



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 05:48 AM EDT

PDB ID : 9MOG / pdb_00009mog
EMDB ID : EMD-48459
Title : Structure of the distal part of the bacteriophage T4 tail
Authors : Fokine, A.; Zhu, J.; Klose, T.; Vago, F.; Arnaud, C.; Wang, Z.; Khare, B.;
Rossmann, M.G.; Chen, Z.; Sun, L.; Fang, Q.; Kuhn, R.; Rao, V.B.
Deposited on : 2024-12-26
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

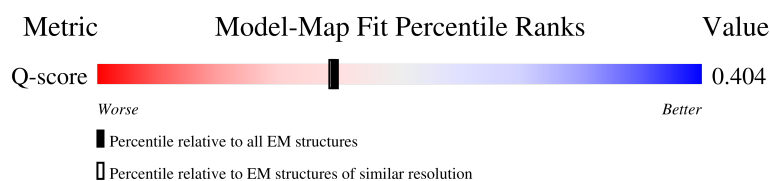
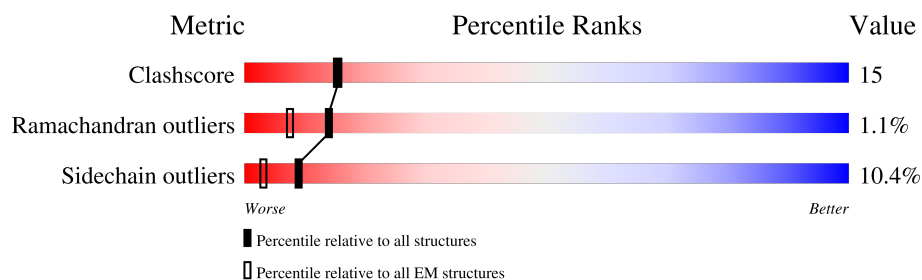
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	S0	527	99% 57% 40%
1	S1	527	98% 58% 37%
1	S2	527	98% 59% 38%
1	S3	527	98% 61% 36%

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Mol	Chain	Length	Quality of chain	
1	S4	527	99%	60%
1	S5	527	97%	61%
1	S6	527	98%	61%
1	S7	527	97%	63%
1	S8	527	97%	60%
1	SA	527	99%	60%
1	SO	527	98%	59%
1	SP	527	97%	60%
1	SQ	527	99%	60%
1	Sv	527	98%	60%
1	Sw	527	98%	64%
1	Sx	527	99%	61%
1	Sy	527	97%	63%
1	Sz	527	98%	60%
2	T1	288	100%	65%
2	T2	288	100%	68%
2	T3	288	100%	65%
2	T4	288	100%	67%
2	T5	288	100%	73%
2	T6	288	100%	69%
2	T7	288	100%	66%
2	T8	288	100%	72%
2	T9	288	100%	67%
2	TF	288	100%	66%
2	TG	288	100%	69%

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Mol	Chain	Length	Quality of chain
2	TH	288	99% 69% 30%
2	Td	288	99% 62% 37%
2	Te	288	99% 68% 30%
2	Tf	288	100% 71% 27%
2	Tg	288	100% 68% 29%
2	Th	288	100% 72% 27%
2	Ti	288	100% 66% 33%
3	UL	219	99% 65% 33%
3	UM	219	100% 63% 35%
3	UN	219	99% 57% 42%
3	Up	219	100% 63% 35%
3	Uq	219	99% 63% 35%
3	Ur	219	99% 61% 36%
3	Us	219	100% 61% 37%
3	Ut	219	99% 68% 30%
3	Uu	219	100% 63% 37%
3	VL	219	99% 63% 36%
3	VM	219	100% 60% 39%
3	VN	219	99% 68% 31%
3	Vp	219	99% 64% 33%
3	Vq	219	99% 64% 34%
3	Vr	219	100% 60% 38%
3	Vs	219	100% 62% 35%
3	Vt	219	99% 64% 34%
3	Vu	219	99% 60% 39%

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Mol	Chain	Length	Quality of chain
4	WI	602	91% 56% 40%
4	WJ	602	88% 58% 38%
4	WK	602	88% 54% 41% 5%
4	Wj	602	92% 54% 41%
4	Wk	602	90% 57% 40%
4	Wl	602	88% 56% 39%
4	Wm	602	88% 57% 37% 5%
4	Wn	602	89% 56% 39% 5%
4	Wo	602	89% 54% 41%
4	XI	602	91% 54% 41% 5%
4	XJ	602	88% 54% 40% 5%
4	XK	602	90% 59% 36% 5%
4	Xj	602	92% 55% 40%
4	Xk	602	90% 57% 39%
4	Xl	602	88% 55% 40%
4	Xm	602	86% 57% 38% 5%
4	Xn	602	89% 58% 37% 5%
4	Xo	602	90% 55% 39% 5%
5	YC	1032	33% 50% 37% 9%
5	YX	1032	30% 50% 38% 9%
5	YY	1032	32% 50% 39% 8%
5	Yc	1032	31% 48% 41% 8%
5	Yx	1032	32% 50% 38% 8%
5	Yy	1032	31% 49% 40% 7%
6	ZD	334	29% 68% 29%

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Mol	Chain	Length	Quality of chain
6	ZE	334	
6	ZZ	334	
6	Za	334	
6	Zb	334	
6	Zc	334	
6	aD	334	
6	aE	334	
6	aZ	334	
6	aa	334	
6	ab	334	
6	ac	334	
7	b0	659	
7	b3	659	
7	b4	659	
7	b5	659	
7	b6	659	
7	b7	659	
7	b8	659	
7	b9	659	
7	bN	659	
7	bO	659	
7	bP	659	
7	bQ	659	
7	bR	659	
7	bY	659	

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Mol	Chain	Length	Quality of chain
7	cA	659	
7	cB	659	
7	cC	659	
7	cD	659	
7	cE	659	
7	cF	659	
7	cG	659	
7	cH	659	
7	cI	659	
7	cJ	659	
7	cK	659	
7	cL	659	
7	cM	659	
7	cN	659	
7	cO	659	
7	cP	659	
7	dS	659	
7	dT	659	
7	dU	659	
7	dV	659	
7	dW	659	
7	dZ	659	
8	eB	660	
8	eU	660	
8	eW	660	

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Mol	Chain	Length	Quality of chain
8	f9	660	
8	fA	660	
8	fB	660	
8	fR	660	
8	fS	660	
8	fU	660	
8	fW	660	
8	fr	660	
8	fs	660	
9	gE	575	
9	gG	575	
9	gH	575	
10	gd	97	
11	h1	163	
11	h2	163	
11	hI	163	
11	hJ	163	
11	hK	163	
11	hL	163	
11	hM	163	
11	hX	163	
11	he	163	
11	hf	163	
11	hg	163	
11	hh	163	

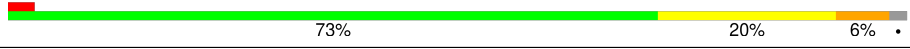
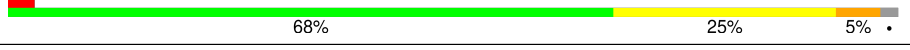
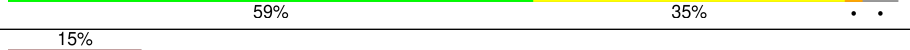
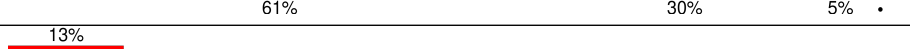
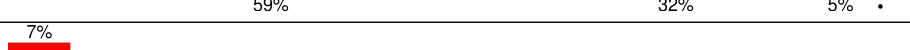
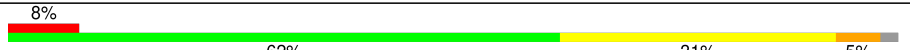
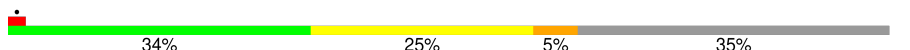
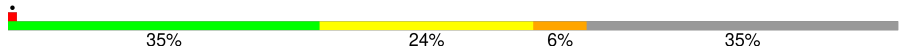
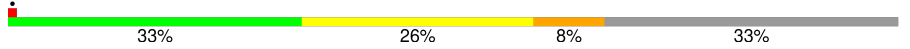
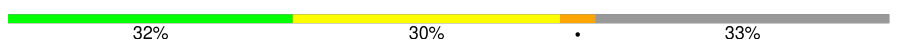
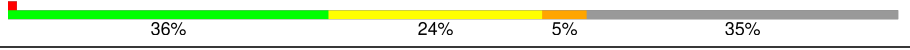
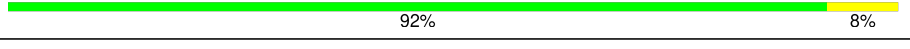
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Mol	Chain	Length	Quality of chain
11	hi	163	
11	hj	163	
11	hk	163	
11	hl	163	
11	hm	163	
11	hn	163	
11	ho	163	
11	hp	163	
11	hq	163	
11	hr	163	
11	hs	163	
11	ht	163	
11	hu	163	
11	hv	163	
11	hw	163	
11	hx	163	
11	hy	163	
11	hz	163	
12	iC	391	
12	iD	391	
12	iF	391	
13	ja	590	
13	jb	590	
13	jc	590	
14	k3	196	

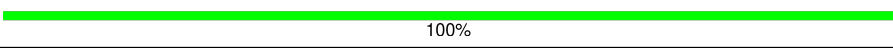
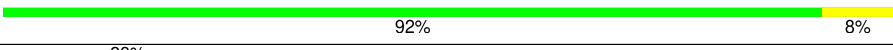
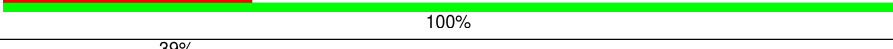
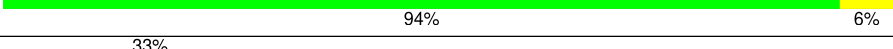
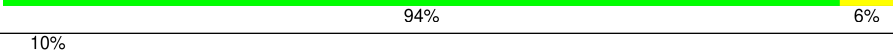
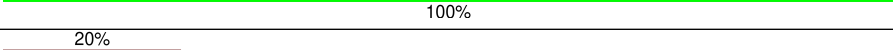
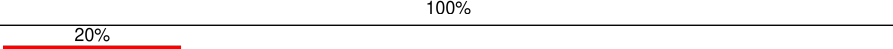
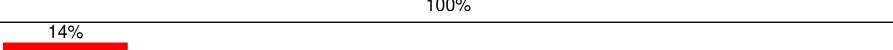
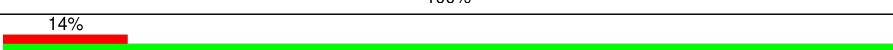
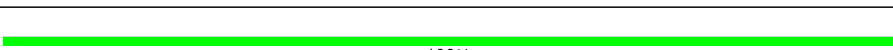
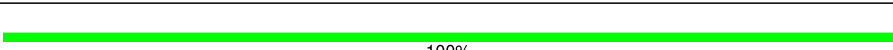
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Mol	Chain	Length	Quality of chain
14	k4	196	
14	k7	196	
14	k8	196	
14	kV	196	
14	lV	196	
15	m1	132	
15	m2	132	
15	m5	132	
15	m6	132	
15	mT	132	
15	nT	132	
16	o0	364	
16	o1	364	
16	o2	364	
16	o6	364	
16	pA	364	
16	pB	364	
17	q3	320	
17	q4	320	
17	q5	320	
17	q7	320	
17	q8	320	
17	q9	320	
18	rc	25	
18	rd	25	

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Mol	Chain	Length	Quality of chain
18	re	25	 84%16%
18	rf	25	 80%20%
18	rg	25	 100%
18	rh	25	 92%8%
19	sQ	18	 28%100%
19	sT	18	 39%94%6%
19	sU	18	 33%94%6%
20	tS	10	 10%100%
20	tX	10	 20%100%
20	tY	10	 20%100%
21	uR	7	 14%86%14%
21	uV	7	 14%100%
21	uW	7	 14%100%
22	vZ	9	 100%
22	va	9	 100%
22	vb	9	 100%

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 652117 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 gp12, short tail fiber protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S0	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	S1	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	S2	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	S3	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	S4	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	S5	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	S6	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	S7	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	S8	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	SA	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	SO	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	SP	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	SQ	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	Sv	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	Sw	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	Sx	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
1	Sy	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Sz	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		

- Molecule 2 is a protein called gp9, baseplate wedge tail fiber connector.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T1	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	T2	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	T3	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	T4	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	T5	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	T6	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	T7	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	T8	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	T9	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	TF	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	TG	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	TH	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	Td	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	Te	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	Tf	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	Tg	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	Th	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
2	Ti	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		

- Molecule 3 is a protein called gp11, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	UL	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	UM	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	UN	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Up	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Uq	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Ur	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Us	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Ut	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Uu	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	VL	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	VM	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	VN	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Vp	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Vq	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Vr	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Vs	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Vt	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
3	Vu	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		

- Molecule 4 is a protein called gp10, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	WI	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	WJ	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	WK	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Wj	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Wk	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Wl	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Wm	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Wn	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Wo	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	XI	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	XJ	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	XK	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Xj	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Xk	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Xl	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Xm	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Xn	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
4	Xo	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		

- Molecule 5 is a protein called gp7, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	YC	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
5	YX	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	YY	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
5	Yc	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
5	Yx	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
5	Yy	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		

- Molecule 6 is a protein called gp8, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	ZD	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
6	ZE	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
6	ZZ	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
6	Za	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
6	Zb	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
6	Zc	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
6	aD	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
6	aE	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
6	aZ	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
6	aa	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
6	ab	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
6	ac	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		

- Molecule 7 is a protein called gp18, tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	b0	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	b3	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	b4	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	b5	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	b6	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	b7	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	b8	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	b9	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	bN	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	bO	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	bP	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	bQ	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	bR	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	bY	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	cA	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	cB	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	cC	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	cD	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	cE	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	cF	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	cG	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
7	cH	655	Total 5000	C 3152	N 841	O 996	S 11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	cI	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
7	cJ	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
7	cK	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
7	cL	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
7	cM	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
7	cN	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
7	cO	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
7	cP	655	Total	C	N	O	S	0	0
			5000	3152	841	996	11		
7	dS	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		
7	dT	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		
7	dU	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		
7	dV	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		
7	dW	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		
7	dZ	647	Total	C	N	O	S	0	0
			4941	3115	833	982	11		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b0	109	ASN	SER	conflict	UNP A0A7S9SVW9
b0	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b0	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b3	109	ASN	SER	conflict	UNP A0A7S9SVW9
b3	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b3	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b4	109	ASN	SER	conflict	UNP A0A7S9SVW9
b4	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b4	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b5	109	ASN	SER	conflict	UNP A0A7S9SVW9
b5	301	GLY	GLU	conflict	UNP A0A7S9SVW9

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Chain	Residue	Modelled	Actual	Comment	Reference
b5	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b6	109	ASN	SER	conflict	UNP A0A7S9SVW9
b6	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b6	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b7	109	ASN	SER	conflict	UNP A0A7S9SVW9
b7	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b7	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b8	109	ASN	SER	conflict	UNP A0A7S9SVW9
b8	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b8	399	VAL	ALA	conflict	UNP A0A7S9SVW9
b9	109	ASN	SER	conflict	UNP A0A7S9SVW9
b9	301	GLY	GLU	conflict	UNP A0A7S9SVW9
b9	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bN	109	ASN	SER	conflict	UNP A0A7S9SVW9
bN	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bN	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bO	109	ASN	SER	conflict	UNP A0A7S9SVW9
bO	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bO	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bP	109	ASN	SER	conflict	UNP A0A7S9SVW9
bP	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bP	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bQ	109	ASN	SER	conflict	UNP A0A7S9SVW9
bQ	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bQ	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bR	109	ASN	SER	conflict	UNP A0A7S9SVW9
bR	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bR	399	VAL	ALA	conflict	UNP A0A7S9SVW9
bY	109	ASN	SER	conflict	UNP A0A7S9SVW9
bY	301	GLY	GLU	conflict	UNP A0A7S9SVW9
bY	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cA	109	ASN	SER	conflict	UNP A0A7S9SVW9
cA	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cA	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cB	109	ASN	SER	conflict	UNP A0A7S9SVW9
cB	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cB	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cC	109	ASN	SER	conflict	UNP A0A7S9SVW9
cC	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cC	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cD	109	ASN	SER	conflict	UNP A0A7S9SVW9
cD	301	GLY	GLU	conflict	UNP A0A7S9SVW9

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Chain	Residue	Modelled	Actual	Comment	Reference
cD	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cE	109	ASN	SER	conflict	UNP A0A7S9SVW9
cE	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cE	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cF	109	ASN	SER	conflict	UNP A0A7S9SVW9
cF	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cF	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cG	109	ASN	SER	conflict	UNP A0A7S9SVW9
cG	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cG	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cH	109	ASN	SER	conflict	UNP A0A7S9SVW9
cH	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cH	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cI	109	ASN	SER	conflict	UNP A0A7S9SVW9
cI	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cI	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cJ	109	ASN	SER	conflict	UNP A0A7S9SVW9
cJ	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cJ	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cK	109	ASN	SER	conflict	UNP A0A7S9SVW9
cK	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cK	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cL	109	ASN	SER	conflict	UNP A0A7S9SVW9
cL	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cL	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cM	109	ASN	SER	conflict	UNP A0A7S9SVW9
cM	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cM	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cN	109	ASN	SER	conflict	UNP A0A7S9SVW9
cN	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cN	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cO	109	ASN	SER	conflict	UNP A0A7S9SVW9
cO	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cO	399	VAL	ALA	conflict	UNP A0A7S9SVW9
cP	109	ASN	SER	conflict	UNP A0A7S9SVW9
cP	301	GLY	GLU	conflict	UNP A0A7S9SVW9
cP	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dS	109	ASN	SER	conflict	UNP A0A7S9SVW9
dS	301	GLY	GLU	conflict	UNP A0A7S9SVW9
dS	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dT	109	ASN	SER	conflict	UNP A0A7S9SVW9
dT	301	GLY	GLU	conflict	UNP A0A7S9SVW9

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Chain	Residue	Modelled	Actual	Comment	Reference
dT	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dU	109	ASN	SER	conflict	UNP A0A7S9SVW9
dU	301	GLY	GLU	conflict	UNP A0A7S9SVW9
dU	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dV	109	ASN	SER	conflict	UNP A0A7S9SVW9
dV	301	GLY	GLU	conflict	UNP A0A7S9SVW9
dV	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dW	109	ASN	SER	conflict	UNP A0A7S9SVW9
dW	301	GLY	GLU	conflict	UNP A0A7S9SVW9
dW	399	VAL	ALA	conflict	UNP A0A7S9SVW9
dZ	109	ASN	SER	conflict	UNP A0A7S9SVW9
dZ	301	GLY	GLU	conflict	UNP A0A7S9SVW9
dZ	399	VAL	ALA	conflict	UNP A0A7S9SVW9

- Molecule 8 is a protein called gp6, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	eB	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
8	eU	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
8	eW	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
8	f9	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
8	fA	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
8	fB	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
8	fR	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
8	fS	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
8	fU	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
8	fW	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
8	fr	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
8	fs	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		

- Molecule 9 is a protein called gp5, baseplate central spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	gE	559	Total	C	N	O	S	0	0
			4321	2681	761	856	23		
9	gG	559	Total	C	N	O	S	0	0
			4321	2681	761	856	23		
9	gH	559	Total	C	N	O	S	0	0
			4321	2681	761	856	23		

- Molecule 10 is a protein called gp5.4, tip of the central spike.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	gd	96	Total	C	N	O	S	0	0
			709	447	120	139	3		

- Molecule 11 is a protein called gp19, tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	h1	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	h2	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hI	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hJ	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hK	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hL	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hM	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hX	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	he	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hf	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hg	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hh	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hi	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hj	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	hk	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hl	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hm	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hn	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	ho	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hp	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hq	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hr	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hs	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	ht	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hu	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hv	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hw	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hx	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hy	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
11	hz	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		

- Molecule 12 is a protein called gp27, baseplate hub protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	iC	375	Total	C	N	O	S	0	0
			3000	1916	491	575	18		
12	iD	375	Total	C	N	O	S	0	0
			3000	1916	491	575	18		
12	iF	375	Total	C	N	O	S	0	0
			3000	1916	491	575	18		

- Molecule 13 is a protein called gp29, tape measure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	ja	20	Total	C	N	O	S	0	0
			137	84	22	30	1		
13	jb	20	Total	C	N	O	S	0	0
			137	84	22	30	1		
13	jc	20	Total	C	N	O	S	0	0
			137	84	22	30	1		

- Molecule 14 is a protein called gp53, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	k3	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
14	k4	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
14	k7	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
14	k8	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
14	kV	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
14	lV	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		

- Molecule 15 is a protein called gp25, baseplate wedge protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m1	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		
15	m2	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		
15	m5	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		
15	m6	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		
15	mT	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		
15	nT	127	Total	C	N	O	S	0	0
			1019	640	171	204	4		

- Molecule 16 is a protein called gp48, baseplate protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	o0	358	Total	C	N	O	S	0	0
			2749	1714	467	559	9		
16	o1	314	Total	C	N	O	S	0	0
			2436	1523	414	491	8		
16	o2	314	Total	C	N	O	S	0	0
			2436	1523	414	491	8		
16	o6	314	Total	C	N	O	S	0	0
			2436	1523	414	491	8		
16	pA	358	Total	C	N	O	S	0	0
			2749	1714	467	559	9		
16	pB	358	Total	C	N	O	S	0	0
			2749	1714	467	559	9		

- Molecule 17 is a protein called gp54, baseplate protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q3	207	Total	C	N	O	S	0	0
			1650	1037	280	321	12		
17	q4	207	Total	C	N	O	S	0	0
			1650	1037	280	321	12		
17	q5	213	Total	C	N	O	S	0	0
			1693	1064	287	330	12		
17	q7	213	Total	C	N	O	S	0	0
			1693	1064	287	330	12		
17	q8	207	Total	C	N	O	S	0	0
			1650	1037	280	321	12		
17	q9	213	Total	C	N	O	S	0	0
			1693	1064	287	330	12		

- Molecule 18 is a protein called unassigned peptide A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	rc	25	Total	C	N	O	0	0
			125	75	25	25		
18	rd	25	Total	C	N	O	0	0
			125	75	25	25		
18	re	25	Total	C	N	O	0	0
			125	75	25	25		
18	rf	25	Total	C	N	O	0	0
			125	75	25	25		
18	rg	25	Total	C	N	O	0	0
			125	75	25	25		
18	rh	25	Total	C	N	O	0	0
			125	75	25	25		

- Molecule 19 is a protein called unassigned peptide B.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	sQ	18	Total	C	N	O	0	0
			90	54	18	18		
19	sT	18	Total	C	N	O	0	0
			90	54	18	18		
19	sU	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 20 is a protein called unassigned peptide C.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	tS	10	Total	C	N	O	0	0
			50	30	10	10		
20	tX	10	Total	C	N	O	0	0
			50	30	10	10		
20	tY	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 21 is a protein called unassigned peptide D.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	uR	7	Total	C	N	O	0	0
			35	21	7	7		
21	uV	7	Total	C	N	O	0	0
			35	21	7	7		
21	uW	7	Total	C	N	O	0	0
			35	21	7	7		

- Molecule 22 is a protein called unassigned peptide E.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	vZ	9	Total	C	N	O	0	0
			45	27	9	9		
22	va	9	Total	C	N	O	0	0
			45	27	9	9		
22	vb	9	Total	C	N	O	0	0
			45	27	9	9		

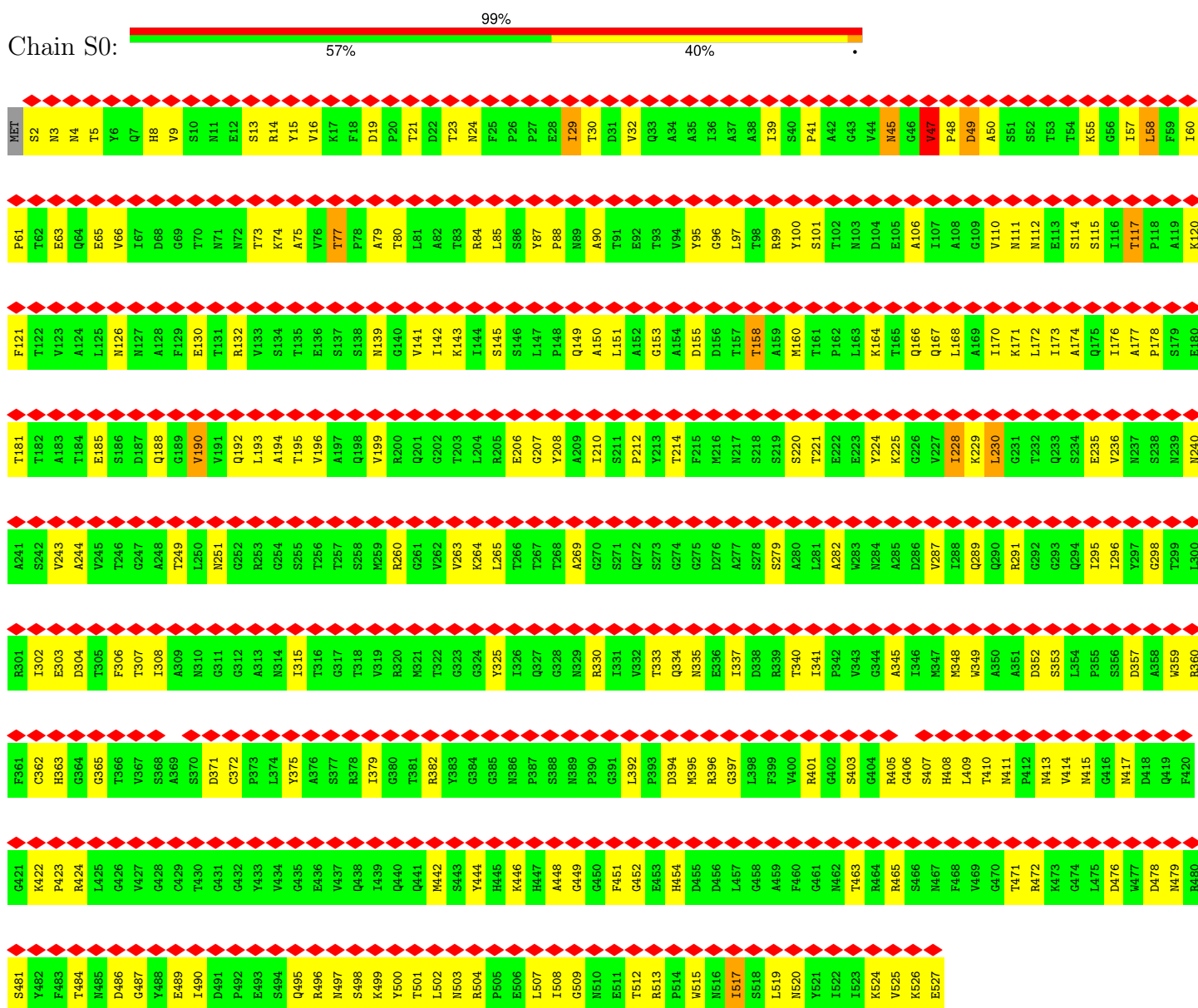
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

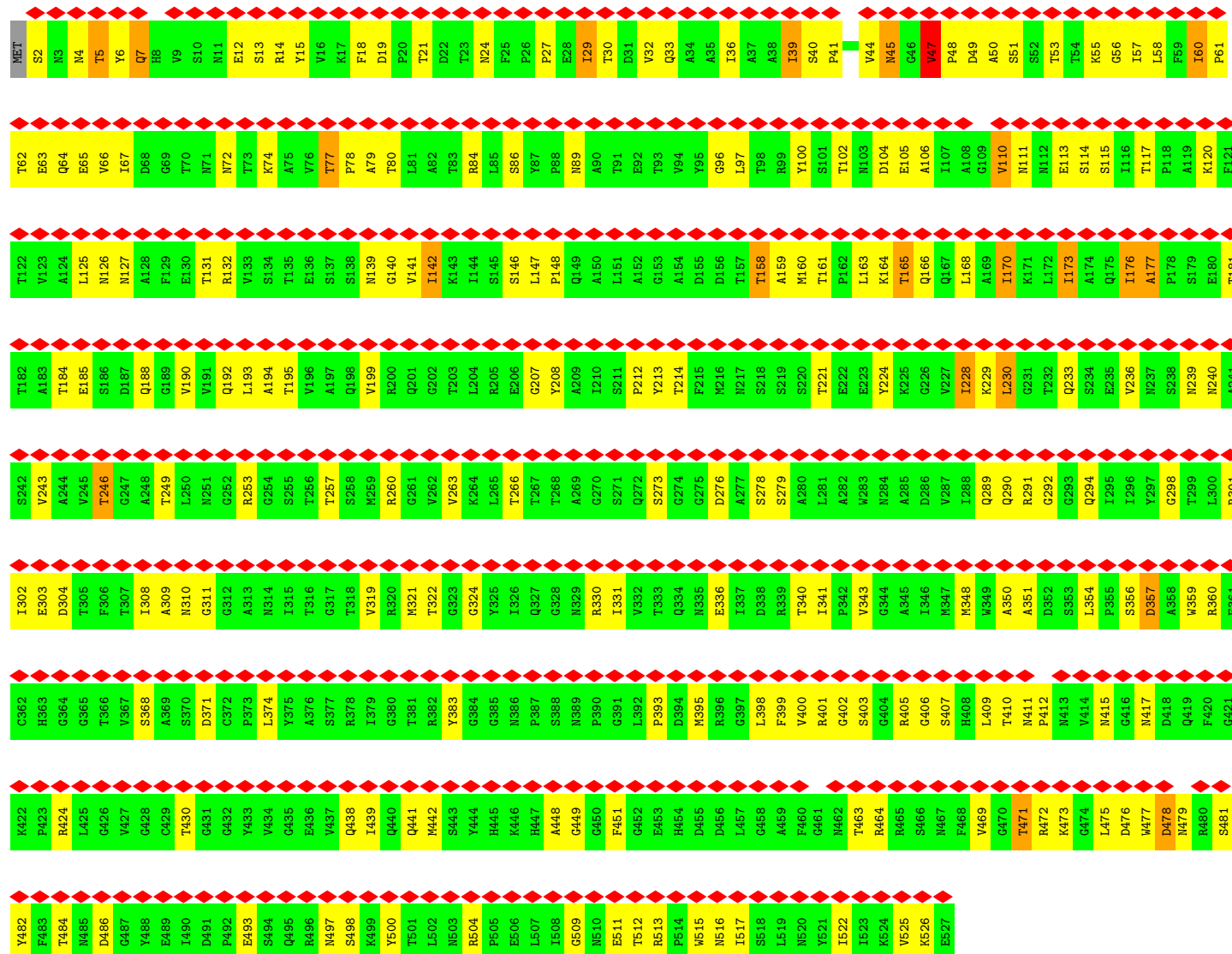
Mol	Chain	Residues	Atoms		AltConf
23	S0	1	Total 1	Zn 1	0
23	S1	1	Total 1	Zn 1	0
23	S4	1	Total 1	Zn 1	0
23	SA	1	Total 1	Zn 1	0
23	SQ	1	Total 1	Zn 1	0
23	Sv	1	Total 1	Zn 1	0

3 Residue-property plots

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: gp12, short tail fiber protein





• Molecule 1: gp12, short tail fiber protein

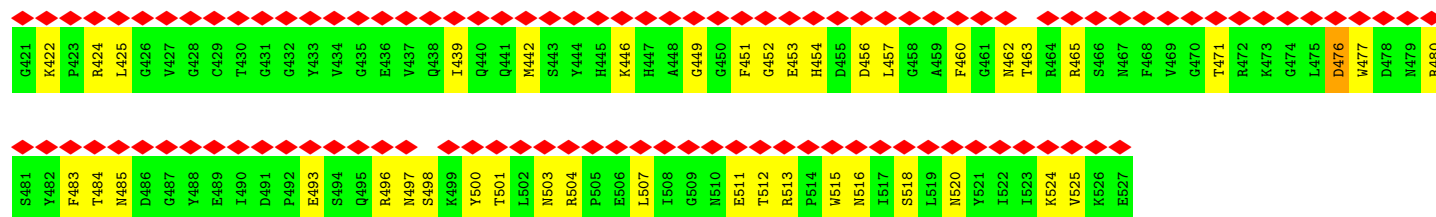


T181	A241	R301	F361	G421	S481
T182	S242	I302	C362	K422	Y482
A183	V243	E303	H363	F423	F483
T184	A244	D304	G364	R424	T484
E185	V245	T305	G365	L425	M485
S186	T246	F306	T366	G426	D486
D187	G247	T307	V367	V427	G487
Q188	A248	I308	S368	G428	Y488
G189	T249	A309	A369	C429	E489
V190	L250	N310	S370	T430	I490
V191	N251	G311	D371	G431	D491
Q192	G252	G312	C372	G432	P492
L193	R253	A313	F373	Y433	E493
A194	G254	N314	L374	V434	S494
T195	S255	I315	Y375	G435	Q495
V196	T256	T316	A376	E436	R496
A197	T257	G317	A377	V437	M497
Q198	S258	T318	R378	Q438	S498
V199	M259	V319	I379	I439	K499
R200	R260	R320	G380	Q440	Y500
Q201	G261	M321	T381	Q441	T501
G202	V262	T322	R382	M442	L502
T203	V263	G323	Y383	S443	N503
L204	K264	G324	G384	Y444	R504
R205	L265	Y325	G385	H445	P505
E206	T266	I326	N386	K446	E506
G207	T267	Q327	P387	H447	L507
Y208	T268	G328	S388	A448	I508
A209	A269	N329	N389	G449	G509
I210	G270	R330	P390	G450	N510
S211	S271	I331	G391	F451	E511
P212	Q272	V332	L392	G452	T512
Y213	G273	T333	P393	E453	R513
T214	G274	Q334	D394	H454	P514
F215	G275	N335	M395	D455	W515
M216	D276	E336	R396	D456	N516
N217	A277	I337	G397	L457	I517
S218	S278	D338	L398	G458	S518
S219	S279	R339	F399	A459	L519
T220	A280	T340	V400	F460	N520
T221	L281	I341	R401	G461	Y521
E222	A282	P342	G402	M462	I522
E223	W283	V343	S403	T463	I523
Y224	N284	G344	G404	R464	K524
K225	A285	R405	R405	R465	V525
G226	D286	I346	G406	S466	K526
V227	V287	M347	S407	M467	E527
I228	I288	M348	H408	F468	
K229	Q289	W349	L409	V469	
L230	Q290	A350	T410	G470	
G231	R291	A351	M411	T471	
T232	G292	D352	P412	R472	
Q233	G293	M413	M413	K473	
S234	Q294	L354	V414	G474	
E235	I295	P355	M415	L475	
V236	I296	G356	G416	D476	
N237	Y297	D357	M417	W477	
S238	G298	D418	D418	D478	
N239	T299	W359	Q419	M479	
N240	L300	R360	F420	R480	

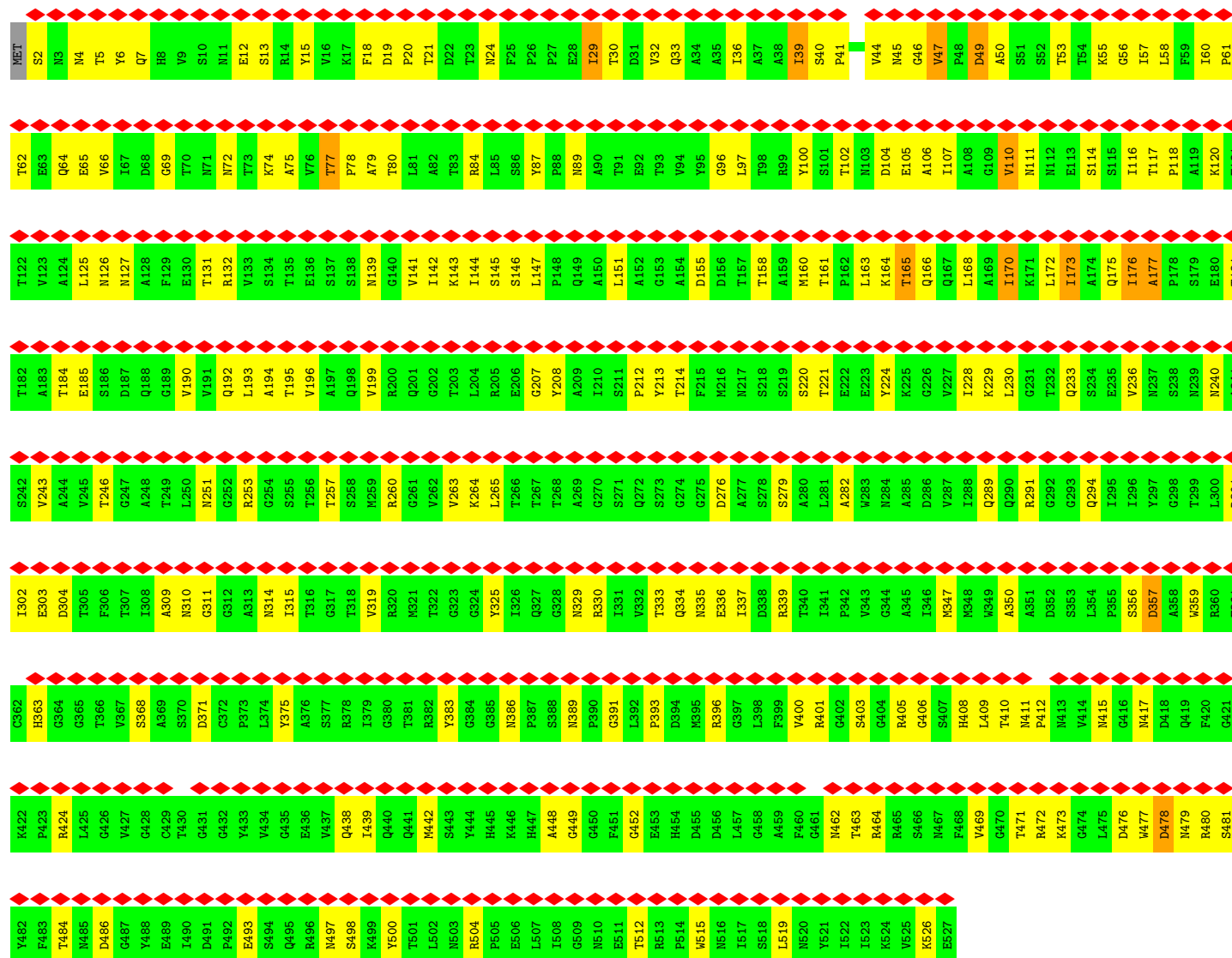
● Molecule 1: gp12, short tail fiber protein



MET	S2	N3	N4	T5	Y6	O7	H8	V9	S10	N11	E12	S13	R14	Y15	V16	K17	F18	D19	P20	T21	D22	T23	N24	F25	P26	P27	E28	I29	T30	D31	V32	Q33	A34	A35	I36	A37	A38	I39	S40	P41	A42	G43	V44	N45	G46	V47	P48	D49	A50	S51	S52	T53	T54	K55	G56	L57	L58	F59	L60
P61	T62	E63	Q64	E65	V66	L67	D68	G69	T70	M71	N72	T73	K74	A75	V76	T77	P78	A79	T80	L81	A82	T83	R84	L85	S86	Y87	P88	N89	A90	T91	E92	T93	V94	Y95	G96	L97	T98	R99	Y100	S101	T102	M103	D104	N105	E106	L107	A108	G109	T110	N111	N112	E113	S114	S115	I116	T117	A118	A119	K120
F121	T122	V123	A124	L125	N126	M127	A128	F129	E130	T131	R132	V133	S134	T135	E136	S137	S138	M139	G140	V141	I142	K143	I144	S145	S146	L147	P148	Q149	A150	L151	A152	G153	A154	D155	D156	T157	T158	A159	M160	T161	P162	L163	K164	T165	Q166	Q167	L168	A169	I170	K171	L172	I173	A174	Q175	I176	A177	S178	S179	E180
T181	T182	A183	T184	E185	S186	D187	Q188	G189	V190	V191	Q192	L193	A194	T195	V196	A197	Q198	V199	R200	Q201	G202	T203	L204	R205	E206	G207	Y208	A209	I210	S211	P212	Y213	T214	F215	H216	M217	S218	S219	S220	T221	E222	E223	Y224	G225	G226	V227	I228	K229	L230	G231	T232	Q233	S234	E235	V236	N237	S238	N239	N240
A241	S242	V243	A244	T245	G246	G247	A248	T249	L250	N251	G252	R253	G254	S255	T256	T257	S258	M259	R260	G261	V262	V263	K264	L265	T266	T267	A268	A269	G270	S271	Q272	G273	G274	D275	D276	A277	S278	S279	A280	L281	A282	W283	N284	A285	D286	V287	I288	Q289	Q290	R291	G292	G293	Q294	I295	I296	Y297	G298	T299	L300
R301	I302	E303	D304	T305	F306	T307	I308	A309	M310	G311	G312	A313	N314	I315	T316	G317	T318	V319	R320	M321	T322	G323	G324	Y325	I326	Q327	G328	N329	R330	I331	V332	T333	Q334	N335	E336	I337	R338	R339	T340	I341	P342	V343	G344	A345	I346	M347	M348	W349	A350	A351	D352	S353	L354	P355	I296	D357	A358	W359	R360
F361	C362	H363	G364	G365	T366	V367	S368	A369	S370	D371	C372	F373	L374	Y375	A376	S377	R378	I379	G380	T381	R382	Y383	G384	G385	N386	P387	S388	N389	P390	G391	L392	P393	D394	M395	R396	G397	L398	P399	V400	R401	G402	S403	G404	R405	G406	S407	H408	L409	T410	M411	P412	M413	V414	M415	G416	M417	D418	Q419	F420



- Molecule 1: gp12, short tail fiber protein



- Molecule 1: gp12, short tail fiber protein

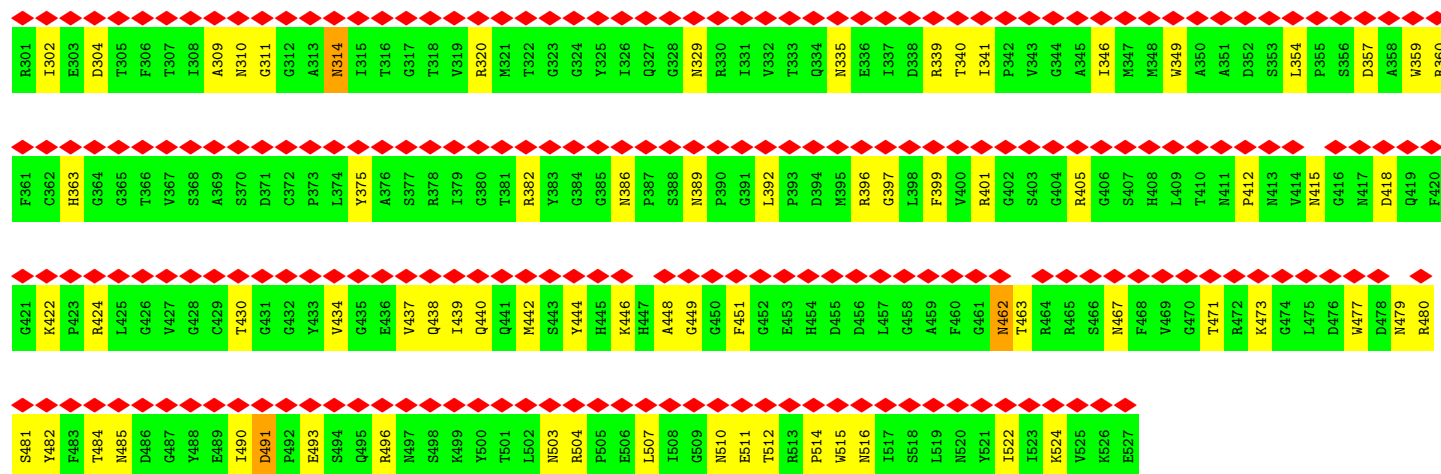


P61	T181	A241	R301	F361	G421	S481
T62	T182	S242	I302	G362	K422	Y482
E63	T122	V243	E303	H363	P423	F483
Q64	V123			G364	R424	T484
E65	A124	A244	D304	G365	L425	N485
V66	L125	T245	T305	T366	G426	D486
I67	N126	G247	F306	V367	V427	G487
D68	N127	Q188	T307	S368	G428	Y488
G69	A128	A248	I308	A369	C429	E489
T70	F129	T249	A309	S370	G430	L490
N71	E130	L250	N310	D371	G431	D491
N72	T131	N251	G311	G372	G432	P492
T73	R132	G252	G312	P373	Y433	E493
K74	V133	A194	A313	L374	Y434	S494
A75	S134	T255	N314	V375	G435	Q495
V76	T135	T256	I315	A376	E436	R496
T77	E136	V196	T316	S377	V437	N497
P78	S137	G197	G317	R378	A438	S498
A79	S138	Q198	T318	I379	T439	K499
T80	N139	V199	V319	G380	Q440	Y500
L81	G140	R200	R320	T381	Q441	T501
A82	V141	Q201	M321	R382	N442	L502
T83	I142	G202	T322	Y383	S443	N503
R84	K143	T203	G323	G384	Y444	R504
L85	I144	R204	G324	G385	H445	P505
S86	S145	L265	Y325	N386	K446	E506
Y87	S146	T267	I326	P387	L447	L507
P88	L147	G207	Q327	S388	A448	T508
N89	P148	Y208	G328	N389	G449	G509
A90	Q149	A209	R329	P390	G450	N510
T91	A150	I210	R330	G391	F451	E511
E92	L151	S211	I331	L392	G452	T512
T93	A152	P212	V332	P393	E453	R513
V94	G153	Y213	T333	D394	H454	P514
Y95	A154	T214	Q334	K395	D455	W515
G96	D155	F215	N335	R396	D456	N516
L97	D156	M216	E336	G397	L457	L517
T98	T157	N217	I337	L398	G458	S518
R99	T158	S218	D338	F399	A459	L519
Y100	A159	S219	R339	V400	F460	N520
S101	M160	S220	T340	R401	G461	Y521
T102	T161	T221	I341	G402	N462	T522
N103	P162	E222	P342	S403	T463	I523
D104	L163	E223	V343	G404	R464	K524
E105	K164	Y224	G344	R405	R465	V525
A106	T165	K225	A345	G406	S466	K526
I107	Q166	G226	I346	S407	N467	E527
A108	Q167	V227	M347	H408	F468	
G109	L168	I228	M348	L409	G470	
V110	A169	K229	W349	T410	T471	
N111	I170	G231	A350	N411	R472	
N112	K171	G232	D352	P412	K473	
E113	L172	Q233	S353	N413	G474	
S114	I173	S234	L354	V414	L475	
S115	A174	E235	P355	N415	D476	
I116	Q175	V236	S356	G416	V477	
T117	I176	N237	D357	N417	D478	
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A119	P178	N239	W359	Q419	R480	
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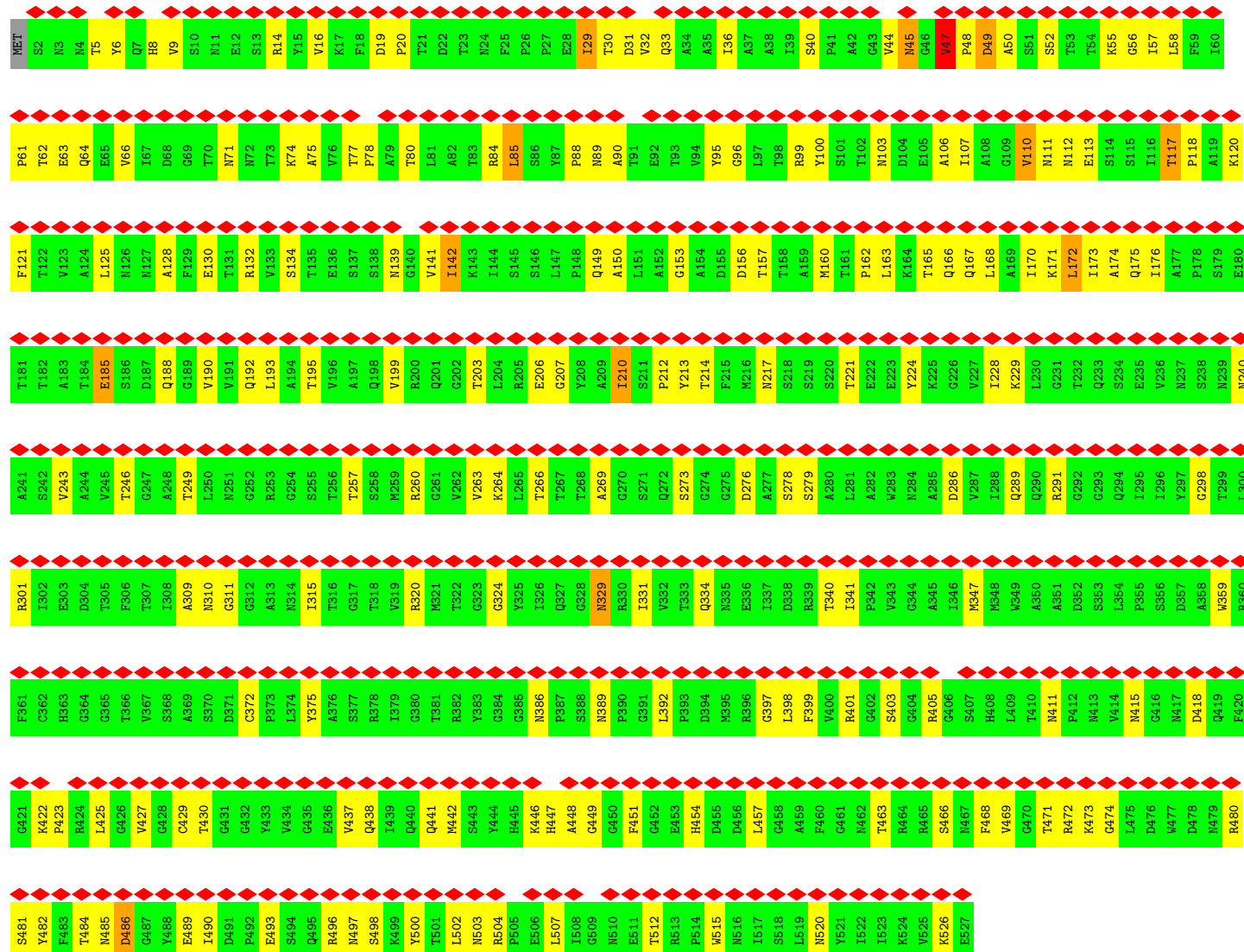
• Molecule 1: gp12, short tail fiber protein

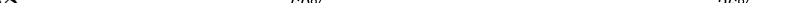


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Y6	V66	N126	S186	T246
Q7	I67	M127	D187	G247
H8	D68	A128	Q188	A248
V9	G69	F129	G189	T249
S10	T70	E130	V190	L250
M11	N71	T131	V191	N251
E12	N72	R132	Q192	G252
S13	T73	V133	L193	R253
R14	K74	S134	A194	E254
Y15	A75	T135	T195	S255
V16	V76	E136	V196	T256
K17	T77	S137	A197	T257
F18	P78	N138	Q198	S258
D19	A79	M139	V199	M259
P20	T80	G140	R200	R260
T21	L81	V141	Q201	G261
D22	A82	I142	G202	V262
T23	T83	K143	T203	V263
N24	R84	I144	L204	K264
F25	L85	S145	R205	L265
P26	S86	S146	E206	T266
P27	Y87	L147	G207	T267
E28	P88	P148	Y208	T268
I29	N89	Q149	A209	A269
T30	A90	A150	I210	G270
D31	T91	L151	S211	S271
V32	E92	A152	P212	Q272
Q33	T93	G153	Y213	Q273
A34	V94	A154	T214	G274
A35	Y95	D155	F215	G275
I36	G96	D156	M216	D276
A37	L97	T157	N217	A277
A38	T98	T158	S218	S278
I39	R99	A159	S219	S279
S40	Y100	M160	S220	S279
P41	S101	T161	T221	L281
A42	T102	P162	E222	A282
G43	N103	L163	E223	W283
V44	D104	K164	Y224	N284
N45	E105	T165	K225	A285
G46	A106	Q166	G226	D286
V47	I107	Q167	V227	T287
P48	A108	L168	I228	I288
D49	G109	A169	K229	K289
A50	V110	I170	L230	A289
S51	M111	K171	G231	Q291
S52	N112	L172	T232	G292
T53	E113	I173	Q233	G293
T54	S114	A174	S234	Q294
K55	S115	Q175	E235	I295
G56	I116	I176	V236	I296
I57	T117	A177	N237	Y297
L58	P118	P178	S238	G298
F59	A119	S179	N239	T299
T60	K120	E180	L300	L300



- Molecule 1: gp12, short tail fiber protein



- Chain S8: 

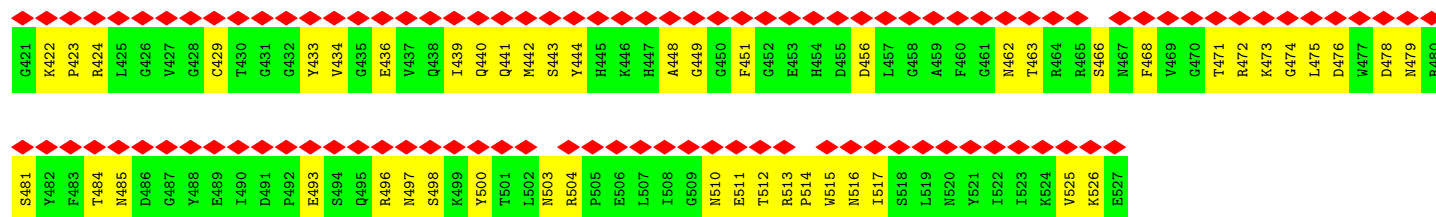


T181	A241	R301	F361	G421	S481
T182	S242	I302	C362	K422	Y482
A183	V243	E303	H363	P423	F483
T184	A244	D304	G364	R424	T484
E185	V245	T305	G365	L425	M485
S186	T246	F306	T366	G426	D486
D187	G247	T307	V367	V427	G487
Q188	A248	I308	S368	G428	Y488
G189	T249	A309	A369	C429	E489
V190	L250	N310	S370	T430	I490
V191	N251	G311	D371	G431	D491
Q192	G252	G312	C372	G432	P492
L193	R253	A313	F373	G433	E493
A194	G254	N314	L374	Y434	S494
T195	S255	I315	Y375	G435	Q495
V196	T256	T316	A376	E436	R496
A197	T257	G317	S377	V437	M497
Q198	S258	T318	R378	Q438	S498
V199	M259	V319	I379	I439	K499
R200	R260	R320	G380	Q440	Y500
Q201	G261	M321	T381	Q441	T501
G202	V262	T322	R382	M442	L502
T203	V263	G323	Y383	S443	N503
L204	K264	G324	G384	Y444	R504
R205	L265	Y325	G385	H445	P505
E206	T266	I326	N386	K446	E506
G207	T267	Q327	P387	H447	L507
Y208	T268	G328	S388	A448	I508
A209	A269	N329	N389	G449	G509
I210	G270	R330	P390	G450	N510
S211	S271	I331	G391	F451	E511
P212	Q272	V332	L392	G452	T512
Y213	S273	T333	P393	E453	R513
T214	G274	Q334	D394	H454	P514
F215	G275	N335	M395	D455	W515
M216	D276	E336	R396	D456	N516
N217	A277	I337	G397	L457	I517
S218	S278	D338	L398	G458	S518
S219	S279	R339	F399	A459	L519
S220	A280	T340	V400	F460	N520
T221	L281	I341	R401	G461	Y521
E222	A282	P342	G402	M462	I522
E223	W283	V343	S403	T463	I523
Y224	N284	G344	G404	R464	K524
K225	A285	A345	R405	R465	W525
G226	D286	I346	G406	S466	K526
V227	V287	M347	S407	M467	E527
I228	I288	M348	H408	F468	
K229	Q289	W349	L409	V469	
L230	Q290	A350	T410	G470	
G231	R291	A351	M411	T471	
T232	G292	P352	P412	R472	
Q233	G293	S353	M413	K473	
S234	Q294	L354	V414	G474	
E235	I295	P355	M415	L475	
V236	I296	G356	G416	D476	
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S238	Q298	A358	D418	D478	
N239	T299	W359	Q419	M479	
N240	L300	R360	F420	R480	

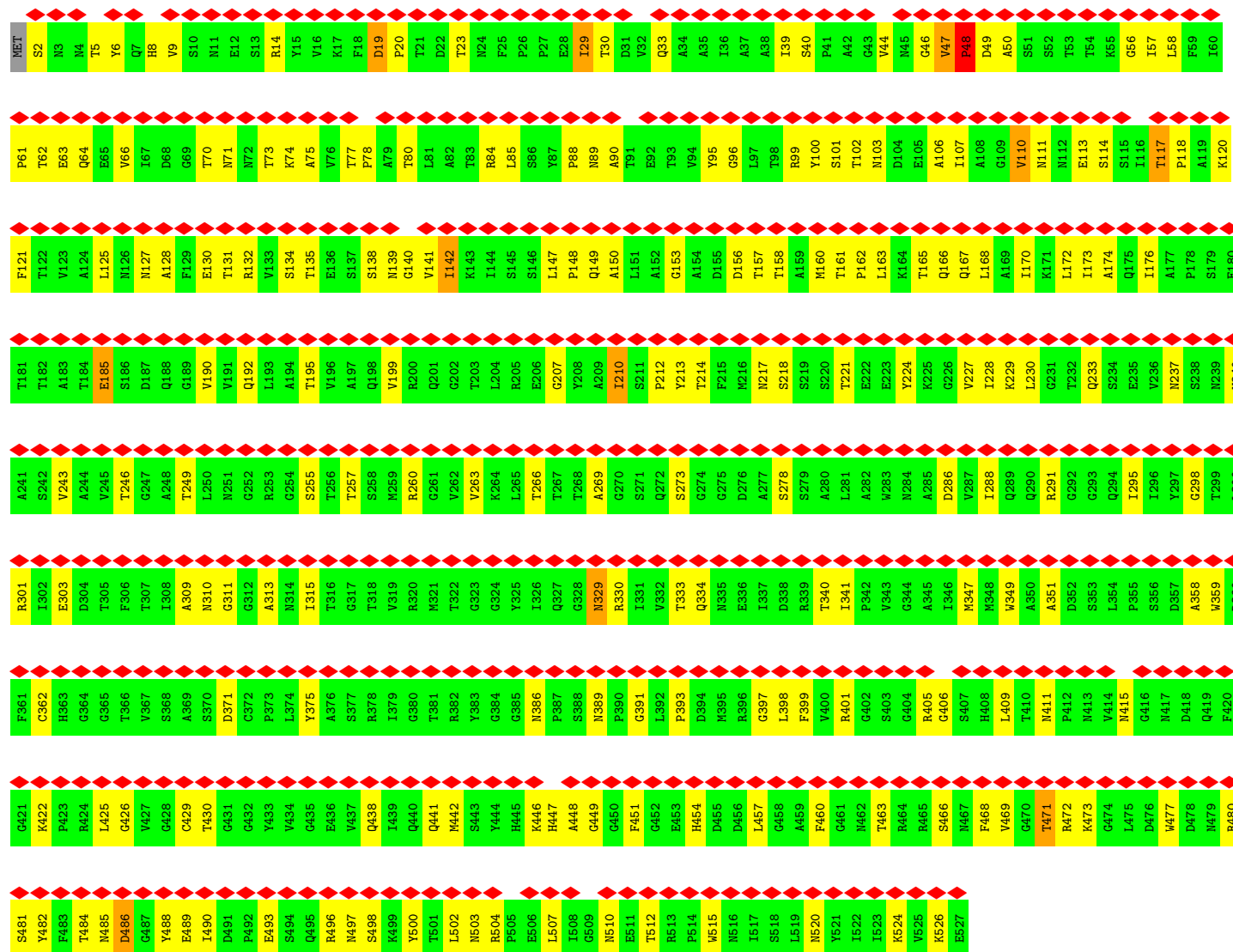
• Molecule 1: gp12, short tail fiber protein



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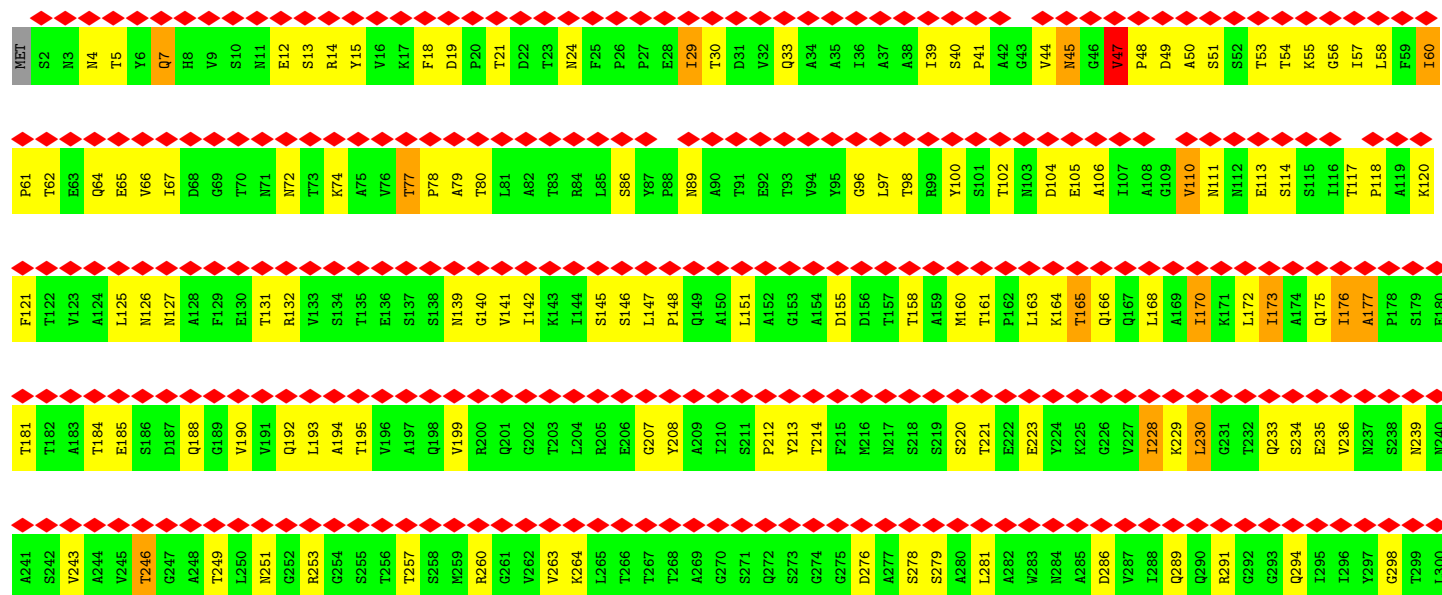


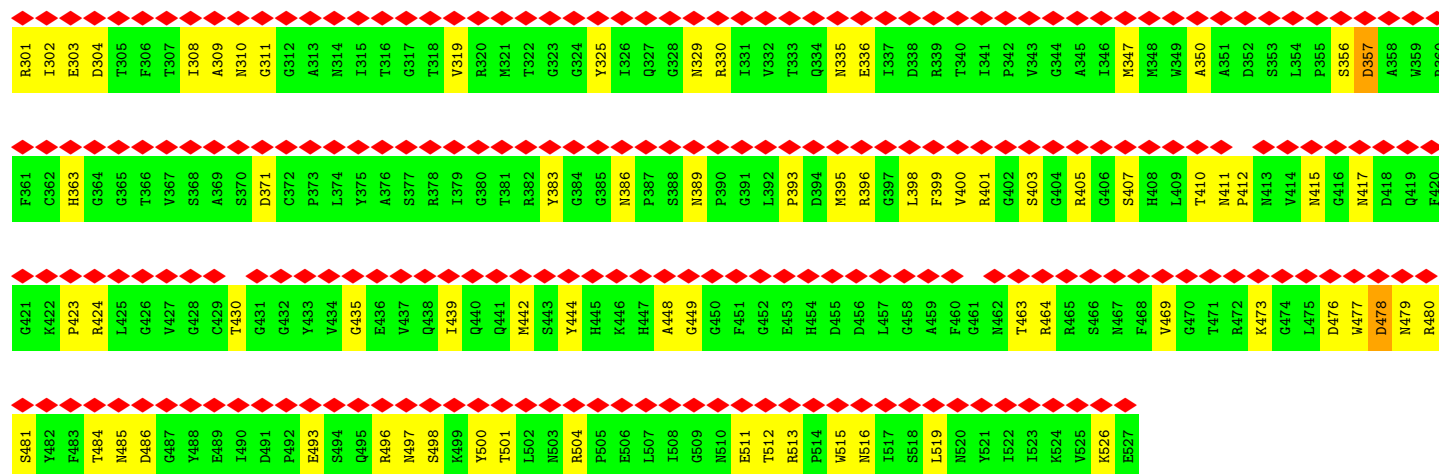
- Molecule 1: gp12, short tail fiber protein



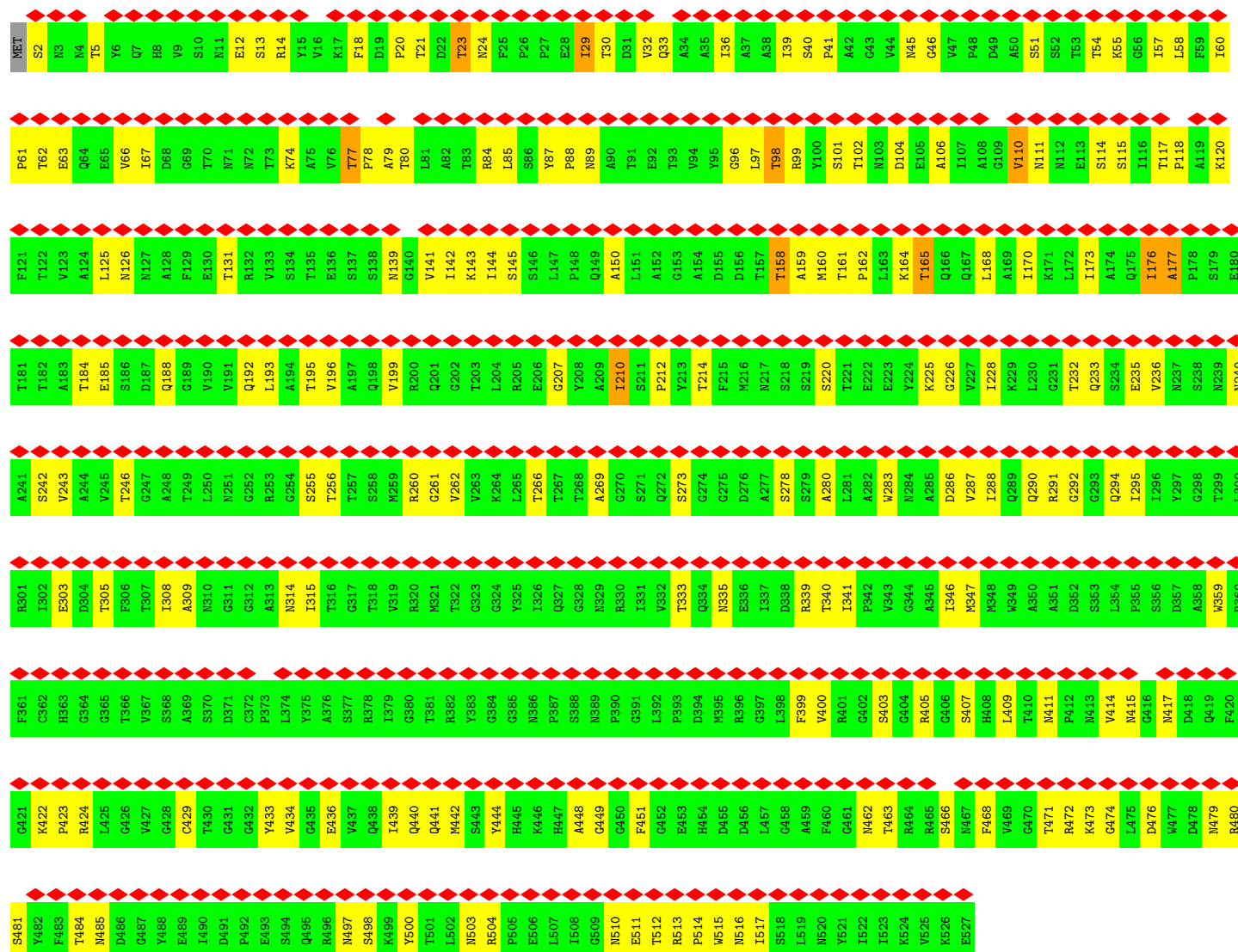
- Molecule 1: gp12, short tail fiber protein

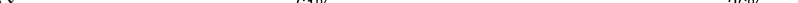






- Molecule 1: gp12, short tail fiber protein



- Chain Sx: 



T181	A241	R301	F361	G421	S481
T182	S242	I302	C362	K422	Y482
A183	V243	E303	H363	P423	F483
T184	A244	D304	G364	R424	T484
E185	V245	F305	T366	L425	M485
S186	T246	T307	V367	G426	D486
D187	G247	I308	S368	V427	G487
Q188	A248	A309	A369	G428	Y488
G189	T249	N310	S370	T430	E489
V190	L250	G311	D371	G431	I490
V191	N251	G312	C372	G432	D491
Q192	G252	A313	F373	Y433	P492
L193	R253	A314	L374	V434	E493
A194	G254	I315	Y375	G435	S494
T195	S255	T316	A376	E436	Q495
V196	T256	G317	S377	V437	R496
A197	T257	T318	R378	Q438	M497
Q198	S258	V319	I379	I439	S498
V199	R260	R320	G380	Q440	K499
R200	G261	M321	T381	Q441	Y500
Q201	V262	T322	T382	M442	T501
G202	V263	G323	Y383	S443	L502
T203	K264	G324	G384	Y444	N503
L204	L265	Y325	G385	H445	R504
R205	T266	I326	N386	K446	P505
E206	T267	Q327	P387	H447	E506
G207	T268	G328	S388	A448	L507
Y208	A269	N329	N389	G449	I508
A209	G270	R330	P390	G450	G509
I210	S271	I331	G391	F451	N510
S211	Q272	T332	L392	G452	E511
P212	S273	T333	P393	E453	T512
Y213	G274	Q334	D394	H454	R513
T214	G275	N335	M395	D455	P514
F215	D276	E336	M396	D456	W515
M216	A277	I337	R396	L457	N516
N217	S278	D338	G397	G458	I517
S218	S279	R339	L398	A459	S518
S219	A280	T340	F399	F460	L519
S220	L281	I341	V400	G461	N520
T221	A282	P342	R401	M462	Y521
E222	W283	V343	G402	T463	I522
E223	N284	G344	S403	R464	I523
Y224	A285	A345	G404	R465	V524
K225	G406	I346	R405	S466	V525
G226	D286	M347	G407	M467	K526
V227	I288	M348	S407	F468	E527
K228	Q289	W349	H408	V469	
K229	Q290	A350	L409	G470	
L230	R291	A351	T410	T471	
G231	G292	D352	M411	R472	
T232	G293	S353	P412	K473	
Q233	Q294	L354	M413	G474	
S234	I295	P355	N415	L475	
E235	V296	S356	G416	D476	
V236	I297	D357	M417	W477	
N237	G298	A358	D418	D478	
S238	T299	W359	Q419	M479	
N239	L300	R360	F420	R480	

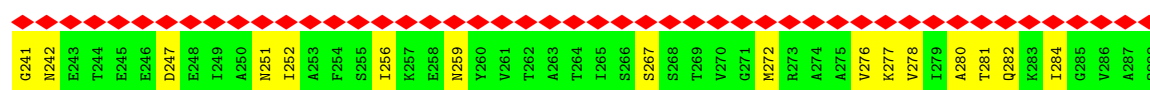
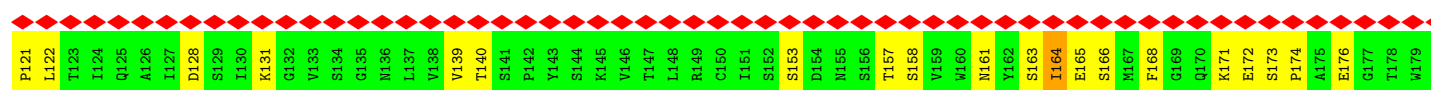
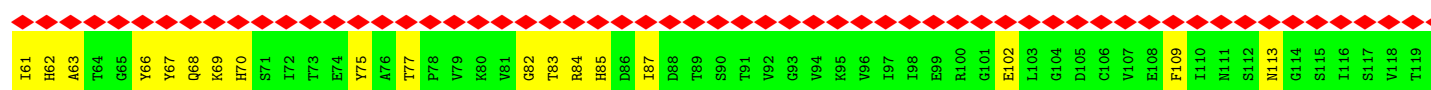
• Molecule 1: gp12, short tail fiber protein



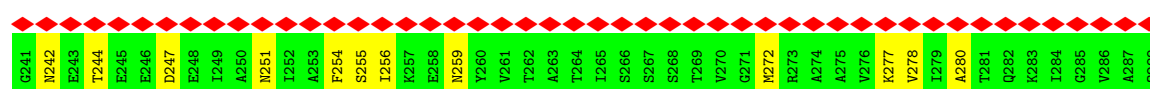
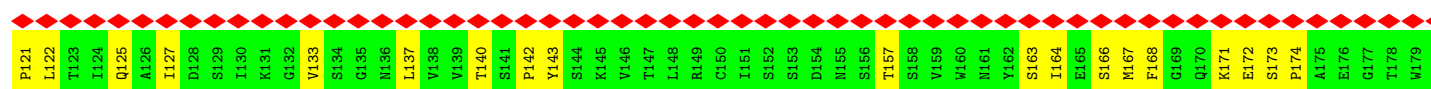
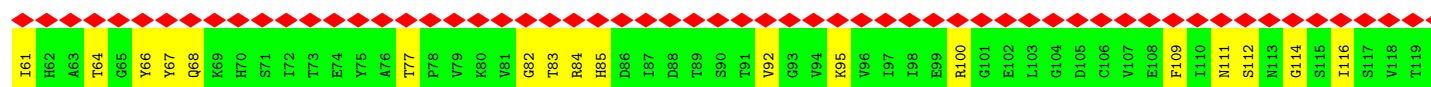
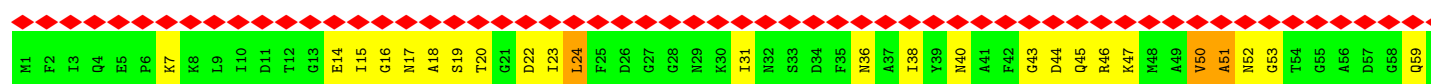
RET	S2	P61	F121	T181	A241	R301	F361
S3	E63	T62	T122	T182	S242	I302	C362
N4	Q64	E63	V123	A183	V243	E303	H363
T5	E65	Q64	A124	T184	A244	D304	G364
Y6	V66	E65	L125	E185	V245	F305	T366
Q7	I67	V66	N126	S186	T246	T307	V367
H8	D68	I67	N127	D187	G247	I308	S368
V9	G69	D68	A128	Q188	A248	A309	A369
S10	T70	G69	F129	G189	T249	N310	S370
N11	T71	T70	E130	V190	L250	G311	D371
E12	N72	N71	T131	V191	N251	G312	C372
S13	T73	N72	R132	Q192	G252	A313	F373
R14	K74	T73	V133	L193	R253	A314	L374
Y15	A75	K74	S134	A194	G254	I315	Y375
V16	A76	A75	T135	T195	S255	T316	A376
K17	V76	V76	E136	V196	T256	G317	S377
F18	T77	T77	S137	A197	T257	T318	R378
D19	P78	P78	S138	Q198	T258	V319	I379
P20	A79	A79	N139	V199	K259	R320	G380
T21	T80	T80	G140	R200	R260	M321	T381
D22	L81	L81	V141	Q201	G261	T322	V262
T23	A82	A82	I142	G202	V262	G323	V263
N24	T83	T83	K143	T203	V263	G324	K264
F25	R84	R84	I144	L204	K264	Y325	L265
P26	L85	L85	S145	R205	L265	I326	T266
P27	S86	S86	S146	E206	T266	Q327	P387
E28	Y87	Y87	L147	G207	T267	G328	S388
I29	P88	P88	P148	Y208	T268	N329	N389
T30	N89	N89	Q149	A209	A269	R330	P390
D31	A90	A90	A150	I210	G270	I331	G391
V32	T91	T91	L151	S211	S271	T332	L392
Q33	E92	E92	A152	P212	Q272	T333	P393
A34	T93	T93	G153	Y213	G273	Q334	D394
A35	V94	V94	A154	T214	G274	N335	M395
I36	Y95	Y95	D155	F215	G275	E336	M396
A37	G96	G96	D156	H216	D276	I337	R396
A38	L97	L97	T157	M217	A277	D338	G397
I39	T98	T98	T158	S218	S278	R339	L398
S40	R99	R99	A159	S219	S279	T340	F399
P41	Y100	Y100	M160	S220	A280	I341	V400
A42	S101	S101	T161	T221	L281	P342	R401
Q43	T102	T102	P162	E222	A282	V343	G402
V44	M103	M103	L163	E223	W283	G344	S403
N45	D104	D104	K164	Y224	N284	A345	G404
G46	E105	E105	T165	K225	A285	R405	R405
V47	A106	A106	Q166	G226	G406	I346	G406
P48	I107	I107	Q167	V227	D286	M347	S407
D49	A108	A108	L168	I228	I288	M348	H408
A50	G109	G109	A169	K229	Q289	W349	L409
S51	V110	V110	I170	L230	Q290	A350	T410
S52	N111	N111	K171	G231	R291	A351	M411
T53	N112	N112	L172	T232	G292	D352	P412
T54	E113	E113	I173	Q233	G293	S353	M413
K55	S114	S114	A174	S234	Q294	L354	V414
G56	S115	S115	Q175	E235	I295	P355	N415
L58	I116	I116	T176	V236	I296	S356	G416
F59	P117	P117	A177	N237	I297	D357	M417
L60	A119	A119	S179	S238	G298	A358	D418
	E180	E180		N239	T299	W359	Q419
					L300	R360	F420



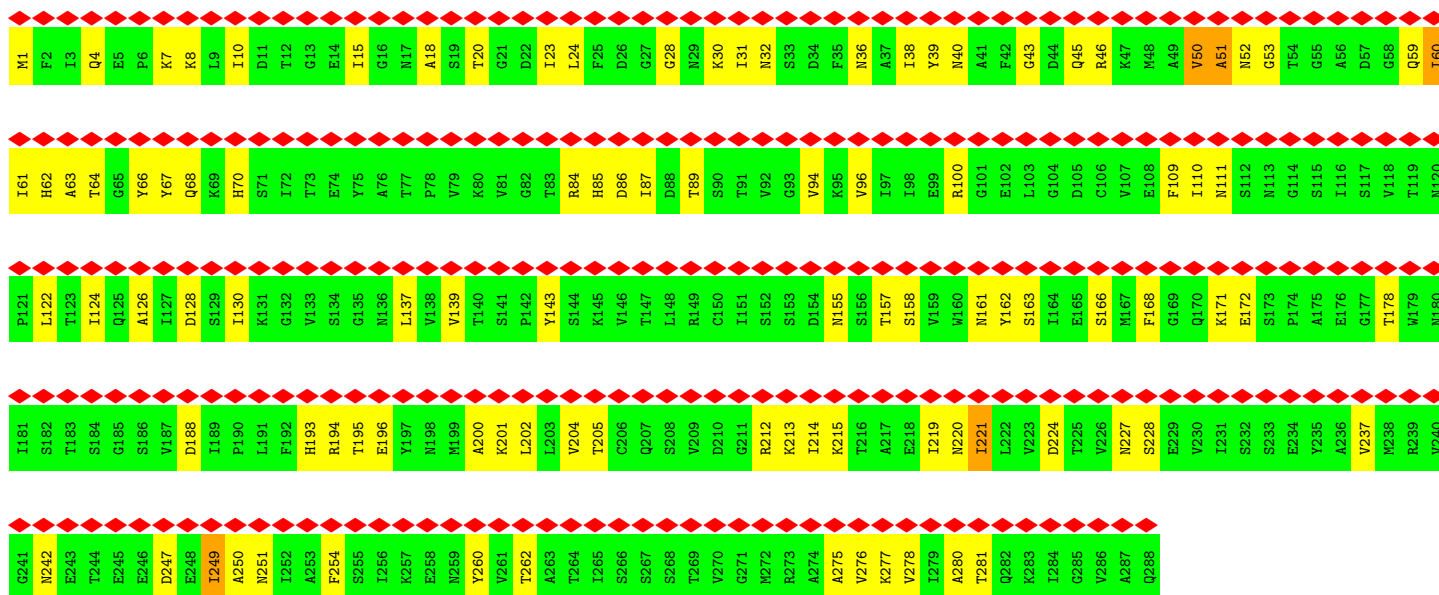
• Molecule 2: gp9, baseplate wedge tail fiber connector



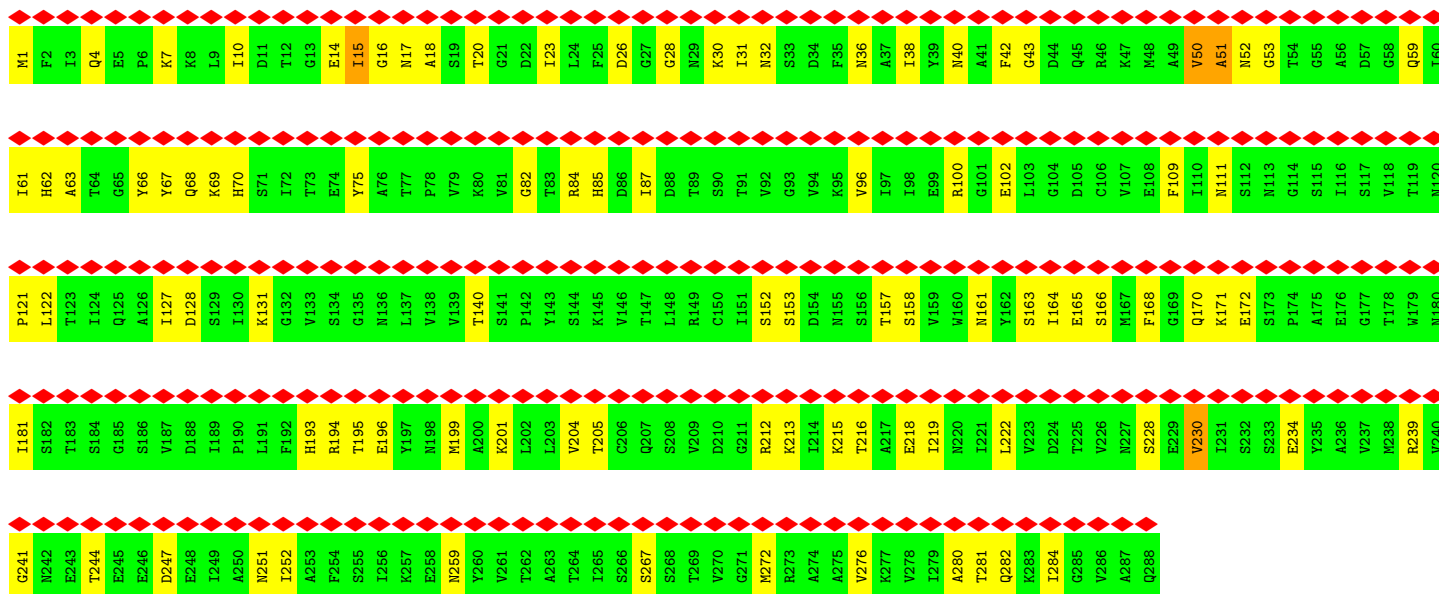
• Molecule 2: gp9, baseplate wedge tail fiber connector



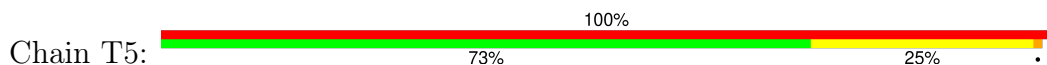
- Molecule 2: gp9, baseplate wedge tail fiber connector

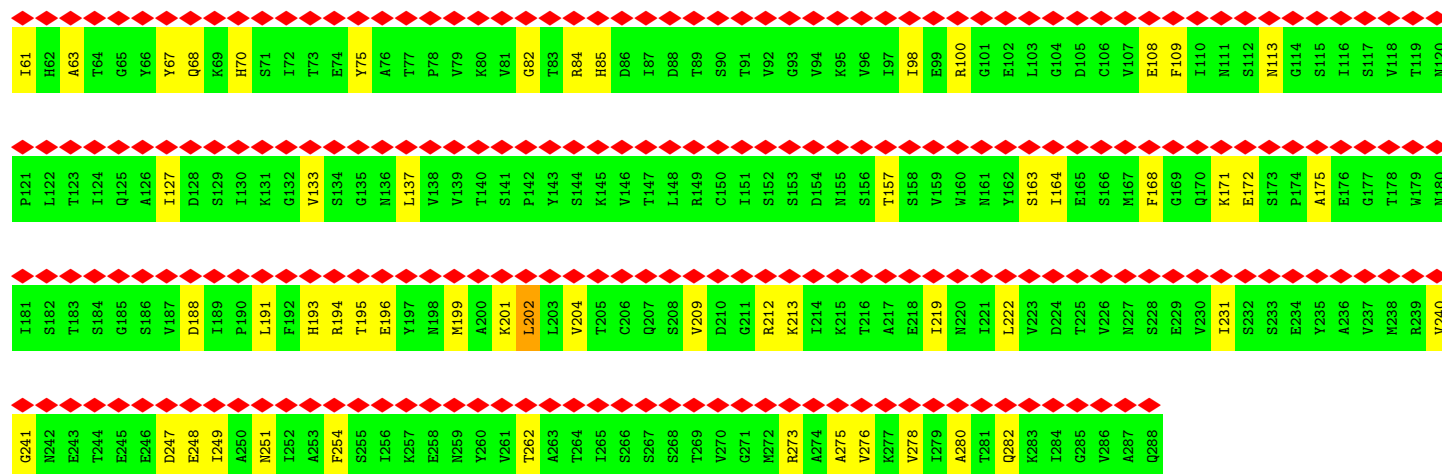


- Molecule 2: gp9, baseplate wedge tail fiber connector

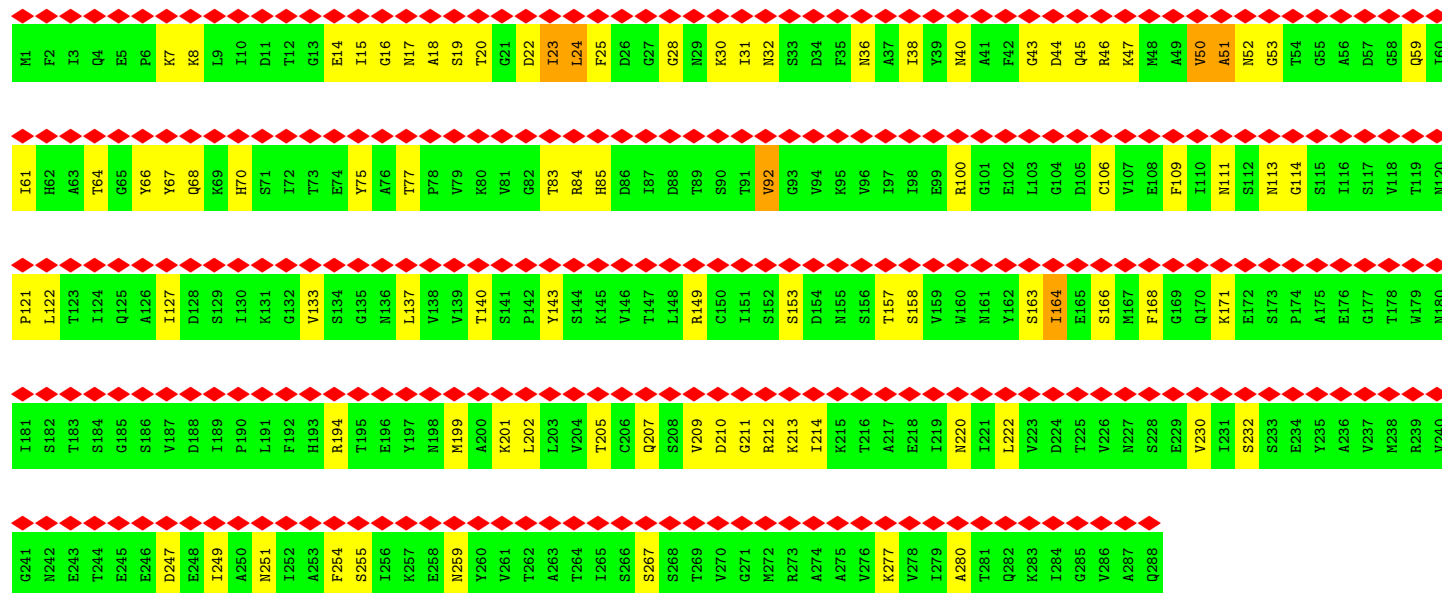


- Molecule 2: gp9, baseplate wedge tail fiber connector

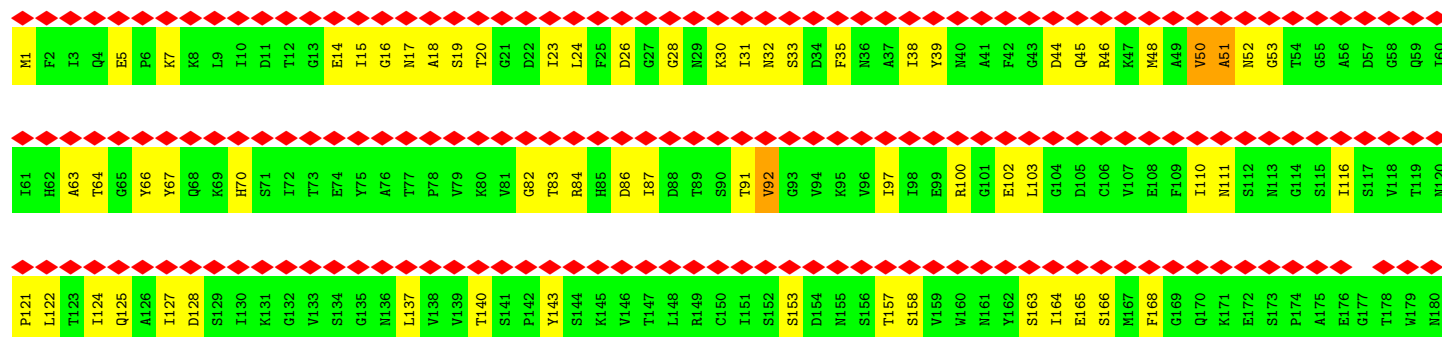


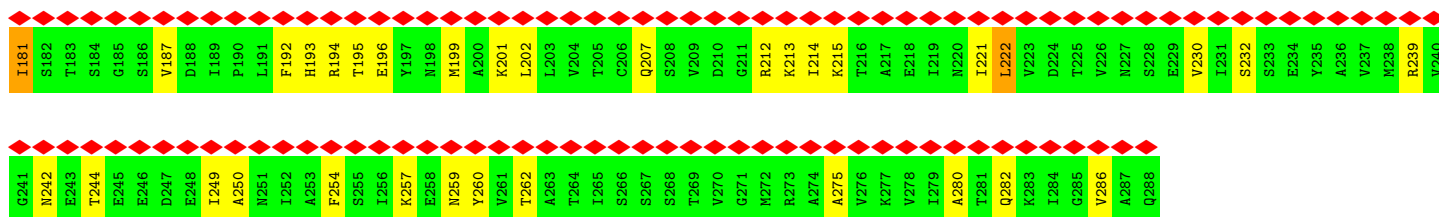


- Molecule 2: gp9, baseplate wedge tail fiber connector

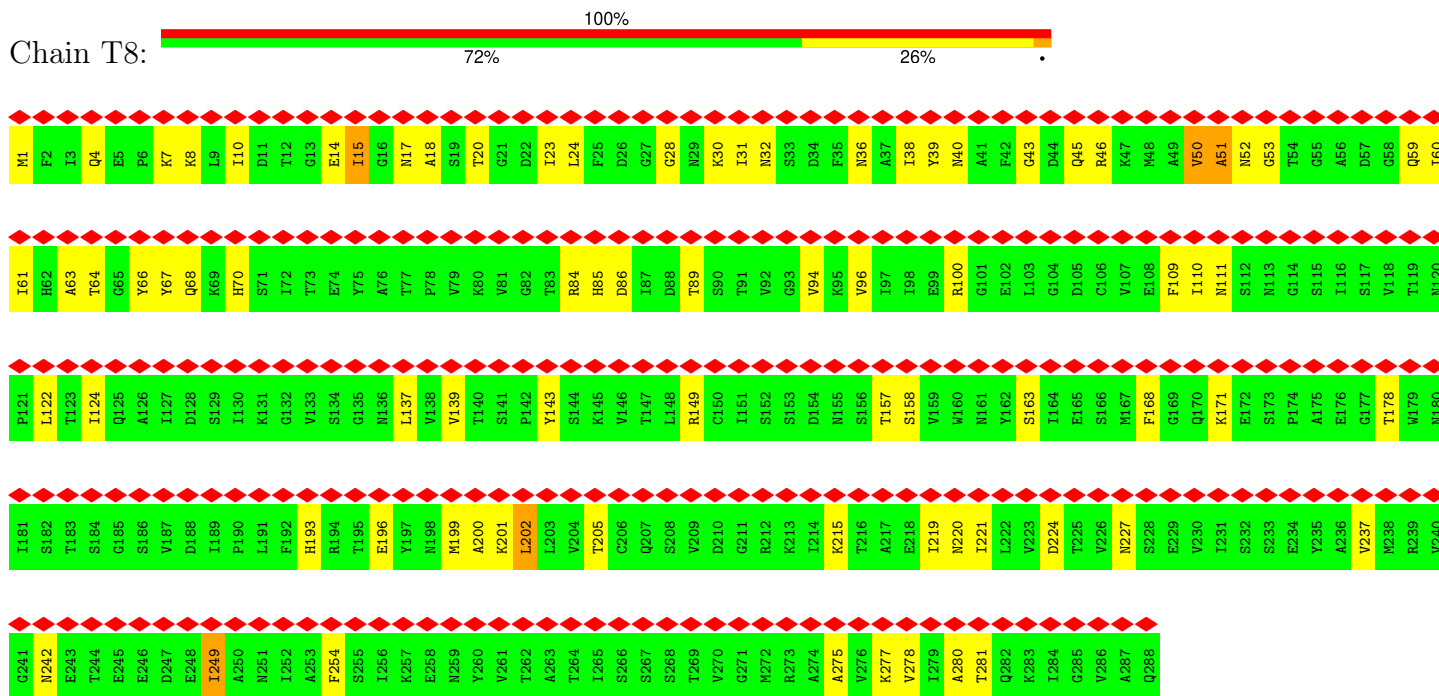


- Molecule 2: gp9, baseplate wedge tail fiber connector

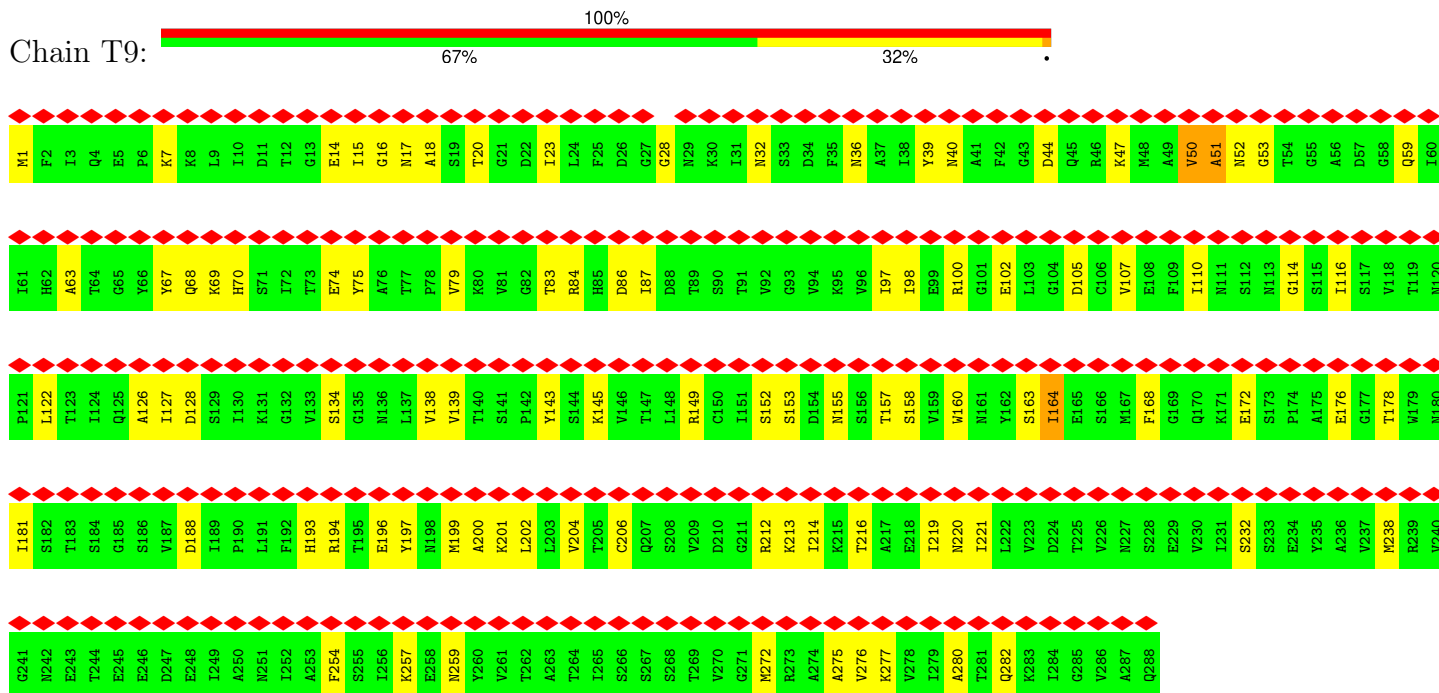




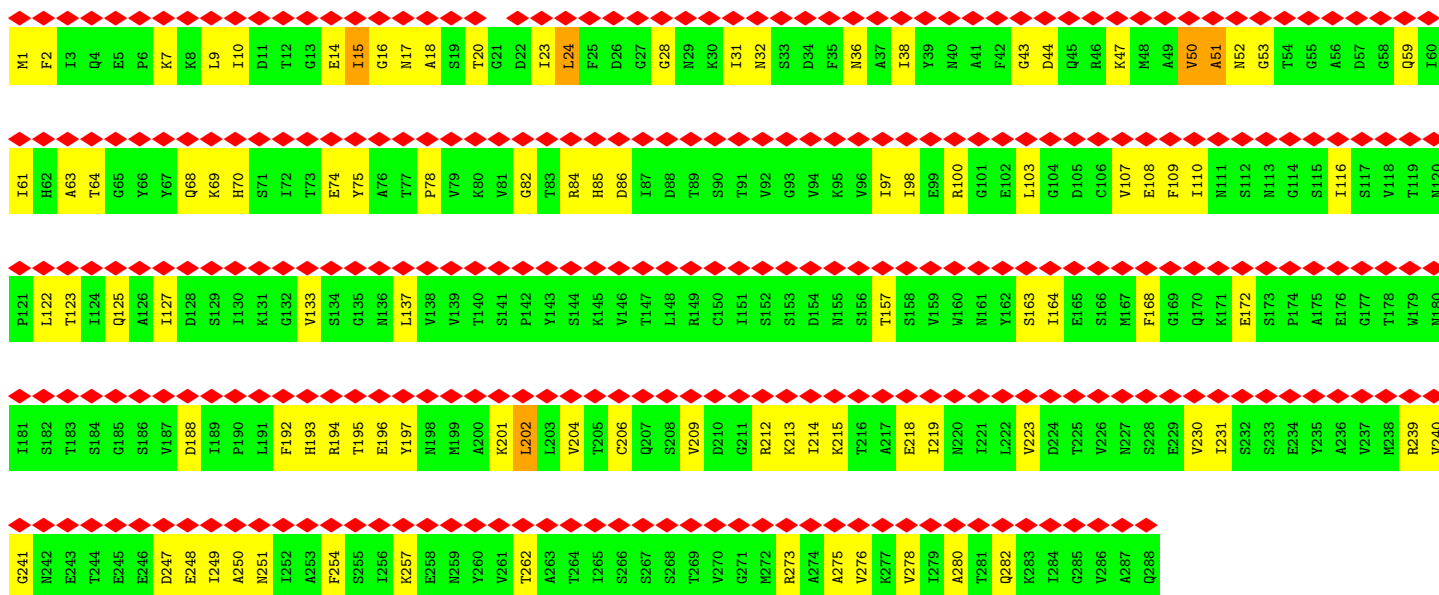
- Molecule 2: gp9, baseplate wedge tail fiber connector



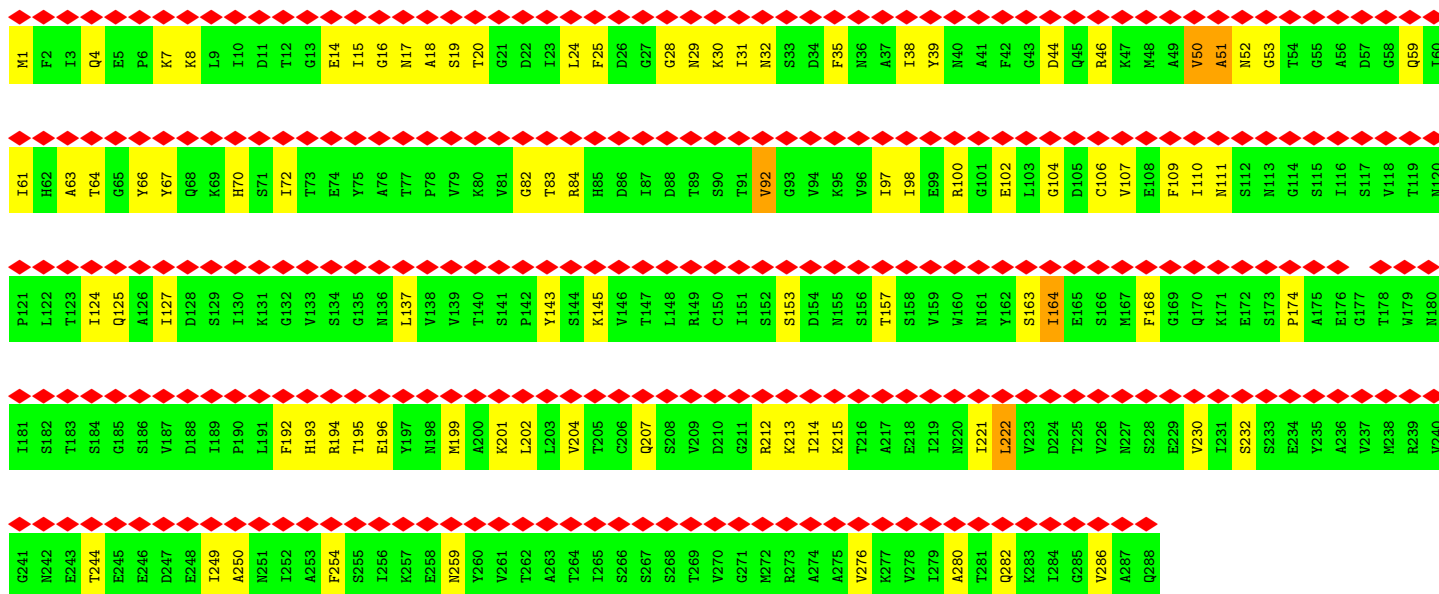
- Molecule 2: gp9, baseplate wedge tail fiber connector



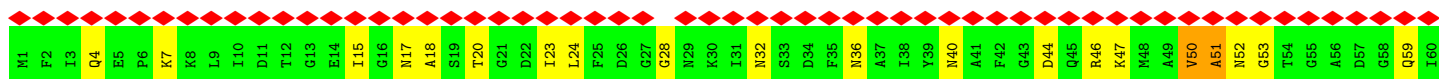
- Molecule 2: gp9, baseplate wedge tail fiber connector

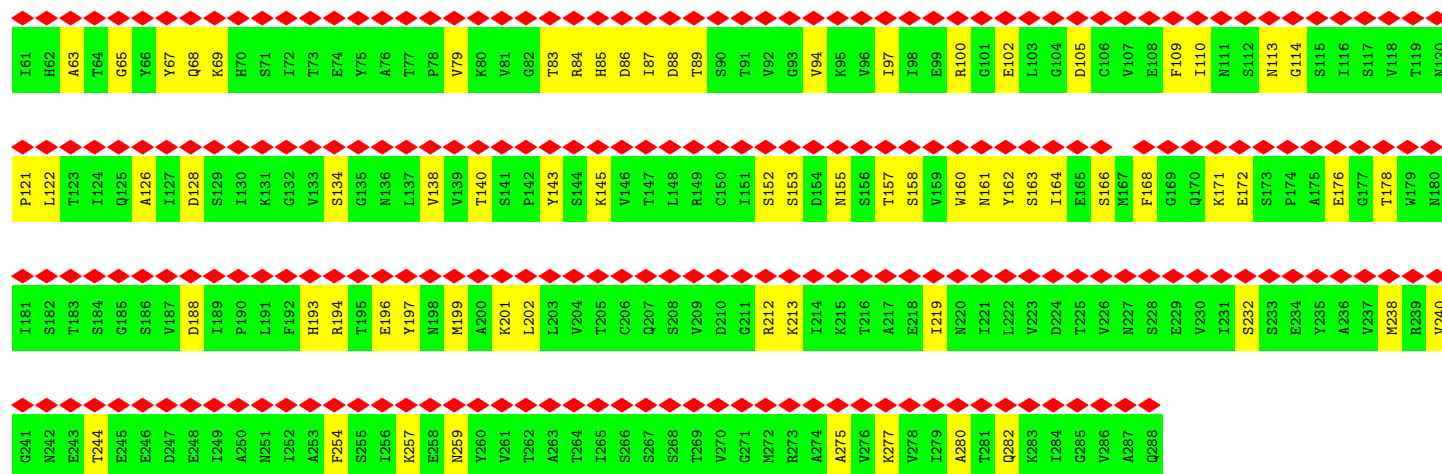


- Molecule 2: gp9, baseplate wedge tail fiber connector

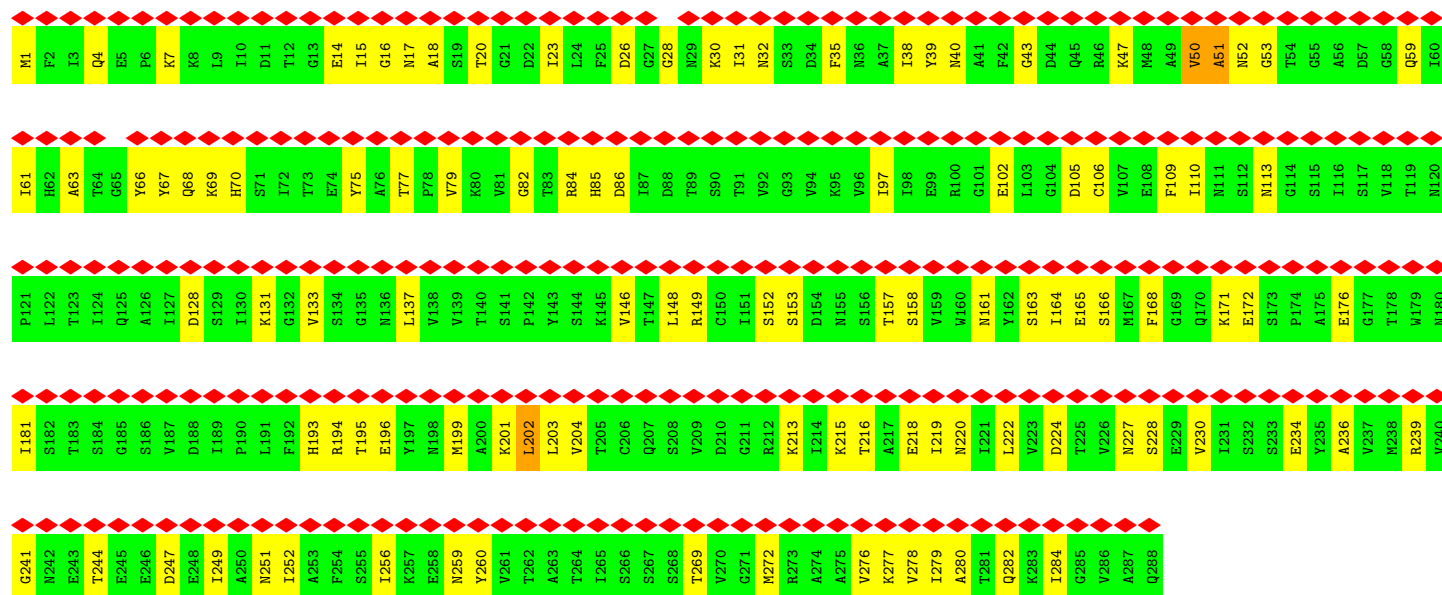


- Molecule 2: gp9, baseplate wedge tail fiber connector

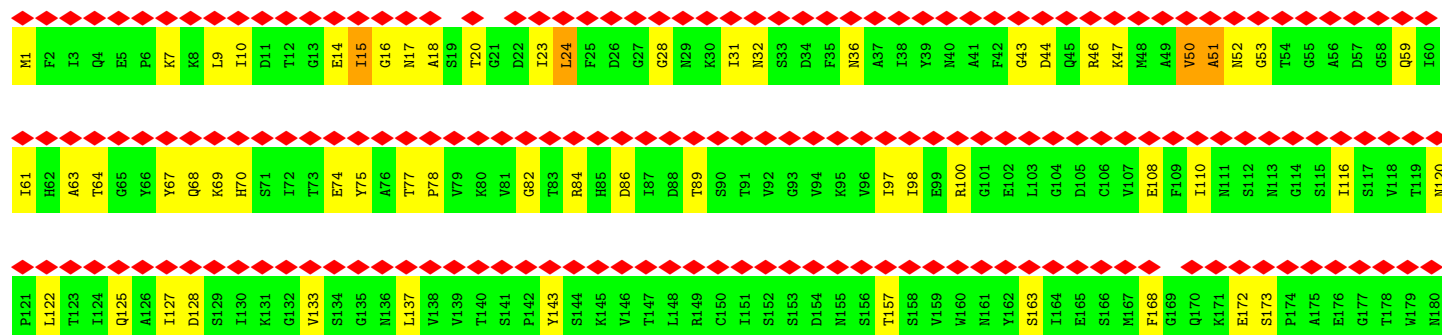




- Molecule 2: gp9, baseplate wedge tail fiber connector



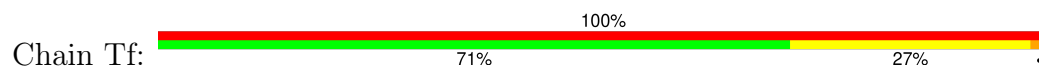
- Molecule 2: gp9, baseplate wedge tail fiber connector



I181	S182	T183	S184	G185	S186	V187	D188	I189	P190	L191	F192	H193	R194	T195	E196	Y197	N198	M199	A200	K201	L202	L203	V204	T205	C206	Q207	S208	V209	D210	G211	R212	K213	I214	K215	T216	A217	E218	I219	N220	I221	L222	V223	D224	T225	V226	N227	S228	E229	V230	I231	S232	S233	E234	Y235	A236	V237	M238	R239	V240
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G241	N242	E243	T244	E245	E246	D247	E248	I249	A250	N251	I252	A253	F254	S255	I256	K257	E258	N259	Y260	V261	T262	A263	T264	I265	S266	S267	S268	T269	V270	G271	M272	R273	A274	A275	V276	K277	V278	I279	A280	T281	Q282	K283	I284	G285	V286	A287	Q288
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- Molecule 2: gp9, baseplate wedge tail fiber connector



M1	F2	I3	Q4	E5	P6	K7	K8	L9	I10	D11	T12	G13	E14	I15	G16	M17	A18	S19	Y20	G21	D22	I23	L24	F25	D26	G27	G28	M29	K30	I31	N32	S33	D34	F35	N36	A37	I38	Y39	N40	A41	F42	G43	D44	Q45	R46	K47	M48	A49	V50	A51	N52	G53	T54	G55	A56	D57	G58	Q59	I60
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I61	H62	A63	T64	G65	Y66	Y67	Q68	K69	H70	S71	I72	T73	E74	Y75	A76	T77	P78	V79	K80	W81	G82	T83	R84	H85	D86	I87	D88	T89	S90	T91	V92	G93	V94	K95	V96	I97	I98	E99	R100	G101	E102	L103	G104	D105	C106	V107	E108	F109	I110	N111	S112	N113	G114	S115	T116	S117	V118	T119	N120
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I181	S182	T183	S184	G185	S186	V187	D188	I189	P190	L191	F192	H193	R194	T195	E196	Y197	N198	M199	A200	K201	L202	L203	V204	T205	C206	Q207	S208	V209	D210	G211	R212	K213	I214	K215	T216	A217	E218	I219	N220	I221	L222	V223	D224	T225	V226	N227	S228	E229	V230	I231	S232	S233	E234	Y235	A236	V237	M238	R239	V240
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G241	N242	E243	T244	E245	E246	D247	E248	I249	A250	N251	I252	A253	F254	S255	I256	K257	E258	N259	Y260	V261	T262	A263	T264	I265	S266	S267	S268	T269	V270	G271	M272	R273	A274	A275	V276	K277	V278	I279	A280	T281	Q282	K283	I284	G285	V286	A287	Q288
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- Molecule 2: gp9, baseplate wedge tail fiber connector



M1	F2	I3	Q4	E5	P6	K7	K8	L9	I10	D11	T12	G13	E14	I15	G16	M17	A18	S19	Y20	G21	D22	I23	L24	F25	D26	G27	G28	N29	K30	I31	N32	S33	D34	F35	N36	A37	I38	Y39	N40	A41	F42	G43	D44	Q45	R46	K47	M48	A49	V50	A51	N52	G53	T54	G55	A56	D57	G58	Q59	I60
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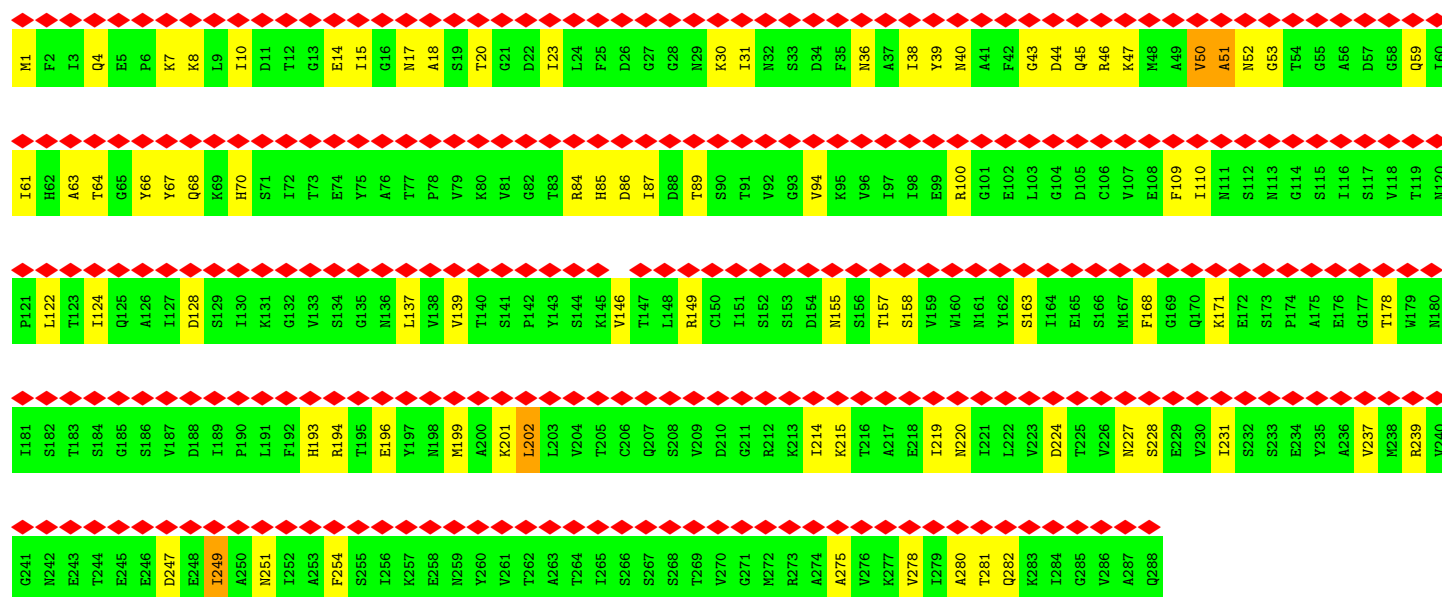
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P121	L122	T123	I124	Q125	A126	I127	D128	S129	I130	K131	G132	V133	S134	G135	N136	L137	V138	V139	T140	S141	P142	Y143	S144	K145	V146	T147	L148	R149	C150	I151	S152	S153	D154	N155	S156	I157	S158	V159	W160	N161	Y162	S163	I164	E165	S166	M167	F168	G169	Q170	K171	E172	S173	P174	A175	E176	G177	T178	W179	N180
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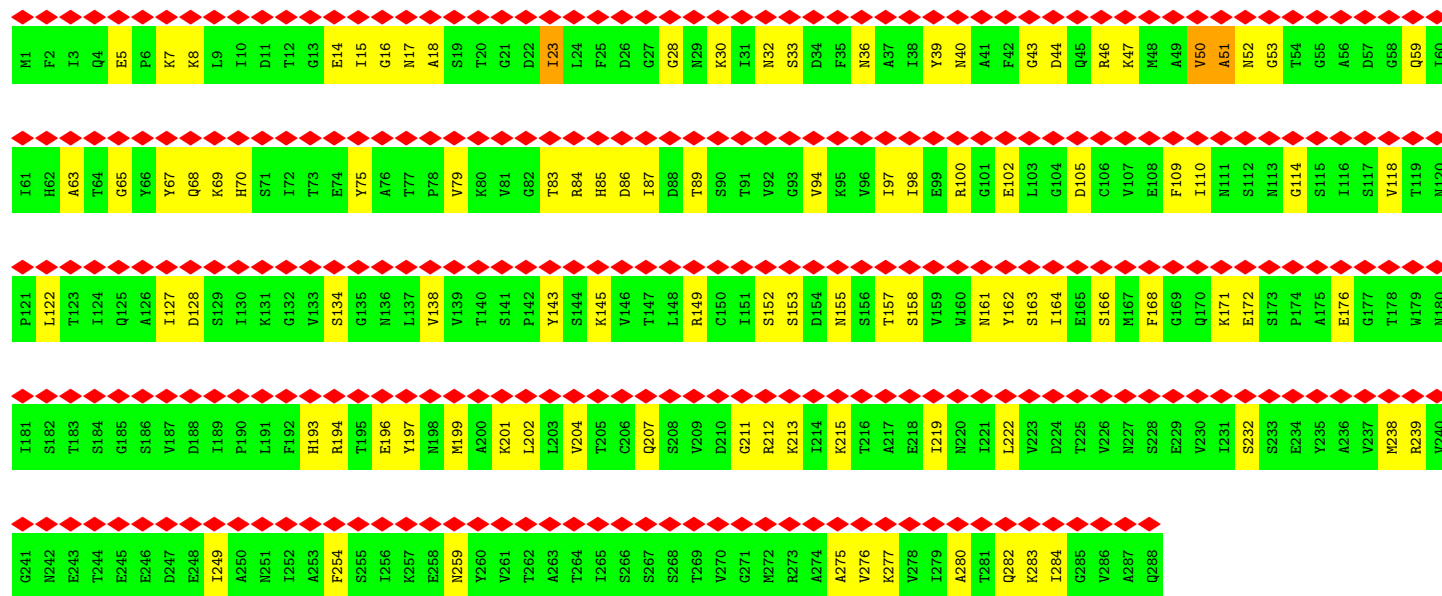
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G241	N242	E243	T244	E245	E246	D247	E248	I249	A250	N251	I252	A253	F254	S255	I256	K257	E258	N259	Y260	V261	T262	A263	T264	I265	S266	S267	S268	T269	V270	G271	M272	R273	A274	A275	V276	K277	V278	I279	A280	T281	Q282	K283	I284	G285	V286	A287	Q288
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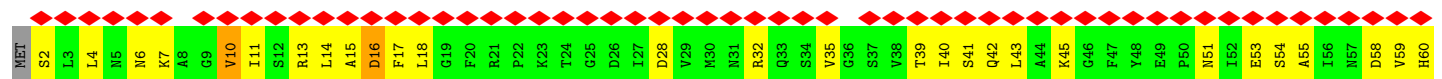
- Molecule 2: gp9, baseplate wedge tail fiber connector

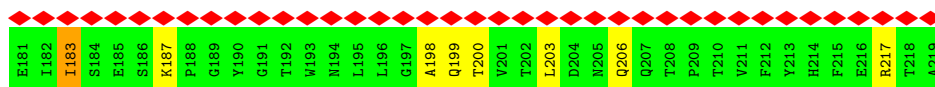
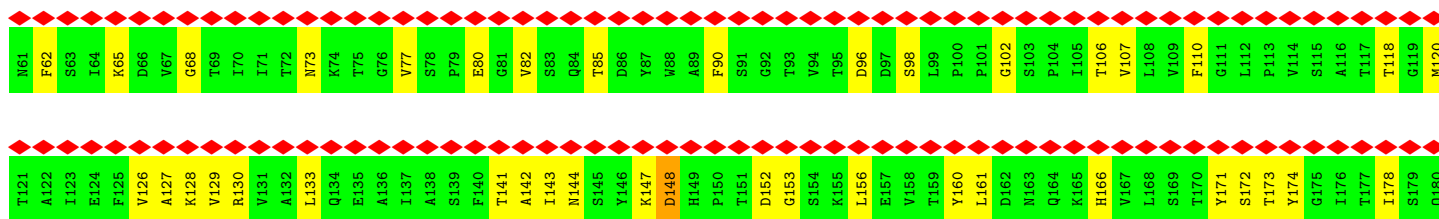


- Molecule 2: gp9, baseplate wedge tail fiber connector

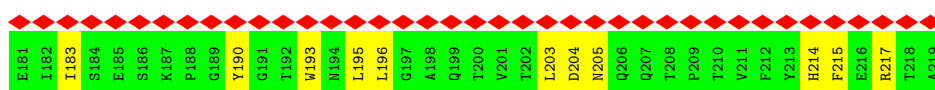
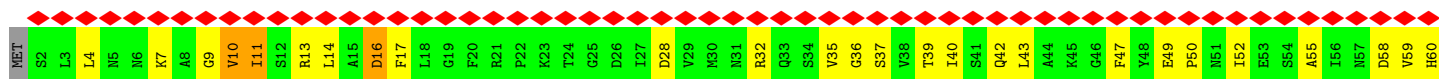


- Molecule 3: gp11, baseplate wedge protein

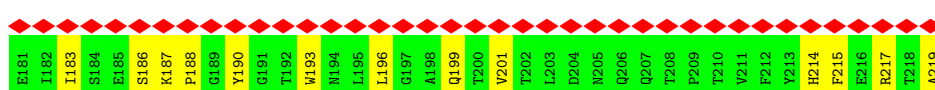
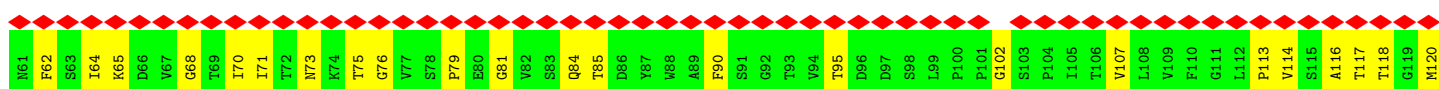




• Molecule 3: gp11, baseplate wedge protein

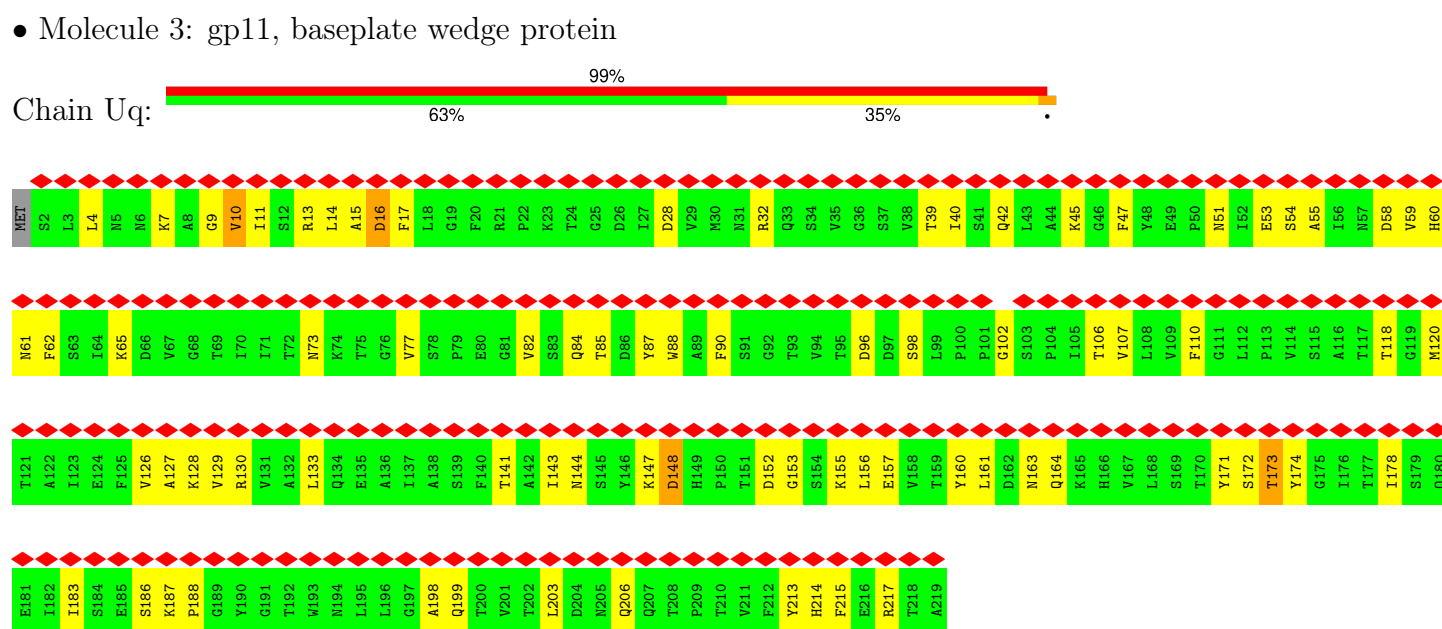
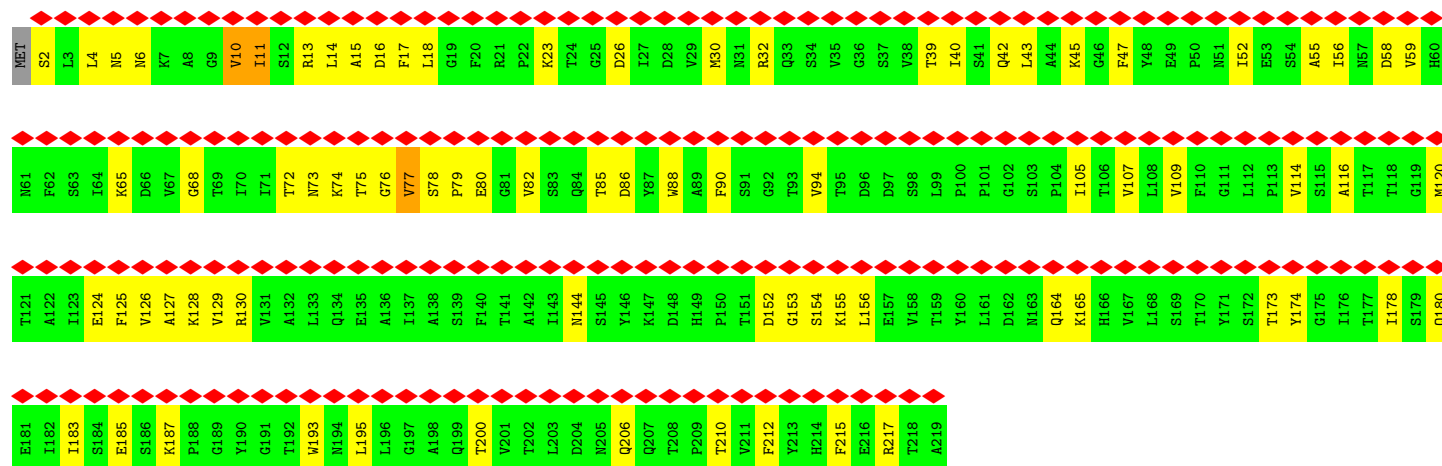


• Molecule 3: gp11, baseplate wedge protein

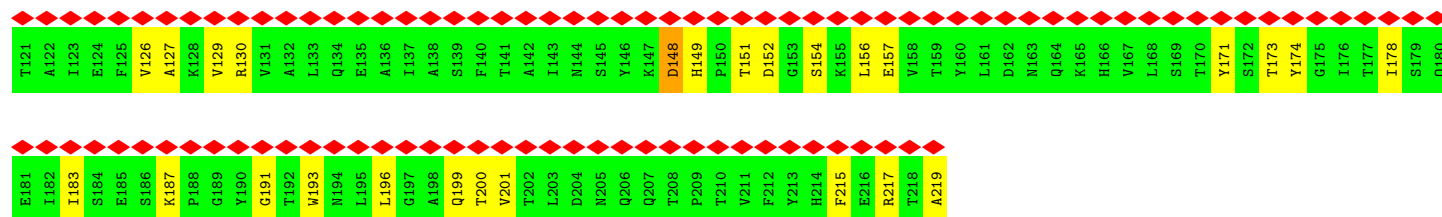


• Molecule 3: gp11, baseplate wedge protein

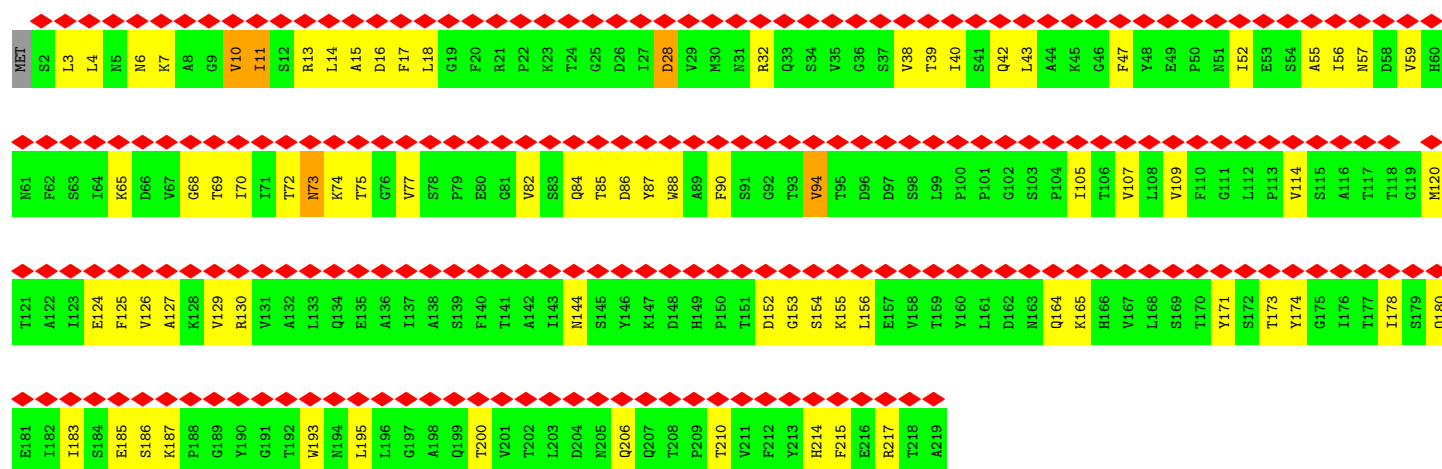




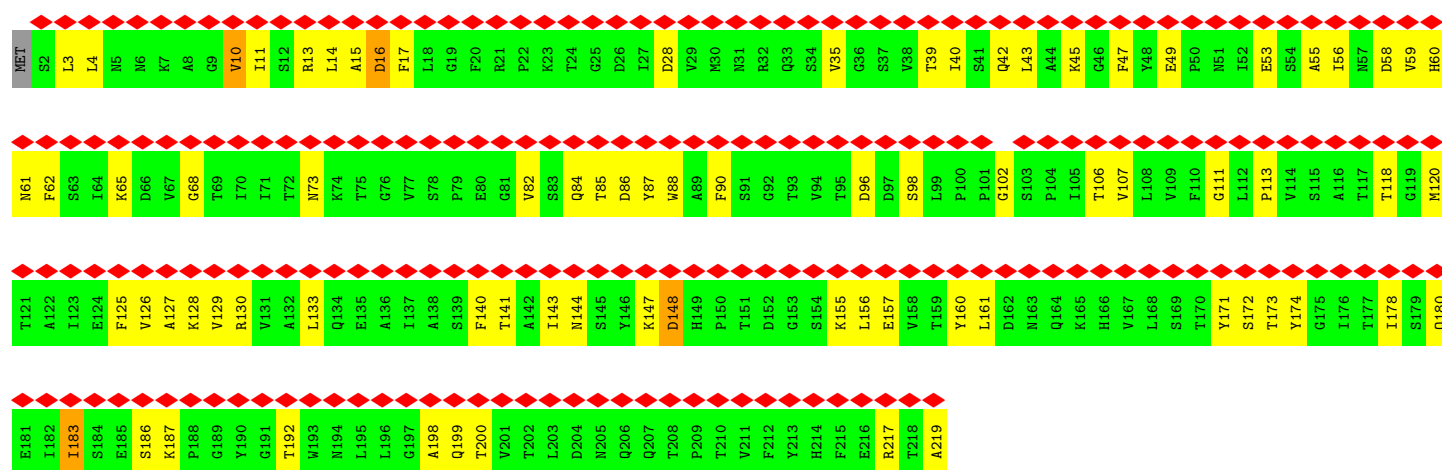
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| | N61 | F62 | S63 | I64 | K65 | D66 | V67 | G68 | T69 | I70 | I71 | T72 | N73 | K74 | T75 | G76 | V77 | S78 | P79 | E80 | G81 | V82 | S83 | Q84 | T85 | D86 | K87 | H88 | A89 | F90 | S91 | G92 | T93 | V94 | T95 | D96 | D97 | S98 | L99 | P100 | P101 | G102 | S103 | P104 | I105 | T106 | V107 | L108 | V109 | F110 | G111 | L112 | P113 | V114 | S115 | A116 | T117 | T118 | G119 | M120 |



• Molecule 3: gp11, baseplate wedge protein

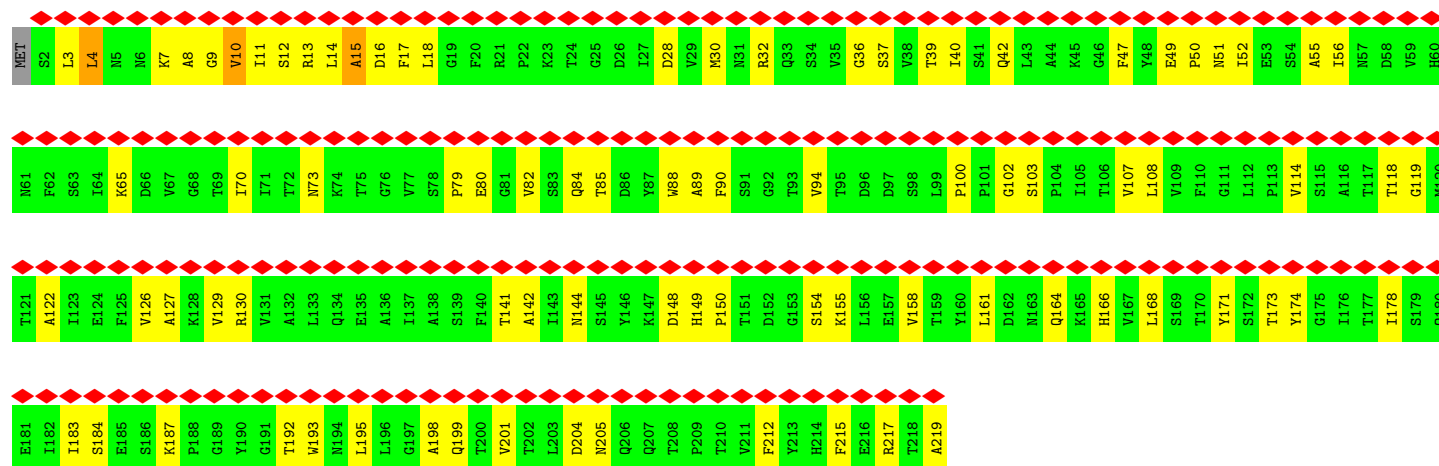


• Molecule 3: gp11, baseplate wedge protein

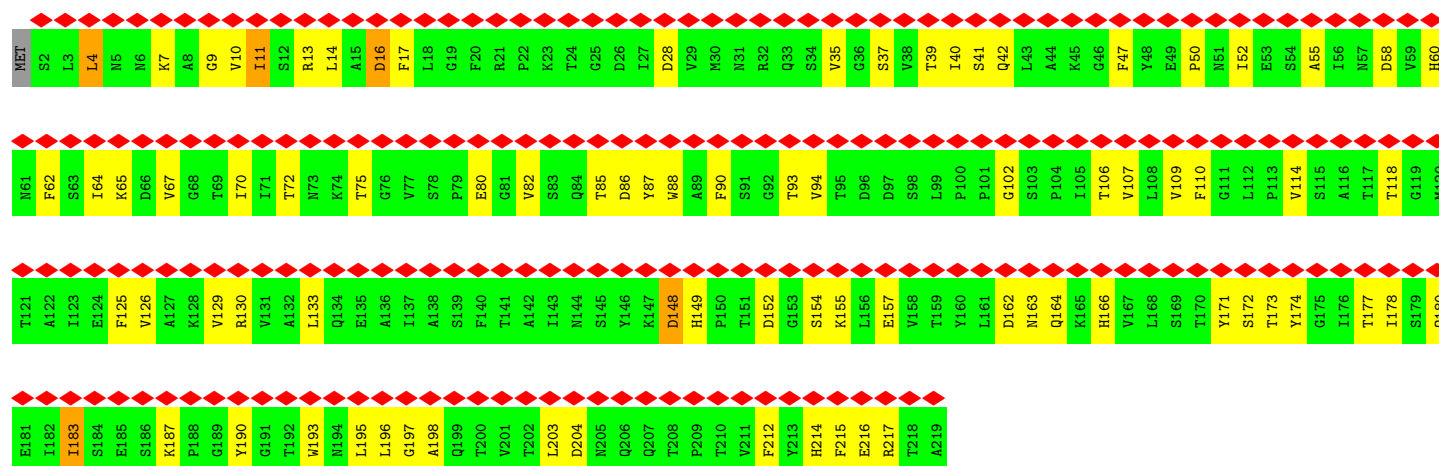


• Molecule 3: gp11, baseplate wedge protein

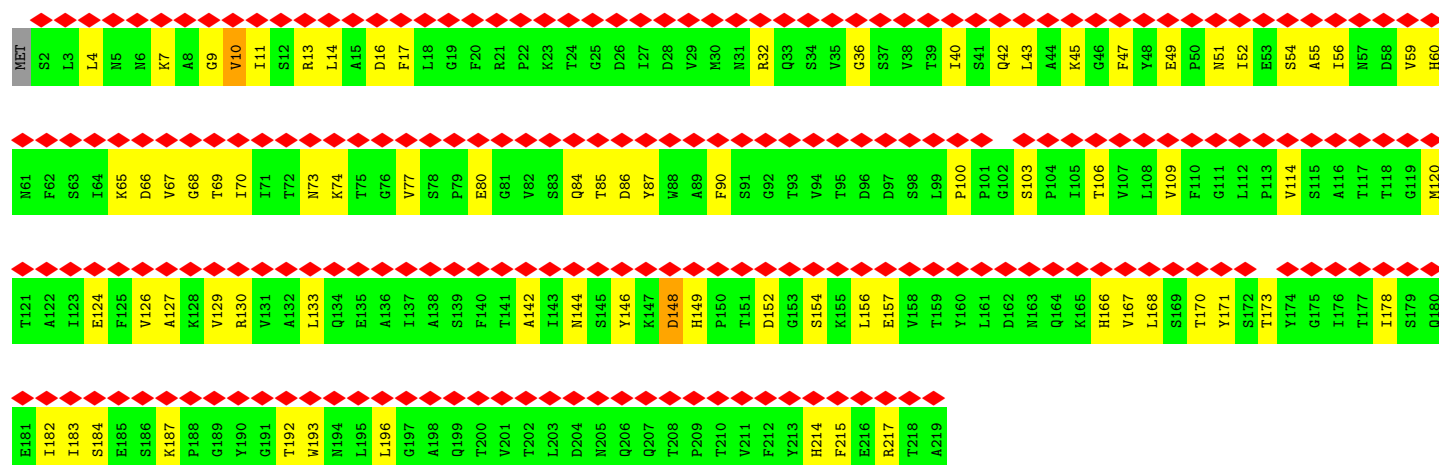




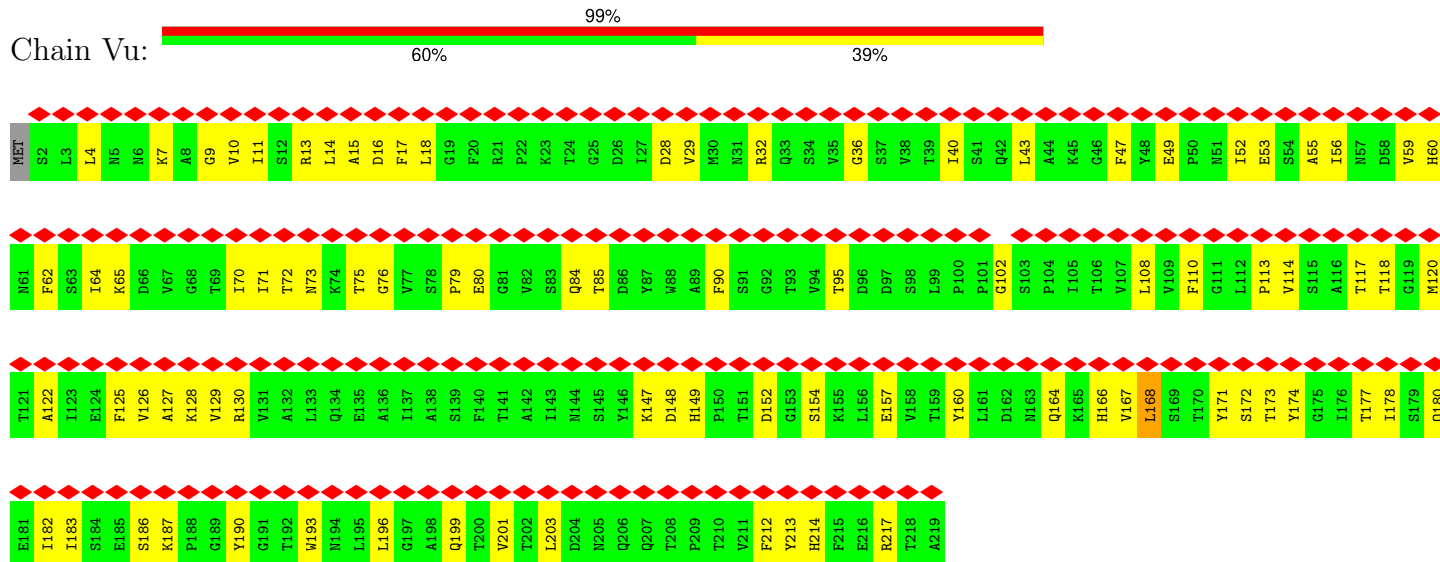
• Molecule 3: gp11, baseplate wedge protein



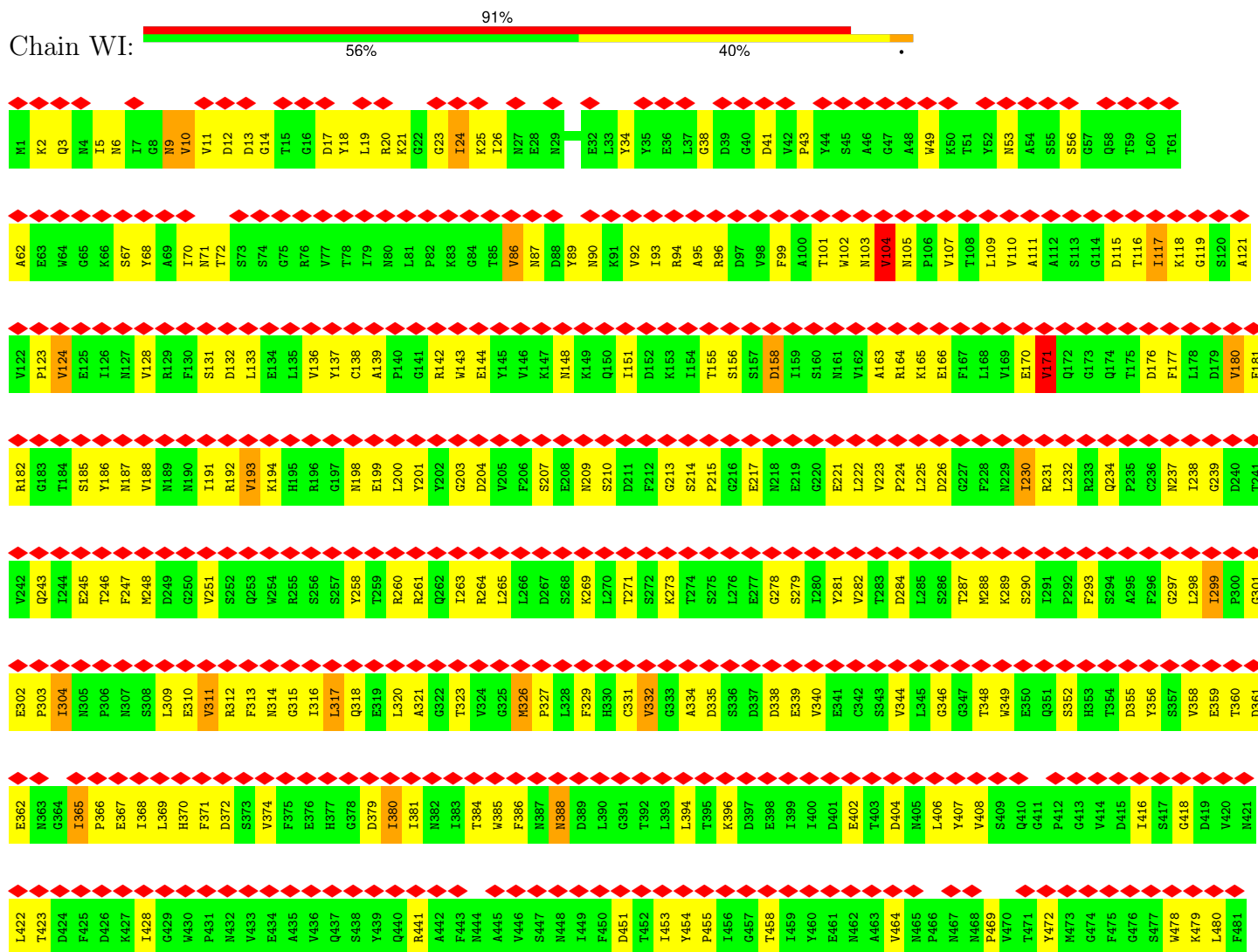
• Molecule 3: gp11, baseplate wedge protein

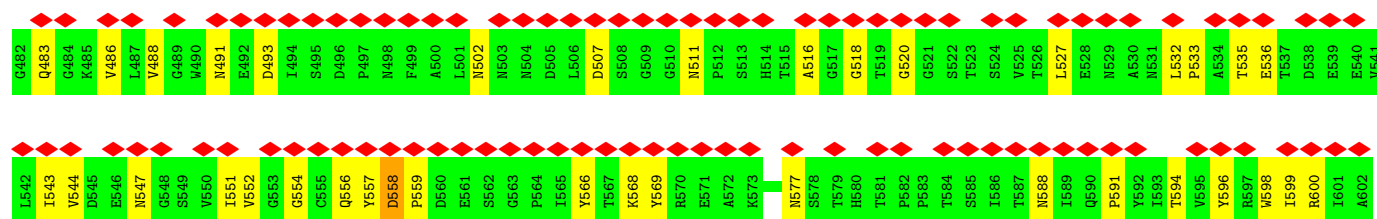


- Molecule 3: gp11, baseplate wedge protein

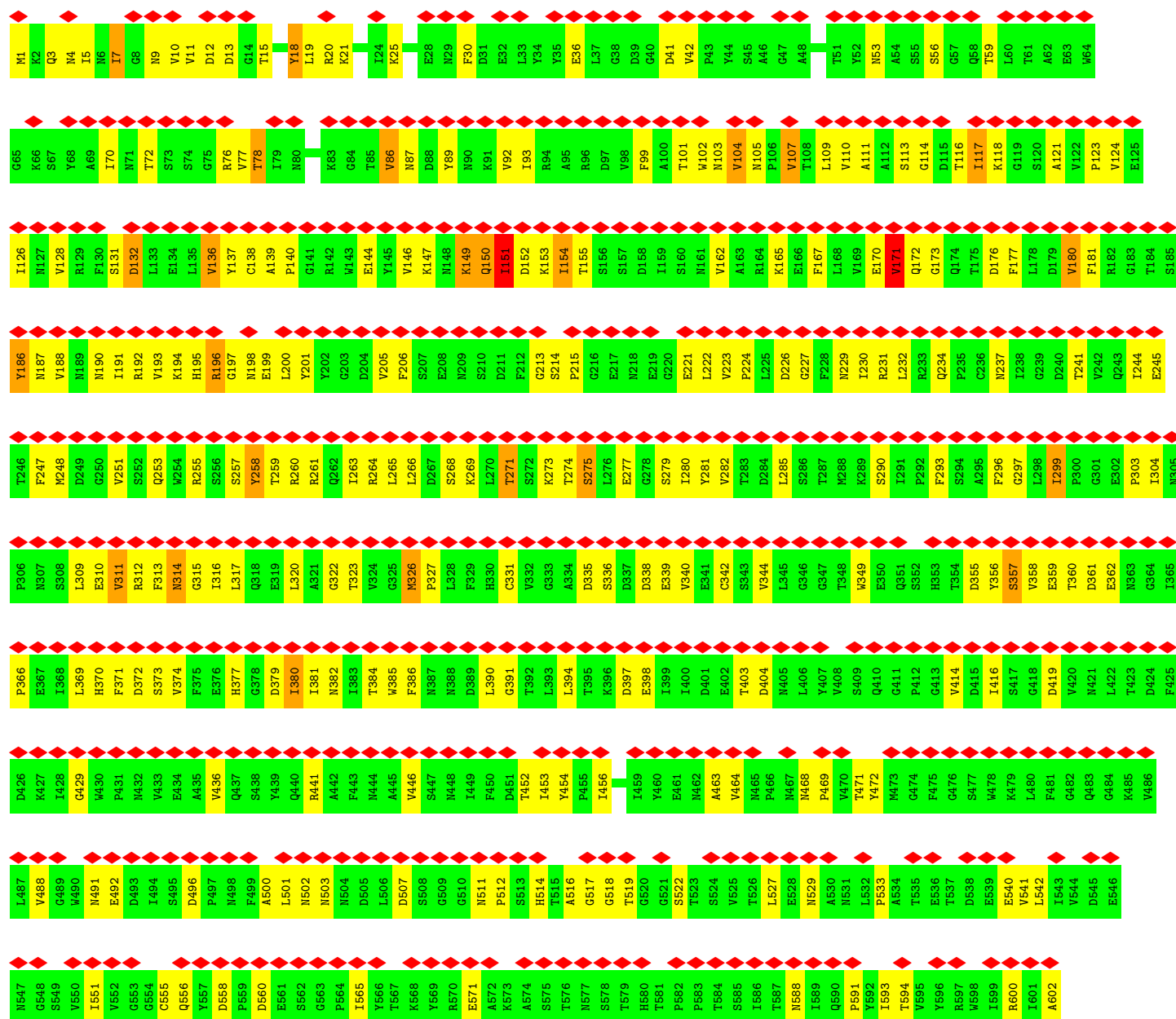
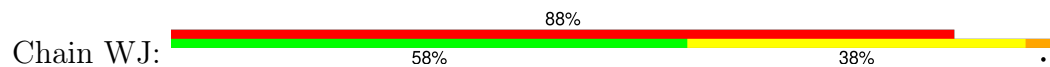


- Molecule 4: gp10, baseplate wedge protein

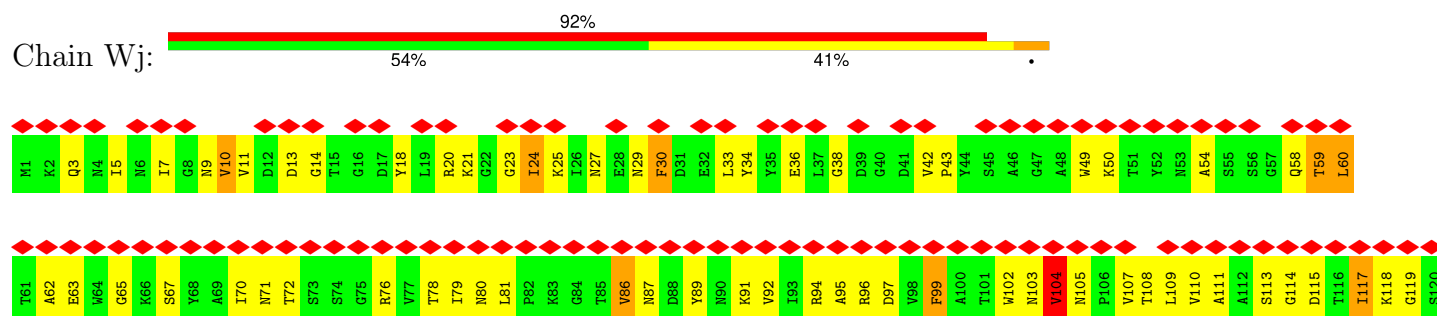
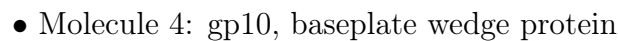


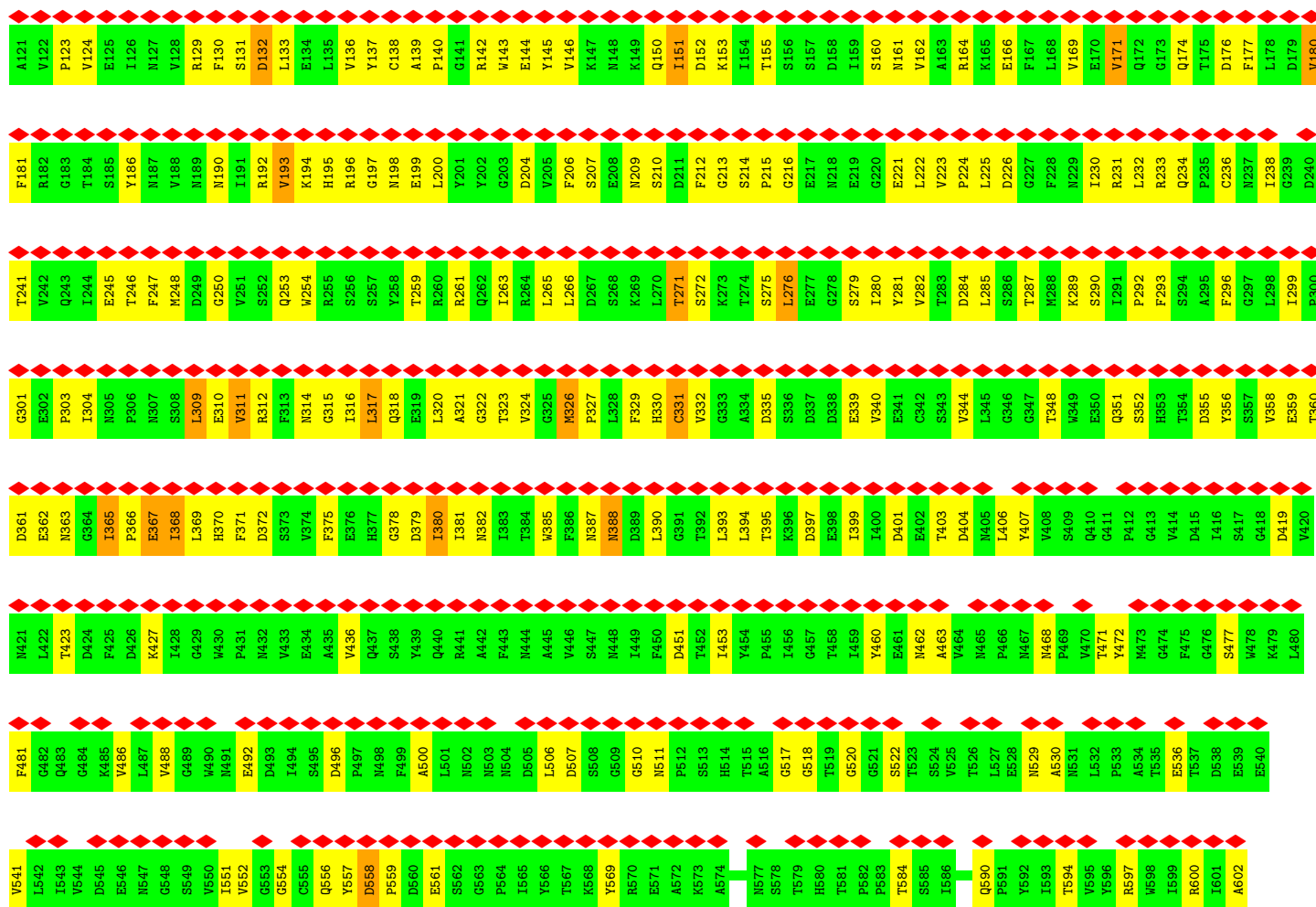


• Molecule 4: gp10, baseplate wedge protein

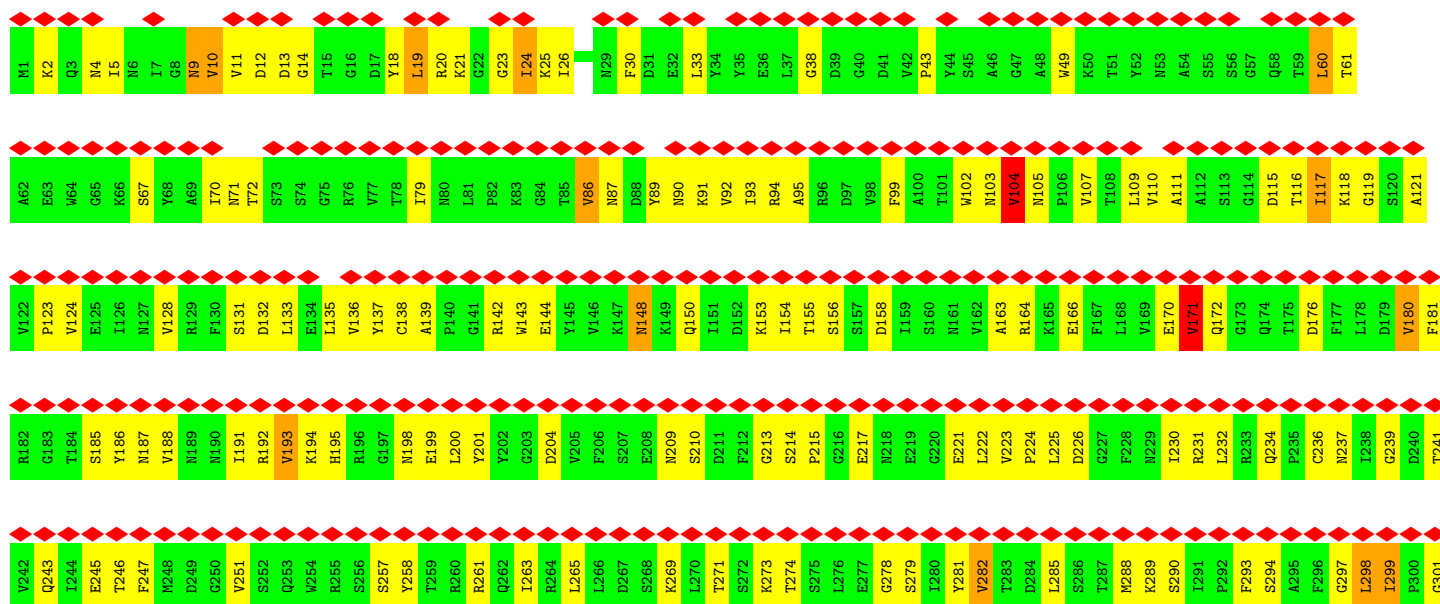


• Molecule 4: gp10, baseplate wedge protein

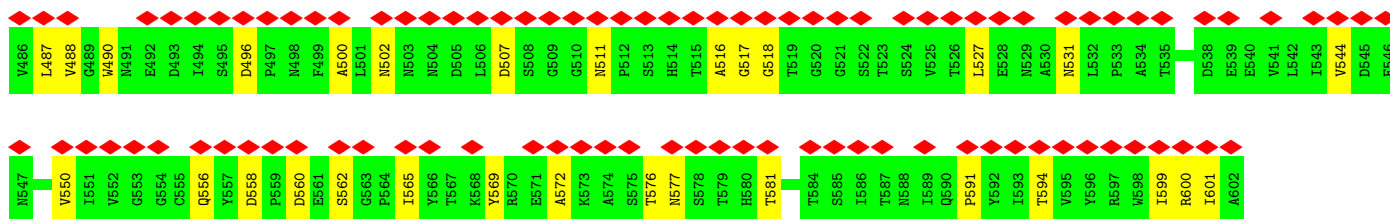




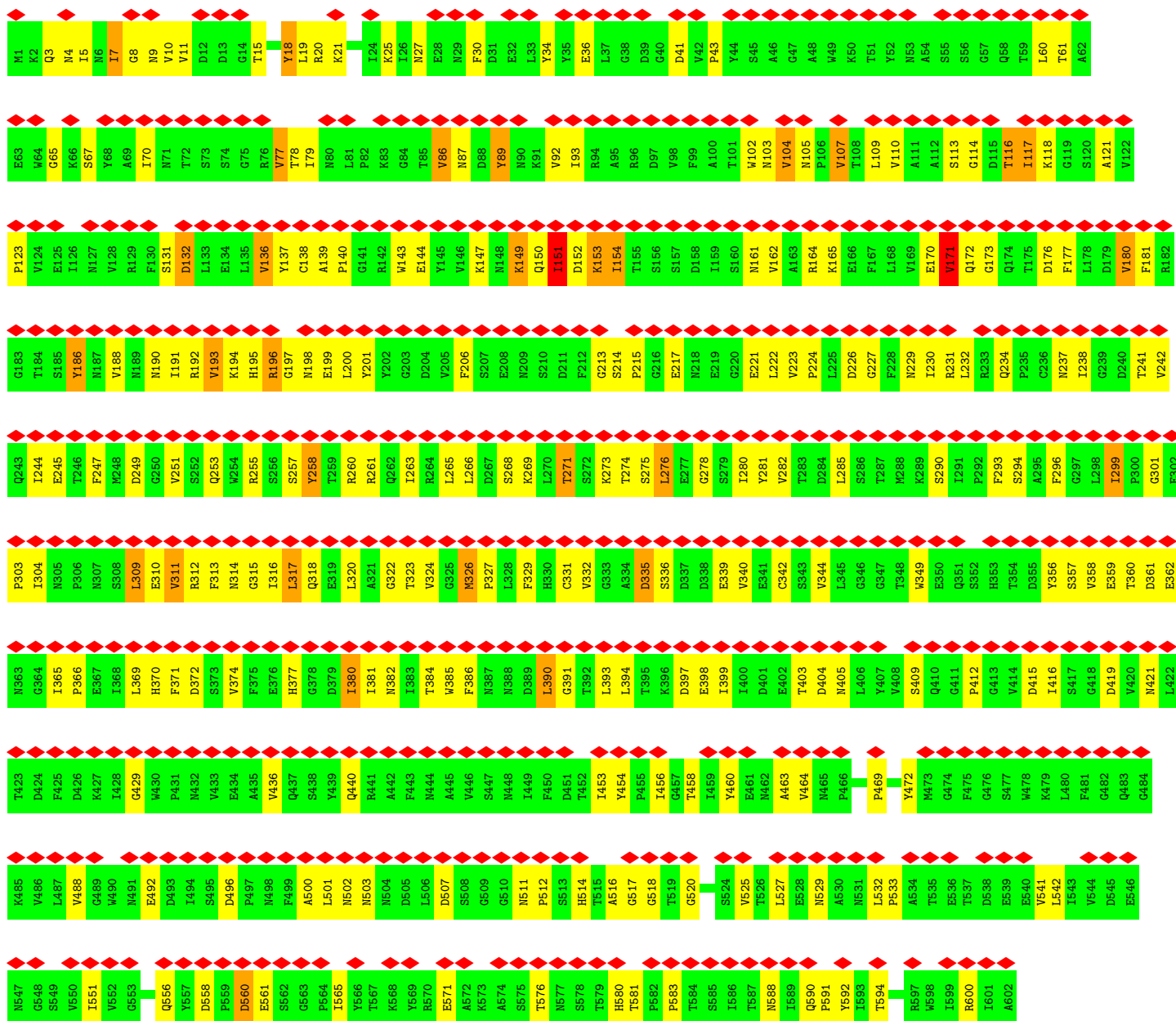
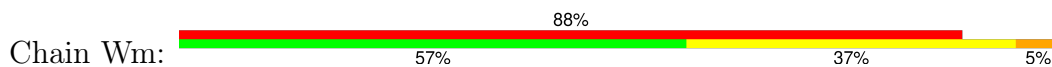
• Molecule 4: gp10, baseplate wedge protein



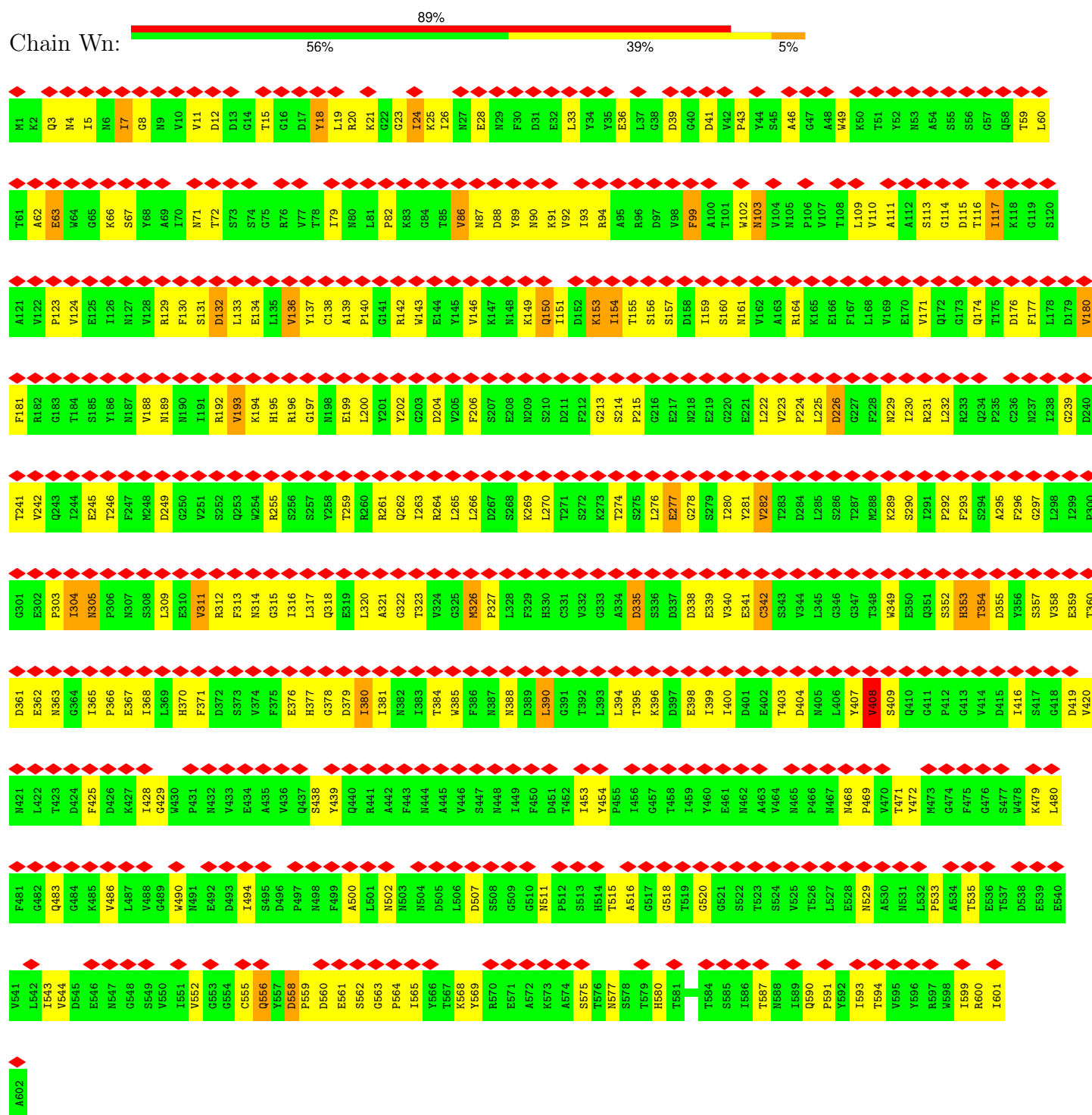




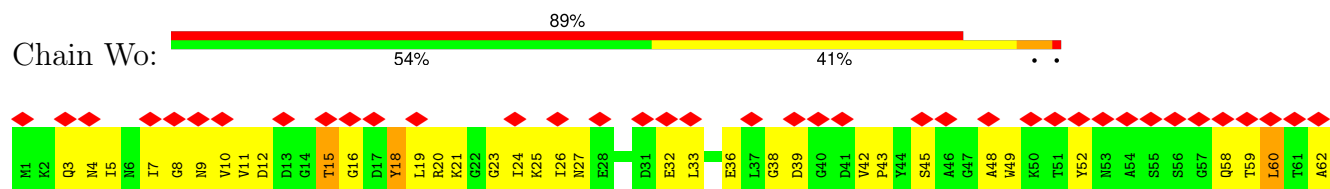
• Molecule 4: gp10, baseplate wedge protein

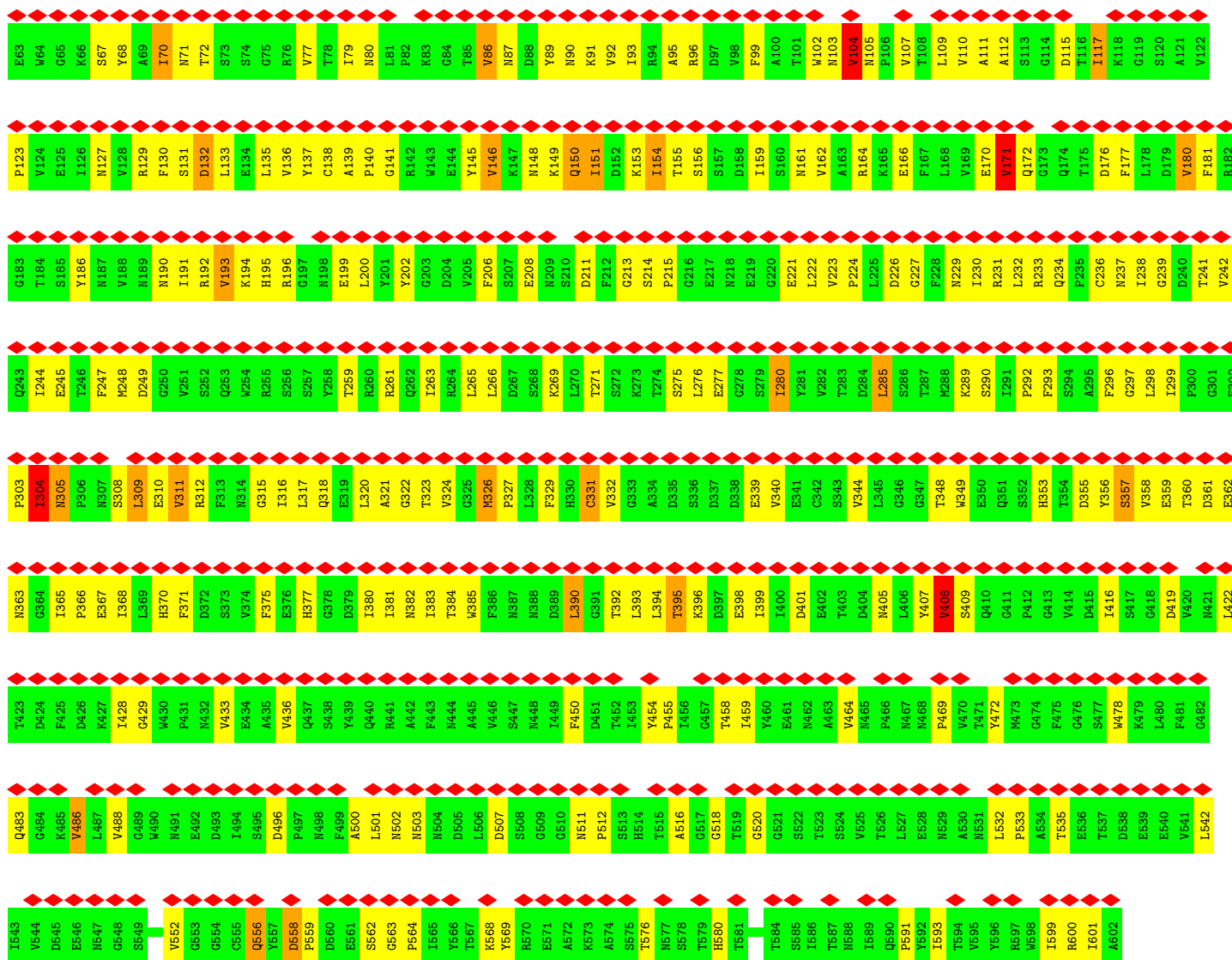


• Molecule 4: gp10, baseplate wedge protein

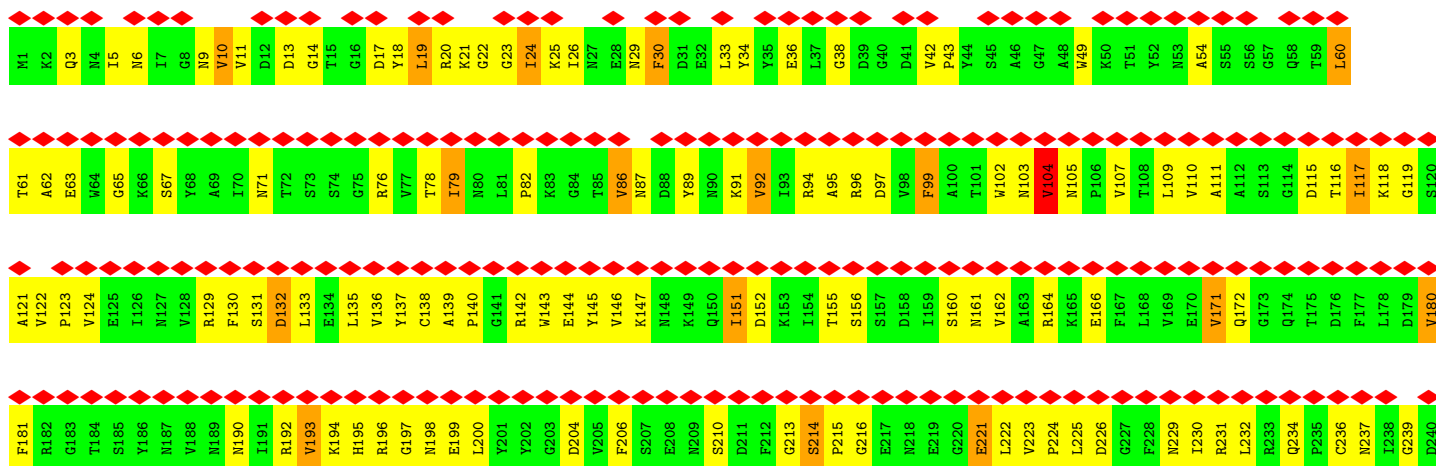


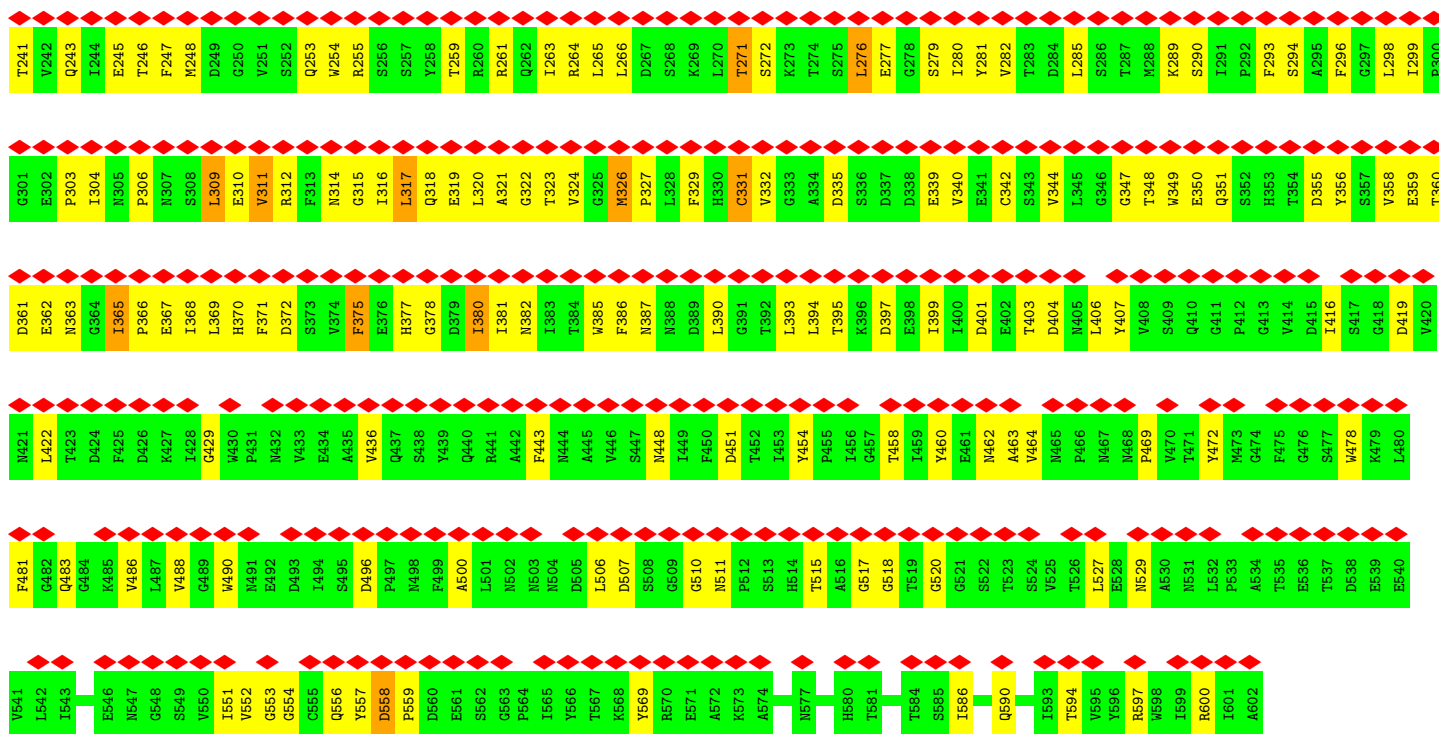
- Molecule 4: gp10, baseplate wedge protein



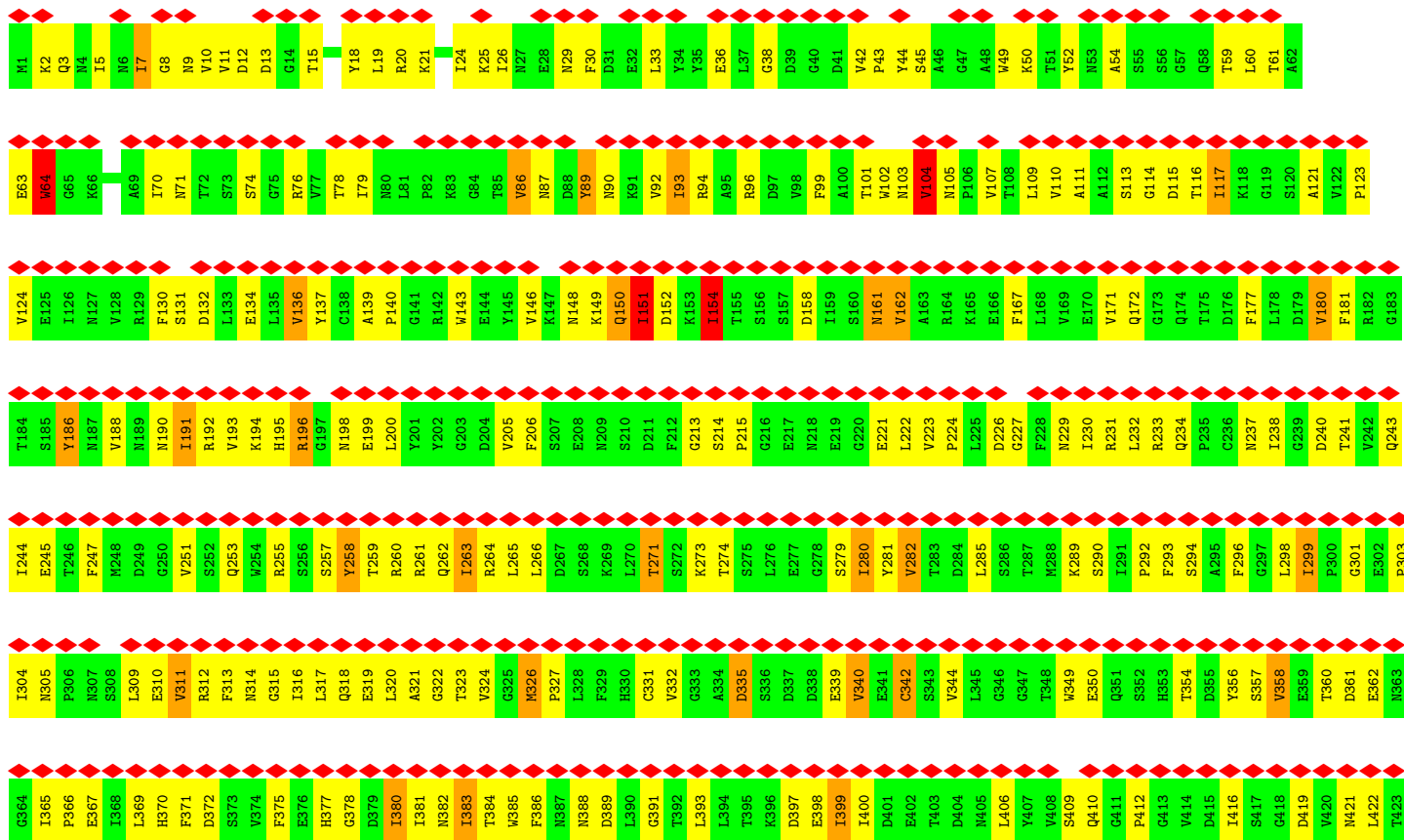
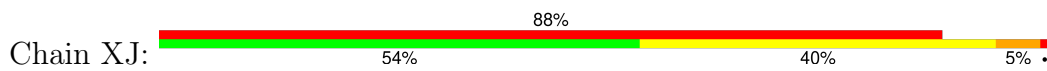


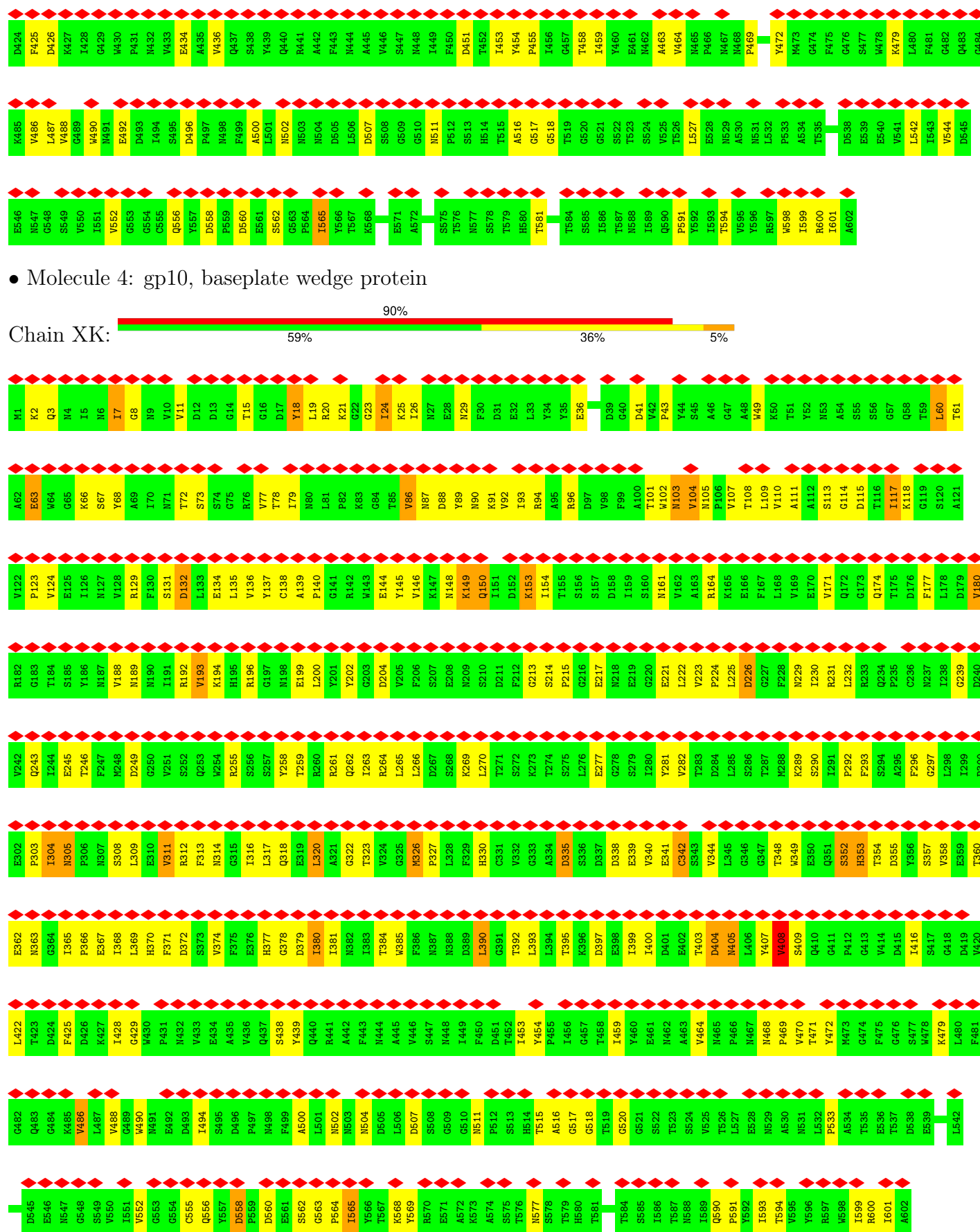
• Molecule 4: gp10, baseplate wedge protein



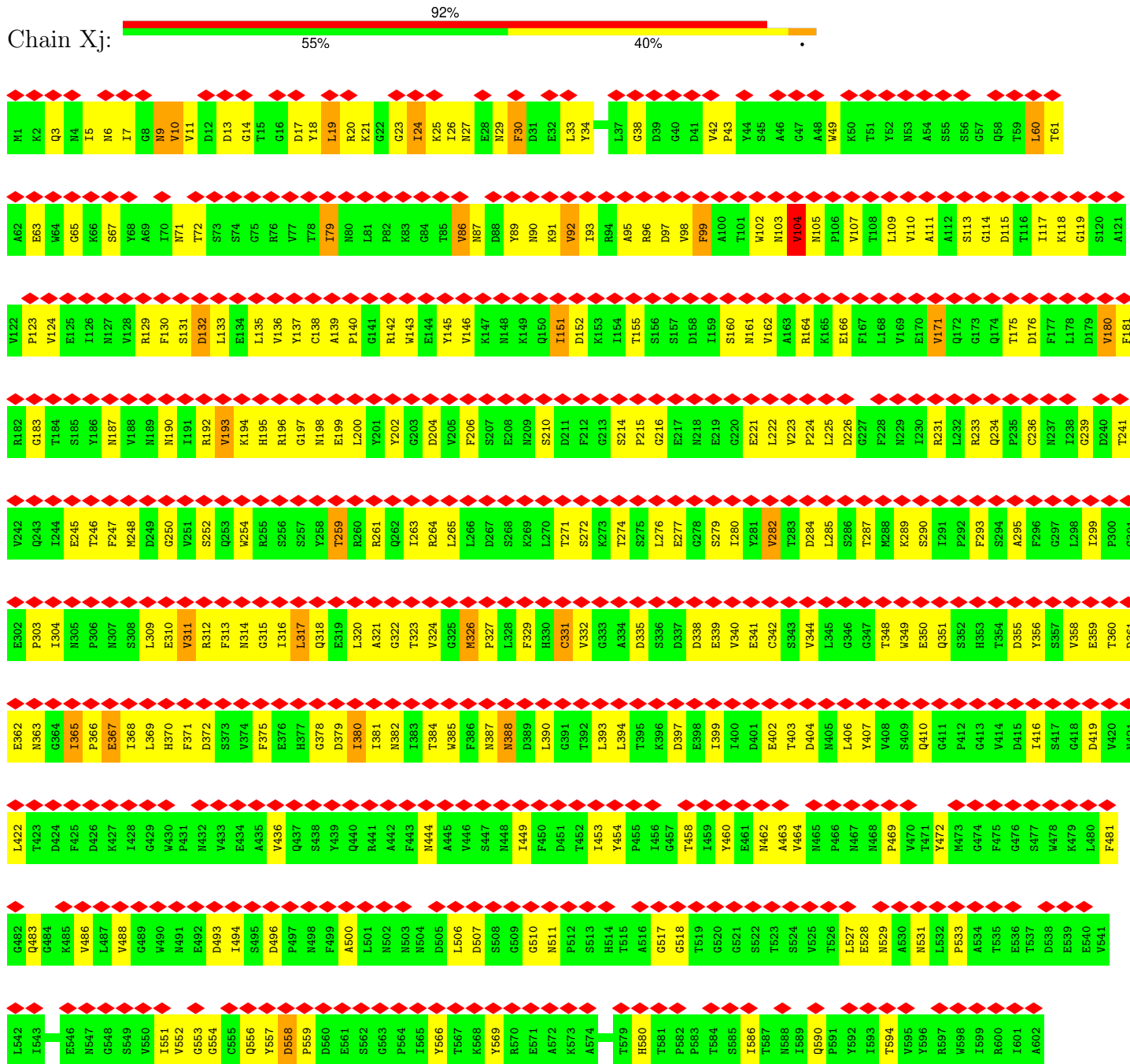


• Molecule 4: gp10, baseplate wedge protein

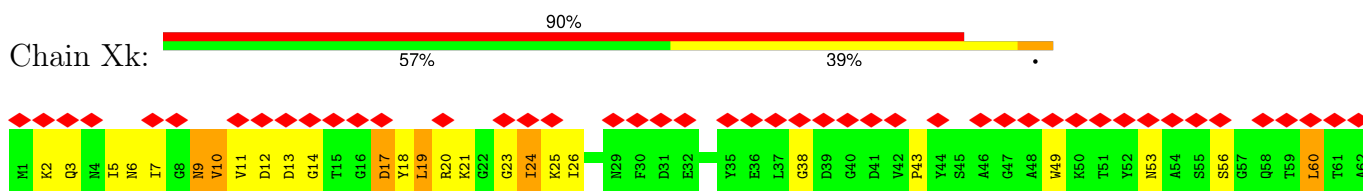


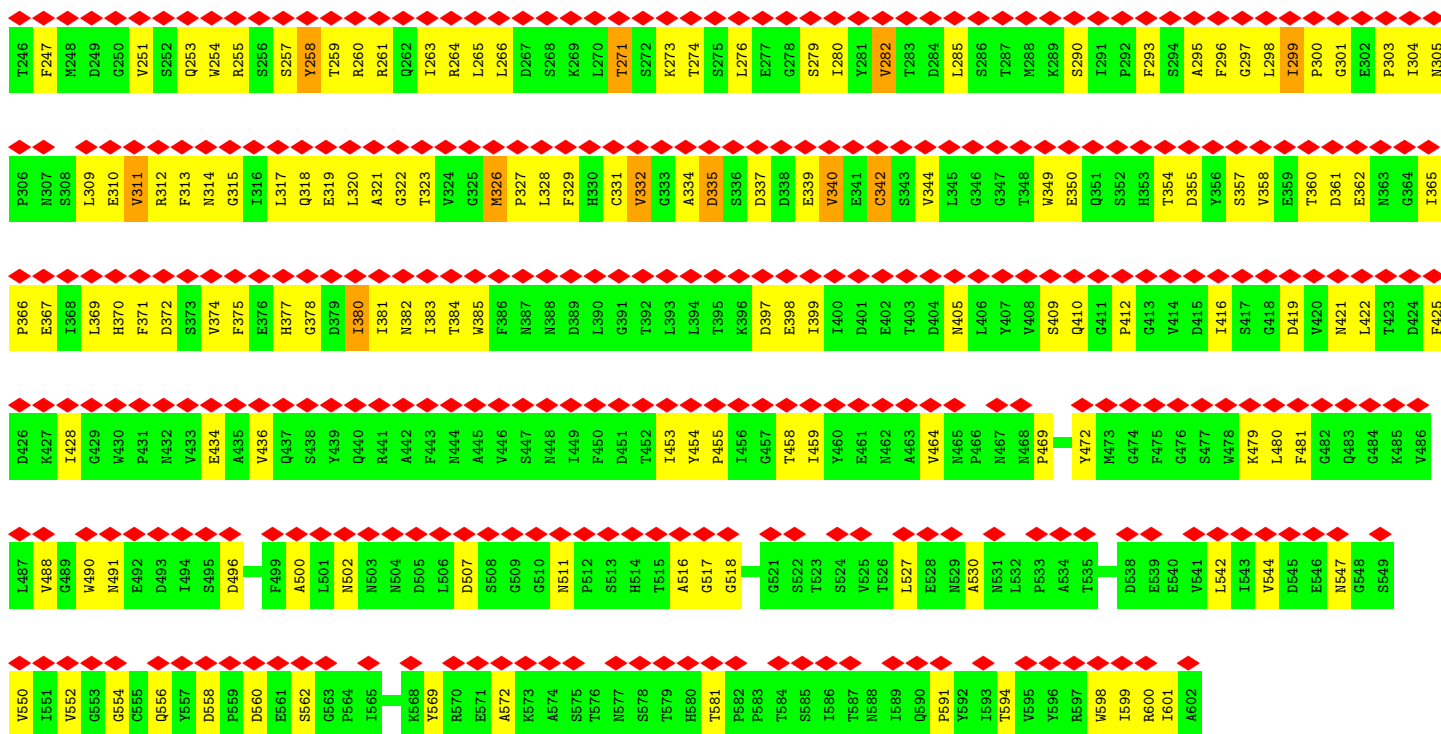


• Molecule 4: gp10, baseplate wedge protein

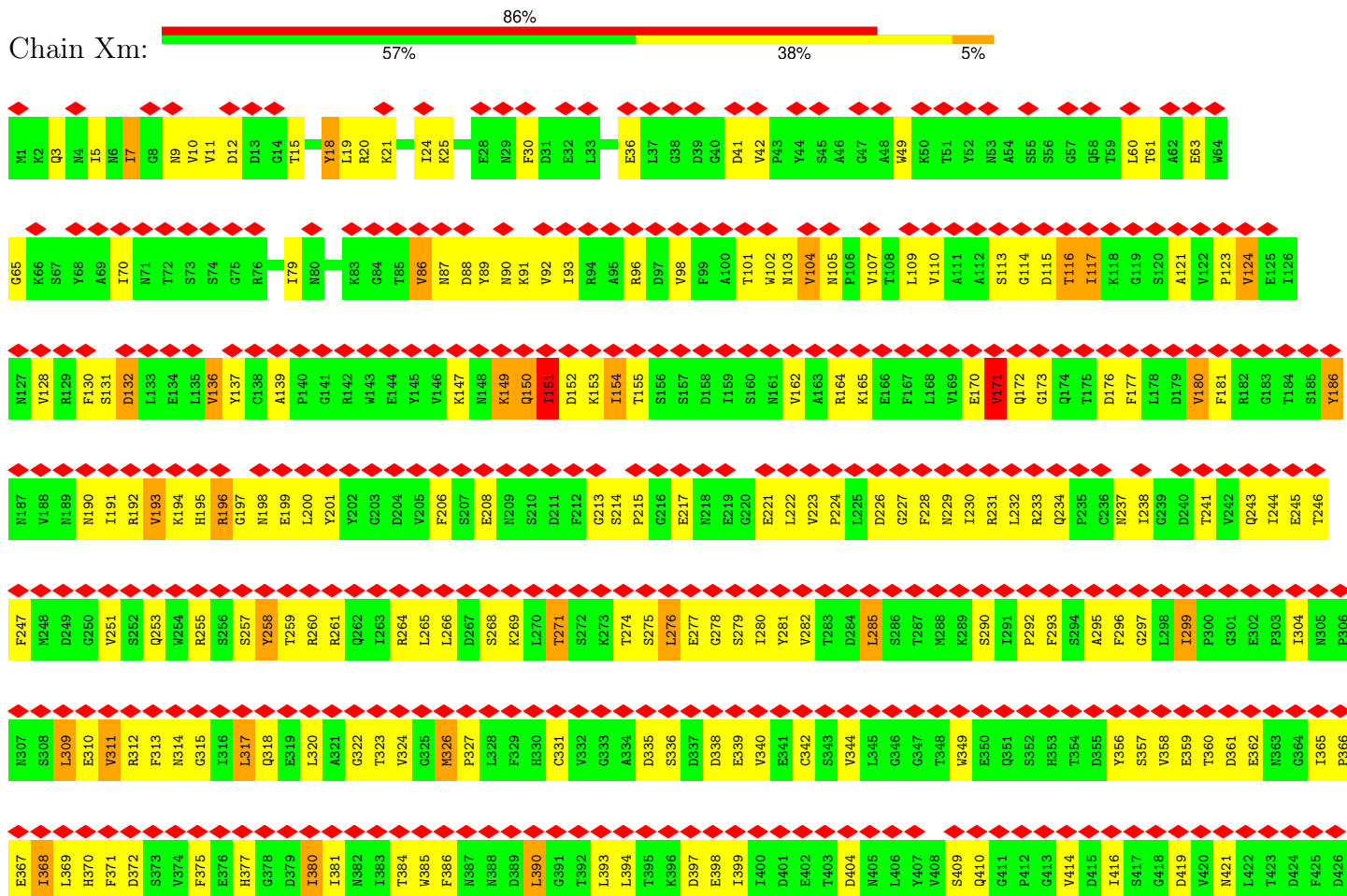


• Molecule 4: gp10, baseplate wedge protein



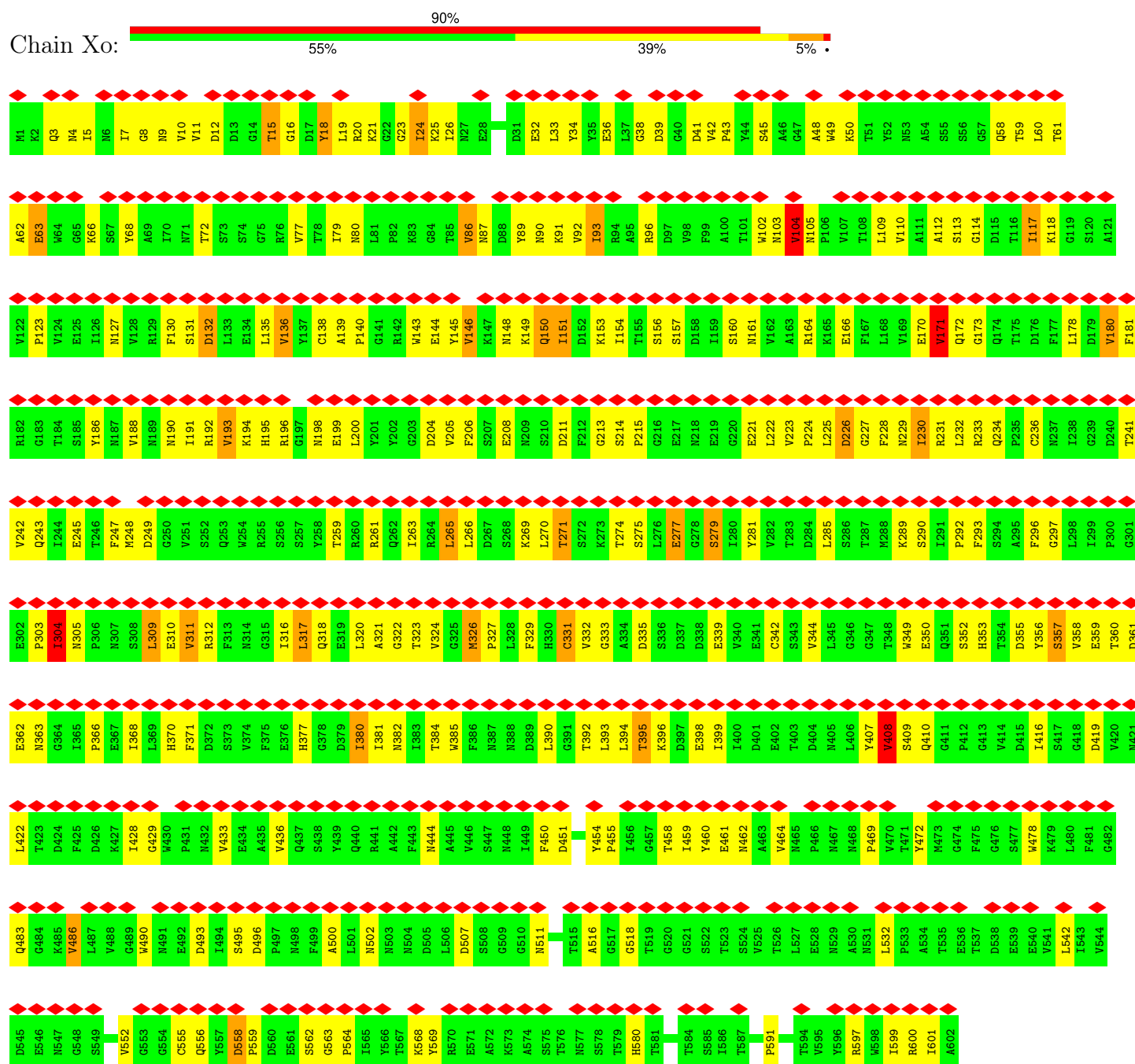


• Molecule 4: gp10, baseplate wedge protein

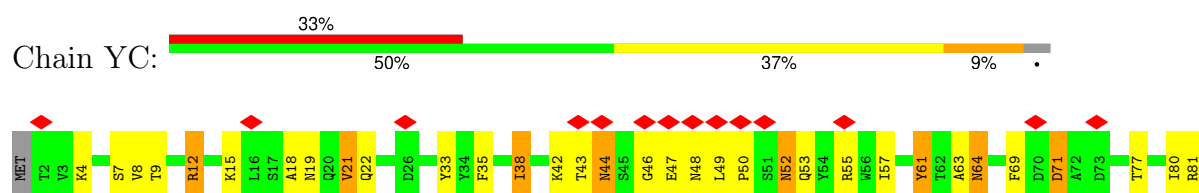




• Molecule 4: gp10, baseplate wedge protein



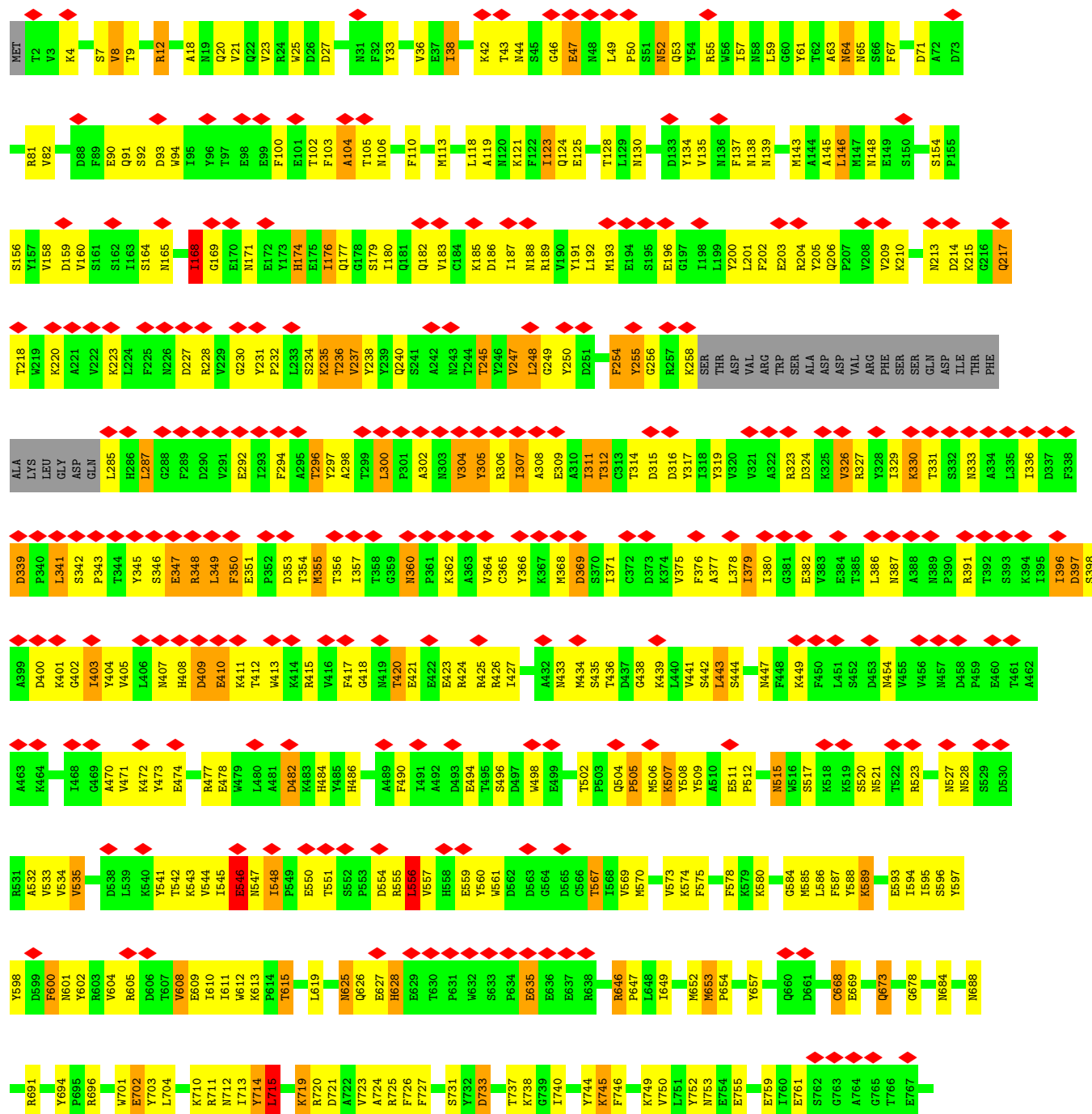
• Molecule 5: gp7, baseplate wedge protein

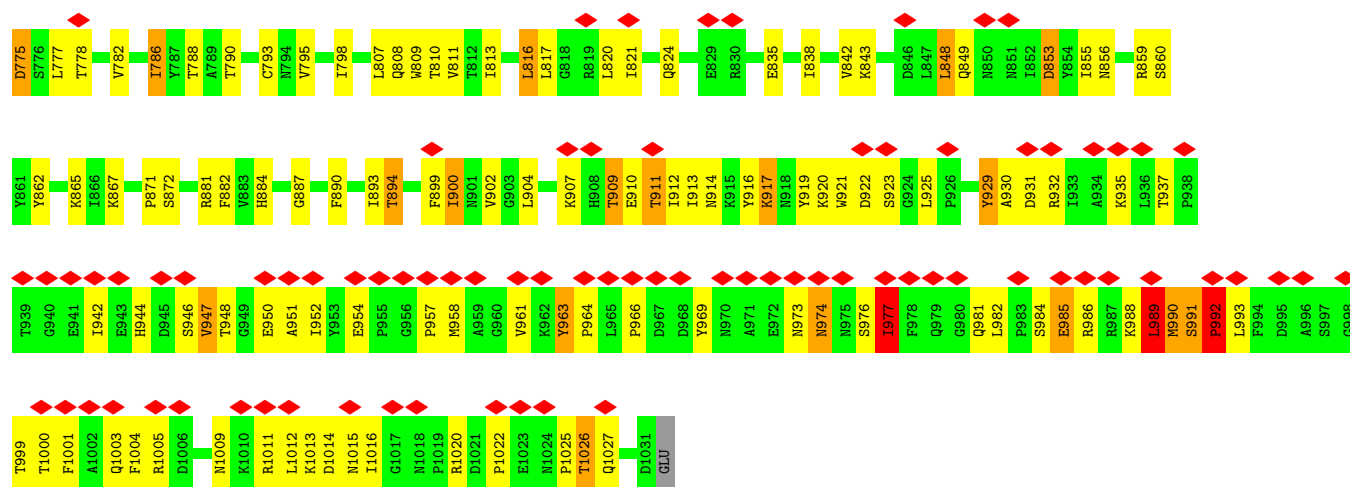




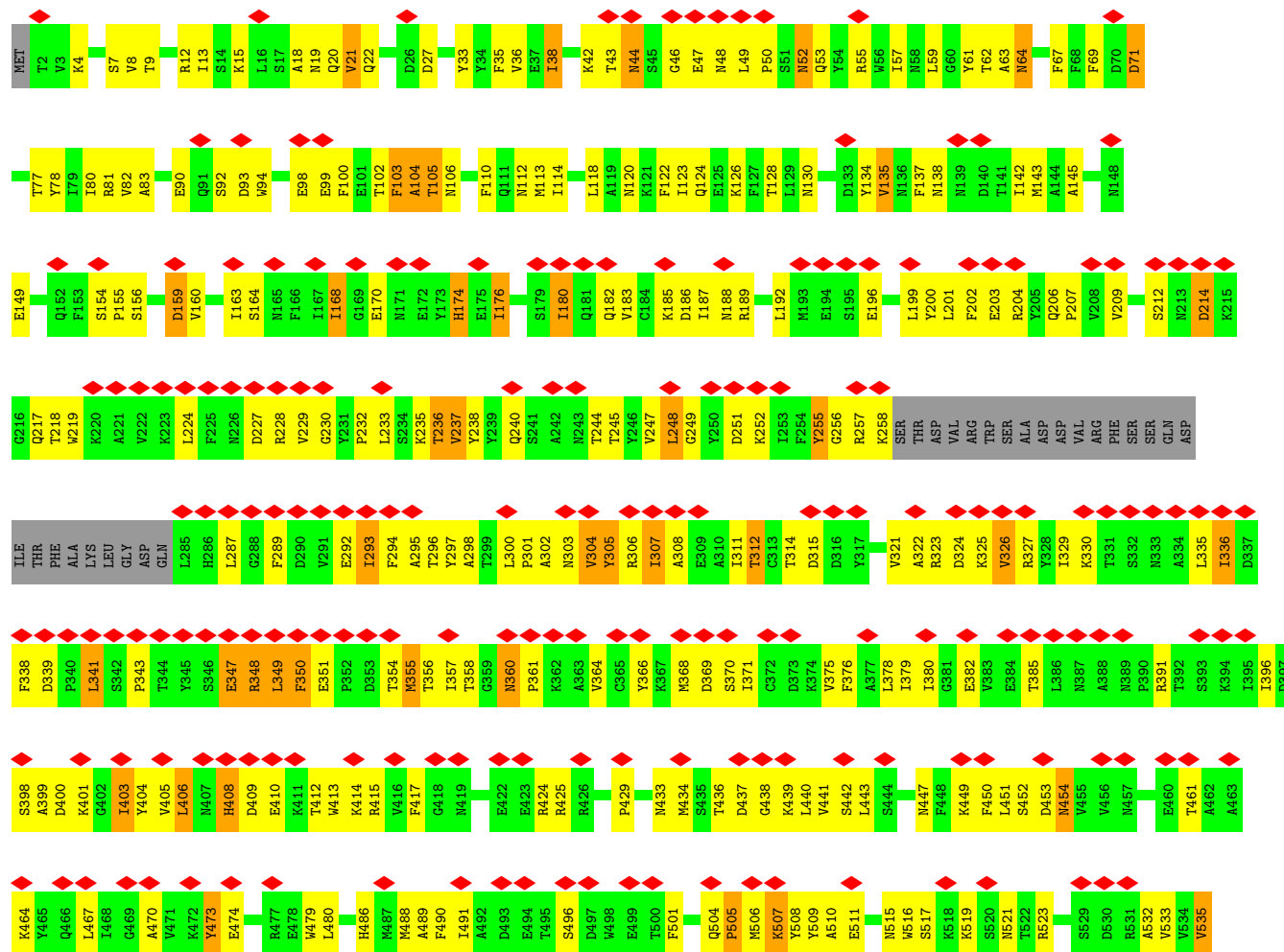


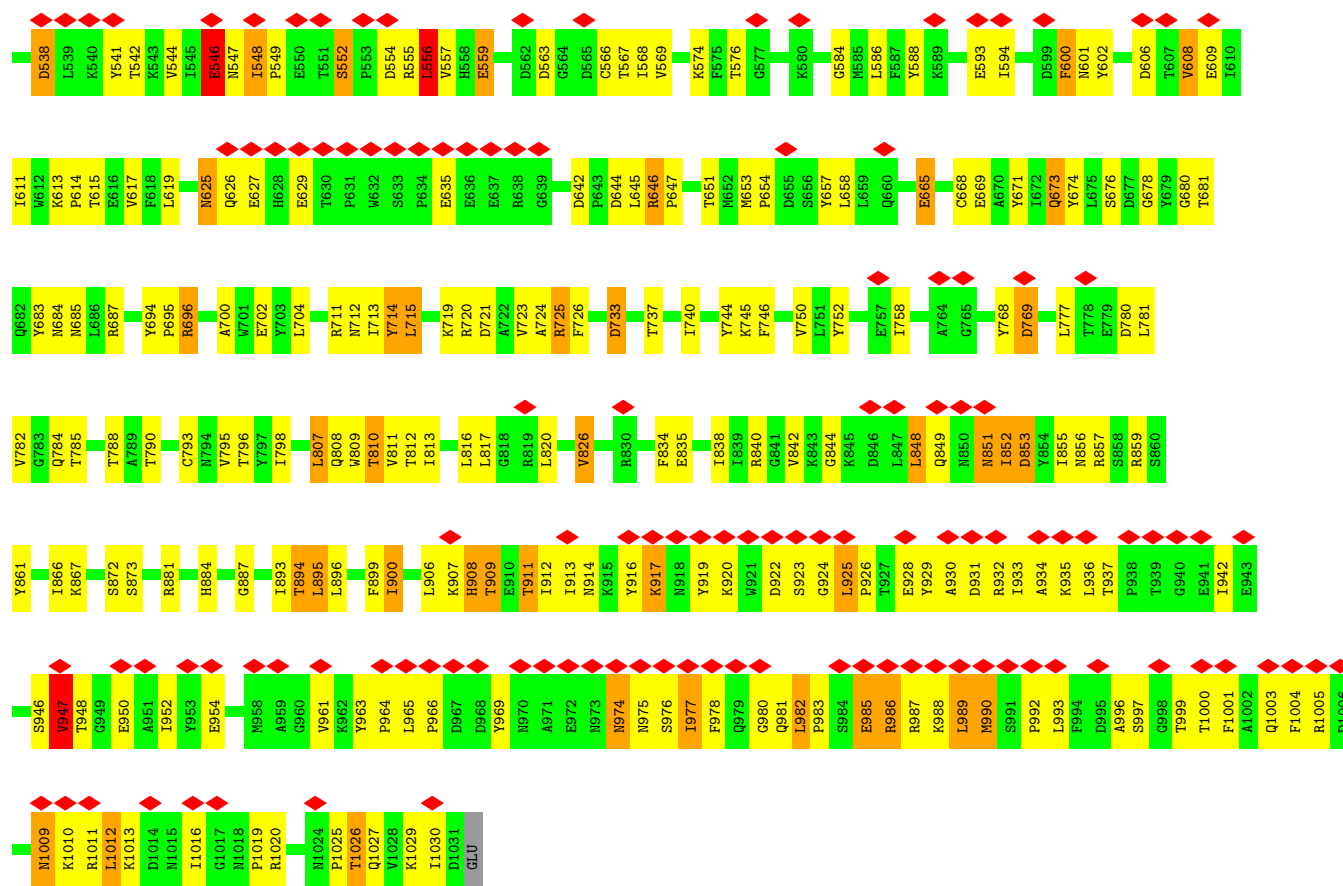
• Molecule 5: gp7, baseplate wedge protein



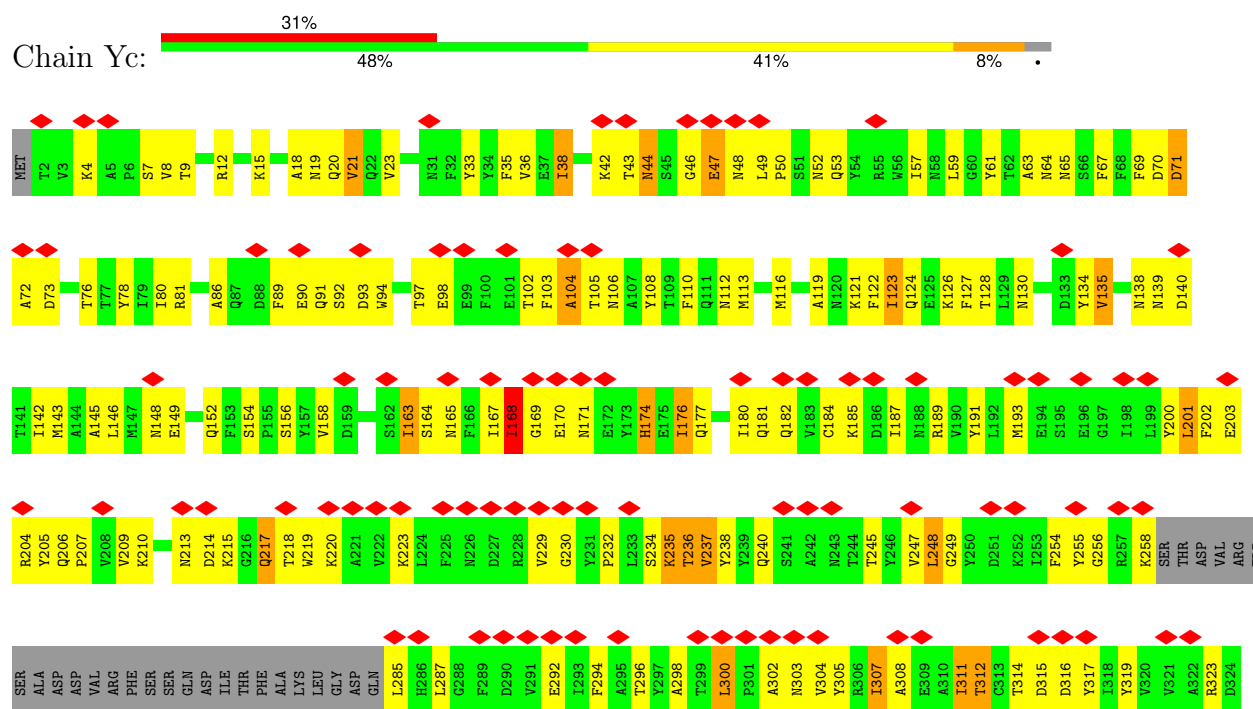


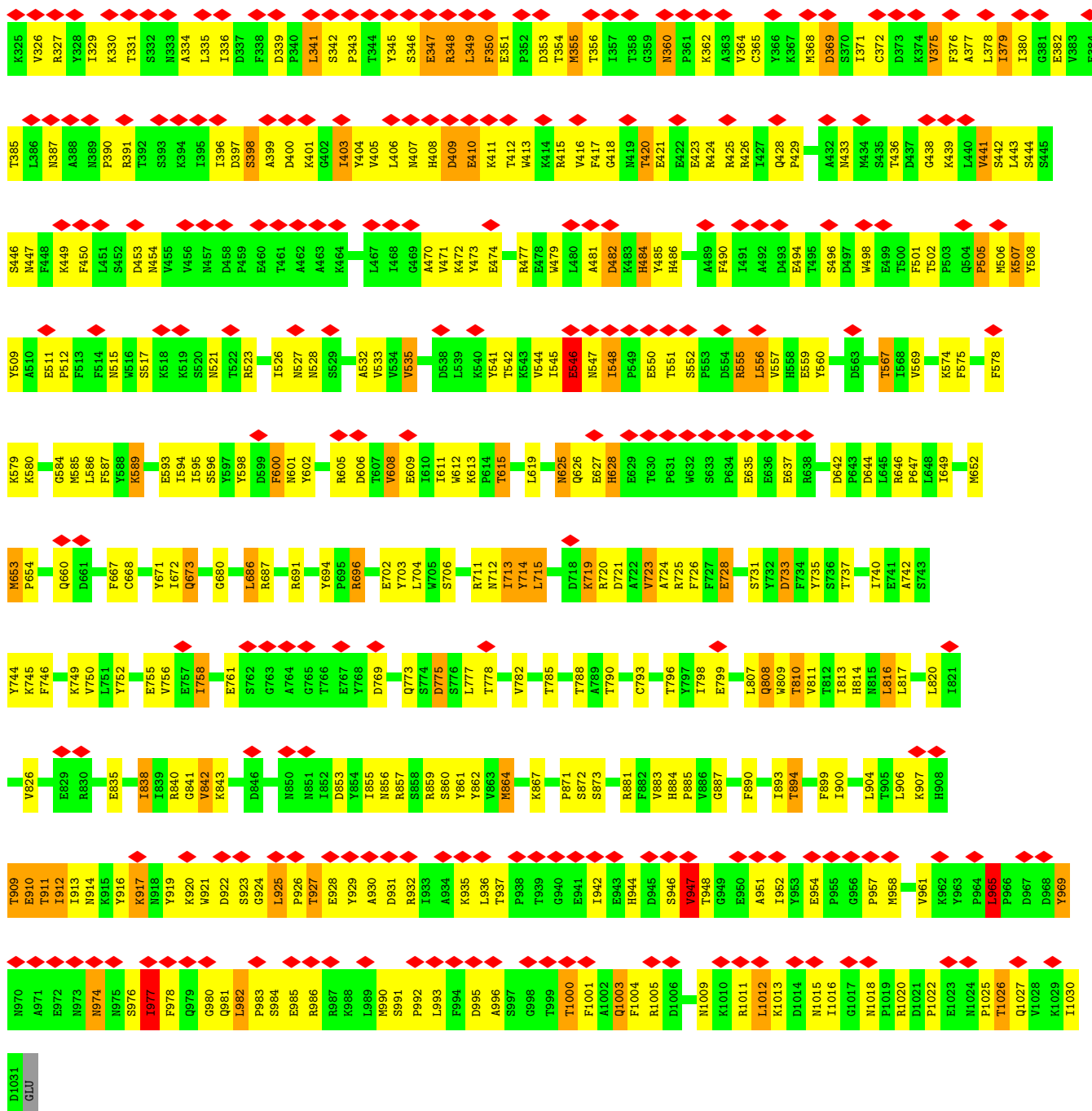
• Molecule 5: gp7, baseplate wedge protein



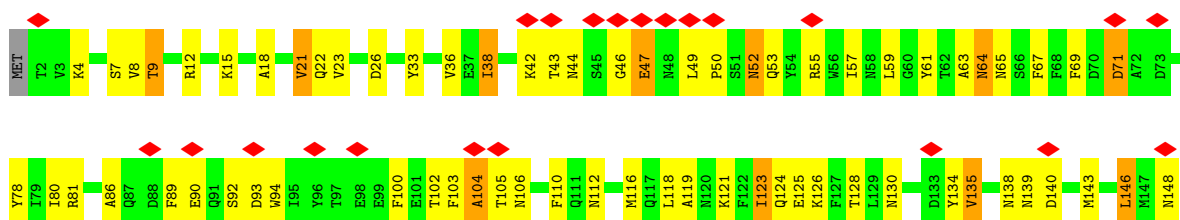


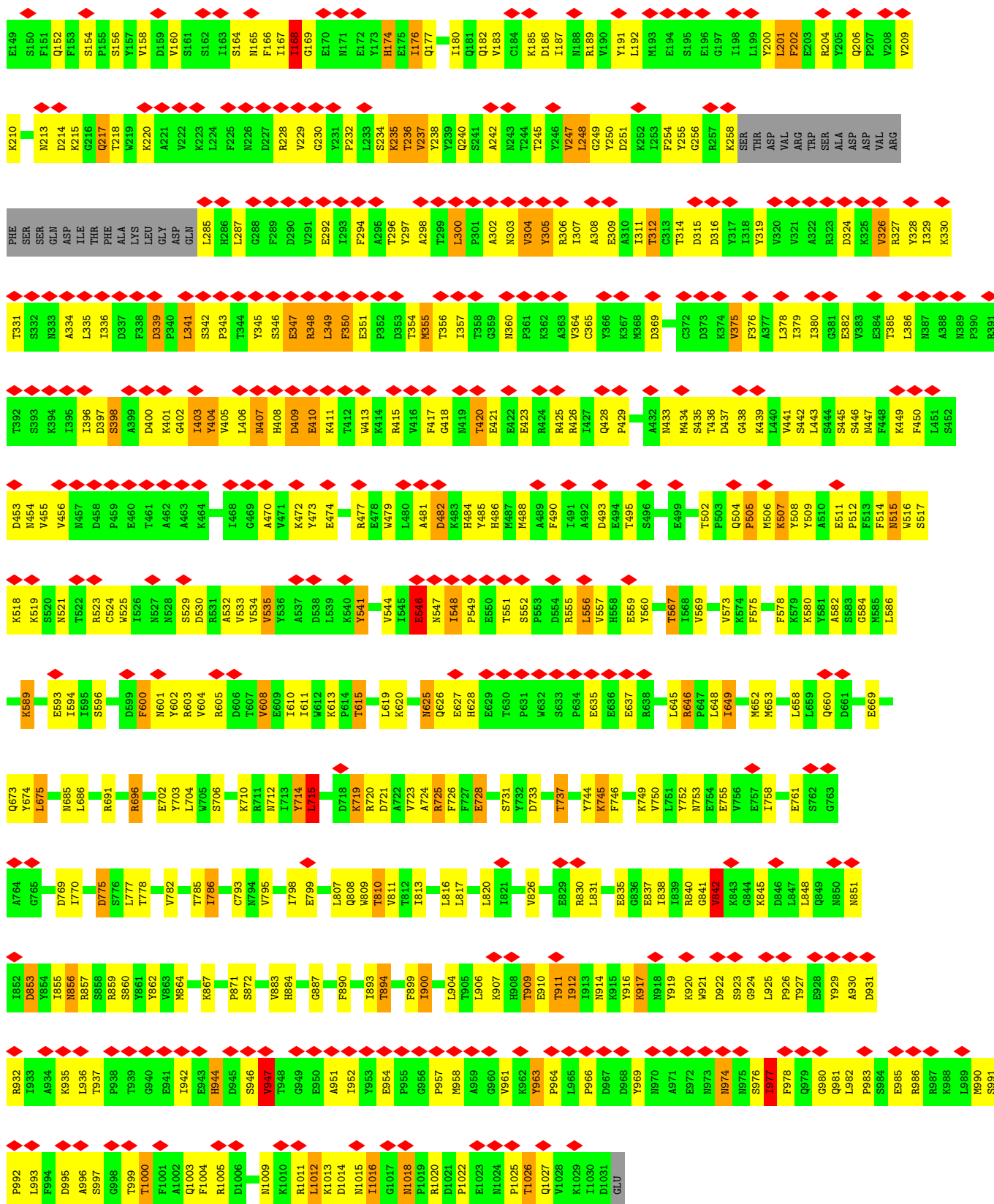
• Molecule 5: gp7, baseplate wedge protein

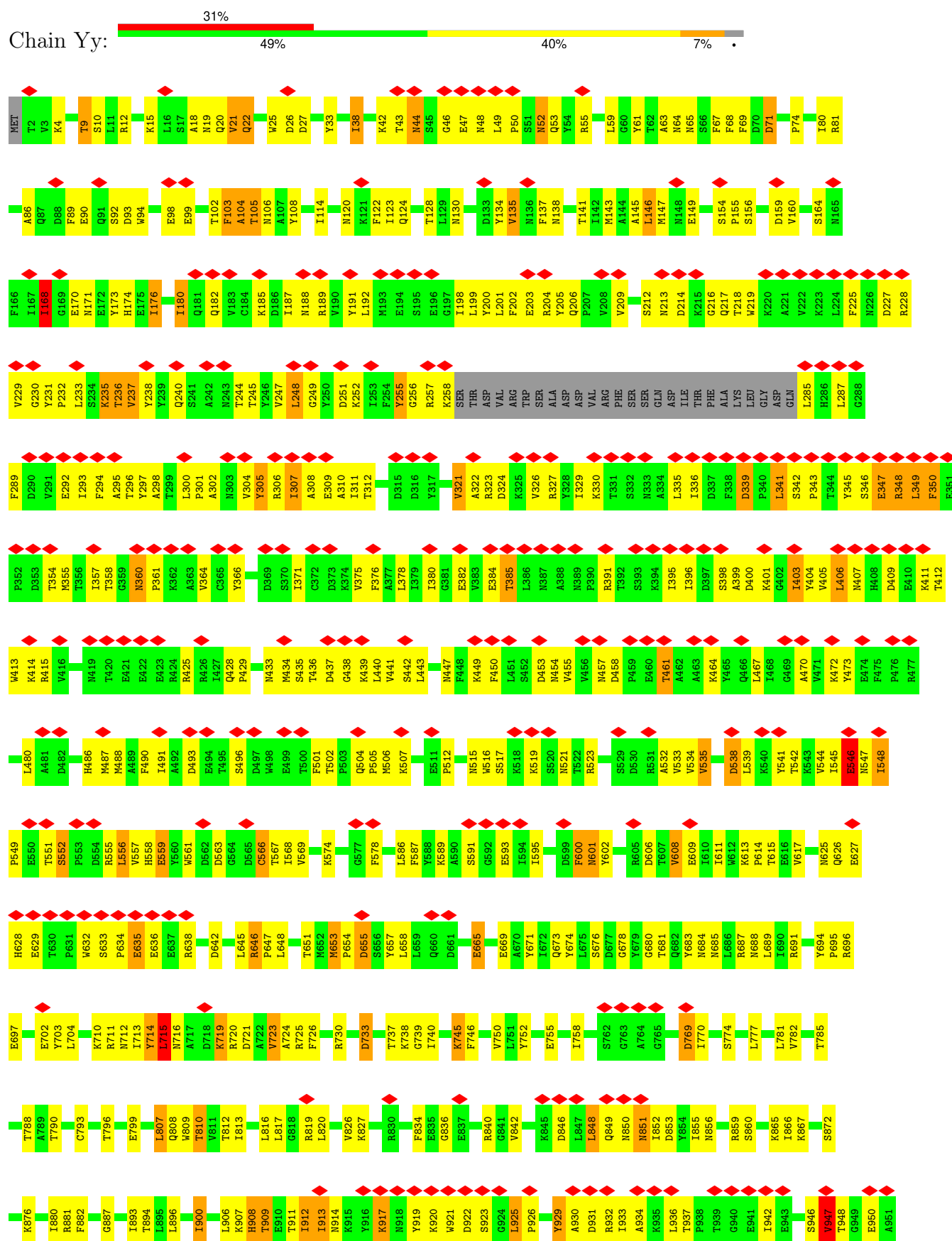


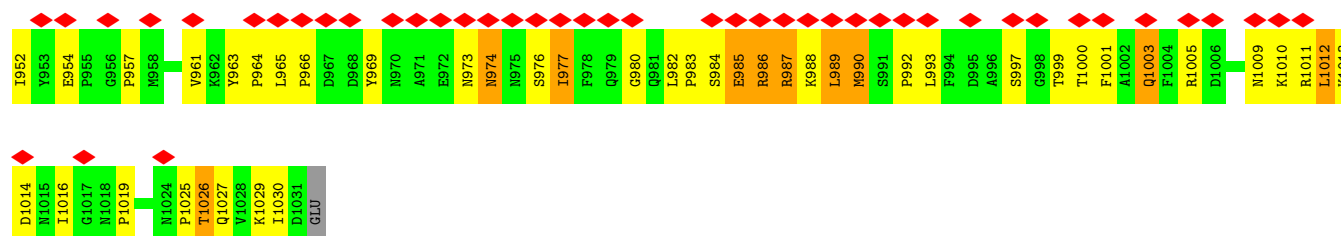


• Molecule 5: gp7, baseplate wedge protein

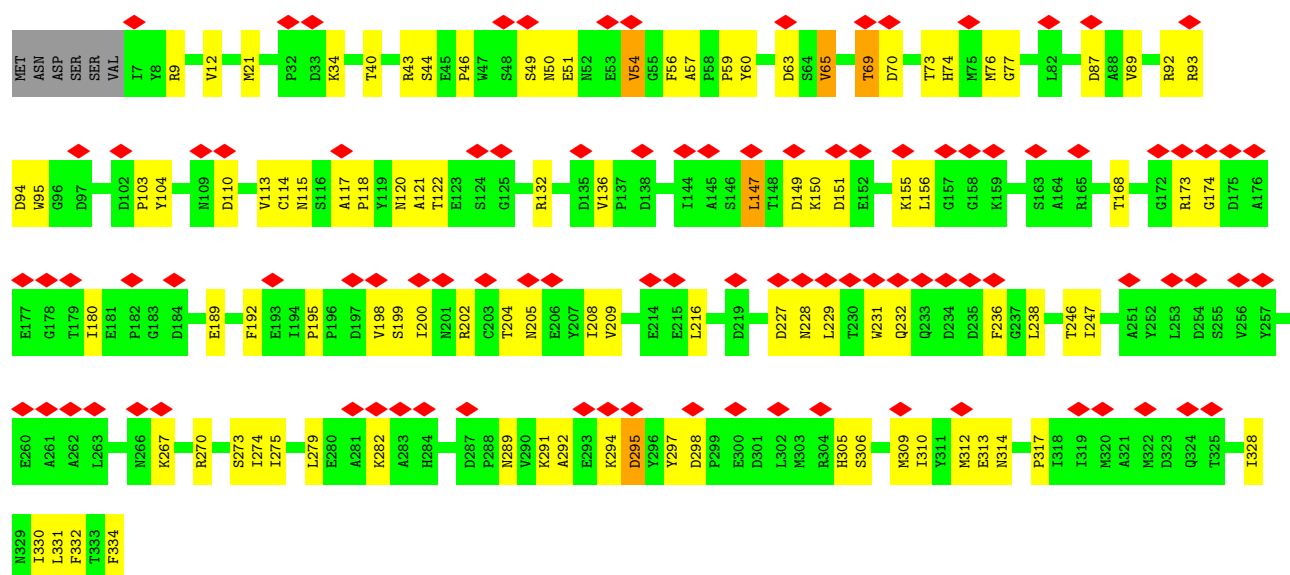




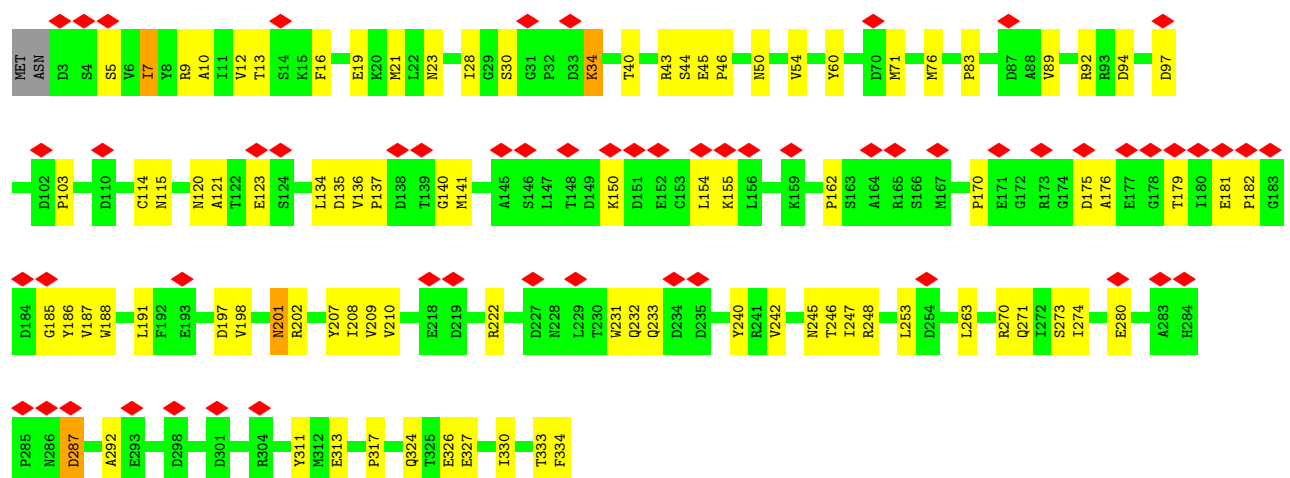
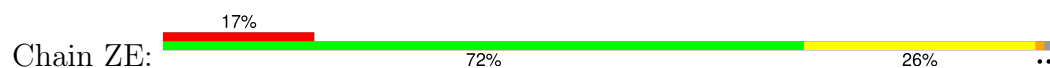




• Molecule 6: gp8, baseplate wedge protein

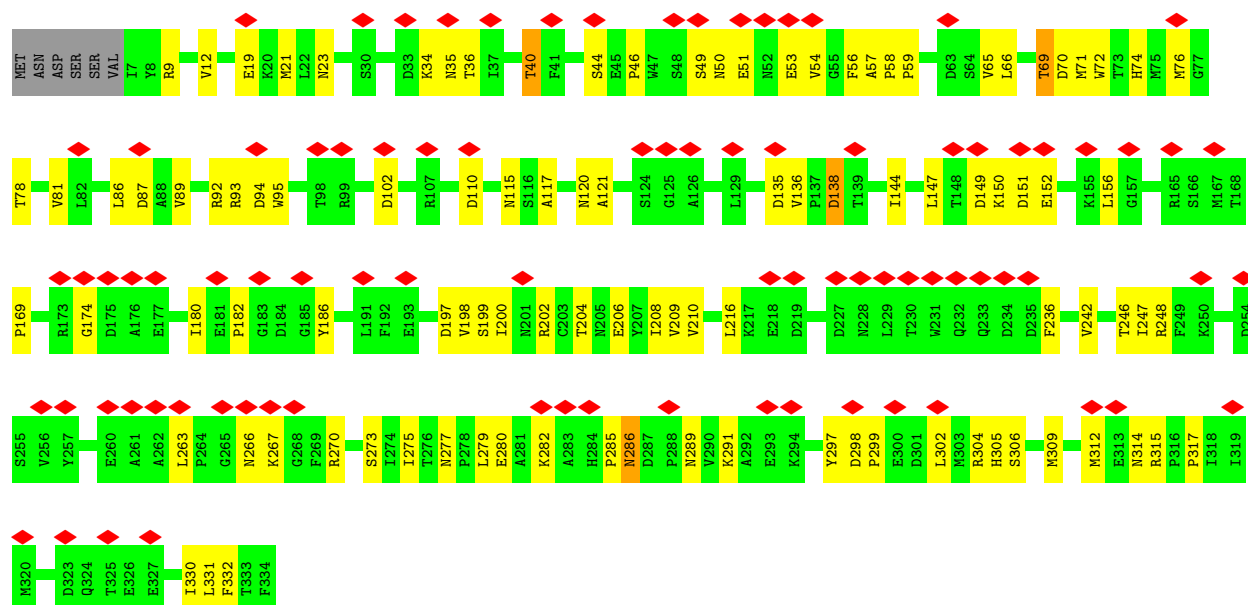


• Molecule 6: gp8, baseplate wedge protein



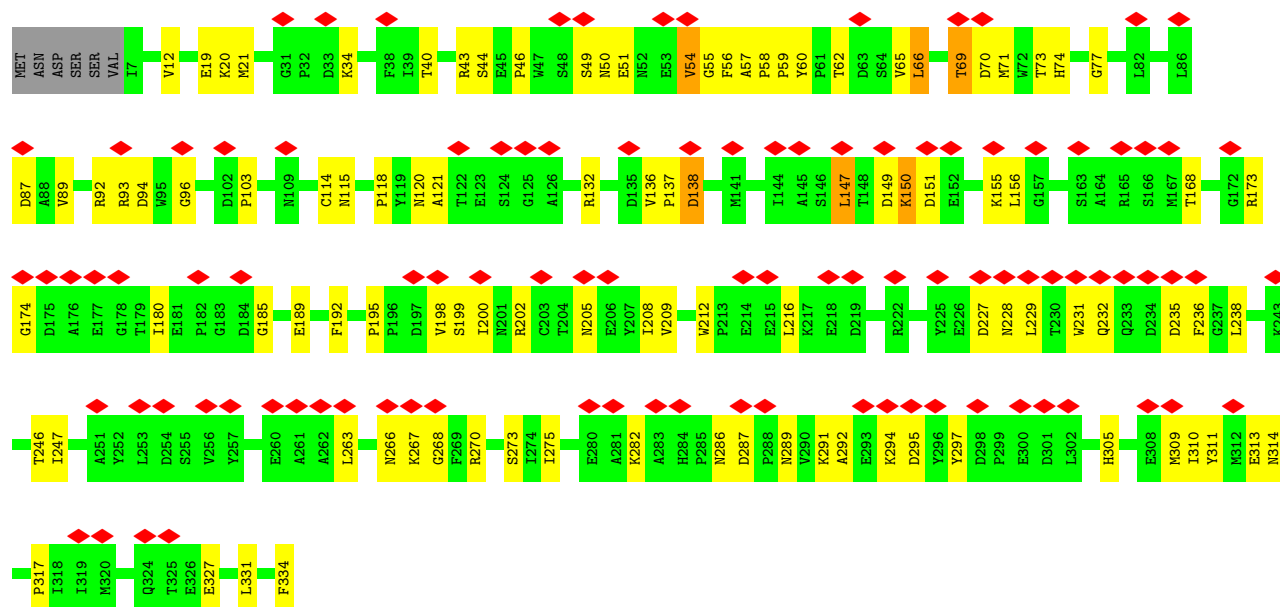
• Molecule 6: gp8, baseplate wedge protein





- Molecule 6: gp8, baseplate wedge protein

Chain Za: 30% 67% 29%



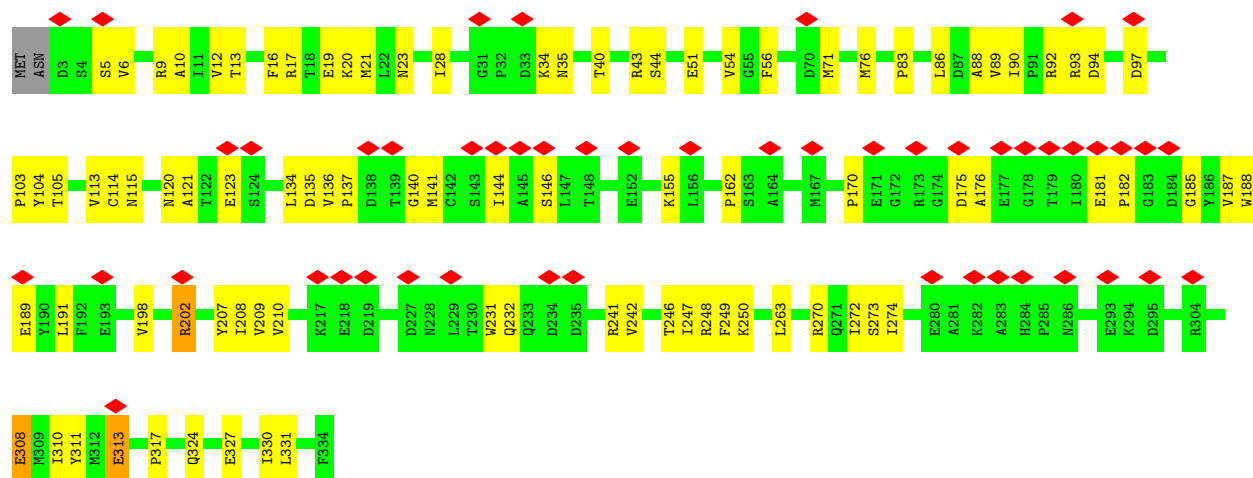
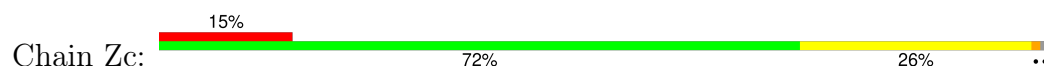
- Molecule 6: gp8, baseplate wedge protein

Chain Zb: 18% 73% 25%

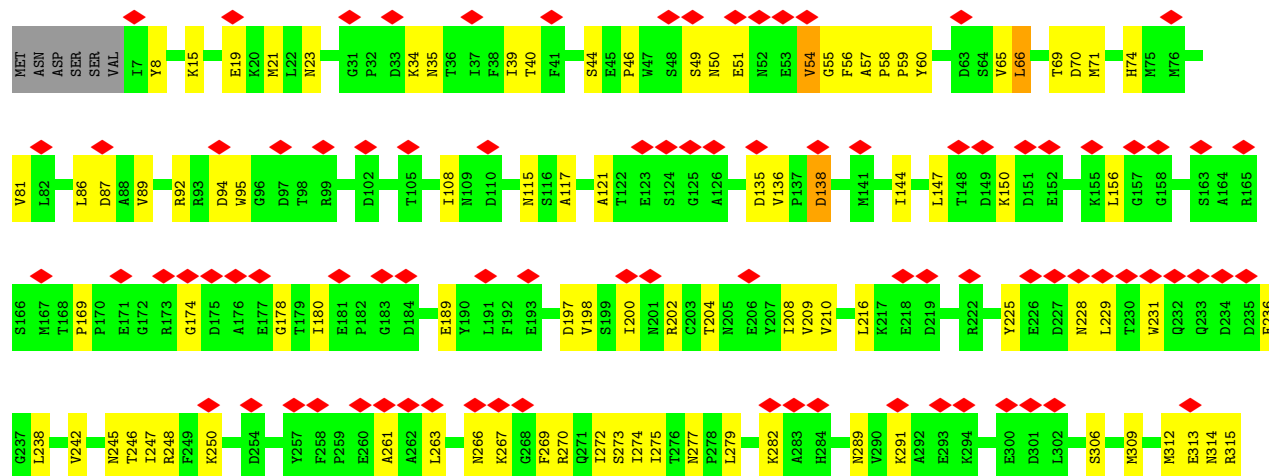


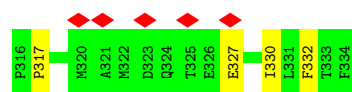


• Molecule 6: gp8, baseplate wedge protein

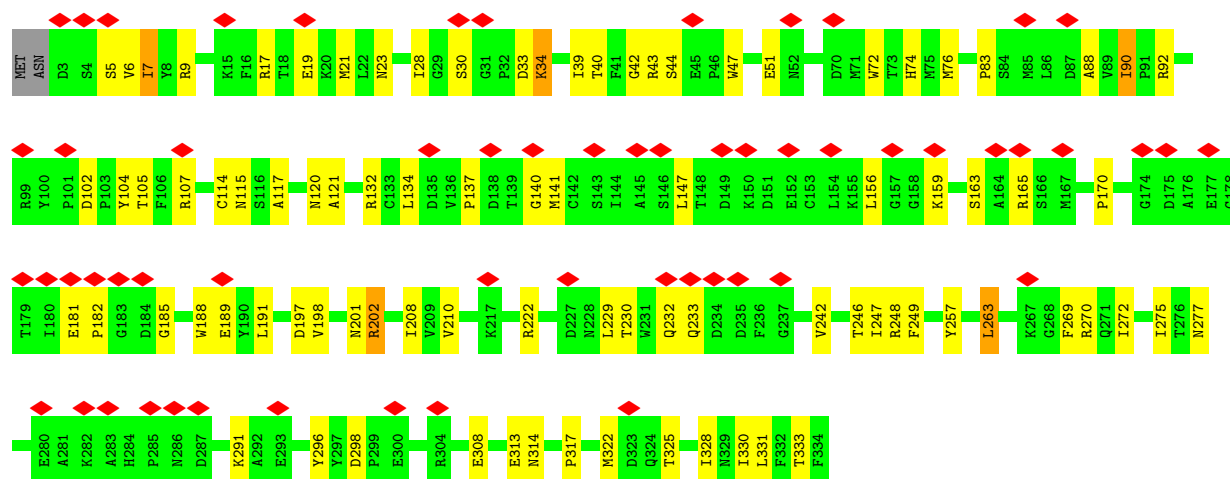
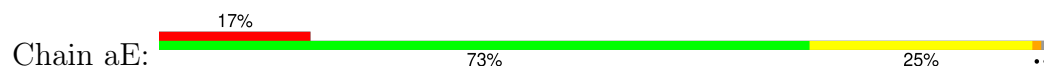


• Molecule 6: gp8, baseplate wedge protein

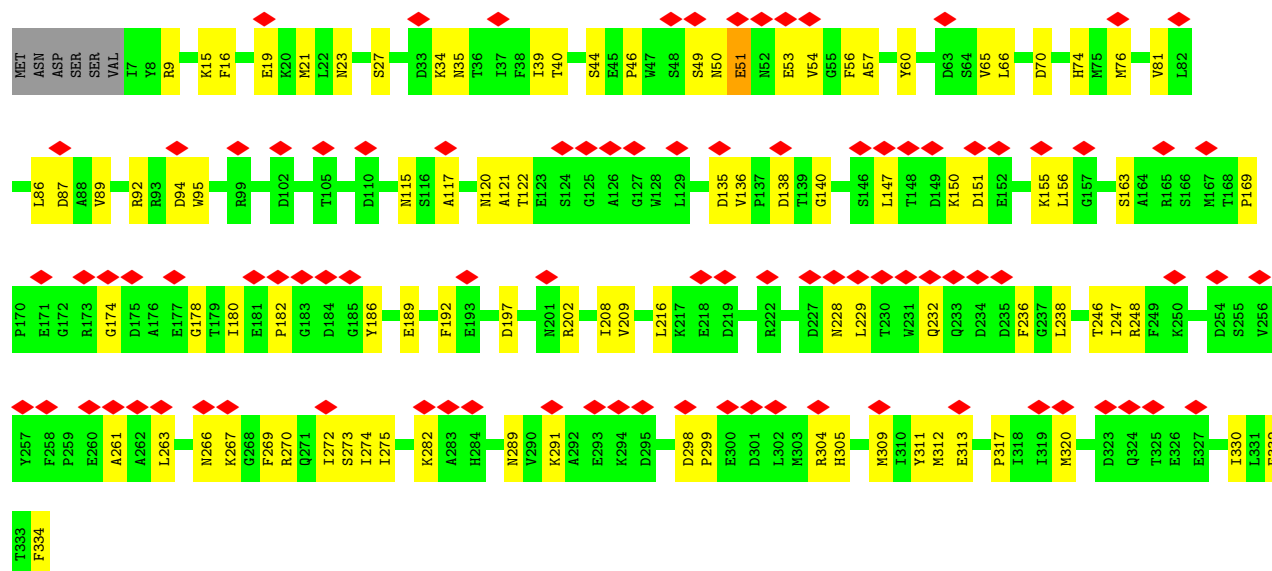




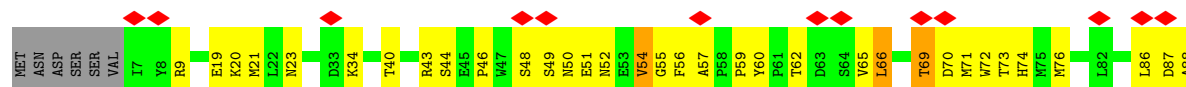
- Molecule 6: gp8, baseplate wedge protein

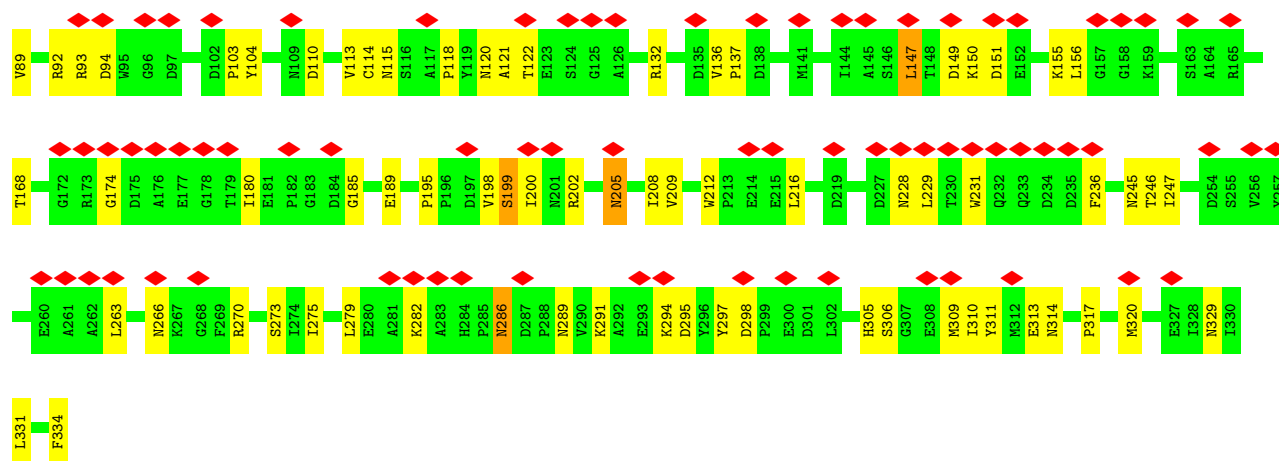


- Molecule 6: gp8, baseplate wedge protein

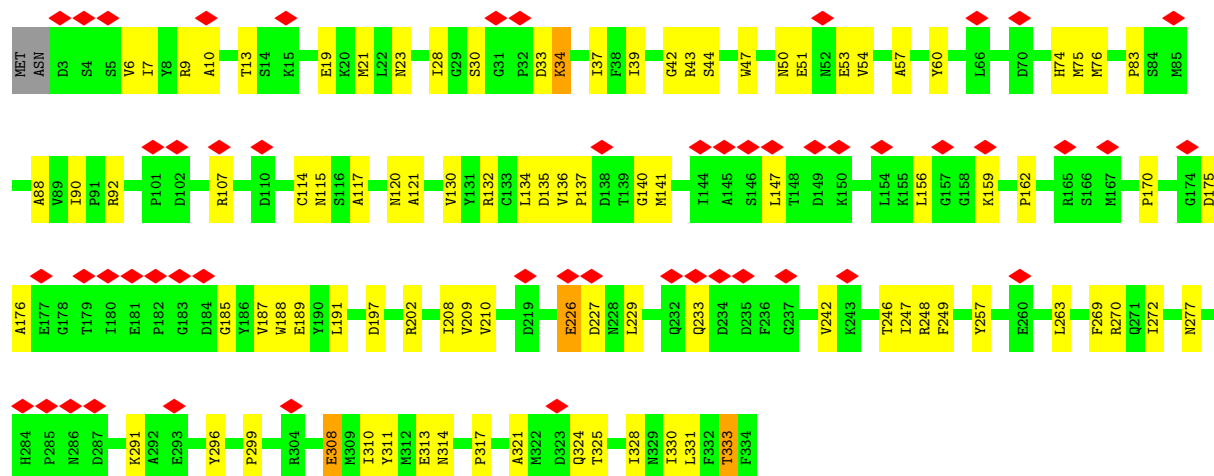


- Molecule 6: gp8, baseplate wedge protein

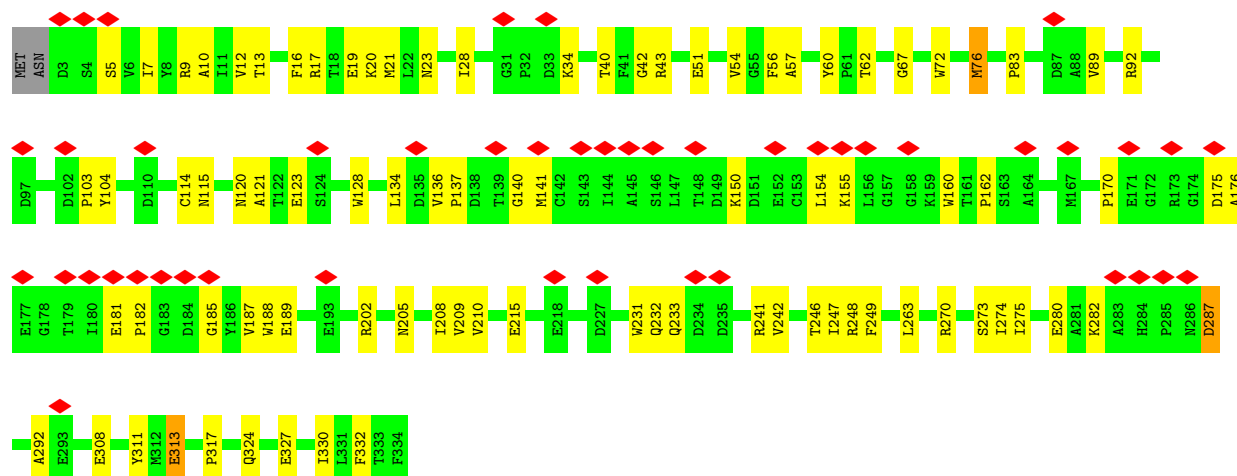
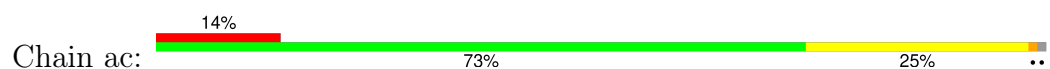




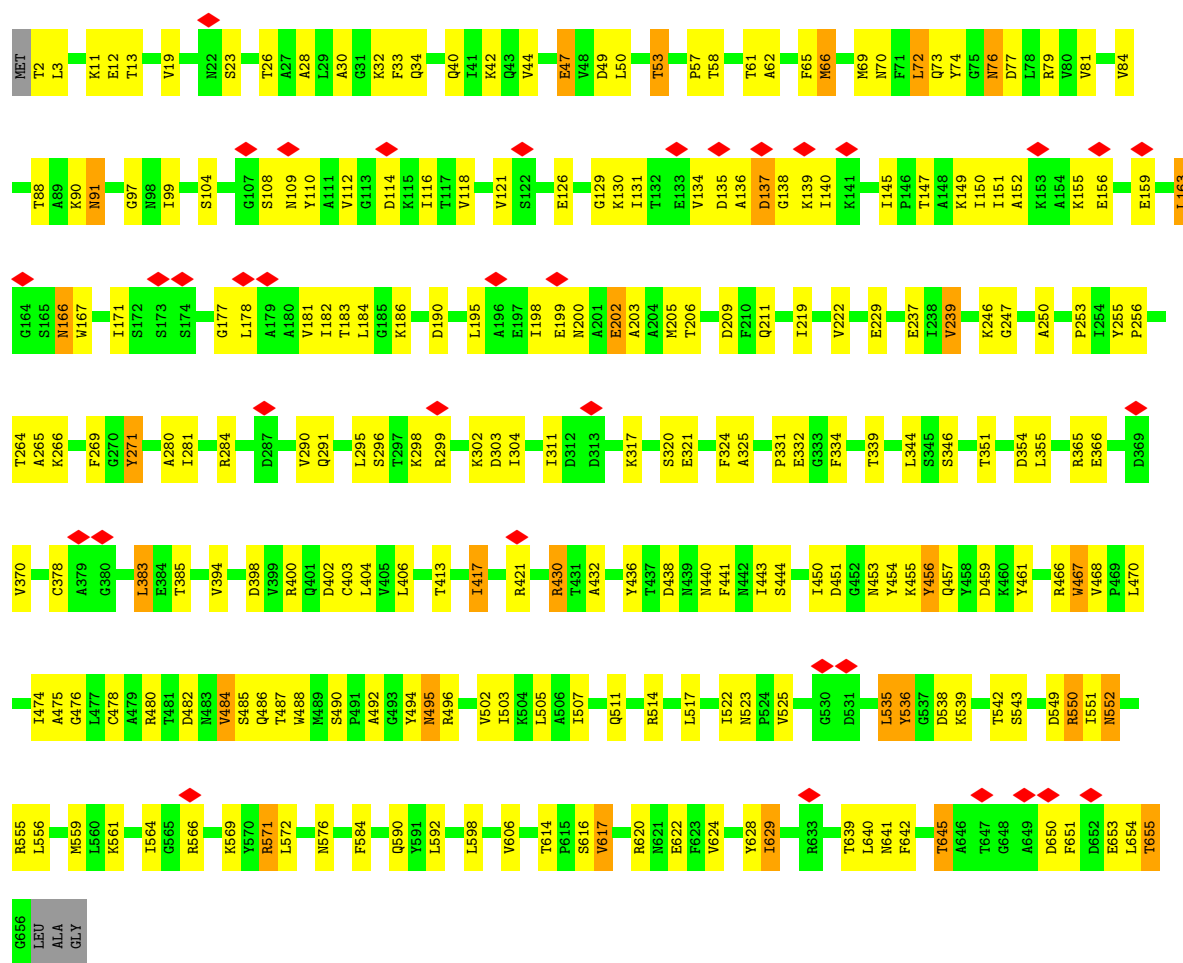
• Molecule 6: gp8, baseplate wedge protein



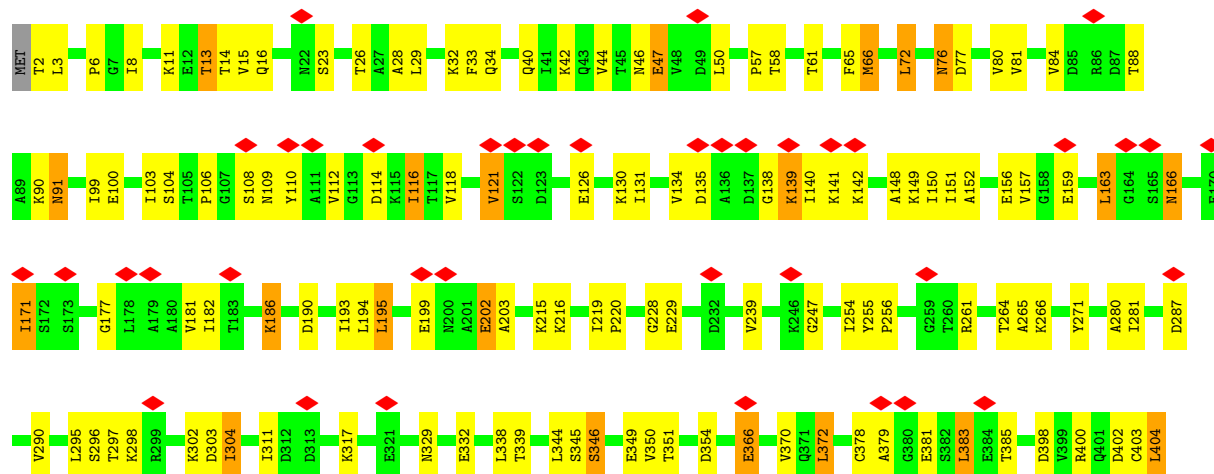
• Molecule 6: gp8, baseplate wedge protein

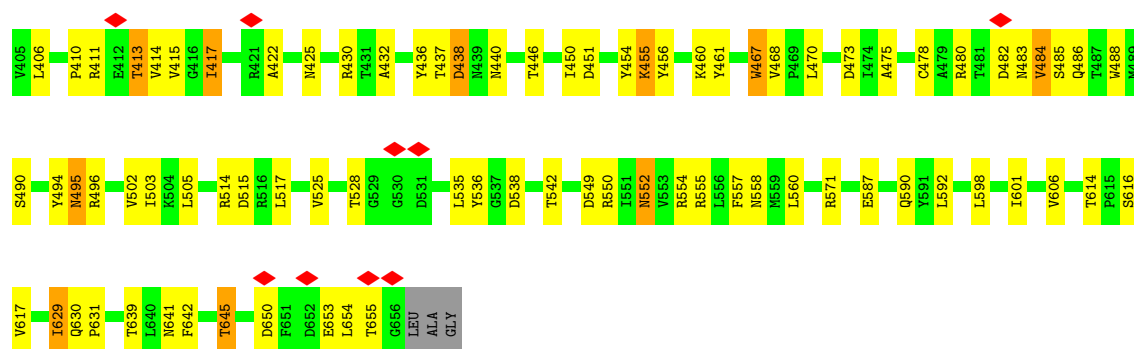


• Molecule 7: gp18, tail sheath protein

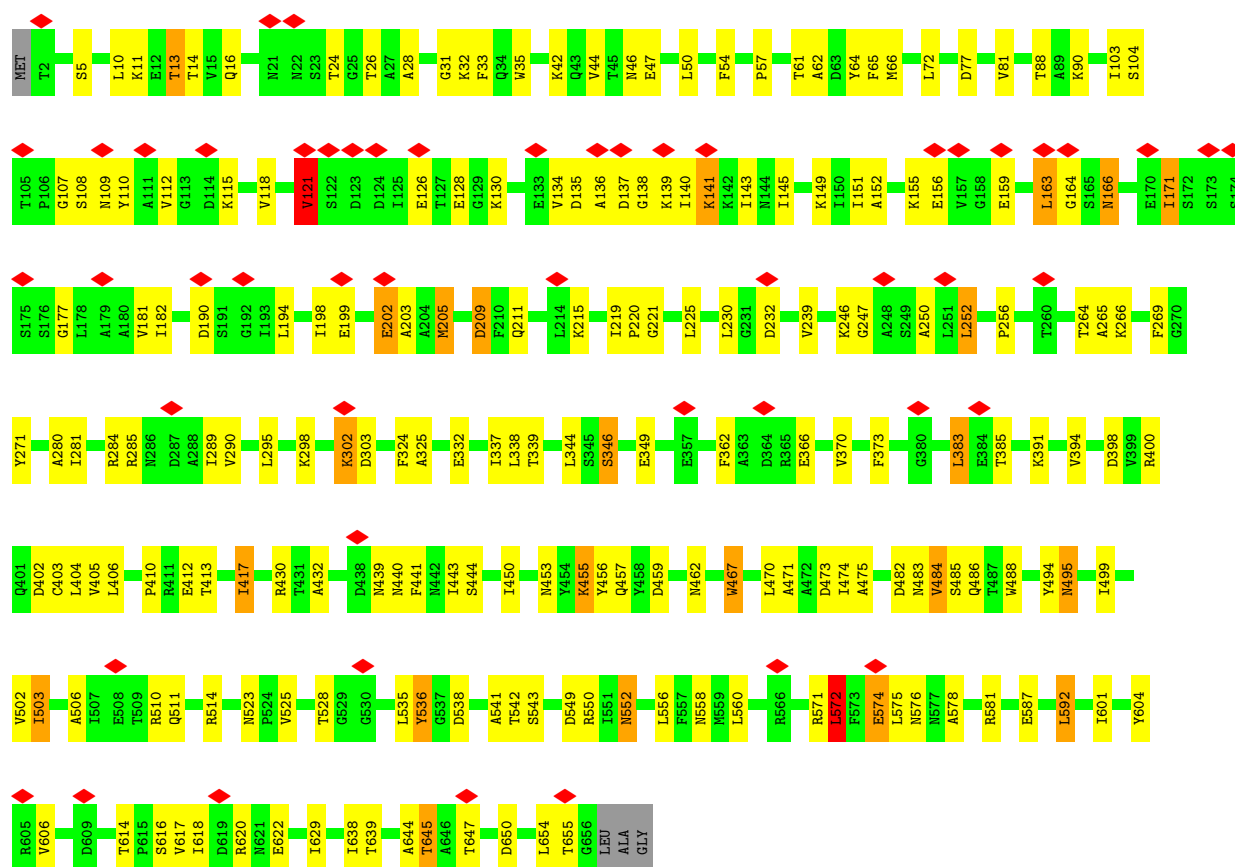


• Molecule 7: gp18, tail sheath protein

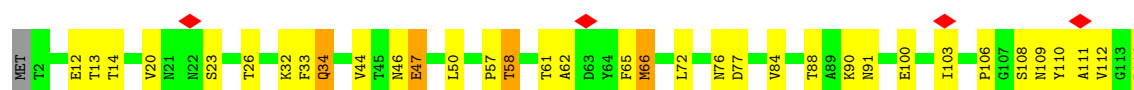


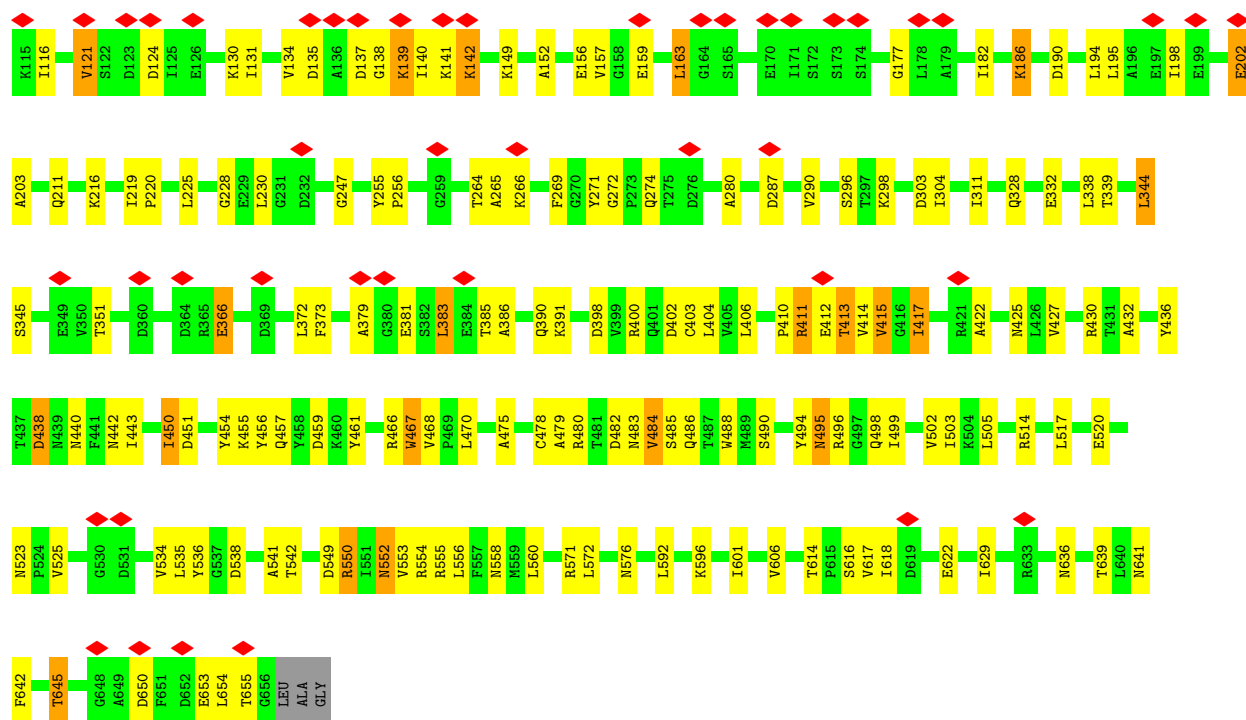


• Molecule 7: gp18, tail sheath protein

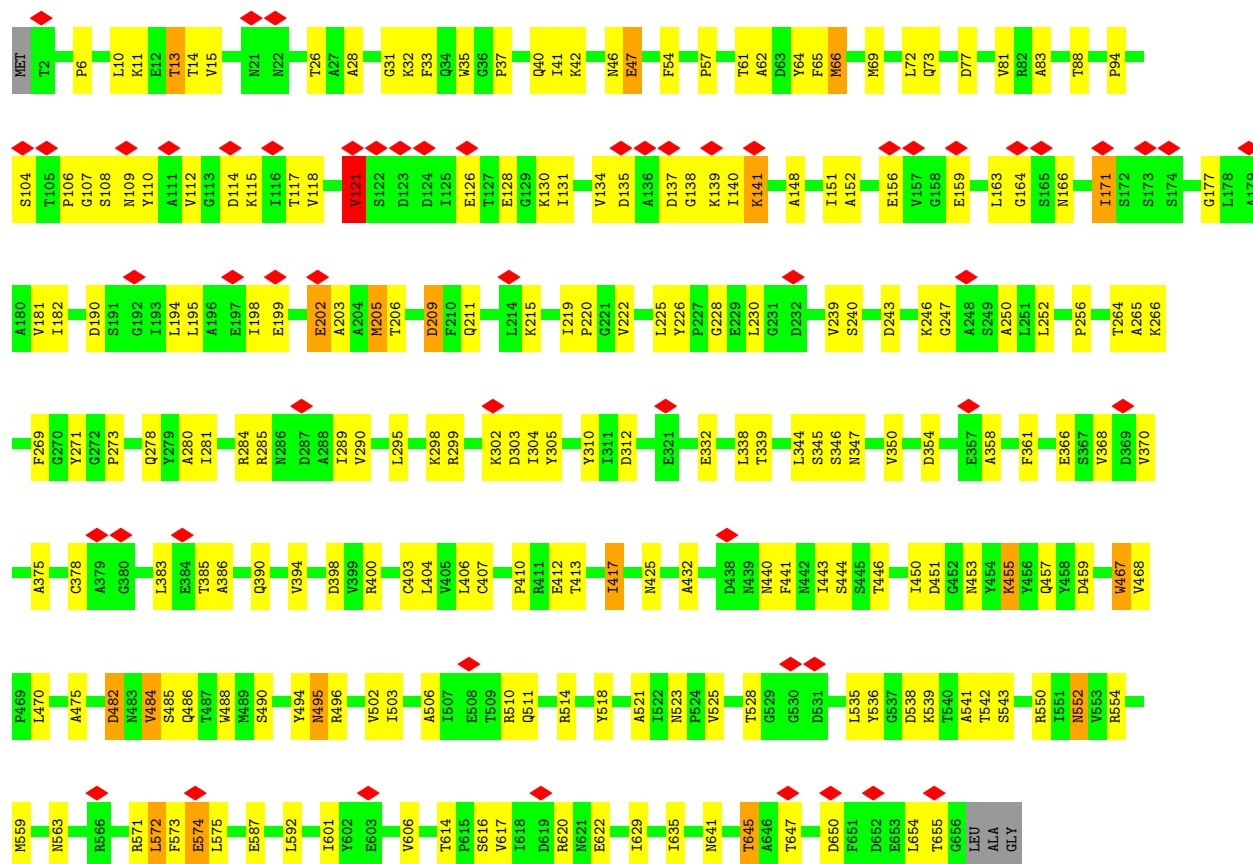


• Molecule 7: gp18, tail sheath protein

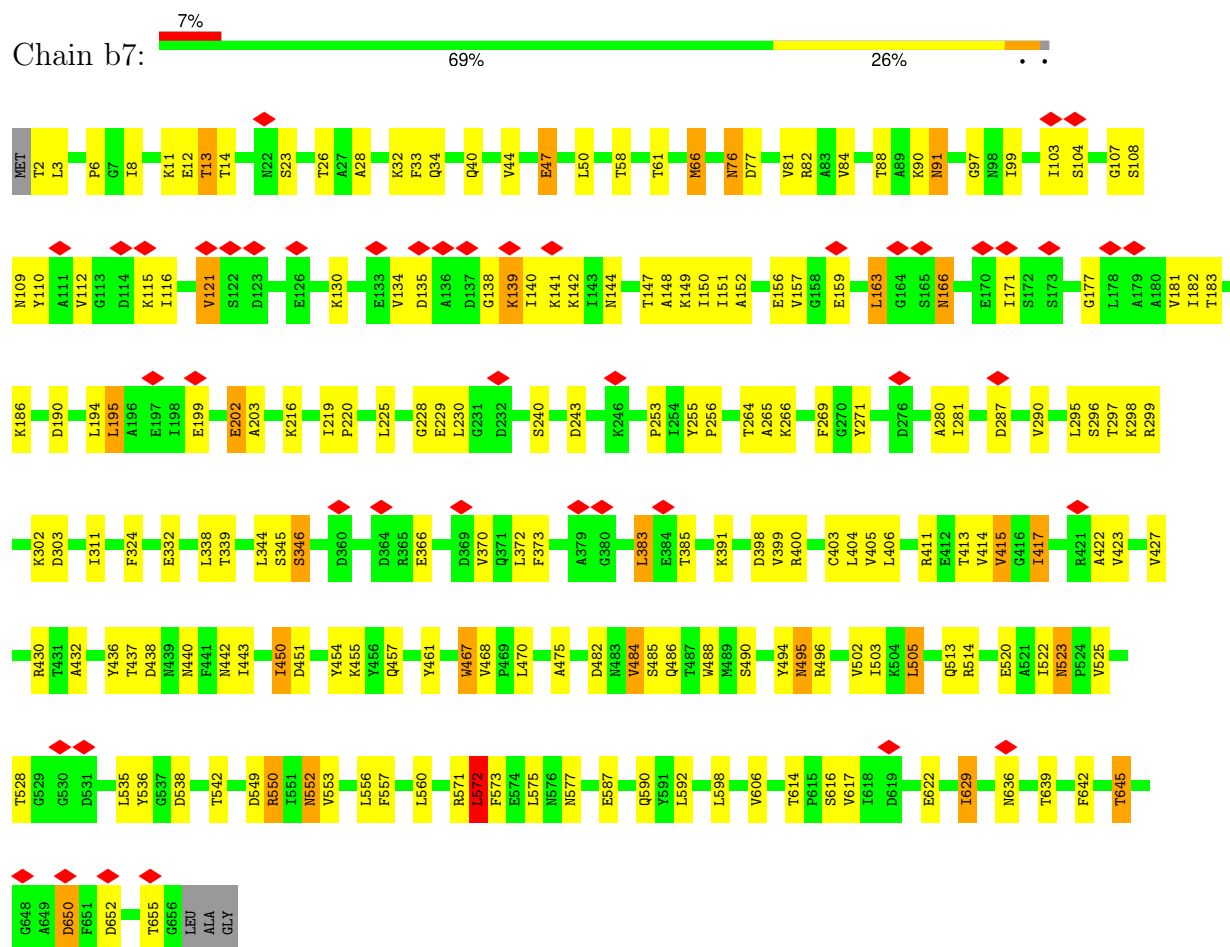




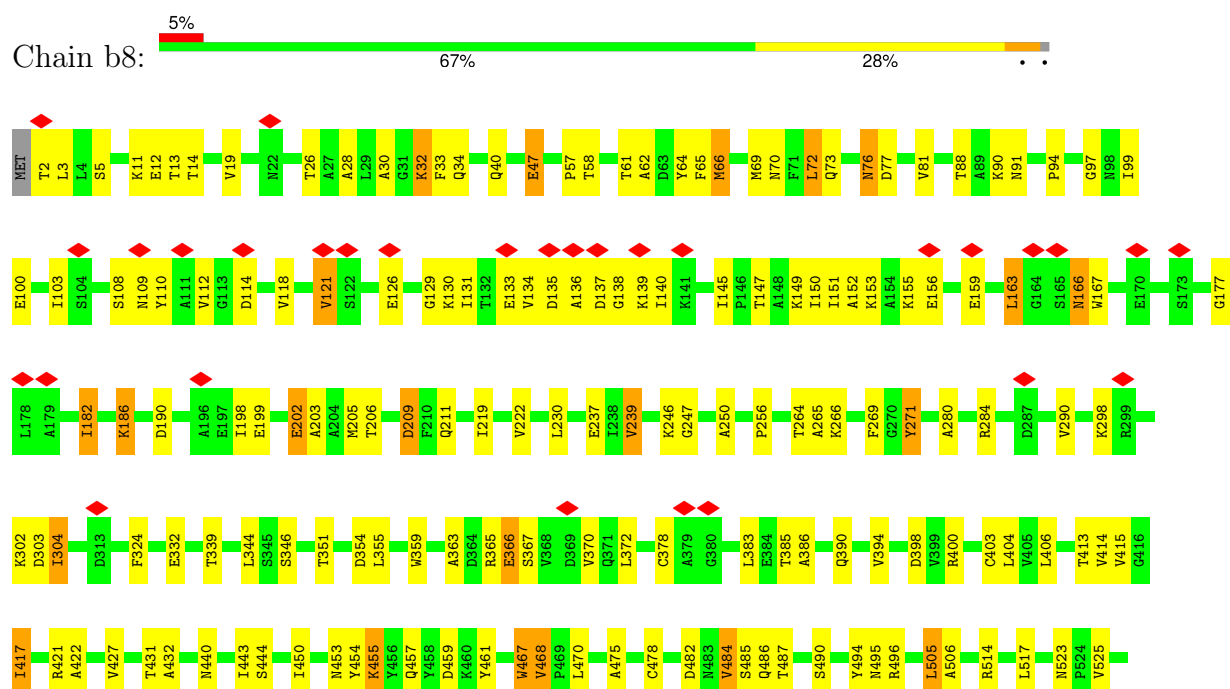
• Molecule 7: gp18, tail sheath protein



- Molecule 7: gp18, tail sheath protein

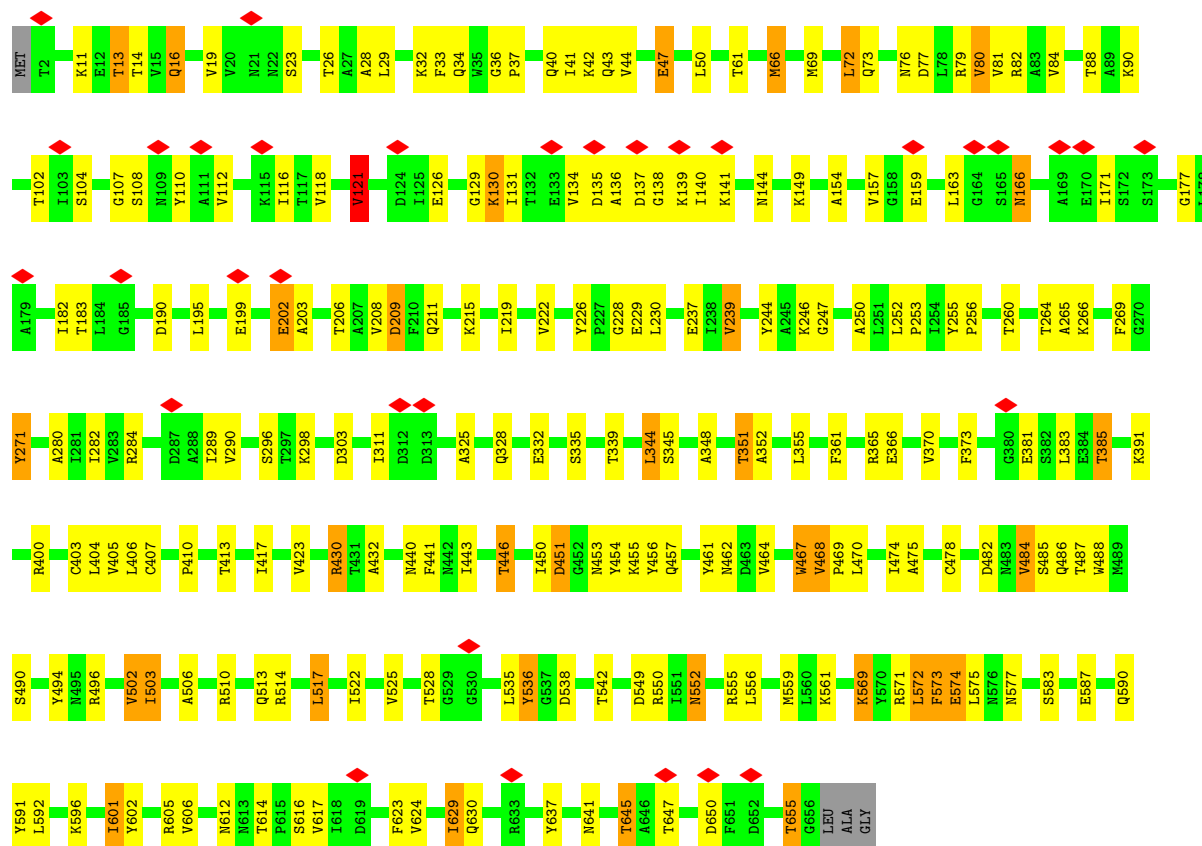


- Molecule 7: gp18, tail sheath protein

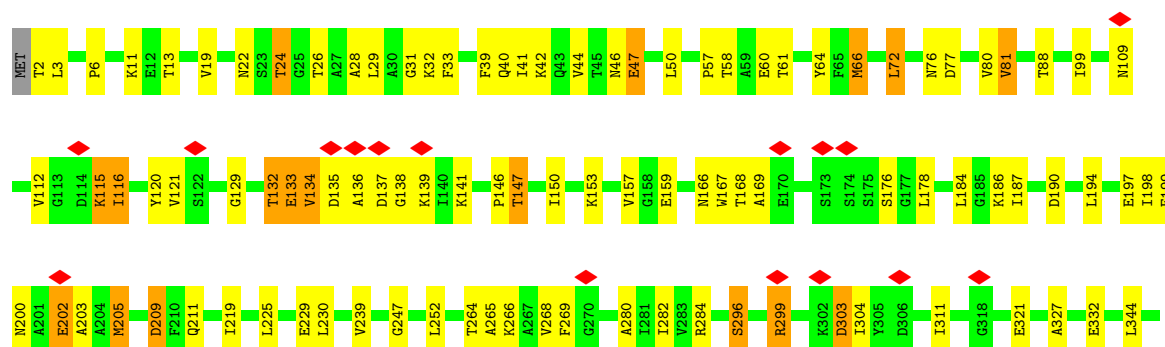


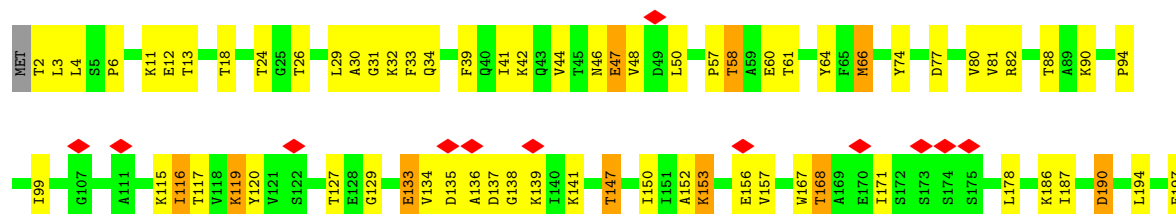


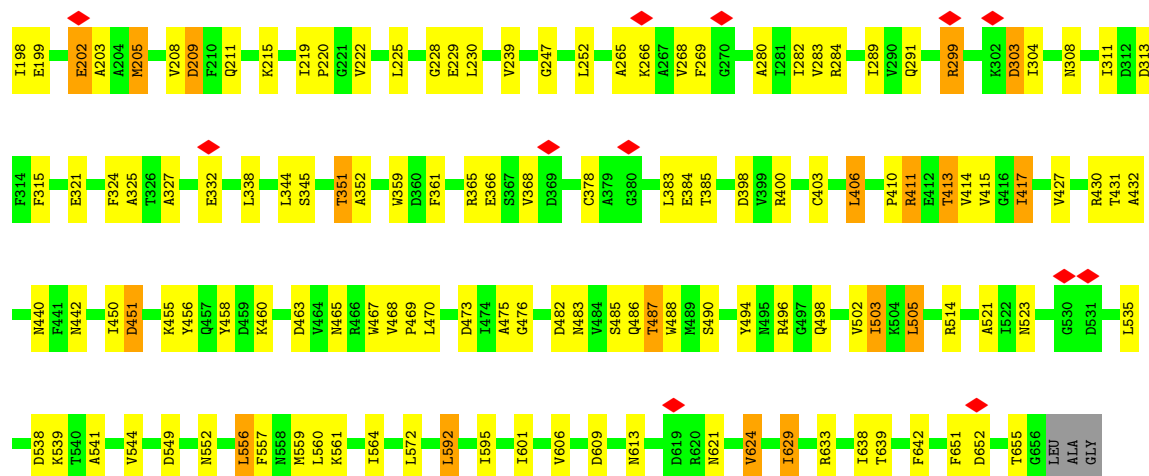
• Molecule 7: gp18, tail sheath protein



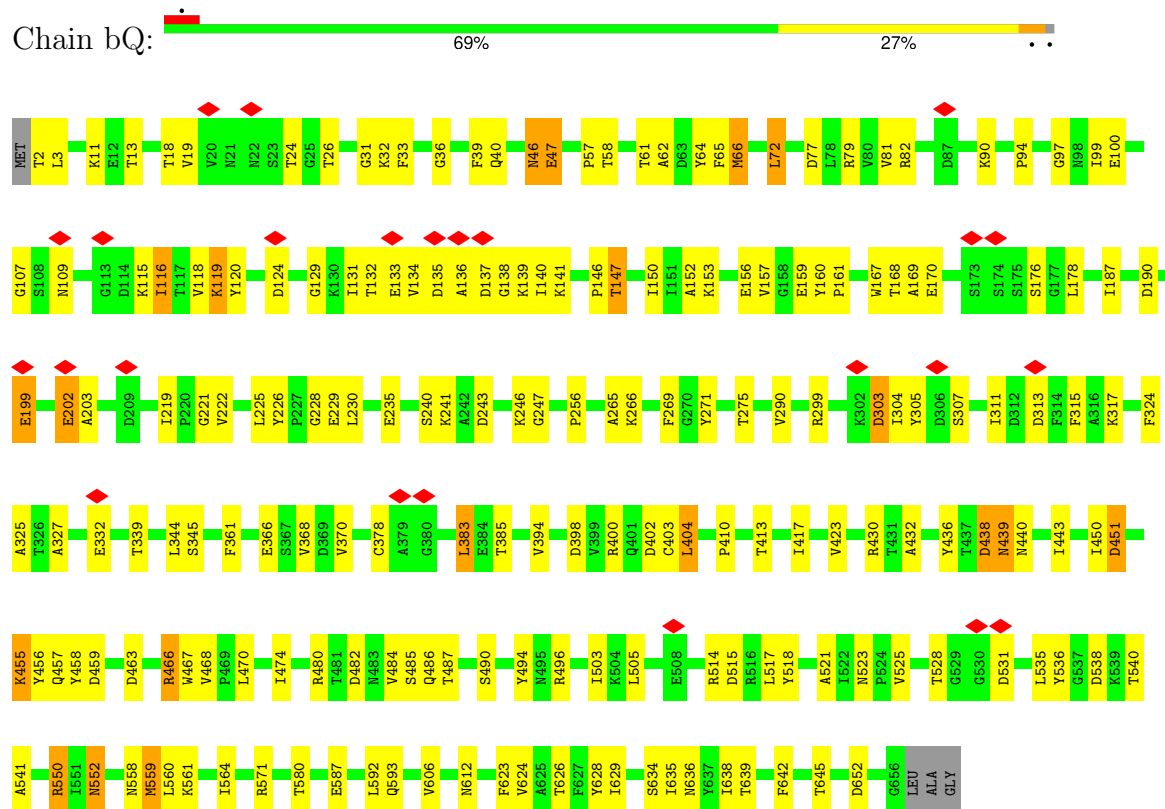
• Molecule 7: gp18, tail sheath protein



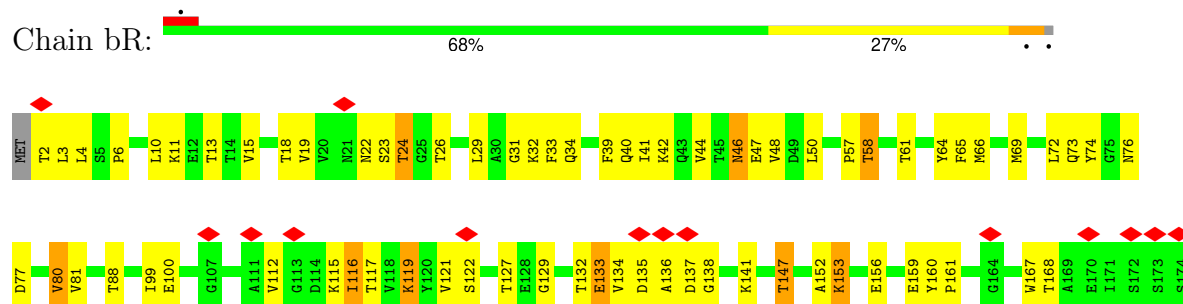


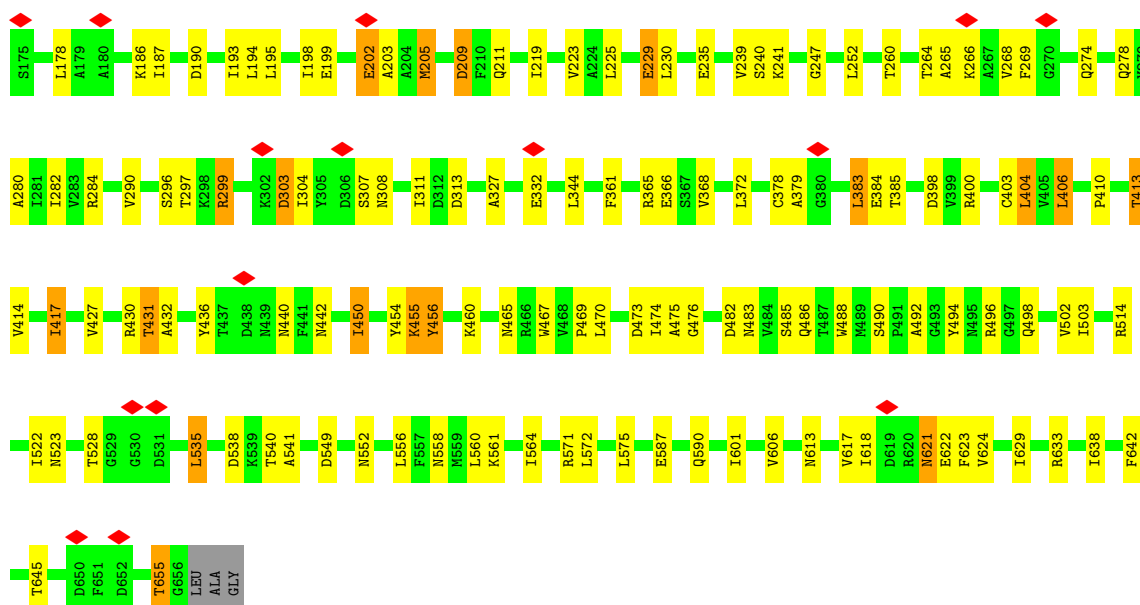


- Molecule 7: gp18, tail sheath protein

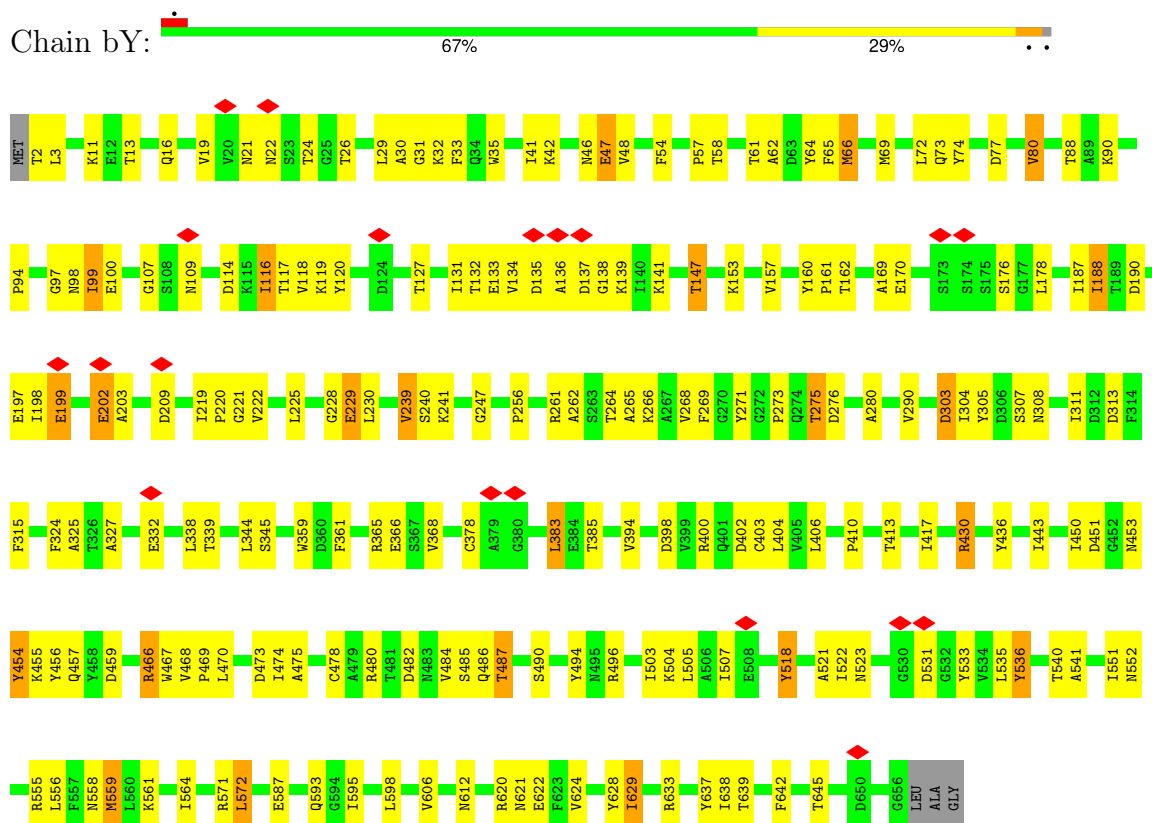


- Molecule 7: gp18, tail sheath protein



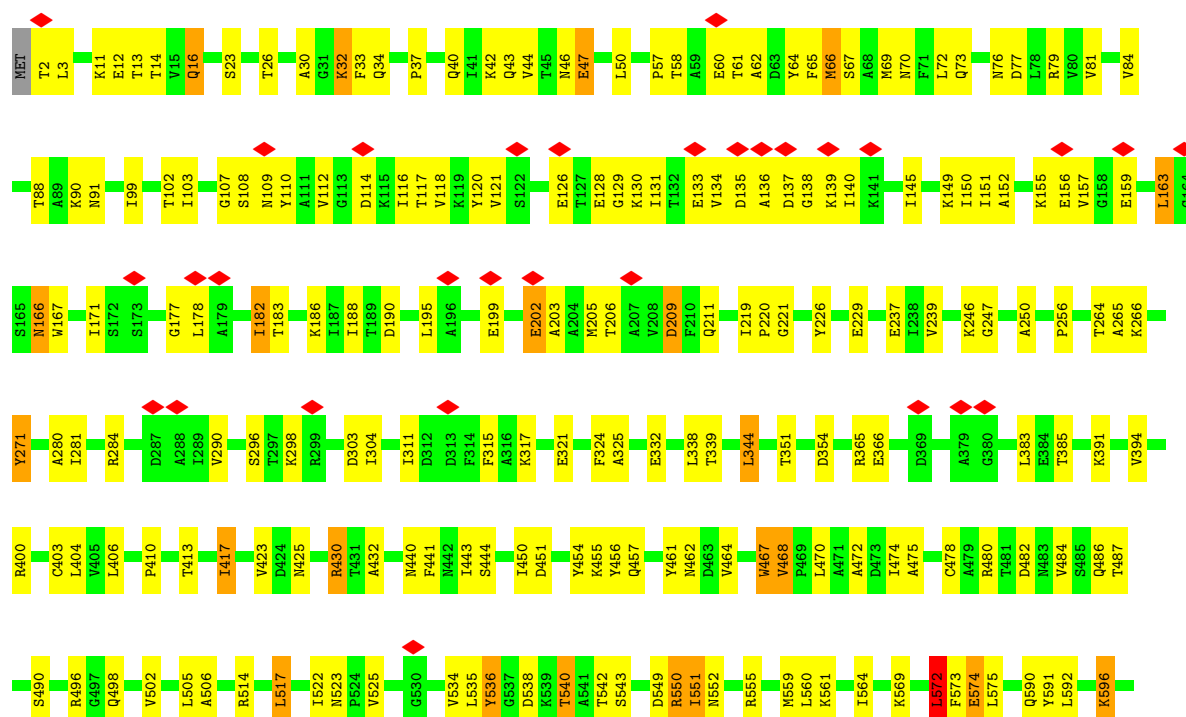


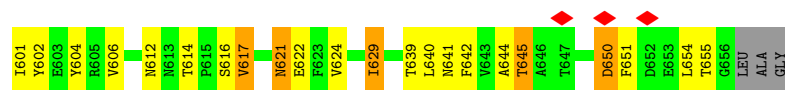
- Molecule 7: gp18, tail sheath protein



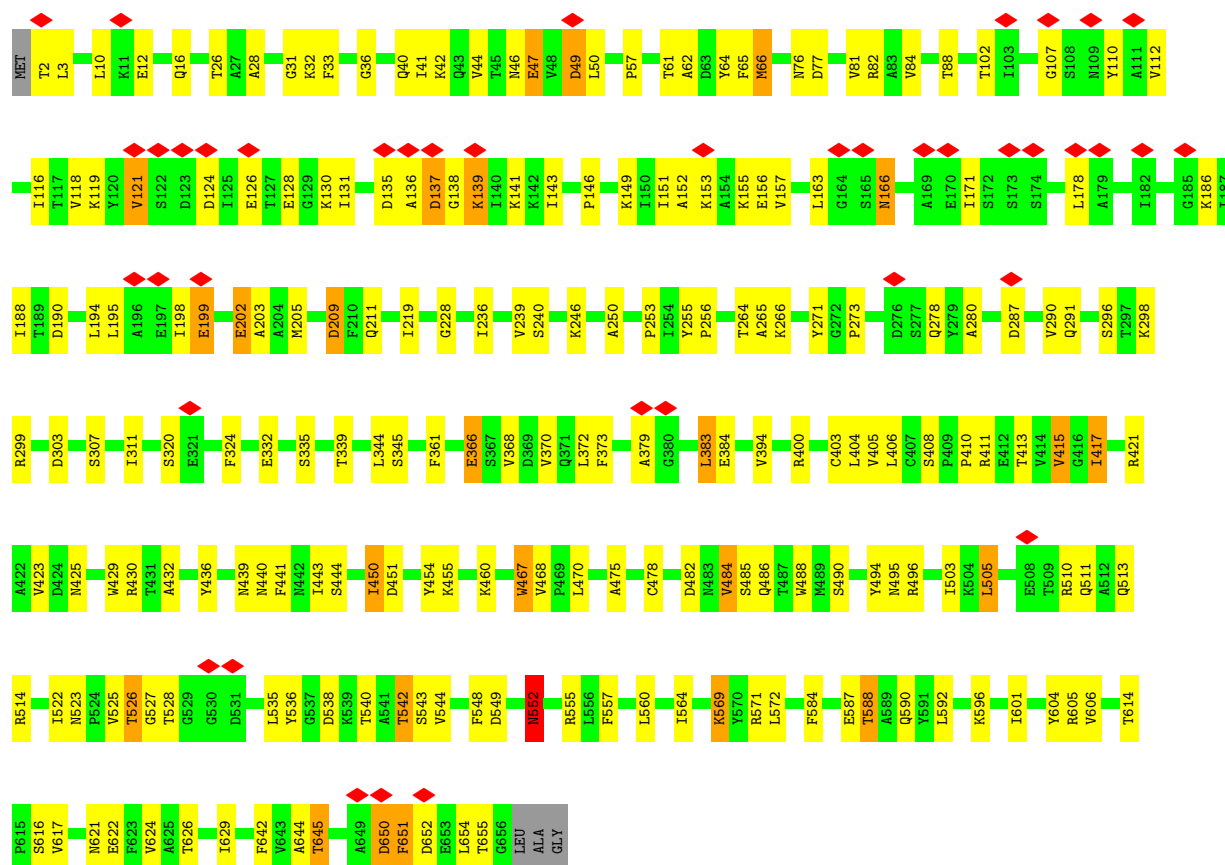
- Molecule 7: gp18, tail sheath protein



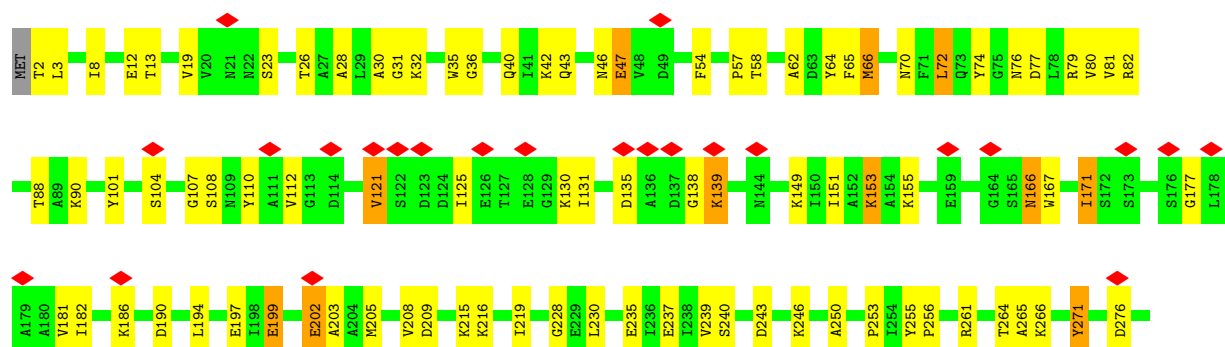


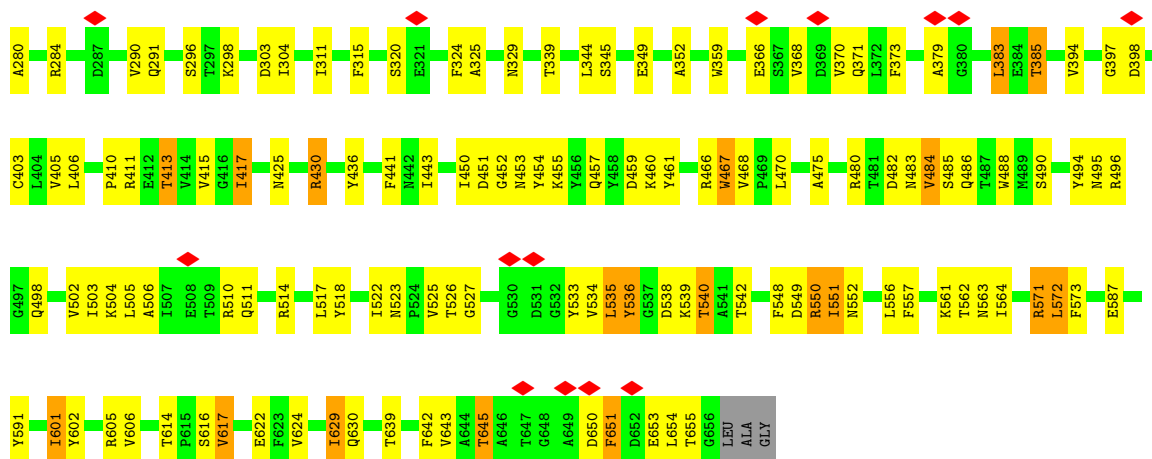


• Molecule 7: gp18, tail sheath protein

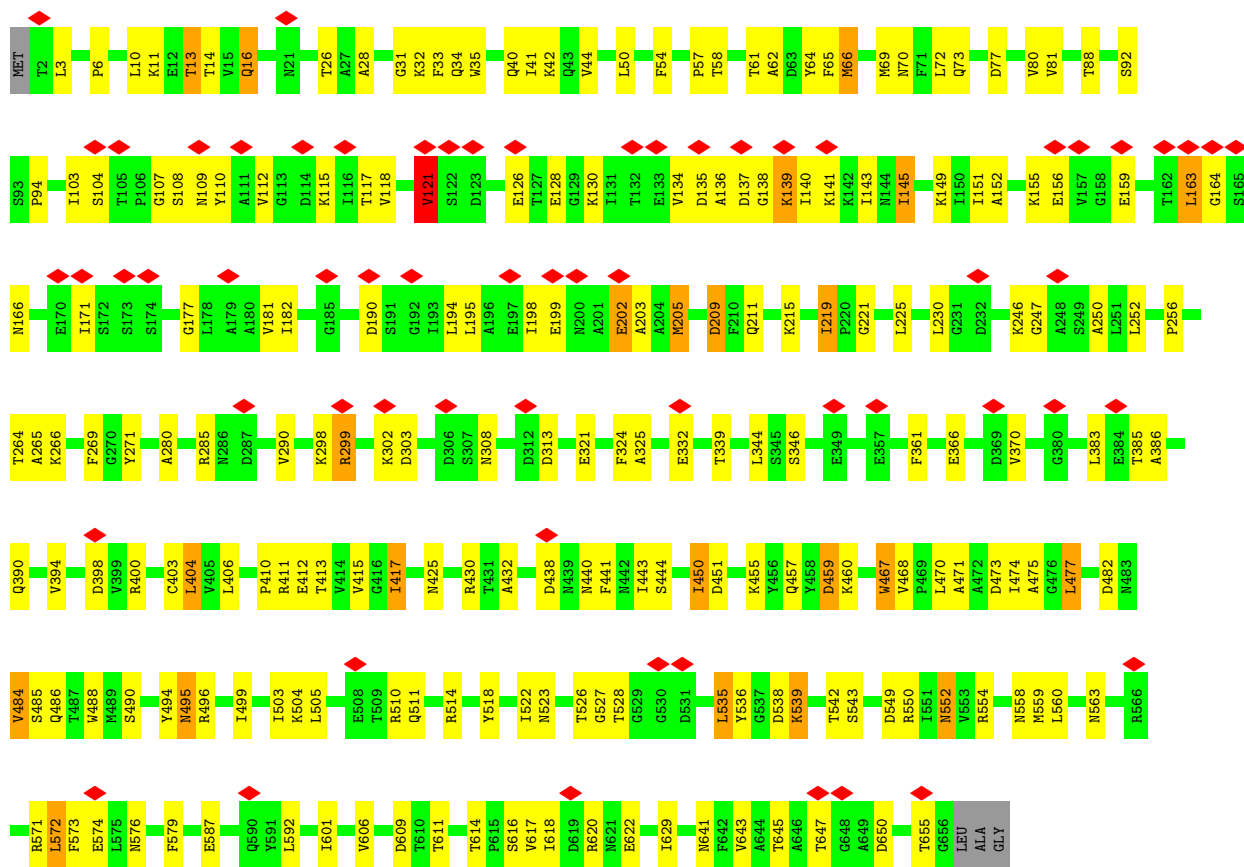


• Molecule 7: gp18, tail sheath protein

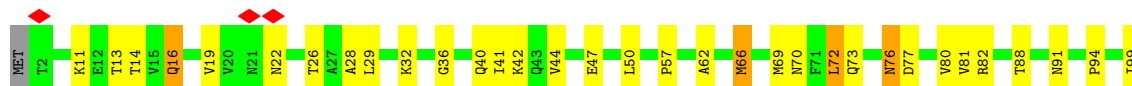


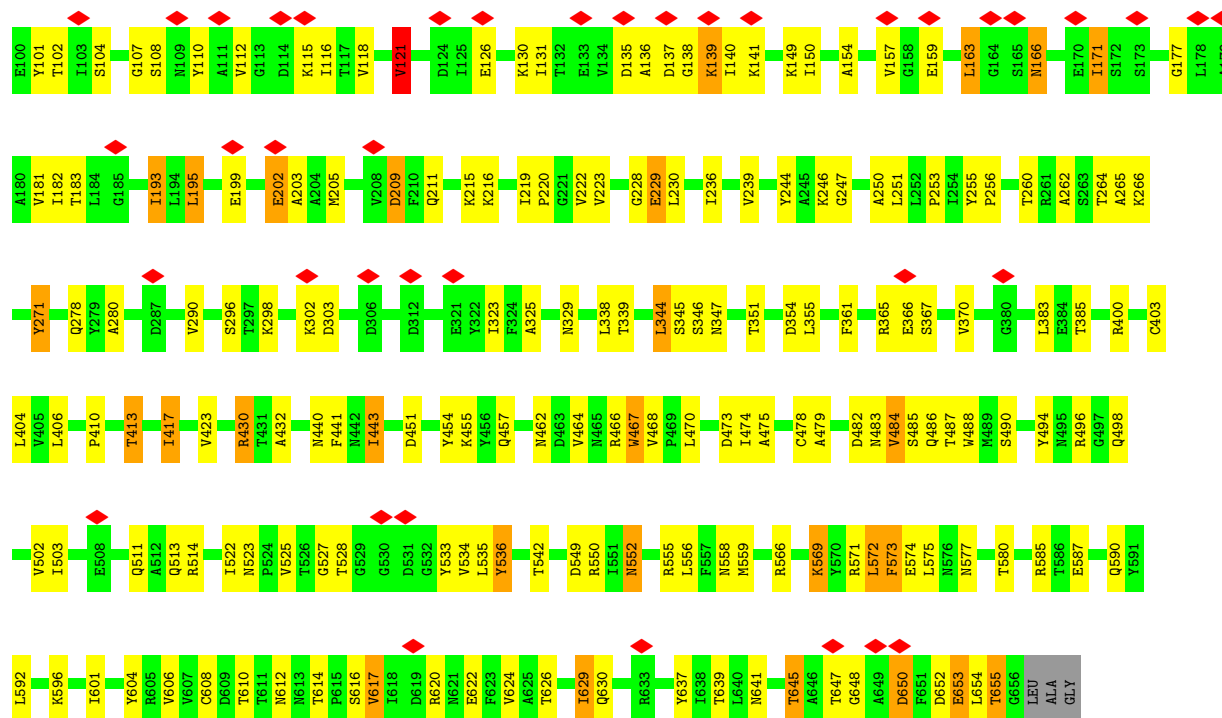


• Molecule 7: gp18, tail sheath protein

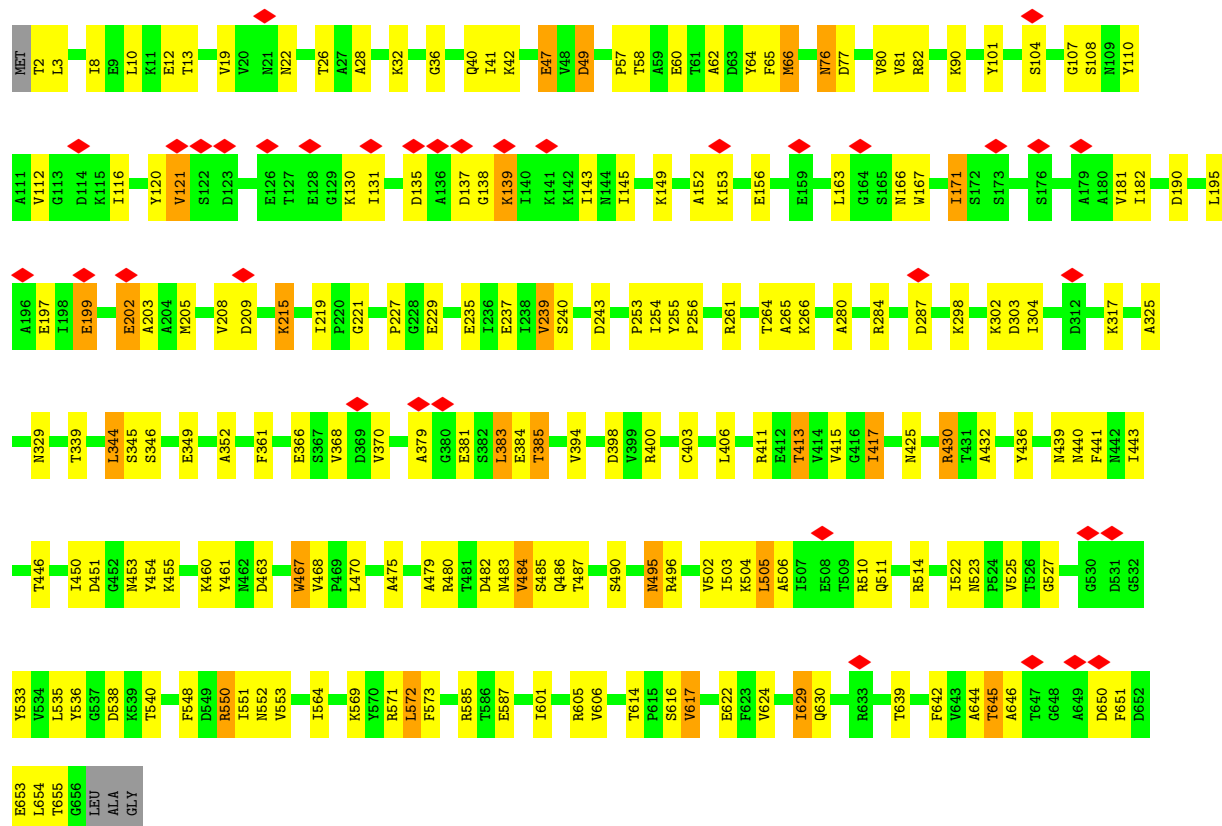


• Molecule 7: gp18, tail sheath protein

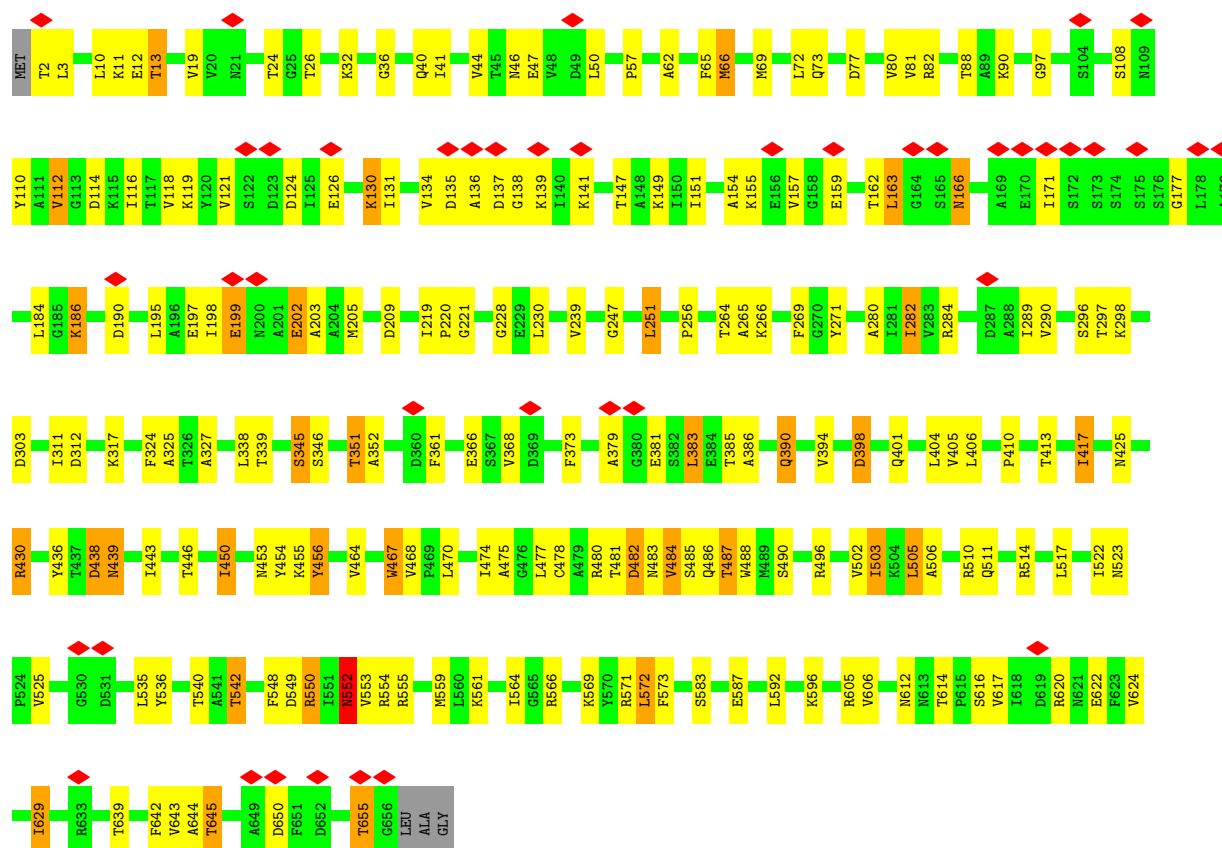




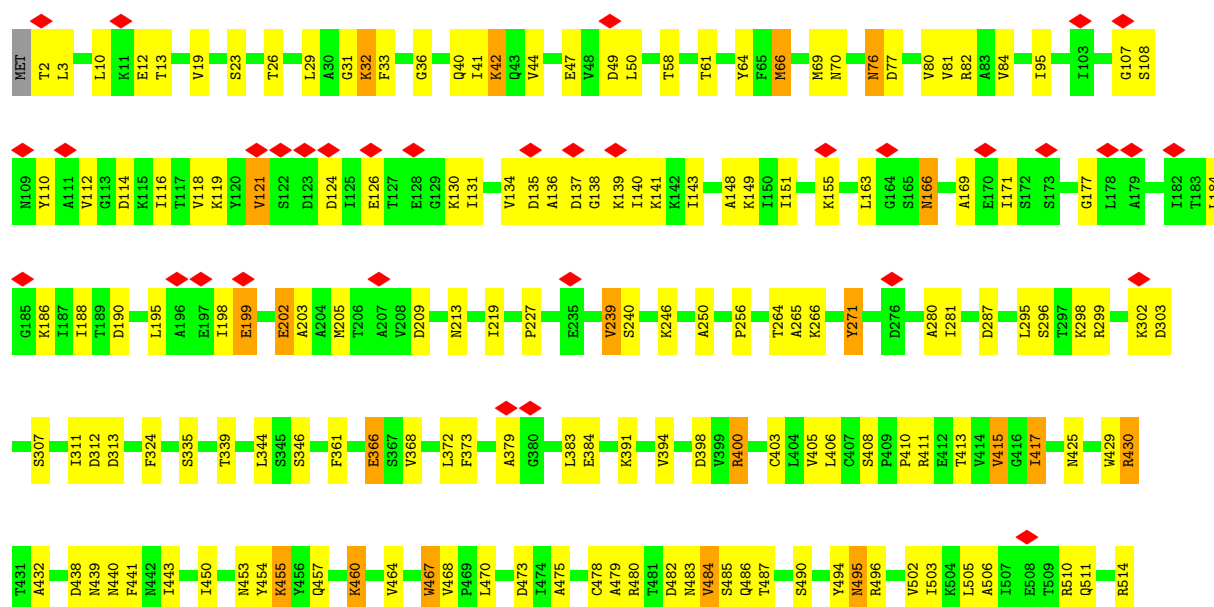
• Molecule 7: gp18, tail sheath protein

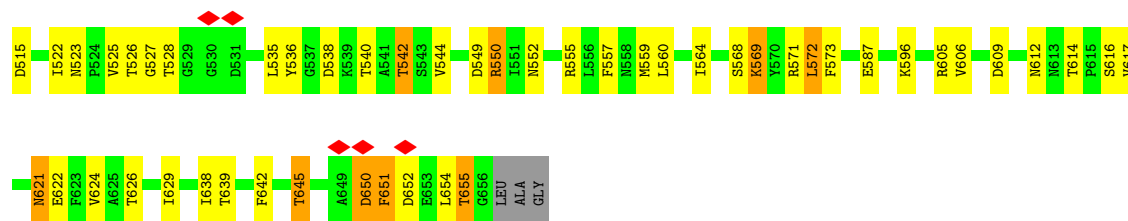


• Molecule 7: gp18, tail sheath protein

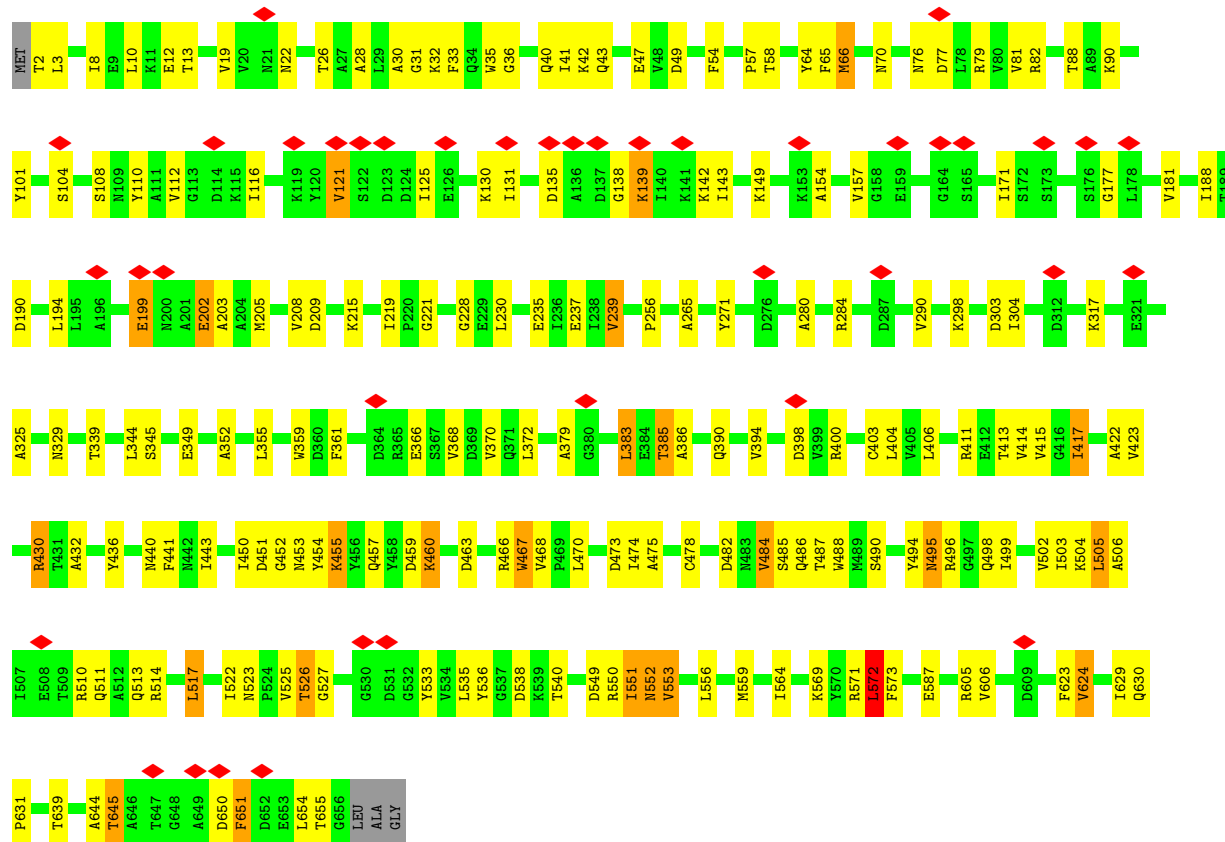


• Molecule 7: gp18, tail sheath protein

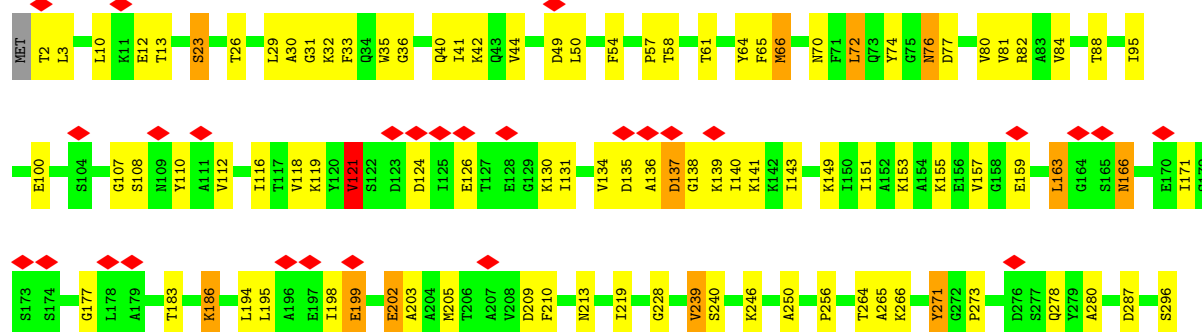


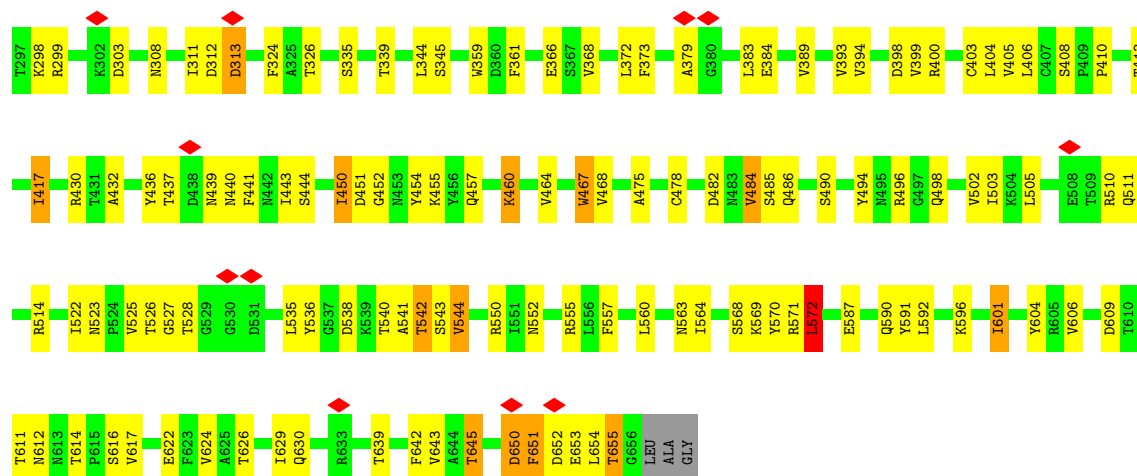


• Molecule 7: gp18, tail sheath protein

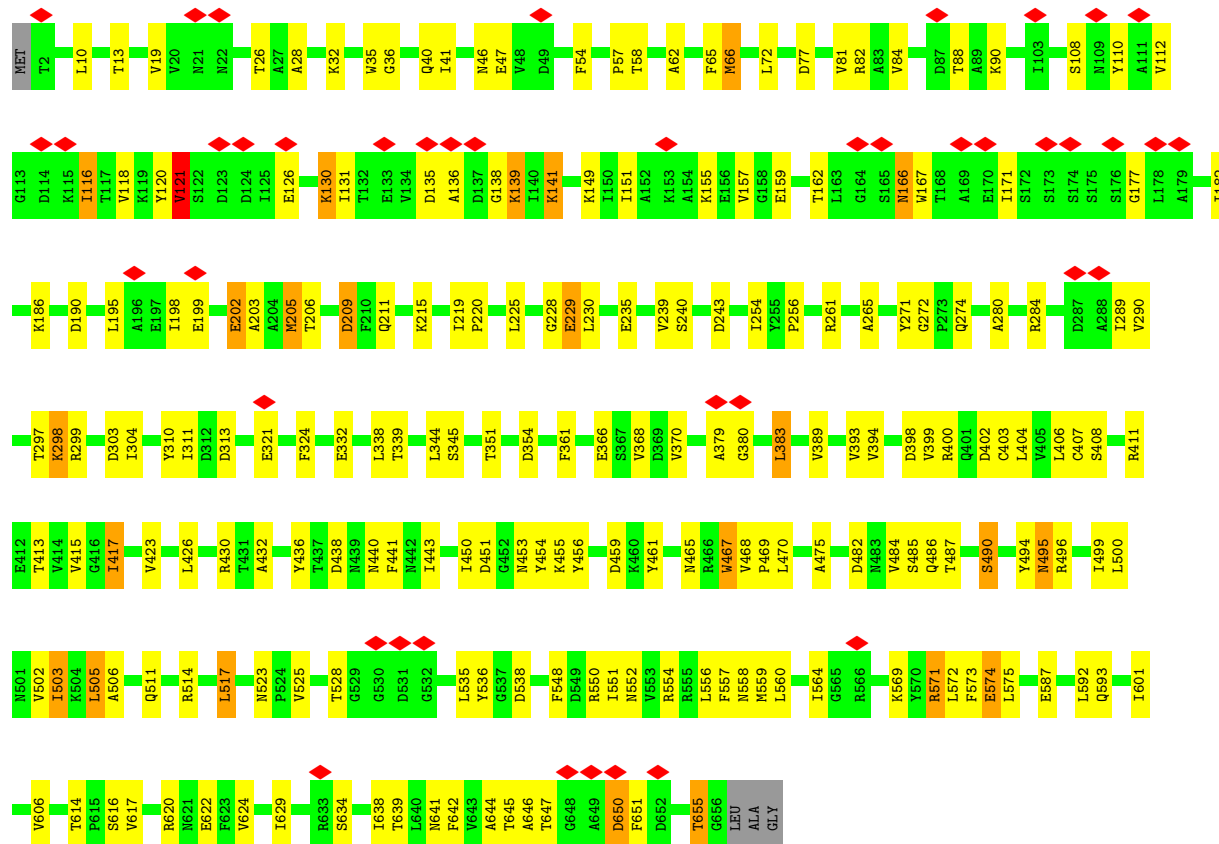


• Molecule 7: gp18, tail sheath protein



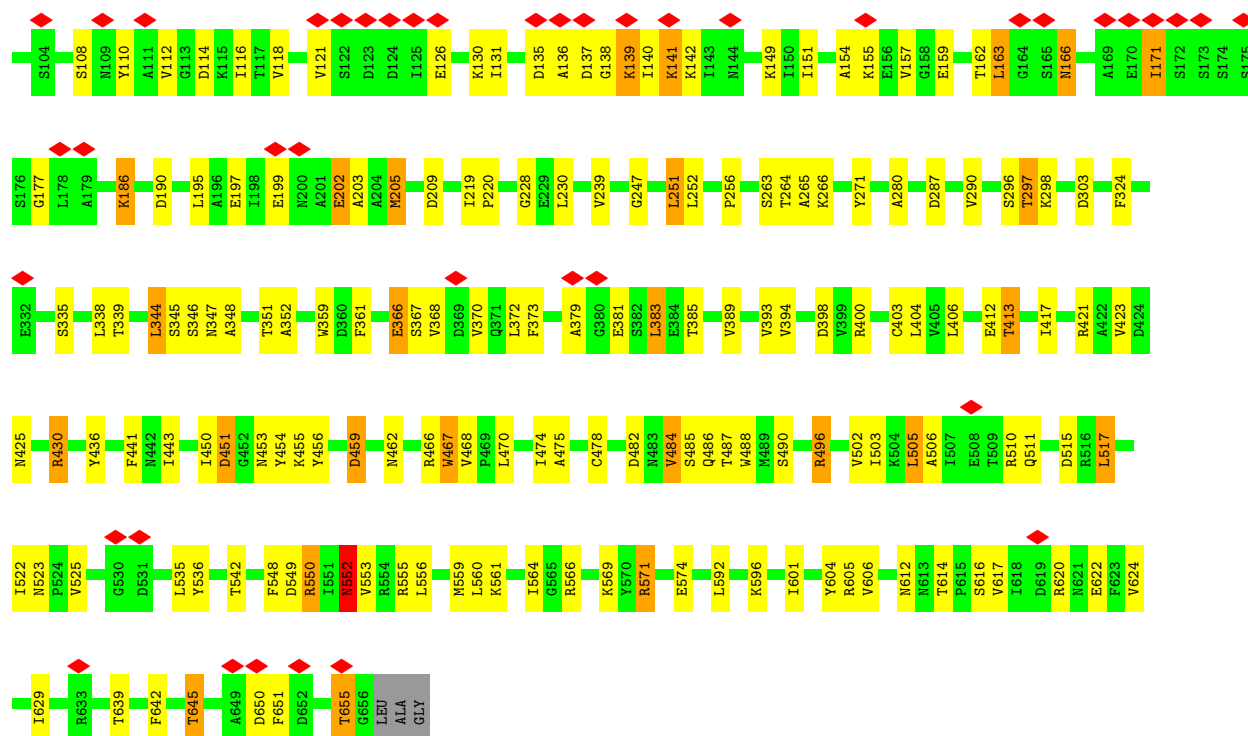


- Molecule 7: gp18, tail sheath protein

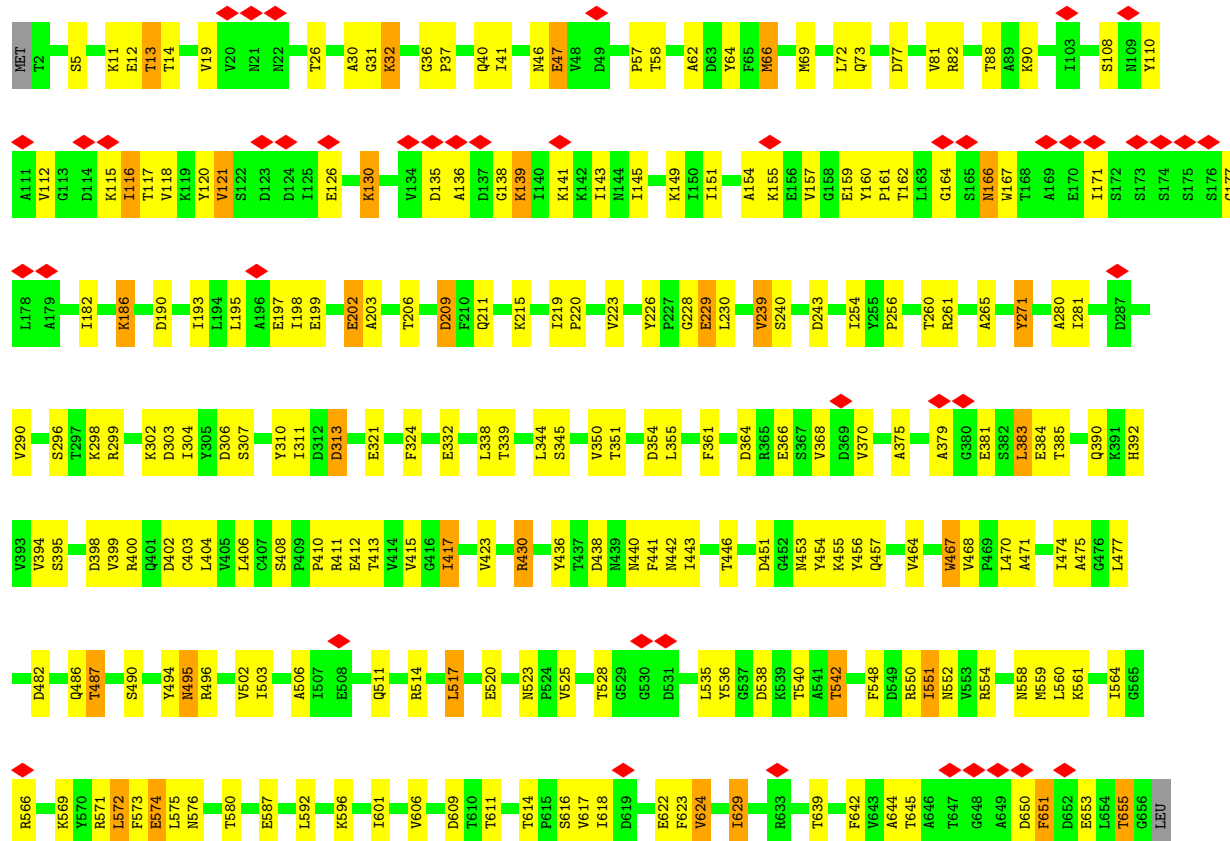


- Molecule 7: gp18, tail sheath protein



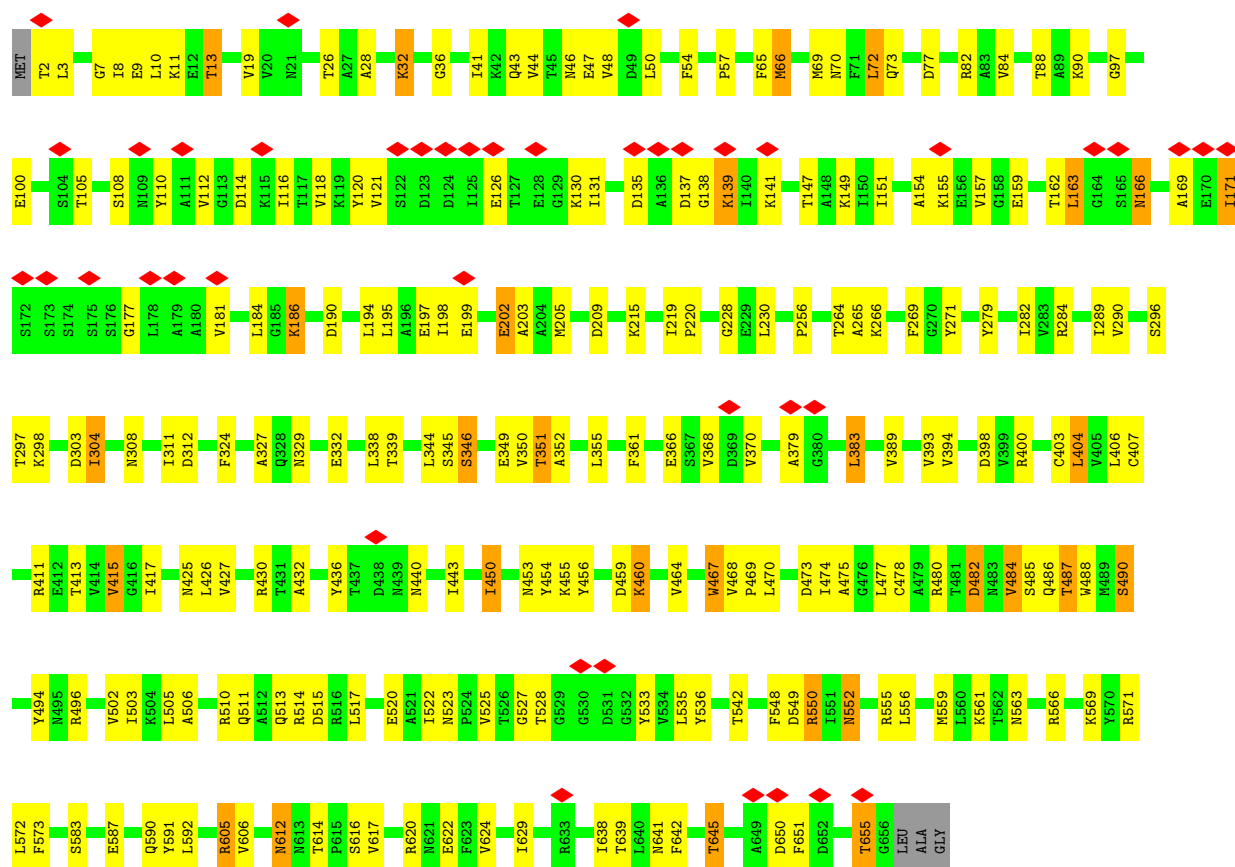


• Molecule 7: gp18, tail sheath protein

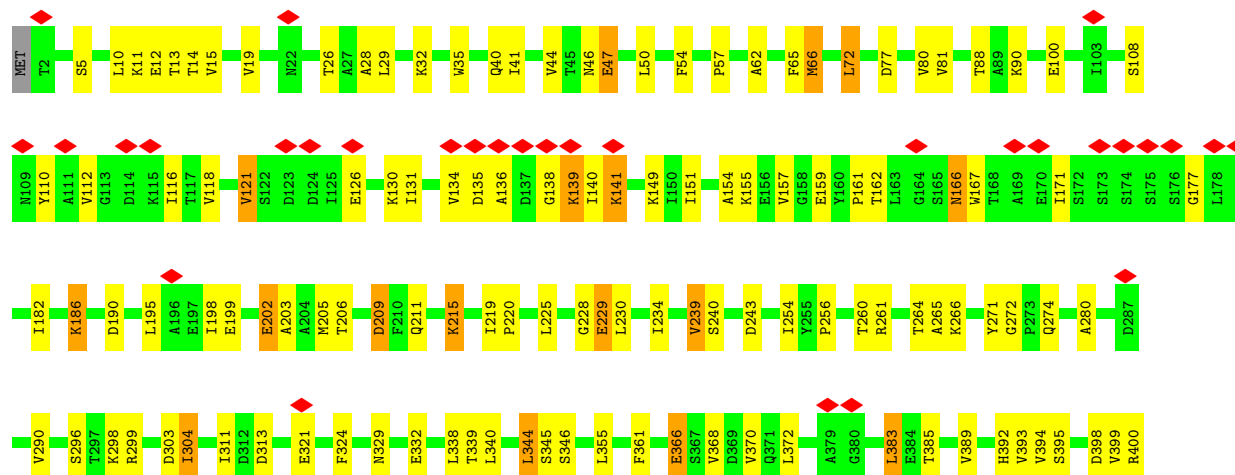


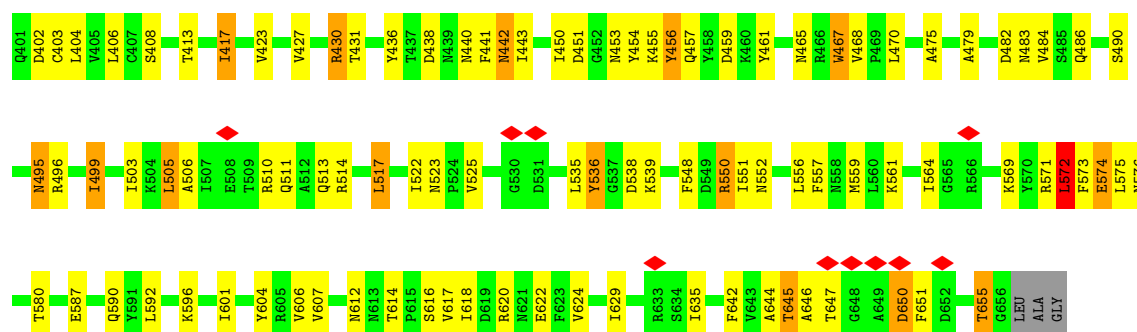
ALA
GLY

- Molecule 7: gp18, tail sheath protein

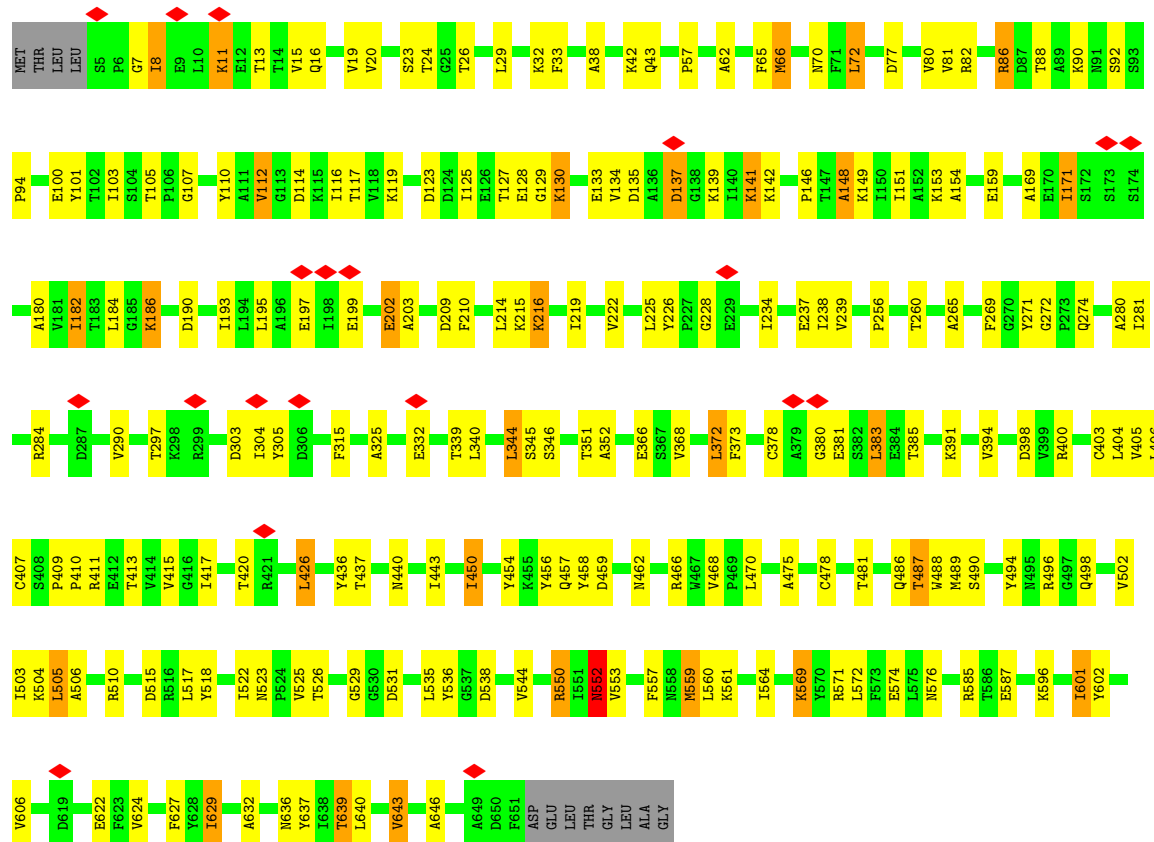


- Molecule 7: gp18, tail sheath protein

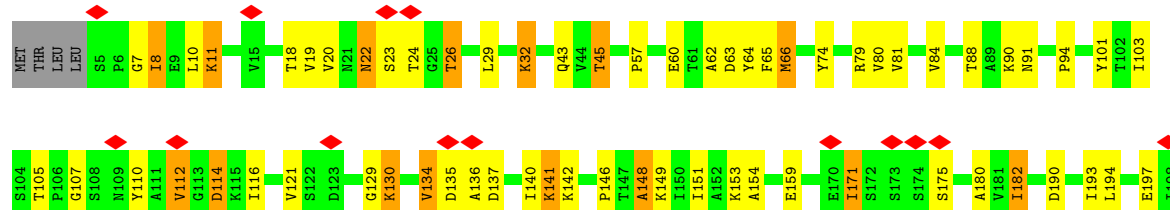


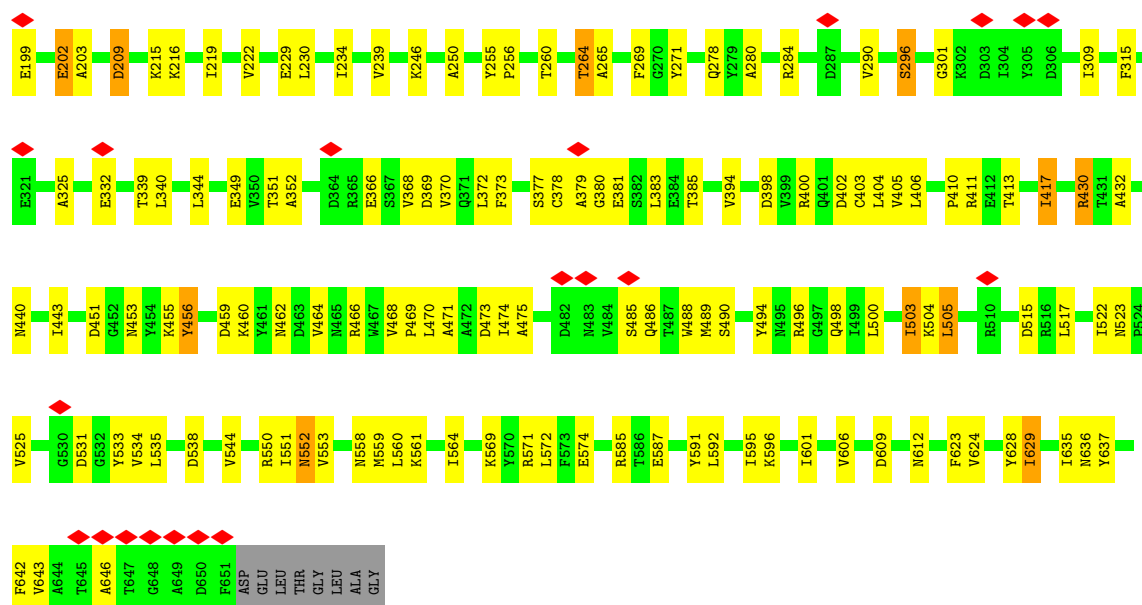


• Molecule 7: gp18, tail sheath protein

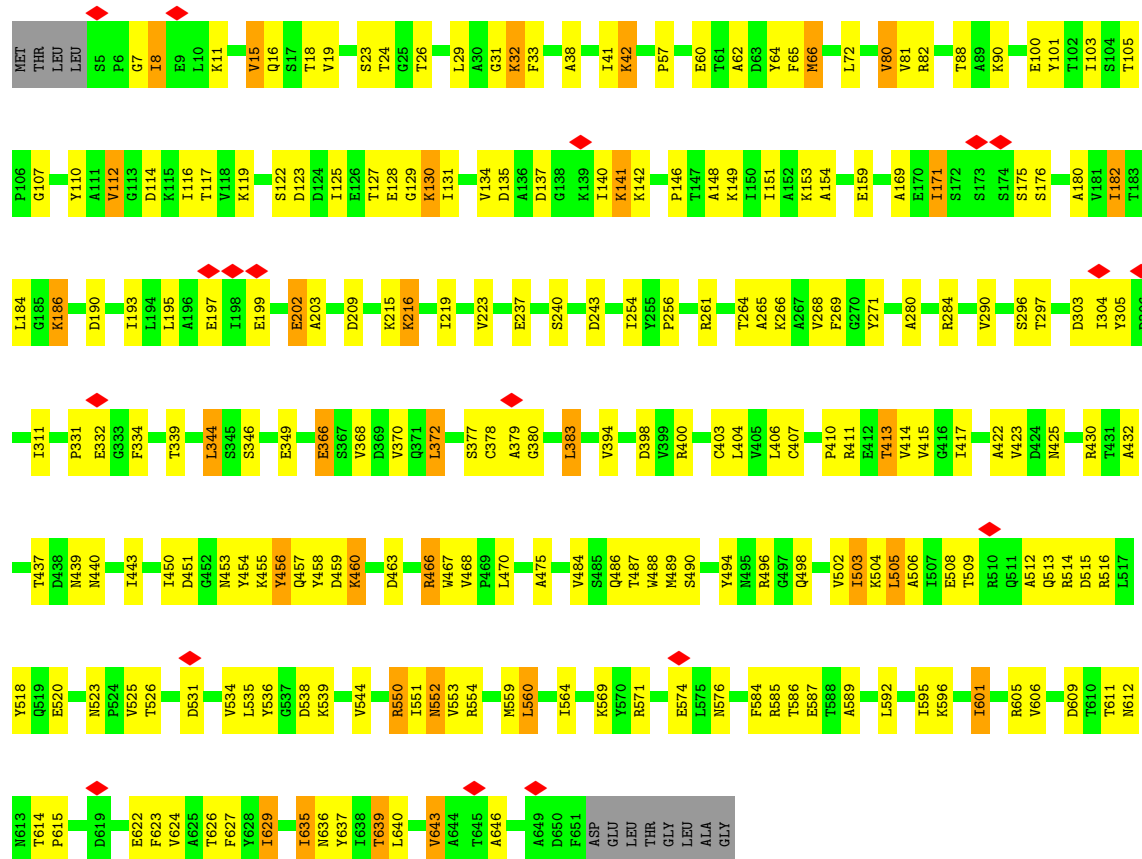


• Molecule 7: gp18, tail sheath protein

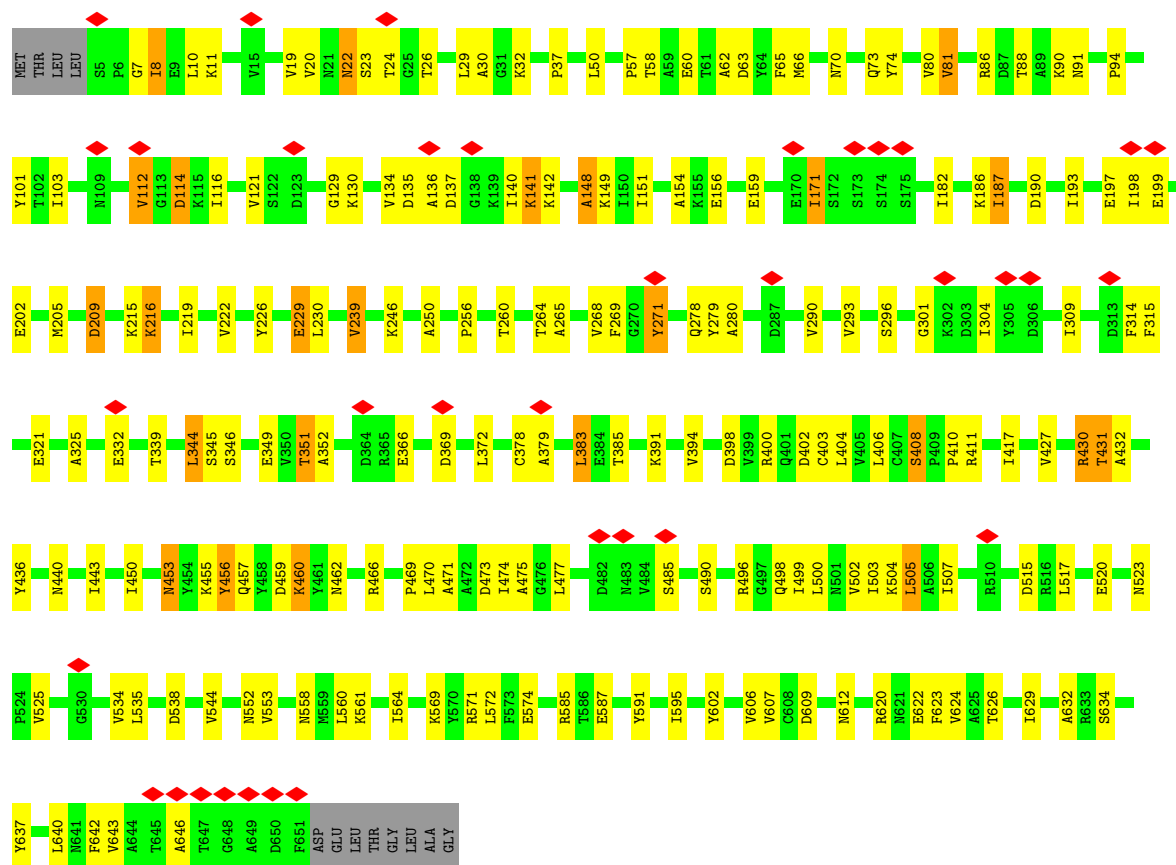




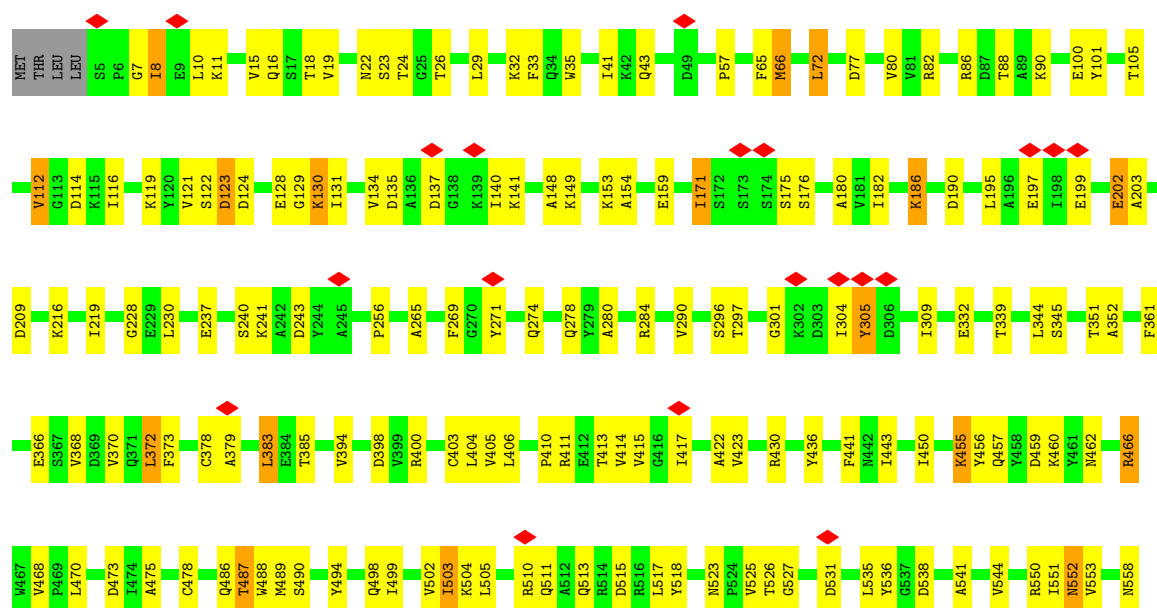
- Molecule 7: gp18, tail sheath protein



- Molecule 7: gp18, tail sheath protein

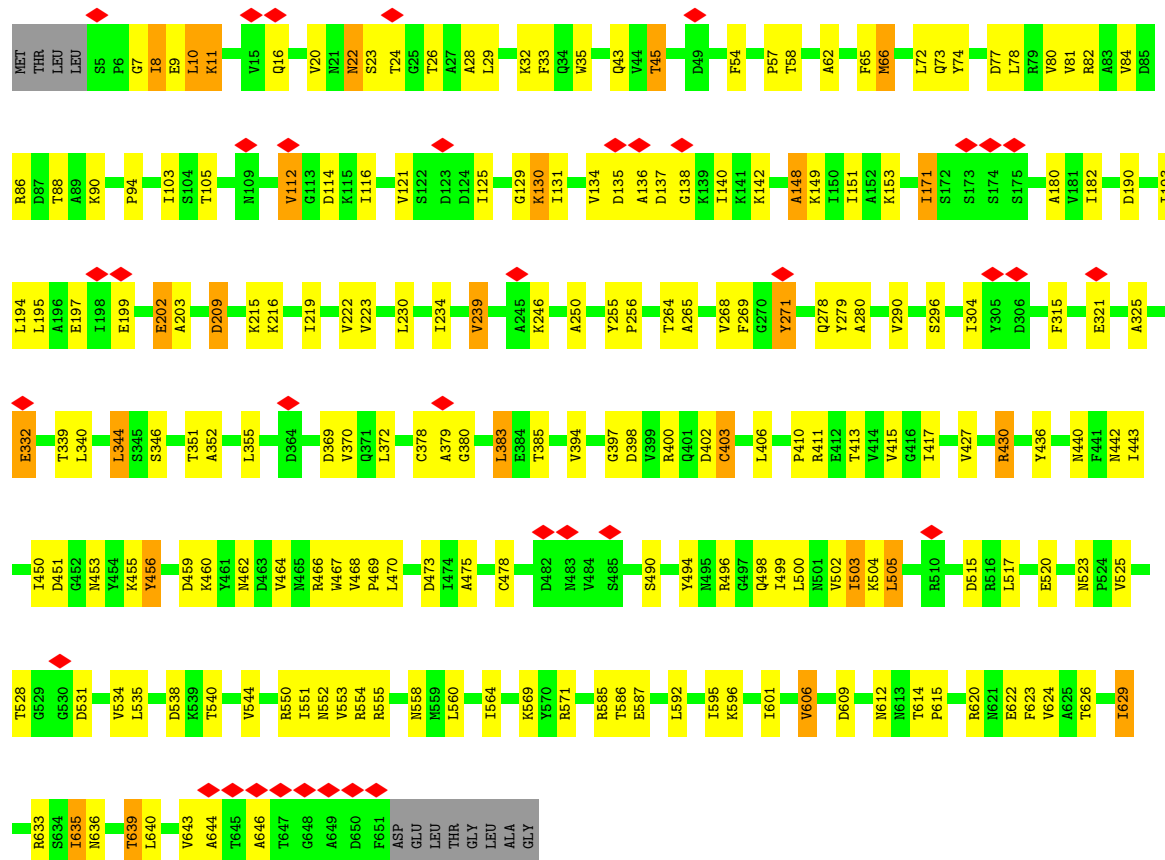


• Molecule 7: gp18, tail sheath protein

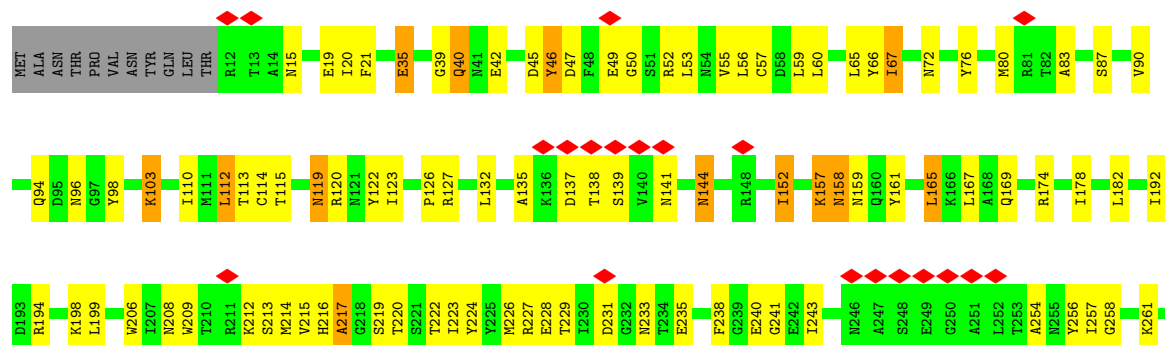


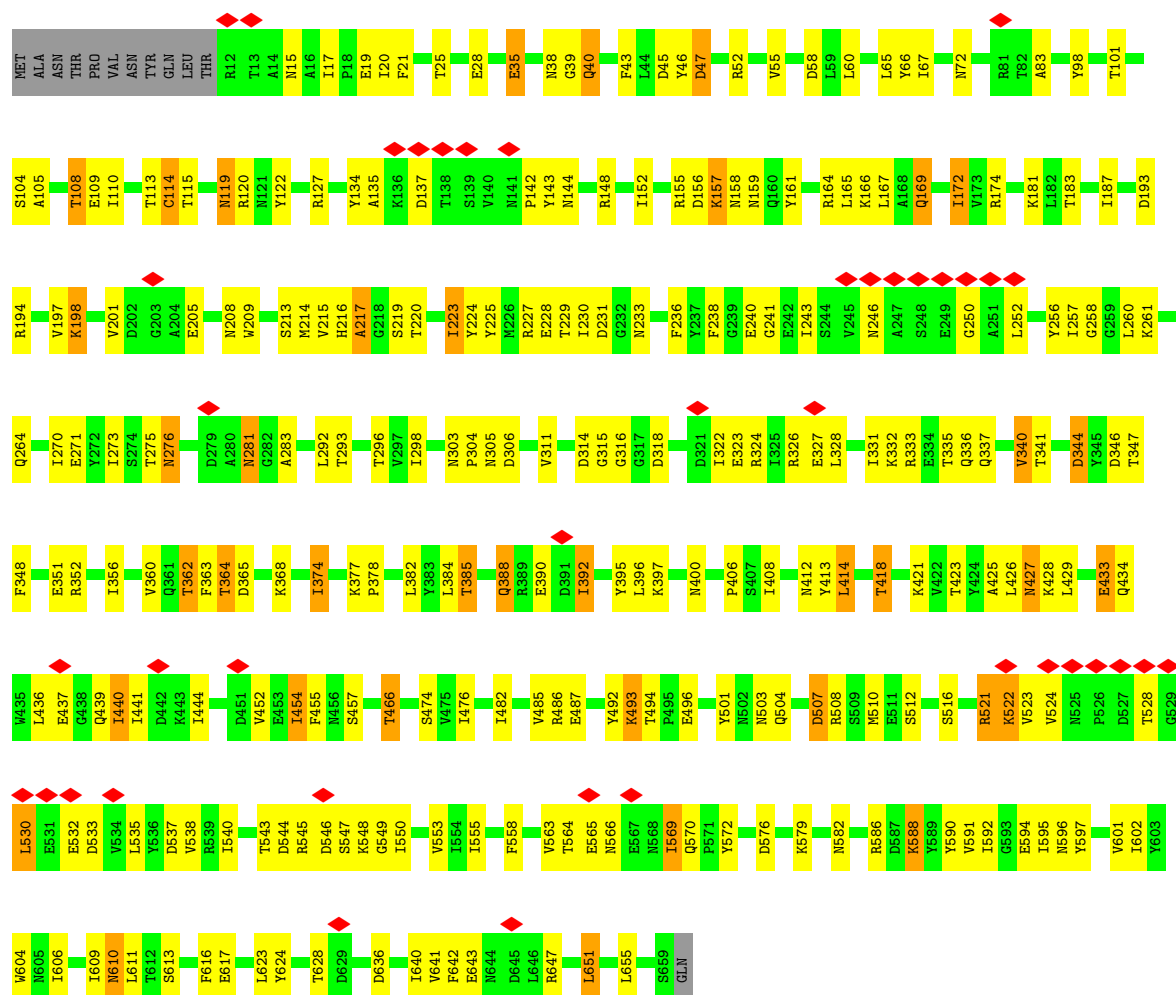


• Molecule 7: gp18, tail sheath protein

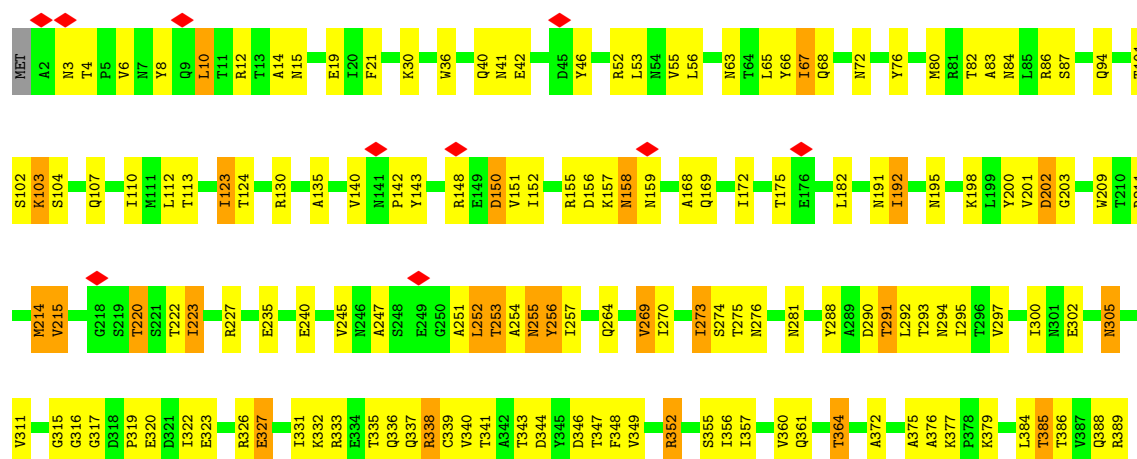


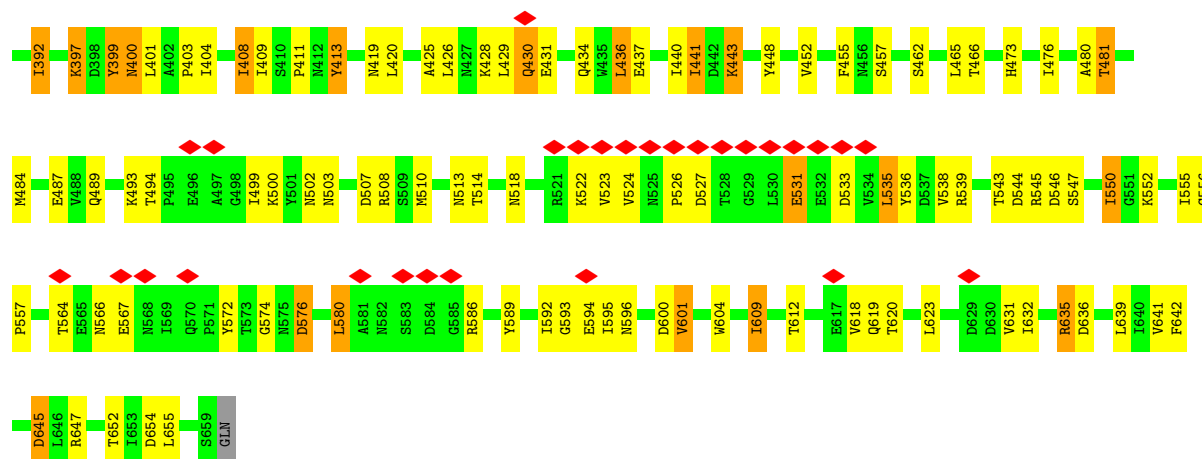
• Molecule 8: gp6, baseplate wedge protein



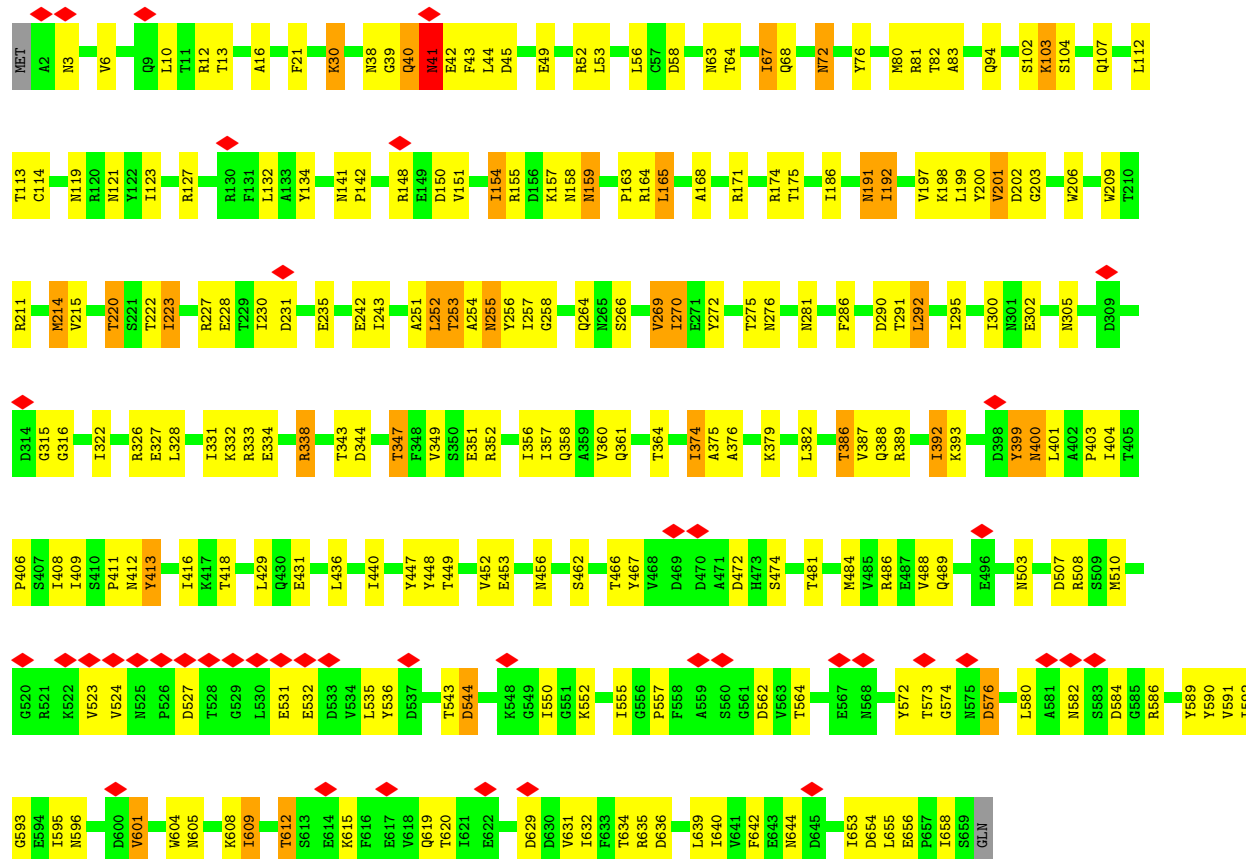


Chain eW:



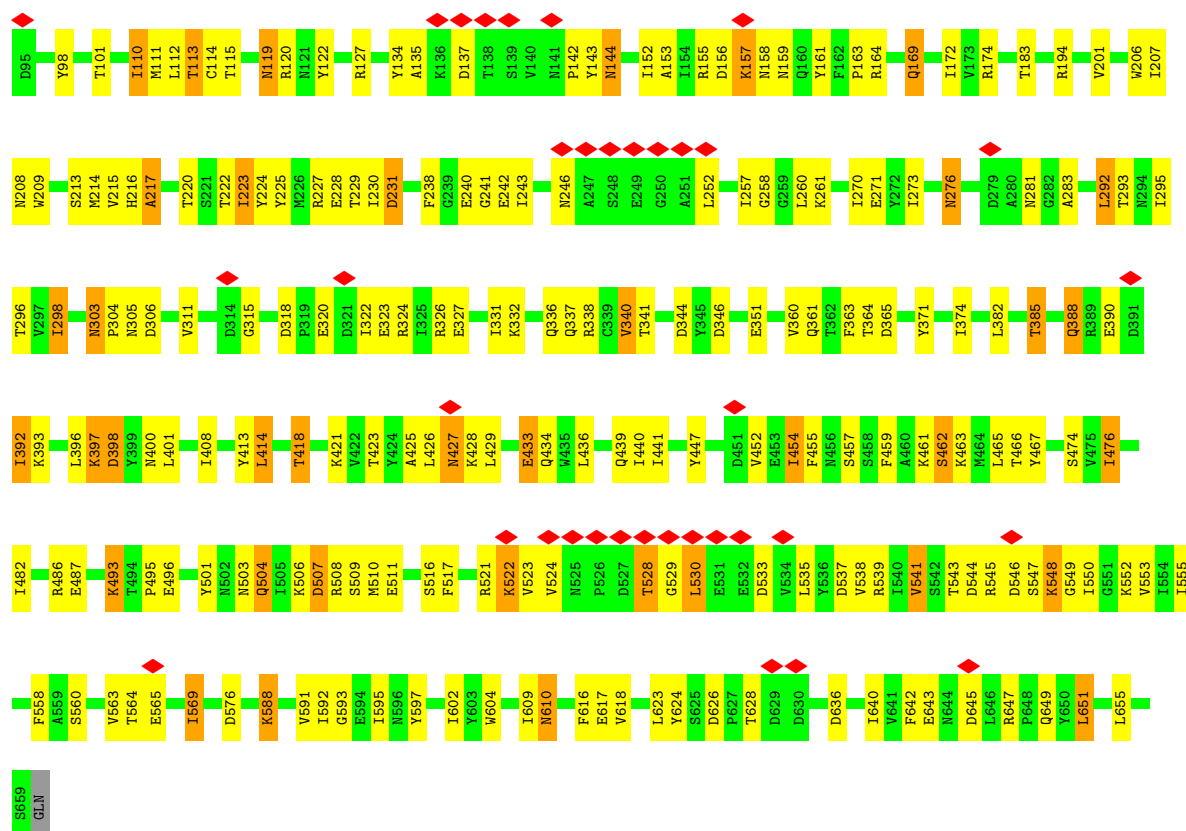


• Molecule 8: gp6, baseplate wedge protein

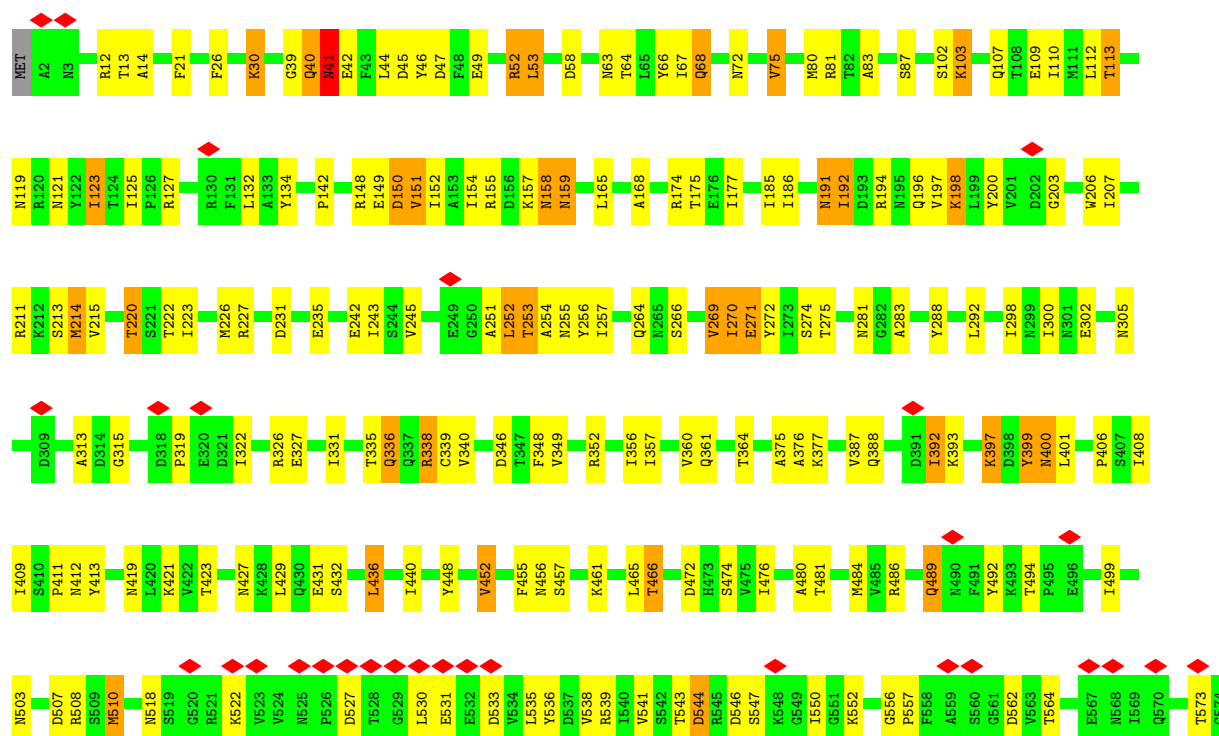


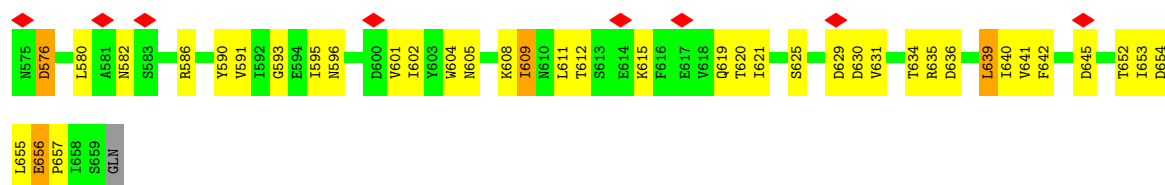
• Molecule 8: gp6, baseplate wedge protein



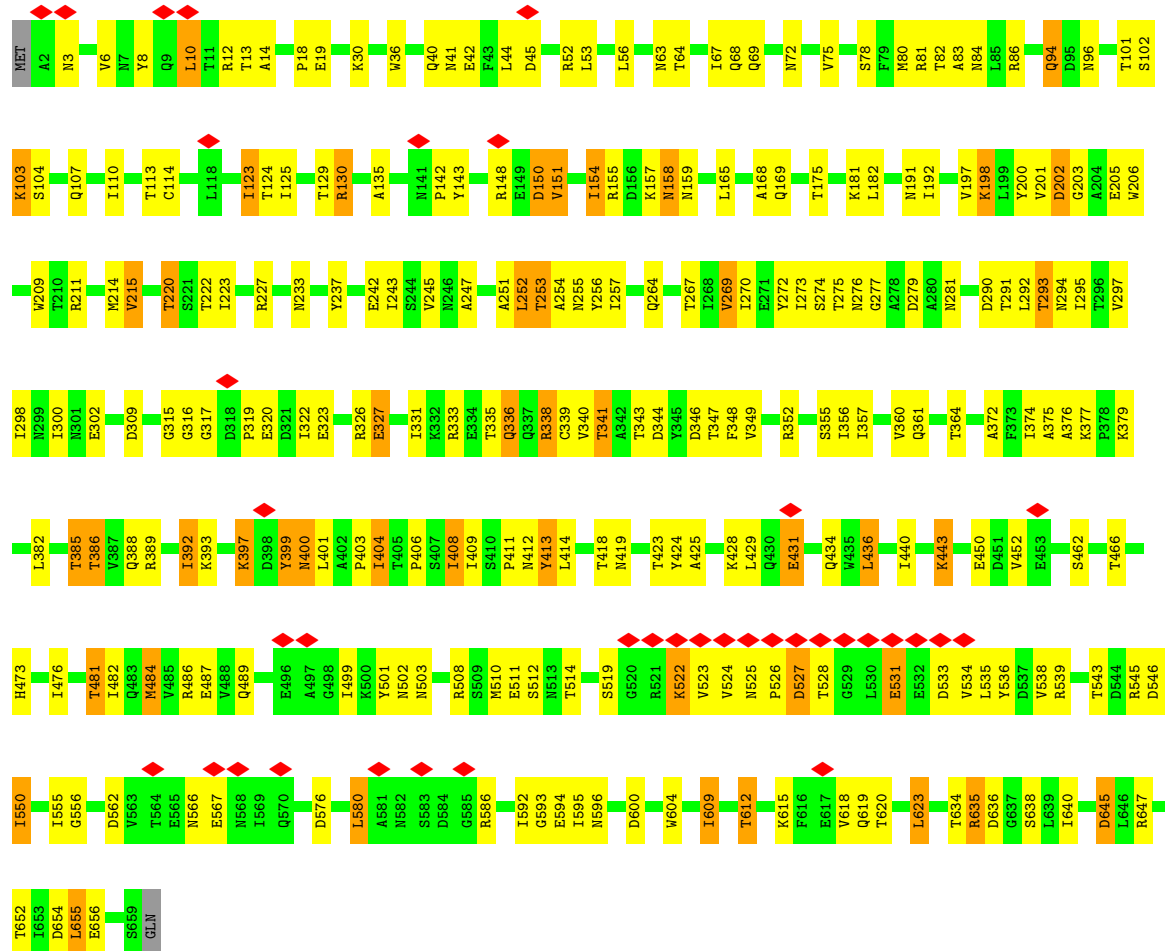


• Molecule 8: gp6, baseplate wedge protein

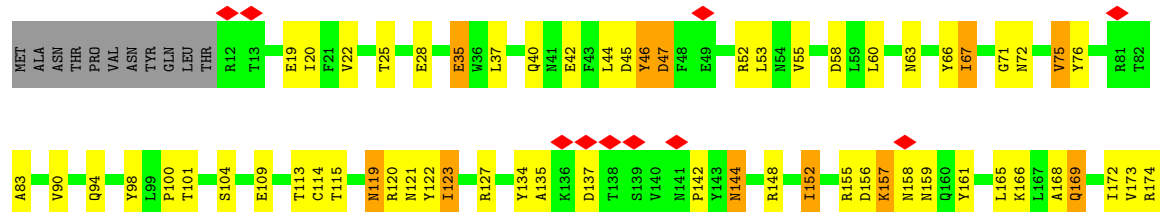


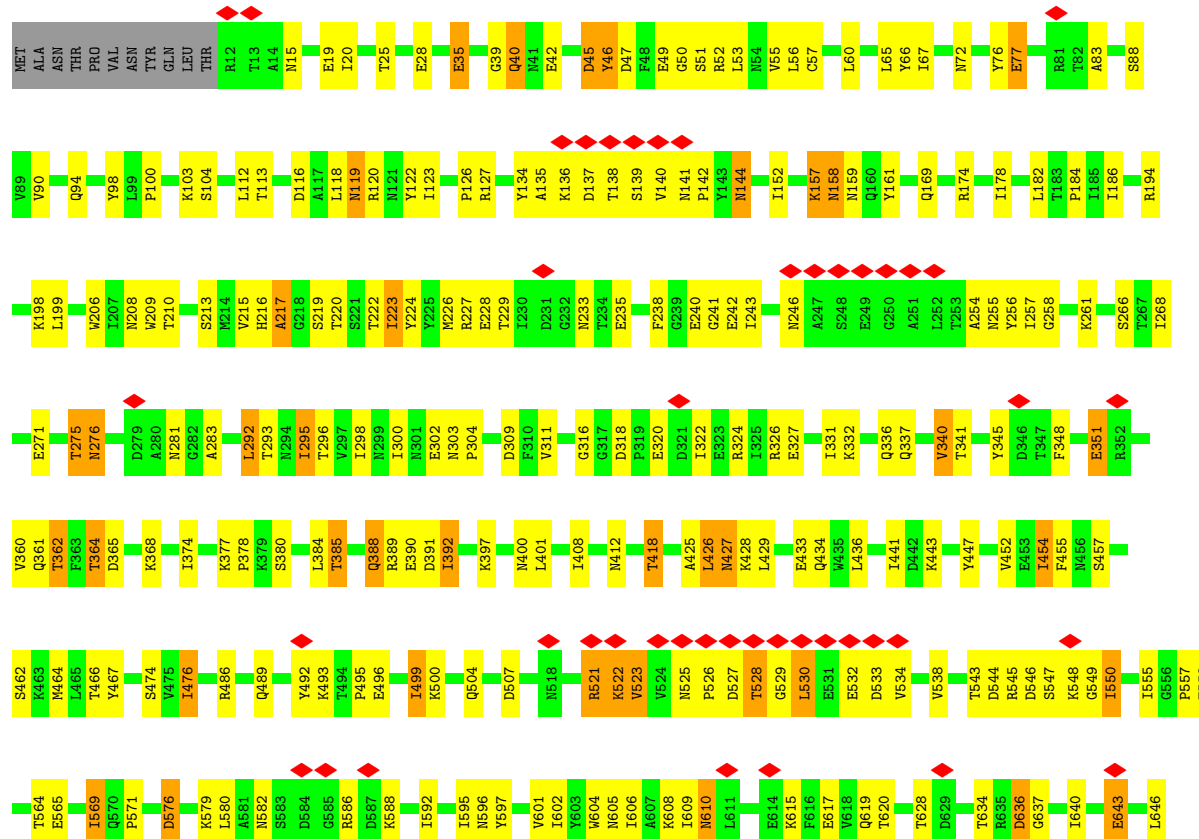


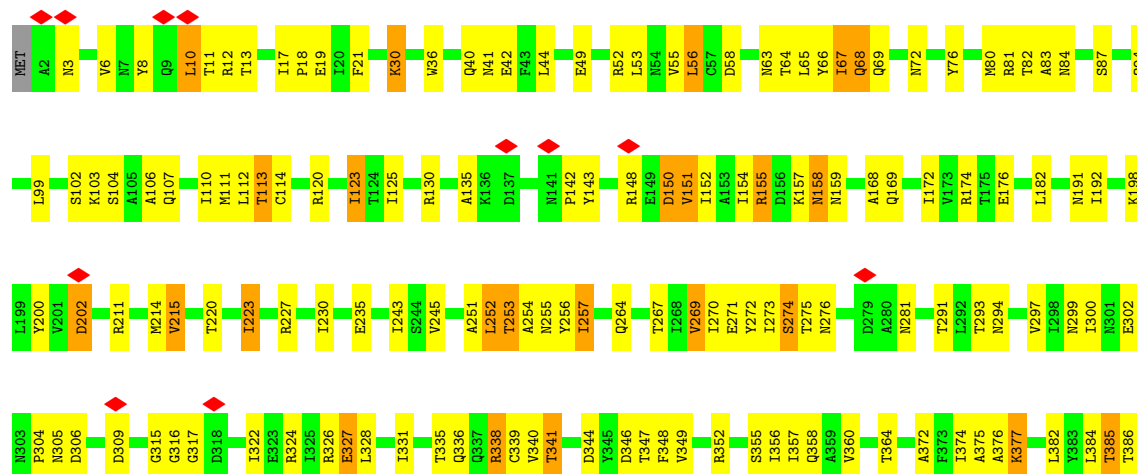
• Molecule 8: gp6, baseplate wedge protein

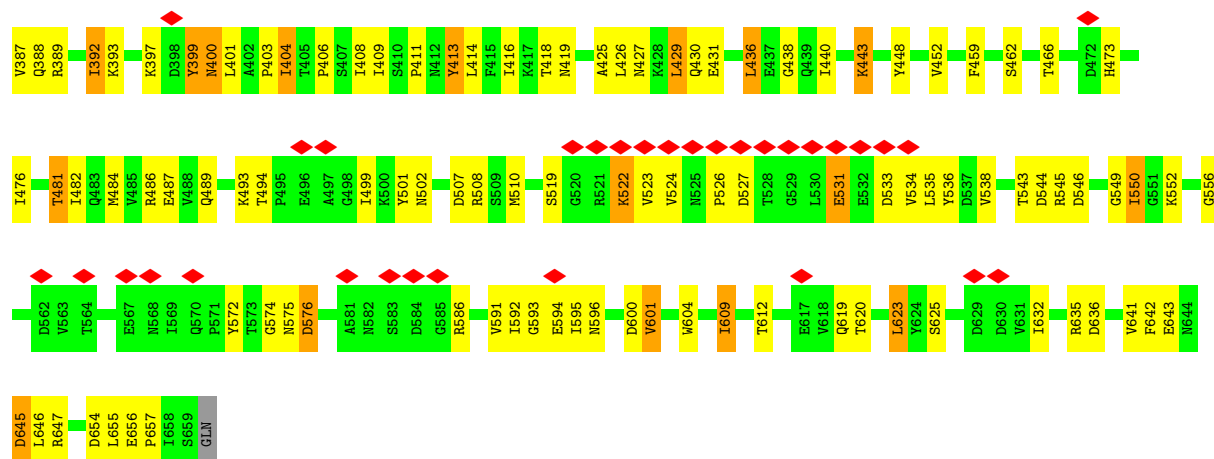


• Molecule 8: gp6, baseplate wedge protein



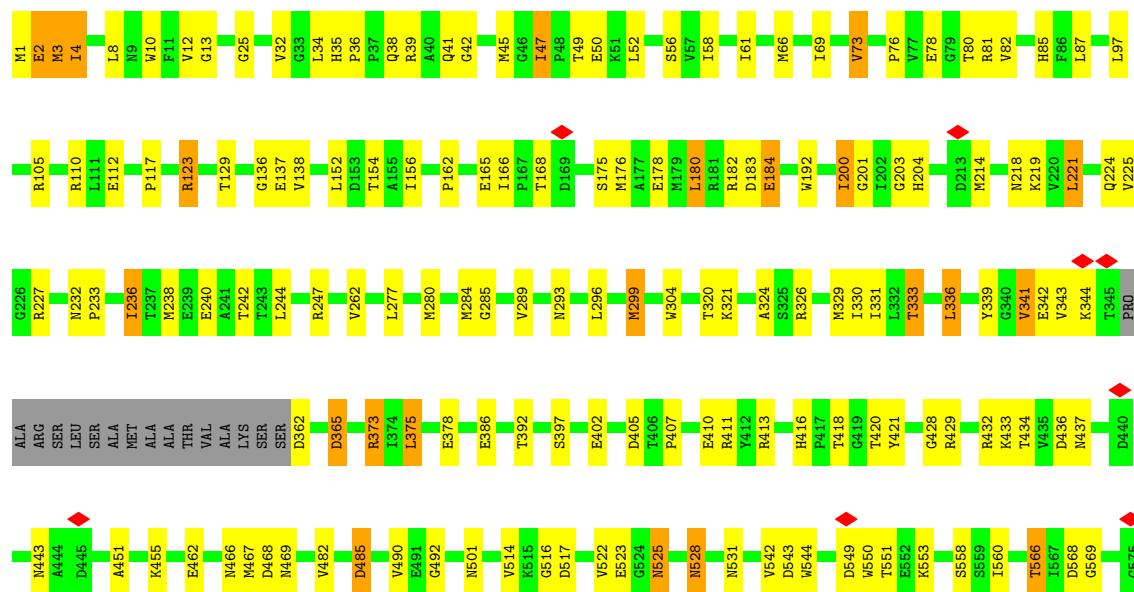






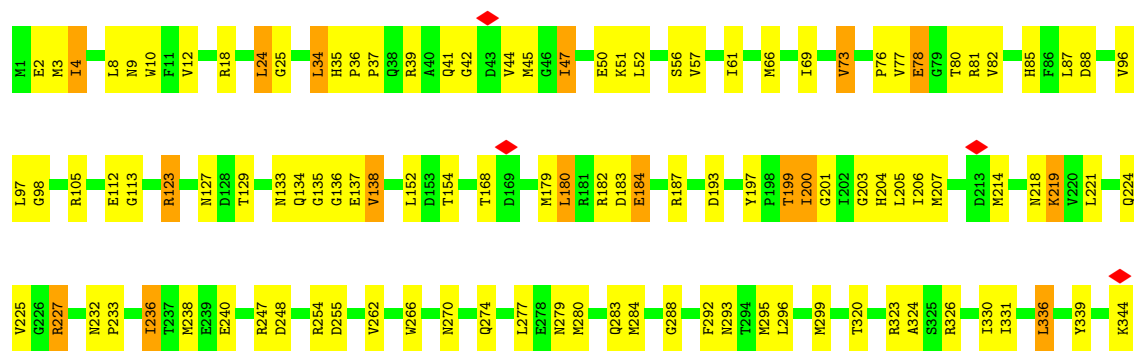
- Molecule 9: gp5, baseplate central spike protein

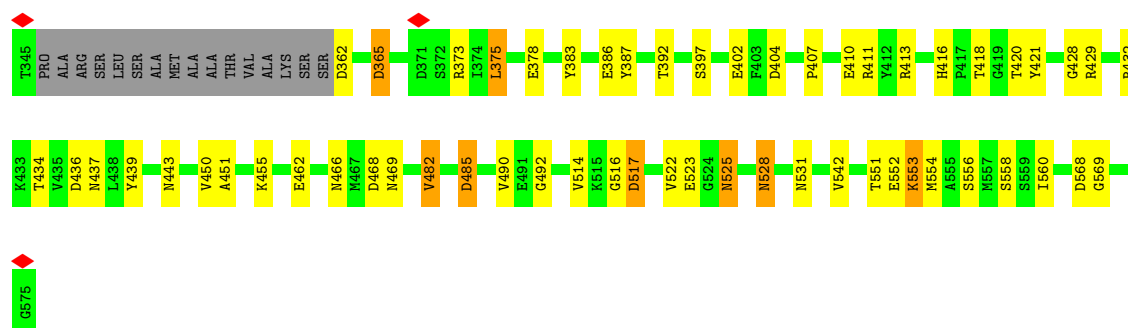
Chain gE: 69% 24%



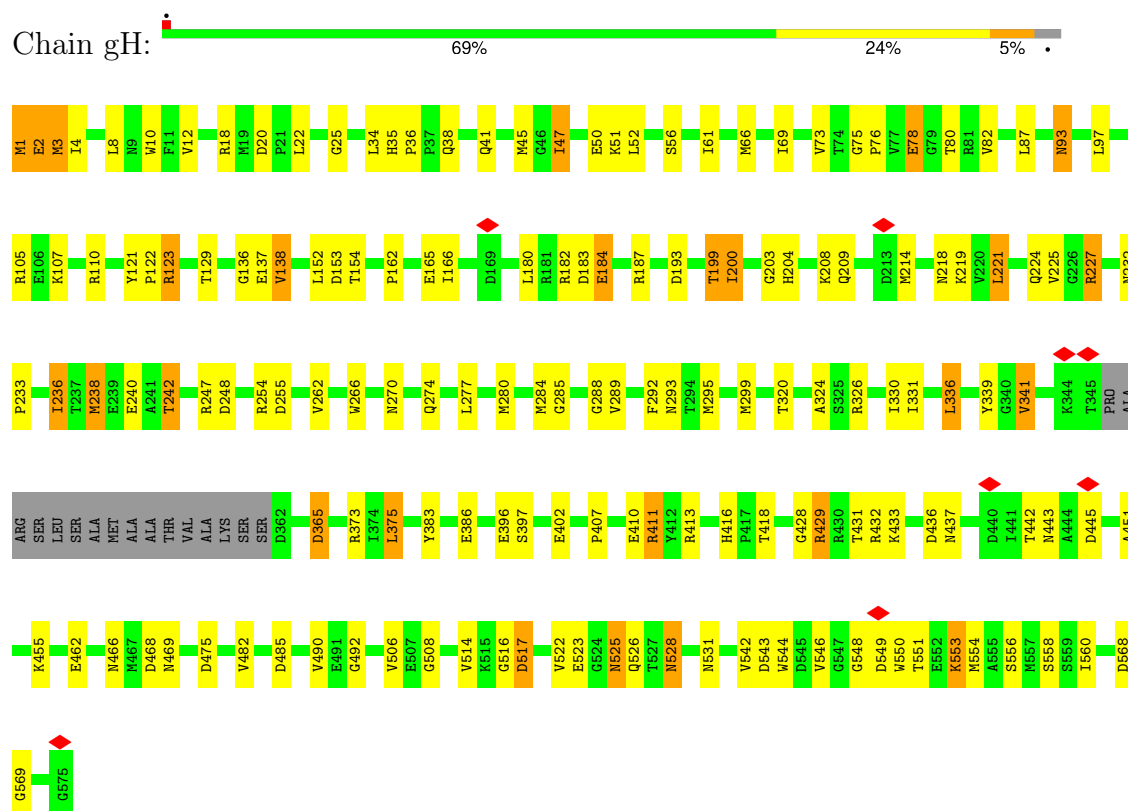
- Molecule 9: gp5, baseplate central spike protein

Chain gG: 68% 25%

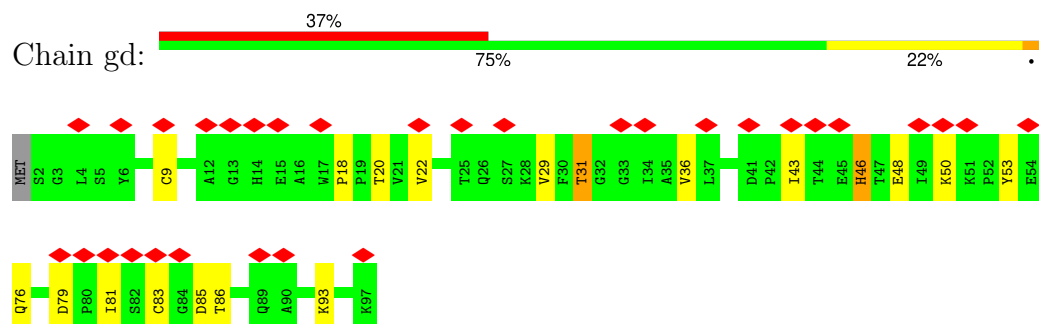




- Molecule 9: gp5, baseplate central spike protein

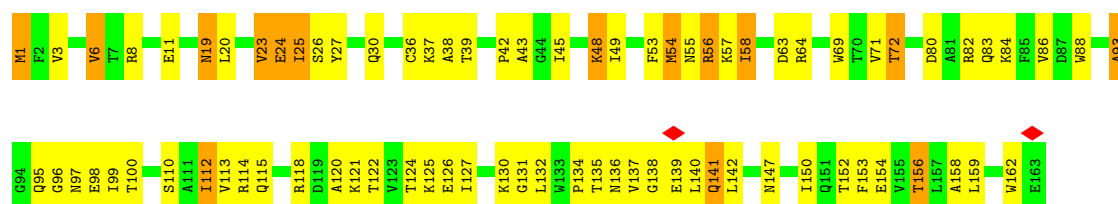


- Molecule 10: gp5.4, tip of the central spike

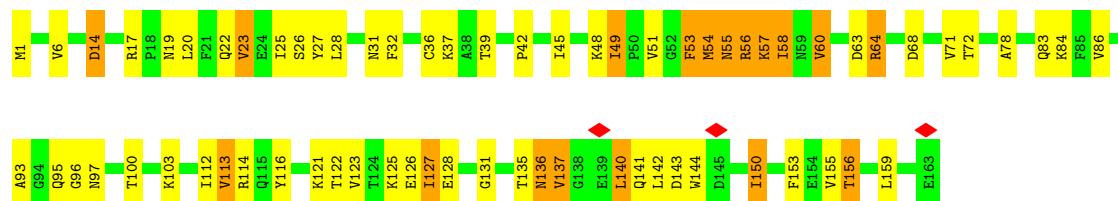


- Molecule 11: gp19, tail tube protein

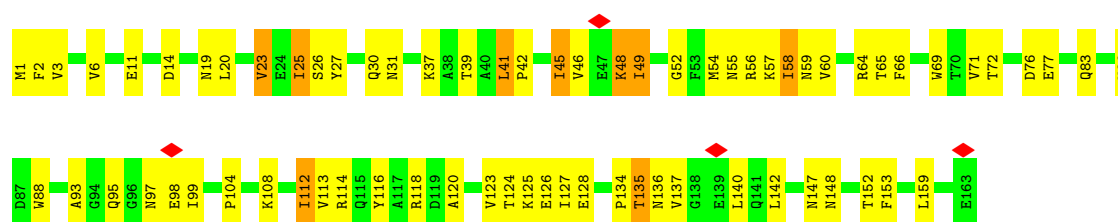




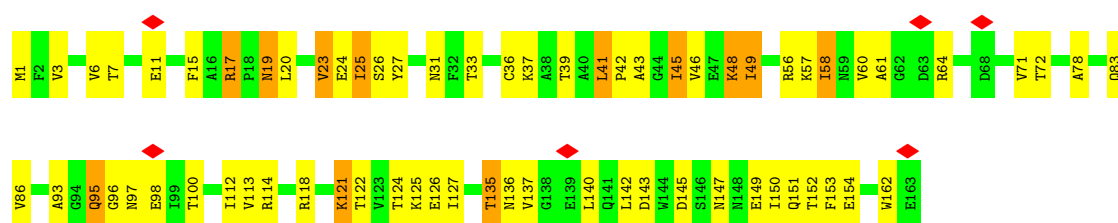
- Molecule 11: gp19, tail tube protein



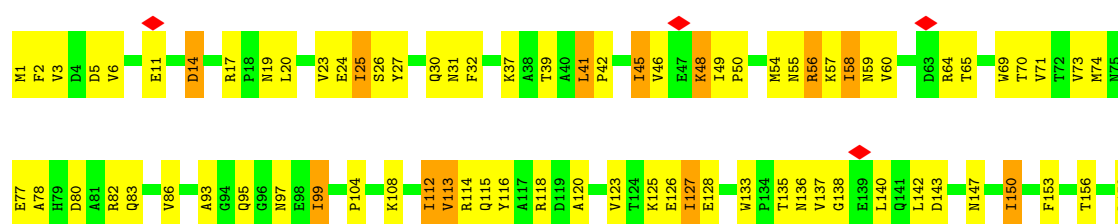
- Molecule 11: gp19, tail tube protein



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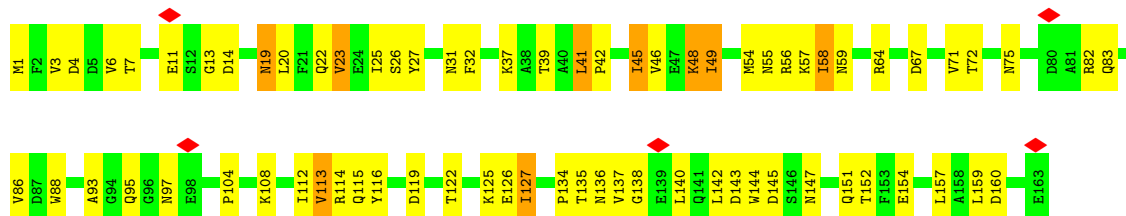


- Molecule 11: gp19, tail tube protein

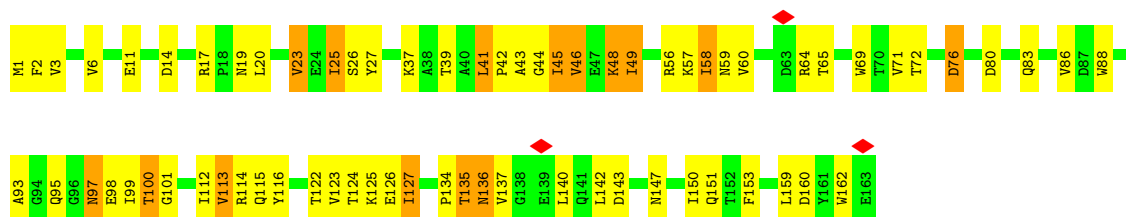




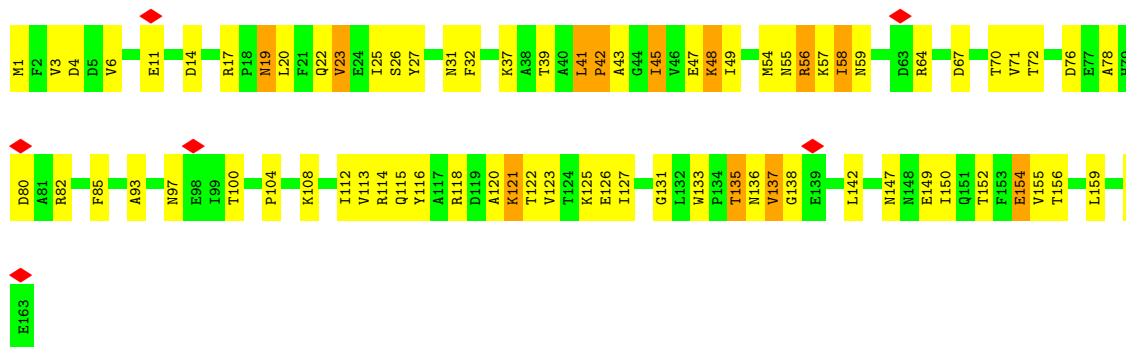
- Molecule 11: gp19, tail tube protein



- Molecule 11: gp19, tail tube protein

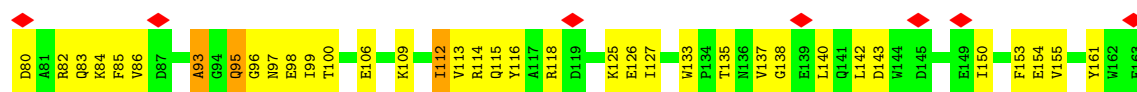


- Molecule 11: gp19, tail tube protein



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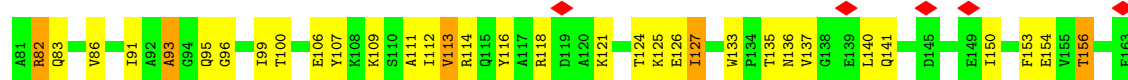
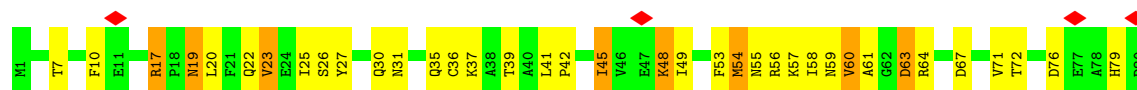




- Molecule 11: gp19, tail tube protein



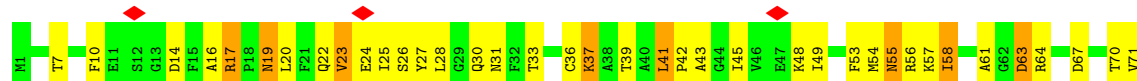
- Molecule 11: gp19, tail tube protein



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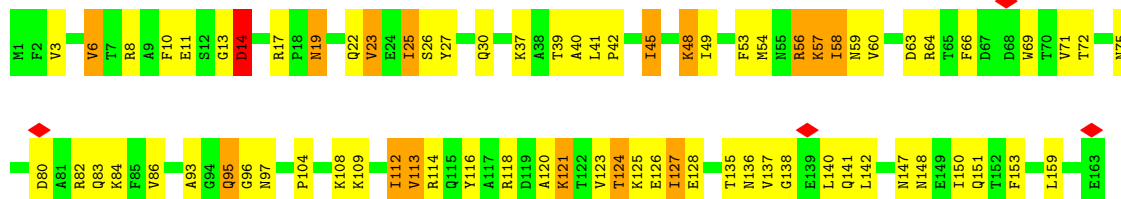


- Molecule 11: gp19, tail tube protein

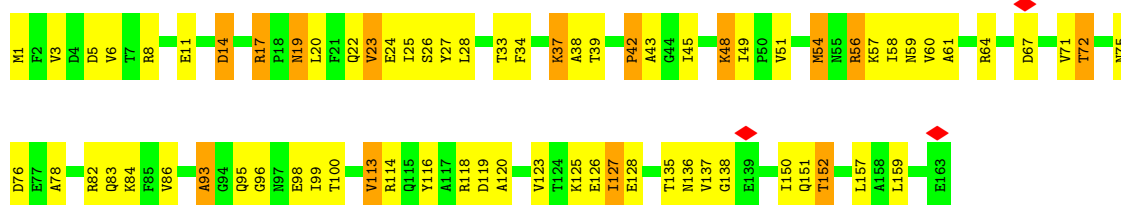




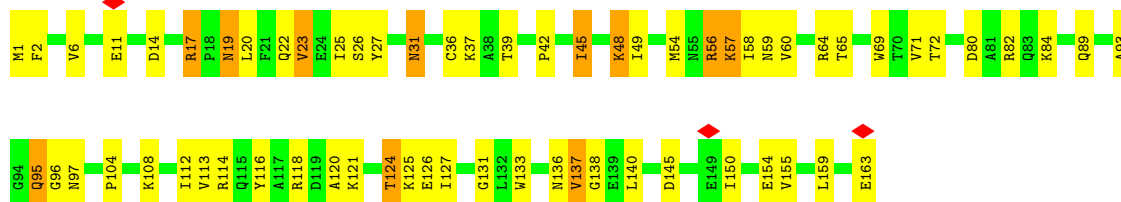
- Molecule 11: gp19, tail tube protein



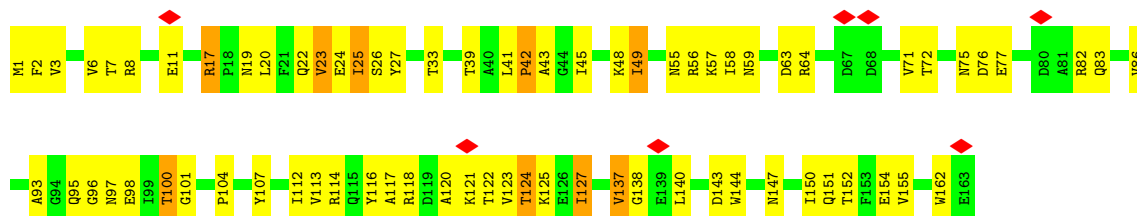
- Molecule 11: gp19, tail tube protein



- Molecule 11: gp19, tail tube protein

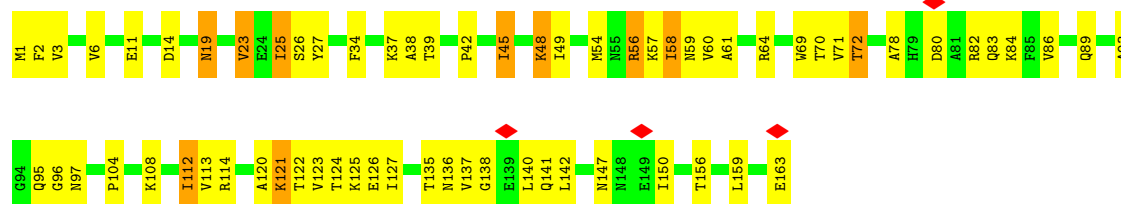


- Molecule 11: gp19, tail tube protein



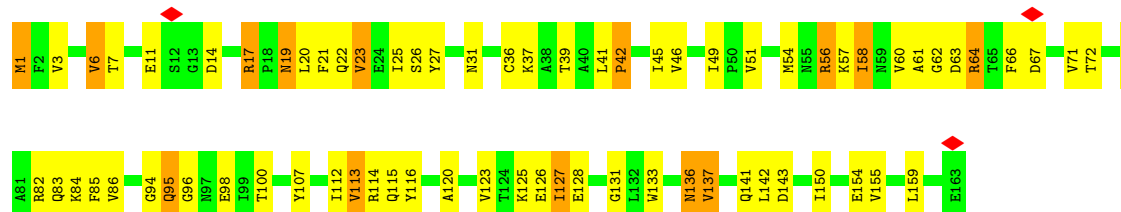
- Molecule 11: gp19, tail tube protein

Chain hn: 



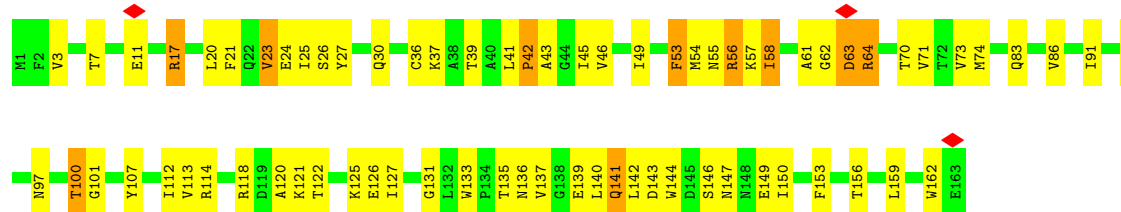
• Molecule 11: gp19, tail tube protein

Chain ho: 



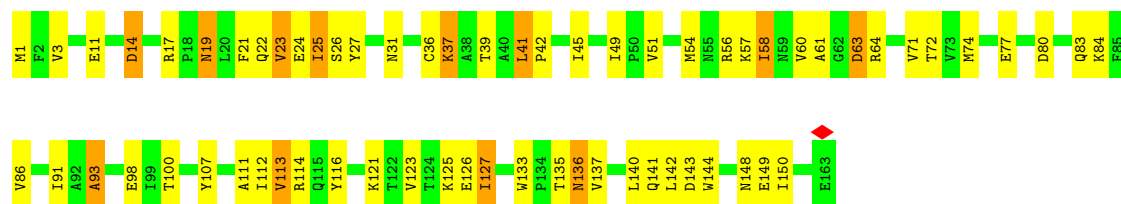
• Molecule 11: gp19, tail tube protein

Chain hp: 



• Molecule 11: gp19, tail tube protein

Chain hq: 



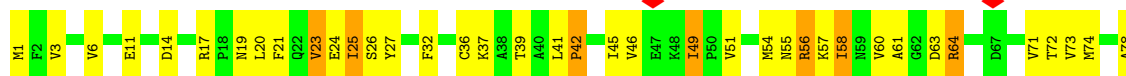
• Molecule 11: gp19, tail tube protein

Chain hr: 

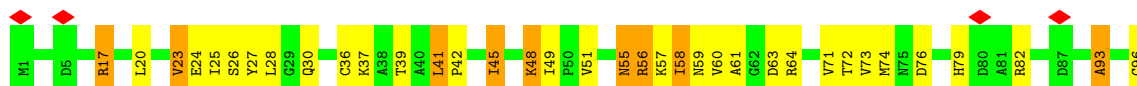




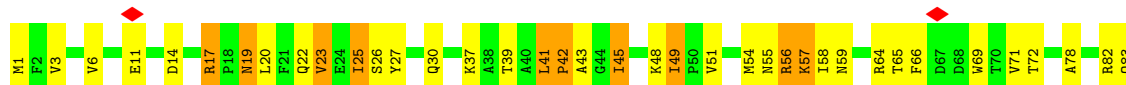
- Molecule 11: gp19, tail tube protein



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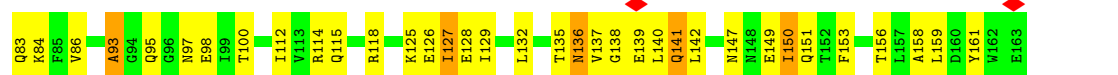
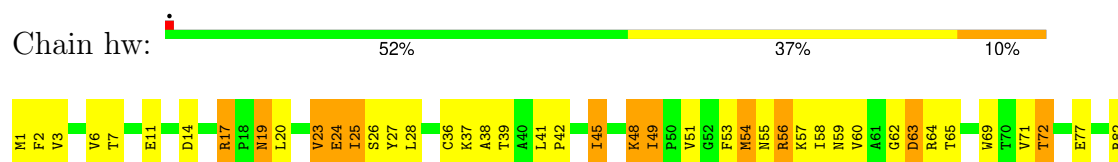


- Molecule 11: gp19, tail tube protein

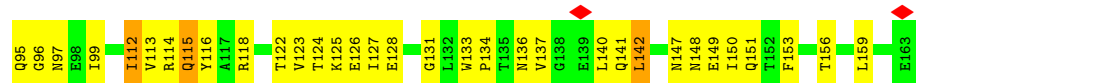
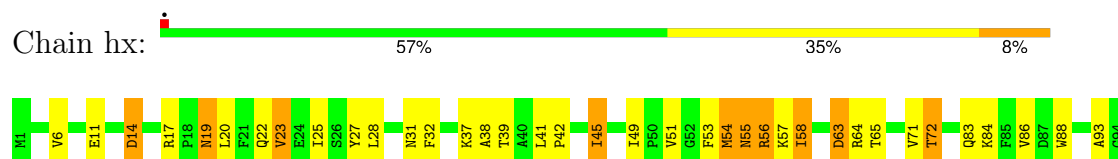


- Molecule 11: gp19, tail tube protein

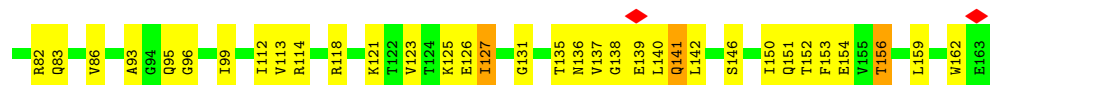
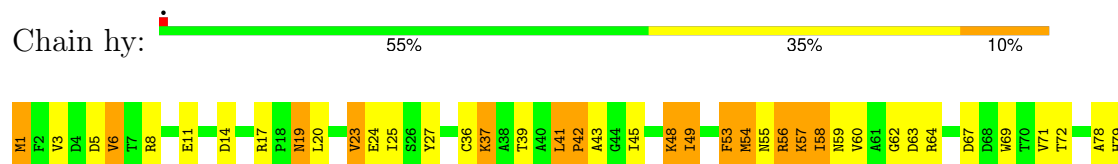




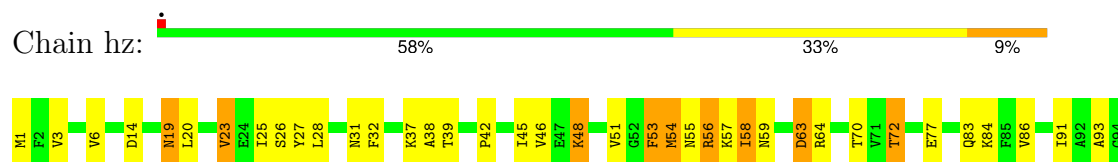
- Molecule 11: gp19, tail tube protein



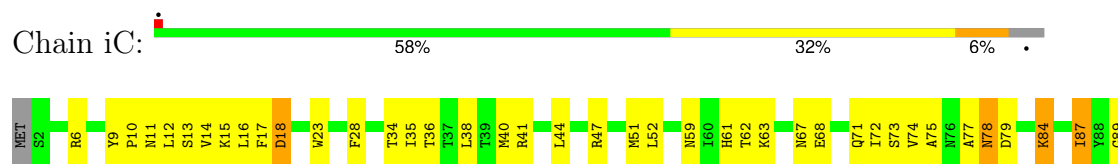
- Molecule 11: gp19, tail tube protein

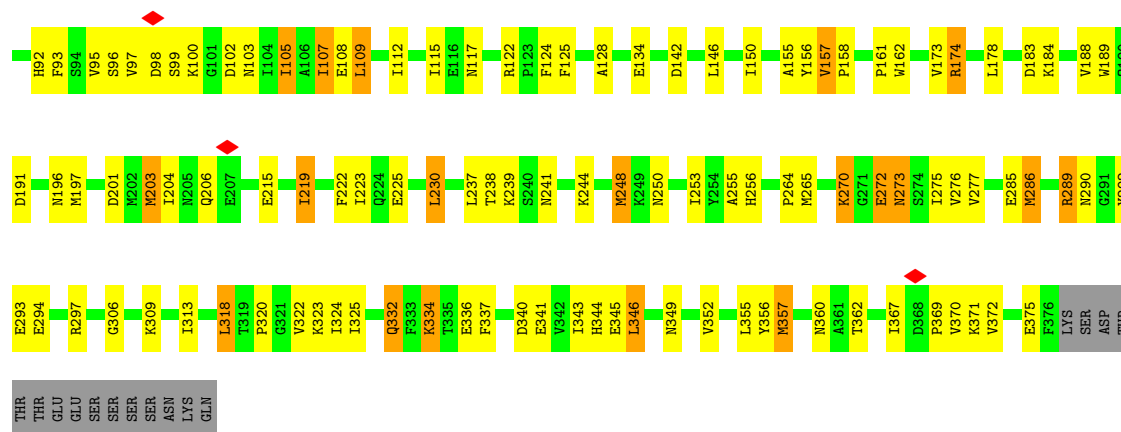


- Molecule 11: gp19, tail tube protein

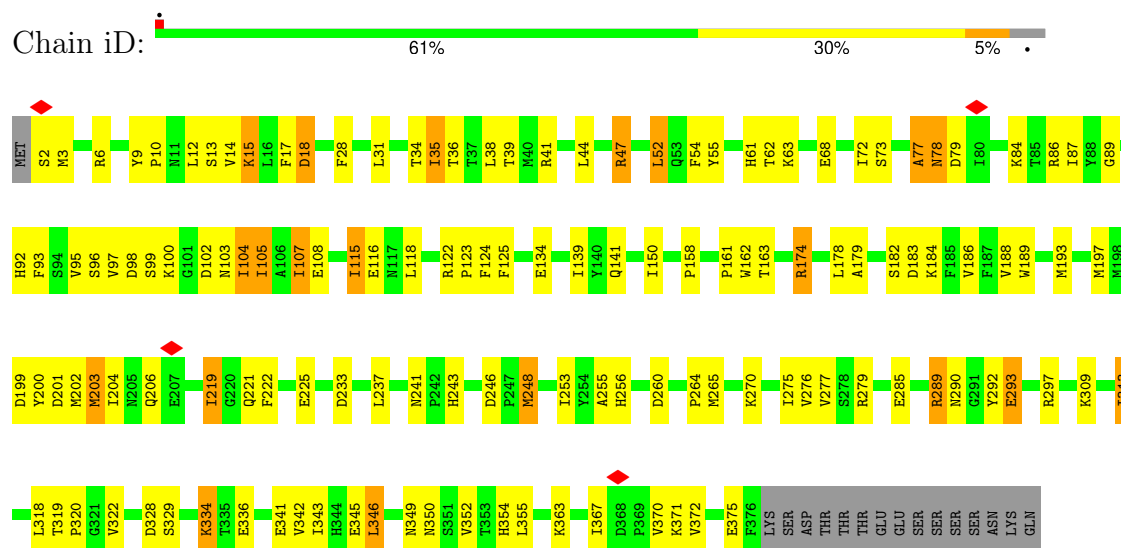


- Molecule 12: gp27, baseplate hub protein

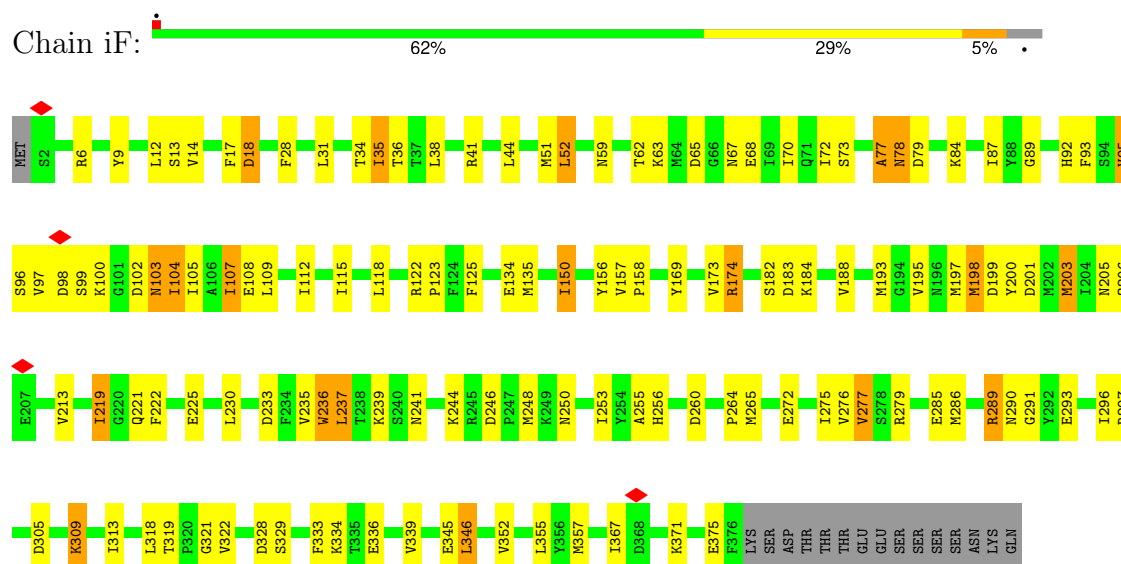




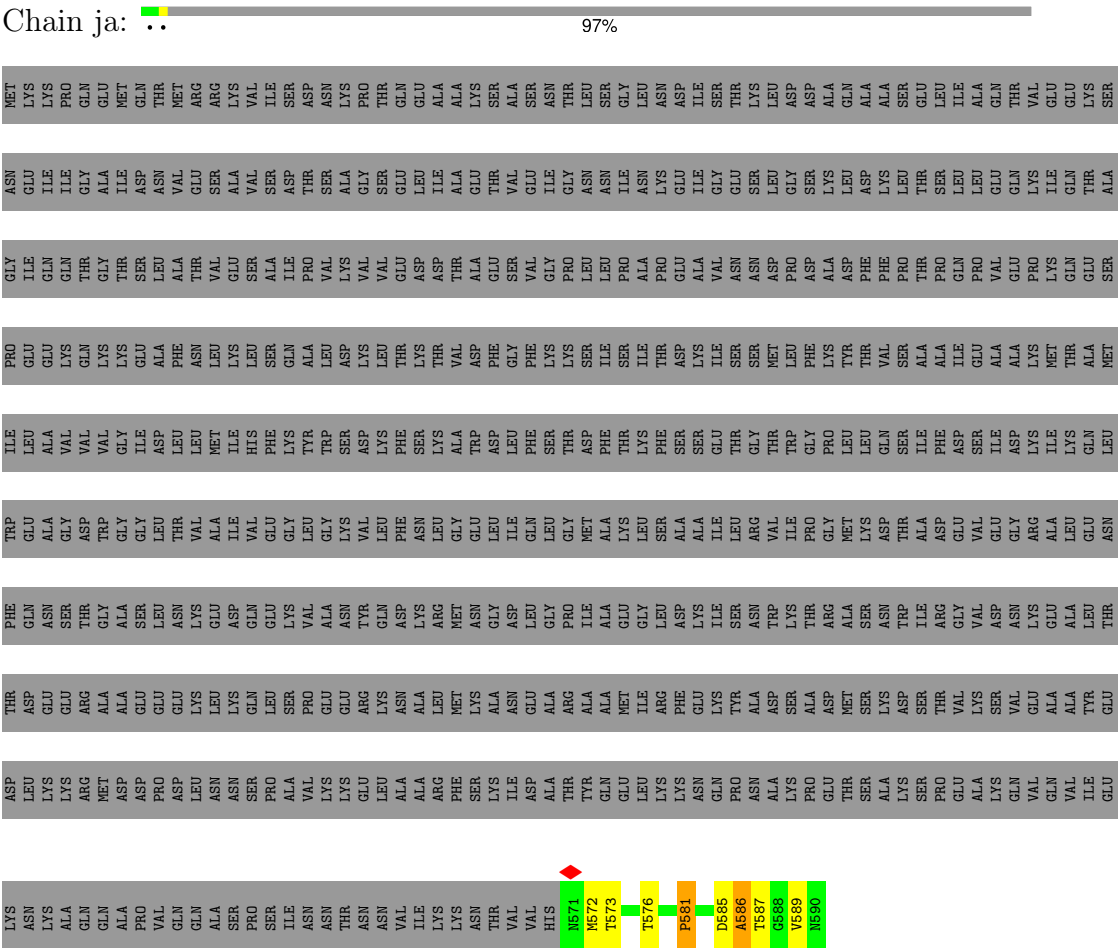
• Molecule 12: gp27, baseplate hub protein



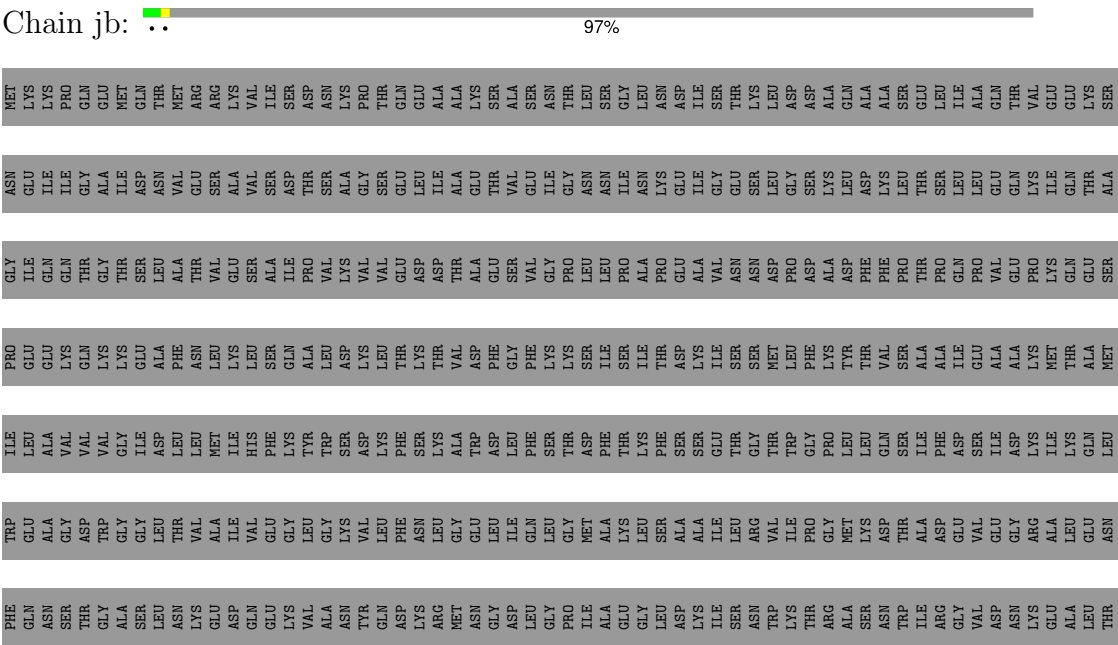
• Molecule 12: gp27, baseplate hub protein

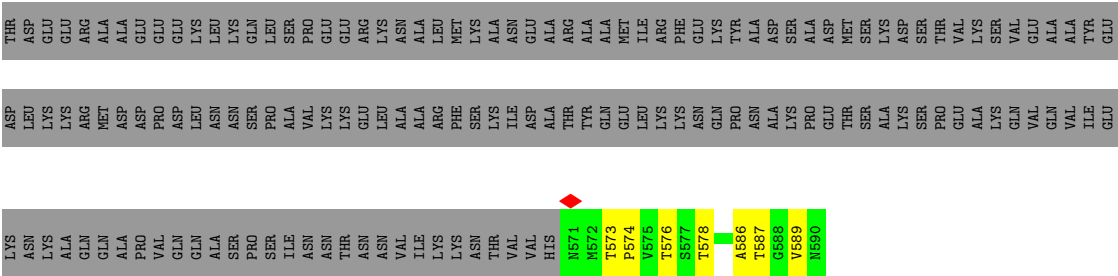


● Molecule 13: gp29, tape measure protein

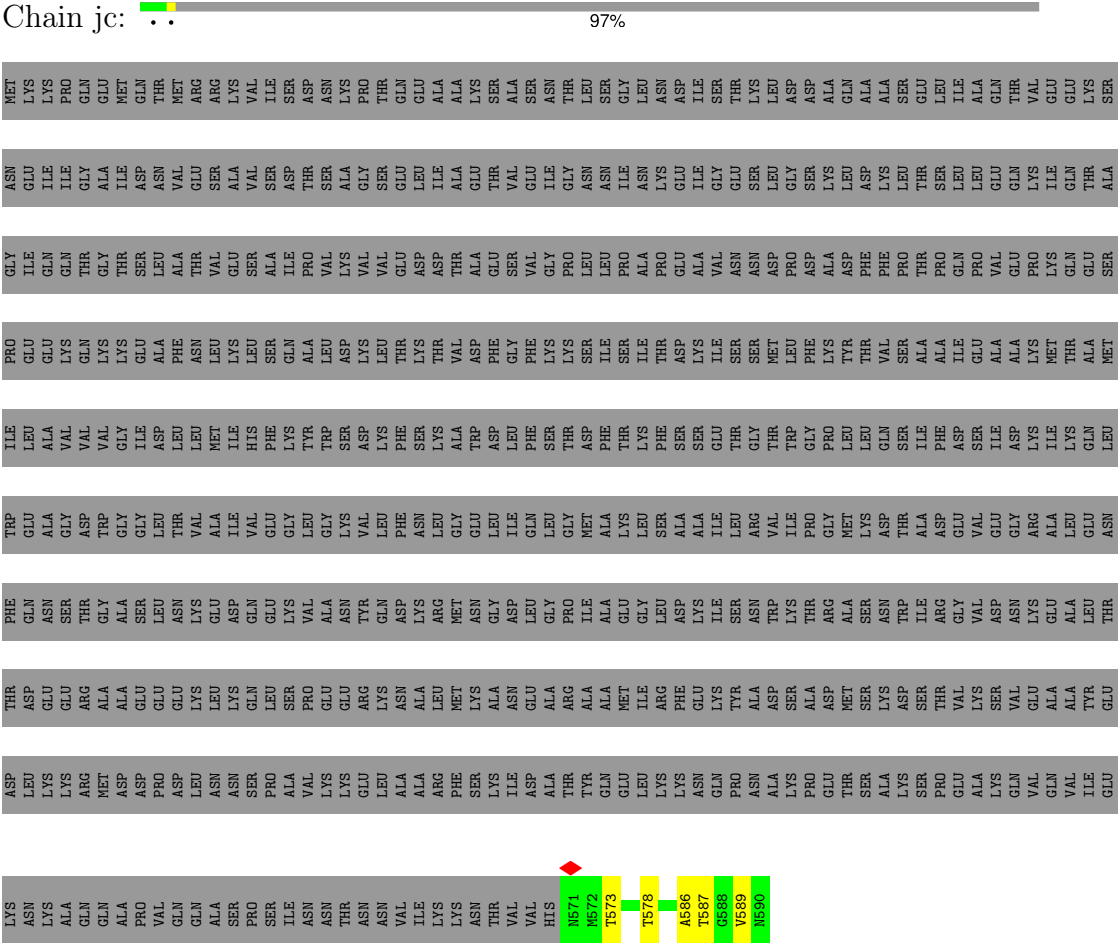


● Molecule 13: gp29, tape measure protein

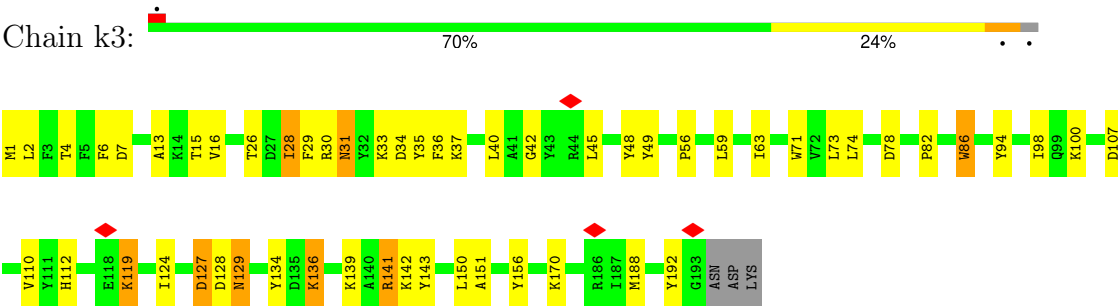




• Molecule 13: gp29, tape measure protein

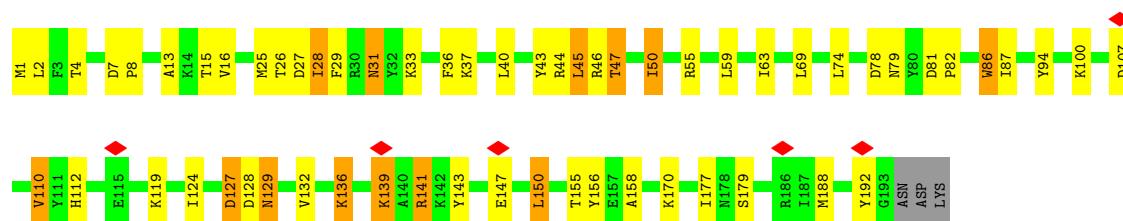


• Molecule 14: gp53, baseplate wedge protein



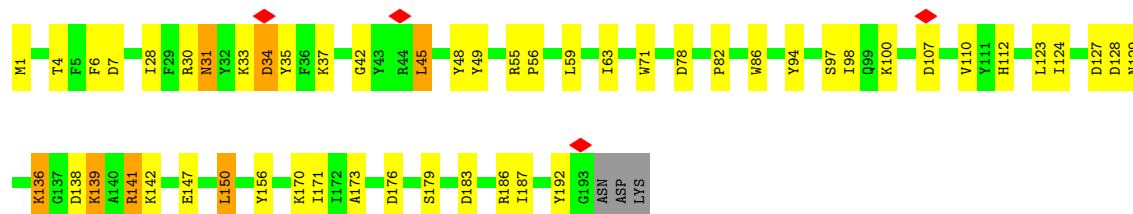
• Molecule 14: gp53, baseplate wedge protein

Chain k4:  68% 24% 7% .



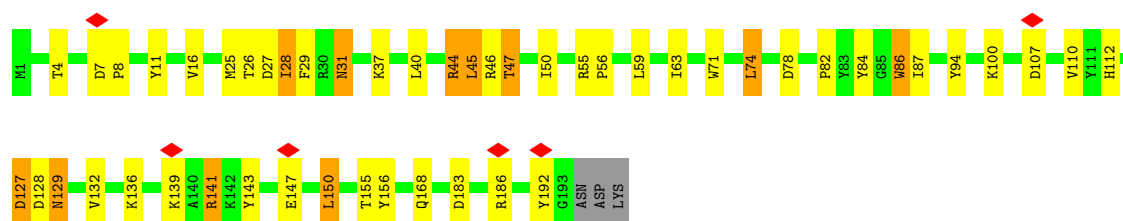
- Molecule 14: gp53, baseplate wedge protein

Chain k7:  72% 23% . .



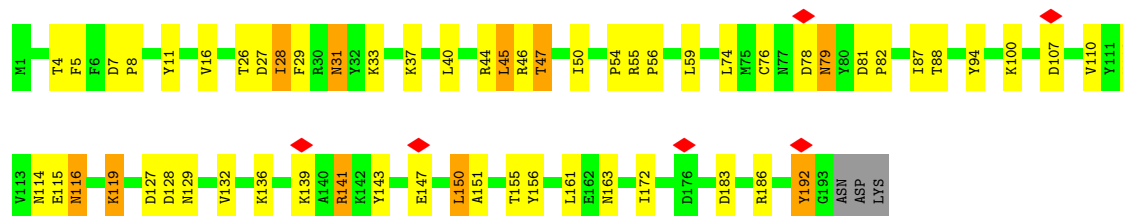
- Molecule 14: gp53, baseplate wedge protein

Chain k8:  73% 20% 6% .



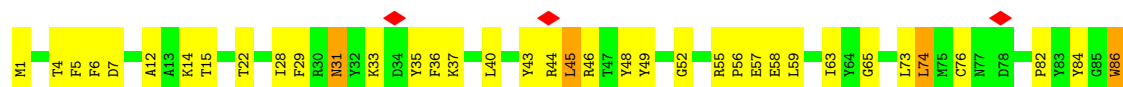
- Molecule 14: gp53, baseplate wedge protein

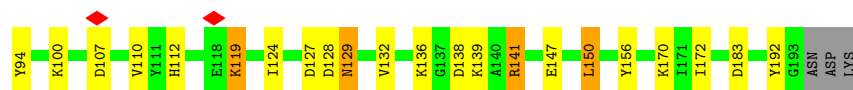
Chain kV:  68% 25% 5% .



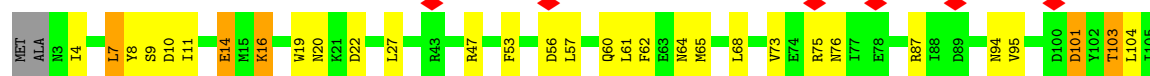
- Molecule 14: gp53, baseplate wedge protein

Chain IV:  68% 26% . .

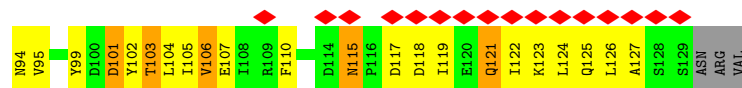
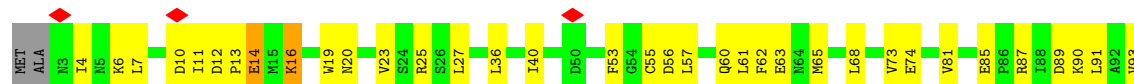




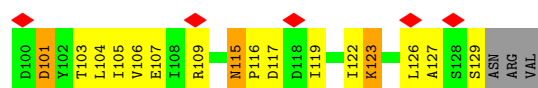
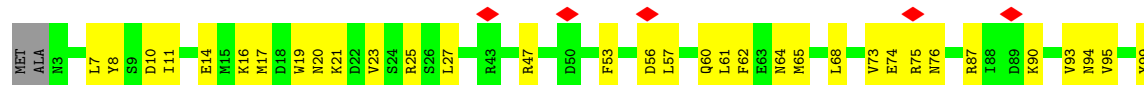
- Molecule 15: gp25, baseplate wedge protein



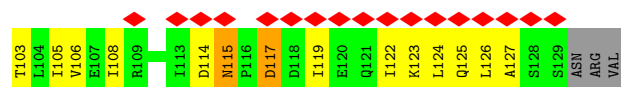
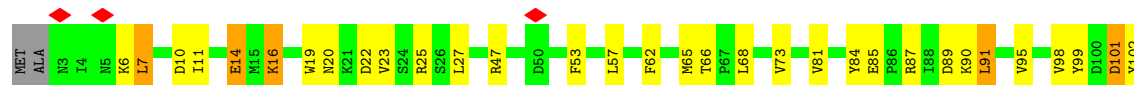
- Molecule 15: gp25, baseplate wedge protein



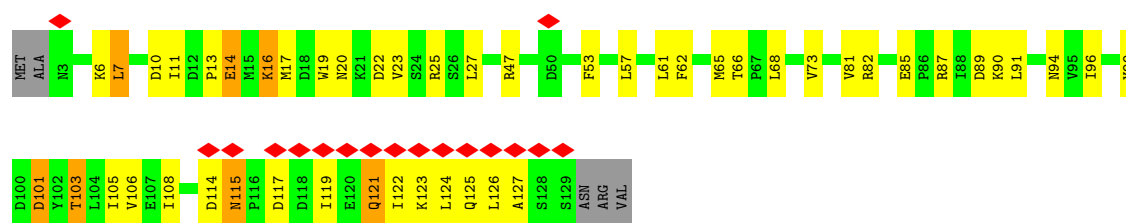
- Molecule 15: gp25, baseplate wedge protein



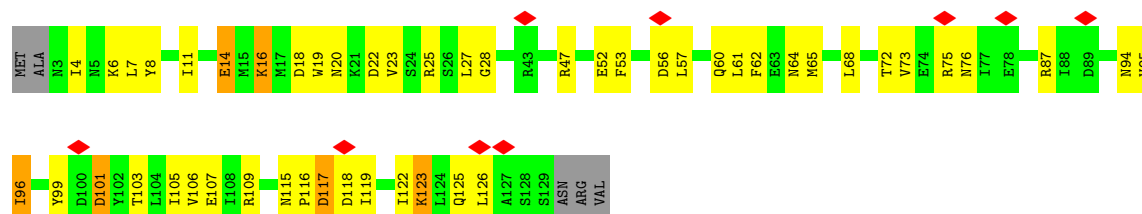
- Molecule 15: gp25, baseplate wedge protein



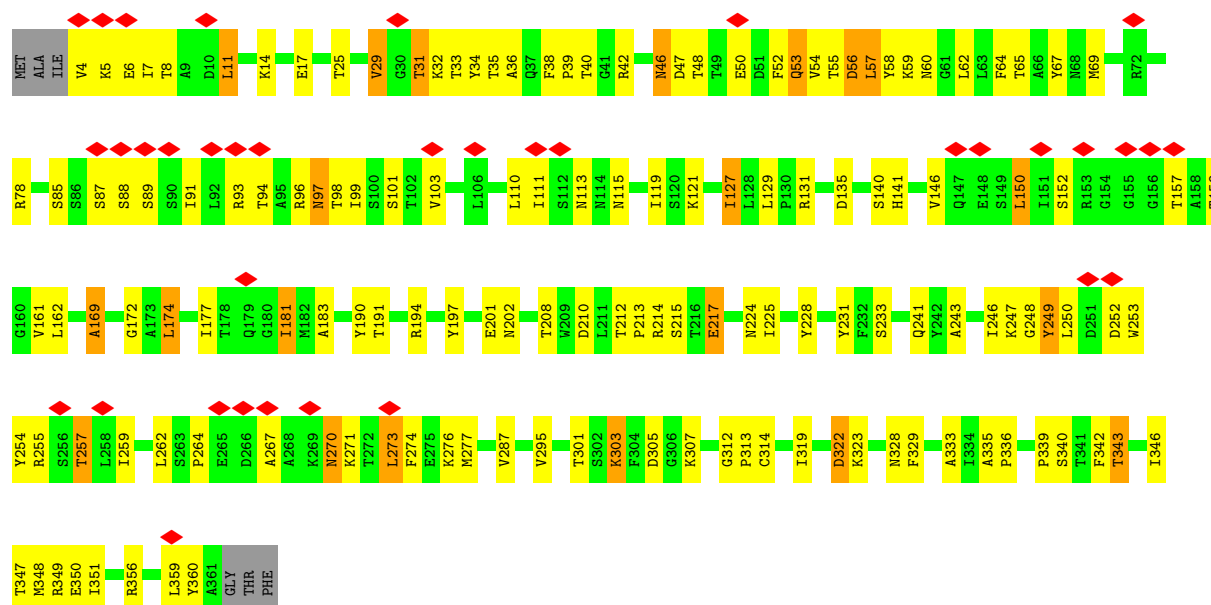
- Molecule 15: gp25, baseplate wedge protein



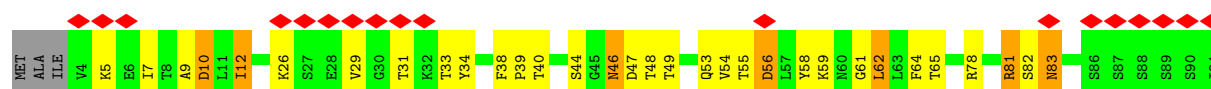
- Molecule 15: gp25, baseplate wedge protein

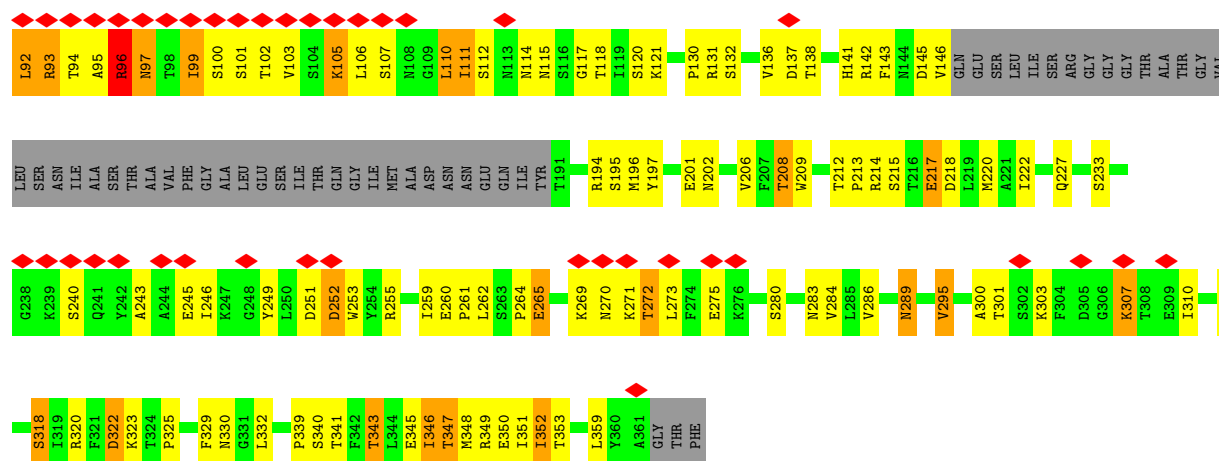


- Molecule 16: gp48, baseplate protein

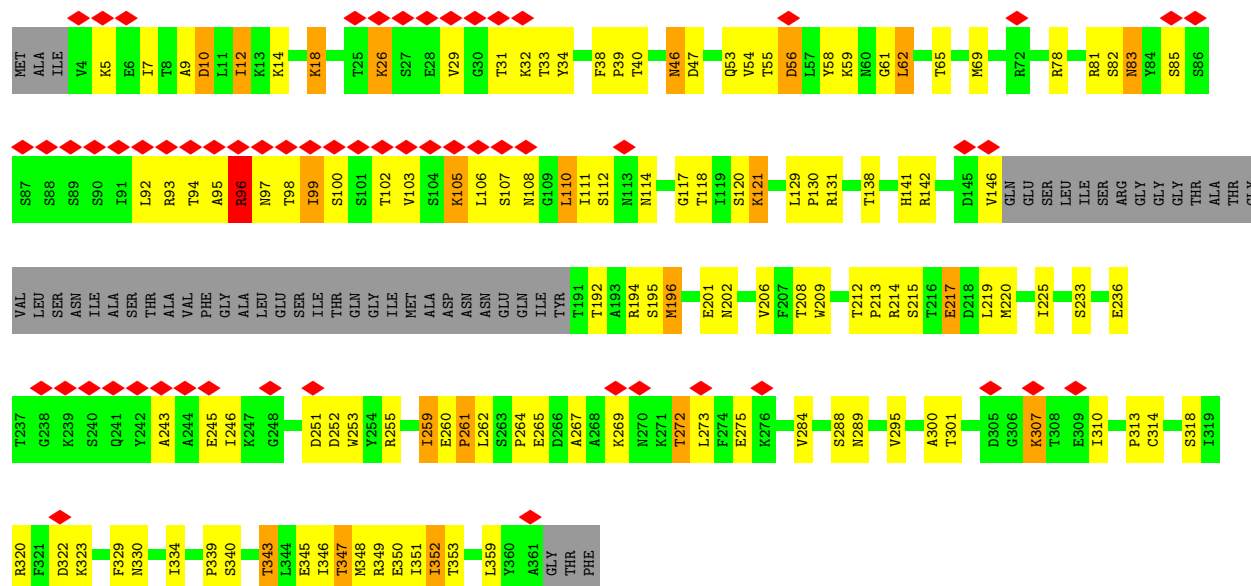


- Molecule 16: gp48, baseplate protein

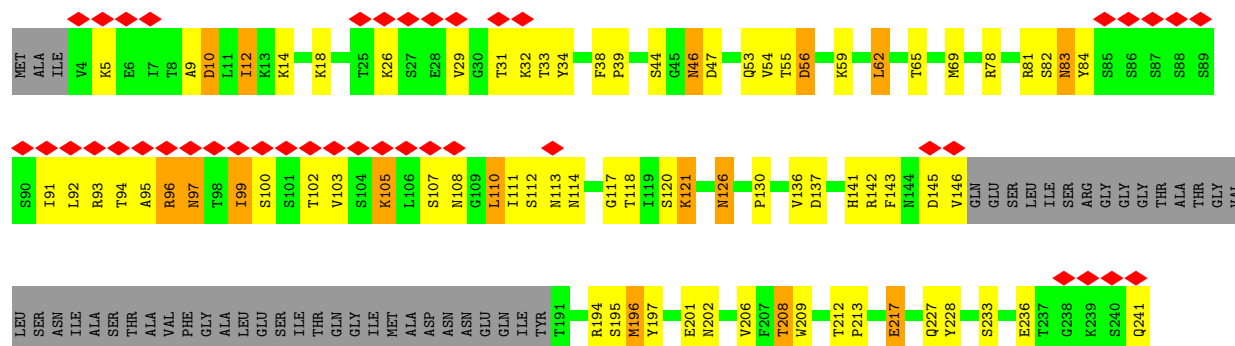


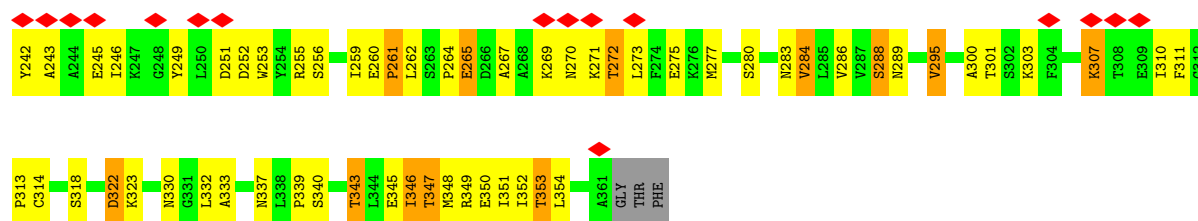


• Molecule 16: gp48, baseplate protein

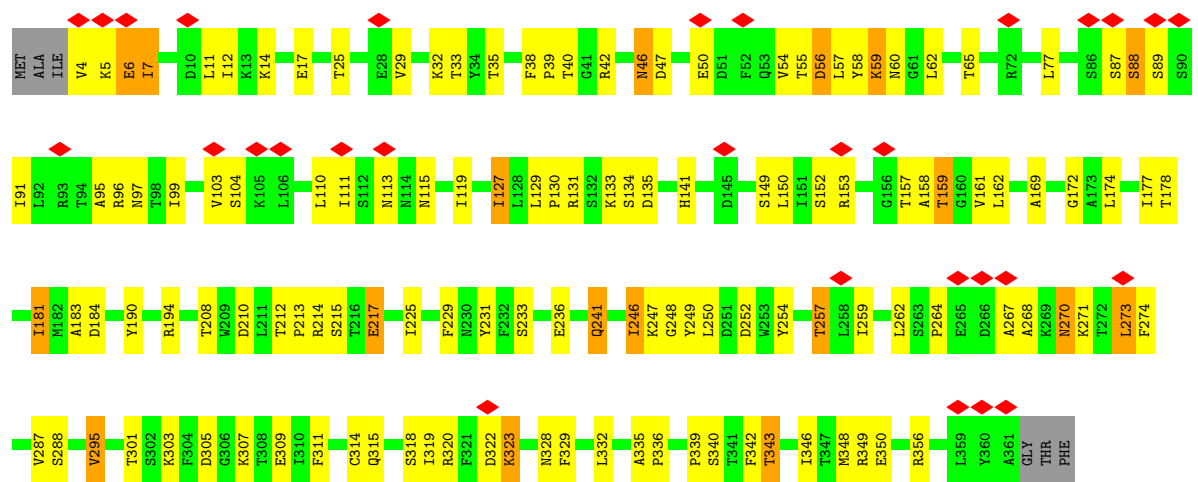


• Molecule 16: gp48, baseplate protein

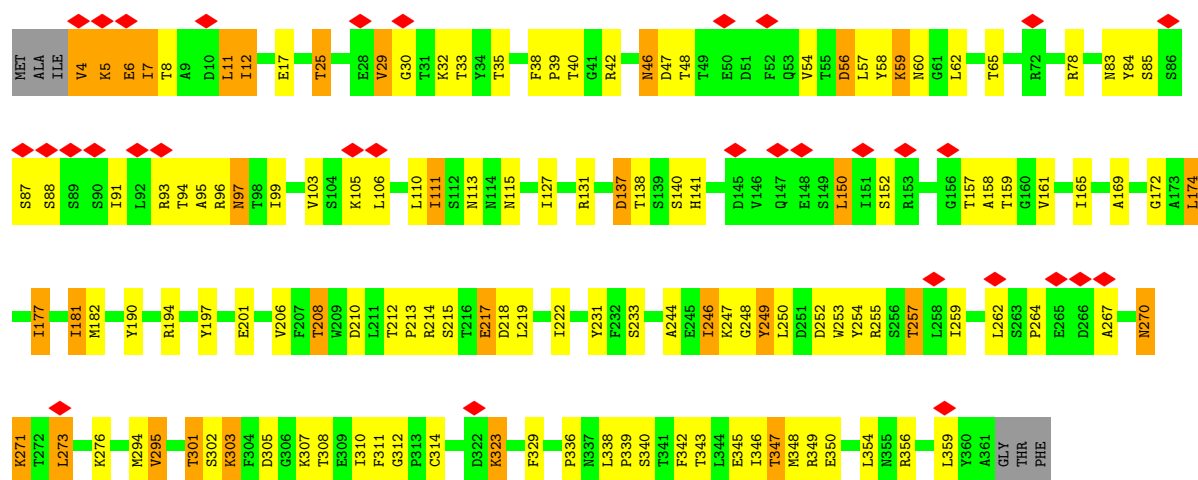




• Molecule 16: gp48, baseplate protein

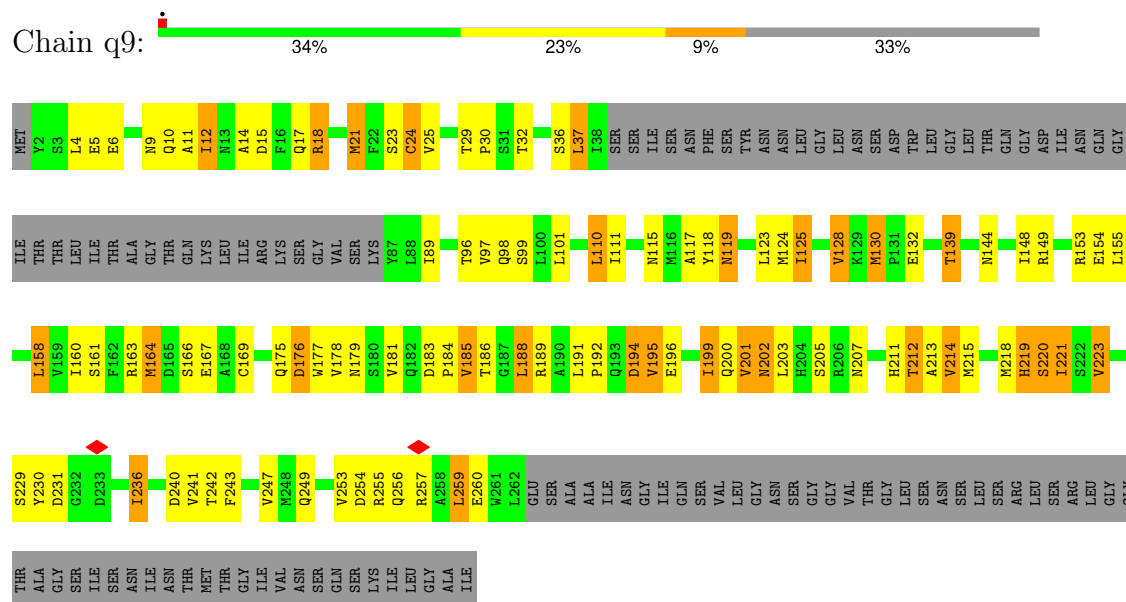


• Molecule 16: gp48, baseplate protein

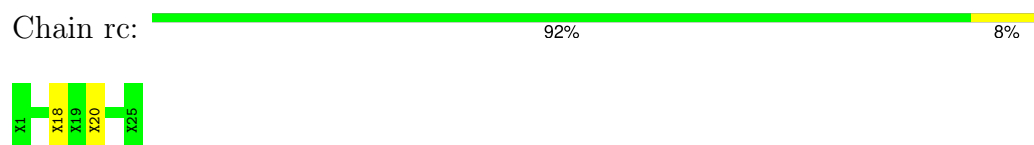


• Molecule 17: gp54, baseplate protein

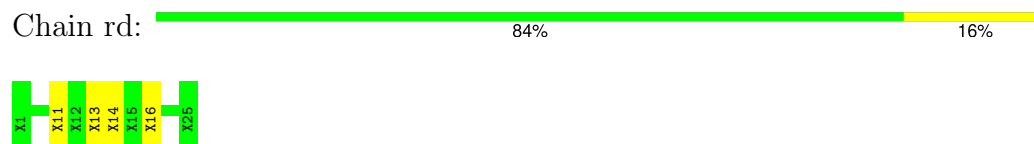




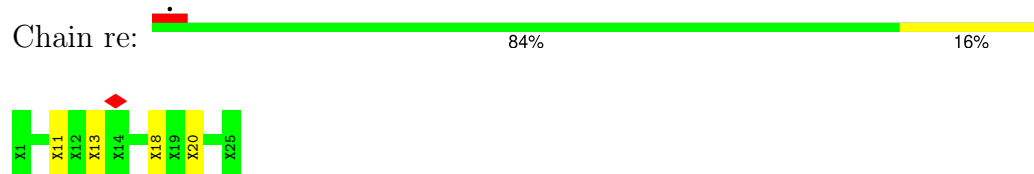
- Molecule 18: unassigned peptide A



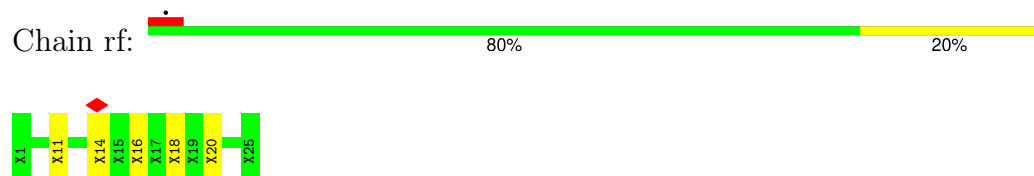
- Molecule 18: unassigned peptide A



- Molecule 18: unassigned peptide A



- Molecule 18: unassigned peptide A



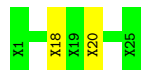
- Molecule 18: unassigned peptide A



There are no outlier residues recorded for this chain.

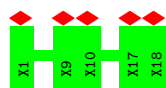
- Molecule 18: unassigned peptide A

Chain rh:  92% 8%



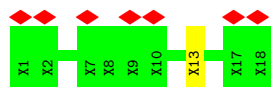
- Molecule 19: unassigned peptide B

Chain sQ:  28% 100%



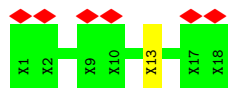
- Molecule 19: unassigned peptide B

Chain sT:  39% 94% 6%



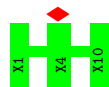
- Molecule 19: unassigned peptide B

Chain sU:  33% 94% 6%



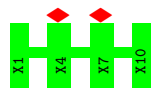
- Molecule 20: unassigned peptide C

Chain tS:  10% 100%



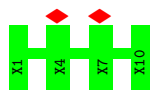
- Molecule 20: unassigned peptide C

Chain tX:  20% 100%

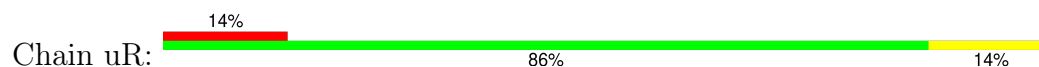


- Molecule 20: unassigned peptide C

Chain tY:  20% 100%



- Molecule 21: unassigned peptide D



- Molecule 21: unassigned peptide D



- Molecule 21: unassigned peptide D



- Molecule 22: unassigned peptide E



There are no outlier residues recorded for this chain.

- Molecule 22: unassigned peptide E



There are no outlier residues recorded for this chain.

- Molecule 22: unassigned peptide E



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	113800	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 ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	646.4, 646.4, 646.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.616, 1.616, 1.616	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	S0	0.11	0/4016	0.31	0/5464
1	S1	0.12	0/4016	0.31	0/5464
1	S2	0.11	0/4016	0.32	0/5464
1	S3	0.12	0/4016	0.31	0/5464
1	S4	0.12	0/4016	0.32	0/5464
1	S5	0.11	0/4016	0.31	0/5464
1	S6	0.11	0/4016	0.29	0/5464
1	S7	0.11	0/4016	0.30	0/5464
1	S8	0.13	0/4016	0.32	0/5464
1	SA	0.11	0/4016	0.30	0/5464
1	SO	0.12	0/4016	0.35	2/5464 (0.0%)
1	SP	0.12	0/4016	0.32	0/5464
1	SQ	0.11	0/4016	0.32	0/5464
1	Sv	0.12	0/4016	0.31	0/5464
1	Sw	0.11	0/4016	0.30	0/5464
1	Sx	0.11	0/4016	0.30	0/5464
1	Sy	0.12	0/4016	0.31	0/5464
1	Sz	0.11	0/4016	0.31	0/5464
2	T1	0.11	0/2205	0.32	0/2988
2	T2	0.11	0/2205	0.30	0/2988
2	T3	0.11	0/2205	0.31	0/2988
2	T4	0.12	0/2205	0.32	0/2988
2	T5	0.12	0/2205	0.31	0/2988
2	T6	0.11	0/2205	0.30	0/2988
2	T7	0.11	0/2205	0.29	0/2988
2	T8	0.11	0/2205	0.29	0/2988
2	T9	0.12	0/2205	0.31	0/2988
2	TF	0.11	0/2205	0.29	0/2988
2	TG	0.11	0/2205	0.30	0/2988
2	TH	0.11	0/2205	0.30	0/2988
2	Td	0.11	0/2205	0.30	0/2988
2	Te	0.11	0/2205	0.31	0/2988

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Tf	0.11	0/2205	0.31	0/2988
2	Tg	0.12	0/2205	0.32	0/2988
2	Th	0.12	0/2205	0.32	1/2988 (0.0%)
2	Ti	0.12	0/2205	0.33	0/2988
3	UL	0.11	0/1700	0.28	0/2318
3	UM	0.11	0/1700	0.29	0/2318
3	UN	0.11	0/1700	0.29	0/2318
3	Up	0.12	0/1700	0.31	0/2318
3	Uq	0.11	0/1700	0.29	0/2318
3	Ur	0.11	0/1700	0.31	0/2318
3	Us	0.12	0/1700	0.31	0/2318
3	Ut	0.10	0/1700	0.29	0/2318
3	Uu	0.11	0/1700	0.28	0/2318
3	VL	0.12	0/1700	0.31	0/2318
3	VM	0.12	0/1700	0.31	0/2318
3	VN	0.10	0/1700	0.29	0/2318
3	Vp	0.11	0/1700	0.28	0/2318
3	Vq	0.11	0/1700	0.29	0/2318
3	Vr	0.11	0/1700	0.30	0/2318
3	Vs	0.11	0/1700	0.29	0/2318
3	Vt	0.11	0/1700	0.29	0/2318
3	Vu	0.11	0/1700	0.29	0/2318
4	WI	0.13	0/4778	0.38	0/6513
4	WJ	0.14	0/4778	0.39	1/6513 (0.0%)
4	WK	0.14	0/4778	0.39	1/6513 (0.0%)
4	Wj	0.13	0/4778	0.38	0/6513
4	Wk	0.13	0/4778	0.39	0/6513
4	Wl	0.13	0/4778	0.39	0/6513
4	Wm	0.13	0/4778	0.39	0/6513
4	Wn	0.13	0/4778	0.40	0/6513
4	Wo	0.14	0/4778	0.39	1/6513 (0.0%)
4	XI	0.13	0/4778	0.38	0/6513
4	XJ	0.13	0/4778	0.39	0/6513
4	XK	0.14	0/4778	0.39	0/6513
4	Xj	0.13	0/4778	0.36	0/6513
4	Xk	0.13	0/4778	0.38	0/6513
4	Xl	0.13	0/4778	0.40	0/6513
4	Xm	0.13	0/4778	0.39	0/6513
4	Xn	0.13	0/4778	0.39	0/6513
4	Xo	0.14	0/4778	0.41	1/6513 (0.0%)
5	YC	0.19	0/8405	0.46	1/11412 (0.0%)
5	YX	0.19	0/8405	0.46	0/11412
5	YY	0.18	0/8405	0.45	0/11412

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	Yc	0.19	0/8405	0.46	0/11412
5	Yx	0.19	0/8405	0.46	0/11412
5	Yy	0.19	0/8405	0.45	2/11412 (0.0%)
6	ZD	0.14	0/2709	0.30	0/3694
6	ZE	0.16	0/2736	0.32	0/3731
6	ZZ	0.14	0/2709	0.29	0/3694
6	Za	0.14	0/2709	0.29	0/3694
6	Zb	0.17	0/2736	0.31	0/3731
6	Zc	0.16	0/2736	0.32	0/3731
6	aD	0.14	0/2709	0.29	0/3694
6	aE	0.17	0/2736	0.31	0/3731
6	aZ	0.14	0/2709	0.29	0/3694
6	aa	0.14	0/2709	0.29	0/3694
6	ab	0.17	0/2736	0.31	0/3731
6	ac	0.17	0/2736	0.30	0/3731
7	b0	0.21	0/5092	0.38	0/6928
7	b3	0.19	0/5092	0.37	0/6928
7	b4	0.19	0/5092	0.36	0/6928
7	b5	0.20	0/5092	0.37	0/6928
7	b6	0.20	0/5092	0.37	0/6928
7	b7	0.20	0/5092	0.38	0/6928
7	b8	0.21	0/5092	0.38	0/6928
7	b9	0.21	0/5092	0.39	1/6928 (0.0%)
7	bN	0.22	0/5092	0.36	0/6928
7	bO	0.22	0/5092	0.37	0/6928
7	bP	0.22	0/5092	0.36	0/6928
7	bQ	0.22	0/5092	0.37	0/6928
7	bR	0.22	0/5092	0.37	0/6928
7	bY	0.22	0/5092	0.38	0/6928
7	cA	0.21	0/5092	0.38	0/6928
7	cB	0.21	0/5092	0.37	0/6928
7	cC	0.21	0/5092	0.37	0/6928
7	cD	0.22	0/5092	0.37	0/6928
7	cE	0.19	0/5092	0.36	0/6928
7	cF	0.21	0/5092	0.39	0/6928
7	cG	0.22	0/5092	0.38	0/6928
7	cH	0.22	0/5092	0.38	0/6928
7	cI	0.22	0/5092	0.38	0/6928
7	cJ	0.21	0/5092	0.38	0/6928
7	cK	0.22	0/5092	0.37	0/6928
7	cL	0.22	0/5092	0.38	0/6928
7	cM	0.22	0/5092	0.37	0/6928
7	cN	0.22	0/5092	0.38	0/6928

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	cO	0.22	0/5092	0.37	0/6928
7	cP	0.22	0/5092	0.38	0/6928
7	dS	0.23	0/5033	0.39	0/6847
7	dT	0.23	0/5033	0.38	0/6847
7	dU	0.23	0/5033	0.39	0/6847
7	dV	0.22	0/5033	0.38	0/6847
7	dW	0.23	0/5033	0.39	0/6847
7	dZ	0.22	0/5033	0.38	0/6847
8	eB	0.22	0/5257	0.39	0/7144
8	eU	0.23	0/5257	0.40	0/7144
8	eW	0.22	0/5257	0.38	0/7144
8	f9	0.23	0/5337	0.40	0/7256
8	fA	0.22	0/5337	0.39	1/7256 (0.0%)
8	fB	0.24	1/5257 (0.0%)	0.39	0/7144
8	fR	0.22	0/5337	0.39	1/7256 (0.0%)
8	fS	0.23	0/5337	0.41	1/7256 (0.0%)
8	fU	0.23	0/5257	0.38	0/7144
8	fW	0.22	0/5257	0.38	0/7144
8	fr	0.22	0/5337	0.38	0/7256
8	fs	0.23	0/5337	0.40	1/7256 (0.0%)
9	gE	0.21	0/4402	0.32	0/5966
9	gG	0.21	0/4402	0.33	0/5966
9	gH	0.21	0/4402	0.33	0/5966
10	gd	0.11	0/724	0.25	0/984
11	h1	0.28	0/1333	0.42	0/1807
11	h2	0.27	0/1333	0.41	0/1807
11	hI	0.27	0/1333	0.43	0/1807
11	hJ	0.27	0/1333	0.43	0/1807
11	hK	0.27	0/1333	0.41	0/1807
11	hL	0.28	0/1333	0.43	0/1807
11	hM	0.27	0/1333	0.42	0/1807
11	hX	0.27	0/1333	0.41	0/1807
11	he	0.22	0/1333	0.40	0/1807
11	hf	0.22	0/1333	0.40	0/1807
11	hg	0.22	0/1333	0.39	0/1807
11	hh	0.22	0/1333	0.40	0/1807
11	hi	0.22	0/1333	0.40	0/1807
11	hj	0.26	0/1333	0.42	0/1807
11	hk	0.27	0/1333	0.43	0/1807
11	hl	0.26	0/1333	0.43	0/1807
11	hm	0.26	0/1333	0.42	0/1807
11	hn	0.26	0/1333	0.42	0/1807
11	ho	0.27	0/1333	0.43	0/1807

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	hp	0.27	0/1333	0.42	0/1807
11	hq	0.27	0/1333	0.39	0/1807
11	hr	0.27	0/1333	0.44	0/1807
11	hs	0.27	0/1333	0.43	0/1807
11	ht	0.22	0/1333	0.39	0/1807
11	hu	0.26	0/1333	0.42	0/1807
11	hv	0.27	0/1333	0.41	0/1807
11	hw	0.28	0/1333	0.43	0/1807
11	hx	0.28	0/1333	0.41	0/1807
11	hy	0.28	0/1333	0.42	0/1807
11	hz	0.28	0/1333	0.43	0/1807
12	iC	0.27	0/3070	0.41	0/4164
12	iD	0.26	0/3070	0.40	0/4164
12	iF	0.27	0/3070	0.41	0/4164
13	ja	0.22	0/139	0.43	0/192
13	jb	0.23	0/139	0.57	0/192
13	jc	0.23	0/139	0.55	0/192
14	k3	0.24	0/1643	0.38	0/2228
14	k4	0.24	0/1643	0.36	0/2228
14	k7	0.25	0/1643	0.39	0/2228
14	k8	0.24	0/1643	0.35	0/2228
14	kV	0.24	0/1643	0.36	0/2228
14	lV	0.24	0/1643	0.38	0/2228
15	m1	0.24	0/1035	0.41	1/1403 (0.1%)
15	m2	0.24	0/1035	0.38	0/1403
15	m5	0.25	0/1035	0.39	0/1403
15	m6	0.23	0/1035	0.40	0/1403
15	mT	0.24	0/1035	0.40	0/1403
15	nT	0.25	0/1035	0.39	0/1403
16	o0	0.24	0/2795	0.45	0/3784
16	o1	0.24	0/2479	0.50	0/3354
16	o2	0.25	0/2479	0.50	0/3354
16	o6	0.24	0/2479	0.50	0/3354
16	pA	0.25	0/2795	0.46	0/3784
16	pB	0.25	0/2795	0.45	0/3784
17	q3	0.28	0/1686	0.44	0/2292
17	q4	0.28	0/1686	0.44	0/2292
17	q5	0.30	0/1729	0.50	0/2349
17	q7	0.29	0/1729	0.50	2/2349 (0.1%)
17	q8	0.28	0/1686	0.48	0/2292
17	q9	0.29	0/1729	0.50	0/2349
All	All	0.19	1/663886 (0.0%)	0.38	18/902721 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	S2	0	1
1	Sx	0	1
5	Yc	0	1
5	Yx	0	1
7	b4	0	1
7	b7	0	1
7	cB	0	1
7	cJ	0	1
7	cK	0	1
7	cP	0	1
7	dV	0	1
16	o1	0	1
16	o2	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	fB	303	ASN	C-O	6.32	1.26	1.23

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	SO	46	GLY	CA-C-N	7.10	124.71	120.24
1	SO	46	GLY	C-N-CA	7.10	124.71	120.24
8	fS	64	THR	N-CA-C	-6.66	105.78	114.04
5	Yy	985	GLU	N-CA-CB	-6.19	107.11	114.17
8	fs	64	THR	N-CA-C	-5.83	106.81	114.04

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	S2	87	TYR	Peptide
1	Sx	87	TYR	Peptide
5	Yc	398	SER	Peptide
5	Yx	398	SER	Peptide
7	b4	572	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S0	3945	0	3828	211	0
1	S1	3945	0	3828	211	0
1	S2	3945	0	3828	206	0
1	S3	3945	0	3828	187	0
1	S4	3945	0	3828	209	0
1	S5	3945	0	3828	190	0
1	S6	3945	0	3828	211	0
1	S7	3945	0	3828	196	0
1	S8	3945	0	3828	198	0
1	SA	3945	0	3828	190	0
1	SO	3945	0	3828	191	0
1	SP	3945	0	3828	195	0
1	SQ	3945	0	3828	197	0
1	Sv	3945	0	3828	203	0
1	Sw	3945	0	3828	185	0
1	Sx	3945	0	3828	206	0
1	Sy	3945	0	3828	196	0
1	Sz	3945	0	3828	202	0
2	T1	2175	0	2157	77	0
2	T2	2175	0	2157	66	0
2	T3	2175	0	2157	74	0
2	T4	2175	0	2157	73	0
2	T5	2175	0	2157	54	0
2	T6	2175	0	2157	66	0
2	T7	2175	0	2157	65	0
2	T8	2175	0	2157	61	0
2	T9	2175	0	2157	61	0
2	TF	2175	0	2157	70	0
2	TG	2175	0	2157	62	0
2	TH	2175	0	2157	64	0
2	Td	2175	0	2157	77	0
2	Te	2175	0	2157	66	0
2	Tf	2175	0	2157	62	0
2	Tg	2175	0	2157	61	0
2	Th	2175	0	2157	65	0
2	Ti	2175	0	2157	68	0
3	UL	1665	0	1638	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	UM	1665	0	1638	78	0
3	UN	1665	0	1638	80	0
3	Up	1665	0	1638	64	0
3	Uq	1665	0	1638	77	0
3	Ur	1665	0	1638	71	0
3	Us	1665	0	1638	74	0
3	Ut	1665	0	1638	57	0
3	Uu	1665	0	1638	65	0
3	VL	1665	0	1638	75	0
3	VM	1665	0	1638	76	0
3	VN	1665	0	1638	63	0
3	Vp	1665	0	1638	69	0
3	Vq	1665	0	1638	72	0
3	Vr	1665	0	1638	74	0
3	Vs	1665	0	1638	79	0
3	Vt	1665	0	1638	70	0
3	Vu	1665	0	1638	77	0
4	WI	4675	0	4446	222	0
4	WJ	4675	0	4447	222	0
4	WK	4675	0	4446	240	0
4	Wj	4675	0	4446	236	0
4	Wk	4675	0	4446	215	0
4	Wl	4675	0	4447	226	0
4	Wm	4675	0	4447	222	0
4	Wn	4675	0	4446	247	0
4	Wo	4675	0	4446	234	0
4	XI	4675	0	4446	239	0
4	XJ	4675	0	4447	244	0
4	XK	4675	0	4446	250	0
4	Xj	4675	0	4446	250	0
4	Xk	4675	0	4446	223	0
4	Xl	4675	0	4447	233	0
4	Xm	4675	0	4447	229	0
4	Xn	4675	0	4446	240	0
4	Xo	4675	0	4446	230	0
5	YC	8199	0	7914	358	0
5	YX	8199	0	7914	358	0
5	YY	8199	0	7914	340	0
5	Yc	8199	0	7914	376	0
5	Yx	8199	0	7914	343	0
5	Yy	8199	0	7914	347	0
6	ZD	2631	0	2509	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	ZE	2658	0	2532	64	0
6	ZZ	2631	0	2509	72	0
6	Za	2631	0	2509	80	0
6	Zb	2658	0	2532	60	0
6	Zc	2658	0	2532	59	0
6	aD	2631	0	2509	68	0
6	aE	2658	0	2532	59	0
6	aZ	2631	0	2509	66	0
6	aa	2631	0	2509	77	0
6	ab	2658	0	2532	59	0
6	ac	2658	0	2532	57	0
7	b0	5000	0	4918	149	0
7	b3	5000	0	4918	114	0
7	b4	5000	0	4918	121	0
7	b5	5000	0	4918	113	0
7	b6	5000	0	4918	119	0
7	b7	5000	0	4918	106	0
7	b8	5000	0	4918	123	0
7	b9	5000	0	4918	128	0
7	bN	5000	0	4918	111	0
7	bO	5000	0	4918	121	0
7	bP	5000	0	4918	118	0
7	bQ	5000	0	4918	120	0
7	bR	5000	0	4918	126	0
7	bY	5000	0	4918	118	0
7	cA	5000	0	4918	143	0
7	cB	5000	0	4918	143	0
7	cC	5000	0	4918	118	0
7	cD	5000	0	4918	126	0
7	cE	5000	0	4918	116	0
7	cF	5000	0	4918	138	0
7	cG	5000	0	4918	118	0
7	cH	5000	0	4918	127	0
7	cI	5000	0	4918	134	0
7	cJ	5000	0	4918	122	0
7	cK	5000	0	4918	123	0
7	cL	5000	0	4918	130	0
7	cM	5000	0	4918	122	0
7	cN	5000	0	4918	137	0
7	cO	5000	0	4918	135	0
7	cP	5000	0	4918	135	0
7	dS	4941	0	4858	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	dT	4941	0	4858	110	0
7	dU	4941	0	4858	138	0
7	dV	4941	0	4858	102	0
7	dW	4941	0	4858	107	0
7	dZ	4941	0	4858	116	0
8	eB	5157	0	5011	172	0
8	eU	5157	0	5011	172	0
8	eW	5157	0	5011	155	0
8	f9	5235	0	5086	151	0
8	fA	5235	0	5086	144	0
8	fB	5157	0	5011	158	0
8	fR	5235	0	5086	132	0
8	fS	5235	0	5086	148	0
8	fU	5157	0	5011	182	0
8	fW	5157	0	5011	154	0
8	fr	5235	0	5086	137	0
8	fs	5235	0	5086	146	0
9	gE	4321	0	4227	107	0
9	gG	4321	0	4227	121	0
9	gH	4321	0	4227	115	0
10	gd	709	0	713	14	0
11	h1	1304	0	1255	50	0
11	h2	1304	0	1255	42	0
11	hI	1304	0	1255	41	0
11	hJ	1304	0	1255	45	0
11	hK	1304	0	1255	53	0
11	hL	1304	0	1255	49	0
11	hM	1304	0	1255	45	0
11	hX	1304	0	1255	51	0
11	he	1304	0	1255	43	0
11	hf	1304	0	1255	45	0
11	hg	1304	0	1255	42	0
11	hh	1304	0	1255	38	0
11	hi	1304	0	1255	45	0
11	hj	1304	0	1255	48	0
11	hk	1304	0	1255	55	0
11	hl	1304	0	1255	42	0
11	hm	1304	0	1255	49	0
11	hn	1304	0	1255	44	0
11	ho	1304	0	1255	42	0
11	hp	1304	0	1255	48	0
11	hq	1304	0	1255	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	hr	1304	0	1255	37	0
11	hs	1304	0	1255	55	0
11	ht	1304	0	1255	38	0
11	hu	1304	0	1255	46	0
11	hv	1304	0	1255	39	0
11	hw	1304	0	1255	50	0
11	hx	1304	0	1255	49	0
11	hy	1304	0	1255	49	0
11	hz	1304	0	1255	44	0
12	iC	3000	0	2928	100	0
12	iD	3000	0	2928	100	0
12	iF	3000	0	2928	79	0
13	ja	137	0	130	4	0
13	jb	137	0	130	4	0
13	jc	137	0	130	2	0
14	k3	1599	0	1544	35	0
14	k4	1599	0	1544	33	0
14	k7	1599	0	1544	31	0
14	k8	1599	0	1544	27	0
14	kV	1599	0	1544	27	0
14	lV	1599	0	1544	36	0
15	m1	1019	0	1015	36	0
15	m2	1019	0	1015	35	0
15	m5	1019	0	1015	38	0
15	m6	1019	0	1015	36	0
15	mT	1019	0	1015	37	0
15	nT	1019	0	1015	36	0
16	o0	2749	0	2715	105	0
16	o1	2436	0	2408	90	0
16	o2	2436	0	2408	85	0
16	o6	2436	0	2408	91	0
16	pA	2749	0	2715	96	0
16	pB	2749	0	2715	100	0
17	q3	1650	0	1569	77	0
17	q4	1650	0	1569	72	0
17	q5	1693	0	1619	82	0
17	q7	1693	0	1619	74	0
17	q8	1650	0	1569	71	0
17	q9	1693	0	1619	84	0
18	rc	125	0	27	1	0
18	rd	125	0	27	3	0
18	re	125	0	27	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	rf	125	0	27	3	0
18	rg	125	0	27	0	0
18	rh	125	0	27	1	0
19	sQ	90	0	22	0	0
19	sT	90	0	22	1	0
19	sU	90	0	22	1	0
20	tS	50	0	12	0	0
20	tX	50	0	12	0	0
20	tY	50	0	12	0	0
21	uR	35	0	10	1	0
21	uV	35	0	10	0	0
21	uW	35	0	10	0	0
22	vZ	45	0	11	0	0
22	va	45	0	11	0	0
22	vb	45	0	11	0	0
23	S0	1	0	0	0	0
23	S1	1	0	0	0	0
23	S4	1	0	0	0	0
23	SA	1	0	0	0	0
23	SQ	1	0	0	0	0
23	Sv	1	0	0	0	0
All	All	652117	0	633080	18930	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 18930 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:hi:82:ARG:HH12	11:hi:138:GLY:HA2	1.34	0.91
1:Sz:2:SER:N	1:Sz:5:THR:HG1	1.70	0.90
1:Sv:173:ILE:HD11	1:Sz:174:ALA:HB2	1.54	0.89
1:S1:173:ILE:HD11	1:S3:174:ALA:HB2	1.55	0.88
2:Te:168:PHE:HA	2:Tg:163:SER:HB3	1.55	0.87

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S0	524/527 (99%)	488 (93%)	34 (6%)	2 (0%)	30	61
1	S1	524/527 (99%)	498 (95%)	22 (4%)	4 (1%)	16	49
1	S2	524/527 (99%)	492 (94%)	31 (6%)	1 (0%)	43	72
1	S3	524/527 (99%)	488 (93%)	33 (6%)	3 (1%)	21	54
1	S4	524/527 (99%)	498 (95%)	22 (4%)	4 (1%)	16	49
1	S5	524/527 (99%)	493 (94%)	27 (5%)	4 (1%)	16	49
1	S6	524/527 (99%)	497 (95%)	25 (5%)	2 (0%)	30	61
1	S7	524/527 (99%)	495 (94%)	27 (5%)	2 (0%)	30	61
1	S8	524/527 (99%)	491 (94%)	30 (6%)	3 (1%)	21	54
1	SA	524/527 (99%)	486 (93%)	36 (7%)	2 (0%)	30	61
1	SO	524/527 (99%)	490 (94%)	31 (6%)	3 (1%)	21	54
1	SP	524/527 (99%)	485 (93%)	36 (7%)	3 (1%)	21	54
1	SQ	524/527 (99%)	485 (93%)	36 (7%)	3 (1%)	21	54
1	Sv	524/527 (99%)	497 (95%)	23 (4%)	4 (1%)	16	49
1	Sw	524/527 (99%)	491 (94%)	31 (6%)	2 (0%)	30	61
1	Sx	524/527 (99%)	498 (95%)	25 (5%)	1 (0%)	43	72
1	Sy	524/527 (99%)	491 (94%)	31 (6%)	2 (0%)	30	61
1	Sz	524/527 (99%)	489 (93%)	32 (6%)	3 (1%)	21	54
2	T1	286/288 (99%)	271 (95%)	13 (4%)	2 (1%)	18	51
2	T2	286/288 (99%)	272 (95%)	12 (4%)	2 (1%)	18	51
2	T3	286/288 (99%)	271 (95%)	12 (4%)	3 (1%)	12	45
2	T4	286/288 (99%)	269 (94%)	15 (5%)	2 (1%)	18	51
2	T5	286/288 (99%)	270 (94%)	14 (5%)	2 (1%)	18	51
2	T6	286/288 (99%)	273 (96%)	11 (4%)	2 (1%)	18	51
2	T7	286/288 (99%)	268 (94%)	16 (6%)	2 (1%)	18	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T8	286/288 (99%)	274 (96%)	9 (3%)	3 (1%)	12	45
2	T9	286/288 (99%)	272 (95%)	12 (4%)	2 (1%)	18	51
2	TF	286/288 (99%)	271 (95%)	13 (4%)	2 (1%)	18	51
2	TG	286/288 (99%)	268 (94%)	16 (6%)	2 (1%)	18	51
2	TH	286/288 (99%)	271 (95%)	13 (4%)	2 (1%)	18	51
2	Td	286/288 (99%)	272 (95%)	12 (4%)	2 (1%)	18	51
2	Te	286/288 (99%)	271 (95%)	13 (4%)	2 (1%)	18	51
2	Tf	286/288 (99%)	272 (95%)	12 (4%)	2 (1%)	18	51
2	Tg	286/288 (99%)	269 (94%)	14 (5%)	3 (1%)	12	45
2	Th	286/288 (99%)	271 (95%)	12 (4%)	3 (1%)	12	45
2	Ti	286/288 (99%)	272 (95%)	12 (4%)	2 (1%)	18	51
3	UL	216/219 (99%)	208 (96%)	7 (3%)	1 (0%)	24	57
3	UM	216/219 (99%)	206 (95%)	9 (4%)	1 (0%)	24	57
3	UN	216/219 (99%)	207 (96%)	8 (4%)	1 (0%)	24	57
3	Up	216/219 (99%)	206 (95%)	8 (4%)	2 (1%)	14	46
3	Uq	216/219 (99%)	208 (96%)	7 (3%)	1 (0%)	24	57
3	Ur	216/219 (99%)	204 (94%)	11 (5%)	1 (0%)	24	57
3	Us	216/219 (99%)	205 (95%)	10 (5%)	1 (0%)	24	57
3	Ut	216/219 (99%)	203 (94%)	12 (6%)	1 (0%)	24	57
3	Uu	216/219 (99%)	206 (95%)	9 (4%)	1 (0%)	24	57
3	VL	216/219 (99%)	205 (95%)	10 (5%)	1 (0%)	24	57
3	VM	216/219 (99%)	208 (96%)	7 (3%)	1 (0%)	24	57
3	VN	216/219 (99%)	205 (95%)	10 (5%)	1 (0%)	24	57
3	Vp	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	14	46
3	Vq	216/219 (99%)	206 (95%)	9 (4%)	1 (0%)	24	57
3	Vr	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	14	46
3	Vs	216/219 (99%)	206 (95%)	9 (4%)	1 (0%)	24	57
3	Vt	216/219 (99%)	207 (96%)	8 (4%)	1 (0%)	24	57
3	Vu	216/219 (99%)	208 (96%)	7 (3%)	1 (0%)	24	57
4	WI	600/602 (100%)	529 (88%)	64 (11%)	7 (1%)	10	41
4	WJ	600/602 (100%)	526 (88%)	66 (11%)	8 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	WK	600/602 (100%)	520 (87%)	74 (12%)	6 (1%)	12	45
4	Wj	600/602 (100%)	528 (88%)	64 (11%)	8 (1%)	9	39
4	Wk	600/602 (100%)	530 (88%)	63 (10%)	7 (1%)	10	41
4	Wl	600/602 (100%)	512 (85%)	80 (13%)	8 (1%)	9	39
4	Wm	600/602 (100%)	523 (87%)	67 (11%)	10 (2%)	7	35
4	Wn	600/602 (100%)	523 (87%)	71 (12%)	6 (1%)	12	45
4	Wo	600/602 (100%)	515 (86%)	79 (13%)	6 (1%)	12	45
4	XI	600/602 (100%)	536 (89%)	57 (10%)	7 (1%)	10	41
4	XJ	600/602 (100%)	511 (85%)	79 (13%)	10 (2%)	7	35
4	XK	600/602 (100%)	520 (87%)	73 (12%)	7 (1%)	10	41
4	Xj	600/602 (100%)	533 (89%)	61 (10%)	6 (1%)	12	45
4	Xk	600/602 (100%)	527 (88%)	66 (11%)	7 (1%)	10	41
4	Xl	600/602 (100%)	515 (86%)	78 (13%)	7 (1%)	10	41
4	Xm	600/602 (100%)	526 (88%)	65 (11%)	9 (2%)	8	37
4	Xn	600/602 (100%)	519 (86%)	75 (12%)	6 (1%)	12	45
4	Xo	600/602 (100%)	523 (87%)	70 (12%)	7 (1%)	10	41
5	YC	1000/1032 (97%)	785 (78%)	191 (19%)	24 (2%)	4	29
5	YX	1000/1032 (97%)	789 (79%)	189 (19%)	22 (2%)	5	30
5	YY	1000/1032 (97%)	787 (79%)	191 (19%)	22 (2%)	5	30
5	Yc	1000/1032 (97%)	795 (80%)	186 (19%)	19 (2%)	6	33
5	Yx	1000/1032 (97%)	792 (79%)	187 (19%)	21 (2%)	5	31
5	Yy	1000/1032 (97%)	785 (78%)	192 (19%)	23 (2%)	5	30
6	ZD	326/334 (98%)	309 (95%)	16 (5%)	1 (0%)	36	65
6	ZE	330/334 (99%)	314 (95%)	16 (5%)	0	100	100
6	ZZ	326/334 (98%)	314 (96%)	10 (3%)	2 (1%)	21	54
6	Za	326/334 (98%)	315 (97%)	10 (3%)	1 (0%)	36	65
6	Zb	330/334 (99%)	311 (94%)	19 (6%)	0	100	100
6	Zc	330/334 (99%)	313 (95%)	17 (5%)	0	100	100
6	aD	326/334 (98%)	314 (96%)	11 (3%)	1 (0%)	36	65
6	aE	330/334 (99%)	311 (94%)	19 (6%)	0	100	100
6	aZ	326/334 (98%)	314 (96%)	11 (3%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	aa	326/334 (98%)	312 (96%)	13 (4%)	1 (0%)	36	65
6	ab	330/334 (99%)	311 (94%)	19 (6%)	0	100	100
6	ac	330/334 (99%)	311 (94%)	19 (6%)	0	100	100
7	b0	653/659 (99%)	579 (89%)	67 (10%)	7 (1%)	11	43
7	b3	653/659 (99%)	581 (89%)	64 (10%)	8 (1%)	10	41
7	b4	653/659 (99%)	569 (87%)	76 (12%)	8 (1%)	10	41
7	b5	653/659 (99%)	578 (88%)	68 (10%)	7 (1%)	11	43
7	b6	653/659 (99%)	568 (87%)	76 (12%)	9 (1%)	9	38
7	b7	653/659 (99%)	576 (88%)	69 (11%)	8 (1%)	10	41
7	b8	653/659 (99%)	577 (88%)	70 (11%)	6 (1%)	14	46
7	b9	653/659 (99%)	574 (88%)	72 (11%)	7 (1%)	11	43
7	bN	653/659 (99%)	582 (89%)	68 (10%)	3 (0%)	24	57
7	bO	653/659 (99%)	582 (89%)	68 (10%)	3 (0%)	24	57
7	bP	653/659 (99%)	575 (88%)	75 (12%)	3 (0%)	24	57
7	bQ	653/659 (99%)	578 (88%)	71 (11%)	4 (1%)	21	54
7	bR	653/659 (99%)	582 (89%)	67 (10%)	4 (1%)	21	54
7	bY	653/659 (99%)	578 (88%)	71 (11%)	4 (1%)	21	54
7	cA	653/659 (99%)	582 (89%)	64 (10%)	7 (1%)	11	43
7	cB	653/659 (99%)	584 (89%)	63 (10%)	6 (1%)	14	46
7	cC	653/659 (99%)	585 (90%)	62 (10%)	6 (1%)	14	46
7	cD	653/659 (99%)	567 (87%)	80 (12%)	6 (1%)	14	46
7	cE	653/659 (99%)	574 (88%)	71 (11%)	8 (1%)	10	41
7	cF	653/659 (99%)	567 (87%)	78 (12%)	8 (1%)	10	41
7	cG	653/659 (99%)	572 (88%)	75 (12%)	6 (1%)	14	46
7	cH	653/659 (99%)	574 (88%)	71 (11%)	8 (1%)	10	41
7	cI	653/659 (99%)	577 (88%)	68 (10%)	8 (1%)	10	41
7	cJ	653/659 (99%)	577 (88%)	70 (11%)	6 (1%)	14	46
7	cK	653/659 (99%)	576 (88%)	70 (11%)	7 (1%)	11	43
7	cL	653/659 (99%)	580 (89%)	68 (10%)	5 (1%)	16	49
7	cM	653/659 (99%)	585 (90%)	61 (9%)	7 (1%)	11	43
7	cN	653/659 (99%)	582 (89%)	66 (10%)	5 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	cO	653/659 (99%)	575 (88%)	70 (11%)	8 (1%)	10	41
7	cP	653/659 (99%)	582 (89%)	65 (10%)	6 (1%)	14	46
7	dS	645/659 (98%)	579 (90%)	61 (10%)	5 (1%)	16	49
7	dT	645/659 (98%)	581 (90%)	57 (9%)	7 (1%)	11	43
7	dU	645/659 (98%)	580 (90%)	60 (9%)	5 (1%)	16	49
7	dV	645/659 (98%)	579 (90%)	58 (9%)	8 (1%)	10	41
7	dW	645/659 (98%)	571 (88%)	68 (10%)	6 (1%)	14	46
7	dZ	645/659 (98%)	585 (91%)	53 (8%)	7 (1%)	11	43
8	eB	646/660 (98%)	564 (87%)	74 (12%)	8 (1%)	10	41
8	eU	646/660 (98%)	572 (88%)	68 (10%)	6 (1%)	14	46
8	eW	646/660 (98%)	573 (89%)	65 (10%)	8 (1%)	10	41
8	f9	656/660 (99%)	597 (91%)	52 (8%)	7 (1%)	11	43
8	fA	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	11	43
8	fB	646/660 (98%)	575 (89%)	65 (10%)	6 (1%)	14	46
8	fR	656/660 (99%)	594 (90%)	56 (8%)	6 (1%)	14	46
8	fS	656/660 (99%)	584 (89%)	65 (10%)	7 (1%)	11	43
8	fU	646/660 (98%)	578 (90%)	62 (10%)	6 (1%)	14	46
8	fW	646/660 (98%)	570 (88%)	70 (11%)	6 (1%)	14	46
8	fr	656/660 (99%)	598 (91%)	52 (8%)	6 (1%)	14	46
8	fs	656/660 (99%)	591 (90%)	59 (9%)	6 (1%)	14	46
9	gE	555/575 (96%)	521 (94%)	33 (6%)	1 (0%)	43	72
9	gG	555/575 (96%)	525 (95%)	29 (5%)	1 (0%)	43	72
9	gH	555/575 (96%)	526 (95%)	28 (5%)	1 (0%)	43	72
10	gd	94/97 (97%)	91 (97%)	3 (3%)	0	100	100
11	h1	161/163 (99%)	137 (85%)	19 (12%)	5 (3%)	3	25
11	h2	161/163 (99%)	137 (85%)	19 (12%)	5 (3%)	3	25
11	hI	161/163 (99%)	134 (83%)	21 (13%)	6 (4%)	2	21
11	hJ	161/163 (99%)	139 (86%)	18 (11%)	4 (2%)	4	28
11	hK	161/163 (99%)	137 (85%)	19 (12%)	5 (3%)	3	25
11	hL	161/163 (99%)	140 (87%)	16 (10%)	5 (3%)	3	25
11	hM	161/163 (99%)	137 (85%)	20 (12%)	4 (2%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	hX	161/163 (99%)	137 (85%)	18 (11%)	6 (4%)	2	21
11	he	161/163 (99%)	133 (83%)	24 (15%)	4 (2%)	4	28
11	hf	161/163 (99%)	139 (86%)	18 (11%)	4 (2%)	4	28
11	hg	161/163 (99%)	135 (84%)	21 (13%)	5 (3%)	3	25
11	hh	161/163 (99%)	139 (86%)	17 (11%)	5 (3%)	3	25
11	hi	161/163 (99%)	133 (83%)	22 (14%)	6 (4%)	2	21
11	hj	161/163 (99%)	132 (82%)	24 (15%)	5 (3%)	3	25
11	hk	161/163 (99%)	135 (84%)	22 (14%)	4 (2%)	4	28
11	hl	161/163 (99%)	133 (83%)	23 (14%)	5 (3%)	3	25
11	hm	161/163 (99%)	135 (84%)	22 (14%)	4 (2%)	4	28
11	hn	161/163 (99%)	135 (84%)	21 (13%)	5 (3%)	3	25
11	ho	161/163 (99%)	133 (83%)	25 (16%)	3 (2%)	6	33
11	hp	161/163 (99%)	139 (86%)	18 (11%)	4 (2%)	4	28
11	hq	161/163 (99%)	134 (83%)	23 (14%)	4 (2%)	4	28
11	hr	161/163 (99%)	132 (82%)	25 (16%)	4 (2%)	4	28
11	hs	161/163 (99%)	136 (84%)	21 (13%)	4 (2%)	4	28
11	ht	161/163 (99%)	139 (86%)	17 (11%)	5 (3%)	3	25
11	hu	161/163 (99%)	133 (83%)	23 (14%)	5 (3%)	3	25
11	hv	161/163 (99%)	139 (86%)	18 (11%)	4 (2%)	4	28
11	hw	161/163 (99%)	135 (84%)	20 (12%)	6 (4%)	2	21
11	hx	161/163 (99%)	136 (84%)	21 (13%)	4 (2%)	4	28
11	hy	161/163 (99%)	133 (83%)	23 (14%)	5 (3%)	3	25
11	hz	161/163 (99%)	135 (84%)	21 (13%)	5 (3%)	3	25
12	iC	373/391 (95%)	343 (92%)	28 (8%)	2 (0%)	24	57
12	iD	373/391 (95%)	347 (93%)	23 (6%)	3 (1%)	16	49
12	iF	373/391 (95%)	344 (92%)	26 (7%)	3 (1%)	16	49
13	ja	18/590 (3%)	13 (72%)	3 (17%)	2 (11%)	0	4
13	jb	18/590 (3%)	12 (67%)	5 (28%)	1 (6%)	1	14
13	jc	18/590 (3%)	12 (67%)	5 (28%)	1 (6%)	1	14
14	k3	191/196 (97%)	166 (87%)	23 (12%)	2 (1%)	12	45
14	k4	191/196 (97%)	166 (87%)	23 (12%)	2 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	k7	191/196 (97%)	162 (85%)	27 (14%)	2 (1%)	12	45
14	k8	191/196 (97%)	168 (88%)	21 (11%)	2 (1%)	12	45
14	kV	191/196 (97%)	166 (87%)	23 (12%)	2 (1%)	12	45
14	IV	191/196 (97%)	165 (86%)	24 (13%)	2 (1%)	12	45
15	m1	125/132 (95%)	106 (85%)	19 (15%)	0	100	100
15	m2	125/132 (95%)	108 (86%)	17 (14%)	0	100	100
15	m5	125/132 (95%)	107 (86%)	18 (14%)	0	100	100
15	m6	125/132 (95%)	112 (90%)	13 (10%)	0	100	100
15	mT	125/132 (95%)	114 (91%)	11 (9%)	0	100	100
15	nT	125/132 (95%)	108 (86%)	17 (14%)	0	100	100
16	o0	356/364 (98%)	279 (78%)	71 (20%)	6 (2%)	7	35
16	o1	310/364 (85%)	248 (80%)	55 (18%)	7 (2%)	5	30
16	o2	310/364 (85%)	242 (78%)	59 (19%)	9 (3%)	3	26
16	o6	310/364 (85%)	243 (78%)	58 (19%)	9 (3%)	3	26
16	pA	356/364 (98%)	274 (77%)	74 (21%)	8 (2%)	5	30
16	pB	356/364 (98%)	275 (77%)	74 (21%)	7 (2%)	6	32
17	q3	203/320 (63%)	170 (84%)	30 (15%)	3 (2%)	8	37
17	q4	203/320 (63%)	175 (86%)	26 (13%)	2 (1%)	12	45
17	q5	209/320 (65%)	179 (86%)	28 (13%)	2 (1%)	12	45
17	q7	209/320 (65%)	178 (85%)	29 (14%)	2 (1%)	12	45
17	q8	203/320 (63%)	168 (83%)	33 (16%)	2 (1%)	12	45
17	q9	209/320 (65%)	178 (85%)	29 (14%)	2 (1%)	12	45
All	All	83368/87019 (96%)	74174 (89%)	8284 (10%)	910 (1%)	14	43

5 of 910 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S1	47	VAL
1	S2	47	VAL
1	S3	47	VAL
1	S4	47	VAL
1	S5	47	VAL

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	S0	426/427 (100%)	404 (95%)	22 (5%)	21	48
1	S1	426/427 (100%)	400 (94%)	26 (6%)	17	45
1	S2	426/427 (100%)	408 (96%)	18 (4%)	26	53
1	S3	426/427 (100%)	404 (95%)	22 (5%)	21	48
1	S4	426/427 (100%)	407 (96%)	19 (4%)	24	51
1	S5	426/427 (100%)	405 (95%)	21 (5%)	22	49
1	S6	426/427 (100%)	407 (96%)	19 (4%)	24	51
1	S7	426/427 (100%)	410 (96%)	16 (4%)	29	55
1	S8	426/427 (100%)	404 (95%)	22 (5%)	21	48
1	SA	426/427 (100%)	406 (95%)	20 (5%)	23	50
1	SO	426/427 (100%)	402 (94%)	24 (6%)	19	47
1	SP	426/427 (100%)	407 (96%)	19 (4%)	24	51
1	SQ	426/427 (100%)	404 (95%)	22 (5%)	21	48
1	Sv	426/427 (100%)	402 (94%)	24 (6%)	19	47
1	Sw	426/427 (100%)	406 (95%)	20 (5%)	23	50
1	Sx	426/427 (100%)	409 (96%)	17 (4%)	28	54
1	Sy	426/427 (100%)	411 (96%)	15 (4%)	32	57
1	Sz	426/427 (100%)	406 (95%)	20 (5%)	23	50
2	T1	244/244 (100%)	237 (97%)	7 (3%)	37	60
2	T2	244/244 (100%)	232 (95%)	12 (5%)	22	49
2	T3	244/244 (100%)	239 (98%)	5 (2%)	48	66
2	T4	244/244 (100%)	238 (98%)	6 (2%)	42	63
2	T5	244/244 (100%)	238 (98%)	6 (2%)	42	63
2	T6	244/244 (100%)	232 (95%)	12 (5%)	22	49
2	T7	244/244 (100%)	232 (95%)	12 (5%)	22	49
2	T8	244/244 (100%)	239 (98%)	5 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T9	244/244 (100%)	237 (97%)	7 (3%)	37	60
2	TF	244/244 (100%)	237 (97%)	7 (3%)	37	60
2	TG	244/244 (100%)	233 (96%)	11 (4%)	24	51
2	TH	244/244 (100%)	237 (97%)	7 (3%)	37	60
2	Td	244/244 (100%)	234 (96%)	10 (4%)	27	53
2	Te	244/244 (100%)	239 (98%)	5 (2%)	48	66
2	Tf	244/244 (100%)	233 (96%)	11 (4%)	24	51
2	Tg	244/244 (100%)	233 (96%)	11 (4%)	24	51
2	Th	244/244 (100%)	240 (98%)	4 (2%)	55	69
2	Ti	244/244 (100%)	236 (97%)	8 (3%)	33	58
3	UL	187/188 (100%)	182 (97%)	5 (3%)	39	61
3	UM	187/188 (100%)	184 (98%)	3 (2%)	55	69
3	UN	187/188 (100%)	185 (99%)	2 (1%)	65	74
3	Up	187/188 (100%)	184 (98%)	3 (2%)	55	69
3	Uq	187/188 (100%)	183 (98%)	4 (2%)	47	65
3	Ur	187/188 (100%)	183 (98%)	4 (2%)	47	65
3	Us	187/188 (100%)	181 (97%)	6 (3%)	34	58
3	Ut	187/188 (100%)	184 (98%)	3 (2%)	55	69
3	Uu	187/188 (100%)	185 (99%)	2 (1%)	65	74
3	VL	187/188 (100%)	185 (99%)	2 (1%)	65	74
3	VM	187/188 (100%)	184 (98%)	3 (2%)	55	69
3	VN	187/188 (100%)	182 (97%)	5 (3%)	39	61
3	Vp	187/188 (100%)	182 (97%)	5 (3%)	39	61
3	Vq	187/188 (100%)	182 (97%)	5 (3%)	39	61
3	Vr	187/188 (100%)	182 (97%)	5 (3%)	39	61
3	Vs	187/188 (100%)	180 (96%)	7 (4%)	30	56
3	Vt	187/188 (100%)	184 (98%)	3 (2%)	55	69
3	Vu	187/188 (100%)	184 (98%)	3 (2%)	55	69
4	WI	519/519 (100%)	485 (93%)	34 (7%)	15	43
4	WJ	519/519 (100%)	483 (93%)	36 (7%)	14	41
4	WK	519/519 (100%)	476 (92%)	43 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Wj	519/519 (100%)	484 (93%)	35 (7%)	15	42
4	Wk	519/519 (100%)	485 (93%)	34 (7%)	15	43
4	Wl	519/519 (100%)	485 (93%)	34 (7%)	15	43
4	Wm	519/519 (100%)	478 (92%)	41 (8%)	11	37
4	Wn	519/519 (100%)	481 (93%)	38 (7%)	13	40
4	Wo	519/519 (100%)	471 (91%)	48 (9%)	8	33
4	XI	519/519 (100%)	479 (92%)	40 (8%)	12	38
4	XJ	519/519 (100%)	475 (92%)	44 (8%)	10	35
4	XK	519/519 (100%)	476 (92%)	43 (8%)	10	35
4	Xj	519/519 (100%)	479 (92%)	40 (8%)	12	38
4	Xk	519/519 (100%)	480 (92%)	39 (8%)	12	39
4	Xl	519/519 (100%)	485 (93%)	34 (7%)	15	43
4	Xm	519/519 (100%)	479 (92%)	40 (8%)	12	38
4	Xn	519/519 (100%)	475 (92%)	44 (8%)	10	35
4	Xo	519/519 (100%)	475 (92%)	44 (8%)	10	35
5	YC	896/921 (97%)	750 (84%)	146 (16%)	2	15
5	YX	896/921 (97%)	756 (84%)	140 (16%)	2	16
5	YY	896/921 (97%)	748 (84%)	148 (16%)	2	14
5	Yc	896/921 (97%)	748 (84%)	148 (16%)	2	14
5	Yx	896/921 (97%)	745 (83%)	151 (17%)	2	13
5	Yy	896/921 (97%)	759 (85%)	137 (15%)	3	16
6	ZD	289/295 (98%)	277 (96%)	12 (4%)	26	53
6	ZE	293/295 (99%)	283 (97%)	10 (3%)	32	57
6	ZZ	289/295 (98%)	278 (96%)	11 (4%)	29	55
6	Za	289/295 (98%)	275 (95%)	14 (5%)	23	50
6	Zb	293/295 (99%)	279 (95%)	14 (5%)	23	50
6	Zc	293/295 (99%)	281 (96%)	12 (4%)	27	53
6	aD	289/295 (98%)	278 (96%)	11 (4%)	29	55
6	aE	293/295 (99%)	282 (96%)	11 (4%)	29	55
6	aZ	289/295 (98%)	280 (97%)	9 (3%)	35	59
6	aa	289/295 (98%)	272 (94%)	17 (6%)	18	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	ab	293/295 (99%)	279 (95%)	14 (5%)	23	50
6	ac	293/295 (99%)	281 (96%)	12 (4%)	27	53
7	b0	534/536 (100%)	469 (88%)	65 (12%)	5	23
7	b3	534/536 (100%)	467 (88%)	67 (12%)	4	22
7	b4	534/536 (100%)	481 (90%)	53 (10%)	7	31
7	b5	534/536 (100%)	476 (89%)	58 (11%)	6	27
7	b6	534/536 (100%)	478 (90%)	56 (10%)	6	29
7	b7	534/536 (100%)	475 (89%)	59 (11%)	6	27
7	b8	534/536 (100%)	472 (88%)	62 (12%)	5	25
7	b9	534/536 (100%)	468 (88%)	66 (12%)	4	23
7	bN	534/536 (100%)	476 (89%)	58 (11%)	6	27
7	bO	534/536 (100%)	477 (89%)	57 (11%)	6	28
7	bP	534/536 (100%)	471 (88%)	63 (12%)	5	24
7	bQ	534/536 (100%)	483 (90%)	51 (10%)	8	32
7	bR	534/536 (100%)	474 (89%)	60 (11%)	6	27
7	bY	534/536 (100%)	475 (89%)	59 (11%)	6	27
7	cA	534/536 (100%)	465 (87%)	69 (13%)	4	22
7	cB	534/536 (100%)	472 (88%)	62 (12%)	5	25
7	cC	534/536 (100%)	470 (88%)	64 (12%)	5	24
7	cD	534/536 (100%)	470 (88%)	64 (12%)	5	24
7	cE	534/536 (100%)	474 (89%)	60 (11%)	6	27
7	cF	534/536 (100%)	468 (88%)	66 (12%)	4	23
7	cG	534/536 (100%)	472 (88%)	62 (12%)	5	25
7	cH	534/536 (100%)	474 (89%)	60 (11%)	6	27
7	cI	534/536 (100%)	472 (88%)	62 (12%)	5	25
7	cJ	534/536 (100%)	479 (90%)	55 (10%)	7	30
7	cK	534/536 (100%)	469 (88%)	65 (12%)	5	23
7	cL	534/536 (100%)	472 (88%)	62 (12%)	5	25
7	cM	534/536 (100%)	469 (88%)	65 (12%)	5	23
7	cN	534/536 (100%)	463 (87%)	71 (13%)	4	21
7	cO	534/536 (100%)	472 (88%)	62 (12%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	cP	534/536 (100%)	462 (86%)	72 (14%)	4	21
7	dS	527/536 (98%)	458 (87%)	69 (13%)	4	21
7	dT	527/536 (98%)	460 (87%)	67 (13%)	4	22
7	dU	527/536 (98%)	457 (87%)	70 (13%)	4	21
7	dV	527/536 (98%)	463 (88%)	64 (12%)	5	23
7	dW	527/536 (98%)	462 (88%)	65 (12%)	4	23
7	dZ	527/536 (98%)	455 (86%)	72 (14%)	3	20
8	eB	567/578 (98%)	495 (87%)	72 (13%)	4	22
8	eU	567/578 (98%)	482 (85%)	85 (15%)	3	17
8	eW	567/578 (98%)	488 (86%)	79 (14%)	3	19
8	f9	576/578 (100%)	487 (84%)	89 (16%)	2	16
8	fA	576/578 (100%)	496 (86%)	80 (14%)	3	19
8	fB	567/578 (98%)	486 (86%)	81 (14%)	3	19
8	fR	576/578 (100%)	489 (85%)	87 (15%)	3	17
8	fS	576/578 (100%)	491 (85%)	85 (15%)	3	17
8	fU	567/578 (98%)	496 (88%)	71 (12%)	4	22
8	fW	567/578 (98%)	489 (86%)	78 (14%)	3	20
8	fr	576/578 (100%)	489 (85%)	87 (15%)	3	17
8	fs	576/578 (100%)	490 (85%)	86 (15%)	3	17
9	gE	474/485 (98%)	417 (88%)	57 (12%)	5	24
9	gG	474/485 (98%)	426 (90%)	48 (10%)	7	30
9	gH	474/485 (98%)	422 (89%)	52 (11%)	6	27
10	gd	78/79 (99%)	75 (96%)	3 (4%)	29	55
11	h1	137/137 (100%)	107 (78%)	30 (22%)	1	6
11	h2	137/137 (100%)	106 (77%)	31 (23%)	1	6
11	hI	137/137 (100%)	112 (82%)	25 (18%)	2	11
11	hJ	137/137 (100%)	107 (78%)	30 (22%)	1	6
11	hK	137/137 (100%)	110 (80%)	27 (20%)	1	8
11	hL	137/137 (100%)	114 (83%)	23 (17%)	2	13
11	hM	137/137 (100%)	110 (80%)	27 (20%)	1	8
11	hX	137/137 (100%)	109 (80%)	28 (20%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	he	137/137 (100%)	115 (84%)	22 (16%)	2	15
11	hf	137/137 (100%)	113 (82%)	24 (18%)	2	12
11	hg	137/137 (100%)	113 (82%)	24 (18%)	2	12
11	hh	137/137 (100%)	114 (83%)	23 (17%)	2	13
11	hi	137/137 (100%)	112 (82%)	25 (18%)	2	11
11	hj	137/137 (100%)	109 (80%)	28 (20%)	1	8
11	hk	137/137 (100%)	115 (84%)	22 (16%)	2	15
11	hl	137/137 (100%)	115 (84%)	22 (16%)	2	15
11	hm	137/137 (100%)	117 (85%)	20 (15%)	3	18
11	hn	137/137 (100%)	115 (84%)	22 (16%)	2	15
11	ho	137/137 (100%)	106 (77%)	31 (23%)	1	6
11	hp	137/137 (100%)	114 (83%)	23 (17%)	2	13
11	hq	137/137 (100%)	111 (81%)	26 (19%)	1	9
11	hr	137/137 (100%)	109 (80%)	28 (20%)	1	8
11	hs	137/137 (100%)	114 (83%)	23 (17%)	2	13
11	ht	137/137 (100%)	115 (84%)	22 (16%)	2	15
11	hu	137/137 (100%)	113 (82%)	24 (18%)	2	12
11	hv	137/137 (100%)	108 (79%)	29 (21%)	1	7
11	hw	137/137 (100%)	105 (77%)	32 (23%)	1	5
11	hx	137/137 (100%)	110 (80%)	27 (20%)	1	8
11	hy	137/137 (100%)	109 (80%)	28 (20%)	1	8
11	hz	137/137 (100%)	110 (80%)	27 (20%)	1	8
12	iC	334/350 (95%)	286 (86%)	48 (14%)	3	18
12	iD	334/350 (95%)	294 (88%)	40 (12%)	5	24
12	iF	334/350 (95%)	290 (87%)	44 (13%)	4	21
13	ja	16/499 (3%)	13 (81%)	3 (19%)	1	10
13	jb	16/499 (3%)	14 (88%)	2 (12%)	4	22
13	jc	16/499 (3%)	14 (88%)	2 (12%)	4	22
14	k3	166/169 (98%)	148 (89%)	18 (11%)	6	28
14	k4	166/169 (98%)	138 (83%)	28 (17%)	2	13
14	k7	166/169 (98%)	148 (89%)	18 (11%)	6	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	k8	166/169 (98%)	139 (84%)	27 (16%)	2	15
14	kV	166/169 (98%)	137 (82%)	29 (18%)	2	12
14	lV	166/169 (98%)	149 (90%)	17 (10%)	7	30
15	m1	119/123 (97%)	104 (87%)	15 (13%)	4	22
15	m2	119/123 (97%)	102 (86%)	17 (14%)	3	19
15	m5	119/123 (97%)	108 (91%)	11 (9%)	8	33
15	m6	119/123 (97%)	106 (89%)	13 (11%)	6	27
15	mT	119/123 (97%)	102 (86%)	17 (14%)	3	19
15	nT	119/123 (97%)	103 (87%)	16 (13%)	4	21
16	o0	309/313 (99%)	267 (86%)	42 (14%)	3	20
16	o1	276/313 (88%)	228 (83%)	48 (17%)	2	12
16	o2	276/313 (88%)	237 (86%)	39 (14%)	3	19
16	o6	276/313 (88%)	228 (83%)	48 (17%)	2	12
16	pA	309/313 (99%)	272 (88%)	37 (12%)	5	24
16	pB	309/313 (99%)	267 (86%)	42 (14%)	3	20
17	q3	183/275 (66%)	148 (81%)	35 (19%)	1	9
17	q4	183/275 (66%)	145 (79%)	38 (21%)	1	7
17	q5	189/275 (69%)	146 (77%)	43 (23%)	1	6
17	q7	189/275 (69%)	147 (78%)	42 (22%)	1	6
17	q8	183/275 (66%)	145 (79%)	38 (21%)	1	7
17	q9	189/275 (69%)	149 (79%)	40 (21%)	1	7
All	All	70917/73573 (96%)	63575 (90%)	7342 (10%)	9	29

5 of 7342 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	cI	572	LEU
16	pB	217	GLU
8	eB	138	THR
16	o6	337	ASN
11	hw	149	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 709 such sidechains are listed below:

Mol	Chain	Res	Type
7	dV	501	ASN
9	gG	526	GLN
8	eB	394	ASN
7	dV	495	ASN
8	fR	336	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

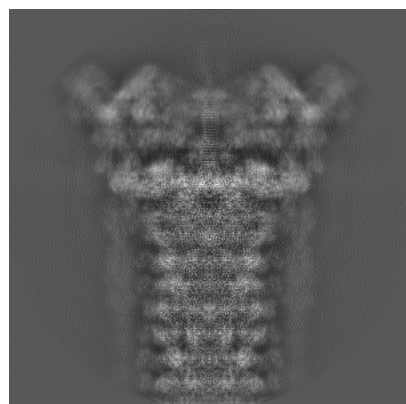
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48459. These allow visual inspection of the internal detail of the map and identification of artifacts.

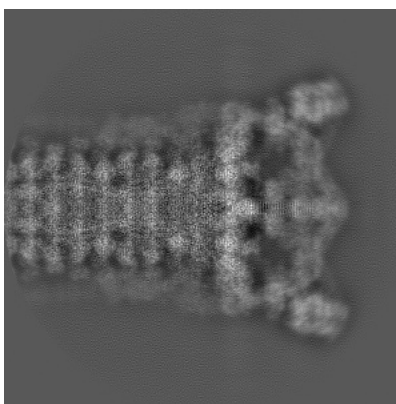
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

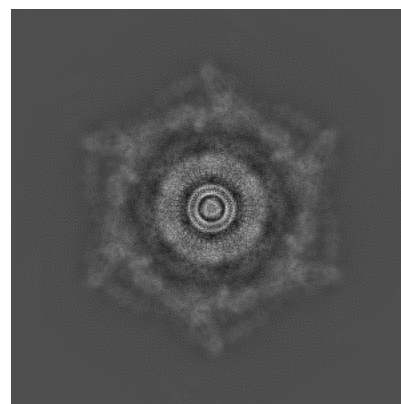
6.1.1 Primary map



X

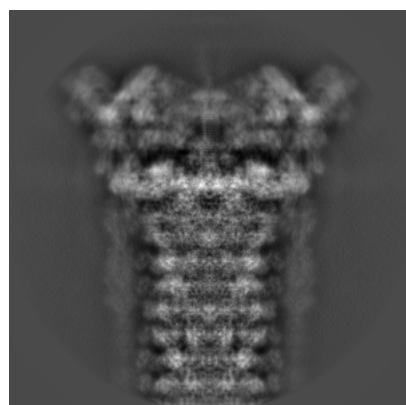


Y

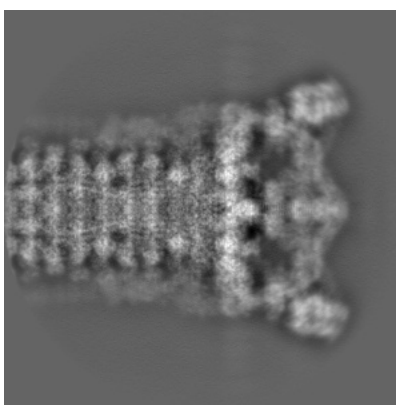


Z

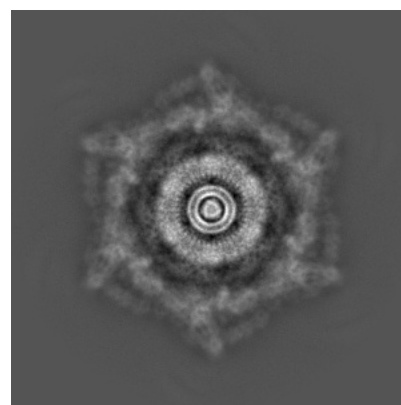
6.1.2 Raw map



X



Y



Z

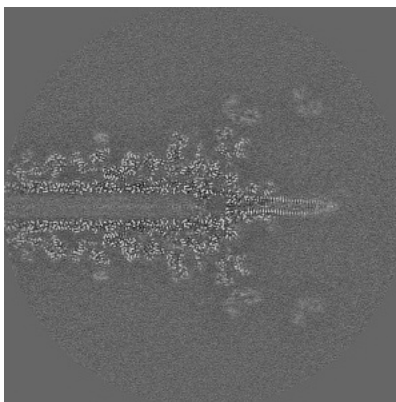
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

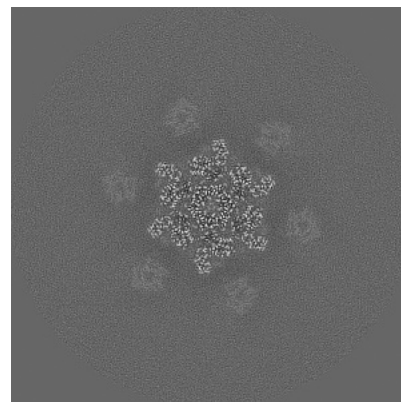
6.2.1 Primary map



X Index: 200

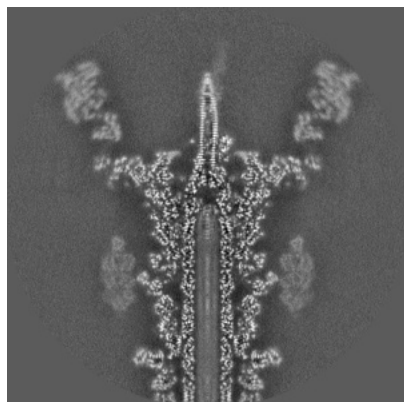


Y Index: 200

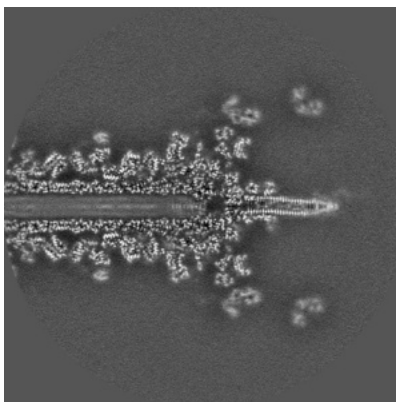


Z Index: 200

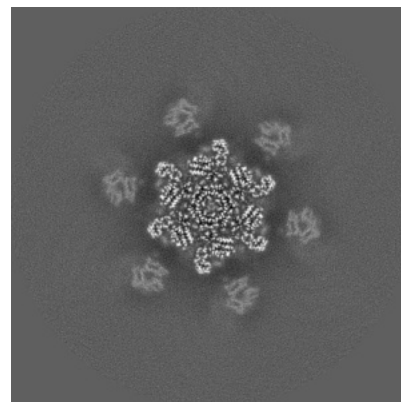
6.2.2 Raw map



X Index: 200



Y Index: 200

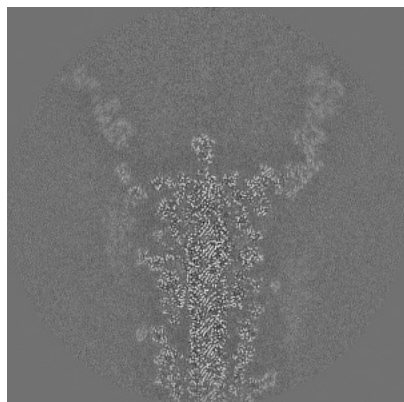


Z Index: 200

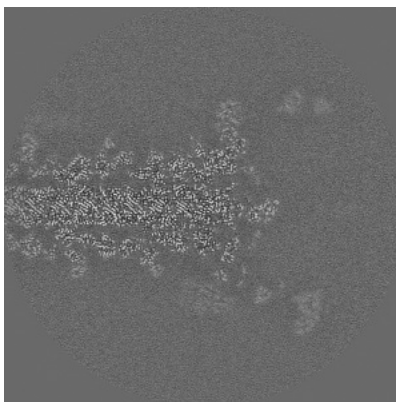
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

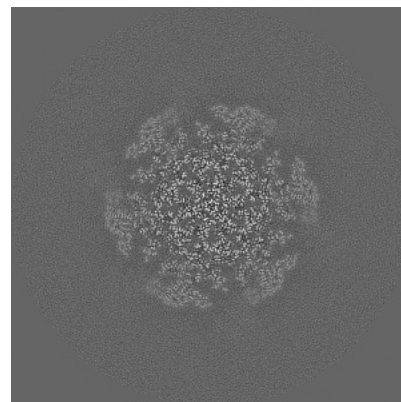
6.3.1 Primary map



X Index: 215

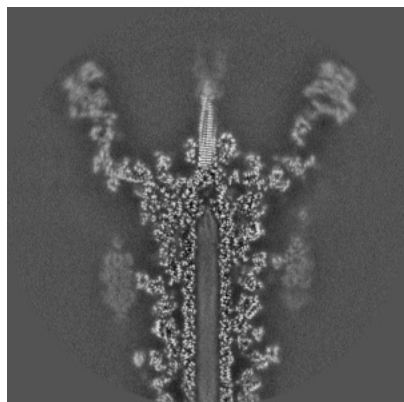


Y Index: 215

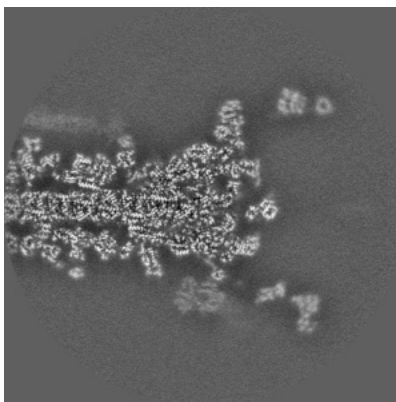


Z Index: 224

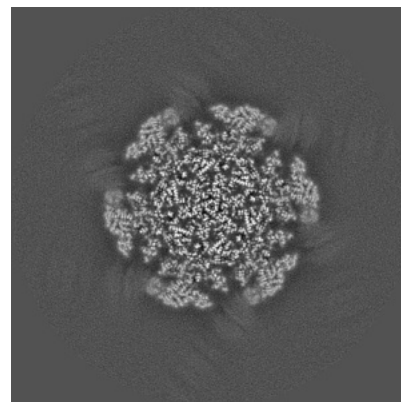
6.3.2 Raw map



X Index: 195



Y Index: 220

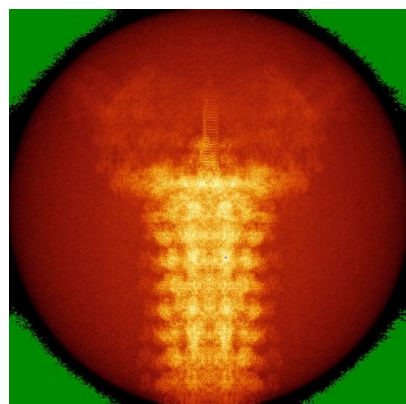


Z Index: 224

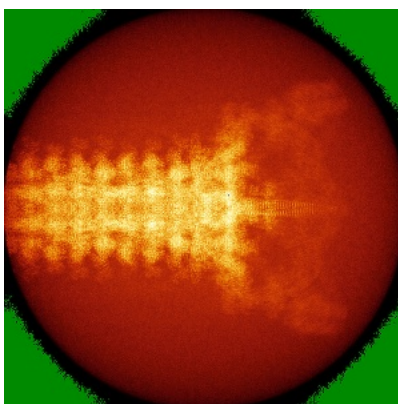
The images above show the largest variance slices of the map in three orthogonal directions.

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

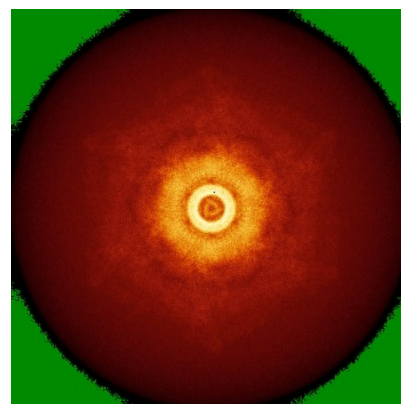
6.4.1 Primary map



X

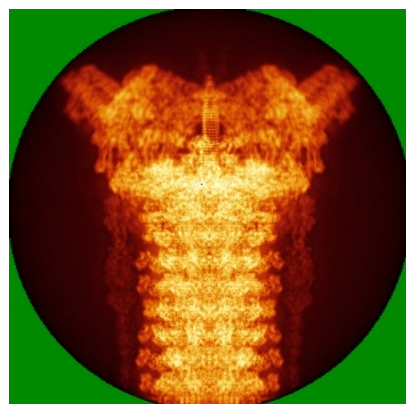


Y

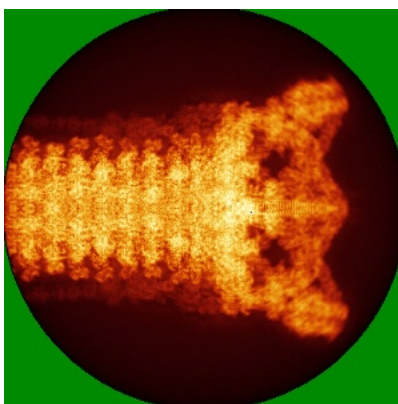


Z

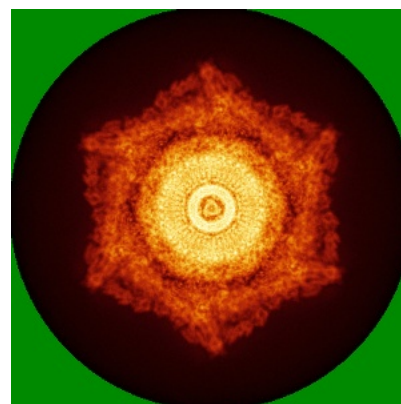
6.4.2 Raw map



X



Y

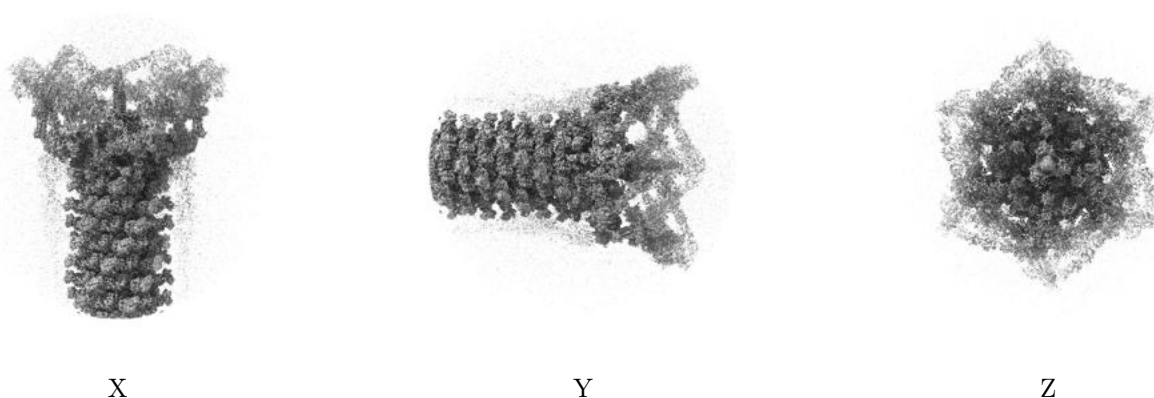


Z

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.

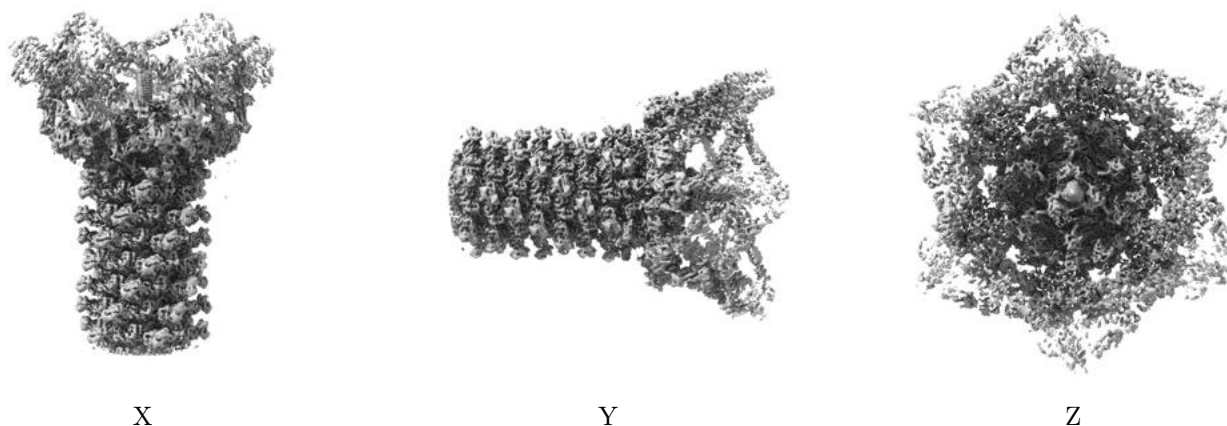
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

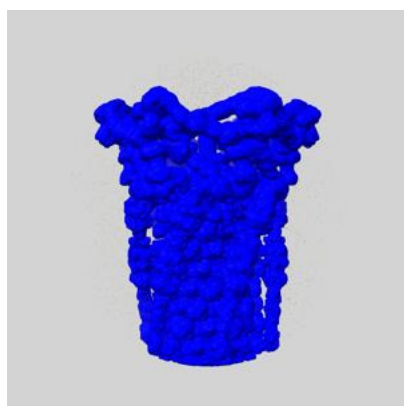
6.6 Mask visualisation [i](#)

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

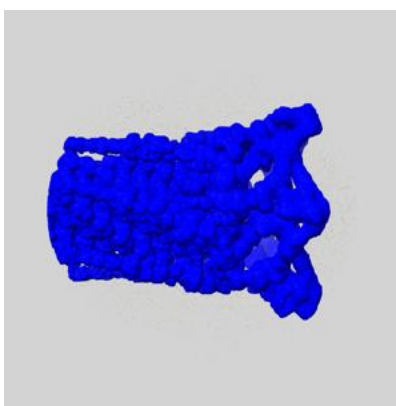
A mask typically either:

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

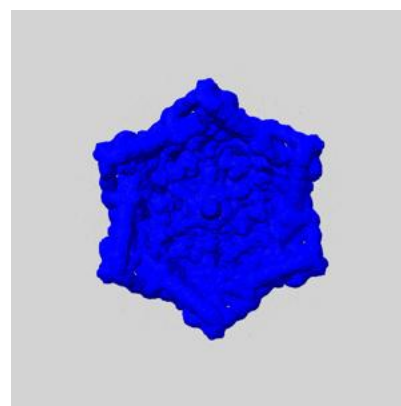
6.6.1 emd_48459_msk_1.map [i](#)



X



Y

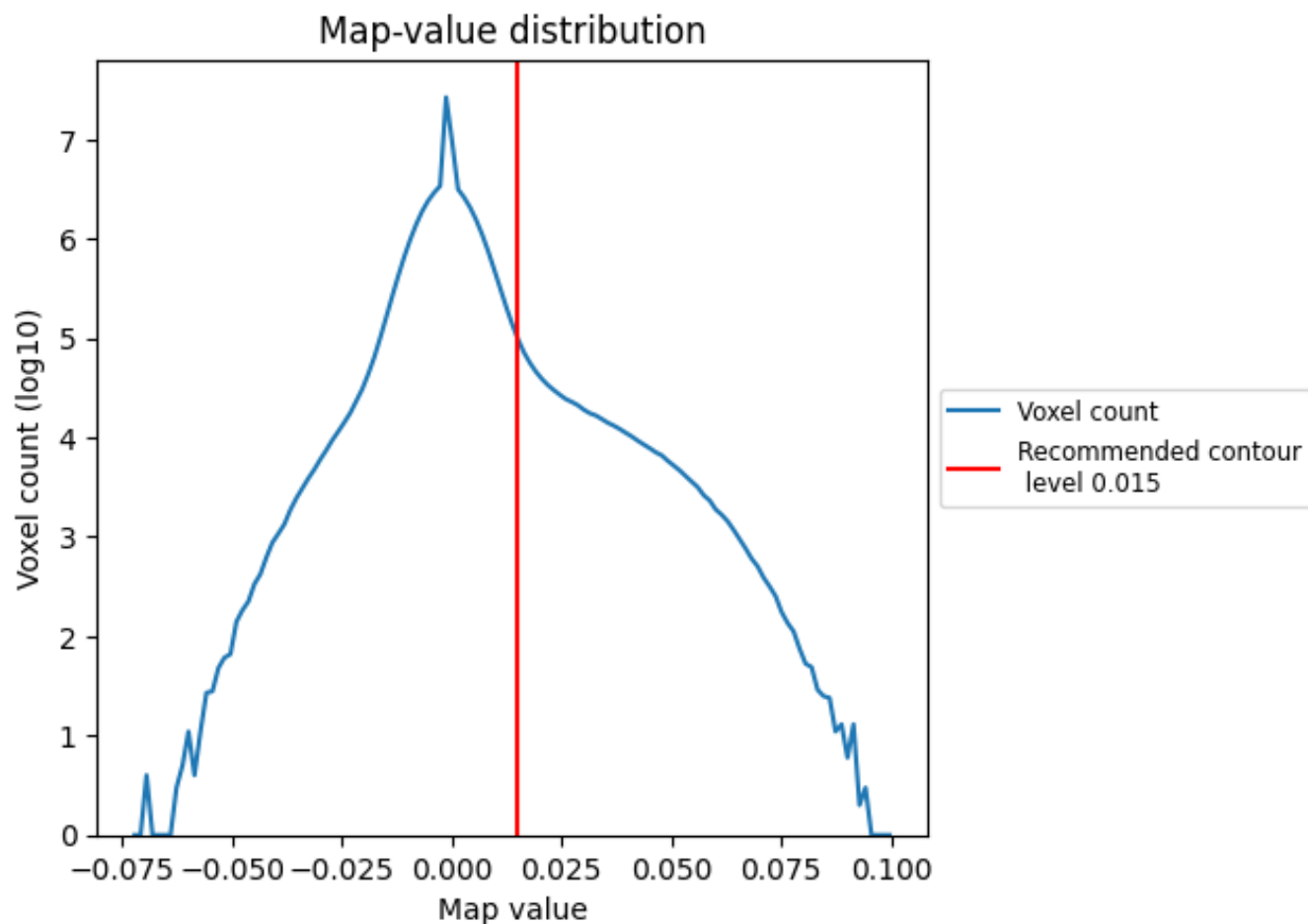


Z

7 Map analysis [i](#)

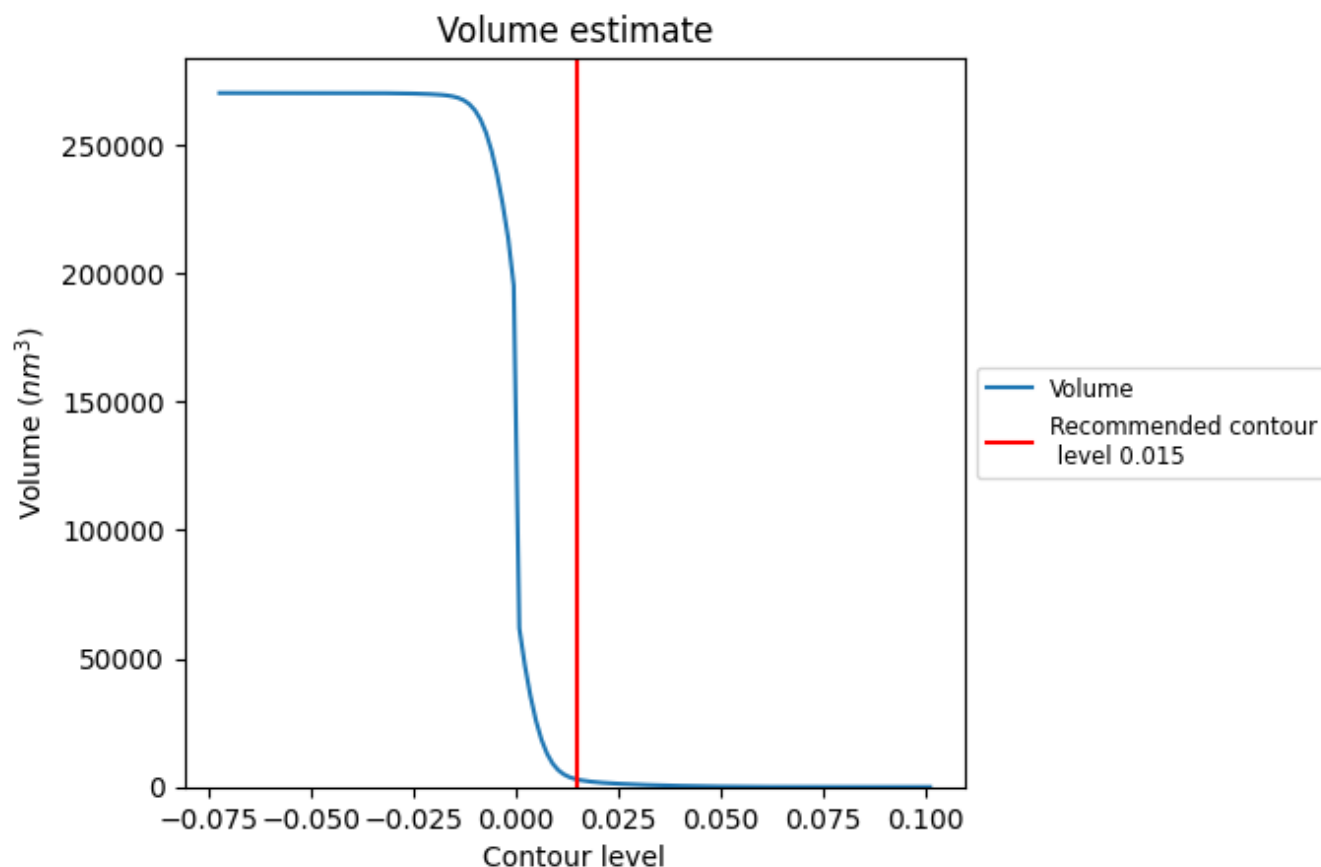
This section contains the results of statistical analysis of the map.

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.

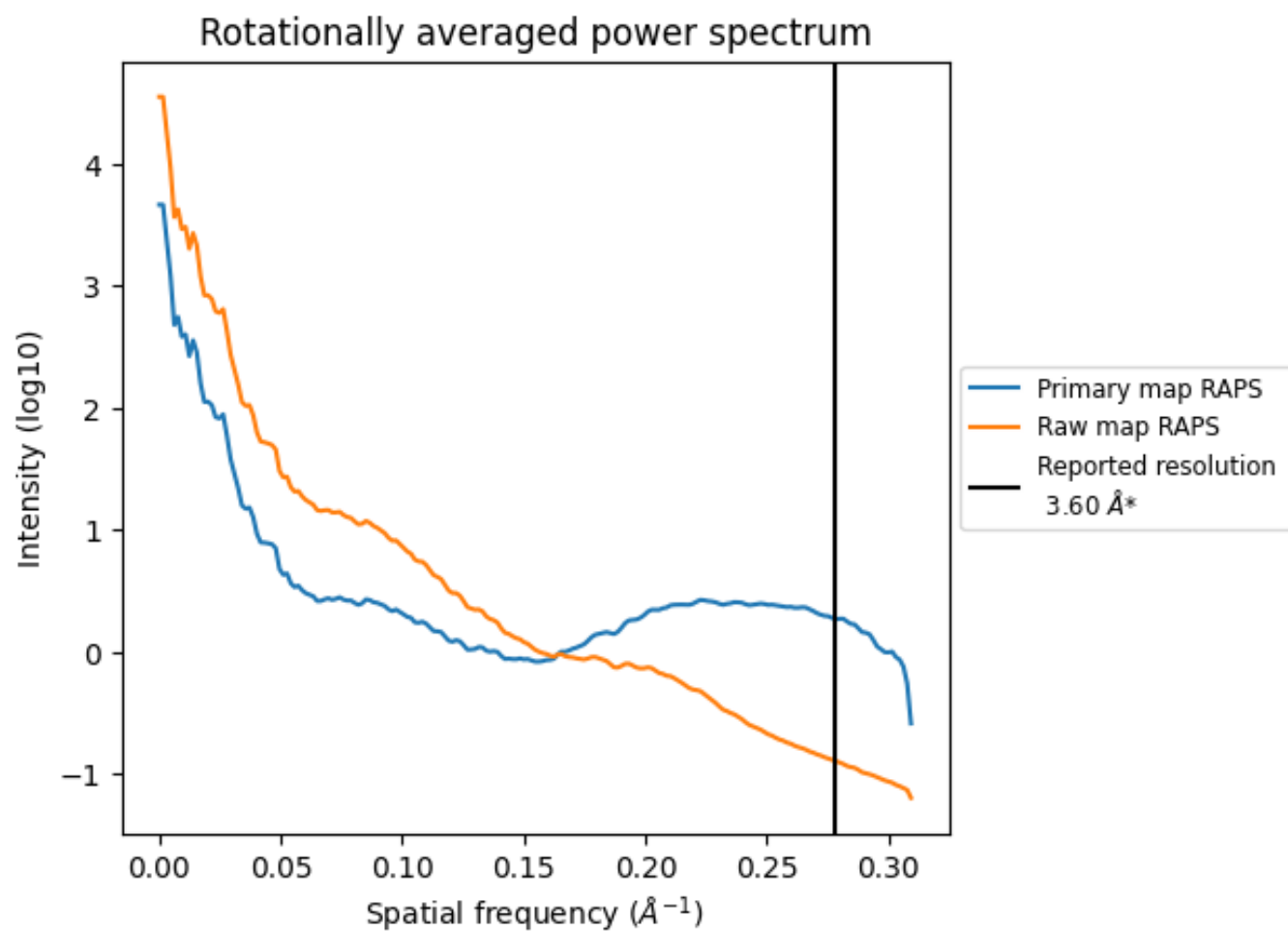
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2938 nm³; this corresponds to an approximate mass of 2654 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 ⓘ

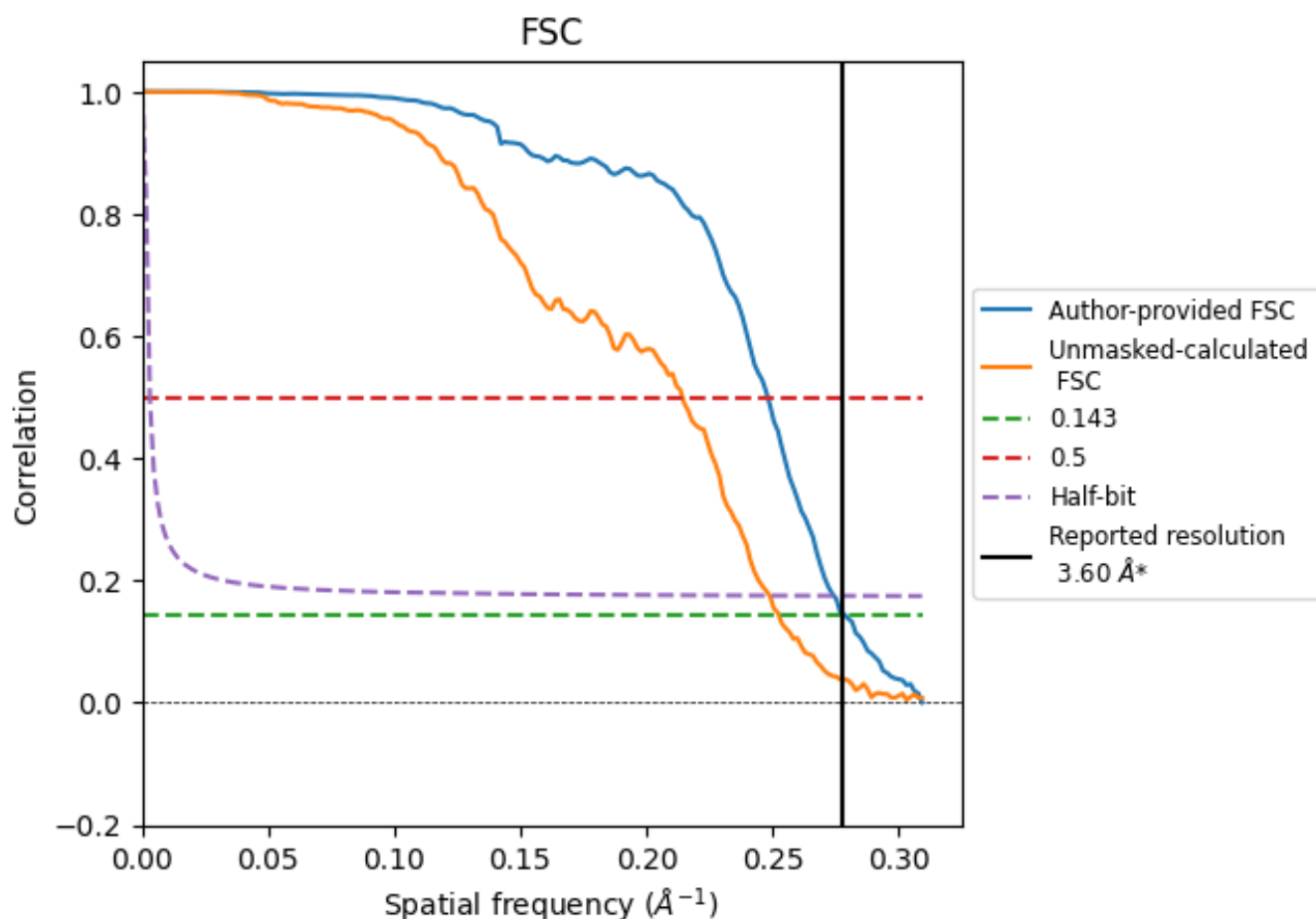


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

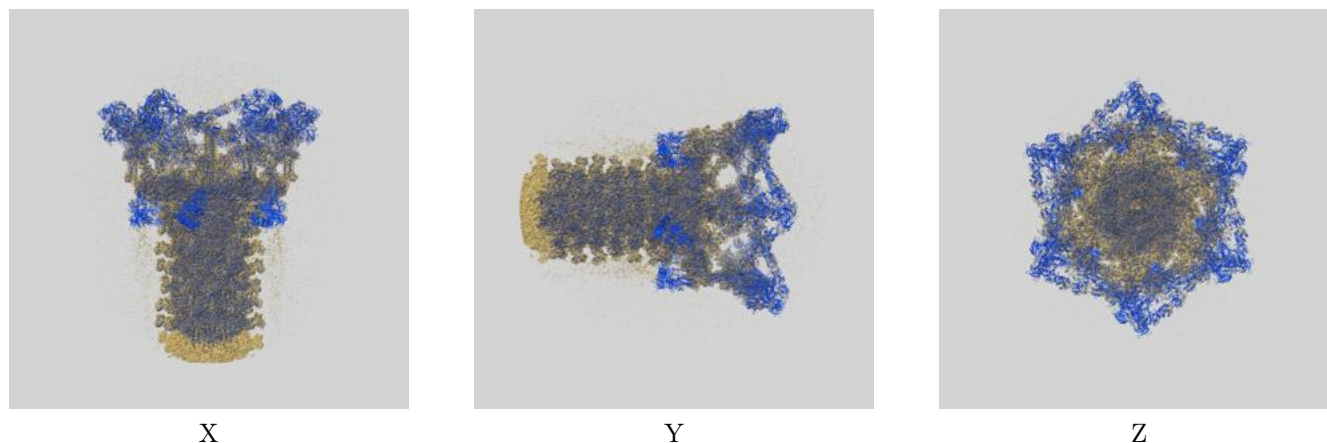
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.03	3.64
Unmasked-calculated*	3.96	4.67	4.02

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

9 Map-model fit [i](#)

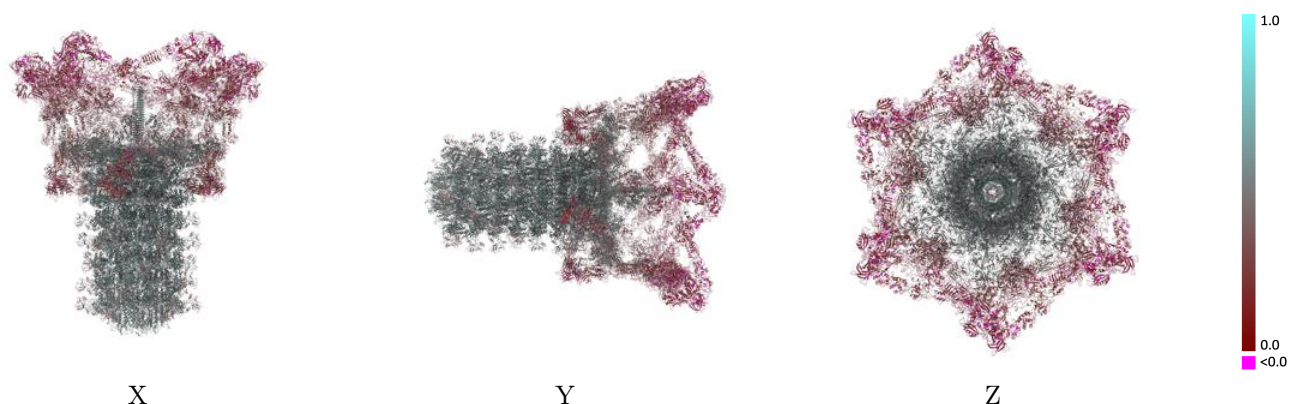
This section contains information regarding the fit between EMDB map EMD-48459 and PDB model 9MOG. Per-residue inclusion information can be found in section [3](#) on page [28](#).

9.1 Map-model overlay [i](#)



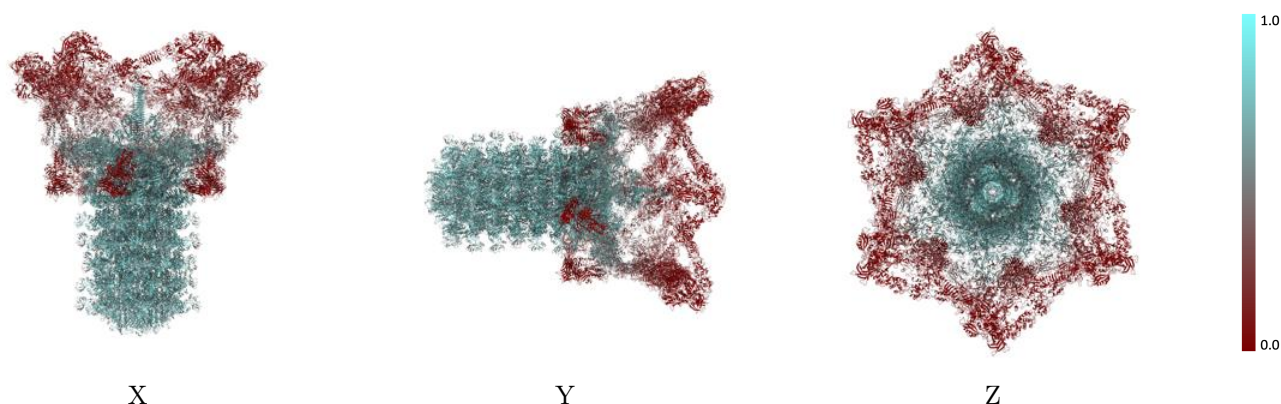
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



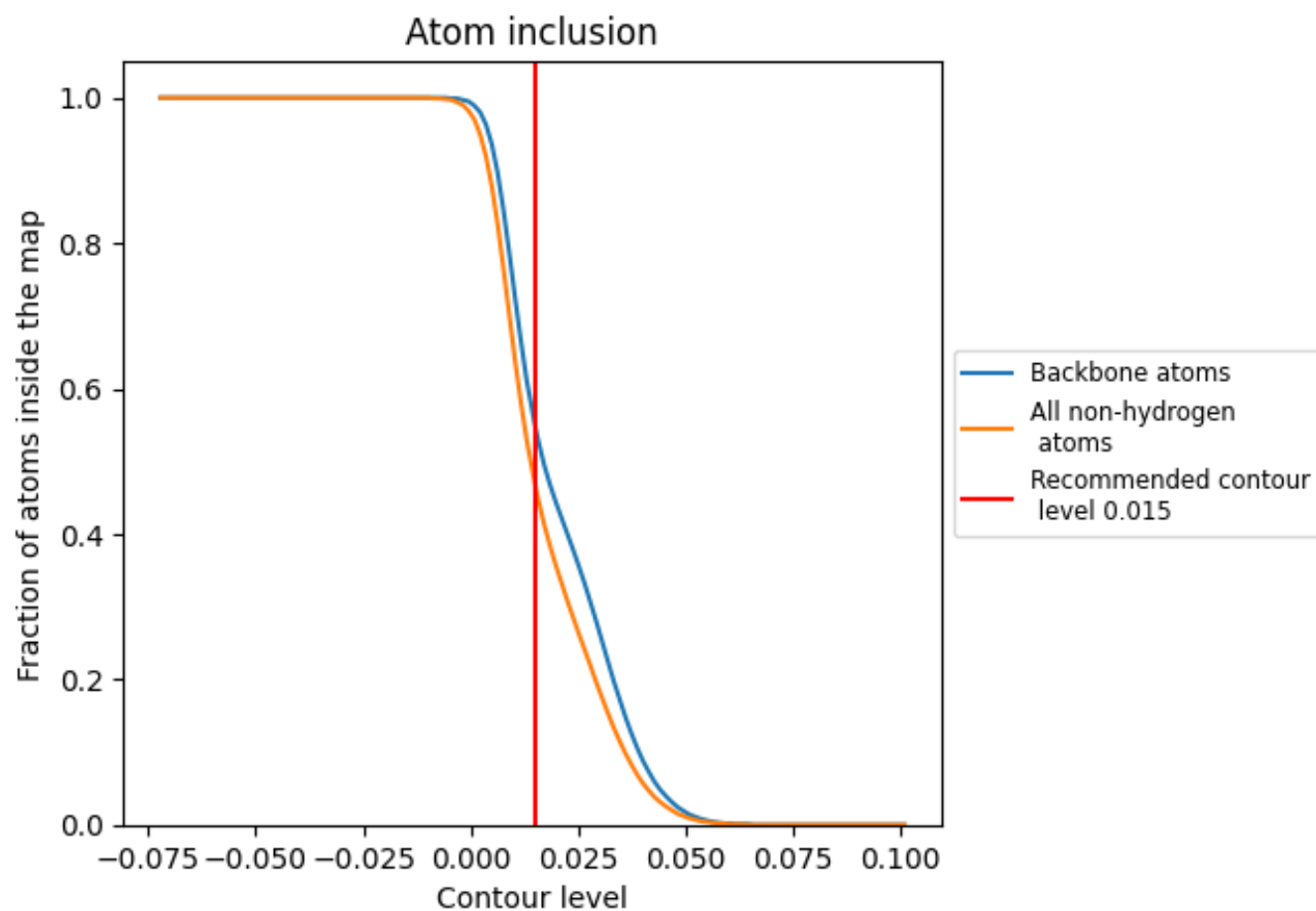
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 47% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4690	 0.4040
S0	 0.0420	 0.1890
S1	 0.0590	 0.2030
S2	 0.0580	 0.1830
S3	 0.0560	 0.1970
S4	 0.0570	 0.2040
S5	 0.0580	 0.1910
S6	 0.0600	 0.1860
S7	 0.0590	 0.1820
S8	 0.0600	 0.1920
SA	 0.0550	 0.1920
SO	 0.0640	 0.1960
SP	 0.0600	 0.1830
SQ	 0.0500	 0.1960
Sv	 0.0570	 0.2010
Sw	 0.0590	 0.1960
Sx	 0.0590	 0.1860
Sy	 0.0630	 0.1790
Sz	 0.0570	 0.1960
T1	 0.0190	 0.2460
T2	 0.0190	 0.2560
T3	 0.0180	 0.2570
T4	 0.0200	 0.2460
T5	 0.0200	 0.2430
T6	 0.0230	 0.2630
T7	 0.0320	 0.2640
T8	 0.0220	 0.2580
T9	 0.0310	 0.2790
TF	 0.0170	 0.2440
TG	 0.0260	 0.2610
TH	 0.0270	 0.2780
Td	 0.0220	 0.2400
Te	 0.0240	 0.2420
Tf	 0.0230	 0.2580
Tg	 0.0330	 0.2620



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Chain	Atom inclusion	Q-score
Th	 0.0230	 0.2640
Ti	 0.0280	 0.2760
UL	 0.0270	 0.1850
UM	 0.0190	 0.1690
UN	 0.0260	 0.1630
Up	 0.0220	 0.1830
Uq	 0.0230	 0.1750
Ur	 0.0250	 0.1580
Us	 0.0210	 0.1640
Ut	 0.0360	 0.1680
Uu	 0.0290	 0.1560
VL	 0.0220	 0.1790
VM	 0.0240	 0.1590
VN	 0.0300	 0.1690
Vp	 0.0210	 0.1850
Vq	 0.0300	 0.1800
Vr	 0.0240	 0.1550
Vs	 0.0160	 0.1640
Vt	 0.0330	 0.1680
Vu	 0.0330	 0.1610
WI	 0.1340	 0.2510
WJ	 0.1610	 0.2510
WK	 0.1630	 0.2650
Wj	 0.1360	 0.2540
Wk	 0.1340	 0.2500
Wl	 0.1580	 0.2640
Wm	 0.1580	 0.2510
Wn	 0.1520	 0.2590
Wo	 0.1610	 0.2640
XI	 0.1370	 0.2480
XJ	 0.1540	 0.2600
XK	 0.1560	 0.2600
Xj	 0.1370	 0.2510
Xk	 0.1360	 0.2490
Xl	 0.1550	 0.2610
Xm	 0.1650	 0.2500
Xn	 0.1560	 0.2600
Xo	 0.1630	 0.2610
YC	 0.5110	 0.4190
YX	 0.5230	 0.4210
YY	 0.5130	 0.4190
Yc	 0.5180	 0.4190

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Chain	Atom inclusion	Q-score
Yx	 0.5130	 0.4190
Yy	 0.5160	 0.4180
ZD	 0.5180	 0.4190
ZE	 0.6070	 0.4770
ZZ	 0.5250	 0.4250
Za	 0.5040	 0.4170
Zb	 0.6070	 0.4740
Zc	 0.6030	 0.4770
aD	 0.5220	 0.4270
aE	 0.6080	 0.4720
aZ	 0.5270	 0.4290
aa	 0.5210	 0.4210
ab	 0.6120	 0.4730
ac	 0.6140	 0.4750
b0	 0.6990	 0.5000
b3	 0.6620	 0.4880
b4	 0.6540	 0.4830
b5	 0.6660	 0.4880
b6	 0.6580	 0.4820
b7	 0.6650	 0.4860
b8	 0.7020	 0.5000
b9	 0.7030	 0.4990
bN	 0.7160	 0.5180
bO	 0.7150	 0.5190
bP	 0.7180	 0.5220
bQ	 0.7140	 0.5170
bR	 0.7150	 0.5170
bY	 0.7150	 0.5200
cA	 0.7000	 0.4970
cB	 0.6960	 0.5000
cC	 0.7110	 0.5050
cD	 0.7100	 0.5060
cE	 0.6580	 0.4850
cF	 0.6990	 0.4970
cG	 0.7070	 0.5060
cH	 0.7010	 0.5040
cI	 0.7090	 0.5030
cJ	 0.7120	 0.5070
cK	 0.7090	 0.5060
cL	 0.7030	 0.5020
cM	 0.7000	 0.5040
cN	 0.7030	 0.5020

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Chain	Atom inclusion	Q-score
cO	 0.6970	 0.5030
cP	 0.7050	 0.5040
dS	 0.7200	 0.5230
dT	 0.7080	 0.5160
dU	 0.7230	 0.5230
dV	 0.7070	 0.5180
dW	 0.7250	 0.5210
dZ	 0.7060	 0.5170
eB	 0.6930	 0.5040
eU	 0.6930	 0.5080
eW	 0.6870	 0.5030
f9	 0.6960	 0.5080
fA	 0.6930	 0.5020
fB	 0.6890	 0.5050
fR	 0.6950	 0.5080
fS	 0.6970	 0.5090
fU	 0.6870	 0.5070
fW	 0.6920	 0.5030
fr	 0.6970	 0.5070
fs	 0.6890	 0.5050
gE	 0.7630	 0.5270
gG	 0.7660	 0.5280
gH	 0.7660	 0.5320
gd	 0.4620	 0.3220
h1	 0.7530	 0.5420
h2	 0.7560	 0.5430
hI	 0.7500	 0.5450
hJ	 0.7370	 0.5400
hK	 0.7510	 0.5440
hL	 0.7520	 0.5430
hM	 0.7590	 0.5430
hX	 0.7400	 0.5400
he	 0.6810	 0.5200
hf	 0.6890	 0.5250
hg	 0.6850	 0.5200
hh	 0.6790	 0.5200
hi	 0.6870	 0.5220
hj	 0.7290	 0.5300
hk	 0.7330	 0.5280
hl	 0.7330	 0.5350
hm	 0.7180	 0.5280
hn	 0.7370	 0.5310

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Chain	Atom inclusion	Q-score
ho	 0.7630	 0.5460
hp	 0.7490	 0.5380
hq	 0.7610	 0.5420
hr	 0.7600	 0.5410
hs	 0.7610	 0.5400
ht	 0.6810	 0.5190
hu	 0.7260	 0.5290
hv	 0.7560	 0.5430
hw	 0.7590	 0.5410
hx	 0.7640	 0.5460
hy	 0.7540	 0.5380
hz	 0.7560	 0.5450
iC	 0.7410	 0.5500
iD	 0.7460	 0.5490
iF	 0.7460	 0.5510
ja	 0.6930	 0.5360
jb	 0.6790	 0.5300
jc	 0.6930	 0.5190
k3	 0.7310	 0.5280
k4	 0.7290	 0.5290
k7	 0.7290	 0.5310
k8	 0.7320	 0.5280
kV	 0.7280	 0.5310
lV	 0.7360	 0.5290
m1	 0.6870	 0.5190
m2	 0.6120	 0.5020
m5	 0.6800	 0.5200
m6	 0.6040	 0.5030
mT	 0.6070	 0.5010
nT	 0.6790	 0.5160
o0	 0.6560	 0.5310
o1	 0.6070	 0.5080
o2	 0.6150	 0.5110
o6	 0.6080	 0.5110
pA	 0.6700	 0.5370
pB	 0.6660	 0.5300
q3	 0.7390	 0.5420
q4	 0.7450	 0.5420
q5	 0.7400	 0.5450
q7	 0.7430	 0.5460
q8	 0.7440	 0.5470
q9	 0.7430	 0.5450

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Chain	Atom inclusion	Q-score
rc	 0.8000	 0.5480
rd	 0.8240	 0.5430
re	 0.7920	 0.5290
rf	 0.8000	 0.5480
rg	 0.8080	 0.5310
rh	 0.8080	 0.5370
sQ	 0.6220	 0.5320
sT	 0.5890	 0.5290
sU	 0.6000	 0.5100
tS	 0.7600	 0.5060
tX	 0.6600	 0.4860
tY	 0.7000	 0.5000
uR	 0.6290	 0.5540
uV	 0.7140	 0.5230
uW	 0.6860	 0.5260
vZ	 0.8440	 0.5900
va	 0.8440	 0.5800
vb	 0.8000	 0.5640