



## wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 10:35 PM UTC

PDB ID : 9MOF / pdb\_00009mof  
EMDB ID : EMD-48458  
Title : Structure of the bacteriophage T4 portal-neck-tail connector complex  
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 : 3.80 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](mailto: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>.

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

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

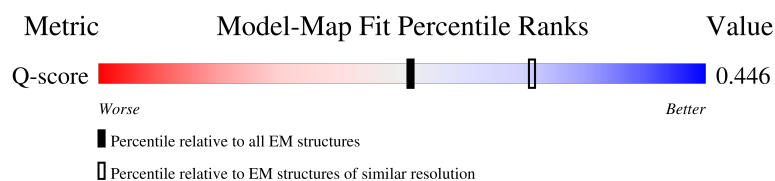
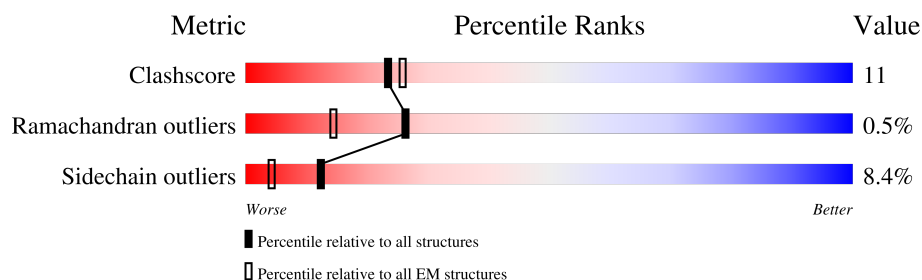
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.








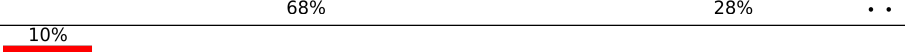
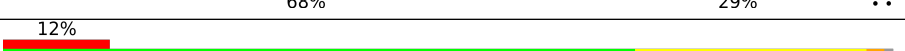


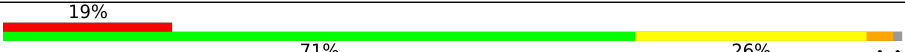






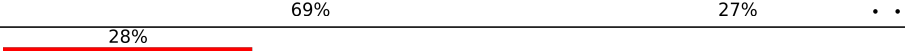
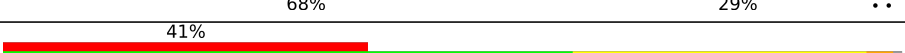

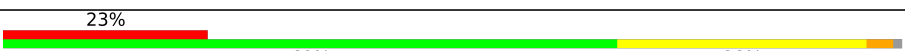
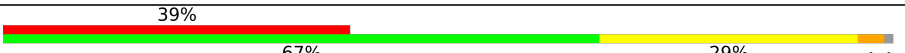




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 ( 3.30 - 4.30 )

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  $\geq 3$ , 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	0	256	
1	k	256	
1	l	256	
1	m	256	

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Mol	Chain	Length	Quality of chain
1	n	256	
1	p	256	
2	1	659	
2	2	659	
2	3	659	
2	4	659	
2	5	659	
2	AD	659	
2	AK	659	
2	AL	659	
2	AM	659	
2	AN	659	
2	AO	659	
2	AP	659	
2	B1	659	
2	B2	659	
2	B3	659	
2	B4	659	
2	B5	659	
2	B6	659	
2	B7	659	
2	Bp	659	
2	Bq	659	
2	Br	659	
2	Bs	659	

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Mol	Chain	Length	Quality of chain
2	Bt	659	
2	Bu	659	
2	Bv	659	
2	Bw	659	
2	Bx	659	
2	By	659	
2	Bz	659	
3	6	163	
3	7	163	
3	8	163	
3	9	163	
3	AA	163	
3	AE	163	
3	AF	163	
3	AG	163	
3	AH	163	
3	AI	163	
3	AJ	163	
3	BX	163	
3	BY	163	
3	BZ	163	
3	Ba	163	
3	Bb	163	
3	Bc	163	
3	Bd	163	





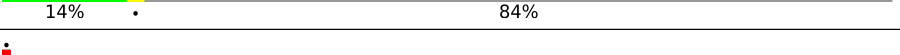
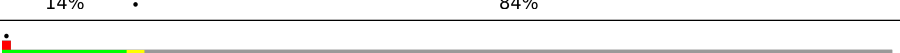









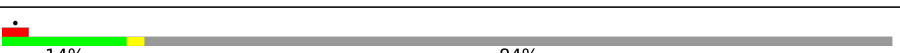





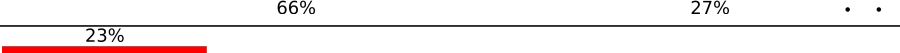



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Mol	Chain	Length	Quality of chain
3	Be	163	
3	Bf	163	
3	Bg	163	
3	Bh	163	
3	Bi	163	
3	Bj	163	
3	Bk	163	
3	Bl	163	
3	Bm	163	
3	Bn	163	
3	Bo	163	
3	o	163	
4	A	487	
4	B	487	
4	C	487	
4	D	487	
4	E	487	
4	F	487	
4	G	487	
4	H	487	
4	I	487	
4	J	487	
4	K	487	
4	L	487	
4	M	487	

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Mol	Chain	Length	Quality of chain
4	N	487	 15% 84%
4	O	487	 13% 84%
4	P	487	 14% 84%
4	Q	487	 14% 84%
4	R	487	 14% 84%
4	S	487	 14% 84%
4	T	487	 14% 84%
4	U	487	 13% 84%
4	V	487	 13% 84%
4	W	487	 13% 84%
4	X	487	 14% 84%
4	Y	487	 14% 84%
4	Z	487	 14% 84%
4	a	487	 14% 84%
4	b	487	 14% 84%
4	c	487	 14% 84%
4	d	487	 14% 84%
4	e	487	 14% 84%
4	f	487	 13% 84%
4	g	487	 13% 84%
4	h	487	 13% 84%
4	i	487	 13% 84%
4	j	487	 14% 84%
5	A0	524	 24% 66% 27%
5	A1	524	 23% 67% 26%




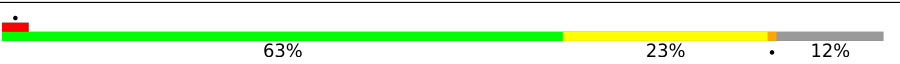
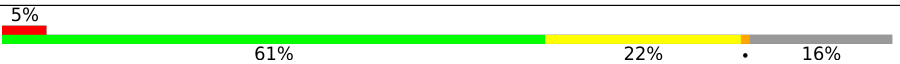

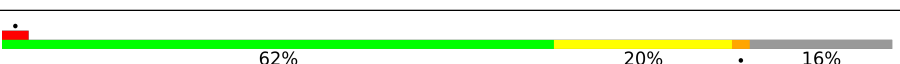
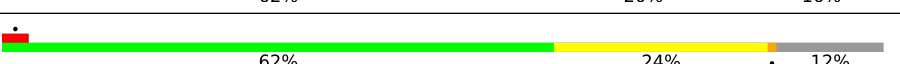
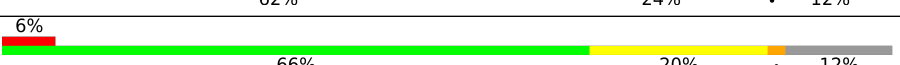
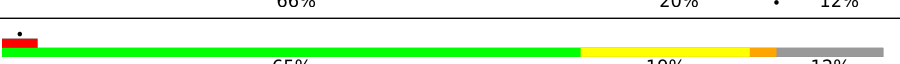
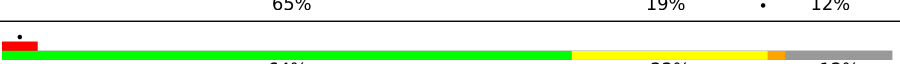
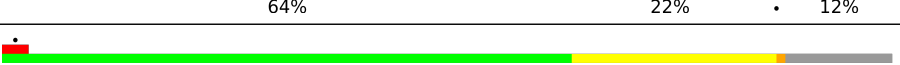

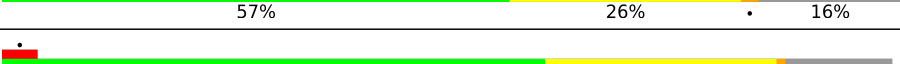



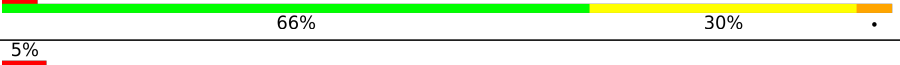

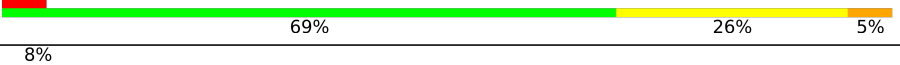
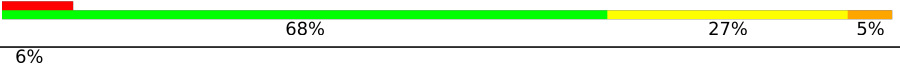


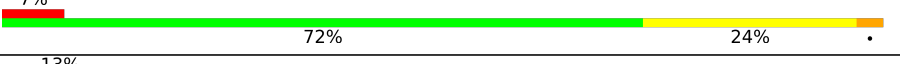

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Mol	Chain	Length	Quality of chain
5	A2	524	
5	A3	524	
5	Av	524	
5	Ax	524	
5	BA	524	
5	BB	524	
5	BD	524	
5	BF	524	
5	BG	524	
5	BH	524	
6	A4	521	
6	A5	521	
6	A7	521	
6	A8	521	
6	A9	521	
6	AV	521	
6	AW	521	
6	AX	521	
6	AZ	521	
6	Ac	521	
6	Ad	521	
6	Ae	521	
6	Af	521	
6	Ag	521	
6	Ah	521	

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Mol	Chain	Length	Quality of chain
6	Ai	521	
6	Aj	521	
6	Ak	521	
6	Am	521	
6	An	521	
6	Ao	521	
6	Ap	521	
6	Au	521	
6	Aw	521	
6	Ay	521	
6	Az	521	
6	BI	521	
6	BJ	521	
6	BK	521	
6	BM	521	
7	A6	309	
7	AY	309	
7	Aa	309	
7	Ab	309	
7	Al	309	
7	Aq	309	
7	Ar	309	
7	As	309	
7	At	309	
7	BC	309	



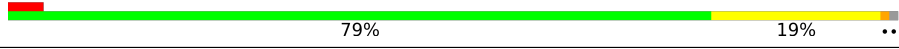

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Mol	Chain	Length	Quality of chain
7	BE	309	
7	BL	309	
8	AB	272	
8	q	272	
8	r	272	
8	s	272	
8	t	272	
8	u	272	
9	AC	176	
9	v	176	
9	w	176	
9	x	176	
9	y	176	
9	z	176	
10	AQ	376	
10	AR	376	
10	AS	376	
10	AT	376	
10	AU	376	
11	BN	80	
11	BO	80	
11	BP	80	
11	BQ	80	
11	BR	80	
11	BS	80	

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Mol	Chain	Length	Quality of chain
11	BT	80	 71%25%..
11	BU	80	 74%25%.
11	BV	80	 79%19%..
11	BW	80	 6%69%28%..

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 435087 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 gp14, neck protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	244	Total 1993	C 1279	N 323	O 387	S 4	0	0
1	k	244	Total 1993	C 1279	N 323	O 387	S 4	0	0
1	l	244	Total 1993	C 1279	N 323	O 387	S 4	0	0
1	m	244	Total 1993	C 1279	N 323	O 387	S 4	0	0
1	n	244	Total 1993	C 1279	N 323	O 387	S 4	0	0
1	p	244	Total 1993	C 1279	N 323	O 387	S 4	0	0

- Molecule 2 is a protein called gp18, tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	2	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	3	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	4	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	5	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	AD	653	Total 4985	C 3142	N 839	O 993	S 11	0	0
2	AK	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	AL	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	AM	655	Total 5000	C 3152	N 841	O 996	S 11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	AN	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	AO	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	AP	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	B1	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	B2	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	B3	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	B4	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	B5	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	B6	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	B7	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	Bp	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	Bq	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	Br	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	Bs	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	Bt	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	Bu	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	Bv	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	Bw	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	Bx	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	By	655	Total 5000	C 3152	N 841	O 996	S 11	0	0
2	Bz	655	Total 5000	C 3152	N 841	O 996	S 11	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	109	ASN	SER	conflict	UNP A0A7S9SVW9
1	301	GLY	GLU	conflict	UNP A0A7S9SVW9
1	399	VAL	ALA	conflict	UNP A0A7S9SVW9
2	109	ASN	SER	conflict	UNP A0A7S9SVW9
2	301	GLY	GLU	conflict	UNP A0A7S9SVW9
2	399	VAL	ALA	conflict	UNP A0A7S9SVW9
3	109	ASN	SER	conflict	UNP A0A7S9SVW9
3	301	GLY	GLU	conflict	UNP A0A7S9SVW9
3	399	VAL	ALA	conflict	UNP A0A7S9SVW9
4	109	ASN	SER	conflict	UNP A0A7S9SVW9
4	301	GLY	GLU	conflict	UNP A0A7S9SVW9
4	399	VAL	ALA	conflict	UNP A0A7S9SVW9
5	109	ASN	SER	conflict	UNP A0A7S9SVW9
5	301	GLY	GLU	conflict	UNP A0A7S9SVW9
5	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AD	109	ASN	SER	conflict	UNP A0A7S9SVW9
AD	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AD	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AK	109	ASN	SER	conflict	UNP A0A7S9SVW9
AK	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AK	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AL	109	ASN	SER	conflict	UNP A0A7S9SVW9
AL	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AL	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AM	109	ASN	SER	conflict	UNP A0A7S9SVW9
AM	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AM	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AN	109	ASN	SER	conflict	UNP A0A7S9SVW9
AN	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AN	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AO	109	ASN	SER	conflict	UNP A0A7S9SVW9
AO	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AO	399	VAL	ALA	conflict	UNP A0A7S9SVW9
AP	109	ASN	SER	conflict	UNP A0A7S9SVW9
AP	301	GLY	GLU	conflict	UNP A0A7S9SVW9
AP	399	VAL	ALA	conflict	UNP A0A7S9SVW9
B1	109	ASN	SER	conflict	UNP A0A7S9SVW9
B1	301	GLY	GLU	conflict	UNP A0A7S9SVW9
B1	399	VAL	ALA	conflict	UNP A0A7S9SVW9
B2	109	ASN	SER	conflict	UNP A0A7S9SVW9
B2	301	GLY	GLU	conflict	UNP A0A7S9SVW9
B2	399	VAL	ALA	conflict	UNP A0A7S9SVW9

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
Bs	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bs	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bs	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bt	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bt	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bt	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bu	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bu	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bu	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bv	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bv	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bv	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bw	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bw	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bw	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bx	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bx	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bx	399	VAL	ALA	conflict	UNP A0A7S9SVW9

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Chain	Residue	Modelled	Actual	Comment	Reference
By	109	ASN	SER	conflict	UNP A0A7S9SVW9
By	301	GLY	GLU	conflict	UNP A0A7S9SVW9
By	399	VAL	ALA	conflict	UNP A0A7S9SVW9
Bz	109	ASN	SER	conflict	UNP A0A7S9SVW9
Bz	301	GLY	GLU	conflict	UNP A0A7S9SVW9
Bz	399	VAL	ALA	conflict	UNP A0A7S9SVW9

- Molecule 3 is a protein called gp19, tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
3	7	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
3	8	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
3	9	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
3	AA	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
3	AE	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	AF	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	AG	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	AH	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	AI	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	AJ	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	BX	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	BY	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	BZ	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Ba	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bb	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Bc	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bd	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Be	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bf	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bg	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bh	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bi	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bj	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bk	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bl	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bm	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bn	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	Bo	163	Total	C	N	O	S	0	0
			1304	828	219	253	4		
3	o	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		

- Molecule 4 is a protein called gpwac, fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	B	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	C	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	D	79	Total	C	N	O	S	0	0
			601	373	102	125	1		
4	E	79	Total	C	N	O	S	0	0
			601	373	102	125	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	G	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	H	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	I	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	J	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	K	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	L	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	M	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	N	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	O	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	P	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	Q	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	R	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	S	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	T	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	U	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	V	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	W	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	X	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	Y	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	Z	79	Total 601	C 373	N 102	O 125	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	b	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	c	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	d	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	e	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	f	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	g	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	h	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	i	79	Total 601	C 373	N 102	O 125	S 1	0	0
4	j	79	Total 601	C 373	N 102	O 125	S 1	0	0

- Molecule 5 is a protein called gp20, portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A0	507	Total 4140	C 2611	N 717	O 790	S 22	0	0
5	A1	507	Total 4140	C 2611	N 717	O 790	S 22	0	0
5	A2	506	Total 4132	C 2607	N 715	O 788	S 22	0	0
5	A3	506	Total 4132	C 2607	N 715	O 788	S 22	0	0
5	Av	506	Total 4132	C 2607	N 715	O 788	S 22	0	0
5	Ax	506	Total 4132	C 2607	N 715	O 788	S 22	0	0
5	BA	500	Total 4074	C 2571	N 707	O 776	S 20	0	0
5	BB	488	Total 3995	C 2517	N 695	O 761	S 22	0	0
5	BD	506	Total 4132	C 2607	N 715	O 788	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	BF	506	Total	C	N	O	S	0	0
			4132	2607	715	788	22		
5	BG	497	Total	C	N	O	S	0	0
			4039	2549	702	768	20		
5	BH	506	Total	C	N	O	S	0	0
			4091	2582	710	779	20		

- Molecule 6 is a protein called gp23, major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A4	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	A5	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	A7	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	A8	440	Total	C	N	O	S	0	0
			3311	2099	564	633	15		
6	A9	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	AV	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	AW	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	AX	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	AZ	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ac	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ad	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ae	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Af	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ag	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ah	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ai	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Aj	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ak	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Am	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	An	440	Total	C	N	O	S	0	0
			3311	2099	564	633	15		
6	Ao	437	Total	C	N	O	S	0	0
			3291	2088	560	628	15		
6	Ap	440	Total	C	N	O	S	0	0
			3311	2099	564	633	15		
6	Au	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Aw	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Ay	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	Az	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	BI	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	BJ	437	Total	C	N	O	S	0	0
			3291	2088	560	628	15		
6	BK	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		
6	BM	456	Total	C	N	O	S	0	0
			3425	2167	584	659	15		

- Molecule 7 is a protein called gp13, neck protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A6	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	AY	308	Total	C	N	O	S	0	0
			2435	1550	412	460	13		
7	Aa	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	Ab	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	Al	308	Total	C	N	O	S	0	0
			2435	1550	412	460	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	Aq	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	Ar	290	Total	C	N	O	S	0	0
			2310	1473	389	437	11		
7	As	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	At	298	Total	C	N	O	S	0	0
			2371	1512	402	445	12		
7	BC	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	BE	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		
7	BL	308	Total	C	N	O	S	0	0
			2438	1551	413	461	13		

- Molecule 8 is a protein called gp15, tail terminator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AB	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		
8	q	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		
8	r	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		
8	s	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		
8	t	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		
8	u	272	Total	C	N	O	S	0	0
			2227	1424	369	425	9		

- Molecule 9 is a protein called gp3, tube terminator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AC	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		
9	v	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		
9	w	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		
9	x	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	y	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		
9	z	175	Total	C	N	O	S	0	0
			1383	890	215	274	4		

- Molecule 10 is a protein called Hoc, highly immunogenic outer capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AQ	96	Total	C	N	O	S	0	0
			805	519	129	152	5		
10	AR	96	Total	C	N	O	S	0	0
			805	519	129	152	5		
10	AS	96	Total	C	N	O	S	0	0
			805	519	129	152	5		
10	AT	96	Total	C	N	O	S	0	0
			805	519	129	152	5		
10	AU	96	Total	C	N	O	S	0	0
			805	519	129	152	5		

- Molecule 11 is a protein called Soc, small outer capsid protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	BN	79	Total	C	N	O	0	0
			636	405	106	125		
11	BO	79	Total	C	N	O	0	0
			636	405	106	125		
11	BP	79	Total	C	N	O	0	0
			636	405	106	125		
11	BQ	79	Total	C	N	O	0	0
			636	405	106	125		
11	BR	79	Total	C	N	O	0	0
			636	405	106	125		
11	BS	79	Total	C	N	O	0	0
			636	405	106	125		
11	BT	79	Total	C	N	O	0	0
			636	405	106	125		
11	BU	79	Total	C	N	O	0	0
			636	405	106	125		
11	BV	79	Total	C	N	O	0	0
			636	405	106	125		
11	BW	79	Total	C	N	O	0	0
			636	405	106	125		

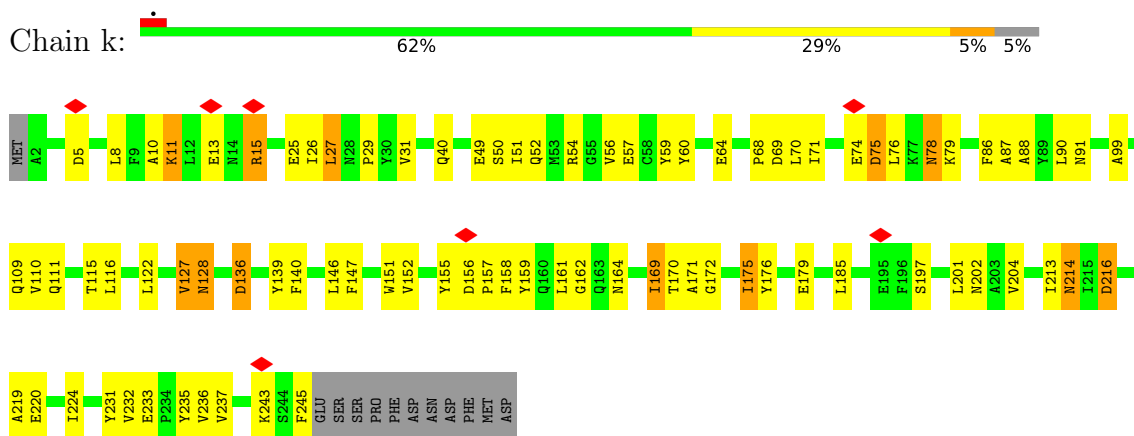
### 3 Residue-property plots

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.

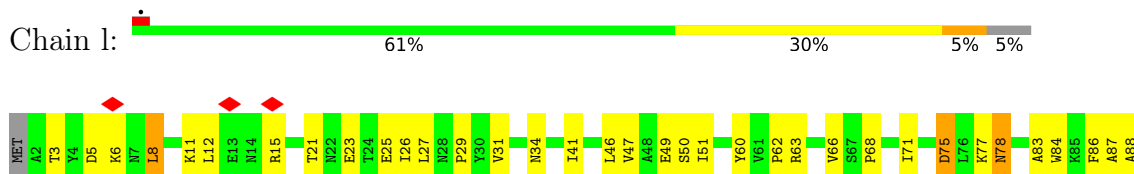
- Molecule 1: gp14, neck protein

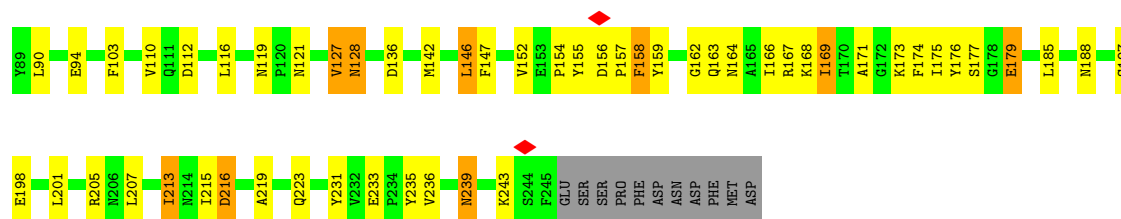


- Molecule 1: gp14, neck protein

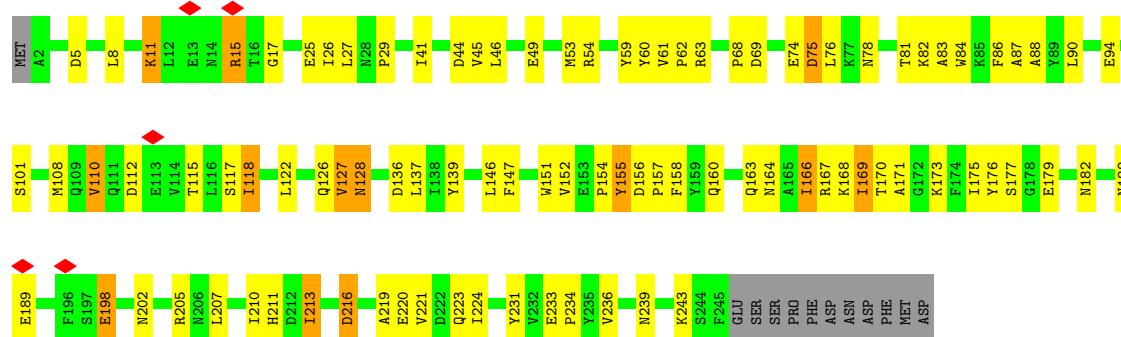


- Molecule 1: gp14, neck protein

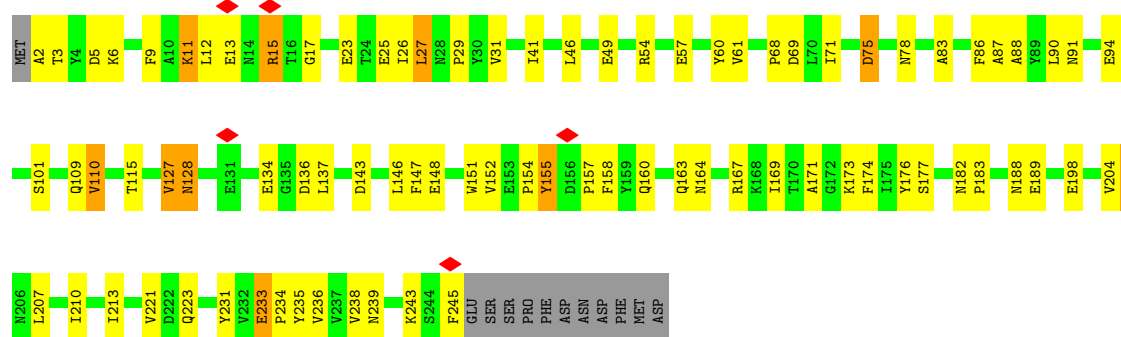




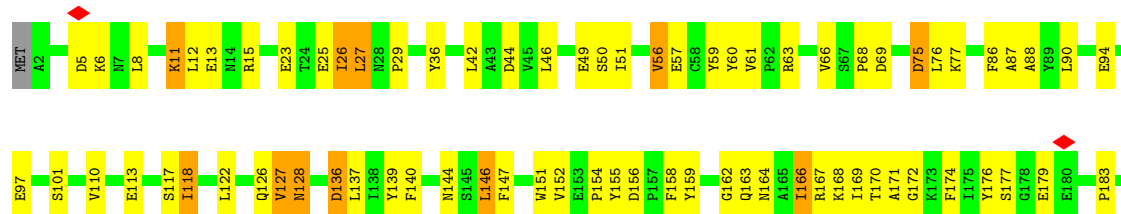
- Molecule 1: gp14, neck protein

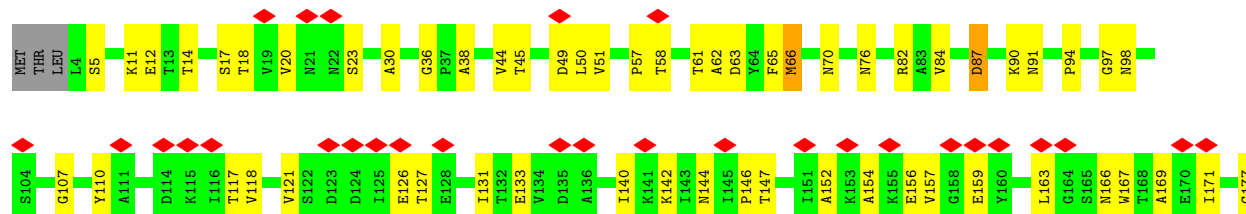


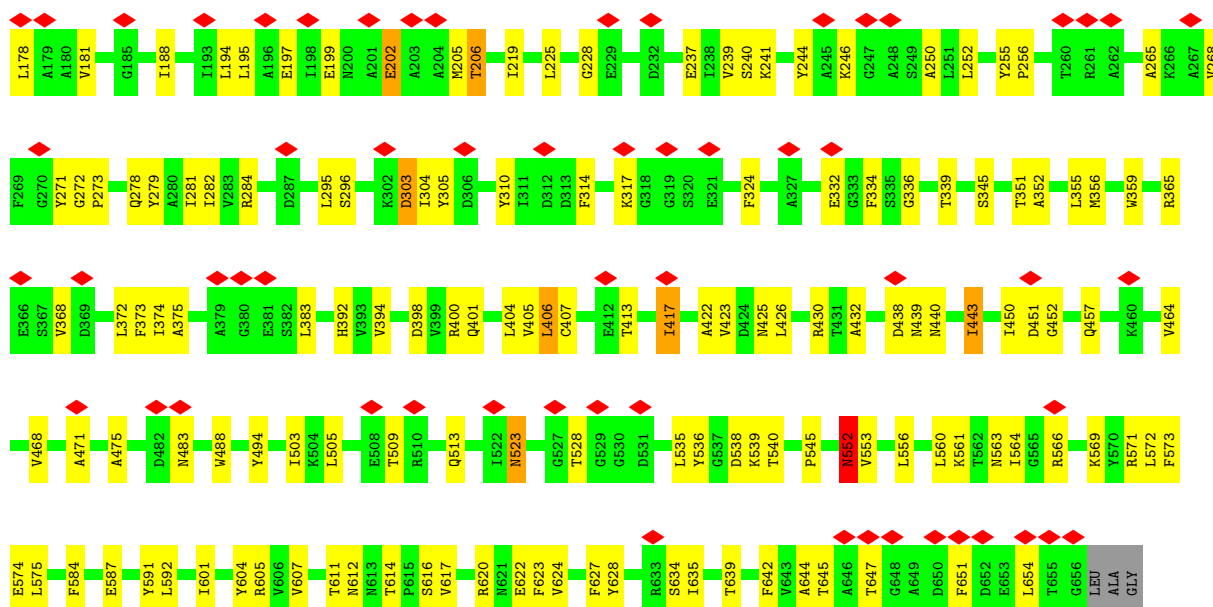
- Molecule 1: gp14, neck protein



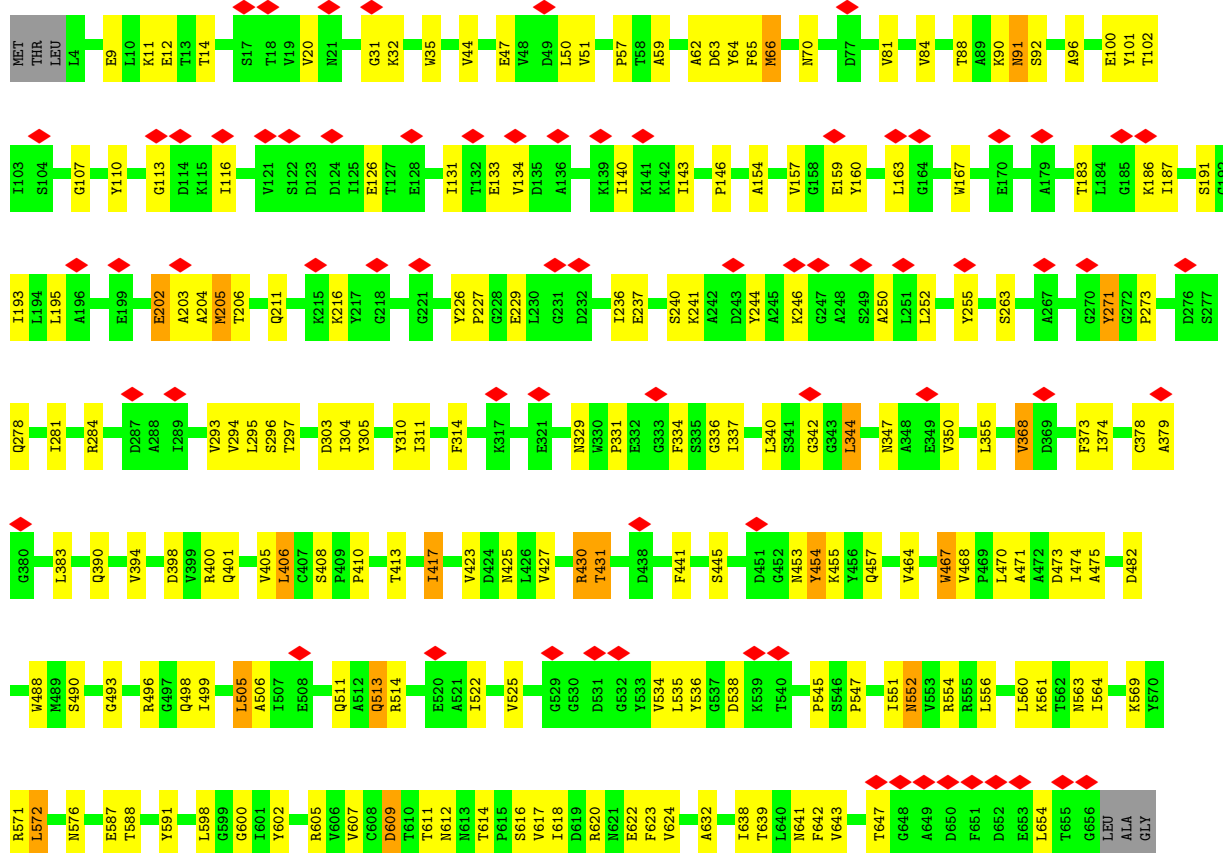
- Molecule 1: gp14, neck protein



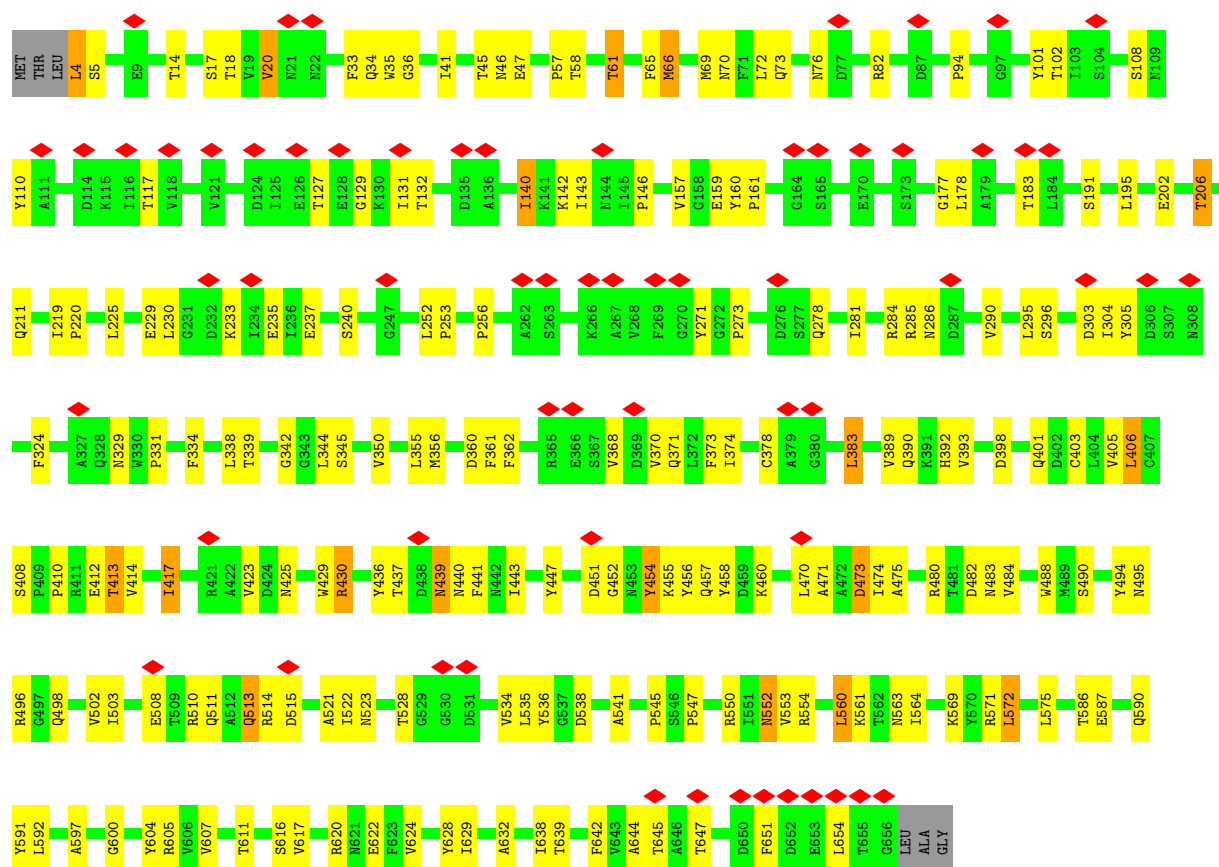




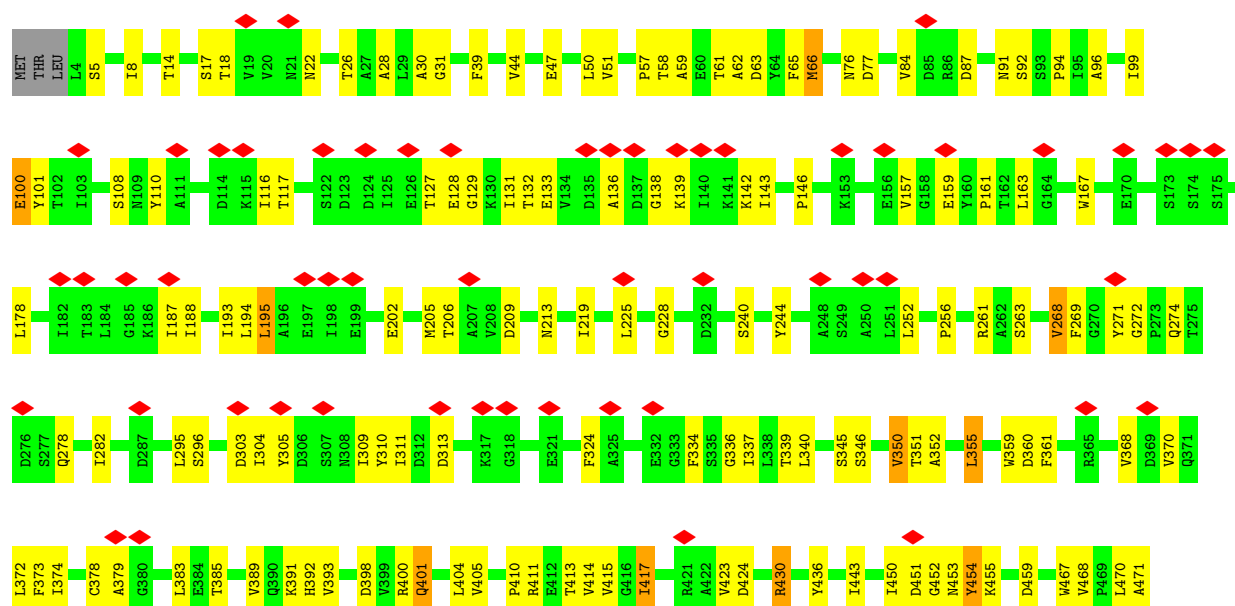
• Molecule 2: gp18, tail sheath protein

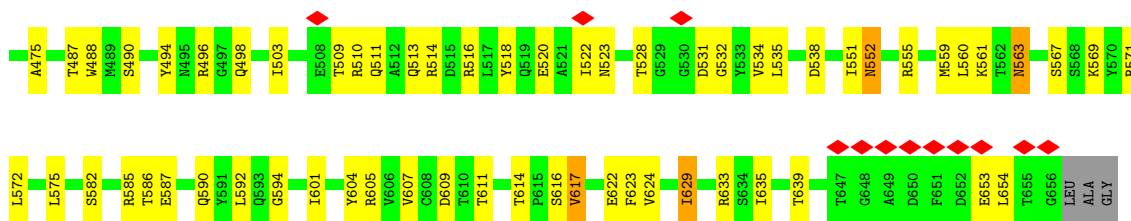


• Molecule 2: gp18, tail sheath protein

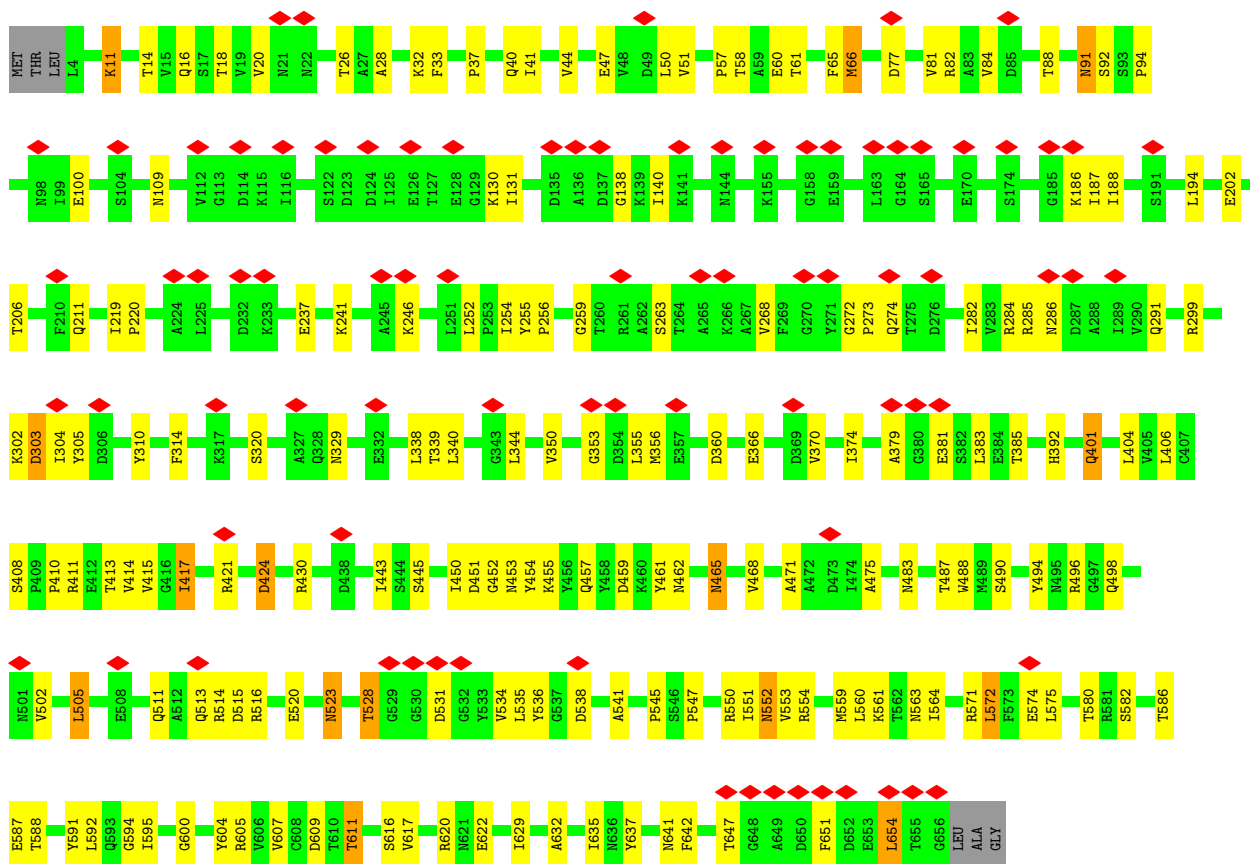
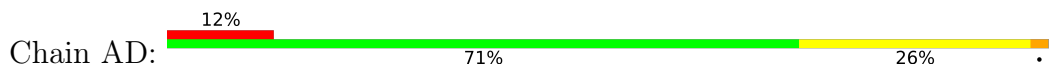


• Molecule 2: gp18, tail sheath protein

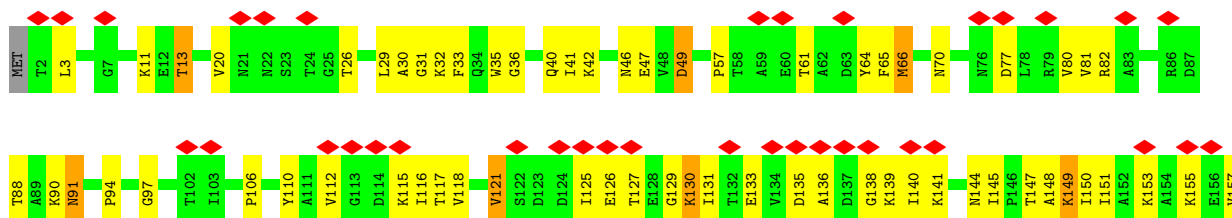


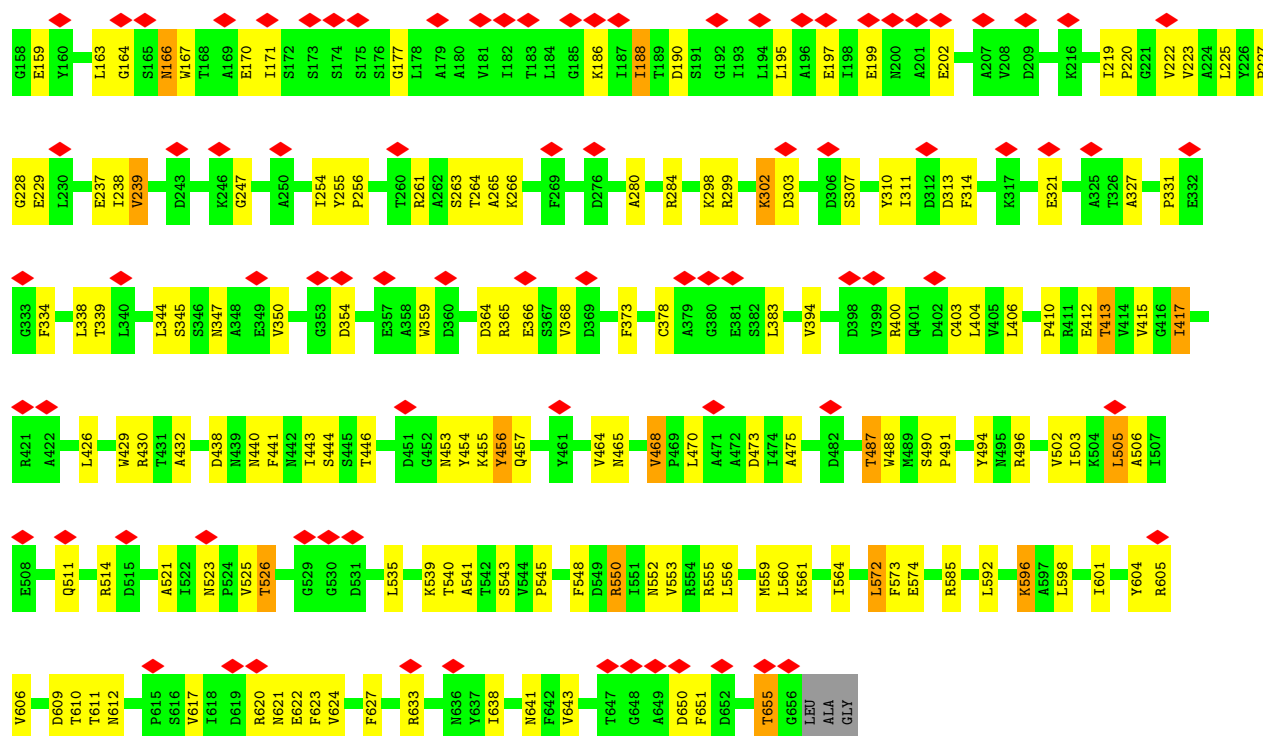


• Molecule 2: gp18, tail sheath protein

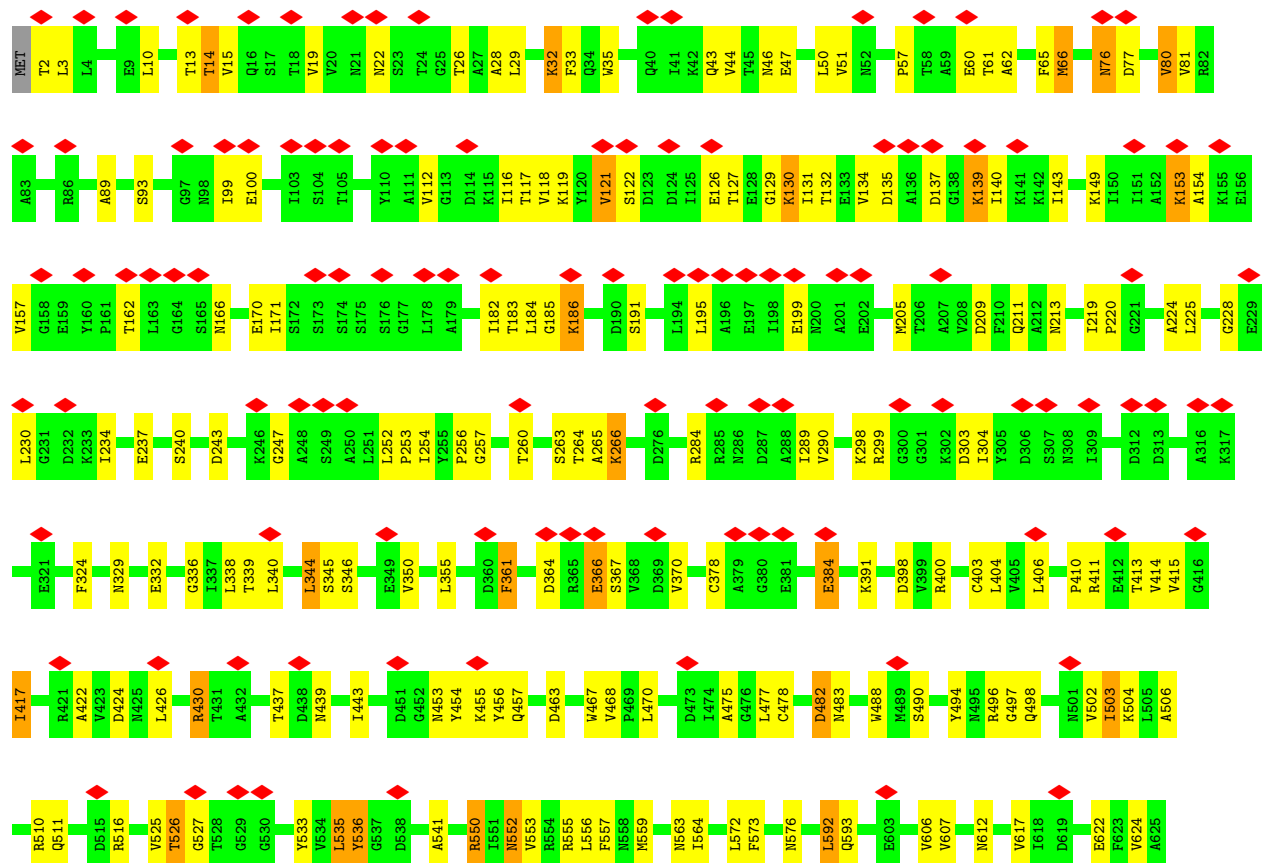


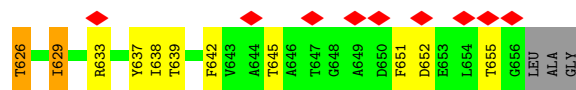
• Molecule 2: gp18, tail sheath protein



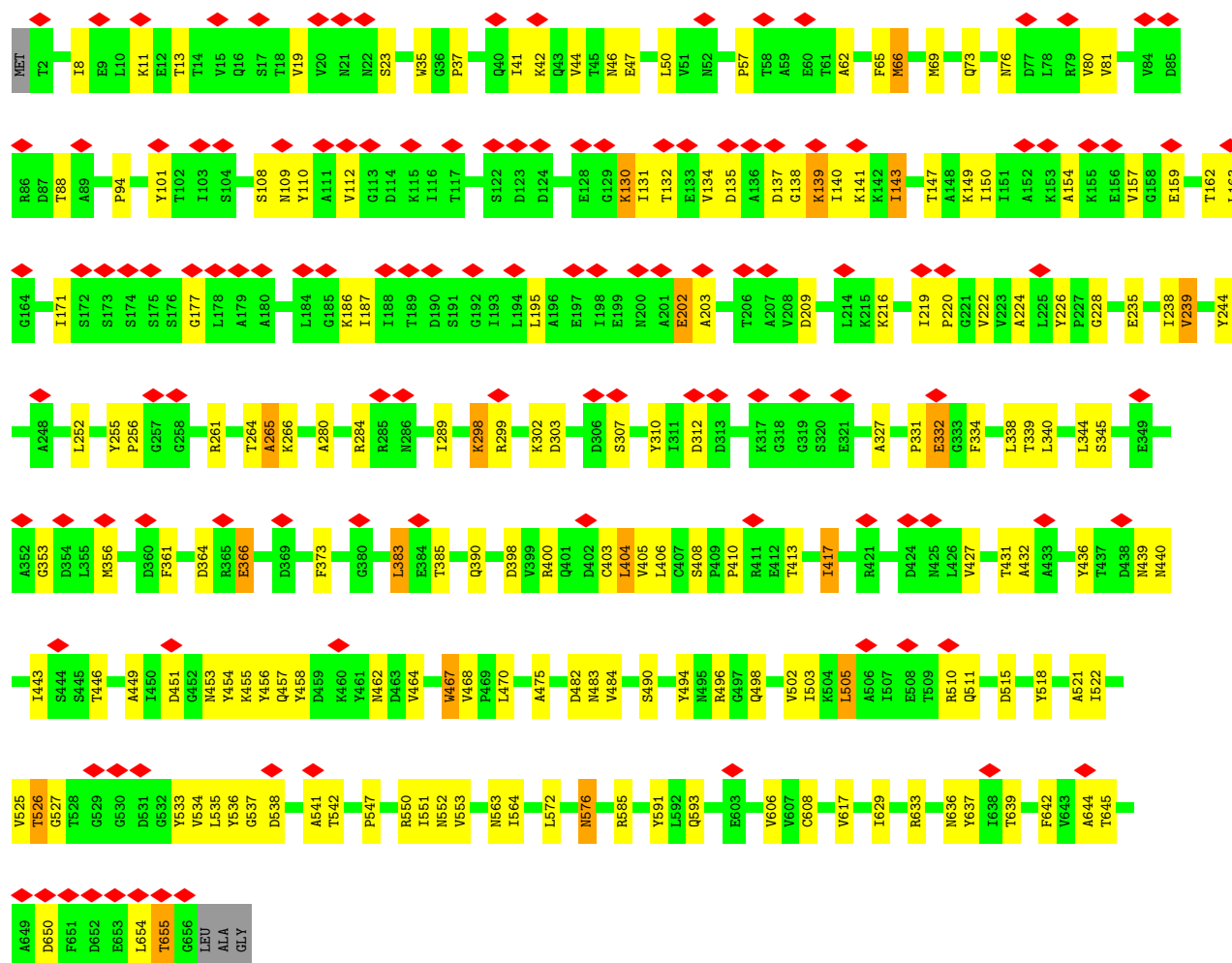
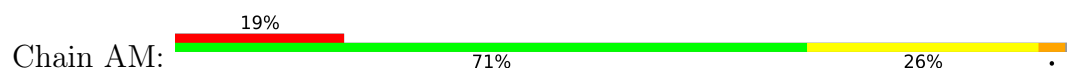


• Molecule 2: gp18, tail sheath protein

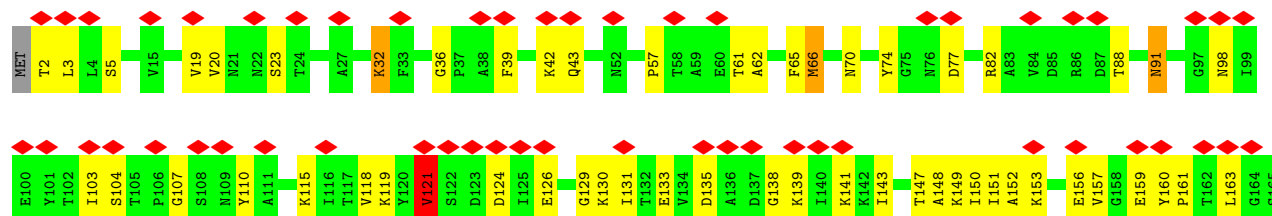


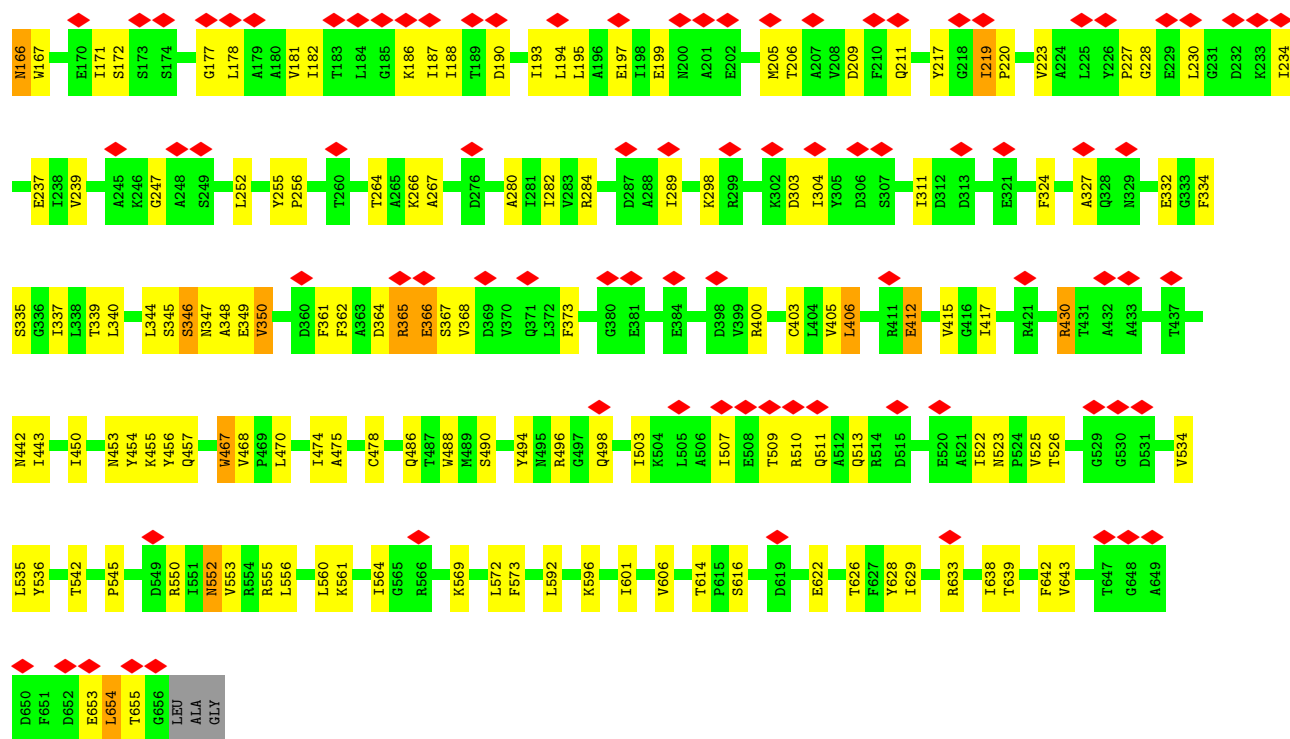


• Molecule 2: gp18, tail sheath protein

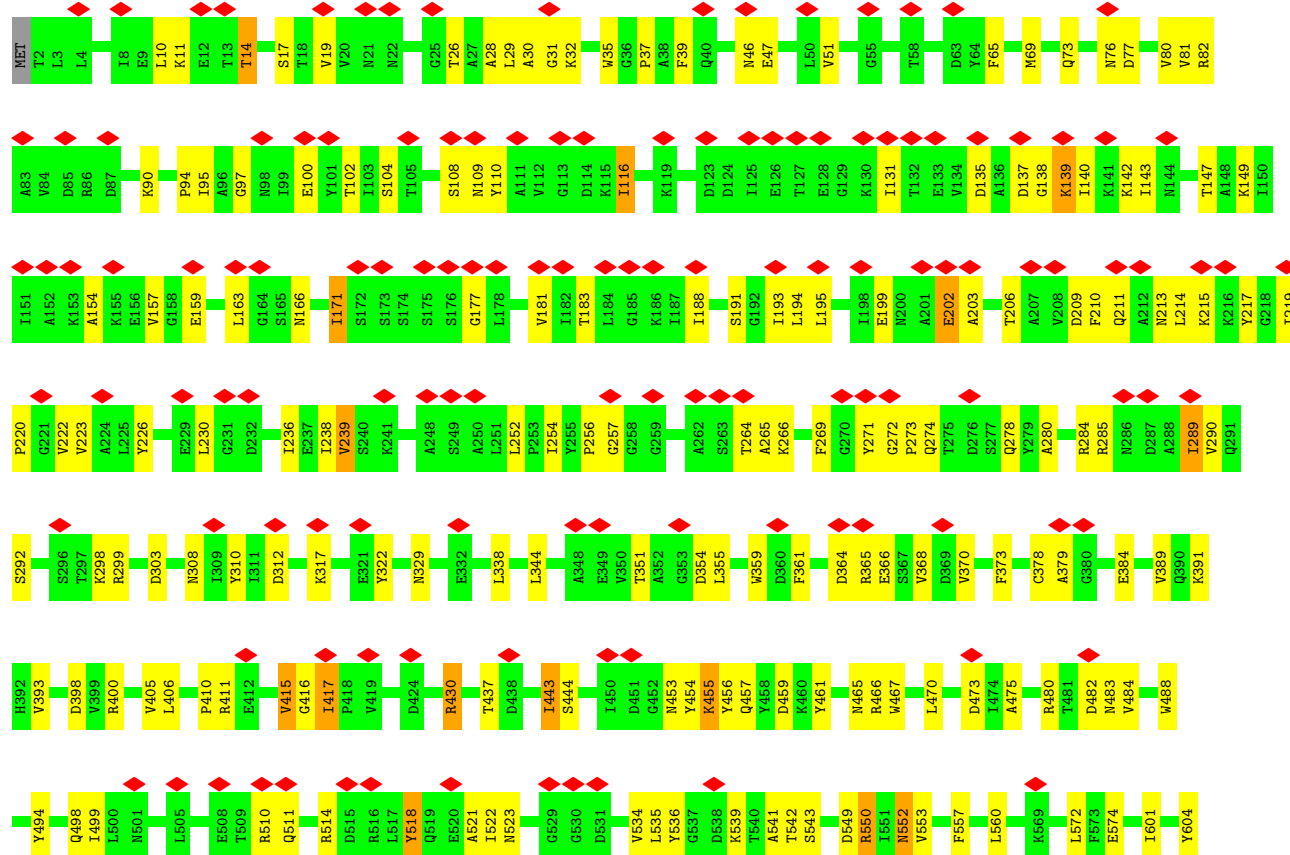


• Molecule 2: gp18, tail sheath protein



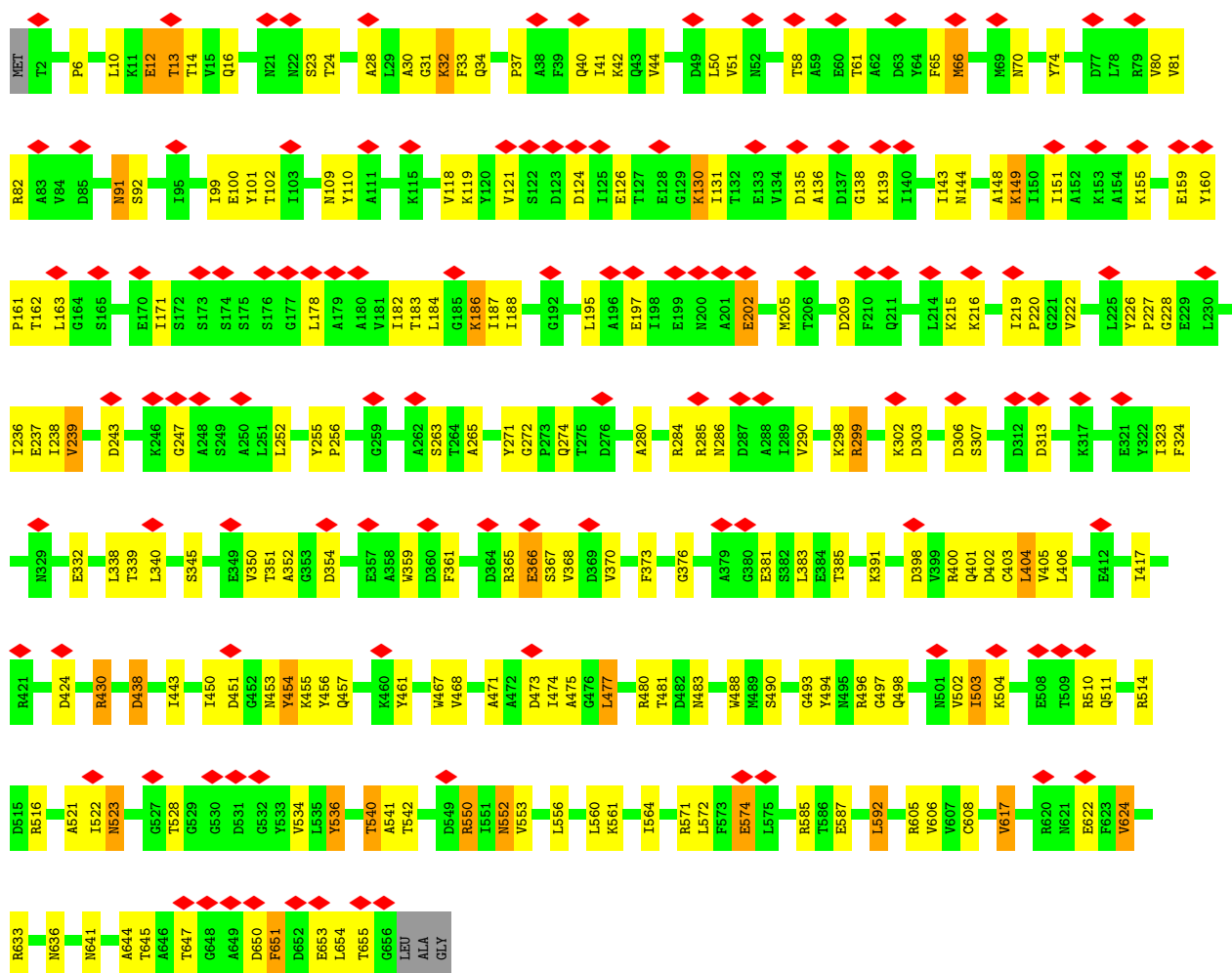


• Molecule 2: gp18, tail sheath protein

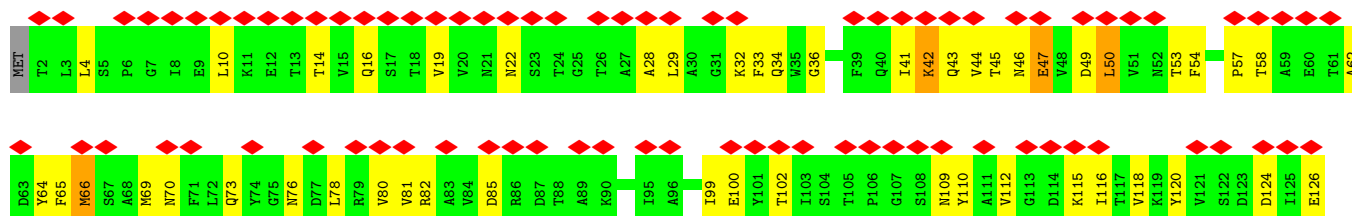


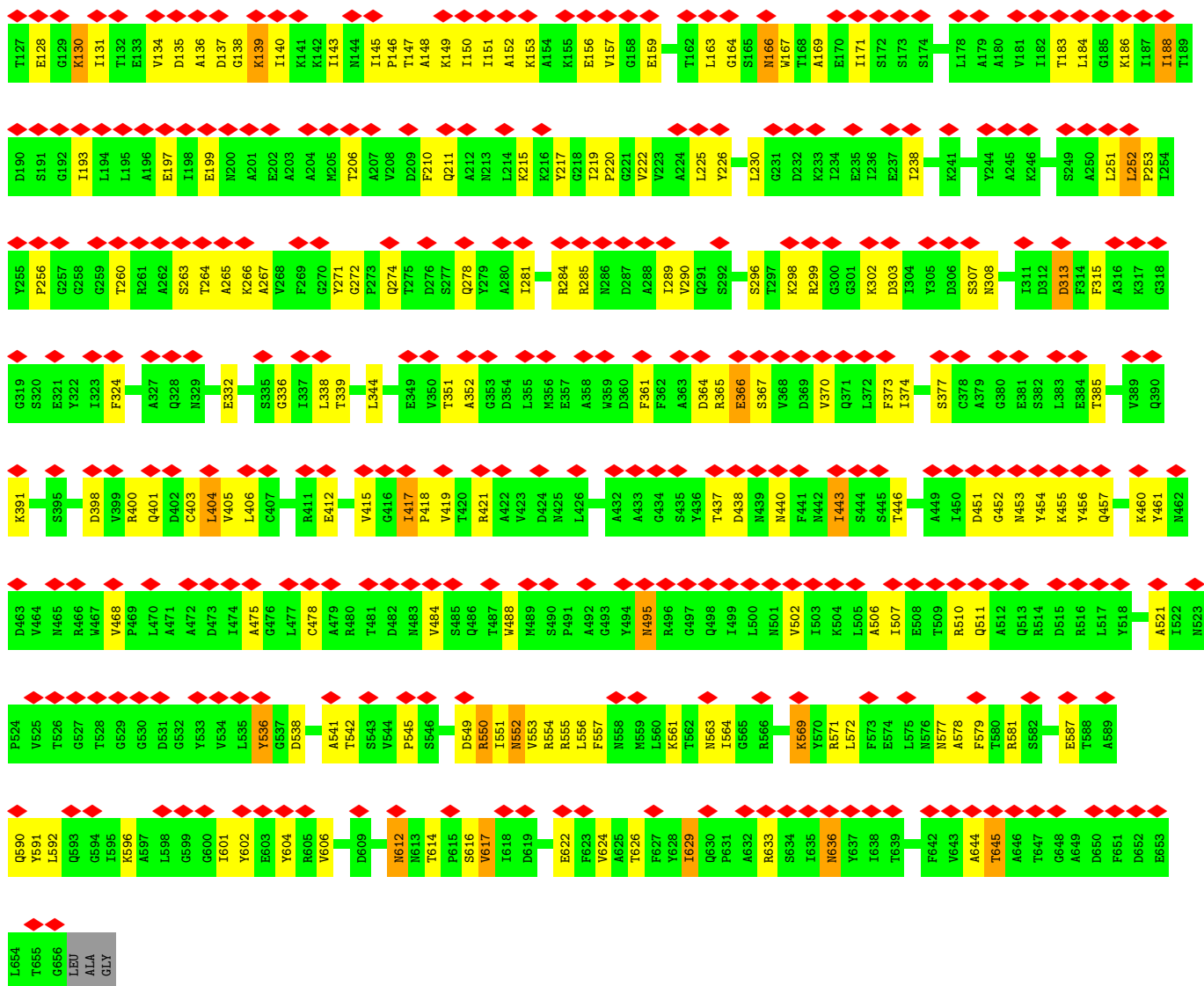


• Molecule 2: gp18, tail sheath protein

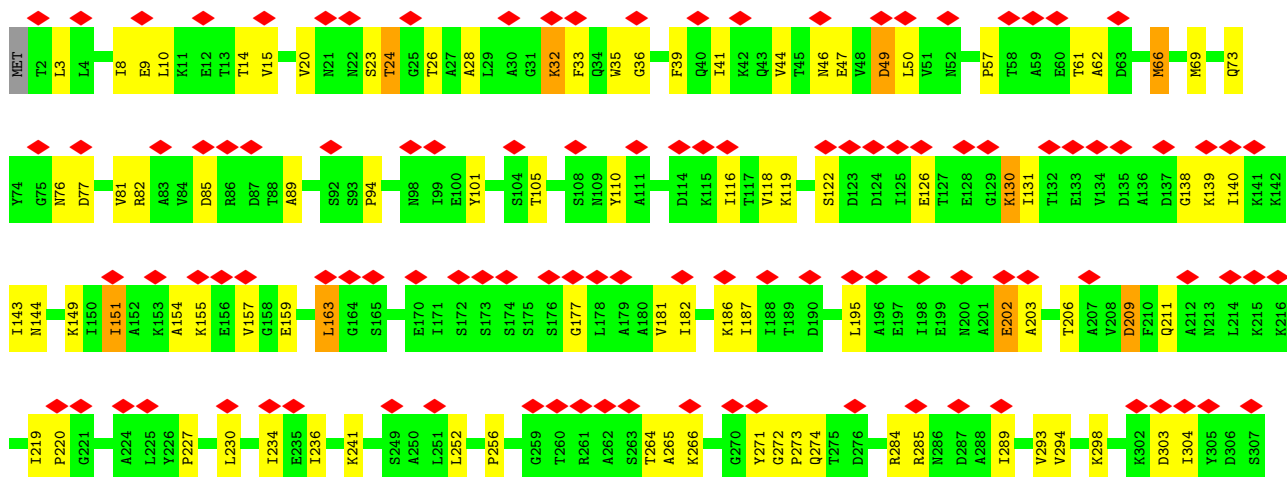


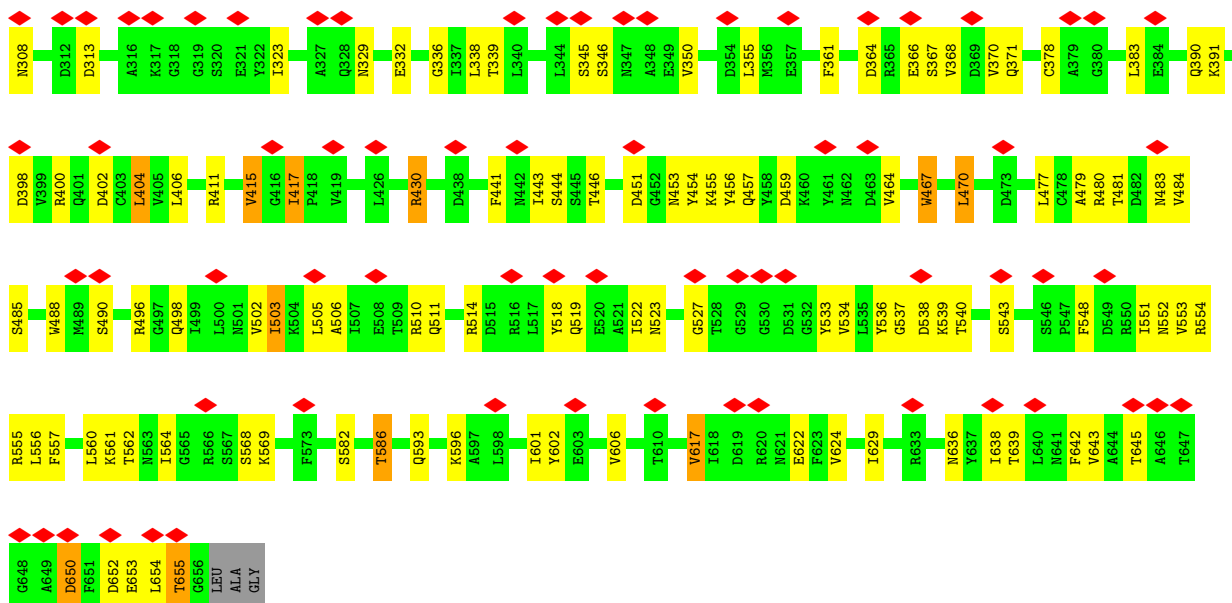
• Molecule 2: gp18, tail sheath protein



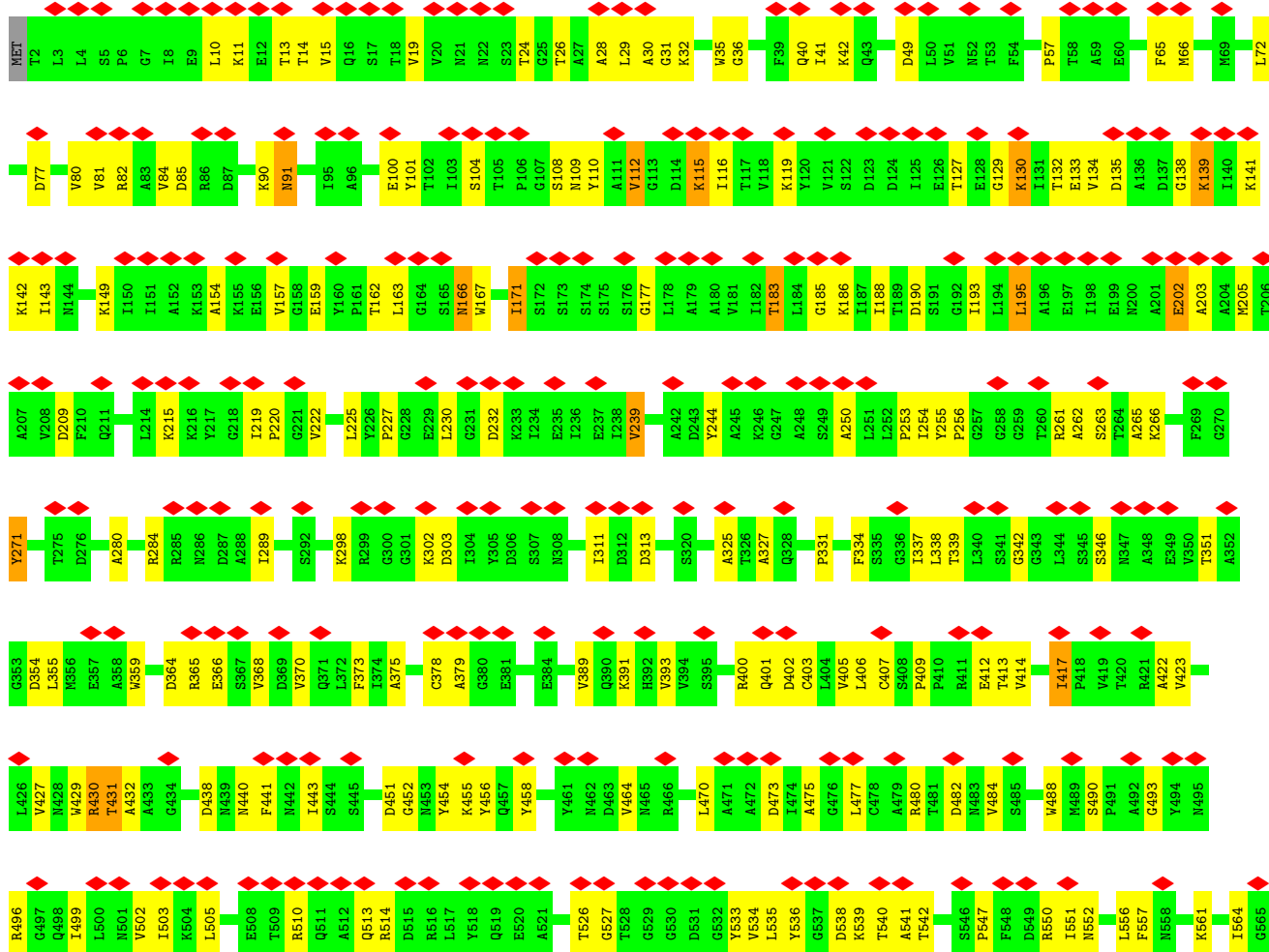
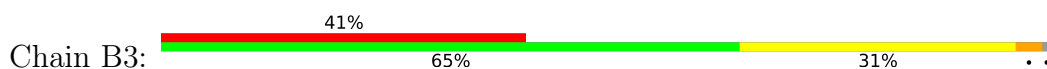


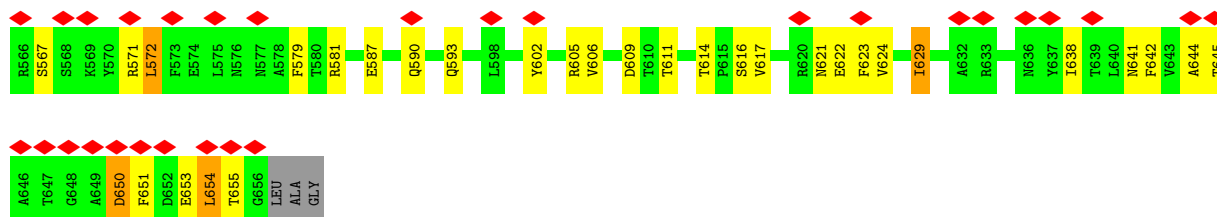
• Molecule 2: gp18, tail sheath protein



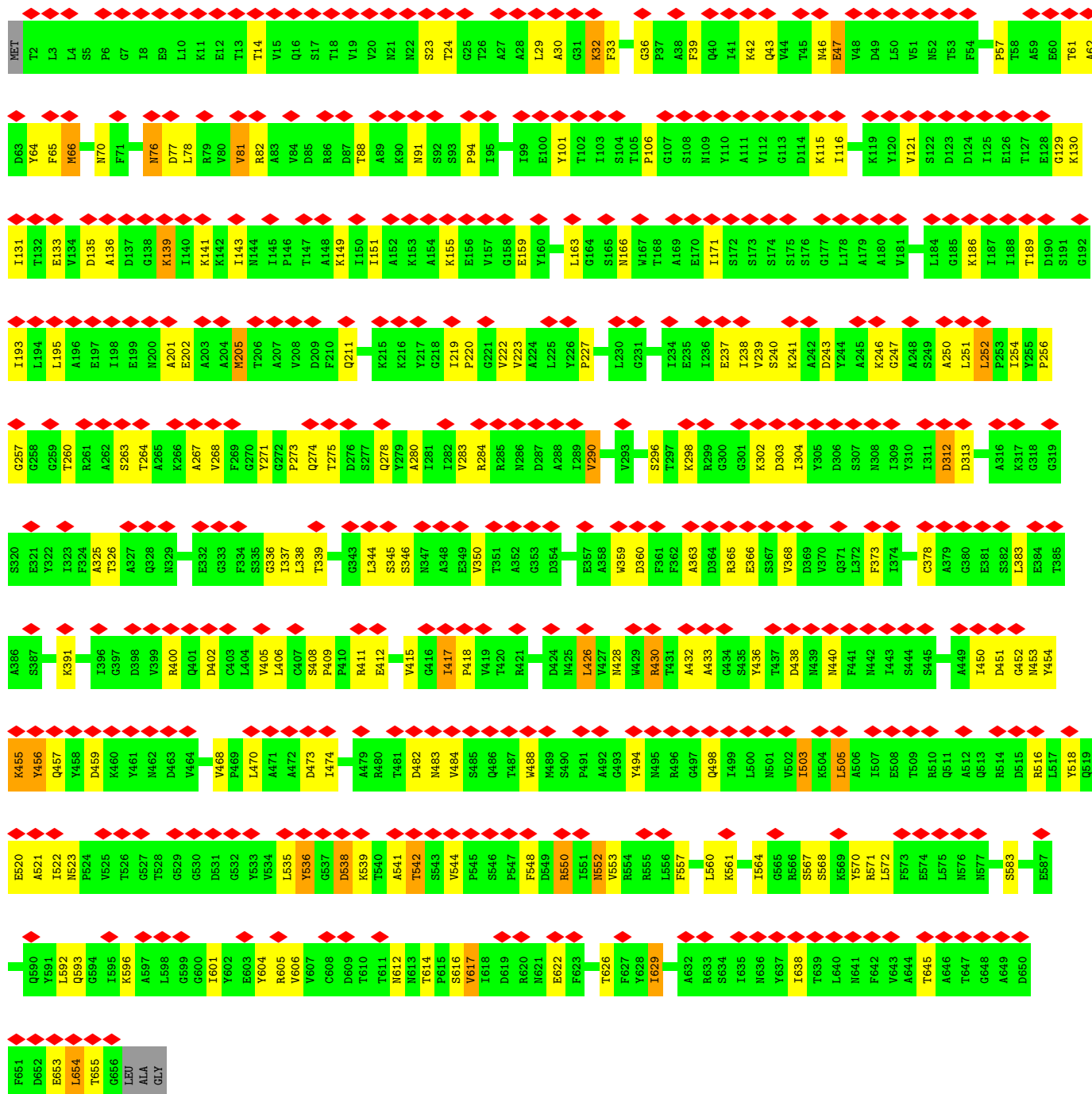


• Molecule 2: gp18, tail sheath protein

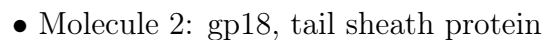




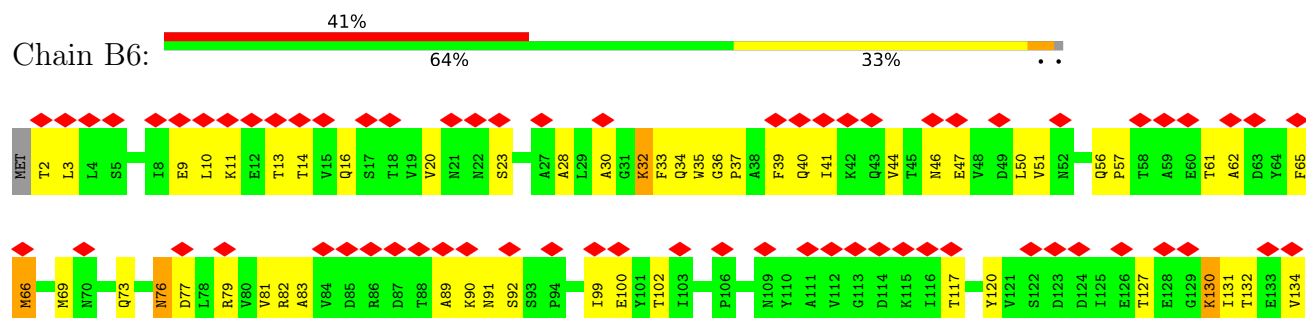
• Molecule 2: gp18, tail sheath protein

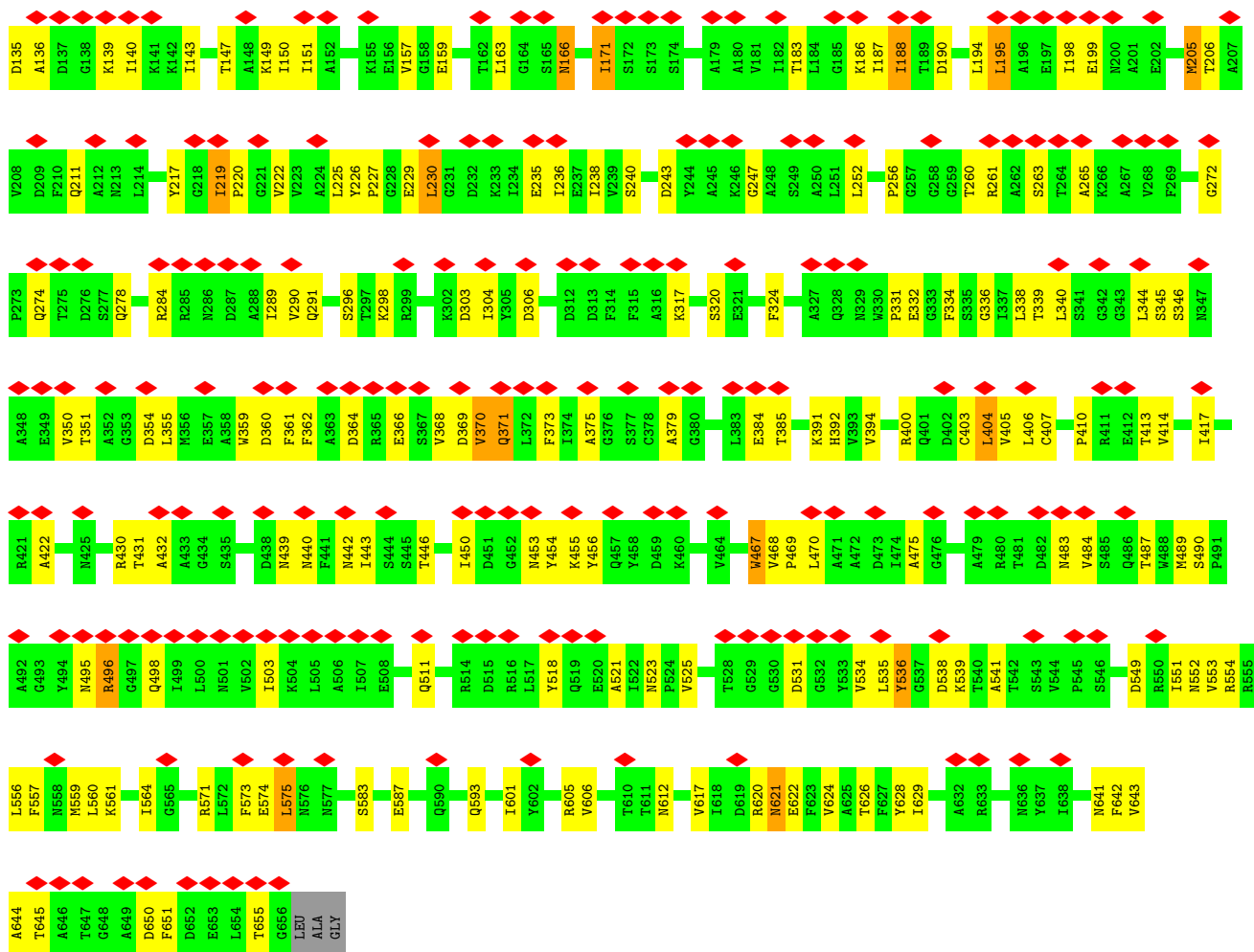


## Chain B5:

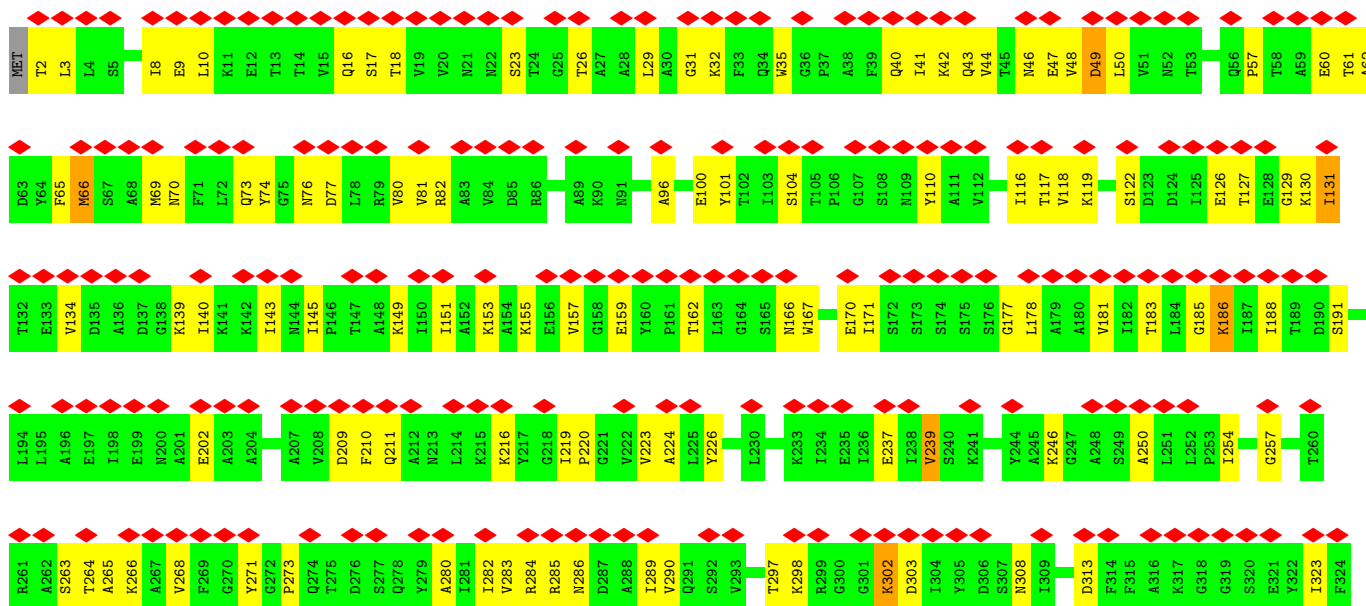


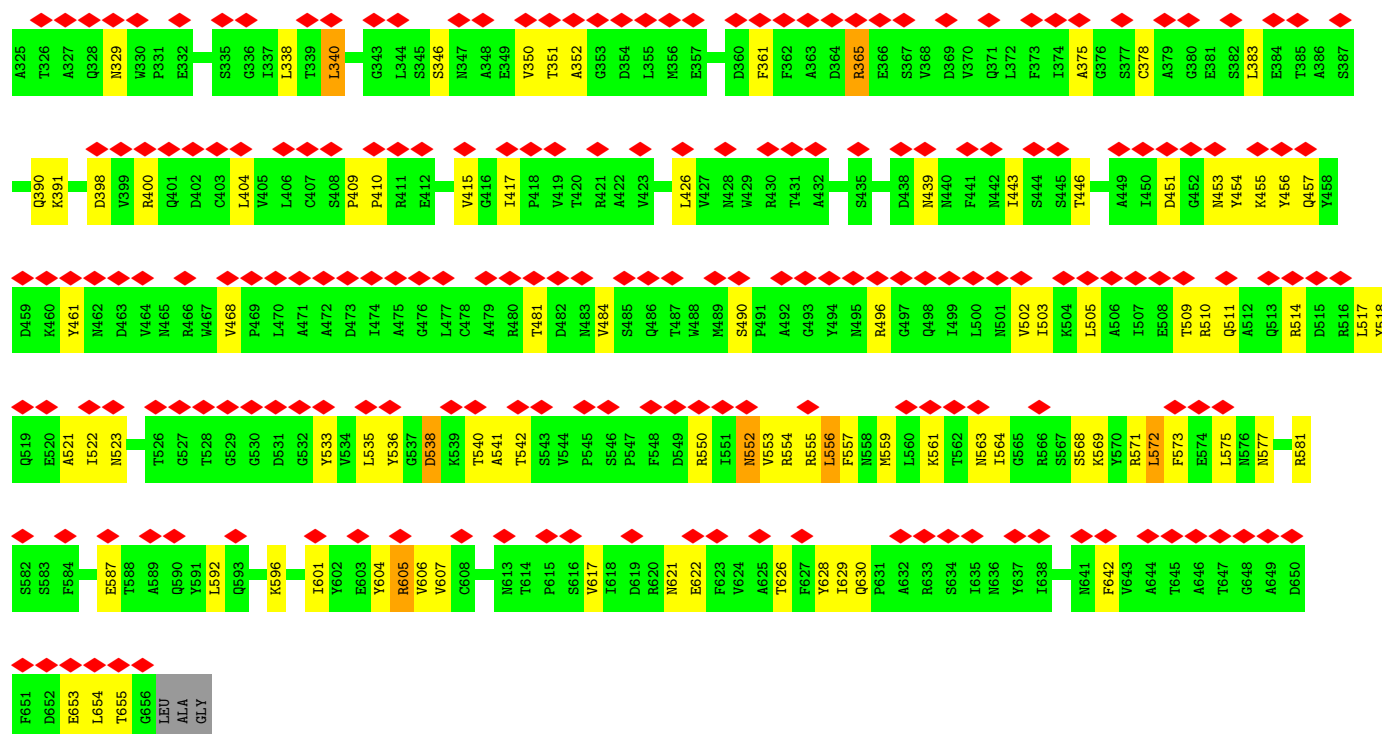
## Chain B6:



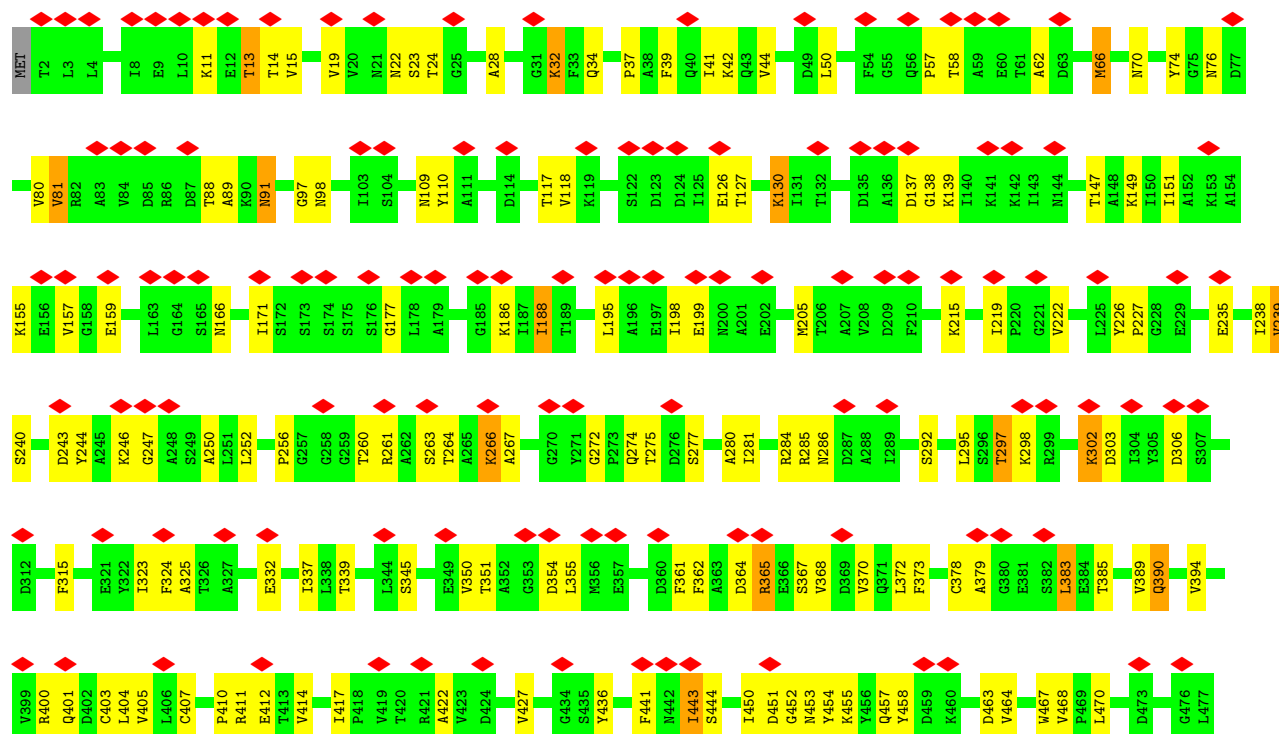


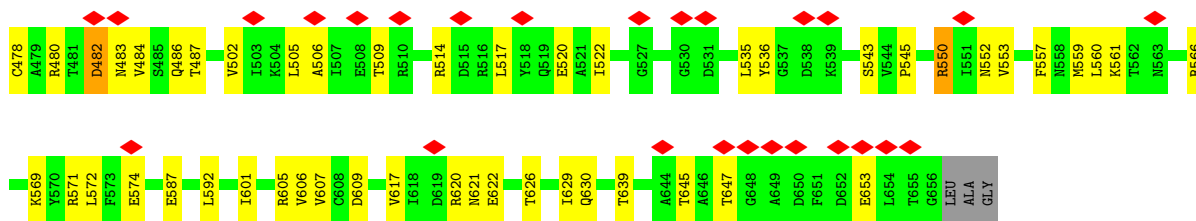
• Molecule 2: gp18, tail sheath protein



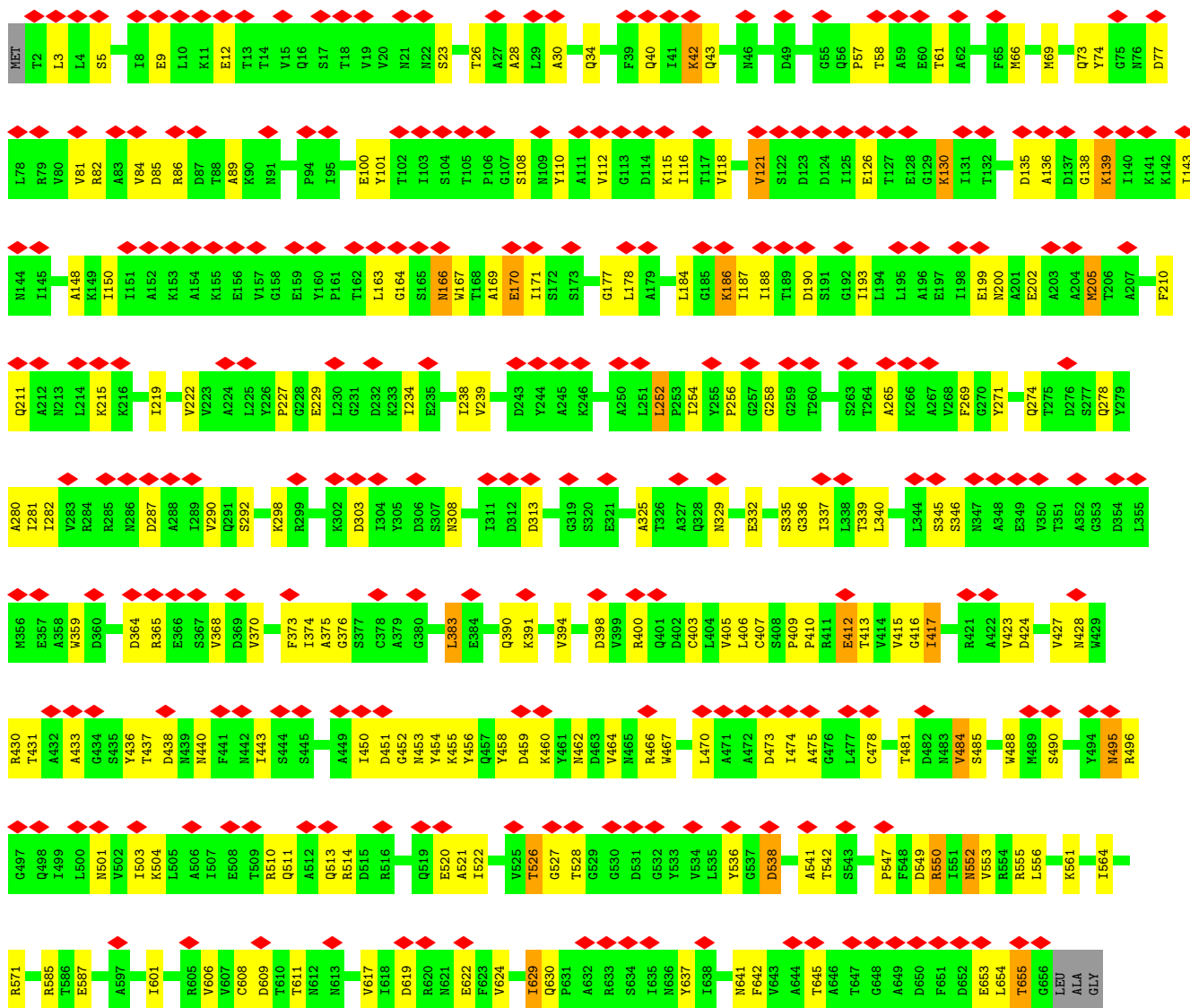
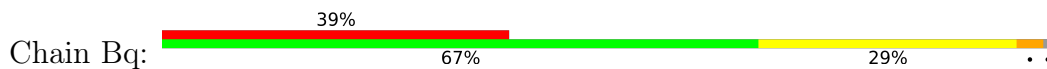


• Molecule 2: gp18, tail sheath protein



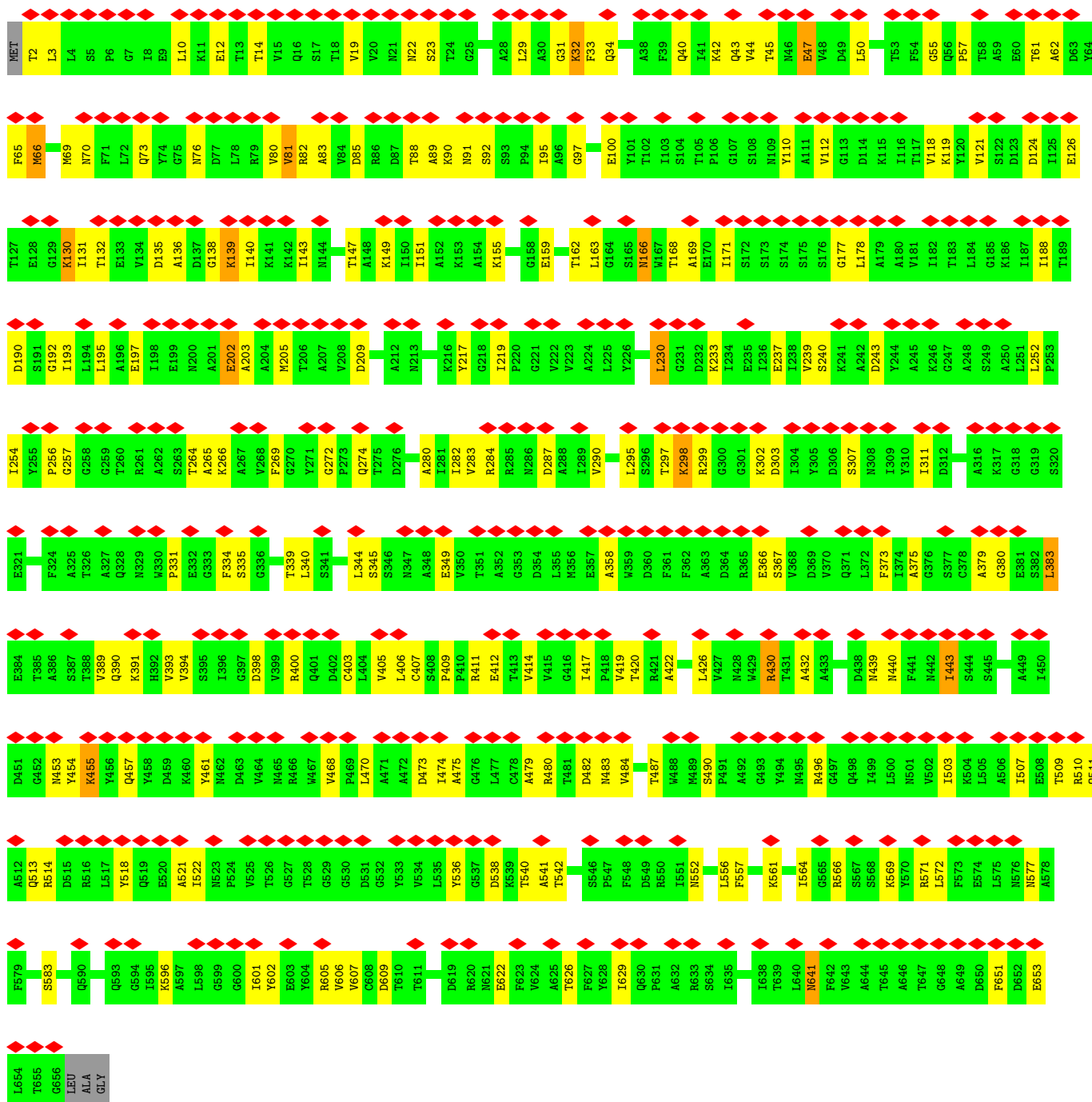


• Molecule 2: gp18, tail sheath protein

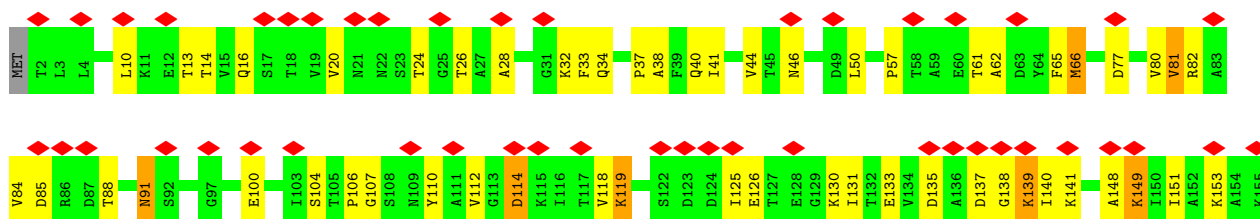


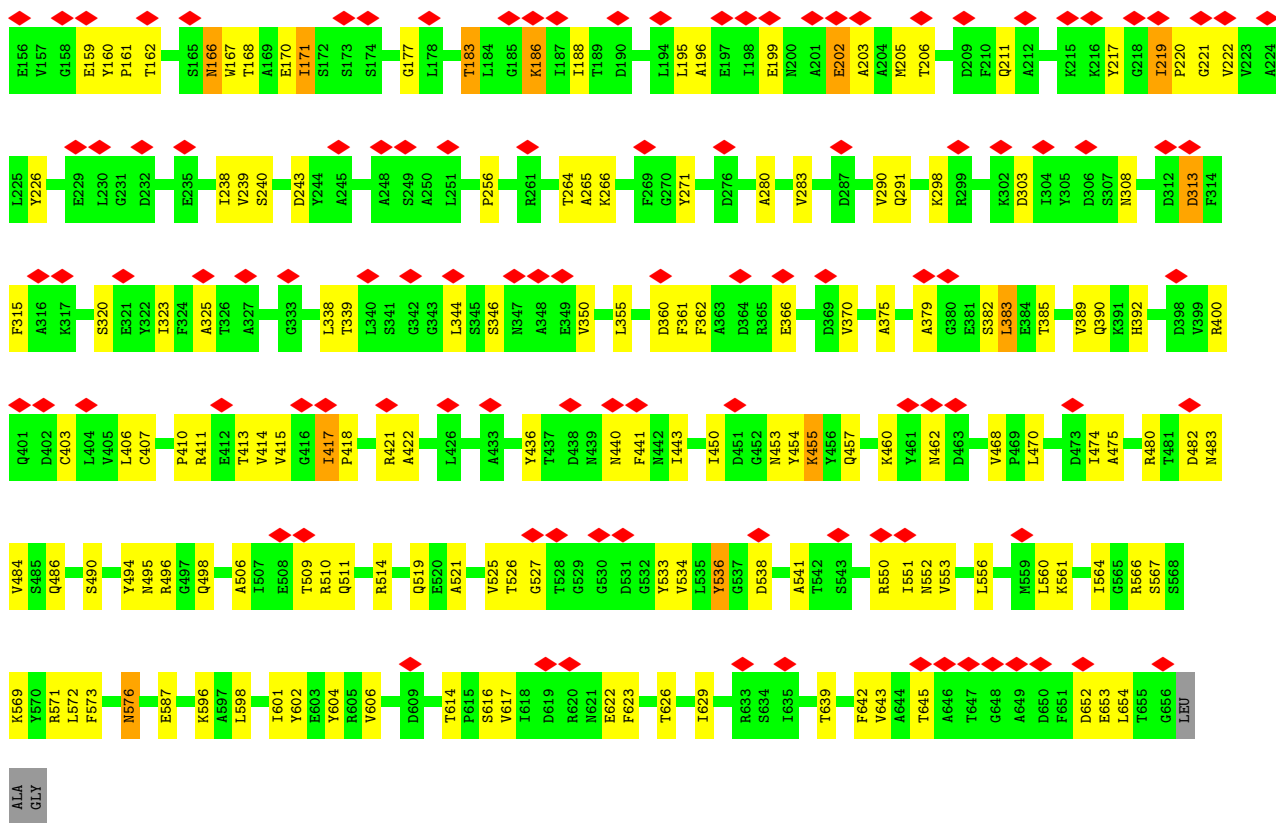
• Molecule 2: gp18, tail sheath protein



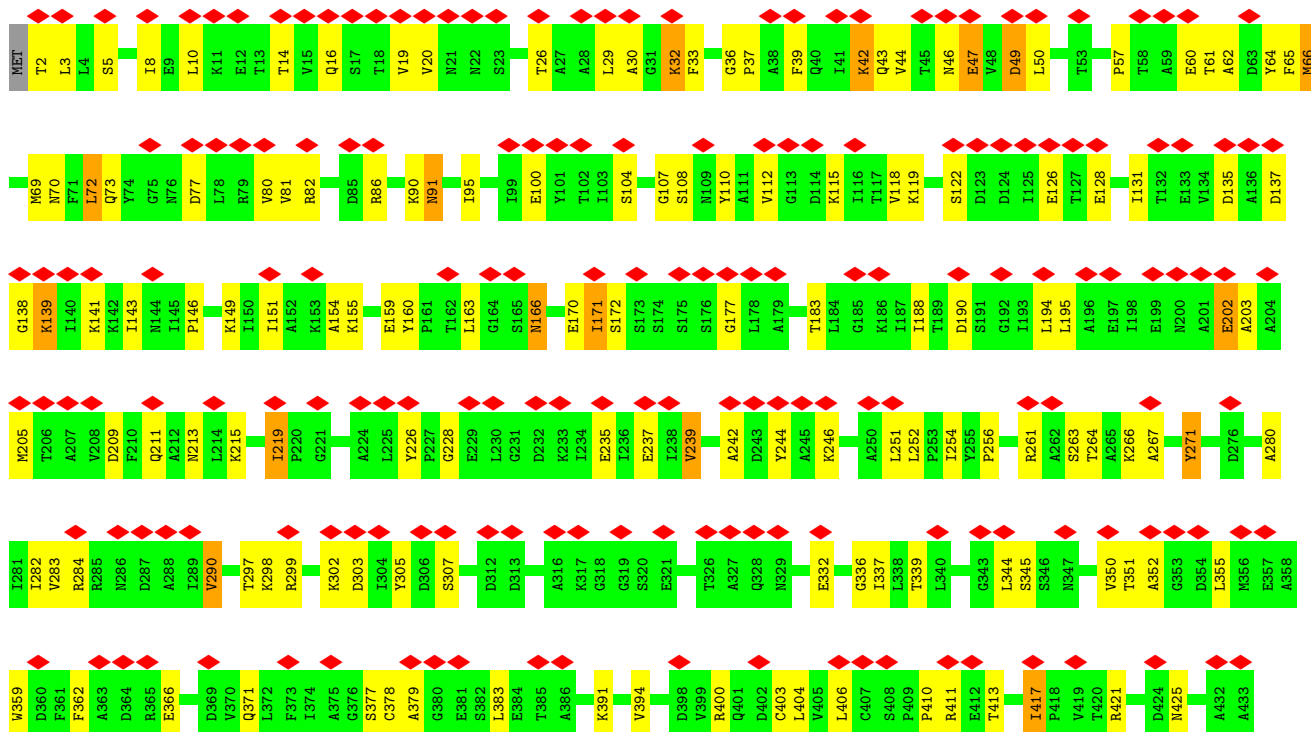


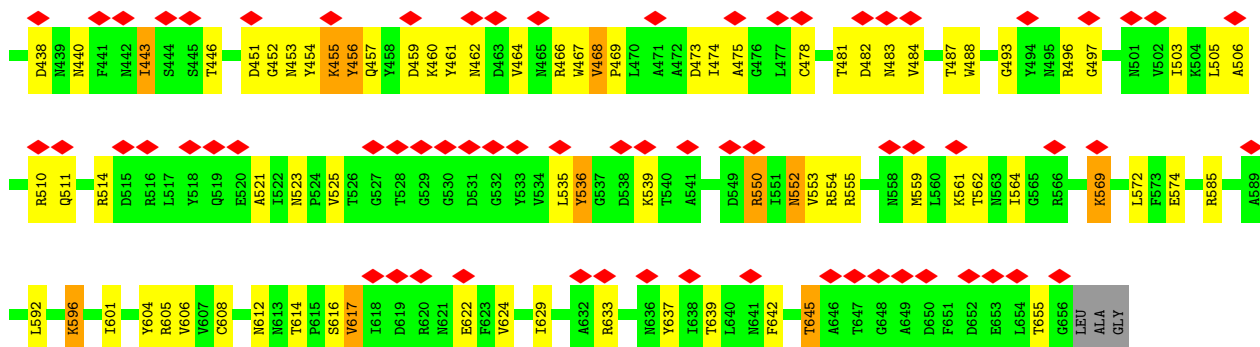
- Molecule 2: gp18, tail sheath protein



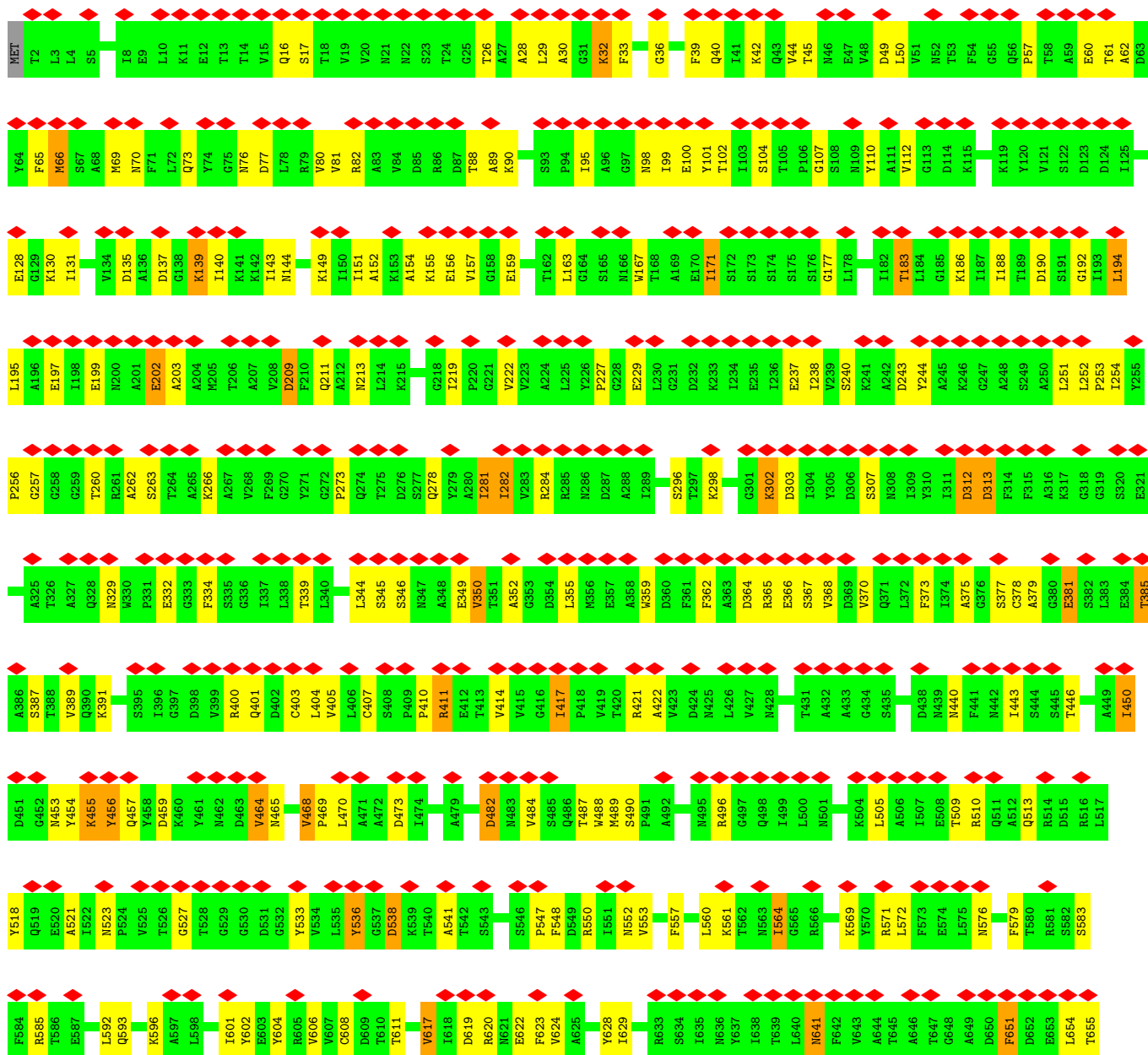


• Molecule 2: gp18, tail sheath protein



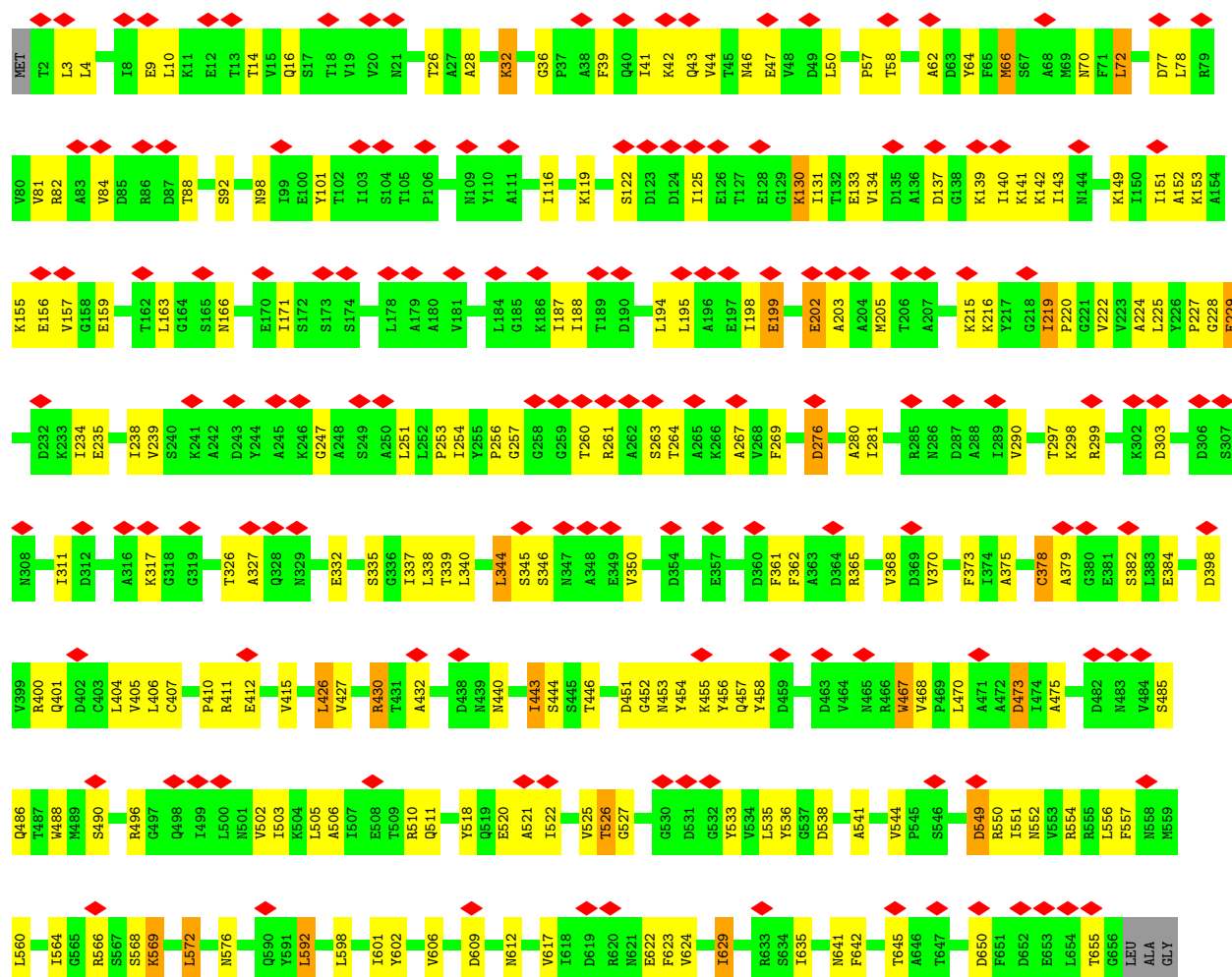


• Molecule 2: gp18, tail sheath protein

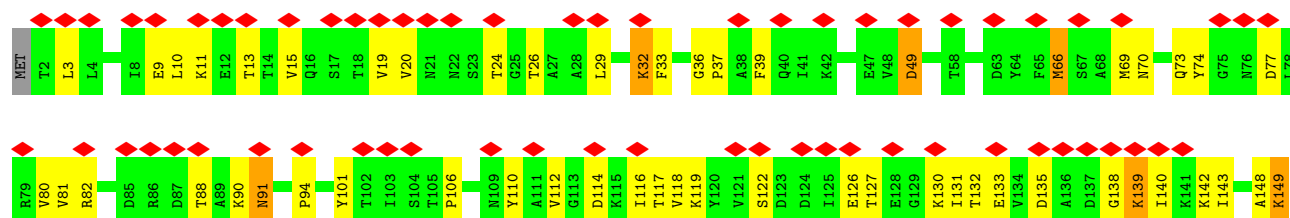


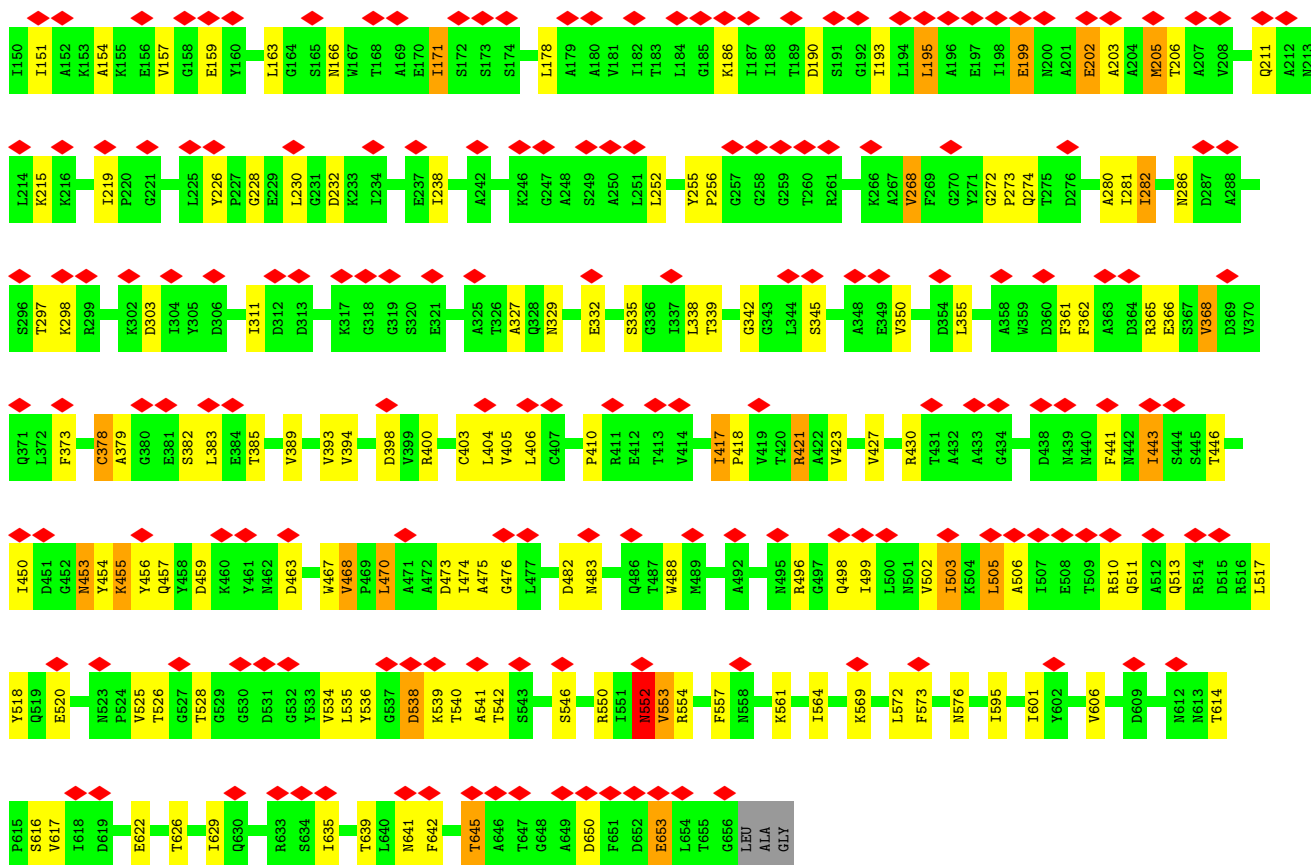


• Molecule 2: gp18, tail sheath protein

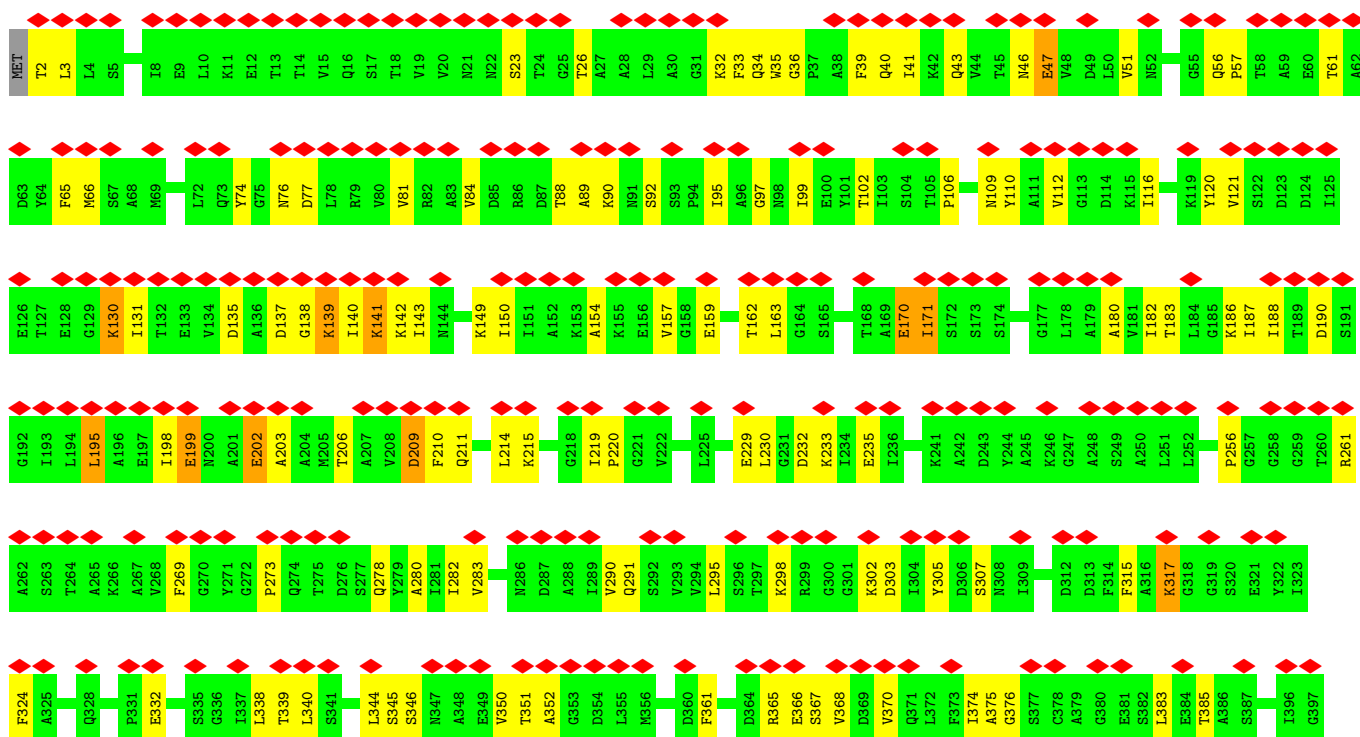


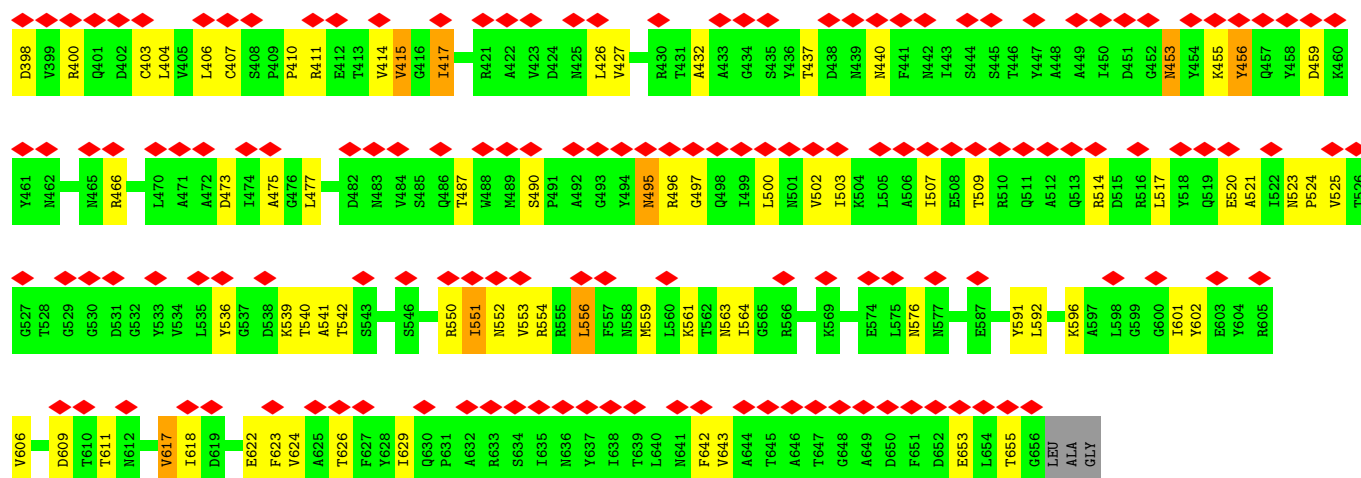
• Molecule 2: gp18, tail sheath protein



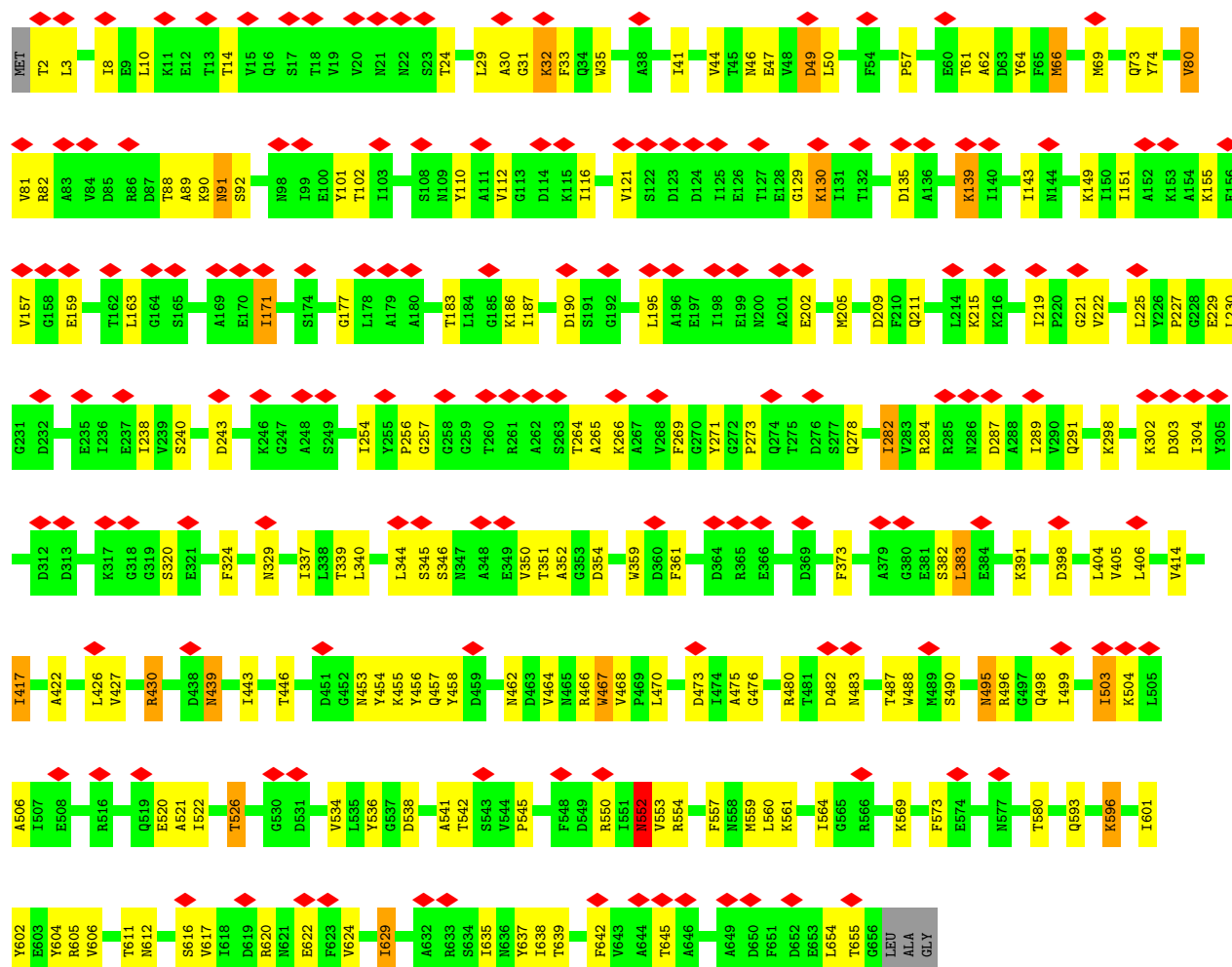


• Molecule 2: gp18, tail sheath protein

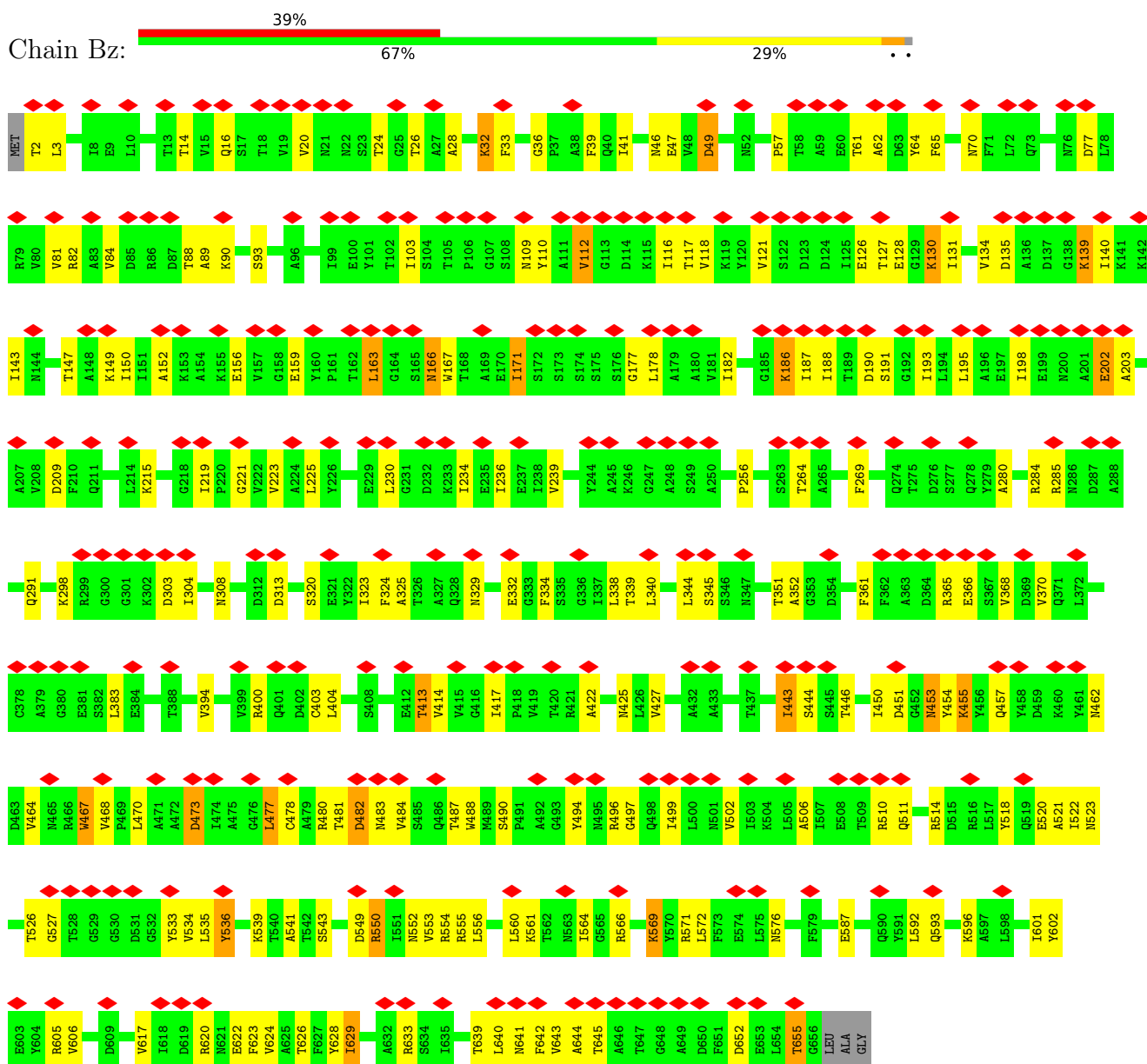




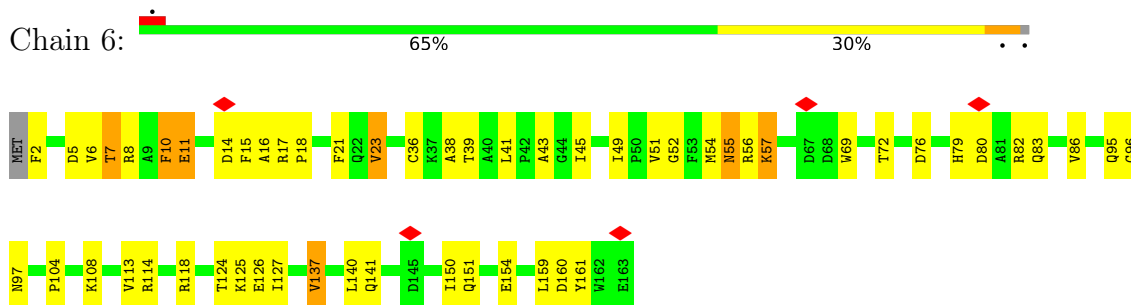
• Molecule 2: gp18, tail sheath protein



• Molecule 2: gp18, tail sheath protein

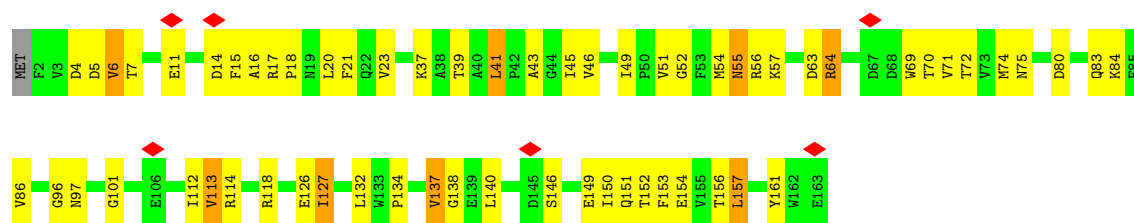


- Molecule 3: gp19, tail tube protein

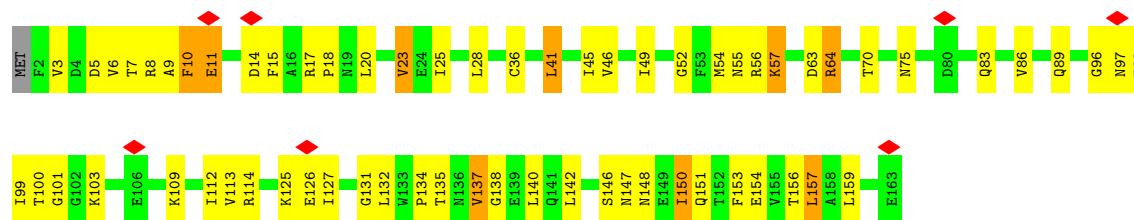


- Molecule 3: gp19, tail tube protein

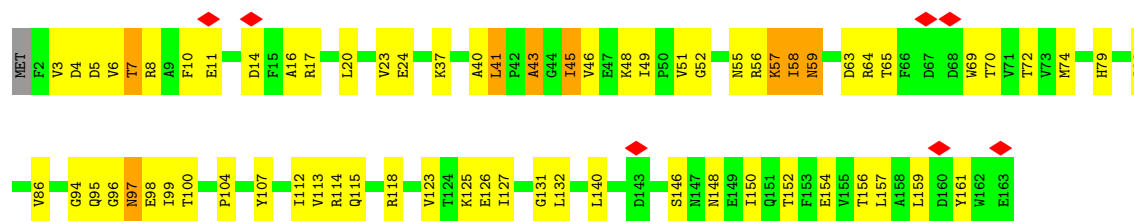




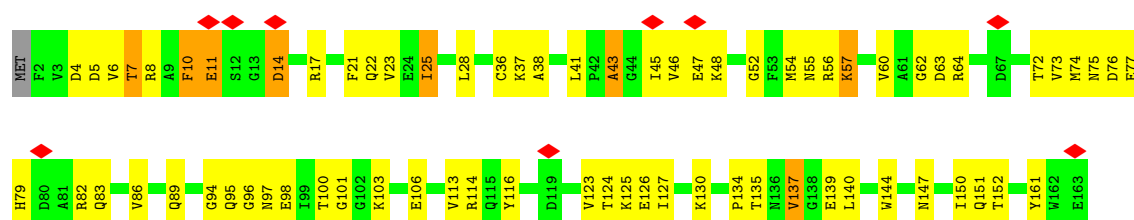
- Molecule 3: gp19, tail tube protein



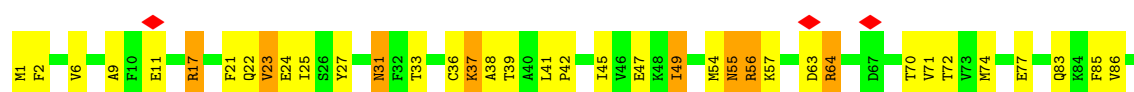
- Molecule 3: gp19, tail tube protein

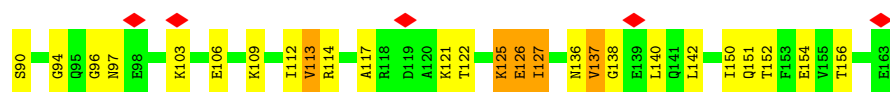


- Molecule 3: gp19, tail tube protein



- Molecule 3: gp19, tail tube protein

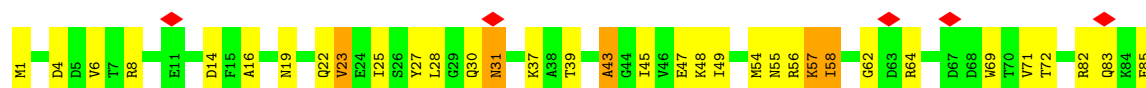




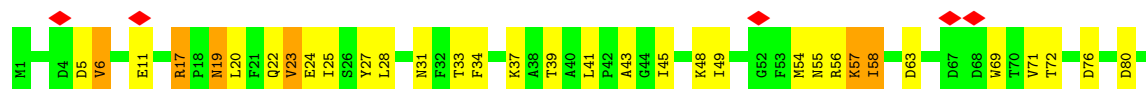
- Molecule 3: gp19, tail tube protein



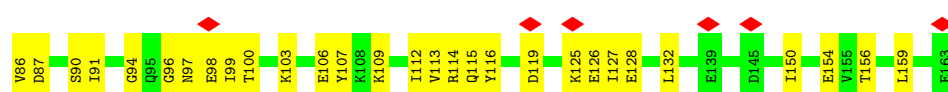
- Molecule 3: gp19, tail tube protein



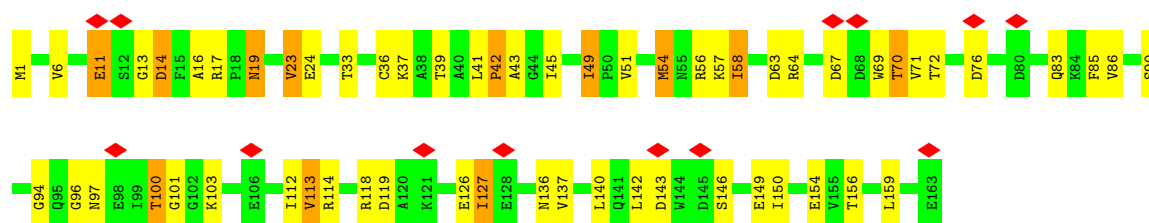
- Molecule 3: gp19, tail tube protein



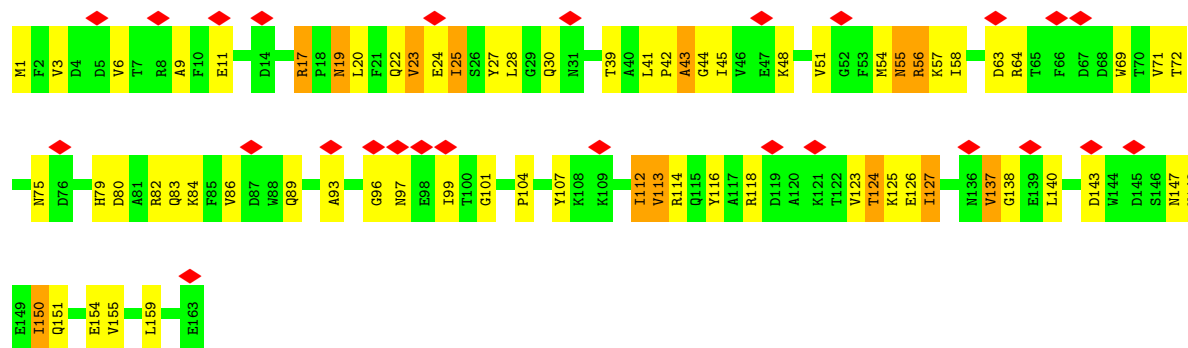
- Molecule 3: gp19, tail tube protein



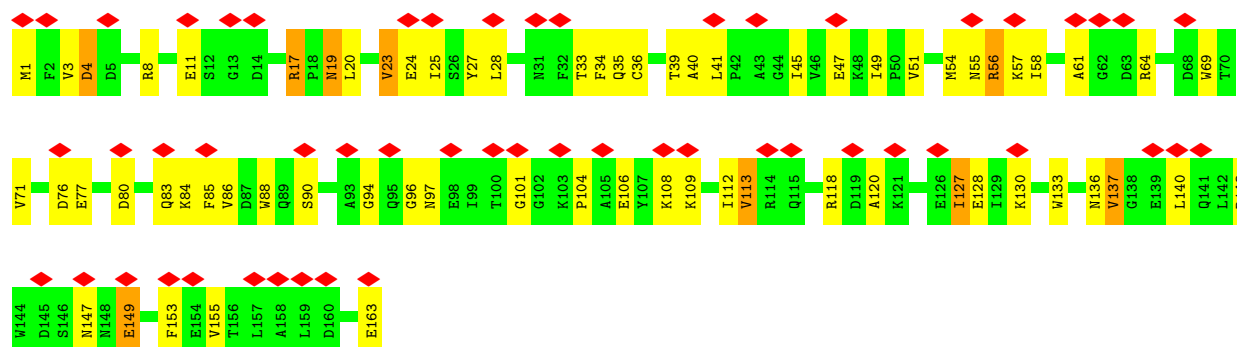
- Molecule 3: gp19, tail tube protein



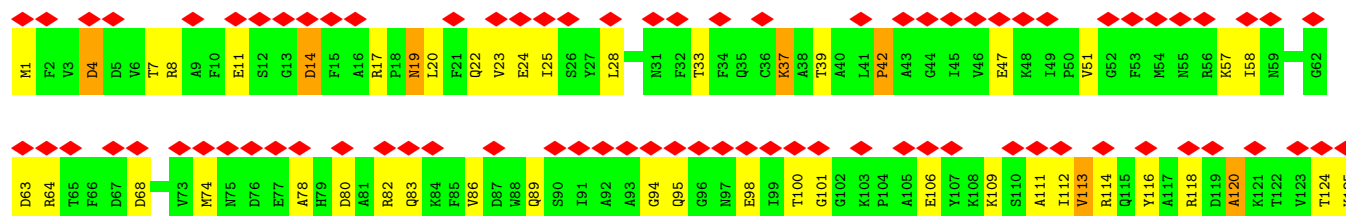
- Molecule 3: gp19, tail tube protein



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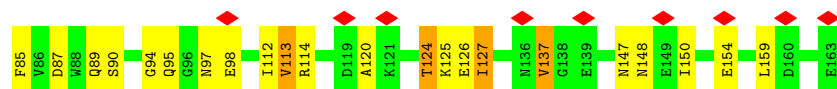
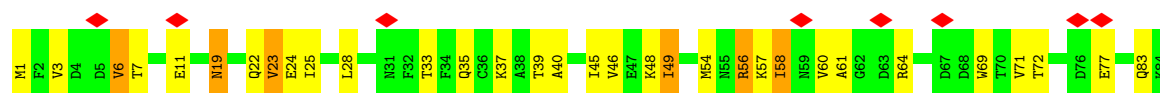


- Molecule 3: gp19, tail tube protein

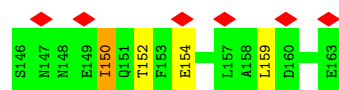
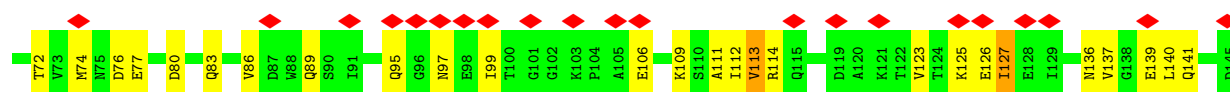
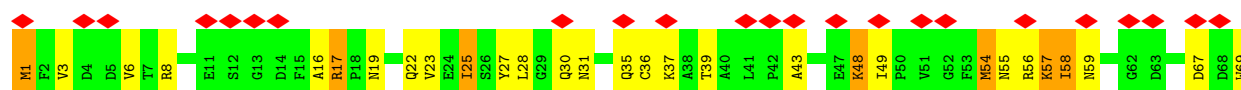




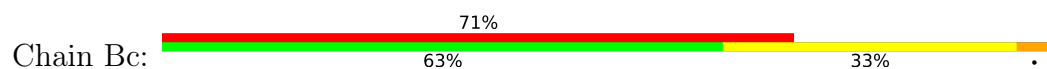
- Molecule 3: gp19, tail tube protein



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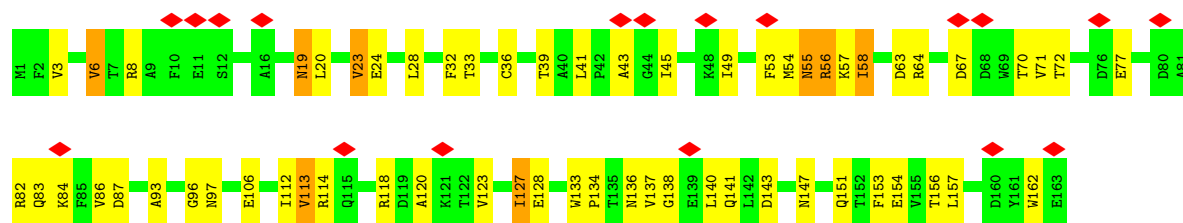


- Molecule 3: gp19, tail tube protein

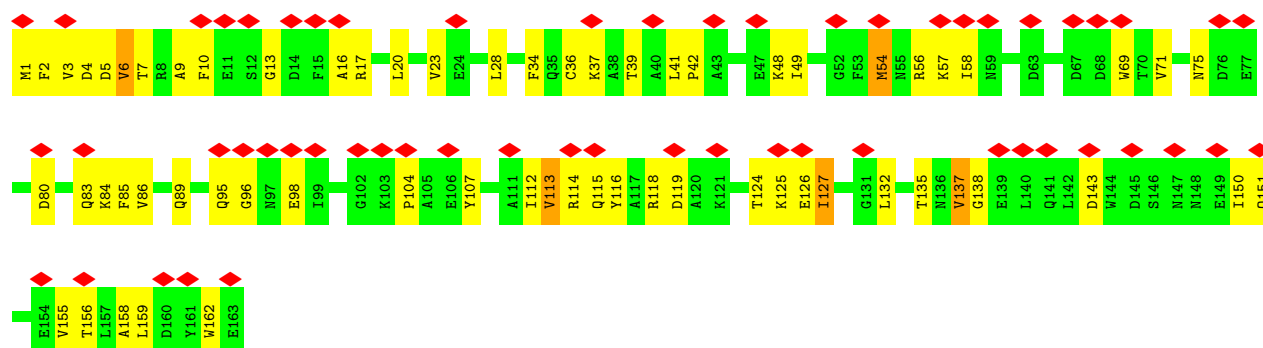


- Molecule 3: gp19, tail tube protein

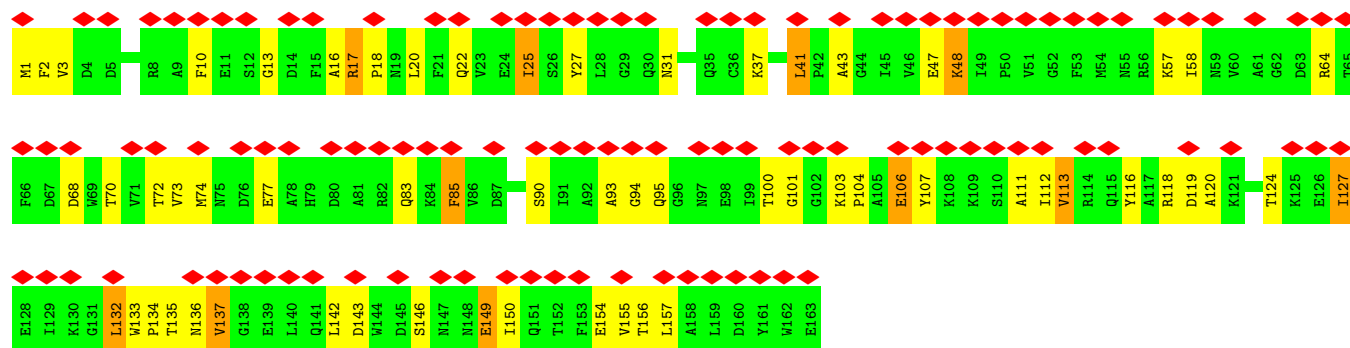




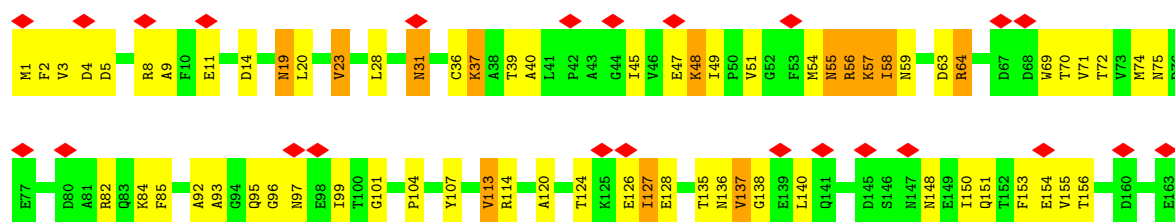
• Molecule 3: gp19, tail tube protein



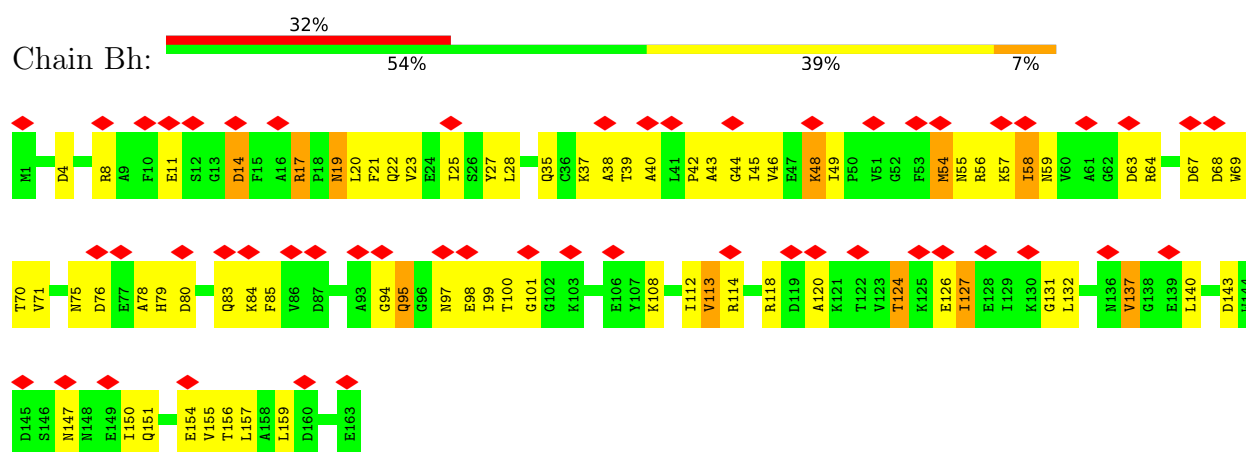
• Molecule 3: gp19, tail tube protein



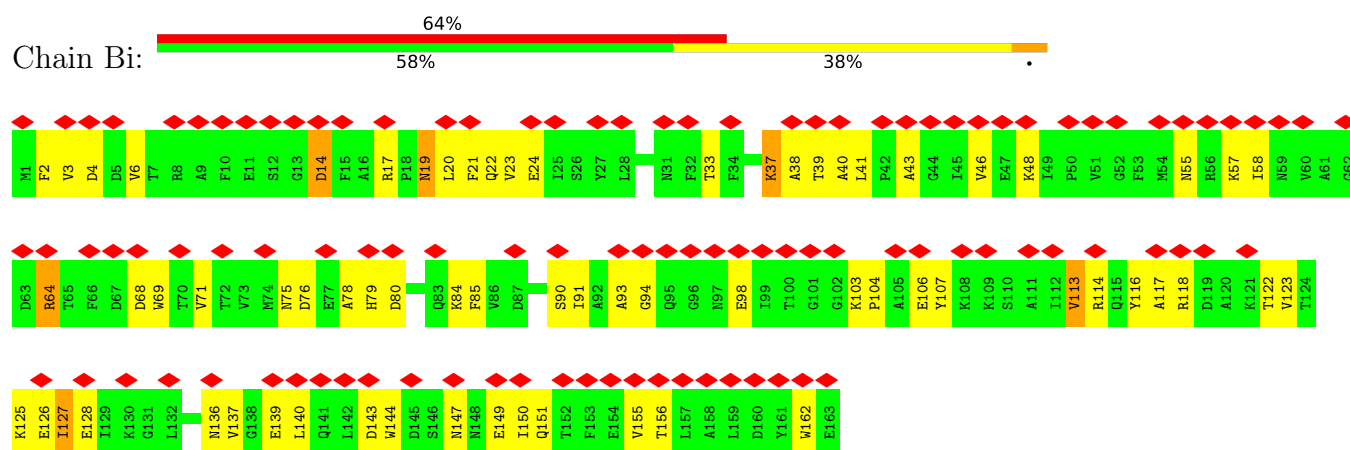
• Molecule 3: gp19, tail tube protein



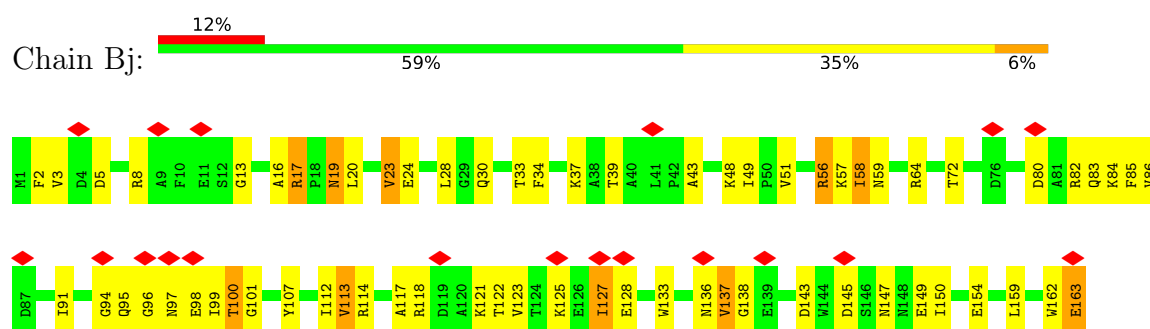
• Molecule 3: gp19, tail tube protein



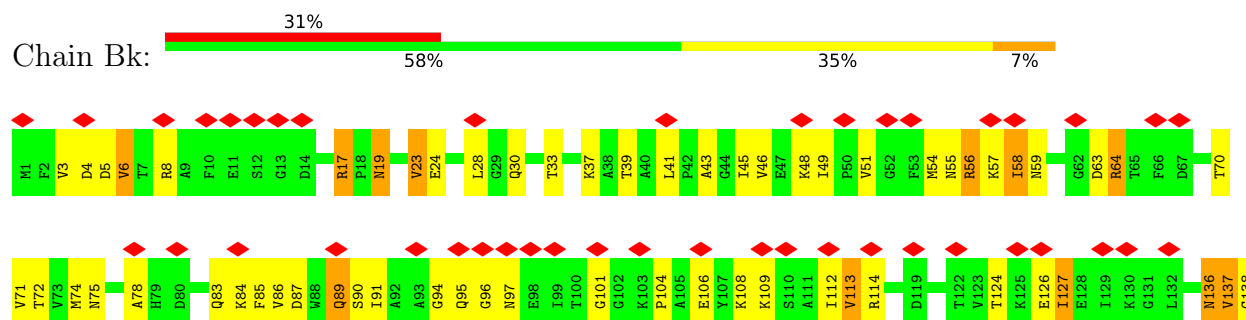
• Molecule 3: gp19, tail tube protein

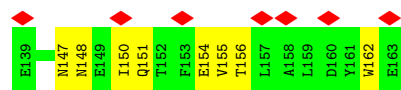


• Molecule 3: gp19, tail tube protein

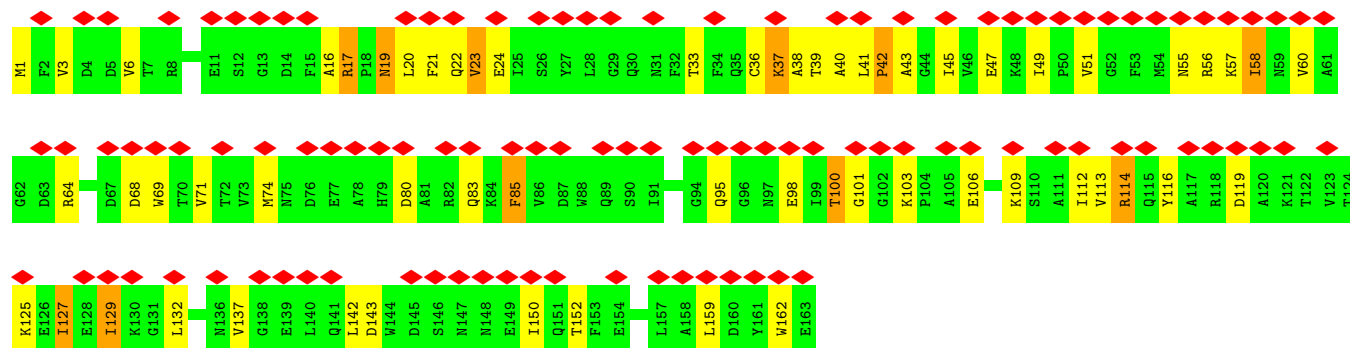


• Molecule 3: gp19, tail tube protein

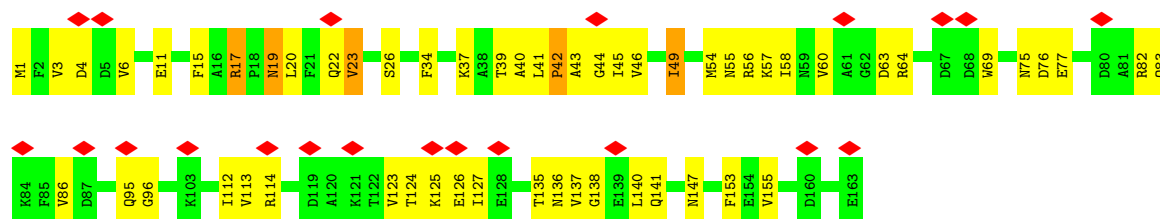




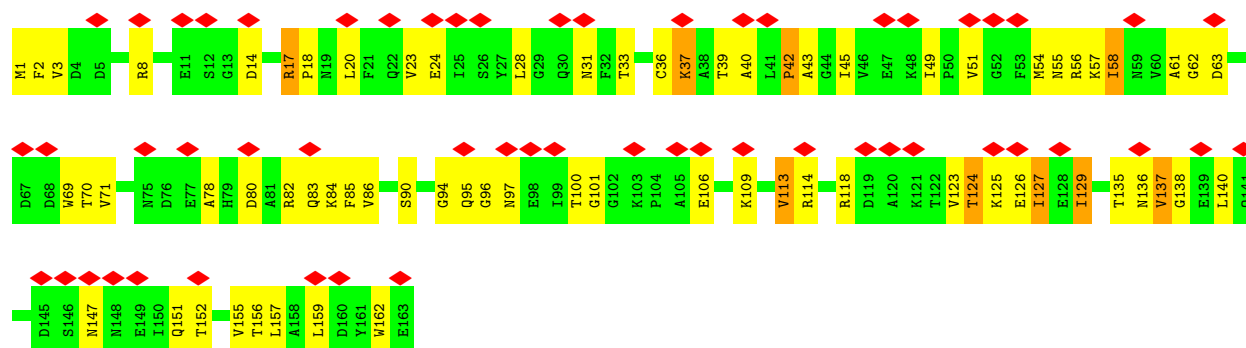
- Molecule 3: gp19, tail tube protein



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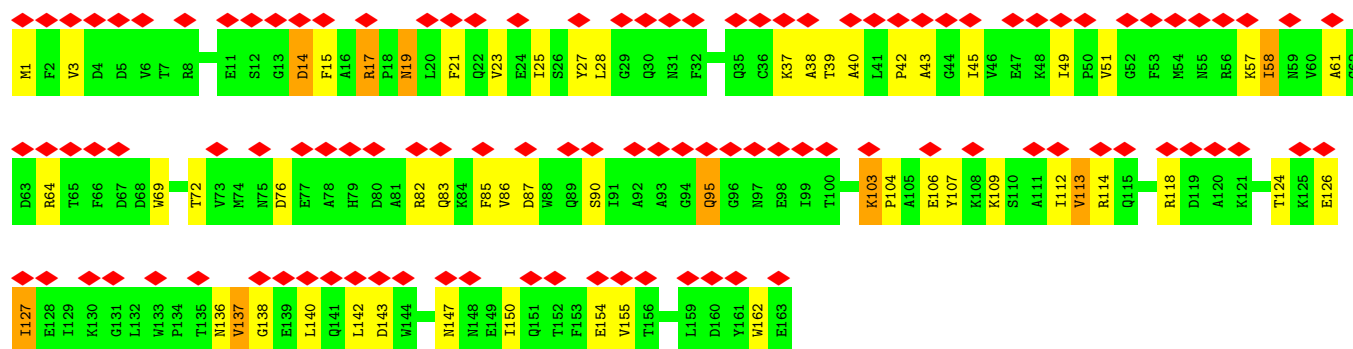


- Molecule 3: gp19, tail tube protein

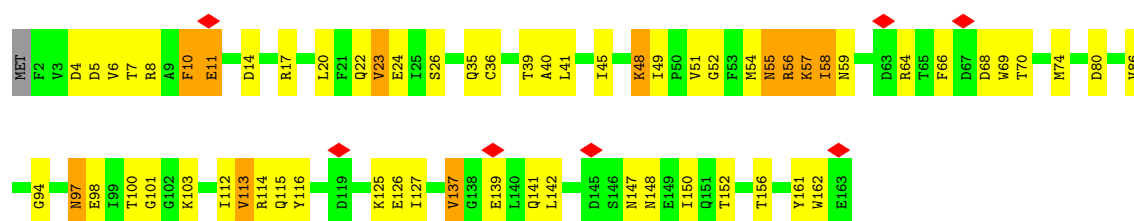


- Molecule 3: gp19, tail tube protein

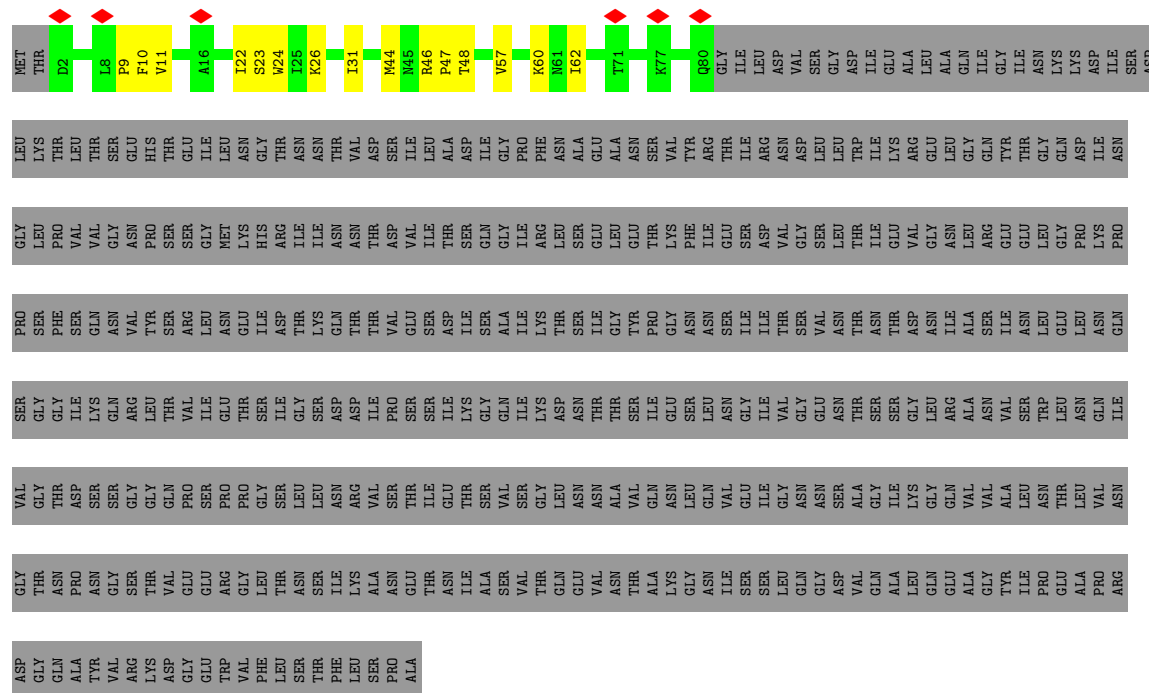




• Molecule 3: gp19, tail tube protein



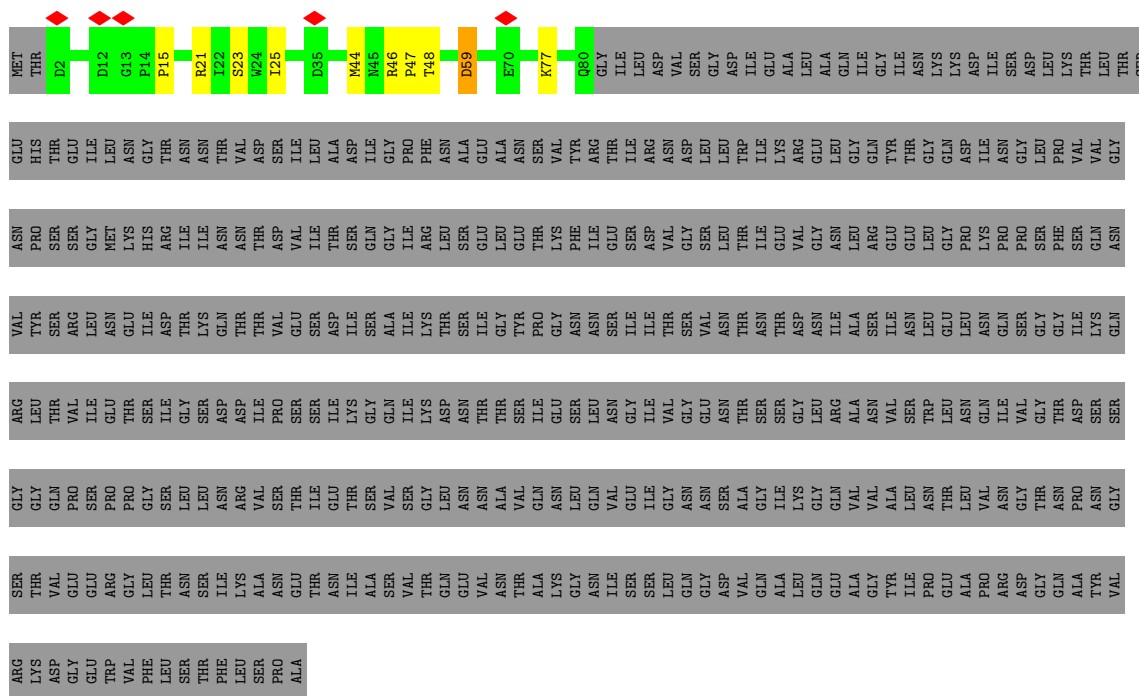
• Molecule 4: gpwac, fibrinin



• Molecule 4: gpwac, fibrinin

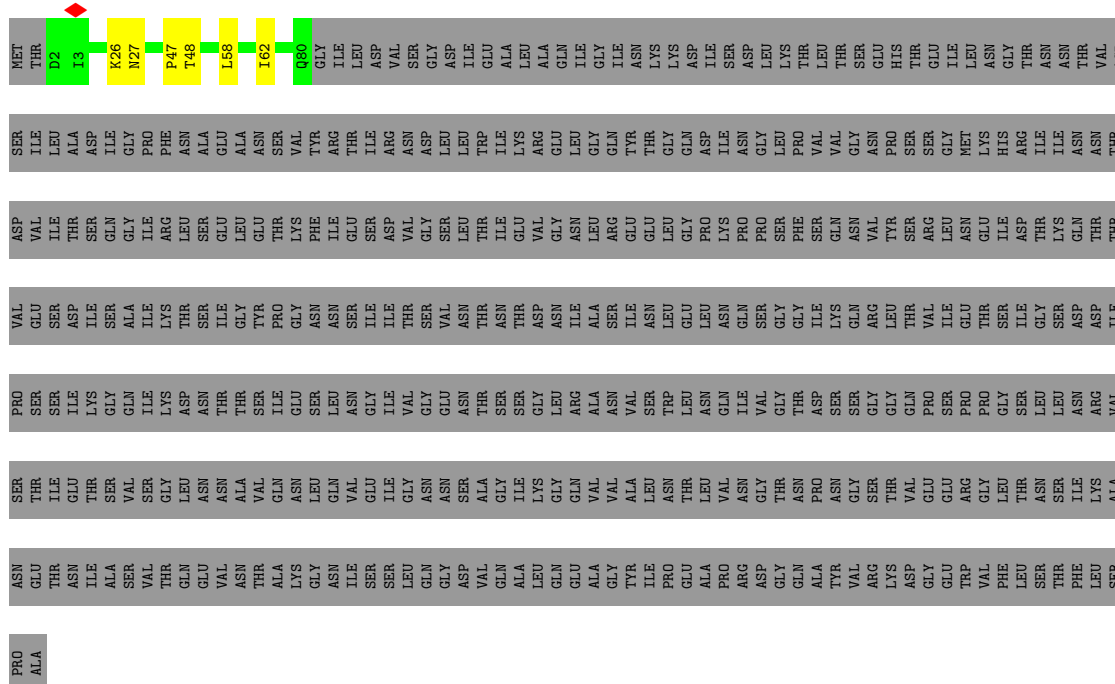






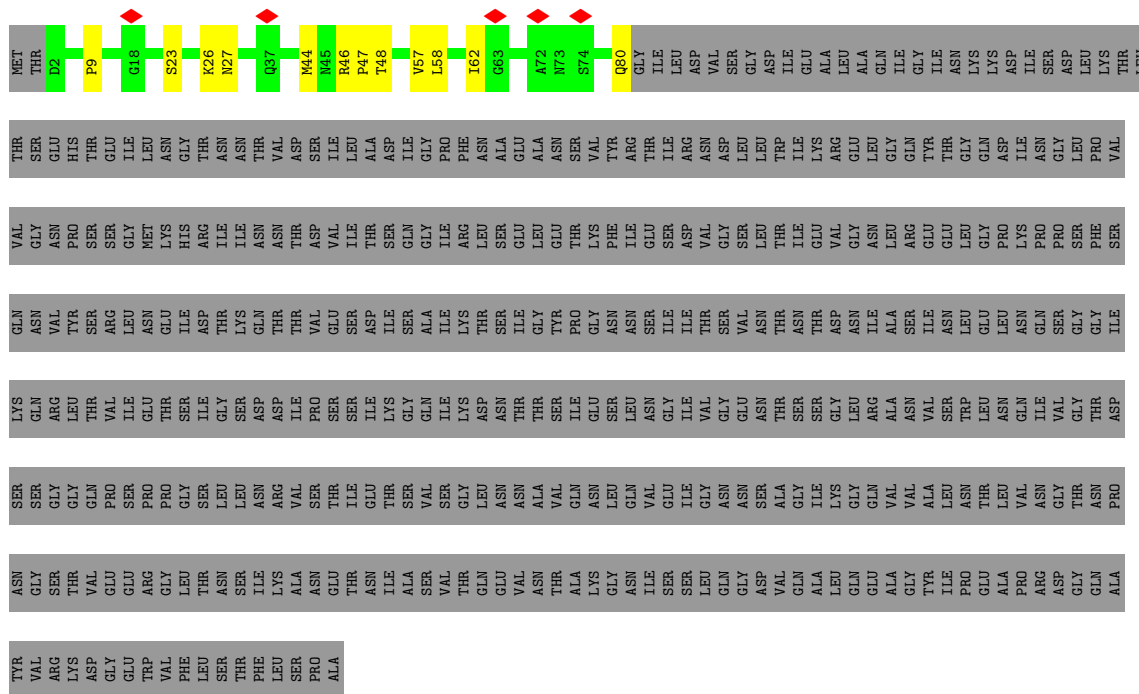
- Molecule 4: gpwac, fibrinin

Chain E:  15% . 84%

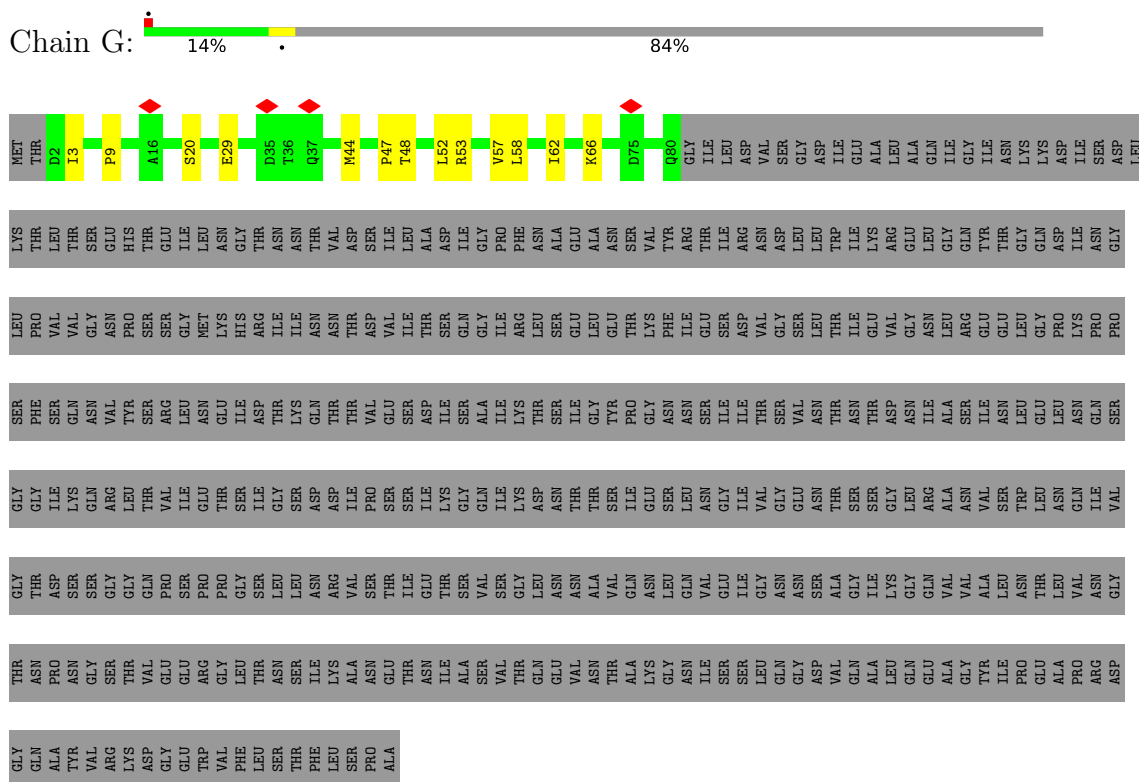


- Molecule 4: gpwac, fibrinin

Chain F:  14% 84%

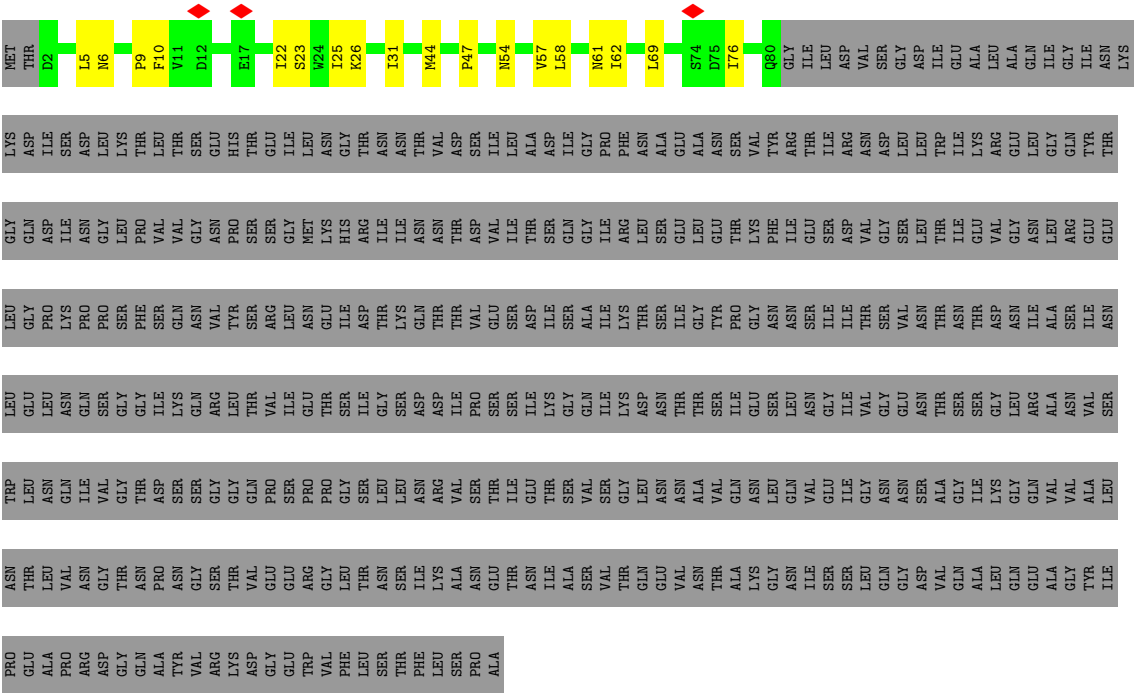


- Molecule 4: gpwac, fibrinin

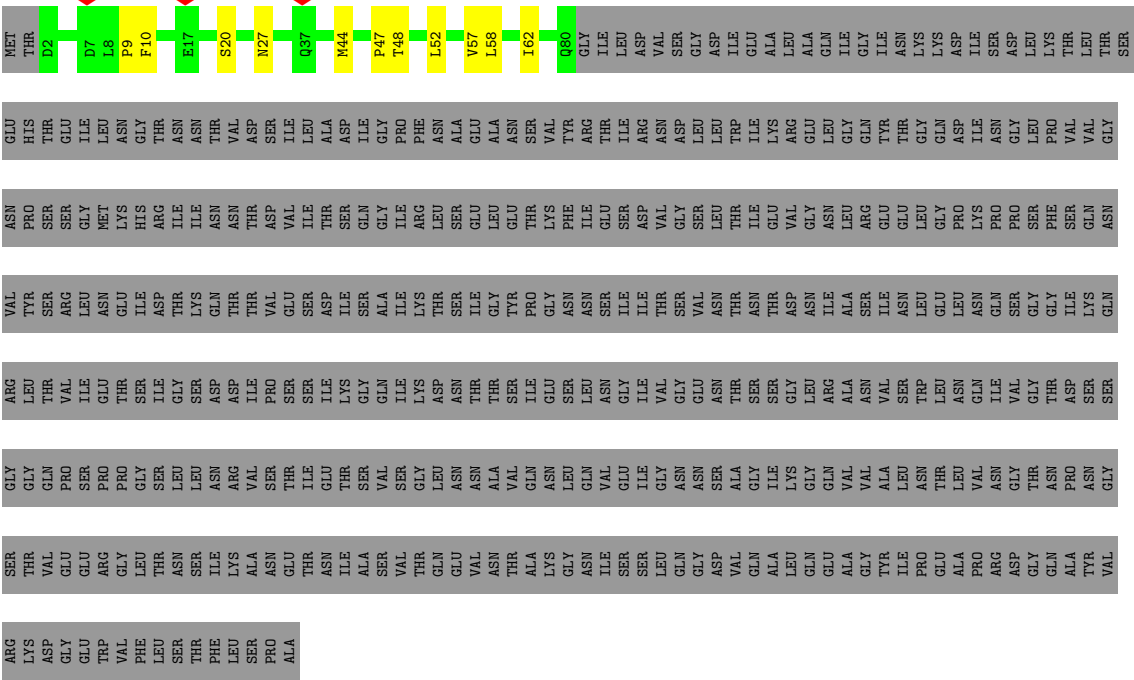


- Molecule 4: gpwac, fibrinin





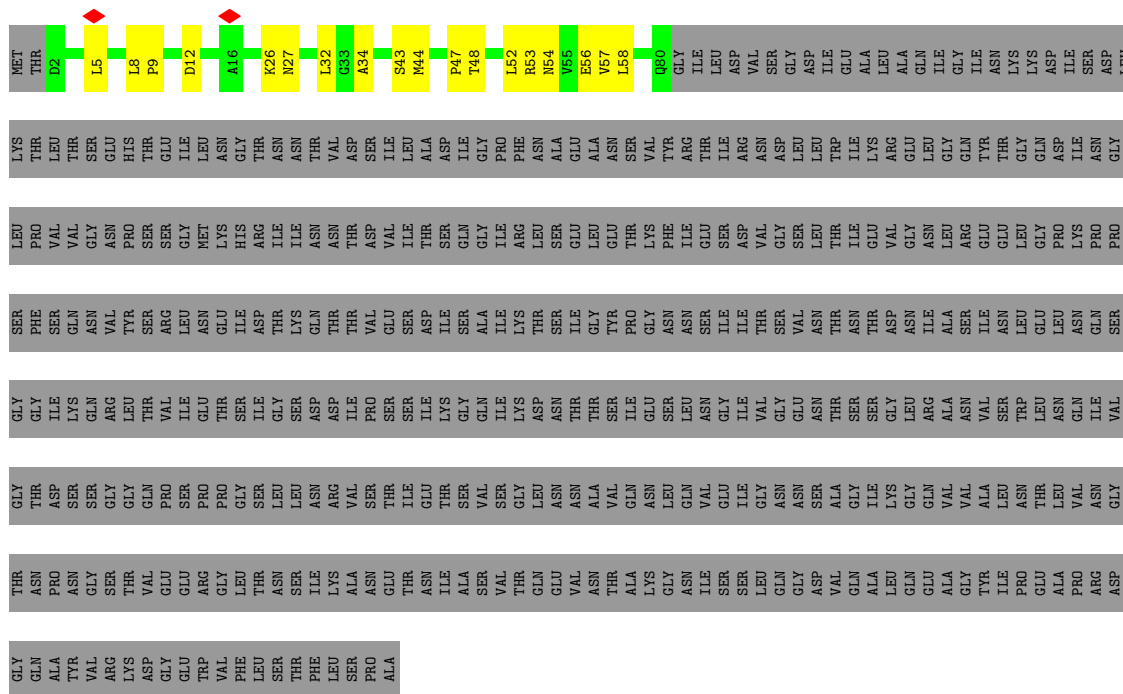
• Molecule 4: gpwac, fibritin



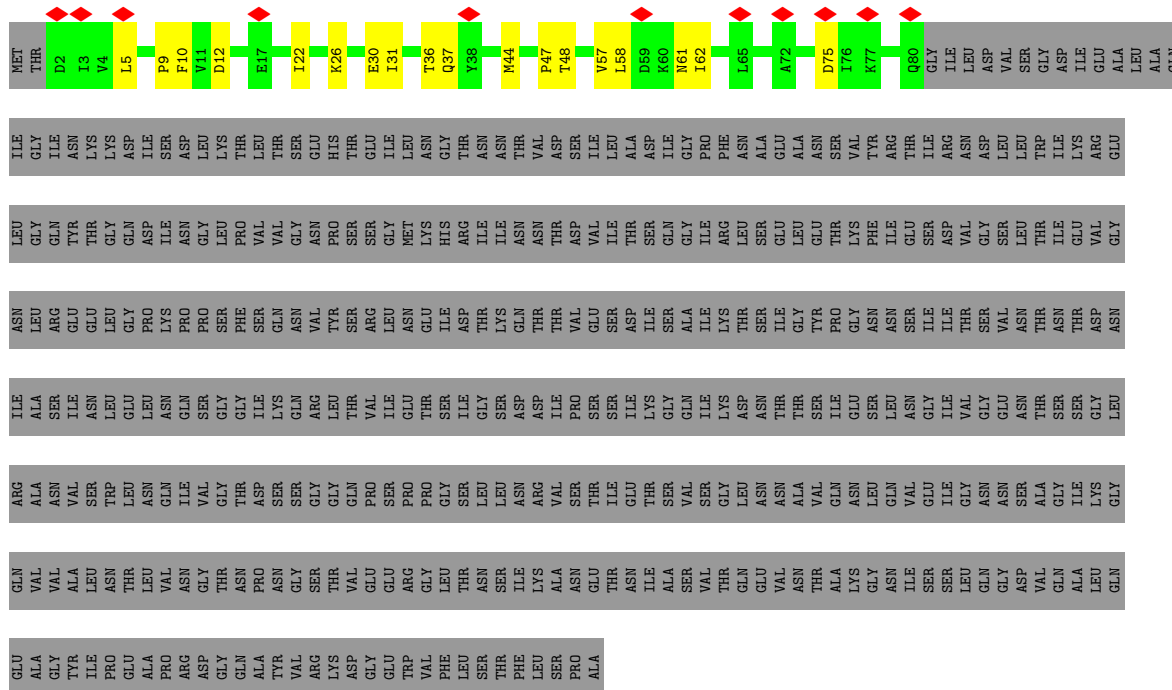
• Molecule 4: gpwac, fibritin





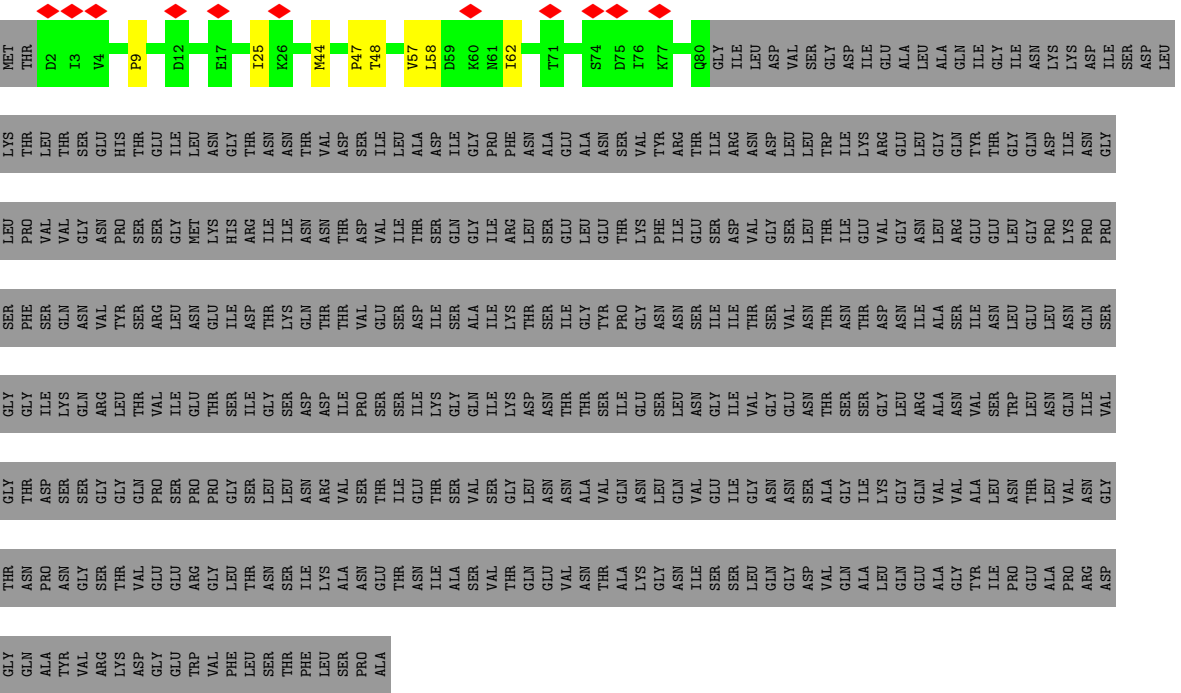


- Molecule 4: gpwac, fibrinin

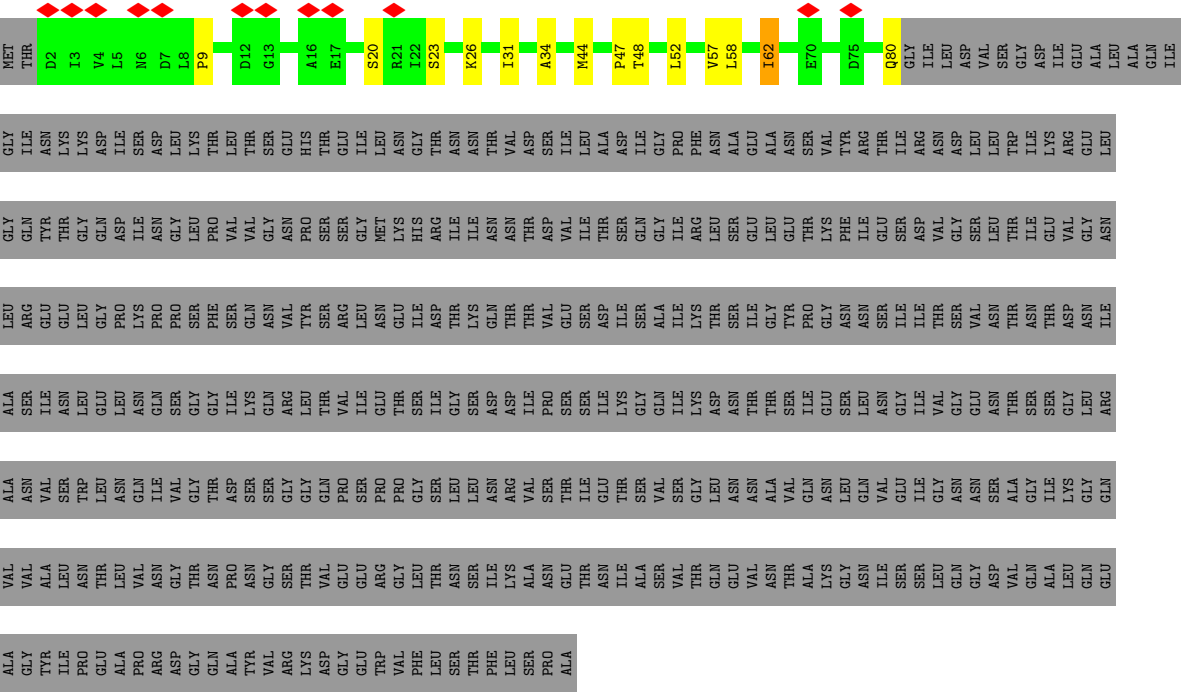


- Molecule 4: gpwac, fibrinin



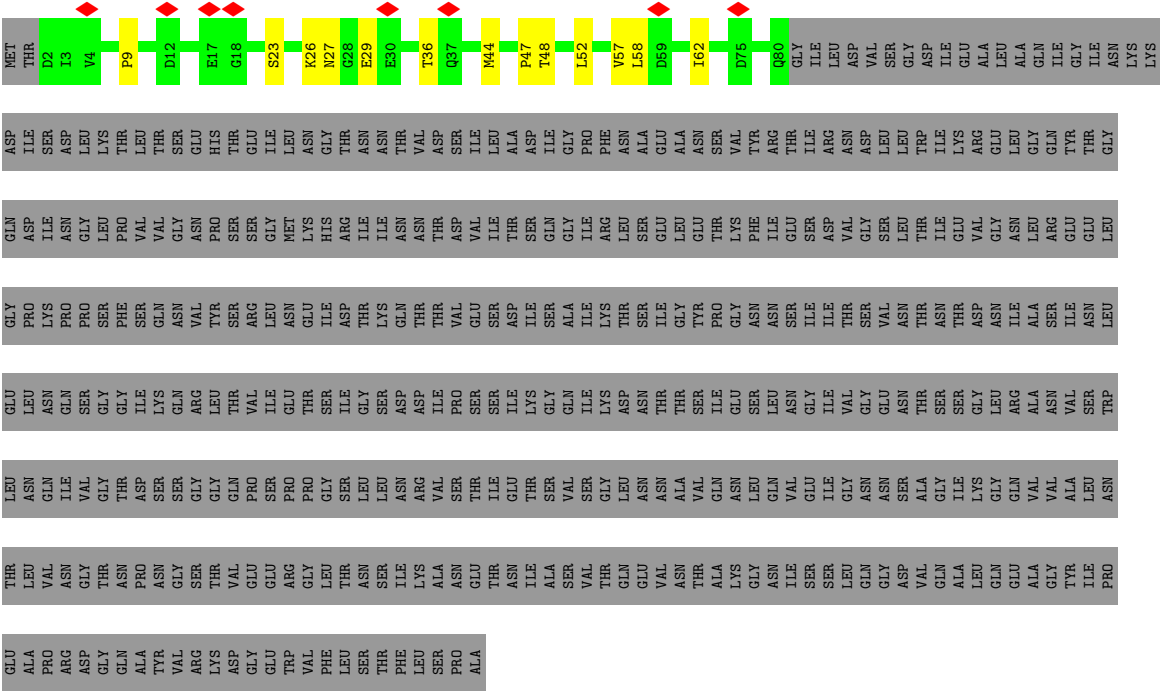


• Molecule 4: gpwac, fibrinin

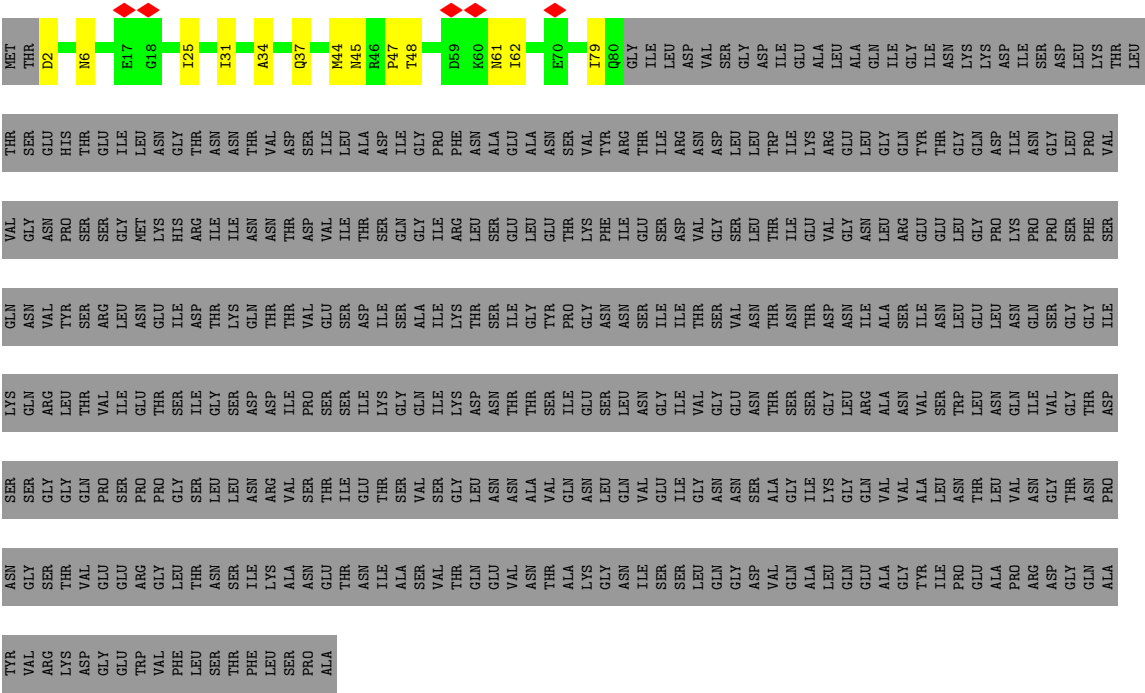


• Molecule 4: gpwac, fibrinin





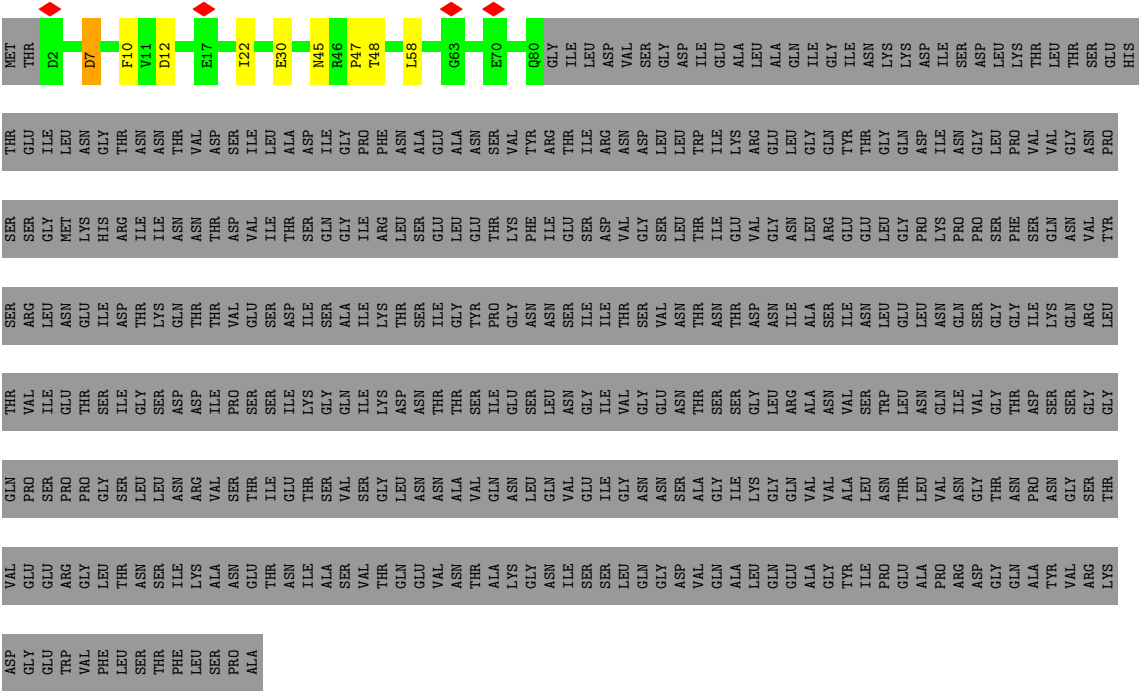
• Molecule 4: gpwac, fibritin



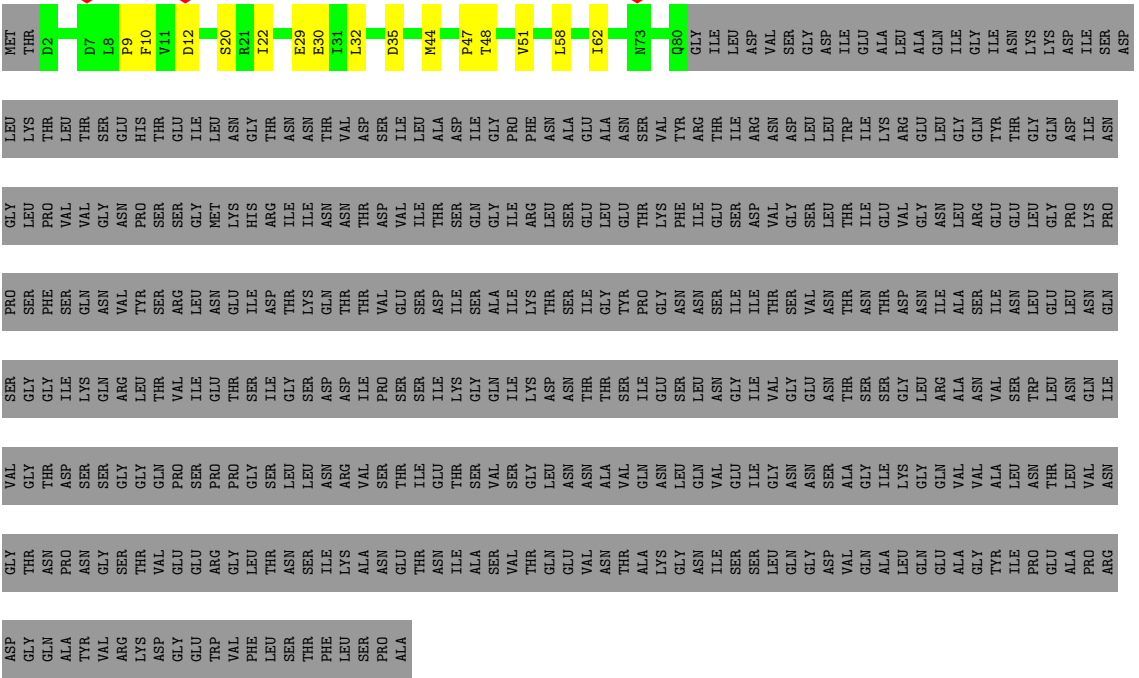
• Molecule 4: gpwac, fibritin







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• Molecule 4: gpwac, fibritin



- Molecule 4: gpwac, fibrinin

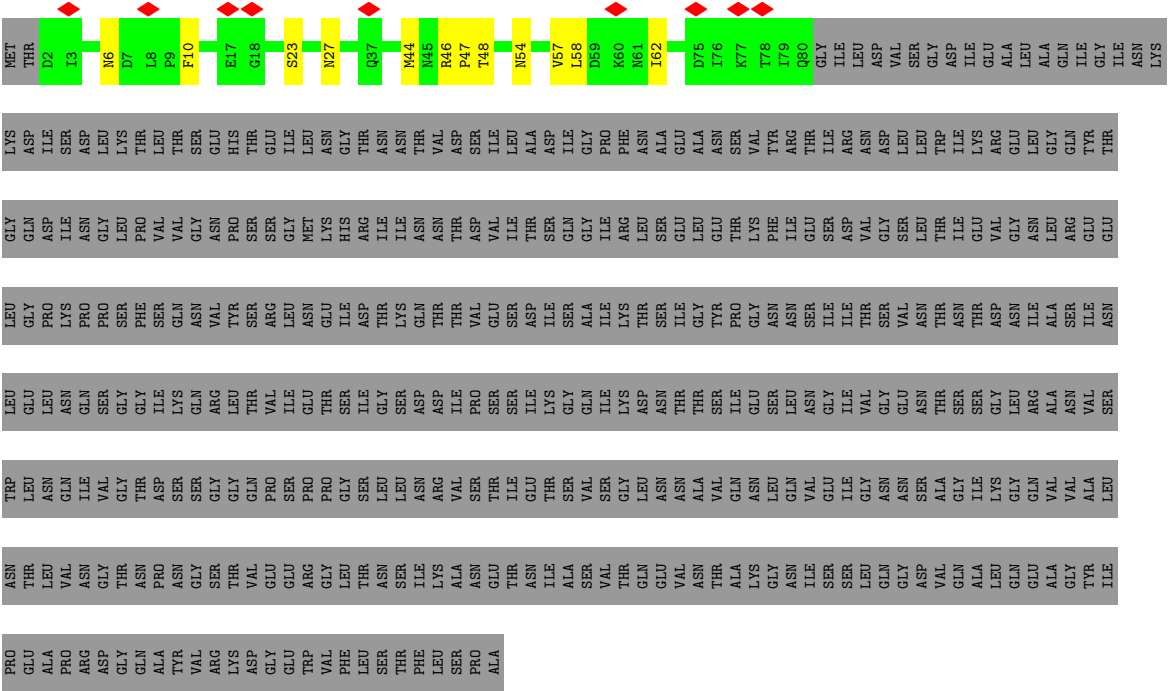


- Molecule 4: gpwac, fibrinin

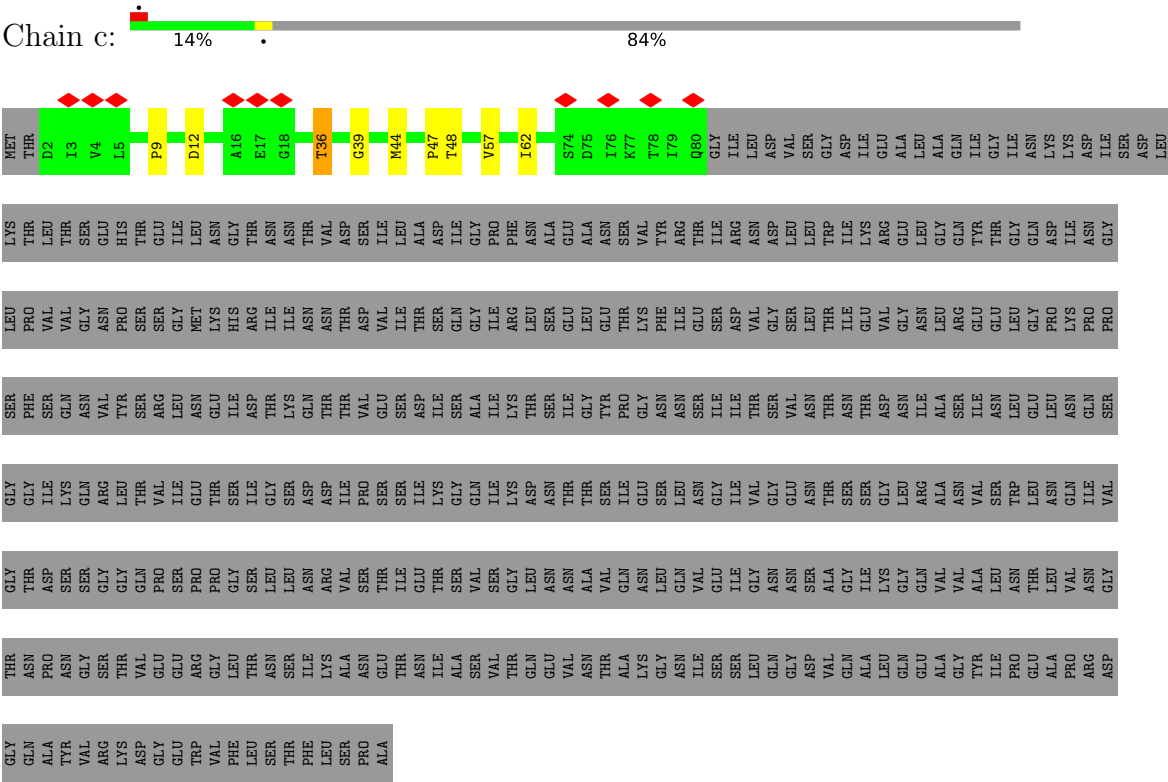






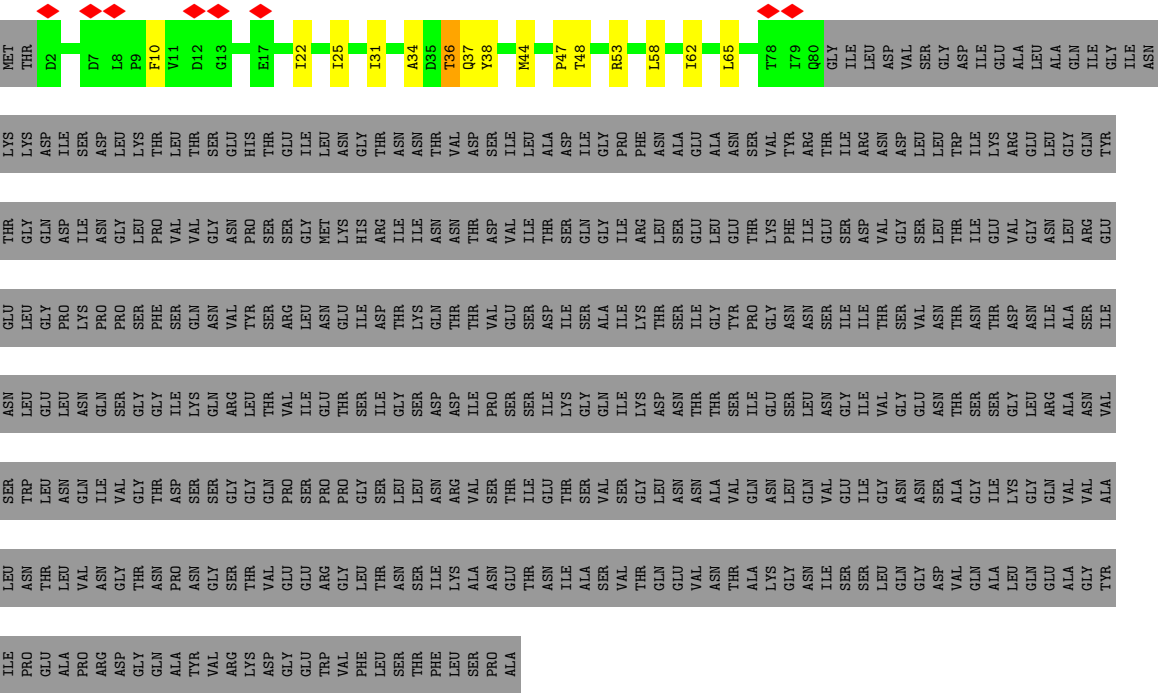


• Molecule 4: gpwac, fibrinin

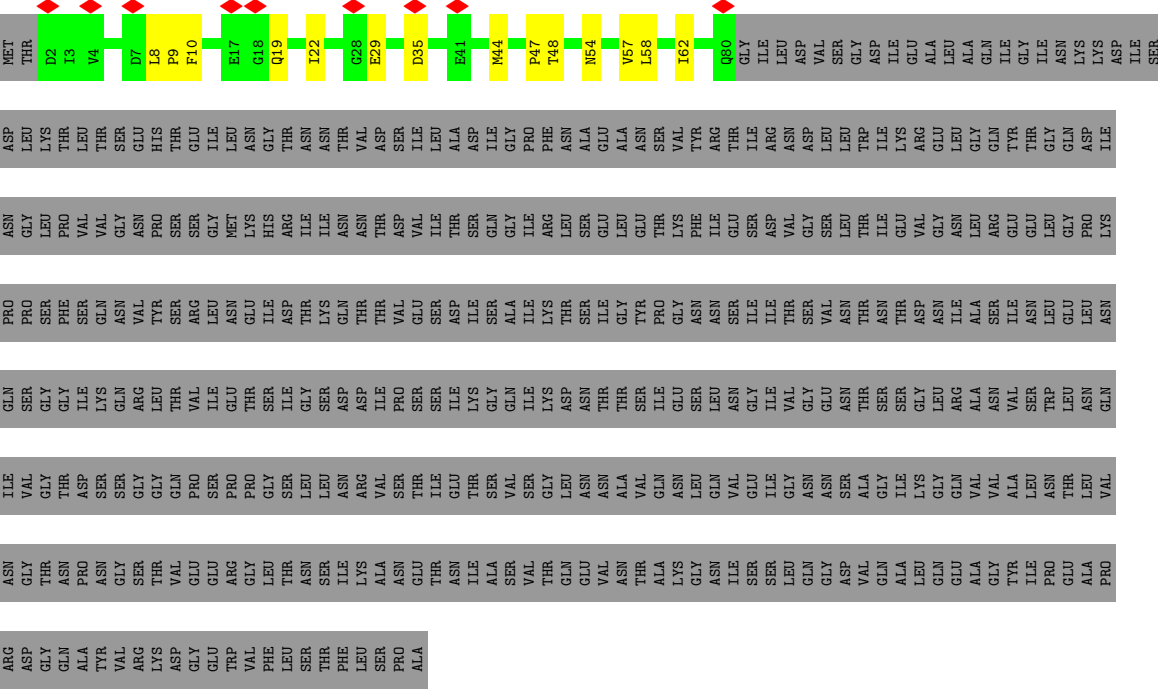


• Molecule 4: gpwac, fibrinin





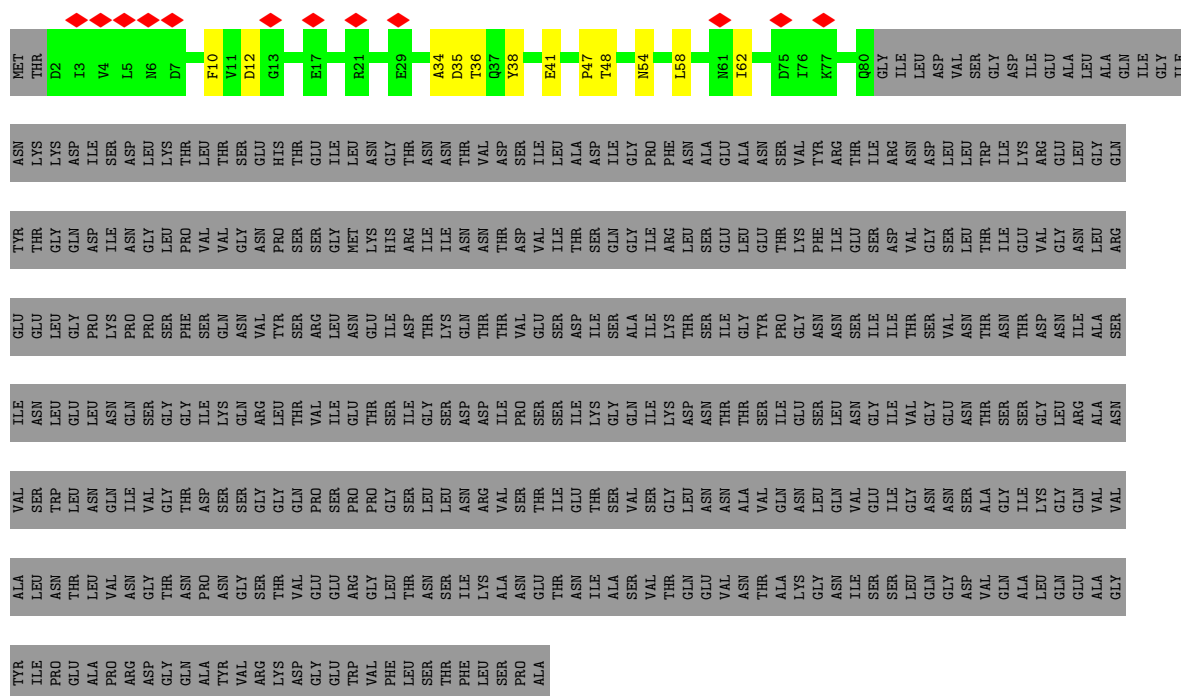
• Molecule 4: gpwac, fibrinin



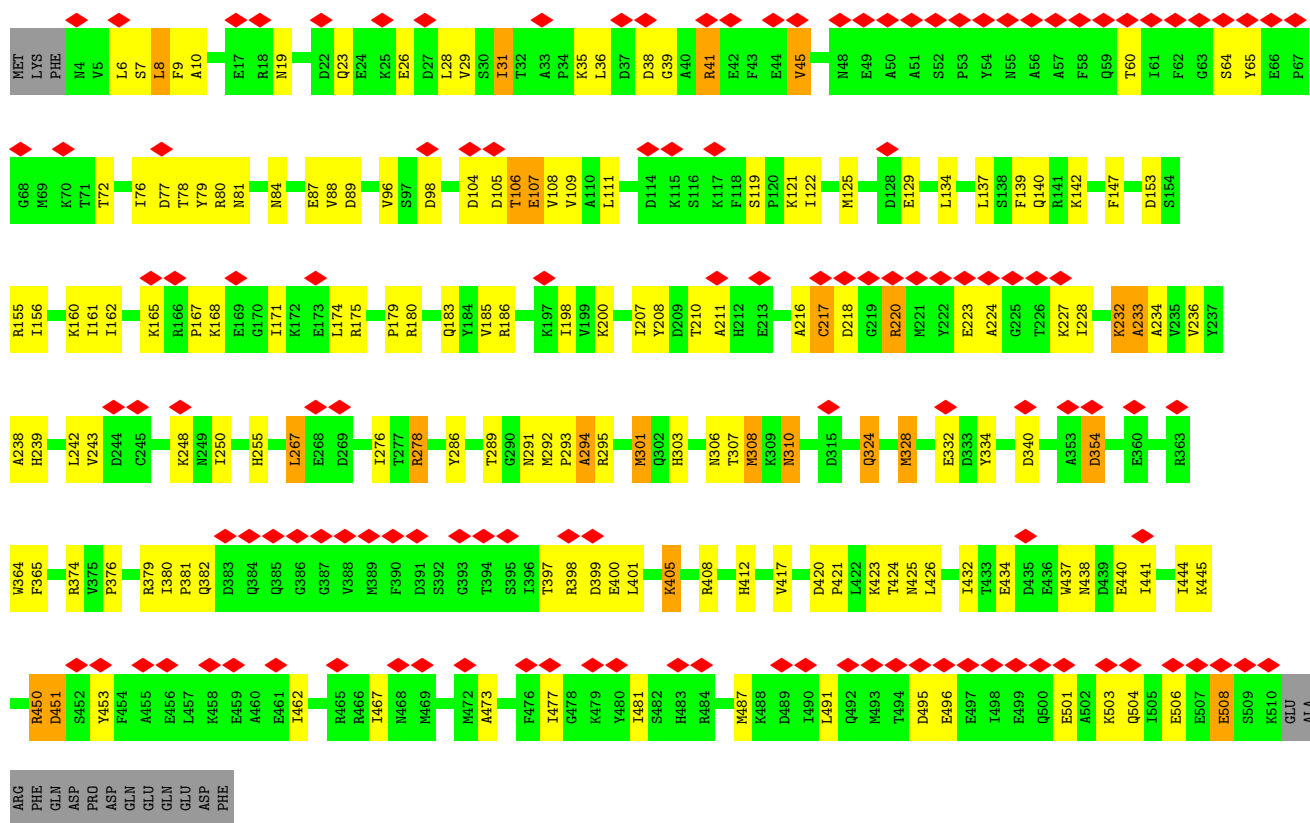
• Molecule 4: gpwac, fibrinin



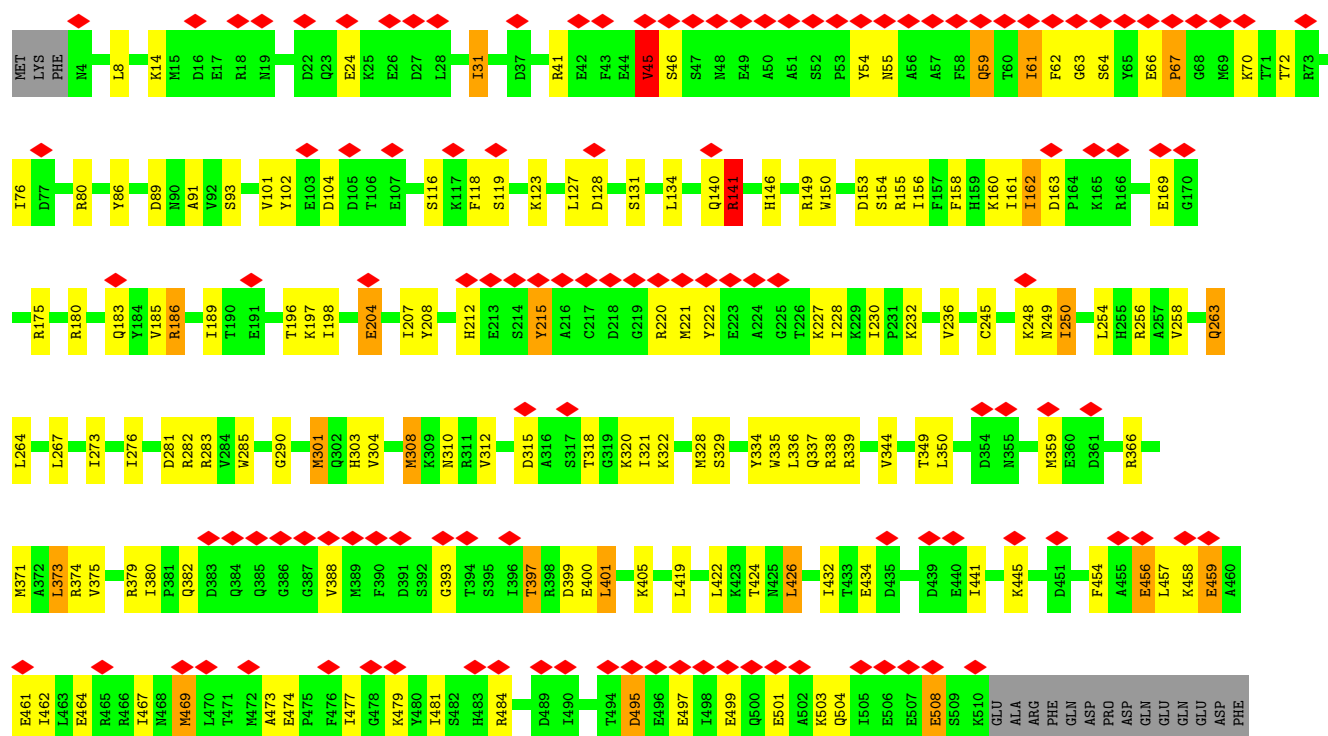




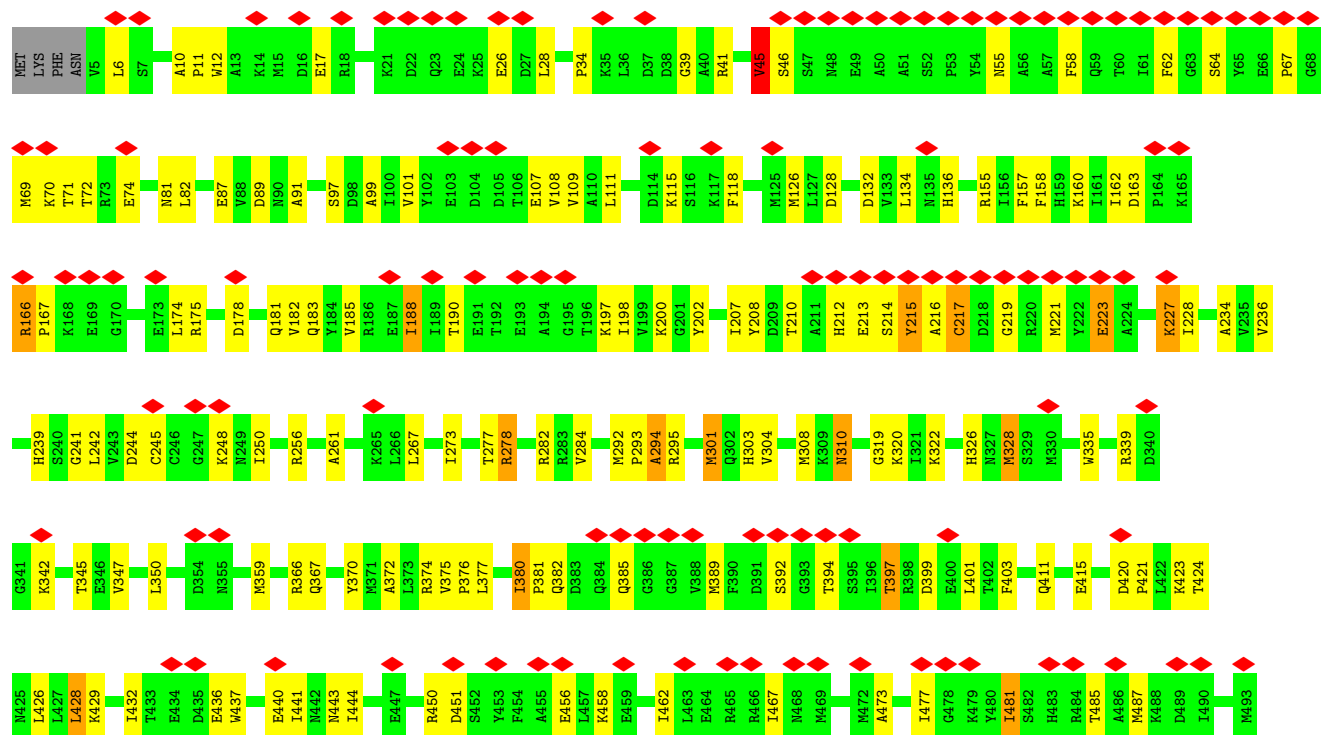
• Molecule 5: gp20, portal protein

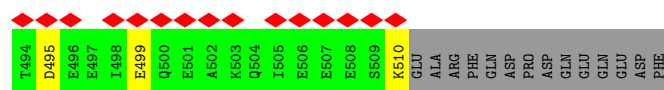


• Molecule 5: gp20, portal protein

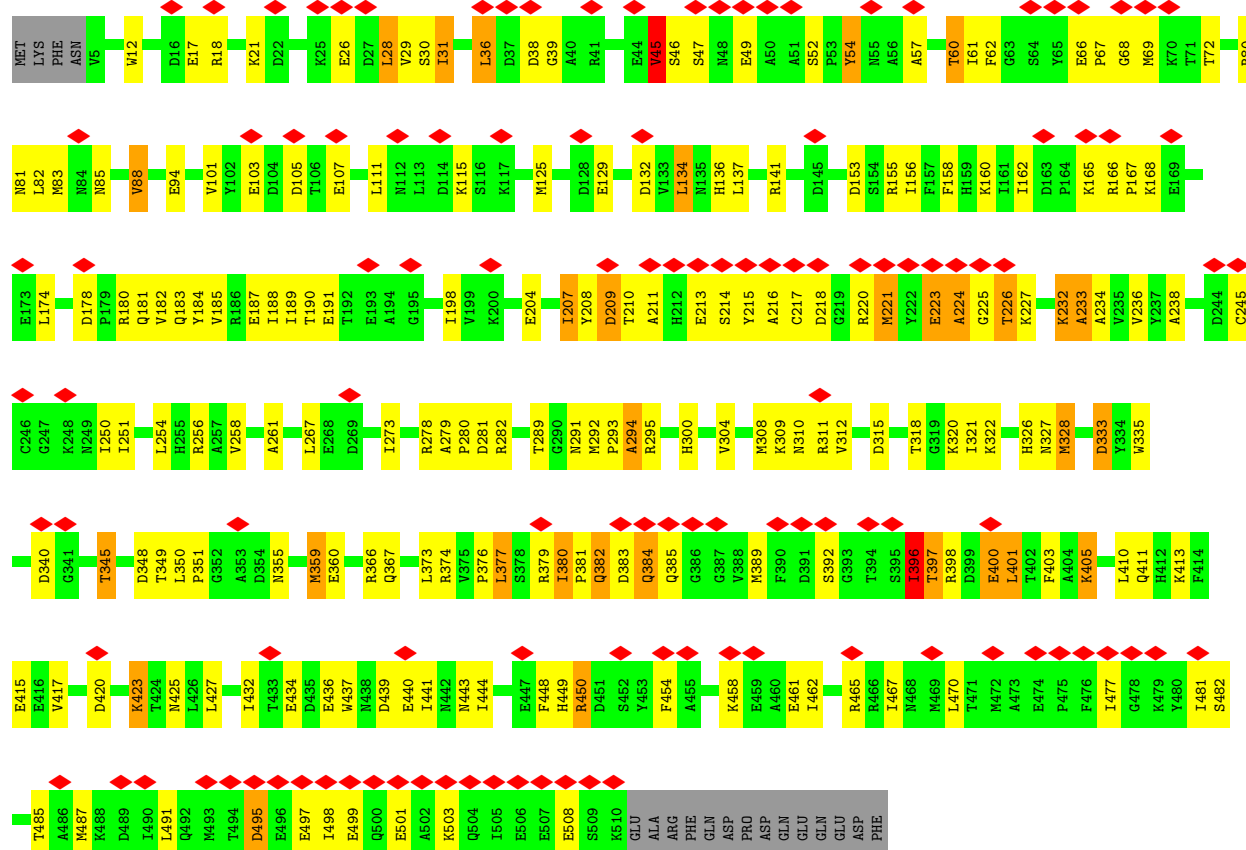


• Molecule 5: gp20, portal protein

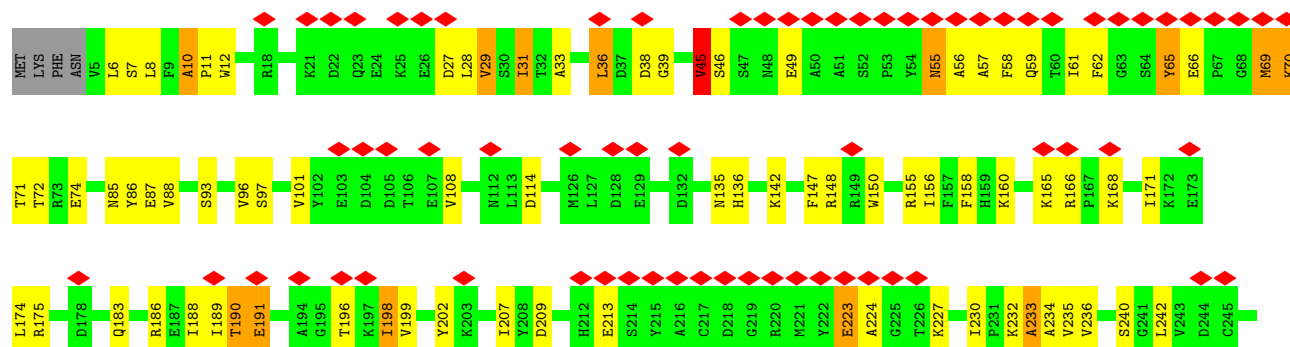


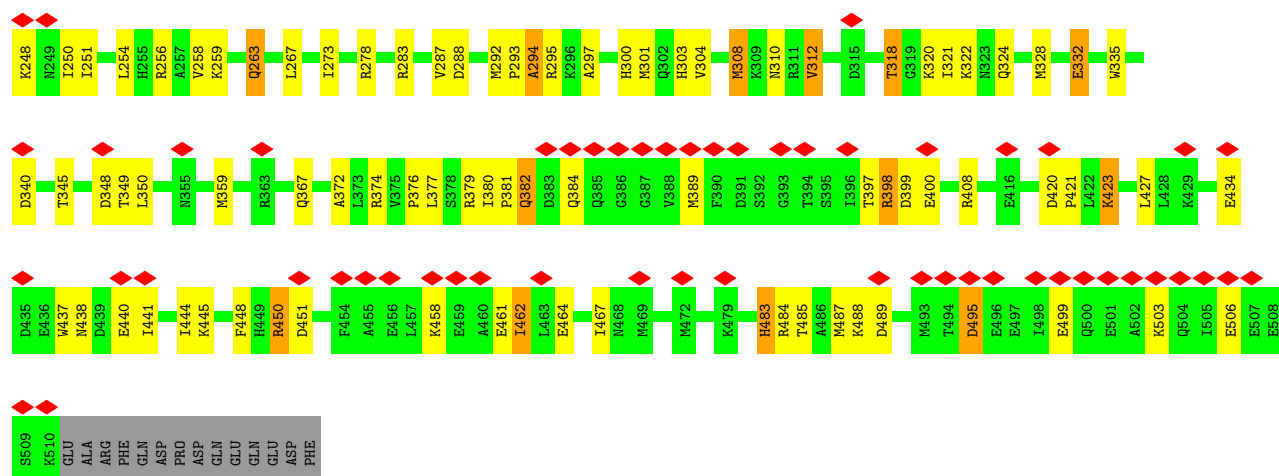


• Molecule 5: gp20, portal protein

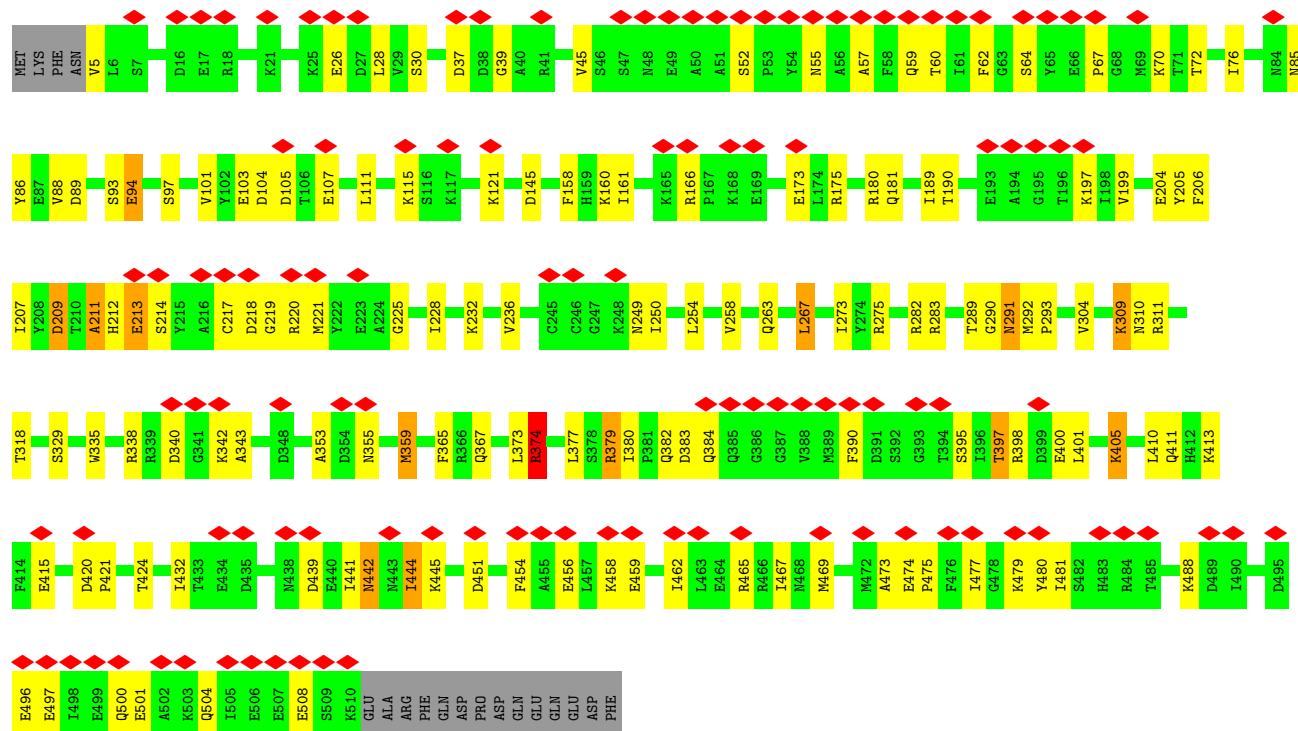
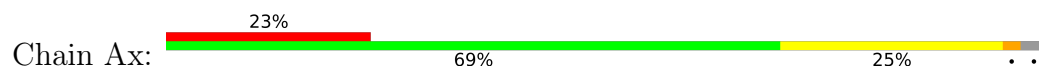


• Molecule 5: gp20, portal protein

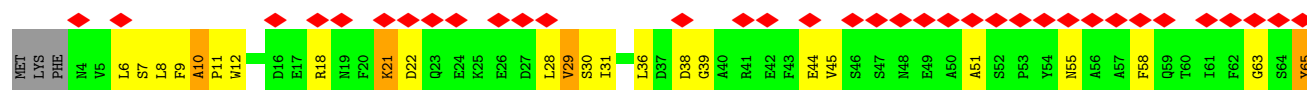


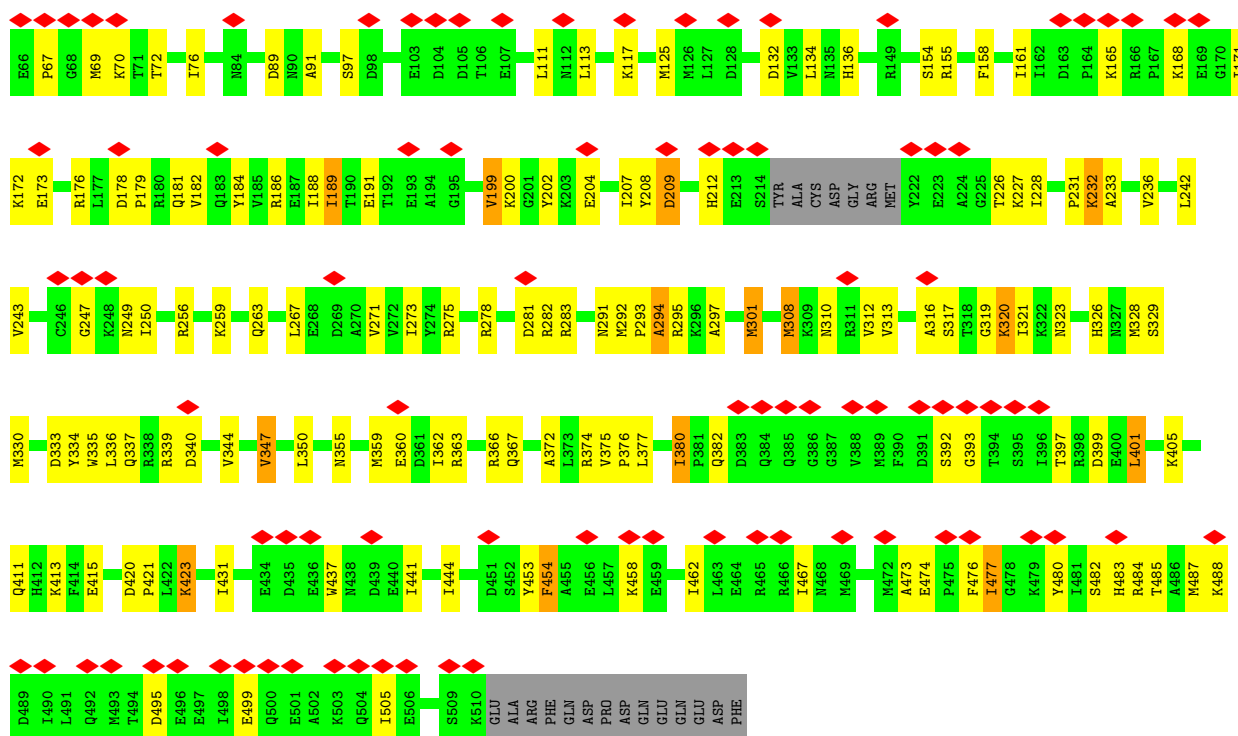


• Molecule 5: gp20, portal protein

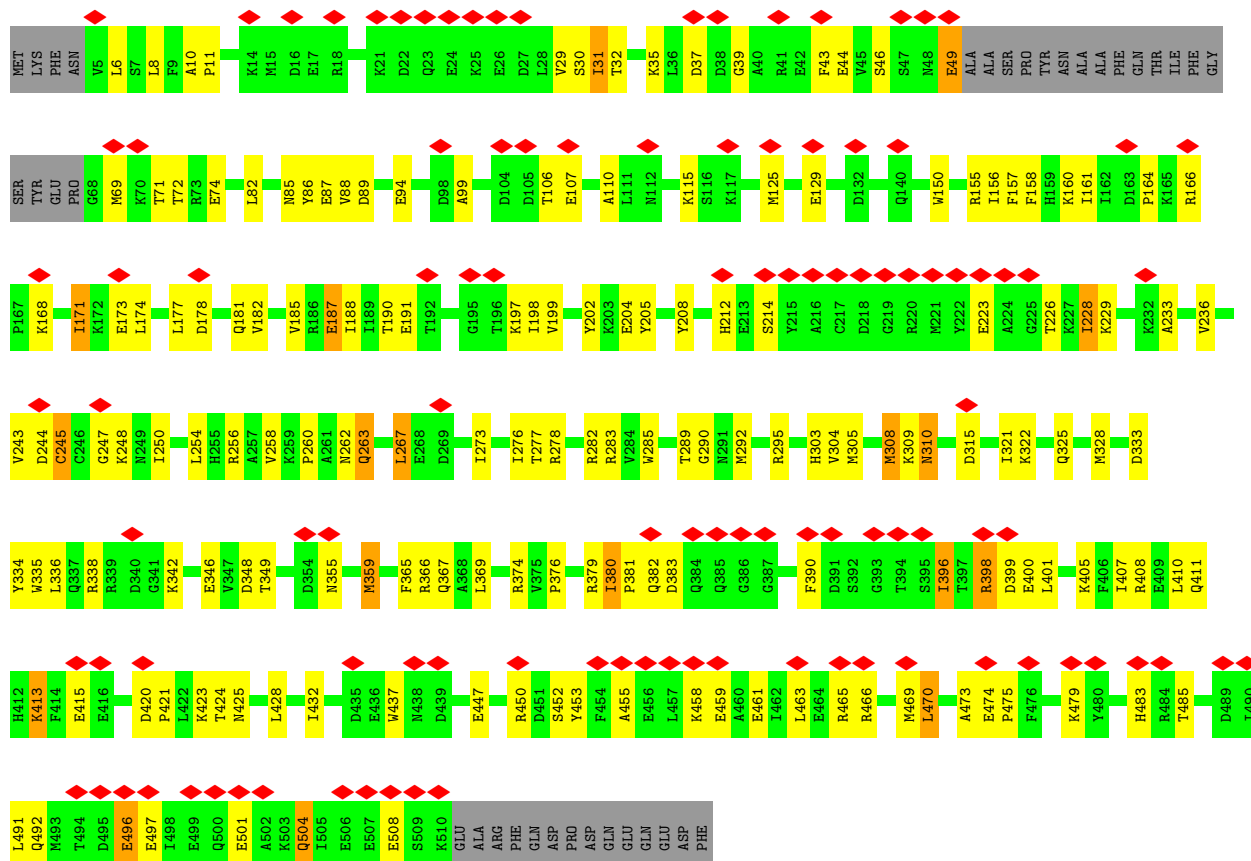


• Molecule 5: gp20, portal protein

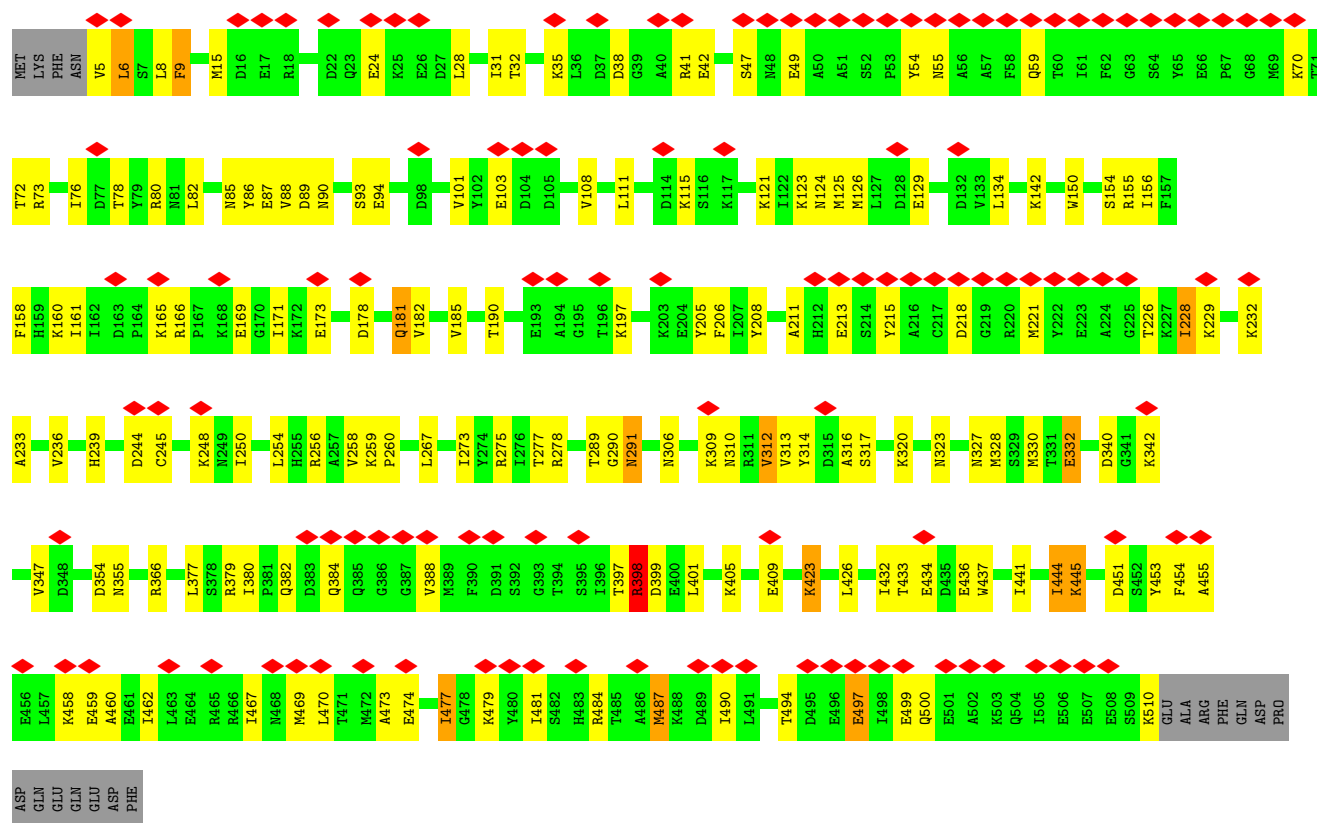




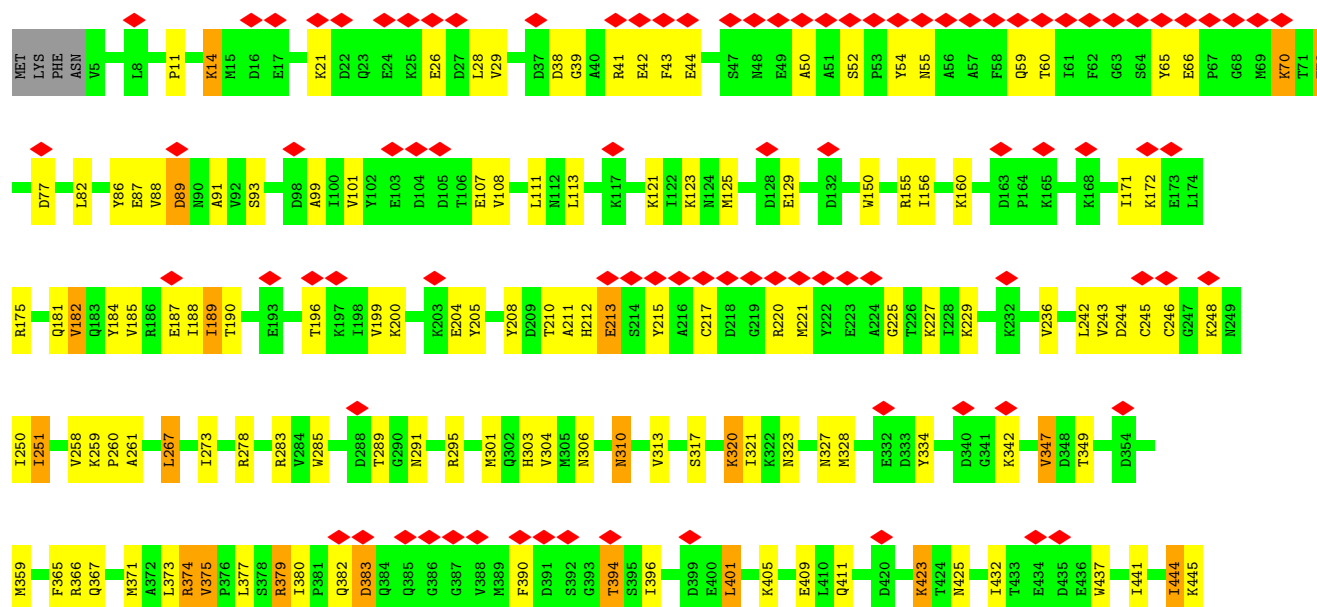
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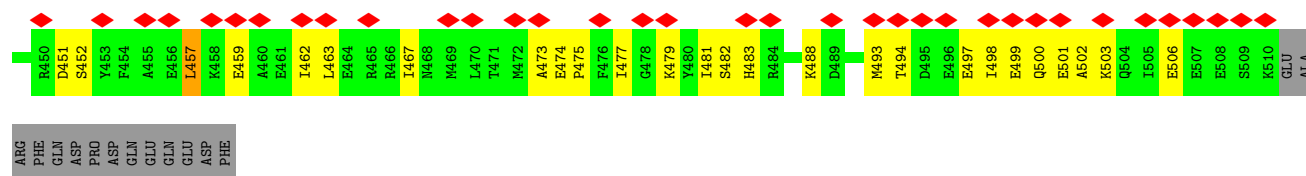


- Molecule 5: gp20, portal protein

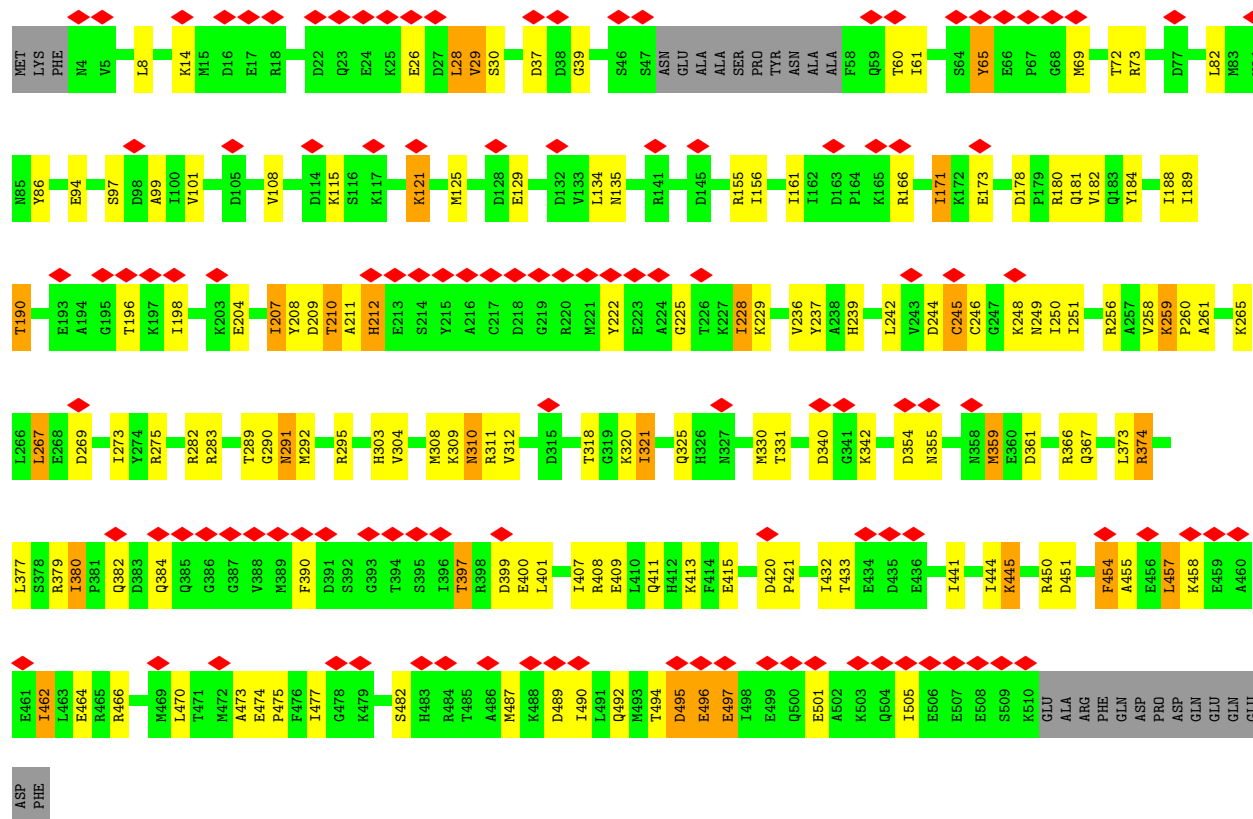


- Molecule 5: gp20, portal protein

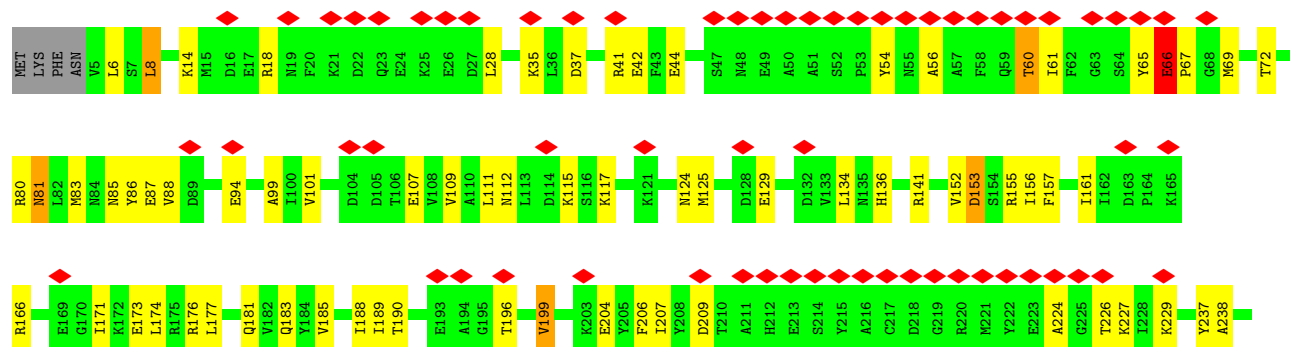


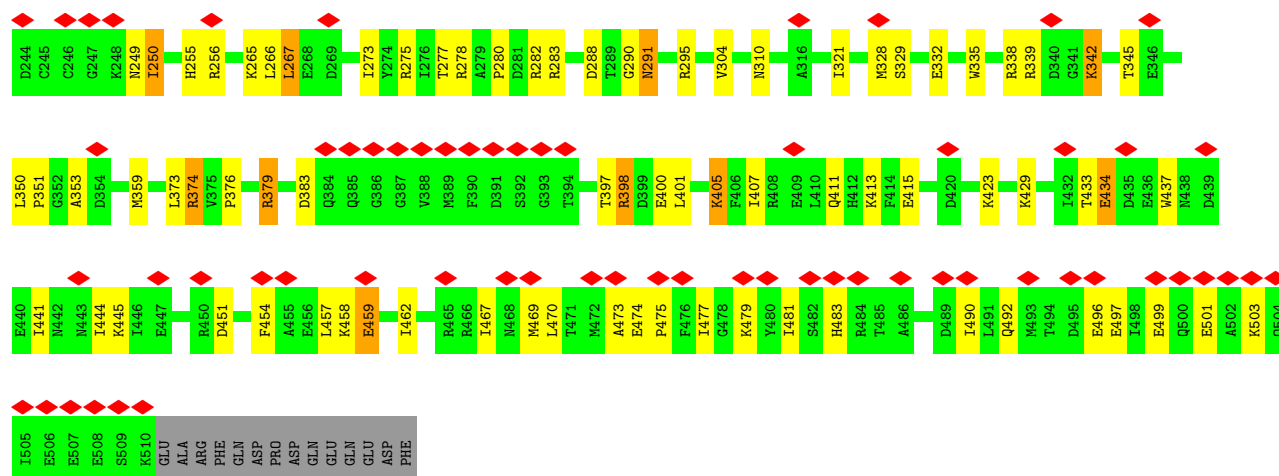


- Molecule 5: gp20, portal protein

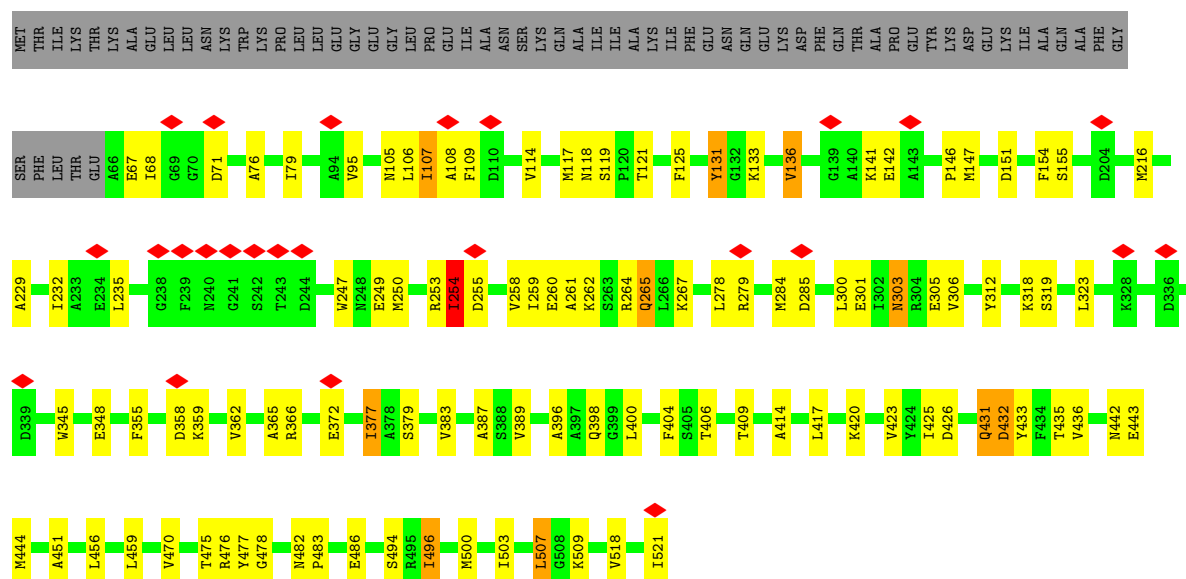


- Molecule 5: gp20, portal protein

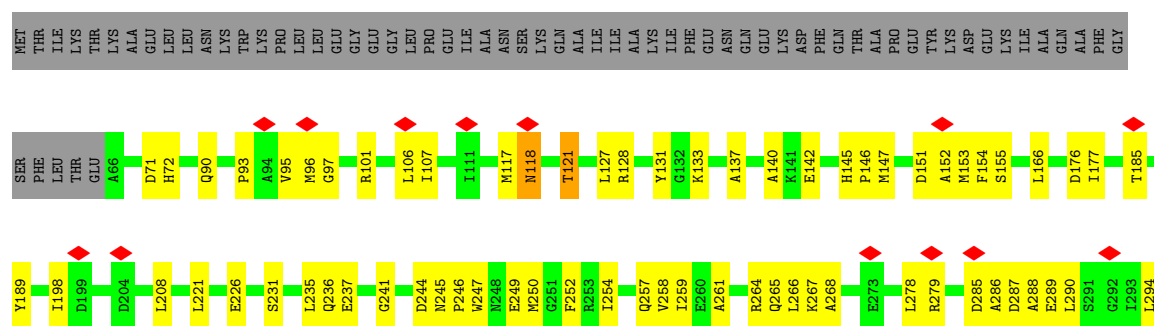


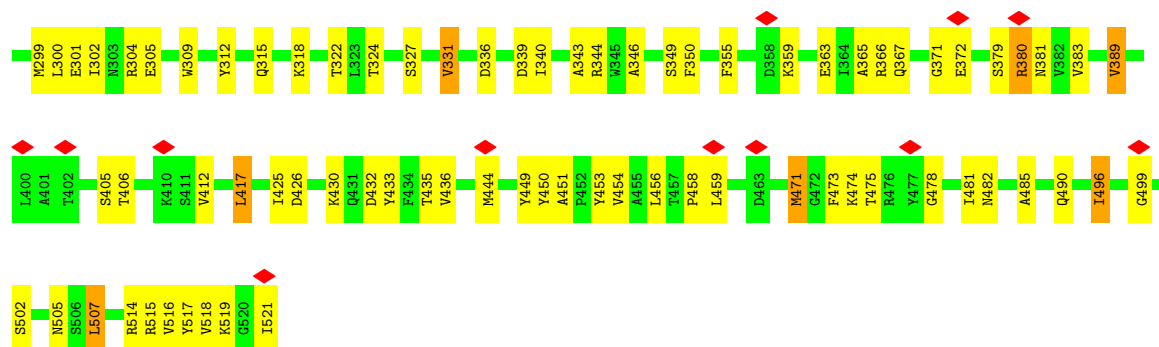


- Molecule 6: gp23, major capsid protein



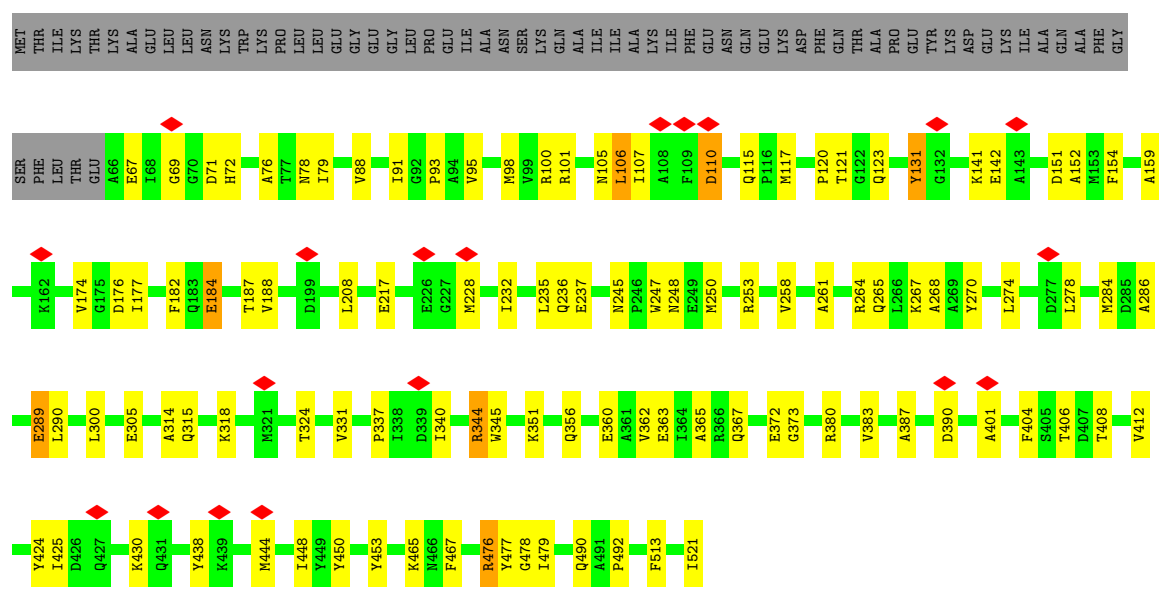
- Molecule 6: gp23, major capsid protein





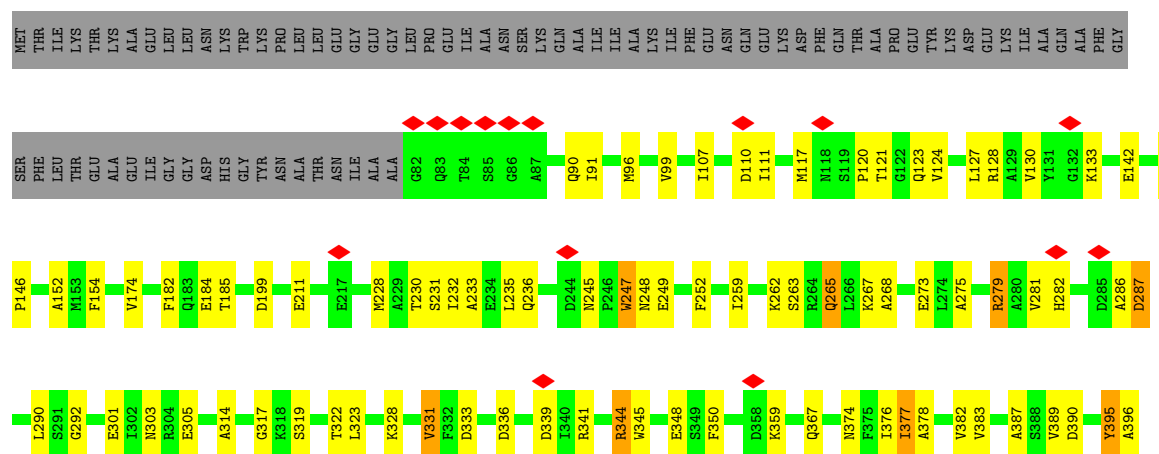
- Molecule 6: gp23, major capsid protein

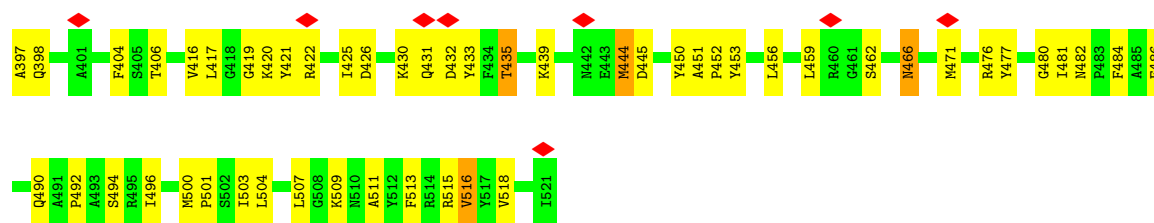
Chain A7: 67% 20% 12%



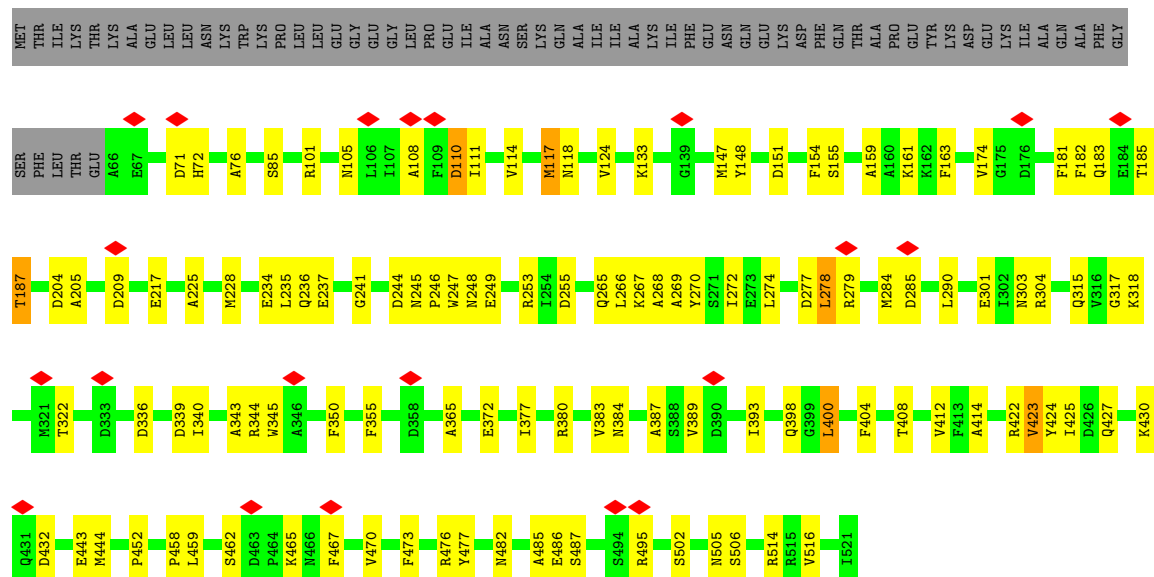
- Molecule 6: gp23, major capsid protein

Chain A8: 58% 24% 16%

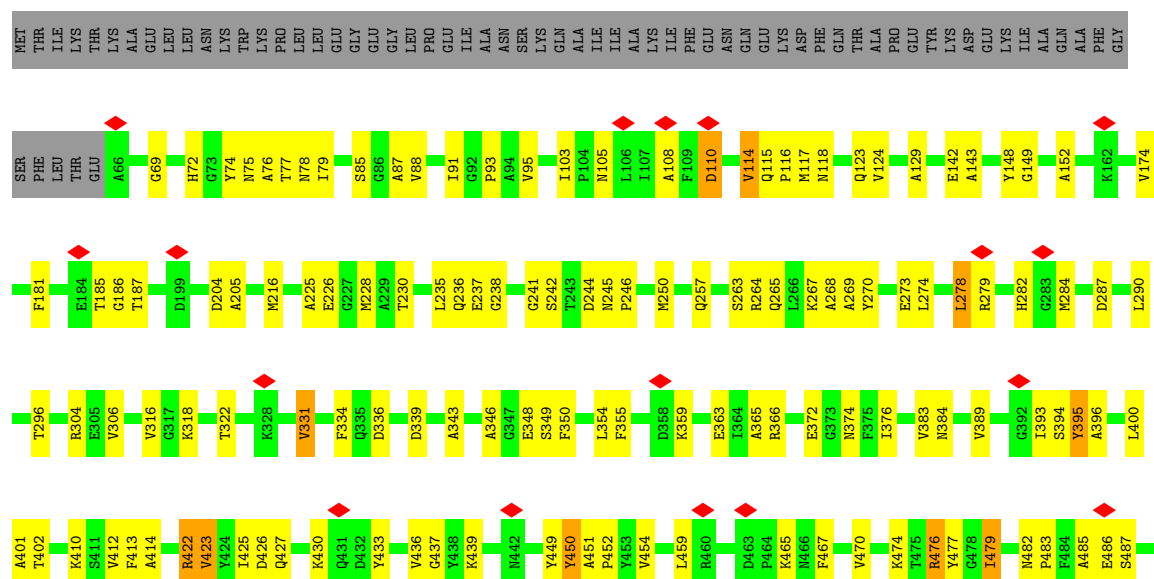




- Molecule 6: gp23, major capsid protein

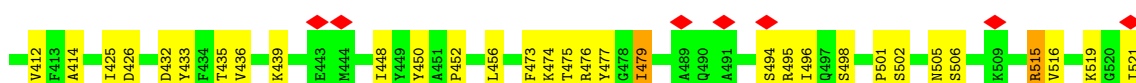
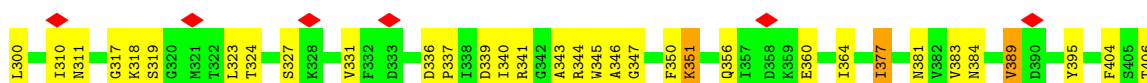
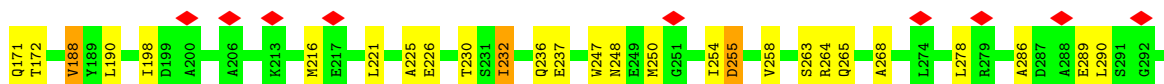
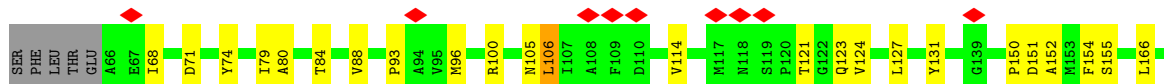
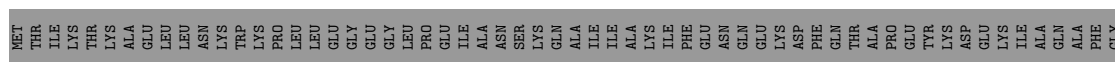


- Molecule 6: gp23, major capsid protein

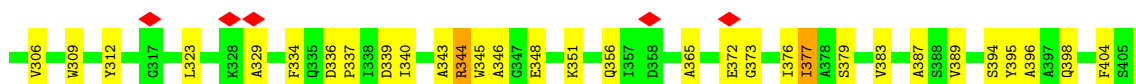
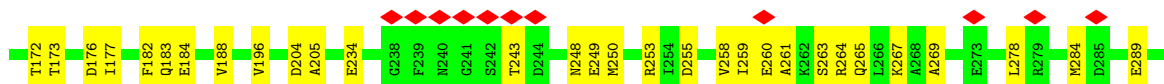
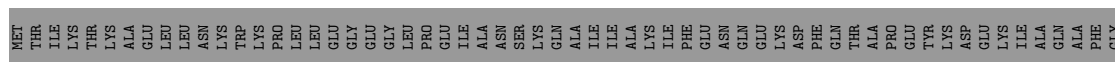




- Molecule 6: gp23, major capsid protein

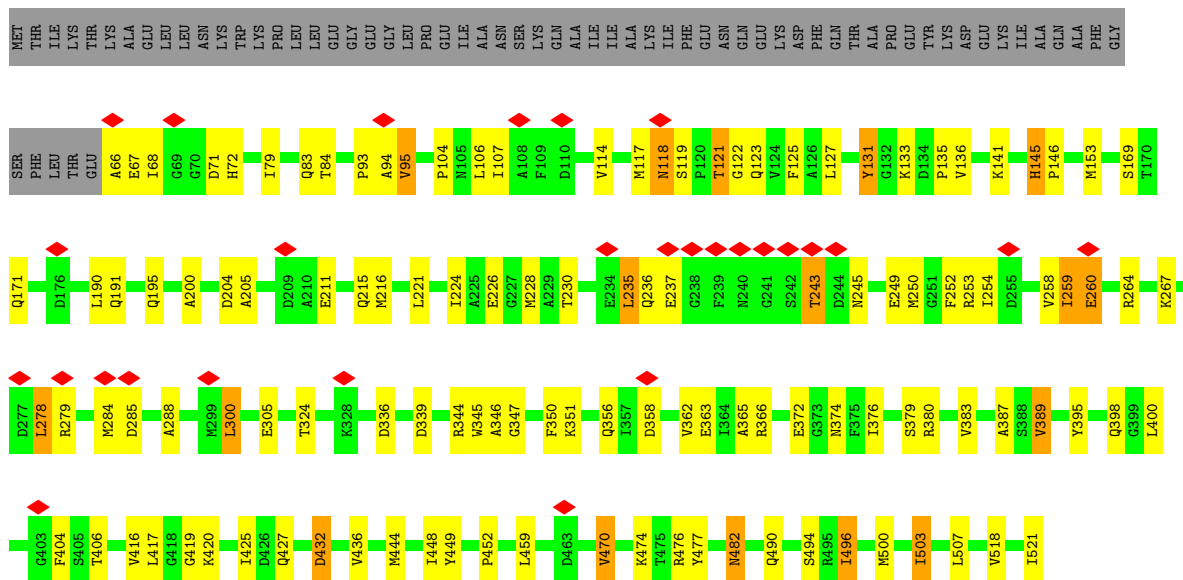


- Molecule 6: gp23, major capsid protein

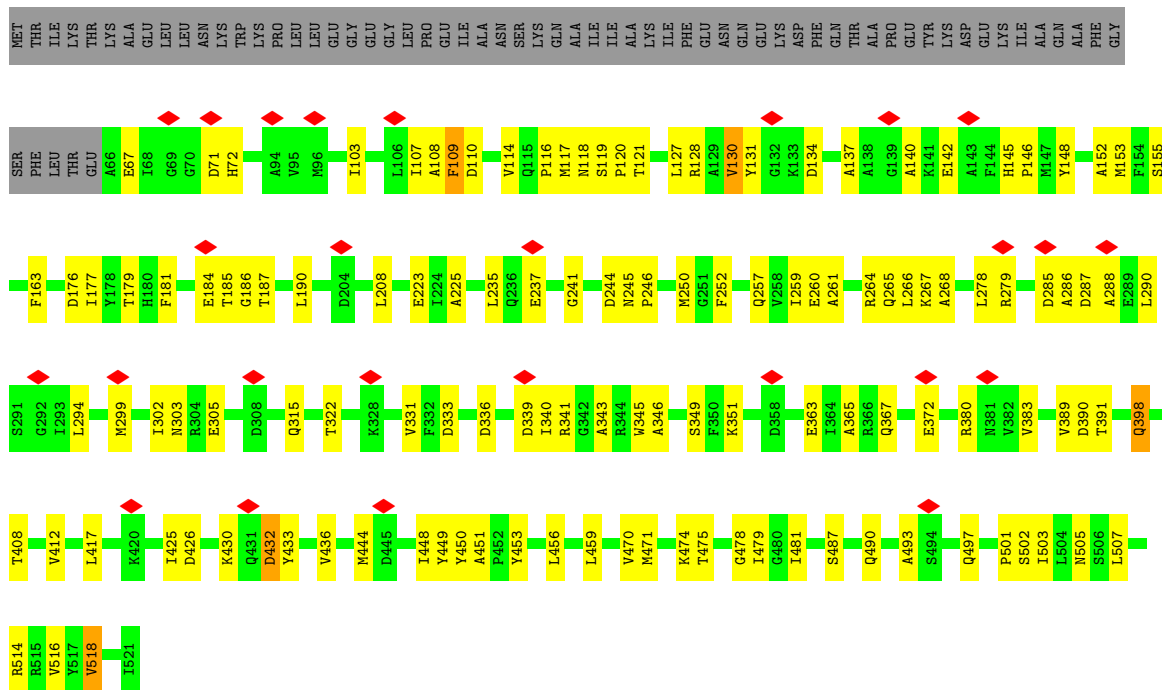


- Molecule 6: gp23, major capsid protein

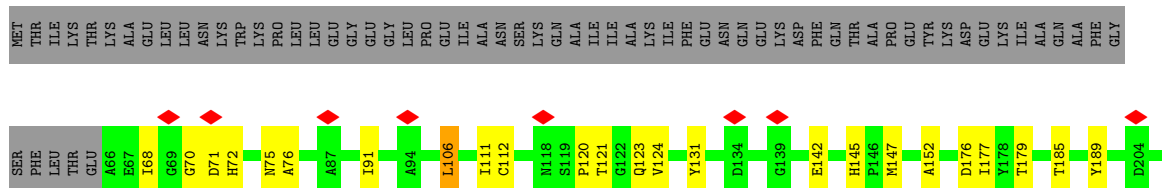


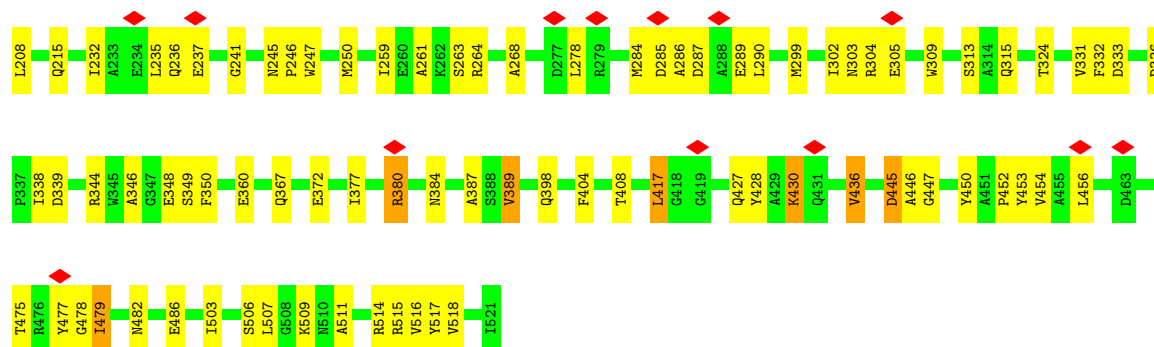


• Molecule 6: gp23, major capsid protein

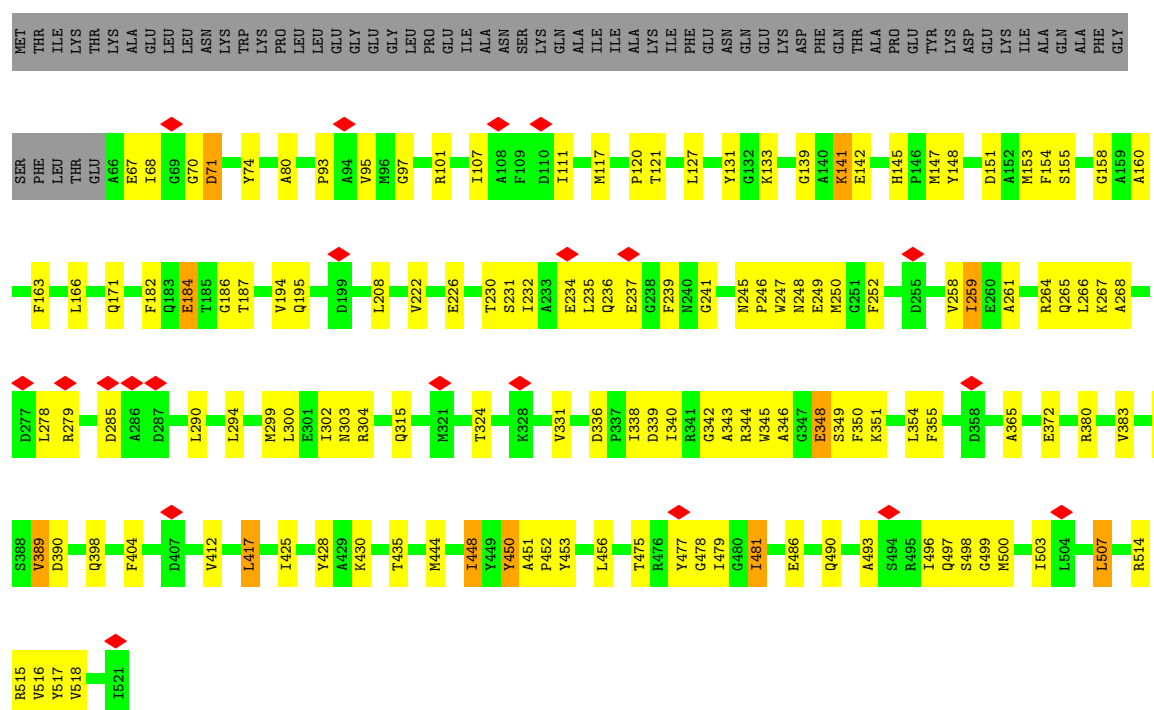


• Molecule 6: gp23, major capsid protein

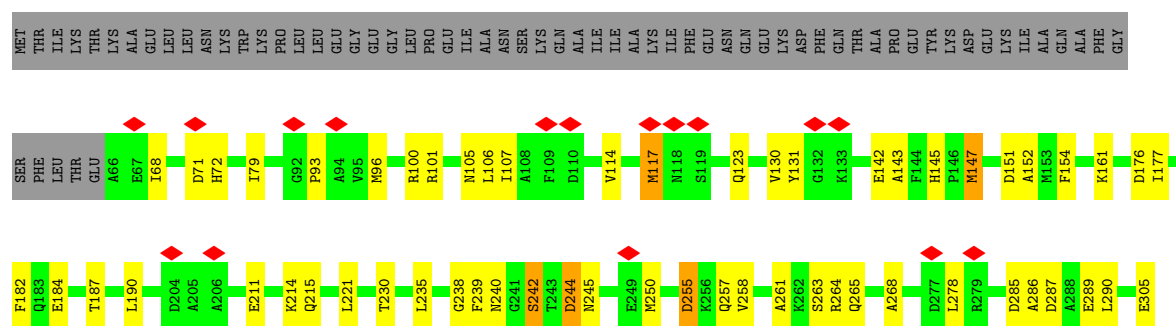


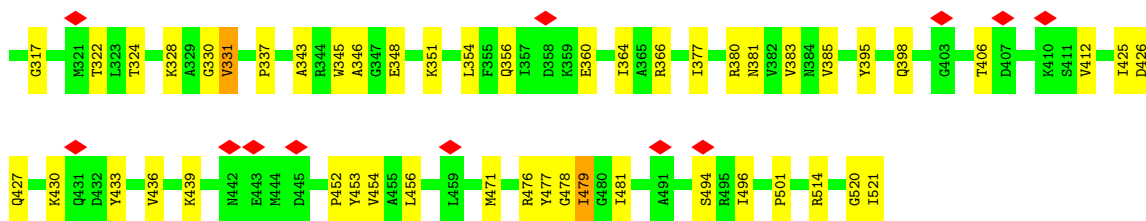


- Molecule 6: gp23, major capsid protein



- Molecule 6: gp23, major capsid protein

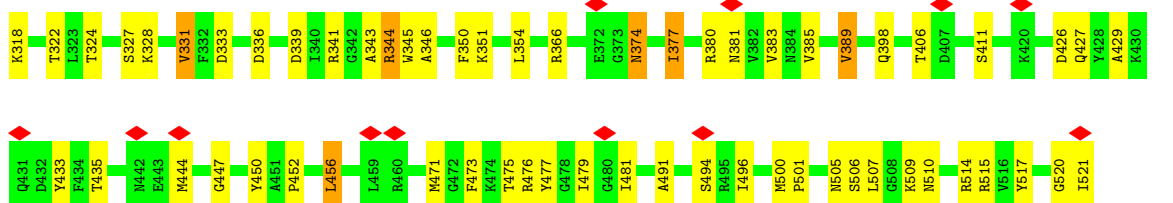
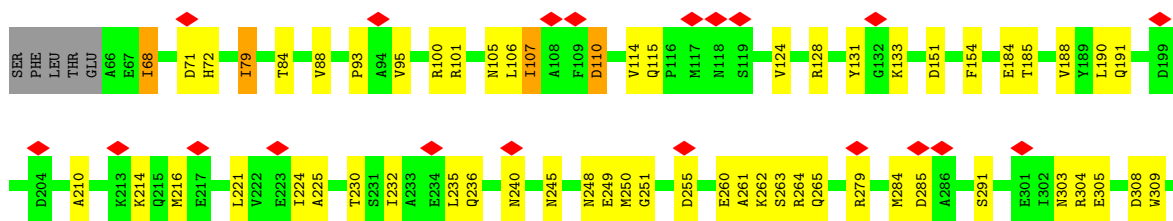




- Molecule 6: gp23, major capsid protein



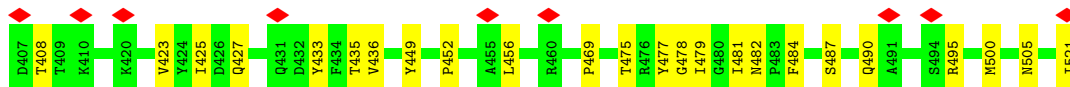
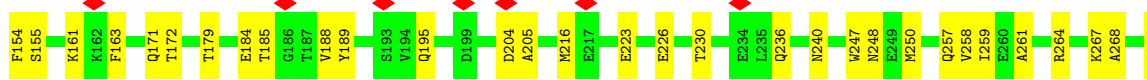
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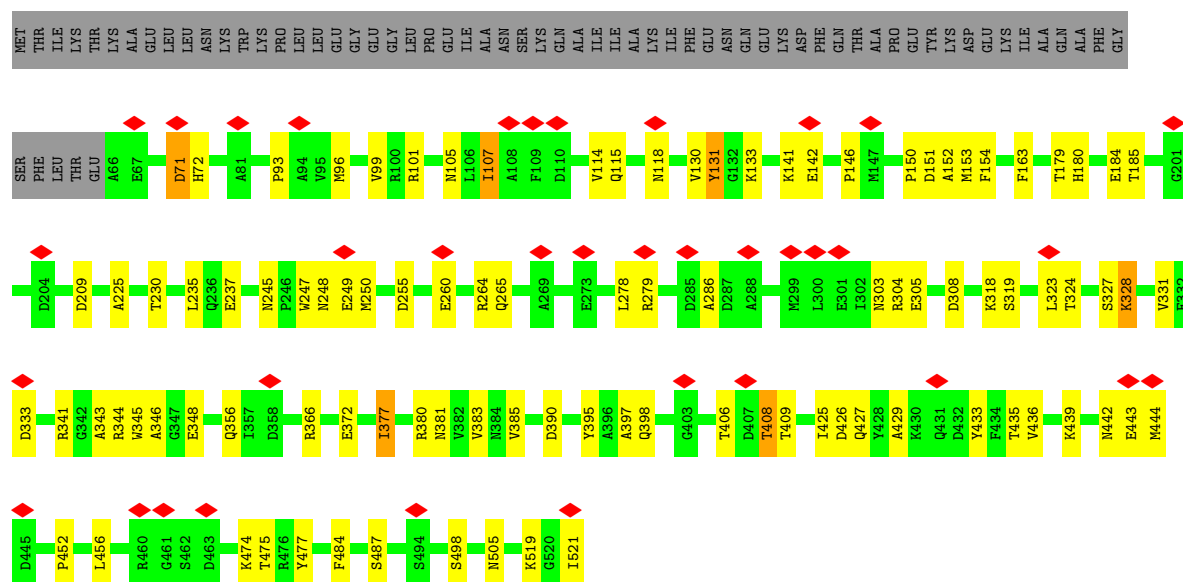
- Molecule 6: gp23, major capsid protein



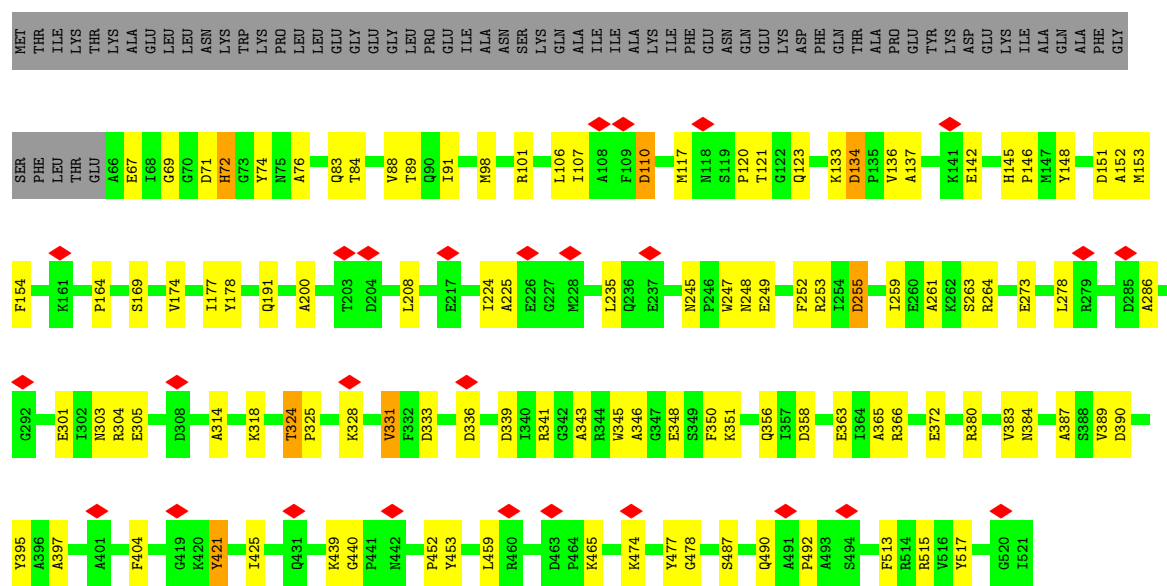
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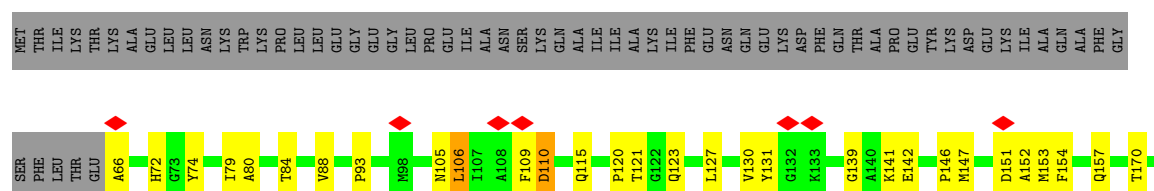
- Molecule 6: gp23, major capsid protein

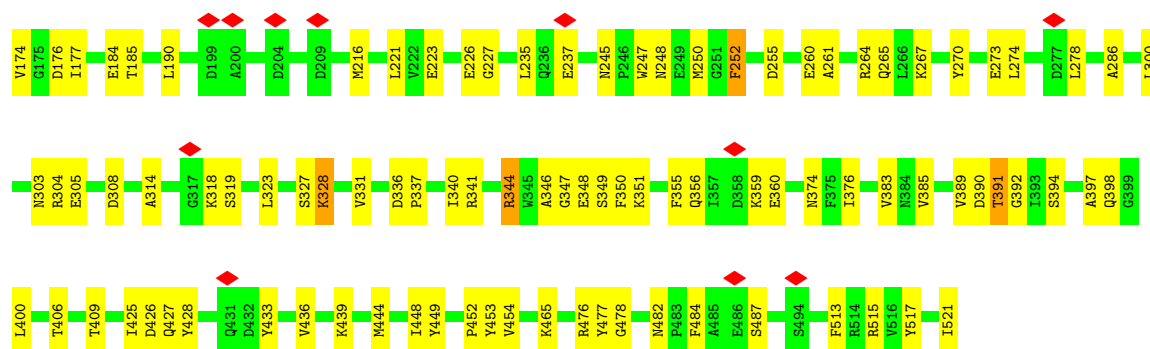


- Molecule 6: gp23, major capsid protein



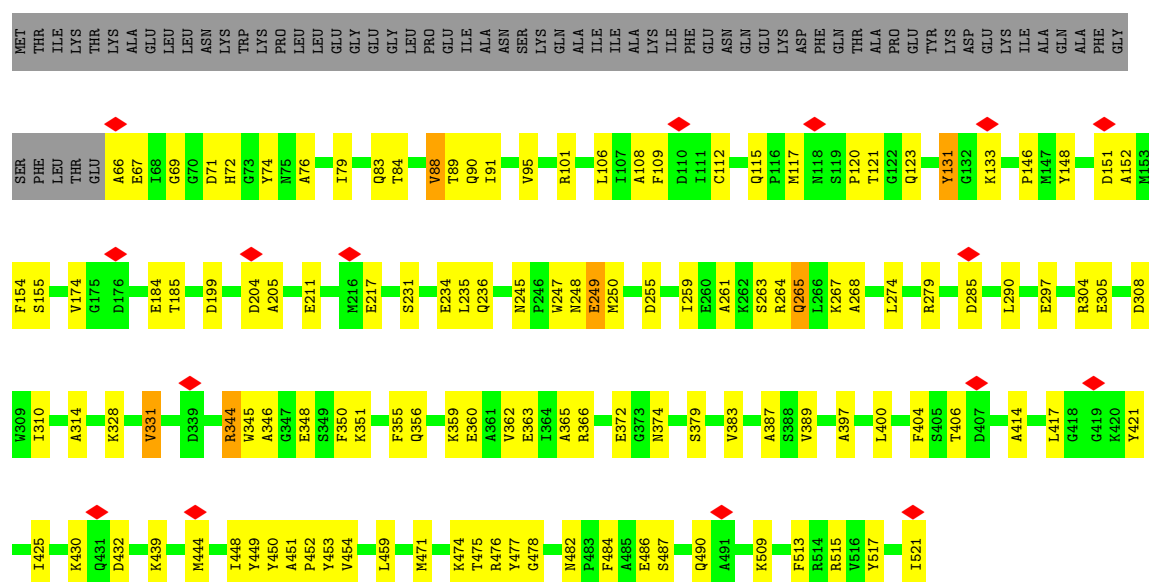
- Molecule 6: gp23, major capsid protein





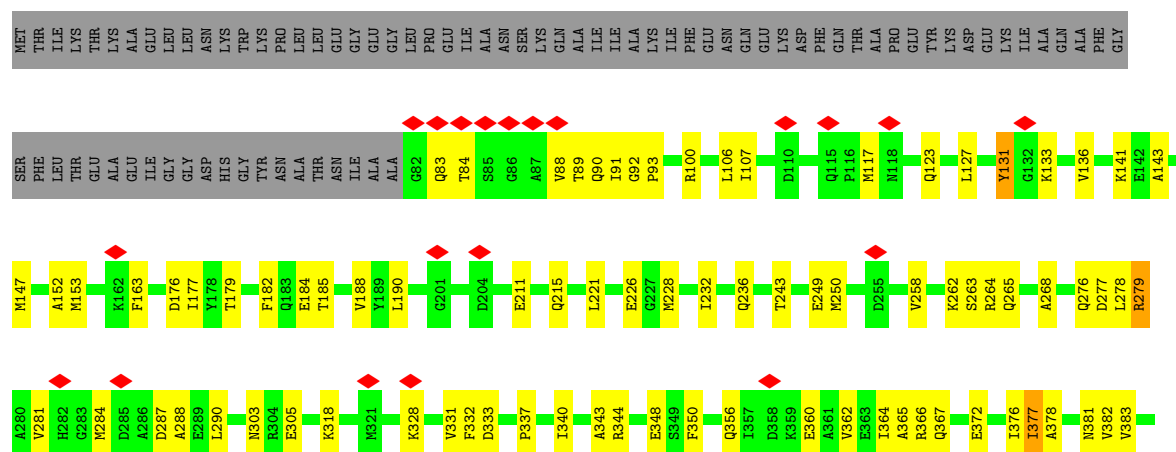
- Molecule 6: gp23, major capsid protein

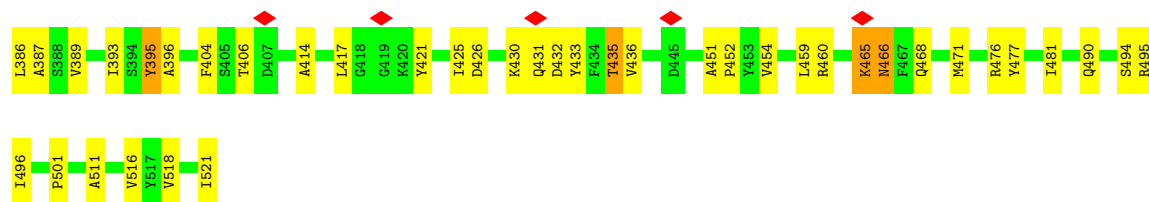
Chain Am: 63% 23% 12%



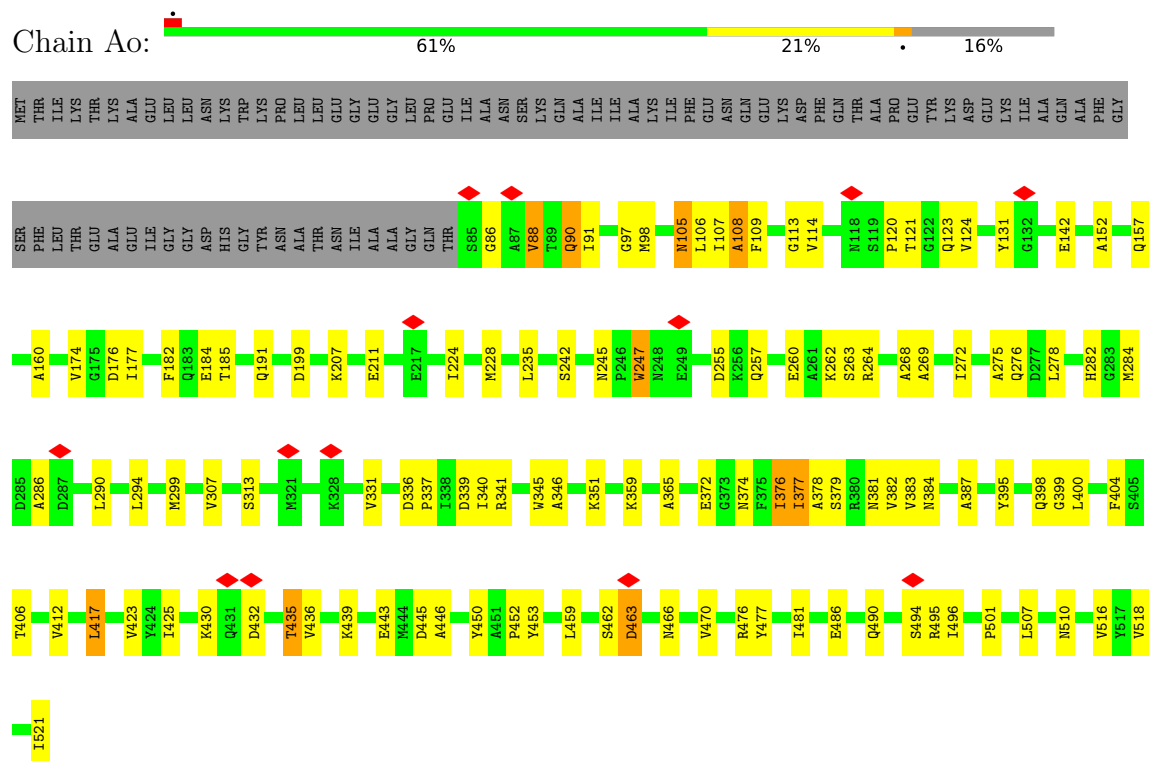
- Molecule 6: gp23, major capsid protein

Chain An: 5% 61% 22% 16%

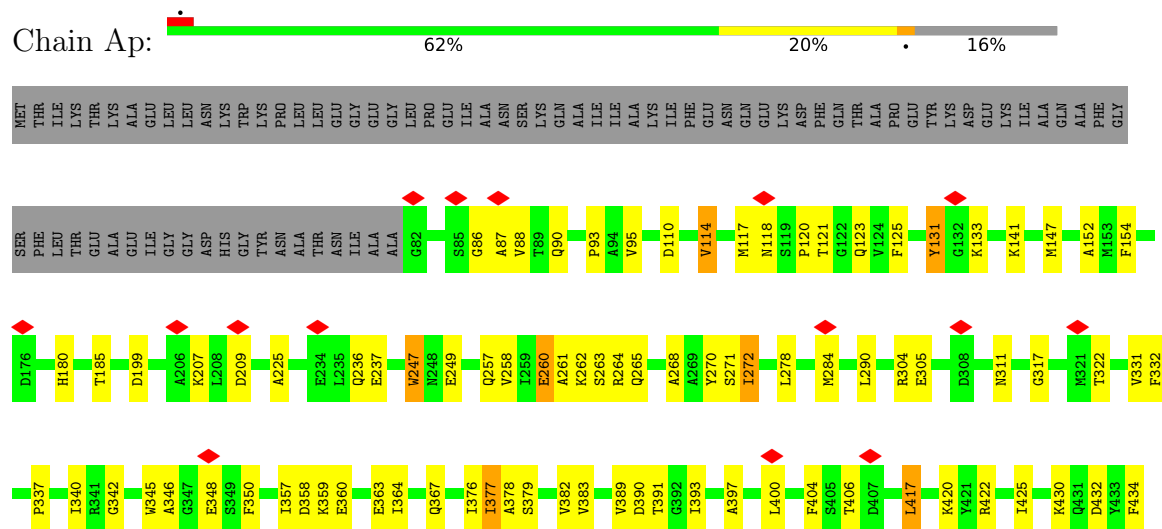




- Molecule 6: gp23, major capsid protein

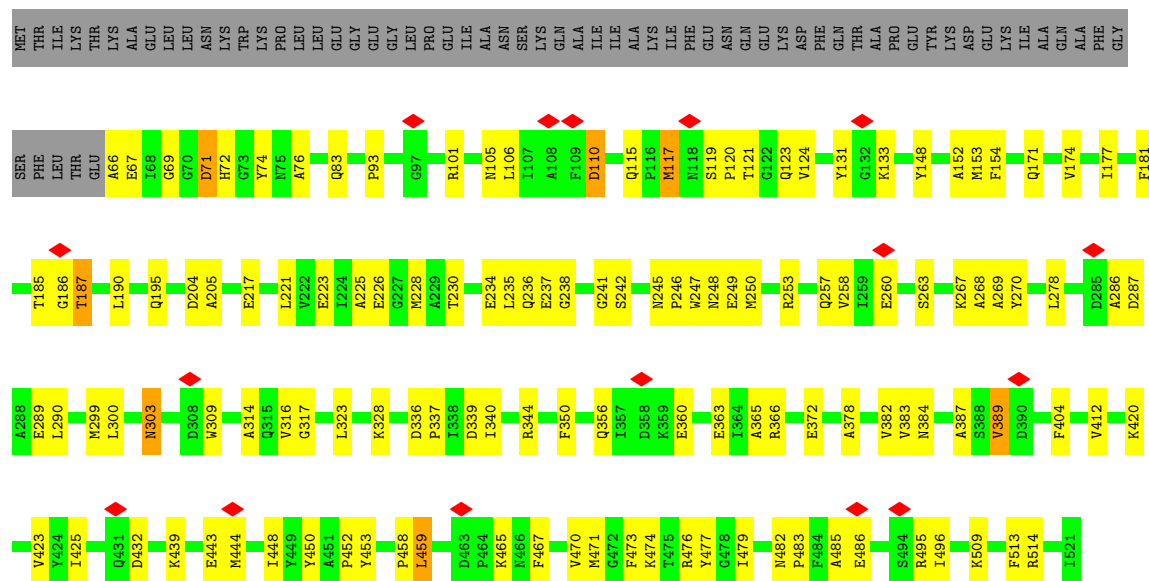


- Molecule 6: gp23, major capsid protein

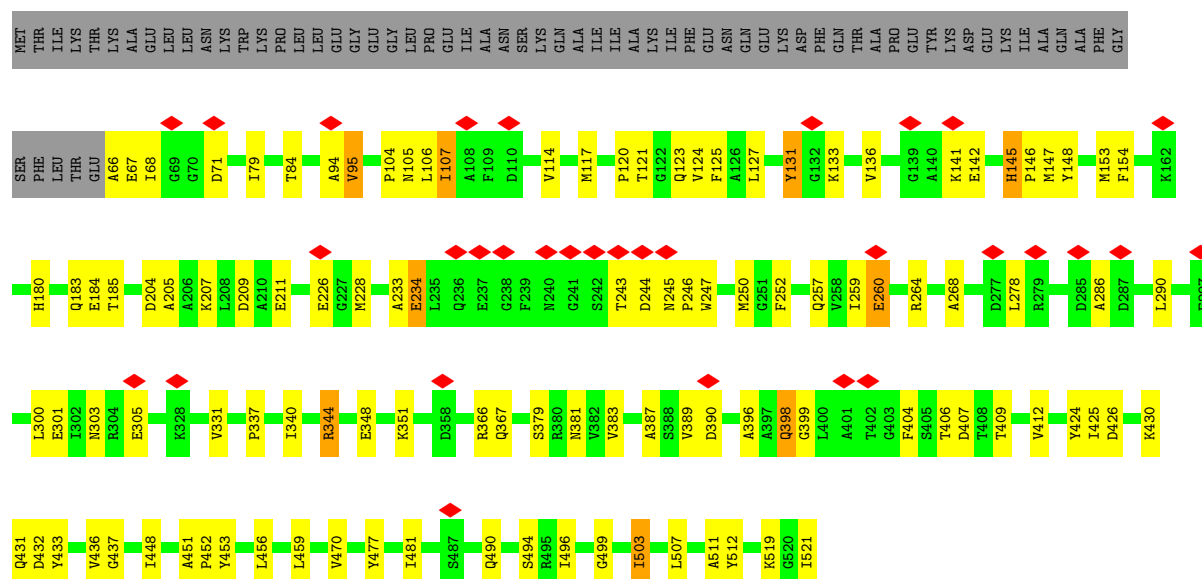




- Molecule 6: gp23, major capsid protein

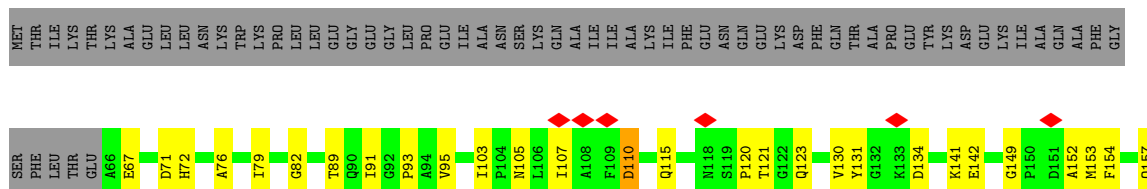


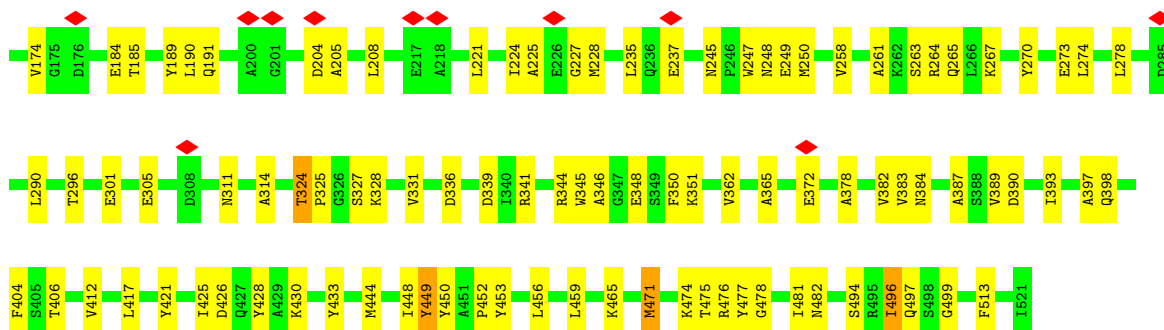
- Molecule 6: gp23, major capsid protein



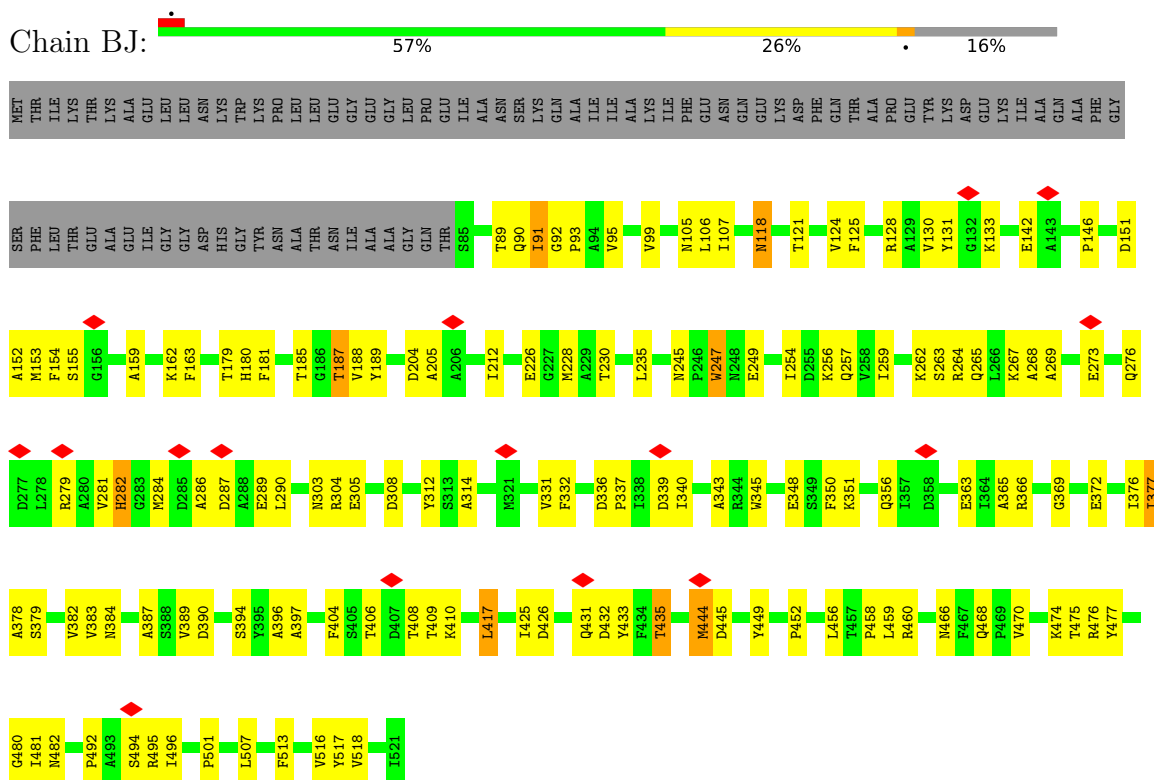
- Molecule 6: gp23, major capsid protein



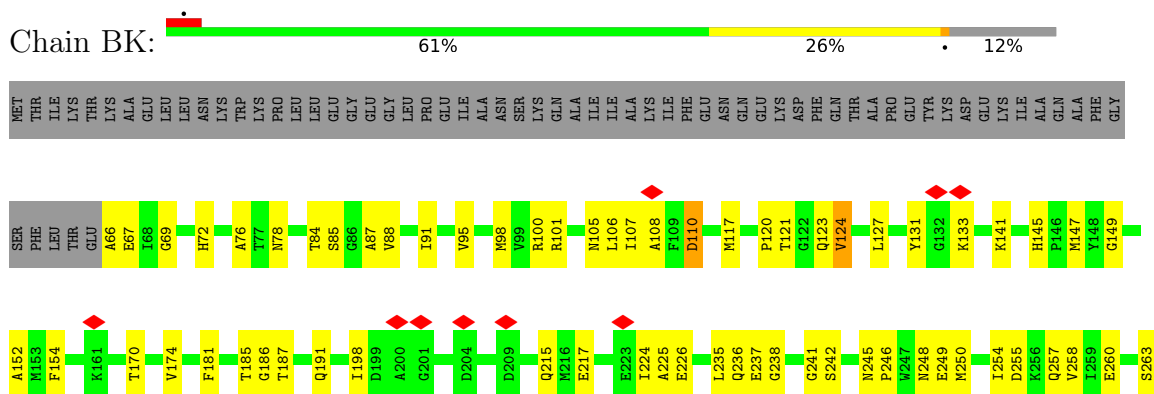


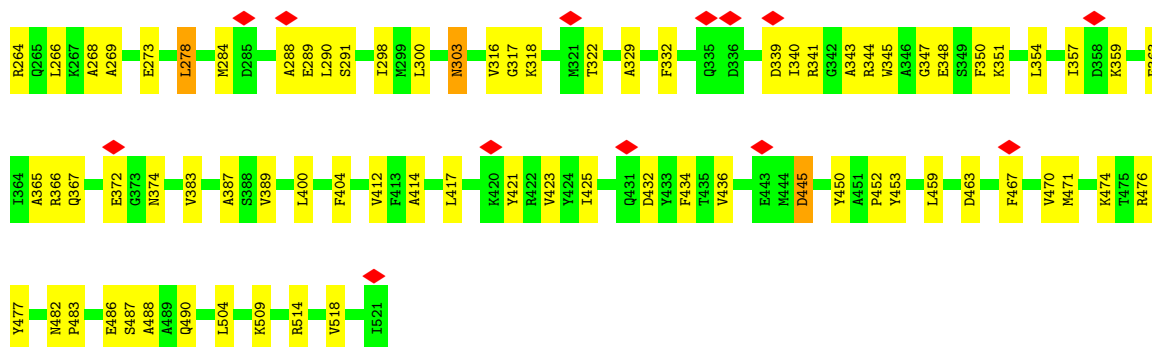


- Molecule 6: gp23, major capsid protein



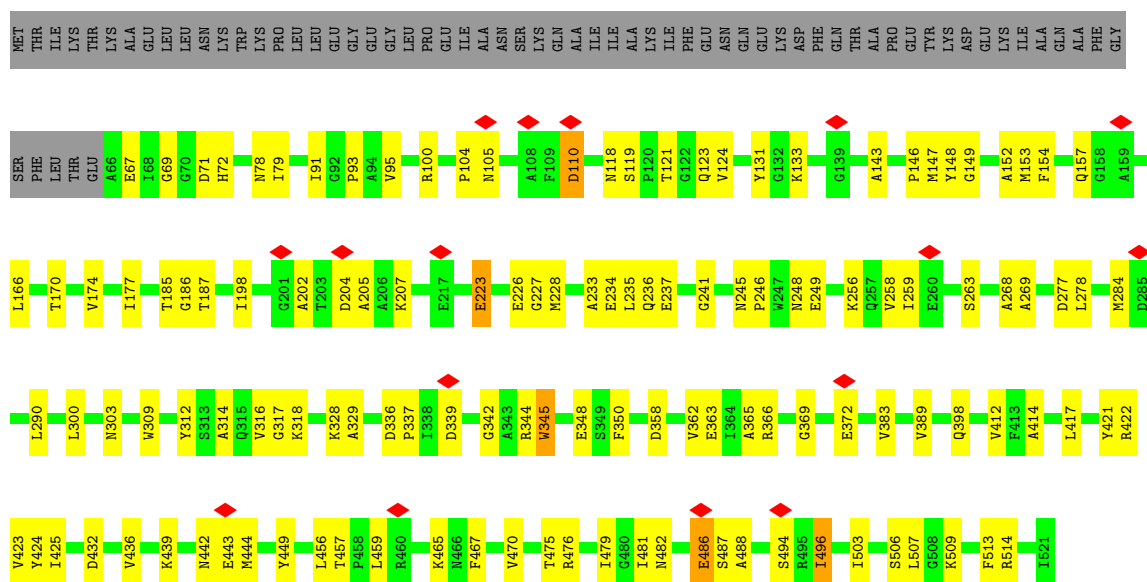
- Molecule 6: gp23, major capsid protein





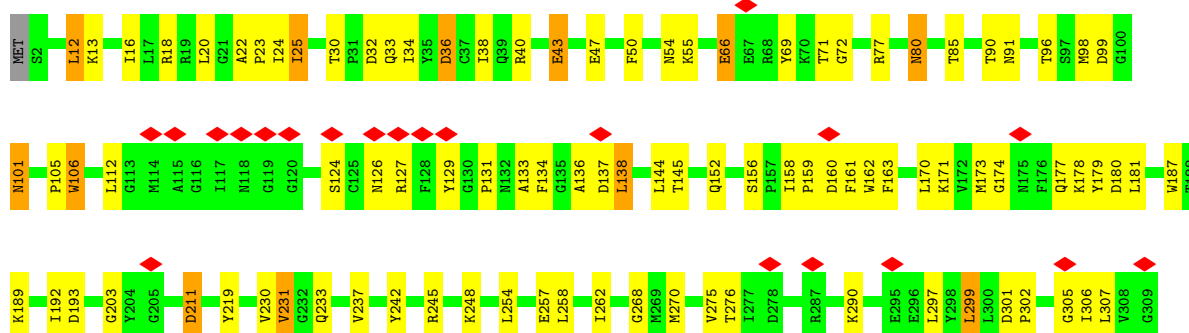
- Molecule 6: gp23, major capsid protein

Chain BM: 63% 24% 12%



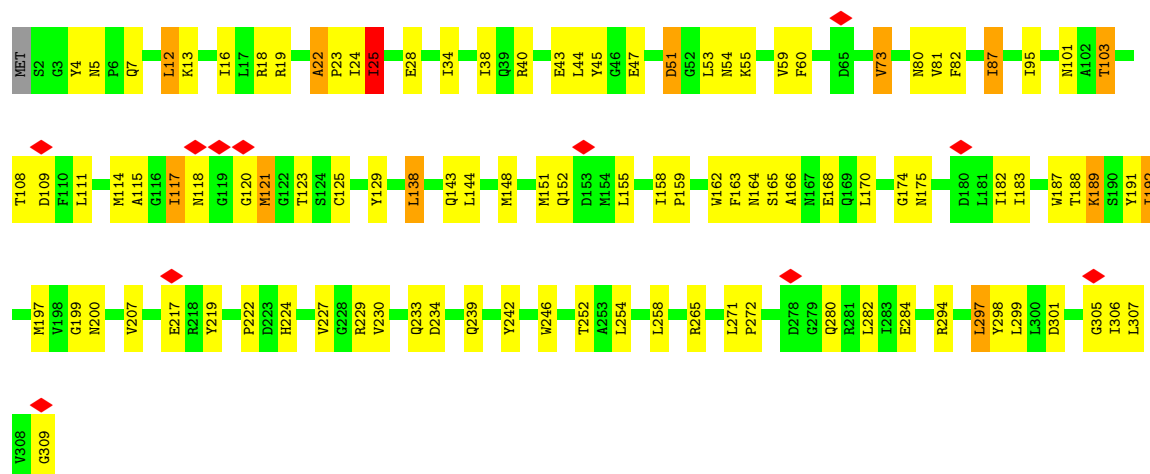
- Molecule 7: gp13, neck protein

Chain A6: 7% 69% 27%

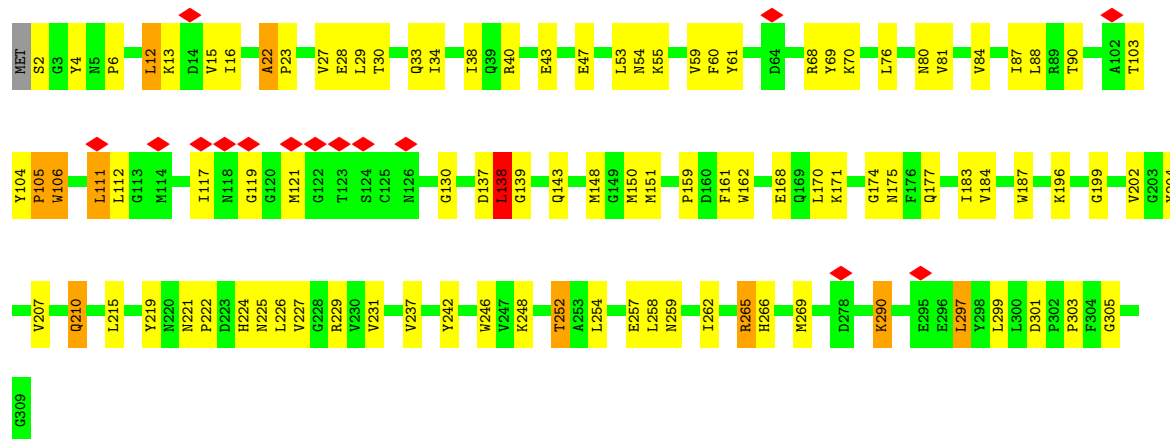


- Molecule 7: gp13, neck protein

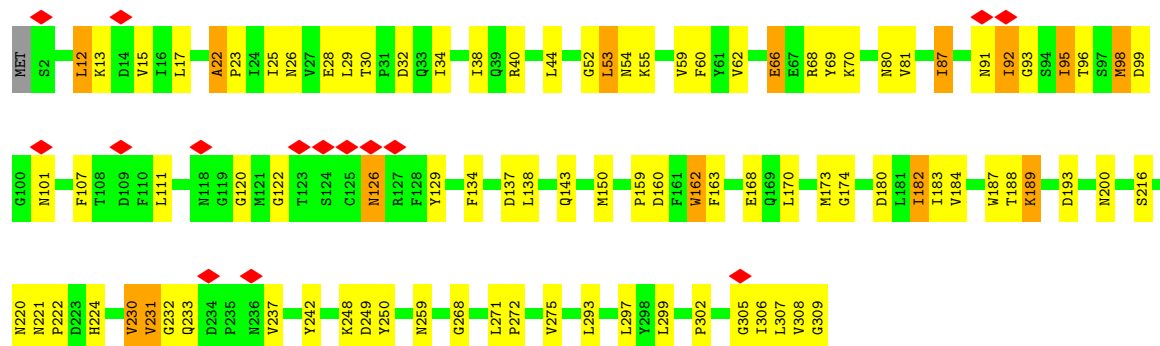
Chain AY: 66% 30% 4%



- Molecule 7: gp13, neck protein

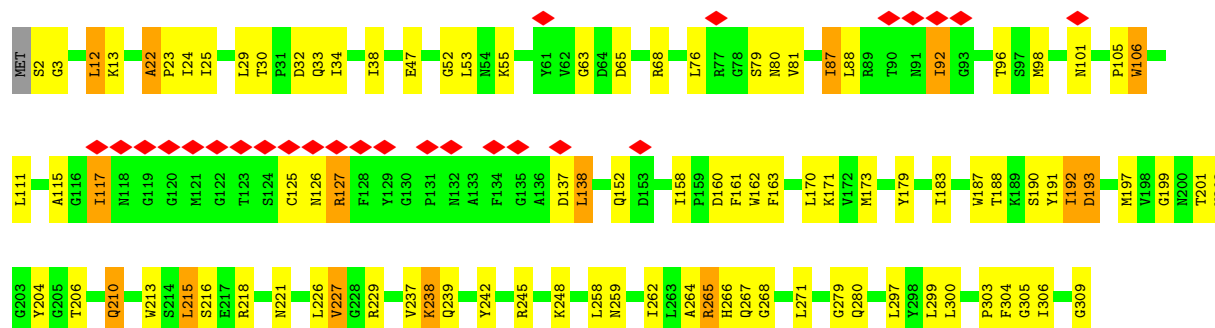


- Molecule 7: gp13, neck protein

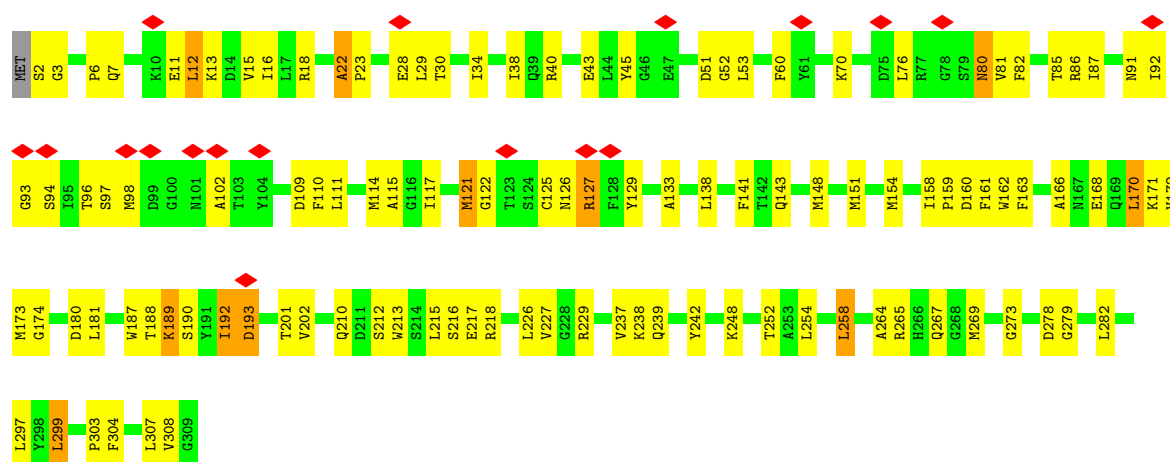


- Molecule 7: gp13, neck protein

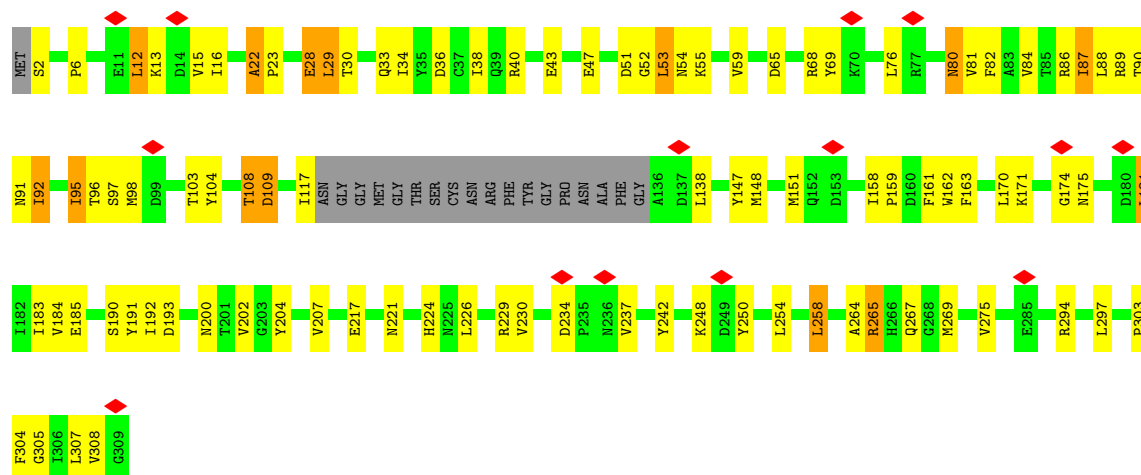




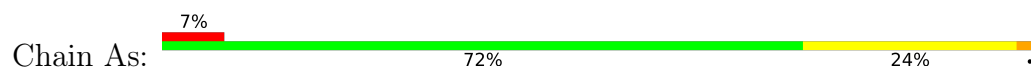
• Molecule 7: gp13, neck protein

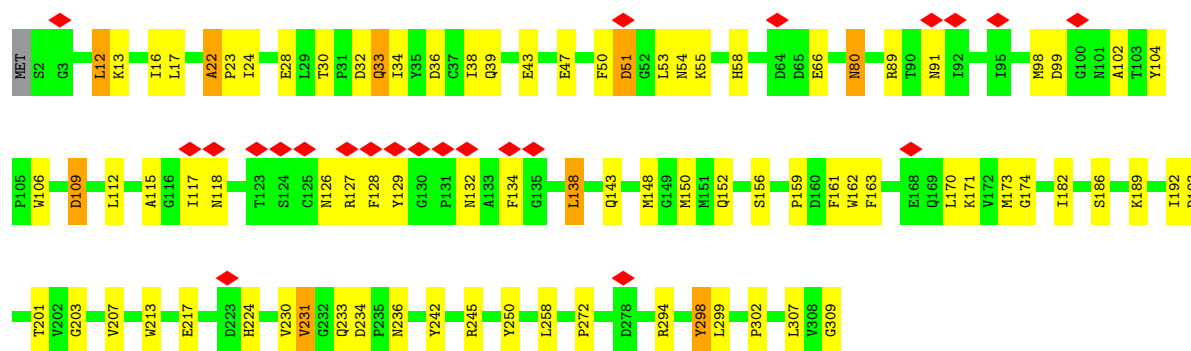


• Molecule 7: gp13, neck protein

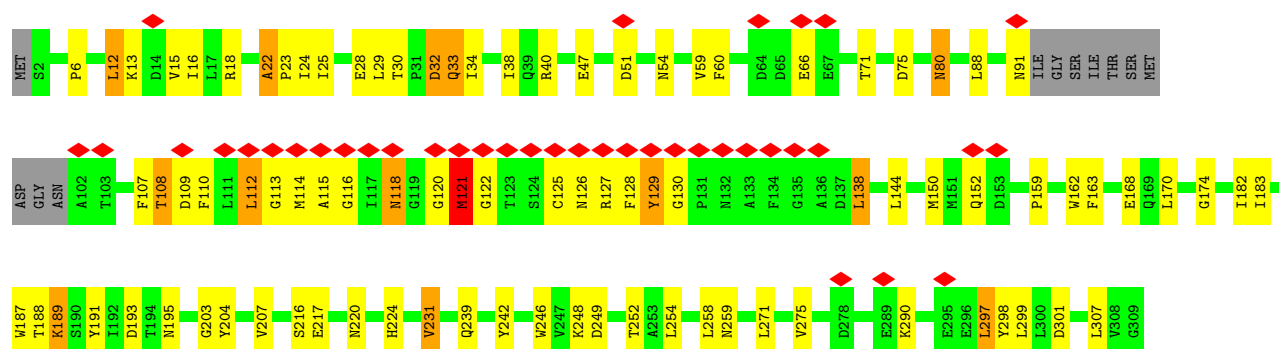


• Molecule 7: gp13, neck protein

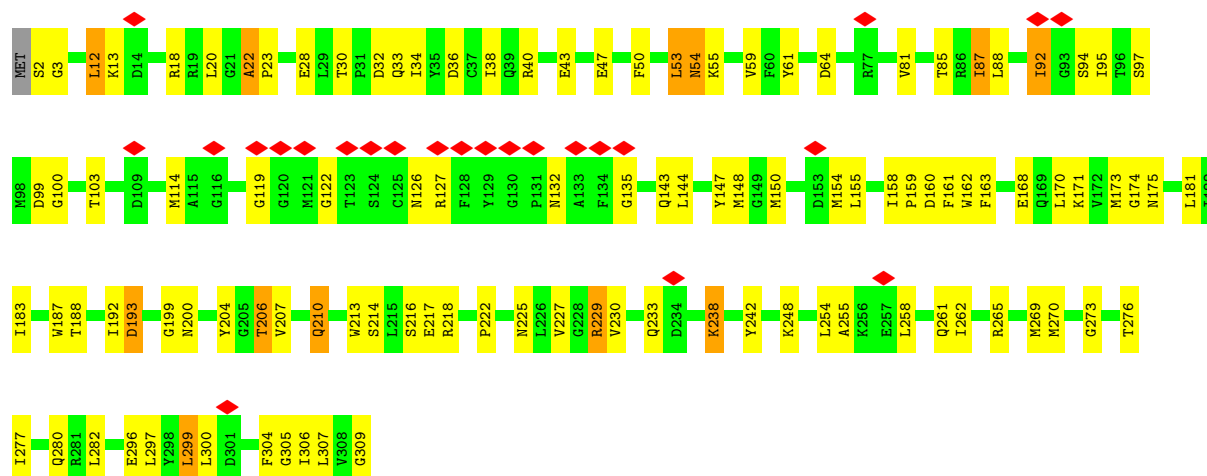




• Molecule 7: gp13, neck protein

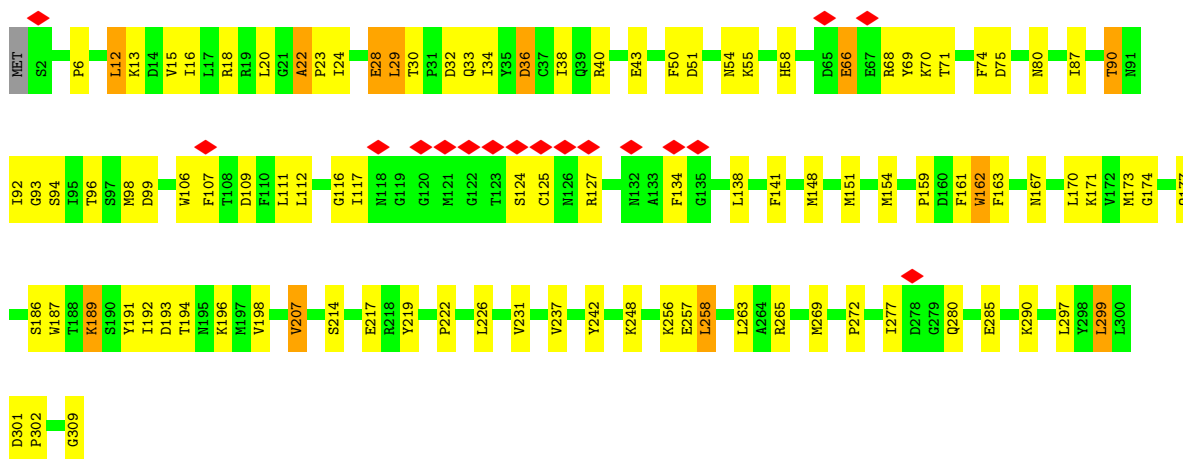


• Molecule 7: gp13, neck protein

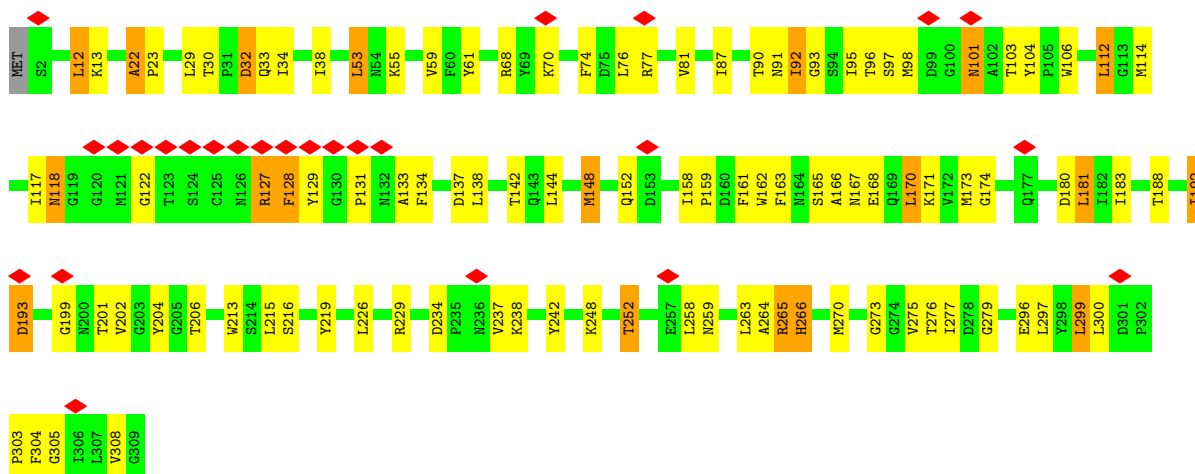


• Molecule 7: gp13, neck protein

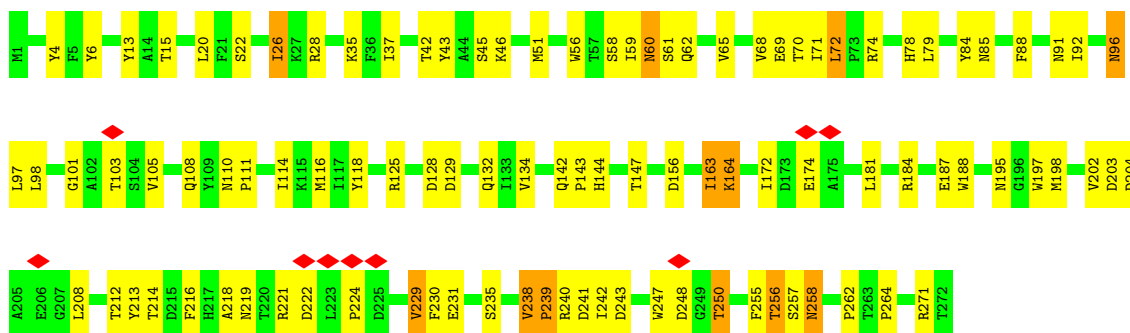




• Molecule 7: gp13, neck protein



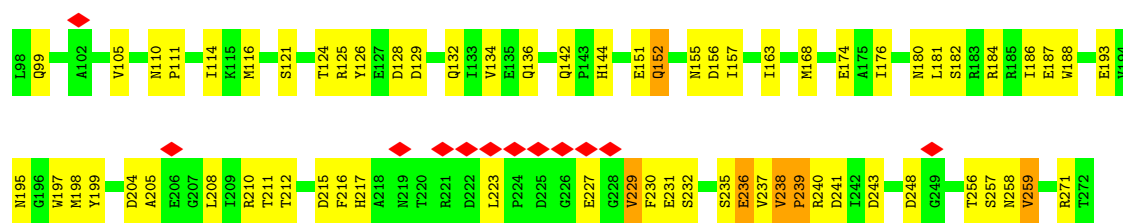
• Molecule 8: gp15, tail terminator protein



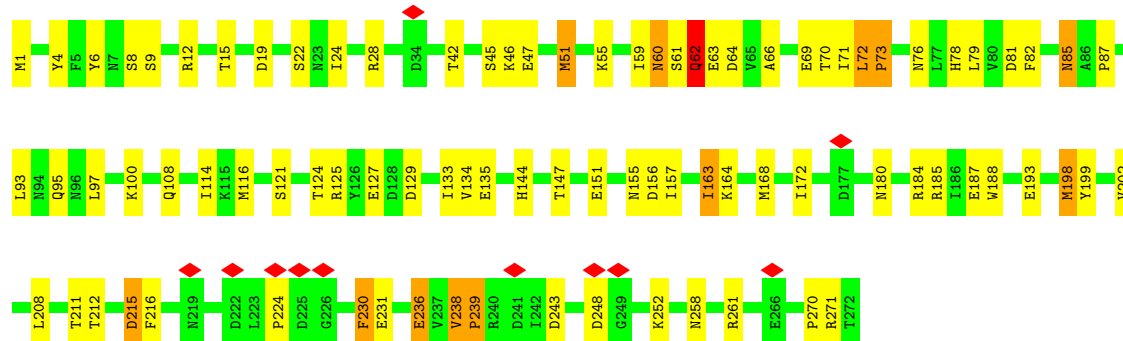
• Molecule 8: gp15, tail terminator protein



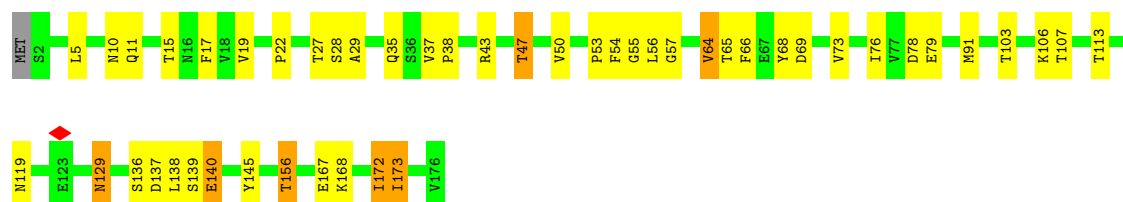
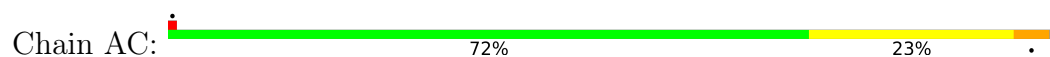




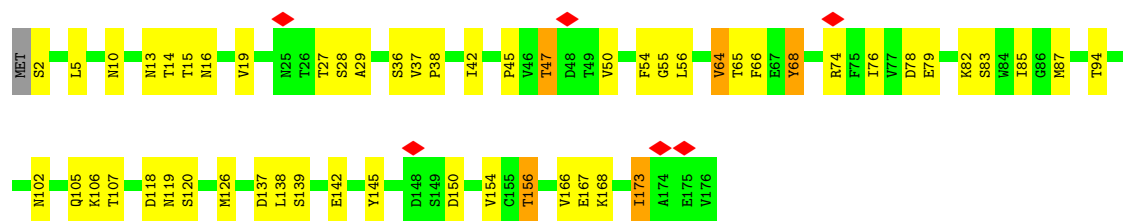
• Molecule 8: gp15, tail terminator protein



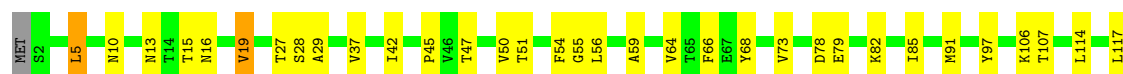
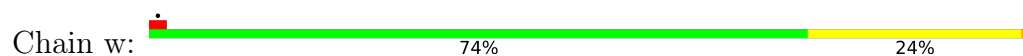
• Molecule 9: gp3, tube terminator protein



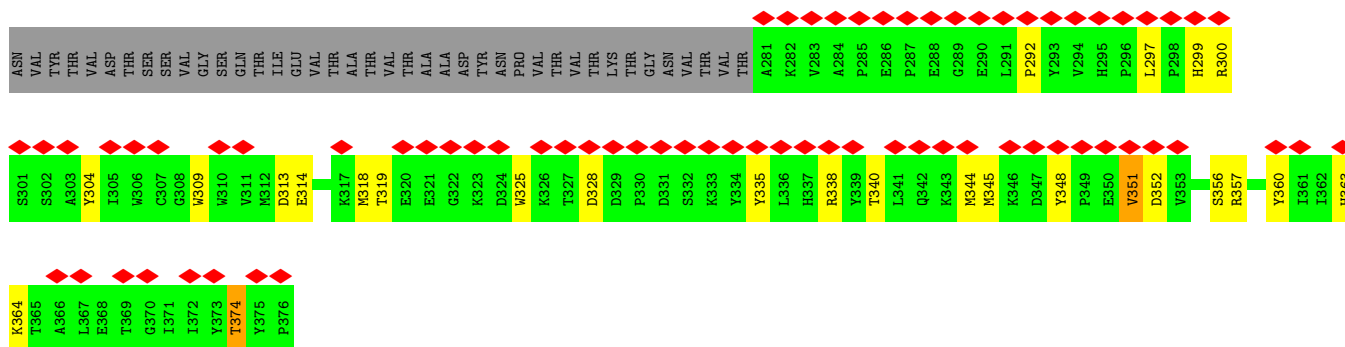
• Molecule 9: gp3, tube terminator protein



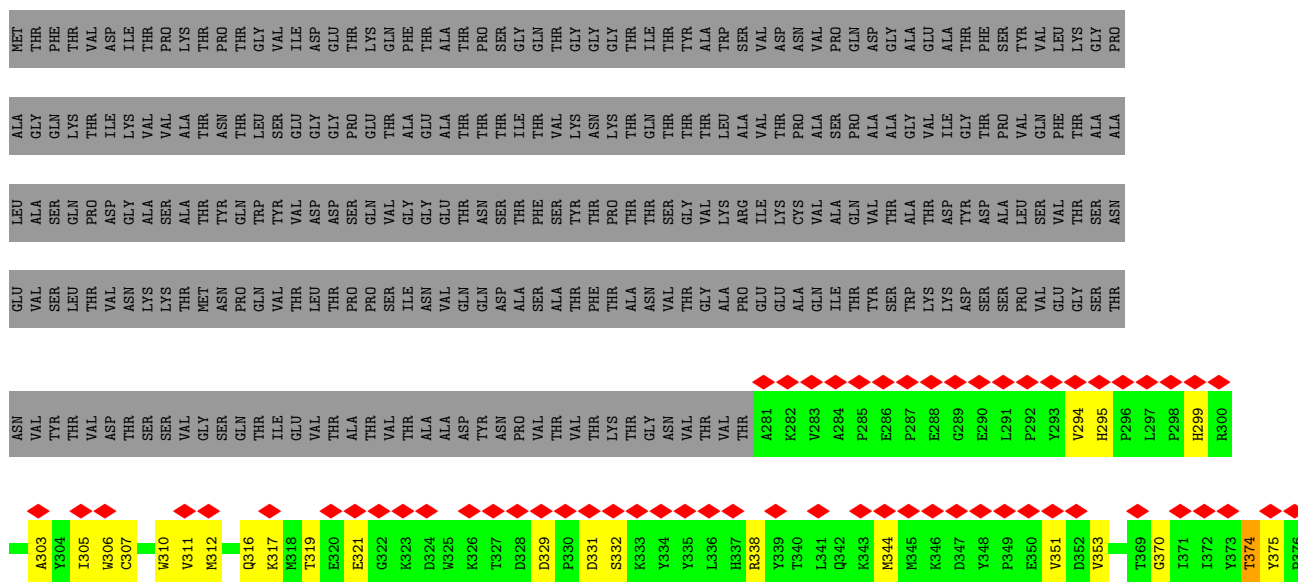
• Molecule 9: gp3, tube terminator protein



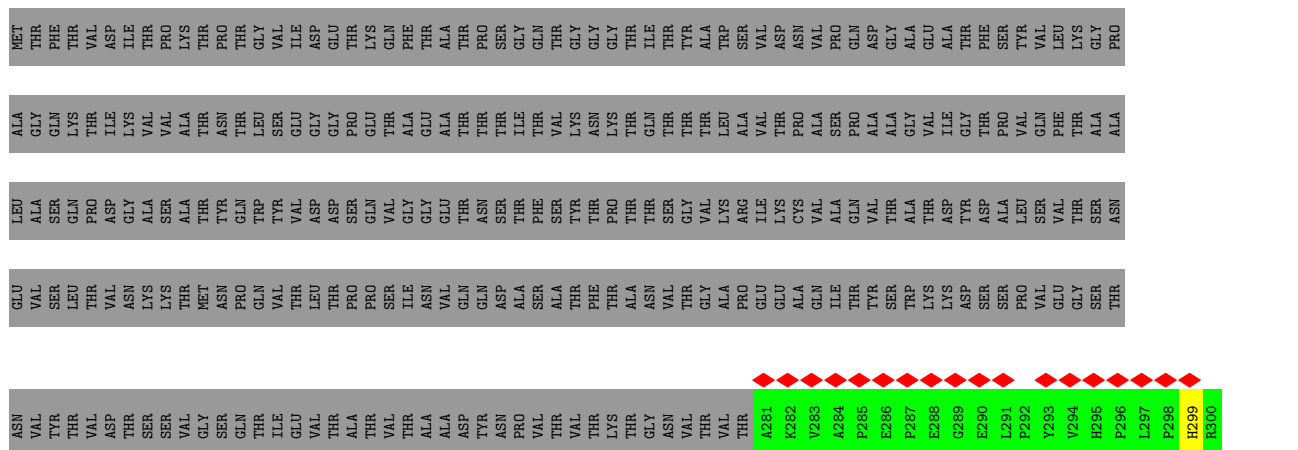




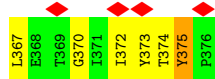
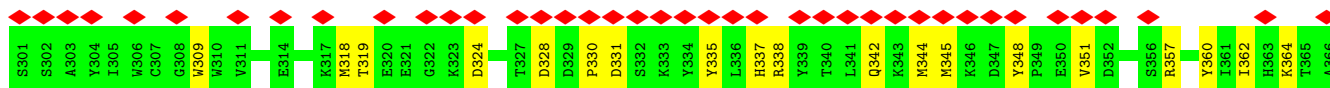
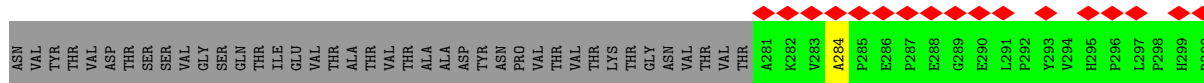
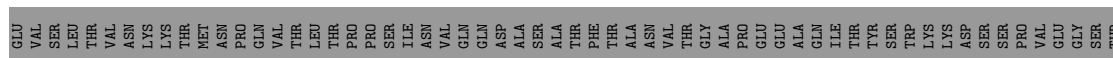
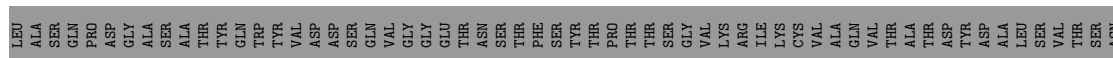
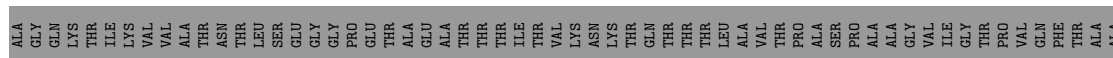
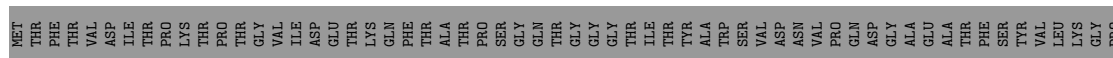
- Molecule 10: Hoc, highly immunogenic outer capsid protein.



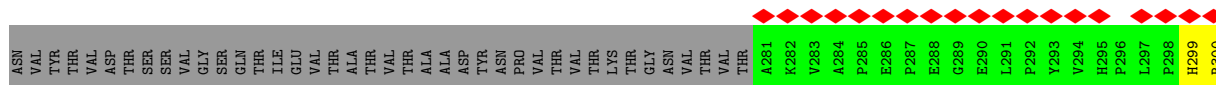
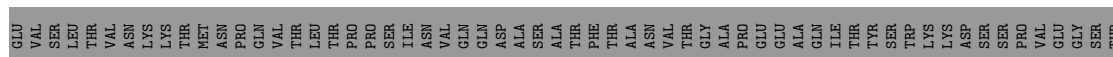
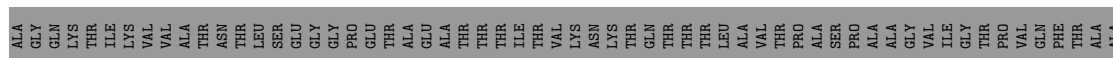
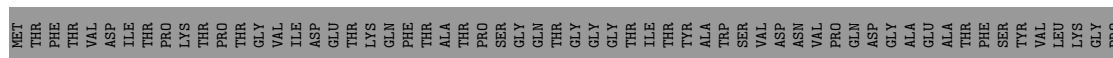
- Molecule 10: Hoc, highly immunogenic outer capsid protein.

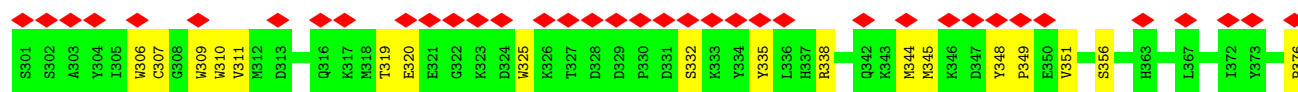


- Molecule 10: Hoc, highly immunogenic outer capsid protein.

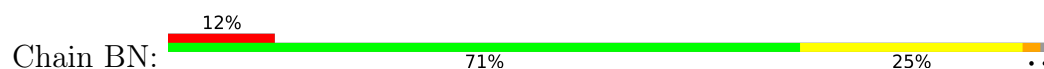


- Molecule 10: Hoc, highly immunogenic outer capsid protein.

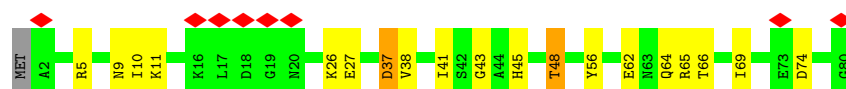
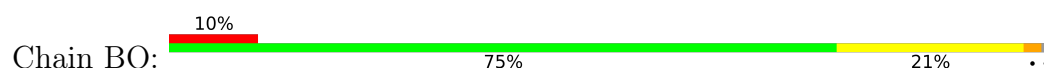




- Molecule 11: Soc, small outer capsid protein



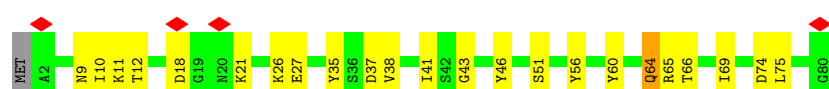
- Molecule 11: Soc, small outer capsid protein



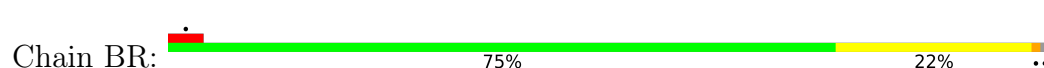
- Molecule 11: Soc, small outer capsid protein



- Molecule 11: Soc, small outer capsid protein




- Molecule 11: Soc, small outer capsid protein

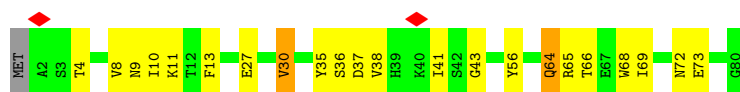


- Molecule 11: Soc, small outer capsid protein




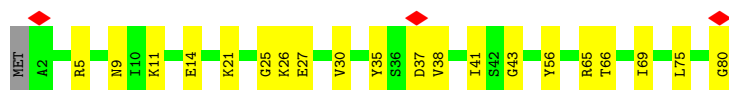
- Molecule 11: Soc, small outer capsid protein

Chain BT:  71% 25% ..




- Molecule 11: Soc, small outer capsid protein

Chain BU:  74% 25% .




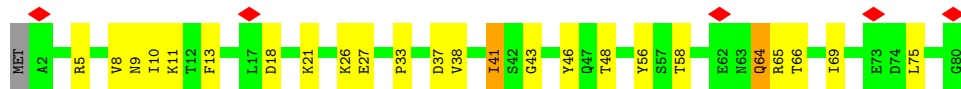
- Molecule 11: Soc, small outer capsid protein

Chain BV:  79% 19% ..



- Molecule 11: Soc, small outer capsid protein

Chain BW:  6% 69% 28% ..



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	69000	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	0.090	Depositor
Minimum map value	-0.059	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	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 [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.12	0/2042	0.40	0/2768
1	k	0.13	0/2042	0.40	0/2768
1	l	0.13	0/2042	0.41	0/2768
1	m	0.12	0/2042	0.38	0/2768
1	n	0.13	0/2042	0.38	0/2768
1	p	0.13	0/2042	0.39	0/2768
2	1	0.11	0/5077	0.31	1/6907 (0.0%)
2	2	0.11	0/5077	0.31	0/6907
2	3	0.11	0/5077	0.32	1/6907 (0.0%)
2	4	0.11	0/5077	0.31	0/6907
2	5	0.11	0/5077	0.31	0/6907
2	AD	0.11	0/5077	0.30	0/6907
2	AK	0.10	0/5092	0.30	0/6928
2	AL	0.11	0/5092	0.31	0/6928
2	AM	0.10	0/5092	0.29	0/6928
2	AN	0.10	0/5092	0.31	0/6928
2	AO	0.11	0/5092	0.32	0/6928
2	AP	0.11	0/5092	0.30	0/6928
2	B1	0.10	0/5092	0.32	0/6928
2	B2	0.11	0/5092	0.30	0/6928
2	B3	0.10	0/5092	0.31	0/6928
2	B4	0.10	0/5092	0.32	1/6928 (0.0%)
2	B5	0.10	0/5092	0.30	0/6928
2	B6	0.10	0/5092	0.29	0/6928
2	B7	0.10	0/5092	0.30	0/6928
2	Bp	0.11	0/5092	0.31	0/6928
2	Bq	0.10	0/5092	0.30	0/6928
2	Br	0.10	0/5092	0.30	0/6928
2	Bs	0.10	0/5092	0.31	0/6928
2	Bt	0.10	0/5092	0.29	0/6928
2	Bu	0.10	0/5092	0.31	0/6928
2	Bv	0.10	0/5092	0.31	0/6928
2	Bw	0.10	0/5092	0.32	1/6928 (0.0%)
2	Bx	0.10	0/5092	0.32	0/6928

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	By	0.11	0/5092	0.32	0/6928
2	Bz	0.10	0/5092	0.32	1/6928 (0.0%)
3	6	0.12	0/1325	0.37	0/1797
3	7	0.12	0/1325	0.35	0/1797
3	8	0.12	0/1325	0.36	0/1797
3	9	0.13	0/1325	0.37	0/1797
3	AA	0.12	0/1325	0.38	1/1797 (0.1%)
3	AE	0.15	0/1333	0.39	0/1807
3	AF	0.12	0/1333	0.32	0/1807
3	AG	0.13	0/1333	0.31	0/1807
3	AH	0.12	0/1333	0.31	0/1807
3	AI	0.11	0/1333	0.34	0/1807
3	AJ	0.11	0/1333	0.33	0/1807
3	BX	0.11	0/1333	0.33	0/1807
3	BY	0.11	0/1333	0.32	0/1807
3	BZ	0.10	0/1333	0.32	0/1807
3	Ba	0.11	0/1333	0.34	0/1807
3	Bb	0.10	0/1333	0.33	0/1807
3	Bc	0.10	0/1333	0.32	0/1807
3	Bd	0.11	0/1333	0.32	0/1807
3	Be	0.11	0/1333	0.33	0/1807
3	Bf	0.10	0/1333	0.29	0/1807
3	Bg	0.11	0/1333	0.34	0/1807
3	Bh	0.11	0/1333	0.34	0/1807
3	Bi	0.11	0/1333	0.32	0/1807
3	Bj	0.11	0/1333	0.33	0/1807
3	Bk	0.11	0/1333	0.32	0/1807
3	Bl	0.12	0/1333	0.33	0/1807
3	Bm	0.15	0/1333	0.38	1/1807 (0.1%)
3	Bn	0.17	0/1333	0.38	0/1807
3	Bo	0.10	0/1333	0.31	0/1807
3	o	0.13	0/1325	0.36	0/1797
4	A	0.11	0/608	0.20	0/825
4	B	0.10	0/608	0.19	0/825
4	C	0.10	0/608	0.21	0/825
4	D	0.09	0/608	0.20	0/825
4	E	0.09	0/608	0.20	0/825
4	F	0.09	0/608	0.19	0/825
4	G	0.09	0/608	0.18	0/825
4	H	0.11	0/608	0.22	0/825
4	I	0.09	0/608	0.21	0/825
4	J	0.09	0/608	0.20	0/825
4	K	0.10	0/608	0.20	0/825

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
4	L	0.09	0/608	0.19	0/825
4	M	0.09	0/608	0.19	0/825
4	N	0.08	0/608	0.17	0/825
4	O	0.10	0/608	0.20	0/825
4	P	0.10	0/608	0.19	0/825
4	Q	0.09	0/608	0.18	0/825
4	R	0.10	0/608	0.22	0/825
4	S	0.09	0/608	0.20	0/825
4	T	0.10	0/608	0.20	0/825
4	U	0.10	0/608	0.19	0/825
4	V	0.09	0/608	0.20	0/825
4	W	0.09	0/608	0.20	0/825
4	X	0.09	0/608	0.21	0/825
4	Y	0.09	0/608	0.19	0/825
4	Z	0.09	0/608	0.20	0/825
4	a	0.09	0/608	0.18	0/825
4	b	0.09	0/608	0.19	0/825
4	c	0.10	0/608	0.21	0/825
4	d	0.09	0/608	0.18	0/825
4	e	0.09	0/608	0.19	0/825
4	f	0.10	0/608	0.20	0/825
4	g	0.10	0/608	0.20	0/825
4	h	0.09	0/608	0.19	0/825
4	i	0.09	0/608	0.20	0/825
4	j	0.10	0/608	0.21	0/825
5	A0	0.12	0/4222	0.33	0/5693
5	A1	0.12	0/4222	0.31	0/5693
5	A2	0.11	0/4214	0.33	0/5682
5	A3	0.12	0/4214	0.33	0/5682
5	Av	0.11	0/4214	0.31	0/5682
5	Ax	0.11	0/4214	0.29	0/5682
5	BA	0.11	0/4153	0.31	0/5600
5	BB	0.11	0/4070	0.30	0/5482
5	BD	0.13	0/4214	0.33	1/5682 (0.0%)
5	BF	0.11	0/4214	0.30	0/5682
5	BG	0.11	0/4116	0.32	0/5548
5	BH	0.11	0/4170	0.29	0/5626
6	A4	0.12	0/3493	0.34	0/4731
6	A5	0.10	0/3493	0.31	0/4731
6	A7	0.11	0/3493	0.31	0/4731
6	A8	0.11	0/3377	0.31	0/4573
6	A9	0.11	0/3493	0.32	0/4731
6	AV	0.12	0/3493	0.32	0/4731

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	AW	0.11	0/3493	0.31	0/4731
6	AX	0.11	0/3493	0.30	0/4731
6	AZ	0.12	0/3493	0.34	2/4731 (0.0%)
6	Ac	0.11	0/3493	0.32	0/4731
6	Ad	0.11	0/3493	0.31	0/4731
6	Ae	0.11	0/3493	0.31	0/4731
6	Af	0.11	0/3493	0.31	0/4731
6	Ag	0.12	0/3493	0.31	0/4731
6	Ah	0.11	0/3493	0.29	0/4731
6	Ai	0.10	0/3493	0.31	1/4731 (0.0%)
6	Aj	0.11	0/3493	0.32	0/4731
6	Ak	0.12	0/3493	0.29	0/4731
6	Am	0.12	0/3493	0.33	0/4731
6	An	0.12	0/3377	0.31	0/4573
6	Ao	0.11	0/3357	0.31	0/4546
6	Ap	0.12	0/3377	0.31	0/4573
6	Au	0.11	0/3493	0.31	0/4731
6	Aw	0.12	0/3493	0.32	0/4731
6	Ay	0.11	0/3493	0.30	0/4731
6	Az	0.11	0/3493	0.31	0/4731
6	BI	0.11	0/3493	0.29	0/4731
6	BJ	0.12	0/3357	0.32	0/4546
6	BK	0.11	0/3493	0.31	0/4731
6	BM	0.12	0/3493	0.34	0/4731
7	A6	0.11	0/2496	0.29	0/3383
7	AY	0.12	0/2493	0.32	0/3379
7	Aa	0.12	0/2496	0.33	0/3383
7	Ab	0.11	0/2496	0.31	0/3383
7	Al	0.13	0/2493	0.34	1/3379 (0.0%)
7	Aq	0.12	0/2496	0.32	0/3383
7	Ar	0.12	0/2363	0.30	0/3203
7	As	0.11	0/2496	0.31	0/3383
7	At	0.12	0/2428	0.31	0/3290
7	BC	0.12	0/2496	0.30	0/3383
7	BE	0.12	0/2496	0.31	0/3383
7	BL	0.12	0/2496	0.32	0/3383
8	AB	0.15	0/2287	0.37	0/3109
8	q	0.16	0/2287	0.38	0/3109
8	r	0.15	0/2287	0.37	0/3109
8	s	0.15	0/2287	0.37	0/3109
8	t	0.14	0/2287	0.37	0/3109
8	u	0.15	0/2287	0.38	0/3109
9	AC	0.13	0/1418	0.33	0/1939

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
9	v	0.13	0/1418	0.32	0/1939
9	w	0.13	0/1418	0.32	0/1939
9	x	0.13	0/1418	0.34	0/1939
9	y	0.12	0/1418	0.31	0/1939
9	z	0.12	0/1418	0.31	0/1939
10	AQ	0.09	0/833	0.27	0/1133
10	AR	0.10	0/833	0.29	0/1133
10	AS	0.09	0/833	0.27	0/1133
10	AT	0.10	0/833	0.31	0/1133
10	AU	0.10	0/833	0.28	0/1133
11	BN	0.10	0/651	0.28	0/880
11	BO	0.10	0/651	0.27	0/880
11	BP	0.11	0/651	0.32	0/880
11	BQ	0.10	0/651	0.31	0/880
11	BR	0.10	0/651	0.32	0/880
11	BS	0.10	0/651	0.29	0/880
11	BT	0.11	0/651	0.30	0/880
11	BU	0.11	0/651	0.30	0/880
11	BV	0.11	0/651	0.29	0/880
11	BW	0.10	0/651	0.30	0/880
All	All	0.11	0/443809	0.31	12/602060 (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
6	A4	0	1
8	s	0	1
8	u	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AZ	118	ASN	CA-C-N	6.56	133.51	121.70
6	AZ	118	ASN	C-N-CA	6.56	133.51	121.70
2	Bw	482	ASP	N-CA-C	-6.35	107.39	114.62
2	3	482	ASP	N-CA-C	-5.92	107.05	114.56
3	Bm	125	LYS	N-CA-C	-5.51	103.63	111.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A4	254	ILE	Peptide
8	s	142	GLN	Peptide
8	u	72	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	0	1993	0	1903	59	0
1	k	1993	0	1903	59	0
1	l	1993	0	1903	60	0
1	m	1993	0	1903	79	0
1	n	1993	0	1903	61	0
1	p	1993	0	1903	73	0
2	1	4985	0	4900	127	0
2	2	4985	0	4900	117	0
2	3	4985	0	4900	120	0
2	4	4985	0	4900	125	0
2	5	4985	0	4900	118	0
2	AD	4985	0	4900	117	0
2	AK	5000	0	4918	125	0
2	AL	5000	0	4918	126	0
2	AM	5000	0	4918	114	0
2	AN	5000	0	4918	118	0
2	AO	5000	0	4918	124	0
2	AP	5000	0	4918	129	0
2	B1	5000	0	4918	142	0
2	B2	5000	0	4918	128	0
2	B3	5000	0	4918	134	0
2	B4	5000	0	4918	131	0
2	B5	5000	0	4918	121	0
2	B6	5000	0	4918	143	0
2	B7	5000	0	4918	113	0
2	Bp	5000	0	4918	125	0
2	Bq	5000	0	4918	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Br	5000	0	4918	117	0
2	Bs	5000	0	4918	126	0
2	Bt	5000	0	4918	136	0
2	Bu	5000	0	4918	136	0
2	Bv	5000	0	4918	133	0
2	Bw	5000	0	4918	119	0
2	Bx	5000	0	4918	115	0
2	By	5000	0	4918	114	0
2	Bz	5000	0	4918	142	0
3	6	1296	0	1243	42	0
3	7	1296	0	1243	41	0
3	8	1296	0	1243	51	0
3	9	1296	0	1243	48	0
3	AA	1296	0	1243	55	0
3	AE	1304	0	1255	44	0
3	AF	1304	0	1255	50	0
3	AG	1304	0	1255	49	0
3	AH	1304	0	1255	46	0
3	AI	1304	0	1255	45	0
3	AJ	1304	0	1255	45	0
3	BX	1304	0	1255	51	0
3	BY	1304	0	1255	46	0
3	BZ	1304	0	1255	39	0
3	Ba	1304	0	1255	40	0
3	Bb	1304	0	1255	47	0
3	Bc	1304	0	1255	39	0
3	Bd	1304	0	1255	50	0
3	Be	1304	0	1255	44	0
3	Bf	1304	0	1255	44	0
3	Bg	1304	0	1255	52	0
3	Bh	1304	0	1255	55	0
3	Bi	1304	0	1255	49	0
3	Bj	1304	0	1255	48	0
3	Bk	1304	0	1255	51	0
3	Bl	1304	0	1255	40	0
3	Bm	1304	0	1255	37	0
3	Bn	1304	0	1255	55	0
3	Bo	1304	0	1255	44	0
3	o	1296	0	1243	50	0
4	A	601	0	600	14	0
4	B	601	0	600	7	0
4	C	601	0	600	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	601	0	600	7	0
4	E	601	0	600	5	0
4	F	601	0	600	10	0
4	G	601	0	600	12	0
4	H	601	0	600	15	0
4	I	601	0	600	9	0
4	J	601	0	600	8	0
4	K	601	0	600	15	0
4	L	601	0	600	16	0
4	M	601	0	600	16	0
4	N	601	0	600	7	0
4	O	601	0	600	12	0
4	P	601	0	600	10	0
4	Q	601	0	600	10	0
4	R	601	0	600	11	0
4	S	601	0	600	8	0
4	T	601	0	600	8	0
4	U	601	0	600	13	0
4	V	601	0	600	11	0
4	W	601	0	600	13	0
4	X	601	0	600	10	0
4	Y	601	0	600	8	0
4	Z	601	0	600	10	0
4	a	601	0	600	11	0
4	b	601	0	600	10	0
4	c	601	0	600	9	0
4	d	601	0	600	9	0
4	e	601	0	600	8	0
4	f	601	0	600	12	0
4	g	601	0	600	12	0
4	h	601	0	600	14	0
4	i	601	0	600	15	0
4	j	601	0	600	11	0
5	A0	4140	0	4075	101	0
5	A1	4140	0	4076	101	0
5	A2	4132	0	4070	92	0
5	A3	4132	0	4070	130	0
5	Av	4132	0	4070	106	0
5	Ax	4132	0	4070	91	0
5	BA	4074	0	4013	103	0
5	BB	3995	0	3948	119	0
5	BD	4132	0	4071	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	BF	4132	0	4070	110	0
5	BG	4039	0	3976	108	0
5	BH	4091	0	4018	91	0
6	A4	3425	0	3371	78	0
6	A5	3425	0	3371	93	0
6	A7	3425	0	3371	78	0
6	A8	3311	0	3271	94	0
6	A9	3425	0	3371	98	0
6	AV	3425	0	3371	105	0
6	AW	3425	0	3371	76	0
6	AX	3425	0	3371	80	0
6	AZ	3425	0	3371	87	0
6	Ac	3425	0	3371	79	0
6	Ad	3425	0	3371	68	0
6	Ae	3425	0	3371	87	0
6	Af	3425	0	3371	76	0
6	Ag	3425	0	3371	88	0
6	Ah	3425	0	3371	81	0
6	Ai	3425	0	3371	72	0
6	Aj	3425	0	3371	77	0
6	Ak	3425	0	3371	91	0
6	Am	3425	0	3371	93	0
6	An	3311	0	3271	85	0
6	Ao	3291	0	3253	90	0
6	Ap	3311	0	3271	84	0
6	Au	3425	0	3371	97	0
6	Aw	3425	0	3371	72	0
6	Ay	3425	0	3371	79	0
6	Az	3425	0	3371	79	0
6	BI	3425	0	3371	89	0
6	BJ	3291	0	3253	95	0
6	BK	3425	0	3371	102	0
6	BM	3425	0	3371	89	0
7	A6	2438	0	2356	79	0
7	AY	2435	0	2352	79	0
7	Aa	2438	0	2356	67	0
7	Ab	2438	0	2356	70	0
7	Al	2435	0	2352	85	0
7	Aq	2438	0	2356	89	0
7	Ar	2310	0	2245	78	0
7	As	2438	0	2356	65	0
7	At	2371	0	2291	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BC	2438	0	2356	85	0
7	BE	2438	0	2356	85	0
7	BL	2438	0	2357	78	0
8	AB	2227	0	2152	70	0
8	q	2227	0	2152	75	0
8	r	2227	0	2152	86	0
8	s	2227	0	2152	75	0
8	t	2227	0	2152	76	0
8	u	2227	0	2152	62	0
9	AC	1383	0	1344	35	0
9	v	1383	0	1344	40	0
9	w	1383	0	1344	31	0
9	x	1383	0	1344	21	0
9	y	1383	0	1344	38	0
9	z	1383	0	1344	32	0
10	AQ	805	0	763	18	0
10	AR	805	0	763	14	0
10	AS	805	0	763	11	0
10	AT	805	0	763	15	0
10	AU	805	0	763	16	0
11	BN	636	0	612	14	0
11	BO	636	0	612	10	0
11	BP	636	0	612	19	0
11	BQ	636	0	612	12	0
11	BR	636	0	612	12	0
11	BS	636	0	612	14	0
11	BT	636	0	612	13	0
11	BU	636	0	612	13	0
11	BV	636	0	612	8	0
11	BW	636	0	612	16	0
All	All	435087	0	426149	9490	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 11.

The worst 5 of 9490 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)
1:l:25:GLU:HG2	1:l:29:PRO:HD3	1.54	0.90
3:Bk:104:PRO:O	3:Bk:108:LYS:HB2	1.72	0.90
1:m:25:GLU:HG2	1:m:29:PRO:HD3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:25:GLU:HG2	1:n:29:PRO:HD3	1.55	0.87
1:k:68:PRO:HA	1:k:75:ASP:HB2	1.57	0.86

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	242/256 (94%)	210 (87%)	31 (13%)	1 (0%)	30	62
1	k	242/256 (94%)	206 (85%)	35 (14%)	1 (0%)	30	62
1	l	242/256 (94%)	205 (85%)	35 (14%)	2 (1%)	16	48
1	m	242/256 (94%)	213 (88%)	28 (12%)	1 (0%)	30	62
1	n	242/256 (94%)	210 (87%)	31 (13%)	1 (0%)	30	62
1	p	242/256 (94%)	211 (87%)	30 (12%)	1 (0%)	30	62
2	1	651/659 (99%)	586 (90%)	62 (10%)	3 (0%)	24	57
2	2	651/659 (99%)	590 (91%)	58 (9%)	3 (0%)	24	57
2	3	651/659 (99%)	584 (90%)	64 (10%)	3 (0%)	24	57
2	4	651/659 (99%)	584 (90%)	65 (10%)	2 (0%)	36	67
2	5	651/659 (99%)	588 (90%)	61 (9%)	2 (0%)	36	67
2	AD	651/659 (99%)	589 (90%)	60 (9%)	2 (0%)	36	67
2	AK	653/659 (99%)	586 (90%)	63 (10%)	4 (1%)	21	54
2	AL	653/659 (99%)	592 (91%)	58 (9%)	3 (0%)	24	57
2	AM	653/659 (99%)	584 (89%)	67 (10%)	2 (0%)	36	67
2	AN	653/659 (99%)	586 (90%)	62 (10%)	5 (1%)	16	48
2	AO	653/659 (99%)	596 (91%)	55 (8%)	2 (0%)	36	67
2	AP	653/659 (99%)	585 (90%)	64 (10%)	4 (1%)	21	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B1	653/659 (99%)	590 (90%)	60 (9%)	3 (0%)	24	57
2	B2	653/659 (99%)	594 (91%)	55 (8%)	4 (1%)	21	54
2	B3	653/659 (99%)	592 (91%)	58 (9%)	3 (0%)	24	57
2	B4	653/659 (99%)	586 (90%)	65 (10%)	2 (0%)	36	67
2	B5	653/659 (99%)	595 (91%)	54 (8%)	4 (1%)	21	54
2	B6	653/659 (99%)	579 (89%)	72 (11%)	2 (0%)	36	67
2	B7	653/659 (99%)	583 (89%)	67 (10%)	3 (0%)	24	57
2	Bp	653/659 (99%)	587 (90%)	63 (10%)	3 (0%)	24	57
2	Bq	653/659 (99%)	591 (90%)	59 (9%)	3 (0%)	24	57
2	Br	653/659 (99%)	588 (90%)	61 (9%)	4 (1%)	21	54
2	Bs	653/659 (99%)	585 (90%)	66 (10%)	2 (0%)	36	67
2	Bt	653/659 (99%)	585 (90%)	65 (10%)	3 (0%)	24	57
2	Bu	653/659 (99%)	592 (91%)	59 (9%)	2 (0%)	36	67
2	Bv	653/659 (99%)	589 (90%)	63 (10%)	1 (0%)	43	73
2	Bw	653/659 (99%)	585 (90%)	66 (10%)	2 (0%)	36	67
2	Bx	653/659 (99%)	591 (90%)	61 (9%)	1 (0%)	43	73
2	By	653/659 (99%)	587 (90%)	63 (10%)	3 (0%)	24	57
2	Bz	653/659 (99%)	581 (89%)	70 (11%)	2 (0%)	36	67
3	6	160/163 (98%)	138 (86%)	18 (11%)	4 (2%)	4	28
3	7	160/163 (98%)	141 (88%)	16 (10%)	3 (2%)	6	32
3	8	160/163 (98%)	139 (87%)	19 (12%)	2 (1%)	9	38
3	9	160/163 (98%)	140 (88%)	17 (11%)	3 (2%)	6	32
3	AA	160/163 (98%)	142 (89%)	13 (8%)	5 (3%)	3	25
3	AE	161/163 (99%)	138 (86%)	21 (13%)	2 (1%)	10	40
3	AF	161/163 (99%)	142 (88%)	18 (11%)	1 (1%)	21	54
3	AG	161/163 (99%)	140 (87%)	20 (12%)	1 (1%)	21	54
3	AH	161/163 (99%)	141 (88%)	19 (12%)	1 (1%)	21	54
3	AI	161/163 (99%)	141 (88%)	18 (11%)	2 (1%)	10	40
3	AJ	161/163 (99%)	141 (88%)	19 (12%)	1 (1%)	21	54
3	BX	161/163 (99%)	141 (88%)	17 (11%)	3 (2%)	6	32
3	BY	161/163 (99%)	141 (88%)	18 (11%)	2 (1%)	10	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	BZ	161/163 (99%)	141 (88%)	18 (11%)	2 (1%)	10	40
3	Ba	161/163 (99%)	140 (87%)	20 (12%)	1 (1%)	21	54
3	Bb	161/163 (99%)	141 (88%)	20 (12%)	0	100	100
3	Bc	161/163 (99%)	138 (86%)	21 (13%)	2 (1%)	10	40
3	Bd	161/163 (99%)	143 (89%)	17 (11%)	1 (1%)	21	54
3	Be	161/163 (99%)	142 (88%)	18 (11%)	1 (1%)	21	54
3	Bf	161/163 (99%)	143 (89%)	18 (11%)	0	100	100
3	Bg	161/163 (99%)	138 (86%)	22 (14%)	1 (1%)	21	54
3	Bh	161/163 (99%)	137 (85%)	23 (14%)	1 (1%)	21	54
3	Bi	161/163 (99%)	141 (88%)	19 (12%)	1 (1%)	21	54
3	Bj	161/163 (99%)	142 (88%)	19 (12%)	0	100	100
3	Bk	161/163 (99%)	137 (85%)	24 (15%)	0	100	100
3	Bl	161/163 (99%)	133 (83%)	27 (17%)	1 (1%)	21	54
3	Bm	161/163 (99%)	142 (88%)	17 (11%)	2 (1%)	10	40
3	Bn	161/163 (99%)	140 (87%)	18 (11%)	3 (2%)	6	32
3	Bo	161/163 (99%)	135 (84%)	25 (16%)	1 (1%)	21	54
3	o	160/163 (98%)	143 (89%)	15 (9%)	2 (1%)	9	38
4	A	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	B	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	C	77/487 (16%)	77 (100%)	0	0	100	100
4	D	77/487 (16%)	77 (100%)	0	0	100	100
4	E	77/487 (16%)	77 (100%)	0	0	100	100
4	F	77/487 (16%)	77 (100%)	0	0	100	100
4	G	77/487 (16%)	75 (97%)	2 (3%)	0	100	100
4	H	77/487 (16%)	77 (100%)	0	0	100	100
4	I	77/487 (16%)	77 (100%)	0	0	100	100
4	J	77/487 (16%)	77 (100%)	0	0	100	100
4	K	77/487 (16%)	77 (100%)	0	0	100	100
4	L	77/487 (16%)	77 (100%)	0	0	100	100
4	M	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	N	77/487 (16%)	75 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	P	77/487 (16%)	77 (100%)	0	0	100	100
4	Q	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	R	77/487 (16%)	75 (97%)	2 (3%)	0	100	100
4	S	77/487 (16%)	74 (96%)	3 (4%)	0	100	100
4	T	77/487 (16%)	75 (97%)	2 (3%)	0	100	100
4	U	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	V	77/487 (16%)	75 (97%)	2 (3%)	0	100	100
4	W	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	X	77/487 (16%)	77 (100%)	0	0	100	100
4	Y	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	Z	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	a	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	b	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	c	77/487 (16%)	77 (100%)	0	0	100	100
4	d	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	e	77/487 (16%)	75 (97%)	2 (3%)	0	100	100
4	f	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	g	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
4	h	77/487 (16%)	75 (97%)	2 (3%)	0	100	100
4	i	77/487 (16%)	77 (100%)	0	0	100	100
4	j	77/487 (16%)	76 (99%)	1 (1%)	0	100	100
5	A0	505/524 (96%)	444 (88%)	54 (11%)	7 (1%)	9	37
5	A1	505/524 (96%)	459 (91%)	40 (8%)	6 (1%)	10	40
5	A2	504/524 (96%)	454 (90%)	43 (8%)	7 (1%)	9	37
5	A3	504/524 (96%)	440 (87%)	56 (11%)	8 (2%)	7	35
5	Av	504/524 (96%)	455 (90%)	44 (9%)	5 (1%)	12	43
5	Ax	504/524 (96%)	461 (92%)	40 (8%)	3 (1%)	21	54
5	BA	496/524 (95%)	445 (90%)	45 (9%)	6 (1%)	10	40
5	BB	484/524 (92%)	445 (92%)	38 (8%)	1 (0%)	43	73
5	BD	504/524 (96%)	459 (91%)	42 (8%)	3 (1%)	21	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	BF	504/524 (96%)	463 (92%)	39 (8%)	2 (0%)	30	62
5	BG	493/524 (94%)	447 (91%)	44 (9%)	2 (0%)	30	62
5	BH	504/524 (96%)	467 (93%)	34 (7%)	3 (1%)	21	54
6	A4	454/521 (87%)	413 (91%)	40 (9%)	1 (0%)	43	73
6	A5	454/521 (87%)	423 (93%)	31 (7%)	0	100	100
6	A7	454/521 (87%)	420 (92%)	34 (8%)	0	100	100
6	A8	438/521 (84%)	396 (90%)	41 (9%)	1 (0%)	43	73
6	A9	454/521 (87%)	413 (91%)	41 (9%)	0	100	100
6	AV	454/521 (87%)	413 (91%)	41 (9%)	0	100	100
6	AW	454/521 (87%)	419 (92%)	35 (8%)	0	100	100
6	AX	454/521 (87%)	419 (92%)	35 (8%)	0	100	100
6	AZ	454/521 (87%)	423 (93%)	30 (7%)	1 (0%)	43	73
6	Ac	454/521 (87%)	415 (91%)	39 (9%)	0	100	100
6	Ad	454/521 (87%)	424 (93%)	30 (7%)	0	100	100
6	Ae	454/521 (87%)	422 (93%)	32 (7%)	0	100	100
6	Af	454/521 (87%)	414 (91%)	40 (9%)	0	100	100
6	Ag	454/521 (87%)	419 (92%)	34 (8%)	1 (0%)	43	73
6	Ah	454/521 (87%)	420 (92%)	34 (8%)	0	100	100
6	Ai	454/521 (87%)	417 (92%)	37 (8%)	0	100	100
6	Aj	454/521 (87%)	415 (91%)	38 (8%)	1 (0%)	43	73
6	Ak	454/521 (87%)	413 (91%)	40 (9%)	1 (0%)	43	73
6	Am	454/521 (87%)	420 (92%)	33 (7%)	1 (0%)	43	73
6	An	438/521 (84%)	404 (92%)	34 (8%)	0	100	100
6	Ao	435/521 (84%)	397 (91%)	36 (8%)	2 (0%)	24	57
6	Ap	438/521 (84%)	406 (93%)	31 (7%)	1 (0%)	43	73
6	Au	454/521 (87%)	419 (92%)	35 (8%)	0	100	100
6	Aw	454/521 (87%)	424 (93%)	29 (6%)	1 (0%)	43	73
6	Ay	454/521 (87%)	421 (93%)	32 (7%)	1 (0%)	43	73
6	Az	454/521 (87%)	422 (93%)	32 (7%)	0	100	100
6	BI	454/521 (87%)	420 (92%)	34 (8%)	0	100	100
6	BJ	435/521 (84%)	398 (92%)	36 (8%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BK	454/521 (87%)	415 (91%)	39 (9%)	0	100	100
6	BM	454/521 (87%)	422 (93%)	31 (7%)	1 (0%)	43	73
7	A6	306/309 (99%)	286 (94%)	20 (6%)	0	100	100
7	AY	306/309 (99%)	276 (90%)	28 (9%)	2 (1%)	18	51
7	Aa	306/309 (99%)	269 (88%)	34 (11%)	3 (1%)	12	43
7	Ab	306/309 (99%)	284 (93%)	21 (7%)	1 (0%)	36	67
7	Al	306/309 (99%)	268 (88%)	36 (12%)	2 (1%)	18	51
7	Aq	306/309 (99%)	266 (87%)	37 (12%)	3 (1%)	12	43
7	Ar	286/309 (93%)	254 (89%)	31 (11%)	1 (0%)	36	67
7	As	306/309 (99%)	276 (90%)	29 (10%)	1 (0%)	36	67
7	At	294/309 (95%)	264 (90%)	27 (9%)	3 (1%)	12	43
7	BC	306/309 (99%)	273 (89%)	32 (10%)	1 (0%)	36	67
7	BE	306/309 (99%)	284 (93%)	20 (6%)	2 (1%)	18	51
7	BL	306/309 (99%)	267 (87%)	37 (12%)	2 (1%)	18	51
8	AB	270/272 (99%)	235 (87%)	31 (12%)	4 (2%)	8	36
8	q	270/272 (99%)	237 (88%)	28 (10%)	5 (2%)	6	32
8	r	270/272 (99%)	236 (87%)	31 (12%)	3 (1%)	11	41
8	s	270/272 (99%)	240 (89%)	28 (10%)	2 (1%)	18	51
8	t	270/272 (99%)	238 (88%)	29 (11%)	3 (1%)	11	41
8	u	270/272 (99%)	237 (88%)	28 (10%)	5 (2%)	6	32
9	AC	173/176 (98%)	152 (88%)	19 (11%)	2 (1%)	10	40
9	v	173/176 (98%)	156 (90%)	15 (9%)	2 (1%)	10	40
9	w	173/176 (98%)	157 (91%)	15 (9%)	1 (1%)	21	54
9	x	173/176 (98%)	158 (91%)	14 (8%)	1 (1%)	21	54
9	y	173/176 (98%)	155 (90%)	16 (9%)	2 (1%)	10	40
9	z	173/176 (98%)	157 (91%)	14 (8%)	2 (1%)	10	40
10	AQ	94/376 (25%)	86 (92%)	8 (8%)	0	100	100
10	AR	94/376 (25%)	88 (94%)	5 (5%)	1 (1%)	11	41
10	AS	94/376 (25%)	85 (90%)	9 (10%)	0	100	100
10	AT	94/376 (25%)	81 (86%)	12 (13%)	1 (1%)	11	41
10	AU	94/376 (25%)	83 (88%)	11 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	BN	77/80 (96%)	71 (92%)	5 (6%)	1 (1%)	9	38
11	BO	77/80 (96%)	72 (94%)	4 (5%)	1 (1%)	9	38
11	BP	77/80 (96%)	69 (90%)	7 (9%)	1 (1%)	9	38
11	BQ	77/80 (96%)	70 (91%)	6 (8%)	1 (1%)	9	38
11	BR	77/80 (96%)	69 (90%)	7 (9%)	1 (1%)	9	38
11	BS	77/80 (96%)	73 (95%)	3 (4%)	1 (1%)	9	38
11	BT	77/80 (96%)	67 (87%)	9 (12%)	1 (1%)	9	38
11	BU	77/80 (96%)	68 (88%)	9 (12%)	0	100	100
11	BV	77/80 (96%)	69 (90%)	7 (9%)	1 (1%)	9	38
11	BW	77/80 (96%)	69 (90%)	7 (9%)	1 (1%)	9	38
All	All	55709/74722 (75%)	50476 (91%)	4964 (9%)	269 (0%)	26	57

5 of 269 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1	62	ALA
2	1	552	ASN
2	2	62	ALA
2	4	552	ASN
2	5	62	ALA

### 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	0	217/229 (95%)	191 (88%)	26 (12%)	5	21
1	k	217/229 (95%)	189 (87%)	28 (13%)	4	20
1	l	217/229 (95%)	193 (89%)	24 (11%)	6	24
1	m	217/229 (95%)	196 (90%)	21 (10%)	8	29
1	n	217/229 (95%)	196 (90%)	21 (10%)	8	29
1	p	217/229 (95%)	195 (90%)	22 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	532/536 (99%)	486 (91%)	46 (9%)	10	33
2	2	532/536 (99%)	495 (93%)	37 (7%)	14	40
2	3	532/536 (99%)	494 (93%)	38 (7%)	13	39
2	4	532/536 (99%)	493 (93%)	39 (7%)	13	39
2	5	532/536 (99%)	496 (93%)	36 (7%)	14	40
2	AD	532/536 (99%)	492 (92%)	40 (8%)	12	38
2	AK	534/536 (100%)	478 (90%)	56 (10%)	6	26
2	AL	534/536 (100%)	489 (92%)	45 (8%)	10	34
2	AM	534/536 (100%)	487 (91%)	47 (9%)	9	33
2	AN	534/536 (100%)	494 (92%)	40 (8%)	12	38
2	AO	534/536 (100%)	487 (91%)	47 (9%)	9	33
2	AP	534/536 (100%)	479 (90%)	55 (10%)	7	27
2	B1	534/536 (100%)	482 (90%)	52 (10%)	8	29
2	B2	534/536 (100%)	491 (92%)	43 (8%)	11	35
2	B3	534/536 (100%)	484 (91%)	50 (9%)	8	30
2	B4	534/536 (100%)	489 (92%)	45 (8%)	10	34
2	B5	534/536 (100%)	490 (92%)	44 (8%)	10	35
2	B6	534/536 (100%)	486 (91%)	48 (9%)	9	32
2	B7	534/536 (100%)	487 (91%)	47 (9%)	9	33
2	Bp	534/536 (100%)	498 (93%)	36 (7%)	15	41
2	Bq	534/536 (100%)	485 (91%)	49 (9%)	8	31
2	Br	534/536 (100%)	484 (91%)	50 (9%)	8	30
2	Bs	534/536 (100%)	494 (92%)	40 (8%)	12	38
2	Bt	534/536 (100%)	482 (90%)	52 (10%)	8	29
2	Bu	534/536 (100%)	481 (90%)	53 (10%)	7	28
2	Bv	534/536 (100%)	484 (91%)	50 (9%)	8	30
2	Bw	534/536 (100%)	478 (90%)	56 (10%)	6	26
2	Bx	534/536 (100%)	489 (92%)	45 (8%)	10	34
2	By	534/536 (100%)	484 (91%)	50 (9%)	8	30
2	Bz	534/536 (100%)	493 (92%)	41 (8%)	12	37
3	6	136/137 (99%)	120 (88%)	16 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	7	136/137 (99%)	120 (88%)	16 (12%)	5	22
3	8	136/137 (99%)	119 (88%)	17 (12%)	4	21
3	9	136/137 (99%)	116 (85%)	20 (15%)	3	17
3	AA	136/137 (99%)	121 (89%)	15 (11%)	6	24
3	AE	137/137 (100%)	118 (86%)	19 (14%)	3	18
3	AF	137/137 (100%)	116 (85%)	21 (15%)	3	16
3	AG	137/137 (100%)	119 (87%)	18 (13%)	4	20
3	AH	137/137 (100%)	118 (86%)	19 (14%)	3	18
3	AI	137/137 (100%)	123 (90%)	14 (10%)	7	27
3	AJ	137/137 (100%)	118 (86%)	19 (14%)	3	18
3	BX	137/137 (100%)	118 (86%)	19 (14%)	3	18
3	BY	137/137 (100%)	120 (88%)	17 (12%)	4	21
3	BZ	137/137 (100%)	117 (85%)	20 (15%)	3	17
3	Ba	137/137 (100%)	120 (88%)	17 (12%)	4	21
3	Bb	137/137 (100%)	122 (89%)	15 (11%)	6	25
3	Bc	137/137 (100%)	125 (91%)	12 (9%)	9	33
3	Bd	137/137 (100%)	120 (88%)	17 (12%)	4	21
3	Be	137/137 (100%)	121 (88%)	16 (12%)	5	22
3	Bf	137/137 (100%)	117 (85%)	20 (15%)	3	17
3	Bg	137/137 (100%)	117 (85%)	20 (15%)	3	17
3	Bh	137/137 (100%)	116 (85%)	21 (15%)	3	16
3	Bi	137/137 (100%)	122 (89%)	15 (11%)	6	25
3	Bj	137/137 (100%)	116 (85%)	21 (15%)	3	16
3	Bk	137/137 (100%)	117 (85%)	20 (15%)	3	17
3	Bl	137/137 (100%)	116 (85%)	21 (15%)	3	16
3	Bm	137/137 (100%)	120 (88%)	17 (12%)	4	21
3	Bn	137/137 (100%)	125 (91%)	12 (9%)	9	33
3	Bo	137/137 (100%)	120 (88%)	17 (12%)	4	21
3	o	136/137 (99%)	115 (85%)	21 (15%)	2	15
4	A	69/419 (16%)	68 (99%)	1 (1%)	59	70
4	B	69/419 (16%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	69/419 (16%)	69 (100%)	0	100	100
4	D	69/419 (16%)	67 (97%)	2 (3%)	37	58
4	E	69/419 (16%)	68 (99%)	1 (1%)	59	70
4	F	69/419 (16%)	68 (99%)	1 (1%)	59	70
4	G	69/419 (16%)	69 (100%)	0	100	100
4	H	69/419 (16%)	69 (100%)	0	100	100
4	I	69/419 (16%)	69 (100%)	0	100	100
4	J	69/419 (16%)	69 (100%)	0	100	100
4	K	69/419 (16%)	68 (99%)	1 (1%)	59	70
4	L	69/419 (16%)	69 (100%)	0	100	100
4	M	69/419 (16%)	69 (100%)	0	100	100
4	N	69/419 (16%)	69 (100%)	0	100	100
4	O	69/419 (16%)	68 (99%)	1 (1%)	59	70
4	P	69/419 (16%)	68 (99%)	1 (1%)	59	70
4	Q	69/419 (16%)	67 (97%)	2 (3%)	37	58
4	R	69/419 (16%)	69 (100%)	0	100	100
4	S	69/419 (16%)	68 (99%)	1 (1%)	59	70
4	T	69/419 (16%)	68 (99%)	1 (1%)	59	70
4	U	69/419 (16%)	69 (100%)	0	100	100
4	V	69/419 (16%)	67 (97%)	2 (3%)	37	58
4	W	69/419 (16%)	67 (97%)	2 (3%)	37	58
4	X	69/419 (16%)	66 (96%)	3 (4%)	26	50
4	Y	69/419 (16%)	67 (97%)	2 (3%)	37	58
4	Z	69/419 (16%)	68 (99%)	1 (1%)	59	70
4	a	69/419 (16%)	69 (100%)	0	100	100
4	b	69/419 (16%)	69 (100%)	0	100	100
4	c	69/419 (16%)	68 (99%)	1 (1%)	59	70
4	d	69/419 (16%)	69 (100%)	0	100	100
4	e	69/419 (16%)	69 (100%)	0	100	100
4	f	69/419 (16%)	67 (97%)	2 (3%)	37	58
4	g	69/419 (16%)	68 (99%)	1 (1%)	59	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	h	69/419 (16%)	67 (97%)	2 (3%)	37	58
4	i	69/419 (16%)	69 (100%)	0	100	100
4	j	69/419 (16%)	69 (100%)	0	100	100
5	A0	449/465 (97%)	400 (89%)	49 (11%)	6	25
5	A1	449/465 (97%)	392 (87%)	57 (13%)	4	21
5	A2	448/465 (96%)	398 (89%)	50 (11%)	6	24
5	A3	448/465 (96%)	390 (87%)	58 (13%)	4	20
5	Av	448/465 (96%)	388 (87%)	60 (13%)	4	19
5	Ax	448/465 (96%)	401 (90%)	47 (10%)	6	26
5	BA	441/465 (95%)	394 (89%)	47 (11%)	6	25
5	BB	435/465 (94%)	393 (90%)	42 (10%)	8	29
5	BD	448/465 (96%)	385 (86%)	63 (14%)	3	18
5	BF	448/465 (96%)	400 (89%)	48 (11%)	6	25
5	BG	436/465 (94%)	385 (88%)	51 (12%)	5	22
5	BH	438/465 (94%)	385 (88%)	53 (12%)	5	21
6	A4	345/400 (86%)	320 (93%)	25 (7%)	13	39
6	A5	345/400 (86%)	326 (94%)	19 (6%)	19	45
6	A7	345/400 (86%)	324 (94%)	21 (6%)	17	43
6	A8	335/400 (84%)	317 (95%)	18 (5%)	20	45
6	A9	345/400 (86%)	330 (96%)	15 (4%)	26	50
6	AV	345/400 (86%)	321 (93%)	24 (7%)	14	40
6	AW	345/400 (86%)	328 (95%)	17 (5%)	22	47
6	AX	345/400 (86%)	314 (91%)	31 (9%)	9	32
6	AZ	345/400 (86%)	312 (90%)	33 (10%)	8	29
6	Ac	345/400 (86%)	324 (94%)	21 (6%)	17	43
6	Ad	345/400 (86%)	323 (94%)	22 (6%)	16	42
6	Ae	345/400 (86%)	319 (92%)	26 (8%)	12	38
6	Af	345/400 (86%)	326 (94%)	19 (6%)	19	45
6	Ag	345/400 (86%)	330 (96%)	15 (4%)	26	50
6	Ah	345/400 (86%)	330 (96%)	15 (4%)	26	50
6	Ai	345/400 (86%)	330 (96%)	15 (4%)	26	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Aj	345/400 (86%)	329 (95%)	16 (5%)	24	48
6	Ak	345/400 (86%)	331 (96%)	14 (4%)	27	51
6	Am	345/400 (86%)	327 (95%)	18 (5%)	21	46
6	An	335/400 (84%)	317 (95%)	18 (5%)	20	45
6	Ao	333/400 (83%)	312 (94%)	21 (6%)	16	42
6	Ap	335/400 (84%)	314 (94%)	21 (6%)	16	42
6	Au	345/400 (86%)	325 (94%)	20 (6%)	18	44
6	Aw	345/400 (86%)	320 (93%)	25 (7%)	13	39
6	Ay	345/400 (86%)	316 (92%)	29 (8%)	10	34
6	Az	345/400 (86%)	322 (93%)	23 (7%)	15	41
6	BI	345/400 (86%)	326 (94%)	19 (6%)	19	45
6	BJ	333/400 (83%)	311 (93%)	22 (7%)	15	41
6	BK	345/400 (86%)	329 (95%)	16 (5%)	24	48
6	BM	345/400 (86%)	328 (95%)	17 (5%)	22	47
7	A6	259/260 (100%)	234 (90%)	25 (10%)	8	29
7	AY	258/260 (99%)	234 (91%)	24 (9%)	8	30
7	Aa	259/260 (100%)	235 (91%)	24 (9%)	8	30
7	Ab	259/260 (100%)	234 (90%)	25 (10%)	8	29
7	Al	258/260 (99%)	236 (92%)	22 (8%)	10	33
7	Aq	259/260 (100%)	234 (90%)	25 (10%)	8	29
7	Ar	247/260 (95%)	228 (92%)	19 (8%)	12	37
7	As	259/260 (100%)	233 (90%)	26 (10%)	7	28
7	At	251/260 (96%)	224 (89%)	27 (11%)	6	25
7	BC	259/260 (100%)	235 (91%)	24 (9%)	8	30
7	BE	259/260 (100%)	238 (92%)	21 (8%)	11	35
7	BL	259/260 (100%)	230 (89%)	29 (11%)	6	24
8	AB	250/250 (100%)	224 (90%)	26 (10%)	7	26
8	q	250/250 (100%)	230 (92%)	20 (8%)	11	36
8	r	250/250 (100%)	226 (90%)	24 (10%)	8	29
8	s	250/250 (100%)	222 (89%)	28 (11%)	6	24
8	t	250/250 (100%)	227 (91%)	23 (9%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	u	250/250 (100%)	229 (92%)	21 (8%)	10	34
9	AC	156/157 (99%)	144 (92%)	12 (8%)	12	37
9	v	156/157 (99%)	148 (95%)	8 (5%)	21	46
9	w	156/157 (99%)	147 (94%)	9 (6%)	18	44
9	x	156/157 (99%)	145 (93%)	11 (7%)	13	39
9	y	156/157 (99%)	144 (92%)	12 (8%)	12	37
9	z	156/157 (99%)	145 (93%)	11 (7%)	13	39
10	AQ	87/319 (27%)	85 (98%)	2 (2%)	44	63
10	AR	87/319 (27%)	85 (98%)	2 (2%)	44	63
10	AS	87/319 (27%)	84 (97%)	3 (3%)	32	55
10	AT	87/319 (27%)	86 (99%)	1 (1%)	65	73
10	AU	87/319 (27%)	86 (99%)	1 (1%)	65	73
11	BN	67/68 (98%)	64 (96%)	3 (4%)	24	48
11	BO	67/68 (98%)	63 (94%)	4 (6%)	17	43
11	BP	67/68 (98%)	64 (96%)	3 (4%)	24	48
11	BQ	67/68 (98%)	64 (96%)	3 (4%)	24	48
11	BR	67/68 (98%)	64 (96%)	3 (4%)	24	48
11	BS	67/68 (98%)	64 (96%)	3 (4%)	24	48
11	BT	67/68 (98%)	63 (94%)	4 (6%)	17	43
11	BU	67/68 (98%)	65 (97%)	2 (3%)	36	57
11	BV	67/68 (98%)	64 (96%)	3 (4%)	24	48
11	BW	67/68 (98%)	64 (96%)	3 (4%)	24	48
All	All	46157/62065 (74%)	42302 (92%)	3855 (8%)	12	34

5 of 3855 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	Az	130	VAL
4	f	36	THR
7	BC	28	GLU
2	Bz	455	LYS
8	u	60	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 468 such sidechains are listed below:

Mol	Chain	Res	Type
2	B1	462	ASN
1	p	121	ASN
7	BC	239	GLN
1	n	182	ASN
4	I	73	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

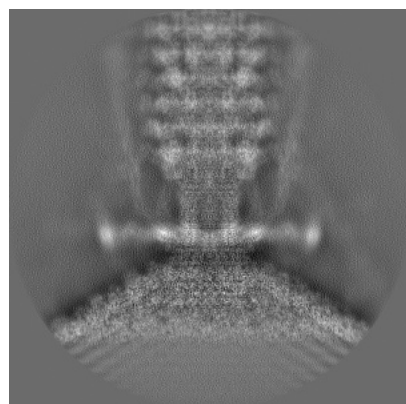
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48458. These allow visual inspection of the internal detail of the map and identification of artifacts.

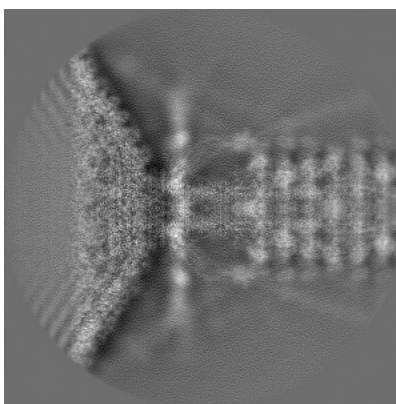
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

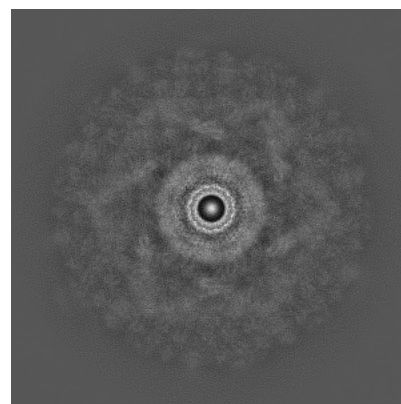
#### 6.1.1 Primary map



X

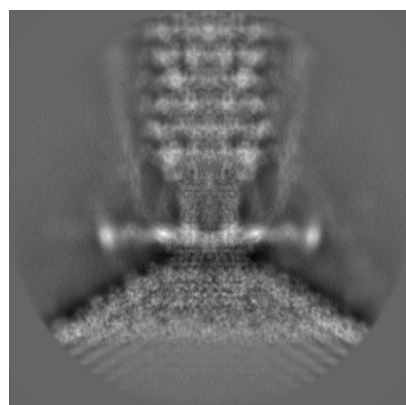


Y

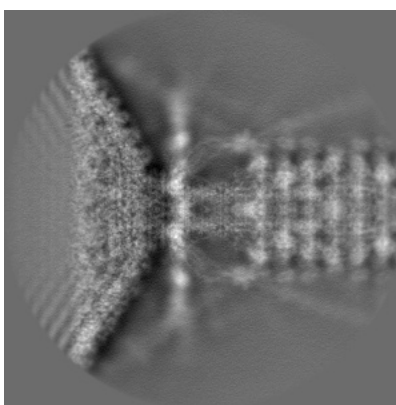


Z

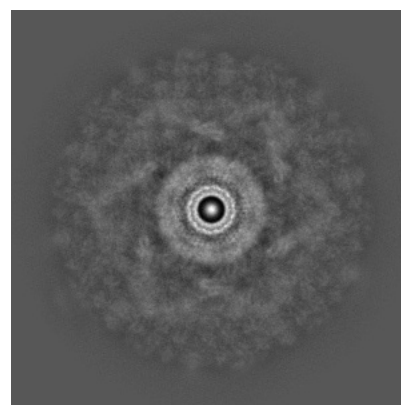
#### 6.1.2 Raw map



X



Y

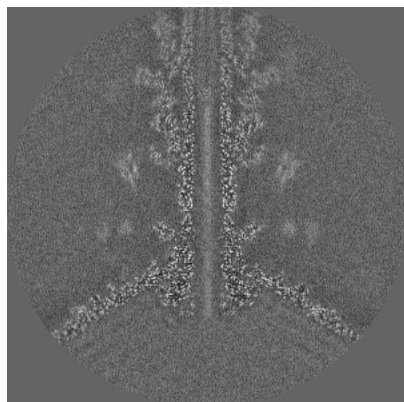


Z

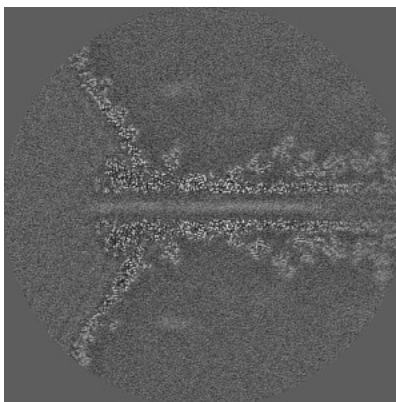
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

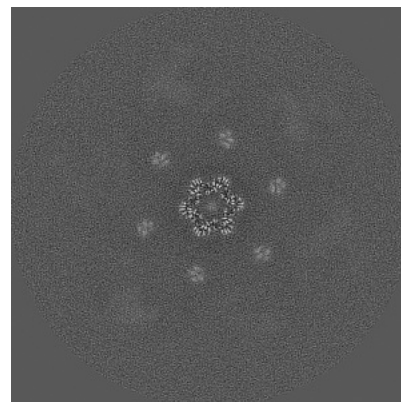
### 6.2.1 Primary map



X Index: 200

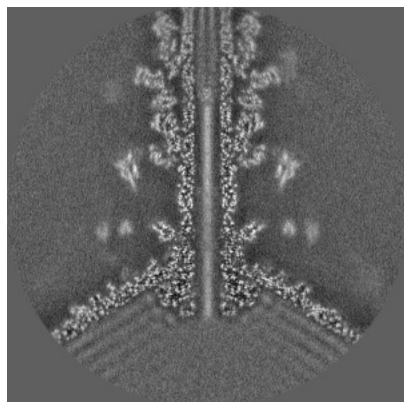


Y Index: 200

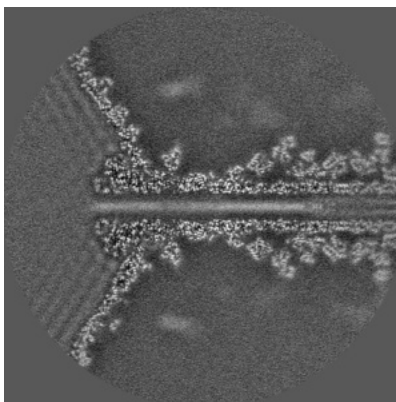


Z Index: 200

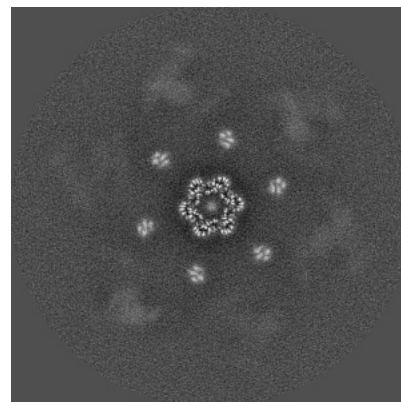
### 6.2.2 Raw map



X Index: 200



Y Index: 200

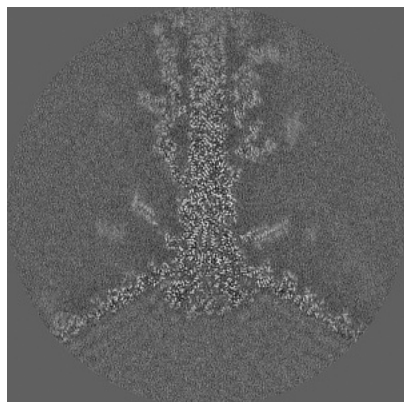


Z Index: 200

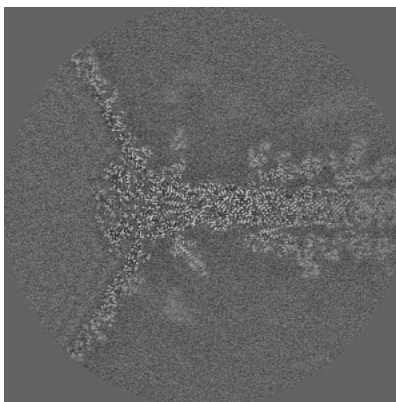
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

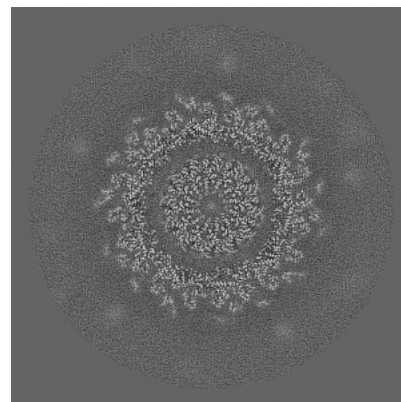
### 6.3.1 Primary map



X Index: 184

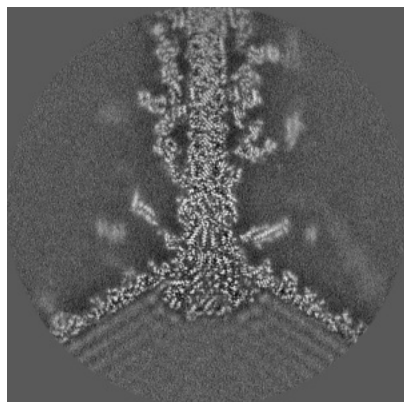


Y Index: 184

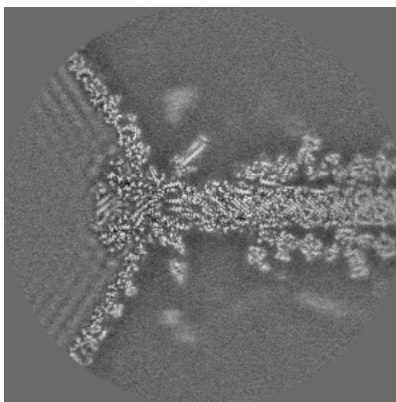


Z Index: 115

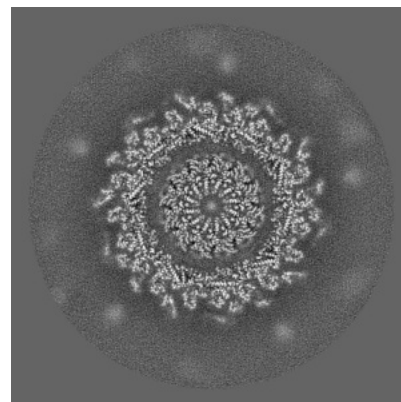
### 6.3.2 Raw map



X Index: 184



Y Index: 215

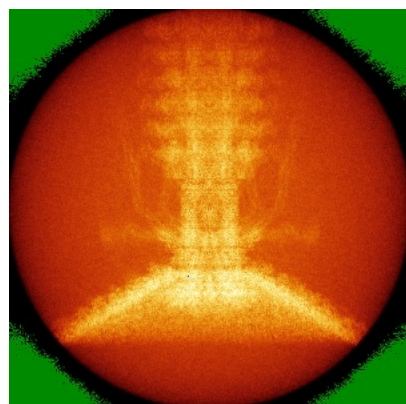


Z Index: 115

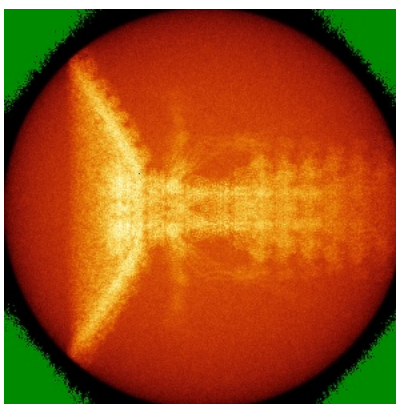
The images above show the largest variance slices of the map in three orthogonal directions.

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

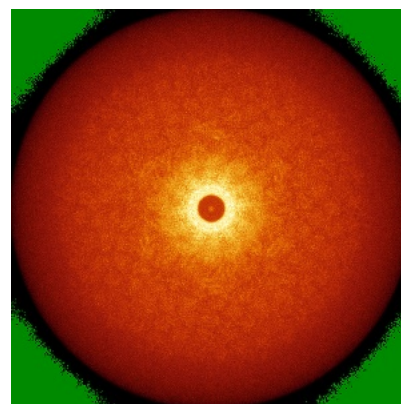
### 6.4.1 Primary map



X

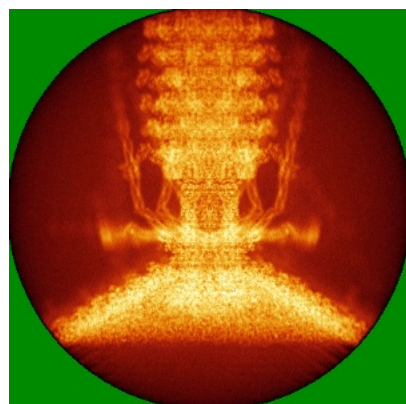


Y

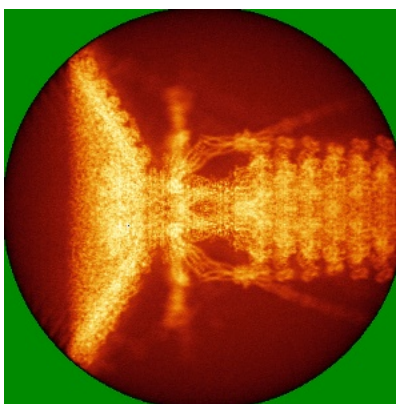


Z

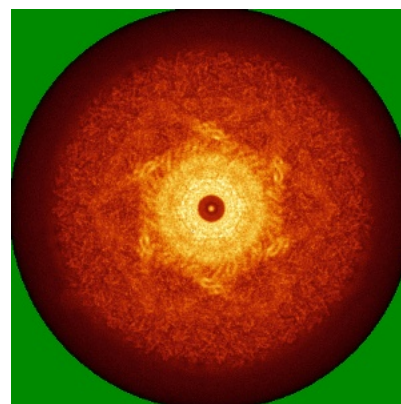
### 6.4.2 Raw map



X



Y



Z

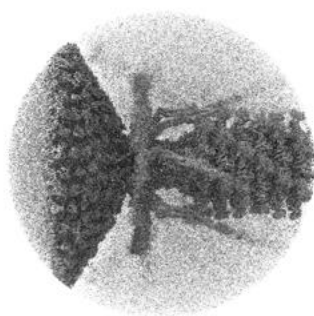
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

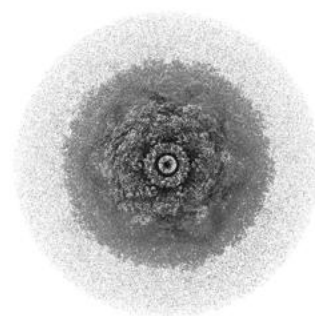
### 6.5.1 Primary map



X



Y



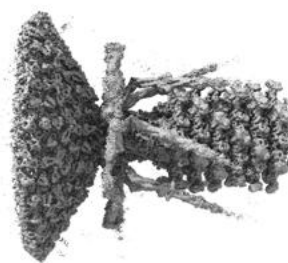
Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

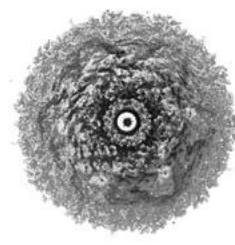
### 6.5.2 Raw map



X



Y



Z

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

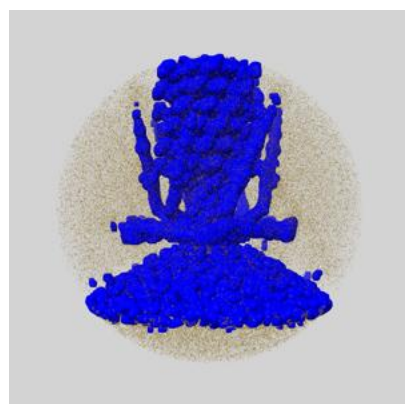
## 6.6 Mask visualisation [i](#)

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

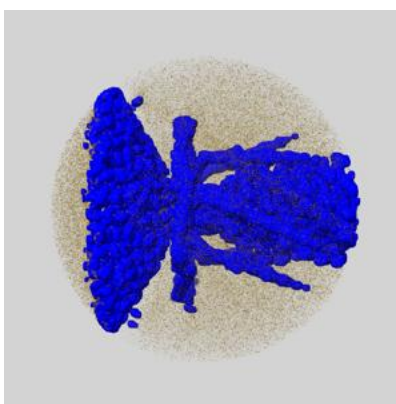
A mask typically either:

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

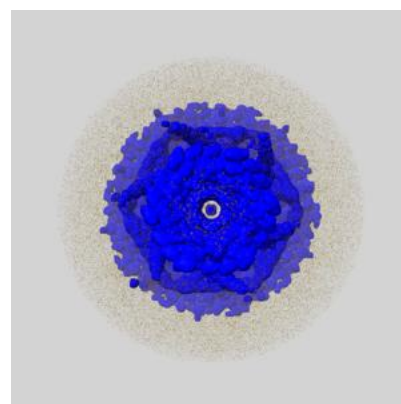
### 6.6.1 emd\_48458\_msk\_1.map [i](#)



X



Y

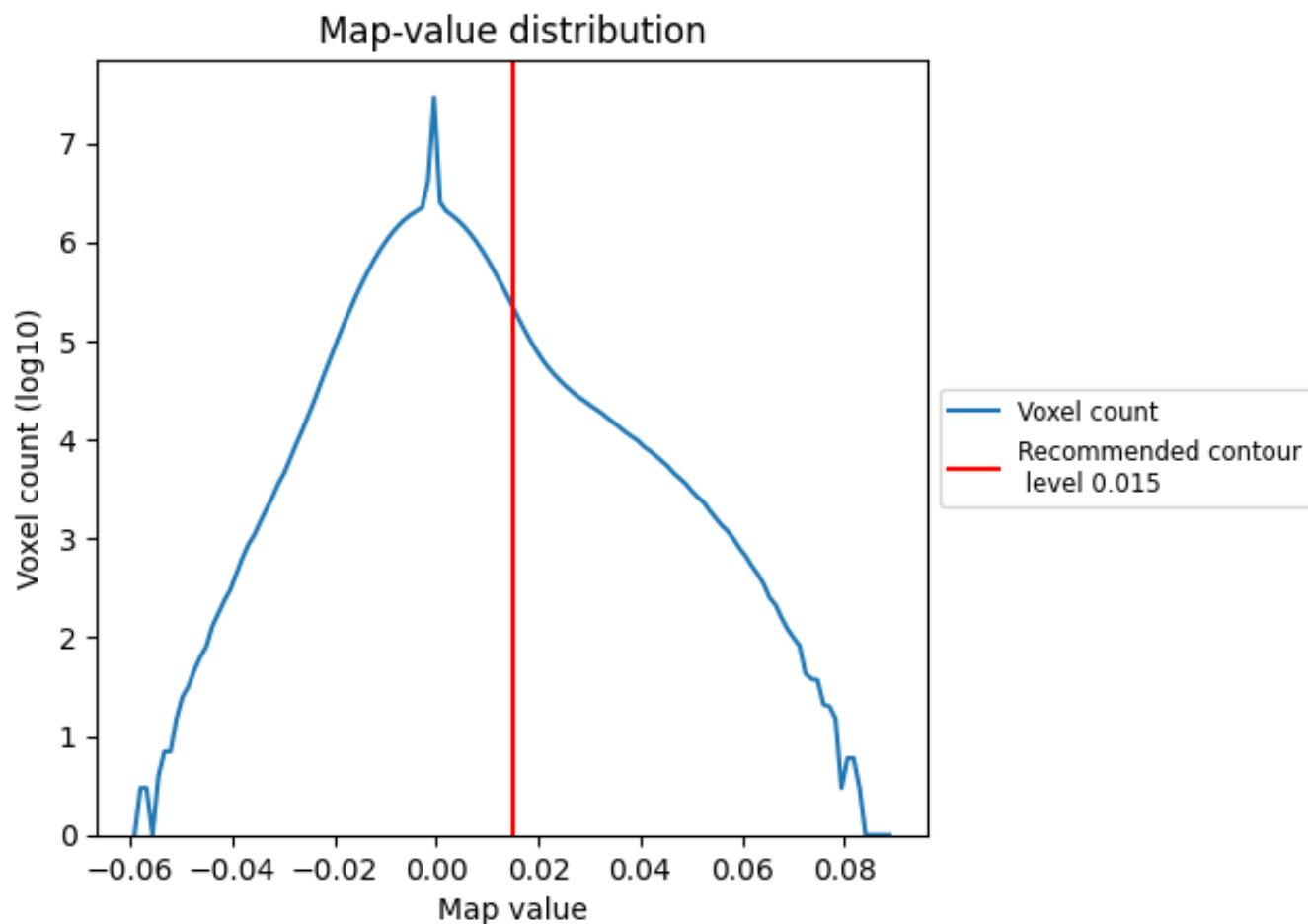


Z

## 7 Map analysis [i](#)

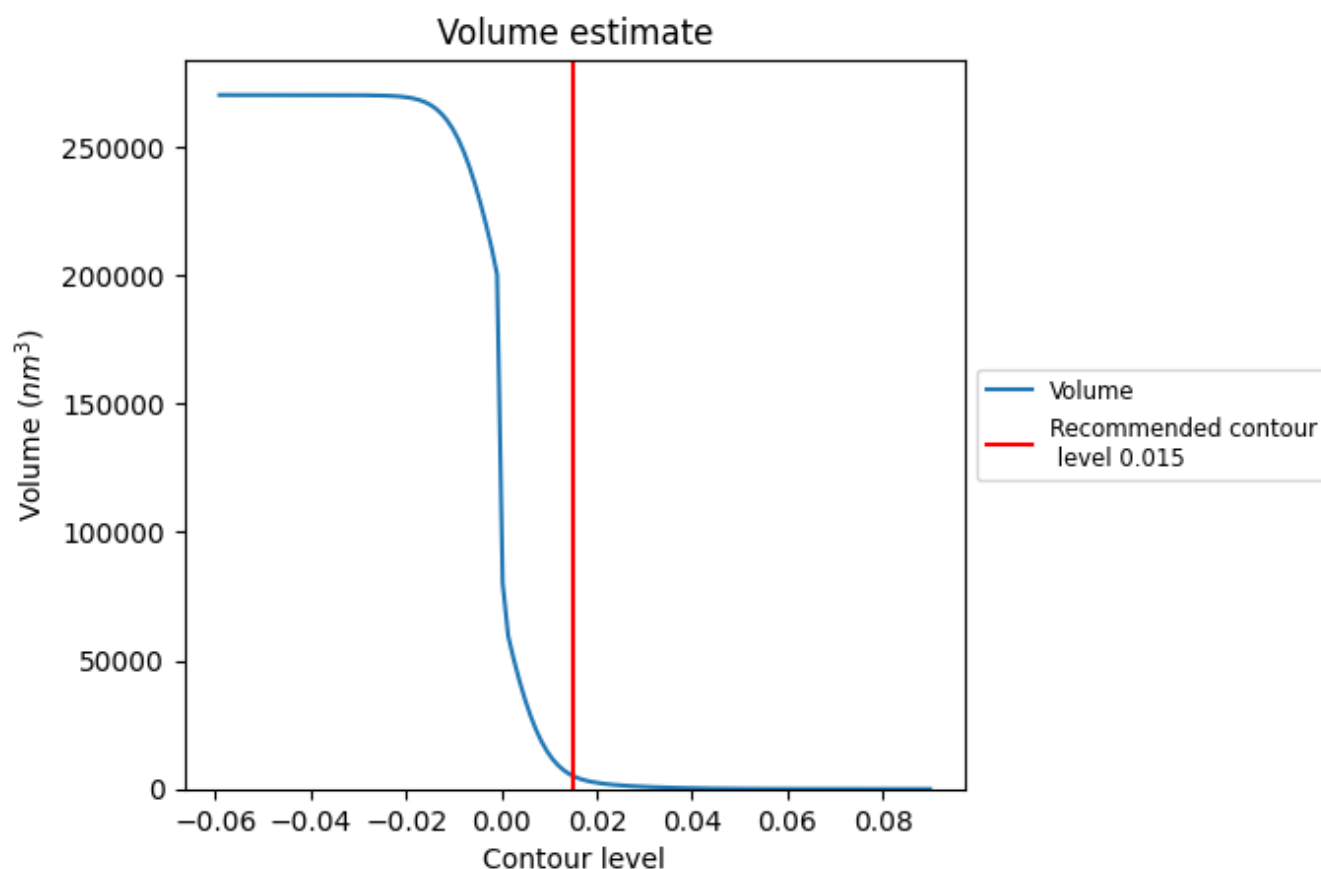
This section contains the results of statistical analysis of the map.

### 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.

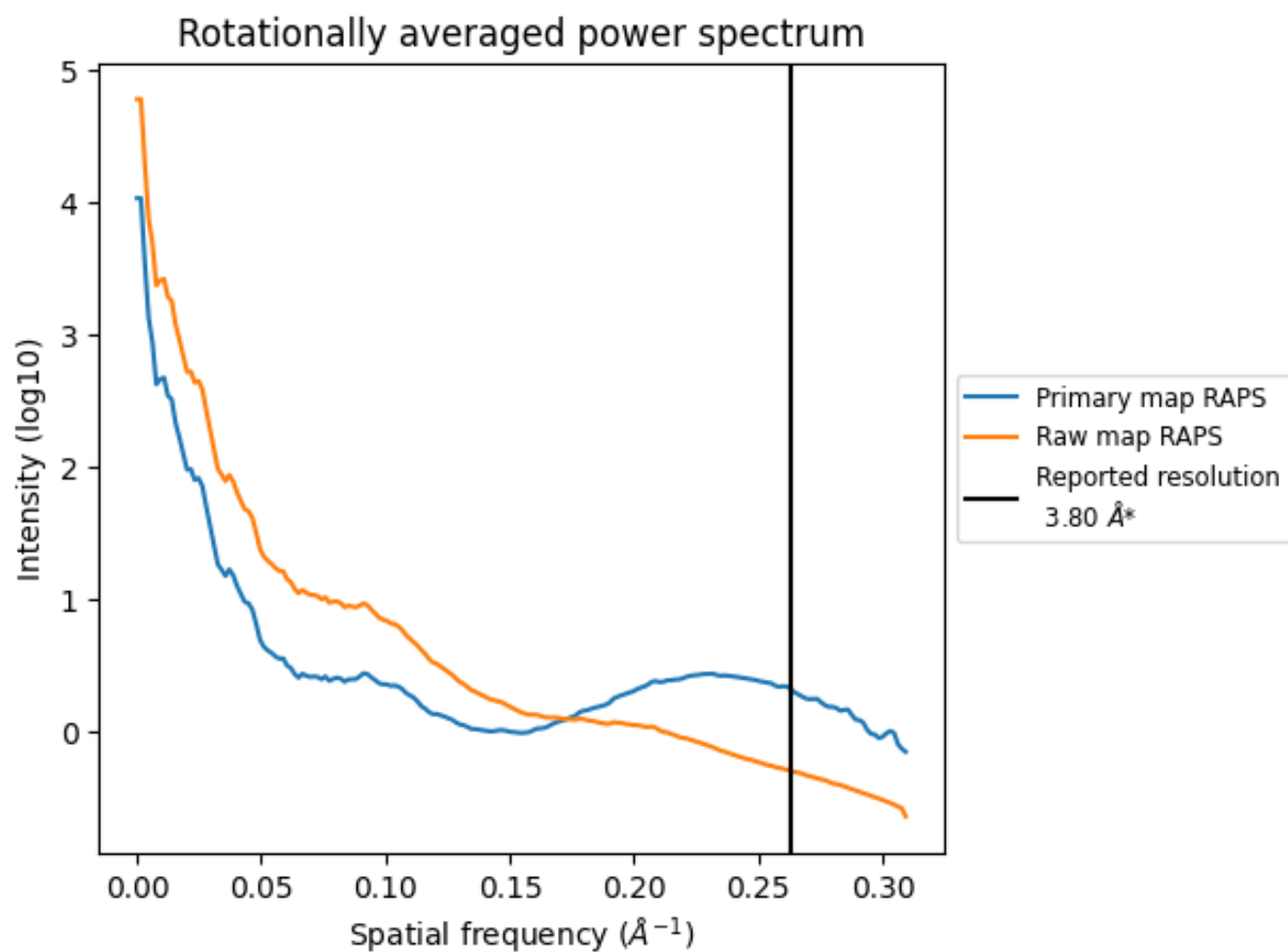
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51411 nm<sup>3</sup>; this corresponds to an approximate mass of 4644 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 ⓘ

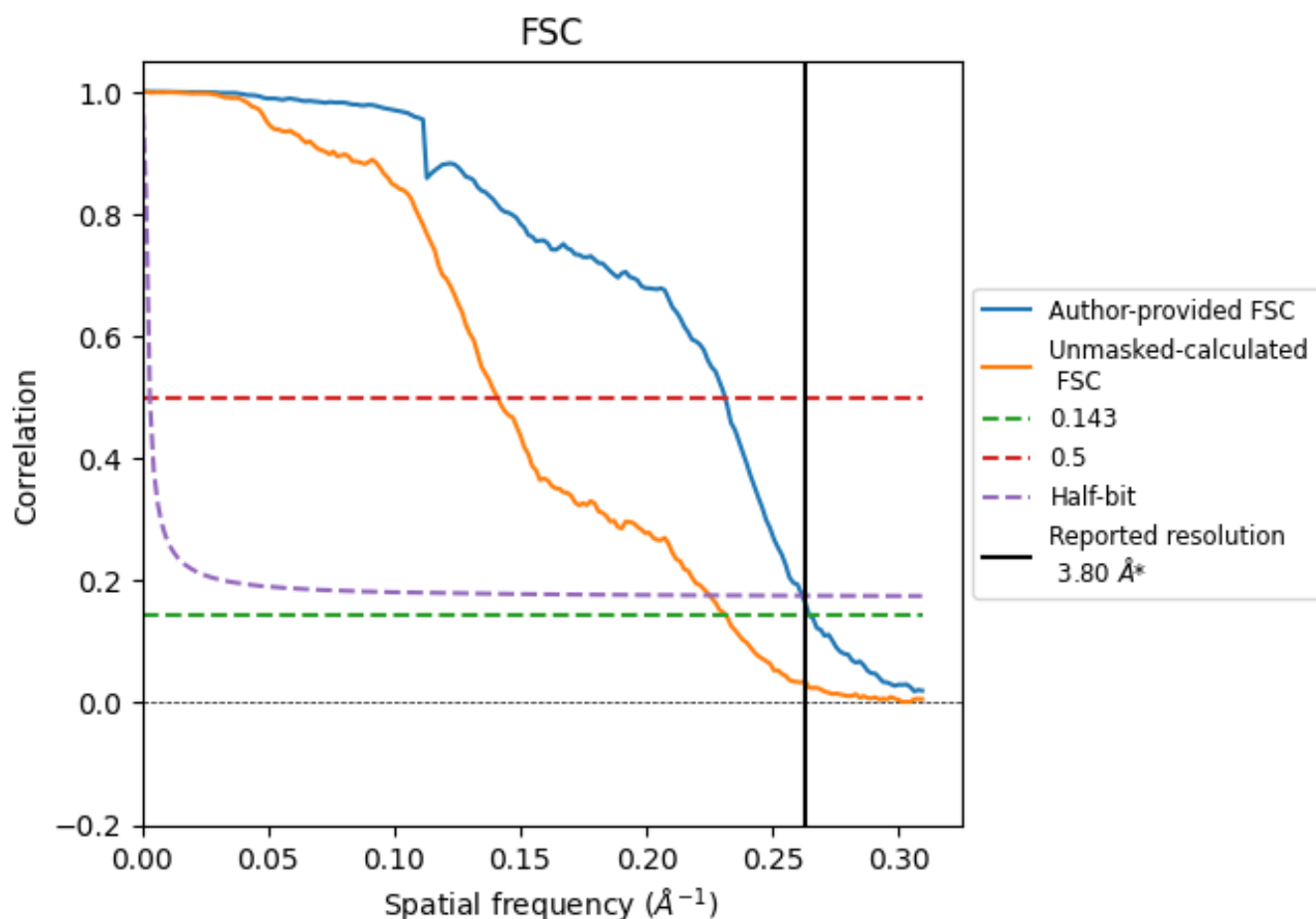


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.33	3.82
Unmasked-calculated*	4.32	7.10	4.44

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.32 differs from the reported value 3.8 by more than 10 %

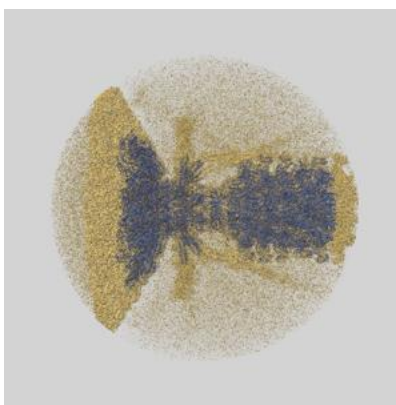
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48458 and PDB model 9MOF. Per-residue inclusion information can be found in section [3](#) on page [23](#).

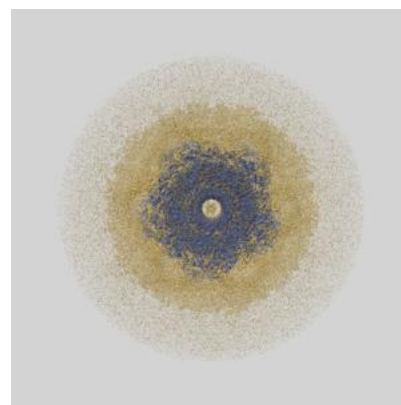
### 9.1 Map-model overlay [i](#)



X



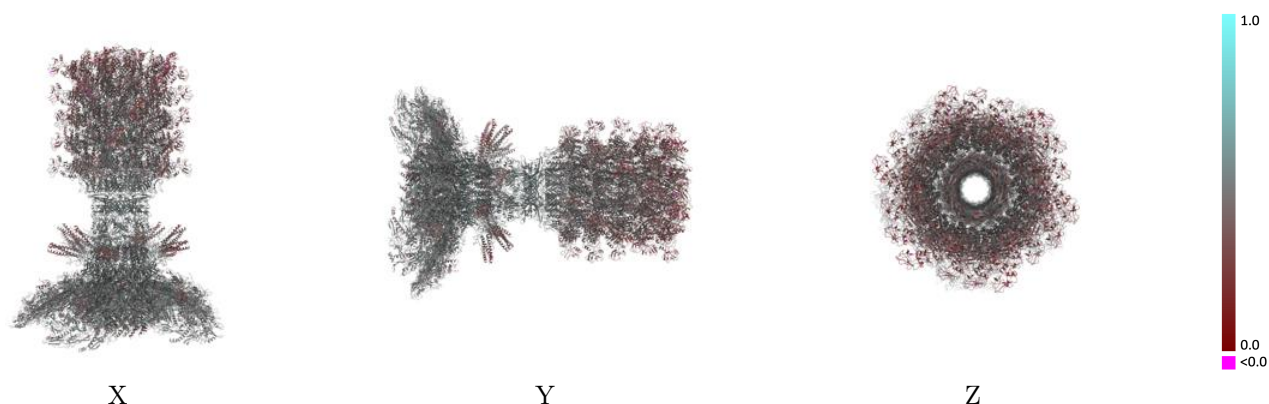
Y



Z

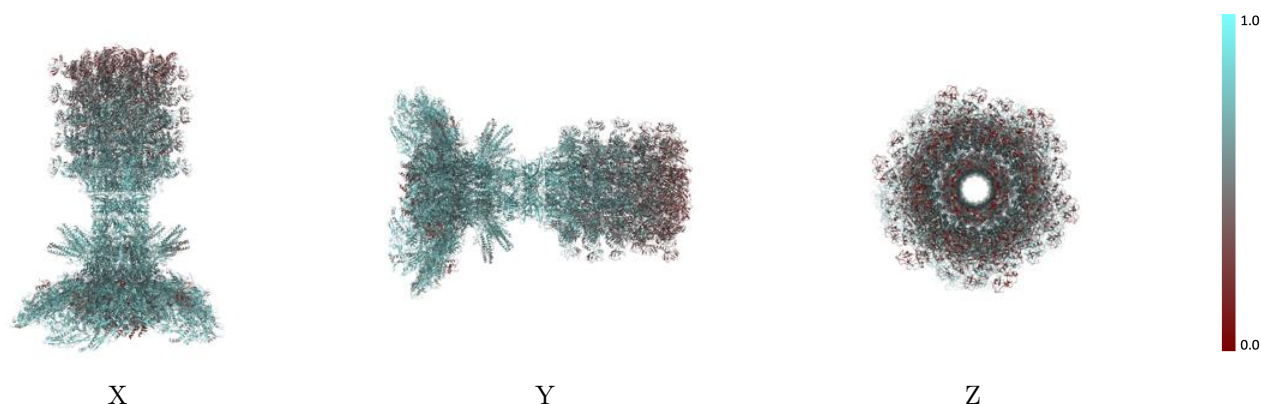
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



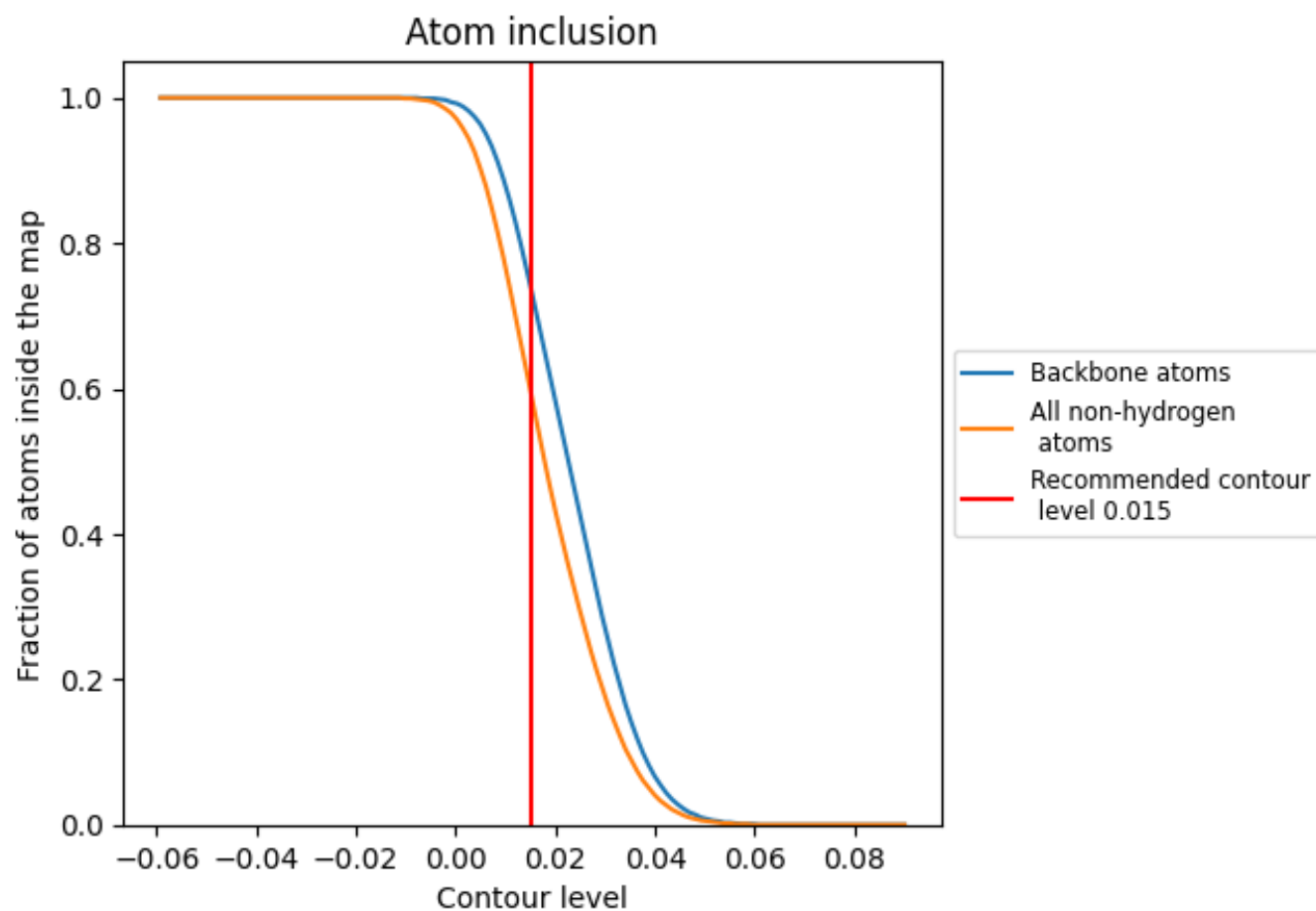
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 74% of all backbone atoms, 60% 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	 0.5960	 0.4460
0	 0.7510	 0.5060
1	 0.6370	 0.4330
2	 0.6330	 0.4280
3	 0.6410	 0.4320
4	 0.6490	 0.4340
5	 0.6450	 0.4300
6	 0.6820	 0.4960
7	 0.6860	 0.4970
8	 0.7000	 0.4940
9	 0.6980	 0.5070
A	 0.6740	 0.4400
A0	 0.5520	 0.4700
A1	 0.5420	 0.4710
A2	 0.5400	 0.4600
A3	 0.5550	 0.4680
A4	 0.6720	 0.4820
A5	 0.6670	 0.4790
A6	 0.6800	 0.4920
A7	 0.6820	 0.4840
A8	 0.6870	 0.4890
A9	 0.6890	 0.4910
AA	 0.6970	 0.5060
AB	 0.7490	 0.4970
AC	 0.7210	 0.5090
AD	 0.6360	 0.4300
AE	 0.6730	 0.4890
AF	 0.6650	 0.4960
AG	 0.6550	 0.4890
AH	 0.6640	 0.4860
AI	 0.6560	 0.4900
AJ	 0.6460	 0.4830
AK	 0.5860	 0.4210
AL	 0.5830	 0.4180
AM	 0.5760	 0.4170























































































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Chain	Atom inclusion	Q-score
AN	 0.5570	 0.4110
AO	 0.5570	 0.4090
AP	 0.5690	 0.4120
AQ	 0.2760	 0.3540
AR	 0.3000	 0.3680
AS	 0.3120	 0.3770
AT	 0.3180	 0.3670
AU	 0.3330	 0.3880
AV	 0.6960	 0.4960
AW	 0.6550	 0.4700
AX	 0.6850	 0.4880
AY	 0.6960	 0.5000
AZ	 0.6840	 0.4940
Aa	 0.6870	 0.5030
Ab	 0.6910	 0.4970
Ac	 0.6690	 0.4750
Ad	 0.6790	 0.4800
Ae	 0.6730	 0.4820
Af	 0.6520	 0.4660
Ag	 0.6540	 0.4700
Ah	 0.6700	 0.4800
Ai	 0.6530	 0.4710
Aj	 0.6610	 0.4760
Ak	 0.6730	 0.4800
Al	 0.6760	 0.4900
Am	 0.6820	 0.4880
An	 0.6790	 0.4850
Ao	 0.6910	 0.4910
Ap	 0.6900	 0.4880
Aq	 0.6780	 0.4940
Ar	 0.7000	 0.4960
As	 0.6730	 0.4950
At	 0.6500	 0.4800
Au	 0.6970	 0.4940
Av	 0.5470	 0.4710
Aw	 0.6750	 0.4860
Ax	 0.5600	 0.4760
Ay	 0.6840	 0.4930
Az	 0.6690	 0.4790
B	 0.6850	 0.4550
B1	 0.3570	 0.3380
B2	 0.5220	 0.3920





















































































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Chain	Atom inclusion	Q-score
B3	 0.4490	 0.3750
B4	 0.3390	 0.3300
B5	 0.5150	 0.3970
B6	 0.4460	 0.3710
B7	 0.3490	 0.3440
BA	 0.5610	 0.4710
BB	 0.5610	 0.4750
BC	 0.6750	 0.4940
BD	 0.5440	 0.4680
BE	 0.6880	 0.4960
BF	 0.5440	 0.4640
BG	 0.5640	 0.4710
BH	 0.5550	 0.4700
BI	 0.6780	 0.4860
BJ	 0.6950	 0.4890
BK	 0.7000	 0.4920
BL	 0.6830	 0.4930
BM	 0.6950	 0.4920
BN	 0.6780	 0.4890
BO	 0.6850	 0.4830
BP	 0.6750	 0.4740
BQ	 0.6720	 0.4710
BR	 0.6850	 0.4870
BS	 0.6740	 0.4720
BT	 0.6830	 0.4730
BU	 0.6590	 0.4660
BV	 0.6990	 0.4950
BW	 0.6820	 0.4820
BX	 0.5800	 0.4750
BY	 0.4890	 0.4440
BZ	 0.3490	 0.4000
Ba	 0.5980	 0.4740
Bb	 0.4960	 0.4430
Bc	 0.3290	 0.3990
Bd	 0.5960	 0.4700
Be	 0.4800	 0.4330
Bf	 0.3290	 0.4020
Bg	 0.5970	 0.4800
Bh	 0.4750	 0.4350
Bi	 0.3450	 0.3830
Bj	 0.5920	 0.4690
Bk	 0.4800	 0.4460















































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Chain	Atom inclusion	Q-score
Bl	 0.3250	 0.3940
Bm	 0.5930	 0.4790
Bn	 0.4710	 0.4370
Bo	 0.3320	 0.3980
Bp	 0.5430	 0.4020
Bq	 0.4620	 0.3810
Br	 0.3510	 0.3370
Bs	 0.5480	 0.4050
Bt	 0.4750	 0.3800
Bu	 0.3620	 0.3440
Bv	 0.5520	 0.4100
Bw	 0.4800	 0.3830
Bx	 0.3650	 0.3360
By	 0.5350	 0.3980
Bz	 0.4580	 0.3770
C	 0.6730	 0.4530
D	 0.6800	 0.4410
E	 0.6800	 0.4370
F	 0.6850	 0.4320
G	 0.7270	 0.4400
H	 0.7020	 0.4370
I	 0.6970	 0.4280
J	 0.6880	 0.4450
K	 0.6980	 0.4290
L	 0.6710	 0.4370
M	 0.6320	 0.3820
N	 0.6190	 0.3890
O	 0.6390	 0.4300
P	 0.6530	 0.4100
Q	 0.6780	 0.4350
R	 0.6810	 0.4310
S	 0.6610	 0.4310
T	 0.6800	 0.4340
U	 0.6510	 0.4330
V	 0.6730	 0.4140
W	 0.6440	 0.4090
X	 0.6420	 0.3940
Y	 0.6510	 0.4250
Z	 0.6590	 0.4080
a	 0.6220	 0.3840
b	 0.6290	 0.4020
c	 0.6120	 0.3760

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Chain	Atom inclusion	Q-score
d	 0.6260	 0.3850
e	 0.6140	 0.3820
f	 0.6370	 0.4130
g	 0.6360	 0.4150
h	 0.6190	 0.4280
i	 0.6000	 0.4120
j	 0.5970	 0.4130
k	 0.7490	 0.4990
l	 0.7400	 0.5020
m	 0.7480	 0.5010
n	 0.7550	 0.5020
o	 0.6970	 0.5070
p	 0.7510	 0.4980
q	 0.7380	 0.4950
r	 0.7460	 0.4980
s	 0.7390	 0.4910
t	 0.7340	 0.4960
u	 0.7410	 0.4940
v	 0.7210	 0.5080
w	 0.7140	 0.5030
x	 0.7200	 0.5080
y	 0.7340	 0.5070
z	 0.7160	 0.5050