wwPDB EM Map/Model Validation Report (i)

Jun 2, 2016 – 11:42 AM EDT

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 EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

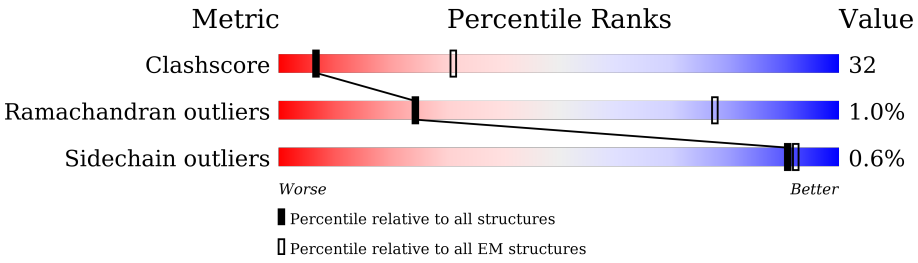
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.11 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	660	46% 53%
1	B	660	43% 53%
1	BH	660	47% 52%
1	BI	660	43% 54%
1	EA	660	47% 53%
1	EB	660	42% 54%
1	GD	660	47% 52%
1	GE	660	44% 53%
1	X	660	47% 53%

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Mol	Chain	Length	Quality of chain
1	Y	660	44% 53%
1	u	660	99%
1	v	660	96%
2	BJ	1032	32% 60%
2	C	1032	34% 59%
2	EC	1032	32% 61%
2	GF	1032	33% 60%
2	Z	1032	35% 58%
2	w	1032	92% 5%
3	CA	334	50% 47%
3	CB	334	55% 43%
3	D	334	51% 47%
3	E	334	56% 43%
3	ED	334	49% 48%
3	EE	334	55% 43%
3	GG	334	50% 47%
3	GH	334	56% 42%
3	a	334	97%
3	b	334	98%
3	x	334	97%
3	y	334	98%
4	AA	288	59% 40%
4	AB	288	61% 37%
4	CC	288	58% 41%
4	CD	288	56% 43%

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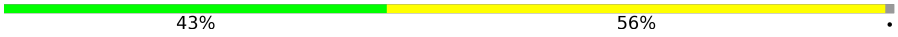
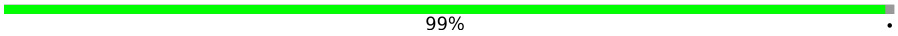
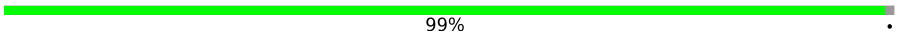
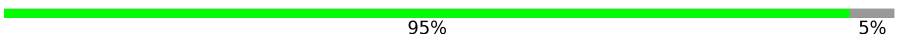
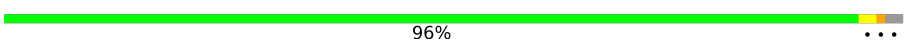
Mol	Chain	Length	Quality of chain
8	IB	163	
8	R	163	
8	S	163	
8	o	163	
8	p	163	
9	BD	132	
9	DG	132	
9	FJ	132	
9	IC	132	
9	T	132	
9	q	132	
10	BE	364	
10	DH	364	
10	GA	364	
10	ID	364	
10	U	364	
10	r	364	
11	BF	196	
11	DI	196	
11	GB	196	
11	IE	196	
11	V	196	
11	s	196	
12	BG	320	
12	DJ	320	

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Mol	Chain	Length	Quality of chain
12	GC	320	24% 35% 40%
12	IF	320	24% 36% 40%
12	W	320	27% 33% 40%
12	t	320	58% 40%
13	YA	575	49% 41% 6%
13	YB	575	49% 41% 6%
13	YC	575	48% 42% 6%
14	YD	391	40% 47% 6% 7%
14	YE	391	38% 48% 6% 7%
14	YF	391	38% 48% 6% 7%
15	ZA	97	76% 22%

2 Entry composition

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 25692	C 15942	N 4536	O 5088	S 126	554	0

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

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

- 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 4254	C 2682	N 720	O 834	S 18	96	0

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

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

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

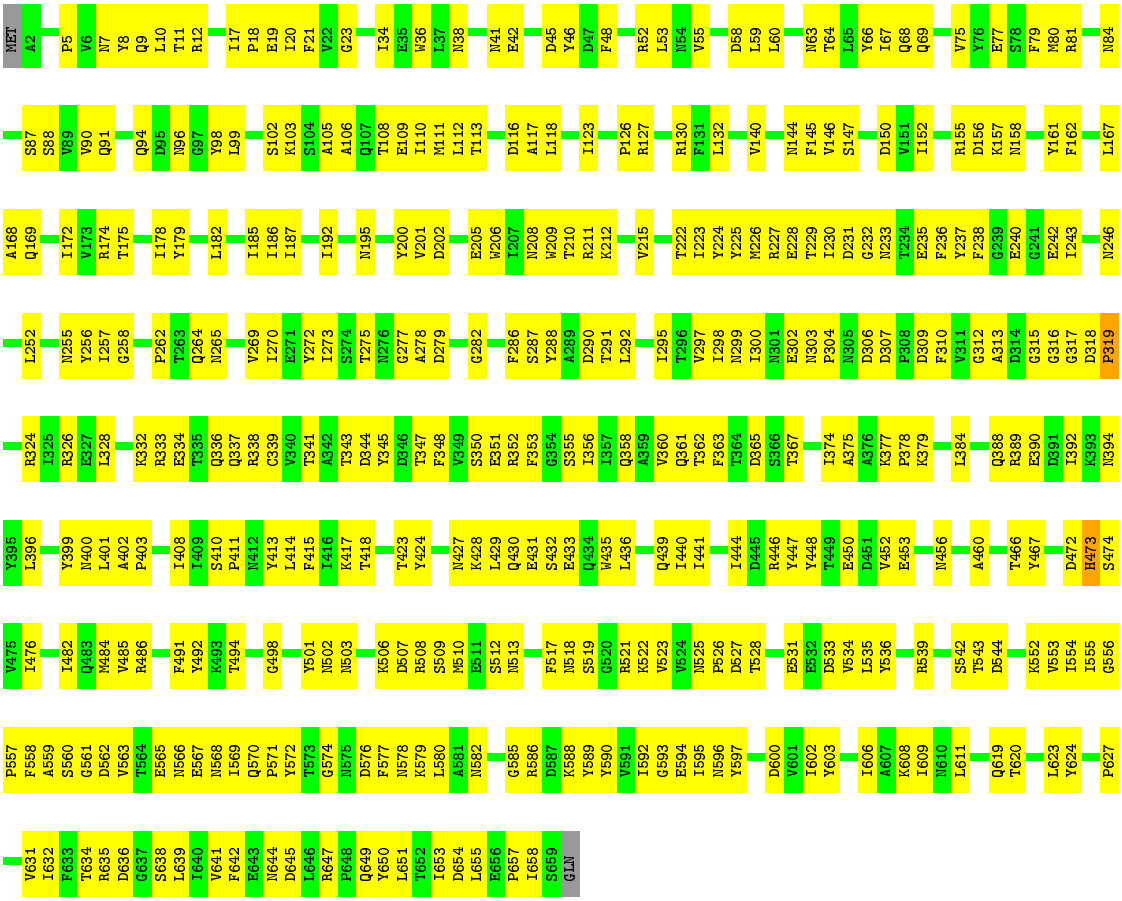
Mol	Chain	Residues	Atoms		AltConf
17	ZA	1	Total 6	Fe 6	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

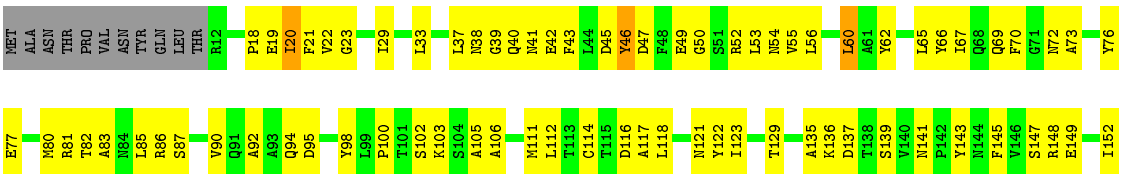
- Molecule 1: Baseplate wedge protein gp6

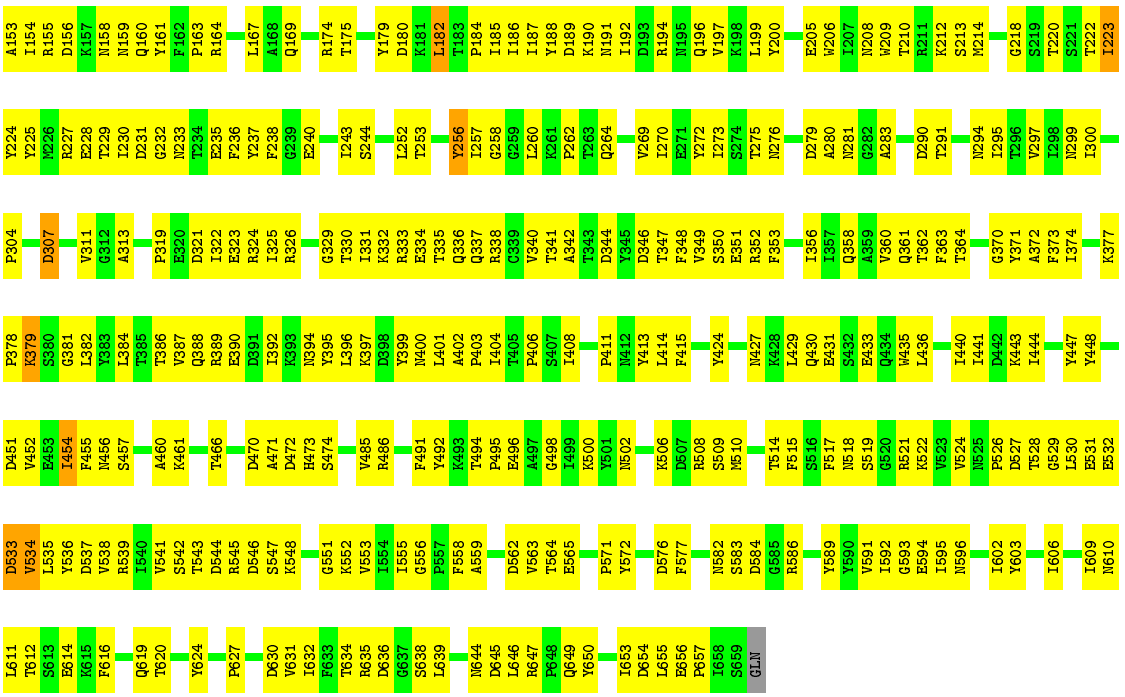
Chain A:



- Molecule 1: Baseplate wedge protein gp6

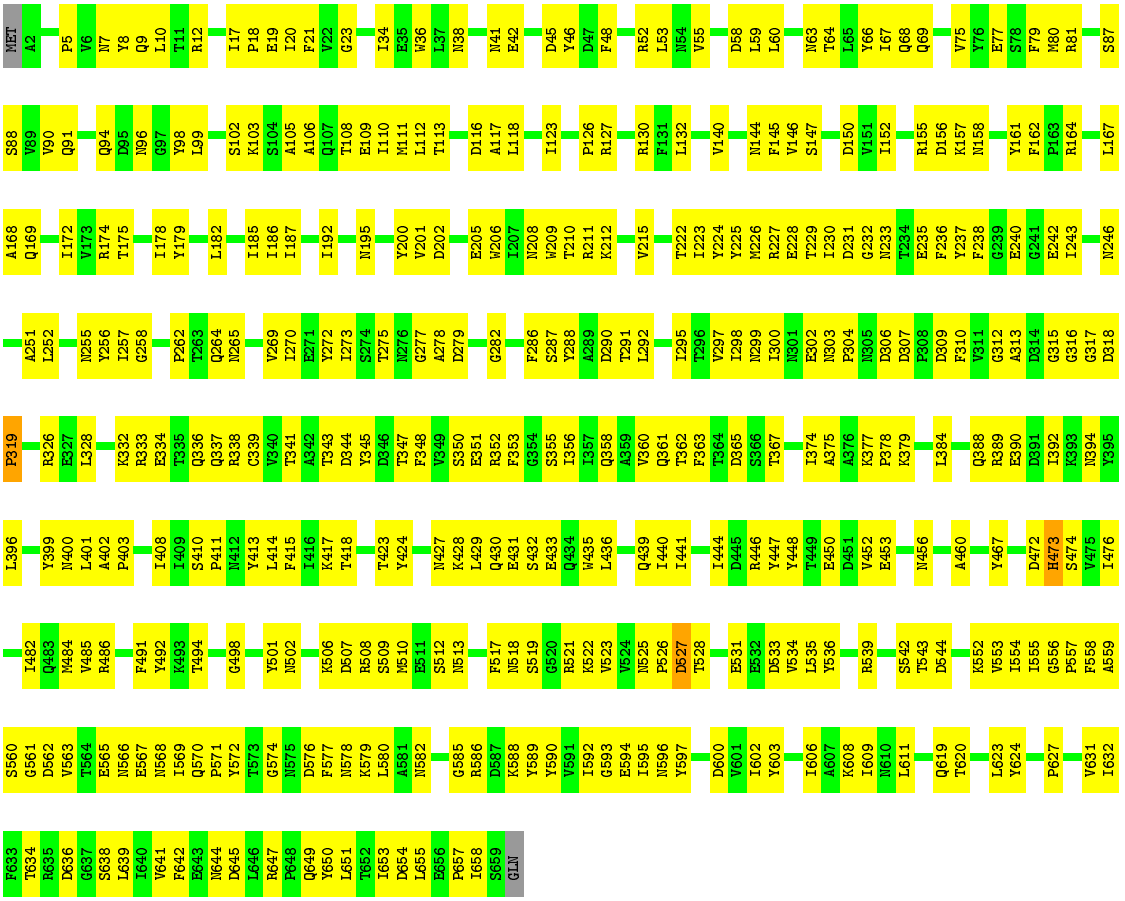
Chain B:





• Molecule 1: Baseplate wedge protein gp6

Chain X:



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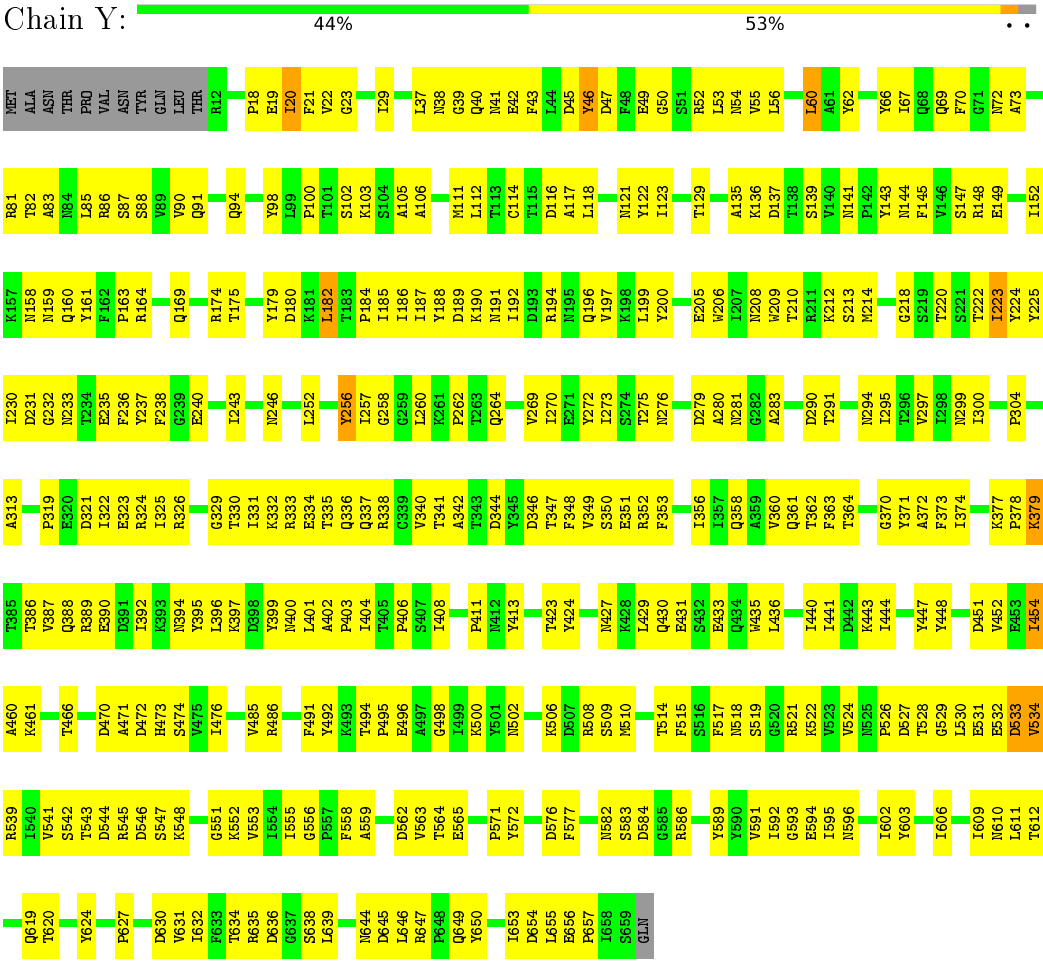
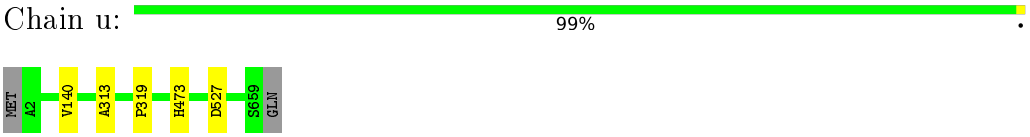
• Molecule 1: Baseplate wedge protein gp6

Chain Y:



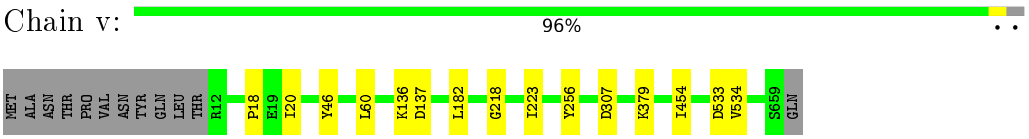
• Molecule 1: Baseplate wedge protein gp6

Chain u:



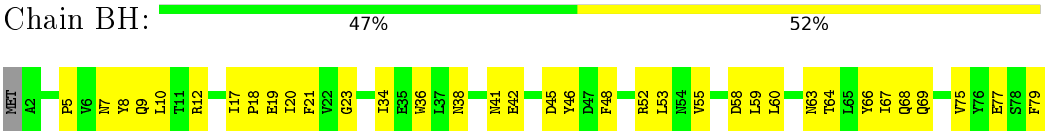
• Molecule 1: Baseplate wedge protein gp6

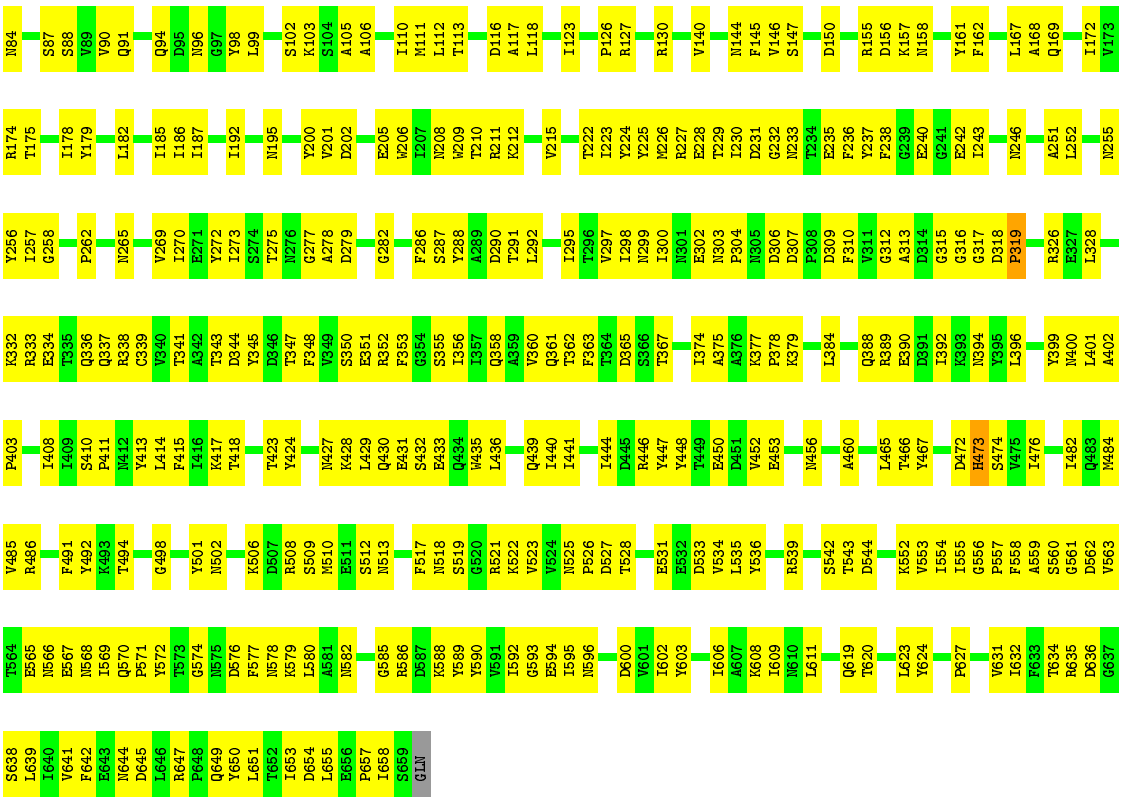
Chain v:



• Molecule 1: Baseplate wedge protein gp6

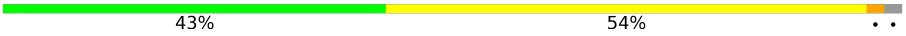
Chain BH:

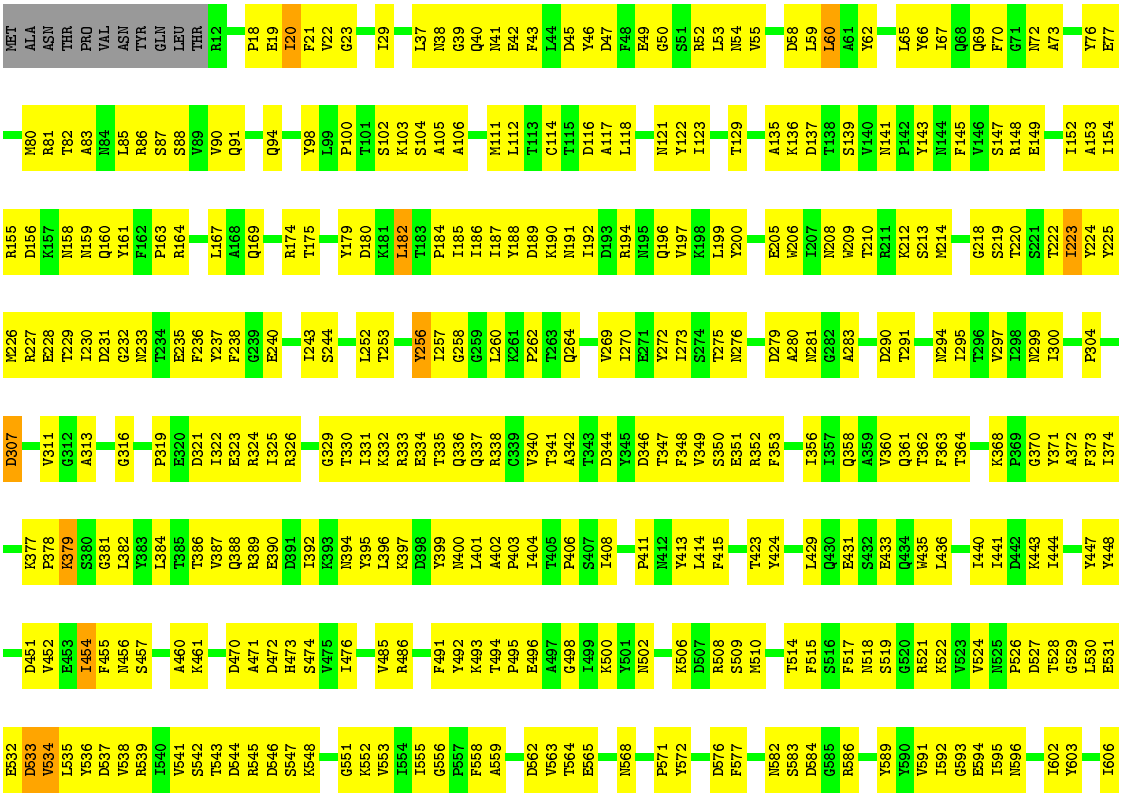




• Molecule 1: Baseplate wedge protein gp6

Chain BI:





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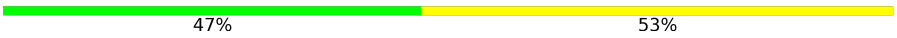
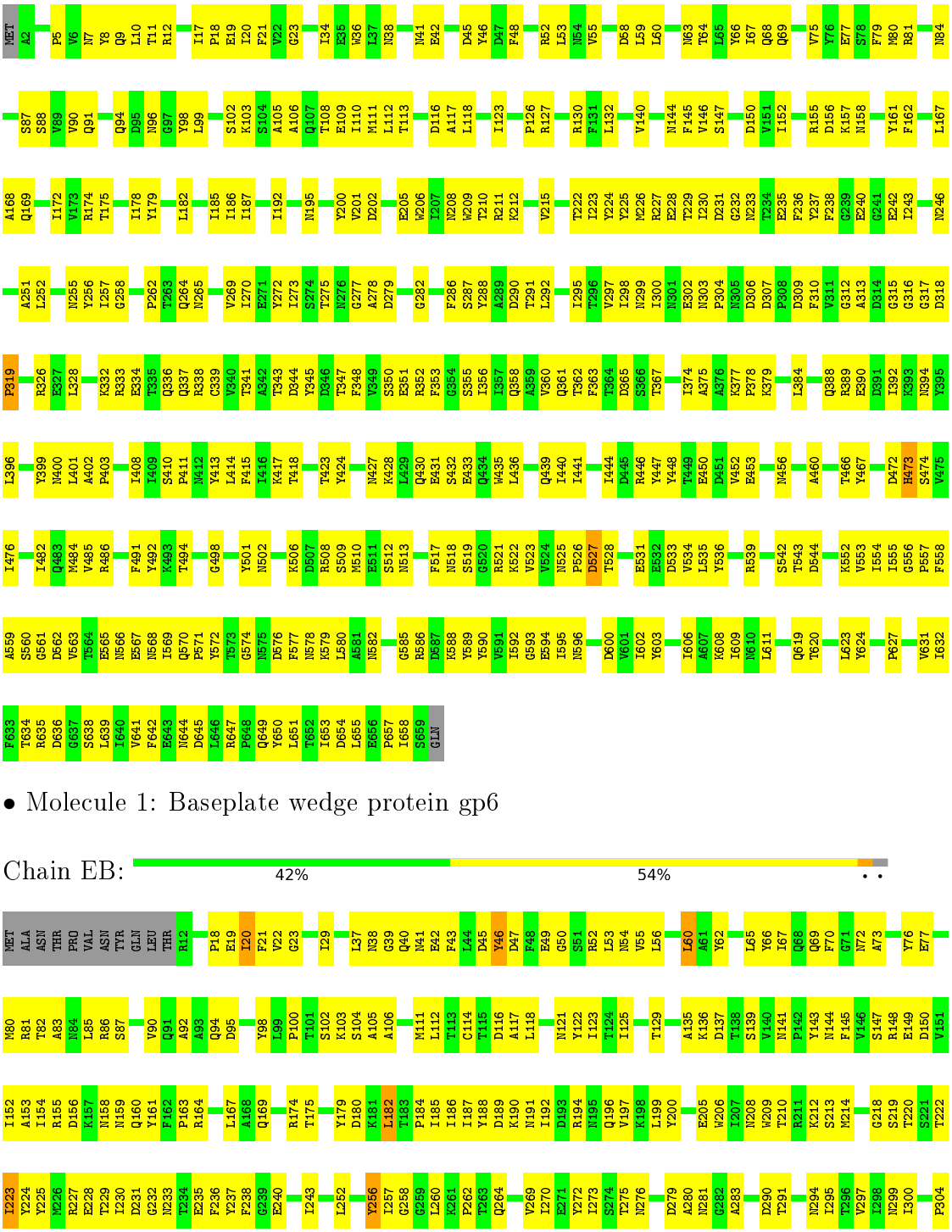
• Molecule 1: Baseplate wedge protein gp6

Chain EA:





• Molecule 1: Baseplate wedge protein gp6

Chain EB:

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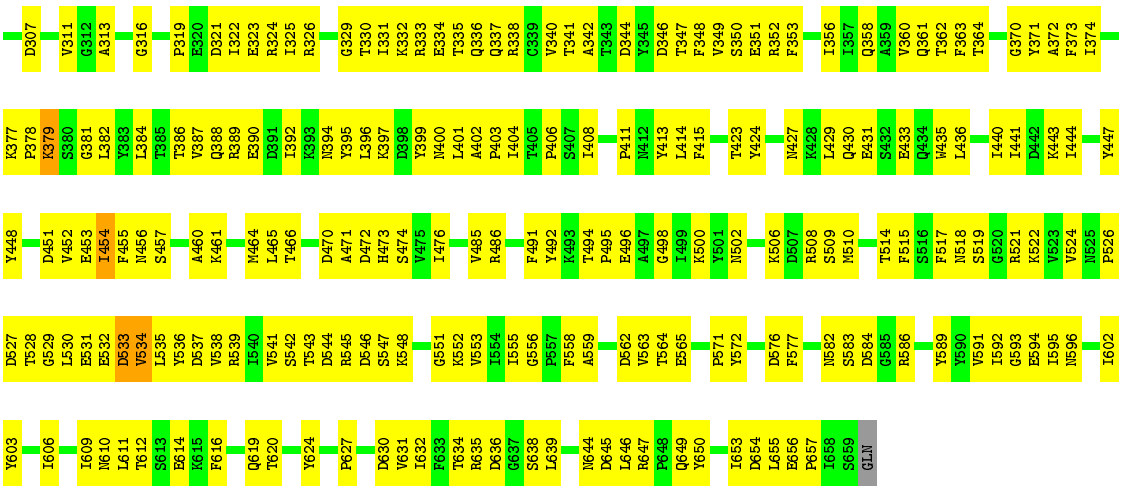
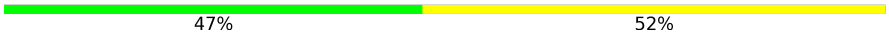
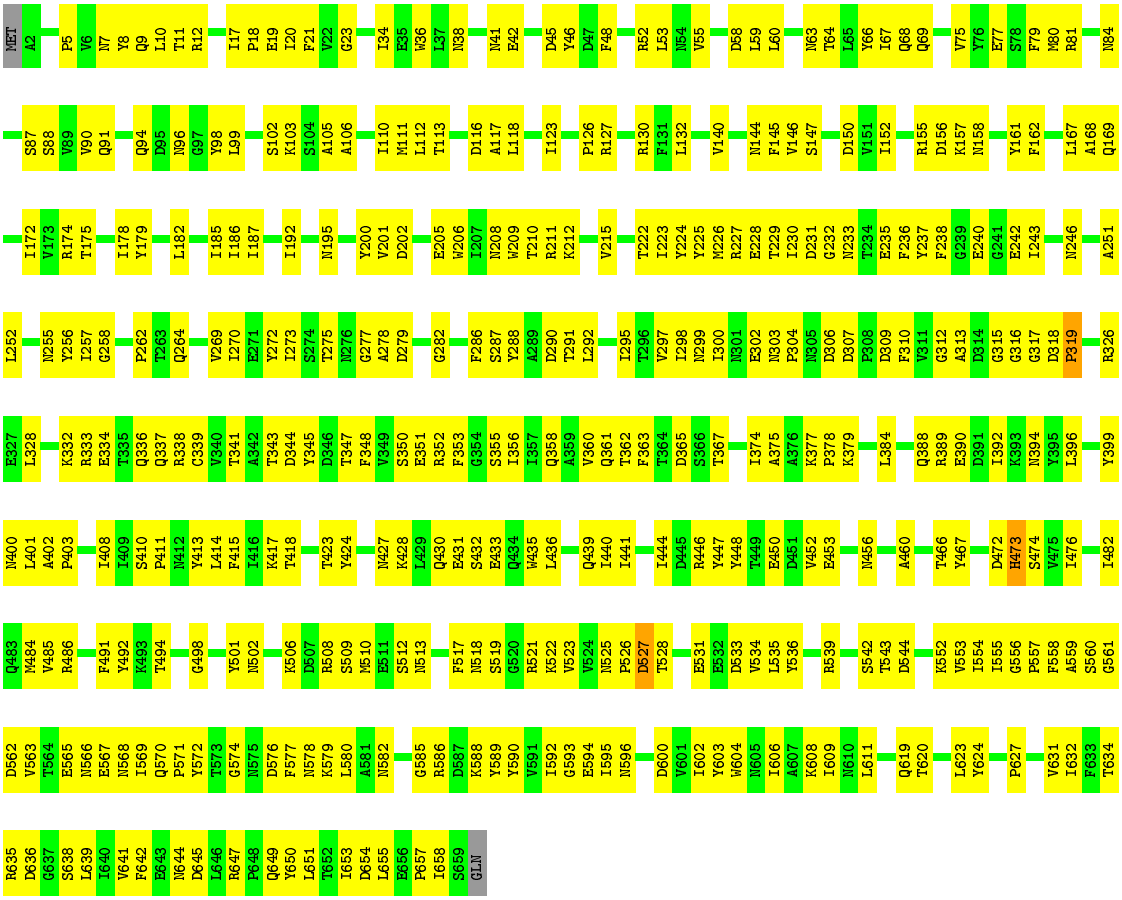


• Molecule 1: Baseplate wedge protein gp6

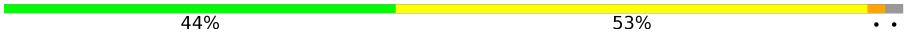
Chain GD:

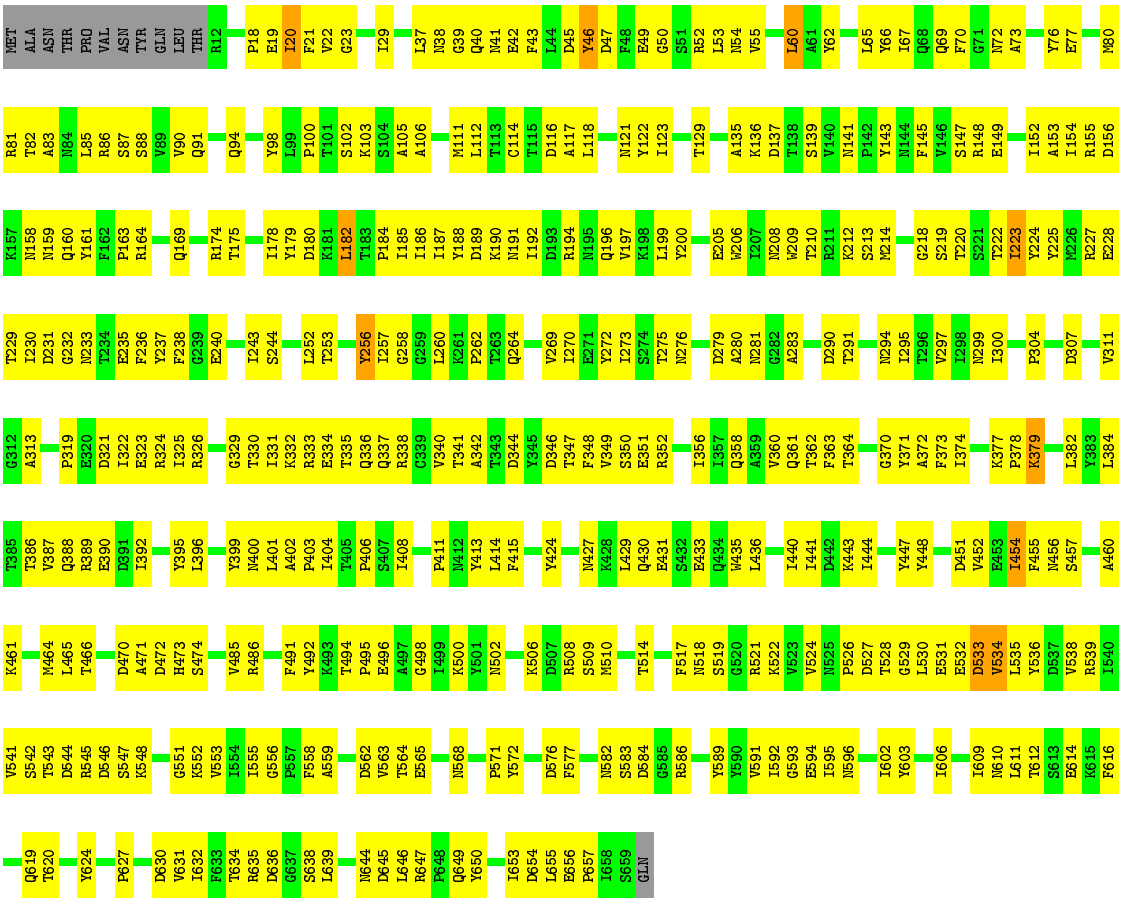




• Molecule 1: Baseplate wedge protein gp6

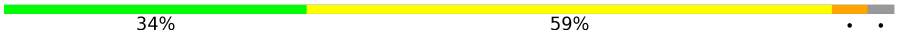
Chain GE:

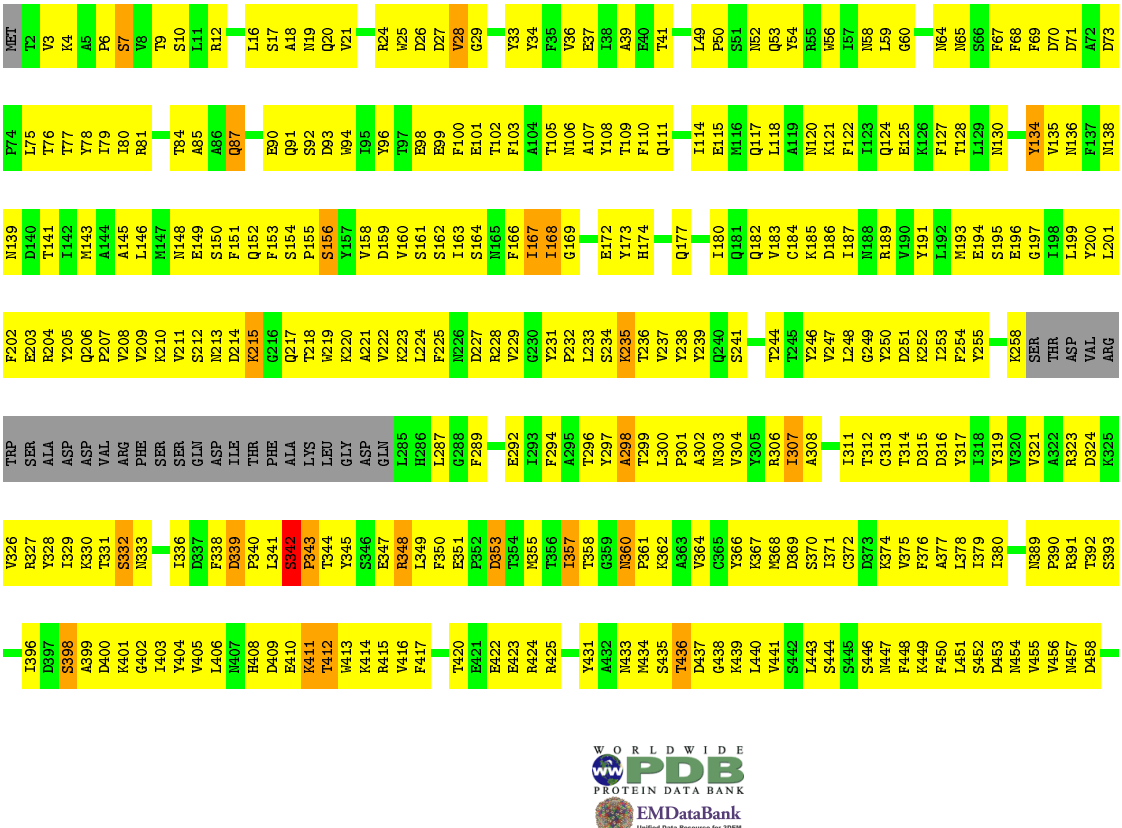




• Molecule 2: Baseplate wedge protein gp7

Chain C:





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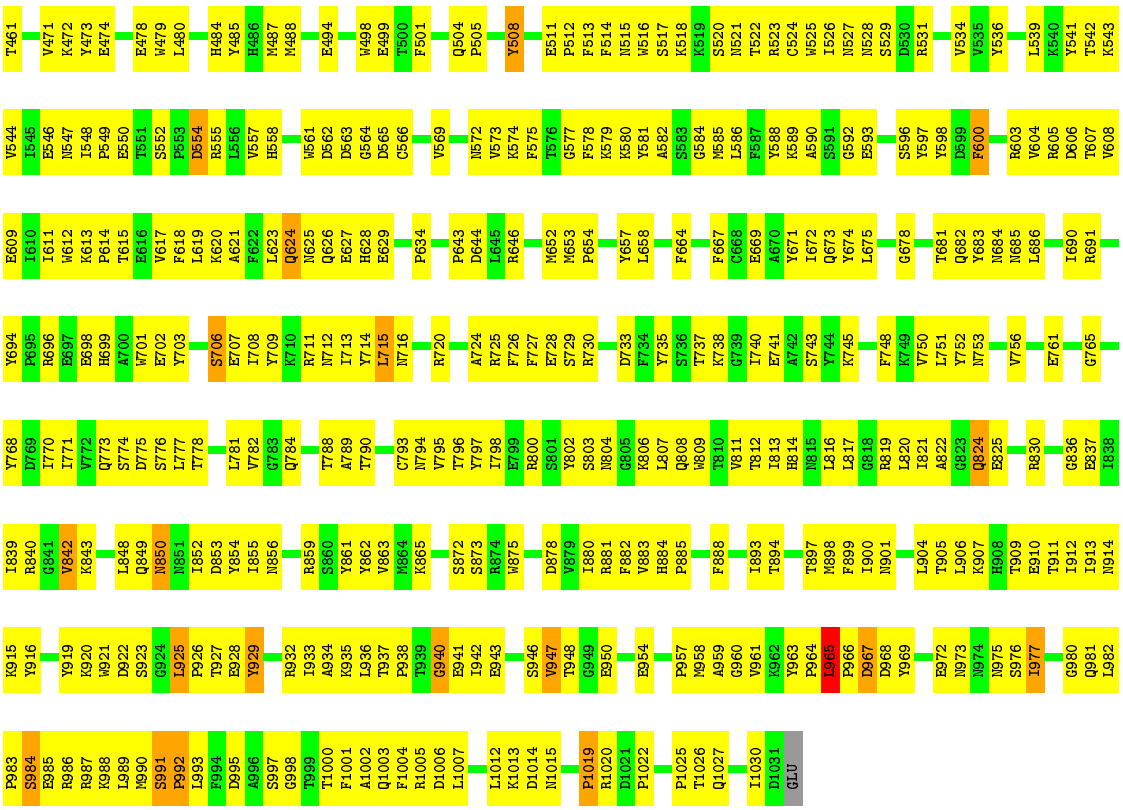
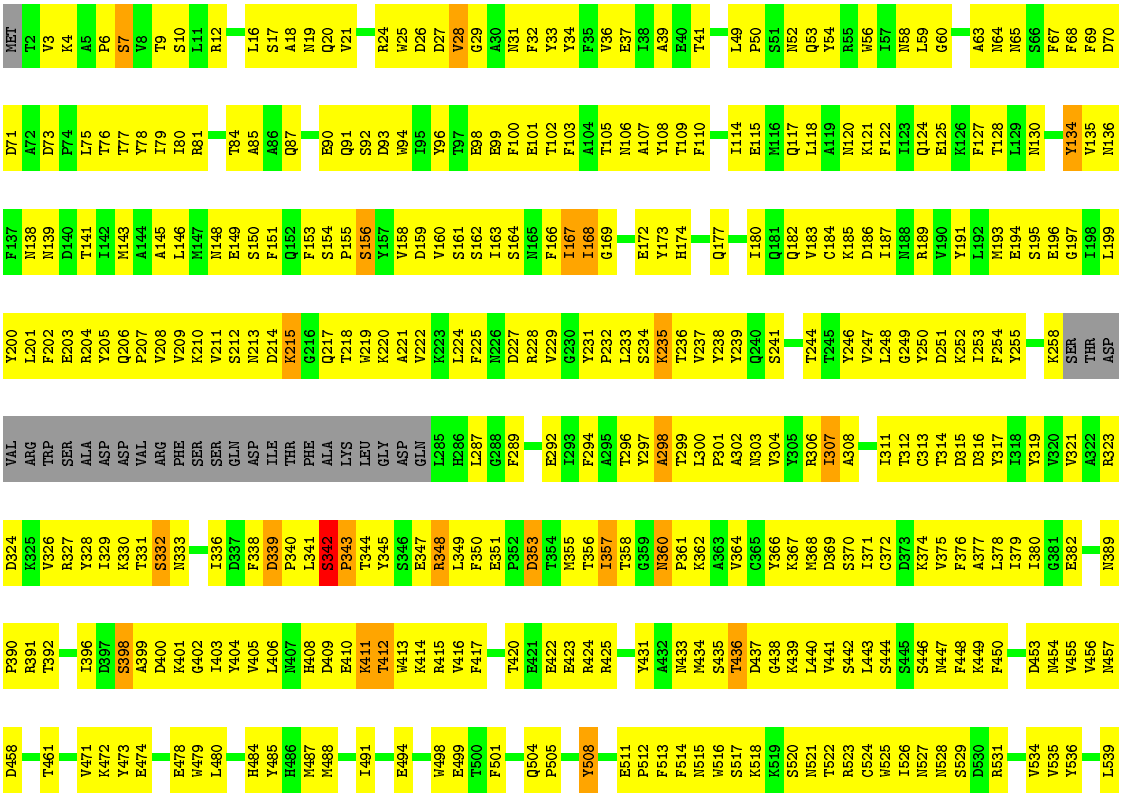


• Molecule 2: Baseplate wedge protein gp7

Chain Z:



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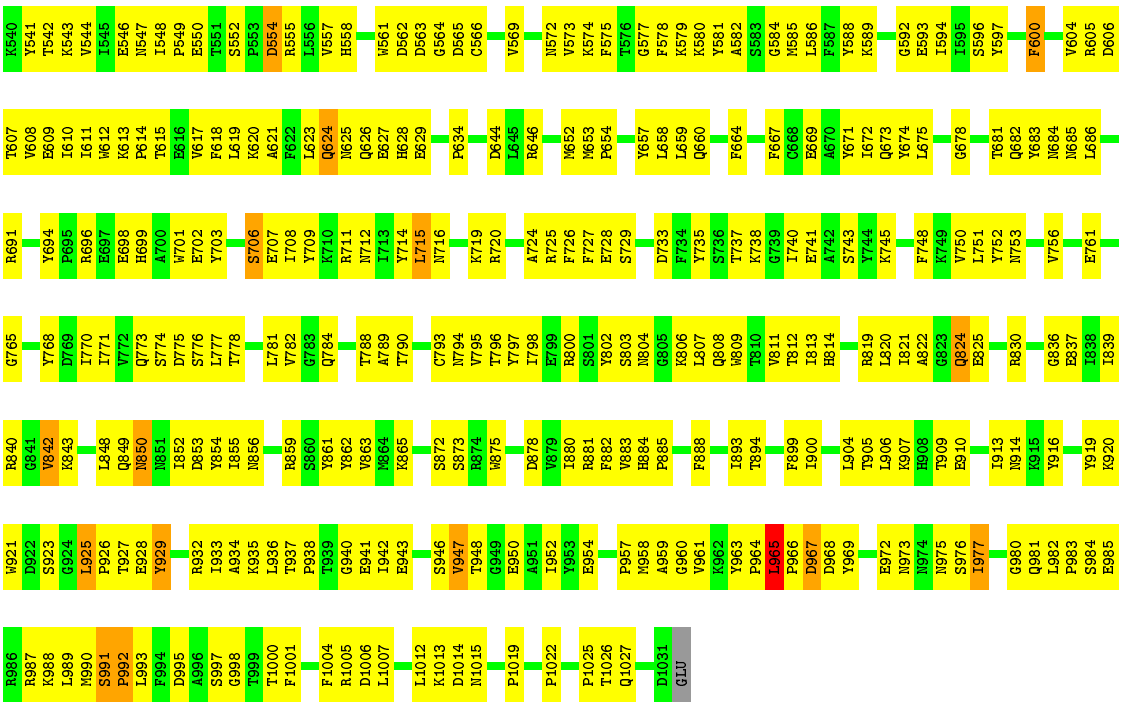
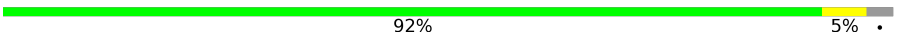
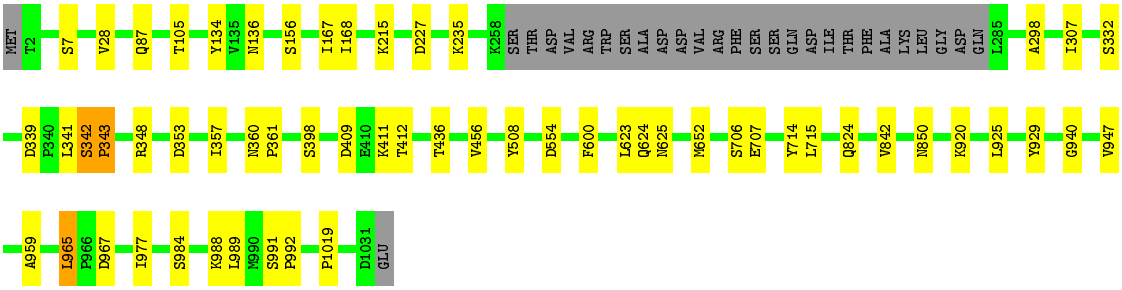


• Molecule 2: Baseplate wedge protein gp7

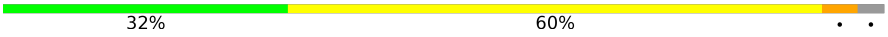
Chain w:

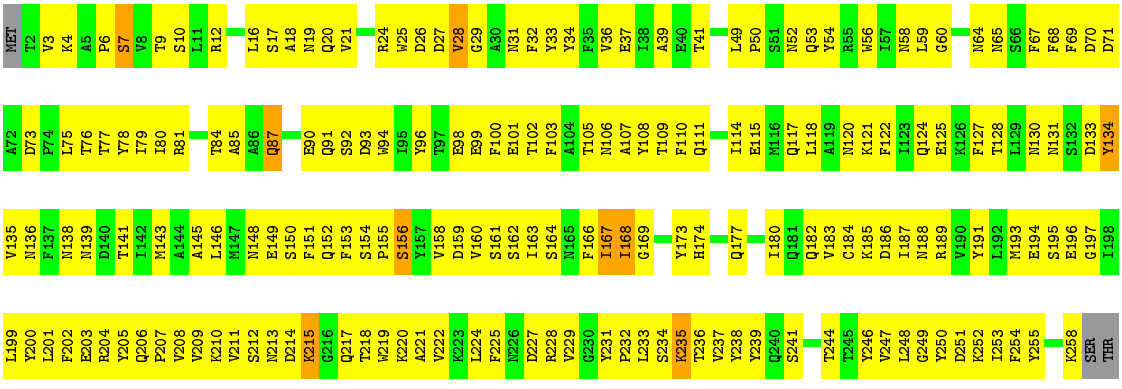


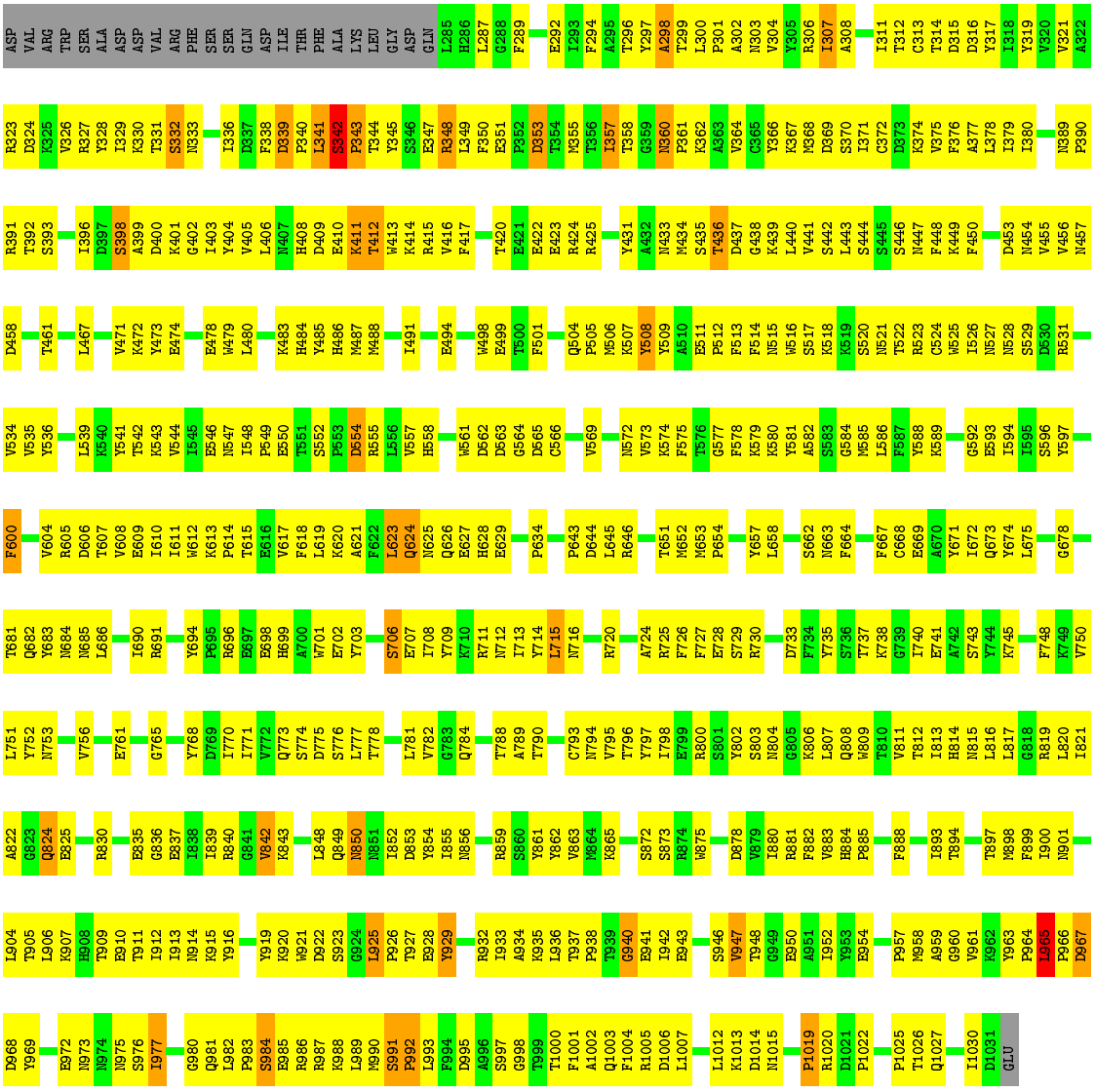


• Molecule 2: Baseplate wedge protein gp7

Chain BJ:

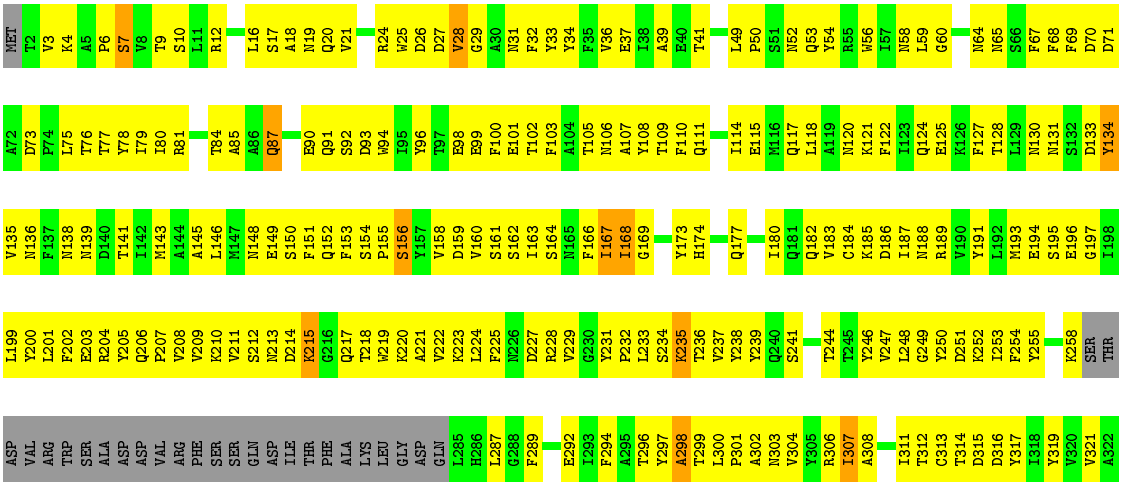






• Molecule 2: Baseplate wedge protein gp7

Chain EC:



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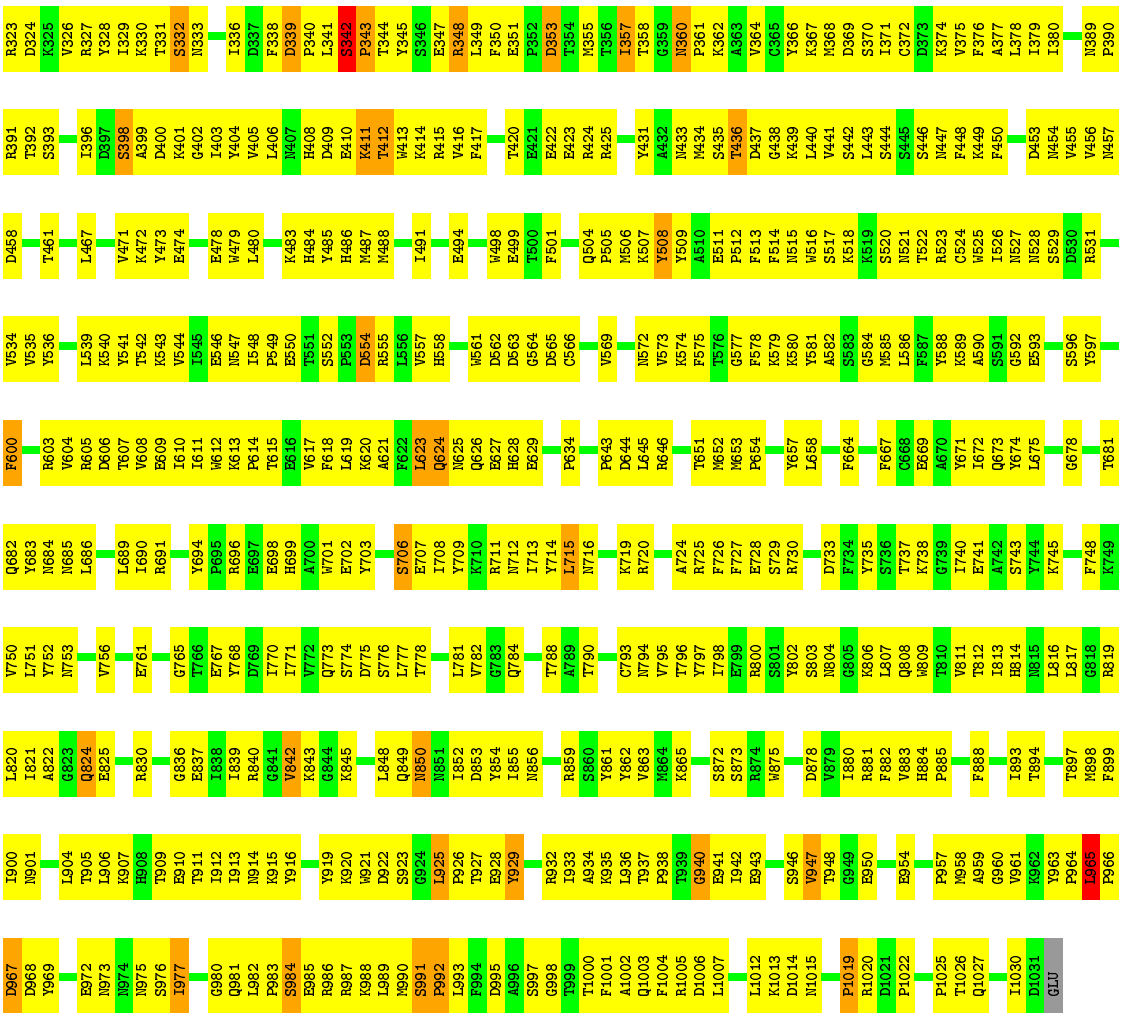
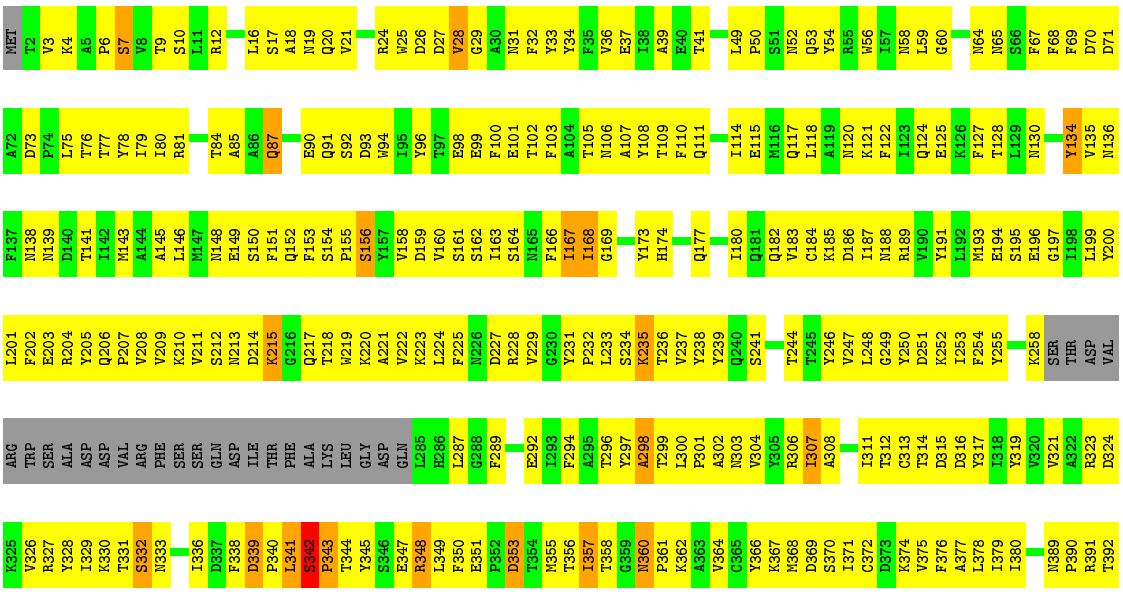


• Molecule 2: Baseplate wedge protein gp7

Chain GF:



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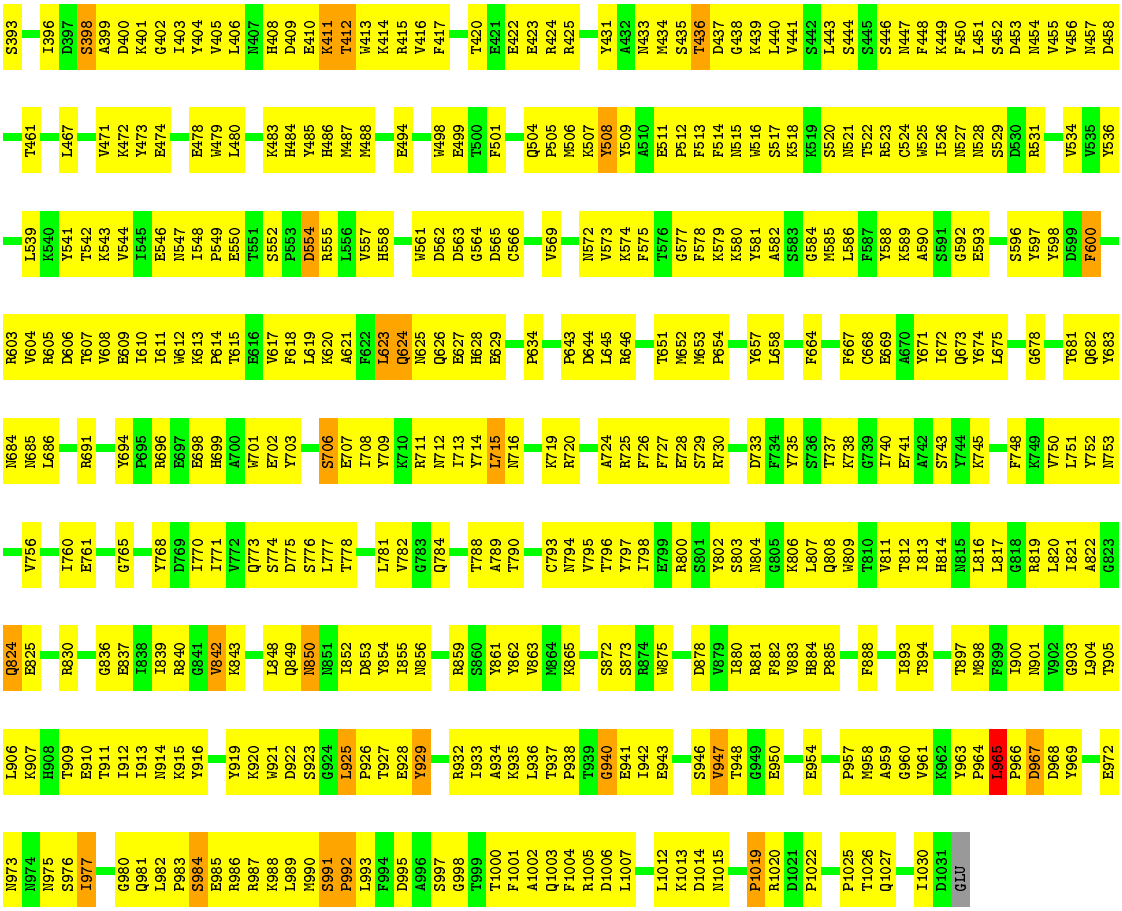
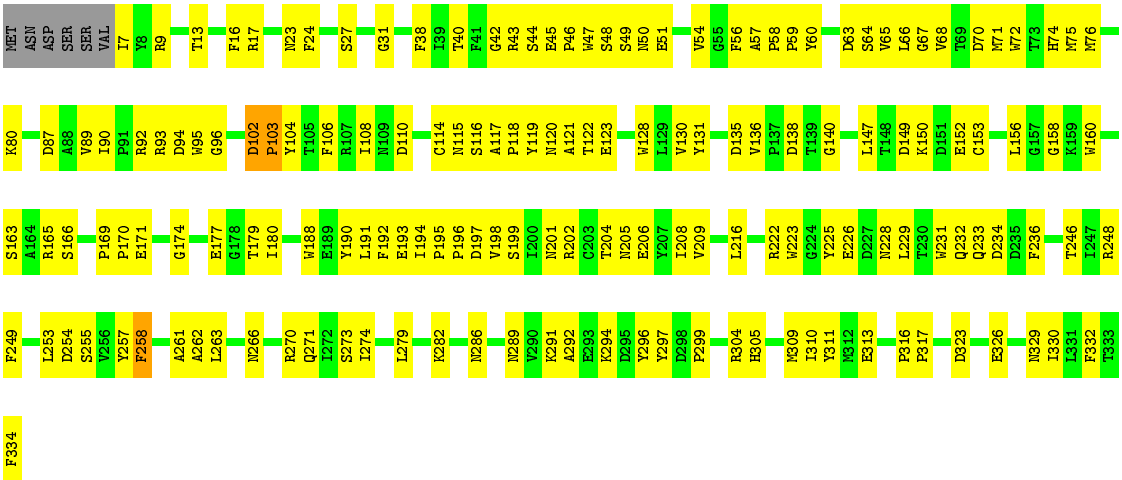


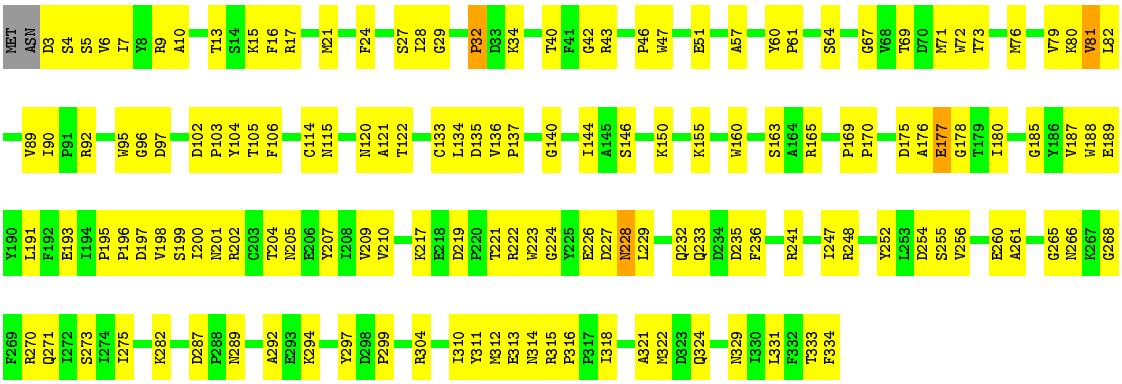
• Molecule 3: Baseplate wedge protein gp8

Chain D:



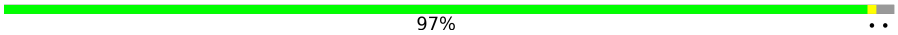
• Molecule 3: Baseplate wedge protein gp8

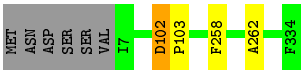
Chain E:



• Molecule 3: Baseplate wedge protein gp8

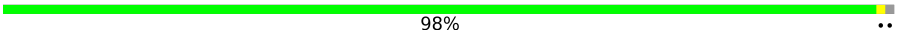
Chain a:

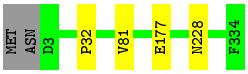




• Molecule 3: Baseplate wedge protein gp8

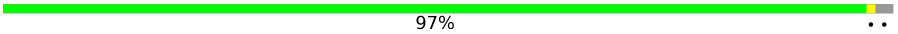
Chain b:

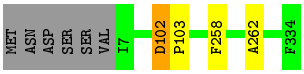




• Molecule 3: Baseplate wedge protein gp8

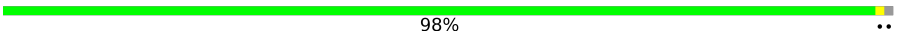
Chain x:

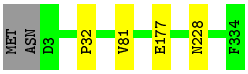




• Molecule 3: Baseplate wedge protein gp8

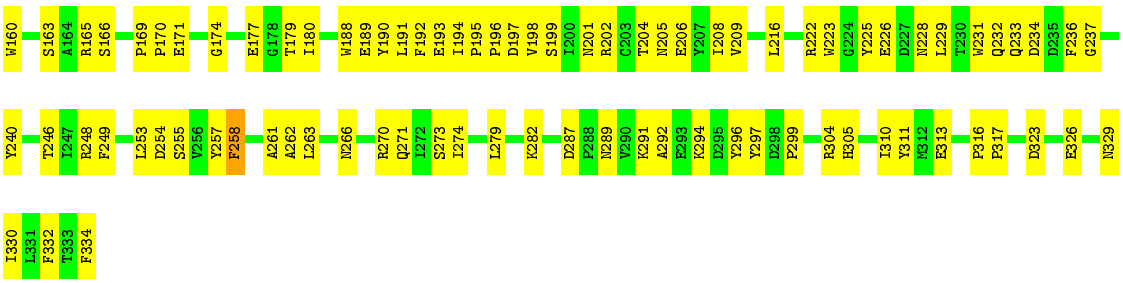
Chain y:





• Molecule 3: Baseplate wedge protein gp8

Chain CA:



• Molecule 3: Baseplate wedge protein gp8

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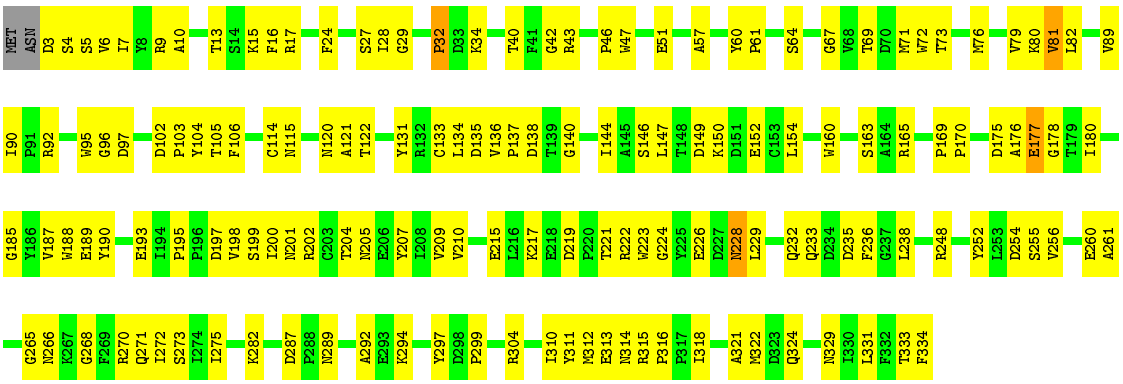

• Molecule 3: Baseplate wedge protein gp8

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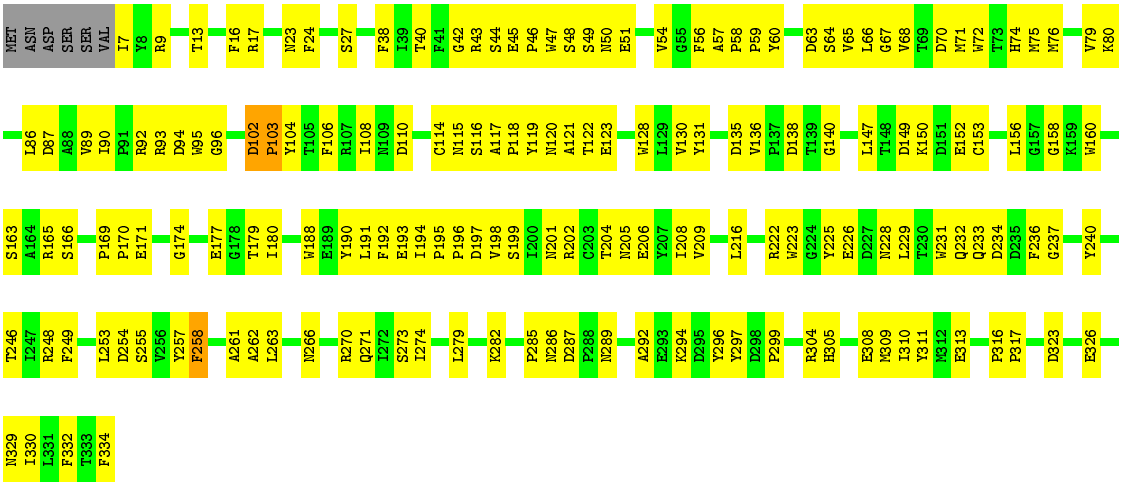

• Molecule 3: Baseplate wedge protein gp8

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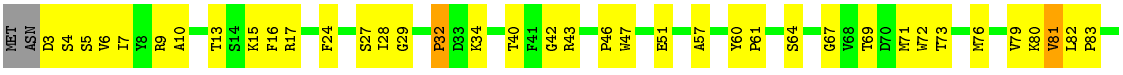

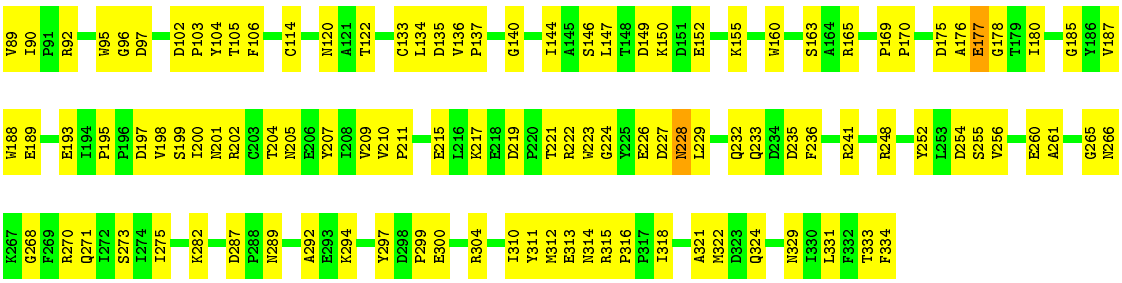

• Molecule 3: Baseplate wedge protein gp8

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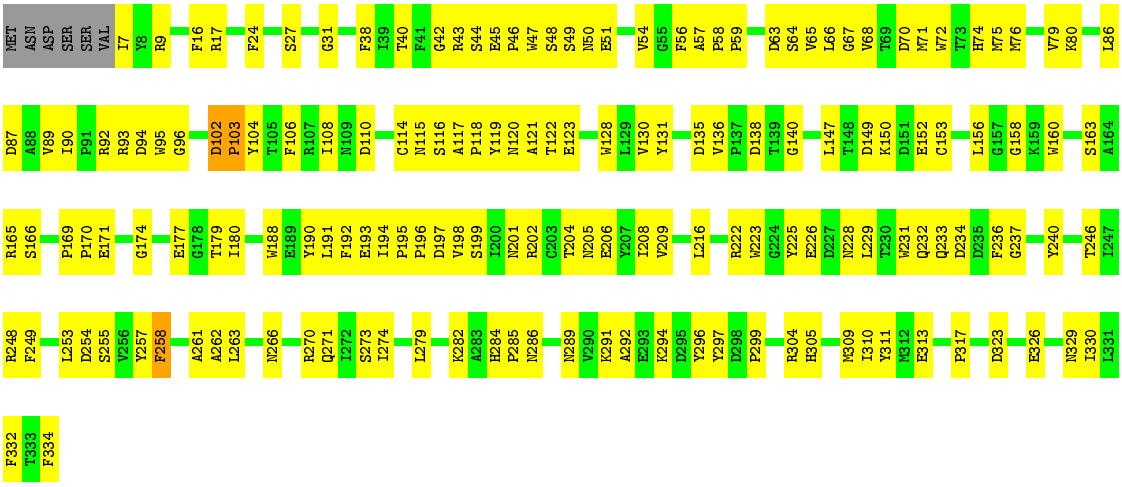
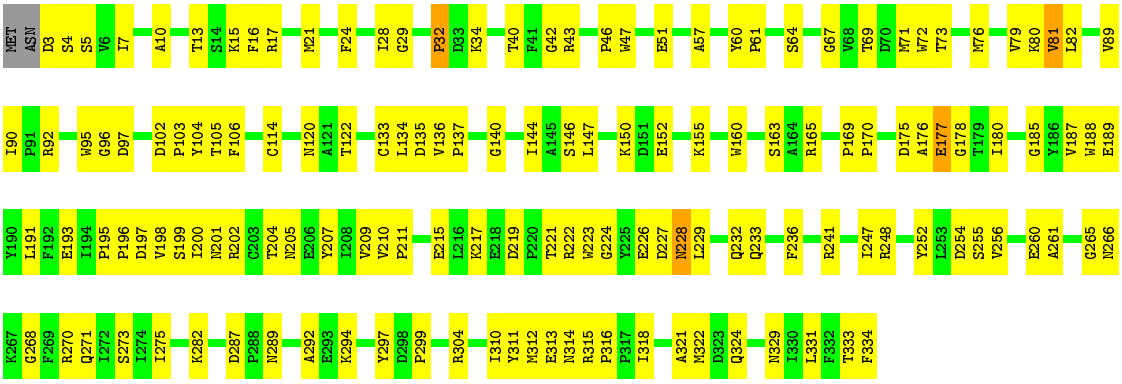


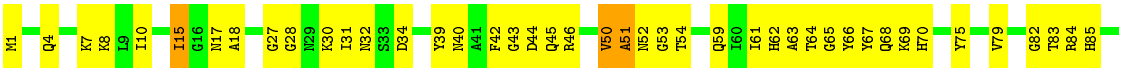
• Molecule 3: Baseplate wedge protein gp8

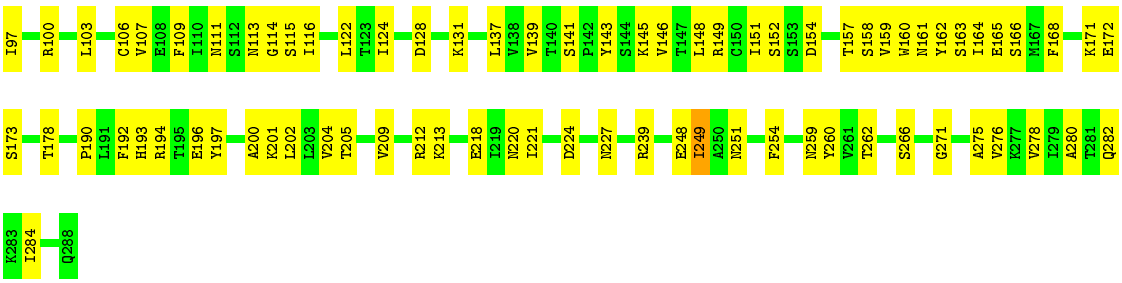
Chain GH:



• Molecule 4: Baseplate wedge protein gp9

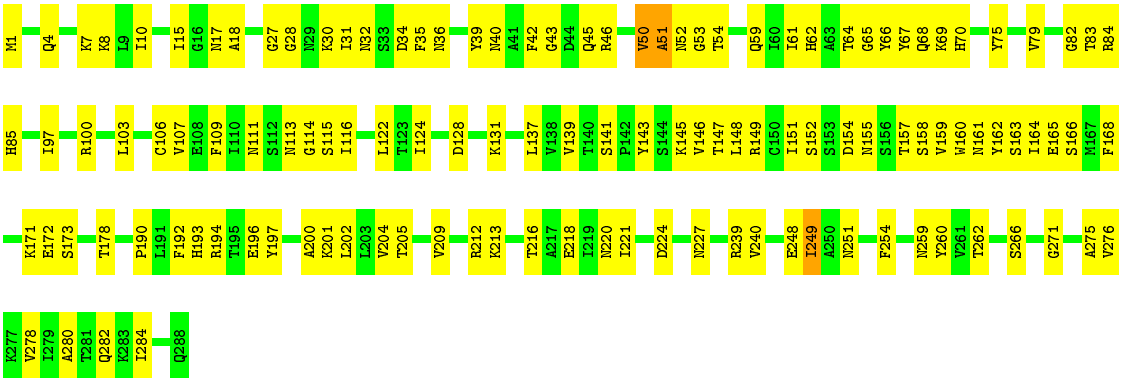
Chain F:





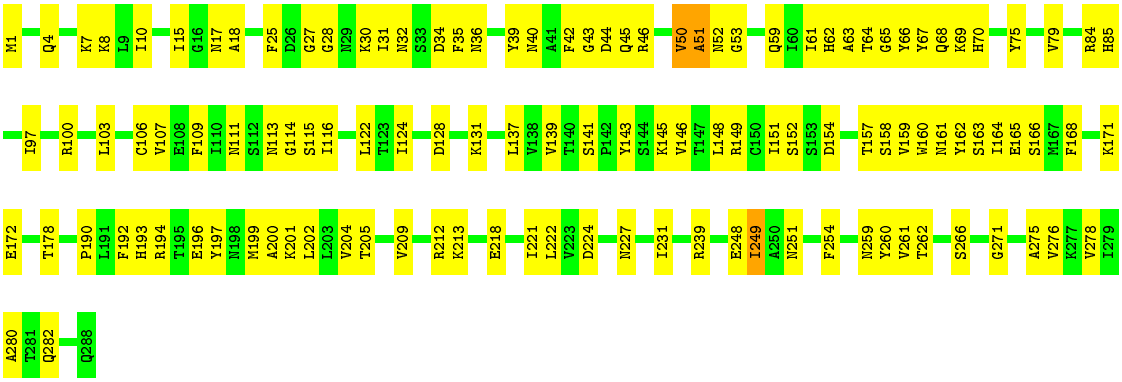
• Molecule 4: Baseplate wedge protein gp9

Chain G:



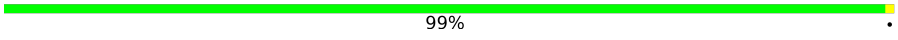
• Molecule 4: Baseplate wedge protein gp9

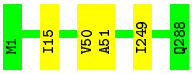
Chain H:



• Molecule 4: Baseplate wedge protein gp9

Chain c:





• Molecule 4: Baseplate wedge protein gp9

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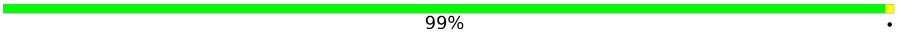

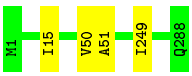

• Molecule 4: Baseplate wedge protein gp9

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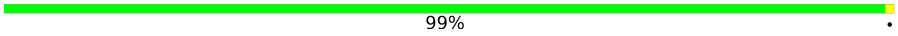
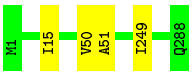
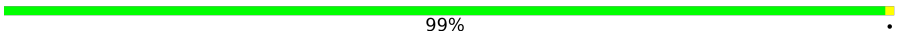
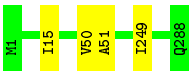




• Molecule 4: Baseplate wedge protein gp9

Chain z:





• Molecule 4: Baseplate wedge protein gp9

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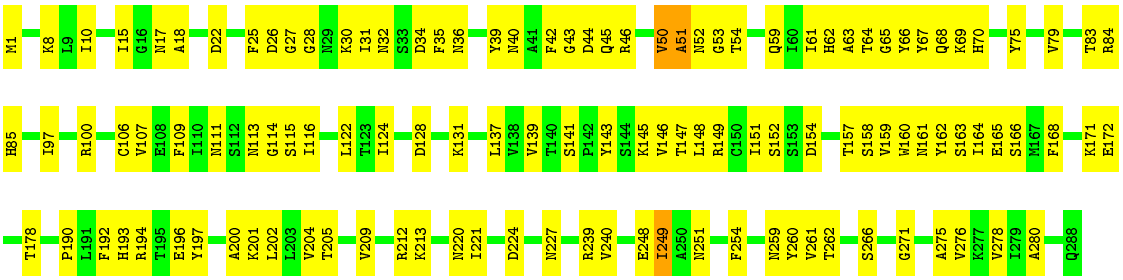
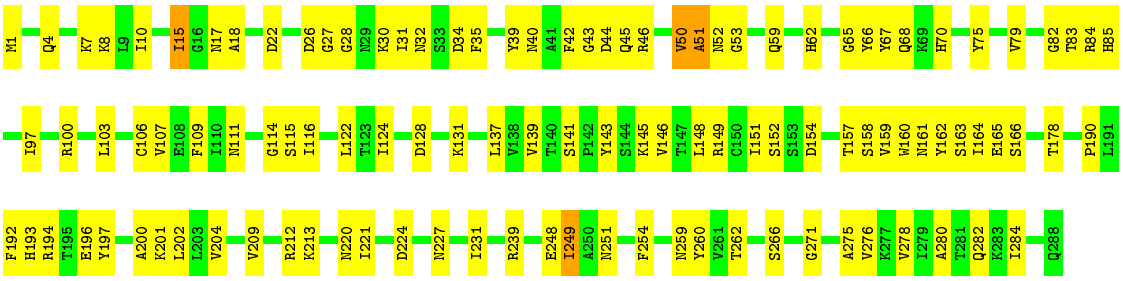


• Molecule 4: Baseplate wedge protein gp9

Chain AB:



• Molecule 4: Baseplate wedge protein gp9

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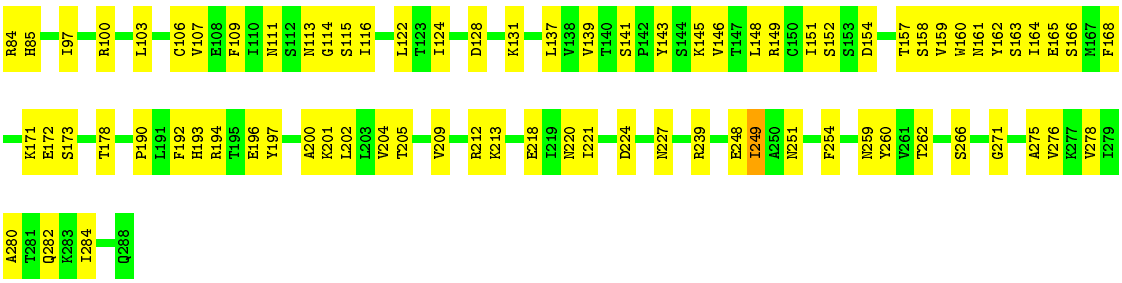
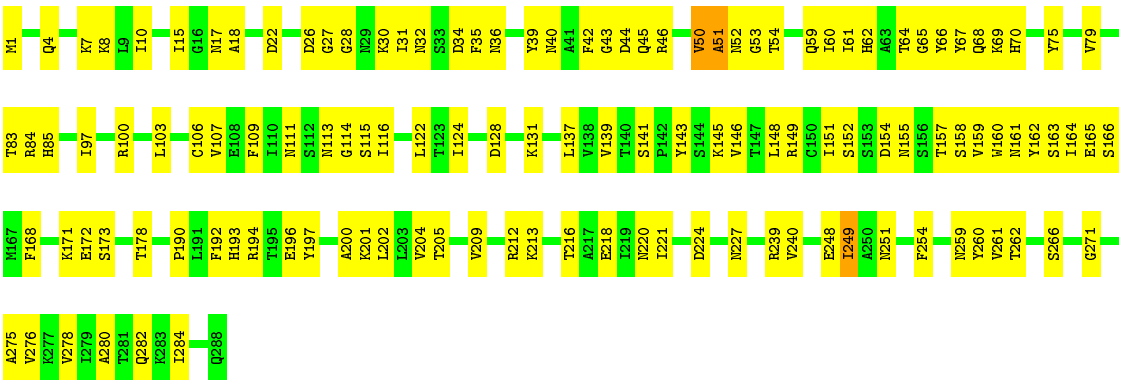


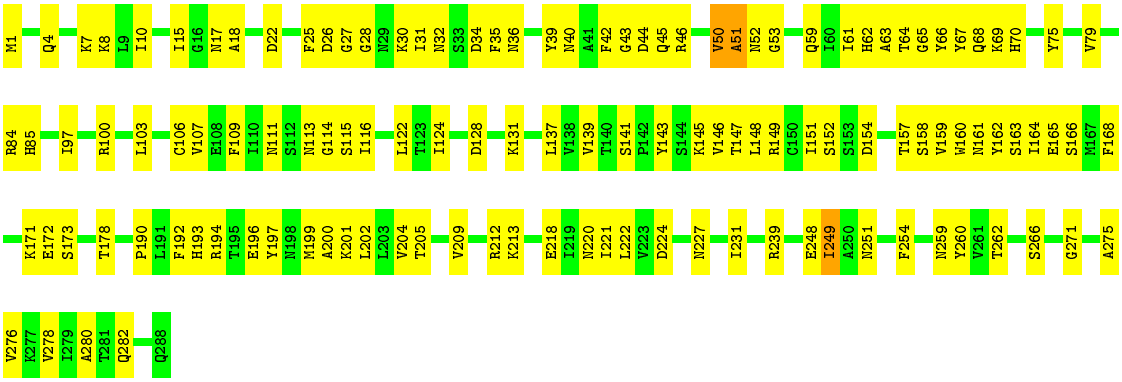
• Molecule 4: Baseplate wedge protein gp9

Chain CD: 56% 43%



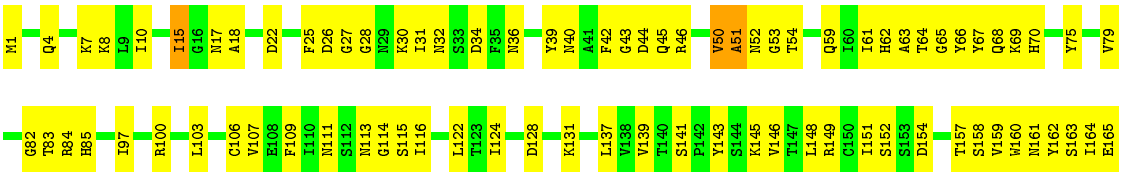
• Molecule 4: Baseplate wedge protein gp9

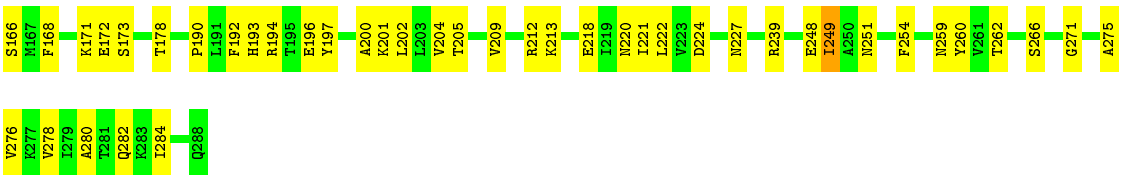
Chain CE: 57% 42%



• Molecule 4: Baseplate wedge protein gp9

Chain EF: 57% 42%





• Molecule 4: Baseplate wedge protein gp9

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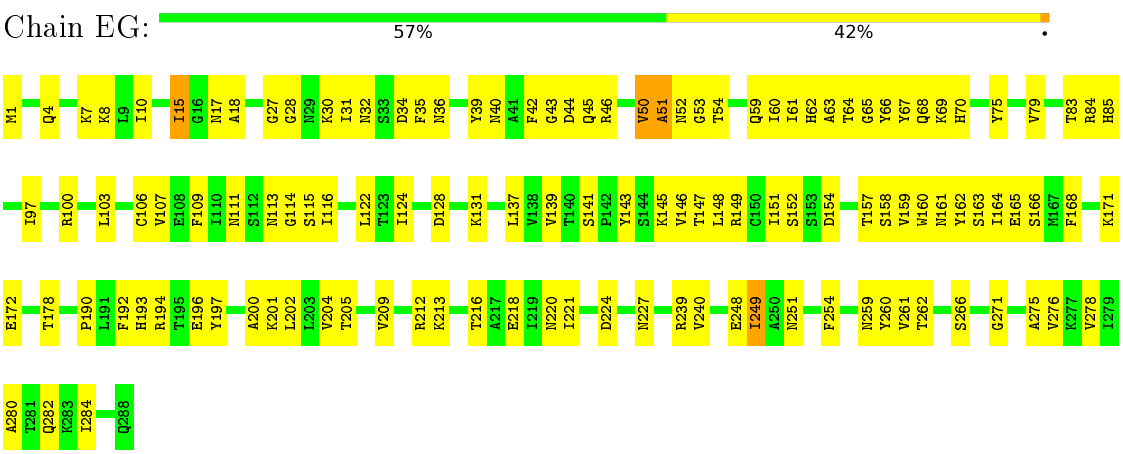

• Molecule 4: Baseplate wedge protein gp9

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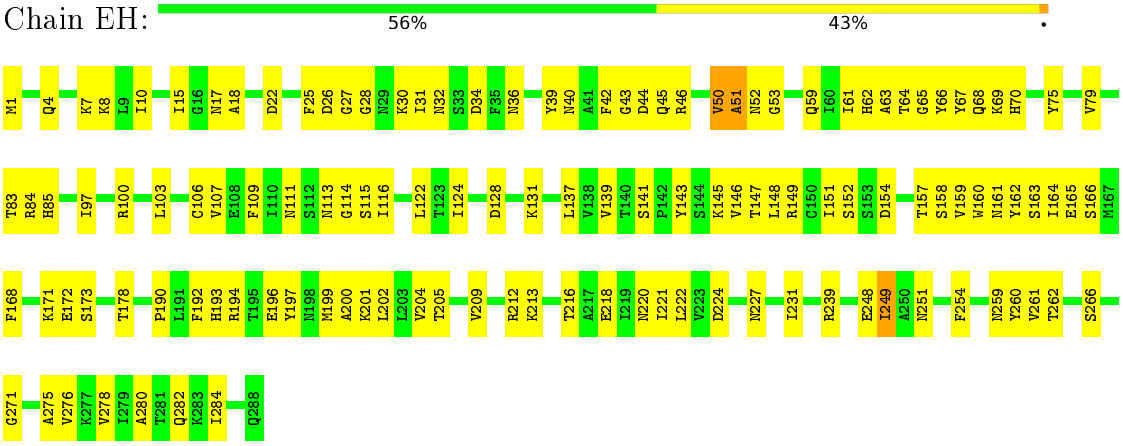
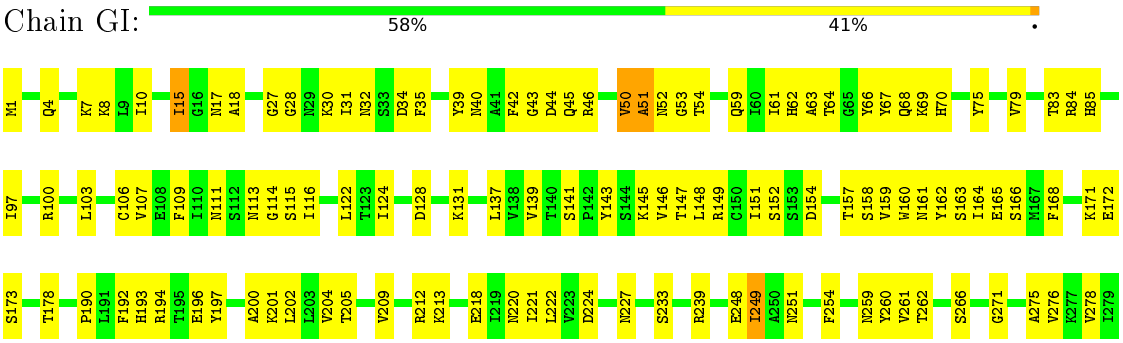
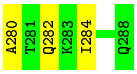


• Molecule 4: Baseplate wedge protein gp9

Chain GI:





• Molecule 4: Baseplate wedge protein gp9

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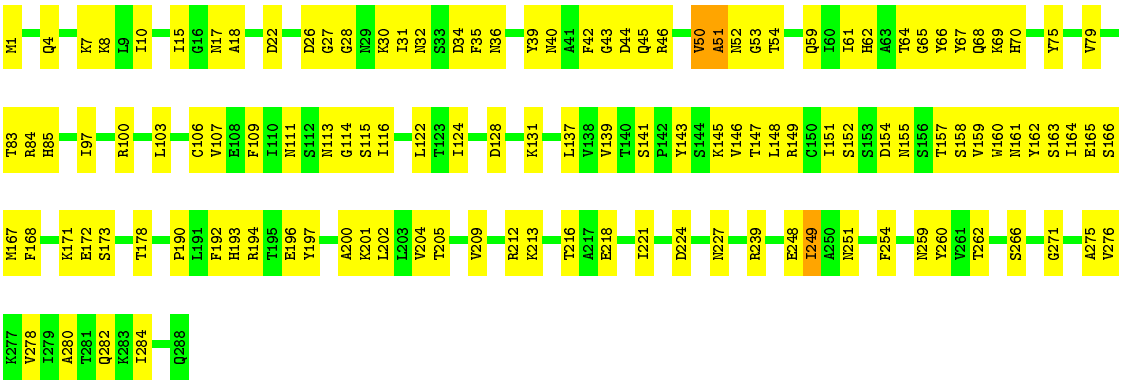

• Molecule 4: Baseplate wedge protein gp9

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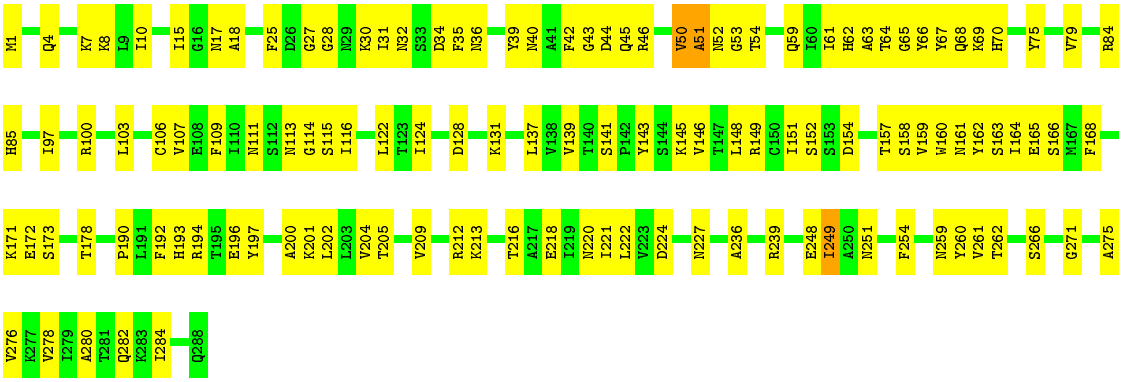
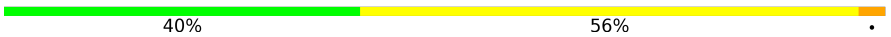
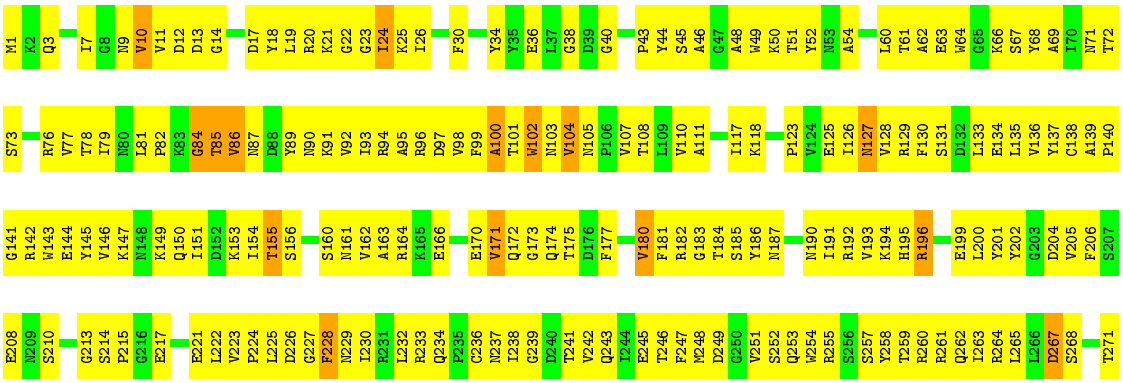
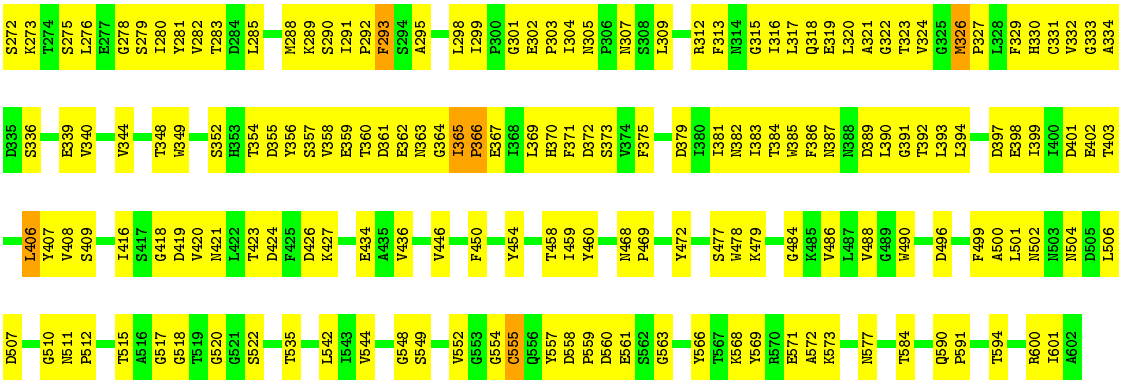


• Molecule 5: Baseplate wedge protein gp10

Chain I:







• Molecule 5: Baseplate wedge protein gp10

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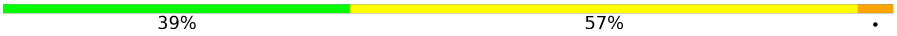

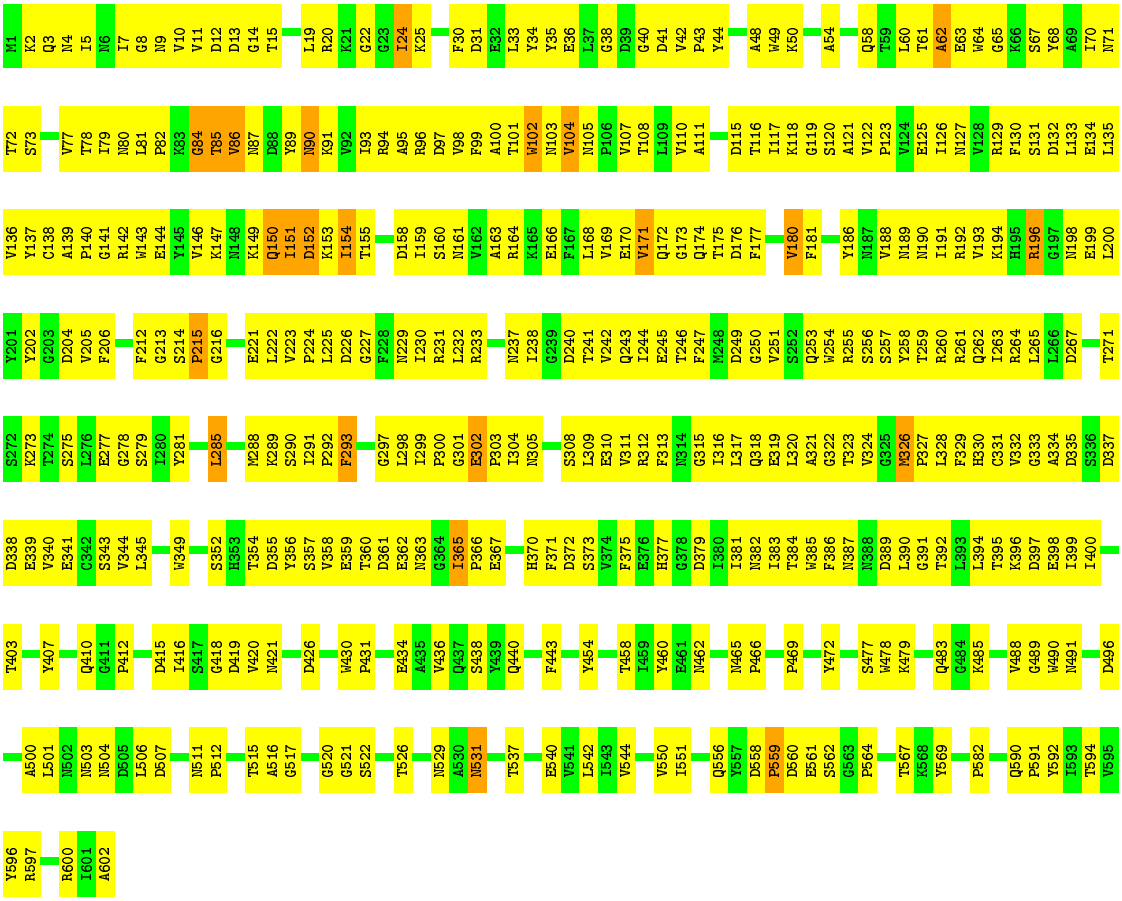

• Molecule 5: Baseplate wedge protein gp10

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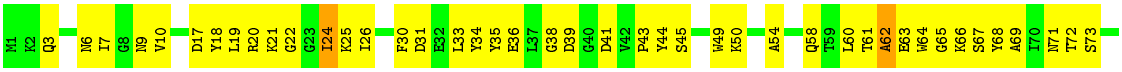

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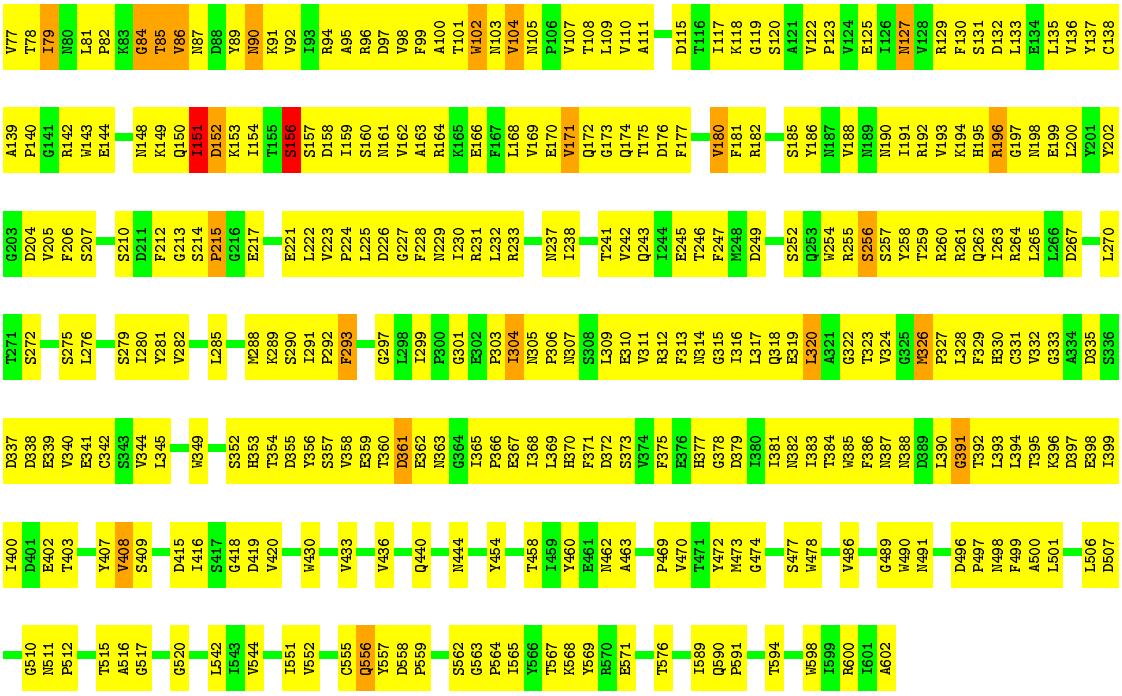

- Molecule 5: Baseplate wedge protein gp10

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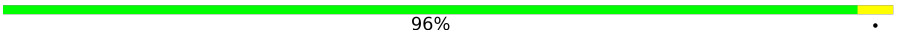

- Molecule 5: Baseplate wedge protein gp10

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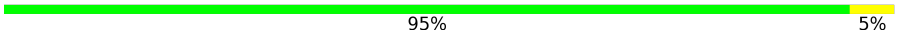
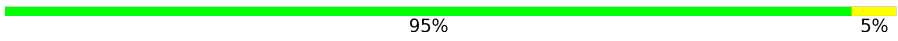
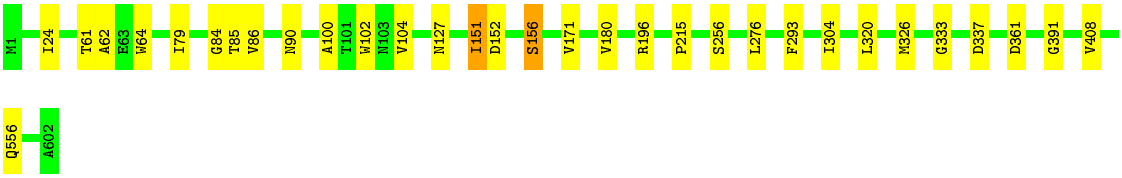


- Molecule 5: Baseplate wedge protein gp10

Chain h:





- Molecule 5: Baseplate wedge protein gp10

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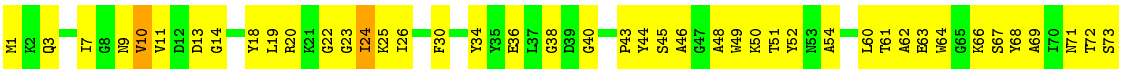
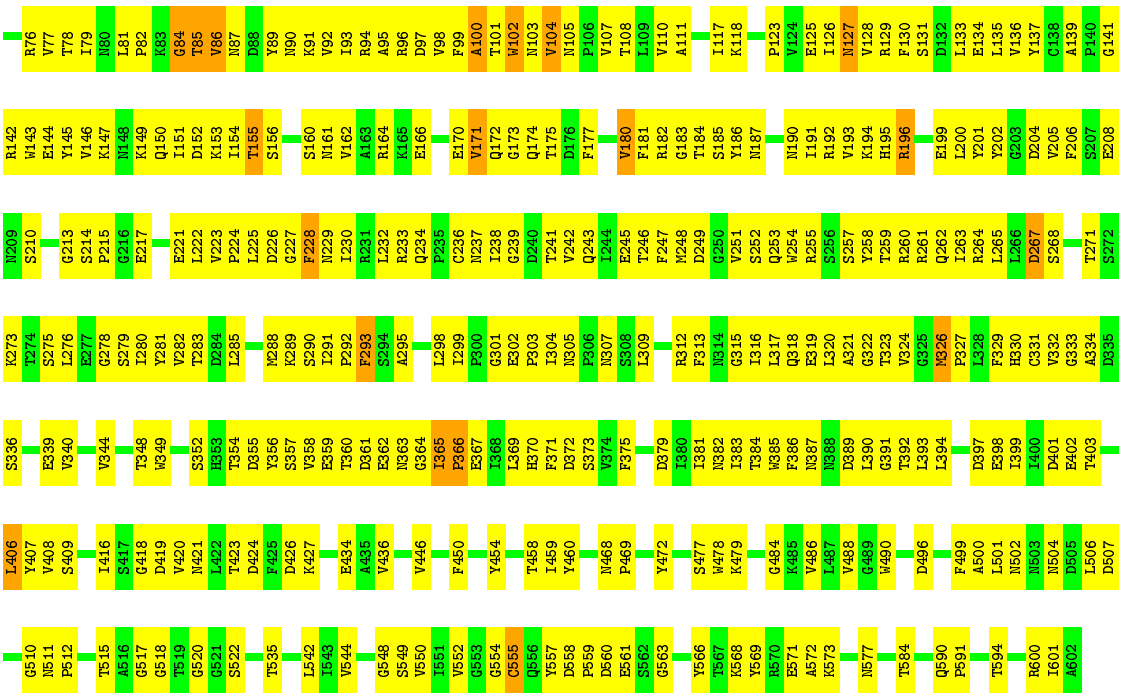
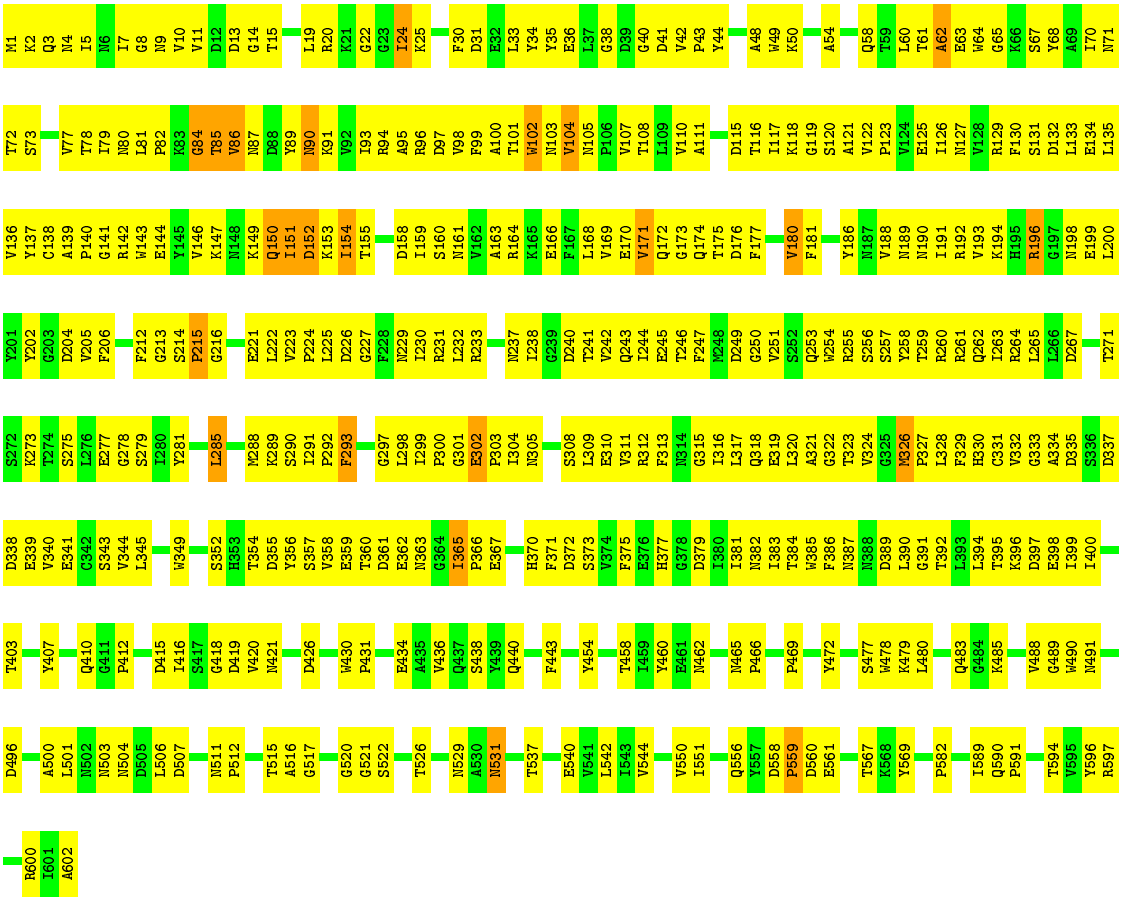




• Molecule 5: Baseplate wedge protein gp10

Chain AD:



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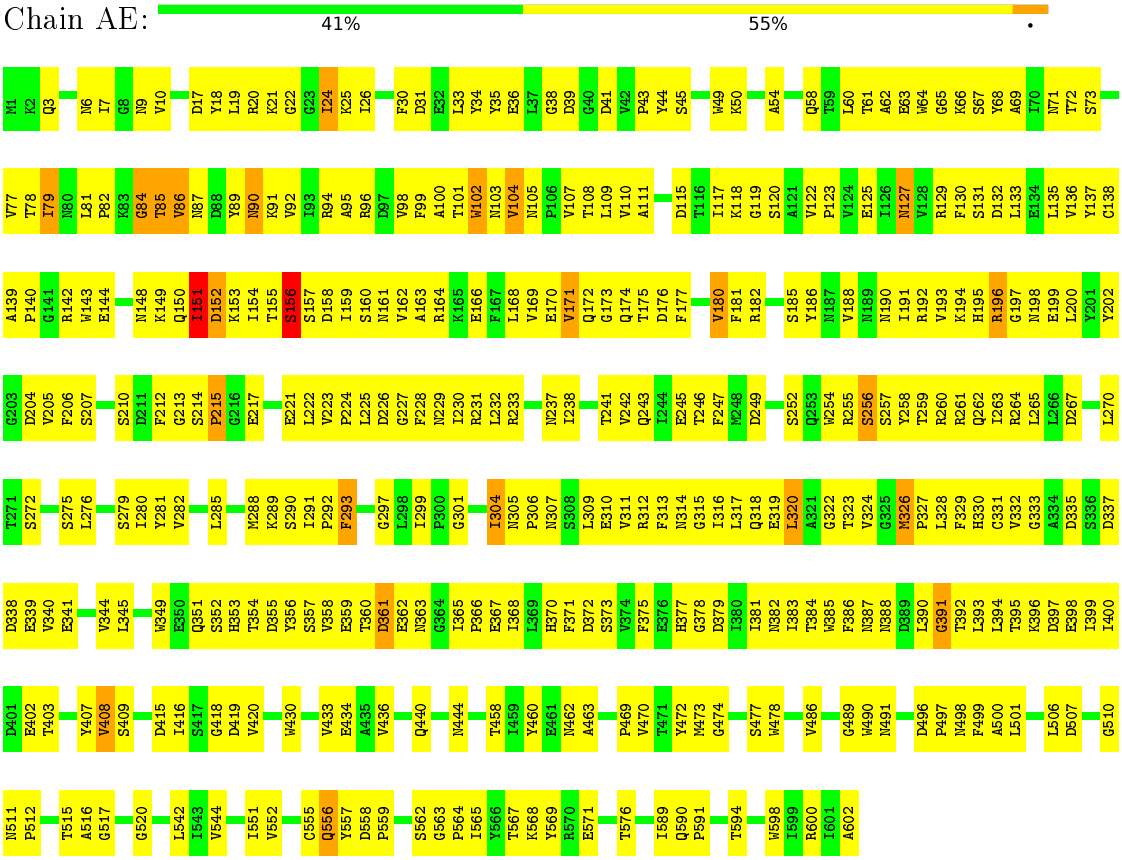
• Molecule 5: Baseplate wedge protein gp10

Chain AE:



• Molecule 5: Baseplate wedge protein gp10

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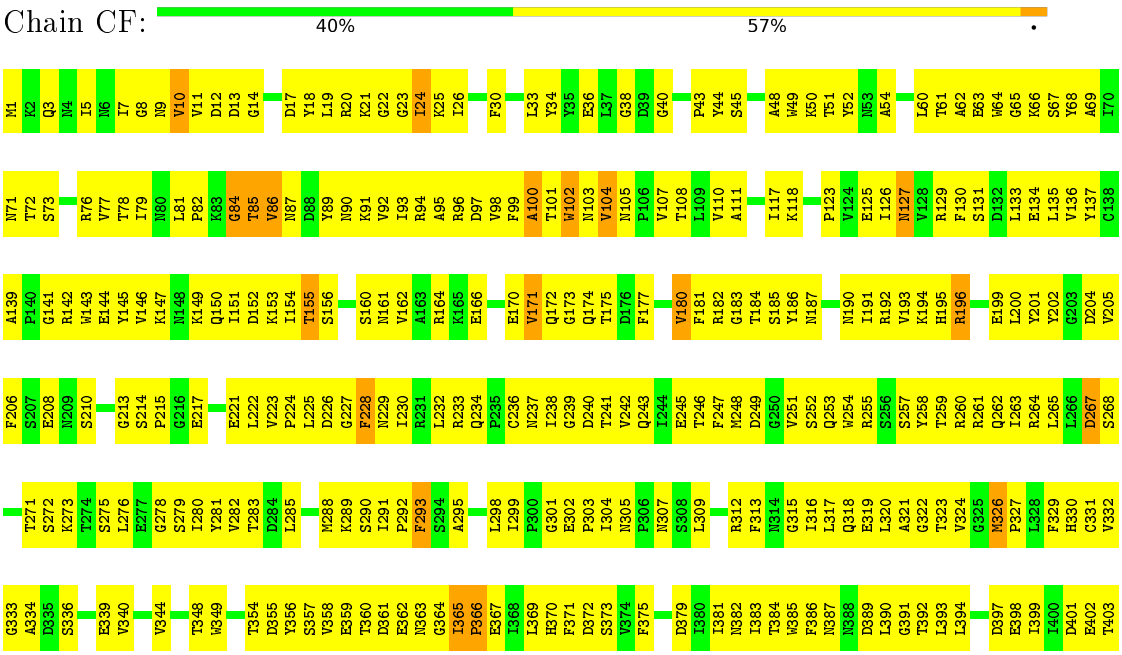

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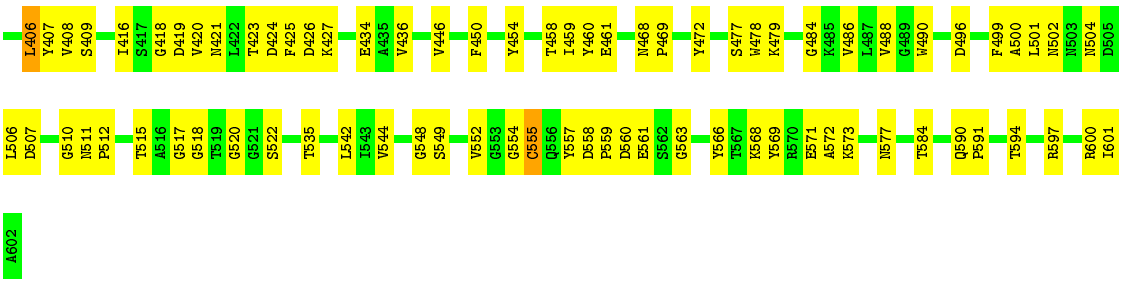
EMDataBank Unified Data Resource for 3DEM



• Molecule 5: Baseplate wedge protein gp10

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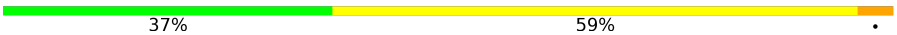
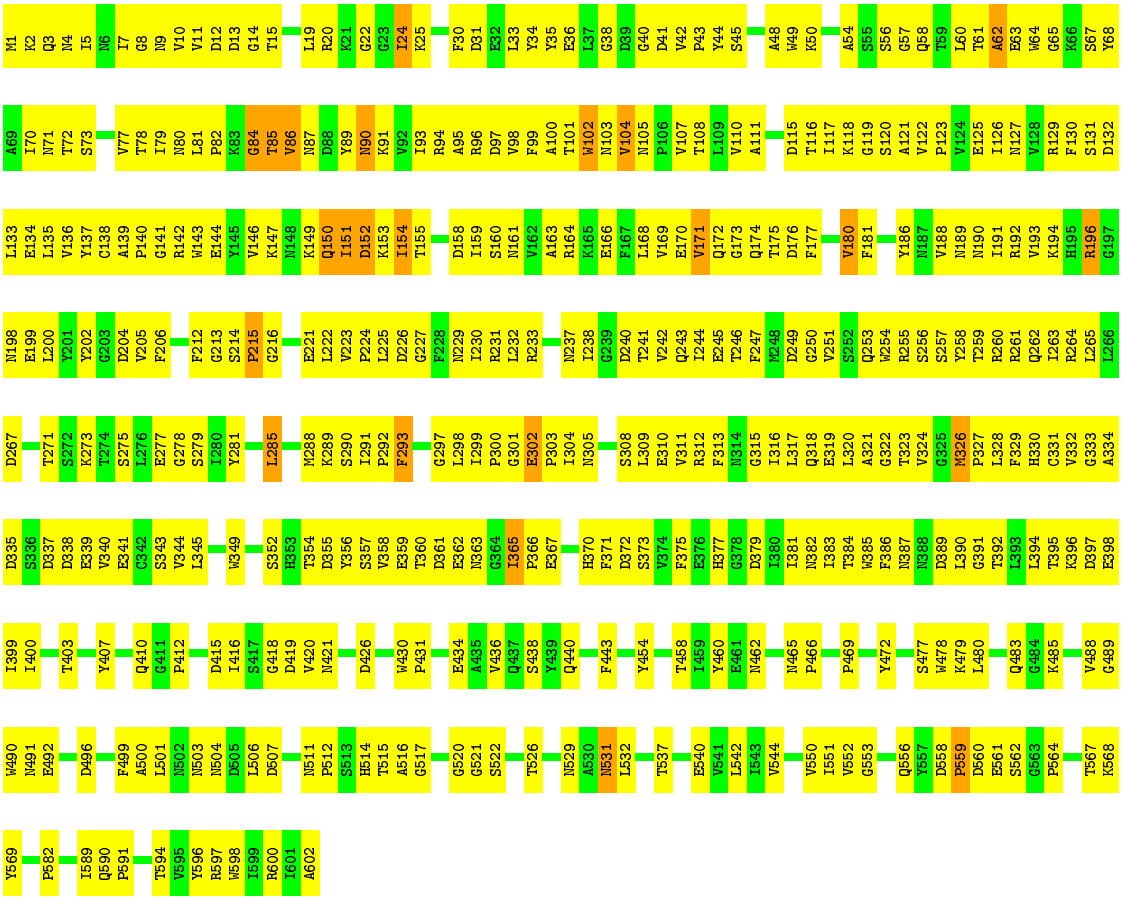
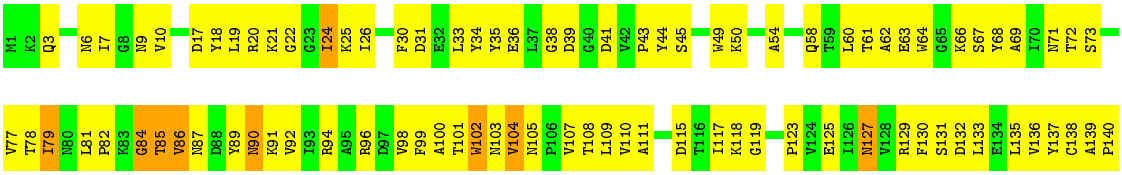




• Molecule 5: Baseplate wedge protein gp10

Chain CH:



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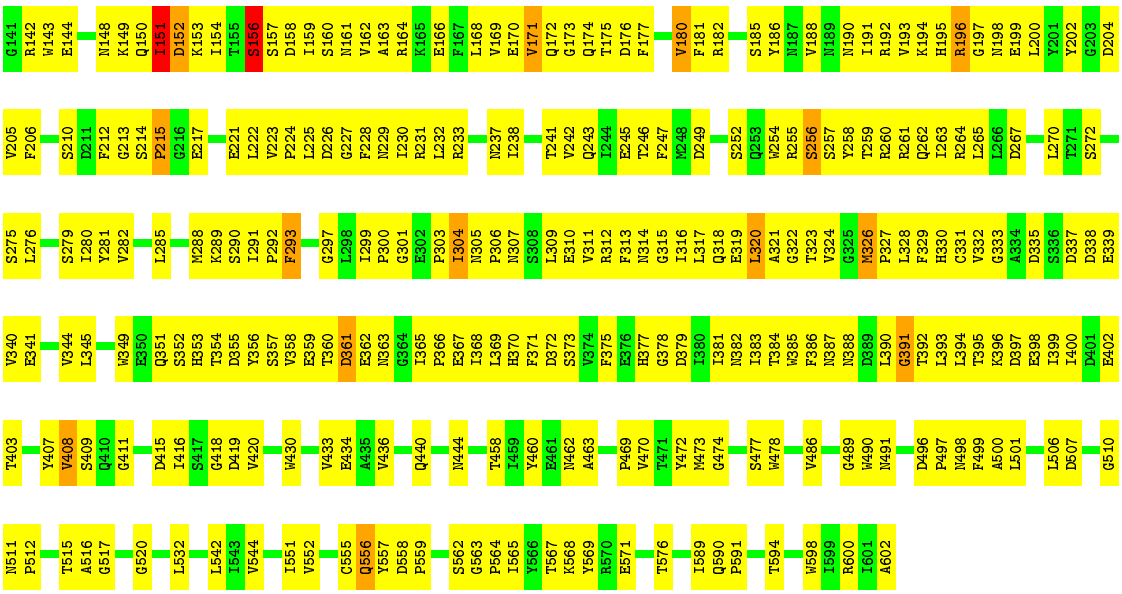
EMDataBank Unified Data Resource for 3DEM



• Molecule 5: Baseplate wedge protein gp10

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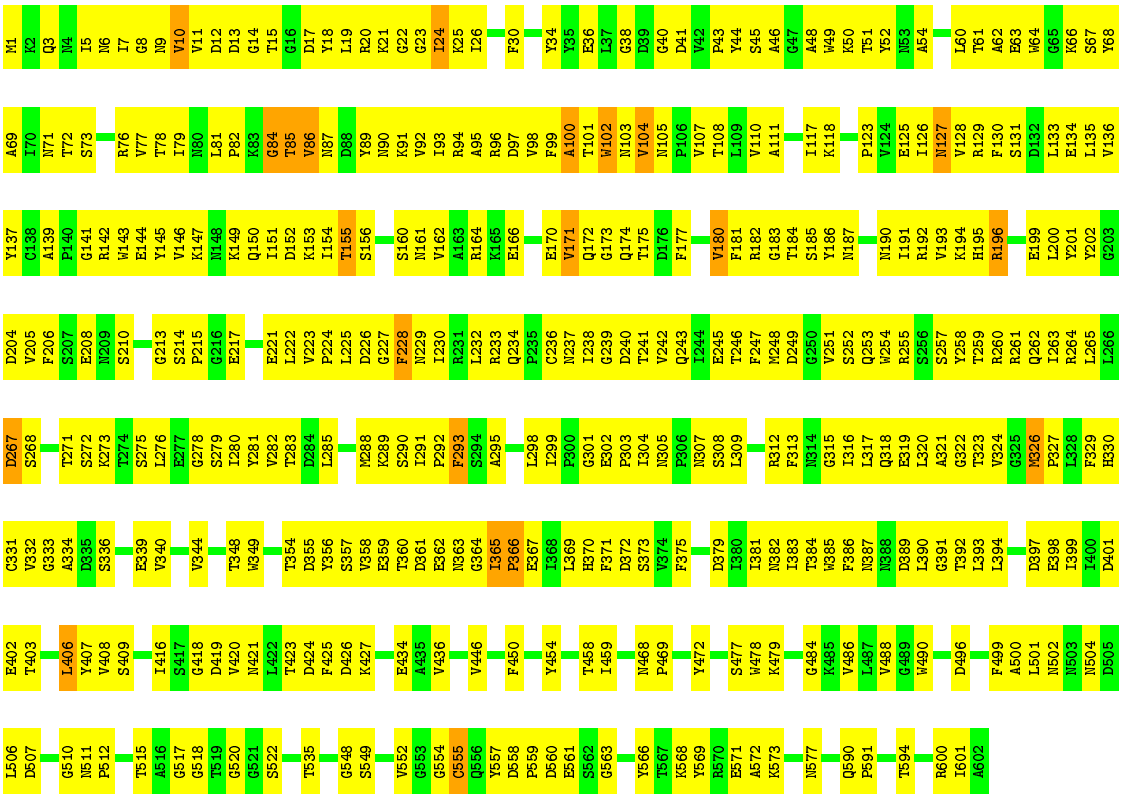

• Molecule 5: Baseplate wedge protein gp10

Chain EJ:

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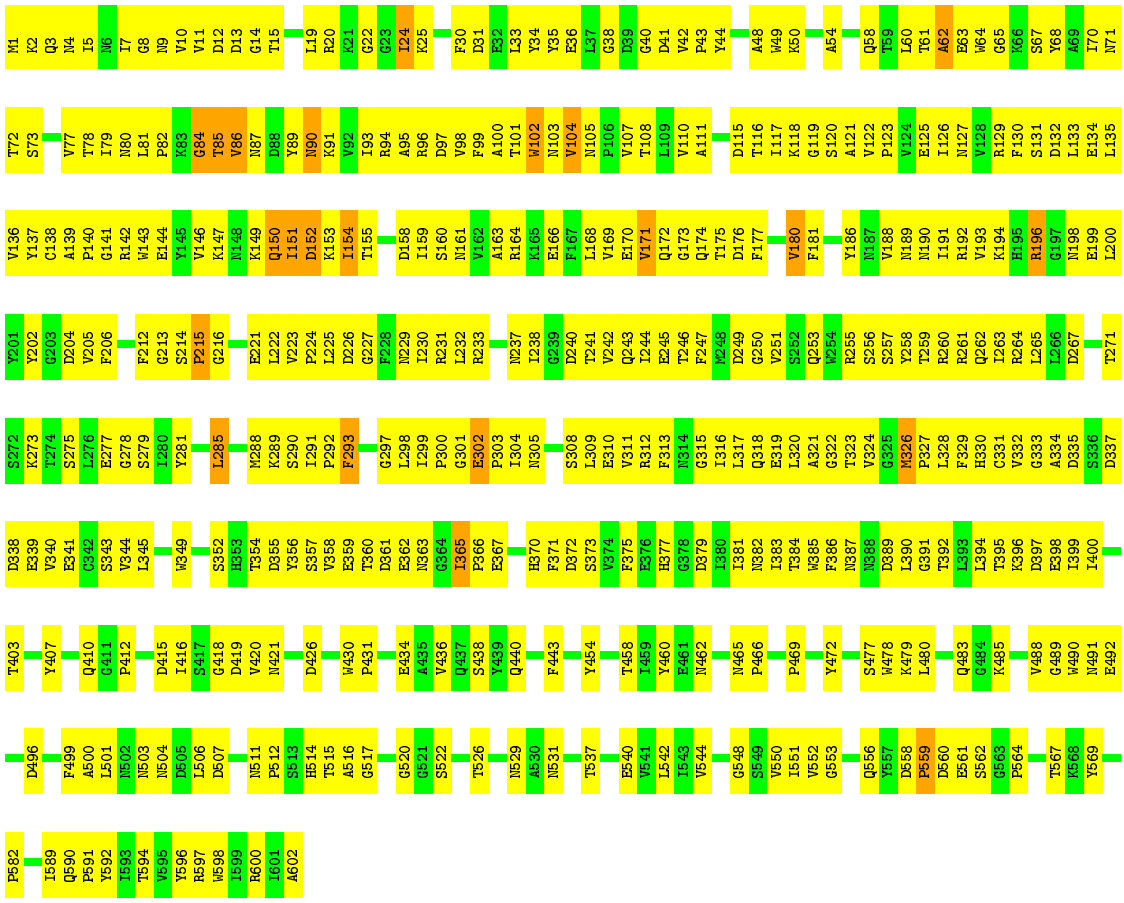
EMDataBank Unified Data Resource for 3DEM



• Molecule 5: Baseplate wedge protein gp10

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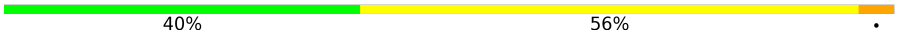

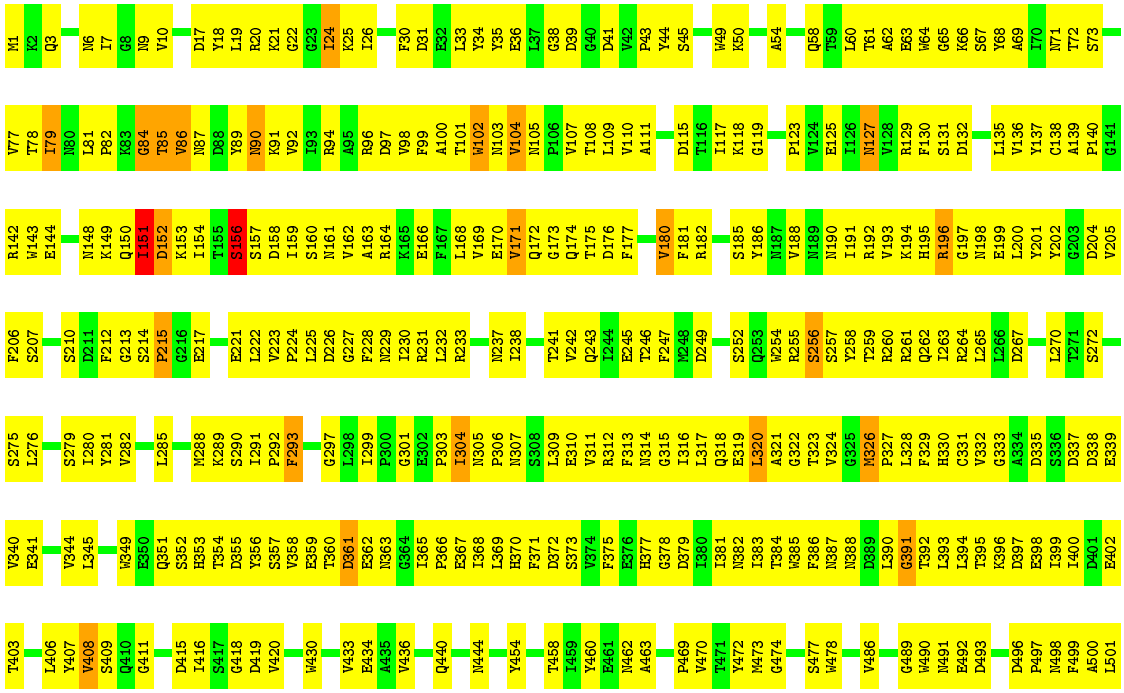

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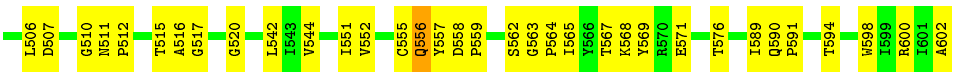

• Molecule 5: Baseplate wedge protein gp10

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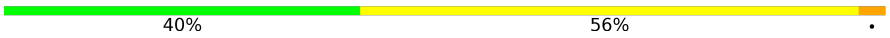

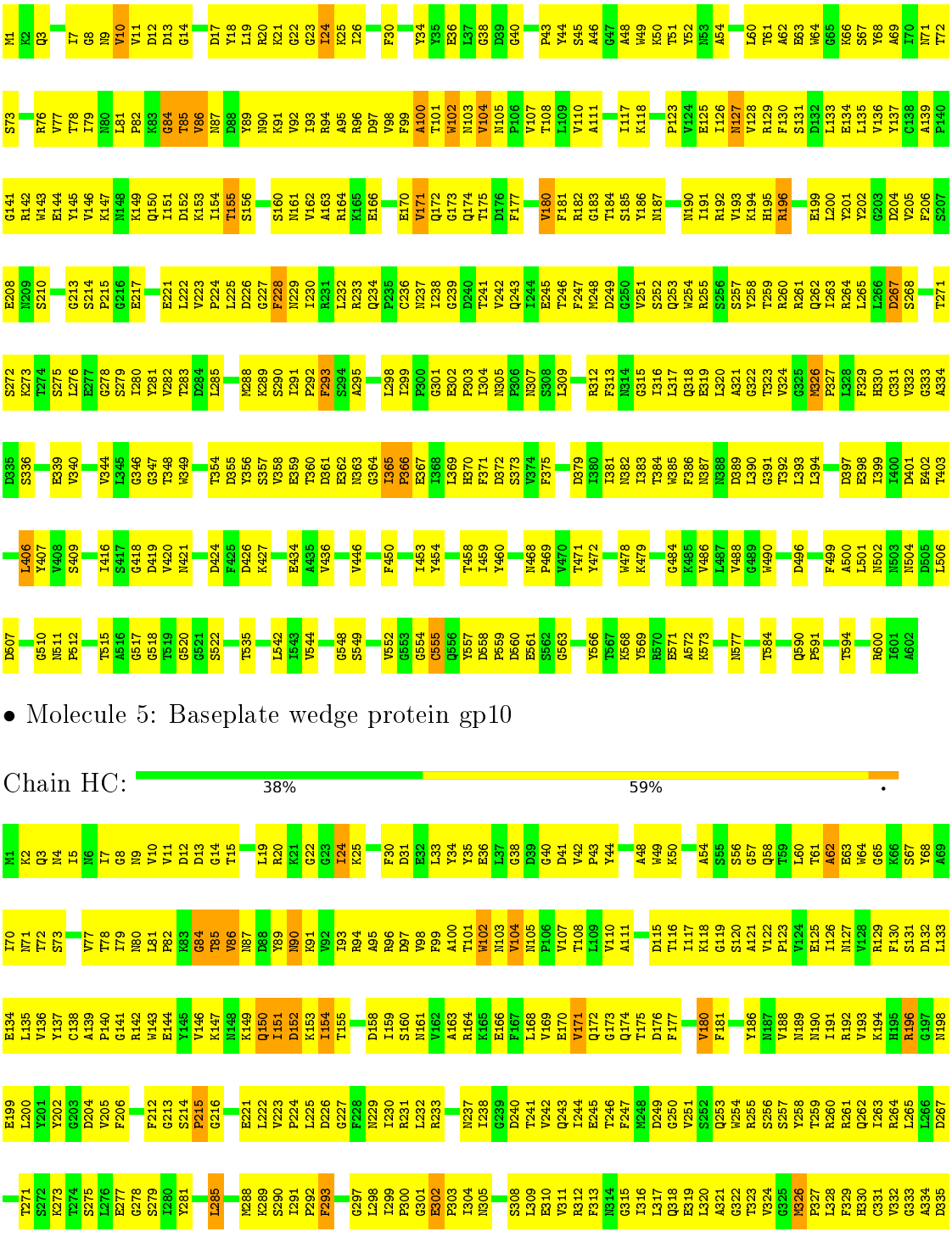

• Molecule 5: Baseplate wedge protein gp10

Chain HC:

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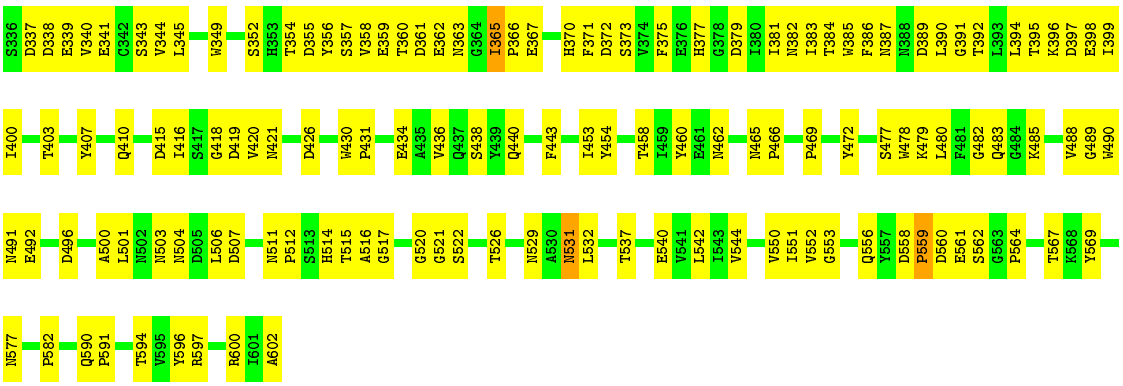
EMDataBank Unified Data Resource for 3DEM



• Molecule 5: Baseplate wedge protein gp10

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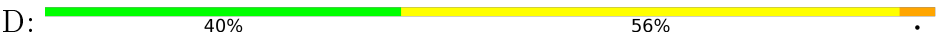

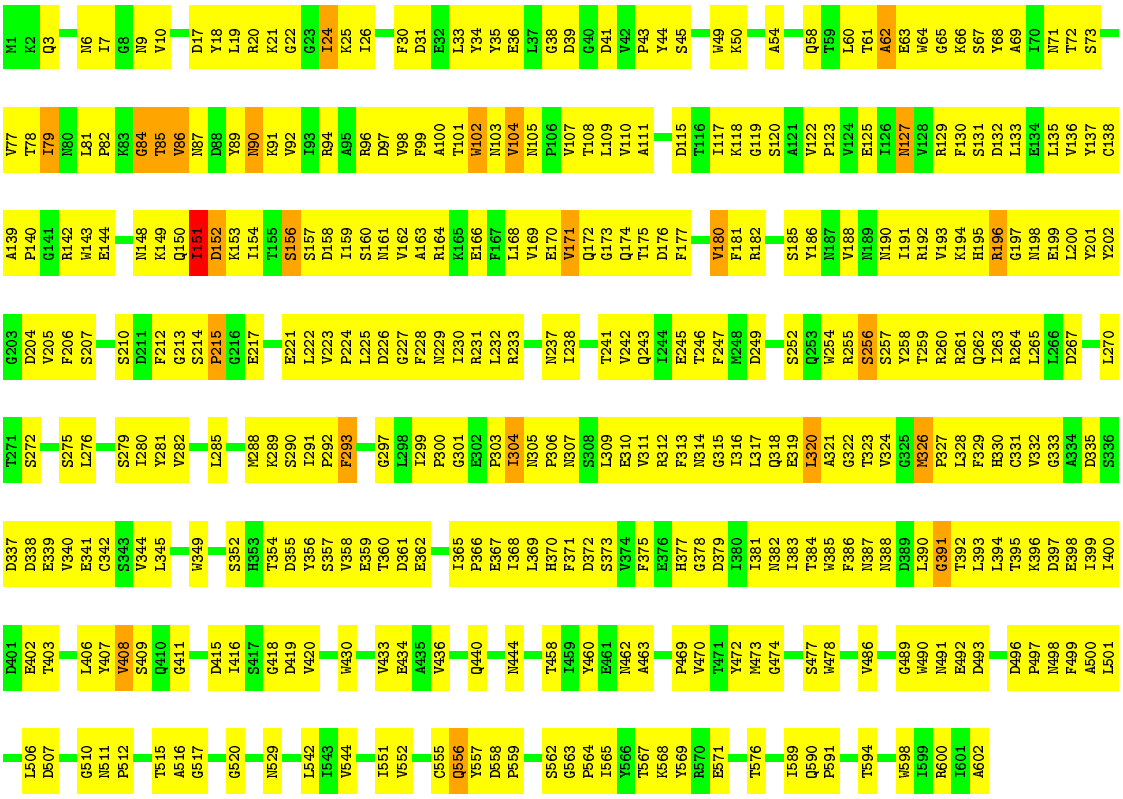

• Molecule 6: Baseplate wedge protein gp11

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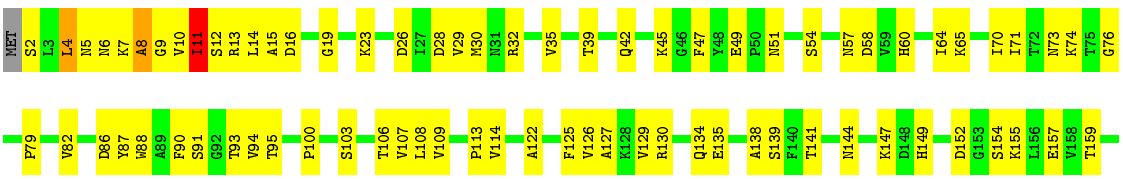

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EMDataBank Unified Data Resource for 3DEM

• Molecule 6: Baseplate wedge protein gp11

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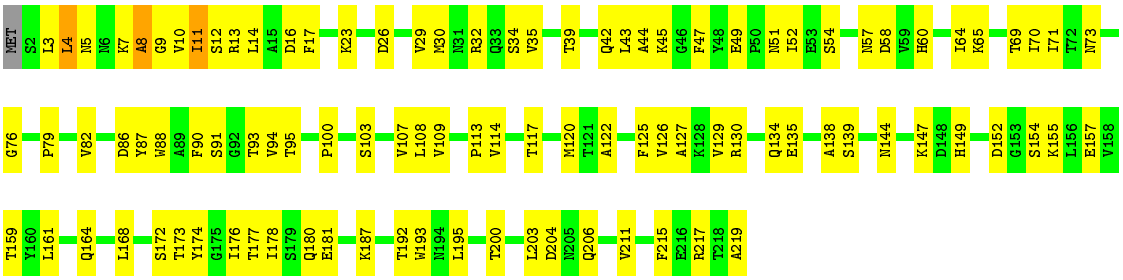

• Molecule 6: Baseplate wedge protein gp11

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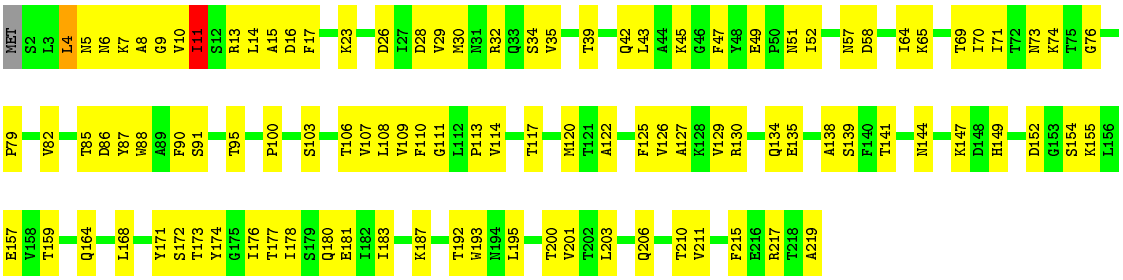

• Molecule 6: Baseplate wedge protein gp11

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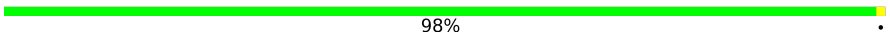

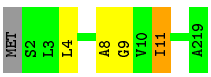

• Molecule 6: Baseplate wedge protein gp11

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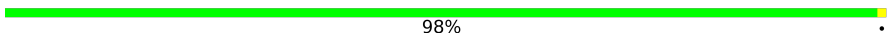

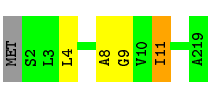

• Molecule 6: Baseplate wedge protein gp11

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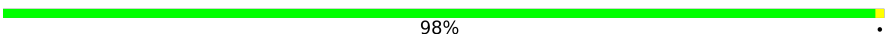

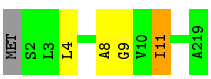

• Molecule 6: Baseplate wedge protein gp11

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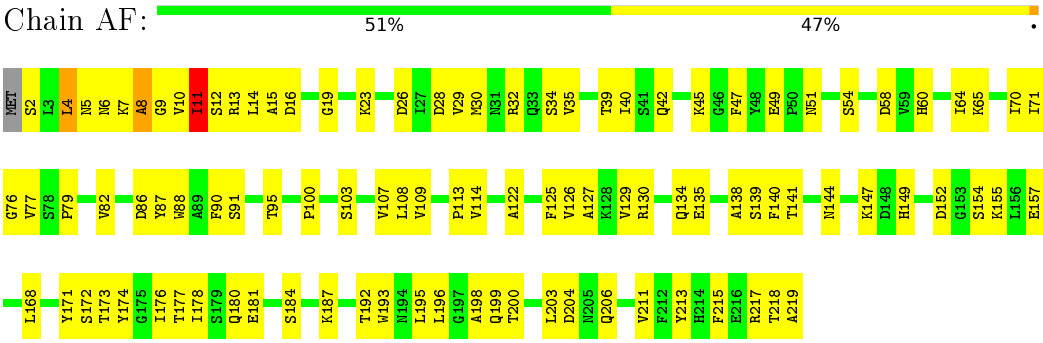

- Molecule 6: Baseplate wedge protein gp11

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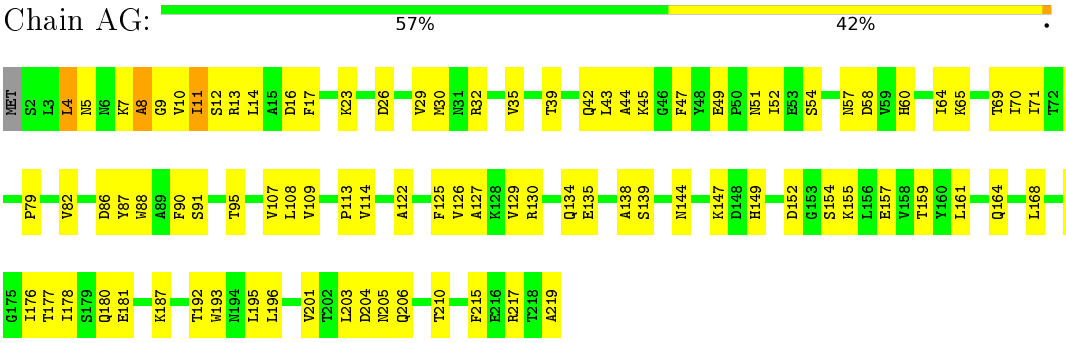

- Molecule 6: Baseplate wedge protein gp11

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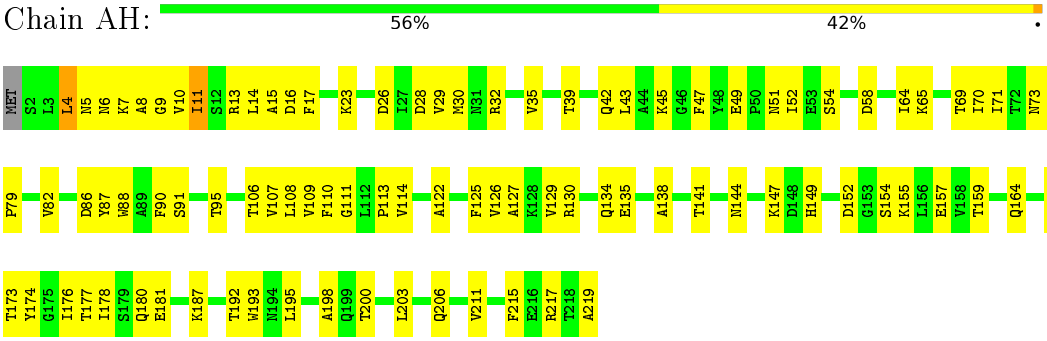

- Molecule 6: Baseplate wedge protein gp11

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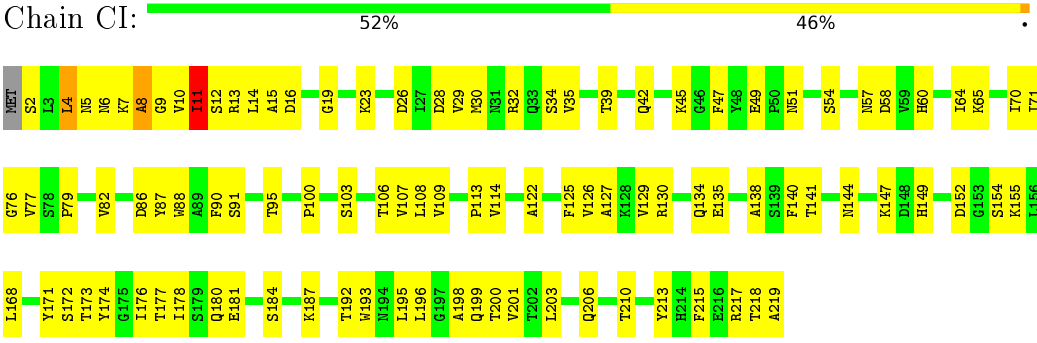

- Molecule 6: Baseplate wedge protein gp11

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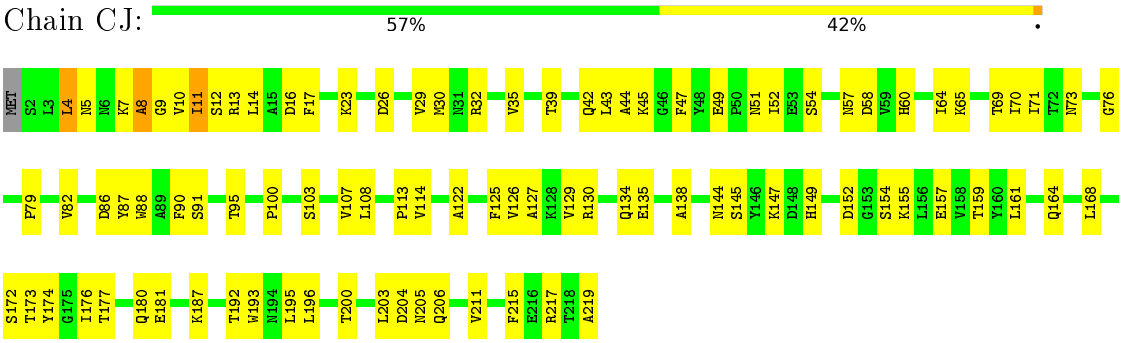

- Molecule 6: Baseplate wedge protein gp11

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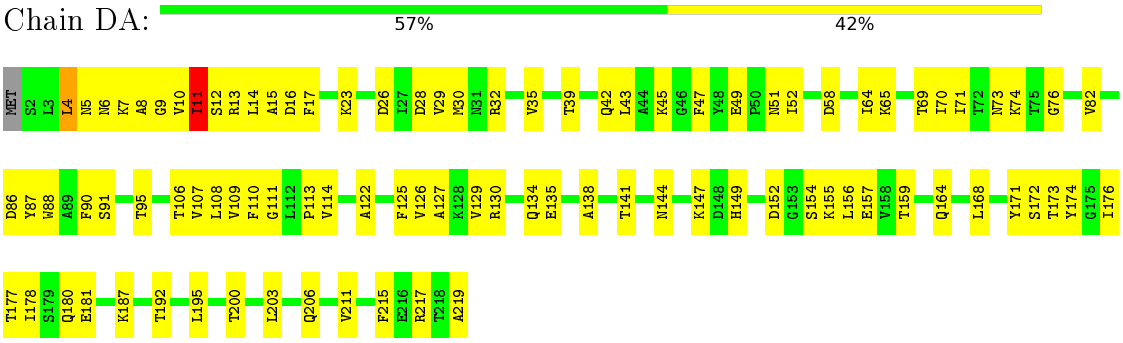

- Molecule 6: Baseplate wedge protein gp11

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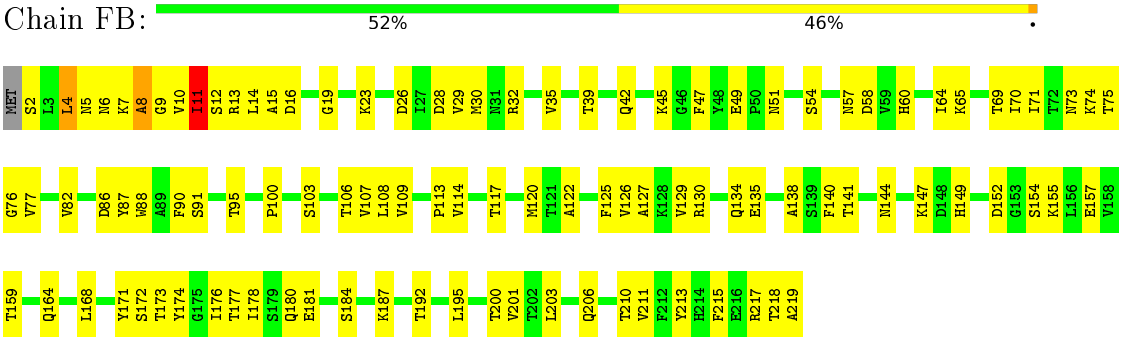

- Molecule 6: Baseplate wedge protein gp11

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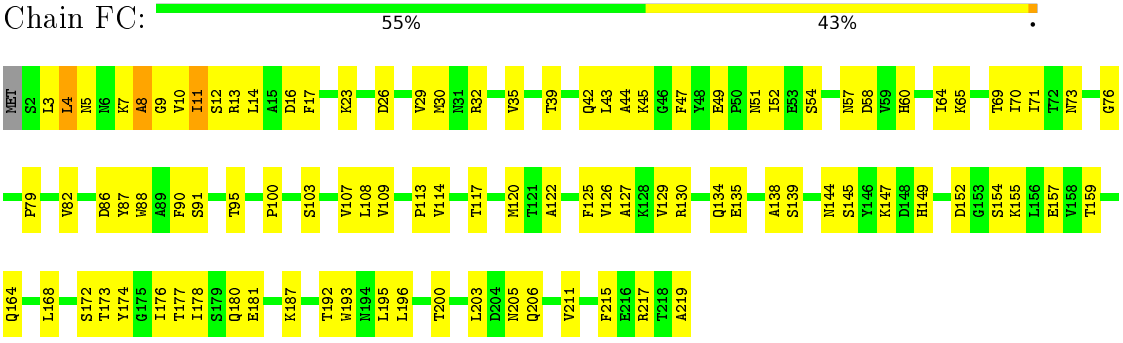

- Molecule 6: Baseplate wedge protein gp11

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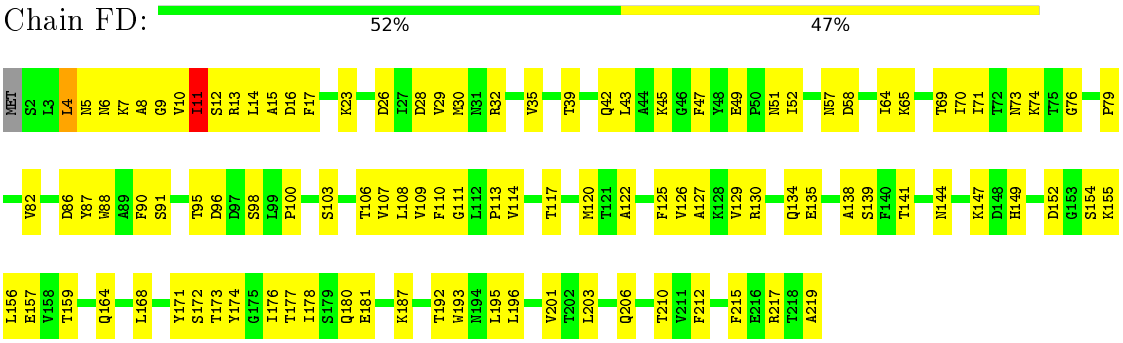

• Molecule 6: Baseplate wedge protein gp11

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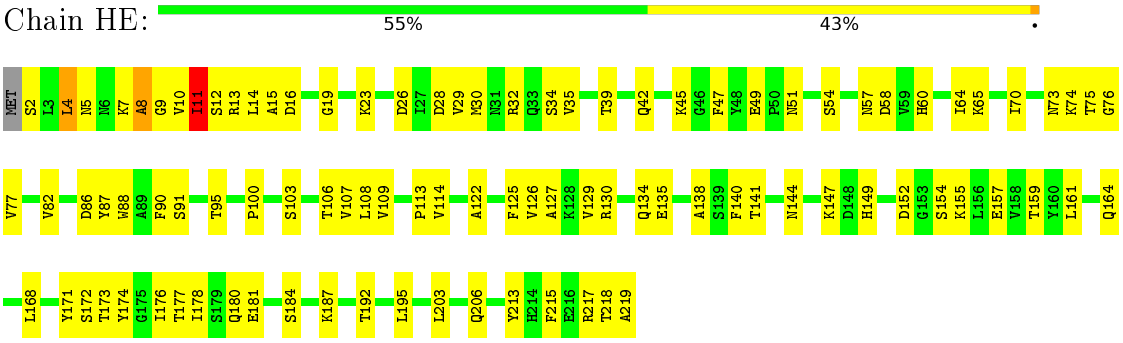

• Molecule 6: Baseplate wedge protein gp11

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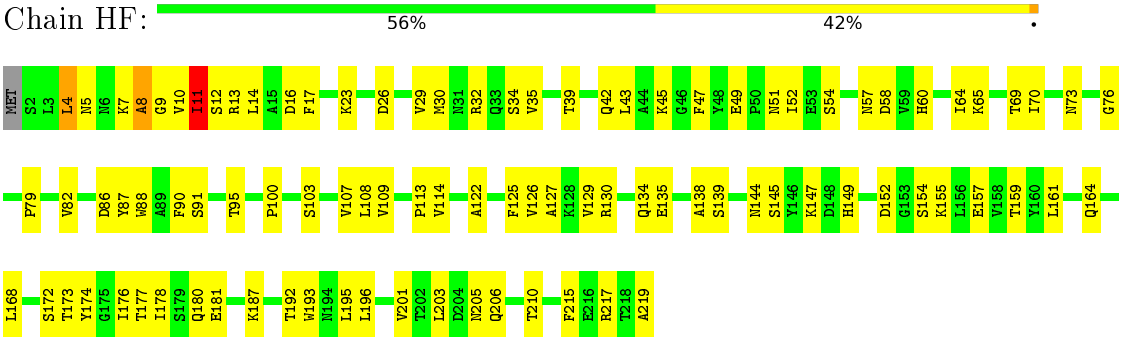

• Molecule 6: Baseplate wedge protein gp11

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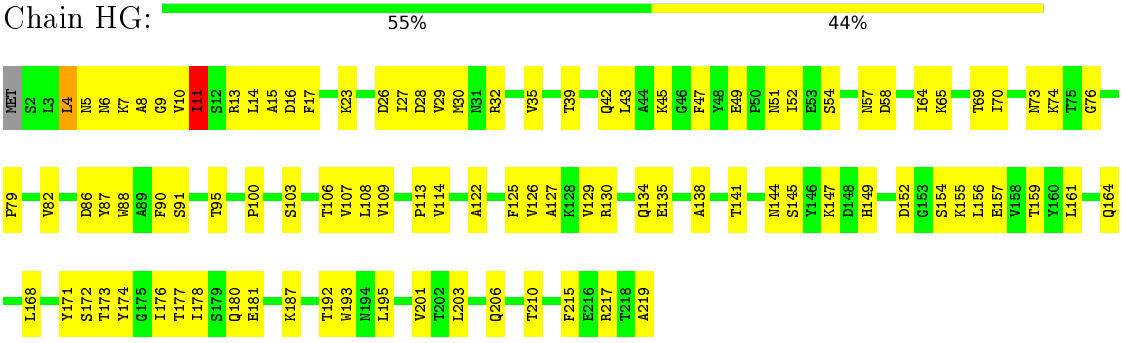

• Molecule 7: Short tail fiber protein gp12

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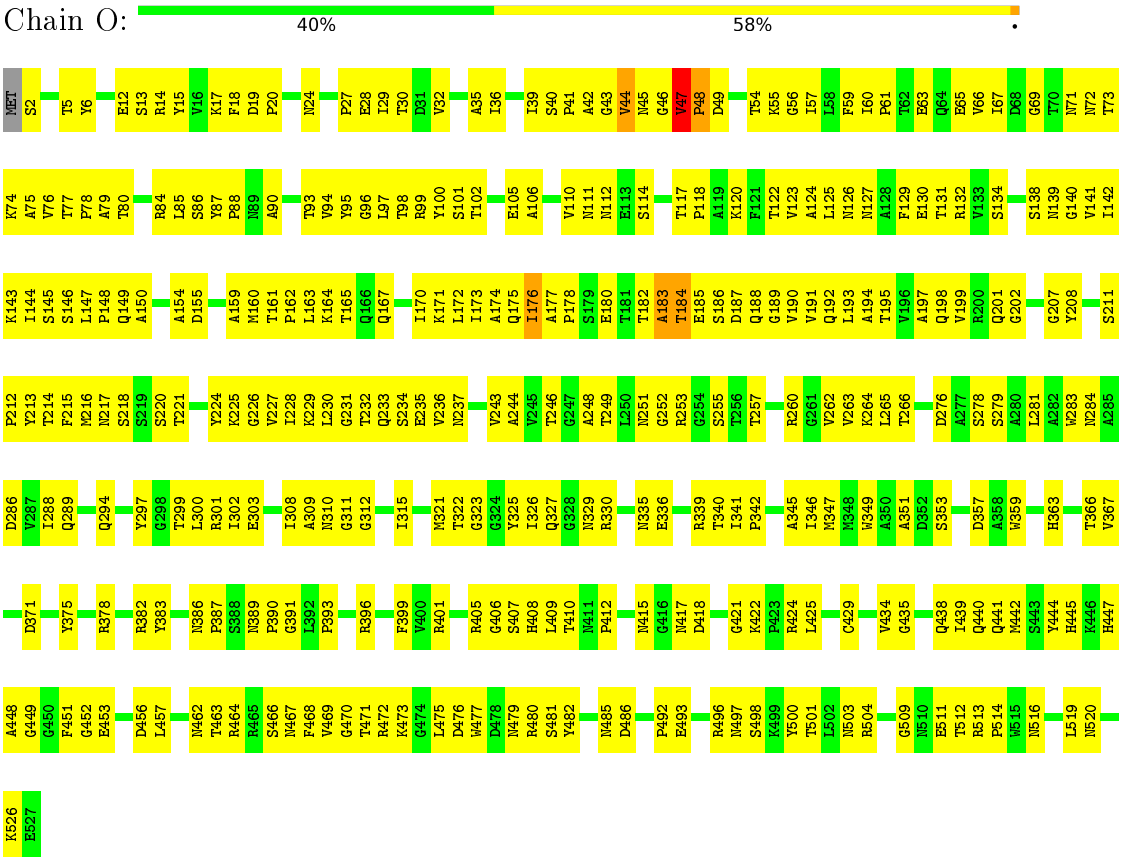

• Molecule 7: Short tail fiber protein gp12

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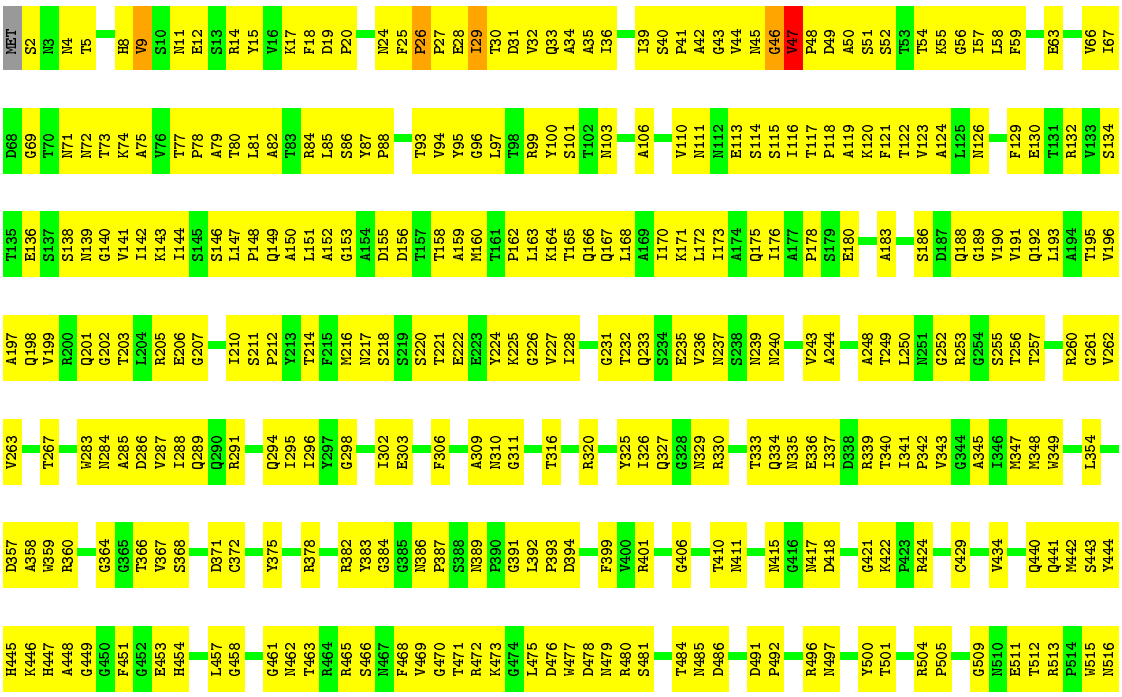

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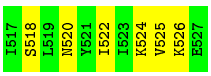

• Molecule 7: Short tail fiber protein gp12

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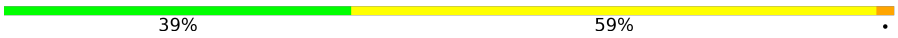

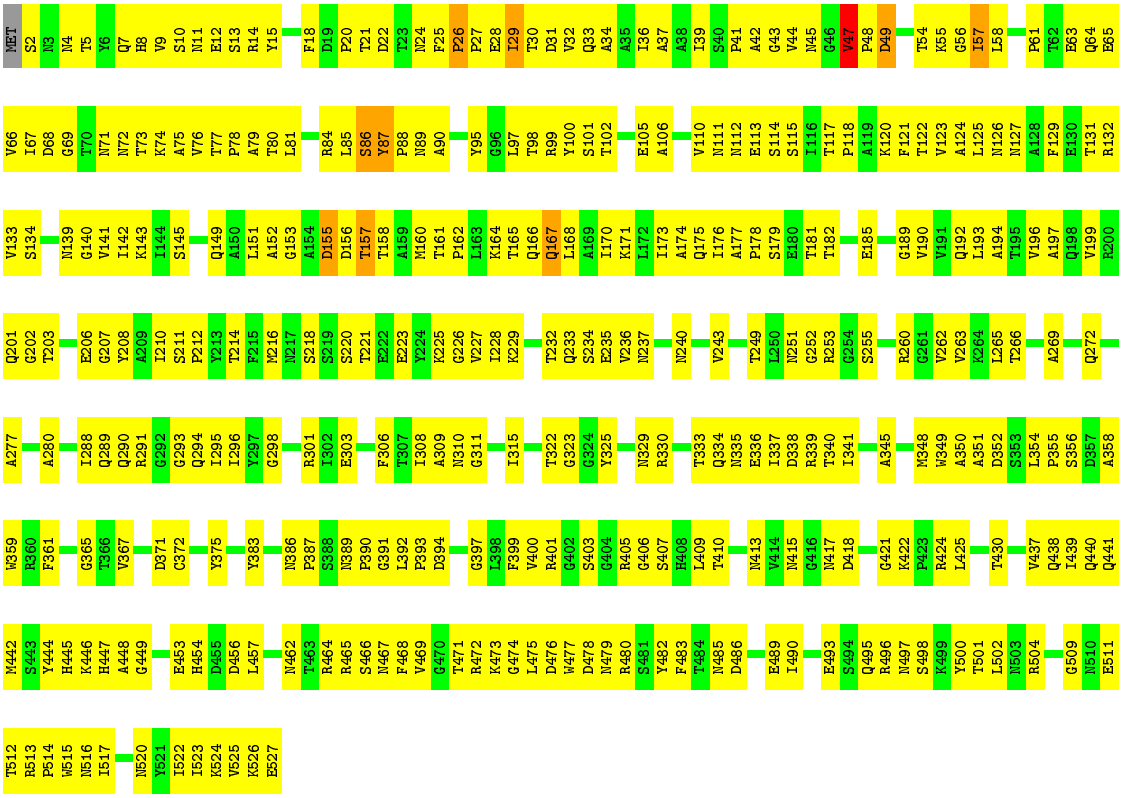

• Molecule 7: Short tail fiber protein gp12

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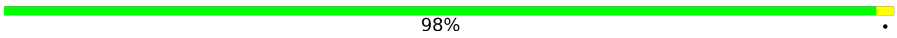

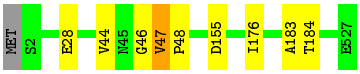

• Molecule 7: Short tail fiber protein gp12

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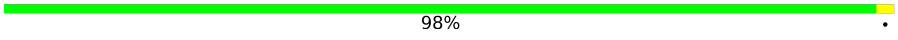

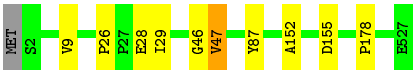

• Molecule 7: Short tail fiber protein gp12

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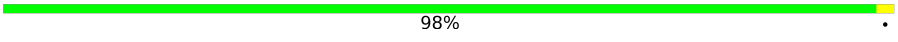

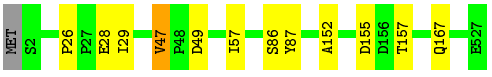

• Molecule 7: Short tail fiber protein gp12

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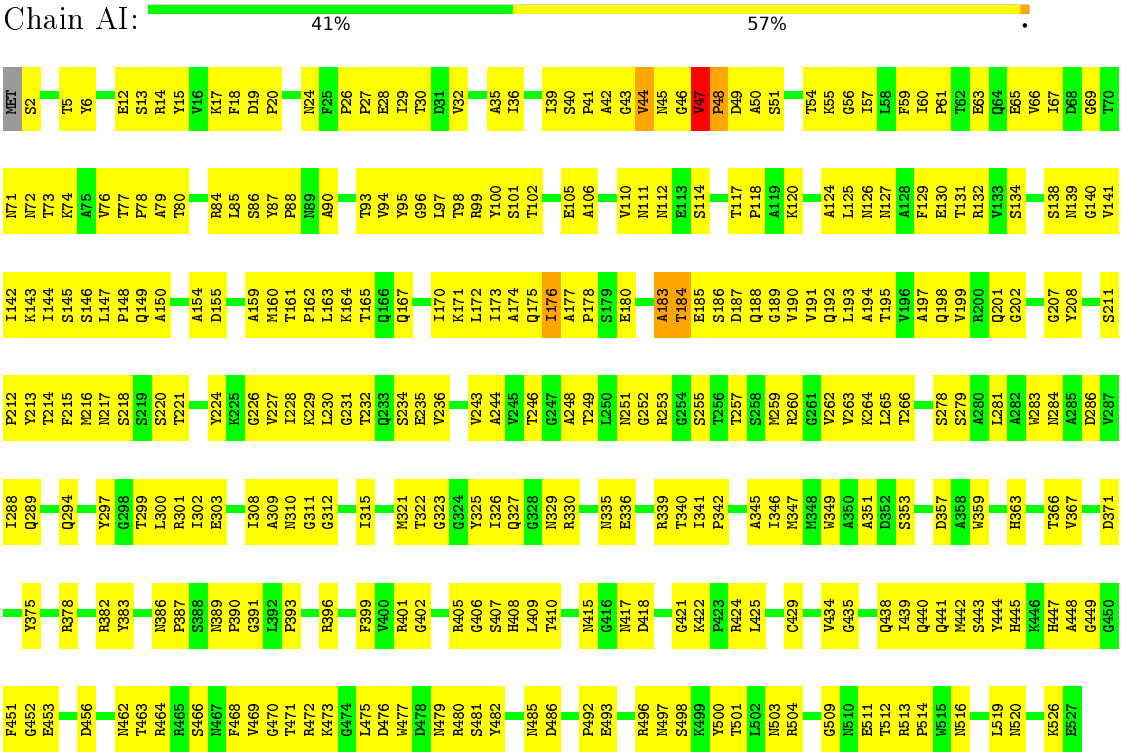

• Molecule 7: Short tail fiber protein gp12

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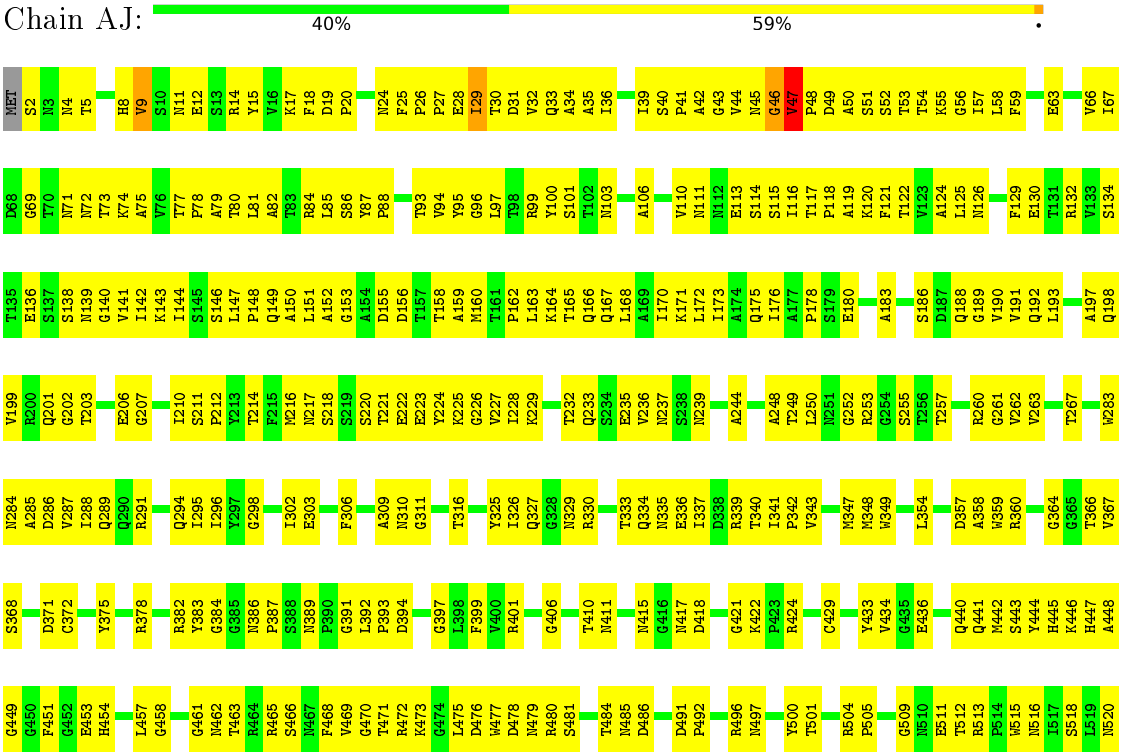

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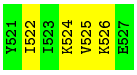

• Molecule 7: Short tail fiber protein gp12

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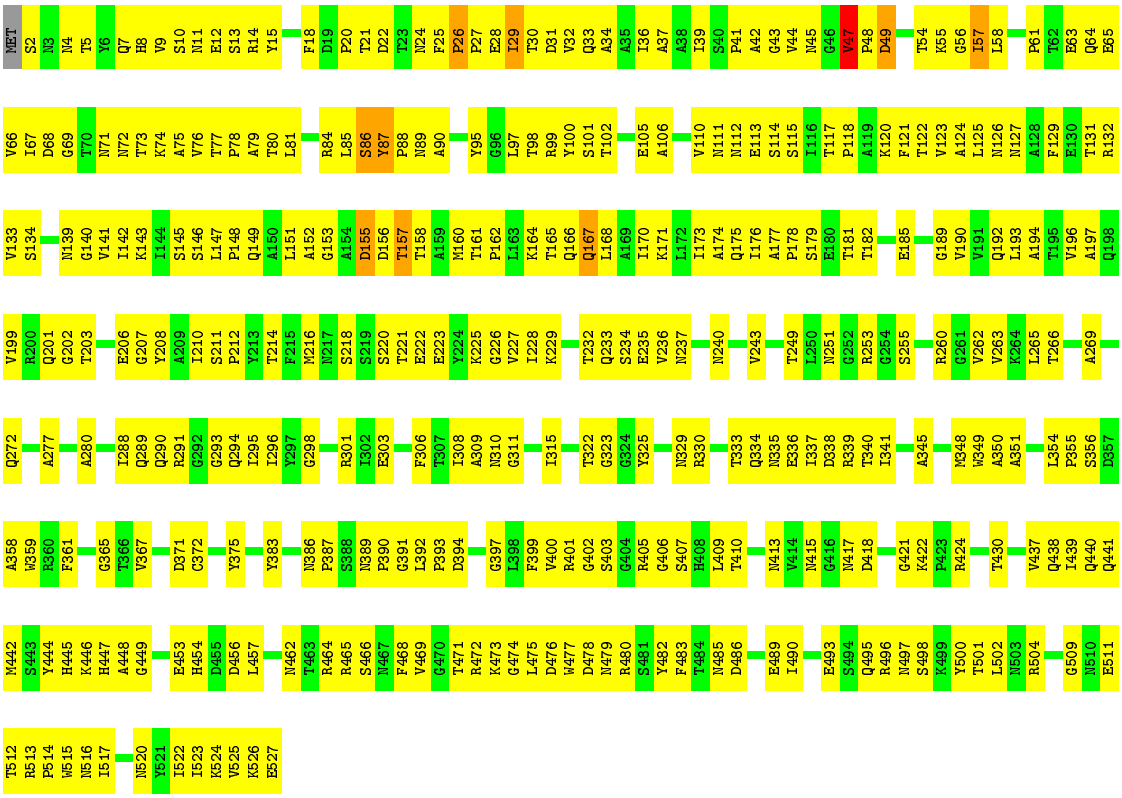

• Molecule 7: Short tail fiber protein gp12

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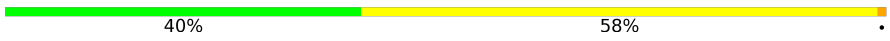

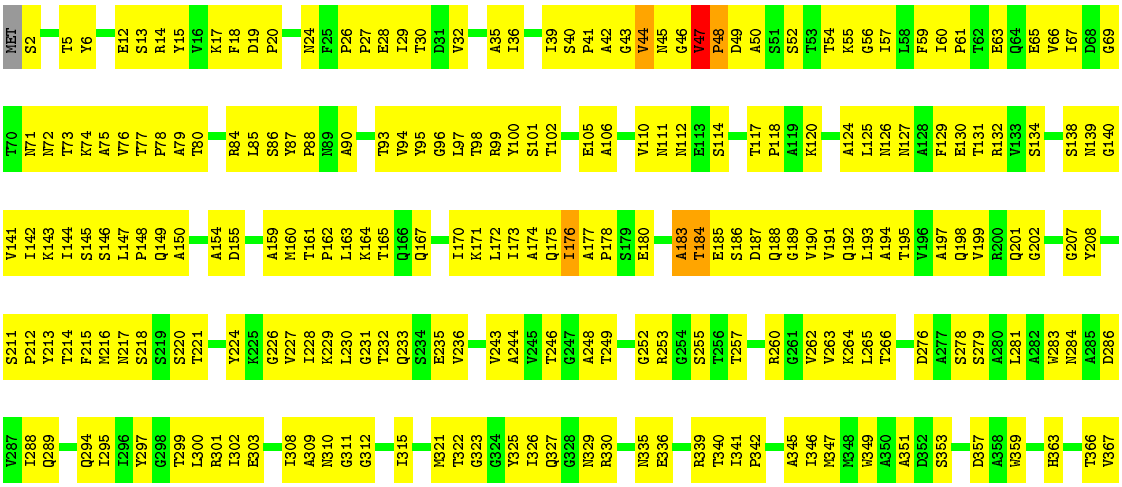

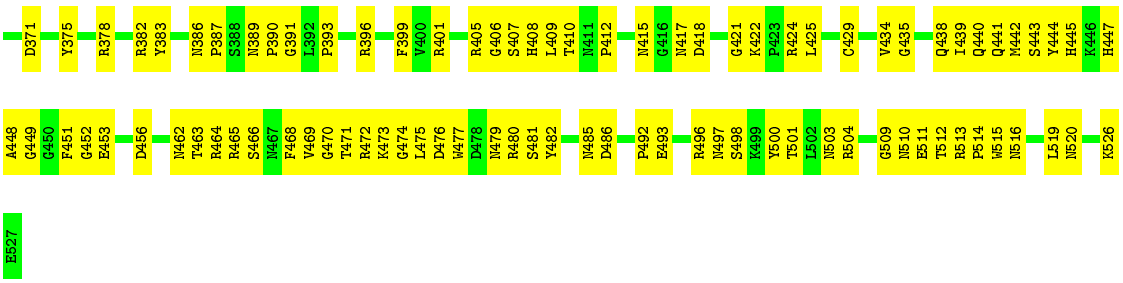

• Molecule 7: Short tail fiber protein gp12

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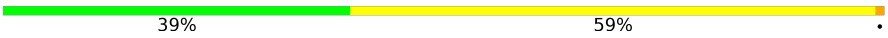
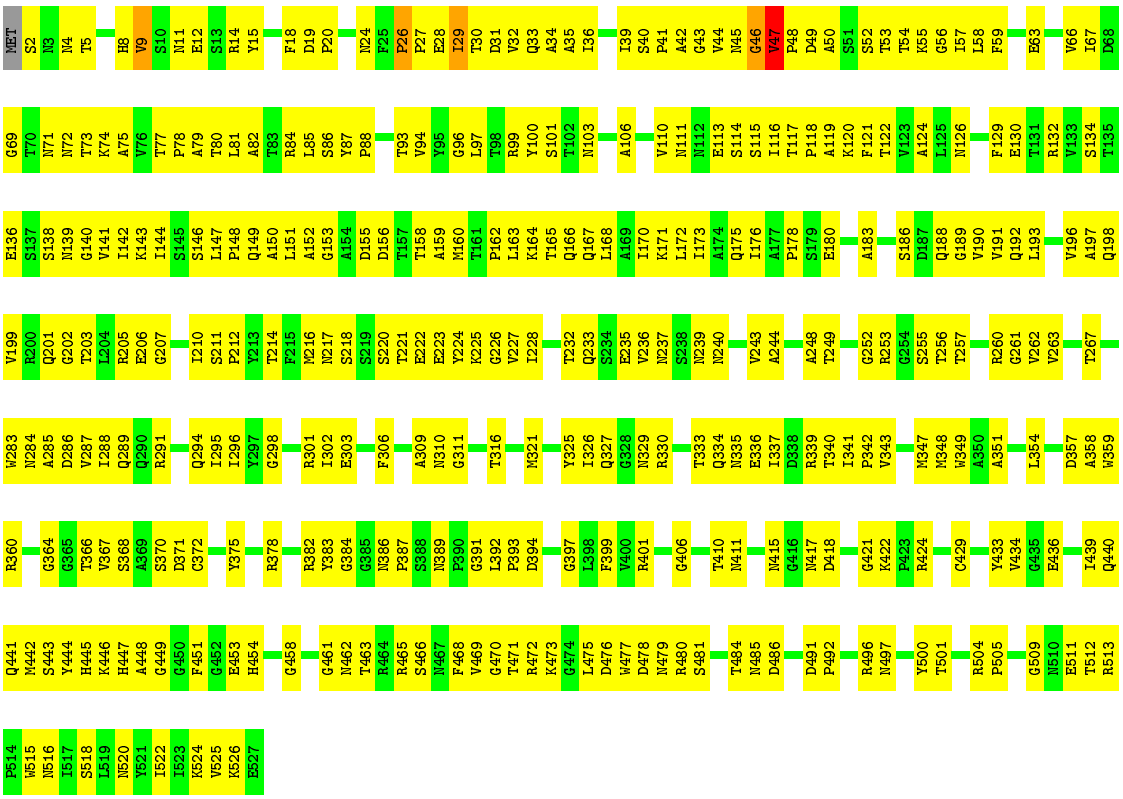
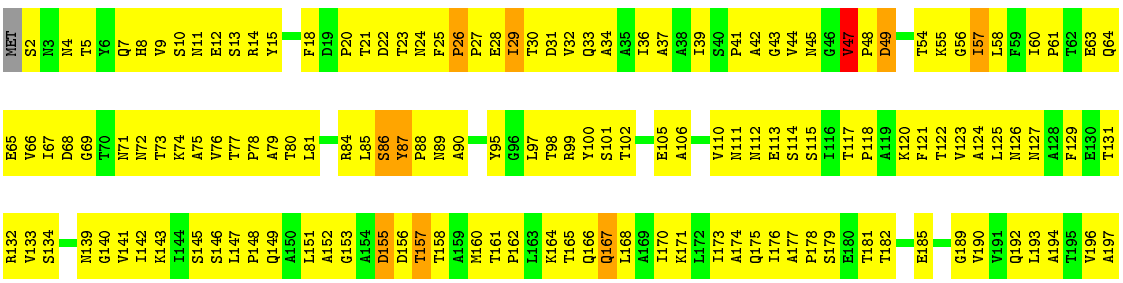


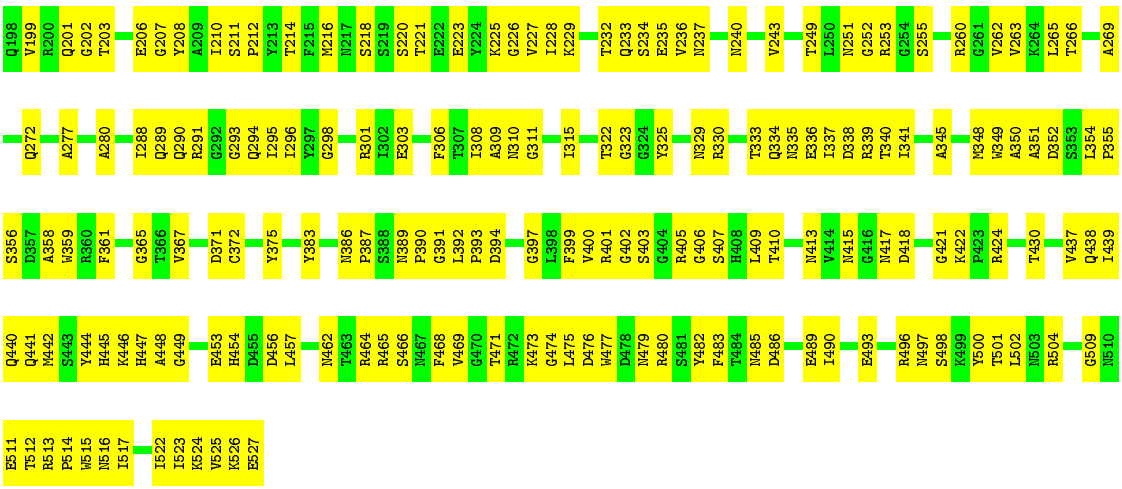


• Molecule 7: Short tail fiber protein gp12

Chain DD:



WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



- Molecule 7: Short tail fiber protein gp12

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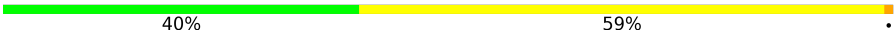

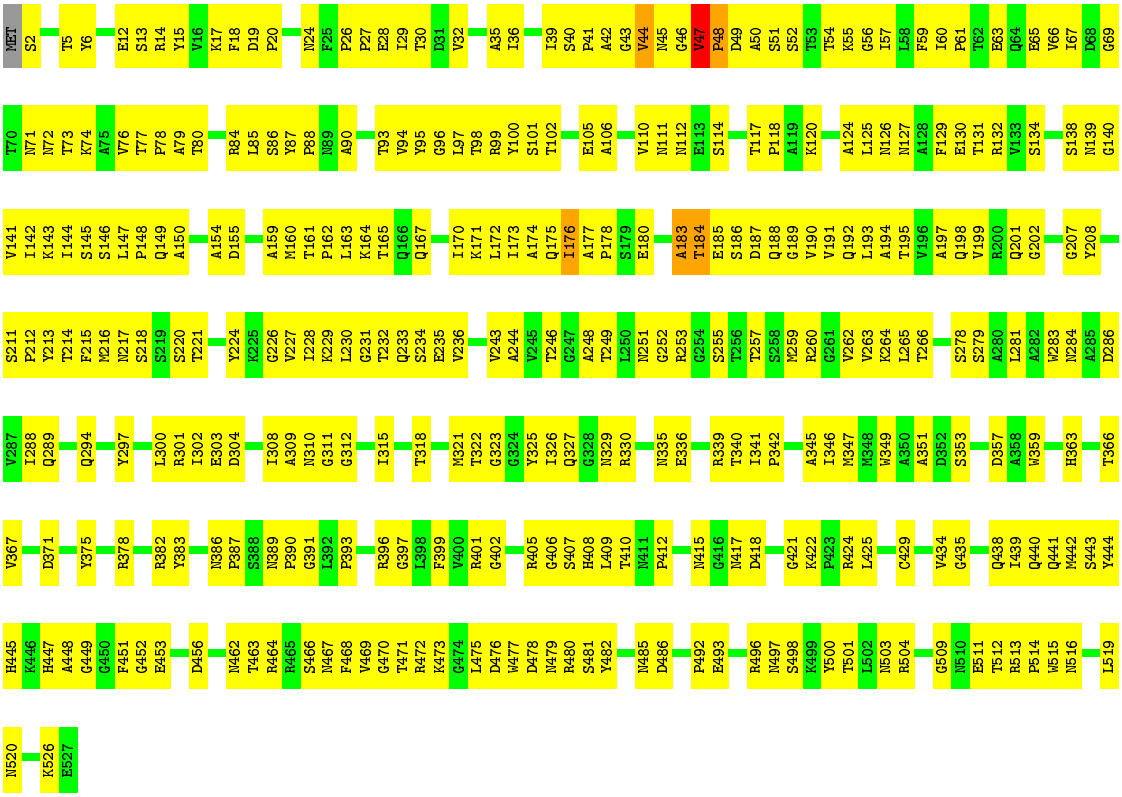

- Molecule 7: Short tail fiber protein gp12

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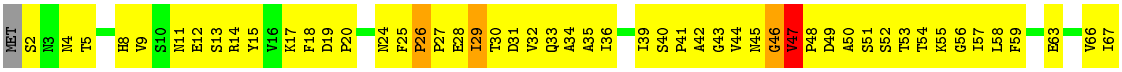
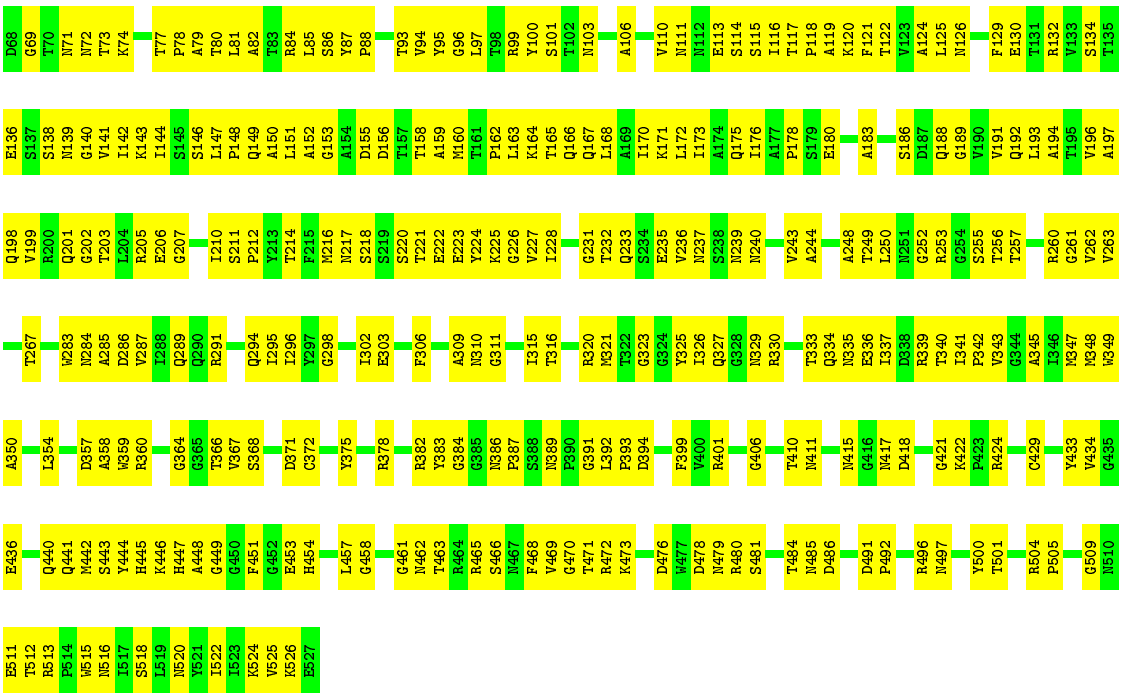
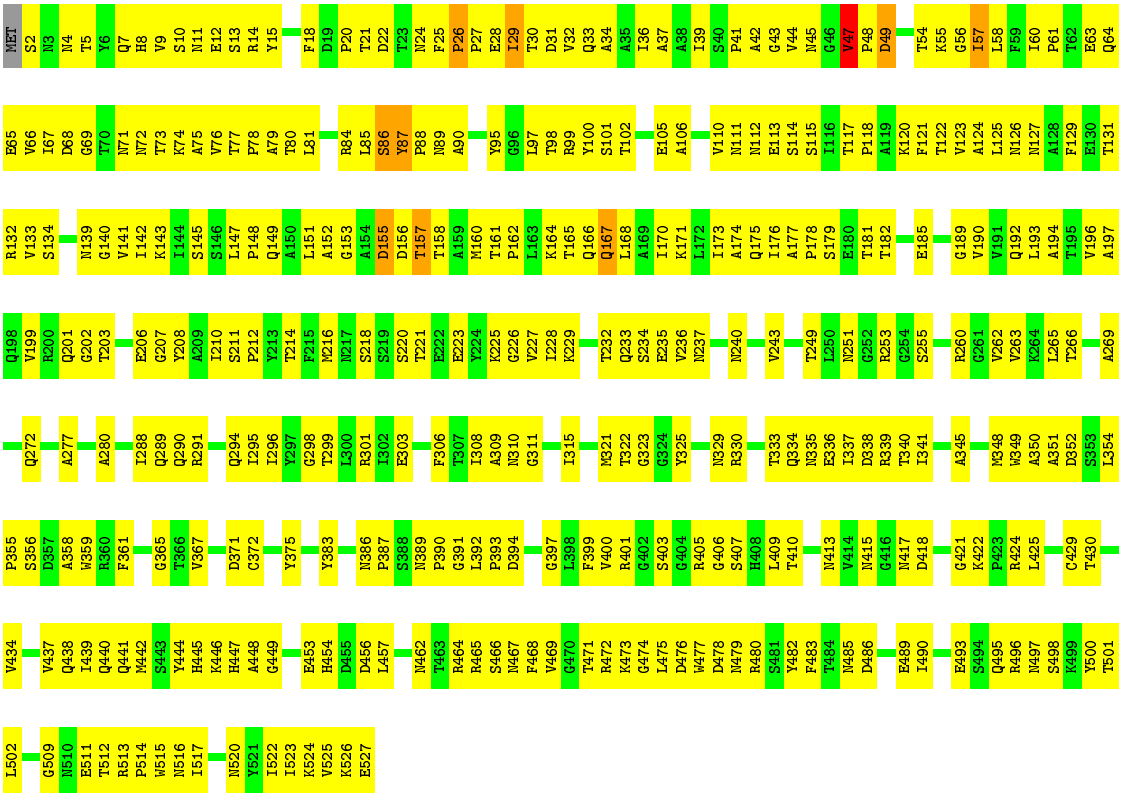




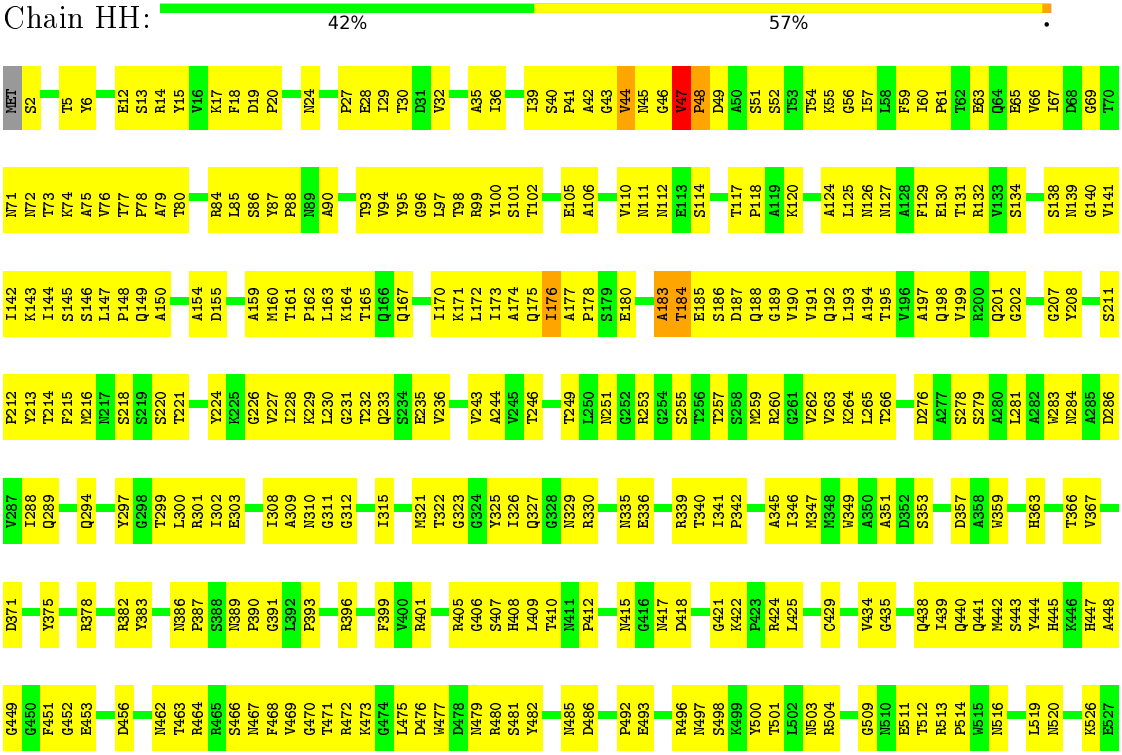
• Molecule 7: Short tail fiber protein gp12

Chain FG:



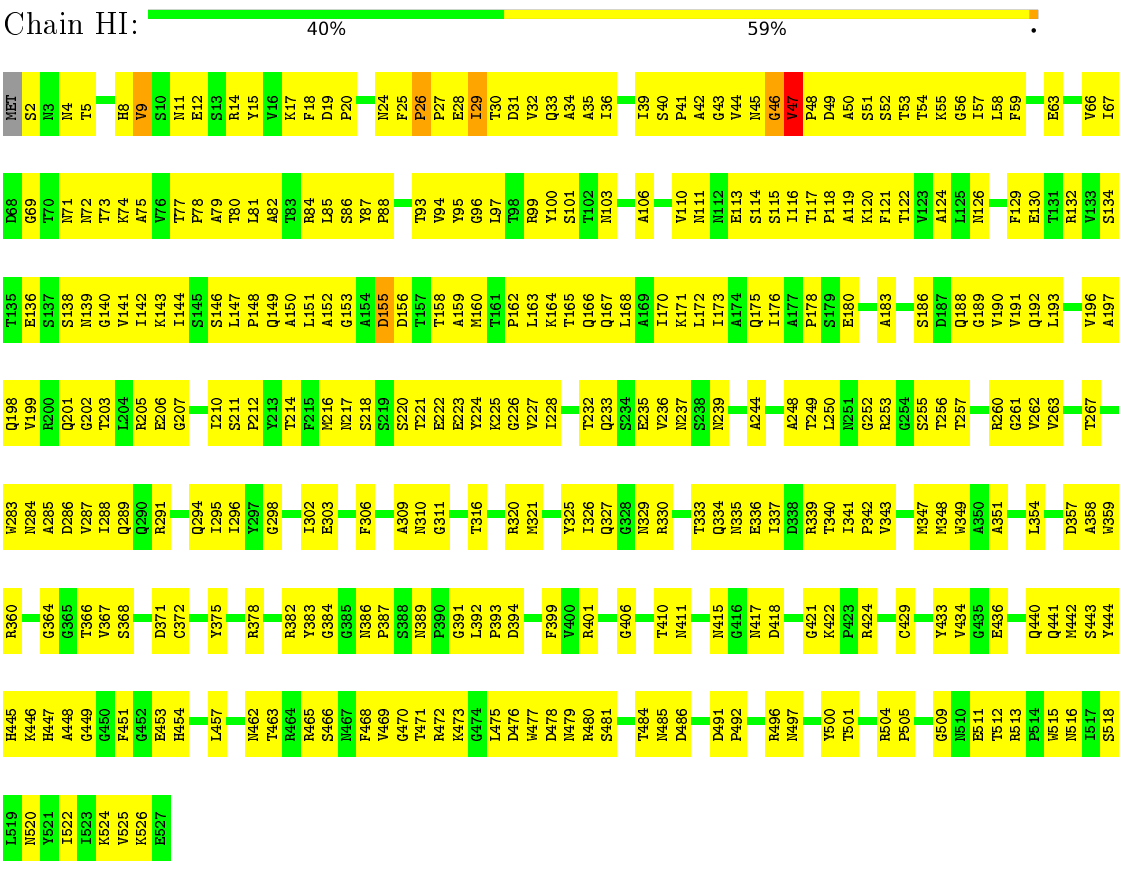
• Molecule 7: Short tail fiber protein gp12

Chain HH:



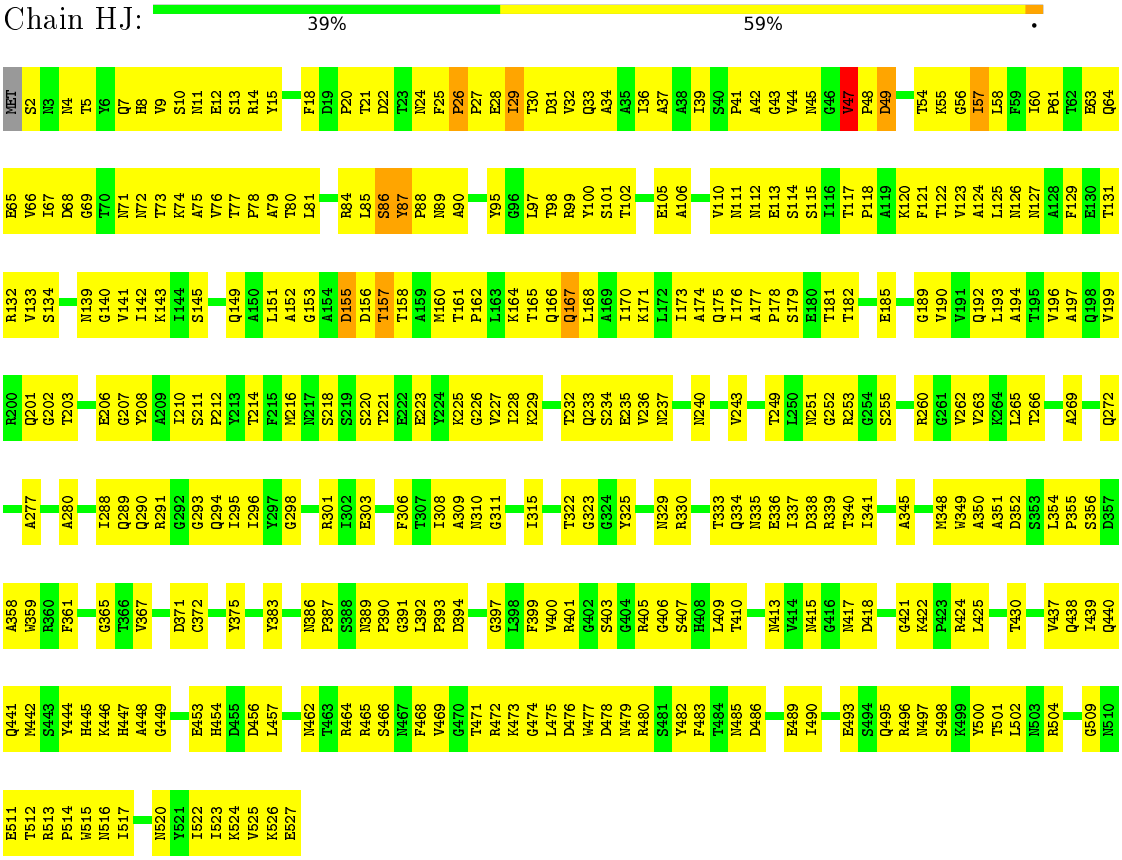
• Molecule 7: Short tail fiber protein gp12

Chain HI:



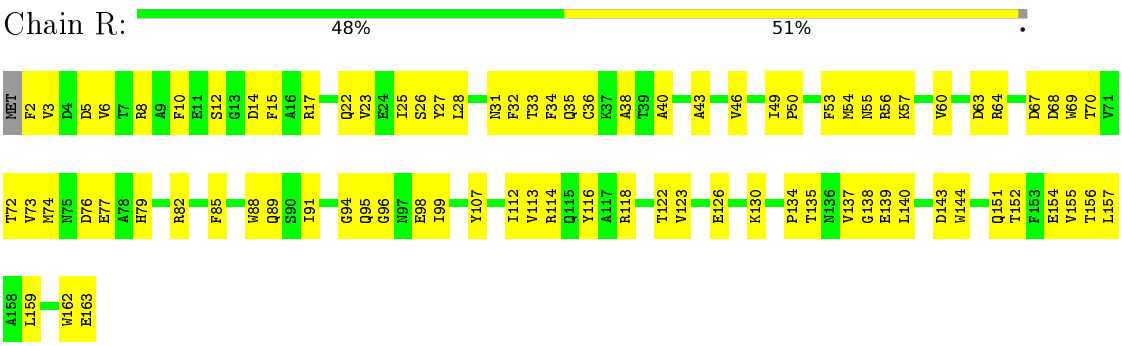
• Molecule 7: Short tail fiber protein gp12

Chain HJ:



• Molecule 8: Tail tube protein gp19

Chain R:



• Molecule 8: Tail tube protein gp19

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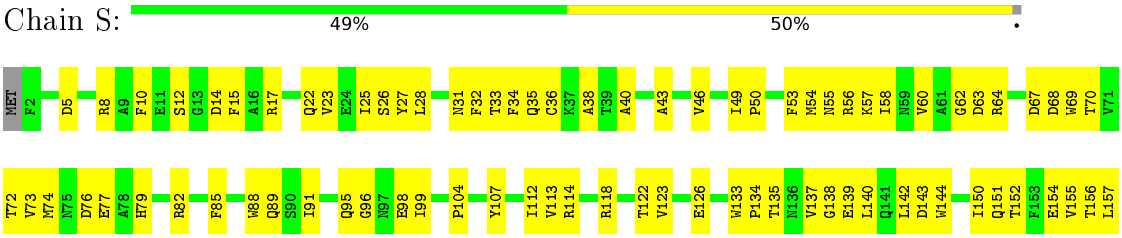
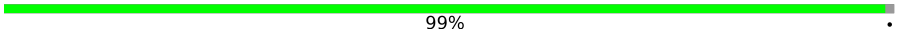


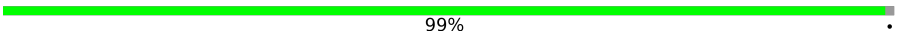
• Molecule 8: Tail tube protein gp19

Chain o:



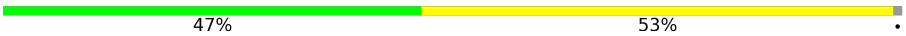
• Molecule 8: Tail tube protein gp19

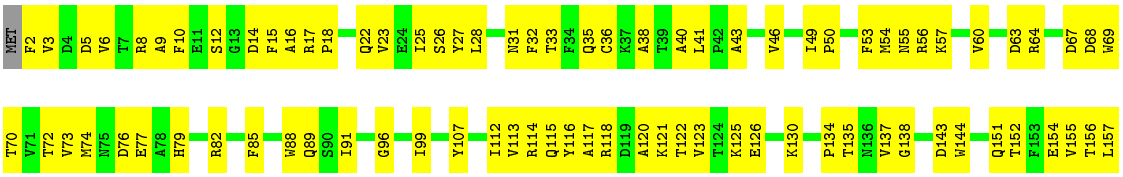
Chain p:



• Molecule 8: Tail tube protein gp19

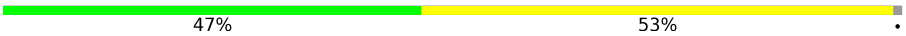
Chain BB:

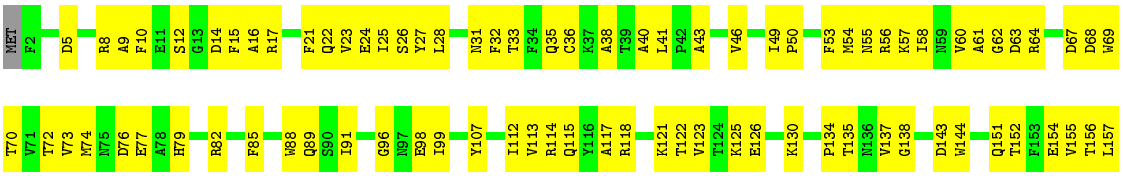




• Molecule 8: Tail tube protein gp19

Chain BC:





• Molecule 8: Tail tube protein gp19

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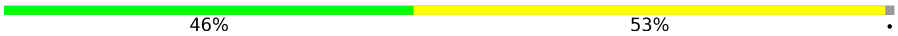
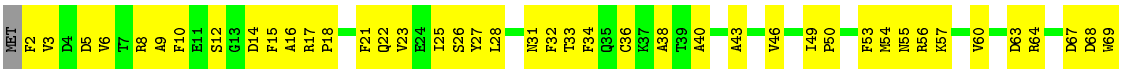
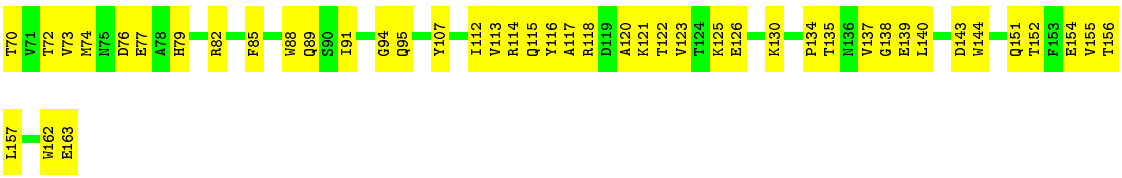




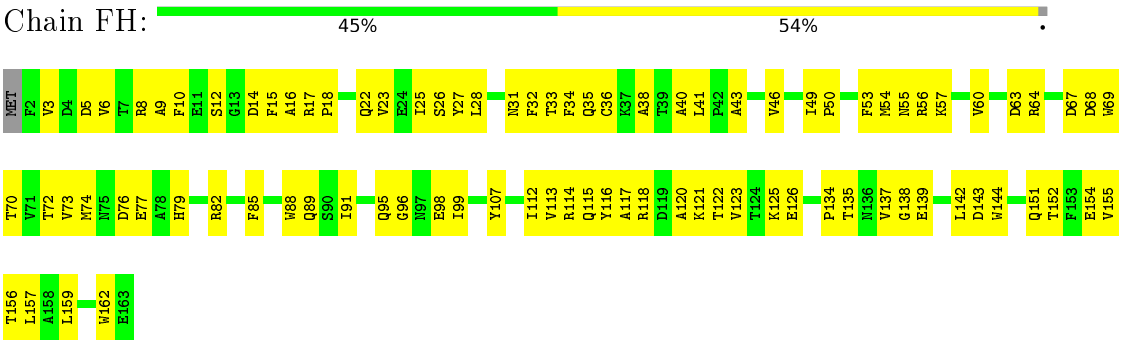


• Molecule 8: Tail tube protein gp19

Chain DF:

• Molecule 8: Tail tube protein gp19

Chain FH:



• Molecule 8: Tail tube protein gp19

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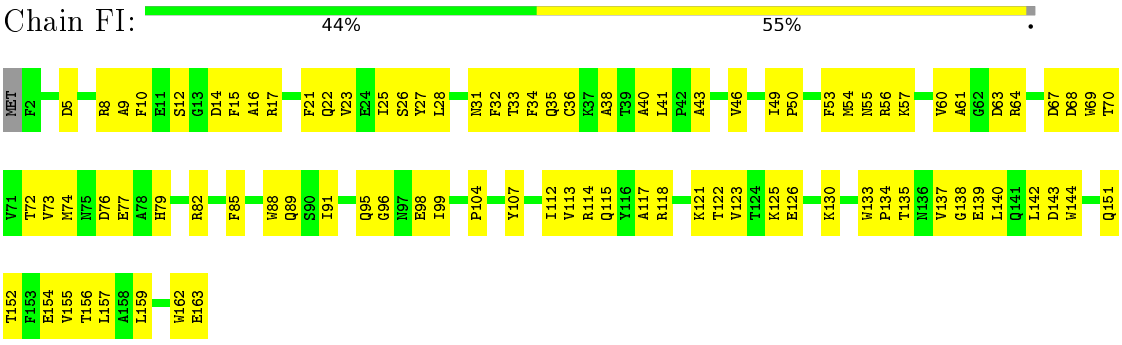

• Molecule 8: Tail tube protein gp19

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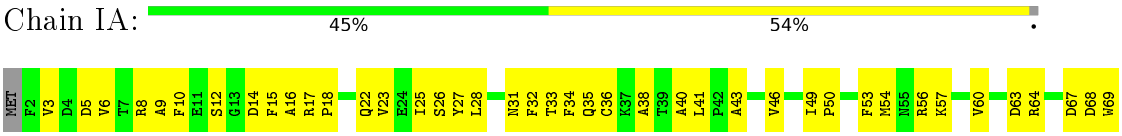

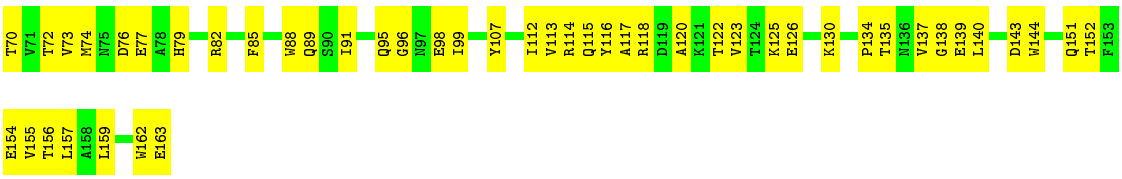

• Molecule 8: Tail tube protein gp19

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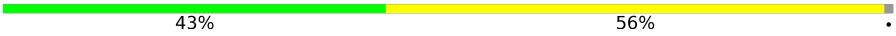

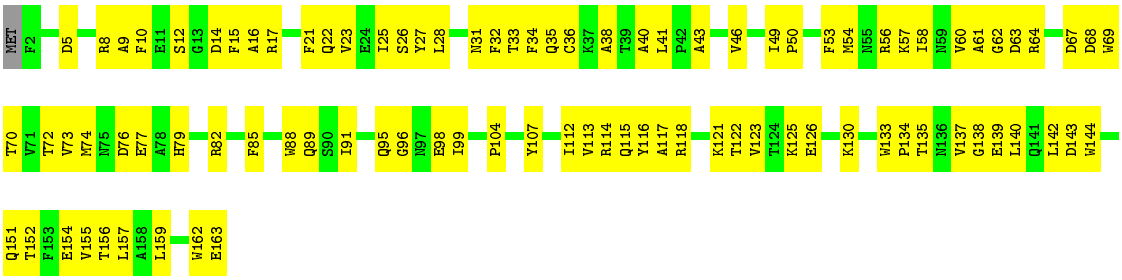

• Molecule 9: Baseplate wedge protein gp25

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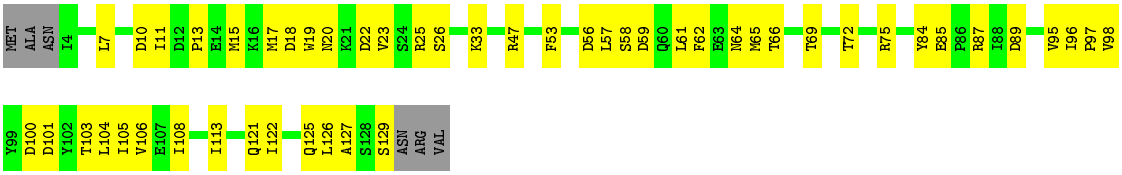

• Molecule 9: Baseplate wedge protein gp25

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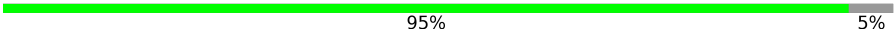

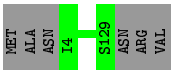

• Molecule 9: Baseplate wedge protein gp25

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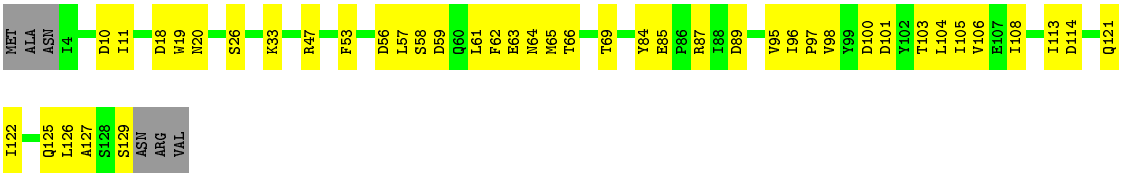
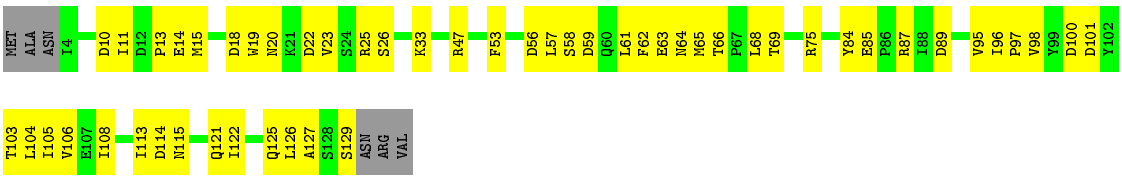


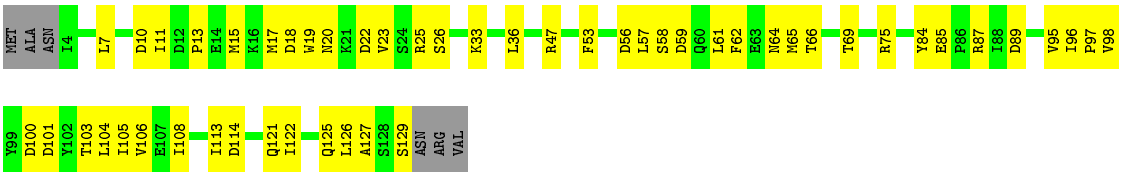
• Molecule 9: Baseplate wedge protein gp25

Chain DG:



• Molecule 9: Baseplate wedge protein gp25

Chain FJ:



• Molecule 9: Baseplate wedge protein gp25

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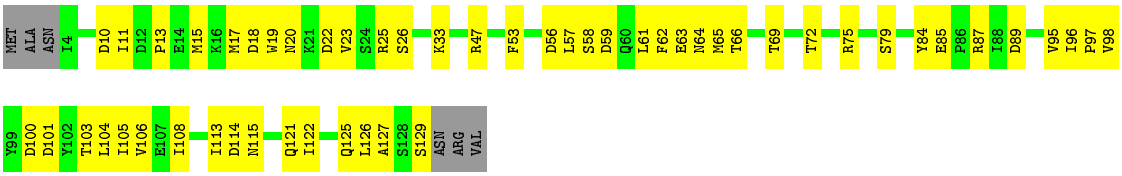
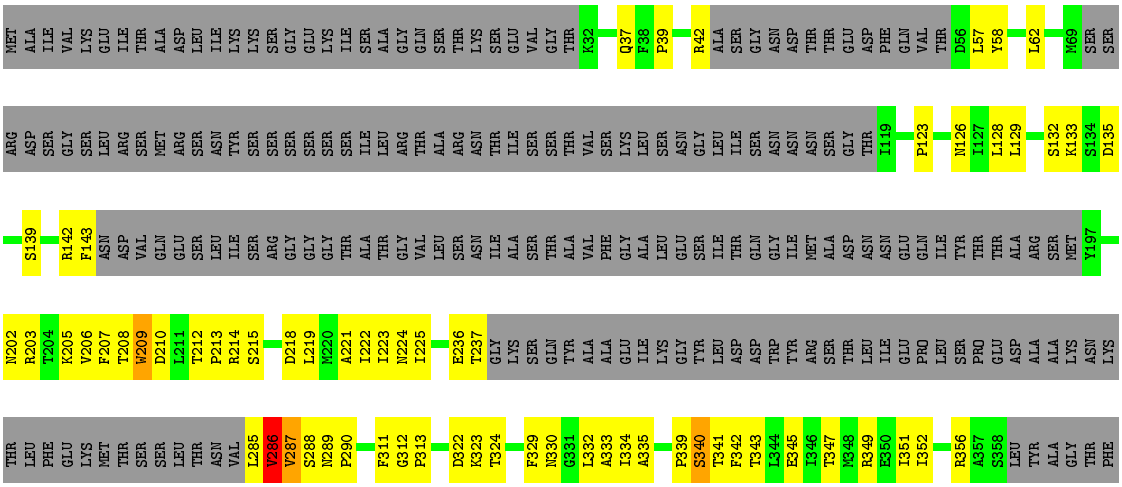


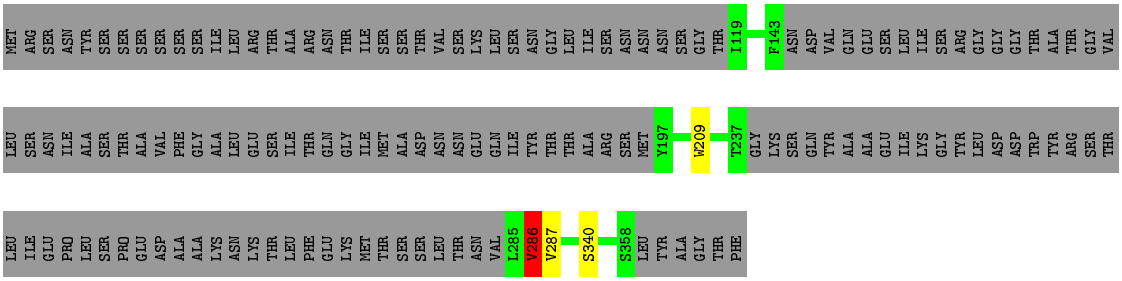
• Molecule 10: Baseplate tail-tube protein gp48

Chain U:



• Molecule 10: Baseplate tail-tube protein gp48

Chain r:



• Molecule 10: Baseplate tail-tube protein gp48

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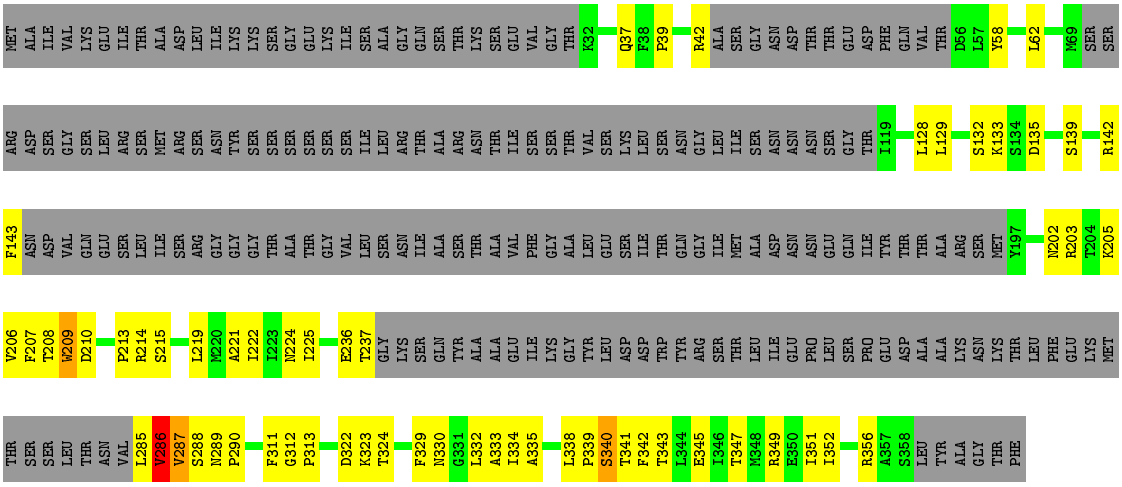

• Molecule 10: Baseplate tail-tube protein gp48

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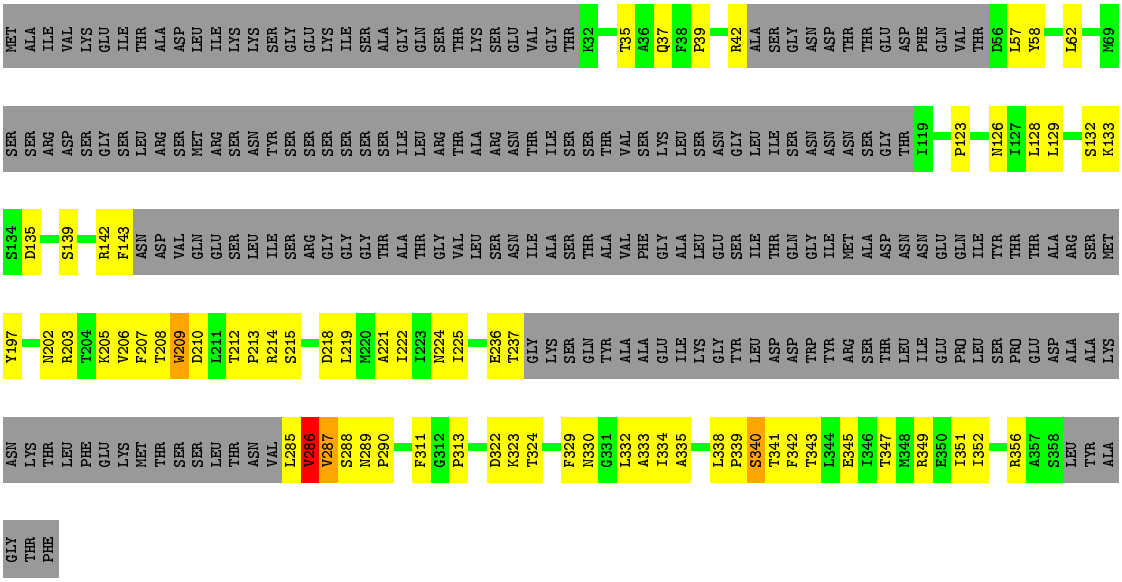

• Molecule 10: Baseplate tail-tube protein gp48

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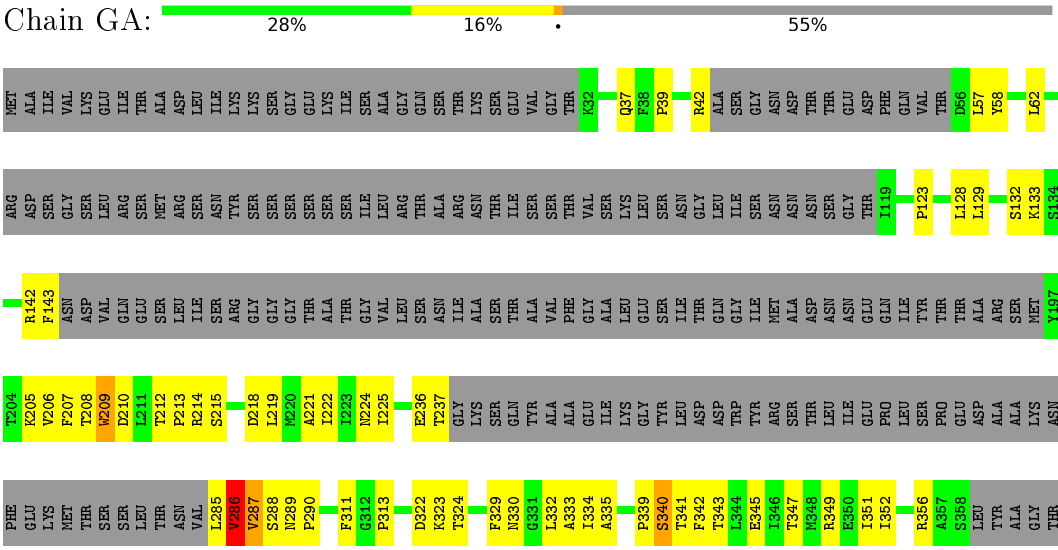

- Molecule 10: Baseplate tail-tube protein gp48

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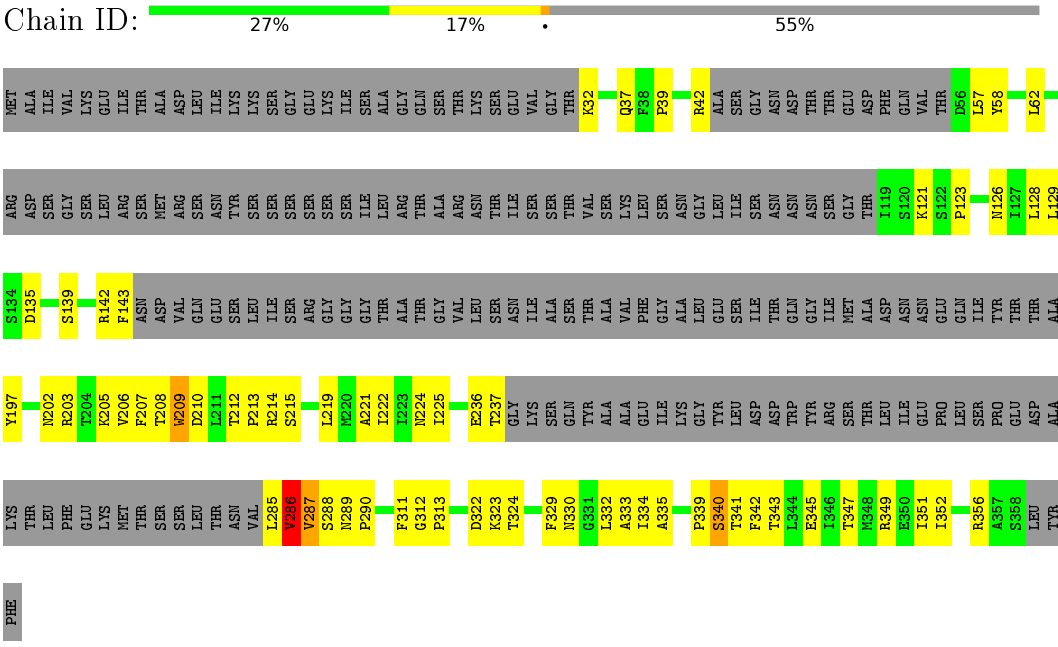
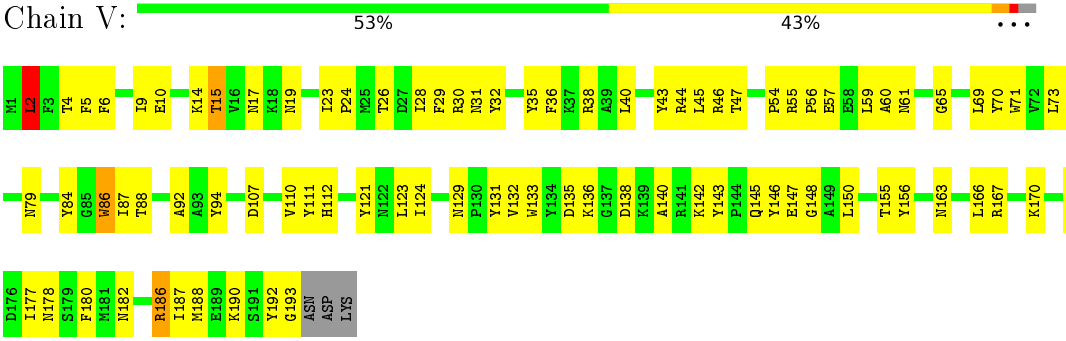


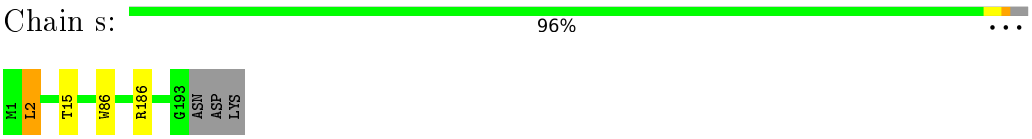
- Molecule 11: Baseplate wedge protein gp53

Chain V:



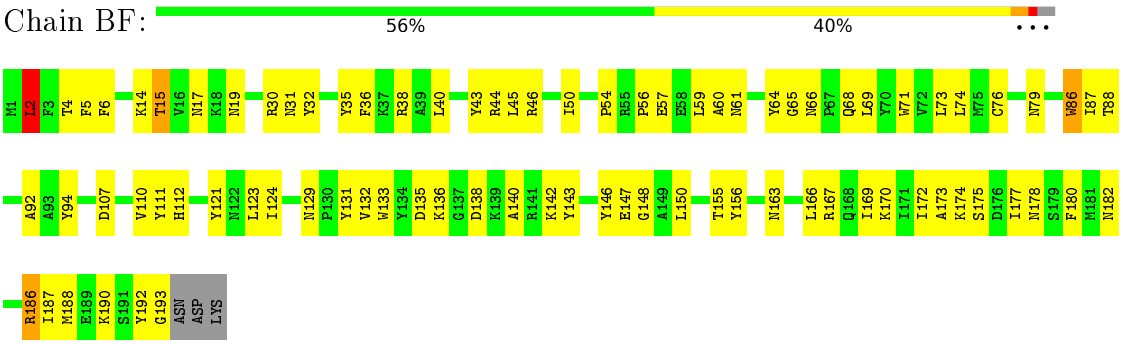
- Molecule 11: Baseplate wedge protein gp53

Chain s:



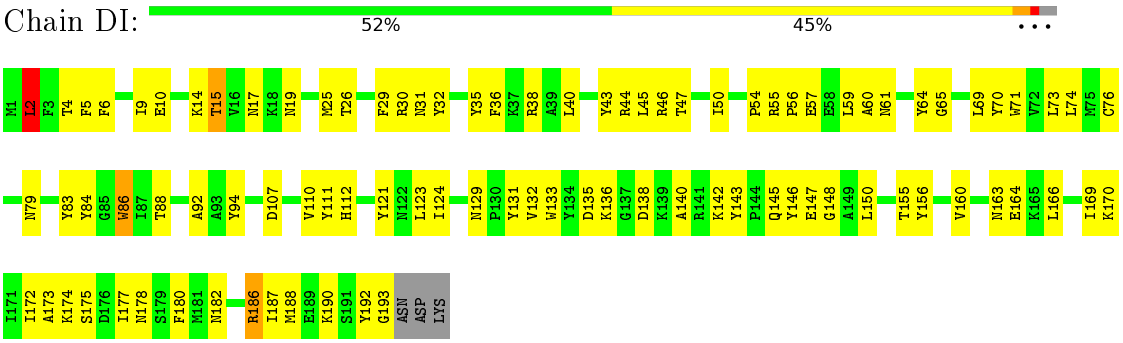
- Molecule 11: Baseplate wedge protein gp53

Chain BF:



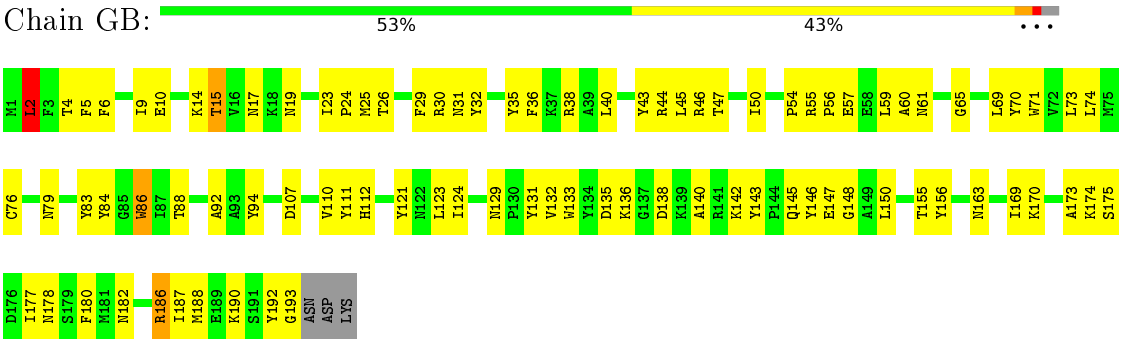
- Molecule 11: Baseplate wedge protein gp53

Chain DI:



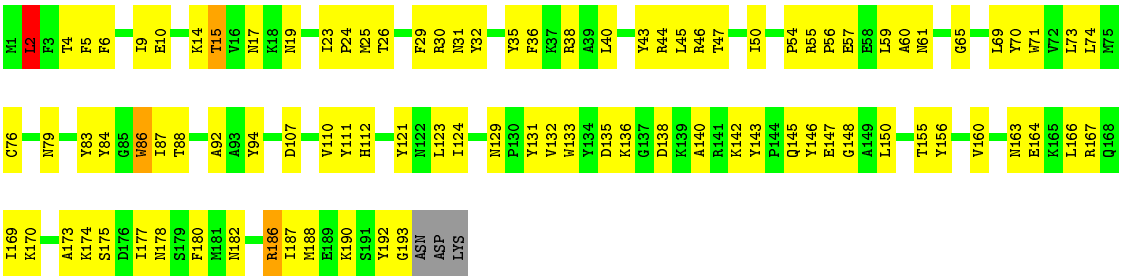
- Molecule 11: Baseplate wedge protein gp53

Chain GB:



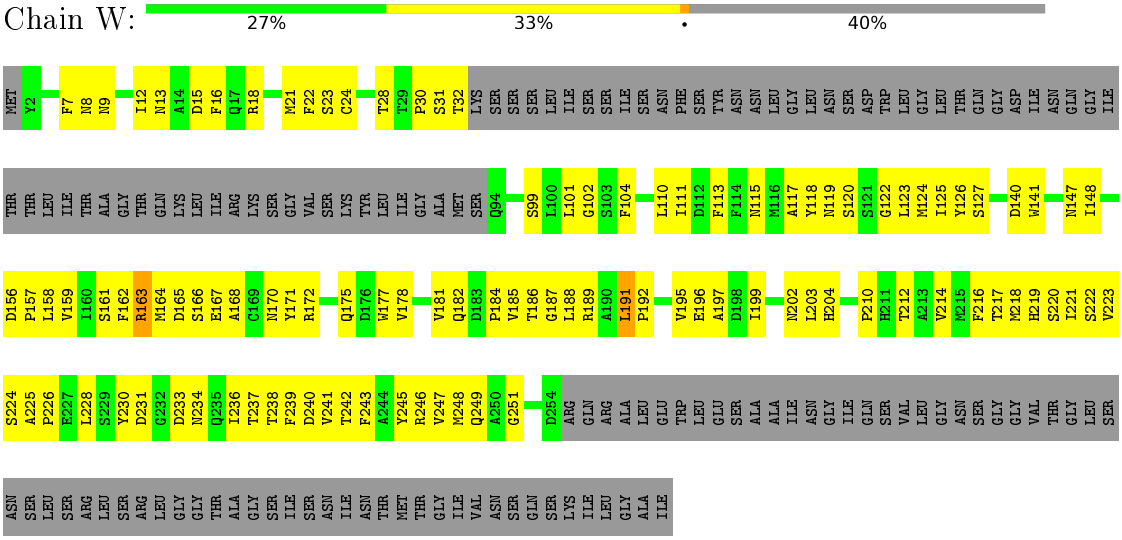
- Molecule 11: Baseplate wedge protein gp53

Chain IE:



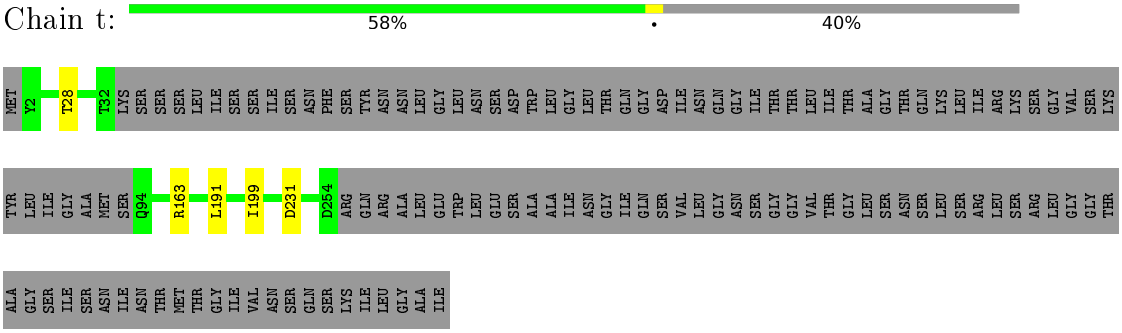
• Molecule 12: Baseplate tail-tube protein gp54

Chain W:



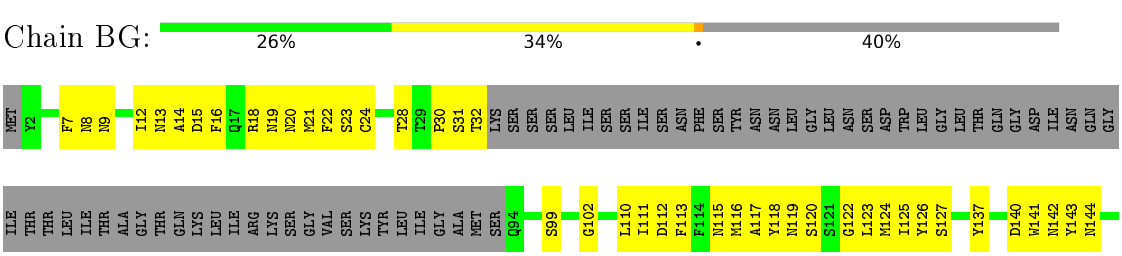
• Molecule 12: Baseplate tail-tube protein gp54

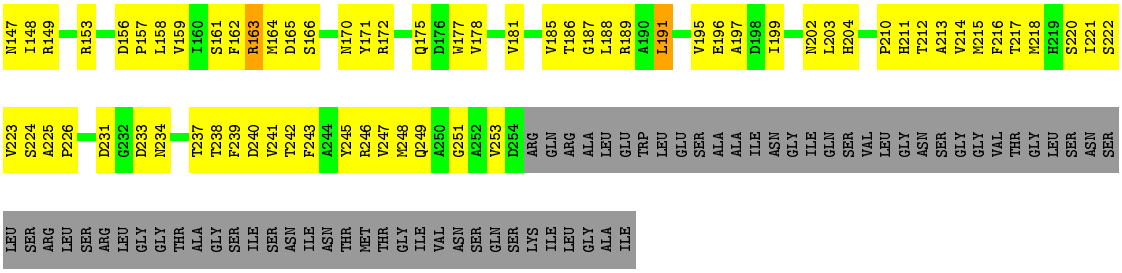
Chain t:



• Molecule 12: Baseplate tail-tube protein gp54

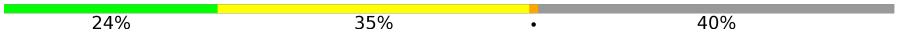
Chain BG:

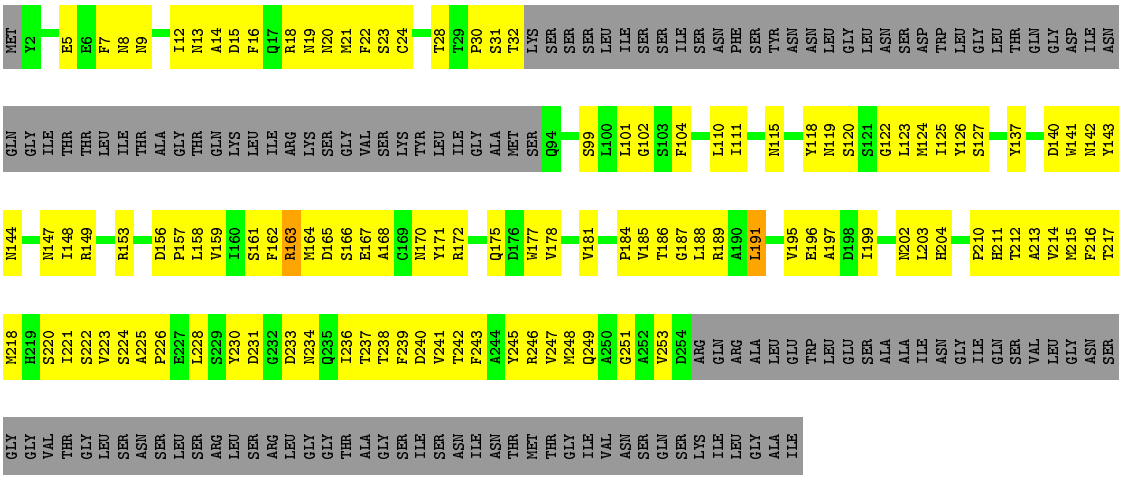




- Molecule 12: Baseplate tail-tube protein gp54

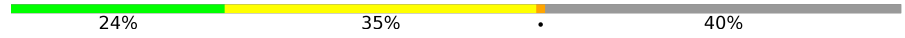
Chain DJ:

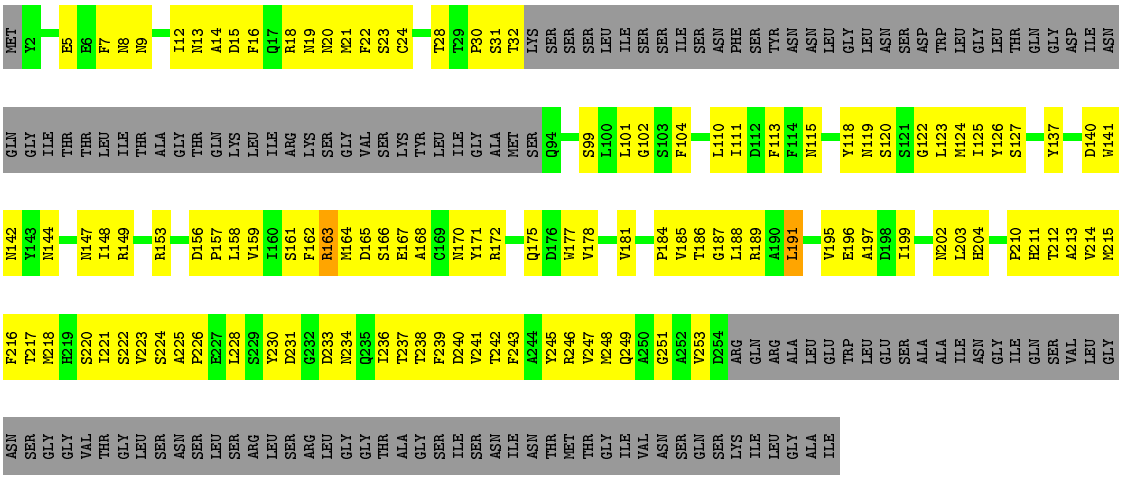




- Molecule 12: Baseplate tail-tube protein gp54

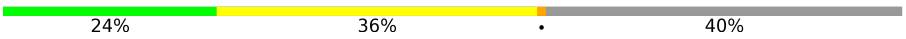
Chain GC:

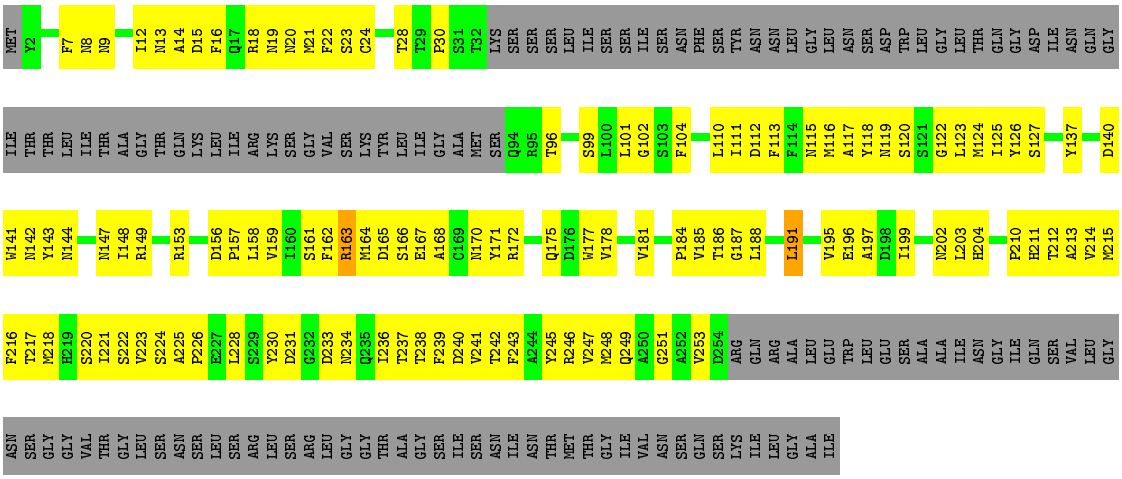




- Molecule 12: Baseplate tail-tube protein gp54

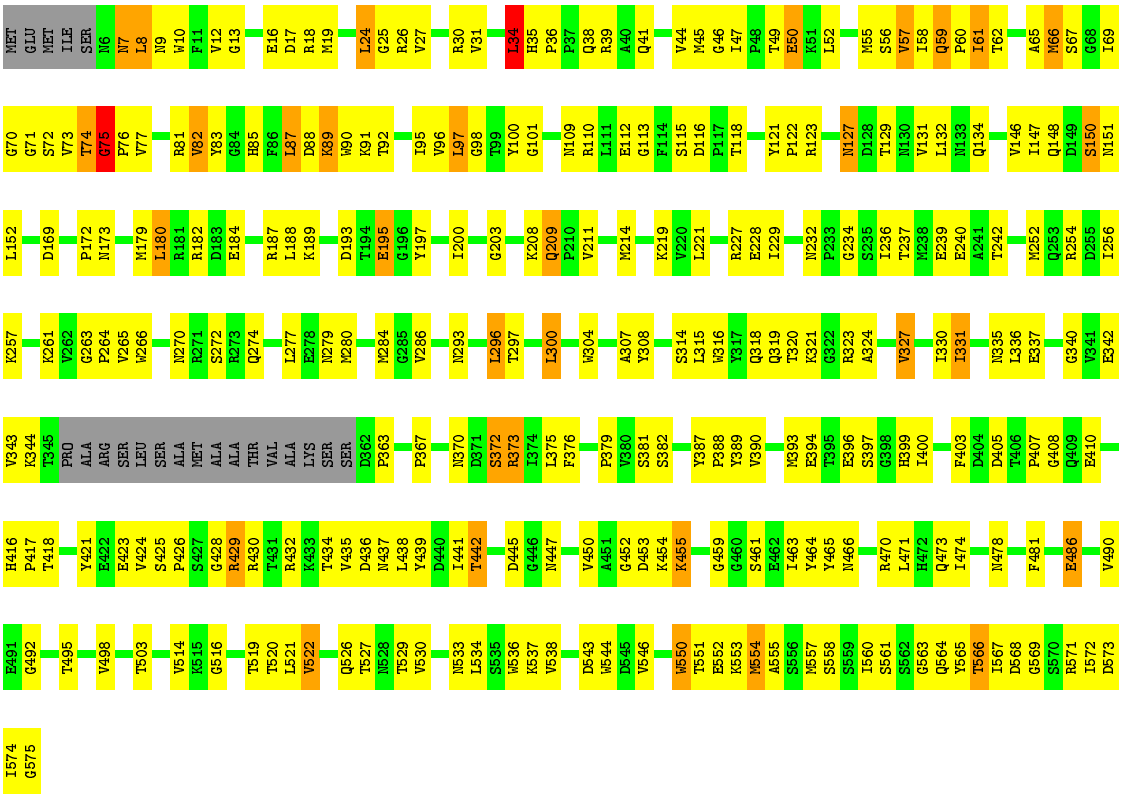
Chain IF:





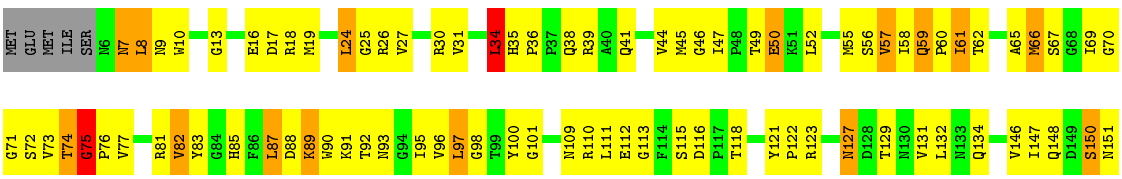
• Molecule 13: Peptidoglycan hydrolase gp5

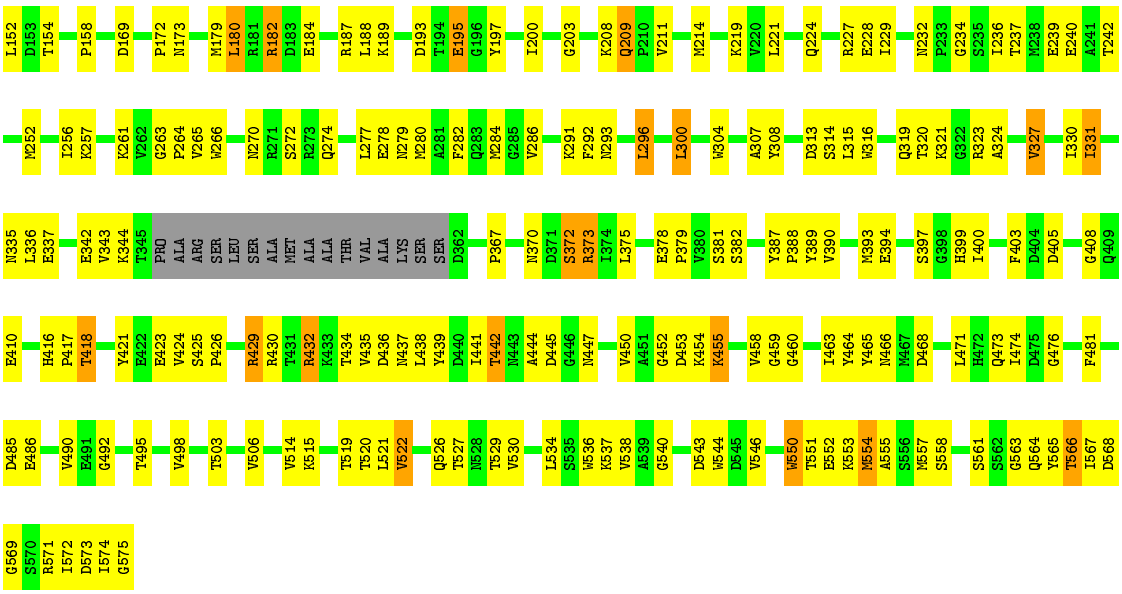
Chain YA:



• Molecule 13: Peptidoglycan hydrolase gp5

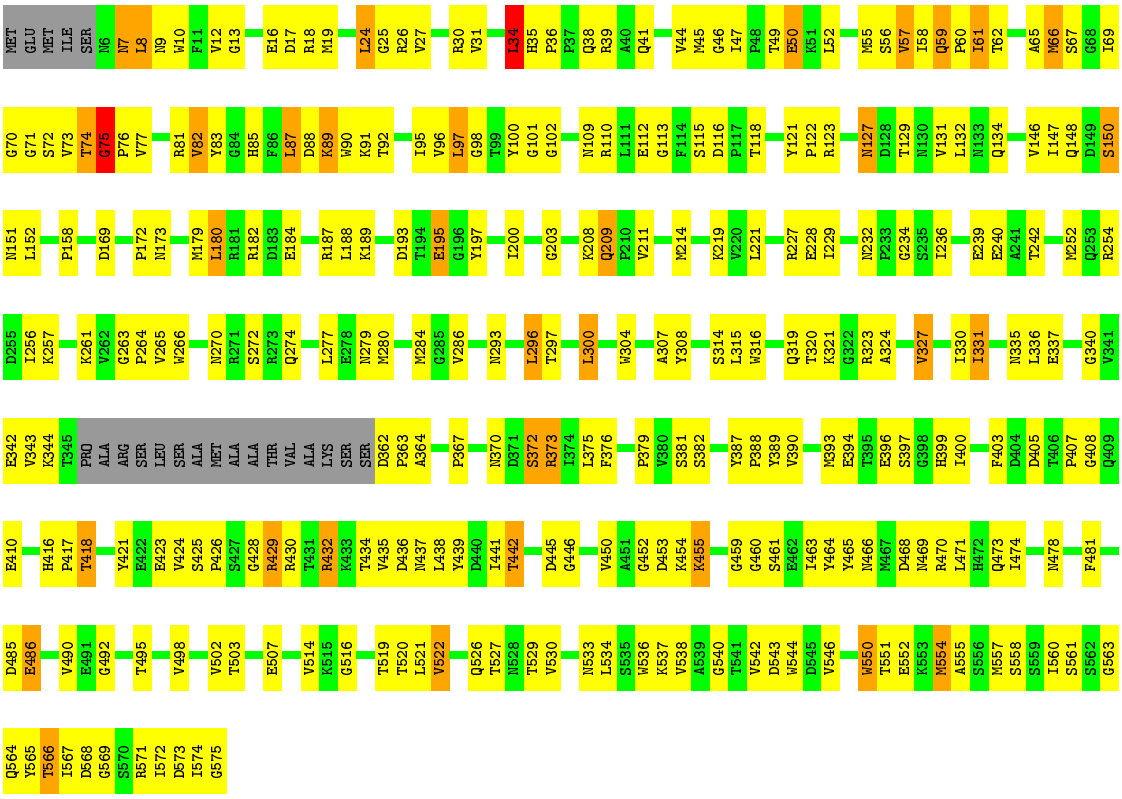
Chain YB:





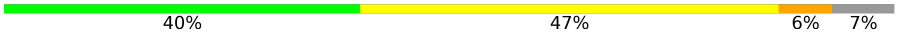
• Molecule 13: Peptidoglycan hydrolase gp5

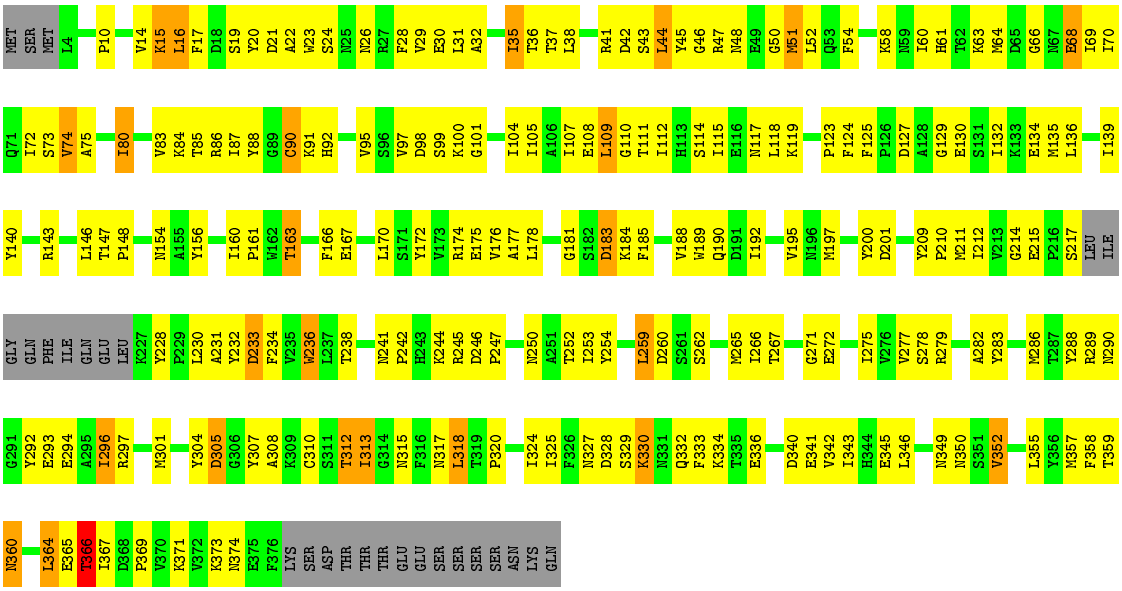
Chain YC:



• Molecule 14: Baseplate hub protein gp27

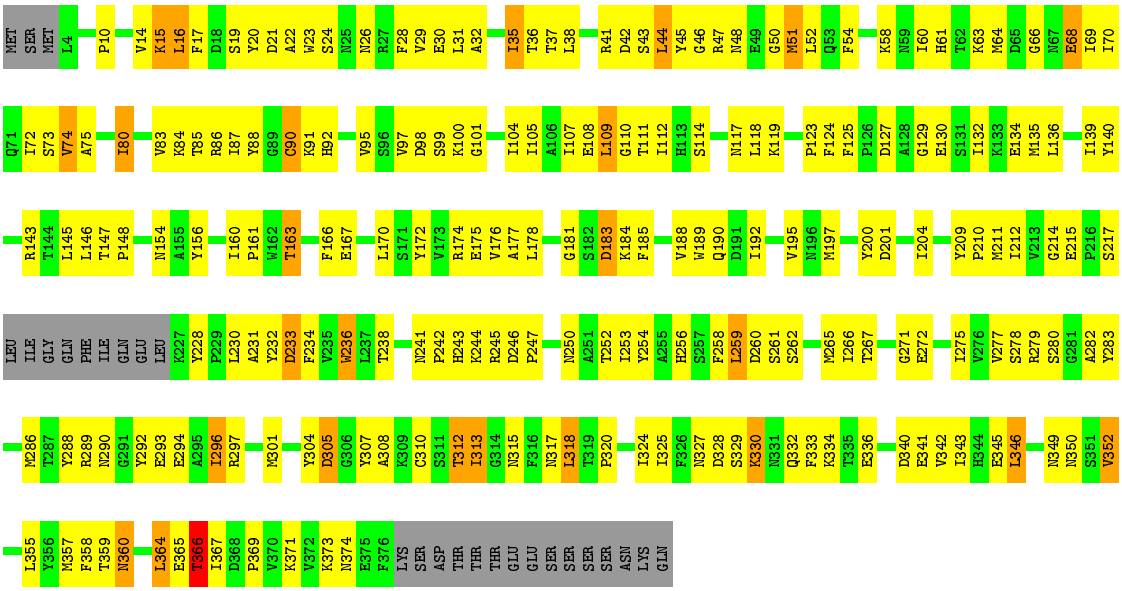
Chain YD:





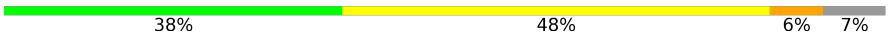
• Molecule 14: Baseplate hub protein gp27

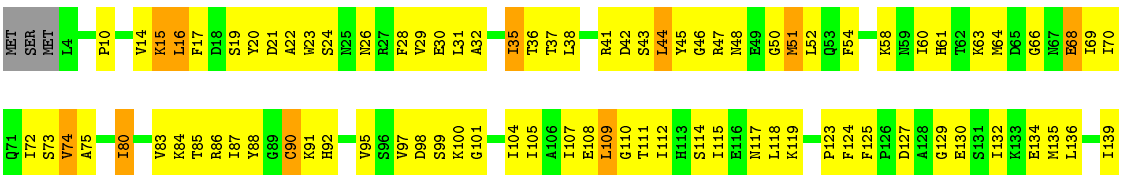
Chain YE:



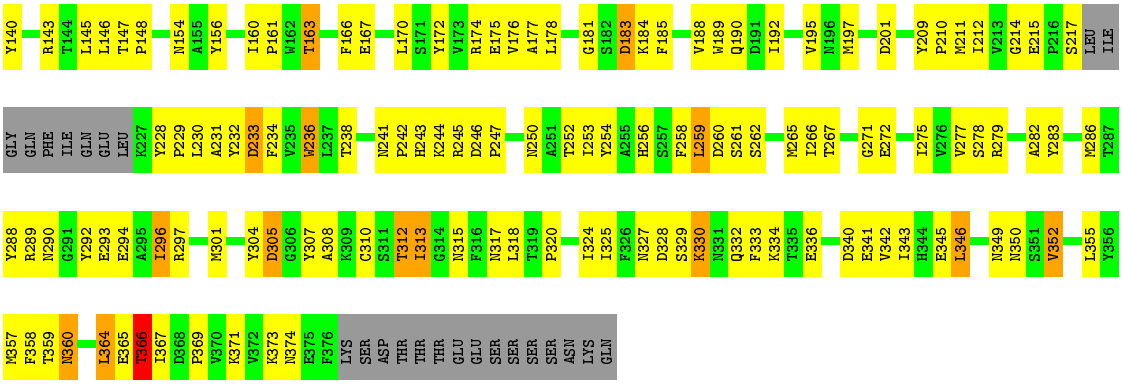
• Molecule 14: Baseplate hub protein gp27

Chain YF:



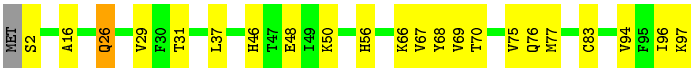


WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



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

Chain ZA:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	37913	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	105000	Depositor
Image detector	Not provided	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(^{o})	Ideal(^{o})
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 (i)

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%)	34	76
1	B	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	24	69
1	BH	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	34	76
1	BI	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	24	69
1	EA	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	34	76
1	EB	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	24	69
1	GD	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	34	76
1	GE	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	24	69
1	X	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	34	76
1	Y	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	24	69
1	u	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	34	76
1	v	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	24	69
2	BJ	1000/1032 (97%)	836 (84%)	144 (14%)	20 (2%)	9	54
2	C	1000/1032 (97%)	836 (84%)	145 (14%)	19 (2%)	10	54
2	EC	1000/1032 (97%)	836 (84%)	145 (14%)	19 (2%)	10	54
2	GF	1000/1032 (97%)	836 (84%)	144 (14%)	20 (2%)	9	54
2	Z	1000/1032 (97%)	837 (84%)	144 (14%)	19 (2%)	10	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	w	1000/1032 (97%)	837 (84%)	143 (14%)	20 (2%)	9 54
3	CA	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	30 73
3	CB	330/334 (99%)	310 (94%)	20 (6%)	0	100 100
3	D	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	30 73
3	E	330/334 (99%)	310 (94%)	20 (6%)	0	100 100
3	ED	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	30 73
3	EE	330/334 (99%)	310 (94%)	20 (6%)	0	100 100
3	GG	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	30 73
3	GH	330/334 (99%)	310 (94%)	20 (6%)	0	100 100
3	a	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	30 73
3	b	330/334 (99%)	310 (94%)	20 (6%)	0	100 100
3	x	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	30 73
3	y	330/334 (99%)	310 (94%)	20 (6%)	0	100 100
4	AA	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	AB	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	CC	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	CD	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	CE	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	EF	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	EG	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	EH	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	F	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	G	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	GI	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	GJ	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	H	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	HA	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	c	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	d	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	e	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59
4	z	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	14 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	AC	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	15 61
5	AD	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	11 55
5	AE	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	8 51
5	CF	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	15 61
5	CG	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	11 55
5	CH	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	8 51
5	EI	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	15 61
5	EJ	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	11 55
5	FA	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	8 51
5	HB	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	15 61
5	HC	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	11 55
5	HD	600/602 (100%)	530 (88%)	58 (10%)	12 (2%)	9 54
5	I	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	15 61
5	J	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	11 55
5	K	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	8 51
5	f	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	15 61
5	g	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	11 55
5	h	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	8 51
6	AF	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	AG	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	AH	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	CI	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	CJ	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	DA	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	FB	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	FC	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	FD	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	HE	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	HF	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	HG	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67
6	L	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	M	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21	67
6	N	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21	67
6	i	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21	67
6	j	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21	67
6	k	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	21	67
7	AI	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	64
7	AJ	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	30	73
7	BA	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	15	61
7	DB	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	64
7	DC	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	30	73
7	DD	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	15	61
7	FE	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	64
7	FF	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	30	73
7	FG	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	15	61
7	HH	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	64
7	HI	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	30	73
7	HJ	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	15	61
7	O	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	64
7	P	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	30	73
7	Q	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	15	61
7	l	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	17	64
7	m	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	30	73
7	n	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	15	61
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%)	30	73
10	DH	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	30	73
10	GA	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	30	73
10	ID	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	30	73
10	U	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	30	73
10	r	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	30	73
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%)	46 82
14	YE	2160/391 (552%)	2070 (96%)	84 (4%)	6 (0%)	46 82
14	YF	2160/391 (552%)	2070 (96%)	84 (4%)	6 (0%)	46 82
15	ZA	564/97 (581%)	540 (96%)	24 (4%)	0	100 100
All	All	69756/58591 (119%)	64970 (93%)	4190 (6%)	596 (1%)	24 67

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	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%)	95 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%)	95 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%)	95 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%)	95 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%)	95 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%)	95 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%)	95	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%)	95	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%)	95	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%)	95	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%)	95	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%)	95	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%)	88	94
10	DH	146/313 (47%)	145 (99%)	1 (1%)	88	94
10	GA	146/313 (47%)	145 (99%)	1 (1%)	88	94
10	ID	146/313 (47%)	145 (99%)	1 (1%)	88	94
10	U	146/313 (47%)	145 (99%)	1 (1%)	88	94
10	r	146/313 (47%)	145 (99%)	1 (1%)	88	94
11	BF	166/169 (98%)	165 (99%)	1 (1%)	90	95
11	DI	166/169 (98%)	165 (99%)	1 (1%)	90	95
11	GB	166/169 (98%)	165 (99%)	1 (1%)	90	95
11	IE	166/169 (98%)	165 (99%)	1 (1%)	90	95
11	V	166/169 (98%)	165 (99%)	1 (1%)	90	95
11	s	166/169 (98%)	165 (99%)	1 (1%)	90	95
12	BG	171/275 (62%)	170 (99%)	1 (1%)	90	95
12	DJ	171/275 (62%)	170 (99%)	1 (1%)	90	95
12	GC	171/275 (62%)	170 (99%)	1 (1%)	90	95
12	IF	171/275 (62%)	170 (99%)	1 (1%)	90	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	W	171/275 (62%)	170 (99%)	1 (1%)	90 95
12	t	171/275 (62%)	170 (99%)	1 (1%)	90 95
13	YA	2814/485 (580%)	2544 (90%)	270 (10%)	10 44
13	YB	2814/485 (580%)	2544 (90%)	270 (10%)	10 44
13	YC	2814/485 (580%)	2544 (90%)	270 (10%)	10 44
14	YD	1944/350 (555%)	1710 (88%)	234 (12%)	6 34
14	YE	1944/350 (555%)	1710 (88%)	234 (12%)	6 34
14	YF	1944/350 (555%)	1710 (88%)	234 (12%)	6 34
15	ZA	468/79 (592%)	450 (96%)	18 (4%)	40 75
All	All	60474/50314 (120%)	58914 (97%)	1560 (3%)	91 81

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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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