



wwPDB EM Map/Model Validation Report ⓘ

Jun 2, 2016 – 12:02 PM EDT

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 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

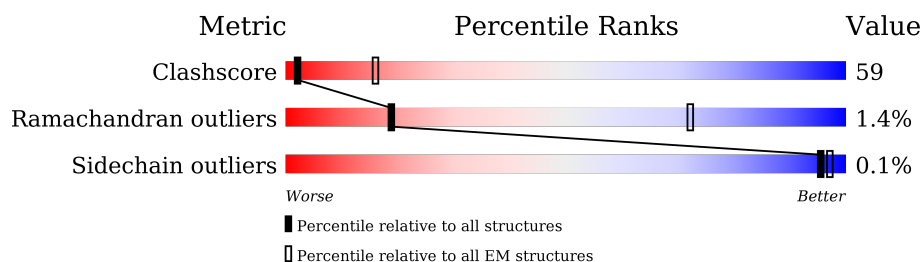
1 Overall quality at a glance

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.



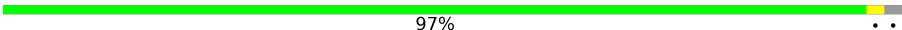
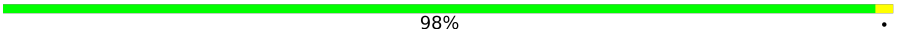
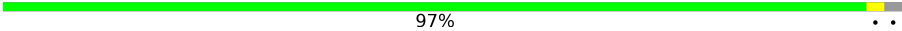








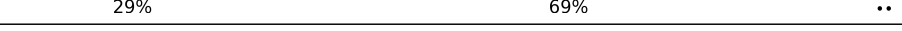






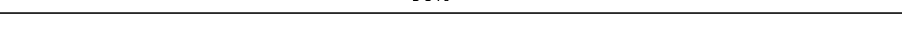
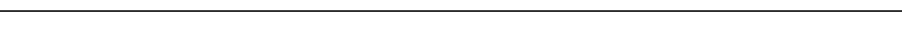

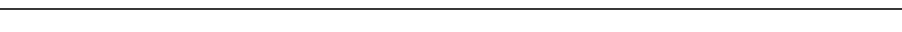
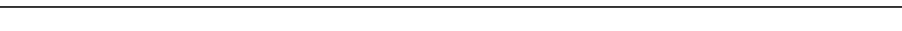


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	660	28% 70% .
1	B	660	23% 73% ..
1	BF	660	28% 70% .
1	BG	660	24% 73% ..
1	EA	660	28% 70% .
1	EB	660	24% 73% ..
1	Q	660	29% 69% .
1	R	660	25% 72% ..
1	g	660	98% .





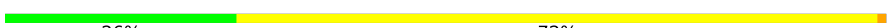
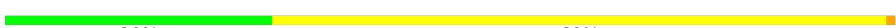







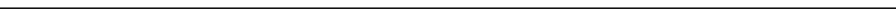











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Mol	Chain	Length	Quality of chain
1	h	660	 97% ..
1	w	660	 98% .
1	x	660	 97% ..
2	C	1032	 17% 75% 5% .
2	CA	1032	 18% 74% 5% .
2	EC	1032	 18% 74% 5% .
2	S	1032	 18% 74% 5% .
2	i	1032	 91% 6% .
2	y	1032	 91% 6% .
3	AA	334	 33% 65% ..
3	CB	334	 28% 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% .





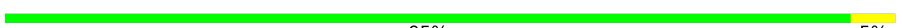








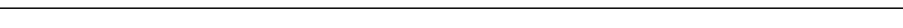






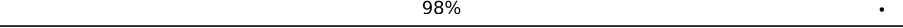
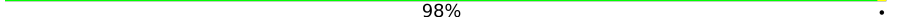
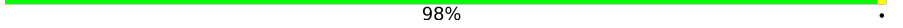
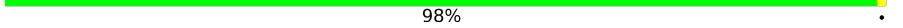
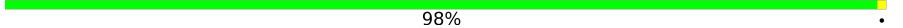
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Mol	Chain	Length	Quality of chain
4	CE	288	 27% 72% .
4	CF	288	 31% 68% .
4	EF	288	 25% 74% .
4	EG	288	 26% 73% .
4	F	288	 26% 72% .
4	FA	288	 30% 69% .
4	G	288	 26% 73% .
4	H	288	 27% 72% .
4	V	288	 27% 71% .
4	W	288	 27% 71% .
4	X	288	 29% 69% .
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% .




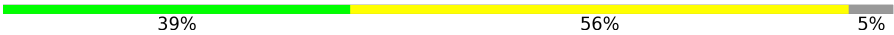
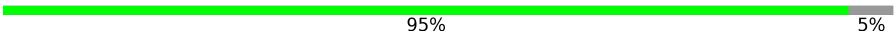
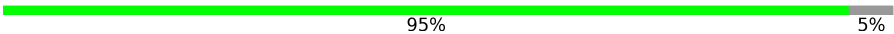
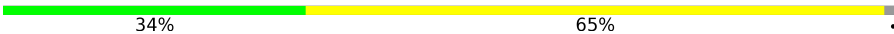
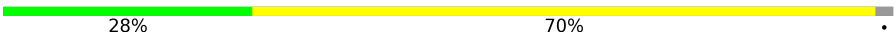
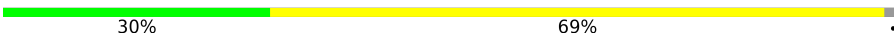
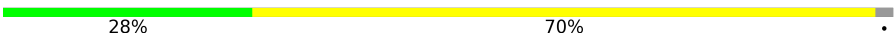
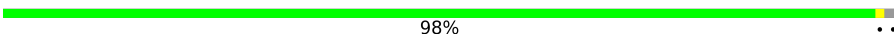
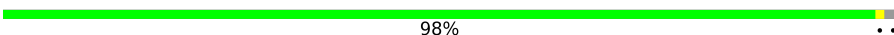
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Mol	Chain	Length	Quality of chain
5	K	602	 27% 70% .
5	Y	602	 32% 63% .
5	Z	602	 32% 63% 5% .
5	a	602	 95% 5% .
5	o	602	 95% 5% .
5	p	602	 94% 6% .
5	q	602	 95% 5% .
6	BA	219	 26% 73% .
6	BB	219	 26% 73% .
6	BC	219	 24% 74% .
6	DC	219	 24% 74% .
6	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		

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

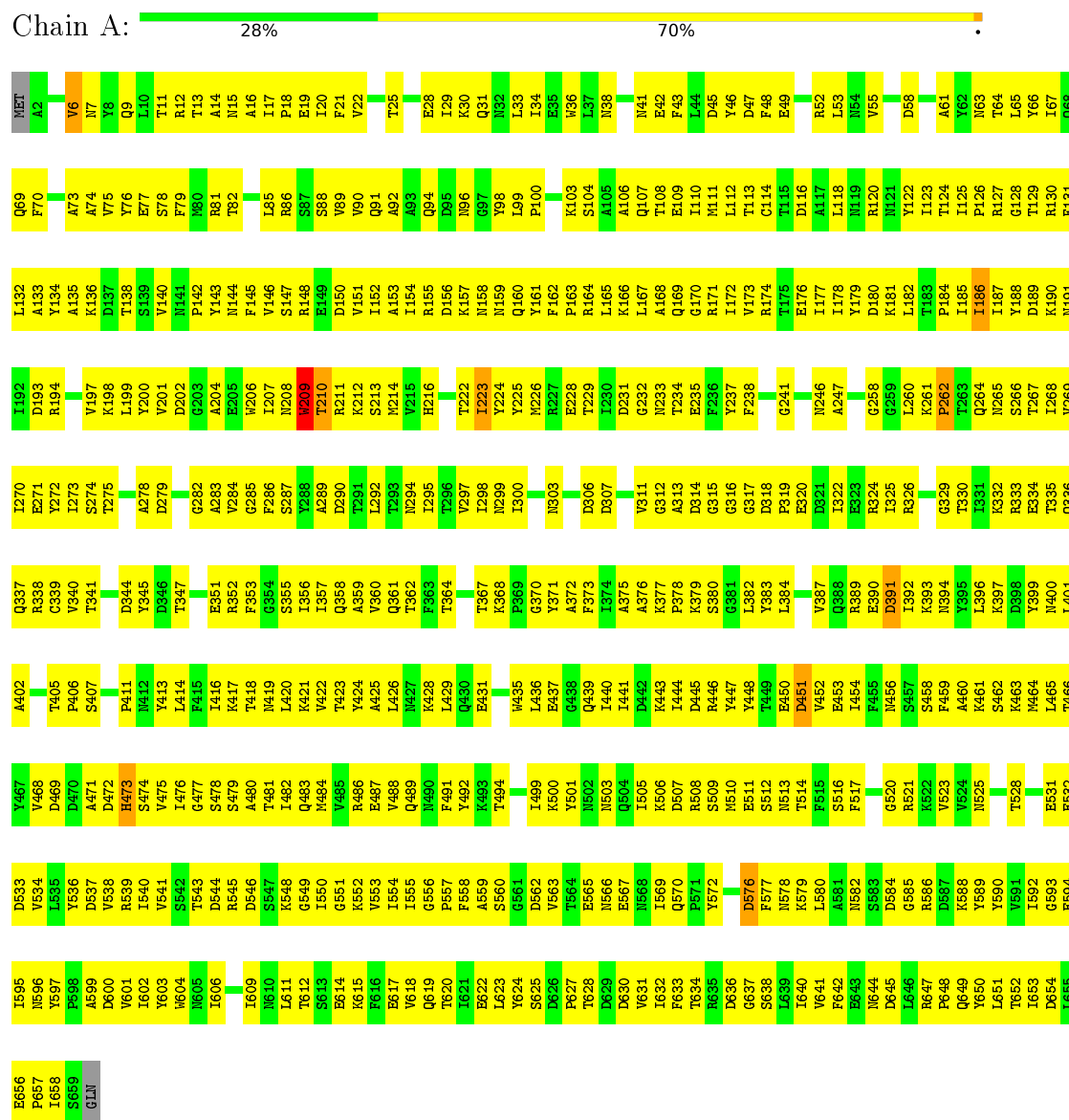
- Molecule 8 is a protein called Baseplate wedge protein gp53.

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 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



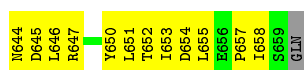
• Molecule 1: Baseplate wedge protein gp6



WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM





- 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%



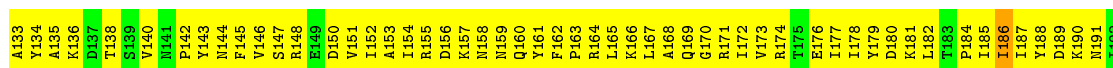
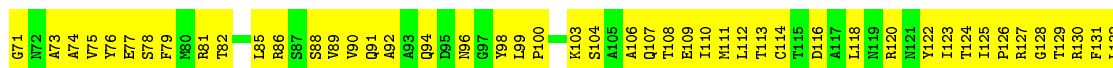
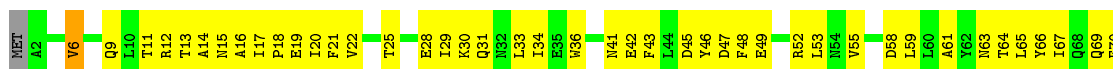
- Molecule 1: Baseplate wedge protein gp6

Chain x: 97%



- Molecule 1: Baseplate wedge protein gp6

Chain BF: 28% 70%



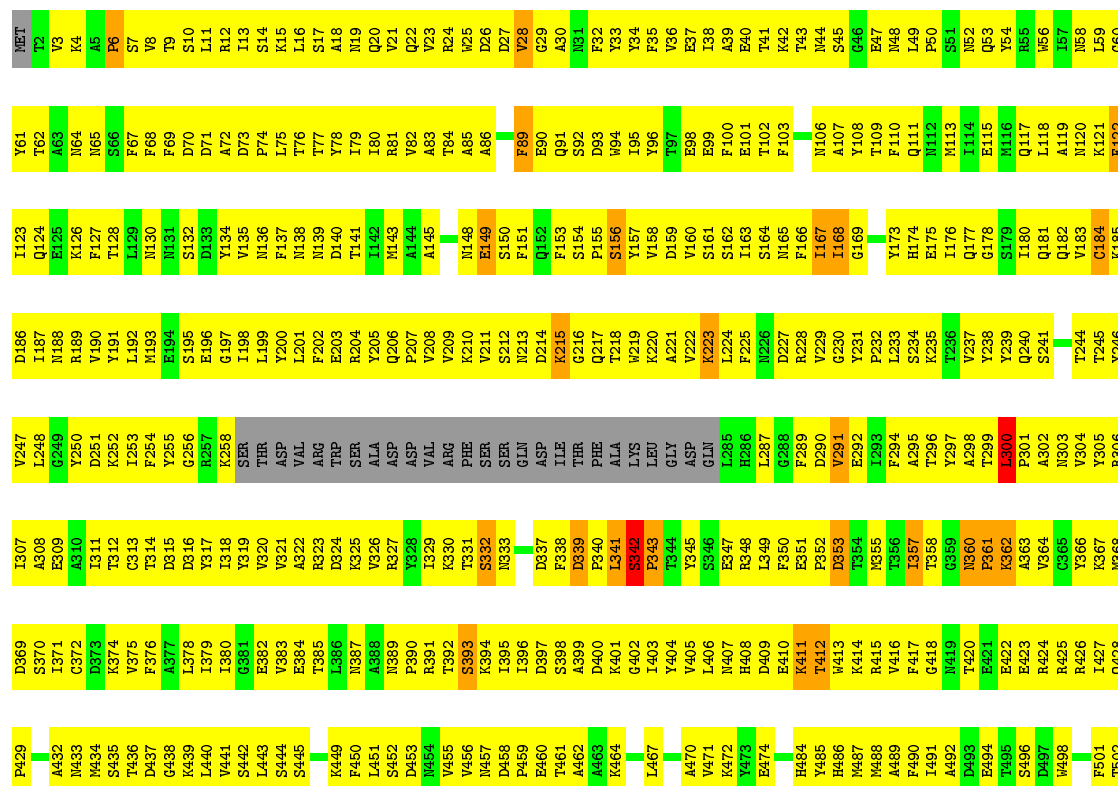
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L639	R446	E323	N255	D193	R130	I67	ALA	V601	R539	D470	T406	C339
I640	Y447	R324	Y256	R194	F131	Q68	ASN	I602	R540	A471	P406	V340
V641	Y448	I325	I257	N195	L132	Q69	THR	I603	V541	D472	S407	T341
E642	T449	R326	G258	Q196	A133	G70	PRO	N604	S542	H473	P411	A342
I644	E450	E327	G259	Q197	Y134	G71	VAL	N605	T543	S474	Y412	T343
D645	D451	L328	L260	K198	A135	I72	ASN	I606	R545	V475	Y413	D444
L646	Y452	G329	K261	Y200	I336	A73	TTR	I609	D646	I476	L414	T345
R647	E453	T330	P262	Y201	L137	A74	GLN	N610	S547	G477	L417	T347
Y650	R648	I331	T263	D202	T138	V75	LEU	L611	R548	S479	K417	E351
L651	F455	R332	Q264	G203	Y140	E77	THR	T612	G549	A480	T418	R352
T652	K397	R333	N265	A204	N141	S78	R12	S613	I550	T481	N419	R353
I653	N400	T335	S266	E205	P142	F79	I17	B614	G551	I482	L420	F354
D654	L401	Q336	I268	I206	Y143	R81	P18	R615	R552	Q483	K421	S354
L655	A402	Q337	V269	I207	N144	T82	E19	T616	V553	N484	V422	S355
R657	T466	R338	E270	N208	F145	L85	I20	B617	I554	V485	T423	T356
I658	Y467	C339	E271	W209	V146	V22	F21	V618	I555	Y486	Y424	T357
S659	Y468	V340	Y272	T210	S147	L86	G23	Q619	G556	E487	A425	Q358
GLN	A342	T341	I273	R211	R148	S87	G24	T620	P557	Y488	L426	A359
Y660	T405	A343	S274	R212	I152	Q91	G24	T621	F558	Q489	N427	V360
L661	P406	D344	T275	S213	A153	V90	F26	L622	S559	F490	K428	Q361
T662	I408	D345	N276	N214	A154	Q92	F26	L623	S560	Y492	L429	T362
V663	I409	D346	A280	W215	R155	A93	E28	S625	G561	K493	E430	T363
S664	S410	T347	N281	A217	R156	T29	I29	D626	V563	T494	E431	T364
F665	P411	F348	G282	G218	N158	Q94	K30	T627	E564	I499	M435	T367
I666	Y413	V349	A283	S219	N159	D85	Q31	T628	E565	L436	L436	R368
L667	L414	S350	V284	S221	Q160	N96	I34	D630	N566	E437	E437	P369
A668	F415	R352	F285	S222	Y161	G97	T34	D631	E567	G438	G438	G370
S479	T416	F353	F286	T223	F162	Y98	E35	V631	N568	Q439	Q439	Y371
Q483	K417	I356	S287	I223	P163	L99	V36	T632	I569	I505	I440	A372
L484	T418	I357	A289	T224	R164	P100	L37	T633	Q570	R506	I441	F373
Y485	L419	Q358	D290	Y225	L165	T101	N38	T634	D507	S507	K443	A375
R486	L420	Q359	T291	R227	K166	S102	G39	D636	R508	N509	I444	A376
E487	Y422	A359	T292	R228	L167	K103	Q40	G637	S509	N510	D445	K377
Y488	Y423	V360	N294	T229	A168	A105	E42	S638	E511	E511	R446	P378
Q489	T424	Q361	I295	T230	Q170	A106	F43	D639	N578	S512	Y447	K379
N490	A425	T362	T296	D231	R171	Q107	L44	I640	K579	N513	Y448	S380
Y492	L426	F363	V297	G232	V173	T108	D45	V641	L580	T514	T449	G381
K493	N427	D365	N299	T234	R174	E109	Y46	T642	A581	F515	E450	G381
P495	Y428	S366	N301	T235	T175	M111	D47	D643	N582	S516	D451	Y383
G498	E431	G370	E302	Y237	E176	L112	F48	D644	S583	F517	V452	L384
I499	S432	Y371	N303	T238	I178	C114	G50	D645	R586	R521	I454	V387
S625	E433	A372	P304	G239	Y179	T115	S51	R647	F455	F455	F455	Q388
D626	Q434	F373	N305	E240	D180	Q649	R52	P648	R389	V524	N456	R389
P627	N435	I374	D306	G241	K181	V650	N54	V650	S457	N525	S457	E390
T628	L436	A375	A313	E242	L182	L651	V55	T652	Y589	N525	S458	D391
D629	N502	I376	D314	T243	T183	N119	—	R590	V590	T528	F459	I392
V631	E503	A376	G315	A247	P184	R120	D58	I592	K393	—	A460	K393
N666	Q504	K377	G316	S248	I185	N121	S59	E531	N394	—	K461	N394
I569	K506	P378	G317	E249	I186	Y122	E594	S462	S462	—	S462	T395
Q570	D507	K379	D318	G250	I187	I123	E595	L396	L396	—	K463	L396
R635	P571	S380	P319	A251	I188	T124	N56	P657	N596	—	M465	K397
D636	D576	G381	E320	L252	R189	—	N63	T658	Y597	—	L465	D396
G637	—	Y383	D321	T253	K190	R127	T64	S659	P598	—	Y467	T399
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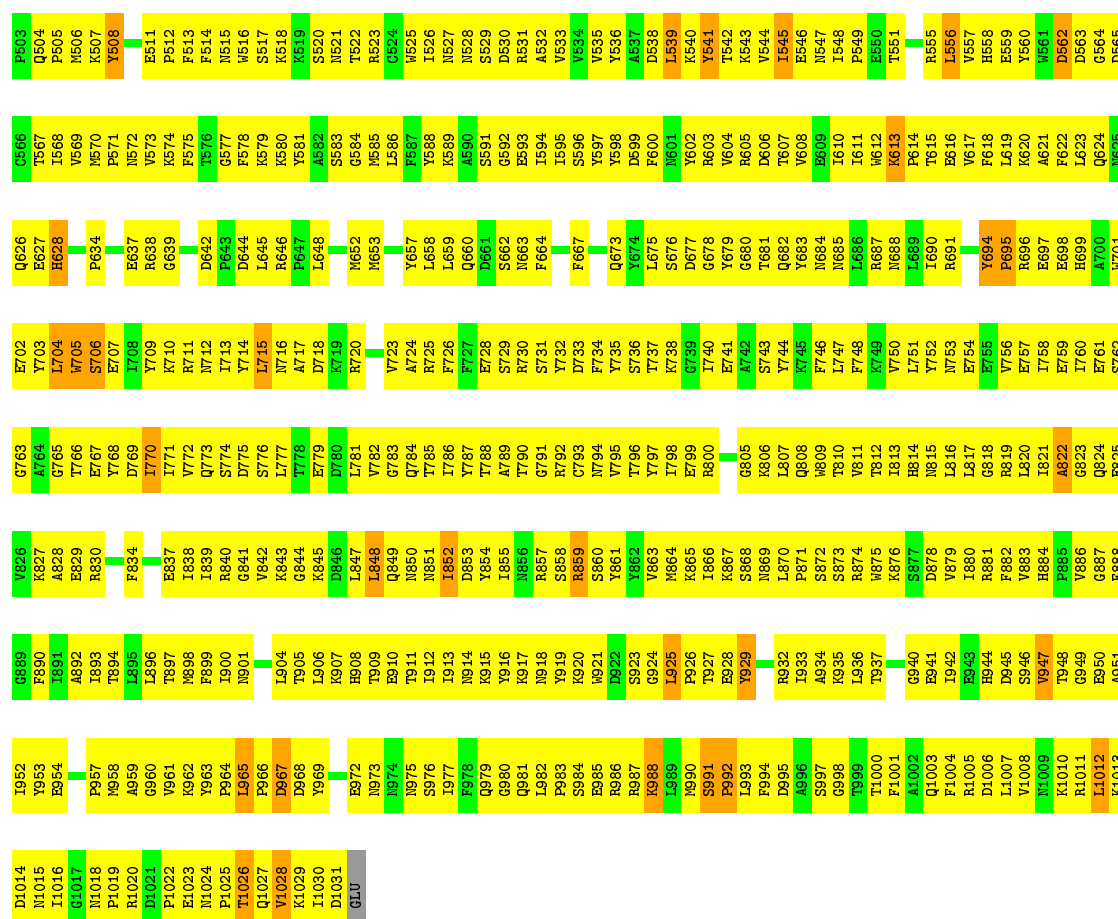
• Molecule 1: Baseplate wedge protein gp6

Chain BG: 24% 73% ..

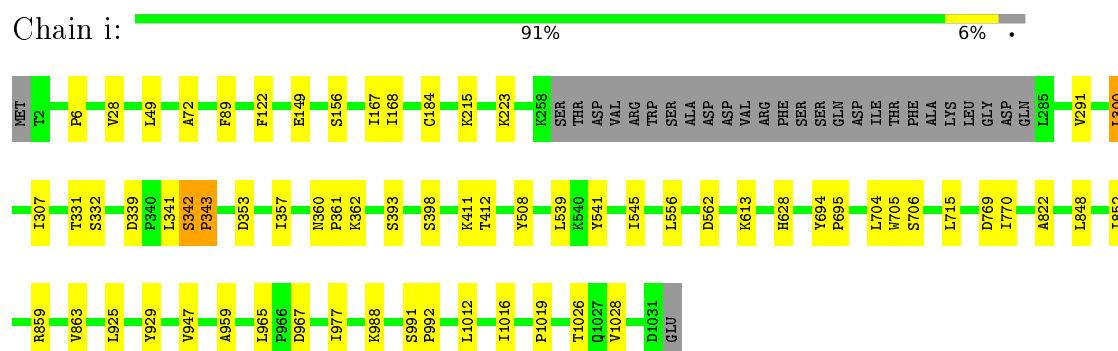
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|------|------|------|-----|
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| R194 | F131 | Q68 | ASN |
| H195 | L132 | Q69 | ALA |
| Q196 | A133 | F70 | THR |
| I197 | Y134 | G71 | PRO |
| K198 | A135 | | VAL |
| L199 | K136 | A74 | ASN |
| Y200 | D137 | V75 | TYR |
| V201 | T138 | Y76 | GLN |
| D202 | S139 | E77 | LEU |
| G203 | V140 | S78 | THR |
| A204 | N141 | F79 | R12 |
| E205 | P142 | M80 | |
| I206 | I143 | R81 | I17 |
| D207 | N144 | T82 | P18 |
| N208 | F145 | | E19 |
| W209 | V146 | L85 | I20 |
| T210 | S147 | R86 | F21 |
| E211 | R148 | S87 | V22 |
| F212 | | S88 | G23 |
| S213 | I152 | V89 | G24 |
| M214 | A153 | V90 | T25 |
| Y215 | I154 | Q91 | F26 |
| W216 | R155 | A92 | Z27 |
| A217 | | A93 | E28 |
| S218 | N158 | Q94 | I29 |
| S219 | N159 | D95 | K30 |
| T220 | Q160 | N96 | Q31 |
| S221 | Y161 | | |
| T222 | F162 | S97 | I34 |
| I223 | P163 | L98 | E35 |
| Y224 | R164 | P100 | W36 |
| Y225 | T165 | T101 | L37 |
| M226 | K166 | S102 | N38 |
| R227 | L167 | K103 | G39 |
| E228 | A168 | S104 | Q40 |
| T229 | Q169 | A105 | N41 |
| I230 | G170 | A106 | E42 |
| D231 | R171 | Q107 | F43 |
| G232 | T172 | T108 | L44 |
| N233 | V173 | E109 | D45 |
| T234 | R174 | I110 | Y46 |
| E235 | T175 | M111 | D47 |
| F236 | E176 | L112 | |
| Y237 | T177 | T113 | G50 |
| F238 | R178 | G114 | S51 |
| G239 | Y179 | T115 | R52 |
| E240 | D180 | D116 | L53 |
| G241 | K181 | A117 | M54 |
| E242 | L182 | L118 | V55 |
| I243 | T183 | N119 | |
| | P184 | R120 | D58 |
| A247 | N185 | N121 | L59 |
| S248 | I186 | Y122 | L60 |
| E249 | I187 | T123 | A61 |
| G250 | Y188 | T124 | Y62 |
| A251 | D189 | | N63 |
| I252 | K190 | R127 | T64 |
| T253 | N191 | G128 | L65 |
| S254 | I192 | T129 | Y66 |

T502	F603	A432	M433	M434	P504	S435	M506	K507	D437	K438	A509	A510	E511	P512	F513	L443	F514	S444	S445	K449	F450	K451	S452	D453	V455	C524	V456	N457	I526	D458	P459	N527	N528	S529	D530	A463	K464	V533	V534	V535	A537	K471	V472	L539	K540	T541	K477	K483	I545	E546	N547	M487	P488	A489	F490	I491	A492	L556	D493	E494	H558	P559	S496	D497	N498	D562	D563	F501	T526	I257	G258	G259	L260	K261	F262	T263	K265	K266	K267	L268	V269	L270	E271	Y272	L273	S274	T275	I276	A280	N281	G282	A283	E285	F286	S287	T288	A289	D290	T291	I294	L295	T296	V297	L298	N299	L300	I301	E302	I303	P304	N305	D306	A313	G315	G316	G317	D318	F319	E320	L382	Y383	L384	E323	K324	L325	Q388	K4	Q389	E327	L328	K330	G329	T330	L331	K332	K333	E334	T335	Q336	Q337	R338	C339	V340	Y272	T341	L273	A342	T343	T344	T345	T346	T347	D346	Y345	T347	F348	V349	S350	E351	F352	F353	I356	L357	Q358	A359	V360	Q361	F362	T364	D365	S366	I301	E302	G370	Y371	A372	F373	L374	A375	A376	K377	G378	K379	I440	S380	G381	L382	Y383	L384	T385	I386	T387	Q388	F389	E390	D391	L392	K393	N394	K395	L396	K397	N400	M401	L402	A403	P404	Y405	T406	T407	S407	I408	T409	S410	T411	H412	P413	V414	S415	G416	T417	K418	D419	N420	V421	K422	T423	Y424	A425	L426	N427	K428	L429	Q430	E431	S432	E433	Q434	N435	L436	A437	N503	Q504	I505	K506	D507	I441	D442	R508	S509	I510	I444	D445	R446	Y447	T448	D449	E450	D451	W452	E453	F454	F455	F456	F457	F458	F459	A460	K461	M462	L463	T464	Y465	Y466	Y467	V468	D469	S470	A471	D472	H473	S474	V475	I476	G477	S478	S479	Q483	M484	V485	R486	E487	W488	Q489	N490	F491	Y492	N493	K494	P495	G498	L499	K500	Y501	N502	N503	Q504	I505	K506	D507	I441	D442	R508	S509	I510	I444	D445	S512	N513	T514	F515	S516	F517	N518	S519	G520	K521	K522	V523	V524	N525	P526	D527	T528	G529	A530	L531	E532	E533	E534	V535	D536	V537	L538	N539	S540	S541	T542	T543	R544	N545	G546	K547	S548	G549	K552	V553	L554	I555	G556	P557	F558	D562	V563	T564	E565	N566	I569	F563	T564	R565	I567	D568	N569	I570	P571	D576	F577	N578	K579	L580	A581	F582	S583	D584	G585	R586	D587	K588	Y589	A590	V591	L592	G593	E594	L595	P596	Y597	E598	A599	D600	V601	L602	V603	M604	N605	L606	A607	K608	L609	N610	L611	T612	S613	E614	K615	F616	Q619	T620	L621	L622	L623	Y624	S625	D626	P627	T628	D629	D630	V631	L632	F633	T634	R635	D636	G637	S638	L639	I640	V641	E643	N644	D645	L646	H647	V650	L651	T652	I653	D654	L655	E656	P657	L658	S659	GLN	L639	I640	V641	E643	N644	D645	L646	H647	V650	L651	T652	I653	D654	L655	E656	P657	L658	S659	GLN	N578	K579	L580	A581	F582	S583	D584	G585	R586	D587	K588	Y589	A590	V591	L592	G593	E594	L595	P596	Y597	E598	A599	D600	V601	L602	V603	M604	N605	L606	A607	K608	L609	N610	L611	T612	S613	E614	K615	F616	Q619	T620	L621	L622	L623	Y624	S625	D626	P627	T628	D629	D630	V631	L632	F633	T634	R635	D636	G637	S638	L639	I640	V641	E643	N644	D645	L646	H647	V650	L651	T652	I653	D654	L655	E656	P657	L658	S659	GLN	S512	N513	T514	F515	S516	F517	N518	S519	G520	K521	K522	V523	V524	N525	P526	D527	T528	G529	A530	L531	E532	E533	E534	V535	D536	V537	L538	N539	S540	S541	T542	T543	R544	N545	G546	K547	S548	G549	K552	V553	L554	I555	G556	P557	F558	D562	V563	T564	E565	N566	I569	F563	T564	R565	I567	D568	N569	I570	P571	D576	F577	N578	K579	L580	A581	F582	S583	D584	G585	R586	D587	K588	Y589	A590	V591	L592	G593	E594	L595	P596	Y597	E598	A599	D600	V601	L602	V603	M604	N605	L606	A607	K608	L609	N610	L611	T612	S613	E614	K615	F616	Q619	T620	L621	L622	L623	Y624	S625	D626	P627	T628	D629	D630	V631	L632	F633	T634	R635	D636	G637	S638	L639	I640	V641	E643	N644	D645	L646	H647	V650	L651	T652	I653	D654	L655	E656	P657	L658	S659	GLN	N578	K579	L580	A581	F582	S583	D584	G585	R586	D587	K588	Y589	A590	V591	L592	G593	E594	L595	P596	Y597	E598	A599	D600	V601	L602	V603	M604	N605	L606	A607	K608	L609	N610	L611	T612	S613	E614	K615	F616	Q619	T620	L621	L622	L623	Y624	S625	D626	P627	T628	D629	D630	V631	L632	F633	T634	R635	D636	G637	S638	L639	I640	V641	E643	N644	D645	L646	H647	V650	L651	T652	I653	D654	L655	E656	P657	L658	S659	GLN	N578	K579	L580	A581	F582	S583	D584	G585	R586	D587	K588	Y589	A590	V591	L592	G593	E594	L595	P596	Y597	E598	A599	D600	V601	L602	V603	M604	N605	L606	A607	K608	L609	N610	L611	T612	S613	E614	K615	F616	Q619	T620	L621	L622	L623	Y624	S625	D626	P627	T628	D629	D630	V631	L632	F633	T634	R635	D636	G637	S638	L639	I640	V641	E643	N644	D645	L646	H647	V650	L651	T652	I653	D654	L655	E656	P657	L658	S659	GLN	N578	K579	L580	A581	F582	S583	D584	G585	R586	D587	K588	Y589	A590	V591	L592	G593	E594	L595	P596	Y597	E598	A599	D600	V601	L602	V603	M604	N605	L606	A607	K608	L609	N610	L611	T612	S613	E614	K615	F616	Q619	T620	L621	L622	L623	Y624	S625	D626	P627	T628	D629	D630	V631	L632	F633	T634	R635	D636	G637	S638	L639	I640	V641	E643	N644	D645	L646	H647	V650	L651	T652	I653	D654	L655	E656	P657	L658	S659	GLN	N578	K579	L580	A581	F582	S583	D584	G585	R586	D587	K588	Y589	A590	V591	L592	G593	E594	L595	P596	Y597	E598	A599	D600	V601	L602	V603	M604	N605	L606	A607	K608	L609	N610	L611	T612	S613	E614	K615	F616	Q619	T620	L621	L622	L623	Y624	S625	D626	P627	T628	D629	D630	V631	L632	F633	T634	R635	D636	G637	S638	L639	I640	V641	E643	N644	D645	L646	H647	V650	L651	T652	I653	D654	L655	E656	P657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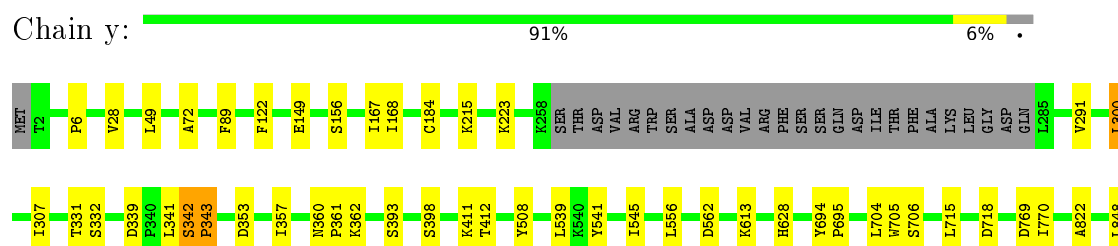


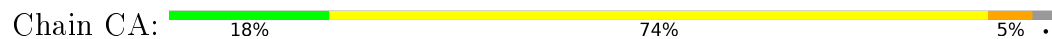


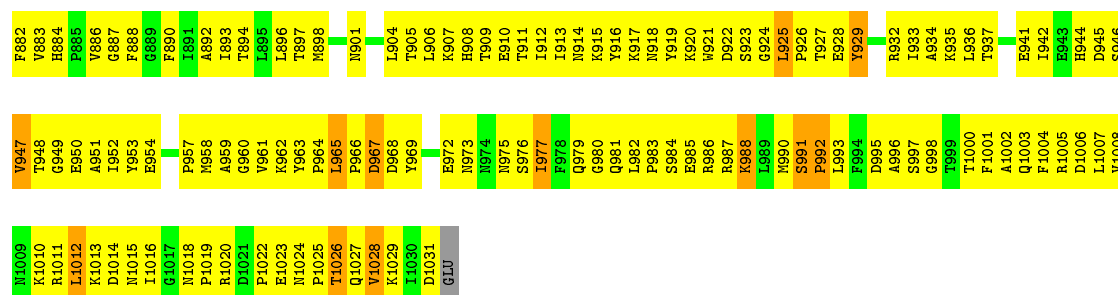
• Molecule 2: Baseplate wedge protein gp7



• Molecule 2: Baseplate wedge protein gp7



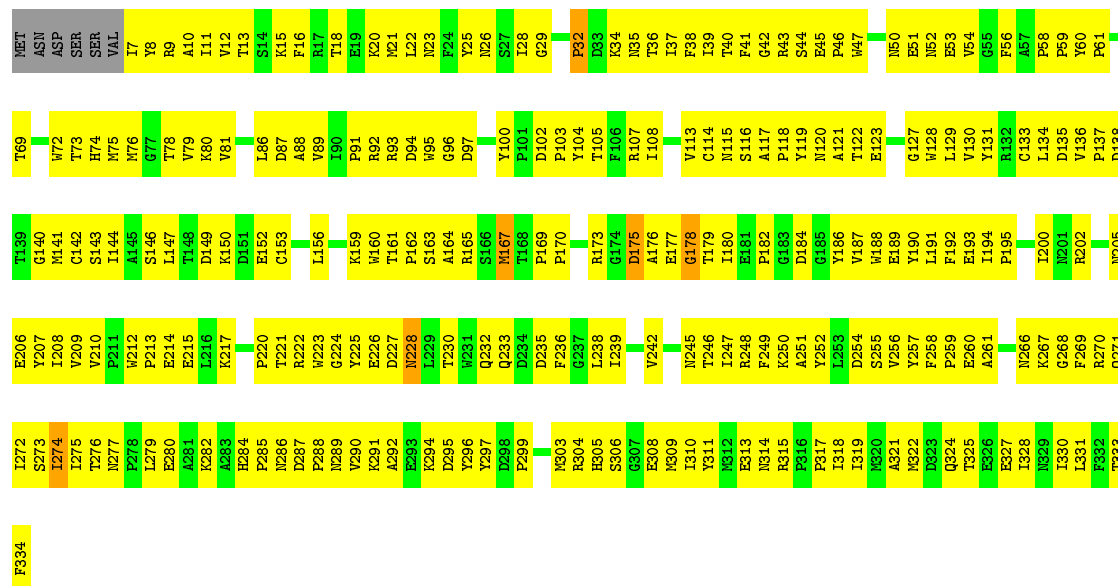




I328
I329
I330
I331
F332
T333
F334

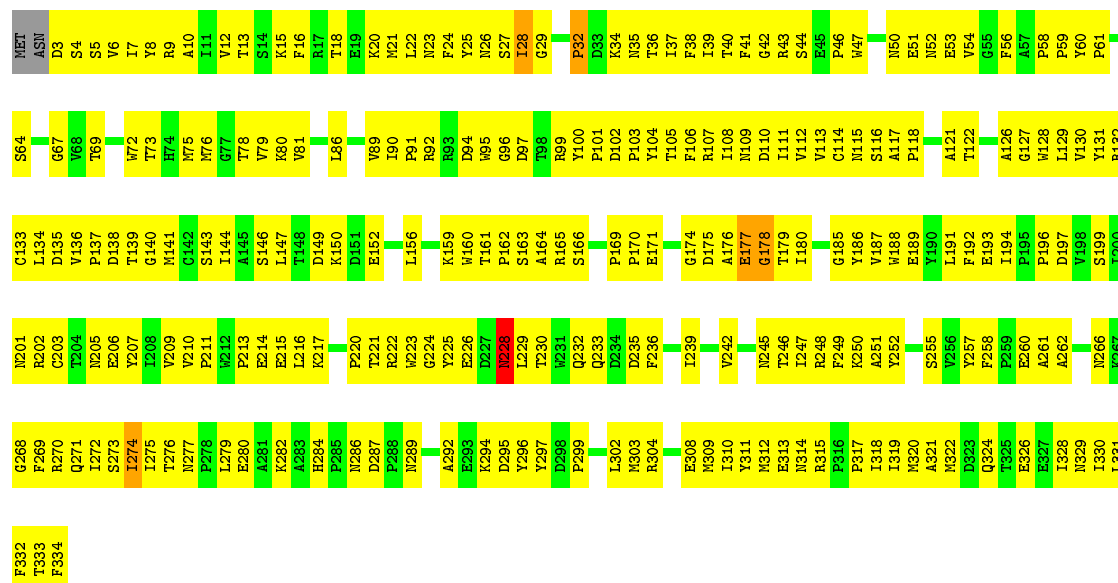
• Molecule 3: Baseplate wedge protein gp8

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%



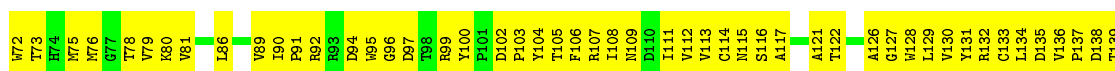
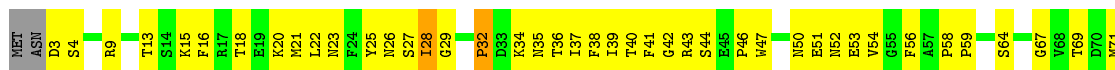
- Molecule 3: Baseplate wedge protein gp8

Chain z: 96%



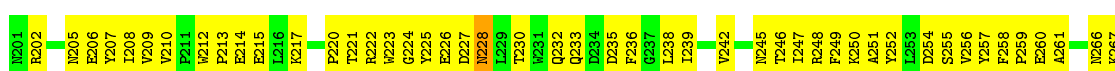
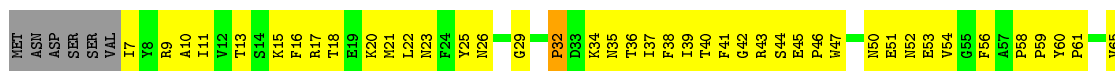
- Molecule 3: Baseplate wedge protein gp8

Chain AA: 33% 65%



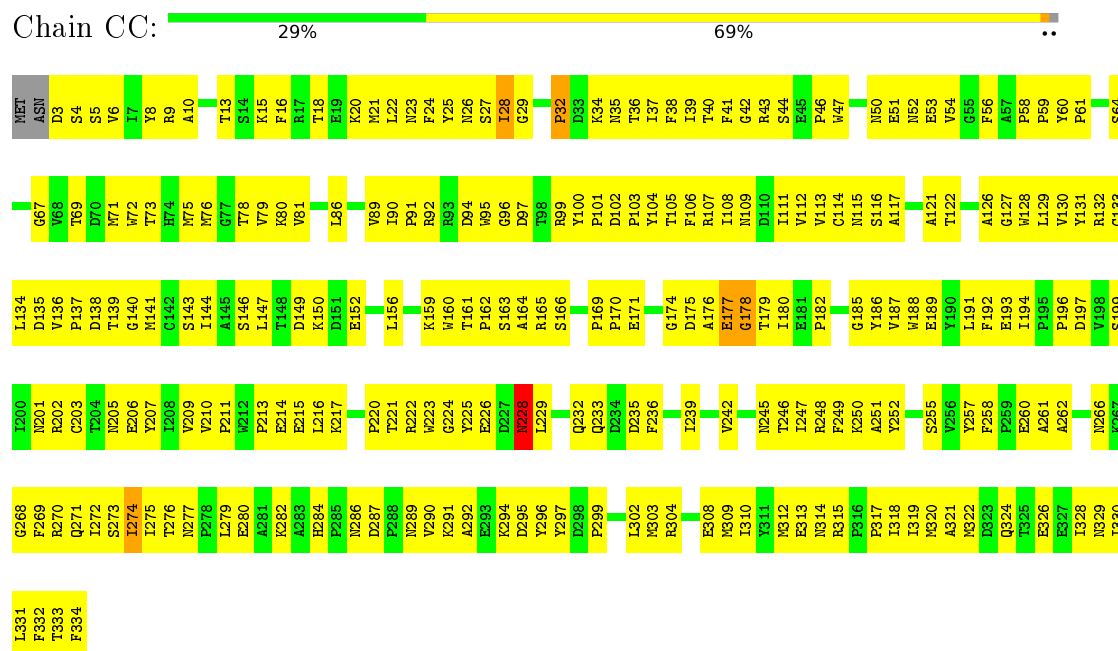
- Molecule 3: Baseplate wedge protein gp8

Chain CB: 28% 69%

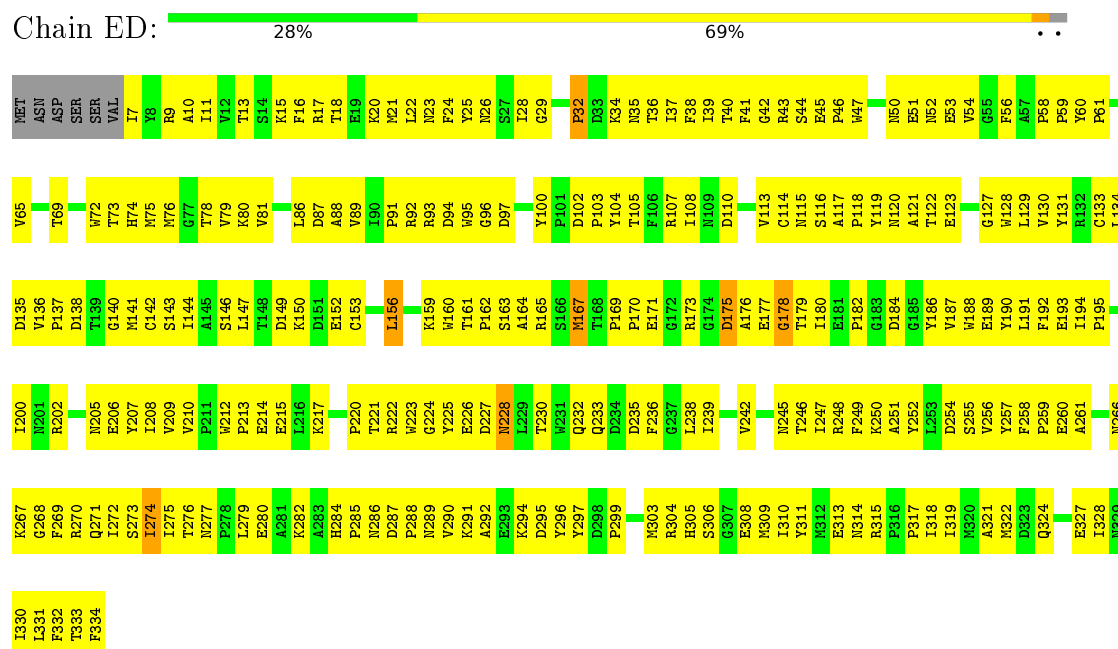




• Molecule 3: Baseplate wedge protein gp8

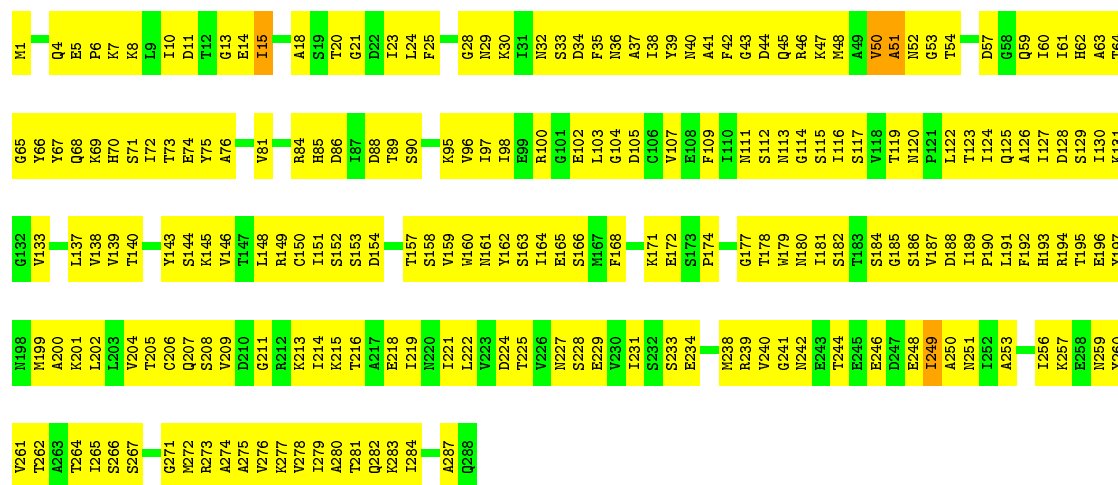


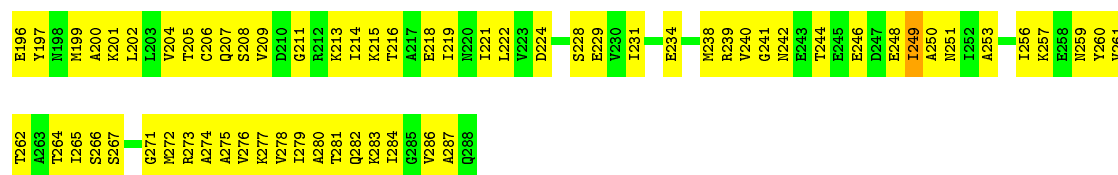
• Molecule 3: Baseplate wedge protein gp8



• Molecule 3: Baseplate wedge protein gp8

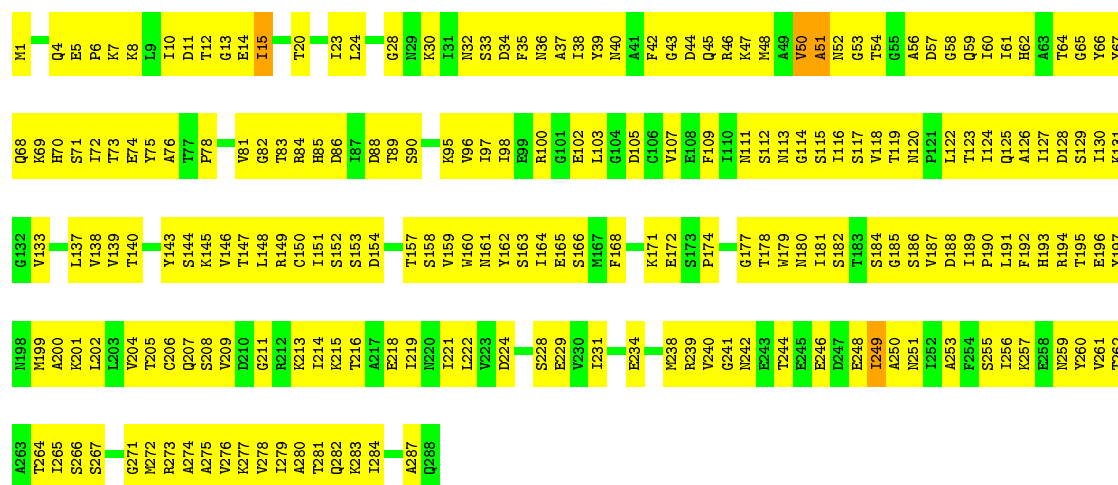
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	Q271	T204	D138	S5
	I272	N205	T139	V6
	S273	E206	G140	I7
	I274	Y207	M141	Y8
	I275	I208	C142	R9
	T276	V209	S143	H75
	I277	V210	I144	M76
	T278	P211	A145	G77
	I279	E212	S146	T78
	E280	P213	L147	V79
	A281	E214	T148	R30
	K282	E215	D149	V81
	K283	L216	K150	T18
	H284	K217	D151	E49
	T285		E152	K20
	N286	P220		M21
	T287	T221	L156	L22
	T288	R222		N23
	N289	H223	K159	F24
		G224	V160	Y25
	A292	T225	T161	N26
	K293	E226	P162	
	K294	D227	S163	I28
	D295	K228	A164	G29
	Y296	L229	R165	
	T297	T230	S166	P32
	T298	H231		D33
	P299	Q232	P169	K34
		Q233	P170	N35
		D234	E171	T36
	L302	D235		I37
K303		F236	G174	F38
R304			D175	I39
	E308	I239	A176	T40
	K309		E177	F41
	T310	V242	G178	N109
	V311		T179	R43
	H312	N245	I180	G44
	E313	T246	E181	S44
	N314	I247	P182	E45
	R315	R248	C114	P46
	P316	F249	G185	W47
	P317	K250	V186	
	T318	A251	V187	N50
	I319	Y252	W188	E51
	K320		E189	N52
	A321	S255	Y190	E53
	K322	V256	L191	V54
	Q323	Y257	F192	G55
	Q324	F258	E193	F56
	T325	P259	I194	A57
	K326	E260	P195	P58
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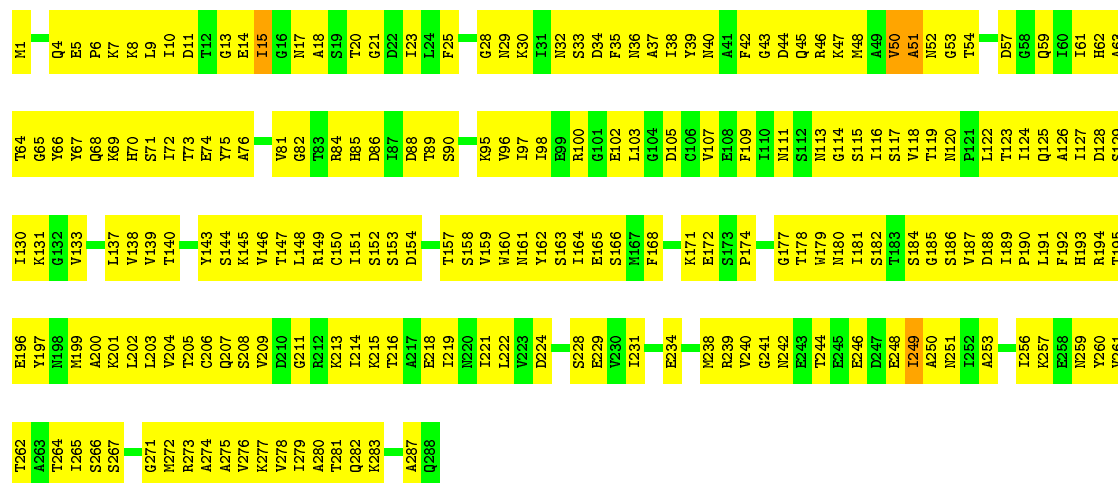
• Molecule 4: Baseplate wedge protein gp9

Chain H: 27% 72%



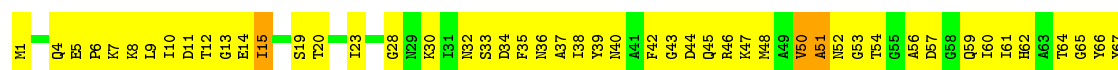
• Molecule 4: Baseplate wedge protein gp9

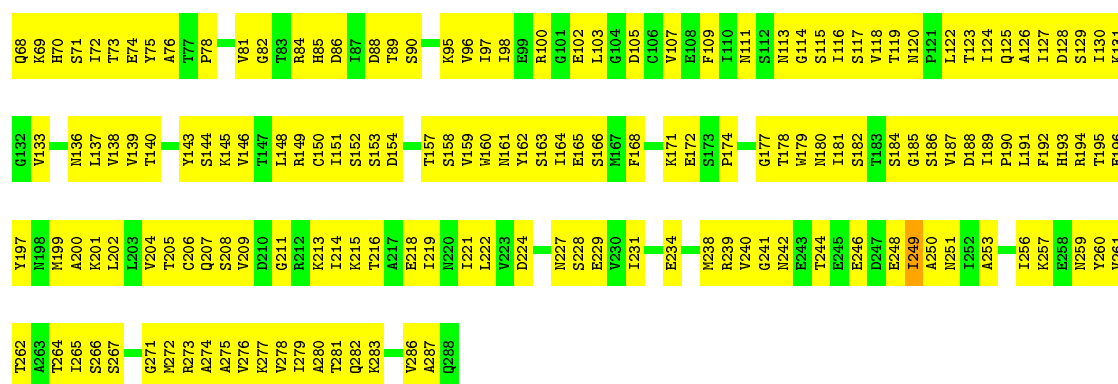
Chain V: 27% 71%



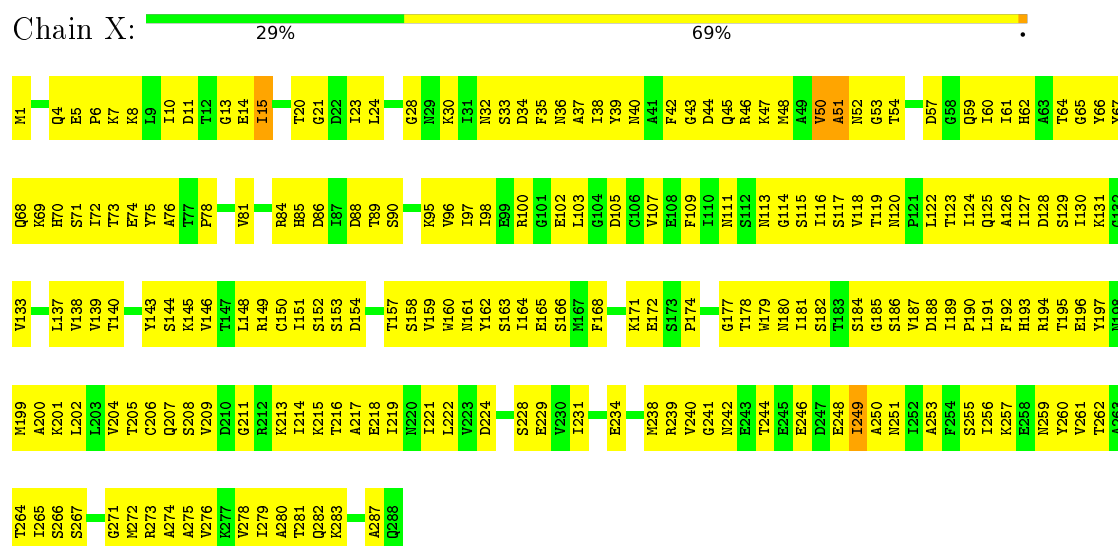
• Molecule 4: Baseplate wedge protein gp9

Chain W: 27% 71%

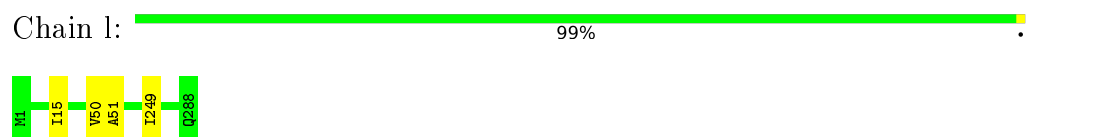




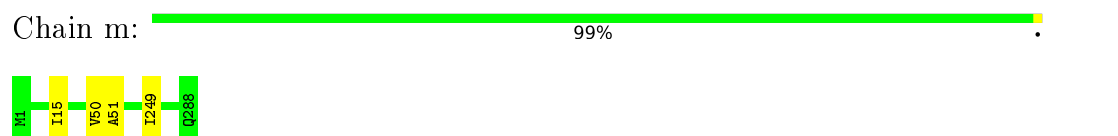
- Molecule 4: Baseplate wedge protein gp9



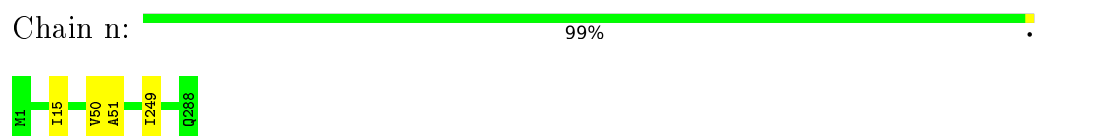
- Molecule 4: Baseplate wedge protein gp9



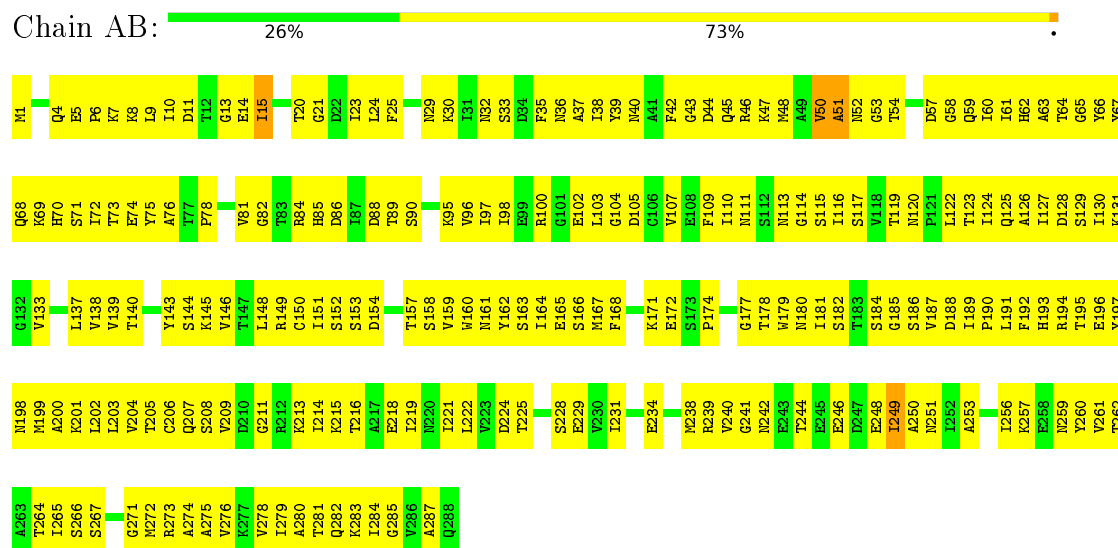
- Molecule 4: Baseplate wedge protein gp9



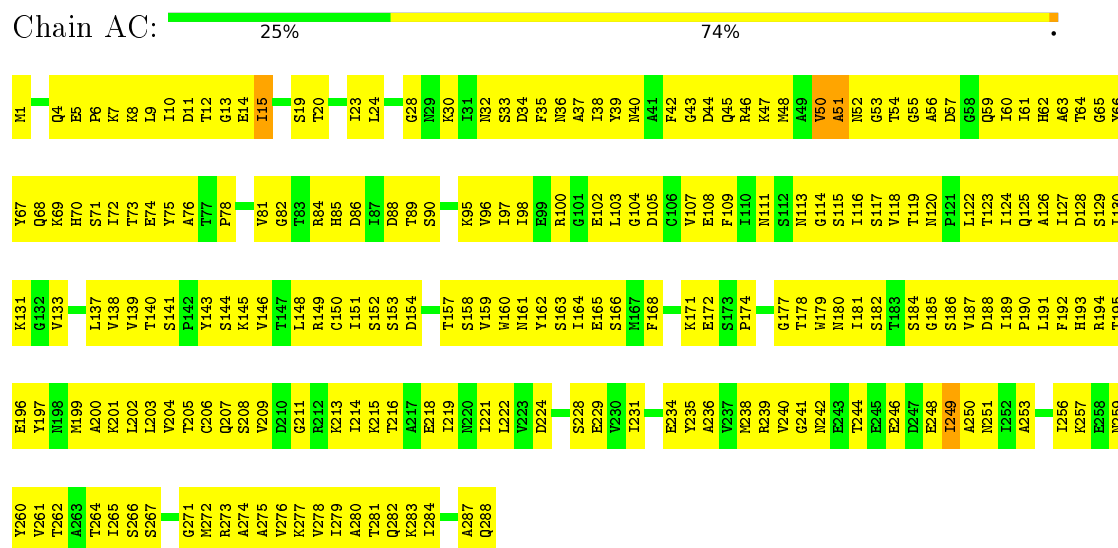
- Molecule 4: Baseplate wedge protein gp9



- Molecule 4: Baseplate wedge protein gp9



- Molecule 4: Baseplate wedge protein gp9



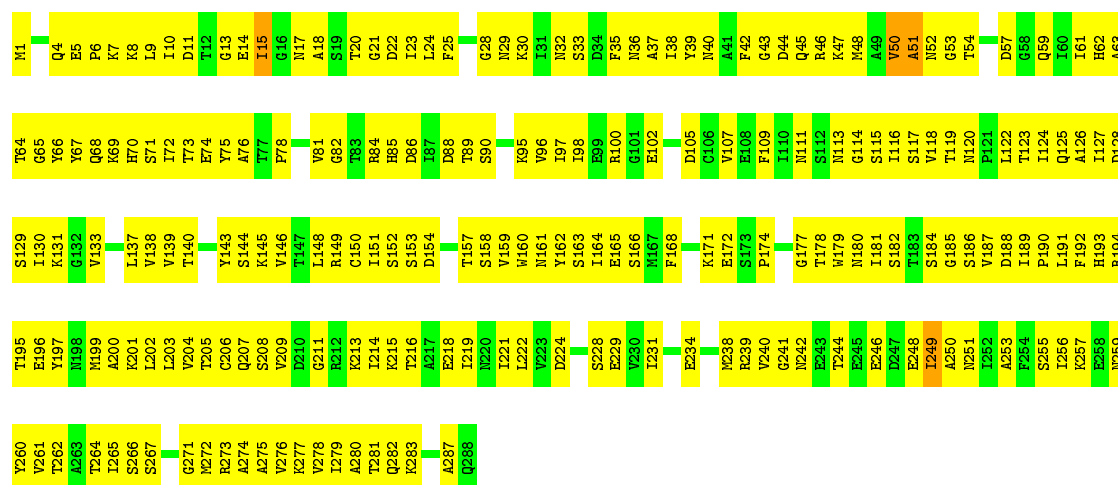
- Molecule 4: Baseplate wedge protein gp9





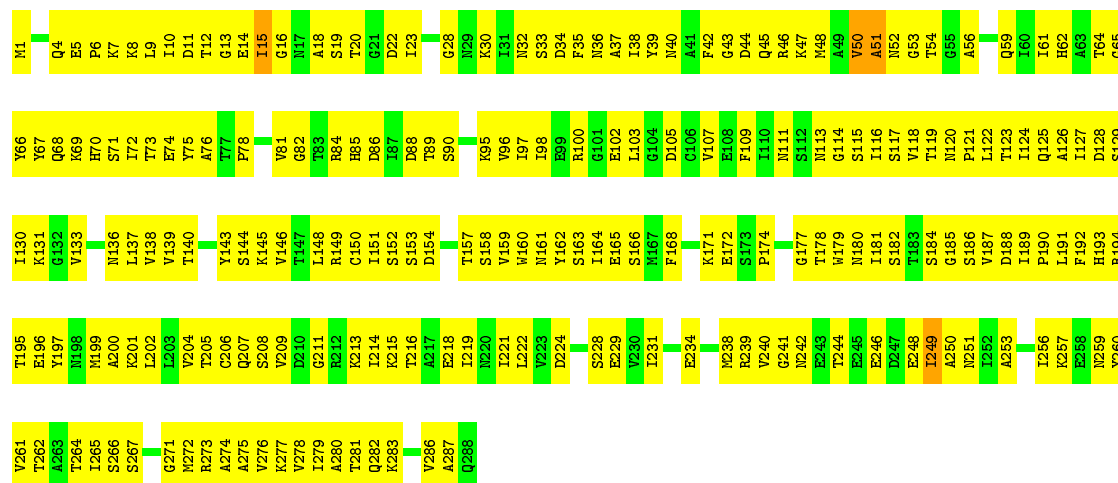
• Molecule 4: Baseplate wedge protein gp9

Chain CD: 27% 72%



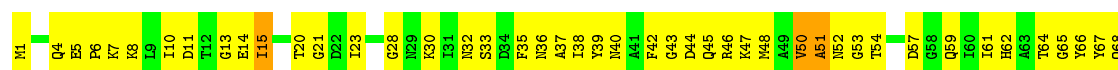
• Molecule 4: Baseplate wedge protein gp9

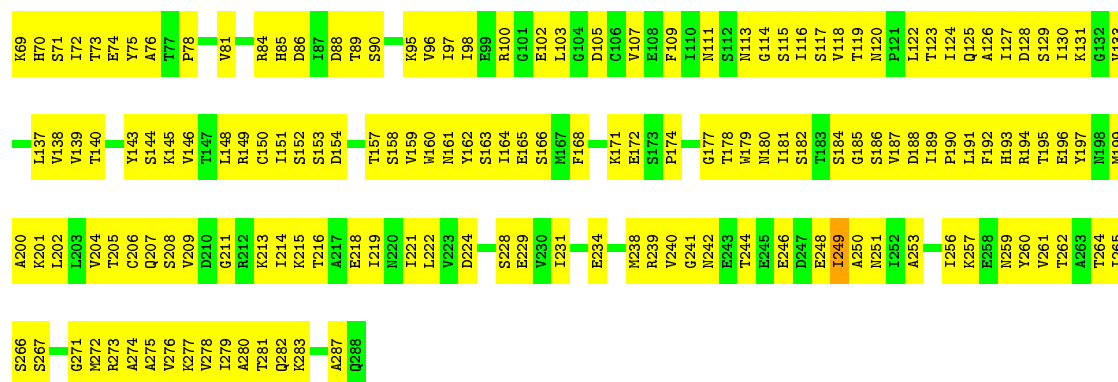
Chain CE: 27% 72%



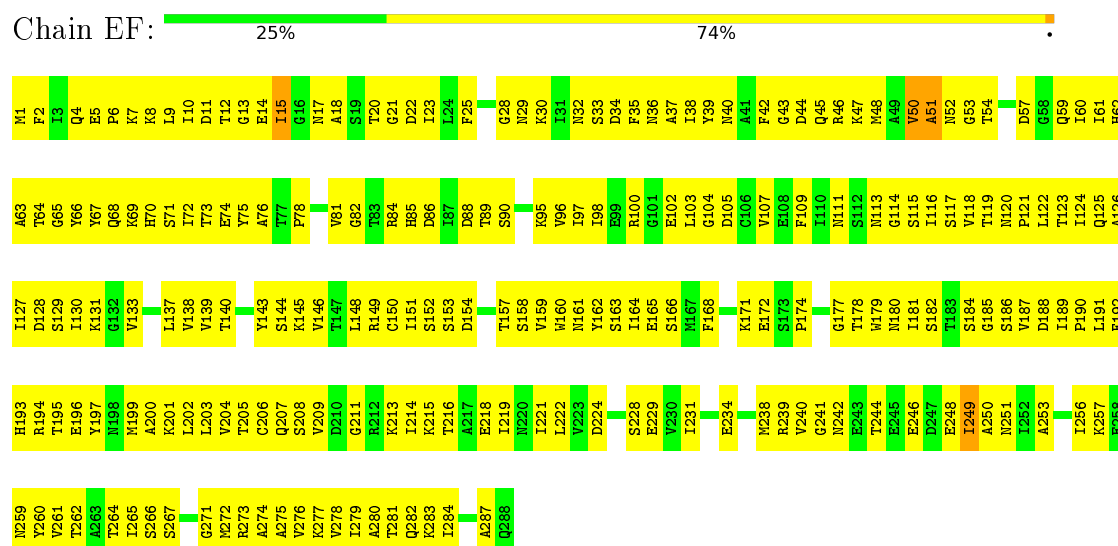
• Molecule 4: Baseplate wedge protein gp9

Chain CF: 31% 68%

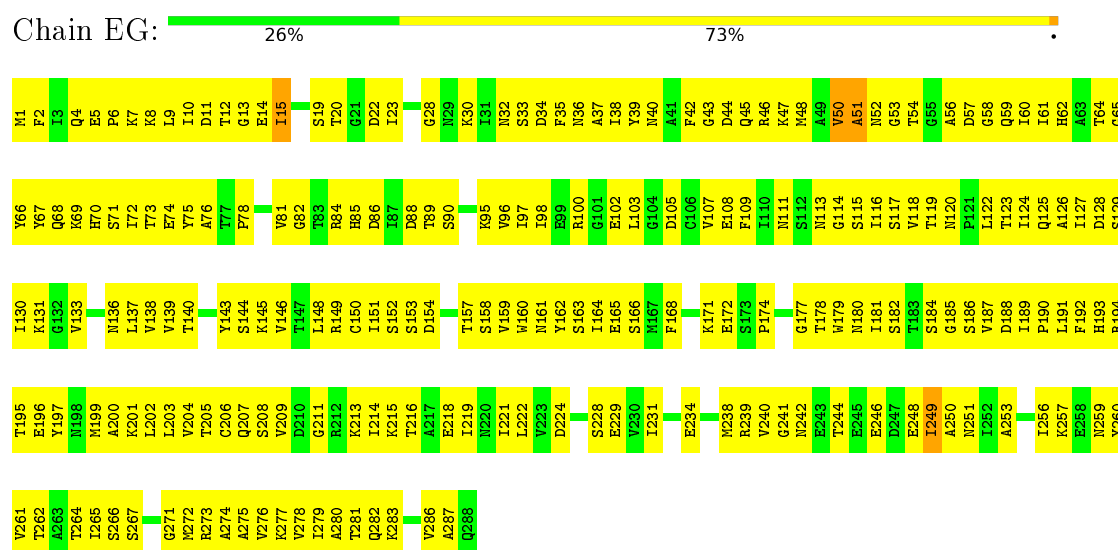




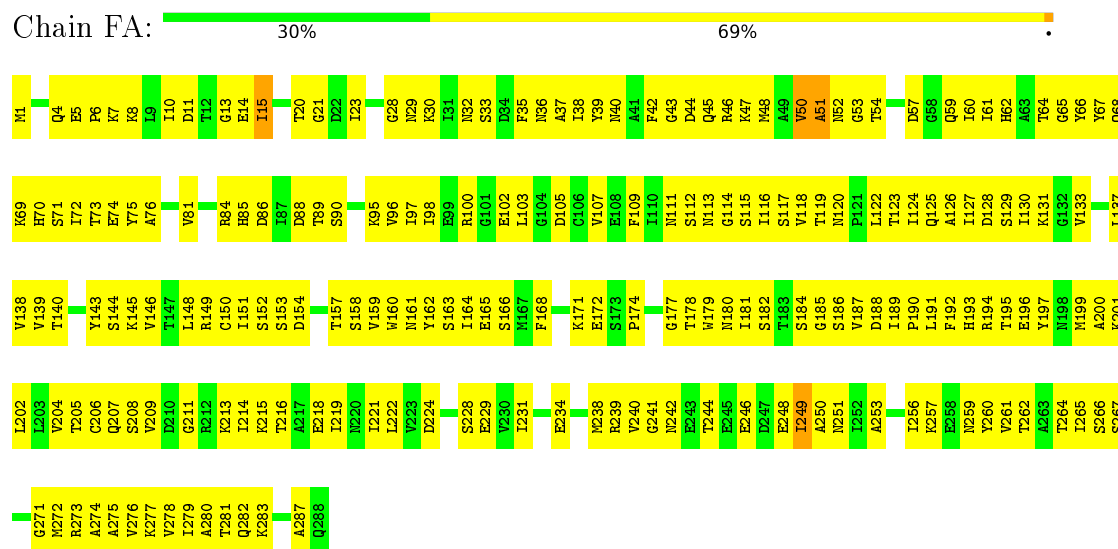
• Molecule 4: Baseplate wedge protein gp9



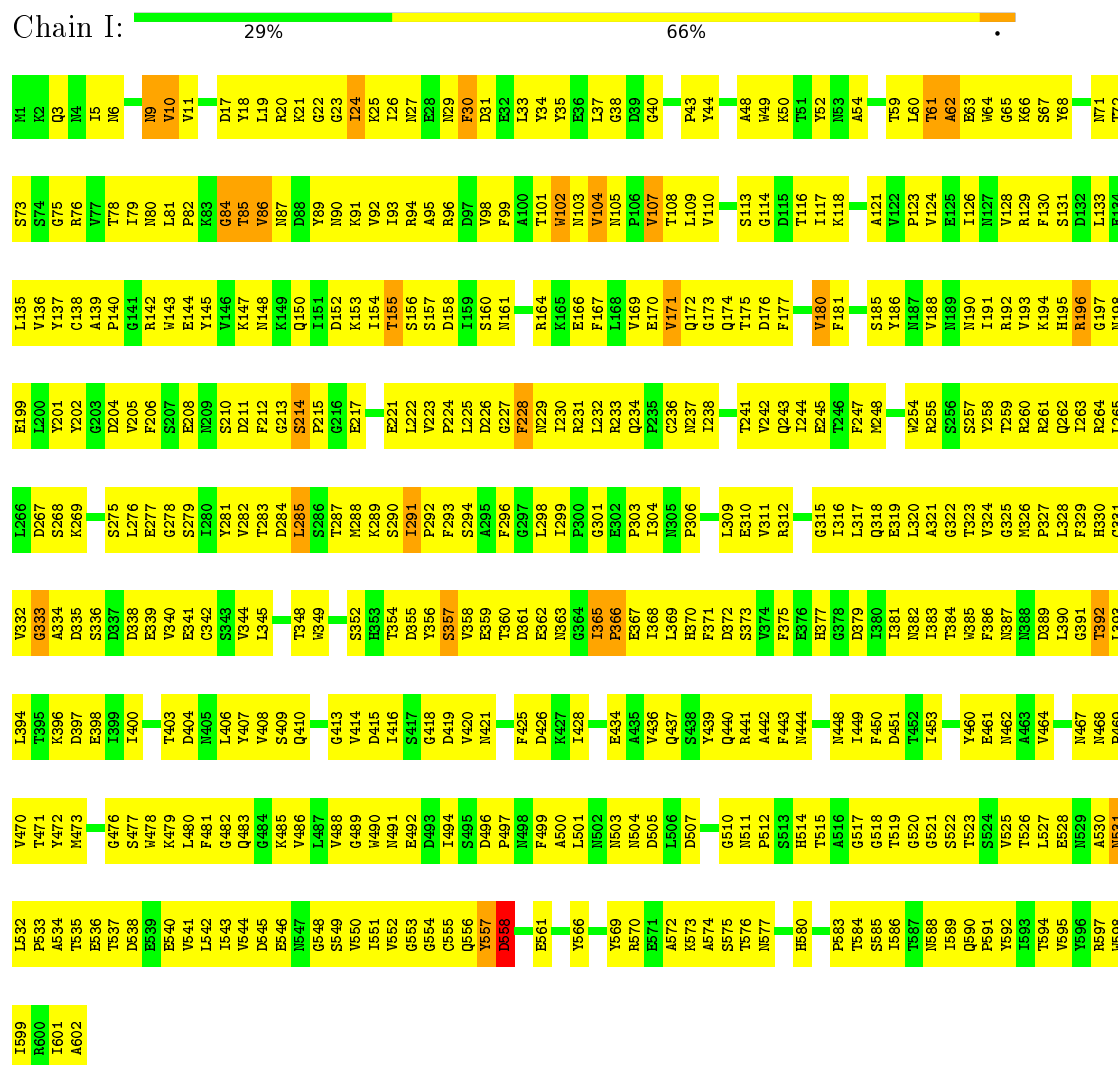
• Molecule 4: Baseplate wedge protein gp9



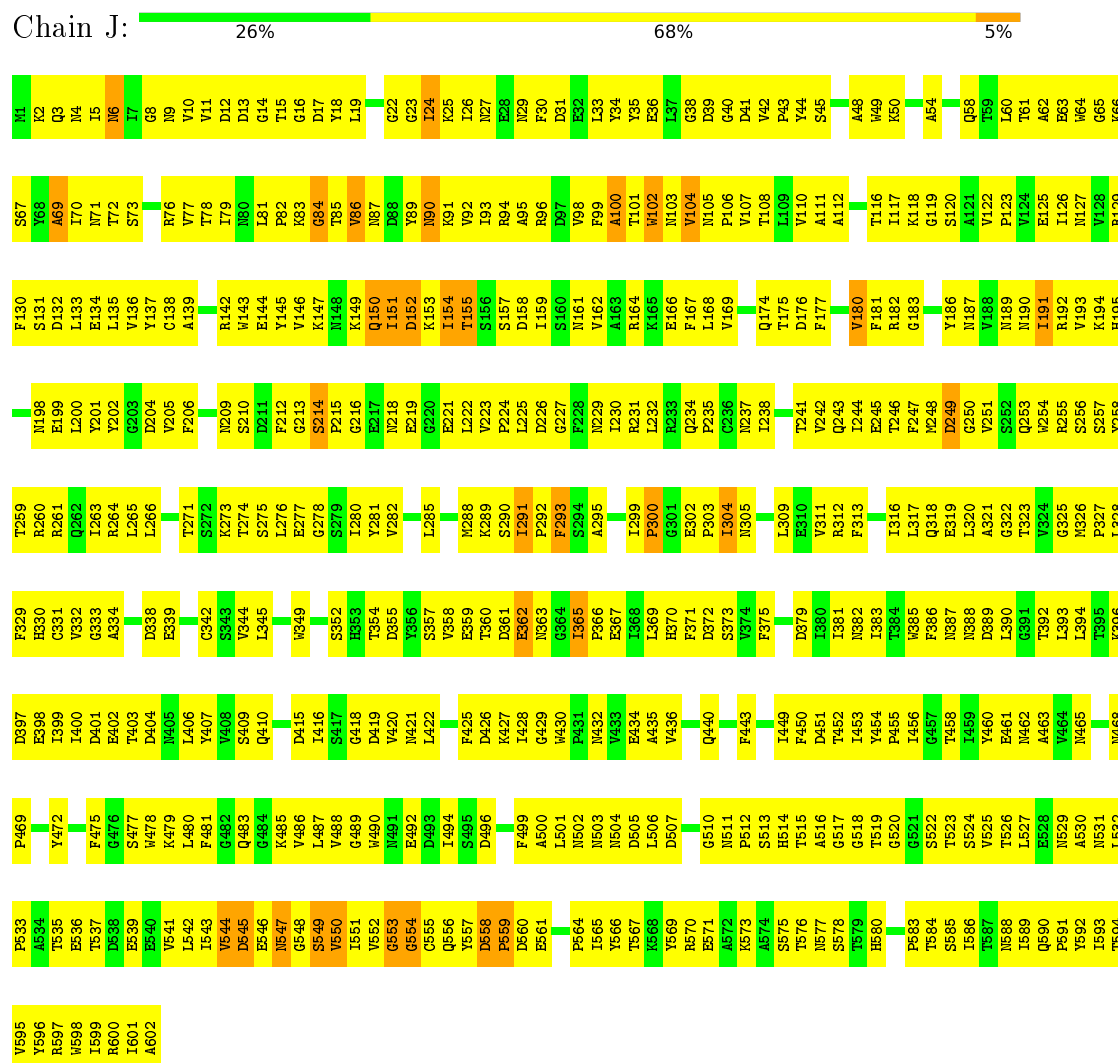
• Molecule 4: Baseplate wedge protein gp9



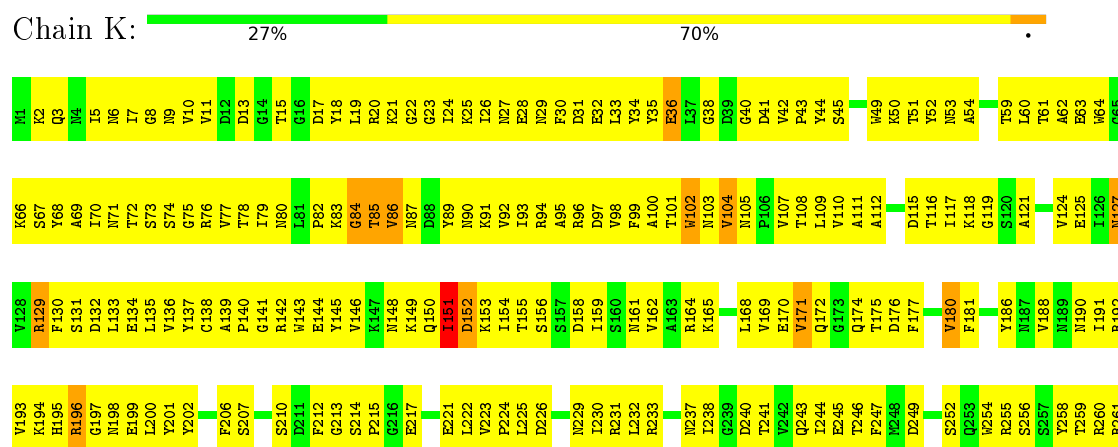
• Molecule 5: Baseplate wedge protein gp10



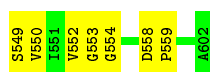
• Molecule 5: Baseplate wedge protein gp10



• Molecule 5: Baseplate wedge protein gp10







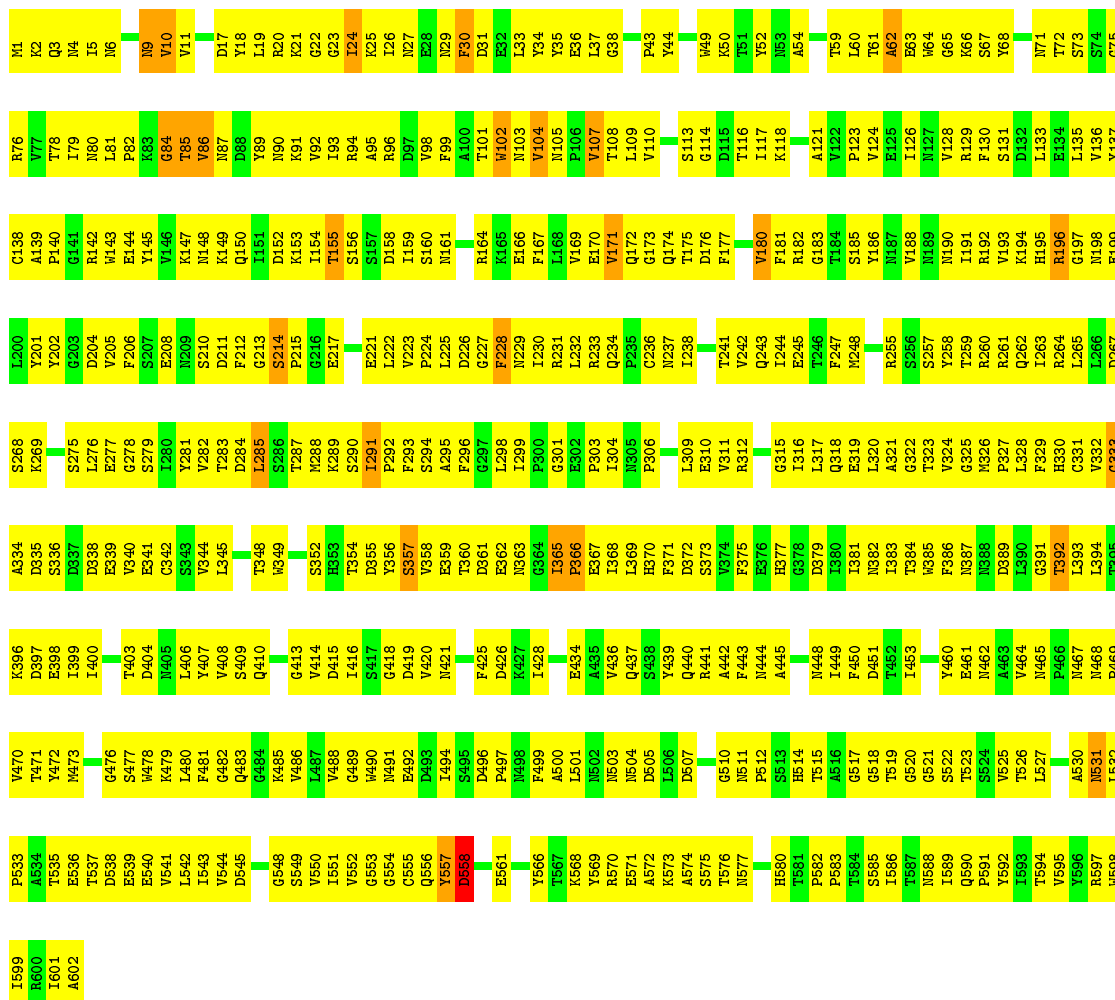
• Molecule 5: Baseplate wedge protein gp10

Chain q: 95% 5%



• Molecule 5: Baseplate wedge protein gp10

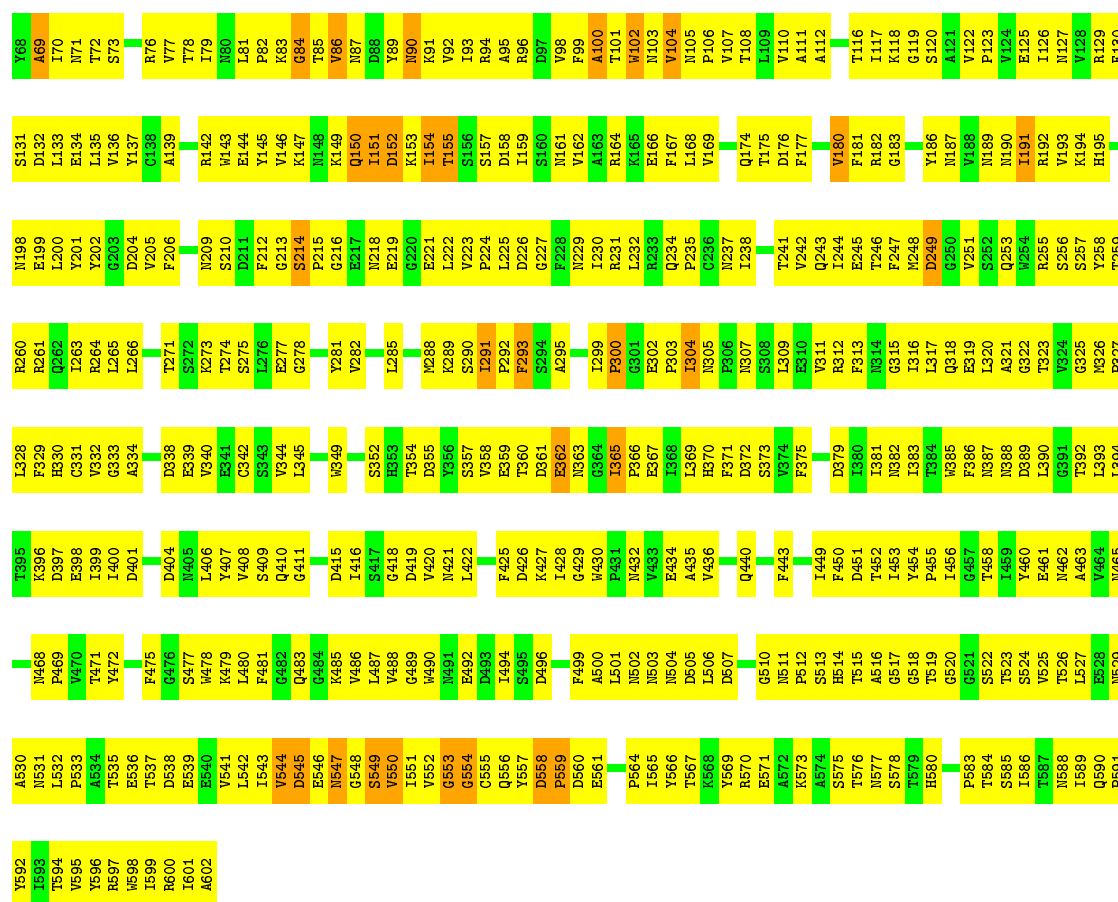
Chain AE: 28% 68% .



• Molecule 5: Baseplate wedge protein gp10

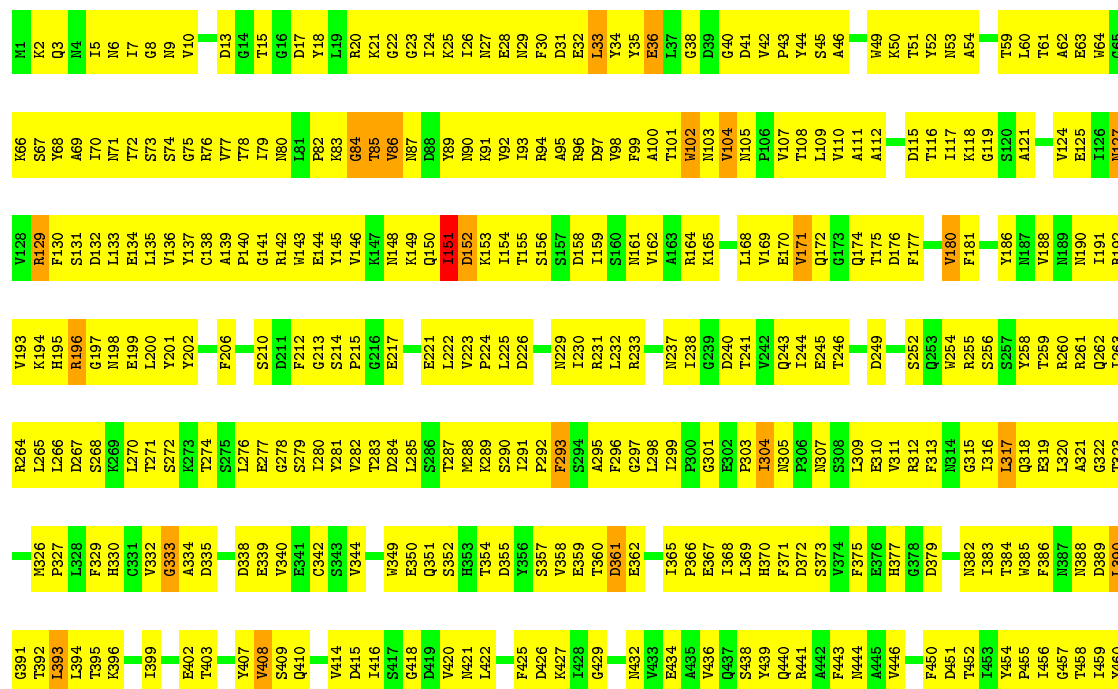
Chain AF: 27% 67% 5%





• Molecule 5: Baseplate wedge protein gp10

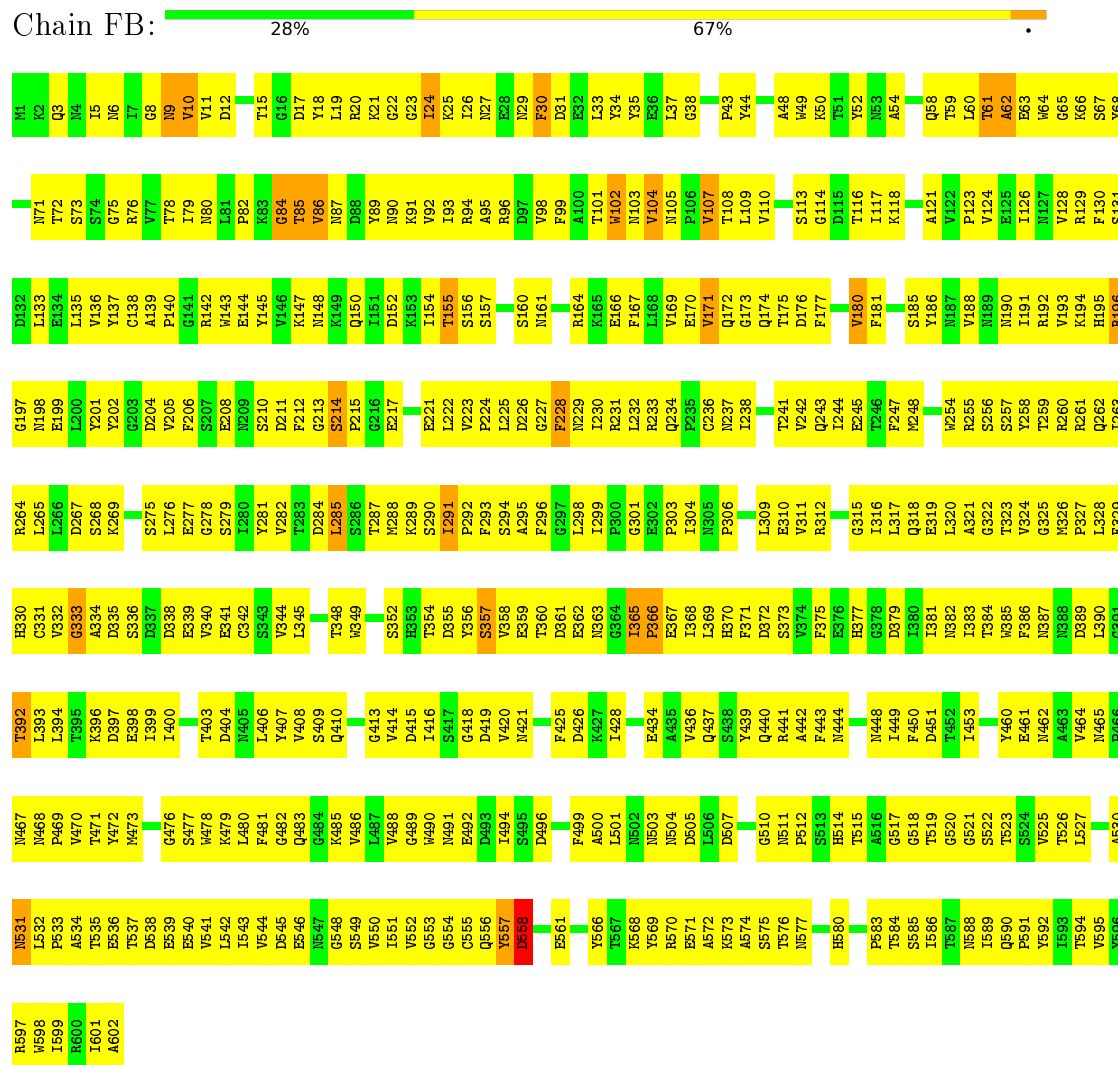
Chain AG: 27% 69%



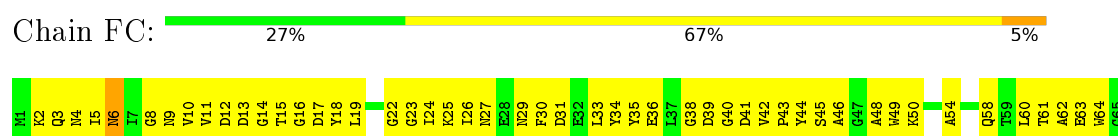
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• Molecule 5: Baseplate wedge protein gp10



• Molecule 5: Baseplate wedge protein gp10



K66	R129	Y258	F329	L394	P469	P533	Y596
S67	F130	T259	H330	T395	P469	A534	R597
Y68	D132	R260	C331	K396	Y472	T535	W598
A69	D133	R261	V332	R397		E536	I599
I70	L133	Q262	G333	E398	F475	T537	R600
N71	E134	L263	A334	I399	G476	D538	I601
T72	L135	R264		I400	S477	E539	A602
S73	V136	L265	D338	D401	W478	E540	
	Y137	L266	E339	D404	K479	V541	
	C138		V340	N405	F480	L542	
R76	G139	T271	E341	L406	F481	L543	
R77	A139	S272	G342	G482	G482	V544	
T78		K273	S343	Y407	Q483	E545	
I79	R142	T274	V344	V408	G484	E546	
N80	W143	S275	L345	S409	K485	N547	
L81	E144	D211		Q410	V486	G548	
P82	Y145	L276			L487	D17	
R83	V146	E277	K349		V550	K83	
K84	K147	G278		D415	V488	V551	
G84	K147			L416	G489	V552	
T85	W148	P215	S352	S417	W490	V553	
R86	K149	G216	R553	G418	N491	G553	
N87	Q150	E217	T354	D419	D492	G554	
D88	L151	E218	V355	V420	D493	C555	
Y89	D152	E219	V356	N421	L494	Y556	
	K153		S357	L422	G495	Y557	
N90	K153	E221	V358		D496	D558	
K91	I154	L222	E359	F425		P559	
V92	T155	V223	T360	D426	F499	P560	
R93	S156	D225	D361	K427	A500	G561	
A95	D158	L226	E362	N501	F501	E562	
R96	I159	L227	R363	N502	N502	E563	
	S160	G227	G364	G429	N503	E564	
D97	S160	E228	T365	P431	N504	E565	
V98	N161	E229	P366	N432	L506	E566	
F99	V162	L230	I367	V433	L506	E567	
A100	R163	L231	R368	V433	L506	E568	
T101	K164	L232	R370	E434	D507	Y569	
W102	K165	L233	E302	A435	G510	R570	
N103	E166	R233	R303	A435	N511	E571	
V104	F167	Q234	I304	Q440	P512	A572	
N105	L168	P235	S373		S513	K573	
P106	V169	C236	V374	F443	H514	A574	
V107		L237	F375	F443	T515	S575	
T108	Q174	N238	E376	I449	A516	N576	
L109	T175	E310	R377	F450	G517	N577	
V110	D176	R311	G376	F450	G518	S578	
A111	F177	F313	D379	T452	T519	T579	
A112		Q243	T380	T452	G520	H580	
	V180	L244	I381	I453	G521	P583	
T116	F181	E245	N382	Y454	S522	T584	
I117	R182	T246	I383	P455	S523	S585	
K118	G183	F247	E319	I456	S524	S586	
G119		D248	T384	T458	V525	N588	
S120	Y186	D249	K385		T526	L589	
A121	N187	G250	A321		L60	Q590	
V122	L188	V251	G322	N463	T527	P591	
P123	N189	S252	T323	A463	E528	Y592	
V124	N190	G253	D389	V464	N529	E593	
E125	I191	N254	G325	N465	A530	E594	
I126	R192	R255	M326		T594	L126	
N127	V193	S256	P327		N531	W64	
V128	K194	S257	L328	N468	L532	G65	

• Molecule 5: Baseplate wedge protein gp10

Chain FD:  26%  70%

V193	T263	K326	G391
K194	R264	P327	T392
L265	L265	L393	L393
R196	L266	L394	L394
I5	D267	F329	T395
N6	L197	H330	K396
I198	L133	G381	
E199	E134	V332	
L200	L135	G383	
T201	T271	A334	
Y202	K273	D335	
	T274		
F206	S275		
S210	L276	D338	
D211	E277	E339	
F212	S279	V340	
G213	E280	E341	
S214	K281	C342	
P215	V282	S343	
G216	T283	V344	
E217	D284	W349	
	N148	E350	
E221	L285	Q351	
L222	S286	S352	
V223	T287	H353	
P224	N288	T354	
L225	S290	D355	
L226	T291	Y356	
N229	F292	V357	
L230	P293	V358	
R231	A295	E359	
L232	S160	T360	
R233	D361	D361	
	L298	E362	
N237	L299	I365	
L238	P300	E434	
G239	G301	E367	
D240	E302	L368	
T241	P303	L369	
V242	I304	H370	
Q243	N305	F371	
L244	P306	D372	
E245	N307	S373	
T246	S308	V374	
T247	E310	E376	
N248	V311	L309	
D249	R312	G378	
	F313	D379	
S252	H314		
Q253	G315	N382	
W254	L316	L383	
R255	L317	T384	
S256	Q318	V385	
S257	H187	V386	
L187	N188	H389	
A121	V183	L220	
T59	Q590	T259	
L60	P591	R260	
T61	Y592	A530	
A62	E593	E63	
E63	L126	W64	
N127		G65	



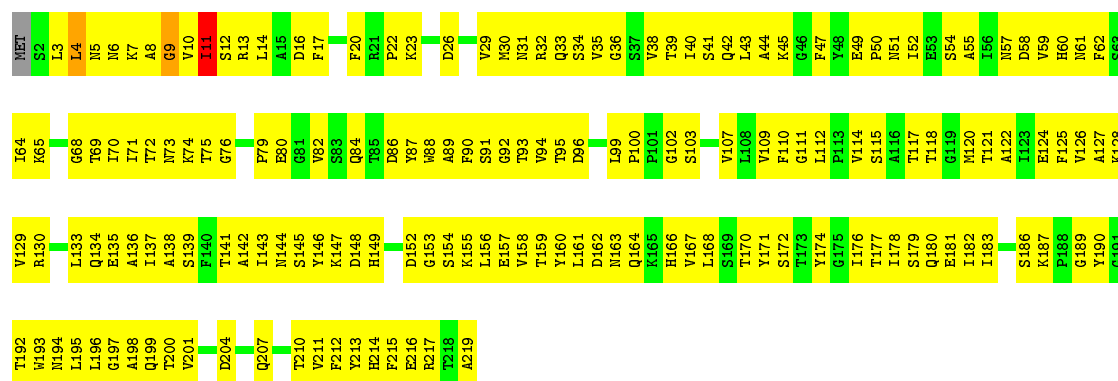
• Molecule 6: Baseplate wedge protein gp11

Chain L: 25% 74%



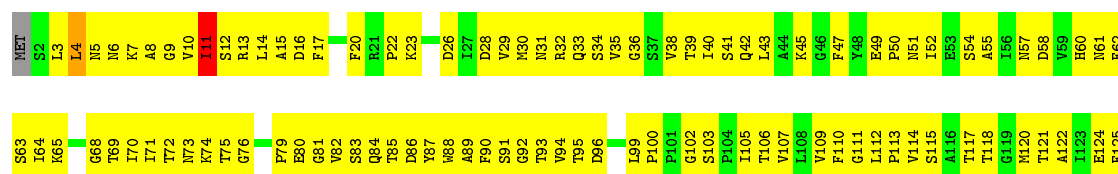
• Molecule 6: Baseplate wedge protein gp11

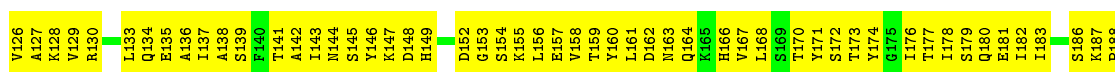
Chain M: 24% 74%



• Molecule 6: Baseplate wedge protein gp11

Chain N: 20% 79%





- 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%



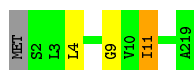
- Molecule 6: Baseplate wedge protein gp11

Chain r: 98%



- Molecule 6: Baseplate wedge protein gp11

Chain s: 98%



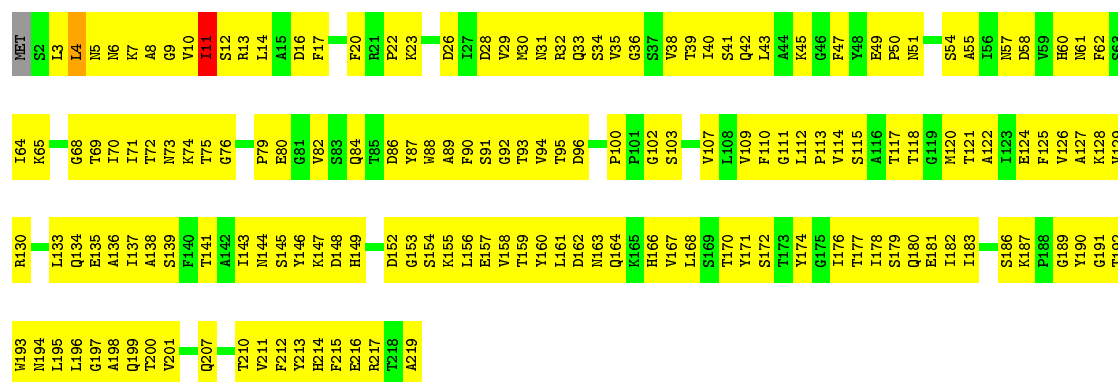
- Molecule 6: Baseplate wedge protein gp11

Chain t: 98%



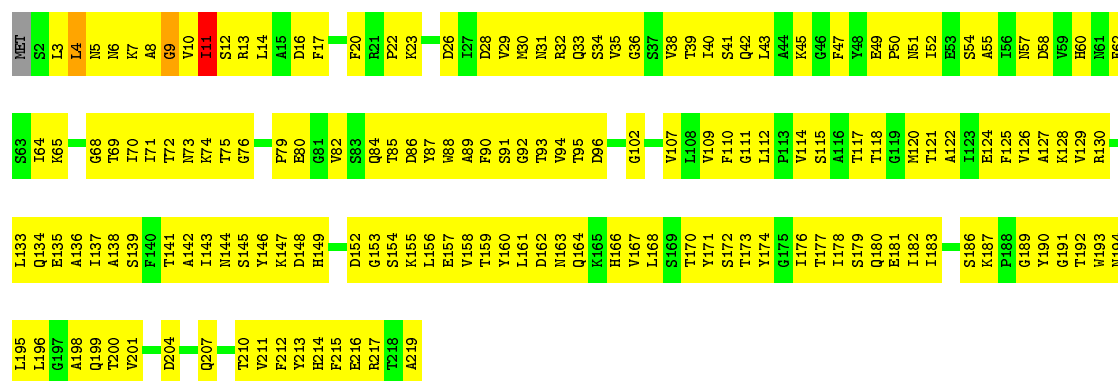
- Molecule 6: Baseplate wedge protein gp11

Chain BA: 26%



• Molecule 6: Baseplate wedge protein gp11

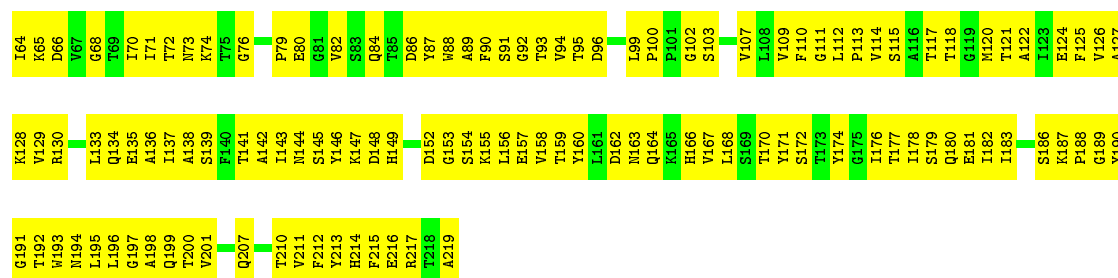
Chain BB: 26% 73%



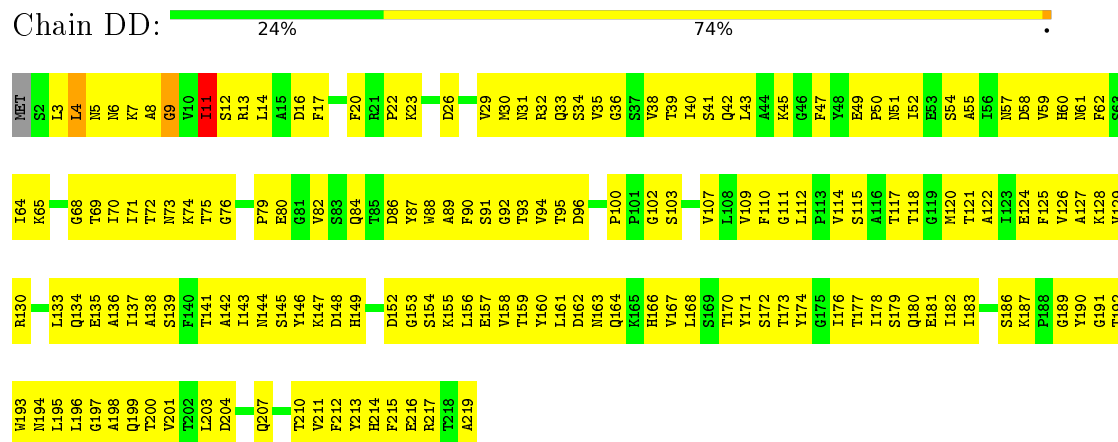
• Molecule 6: Baseplate wedge protein gp11

Chain BC: 24% 74%

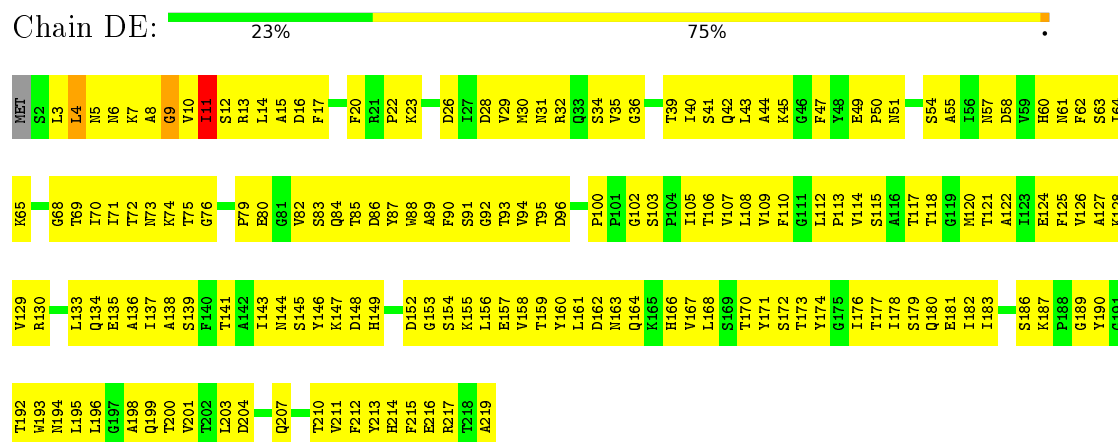




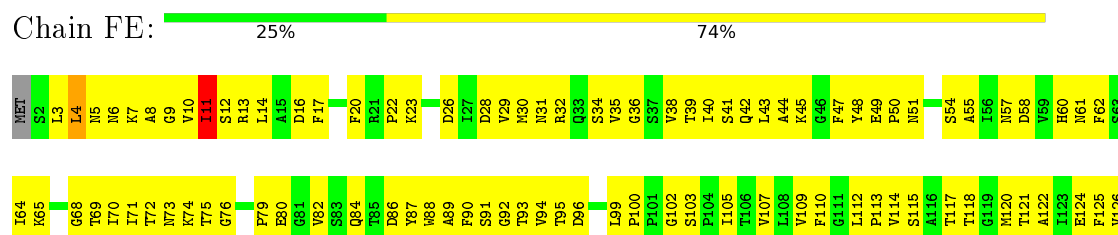
• Molecule 6: Baseplate wedge protein gp11

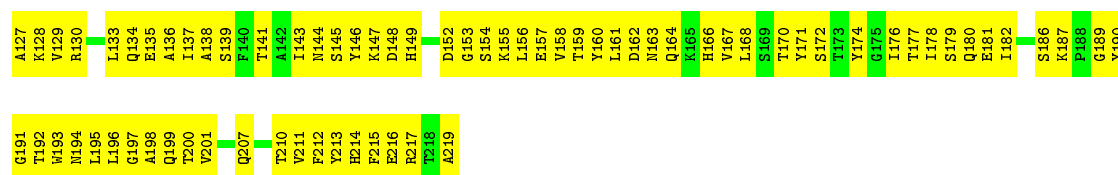


• Molecule 6: Baseplate wedge protein gp11

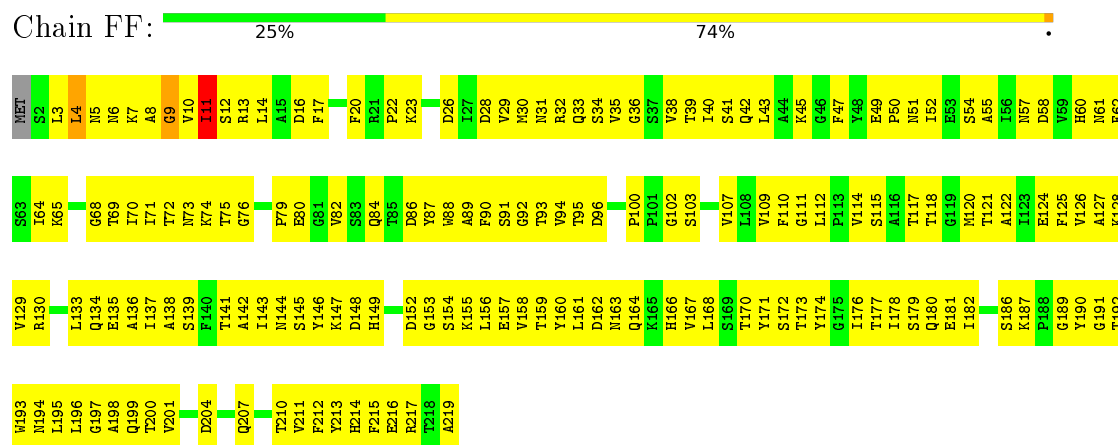


• Molecule 6: Baseplate wedge protein gp11

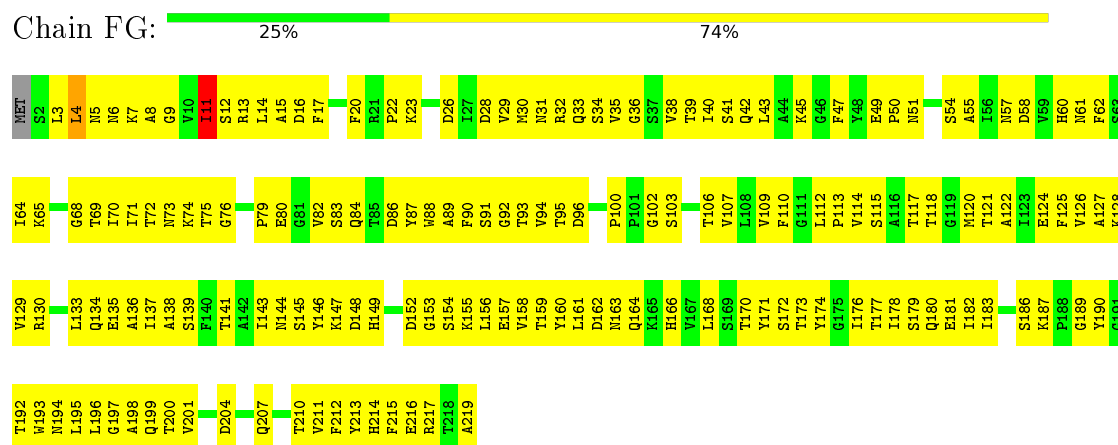




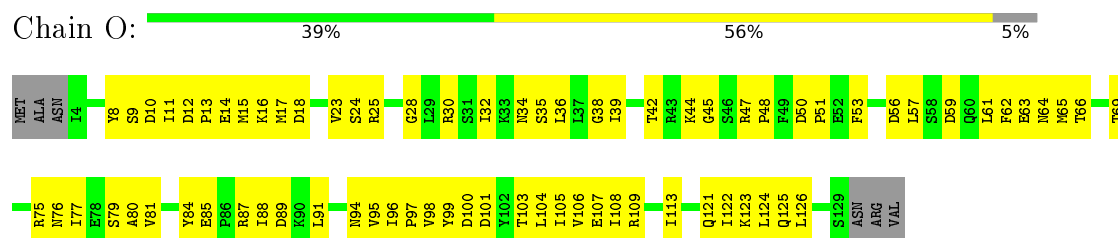
• Molecule 6: Baseplate wedge protein gp11



• Molecule 6: Baseplate wedge protein gp11

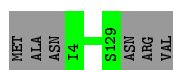


• Molecule 7: Baseplate wedge protein gp25



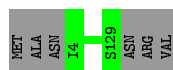
• Molecule 7: Baseplate wedge protein gp25





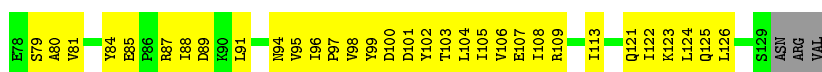
- Molecule 7: Baseplate wedge protein gp25

Chain u: 95% 5%



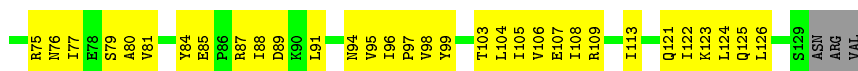
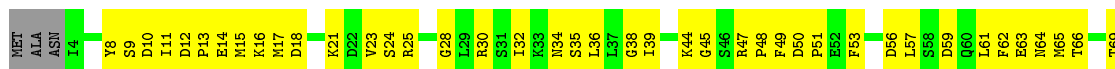
- Molecule 7: Baseplate wedge protein gp25

Chain BD: 43% 52% 5%



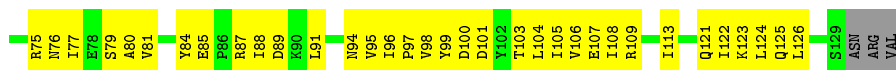
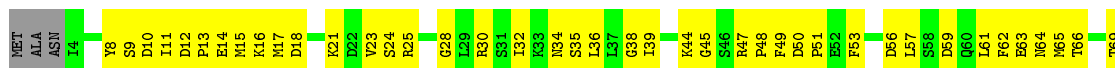
- Molecule 7: Baseplate wedge protein gp25

Chain DF: 40% 55% 5%



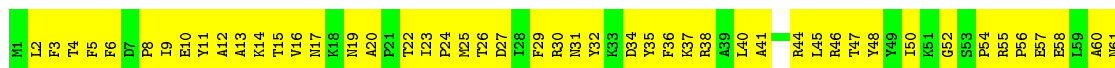
- Molecule 7: Baseplate wedge protein gp25

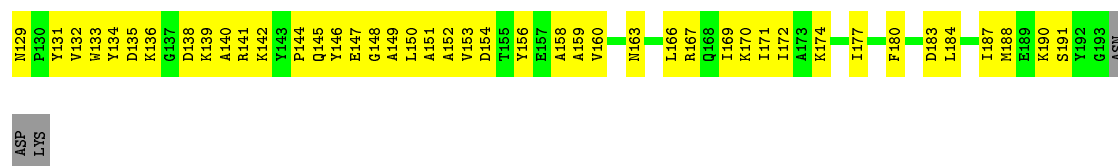
Chain GA: 39% 57% 5%



- Molecule 8: Baseplate wedge protein gp53

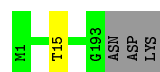
Chain P: 28% 70% 2%





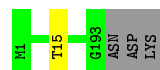
• Molecule 8: Baseplate wedge protein gp53

Chain f: 98%



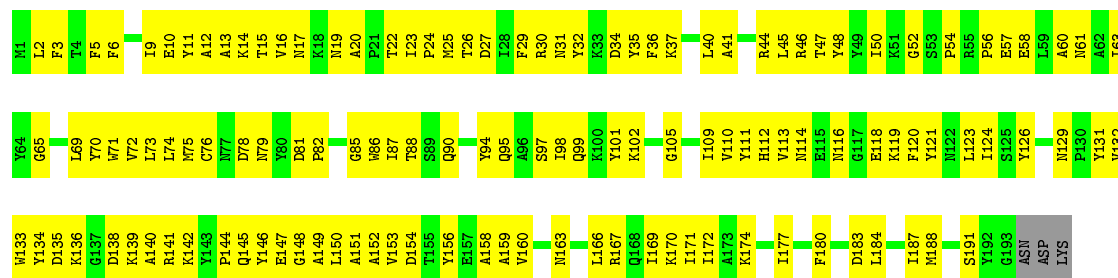
• Molecule 8: Baseplate wedge protein gp53

Chain v: 98%



• Molecule 8: Baseplate wedge protein gp53

Chain BE: 34% 65%



• Molecule 8: Baseplate wedge protein gp53

Chain DG: 28% 70%



ASP
LYS

• Molecule 8: Baseplate wedge protein gp53

Chain GB: 30% 69%

LYS	M1	L2	F3	T4	F5	F6	D7	P8	I9	E10	Y11	A12	A13	K14	T15	V16	M17	N18	N19	A20	F21	T22	T23	P24	N25	T26	D27	I28	F29	R30	N31	Y32	F33	D34	Y35	F36	K37	R38	A39	L40	A41		R44	L45	R46	T47	Y48	Y49	I50	K51	G52	S53	P54	R55	P56	E57	E58	L59	A60	M61
	A62	I63	Y64	G65		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	Q99	K100	R101	K102		G105		I109	V110	Y111	H112	V113	N114	E115	N116	G117	E118	K119	F120	Y121	N122	L123	I124	S125	Y126		N129
	P130	Y131	V132	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

4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	5176	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 ($e^-/\text{\AA}^2$)	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 ⓘ

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	656/660 (99%)	590 (90%)	59 (9%)	7 (1%)	17	63
1	B	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	34	77
1	BF	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	17	63
1	BG	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	34	77
1	EA	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	17	63
1	EB	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	34	77
1	Q	656/660 (99%)	590 (90%)	59 (9%)	7 (1%)	17	63
1	R	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	34	77
1	g	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	17	63
1	h	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	34	77
1	w	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	17	63
1	x	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	34	77
2	C	1000/1032 (97%)	817 (82%)	155 (16%)	28 (3%)	6	44
2	CA	1000/1032 (97%)	818 (82%)	154 (15%)	28 (3%)	6	44
2	EC	1000/1032 (97%)	818 (82%)	155 (16%)	27 (3%)	6	45
2	S	1000/1032 (97%)	818 (82%)	154 (15%)	28 (3%)	6	44
2	i	1000/1032 (97%)	818 (82%)	155 (16%)	27 (3%)	6	45
2	y	1000/1032 (97%)	818 (82%)	154 (15%)	28 (3%)	6	44
3	AA	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	46	83
3	CB	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	CC	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	46	83
3	D	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	E	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	46	83
3	ED	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	EE	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	46	83
3	T	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	U	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	46	83
3	j	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	k	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	46	83
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%)	14	58
4	AC	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	AD	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	CD	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	CE	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	CF	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	EF	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	EG	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	F	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	FA	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	G	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	H	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	V	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	W	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	X	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	l	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	m	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
4	n	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	14	58
5	AE	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	8	48
5	AF	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	11	53
5	AG	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	51
5	CG	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	8	48
5	DA	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	11	53
5	DB	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	51
5	FB	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	8	48
5	FC	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	11	53
5	FD	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	51
5	I	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	8	48
5	J	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	11	53
5	K	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	51
5	Y	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	8	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Z	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	11	53
5	a	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	51
5	o	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	8	48
5	p	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	11	53
5	q	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	9	51
6	BA	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	BB	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	BC	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	DC	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	DD	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	DE	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	FE	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	FF	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	FG	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	L	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	M	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	N	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	b	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	c	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	d	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	r	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	s	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
6	t	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	21	67
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%)	19	58

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%)	95	97
2	CA	896/921 (97%)	894 (100%)	2 (0%)	95	97
2	EC	896/921 (97%)	894 (100%)	2 (0%)	95	97
2	S	896/921 (97%)	894 (100%)	2 (0%)	95	97
2	i	896/921 (97%)	894 (100%)	2 (0%)	95	97
2	y	896/921 (97%)	894 (100%)	2 (0%)	95	97
3	AA	293/295 (99%)	291 (99%)	2 (1%)	88	94
3	CB	289/295 (98%)	288 (100%)	1 (0%)	94	96
3	CC	293/295 (99%)	291 (99%)	2 (1%)	88	94
3	D	289/295 (98%)	287 (99%)	2 (1%)	88	94
3	E	293/295 (99%)	291 (99%)	2 (1%)	88	94
3	ED	289/295 (98%)	287 (99%)	2 (1%)	88	94
3	EE	293/295 (99%)	291 (99%)	2 (1%)	88	94
3	T	289/295 (98%)	287 (99%)	2 (1%)	88	94
3	U	293/295 (99%)	291 (99%)	2 (1%)	88	94
3	j	289/295 (98%)	287 (99%)	2 (1%)	88	94
3	k	293/295 (99%)	291 (99%)	2 (1%)	88	94
3	z	289/295 (98%)	287 (99%)	2 (1%)	88	94
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%)	95	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%)	95	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%)	95	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%)	95	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%)	95	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%)	95	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%)	90	95
8	DG	166/169 (98%)	165 (99%)	1 (1%)	90	95
8	GB	166/169 (98%)	165 (99%)	1 (1%)	90	95
8	P	166/169 (98%)	165 (99%)	1 (1%)	90	95
8	f	166/169 (98%)	165 (99%)	1 (1%)	90	95
8	v	166/169 (98%)	165 (99%)	1 (1%)	90	95
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