



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 08:47 AM EDT

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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

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

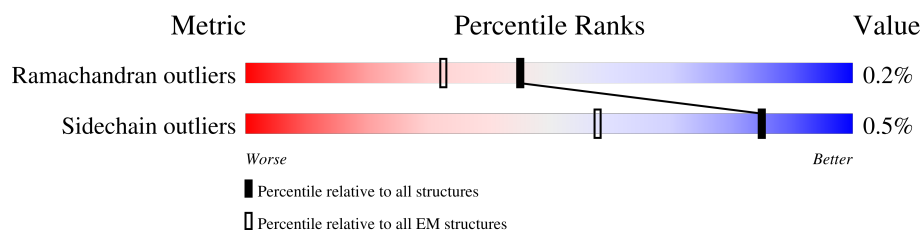
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 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	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	a1	38	
1	a2	38	
1	a5	38	
1	a6	38	
1	a7	38	
1	b1	38	
1	b2	38	
1	b5	38	
1	b6	38	

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Mol	Chain	Length	Quality of chain
1	b7	38	
1	c	38	
1	d	38	
1	d1	38	
1	d2	38	
1	d5	38	
1	d6	38	
1	d7	38	
1	e	38	
1	e1	38	
1	e2	38	
1	e5	38	
1	e6	38	
1	e7	38	
1	f	38	
1	g	38	
2	a	202	
2	b	202	
2	h	202	
2	i	202	
2	j	202	
2	k	202	
2	l	202	
2	m	202	
2	n	202	

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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	

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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%

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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%

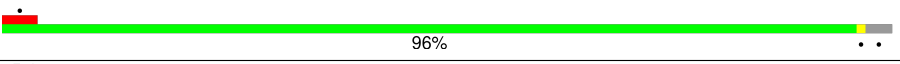
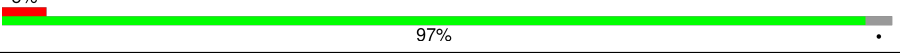
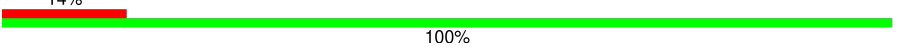
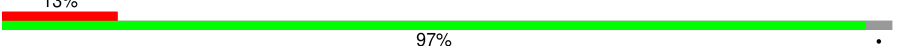
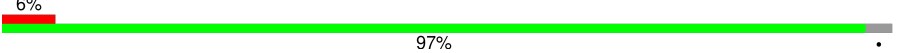

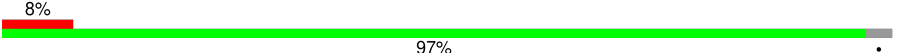
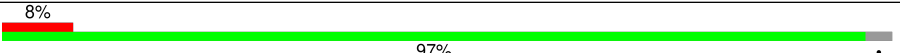
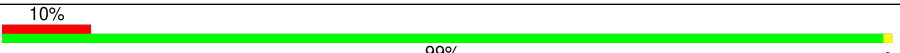
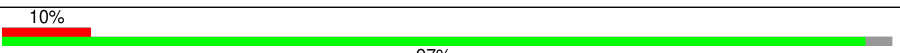
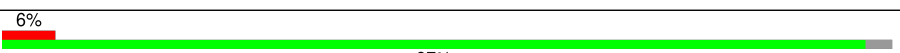
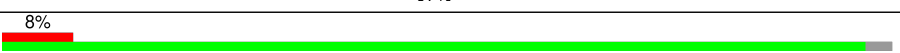
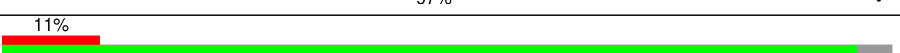
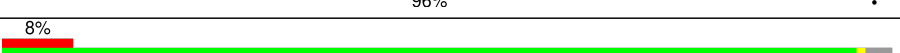
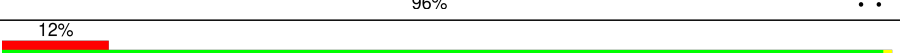
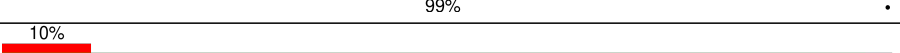
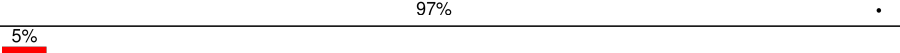
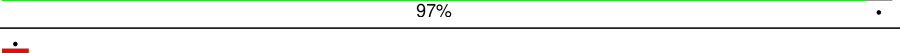
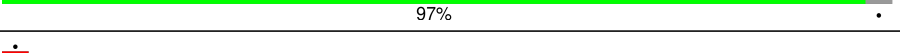
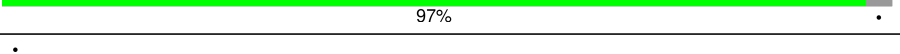
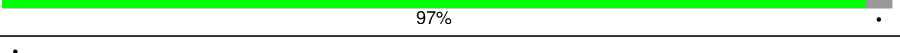
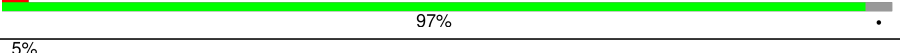
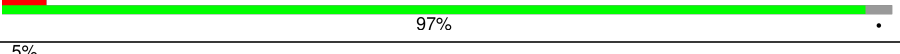
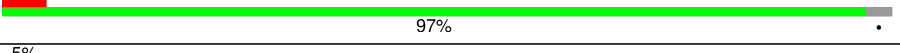
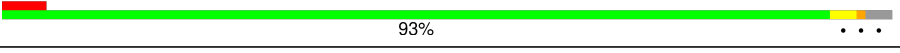
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Mol	Chain	Length	Quality of chain
6	u2	137	23% 99%
6	u5	137	20% 99%
6	u6	137	21% 99%
6	u7	137	20% 99%
6	v1	137	15% 98%
6	v2	137	27% 99%
6	v5	137	20% 99%
6	v6	137	24% 99%
6	v7	137	18% 99%
7	03	230	97%
7	13	230	5% 97%
7	23	230	97%
7	33	230	5% 97%
7	43	230	5% 97%
7	53	230	96%
7	63	230	5% 97%
7	73	230	5% 97%
7	83	230	5% 97%
7	93	230	6% 97%
7	A3	230	5% 97%
7	B3	230	5% 97%
7	C3	230	97%
7	D3	230	97%
7	E3	230	5% 97%
7	F3	230	7% 97%

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Mol	Chain	Length	Quality of chain
7	G3	230	
7	J3	230	
7	K3	230	
7	L3	230	
7	M3	230	
7	N3	230	
7	O3	230	
7	P3	230	
7	Q3	230	
7	R3	230	
7	S3	230	
7	T3	230	
7	U3	230	
7	V3	230	
7	W3	230	
7	X3	230	
7	Y3	230	
7	Z3	230	
7	a3	230	
7	b3	230	
7	c3	230	
7	d3	230	
7	e3	230	
7	f3	230	
7	g3	230	

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Mol	Chain	Length	Quality of chain
7	h3	230	
7	i3	230	
7	j3	230	
7	k3	230	
7	l3	230	
7	m3	230	
7	n3	230	
7	o3	230	
7	p3	230	
7	q3	230	
7	r3	230	
7	s3	230	
7	t3	230	
7	u3	230	
7	v3	230	
7	w3	230	
7	x3	230	
7	y3	230	
7	z3	230	
8	AA	420	
8	AB	420	
8	AC	420	
8	AD	420	
8	AE	420	
8	AF	420	

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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		

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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		

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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		

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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		

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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		

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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		

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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		

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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		

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

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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		

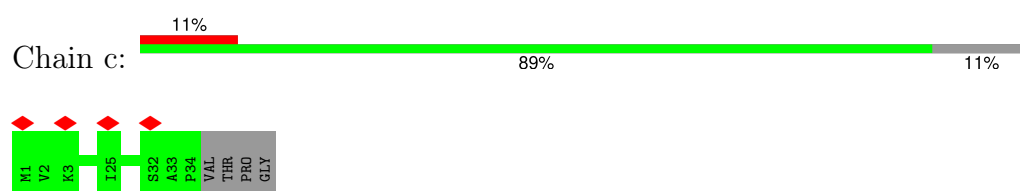
- Molecule 10 is a protein called Tail-tube, gp21.

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		

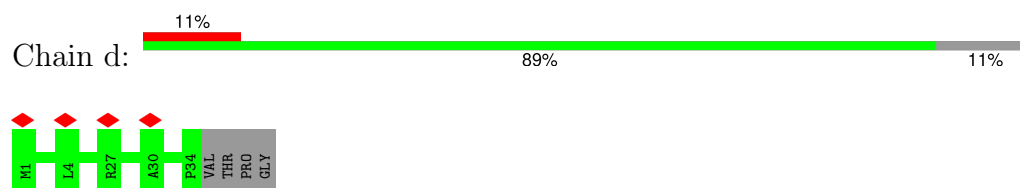
3 Residue-property plots [i](#)

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.

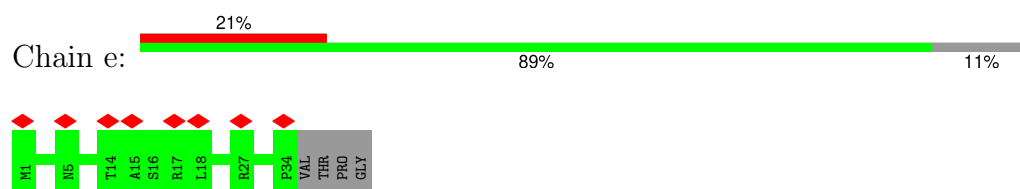
- Molecule 1: Linking protein 2, gp128



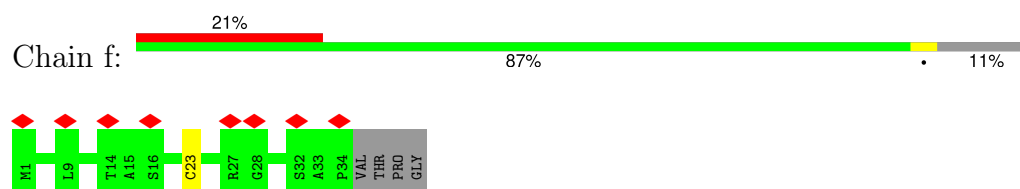
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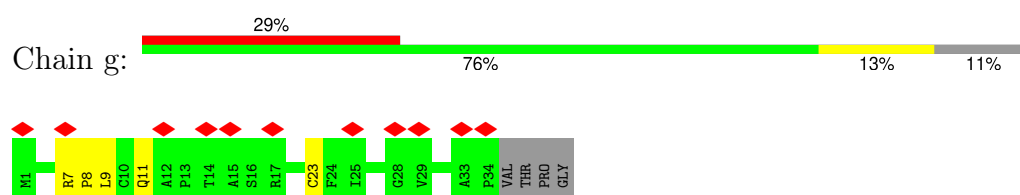
- Molecule 1: Linking protein 2, gp128



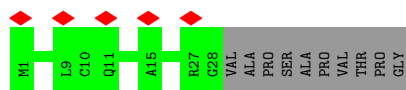
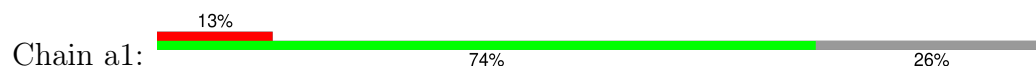
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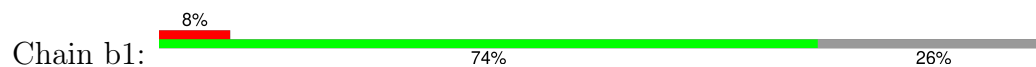
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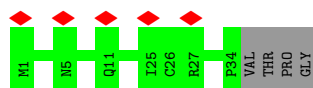
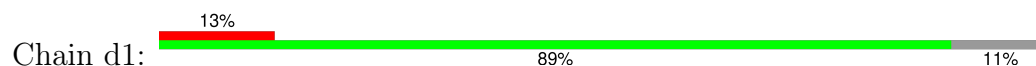
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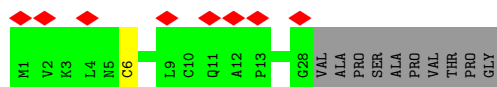
- Molecule 1: Linking protein 2, gp128



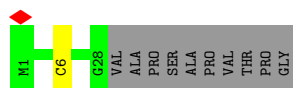
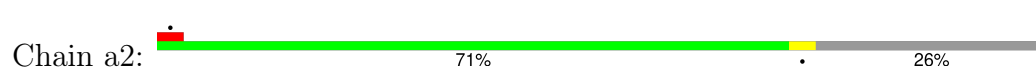
- Molecule 1: Linking protein 2, gp128



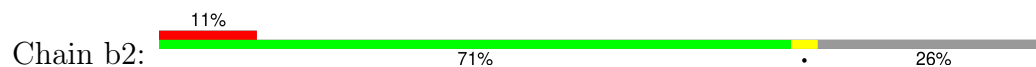
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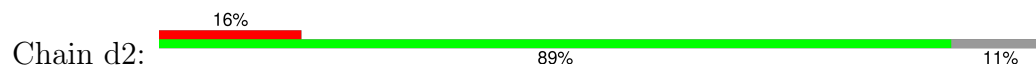
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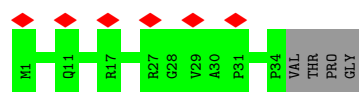


- Molecule 1: Linking protein 2, gp128

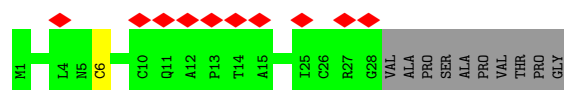


- Molecule 1: Linking protein 2, gp128

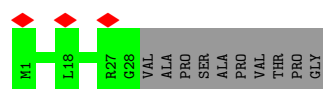
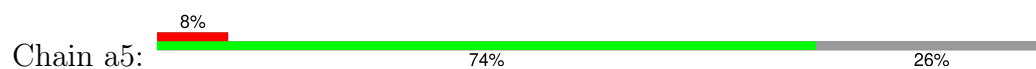




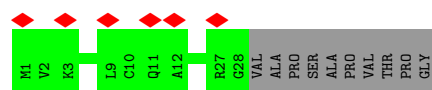
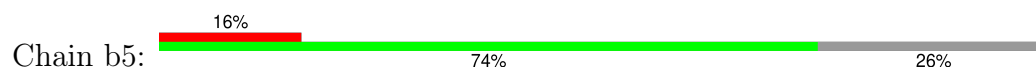
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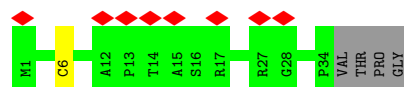
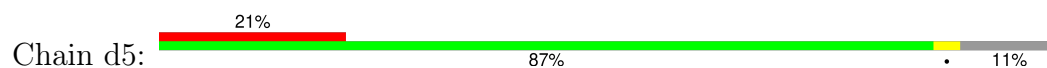
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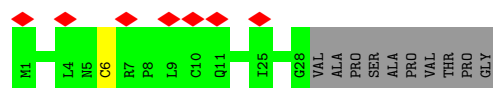
- Molecule 1: Linking protein 2, gp128



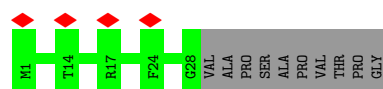
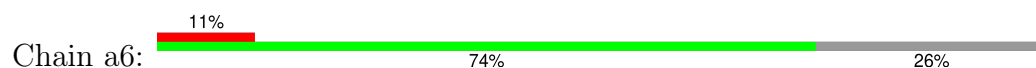
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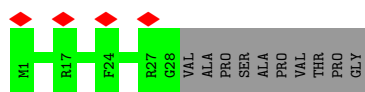
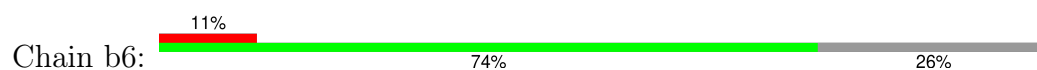
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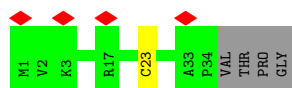
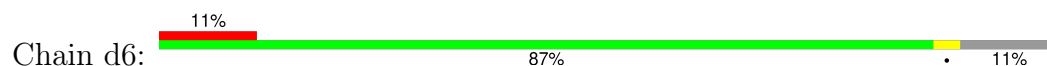
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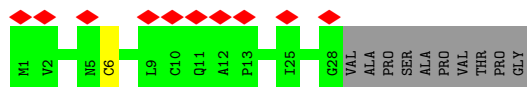
- Molecule 1: Linking protein 2, gp128



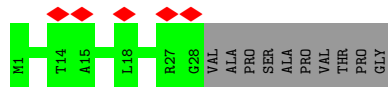
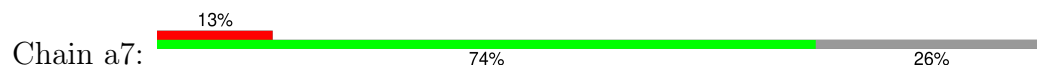
- Molecule 1: Linking protein 2, gp128



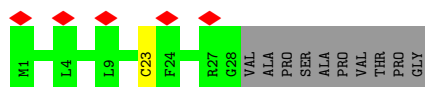
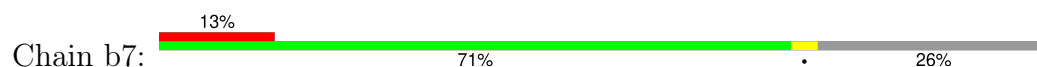
- Molecule 1: Linking protein 2, gp128



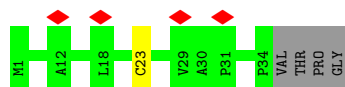
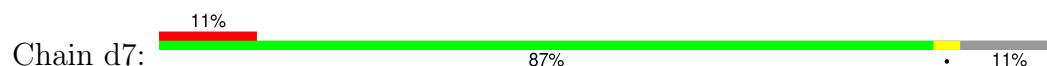
- Molecule 1: Linking protein 2, gp128



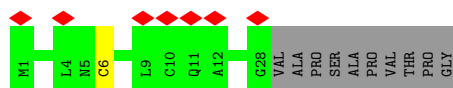
- Molecule 1: Linking protein 2, gp128



- Molecule 1: Linking protein 2, gp128

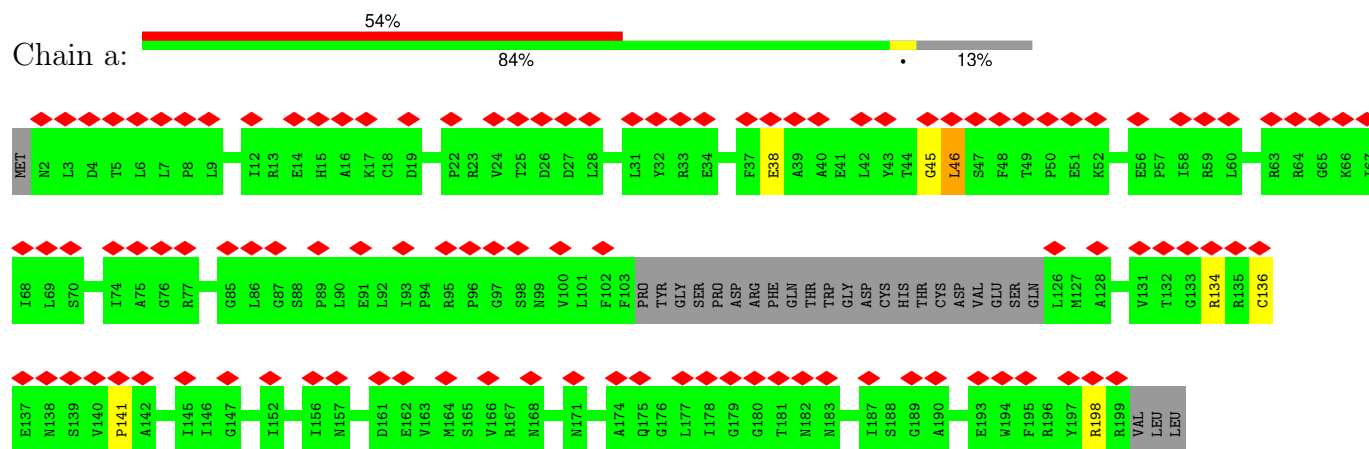


- Molecule 1: Linking protein 2, gp128



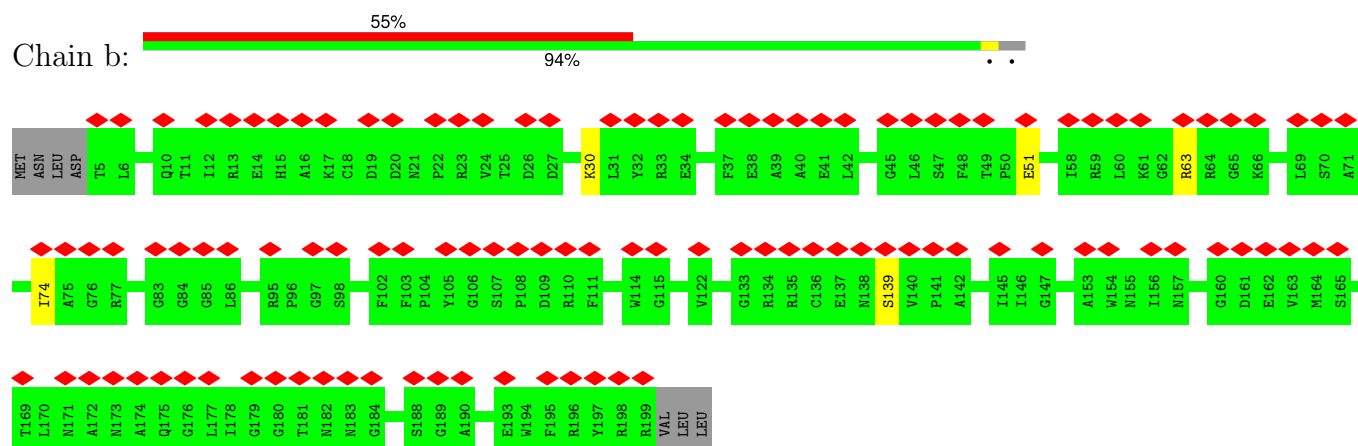
- Molecule 2: Neck 1 protein, gp14

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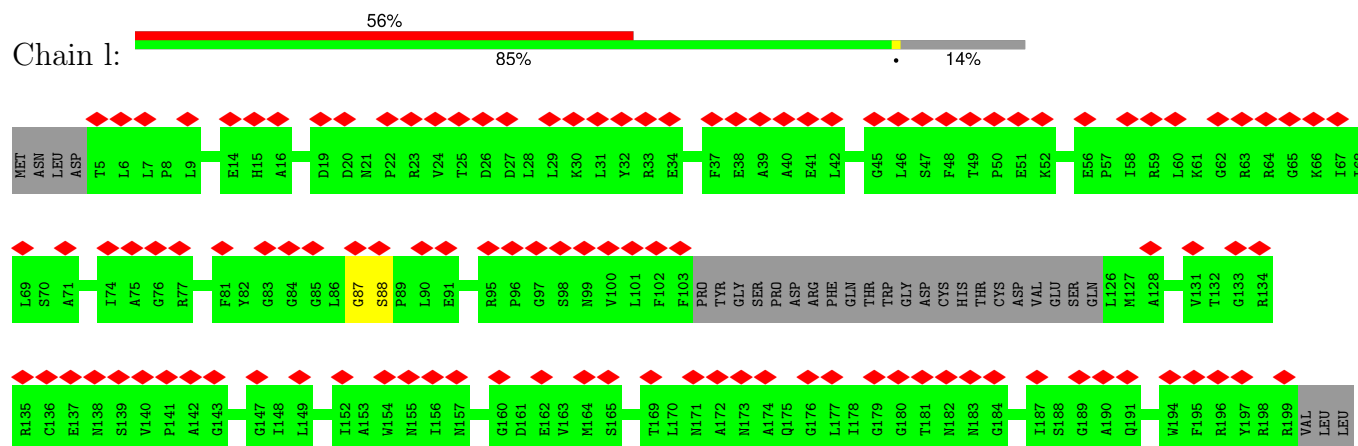
- Molecule 2: Neck 1 protein, gp14

Chain b:



- Molecule 2: Neck 1 protein, gp14

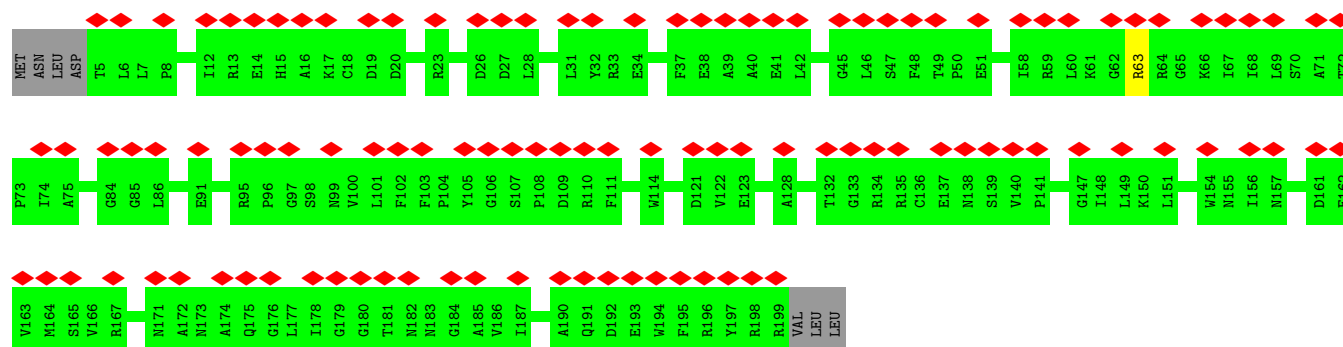
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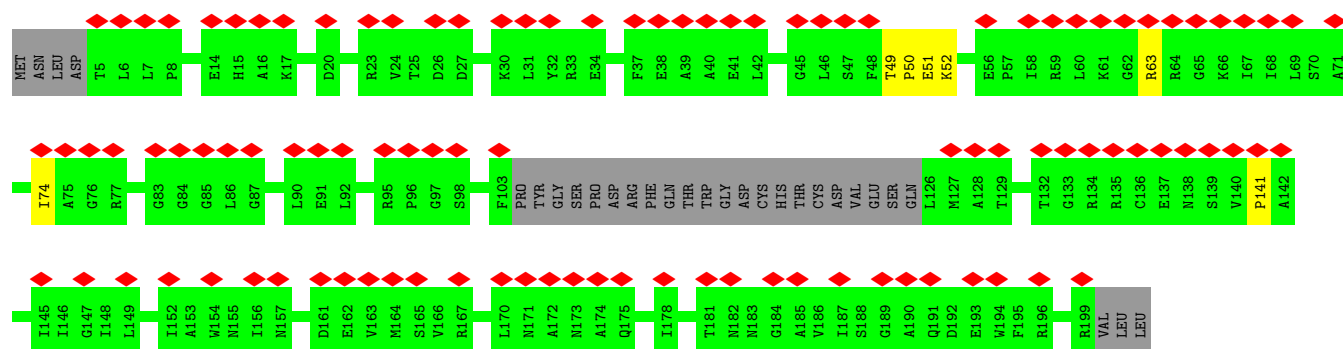
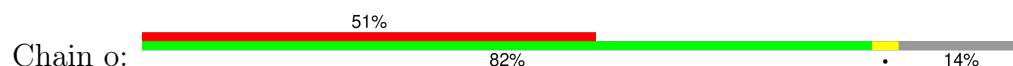
- Molecule 2: Neck 1 protein, gp14

Chain n:

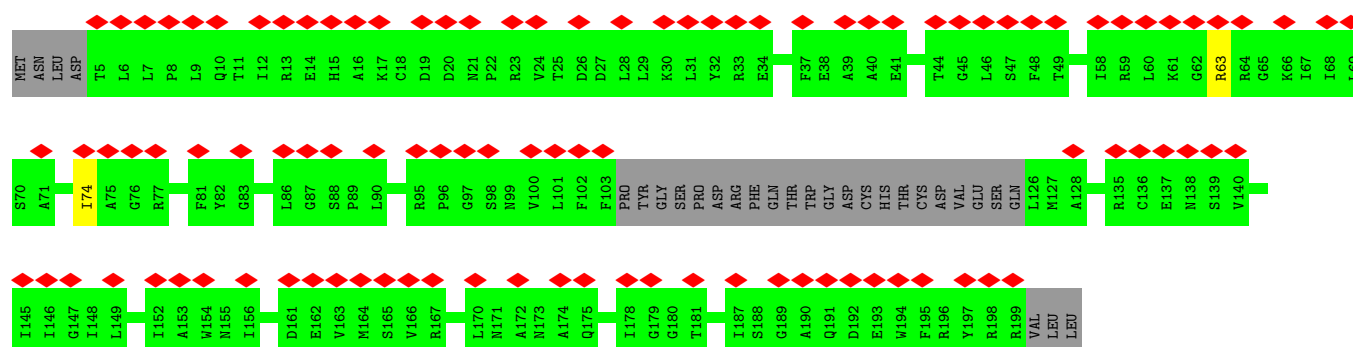
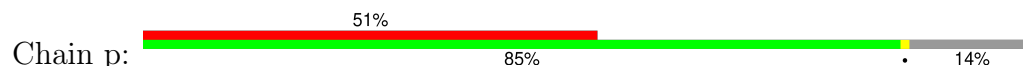




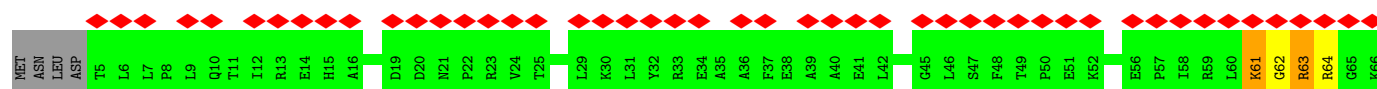
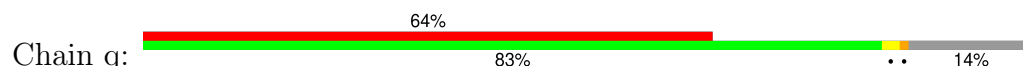
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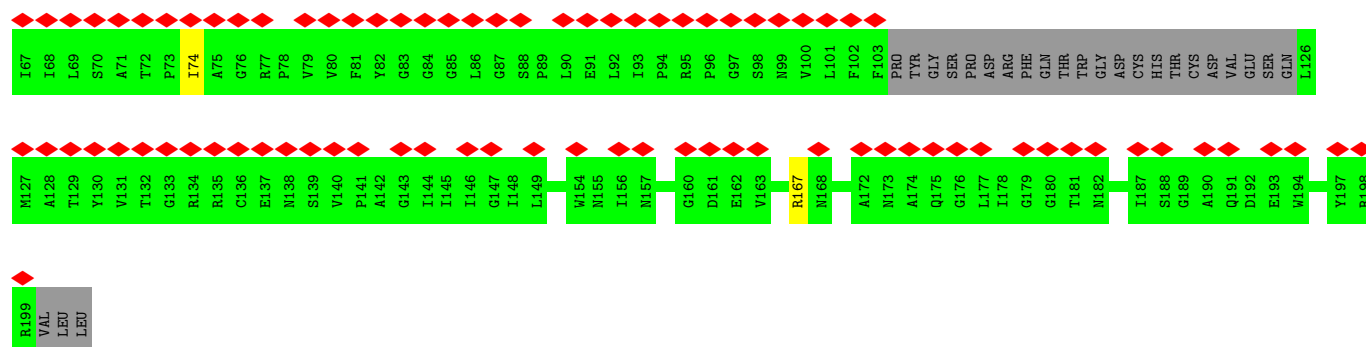


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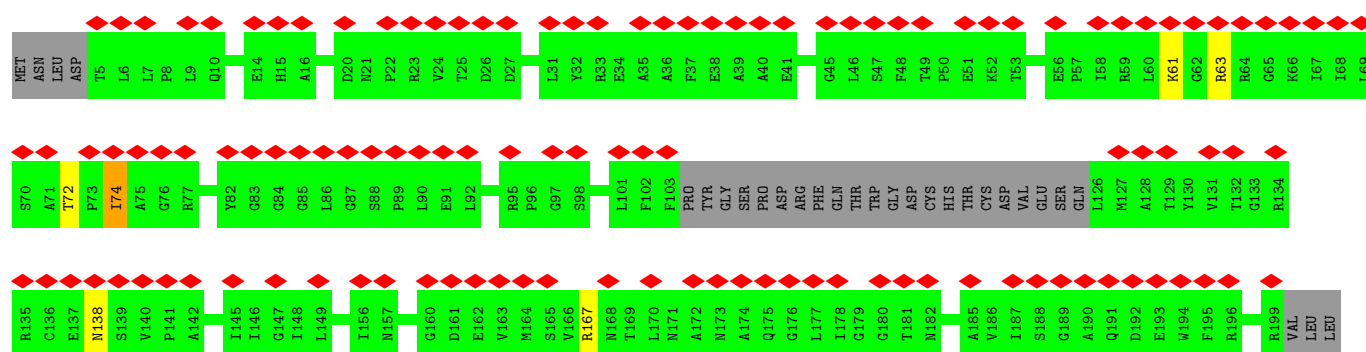
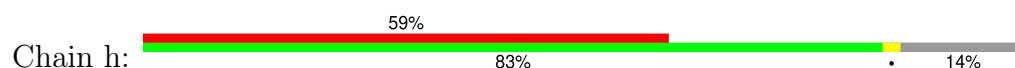


• Molecule 2: Neck 1 protein, gp14

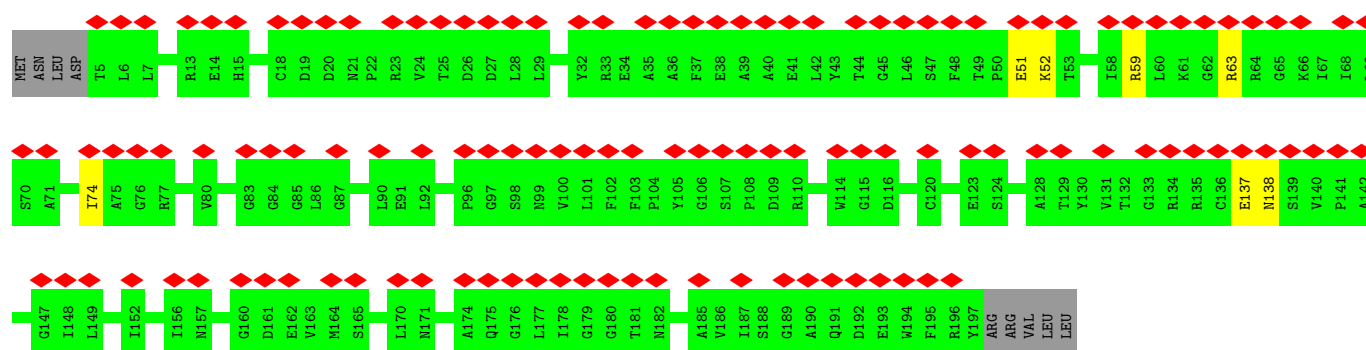
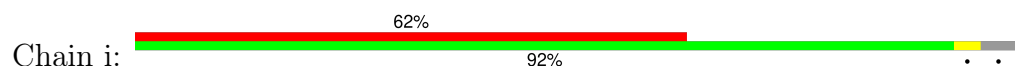




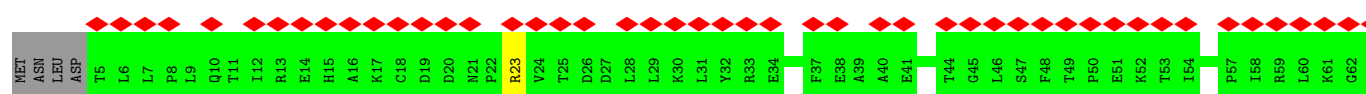
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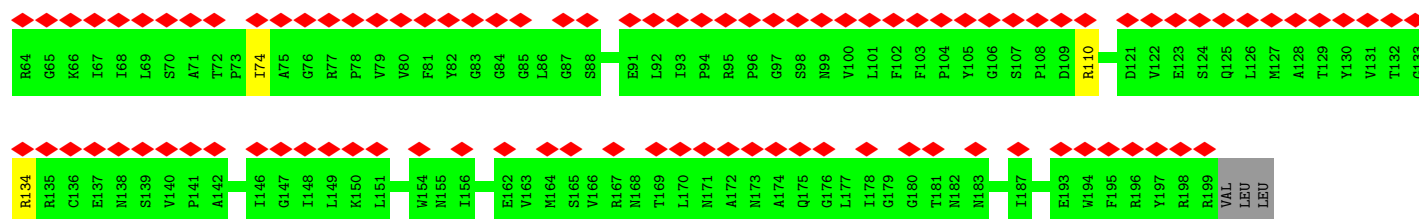


- Molecule 2: Neck 1 protein, gp14

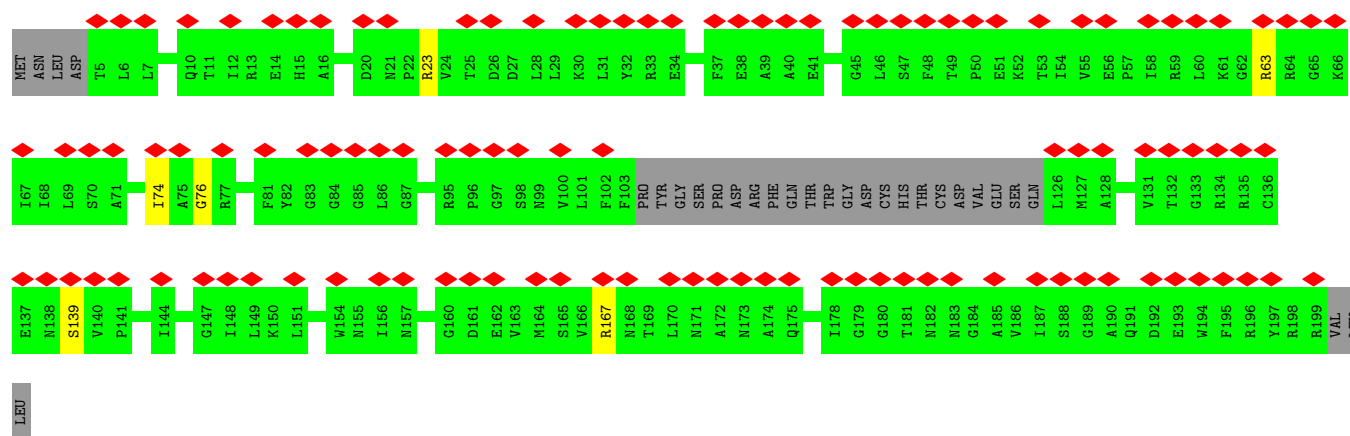
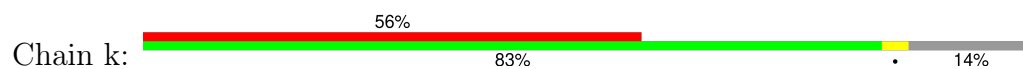


- Molecule 2: Neck 1 protein, gp14

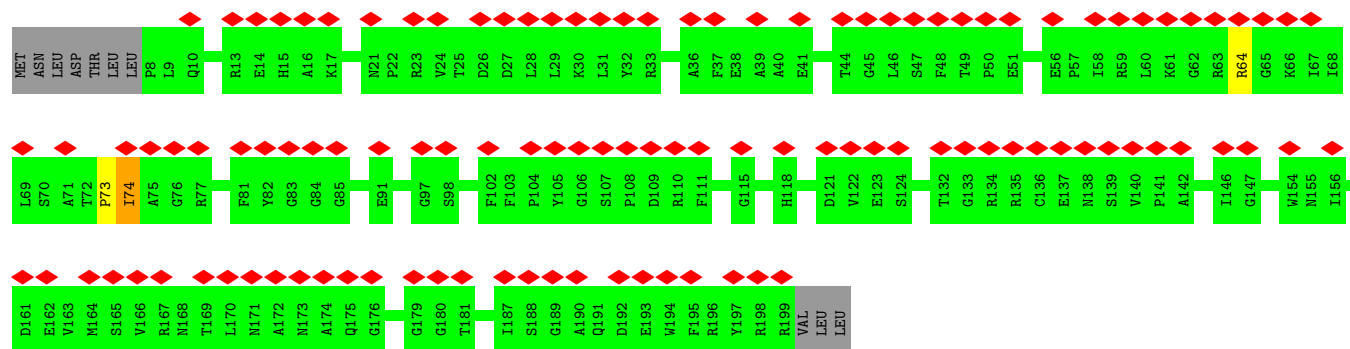




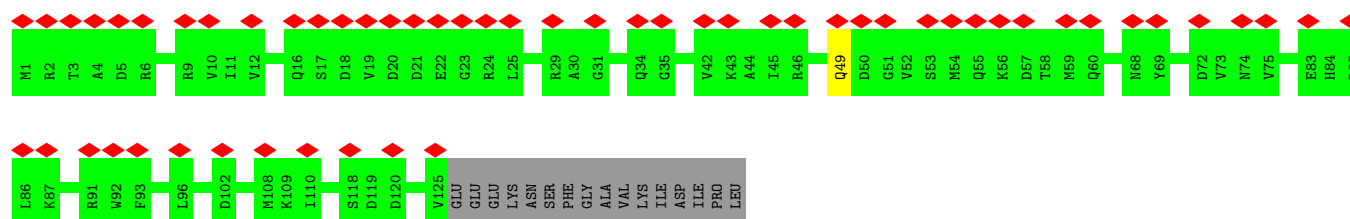
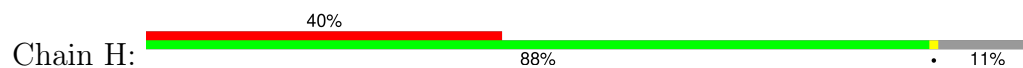
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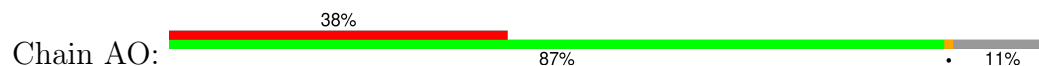
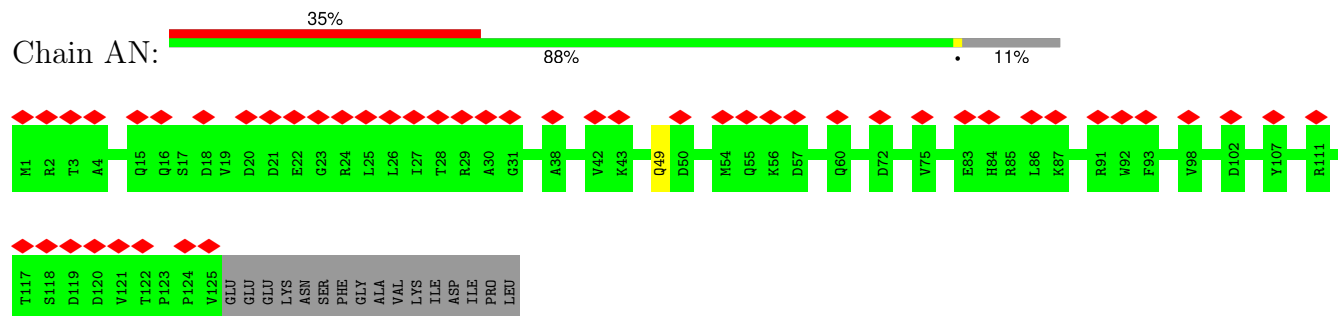
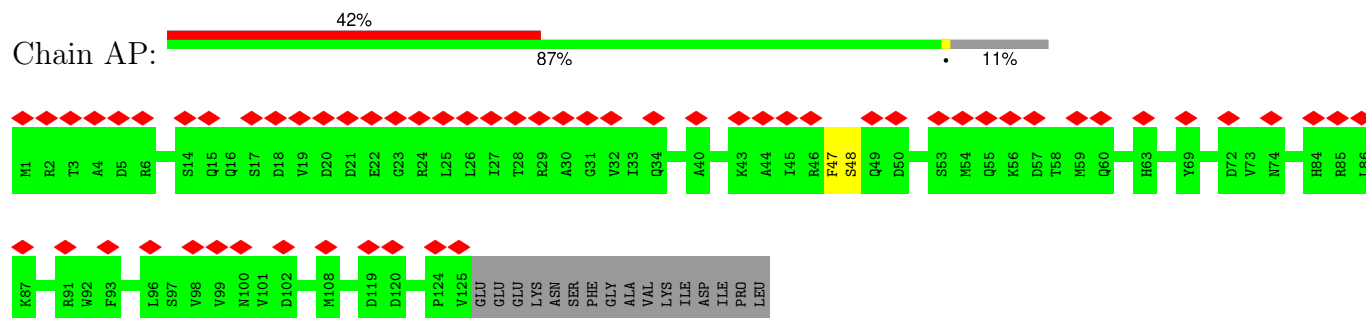
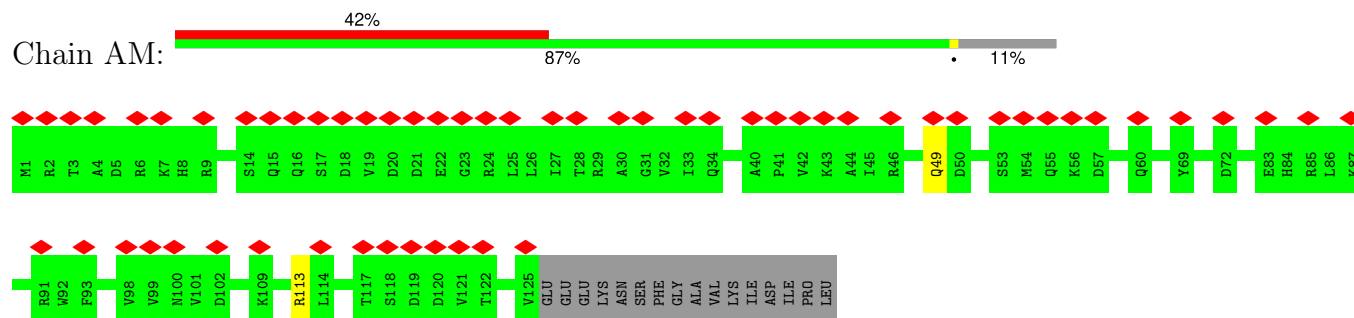
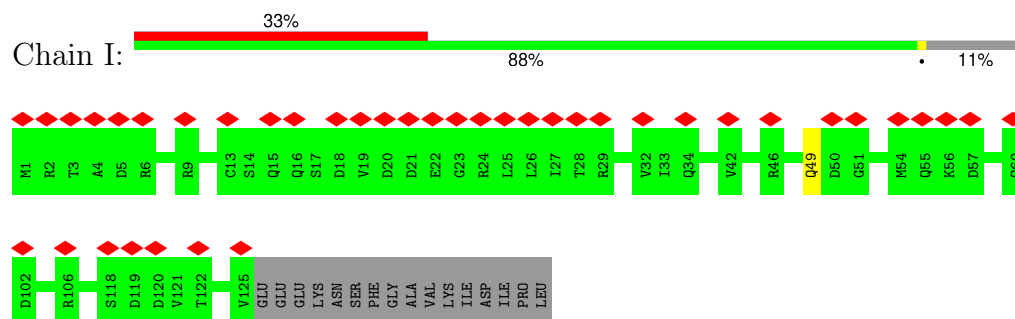


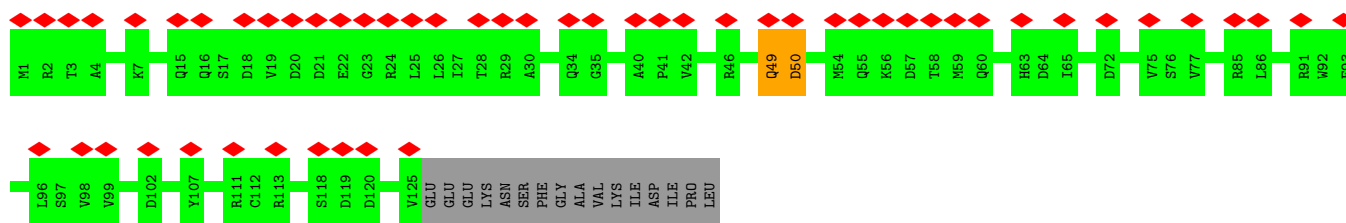
• Molecule 2: Neck 1 protein, gp14



• Molecule 3: Neck 2 protein, gp15

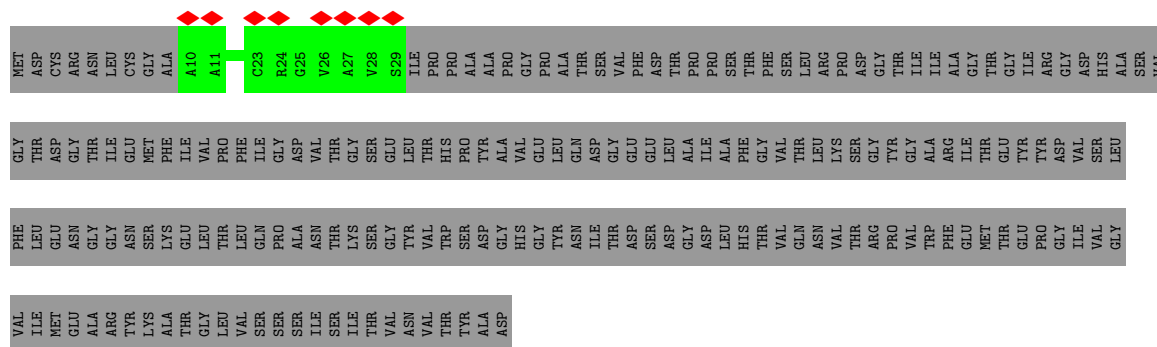






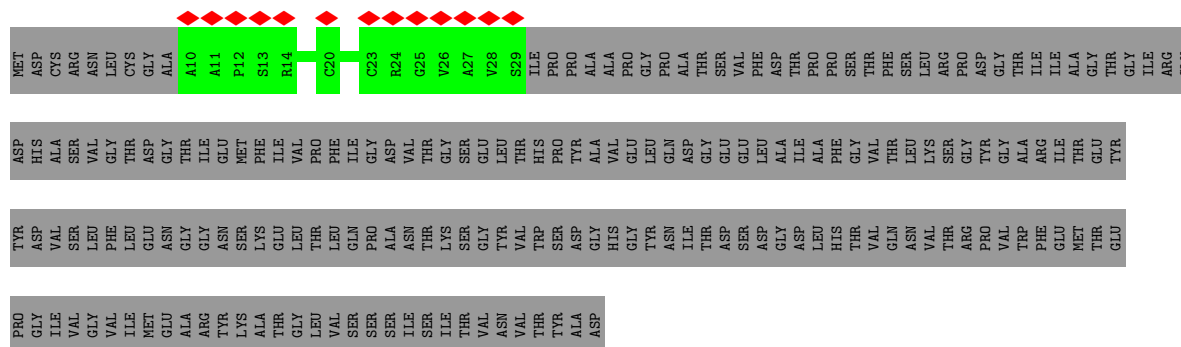
• Molecule 4: Linking protein 1, gp16

Chain f1: 9% 91%



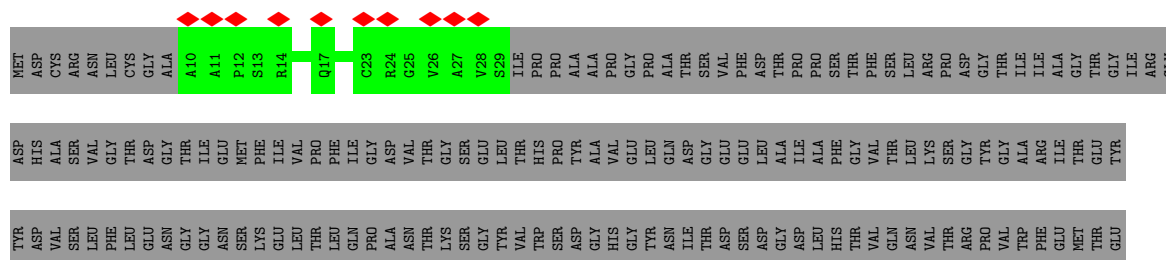
• Molecule 4: Linking protein 1, gp16

Chain f2: 6% 9% 91%



• Molecule 4: Linking protein 1, gp16

Chain f5: 5% 9% 91%





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THR LYS GLU TYR ALA GLU SER LEU ALA HIS PHE PHE THR GLU SER GLU LEU ALA ALA MET LYS SER LEU ALA ARG HIS VAL VAL ARG LYS MET LYS MET LYS VAL ARG GLY ILE THR ASP THR ASP HIS ASP THR LYS ARG LYS THR ALA ILE GLN LEU LYS GLN ARG ASN MET MET HIS GLU PHE ARG LYS VAL ASP THR ASP VAL ASP THR ASP VAL ASP THR ASP THR ILE ASP E183 V184 C186

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• Molecule 5: Major capsid protein, gp9



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• Molecule 5: Major capsid protein, gp9

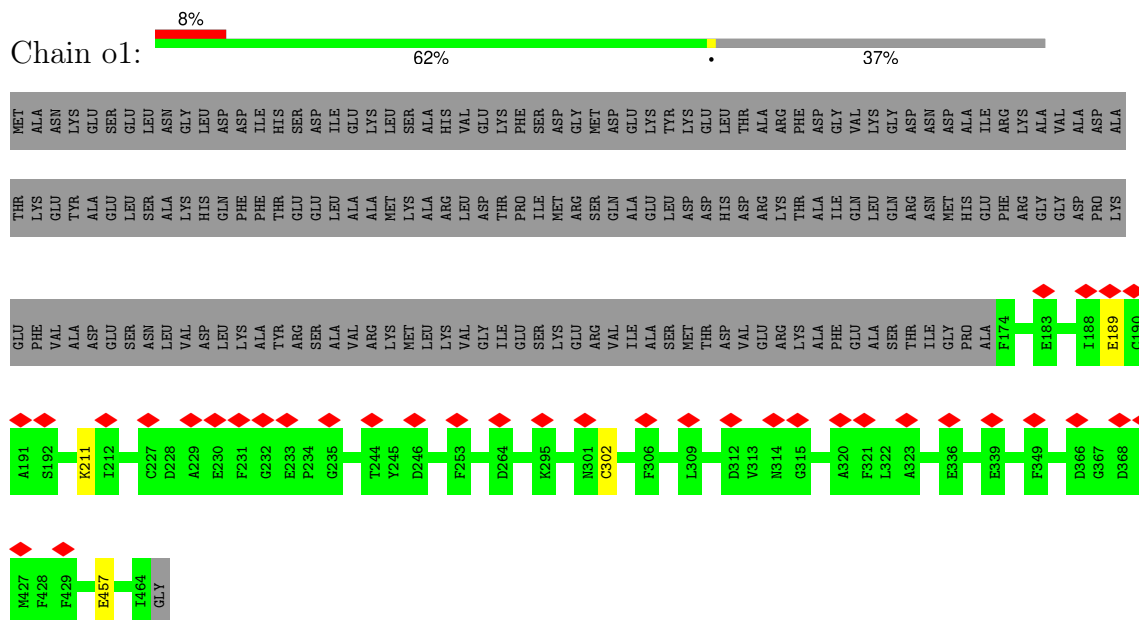


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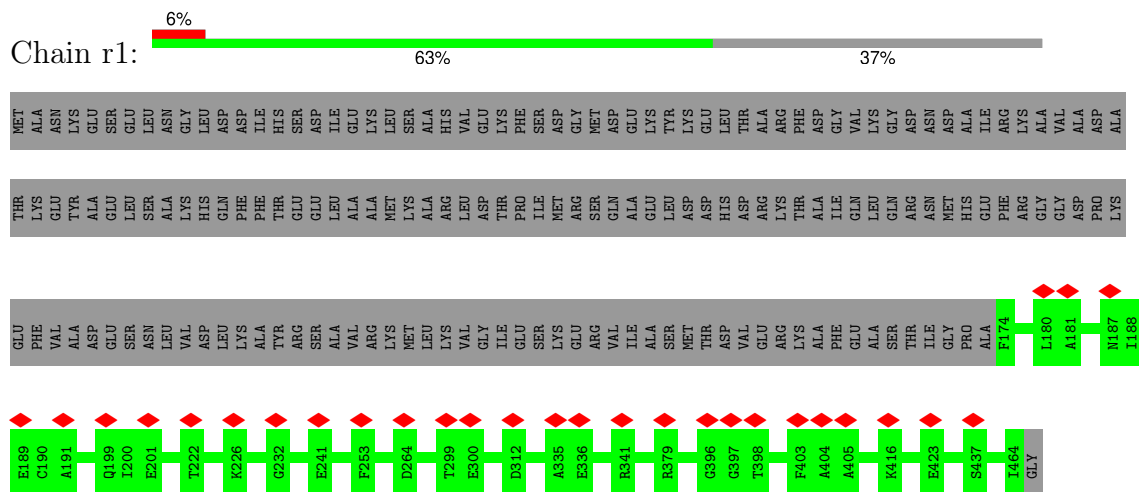
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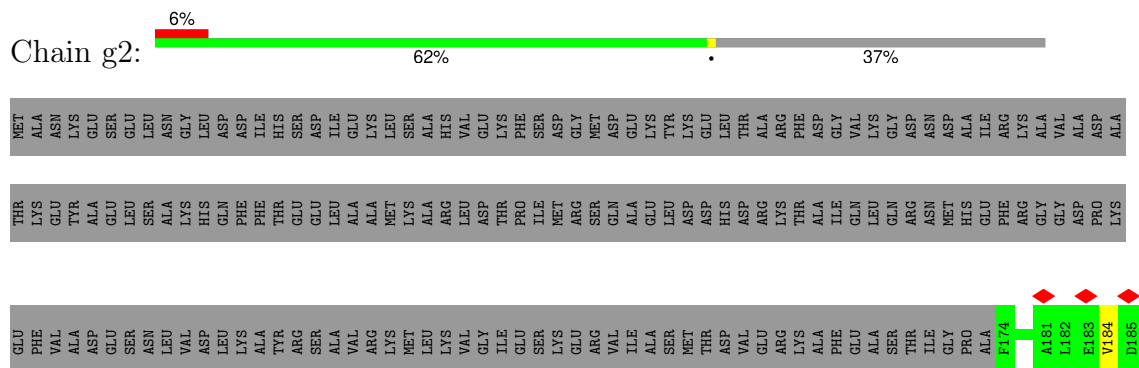
- Molecule 5: Major capsid protein, gp9

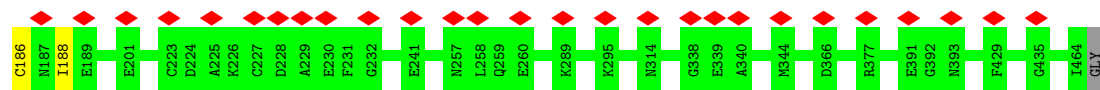


- Molecule 5: Major capsid protein, gp9

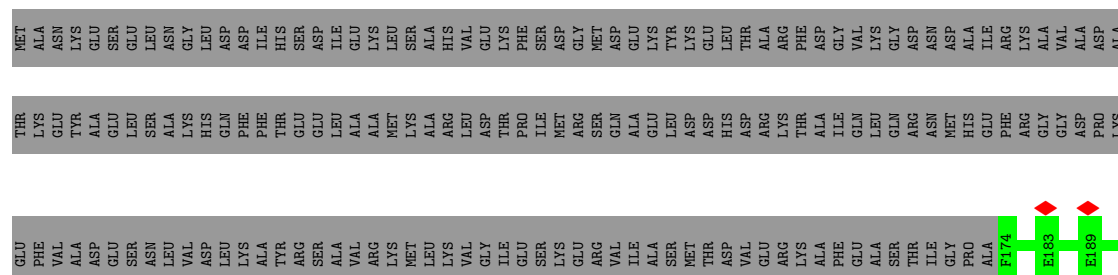


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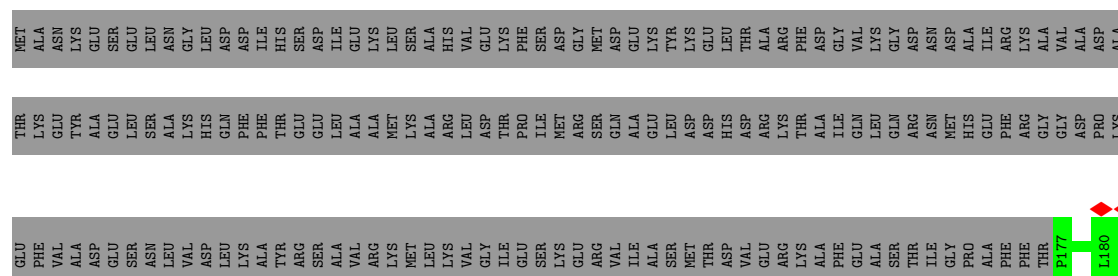




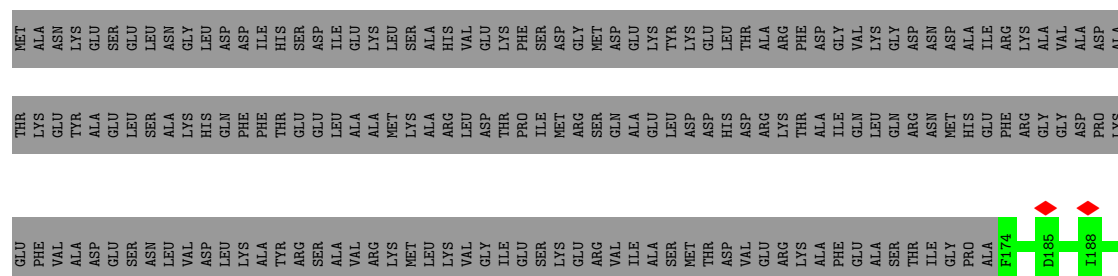
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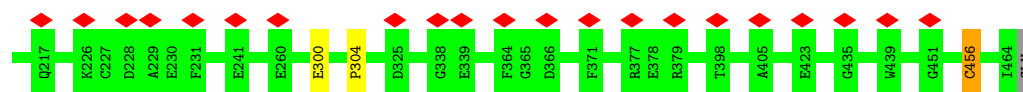


- Molecule 5: Major capsid protein, gp9

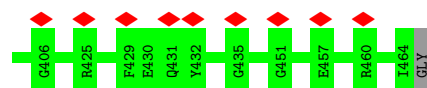
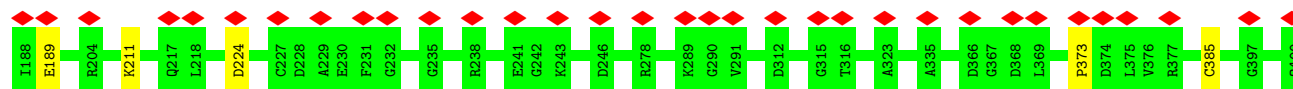
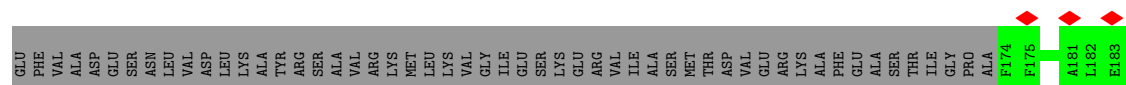
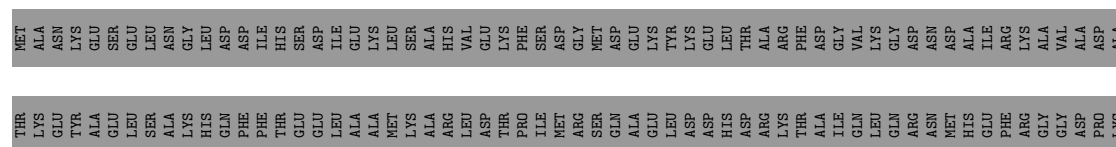


- Molecule 5: Major capsid protein, gp9

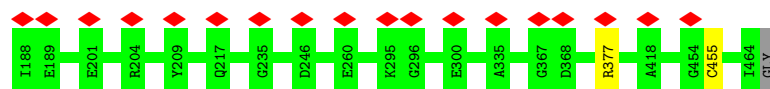
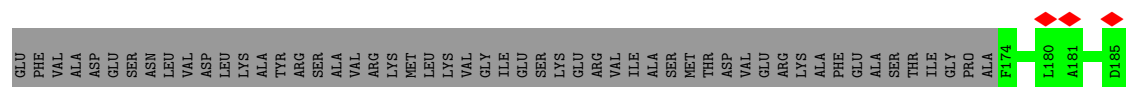
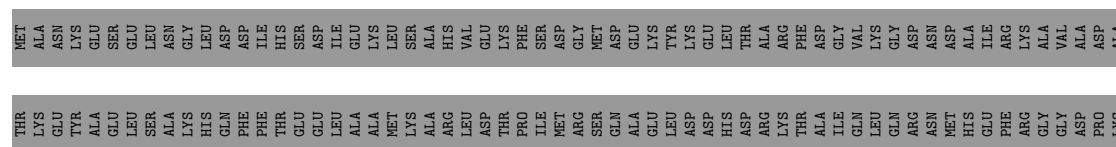




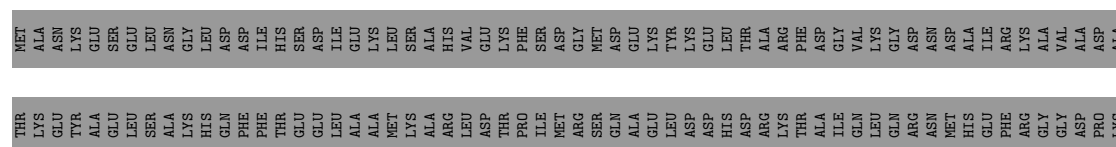
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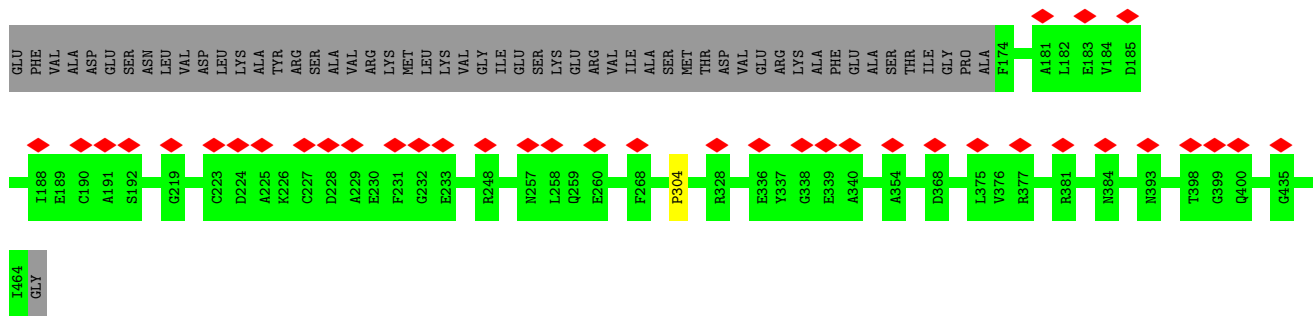


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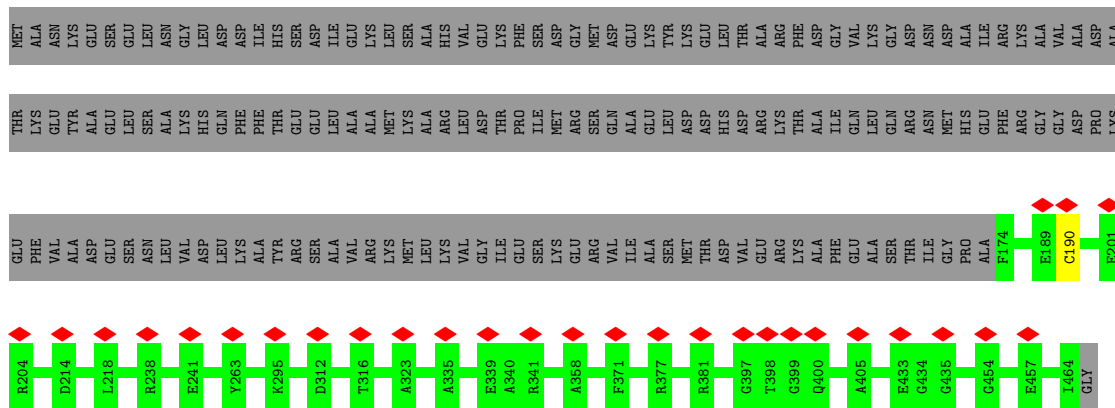


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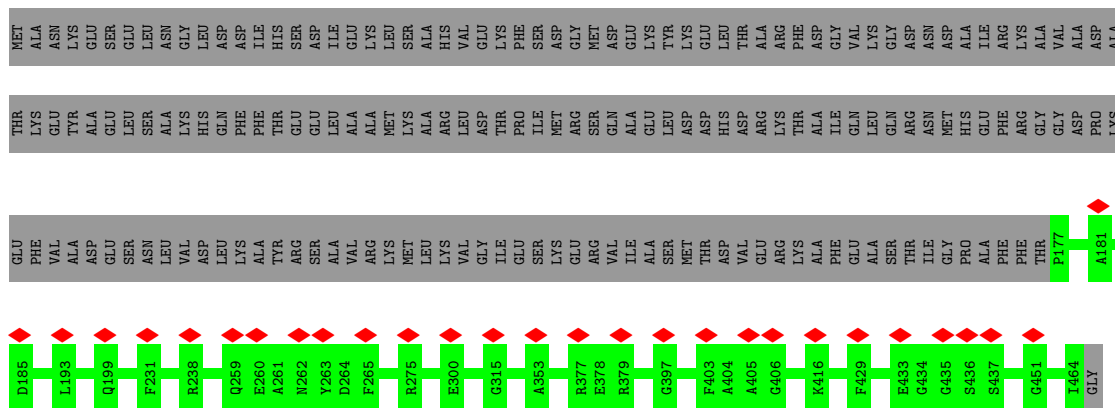




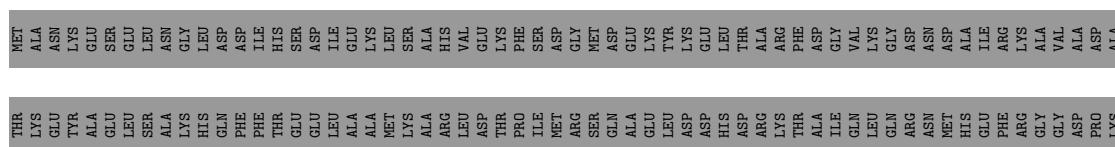
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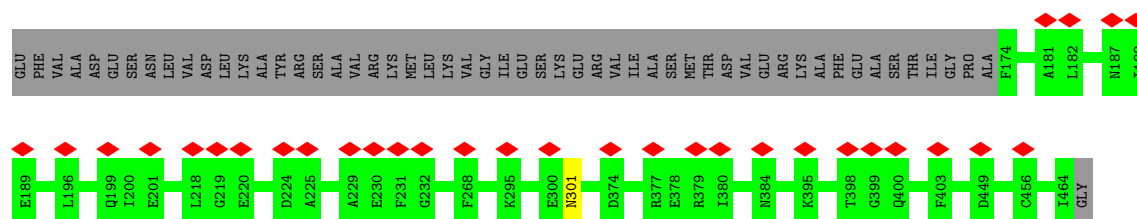


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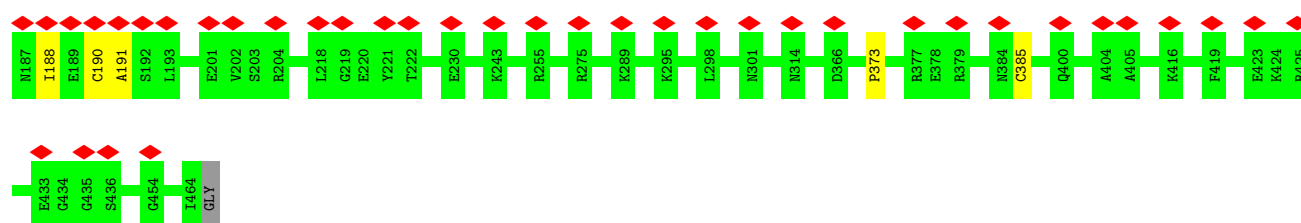
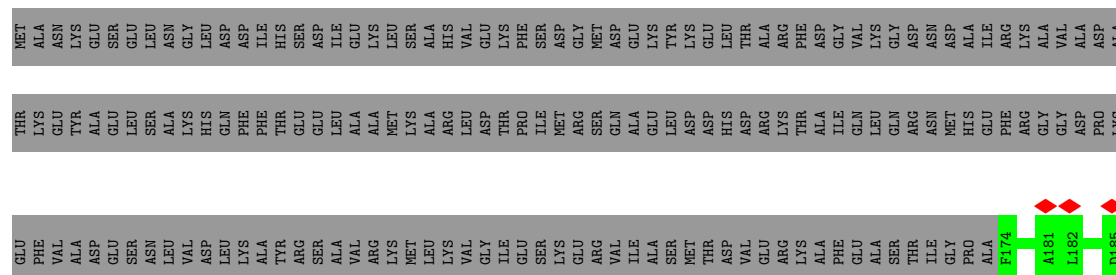


- Molecule 5: Major capsid protein, gp9

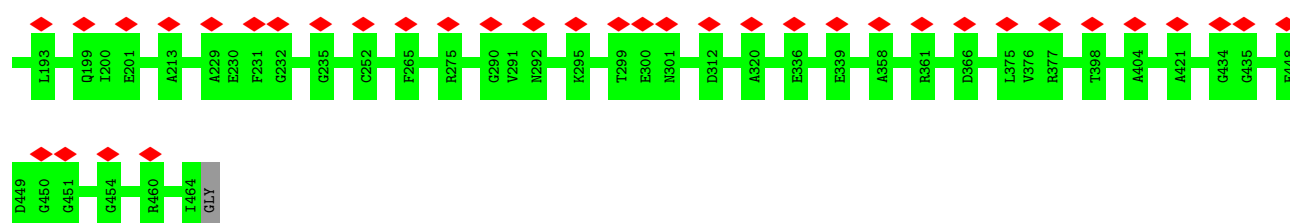
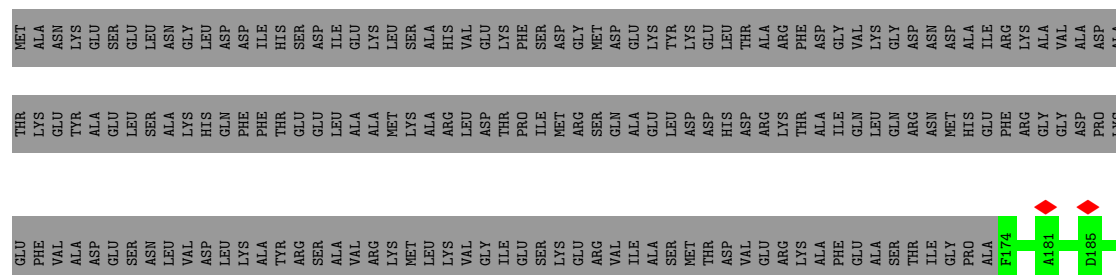




• Molecule 5: Major capsid protein, gp9

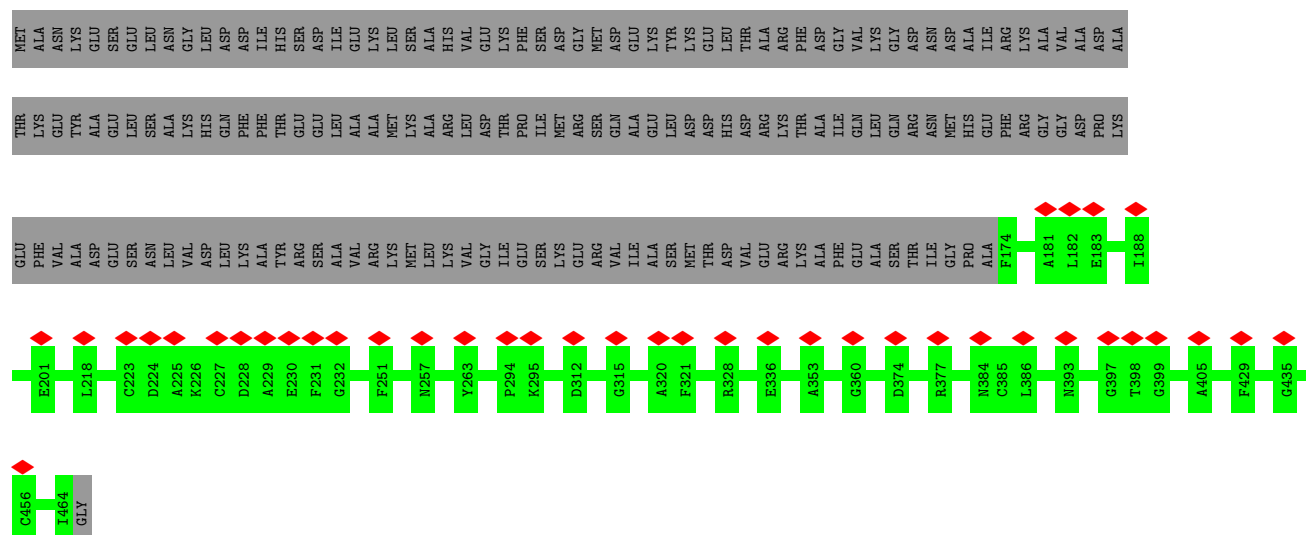


• Molecule 5: Major capsid protein, gp9

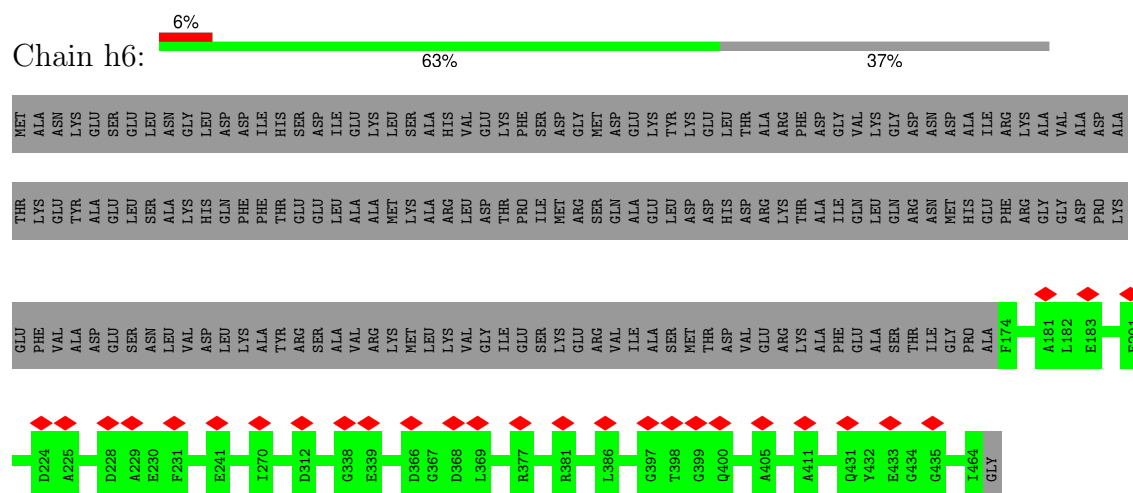


• Molecule 5: Major capsid protein, gp9

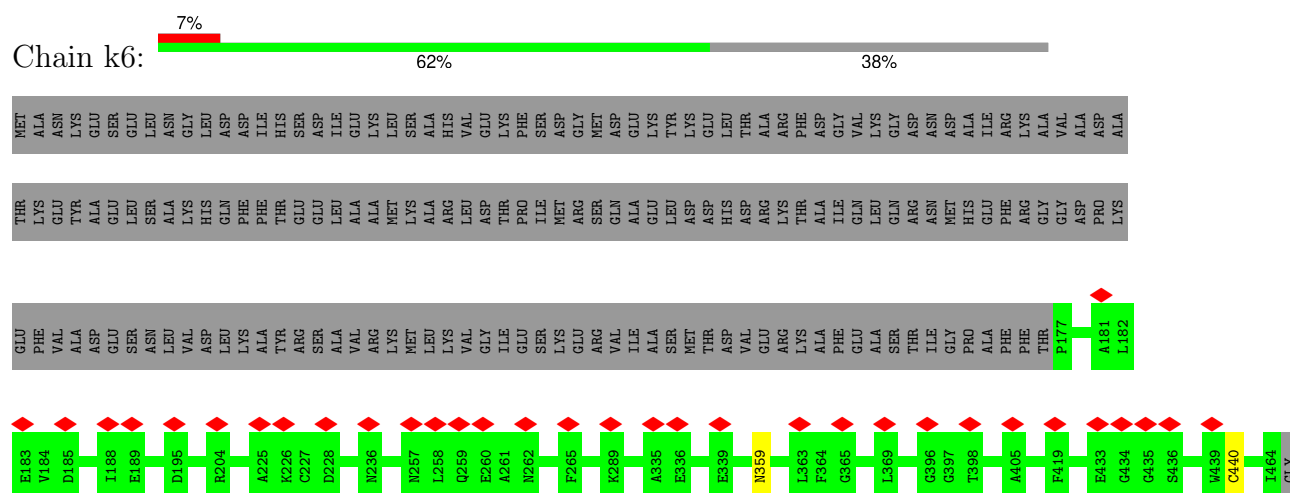




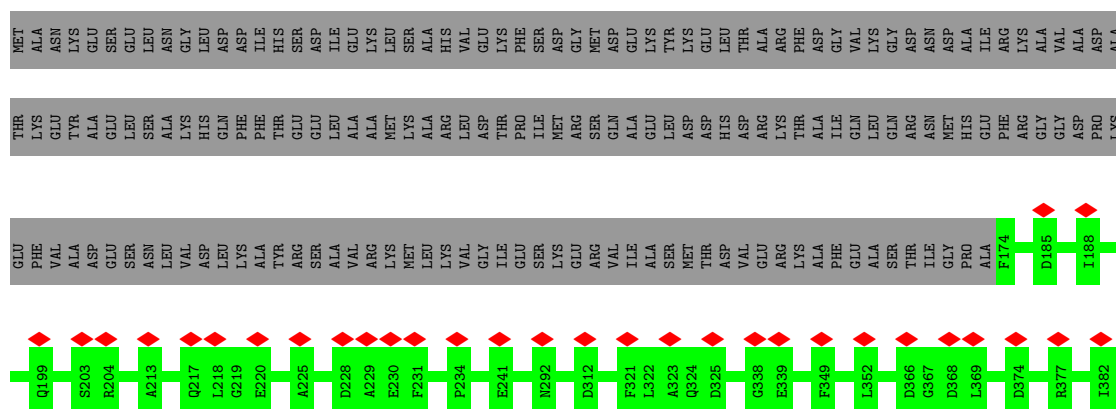
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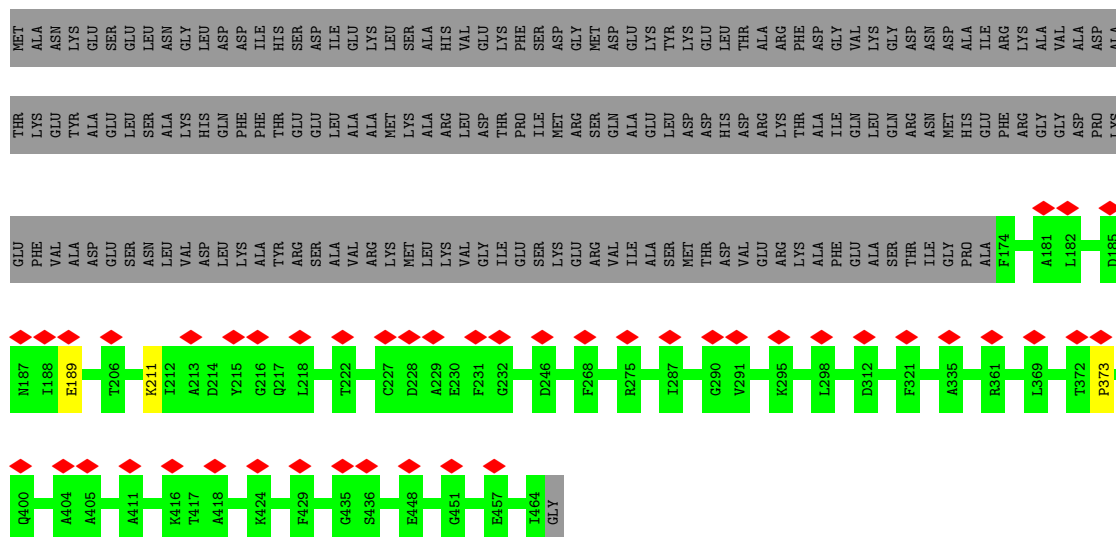
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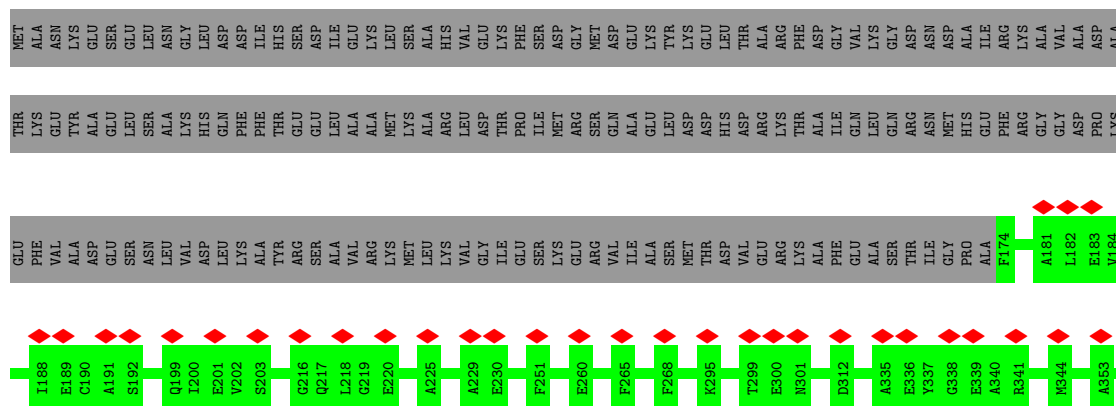
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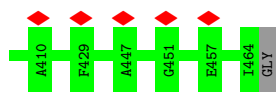


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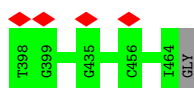
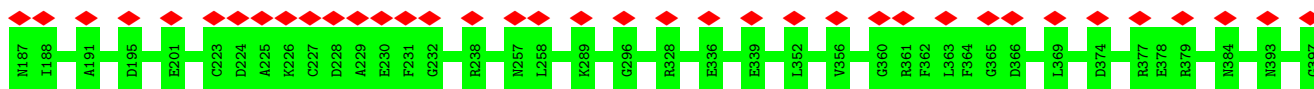
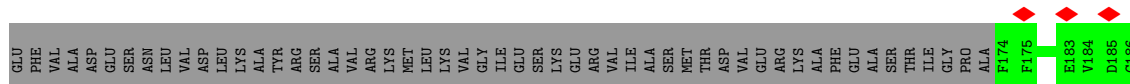


• Molecule 5: Major capsid protein, gp9

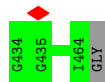
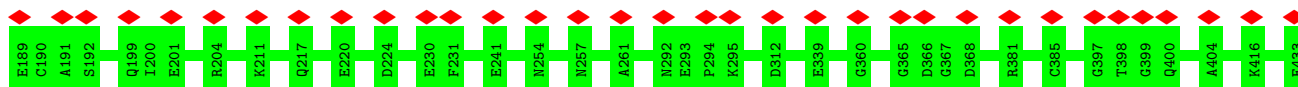
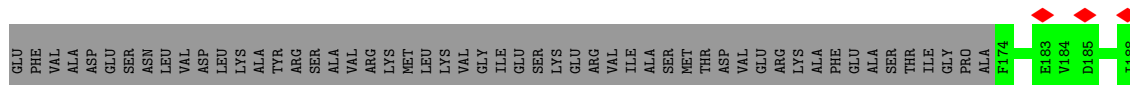
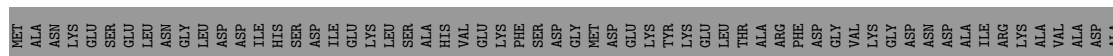




- Molecule 5: Major capsid protein, gp9



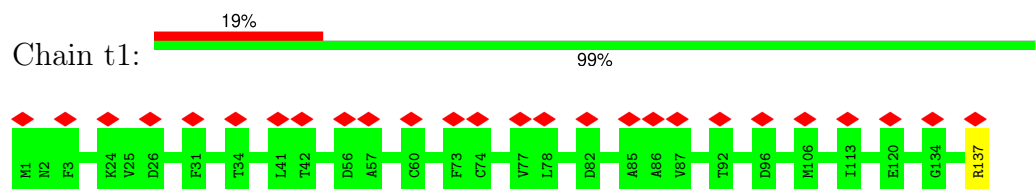
- Molecule 5: Major capsid protein, gp9



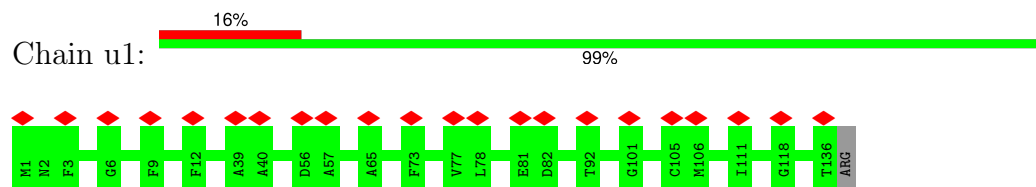
- Molecule 5: Major capsid protein, gp9



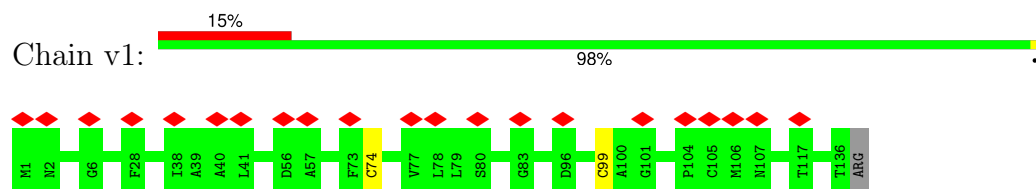
● Molecule 6: Minor capsid protein, gp10



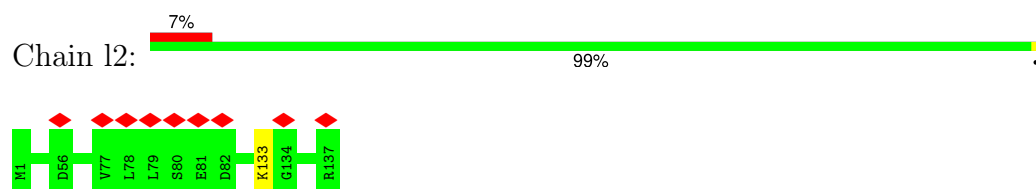
● Molecule 6: Minor capsid protein, gp10



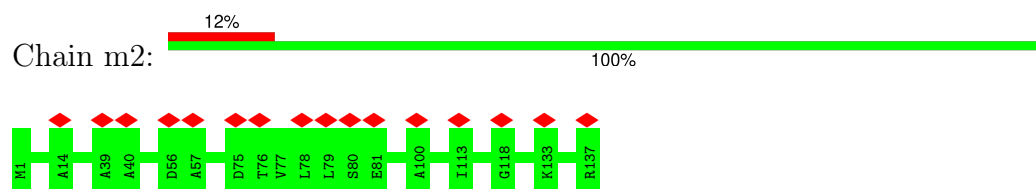
● Molecule 6: Minor capsid protein, gp10



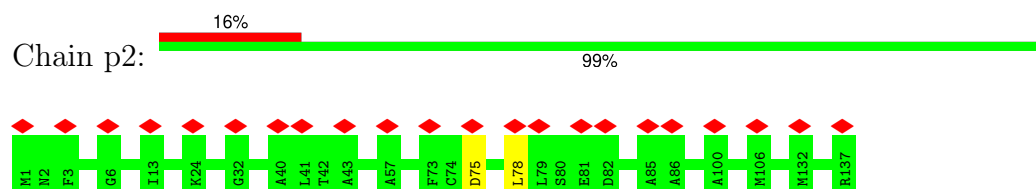
● Molecule 6: Minor capsid protein, gp10



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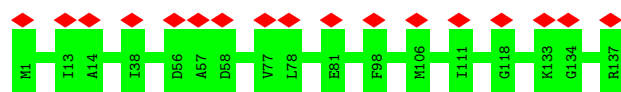


● Molecule 6: Minor capsid protein, gp10

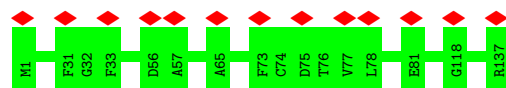


● Molecule 6: Minor capsid protein, gp10

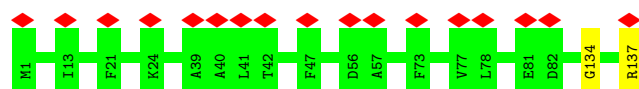




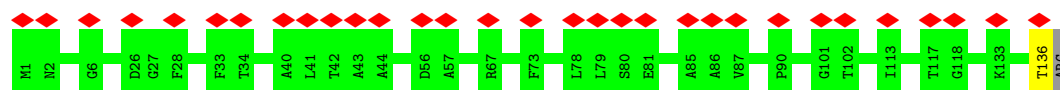
- Molecule 6: Minor capsid protein, gp10



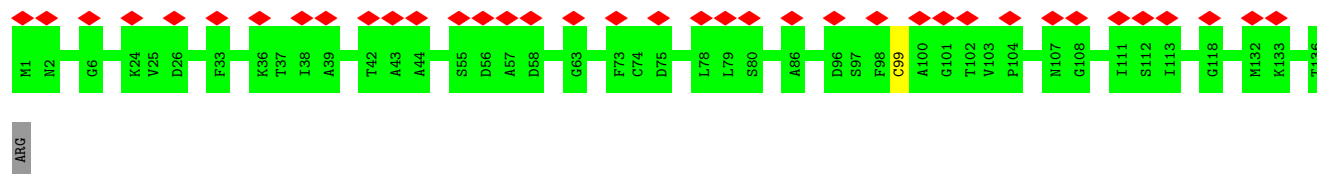
- Molecule 6: Minor capsid protein, gp10



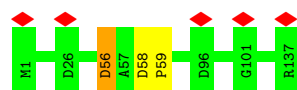
- Molecule 6: Minor capsid protein, gp10



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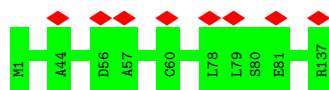


- Molecule 6: Minor capsid protein, gp10

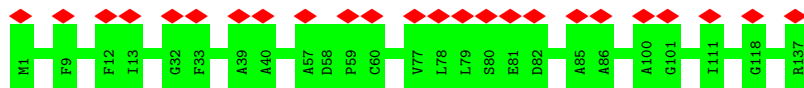


- Molecule 6: Minor capsid protein, gp10

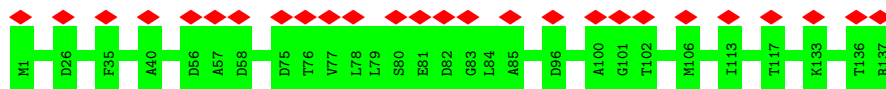




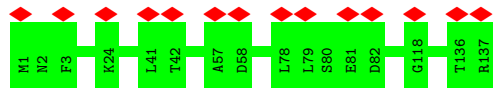
- Molecule 6: Minor capsid protein, gp10



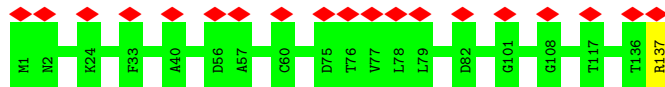
- Molecule 6: Minor capsid protein, gp10



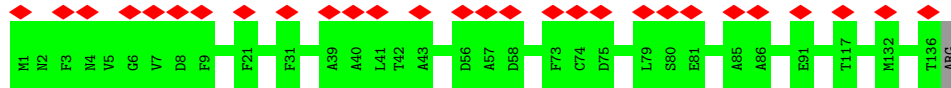
- Molecule 6: Minor capsid protein, gp10



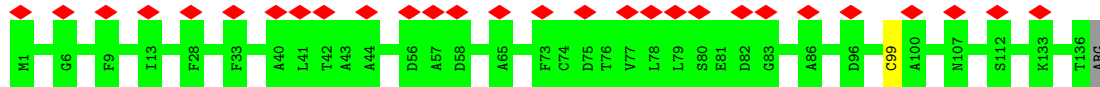
- Molecule 6: Minor capsid protein, gp10



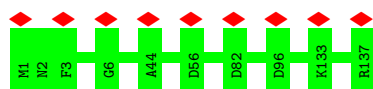
- Molecule 6: Minor capsid protein, gp10



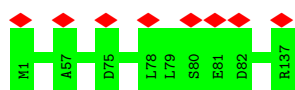
- Molecule 6: Minor capsid protein, gp10



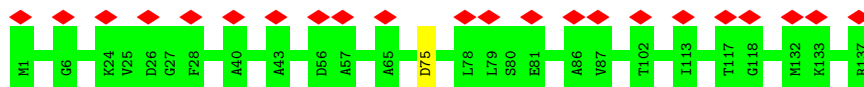
- Molecule 6: Minor capsid protein, gp10



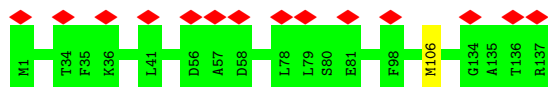
- Molecule 6: Minor capsid protein, gp10



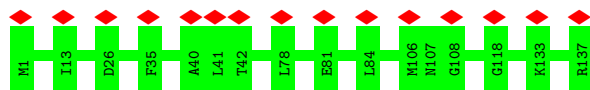
- Molecule 6: Minor capsid protein, gp10



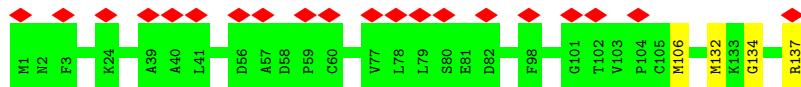
- Molecule 6: Minor capsid protein, gp10



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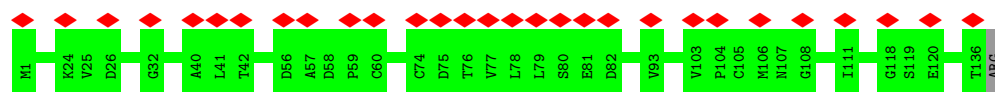


- Molecule 6: Minor capsid protein, gp10

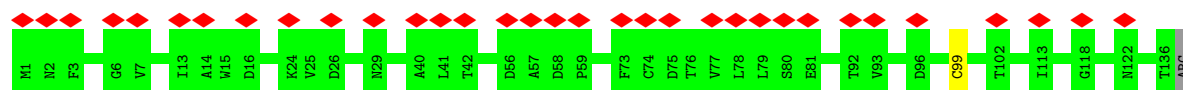


- Molecule 6: Minor capsid protein, gp10

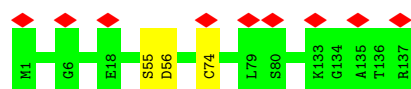




- Molecule 6: Minor capsid protein, gp10



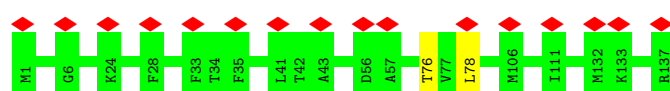
- Molecule 6: Minor capsid protein, gp10



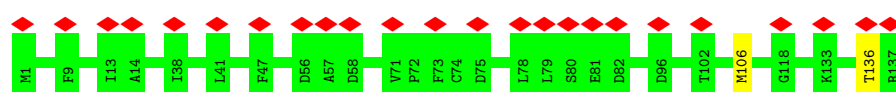
- Molecule 6: Minor capsid protein, gp10



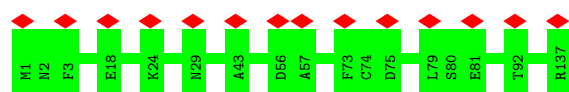
- Molecule 6: Minor capsid protein, gp10



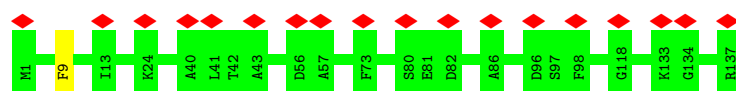
- Molecule 6: Minor capsid protein, gp10



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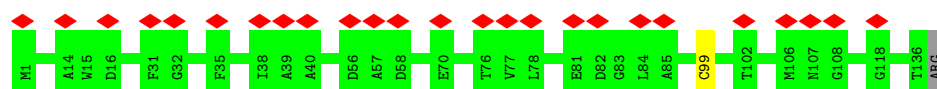
- Molecule 6: Minor capsid protein, gp10



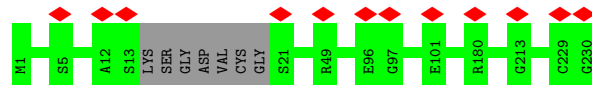
- Molecule 6: Minor capsid protein, gp10



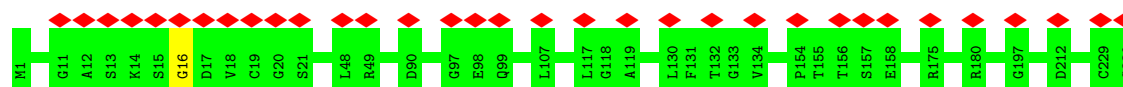
- Molecule 6: Minor capsid protein, gp10



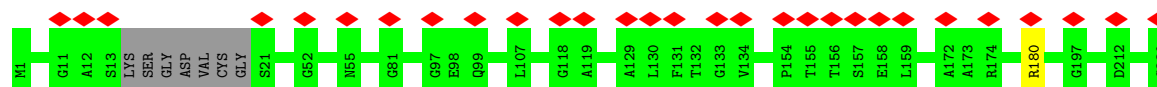
- Molecule 7: Collar sheath protein, gp13



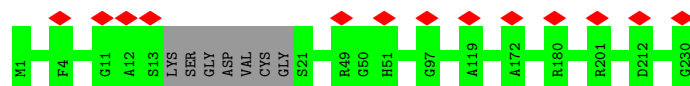
- Molecule 7: Collar sheath protein, gp13



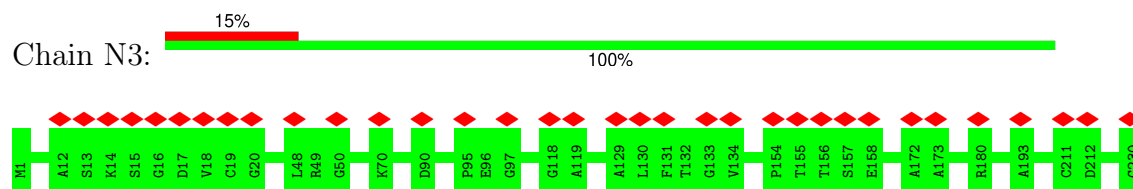
- Molecule 7: Collar sheath protein, gp13



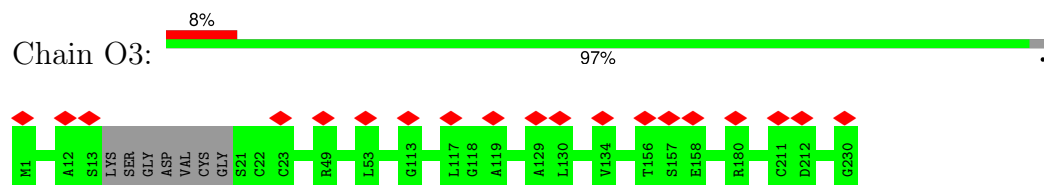
- Molecule 7: Collar sheath protein, gp13



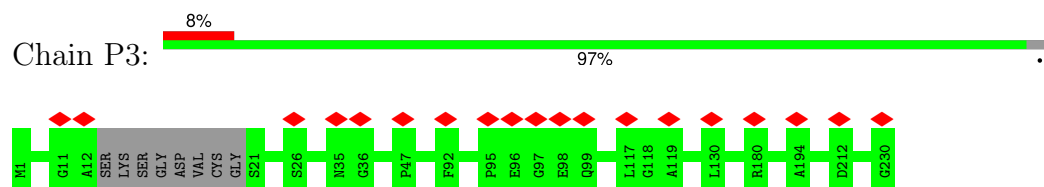
- Molecule 7: Collar sheath protein, gp13



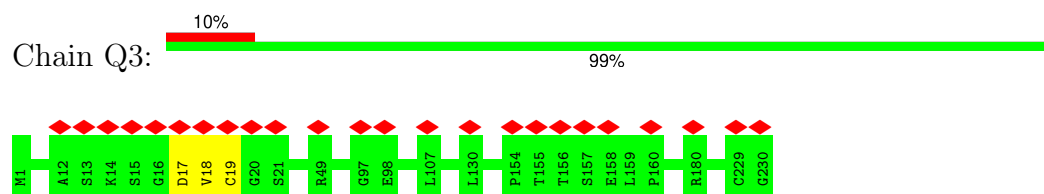
- Molecule 7: Collar sheath protein, gp13



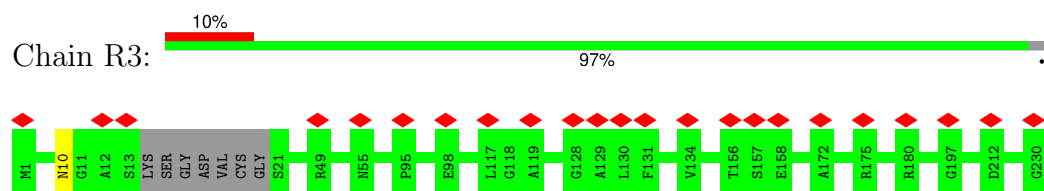
- Molecule 7: Collar sheath protein, gp13



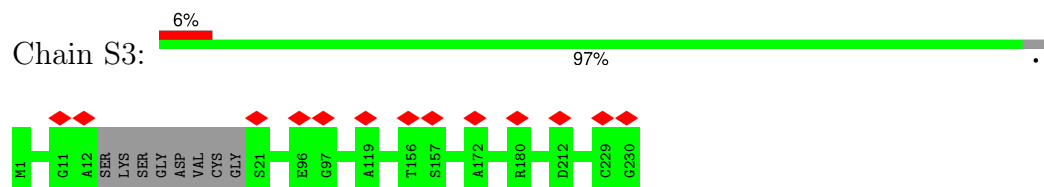
- Molecule 7: Collar sheath protein, gp13



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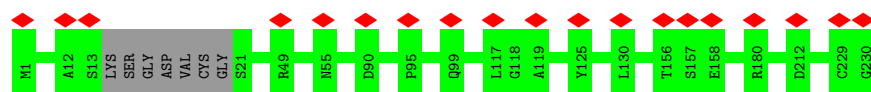


- Molecule 7: Collar sheath protein, gp13

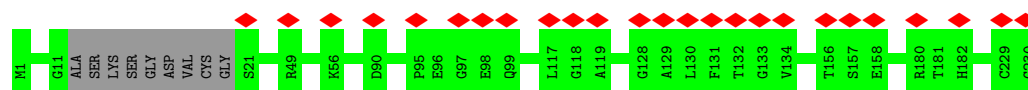


- Molecule 7: Collar sheath protein, gp13

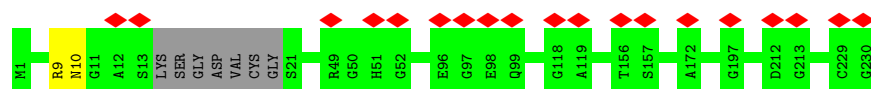




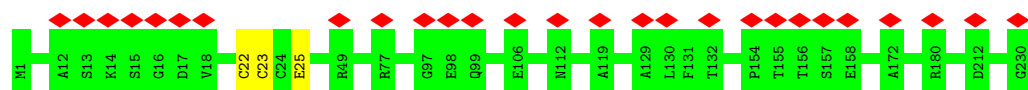
- Molecule 7: Collar sheath protein, gp13



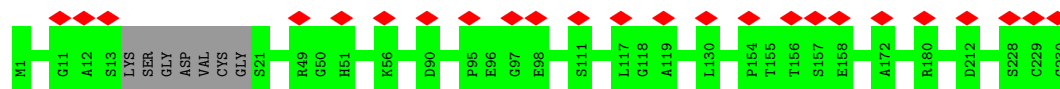
- Molecule 7: Collar sheath protein, gp13



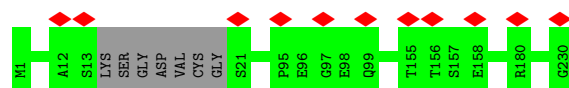
- Molecule 7: Collar sheath protein, gp13



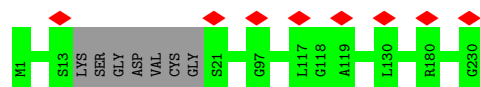
- Molecule 7: Collar sheath protein, gp13



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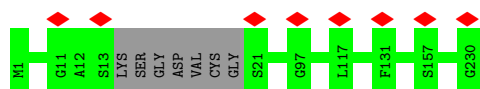


- Molecule 7: Collar sheath protein, gp13



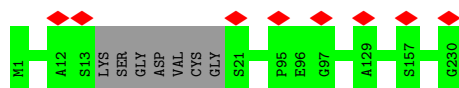
- Molecule 7: Collar sheath protein, gp13

Chain a3:  97%



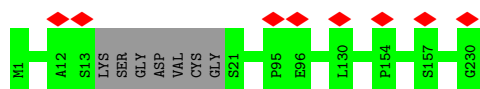
- Molecule 7: Collar sheath protein, gp13

Chain b3:  97%



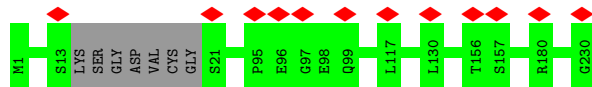
- Molecule 7: Collar sheath protein, gp13

Chain c3:  97%



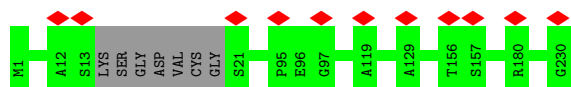
- Molecule 7: Collar sheath protein, gp13

Chain d3:  97%



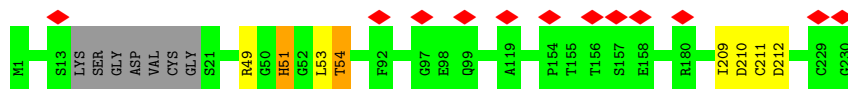
- Molecule 7: Collar sheath protein, gp13

Chain e3:  97%



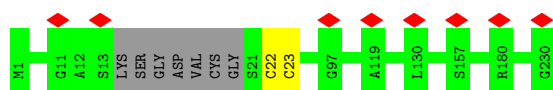
- Molecule 7: Collar sheath protein, gp13

Chain f3:  93%

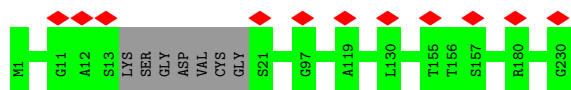


- Molecule 7: Collar sheath protein, gp13

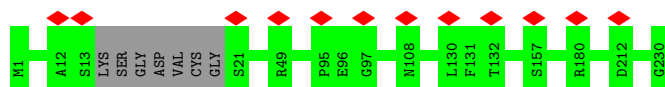
Chain g3:  96%



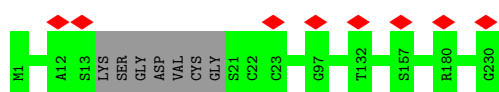
- Molecule 7: Collar sheath protein, gp13



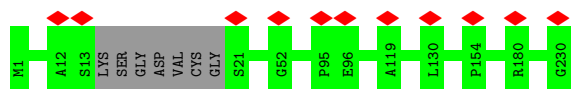
- Molecule 7: Collar sheath protein, gp13



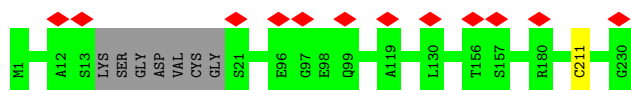
- Molecule 7: Collar sheath protein, gp13



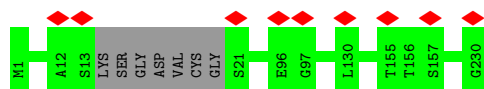
- Molecule 7: Collar sheath protein, gp13



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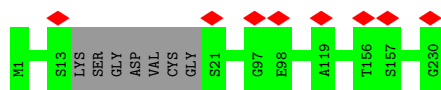


- Molecule 7: Collar sheath protein, gp13

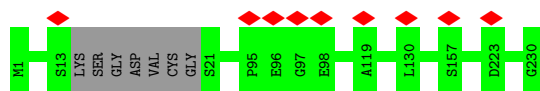


- Molecule 7: Collar sheath protein, gp13

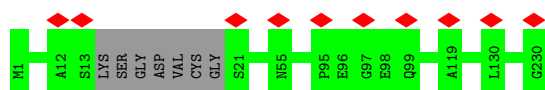




- Molecule 7: Collar sheath protein, gp13



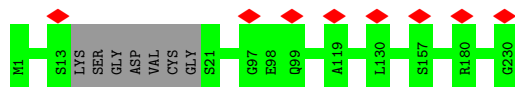
- Molecule 7: Collar sheath protein, gp13



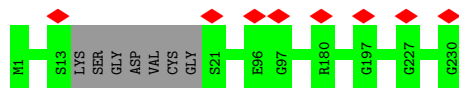
- Molecule 7: Collar sheath protein, gp13



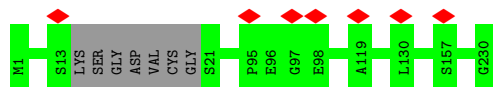
- Molecule 7: Collar sheath protein, gp13



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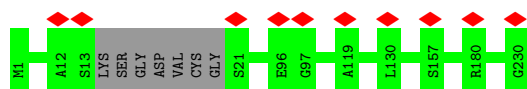


- Molecule 7: Collar sheath protein, gp13



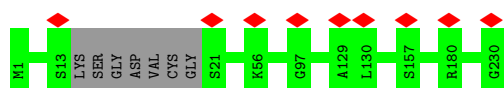
- Molecule 7: Collar sheath protein, gp13

Chain u3:  97%



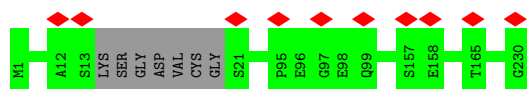
- Molecule 7: Collar sheath protein, gp13

Chain v3:  97%



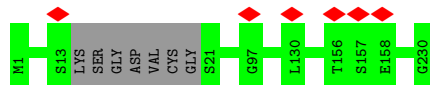
- Molecule 7: Collar sheath protein, gp13

Chain w3:  97%



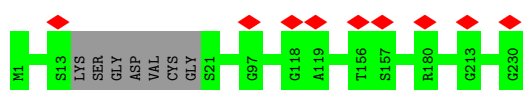
- Molecule 7: Collar sheath protein, gp13

Chain x3:  97%



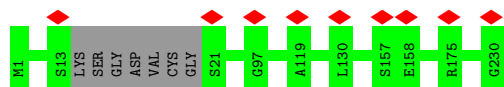
- Molecule 7: Collar sheath protein, gp13

Chain y3:  97%



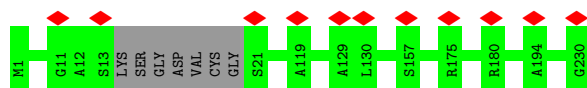
- Molecule 7: Collar sheath protein, gp13

Chain z3:  97%



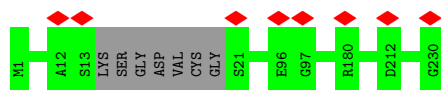
- Molecule 7: Collar sheath protein, gp13

Chain 13:  5% 97%



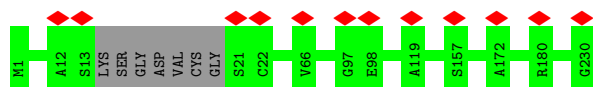
- Molecule 7: Collar sheath protein, gp13

Chain 23:  97%



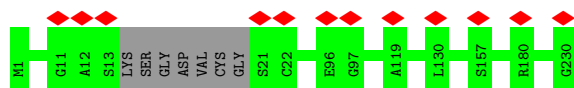
- Molecule 7: Collar sheath protein, gp13

Chain 33:  97%



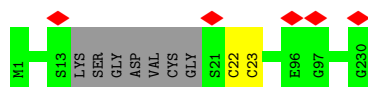
- Molecule 7: Collar sheath protein, gp13

Chain 43:  97%



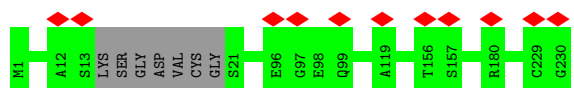
- Molecule 7: Collar sheath protein, gp13

Chain 53:  96%



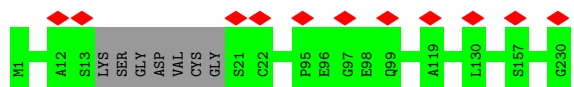
- Molecule 7: Collar sheath protein, gp13

Chain 63:  97%



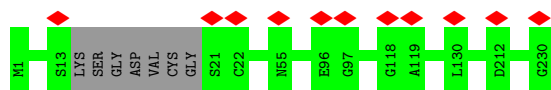
- Molecule 7: Collar sheath protein, gp13

Chain 73:  97%

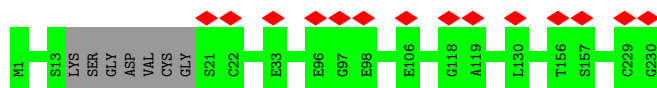


- Molecule 7: Collar sheath protein, gp13

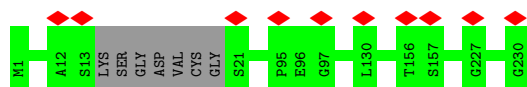
Chain 83:  97%



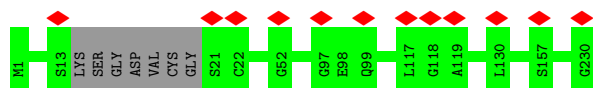
- Molecule 7: Collar sheath protein, gp13



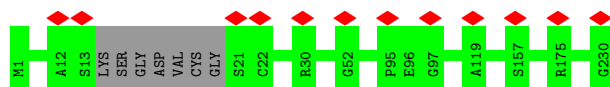
- Molecule 7: Collar sheath protein, gp13



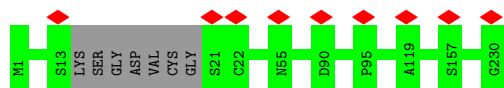
- Molecule 7: Collar sheath protein, gp13



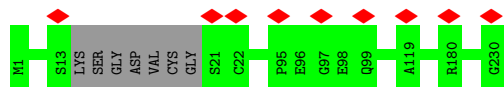
- Molecule 7: Collar sheath protein, gp13



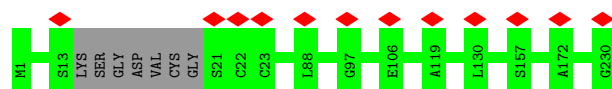
- Molecule 7: Collar sheath protein, gp13



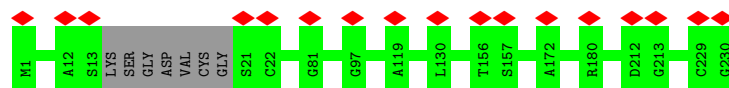
- Molecule 7: Collar sheath protein, gp13



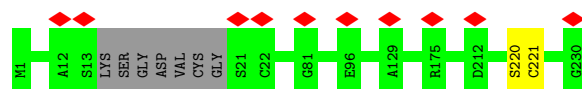
- Molecule 7: Collar sheath protein, gp13



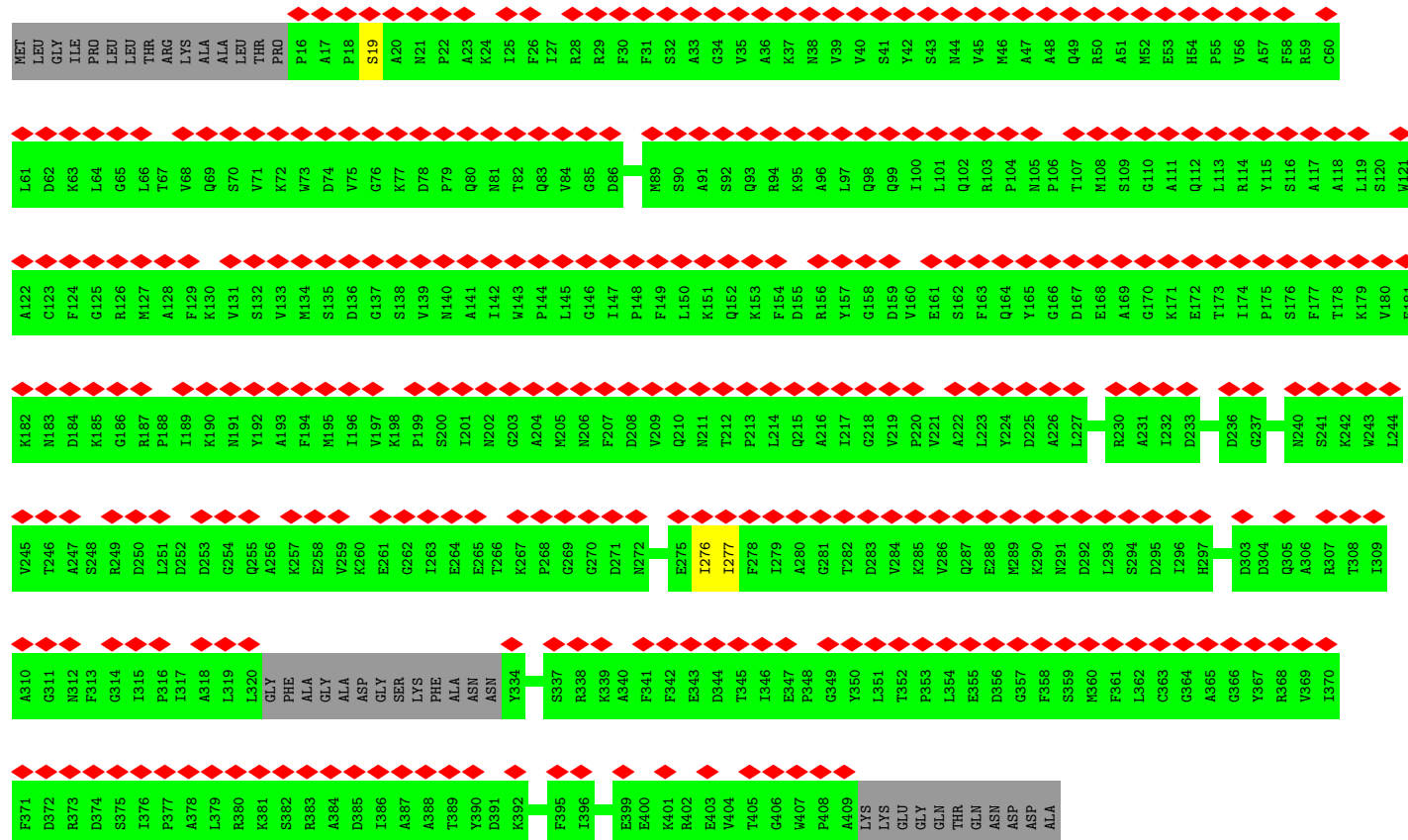
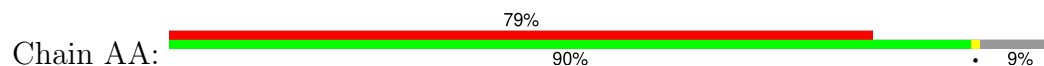
- Molecule 7: Collar sheath protein, gp13



- Molecule 7: Collar sheath protein, gp13

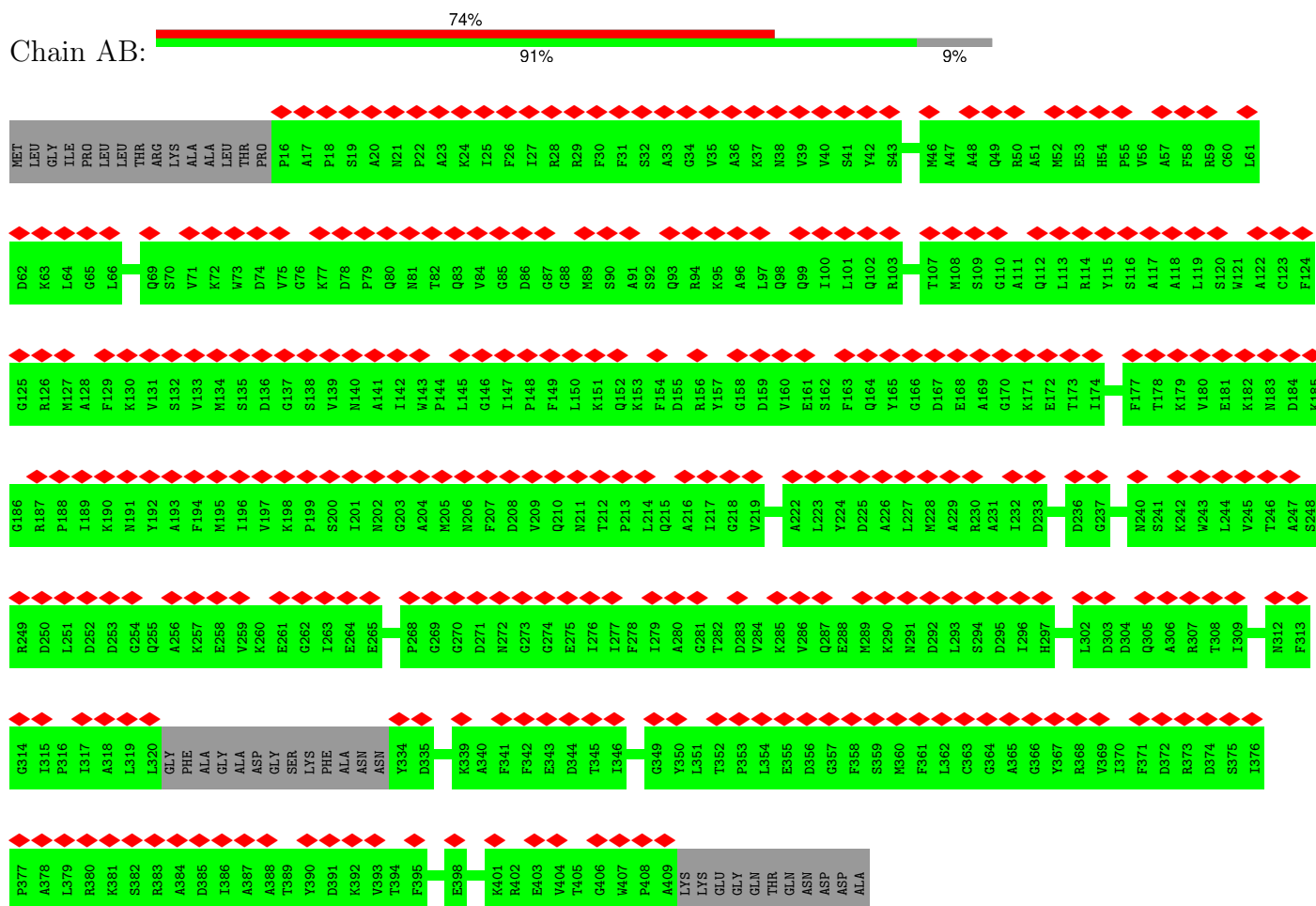


- Molecule 8: Portal protein, gp7



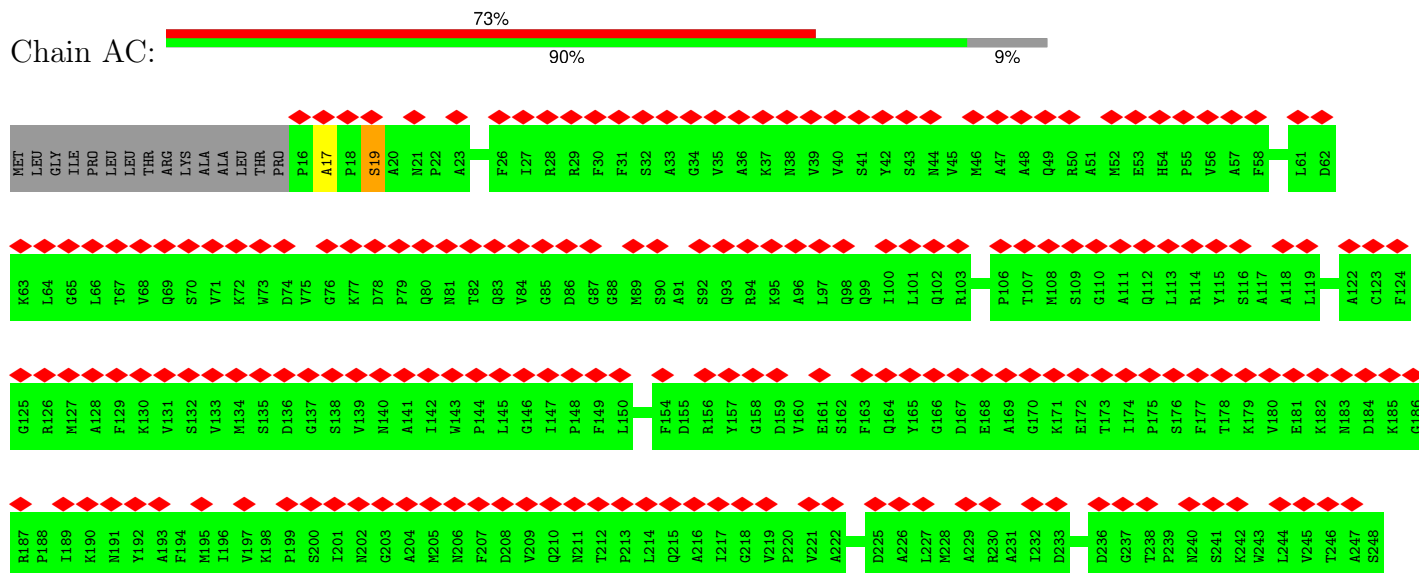
- Molecule 8: Portal protein, gp7

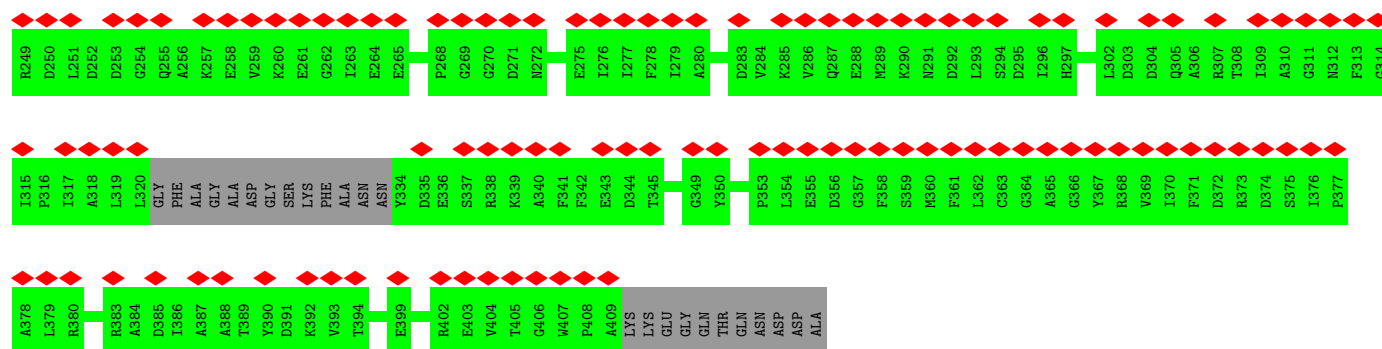
Chain AB:

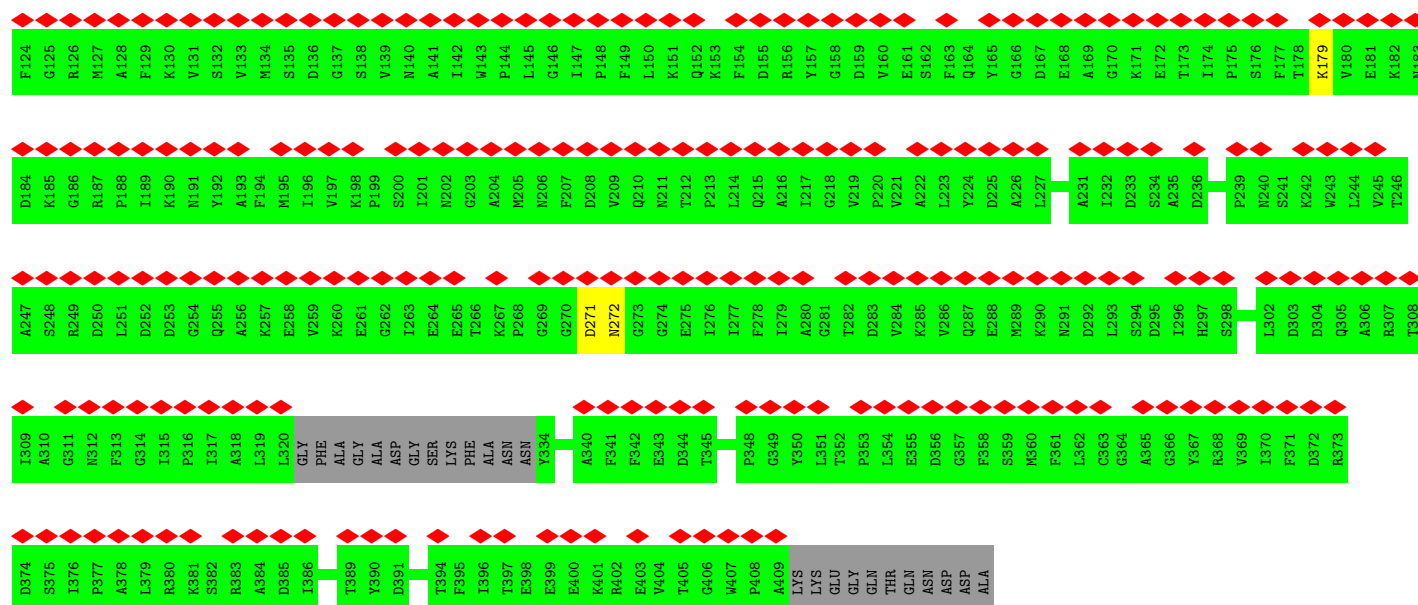


- Molecule 8: Portal protein, gp7

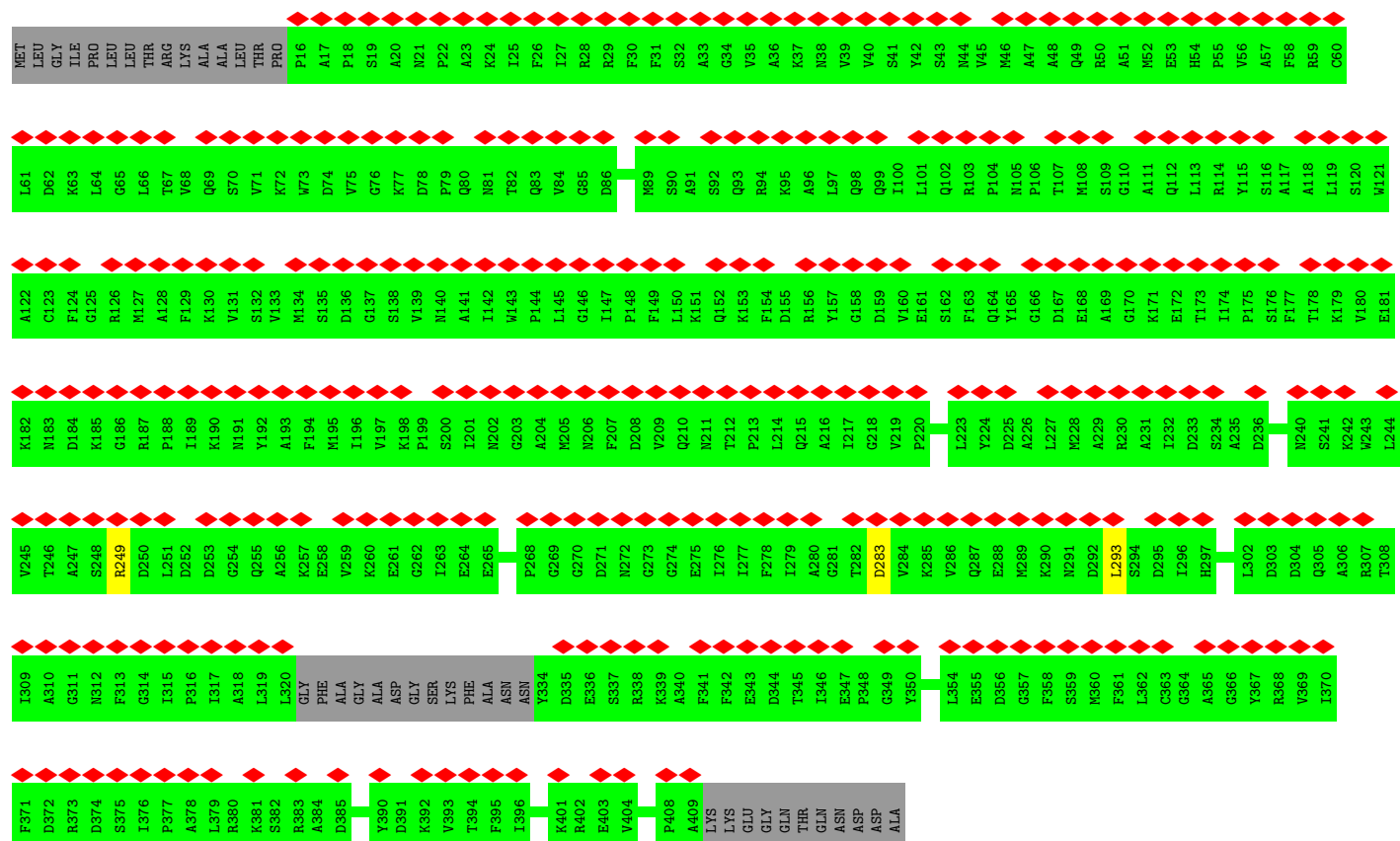
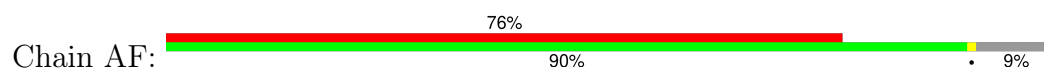
Chain AC:



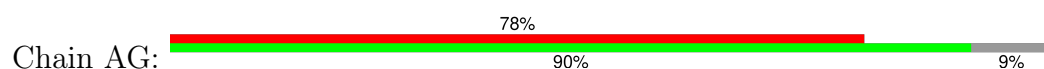


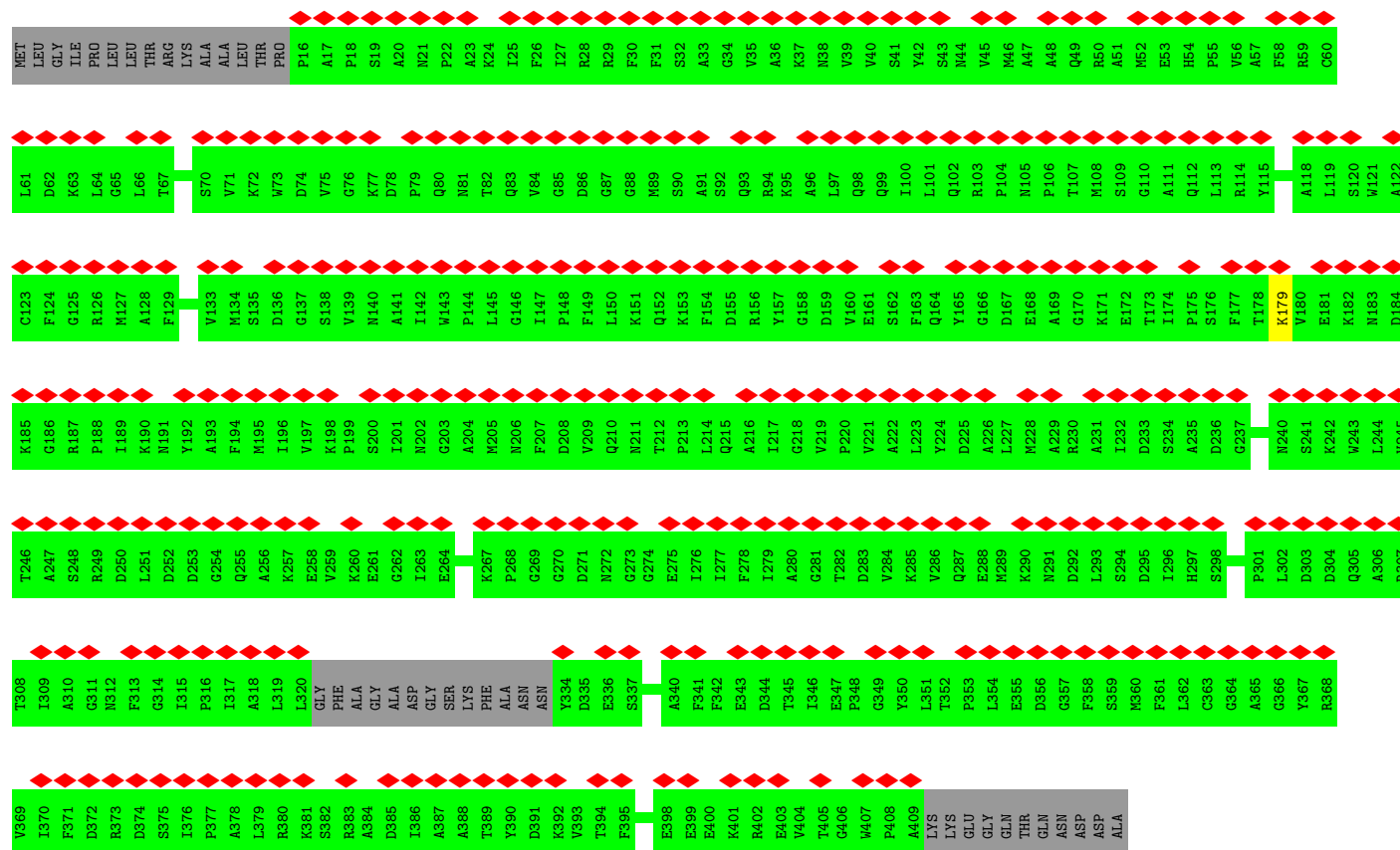


• Molecule 8: Portal protein, gp7

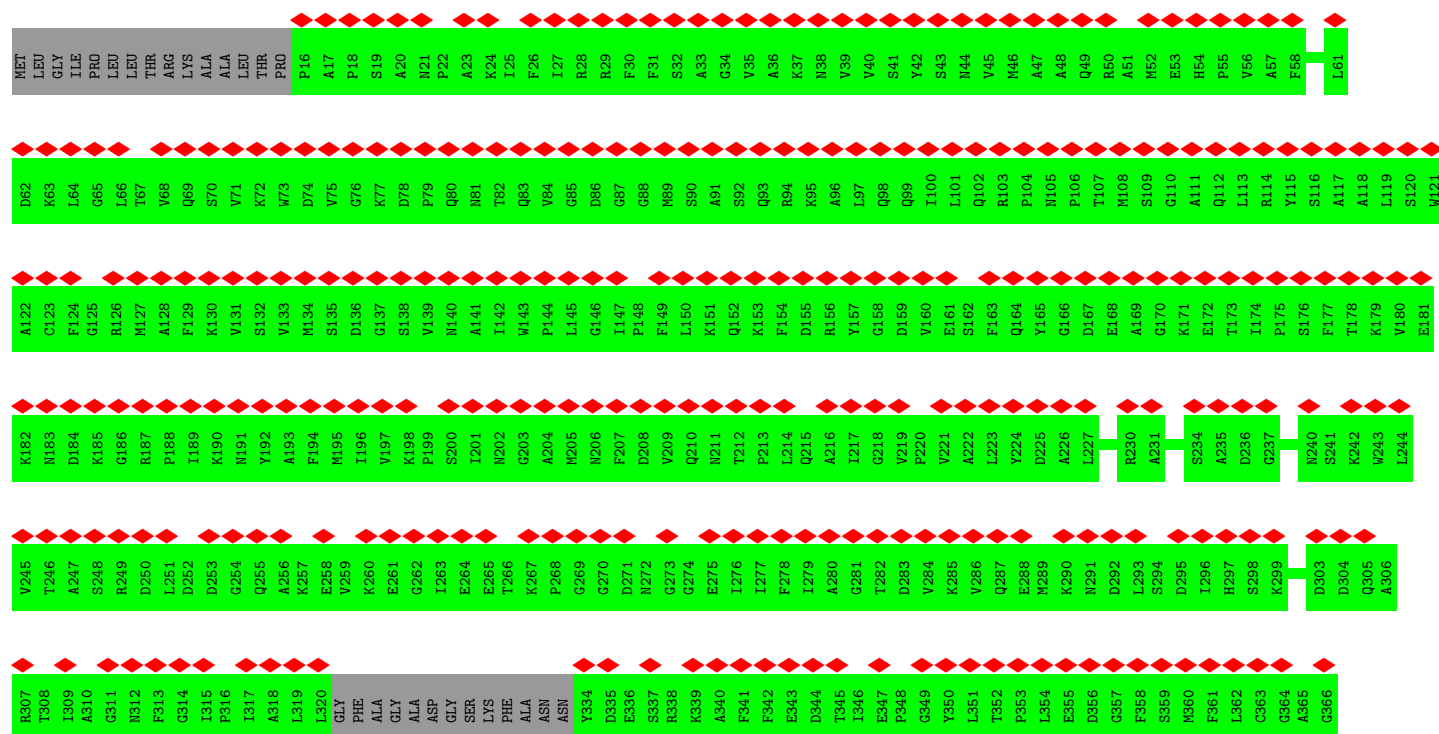
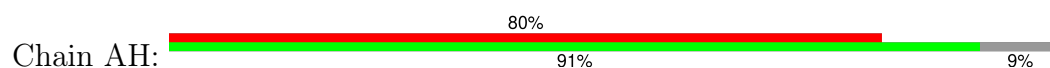


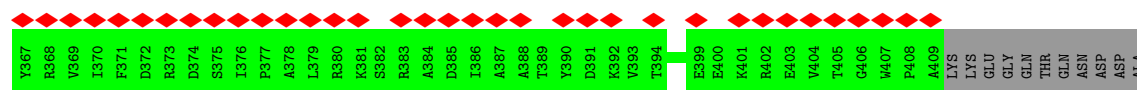
• Molecule 8: Portal protein, gp7



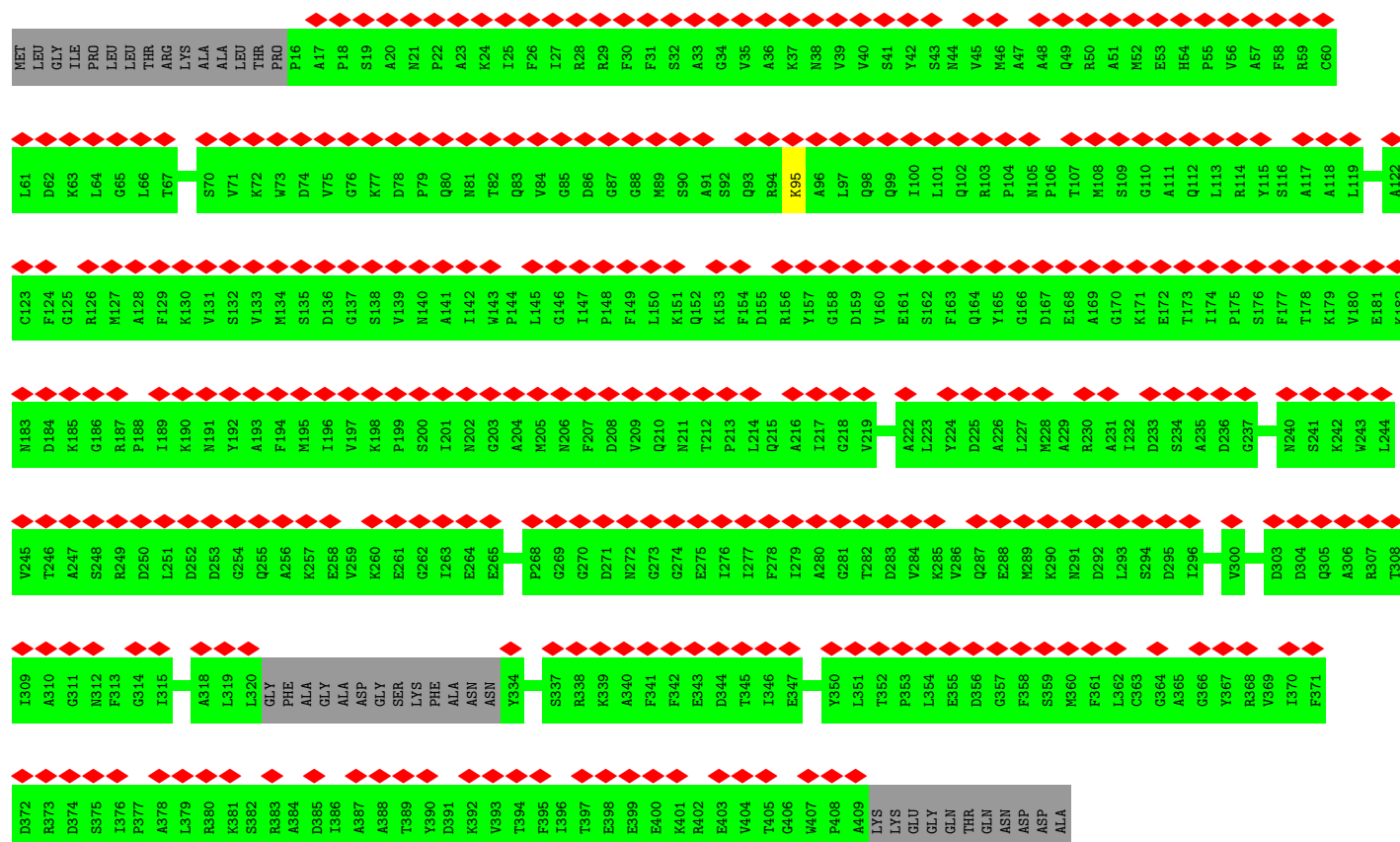
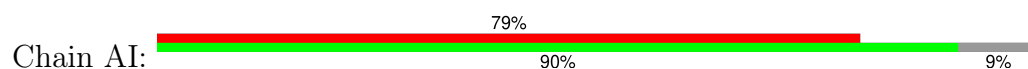


• Molecule 8: Portal protein, gp7

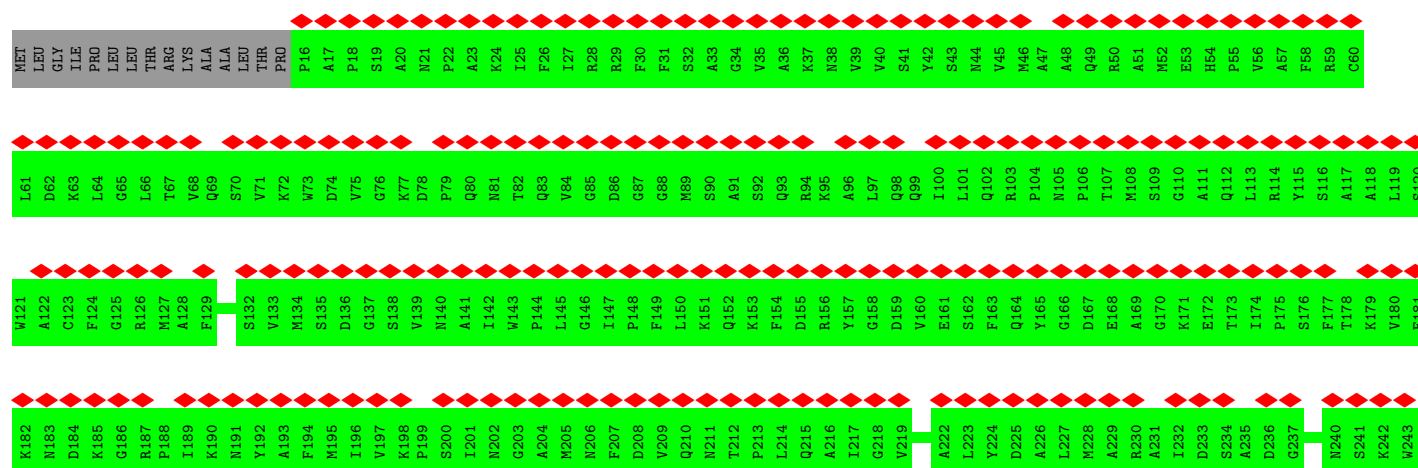
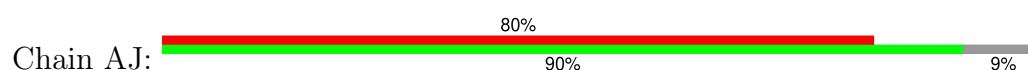


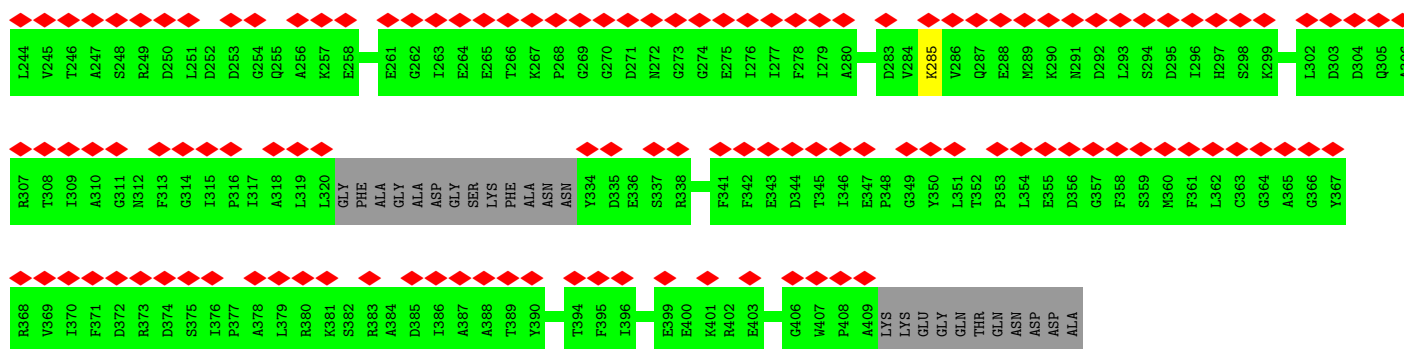


• Molecule 8: Portal protein, gp7

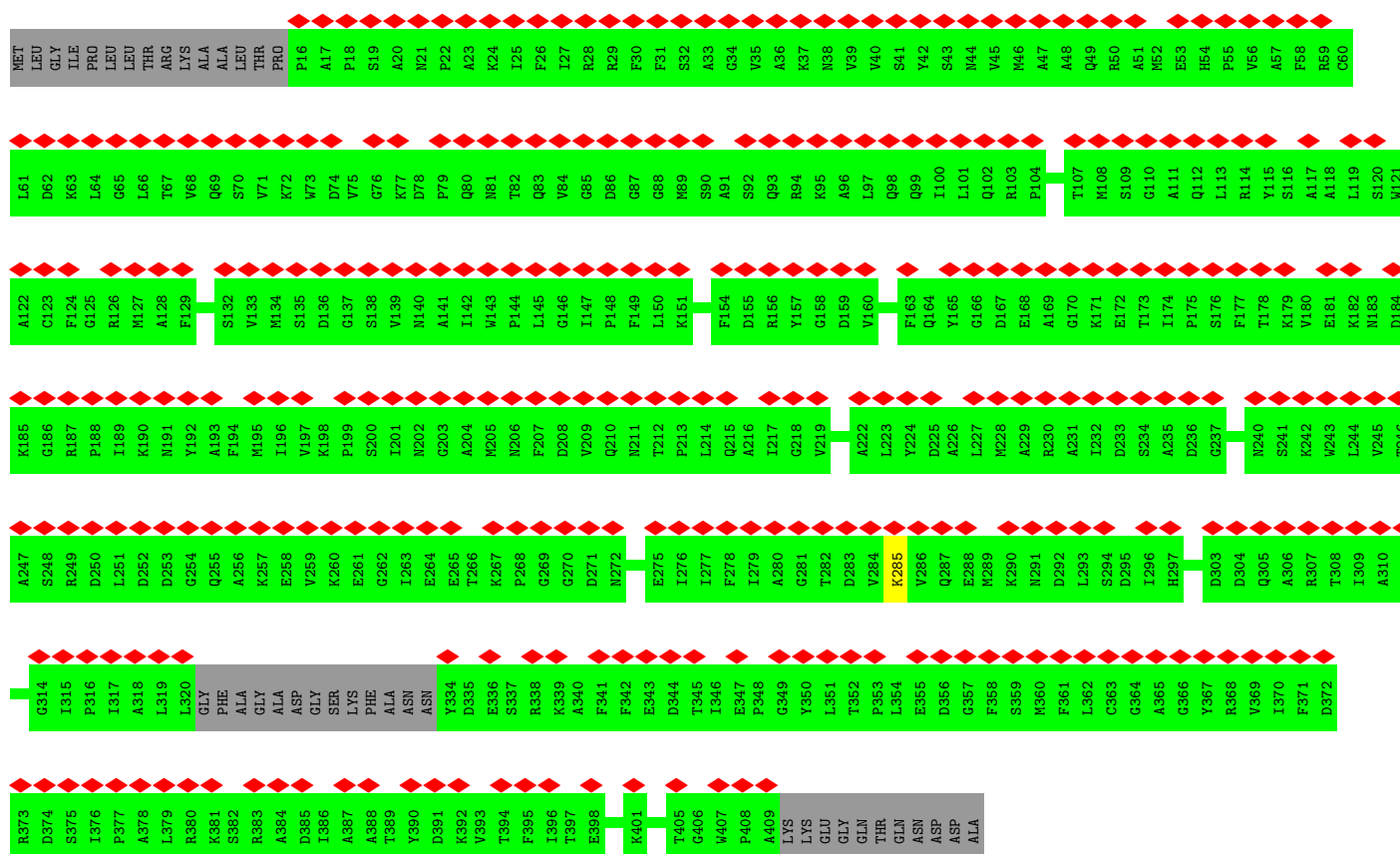
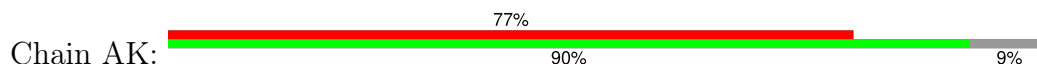


• Molecule 8: Portal protein, gp7

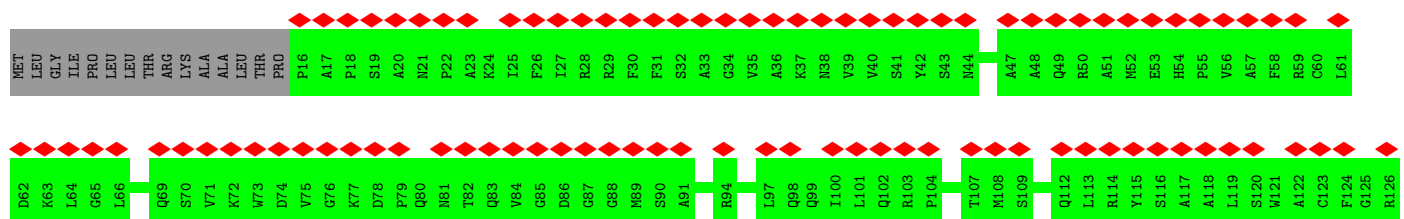
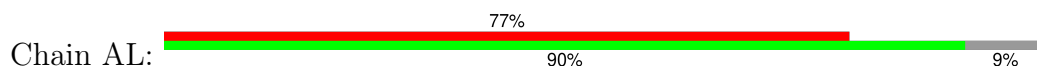


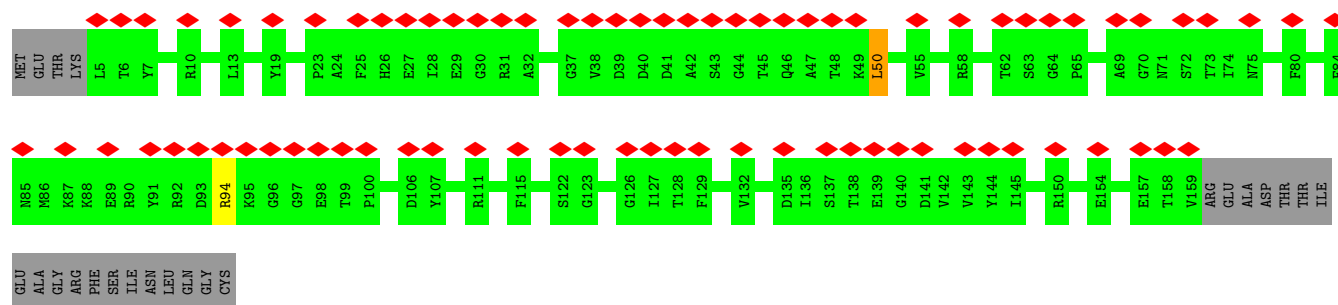


• Molecule 8: Portal protein, gp7

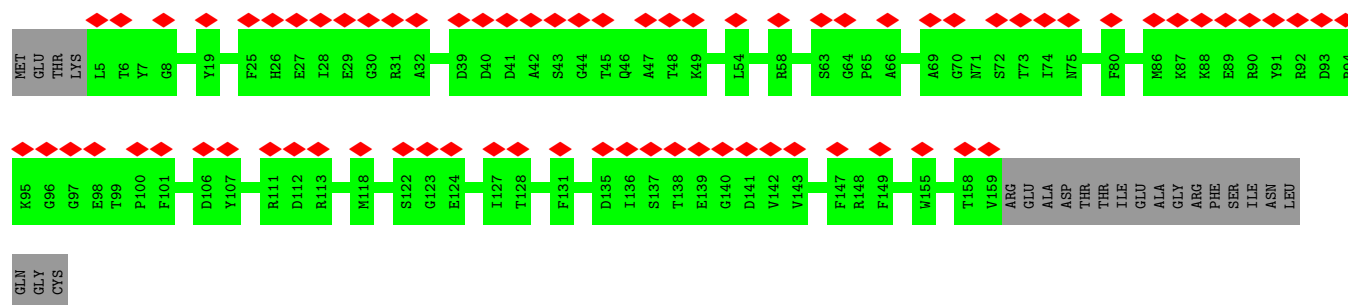
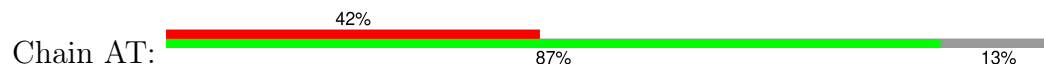


• Molecule 8: Portal protein, gp7

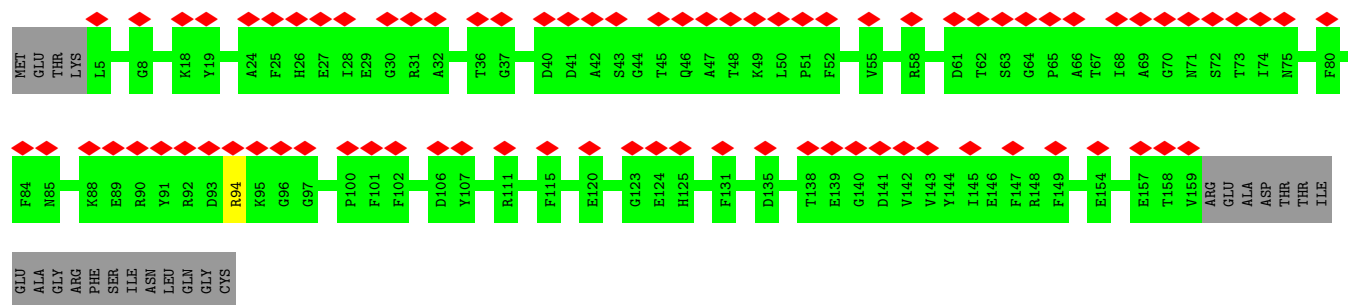




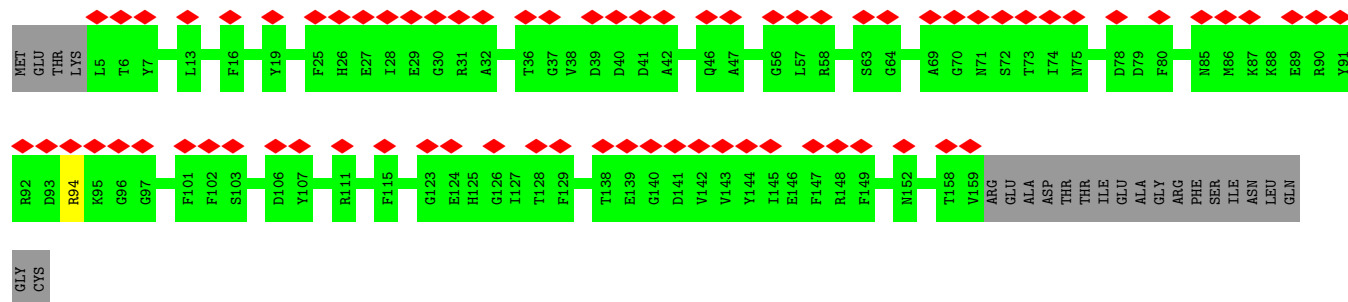
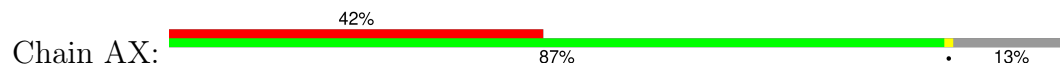
- Molecule 9: Tail-terminator protein, gp18



- Molecule 9: Tail-terminator protein, gp18

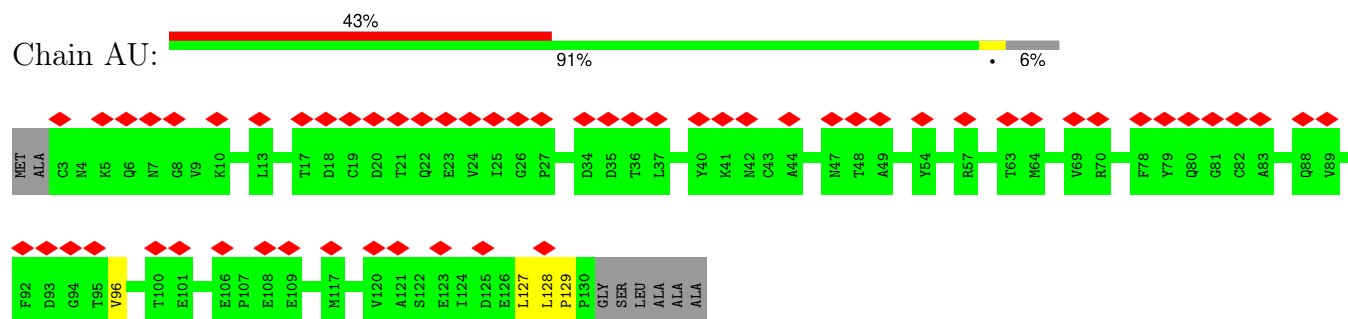


- Molecule 9: Tail-terminator protein, gp18



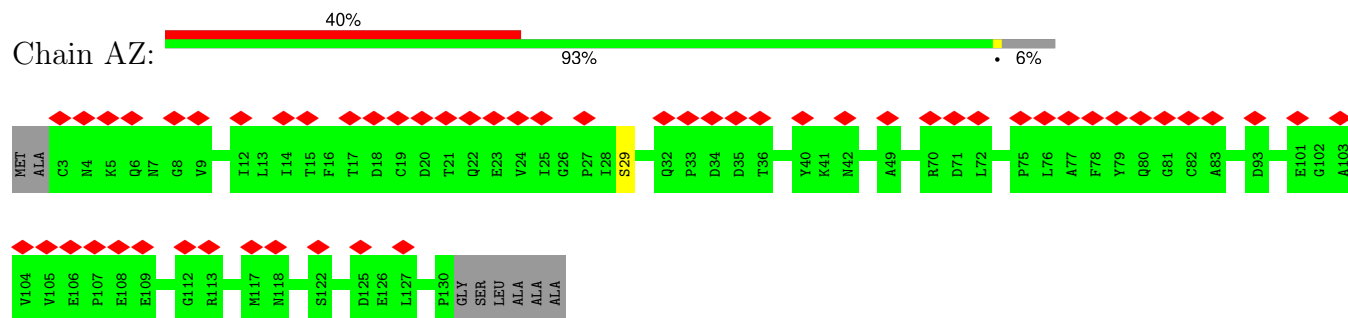
- Molecule 10: Tail-tube, gp21

Chain AU:



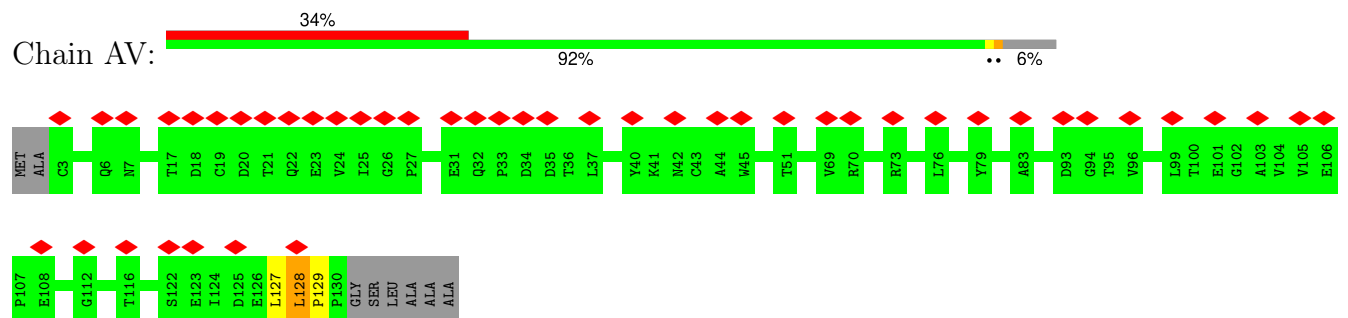
- Molecule 10: Tail-tube, gp21

Chain AZ:



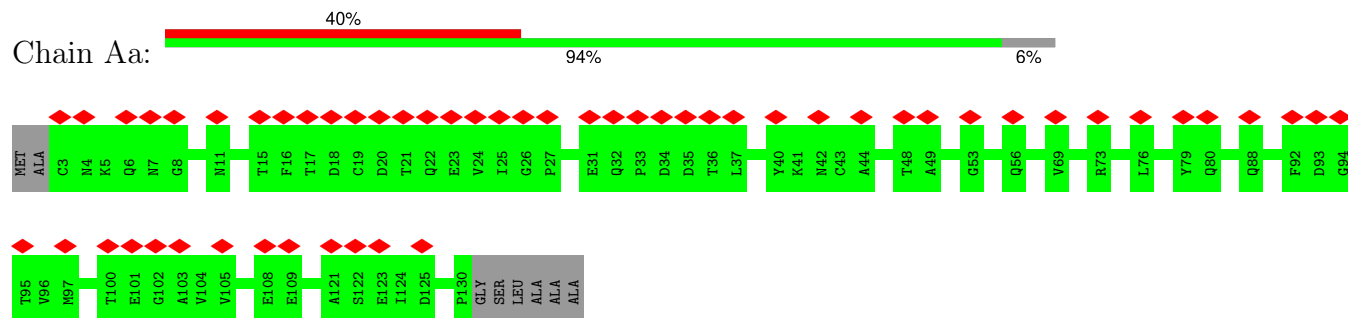
- Molecule 10: Tail-tube, gp21

Chain AV:



- Molecule 10: Tail-tube, gp21

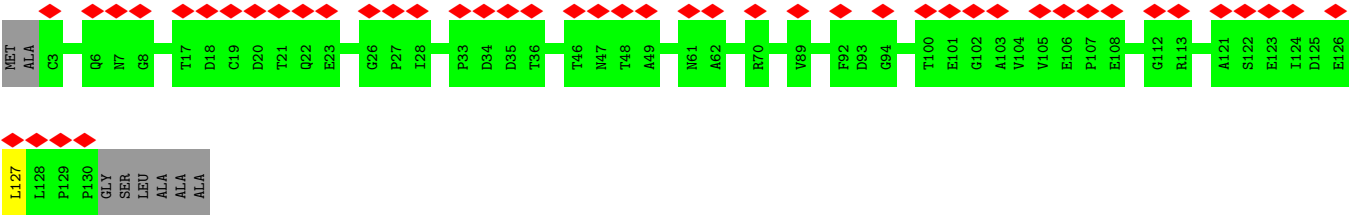
Chain Aa:



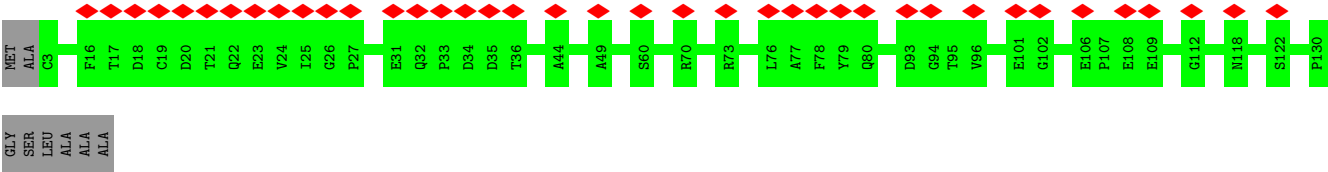
- Molecule 10: Tail-tube, gp21

Chain AY:





• Molecule 10: Tail-tube, gp21



4 Experimental information

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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.483	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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	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(°)	Ideal(°)
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

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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%)	3	22
2	a	172/202 (85%)	128 (74%)	40 (23%)	4 (2%)	5	29
2	b	193/202 (96%)	160 (83%)	30 (16%)	3 (2%)	8	37
2	h	169/202 (84%)	144 (85%)	23 (14%)	2 (1%)	11	44
2	i	191/202 (95%)	162 (85%)	26 (14%)	3 (2%)	8	37
2	j	193/202 (96%)	152 (79%)	40 (21%)	1 (0%)	25	64
2	k	169/202 (84%)	126 (75%)	41 (24%)	2 (1%)	11	44
2	l	169/202 (84%)	146 (86%)	22 (13%)	1 (1%)	22	60
2	m	190/202 (94%)	153 (80%)	35 (18%)	2 (1%)	12	46
2	n	193/202 (96%)	160 (83%)	33 (17%)	0	100	100
2	o	169/202 (84%)	140 (83%)	25 (15%)	4 (2%)	5	28
2	p	169/202 (84%)	143 (85%)	25 (15%)	1 (1%)	22	60
2	q	169/202 (84%)	141 (83%)	24 (14%)	4 (2%)	5	28
3	AM	123/141 (87%)	113 (92%)	9 (7%)	1 (1%)	16	54
3	AN	123/141 (87%)	115 (94%)	7 (6%)	1 (1%)	16	54
3	AO	123/141 (87%)	114 (93%)	7 (6%)	2 (2%)	8	37
3	AP	123/141 (87%)	114 (93%)	8 (6%)	1 (1%)	16	54
3	H	123/141 (87%)	115 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	123/141 (87%)	116 (94%)	6 (5%)	1 (1%)	16	54
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%)	37	72
5	h2	289/465 (62%)	248 (86%)	41 (14%)	0	100	100
5	h5	289/465 (62%)	246 (85%)	42 (14%)	1 (0%)	37	72
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%)	37	72
5	k7	286/465 (62%)	258 (90%)	28 (10%)	0	100	100
5	n1	289/465 (62%)	254 (88%)	34 (12%)	1 (0%)	37	72
5	n2	289/465 (62%)	248 (86%)	39 (14%)	2 (1%)	19	56
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%)	19	56
5	o2	289/465 (62%)	249 (86%)	37 (13%)	3 (1%)	13	49
5	o5	289/465 (62%)	250 (86%)	37 (13%)	2 (1%)	19	56
5	o6	289/465 (62%)	250 (86%)	37 (13%)	2 (1%)	19	56
5	o7	289/465 (62%)	248 (86%)	38 (13%)	3 (1%)	13	49

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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%)	8	39
6	l6	135/137 (98%)	122 (90%)	13 (10%)	0	100	100
6	l7	135/137 (98%)	122 (90%)	12 (9%)	1 (1%)	19	56
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%)	19	56
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

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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%)	19	56
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%)	25	64
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

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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%)	30	68
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%)	14	51
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%)	30	68
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%)	9	40
7	g3	219/230 (95%)	205 (94%)	12 (6%)	2 (1%)	14	51
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

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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%)	37	72
8	AB	377/420 (90%)	333 (88%)	44 (12%)	0	100	100
8	AC	377/420 (90%)	332 (88%)	43 (11%)	2 (0%)	25	64
8	AD	377/420 (90%)	334 (89%)	43 (11%)	0	100	100
8	AE	377/420 (90%)	322 (85%)	54 (14%)	1 (0%)	37	72
8	AF	377/420 (90%)	336 (89%)	40 (11%)	1 (0%)	37	72
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%)	19	56
9	AR	153/178 (86%)	142 (93%)	11 (7%)	0	100	100
9	AS	153/178 (86%)	141 (92%)	10 (6%)	2 (1%)	10	42
9	AT	153/178 (86%)	141 (92%)	12 (8%)	0	100	100
9	AW	153/178 (86%)	143 (94%)	9 (6%)	1 (1%)	19	56
9	AX	153/178 (86%)	141 (92%)	11 (7%)	1 (1%)	19	56
10	AU	126/136 (93%)	115 (91%)	9 (7%)	2 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AV	126/136 (93%)	115 (91%)	9 (7%)	2 (2%)	8	37
10	AY	126/136 (93%)	114 (90%)	12 (10%)	0	100	100
10	AZ	126/136 (93%)	115 (91%)	10 (8%)	1 (1%)	16	54
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%)	45	78

All (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
2	a	45	GLY
2	a	46	LEU
2	h	74	ILE
2	k	139	SER
2	m	74	ILE
6	v1	74	CYS
7	W3	23	CYS
7	f3	49	ARG
7	f3	51	HIS
7	g3	23	CYS
5	h5	190	CYS
6	l5	56	ASP
6	l7	74	CYS
3	AO	49	GLN
9	AX	94	ARG
2	a	136	CYS
2	b	74	ILE
2	b	139	SER
2	q	63	ARG
2	i	137	GLU
2	i	138	ASN
3	I	49	GLN
5	n1	301	ASN
5	o1	189	GLU
5	o2	189	GLU

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Mol	Chain	Res	Type
6	p2	78	LEU
5	o6	189	GLU
8	AE	271	ASP
3	AP	48	SER
9	AS	94	ARG
10	AV	129	PRO
9	AW	94	ARG
2	a	141	PRO
2	b	51	GLU
2	q	61	LYS
2	q	62	GLY
2	m	73	PRO
5	o1	373	PRO
5	n2	304	PRO
5	o2	224	ASP
5	o2	373	PRO
7	Q3	18	VAL
7	g3	22	CYS
7	53	23	CYS
6	l5	59	PRO
5	o5	191	ALA
5	o7	191	ALA
5	o7	373	PRO
8	AC	17	ALA
8	AF	283	ASP
3	AM	49	GLN
2	l	87	GLY
2	o	49	THR
2	h	138	ASN
5	h1	191	ALA
5	n2	456	CYS
7	K3	16	GLY
5	o5	373	PRO
5	k6	359	ASN
5	o6	373	PRO
5	o7	224	ASP
8	AA	19	SER
8	AC	19	SER
10	AU	129	PRO
10	AV	128	LEU
2	o	141	PRO
2	p	74	ILE

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Mol	Chain	Res	Type
7	Q3	17	ASP
10	AU	128	LEU
9	AS	50	LEU
2	o	74	ILE
1	g	8	PRO
2	k	74	ILE
9	AQ	51	PRO
2	q	74	ILE
2	i	74	ILE
2	j	74	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a1	25/32 (78%)	25 (100%)	0	100	100
1	a2	25/32 (78%)	24 (96%)	1 (4%)	27	48
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%)	27	48
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%)	27	48
1	c	29/32 (91%)	29 (100%)	0	100	100
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%)	32	53
1	d6	29/32 (91%)	28 (97%)	1 (3%)	32	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d7	29/32 (91%)	28 (97%)	1 (3%)	32	53
1	e	29/32 (91%)	29 (100%)	0	100	100
1	e1	25/32 (78%)	24 (96%)	1 (4%)	27	48
1	e2	25/32 (78%)	24 (96%)	1 (4%)	27	48
1	e5	25/32 (78%)	24 (96%)	1 (4%)	27	48
1	e6	25/32 (78%)	24 (96%)	1 (4%)	27	48
1	e7	25/32 (78%)	24 (96%)	1 (4%)	27	48
1	f	29/32 (91%)	28 (97%)	1 (3%)	32	53
1	g	29/32 (91%)	25 (86%)	4 (14%)	3	14
2	a	144/168 (86%)	140 (97%)	4 (3%)	38	59
2	b	161/168 (96%)	159 (99%)	2 (1%)	67	79
2	h	141/168 (84%)	136 (96%)	5 (4%)	31	52
2	i	159/168 (95%)	155 (98%)	4 (2%)	42	62
2	j	161/168 (96%)	158 (98%)	3 (2%)	52	69
2	k	141/168 (84%)	138 (98%)	3 (2%)	48	67
2	l	141/168 (84%)	140 (99%)	1 (1%)	81	87
2	m	158/168 (94%)	156 (99%)	2 (1%)	65	77
2	n	161/168 (96%)	160 (99%)	1 (1%)	84	88
2	o	141/168 (84%)	138 (98%)	3 (2%)	48	67
2	p	141/168 (84%)	140 (99%)	1 (1%)	81	87
2	q	141/168 (84%)	137 (97%)	4 (3%)	38	59
3	AM	114/128 (89%)	113 (99%)	1 (1%)	75	83
3	AN	114/128 (89%)	114 (100%)	0	100	100
3	AO	114/128 (89%)	112 (98%)	2 (2%)	54	71
3	AP	114/128 (89%)	113 (99%)	1 (1%)	75	83
3	H	114/128 (89%)	113 (99%)	1 (1%)	75	83
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	65	77
5	g5	235/379 (62%)	234 (100%)	1 (0%)	89	90
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%)	32	53
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%)	89	90
5	k7	232/379 (61%)	230 (99%)	2 (1%)	75	83
5	n1	235/379 (62%)	234 (100%)	1 (0%)	89	90
5	n2	235/379 (62%)	233 (99%)	2 (1%)	75	83
5	n5	235/379 (62%)	234 (100%)	1 (0%)	89	90
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%)	65	77
5	o2	235/379 (62%)	233 (99%)	2 (1%)	75	83
5	o5	235/379 (62%)	232 (99%)	3 (1%)	65	77
5	o6	235/379 (62%)	233 (99%)	2 (1%)	75	83
5	o7	235/379 (62%)	232 (99%)	3 (1%)	65	77
5	r1	235/379 (62%)	235 (100%)	0	100	100
5	r2	235/379 (62%)	233 (99%)	2 (1%)	75	83
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%)	89	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	l1	112/112 (100%)	111 (99%)	1 (1%)	75	83
6	l2	112/112 (100%)	111 (99%)	1 (1%)	75	83
6	l5	112/112 (100%)	110 (98%)	2 (2%)	54	71
6	l6	112/112 (100%)	112 (100%)	0	100	100
6	l7	112/112 (100%)	110 (98%)	2 (2%)	54	71
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%)	75	83
6	p5	112/112 (100%)	112 (100%)	0	100	100
6	p6	112/112 (100%)	111 (99%)	1 (1%)	75	83
6	p7	112/112 (100%)	110 (98%)	2 (2%)	54	71
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%)	75	83
6	q7	112/112 (100%)	110 (98%)	2 (2%)	54	71
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%)	75	83
6	t2	112/112 (100%)	111 (99%)	1 (1%)	75	83
6	t5	112/112 (100%)	111 (99%)	1 (1%)	75	83
6	t6	112/112 (100%)	109 (97%)	3 (3%)	40	60
6	t7	112/112 (100%)	111 (99%)	1 (1%)	75	83
6	u1	111/112 (99%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	u2	111/112 (99%)	110 (99%)	1 (1%)	75	83
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%)	75	83
6	v2	111/112 (99%)	110 (99%)	1 (1%)	75	83
6	v5	111/112 (99%)	110 (99%)	1 (1%)	75	83
6	v6	111/112 (99%)	110 (99%)	1 (1%)	75	83
6	v7	111/112 (99%)	110 (99%)	1 (1%)	75	83
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%)	86	89
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%)	70	80
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%)	86	89
7	M3	186/191 (97%)	186 (100%)	0	100	100
7	N3	191/191 (100%)	191 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	86	89
7	R3	186/191 (97%)	185 (100%)	1 (0%)	86	89
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%)	70	80
7	W3	191/191 (100%)	189 (99%)	2 (1%)	73	81
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%)	28	50
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%)	86	89
7	m3	186/191 (97%)	186 (100%)	0	100	100
7	n3	186/191 (97%)	186 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	84	88
8	AB	311/339 (92%)	311 (100%)	0	100	100
8	AC	311/339 (92%)	310 (100%)	1 (0%)	91	91
8	AD	311/339 (92%)	311 (100%)	0	100	100
8	AE	311/339 (92%)	310 (100%)	1 (0%)	91	91
8	AF	311/339 (92%)	310 (100%)	1 (0%)	91	91
8	AG	311/339 (92%)	310 (100%)	1 (0%)	91	91
8	AH	311/339 (92%)	311 (100%)	0	100	100
8	AI	311/339 (92%)	310 (100%)	1 (0%)	91	91
8	AJ	311/339 (92%)	310 (100%)	1 (0%)	91	91
8	AK	311/339 (92%)	310 (100%)	1 (0%)	91	91
8	AL	311/339 (92%)	310 (100%)	1 (0%)	91	91
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%)	81	87
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%)	54	71
10	AV	113/116 (97%)	111 (98%)	2 (2%)	54	71
10	AY	113/116 (97%)	112 (99%)	1 (1%)	75	83
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	31110/37451 (83%)	30961 (100%)	149 (0%)	85 89

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	23	CYS
1	g	7	ARG
1	g	9	LEU
1	g	11	GLN
1	g	23	CYS
2	a	38	GLU
2	a	46	LEU
2	a	134	ARG
2	a	198	ARG
2	b	30	LYS
2	b	63	ARG
2	l	88	SER
2	n	63	ARG
2	o	51	GLU
2	o	52	LYS
2	o	63	ARG
2	p	63	ARG
2	q	61	LYS
2	q	63	ARG
2	q	64	ARG
2	q	167	ARG
2	h	61	LYS
2	h	63	ARG
2	h	72	THR
2	h	74	ILE
2	h	167	ARG
2	i	51	GLU
2	i	52	LYS
2	i	59	ARG
2	i	63	ARG
2	j	23	ARG
2	j	110	ARG
2	j	134	ARG
2	k	23	ARG
2	k	63	ARG
2	k	167	ARG
2	m	64	ARG

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Mol	Chain	Res	Type
2	m	74	ILE
3	H	49	GLN
1	e1	6	CYS
5	h1	184	VAL
5	h1	186	CYS
5	h1	189	GLU
5	h1	190	CYS
5	h1	302	CYS
5	h1	385	CYS
5	h1	455	CYS
5	h1	457	GLU
6	l1	99	CYS
5	n1	305	VAL
5	o1	211	LYS
5	o1	302	CYS
5	o1	457	GLU
6	t1	137	ARG
6	v1	99	CYS
1	a2	6	CYS
1	b2	25	ILE
1	e2	6	CYS
5	g2	184	VAL
5	g2	186	CYS
5	g2	188	ILE
6	l2	133	LYS
5	n2	300	GLU
5	n2	456	CYS
5	o2	211	LYS
5	o2	385	CYS
6	p2	75	ASP
5	r2	377	ARG
5	r2	455	CYS
6	t2	137	ARG
6	u2	136	THR
6	v2	99	CYS
7	L3	180	ARG
7	Q3	19	CYS
7	R3	10	ASN
7	V3	9	ARG
7	V3	10	ASN
7	W3	22	CYS
7	W3	25	GLU

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Mol	Chain	Res	Type
7	f3	51	HIS
7	f3	53	LEU
7	f3	54	THR
7	f3	209	ILE
7	f3	210	ASP
7	f3	211	CYS
7	f3	212	ASP
7	l3	211	CYS
7	53	22	CYS
7	G3	220	SER
7	G3	221	CYS
1	d5	6	CYS
1	e5	6	CYS
5	g5	304	PRO
6	l5	56	ASP
6	l5	58	ASP
5	n5	301	ASN
5	o5	188	ILE
5	o5	190	CYS
5	o5	385	CYS
6	t5	137	ARG
6	v5	99	CYS
1	d6	23	CYS
1	e6	6	CYS
5	k6	440	CYS
5	o6	211	LYS
5	o6	385	CYS
6	p6	75	ASP
6	q6	106	MET
6	t6	106	MET
6	t6	132	MET
6	t6	137	ARG
6	v6	99	CYS
1	b7	23	CYS
1	d7	23	CYS
1	e7	6	CYS
5	k7	289	LYS
5	k7	440	CYS
6	l7	55	SER
6	l7	56	ASP
5	o7	189	GLU
5	o7	190	CYS

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Mol	Chain	Res	Type
5	o7	211	LYS
6	p7	76	THR
6	p7	78	LEU
6	q7	106	MET
6	q7	136	THR
5	r7	377	ARG
6	t7	9	PHE
6	v7	99	CYS
8	AA	276	ILE
8	AA	277	ILE
8	AC	19	SER
8	AE	179	LYS
8	AF	249	ARG
8	AG	179	LYS
8	AI	95	LYS
8	AJ	285	LYS
8	AK	285	LYS
8	AL	179	LYS
3	AM	113	ARG
10	AU	96	VAL
10	AU	127	LEU
3	AP	47	PHE
9	AS	50	LEU
10	AV	127	LEU
10	AV	128	LEU
3	AO	49	GLN
3	AO	50	ASP
10	AY	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (384) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	158	ASN
2	a	191	GLN
2	b	10	GLN
2	b	15	HIS
2	l	138	ASN
2	l	158	ASN
2	n	191	GLN
2	q	99	ASN
2	q	138	ASN
2	h	10	GLN

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Mol	Chain	Res	Type
2	h	191	GLN
2	i	15	HIS
2	i	138	ASN
2	j	10	GLN
2	j	155	ASN
2	j	158	ASN
2	m	155	ASN
2	m	175	GLN
3	H	8	HIS
3	H	68	ASN
3	I	8	HIS
3	I	15	GLN
3	I	16	GLN
3	I	49	GLN
3	I	55	GLN
3	I	60	GLN
1	e1	5	ASN
5	g1	187	ASN
5	g1	277	HIS
5	g1	292	ASN
5	h1	236	ASN
5	h1	280	ASN
5	h1	314	ASN
5	h1	346	GLN
5	h1	359	ASN
5	h1	431	GLN
5	k1	324	GLN
5	k1	346	GLN
5	k1	359	ASN
5	k1	431	GLN
5	k1	458	HIS
6	l1	122	ASN
6	m1	127	GLN
5	n1	280	ASN
5	n1	283	GLN
5	o1	301	ASN
5	o1	314	ASN
5	o1	346	GLN
5	o1	384	ASN
5	o1	458	HIS
6	p1	122	ASN
5	r1	254	ASN

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Mol	Chain	Res	Type
5	r1	282	ASN
5	r1	283	GLN
5	r1	292	ASN
5	r1	359	ASN
6	t1	127	GLN
6	u1	109	GLN
6	u1	125	ASN
6	v1	48	ASN
6	v1	127	GLN
1	e2	5	ASN
4	f2	17	GLN
5	g2	274	GLN
5	g2	292	ASN
5	g2	359	ASN
5	g2	384	ASN
5	g2	393	ASN
5	h2	280	ASN
5	h2	346	GLN
5	h2	359	ASN
5	k2	259	GLN
5	k2	324	GLN
5	k2	346	GLN
5	k2	431	GLN
5	k2	458	HIS
6	m2	127	GLN
5	n2	292	ASN
5	n2	324	GLN
5	o2	217	GLN
5	o2	314	ASN
5	o2	346	GLN
5	o2	384	ASN
5	o2	458	HIS
6	p2	2	ASN
6	p2	122	ASN
6	p2	127	GLN
5	r2	254	ASN
5	r2	282	ASN
5	r2	292	ASN
5	r2	384	ASN
6	t2	127	GLN
6	u2	122	ASN
6	u2	127	GLN

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Mol	Chain	Res	Type
6	v2	107	ASN
7	J3	142	ASN
7	K3	108	ASN
7	M3	142	ASN
7	M3	218	HIS
7	N3	108	ASN
7	P3	142	ASN
7	P3	218	HIS
7	R3	112	ASN
7	R3	120	ASN
7	S3	142	ASN
7	S3	182	HIS
7	T3	55	ASN
7	V3	10	ASN
7	V3	142	ASN
7	Y3	55	ASN
7	Z3	55	ASN
7	a3	51	HIS
7	b3	55	ASN
7	d3	51	HIS
7	d3	120	ASN
7	d3	182	HIS
7	e3	55	ASN
7	f3	144	ASN
7	f3	182	HIS
7	f3	214	ASN
7	h3	55	ASN
7	j3	55	ASN
7	j3	182	HIS
7	k3	51	HIS
7	k3	55	ASN
7	m3	182	HIS
7	n3	108	ASN
7	o3	55	ASN
7	o3	108	ASN
7	p3	55	ASN
7	p3	120	ASN
7	q3	10	ASN
7	q3	112	ASN
7	s3	55	ASN
7	s3	120	ASN
7	t3	112	ASN

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Mol	Chain	Res	Type
7	u3	51	HIS
7	u3	108	ASN
7	v3	55	ASN
7	w3	112	ASN
7	w3	142	ASN
7	x3	55	ASN
7	x3	108	ASN
7	y3	55	ASN
7	13	55	ASN
7	23	55	ASN
7	23	120	ASN
7	43	142	ASN
7	53	120	ASN
7	83	120	ASN
7	03	55	ASN
7	A3	55	ASN
7	B3	161	GLN
7	D3	55	ASN
7	D3	120	ASN
7	E3	161	GLN
7	G3	120	ASN
5	g5	187	ASN
5	g5	277	HIS
5	g5	280	ASN
5	g5	292	ASN
5	g5	359	ASN
5	h5	314	ASN
5	h5	346	GLN
5	h5	359	ASN
5	h5	431	GLN
5	h5	444	GLN
5	k5	217	GLN
5	k5	259	GLN
5	k5	324	GLN
5	k5	346	GLN
5	k5	359	ASN
5	k5	431	GLN
5	k5	458	HIS
6	m5	127	GLN
5	n5	199	GLN
5	n5	280	ASN
5	n5	301	ASN

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Mol	Chain	Res	Type
5	o5	178	GLN
5	o5	314	ASN
5	o5	346	GLN
5	o5	384	ASN
6	p5	122	ASN
6	p5	127	GLN
5	r5	277	HIS
5	r5	292	ASN
5	r5	347	ASN
5	r5	384	ASN
6	t5	127	GLN
6	u5	4	ASN
6	u5	122	ASN
6	u5	127	GLN
6	v5	127	GLN
5	g6	187	ASN
5	g6	292	ASN
5	g6	346	GLN
5	h6	280	ASN
5	h6	282	ASN
5	h6	314	ASN
5	h6	346	GLN
5	h6	359	ASN
5	h6	431	GLN
5	k6	324	GLN
5	k6	346	GLN
5	k6	431	GLN
5	k6	458	HIS
6	l6	4	ASN
6	l6	122	ASN
6	m6	52	HIS
6	m6	107	ASN
6	m6	127	GLN
5	n6	280	ASN
5	n6	324	GLN
5	o6	178	GLN
5	o6	217	GLN
5	o6	259	GLN
5	o6	282	ASN
5	o6	314	ASN
5	o6	346	GLN
5	o6	384	ASN

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Mol	Chain	Res	Type
6	p6	122	ASN
5	r6	254	ASN
5	r6	280	ASN
5	r6	282	ASN
5	r6	292	ASN
5	r6	359	ASN
5	r6	384	ASN
6	s6	109	GLN
6	t6	127	GLN
6	u6	4	ASN
6	u6	125	ASN
6	u6	127	GLN
6	v6	107	ASN
6	v6	127	GLN
5	g7	187	ASN
5	g7	292	ASN
5	g7	324	GLN
5	g7	359	ASN
5	g7	384	ASN
5	h7	314	ASN
5	h7	346	GLN
5	h7	359	ASN
5	k7	259	GLN
5	k7	324	GLN
5	k7	458	HIS
6	m7	107	ASN
6	m7	127	GLN
5	n7	280	ASN
5	n7	324	GLN
5	o7	178	GLN
5	o7	217	GLN
5	o7	280	ASN
5	o7	282	ASN
5	o7	314	ASN
5	o7	346	GLN
5	o7	384	ASN
5	o7	458	HIS
6	p7	109	GLN
6	p7	122	ASN
6	p7	127	GLN
5	r7	277	HIS
5	r7	280	ASN

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Mol	Chain	Res	Type
5	r7	282	ASN
5	r7	292	ASN
5	r7	384	ASN
6	s7	122	ASN
6	t7	48	ASN
6	t7	127	GLN
6	u7	4	ASN
6	u7	122	ASN
8	AA	38	ASN
8	AA	69	GLN
8	AA	81	ASN
8	AA	140	ASN
8	AA	191	ASN
8	AA	206	ASN
8	AA	255	GLN
8	AA	291	ASN
8	AB	38	ASN
8	AB	69	GLN
8	AB	81	ASN
8	AB	112	GLN
8	AB	140	ASN
8	AB	183	ASN
8	AB	202	ASN
8	AB	255	GLN
8	AB	291	ASN
8	AC	44	ASN
8	AC	69	GLN
8	AC	98	GLN
8	AC	99	GLN
8	AC	191	ASN
8	AC	202	ASN
8	AC	211	ASN
8	AC	291	ASN
8	AD	44	ASN
8	AD	81	ASN
8	AD	99	GLN
8	AD	112	GLN
8	AD	140	ASN
8	AD	183	ASN
8	AD	202	ASN
8	AD	240	ASN
8	AD	305	GLN

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Mol	Chain	Res	Type
8	AE	44	ASN
8	AE	69	GLN
8	AE	112	GLN
8	AE	183	ASN
8	AE	202	ASN
8	AE	215	GLN
8	AE	240	ASN
8	AE	291	ASN
8	AE	312	ASN
8	AF	38	ASN
8	AF	44	ASN
8	AF	69	GLN
8	AF	93	GLN
8	AF	152	GLN
8	AF	202	ASN
8	AF	312	ASN
8	AG	38	ASN
8	AG	69	GLN
8	AG	81	ASN
8	AG	98	GLN
8	AG	112	GLN
8	AG	140	ASN
8	AG	164	GLN
8	AG	191	ASN
8	AG	202	ASN
8	AG	206	ASN
8	AG	272	ASN
8	AH	112	GLN
8	AH	140	ASN
8	AH	164	GLN
8	AH	240	ASN
8	AH	312	ASN
8	AI	69	GLN
8	AI	81	ASN
8	AI	140	ASN
8	AI	202	ASN
8	AI	211	ASN
8	AI	272	ASN
8	AJ	69	GLN
8	AJ	112	GLN
8	AJ	202	ASN
8	AK	69	GLN

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Mol	Chain	Res	Type
8	AK	99	GLN
8	AK	152	GLN
8	AK	183	ASN
8	AK	191	ASN
8	AK	202	ASN
8	AK	272	ASN
8	AL	102	GLN
8	AL	140	ASN
8	AL	164	GLN
8	AL	211	ASN
8	AL	255	GLN
3	AM	68	ASN
3	AM	74	ASN
9	AQ	125	HIS
10	AU	6	GLN
10	AU	42	ASN
9	AR	151	GLN
3	AP	8	HIS
10	AZ	6	GLN
10	AZ	56	GLN
10	AZ	80	GLN
3	AN	8	HIS
3	AN	68	ASN
3	AN	74	ASN
9	AS	85	ASN
9	AS	151	GLN
10	AV	6	GLN
10	AV	42	ASN
10	AV	84	GLN
9	AT	151	GLN
10	Aa	6	GLN
10	Aa	84	GLN
3	AO	49	GLN
3	AO	68	ASN
10	AY	6	GLN
10	AY	42	ASN
9	AX	151	GLN
10	Ab	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

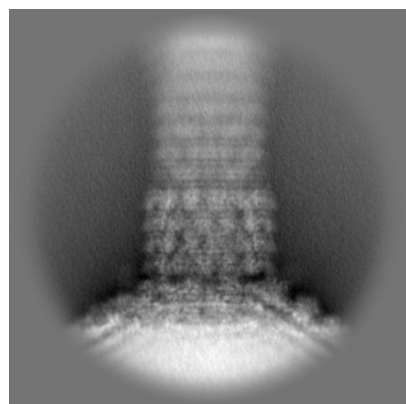
6 Map visualisation [i](#)

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.

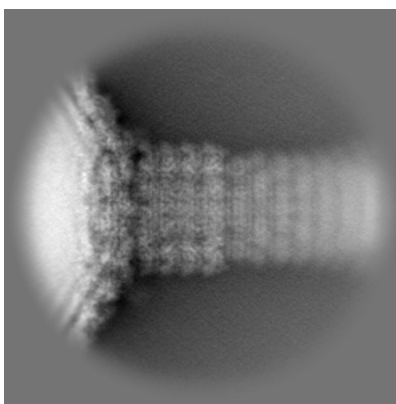
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

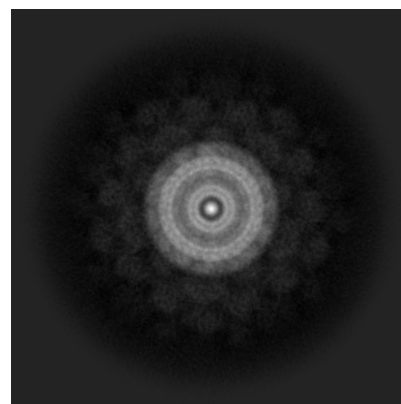
6.1.1 Primary map



X

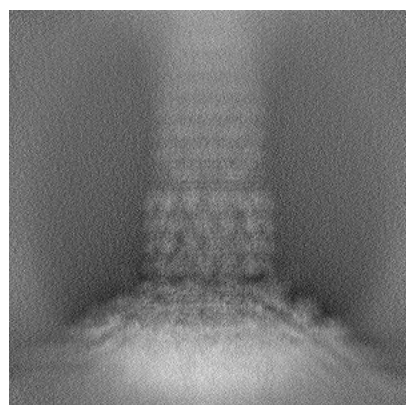


Y

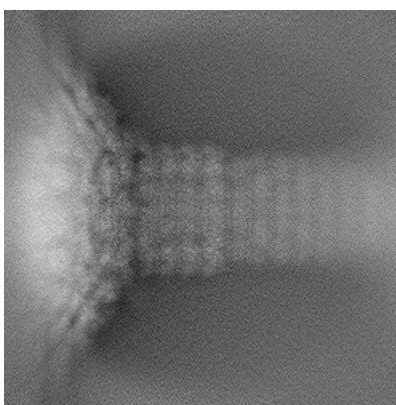


Z

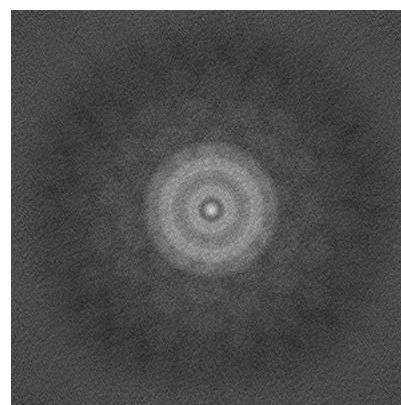
6.1.2 Raw map



X



Y

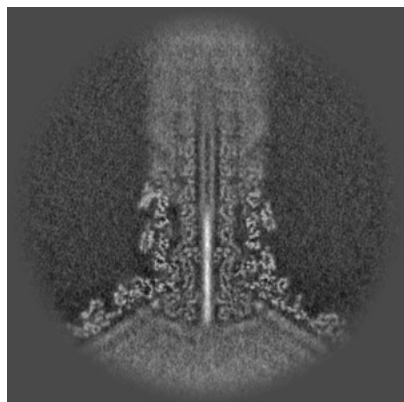


Z

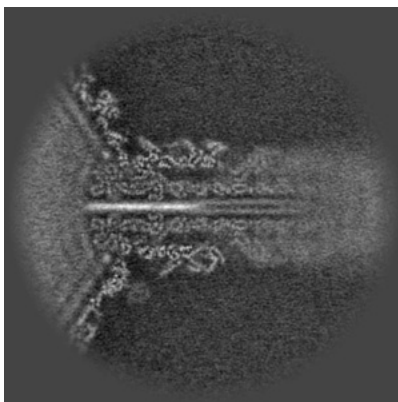
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

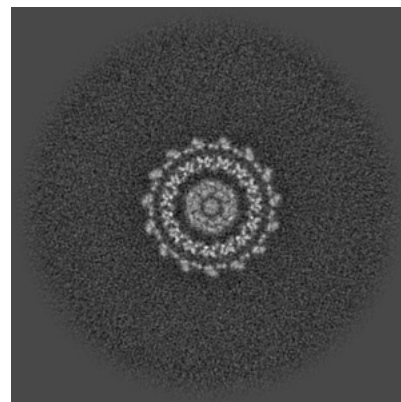
6.2.1 Primary map



X Index: 300

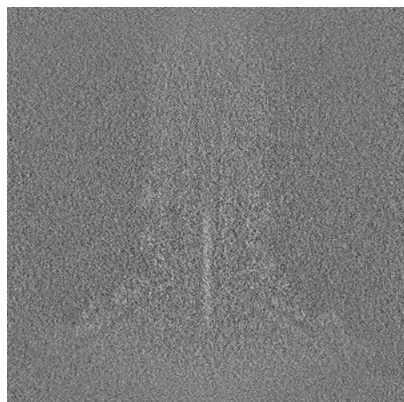


Y Index: 300

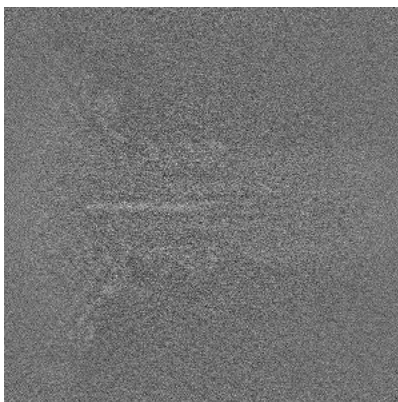


Z Index: 300

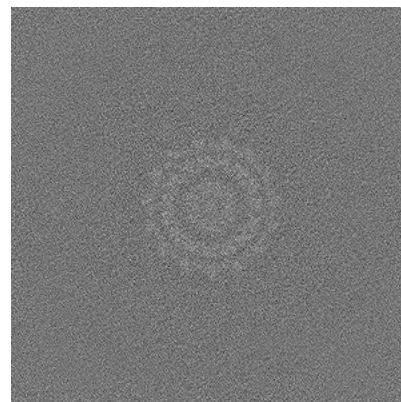
6.2.2 Raw map



X Index: 300



Y Index: 300

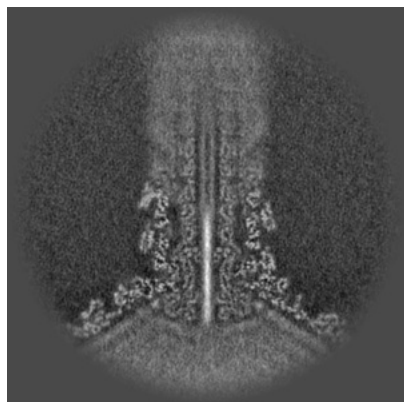


Z Index: 300

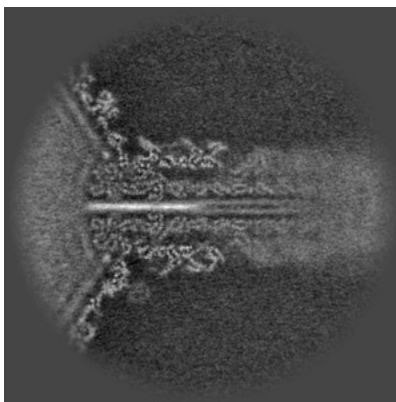
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

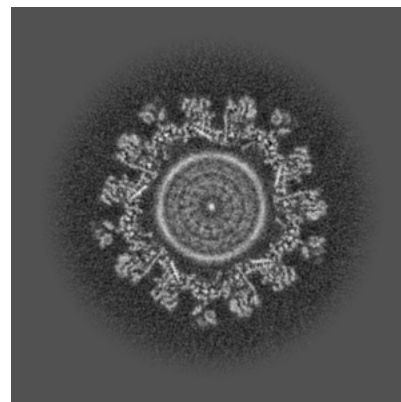
6.3.1 Primary map



X Index: 300

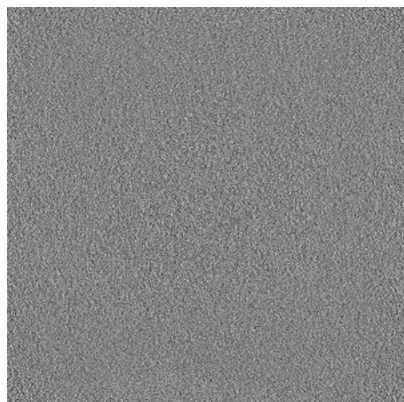


Y Index: 299

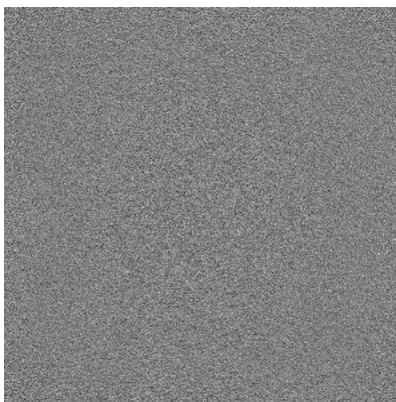


Z Index: 155

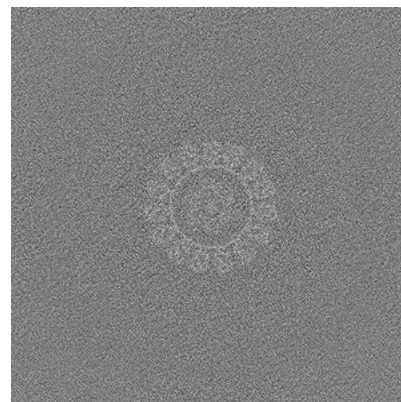
6.3.2 Raw map



X Index: 0



Y Index: 0

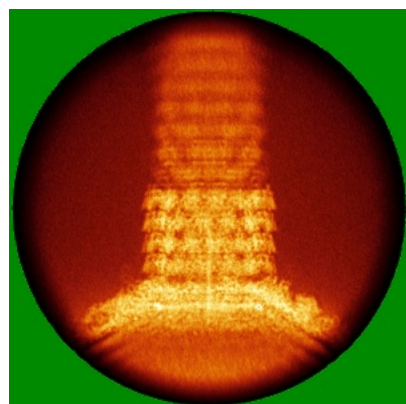


Z Index: 280

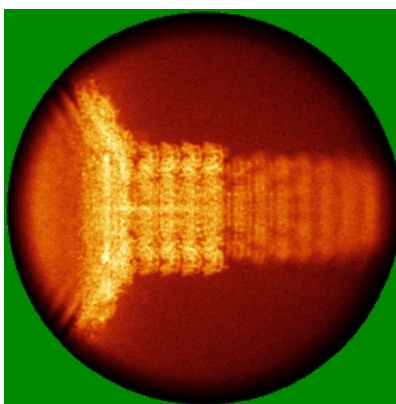
The images above show the largest variance slices of the map in three orthogonal directions.

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

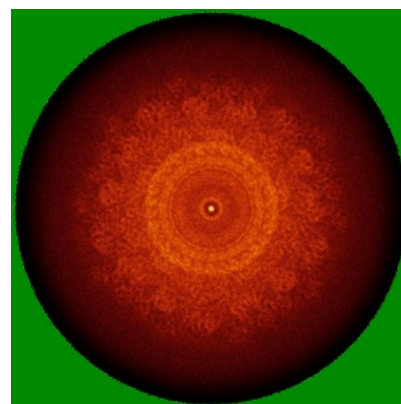
6.4.1 Primary map



X

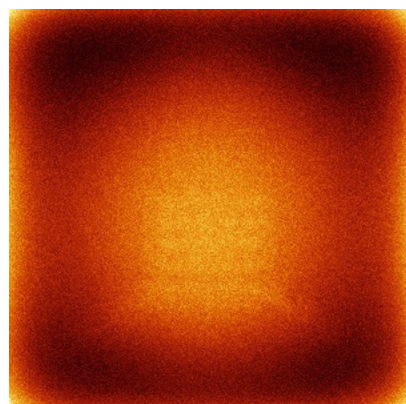


Y

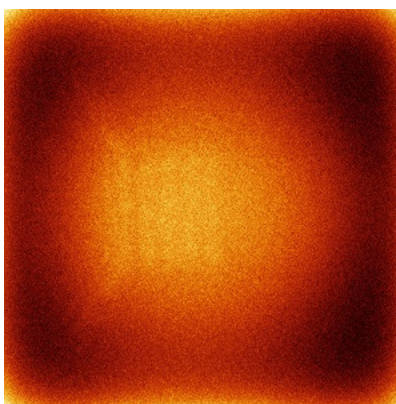


Z

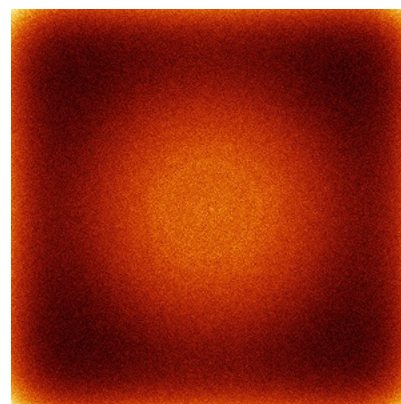
6.4.2 Raw map



X



Y

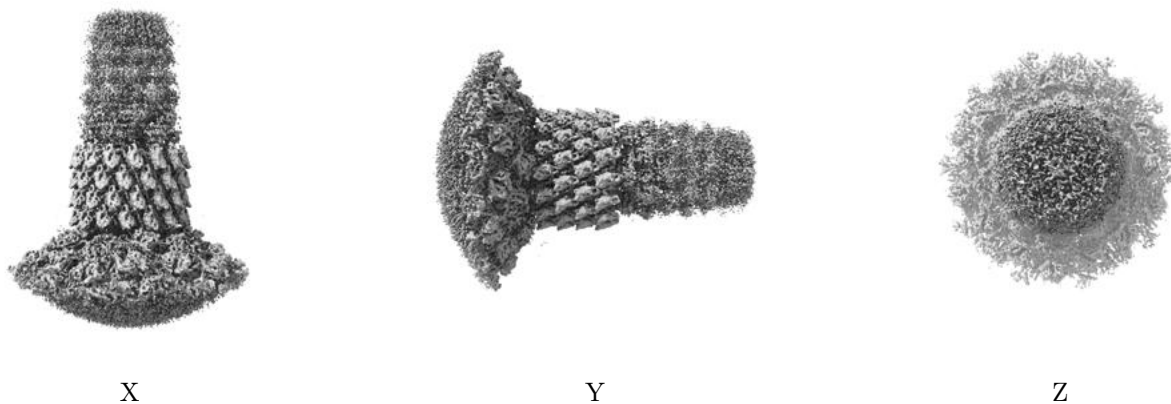


Z

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.

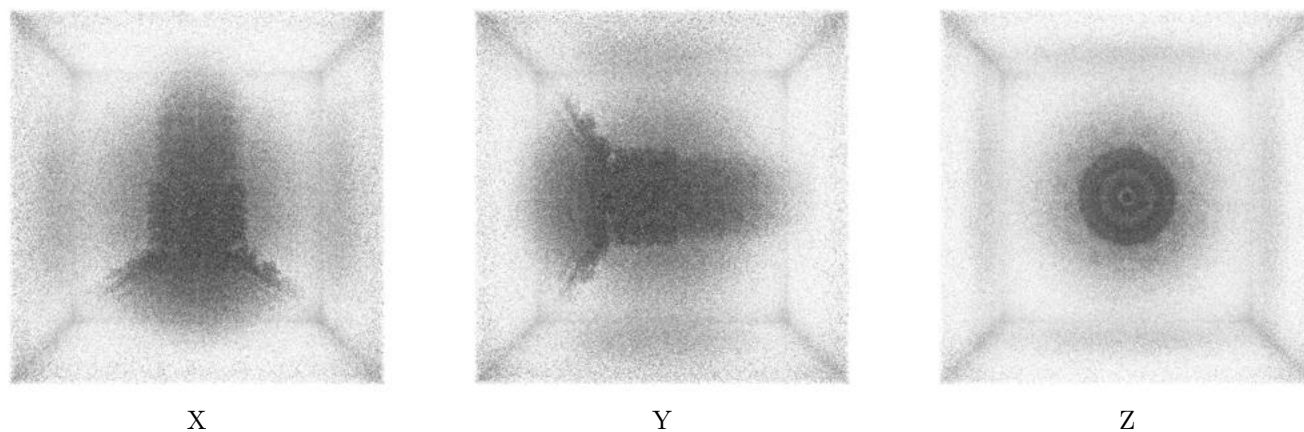
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

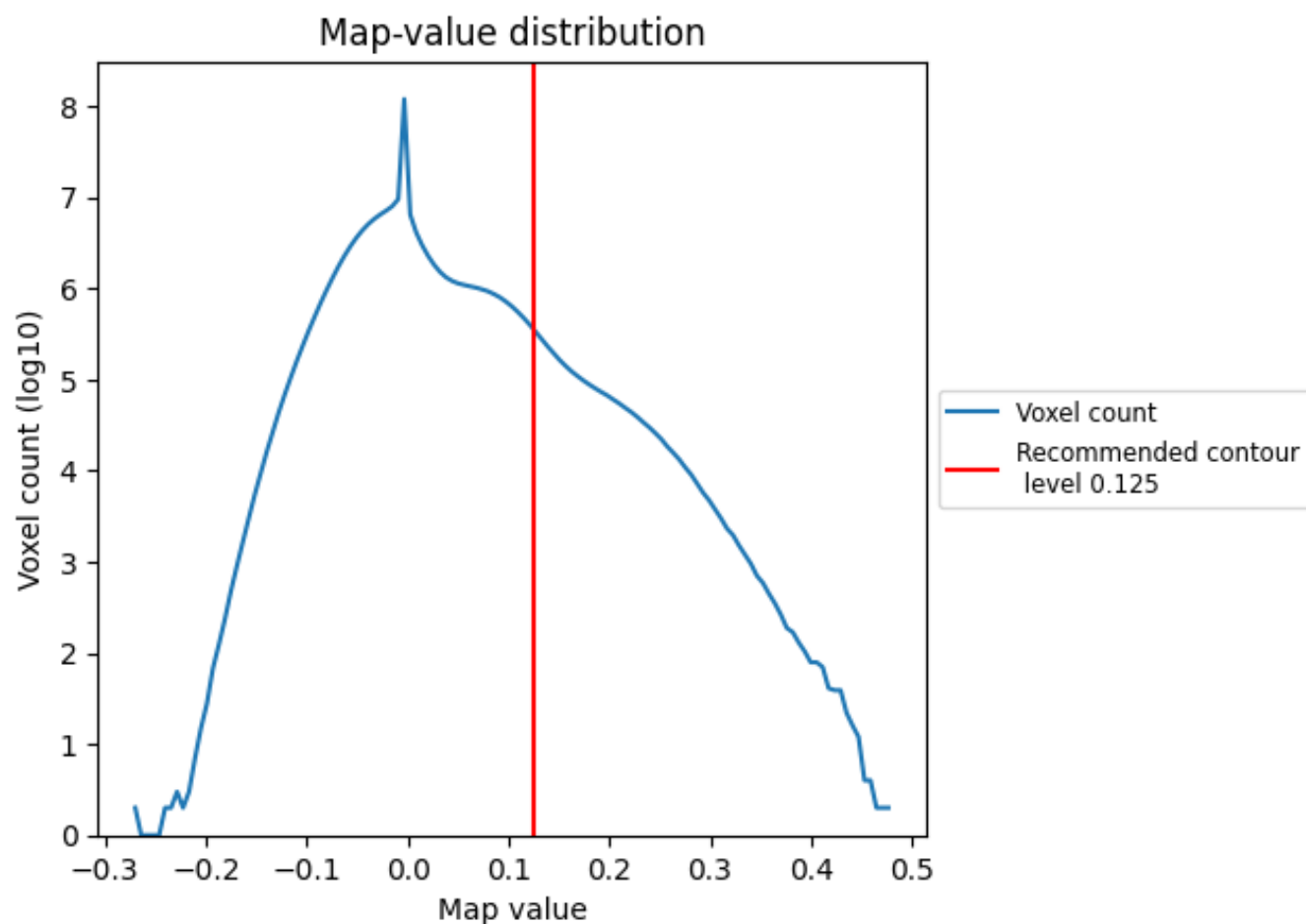
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

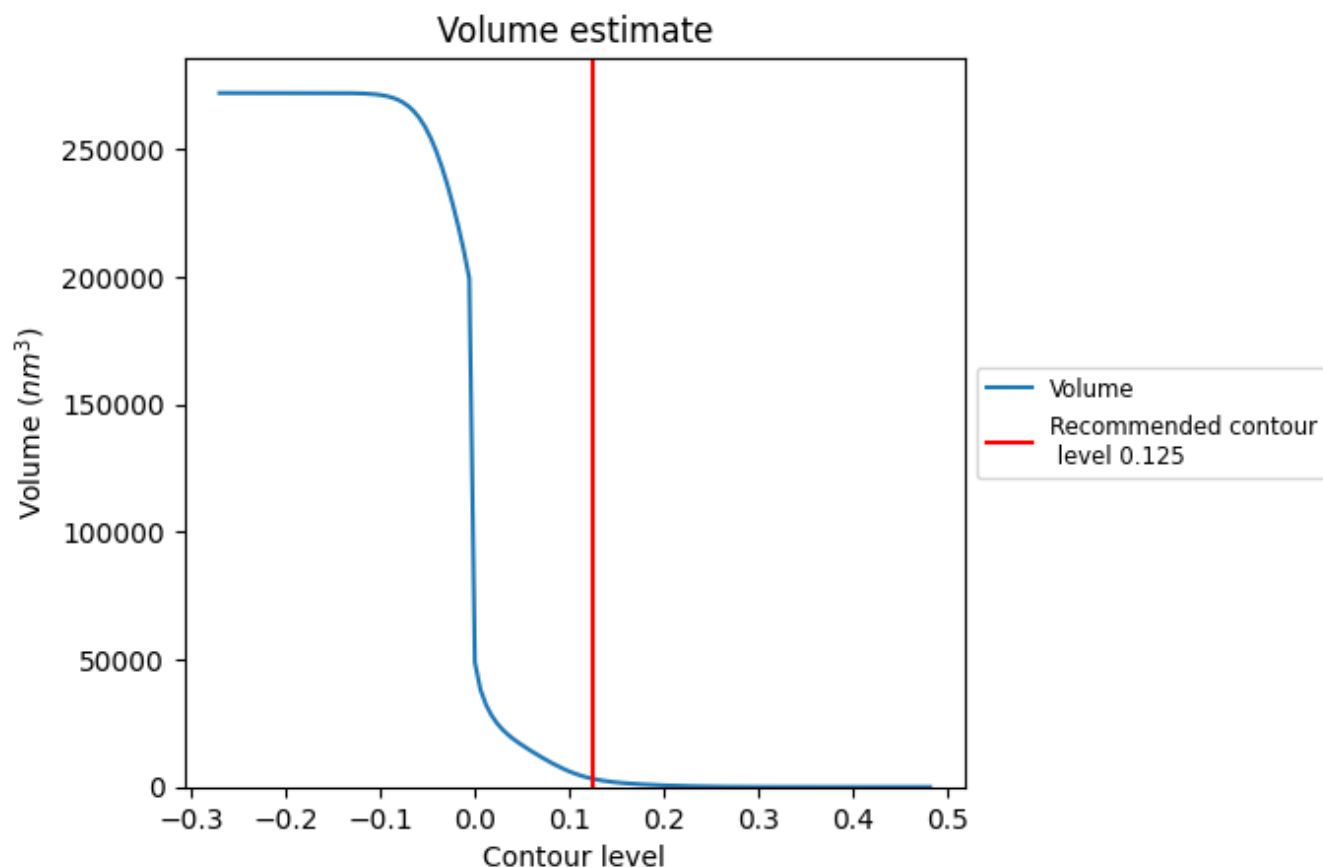
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

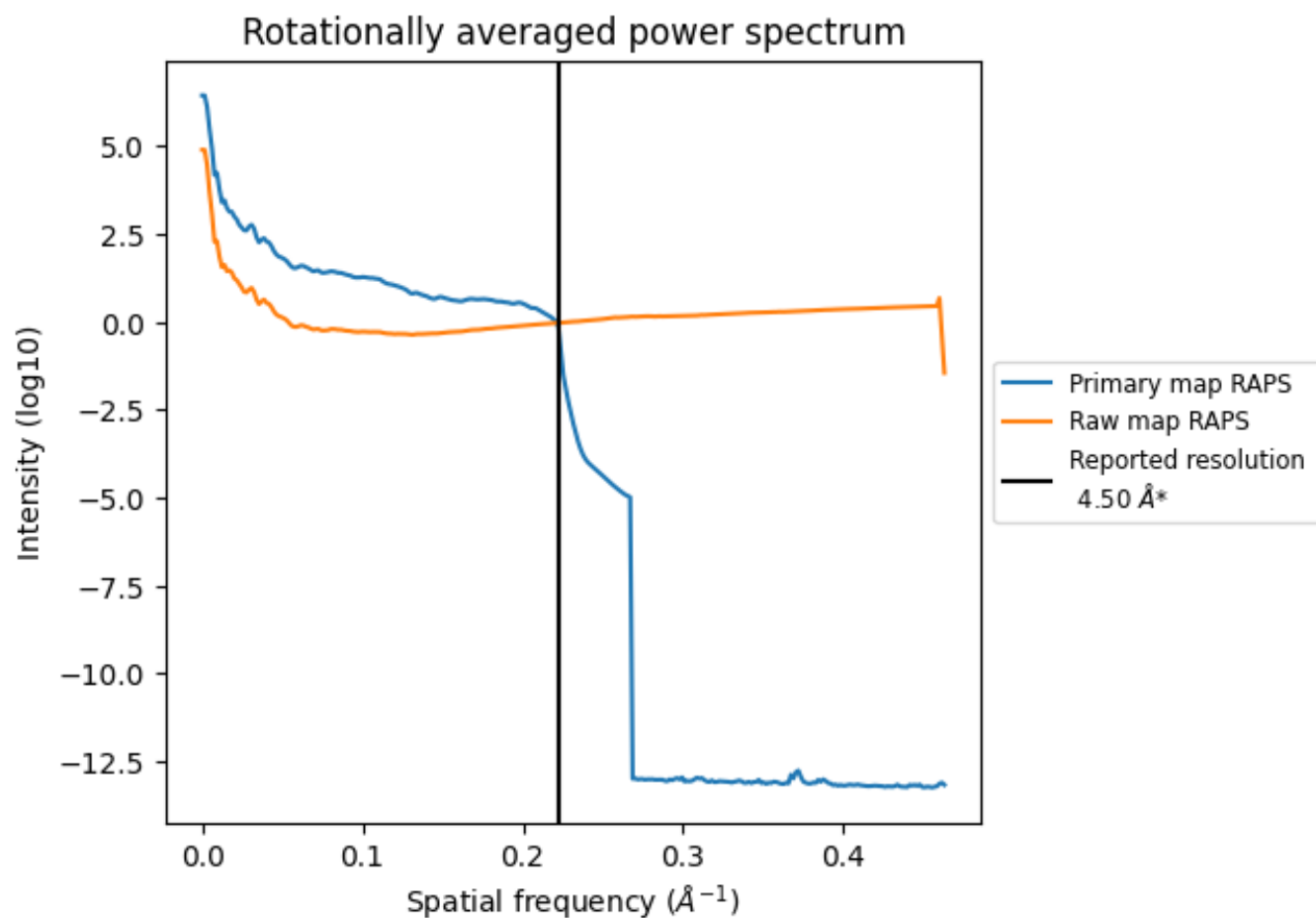
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3249 nm³; 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 ⓘ

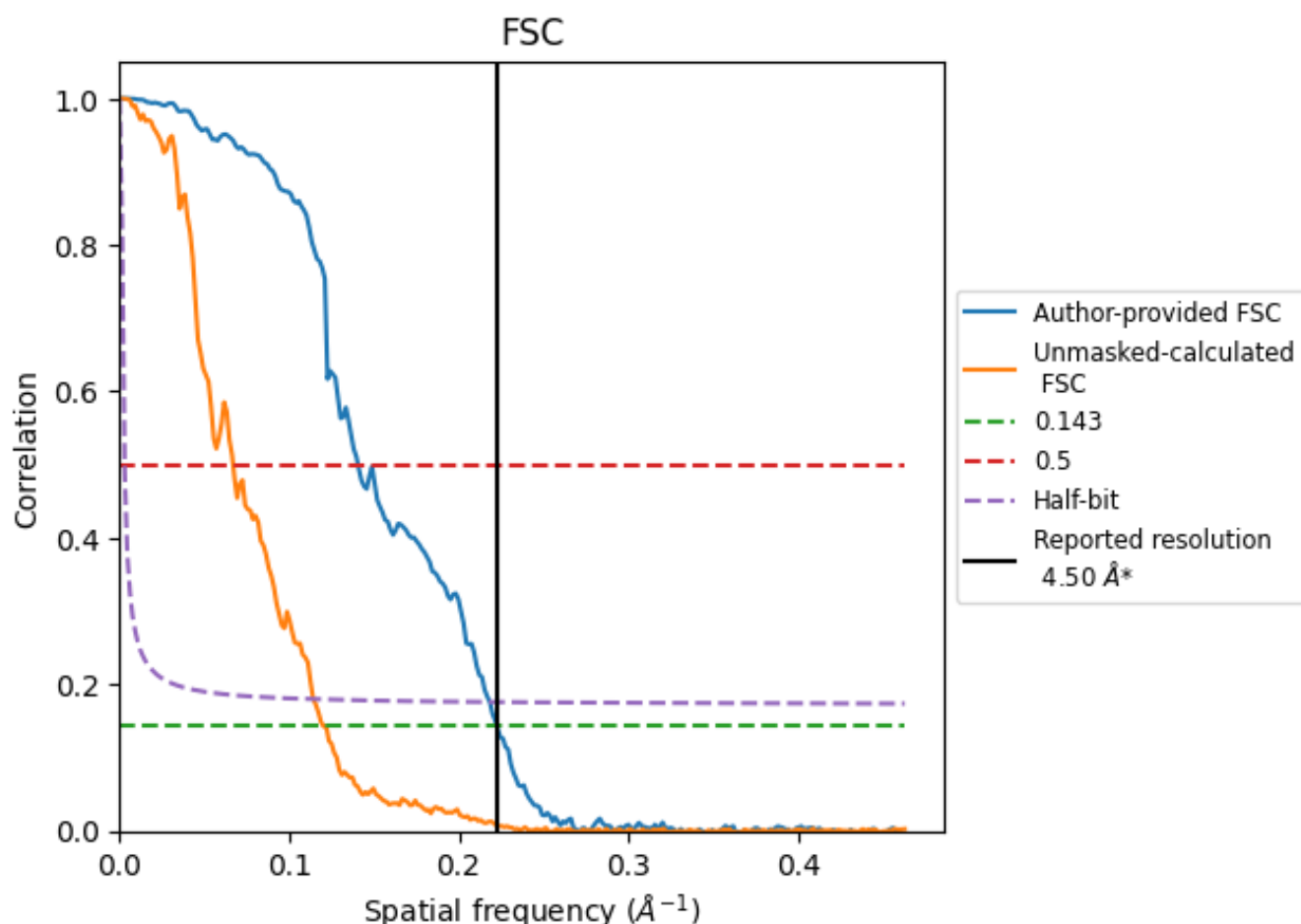


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

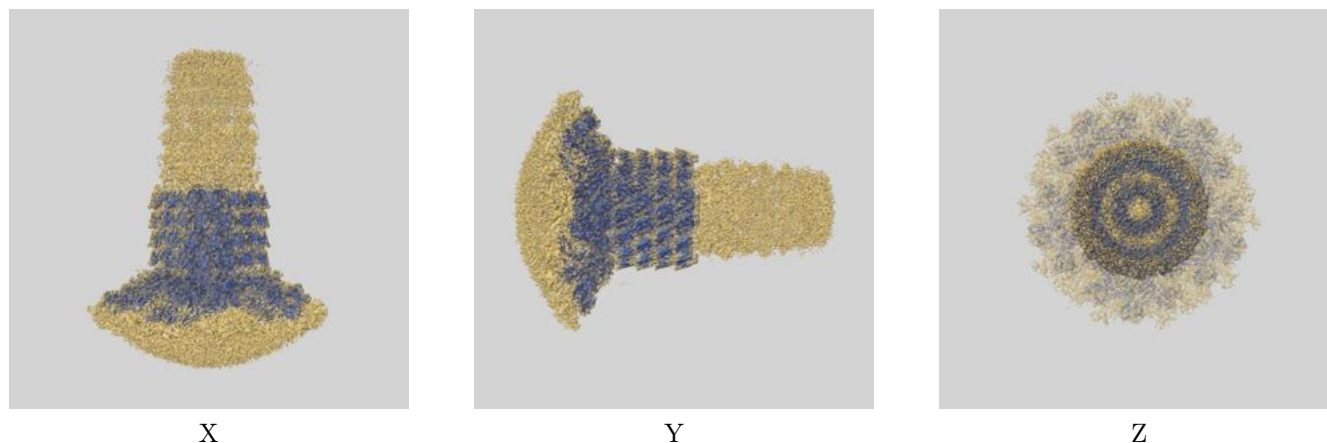
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.49	7.11	4.58
Unmasked-calculated*	8.32	14.93	8.75

*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 [i](#)

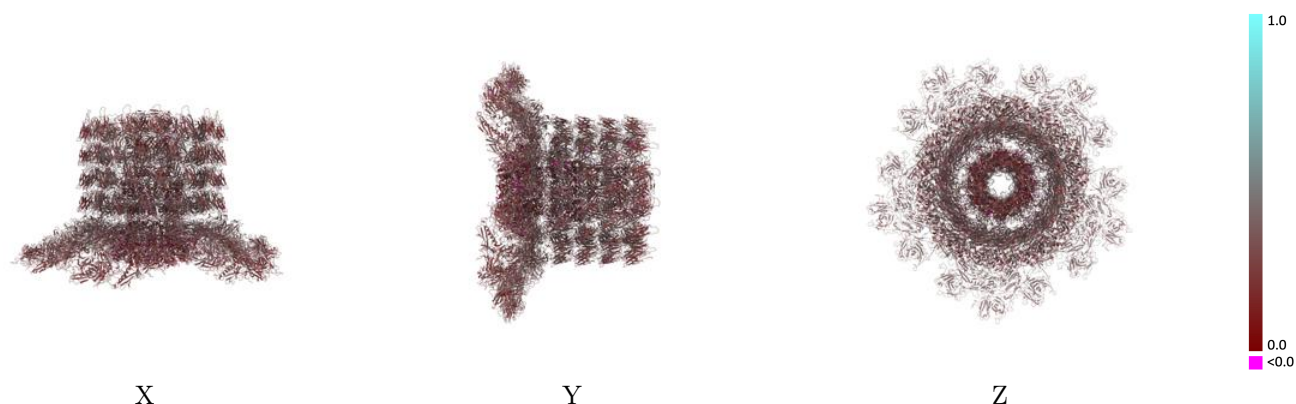
This section contains information regarding the fit between EMDB map EMD-29541 and PDB model 8FXR. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



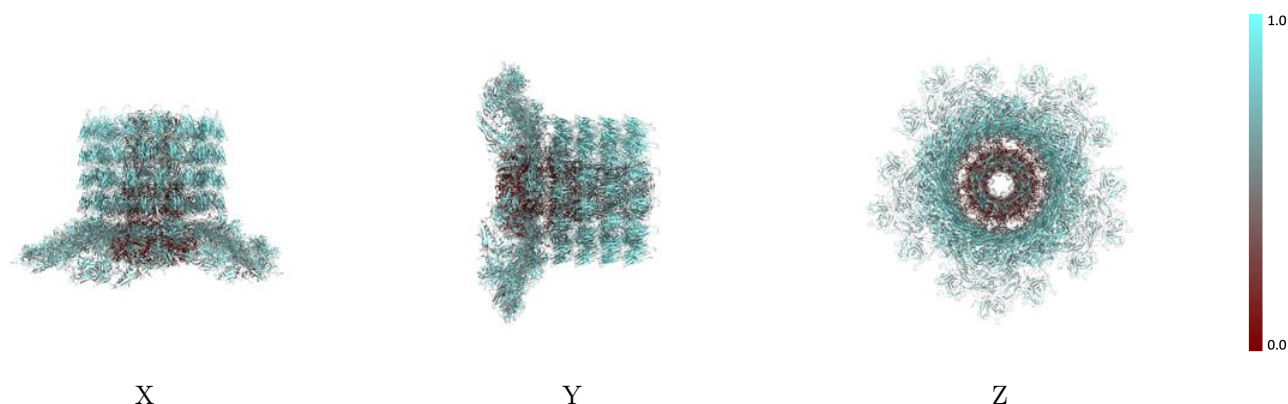
The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



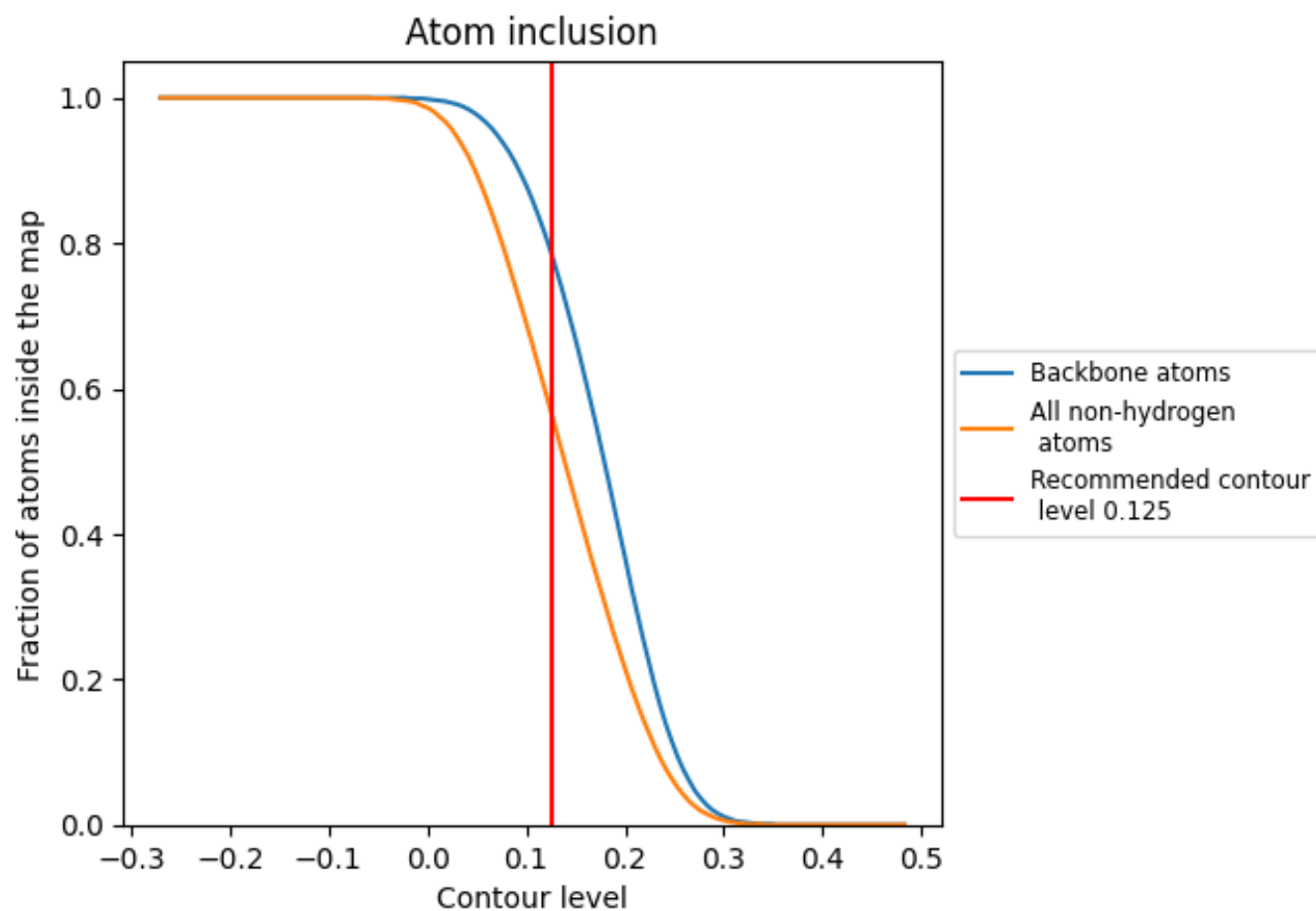
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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	Q-score
All	 0.5690	 0.3020
03	 0.7500	 0.3050
13	 0.7310	 0.3340
23	 0.7580	 0.3370
33	 0.7540	 0.3070
43	 0.7590	 0.3150
53	 0.7710	 0.3000
63	 0.7590	 0.3060
73	 0.7580	 0.3110
83	 0.7510	 0.3070
93	 0.7500	 0.3100
A3	 0.7620	 0.3100
AA	 0.1490	 0.2130
AB	 0.1960	 0.2120
AC	 0.1960	 0.2240
AD	 0.1820	 0.1930
AE	 0.1580	 0.1970
AF	 0.1760	 0.2140
AG	 0.1660	 0.1990
AH	 0.1600	 0.1910
AI	 0.1590	 0.1980
AJ	 0.1660	 0.2030
AK	 0.1750	 0.2160
AL	 0.1650	 0.2030
AM	 0.4150	 0.2730
AN	 0.4440	 0.2640
AO	 0.4430	 0.2510
AP	 0.4190	 0.2670
AQ	 0.3860	 0.2610
AR	 0.4060	 0.2600
AS	 0.3980	 0.2450
AT	 0.3850	 0.2520
AU	 0.3990	 0.2560
AV	 0.4740	 0.2520
AW	 0.3870	 0.2580























































































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Chain	Atom inclusion	Q-score
AX	0.4070	0.2550
AY	0.4480	0.2550
AZ	0.4180	0.2550
Aa	0.4240	0.2490
Ab	0.4780	0.2590
B3	0.7530	0.3140
C3	0.7540	0.3150
D3	0.7580	0.3090
E3	0.7440	0.3050
F3	0.7570	0.3100
G3	0.7390	0.3090
H	0.4320	0.2750
I	0.4710	0.2750
J3	0.7010	0.3560
K3	0.6380	0.3280
L3	0.6450	0.3350
M3	0.6900	0.3510
N3	0.6250	0.3310
O3	0.6580	0.3380
P3	0.6760	0.3480
Q3	0.6630	0.3360
R3	0.6480	0.3410
S3	0.6980	0.3520
T3	0.6710	0.3390
U3	0.6530	0.3300
V3	0.6850	0.3500
W3	0.6500	0.3340
X3	0.6610	0.3360
Y3	0.7270	0.3360
Z3	0.7380	0.3440
a	0.3030	0.2270
a1	0.5960	0.3750
a2	0.6260	0.3770
a3	0.7350	0.3330
a5	0.6010	0.3900
a6	0.6260	0.3870
a7	0.5910	0.3600
b	0.3580	0.2620
b1	0.6210	0.3620
b2	0.5960	0.3680
b3	0.7200	0.3350
b5	0.5520	0.3740





















































































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Chain	Atom inclusion	Q-score
b6	 0.5620	 0.3510
b7	 0.6010	 0.3530
c	 0.6000	 0.3710
c3	 0.7350	 0.3420
d	 0.6130	 0.3740
d1	 0.5830	 0.3600
d2	 0.5750	 0.3630
d3	 0.7300	 0.3350
d5	 0.5540	 0.3640
d6	 0.6130	 0.3610
d7	 0.5920	 0.3560
e	 0.5500	 0.3620
e1	 0.5270	 0.3420
e2	 0.5370	 0.3420
e3	 0.7240	 0.3370
e5	 0.5760	 0.3610
e6	 0.5320	 0.3440
e7	 0.5320	 0.3410
f	 0.5580	 0.3600
f1	 0.4190	 0.3410
f2	 0.3600	 0.3010
f3	 0.7340	 0.3430
f5	 0.3900	 0.3540
f6	 0.3820	 0.3630
f7	 0.4630	 0.3460
g	 0.5420	 0.3690
g1	 0.6110	 0.3210
g2	 0.6270	 0.3200
g3	 0.7210	 0.3400
g5	 0.6190	 0.3270
g6	 0.5950	 0.3200
g7	 0.5980	 0.3280
h	 0.2850	 0.2560
h1	 0.6290	 0.3350
h2	 0.6230	 0.3340
h3	 0.7470	 0.3470
h5	 0.6250	 0.3420
h6	 0.6180	 0.3360
h7	 0.6160	 0.3350
i	 0.3180	 0.2680
i3	 0.7240	 0.3390
j	 0.2500	 0.2440





















































































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Chain	Atom inclusion	Q-score
j3	 0.7140	 0.3370
k	 0.3090	 0.2730
k1	 0.5980	 0.3310
k2	 0.5940	 0.3230
k3	 0.7190	 0.3420
k5	 0.6170	 0.3360
k6	 0.5970	 0.3300
k7	 0.6020	 0.3310
l	 0.3160	 0.2590
l1	 0.7120	 0.3360
l2	 0.6710	 0.3550
l3	 0.7340	 0.3460
l5	 0.6900	 0.3480
l6	 0.6840	 0.3390
l7	 0.6880	 0.3430
m	 0.3560	 0.2640
m1	 0.6630	 0.3480
m2	 0.6490	 0.3560
m3	 0.7170	 0.3300
m5	 0.6600	 0.3510
m6	 0.6650	 0.3480
m7	 0.6550	 0.3500
n	 0.3730	 0.2680
n1	 0.6180	 0.3160
n2	 0.6280	 0.3240
n3	 0.7620	 0.3390
n5	 0.6160	 0.3230
n6	 0.6140	 0.3240
n7	 0.6340	 0.3230
o	 0.3390	 0.2640
o1	 0.6110	 0.2990
o2	 0.5920	 0.2930
o3	 0.7560	 0.3340
o5	 0.6010	 0.2970
o6	 0.6110	 0.3050
o7	 0.6310	 0.3040
p	 0.3650	 0.2810
p1	 0.6160	 0.3140
p2	 0.6220	 0.3180
p3	 0.7480	 0.3340
p5	 0.6080	 0.3110
p6	 0.6180	 0.3200

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Chain	Atom inclusion	Q-score
p7	 0.6310	 0.3180
q	 0.2510	 0.2540
q1	 0.6030	 0.3030
q2	 0.6170	 0.3080
q3	 0.7340	 0.3320
q5	 0.5950	 0.3000
q6	 0.6400	 0.3060
q7	 0.6090	 0.3060
r1	 0.6190	 0.3080
r2	 0.6390	 0.3110
r3	 0.7570	 0.3410
r5	 0.6010	 0.3070
r6	 0.6030	 0.2980
r7	 0.6220	 0.3090
s1	 0.6480	 0.3190
s2	 0.6390	 0.3140
s3	 0.7500	 0.3330
s5	 0.6520	 0.3110
s6	 0.6450	 0.3130
s7	 0.6330	 0.3110
t1	 0.5880	 0.2920
t2	 0.6260	 0.2980
t3	 0.7580	 0.3310
t5	 0.6210	 0.3090
t6	 0.6220	 0.3000
t7	 0.6320	 0.3000
u1	 0.5920	 0.2890
u2	 0.5520	 0.2810
u3	 0.7510	 0.3350
u5	 0.5880	 0.2850
u6	 0.5560	 0.2870
u7	 0.5780	 0.2810
v1	 0.6090	 0.2830
v2	 0.5540	 0.2870
v3	 0.7460	 0.3300
v5	 0.5840	 0.2780
v6	 0.5620	 0.2740
v7	 0.5810	 0.2830
w3	 0.7620	 0.3330
x3	 0.7530	 0.3410
y3	 0.7500	 0.3350
z3	 0.7530	 0.3360