



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

Feb 1, 2018 – 12:22 PM EST

PDB ID : 5IV7  
EMDB ID: : EMD-3396  
Title : Cryo-electron microscopy structure of the star-shaped, hubless post-attachment T4 baseplate  
Authors : Taylor, N.M.I.; Guerrero-Ferreira, R.C.; Goldie, K.N.; Stahlberg, H.; Leiman, P.G.  
Deposited on : 2016-03-19  
Resolution : 6.77 Å(reported)  
Based on PDB ID : 5IV5

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

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

A user guide is available at

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

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

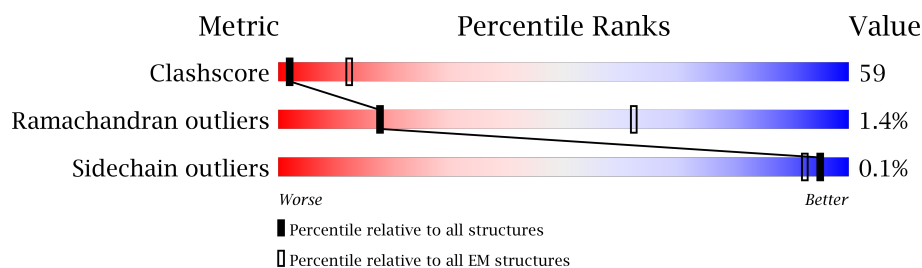
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.77 Å.

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



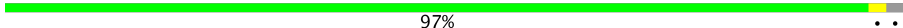
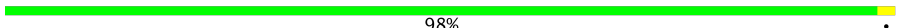
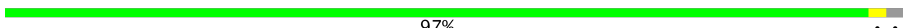

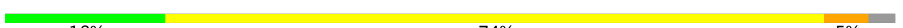
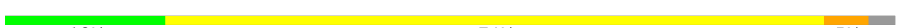







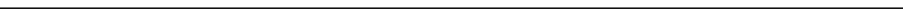





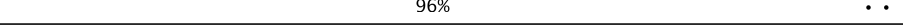
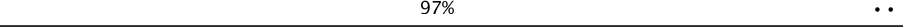
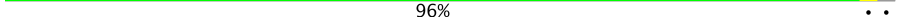



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	660	
1	B	660	
1	BF	660	
1	BG	660	
1	EA	660	
1	EB	660	
1	Q	660	
1	R	660	
1	g	660	




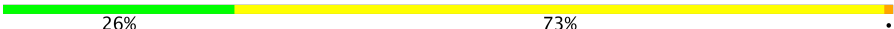
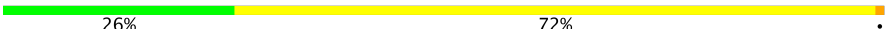
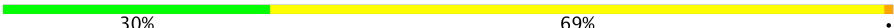
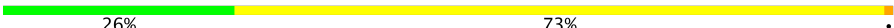


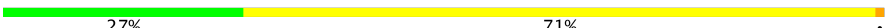
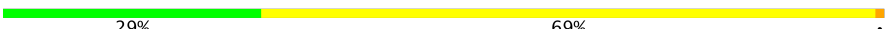

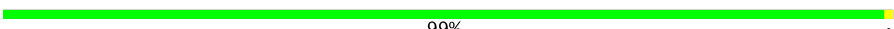
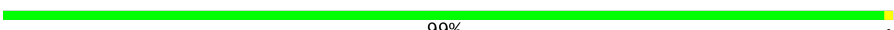


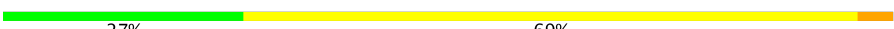
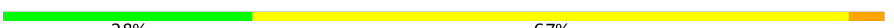

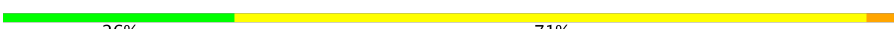
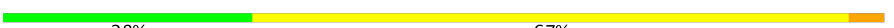

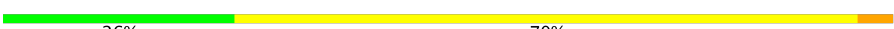


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Mol	Chain	Length	Quality of chain
1	h	660	 97% ..
1	w	660	 98% .
1	x	660	 97% ..
2	C	1032	 17% 75% 5% .
2	CA	1032	 18% 74% 5% .
2	EC	1032	 18% 74% 5% .
2	S	1032	 18% 74% 5% .
2	i	1032	 91% 6% .
2	y	1032	 91% 6% .
3	AA	334	 33% 65% ..
3	CB	334	 28% 69% ..
3	CC	334	 29% 69% ..
3	D	334	 28% 69% ..
3	E	334	 28% 69% ..
3	ED	334	 28% 69% ..
3	EE	334	 30% 68% ..
3	T	334	 28% 68% ..
3	U	334	 28% 69% ..
3	j	334	 96% ..
3	k	334	 97% ..
3	z	334	 96% ..
4	AB	288	 26% 73% .
4	AC	288	 25% 74% .
4	AD	288	 27% 71% .
4	CD	288	 27% 72% .

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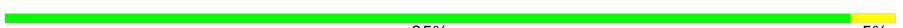








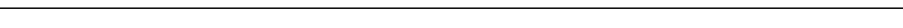






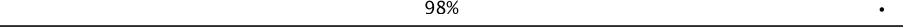
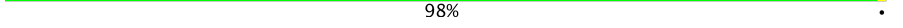

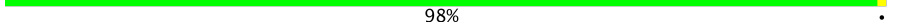
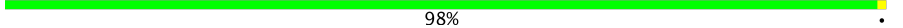
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Mol	Chain	Length	Quality of chain
4	CE	288	 27% 72% .
4	CF	288	 31% 68% .
4	EF	288	 25% 74% .
4	EG	288	 26% 73% .
4	F	288	 26% 72% .
4	FA	288	 30% 69% .
4	G	288	 26% 73% .
4	H	288	 27% 72% .
4	V	288	 27% 71% .
4	W	288	 27% 71% .
4	X	288	 29% 69% .
4	l	288	 99% .
4	m	288	 99% .
4	n	288	 99% .
5	AE	602	 28% 68% .
5	AF	602	 27% 67% 5% .
5	AG	602	 27% 69% .
5	CG	602	 28% 67% .
5	DA	602	 27% 67% 5% .
5	DB	602	 26% 71% .
5	FB	602	 28% 67% .
5	FC	602	 27% 67% 5% .
5	FD	602	 26% 70% .
5	I	602	 29% 66% .
5	J	602	 26% 68% 5% .

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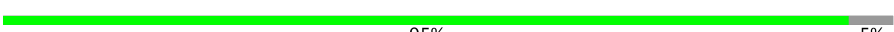

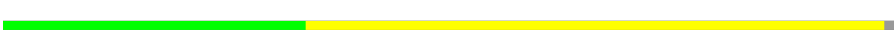







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Mol	Chain	Length	Quality of chain
5	K	602	 27% 70% .
5	Y	602	 32% 63% .
5	Z	602	 32% 63% 5% .
5	a	602	 95% 5% .
5	o	602	 95% 5% .
5	p	602	 94% 6% .
5	q	602	 95% 5% .
6	BA	219	 26% 73% .
6	BB	219	 26% 73% .
6	BC	219	 24% 74% .
6	DC	219	 24% 74% .
6	DD	219	 24% 74% .
6	DE	219	 23% 75% .
6	FE	219	 25% 74% .
6	FF	219	 25% 74% .
6	FG	219	 25% 74% .
6	L	219	 25% 74% .
6	M	219	 24% 74% .
6	N	219	 20% 79% .
6	b	219	 98% .
6	c	219	 98% .
6	d	219	 98% .
6	r	219	 98% .
6	s	219	 98% .
6	t	219	 98% .

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Mol	Chain	Length	Quality of chain
7	BD	132	 43%52%5%
7	DF	132	 40%55%5%
7	GA	132	 39%57%5%
7	O	132	 39%56%5%
7	e	132	 95%5%
7	u	132	 95%5%
8	BE	196	 34%65%. .
8	DG	196	 28%70%. .
8	GB	196	 30%69%. .
8	P	196	 28%70%. .
8	f	196	 98%. .
8	v	196	 98%. .

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 312210 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	Q	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
1	R	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
1	g	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
1	h	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
1	w	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
1	x	648	Total	C	N	O	S	0	0
			5157	3259	854	1034	10		
1	BF	658	Total	C	N	O	S	0	0
			5235	3308	867	1050	10		
1	BG	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		

- 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	S	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		
2	i	1004	Total	C	N	O	S	0	0
			8199	5247	1347	1578	27		

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

- 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	T	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	U	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	j	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	k	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	z	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	AA	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	CB	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	CC	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		

- 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	V	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	W	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	X	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	l	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	m	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	n	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	AC	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	AD	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	CF	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	FA	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	Y	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	Z	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	a	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	o	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	p	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	q	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	AF	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	AG	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	DA	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	DB	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	FB	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	FC	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	FD	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	b	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	c	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	d	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	r	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	s	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	t	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	BA	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	BB	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	BC	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	DC	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	DD	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	DE	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	FE	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	FF	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	FG	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		

- Molecule 7 is a protein called Baseplate wedge protein gp25.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
7	e	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
7	u	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
7	BD	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
7	DF	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
7	GA	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		

- Molecule 8 is a protein called Baseplate wedge protein gp53.

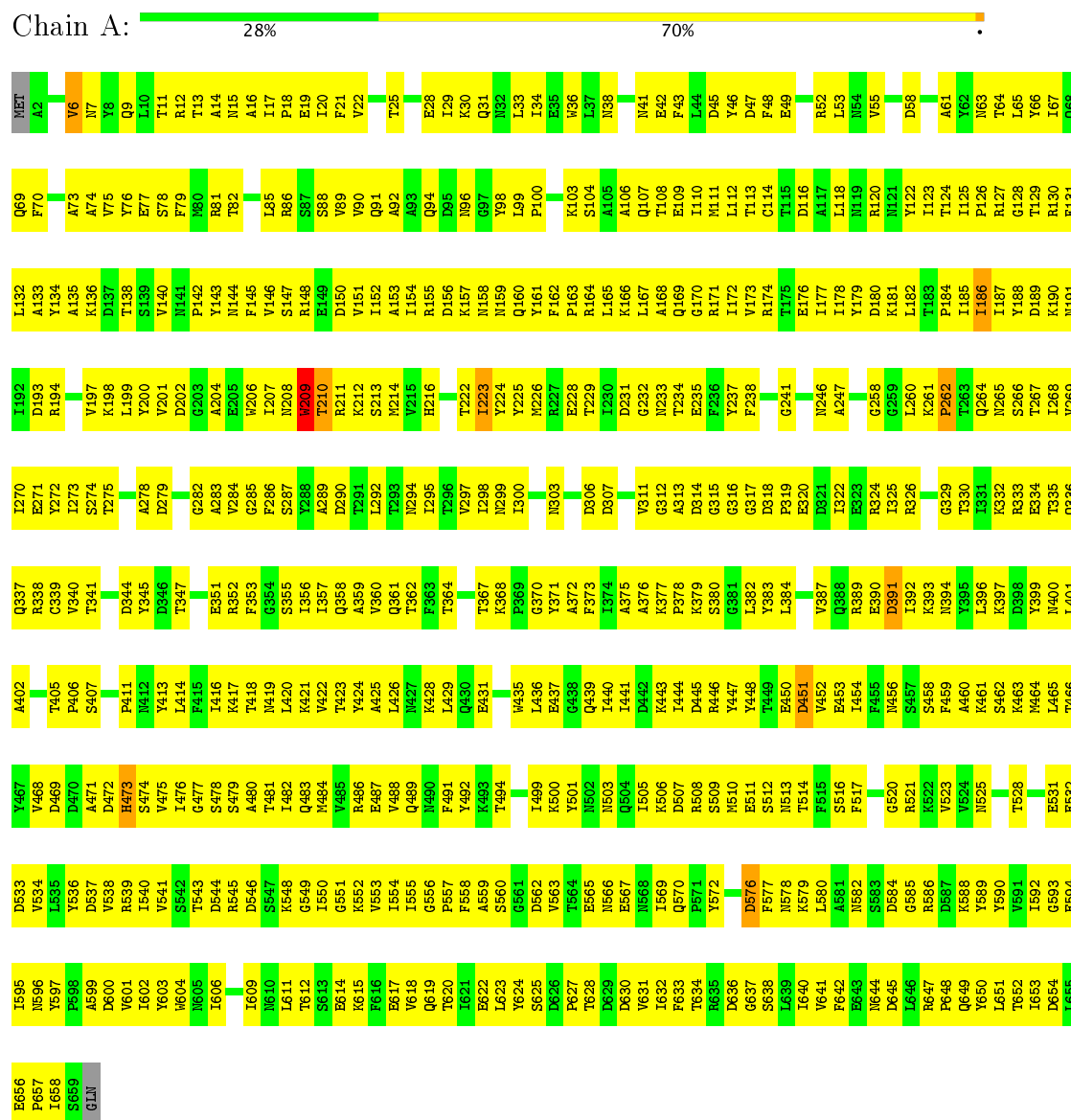
Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
8	f	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
8	v	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
8	BE	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
8	DG	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
8	GB	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

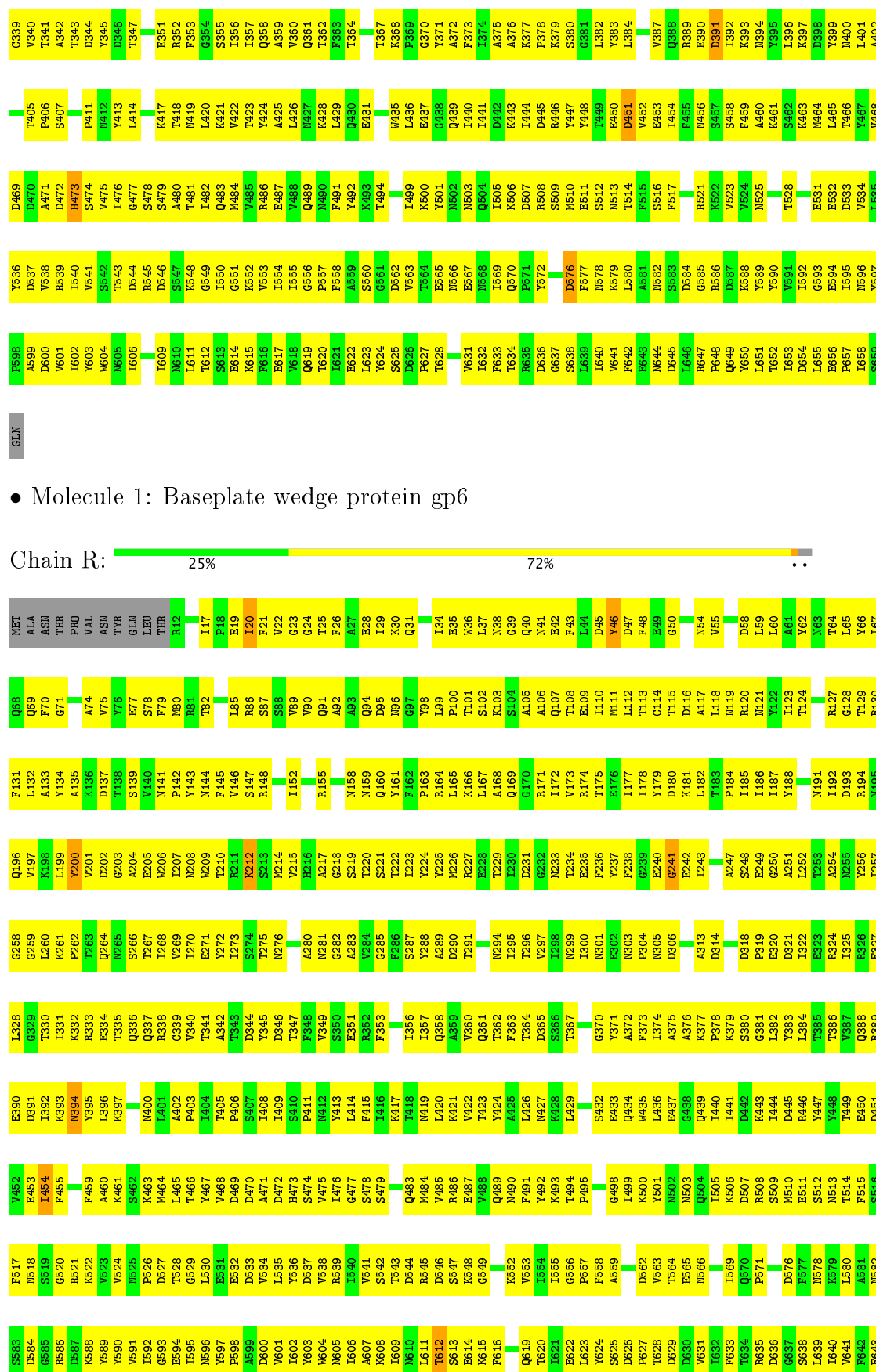
#### • Molecule 1: Baseplate wedge protein gp6

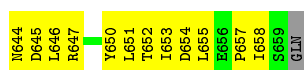


#### • Molecule 1: Baseplate wedge protein gp6







- Molecule 1: Baseplate wedge protein gp6

Chain g: 98%



- Molecule 1: Baseplate wedge protein gp6

Chain h: 97%



- Molecule 1: Baseplate wedge protein gp6

Chain w: 98%



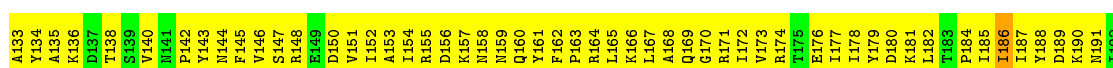
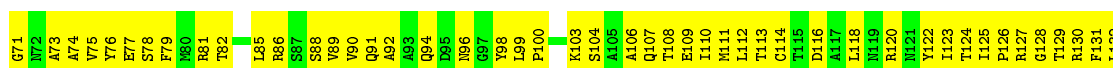
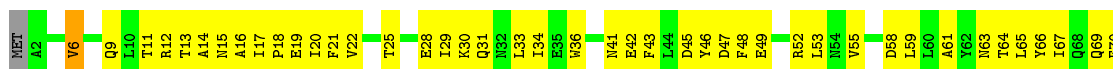
- Molecule 1: Baseplate wedge protein gp6

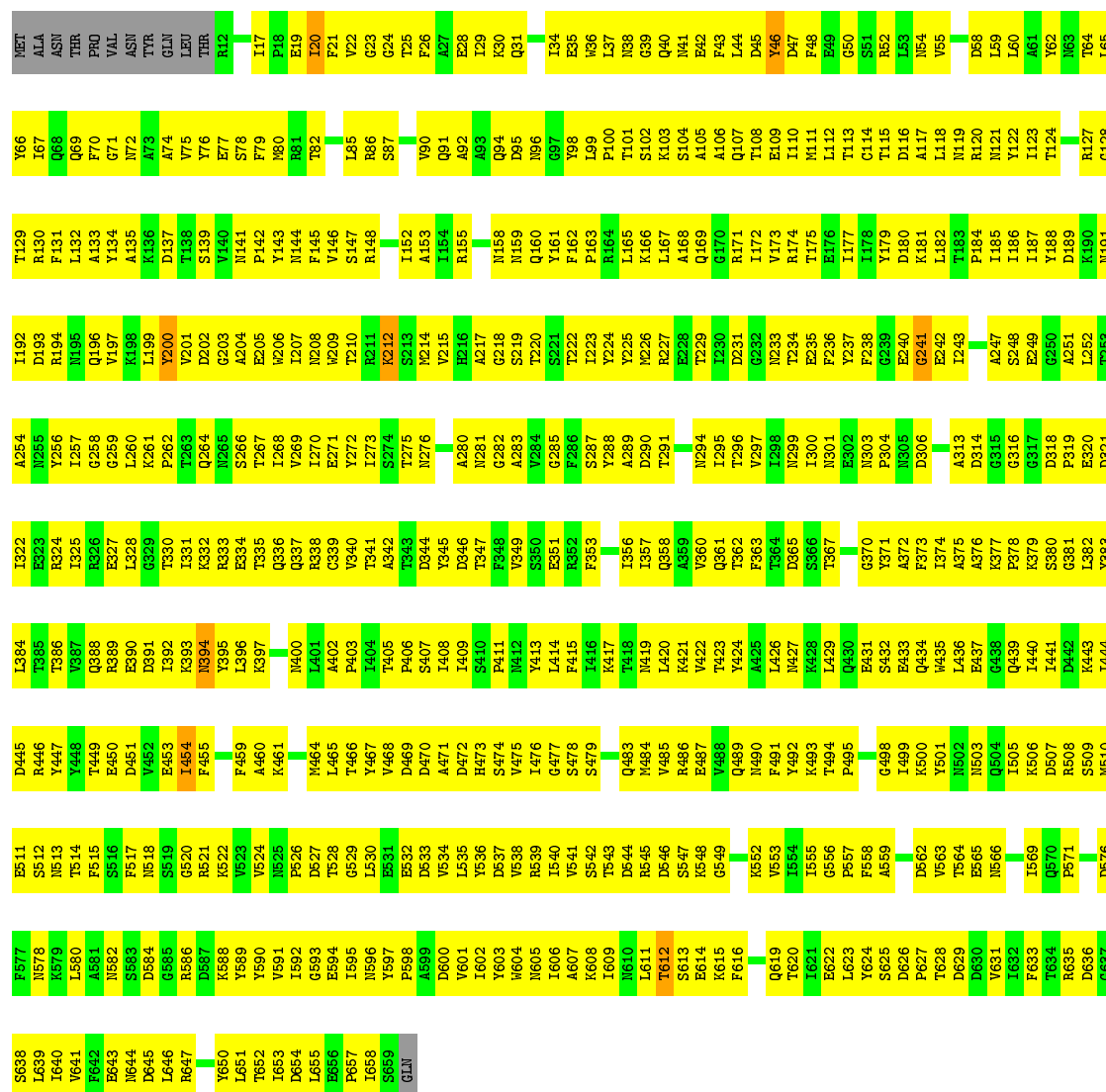
Chain x: 97%



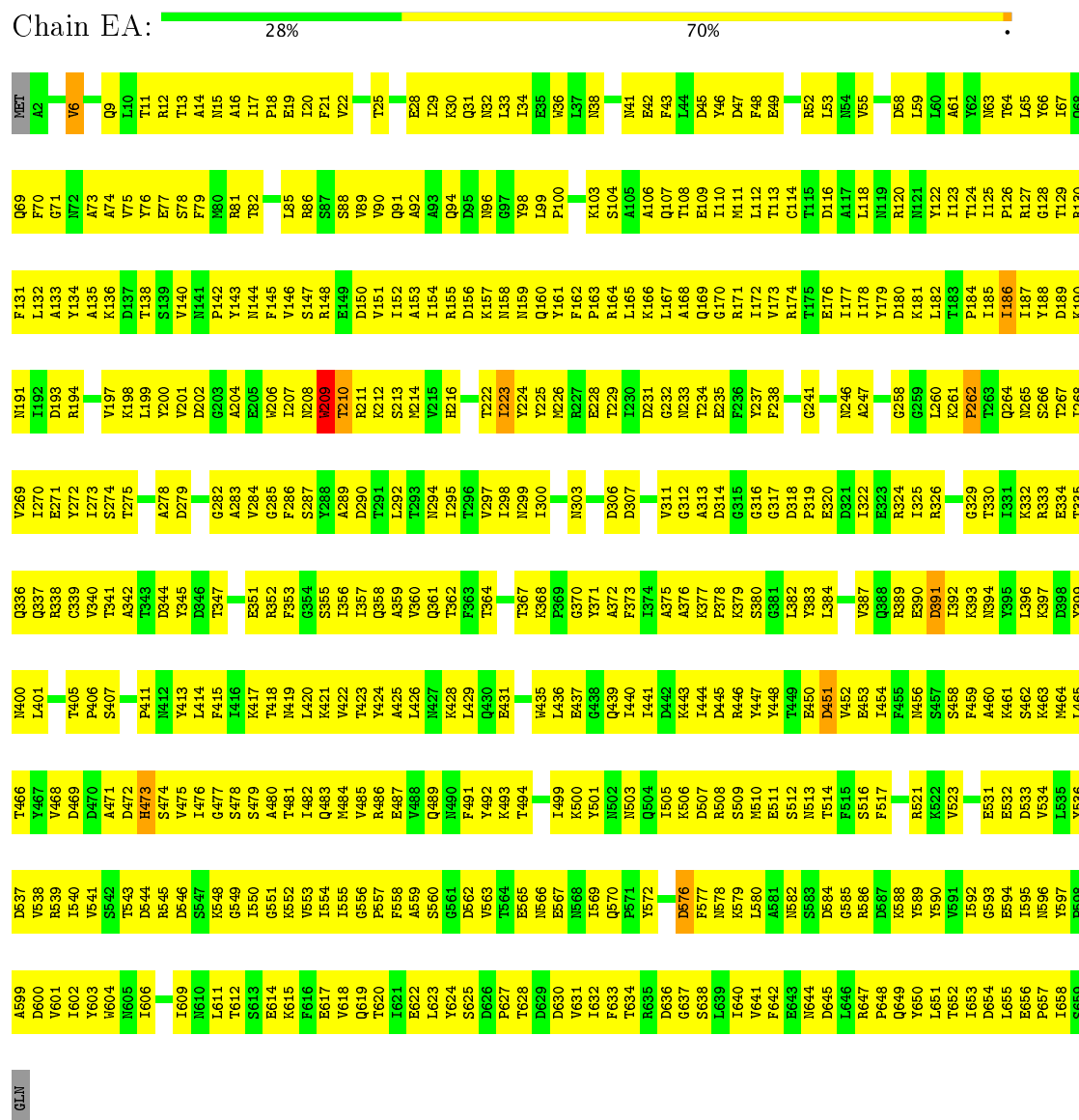
- Molecule 1: Baseplate wedge protein gp6

Chain BF: 28% 70%





- Molecule 1: Baseplate wedge protein gp6





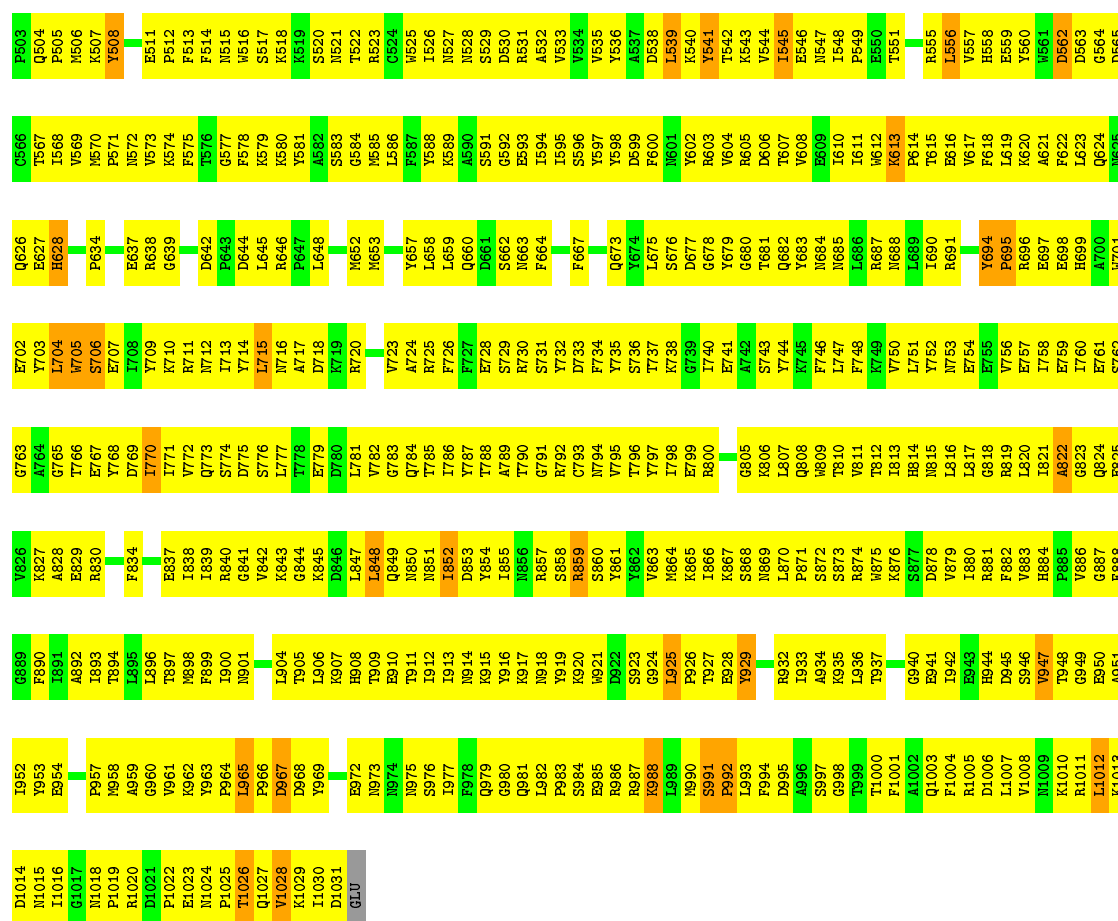
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A433	S370	A308	L248	I187	Q124	T62	T2
N432	C372	E309	G249	N188	E125	A63	V3
M494	I371	I311	Y250	R189	K126	N64	K4
S495	D373	T312	K251	V190	F127	G65	A5
T436	K374	C313	K252	Y191	T128	S66	P6
D437	V375	C314	K253	L192	L129	F67	S7
G438	A377	D315	Y255	M193	M130	F68	V8
K439	L378	D316	G256	E194	N131	F69	T9
L440	L379	Y317	K257	S195	S132	D70	S10
V441	I380	I318	K258	E196	D133	D71	L11
S442	G381	Y319	SER	G197	Y134	A72	R12
L443	E382	V320	THR	L198	V135	D73	I13
S444	V383	V321	ASP	Y200	F137	P74	S14
S445	A322	A322	VAL	L201	N138	L75	K15
	T385	R323	ARG	F202	T77	T78	S17
	D386	D324	TRP	E203	D140	Y78	A18
	K387	K325	SER	R204	T141	I79	N19
	L451	V326	ALA	Y205	I142	I80	Q20
	S452	Y328	ASP	Q206	M143	R81	V21
	D453	I329	VAL	V207	A144	B82	Q22
	M454	K330	ARG	A83	A145	T84	V23
	V455	T331	PHE	A85		A86	R24
	S456	S332	SER	D210	E148		K25
	N457	N333		V211	E149		D26
	D458	I335	SER	S212	S150		I27
	P459	L396	GLN	N213	F151	F89	V28
	E460	D397	ASP	D214	Q152	Q91	G29
	T461	S398	ILE	K215	F153	Q92	A30
	A462	A399	THR	G216	S154	S92	N31
	D463	D400	PHE	Q217	P155	D93	F32
	K464	K401	ALA	T218	S156	N94	I33
	L467	G402	LEU	K220	Y157	Y96	F34
		L403	GLY	A221	D159	T97	V36
	A470	Y404	ASP	V222	V160	E98	E37
	V471	L406	GLN	K223	S161	E99	I38
	K472	M407	L285	L224	S162	F100	A39
	Y473	R408	H286	F225	I163	E101	E40
	E474	D409	L287	N226	S164	T102	T41
		E410	G288	D227	N165	F103	K42
	H484	T411	F289	R228	F166		T43
	Y485	T412	D290	V229	I167		T44
	H486	M413	V291	G230	I168	N106	N44
	M487	K414	E292	Y231	G169	A107	S45
	M488	R415	I293	P232		Y108	E46
	A489	V416	F294	Y231		T109	E47
	F490	F417	A295	L233	H174	F110	N48
	I491	T358	T296	S234	Q111	Q111	L49
	A492	G399	T297	K235	E175	M112	P50
	D493	N360	A298	T236	I176	M113	S51
	E494	P361	T299	V237	Q177	I114	N52
	T495	K362	L300	Y238	G178	M116	Y54
	S496	E422	P301	Y239	S179	Q117	R55
	M497	E423	A302	Q240	I180	Q117	A56
	W498	R425	V364	S241	Q181	L118	I57
		R426	G365		Q182	A119	N58
	F501	I427	Y366	T244	C183	N120	F1004
		T502	K367	T245	C184	K121	R1005
			M368	Y246	K185	F122	D1006

• Molecule 2: Baseplate wedge protein gp7

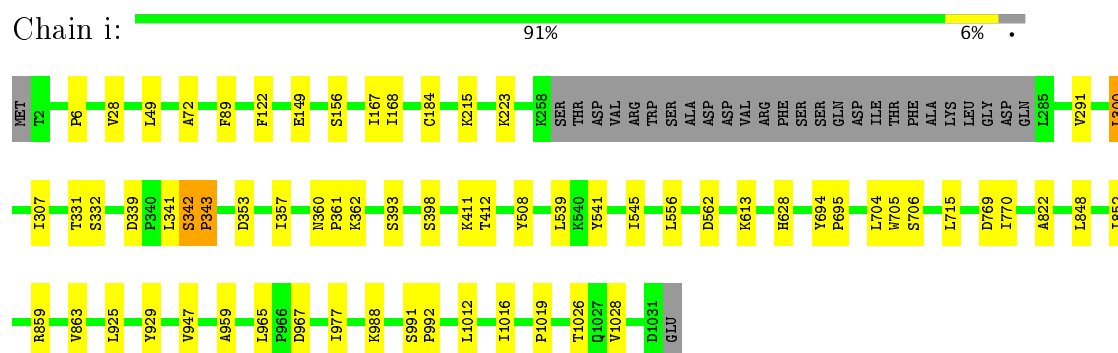
Chain S: 18% 74% 5% •

P429	D369	T307	V247	D186	I123	Y61	MET
A432	S370	A308	L248	I187	Q124	T62	V3
M433	S371	E309	G249	N188	A63	A63	K4
M434	C372	A310	D250	R189	K126	N64	A5
S435	D373	T311	K251	Y190	F127	N65	P6
T436	K374	T312	K252	Y191	T128	S66	S7
T437	V375	C313	T253	L192	L129	F67	V8
T438	F376	T314	F254	M193	M130	F68	T9
G439	A377	D315	Y255	E194	M131	D70	S10
K439	L378	D316	G256	S195	S132	D71	L11
L440	L379	Y317	R357	E196	D133	D71	L11
V441	I380	I318	K258	I197	Y134	A72	R12
S442	G381	Y319	SER	SER	V135	D73	I13
L443	E382	V320	THR	I198	M136	P74	K14
S444	V383	V321	ASP	Y200	F137	L75	S15
S445	E384	A322	VAL	L201	N138	T76	L16
T446	T385	R323	ARG	F202	M139	T77	S17
K449	L386	D324	TRP	E203	D140	Y78	A18
F450	N387	K325	SER	R204	T141	I79	M19
L451	A388	V326	ALA	Y205	I142	I80	Q20
S452	N389	R327	ASP	Q206	M143	R81	V21
D453	P390	Y328	ASP	P207	A144	V82	Q22
M454	R391	T329	VAL	V208	A145	A83	V23
V455	T392	K330	ARG	V209		T84	R24
F456	S393	T331	PHE	K210	M148	A86	K25
M457	K394	S332	SER	V211	E149		D26
D458	L395	N333	SER	S212	S150	F89	V28
F459	L396		GLN	N213	F151	E90	G29
E460	D397	D337	ASP	D214	O152	Q91	A30
T461	S398	F338	ILE	K215	F153	S92	N31
A462	A399	D339	THR	G216	S154	D93	F32
A463	D400	P340	PHE	Q217	P155	N94	V33
K464	K401	L341	ALA	T218	A156	V94	V34
	G402	S342	LVS	Y219	S157	I95	V34
	L403	P343	LEU	K220	V158	Y96	F35
L467	Y404	T344	GLY	A221	D159	T97	V36
A470	V405	Y345	ASP	V222	V160	E98	E37
K471	L406	S346	GLN	K223	S161	E99	T38
V472	N407	E347	L285	L224	S162	F100	A39
Y473	H408	R348	H286	F225	I163	E101	E40
E474	D409	L349	L287	T226	S164	T102	T41
	E410	F350	G358	D227	N165	F103	K42
H484	K411	E351	F289	R228	F166		T43
Y485	T412	P352	D290	V229	I167	N106	N44
H486	K413	D353	V291	G230	I168	A107	S45
M487	H414	T354	E292	T231	G169	Y108	G46
M488	R415	K355	T393	P232		T109	E47
A489	V416	T356	F294	L233	Y173	F110	N48
F490	F417	I357	A295	S234	H174	Q111	L49
L491	G418	T358	T296	K235	E175	M112	P50
A492	H419	G359	Y297	T236	I176	M113	S51
D493	T420	N360	A298	V237	Q177	I114	N52
E494	E421	P361	T299	Y238	G178	E115	O53
T495	E422	K362	L300	Y239	S179	M116	Y54
S496	E423	A364	P301	Q240	I180	Q117	R55
D497	R424	V364	A302	S241	Q181	L118	W56
W498	R425	G365	N303	T244	Q182	A119	N58
	R426	T367	V304		V183	N120	V57
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F501	O428		R306	V246	K185	F420	O60

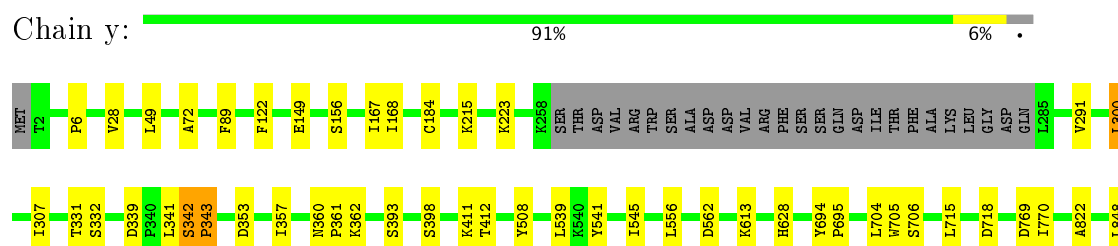




### • Molecule 2: Baseplate wedge protein gp7



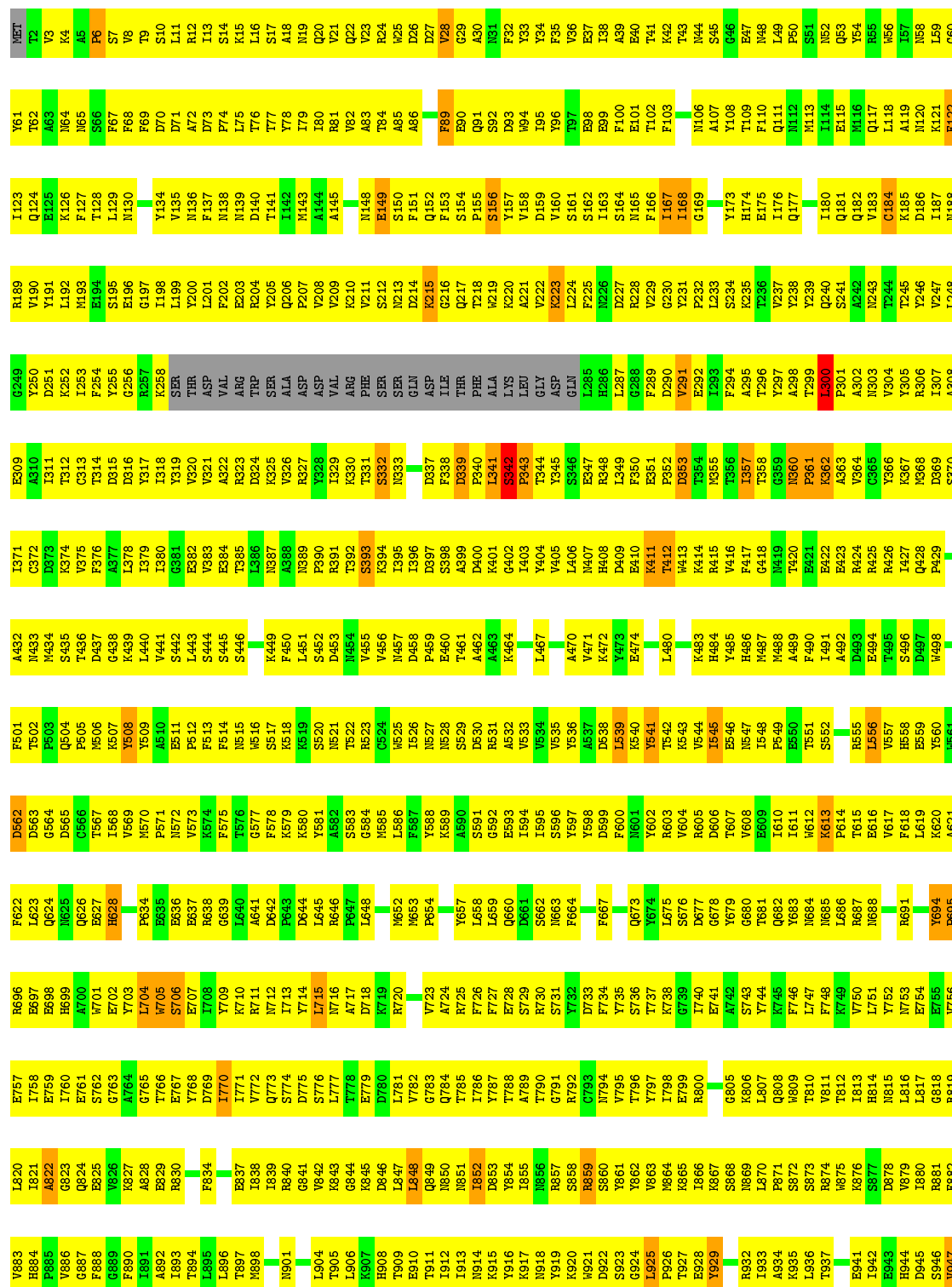
### • Molecule 2: Baseplate wedge protein gp7





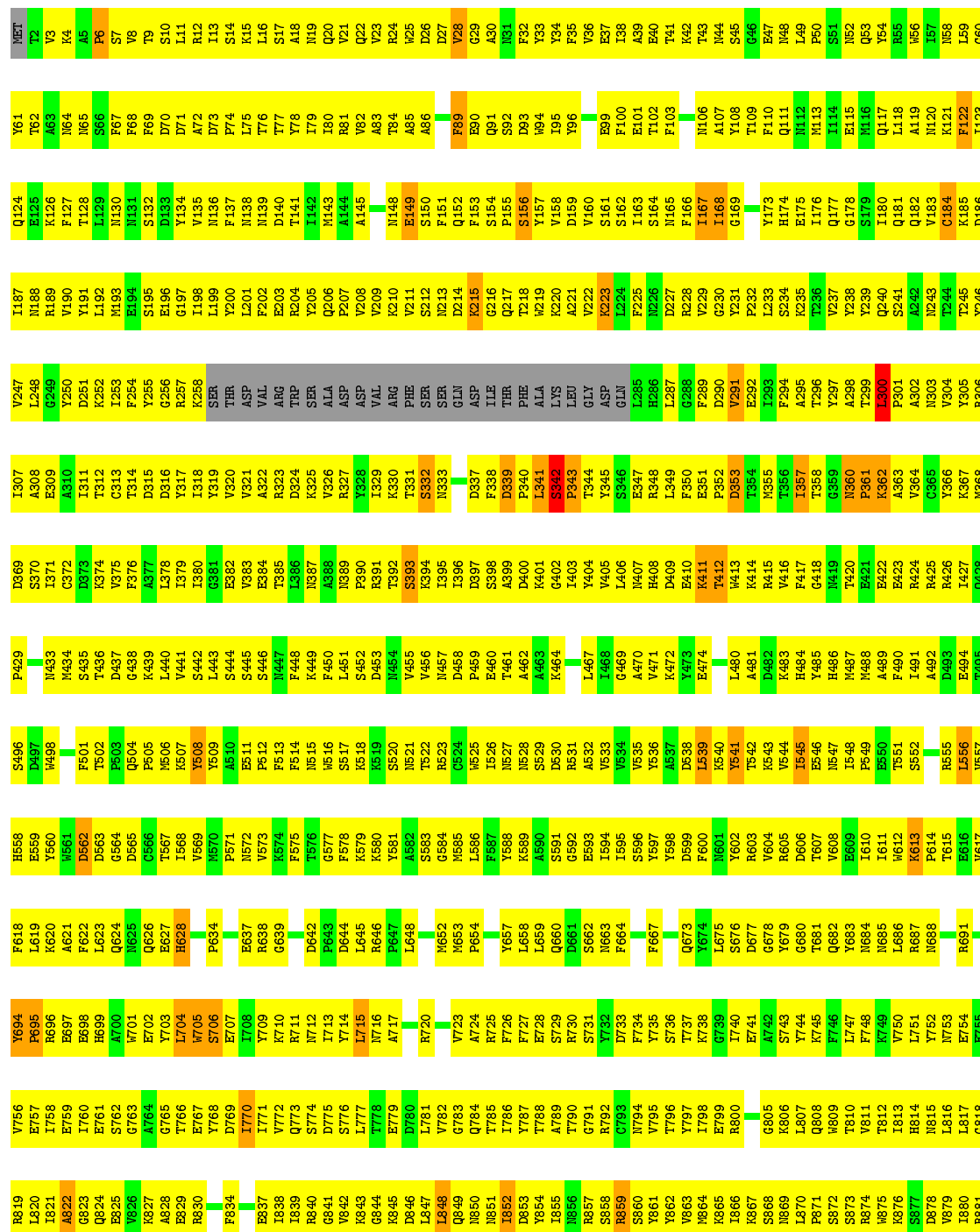
• Molecule 2: Baseplate wedge protein gp7

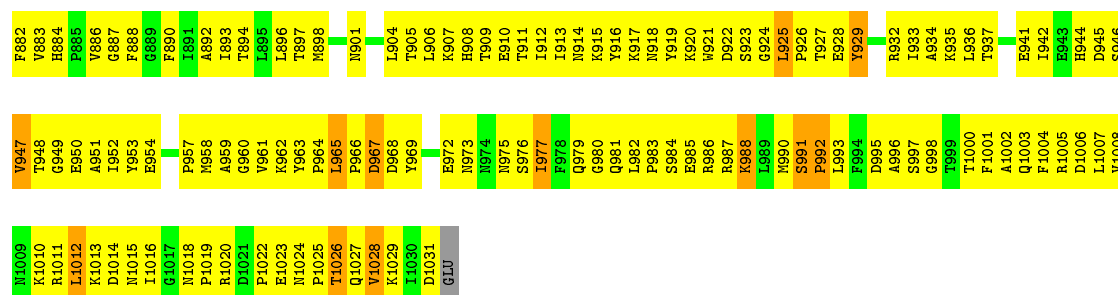
Chain CA: 18% 74% 5%



- Molecule 2: Baseplate wedge protein gp7

Chain EC:  18% 74% 5%

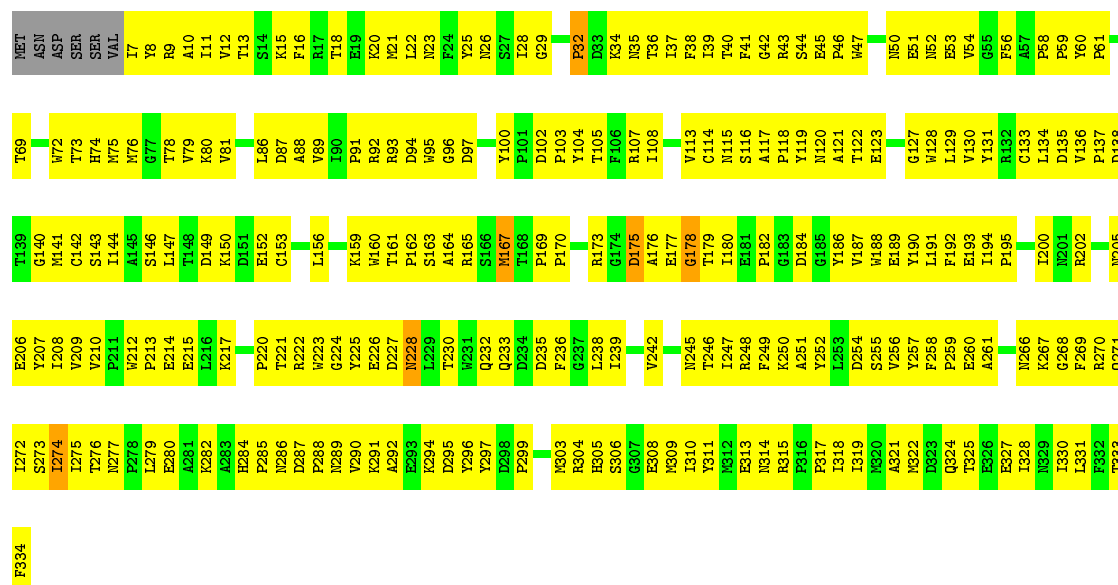




I328  
I329  
I330  
I331  
F332  
T333  
F334

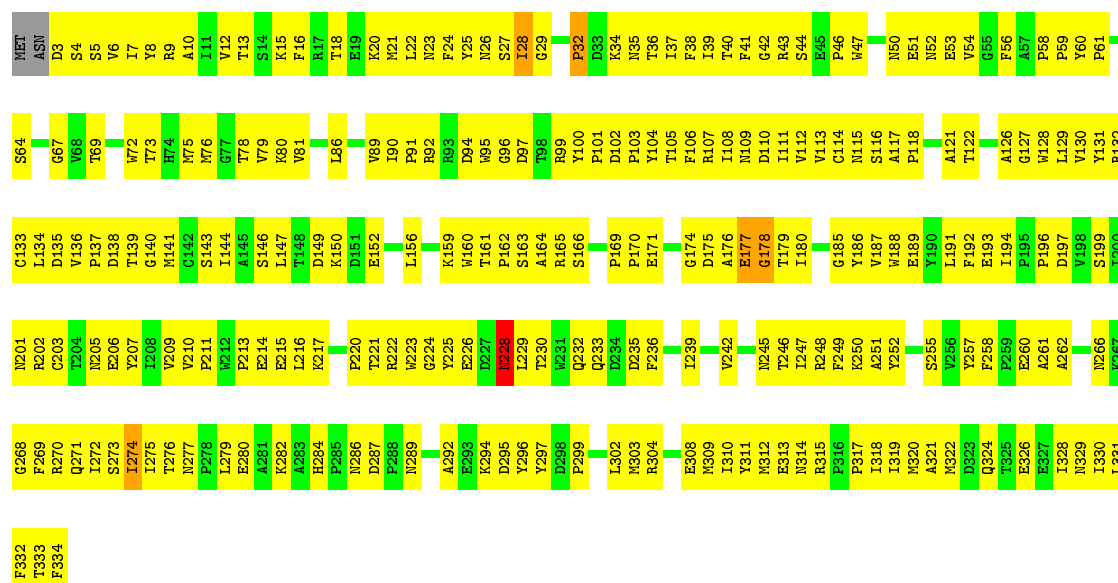
• Molecule 3: Baseplate wedge protein gp8

Chain T:  28% 68%



• Molecule 3: Baseplate wedge protein gp8

Chain U:  28% 69%



• Molecule 3: Baseplate wedge protein gp8

Chain j:  96%



• Molecule 3: Baseplate wedge protein gp8

Chain k: 97%



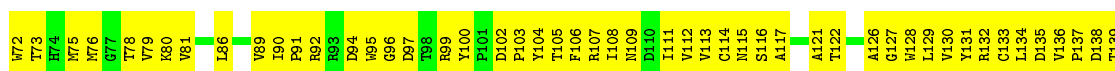
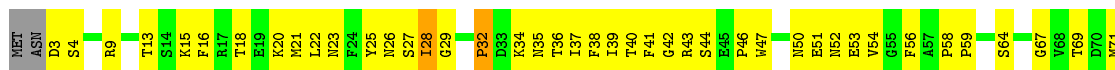
• Molecule 3: Baseplate wedge protein gp8

Chain z: 96%



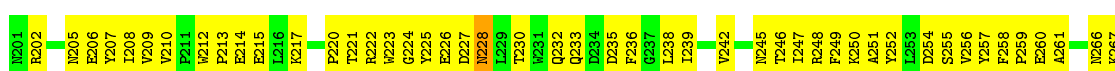
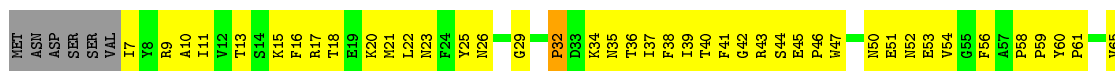
• Molecule 3: Baseplate wedge protein gp8

Chain AA: 33% 65%



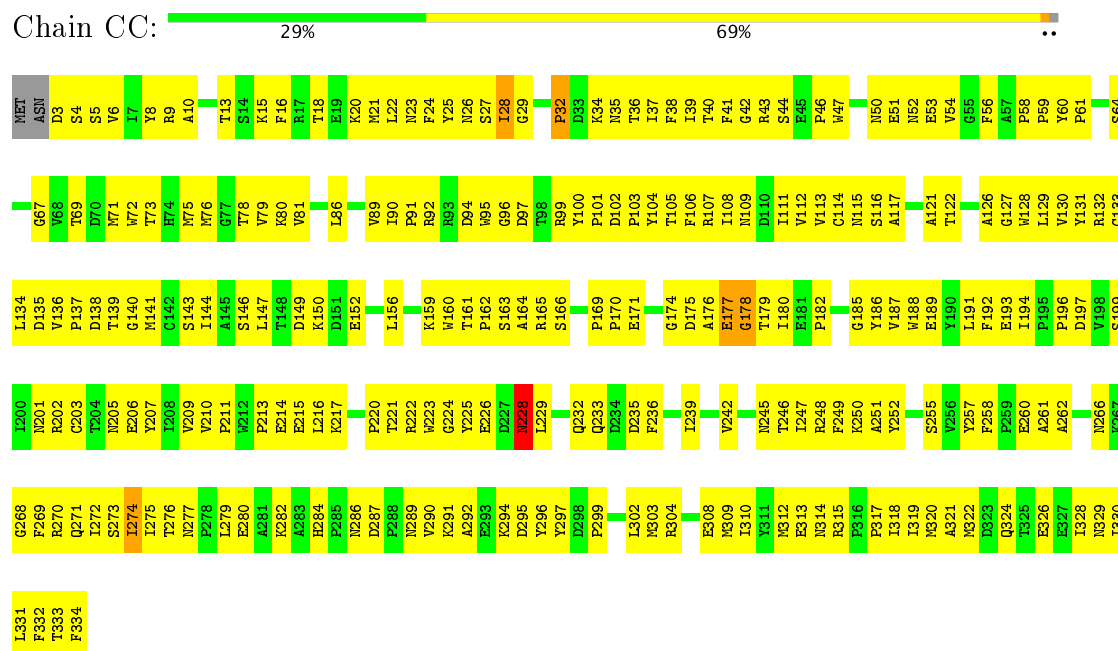
• Molecule 3: Baseplate wedge protein gp8

Chain CB: 28% 69%

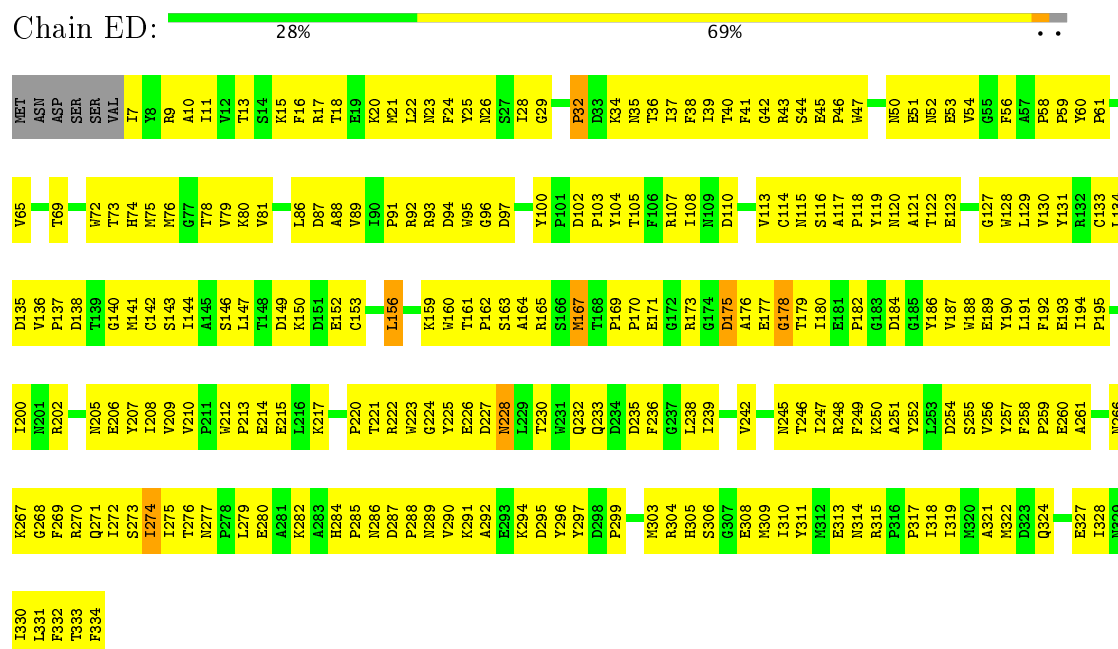




• Molecule 3: Baseplate wedge protein gp8

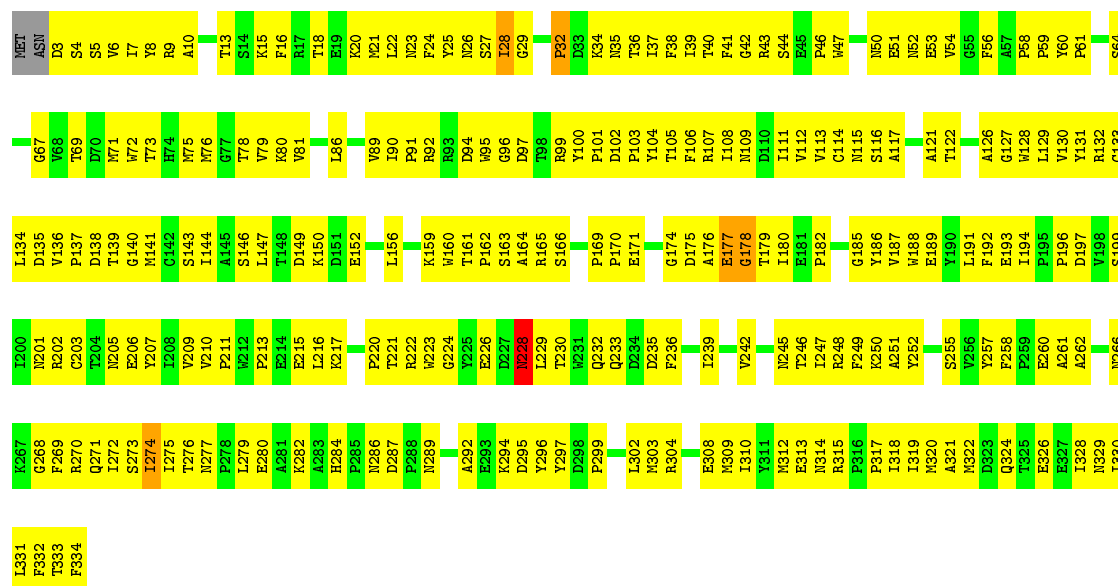


• Molecule 3: Baseplate wedge protein gp8



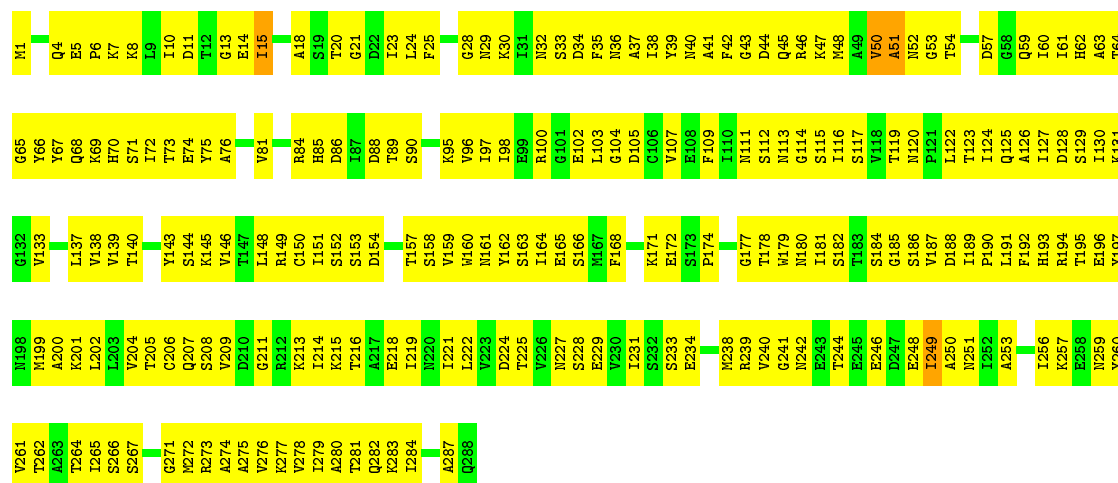
• Molecule 3: Baseplate wedge protein gp8

Chain EE:  30% 68%



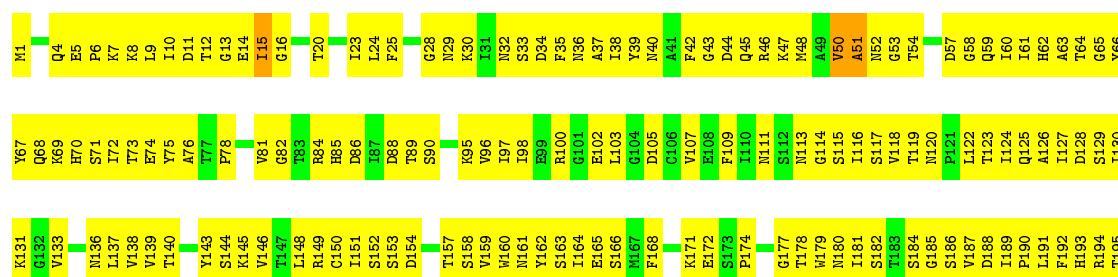
• Molecule 4: Baseplate wedge protein gp9

Chain F:  26% 72%

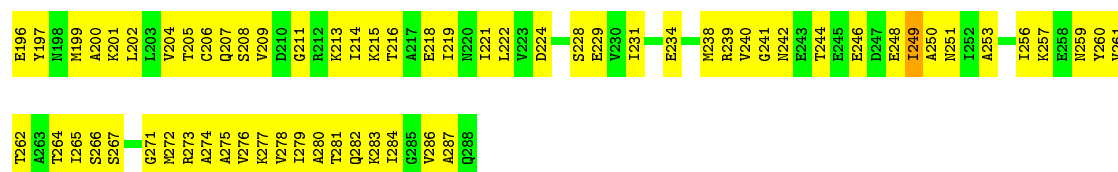


• Molecule 4: Baseplate wedge protein gp9

Chain G:  26% 73%

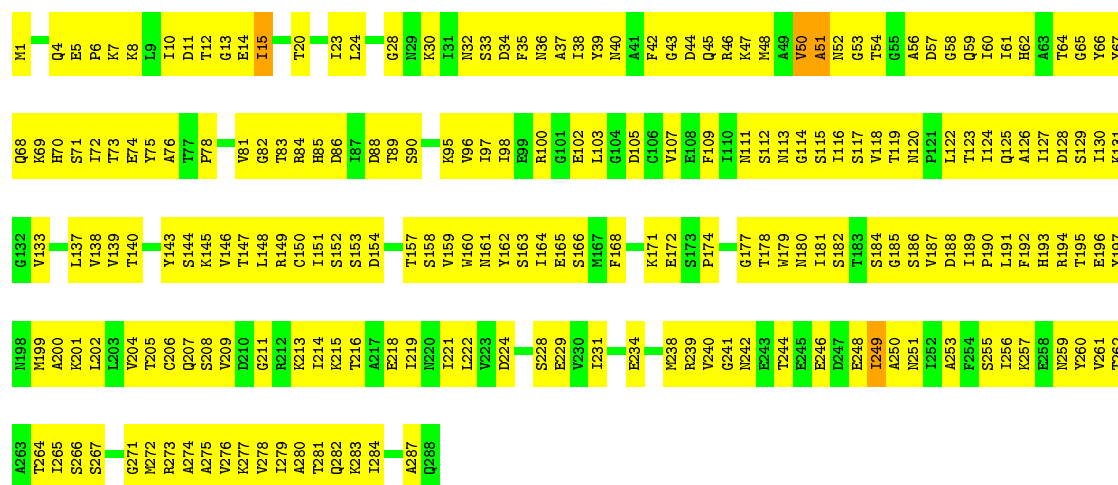






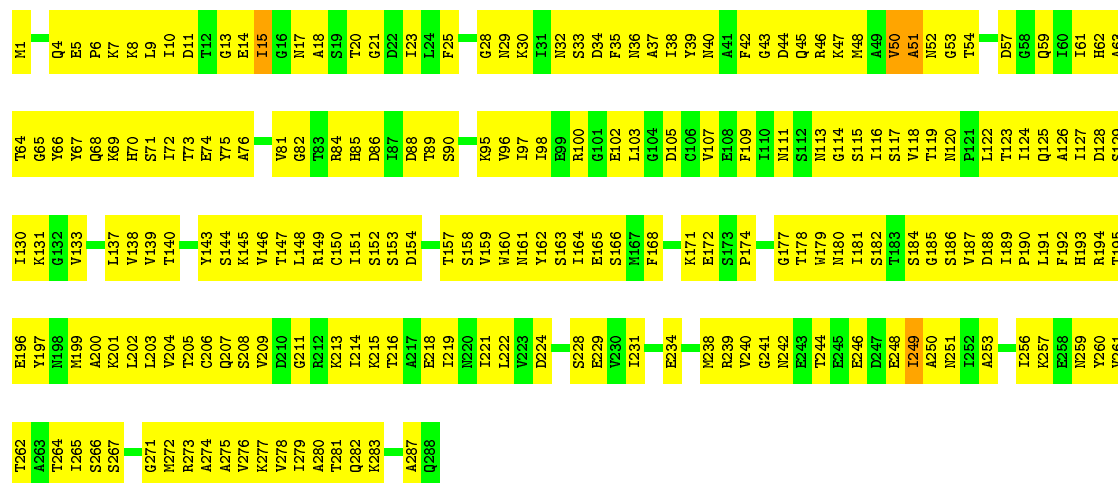
• Molecule 4: Baseplate wedge protein gp9

Chain H: 27% 72%



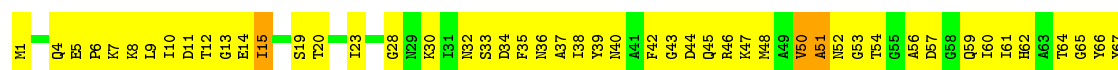
• Molecule 4: Baseplate wedge protein gp9

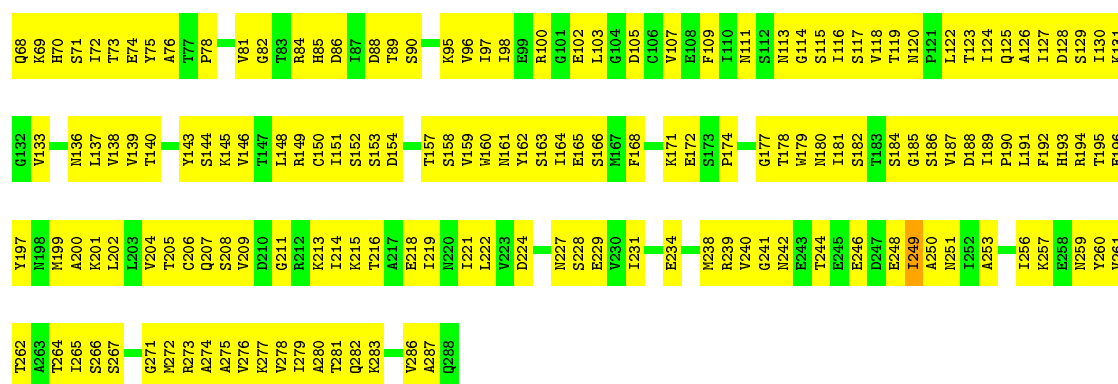
Chain V: 27% 71%



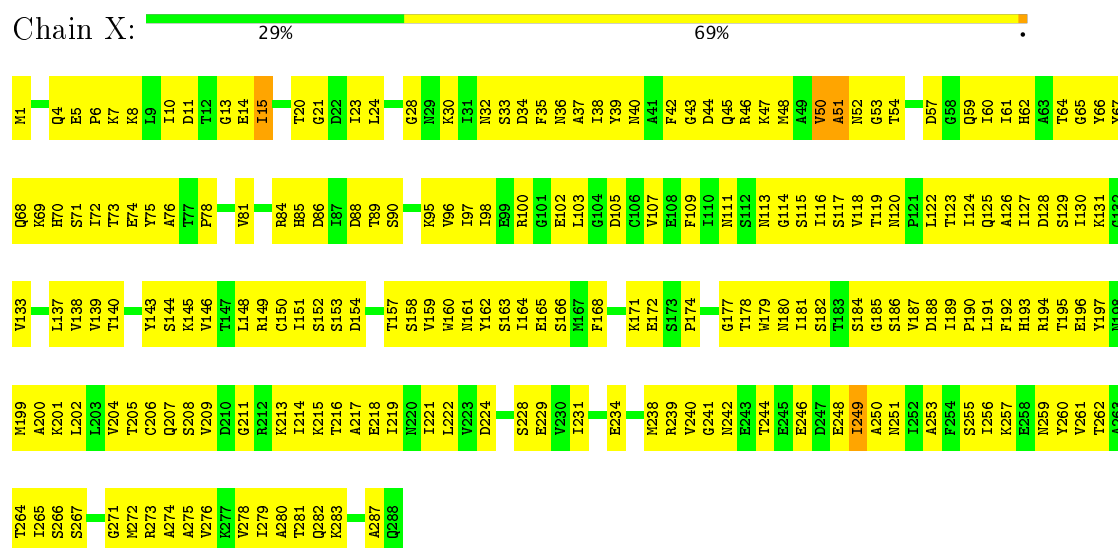
• Molecule 4: Baseplate wedge protein gp9

Chain W: 27% 71%

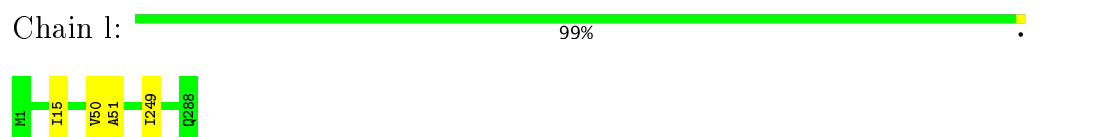




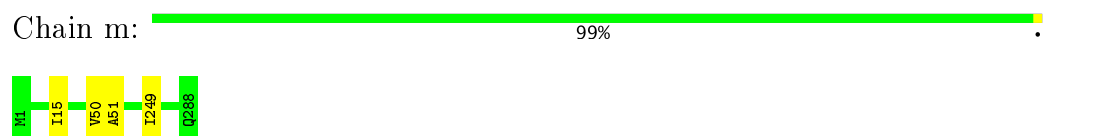
• Molecule 4: Baseplate wedge protein gp9



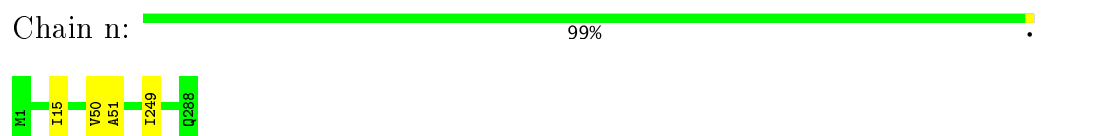
• Molecule 4: Baseplate wedge protein gp9



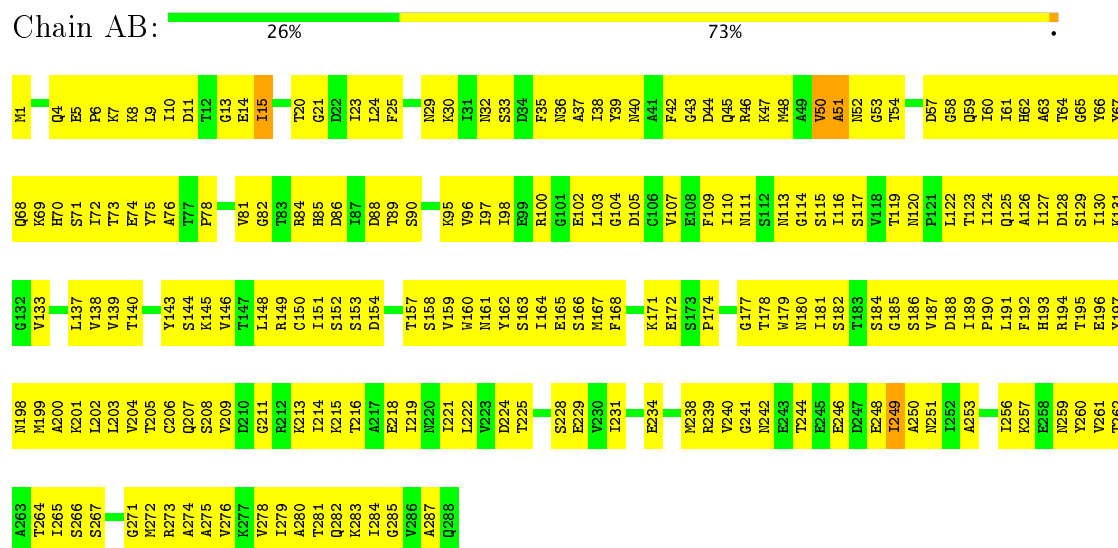
• Molecule 4: Baseplate wedge protein gp9



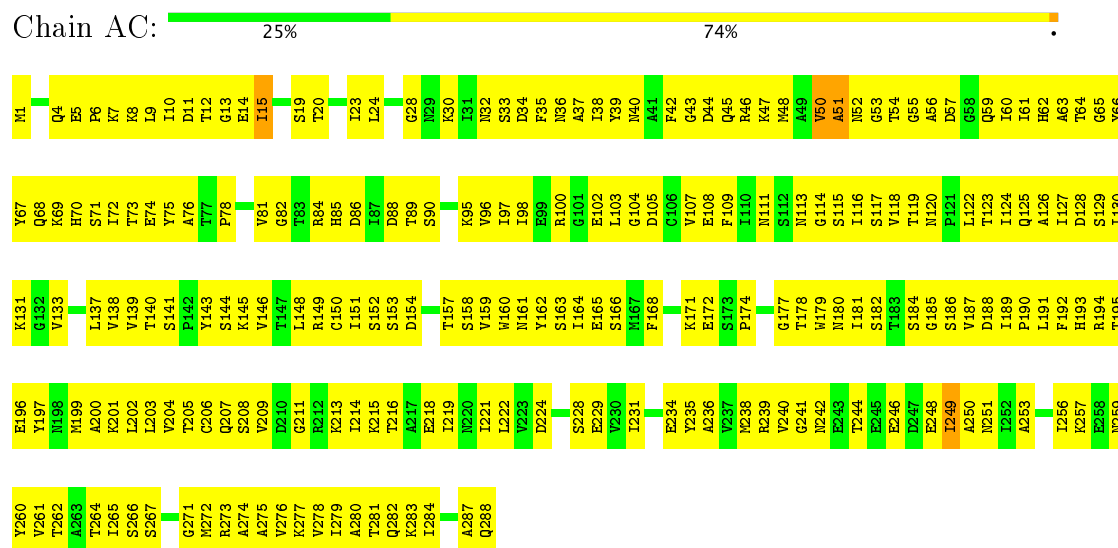
• Molecule 4: Baseplate wedge protein gp9



- Molecule 4: Baseplate wedge protein gp9



- Molecule 4: Baseplate wedge protein gp9



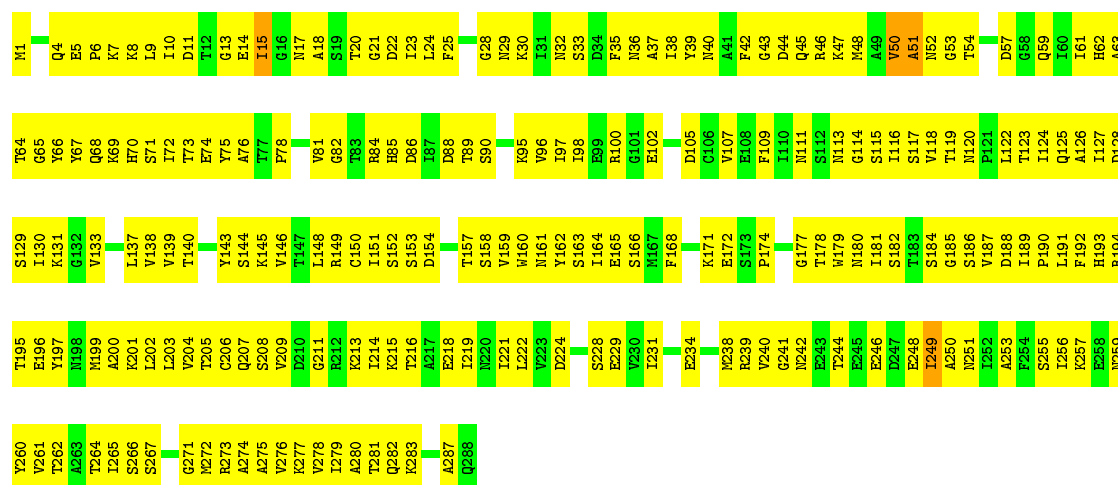
- Molecule 4: Baseplate wedge protein gp9





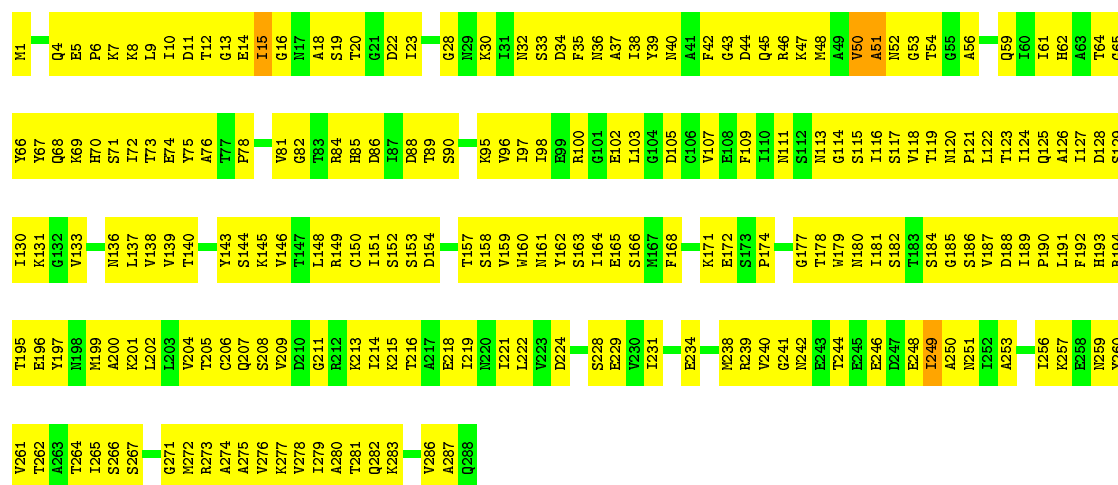
• Molecule 4: Baseplate wedge protein gp9

Chain CD: 27% 72%



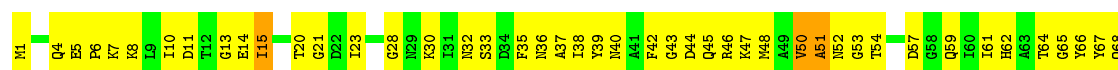
• Molecule 4: Baseplate wedge protein gp9

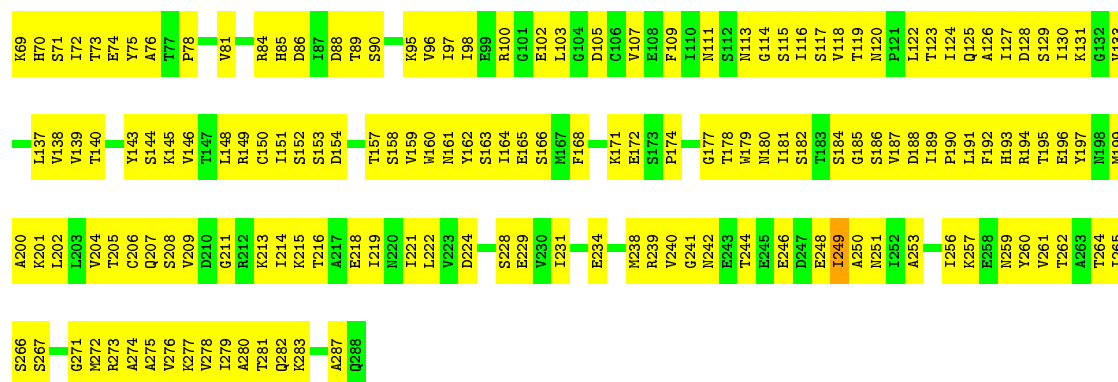
Chain CE: 27% 72%



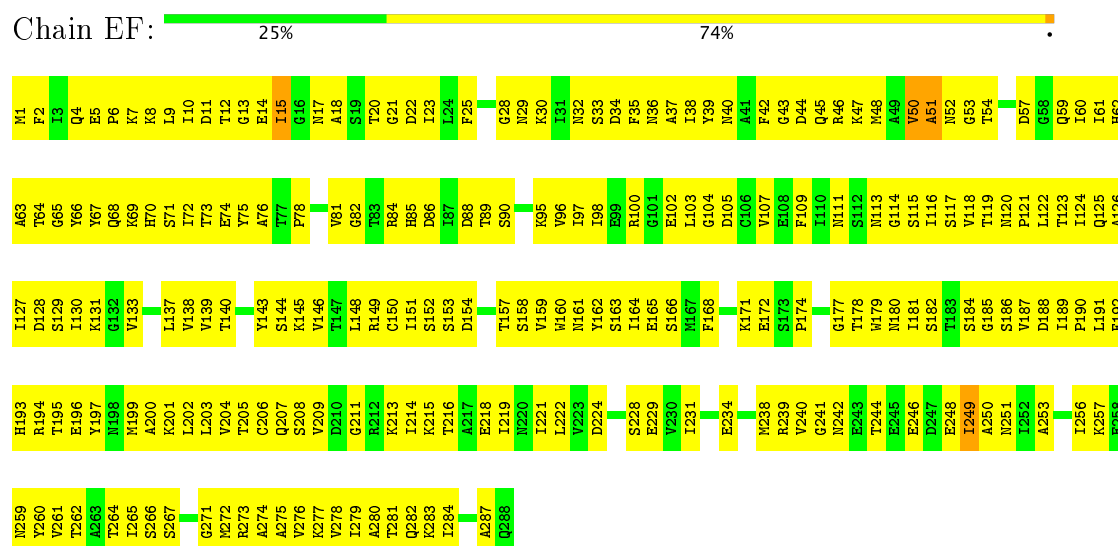
• Molecule 4: Baseplate wedge protein gp9

Chain CF: 31% 68%

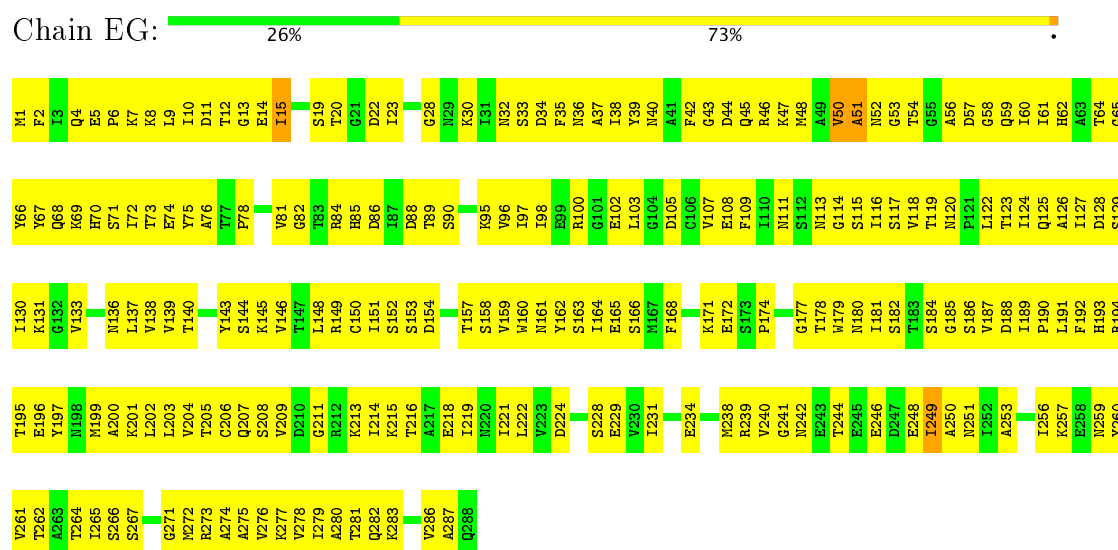




### • Molecule 4: Baseplate wedge protein gp9

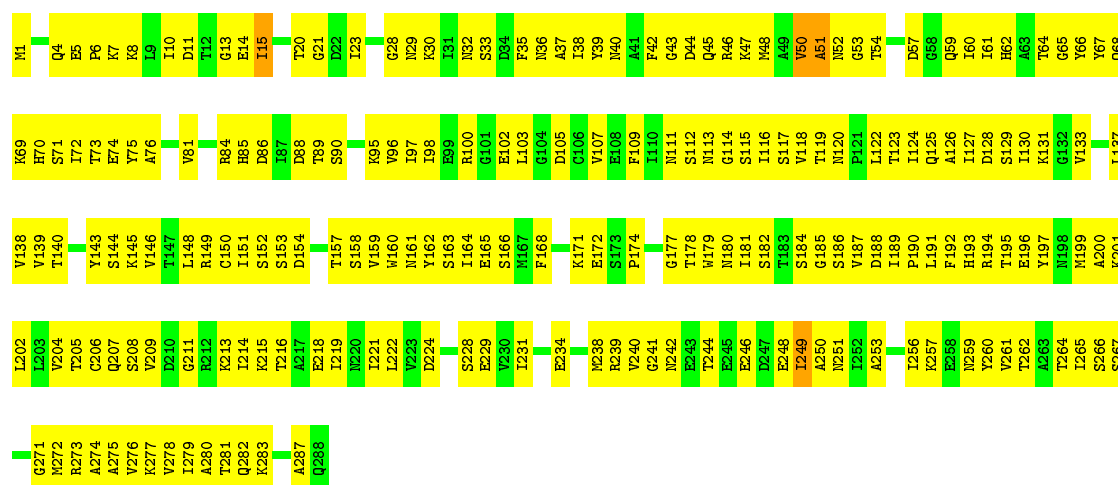


### • Molecule 4: Baseplate wedge protein gp9



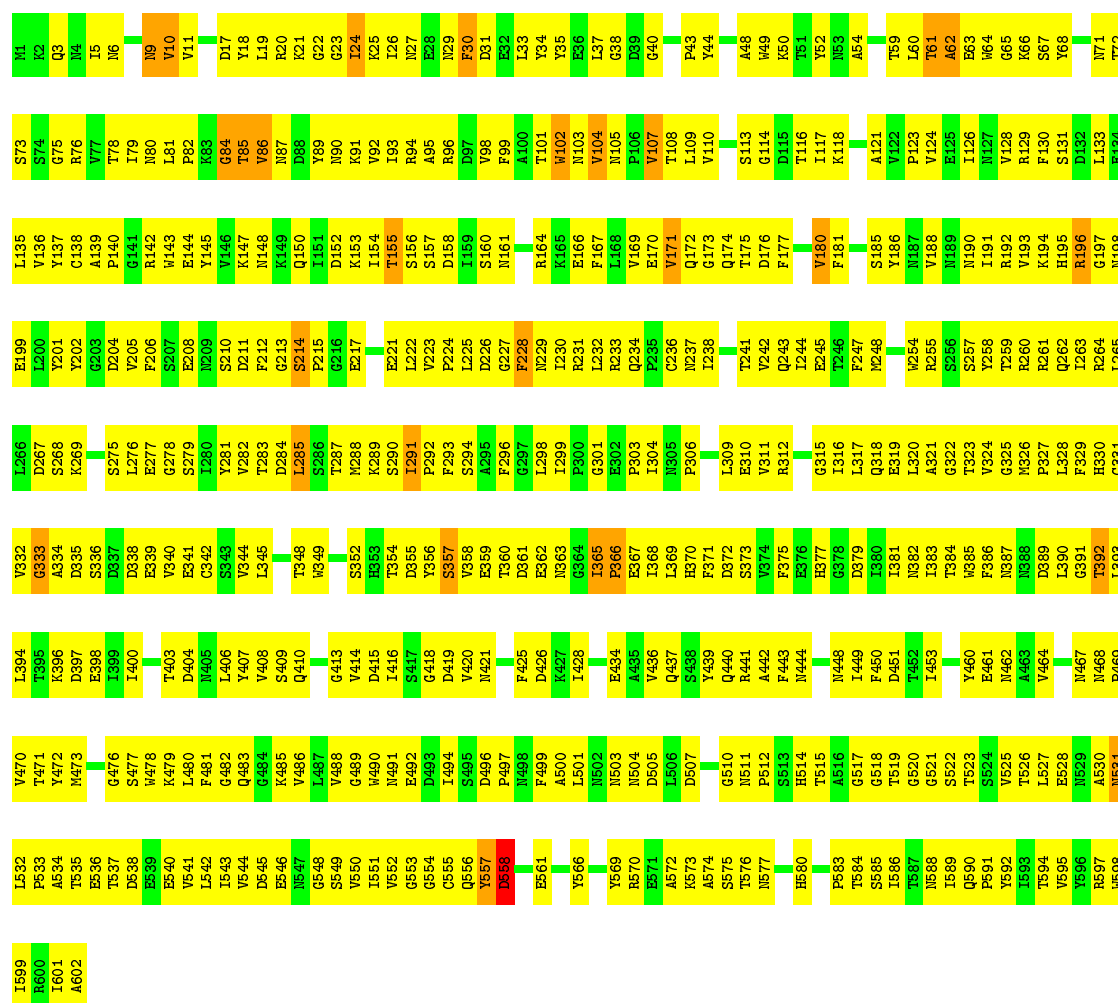
### • Molecule 4: Baseplate wedge protein gp9

Chain FA: 

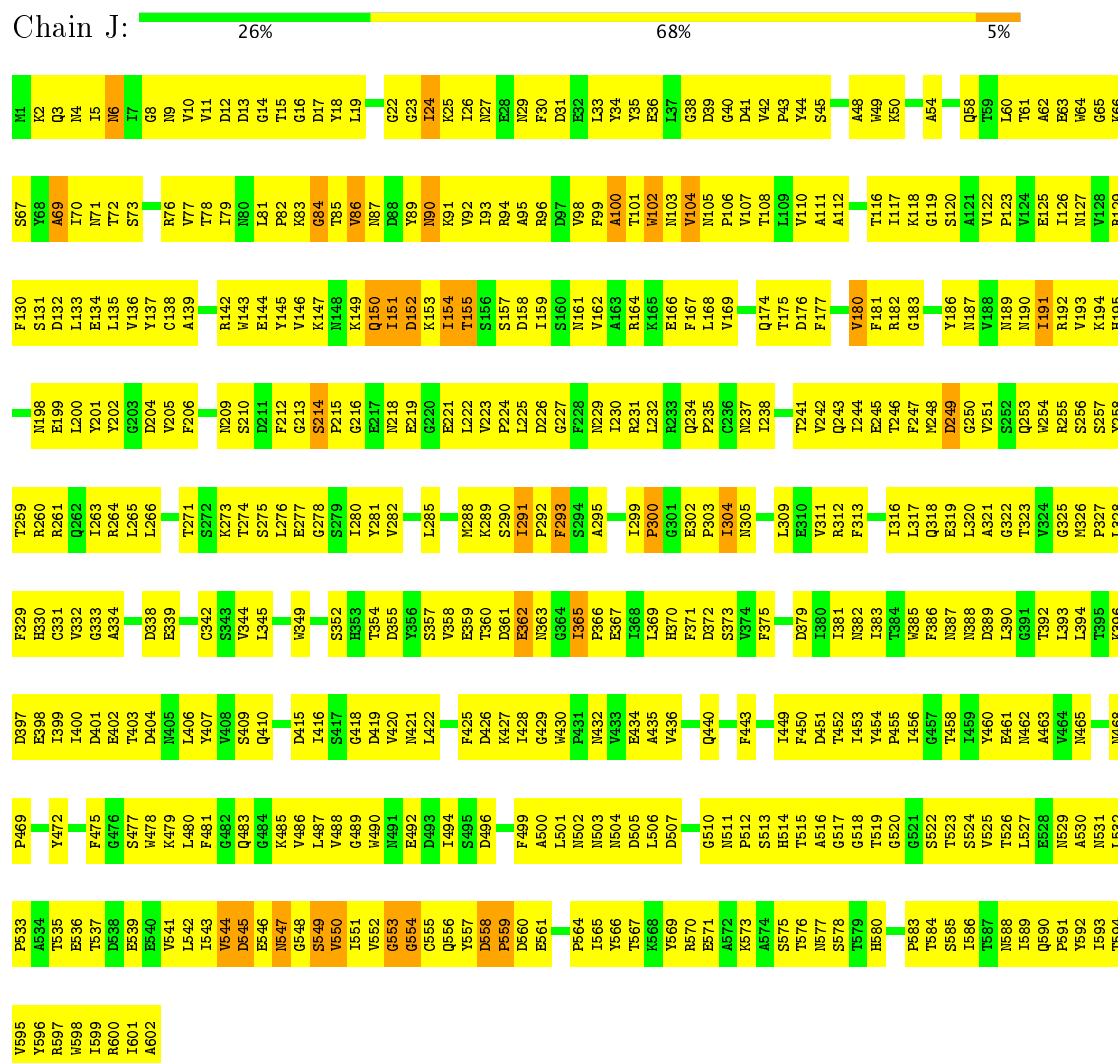


- Molecule 5: Baseplate wedge protein gp10

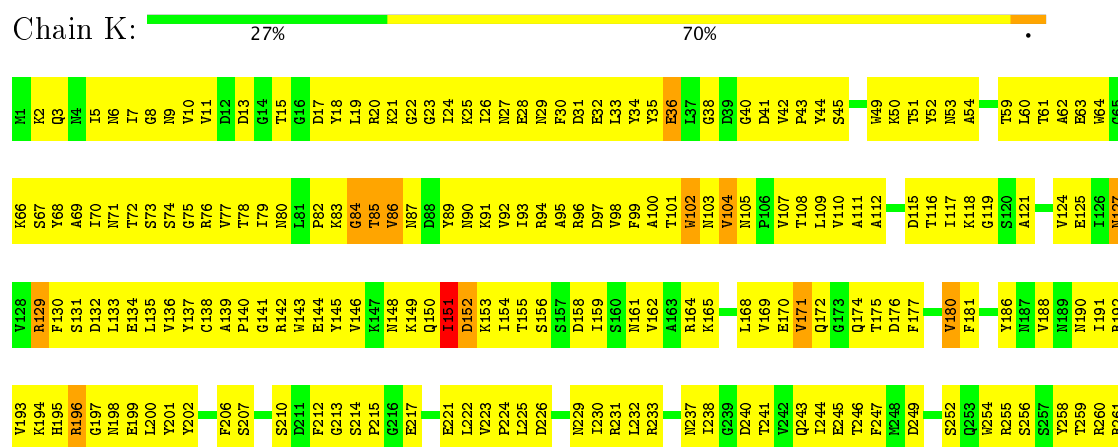
Chain I:  29% 66% .



• Molecule 5: Baseplate wedge protein gp10

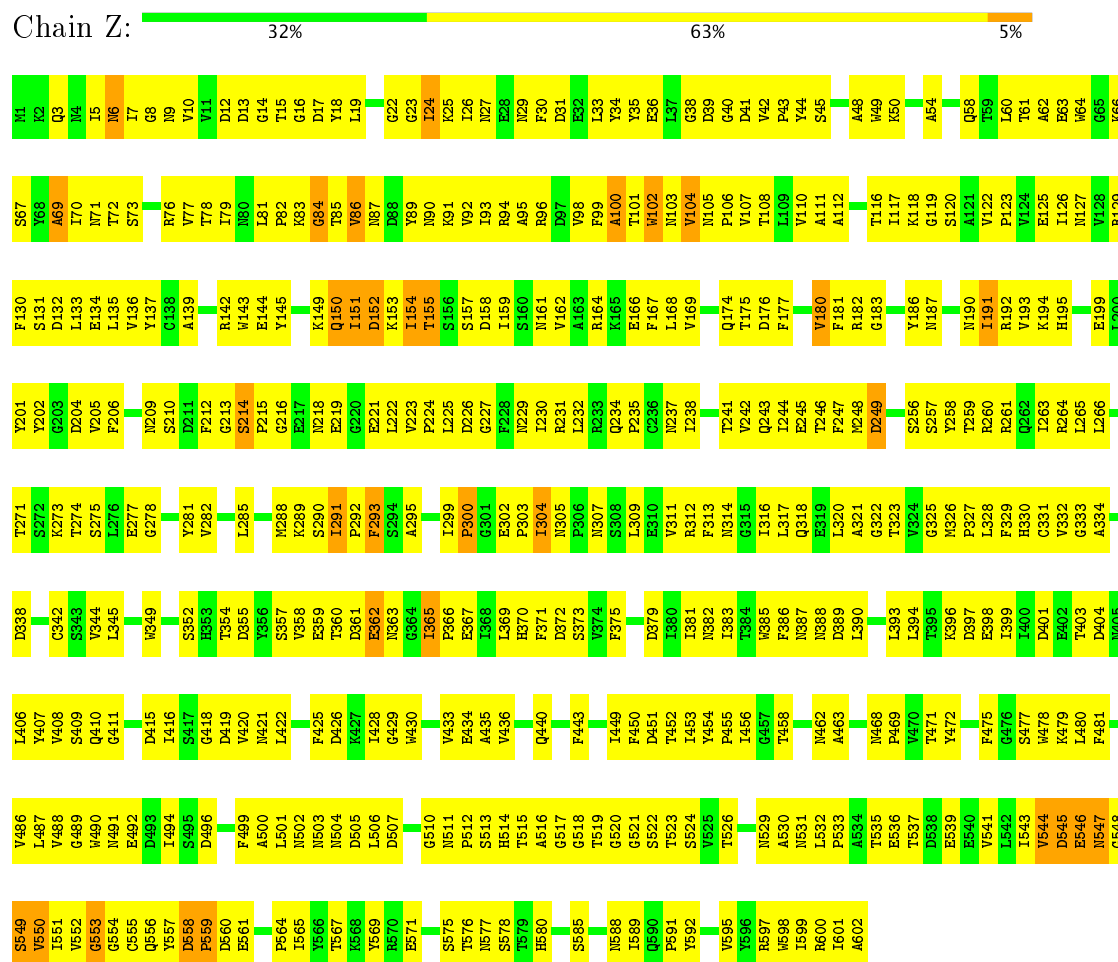


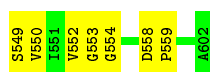
• Molecule 5: Baseplate wedge protein gp10











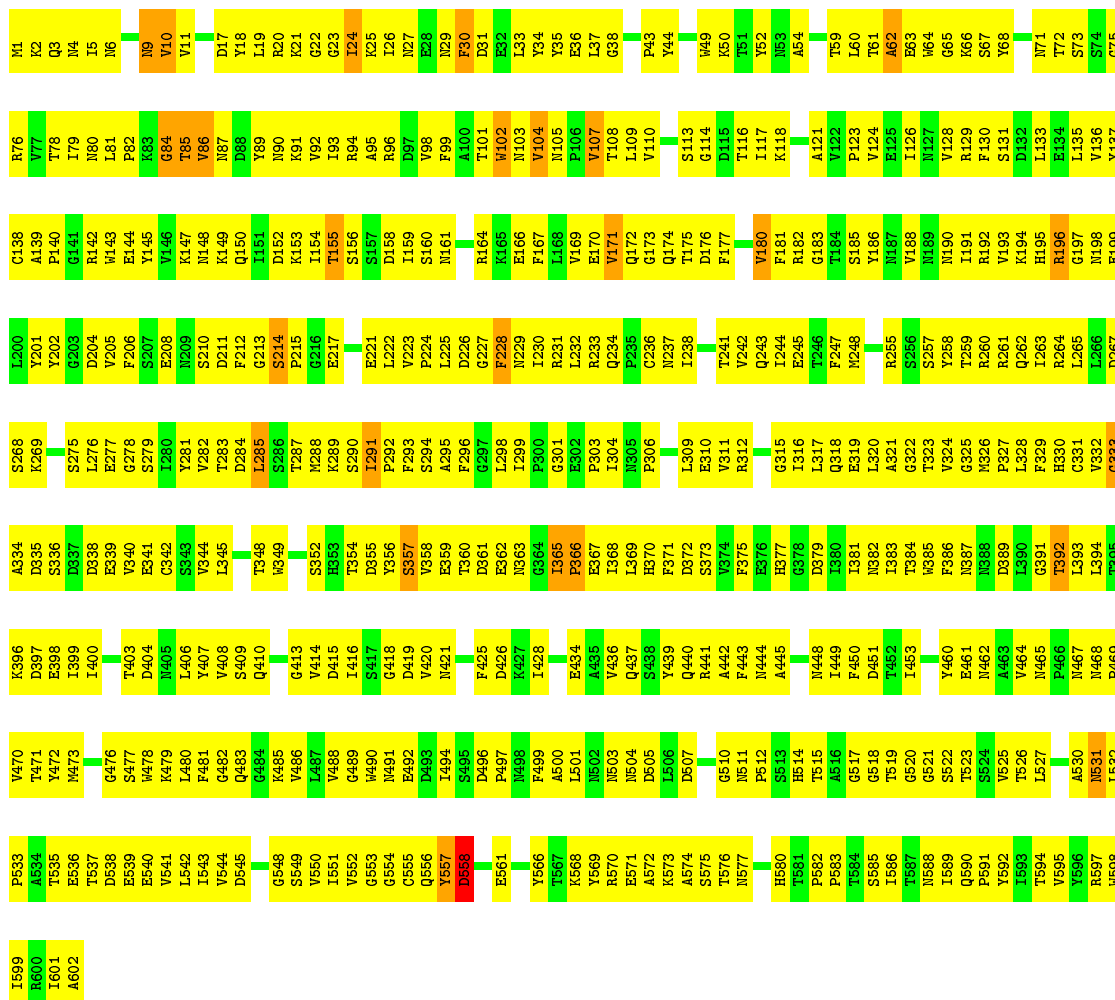
• Molecule 5: Baseplate wedge protein gp10

Chain q: 95% 5%



• Molecule 5: Baseplate wedge protein gp10

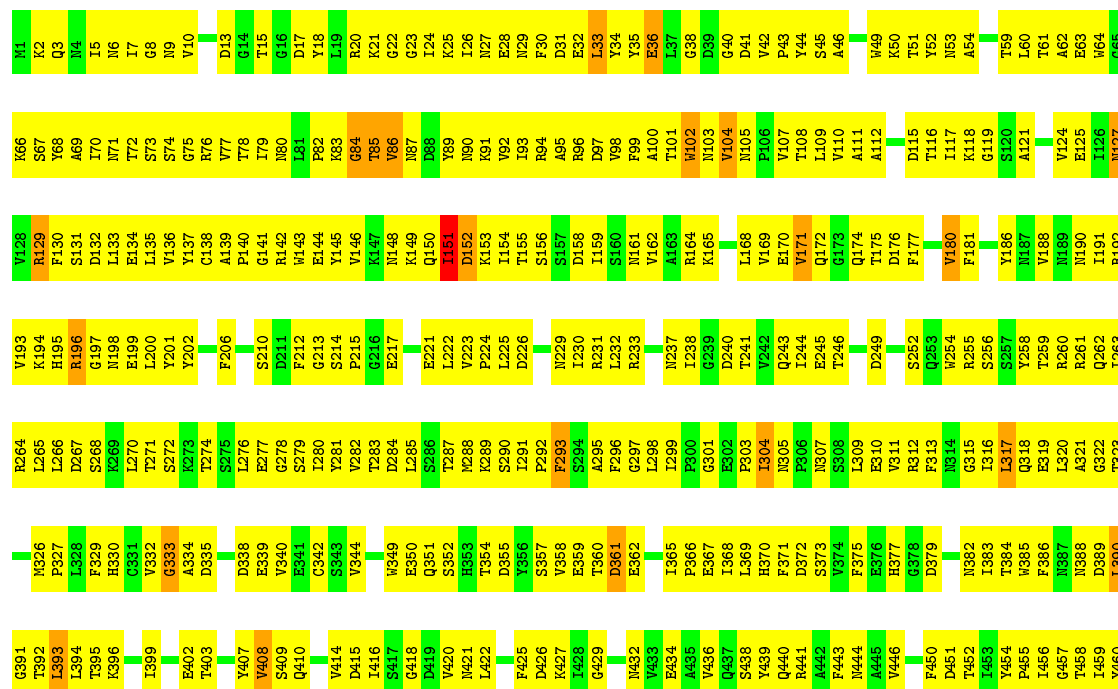
Chain AE: 28% 68%



• Molecule 5: Baseplate wedge protein gp10

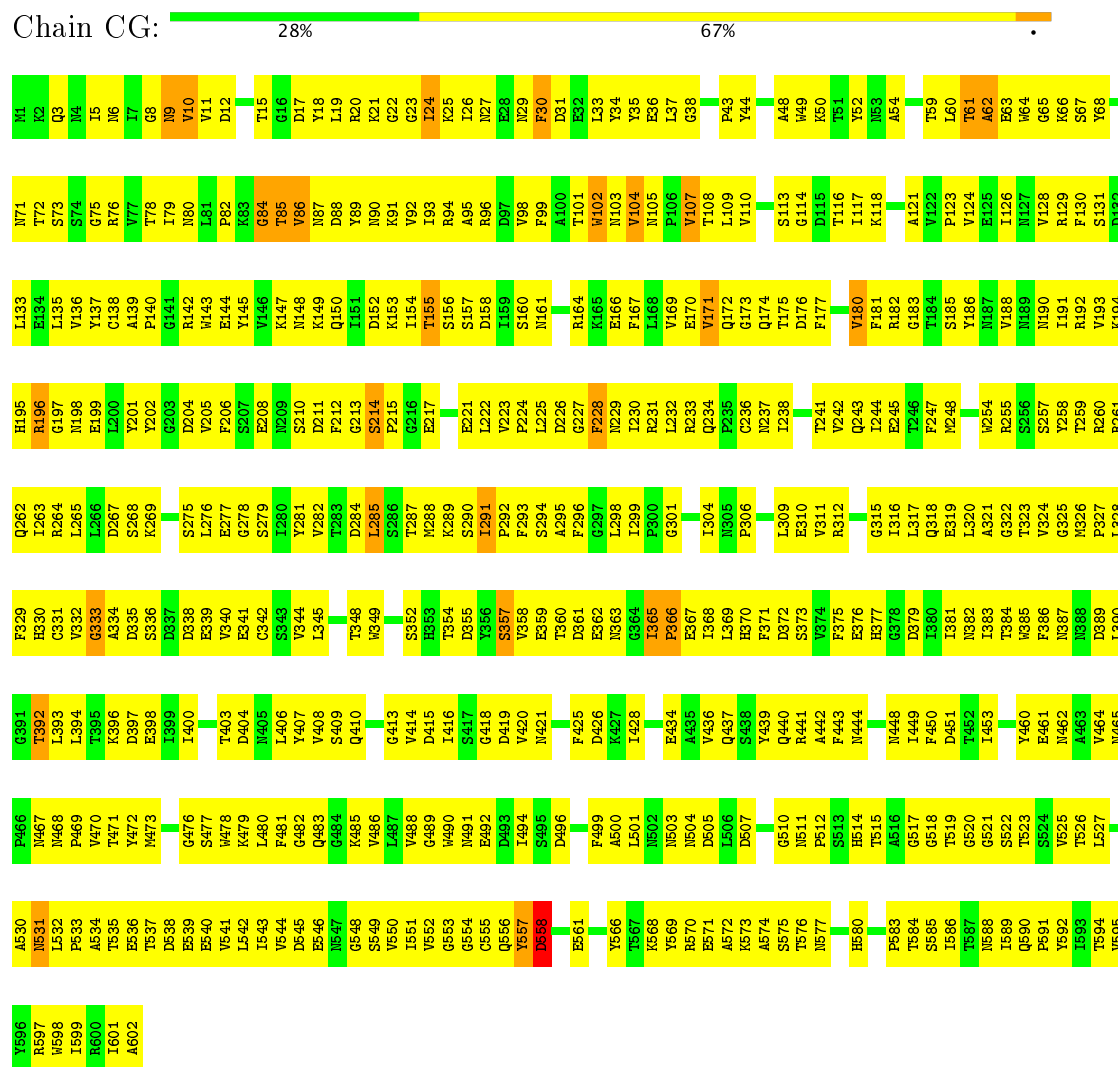
Chain AF: 27% 67% 5%



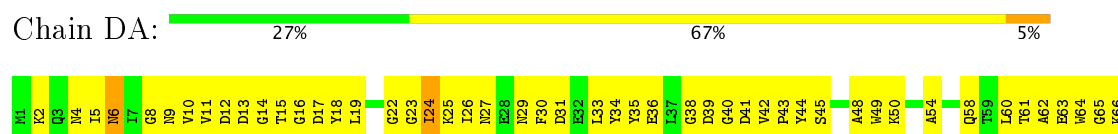




• Molecule 5: Baseplate wedge protein gp10



• Molecule 5: Baseplate wedge protein gp10



S67	F130	T259	F329	L384	P469	P533	V595
T68	S131	R260	H330	L394	P469	A534	V596
A70	D132	R261	C331	D397	Y472	T535	V597
L71	L133	Q262	V331	E398	Y472	T536	W598
W71	E134	R263	G333	I399	F475	T537	I599
T72	L135	R264	A334	I400	G476	D538	R600
S73	V136	L265	G334	D401	S477	E539	I601
	Y137	L266	D338	D404	W478	E540	A602
R76	C138	D267	E339	D404	K479	V541	
V77	A139	T271	V340	N405	K479	I542	
T78		S272	E341	L406	F481	I543	
I79	R142	K273	G342	Y407	F482	V544	
N80	W143	R274	S343	W408	Q483	D545	
L81	E144	T274	V344	S409	G484	E546	
P82	Y145	S275	I345	Q410	K485	N547	
K83	V146	L276			W486	S549	
E84	K147	E277	K349	D415	W488	I551	
	K148	G278	S352	S417	W489	V552	
T85	W149		R353	G418	W490	G553	
W86	Q150		T354	D419	K491	G554	
N87	L151	Y281	D355	W420	D492	C555	
D88	D152	V282	V356	N421	D493	Q556	
Y89	K153	E219	L285	L422	W494	Y557	
N90	D154	E221			S495	D558	
K91	I154	L222			D496	P559	
V92	T155	V223				D560	
I93	S156	P224				E561	
R94	S157	P225			F499		
A95	D158	D226			A500		
N96	I159	D227			I501		
D97	S160	G227			N502		
V98	N161	F228			N503		
F99	V162	N229			N504		
A100	A163	L230			D505		
T101	R164	L231			L506		
N102	K165	L232			Y569		
N103	E166	G301			E571		
W104	F167	E302			A572		
N105	L168	R370			A574		
P106	V169	F371			T576		
		D372			S578		
T107		N305			T579		
		L238			H580		
L108	Q174						
L109	T175						
V110	D176						
A111	F177						
A112							
T116	V180						
I117	R181						
K118	R182						
G119	G183						
S120							
A121	Y186						
V122	N187						
P123	V188						
N124	N189						
E125	I191						
I126	R192						
N127	V193						
V128	K194						
R129	H195						

• Molecule 5: Baseplate wedge protein gp10

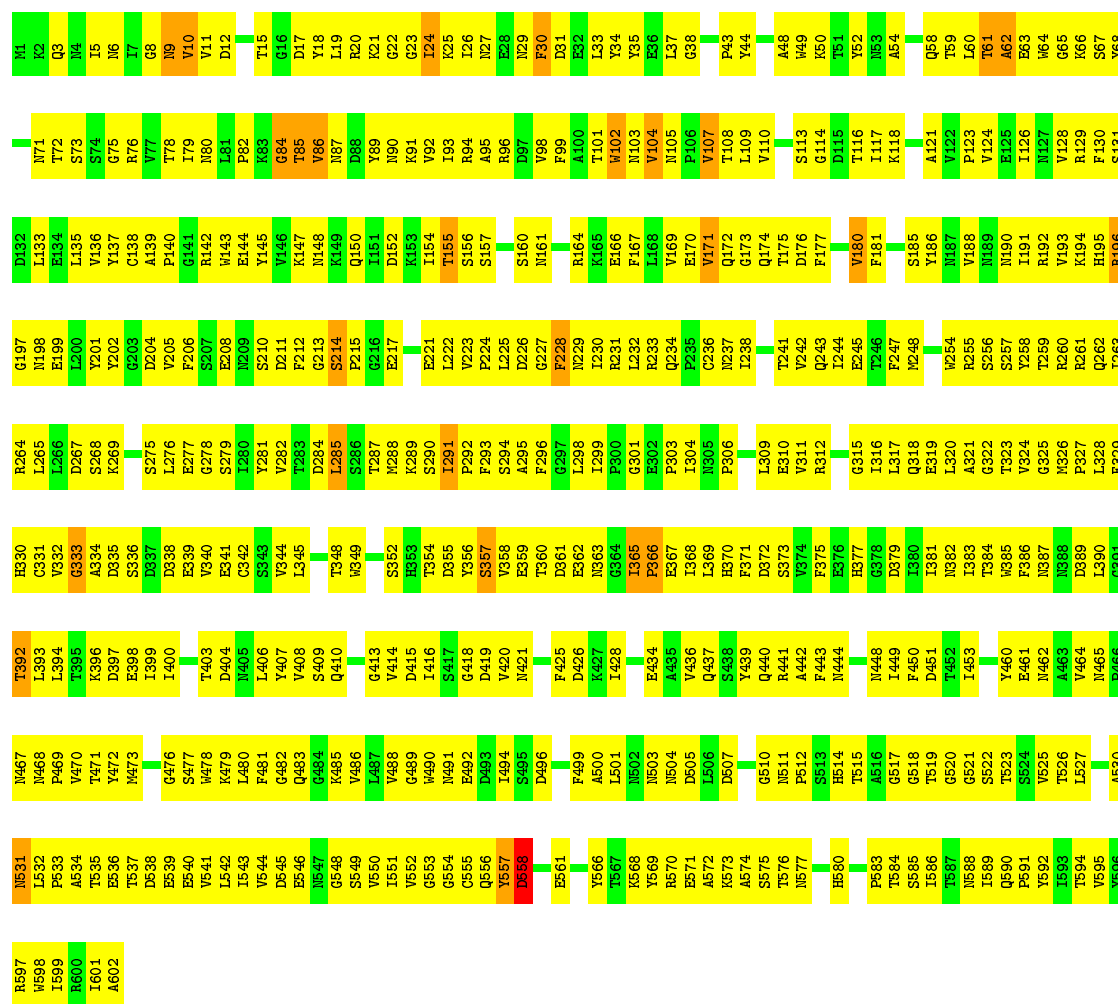
Chain DB:  26% 71%

V41	A62	V124	H189	T259	E319	F386
K2	B63	E125	N190	R260	L320	N387
Q3	W64	I126	I191	R261	A321	N388
I4	G65	N127	R192	Q262	G322	D389
I5	K66	V128	K193	L263	T323	L390
N6	S67	R129	K194	R264	G391	G391
I7	V68	F130	H195	L265	N326	T392
Q8	A69	D131	R196	L266	F327	T393
		S132	G197	D267	L328	L394
V10	N71	L133	N198	S268	F329	K395
V11	T72	E134	K199	K269	H330	
D12	S73	L135	L200	L270	G331	
D13	S74	V136	Y201	T271	V332	
G14	G75	Y137	I202	S272	G333	
T15	R76	C138	F206	K273	A334	
G16	V77	A139		T274	D335	
D17	P140	P141		S275		
Y18	T78	G141		L276	D338	
L19	W80	R142		E277	E339	
R20	L81	W143		G278	V340	
K21	P82	E144		S279	E341	
G22	K83	Y145		T280	C342	
G23	G84	V146		Y281	S343	
I24	T85	K147		V282	V344	
K25	W86	N148		T283		
T26	N87	K149		D284	W349	
N27	D88	Q150		L285	E350	
E28	Y89	T151		S286	Q351	
N29	N90	D152		T287	N420	
F30	K91	K153		N288	H353	
D31	V92	I154		K289	T354	
E32	I93	T155		S290	D355	
L33	R94	S156		L291	F356	
Y34	A95	S157		P292	S357	
E36	D97	I159		S294	V358	
L37	V98	S160		A295	E359	
G38	F99	N161		F296	T360	
D39	A100	V162		G297	D361	
G40	T101	A163		L298	E362	
D41	W102	R164		L299		
V42	N103	K165		G301	P365	
P43	W104			P300	E366	
Y44	N105			E302	E367	
S45	P106			P303	L368	
	V107			T241	L369	
A48	T108			Y242	H370	
W49	L109			Q243	F371	
K50	Q172			N305	Q440	
T51	V110			E245	R441	
Y52	A111			T246	D372	
N53	A112			F247	S373	
A54	D115			K248	Y374	
S45	T116			D249	F375	
S55	I117			V311	E376	
S56	K118			R312	H377	
G58	G119			S313	G378	
T59	S120			S252	D379	
L60	A121			W254		
T61				R255		
				S256		
				T257		
				V258		



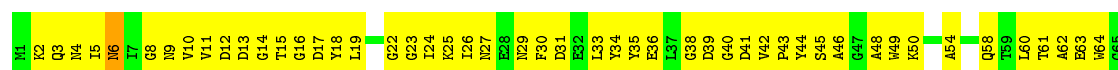
• Molecule 5: Baseplate wedge protein gp10

Chain FB: 28% 67%



• Molecule 5: Baseplate wedge protein gp10

Chain FC: 27% 67% 5%



K66	R129	H195	Y258	F329	L394	P469	P533	Y596
S67	F130	H196	T299	H330	T395	P470	A534	R597
<b>Y68</b>	<b>D132</b>	N198	R260	C331	K396	Y472	T535	W598
<b>A69</b>	<b>D133</b>	E199	R261	V332	R397		E536	I599
I70	L133	L200	Q262	G333	E398	G475	D537	R600
N71	E134	Y201	L263	A334	I399	F476	D538	I601
T72	L135	Y202	R264		I400	S477	E539	A602
<b>S73</b>	<b>V136</b>	<b>Q203</b>	L266	D638	D401	W478	E540	
	<b>Y137</b>	<b>D204</b>	L266	E339	D404	K479	V541	
	<b>C138</b>	<b>F206</b>	T271	V340	N405	F480	I542	
R76	<b>A139</b>		T272	G342	E341	F481	I543	
T78	R142	Y209	K273	G343	L406	Q482	V544	
I79	W143	S210	T274	V344	Y407	Q483	E545	
<b>N80</b>	E144	D211	S275	L345	V408	Q484	E546	
L81	F145	E212	T276		S409	K485	N547	
P82	V146	G213	E277	K349	Q410	V486	G548	
<b>K84</b>	<b>K147</b>	<b>S214</b>	G278		D415	V488	S549	
<b>R85</b>	<b>W148</b>	P215			D416	Q489	V551	
<b>T86</b>	<b>K149</b>	G216	Y281	S352	S417	W490	V552	
N87	Q150	E217	V292	R353	G418	P491	G553	
<b>D88</b>	<b>D151</b>	<b>E218</b>	D291	T354	D419	A500	G554	
<b>Y89</b>	<b>D152</b>	<b>E219</b>	L285	V356	V420	D493	C555	
	<b>K153</b>	<b>E220</b>		<b>S357</b>	N421	L494	Y556	
K91	I154	E221	M288	G364	L422	S495	Y557	
V92	T155	L222	K289	T365	F425	D496	D558	
R93	S156	V223	S290	P366	D426		P559	
A95	D158	L225	I291	R367	K427	F499	P560	
R96	I159	D226	P292	E362	V428	A501	N502	
<b>N97</b>	<b>S160</b>	<b>G227</b>	F293	N363	G429	N503	P564	
V98	N161	<b>F228</b>	A295	G364	Q430	N504	I565	
F99	V162	N229	I299	L369	P431	D507	V566	
<b>A100</b>	<b>R163</b>	L230	P300	L368	N432		T567	
T101	K164	L232	R231	E370	V433	L506	V568	
<b>N102</b>	<b>K165</b>	<b>L233</b>	G302	R370	E434		Y569	
<b>N103</b>	<b>E166</b>	<b>Q234</b>	E303	F371	A435	G510	R570	
<b>V104</b>	<b>F167</b>	P235	I304	D372	V436	N511	E571	
N105	V169	C236	N305	S373	Q440	P512	K573	
V107		L237	L309	V374	F443	S513	A574	
T108	Q174	N238	E310	F375	I449	H514	T576	
L109	T175	T241	V311	E376	F450	T515	N577	
V110	D176	V242	R312	R377	D451	G517	S578	
A111	F177	Q243	F313	G378	T452	G518	T579	
	<b>V180</b>	L244		I380	T453	T519	H580	
T116	F181	E245	I316	I381	Y454	G520	P583	
I117	R182	T246	L317	N382	P455	G521	T584	
K118	G183	F247	Q318	I383	I456	S522	S585	
G119		E248	E319	T384	T458	T523		
S120	Y186	D249	L320	K385	V458	V524	N588	
<b>A121</b>	<b>N187</b>	<b>G250</b>	A321	N386	V458	V525	I589	
V122	V188	V251	G322	T387	N463	L527	T590	
P123	N189	<b>S252</b>	T323	N388	A463	E528	P591	
<b>V124</b>	<b>N190</b>	<b>Q253</b>	V324	D389	V464	N529	Y592	
E125	<b>I191</b>	N254	G325	L390	N465	A530	<b>I593</b>	
I126	R192	R255	M326	G391	T468	N531	T594	
N127	V193	S256	P327	L393	N468	L532	V595	
<b>V128</b>	K194	S257	L328					

• Molecule 5: Baseplate wedge protein gp10

Chain FD: 26% 70%

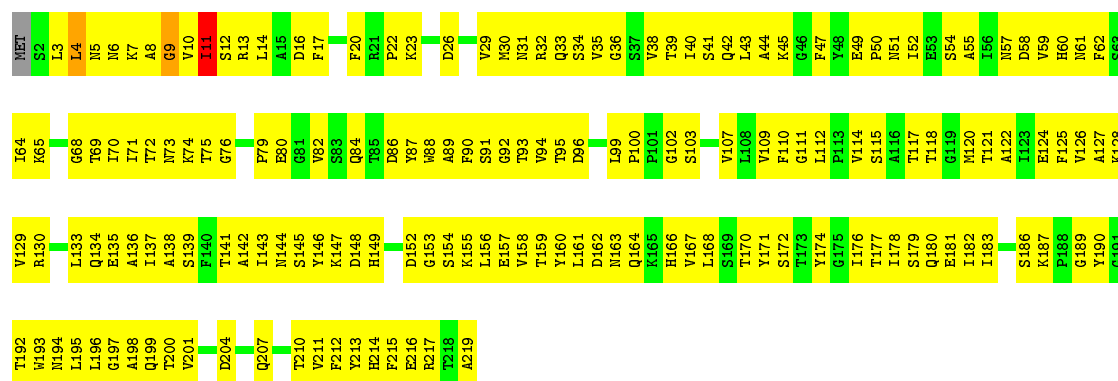
V193	T263	G391	V128	K66	V193	T263	G391
K194	R264	K326	R129	S67	K194	R264	K326
F130	L265	P327	F130	Y68	F130	L265	P327
<b>L196</b>	<b>L266</b>	<b>L394</b>	<b>S131</b>	<b>A69</b>	<b>L196</b>	<b>L266</b>	<b>L394</b>
I5	D267	T295	D132	I70	I5	D267	T295
N6	G197	T296	D133	N71	N6	G197	T296
N198	L198	K396	L133	T72	N198	L198	K396
E199	E134	<b>G391</b>	E134	T72	E199	E134	<b>G391</b>
L200	L136	V332	L136	S73	L200	L136	V332
Y201	T271	<b>G333</b>	Y201	S74	Y201	T271	<b>G333</b>
Y202	K273	A334	Y202	G75	Y202	K273	A334
	T274	D335		R76		T274	D335
F206	<b>S275</b>		F206	V77	F206	<b>S275</b>	
S210	L276	D338	S210	T78	S210	L276	D338
D211	E277	E339	D211	I79	D211	E277	E339
F212	S279	V340	F212	N80	F212	S279	V340
G213	E280	E341	G213	<b>L81</b>	G213	E280	E341
S214	K281	C342	S214	P82	S214	K281	C342
P215	V282	S343	P215	<b>G84</b>	P215	V282	S343
<b>G216</b>	<b>T283</b>	V344	<b>G216</b>	T85	<b>G216</b>	<b>T283</b>	V344
E217	D284	W349	E217	<b>R86</b>	E217	D284	W349
E221	L285	E350	E221	N87	E221	L285	E350
V223	<b>S286</b>	Q351	V223	<b>D88</b>	V223	<b>S286</b>	Q351
P224	T287	S352	P224	<b>N90</b>	P224	T287	S352
V225	M288	<b>H353</b>	V225	<b>I151</b>	V225	M288	<b>H353</b>
L225	K289	T354	L225	K91	L225	K289	T354
S290	S290	D355	S290	V92	S290	S290	D355
P292	F292	Y356	P292	I93	P292	F292	Y356
F293	S294	V357	F293	R94	F293	S294	V357
A295	<b>S294</b>	E359	A295	R96	A295	<b>S294</b>	E359
T360	T360	T360	T360	D97	T360	T360	T360
<b>D361</b>	<b>F296</b>	<b>D361</b>	<b>D361</b>	V98	<b>D361</b>	<b>F296</b>	<b>D361</b>
G297	G297	E362	G297	F99	G297	G297	E362
L298	L298	A100	L298	A100	L298	L298	A100
I299	I299	V102	I299	T101	I299	I299	V102
<b>P300</b>	<b>G301</b>	<b>A163</b>	<b>P300</b>	<b>W102</b>	<b>P300</b>	<b>G301</b>	<b>A163</b>
E302	E302	R164	E302	N103	E302	E302	R164
<b>E303</b>	<b>E303</b>	K165	<b>E303</b>	V104	<b>E303</b>	<b>E303</b>	K165
L168	L168	L168	L168	N105	L168	L168	L168
V169	V169	V169	V169	P106	V169	V169	V169
E170	E170	E170	E170	V107	E170	E170	E170
V171	V171	V171	V171	T108	V171	V171	V171
<b>Q172</b>	<b>P106</b>	<b>Q172</b>	<b>Q172</b>	L109	<b>Q172</b>	<b>P106</b>	<b>Q172</b>
G173	G173	G173	G173	V110	G173	G173	G173
Q174	Q174	Q174	Q174	A111	Q174	Q174	Q174
D176	D176	D176	D176	A112	D176	D176	D176
F177	F177	F177	F177	D115	F177	F177	F177
<b>V180</b>	<b>V180</b>	<b>V180</b>	<b>V180</b>	T116	<b>V180</b>	<b>V180</b>	<b>V180</b>
F181	F181	F181	F181	I117	F181	F181	F181
				K118			
Y186	Y186	Y186	Y186	G119	Y186	Y186	Y186
<b>N187</b>	<b>N187</b>	<b>N187</b>	<b>N187</b>	A121	<b>N187</b>	<b>N187</b>	<b>N187</b>
<b>H188</b>	<b>H188</b>	<b>H188</b>	<b>H188</b>	T59	<b>H188</b>	<b>H188</b>	<b>H188</b>
<b>V189</b>	<b>V189</b>	<b>V189</b>	<b>V189</b>	L60	<b>V189</b>	<b>V189</b>	<b>V189</b>
<b>N190</b>	<b>N190</b>	<b>N190</b>	<b>N190</b>	T61	<b>N190</b>	<b>N190</b>	<b>N190</b>
<b>E125</b>	<b>E125</b>	<b>E125</b>	<b>E125</b>	A62	<b>E125</b>	<b>E125</b>	<b>E125</b>
<b>I126</b>	<b>I126</b>	<b>I126</b>	<b>I126</b>	E63	<b>I126</b>	<b>I126</b>	<b>I126</b>
<b>N127</b>	<b>N127</b>	<b>N127</b>	<b>N127</b>	W64	<b>N127</b>	<b>N127</b>	<b>N127</b>
				G65			



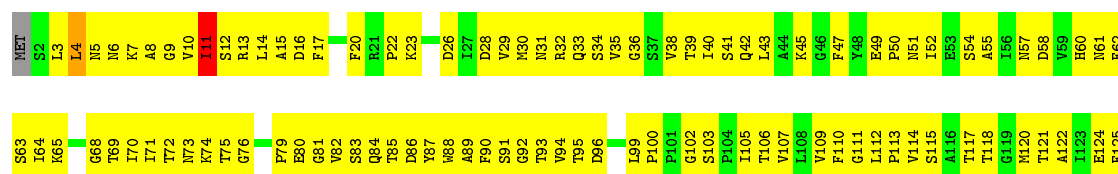
• Molecule 6: Baseplate wedge protein gp11



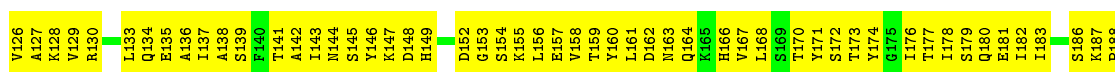
• Molecule 6: Baseplate wedge protein gp11



• Molecule 6: Baseplate wedge protein gp11







- Molecule 6: Baseplate wedge protein gp11

Chain b: 98%



- Molecule 6: Baseplate wedge protein gp11

Chain c: 98%



- Molecule 6: Baseplate wedge protein gp11

Chain d: 98%



- Molecule 6: Baseplate wedge protein gp11

Chain r: 98%



- Molecule 6: Baseplate wedge protein gp11

Chain s: 98%



- Molecule 6: Baseplate wedge protein gp11

Chain t: 98%

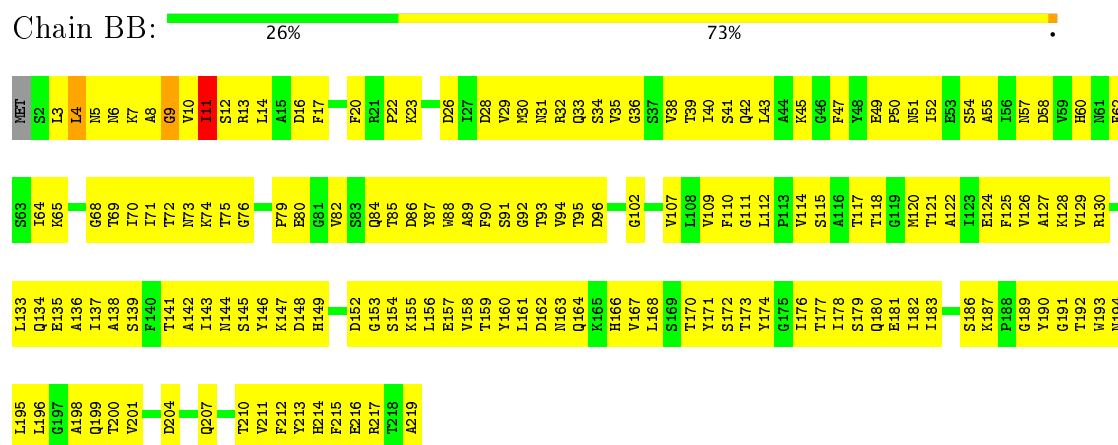


- Molecule 6: Baseplate wedge protein gp11

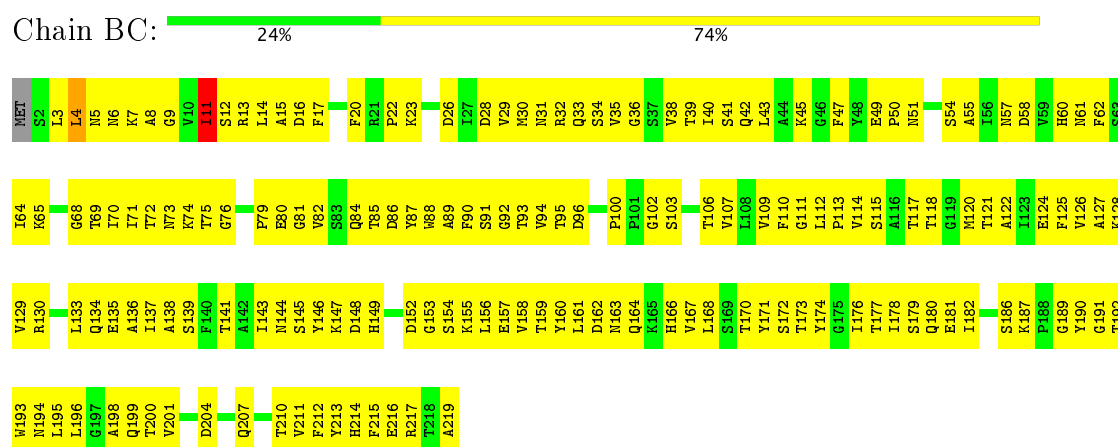
Chain BA: 26%



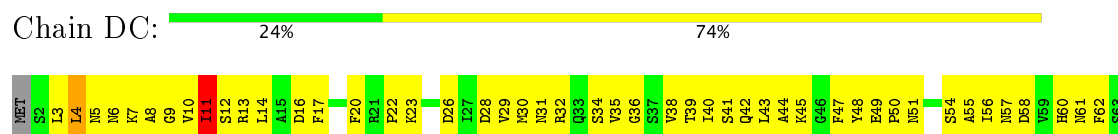
• Molecule 6: Baseplate wedge protein gp11

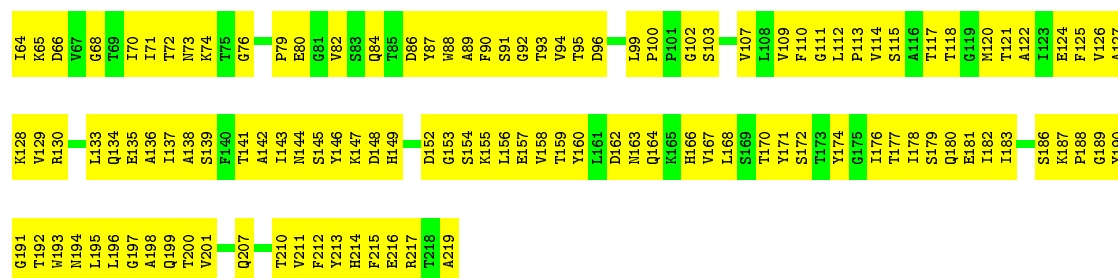


• Molecule 6: Baseplate wedge protein gp11

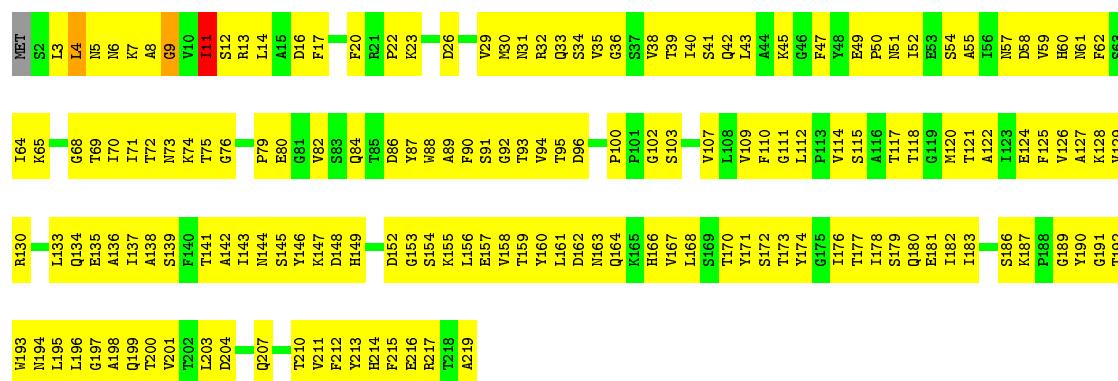


• Molecule 6: Baseplate wedge protein gp11

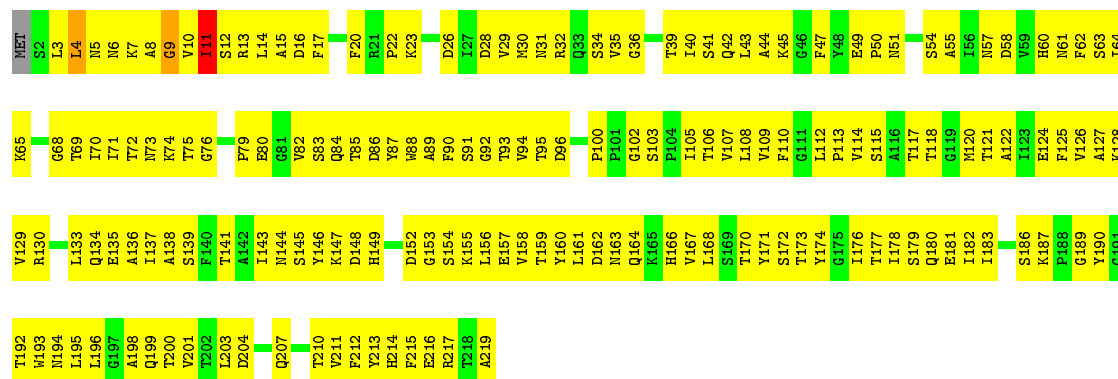




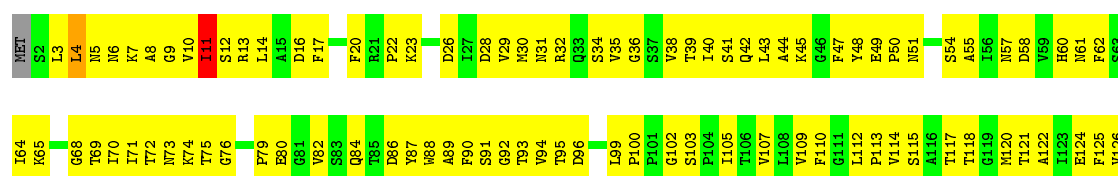
- Molecule 6: Baseplate wedge protein gp11

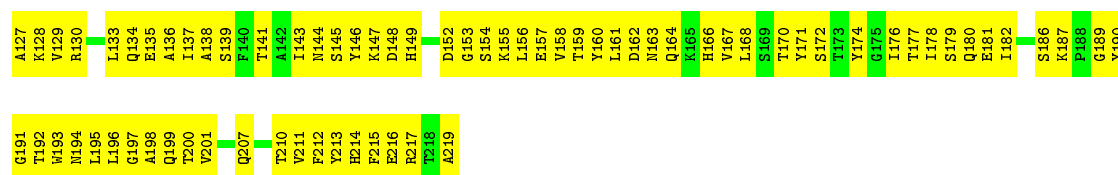


- Molecule 6: Baseplate wedge protein gp11



- Molecule 6: Baseplate wedge protein gp11





• Molecule 6: Baseplate wedge protein gp11

Chain FF: 25% 74%



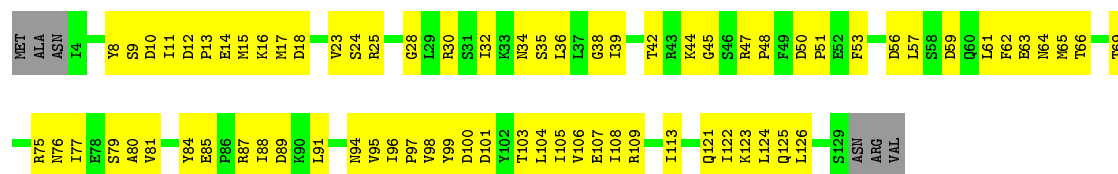
• Molecule 6: Baseplate wedge protein gp11

Chain FG: 25% 74%



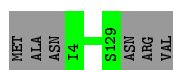
• Molecule 7: Baseplate wedge protein gp25

Chain O: 39% 56% 5%



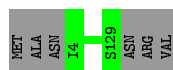
• Molecule 7: Baseplate wedge protein gp25

Chain e: 95% 5%



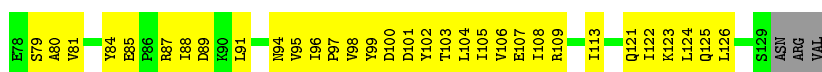
• Molecule 7: Baseplate wedge protein gp25

Chain u: 95% 5%



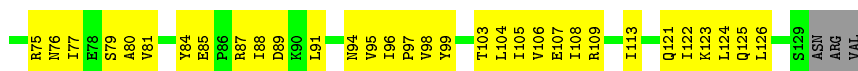
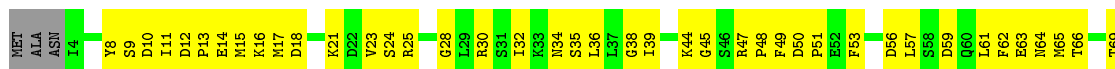
• Molecule 7: Baseplate wedge protein gp25

Chain BD: 43% 52% 5%



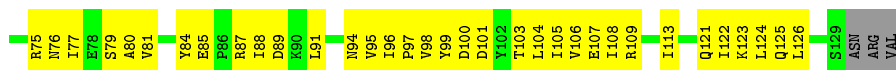
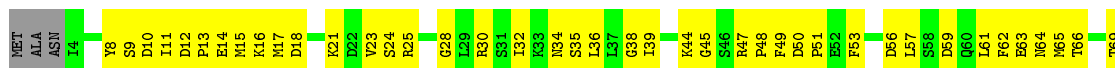
• Molecule 7: Baseplate wedge protein gp25

Chain DF: 40% 55% 5%



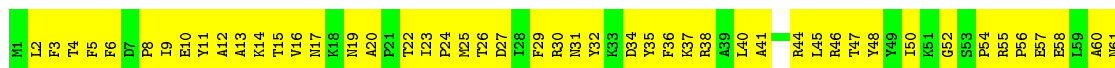
• Molecule 7: Baseplate wedge protein gp25

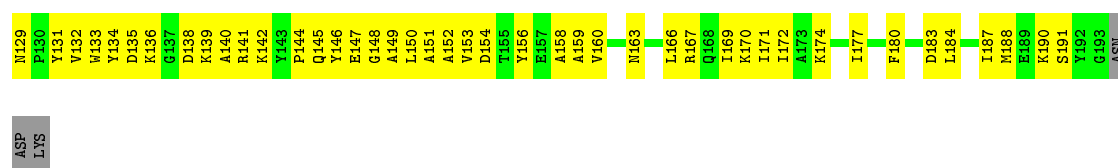
Chain GA: 39% 57% 5%



• Molecule 8: Baseplate wedge protein gp53

Chain P: 28% 70% 2%





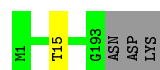
• Molecule 8: Baseplate wedge protein gp53

Chain f: 98%



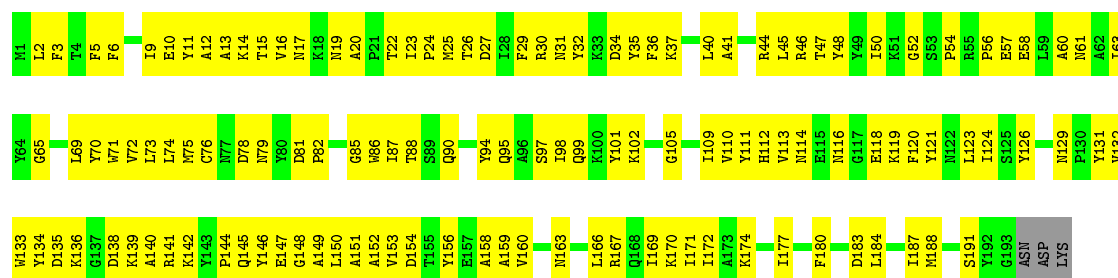
• Molecule 8: Baseplate wedge protein gp53

Chain v: 98%



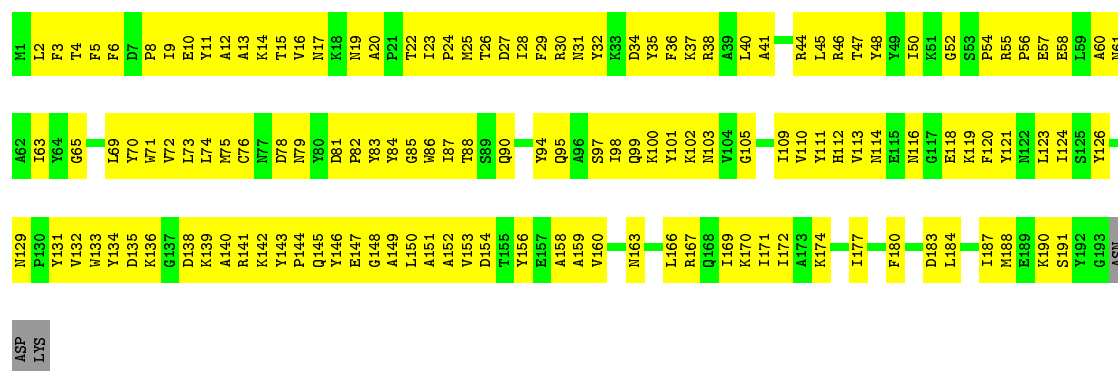
• Molecule 8: Baseplate wedge protein gp53

Chain BE: 34% 65%



• Molecule 8: Baseplate wedge protein gp53

Chain DG: 28% 70%



• Molecule 8: Baseplate wedge protein gp53

Chain GB: 30% 69%

LYS	M1	A62	P130	Y131	I163	L69	Y70	W71	V72	L73	L74	M75	C76	H77	D78	N79	Y80	D81	P82	Y83	Y84	G85	W86	I87	T88	S89	Q90		Y94	Q95	A96	S97	I98	K100	R101	K102		G105		I109	V110	Y111	H112	V113	N114	E115	N116	G117	E118	K119	F120	Y121	N122	L123	I124	S125	Y126		N129																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
	L2	I63	Y132	W133	Y134	D135	K136	G137	D138	K139	A140	R141	K142	H143	P144	Q145	Y146	E147	G148	A149	L150	A151	A152	V153	D154	T155	Y156	E157	A158	A159	V160		N163		L166	R167	Q168	I169	K170	I171	I172	A173	K174		I177		F180		D183	L184		I187	M188	E189	K190	S191	Y192	G193	ASN	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	5176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	37700	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.45	0/5337	0.63	1/7256 (0.0%)
1	B	0.47	0/5257	0.65	0/7144
1	BF	0.45	0/5337	0.63	1/7256 (0.0%)
1	BG	0.47	0/5257	0.65	0/7144
1	EA	0.45	0/5337	0.63	1/7256 (0.0%)
1	EB	0.47	0/5257	0.65	0/7144
1	Q	0.45	0/5337	0.63	1/7256 (0.0%)
1	R	0.47	0/5257	0.65	0/7144
1	g	0.45	0/5337	0.63	1/7256 (0.0%)
1	h	0.47	0/5257	0.65	0/7144
1	w	0.45	0/5337	0.63	1/7256 (0.0%)
1	x	0.47	0/5257	0.65	0/7144
2	C	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
2	CA	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
2	EC	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
2	S	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
2	i	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
2	y	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
3	AA	0.56	0/2736	0.79	3/3731 (0.1%)
3	CB	0.56	0/2709	0.79	3/3694 (0.1%)
3	CC	0.56	0/2736	0.79	3/3731 (0.1%)
3	D	0.56	0/2709	0.79	3/3694 (0.1%)
3	E	0.56	0/2736	0.79	3/3731 (0.1%)
3	ED	0.56	0/2709	0.79	3/3694 (0.1%)
3	EE	0.56	0/2736	0.79	3/3731 (0.1%)
3	T	0.56	0/2709	0.79	3/3694 (0.1%)
3	U	0.56	0/2736	0.79	3/3731 (0.1%)
3	j	0.56	0/2709	0.79	3/3694 (0.1%)
3	k	0.56	0/2736	0.79	3/3731 (0.1%)
3	z	0.56	0/2709	0.80	3/3694 (0.1%)
4	AB	0.40	0/2205	0.58	0/2988
4	AC	0.40	0/2205	0.58	0/2988
4	AD	0.40	0/2205	0.58	0/2988
4	CD	0.40	0/2205	0.58	0/2988

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
4	CE	0.40	0/2205	0.58	0/2988
4	CF	0.40	0/2205	0.58	0/2988
4	EF	0.40	0/2205	0.58	0/2988
4	EG	0.40	0/2205	0.58	0/2988
4	F	0.40	0/2205	0.58	0/2988
4	FA	0.40	0/2205	0.58	0/2988
4	G	0.40	0/2205	0.58	0/2988
4	H	0.40	0/2205	0.58	0/2988
4	V	0.40	0/2205	0.58	0/2988
4	W	0.40	0/2205	0.58	0/2988
4	X	0.40	0/2205	0.58	0/2988
4	l	0.40	0/2205	0.58	0/2988
4	m	0.40	0/2205	0.58	0/2988
4	n	0.40	0/2205	0.58	0/2988
5	AE	0.42	0/4777	0.68	4/6510 (0.1%)
5	AF	0.43	0/4778	0.71	3/6513 (0.0%)
5	AG	0.44	0/4778	0.69	3/6513 (0.0%)
5	CG	0.42	0/4777	0.68	4/6510 (0.1%)
5	DA	0.43	0/4778	0.71	3/6513 (0.0%)
5	DB	0.44	0/4778	0.69	3/6513 (0.0%)
5	FB	0.42	0/4777	0.68	4/6510 (0.1%)
5	FC	0.43	0/4778	0.71	3/6513 (0.0%)
5	FD	0.44	0/4778	0.69	3/6513 (0.0%)
5	I	0.42	0/4777	0.68	4/6510 (0.1%)
5	J	0.43	0/4778	0.71	3/6513 (0.0%)
5	K	0.44	0/4778	0.69	3/6513 (0.0%)
5	Y	0.42	0/4777	0.68	4/6510 (0.1%)
5	Z	0.43	0/4778	0.71	3/6513 (0.0%)
5	a	0.44	0/4778	0.69	3/6513 (0.0%)
5	o	0.42	0/4777	0.68	4/6510 (0.1%)
5	p	0.43	0/4778	0.71	3/6513 (0.0%)
5	q	0.44	0/4778	0.69	3/6513 (0.0%)
6	BA	0.42	0/1700	0.62	0/2318
6	BB	0.42	0/1700	0.62	0/2318
6	BC	0.42	0/1700	0.63	0/2318
6	DC	0.42	0/1700	0.62	0/2318
6	DD	0.42	0/1700	0.62	0/2318
6	DE	0.42	0/1700	0.62	0/2318
6	FE	0.42	0/1700	0.62	0/2318
6	FF	0.42	0/1700	0.62	0/2318
6	FG	0.42	0/1700	0.62	0/2318
6	L	0.42	0/1700	0.62	0/2318
6	M	0.42	0/1700	0.62	0/2318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
6	N	0.42	0/1700	0.62	0/2318
6	b	0.42	0/1700	0.62	0/2318
6	c	0.42	0/1700	0.62	0/2318
6	d	0.42	0/1700	0.63	0/2318
6	r	0.42	0/1700	0.62	0/2318
6	s	0.42	0/1700	0.62	0/2318
6	t	0.42	0/1700	0.62	0/2318
7	BD	0.35	0/1027	0.58	0/1392
7	DF	0.35	0/1027	0.57	0/1392
7	GA	0.35	0/1027	0.58	0/1392
7	O	0.35	0/1027	0.58	0/1392
7	e	0.35	0/1027	0.57	0/1392
7	u	0.35	0/1027	0.58	0/1392
8	BE	0.48	0/1643	0.62	0/2228
8	DG	0.48	0/1643	0.62	0/2228
8	GB	0.48	0/1643	0.62	0/2228
8	P	0.48	0/1643	0.62	0/2228
8	f	0.48	0/1643	0.62	0/2228
8	v	0.48	0/1643	0.62	0/2228
All	All	0.46	18/318972 (0.0%)	0.68	144/433866 (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	6
1	B	0	7
1	BF	0	6
1	BG	0	7
1	EA	0	6
1	EB	0	7
1	Q	0	6
1	R	0	7
1	g	0	6
1	h	0	7
1	w	0	6
1	x	0	7
2	C	0	31
2	CA	0	31
2	EC	0	31

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	S	0	31
2	i	0	31
2	y	0	31
3	AA	0	4
3	CB	0	3
3	CC	0	4
3	D	0	3
3	E	0	4
3	ED	0	3
3	EE	0	4
3	T	0	3
3	U	0	4
3	j	0	3
3	k	0	4
3	z	0	3
5	AE	0	16
5	AF	0	24
5	AG	0	15
5	CG	0	16
5	DA	0	24
5	DB	0	15
5	FB	0	16
5	FC	0	24
5	FD	0	15
5	I	0	16
5	J	0	24
5	K	0	15
5	Y	0	16
5	Z	0	24
5	a	0	15
5	o	0	16
5	p	0	24
5	q	0	15
6	BA	0	2
6	BB	0	2
6	BC	0	2
6	DC	0	2
6	DD	0	2
6	DE	0	2
6	FE	0	2
6	FF	0	2
6	FG	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	L	0	2
6	M	0	2
6	N	0	2
6	b	0	2
6	c	0	2
6	d	0	2
6	r	0	2
6	s	0	2
6	t	0	2
All	All	0	672

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	613	LYS	C-N	6.92	1.47	1.34
2	i	613	LYS	C-N	6.91	1.47	1.34
2	EC	613	LYS	C-N	6.91	1.47	1.34
2	y	613	LYS	C-N	6.90	1.47	1.34
2	CA	613	LYS	C-N	6.90	1.47	1.34

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AG	317	LEU	CA-CB-CG	7.88	133.42	115.30
5	DB	317	LEU	CA-CB-CG	7.87	133.41	115.30
5	q	317	LEU	CA-CB-CG	7.86	133.39	115.30
5	FD	317	LEU	CA-CB-CG	7.86	133.39	115.30
5	K	317	LEU	CA-CB-CG	7.85	133.35	115.30

There are no chirality outliers.

5 of 672 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ILE	Peptide
1	A	209	TRP	Peptide
1	A	262	PRO	Peptide
1	A	451	ASP	Peptide
1	A	6	VAL	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5235	0	5086	571	0
1	B	5157	0	5011	707	0
1	BF	5235	0	5086	561	0
1	BG	5157	0	5011	654	0
1	EA	5235	0	5086	570	0
1	EB	5157	0	5011	666	0
1	Q	5235	0	5086	548	0
1	R	5157	0	5011	664	0
1	g	5235	0	5086	0	0
1	h	5157	0	5011	0	0
1	w	5235	0	5086	0	0
1	x	5157	0	5011	0	0
2	C	8199	0	7912	1295	0
2	CA	8199	0	7912	1268	0
2	EC	8199	0	7912	1255	0
2	S	8199	0	7912	1186	0
2	i	8199	0	7912	0	0
2	y	8199	0	7912	0	0
3	AA	2658	0	2532	242	0
3	CB	2631	0	2509	320	0
3	CC	2658	0	2532	317	0
3	D	2631	0	2509	344	0
3	E	2658	0	2532	357	0
3	ED	2631	0	2509	324	0
3	EE	2658	0	2532	328	0
3	T	2631	0	2509	320	0
3	U	2658	0	2532	344	0
3	j	2631	0	2509	0	0
3	k	2658	0	2532	0	0
3	z	2631	0	2509	0	0
4	AB	2175	0	2157	336	0
4	AC	2175	0	2157	337	0
4	AD	2175	0	2157	334	0
4	CD	2175	0	2157	282	0
4	CE	2175	0	2157	281	0
4	CF	2175	0	2157	260	0
4	EF	2175	0	2157	288	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	EG	2175	0	2157	281	0
4	F	2175	0	2157	323	0
4	FA	2175	0	2157	275	0
4	G	2175	0	2157	313	0
4	H	2175	0	2157	309	0
4	V	2175	0	2157	280	0
4	W	2175	0	2157	276	0
4	X	2175	0	2157	272	0
4	l	2175	0	2157	0	0
4	m	2175	0	2157	0	0
4	n	2175	0	2157	0	0
5	AE	4675	0	4445	630	0
5	AF	4675	0	4446	649	0
5	AG	4675	0	4446	644	0
5	CG	4675	0	4445	640	0
5	DA	4675	0	4446	659	0
5	DB	4675	0	4446	676	0
5	FB	4675	0	4445	645	0
5	FC	4675	0	4446	655	0
5	FD	4675	0	4446	666	0
5	I	4675	0	4445	641	0
5	J	4675	0	4446	654	0
5	K	4675	0	4446	680	0
5	Y	4675	0	4445	542	0
5	Z	4675	0	4446	560	0
5	a	4675	0	4446	0	0
5	o	4675	0	4445	0	0
5	p	4675	0	4446	0	0
5	q	4675	0	4446	0	0
6	BA	1665	0	1638	235	0
6	BB	1665	0	1638	255	0
6	BC	1665	0	1638	239	0
6	DC	1665	0	1638	253	0
6	DD	1665	0	1638	264	0
6	DE	1665	0	1638	268	0
6	FE	1665	0	1638	235	0
6	FF	1665	0	1638	246	0
6	FG	1665	0	1638	241	0
6	L	1665	0	1638	234	0
6	M	1665	0	1638	257	0
6	N	1665	0	1638	254	0
6	b	1665	0	1638	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	c	1665	0	1638	0	0
6	d	1665	0	1638	0	0
6	r	1665	0	1638	0	0
6	s	1665	0	1638	0	0
6	t	1665	0	1638	0	0
7	BD	1011	0	1009	61	0
7	DF	1011	0	1009	76	0
7	GA	1011	0	1009	80	0
7	O	1011	0	1009	81	0
7	e	1011	0	1009	0	0
7	u	1011	0	1009	0	0
8	BE	1599	0	1544	143	0
8	DG	1599	0	1544	163	0
8	GB	1599	0	1544	175	0
8	P	1599	0	1544	176	0
8	f	1599	0	1544	0	0
8	v	1599	0	1544	0	0
All	All	312210	0	301950	26167	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 59.

The worst 5 of 26167 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)
2:C:81:ARG:HD2	2:C:94:TRP:HB3	1.29	1.15
5:AE:33:LEU:HA	5:AF:43:PRO:HG3	1.27	1.14
2:S:81:ARG:HD2	2:S:94:TRP:HB3	1.29	1.13
5:AG:316:ILE:HD11	6:BB:7:LYS:HG3	1.33	1.11
2:CA:81:ARG:HD2	2:CA:94:TRP:HB3	1.29	1.10

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%)	590 (90%)	59 (9%)	7 (1%)	17	60
1	B	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	32	74
1	BF	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	17	60
1	BG	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	32	74
1	EA	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	17	60
1	EB	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	32	74
1	Q	656/660 (99%)	590 (90%)	59 (9%)	7 (1%)	17	60
1	R	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	32	74
1	g	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	17	60
1	h	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	32	74
1	w	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	17	60
1	x	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	32	74
2	C	1000/1032 (97%)	817 (82%)	155 (16%)	28 (3%)	6	39
2	CA	1000/1032 (97%)	818 (82%)	154 (15%)	28 (3%)	6	39
2	EC	1000/1032 (97%)	818 (82%)	155 (16%)	27 (3%)	6	40
2	S	1000/1032 (97%)	818 (82%)	154 (15%)	28 (3%)	6	39
2	i	1000/1032 (97%)	818 (82%)	155 (16%)	27 (3%)	6	40
2	y	1000/1032 (97%)	818 (82%)	154 (15%)	28 (3%)	6	39
3	AA	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	44	81
3	CB	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	CC	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	44	81
3	D	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	E	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	44	81
3	ED	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	EE	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	44	81
3	T	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	U	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	44	81
3	j	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	k	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	44	81
3	z	326/334 (98%)	307 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AB	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	AC	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	AD	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	CD	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	CE	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	CF	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	EF	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	EG	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	F	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	FA	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	G	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	H	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	V	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	W	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	X	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	l	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	m	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
4	n	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	13	54
5	AE	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	7	43
5	AF	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	10	49
5	AG	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	46
5	CG	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	7	43
5	DA	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	10	49
5	DB	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	46
5	FB	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	7	43
5	FC	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	10	49
5	FD	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	46
5	I	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	7	43
5	J	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	10	49
5	K	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	46
5	Y	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	7	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Z	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	10	49
5	a	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	46
5	o	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	7	43
5	p	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	10	49
5	q	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	46
6	BA	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	BB	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	BC	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	DC	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	DD	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	DE	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	FE	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	FF	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	FG	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	L	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	M	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	N	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	b	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	c	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	d	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	r	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	s	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
6	t	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	20	63
7	BD	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
7	DF	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
7	GA	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
7	O	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
7	e	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
7	u	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
8	BE	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
8	DG	191/196 (97%)	172 (90%)	19 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	GB	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
8	P	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
8	f	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
8	v	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
All	All	39462/40050 (98%)	35197 (89%)	3703 (9%)	562 (1%)	18	54

5 of 562 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	249	ILE
4	G	249	ILE
4	H	249	ILE
5	I	10	VAL
5	I	24	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	576/578 (100%)	576 (100%)	0	100	100
1	B	567/578 (98%)	567 (100%)	0	100	100
1	BF	576/578 (100%)	576 (100%)	0	100	100
1	BG	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	Q	576/578 (100%)	576 (100%)	0	100	100
1	R	567/578 (98%)	567 (100%)	0	100	100
1	g	576/578 (100%)	576 (100%)	0	100	100
1	h	567/578 (98%)	567 (100%)	0	100	100
1	w	576/578 (100%)	576 (100%)	0	100	100
1	x	567/578 (98%)	567 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	896/921 (97%)	894 (100%)	2 (0%)	94	97
2	CA	896/921 (97%)	894 (100%)	2 (0%)	94	97
2	EC	896/921 (97%)	894 (100%)	2 (0%)	94	97
2	S	896/921 (97%)	894 (100%)	2 (0%)	94	97
2	i	896/921 (97%)	894 (100%)	2 (0%)	94	97
2	y	896/921 (97%)	894 (100%)	2 (0%)	94	97
3	AA	293/295 (99%)	291 (99%)	2 (1%)	87	93
3	CB	289/295 (98%)	288 (100%)	1 (0%)	94	96
3	CC	293/295 (99%)	291 (99%)	2 (1%)	87	93
3	D	289/295 (98%)	287 (99%)	2 (1%)	87	93
3	E	293/295 (99%)	291 (99%)	2 (1%)	87	93
3	ED	289/295 (98%)	287 (99%)	2 (1%)	87	93
3	EE	293/295 (99%)	291 (99%)	2 (1%)	87	93
3	T	289/295 (98%)	287 (99%)	2 (1%)	87	93
3	U	293/295 (99%)	291 (99%)	2 (1%)	87	93
3	j	289/295 (98%)	287 (99%)	2 (1%)	87	93
3	k	293/295 (99%)	291 (99%)	2 (1%)	87	93
3	z	289/295 (98%)	287 (99%)	2 (1%)	87	93
4	AB	244/244 (100%)	244 (100%)	0	100	100
4	AC	244/244 (100%)	244 (100%)	0	100	100
4	AD	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	CF	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	F	244/244 (100%)	244 (100%)	0	100	100
4	FA	244/244 (100%)	244 (100%)	0	100	100
4	G	244/244 (100%)	244 (100%)	0	100	100
4	H	244/244 (100%)	244 (100%)	0	100	100
4	V	244/244 (100%)	244 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	W	244/244 (100%)	244 (100%)	0	100	100
4	X	244/244 (100%)	244 (100%)	0	100	100
4	l	244/244 (100%)	244 (100%)	0	100	100
4	m	244/244 (100%)	244 (100%)	0	100	100
4	n	244/244 (100%)	244 (100%)	0	100	100
5	AE	519/519 (100%)	519 (100%)	0	100	100
5	AF	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	AG	519/519 (100%)	519 (100%)	0	100	100
5	CG	519/519 (100%)	519 (100%)	0	100	100
5	DA	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	DB	519/519 (100%)	519 (100%)	0	100	100
5	FB	519/519 (100%)	519 (100%)	0	100	100
5	FC	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	FD	519/519 (100%)	519 (100%)	0	100	100
5	I	519/519 (100%)	519 (100%)	0	100	100
5	J	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	K	519/519 (100%)	519 (100%)	0	100	100
5	Y	519/519 (100%)	519 (100%)	0	100	100
5	Z	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	a	519/519 (100%)	519 (100%)	0	100	100
5	o	519/519 (100%)	519 (100%)	0	100	100
5	p	519/519 (100%)	518 (100%)	1 (0%)	94	97
5	q	519/519 (100%)	519 (100%)	0	100	100
6	BA	187/188 (100%)	187 (100%)	0	100	100
6	BB	187/188 (100%)	187 (100%)	0	100	100
6	BC	187/188 (100%)	187 (100%)	0	100	100
6	DC	187/188 (100%)	187 (100%)	0	100	100
6	DD	187/188 (100%)	187 (100%)	0	100	100
6	DE	187/188 (100%)	187 (100%)	0	100	100
6	FE	187/188 (100%)	187 (100%)	0	100	100
6	FF	187/188 (100%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	FG	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	b	187/188 (100%)	187 (100%)	0	100	100
6	c	187/188 (100%)	187 (100%)	0	100	100
6	d	187/188 (100%)	187 (100%)	0	100	100
6	r	187/188 (100%)	187 (100%)	0	100	100
6	s	187/188 (100%)	187 (100%)	0	100	100
6	t	187/188 (100%)	187 (100%)	0	100	100
7	BD	118/123 (96%)	118 (100%)	0	100	100
7	DF	118/123 (96%)	118 (100%)	0	100	100
7	GA	118/123 (96%)	118 (100%)	0	100	100
7	O	118/123 (96%)	118 (100%)	0	100	100
7	e	118/123 (96%)	118 (100%)	0	100	100
7	u	118/123 (96%)	118 (100%)	0	100	100
8	BE	166/169 (98%)	165 (99%)	1 (1%)	89	94
8	DG	166/169 (98%)	165 (99%)	1 (1%)	89	94
8	GB	166/169 (98%)	165 (99%)	1 (1%)	89	94
8	P	166/169 (98%)	165 (99%)	1 (1%)	89	94
8	f	166/169 (98%)	165 (99%)	1 (1%)	89	94
8	v	166/169 (98%)	165 (99%)	1 (1%)	89	94
All	All	34530/34872 (99%)	34483 (100%)	47 (0%)	95	97

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	k	274	ILE
3	z	28	ILE
3	EE	28	ILE
8	v	15	THR
3	z	274	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 671 such sidechains are listed below:

Mol	Chain	Res	Type
5	p	377	HIS
3	z	314	ASN
4	FA	193	HIS
5	q	195	HIS
1	w	216	HIS

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	i	1
2	CA	1
5	AE	1
2	y	1
5	I	1
2	C	1
2	S	1
2	EC	1

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Mol	Chain	Number of breaks
5	o	1
5	Y	1
5	FB	1
5	CG	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	570:ARG	C	571:GLU	N	3.75
1	Y	570:ARG	C	571:GLU	N	3.75
1	o	570:ARG	C	571:GLU	N	3.75
1	CG	570:ARG	C	571:GLU	N	3.75
1	FB	570:ARG	C	571:GLU	N	3.75