



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 1, 2018 – 04:32 PM EST

PDB ID : 5IV5  
EMDB ID: : EMD-3374  
Title : Cryo-electron microscopy structure of the hexagonal pre-attachment T4 baseplate-tail tube complex  
Authors : Taylor, N.M.I.; Guerrero-Ferreira, R.C.; Goldie, K.N.; Stahlberg, H.; Leiman, P.G.  
Deposited on : 2016-03-19  
Resolution : 4.11 Å(reported)  
Based on PDB ID : 4KU0, 1H6W, 1OCY, 1K28, 3H2T, 4HRZ, 1N7Z, 1S2E, 1EL6, 2FKK

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

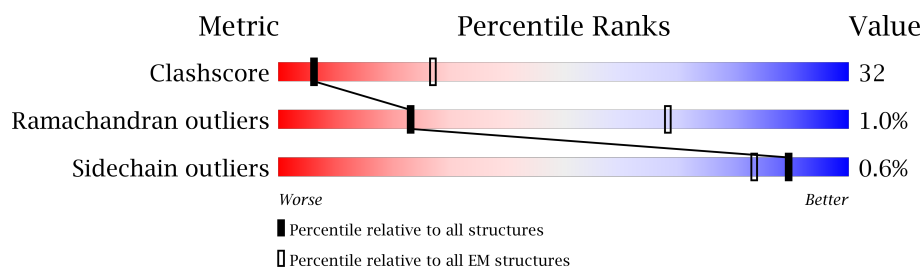
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.11 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.




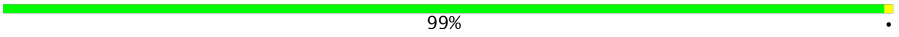
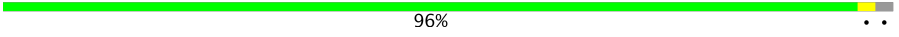

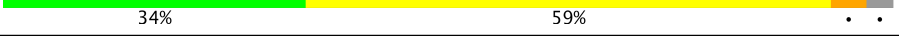
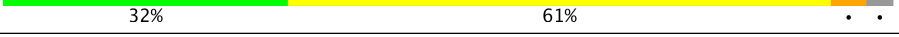
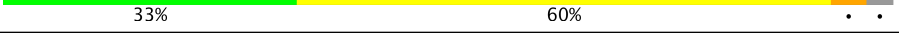

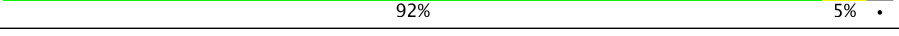

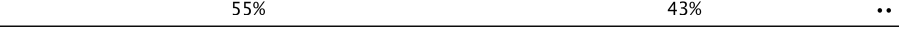
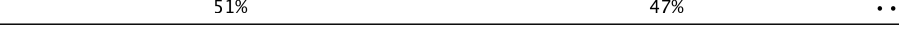

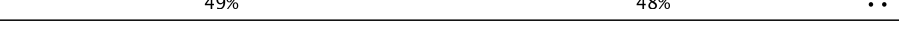


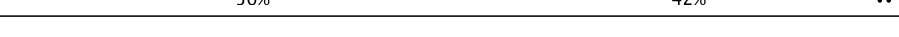
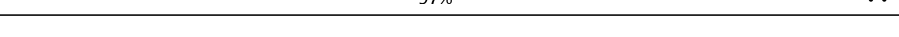
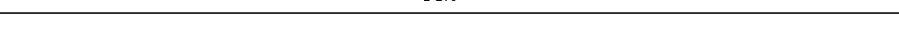






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	660	
1	B	660	
1	BH	660	
1	BI	660	
1	EA	660	
1	EB	660	
1	GD	660	
1	GE	660	
1	X	660	














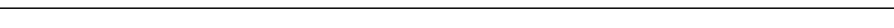











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Mol	Chain	Length	Quality of chain
1	Y	660	
1	u	660	
1	v	660	
2	BJ	1032	
2	C	1032	
2	EC	1032	
2	GF	1032	
2	Z	1032	
2	w	1032	
3	CA	334	
3	CB	334	
3	D	334	
3	E	334	
3	ED	334	
3	EE	334	
3	GG	334	
3	GH	334	
3	a	334	
3	b	334	
3	x	334	
3	y	334	
4	AA	288	
4	AB	288	
4	CC	288	
4	CD	288	




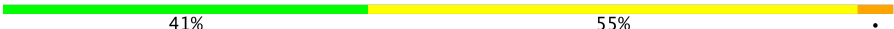
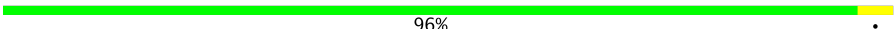

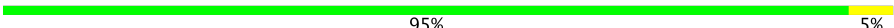















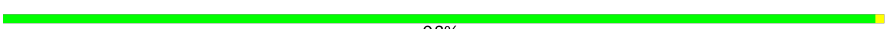


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Mol	Chain	Length	Quality of chain
4	CE	288	 57% 42% .
4	EF	288	 57% 42% .
4	EG	288	 57% 42% .
4	EH	288	 56% 43% .
4	F	288	 59% 40% .
4	G	288	 57% 42% .
4	GI	288	 58% 41% .
4	GJ	288	 57% 42% .
4	H	288	 58% 41% .
4	HA	288	 57% 42% .
4	c	288	 99% .
4	d	288	 99% .
4	e	288	 99% .
4	z	288	 99% .
5	AC	602	 41% 55% .
5	AD	602	 39% 57% .
5	AE	602	 41% 55% .
5	CF	602	 40% 57% .
5	CG	602	 37% 59% .
5	CH	602	 41% 55% .
5	EI	602	 40% 56% .
5	EJ	602	 38% 59% .
5	FA	602	 40% 56% .
5	HB	602	 40% 56% .
5	HC	602	 38% 59% .





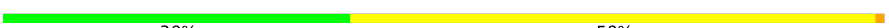
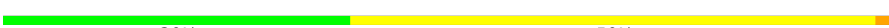







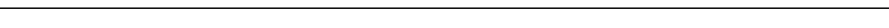


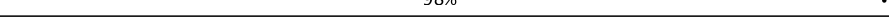
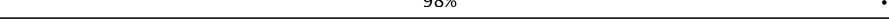
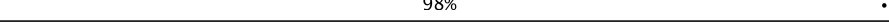






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Mol	Chain	Length	Quality of chain
5	HD	602	 40% 56% .
5	I	602	 40% 56% .
5	J	602	 39% 57% .
5	K	602	 41% 55% .
5	f	602	 96% .
5	g	602	 95% 5%
5	h	602	 95% 5%
6	AF	219	 51% 47% .
6	AG	219	 57% 42% .
6	AH	219	 56% 42% .
6	CI	219	 52% 46% .
6	CJ	219	 57% 42% .
6	DA	219	 57% 42%
6	FB	219	 52% 46% .
6	FC	219	 55% 43% .
6	FD	219	 52% 47%
6	HE	219	 55% 43% .
6	HF	219	 56% 42% .
6	HG	219	 55% 44%
6	L	219	 53% 45% .
6	M	219	 54% 44% .
6	N	219	 52% 47%
6	i	219	 98% .
6	j	219	 98% .
6	k	219	 98% .




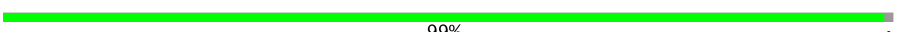
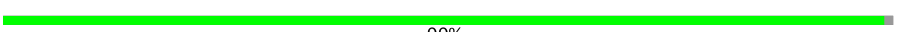







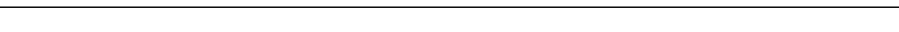

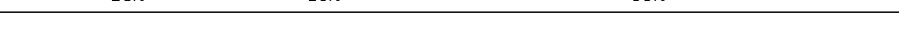

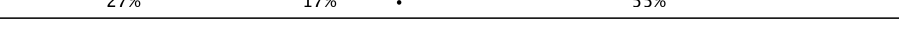






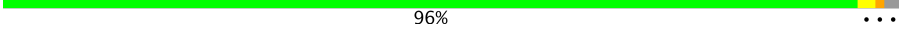
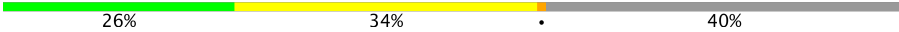
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Mol	Chain	Length	Quality of chain
7	AI	527	 41% 57%
7	AJ	527	 40% 59%
7	BA	527	 39% 59%
7	DB	527	 40% 58%
7	DC	527	 39% 59%
7	DD	527	 39% 59%
7	FE	527	 40% 59%
7	FF	527	 39% 61%
7	FG	527	 38% 60%
7	HH	527	 42% 57%
7	HI	527	 40% 59%
7	HJ	527	 39% 59%
7	O	527	 40% 58%
7	P	527	 39% 60%
7	Q	527	 39% 59%
7	l	527	 98%
7	m	527	 98%
7	n	527	 98%
8	BB	163	 47% 53%
8	BC	163	 47% 53%
8	DE	163	 46% 53%
8	DF	163	 44% 56%
8	FH	163	 45% 54%
8	FI	163	 44% 55%
8	IA	163	 45% 54%


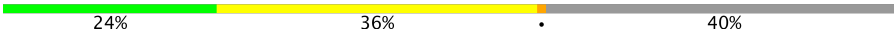






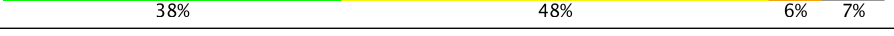

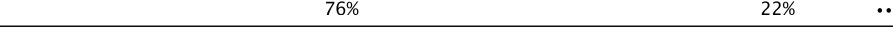
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Mol	Chain	Length	Quality of chain
8	IB	163	
8	R	163	
8	S	163	
8	o	163	
8	p	163	
9	BD	132	
9	DG	132	
9	FJ	132	
9	IC	132	
9	T	132	
9	q	132	
10	BE	364	
10	DH	364	
10	GA	364	
10	ID	364	
10	U	364	
10	r	364	
11	BF	196	
11	DI	196	
11	GB	196	
11	IE	196	
11	V	196	
11	s	196	
12	BG	320	
12	DJ	320	

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Mol	Chain	Length	Quality of chain
12	GC	320	
12	IF	320	
12	W	320	
12	t	320	
13	YA	575	
13	YB	575	
13	YC	575	
14	YD	391	
14	YE	391	
14	YF	391	
15	ZA	97	

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 549576 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 Baseplate wedge protein gp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
1	B	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
1	X	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
1	Y	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
1	u	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
1	v	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
1	BH	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
1	BI	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
1	EA	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
1	EB	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
1	GD	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
1	GE	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		

- Molecule 2 is a protein called Baseplate wedge protein gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
2	Z	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
2	w	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BJ	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
2	EC	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
2	GF	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		

- Molecule 3 is a protein called Baseplate wedge protein gp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	E	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	a	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	b	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	x	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	y	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	CA	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	CB	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	ED	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	EE	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	GG	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	GH	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		

- Molecule 4 is a protein called Baseplate wedge protein gp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	G	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	c	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	d	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	e	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	z	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	AA	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	AB	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	CC	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	CD	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	CE	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	EF	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	EG	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	EH	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	GI	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	GJ	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	HA	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		

- Molecule 5 is a protein called Baseplate wedge protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	J	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	K	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	g	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	h	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	AC	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	AD	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	AE	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	CF	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	CG	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	CH	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	EI	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	EJ	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	FA	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	HB	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	HC	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	HD	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		

- Molecule 6 is a protein called Baseplate wedge protein gp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	M	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	N	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	i	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	k	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	AF	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	AG	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	AH	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	CI	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	CJ	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	DA	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	FB	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	FC	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	FD	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	HE	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	HF	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	HG	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		

- Molecule 7 is a protein called Short tail fiber protein gp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	P	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	Q	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	l	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	m	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	n	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	AI	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	AJ	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	BA	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	DB	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	DC	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	DD	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	FE	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	FF	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	FG	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	HH	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	HI	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		
7	HJ	526	Total	C	N	O	S	0	0
			3945	2429	702	803	11		

- Molecule 8 is a protein called Tail tube protein gp19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
8	S	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
8	o	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
8	p	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
8	BB	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
8	BC	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	DE	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
8	DF	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
8	FH	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
8	FI	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
8	IA	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		
8	IB	162	Total	C	N	O	S	0	0
			1296	823	218	252	3		

- Molecule 9 is a protein called Baseplate wedge protein gp25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
9	q	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
9	BD	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
9	DG	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
9	FJ	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
9	IC	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		

- Molecule 10 is a protein called Baseplate tail-tube protein gp48.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	165	Total	C	N	O	S	0	0
			1317	846	219	247	5		
10	r	165	Total	C	N	O	S	0	0
			1317	846	219	247	5		
10	BE	165	Total	C	N	O	S	0	0
			1317	846	219	247	5		
10	DH	165	Total	C	N	O	S	0	0
			1317	846	219	247	5		
10	GA	165	Total	C	N	O	S	0	0
			1317	846	219	247	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	ID	165	Total	C	N	O	S	0	0
			1317	846	219	247	5		

- Molecule 11 is a protein called Baseplate wedge protein gp53.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
11	s	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
11	BF	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
11	DI	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
11	GB	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
11	IE	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		

- Molecule 12 is a protein called Baseplate tail-tube protein gp54.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	W	192	Total	C	N	O	S	0	0
			1524	955	257	301	11		
12	t	192	Total	C	N	O	S	0	0
			1524	955	257	301	11		
12	BG	192	Total	C	N	O	S	0	0
			1524	955	257	301	11		
12	DJ	192	Total	C	N	O	S	0	0
			1524	955	257	301	11		
12	GC	192	Total	C	N	O	S	0	0
			1524	955	257	301	11		
12	IF	192	Total	C	N	O	S	0	0
			1524	955	257	301	11		

- Molecule 13 is a protein called Peptidoglycan hydrolase gp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	YA	554	Total	C	N	O	S	554	0
			25692	15942	4536	5088	126		
13	YB	554	Total	C	N	O	S	554	0
			25692	15942	4536	5088	126		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	YC	554	Total	C	N	O	S	554	0
			25692	15942	4536	5088	126		

- Molecule 14 is a protein called Baseplate hub protein gp27.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	YD	364	Total	C	N	O	S	364	0
			17472	11148	2868	3354	102		
14	YE	364	Total	C	N	O	S	364	0
			17472	11148	2868	3354	102		
14	YF	364	Total	C	N	O	S	364	0
			17472	11148	2868	3354	102		

- Molecule 15 is a protein called Uncharacterized 10.2 kDa protein in segC-Gp6 intergenic region.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	ZA	96	Total	C	N	O	S	96	0
			4254	2682	720	834	18		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	AI	1	Total	Zn	0
			1	1	
16	FE	1	Total	Zn	0
			1	1	
16	O	1	Total	Zn	0
			1	1	
16	l	1	Total	Zn	0
			1	1	
16	HH	1	Total	Zn	0
			1	1	
16	DB	1	Total	Zn	0
			1	1	

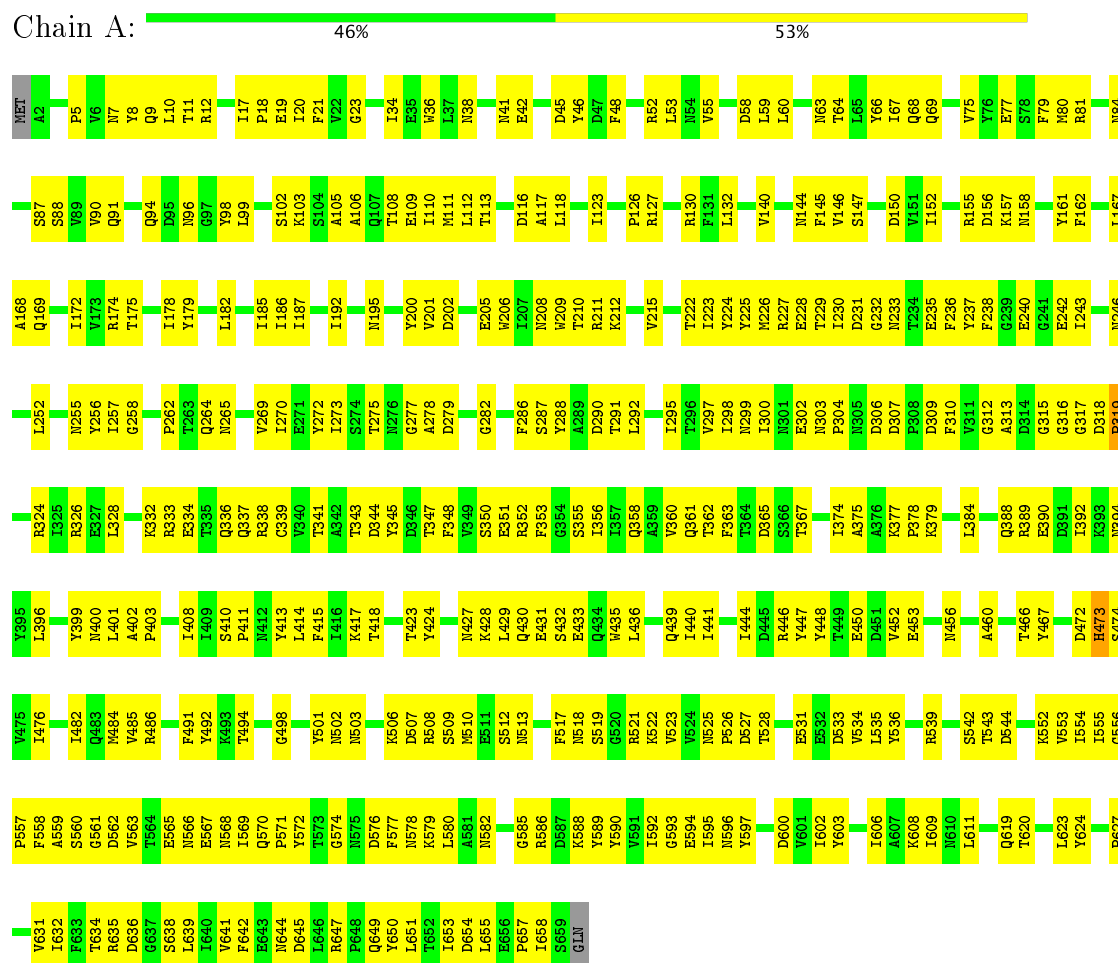
- Molecule 17 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
17	ZA	1	Total	Fe	1
			6	6	

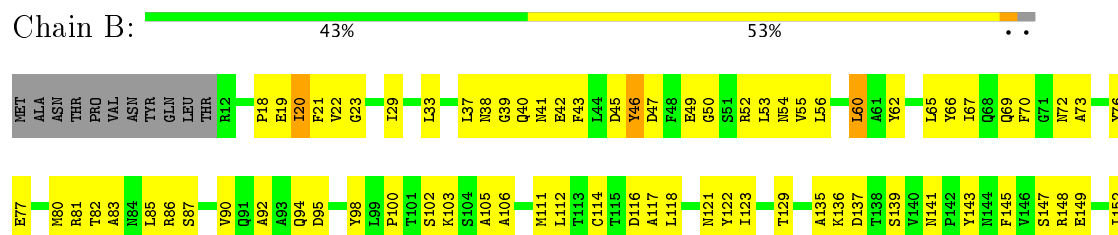
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: Baseplate wedge protein gp6



#### • Molecule 1: Baseplate wedge protein gp6

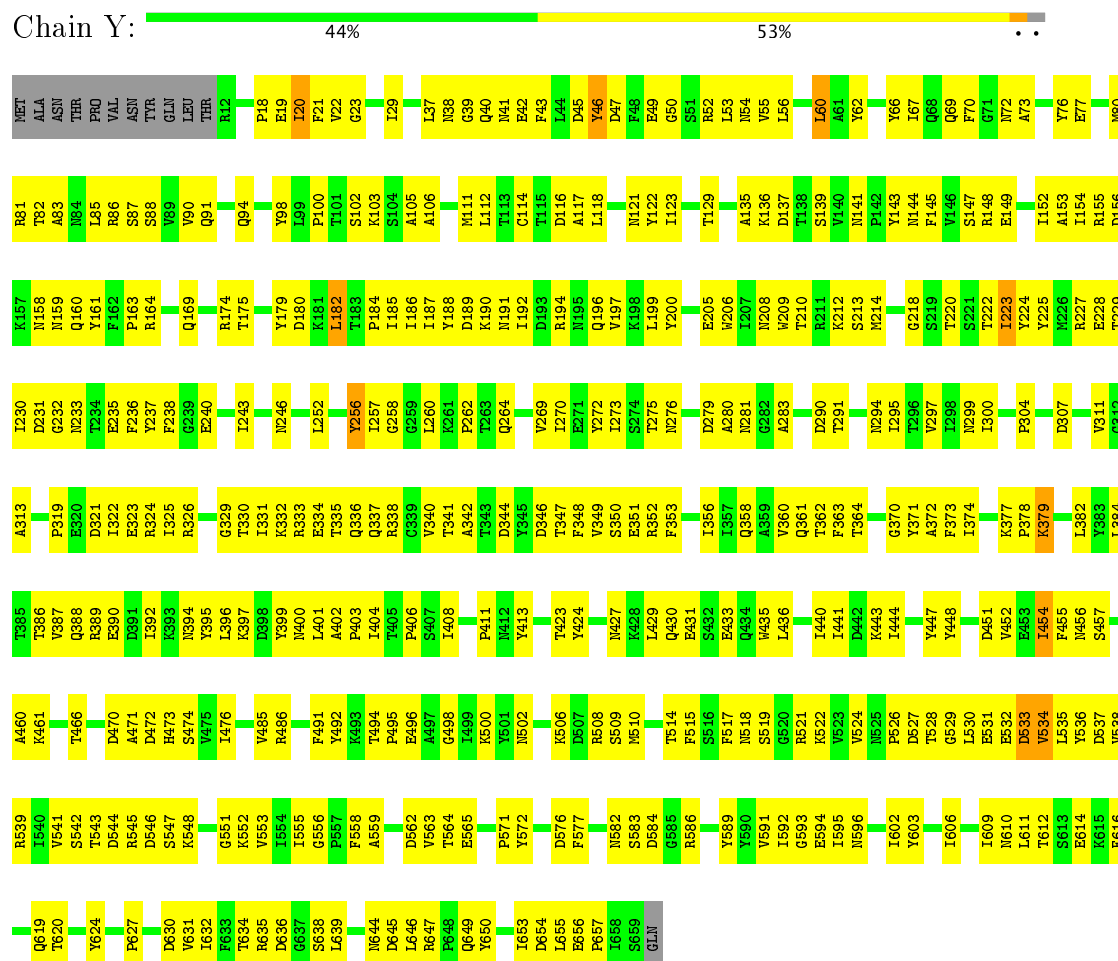


F633	S560	L396	P319	MET	S88	A168	A251	P326	L396	I482	G561	F633	Y224	P304	D451	P378	P304	Y224	A153
T634	G561	Y399	R326	A2	V89	Q169	L252	R327	Y399	Q483	D562	T634	Y225	P307	V452	K379	P307	Y225	I154
R635	D562	M400	R327	P5	V90	I172	L252	E327	M400	E327	D563	R635	D226	D307	Y535	S380	D307	D226	R155
D636	V563	L401	L328	N7	Q94	V173	N255	L328	L401	N7	E327	D636	E228	V311	Y536	G381	V311	E228	D156
G637	T654	A402	L328	N7	Q94	V173	N255	L328	A402	N7	E327	G637	T629	G312	Y538	L382	G312	T629	N158
S638	E565	P403	L328	N7	Q94	V173	N255	L328	P403	N7	E327	S638	I230	A313	Y539	L384	A313	I230	N159
L639	N566	P403	L328	N7	Q94	V173	N255	L328	P403	N7	E327	L639	D231	A313	Y540	L384	A313	D231	Q160
I640	E567	P403	L328	N7	Q94	V173	N255	L328	P403	N7	E327	I640	D232	A313	Y541	L384	A313	D232	Y161
V641	N568	L408	E334	R11	G97	L110	T620	E334	L408	R11	E334	V641	D233	P319	Y542	T386	P319	D233	F162
F642	F569	I409	T335	R11	G97	L110	T620	T335	I409	R11	E334	F642	D234	D321	Y543	Q388	D321	D234	P163
E643	Q570	S410	T335	R11	G97	L110	T620	T335	S410	R11	E334	E643	D235	D321	Y544	Q388	D321	D235	R164
N644	P571	P411	Q337	Q264	N265	L182	T175	Q337	P411	Q337	E334	N644	D236	D321	Y545	Q388	D321	D236	E235
D645	Y572	G498	R338	N265	L182	T175	T175	R338	G498	N265	E334	D645	D237	D321	Y546	Q388	D321	D237	E236
L646	T573	Y501	C339	N265	L182	T175	T175	C339	Y501	N265	E334	L646	D238	D321	Y547	Q388	D321	D238	L167
R647	G574	N502	V340	T269	S104	I186	T270	V340	G574	N502	E334	R647	D239	D321	Y548	Q388	D321	D239	A168
P648	N575	N502	T341	T270	S104	I186	T270	T341	N575	N502	E334	P648	D240	D321	Y549	Q388	D321	D240	Q169
Q649	D576	K506	T341	T270	S104	I186	T270	T341	D576	K506	E334	Q649	D241	D321	Y550	Q388	D321	D241	E240
Y650	F577	D507	D344	I273	S274	N195	T275	D344	F577	D507	E334	Y650	D242	D321	Y551	Q388	D321	D242	E241
L651	N578	R508	T345	I273	S274	N195	T275	T345	N578	R508	E334	L651	D243	D321	Y552	Q388	D321	D243	E242
T652	K579	S509	T345	I273	S274	N195	T275	T345	K579	S509	E334	T652	D244	D321	Y553	Q388	D321	D244	E243
I653	L580	N510	F348	I273	S274	N195	T275	F348	L580	N510	E334	I653	D245	D321	Y554	Q388	D321	D245	E244
D654	A581	E511	T347	I273	S274	N195	T275	T347	A581	E511	E334	D654	D246	D321	Y555	Q388	D321	D246	E245
L655	N582	S512	V349	A278	D279	E205	T275	V349	N582	S512	E334	L655	D247	D321	Y556	Q388	D321	D247	E246
E656	K585	N513	S350	D279	E205	T275	T275	S350	E656	K585	E334	E656	D248	D321	Y557	Q388	D321	D248	E247
P657	R586	F517	R352	G282	E205	T275	T275	R352	P657	R586	E334	P657	D249	D321	Y558	Q388	D321	D249	E248
I658	D587	N518	F353	G282	E205	T275	T275	F353	I658	D587	E334	I658	D250	D321	Y559	Q388	D321	D250	E249
S659	Y589	S519	G354	S286	E205	T275	T275	G354	S659	Y589	E334	S659	D251	D321	Y560	Q388	D321	D251	E250
L660	Y590	G520	S355	S286	E205	T275	T275	S355	L660	Y590	E334	L660	D252	D321	Y561	Q388	D321	D252	E251
Y661	F591	R521	T356	T288	E205	T275	T275	T356	Y661	F591	E334	Y661	D253	D321	Y562	Q388	D321	D253	E252
T662	I592	K522	T357	D289	E205	T275	T275	T357	T662	I592	E334	T662	D254	D321	Y563	Q388	D321	D254	E253
E663	G593	V523	Q358	D290	E205	T275	T275	Q358	E663	G593	E334	E663	D255	D321	Y564	Q388	D321	D255	E254
S664	E594	N524	V360	T291	E205	T275	T275	V360	S664	E594	E334	S664	D256	D321	Y565	Q388	D321	D256	E255
N665	I595	P526	Q361	T291	E205	T275	T275	Q361	N665	I595	E334	N665	D257	D321	Y566	Q388	D321	D257	E256
Y666	N596	P526	T362	L292	E205	T275	T275	T362	Y666	N596	E334	Y666	D258	D321	Y567	Q388	D321	D258	E257
Y667	S597	T528	F363	L292	E205	T275	T275	F363	Y667	S597	E334	Y667	D259	D321	Y568	Q388	D321	D259	E258
D600	D600	E531	T364	L292	E205	T275	T275	T364	D600	D600	E334	D600	D260	D321	Y569	Q388	D321	D260	E259
V601	V601	E532	D365	L292	E205	T275	T275	D365	V601	V601	E334	V601	D261	D321	Y570	Q388	D321	D261	E260
I602	I602	E533	S366	L292	E205	T275	T275	S366	I602	I602	E334	I602	D262	D321	Y571	Q388	D321	D262	E261
Y603	Y603	D533	T367	L292	E205	T275	T275	T367	Y603	Y603	E334	Y603	D263	D321	Y572	Q388	D321	D263	E262
L606	L606	L535	T374	L292	E205	T275	T275	T374	L606	L606	E334	L606	D264	D321	Y573	Q388	D321	D264	E263
A607	A607	Y536	A375	L292	E205	T275	T275	A375	A607	A607	E334	A607	D265	D321	Y574	Q388	D321	D265	E264
R608	R608	E534	D445	L292	E205	T275	T275	D445	R608	R608	E334	R608	D266	D321	Y575	Q388	D321	D266	E265
I609	I609	R539	R446	L292	E205	T275	T275	R446	I609	I609	E334	I609	D267	D321	Y576	Q388	D321	D267	E266
N610	N610	D533	Y447	L292	E205	T275	T275	Y447	N610	N610	E334	N610	D268	D321	Y577	Q388	D321	D268	E267
L611	L611	S542	Y448	L292	E205	T275	T275	Y448	L611	L611	E334	L611	D269	D321	Y578	Q388	D321	D269	E268
Q619	Q619	T543	T449	L292	E205	T275	T275	T449	Q619	Q619	E334	Q619	D270	D321	Y579	Q388	D321	D270	E269
T620	T620	D544	E450	L292	E205	T275	T275	E450	T620	T620	E334	T620	D271	D321	Y580	Q388	D321	D271	E270
L623	L623	K552	D451	L292	E205	T275	T275	D451	L623	L623	E334	L623	D272	D321	Y581	Q388	D321	D272	E271
Y624	Y624	I554	A376	L292	E205	T275	T275	A376	Y624	Y624	E334	Y624	D273	D321	Y582	Q388	D321	D273	E272
E625	E625	I555	R389	L292	E205	T275	T275	R389	E625	E625	E334	E625	D274	D321	Y583	Q388	D321	D274	E273
P627	P627	G556	D472	L292	E205	T275	T275	D472	P627	P627	E334	P627	D275	D321	Y584	Q388	D321	D275	E274
V631	V631	P557	R473	L292	E205	T275	T275	R473	V631	V631	E334	V631	D276	D321	Y585	Q388	D321	D276	E275
I632	I632	F558	S474	L292	E205	T275	T275	S474	I632	I632	E334	I632	D277	D321	Y586	Q388	D321	D277	E276
E633	E633	A559	V475	L292	E205	T275	T275	V475	E633	E633	E334	E633	D278	D321	Y587	Q388	D321	D278	E277
L634	L634	E559	I476	L292	E205	T275	T275	I476	L634	L634	E334	L634	D279	D321	Y588	Q388	D321	D279	E278

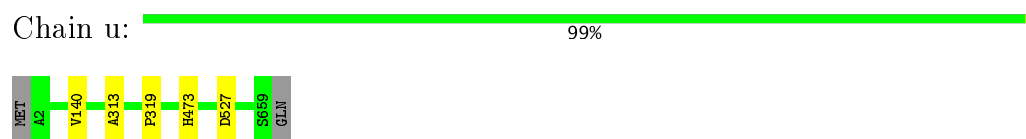
• Molecule 1: Baseplate wedge protein gp6

Chain X: 47% 53%

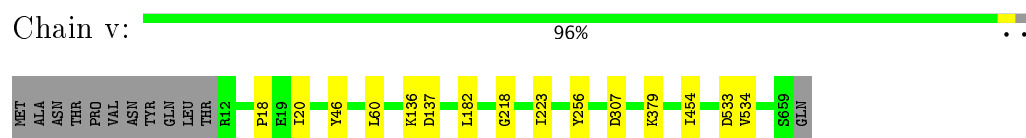
- Molecule 1: Baseplate wedge protein gp6



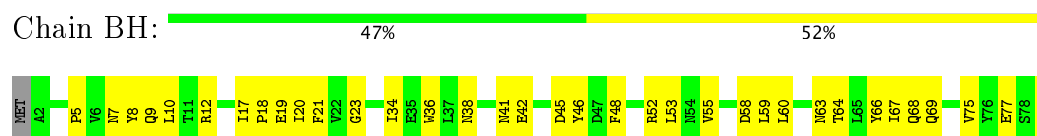
- Molecule 1: Baseplate wedge protein gp6

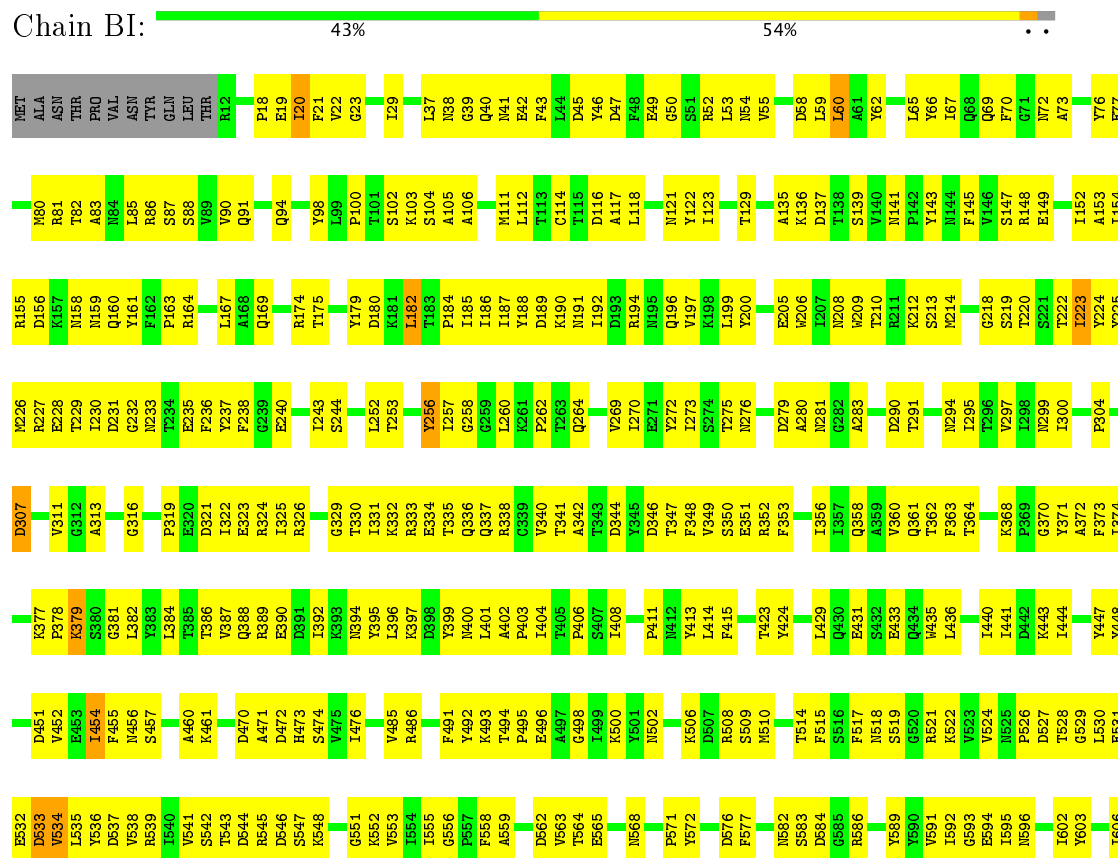


- Molecule 1: Baseplate wedge protein gp6



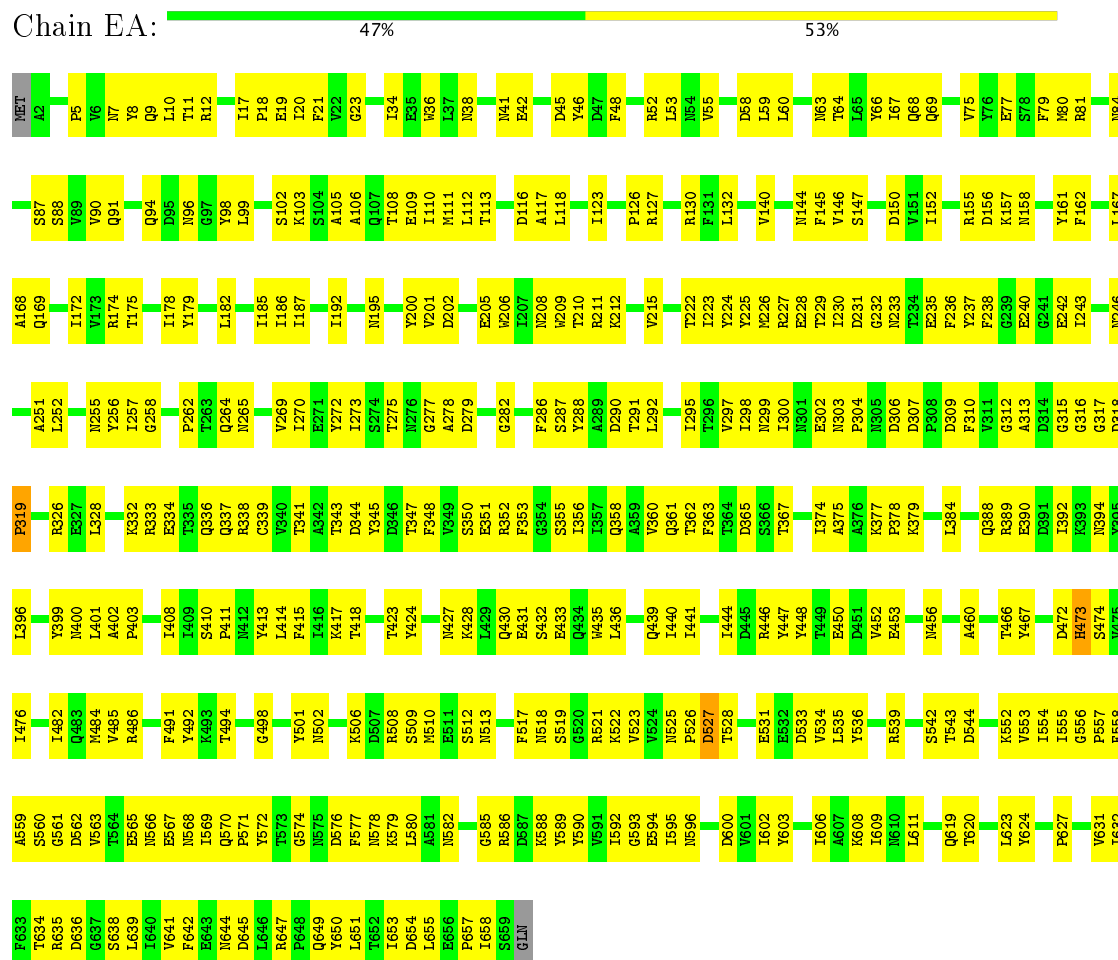
- Molecule 1: Baseplate wedge protein gp6



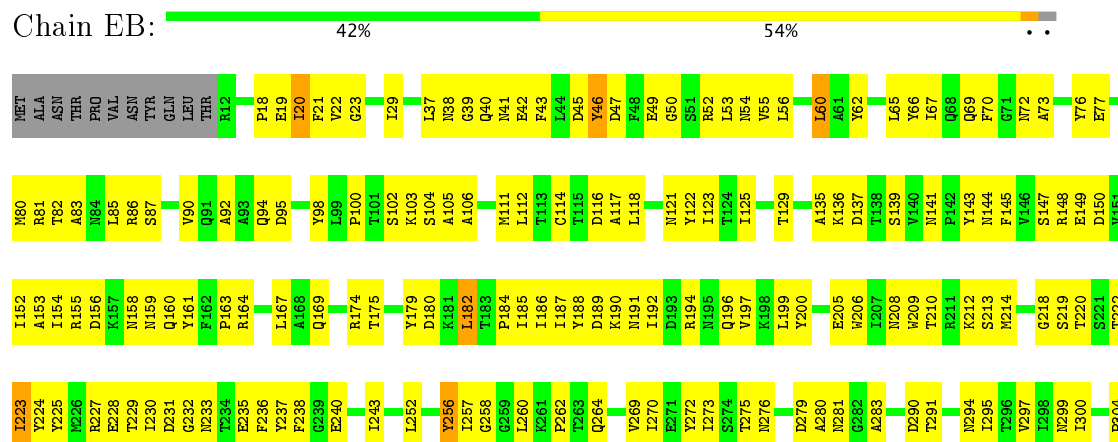




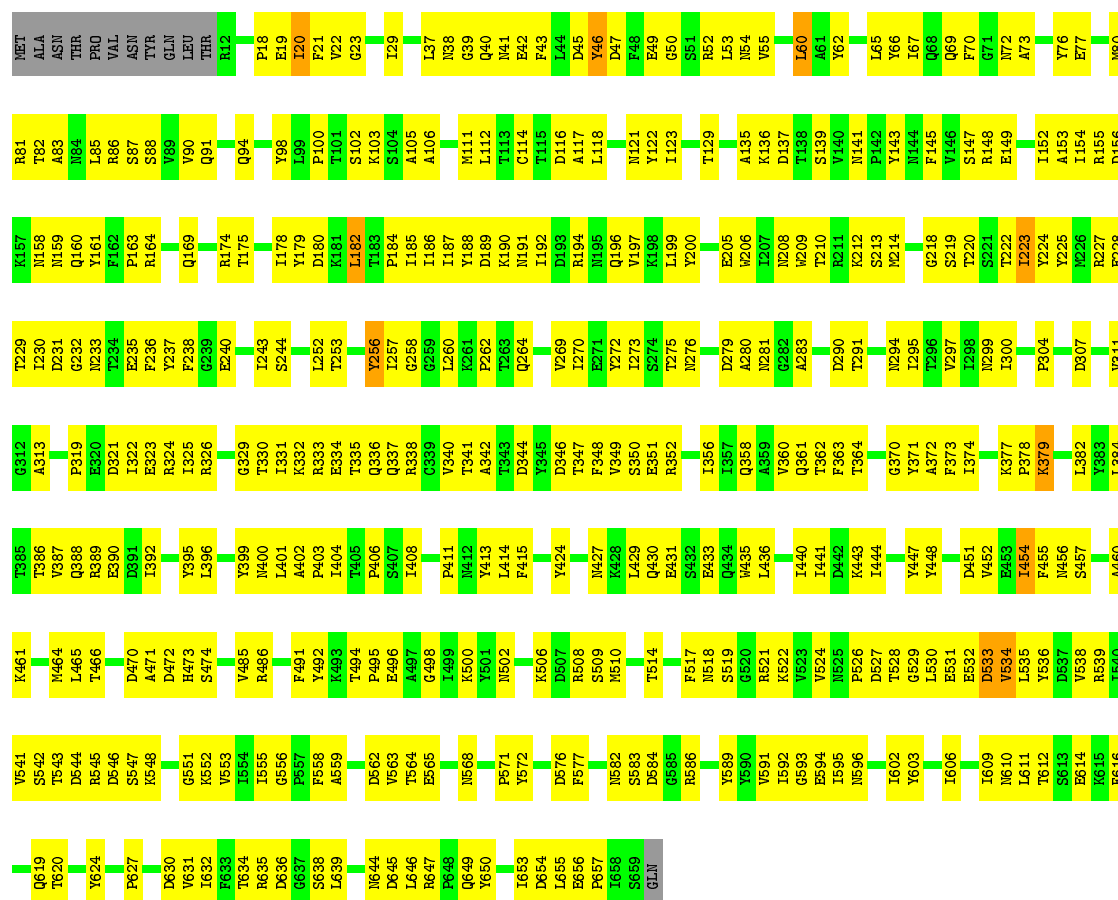
• Molecule 1: Baseplate wedge protein gp6



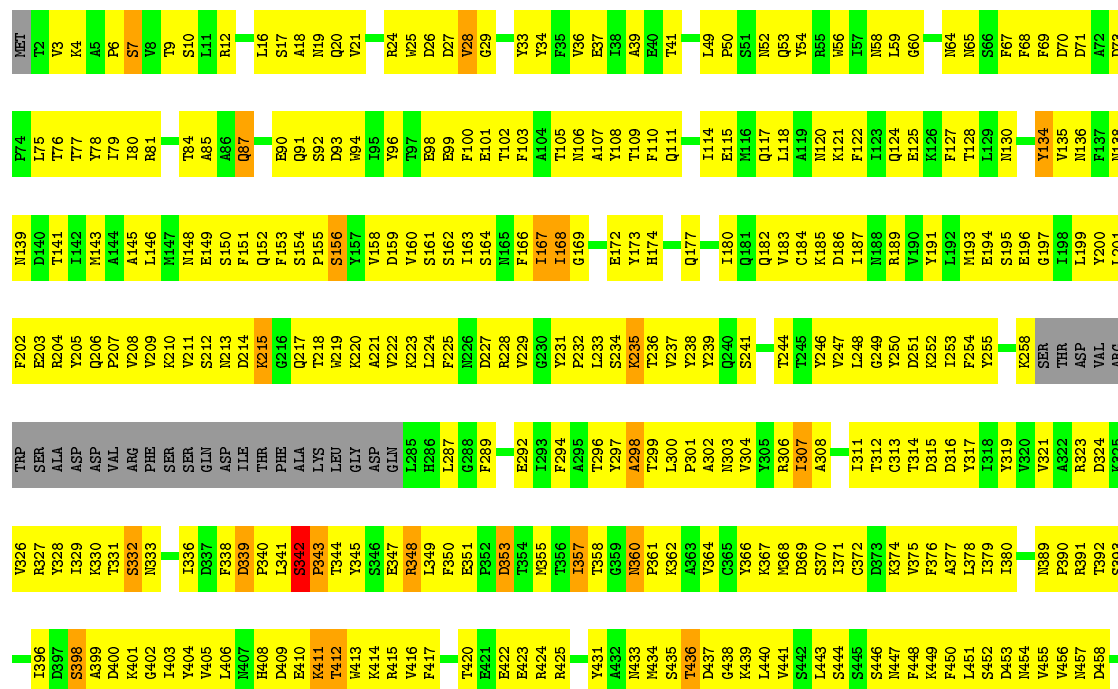
• Molecule 1: Baseplate wedge protein gp6

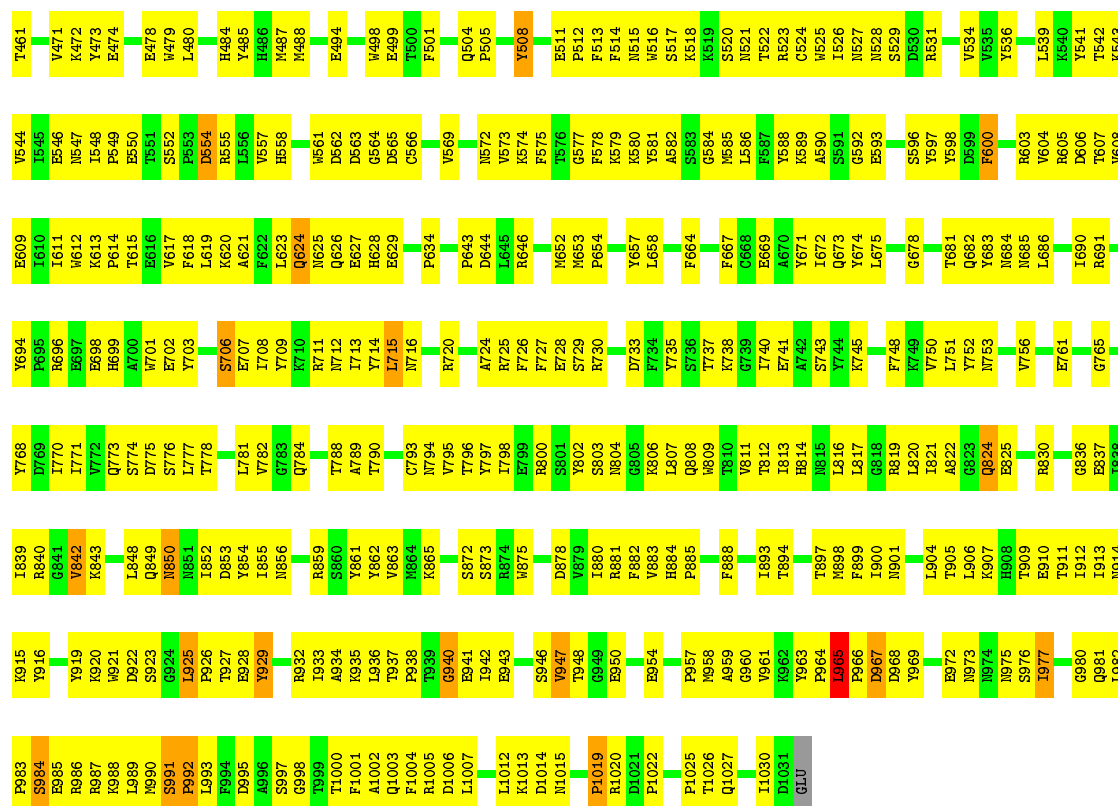






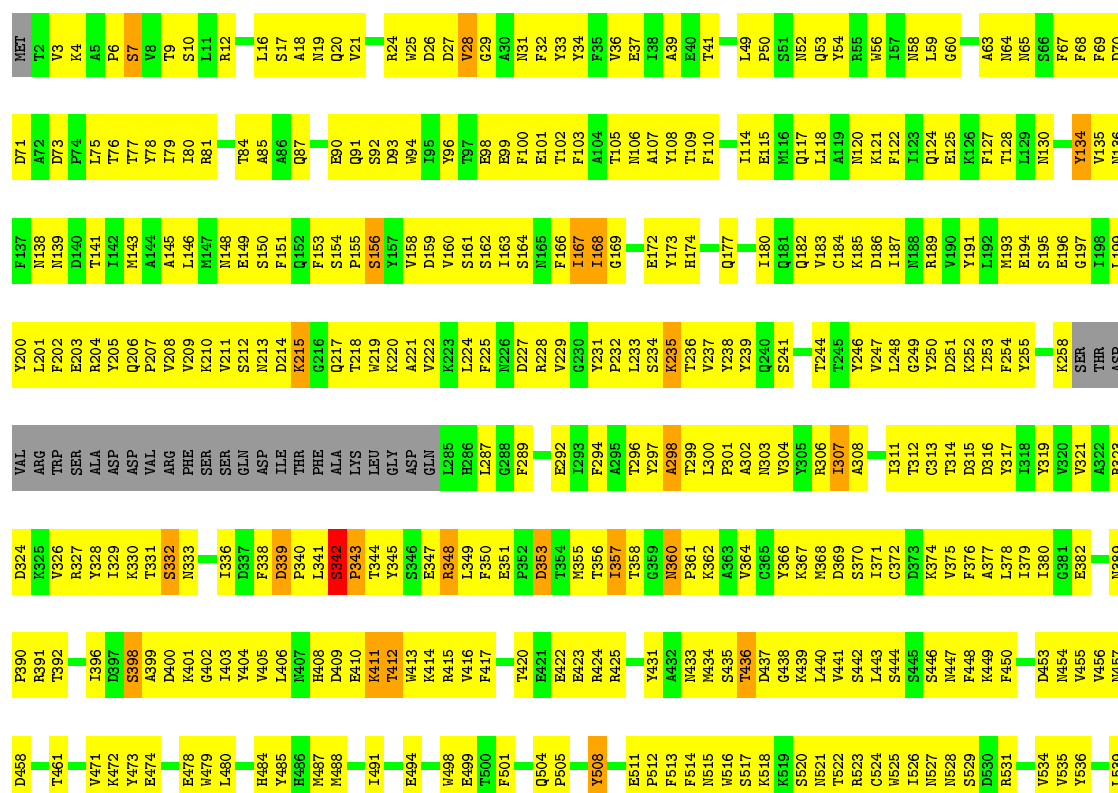
• Molecule 2: Baseplate wedge protein gp7

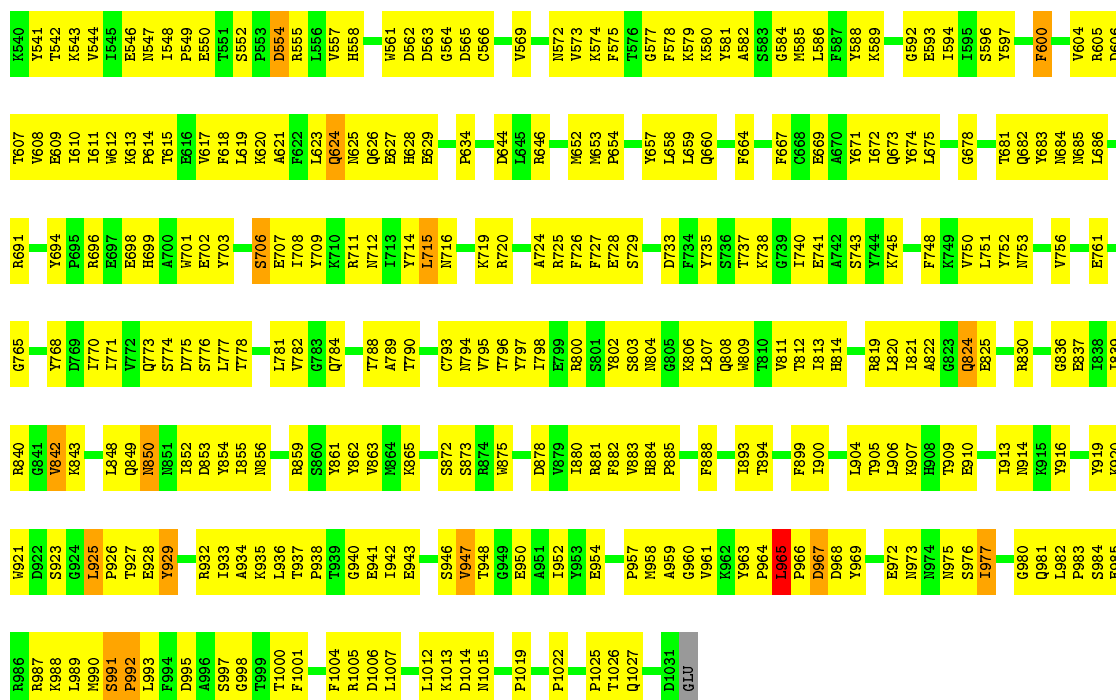




### • Molecule 2: Baseplate wedge protein gp7

Chain Z: 35% 58%





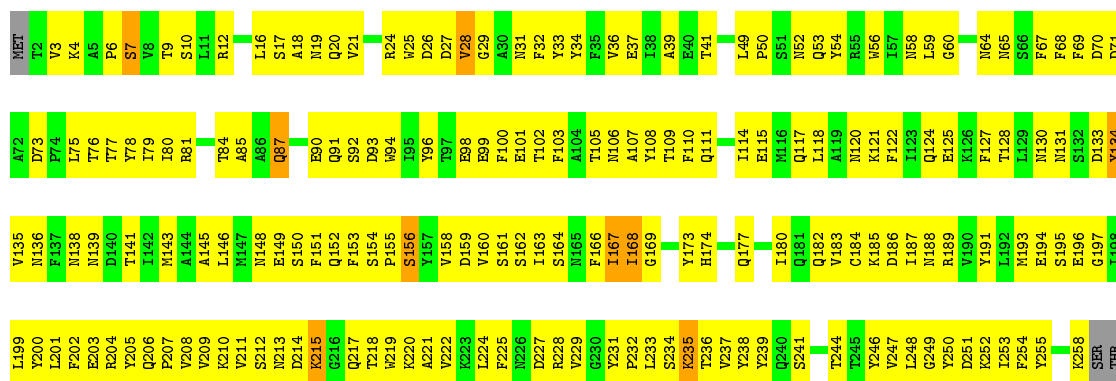
• Molecule 2: Baseplate wedge protein gp7

Chain w: 92% 5% .



• Molecule 2: Baseplate wedge protein gp7

Chain BJ: 32% 60% . .



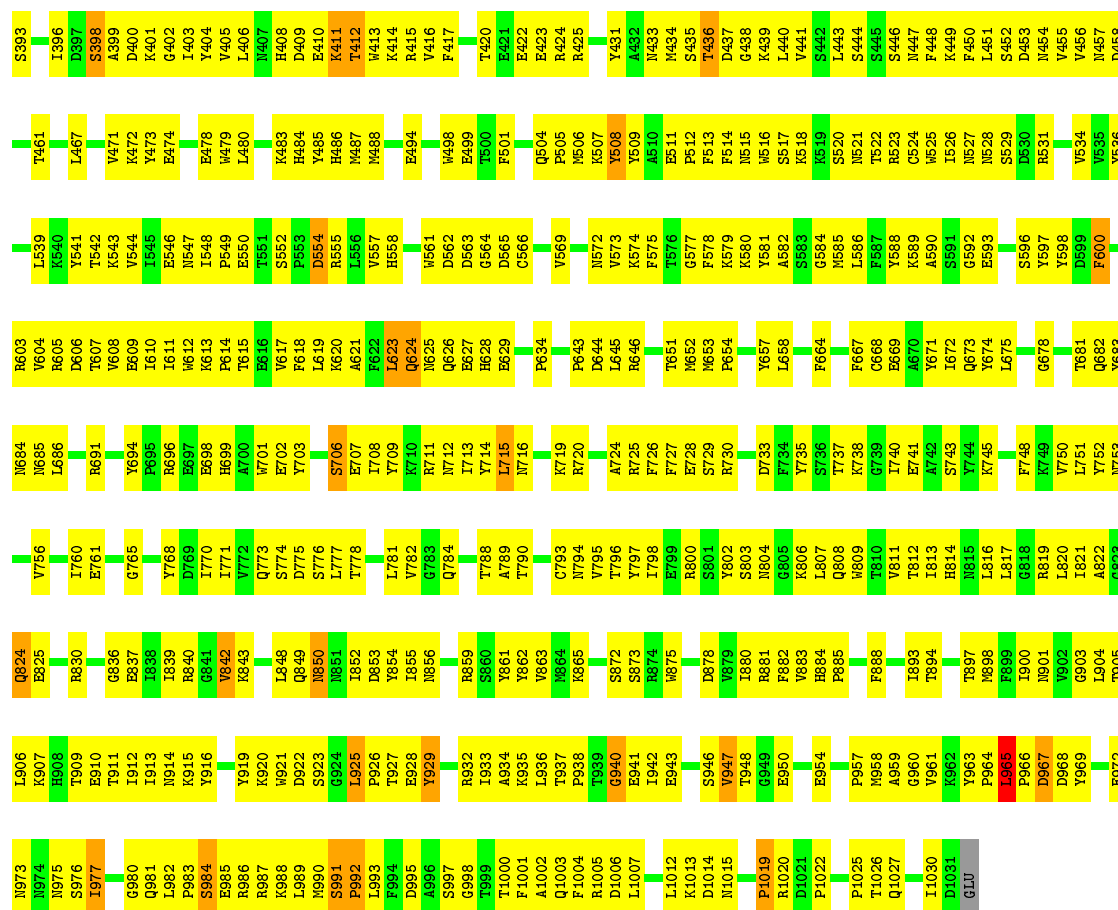
ASP	R391	D458	V534	T681	L751	A822	L904	D968	L1012	L49	Q177	V135	L199	ASP
VAL	T392	T461	V535	Q682	T752	G823	T905	T969	L1013	P50	T177	M136	T200	VAL
ARG	S393		V536	M683	N753	Q824	L906	E972	D1014	S51	F137	F137	L201	ARG
TRP			V326	M685	V756	E825	K907	E974	N1015	N52	M139	M139	E203	TRP
SER			V328	L686	E761	B830	T909	N974	E950	Q53	A5	A5	R204	SER
ALA			V329				E910	N975	E951	Q54	P6	P6	Y205	ALA
ASP			V330				T911	S976	E952	Q55	S7	S7	Y206	ASP
ASP			V331				T912	S977	E953	Q56	V8	V8	Q207	ASP
VAL			V332				T913		E954	Q57	T9	T9	V208	VAL
ARG			V333				T914		E955	Q58	S10	S10	V209	ARG
PHE							T915		E956	Q59	L11	L11	K210	PHE
SER							T916		E957	Q60	N981	N981	K211	SER
SER							T917		E958	Q61	L982	L982	K212	SER
GLN							T918		E959	Q62	P983	P983	S212	GLN
ASP							T919		E960	Q63	S984	S984	E149	ASP
ASP							T920		E961	Q64	E985	E985	S150	ASP
ILE							T921		E962	Q65	A18	A18	D214	ILE
THR							T922		E963	Q66	N19	N19	K215	THR
PHE							T923		E964	Q67	Q20	Q20	G216	PHE
ALA							T924		E965	Q68	R987	R987	Q217	ALA
LYS							T925		E966	Q69	K988	K988	Q218	LYS
LEU							T926		E967	Q70	L989	L989	T219	LEU
ASP							T927		E968	Q71	N990	N990	K220	ASP
GLY							T928		E969	Q72	S991	S991	A221	GLY
GLN							T929		E970	Q73	E992	E992	K222	GLN
L285							T930		E971	Q74	F993	F993	V223	L285
H286							T931		E972	Q75	D994	D994	L224	H286
L287							T932		E973	Q76	N995	N995	F225	L287
G288							T933		E974	Q77	A996	A996	K226	G288
F289							T934		E975	Q78	S997	S997	N227	F289
E292							T935		E976	Q79	N998	N998	R228	E292
L293							T936		E977	Q80	T1000	T1000	V229	L293
F294							T937		E978	Q81	F1001	F1001	G230	F294
A295							T938		E979	Q82	A1002	A1002	T231	A295
T296							T939		E980	Q83	Q1003	Q1003	P232	T296
Y297							T940		E981	Q84	F1004	F1004	L233	Y297
A298							T941		E982	Q85	R1005	R1005	S234	A298
T299							T942		E983	Q86	D1006	D1006	K235	T299
L300							T943		E984	Q87	L1007	L1007	T236	L300
P301							T944		E985	Q88			Y237	P301
N303							T945		E986	Q89	L1012	L1012	Y238	N303
V304							T946		E987	Q90	D1013	D1013	Y239	V304
Y305							T947		E988	Q91	N1014	N1014	Q240	Y305
R306							T948		E989	Q92	E949	E949	S241	R306
A307							T949		E990	Q93	E950	E950	T244	A307
T308							T950		E991	Q94	A951	A951	T245	T308
G309							T951		E992	Q95	R1019	R1019	Y246	G309
N360							T952		E993	Q96	R1020	R1020	Y247	N360
P361							T953		E994	Q97	D1021	D1021	V248	P361
K362							T954		E995	Q98	P1022	P1022	L249	K362
M368							T955		E996	Q99	E954	E954	T250	M368
S370							T956		E997	Q100	P957	P957	Q249	S370
I371							T957		E998	Q101	N958	N958	Y251	I371
C372							T958		E999	Q102	N959	N959	K252	C372
D373							T959		E1000	Q103	A960	A960	L253	D373
K374							T960		E1001	Q104	V961	V961	F254	K374
N447							T961		E1002	Q105	N962	N962	Y255	N447
F448							T962		E1003	Q106	D1031	D1031	K258	F448
K449							T963		E1004	Q107	GLU	GLU	SER	K449
F450							T964		E1005	Q108			V321	F450
I526							T965		E1006	Q109			N389	I526
N527							T966		E1007	Q110			V320	N527
N528							T967		E1008	Q111			N457	N528
S529							T968		E1009	Q112				S529
D453							T969		E1010	Q113				D453
N454							T970		E1011	Q114				N454
V455							T971		E1012	Q115				V455
N389							T972		E1013	Q116				N389
P390							T973		E1014	Q117				P390

• Molecule 2: Baseplate wedge protein gp7

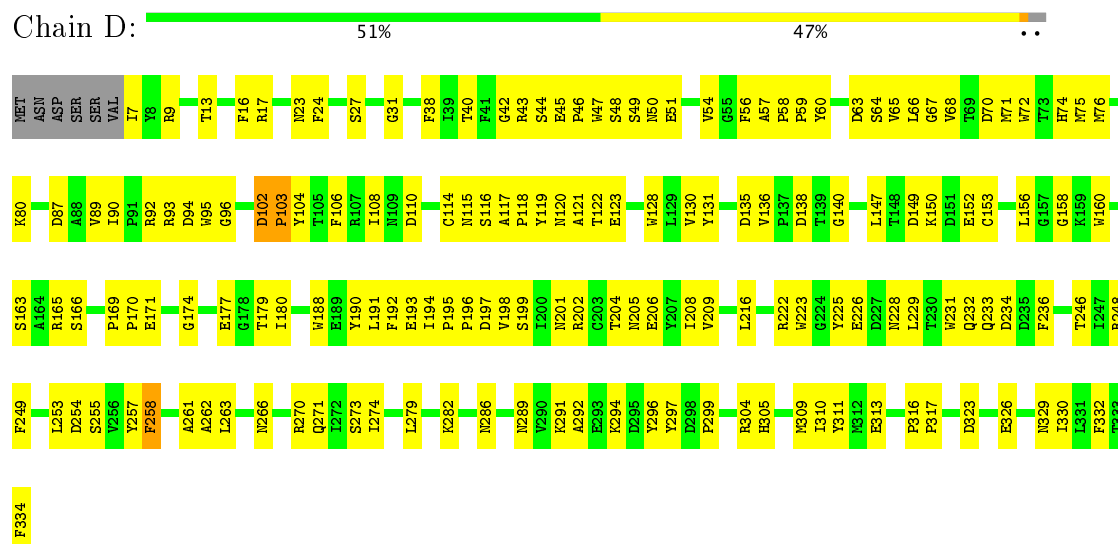
Chain EC: 32% 61%

MET	A72	V135	L199	ASP
T2	D73	M136	T200	VAL
V3	F74	F137	L201	ARG
K4	L75	N138	F202	TRP
A5	T76	M139	E203	SER
P6	T77	D140	R204	ALA
S7	T78	T141	Y205	ASP
V8	T79	T142	Q206	ASP
T9	T80	M143	V207	VAL
S10	R81	A144	V208	ARG
L11		A145	V209	PHE
R12		L146	K210	SER
L16		M147	K211	SER
S17		N148	S212	GLN
A18		E149	N213	ASP
N19		S150	D214	ASP
Q20		F151	K215	THR
R21		Q152	G216	PHE
S22		F153	Q217	ALA
D93		S154	Q218	LYS
N94		P155	T219	LYS
S156		S157	K220	GLY
Y157		T158	A221	ASP
T97		D159	V222	GLN
E98		V160	K223	L285
E99		S161	L224	H286
F100		S162	F225	L287
E101		I163	N226	G288
F102		S164	D227	F289
F103		T103	R228	F289
T104		F104	V229	E292
A105		M165	G230	L293
F106		F166	T231	F294
N106		I167	P232	A295
A107		T168	L233	T296
Y108		G169	L234	Y297
F110		Y173	S234	A298
Q111		H174	T236	T299
			Y237	L300
			Y238	P301
			Q240	N303
			S241	V304
			T244	Y305
			T245	R306
			Y246	A307
			V247	T308
			L248	
			Q249	T311
			Y250	T312
			K251	C313
			T252	T314
			L253	D315
			F254	D316
			Y255	Y317
			E194	T318
			S195	Y319
			E196	T320
			S132	V321
			D133	V321
			D133	A322

R323	R391	D458	V534	P600	Q682	V750	L820	I900	D967	I900	D967	R323
D324	T392	D459	V535	R603	Y683	L751	I821	I901	D968	I901	D968	D324
R325	S393	T461	Y536	R604	N685	Y752	A822	N901	Y969	N901	Y969	R325
V326	I396	L467	L539	R605	L686	Y753	G823	L904	E972	L904	E972	V326
R327	I397	L467	L540	R606	L687	V756	E824	T905	A973	T905	A973	R327
R328	S398	V471	Y541	R607	L689	E761	R830	L906	R974	L906	R974	R328
R329	A399	K472	T542	R608	L690	E762	G836	R907	S975	R907	S975	R329
K330	D400	K473	K543	R609	R691	E763	G837	T908	S976	T908	S976	K330
T331	K401	E474	Y544	R610	R692	E764	R831	R908	I977	R908	I977	T331
S332	G402	E475	I545	R611	Y694	T765	G832	E909	I978	E909	I978	S332
N333	I403	E476	E546	R612	P695	T766	G833	E910	I979	E910	I979	N333
T336	Y404	L480	I547	R613	R696	T767	I838	E911	I980	E911	I980	T336
D337	V405	L481	I548	R614	E697	T768	R839	Q981	A886	Q981	A886	D337
F338	L406	L482	I549	R615	E698	T769	R840	Q982	A887	Q982	A887	F338
R339	H408	L483	T551	R616	R699	T770	G841	P983	S984	P983	S984	R339
P340	D409	L484	Y485	R617	E700	T771	K842	Q984	S985	Q984	S985	P340
L341	E410	L485	S552	R618	Y701	T772	G843	Q985	N986	Q985	N986	L341
S342	K411	L486	P653	R619	E702	T773	K844	Q986	N987	Q986	N987	S342
P343	T412	L487	D554	R620	Y703	T774	K845	Q987	N988	Q987	N988	P343
R344	Y413	L488	R555	R621	S706	T775	L848	Q988	N989	Q988	N989	R344
E345	K414	L489	I556	R622	E707	T776	G849	Q989	N990	Q989	N990	E345
S346	R415	L490	V557	R623	Y708	T777	K850	Q990	N991	Q990	N991	S346
R347	V416	L491	H558	R624	I709	T778	R851	Q991	N992	Q991	N992	R347
R348	F417	L492	E559	R625	Y710	T779	R852	Q992	N993	Q992	N993	R348
F350	L420	L493	D560	R626	K710	T780	R853	Q993	N994	Q993	N994	F350
E351	T421	L494	D561	R627	R711	T781	D854	Q994	N995	Q994	N995	E351
P352	E422	L495	D562	R628	Y712	T782	R855	Q995	N996	Q995	N996	P352
D353	E423	L496	G564	R629	E713	T783	R856	Q996	N997	Q996	N997	D353
T354	E424	L497	D565	R630	Y714	T784	R857	Q997	N998	Q997	N998	T354
K355	E425	L498	C566	R631	L715	T785	R858	Q998	N999	Q998	N999	K355
R356	R424	L499	Q504	R632	Y716	T786	R859	Q999	N1000	Q999	N1000	R356
S357	R425	L500	P505	R633	K717	T787	R860	Q1001	N1001	Q1001	N1001	S357
T358	Y431	L501	N506	R634	R720	T788	R861	Q1002	N1002	Q1002	N1002	T358
G359	M432	L502	N507	R635	K721	T789	R862	Q1003	N1003	Q1003	N1003	G359
K360	M433	L503	V508	R636	L645	T790	R863	Q1004	N1004	Q1004	N1004	K360
P361	M434	L504	K574	R637	R646	T791	R864	Q1005	N1005	Q1005	N1005	P361
K362	S435	L505	P575	R638	T651	T792	R865	Q1006	N1006	Q1006	N1006	K362
A363	T436	L506	T576	R639	R652	T793	R866	Q1007	N1007	Q1007	N1007	A363
V364	S436	L507	G577	R640	R653	T794	R867	Q1008	N1008	Q1008	N1008	V364
R365	D437	L508	F578	R641	P654	T795	R868	Q1009	N1009	Q1009	N1009	R365
K366	G438	L509	K579	R642	R655	T796	R869	Q1010	N1010	Q1010	N1010	K366
L367	K439	L510	N510	R643	R656	T797	R870	Q1011	N1011	Q1011	N1011	L367
S368	L440	L511	E511	R644	T657	T798	R871	Q1012	N1012	Q1012	N1012	S368
D369	V441	L512	S512	R645	L658	T799	R872	Q1013	N1013	Q1013	N1013	D369
I370	S442	L513	G513	R646	R659	T800	R873	Q1014	N1014	Q1014	N1014	I370
N371	S443	L514	M514	R647	T660	T801	R874	Q1015	N1015	Q1015	N1015	N371
K372	S444	L515	M515	R648	T661	T802	R875	Q1016	N1016	Q1016	N1016	K372
G373	S445	L516	P516	R649	T662	T803	R876	Q1017	N1017	Q1017	N1017	G373
K374	S446	L517	S517	R650	T663	T804	R877	Q1018	N1018	Q1018	N1018	K374
V375	M447	L518	K518	R651	T664	T805	R878	Q1019	N1019	Q1019	N1019	V375
A376	K448	L519	N519	R652	T665	T806	R879	Q1020	N1020	Q1020	N1020	A376
F377	F449	L520	M520	R653	T666	T807	R880	Q1021	N1021	Q1021	N1021	F377
A378	F450	L521	M521	R654	T667	T808	R881	Q1022	N1022	Q1022	N1022	A378
L379	D453	L522	P522	R655	T668	T809	R882	Q1023	N1023	Q1023	N1023	L379
I380	M454	L523	S523	R656	T669	T810	R883	Q1024	N1024	Q1024	N1024	I380
N389	V455	L524	K524	R657	T670	T811	R884	Q1025	N1025	Q1025	N1025	N389
P390	F456	L525	N525	R658	T671	T812	R885	Q1026	N1026	Q1026	N1026	P390
T392	M457	L526	S526	R659	T672	T813	R886	Q1027	N1027	Q1027	N1027	T392
		L527	E527	R660	T673	T814	R887	Q1028	N1028	Q1028	N1028	
		L528	G528	R661	T674	T815	R888	Q1029	N1029	Q1029	N1029	
		L529	H529	R662	T675	T816	R889	Q1030	N1030	Q1030	N1030	
		L530	I530	R663	T676	T817	R890	Q1031	N1031	Q1031	N1031	
		L531	J531	R664	T677	T818	R891	Q1032	N1032	Q1032	N1032	
		L532	K532	R665	T678	T819	R892	Q1033	N1033	Q1033	N1033	
		L533	L533	R666	T679	T820	R893	Q1034	N1034	Q1034	N1034	
		L534	M534	R667	T680	T821	R894	Q1035	N1035	Q1035	N1035	
		L535	N535	R668	T681	T822	R895	Q1036	N1036	Q1036	N1036	
		L536	O536	R669	T682	T823	R896	Q1037	N1037	Q1037	N1037	
		L537	P537	R670	T683	T824	R897	Q1038	N1038	Q1038	N1038	
		L538	Q538	R671	T684	T825	R898	Q1039	N1039	Q1039	N1039	
		L539	R539	R672	T685	T826	R899	Q1040	N1040	Q1040	N1040	
		L540	S539	R673	T686	T827	R900	Q1041	N1041	Q1041	N1041	
		L541	T539	R674	T687	T828	R901	Q1042	N1042	Q1042	N1042	
		L542	V539	R675	T688	T829	R902	Q1043	N1043	Q1043	N1043	
		L543	W539	R676	T689	T830	R903	Q1044	N1044	Q1044	N1044	
		L544	X539	R677	T690	T831	R904	Q1045	N1045	Q1045	N1045	
		L545	Y539	R678	T691	T832	R905	Q1046	N1046	Q1046	N1046	
		L546	Z539	R679	T692	T833	R906	Q1047	N1047	Q1047	N1047	
		L547	A540	R680	T693	T834	R907	Q1048	N1048	Q1048	N1048	
		L548	C540	R681	T694	T835	R908	Q1049	N1049	Q1049	N1049	
		L549	D540	R682	T695	T836	R909	Q1050	N1050	Q1050	N1050	
		L550	E540	R683	T696	T837	R910	Q1051	N1051	Q1051	N1051	
		L551	F540	R684	T697	T838	R911	Q1052	N1052	Q1052	N1052	
		L552	G540	R685	T698	T839	R912	Q1053	N1053	Q1053	N1053	
		L553	H540	R686	T699	T840	R913	Q1054	N1054	Q1054	N1054	
		L554	I540	R687	T700	T841	R914	Q1055	N1055	Q1055	N1055	
		L555	J540	R688	T701	T842	R915	Q1056	N1056	Q1056	N1056	
		L556	K540	R689	T702	T843	R916	Q1057	N1057	Q1057	N1057	
		L557	L541	R690	T703	T844	R917	Q1058	N1058	Q1058	N1058	
		L558	M541	R691	T704	T845	R918	Q1059	N1059	Q1059	N1059	
		L559	N541	R692	T705	T846	R919	Q1060	N1060	Q1060	N1060	
		L560	O541	R693	T706	T847	R920	Q1061	N1061	Q1061	N1061	
		L561	P541	R694	T707	T848	R921	Q1062	N1062	Q1062	N1062	
		L562	Q541	R695	T708	T849	R922	Q1063	N1063	Q1063	N1063	
		L563	R541	R696	T709	T850	R923	Q1064	N1064	Q1064	N1064	
		L564	S541	R697	T710	T851	R924	Q1065	N1065	Q1065	N1065	
		L565	T541	R698	T711	T852	R925	Q1066	N1066	Q1066	N1066	
		L566	V541	R699	T712	T853	R926	Q1067	N1067	Q1067	N1067	
		L567	W541	R700	T713	T854	R927	Q1068	N1068	Q1068	N1068	
		L568	X541	R701	T714	T855	R928	Q1069	N1069	Q1069	N1069	
		L569	Y541	R702	T715	T856	R929	Q1070	N1070	Q1070	N1070	
		L570	Z541	R703	T716	T857	R930	Q1071	N1071	Q1071	N1071	
		L571	A542	R704	T717	T858	R931	Q1072	N1072	Q1072	N1072	
		L572	C542	R705	T718	T859	R932	Q1073	N1073	Q1073	N1073	
		L573	D542	R706	T719	T860	R933	Q1074	N1074	Q1074	N1074	
		L574	E542	R707	T720	T861	R934	Q1075	N1075	Q1075	N1075	
		L575	F542	R708	T721	T862	R935	Q1076	N1076	Q1076	N1076	
		L576	G542	R709	T722	T863	R936	Q1077	N1077	Q1077	N1077	
		L577	H542	R710	T723	T864	R937	Q1078	N1078	Q1078	N1078	
		L578	I542	R711	T724	T865	R938	Q1079	N1079	Q1079	N1079	
		L579	J542	R712	T725	T866	R939	Q1080	N1080	Q1080	N1080	
		L580	K542	R713	T726	T867	R940	Q1081	N1081	Q1081	N1081	
		L581	L543	R714	T727	T868	R941	Q1082	N1082	Q1082	N1082	
		L582	M543	R715								

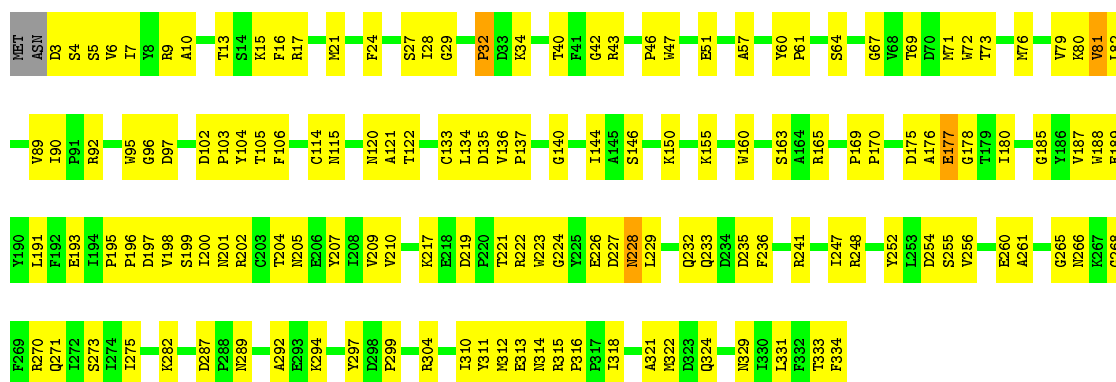


### • Molecule 3: Baseplate wedge protein gp8



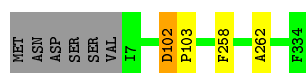
### • Molecule 3: Baseplate wedge protein gp8





• Molecule 3: Baseplate wedge protein gp8

Chain a: 97%



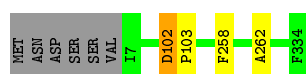
• Molecule 3: Baseplate wedge protein gp8

Chain b: 98%



• Molecule 3: Baseplate wedge protein gp8

Chain x: 97%



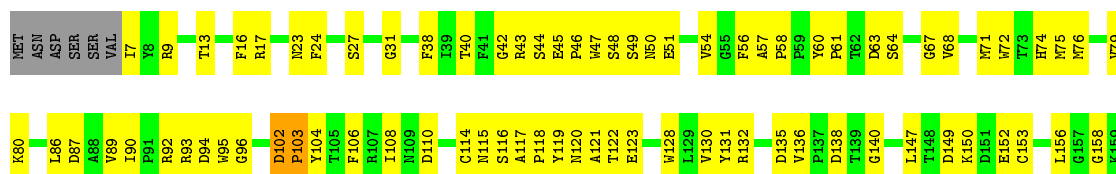
• Molecule 3: Baseplate wedge protein gp8

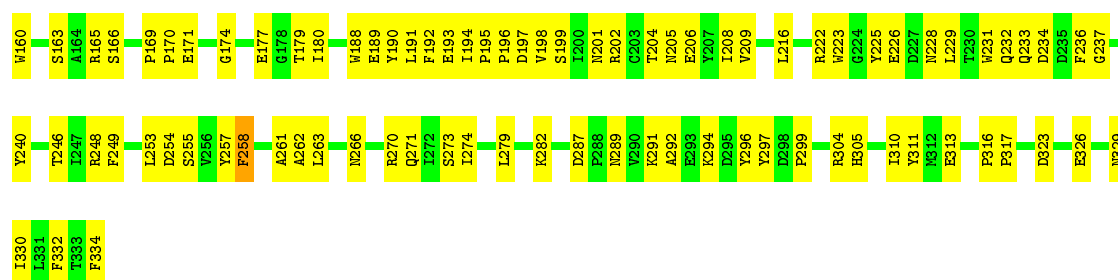
Chain y: 98%



• Molecule 3: Baseplate wedge protein gp8

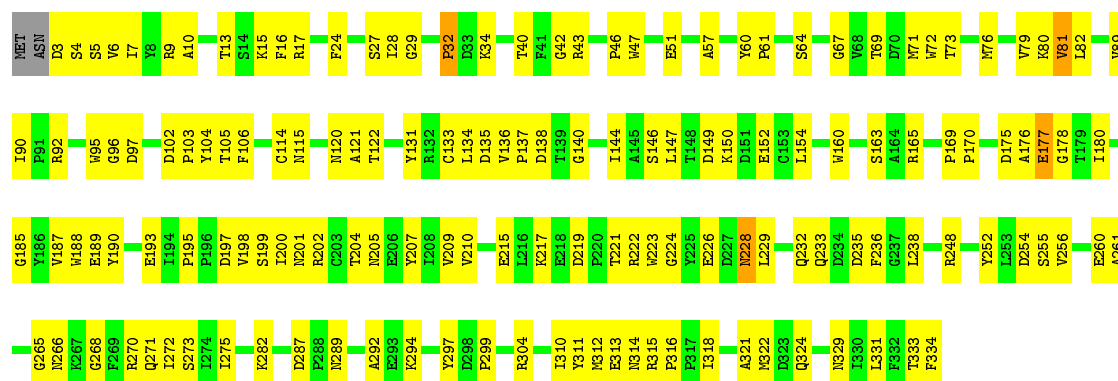
Chain CA: 50% 47%





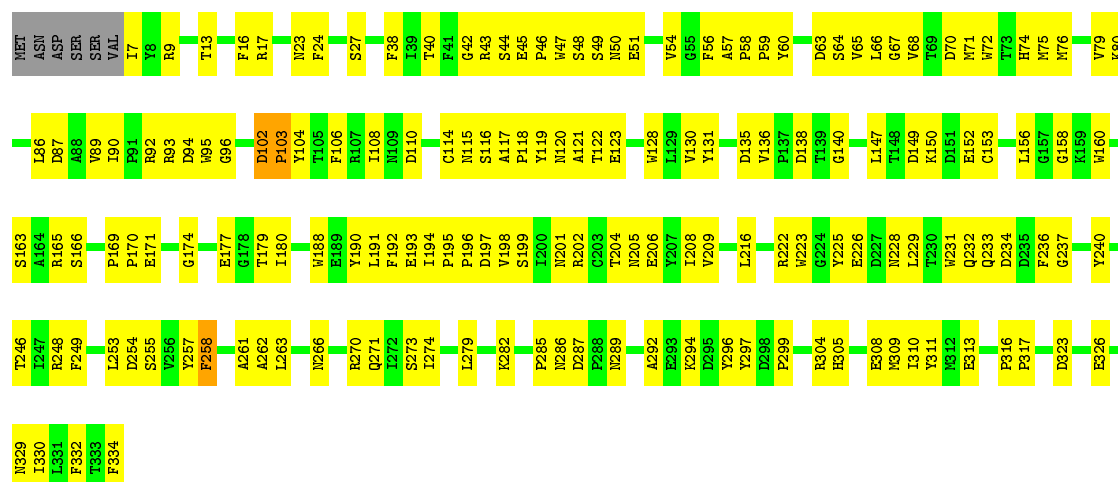
• Molecule 3: Baseplate wedge protein gp8

Chain CB: 55% 43%



• Molecule 3: Baseplate wedge protein gp8

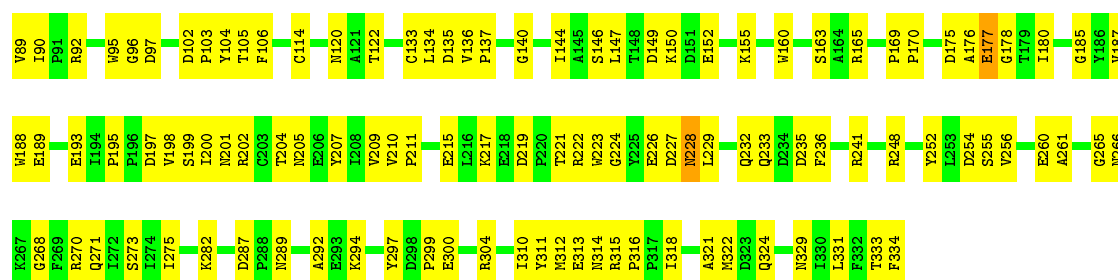
Chain ED: 49% 48%



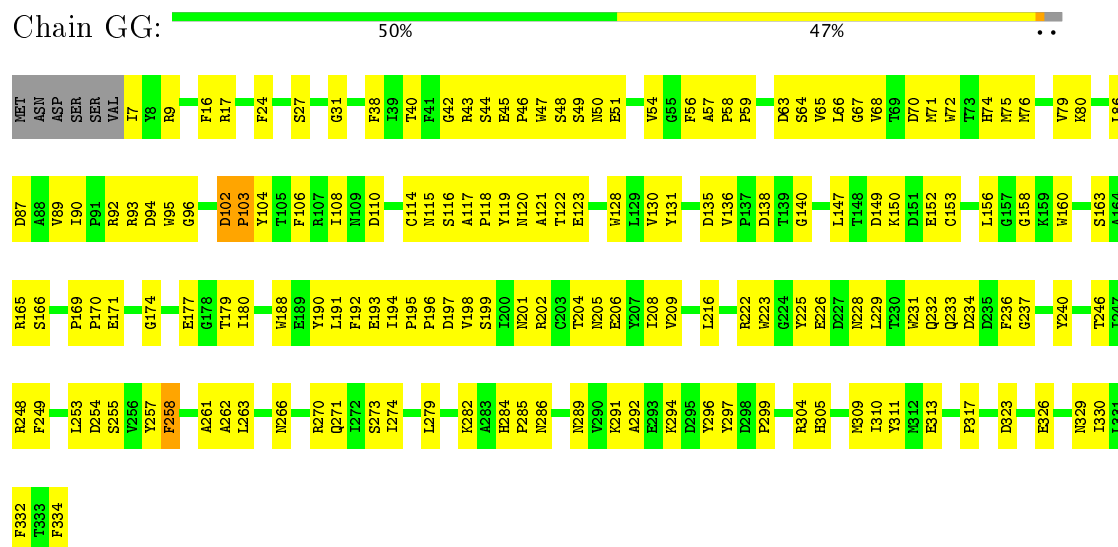
• Molecule 3: Baseplate wedge protein gp8

Chain EE: 55% 43%

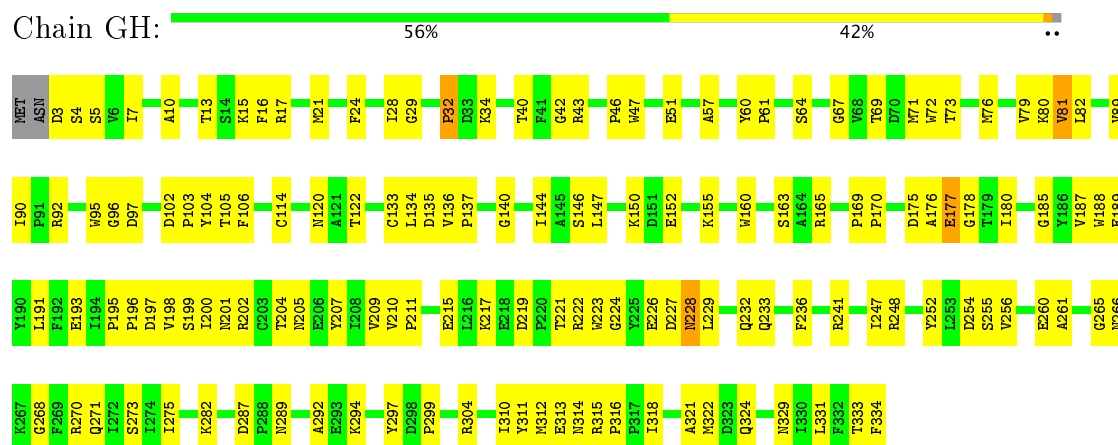




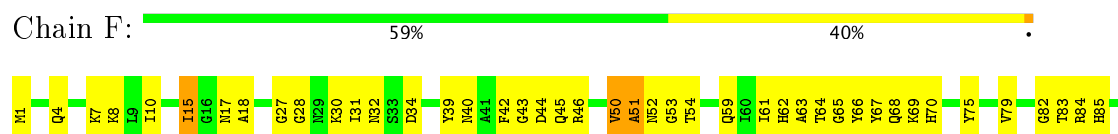
• Molecule 3: Baseplate wedge protein gp8



• Molecule 3: Baseplate wedge protein gp8

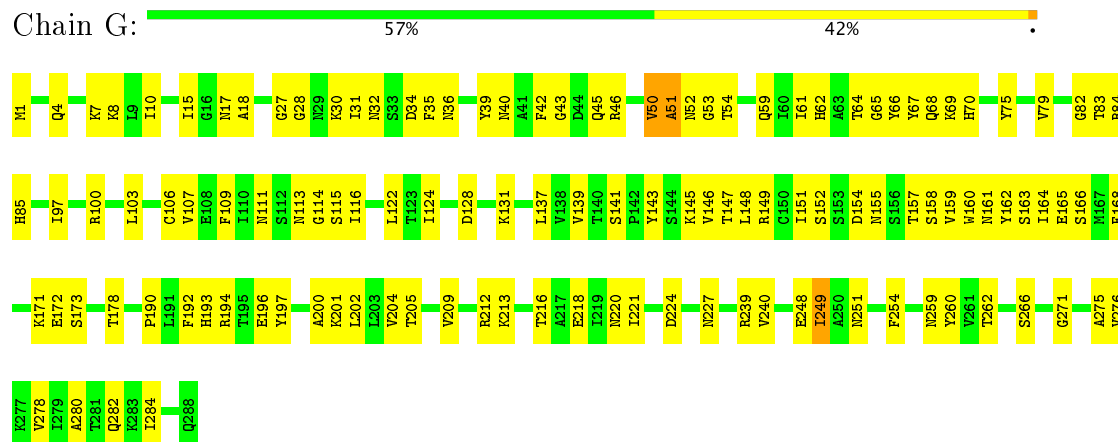


• Molecule 4: Baseplate wedge protein gp9

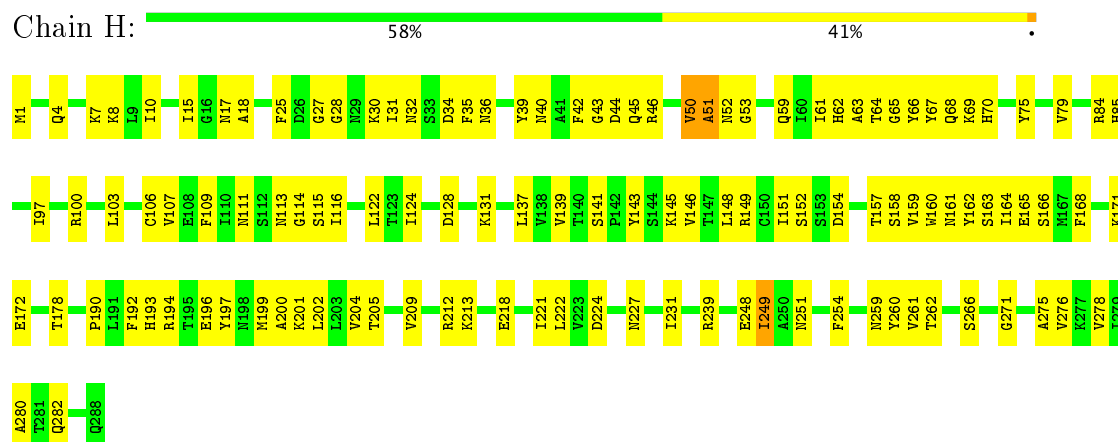




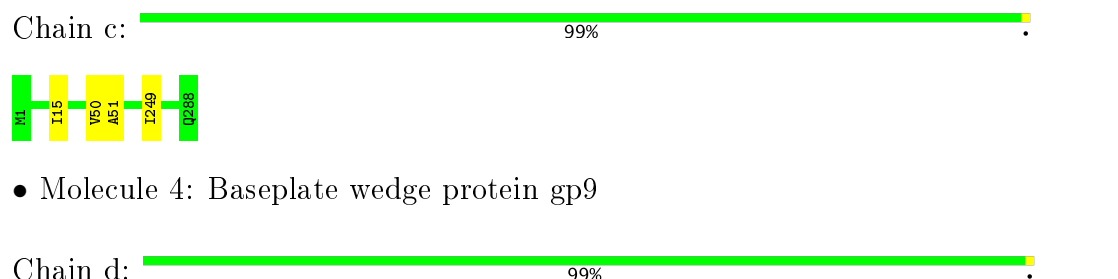
- Molecule 4: Baseplate wedge protein gp9



- Molecule 4: Baseplate wedge protein gp9



- Molecule 4: Baseplate wedge protein gp9



- Molecule 4: Baseplate wedge protein gp9



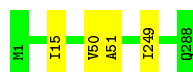
- Molecule 4: Baseplate wedge protein gp9

Chain e: 99%



- Molecule 4: Baseplate wedge protein gp9

Chain z: 99%



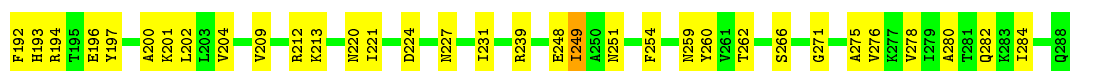
- Molecule 4: Baseplate wedge protein gp9

Chain AA: 59% 40%



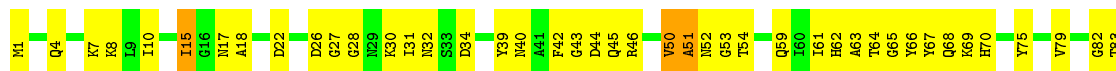
- Molecule 4: Baseplate wedge protein gp9

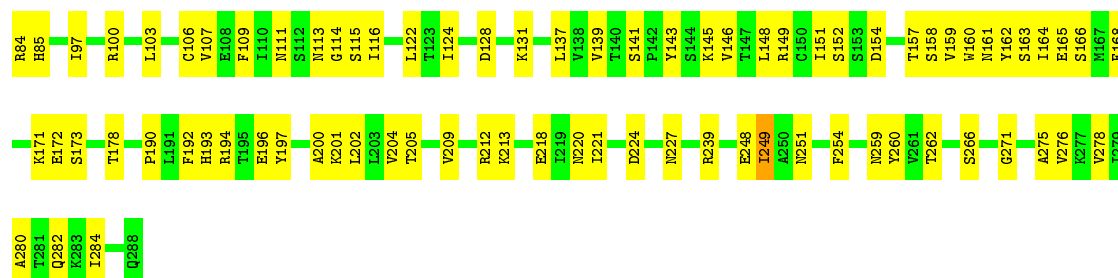
Chain AB: 61% 37%



- Molecule 4: Baseplate wedge protein gp9

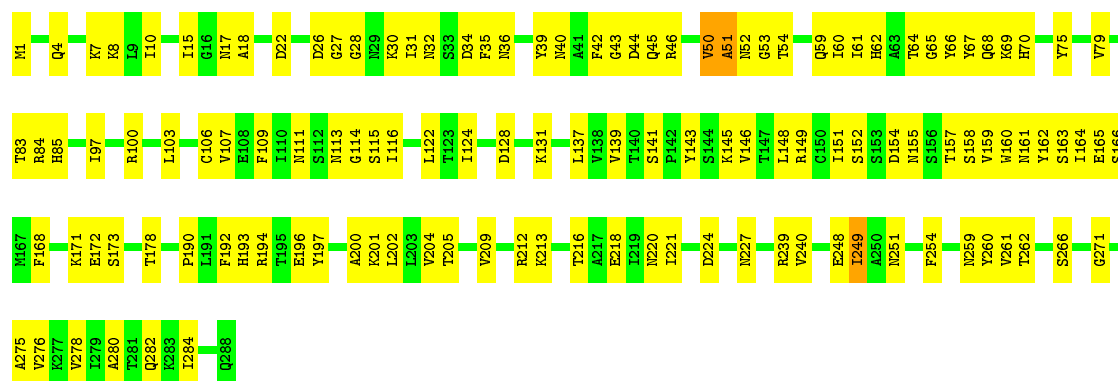
Chain CC: 58% 41%





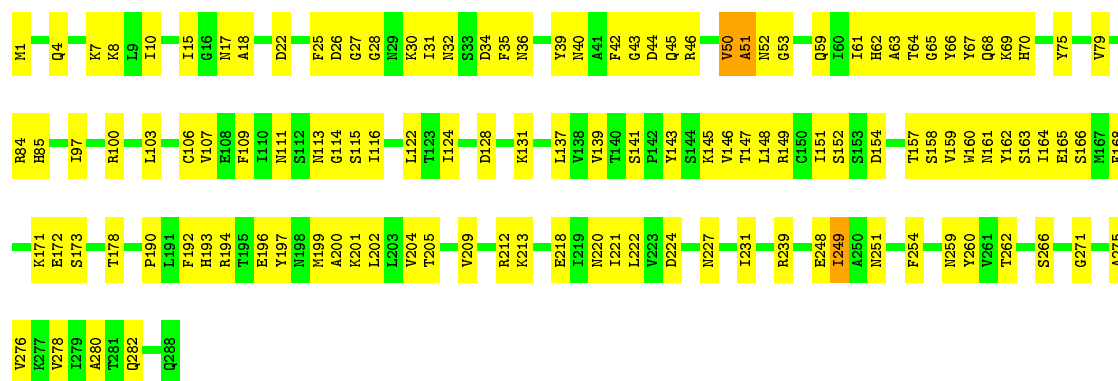
• Molecule 4: Baseplate wedge protein gp9

Chain CD: 56% 43%



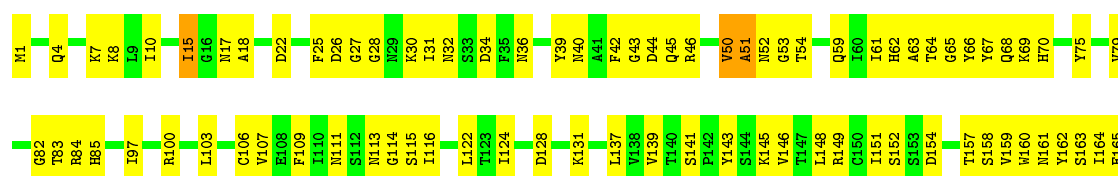
• Molecule 4: Baseplate wedge protein gp9

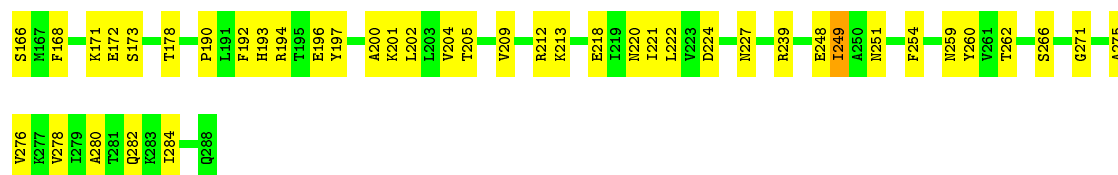
Chain CE: 57% 42%



• Molecule 4: Baseplate wedge protein gp9

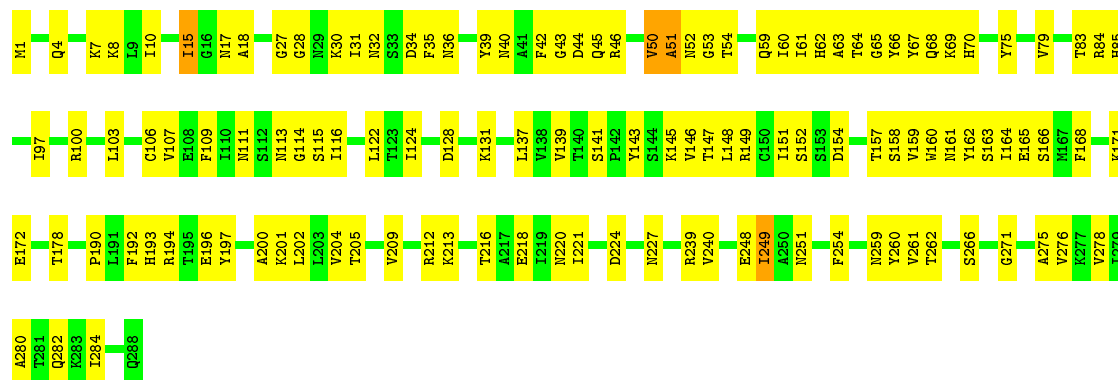
Chain EF: 57% 42%





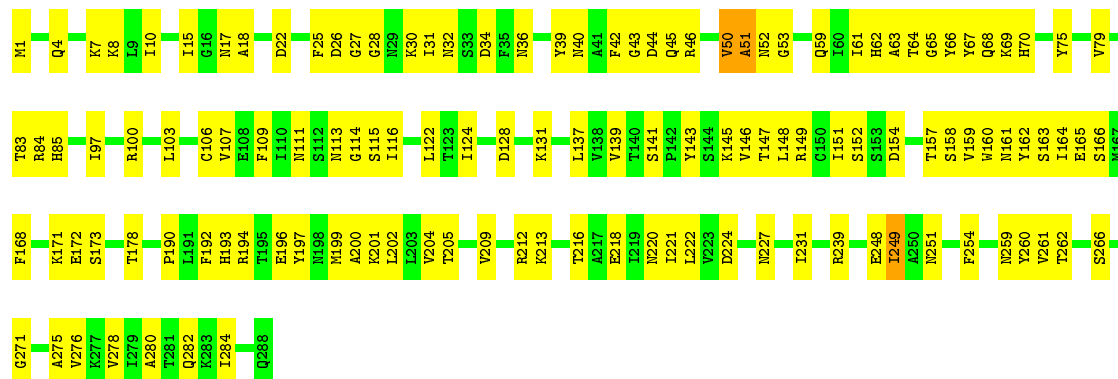
• Molecule 4: Baseplate wedge protein gp9

Chain EG: 57% 42%



• Molecule 4: Baseplate wedge protein gp9

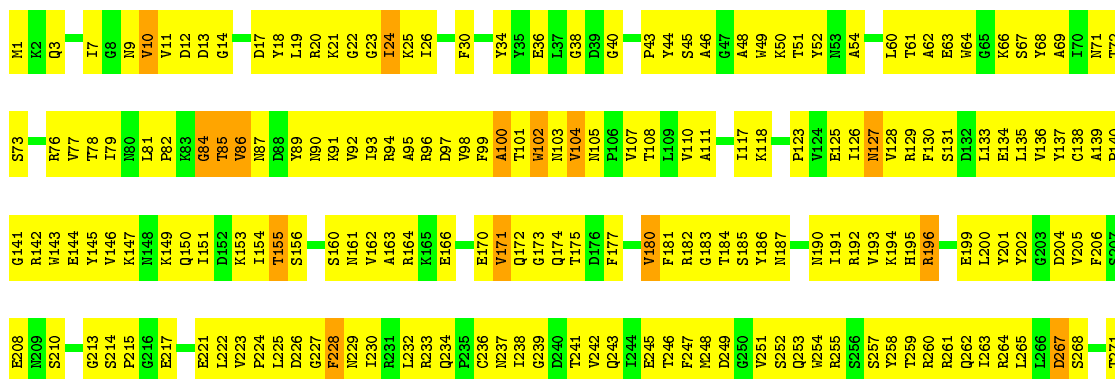
Chain EH: 56% 43%

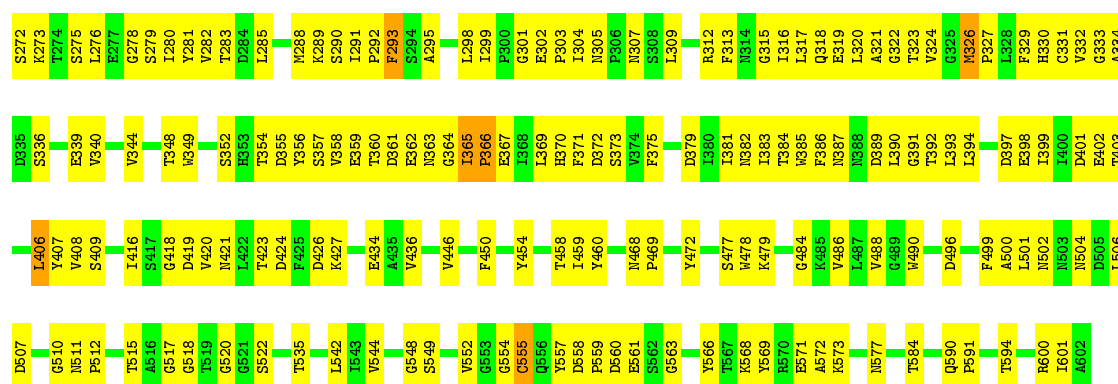


• Molecule 4: Baseplate wedge protein gp9

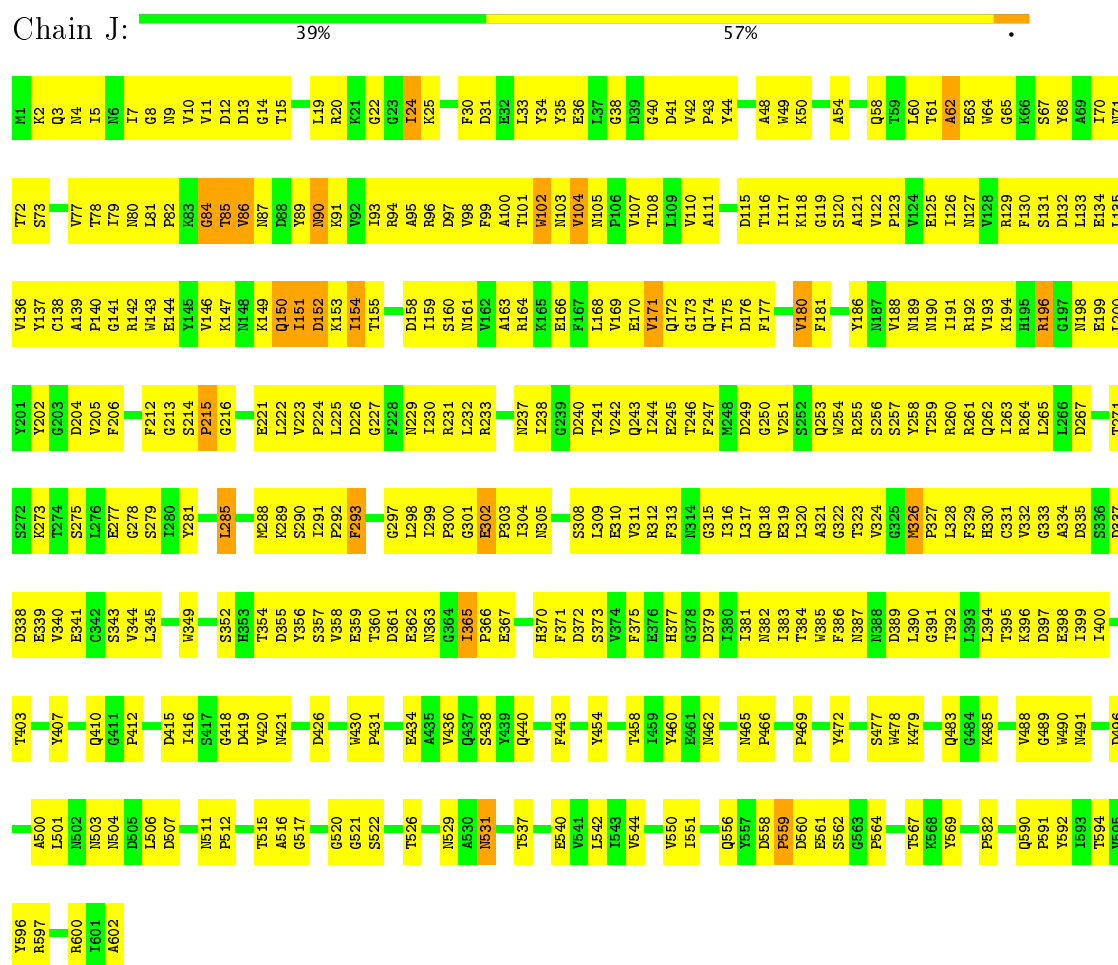
Chain GI: 58% 41%



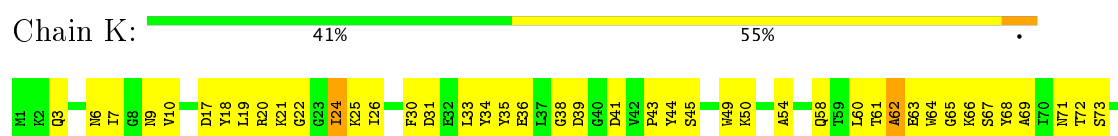




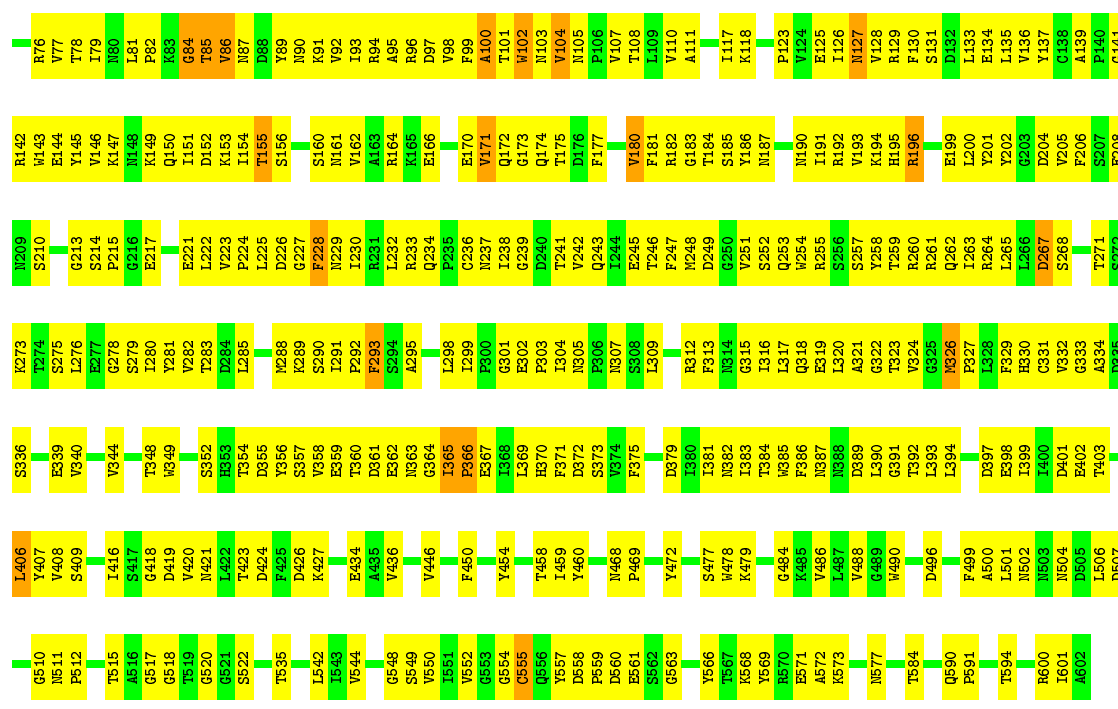
• Molecule 5: Baseplate wedge protein gp10



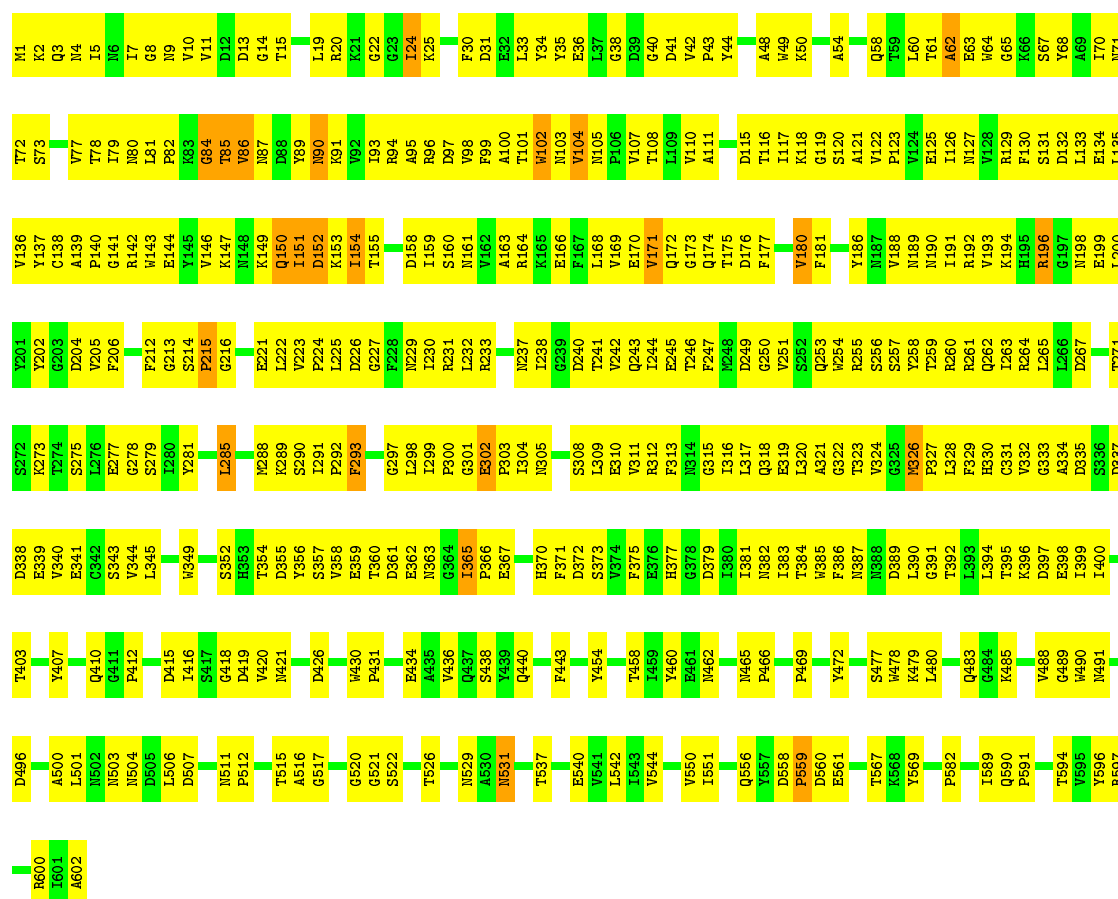
• Molecule 5: Baseplate wedge protein gp10



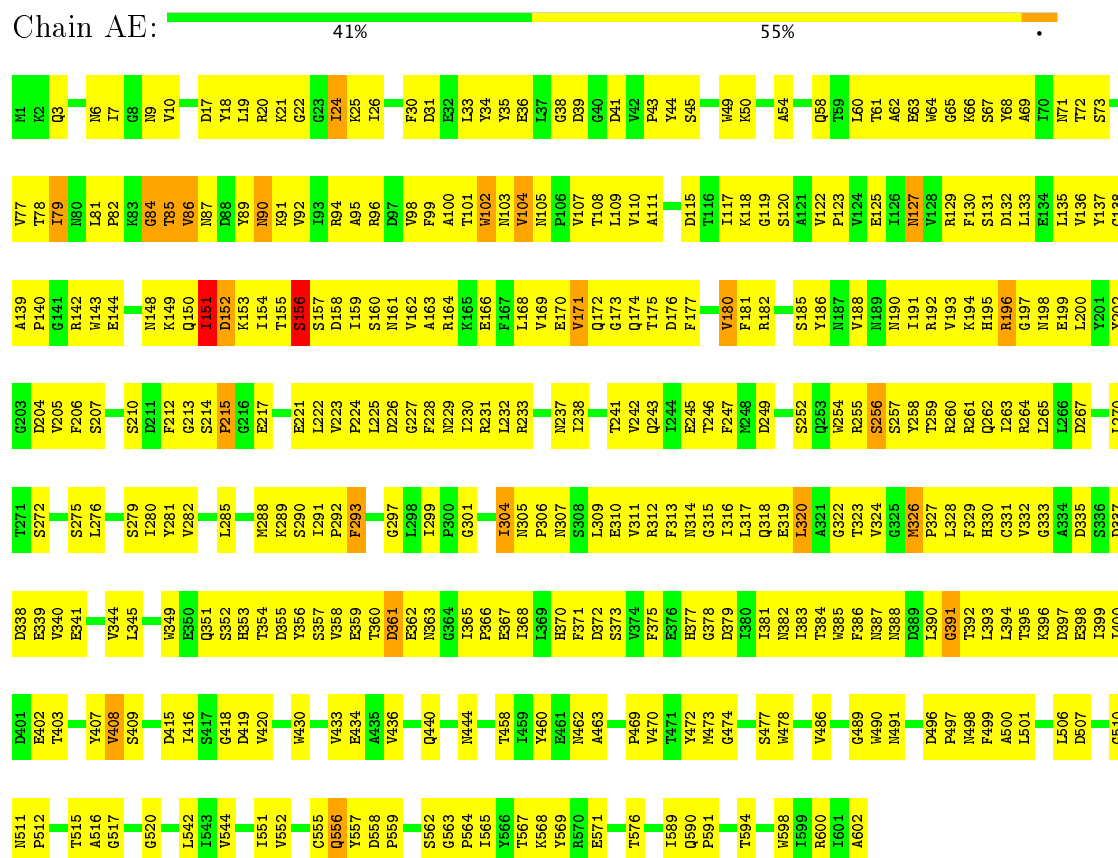




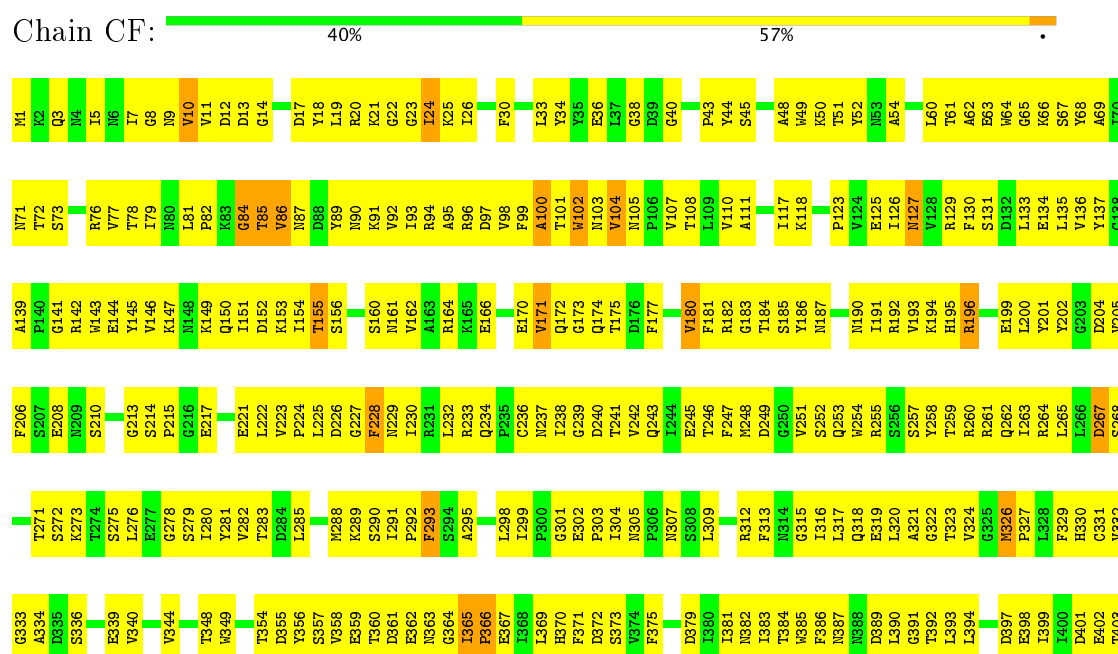
Chain AD:

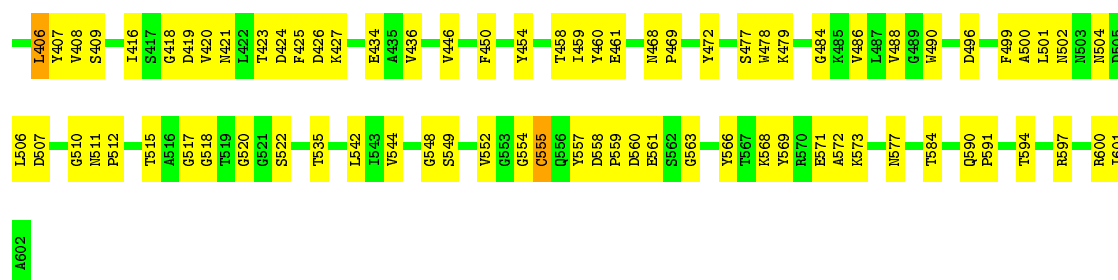


• Molecule 5: Baseplate wedge protein gp10

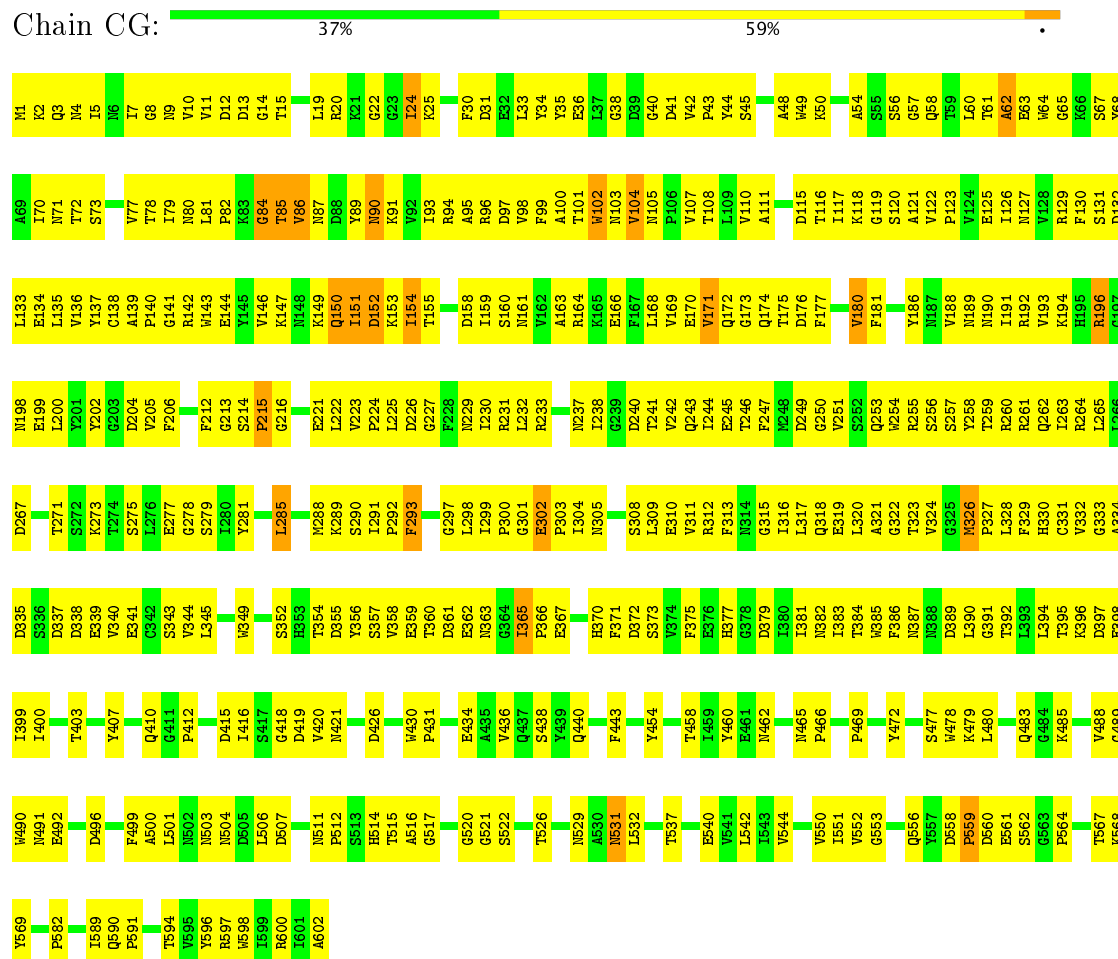


• Molecule 5: Baseplate wedge protein gp10

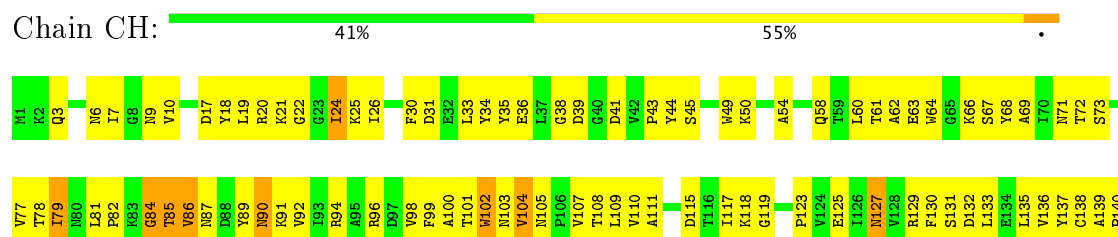


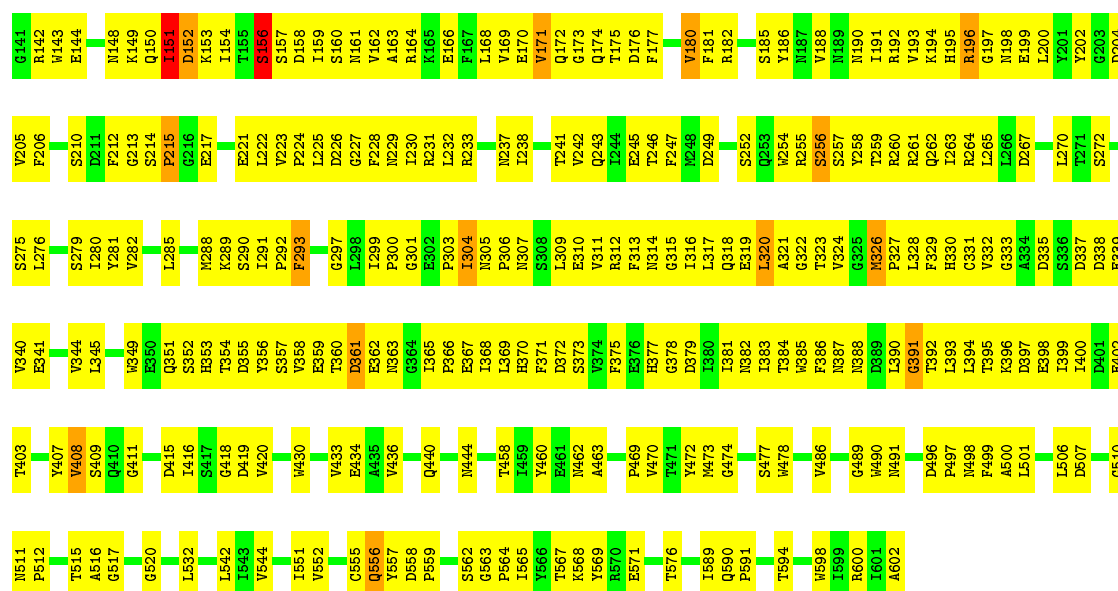


• Molecule 5: Baseplate wedge protein gp10



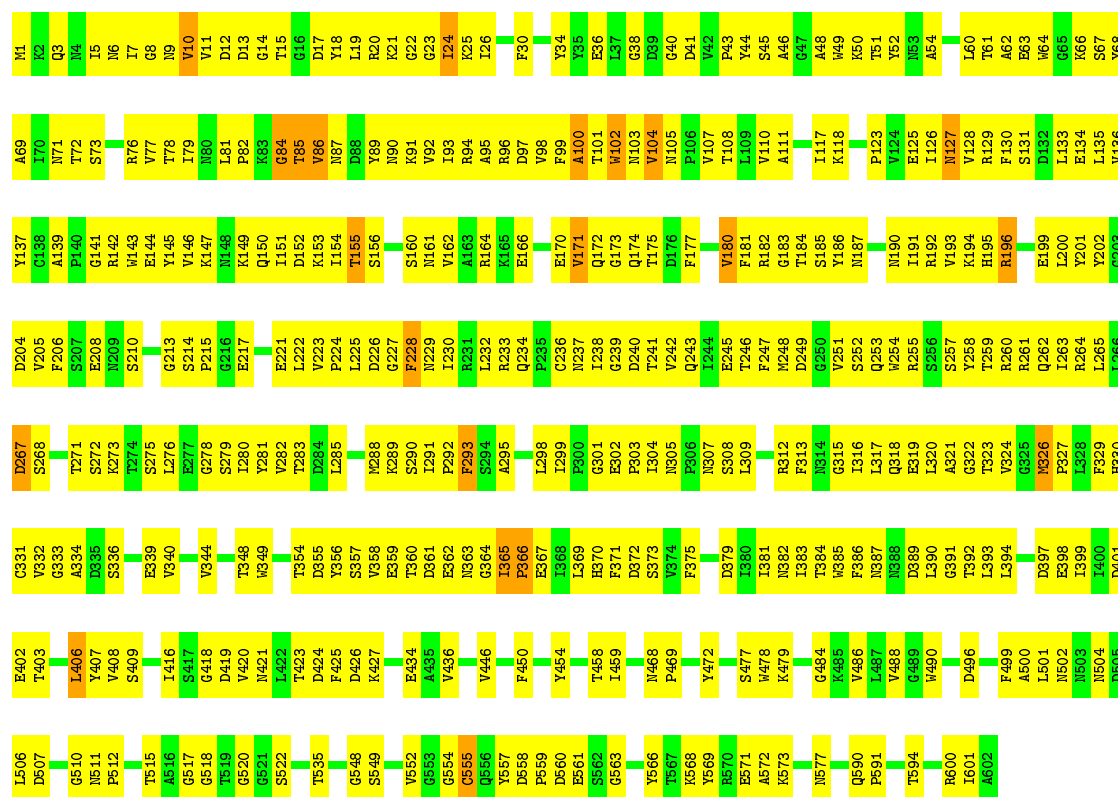
• Molecule 5: Baseplate wedge protein gp10





• Molecule 5: Baseplate wedge protein gp10

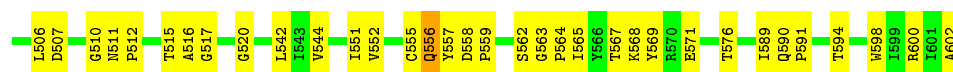
Chain EI: 40% 56%



• Molecule 5: Baseplate wedge protein gp10

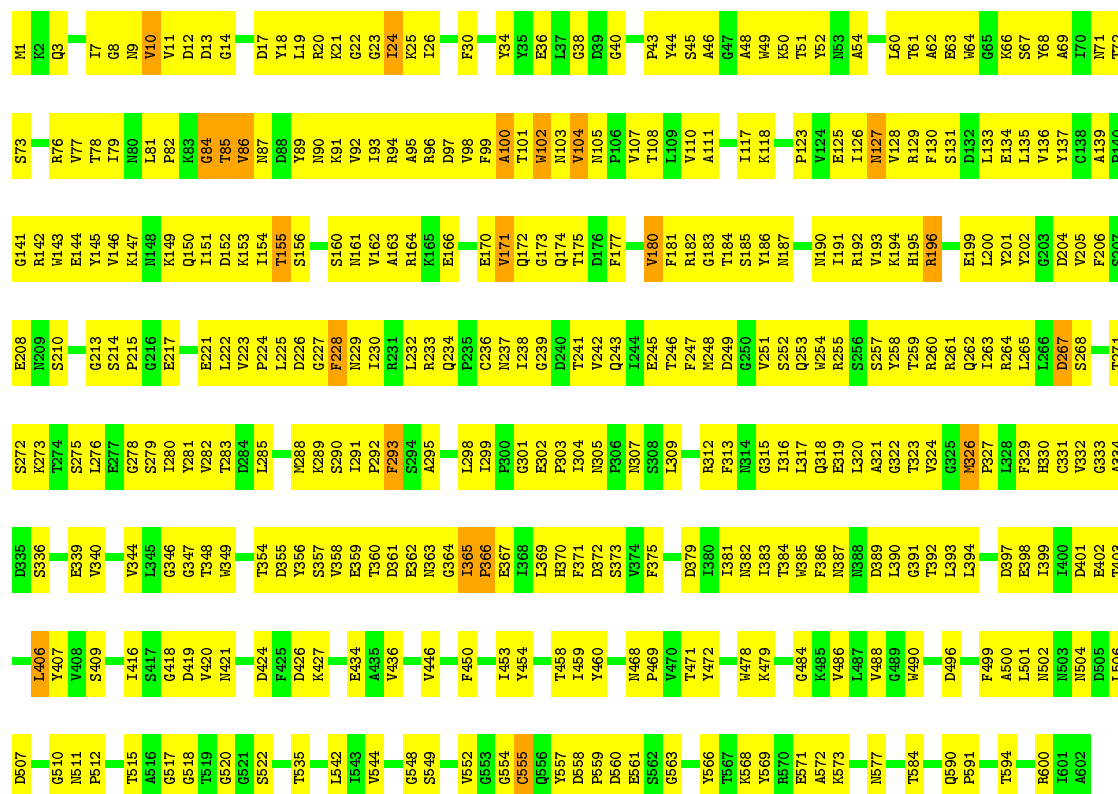
Chain EJ: 38% 59%





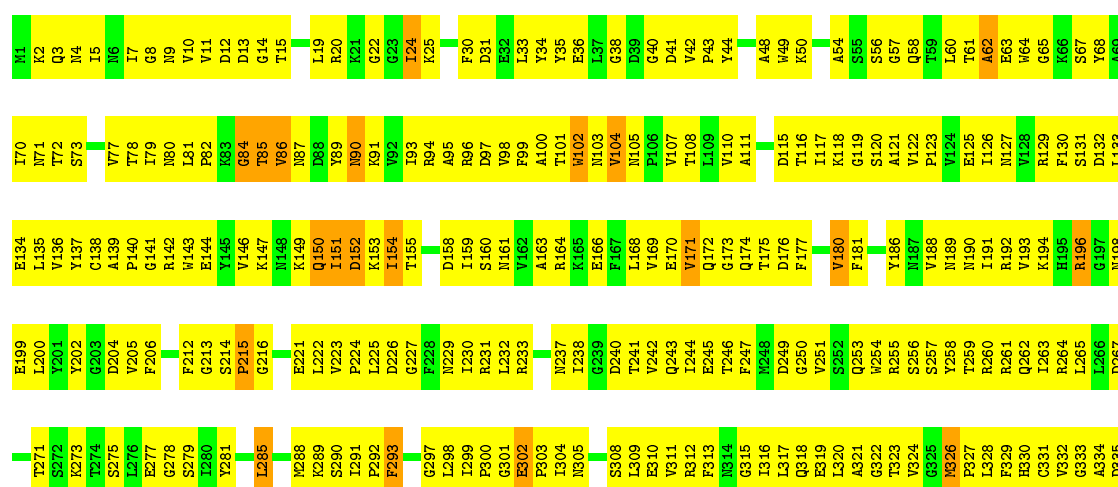
• Molecule 5: Baseplate wedge protein gp10

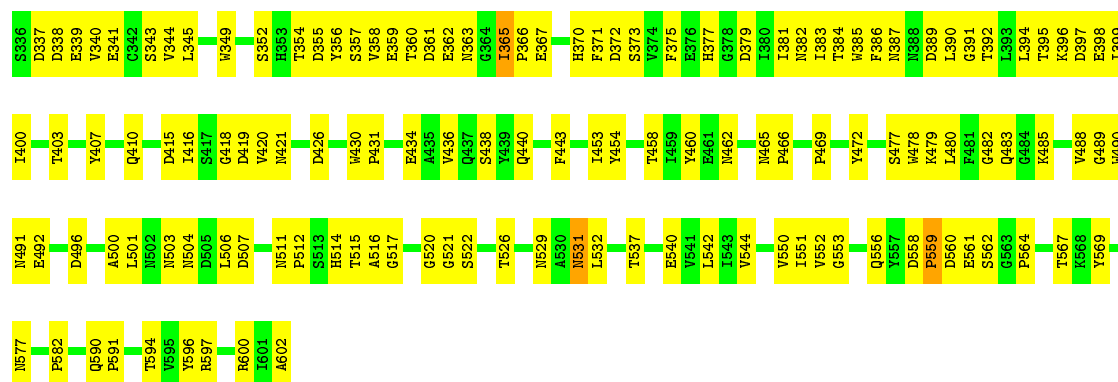
Chain HB:



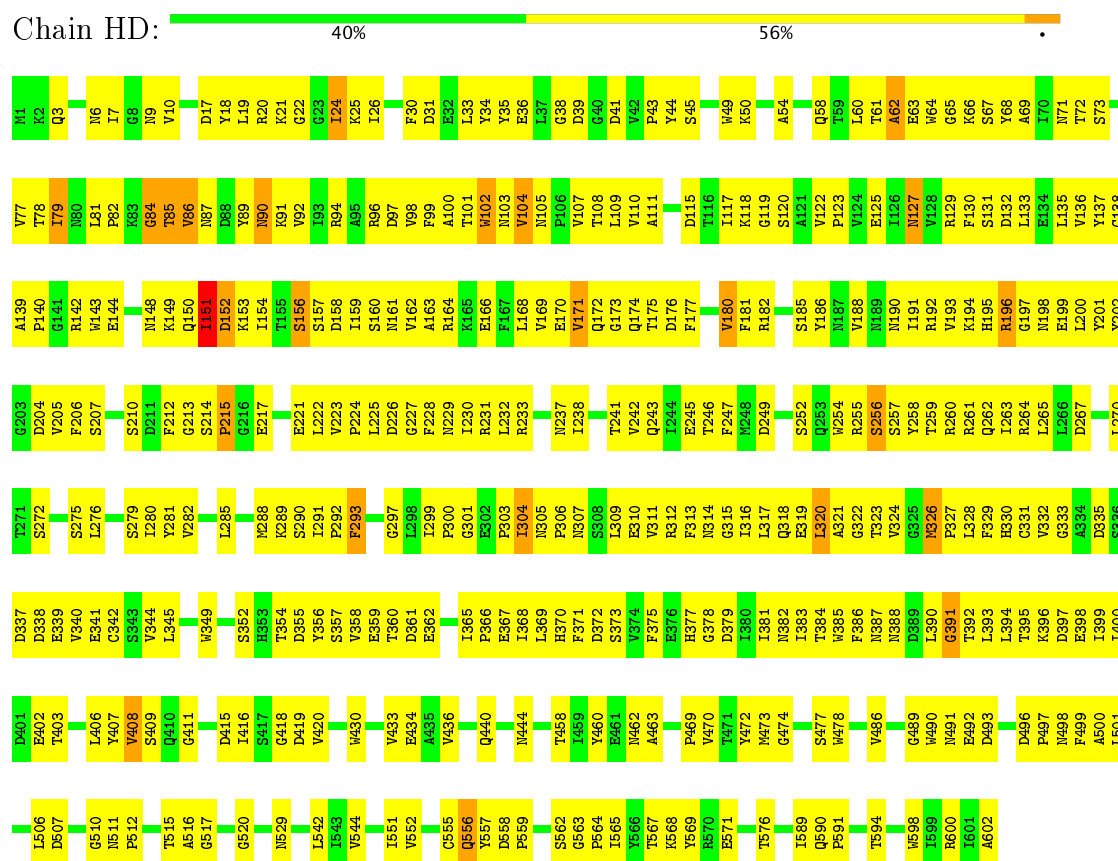
• Molecule 5: Baseplate wedge protein gp10

Chain HC:

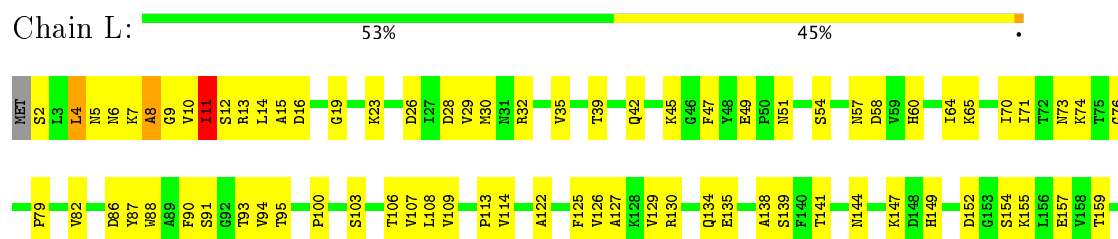


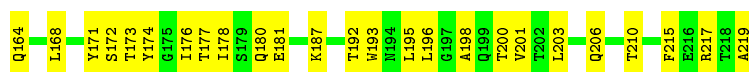


• Molecule 5: Baseplate wedge protein gp10



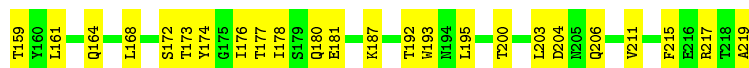
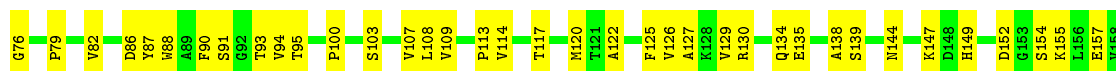
• Molecule 6: Baseplate wedge protein gp11





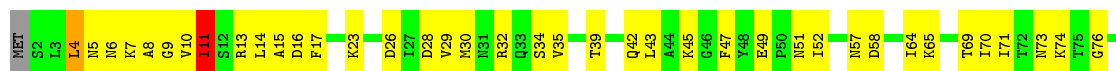
- Molecule 6: Baseplate wedge protein gp11

Chain M: 54% 44%



- Molecule 6: Baseplate wedge protein gp11

Chain N: 52% 47%



- Molecule 6: Baseplate wedge protein gp11

Chain i: 98%



- Molecule 6: Baseplate wedge protein gp11

Chain j: 98%

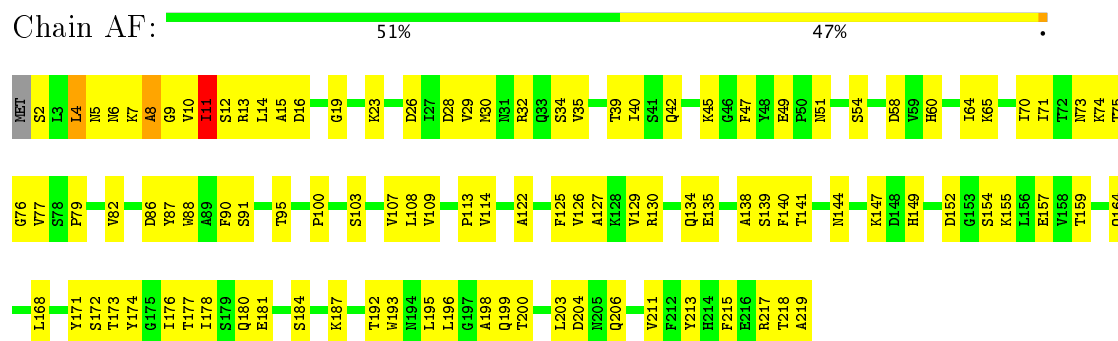


- Molecule 6: Baseplate wedge protein gp11

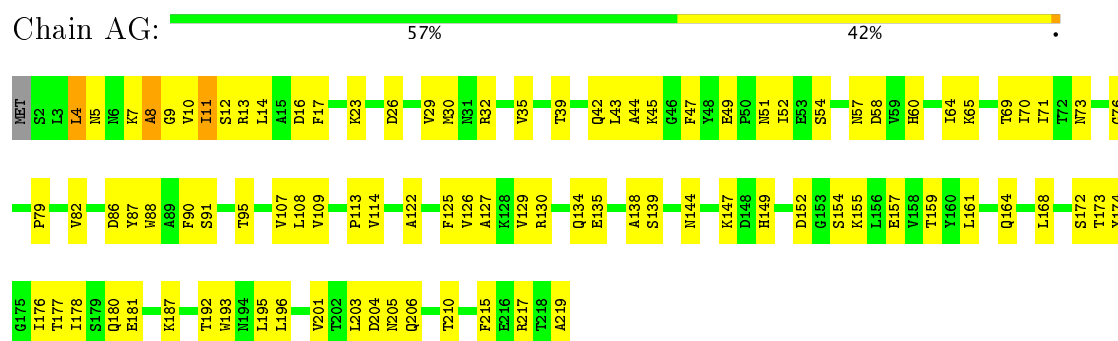
Chain k: 98%



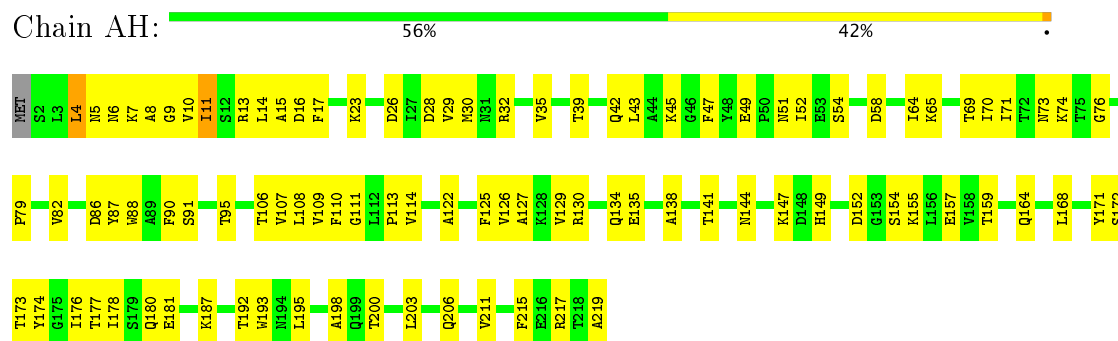
- Molecule 6: Baseplate wedge protein gp11



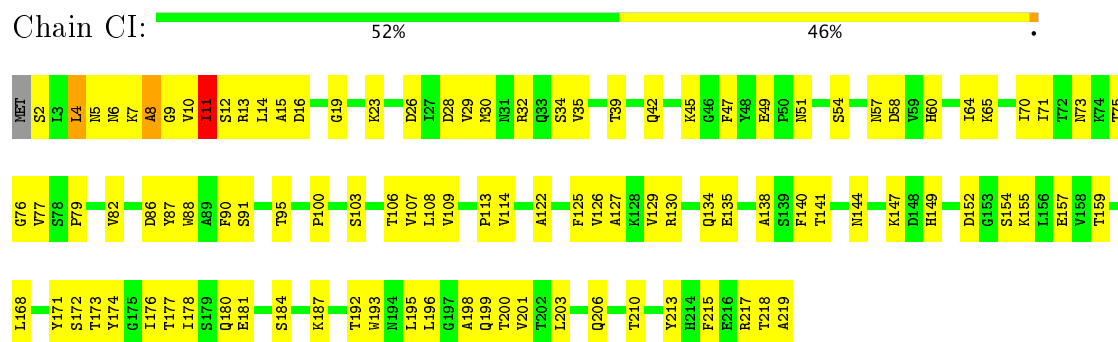
- Molecule 6: Baseplate wedge protein gp11



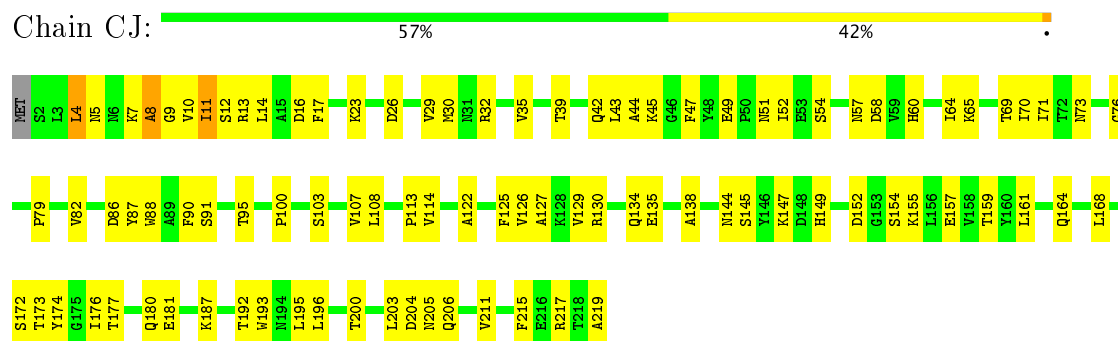
- Molecule 6: Baseplate wedge protein gp11



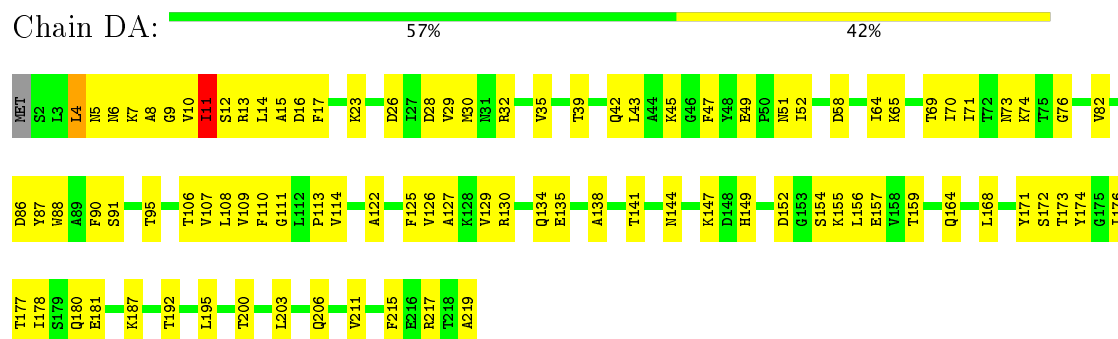
- Molecule 6: Baseplate wedge protein gp11



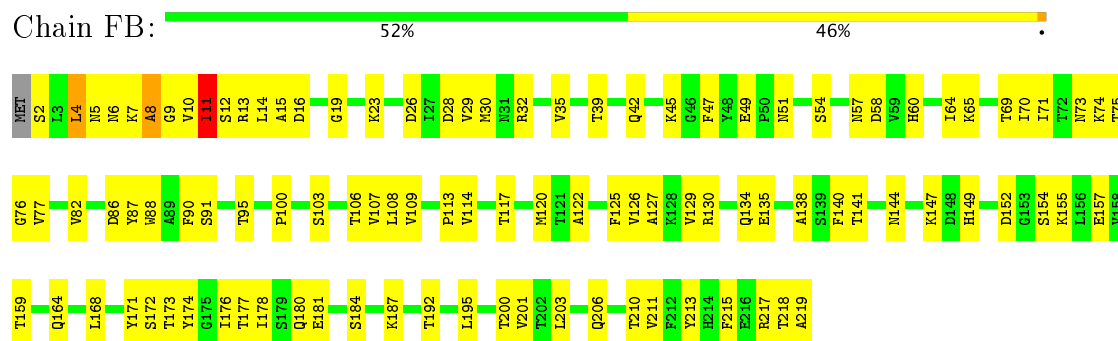
- Molecule 6: Baseplate wedge protein gp11



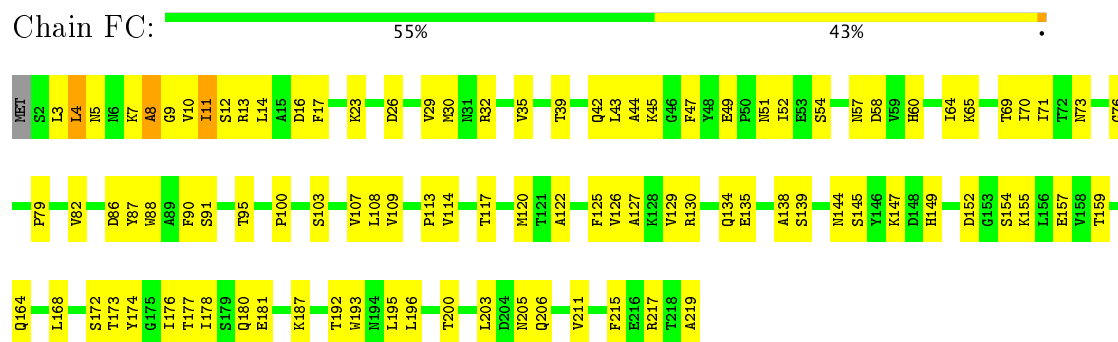
- Molecule 6: Baseplate wedge protein gp11



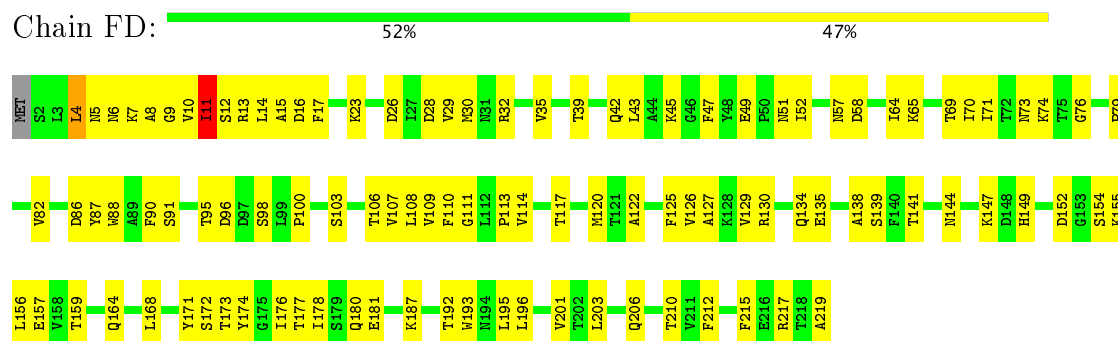
- Molecule 6: Baseplate wedge protein gp11



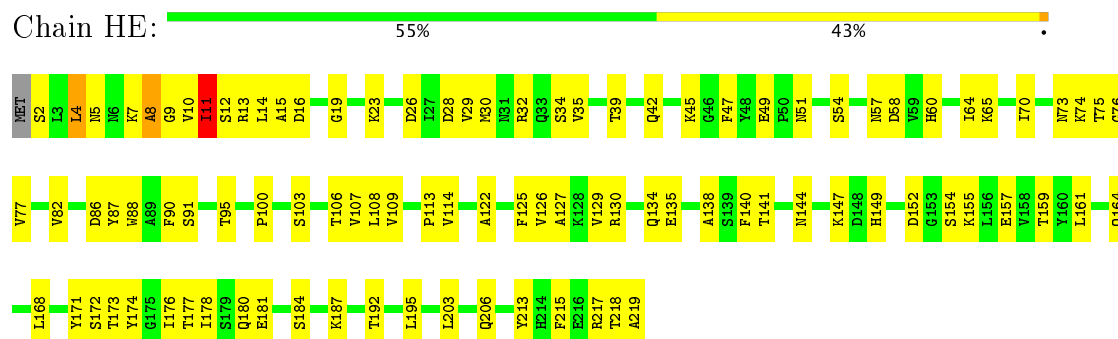
- Molecule 6: Baseplate wedge protein gp11



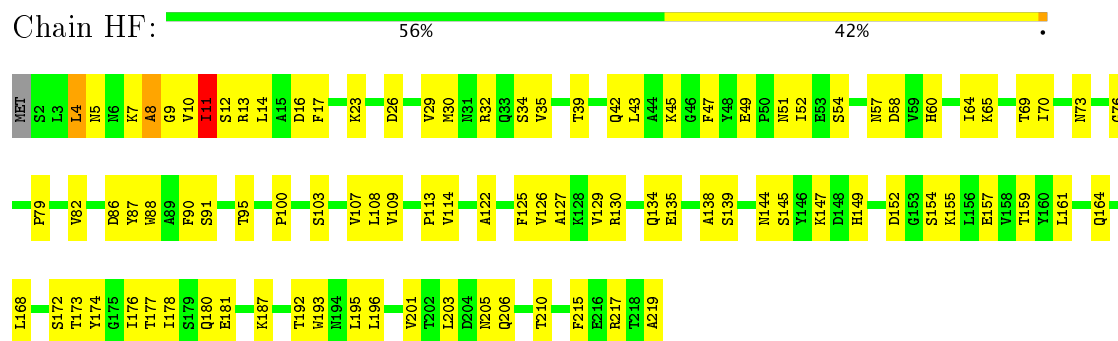
- Molecule 6: Baseplate wedge protein gp11



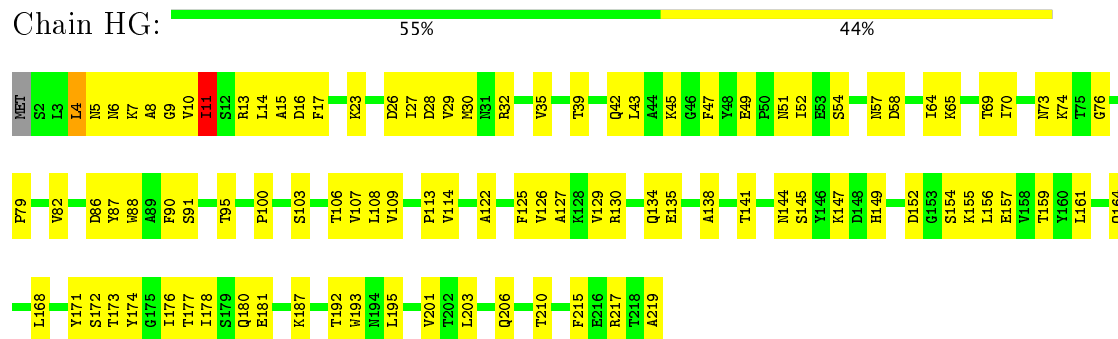
- Molecule 6: Baseplate wedge protein gp11



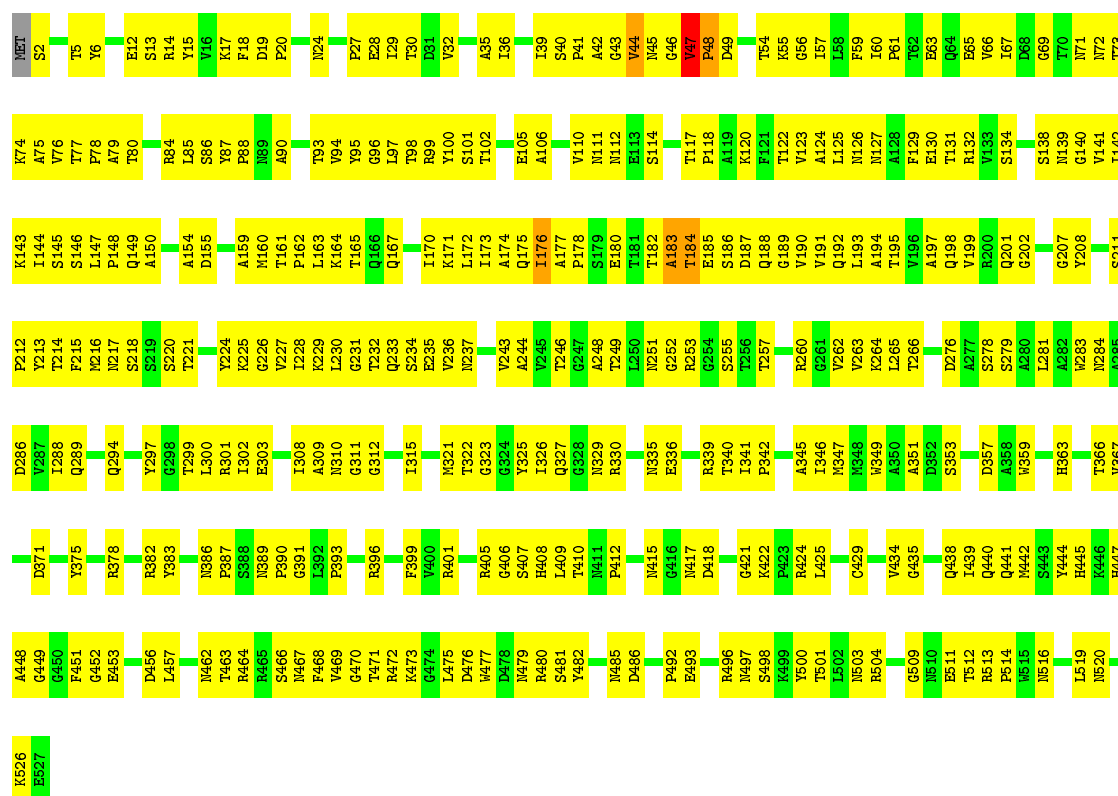
- Molecule 6: Baseplate wedge protein gp11



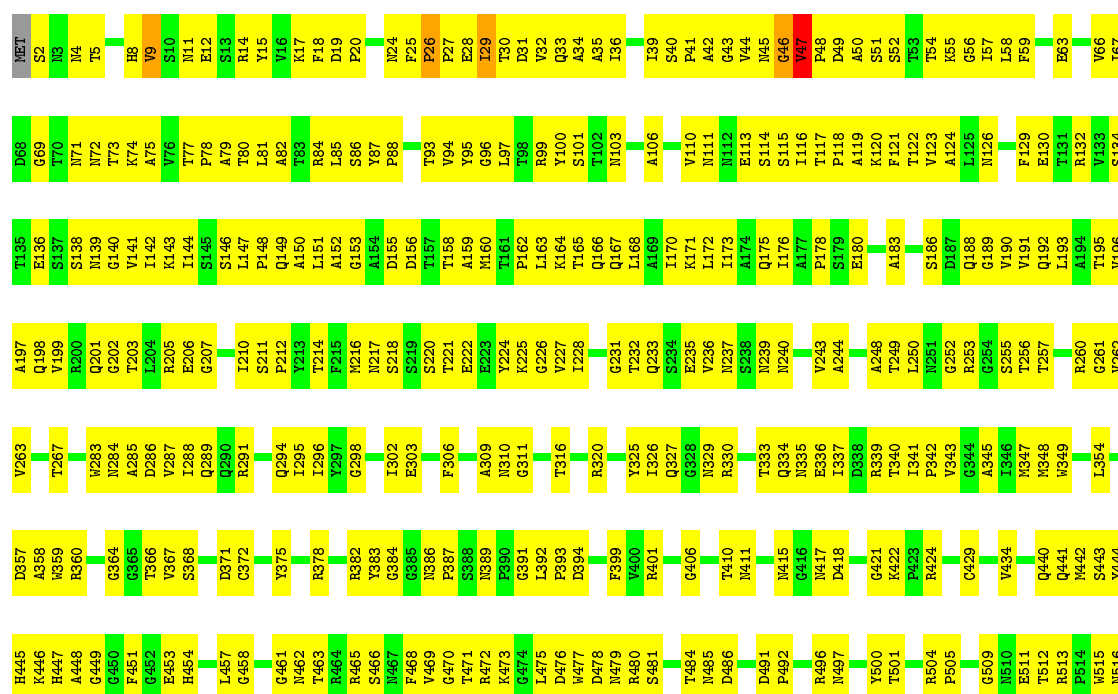
- Molecule 6: Baseplate wedge protein gp11



- Molecule 7: Short tail fiber protein gp12

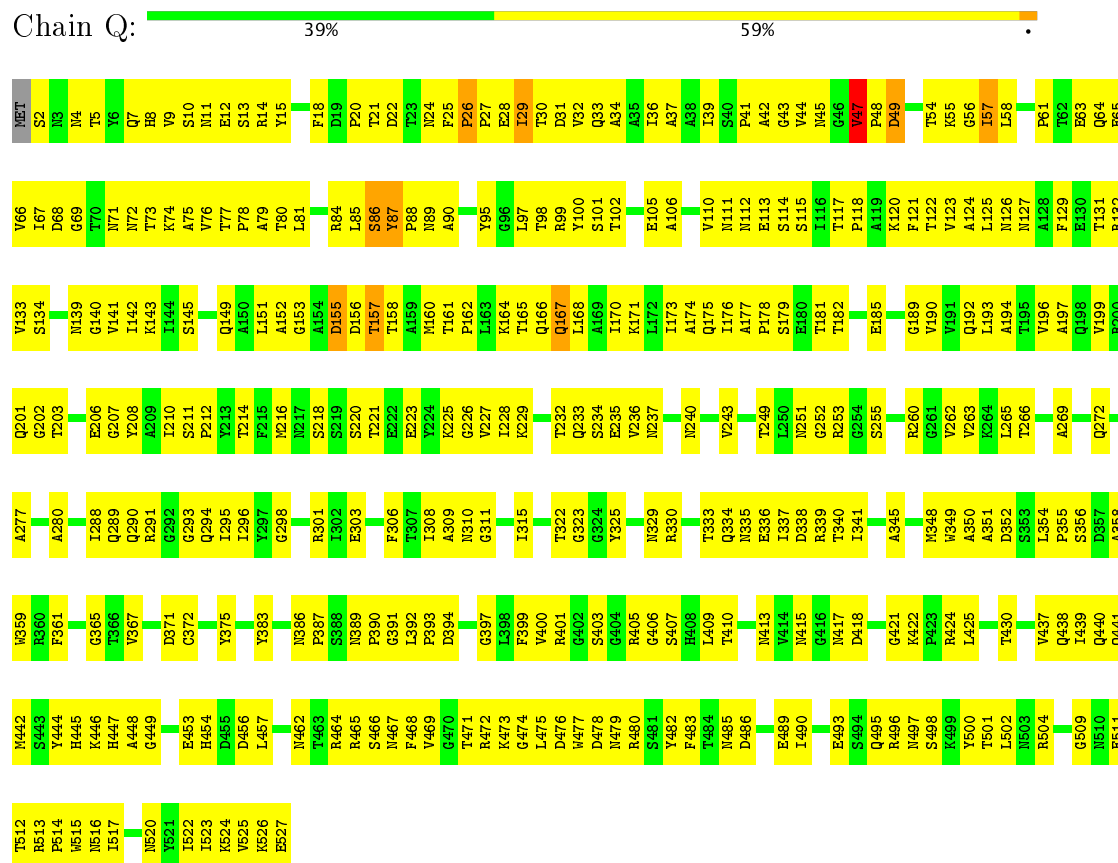
Chain O:  40% 58%

• Molecule 7: Short tail fiber protein gp12

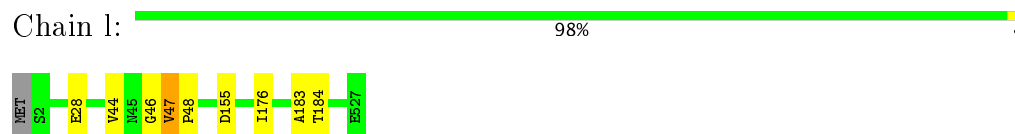
Chain P:  39% 60%



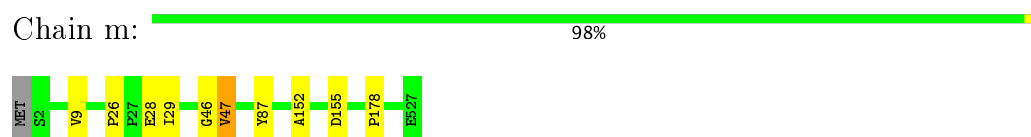
• Molecule 7: Short tail fiber protein gp12



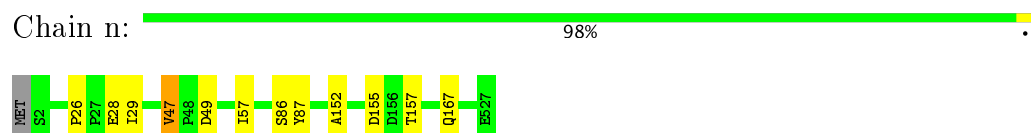
• Molecule 7: Short tail fiber protein gp12



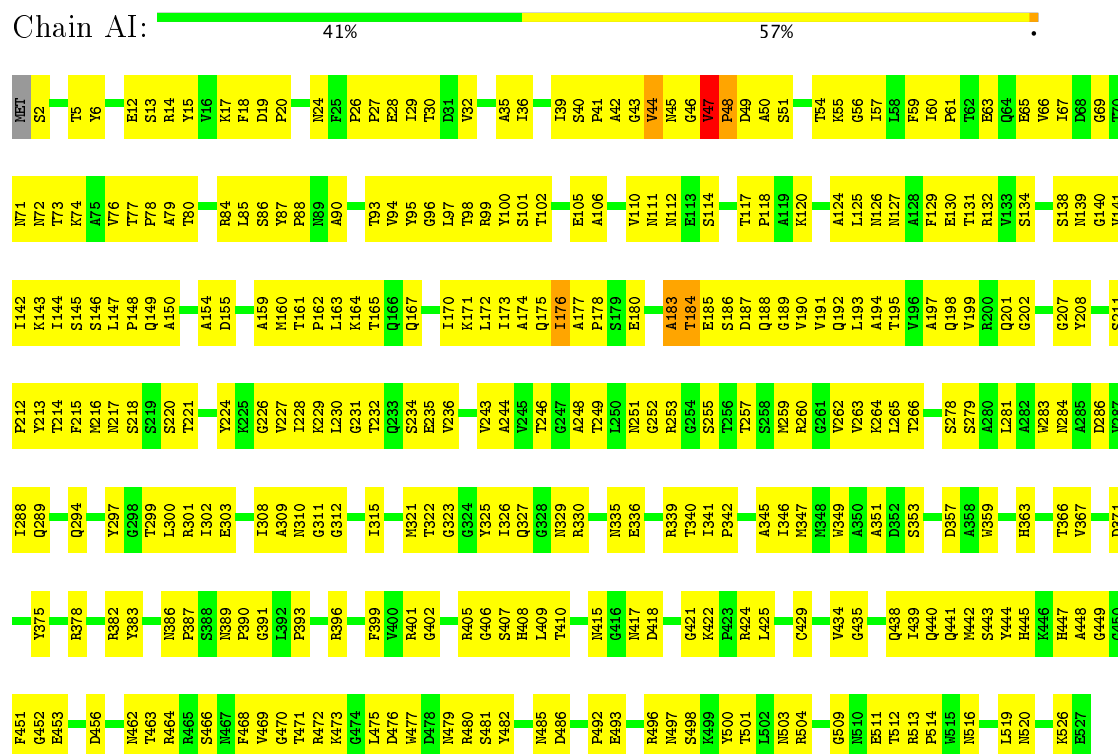
• Molecule 7: Short tail fiber protein gp12



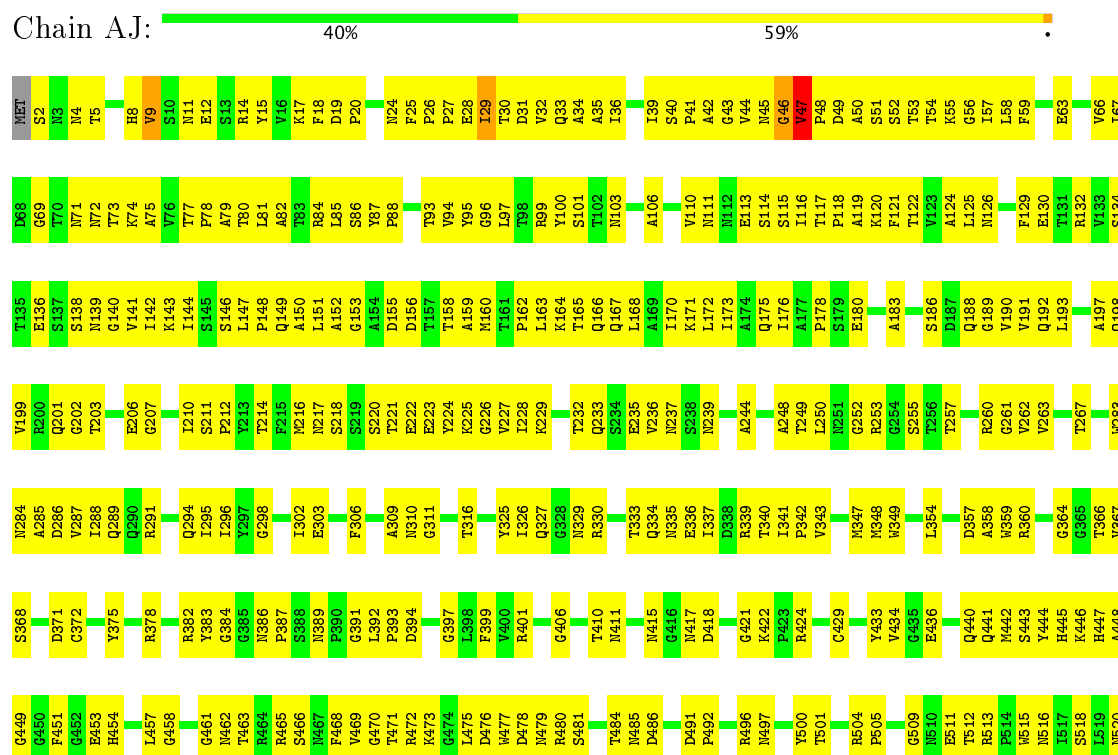
• Molecule 7: Short tail fiber protein gp12



• Molecule 7: Short tail fiber protein gp12



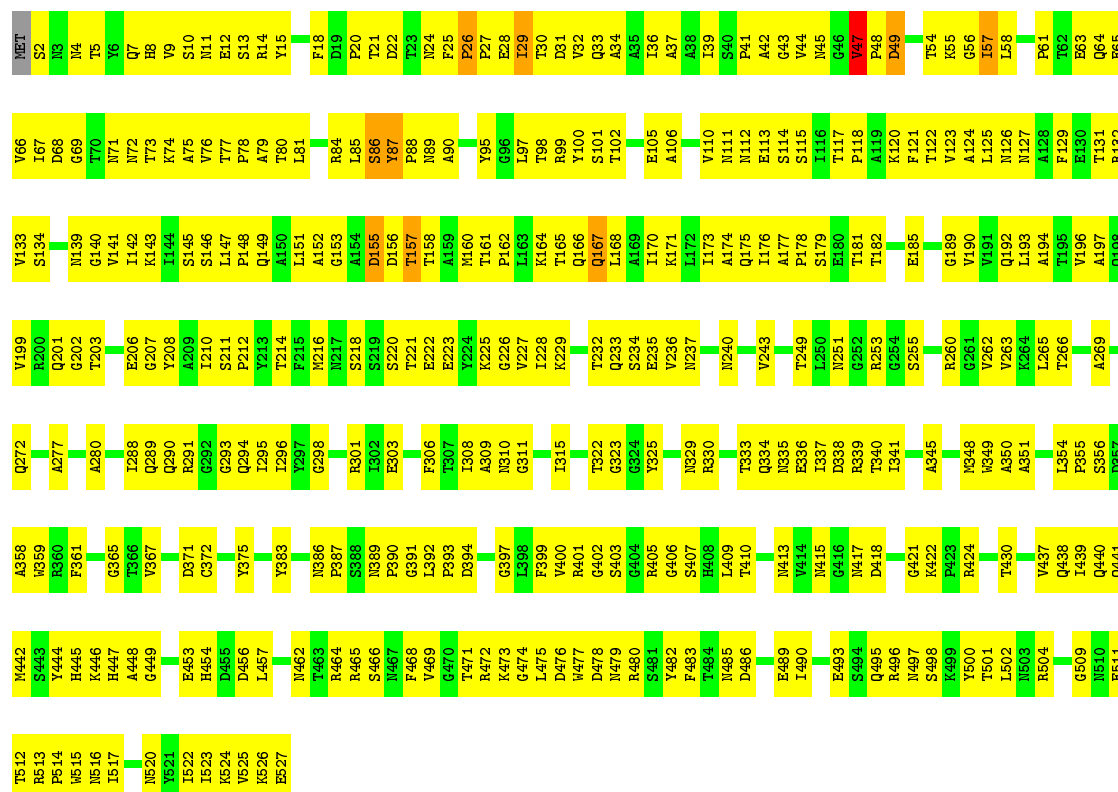
• Molecule 7: Short tail fiber protein gp12



V521  
V522  
V523  
V524  
V525  
V526  
V527

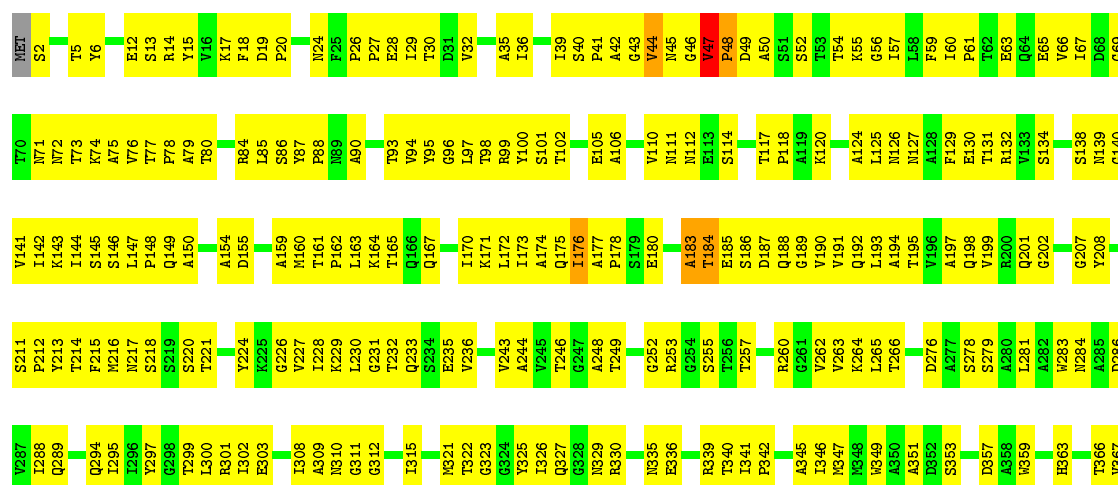
• Molecule 7: Short tail fiber protein gp12

Chain BA: 39% 59%

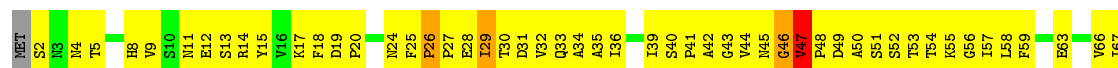


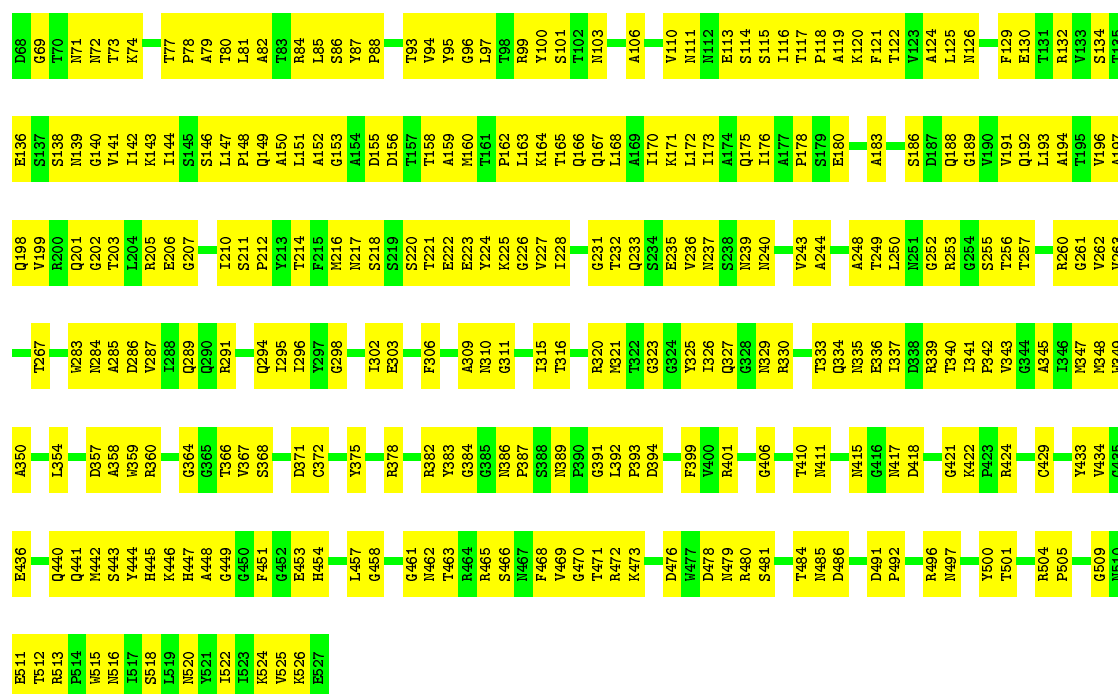
• Molecule 7: Short tail fiber protein gp12

Chain DB: 40% 58%

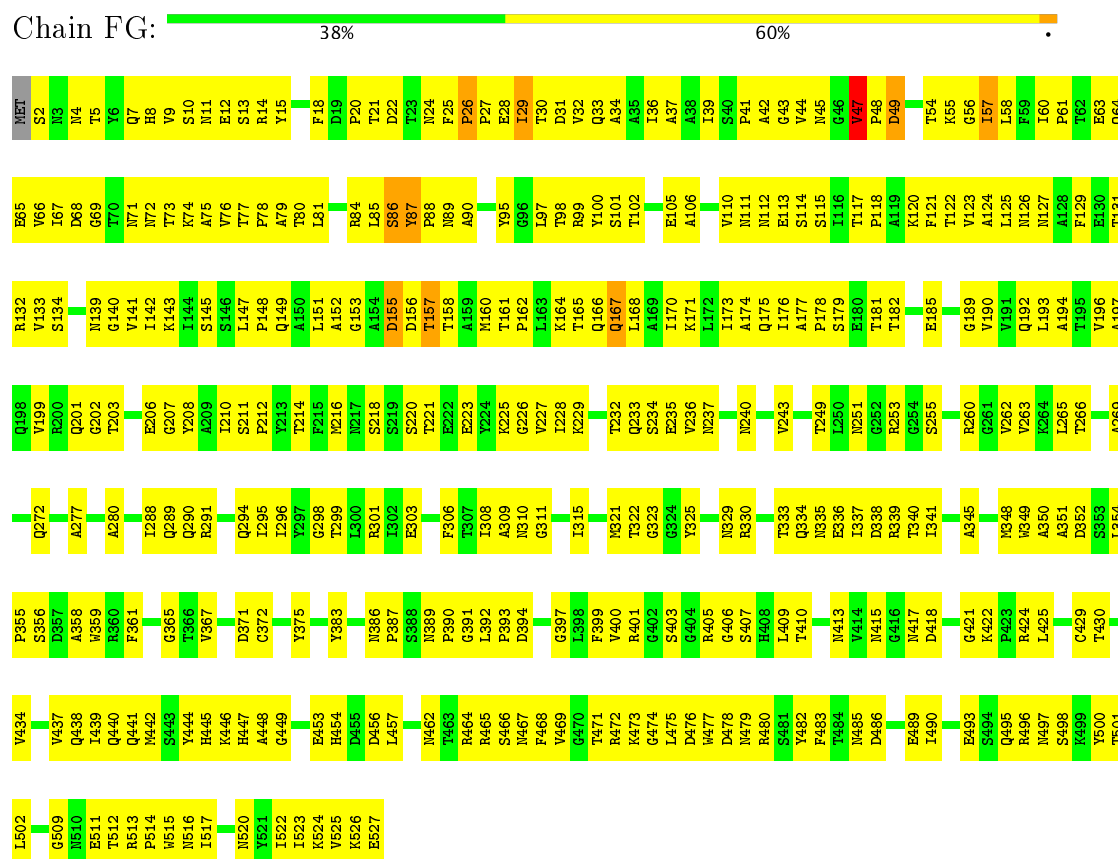






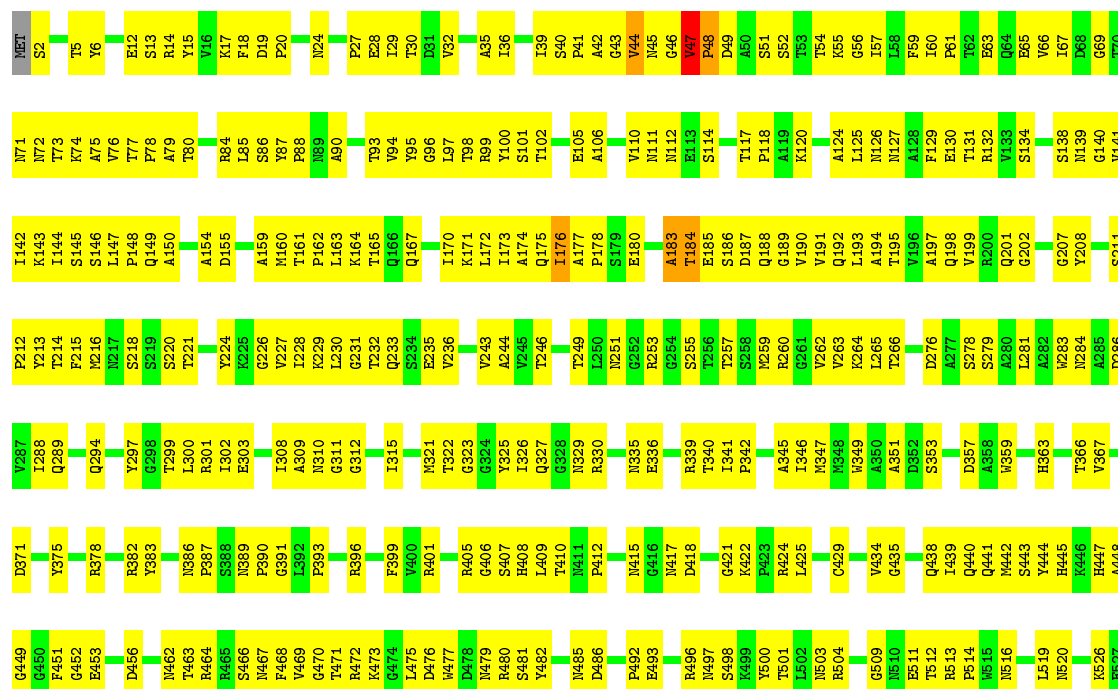


• Molecule 7: Short tail fiber protein gp12



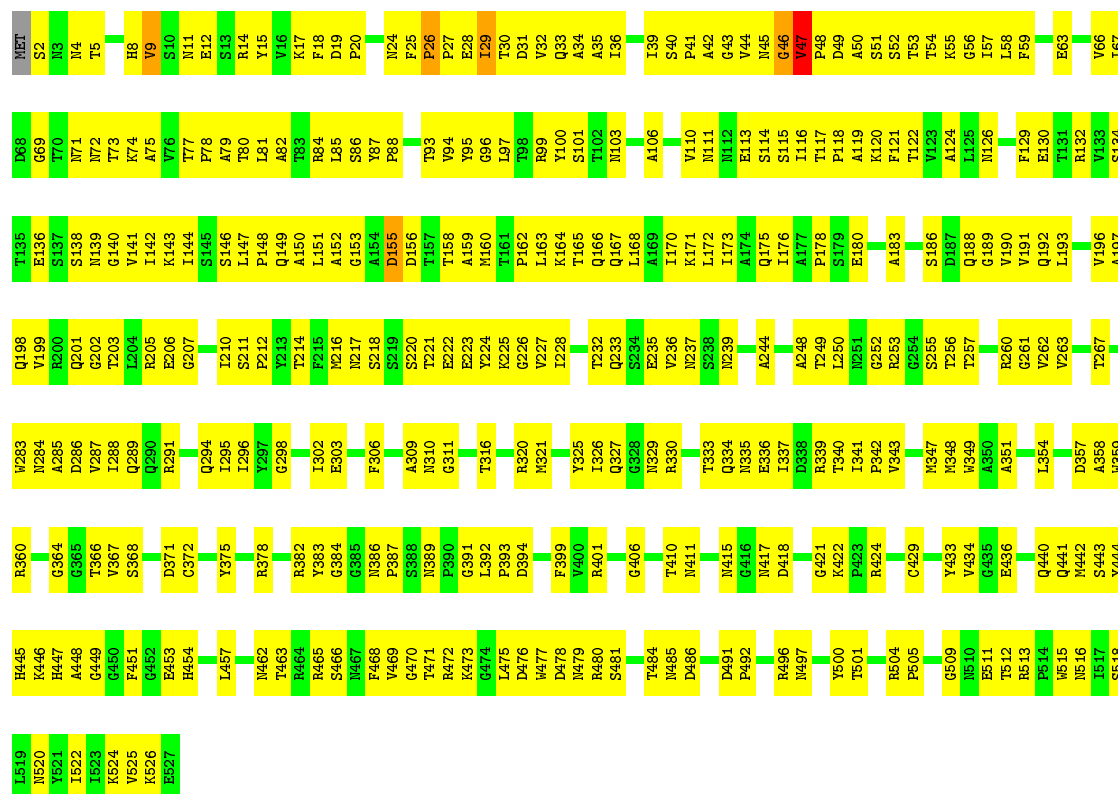
• Molecule 7: Short tail fiber protein gp12

Chain HH:  42% 57%

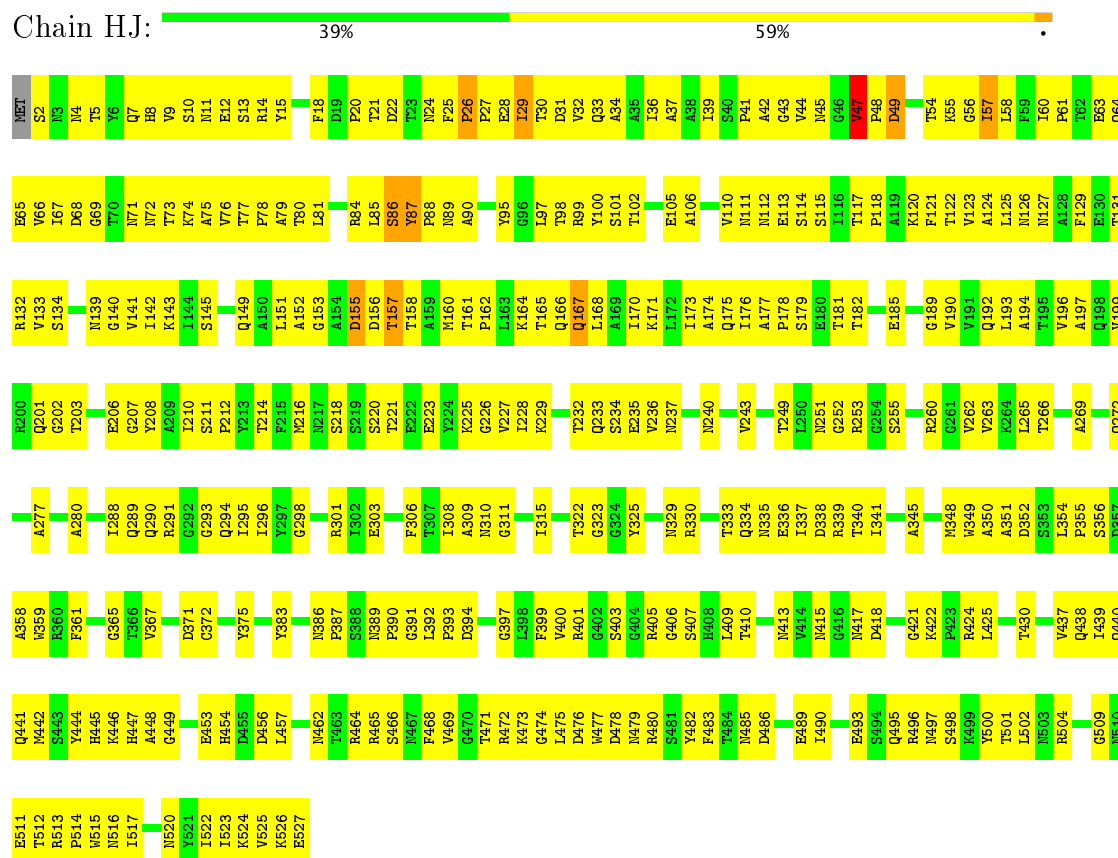


# • Molecule 7: Short tail fiber protein gp12

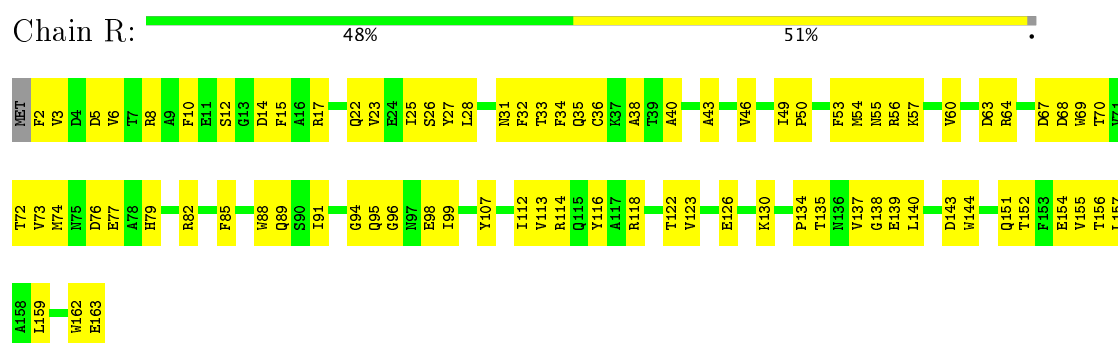
Chain HI:  40% 59%



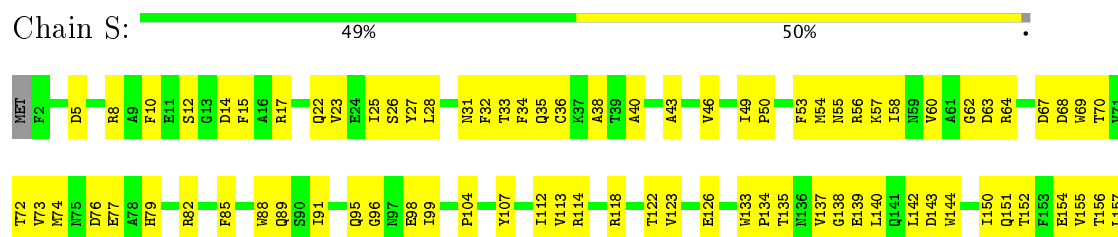
- Molecule 7: Short tail fiber protein gp12



- Molecule 8: Tail tube protein gp19



- Molecule 8: Tail tube protein gp19





- Molecule 8: Tail tube protein gp19

Chain o: 99%



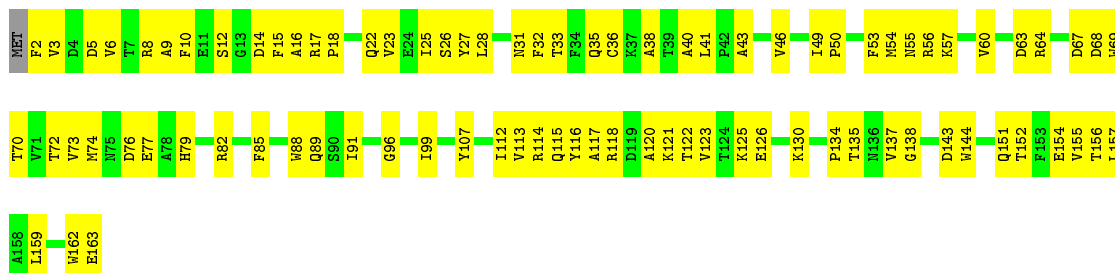
- Molecule 8: Tail tube protein gp19

Chain p: 99%



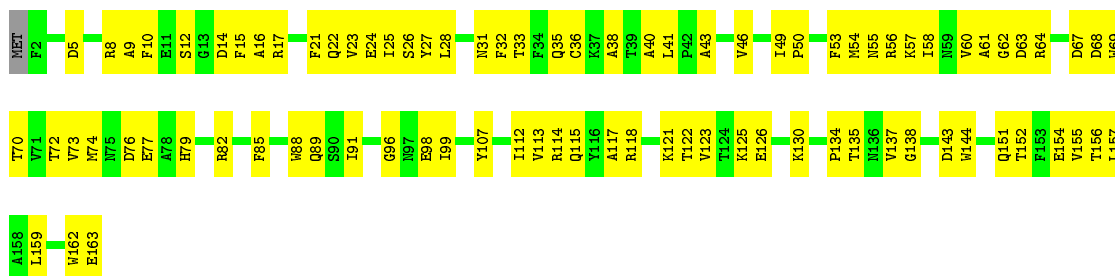
- Molecule 8: Tail tube protein gp19

Chain BB: 47%



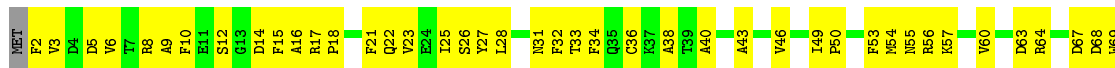
- Molecule 8: Tail tube protein gp19

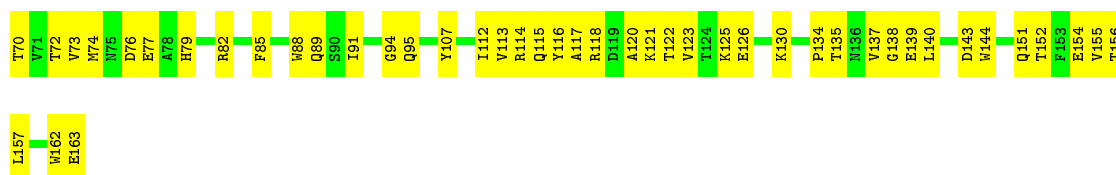
Chain BC: 47%



- Molecule 8: Tail tube protein gp19

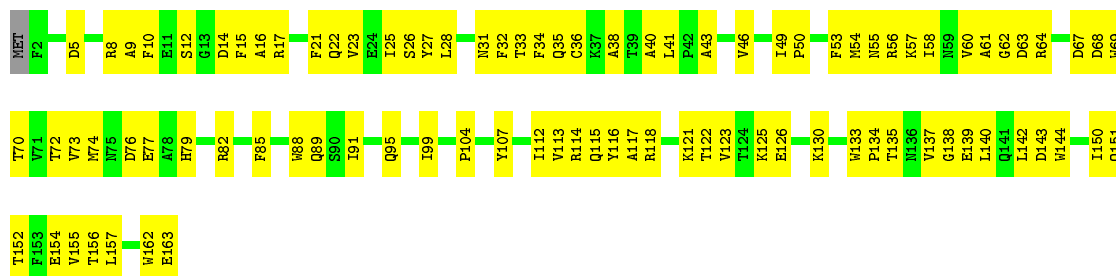
Chain DE: 46%





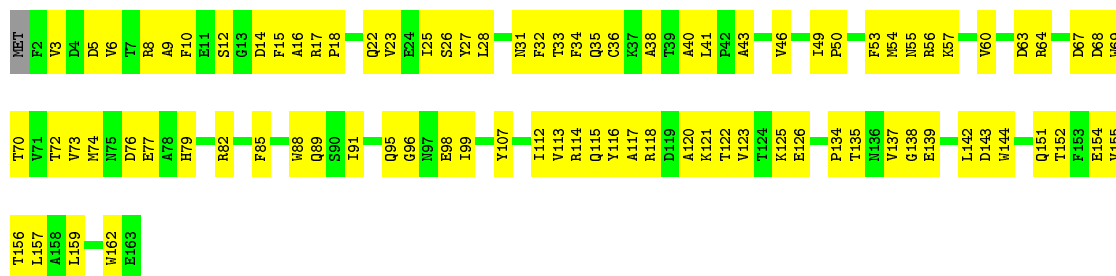
- Molecule 8: Tail tube protein gp19

Chain DF: 44% 56%



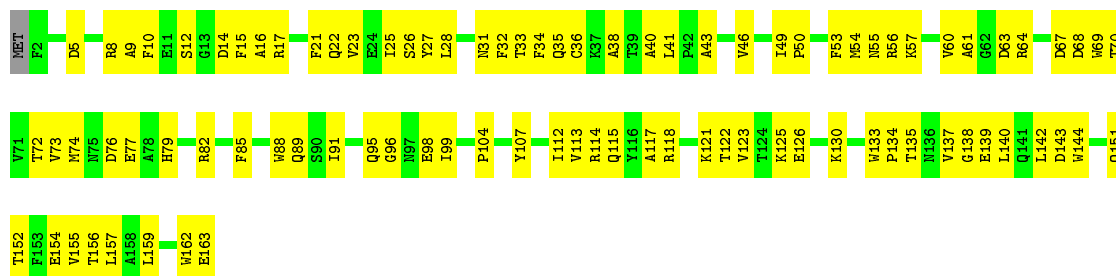
- Molecule 8: Tail tube protein gp19

Chain FH: 45% 54%



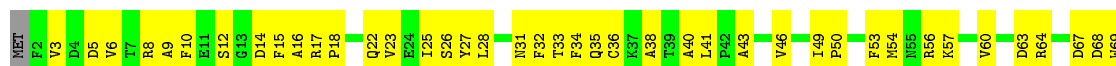
- Molecule 8: Tail tube protein gp19

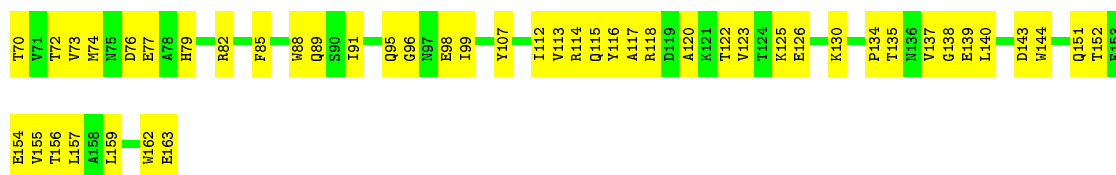
Chain FI: 44% 55%



- Molecule 8: Tail tube protein gp19

Chain IA: 45% 54%

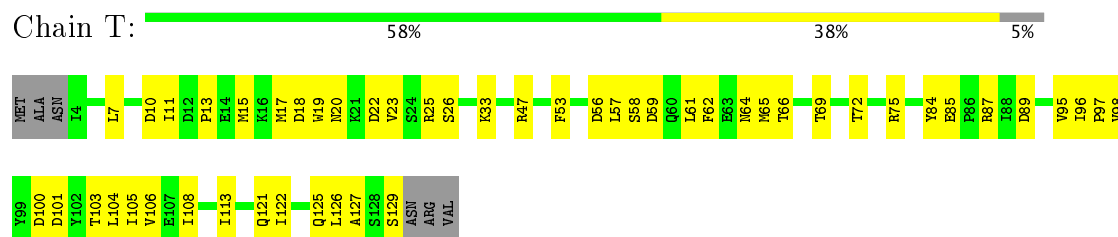




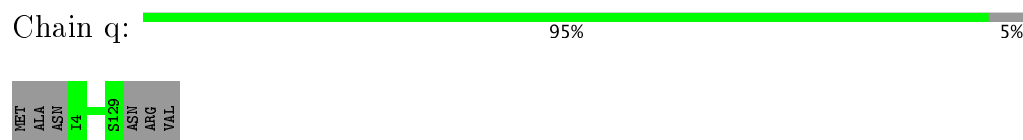
- Molecule 8: Tail tube protein gp19



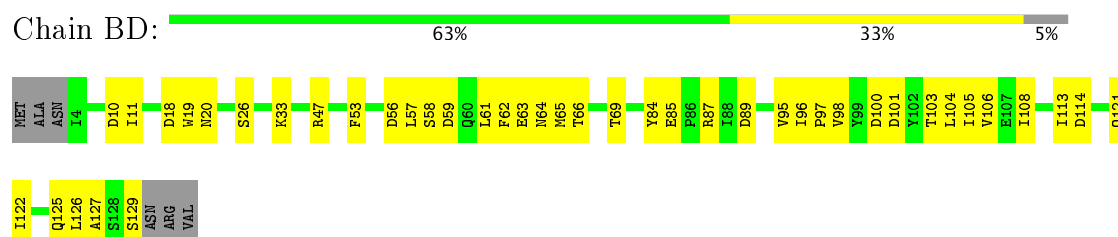
- Molecule 9: Baseplate wedge protein gp25



- Molecule 9: Baseplate wedge protein gp25



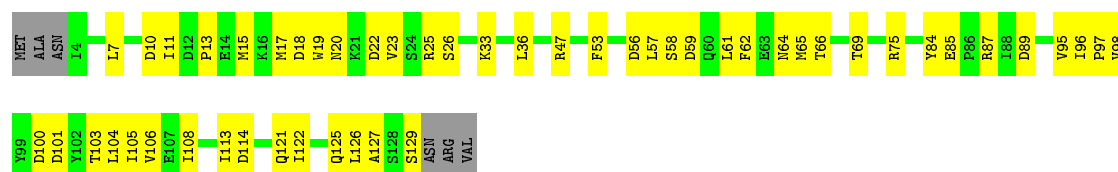
- Molecule 9: Baseplate wedge protein gp25



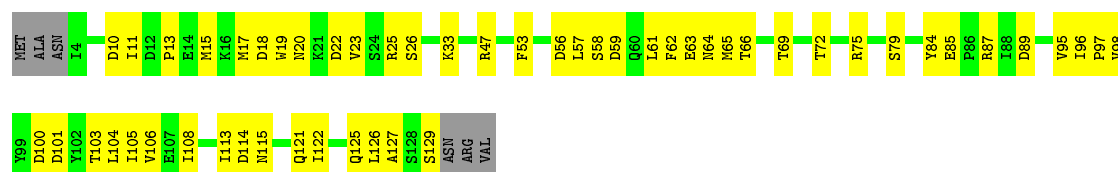
- Molecule 9: Baseplate wedge protein gp25



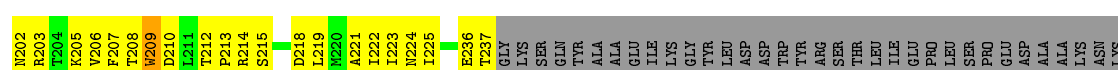
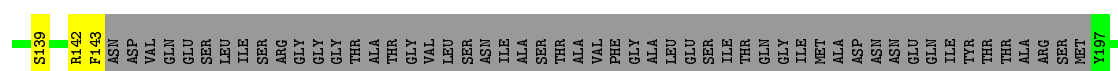
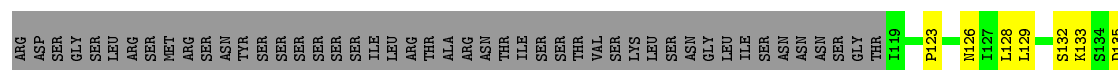
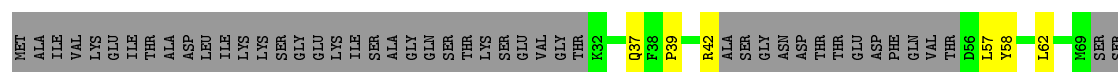
- Molecule 9: Baseplate wedge protein gp25



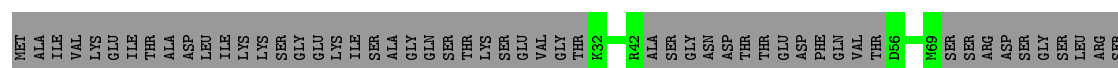
- Molecule 9: Baseplate wedge protein gp25

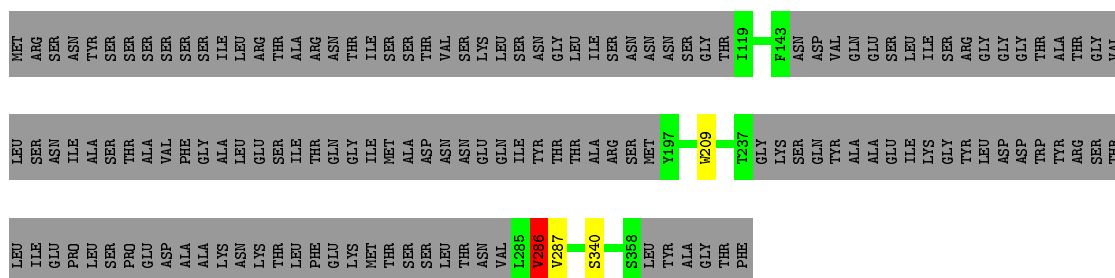


- Molecule 10: Baseplate tail-tube protein gp48

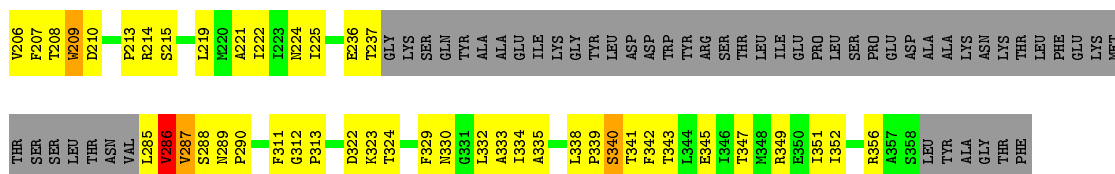
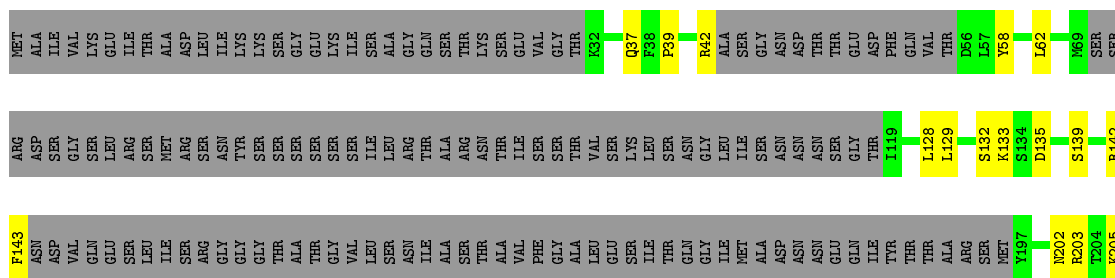
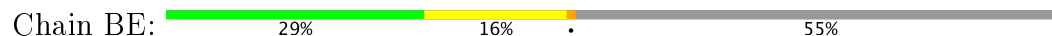


- Molecule 10: Baseplate tail-tube protein gp48

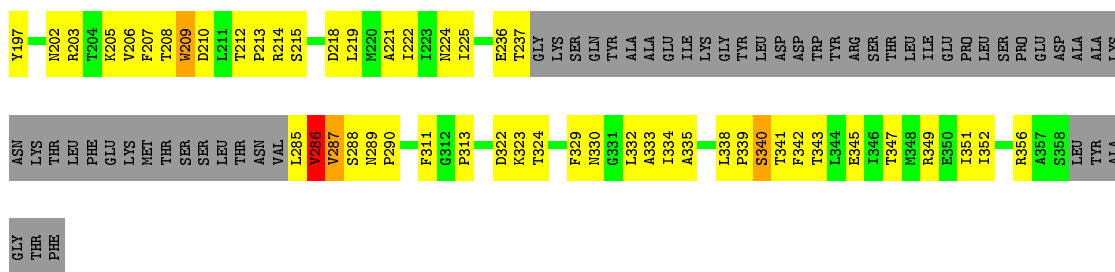
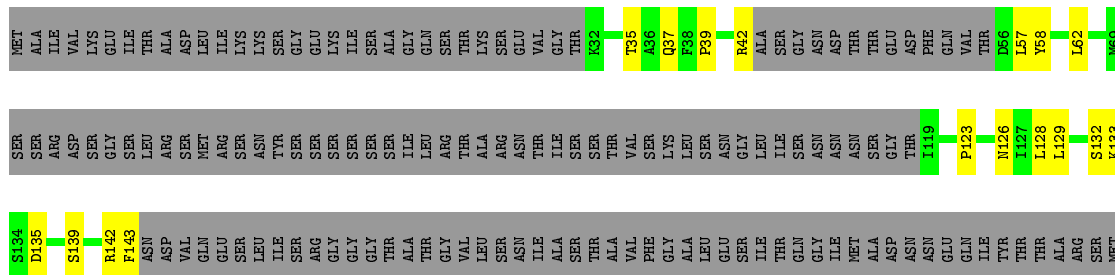




- Molecule 10: Baseplate tail-tube protein gp48



- Molecule 10: Baseplate tail-tube protein gp48



- Molecule 10: Baseplate tail-tube protein gp48



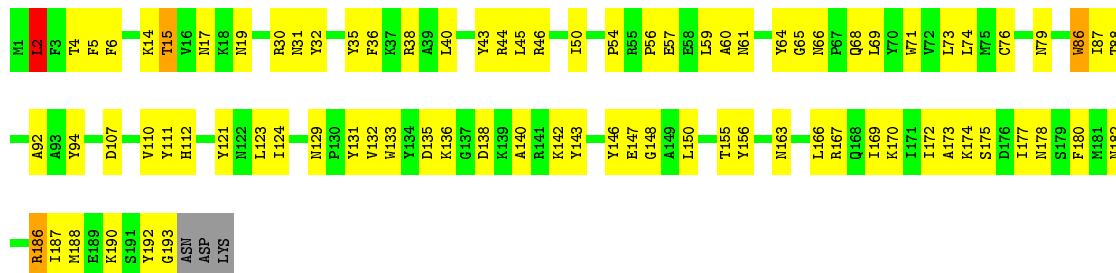
- Molecule 11: Baseplate wedge protein gp53

Chain s:  96%



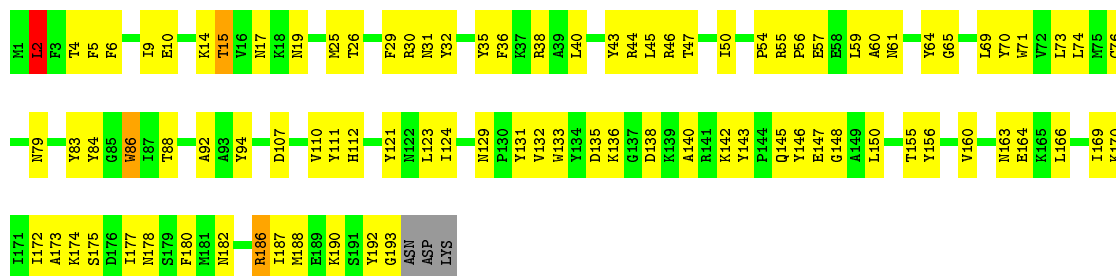
- Molecule 11: Baseplate wedge protein gp53

Chain BF:  56% 40%



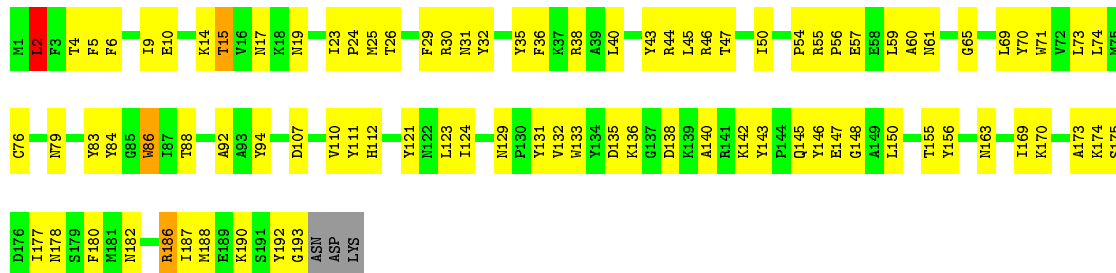
- Molecule 11: Baseplate wedge protein gp53

Chain DI:  52% 45%



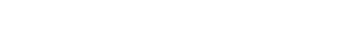
- Molecule 11: Baseplate wedge protein gp53

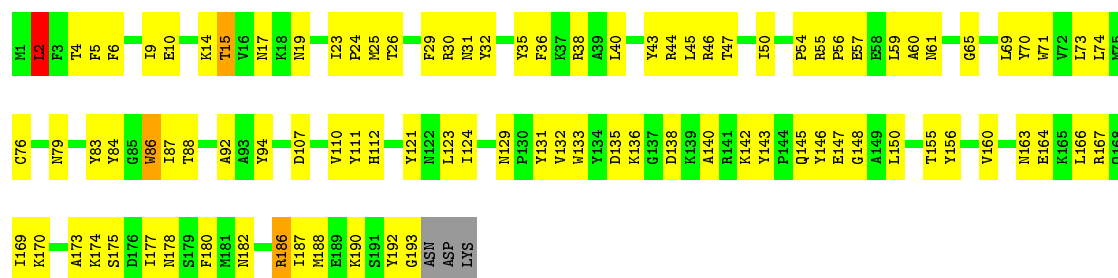
Chain GB:  53% 43%



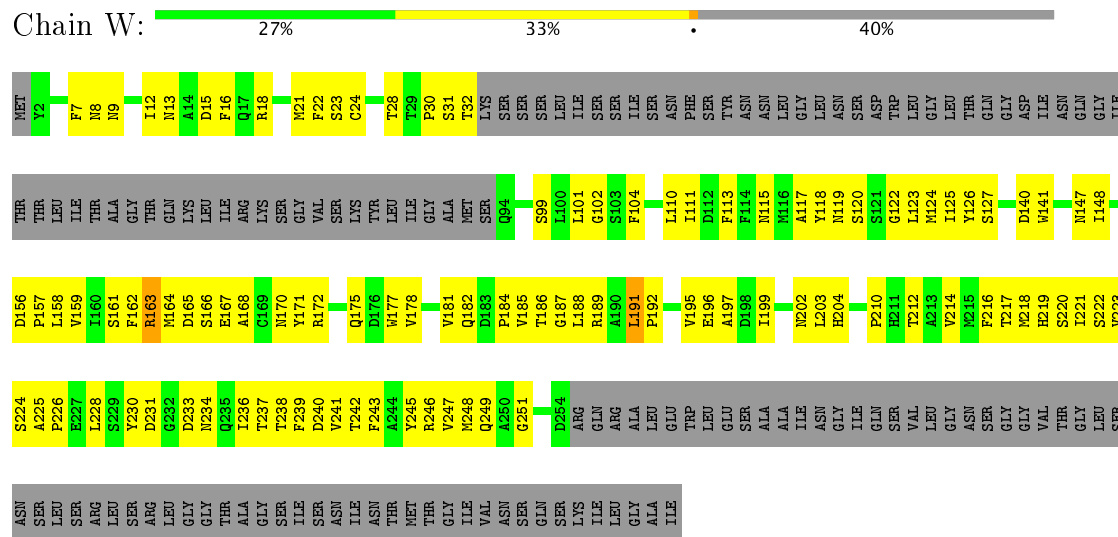
- Molecule 11: Baseplate wedge protein gp53

Chain IE:  51% 46%

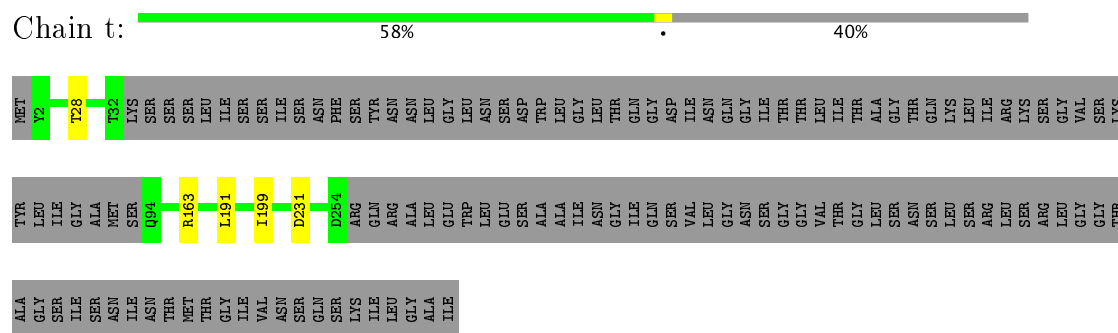




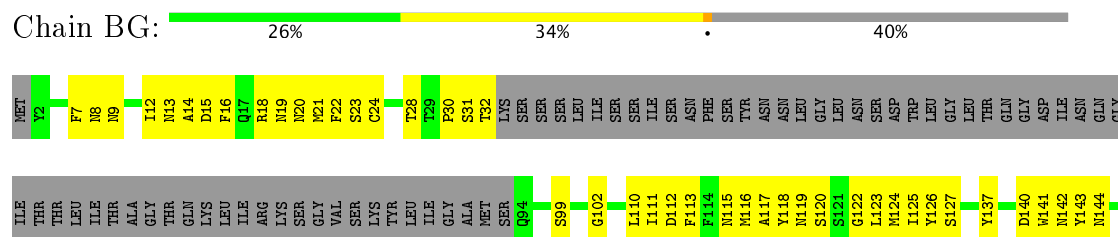
- Molecule 12: Baseplate tail-tube protein gp54

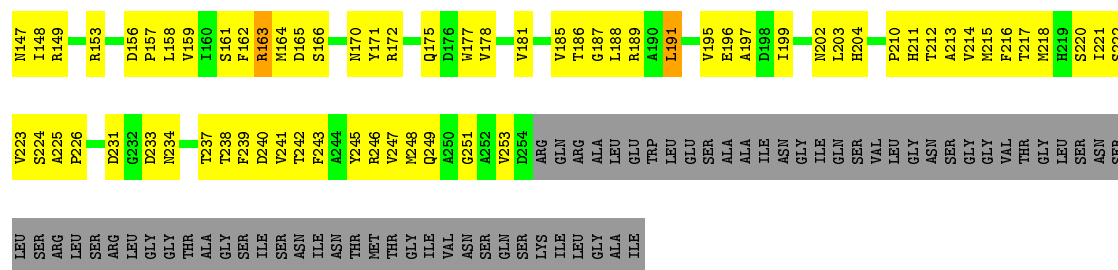


- Molecule 12: Baseplate tail-tube protein gp54

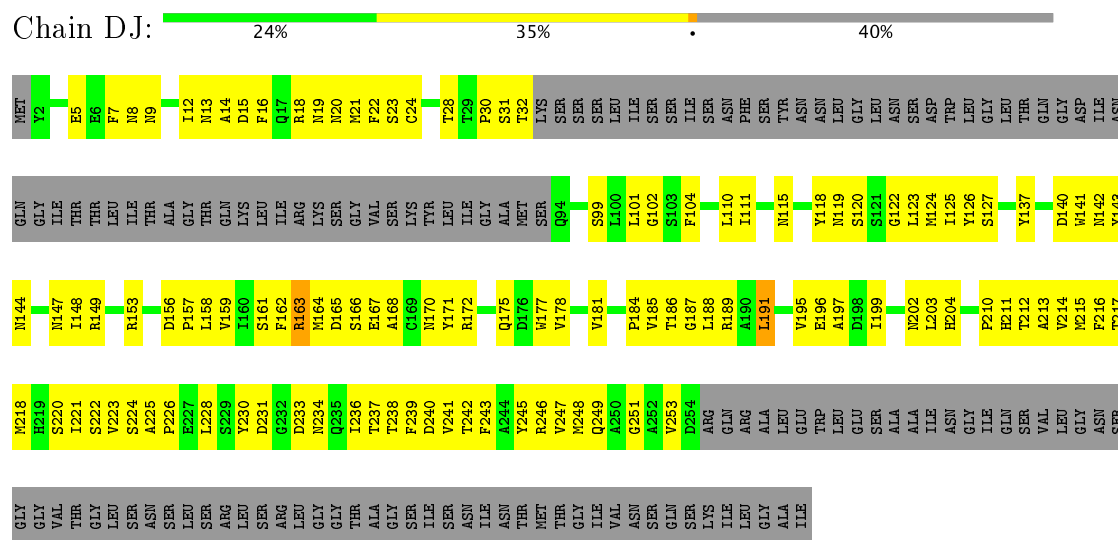


- Molecule 12: Baseplate tail-tube protein gp54

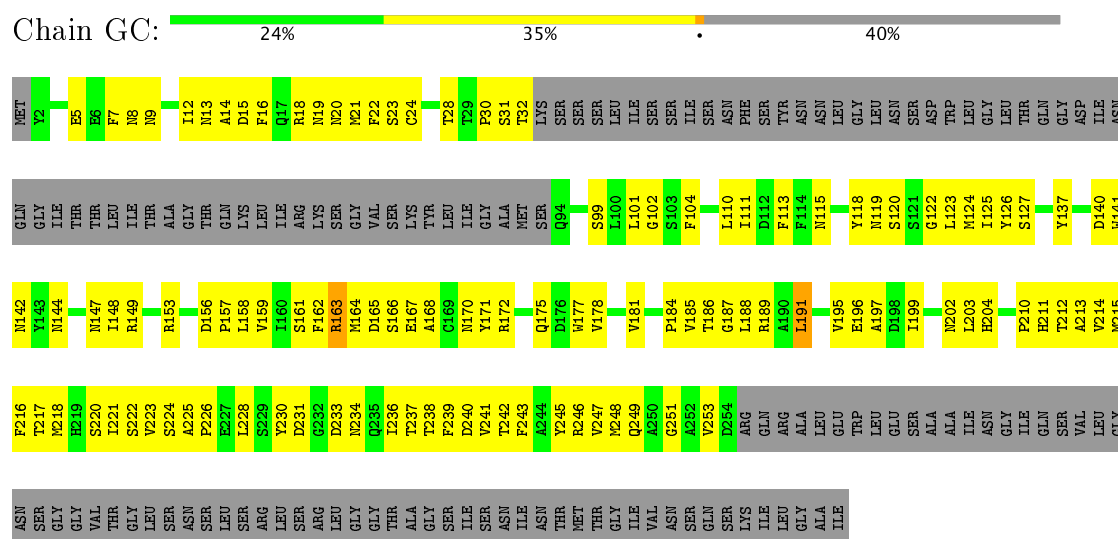




- Molecule 12: Baseplate tail-tube protein gp54

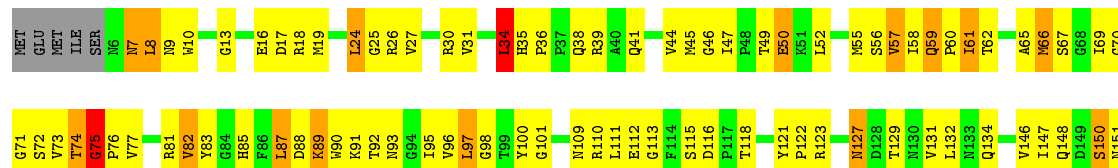


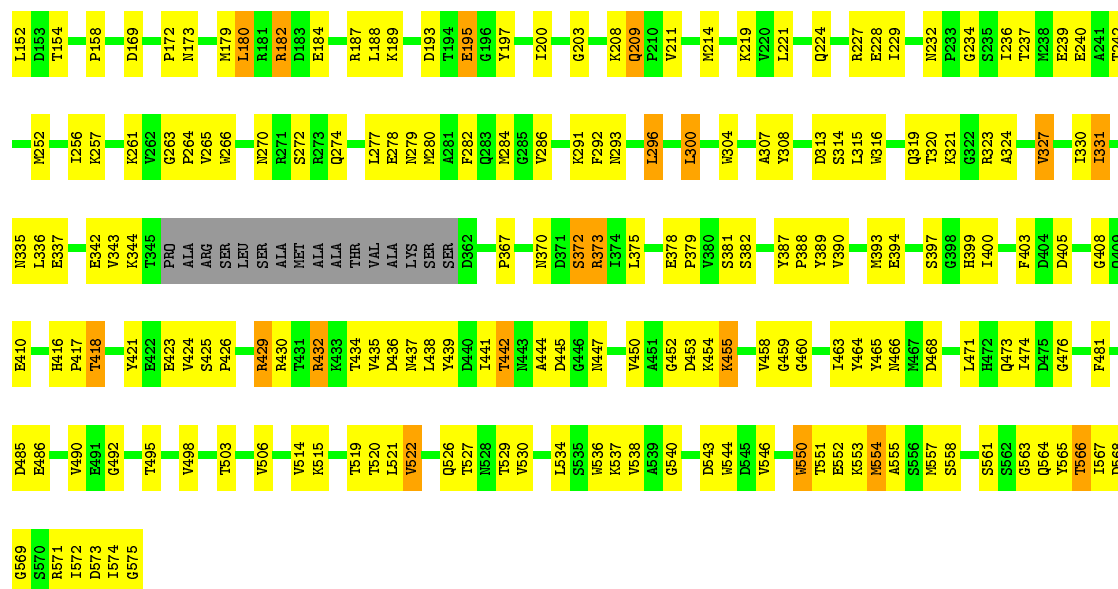
- Molecule 12: Baseplate tail-tube protein gp54



- Molecule 12: Baseplate tail-tube protein gp54

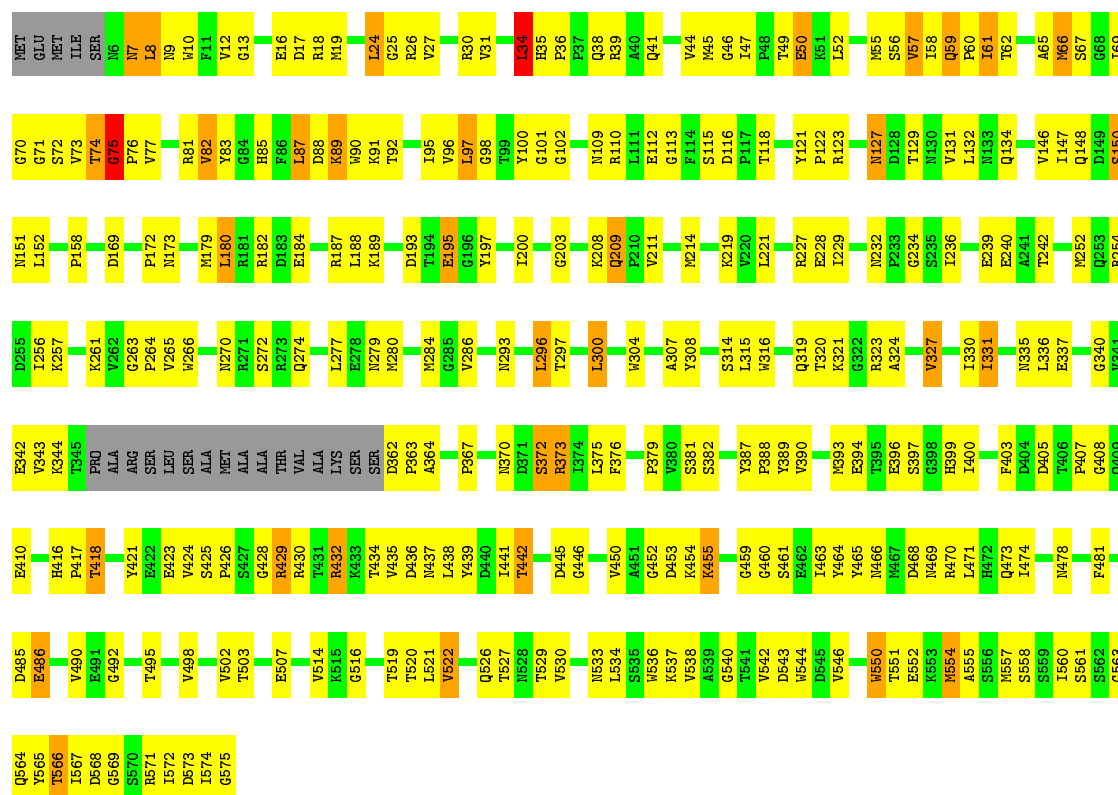






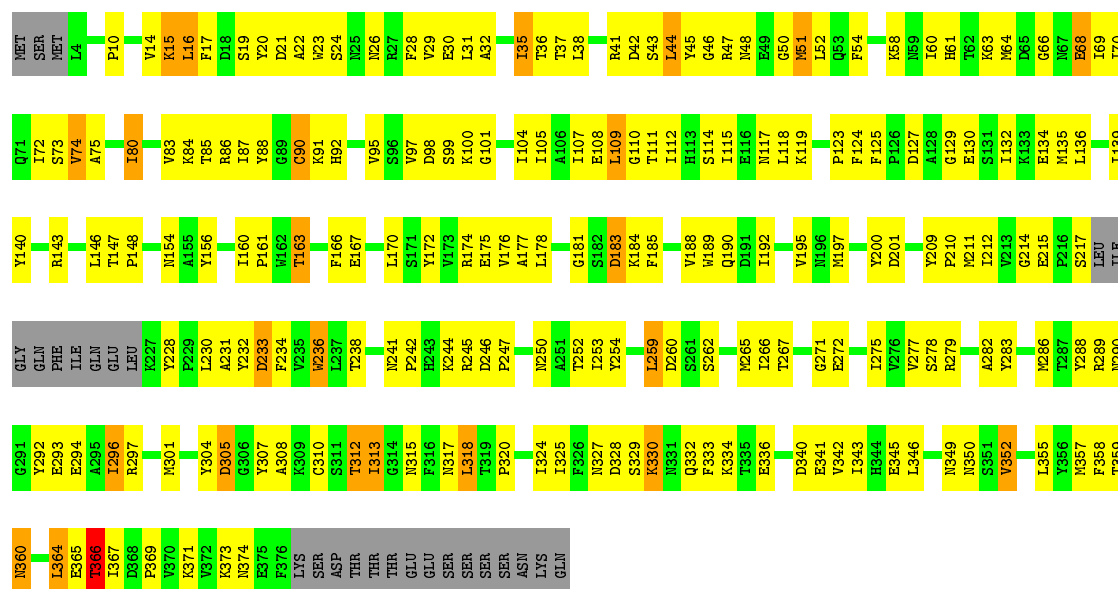
• Molecule 13: Peptidoglycan hydrolase gp5

Chain YC: 48% 42% 6% .



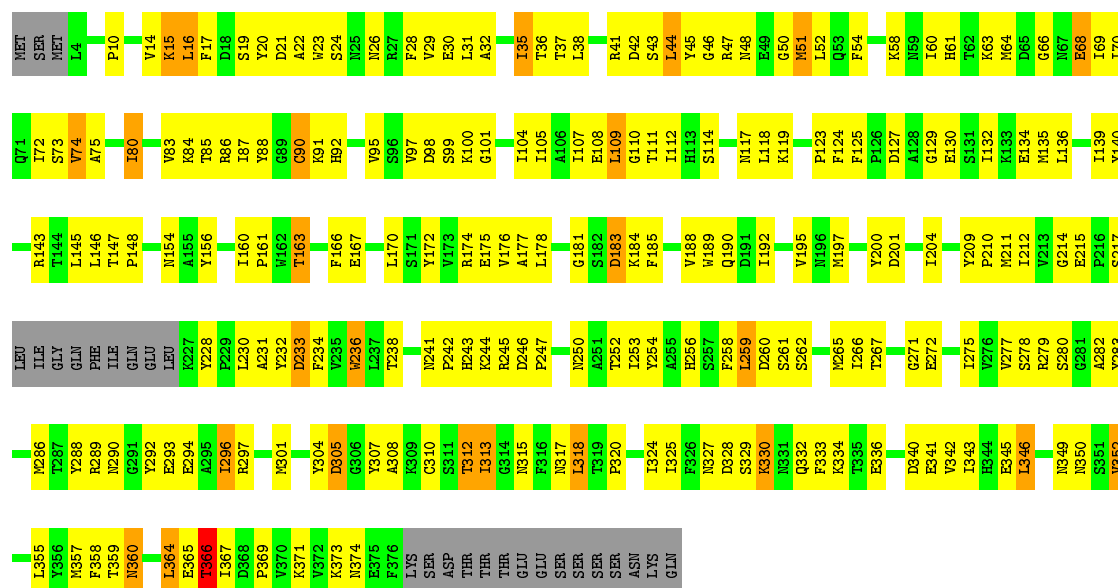
• Molecule 14: Baseplate hub protein gp27

Chain YD: 40% 47% 6% 7%



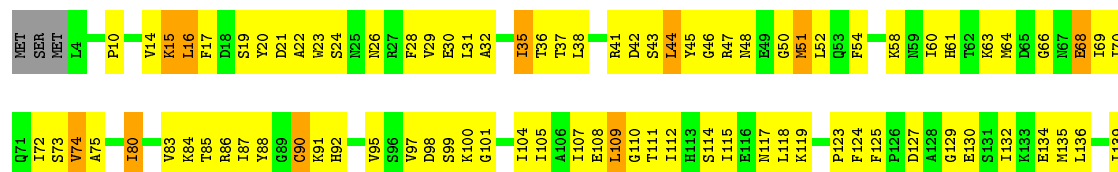
• Molecule 14: Baseplate hub protein gp27

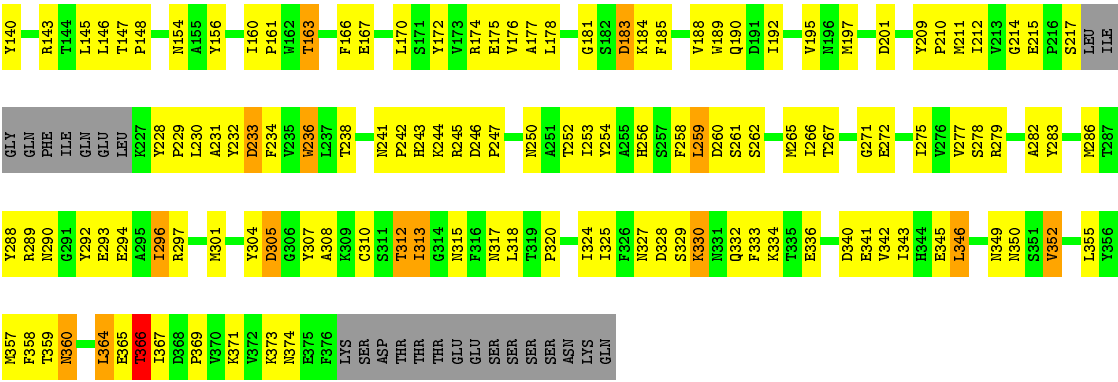
Chain YE: 38% 48% 6% 7%



• Molecule 14: Baseplate hub protein gp27

Chain YF: 38% 48% 6% 7%





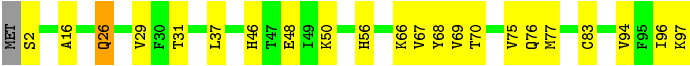
- Molecule 15: Uncharacterized 10.2 kDa protein in segC-Gp6 intergenic region

Chain ZA: 

76%

22%

..



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	37913	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	37700	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.75	0/5337	0.66	1/7256 (0.0%)
1	B	0.71	1/5257 (0.0%)	0.66	1/7144 (0.0%)
1	BH	0.75	0/5337	0.66	1/7256 (0.0%)
1	BI	0.71	1/5257 (0.0%)	0.65	1/7144 (0.0%)
1	EA	0.75	0/5337	0.66	1/7256 (0.0%)
1	EB	0.71	1/5257 (0.0%)	0.65	1/7144 (0.0%)
1	GD	0.75	0/5337	0.66	1/7256 (0.0%)
1	GE	0.71	1/5257 (0.0%)	0.65	1/7144 (0.0%)
1	X	0.75	0/5337	0.66	1/7256 (0.0%)
1	Y	0.71	1/5257 (0.0%)	0.66	1/7144 (0.0%)
1	u	0.75	0/5337	0.66	1/7256 (0.0%)
1	v	0.71	1/5257 (0.0%)	0.65	1/7144 (0.0%)
10	BE	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
10	DH	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
10	GA	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
10	ID	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
10	U	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
10	r	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
11	BF	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
11	DI	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
11	GB	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
11	IE	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
11	V	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
11	s	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
12	BG	0.62	1/1557 (0.1%)	0.68	3/2118 (0.1%)
12	DJ	0.62	1/1557 (0.1%)	0.68	4/2118 (0.2%)
12	GC	0.62	1/1557 (0.1%)	0.68	3/2118 (0.1%)
12	IF	0.63	1/1557 (0.1%)	0.68	3/2118 (0.1%)
12	W	0.62	1/1557 (0.1%)	0.68	3/2118 (0.1%)
12	t	0.62	1/1557 (0.1%)	0.68	3/2118 (0.1%)
13	YA	0.49	0/26166	0.60	24/35454 (0.1%)
13	YB	0.49	0/26166	0.60	24/35454 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
13	YC	0.49	0/26166	0.60	24/35454 (0.1%)
14	YD	0.61	0/17880	0.64	6/24252 (0.0%)
14	YE	0.61	0/17880	0.64	6/24252 (0.0%)
14	YF	0.61	0/17880	0.64	6/24252 (0.0%)
15	ZA	0.33	0/4344	0.54	0/5904
2	BJ	0.65	2/8405 (0.0%)	0.73	2/11412 (0.0%)
2	C	0.65	2/8405 (0.0%)	0.74	2/11412 (0.0%)
2	EC	0.65	2/8405 (0.0%)	0.74	2/11412 (0.0%)
2	GF	0.65	2/8405 (0.0%)	0.74	2/11412 (0.0%)
2	Z	0.65	2/8405 (0.0%)	0.74	2/11412 (0.0%)
2	w	0.65	2/8405 (0.0%)	0.74	2/11412 (0.0%)
3	CA	0.70	1/2709 (0.0%)	0.57	0/3694
3	CB	0.68	1/2736 (0.0%)	0.62	0/3731
3	D	0.70	1/2709 (0.0%)	0.57	0/3694
3	E	0.68	1/2736 (0.0%)	0.62	0/3731
3	ED	0.70	1/2709 (0.0%)	0.57	0/3694
3	EE	0.68	1/2736 (0.0%)	0.62	0/3731
3	GG	0.70	1/2709 (0.0%)	0.57	0/3694
3	GH	0.68	1/2736 (0.0%)	0.62	0/3731
3	a	0.70	1/2709 (0.0%)	0.57	0/3694
3	b	0.68	1/2736 (0.0%)	0.62	0/3731
3	x	0.70	1/2709 (0.0%)	0.57	0/3694
3	y	0.68	1/2736 (0.0%)	0.62	0/3731
4	AA	0.28	0/2205	0.48	0/2988
4	AB	0.28	0/2205	0.48	0/2988
4	CC	0.28	0/2205	0.48	0/2988
4	CD	0.28	0/2205	0.48	0/2988
4	CE	0.28	0/2205	0.48	0/2988
4	EF	0.28	0/2205	0.48	0/2988
4	EG	0.28	0/2205	0.48	0/2988
4	EH	0.28	0/2205	0.48	0/2988
4	F	0.28	0/2205	0.48	0/2988
4	G	0.28	0/2205	0.48	0/2988
4	GI	0.28	0/2205	0.48	0/2988
4	GJ	0.28	0/2205	0.48	0/2988
4	H	0.28	0/2205	0.48	0/2988
4	HA	0.28	0/2205	0.48	0/2988
4	c	0.28	0/2205	0.48	0/2988
4	d	0.28	0/2205	0.48	0/2988
4	e	0.28	0/2205	0.48	0/2988
4	z	0.28	0/2205	0.48	0/2988
5	AC	0.48	0/4778	0.68	2/6513 (0.0%)
5	AD	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
5	AE	0.50	0/4778	0.70	3/6513 (0.0%)
5	CF	0.48	0/4778	0.68	2/6513 (0.0%)
5	CG	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	CH	0.50	0/4778	0.70	3/6513 (0.0%)
5	EI	0.48	0/4778	0.68	2/6513 (0.0%)
5	EJ	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	FA	0.50	0/4778	0.70	3/6513 (0.0%)
5	HB	0.48	0/4778	0.68	2/6513 (0.0%)
5	HC	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	HD	0.50	0/4778	0.70	4/6513 (0.1%)
5	I	0.48	0/4778	0.68	2/6513 (0.0%)
5	J	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	K	0.50	0/4778	0.70	4/6513 (0.1%)
5	f	0.48	0/4778	0.68	2/6513 (0.0%)
5	g	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	h	0.50	0/4778	0.70	4/6513 (0.1%)
6	AF	0.34	0/1700	0.51	0/2318
6	AG	0.34	0/1700	0.51	0/2318
6	AH	0.34	0/1700	0.51	0/2318
6	CI	0.34	0/1700	0.51	0/2318
6	CJ	0.34	0/1700	0.51	0/2318
6	DA	0.34	0/1700	0.51	0/2318
6	FB	0.34	0/1700	0.51	0/2318
6	FC	0.34	0/1700	0.51	0/2318
6	FD	0.34	0/1700	0.51	0/2318
6	HE	0.34	0/1700	0.51	0/2318
6	HF	0.34	0/1700	0.51	0/2318
6	HG	0.34	0/1700	0.51	0/2318
6	L	0.34	0/1700	0.51	0/2318
6	M	0.34	0/1700	0.51	0/2318
6	N	0.34	0/1700	0.51	0/2318
6	i	0.34	0/1700	0.51	0/2318
6	j	0.34	0/1700	0.51	0/2318
6	k	0.34	0/1700	0.51	0/2318
7	AI	0.39	0/4016	0.61	0/5464
7	AJ	0.39	1/4016 (0.0%)	0.61	0/5464
7	BA	0.40	1/4016 (0.0%)	0.60	0/5464
7	DB	0.39	0/4016	0.61	0/5464
7	DC	0.39	1/4016 (0.0%)	0.60	0/5464
7	DD	0.40	1/4016 (0.0%)	0.60	0/5464
7	FE	0.39	0/4016	0.61	0/5464
7	FF	0.39	1/4016 (0.0%)	0.60	0/5464
7	FG	0.40	1/4016 (0.0%)	0.60	0/5464

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
7	HH	0.39	0/4016	0.61	0/5464
7	HI	0.39	1/4016 (0.0%)	0.60	0/5464
7	HJ	0.40	1/4016 (0.0%)	0.60	0/5464
7	O	0.39	0/4016	0.61	0/5464
7	P	0.39	1/4016 (0.0%)	0.60	0/5464
7	Q	0.40	1/4016 (0.0%)	0.60	0/5464
7	l	0.39	0/4016	0.61	0/5464
7	m	0.39	1/4016 (0.0%)	0.61	0/5464
7	n	0.40	1/4016 (0.0%)	0.60	0/5464
8	BB	0.45	0/1325	0.58	0/1797
8	BC	0.45	0/1325	0.58	0/1797
8	DE	0.44	0/1325	0.58	0/1797
8	DF	0.45	0/1325	0.58	0/1797
8	FH	0.44	0/1325	0.58	0/1797
8	FI	0.44	0/1325	0.58	0/1797
8	IA	0.44	0/1325	0.58	0/1797
8	IB	0.45	0/1325	0.58	0/1797
8	R	0.44	0/1325	0.58	0/1797
8	S	0.45	0/1325	0.58	0/1797
8	o	0.44	0/1325	0.58	0/1797
8	p	0.44	0/1325	0.58	0/1797
9	BD	0.55	0/1027	0.59	0/1392
9	DG	0.55	0/1027	0.59	0/1392
9	FJ	0.55	0/1027	0.59	0/1392
9	IC	0.55	0/1027	0.59	0/1392
9	T	0.55	0/1027	0.59	0/1392
9	q	0.55	0/1027	0.59	0/1392
All	All	0.55	66/561066 (0.0%)	0.63	226/762456 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	8
1	BH	0	1
1	BI	0	8
1	EA	0	1
1	EB	0	8
1	GD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	GE	0	8
1	X	0	1
1	Y	0	8
1	u	0	1
1	v	0	8
10	BE	0	1
10	DH	0	1
10	GA	0	1
10	ID	0	1
10	U	0	1
10	r	0	1
11	BF	0	1
11	DI	0	1
11	GB	0	1
11	IE	0	1
11	V	0	1
11	s	0	1
13	YA	0	7
13	YB	0	7
13	YC	0	7
14	YD	0	6
14	YE	0	6
14	YF	0	6
2	BJ	0	38
2	C	0	38
2	EC	0	38
2	GF	0	38
2	Z	0	38
2	w	0	38
3	CA	0	2
3	CB	0	3
3	D	0	2
3	E	0	3
3	ED	0	2
3	EE	0	3
3	GG	0	2
3	GH	0	3
3	a	0	2
3	b	0	3
3	x	0	2
3	y	0	3
5	AC	0	17

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	AD	0	13
5	AE	0	16
5	CF	0	17
5	CG	0	13
5	CH	0	16
5	EI	0	17
5	EJ	0	13
5	FA	0	16
5	HB	0	17
5	HC	0	13
5	HD	0	16
5	I	0	17
5	J	0	13
5	K	0	16
5	f	0	17
5	g	0	13
5	h	0	16
6	AF	0	3
6	AG	0	3
6	AH	0	3
6	CI	0	3
6	CJ	0	3
6	DA	0	3
6	FB	0	3
6	FC	0	3
6	FD	0	3
6	HE	0	3
6	HF	0	3
6	HG	0	3
6	L	0	3
6	M	0	3
6	N	0	3
6	i	0	3
6	j	0	3
6	k	0	3
7	AI	0	4
7	AJ	0	6
7	BA	0	5
7	DB	0	4
7	DC	0	6
7	DD	0	5
7	FE	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	FF	0	6
7	FG	0	5
7	HH	0	4
7	HI	0	6
7	HJ	0	5
7	O	0	4
7	P	0	6
7	Q	0	5
7	l	0	4
7	m	0	6
7	n	0	5
All	All	0	783

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CA	258	PHE	C-N	-20.87	0.94	1.34
3	ED	258	PHE	C-N	-20.85	0.94	1.34
3	GG	258	PHE	C-N	-20.84	0.94	1.34
3	x	258	PHE	C-N	-20.84	0.94	1.34
3	a	258	PHE	C-N	-20.82	0.94	1.34

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	BF	186	ARG	NE-CZ-NH1	-11.68	114.46	120.30
11	s	186	ARG	NE-CZ-NH1	-11.58	114.51	120.30
11	GB	186	ARG	NE-CZ-NH1	-11.56	114.52	120.30
11	V	186	ARG	NE-CZ-NH1	-11.54	114.53	120.30
11	DI	186	ARG	NE-CZ-NH1	-11.50	114.55	120.30

There are no chirality outliers.

5 of 783 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ALA	Peptide
1	B	136	LYS	Peptide
1	B	137	ASP	Peptide
1	B	18	PRO	Peptide
1	B	20	ILE	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	A	5235	0	5086	352	0
1	B	5157	0	5011	344	0
1	BH	5235	0	5086	346	0
1	BI	5157	0	5011	350	0
1	EA	5235	0	5086	350	0
1	EB	5157	0	5011	355	0
1	GD	5235	0	5086	349	0
1	GE	5157	0	5011	345	0
1	X	5235	0	5086	345	0
1	Y	5157	0	5011	332	0
1	u	5235	0	5086	0	0
1	v	5157	0	5011	0	0
2	BJ	8199	0	7912	753	0
2	C	8199	0	7912	712	0
2	EC	8199	0	7912	744	0
2	GF	8199	0	7912	735	0
2	Z	8199	0	7912	641	0
2	w	8199	0	7912	0	0
3	CA	2631	0	2509	153	0
3	CB	2658	0	2534	131	0
3	D	2631	0	2509	160	0
3	E	2658	0	2534	140	0
3	ED	2631	0	2509	168	0
3	EE	2658	0	2534	142	0
3	GG	2631	0	2509	163	0
3	GH	2658	0	2534	136	0
3	a	2631	0	2509	0	0
3	b	2658	0	2534	0	0
3	x	2631	0	2509	0	0
3	y	2658	0	2534	0	0
4	AA	2175	0	2157	102	0
4	AB	2175	0	2157	95	0
4	CC	2175	0	2157	113	0
4	CD	2175	0	2157	119	0
4	CE	2175	0	2157	117	0
4	EF	2175	0	2157	121	0
4	EG	2175	0	2157	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	EH	2175	0	2157	120	0
4	F	2175	0	2157	114	0
4	G	2175	0	2157	117	0
4	GI	2175	0	2157	120	0
4	GJ	2175	0	2157	115	0
4	H	2175	0	2157	113	0
4	HA	2175	0	2157	119	0
4	c	2175	0	2157	0	0
4	d	2175	0	2157	0	0
4	e	2175	0	2157	0	0
4	z	2175	0	2157	0	0
5	AC	4675	0	4446	445	0
5	AD	4675	0	4446	456	0
5	AE	4675	0	4446	468	0
5	CF	4675	0	4446	454	0
5	CG	4675	0	4446	473	0
5	CH	4675	0	4446	475	0
5	EI	4675	0	4446	462	0
5	EJ	4675	0	4446	470	0
5	FA	4675	0	4446	487	0
5	HB	4675	0	4446	467	0
5	HC	4675	0	4446	475	0
5	HD	4675	0	4446	475	0
5	I	4675	0	4446	457	0
5	J	4675	0	4446	460	0
5	K	4675	0	4446	483	0
5	f	4675	0	4446	0	0
5	g	4675	0	4446	0	0
5	h	4675	0	4446	0	0
6	AF	1665	0	1638	119	0
6	AG	1665	0	1638	101	0
6	AH	1665	0	1638	106	0
6	CI	1665	0	1638	110	0
6	CJ	1665	0	1638	101	0
6	DA	1665	0	1638	99	0
6	FB	1665	0	1638	113	0
6	FC	1665	0	1638	107	0
6	FD	1665	0	1638	107	0
6	HE	1665	0	1638	109	0
6	HF	1665	0	1638	102	0
6	HG	1665	0	1638	108	0
6	L	1665	0	1638	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	1665	0	1638	106	0
6	N	1665	0	1638	107	0
6	i	1665	0	1638	0	0
6	j	1665	0	1638	0	0
6	k	1665	0	1638	0	0
7	AI	3945	0	3828	399	0
7	AJ	3945	0	3828	389	0
7	BA	3945	0	3828	419	0
7	DB	3945	0	3828	407	0
7	DC	3945	0	3828	398	0
7	DD	3945	0	3828	421	0
7	FE	3945	0	3828	412	0
7	FF	3945	0	3828	396	0
7	FG	3945	0	3828	427	0
7	HH	3945	0	3828	401	0
7	HI	3945	0	3828	401	0
7	HJ	3945	0	3828	425	0
7	O	3945	0	3828	410	0
7	P	3945	0	3828	403	0
7	Q	3945	0	3828	424	0
7	l	3945	0	3828	0	0
7	m	3945	0	3828	0	0
7	n	3945	0	3828	0	0
8	BB	1296	0	1243	80	0
8	BC	1296	0	1243	76	0
8	DE	1296	0	1243	89	0
8	DF	1296	0	1243	89	0
8	FH	1296	0	1243	92	0
8	FI	1296	0	1243	90	0
8	IA	1296	0	1243	88	0
8	IB	1296	0	1243	94	0
8	R	1296	0	1243	77	0
8	S	1296	0	1243	78	0
8	o	1296	0	1243	0	0
8	p	1296	0	1243	0	0
9	BD	1011	0	1009	38	0
9	DG	1011	0	1009	51	0
9	FJ	1011	0	1009	50	0
9	IC	1011	0	1009	51	0
9	T	1011	0	1009	47	0
9	q	1011	0	1009	0	0
10	BE	1317	0	1296	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	DH	1317	0	1296	79	0
10	GA	1317	0	1296	78	0
10	ID	1317	0	1296	86	0
10	U	1317	0	1296	83	0
10	r	1317	0	1296	0	0
11	BF	1599	0	1544	89	0
11	DI	1599	0	1544	114	0
11	GB	1599	0	1544	108	0
11	IE	1599	0	1544	108	0
11	V	1599	0	1544	112	0
11	s	1599	0	1544	0	0
12	BG	1524	0	1439	117	0
12	DJ	1524	0	1439	135	0
12	GC	1524	0	1439	136	0
12	IF	1524	0	1439	140	0
12	W	1524	0	1439	109	0
12	t	1524	0	1439	0	0
13	YA	25692	0	21556	1614	0
13	YB	25692	0	21769	1791	0
13	YC	25692	0	21586	1892	0
14	YD	17472	0	15252	1037	0
14	YE	17472	0	15217	1072	0
14	YF	17472	0	15224	1053	0
15	ZA	4254	0	4245	108	0
16	AI	1	0	0	0	0
16	DB	1	0	0	0	0
16	FE	1	0	0	0	0
16	HH	1	0	0	0	0
16	O	1	0	0	0	0
16	l	1	0	0	0	0
17	ZA	6	0	0	0	0
All	All	549576	0	517047	29063	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 32.

The worst 5 of 29063 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)
7:O:24:ASN:HD22	7:Q:41:PRO:HA	1.18	1.06
2:BJ:935:LYS:HD2	2:BJ:954:GLU:HG2	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:FE:24:ASN:HD22	7:FG:41:PRO:HA	1.17	1.04
2:EC:935:LYS:HD2	2:EC:954:GLU:HG2	1.39	1.04
7:AI:24:ASN:HD22	7:BA:41:PRO:HA	1.17	1.03

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	A	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	32	73
1	B	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	22	65
1	BH	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	32	73
1	BI	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	22	65
1	EA	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	32	73
1	EB	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	22	65
1	GD	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	32	73
1	GE	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	22	65
1	X	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	32	73
1	Y	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	22	65
1	u	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	32	73
1	v	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	22	65
2	BJ	1000/1032 (97%)	836 (84%)	144 (14%)	20 (2%)	9	48
2	C	1000/1032 (97%)	836 (84%)	145 (14%)	19 (2%)	9	49
2	EC	1000/1032 (97%)	836 (84%)	145 (14%)	19 (2%)	9	49
2	GF	1000/1032 (97%)	836 (84%)	144 (14%)	20 (2%)	9	48
2	Z	1000/1032 (97%)	837 (84%)	144 (14%)	19 (2%)	9	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	w	1000/1032 (97%)	837 (84%)	143 (14%)	20 (2%)	9	48
3	CA	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	28	70
3	CB	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
3	D	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	28	70
3	E	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
3	ED	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	28	70
3	EE	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
3	GG	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	28	70
3	GH	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
3	a	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	28	70
3	b	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
3	x	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	28	70
3	y	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
4	AA	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	AB	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	CC	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	CD	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	CE	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	EF	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	EG	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	EH	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	F	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	G	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	GI	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	GJ	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	H	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	HA	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	c	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	d	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	e	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54
4	z	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	13	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AC	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	14	55
5	AD	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	10	50
5	AE	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	8	46
5	CF	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	14	55
5	CG	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	10	50
5	CH	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	8	46
5	EI	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	14	55
5	EJ	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	10	50
5	FA	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	8	46
5	HB	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	14	55
5	HC	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	10	50
5	HD	600/602 (100%)	530 (88%)	58 (10%)	12 (2%)	9	48
5	I	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	14	55
5	J	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	10	50
5	K	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	8	46
5	f	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	14	55
5	g	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	10	50
5	h	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	8	46
6	AF	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	AG	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	AH	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	CI	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	CJ	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	DA	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	FB	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	FC	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	FD	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	HE	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	HF	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	HG	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	L	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	M	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	N	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	i	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	j	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
6	k	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	20	62
7	AI	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	59
7	AJ	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	28	70
7	BA	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	14	55
7	DB	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	59
7	DC	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	28	70
7	DD	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	14	55
7	FE	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	59
7	FF	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	28	70
7	FG	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	14	55
7	HH	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	59
7	HI	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	28	70
7	HJ	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	14	55
7	O	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	59
7	P	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	28	70
7	Q	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	14	55
7	l	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	59
7	m	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	28	70
7	n	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	14	55
8	BB	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	BC	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	DE	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	DF	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	FH	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	FI	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	IA	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	IB	160/163 (98%)	147 (92%)	13 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	R	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	S	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	o	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	p	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
9	BD	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
9	DG	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
9	FJ	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
9	IC	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
9	T	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
9	q	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
10	BE	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	28	70
10	DH	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	28	70
10	GA	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	28	70
10	ID	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	28	70
10	U	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	28	70
10	r	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	28	70
11	BF	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
11	DI	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
11	GB	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
11	IE	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
11	V	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
11	s	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
12	BG	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
12	DJ	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
12	GC	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
12	IF	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
12	W	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
12	t	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
13	YA	3276/575 (570%)	3186 (97%)	90 (3%)	0	100	100
13	YB	3276/575 (570%)	3186 (97%)	90 (3%)	0	100	100
13	YC	3276/575 (570%)	3186 (97%)	90 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	YD	2160/391 (552%)	2070 (96%)	84 (4%)	6 (0%)	44	80
14	YE	2160/391 (552%)	2070 (96%)	84 (4%)	6 (0%)	44	80
14	YF	2160/391 (552%)	2070 (96%)	84 (4%)	6 (0%)	44	80
15	ZA	564/97 (581%)	540 (96%)	24 (4%)	0	100	100
All	All	69756/58591 (119%)	64970 (93%)	4190 (6%)	596 (1%)	23	62

5 of 596 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	343	PRO
4	F	249	ILE
4	G	249	ILE
4	H	249	ILE
5	I	10	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	576/578 (100%)	576 (100%)	0	100	100
1	B	567/578 (98%)	567 (100%)	0	100	100
1	BH	576/578 (100%)	576 (100%)	0	100	100
1	BI	567/578 (98%)	567 (100%)	0	100	100
1	EA	576/578 (100%)	576 (100%)	0	100	100
1	EB	567/578 (98%)	567 (100%)	0	100	100
1	GD	576/578 (100%)	576 (100%)	0	100	100
1	GE	567/578 (98%)	567 (100%)	0	100	100
1	X	576/578 (100%)	576 (100%)	0	100	100
1	Y	567/578 (98%)	567 (100%)	0	100	100
1	u	576/578 (100%)	576 (100%)	0	100	100
1	v	567/578 (98%)	567 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BJ	896/921 (97%)	896 (100%)	0	100	100
2	C	896/921 (97%)	896 (100%)	0	100	100
2	EC	896/921 (97%)	896 (100%)	0	100	100
2	GF	896/921 (97%)	896 (100%)	0	100	100
2	Z	896/921 (97%)	896 (100%)	0	100	100
2	w	896/921 (97%)	896 (100%)	0	100	100
3	CA	289/295 (98%)	289 (100%)	0	100	100
3	CB	293/295 (99%)	293 (100%)	0	100	100
3	D	289/295 (98%)	289 (100%)	0	100	100
3	E	293/295 (99%)	293 (100%)	0	100	100
3	ED	289/295 (98%)	289 (100%)	0	100	100
3	EE	293/295 (99%)	293 (100%)	0	100	100
3	GG	289/295 (98%)	289 (100%)	0	100	100
3	GH	293/295 (99%)	293 (100%)	0	100	100
3	a	289/295 (98%)	289 (100%)	0	100	100
3	b	293/295 (99%)	293 (100%)	0	100	100
3	x	289/295 (98%)	289 (100%)	0	100	100
3	y	293/295 (99%)	293 (100%)	0	100	100
4	AA	244/244 (100%)	244 (100%)	0	100	100
4	AB	244/244 (100%)	244 (100%)	0	100	100
4	CC	244/244 (100%)	244 (100%)	0	100	100
4	CD	244/244 (100%)	244 (100%)	0	100	100
4	CE	244/244 (100%)	244 (100%)	0	100	100
4	EF	244/244 (100%)	244 (100%)	0	100	100
4	EG	244/244 (100%)	244 (100%)	0	100	100
4	EH	244/244 (100%)	244 (100%)	0	100	100
4	F	244/244 (100%)	244 (100%)	0	100	100
4	G	244/244 (100%)	244 (100%)	0	100	100
4	GI	244/244 (100%)	244 (100%)	0	100	100
4	GJ	244/244 (100%)	244 (100%)	0	100	100
4	H	244/244 (100%)	244 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	HA	244/244 (100%)	244 (100%)	0	100	100
4	c	244/244 (100%)	244 (100%)	0	100	100
4	d	244/244 (100%)	244 (100%)	0	100	100
4	e	244/244 (100%)	244 (100%)	0	100	100
4	z	244/244 (100%)	244 (100%)	0	100	100
5	AC	519/519 (100%)	519 (100%)	0	100	100
5	AD	519/519 (100%)	519 (100%)	0	100	100
5	AE	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	CF	519/519 (100%)	519 (100%)	0	100	100
5	CG	519/519 (100%)	519 (100%)	0	100	100
5	CH	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	EI	519/519 (100%)	519 (100%)	0	100	100
5	EJ	519/519 (100%)	519 (100%)	0	100	100
5	FA	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	HB	519/519 (100%)	519 (100%)	0	100	100
5	HC	519/519 (100%)	519 (100%)	0	100	100
5	HD	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	I	519/519 (100%)	519 (100%)	0	100	100
5	J	519/519 (100%)	519 (100%)	0	100	100
5	K	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	f	519/519 (100%)	519 (100%)	0	100	100
5	g	519/519 (100%)	519 (100%)	0	100	100
5	h	519/519 (100%)	518 (100%)	1 (0%)	94	97
6	AF	187/188 (100%)	187 (100%)	0	100	100
6	AG	187/188 (100%)	187 (100%)	0	100	100
6	AH	187/188 (100%)	187 (100%)	0	100	100
6	CI	187/188 (100%)	187 (100%)	0	100	100
6	CJ	187/188 (100%)	187 (100%)	0	100	100
6	DA	187/188 (100%)	187 (100%)	0	100	100
6	FB	187/188 (100%)	187 (100%)	0	100	100
6	FC	187/188 (100%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	FD	187/188 (100%)	187 (100%)	0	100	100
6	HE	187/188 (100%)	187 (100%)	0	100	100
6	HF	187/188 (100%)	187 (100%)	0	100	100
6	HG	187/188 (100%)	187 (100%)	0	100	100
6	L	187/188 (100%)	187 (100%)	0	100	100
6	M	187/188 (100%)	187 (100%)	0	100	100
6	N	187/188 (100%)	187 (100%)	0	100	100
6	i	187/188 (100%)	187 (100%)	0	100	100
6	j	187/188 (100%)	187 (100%)	0	100	100
6	k	187/188 (100%)	187 (100%)	0	100	100
7	AI	426/427 (100%)	426 (100%)	0	100	100
7	AJ	426/427 (100%)	425 (100%)	1 (0%)	94	97
7	BA	426/427 (100%)	426 (100%)	0	100	100
7	DB	426/427 (100%)	426 (100%)	0	100	100
7	DC	426/427 (100%)	425 (100%)	1 (0%)	94	97
7	DD	426/427 (100%)	426 (100%)	0	100	100
7	FE	426/427 (100%)	426 (100%)	0	100	100
7	FF	426/427 (100%)	425 (100%)	1 (0%)	94	97
7	FG	426/427 (100%)	426 (100%)	0	100	100
7	HH	426/427 (100%)	426 (100%)	0	100	100
7	HI	426/427 (100%)	425 (100%)	1 (0%)	94	97
7	HJ	426/427 (100%)	426 (100%)	0	100	100
7	O	426/427 (100%)	426 (100%)	0	100	100
7	P	426/427 (100%)	425 (100%)	1 (0%)	94	97
7	Q	426/427 (100%)	426 (100%)	0	100	100
7	l	426/427 (100%)	426 (100%)	0	100	100
7	m	426/427 (100%)	425 (100%)	1 (0%)	94	97
7	n	426/427 (100%)	426 (100%)	0	100	100
8	BB	136/137 (99%)	136 (100%)	0	100	100
8	BC	136/137 (99%)	136 (100%)	0	100	100
8	DE	136/137 (99%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	DF	136/137 (99%)	136 (100%)	0	100	100
8	FH	136/137 (99%)	136 (100%)	0	100	100
8	FI	136/137 (99%)	136 (100%)	0	100	100
8	IA	136/137 (99%)	136 (100%)	0	100	100
8	IB	136/137 (99%)	136 (100%)	0	100	100
8	R	136/137 (99%)	136 (100%)	0	100	100
8	S	136/137 (99%)	136 (100%)	0	100	100
8	o	136/137 (99%)	136 (100%)	0	100	100
8	p	136/137 (99%)	136 (100%)	0	100	100
9	BD	118/123 (96%)	118 (100%)	0	100	100
9	DG	118/123 (96%)	118 (100%)	0	100	100
9	FJ	118/123 (96%)	118 (100%)	0	100	100
9	IC	118/123 (96%)	118 (100%)	0	100	100
9	T	118/123 (96%)	118 (100%)	0	100	100
9	q	118/123 (96%)	118 (100%)	0	100	100
10	BE	146/313 (47%)	145 (99%)	1 (1%)	87	94
10	DH	146/313 (47%)	145 (99%)	1 (1%)	87	94
10	GA	146/313 (47%)	145 (99%)	1 (1%)	87	94
10	ID	146/313 (47%)	145 (99%)	1 (1%)	87	94
10	U	146/313 (47%)	145 (99%)	1 (1%)	87	94
10	r	146/313 (47%)	145 (99%)	1 (1%)	87	94
11	BF	166/169 (98%)	165 (99%)	1 (1%)	89	95
11	DI	166/169 (98%)	165 (99%)	1 (1%)	89	95
11	GB	166/169 (98%)	165 (99%)	1 (1%)	89	95
11	IE	166/169 (98%)	165 (99%)	1 (1%)	89	95
11	V	166/169 (98%)	165 (99%)	1 (1%)	89	95
11	s	166/169 (98%)	165 (99%)	1 (1%)	89	95
12	BG	171/275 (62%)	170 (99%)	1 (1%)	89	95
12	DJ	171/275 (62%)	170 (99%)	1 (1%)	89	95
12	GC	171/275 (62%)	170 (99%)	1 (1%)	89	95
12	IF	171/275 (62%)	170 (99%)	1 (1%)	89	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	W	171/275 (62%)	170 (99%)	1 (1%)	89	95
12	t	171/275 (62%)	170 (99%)	1 (1%)	89	95
13	YA	2814/485 (580%)	2544 (90%)	270 (10%)	10	40
13	YB	2814/485 (580%)	2544 (90%)	270 (10%)	10	40
13	YC	2814/485 (580%)	2544 (90%)	270 (10%)	10	40
14	YD	1944/350 (555%)	1710 (88%)	234 (12%)	6	31
14	YE	1944/350 (555%)	1710 (88%)	234 (12%)	6	31
14	YF	1944/350 (555%)	1710 (88%)	234 (12%)	6	31
15	ZA	468/79 (592%)	450 (96%)	18 (4%)	38	70
All	All	60474/50314 (120%)	58914 (97%)	1560 (3%)	89	77

5 of 1560 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	YC	209[D]	GLN
14	YD	44[D]	LEU
14	YF	241[B]	ASN
13	YC	327[A]	VAL
13	YC	455[A]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 602 such sidechains are listed below:

Mol	Chain	Res	Type
6	AF	31	ASN
4	CC	111	ASN
5	HC	514	HIS
7	AI	389	ASN
1	BH	246	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	YA	17
13	YC	17
13	YB	17
14	YD	5
14	YF	5
15	ZA	5
14	YE	5
2	GF	1
5	g	1
7	BA	1
3	CA	1
1	B	1
1	EB	1
3	GG	1
3	D	1
1	GE	1

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Mol	Chain	Number of breaks
7	DD	1
5	J	1
7	HJ	1
1	BI	1
2	w	1
7	n	1
3	x	1
2	BJ	1
5	CG	1
5	AD	1
1	v	1
2	Z	1
3	a	1
5	HC	1
7	Q	1
3	ED	1
2	C	1
7	FG	1
2	EC	1
1	Y	1
5	EJ	1

The worst 5 of 101 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	YA	76[E]:PRO	C	77[E]:VAL	N	10.44
1	YB	76[E]:PRO	C	77[E]:VAL	N	10.44
1	YC	76[E]:PRO	C	77[E]:VAL	N	10.44
1	YC	76[B]:PRO	C	77[B]:VAL	N	9.41
1	YA	76[B]:PRO	C	77[B]:VAL	N	9.40