



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:58 AM UTC

PDB ID : 8FWG / pdb_00008fwg
EMDB ID : EMD-29504
Title : Structure of neck and portal vertex of Agrobacterium phage Milano, C5 symmetry
Authors : Sonani, R.R.; Wang, F.; Esteves, N.C.; Kelly, R.J.; Sebastian, A.; Kreutzberger, M.A.B.; Leiman, P.G.; Scharf, B.E.; Egelman, E.H.
Deposited on : 2023-01-22
Resolution : 3.45 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

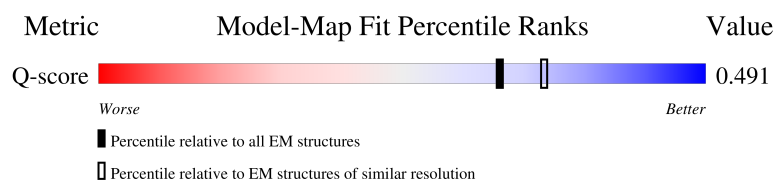
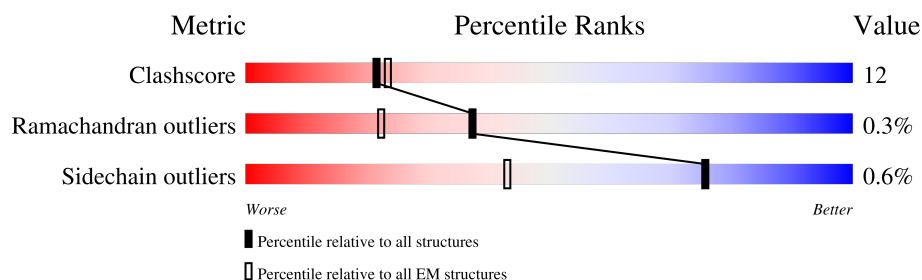
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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.



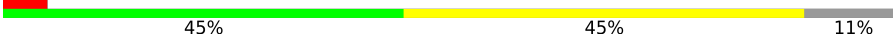
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13836 (2.95 - 3.95)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a1	38	
1	a2	38	
1	a5	38	
1	a6	38	

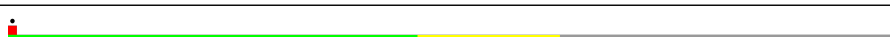
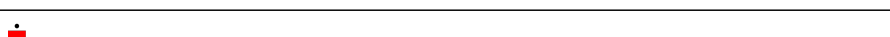
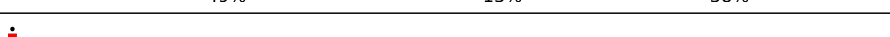
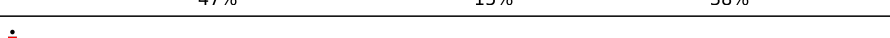
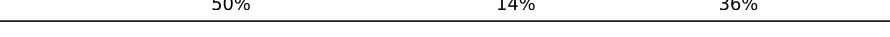
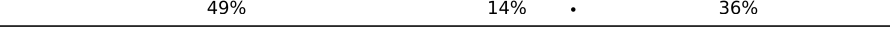
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Mol	Chain	Length	Quality of chain
1	a7	38	
1	b1	38	
1	b2	38	
1	b5	38	
1	b6	38	
1	b7	38	
1	c	38	
1	d	38	
1	d1	38	
1	d2	38	
1	d5	38	
1	d6	38	
1	d7	38	
1	e	38	
1	e1	38	
1	e2	38	
1	e5	38	
1	e6	38	
1	e7	38	
1	f	38	
1	g	38	
2	f1	217	
2	f2	217	
2	f5	217	
2	f6	217	

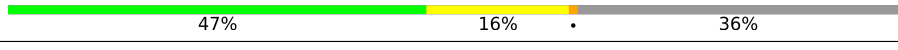
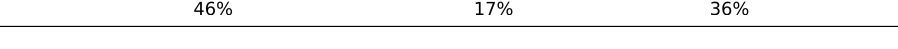
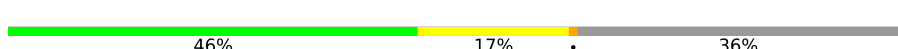
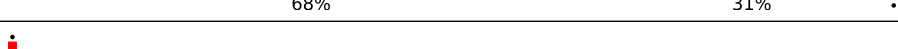
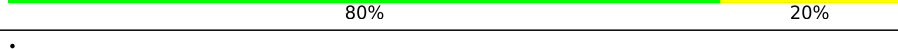
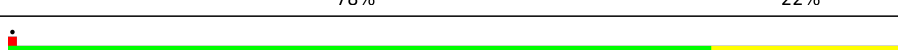
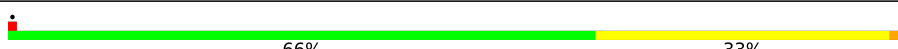
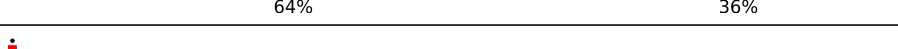
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Mol	Chain	Length	Quality of chain
2	f7	217	 6% 91%
3	g1	465	 52% 11% 36%
3	g2	465	 51% 12% 36%
3	g5	465	 53% 11% 36%
3	g6	465	 51% 13% 36%
3	g7	465	 51% 13% 36%
3	h1	465	 50% 14% 36%
3	h2	465	 52% 11% 36%
3	h5	465	 49% 15% 36%
3	h6	465	 47% 16% 36%
3	h7	465	 49% 15% 36%
3	k1	465	 46% 16% 38%
3	k2	465	 47% 15% 38%
3	k5	465	 49% 13% 38%
3	k6	465	 47% 15% 38%
3	k7	465	 47% 15% 38%
3	n1	465	 50% 14% 36%
3	n2	465	 52% 12% 36%
3	n5	465	 49% 14% 36%
3	n6	465	 48% 16% 36%
3	n7	465	 48% 16% 36%
3	o1	465	 48% 15% 36%
3	o2	465	 47% 16% 36%
3	o5	465	 47% 16% 36%
3	o6	465	 46% 17% 36%

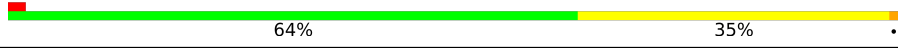
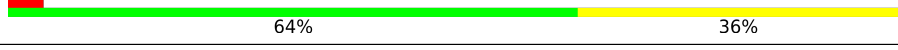
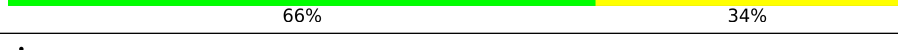
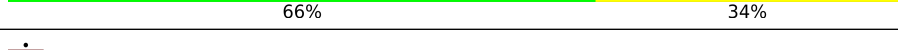
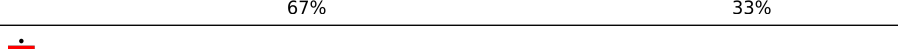
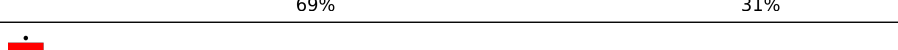
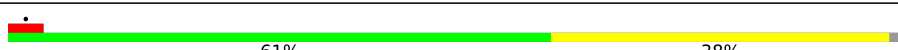
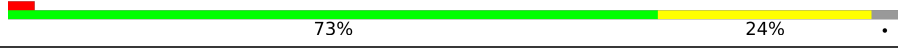
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Mol	Chain	Length	Quality of chain
3	o7	465	
3	r1	465	
3	r2	465	
3	r5	465	
3	r6	465	
3	r7	465	
4	l1	137	
4	l2	137	
4	l5	137	
4	l6	137	
4	l7	137	
4	m1	137	
4	m2	137	
4	m5	137	
4	m6	137	
4	m7	137	
4	p1	137	
4	p2	137	
4	p5	137	
4	p6	137	
4	p7	137	
4	q1	137	
4	q2	137	
4	q5	137	
4	q6	137	

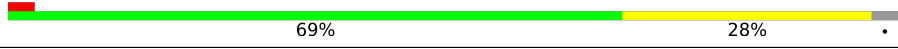
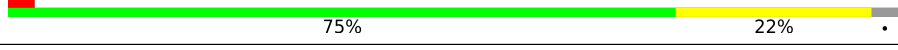
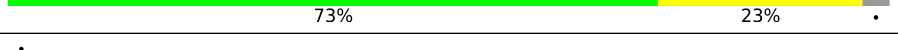
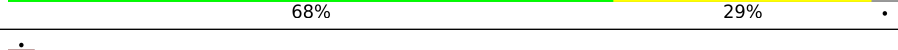
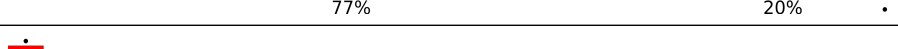
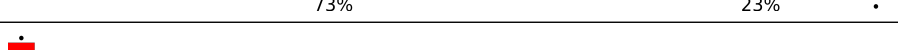
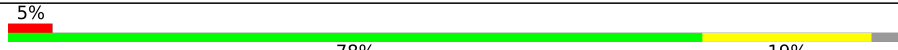
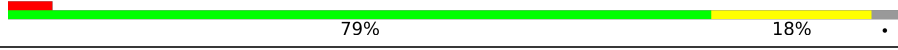
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Mol	Chain	Length	Quality of chain
4	q7	137	 70%30%
4	s1	137	 62%37%
4	s2	137	 64%35%
4	s5	137	 64%36%
4	s6	137	 61%37%
4	s7	137	 59%39%
4	t1	137	 66%34%
4	t2	137	 66%34%
4	t5	137	 67%33%
4	t6	137	 69%31%
4	t7	137	 74%24%
4	u1	137	 7%68%31%
4	u2	137	 5%61%36%
4	u5	137	 68%31%
4	u6	137	 65%34%
4	u7	137	 61%38%
4	v1	137	 69%28%
4	v2	137	 5%70%28%
4	v5	137	 71%28%
4	v6	137	 69%31%
4	v7	137	 69%29%
5	03	230	 73%24%
5	13	230	 77%20%
5	23	230	 76%21%
5	33	230	 71%26%

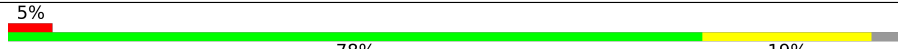
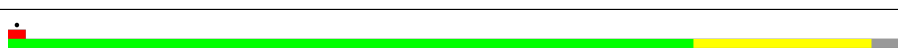
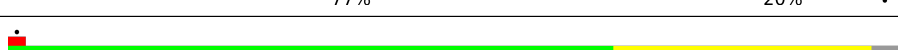
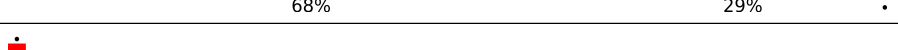
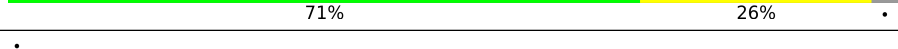
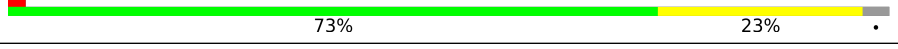
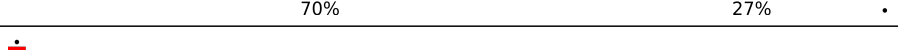
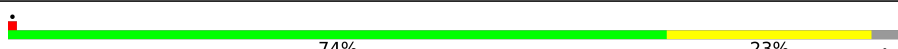
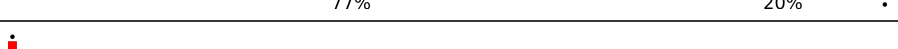
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Mol	Chain	Length	Quality of chain
5	43	230	
5	53	230	
5	63	230	
5	73	230	
5	83	230	
5	93	230	
5	A3	230	
5	B3	230	
5	C3	230	
5	D3	230	
5	E3	230	
5	F3	230	
5	G3	230	
5	J3	230	
5	K3	230	
5	L3	230	
5	M3	230	
5	N3	230	
5	O3	230	
5	P3	230	
5	Q3	230	
5	R3	230	
5	S3	230	
5	T3	230	
5	U3	230	

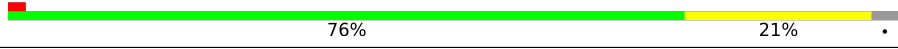
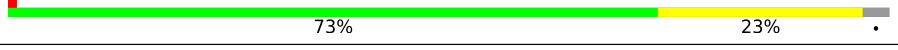
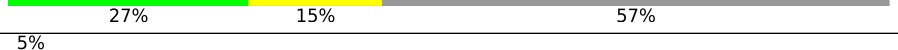
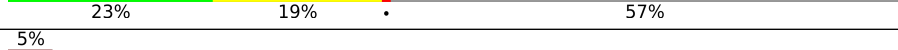
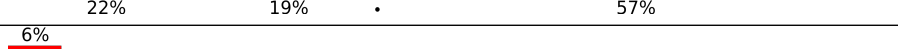
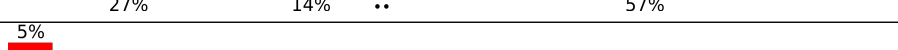
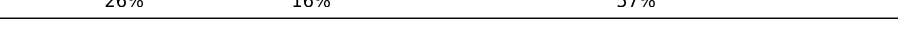
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Mol	Chain	Length	Quality of chain
5	V3	230	
5	W3	230	
5	X3	230	
5	Y3	230	
5	Z3	230	
5	a3	230	
5	b3	230	
5	c3	230	
5	d3	230	
5	e3	230	
5	f3	230	
5	g3	230	
5	h3	230	
5	i3	230	
5	j3	230	
5	k3	230	
5	l3	230	
5	m3	230	
5	n3	230	
5	o3	230	
5	p3	230	
5	q3	230	
5	r3	230	
5	s3	230	
5	t3	230	

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Mol	Chain	Length	Quality of chain
5	u3	230	
5	v3	230	
5	w3	230	
5	x3	230	
5	y3	230	
5	z3	230	
6	A4	202	
6	B4	202	
6	C4	202	
6	D4	202	
6	E4	202	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 221120 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 Linking protein 2, gp128.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a1	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	b1	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	d1	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
1	e1	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	a2	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	b2	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	d2	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
1	e2	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	a5	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	b5	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	d5	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
1	e5	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	a6	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	b6	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	d6	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
1	e6	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	a7	28	Total	C	N	O	S	0	0
			209	131	40	33	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	b7	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	d7	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
1	e7	28	Total	C	N	O	S	0	0
			209	131	40	33	5		
1	c	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
1	d	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
1	e	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
1	f	34	Total	C	N	O	S	0	0
			246	155	46	40	5		
1	g	34	Total	C	N	O	S	0	0
			246	155	46	40	5		

- Molecule 2 is a protein called Linking protein 1, gp16.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	f1	20	Total	C	N	O	S	0	0
			140	88	27	23	2		
2	f2	20	Total	C	N	O	S	0	0
			140	88	27	23	2		
2	f5	20	Total	C	N	O	S	0	0
			140	88	27	23	2		
2	f6	20	Total	C	N	O	S	0	0
			140	88	27	23	2		
2	f7	20	Total	C	N	O	S	0	0
			140	88	27	23	2		

- Molecule 3 is a protein called Major capsid protein, gp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	g1	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	h1	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	k1	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
3	n1	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	o1	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	r1	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	g2	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	h2	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	k2	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
3	n2	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	o2	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	r2	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	g5	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	h5	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	k5	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
3	n5	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	o5	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	r5	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	g6	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	h6	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	k6	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
3	n6	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	o6	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	r6	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	g7	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	h7	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	k7	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
3	n7	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	o7	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		
3	r7	299	Total	C	N	O	S	0	0
			2337	1483	397	441	16		

- Molecule 4 is a protein called Minor capsid protein, gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	l1	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	m1	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	p1	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	q1	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	s1	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	t1	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	u1	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
4	v1	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
4	l2	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	m2	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	p2	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	q2	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	s2	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	t2	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	u2	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
4	v2	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
4	l5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	m5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	p5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	q5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	s5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	t5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	u5	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
4	v5	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
4	l6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	m6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	p6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	q6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	s6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	t6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	u6	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
4	v6	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
4	l7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	m7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	p7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	q7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	s7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	t7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
4	u7	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
4	v7	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		

- Molecule 5 is a protein called Collar sheath protein, gp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	K3	230	Total	C	N	O	S	0	0
			1723	1090	287	337	9		
5	L3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	M3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	N3	230	Total	C	N	O	S	0	0
			1723	1090	287	337	9		
5	O3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	P3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	Q3	230	Total	C	N	O	S	0	0
			1723	1090	287	337	9		
5	R3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	S3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	T3	230	Total	C	N	O	S	0	0
			1723	1090	287	337	9		
5	U3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	V3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	W3	230	Total	C	N	O	S	0	0
			1723	1090	287	337	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	X3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	Y3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	Z3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	a3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	b3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	c3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	d3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	e3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	f3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	g3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	h3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	i3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	j3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	k3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	l3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	m3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	n3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	o3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	p3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	q3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	r3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	s3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	t3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	u3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	v3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	w3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	x3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	y3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	z3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	13	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	23	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	33	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	43	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	53	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	63	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	73	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	83	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	93	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	03	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	A3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	B3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0
5	C3	223	Total 1679	C 1065	N 279	O 327	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	D3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	E3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	F3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
5	G3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		

- Molecule 6 is a protein called Neck 1 protein, gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A4	87	Total	C	N	O	S	0	0
			671	429	120	118	4		
6	B4	87	Total	C	N	O	S	0	0
			671	429	120	118	4		
6	C4	87	Total	C	N	O	S	0	0
			671	429	120	118	4		
6	D4	87	Total	C	N	O	S	0	0
			671	429	120	118	4		
6	E4	87	Total	C	N	O	S	0	0
			671	429	120	118	4		

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.

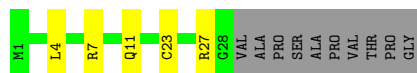
- Molecule 1: Linking protein 2, gp128

Chain a1: 



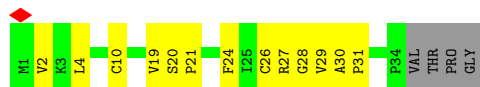
- Molecule 1: Linking protein 2, gp128

Chain b1: 



- Molecule 1: Linking protein 2, gp128

Chain d1: 



- Molecule 1: Linking protein 2, gp128

Chain e1: 

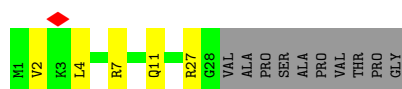


- Molecule 1: Linking protein 2, gp128

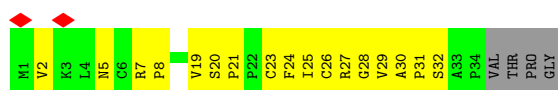
Chain a2: 



- Molecule 1: Linking protein 2, gp128



- Molecule 1: Linking protein 2, gp128



- Molecule 1: Linking protein 2, gp128



- Molecule 1: Linking protein 2, gp128



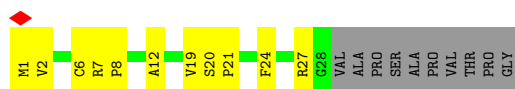
- Molecule 1: Linking protein 2, gp128



- Molecule 1: Linking protein 2, gp128

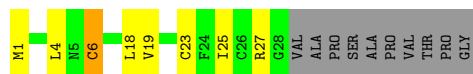


- Molecule 1: Linking protein 2, gp128



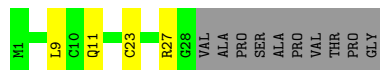
- Molecule 1: Linking protein 2, gp128

Chain a6:  53% 18% 26%



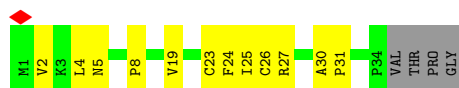
- Molecule 1: Linking protein 2, gp128

Chain b6:  63% 11% 26%



- Molecule 1: Linking protein 2, gp128

Chain d6:  58% 32% 11%



- Molecule 1: Linking protein 2, gp128

Chain e6:  47% 26% 26%



- Molecule 1: Linking protein 2, gp128

Chain a7:  53% 18% 26%



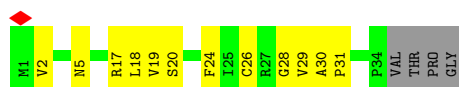
- Molecule 1: Linking protein 2, gp128

Chain b7:  66% 8% 26%



- Molecule 1: Linking protein 2, gp128

Chain d7:  58% 32% 11%



- Molecule 1: Linking protein 2, gp128



- Molecule 1: Linking protein 2, gp128



- Molecule 1: Linking protein 2, gp128



- Molecule 1: Linking protein 2, gp128



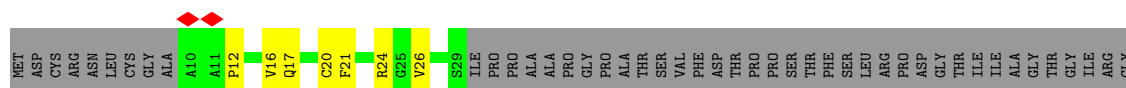
- Molecule 1: Linking protein 2, gp128

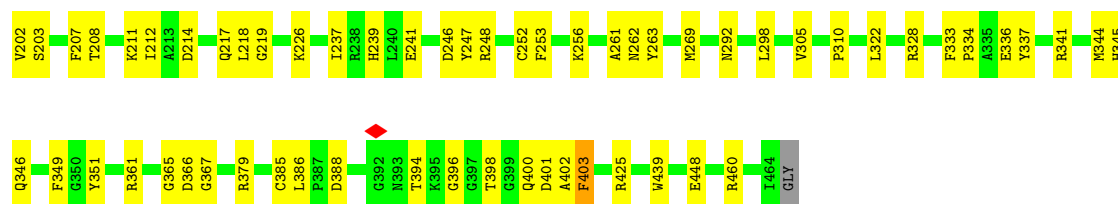


- Molecule 1: Linking protein 2, gp128

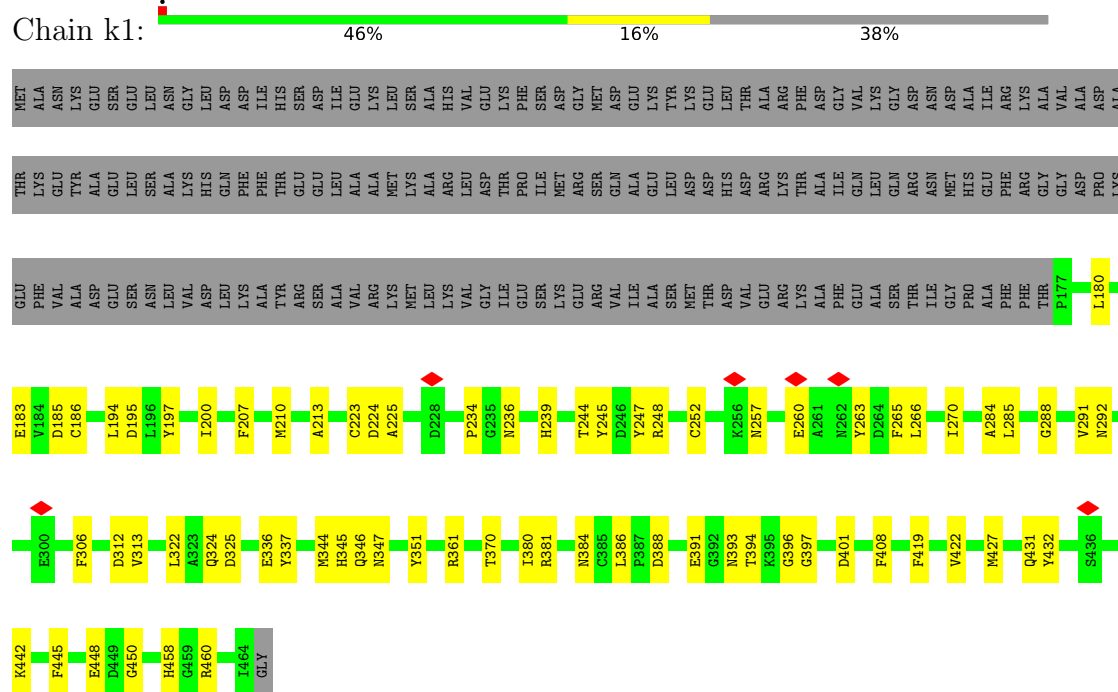


- Molecule 2: Linking protein 1, gp16

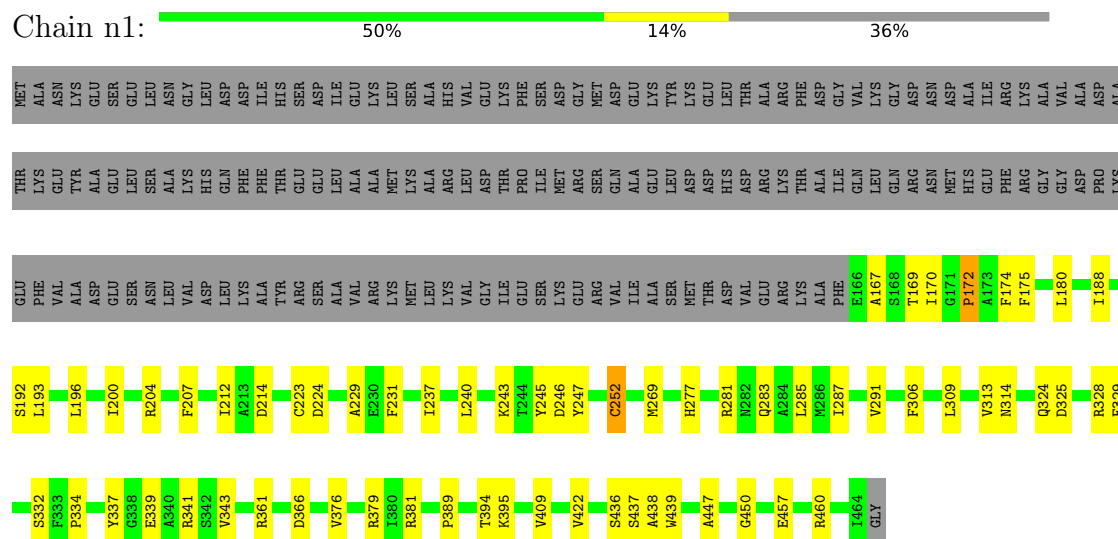




• Molecule 3: Major capsid protein, gp9

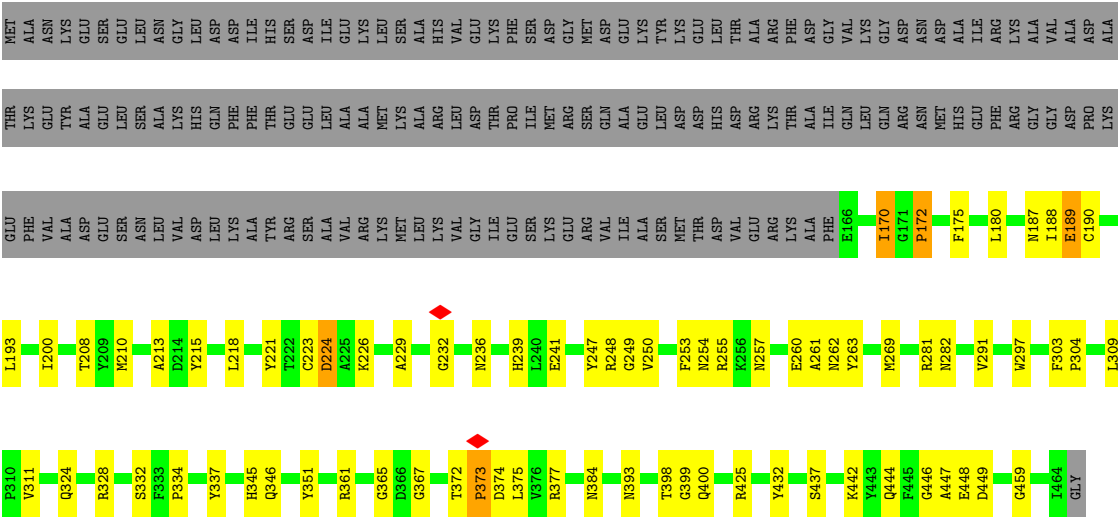


• Molecule 3: Major capsid protein, gp9

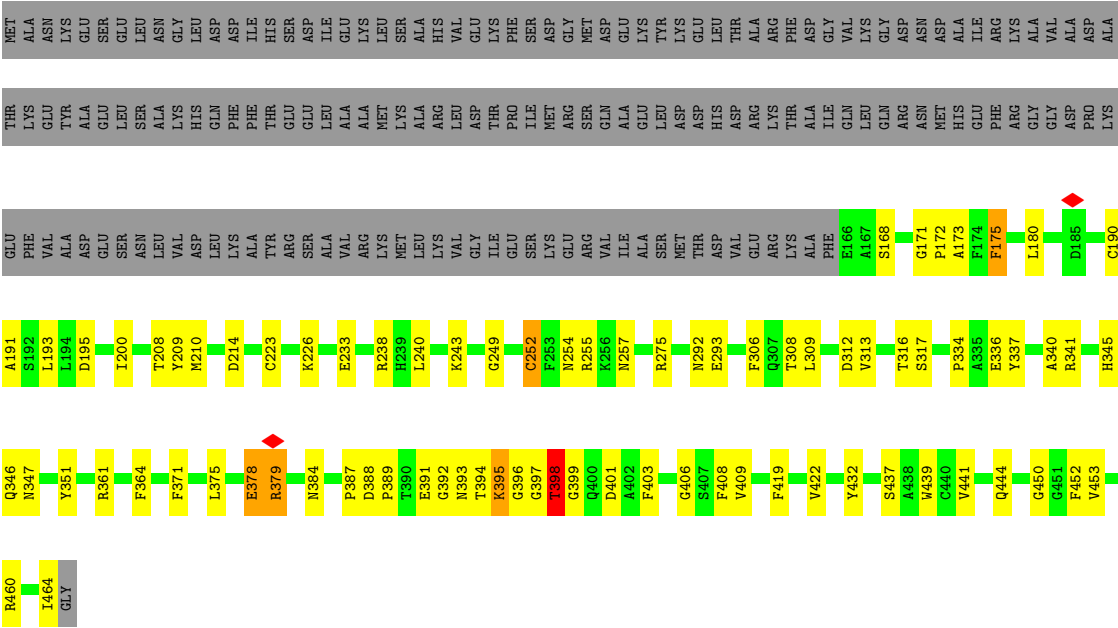


• Molecule 3: Major capsid protein, gp9

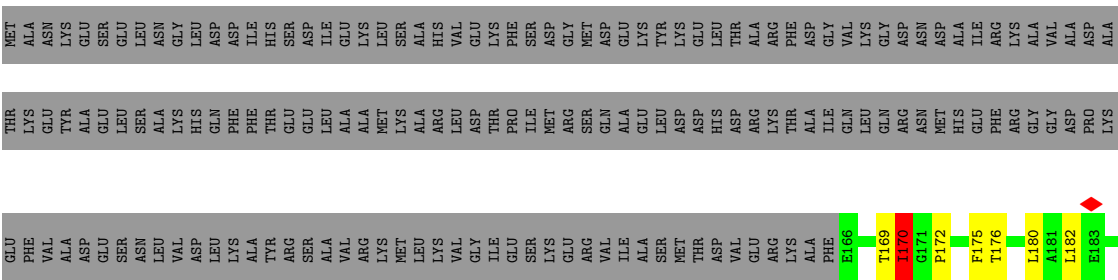




• Molecule 3: Major capsid protein, gp9

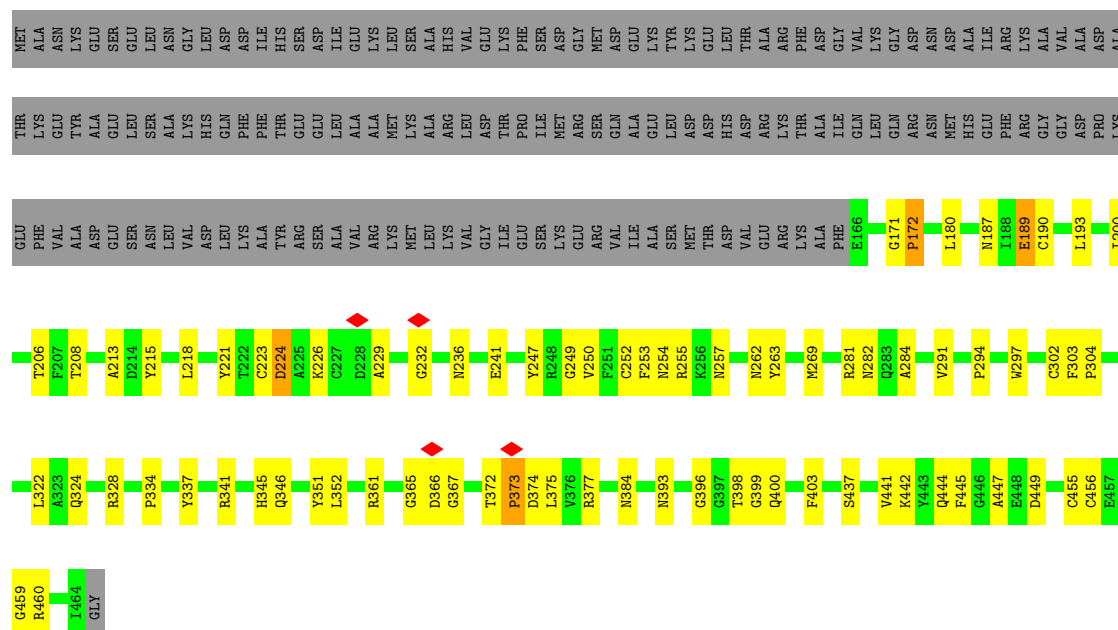


• Molecule 3: Major capsid protein, gp9

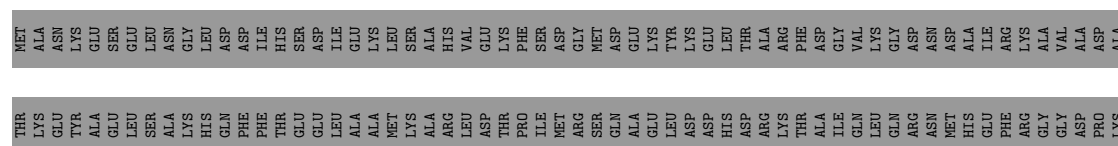


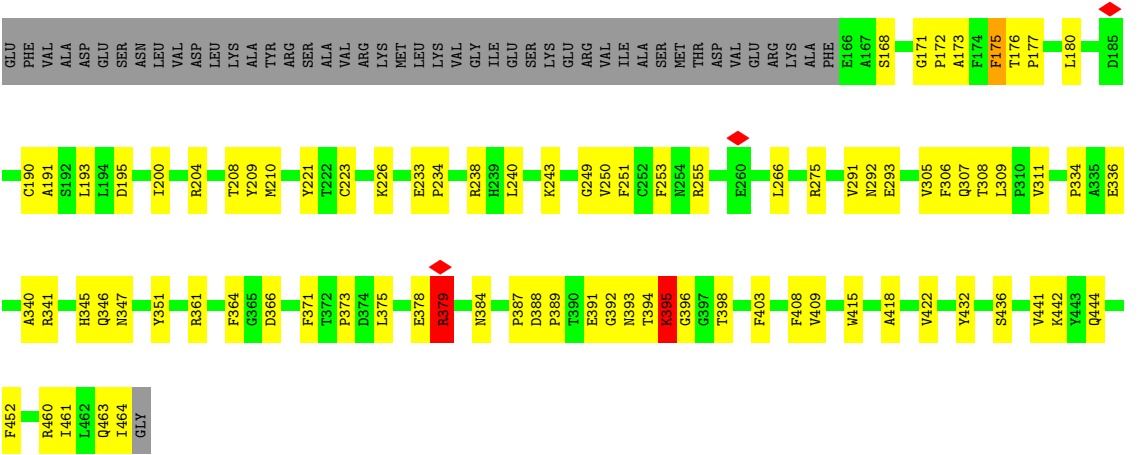
R341	F207	GLU	THR	MET
D366	T208	PHE	LYS	ALA
L375	I212	ALA	GLU	LYS
R379	A213	ASP	TYR	GLY
T394	D214	GLU	ALA	LYS
K395	Q217	SER	LEU	GLU
V422	Q218	ASN	SER	LEU
M427	L218	LEU	ALA	GLY
S436	G219	VAL	LYS	ASN
W439	C223	ASP	HIS	GLY
A447	D224	LEU	GLN	ASP
G450	A229	LYS	PHE	ASP
R460	E230	ALA	PHE	ILE
I464	F231	VAL	THR	SER
GLY	G232	ARG	GLU	ASP
	E233	LYS	LEU	LYS
	I237	MET	ALA	SER
	L240	LEU	ALA	ALA
	E241	LYS	ARG	ALA
	G242	VAL	LEU	GLY
	K243	GLY	ASP	ILE
	T244	GLU	THR	THR
	Y245	SER	PRO	PHE
	D246	LYS	ILE	SER
	Y247	GLU	MET	ASP
	M269	ARG	ARG	GLY
	H277	ILE	GLN	MET
	R281	ALA	ALA	ASP
	L285	VAL	LEU	GLY
	V291	GLU	ASP	LYS
	F306	ARG	ARG	ARG
	L309	LYS	LYS	PHE
	V313	PHE	ILE	GLY
	N314	ILE	GLN	VAL
	Q324	I170	LEU	LYS
	D325	G171	GLN	GLY
	R328	P172	ARG	ASP
	F329	F175	MET	ASN
	S332	L180	HIS	ALA
	F333	I188	GLU	ALA
	P334	L196	PHE	LYS
	A395	T200	ARG	ALA
			THR	LYS

Response	Percentage
Yes	47%
No	16%
Don't know	36%

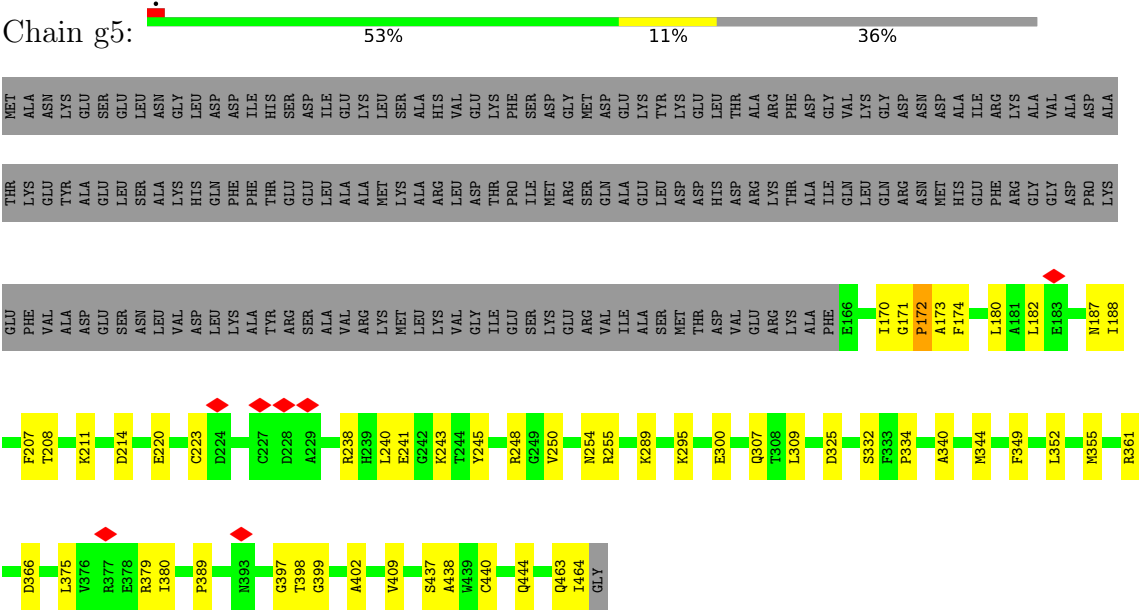


Response	Percentage
Yes	46%
No	17%
Don't know	36%

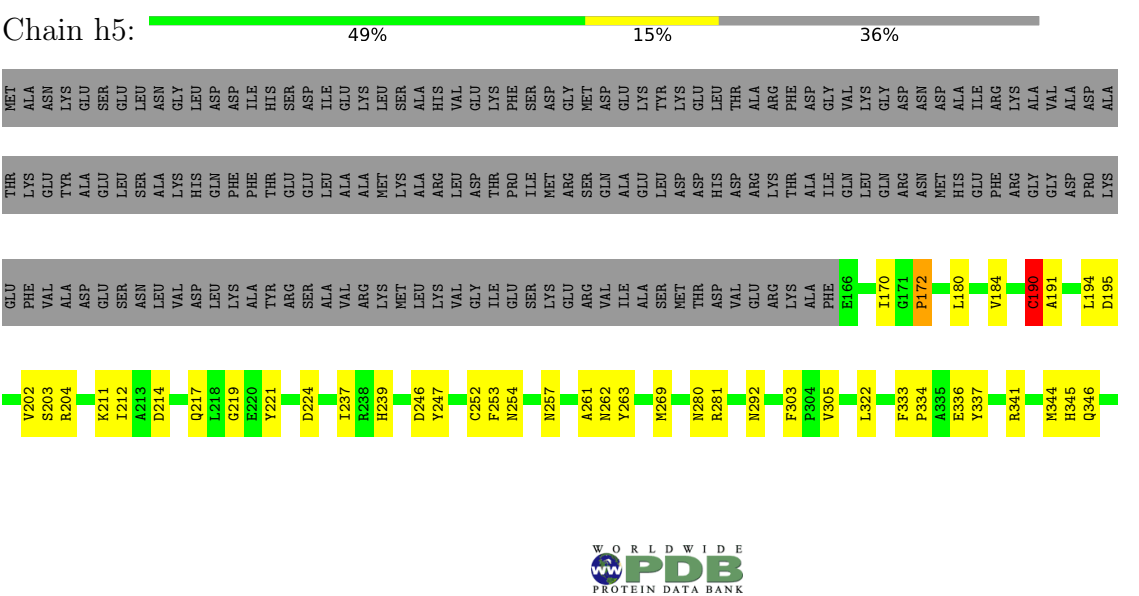




• Molecule 3: Major capsid protein, gp9

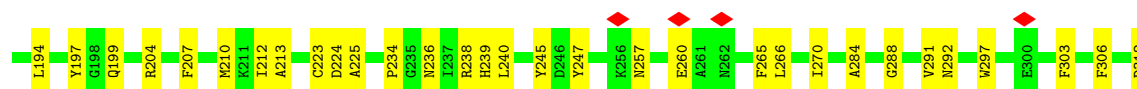
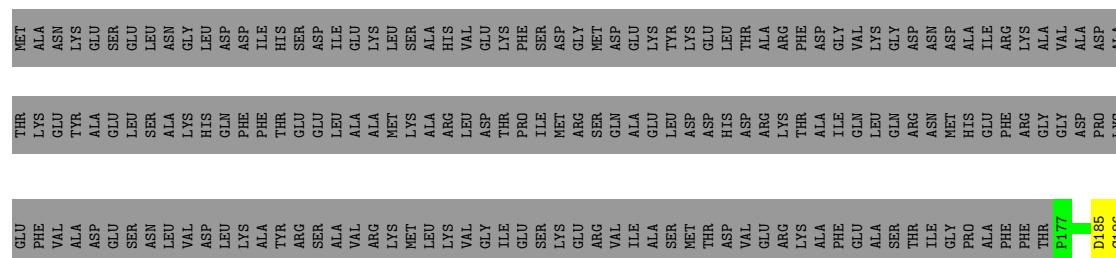


• Molecule 3: Major capsid protein, gp9

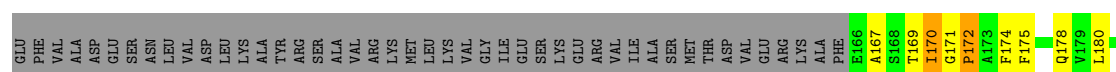
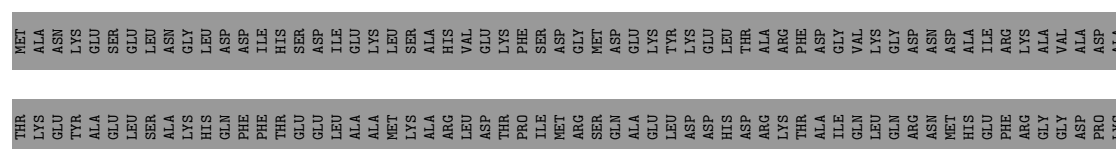




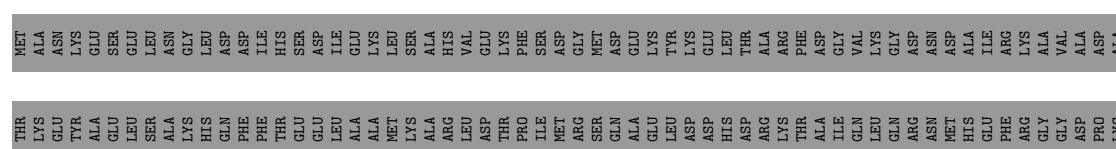
- Molecule 3: Major capsid protein, gp9

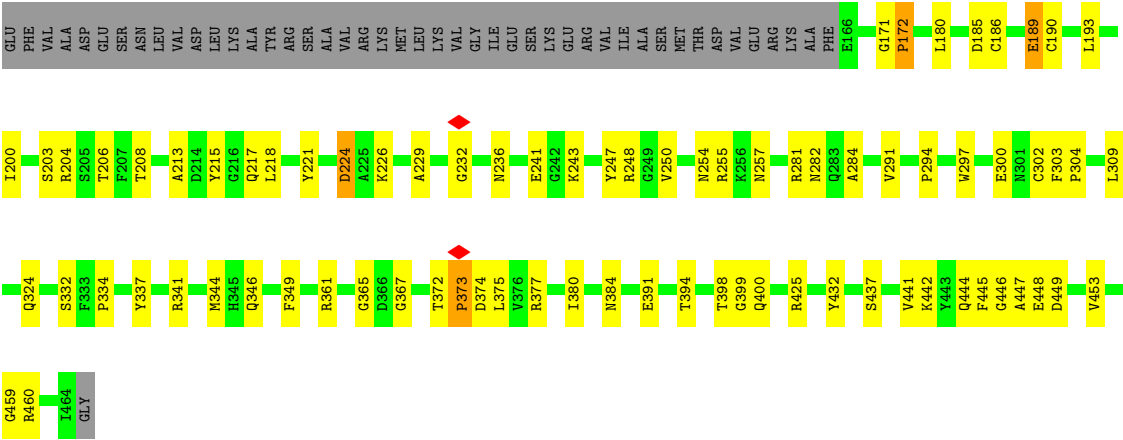


- Molecule 3: Major capsid protein, gp9

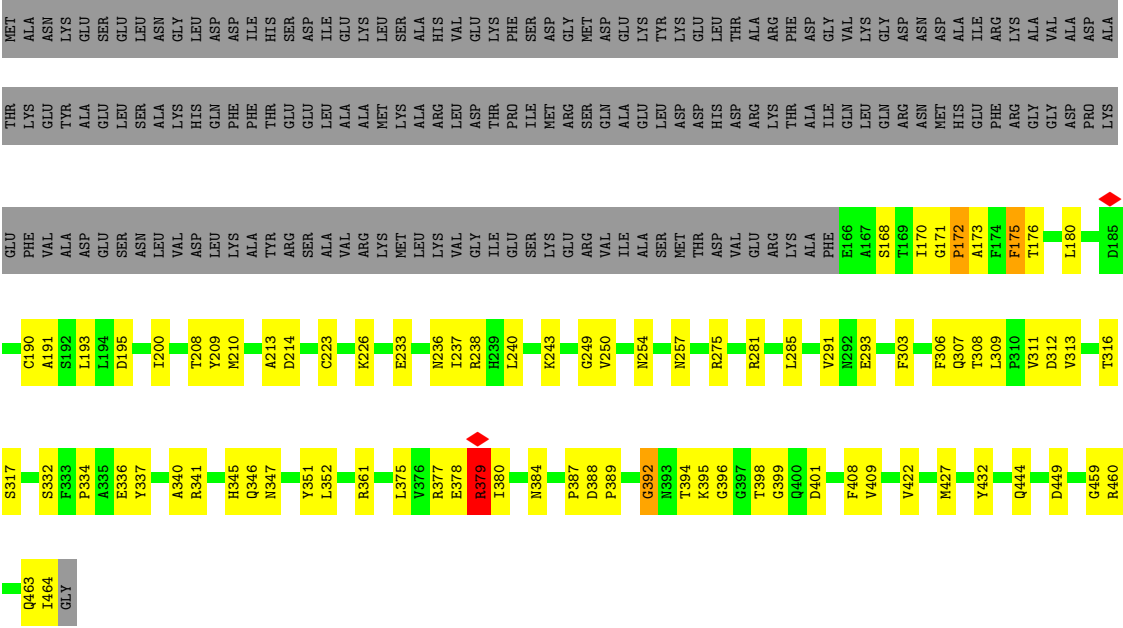


- Molecule 3: Major capsid protein, gp9

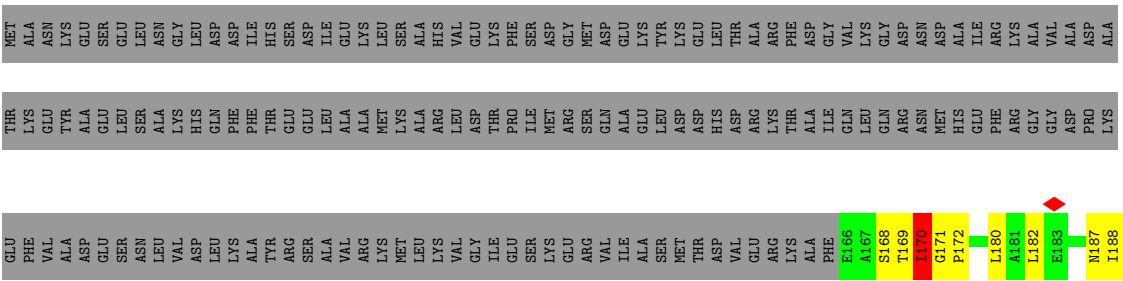




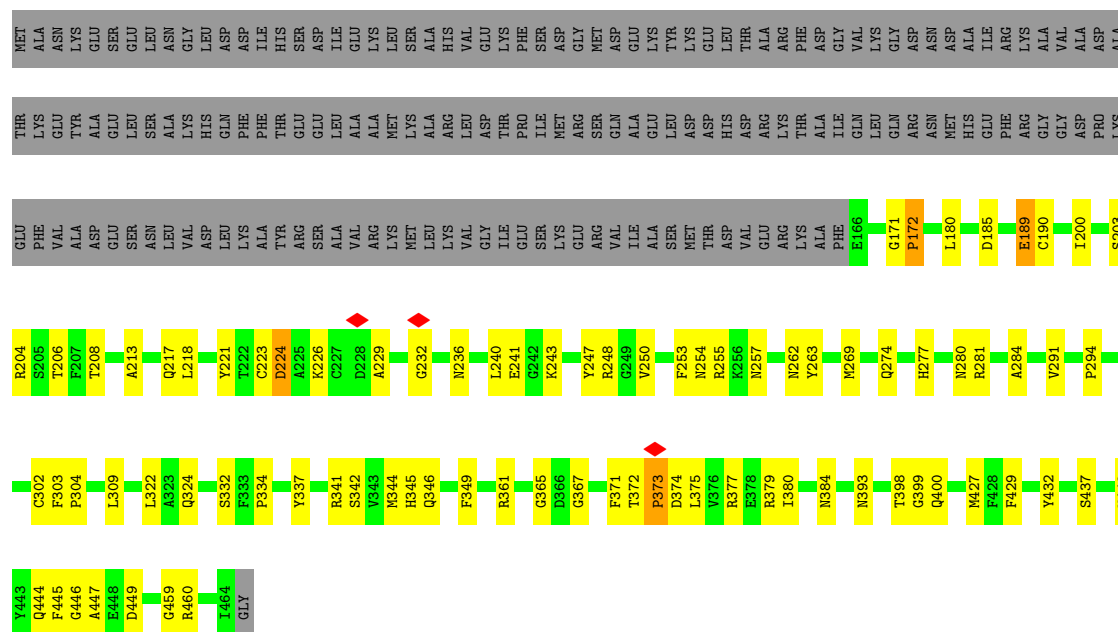
• Molecule 3: Major capsid protein, gp9



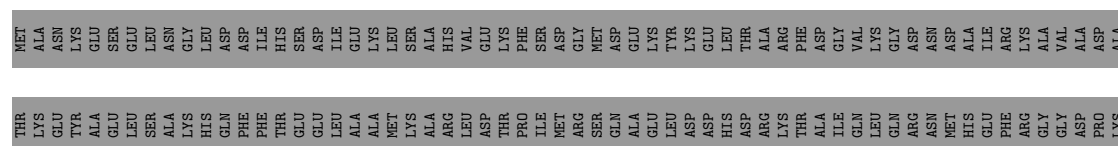
• Molecule 3: Major capsid protein, gp9

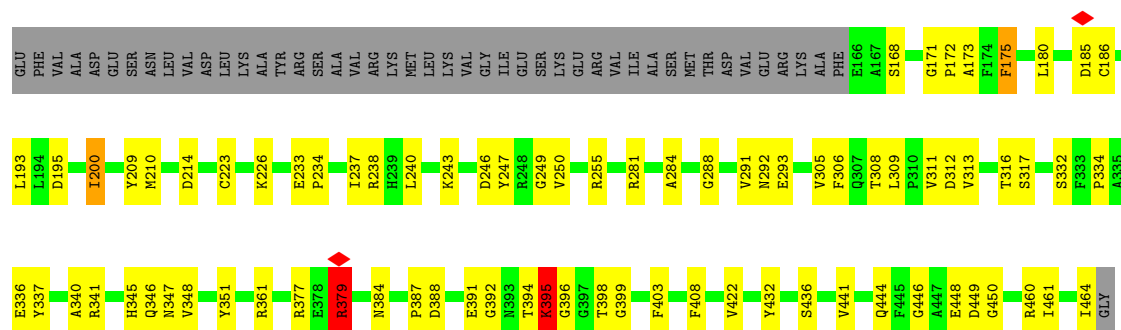


- Molecule 3: Major capsid protein, gp9



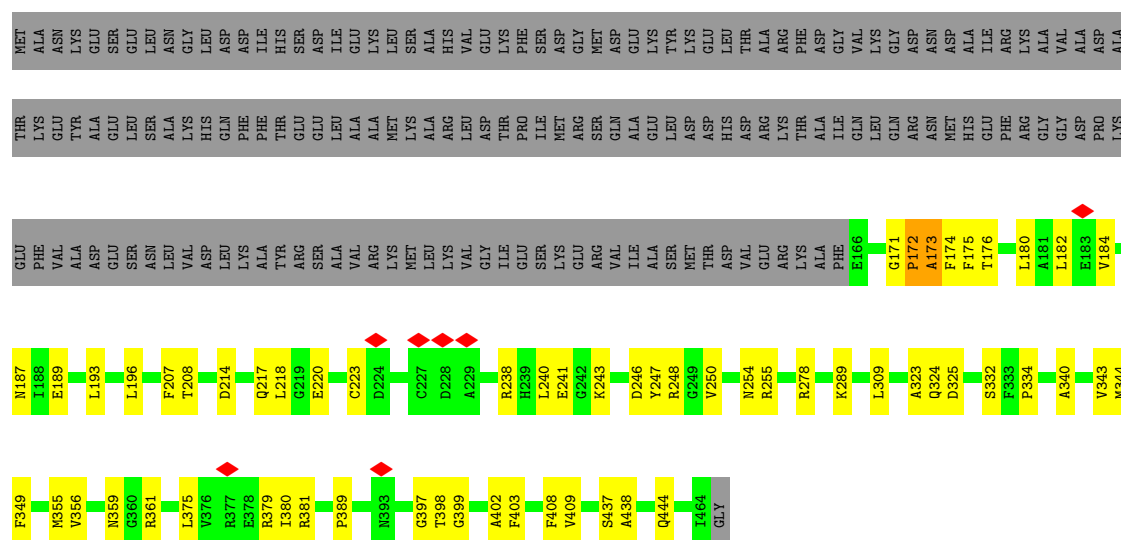
- Molecule 3: Major capsid protein, gp9





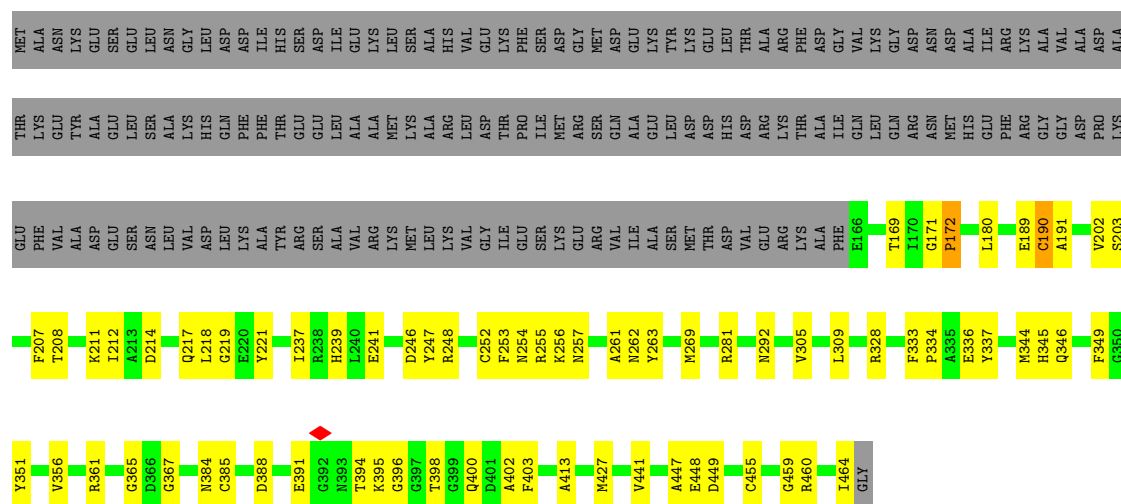
• Molecule 3: Major capsid protein, gp9

Chain g7: 51% 13% 36%



• Molecule 3: Major capsid protein, gp9

Chain h7: 49% 15% 36%



• Molecule 3: Major capsid protein, gp9



MET	THR	GLU	PHE	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL	GLU	THR	LYS	GLU	VAL</
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• Molecule 3: Major capsid protein, gp9

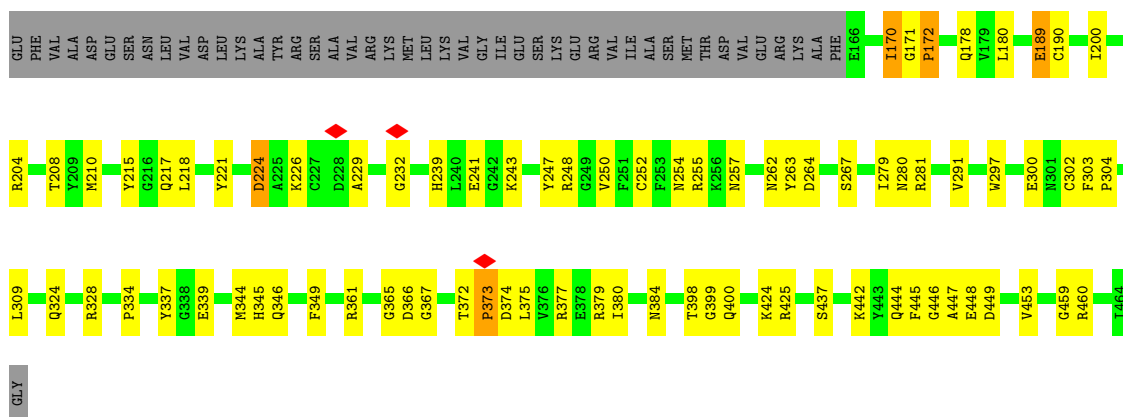


MET	LYS	THR	GLU	PHE	GLU	ASN	GLY	LYS	THR	ALA	GLU	SER	GLU	LEU	ASN	GLY	ASP	ASP	ILE	HIS	SER	GLU	ASP	ILE	GLY	LYS	VAL	GLY	ASP	ASN	ASP	ALA	ILE	ARG	LYS	THR	GLY	VAL	ALA	ASP	PRO	VAL	ALA				
THR	LYS	GLU	TYR	ALA	GLU	GLU	SER	LEU	SER	LEU	ALA	ALA	HIS	GLN	PHE	PHE	THR	GLU	ASP	LEU	ALA	VAL	ARG	SER	ALA	VAL	ARG	VAL	GLY	ASP	THR	ASP	GLN	LYS	THR	ALA	ILE	ARG	LYS	THR	GLY	VAL	ALA	ASP	PRO	VAL	ALA
GLU	PHE	VAL	ALA	ASP	GLU	GLU	SER	ASN	ASN	LEU	VAL	VAL	ASP	LEU	GLN	ALA	TYR	THR	ARG	SER	ALA	VAL	ARG	SER	ALA	VAL	ARG	VAL	GLY	ASP	THR	ASP	GLN	LYS	THR	ALA	ILE	ARG	LYS	THR	GLY	VAL	ALA	ASP	PRO	VAL	ALA
L193	L196	I200	R204	F207	T208	D214	L218	G219	E220	C223	D224	F231	L240	E241	G242	K243	T244	Y245	D246	Y247	R248	G249	V250	I251	H277	R281	N282	Q283	A284	L285	N286	I287	V291	F306	L309	V313	N314	G315	S317	Q324	D325						
R328	F329	S332	F333	P334	A335	E336	E339	A340	R341	S342	V343	Q346	D357	R361	R377	E378	R379	I380	R381	P389	N393	T394	K395	G396	G397	T398	D401	V409	F419	V422	M427	Q431	S437	A438	V439	Y443	Q444	F445	G446	A447	G450						
R460	I464	GLY																																													

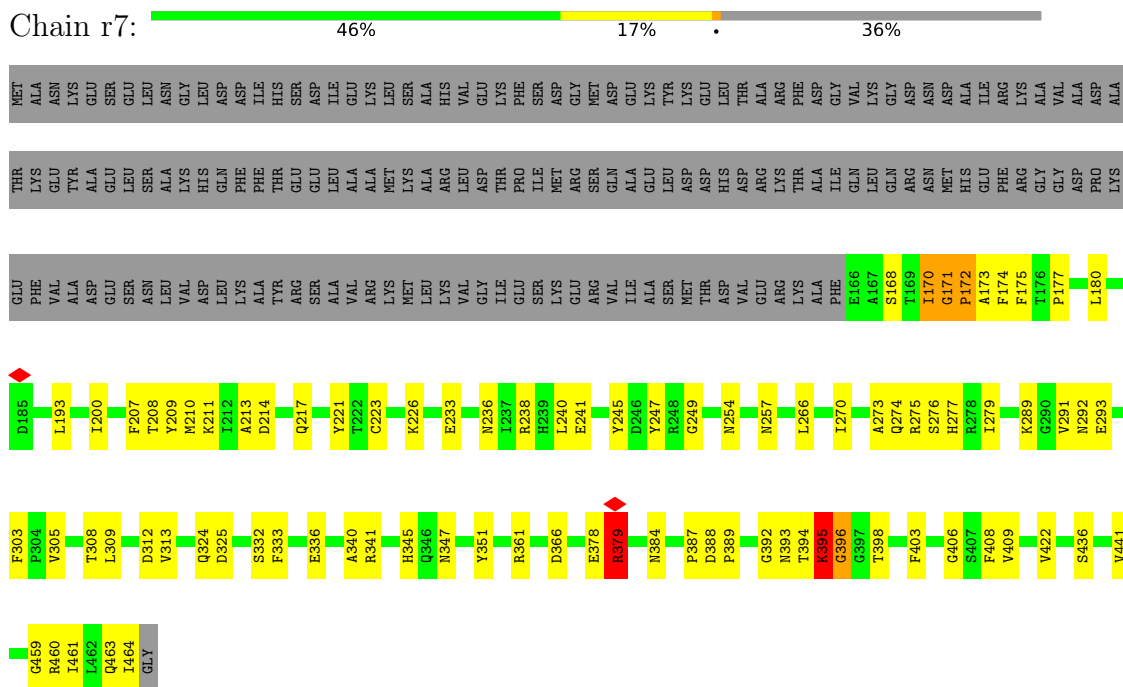
• Molecule 3: Major capsid protein, gp9



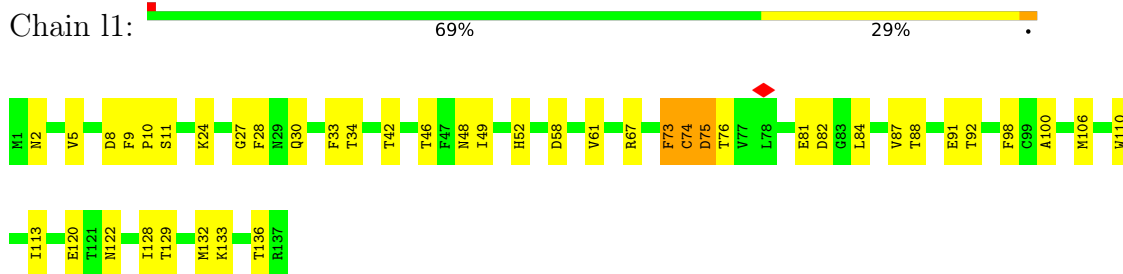
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THR	LYS	GLU	TYR	ALA	GLU	GLU	SER	LEU	SER	LEU	ALA	ALA	HIS	GLN	PHE	PHE	THR	GLU	ASP	LEU	ALA	ALA	ARG	VAL	GLY	ASP	THR	ASP	GLN	LYS	THR	ALA	ILE	ARG	LYS	THR	GLY	VAL	ALA	ASP	PRO	VAL	ALA
GLU	PHE	VAL	ALA	ASP	GLU	GLU	SER	ASN	ASN	LEU	VAL	VAL	ASP	LEU	GLN	ALA	TYR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



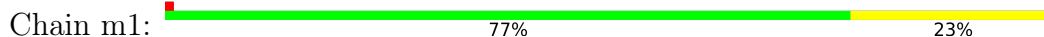
- Molecule 3: Major capsid protein, gp9



- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10





- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10

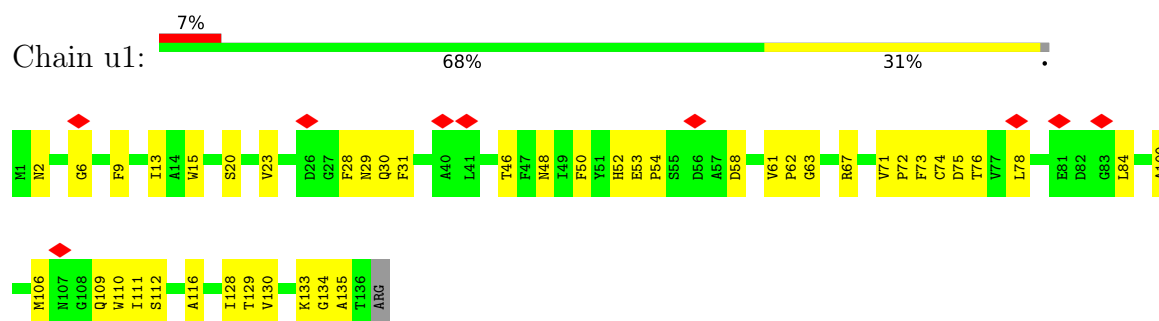


- Molecule 4: Minor capsid protein, gp10

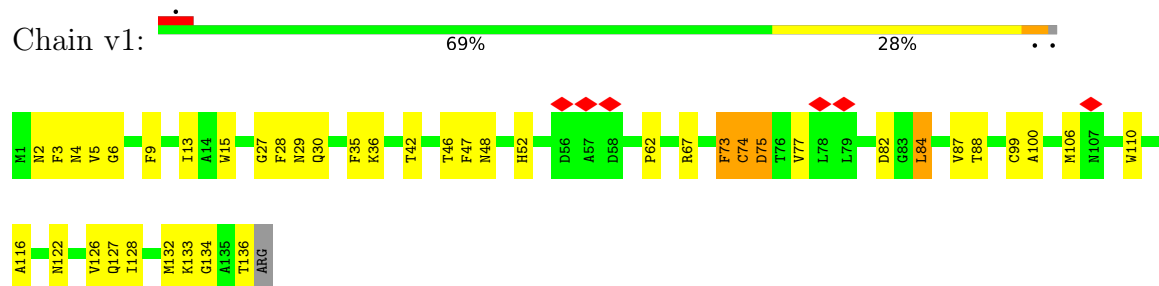


- Molecule 4: Minor capsid protein, gp10

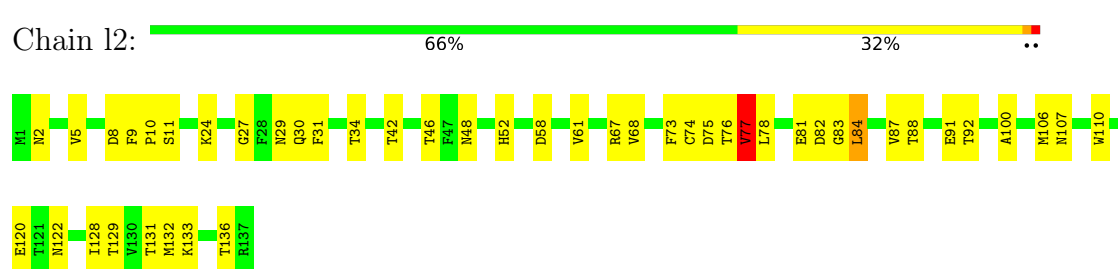




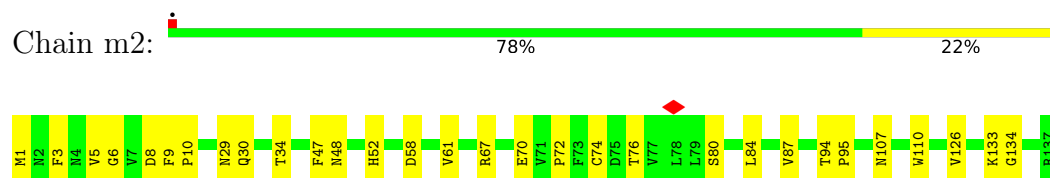
- Molecule 4: Minor capsid protein, gp10



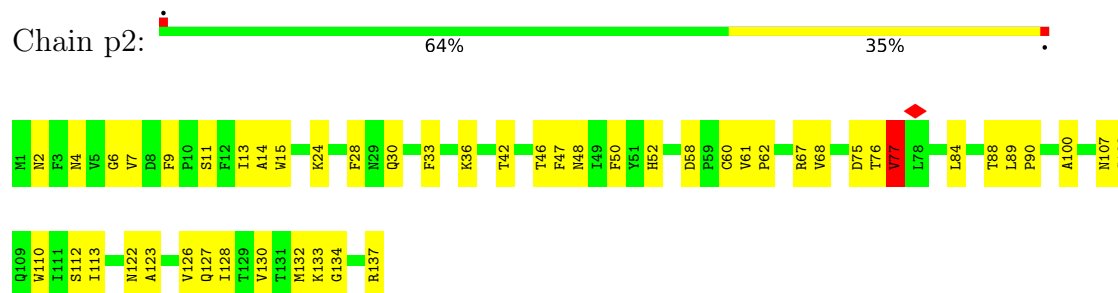
- Molecule 4: Minor capsid protein, gp10



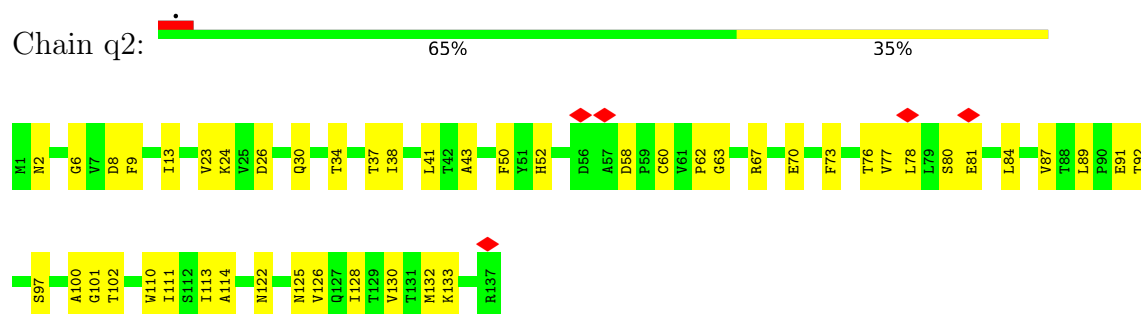
- Molecule 4: Minor capsid protein, gp10



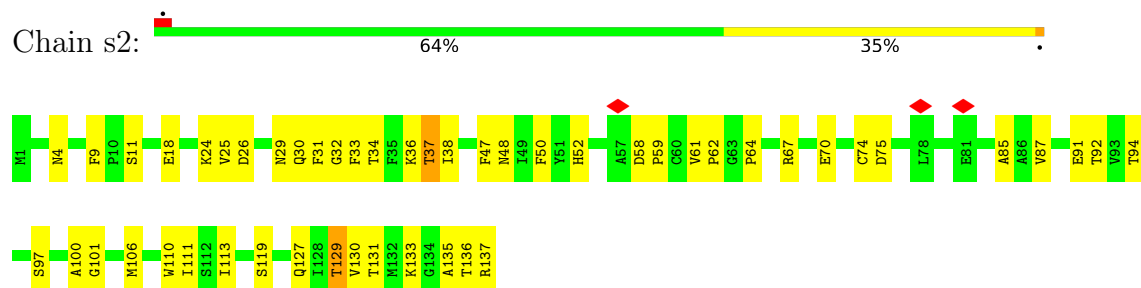
- Molecule 4: Minor capsid protein, gp10



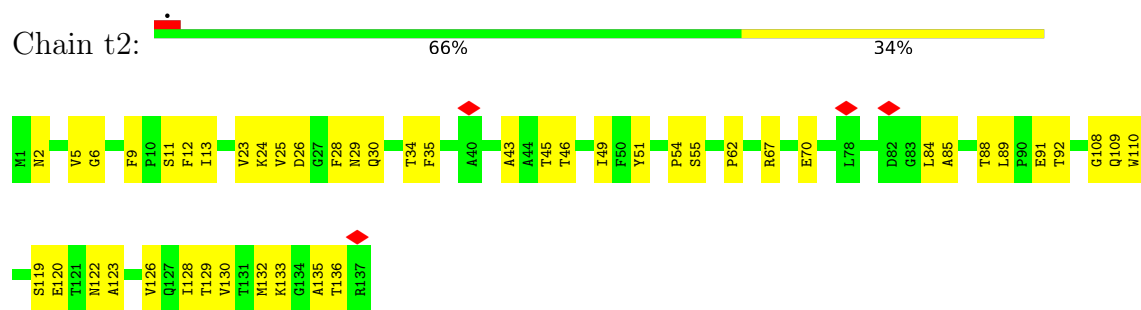
- Molecule 4: Minor capsid protein, gp10



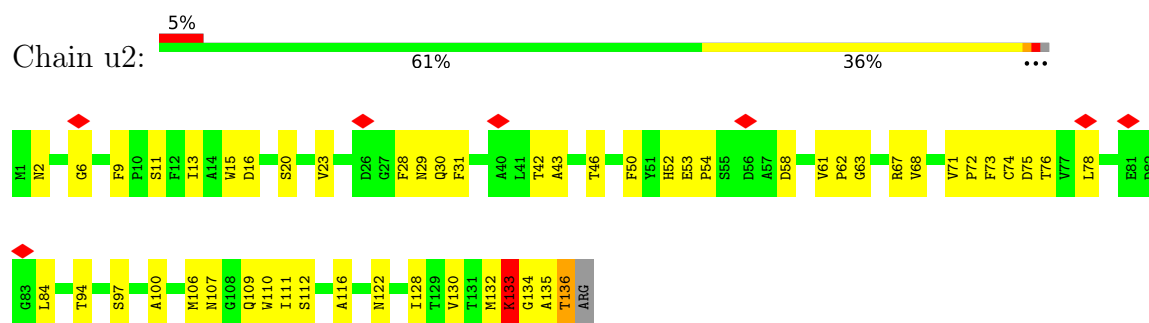
- Molecule 4: Minor capsid protein, gp10



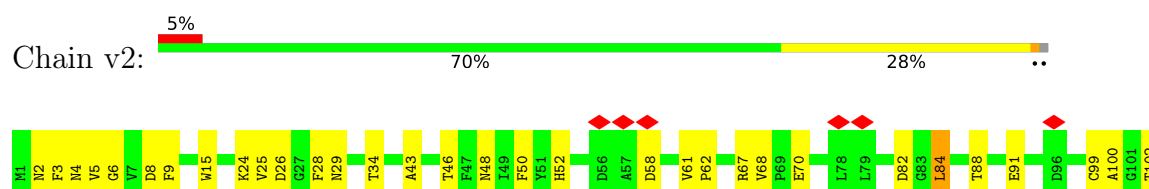
- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10

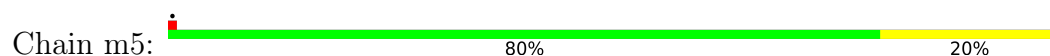




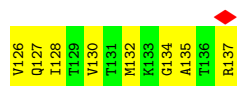
- Molecule 4: Minor capsid protein, gp10



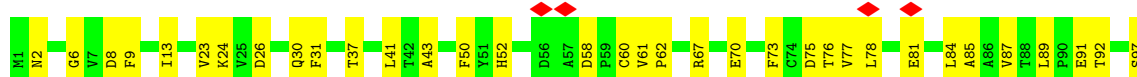
- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10

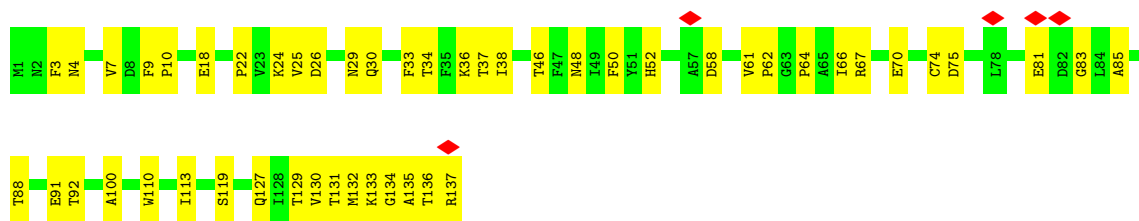


- Molecule 4: Minor capsid protein, gp10

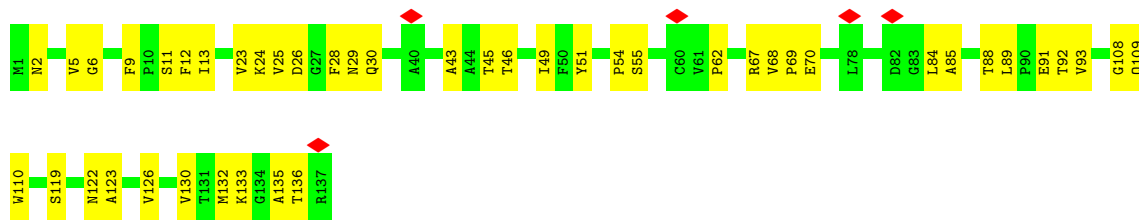


- Molecule 4: Minor capsid protein, gp10

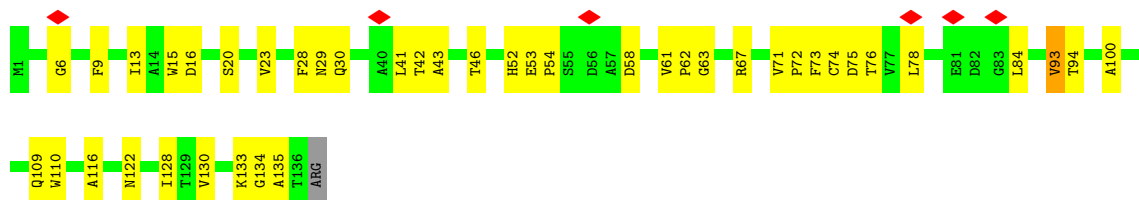




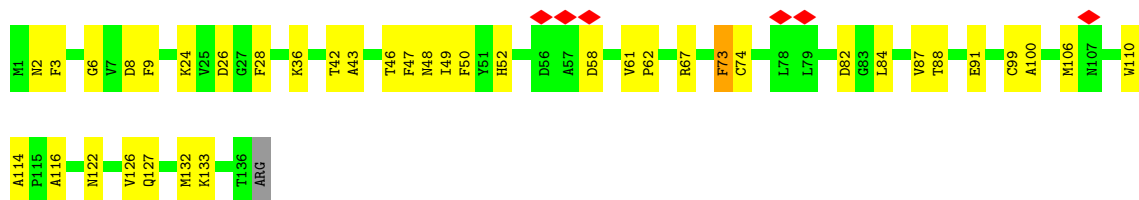
- Molecule 4: Minor capsid protein, gp10



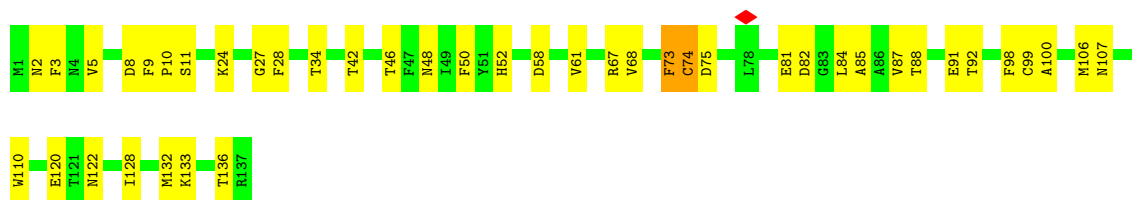
- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10

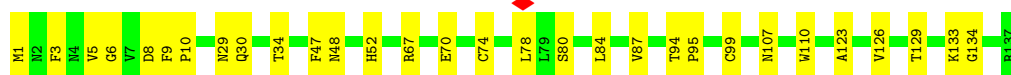


- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10

Chain m6:  78% 22%



- Molecule 4: Minor capsid protein, gp10

Chain p6:  64% 36%



- Molecule 4: Minor capsid protein, gp10

Chain q6:  66% 34%



- Molecule 4: Minor capsid protein, gp10

Chain s6:  61% 37%



- Molecule 4: Minor capsid protein, gp10

Chain t6:  69% 31%

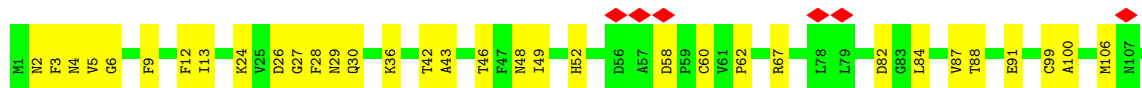




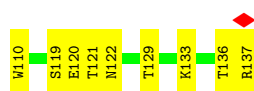
- Molecule 4: Minor capsid protein, gp10



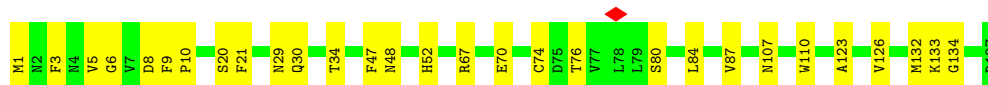
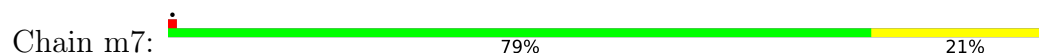
- Molecule 4: Minor capsid protein, gp10



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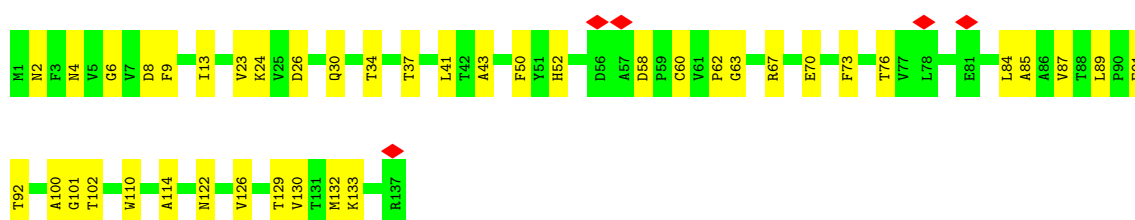


- Molecule 4: Minor capsid protein, gp10

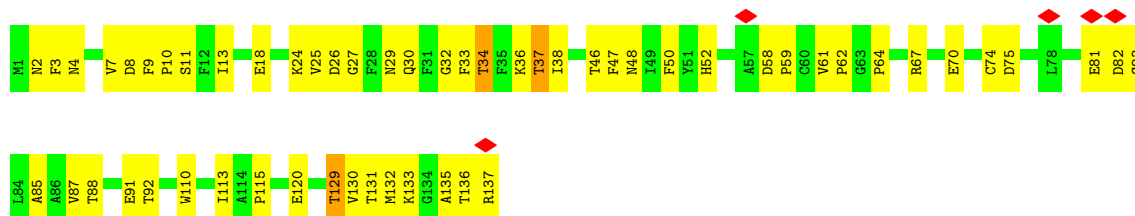




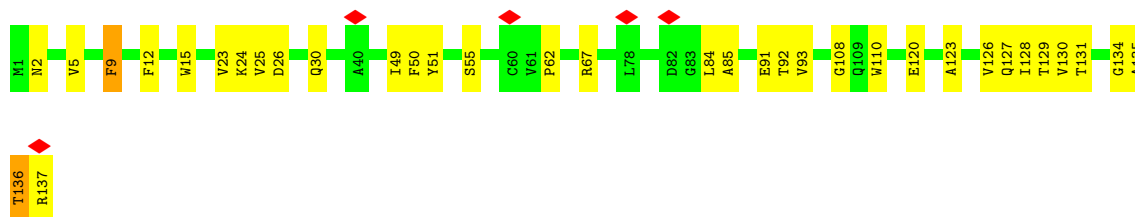
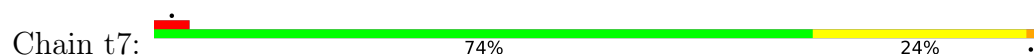
- Molecule 4: Minor capsid protein, gp10



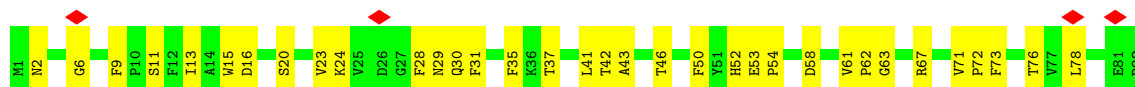
- Molecule 4: Minor capsid protein, gp10

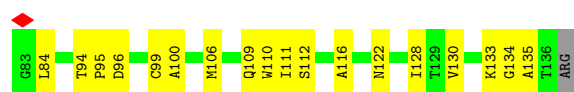


- Molecule 4: Minor capsid protein, gp10

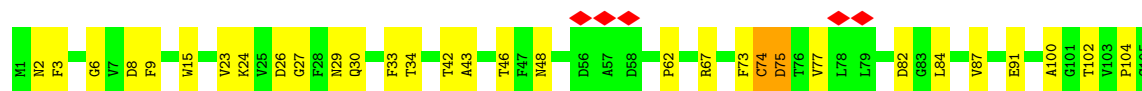


- Molecule 4: Minor capsid protein, gp10

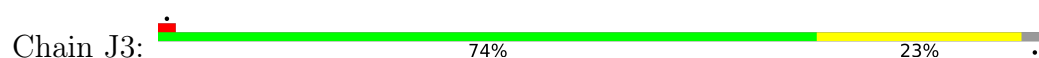




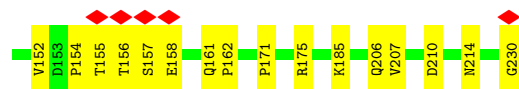
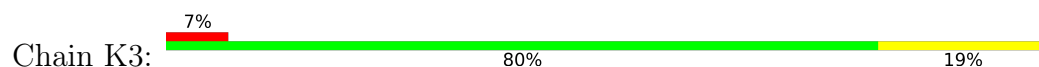
- Molecule 4: Minor capsid protein, gp10



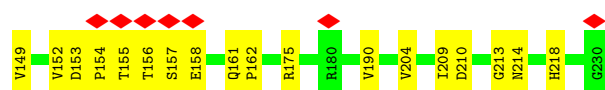
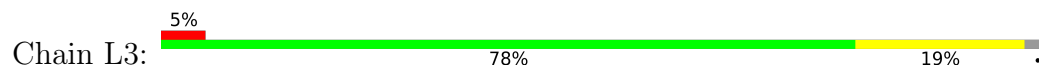
- Molecule 5: Collar sheath protein, gp13



- Molecule 5: Collar sheath protein, gp13

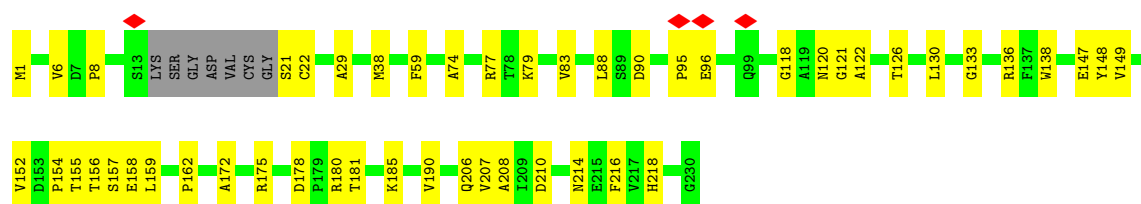


- Molecule 5: Collar sheath protein, gp13



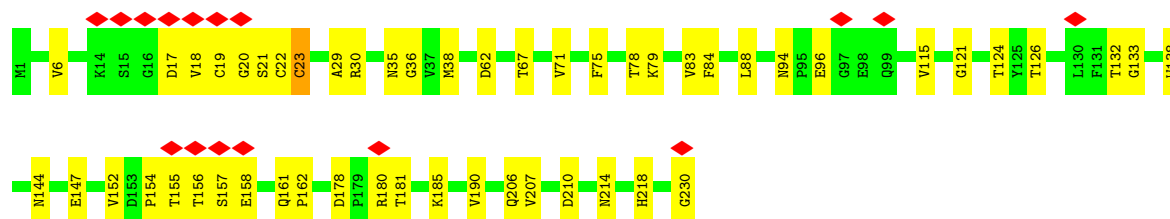
- Molecule 5: Collar sheath protein, gp13

Chain M3:  75% 22%



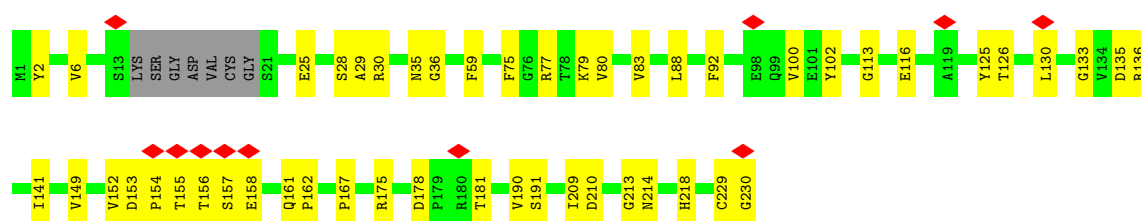
- Molecule 5: Collar sheath protein, gp13

Chain N3:  7% 77% 22%



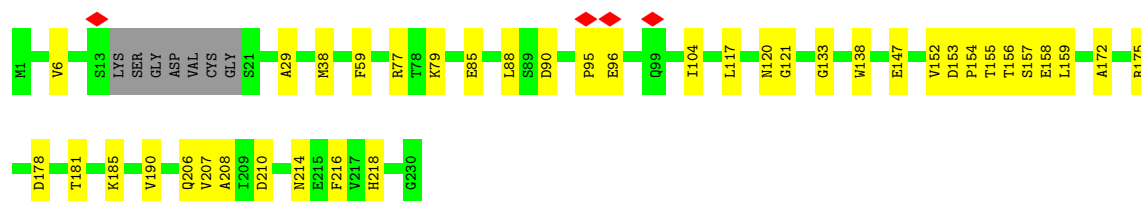
- Molecule 5: Collar sheath protein, gp13

Chain O3:  5% 75% 22%



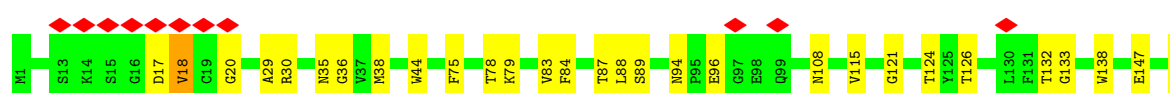
- Molecule 5: Collar sheath protein, gp13

Chain P3:  80% 17%



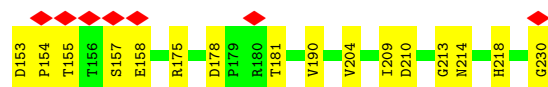
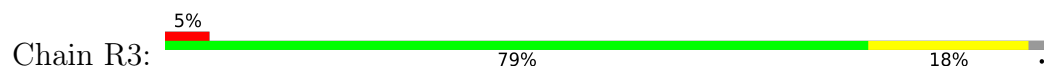
- Molecule 5: Collar sheath protein, gp13

Chain Q3:  7% 77% 23%

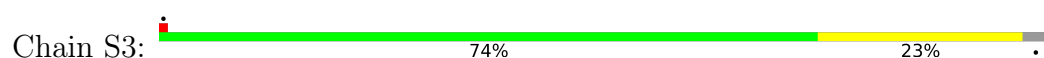




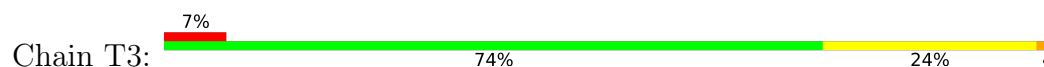
- Molecule 5: Collar sheath protein, gp13



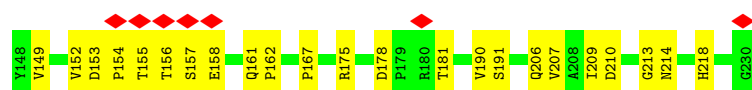
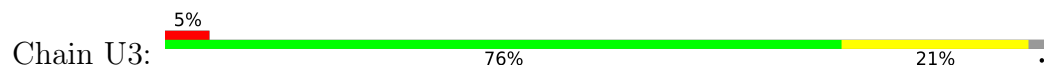
- Molecule 5: Collar sheath protein, gp13



- Molecule 5: Collar sheath protein, gp13

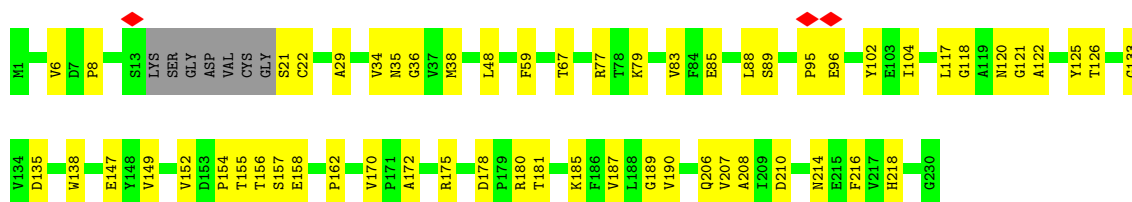


- Molecule 5: Collar sheath protein, gp13



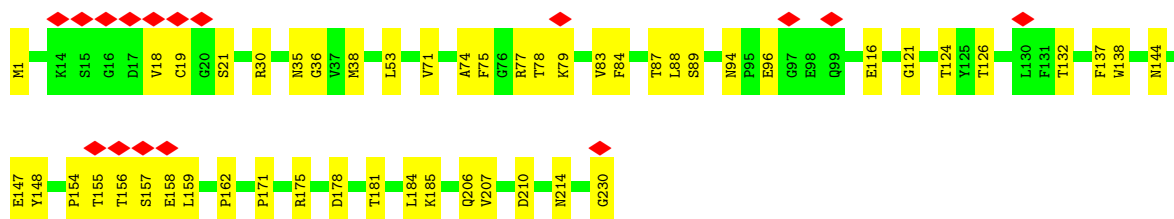
- Molecule 5: Collar sheath protein, gp13

Chain V3:  72% 25%



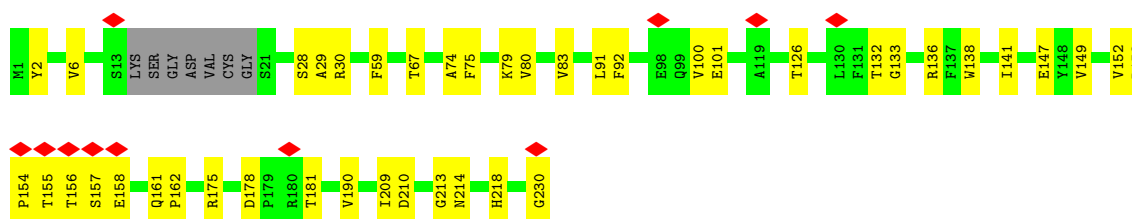
- Molecule 5: Collar sheath protein, gp13

Chain W3:  7% 78% 22%



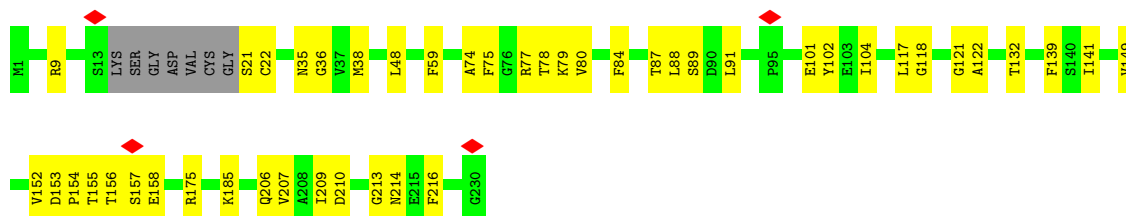
- Molecule 5: Collar sheath protein, gp13

Chain X3:  5% 78% 19%



- Molecule 5: Collar sheath protein, gp13

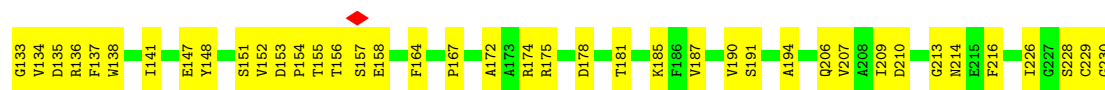
Chain Y3:  77% 20%



- Molecule 5: Collar sheath protein, gp13

Chain Z3:  68% 29%

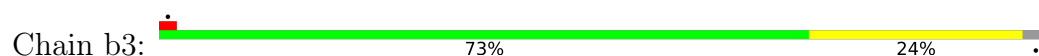




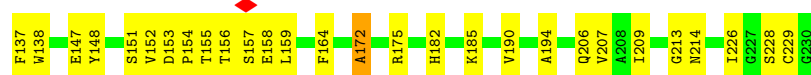
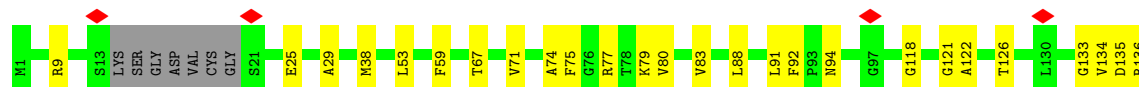
- Molecule 5: Collar sheath protein, gp13



- Molecule 5: Collar sheath protein, gp13



- Molecule 5: Collar sheath protein, gp13

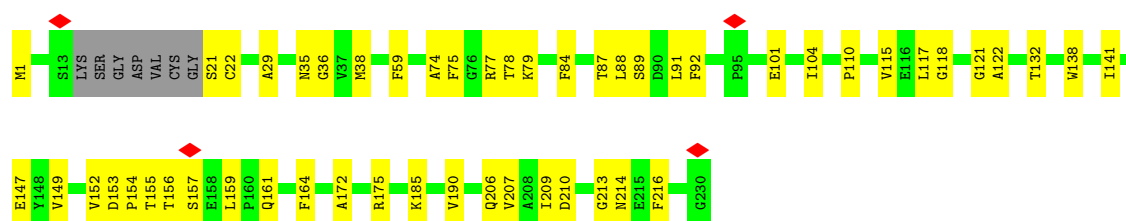


- Molecule 5: Collar sheath protein, gp13



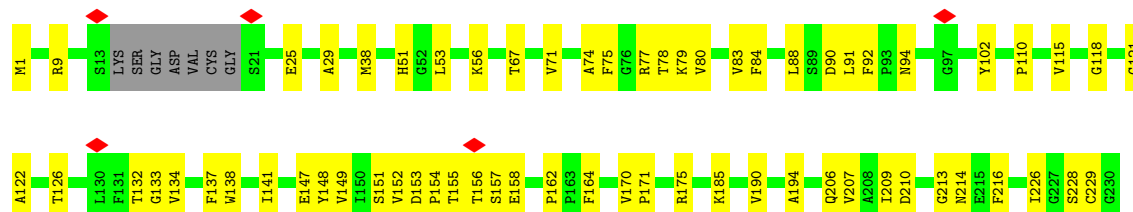
- Molecule 5: Collar sheath protein, gp13

Chain e3:  74% 23%



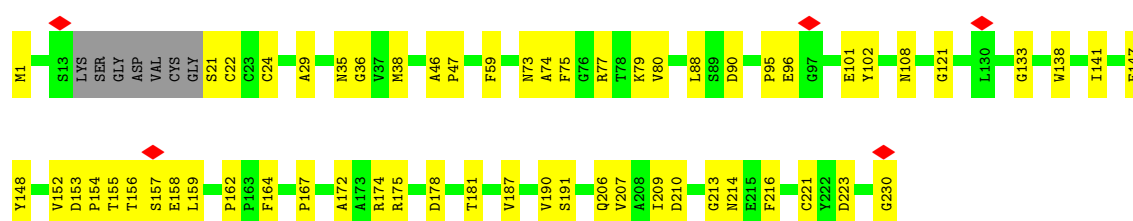
• Molecule 5: Collar sheath protein, gp13

Chain f3:  69% 28%



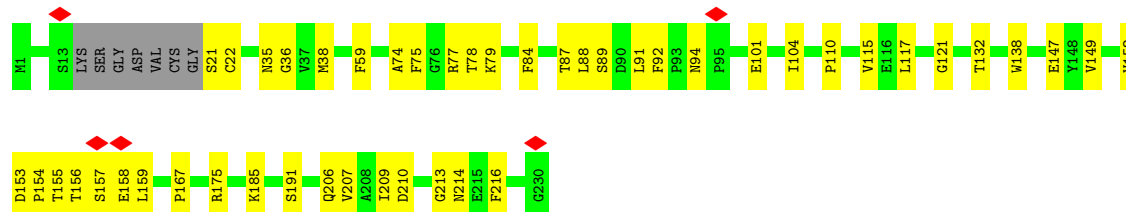
• Molecule 5: Collar sheath protein, gp13

Chain g3:  71% 26%



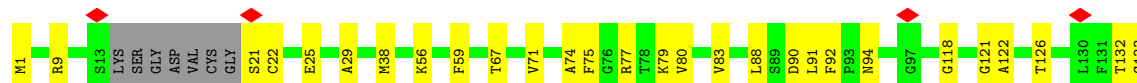
• Molecule 5: Collar sheath protein, gp13

Chain h3:  77% 20%



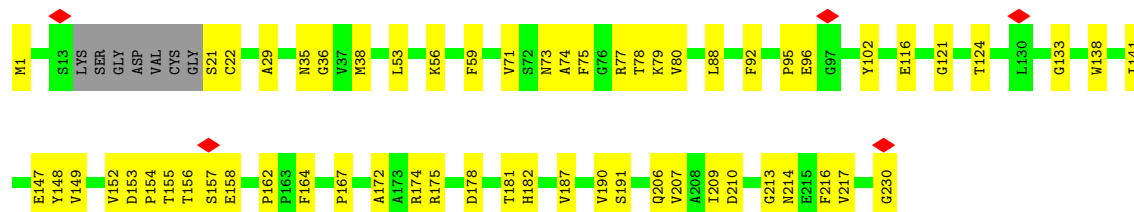
• Molecule 5: Collar sheath protein, gp13

Chain i3:  70% 27%

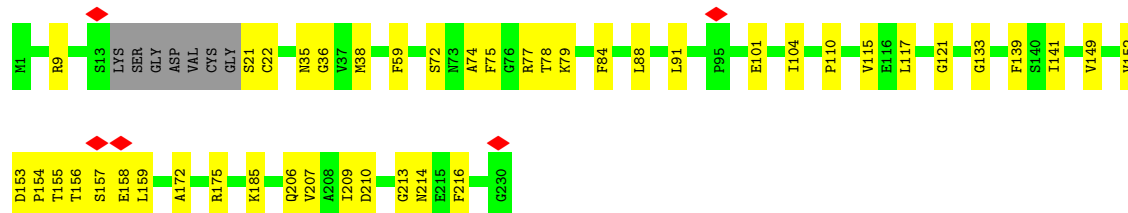
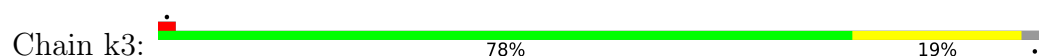




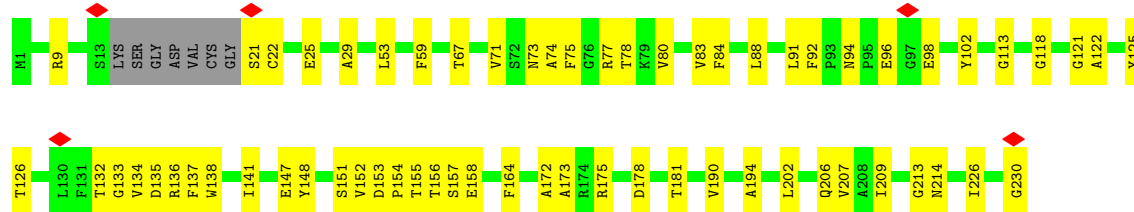
- Molecule 5: Collar sheath protein, gp13



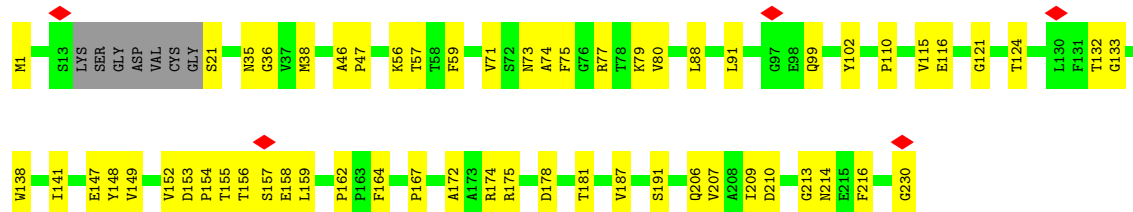
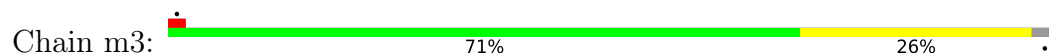
- Molecule 5: Collar sheath protein, gp13



- Molecule 5: Collar sheath protein, gp13

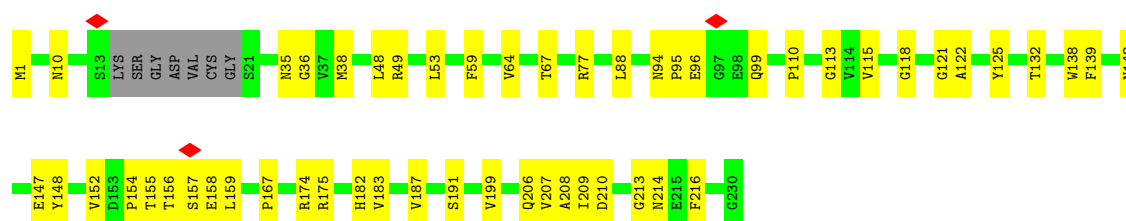


- Molecule 5: Collar sheath protein, gp13



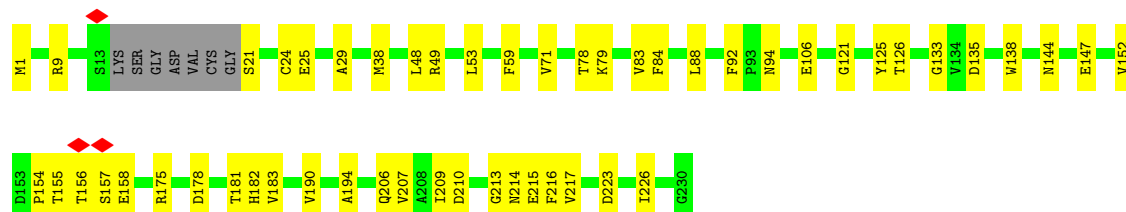
- Molecule 5: Collar sheath protein, gp13

Chain n3:  74% 23%



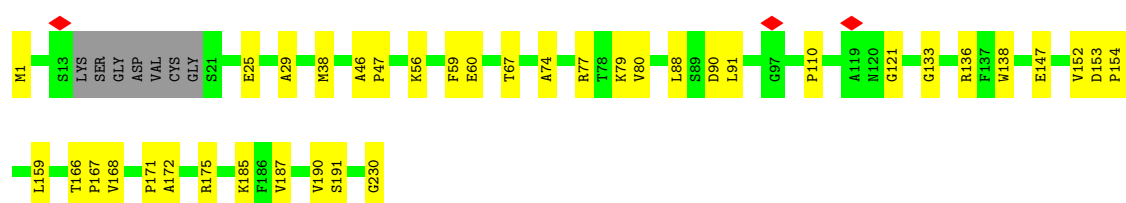
- Molecule 5: Collar sheath protein, gp13

Chain o3:  74% 23%



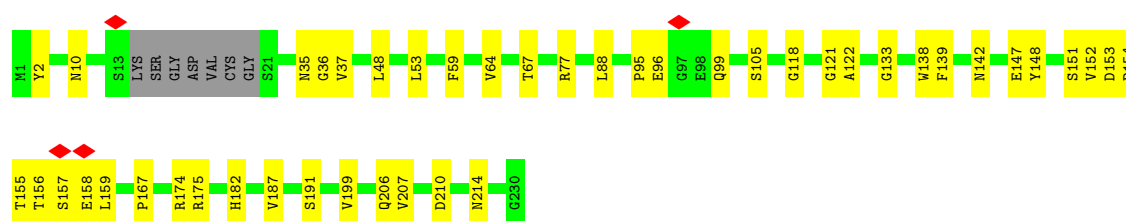
- Molecule 5: Collar sheath protein, gp13

Chain p3:  80% 17%



- Molecule 5: Collar sheath protein, gp13

Chain q3:  77% 20%



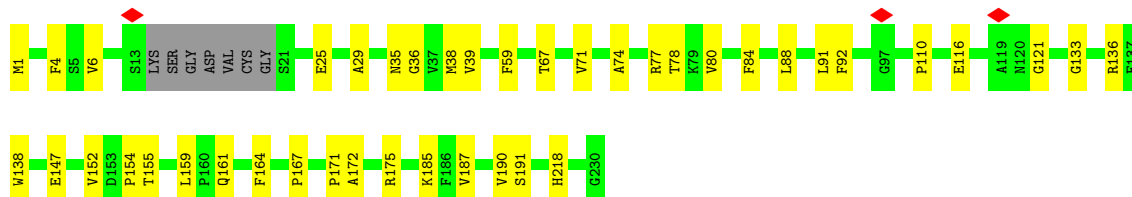
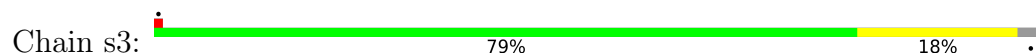
- Molecule 5: Collar sheath protein, gp13

Chain r3:  75% 22%

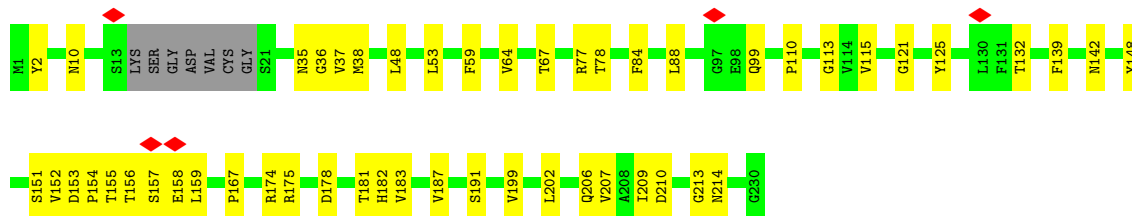
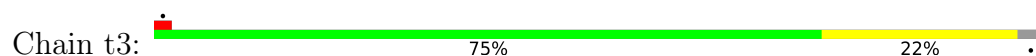




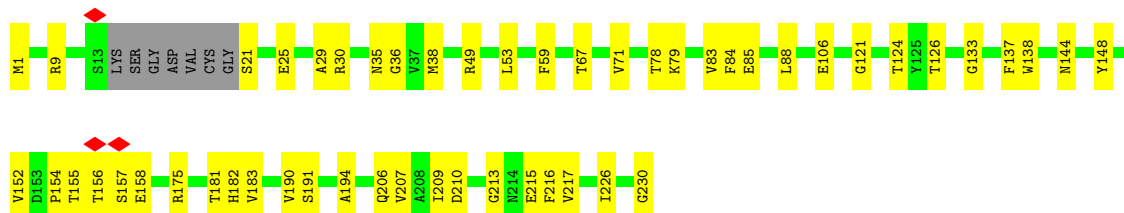
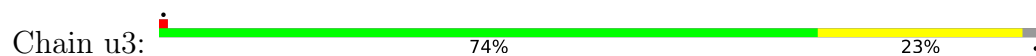
- Molecule 5: Collar sheath protein, gp13



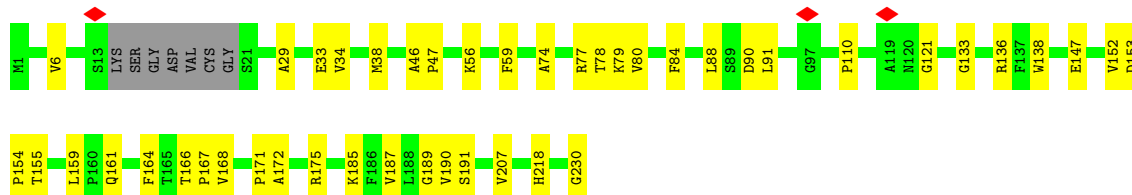
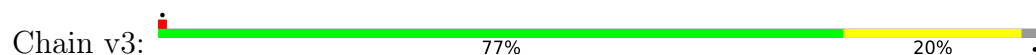
- Molecule 5: Collar sheath protein, gp13



- Molecule 5: Collar sheath protein, gp13

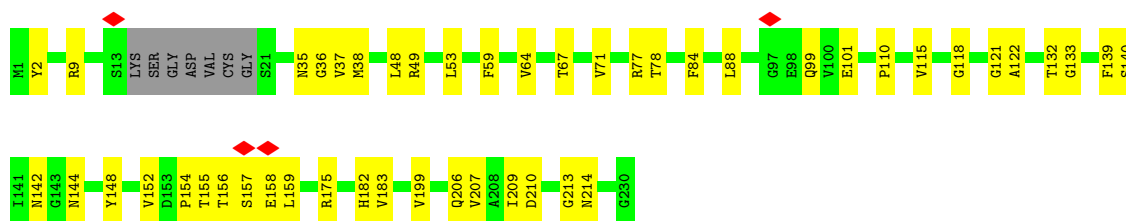


- Molecule 5: Collar sheath protein, gp13



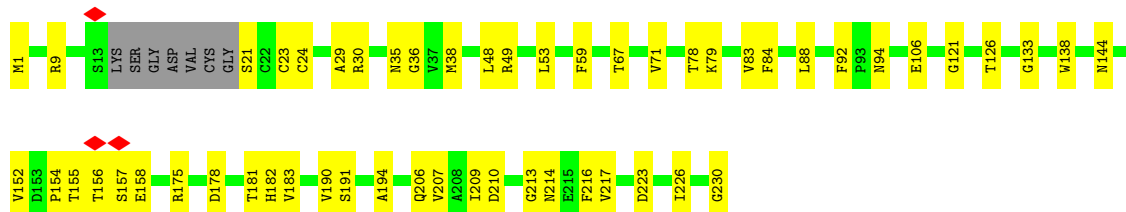
- Molecule 5: Collar sheath protein, gp13

Chain w3:  76% 21%



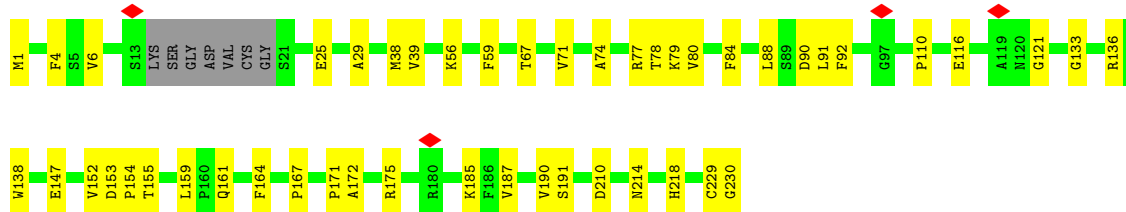
- Molecule 5: Collar sheath protein, gp13

Chain x3:  73% 23%



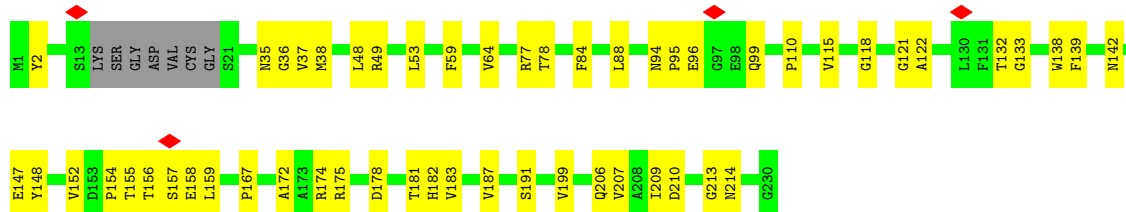
- Molecule 5: Collar sheath protein, gp13

Chain y3:  76% 21%



- Molecule 5: Collar sheath protein, gp13

Chain z3:  73% 23%



- Molecule 5: Collar sheath protein, gp13

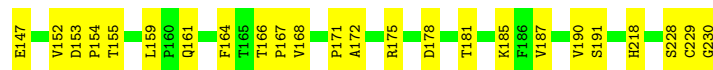
Chain 13:  77% 20%





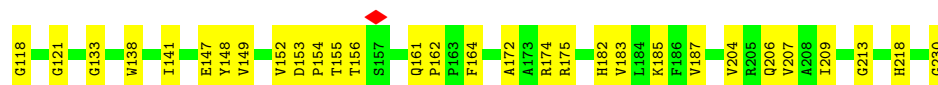
- Molecule 5: Collar sheath protein, gp13

Chain 23: 76% 21%



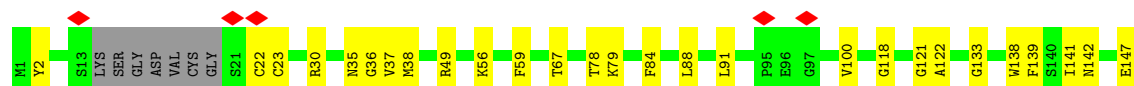
- Molecule 5: Collar sheath protein, gp13

Chain 33: 71% 26%



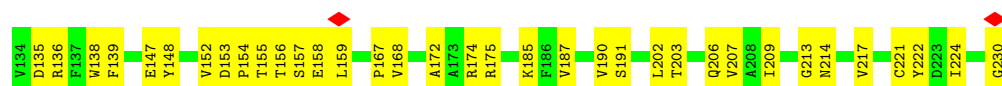
- Molecule 5: Collar sheath protein, gp13

Chain 43: 76% 21%



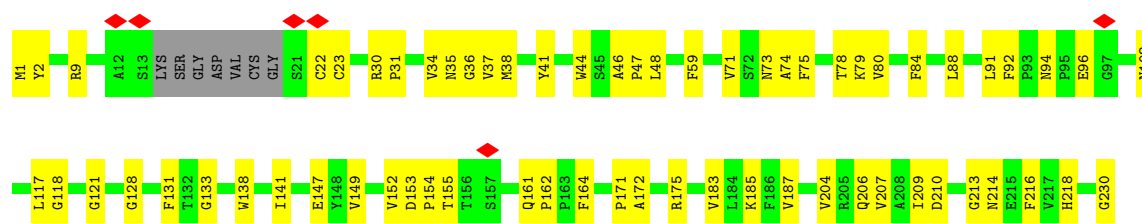
- Molecule 5: Collar sheath protein, gp13

Chain 53: 70% 27%



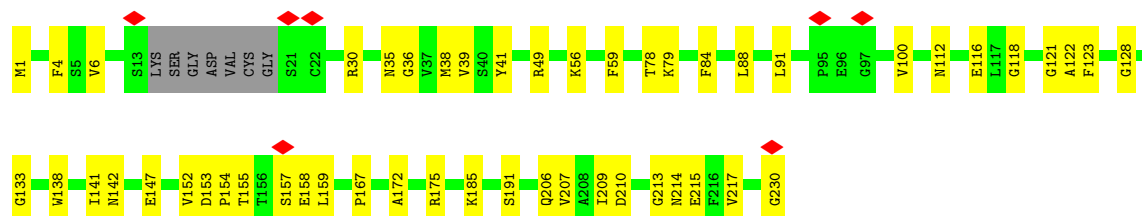
- Molecule 5: Collar sheath protein, gp13

Chain 63: 



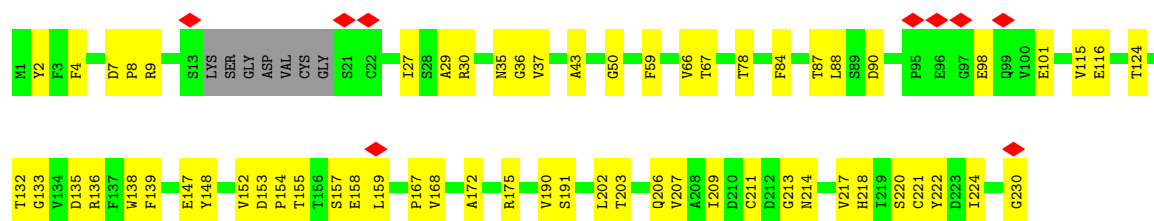
- Molecule 5: Collar sheath protein, gp13

Chain 73: 



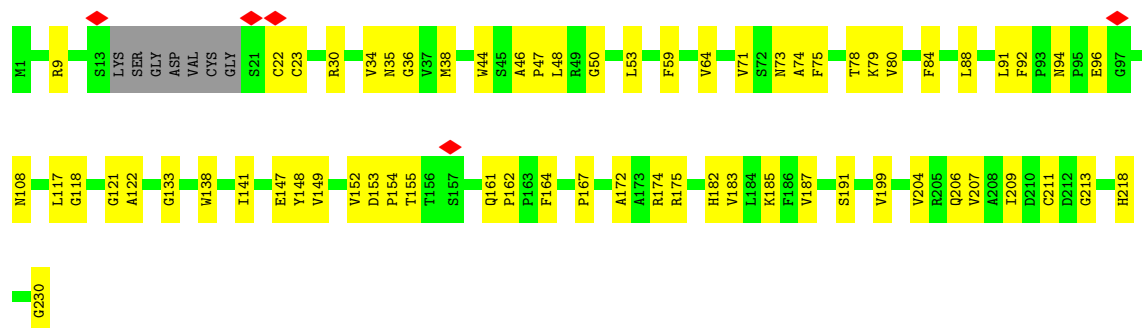
- Molecule 5: Collar sheath protein, gp13

Chain 83: 



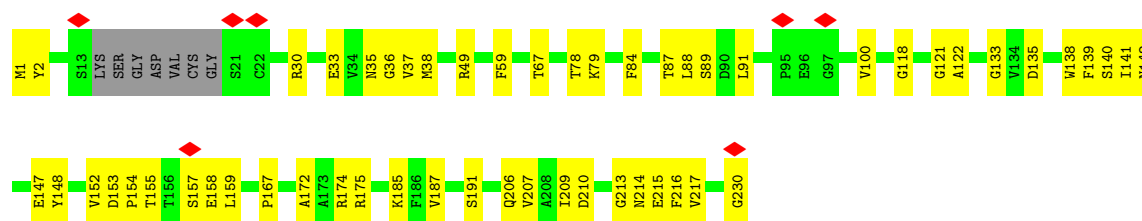
- Molecule 5: Collar sheath protein, gp13

Chain 93: 

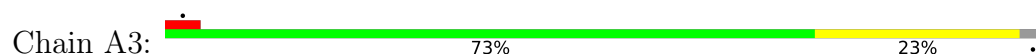


- Molecule 5: Collar sheath protein, gp13

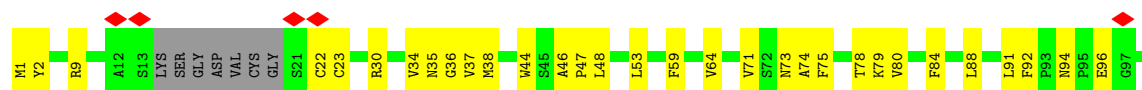
Chain 03: 



• Molecule 5: Collar sheath protein, gp13

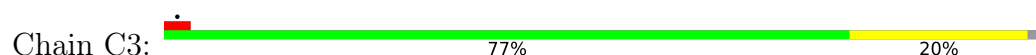


• Molecule 5: Collar sheath protein, gp13

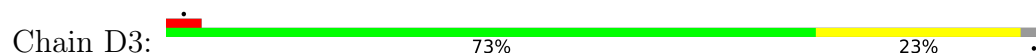


G230

• Molecule 5: Collar sheath protein, gp13

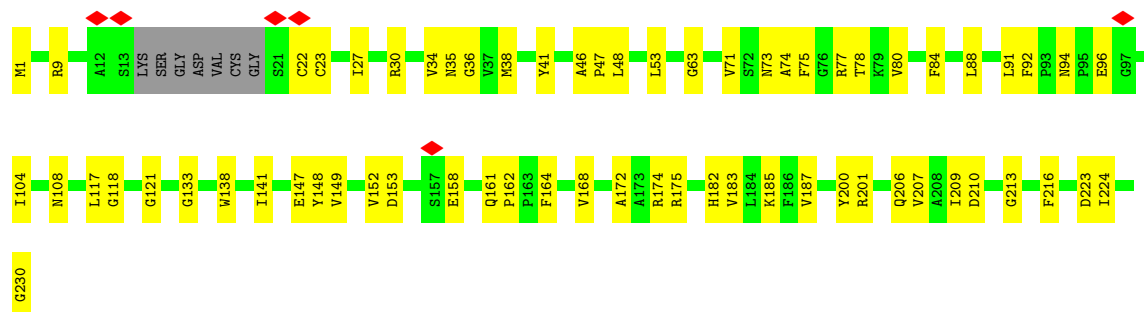


• Molecule 5: Collar sheath protein, gp13

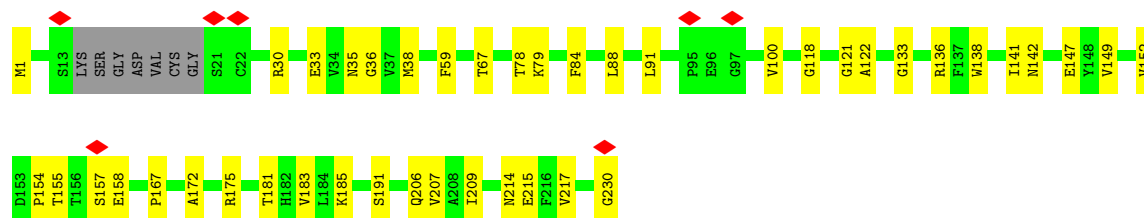
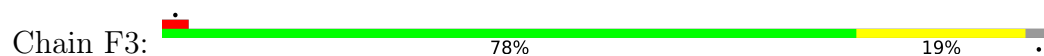




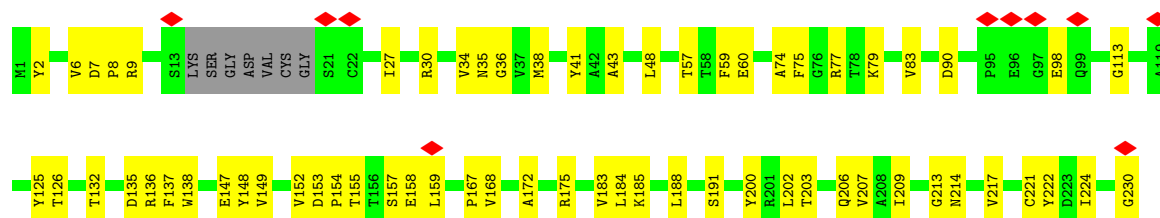
- Molecule 5: Collar sheath protein, gp13



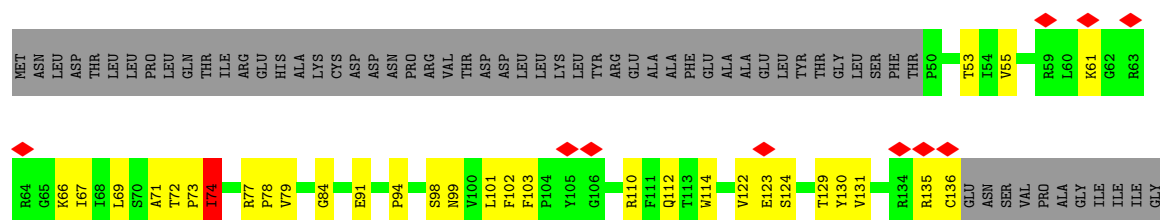
- Molecule 5: Collar sheath protein, gp13



- Molecule 5: Collar sheath protein, gp13



- Molecule 6: Neck 1 protein, gp14



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• Molecule 6: Neck 1 protein, gp14

Chain B4: 5% 23% 19% 57%

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I60

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S98
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Y100
L101
F102
F103
P104
Y105
G106
D109
R110
F111
Q112
W114
G115
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E123
S124
M127
A128
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• Molecule 6: Neck 1 protein, gp14

Chain C4: 5% 22% 19% 57%

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R59
K61
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R63
R64
G66
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L69
T72
P73
I74
R77
P78
V79
G84
G87
L90
E91
P94
S98
N99
F102
F103
P104
Y105
G106
D109
R110
F111
Q112
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V122
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• Molecule 6: Neck 1 protein, gp14

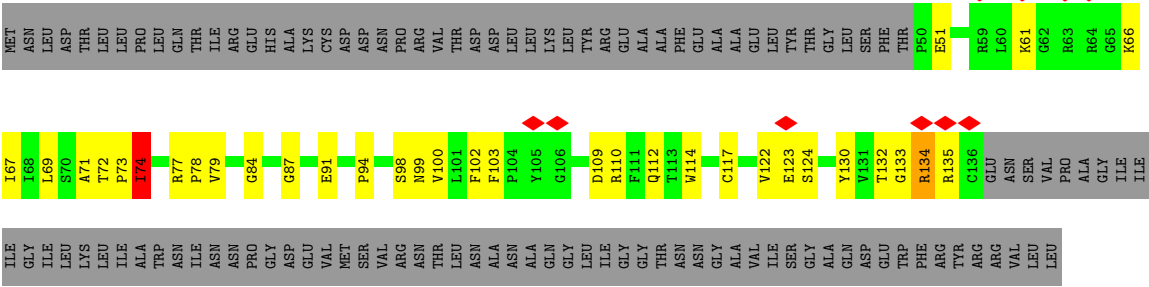
Chain D4: 6% 27% 14% 57%

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G66

R66
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I68
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A75
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R77
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V80
F81
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G87
E91
P94
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F103
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G106
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D108
D109
Q112
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• Molecule 6: Neck 1 protein, gp14



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	10086	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.857	Depositor
Minimum map value	-0.549	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	648.0, 648.0, 648.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	a1	0.28	0/213	0.53	0/288
1	a2	0.25	0/213	0.50	0/288
1	a5	0.29	0/213	0.52	0/288
1	a6	0.28	0/213	0.51	0/288
1	a7	0.22	0/213	0.49	0/288
1	b1	0.29	0/213	0.48	0/288
1	b2	0.20	0/213	0.45	0/288
1	b5	0.22	0/213	0.46	0/288
1	b6	0.20	0/213	0.46	0/288
1	b7	0.21	0/213	0.43	0/288
1	c	0.27	0/252	0.63	0/344
1	d	0.26	0/252	0.60	0/344
1	d1	0.25	0/252	0.55	0/344
1	d2	0.22	0/252	0.56	0/344
1	d5	0.20	0/252	0.58	0/344
1	d6	0.20	0/252	0.57	0/344
1	d7	0.22	0/252	0.57	0/344
1	e	0.22	0/252	0.58	0/344
1	e1	0.24	0/213	0.55	0/288
1	e2	0.22	0/213	0.53	0/288
1	e5	0.24	0/213	0.54	0/288
1	e6	0.22	0/213	0.54	0/288
1	e7	0.22	0/213	0.54	0/288
1	f	0.28	0/252	0.59	0/344
1	g	0.30	0/252	0.61	0/344
2	f1	0.23	0/142	0.52	0/192
2	f2	0.23	0/142	0.54	0/192
2	f5	0.25	0/142	0.61	0/192
2	f6	0.24	0/142	0.57	0/192
2	f7	0.25	0/142	0.52	0/192
3	g1	0.26	0/2396	0.49	0/3243
3	g2	0.28	0/2396	0.50	1/3243 (0.0%)
3	g5	0.24	0/2396	0.47	0/3243
3	g6	0.26	0/2396	0.49	0/3243

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	g7	0.26	0/2396	0.49	0/3243
3	h1	0.36	0/2396	0.52	0/3243
3	h2	0.35	0/2396	0.56	3/3243 (0.1%)
3	h5	0.35	0/2396	0.52	0/3243
3	h6	0.34	0/2396	0.53	1/3243 (0.0%)
3	h7	0.33	0/2396	0.54	2/3243 (0.1%)
3	k1	0.23	0/2313	0.43	0/3128
3	k2	0.24	0/2313	0.44	0/3128
3	k5	0.23	0/2313	0.43	0/3128
3	k6	0.24	0/2313	0.44	0/3128
3	k7	0.25	0/2313	0.49	0/3128
3	n1	0.29	0/2396	0.53	1/3243 (0.0%)
3	n2	0.28	0/2396	0.49	0/3243
3	n5	0.28	0/2396	0.53	1/3243 (0.0%)
3	n6	0.28	0/2396	0.50	0/3243
3	n7	0.27	0/2396	0.50	0/3243
3	o1	0.23	0/2396	0.47	0/3243
3	o2	0.22	0/2396	0.46	0/3243
3	o5	0.22	0/2396	0.47	0/3243
3	o6	0.22	0/2396	0.47	0/3243
3	o7	0.22	0/2396	0.46	0/3243
3	r1	0.27	0/2396	0.50	0/3243
3	r2	0.26	0/2396	0.52	2/3243 (0.1%)
3	r5	0.28	0/2396	0.51	1/3243 (0.0%)
3	r6	0.28	0/2396	0.52	1/3243 (0.0%)
3	r7	0.29	0/2396	0.58	2/3243 (0.1%)
4	l1	0.25	0/1052	0.48	0/1443
4	l2	0.29	0/1052	0.46	0/1443
4	l5	0.25	0/1052	0.47	0/1443
4	l6	0.27	0/1052	0.47	0/1443
4	l7	0.25	0/1052	0.46	0/1443
4	m1	0.25	0/1052	0.45	0/1443
4	m2	0.26	0/1052	0.43	0/1443
4	m5	0.25	0/1052	0.42	0/1443
4	m6	0.24	0/1052	0.44	0/1443
4	m7	0.26	0/1052	0.46	0/1443
4	p1	0.25	0/1052	0.47	0/1443
4	p2	0.24	0/1052	0.52	1/1443 (0.1%)
4	p5	0.25	0/1052	0.48	0/1443
4	p6	0.25	0/1052	0.53	1/1443 (0.1%)
4	p7	0.25	0/1052	0.53	1/1443 (0.1%)
4	q1	0.24	0/1052	0.46	0/1443
4	q2	0.23	0/1052	0.46	0/1443

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	q5	0.24	0/1052	0.45	0/1443
4	q6	0.24	0/1052	0.45	0/1443
4	q7	0.24	0/1052	0.46	0/1443
4	s1	0.23	0/1052	0.45	0/1443
4	s2	0.24	0/1052	0.45	0/1443
4	s5	0.23	0/1052	0.44	0/1443
4	s6	0.23	0/1052	0.45	0/1443
4	s7	0.21	0/1052	0.44	0/1443
4	t1	0.19	0/1052	0.48	0/1443
4	t2	0.19	0/1052	0.46	0/1443
4	t5	0.19	0/1052	0.45	0/1443
4	t6	0.20	0/1052	0.45	0/1443
4	t7	0.28	0/1052	0.57	1/1443 (0.1%)
4	u1	0.18	0/1040	0.44	0/1429
4	u2	0.25	0/1040	0.47	1/1429 (0.1%)
4	u5	0.19	0/1040	0.44	0/1429
4	u6	0.20	0/1040	0.47	0/1429
4	u7	0.19	0/1040	0.46	0/1429
4	v1	0.21	0/1040	0.46	0/1429
4	v2	0.24	0/1040	0.52	1/1429 (0.1%)
4	v5	0.23	0/1040	0.47	0/1429
4	v6	0.20	0/1040	0.49	0/1429
4	v7	0.23	0/1040	0.49	0/1429
5	03	0.18	0/1723	0.37	0/2353
5	13	0.21	0/1723	0.39	0/2353
5	23	0.22	0/1723	0.44	0/2353
5	33	0.19	0/1723	0.39	0/2353
5	43	0.19	0/1723	0.38	0/2353
5	53	0.18	0/1723	0.40	0/2353
5	63	0.18	0/1723	0.38	0/2353
5	73	0.18	0/1723	0.38	0/2353
5	83	0.18	0/1723	0.40	0/2353
5	93	0.19	0/1723	0.39	0/2353
5	A3	0.18	0/1723	0.40	0/2353
5	B3	0.19	0/1723	0.41	0/2353
5	C3	0.19	0/1723	0.38	0/2353
5	D3	0.18	0/1723	0.40	0/2353
5	E3	0.19	0/1723	0.38	0/2353
5	F3	0.18	0/1723	0.38	0/2353
5	G3	0.21	0/1723	0.47	0/2353
5	J3	0.23	0/1723	0.39	0/2353
5	K3	0.22	0/1768	0.41	0/2414
5	L3	0.21	0/1723	0.39	0/2353

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	M3	0.24	0/1723	0.40	0/2353
5	N3	0.30	0/1768	0.50	2/2414 (0.1%)
5	O3	0.22	0/1723	0.38	0/2353
5	P3	0.24	0/1723	0.39	0/2353
5	Q3	0.23	0/1768	0.48	1/2414 (0.0%)
5	R3	0.21	0/1723	0.38	0/2353
5	S3	0.24	0/1723	0.39	0/2353
5	T3	0.26	0/1768	0.46	1/2414 (0.0%)
5	U3	0.22	0/1723	0.39	0/2353
5	V3	0.24	0/1723	0.39	0/2353
5	W3	0.23	0/1768	0.48	0/2414
5	X3	0.22	0/1723	0.39	0/2353
5	Y3	0.23	0/1723	0.38	0/2353
5	Z3	0.23	0/1723	0.40	0/2353
5	a3	0.22	0/1723	0.39	0/2353
5	b3	0.23	0/1723	0.39	0/2353
5	c3	0.27	0/1723	0.44	0/2353
5	d3	0.22	0/1723	0.39	0/2353
5	e3	0.23	0/1723	0.38	0/2353
5	f3	0.29	0/1723	0.44	0/2353
5	g3	0.22	0/1723	0.39	0/2353
5	h3	0.23	0/1723	0.39	0/2353
5	i3	0.28	0/1723	0.44	0/2353
5	j3	0.22	0/1723	0.39	0/2353
5	k3	0.24	0/1723	0.39	0/2353
5	l3	0.28	0/1723	0.44	0/2353
5	m3	0.22	0/1723	0.39	0/2353
5	n3	0.21	0/1723	0.39	0/2353
5	o3	0.21	0/1723	0.39	0/2353
5	p3	0.21	0/1723	0.42	0/2353
5	q3	0.21	0/1723	0.39	0/2353
5	r3	0.22	0/1723	0.39	0/2353
5	s3	0.21	0/1723	0.42	0/2353
5	t3	0.21	0/1723	0.39	0/2353
5	u3	0.21	0/1723	0.38	0/2353
5	v3	0.21	0/1723	0.42	0/2353
5	w3	0.21	0/1723	0.38	0/2353
5	x3	0.21	0/1723	0.38	0/2353
5	y3	0.22	0/1723	0.42	0/2353
5	z3	0.21	0/1723	0.39	0/2353
6	A4	0.21	0/689	0.50	0/934
6	B4	0.23	0/689	0.59	1/934 (0.1%)
6	C4	0.22	0/689	0.51	0/934

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
6	D4	0.26	0/689	0.67	0/934
6	E4	0.23	0/689	0.53	0/934
All	All	0.24	0/226900	0.45	26/309170 (0.0%)

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q3	20	GLY	N-CA-C	10.56	125.90	111.54
5	N3	23	CYS	CA-C-N	-7.93	110.36	122.09
5	N3	23	CYS	C-N-CA	-7.93	110.36	122.09
6	B4	135	ARG	N-CA-C	7.77	121.04	108.76
3	h2	386	LEU	CA-C-N	-7.20	112.22	119.99

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a1	209	0	222	13	0
1	a2	209	0	222	9	0
1	a5	209	0	222	13	0
1	a6	209	0	222	11	0
1	a7	209	0	222	10	0
1	b1	209	0	222	6	0
1	b2	209	0	222	6	0
1	b5	209	0	222	4	0
1	b6	209	0	222	4	0
1	b7	209	0	222	4	0
1	c	246	0	260	17	0
1	d	246	0	260	14	0
1	d1	246	0	260	12	0
1	d2	246	0	260	17	0
1	d5	246	0	260	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d6	246	0	260	16	0
1	d7	246	0	260	10	0
1	e	246	0	260	14	0
1	e1	209	0	222	12	0
1	e2	209	0	222	8	0
1	e5	209	0	222	16	0
1	e6	209	0	222	13	0
1	e7	209	0	222	11	0
1	f	246	0	260	18	0
1	g	246	0	260	16	0
2	f1	140	0	144	12	0
2	f2	140	0	144	10	0
2	f5	140	0	144	13	0
2	f6	140	0	144	10	0
2	f7	140	0	144	12	0
3	g1	2337	0	2203	50	0
3	g2	2337	0	2204	54	0
3	g5	2337	0	2203	52	0
3	g6	2337	0	2203	52	0
3	g7	2337	0	2203	52	0
3	h1	2337	0	2201	65	0
3	h2	2337	0	2202	55	0
3	h5	2337	0	2201	63	0
3	h6	2337	0	2201	66	0
3	h7	2337	0	2201	57	0
3	k1	2257	0	2128	57	0
3	k2	2257	0	2129	52	0
3	k5	2257	0	2128	43	0
3	k6	2257	0	2128	52	0
3	k7	2257	0	2128	60	0
3	n1	2337	0	2202	59	0
3	n2	2337	0	2202	50	0
3	n5	2337	0	2202	65	0
3	n6	2337	0	2202	67	0
3	n7	2337	0	2202	68	0
3	o1	2337	0	2203	69	0
3	o2	2337	0	2203	69	0
3	o5	2337	0	2203	67	0
3	o6	2337	0	2203	74	0
3	o7	2337	0	2203	65	0
3	r1	2337	0	2204	69	0
3	r2	2337	0	2204	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	r5	2337	0	2204	72	0
3	r6	2337	0	2204	75	0
3	r7	2337	0	2204	72	0
4	l1	1023	0	972	38	0
4	l2	1023	0	972	34	0
4	l5	1023	0	972	38	0
4	l6	1023	0	972	40	0
4	l7	1023	0	972	35	0
4	m1	1023	0	973	26	0
4	m2	1023	0	973	27	0
4	m5	1023	0	973	27	0
4	m6	1023	0	973	29	0
4	m7	1023	0	973	31	0
4	p1	1023	0	974	35	0
4	p2	1023	0	974	43	0
4	p5	1023	0	974	36	0
4	p6	1023	0	974	42	0
4	p7	1023	0	974	39	0
4	q1	1023	0	974	42	0
4	q2	1023	0	974	36	0
4	q5	1023	0	974	41	0
4	q6	1023	0	974	39	0
4	q7	1023	0	974	36	0
4	s1	1023	0	974	47	0
4	s2	1023	0	974	45	0
4	s5	1023	0	974	47	0
4	s6	1023	0	974	46	0
4	s7	1023	0	974	51	0
4	t1	1023	0	975	38	0
4	t2	1023	0	975	38	0
4	t5	1023	0	975	37	0
4	t6	1023	0	975	32	0
4	t7	1023	0	975	30	0
4	u1	1011	0	961	36	0
4	u2	1011	0	961	39	0
4	u5	1011	0	961	35	0
4	u6	1011	0	961	38	0
4	u7	1011	0	961	39	0
4	v1	1011	0	961	41	0
4	v2	1011	0	961	36	0
4	v5	1011	0	961	34	0
4	v6	1011	0	961	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	v7	1011	0	961	42	0
5	03	1679	0	1610	41	0
5	13	1679	0	1610	31	0
5	23	1679	0	1610	32	0
5	33	1679	0	1610	41	0
5	43	1679	0	1610	37	0
5	53	1679	0	1610	45	0
5	63	1679	0	1610	44	0
5	73	1679	0	1610	38	0
5	83	1679	0	1610	44	0
5	93	1679	0	1610	44	0
5	A3	1679	0	1610	39	0
5	B3	1679	0	1610	47	0
5	C3	1679	0	1610	37	0
5	D3	1679	0	1610	39	0
5	E3	1679	0	1610	44	0
5	F3	1679	0	1610	33	0
5	G3	1679	0	1610	43	0
5	J3	1679	0	1610	33	0
5	K3	1723	0	1652	32	0
5	L3	1679	0	1610	29	0
5	M3	1679	0	1610	32	0
5	N3	1723	0	1654	41	0
5	O3	1679	0	1611	34	0
5	P3	1679	0	1610	24	0
5	Q3	1723	0	1652	32	0
5	R3	1679	0	1610	26	0
5	S3	1679	0	1610	35	0
5	T3	1723	0	1652	42	0
5	U3	1679	0	1610	31	0
5	V3	1679	0	1610	36	0
5	W3	1723	0	1652	35	0
5	X3	1679	0	1610	28	0
5	Y3	1679	0	1609	29	0
5	Z3	1679	0	1609	45	0
5	a3	1679	0	1609	41	0
5	b3	1679	0	1609	35	0
5	c3	1679	0	1609	34	0
5	d3	1679	0	1609	42	0
5	e3	1679	0	1609	30	0
5	f3	1679	0	1609	39	0
5	g3	1679	0	1609	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	h3	1679	0	1609	28	0
5	i3	1679	0	1609	41	0
5	j3	1679	0	1609	40	0
5	k3	1679	0	1609	27	0
5	l3	1679	0	1609	44	0
5	m3	1679	0	1609	42	0
5	n3	1679	0	1609	32	0
5	o3	1679	0	1609	37	0
5	p3	1679	0	1609	25	0
5	q3	1679	0	1609	29	0
5	r3	1679	0	1609	35	0
5	s3	1679	0	1609	26	0
5	t3	1679	0	1609	30	0
5	u3	1679	0	1609	37	0
5	v3	1679	0	1609	27	0
5	w3	1679	0	1609	32	0
5	x3	1679	0	1610	37	0
5	y3	1679	0	1610	31	0
5	z3	1679	0	1609	32	0
6	A4	671	0	677	27	0
6	B4	671	0	677	33	0
6	C4	671	0	678	38	0
6	D4	671	0	678	23	0
6	E4	671	0	677	25	0
All	All	221120	0	211352	5052	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 5052 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:l6:74:CYS:O	4:l6:74:CYS:SG	2.01	1.18
4:v7:73:PHE:CZ	4:v7:104:PRO:HG2	1.80	1.14
3:g1:172:PRO:HB3	4:s1:5:VAL:HA	1.35	1.06
4:l5:74:CYS:O	4:l5:74:CYS:SG	2.14	1.05
1:d7:5:ASN:HD22	4:p7:7:VAL:HG11	1.19	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a1	26/38 (68%)	24 (92%)	2 (8%)	0	100	100
1	a2	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
1	a5	26/38 (68%)	24 (92%)	2 (8%)	0	100	100
1	a6	26/38 (68%)	24 (92%)	2 (8%)	0	100	100
1	a7	26/38 (68%)	24 (92%)	2 (8%)	0	100	100
1	b1	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
1	b2	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
1	b5	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
1	b6	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
1	b7	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
1	c	32/38 (84%)	29 (91%)	3 (9%)	0	100	100
1	d	32/38 (84%)	29 (91%)	3 (9%)	0	100	100
1	d1	32/38 (84%)	24 (75%)	8 (25%)	0	100	100
1	d2	32/38 (84%)	26 (81%)	6 (19%)	0	100	100
1	d5	32/38 (84%)	25 (78%)	7 (22%)	0	100	100
1	d6	32/38 (84%)	25 (78%)	7 (22%)	0	100	100
1	d7	32/38 (84%)	24 (75%)	8 (25%)	0	100	100
1	e	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
1	e1	26/38 (68%)	19 (73%)	7 (27%)	0	100	100
1	e2	26/38 (68%)	22 (85%)	4 (15%)	0	100	100
1	e5	26/38 (68%)	21 (81%)	5 (19%)	0	100	100
1	e6	26/38 (68%)	19 (73%)	7 (27%)	0	100	100
1	e7	26/38 (68%)	18 (69%)	8 (31%)	0	100	100
1	f	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
1	g	32/38 (84%)	31 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	f1	18/217 (8%)	15 (83%)	3 (17%)	0	100	100
2	f2	18/217 (8%)	16 (89%)	2 (11%)	0	100	100
2	f5	18/217 (8%)	12 (67%)	6 (33%)	0	100	100
2	f6	18/217 (8%)	15 (83%)	3 (17%)	0	100	100
2	f7	18/217 (8%)	16 (89%)	2 (11%)	0	100	100
3	g1	297/465 (64%)	253 (85%)	43 (14%)	1 (0%)	36	67
3	g2	297/465 (64%)	251 (84%)	44 (15%)	2 (1%)	18	51
3	g5	297/465 (64%)	250 (84%)	46 (16%)	1 (0%)	36	67
3	g6	297/465 (64%)	250 (84%)	46 (16%)	1 (0%)	36	67
3	g7	297/465 (64%)	252 (85%)	43 (14%)	2 (1%)	18	51
3	h1	297/465 (64%)	243 (82%)	51 (17%)	3 (1%)	12	44
3	h2	297/465 (64%)	242 (82%)	50 (17%)	5 (2%)	7	35
3	h5	297/465 (64%)	242 (82%)	53 (18%)	2 (1%)	18	51
3	h6	297/465 (64%)	241 (81%)	54 (18%)	2 (1%)	18	51
3	h7	297/465 (64%)	247 (83%)	48 (16%)	2 (1%)	18	51
3	k1	286/465 (62%)	251 (88%)	35 (12%)	0	100	100
3	k2	286/465 (62%)	248 (87%)	37 (13%)	1 (0%)	36	67
3	k5	286/465 (62%)	248 (87%)	38 (13%)	0	100	100
3	k6	286/465 (62%)	251 (88%)	34 (12%)	1 (0%)	36	67
3	k7	286/465 (62%)	249 (87%)	36 (13%)	1 (0%)	36	67
3	n1	297/465 (64%)	247 (83%)	49 (16%)	1 (0%)	36	67
3	n2	297/465 (64%)	243 (82%)	52 (18%)	2 (1%)	18	51
3	n5	297/465 (64%)	245 (82%)	50 (17%)	2 (1%)	18	51
3	n6	297/465 (64%)	246 (83%)	49 (16%)	2 (1%)	18	51
3	n7	297/465 (64%)	249 (84%)	46 (16%)	2 (1%)	18	51
3	o1	297/465 (64%)	248 (84%)	45 (15%)	4 (1%)	9	39
3	o2	297/465 (64%)	245 (82%)	47 (16%)	5 (2%)	7	35
3	o5	297/465 (64%)	245 (82%)	47 (16%)	5 (2%)	7	35
3	o6	297/465 (64%)	242 (82%)	50 (17%)	5 (2%)	7	35
3	o7	297/465 (64%)	248 (84%)	45 (15%)	4 (1%)	9	39
3	r1	297/465 (64%)	254 (86%)	42 (14%)	1 (0%)	36	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	r2	297/465 (64%)	251 (84%)	45 (15%)	1 (0%)	36	67
3	r5	297/465 (64%)	250 (84%)	44 (15%)	3 (1%)	12	44
3	r6	297/465 (64%)	252 (85%)	44 (15%)	1 (0%)	36	67
3	r7	297/465 (64%)	255 (86%)	37 (12%)	5 (2%)	7	35
4	l1	135/137 (98%)	119 (88%)	16 (12%)	0	100	100
4	l2	135/137 (98%)	117 (87%)	15 (11%)	3 (2%)	5	30
4	l5	135/137 (98%)	120 (89%)	14 (10%)	1 (1%)	18	51
4	l6	135/137 (98%)	119 (88%)	15 (11%)	1 (1%)	18	51
4	l7	135/137 (98%)	121 (90%)	13 (10%)	1 (1%)	18	51
4	m1	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
4	m2	135/137 (98%)	119 (88%)	16 (12%)	0	100	100
4	m5	135/137 (98%)	118 (87%)	17 (13%)	0	100	100
4	m6	135/137 (98%)	119 (88%)	16 (12%)	0	100	100
4	m7	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
4	p1	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	18	51
4	p2	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	18	51
4	p5	135/137 (98%)	110 (82%)	24 (18%)	1 (1%)	18	51
4	p6	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	18	51
4	p7	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	18	51
4	q1	135/137 (98%)	120 (89%)	15 (11%)	0	100	100
4	q2	135/137 (98%)	119 (88%)	16 (12%)	0	100	100
4	q5	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
4	q6	135/137 (98%)	122 (90%)	13 (10%)	0	100	100
4	q7	135/137 (98%)	120 (89%)	15 (11%)	0	100	100
4	s1	135/137 (98%)	125 (93%)	10 (7%)	0	100	100
4	s2	135/137 (98%)	124 (92%)	10 (7%)	1 (1%)	18	51
4	s5	135/137 (98%)	125 (93%)	10 (7%)	0	100	100
4	s6	135/137 (98%)	124 (92%)	10 (7%)	1 (1%)	18	51
4	s7	135/137 (98%)	125 (93%)	10 (7%)	0	100	100
4	t1	135/137 (98%)	121 (90%)	14 (10%)	0	100	100
4	t2	135/137 (98%)	123 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	t5	135/137 (98%)	122 (90%)	13 (10%)	0	100	100
4	t6	135/137 (98%)	124 (92%)	11 (8%)	0	100	100
4	t7	135/137 (98%)	119 (88%)	16 (12%)	0	100	100
4	u1	134/137 (98%)	119 (89%)	15 (11%)	0	100	100
4	u2	134/137 (98%)	118 (88%)	16 (12%)	0	100	100
4	u5	134/137 (98%)	118 (88%)	16 (12%)	0	100	100
4	u6	134/137 (98%)	119 (89%)	15 (11%)	0	100	100
4	u7	134/137 (98%)	119 (89%)	15 (11%)	0	100	100
4	v1	134/137 (98%)	113 (84%)	19 (14%)	2 (2%)	8	37
4	v2	134/137 (98%)	111 (83%)	23 (17%)	0	100	100
4	v5	134/137 (98%)	113 (84%)	21 (16%)	0	100	100
4	v6	134/137 (98%)	114 (85%)	20 (15%)	0	100	100
4	v7	134/137 (98%)	113 (84%)	20 (15%)	1 (1%)	18	51
5	03	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
5	13	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
5	23	219/230 (95%)	192 (88%)	27 (12%)	0	100	100
5	33	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
5	43	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
5	53	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
5	63	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
5	73	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
5	83	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
5	93	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
5	A3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
5	B3	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
5	C3	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
5	D3	219/230 (95%)	204 (93%)	15 (7%)	0	100	100
5	E3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
5	F3	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
5	G3	219/230 (95%)	203 (93%)	16 (7%)	0	100	100
5	J3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	K3	228/230 (99%)	210 (92%)	18 (8%)	0	100	100
5	L3	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
5	M3	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
5	N3	228/230 (99%)	207 (91%)	20 (9%)	1 (0%)	30	62
5	O3	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
5	P3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
5	Q3	228/230 (99%)	206 (90%)	21 (9%)	1 (0%)	30	62
5	R3	219/230 (95%)	203 (93%)	16 (7%)	0	100	100
5	S3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
5	T3	228/230 (99%)	206 (90%)	20 (9%)	2 (1%)	14	46
5	U3	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
5	V3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
5	W3	228/230 (99%)	206 (90%)	22 (10%)	0	100	100
5	X3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
5	Y3	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
5	Z3	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
5	a3	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
5	b3	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
5	c3	219/230 (95%)	196 (90%)	22 (10%)	1 (0%)	24	57
5	d3	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
5	e3	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
5	f3	219/230 (95%)	195 (89%)	24 (11%)	0	100	100
5	g3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
5	h3	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
5	i3	219/230 (95%)	196 (90%)	23 (10%)	0	100	100
5	j3	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
5	k3	219/230 (95%)	198 (90%)	21 (10%)	0	100	100
5	l3	219/230 (95%)	196 (90%)	22 (10%)	1 (0%)	24	57
5	m3	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
5	n3	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
5	o3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	p3	219/230 (95%)	192 (88%)	27 (12%)	0	100	100
5	q3	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
5	r3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
5	s3	219/230 (95%)	192 (88%)	27 (12%)	0	100	100
5	t3	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
5	u3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
5	v3	219/230 (95%)	191 (87%)	28 (13%)	0	100	100
5	w3	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
5	x3	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
5	y3	219/230 (95%)	192 (88%)	27 (12%)	0	100	100
5	z3	219/230 (95%)	197 (90%)	22 (10%)	0	100	100
6	A4	85/202 (42%)	66 (78%)	18 (21%)	1 (1%)	10	41
6	B4	85/202 (42%)	72 (85%)	12 (14%)	1 (1%)	10	41
6	C4	85/202 (42%)	67 (79%)	15 (18%)	3 (4%)	3	23
6	D4	85/202 (42%)	71 (84%)	11 (13%)	3 (4%)	3	23
6	E4	85/202 (42%)	71 (84%)	13 (15%)	1 (1%)	10	41
All	All	28655/36275 (79%)	25176 (88%)	3381 (12%)	98 (0%)	37	67

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	h1	172	PRO
4	p1	78	LEU
3	g2	457	GLU
3	h2	191	ALA
4	l2	75	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a1	25/32 (78%)	24 (96%)	1 (4%)	28	55
1	a2	25/32 (78%)	24 (96%)	1 (4%)	28	55
1	a5	25/32 (78%)	23 (92%)	2 (8%)	11	36
1	a6	25/32 (78%)	24 (96%)	1 (4%)	28	55
1	a7	25/32 (78%)	24 (96%)	1 (4%)	28	55
1	b1	25/32 (78%)	25 (100%)	0	100	100
1	b2	25/32 (78%)	25 (100%)	0	100	100
1	b5	25/32 (78%)	25 (100%)	0	100	100
1	b6	25/32 (78%)	25 (100%)	0	100	100
1	b7	25/32 (78%)	25 (100%)	0	100	100
1	c	29/32 (91%)	28 (97%)	1 (3%)	32	59
1	d	29/32 (91%)	29 (100%)	0	100	100
1	d1	29/32 (91%)	29 (100%)	0	100	100
1	d2	29/32 (91%)	29 (100%)	0	100	100
1	d5	29/32 (91%)	29 (100%)	0	100	100
1	d6	29/32 (91%)	29 (100%)	0	100	100
1	d7	29/32 (91%)	29 (100%)	0	100	100
1	e	29/32 (91%)	29 (100%)	0	100	100
1	e1	25/32 (78%)	25 (100%)	0	100	100
1	e2	25/32 (78%)	25 (100%)	0	100	100
1	e5	25/32 (78%)	25 (100%)	0	100	100
1	e6	25/32 (78%)	25 (100%)	0	100	100
1	e7	25/32 (78%)	25 (100%)	0	100	100
1	f	29/32 (91%)	29 (100%)	0	100	100
1	g	29/32 (91%)	29 (100%)	0	100	100
2	f1	15/175 (9%)	15 (100%)	0	100	100
2	f2	15/175 (9%)	15 (100%)	0	100	100
2	f5	15/175 (9%)	15 (100%)	0	100	100
2	f6	15/175 (9%)	15 (100%)	0	100	100
2	f7	15/175 (9%)	15 (100%)	0	100	100
3	g1	240/379 (63%)	239 (100%)	1 (0%)	84	81
3	g2	240/379 (63%)	236 (98%)	4 (2%)	53	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	g5	240/379 (63%)	240 (100%)	0	100	100
3	g6	240/379 (63%)	238 (99%)	2 (1%)	73	77
3	g7	240/379 (63%)	238 (99%)	2 (1%)	73	77
3	h1	240/379 (63%)	234 (98%)	6 (2%)	42	64
3	h2	240/379 (63%)	234 (98%)	6 (2%)	42	64
3	h5	240/379 (63%)	234 (98%)	6 (2%)	42	64
3	h6	240/379 (63%)	234 (98%)	6 (2%)	42	64
3	h7	240/379 (63%)	239 (100%)	1 (0%)	84	81
3	k1	232/379 (61%)	231 (100%)	1 (0%)	84	81
3	k2	232/379 (61%)	231 (100%)	1 (0%)	84	81
3	k5	232/379 (61%)	232 (100%)	0	100	100
3	k6	232/379 (61%)	232 (100%)	0	100	100
3	k7	232/379 (61%)	232 (100%)	0	100	100
3	n1	240/379 (63%)	238 (99%)	2 (1%)	73	77
3	n2	240/379 (63%)	238 (99%)	2 (1%)	73	77
3	n5	240/379 (63%)	238 (99%)	2 (1%)	73	77
3	n6	240/379 (63%)	239 (100%)	1 (0%)	84	81
3	n7	240/379 (63%)	240 (100%)	0	100	100
3	o1	240/379 (63%)	239 (100%)	1 (0%)	84	81
3	o2	240/379 (63%)	240 (100%)	0	100	100
3	o5	240/379 (63%)	240 (100%)	0	100	100
3	o6	240/379 (63%)	240 (100%)	0	100	100
3	o7	240/379 (63%)	239 (100%)	1 (0%)	84	81
3	r1	240/379 (63%)	234 (98%)	6 (2%)	42	64
3	r2	240/379 (63%)	234 (98%)	6 (2%)	42	64
3	r5	240/379 (63%)	235 (98%)	5 (2%)	47	66
3	r6	240/379 (63%)	236 (98%)	4 (2%)	53	70
3	r7	240/379 (63%)	236 (98%)	4 (2%)	53	70
4	l1	112/112 (100%)	108 (96%)	4 (4%)	31	58
4	l2	112/112 (100%)	107 (96%)	5 (4%)	24	52
4	l5	112/112 (100%)	110 (98%)	2 (2%)	51	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	l6	112/112 (100%)	110 (98%)	2 (2%)	51	70
4	l7	112/112 (100%)	110 (98%)	2 (2%)	51	70
4	m1	112/112 (100%)	112 (100%)	0	100	100
4	m2	112/112 (100%)	112 (100%)	0	100	100
4	m5	112/112 (100%)	112 (100%)	0	100	100
4	m6	112/112 (100%)	112 (100%)	0	100	100
4	m7	112/112 (100%)	112 (100%)	0	100	100
4	p1	112/112 (100%)	110 (98%)	2 (2%)	51	70
4	p2	112/112 (100%)	110 (98%)	2 (2%)	51	70
4	p5	112/112 (100%)	110 (98%)	2 (2%)	51	70
4	p6	112/112 (100%)	110 (98%)	2 (2%)	51	70
4	p7	112/112 (100%)	110 (98%)	2 (2%)	51	70
4	q1	112/112 (100%)	111 (99%)	1 (1%)	70	76
4	q2	112/112 (100%)	112 (100%)	0	100	100
4	q5	112/112 (100%)	112 (100%)	0	100	100
4	q6	112/112 (100%)	112 (100%)	0	100	100
4	q7	112/112 (100%)	112 (100%)	0	100	100
4	s1	112/112 (100%)	111 (99%)	1 (1%)	70	76
4	s2	112/112 (100%)	110 (98%)	2 (2%)	51	70
4	s5	112/112 (100%)	111 (99%)	1 (1%)	70	76
4	s6	112/112 (100%)	110 (98%)	2 (2%)	51	70
4	s7	112/112 (100%)	109 (97%)	3 (3%)	39	63
4	t1	112/112 (100%)	112 (100%)	0	100	100
4	t2	112/112 (100%)	112 (100%)	0	100	100
4	t5	112/112 (100%)	112 (100%)	0	100	100
4	t6	112/112 (100%)	112 (100%)	0	100	100
4	t7	112/112 (100%)	110 (98%)	2 (2%)	51	70
4	u1	111/112 (99%)	111 (100%)	0	100	100
4	u2	111/112 (99%)	108 (97%)	3 (3%)	39	63
4	u5	111/112 (99%)	109 (98%)	2 (2%)	51	70
4	u6	111/112 (99%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	u7	111/112 (99%)	109 (98%)	2 (2%)	51	70
4	v1	111/112 (99%)	109 (98%)	2 (2%)	51	70
4	v2	111/112 (99%)	110 (99%)	1 (1%)	70	76
4	v5	111/112 (99%)	109 (98%)	2 (2%)	51	70
4	v6	111/112 (99%)	111 (100%)	0	100	100
4	v7	111/112 (99%)	110 (99%)	1 (1%)	70	76
5	03	186/191 (97%)	185 (100%)	1 (0%)	81	81
5	13	186/191 (97%)	186 (100%)	0	100	100
5	23	186/191 (97%)	186 (100%)	0	100	100
5	33	186/191 (97%)	186 (100%)	0	100	100
5	43	186/191 (97%)	186 (100%)	0	100	100
5	53	186/191 (97%)	186 (100%)	0	100	100
5	63	186/191 (97%)	186 (100%)	0	100	100
5	73	186/191 (97%)	186 (100%)	0	100	100
5	83	186/191 (97%)	186 (100%)	0	100	100
5	93	186/191 (97%)	186 (100%)	0	100	100
5	A3	186/191 (97%)	186 (100%)	0	100	100
5	B3	186/191 (97%)	186 (100%)	0	100	100
5	C3	186/191 (97%)	186 (100%)	0	100	100
5	D3	186/191 (97%)	186 (100%)	0	100	100
5	E3	186/191 (97%)	186 (100%)	0	100	100
5	F3	186/191 (97%)	186 (100%)	0	100	100
5	G3	186/191 (97%)	186 (100%)	0	100	100
5	J3	186/191 (97%)	186 (100%)	0	100	100
5	K3	191/191 (100%)	190 (100%)	1 (0%)	81	81
5	L3	186/191 (97%)	186 (100%)	0	100	100
5	M3	186/191 (97%)	186 (100%)	0	100	100
5	N3	191/191 (100%)	190 (100%)	1 (0%)	81	81
5	O3	186/191 (97%)	186 (100%)	0	100	100
5	P3	186/191 (97%)	186 (100%)	0	100	100
5	Q3	191/191 (100%)	191 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R3	186/191 (97%)	186 (100%)	0	100	100
5	S3	186/191 (97%)	185 (100%)	1 (0%)	81	81
5	T3	191/191 (100%)	188 (98%)	3 (2%)	55	71
5	U3	186/191 (97%)	186 (100%)	0	100	100
5	V3	186/191 (97%)	186 (100%)	0	100	100
5	W3	191/191 (100%)	191 (100%)	0	100	100
5	X3	186/191 (97%)	186 (100%)	0	100	100
5	Y3	186/191 (97%)	186 (100%)	0	100	100
5	Z3	186/191 (97%)	186 (100%)	0	100	100
5	a3	186/191 (97%)	186 (100%)	0	100	100
5	b3	186/191 (97%)	186 (100%)	0	100	100
5	c3	186/191 (97%)	186 (100%)	0	100	100
5	d3	186/191 (97%)	186 (100%)	0	100	100
5	e3	186/191 (97%)	186 (100%)	0	100	100
5	f3	186/191 (97%)	185 (100%)	1 (0%)	81	81
5	g3	186/191 (97%)	186 (100%)	0	100	100
5	h3	186/191 (97%)	186 (100%)	0	100	100
5	i3	186/191 (97%)	186 (100%)	0	100	100
5	j3	186/191 (97%)	186 (100%)	0	100	100
5	k3	186/191 (97%)	186 (100%)	0	100	100
5	l3	186/191 (97%)	186 (100%)	0	100	100
5	m3	186/191 (97%)	186 (100%)	0	100	100
5	n3	186/191 (97%)	186 (100%)	0	100	100
5	o3	186/191 (97%)	186 (100%)	0	100	100
5	p3	186/191 (97%)	186 (100%)	0	100	100
5	q3	186/191 (97%)	186 (100%)	0	100	100
5	r3	186/191 (97%)	186 (100%)	0	100	100
5	s3	186/191 (97%)	186 (100%)	0	100	100
5	t3	186/191 (97%)	186 (100%)	0	100	100
5	u3	186/191 (97%)	186 (100%)	0	100	100
5	v3	186/191 (97%)	186 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	w3	186/191 (97%)	186 (100%)	0	100	100
5	x3	186/191 (97%)	186 (100%)	0	100	100
5	y3	186/191 (97%)	186 (100%)	0	100	100
5	z3	186/191 (97%)	186 (100%)	0	100	100
6	A4	73/168 (44%)	72 (99%)	1 (1%)	59	72
6	B4	73/168 (44%)	70 (96%)	3 (4%)	27	54
6	C4	73/168 (44%)	71 (97%)	2 (3%)	39	63
6	D4	73/168 (44%)	67 (92%)	6 (8%)	10	35
6	E4	73/168 (44%)	71 (97%)	2 (3%)	39	63
All	All	23920/29825 (80%)	23771 (99%)	149 (1%)	76	80

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	h6	403	PHE
4	t7	9	PHE
4	p6	75	ASP
3	h7	455	CYS
4	p2	77	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 355 such sidechains are listed below:

Mol	Chain	Res	Type
3	k5	324	GLN
3	o6	346	GLN
4	m5	127	GLN
4	u5	125	ASN
4	s6	127	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

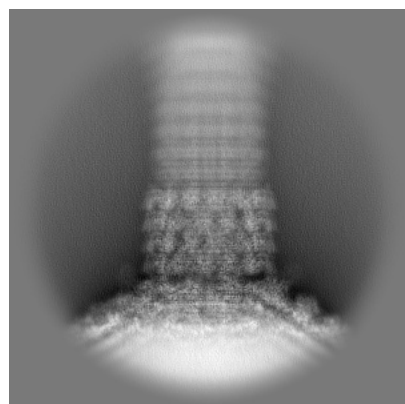
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29504. These allow visual inspection of the internal detail of the map and identification of artifacts.

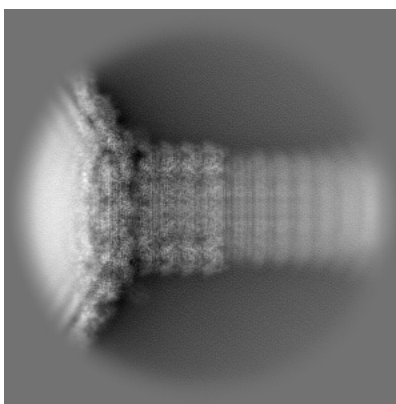
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

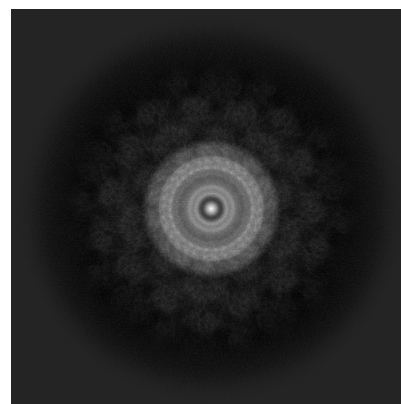
6.1.1 Primary map



X

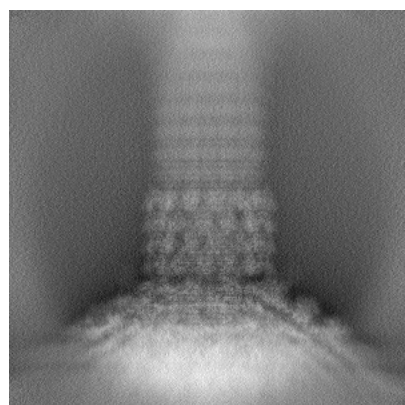


Y

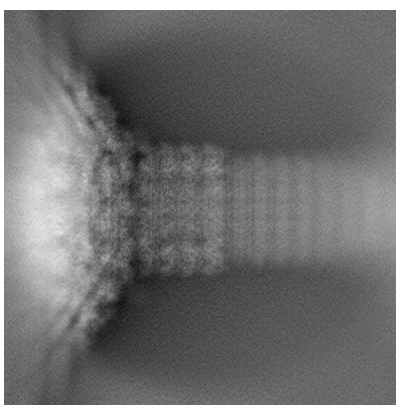


Z

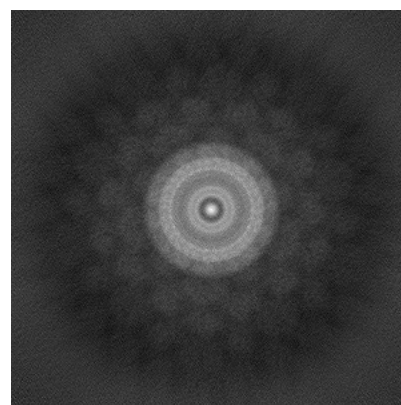
6.1.2 Raw map



X



Y

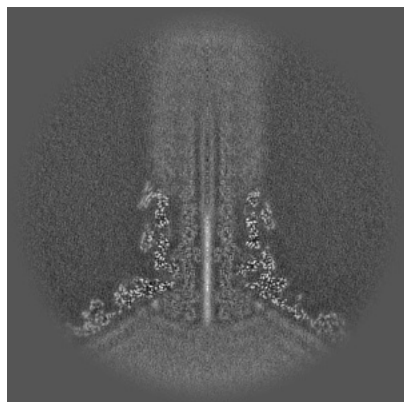


Z

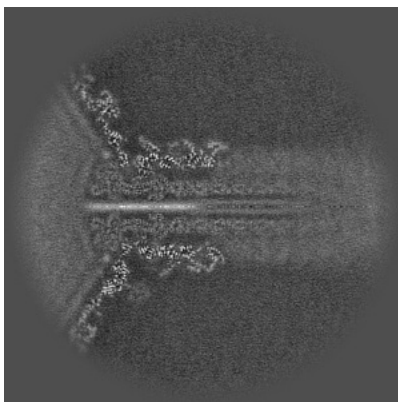
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

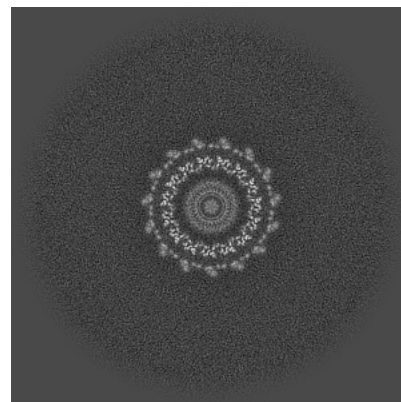
6.2.1 Primary map



X Index: 300

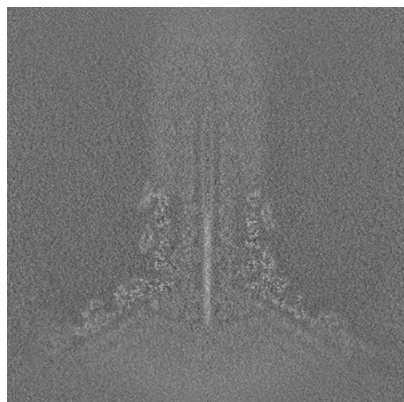


Y Index: 300

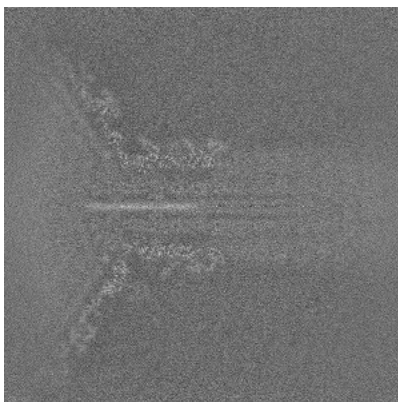


Z Index: 300

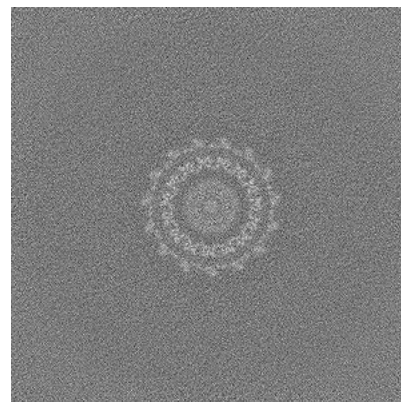
6.2.2 Raw map



X Index: 300



Y Index: 300

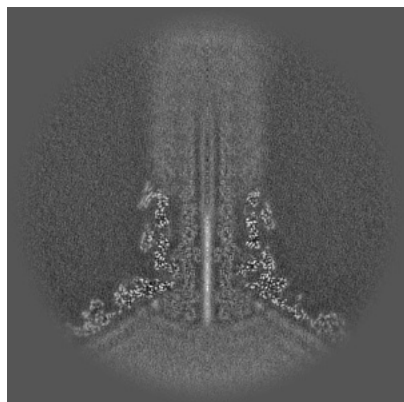


Z Index: 300

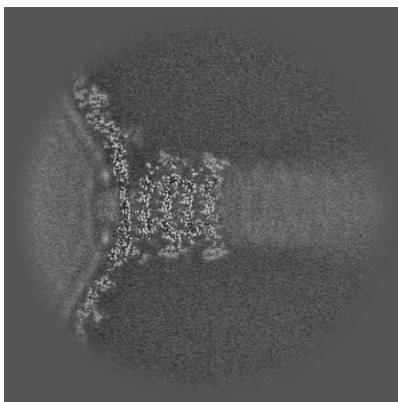
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

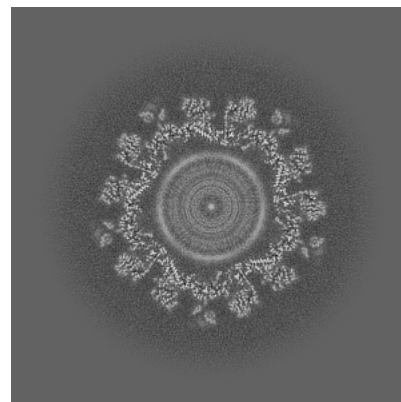
6.3.1 Primary map



X Index: 300

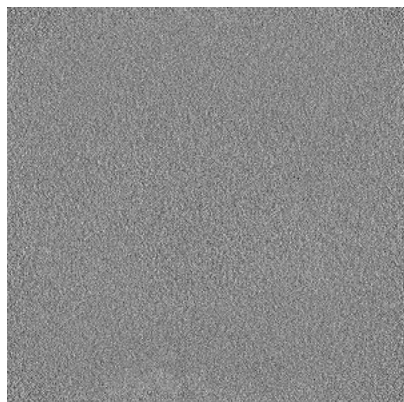


Y Index: 239

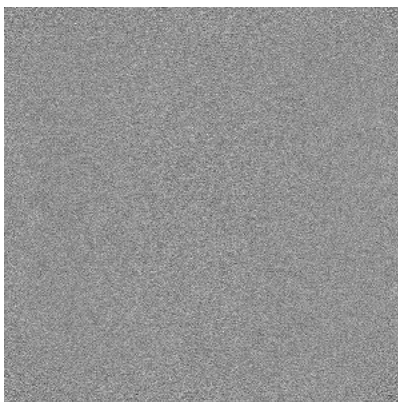


Z Index: 156

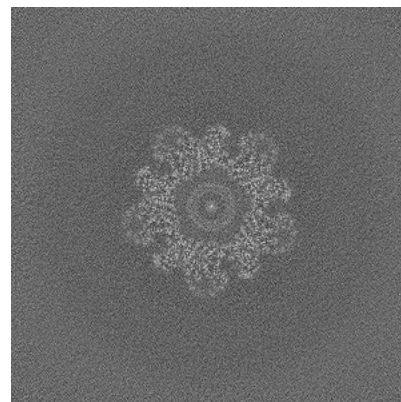
6.3.2 Raw map



X Index: 0



Y Index: 0

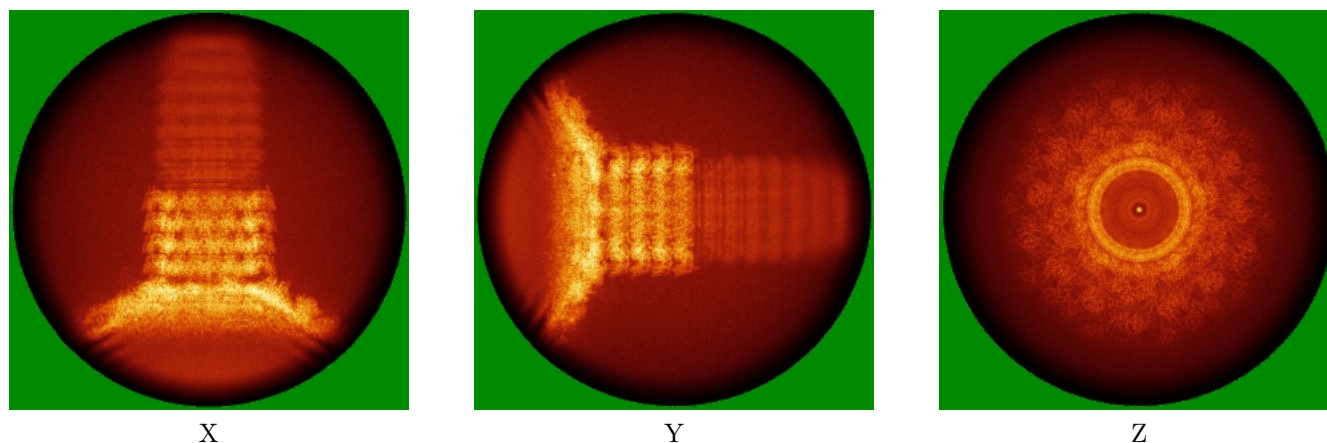


Z Index: 179

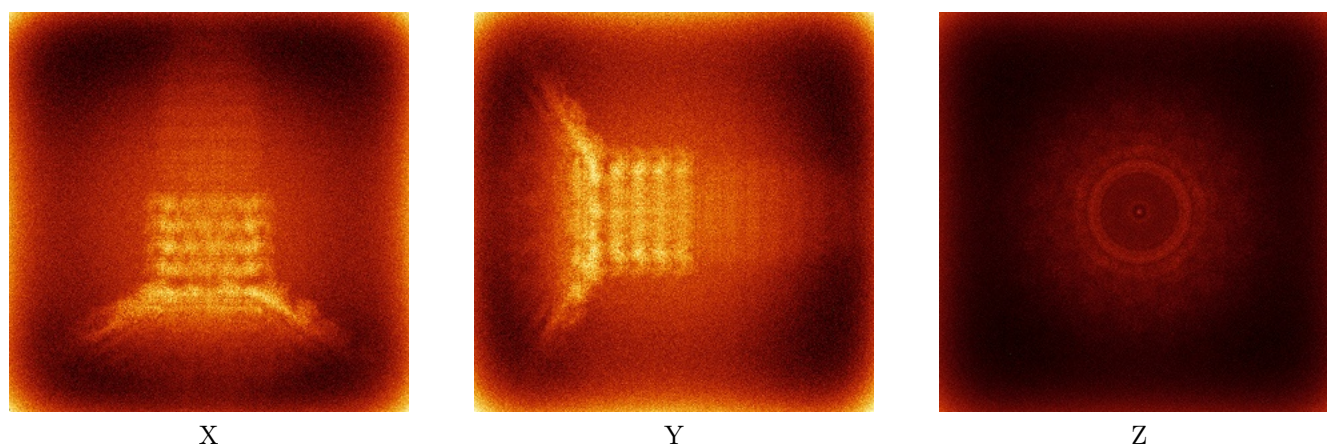
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

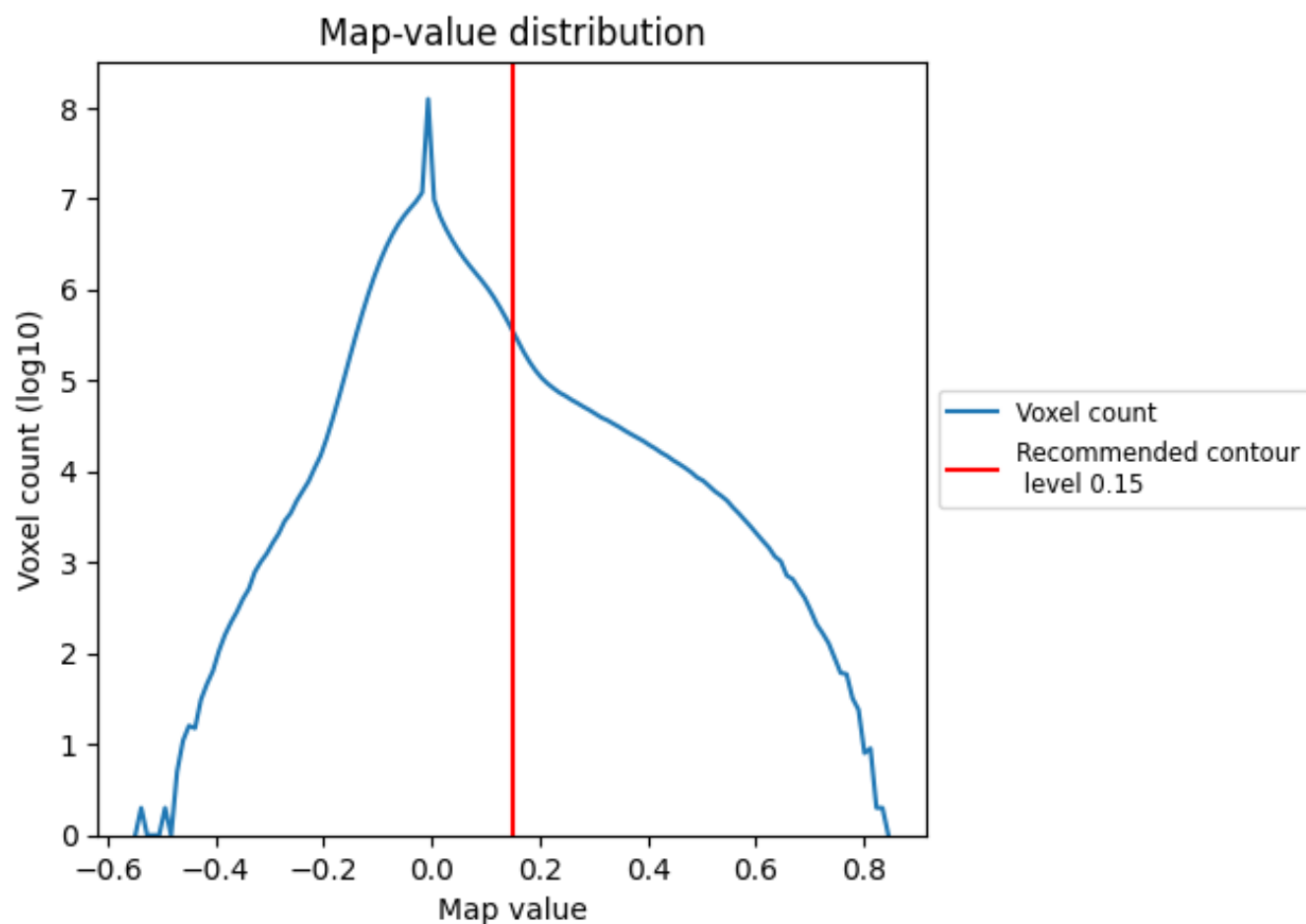
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

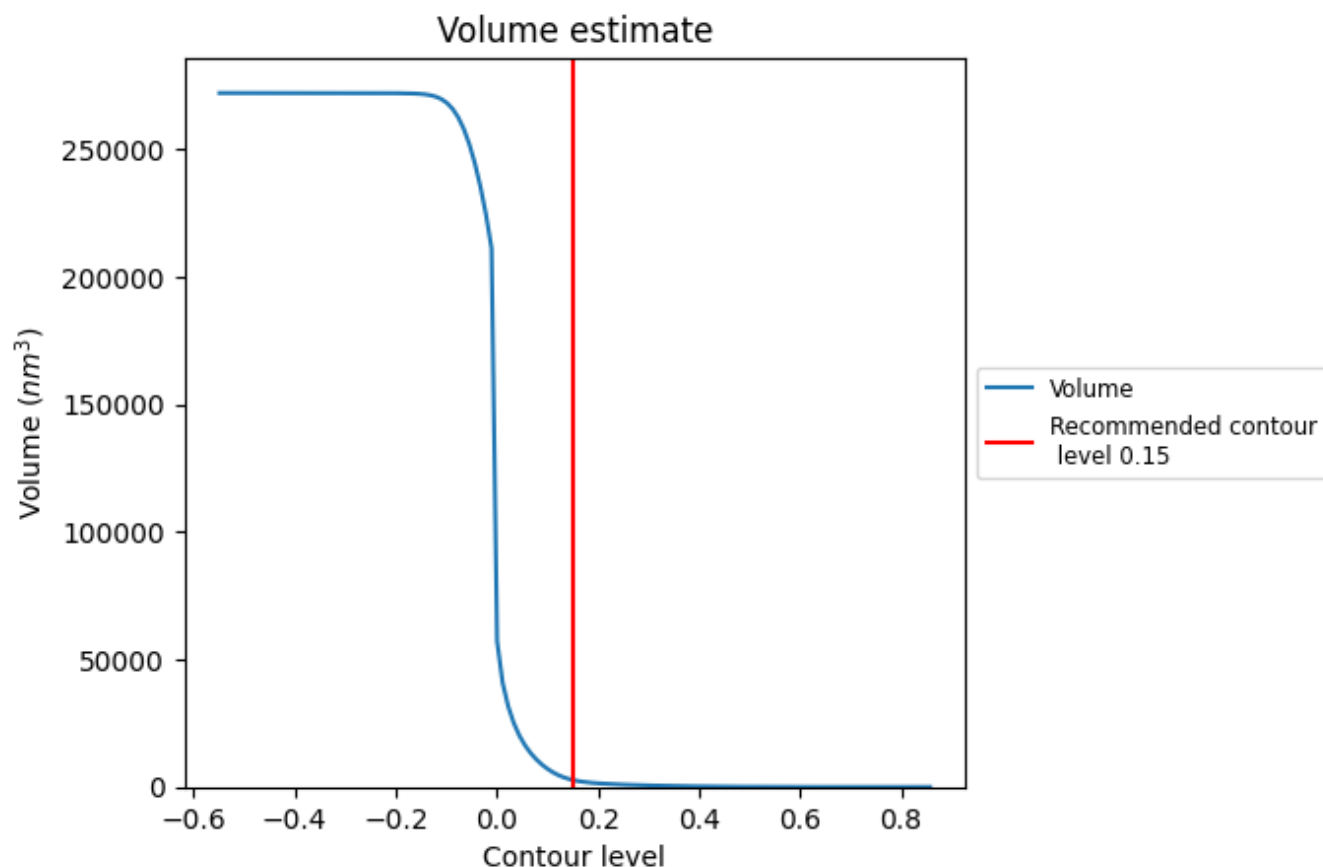
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

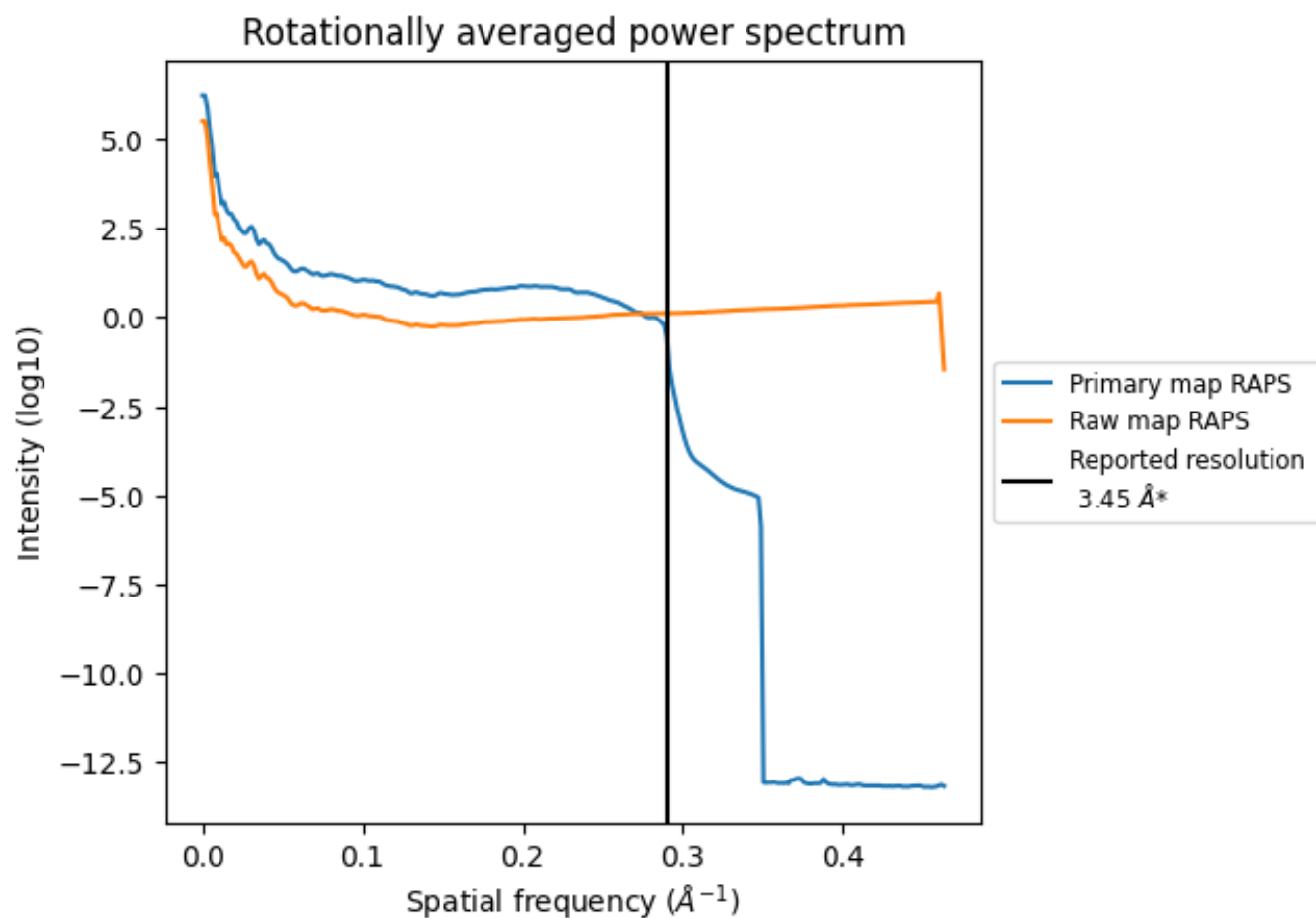
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2752 nm^3 ; this corresponds to an approximate mass of 2486 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

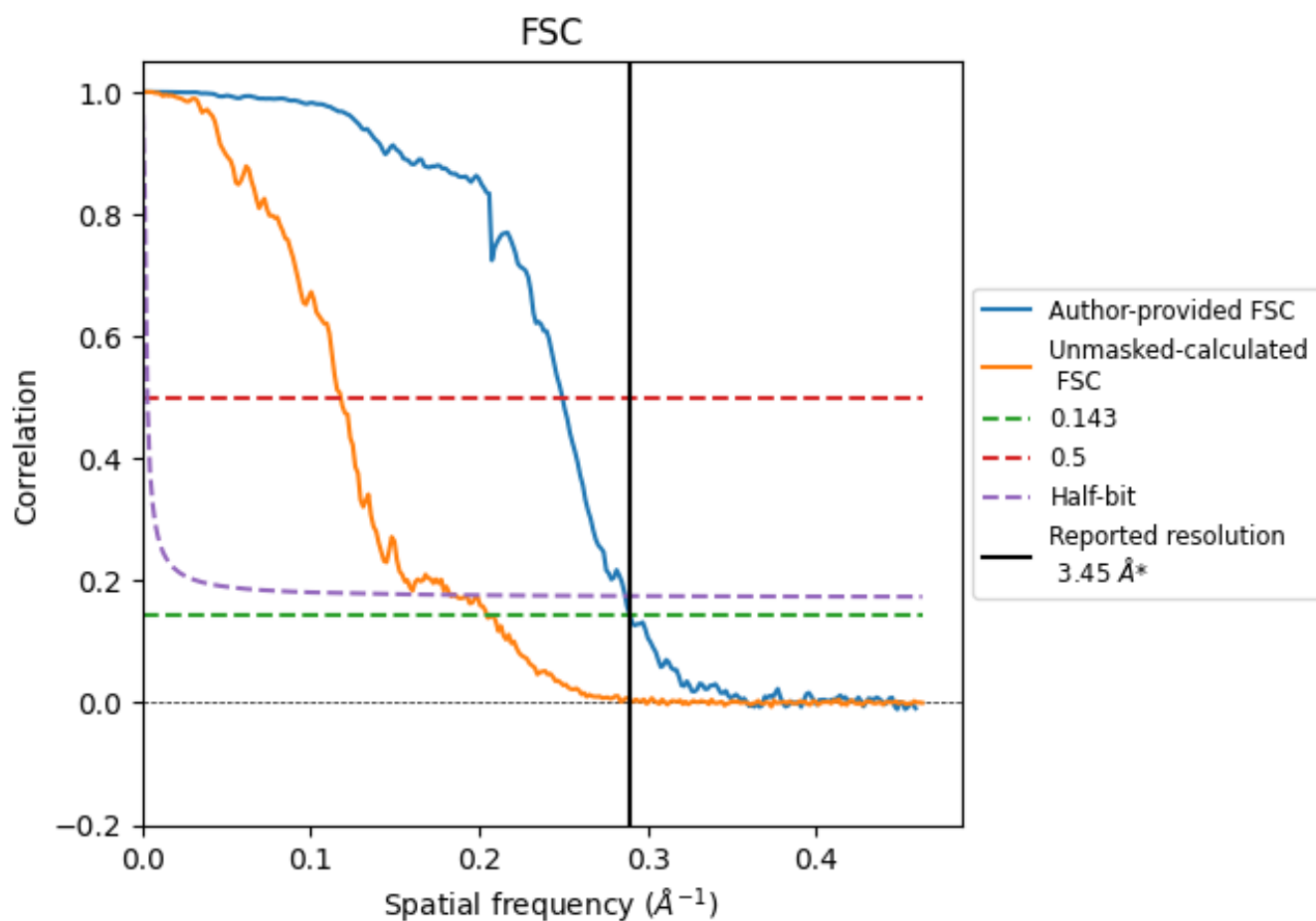


*Reported resolution corresponds to spatial frequency of $0.290 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.290 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

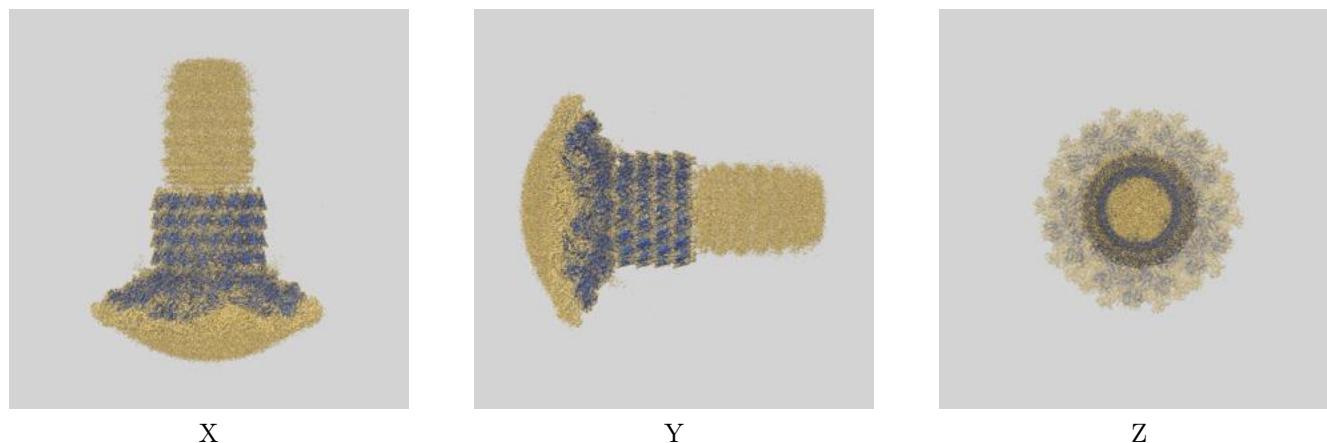
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.45	4.01	3.49
Unmasked-calculated*	4.89	8.49	5.46

*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 4.89 differs from the reported value 3.45 by more than 10 %

9 Map-model fit [i](#)

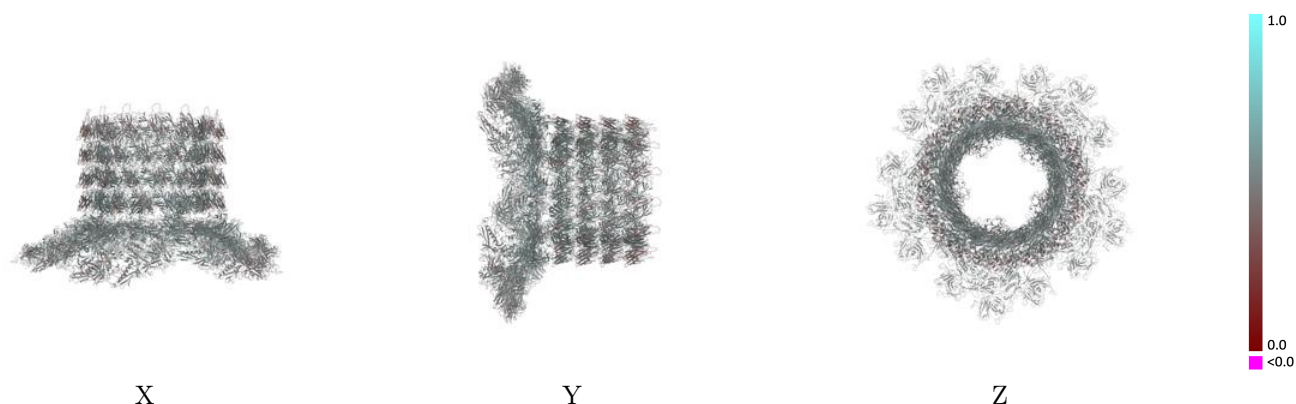
This section contains information regarding the fit between EMDB map EMD-29504 and PDB model 8FWG. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



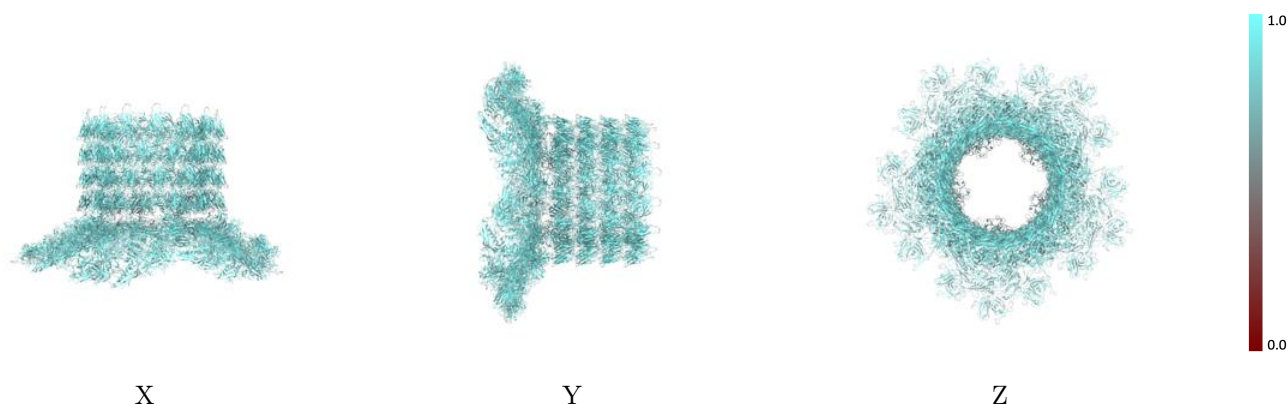
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



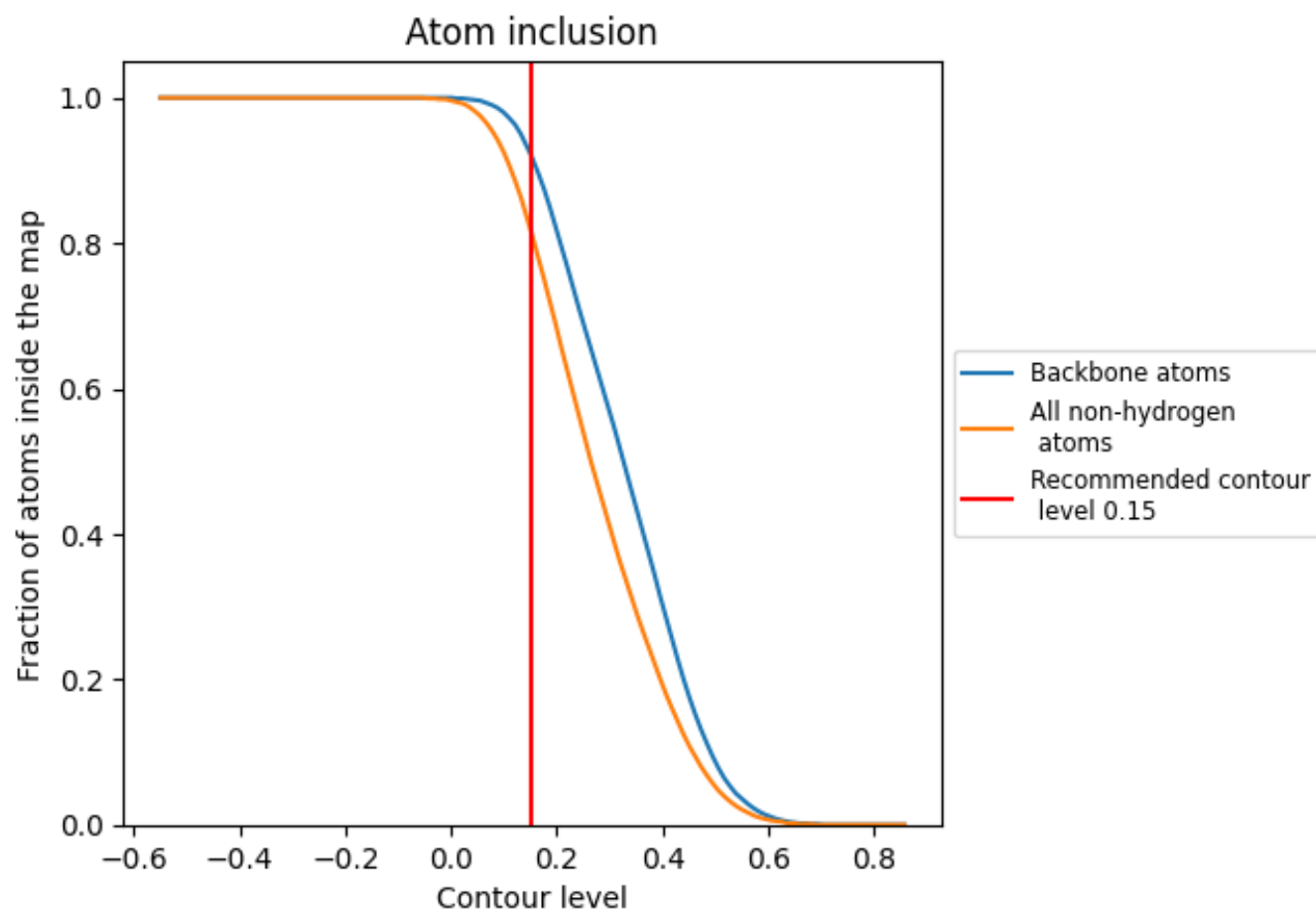
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8190	 0.4910
03	 0.8310	 0.4670
13	 0.8610	 0.4970
23	 0.8580	 0.4900
33	 0.8270	 0.4600
43	 0.8280	 0.4650
53	 0.8440	 0.4610
63	 0.8330	 0.4570
73	 0.8290	 0.4680
83	 0.8360	 0.4610
93	 0.8310	 0.4590
A3	 0.8390	 0.4630
A4	 0.6250	 0.4810
B3	 0.8320	 0.4590
B4	 0.6270	 0.4770
C3	 0.8310	 0.4670
C4	 0.6300	 0.4730
D3	 0.8390	 0.4630
D4	 0.6040	 0.4550
E3	 0.8300	 0.4630
E4	 0.6220	 0.4700
F3	 0.8330	 0.4670
G3	 0.8220	 0.4520
J3	 0.8550	 0.5110
K3	 0.8010	 0.4930
L3	 0.8050	 0.4920
M3	 0.8470	 0.5120
N3	 0.7990	 0.4960
O3	 0.8050	 0.4920
P3	 0.8560	 0.5130
Q3	 0.8060	 0.4960
R3	 0.8100	 0.4950
S3	 0.8590	 0.5120
T3	 0.8070	 0.4930
U3	 0.8020	 0.4950



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Chain	Atom inclusion	Q-score
V3	 0.8560	 0.5120
W3	 0.7950	 0.4910
X3	 0.8100	 0.4930
Y3	 0.8490	 0.4960
Z3	 0.8550	 0.4910
a1	 0.8330	 0.5290
a2	 0.8370	 0.5290
a3	 0.8420	 0.4930
a5	 0.8330	 0.5250
a6	 0.8180	 0.5270
a7	 0.8470	 0.5270
b1	 0.7680	 0.5240
b2	 0.7540	 0.5130
b3	 0.8500	 0.4960
b5	 0.7830	 0.5170
b6	 0.7680	 0.5170
b7	 0.7730	 0.5190
c	 0.8000	 0.5160
c3	 0.8480	 0.4890
d	 0.7920	 0.4970
d1	 0.8000	 0.5020
d2	 0.7790	 0.4870
d3	 0.8500	 0.4960
d5	 0.7920	 0.5040
d6	 0.7870	 0.5010
d7	 0.7920	 0.4990
e	 0.7960	 0.5000
e1	 0.7390	 0.4810
e2	 0.7630	 0.4870
e3	 0.8520	 0.4960
e5	 0.7630	 0.4830
e6	 0.7490	 0.4860
e7	 0.7590	 0.4840
f	 0.8000	 0.5090
f1	 0.6990	 0.5180
f2	 0.7130	 0.5200
f3	 0.8480	 0.4900
f5	 0.6990	 0.5120
f6	 0.7130	 0.5170
f7	 0.7060	 0.5150
g	 0.7960	 0.5010
g1	 0.8200	 0.5060

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Chain	Atom inclusion	Q-score
g2	 0.8250	 0.5060
g3	 0.8450	 0.4950
g5	 0.8200	 0.5040
g6	 0.8240	 0.5040
g7	 0.8190	 0.5030
h1	 0.8380	 0.5170
h2	 0.8410	 0.5190
h3	 0.8480	 0.4970
h5	 0.8410	 0.5180
h6	 0.8420	 0.5170
h7	 0.8400	 0.5160
i3	 0.8530	 0.4920
j3	 0.8500	 0.4930
k1	 0.8150	 0.5140
k2	 0.8170	 0.5160
k3	 0.8480	 0.4960
k5	 0.8160	 0.5150
k6	 0.8160	 0.5170
k7	 0.8140	 0.5100
l1	 0.8530	 0.5170
l2	 0.8540	 0.5160
l3	 0.8530	 0.4890
l5	 0.8530	 0.5170
l6	 0.8570	 0.5170
l7	 0.8490	 0.5140
m1	 0.8420	 0.5130
m2	 0.8430	 0.5140
m3	 0.8490	 0.4950
m5	 0.8450	 0.5170
m6	 0.8510	 0.5140
m7	 0.8500	 0.5150
n1	 0.8400	 0.5090
n2	 0.8390	 0.5090
n3	 0.8620	 0.4890
n5	 0.8410	 0.5100
n6	 0.8450	 0.5120
n7	 0.8410	 0.5100
o1	 0.8010	 0.4790
o2	 0.8030	 0.4790
o3	 0.8650	 0.4960
o5	 0.8000	 0.4800
o6	 0.8040	 0.4790

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Chain	Atom inclusion	Q-score
o7	 0.7990	 0.4820
p1	 0.8030	 0.4890
p2	 0.8030	 0.4860
p3	 0.8550	 0.4890
p5	 0.8050	 0.4860
p6	 0.8010	 0.4870
p7	 0.8030	 0.4840
q1	 0.7660	 0.4690
q2	 0.7640	 0.4680
q3	 0.8590	 0.4890
q5	 0.7620	 0.4660
q6	 0.7580	 0.4690
q7	 0.7680	 0.4690
r1	 0.8030	 0.4940
r2	 0.8010	 0.4920
r3	 0.8630	 0.4960
r5	 0.8090	 0.4930
r6	 0.8110	 0.4920
r7	 0.8060	 0.4870
s1	 0.7940	 0.4890
s2	 0.7970	 0.4890
s3	 0.8550	 0.4910
s5	 0.7940	 0.4900
s6	 0.7950	 0.4900
s7	 0.7930	 0.4890
t1	 0.7860	 0.4690
t2	 0.7860	 0.4710
t3	 0.8590	 0.4890
t5	 0.7880	 0.4700
t6	 0.7850	 0.4720
t7	 0.7730	 0.4670
u1	 0.7160	 0.4480
u2	 0.7170	 0.4490
u3	 0.8660	 0.4960
u5	 0.7180	 0.4520
u6	 0.7170	 0.4490
u7	 0.7190	 0.4490
v1	 0.7040	 0.4500
v2	 0.7160	 0.4490
v3	 0.8600	 0.4890
v5	 0.7180	 0.4540
v6	 0.7090	 0.4530

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Chain	Atom inclusion	Q-score
v7	 0.6980	 0.4460
w3	 0.8670	 0.4900
x3	 0.8640	 0.4960
y3	 0.8530	 0.4880
z3	 0.8630	 0.4910