wwPDB EM Validation Summary Report

Nov 28, 2023 – 03:27 AM EST

PDB ID	:	8FXR
EMDB ID	:	EMD-29541
Title	:	Structure of neck with portal vertex of capsid of Agrobacterium phage Milano
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	:	2023-01-25
Resolution	:	4.50 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:

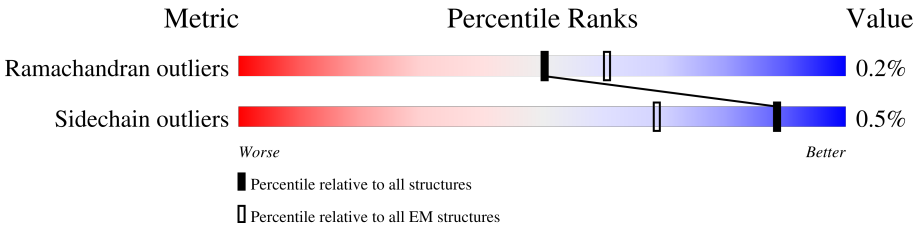
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	a1	38	13% 74% 26%
1	a2	38	71% 26%
1	a5	38	8% 74% 26%
1	a6	38	11% 74% 26%
1	a7	38	13% 74% 26%
1	b1	38	8% 74% 26%
1	b2	38	11% 71% 26%
1	b5	38	16% 74% 26%
1	b6	38	11% 74% 26%

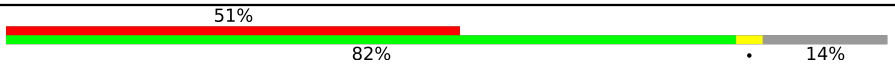
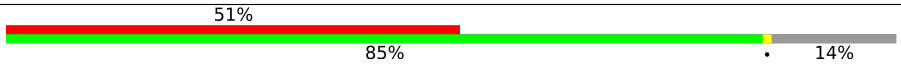
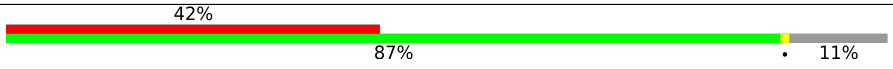
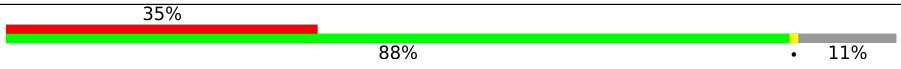
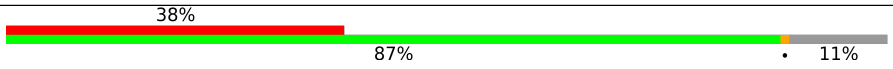
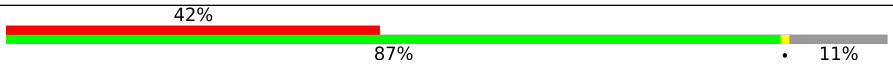
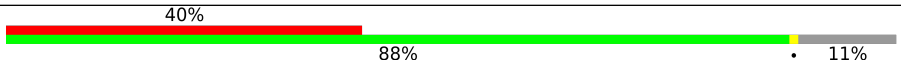
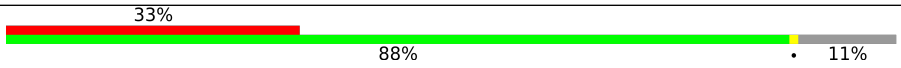
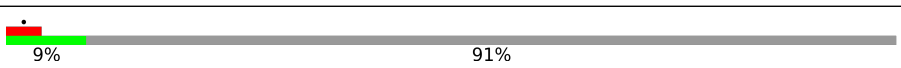
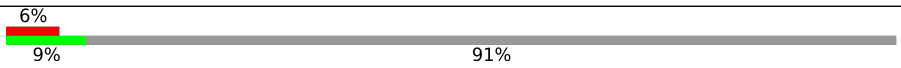
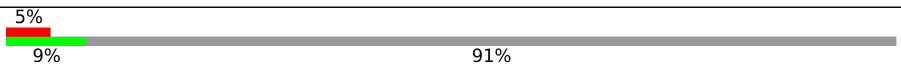
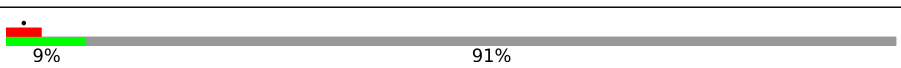
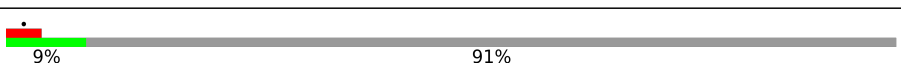
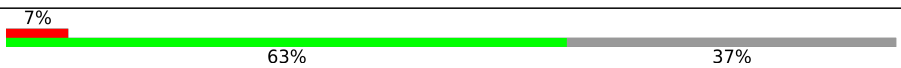
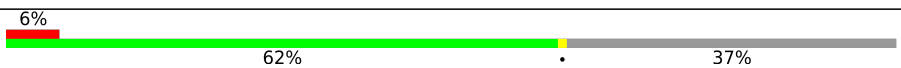
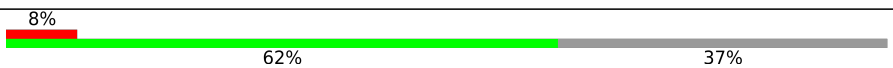
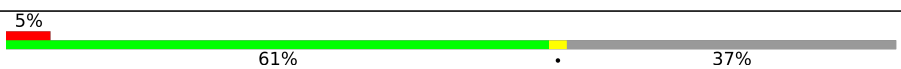
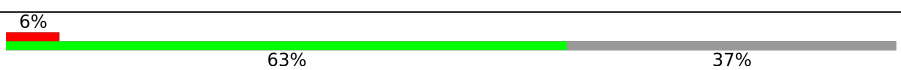
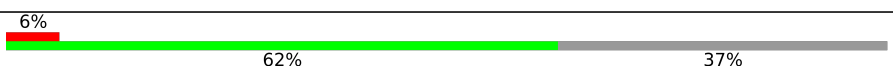
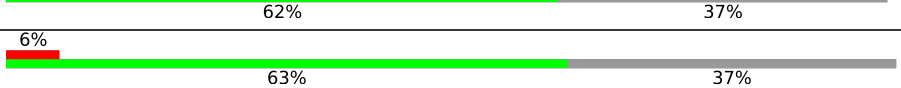
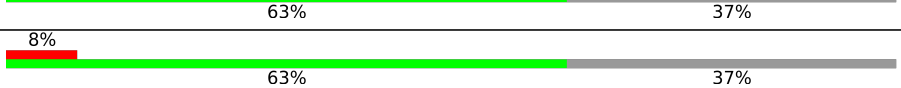
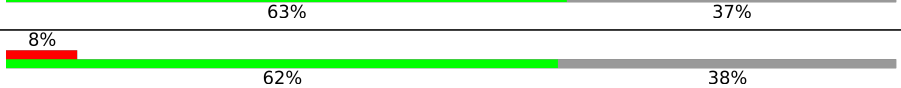
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	b7	38	13% 71% 26%
1	c	38	11% 89% 11%
1	d	38	11% 89% 11%
1	d1	38	13% 89% 11%
1	d2	38	16% 89% 11%
1	d5	38	21% 87% 11%
1	d6	38	11% 87% 11%
1	d7	38	11% 87% 11%
1	e	38	21% 89% 11%
1	e1	38	21% 71% 26%
1	e2	38	26% 71% 26%
1	e5	38	18% 71% 26%
1	e6	38	26% 71% 26%
1	e7	38	18% 71% 26%
1	f	38	21% 87% 11%
1	g	38	29% 76% 13% 11%
2	a	202	54% 84% 13%
2	b	202	55% 94%
2	h	202	59% 83% 14%
2	i	202	62% 92%
2	j	202	72% 95%
2	k	202	56% 83% 14%
2	l	202	56% 85% 14%
2	m	202	55% 94% 5%
2	n	202	55% 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	o	202	
2	p	202	
2	q	202	
3	AM	141	
3	AN	141	
3	AO	141	
3	AP	141	
3	H	141	
3	I	141	
4	f1	217	
4	f2	217	
4	f5	217	
4	f6	217	
4	f7	217	
5	g1	465	
5	g2	465	
5	g5	465	
5	g6	465	
5	g7	465	
5	h1	465	
5	h2	465	
5	h5	465	
5	h6	465	
5	h7	465	
5	k1	465	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	k2	465	8% 62% 38%
5	k5	465	6% 62% 38%
5	k6	465	7% 62% 38%
5	k7	465	7% 62% 38%
5	n1	465	7% 62% 37%
5	n2	465	5% 62% 37%
5	n5	465	7% 62% 37%
5	n6	465	8% 63% 37%
5	n7	465	5% 63% 37%
5	o1	465	8% 62% 37%
5	o2	465	10% 62% 37%
5	o5	465	9% 62% 37%
5	o6	465	10% 62% 37%
5	o7	465	6% 61% 37%
5	r1	465	6% 63% 37%
5	r2	465	5% 62% 37%
5	r5	465	8% 63% 37%
5	r6	465	9% 63% 37%
5	r7	465	6% 62% 37%
6	l1	137	5% 99%
6	l2	137	7% 99%
6	l5	137	98%
6	l6	137	7% 100%
6	l7	137	7% 98%
6	m1	137	6% 100%

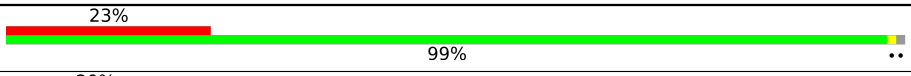
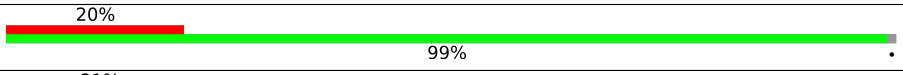
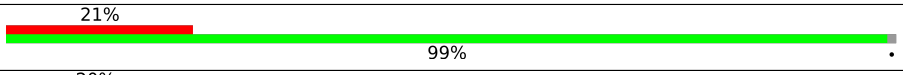
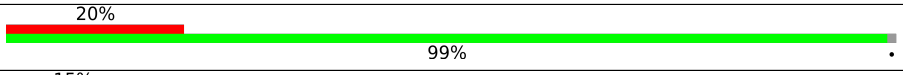
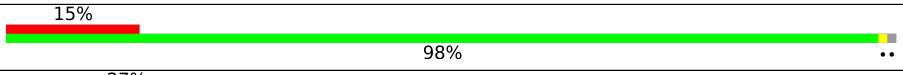
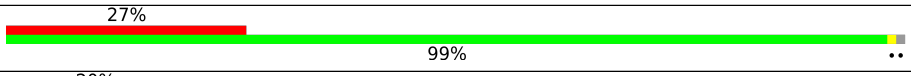
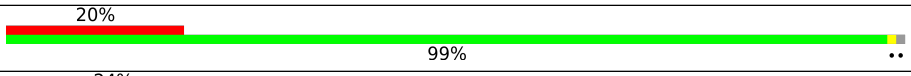
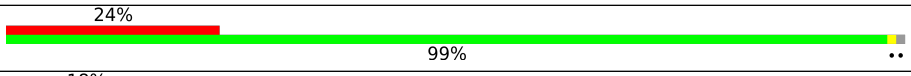
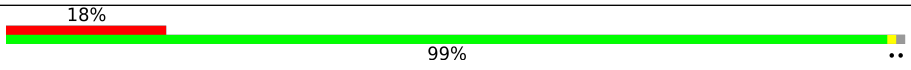
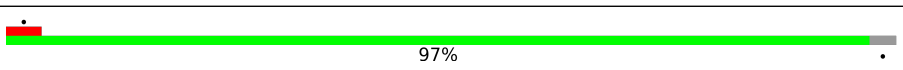
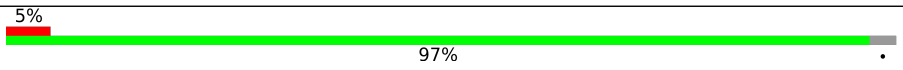
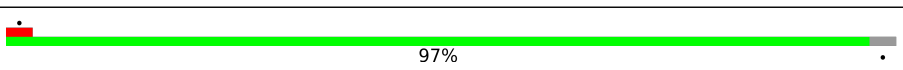
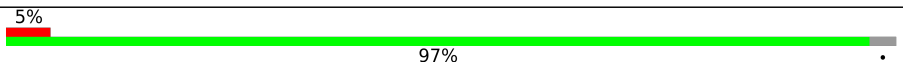
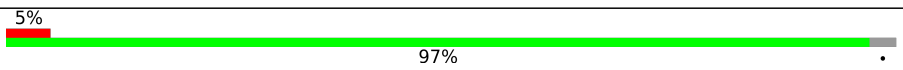
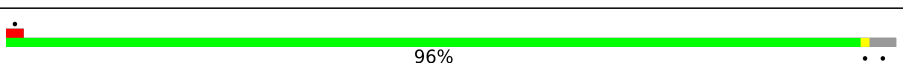
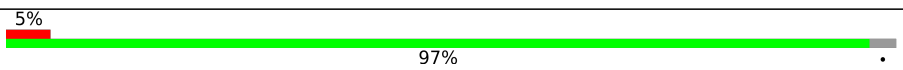
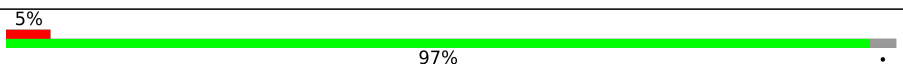
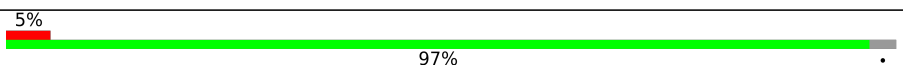
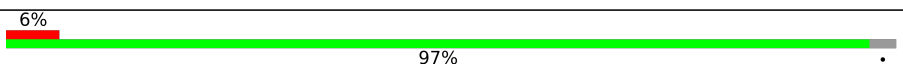
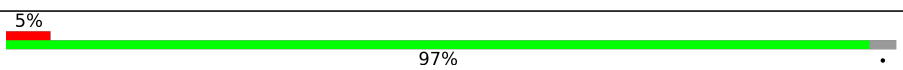
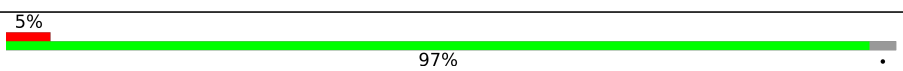
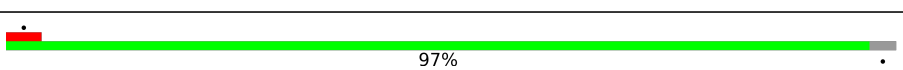
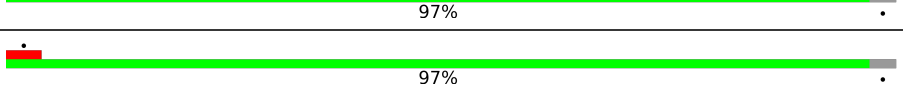
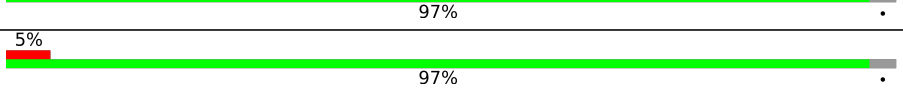
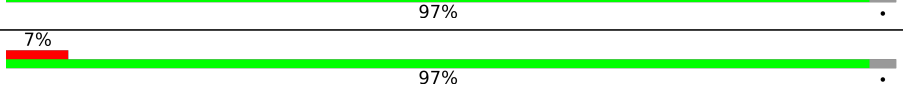
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	m2	137	12% 100%
6	m5	137	6% 100%
6	m6	137	6% 100%
6	m7	137	10% 100%
6	p1	137	14% 100%
6	p2	137	16% 99%
6	p5	137	18% 100%
6	p6	137	16% 99%
6	p7	137	12% 99%
6	q1	137	18% 100%
6	q2	137	12% 100%
6	q5	137	19% 100%
6	q6	137	10% 99%
6	q7	137	18% 99%
6	s1	137	9% 100%
6	s2	137	9% 100%
6	s5	137	10% 100%
6	s6	137	11% 100%
6	s7	137	10% 100%
6	t1	137	19% 99%
6	t2	137	12% 99%
6	t5	137	14% 99%
6	t6	137	15% 97%
6	t7	137	13% 99%
6	u1	137	16% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	u2	137	
6	u5	137	
6	u6	137	
6	u7	137	
6	v1	137	
6	v2	137	
6	v5	137	
6	v6	137	
6	v7	137	
7	03	230	
7	13	230	
7	23	230	
7	33	230	
7	43	230	
7	53	230	
7	63	230	
7	73	230	
7	83	230	
7	93	230	
7	A3	230	
7	B3	230	
7	C3	230	
7	D3	230	
7	E3	230	
7	F3	230	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	G3	230	96%
7	J3	230	5% 97%
7	K3	230	14% 100%
7	L3	230	13% 97%
7	M3	230	6% 97%
7	N3	230	15% 100%
7	O3	230	8% 97%
7	P3	230	8% 97%
7	Q3	230	10% 99%
7	R3	230	10% 97%
7	S3	230	6% 97%
7	T3	230	8% 97%
7	U3	230	11% 96%
7	V3	230	8% 96%
7	W3	230	12% 99%
7	X3	230	10% 97%
7	Y3	230	5% 97%
7	Z3	230	97%
7	a3	230	97%
7	b3	230	97%
7	c3	230	97%
7	d3	230	5% 97%
7	e3	230	5% 97%
7	f3	230	5% 93%
7	g3	230	96%

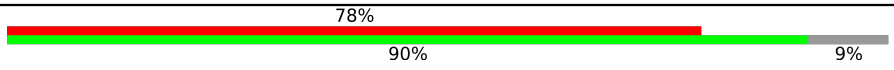
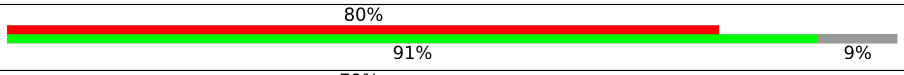
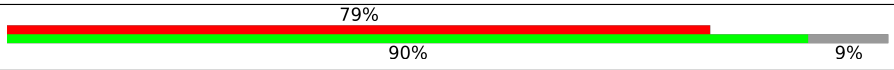
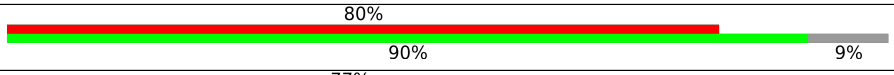
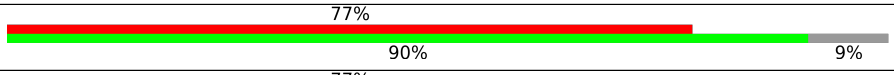
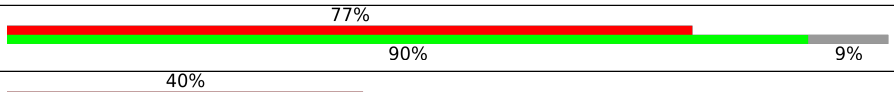
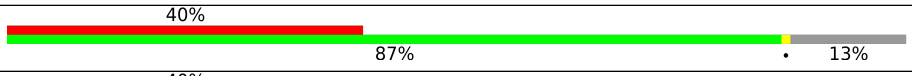
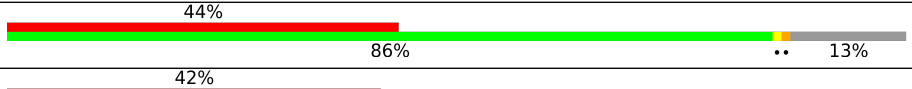
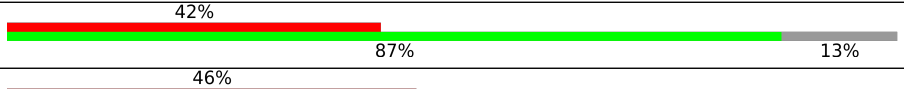
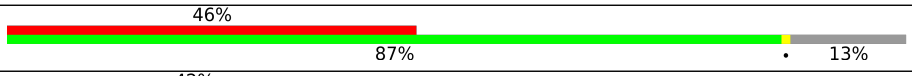
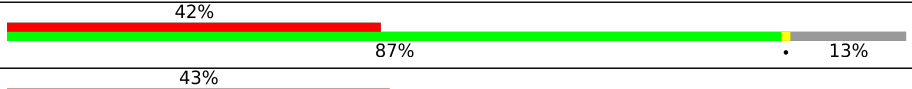
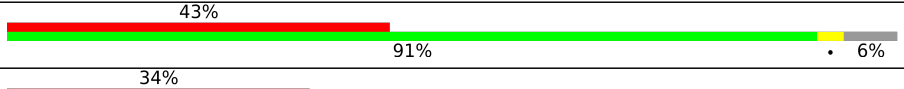
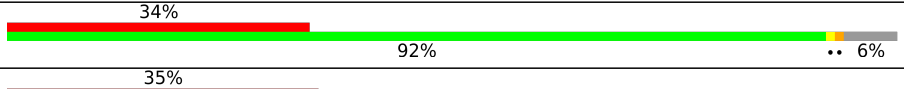
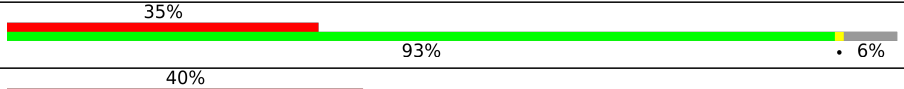
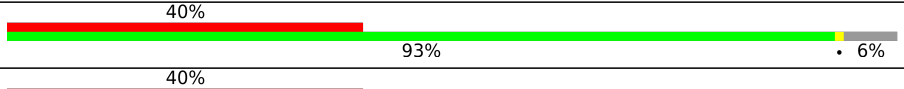
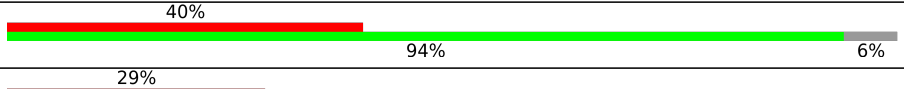
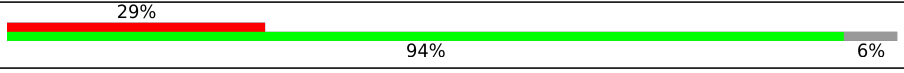
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	h3	230	5% 97%
7	i3	230	5% 97%
7	j3	230	97%
7	k3	230	5% 97%
7	l3	230	5% 97%
7	m3	230	97%
7	n3	230	97%
7	o3	230	97%
7	p3	230	97%
7	q3	230	5% 97%
7	r3	230	97%
7	s3	230	97%
7	t3	230	97%
7	u3	230	97%
7	v3	230	97%
7	w3	230	97%
7	x3	230	97%
7	y3	230	97%
7	z3	230	97%
8	AA	420	79% 90% 9%
8	AB	420	74% 91% 9%
8	AC	420	73% 90% 9%
8	AD	420	76% 91% 9%
8	AE	420	78% 90% 9%
8	AF	420	76% 90% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	AG	420	
8	AH	420	
8	AI	420	
8	AJ	420	
8	AK	420	
8	AL	420	
9	AQ	178	
9	AR	178	
9	AS	178	
9	AT	178	
9	AW	178	
9	AX	178	
10	AU	136	
10	AV	136	
10	AY	136	
10	AZ	136	
10	Aa	136	
10	Ab	136	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 287884 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	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		
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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
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		
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		

- Molecule 2 is a protein called Neck 1 protein, gp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	176	Total	C	N	O	S	0	0
			1357	862	243	248	4		
2	b	195	Total	C	N	O	S	0	0
			1509	955	269	279	6		
2	l	173	Total	C	N	O	S	0	0
			1333	848	239	242	4		
2	n	195	Total	C	N	O	S	0	0
			1509	955	269	279	6		
2	o	173	Total	C	N	O	S	0	0
			1333	848	239	242	4		
2	p	173	Total	C	N	O	S	0	0
			1333	848	239	242	4		
2	q	173	Total	C	N	O	S	0	0
			1333	848	239	242	4		
2	h	173	Total	C	N	O	S	0	0
			1333	848	239	242	4		
2	i	193	Total	C	N	O	S	0	0
			1487	943	261	277	6		
2	j	195	Total	C	N	O	S	0	0
			1509	955	269	279	6		
2	k	173	Total	C	N	O	S	0	0
			1333	848	239	242	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	192	Total	C	N	O	S	0	0
			1486	939	266	275	6		

- Molecule 3 is a protein called Neck 2 protein, gp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	I	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	AM	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	AP	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	AN	125	Total	C	N	O	S	0	0
			997	621	183	185	8		
3	AO	125	Total	C	N	O	S	0	0
			997	621	183	185	8		

- Molecule 4 is a protein called Linking protein 1, gp16.

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

- Molecule 5 is a protein called Major capsid protein, gp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g1	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	h1	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	k1	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	n1	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	o1	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	r1	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	g2	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	h2	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	k2	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
5	n2	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	o2	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	r2	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	g5	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	h5	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	k5	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
5	n5	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	o5	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	r5	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	g6	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	h6	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	k6	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
5	n6	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	o6	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	r6	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g7	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	h7	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	k7	288	Total	C	N	O	S	0	0
			2257	1430	386	425	16		
5	n7	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	o7	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		
5	r7	291	Total	C	N	O	S	0	0
			2286	1452	389	429	16		

- Molecule 6 is a protein called Minor capsid protein, gp10.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	t2	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	u2	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
6	v2	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
6	l5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	m5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	p5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	q5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	s5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	t5	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	u5	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
6	v5	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
6	l6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	m6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	p6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	q6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	s6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	t6	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	u6	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
6	v6	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
6	l7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	m7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	p7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	q7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	s7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	t7	137	Total	C	N	O	S	0	0
			1023	655	160	201	7		
6	u7	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		
6	v7	136	Total	C	N	O	S	0	0
			1011	649	156	199	7		

- Molecule 7 is a protein called Collar sheath protein, gp13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	K3	230	Total	C	N	O	S	0	0
			1723	1090	287	337	9		
7	L3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	M3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	N3	230	Total	C	N	O	S	0	0
			1723	1090	287	337	9		
7	O3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	P3	222	Total	C	N	O	S	0	0
			1673	1062	278	325	8		
7	Q3	230	Total	C	N	O	S	0	0
			1723	1090	287	337	9		
7	R3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	S3	222	Total	C	N	O	S	0	0
			1673	1062	278	325	8		
7	T3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	U3	221	Total	C	N	O	S	0	0
			1668	1059	277	324	8		
7	V3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W3	230	Total	C	N	O	S	0	0
			1723	1090	287	337	9		
7	X3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	Y3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	Z3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	a3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	b3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	c3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	d3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	e3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	f3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	g3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	h3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	i3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	j3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	k3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	l3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	m3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	n3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	o3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	p3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	q3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	r3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	s3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	t3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	u3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	v3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	w3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	x3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	y3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	z3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	13	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	23	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	33	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	43	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	53	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	63	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	73	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	83	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	93	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	03	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	A3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	B3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	D3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	E3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	F3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		
7	G3	223	Total	C	N	O	S	0	0
			1679	1065	279	327	8		

- Molecule 8 is a protein called Portal protein, gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AA	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AB	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AC	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AD	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AE	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AF	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AG	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AH	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AI	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AJ	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AK	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		
8	AL	381	Total	C	N	O	S	0	0
			2938	1860	504	560	14		

- Molecule 9 is a protein called Tail-terminator protein, gp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AQ	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
9	AR	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
9	AS	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
9	AT	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
9	AW	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		
9	AX	155	Total	C	N	O	S	0	0
			1251	798	207	243	3		

- Molecule 10 is a protein called Tail-tube, gp21.

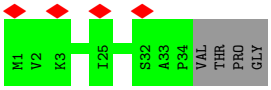
Mol	Chain	Residues	Atoms					AltConf	Trace
10	AU	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
10	AZ	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
10	AV	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
10	Aa	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
10	AY	128	Total	C	N	O	S	0	0
			977	606	162	202	7		
10	Ab	128	Total	C	N	O	S	0	0
			977	606	162	202	7		

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.

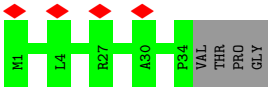
• Molecule 1: Linking protein 2, gp128

Chain c:



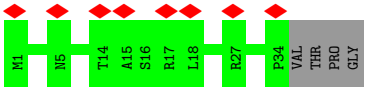
• Molecule 1: Linking protein 2, gp128

Chain d:



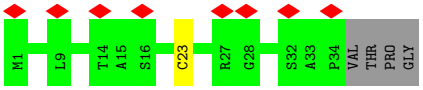
• Molecule 1: Linking protein 2, gp128

Chain e:



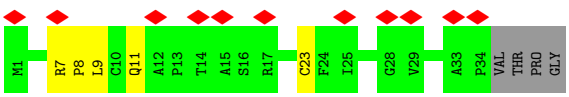
• Molecule 1: Linking protein 2, gp128

Chain f:



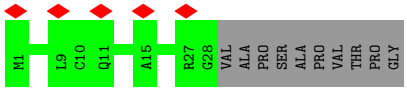
• Molecule 1: Linking protein 2, gp128

Chain g:



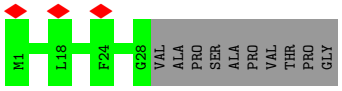
• Molecule 1: Linking protein 2, gp128

Chain a1:



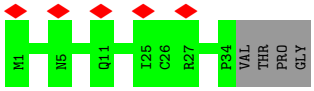
• Molecule 1: Linking protein 2, gp128

Chain b1:



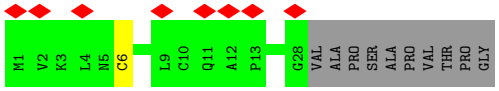
• Molecule 1: Linking protein 2, gp128

Chain d1:



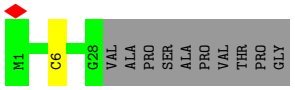
• Molecule 1: Linking protein 2, gp128

Chain e1:



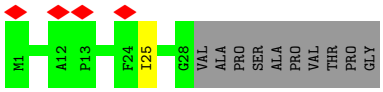
• Molecule 1: Linking protein 2, gp128

Chain a2:



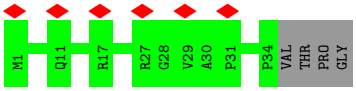
• Molecule 1: Linking protein 2, gp128

Chain b2:



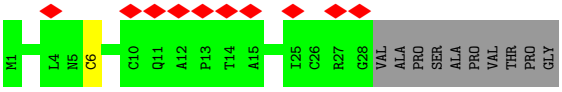
• Molecule 1: Linking protein 2, gp128

Chain d2:



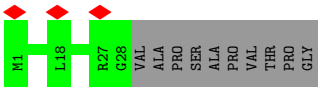
• Molecule 1: Linking protein 2, gp128

Chain e2:



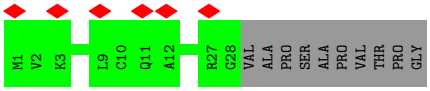
• Molecule 1: Linking protein 2, gp128

Chain a5:



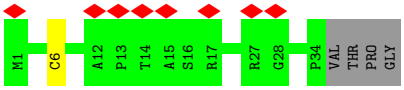
• Molecule 1: Linking protein 2, gp128

Chain b5:



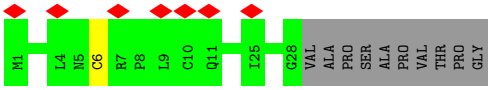
• Molecule 1: Linking protein 2, gp128

Chain d5:



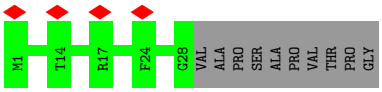
• Molecule 1: Linking protein 2, gp128

Chain e5:



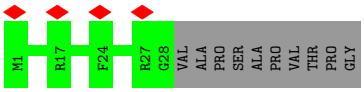
• Molecule 1: Linking protein 2, gp128

Chain a6:



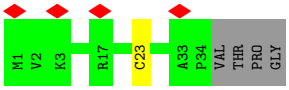
• Molecule 1: Linking protein 2, gp128

Chain b6:



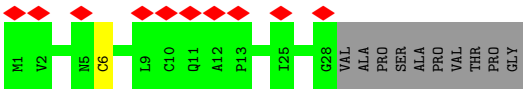
• Molecule 1: Linking protein 2, gp128

Chain d6:



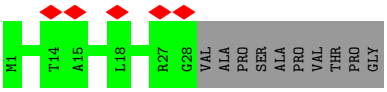
• Molecule 1: Linking protein 2, gp128

Chain e6:



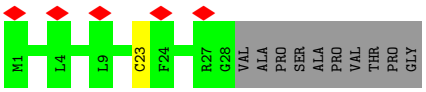
• Molecule 1: Linking protein 2, gp128

Chain a7:



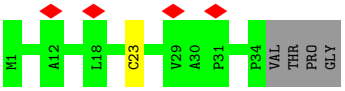
• Molecule 1: Linking protein 2, gp128

Chain b7:



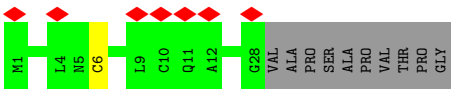
• Molecule 1: Linking protein 2, gp128

Chain d7:



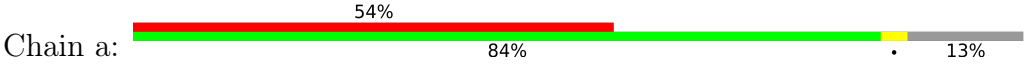
• Molecule 1: Linking protein 2, gp128

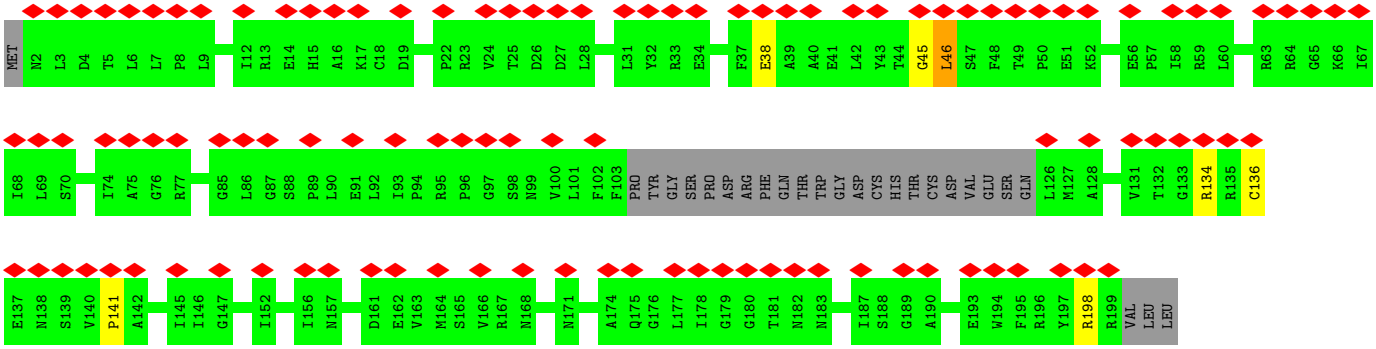
Chain e7:



• Molecule 2: Neck 1 protein, gp14

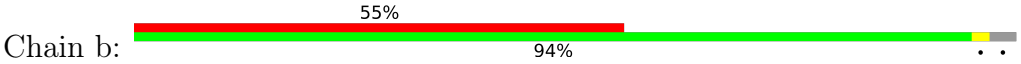
Chain a:

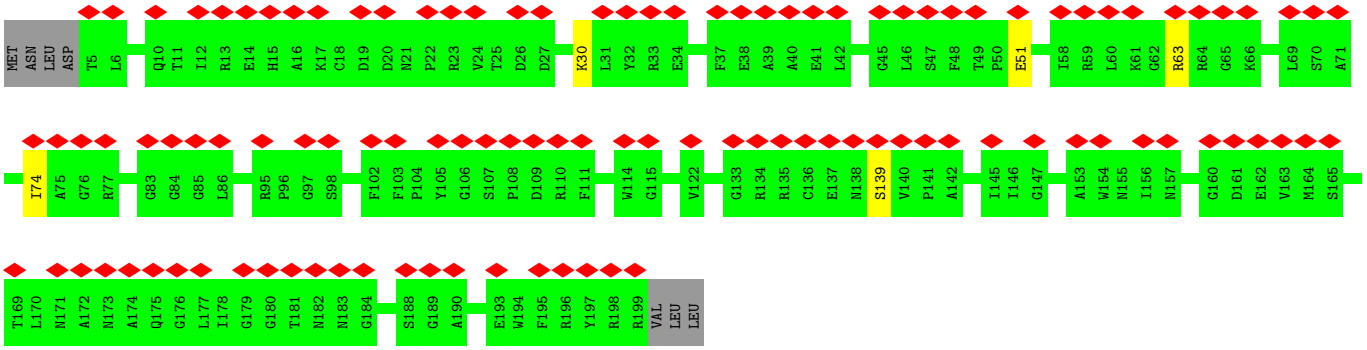




• Molecule 2: Neck 1 protein, gp14

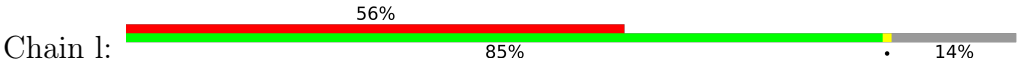
Chain b:

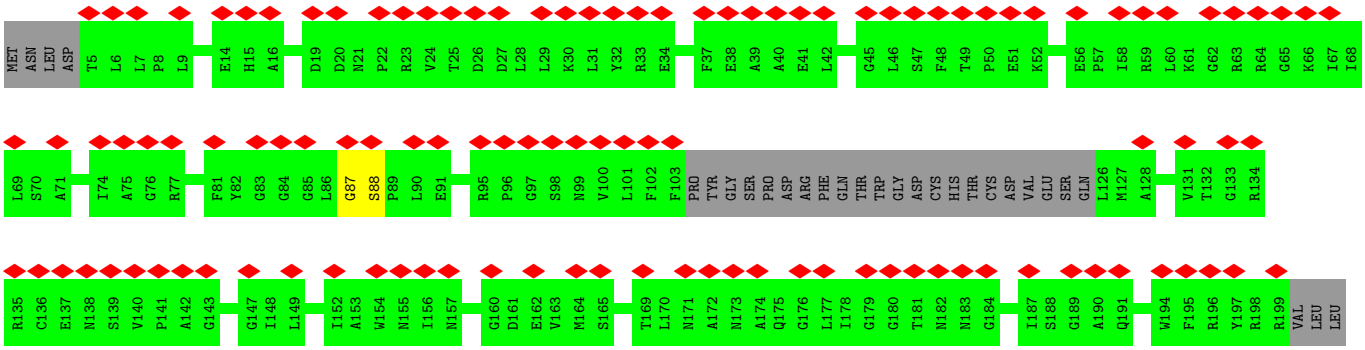




• Molecule 2: Neck 1 protein, gp14

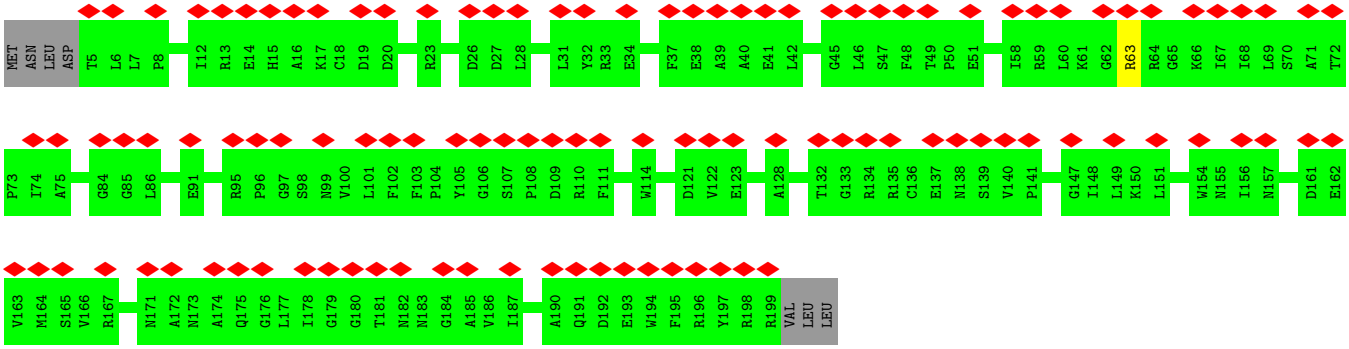
Chain l:





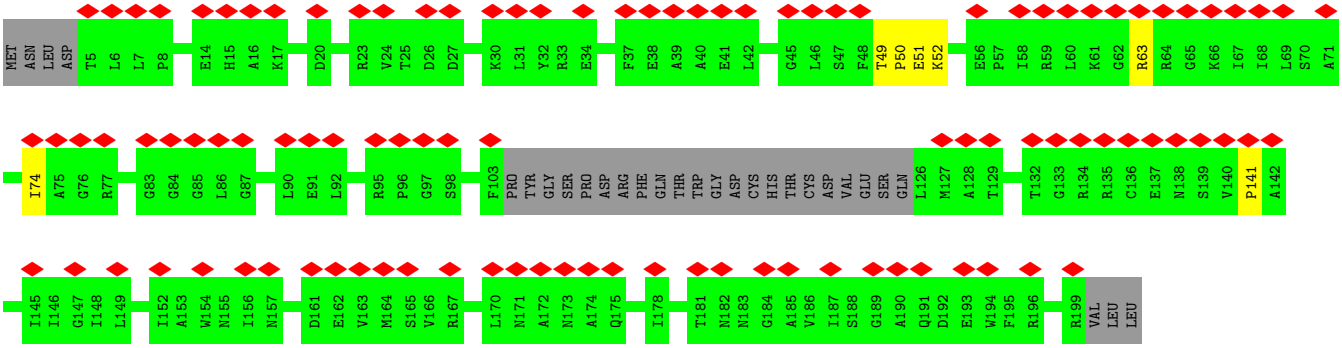
• Molecule 2: Neck 1 protein, gp14

Chain n:



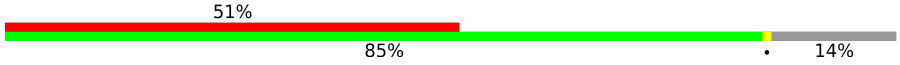
• Molecule 2: Neck 1 protein, gp14

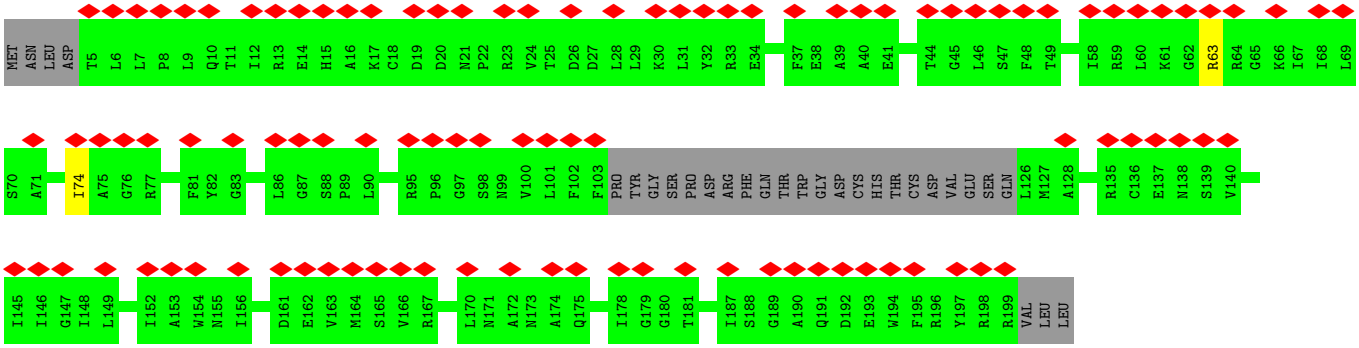
Chain o:



• Molecule 2: Neck 1 protein, gp14

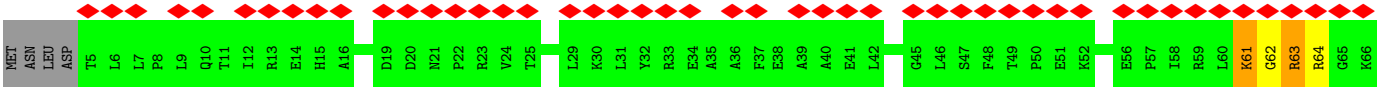
Chain p:

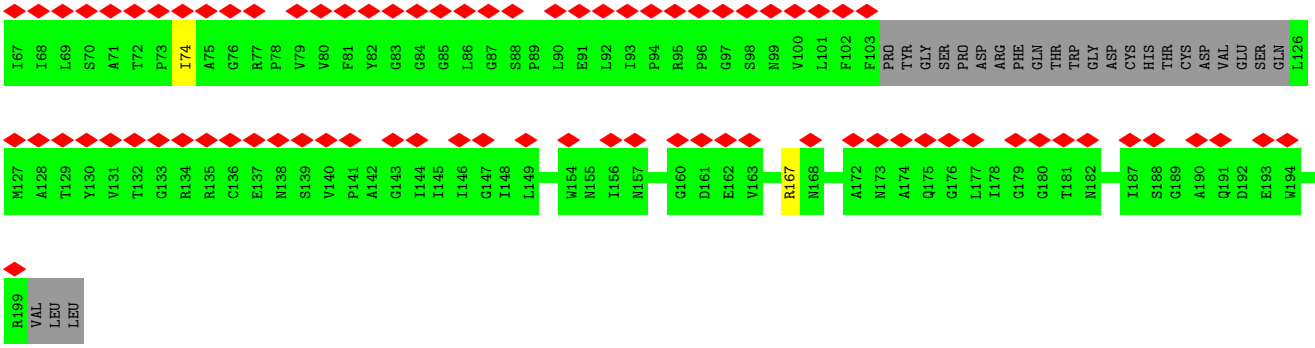




• Molecule 2: Neck 1 protein, gp14

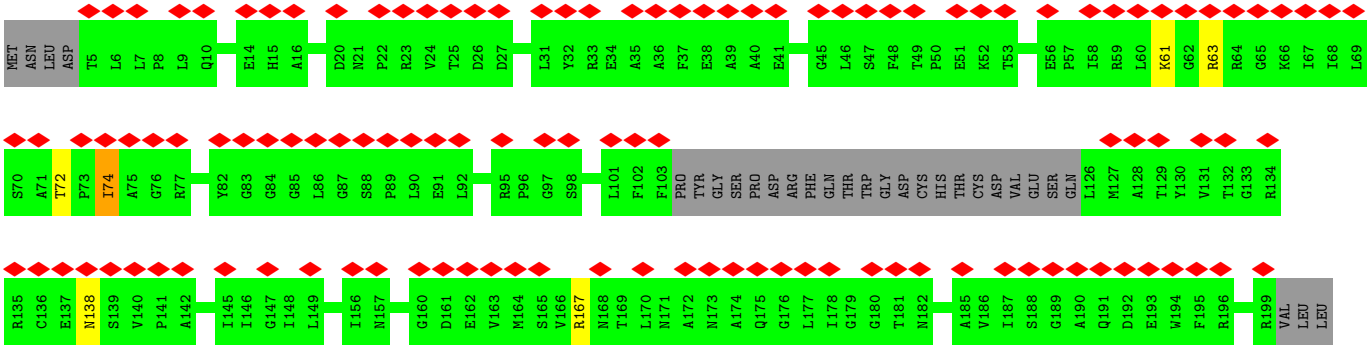
Chain q:





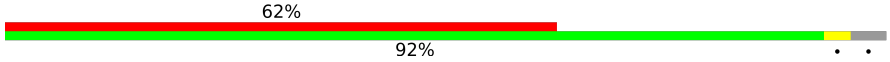
• Molecule 2: Neck 1 protein, gp14

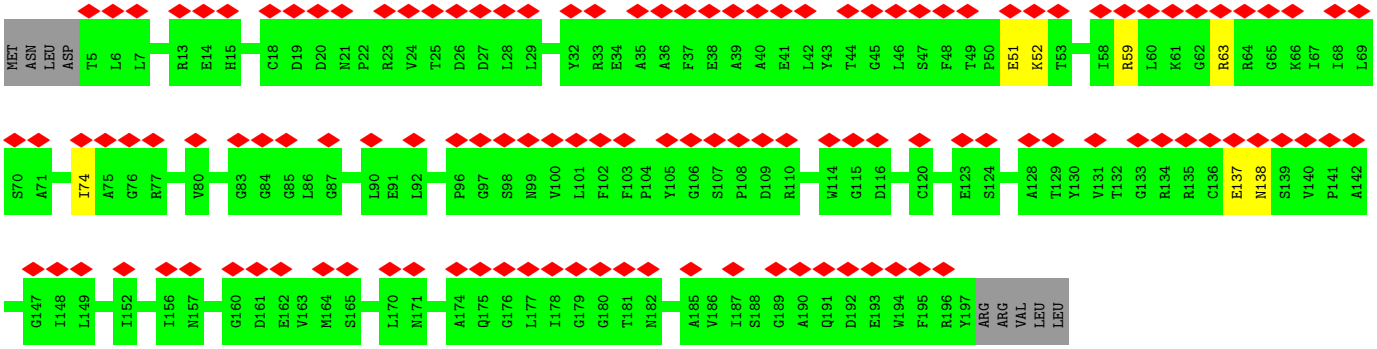
Chain h:



• Molecule 2: Neck 1 protein, gp14

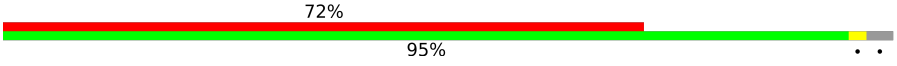
Chain i:

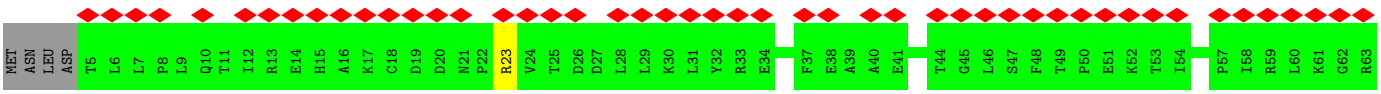


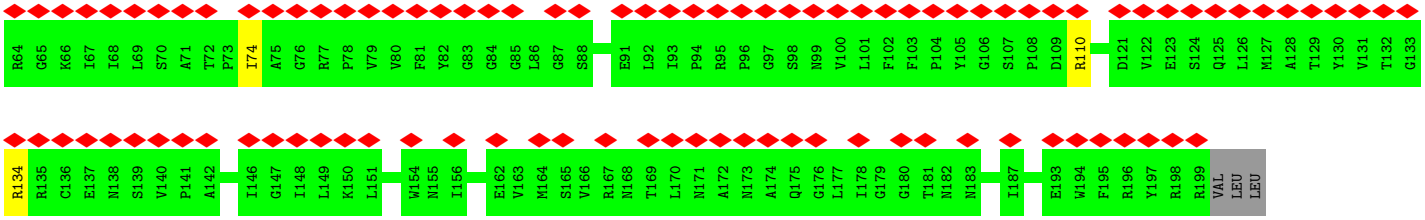


• Molecule 2: Neck 1 protein, gp14

Chain j:





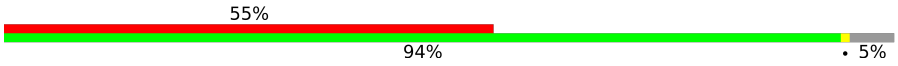


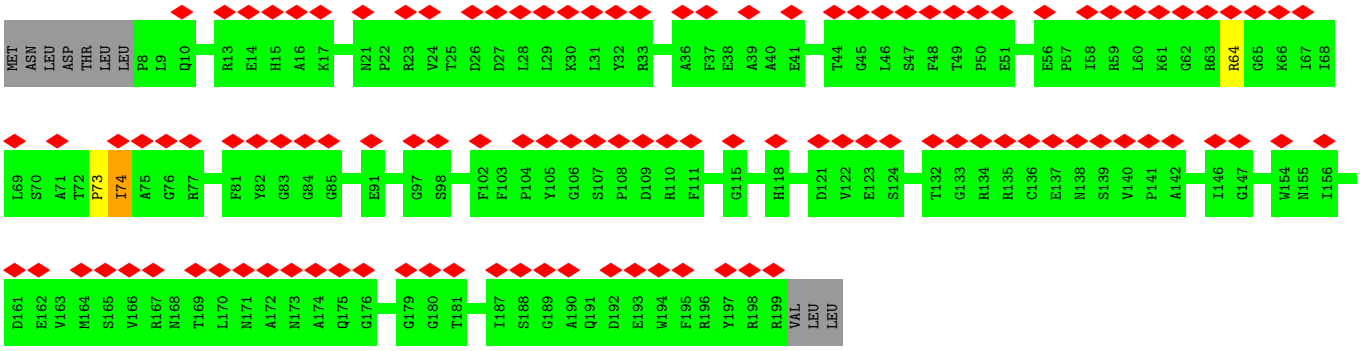
• Molecule 2: Neck 1 protein, gp14

Chain k:

• Molecule 2: Neck 1 protein, gp14

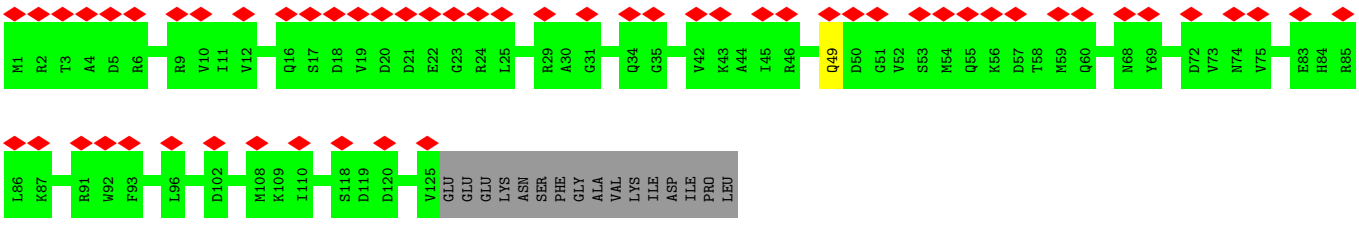
Chain m:





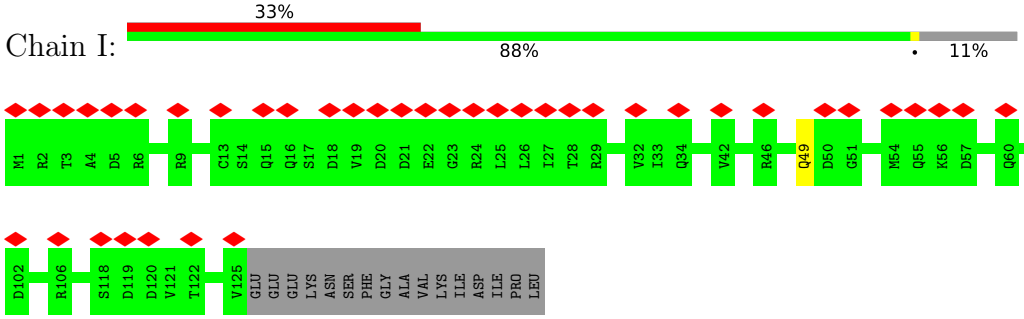
• Molecule 3: Neck 2 protein, gp15

Chain H:



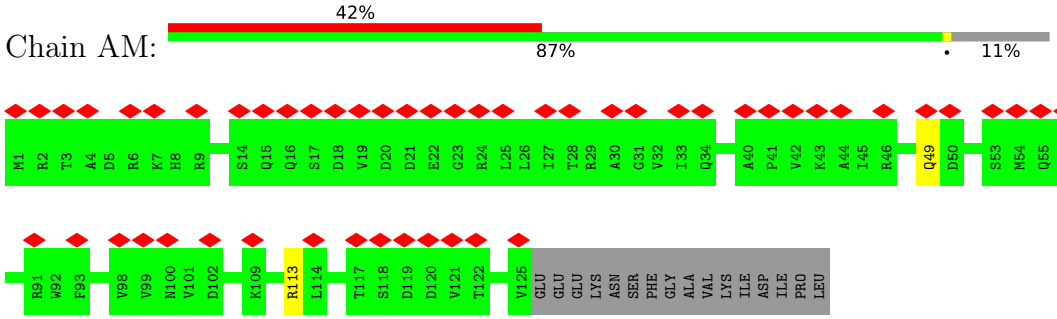
• Molecule 3: Neck 2 protein, gp15

Chain I:



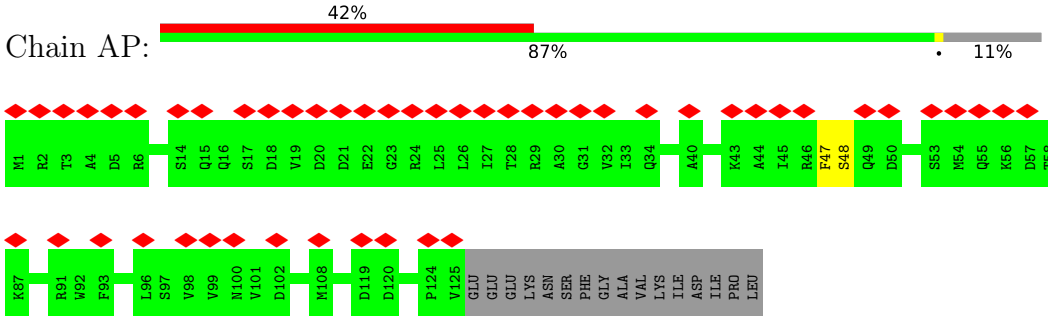
• Molecule 3: Neck 2 protein, gp15

Chain AM:



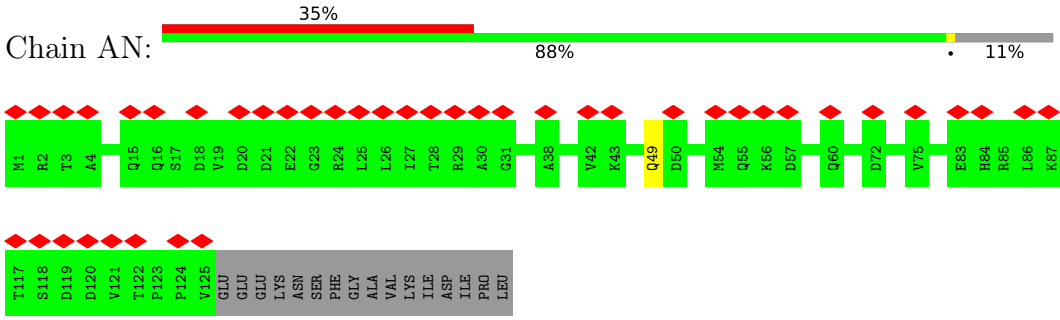
• Molecule 3: Neck 2 protein, gp15

Chain AP:



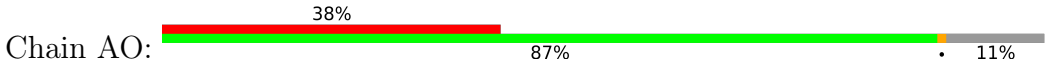
• Molecule 3: Neck 2 protein, gp15

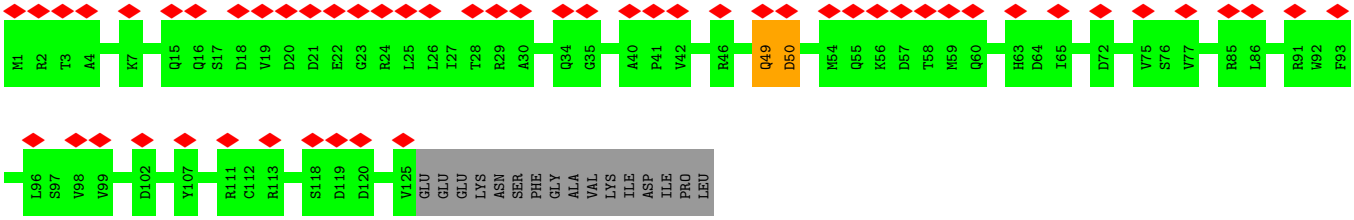
Chain AN:



• Molecule 3: Neck 2 protein, gp15

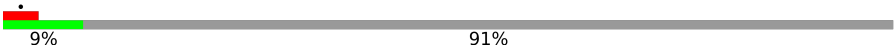
Chain AO:

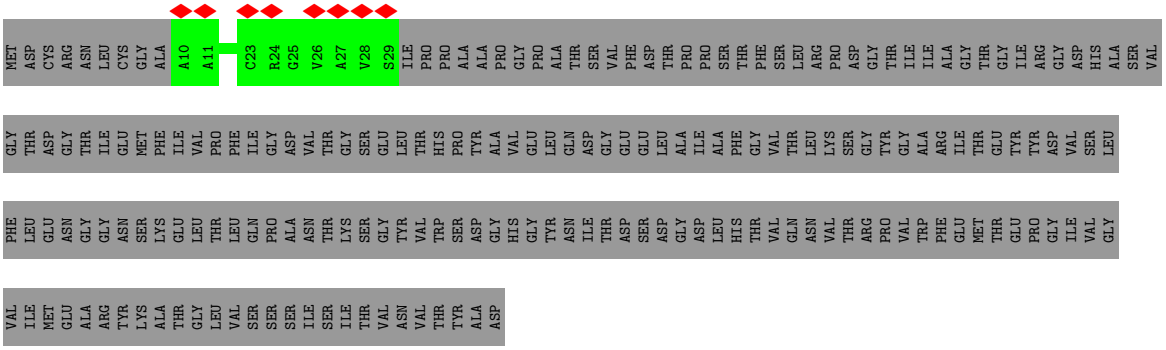




• Molecule 4: Linking protein 1, gp16

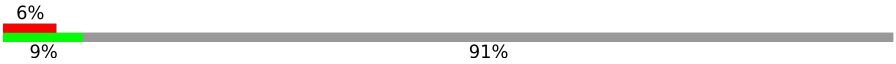
Chain f1:

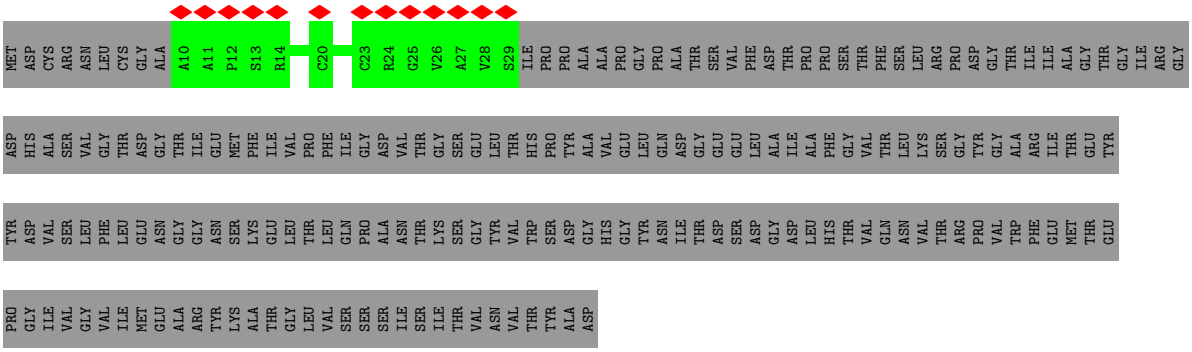




• Molecule 4: Linking protein 1, gp16

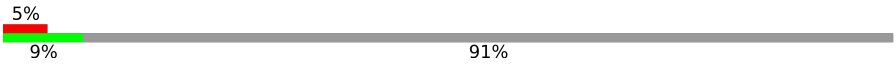
Chain f2:

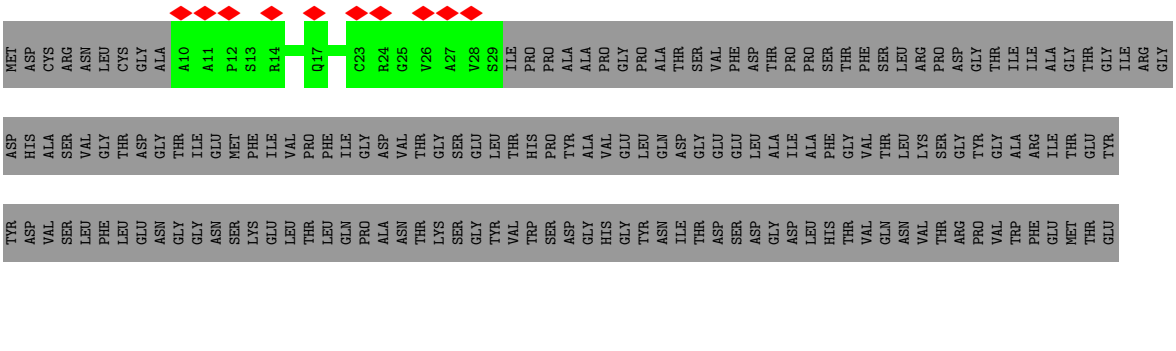


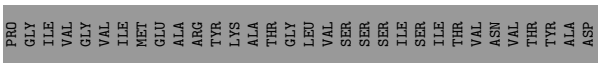


• Molecule 4: Linking protein 1, gp16

Chain f5:

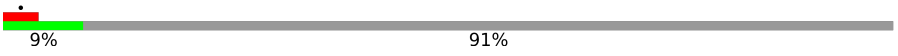


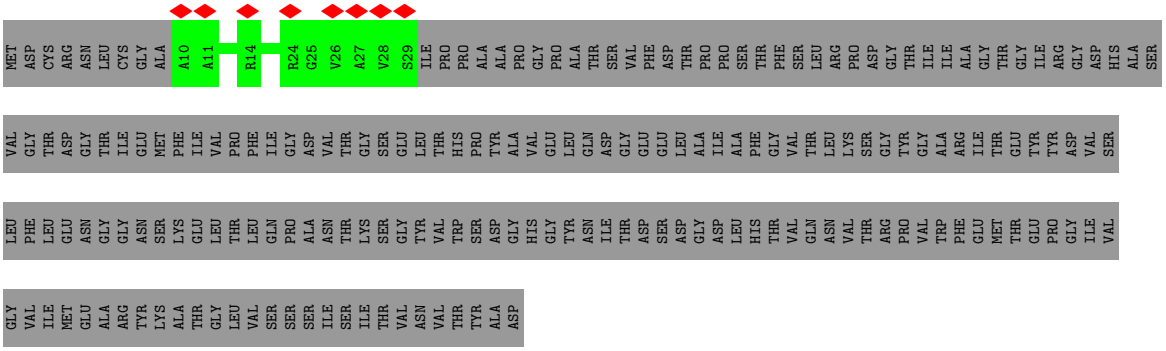




• Molecule 4: Linking protein 1, gp16

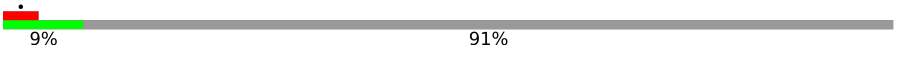
Chain f6:

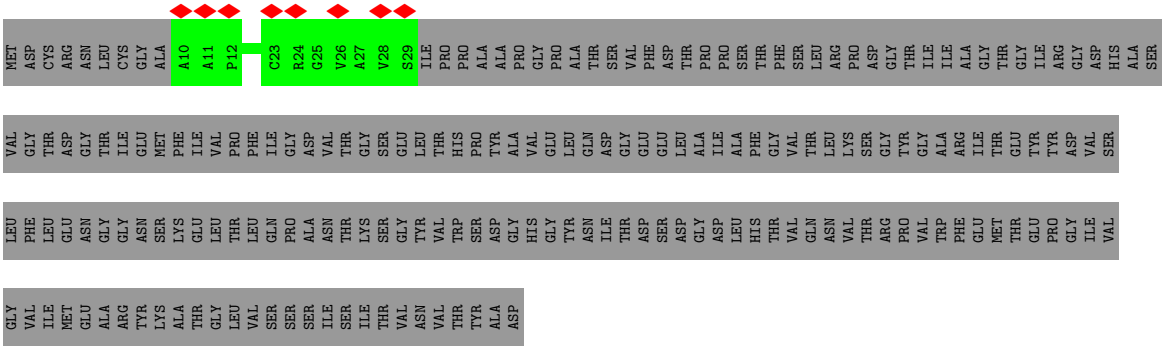




• Molecule 4: Linking protein 1, gp16

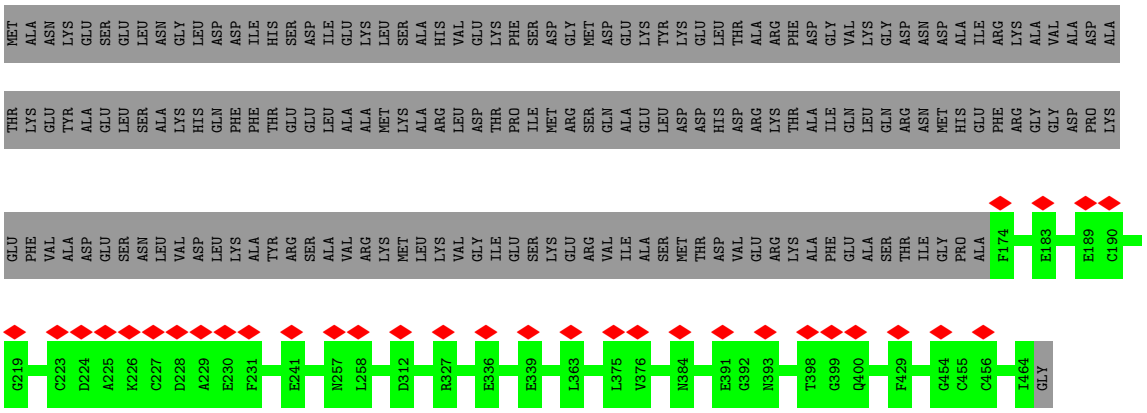
Chain f7:





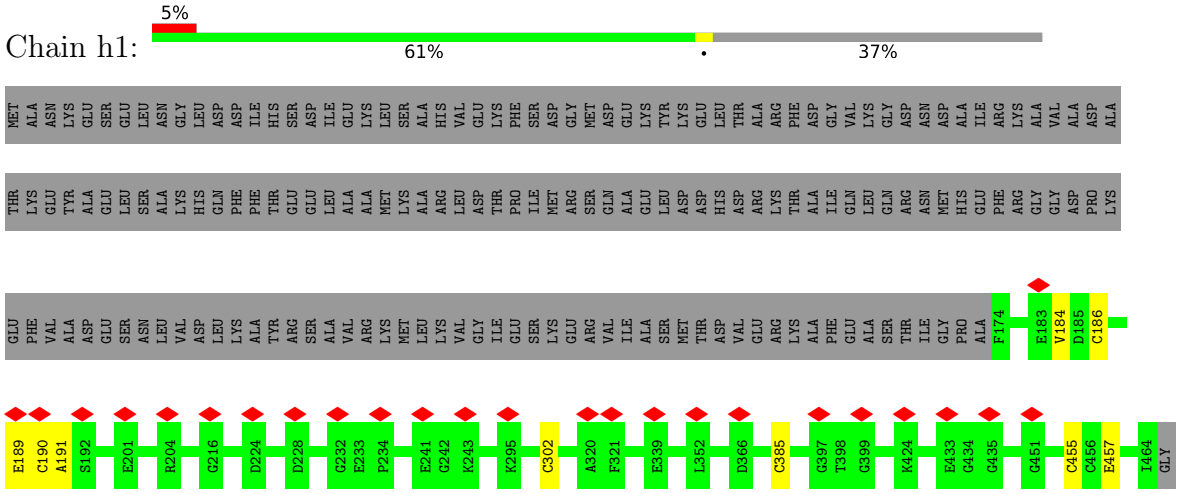
• Molecule 5: Major capsid protein, gp9

Chain g1:



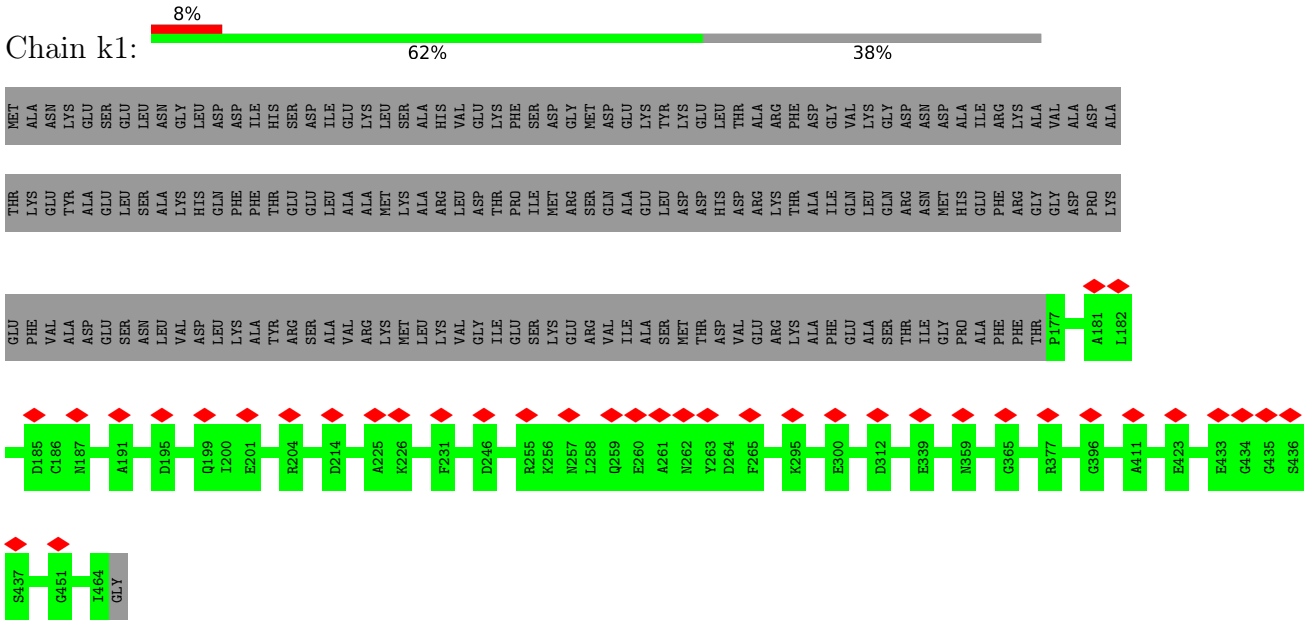
• Molecule 5: Major capsid protein, gp9

Chain h1:



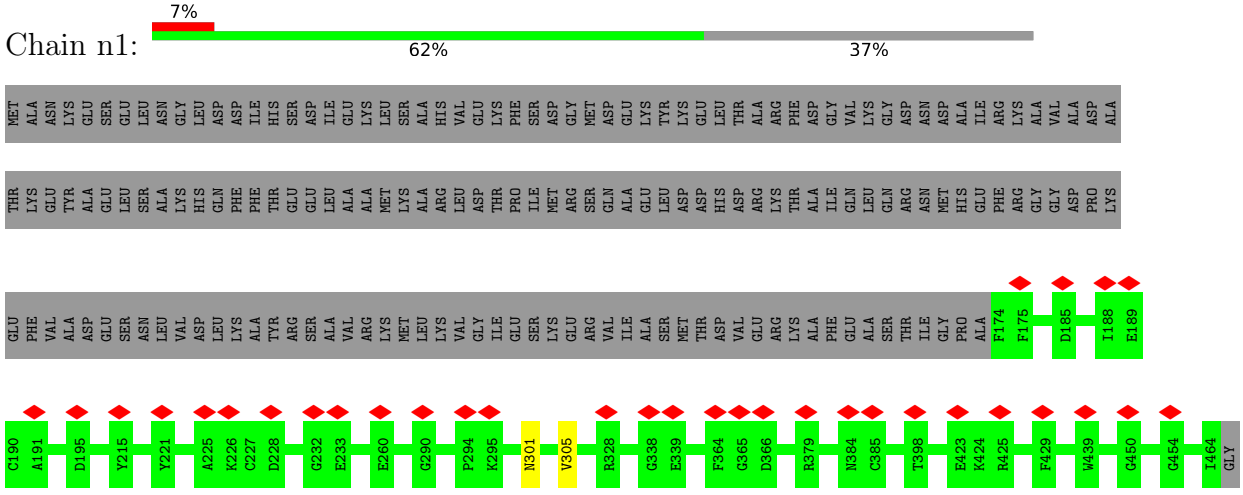
• Molecule 5: Major capsid protein, gp9

Chain k1:



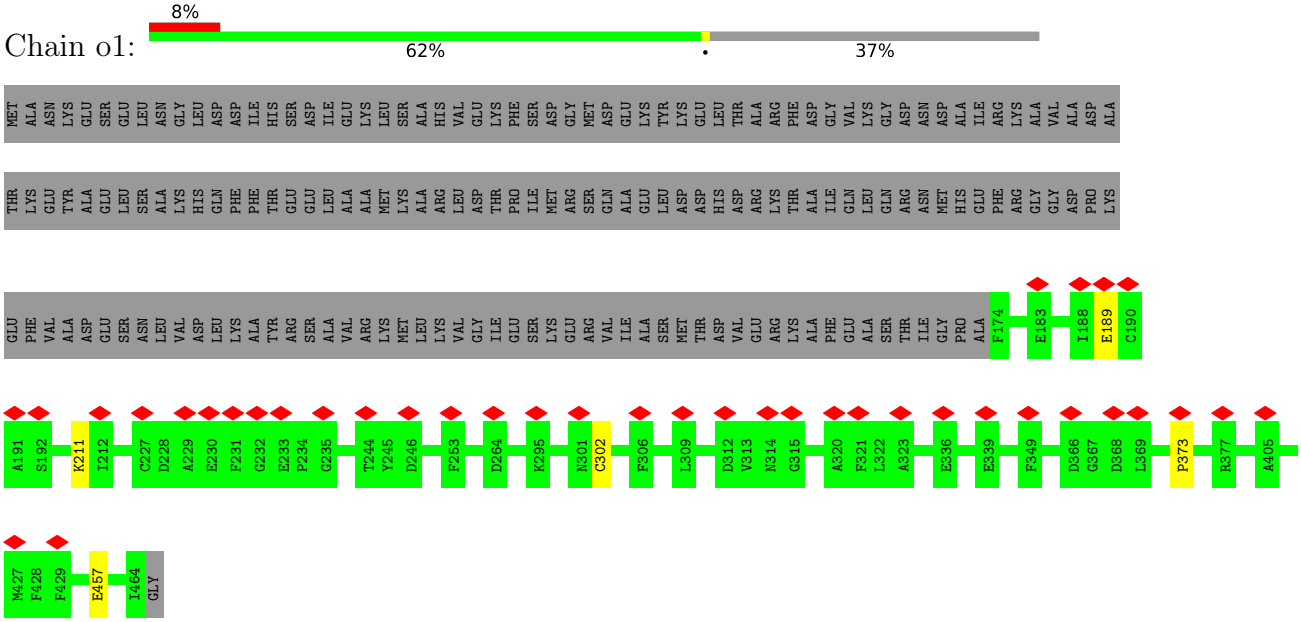
• Molecule 5: Major capsid protein, gp9

Chain n1:



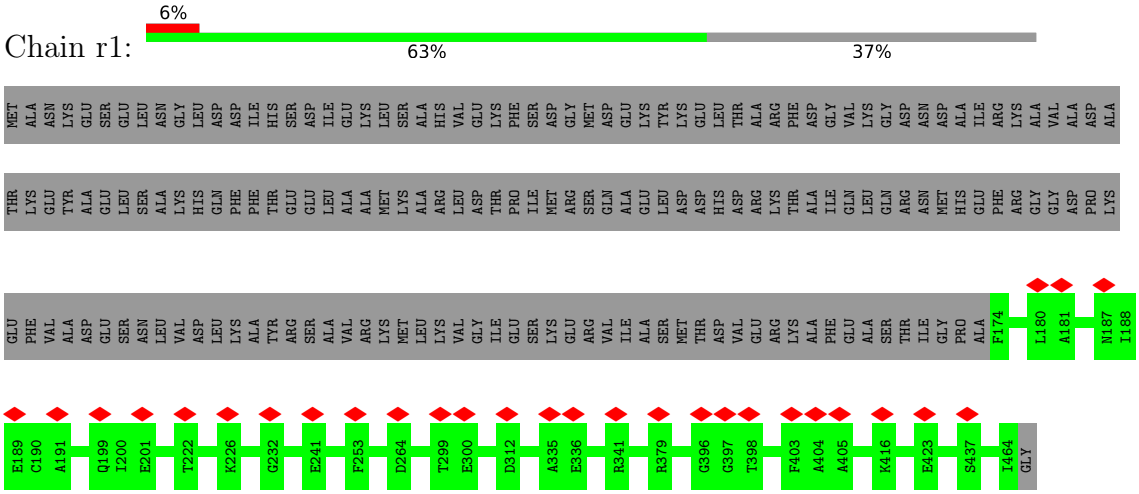
• Molecule 5: Major capsid protein, gp9

Chain o1:



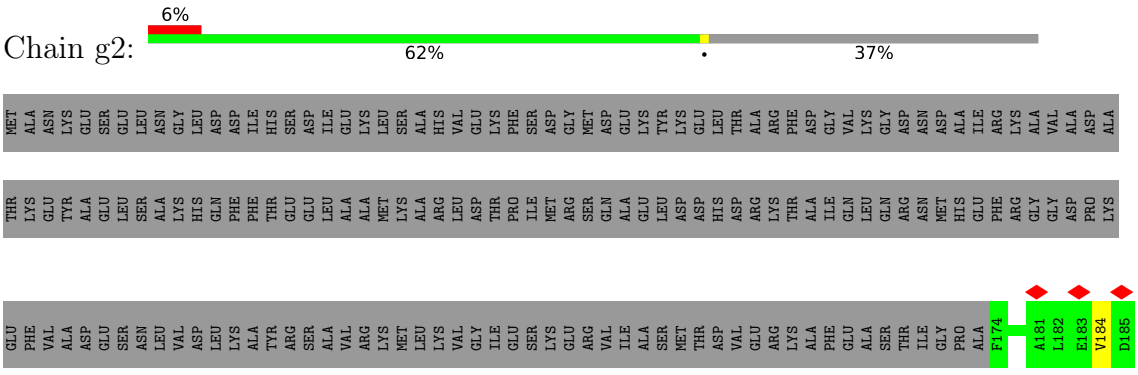
• Molecule 5: Major capsid protein, gp9

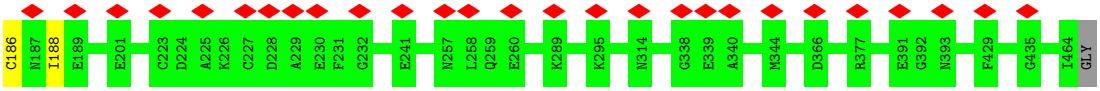
Chain r1:



• Molecule 5: Major capsid protein, gp9

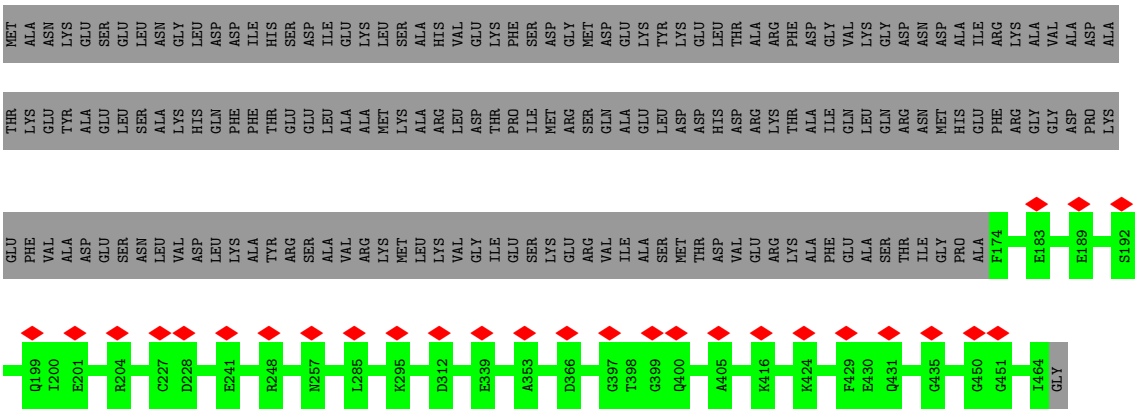
Chain g2:





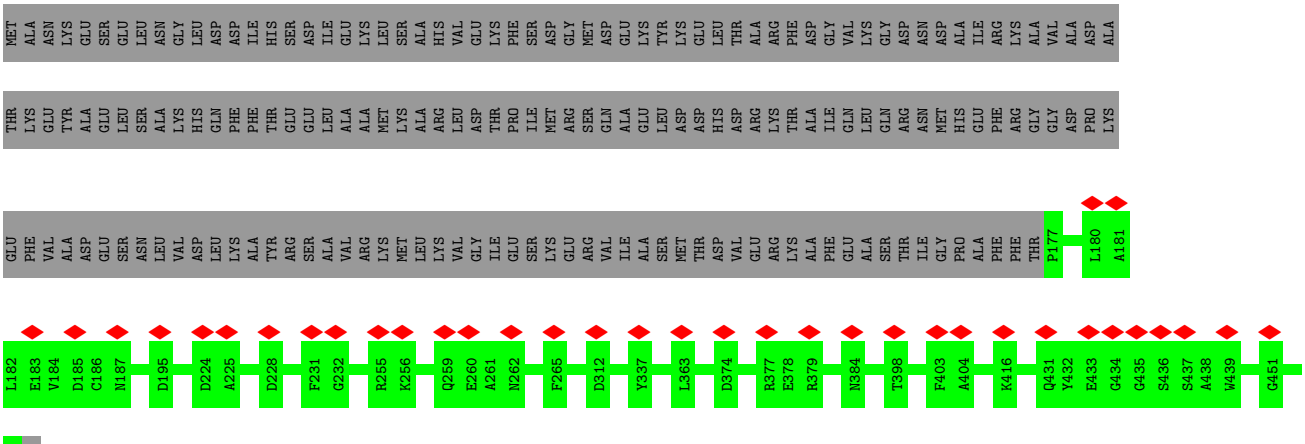
• Molecule 5: Major capsid protein, gp9

Chain h2:



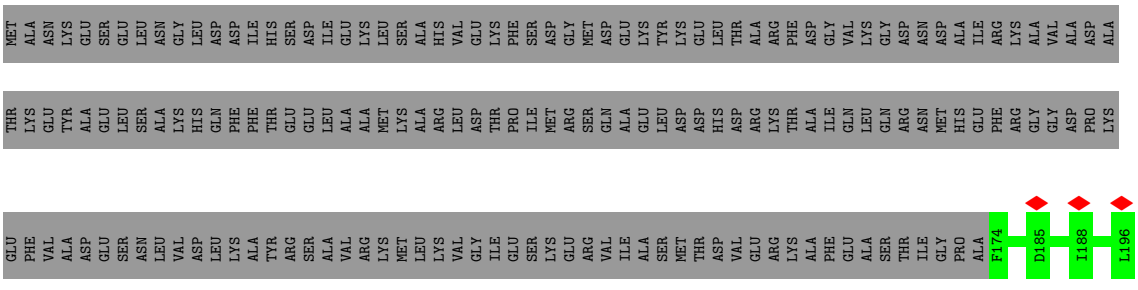
• Molecule 5: Major capsid protein, gp9

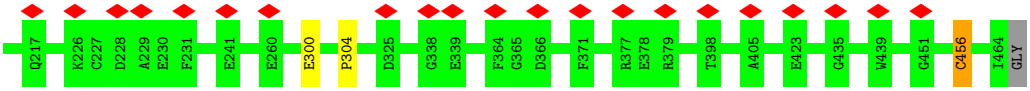
Chain k2:



• Molecule 5: Major capsid protein, gp9

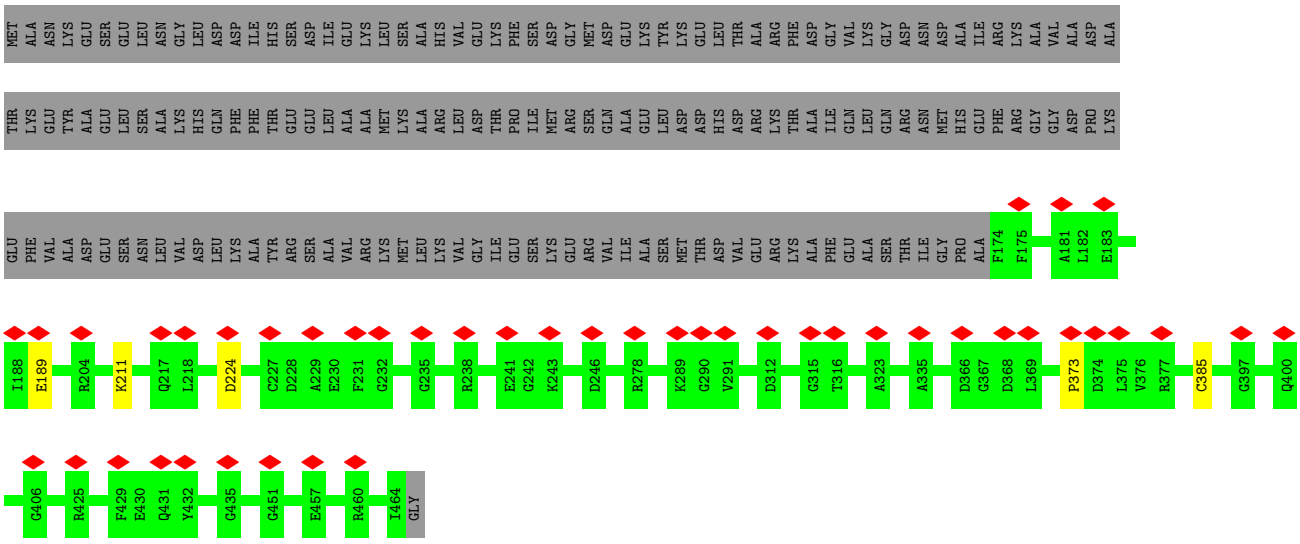
Chain n2:





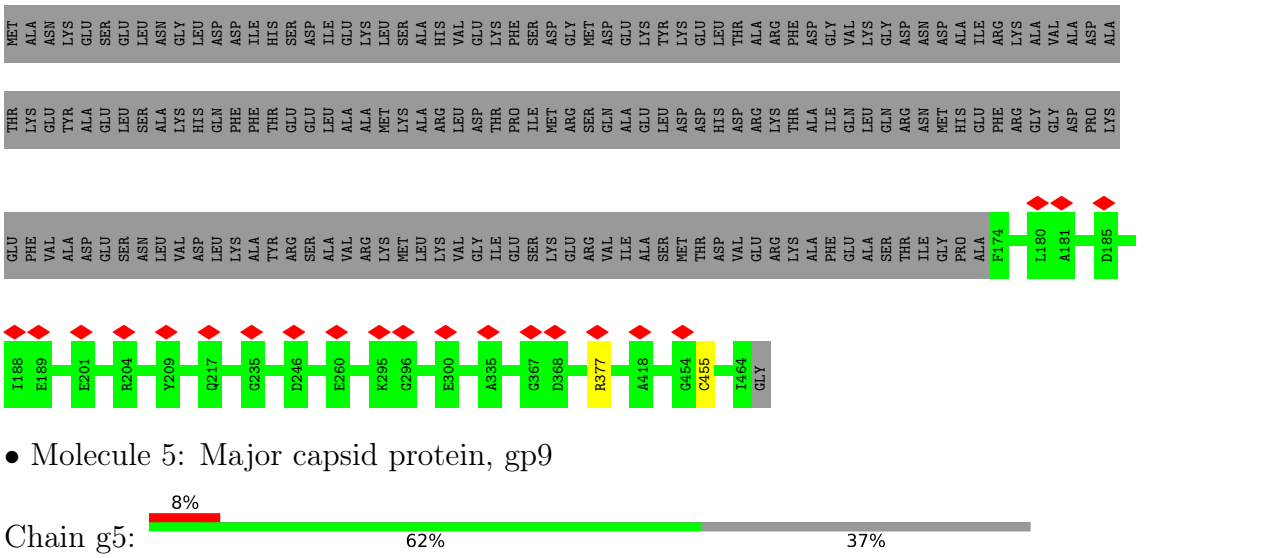
• Molecule 5: Major capsid protein, gp9

Chain o2:



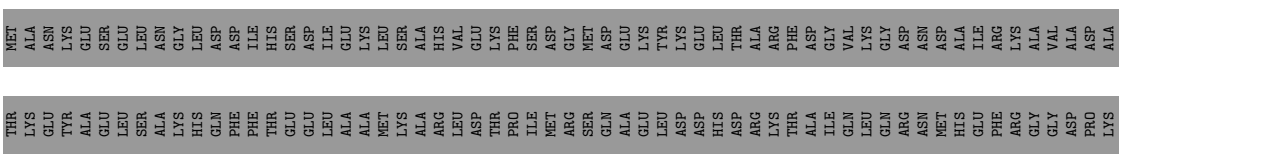
• Molecule 5: Major capsid protein, gp9

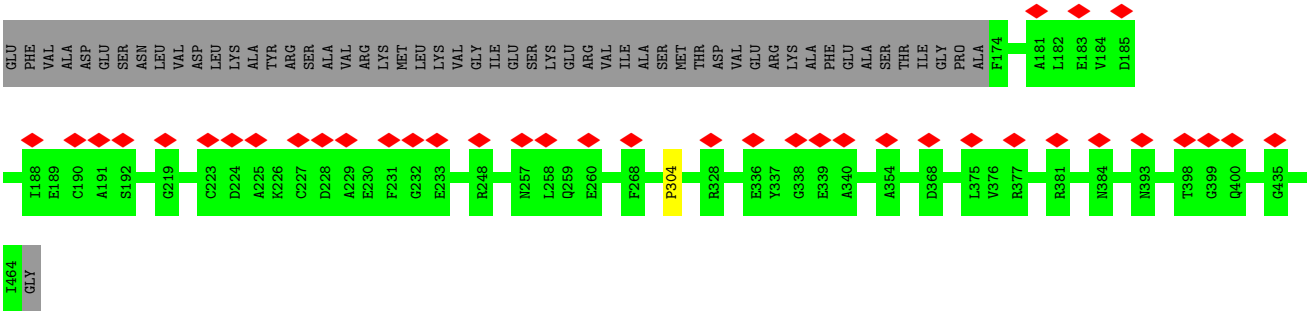
Chain r2:



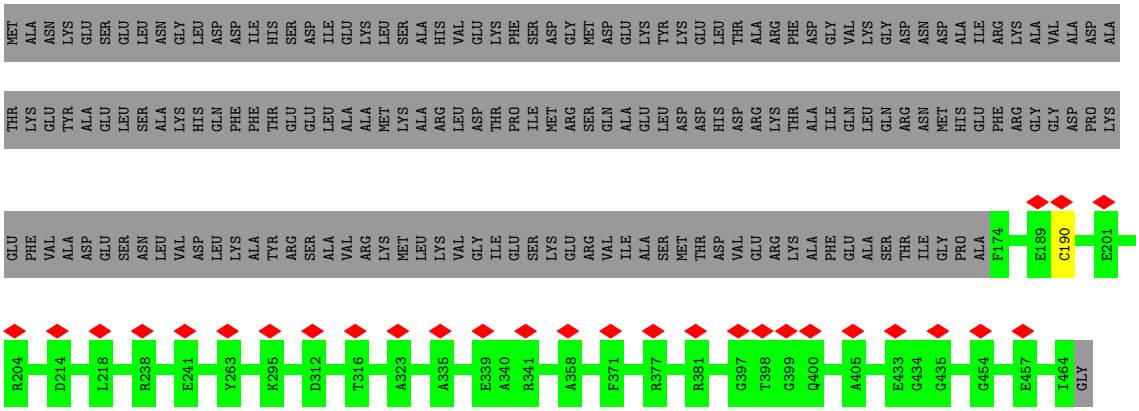
• Molecule 5: Major capsid protein, gp9

Chain g5:

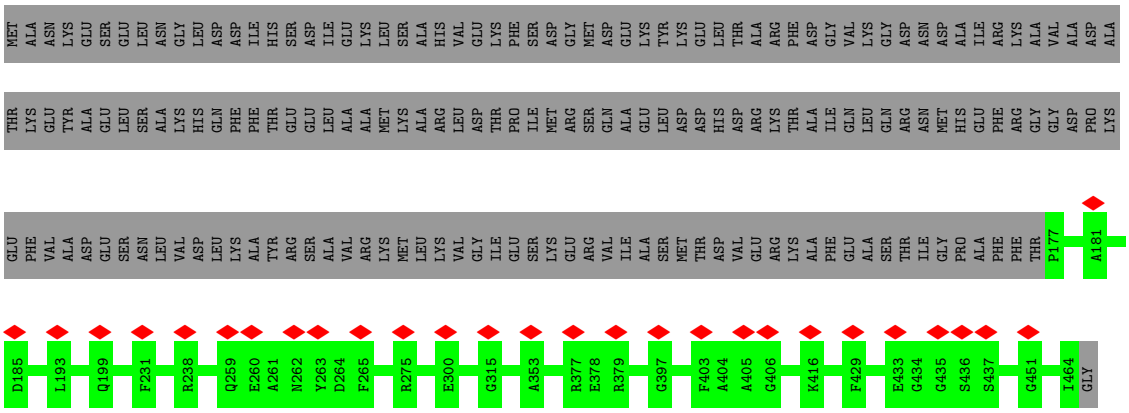




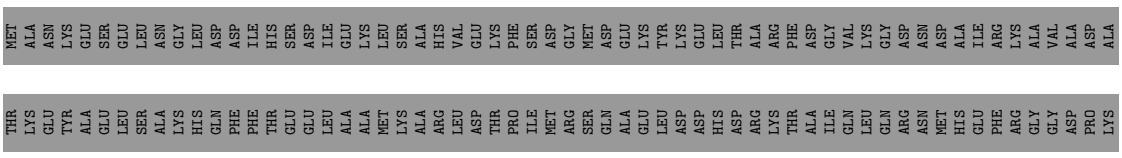
• Molecule 5: Major capsid protein, gp9

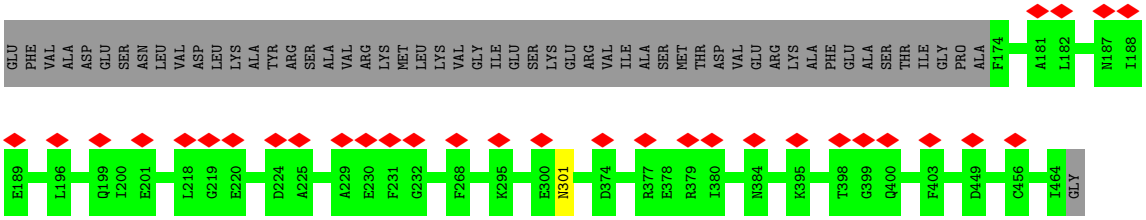


• Molecule 5: Major capsid protein, gp9



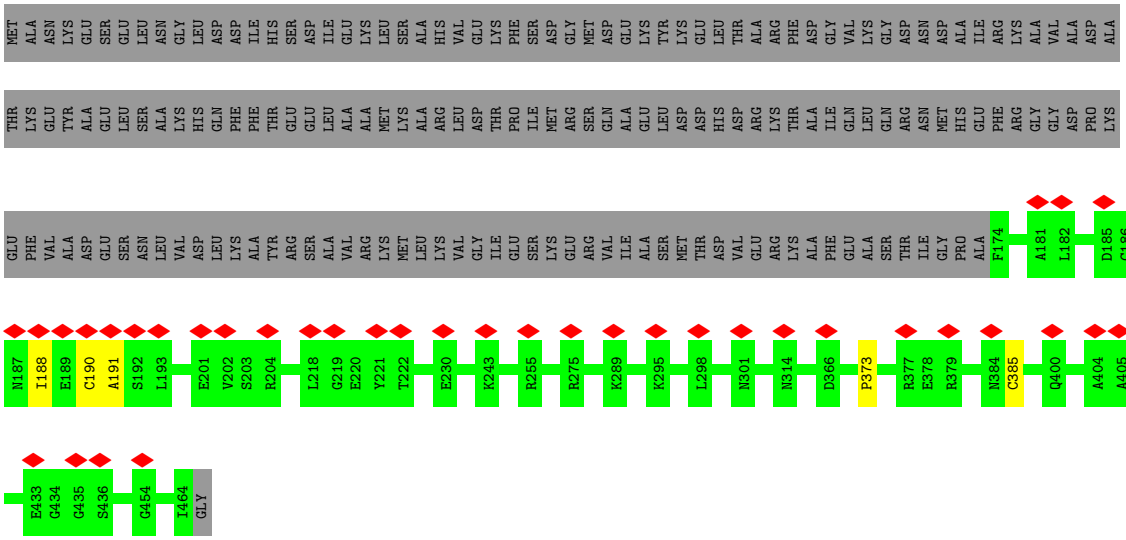
• Molecule 5: Major capsid protein, gp9





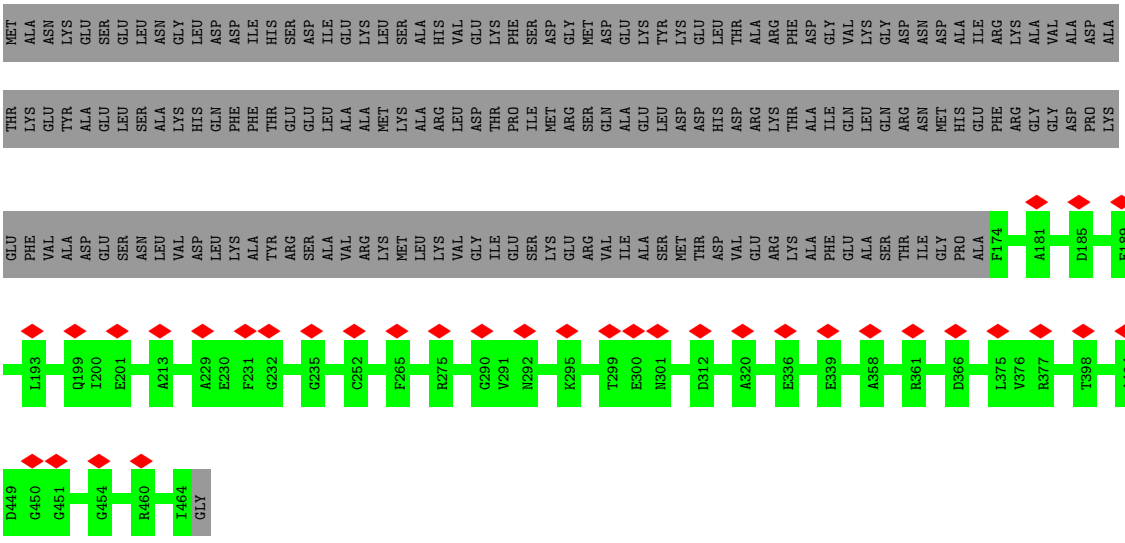
• Molecule 5: Major capsid protein, gp9

Chain o5:



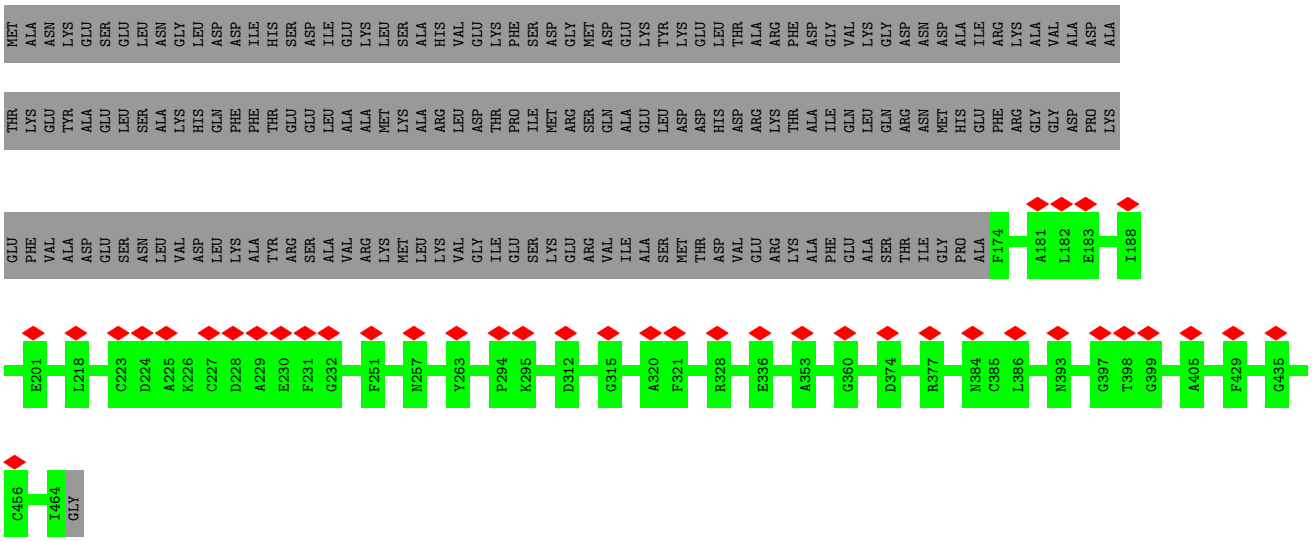
• Molecule 5: Major capsid protein, gp9

Chain r5:



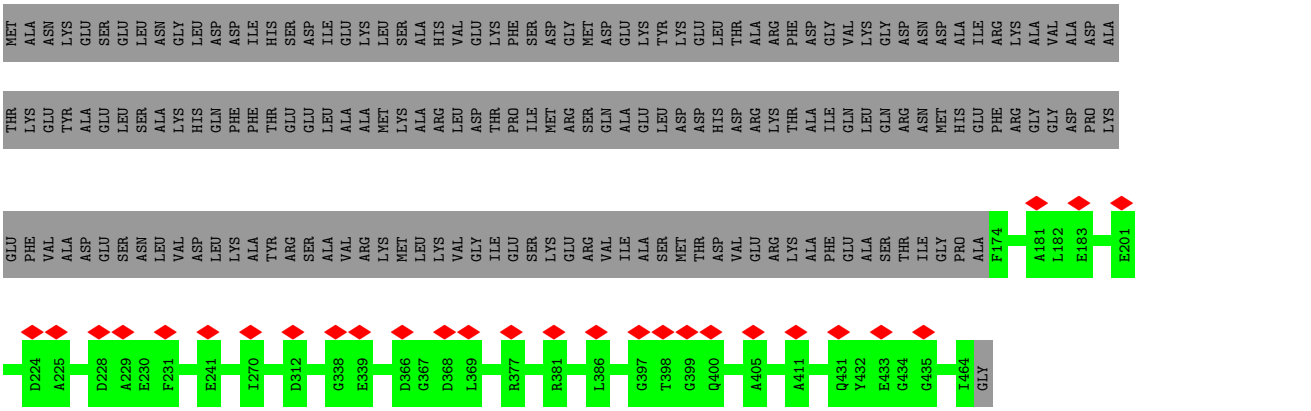
• Molecule 5: Major capsid protein, gp9

Chain g6:



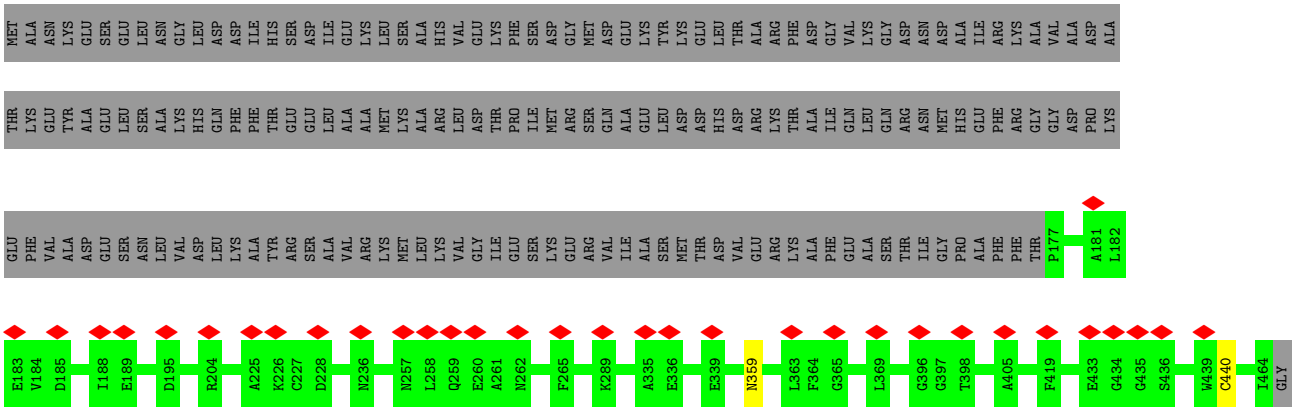
• Molecule 5: Major capsid protein, gp9

Chain h6:



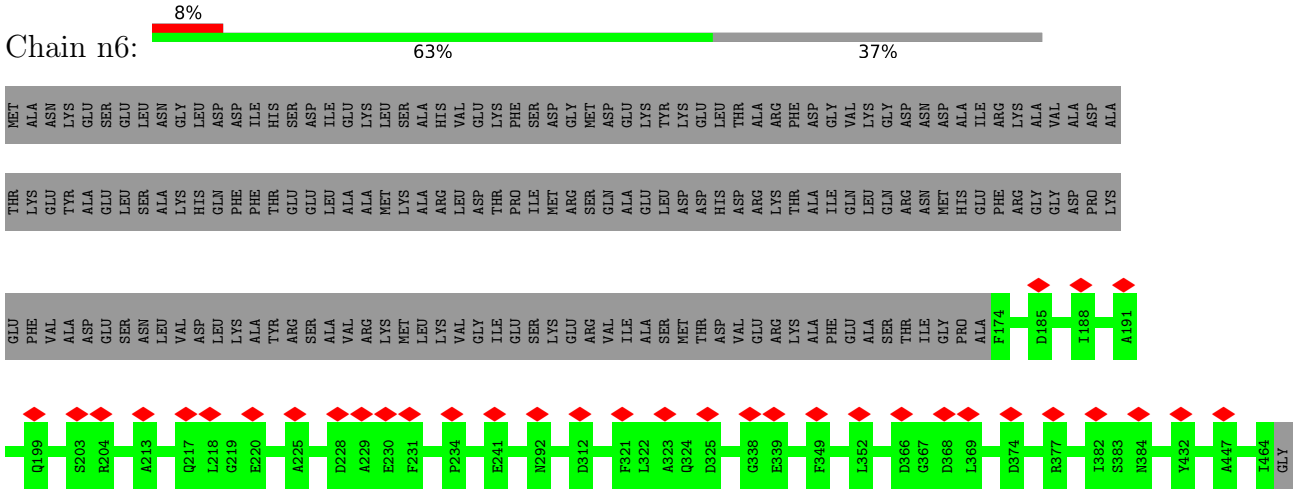
• Molecule 5: Major capsid protein, gp9

Chain k6:



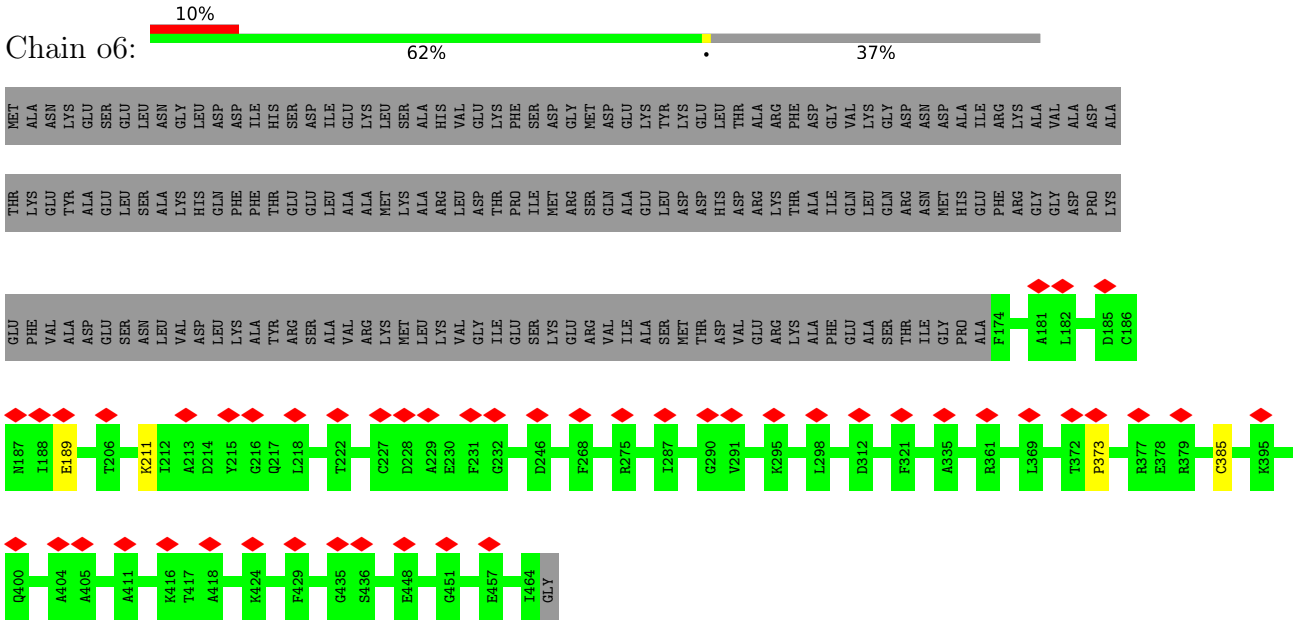
• Molecule 5: Major capsid protein, gp9

Chain n6:



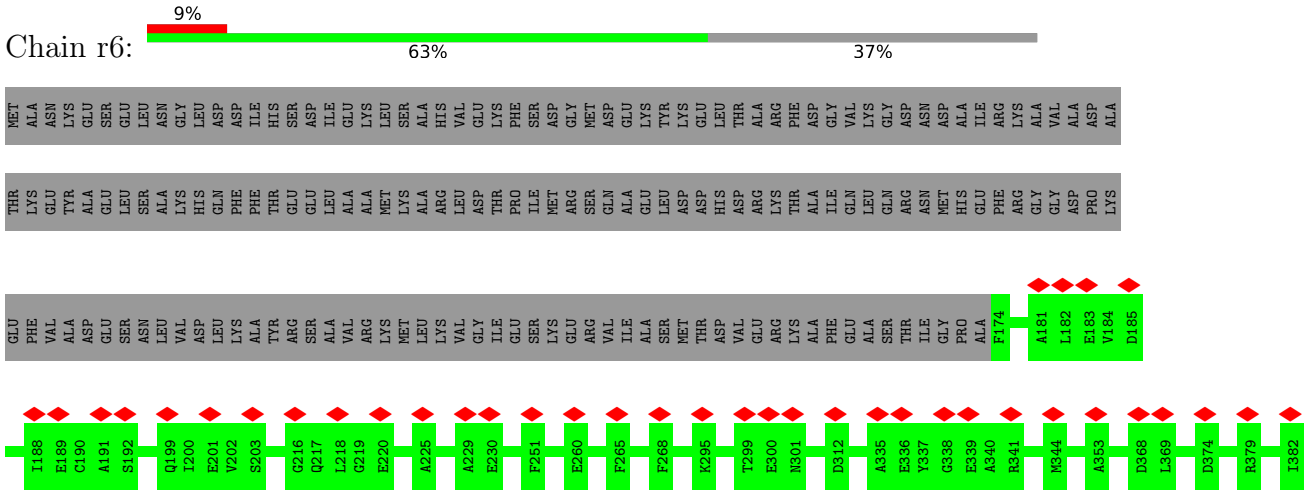
• Molecule 5: Major capsid protein, gp9

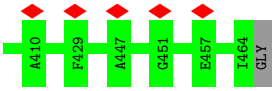
Chain o6:



• Molecule 5: Major capsid protein, gp9

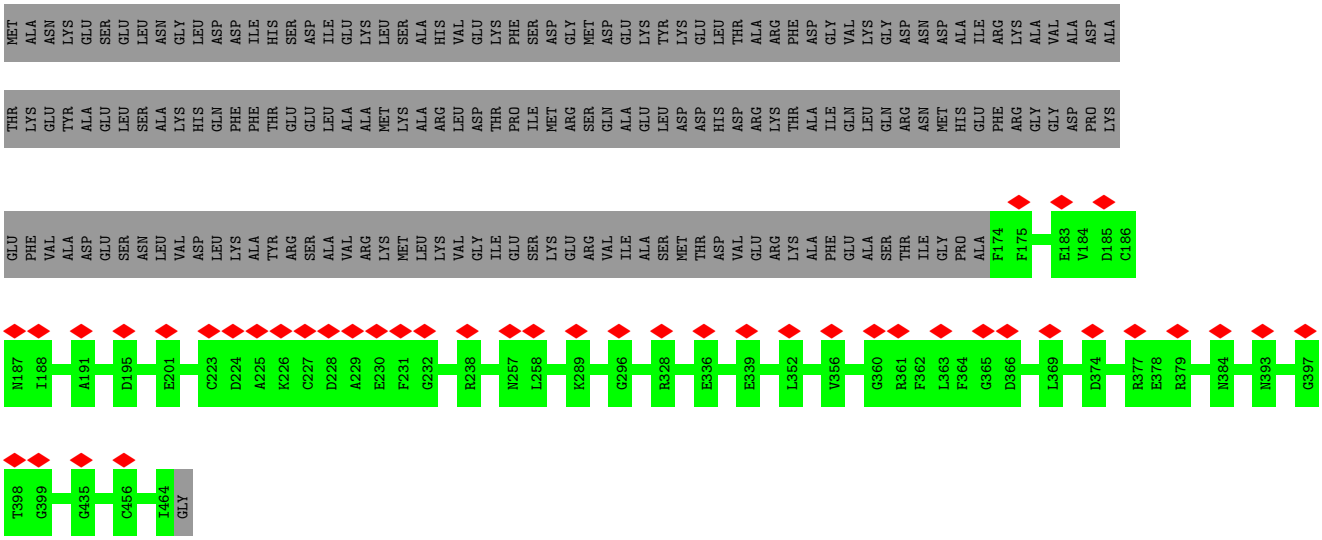
Chain r6:





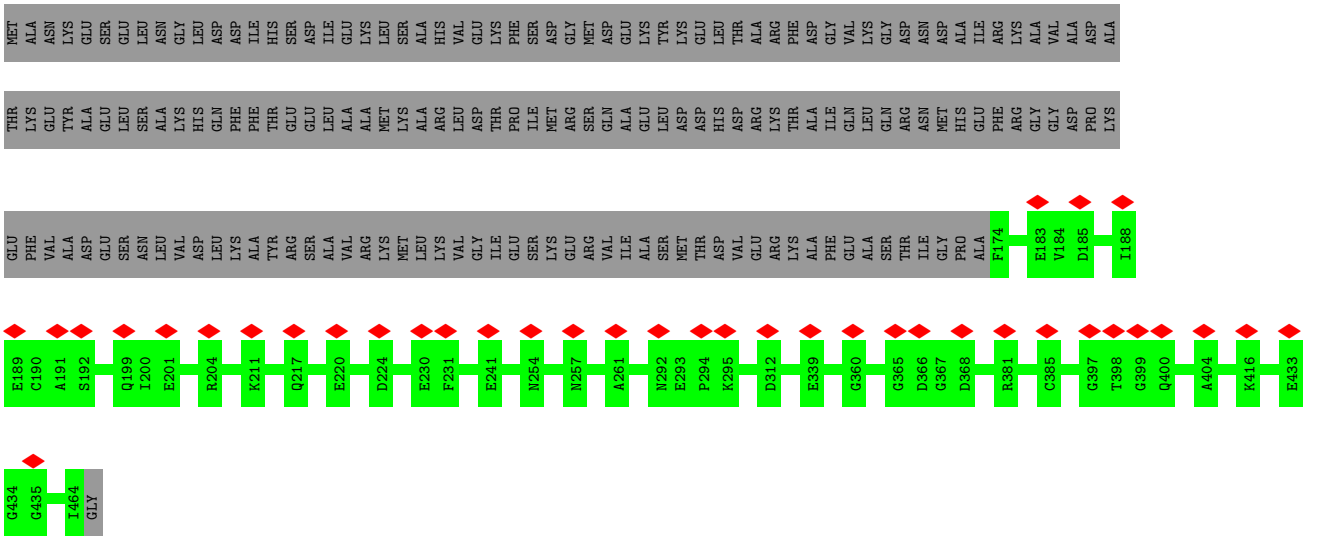
• Molecule 5: Major capsid protein, gp9

Chain g7:



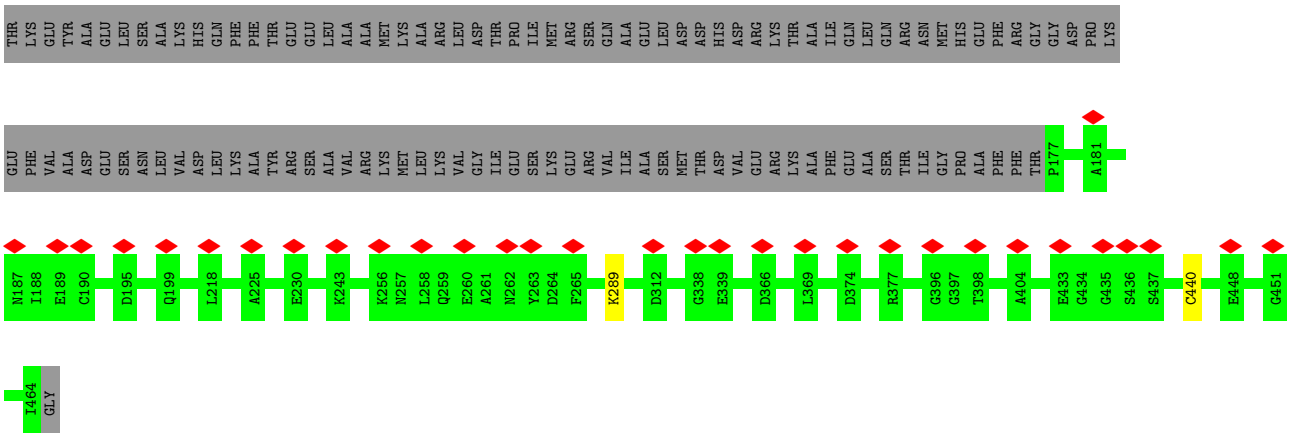
• Molecule 5: Major capsid protein, gp9

Chain h7:

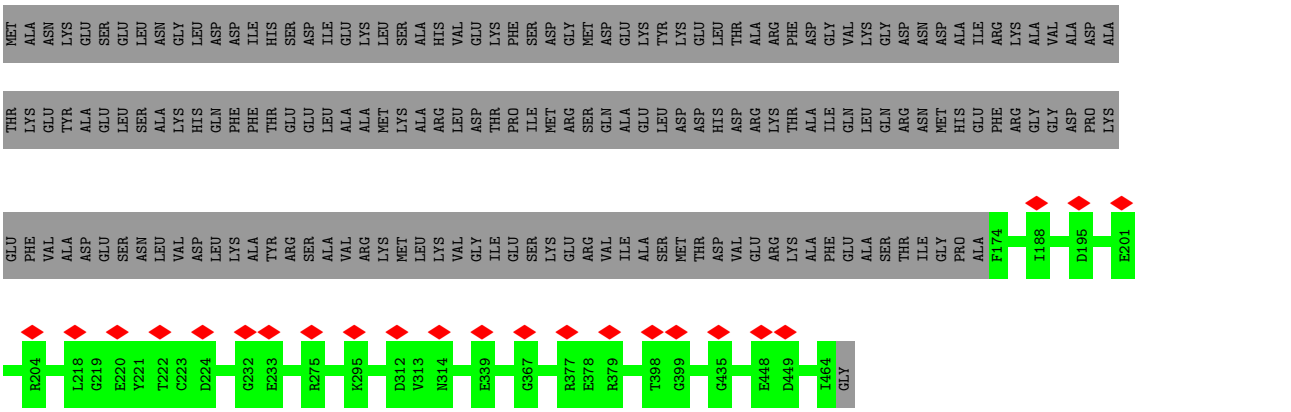


• Molecule 5: Major capsid protein, gp9

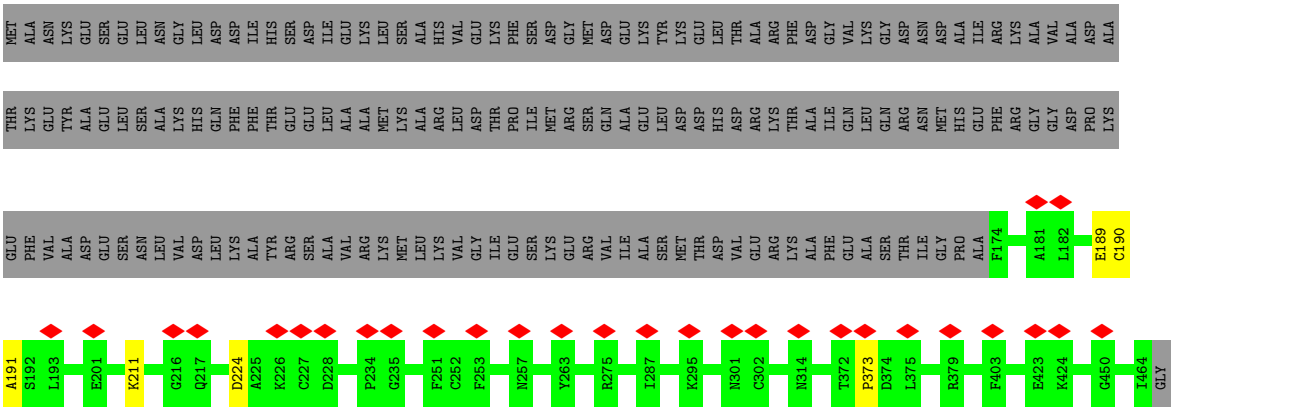
Chain k7:



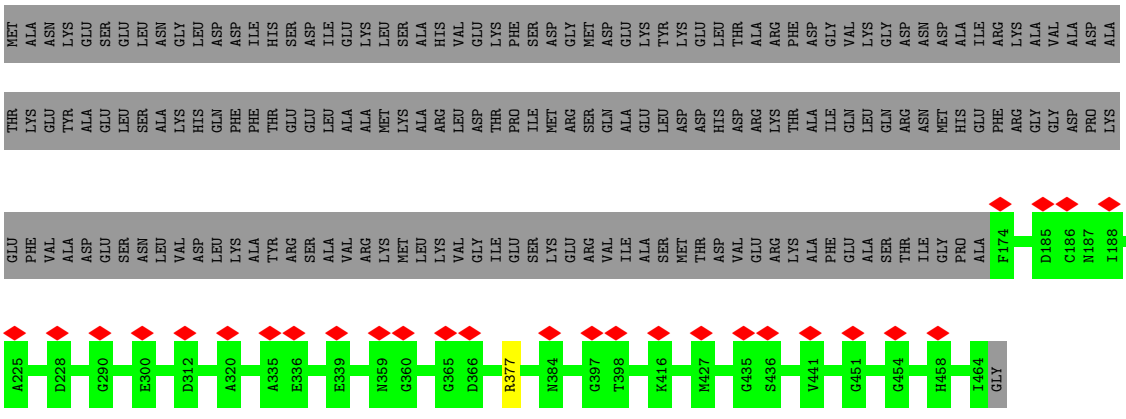
• Molecule 5: Major capsid protein, gp9



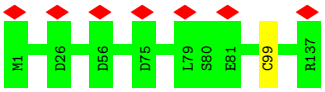
• Molecule 5: Major capsid protein, gp9



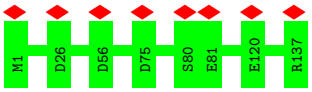
• Molecule 5: Major capsid protein, gp9



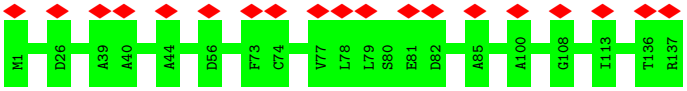
• Molecule 6: Minor capsid protein, gp10



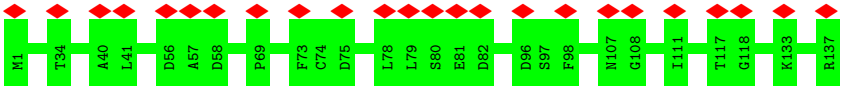
• Molecule 6: Minor capsid protein, gp10



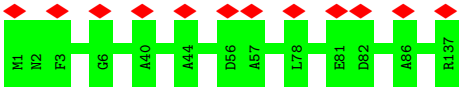
• Molecule 6: Minor capsid protein, gp10



• Molecule 6: Minor capsid protein, gp10

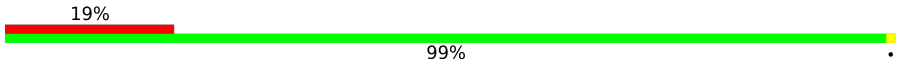


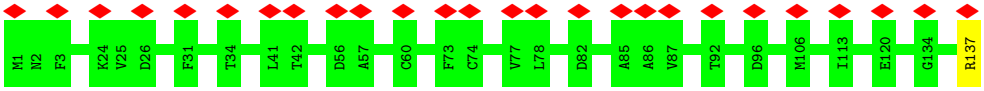
• Molecule 6: Minor capsid protein, gp10



• Molecule 6: Minor capsid protein, gp10

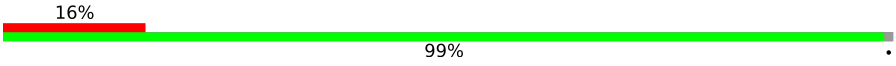
Chain t1:

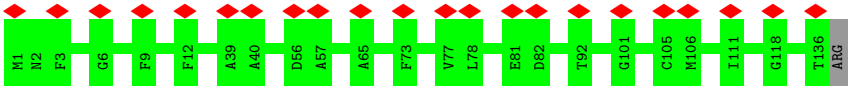




• Molecule 6: Minor capsid protein, gp10

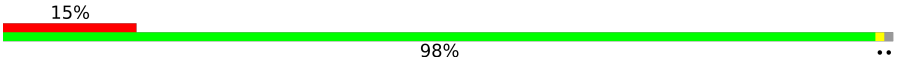
Chain u1:

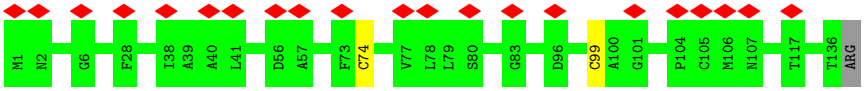




• Molecule 6: Minor capsid protein, gp10

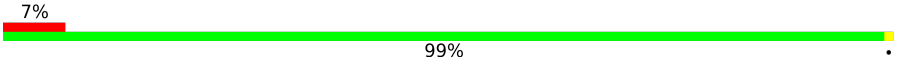
Chain v1:

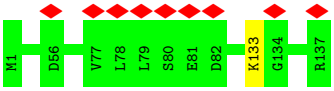




• Molecule 6: Minor capsid protein, gp10

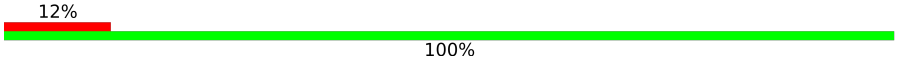
Chain l2:

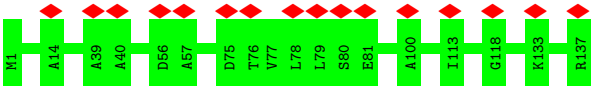




• Molecule 6: Minor capsid protein, gp10

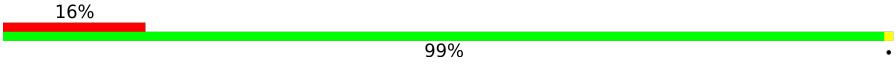
Chain m2:

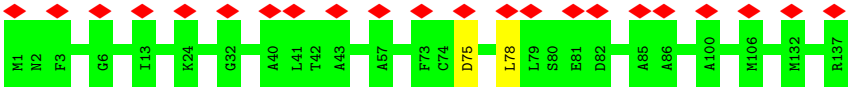




• Molecule 6: Minor capsid protein, gp10

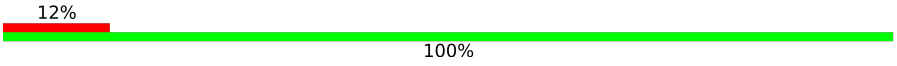
Chain p2:

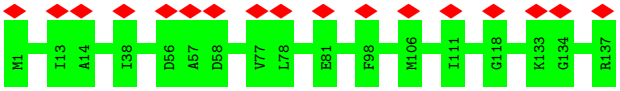




• Molecule 6: Minor capsid protein, gp10

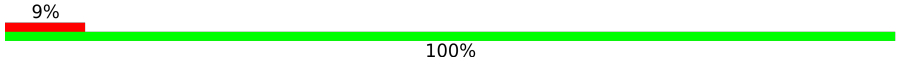
Chain q2:

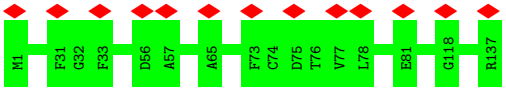




• Molecule 6: Minor capsid protein, gp10

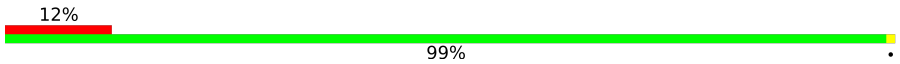
Chain s2:

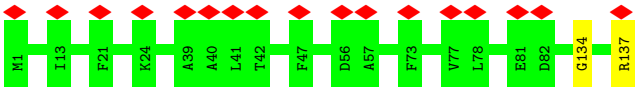




• Molecule 6: Minor capsid protein, gp10

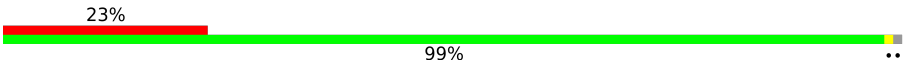
Chain t2:

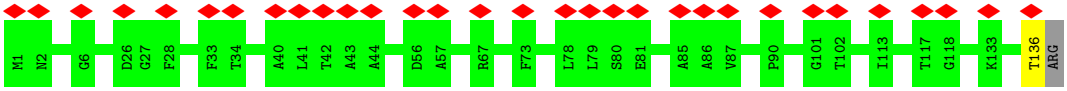




• Molecule 6: Minor capsid protein, gp10

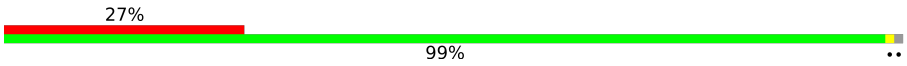
Chain u2:

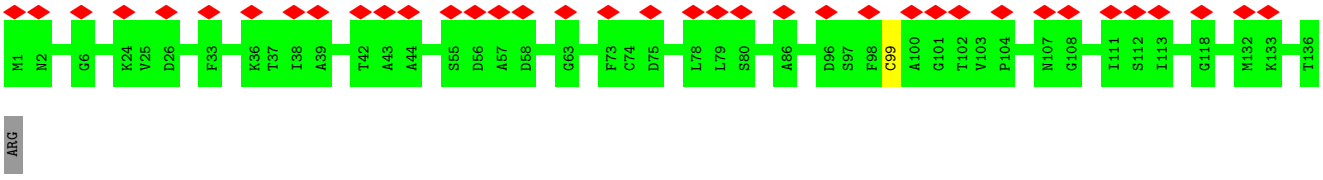




• Molecule 6: Minor capsid protein, gp10

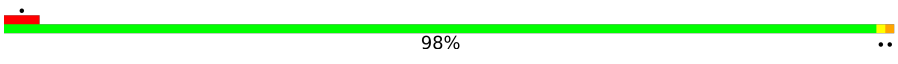
Chain v2:

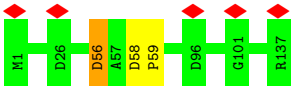




• Molecule 6: Minor capsid protein, gp10

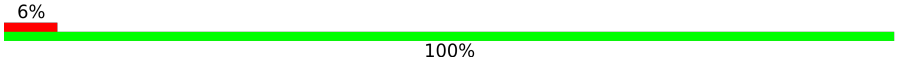
Chain l5:

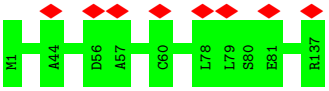




• Molecule 6: Minor capsid protein, gp10

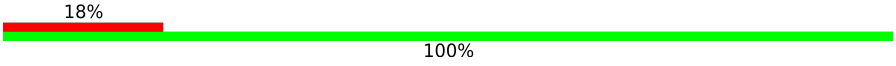
Chain m5:

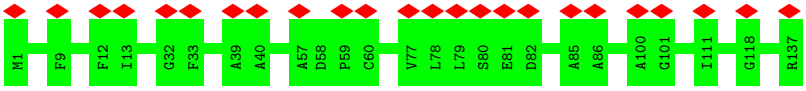




• Molecule 6: Minor capsid protein, gp10

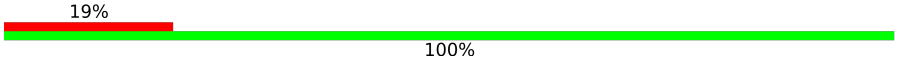
Chain p5:

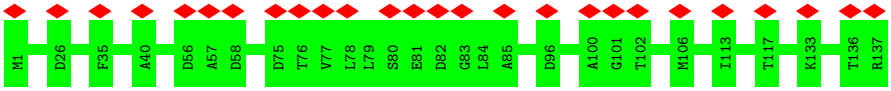




• Molecule 6: Minor capsid protein, gp10

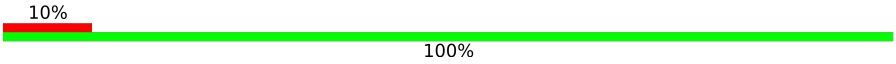
Chain q5:

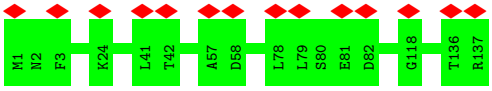




• Molecule 6: Minor capsid protein, gp10

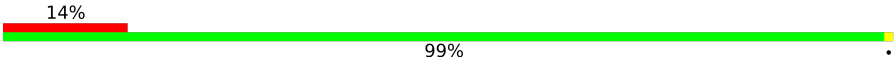
Chain s5:

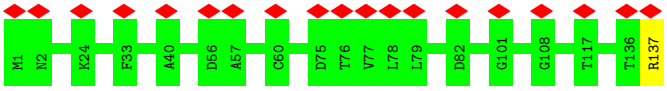




• Molecule 6: Minor capsid protein, gp10

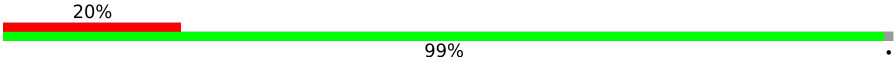
Chain t5:

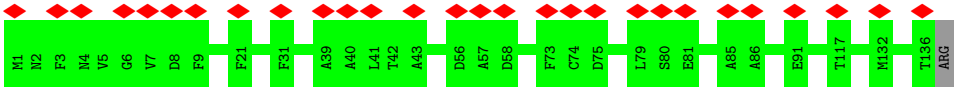




• Molecule 6: Minor capsid protein, gp10

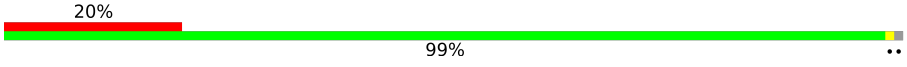
Chain u5:

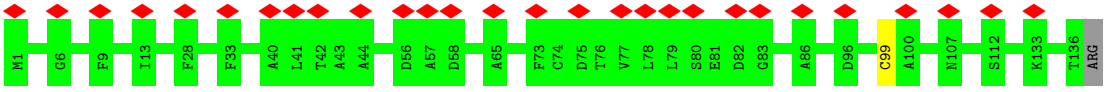




• Molecule 6: Minor capsid protein, gp10

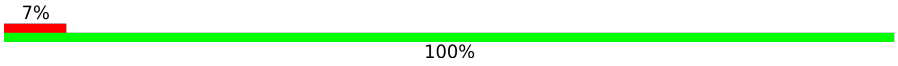
Chain v5:

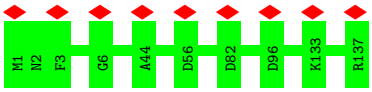




• Molecule 6: Minor capsid protein, gp10

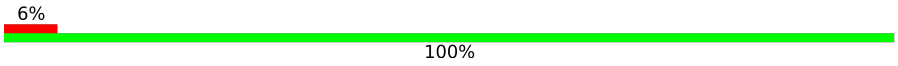
Chain l6:

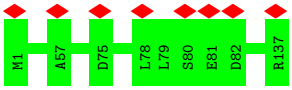




• Molecule 6: Minor capsid protein, gp10

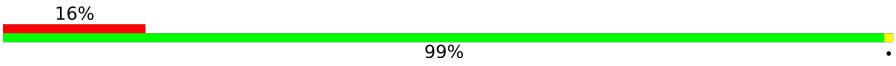
Chain m6:

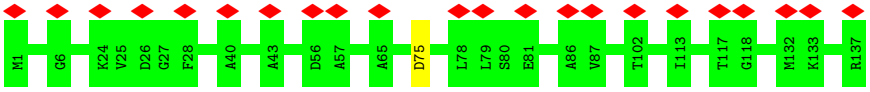




• Molecule 6: Minor capsid protein, gp10

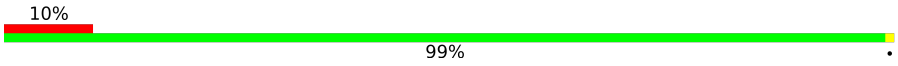
Chain p6:

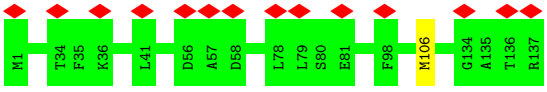




• Molecule 6: Minor capsid protein, gp10

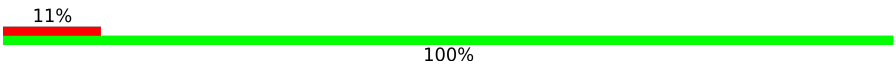
Chain q6:

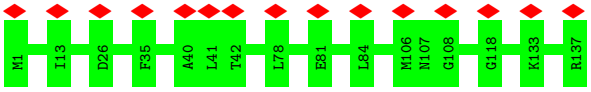




• Molecule 6: Minor capsid protein, gp10

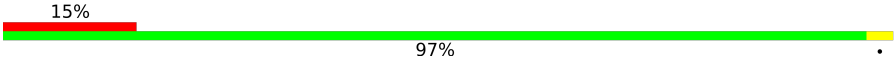
Chain s6:

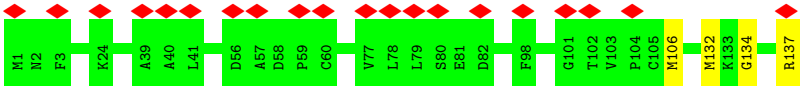




• Molecule 6: Minor capsid protein, gp10

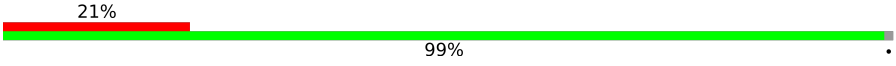
Chain t6:

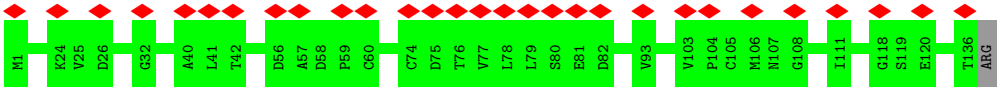




• Molecule 6: Minor capsid protein, gp10

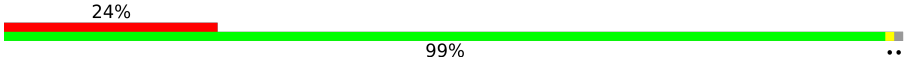
Chain u6:

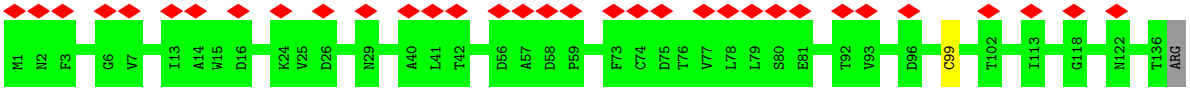




• Molecule 6: Minor capsid protein, gp10

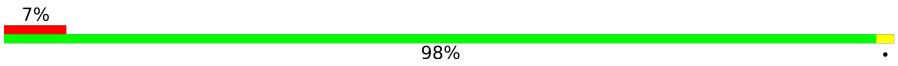
Chain v6:

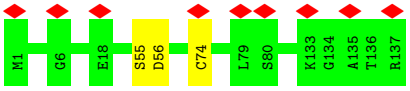




• Molecule 6: Minor capsid protein, gp10

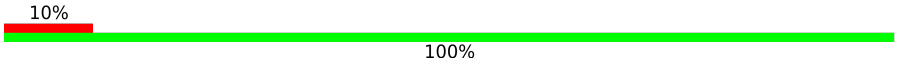
Chain l7:

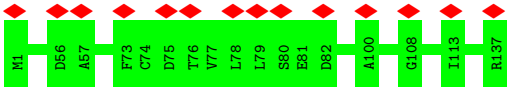




• Molecule 6: Minor capsid protein, gp10

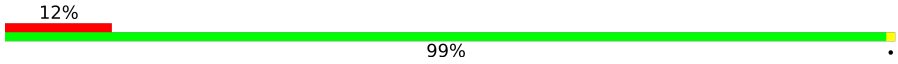
Chain m7:

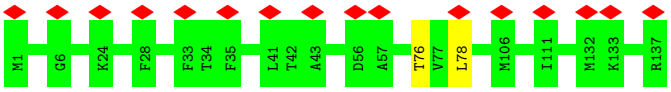




• Molecule 6: Minor capsid protein, gp10

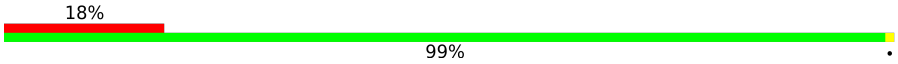
Chain p7:

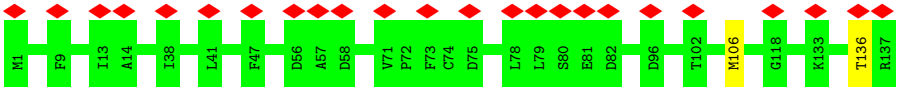




• Molecule 6: Minor capsid protein, gp10

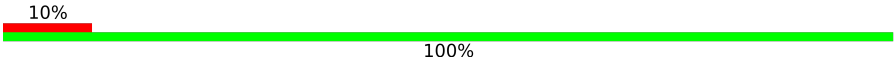
Chain q7:

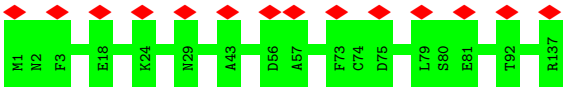




• Molecule 6: Minor capsid protein, gp10

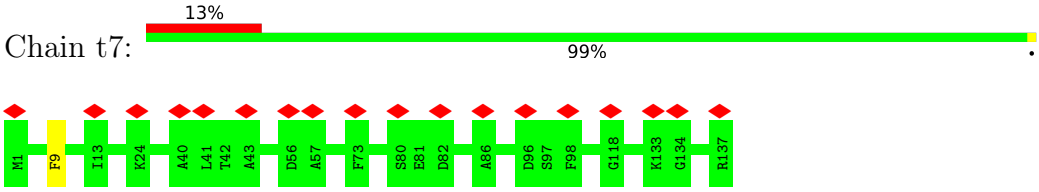
Chain s7:





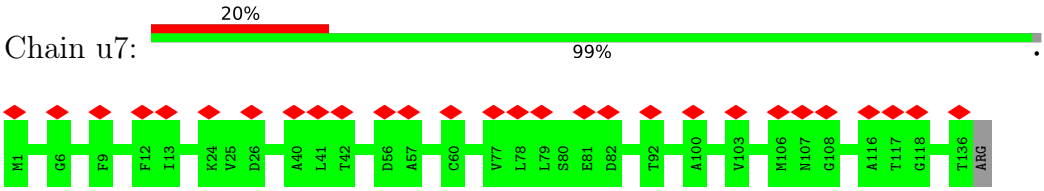
• Molecule 6: Minor capsid protein, gp10

Chain t7:



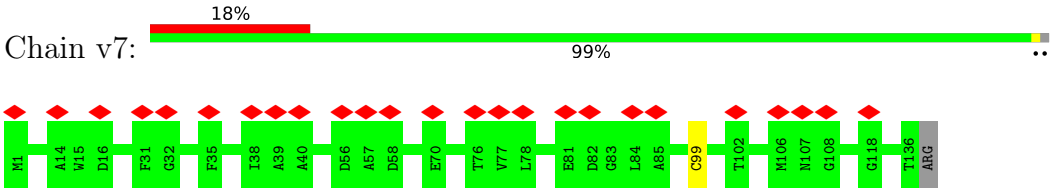
• Molecule 6: Minor capsid protein, gp10

Chain u7:



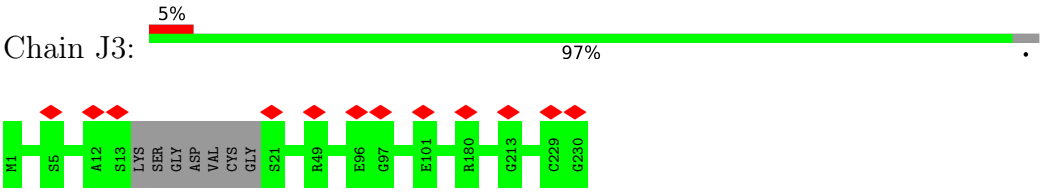
• Molecule 6: Minor capsid protein, gp10

Chain v7:



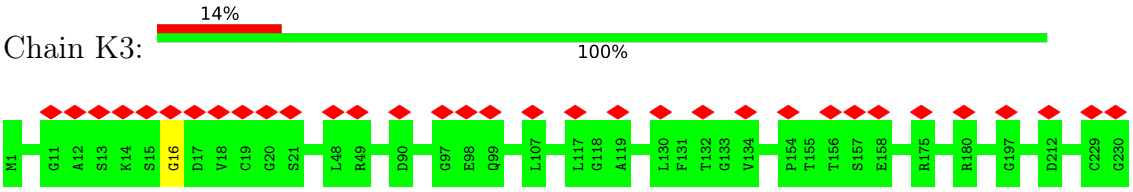
• Molecule 7: Collar sheath protein, gp13

Chain J3:



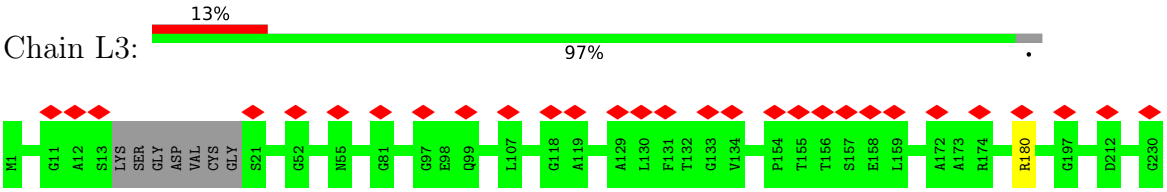
• Molecule 7: Collar sheath protein, gp13

Chain K3:



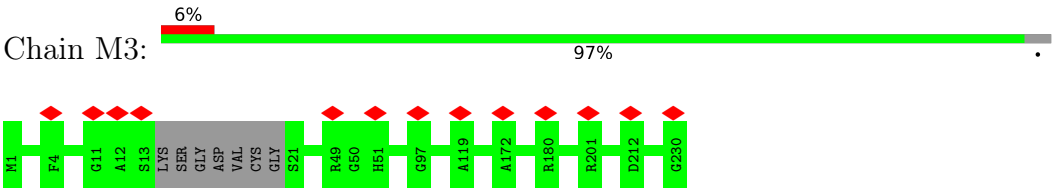
• Molecule 7: Collar sheath protein, gp13

Chain L3:



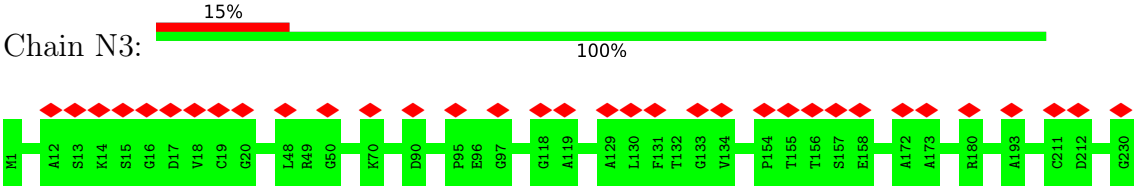
• Molecule 7: Collar sheath protein, gp13

Chain M3:



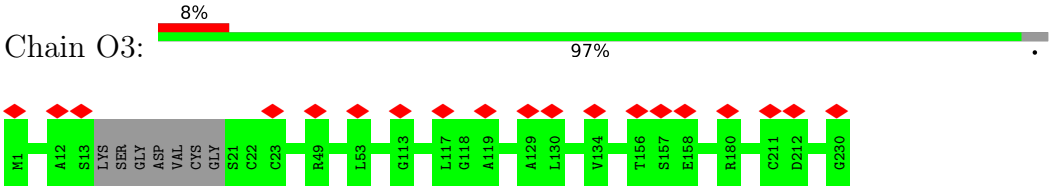
• Molecule 7: Collar sheath protein, gp13

Chain N3:



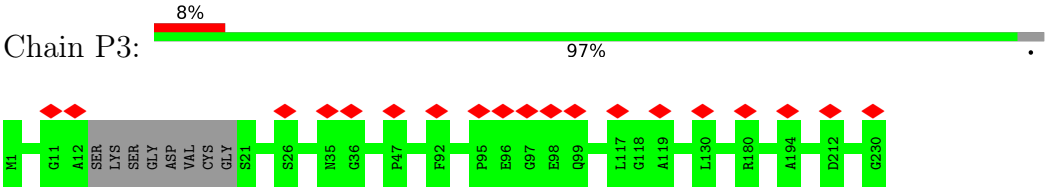
• Molecule 7: Collar sheath protein, gp13

Chain O3:



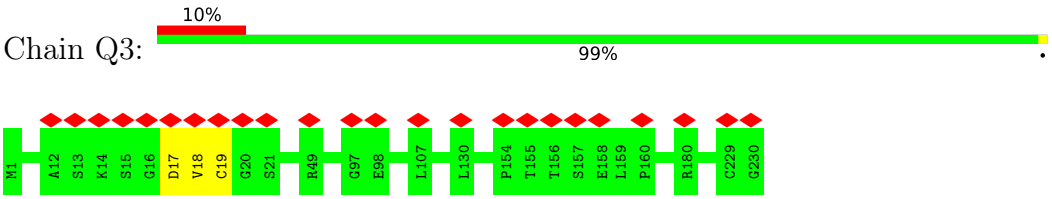
• Molecule 7: Collar sheath protein, gp13

Chain P3:



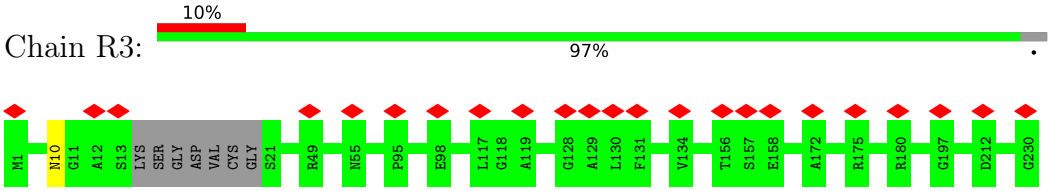
• Molecule 7: Collar sheath protein, gp13

Chain Q3:



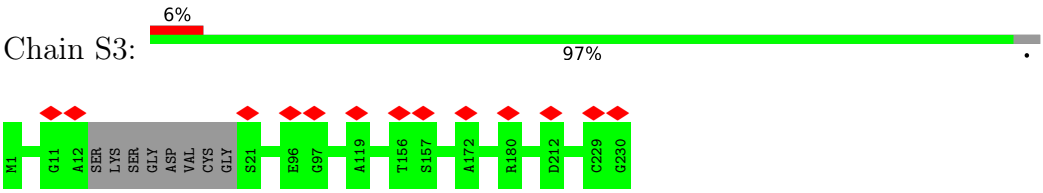
• Molecule 7: Collar sheath protein, gp13

Chain R3:



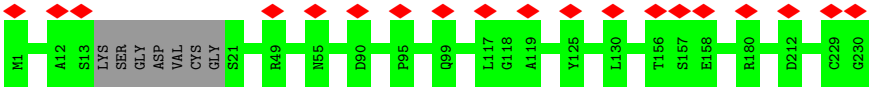
• Molecule 7: Collar sheath protein, gp13

Chain S3:



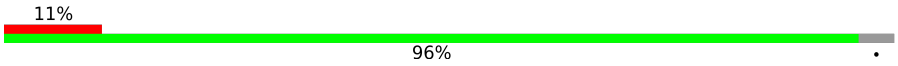
• Molecule 7: Collar sheath protein, gp13

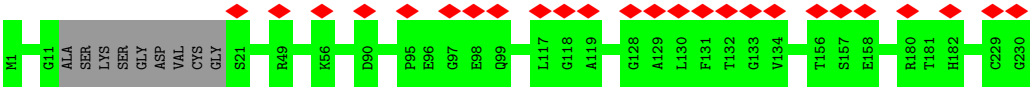
Chain T3:



• Molecule 7: Collar sheath protein, gp13

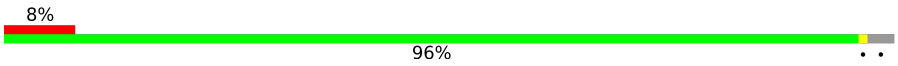
Chain U3:

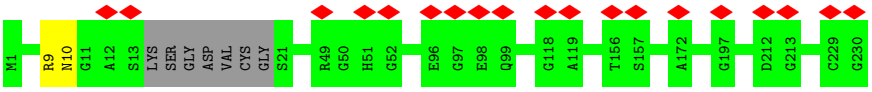




• Molecule 7: Collar sheath protein, gp13

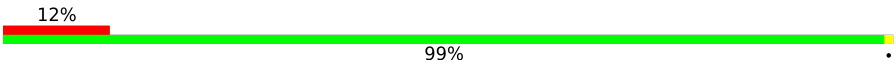
Chain V3:

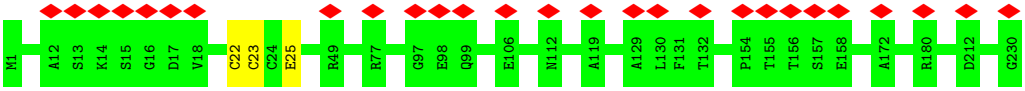




• Molecule 7: Collar sheath protein, gp13

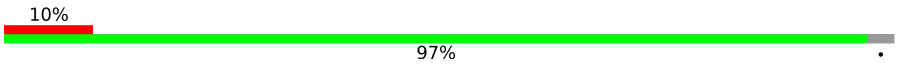
Chain W3:

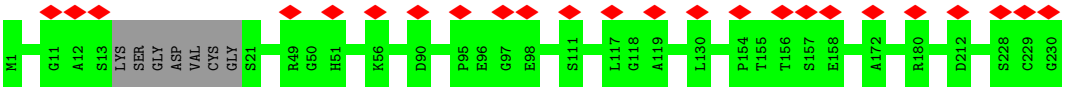




• Molecule 7: Collar sheath protein, gp13

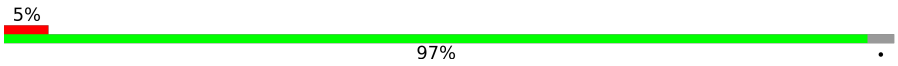
Chain X3:

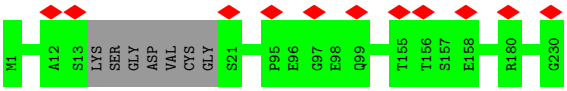




• Molecule 7: Collar sheath protein, gp13

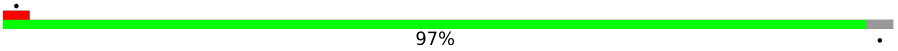
Chain Y3:

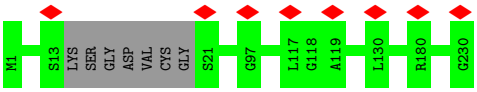




• Molecule 7: Collar sheath protein, gp13

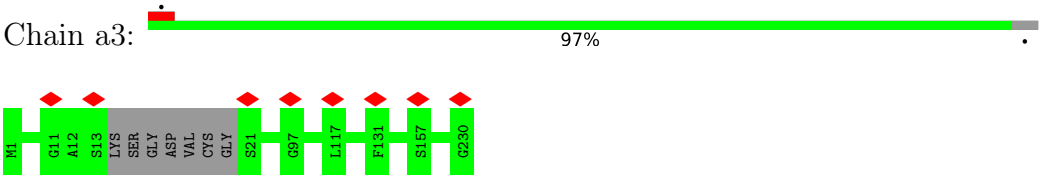
Chain Z3:





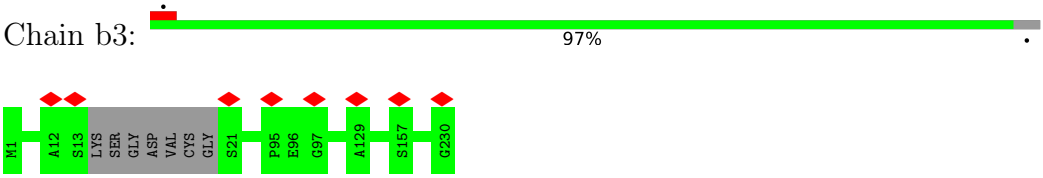
• Molecule 7: Collar sheath protein, gp13

Chain a3:



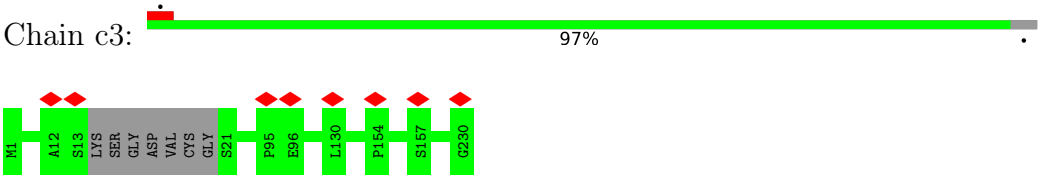
• Molecule 7: Collar sheath protein, gp13

Chain b3:



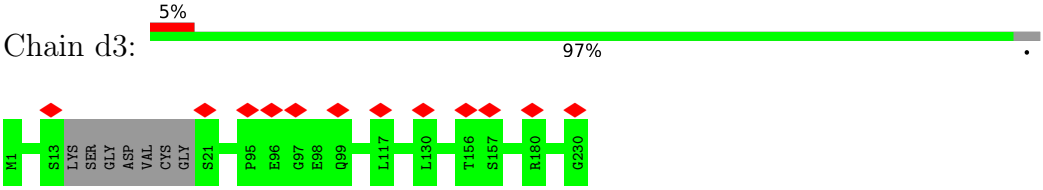
• Molecule 7: Collar sheath protein, gp13

Chain c3:



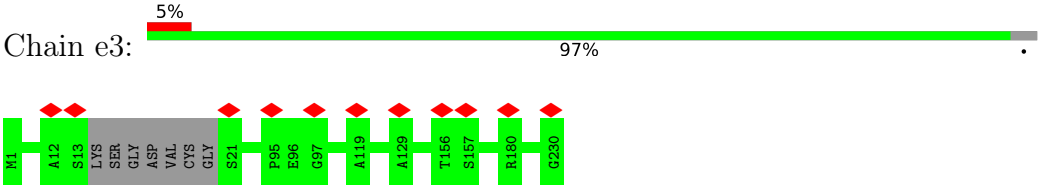
• Molecule 7: Collar sheath protein, gp13

Chain d3:



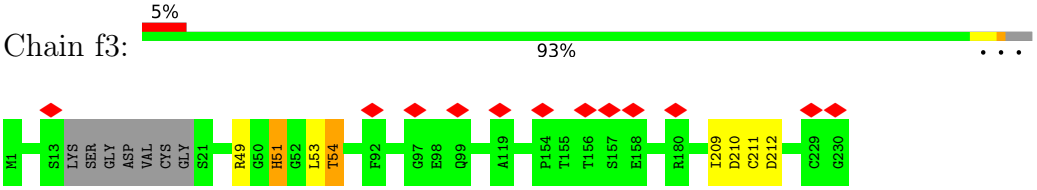
• Molecule 7: Collar sheath protein, gp13

Chain e3:



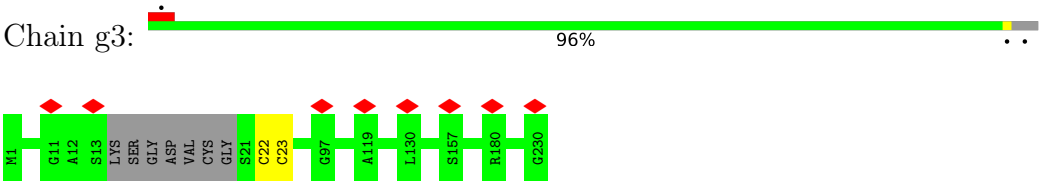
• Molecule 7: Collar sheath protein, gp13

Chain f3:



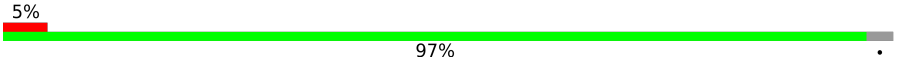
• Molecule 7: Collar sheath protein, gp13

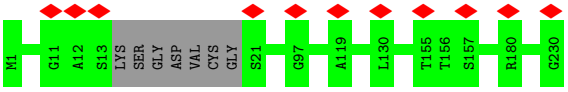
Chain g3:



• Molecule 7: Collar sheath protein, gp13

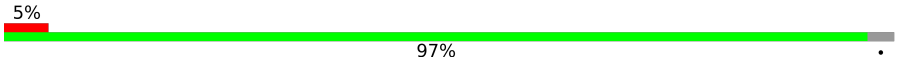
Chain h3:

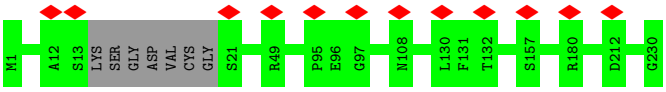




• Molecule 7: Collar sheath protein, gp13

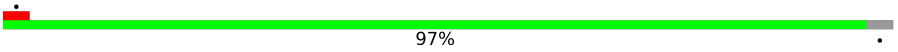
Chain i3:

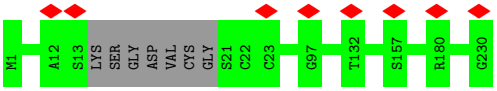




• Molecule 7: Collar sheath protein, gp13

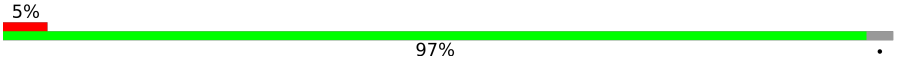
Chain j3:

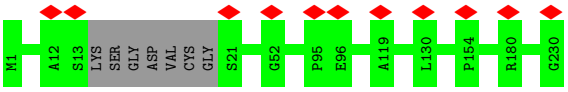




• Molecule 7: Collar sheath protein, gp13

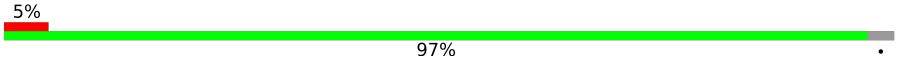
Chain k3:

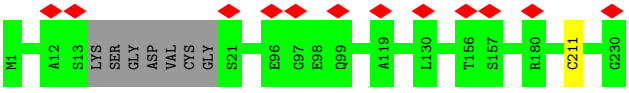




• Molecule 7: Collar sheath protein, gp13

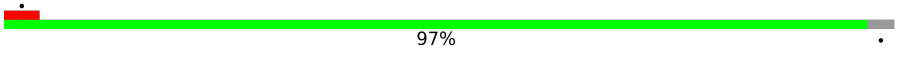
Chain l3:

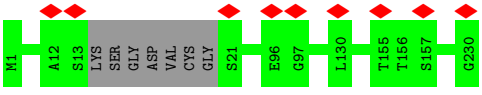




• Molecule 7: Collar sheath protein, gp13

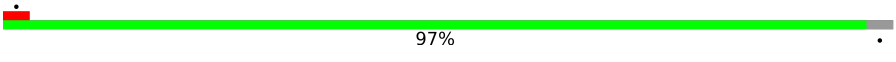
Chain m3:

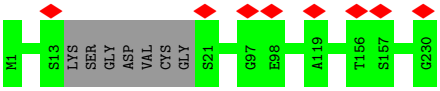




• Molecule 7: Collar sheath protein, gp13

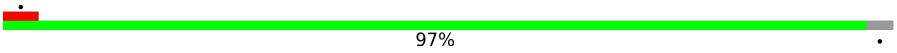
Chain n3:

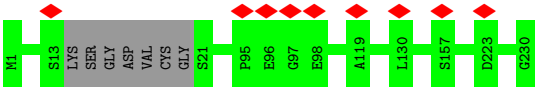




• Molecule 7: Collar sheath protein, gp13

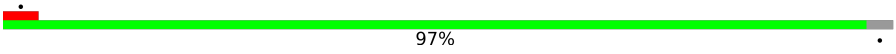
Chain o3:

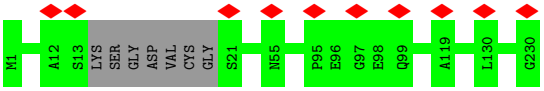




• Molecule 7: Collar sheath protein, gp13

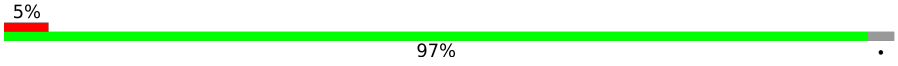
Chain p3:

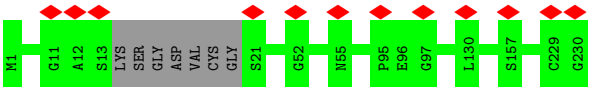




• Molecule 7: Collar sheath protein, gp13

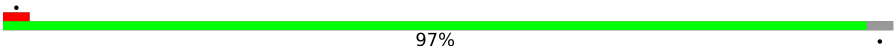
Chain q3:

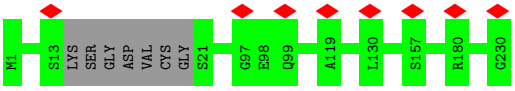




• Molecule 7: Collar sheath protein, gp13

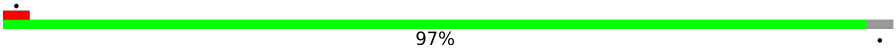
Chain r3:

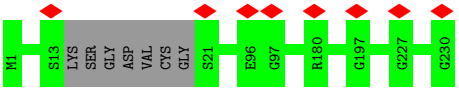




• Molecule 7: Collar sheath protein, gp13

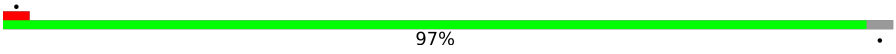
Chain s3:

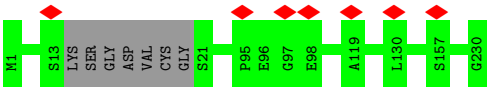




• Molecule 7: Collar sheath protein, gp13

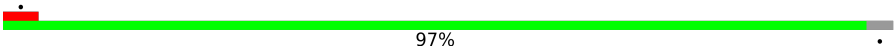
Chain t3:

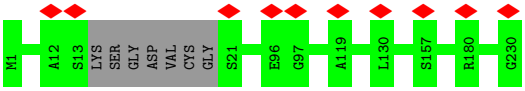




• Molecule 7: Collar sheath protein, gp13

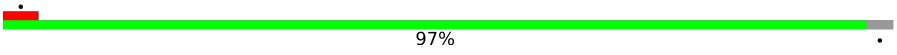
Chain u3:

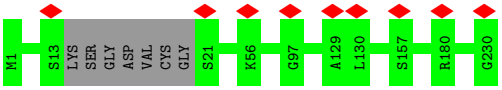




• Molecule 7: Collar sheath protein, gp13

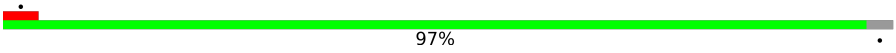
Chain v3:

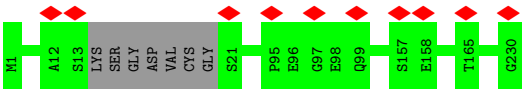




• Molecule 7: Collar sheath protein, gp13

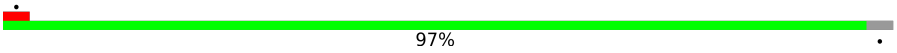
Chain w3:

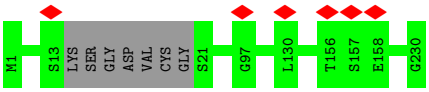




• Molecule 7: Collar sheath protein, gp13

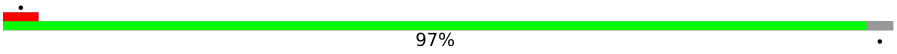
Chain x3:

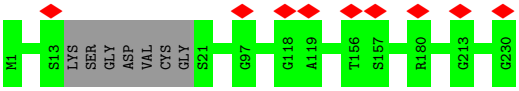




• Molecule 7: Collar sheath protein, gp13

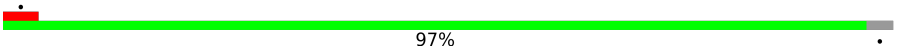
Chain y3:

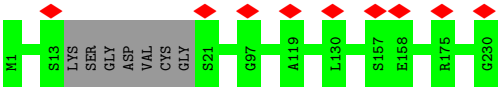




• Molecule 7: Collar sheath protein, gp13

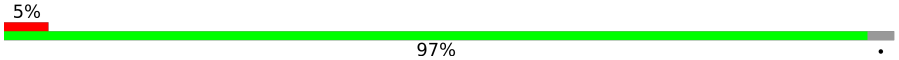
Chain z3:

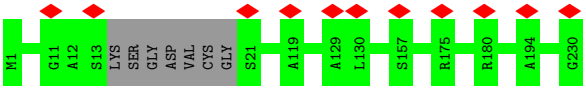




• Molecule 7: Collar sheath protein, gp13

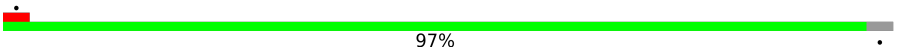
Chain 13:

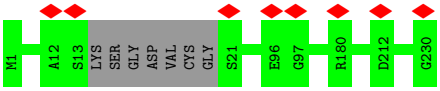




• Molecule 7: Collar sheath protein, gp13

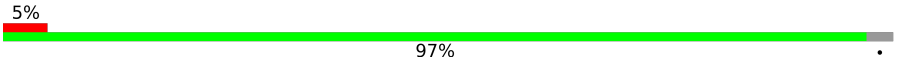
Chain 23:

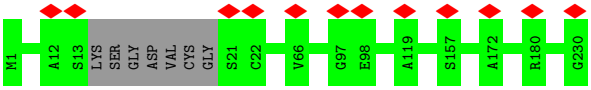




• Molecule 7: Collar sheath protein, gp13

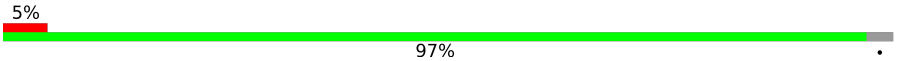
Chain 33:

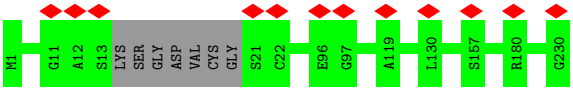




• Molecule 7: Collar sheath protein, gp13

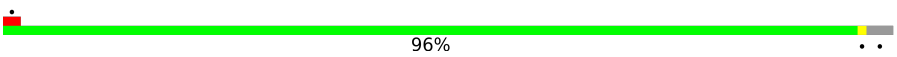
Chain 43:

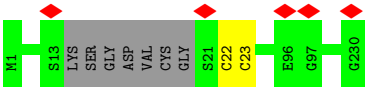




• Molecule 7: Collar sheath protein, gp13

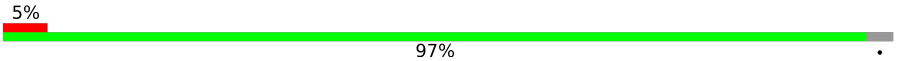
Chain 53:

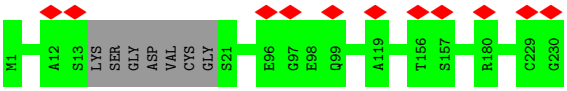




• Molecule 7: Collar sheath protein, gp13

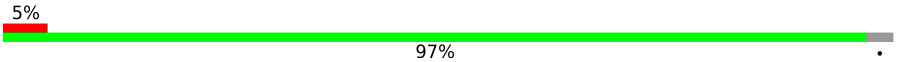
Chain 63:

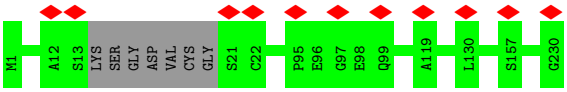




• Molecule 7: Collar sheath protein, gp13

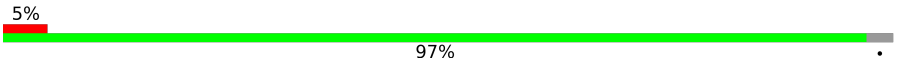
Chain 73:

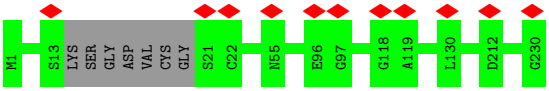




• Molecule 7: Collar sheath protein, gp13

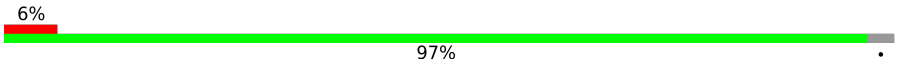
Chain 83:

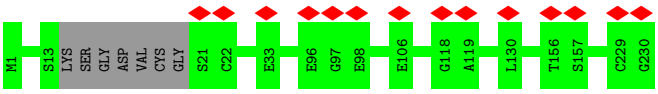




• Molecule 7: Collar sheath protein, gp13

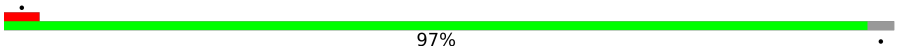
Chain 93:

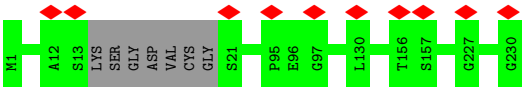




• Molecule 7: Collar sheath protein, gp13

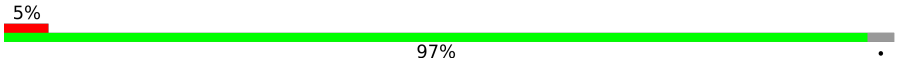
Chain 03:

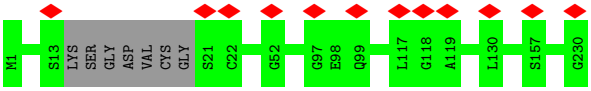




• Molecule 7: Collar sheath protein, gp13

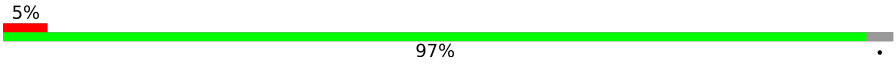
Chain A3:

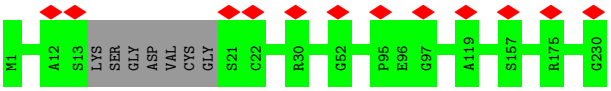




• Molecule 7: Collar sheath protein, gp13

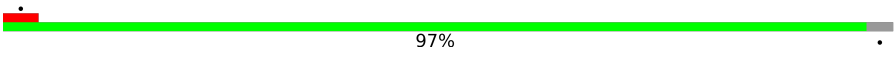
Chain B3:

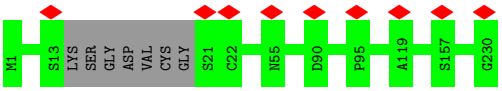




• Molecule 7: Collar sheath protein, gp13

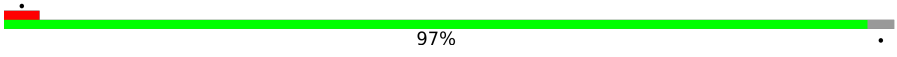
Chain C3:

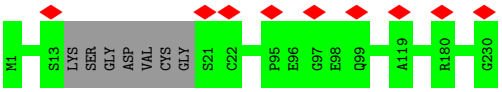




• Molecule 7: Collar sheath protein, gp13

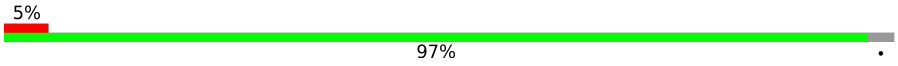
Chain D3:

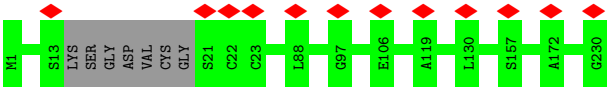




• Molecule 7: Collar sheath protein, gp13

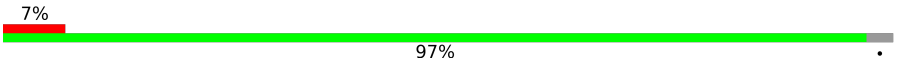
Chain E3:

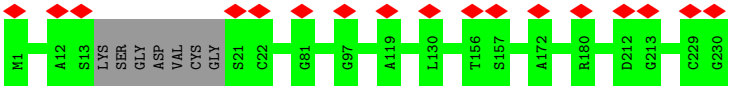




• Molecule 7: Collar sheath protein, gp13

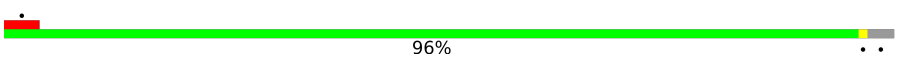
Chain F3:

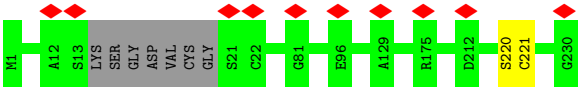




• Molecule 7: Collar sheath protein, gp13

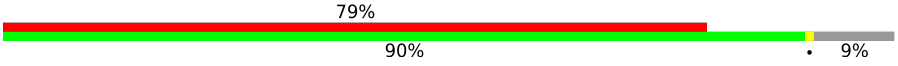
Chain G3:

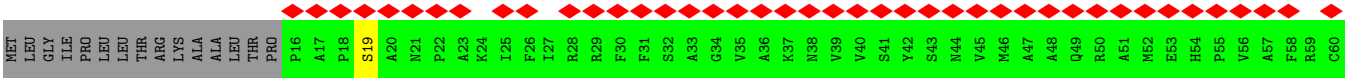


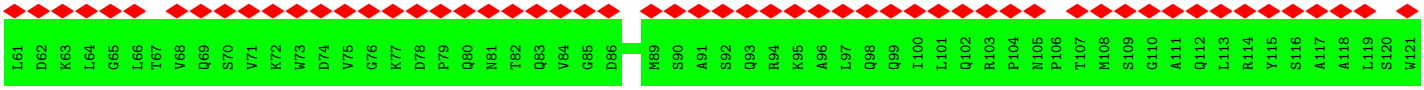


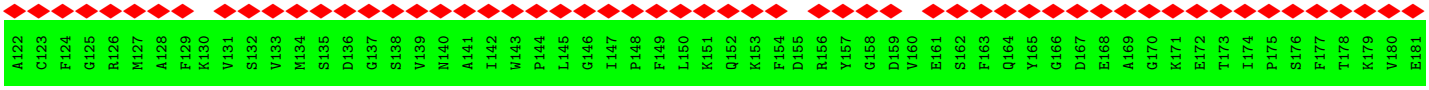
• Molecule 8: Portal protein, gp7

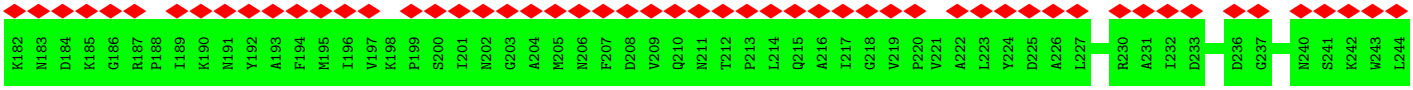
Chain AA:

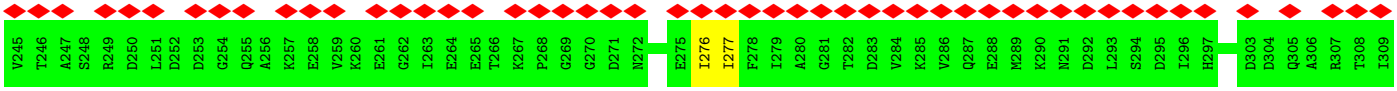


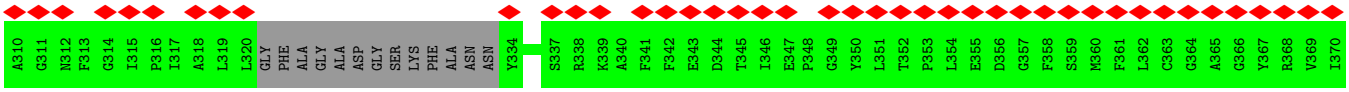


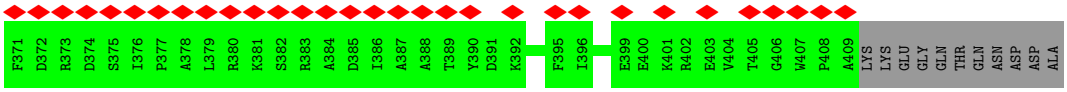






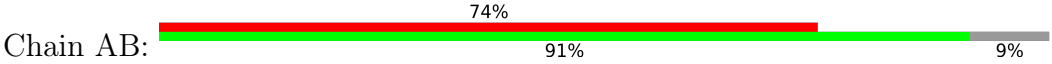


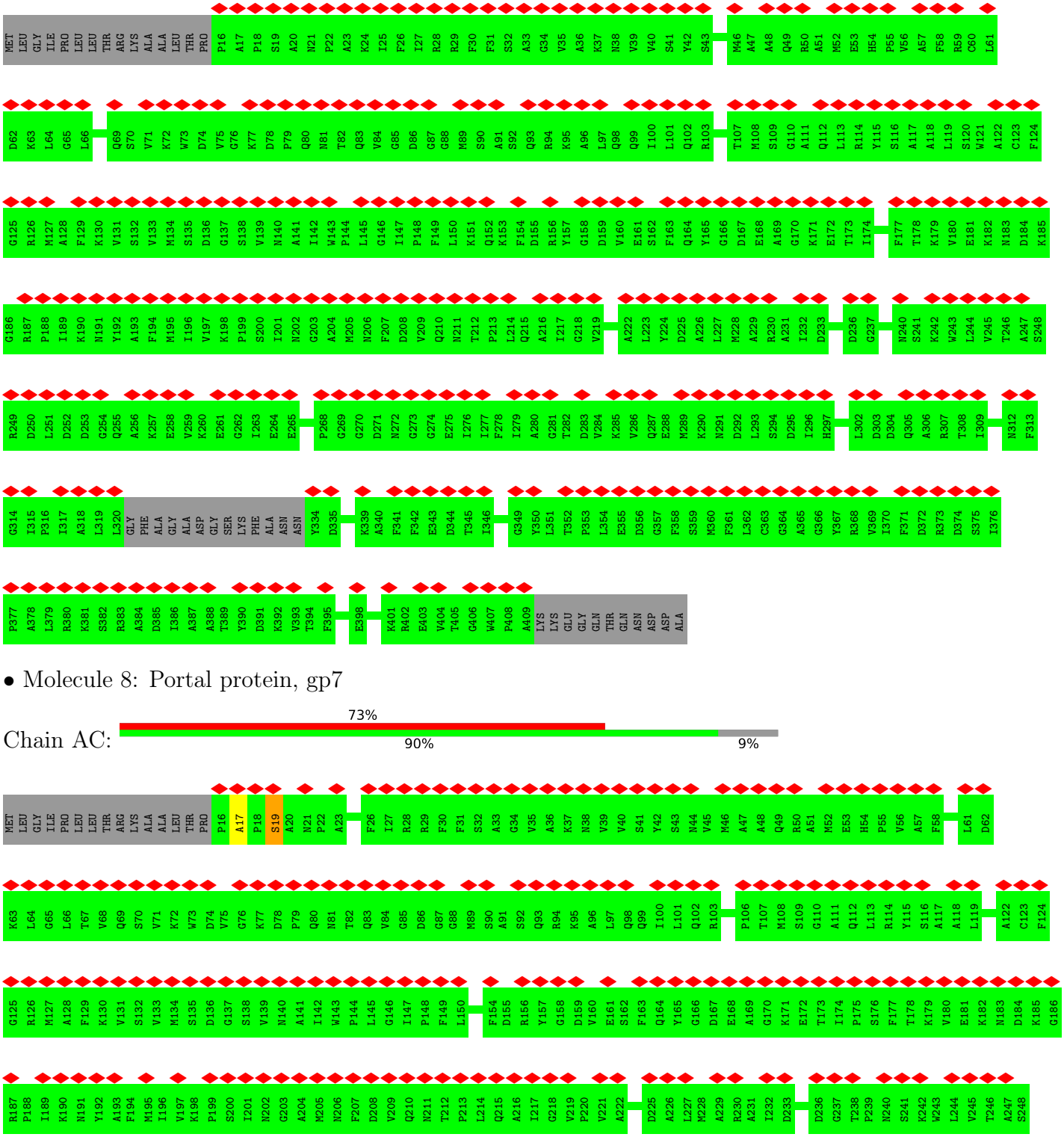




• Molecule 8: Portal protein, gp7

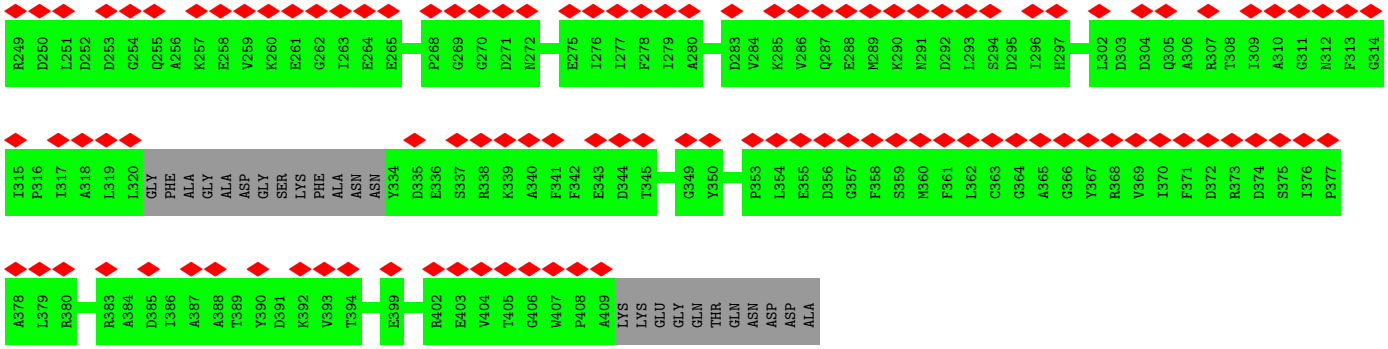
Chain AB:





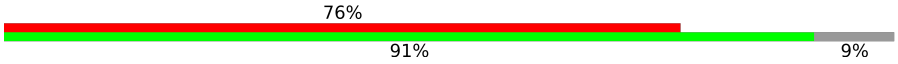
• Molecule 8: Portal protein, gp7

Chain AC:



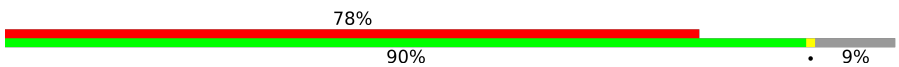
• Molecule 8: Portal protein, gp7

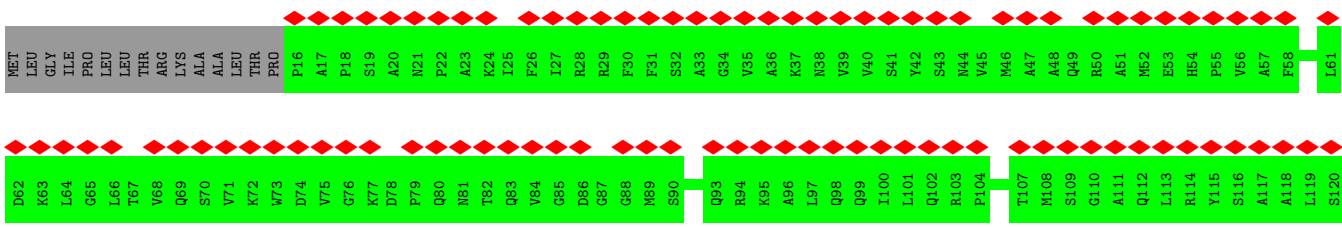
Chain AD:

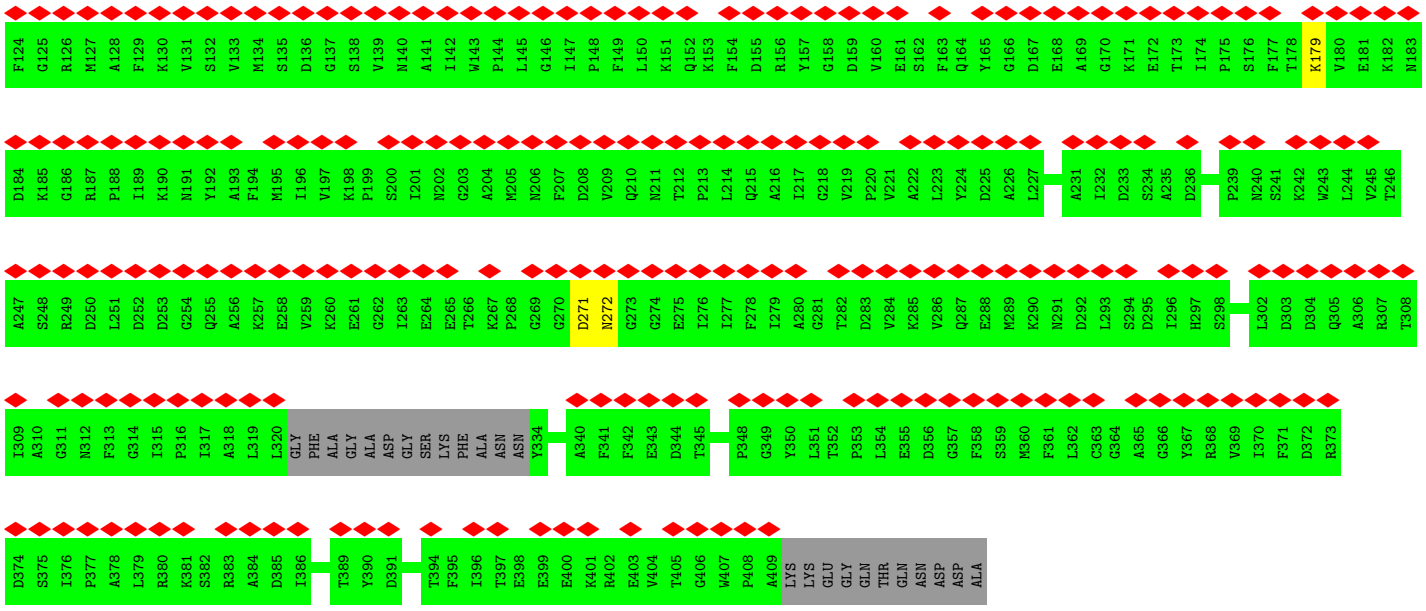


• Molecule 8: Portal protein, gp7

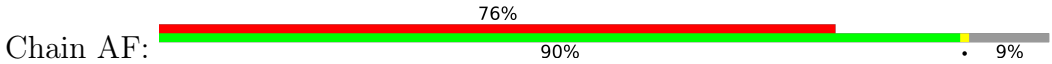
Chain AE:

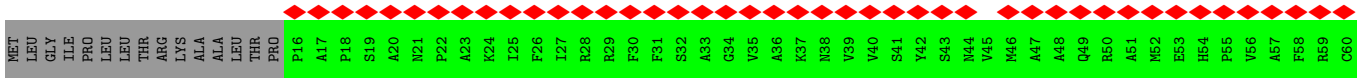




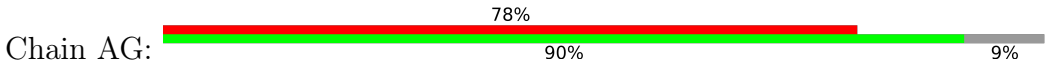


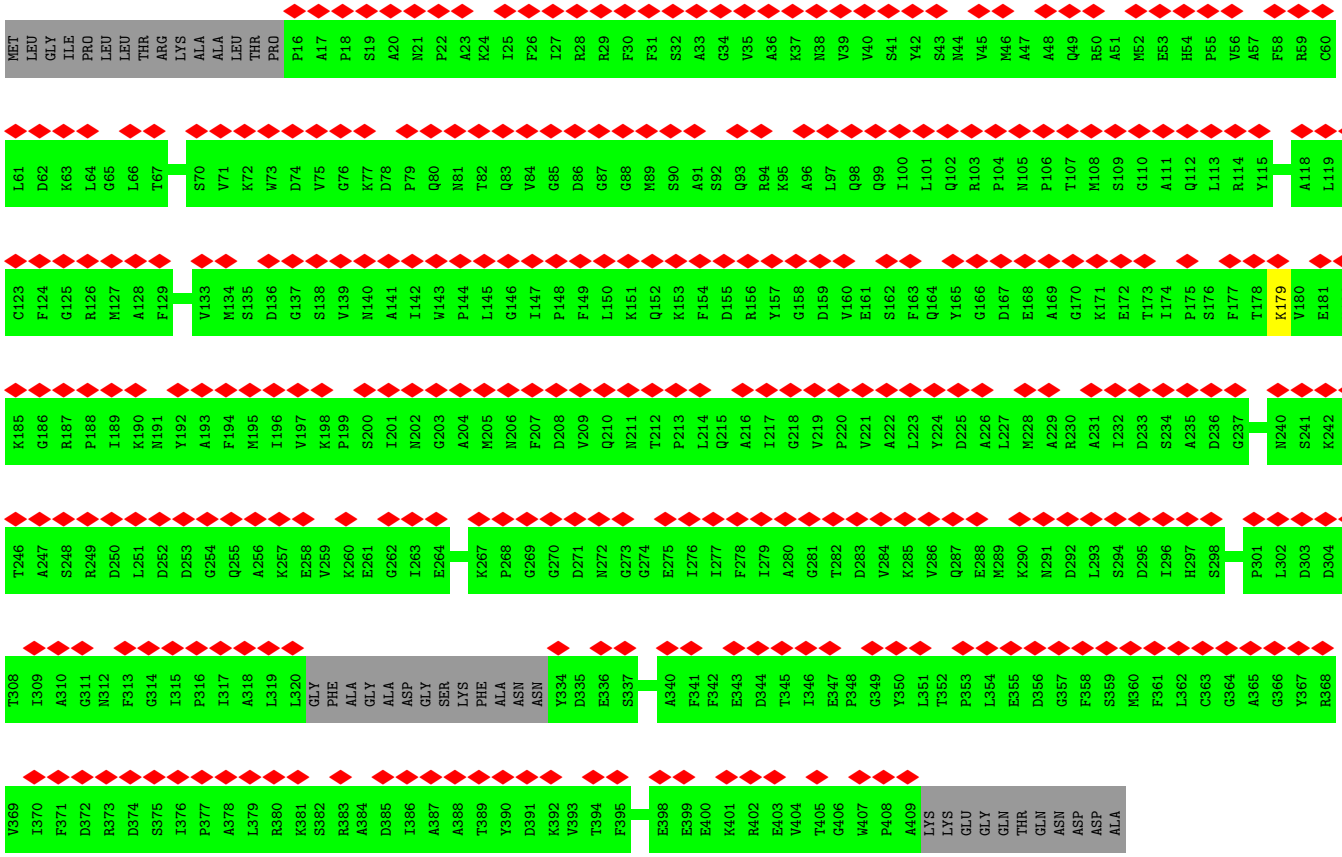
• Molecule 8: Portal protein, gp7





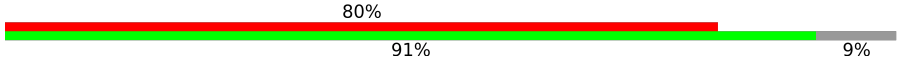
• Molecule 8: Portal protein, gp7

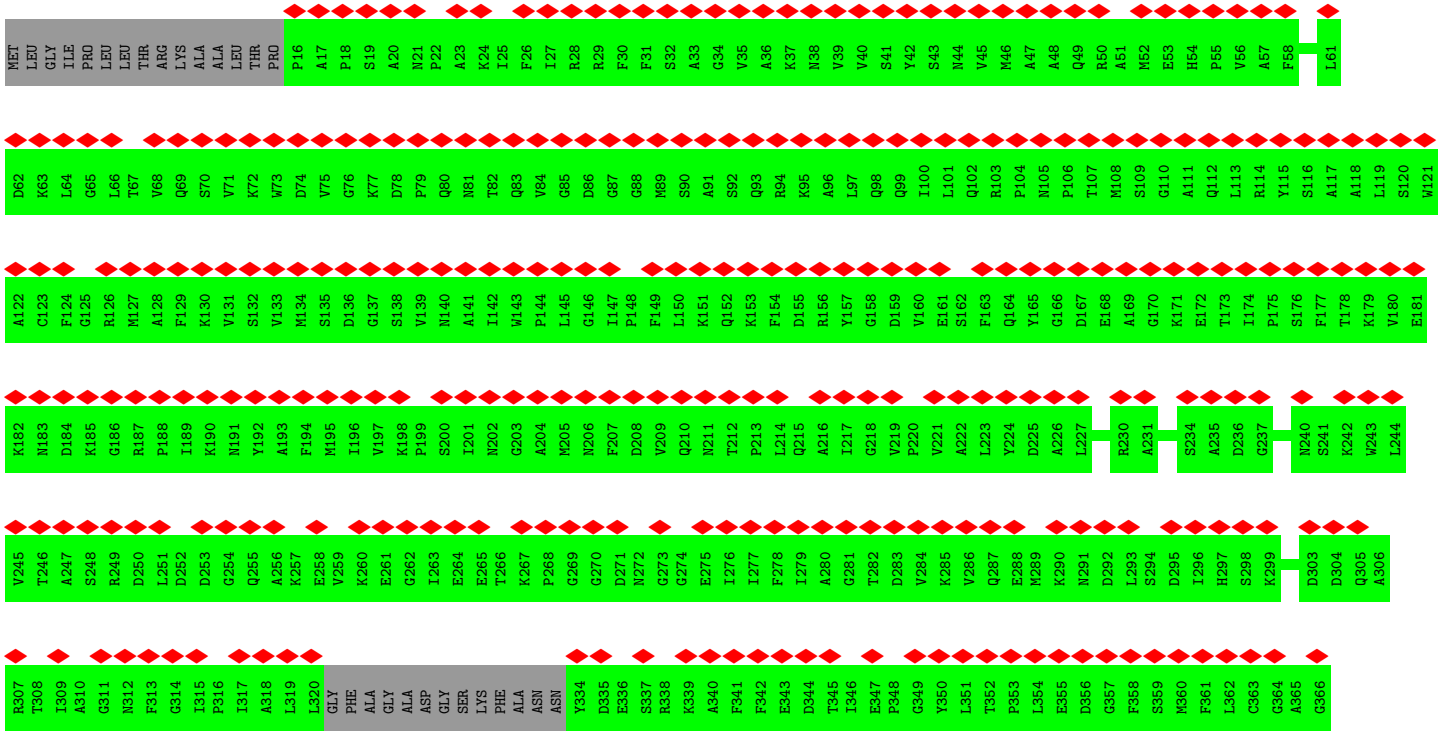


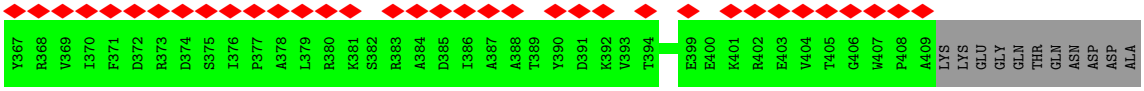


• Molecule 8: Portal protein, gp7

Chain AH:

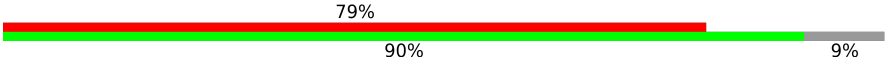


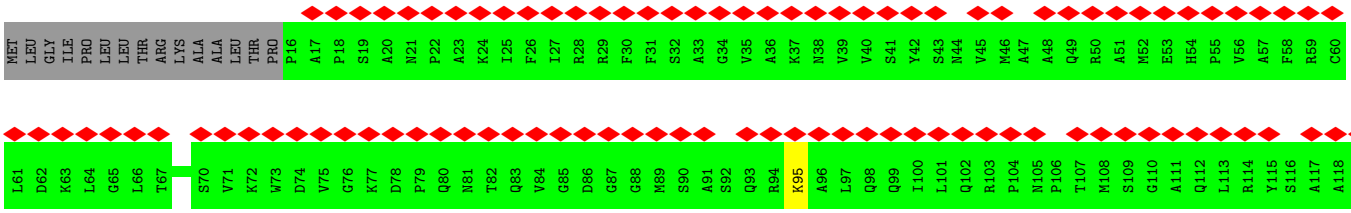




• Molecule 8: Portal protein, gp7

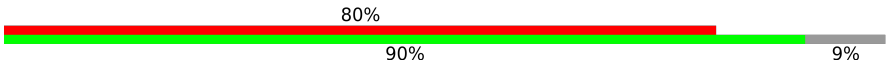
Chain AI:

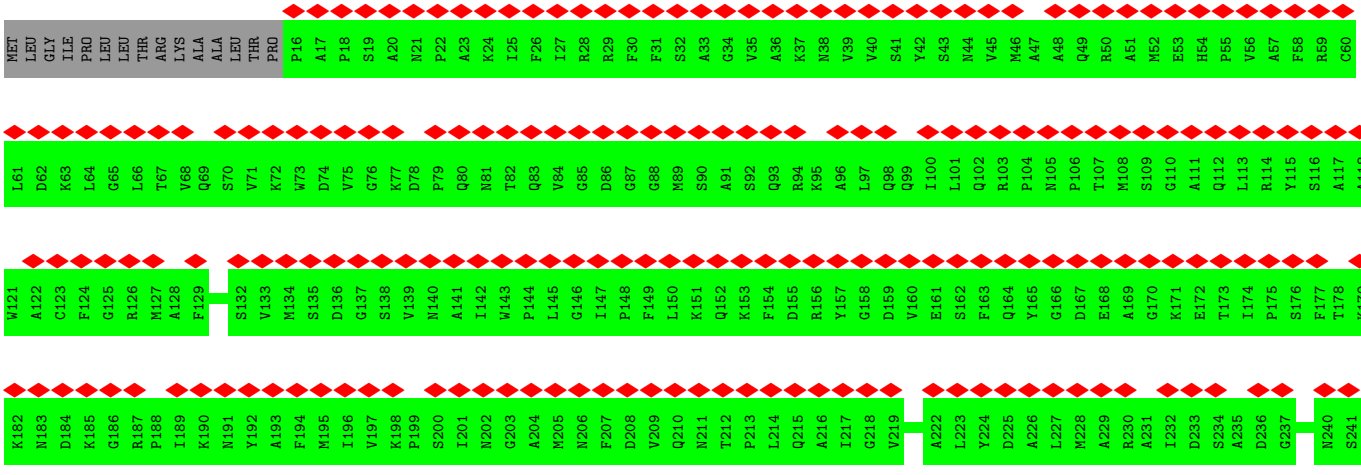


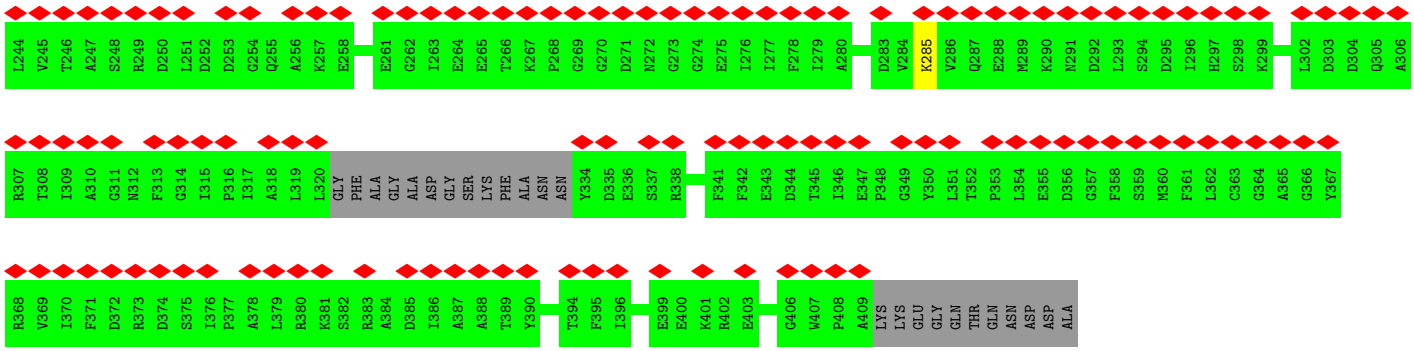


• Molecule 8: Portal protein, gp7

Chain AJ:

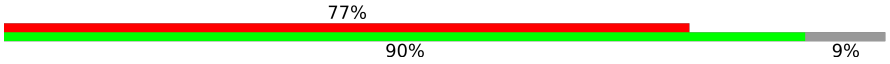


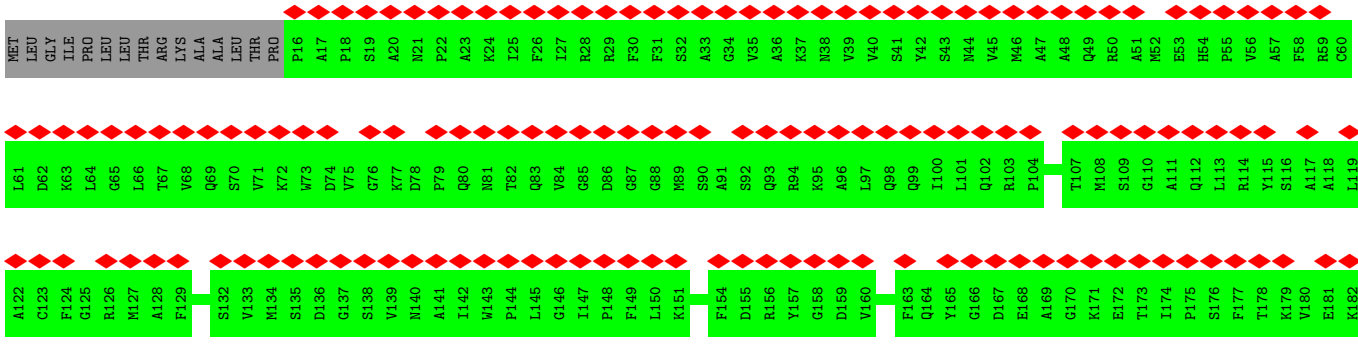




• Molecule 8: Portal protein, gp7

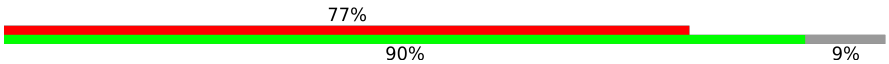
Chain AK:

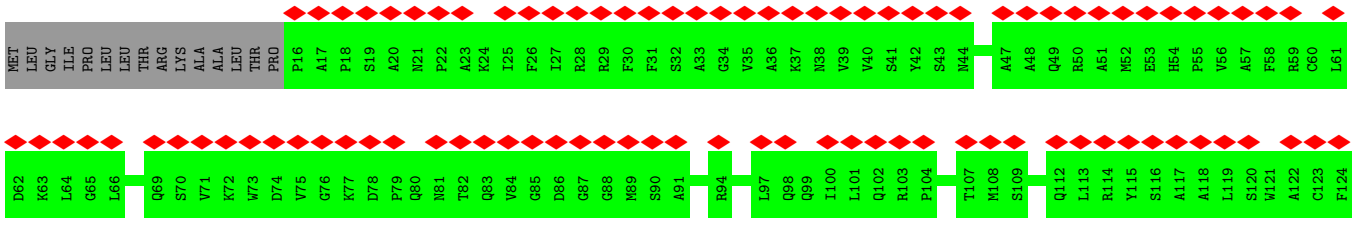


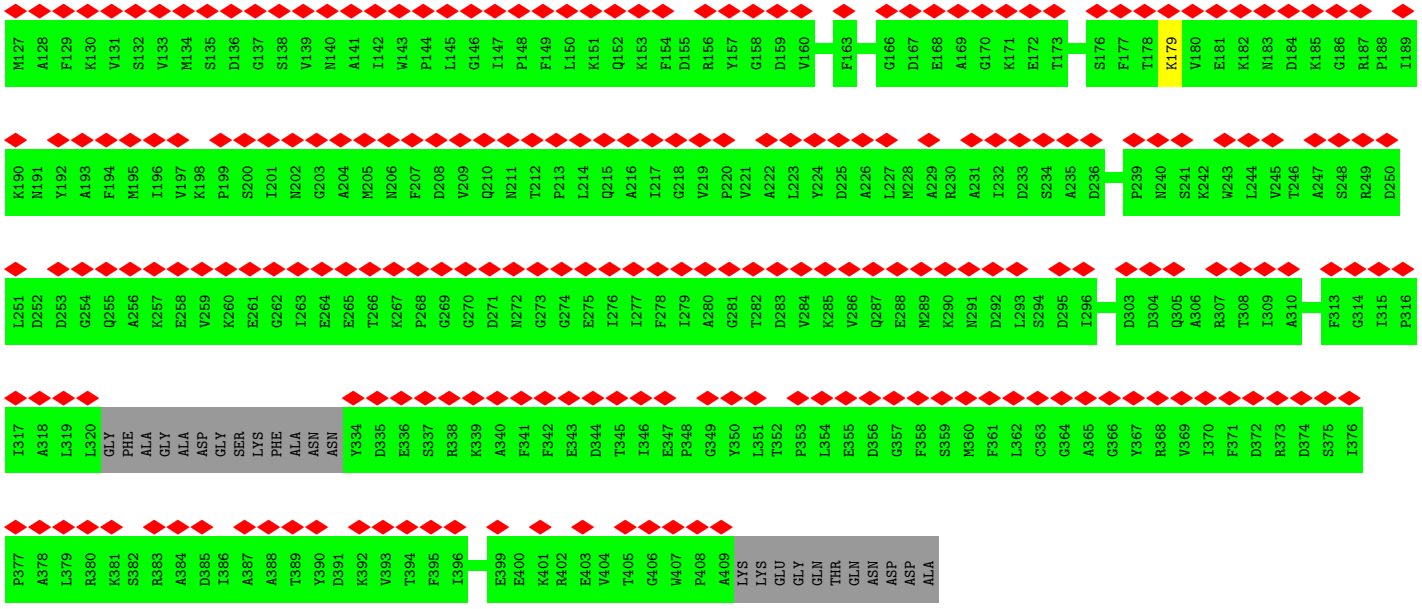


• Molecule 8: Portal protein, gp7

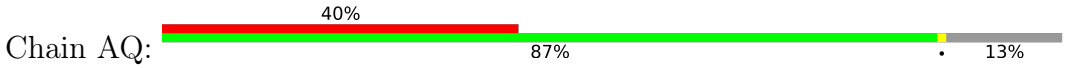
Chain AL:

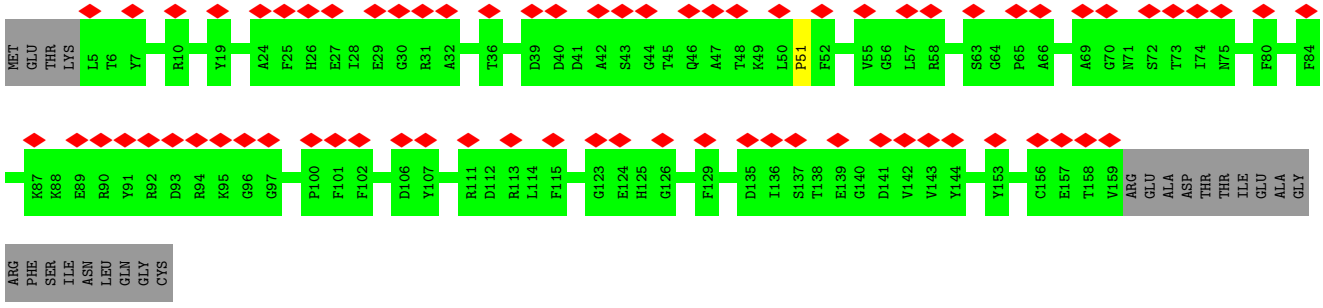




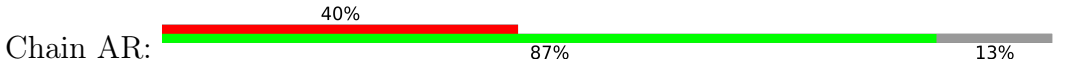


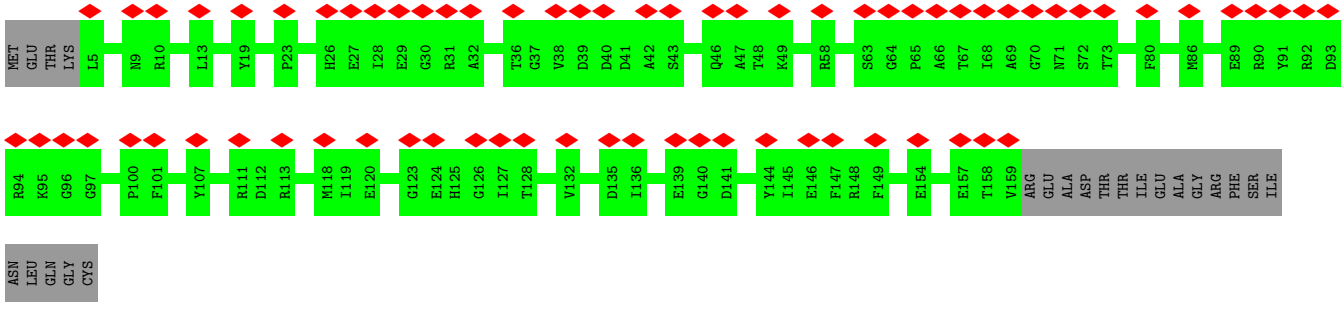
• Molecule 9: Tail-terminator protein, gp18



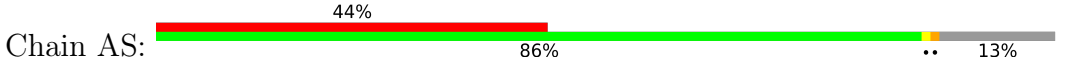


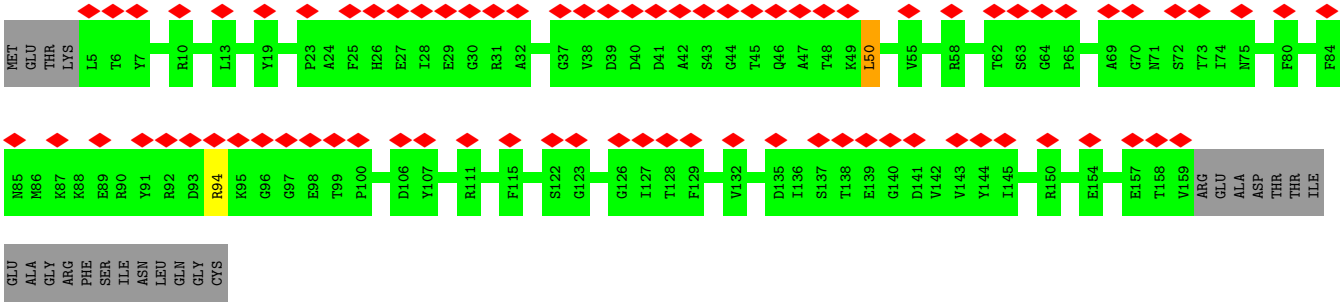
• Molecule 9: Tail-terminator protein, gp18





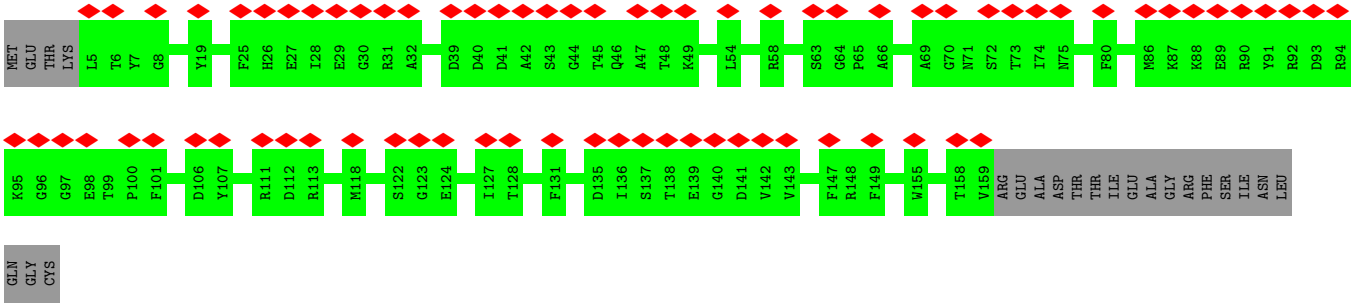
• Molecule 9: Tail-terminator protein, gp18





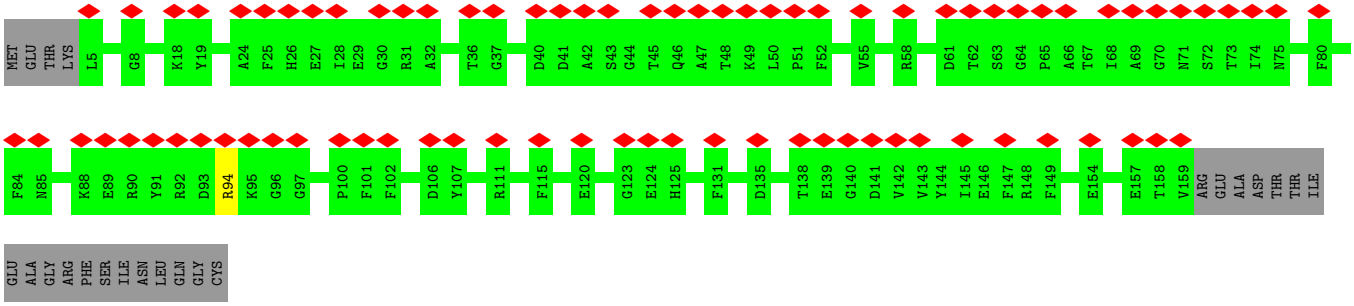
• Molecule 9: Tail-terminator protein, gp18

Chain AT:



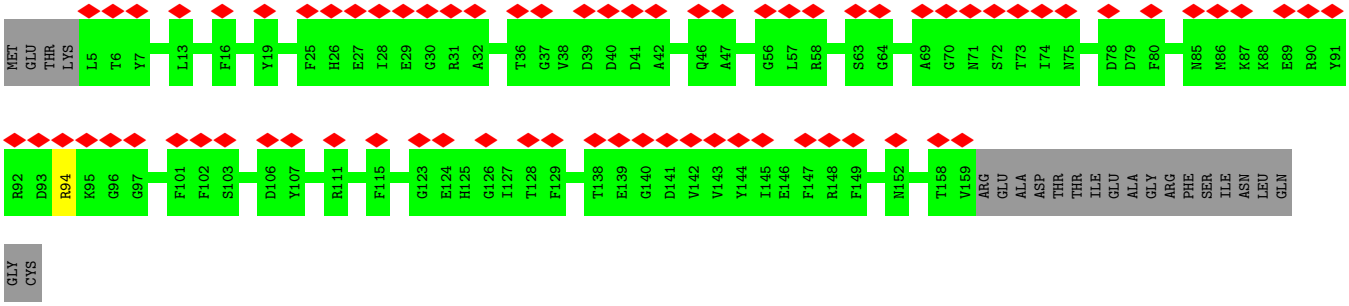
• Molecule 9: Tail-terminator protein, gp18

Chain AW:



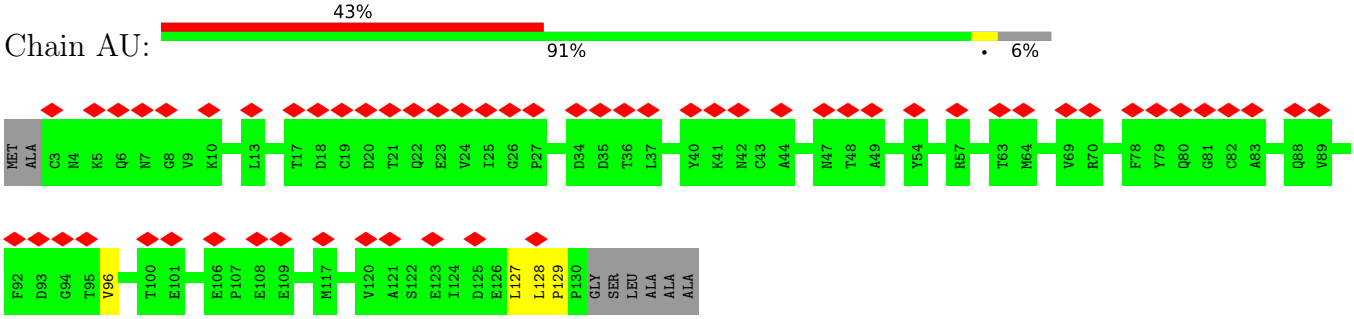
• Molecule 9: Tail-terminator protein, gp18

Chain AX:



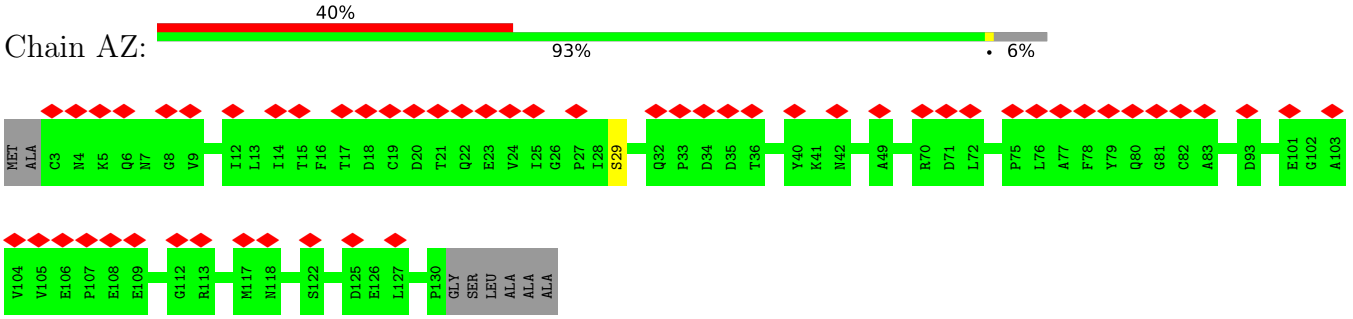
• Molecule 10: Tail-tube, gp21

Chain AU:



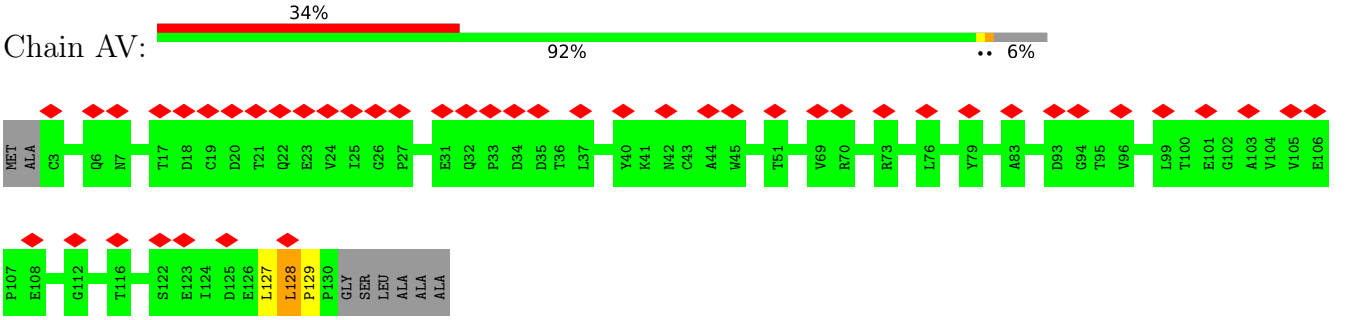
• Molecule 10: Tail-tube, gp21

Chain AZ:



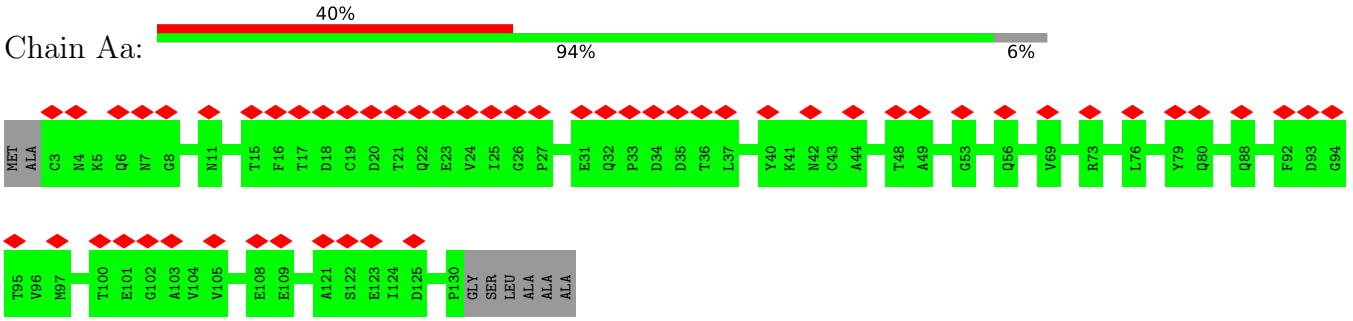
• Molecule 10: Tail-tube, gp21

Chain AV:



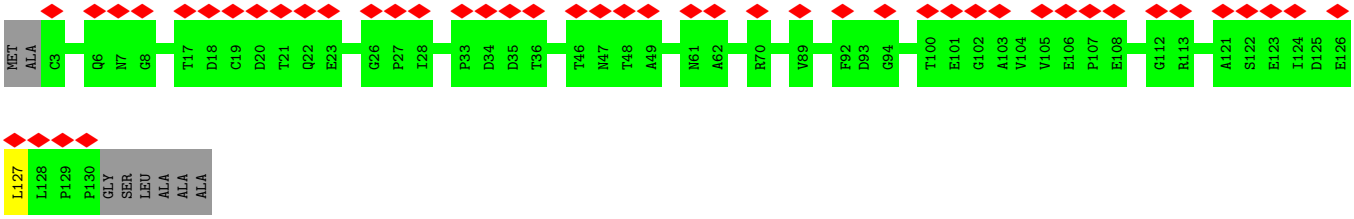
• Molecule 10: Tail-tube, gp21

Chain Aa:



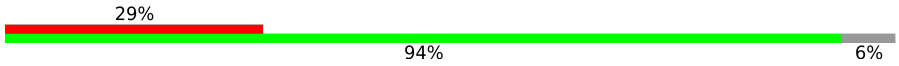
• Molecule 10: Tail-tube, gp21

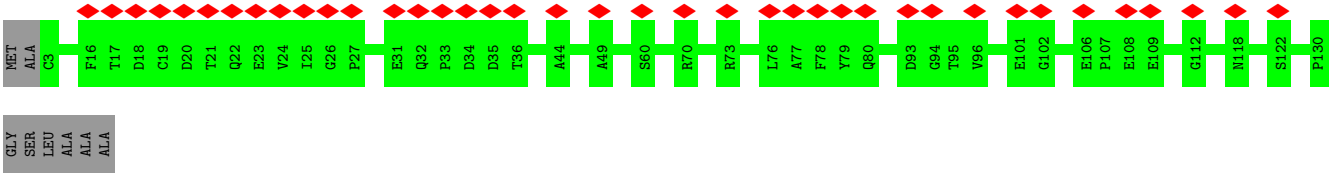
Chain AY:



• Molecule 10: Tail-tube, gp21

Chain Ab:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10083	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	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	0.483	Depositor
Minimum map value	-0.270	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.125	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	0.27	0/213	0.49	0/288
1	a2	0.31	0/213	0.53	0/288
1	a5	0.39	0/213	0.52	0/288
1	a6	0.31	0/213	0.52	0/288
1	a7	0.36	0/213	0.49	0/288
1	b1	0.26	0/213	0.50	0/288
1	b2	0.28	0/213	0.47	0/288
1	b5	0.25	0/213	0.50	0/288
1	b6	0.26	0/213	0.49	0/288
1	b7	0.26	0/213	0.57	0/288
1	c	0.30	0/252	0.52	0/344
1	d	0.35	0/252	0.59	0/344
1	d1	0.32	0/252	0.59	0/344
1	d2	0.27	0/252	0.58	0/344
1	d5	0.35	0/252	0.61	0/344
1	d6	0.32	0/252	0.59	0/344
1	d7	0.33	0/252	0.61	0/344
1	e	0.34	0/252	0.58	0/344
1	e1	0.25	0/213	0.50	0/288
1	e2	0.27	0/213	0.49	0/288
1	e5	0.25	0/213	0.51	0/288
1	e6	0.27	0/213	0.49	0/288
1	e7	0.26	0/213	0.51	0/288
1	f	0.32	0/252	0.64	0/344
1	g	0.35	0/252	0.54	0/344
2	a	0.36	0/1382	0.52	0/1875
2	b	0.30	0/1542	0.51	0/2096
2	h	0.26	0/1358	0.53	0/1842
2	i	0.26	0/1520	0.52	0/2068
2	j	0.29	0/1542	0.56	0/2096
2	k	0.27	0/1358	0.56	1/1842 (0.1%)
2	l	0.29	0/1358	0.52	0/1842
2	m	0.29	0/1519	0.54	0/2063
2	n	0.27	0/1542	0.53	0/2096

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	o	0.25	0/1358	0.48	0/1842
2	p	0.28	0/1358	0.48	0/1842
2	q	0.25	0/1358	0.50	0/1842
3	AM	0.25	0/1017	0.47	0/1381
3	AN	0.24	0/1017	0.47	0/1381
3	AO	0.27	0/1017	0.53	0/1381
3	AP	0.24	0/1017	0.46	0/1381
3	H	0.24	0/1017	0.46	0/1381
3	I	0.24	0/1017	0.46	0/1381
4	f1	0.25	0/142	0.46	0/192
4	f2	0.33	0/142	0.58	0/192
4	f5	0.33	0/142	0.55	0/192
4	f6	0.25	0/142	0.47	0/192
4	f7	0.34	0/142	0.51	0/192
5	g1	0.26	0/2344	0.46	0/3171
5	g2	0.26	0/2344	0.47	0/3171
5	g5	0.27	0/2344	0.47	0/3171
5	g6	0.26	0/2344	0.46	0/3171
5	g7	0.26	0/2344	0.46	0/3171
5	h1	0.28	0/2344	0.51	0/3171
5	h2	0.28	0/2344	0.50	0/3171
5	h5	0.27	0/2344	0.49	0/3171
5	h6	0.27	0/2344	0.48	0/3171
5	h7	0.27	0/2344	0.50	0/3171
5	k1	0.26	0/2313	0.46	0/3128
5	k2	0.26	0/2313	0.47	0/3128
5	k5	0.27	0/2313	0.47	0/3128
5	k6	0.26	0/2313	0.48	0/3128
5	k7	0.27	0/2313	0.48	0/3128
5	n1	0.27	0/2344	0.48	0/3171
5	n2	0.27	0/2344	0.48	0/3171
5	n5	0.27	0/2344	0.48	0/3171
5	n6	0.25	0/2344	0.48	0/3171
5	n7	0.26	0/2344	0.48	0/3171
5	o1	0.27	0/2344	0.48	0/3171
5	o2	0.26	0/2344	0.47	0/3171
5	o5	0.26	0/2344	0.47	0/3171
5	o6	0.25	0/2344	0.47	0/3171
5	o7	0.26	0/2344	0.47	0/3171
5	r1	0.26	0/2344	0.50	0/3171
5	r2	0.26	0/2344	0.47	0/3171
5	r5	0.26	0/2344	0.47	0/3171
5	r6	0.26	0/2344	0.47	0/3171

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	r7	0.27	0/2344	0.50	0/3171
6	l1	0.27	0/1052	0.49	0/1443
6	l2	0.28	0/1052	0.51	0/1443
6	l5	0.28	0/1052	0.49	0/1443
6	l6	0.28	0/1052	0.50	0/1443
6	l7	0.28	0/1052	0.50	0/1443
6	m1	0.26	0/1052	0.50	0/1443
6	m2	0.26	0/1052	0.49	0/1443
6	m5	0.26	0/1052	0.50	0/1443
6	m6	0.26	0/1052	0.48	0/1443
6	m7	0.26	0/1052	0.49	0/1443
6	p1	0.26	0/1052	0.49	0/1443
6	p2	0.26	0/1052	0.49	0/1443
6	p5	0.26	0/1052	0.49	0/1443
6	p6	0.26	0/1052	0.49	0/1443
6	p7	0.27	0/1052	0.48	0/1443
6	q1	0.26	0/1052	0.49	0/1443
6	q2	0.26	0/1052	0.48	0/1443
6	q5	0.26	0/1052	0.48	0/1443
6	q6	0.27	0/1052	0.50	0/1443
6	q7	0.27	0/1052	0.50	0/1443
6	s1	0.26	0/1052	0.47	0/1443
6	s2	0.27	0/1052	0.48	0/1443
6	s5	0.26	0/1052	0.47	0/1443
6	s6	0.26	0/1052	0.47	0/1443
6	s7	0.26	0/1052	0.47	0/1443
6	t1	0.26	0/1052	0.51	0/1443
6	t2	0.27	0/1052	0.52	1/1443 (0.1%)
6	t5	0.26	0/1052	0.49	0/1443
6	t6	0.27	0/1052	0.51	1/1443 (0.1%)
6	t7	0.27	0/1052	0.52	0/1443
6	u1	0.25	0/1040	0.50	0/1429
6	u2	0.26	0/1040	0.52	0/1429
6	u5	0.25	0/1040	0.50	0/1429
6	u6	0.26	0/1040	0.50	0/1429
6	u7	0.25	0/1040	0.51	0/1429
6	v1	0.26	0/1040	0.50	0/1429
6	v2	0.26	0/1040	0.49	0/1429
6	v5	0.26	0/1040	0.49	0/1429
6	v6	0.26	0/1040	0.51	0/1429
6	v7	0.27	0/1040	0.49	0/1429
7	03	0.25	0/1723	0.46	0/2353
7	13	0.25	0/1723	0.46	0/2353

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
7	23	0.25	0/1723	0.47	0/2353
7	33	0.25	0/1723	0.45	0/2353
7	43	0.26	0/1723	0.46	0/2353
7	53	0.26	0/1723	0.46	0/2353
7	63	0.25	0/1723	0.45	0/2353
7	73	0.25	0/1723	0.47	0/2353
7	83	0.25	0/1723	0.46	0/2353
7	93	0.25	0/1723	0.45	0/2353
7	A3	0.25	0/1723	0.45	0/2353
7	B3	0.26	0/1723	0.44	0/2353
7	C3	0.25	0/1723	0.46	0/2353
7	D3	0.25	0/1723	0.45	0/2353
7	E3	0.25	0/1723	0.45	0/2353
7	F3	0.25	0/1723	0.46	0/2353
7	G3	0.26	0/1723	0.48	0/2353
7	J3	0.26	0/1723	0.46	0/2353
7	K3	0.28	0/1768	0.48	0/2414
7	L3	0.26	0/1723	0.47	0/2353
7	M3	0.27	0/1723	0.47	0/2353
7	N3	0.26	0/1768	0.47	0/2414
7	O3	0.25	0/1723	0.47	0/2353
7	P3	0.27	0/1717	0.47	0/2345
7	Q3	0.28	0/1768	0.47	0/2414
7	R3	0.28	0/1723	0.48	0/2353
7	S3	0.26	0/1717	0.46	0/2345
7	T3	0.26	0/1723	0.47	0/2353
7	U3	0.26	0/1712	0.47	0/2338
7	V3	0.26	0/1723	0.47	0/2353
7	W3	0.26	0/1768	0.49	0/2414
7	X3	0.26	0/1723	0.47	0/2353
7	Y3	0.25	0/1723	0.46	0/2353
7	Z3	0.26	0/1723	0.45	0/2353
7	a3	0.27	0/1723	0.47	0/2353
7	b3	0.26	0/1723	0.46	0/2353
7	c3	0.26	0/1723	0.47	0/2353
7	d3	0.26	0/1723	0.46	0/2353
7	e3	0.25	0/1723	0.46	0/2353
7	f3	0.26	0/1723	0.49	0/2353
7	g3	0.26	0/1723	0.46	0/2353
7	h3	0.25	0/1723	0.45	0/2353
7	i3	0.26	0/1723	0.46	0/2353
7	j3	0.26	0/1723	0.47	0/2353
7	k3	0.25	0/1723	0.46	0/2353

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	l3	0.25	0/1723	0.46	0/2353
7	m3	0.26	0/1723	0.45	0/2353
7	n3	0.26	0/1723	0.46	0/2353
7	o3	0.26	0/1723	0.47	0/2353
7	p3	0.25	0/1723	0.46	0/2353
7	q3	0.26	0/1723	0.45	0/2353
7	r3	0.25	0/1723	0.46	0/2353
7	s3	0.25	0/1723	0.46	0/2353
7	t3	0.25	0/1723	0.46	0/2353
7	u3	0.25	0/1723	0.47	0/2353
7	v3	0.25	0/1723	0.46	0/2353
7	w3	0.25	0/1723	0.45	0/2353
7	x3	0.25	0/1723	0.46	0/2353
7	y3	0.25	0/1723	0.46	0/2353
7	z3	0.25	0/1723	0.45	0/2353
8	AA	0.25	0/3000	0.46	0/4056
8	AB	0.26	0/3000	0.48	0/4056
8	AC	0.25	0/3000	0.46	0/4056
8	AD	0.25	0/3000	0.46	0/4056
8	AE	0.27	0/3000	0.50	1/4056 (0.0%)
8	AF	0.26	0/3000	0.47	1/4056 (0.0%)
8	AG	0.26	0/3000	0.47	0/4056
8	AH	0.26	0/3000	0.46	0/4056
8	AI	0.26	0/3000	0.47	0/4056
8	AJ	0.26	0/3000	0.47	0/4056
8	AK	0.25	0/3000	0.46	0/4056
8	AL	0.27	0/3000	0.51	0/4056
9	AQ	0.25	0/1281	0.46	0/1734
9	AR	0.25	0/1281	0.44	0/1734
9	AS	0.26	0/1281	0.49	0/1734
9	AT	0.25	0/1281	0.47	0/1734
9	AW	0.25	0/1281	0.45	0/1734
9	AX	0.26	0/1281	0.49	0/1734
10	AU	0.25	0/993	0.49	0/1358
10	AV	0.25	0/993	0.49	0/1358
10	AY	0.25	0/993	0.51	0/1358
10	AZ	0.25	0/993	0.50	0/1358
10	Aa	0.25	0/993	0.47	0/1358
10	Ab	0.26	0/993	0.49	0/1358
All	All	0.26	0/295028	0.48	5/401464 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	k	76	GLY	C-N-CA	-5.88	107.01	121.70
6	t6	134	GLY	N-CA-C	5.17	126.02	113.10
8	AE	272	ASN	N-CA-C	-5.16	97.07	111.00
6	t2	134	GLY	N-CA-C	5.04	125.71	113.10
8	AF	293	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a1	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
1	a2	26/38 (68%)	24 (92%)	2 (8%)	0	100	100
1	a5	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
1	a6	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
1	a7	26/38 (68%)	25 (96%)	1 (4%)	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%)	26 (100%)	0	0	100	100
1	b7	26/38 (68%)	25 (96%)	1 (4%)	0	100	100
1	c	32/38 (84%)	31 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	d	32/38 (84%)	32 (100%)	0	0	100	100
1	d1	32/38 (84%)	26 (81%)	6 (19%)	0	100	100
1	d2	32/38 (84%)	27 (84%)	5 (16%)	0	100	100
1	d5	32/38 (84%)	29 (91%)	3 (9%)	0	100	100
1	d6	32/38 (84%)	27 (84%)	5 (16%)	0	100	100
1	d7	32/38 (84%)	25 (78%)	7 (22%)	0	100	100
1	e	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
1	e1	26/38 (68%)	21 (81%)	5 (19%)	0	100	100
1	e2	26/38 (68%)	20 (77%)	6 (23%)	0	100	100
1	e5	26/38 (68%)	22 (85%)	4 (15%)	0	100	100
1	e6	26/38 (68%)	19 (73%)	7 (27%)	0	100	100
1	e7	26/38 (68%)	20 (77%)	6 (23%)	0	100	100
1	f	32/38 (84%)	31 (97%)	1 (3%)	0	100	100
1	g	32/38 (84%)	26 (81%)	5 (16%)	1 (3%)	4	31
2	a	172/202 (85%)	128 (74%)	40 (23%)	4 (2%)	6	37
2	b	193/202 (96%)	160 (83%)	30 (16%)	3 (2%)	9	45
2	h	169/202 (84%)	144 (85%)	23 (14%)	2 (1%)	13	50
2	i	191/202 (95%)	162 (85%)	26 (14%)	3 (2%)	9	45
2	j	193/202 (96%)	152 (79%)	40 (21%)	1 (0%)	29	68
2	k	169/202 (84%)	126 (75%)	41 (24%)	2 (1%)	13	50
2	l	169/202 (84%)	146 (86%)	22 (13%)	1 (1%)	25	65
2	m	190/202 (94%)	153 (80%)	35 (18%)	2 (1%)	14	52
2	n	193/202 (96%)	160 (83%)	33 (17%)	0	100	100
2	o	169/202 (84%)	140 (83%)	25 (15%)	4 (2%)	6	36
2	p	169/202 (84%)	143 (85%)	25 (15%)	1 (1%)	25	65
2	q	169/202 (84%)	141 (83%)	24 (14%)	4 (2%)	6	36
3	AM	123/141 (87%)	113 (92%)	9 (7%)	1 (1%)	19	60
3	AN	123/141 (87%)	115 (94%)	7 (6%)	1 (1%)	19	60
3	AO	123/141 (87%)	114 (93%)	7 (6%)	2 (2%)	9	45
3	AP	123/141 (87%)	114 (93%)	8 (6%)	1 (1%)	19	60
3	H	123/141 (87%)	115 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	I	123/141 (87%)	116 (94%)	6 (5%)	1 (1%)	19 60
4	f1	18/217 (8%)	16 (89%)	2 (11%)	0	100 100
4	f2	18/217 (8%)	14 (78%)	4 (22%)	0	100 100
4	f5	18/217 (8%)	13 (72%)	5 (28%)	0	100 100
4	f6	18/217 (8%)	15 (83%)	3 (17%)	0	100 100
4	f7	18/217 (8%)	15 (83%)	3 (17%)	0	100 100
5	g1	289/465 (62%)	256 (89%)	33 (11%)	0	100 100
5	g2	289/465 (62%)	255 (88%)	34 (12%)	0	100 100
5	g5	289/465 (62%)	255 (88%)	34 (12%)	0	100 100
5	g6	289/465 (62%)	257 (89%)	32 (11%)	0	100 100
5	g7	289/465 (62%)	258 (89%)	31 (11%)	0	100 100
5	h1	289/465 (62%)	240 (83%)	48 (17%)	1 (0%)	41 76
5	h2	289/465 (62%)	248 (86%)	41 (14%)	0	100 100
5	h5	289/465 (62%)	246 (85%)	42 (14%)	1 (0%)	41 76
5	h6	289/465 (62%)	242 (84%)	47 (16%)	0	100 100
5	h7	289/465 (62%)	248 (86%)	41 (14%)	0	100 100
5	k1	286/465 (62%)	263 (92%)	23 (8%)	0	100 100
5	k2	286/465 (62%)	257 (90%)	29 (10%)	0	100 100
5	k5	286/465 (62%)	261 (91%)	25 (9%)	0	100 100
5	k6	286/465 (62%)	257 (90%)	28 (10%)	1 (0%)	41 76
5	k7	286/465 (62%)	258 (90%)	28 (10%)	0	100 100
5	n1	289/465 (62%)	254 (88%)	34 (12%)	1 (0%)	41 76
5	n2	289/465 (62%)	248 (86%)	39 (14%)	2 (1%)	22 62
5	n5	289/465 (62%)	248 (86%)	41 (14%)	0	100 100
5	n6	289/465 (62%)	254 (88%)	35 (12%)	0	100 100
5	n7	289/465 (62%)	255 (88%)	34 (12%)	0	100 100
5	o1	289/465 (62%)	249 (86%)	38 (13%)	2 (1%)	22 62
5	o2	289/465 (62%)	249 (86%)	37 (13%)	3 (1%)	15 54
5	o5	289/465 (62%)	250 (86%)	37 (13%)	2 (1%)	22 62
5	o6	289/465 (62%)	250 (86%)	37 (13%)	2 (1%)	22 62
5	o7	289/465 (62%)	248 (86%)	38 (13%)	3 (1%)	15 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	r1	289/465 (62%)	262 (91%)	27 (9%)	0	100	100
5	r2	289/465 (62%)	261 (90%)	28 (10%)	0	100	100
5	r5	289/465 (62%)	259 (90%)	30 (10%)	0	100	100
5	r6	289/465 (62%)	261 (90%)	28 (10%)	0	100	100
5	r7	289/465 (62%)	262 (91%)	27 (9%)	0	100	100
6	l1	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
6	l2	135/137 (98%)	118 (87%)	17 (13%)	0	100	100
6	l5	135/137 (98%)	118 (87%)	15 (11%)	2 (2%)	10	46
6	l6	135/137 (98%)	122 (90%)	13 (10%)	0	100	100
6	l7	135/137 (98%)	122 (90%)	12 (9%)	1 (1%)	22	62
6	m1	135/137 (98%)	122 (90%)	13 (10%)	0	100	100
6	m2	135/137 (98%)	121 (90%)	14 (10%)	0	100	100
6	m5	135/137 (98%)	122 (90%)	13 (10%)	0	100	100
6	m6	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
6	m7	135/137 (98%)	124 (92%)	11 (8%)	0	100	100
6	p1	135/137 (98%)	119 (88%)	16 (12%)	0	100	100
6	p2	135/137 (98%)	114 (84%)	20 (15%)	1 (1%)	22	62
6	p5	135/137 (98%)	115 (85%)	20 (15%)	0	100	100
6	p6	135/137 (98%)	115 (85%)	20 (15%)	0	100	100
6	p7	135/137 (98%)	116 (86%)	19 (14%)	0	100	100
6	q1	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
6	q2	135/137 (98%)	124 (92%)	11 (8%)	0	100	100
6	q5	135/137 (98%)	121 (90%)	14 (10%)	0	100	100
6	q6	135/137 (98%)	119 (88%)	16 (12%)	0	100	100
6	q7	135/137 (98%)	124 (92%)	11 (8%)	0	100	100
6	s1	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
6	s2	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
6	s5	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
6	s6	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
6	s7	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
6	t1	135/137 (98%)	121 (90%)	14 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	t2	135/137 (98%)	125 (93%)	10 (7%)	0	100	100
6	t5	135/137 (98%)	122 (90%)	13 (10%)	0	100	100
6	t6	135/137 (98%)	124 (92%)	11 (8%)	0	100	100
6	t7	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
6	u1	134/137 (98%)	116 (87%)	18 (13%)	0	100	100
6	u2	134/137 (98%)	121 (90%)	13 (10%)	0	100	100
6	u5	134/137 (98%)	121 (90%)	13 (10%)	0	100	100
6	u6	134/137 (98%)	121 (90%)	13 (10%)	0	100	100
6	u7	134/137 (98%)	121 (90%)	13 (10%)	0	100	100
6	v1	134/137 (98%)	117 (87%)	16 (12%)	1 (1%)	22	62
6	v2	134/137 (98%)	114 (85%)	20 (15%)	0	100	100
6	v5	134/137 (98%)	117 (87%)	17 (13%)	0	100	100
6	v6	134/137 (98%)	113 (84%)	21 (16%)	0	100	100
6	v7	134/137 (98%)	114 (85%)	20 (15%)	0	100	100
7	03	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
7	13	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
7	23	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
7	33	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
7	43	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
7	53	219/230 (95%)	204 (93%)	14 (6%)	1 (0%)	29	68
7	63	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
7	73	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
7	83	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
7	93	219/230 (95%)	208 (95%)	11 (5%)	0	100	100
7	A3	219/230 (95%)	204 (93%)	15 (7%)	0	100	100
7	B3	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
7	C3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
7	D3	219/230 (95%)	204 (93%)	15 (7%)	0	100	100
7	E3	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
7	F3	219/230 (95%)	203 (93%)	16 (7%)	0	100	100
7	G3	219/230 (95%)	204 (93%)	15 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	J3	219/230 (95%)	203 (93%)	16 (7%)	0	100	100
7	K3	228/230 (99%)	212 (93%)	15 (7%)	1 (0%)	34	72
7	L3	219/230 (95%)	203 (93%)	16 (7%)	0	100	100
7	M3	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
7	N3	228/230 (99%)	210 (92%)	18 (8%)	0	100	100
7	O3	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
7	P3	218/230 (95%)	207 (95%)	11 (5%)	0	100	100
7	Q3	228/230 (99%)	212 (93%)	14 (6%)	2 (1%)	17	56
7	R3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
7	S3	218/230 (95%)	205 (94%)	13 (6%)	0	100	100
7	T3	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
7	U3	217/230 (94%)	200 (92%)	17 (8%)	0	100	100
7	V3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
7	W3	228/230 (99%)	205 (90%)	22 (10%)	1 (0%)	34	72
7	X3	219/230 (95%)	204 (93%)	15 (7%)	0	100	100
7	Y3	219/230 (95%)	203 (93%)	16 (7%)	0	100	100
7	Z3	219/230 (95%)	203 (93%)	16 (7%)	0	100	100
7	a3	219/230 (95%)	204 (93%)	15 (7%)	0	100	100
7	b3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
7	c3	219/230 (95%)	200 (91%)	19 (9%)	0	100	100
7	d3	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
7	e3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
7	f3	219/230 (95%)	200 (91%)	16 (7%)	3 (1%)	11	47
7	g3	219/230 (95%)	205 (94%)	12 (6%)	2 (1%)	17	56
7	h3	219/230 (95%)	204 (93%)	15 (7%)	0	100	100
7	i3	219/230 (95%)	204 (93%)	15 (7%)	0	100	100
7	j3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
7	k3	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
7	l3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
7	m3	219/230 (95%)	204 (93%)	15 (7%)	0	100	100
7	n3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	o3	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
7	p3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
7	q3	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
7	r3	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
7	s3	219/230 (95%)	203 (93%)	16 (7%)	0	100	100
7	t3	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
7	u3	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
7	v3	219/230 (95%)	201 (92%)	18 (8%)	0	100	100
7	w3	219/230 (95%)	202 (92%)	17 (8%)	0	100	100
7	x3	219/230 (95%)	205 (94%)	14 (6%)	0	100	100
7	y3	219/230 (95%)	199 (91%)	20 (9%)	0	100	100
7	z3	219/230 (95%)	206 (94%)	13 (6%)	0	100	100
8	AA	377/420 (90%)	326 (86%)	50 (13%)	1 (0%)	41	76
8	AB	377/420 (90%)	333 (88%)	44 (12%)	0	100	100
8	AC	377/420 (90%)	332 (88%)	43 (11%)	2 (0%)	29	68
8	AD	377/420 (90%)	334 (89%)	43 (11%)	0	100	100
8	AE	377/420 (90%)	322 (85%)	54 (14%)	1 (0%)	41	76
8	AF	377/420 (90%)	336 (89%)	40 (11%)	1 (0%)	41	76
8	AG	377/420 (90%)	335 (89%)	42 (11%)	0	100	100
8	AH	377/420 (90%)	334 (89%)	43 (11%)	0	100	100
8	AI	377/420 (90%)	330 (88%)	47 (12%)	0	100	100
8	AJ	377/420 (90%)	331 (88%)	46 (12%)	0	100	100
8	AK	377/420 (90%)	327 (87%)	50 (13%)	0	100	100
8	AL	377/420 (90%)	335 (89%)	42 (11%)	0	100	100
9	AQ	153/178 (86%)	139 (91%)	13 (8%)	1 (1%)	22	62
9	AR	153/178 (86%)	142 (93%)	11 (7%)	0	100	100
9	AS	153/178 (86%)	141 (92%)	10 (6%)	2 (1%)	12	48
9	AT	153/178 (86%)	141 (92%)	12 (8%)	0	100	100
9	AW	153/178 (86%)	143 (94%)	9 (6%)	1 (1%)	22	62
9	AX	153/178 (86%)	141 (92%)	11 (7%)	1 (1%)	22	62
10	AU	126/136 (93%)	115 (91%)	9 (7%)	2 (2%)	9	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	AV	126/136 (93%)	115 (91%)	9 (7%)	2 (2%)	9 45
10	AY	126/136 (93%)	114 (90%)	12 (10%)	0	100 100
10	AZ	126/136 (93%)	115 (91%)	10 (8%)	1 (1%)	19 60
10	Aa	126/136 (93%)	121 (96%)	5 (4%)	0	100 100
10	Ab	126/136 (93%)	118 (94%)	8 (6%)	0	100 100
All	All	37099/45459 (82%)	33364 (90%)	3653 (10%)	82 (0%)	50 81

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	o	50	PRO
7	f3	54	THR
10	AZ	29	SER
3	AN	49	GLN
3	AO	50	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a1	25/32 (78%)	25 (100%)	0	100 100
1	a2	25/32 (78%)	24 (96%)	1 (4%)	31 56
1	a5	25/32 (78%)	25 (100%)	0	100 100
1	a6	25/32 (78%)	25 (100%)	0	100 100
1	a7	25/32 (78%)	25 (100%)	0	100 100
1	b1	25/32 (78%)	25 (100%)	0	100 100
1	b2	25/32 (78%)	24 (96%)	1 (4%)	31 56
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%)	24 (96%)	1 (4%)	31 56
1	c	29/32 (91%)	29 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	28 (97%)	1 (3%)	37	61
1	d6	29/32 (91%)	28 (97%)	1 (3%)	37	61
1	d7	29/32 (91%)	28 (97%)	1 (3%)	37	61
1	e	29/32 (91%)	29 (100%)	0	100	100
1	e1	25/32 (78%)	24 (96%)	1 (4%)	31	56
1	e2	25/32 (78%)	24 (96%)	1 (4%)	31	56
1	e5	25/32 (78%)	24 (96%)	1 (4%)	31	56
1	e6	25/32 (78%)	24 (96%)	1 (4%)	31	56
1	e7	25/32 (78%)	24 (96%)	1 (4%)	31	56
1	f	29/32 (91%)	28 (97%)	1 (3%)	37	61
1	g	29/32 (91%)	25 (86%)	4 (14%)	3	19
2	a	144/168 (86%)	140 (97%)	4 (3%)	43	65
2	b	161/168 (96%)	159 (99%)	2 (1%)	71	84
2	h	141/168 (84%)	136 (96%)	5 (4%)	36	60
2	i	159/168 (95%)	155 (98%)	4 (2%)	47	68
2	j	161/168 (96%)	158 (98%)	3 (2%)	57	75
2	k	141/168 (84%)	138 (98%)	3 (2%)	53	72
2	l	141/168 (84%)	140 (99%)	1 (1%)	84	90
2	m	158/168 (94%)	156 (99%)	2 (1%)	69	82
2	n	161/168 (96%)	160 (99%)	1 (1%)	86	92
2	o	141/168 (84%)	138 (98%)	3 (2%)	53	72
2	p	141/168 (84%)	140 (99%)	1 (1%)	84	90
2	q	141/168 (84%)	137 (97%)	4 (3%)	43	65
3	AM	114/128 (89%)	113 (99%)	1 (1%)	78	87
3	AN	114/128 (89%)	114 (100%)	0	100	100
3	AO	114/128 (89%)	112 (98%)	2 (2%)	59	77
3	AP	114/128 (89%)	113 (99%)	1 (1%)	78	87
3	H	114/128 (89%)	113 (99%)	1 (1%)	78	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	114/128 (89%)	114 (100%)	0	100	100
4	f1	15/175 (9%)	15 (100%)	0	100	100
4	f2	15/175 (9%)	15 (100%)	0	100	100
4	f5	15/175 (9%)	15 (100%)	0	100	100
4	f6	15/175 (9%)	15 (100%)	0	100	100
4	f7	15/175 (9%)	15 (100%)	0	100	100
5	g1	235/379 (62%)	235 (100%)	0	100	100
5	g2	235/379 (62%)	232 (99%)	3 (1%)	69	82
5	g5	235/379 (62%)	234 (100%)	1 (0%)	91	94
5	g6	235/379 (62%)	235 (100%)	0	100	100
5	g7	235/379 (62%)	235 (100%)	0	100	100
5	h1	235/379 (62%)	227 (97%)	8 (3%)	37	61
5	h2	235/379 (62%)	235 (100%)	0	100	100
5	h5	235/379 (62%)	235 (100%)	0	100	100
5	h6	235/379 (62%)	235 (100%)	0	100	100
5	h7	235/379 (62%)	235 (100%)	0	100	100
5	k1	232/379 (61%)	232 (100%)	0	100	100
5	k2	232/379 (61%)	232 (100%)	0	100	100
5	k5	232/379 (61%)	232 (100%)	0	100	100
5	k6	232/379 (61%)	231 (100%)	1 (0%)	91	94
5	k7	232/379 (61%)	230 (99%)	2 (1%)	78	87
5	n1	235/379 (62%)	234 (100%)	1 (0%)	91	94
5	n2	235/379 (62%)	233 (99%)	2 (1%)	78	87
5	n5	235/379 (62%)	234 (100%)	1 (0%)	91	94
5	n6	235/379 (62%)	235 (100%)	0	100	100
5	n7	235/379 (62%)	235 (100%)	0	100	100
5	o1	235/379 (62%)	232 (99%)	3 (1%)	69	82
5	o2	235/379 (62%)	233 (99%)	2 (1%)	78	87
5	o5	235/379 (62%)	232 (99%)	3 (1%)	69	82
5	o6	235/379 (62%)	233 (99%)	2 (1%)	78	87
5	o7	235/379 (62%)	232 (99%)	3 (1%)	69	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	r1	235/379 (62%)	235 (100%)	0	100 100
5	r2	235/379 (62%)	233 (99%)	2 (1%)	78 87
5	r5	235/379 (62%)	235 (100%)	0	100 100
5	r6	235/379 (62%)	235 (100%)	0	100 100
5	r7	235/379 (62%)	234 (100%)	1 (0%)	91 94
6	l1	112/112 (100%)	111 (99%)	1 (1%)	78 87
6	l2	112/112 (100%)	111 (99%)	1 (1%)	78 87
6	l5	112/112 (100%)	110 (98%)	2 (2%)	59 77
6	l6	112/112 (100%)	112 (100%)	0	100 100
6	l7	112/112 (100%)	110 (98%)	2 (2%)	59 77
6	m1	112/112 (100%)	112 (100%)	0	100 100
6	m2	112/112 (100%)	112 (100%)	0	100 100
6	m5	112/112 (100%)	112 (100%)	0	100 100
6	m6	112/112 (100%)	112 (100%)	0	100 100
6	m7	112/112 (100%)	112 (100%)	0	100 100
6	p1	112/112 (100%)	112 (100%)	0	100 100
6	p2	112/112 (100%)	111 (99%)	1 (1%)	78 87
6	p5	112/112 (100%)	112 (100%)	0	100 100
6	p6	112/112 (100%)	111 (99%)	1 (1%)	78 87
6	p7	112/112 (100%)	110 (98%)	2 (2%)	59 77
6	q1	112/112 (100%)	112 (100%)	0	100 100
6	q2	112/112 (100%)	112 (100%)	0	100 100
6	q5	112/112 (100%)	112 (100%)	0	100 100
6	q6	112/112 (100%)	111 (99%)	1 (1%)	78 87
6	q7	112/112 (100%)	110 (98%)	2 (2%)	59 77
6	s1	112/112 (100%)	112 (100%)	0	100 100
6	s2	112/112 (100%)	112 (100%)	0	100 100
6	s5	112/112 (100%)	112 (100%)	0	100 100
6	s6	112/112 (100%)	112 (100%)	0	100 100
6	s7	112/112 (100%)	112 (100%)	0	100 100
6	t1	112/112 (100%)	111 (99%)	1 (1%)	78 87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	t2	112/112 (100%)	111 (99%)	1 (1%)	78 87
6	t5	112/112 (100%)	111 (99%)	1 (1%)	78 87
6	t6	112/112 (100%)	109 (97%)	3 (3%)	44 66
6	t7	112/112 (100%)	111 (99%)	1 (1%)	78 87
6	u1	111/112 (99%)	111 (100%)	0	100 100
6	u2	111/112 (99%)	110 (99%)	1 (1%)	78 87
6	u5	111/112 (99%)	111 (100%)	0	100 100
6	u6	111/112 (99%)	111 (100%)	0	100 100
6	u7	111/112 (99%)	111 (100%)	0	100 100
6	v1	111/112 (99%)	110 (99%)	1 (1%)	78 87
6	v2	111/112 (99%)	110 (99%)	1 (1%)	78 87
6	v5	111/112 (99%)	110 (99%)	1 (1%)	78 87
6	v6	111/112 (99%)	110 (99%)	1 (1%)	78 87
6	v7	111/112 (99%)	110 (99%)	1 (1%)	78 87
7	03	186/191 (97%)	186 (100%)	0	100 100
7	13	186/191 (97%)	186 (100%)	0	100 100
7	23	186/191 (97%)	186 (100%)	0	100 100
7	33	186/191 (97%)	186 (100%)	0	100 100
7	43	186/191 (97%)	186 (100%)	0	100 100
7	53	186/191 (97%)	185 (100%)	1 (0%)	88 93
7	63	186/191 (97%)	186 (100%)	0	100 100
7	73	186/191 (97%)	186 (100%)	0	100 100
7	83	186/191 (97%)	186 (100%)	0	100 100
7	93	186/191 (97%)	186 (100%)	0	100 100
7	A3	186/191 (97%)	186 (100%)	0	100 100
7	B3	186/191 (97%)	186 (100%)	0	100 100
7	C3	186/191 (97%)	186 (100%)	0	100 100
7	D3	186/191 (97%)	186 (100%)	0	100 100
7	E3	186/191 (97%)	186 (100%)	0	100 100
7	F3	186/191 (97%)	186 (100%)	0	100 100
7	G3	186/191 (97%)	184 (99%)	2 (1%)	73 85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	J3	186/191 (97%)	186 (100%)	0	100	100
7	K3	191/191 (100%)	191 (100%)	0	100	100
7	L3	186/191 (97%)	185 (100%)	1 (0%)	88	93
7	M3	186/191 (97%)	186 (100%)	0	100	100
7	N3	191/191 (100%)	191 (100%)	0	100	100
7	O3	186/191 (97%)	186 (100%)	0	100	100
7	P3	185/191 (97%)	185 (100%)	0	100	100
7	Q3	191/191 (100%)	190 (100%)	1 (0%)	88	93
7	R3	186/191 (97%)	185 (100%)	1 (0%)	88	93
7	S3	185/191 (97%)	185 (100%)	0	100	100
7	T3	186/191 (97%)	186 (100%)	0	100	100
7	U3	185/191 (97%)	185 (100%)	0	100	100
7	V3	186/191 (97%)	184 (99%)	2 (1%)	73	85
7	W3	191/191 (100%)	189 (99%)	2 (1%)	76	86
7	X3	186/191 (97%)	186 (100%)	0	100	100
7	Y3	186/191 (97%)	186 (100%)	0	100	100
7	Z3	186/191 (97%)	186 (100%)	0	100	100
7	a3	186/191 (97%)	186 (100%)	0	100	100
7	b3	186/191 (97%)	186 (100%)	0	100	100
7	c3	186/191 (97%)	186 (100%)	0	100	100
7	d3	186/191 (97%)	186 (100%)	0	100	100
7	e3	186/191 (97%)	186 (100%)	0	100	100
7	f3	186/191 (97%)	179 (96%)	7 (4%)	33	58
7	g3	186/191 (97%)	186 (100%)	0	100	100
7	h3	186/191 (97%)	186 (100%)	0	100	100
7	i3	186/191 (97%)	186 (100%)	0	100	100
7	j3	186/191 (97%)	186 (100%)	0	100	100
7	k3	186/191 (97%)	186 (100%)	0	100	100
7	l3	186/191 (97%)	185 (100%)	1 (0%)	88	93
7	m3	186/191 (97%)	186 (100%)	0	100	100
7	n3	186/191 (97%)	186 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	o3	186/191 (97%)	186 (100%)	0	100	100
7	p3	186/191 (97%)	186 (100%)	0	100	100
7	q3	186/191 (97%)	186 (100%)	0	100	100
7	r3	186/191 (97%)	186 (100%)	0	100	100
7	s3	186/191 (97%)	186 (100%)	0	100	100
7	t3	186/191 (97%)	186 (100%)	0	100	100
7	u3	186/191 (97%)	186 (100%)	0	100	100
7	v3	186/191 (97%)	186 (100%)	0	100	100
7	w3	186/191 (97%)	186 (100%)	0	100	100
7	x3	186/191 (97%)	186 (100%)	0	100	100
7	y3	186/191 (97%)	186 (100%)	0	100	100
7	z3	186/191 (97%)	186 (100%)	0	100	100
8	AA	311/339 (92%)	309 (99%)	2 (1%)	86	92
8	AB	311/339 (92%)	311 (100%)	0	100	100
8	AC	311/339 (92%)	310 (100%)	1 (0%)	92	95
8	AD	311/339 (92%)	311 (100%)	0	100	100
8	AE	311/339 (92%)	310 (100%)	1 (0%)	92	95
8	AF	311/339 (92%)	310 (100%)	1 (0%)	92	95
8	AG	311/339 (92%)	310 (100%)	1 (0%)	92	95
8	AH	311/339 (92%)	311 (100%)	0	100	100
8	AI	311/339 (92%)	310 (100%)	1 (0%)	92	95
8	AJ	311/339 (92%)	310 (100%)	1 (0%)	92	95
8	AK	311/339 (92%)	310 (100%)	1 (0%)	92	95
8	AL	311/339 (92%)	310 (100%)	1 (0%)	92	95
9	AQ	134/153 (88%)	134 (100%)	0	100	100
9	AR	134/153 (88%)	134 (100%)	0	100	100
9	AS	134/153 (88%)	133 (99%)	1 (1%)	84	90
9	AT	134/153 (88%)	134 (100%)	0	100	100
9	AW	134/153 (88%)	134 (100%)	0	100	100
9	AX	134/153 (88%)	134 (100%)	0	100	100
10	AU	113/116 (97%)	111 (98%)	2 (2%)	59	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	AV	113/116 (97%)	111 (98%)	2 (2%)	59 77
10	AY	113/116 (97%)	112 (99%)	1 (1%)	78 87
10	AZ	113/116 (97%)	113 (100%)	0	100 100
10	Aa	113/116 (97%)	113 (100%)	0	100 100
10	Ab	113/116 (97%)	113 (100%)	0	100 100
All	All	31110/37451 (83%)	30961 (100%)	149 (0%)	89 93

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

Mol	Chain	Res	Type
5	k7	289	LYS
9	AS	50	LEU
5	o7	189	GLU
8	AA	277	ILE
6	l1	99	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 384 such sidechains are listed below:

Mol	Chain	Res	Type
6	u6	127	GLN
8	AB	291	ASN
5	g7	384	ASN
5	r7	277	HIS
8	AD	183	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

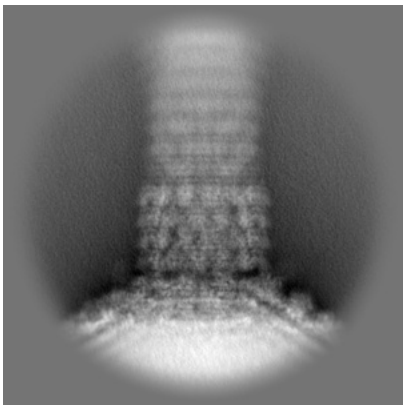
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29541. These allow visual inspection of the internal detail of the map and identification of artifacts.

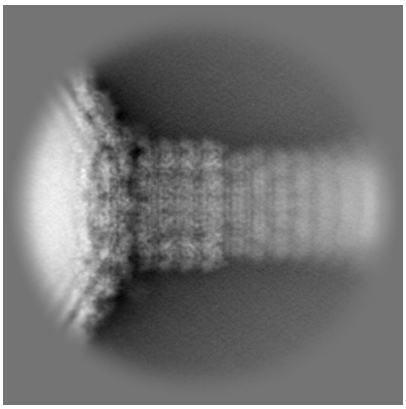
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

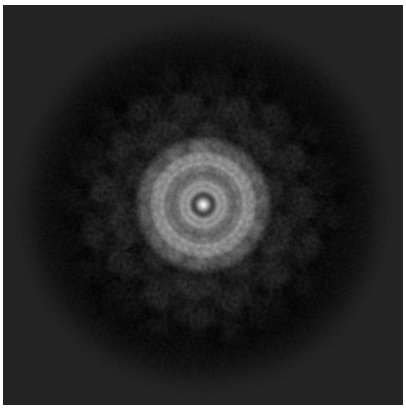
6.1.1 Primary map



X

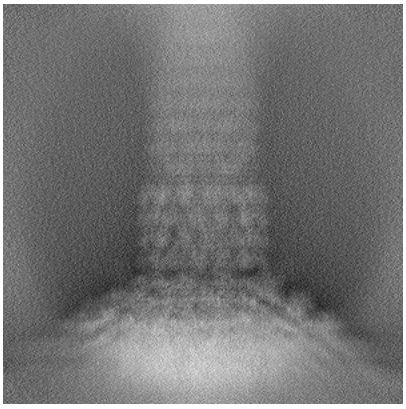


Y

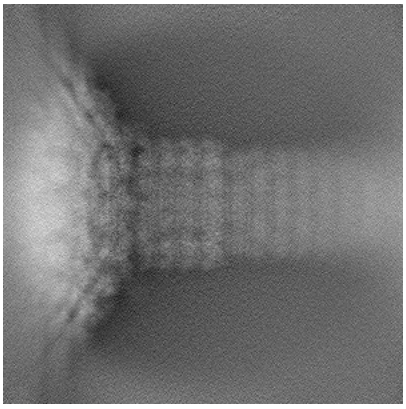


Z

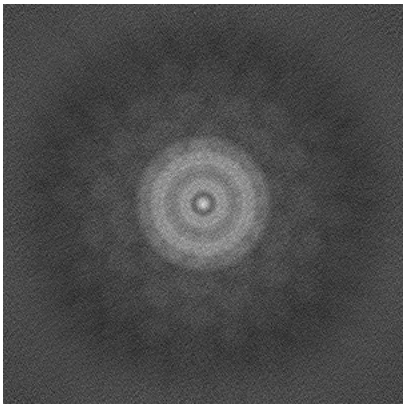
6.1.2 Raw map



X



Y

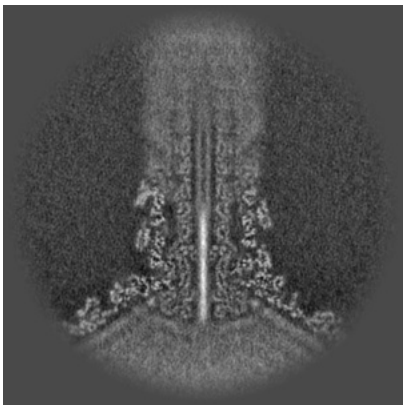


Z

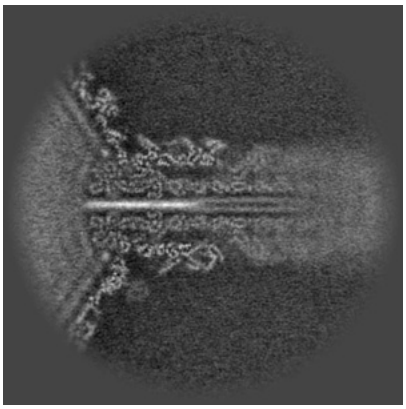
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

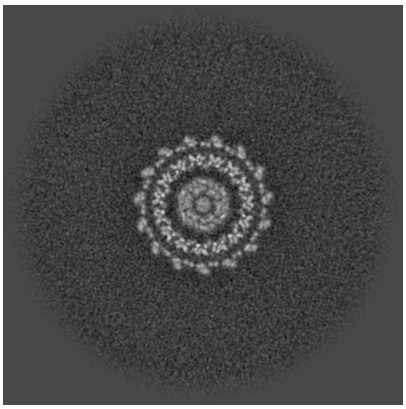
6.2.1 Primary map



X Index: 300

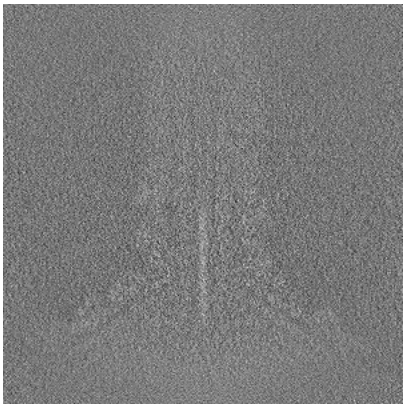


Y Index: 300

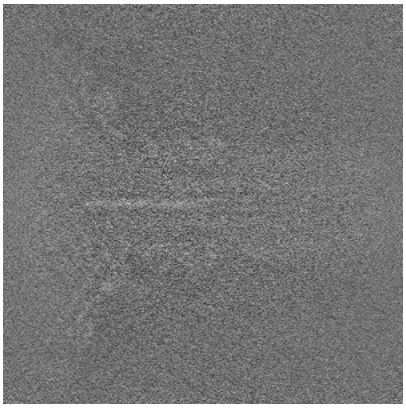


Z Index: 300

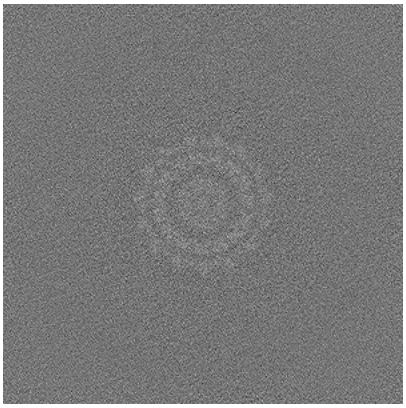
6.2.2 Raw map



X Index: 300



Y Index: 300

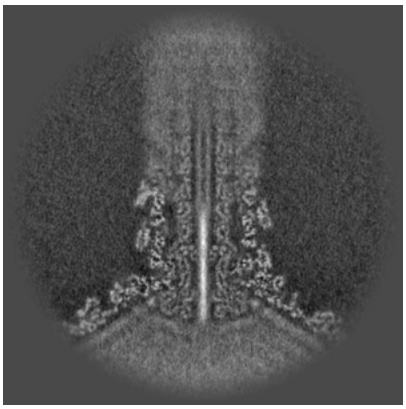


Z Index: 300

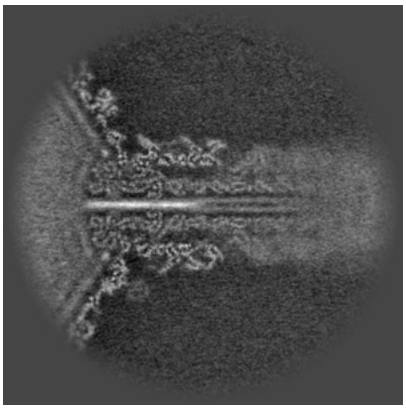
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

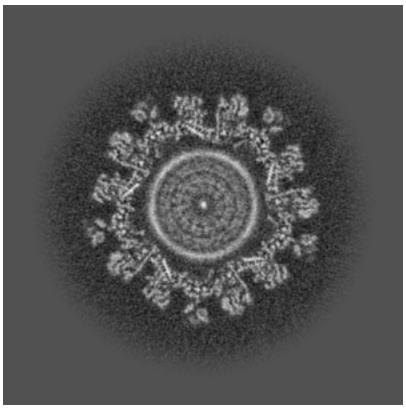
6.3.1 Primary map



X Index: 300

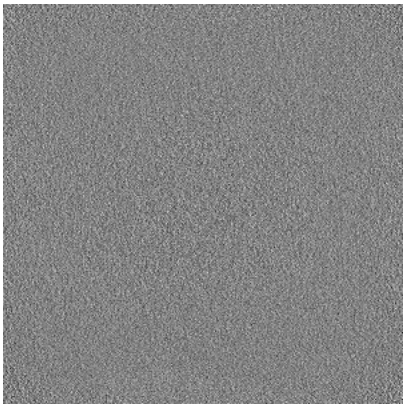


Y Index: 299

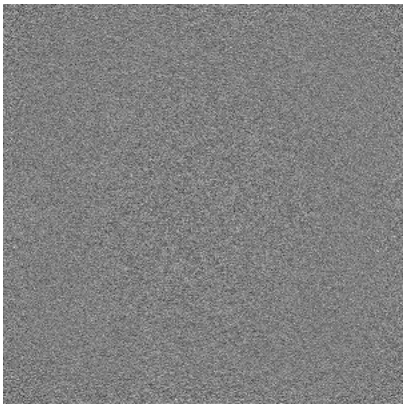


Z Index: 155

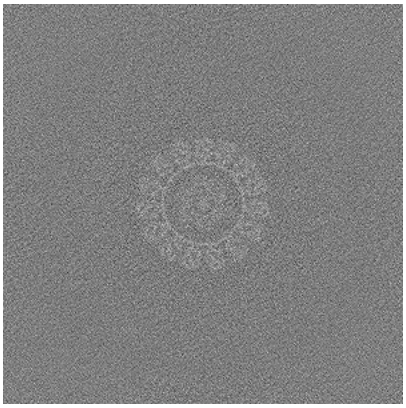
6.3.2 Raw map



X Index: 0



Y Index: 0

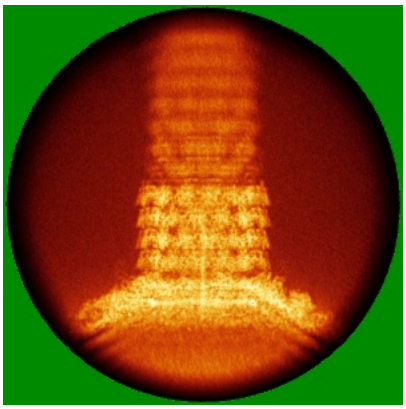


Z Index: 280

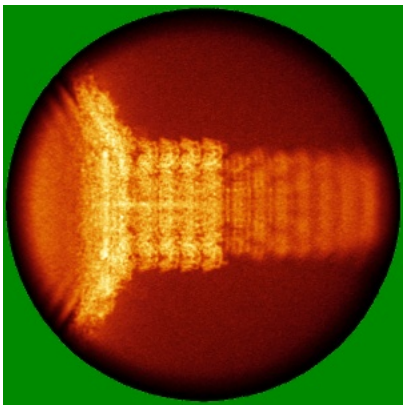
The images above show the largest variance slices of the map in three orthogonal directions.

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

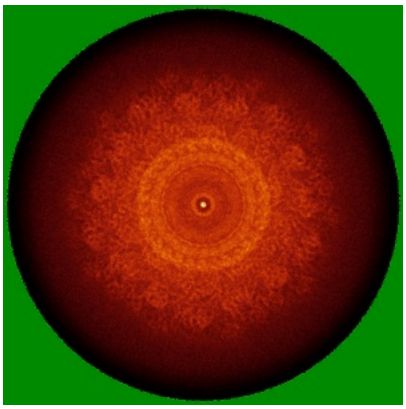
6.4.1 Primary map



X

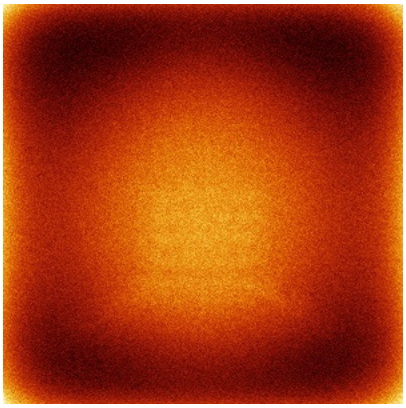


Y

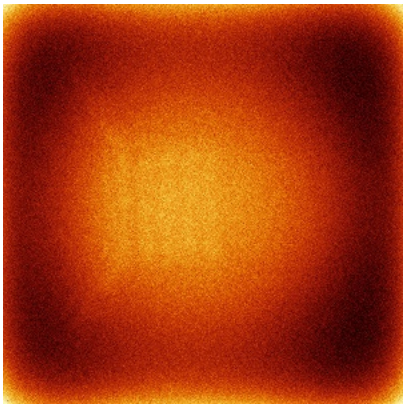


Z

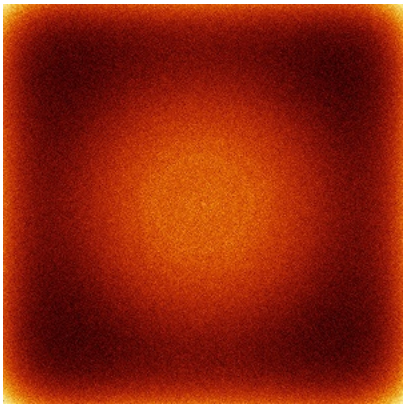
6.4.2 Raw map



X



Y

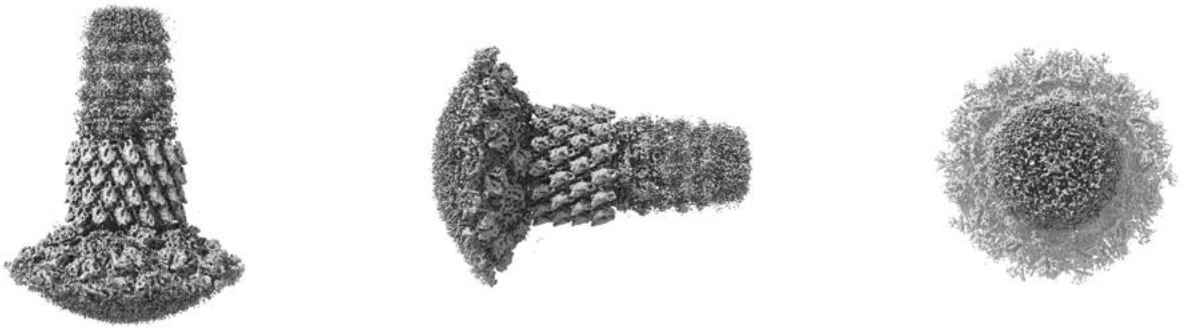


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

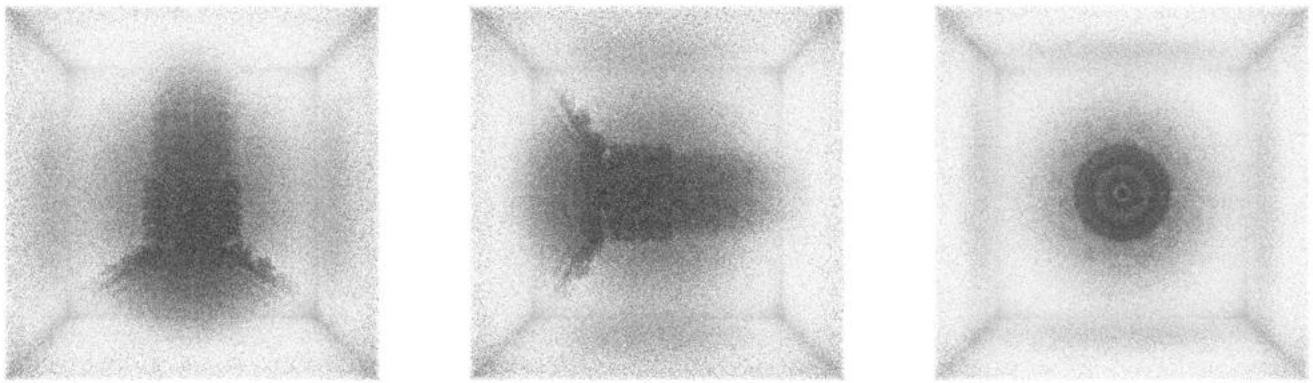
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

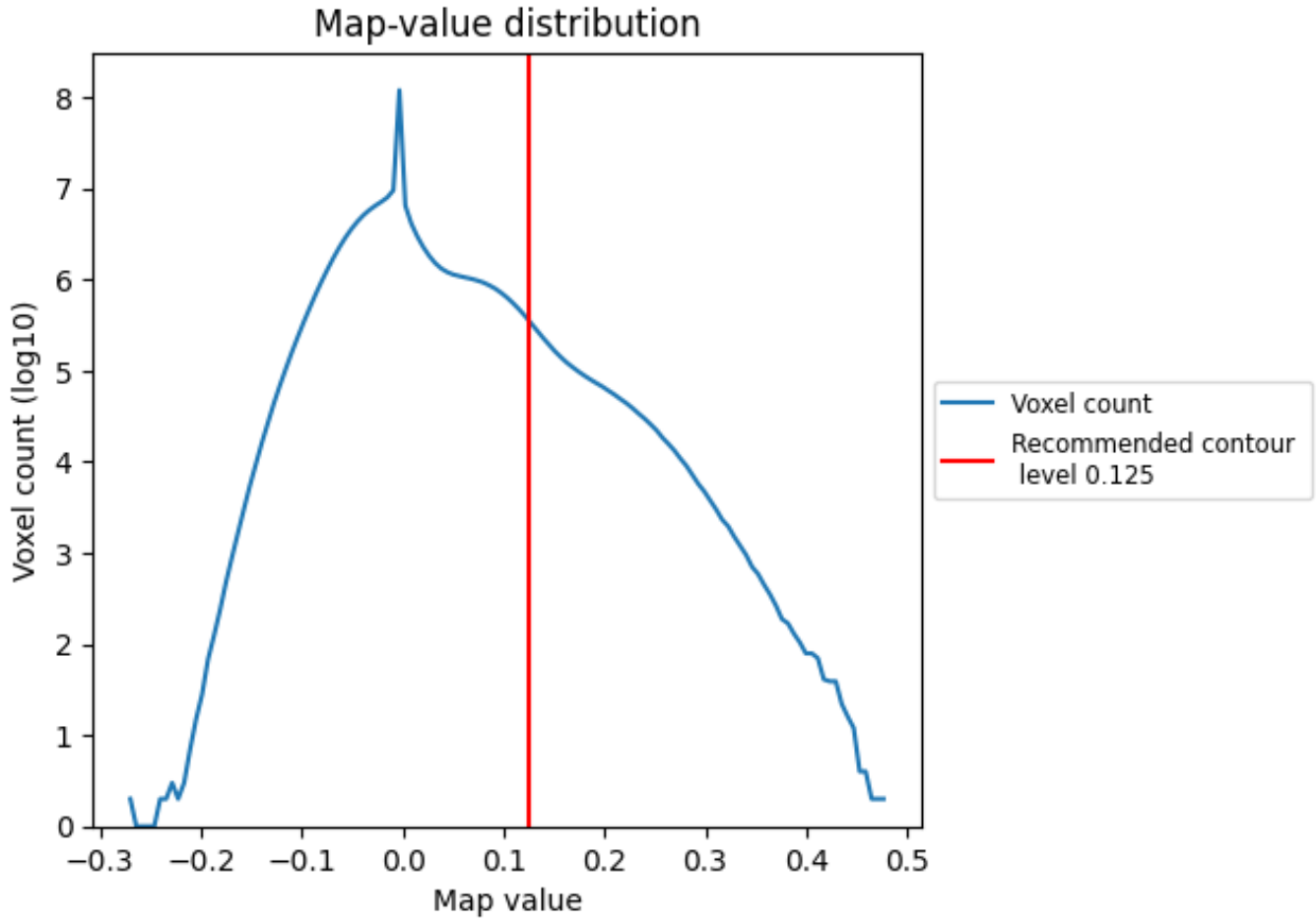
6.6 Mask visualisation (i)

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

7 Map analysis

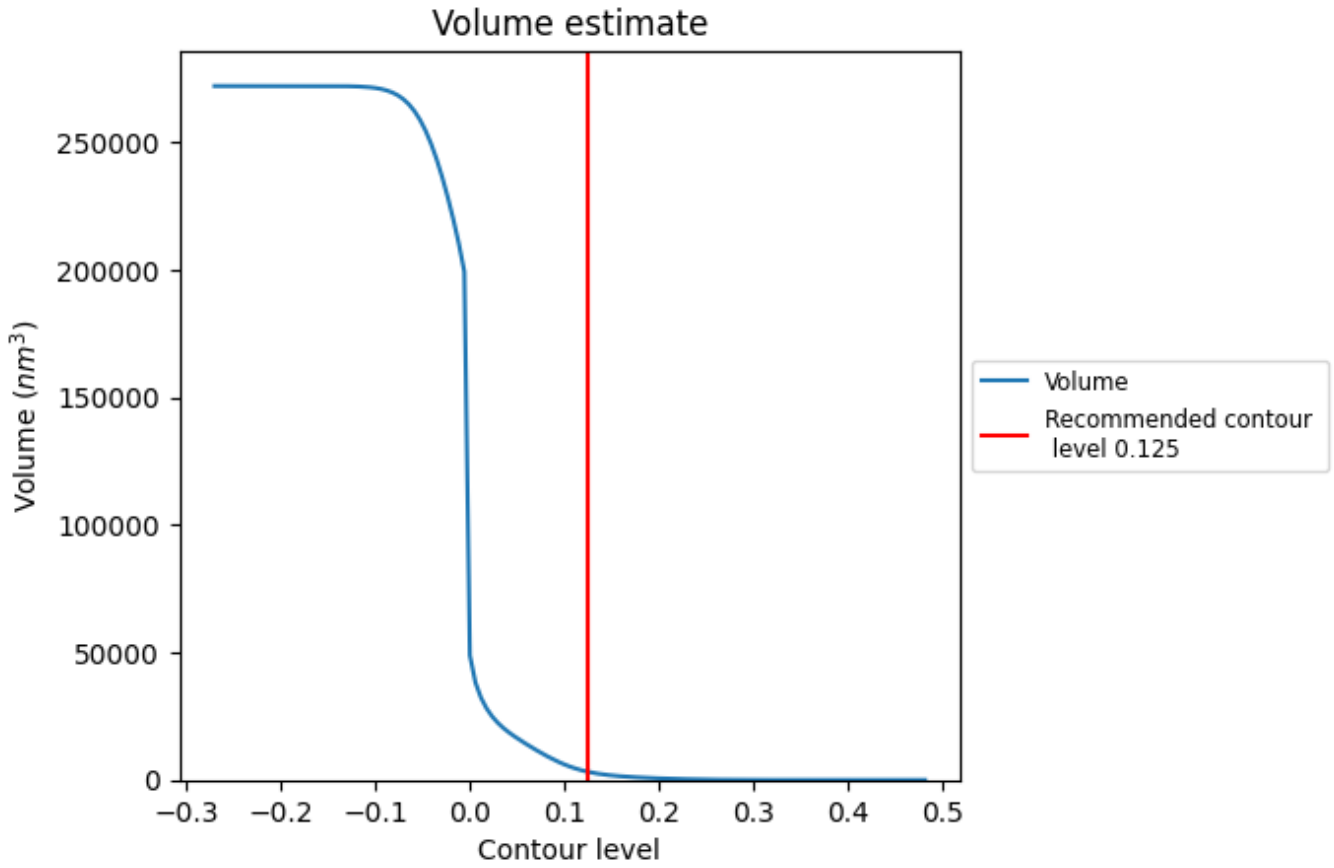
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

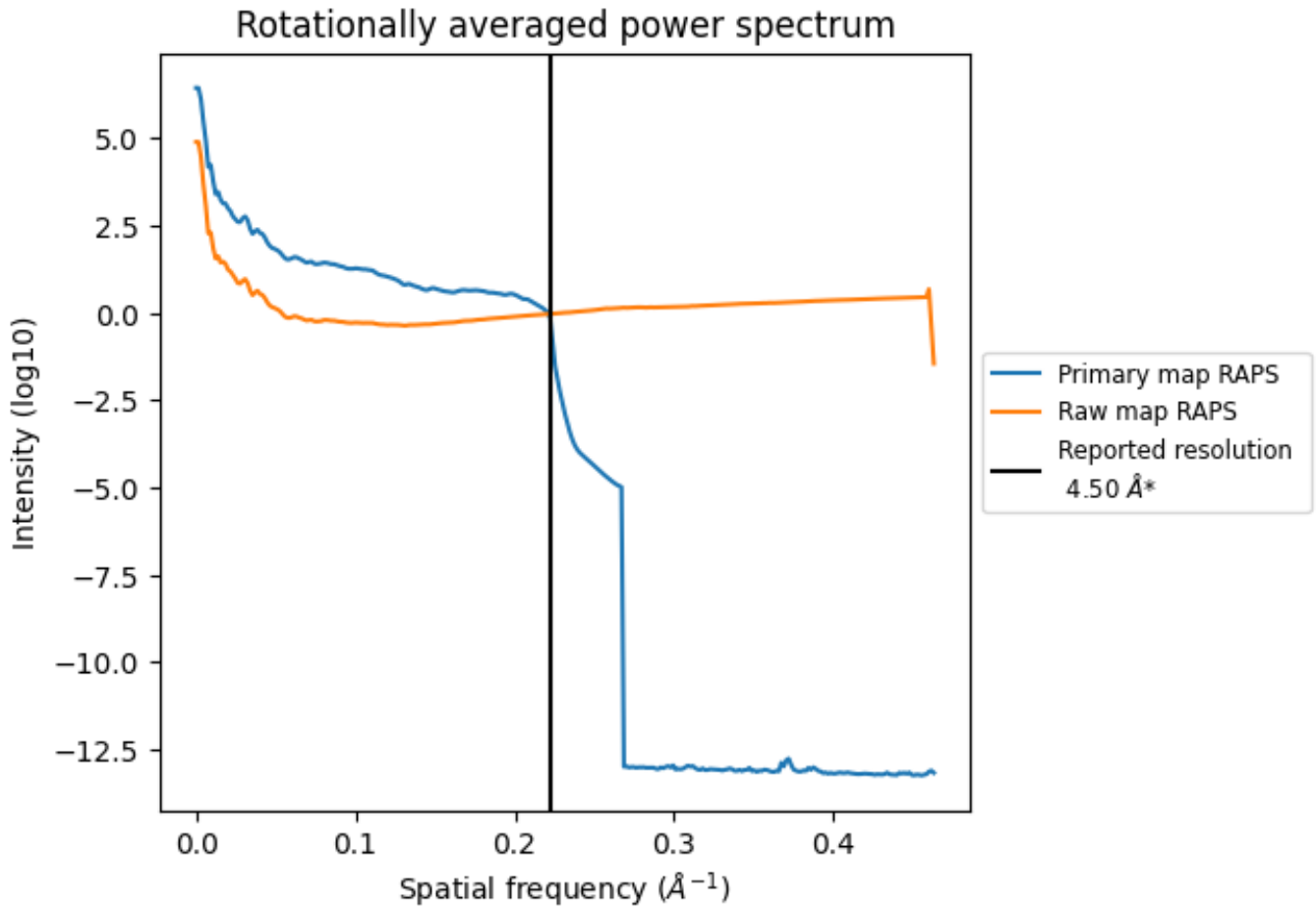
7.2 Volume estimate



The volume at the recommended contour level is 3249 nm^3; this corresponds to an approximate mass of 2935 kDa.

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

7.3 Rotationally averaged power spectrum (i)

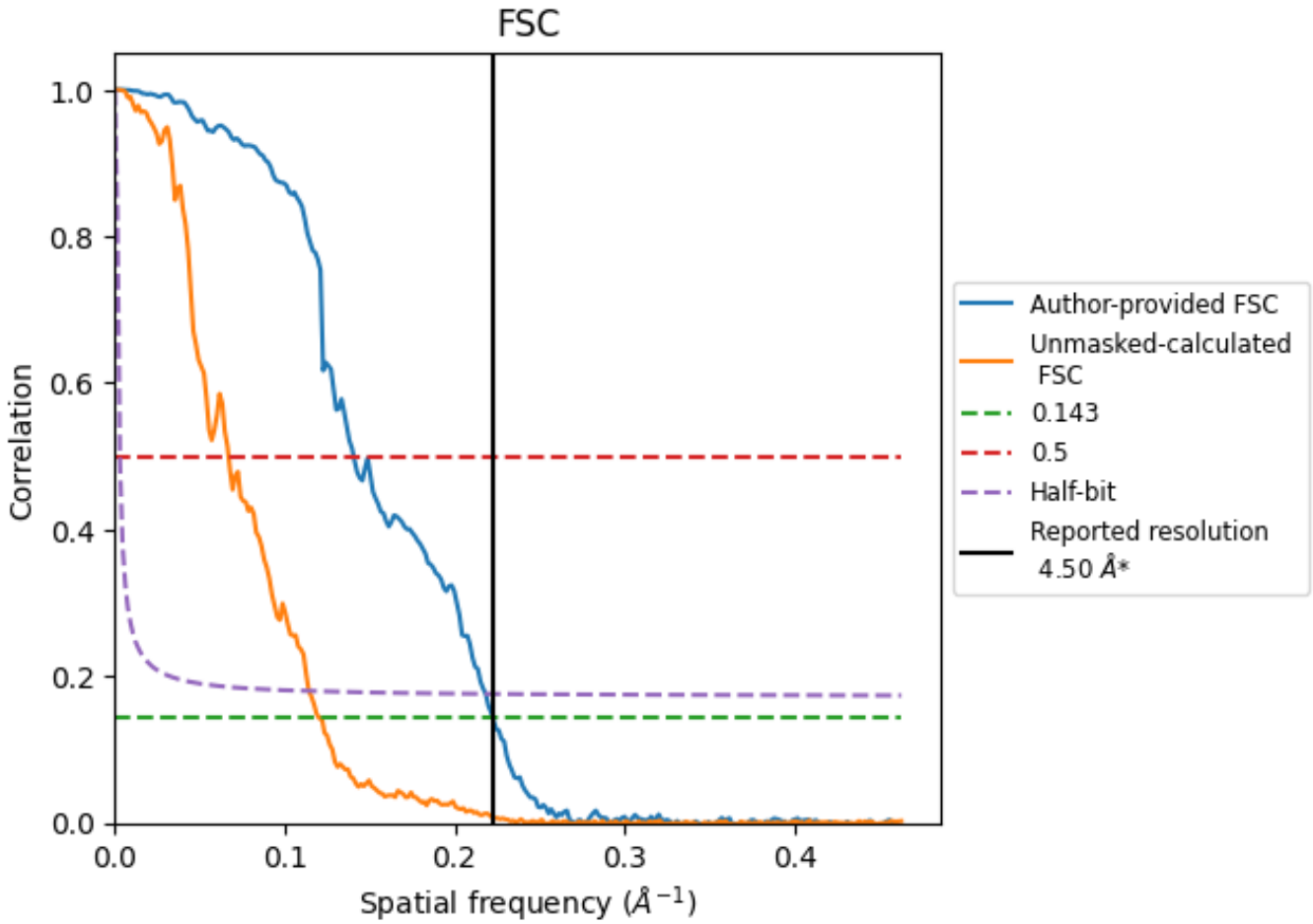


*Reported resolution corresponds to spatial frequency of 0.222 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.49	7.11	4.58
Unmasked-calculated*	8.32	14.93	8.75

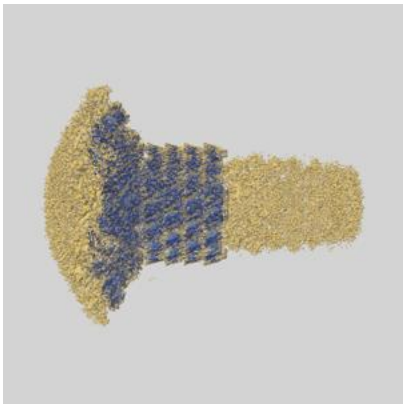
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.32 differs from the reported value 4.5 by more than 10 %

9 Map-model fit

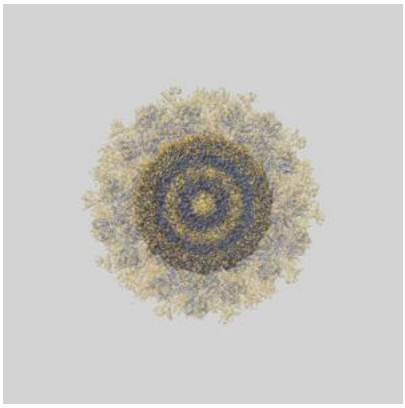
This section contains information regarding the fit between EMDB map EMD-29541 and PDB model 8FXR. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay

X



Y



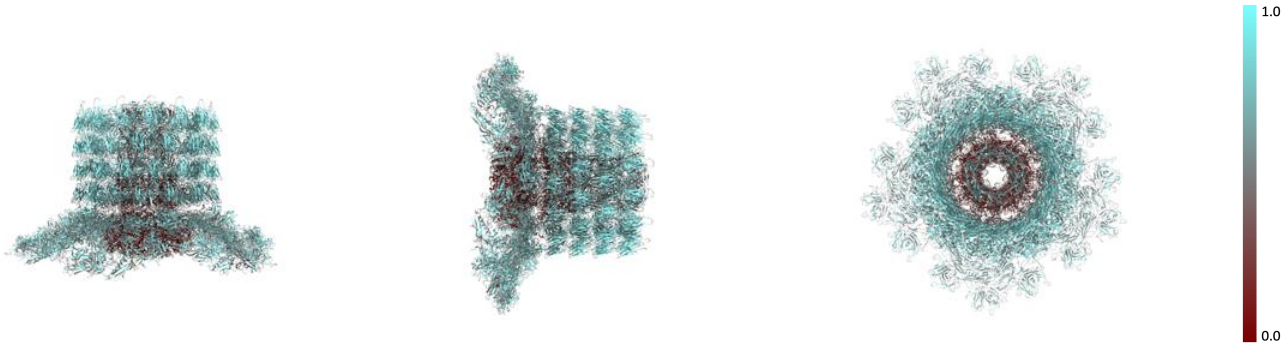
Z

The images above show the 3D surface view of the map at the recommended contour level 0.125 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

This section was not generated.

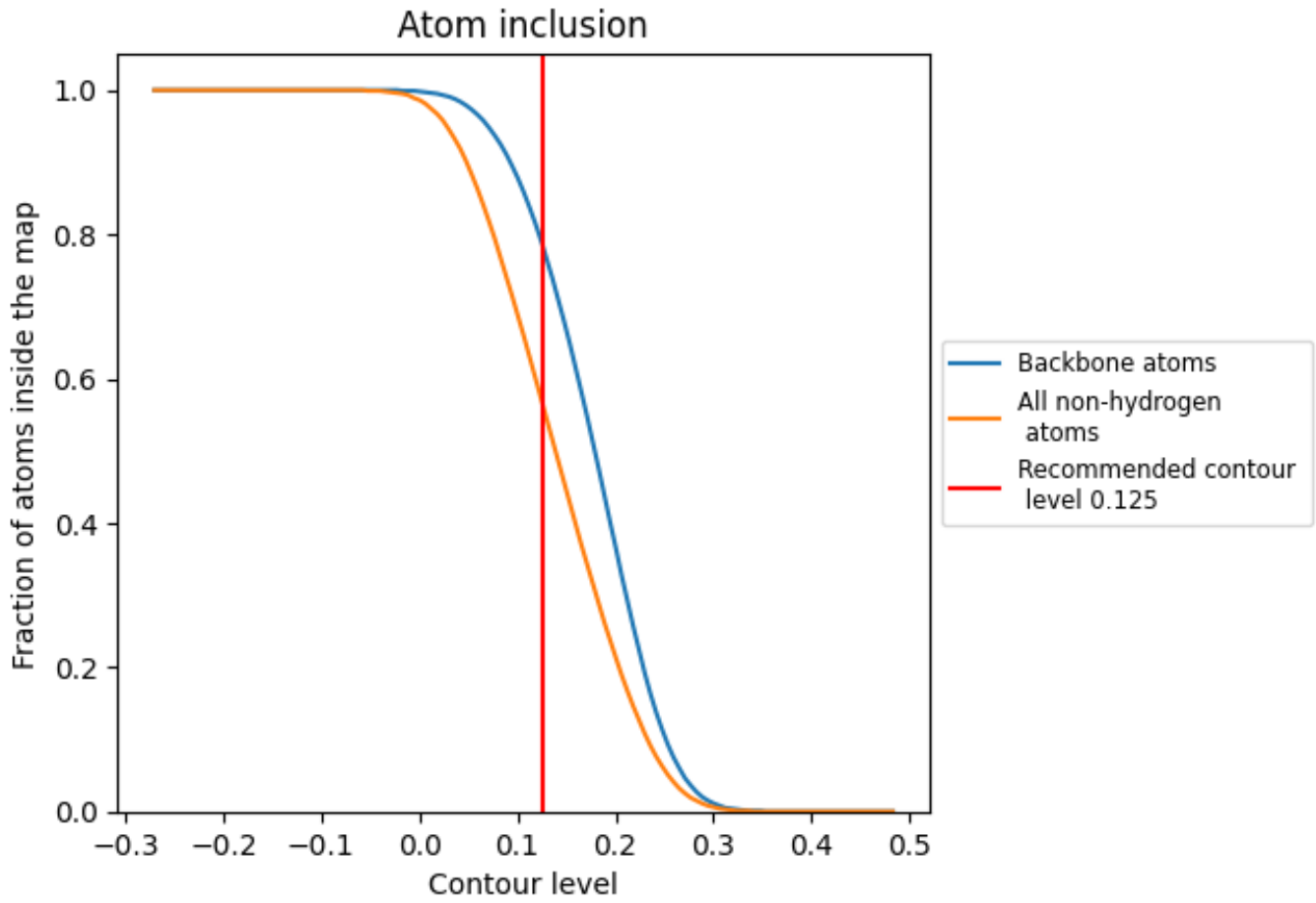
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.125).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 57% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.5690
03	0.7500
13	0.7310
23	0.7580
33	0.7540
43	0.7590
53	0.7710
63	0.7590
73	0.7580
83	0.7510
93	0.7500
A3	0.7620
AA	0.1490
AB	0.1960
AC	0.1960
AD	0.1820
AE	0.1580
AF	0.1760
AG	0.1660
AH	0.1600
AI	0.1590
AJ	0.1660
AK	0.1750
AL	0.1650
AM	0.4150
AN	0.4440
AO	0.4430
AP	0.4190
AQ	0.3860
AR	0.4060
AS	0.3980
AT	0.3850
AU	0.3990
AV	0.4740
AW	0.3870

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
AX	0.4070
AY	0.4480
AZ	0.4180
Aa	0.4240
Ab	0.4780
B3	0.7530
C3	0.7540
D3	0.7580
E3	0.7440
F3	0.7570
G3	0.7390
H	0.4320
I	0.4710
J3	0.7010
K3	0.6380
L3	0.6450
M3	0.6900
N3	0.6250
O3	0.6580
P3	0.6760
Q3	0.6630
R3	0.6480
S3	0.6980
T3	0.6710
U3	0.6530
V3	0.6850
W3	0.6500
X3	0.6610
Y3	0.7270
Z3	0.7380
a	0.3030
a1	0.5960
a2	0.6260
a3	0.7350
a5	0.6010
a6	0.6260
a7	0.5910
b	0.3580
b1	0.6210
b2	0.5960
b3	0.7200
b5	0.5520

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
b6	0.5620
b7	0.6010
c	0.6000
c3	0.7350
d	0.6130
d1	0.5830
d2	0.5750
d3	0.7300
d5	0.5540
d6	0.6130
d7	0.5920
e	0.5500
e1	0.5270
e2	0.5370
e3	0.7240
e5	0.5760
e6	0.5320
e7	0.5320
f	0.5580
f1	0.4190
f2	0.3600
f3	0.7340
f5	0.3900
f6	0.3820
f7	0.4630
g	0.5420
g1	0.6110
g2	0.6270
g3	0.7210
g5	0.6190
g6	0.5950
g7	0.5980
h	0.2850
h1	0.6290
h2	0.6230
h3	0.7470
h5	0.6250
h6	0.6180
h7	0.6160
i	0.3180
i3	0.7240
j	0.2500

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
j3	0.7140
k	0.3090
k1	0.5980
k2	0.5940
k3	0.7190
k5	0.6170
k6	0.5970
k7	0.6020
l	0.3160
l1	0.7120
l2	0.6710
l3	0.7340
l5	0.6900
l6	0.6840
l7	0.6880
m	0.3560
m1	0.6630
m2	0.6490
m3	0.7170
m5	0.6600
m6	0.6650
m7	0.6550
n	0.3730
n1	0.6180
n2	0.6280
n3	0.7620
n5	0.6160
n6	0.6140
n7	0.6340
o	0.3390
o1	0.6110
o2	0.5920
o3	0.7560
o5	0.6010
o6	0.6110
o7	0.6310
p	0.3650
p1	0.6160
p2	0.6220
p3	0.7480
p5	0.6080
p6	0.6180

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
p7	0.6310
q	0.2510
q1	0.6030
q2	0.6170
q3	0.7340
q5	0.5950
q6	0.6400
q7	0.6090
r1	0.6190
r2	0.6390
r3	0.7570
r5	0.6010
r6	0.6030
r7	0.6220
s1	0.6480
s2	0.6390
s3	0.7500
s5	0.6520
s6	0.6450
s7	0.6330
t1	0.5880
t2	0.6260
t3	0.7580
t5	0.6210
t6	0.6220
t7	0.6320
u1	0.5920
u2	0.5520
u3	0.7510
u5	0.5880
u6	0.5560
u7	0.5780
v1	0.6090
v2	0.5540
v3	0.7460
v5	0.5840
v6	0.5620
v7	0.5810
w3	0.7620
x3	0.7530
y3	0.7500
z3	0.7530