Full wwPDB EM Validation Report

Apr 9, 2025 – 02:38 PM JST

PDB ID	:	9LBZ / pdb_00009lbz
EMDB ID	:	EMD-62959
Title	:	unique-vertex of mature phage N4
Authors	:	Liu, H.; Chen, W.
Deposited on	:	2025-01-03
Resolution	:	4.00 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:

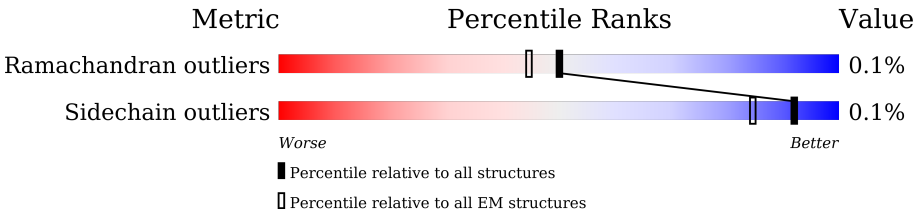
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 4.00 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	A	763	16% 85% 15%
1	B	763	14% 86% 14%
1	C	763	14% 85% 15%
1	D	763	15% 85% 15%
1	E	763	15% 85% 15%
1	F	763	14% 85% 15%
1	G	763	15% 85% 15%
1	H	763	14% 85% 15%
1	I	763	14% 87% 13%

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Mol	Chain	Length	Quality of chain
1	J	763	15% 85% 15%
1	K	763	14% 85% 15%
1	L	763	15% 87% 13%
2	M	401	9% 100%
2	N	401	7% 100%
2	O	401	11% 100%
2	P	401	8% 100%
2	Q	401	8% 100%
2	R	401	100%
2	S	401	6% 100%
2	T	401	100%
2	U	401	5% 100%
2	V	401	100%
2	W	401	100%
2	X	401	100%
2	Y	401	100%
2	Z	401	100%
2	a	401	100%
2	b	401	5% 94% 6%
2	c	401	94% 6%
2	d	401	6% 94% 6%
2	e	401	94% 6%
2	f	401	5% 94% 6%
2	g	401	5% 100%
2	h	401	5% 100%

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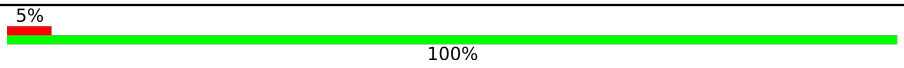
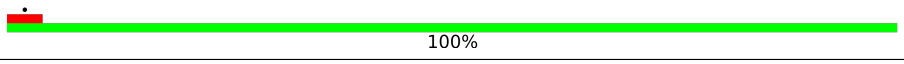
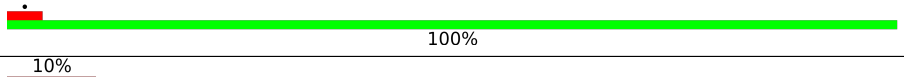
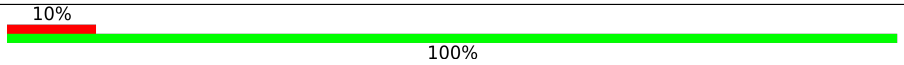
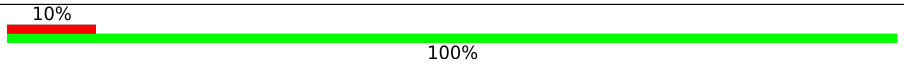
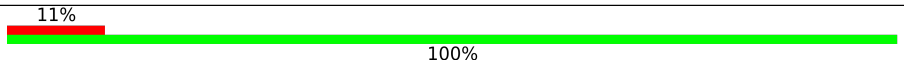
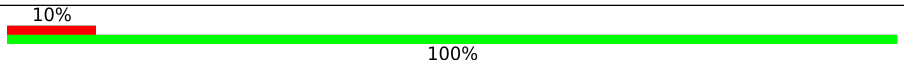
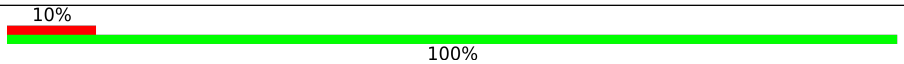
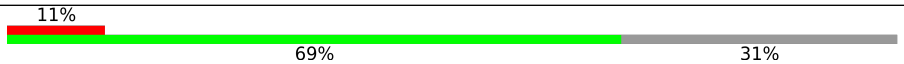
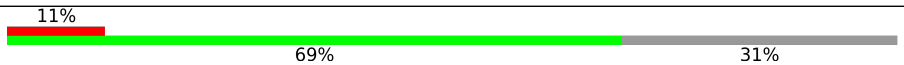
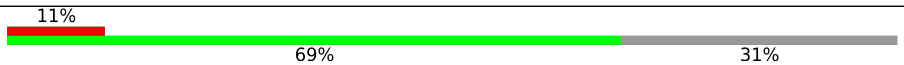
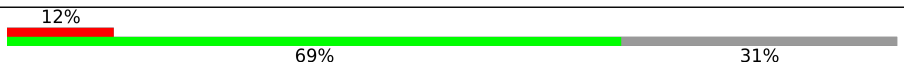
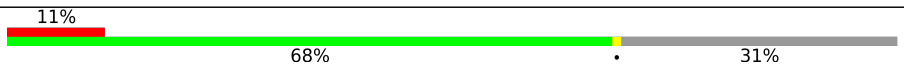
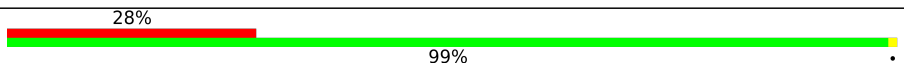
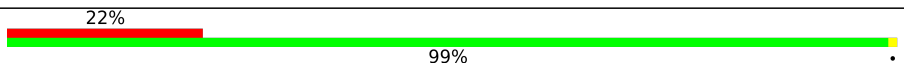
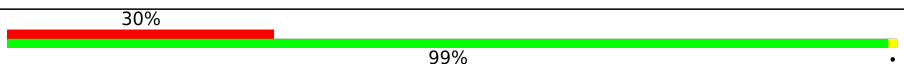
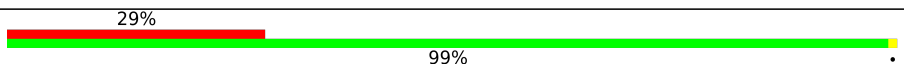
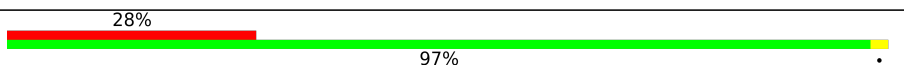
Mol	Chain	Length	Quality of chain
2	i	401	
2	j	401	
2	k	401	
2	l	401	
2	m	401	
2	n	401	
2	o	401	
2	p	401	
3	q	279	
3	r	279	
3	s	279	
3	t	279	
3	u	279	
3	v	279	
3	w	279	
3	x	279	
3	y	279	
3	z	279	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 171453 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 Probable portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	648	Total 5153	C 3236	N 902	O 993	S 22	0	0
1	B	657	Total 5217	C 3276	N 912	O 1007	S 22	0	0
1	C	648	Total 5153	C 3236	N 902	O 993	S 22	0	0
1	D	648	Total 5153	C 3236	N 902	O 993	S 22	0	0
1	E	648	Total 5153	C 3236	N 902	O 993	S 22	0	0
1	F	648	Total 5153	C 3236	N 902	O 993	S 22	0	0
1	G	648	Total 5153	C 3236	N 902	O 993	S 22	0	0
1	H	647	Total 5144	C 3231	N 901	O 990	S 22	0	0
1	I	662	Total 5253	C 3297	N 917	O 1016	S 23	0	0
1	J	648	Total 5153	C 3236	N 902	O 993	S 22	0	0
1	K	648	Total 5153	C 3236	N 902	O 993	S 22	0	0
1	L	664	Total 5270	C 3306	N 921	O 1020	S 23	0	0

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	401	Total 3093	C 1953	N 521	O 603	S 16	0	0
2	N	401	Total 3093	C 1953	N 521	O 603	S 16	0	0
2	O	401	Total 3093	C 1953	N 521	O 603	S 16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	Q	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	R	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	S	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	T	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	U	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	V	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	W	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	X	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	Y	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	Z	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	a	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	b	378	Total	C	N	O	S	0	0
			2924	1854	492	564	14		
2	c	376	Total	C	N	O	S	0	0
			2908	1845	489	560	14		
2	d	377	Total	C	N	O	S	0	0
			2915	1849	490	562	14		
2	e	376	Total	C	N	O	S	0	0
			2908	1845	489	560	14		
2	f	377	Total	C	N	O	S	0	0
			2915	1849	490	562	14		
2	g	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	h	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	i	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	j	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	l	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	m	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	n	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	o	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		
2	p	401	Total	C	N	O	S	0	0
			3093	1953	521	603	16		

- Molecule 3 is a protein called 32 kDa protein.

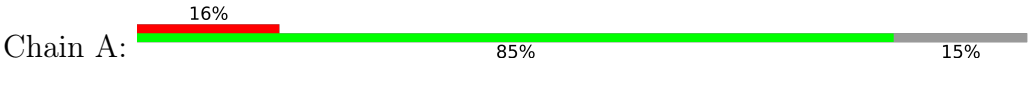
Mol	Chain	Residues	Atoms					AltConf	Trace
3	q	193	Total	C	N	O	S	0	0
			1446	912	242	289	3		
3	r	193	Total	C	N	O	S	0	0
			1446	912	242	289	3		
3	s	193	Total	C	N	O	S	0	0
			1446	912	242	289	3		
3	t	193	Total	C	N	O	S	0	0
			1446	912	242	289	3		
3	u	193	Total	C	N	O	S	0	0
			1446	912	242	289	3		
3	v	278	Total	C	N	O	S	0	0
			2044	1288	337	416	3		
3	w	278	Total	C	N	O	S	0	0
			2044	1288	337	416	3		
3	x	278	Total	C	N	O	S	0	0
			2044	1288	337	416	3		
3	y	278	Total	C	N	O	S	0	0
			2044	1288	337	416	3		
3	z	278	Total	C	N	O	S	0	0
			2044	1288	337	416	3		

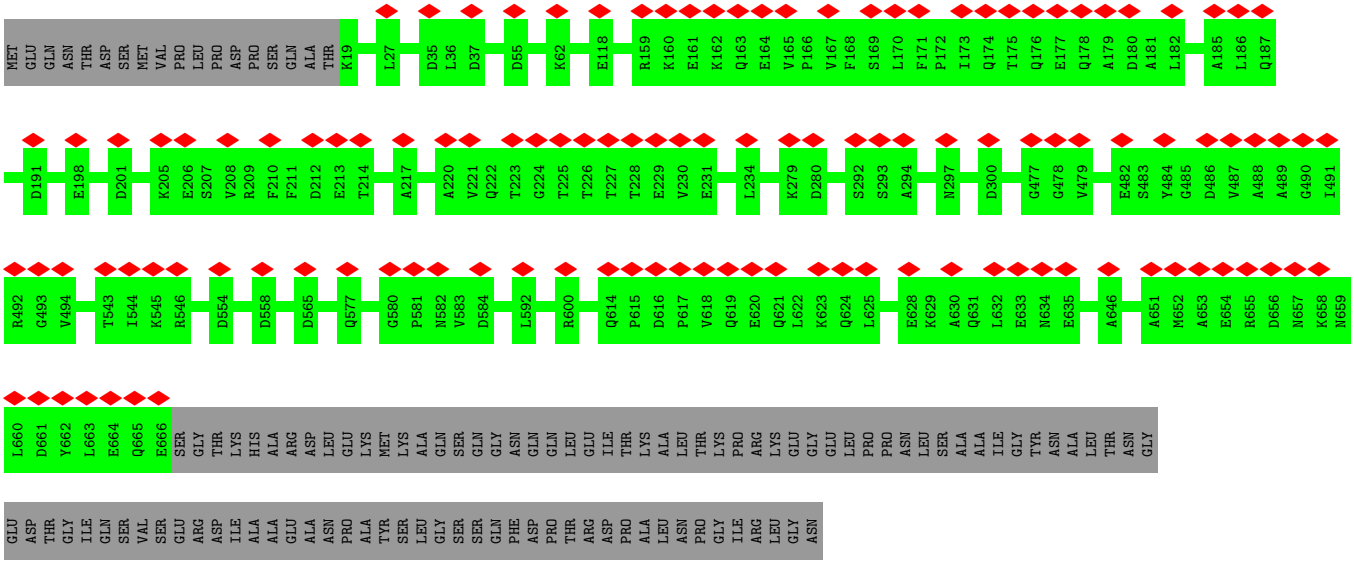
3 Residue-property plots (i)

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: Probable portal protein

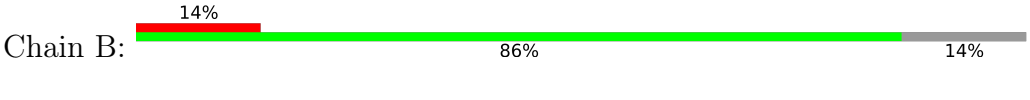
Chain A:

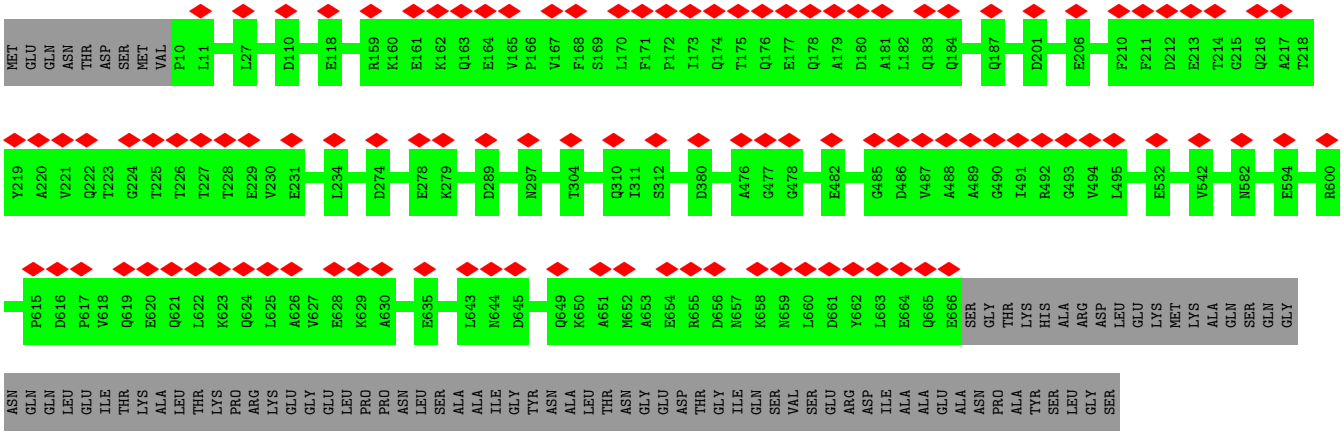


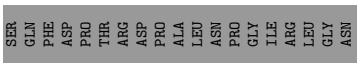


• Molecule 1: Probable portal protein

Chain B:

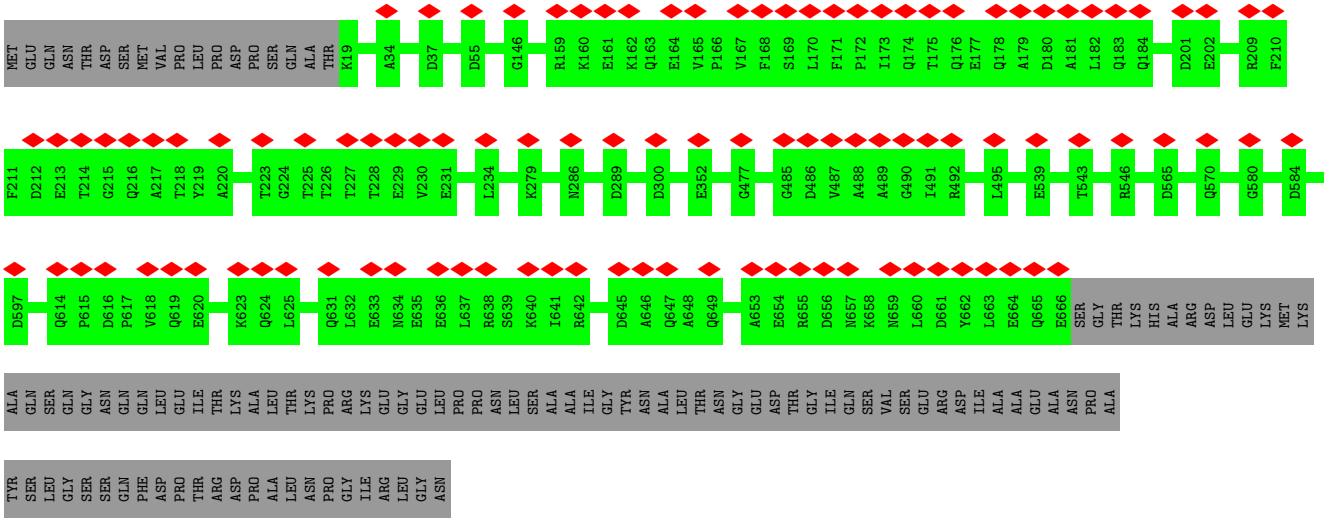






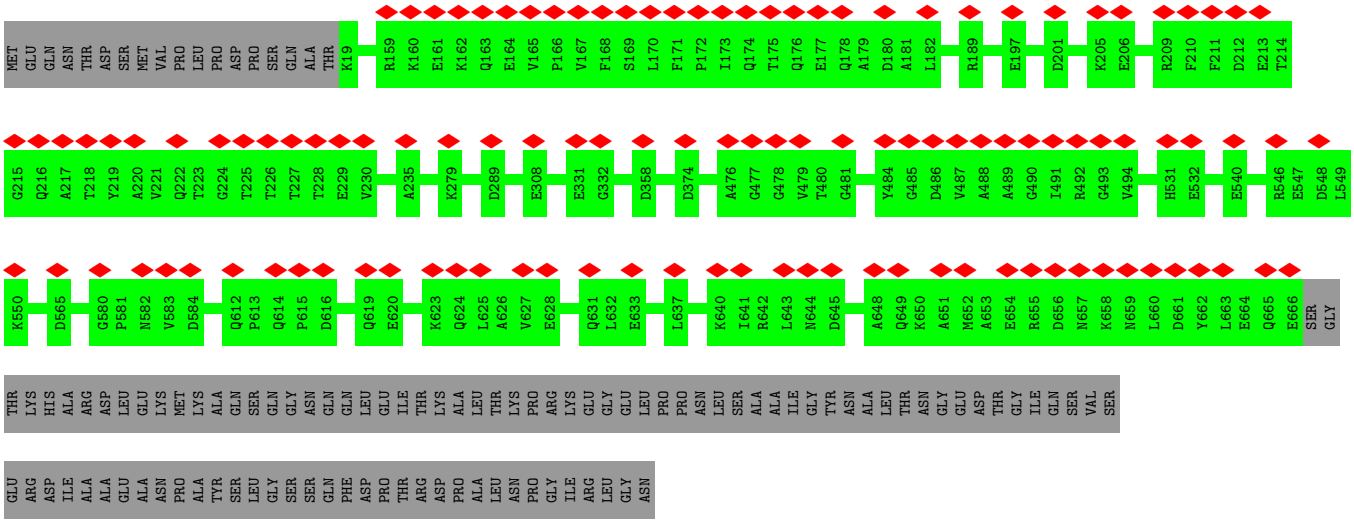
• Molecule 1: Probable portal protein

Chain C:



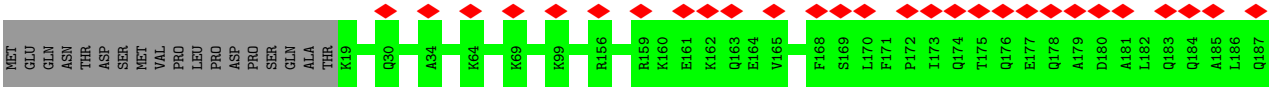
• Molecule 1: Probable portal protein

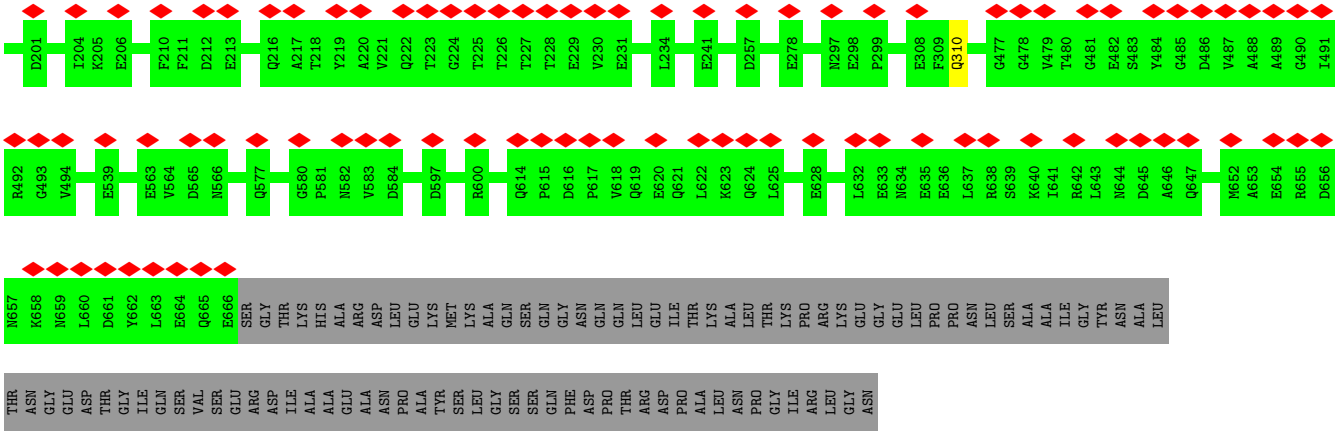
Chain D:



• Molecule 1: Probable portal protein

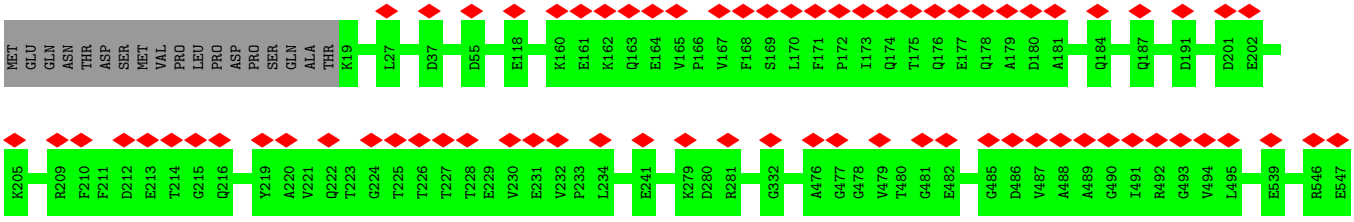
Chain E:





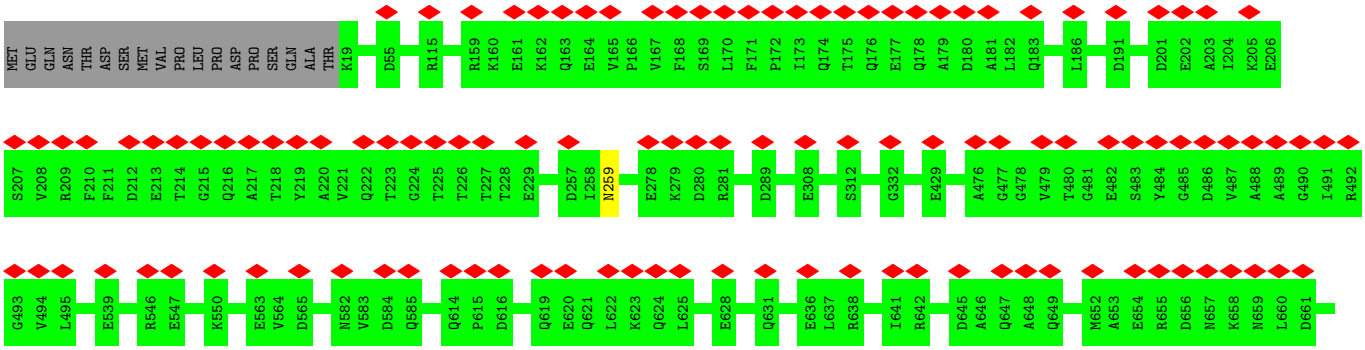
• Molecule 1: Probable portal protein

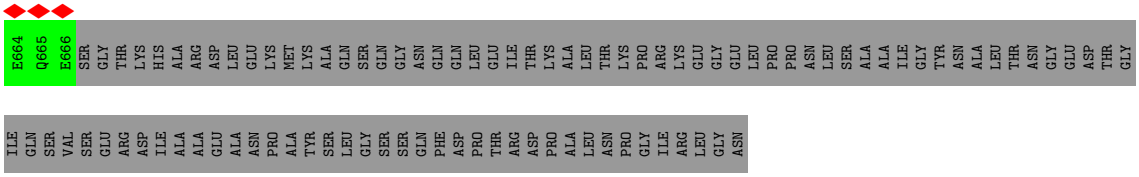
Chain F:



• Molecule 1: Probable portal protein

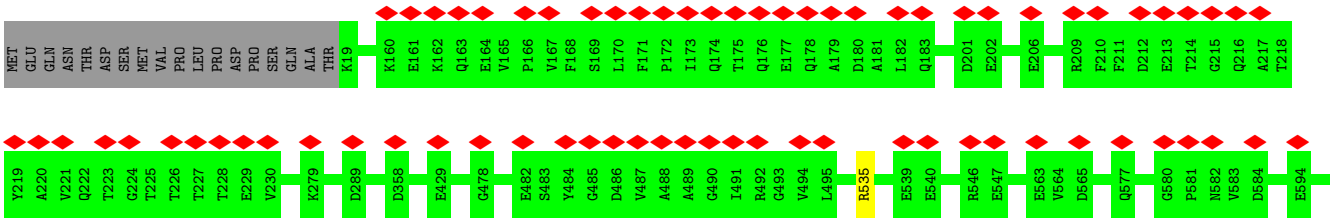
Chain G:





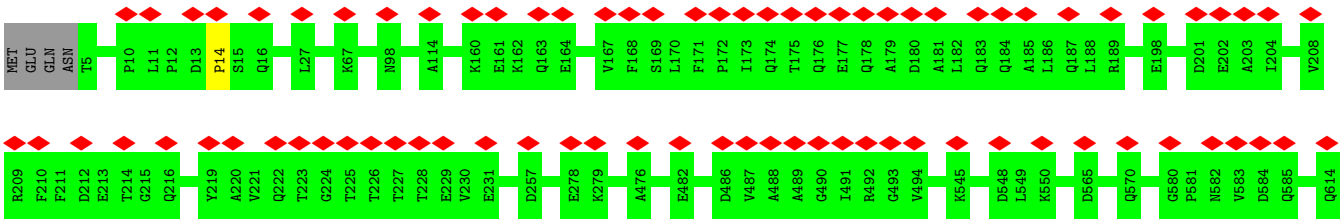
• Molecule 1: Probable portal protein

Chain H:



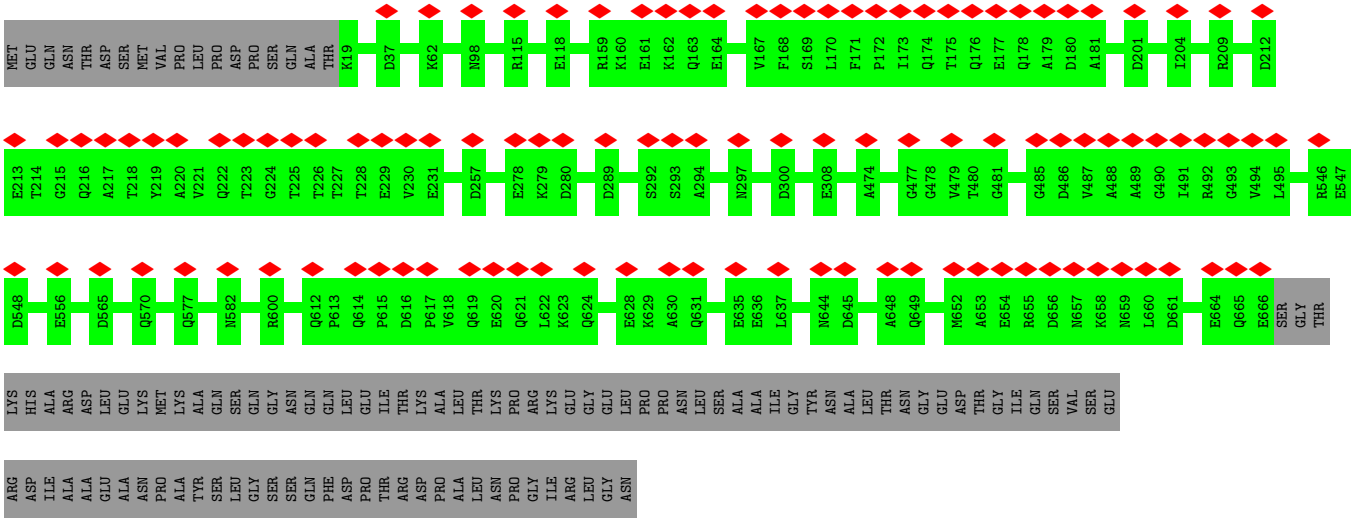
• Molecule 1: Probable portal protein

Chain I:



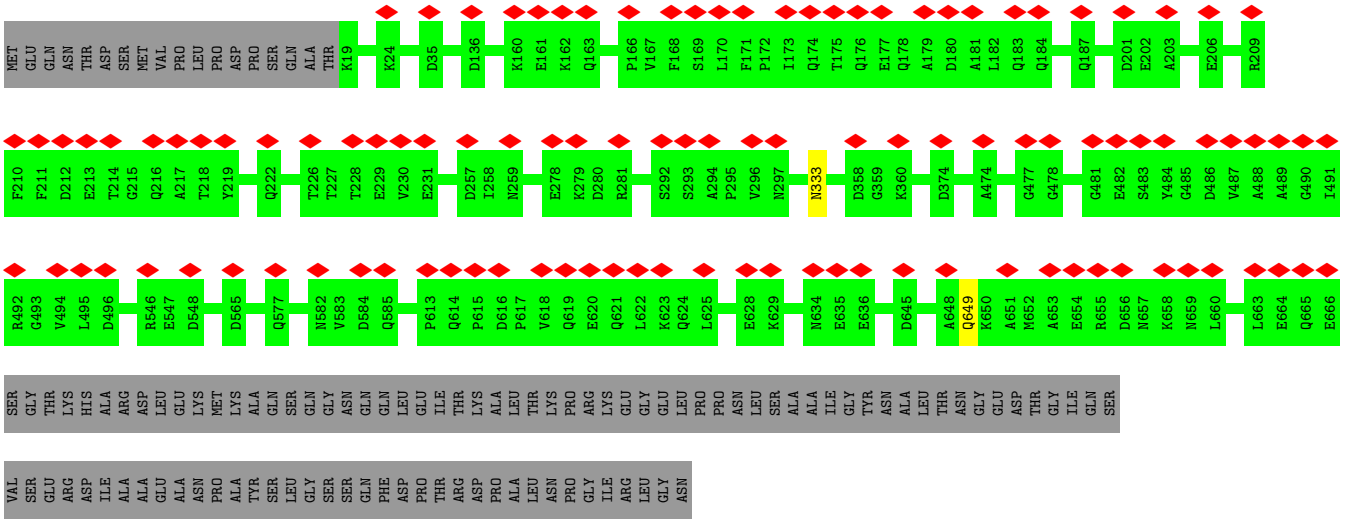
• Molecule 1: Probable portal protein

Chain J:



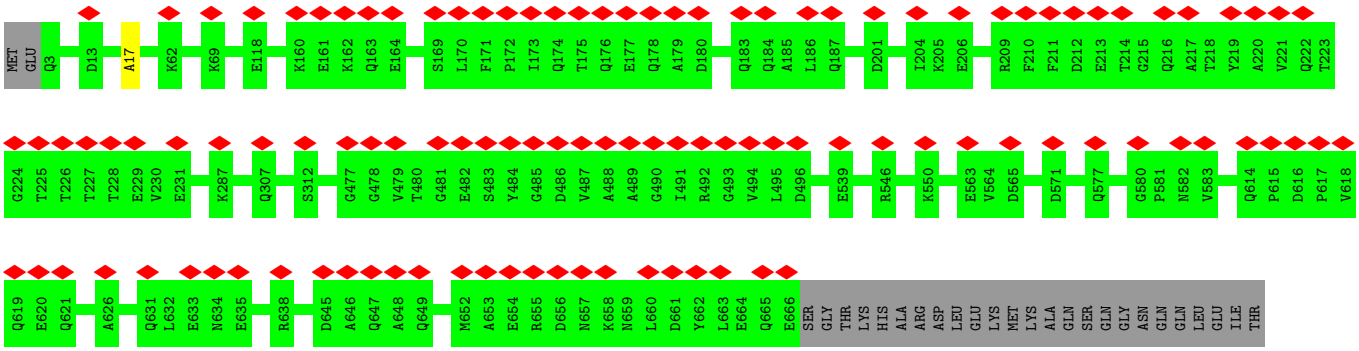
• Molecule 1: Probable portal protein

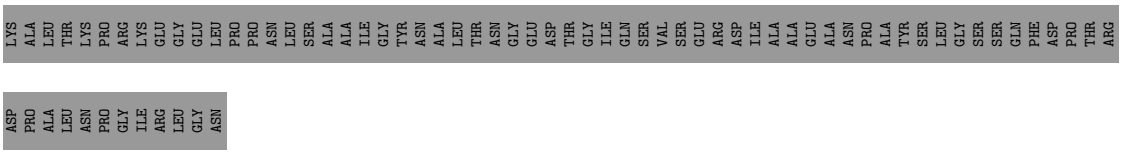
Chain K:



• Molecule 1: Probable portal protein

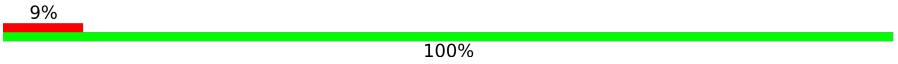
Chain L:

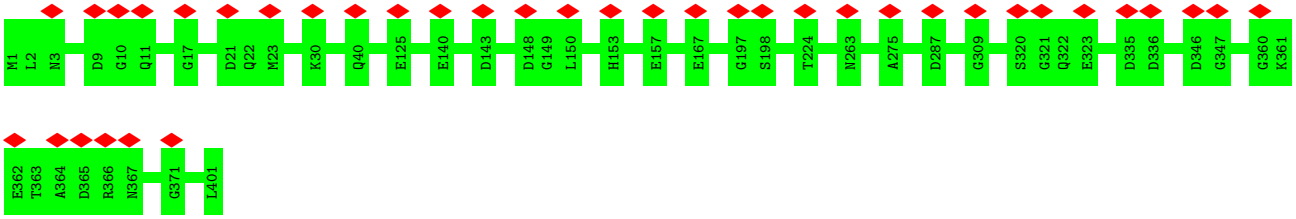




• Molecule 2: Major capsid protein

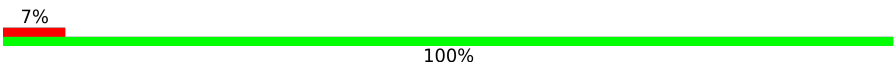
Chain M:

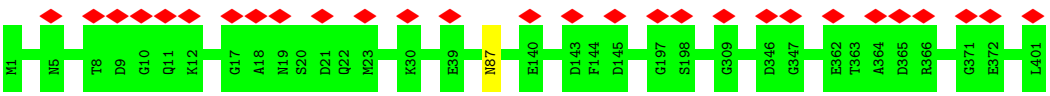




• Molecule 2: Major capsid protein

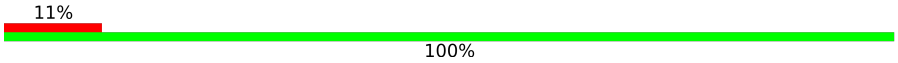
Chain N:

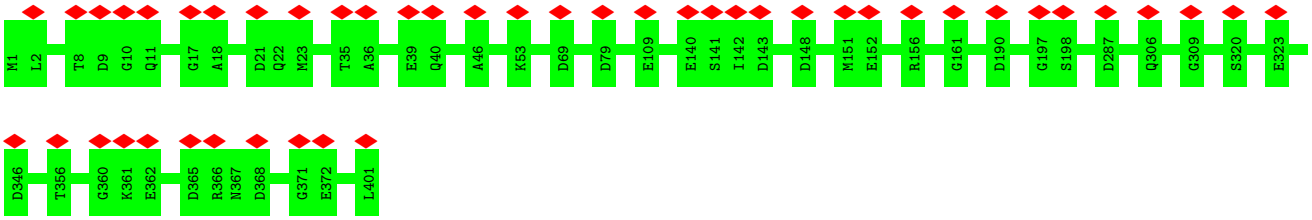




• Molecule 2: Major capsid protein

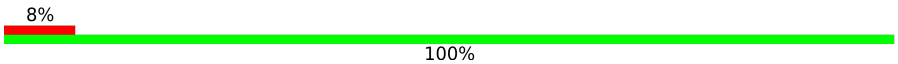
Chain O:

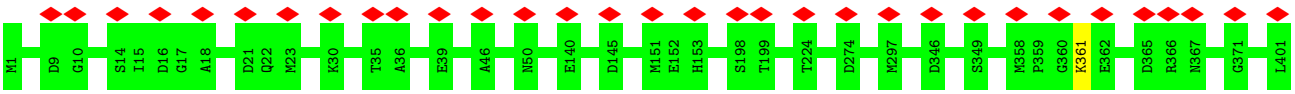




• Molecule 2: Major capsid protein

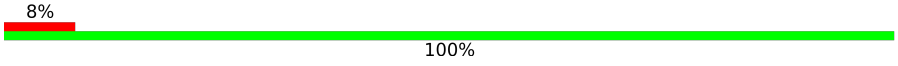
Chain P:

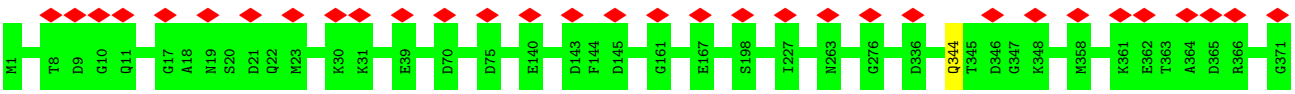




• Molecule 2: Major capsid protein

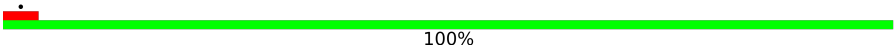
Chain Q:

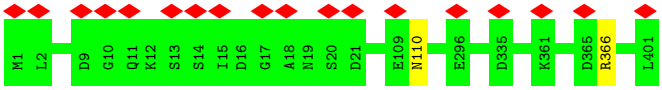




• Molecule 2: Major capsid protein

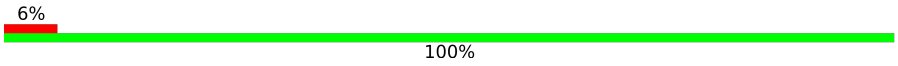
Chain R:

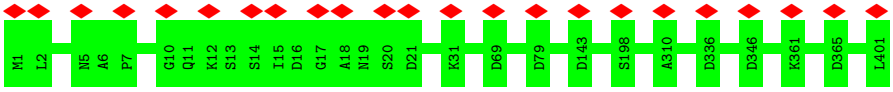




• Molecule 2: Major capsid protein

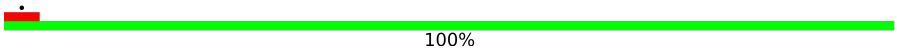
Chain S:

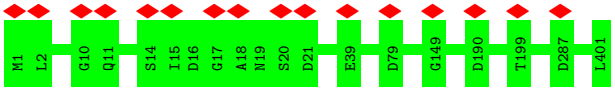




• Molecule 2: Major capsid protein

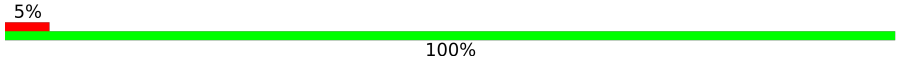
Chain T:

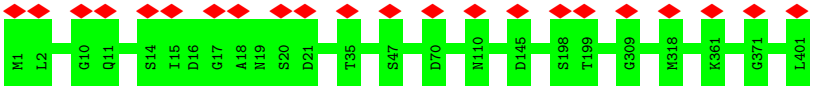




• Molecule 2: Major capsid protein

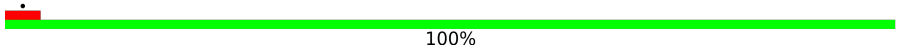
Chain U:

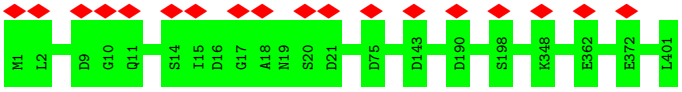




• Molecule 2: Major capsid protein

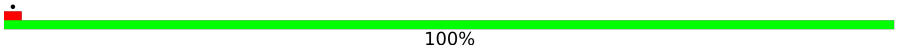
Chain V:

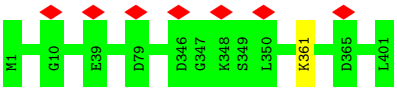




• Molecule 2: Major capsid protein

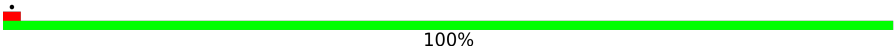
Chain W:

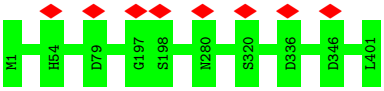




• Molecule 2: Major capsid protein

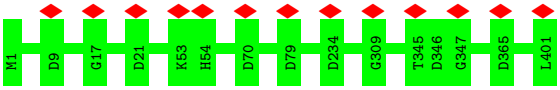
Chain X:





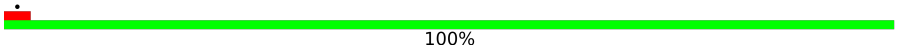
• Molecule 2: Major capsid protein

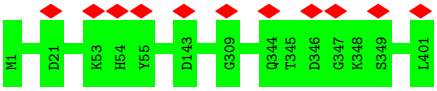
Chain Y:



• Molecule 2: Major capsid protein

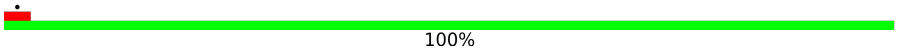
Chain Z:

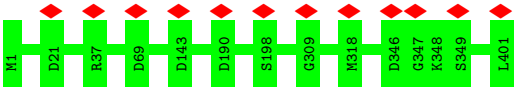




• Molecule 2: Major capsid protein

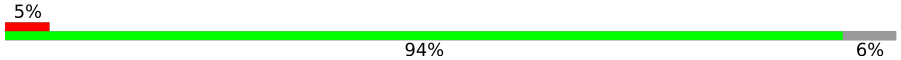
Chain a:

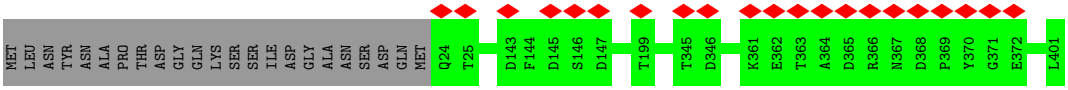




• Molecule 2: Major capsid protein

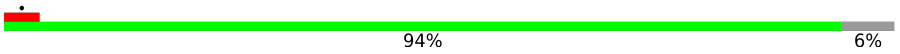
Chain b:

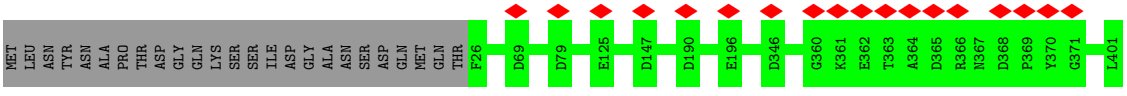




• Molecule 2: Major capsid protein

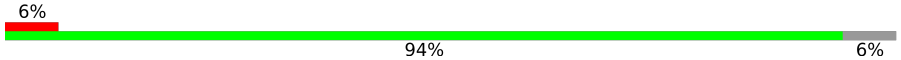
Chain c:

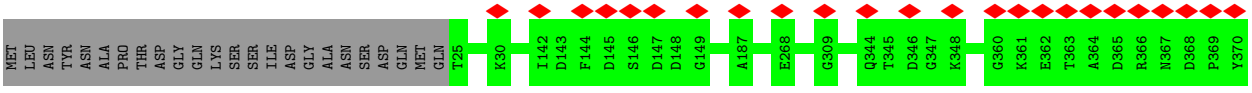




• Molecule 2: Major capsid protein

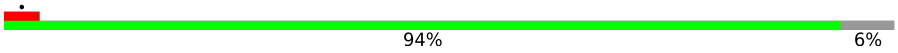
Chain d:

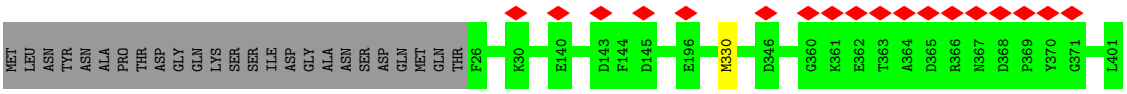




• Molecule 2: Major capsid protein

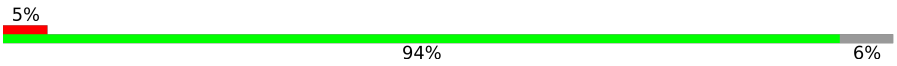
Chain e:

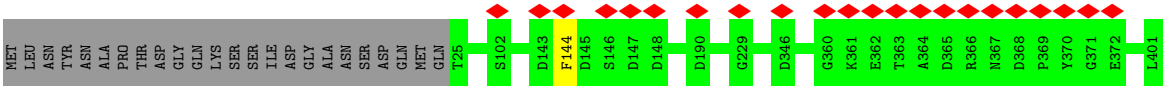




• Molecule 2: Major capsid protein

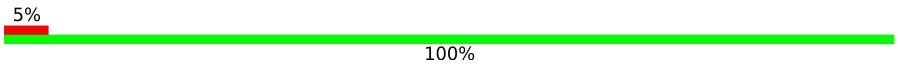
Chain f:

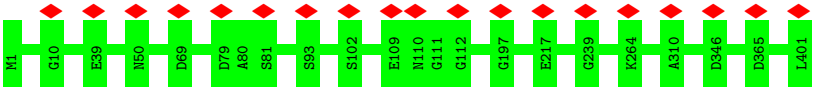




• Molecule 2: Major capsid protein

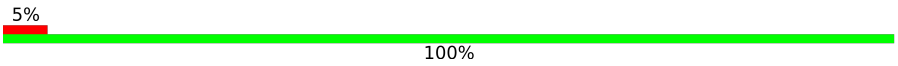
Chain g:

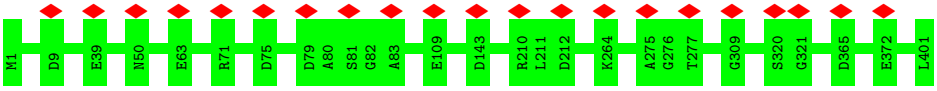




• Molecule 2: Major capsid protein

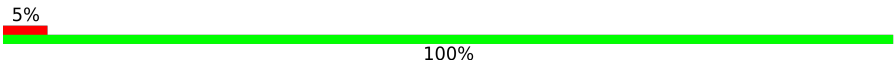
Chain h:

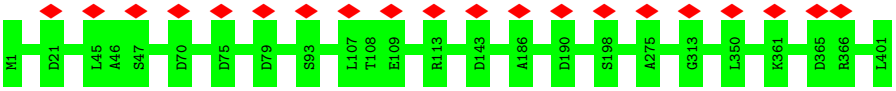




• Molecule 2: Major capsid protein

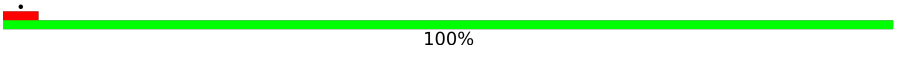
Chain i:

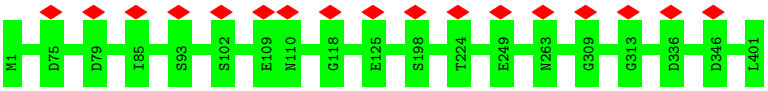




• Molecule 2: Major capsid protein

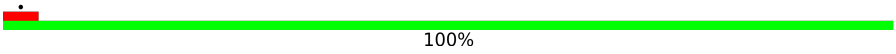
Chain j:

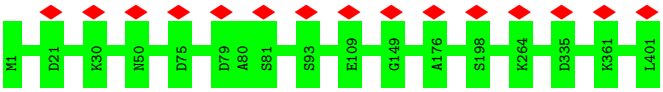




• Molecule 2: Major capsid protein

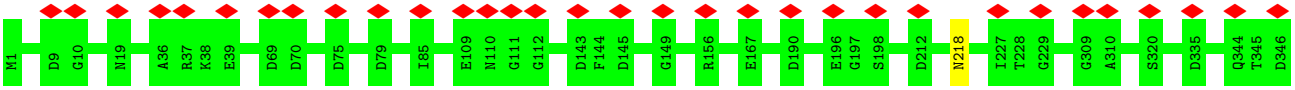
Chain k:

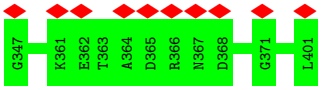




• Molecule 2: Major capsid protein

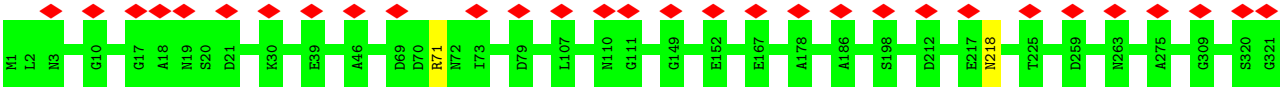
Chain l:

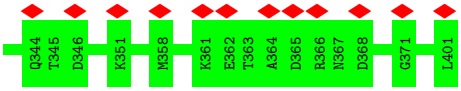




• Molecule 2: Major capsid protein

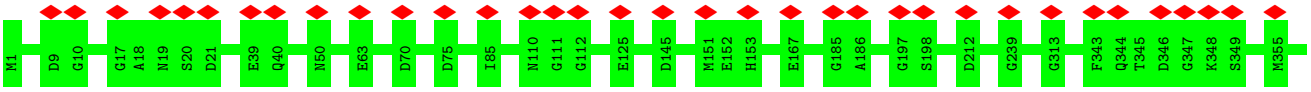
Chain m:

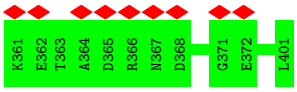




• Molecule 2: Major capsid protein

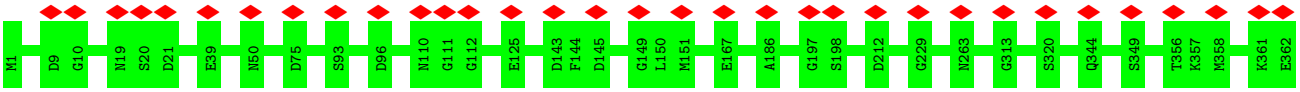
Chain n:

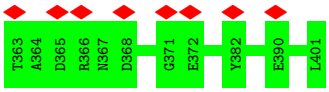




• Molecule 2: Major capsid protein

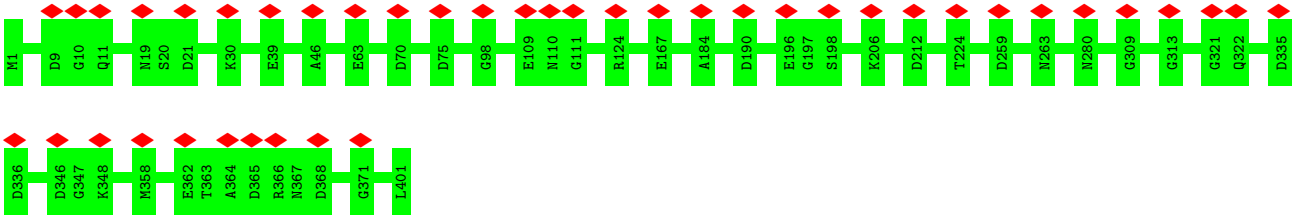
Chain o:





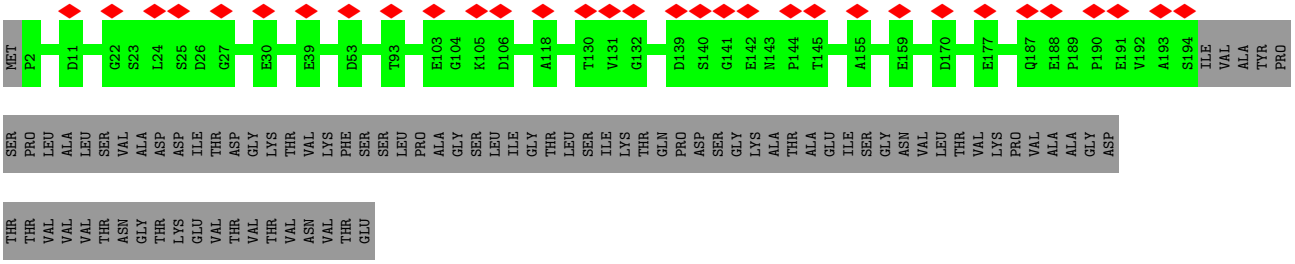
• Molecule 2: Major capsid protein

Chain p:



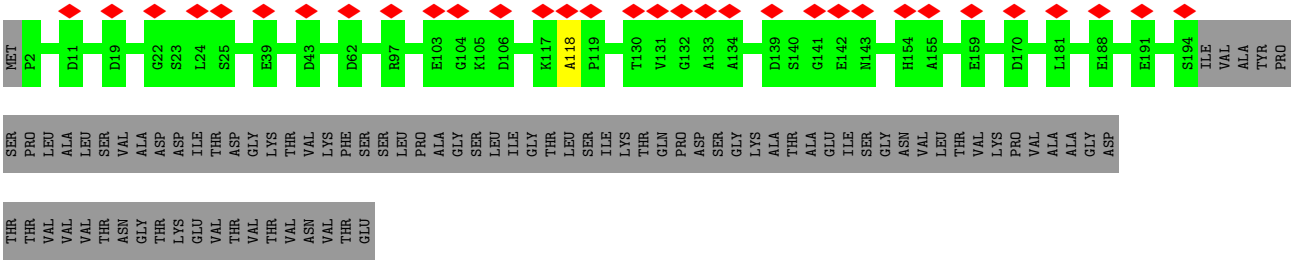
• Molecule 3: 32 kDa protein

Chain q:



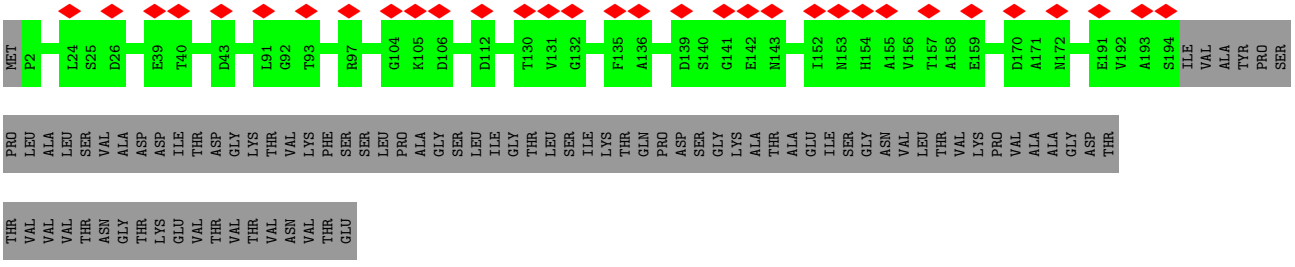
• Molecule 3: 32 kDa protein

Chain r:



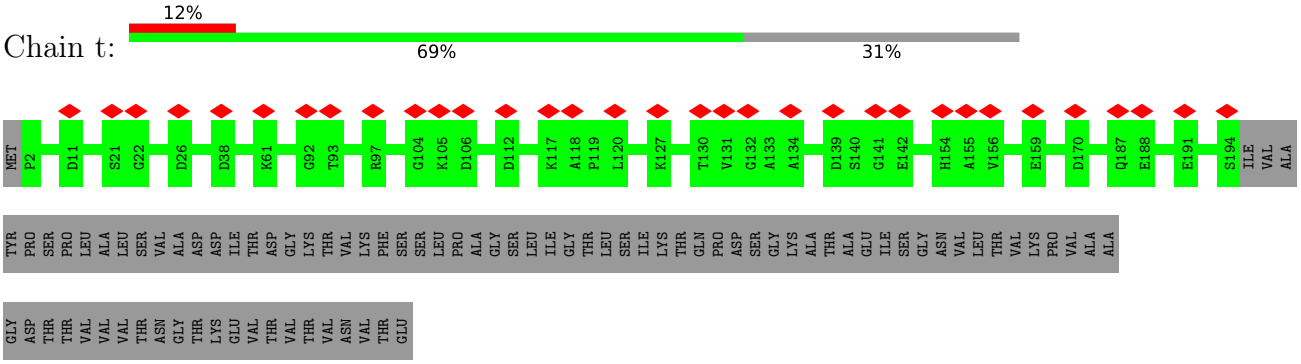
• Molecule 3: 32 kDa protein

Chain s:



• Molecule 3: 32 kDa protein

Chain t:

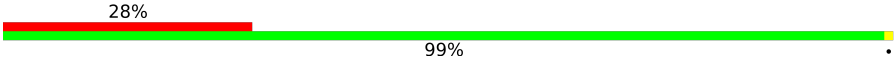


• Molecule 3: 32 kDa protein

Chain u:

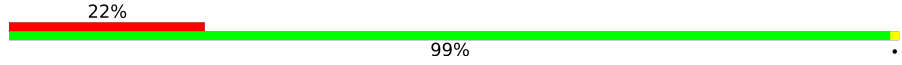
• Molecule 3: 32 kDa protein

Chain v:



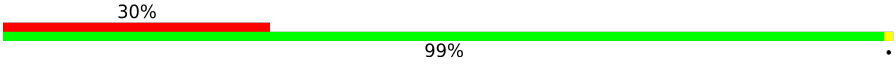
• Molecule 3: 32 kDa protein

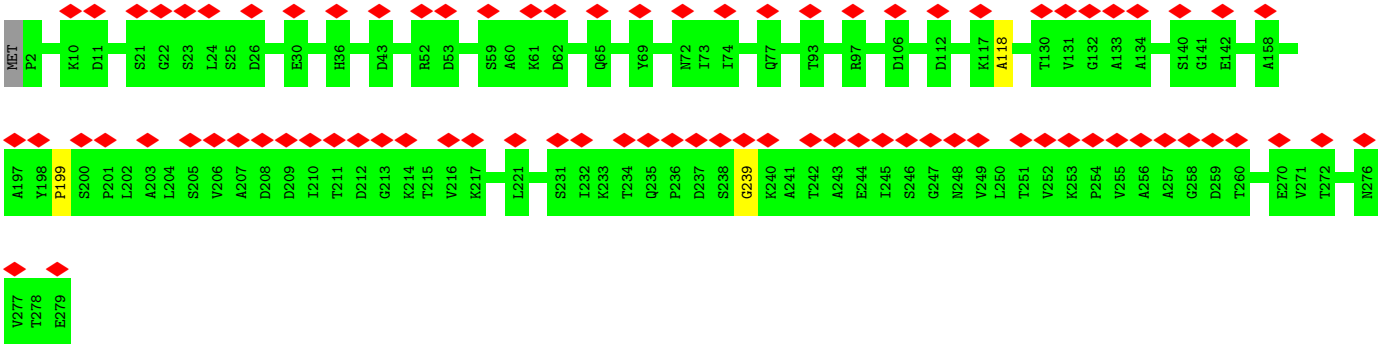
Chain w:



• Molecule 3: 32 kDa protein

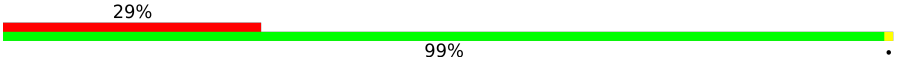
Chain x:

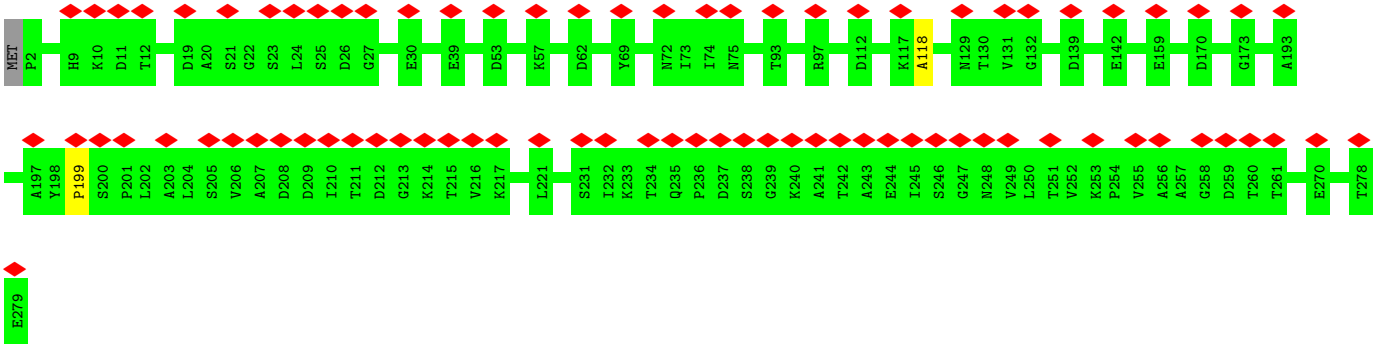




• Molecule 3: 32 kDa protein

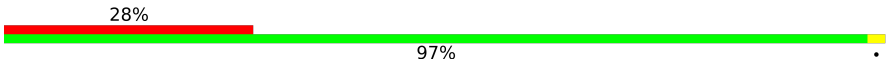
Chain y:

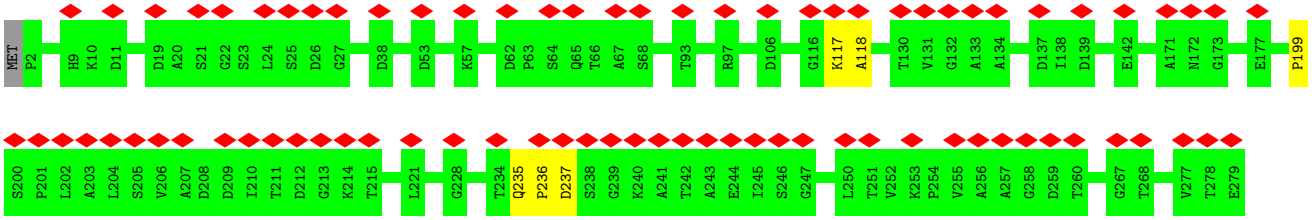




• Molecule 3: 32 kDa protein

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15466	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 ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	49.122	Depositor
Minimum map value	-32.985	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	2.464	Depositor
Recommended contour level	6	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.30	0/5248	0.51	0/7105
1	B	0.30	0/5315	0.51	0/7199
1	C	0.30	0/5248	0.51	0/7105
1	D	0.30	0/5248	0.51	0/7105
1	E	0.31	0/5248	0.52	0/7105
1	F	0.30	0/5248	0.50	0/7105
1	G	0.30	0/5248	0.50	0/7105
1	H	0.30	0/5239	0.50	0/7093
1	I	0.31	0/5351	0.51	0/7249
1	J	0.30	0/5248	0.50	0/7105
1	K	0.31	0/5248	0.51	0/7105
1	L	0.30	0/5368	0.51	0/7272
2	M	0.28	0/3152	0.50	0/4264
2	N	0.28	0/3152	0.50	0/4264
2	O	0.28	0/3152	0.51	0/4264
2	P	0.29	0/3152	0.51	0/4264
2	Q	0.28	0/3152	0.51	0/4264
2	R	0.30	0/3152	0.51	0/4264
2	S	0.31	0/3152	0.51	0/4264
2	T	0.31	0/3152	0.51	0/4264
2	U	0.30	0/3152	0.51	0/4264
2	V	0.30	0/3152	0.52	0/4264
2	W	0.32	0/3152	0.51	0/4264
2	X	0.33	0/3152	0.54	0/4264
2	Y	0.31	0/3152	0.51	0/4264
2	Z	0.32	0/3152	0.52	0/4264
2	a	0.32	0/3152	0.53	0/4264
2	b	0.31	0/2981	0.51	0/4033
2	c	0.32	0/2965	0.53	0/4011
2	d	0.31	0/2972	0.51	0/4021
2	e	0.32	0/2965	0.52	0/4011
2	f	0.32	0/2972	0.52	0/4021
2	g	0.29	0/3152	0.51	0/4264
2	h	0.29	0/3152	0.51	0/4264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
2	i	0.29	0/3152	0.50	0/4264
2	j	0.29	0/3152	0.50	0/4264
2	k	0.30	0/3152	0.51	0/4264
2	l	0.28	0/3152	0.51	0/4264
2	m	0.28	0/3152	0.51	0/4264
2	n	0.28	0/3152	0.51	0/4264
2	o	0.28	0/3152	0.50	0/4264
2	p	0.28	0/3152	0.51	0/4264
3	q	0.26	0/1476	0.47	0/2018
3	r	0.27	0/1476	0.47	0/2018
3	s	0.26	0/1476	0.47	0/2018
3	t	0.26	0/1476	0.47	0/2018
3	u	0.26	0/1476	0.47	0/2018
3	v	0.26	0/2081	0.50	0/2850
3	w	0.26	0/2081	0.49	0/2850
3	x	0.26	0/2081	0.49	0/2850
3	y	0.26	0/2081	0.47	0/2850
3	z	0.27	0/2081	0.48	0/2850
All	All	0.30	0/174697	0.51	0/236690

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	646/763 (85%)	628 (97%)	18 (3%)	0	100	100
1	B	655/763 (86%)	636 (97%)	19 (3%)	0	100	100
1	C	646/763 (85%)	628 (97%)	18 (3%)	0	100	100
1	D	646/763 (85%)	624 (97%)	22 (3%)	0	100	100
1	E	646/763 (85%)	624 (97%)	22 (3%)	0	100	100
1	F	646/763 (85%)	622 (96%)	24 (4%)	0	100	100
1	G	646/763 (85%)	629 (97%)	17 (3%)	0	100	100
1	H	645/763 (84%)	625 (97%)	20 (3%)	0	100	100
1	I	660/763 (86%)	636 (96%)	23 (4%)	1 (0%)	44	76
1	J	646/763 (85%)	621 (96%)	25 (4%)	0	100	100
1	K	646/763 (85%)	625 (97%)	21 (3%)	0	100	100
1	L	662/763 (87%)	639 (96%)	22 (3%)	1 (0%)	44	76
2	M	399/401 (100%)	387 (97%)	12 (3%)	0	100	100
2	N	399/401 (100%)	386 (97%)	13 (3%)	0	100	100
2	O	399/401 (100%)	389 (98%)	10 (2%)	0	100	100
2	P	399/401 (100%)	384 (96%)	14 (4%)	1 (0%)	37	71
2	Q	399/401 (100%)	389 (98%)	10 (2%)	0	100	100
2	R	399/401 (100%)	388 (97%)	11 (3%)	0	100	100
2	S	399/401 (100%)	384 (96%)	15 (4%)	0	100	100
2	T	399/401 (100%)	382 (96%)	17 (4%)	0	100	100
2	U	399/401 (100%)	385 (96%)	14 (4%)	0	100	100
2	V	399/401 (100%)	385 (96%)	14 (4%)	0	100	100
2	W	399/401 (100%)	375 (94%)	24 (6%)	0	100	100
2	X	399/401 (100%)	377 (94%)	22 (6%)	0	100	100
2	Y	399/401 (100%)	379 (95%)	20 (5%)	0	100	100
2	Z	399/401 (100%)	383 (96%)	16 (4%)	0	100	100
2	a	399/401 (100%)	369 (92%)	30 (8%)	0	100	100
2	b	376/401 (94%)	354 (94%)	22 (6%)	0	100	100
2	c	374/401 (93%)	357 (96%)	17 (4%)	0	100	100
2	d	375/401 (94%)	350 (93%)	25 (7%)	0	100	100
2	e	374/401 (93%)	357 (96%)	16 (4%)	1 (0%)	37	71
2	f	375/401 (94%)	347 (92%)	28 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	g	399/401 (100%)	387 (97%)	12 (3%)	0	100	100
2	h	399/401 (100%)	387 (97%)	12 (3%)	0	100	100
2	i	399/401 (100%)	387 (97%)	12 (3%)	0	100	100
2	j	399/401 (100%)	387 (97%)	12 (3%)	0	100	100
2	k	399/401 (100%)	390 (98%)	9 (2%)	0	100	100
2	l	399/401 (100%)	386 (97%)	13 (3%)	0	100	100
2	m	399/401 (100%)	386 (97%)	13 (3%)	0	100	100
2	n	399/401 (100%)	386 (97%)	13 (3%)	0	100	100
2	o	399/401 (100%)	388 (97%)	11 (3%)	0	100	100
2	p	399/401 (100%)	390 (98%)	9 (2%)	0	100	100
3	q	191/279 (68%)	185 (97%)	6 (3%)	0	100	100
3	r	191/279 (68%)	184 (96%)	6 (3%)	1 (0%)	25	61
3	s	191/279 (68%)	184 (96%)	7 (4%)	0	100	100
3	t	191/279 (68%)	184 (96%)	7 (4%)	0	100	100
3	u	191/279 (68%)	181 (95%)	8 (4%)	2 (1%)	13	47
3	v	276/279 (99%)	264 (96%)	10 (4%)	2 (1%)	19	55
3	w	276/279 (99%)	264 (96%)	10 (4%)	2 (1%)	19	55
3	x	276/279 (99%)	262 (95%)	11 (4%)	3 (1%)	12	45
3	y	276/279 (99%)	263 (95%)	11 (4%)	2 (1%)	19	55
3	z	276/279 (99%)	263 (95%)	8 (3%)	5 (2%)	7	36
All	All	21974/23976 (92%)	21152 (96%)	801 (4%)	21 (0%)	50	81

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	14	PRO
2	e	330	MET
3	v	199	PRO
3	v	234	THR
3	w	199	PRO
3	x	199	PRO
3	y	199	PRO
3	z	117	LYS
3	z	118	ALA
3	z	199	PRO

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Mol	Chain	Res	Type
3	u	117	LYS
3	y	118	ALA
3	z	236	PRO
2	P	361	LYS
3	r	118	ALA
3	x	118	ALA
3	x	239	GLY
3	z	237	ASP
3	u	118	ALA
3	w	118	ALA
1	L	17	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	558/652 (86%)	558 (100%)	0	100	100
1	B	566/652 (87%)	566 (100%)	0	100	100
1	C	558/652 (86%)	558 (100%)	0	100	100
1	D	558/652 (86%)	558 (100%)	0	100	100
1	E	558/652 (86%)	557 (100%)	1 (0%)	92	93
1	F	558/652 (86%)	558 (100%)	0	100	100
1	G	558/652 (86%)	557 (100%)	1 (0%)	92	93
1	H	557/652 (85%)	556 (100%)	1 (0%)	92	93
1	I	571/652 (88%)	571 (100%)	0	100	100
1	J	558/652 (86%)	558 (100%)	0	100	100
1	K	558/652 (86%)	556 (100%)	2 (0%)	89	91
1	L	573/652 (88%)	573 (100%)	0	100	100
2	M	333/333 (100%)	333 (100%)	0	100	100
2	N	333/333 (100%)	332 (100%)	1 (0%)	91	92
2	O	333/333 (100%)	333 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	333/333 (100%)	333 (100%)	0	100	100
2	Q	333/333 (100%)	332 (100%)	1 (0%)	91	92
2	R	333/333 (100%)	331 (99%)	2 (1%)	84	88
2	S	333/333 (100%)	333 (100%)	0	100	100
2	T	333/333 (100%)	333 (100%)	0	100	100
2	U	333/333 (100%)	333 (100%)	0	100	100
2	V	333/333 (100%)	333 (100%)	0	100	100
2	W	333/333 (100%)	332 (100%)	1 (0%)	91	92
2	X	333/333 (100%)	333 (100%)	0	100	100
2	Y	333/333 (100%)	333 (100%)	0	100	100
2	Z	333/333 (100%)	333 (100%)	0	100	100
2	a	333/333 (100%)	333 (100%)	0	100	100
2	b	314/333 (94%)	314 (100%)	0	100	100
2	c	312/333 (94%)	312 (100%)	0	100	100
2	d	313/333 (94%)	313 (100%)	0	100	100
2	e	312/333 (94%)	312 (100%)	0	100	100
2	f	313/333 (94%)	312 (100%)	1 (0%)	91	92
2	g	333/333 (100%)	333 (100%)	0	100	100
2	h	333/333 (100%)	333 (100%)	0	100	100
2	i	333/333 (100%)	333 (100%)	0	100	100
2	j	333/333 (100%)	333 (100%)	0	100	100
2	k	333/333 (100%)	333 (100%)	0	100	100
2	l	333/333 (100%)	332 (100%)	1 (0%)	91	92
2	m	333/333 (100%)	331 (99%)	2 (1%)	84	88
2	n	333/333 (100%)	333 (100%)	0	100	100
2	o	333/333 (100%)	333 (100%)	0	100	100
2	p	333/333 (100%)	333 (100%)	0	100	100
3	q	161/232 (69%)	161 (100%)	0	100	100
3	r	161/232 (69%)	161 (100%)	0	100	100
3	s	161/232 (69%)	161 (100%)	0	100	100
3	t	161/232 (69%)	161 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	u	161/232 (69%)	160 (99%)	1 (1%)	84 88
3	v	231/232 (100%)	231 (100%)	0	100 100
3	w	231/232 (100%)	231 (100%)	0	100 100
3	x	231/232 (100%)	231 (100%)	0	100 100
3	y	231/232 (100%)	231 (100%)	0	100 100
3	z	231/232 (100%)	230 (100%)	1 (0%)	89 91
All	All	18580/20134 (92%)	18564 (100%)	16 (0%)	92 94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	310	GLN
1	G	259	ASN
1	H	535	ARG
1	K	333	ASN
1	K	649	GLN
2	N	87	ASN
2	Q	344	GLN
2	R	110	ASN
2	R	366	ARG
2	W	361	LYS
2	f	144	PHE
2	l	218	ASN
2	m	71	ARG
2	m	218	ASN
3	u	172	ASN
3	z	235	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	116	GLN
1	C	462	GLN
1	C	567	GLN
1	E	124	GLN
1	E	567	GLN
1	F	124	GLN
1	F	657	ASN
1	G	116	GLN

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Mol	Chain	Res	Type
1	G	259	ASN
1	G	624	GLN
1	H	117	ASN
1	I	116	GLN
1	I	409	GLN
1	I	524	ASN
1	J	307	GLN
1	K	462	GLN
1	K	644	ASN
1	L	116	GLN
1	L	567	GLN
2	N	171	GLN
2	P	171	GLN
2	P	344	GLN
2	Q	344	GLN
2	U	171	GLN
2	V	344	GLN
2	W	171	GLN
2	X	344	GLN
2	Y	322	GLN
2	a	115	ASN
2	b	99	ASN
2	b	171	GLN
2	b	306	GLN
2	b	367	ASN
2	d	171	GLN
2	g	171	GLN
2	i	171	GLN
2	k	171	GLN
2	m	171	GLN
2	n	72	ASN
2	p	171	GLN
3	s	72	ASN
3	v	72	ASN
3	w	72	ASN
3	x	72	ASN
3	y	72	ASN
3	z	72	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.

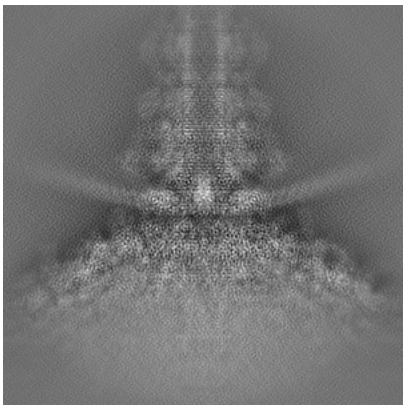
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62959. These allow visual inspection of the internal detail of the map and identification of artifacts.

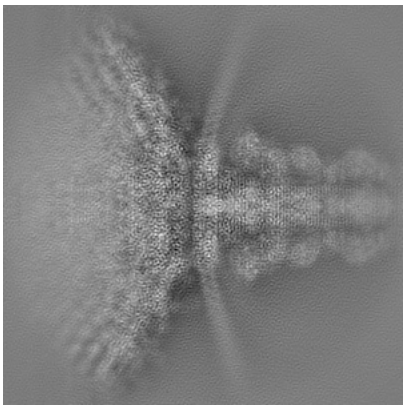
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

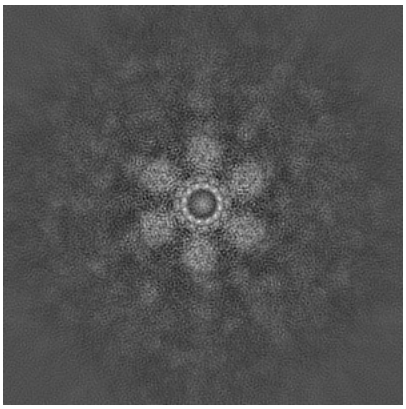
6.1.1 Primary map



X

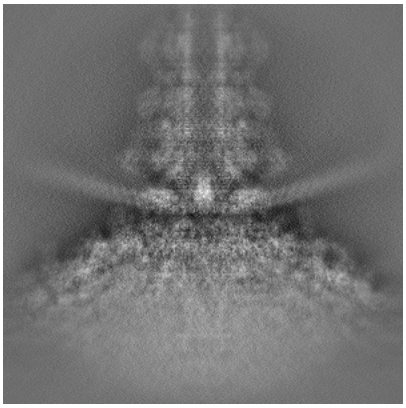


Y

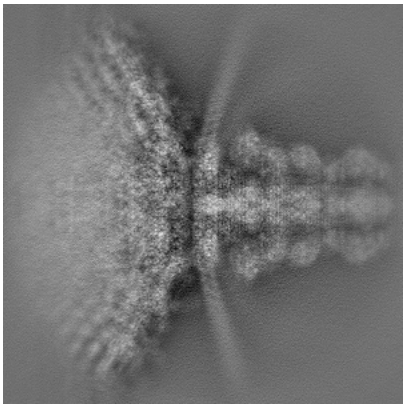


Z

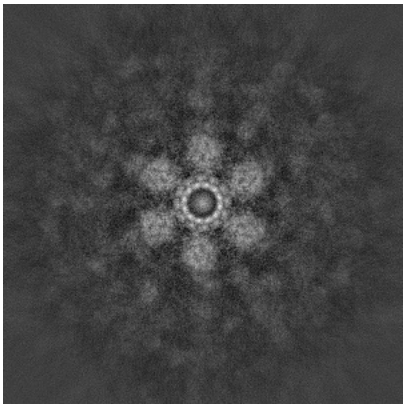
6.1.2 Raw map



X



Y

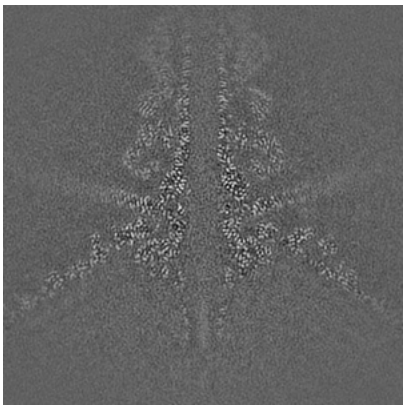


Z

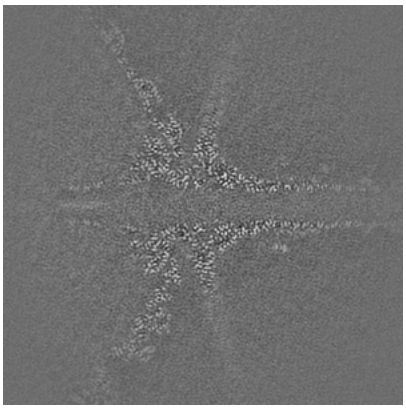
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

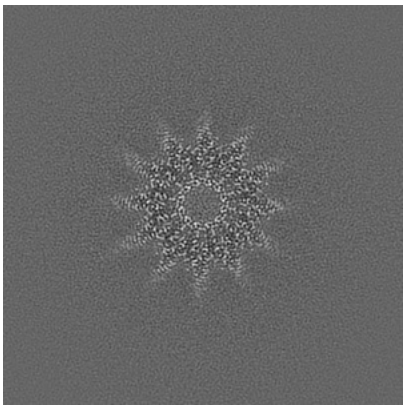
6.2.1 Primary map



X Index: 240

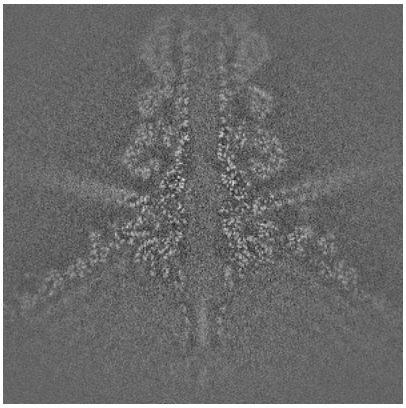


Y Index: 240

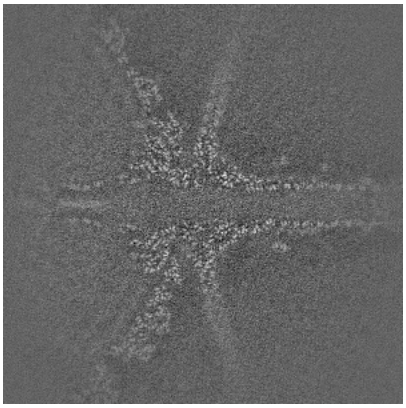


Z Index: 240

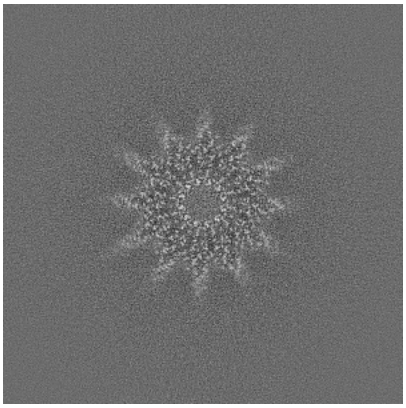
6.2.2 Raw map



X Index: 240



Y Index: 240

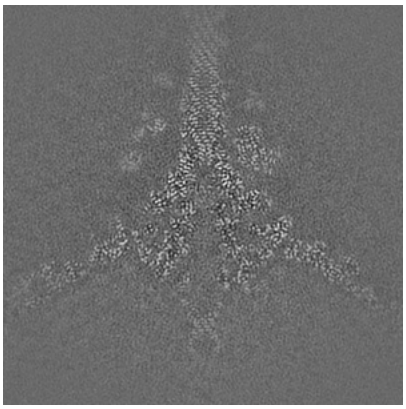


Z Index: 240

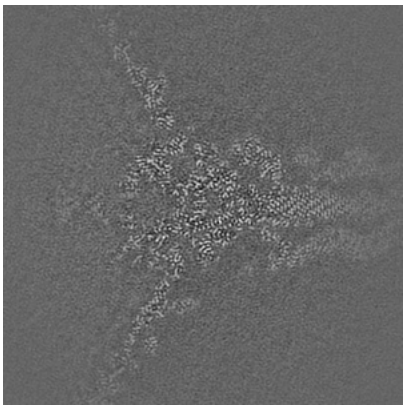
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

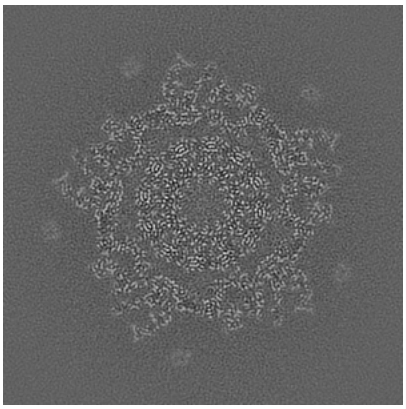
6.3.1 Primary map



X Index: 257

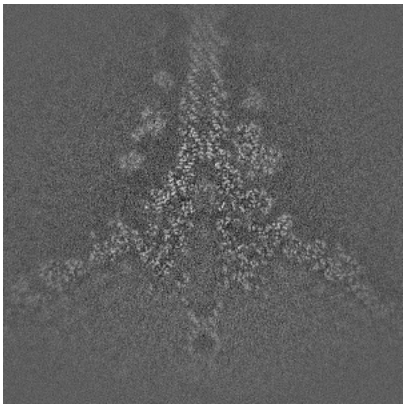


Y Index: 263

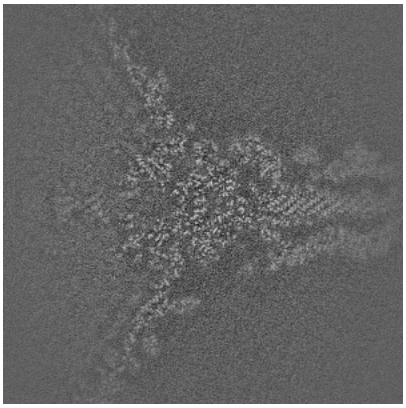


Z Index: 184

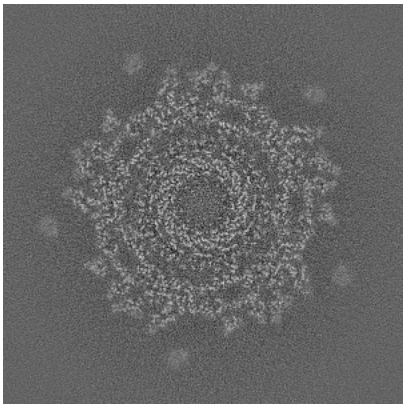
6.3.2 Raw map



X Index: 256



Y Index: 263

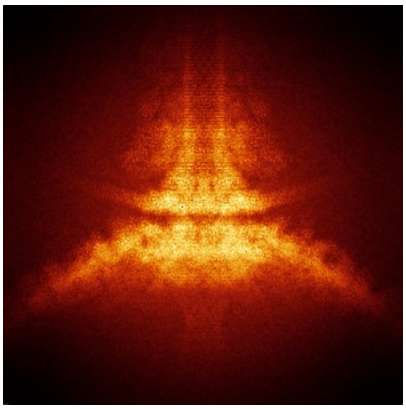


Z Index: 188

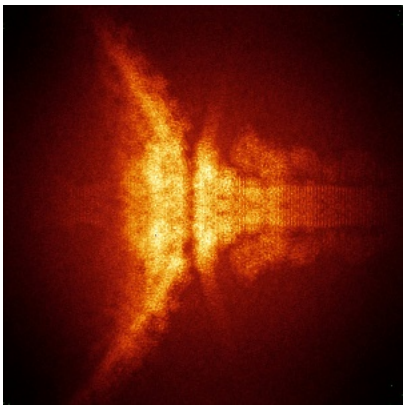
The images above show the largest variance slices of the map in three orthogonal directions.

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

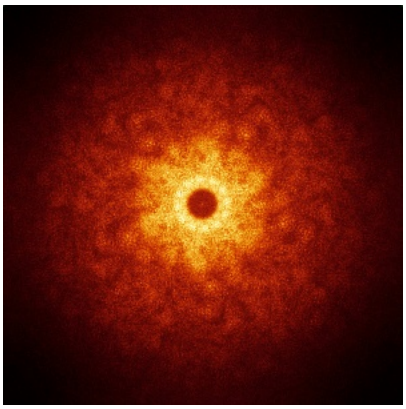
6.4.1 Primary map



X

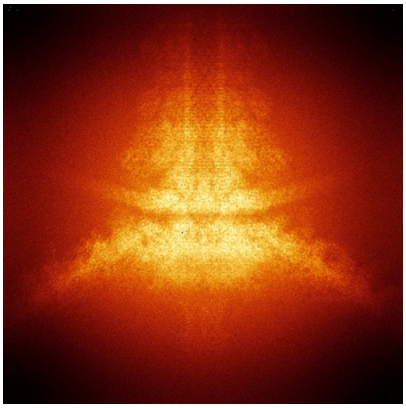


Y

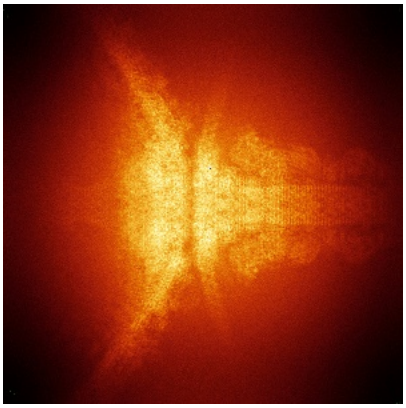


Z

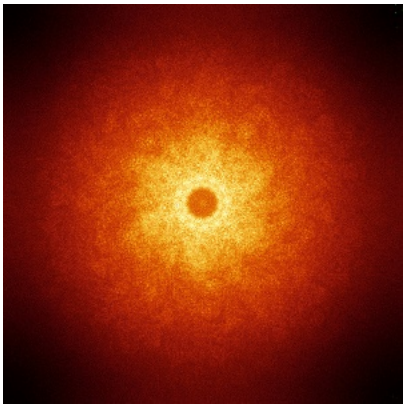
6.4.2 Raw map



X



Y

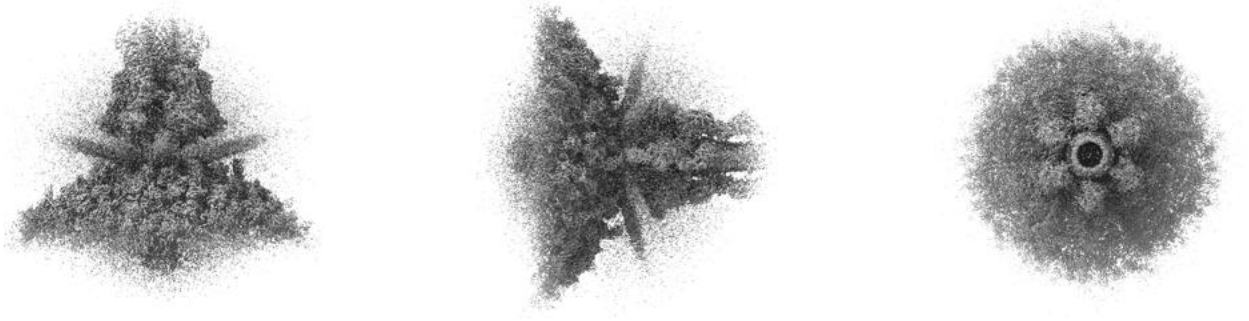


Z

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)

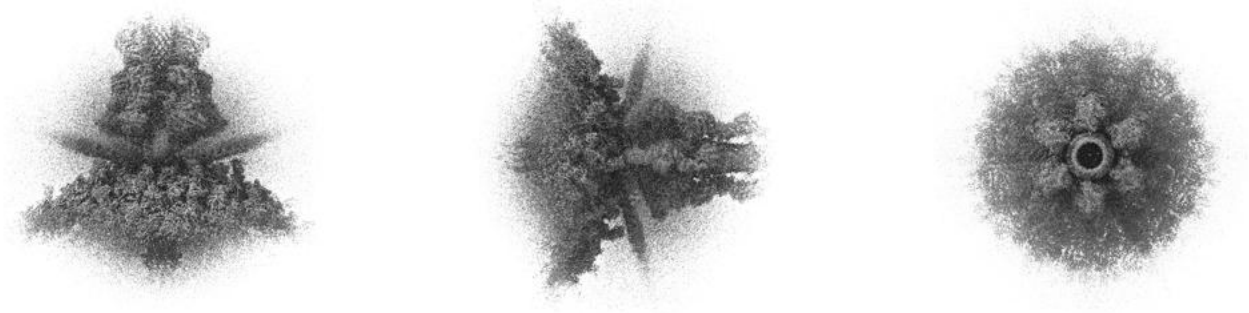
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. 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.

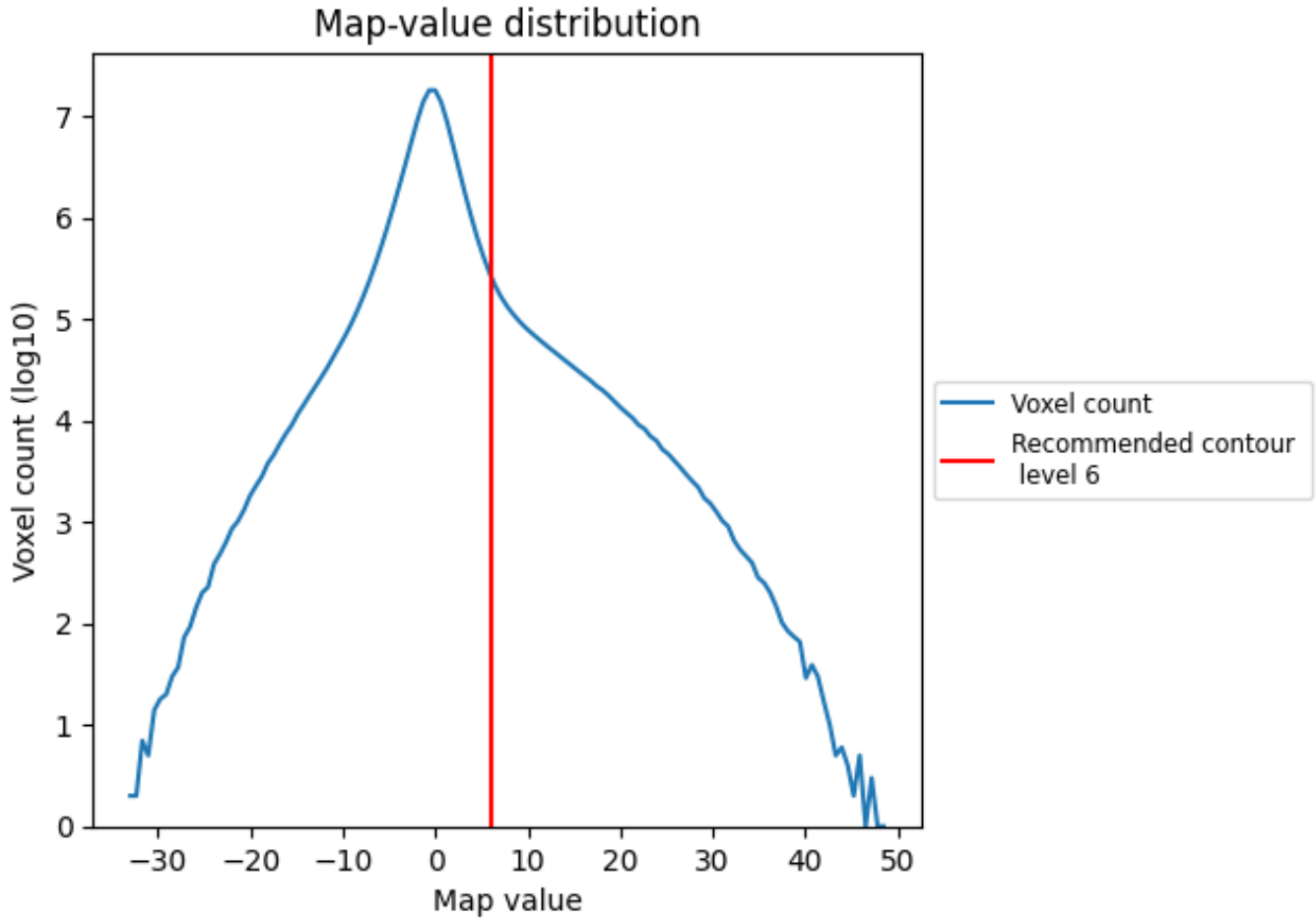
6.6 Mask visualisation (i)

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

7 Map analysis

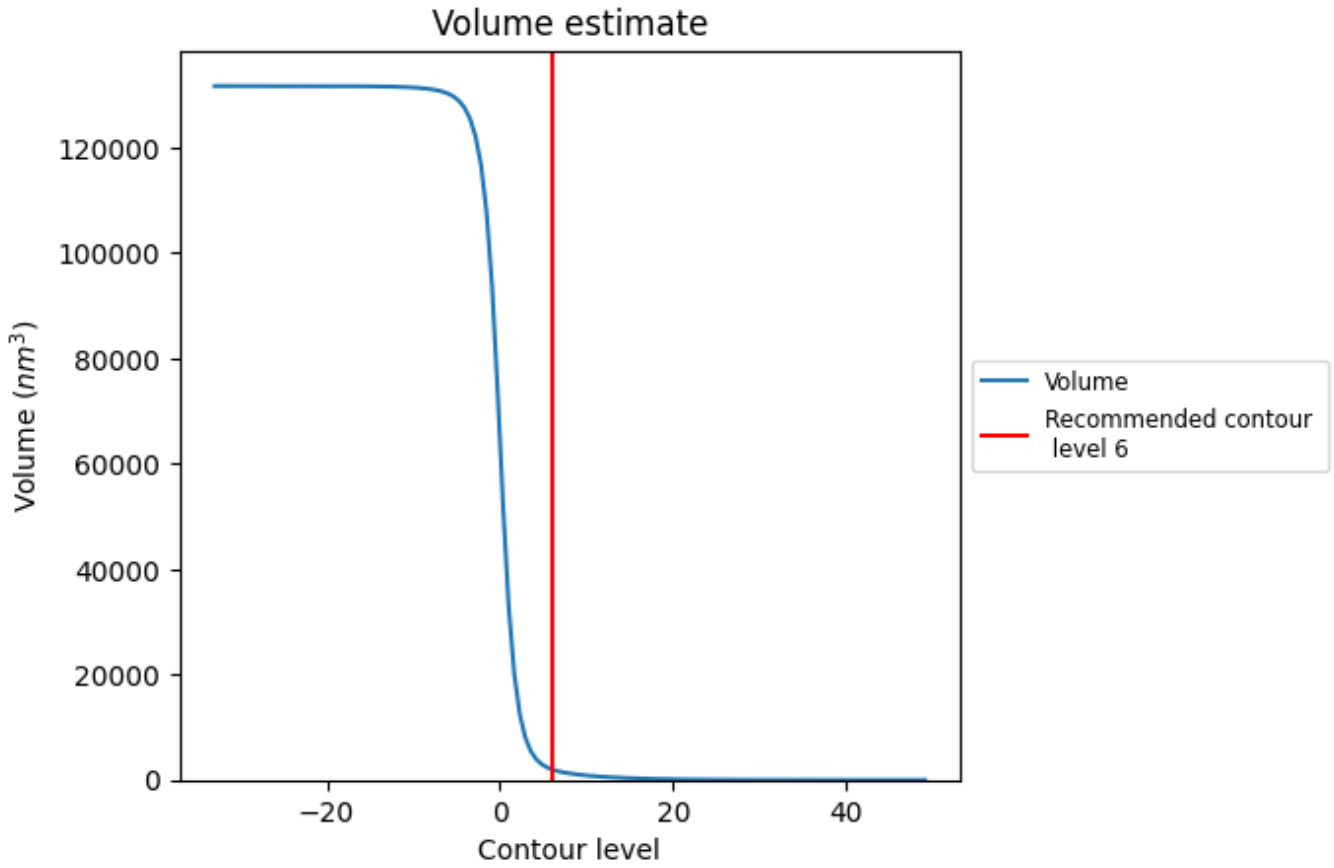
This section contains the results of statistical analysis of the map.

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.

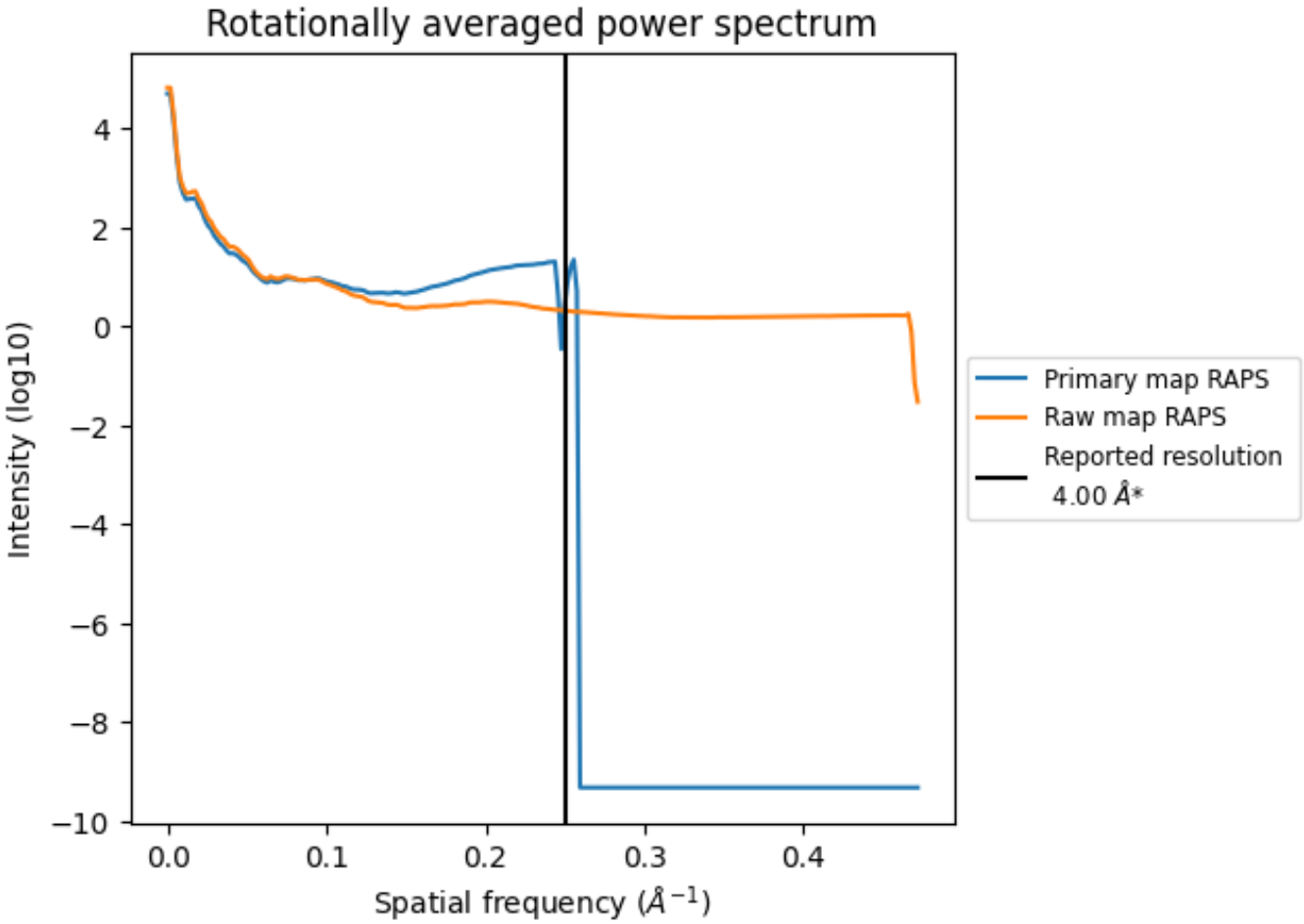
7.2 Volume estimate



The volume at the recommended contour level is 2011 nm^3; this corresponds to an approximate mass of 1817 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)

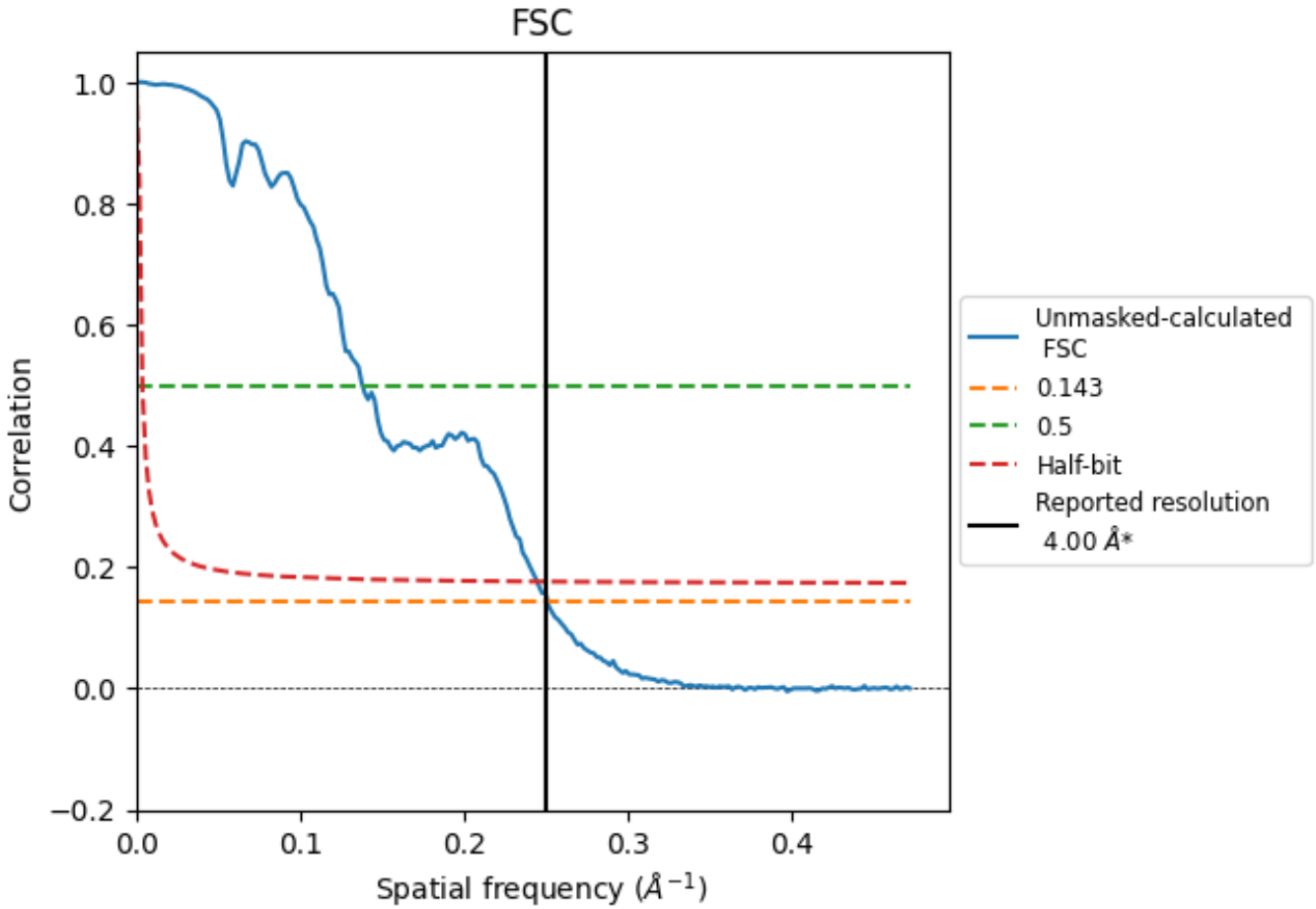


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

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 0.250 Å^{-1}

8.2 Resolution estimates (i)

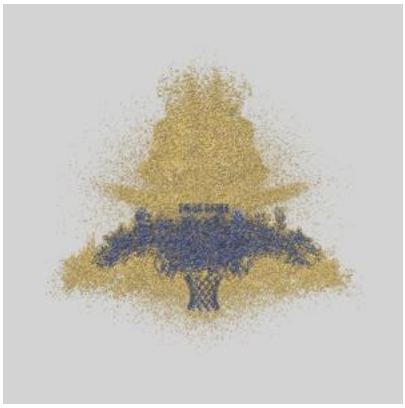
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	7.25	4.09

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

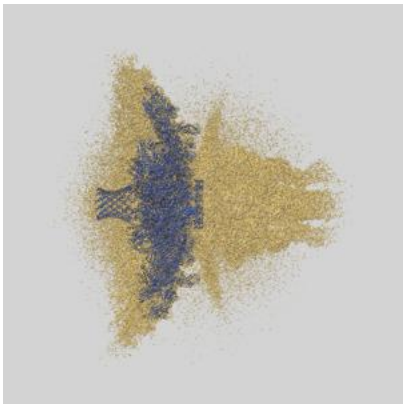
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62959 and PDB model 9LBZ. Per-residue inclusion information can be found in section 3 on page 8.

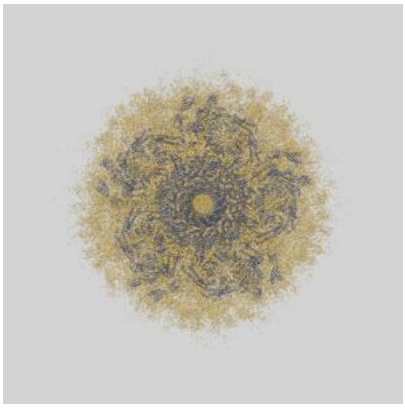
9.1 Map-model overlay



X



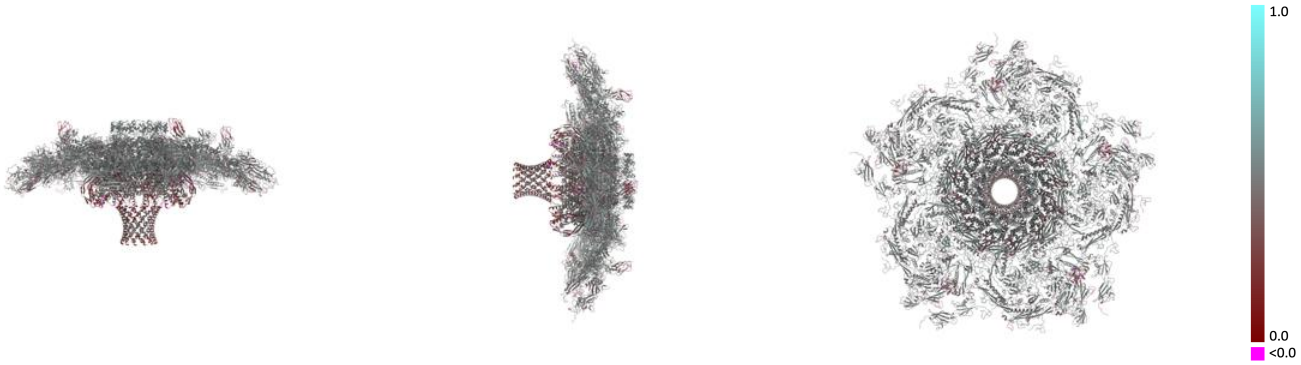
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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.

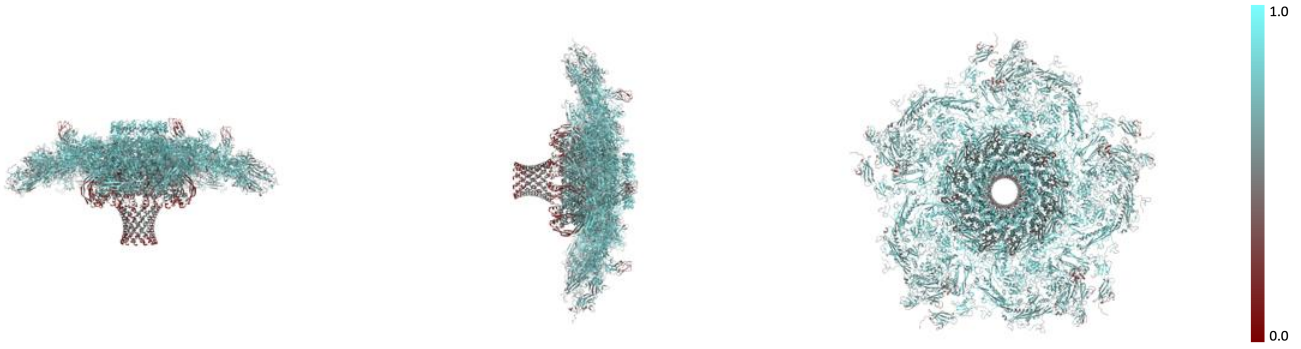
9.2 Q-score mapped to coordinate model (i)



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.

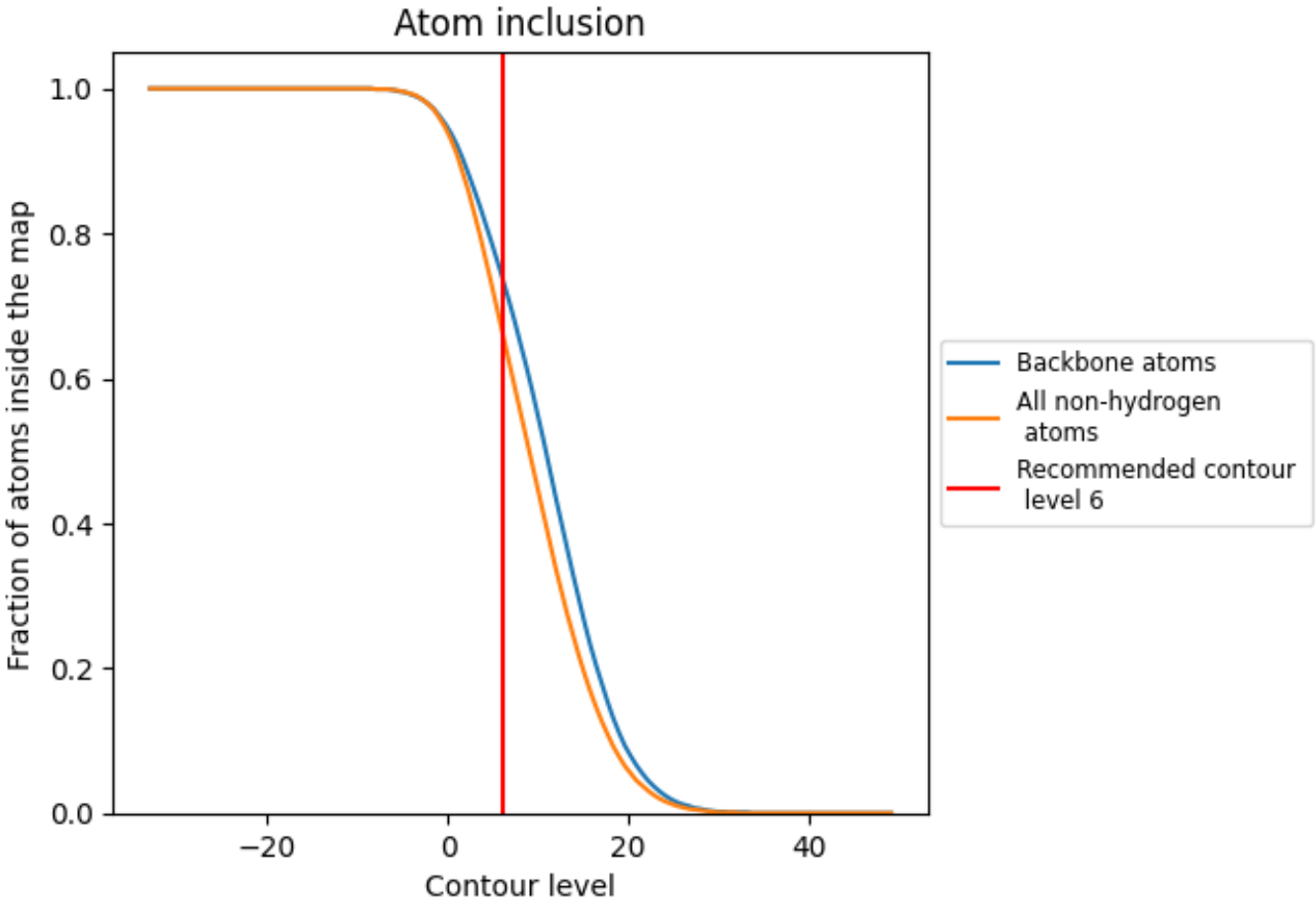
9.3 Atom inclusion mapped to coordinate model (i)



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 (6).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 67% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6660	0.4580
A	0.6380	0.4360
B	0.6370	0.4430
C	0.6500	0.4420
D	0.6390	0.4350
E	0.6360	0.4370
F	0.6430	0.4410
G	0.6370	0.4380
H	0.6440	0.4430
I	0.6440	0.4420
J	0.6410	0.4440
K	0.6400	0.4400
L	0.6450	0.4400
M	0.6620	0.4730
N	0.6770	0.4800
O	0.6570	0.4750
P	0.6690	0.4770
Q	0.6690	0.4780
R	0.7190	0.4650
S	0.7230	0.4710
T	0.7210	0.4720
U	0.7100	0.4680
V	0.7220	0.4750
W	0.7510	0.4870
X	0.7560	0.4890
Y	0.7610	0.4880
Z	0.7560	0.4860
a	0.7550	0.4890
b	0.7310	0.4840
c	0.7390	0.4850
d	0.7270	0.4790
e	0.7430	0.4840
f	0.7380	0.4840
g	0.7120	0.4760
h	0.7180	0.4790

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.7050	0.4730
j	0.7190	0.4800
k	0.7240	0.4830
l	0.6480	0.4570
m	0.6430	0.4580
n	0.6250	0.4500
o	0.6430	0.4560
p	0.6400	0.4540
q	0.5900	0.4630
r	0.5990	0.4650
s	0.5870	0.4540
t	0.5850	0.4530
u	0.5880	0.4600
v	0.5280	0.4180
w	0.5490	0.4150
x	0.5140	0.4120
y	0.5210	0.4100
z	0.5190	0.4080