



## wwPDB EM Validation Summary Report ⓘ

May 5, 2025 – 06:59 pm BST

PDB ID : 9F4B / pdb\_00009f4b  
EMDB ID : EMD-50187  
Title : Pre-assembled baseplate cup of Klebsiella phage KP1 variant vB\_Kpn\_Lilla1  
Authors : Orlova, E.V.; Isupov, M.N.  
Deposited on : 2024-04-26  
Resolution : 3.36 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

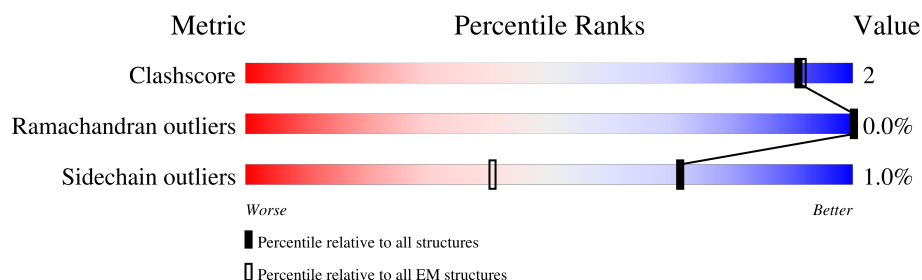
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

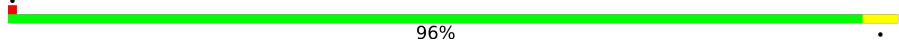
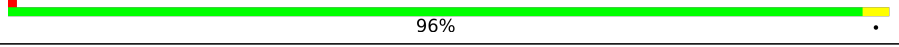
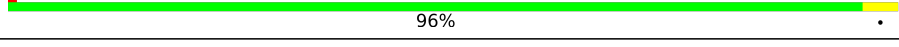
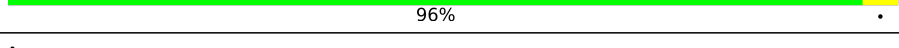
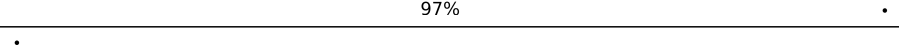
The reported resolution of this entry is 3.36 Å.

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.



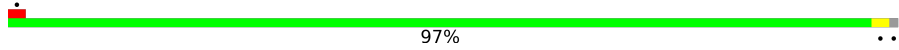
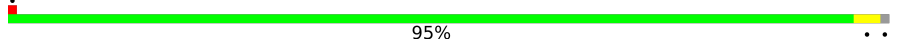
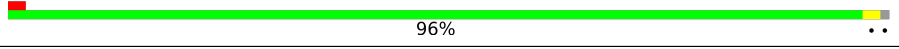
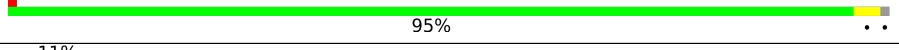


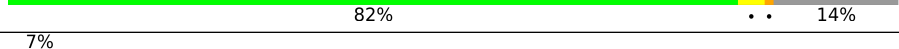
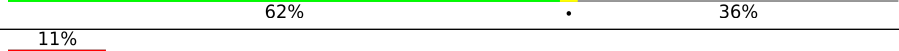
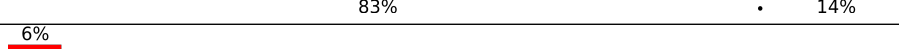
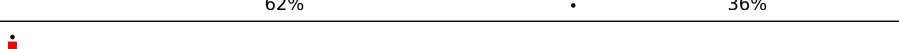
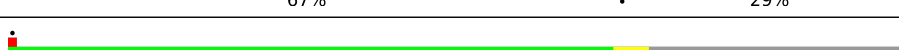

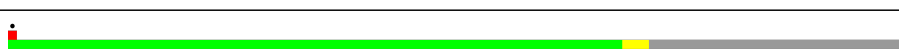

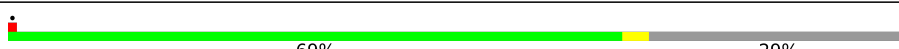
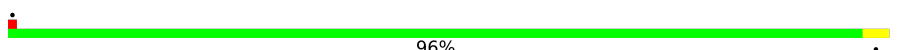
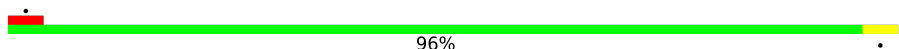
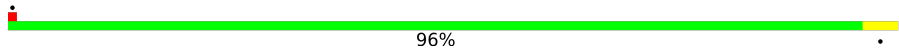
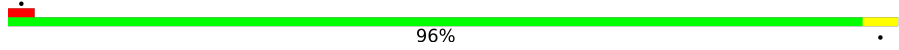
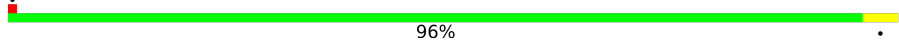
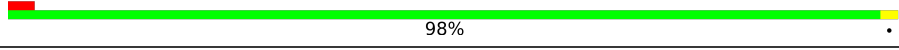
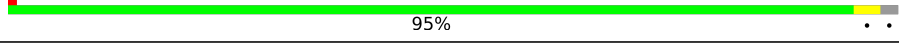
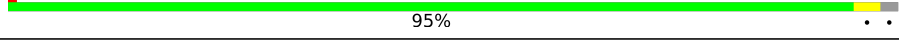
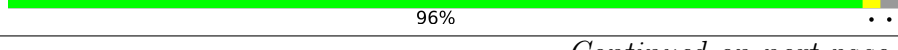

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AM	655	
1	AN	655	
1	AO	655	
1	AP	655	
1	AQ	655	
1	AR	655	
1	AS	655	
1	AT	655	

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Mol	Chain	Length	Quality of chain
1	AU	655	 97%
1	AV	655	 95%
1	AW	655	 96%
1	AX	655	 95%
2	BK	350	 11% 83% 14%
2	BL	350	 7% 63% 36%
2	BM	350	 12% 82% 14%
2	BN	350	 7% 62% 36%
2	BO	350	 11% 83% 14%
2	BP	350	 6% 62% 36%
3	BQ	308	 67% 29%
3	BR	308	 68% 29%
3	BS	308	 69% 29%
3	BT	308	 69% 29%
3	BU	308	 68% 29%
3	BV	308	 69% 29%
4	AG	212	 96%
4	AH	212	 96%
4	AI	212	 96%
4	AJ	212	 96%
4	AK	212	 96%
4	AL	212	 98%
5	BB	576	 95%
5	BC	576	 95%
5	BD	576	 96%

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Mol	Chain	Length	Quality of chain
6	BA	97	
7	A0	1032	
7	A1	1032	
7	A2	1032	
7	A3	1032	
7	AY	1032	
7	AZ	1032	
8	A4	341	
8	A5	341	
8	A6	341	
8	A7	341	
8	A8	341	
8	A9	341	
8	Aa	341	
8	Ab	341	
8	Ac	341	
8	Ad	341	
8	Ae	341	
8	Af	341	
9	LA	303	
9	LB	303	
9	LC	303	
9	LD	303	
9	LE	303	
9	LF	303	

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Mol	Chain	Length	Quality of chain
9	LG	303	93% 98% .
9	LH	303	81% 99% .
9	LI	303	90% 99% .
9	LJ	303	93% 98% .
9	LK	303	82% 99% .
9	LL	303	91% 99% .
9	LM	303	93% 97% .
9	LN	303	83% 99% .
9	LO	303	90% 98% .
9	LP	303	93% 98% .
9	LQ	303	82% 99% .
9	LR	303	91% 99% .
10	FA	607	26% 95% 5%
10	FB	607	23% 97% .
10	FC	607	24% 97% .
10	FJ	607	25% 95% 5%
10	FK	607	30% 96% .
10	FL	607	26% 97% .
10	FS	607	26% 95% 5%
10	FT	607	24% 96% .
10	FU	607	23% 97% .
10	Fb	607	25% 95% 5%
10	Fc	607	30% 96% .
10	Fd	607	25% 96% .
10	Fk	607	27% 95% 5%

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Mol	Chain	Length	Quality of chain
10	F1	607	24% 96% .
10	Fm	607	25% 97% .
10	Ft	607	24% 95% 5%
10	Fu	607	30% 97% .
10	Fv	607	25% 96% .
11	FD	223	56% 98% .
11	FE	223	58% 99% .
11	FF	223	52% 96% .
11	FM	223	57% 98% .
11	FN	223	55% 99% .
11	FO	223	59% 96% .
11	FV	223	57% 98% .
11	FW	223	61% 99% .
11	FX	223	50% 96% .
11	Fe	223	56% 98% .
11	Ff	223	55% 99% .
11	Fg	223	55% 96% .
11	Fn	223	57% 98% .
11	Fo	223	60% 99% .
11	Fp	223	52% 96% .
11	Fw	223	56% 98% .
11	Fx	223	59% 99% .
11	Fy	223	56% 96% .
12	F1	448	59% 96% .
12	F2	448	55% 96% .

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Mol	Chain	Length	Quality of chain
12	FG	448	48% 97% .
12	FH	448	50% 95% .
12	FI	448	52% 95% .
12	FP	448	52% 97% .
12	FQ	448	59% 96% .
12	FR	448	57% 95% .
12	FY	448	48% 97% .
12	FZ	448	49% 95% .
12	Fa	448	50% 96% .
12	Fh	448	53% 97% .
12	Fi	448	59% 96% .
12	Fj	448	57% 96% .
12	Fq	448	48% 97% .
12	Fr	448	50% 95% .
12	Fs	448	53% 96% .
12	Fz	448	52% 97% .
13	B1	163	. 96% ..
13	B2	163	. 98% ..
13	B3	163	6% 98% ..
13	B4	163	6% 97% ..
13	B5	163	8% 98% ..
13	B6	163	6% 96% ..
13	B7	163	9% 98% ..
13	B8	163	8% 98% ..
13	BW	163	. 97% ..

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Mol	Chain	Length	Quality of chain
13	BX	163	 96%
13	BY	163	 95%
13	BZ	163	 95%
14	AA	136	 96%
14	AB	136	 96%
14	AC	136	 93% 7%
14	AD	136	 95%
14	AE	136	 96%
14	AF	136	 95%
15	BE	380	 95% 5%
15	BF	380	 96%
15	BG	380	 96%
16	BH	577	 6% 94%
16	BI	577	 6% 94%
16	BJ	577	 6% 94%



## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 440315 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	AT	646	Total	C	N	O	S	0	0
			5125	3252	853	1009	11		
1	AV	646	Total	C	N	O	S	0	0
			5125	3252	853	1009	11		
1	AX	646	Total	C	N	O	S	0	0
			5125	3252	853	1009	11		
1	AS	648	Total	C	N	O	S	0	0
			5145	3265	856	1013	11		
1	AU	648	Total	C	N	O	S	0	0
			5145	3265	856	1013	11		
1	AW	648	Total	C	N	O	S	0	0
			5145	3265	856	1013	11		
1	AN	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
1	AP	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
1	AR	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
1	AM	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
1	AO	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
1	AQ	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		

- Molecule 2 is a protein called Baseplate tail tube cap.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BL	225	Total	C	N	O	S	0	0
			1790	1131	311	342	6		
2	BN	225	Total	C	N	O	S	0	0
			1790	1131	311	342	6		
2	BP	225	Total	C	N	O	S	0	0
			1790	1131	311	342	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BK	301	Total	C	N	O	S	0	0
			2323	1455	399	461	8		
2	BM	301	Total	C	N	O	S	0	0
			2323	1455	399	461	8		
2	BO	301	Total	C	N	O	S	0	0
			2323	1455	399	461	8		

- Molecule 3 is a protein called Baseplate subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BQ	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		
3	BR	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		
3	BS	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		
3	BT	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		
3	BU	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		
3	BV	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		

- Molecule 4 is a protein called Baseplate wedge subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AH	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		
4	AJ	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		
4	AL	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		
4	AG	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		
4	AI	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		
4	AK	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		

- Molecule 5 is a protein called Baseplate central spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BB	564	Total	C	N	O	S	0	0
			4354	2709	753	871	21		
5	BC	564	Total	C	N	O	S	0	0
			4354	2709	753	871	21		
5	BD	564	Total	C	N	O	S	0	0
			4354	2709	753	871	21		

- Molecule 6 is a protein called Phospholipase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BA	97	Total	C	N	O	S	0	0
			706	440	122	140	4		

- Molecule 7 is a protein called Baseplate wedge protein gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AY	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
7	A2	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
7	AZ	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
7	A0	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
7	A1	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
7	A3	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	530	ALA	SER	conflict	UNP A0A2K9V5T9
AY	532	HIS	ASN	conflict	UNP A0A2K9V5T9
AY	536	ILE	VAL	conflict	UNP A0A2K9V5T9
A2	530	ALA	SER	conflict	UNP A0A2K9V5T9
A2	532	HIS	ASN	conflict	UNP A0A2K9V5T9
A2	536	ILE	VAL	conflict	UNP A0A2K9V5T9
AZ	530	ALA	SER	conflict	UNP A0A2K9V5T9
AZ	532	HIS	ASN	conflict	UNP A0A2K9V5T9
AZ	536	ILE	VAL	conflict	UNP A0A2K9V5T9
A0	530	ALA	SER	conflict	UNP A0A2K9V5T9
A0	532	HIS	ASN	conflict	UNP A0A2K9V5T9

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Chain	Residue	Modelled	Actual	Comment	Reference
A0	536	ILE	VAL	conflict	UNP A0A2K9V5T9
A1	530	ALA	SER	conflict	UNP A0A2K9V5T9
A1	532	HIS	ASN	conflict	UNP A0A2K9V5T9
A1	536	ILE	VAL	conflict	UNP A0A2K9V5T9
A3	530	ALA	SER	conflict	UNP A0A2K9V5T9
A3	532	HIS	ASN	conflict	UNP A0A2K9V5T9
A3	536	ILE	VAL	conflict	UNP A0A2K9V5T9

- Molecule 8 is a protein called Baseplate wedge subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ad	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	Ac	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	Ab	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	Aa	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	Ae	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	Af	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	A4	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
8	A5	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
8	A6	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
8	A7	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
8	A8	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
8	A9	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		

- Molecule 9 is a protein called Baseplate wedge tail fiber connector.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LA	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LB	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	LC	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LD	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LE	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LF	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LG	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LH	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LI	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LJ	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LK	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LL	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LM	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LN	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LO	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LP	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LQ	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LR	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		

- Molecule 10 is a protein called Baseplate wedge protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	FA	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FB	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FC	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	FJ	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FK	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FL	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FS	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FT	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FU	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fb	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fc	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fd	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fk	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fl	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fm	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Ft	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fu	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fv	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		

- Molecule 11 is a protein called Baseplate wedge subunit and tail pin.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	FD	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FE	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FF	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FM	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	FN	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FO	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FV	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FW	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FX	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fe	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Ff	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fg	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fn	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fo	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fp	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fw	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fx	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fy	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		

- Molecule 12 is a protein called Gp12 short tail fibers.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	FG	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	FI	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		
12	FH	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		
12	FP	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	FR	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	FQ	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		
12	FY	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	Fa	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		
12	FZ	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		
12	Fh	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	Fj	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		
12	Fi	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		
12	Fq	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	Fs	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		
12	Fr	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		
12	Fz	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	F2	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		
12	F1	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		

- Molecule 13 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BW	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	BX	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	BY	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	BZ	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B1	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B2	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	B3	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B4	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B5	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B6	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B7	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B8	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		

- Molecule 14 is a protein called IraD/Gp25-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AA	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		
14	AB	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		
14	AC	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		
14	AD	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		
14	AE	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		
14	AF	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		

- Molecule 15 is a protein called Putative baseplate hub subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BE	379	Total	C	N	O	S	0	0
			3055	1945	511	583	16		
15	BF	379	Total	C	N	O	S	0	0
			3055	1945	511	583	16		
15	BG	379	Total	C	N	O	S	0	0
			3055	1945	511	583	16		

- Molecule 16 is a protein called Baseplate hub subunit tail length determinator.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BH	33	Total	C	N	O	S	0	0
			242	147	43	50	2		
16	BI	33	Total	C	N	O	S	0	0
			242	147	43	50	2		
16	BJ	33	Total	C	N	O	S	0	0
			242	147	43	50	2		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BH	87	VAL	ALA	conflict	UNP A0A2K9V5Z4
BH	530	THR	ALA	conflict	UNP A0A2K9V5Z4
BH	555	TYR	HIS	conflict	UNP A0A2K9V5Z4
BH	559	THR	MET	conflict	UNP A0A2K9V5Z4
BI	87	VAL	ALA	conflict	UNP A0A2K9V5Z4
BI	530	THR	ALA	conflict	UNP A0A2K9V5Z4
BI	555	TYR	HIS	conflict	UNP A0A2K9V5Z4
BI	559	THR	MET	conflict	UNP A0A2K9V5Z4
BJ	87	VAL	ALA	conflict	UNP A0A2K9V5Z4
BJ	530	THR	ALA	conflict	UNP A0A2K9V5Z4
BJ	555	TYR	HIS	conflict	UNP A0A2K9V5Z4
BJ	559	THR	MET	conflict	UNP A0A2K9V5Z4

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
17	BB	1	Total	Cl	0
			1	1	

- Molecule 18 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	FA	1	Total	K	0
			1	1	
18	FJ	1	Total	K	0
			1	1	
18	FS	1	Total	K	0
			1	1	
18	Fb	1	Total	K	0
			1	1	
18	Fk	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
18	Ft	1	Total	K	0
			1	1	

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

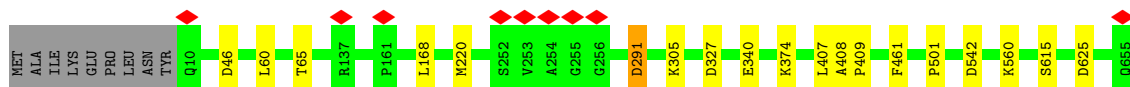
Mol	Chain	Residues	Atoms		AltConf
19	FB	1	Total	Zn	0
			1	1	
19	FK	1	Total	Zn	0
			1	1	
19	FT	1	Total	Zn	0
			1	1	
19	Fc	1	Total	Zn	0
			1	1	
19	Fl	1	Total	Zn	0
			1	1	
19	FG	1	Total	Zn	0
			1	1	

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

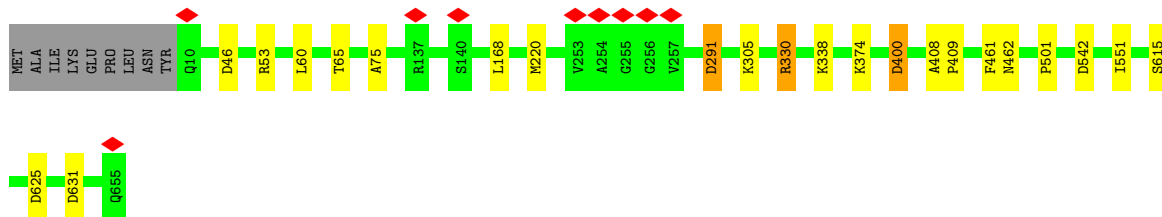
- Molecule 1: Baseplate wedge protein gp6

Chain AT:  96%



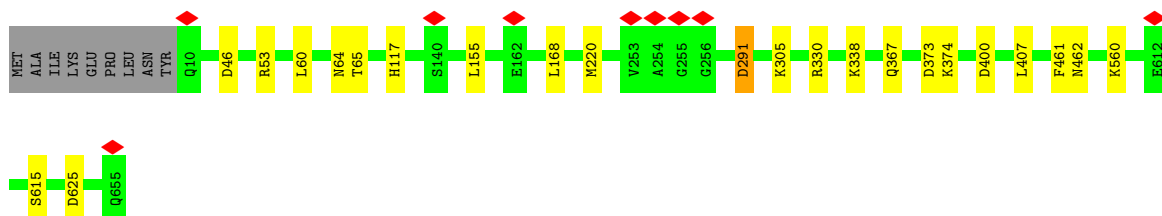
- Molecule 1: Baseplate wedge protein gp6

Chain AV:  95%



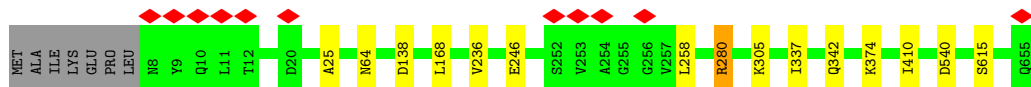
- Molecule 1: Baseplate wedge protein gp6

Chain AX:  95%

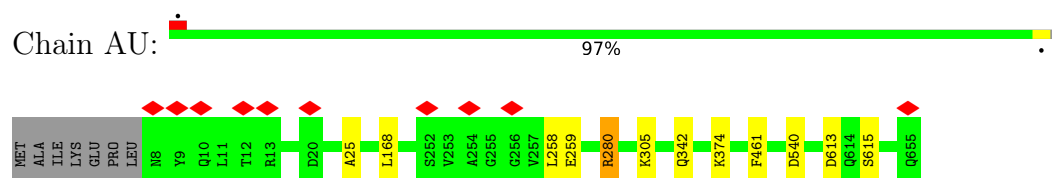


- Molecule 1: Baseplate wedge protein gp6

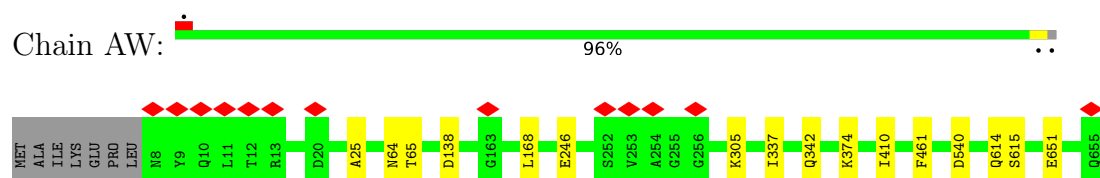
Chain AS:  97%



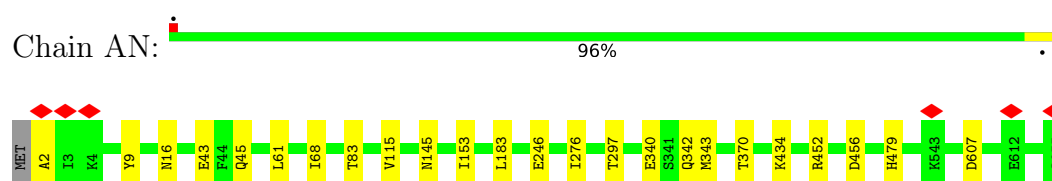
- Molecule 1: Baseplate wedge protein gp6



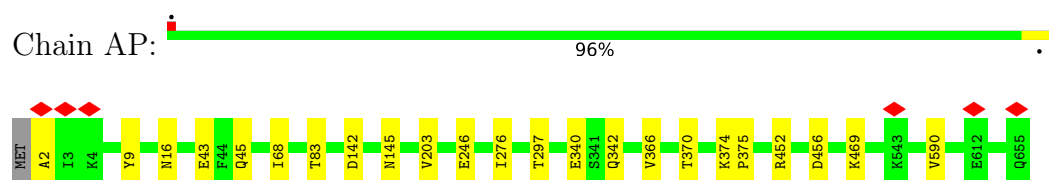
- Molecule 1: Baseplate wedge protein gp6



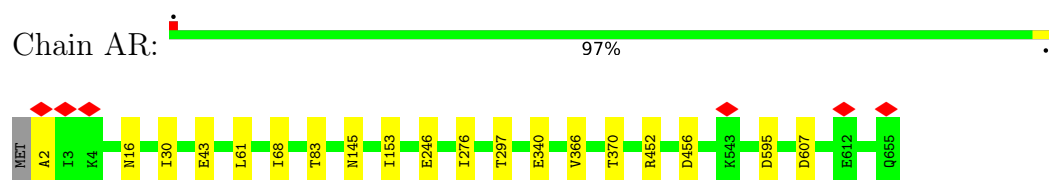
- Molecule 1: Baseplate wedge protein gp6



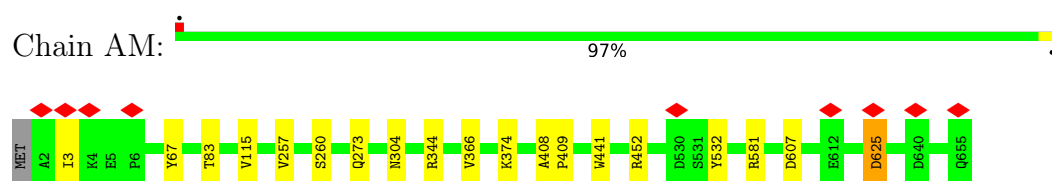
- Molecule 1: Baseplate wedge protein gp6



- Molecule 1: Baseplate wedge protein gp6



- Molecule 1: Baseplate wedge protein gp6



- Molecule 1: Baseplate wedge protein gp6

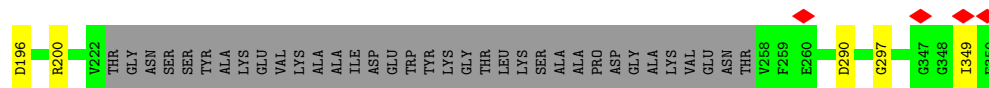
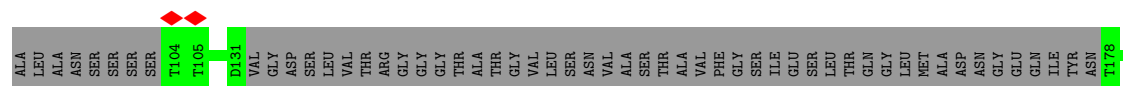
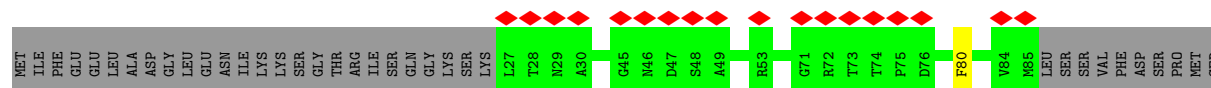




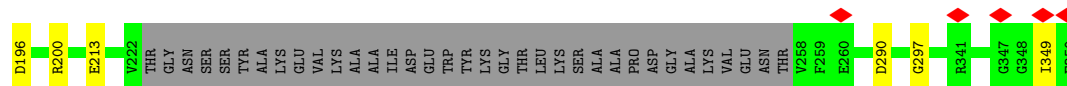
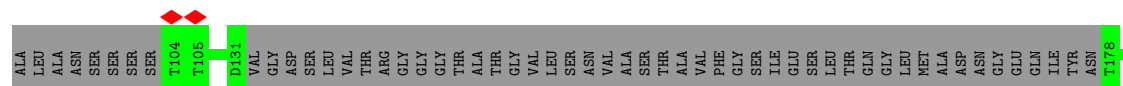
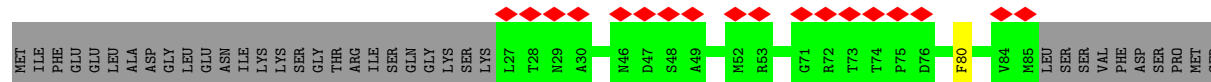
- Molecule 1: Baseplate wedge protein gp6



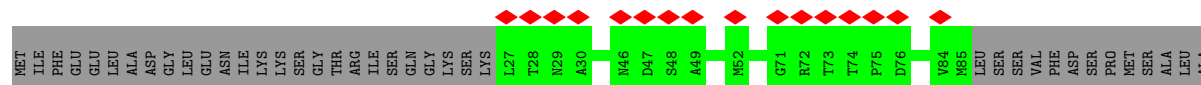
- Molecule 2: Baseplate tail tube cap

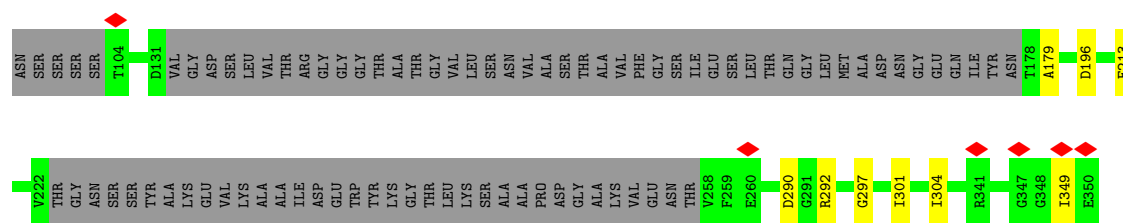


- Molecule 2: Baseplate tail tube cap



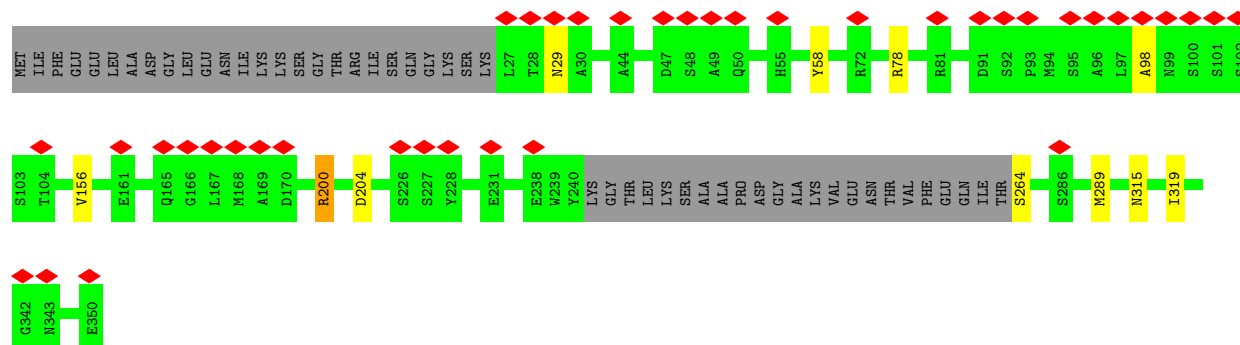
- Molecule 2: Baseplate tail tube cap





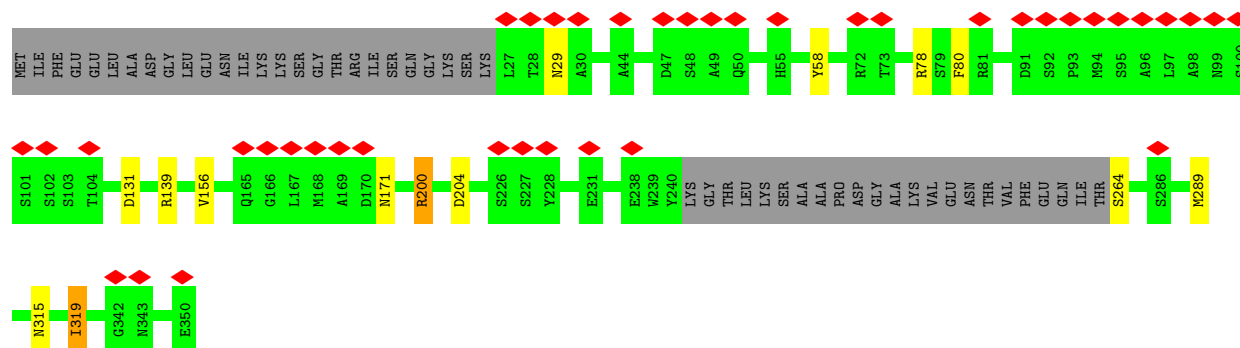
- Molecule 2: Baseplate tail tube cap

Chain BK: 11% 83% 14%



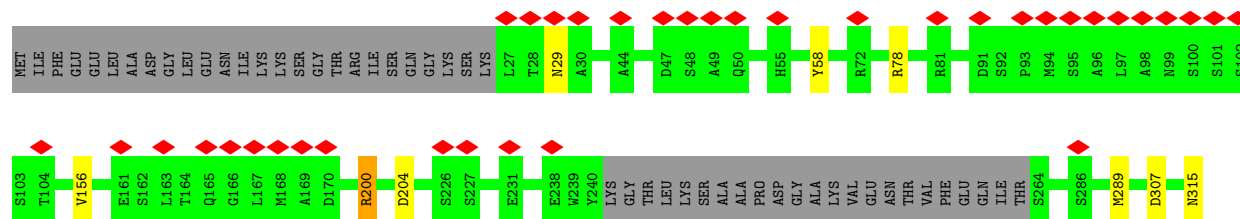
- Molecule 2: Baseplate tail tube cap

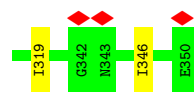
Chain BM: 12% 82% 14%



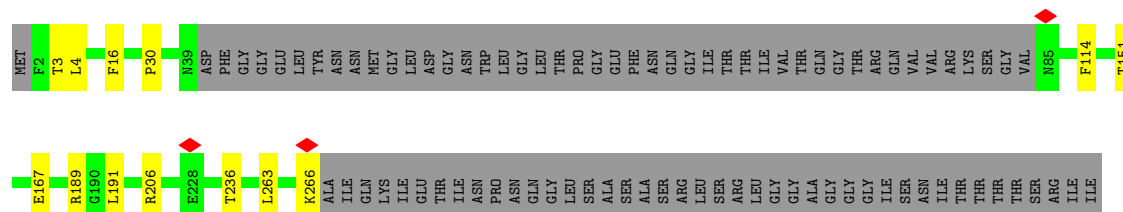
- Molecule 2: Baseplate tail tube cap

Chain BO: 11% 83% 14%

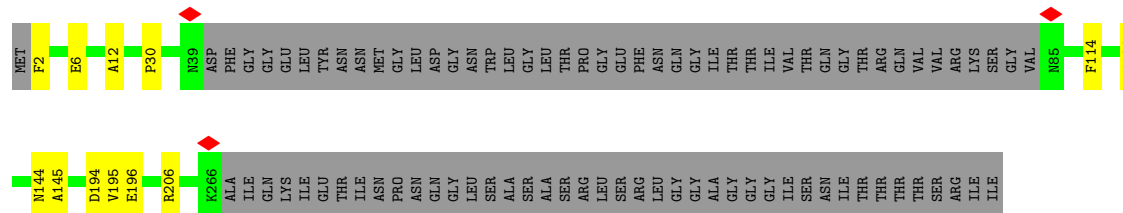




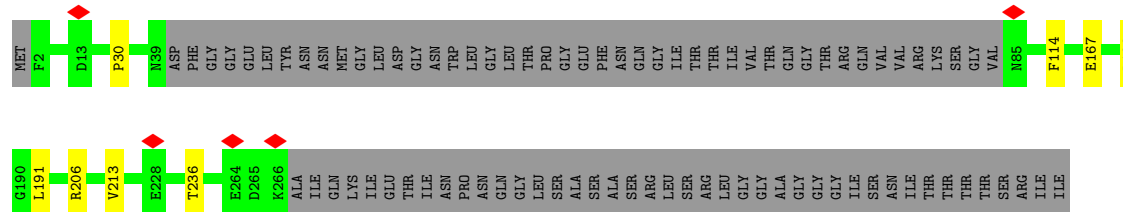
- Molecule 3: Baseplate subunit



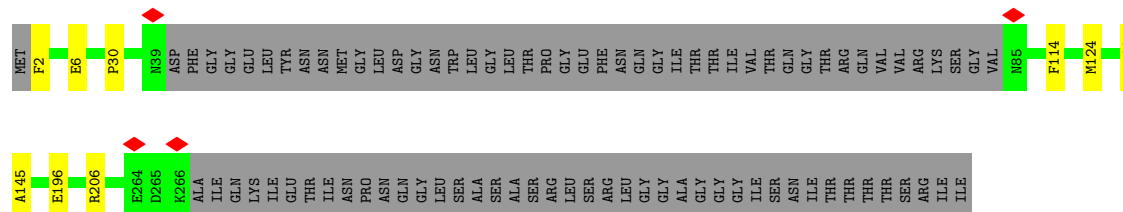
- Molecule 3: Baseplate subunit



- Molecule 3: Baseplate subunit

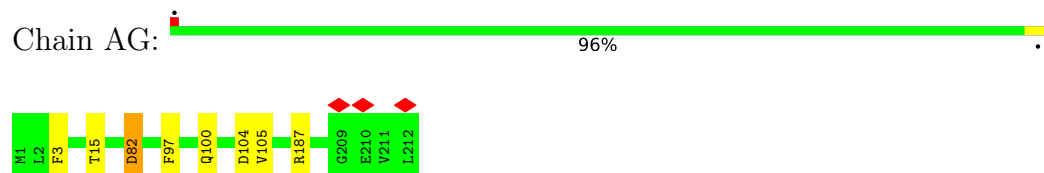


- Molecule 3: Baseplate subunit

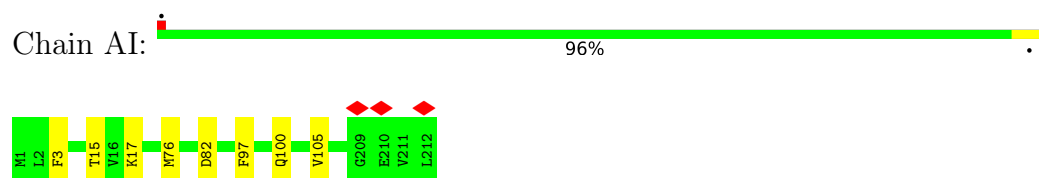


- Molecule 3: Baseplate subunit

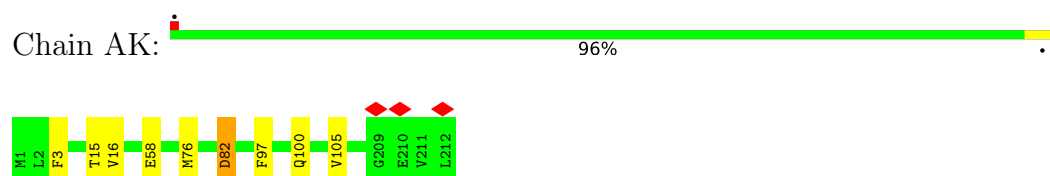




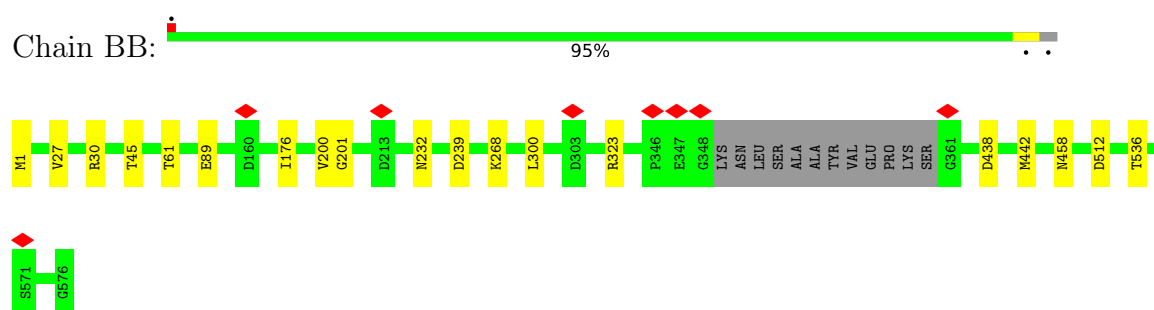
- Molecule 4: Baseplate wedge subunit



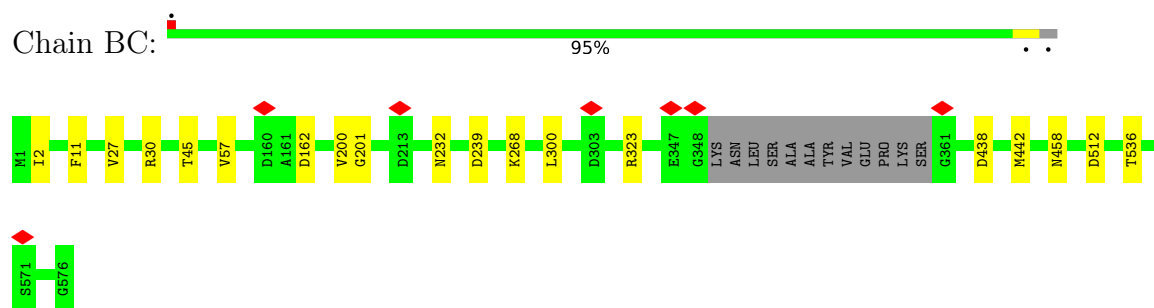
- Molecule 4: Baseplate wedge subunit



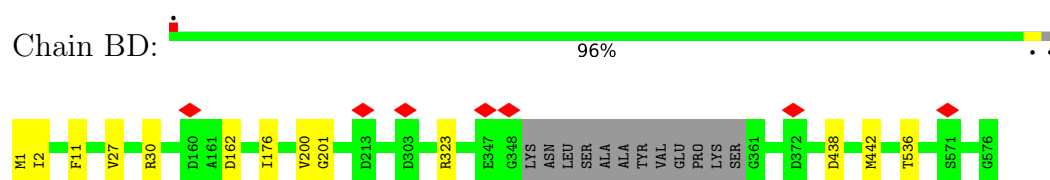
- Molecule 5: Baseplate central spike protein



- Molecule 5: Baseplate central spike protein

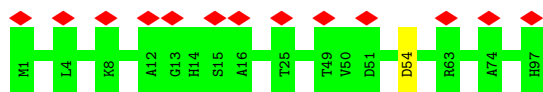


- Molecule 5: Baseplate central spike protein

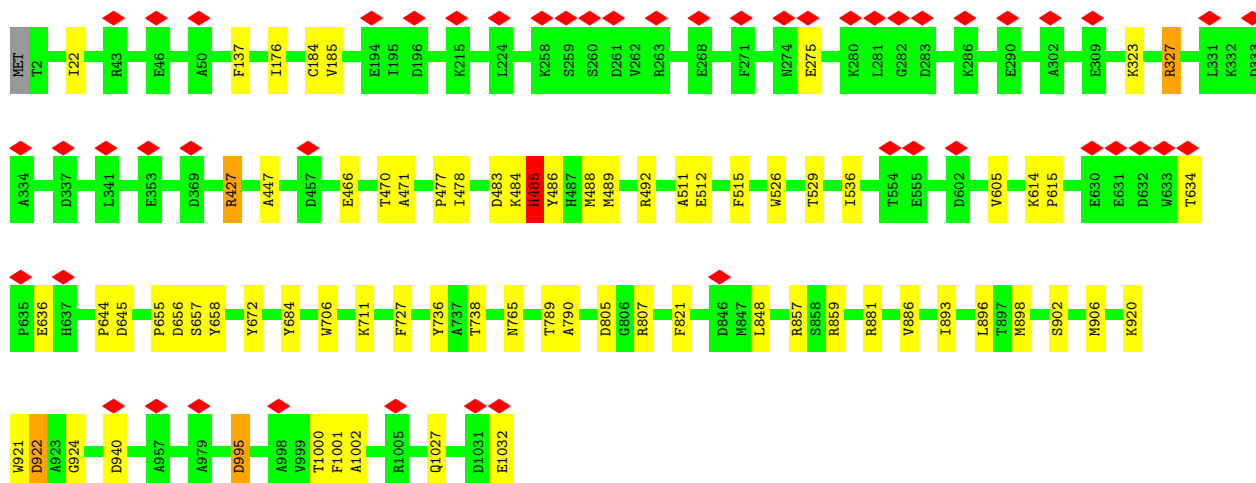


- Molecule 6: Phospholipase

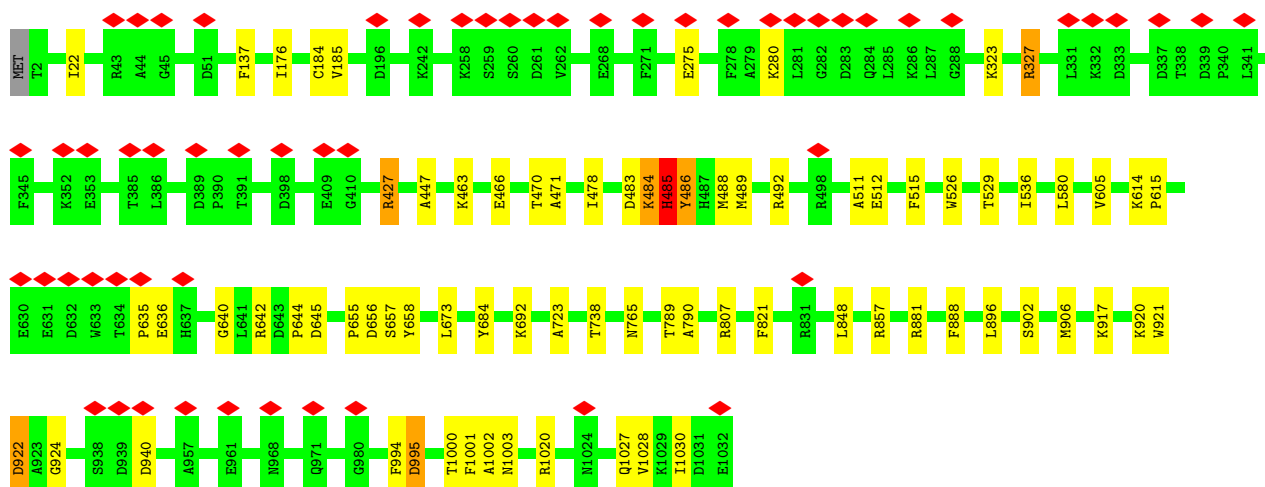




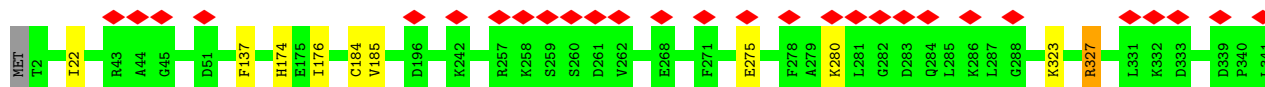
• Molecule 7: Baseplate wedge protein gp7

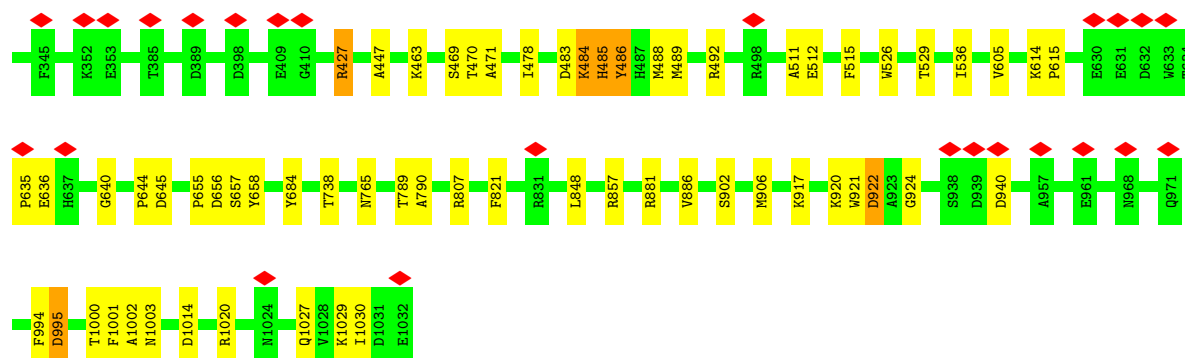


• Molecule 7: Baseplate wedge protein gp7

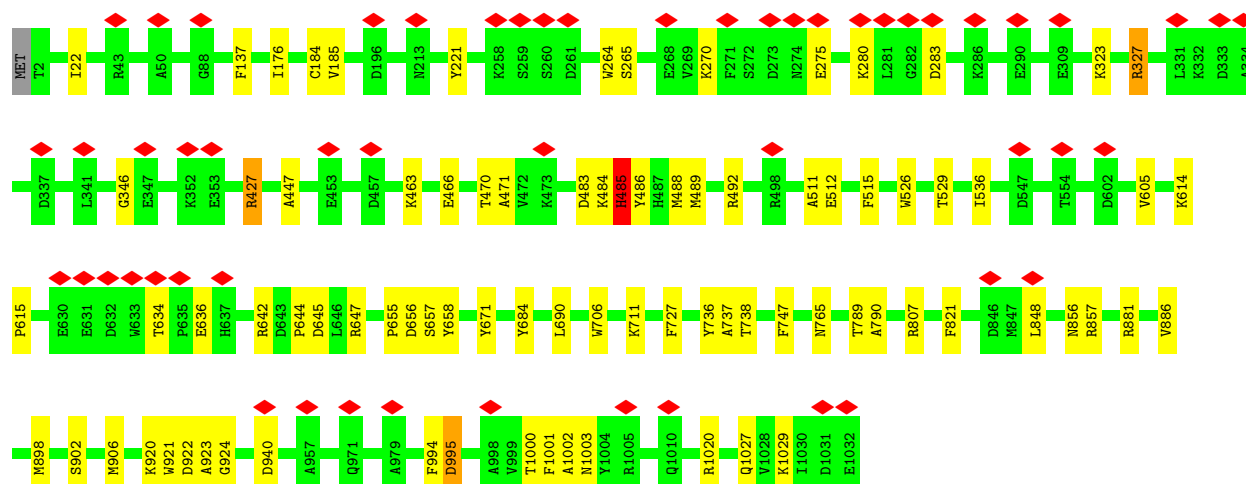


• Molecule 7: Baseplate wedge protein gp7

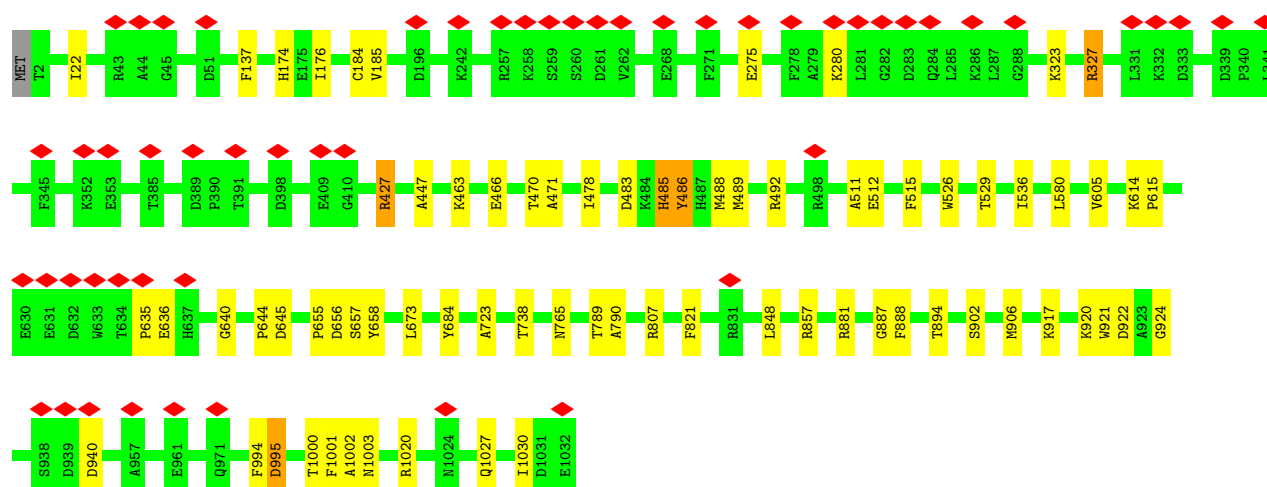




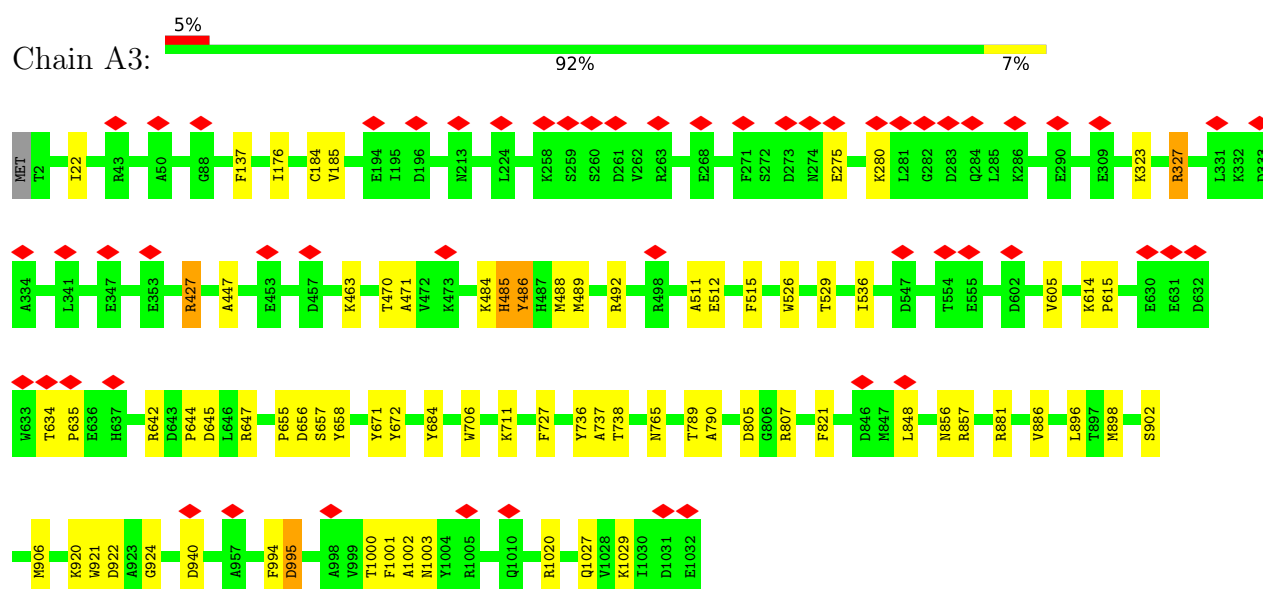
• Molecule 7: Baseplate wedge protein gp7



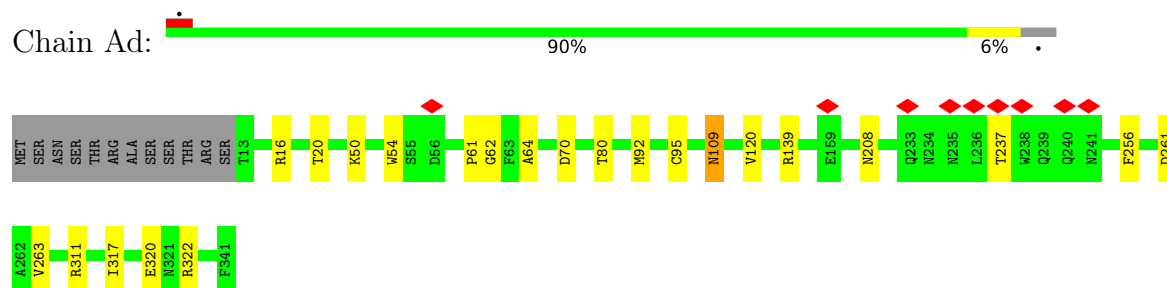
• Molecule 7: Baseplate wedge protein gp7



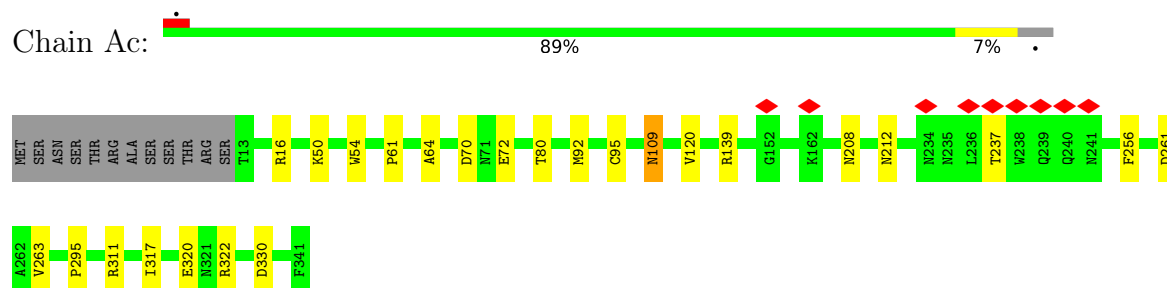
• Molecule 7: Baseplate wedge protein gp7



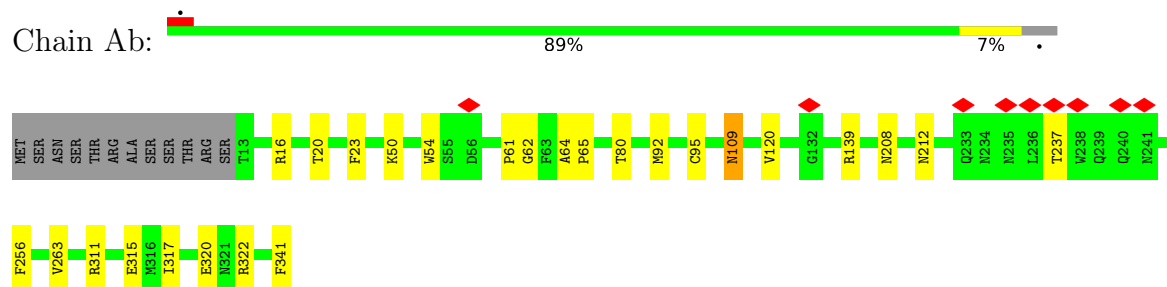
- Molecule 8: Baseplate wedge subunit




- Molecule 8: Baseplate wedge subunit

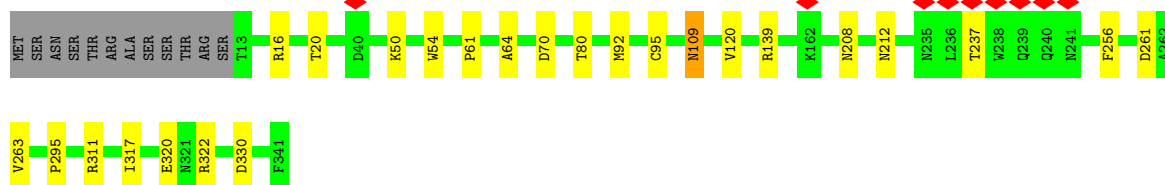


- Molecule 8: Baseplate wedge subunit




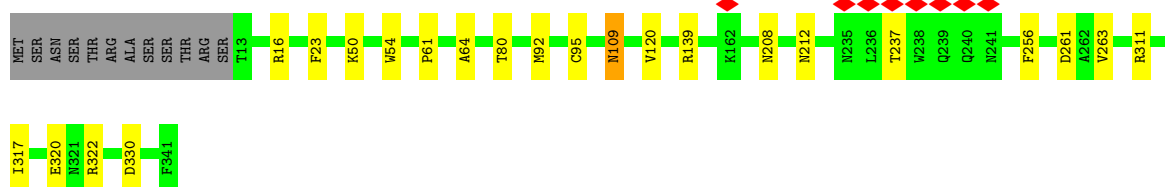
- Molecule 8: Baseplate wedge subunit

Chain Aa:  89% 7% .




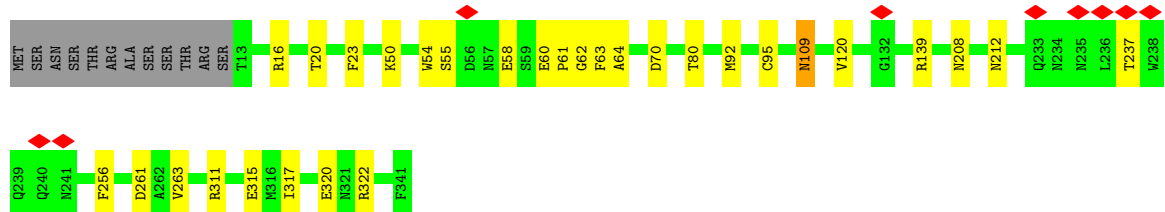
- Molecule 8: Baseplate wedge subunit

Chain Ae:  90% 6% .




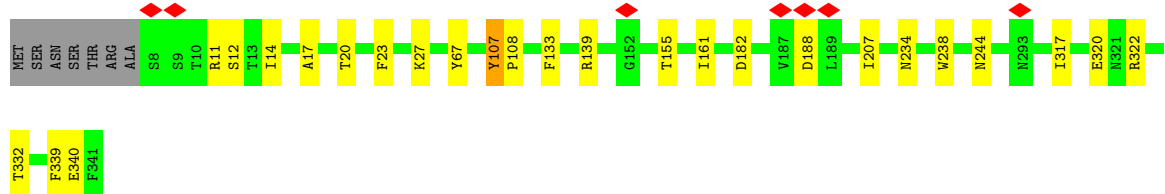
- Molecule 8: Baseplate wedge subunit

Chain Af:  88% 9% .



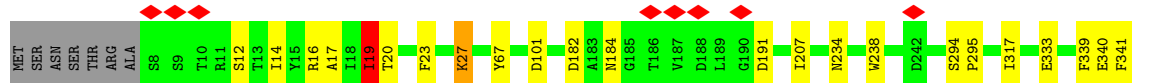
- Molecule 8: Baseplate wedge subunit

Chain A4:  90% 7% .




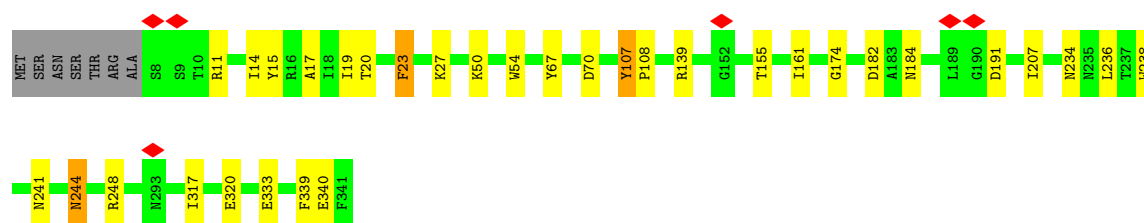
- Molecule 8: Baseplate wedge subunit

Chain A5:  91% 6% .




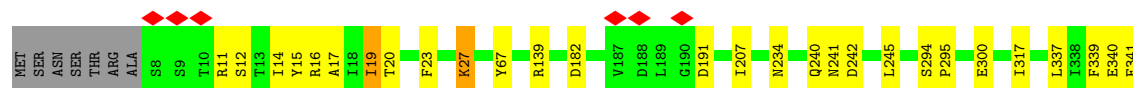
- Molecule 8: Baseplate wedge subunit

Chain A6:  88% 9% ..



- Molecule 8: Baseplate wedge subunit

Chain A7:  90% 8% ..



- Molecule 8: Baseplate wedge subunit

Chain A8:  89% 8% ..



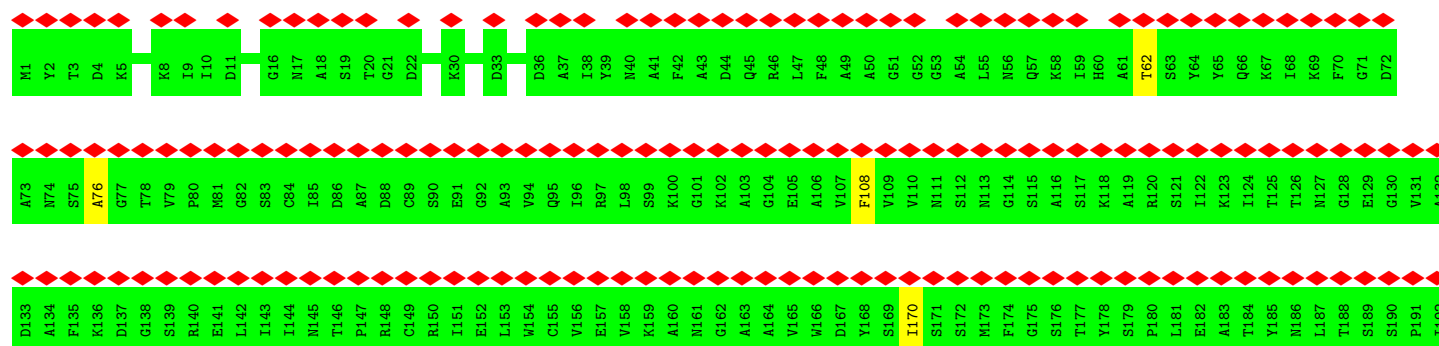
- Molecule 8: Baseplate wedge subunit

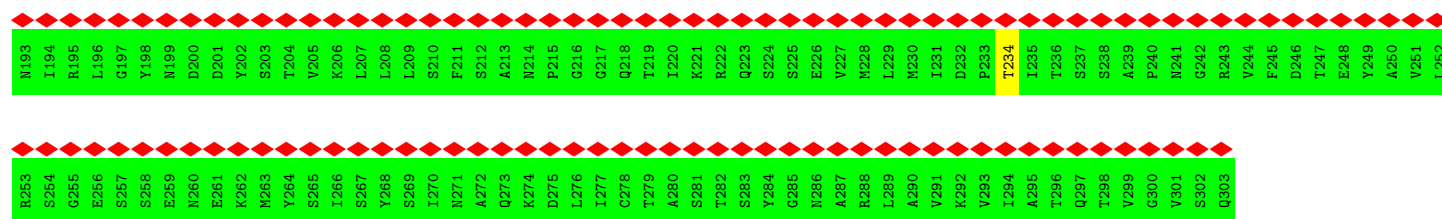
Chain A9:  91% 6% ..



- Molecule 9: Baseplate wedge tail fiber connector

Chain LA:  93% 98% ..





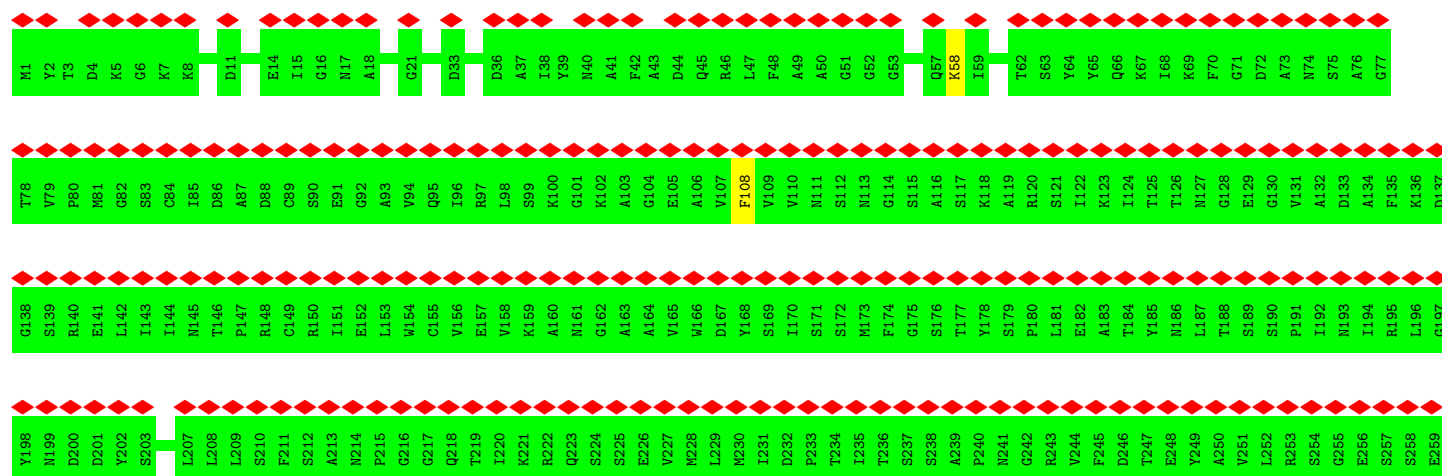
• Molecule 9: Baseplate wedge tail fiber connector

Chain LB: 82%  
99%

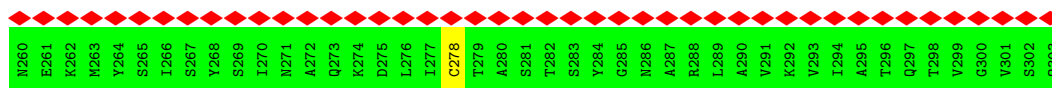


• Molecule 9: Baseplate wedge tail fiber connector

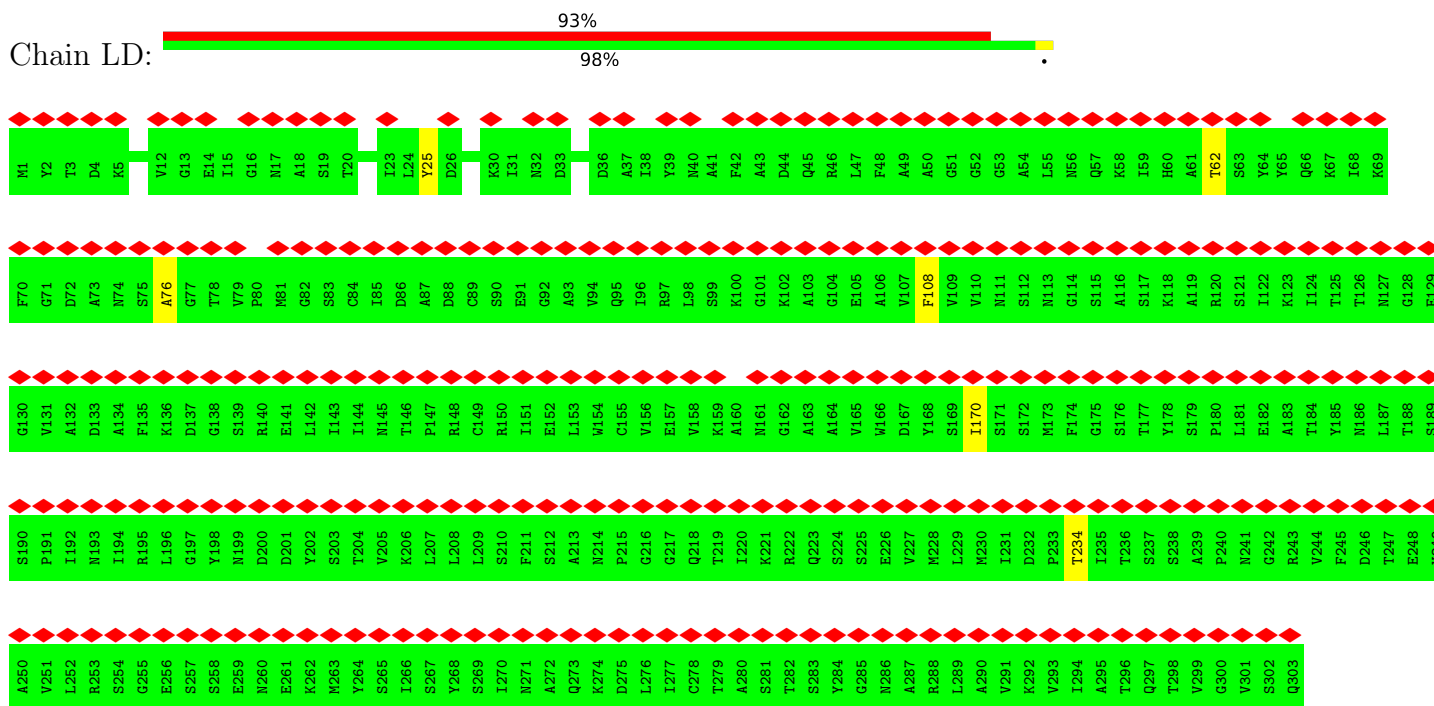
Chain LC: 90%  
99%



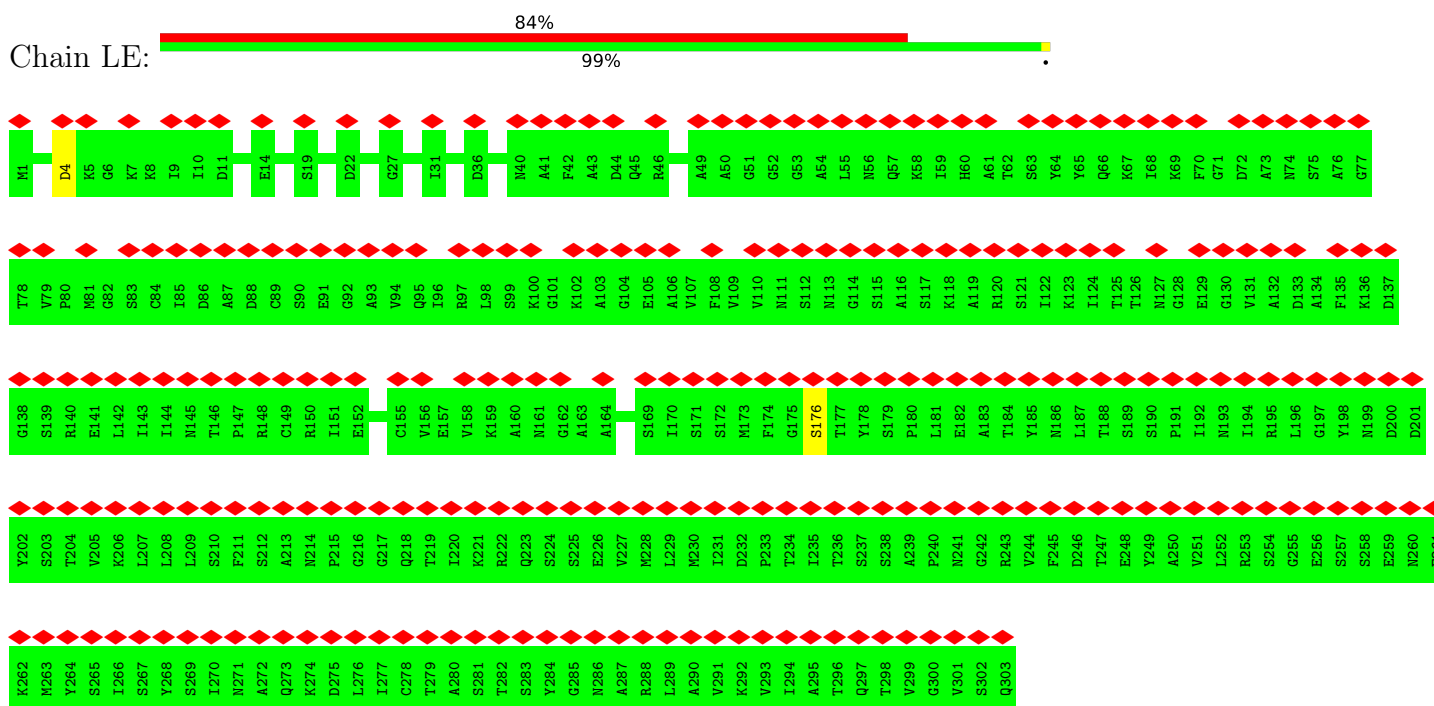




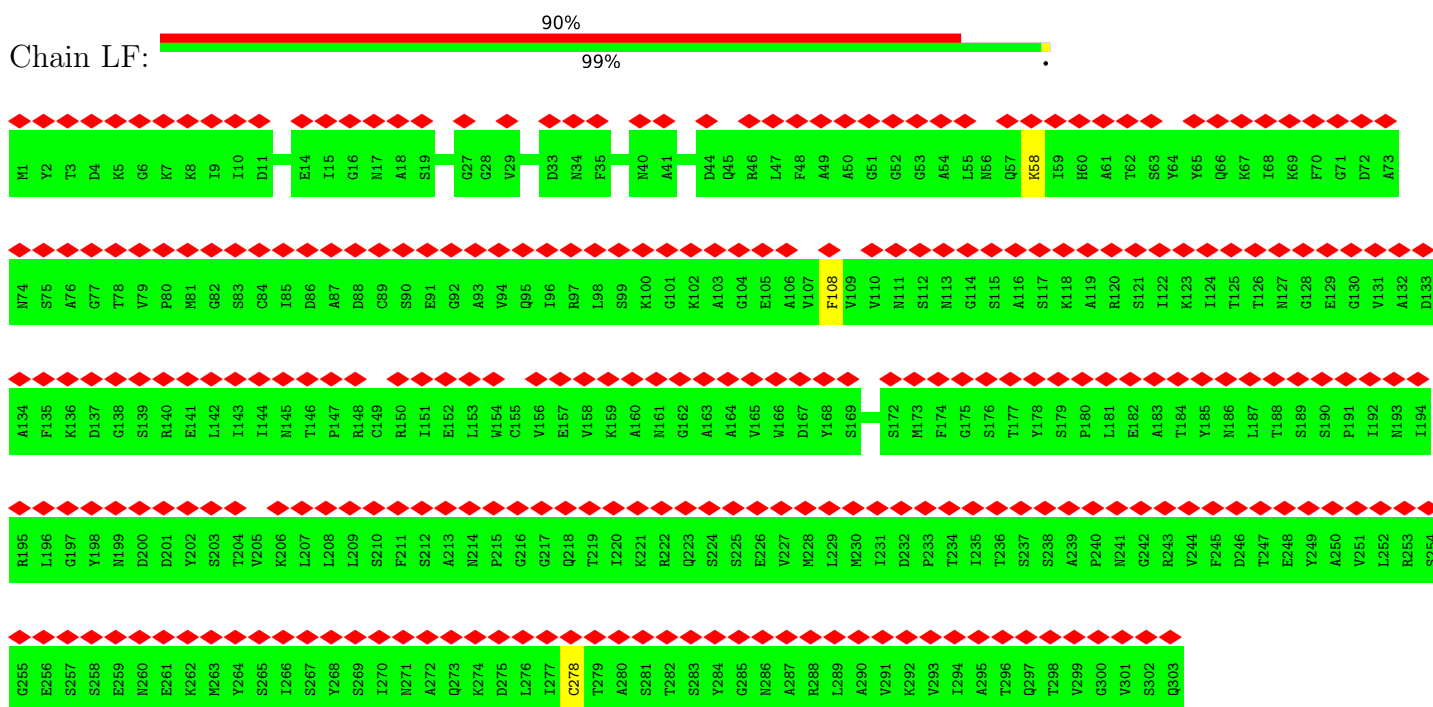
• Molecule 9: Baseplate wedge tail fiber connector



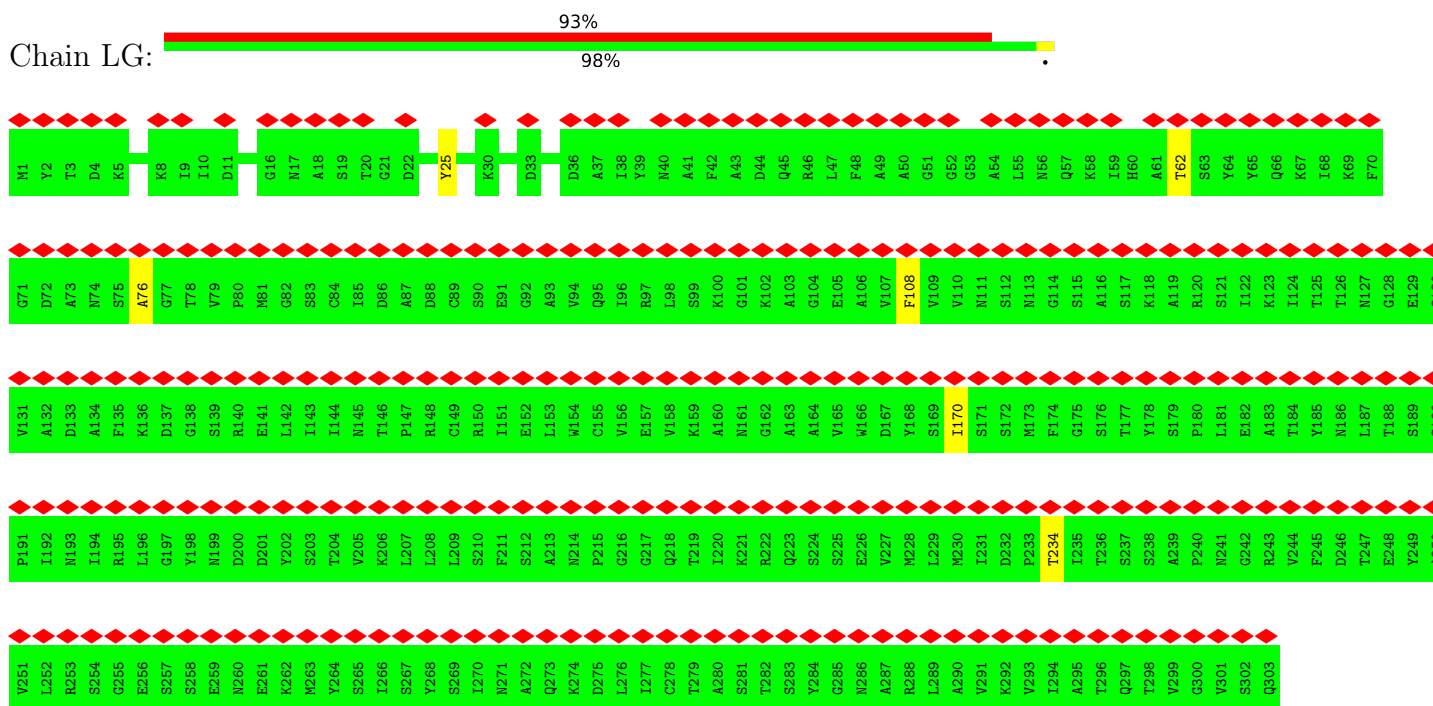
• Molecule 9: Baseplate wedge tail fiber connector



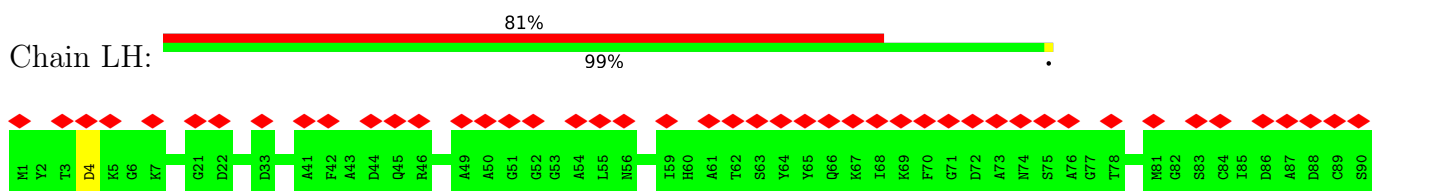
• Molecule 9: Baseplate wedge tail fiber connector

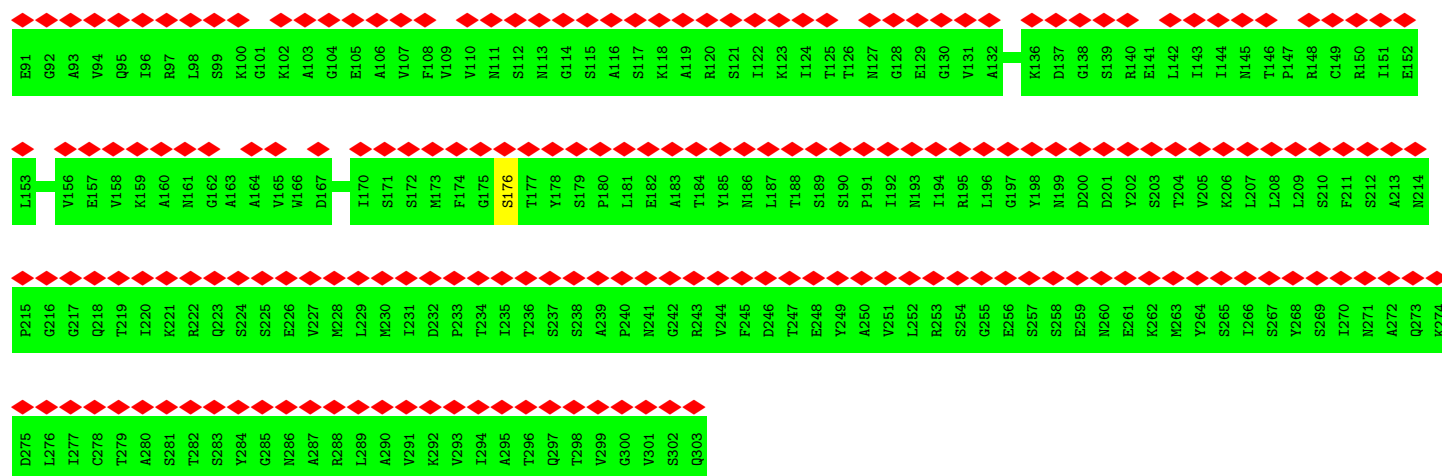


• Molecule 9: Baseplate wedge tail fiber connector

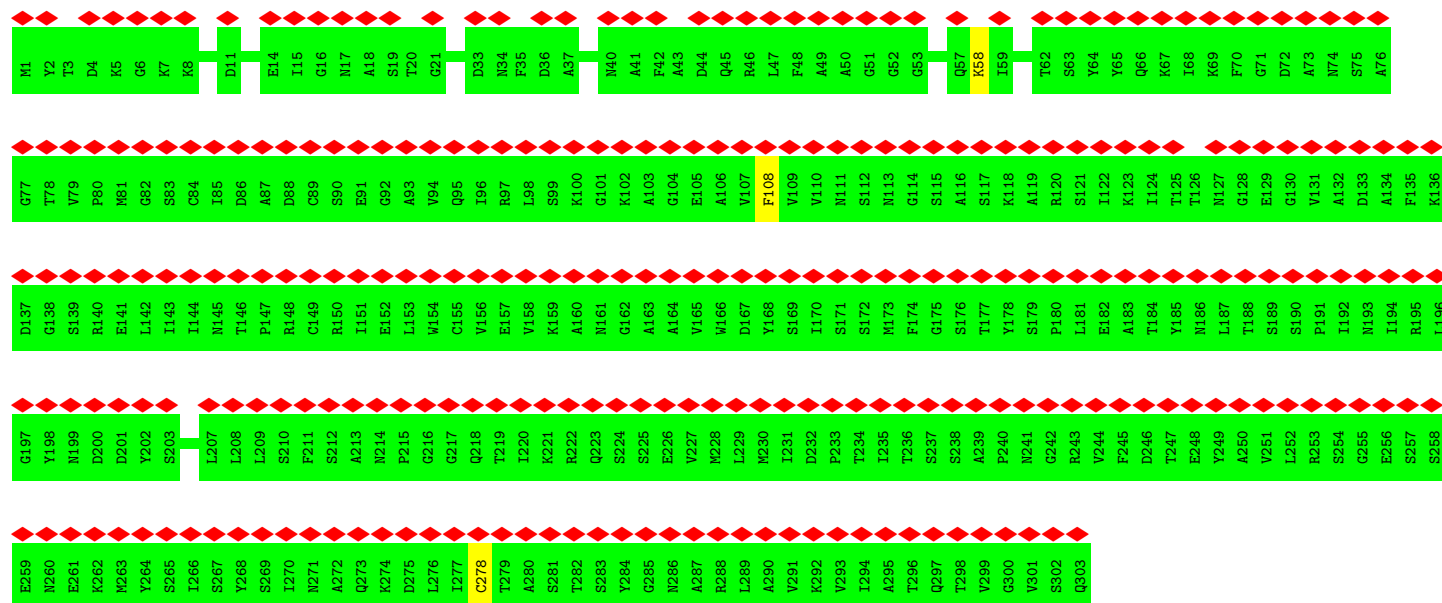


• Molecule 9: Baseplate wedge tail fiber connector



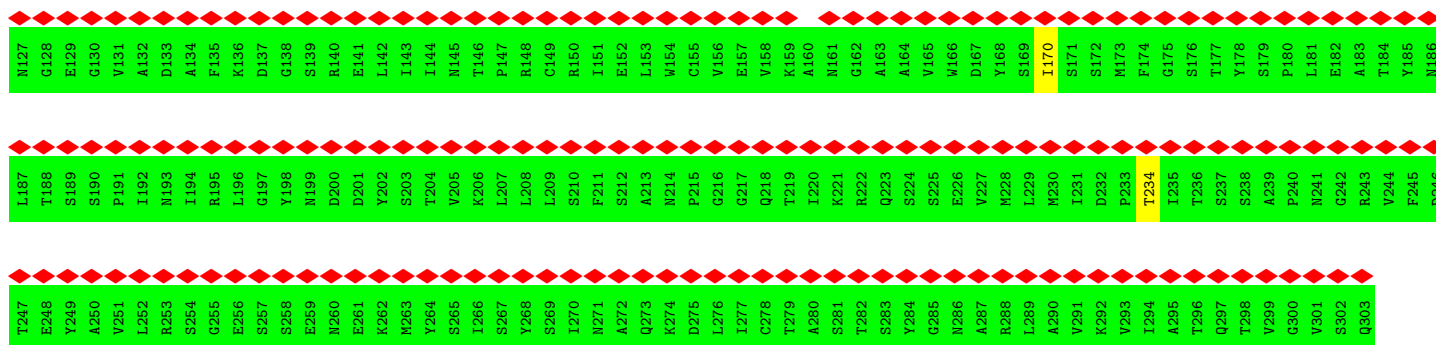


• Molecule 9: Baseplate wedge tail fiber connector



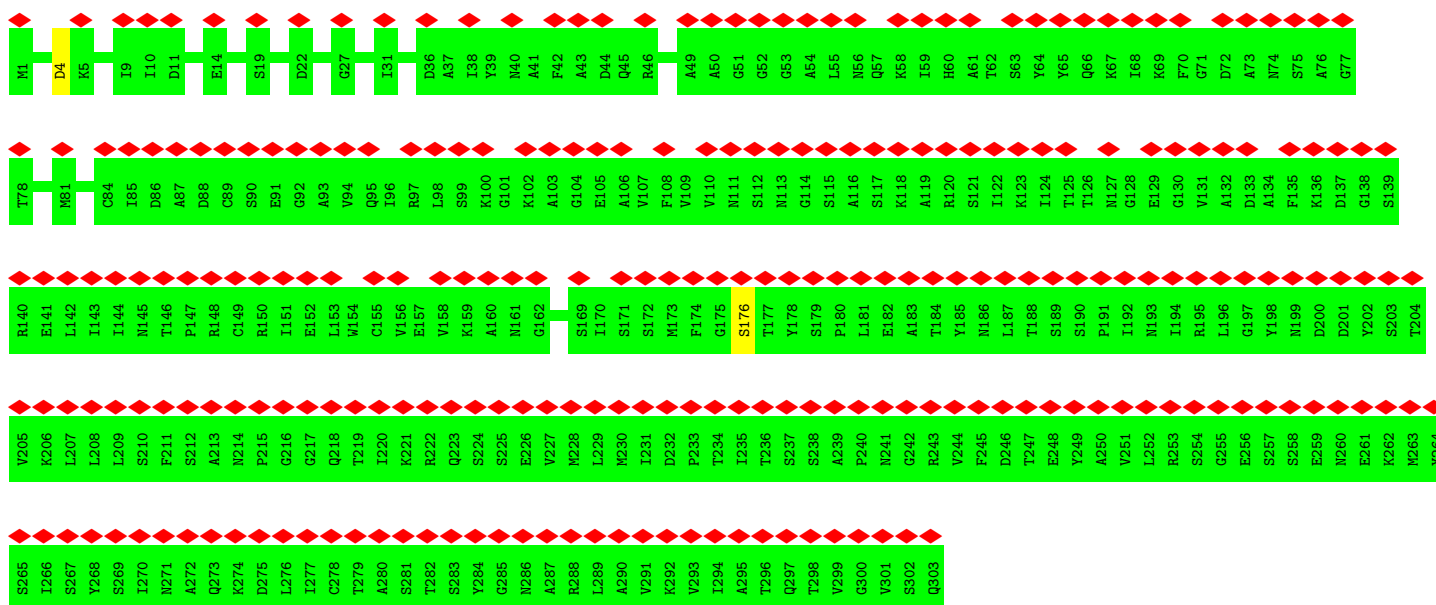
• Molecule 9: Baseplate wedge tail fiber connector





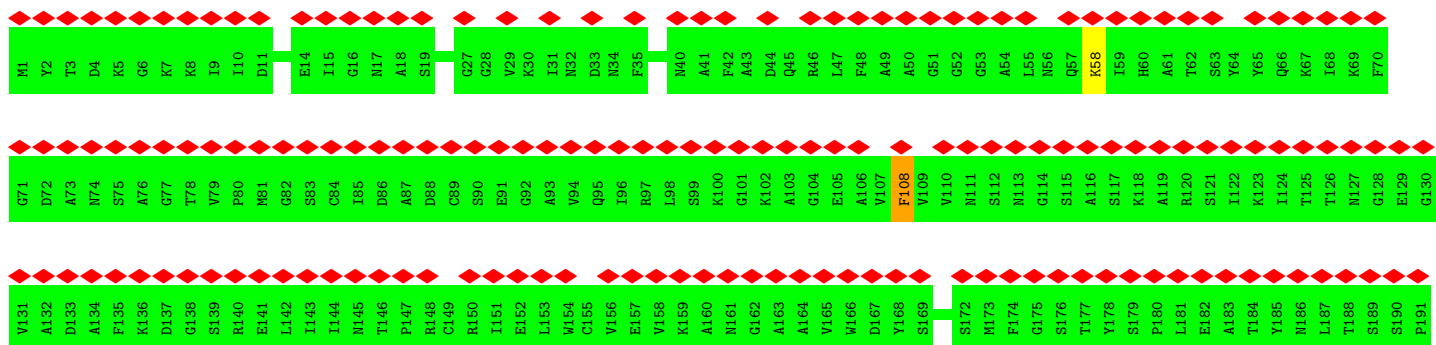
• Molecule 9: Baseplate wedge tail fiber connector

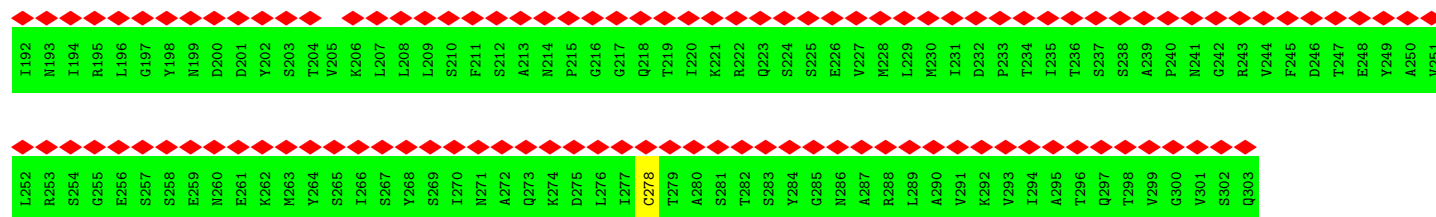
Chain LK: 82% 99%



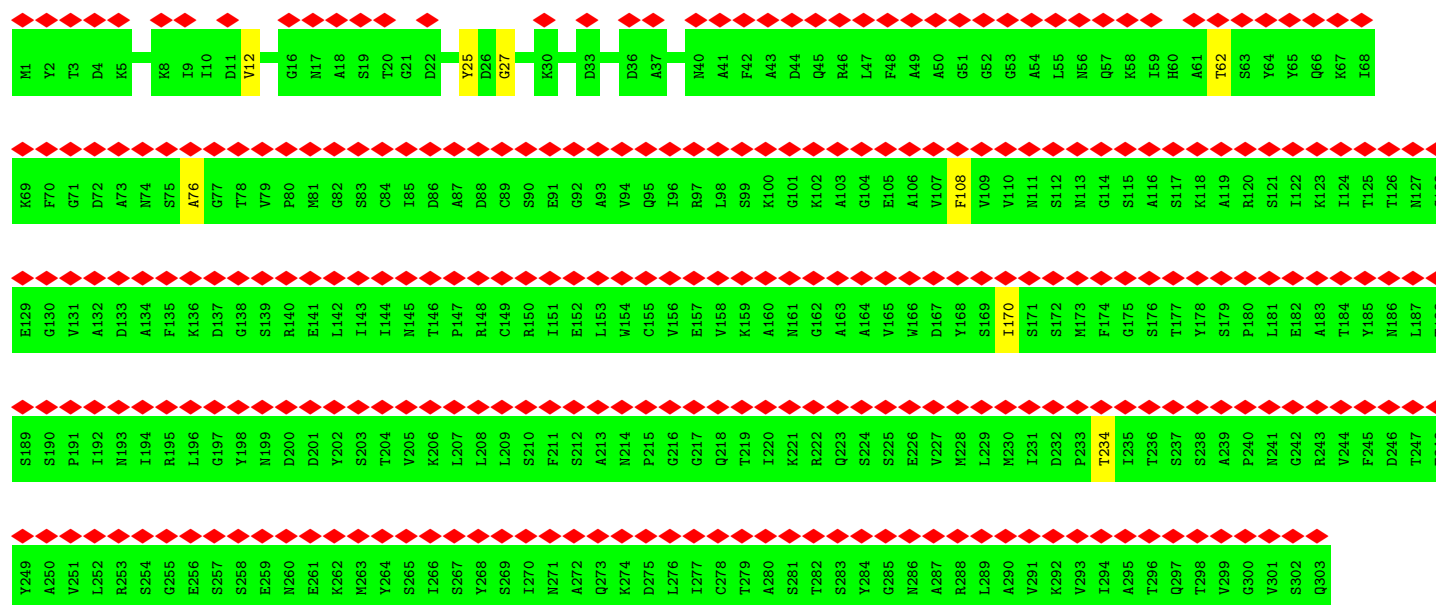
• Molecule 9: Baseplate wedge tail fiber connector

Chain LL: 91% 99%

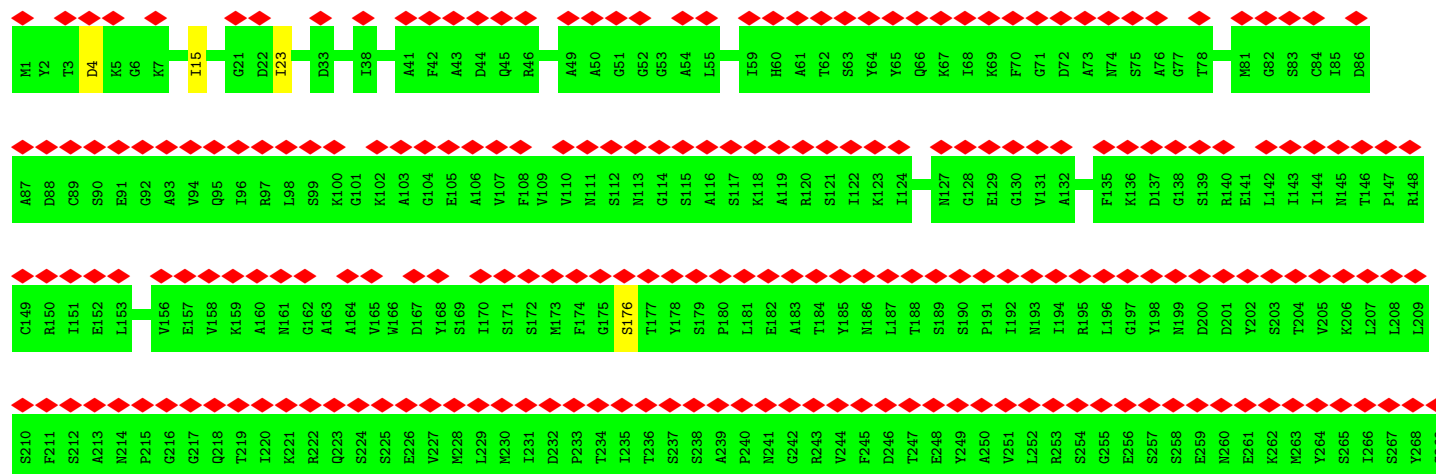
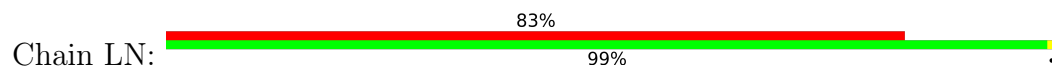


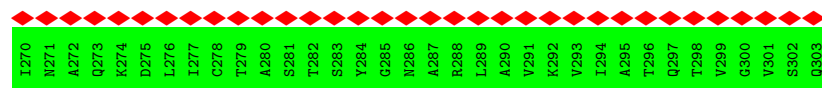


• Molecule 9: Baseplate wedge tail fiber connector

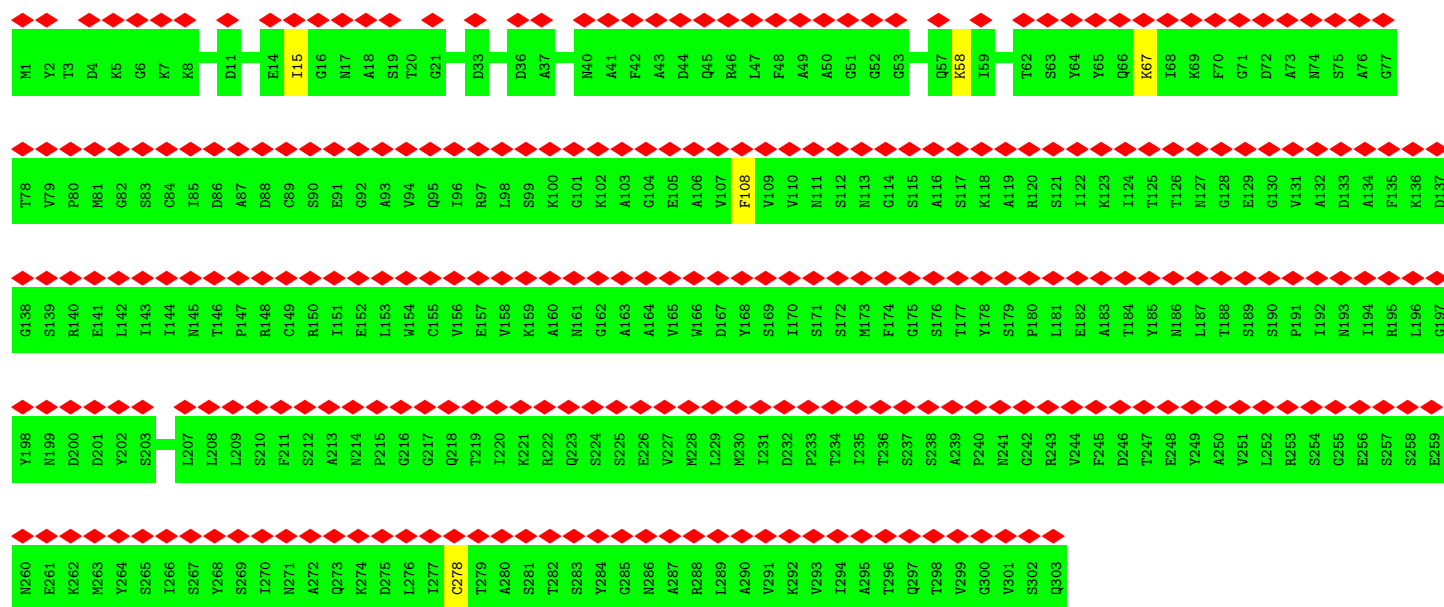
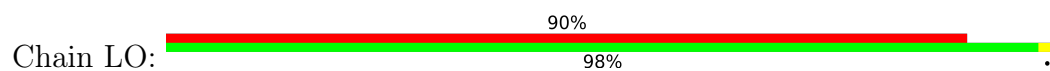


• Molecule 9: Baseplate wedge tail fiber connector

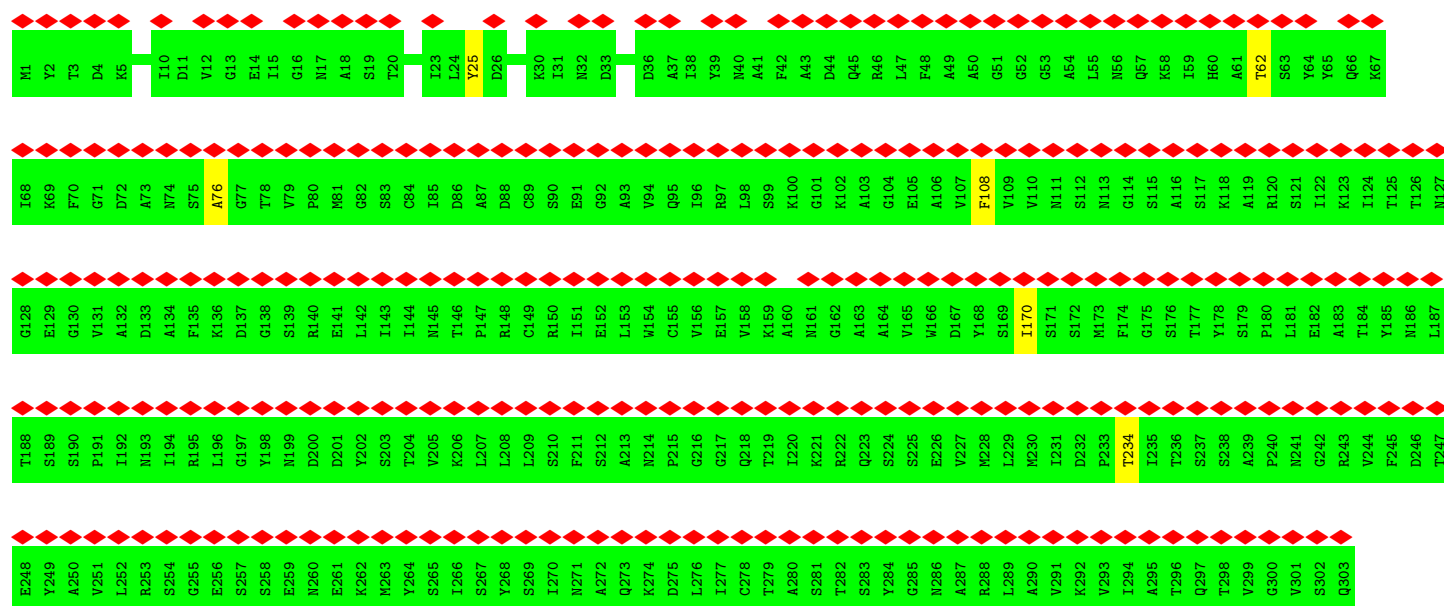




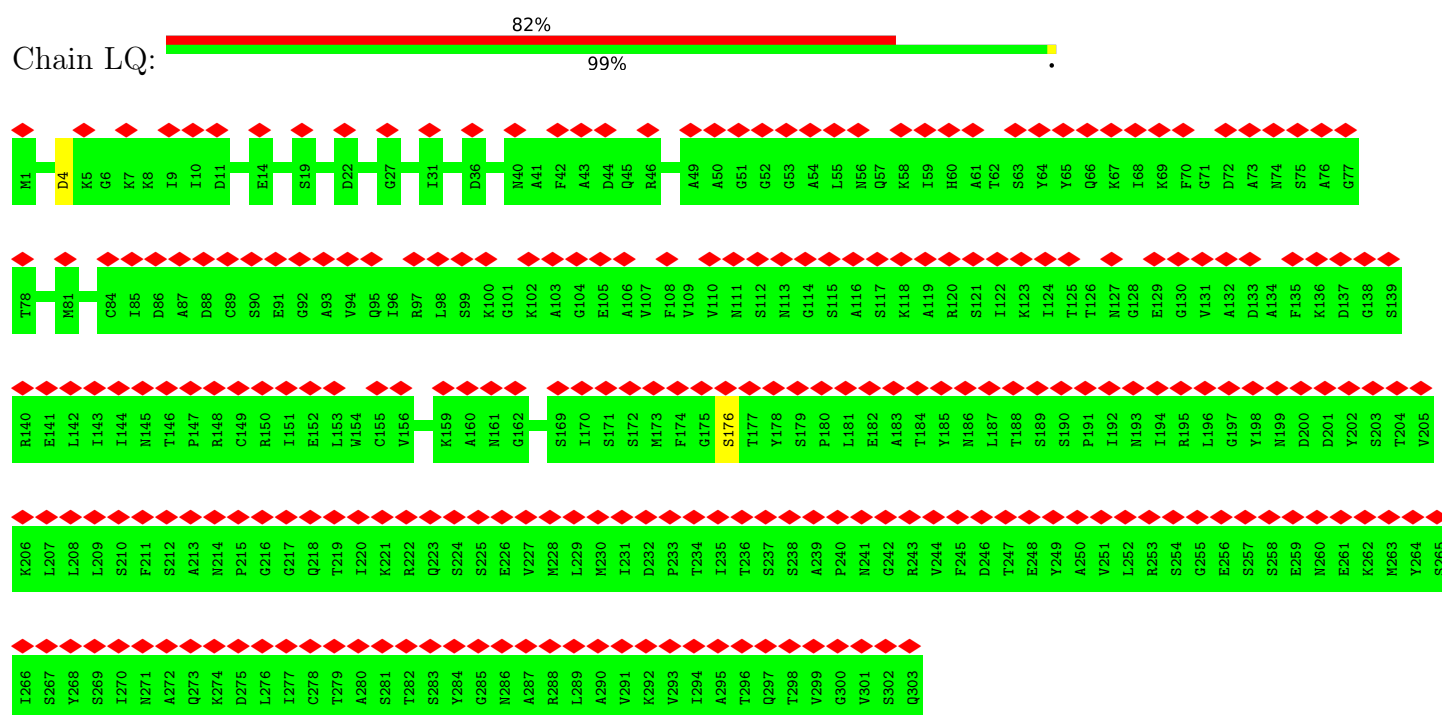
• Molecule 9: Baseplate wedge tail fiber connector



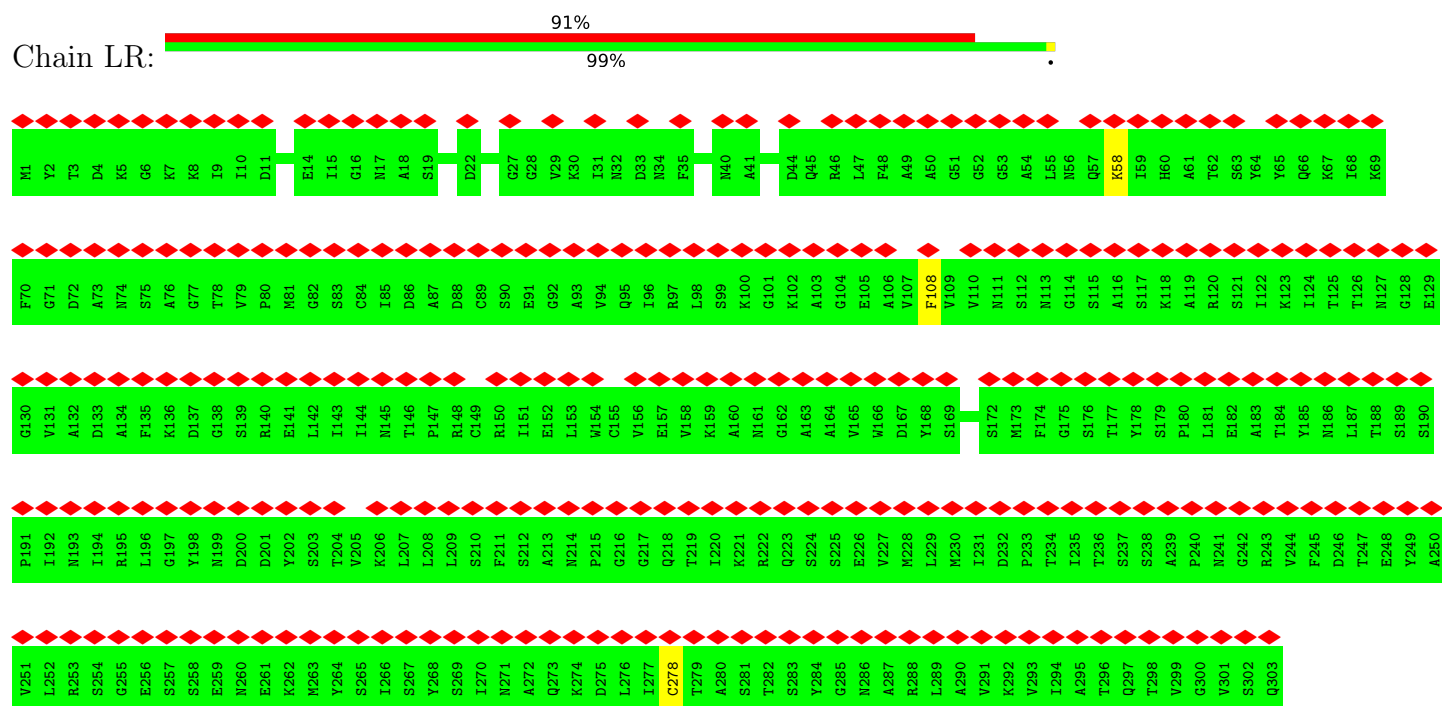
• Molecule 9: Baseplate wedge tail fiber connector



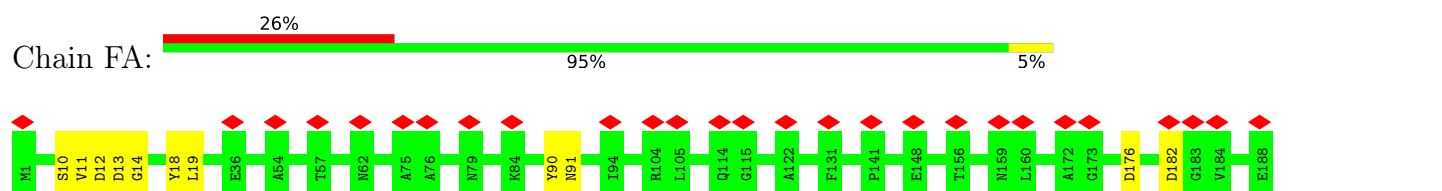
• Molecule 9: Baseplate wedge tail fiber connector

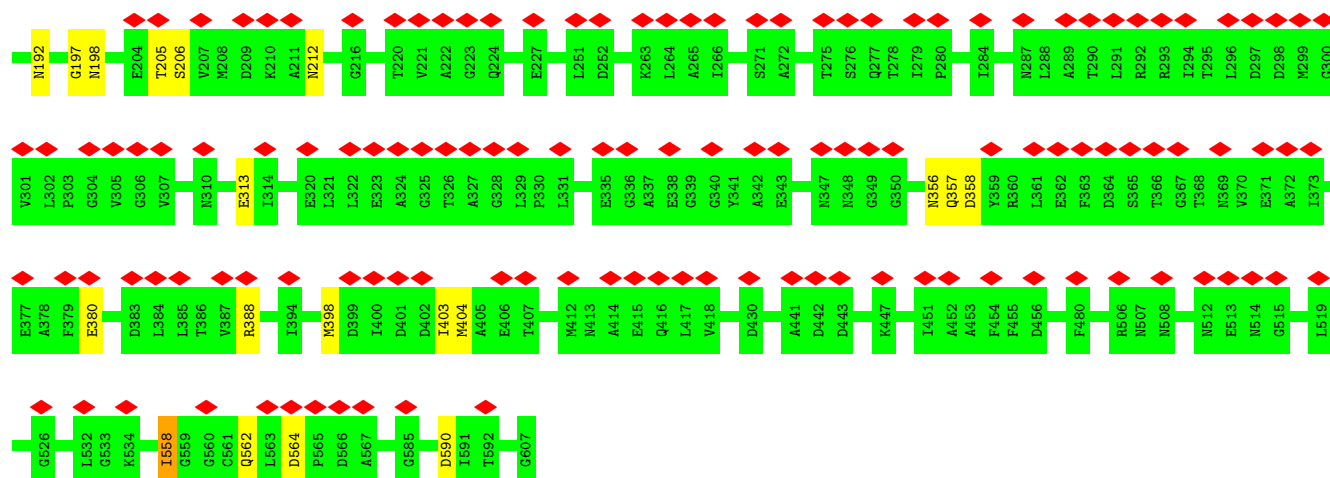


• Molecule 9: Baseplate wedge tail fiber connector

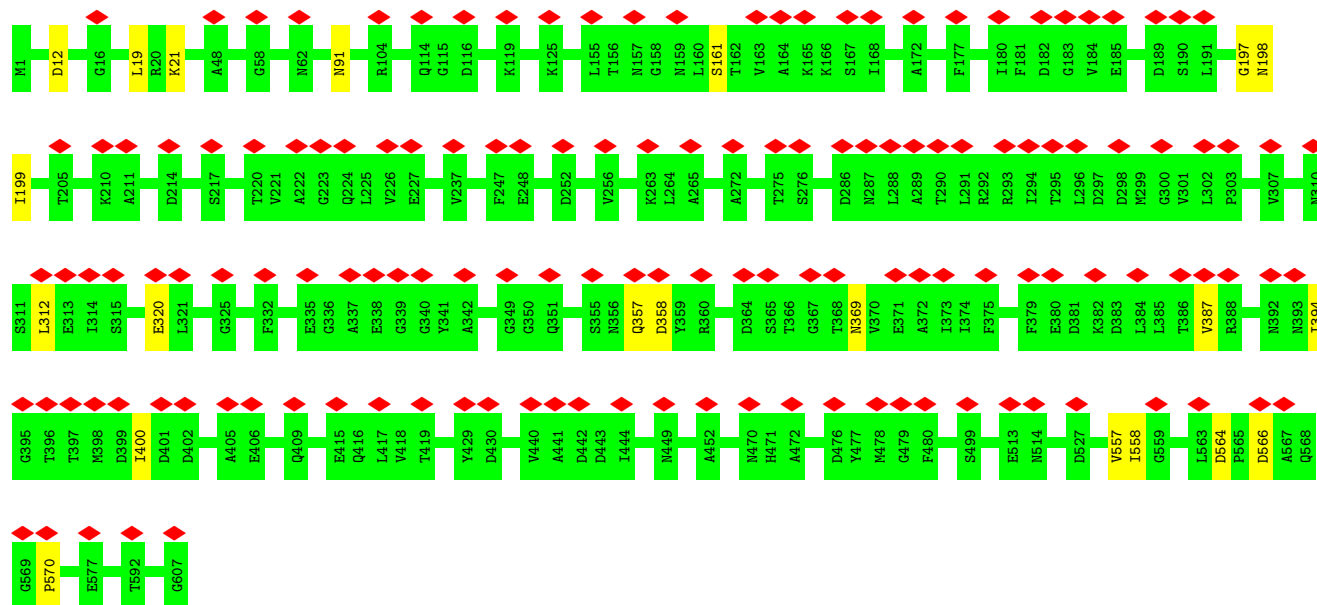


• Molecule 10: Baseplate wedge protein gp10

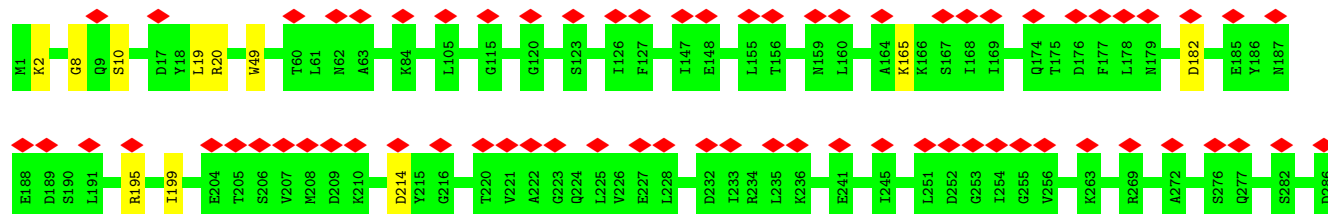




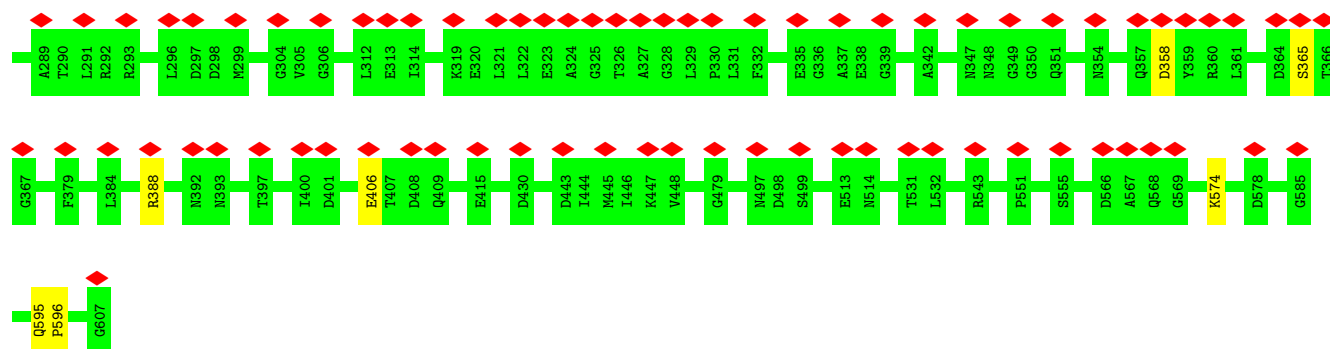
- Molecule 10: Baseplate wedge protein gp10



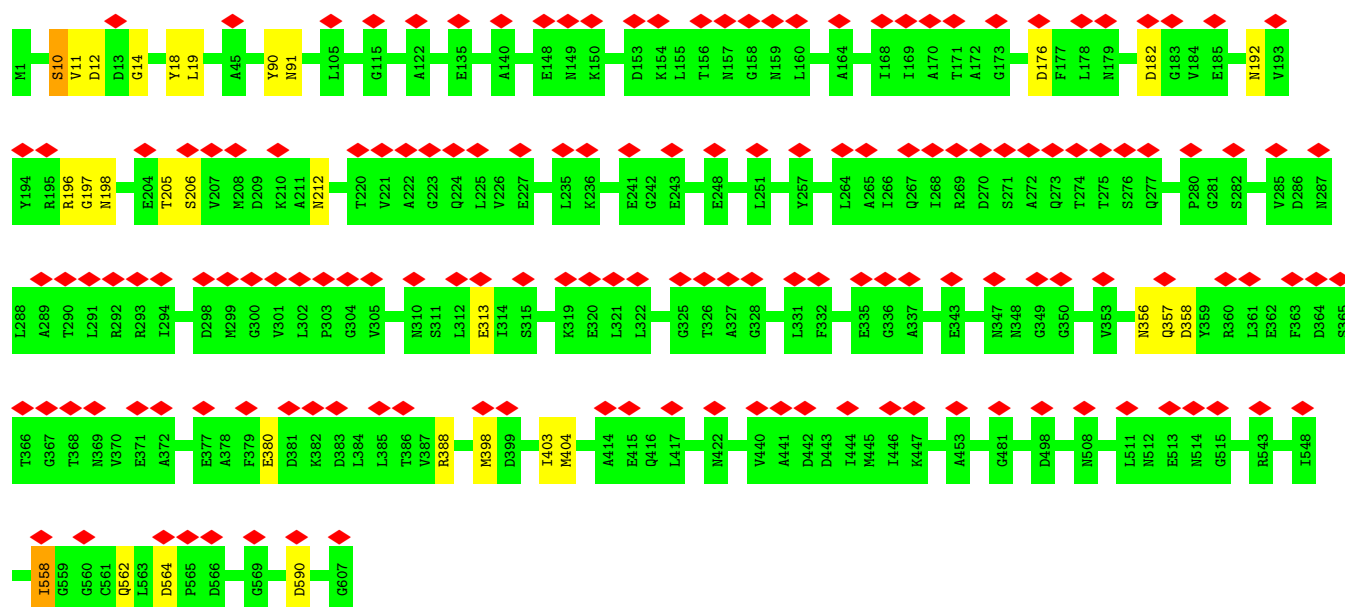
- Molecule 10: Baseplate wedge protein gp10



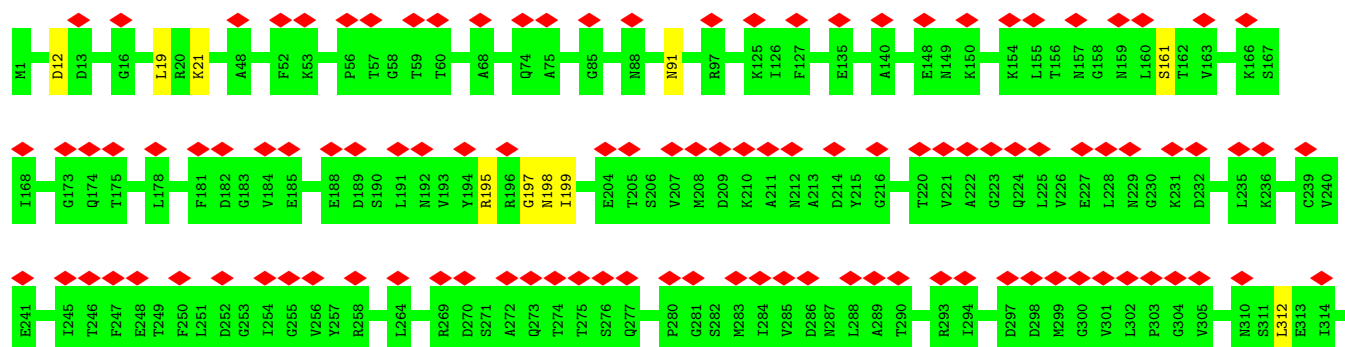


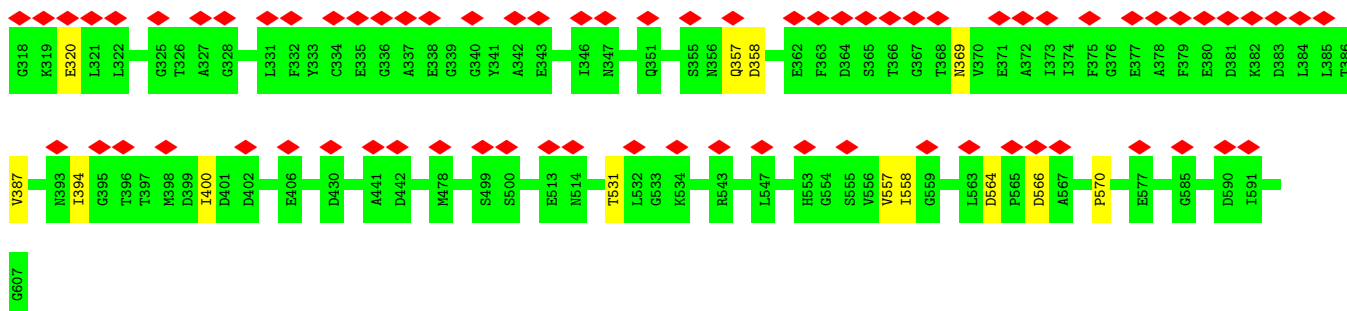


• Molecule 10: Baseplate wedge protein gp10

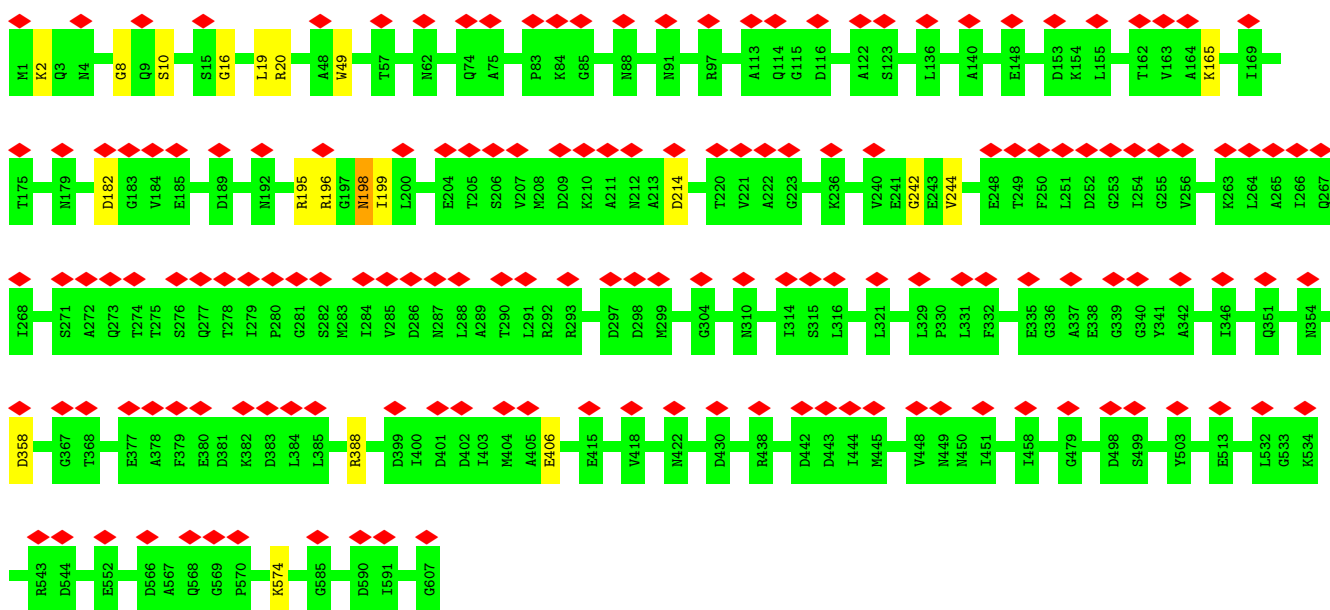


• Molecule 10: Baseplate wedge protein gp10

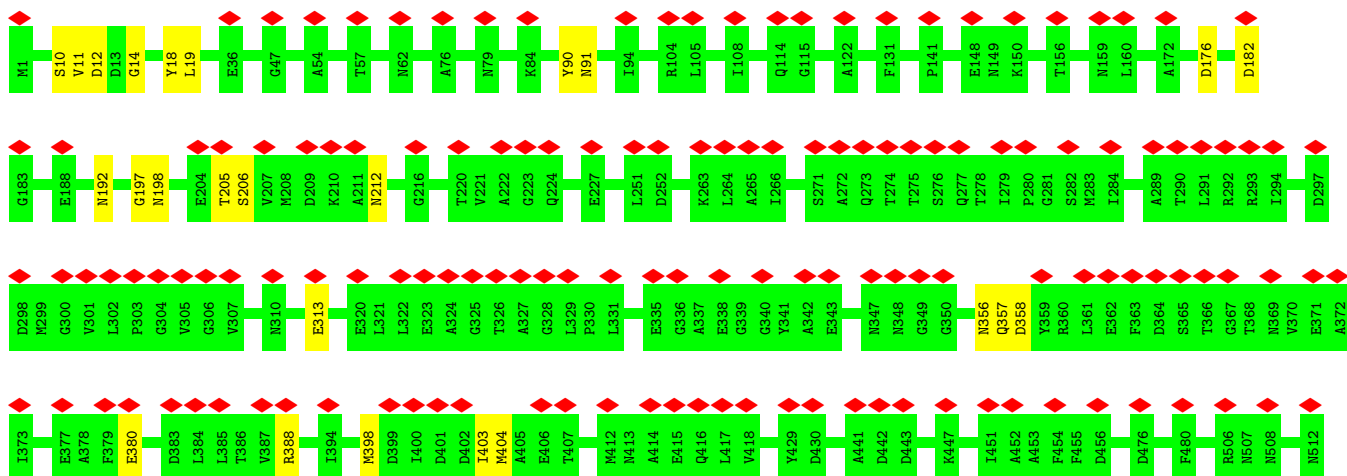


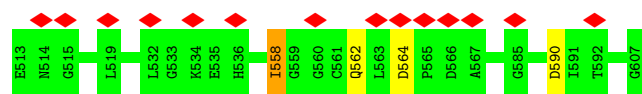


• Molecule 10: Baseplate wedge protein gp10

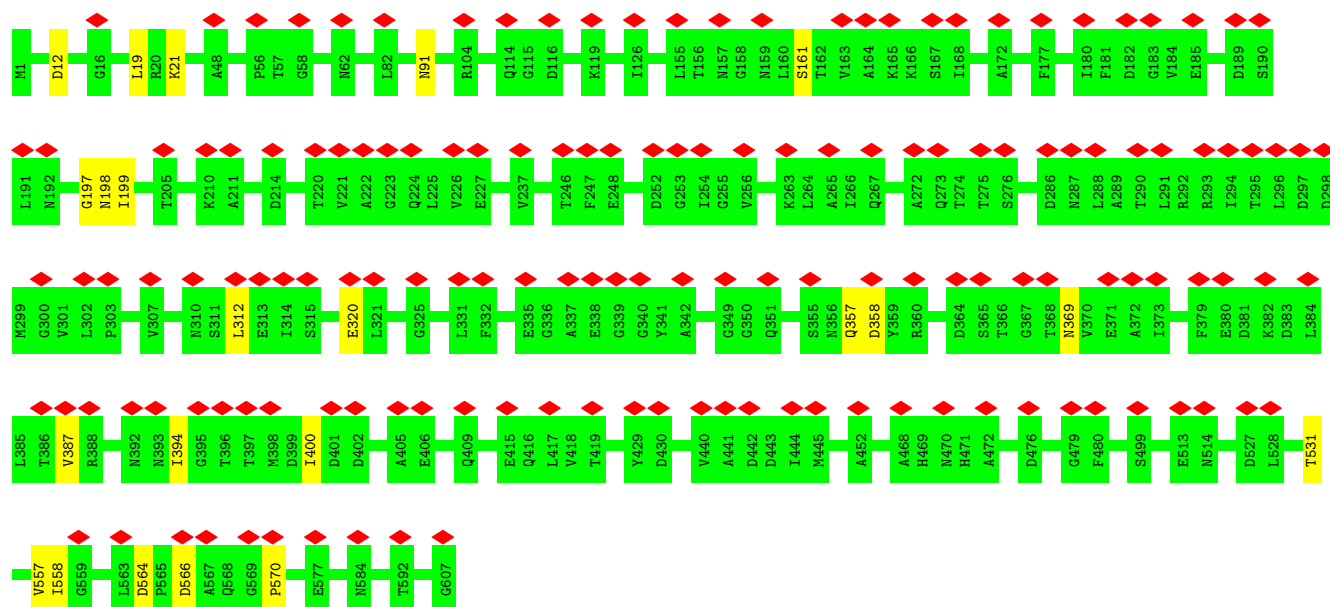


• Molecule 10: Baseplate wedge protein gp10

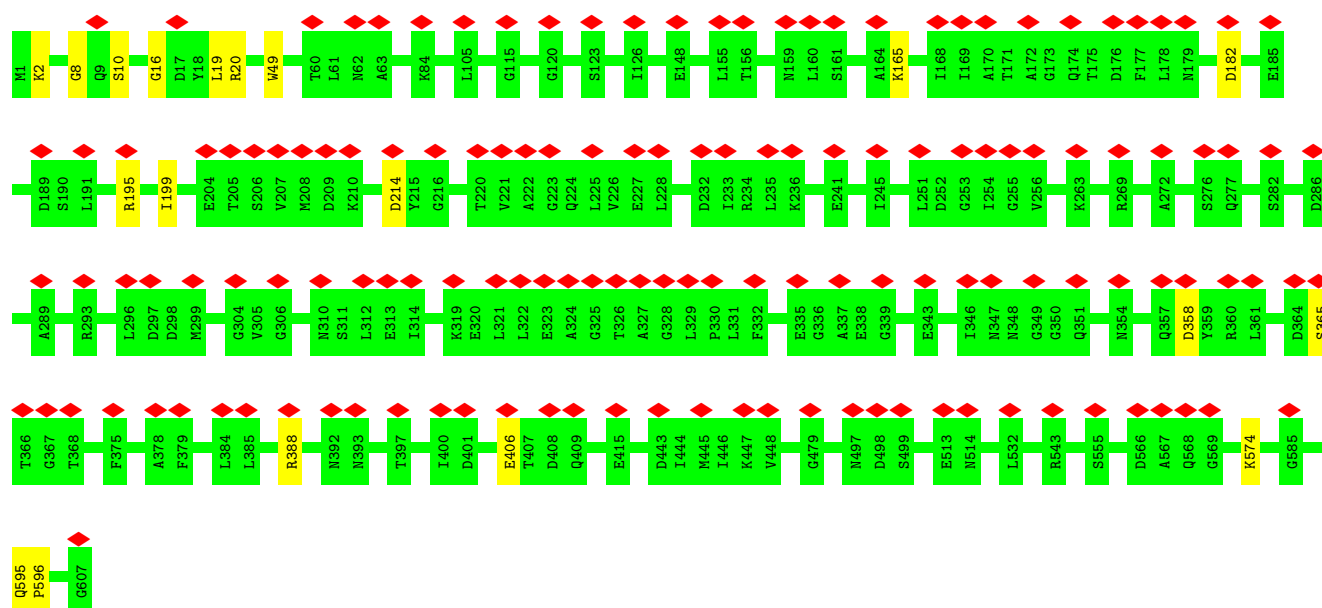




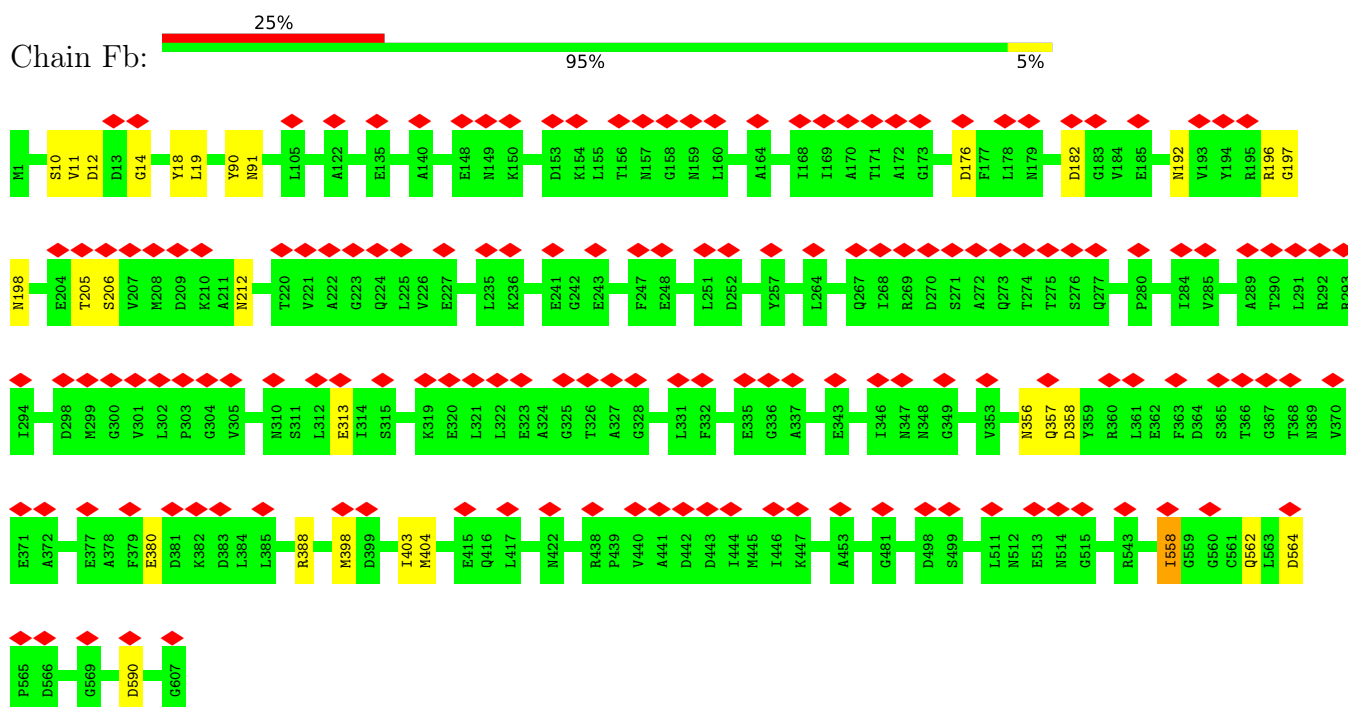
• Molecule 10: Baseplate wedge protein gp10



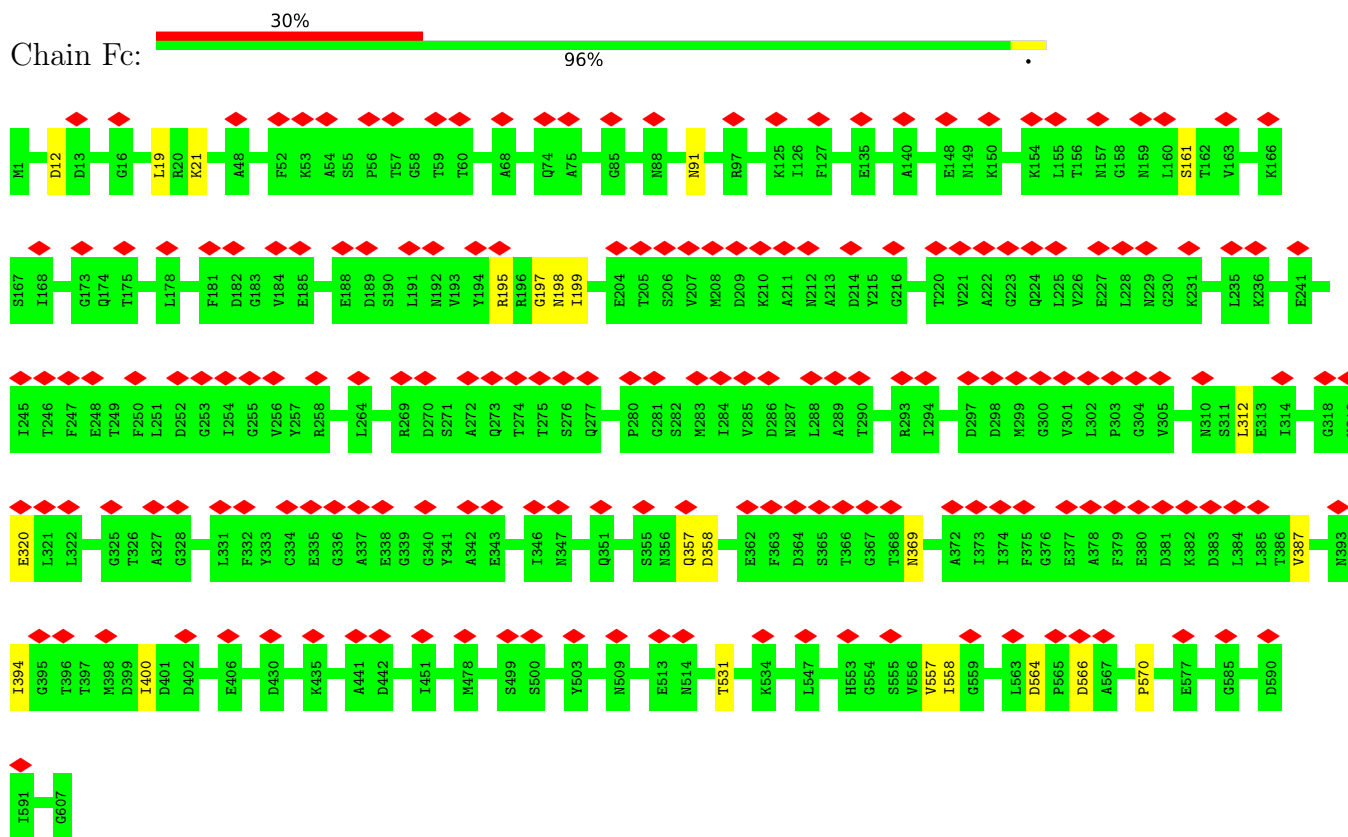
• Molecule 10: Baseplate wedge protein gp10



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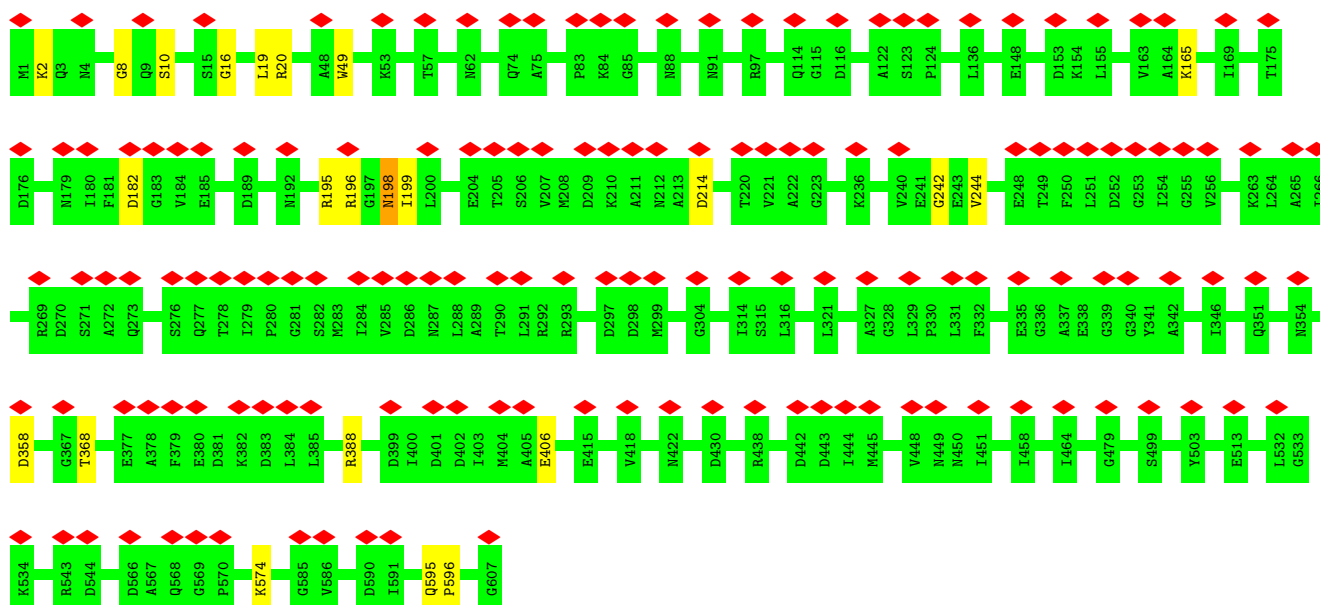


• Molecule 10: Baseplate wedge protein gp10



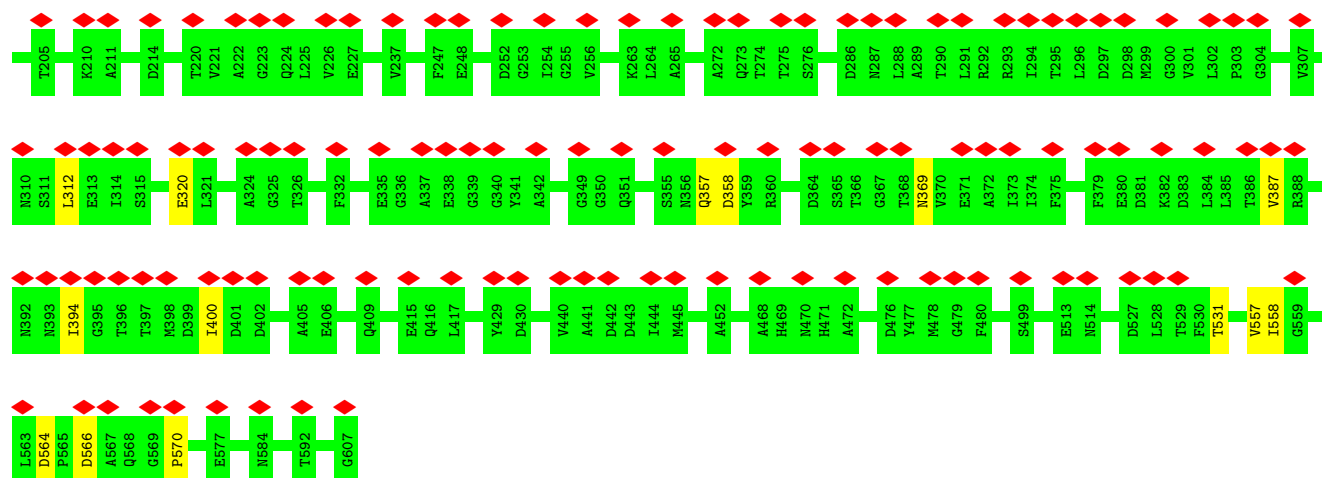
• Molecule 10: Baseplate wedge protein gp10



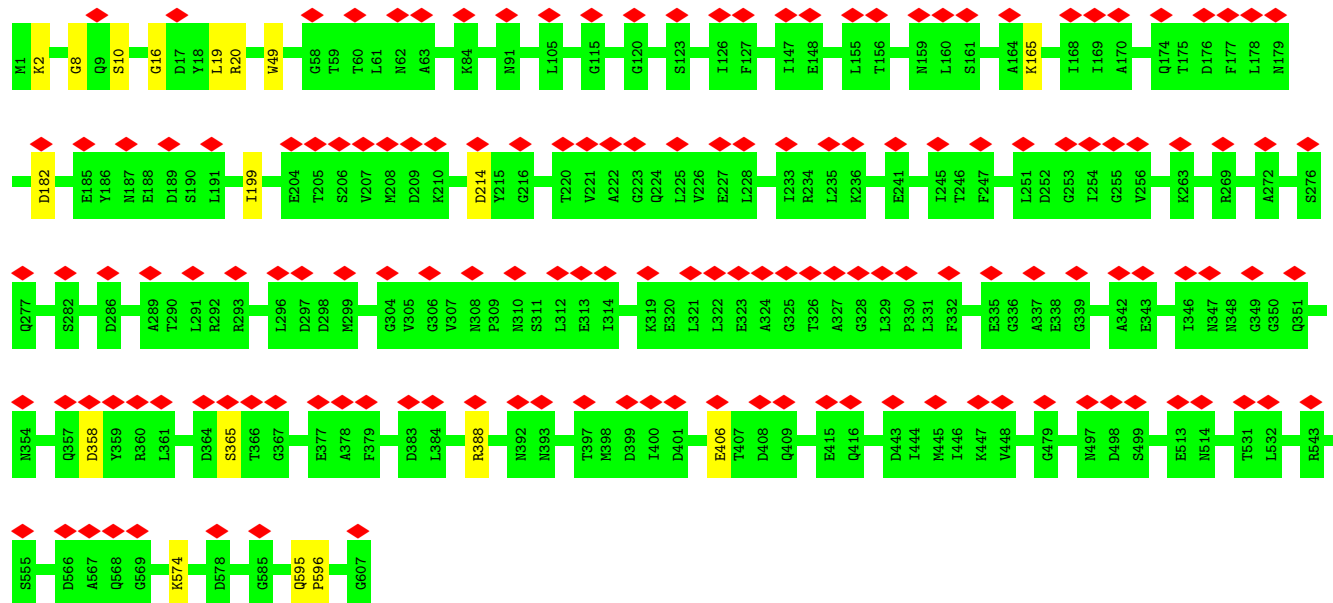


• Molecule 10: Baseplate wedge protein gp10

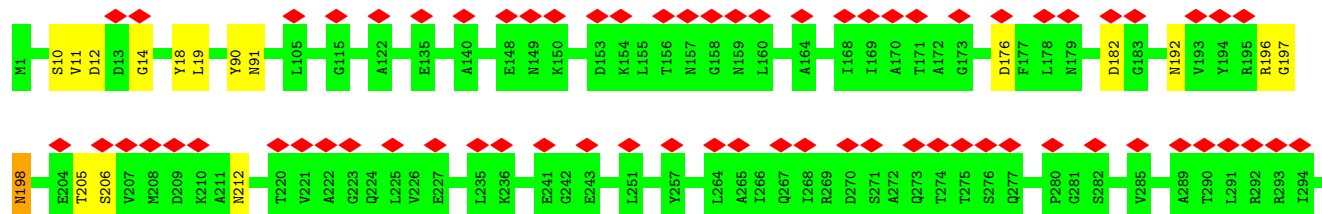


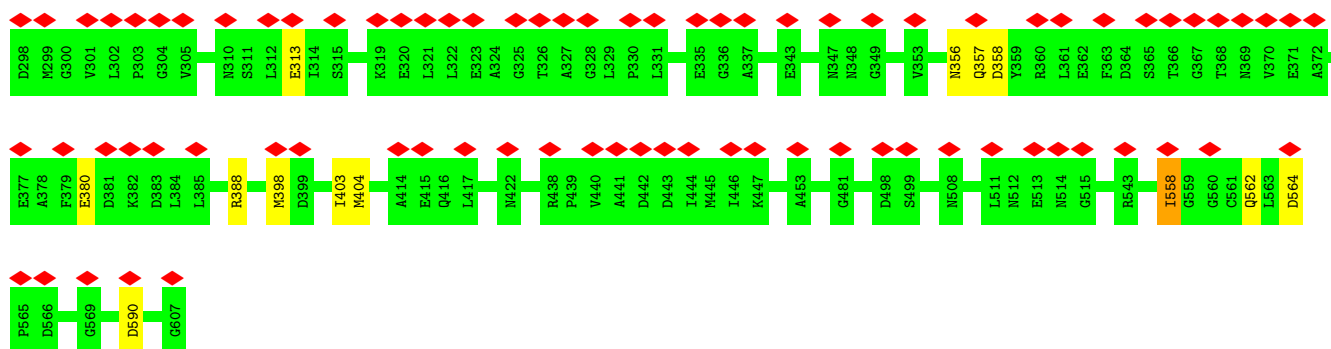


• Molecule 10: Baseplate wedge protein gp10

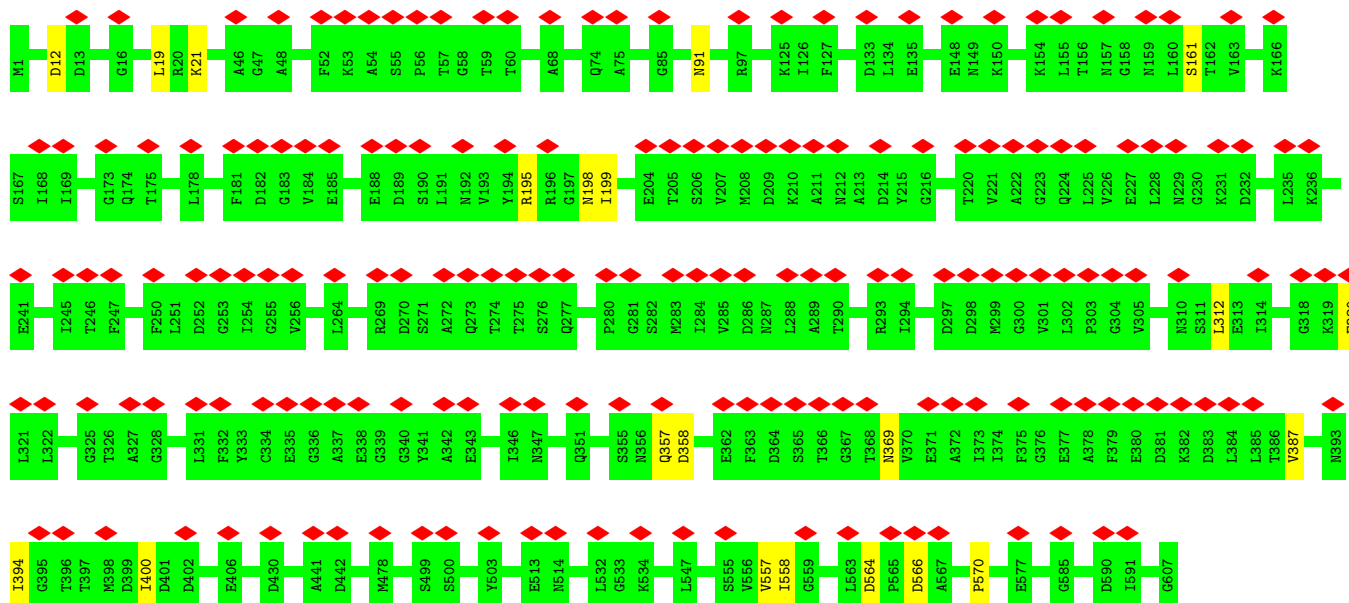


• Molecule 10: Baseplate wedge protein gp10

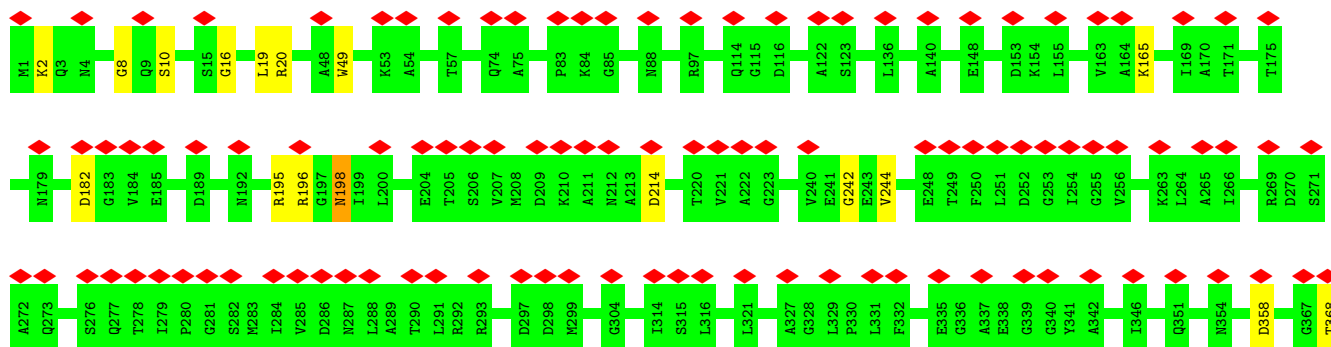


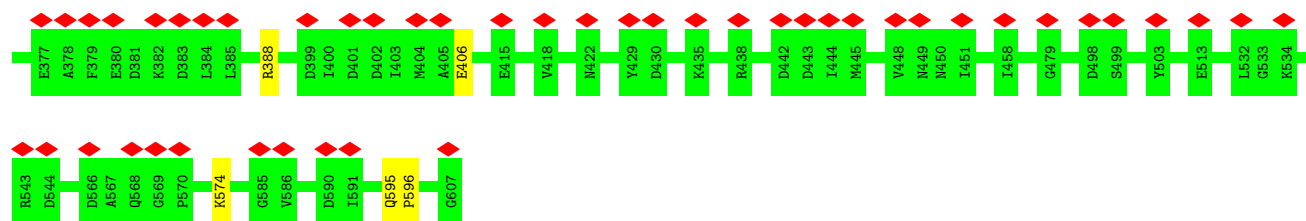


• Molecule 10: Baseplate wedge protein gp10

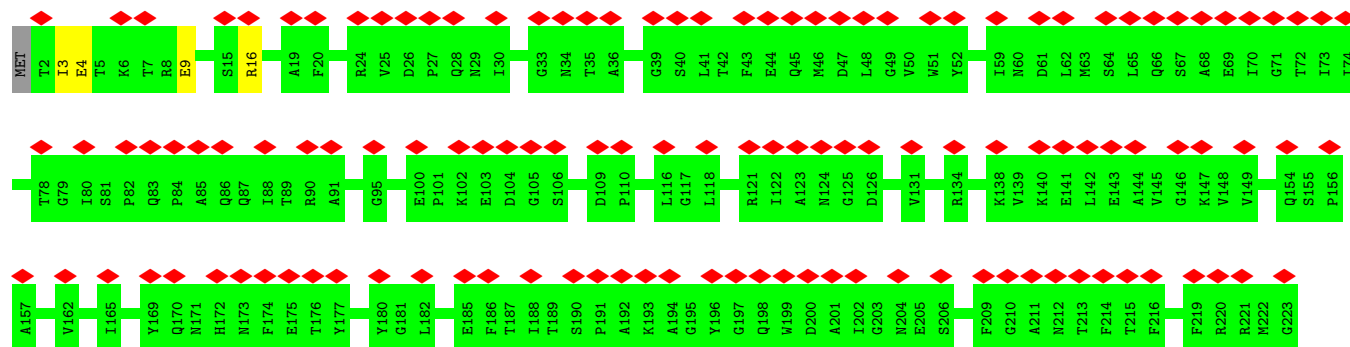


• Molecule 10: Baseplate wedge protein gp10

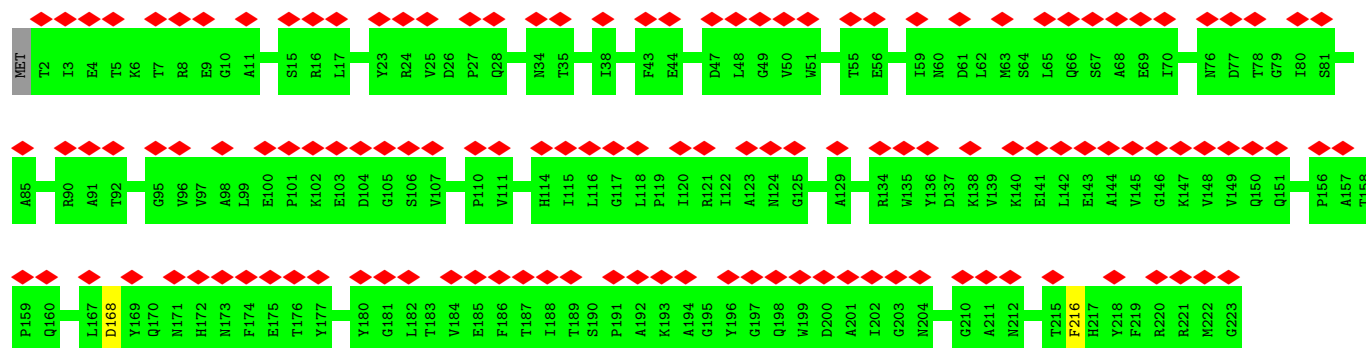




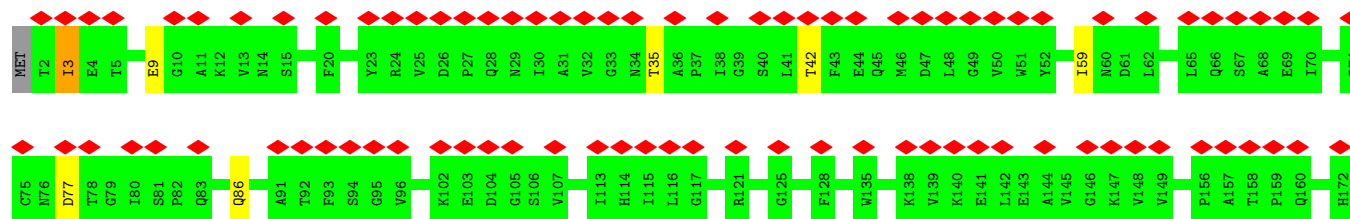
• Molecule 11: Baseplate wedge subunit and tail pin



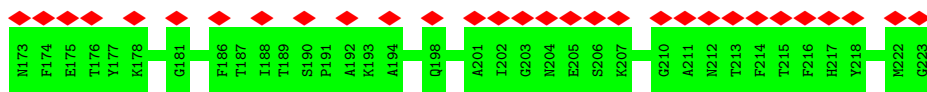
• Molecule 11: Baseplate wedge subunit and tail pin



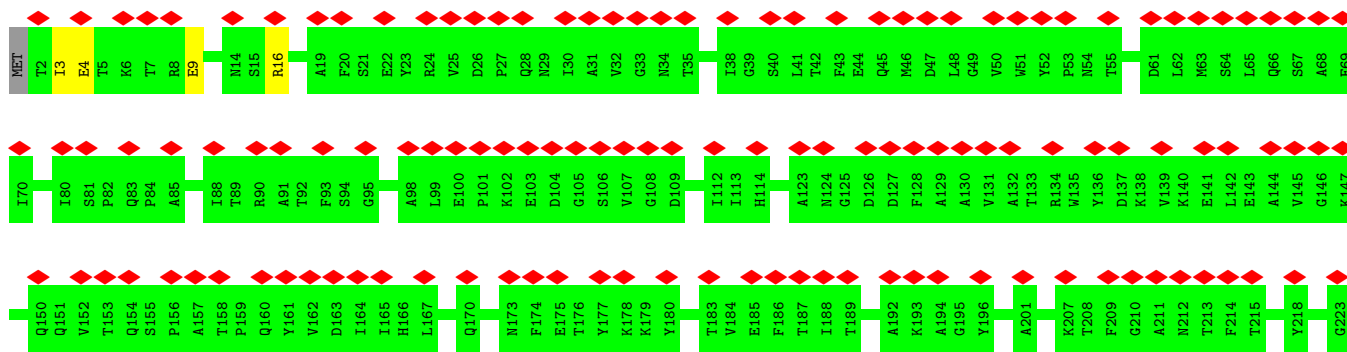
• Molecule 11: Baseplate wedge subunit and tail pin



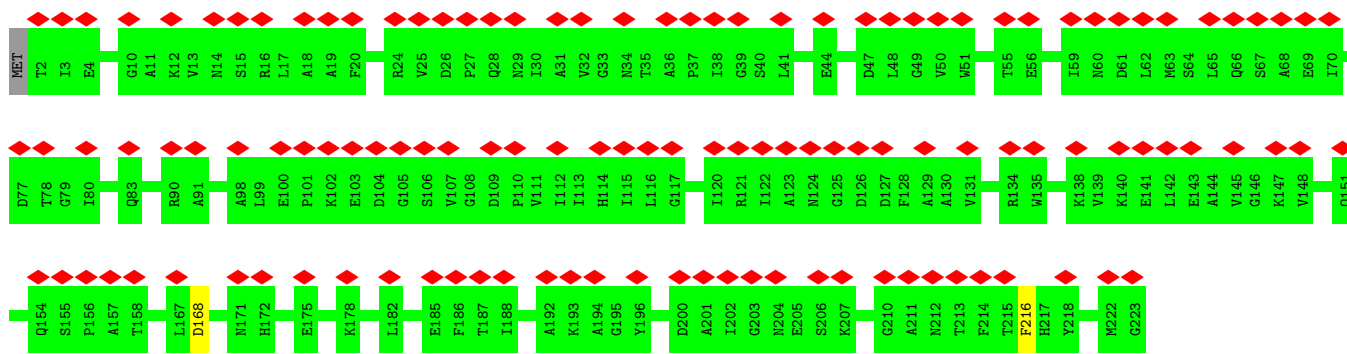




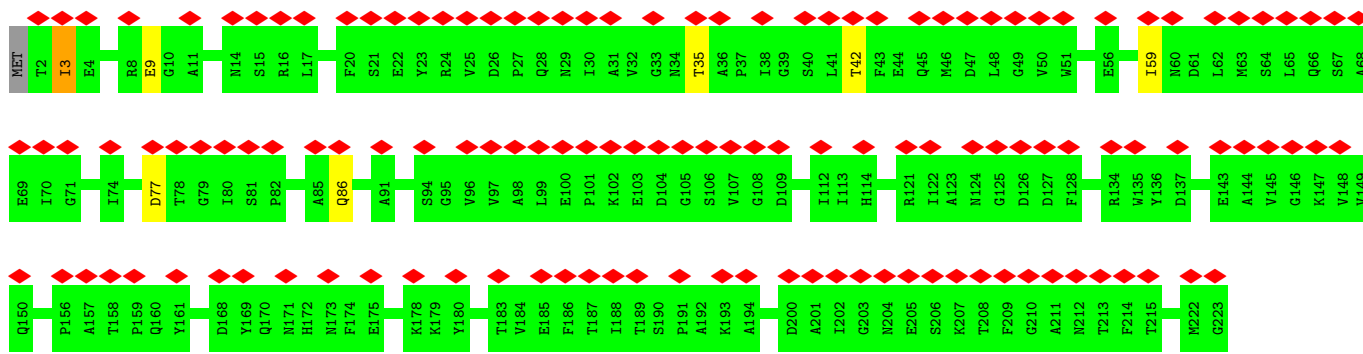
- Molecule 11: Baseplate wedge subunit and tail pin



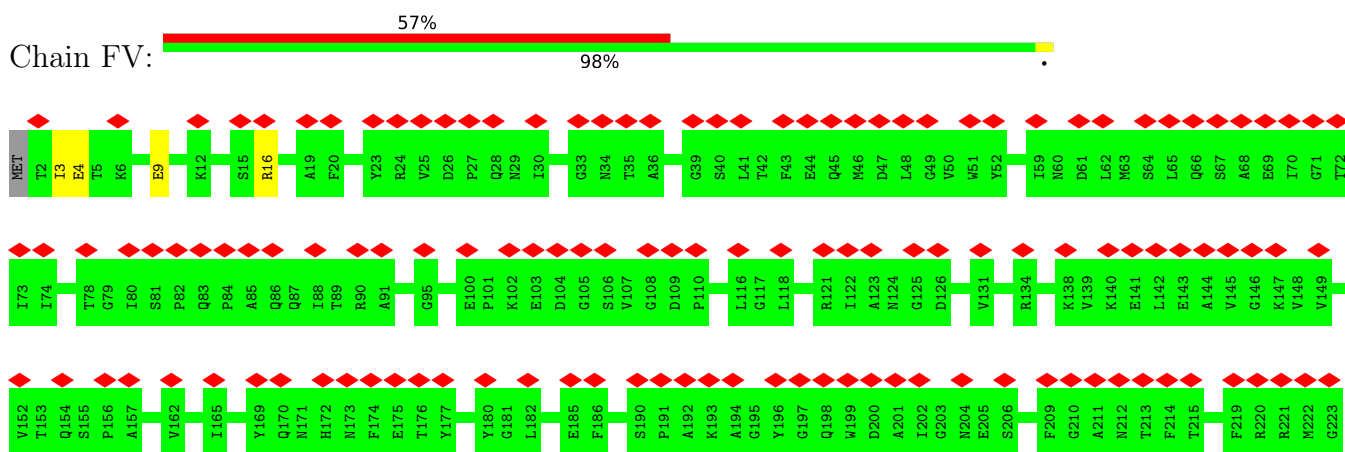
- Molecule 11: Baseplate wedge subunit and tail pin



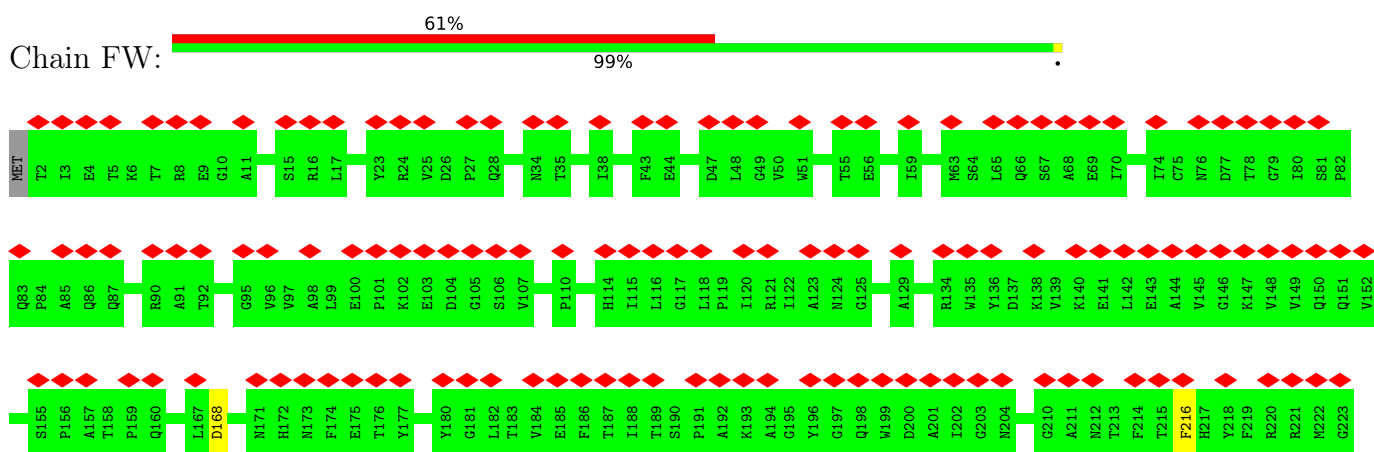
- Molecule 11: Baseplate wedge subunit and tail pin



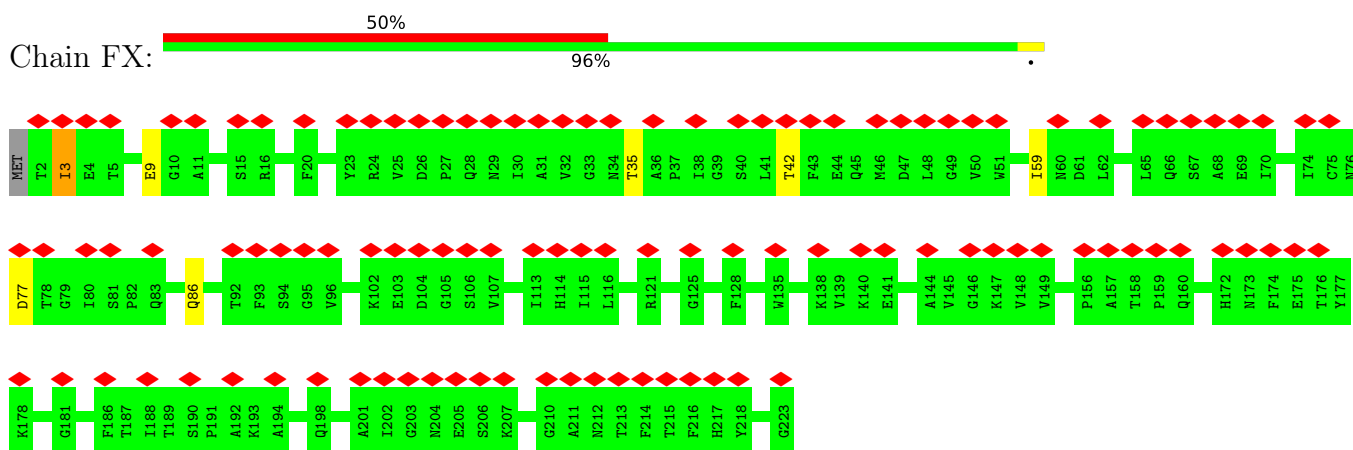
- Molecule 11: Baseplate wedge subunit and tail pin



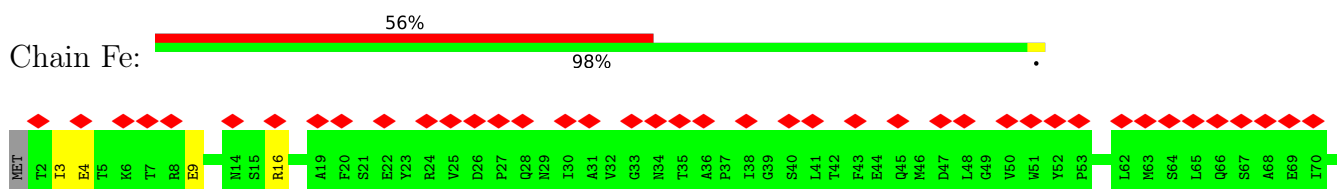
- Molecule 11: Baseplate wedge subunit and tail pin

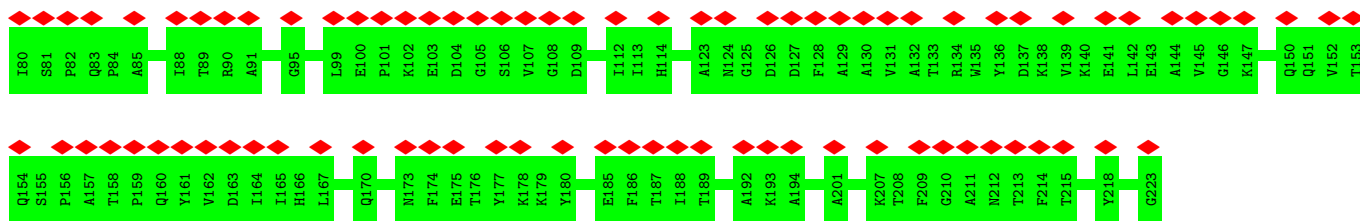


- Molecule 11: Baseplate wedge subunit and tail pin

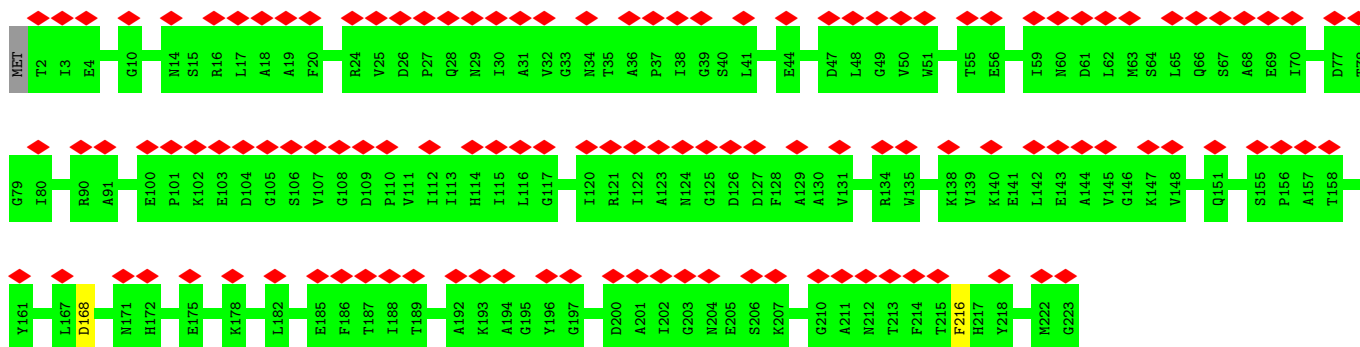


- Molecule 11: Baseplate wedge subunit and tail pin

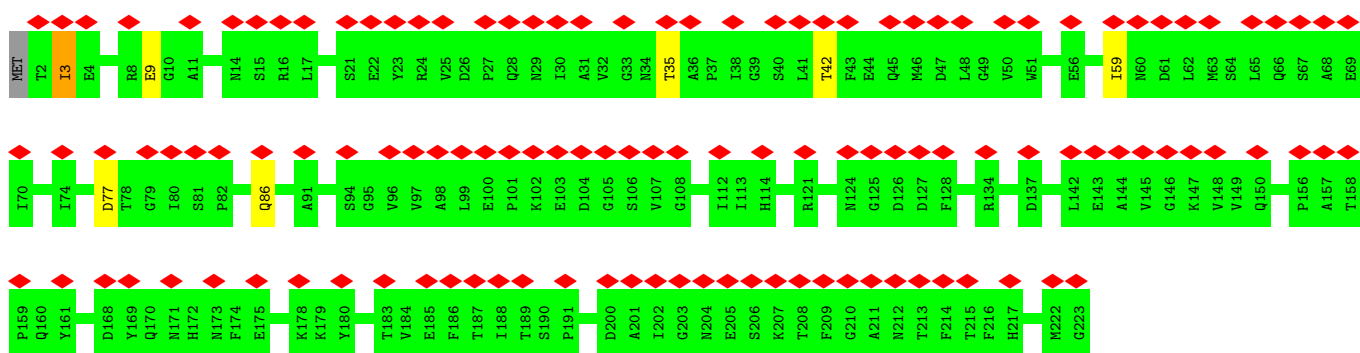




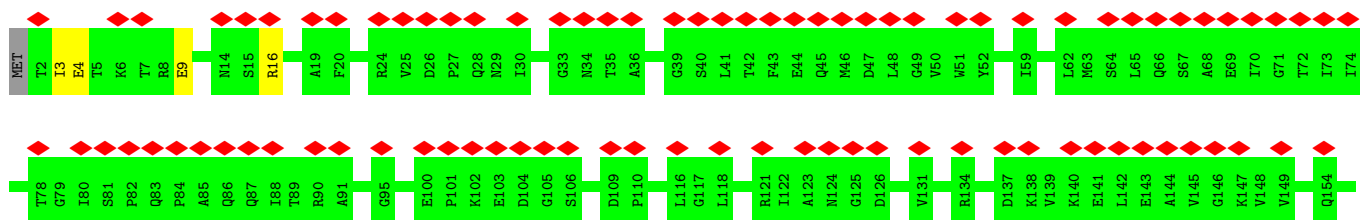
- Molecule 11: Baseplate wedge subunit and tail pin

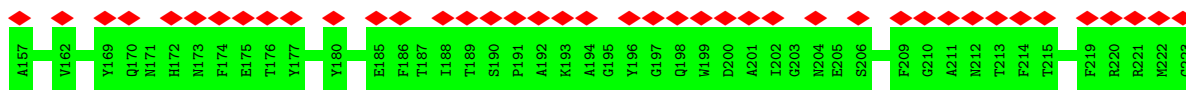


- Molecule 11: Baseplate wedge subunit and tail pin



- Molecule 11: Baseplate wedge subunit and tail pin

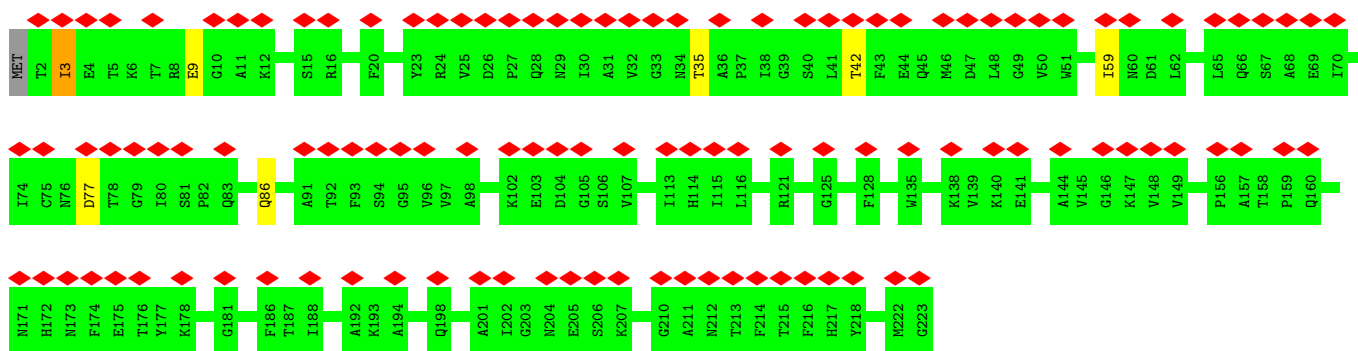




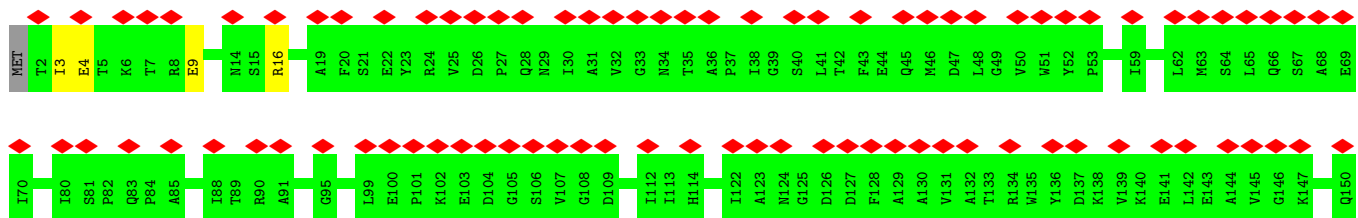
- Molecule 11: Baseplate wedge subunit and tail pin

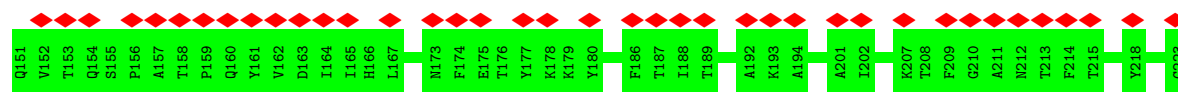


- Molecule 11: Baseplate wedge subunit and tail pin

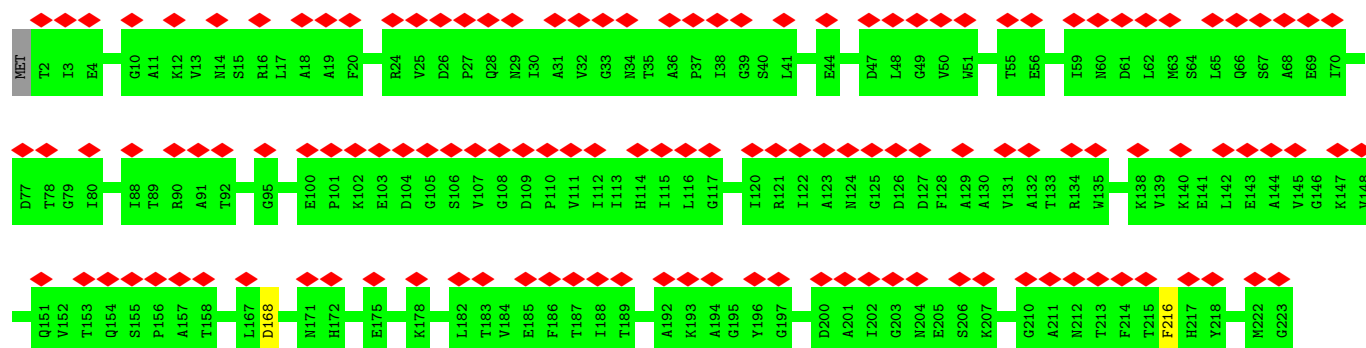


- Molecule 11: Baseplate wedge subunit and tail pin

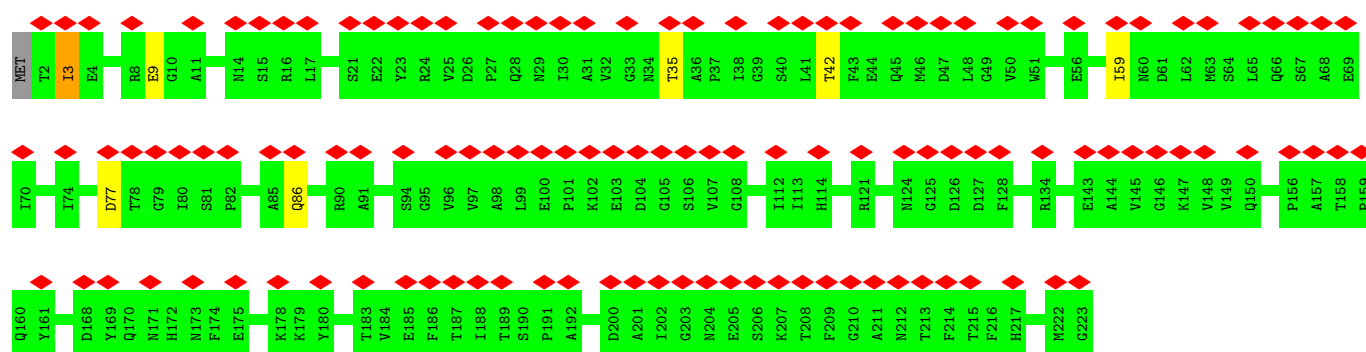




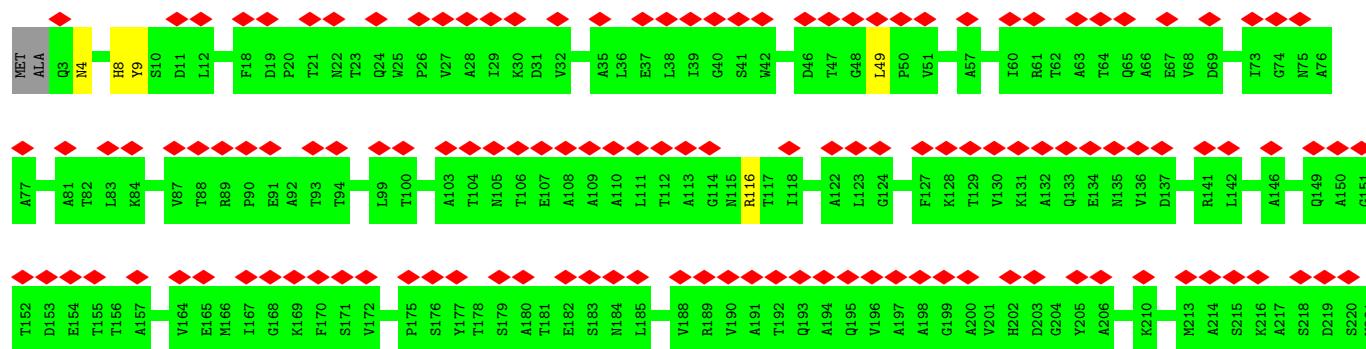
- Molecule 11: Baseplate wedge subunit and tail pin

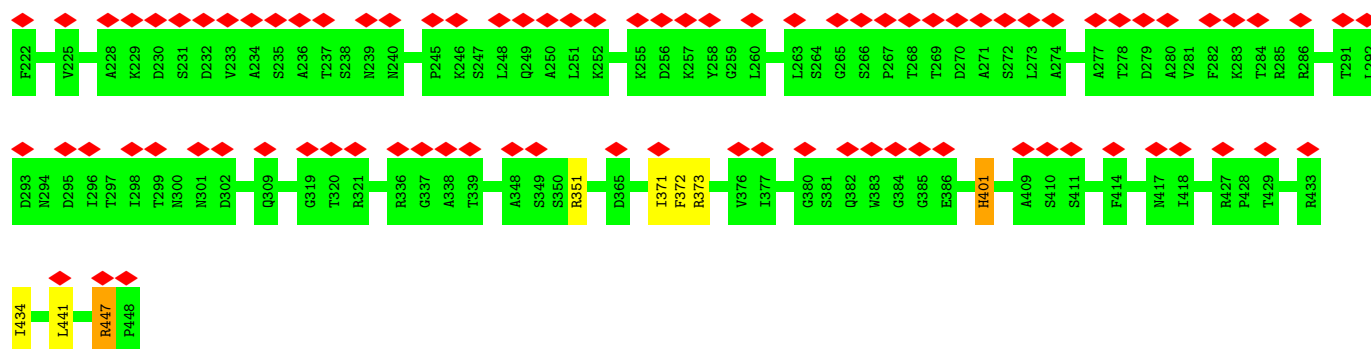


- Molecule 11: Baseplate wedge subunit and tail pin

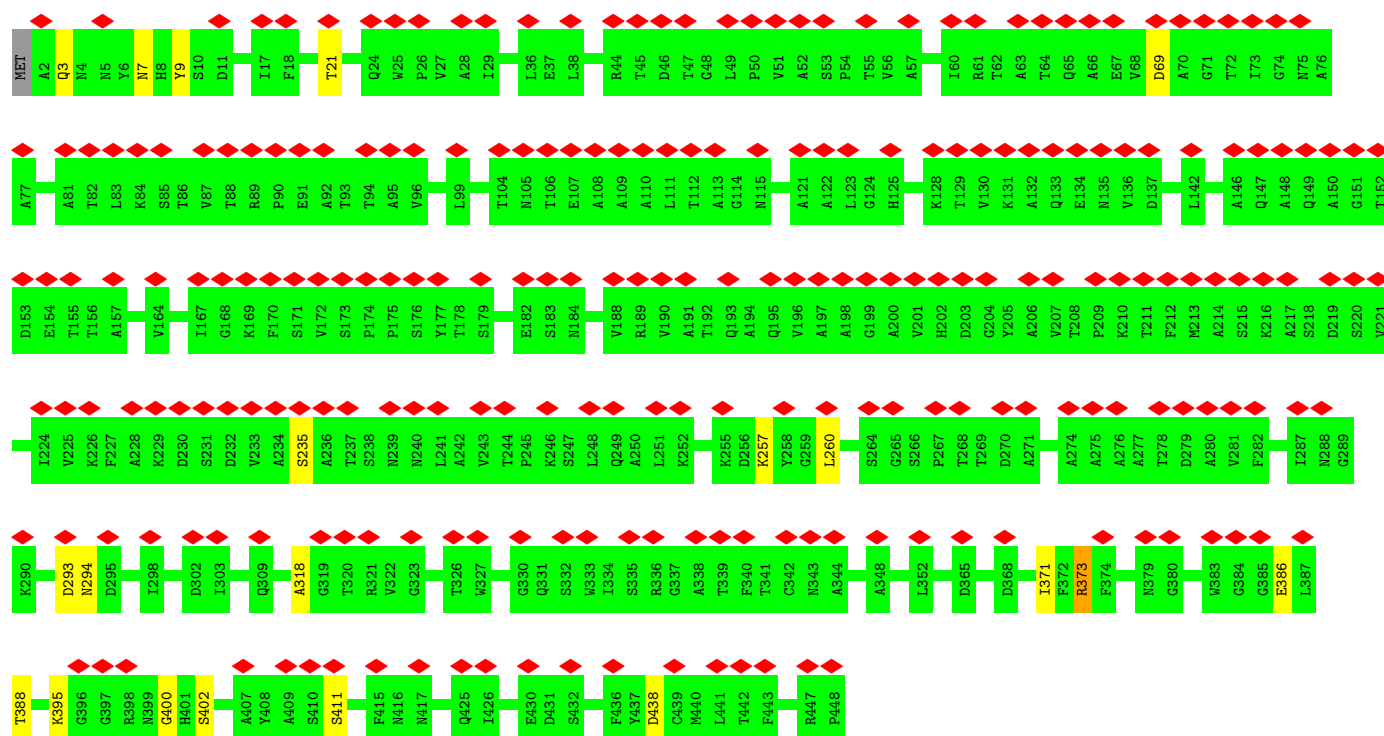


- Molecule 12: Gp12 short tail fibers

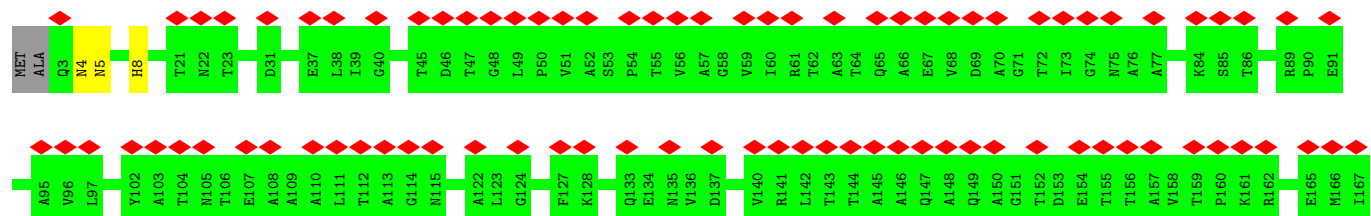


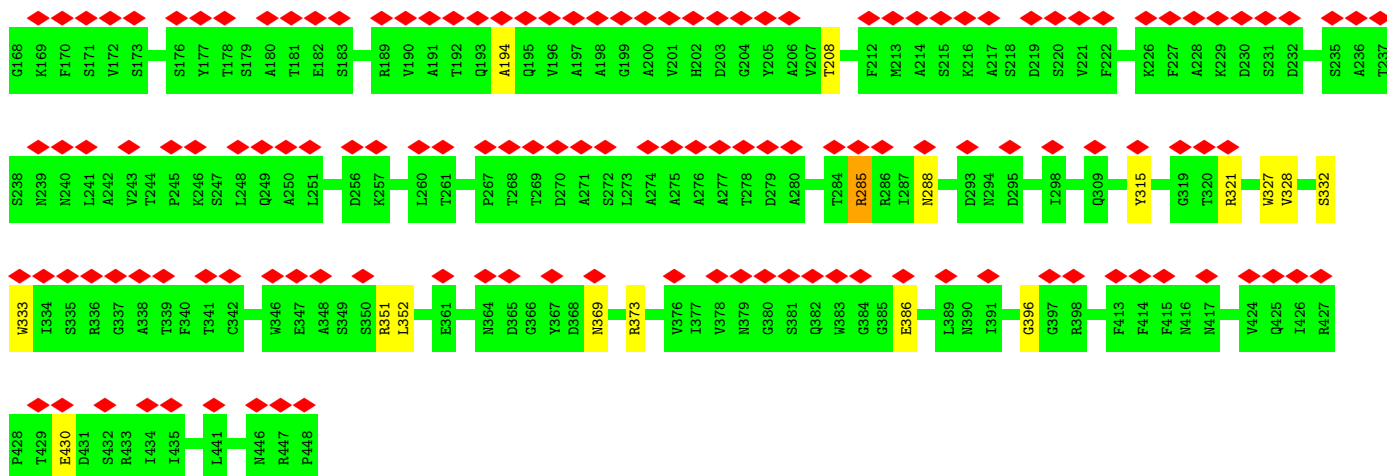


- Molecule 12: Gp12 short tail fibers



- Molecule 12: Gp12 short tail fibers





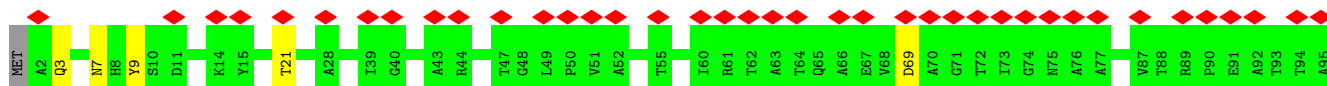
• Molecule 12: Gp12 short tail fibers

Chain FP: 52% 97%



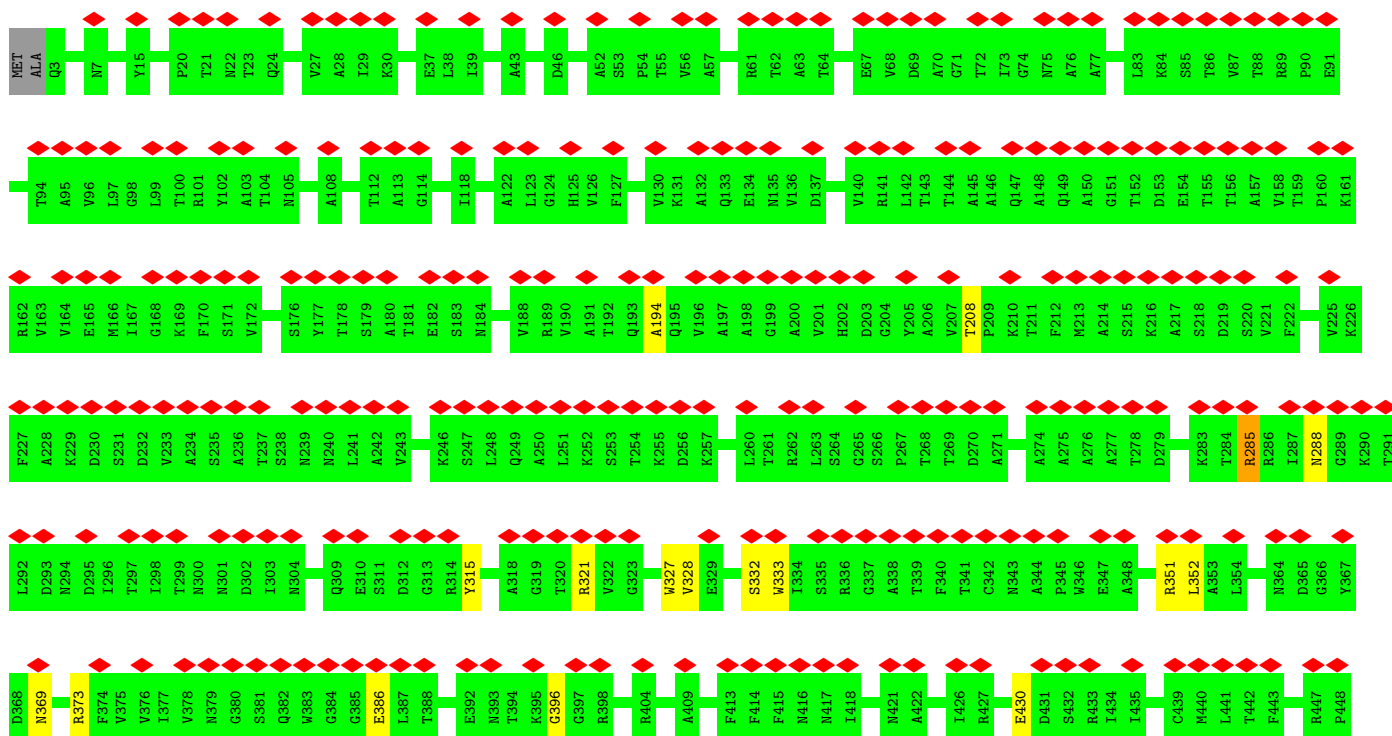
• Molecule 12: Gp12 short tail fibers

Chain FR: 57% 95%





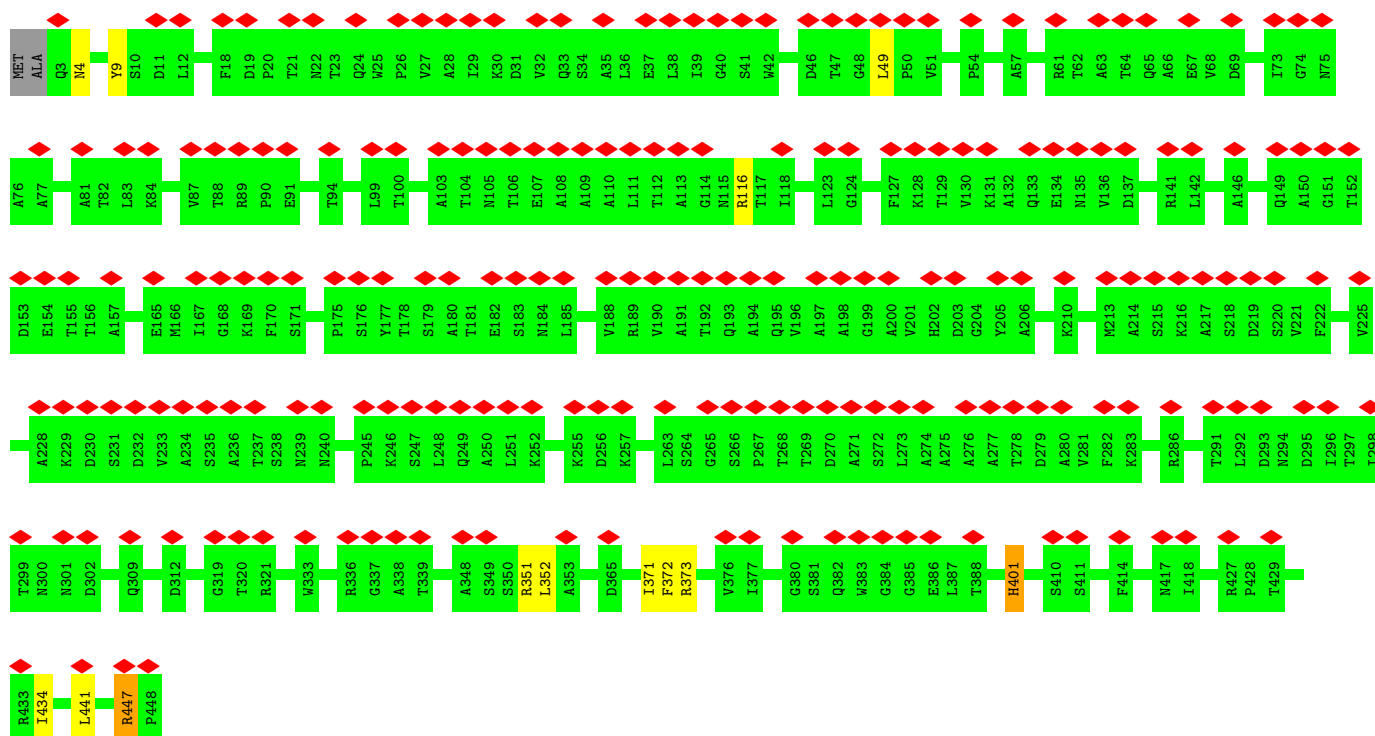
• Molecule 12: Gp12 short tail fibers



• Molecule 12: Gp12 short tail fibers





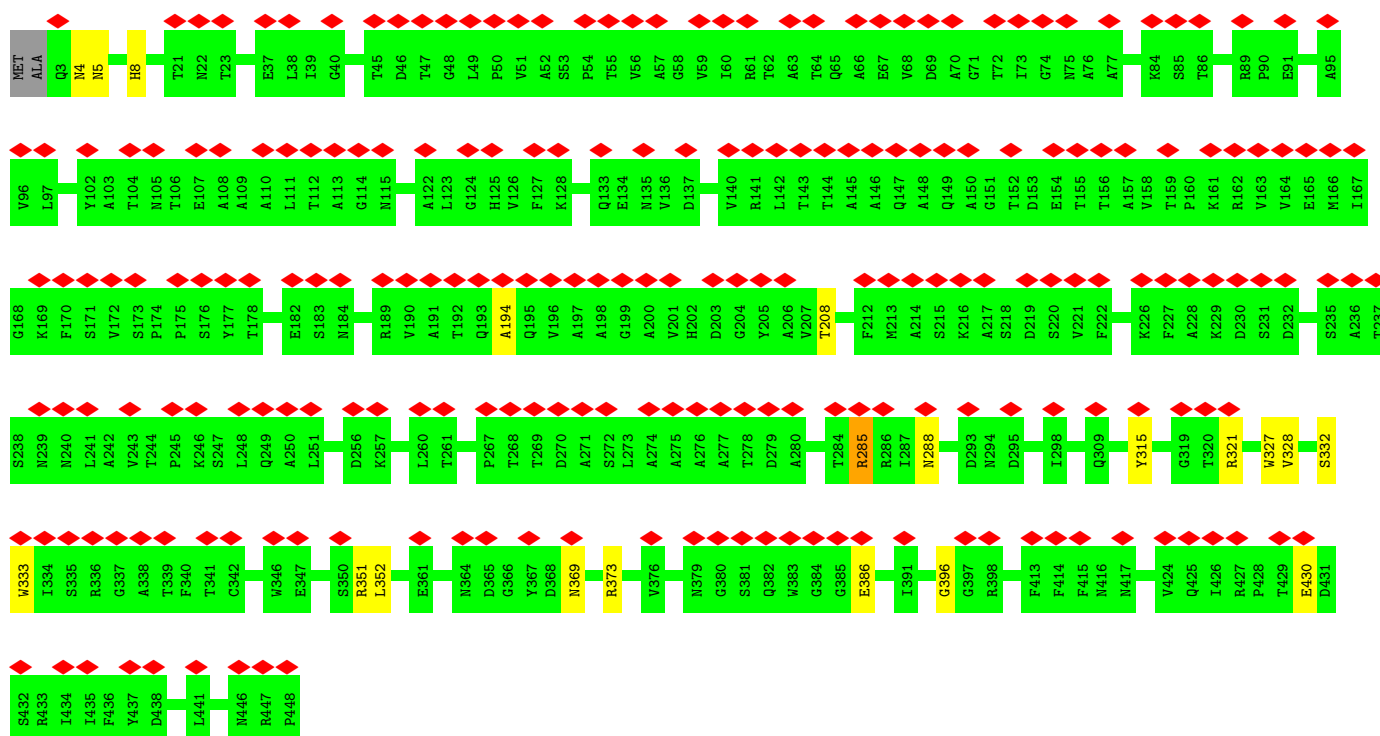


• Molecule 12: Gp12 short tail fibers



• Molecule 12: Gp12 short tail fibers

Chain FZ: 

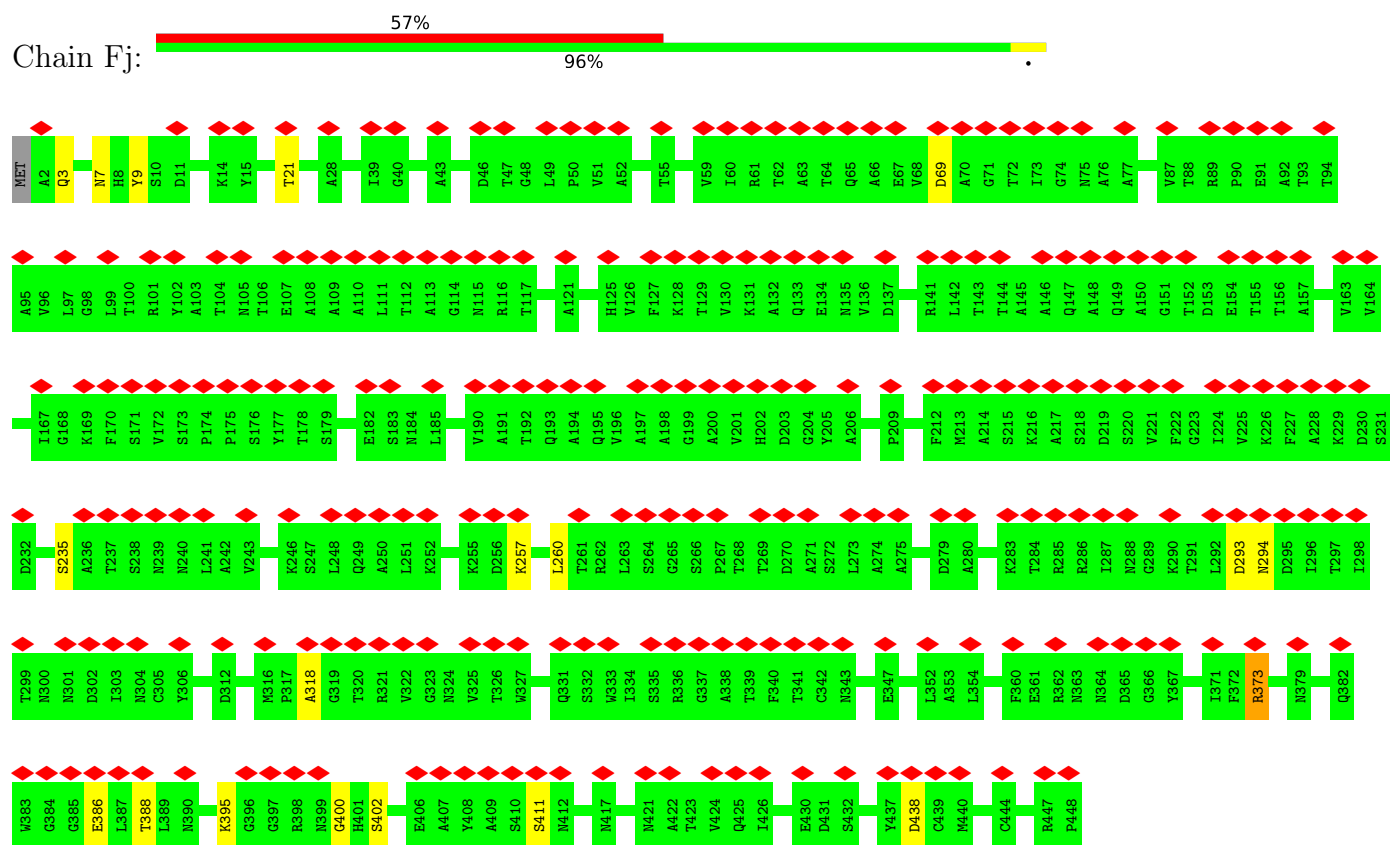


• Molecule 12: Gp12 short tail fibers

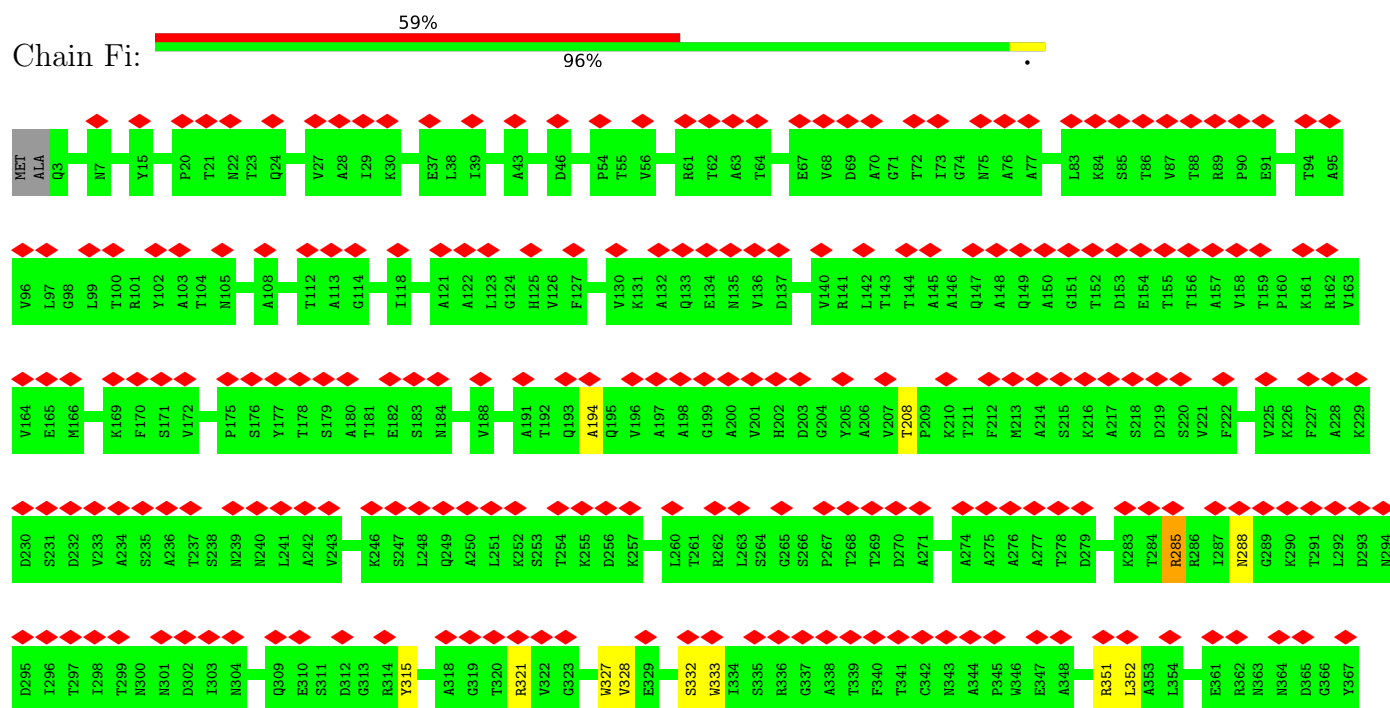
Chain Fh: 

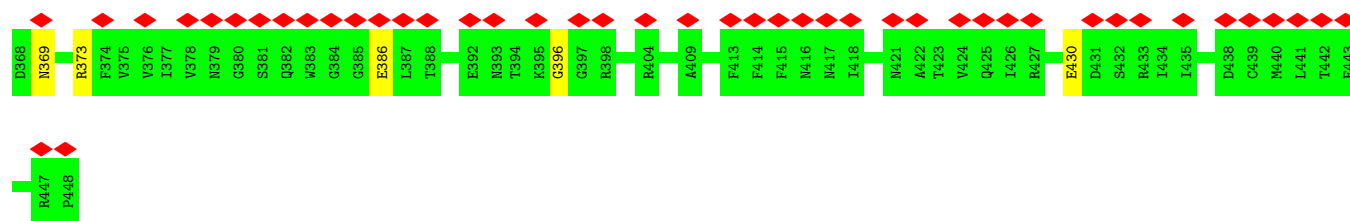


- Molecule 12: Gp12 short tail fibers

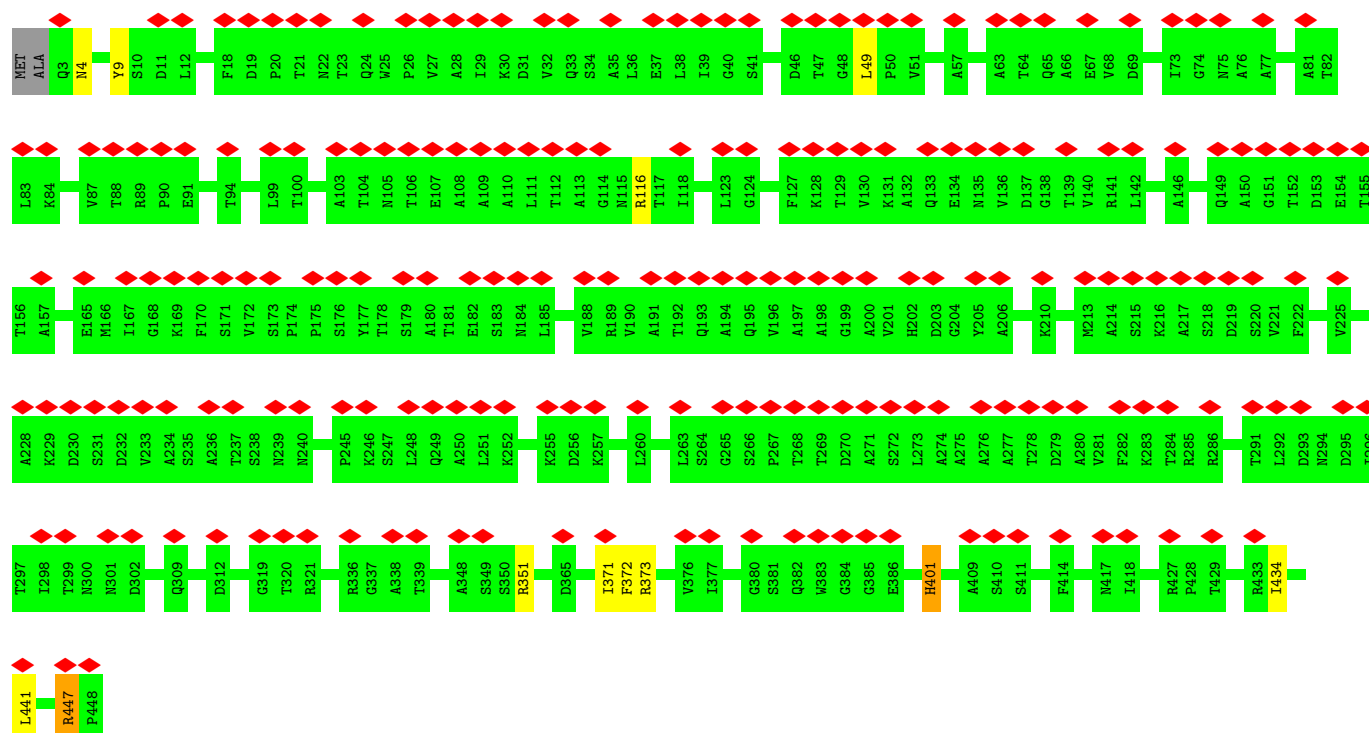


- Molecule 12: Gp12 short tail fibers

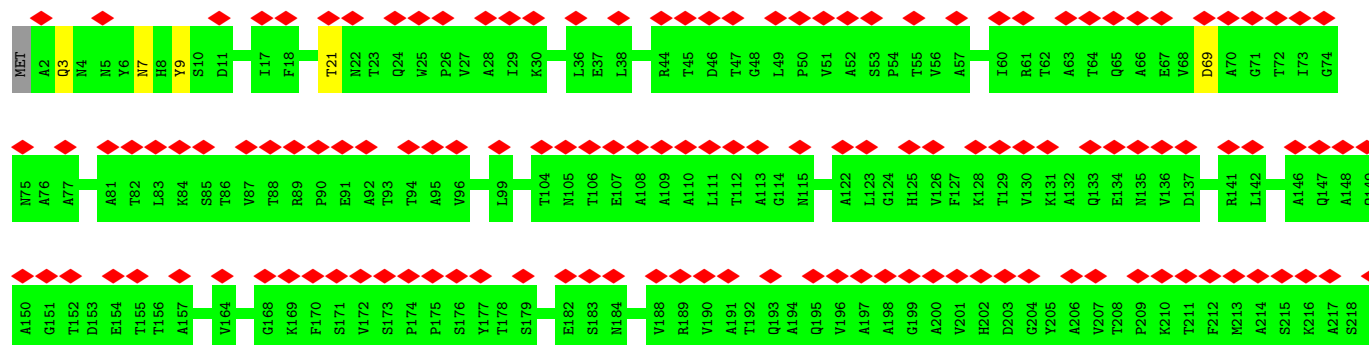




• Molecule 12: Gp12 short tail fibers

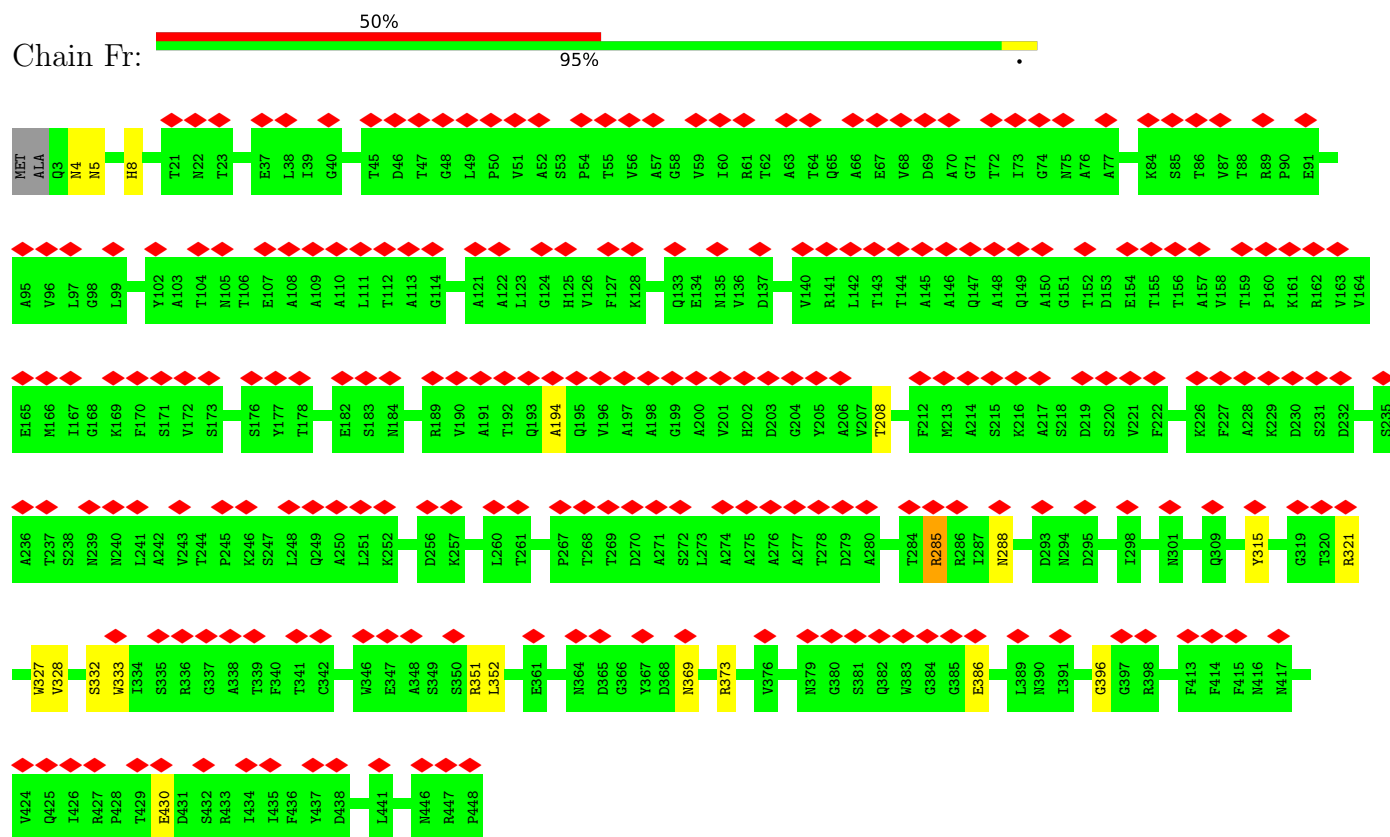


• Molecule 12: Gp12 short tail fibers

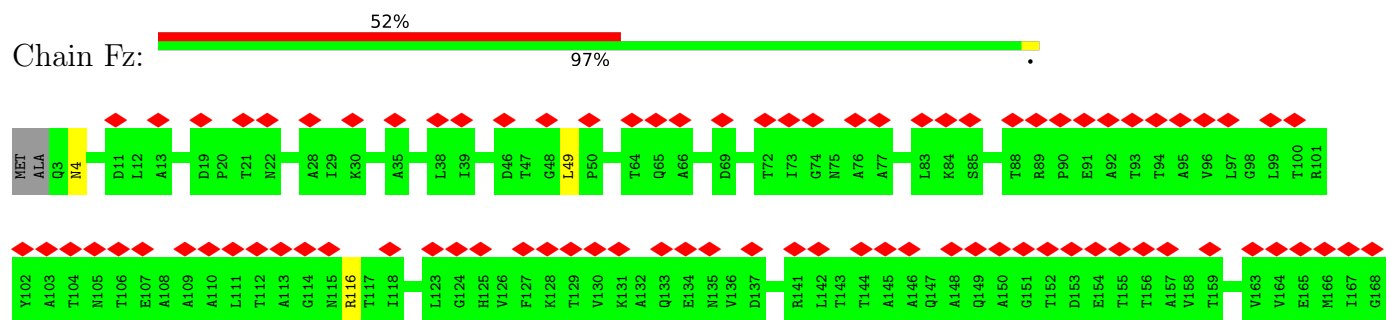


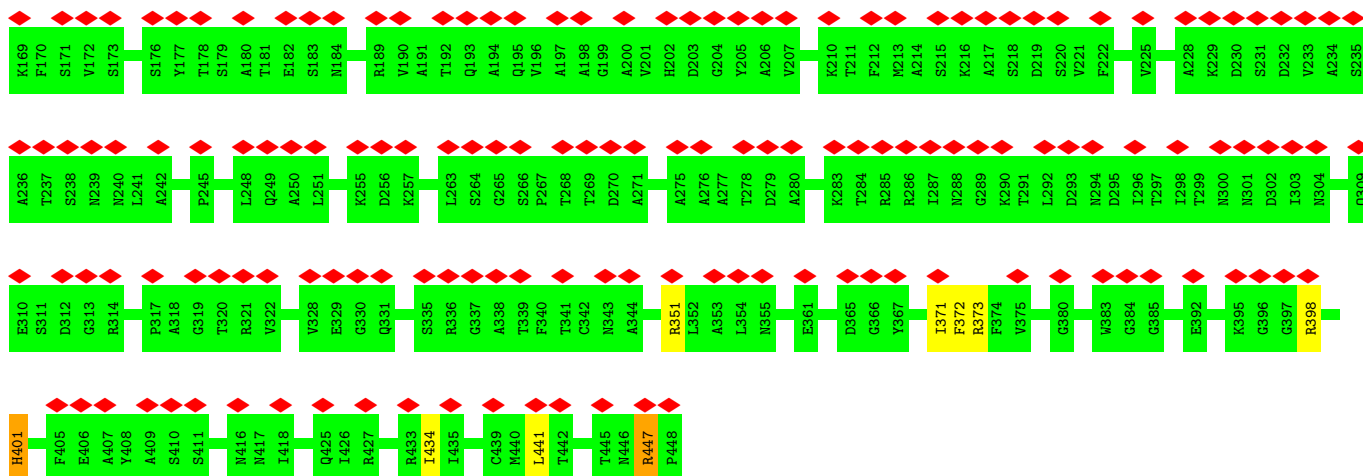


• Molecule 12: Gp12 short tail fibers

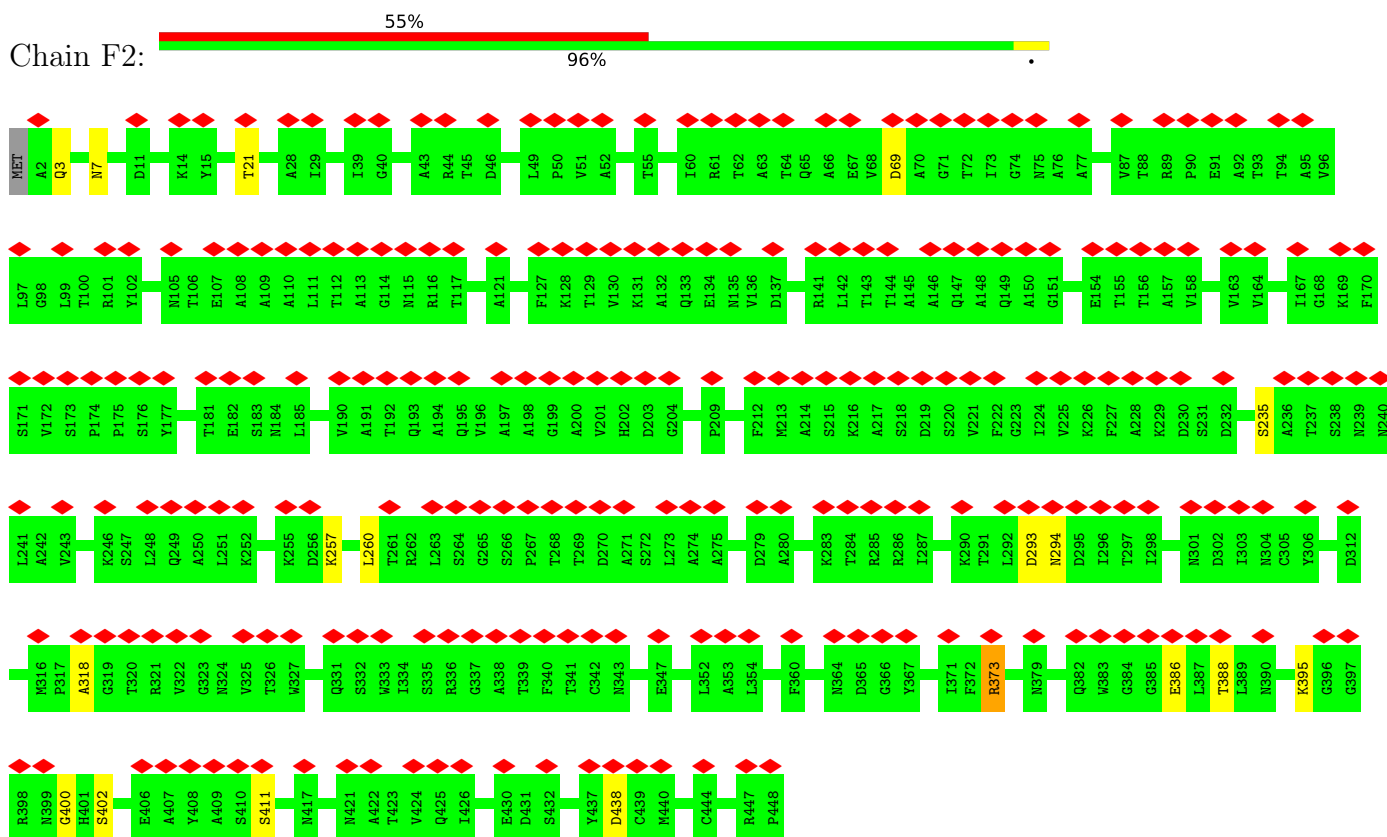


• Molecule 12: Gp12 short tail fibers

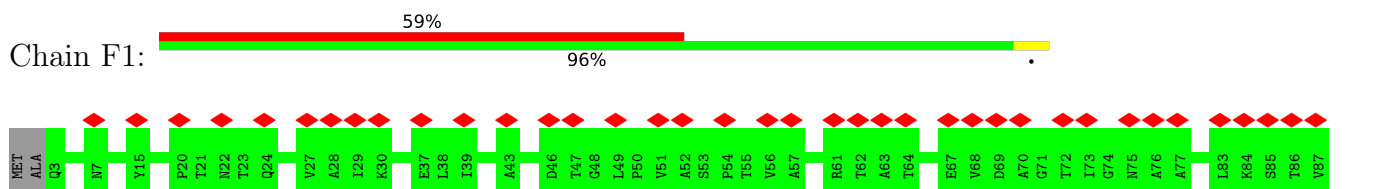


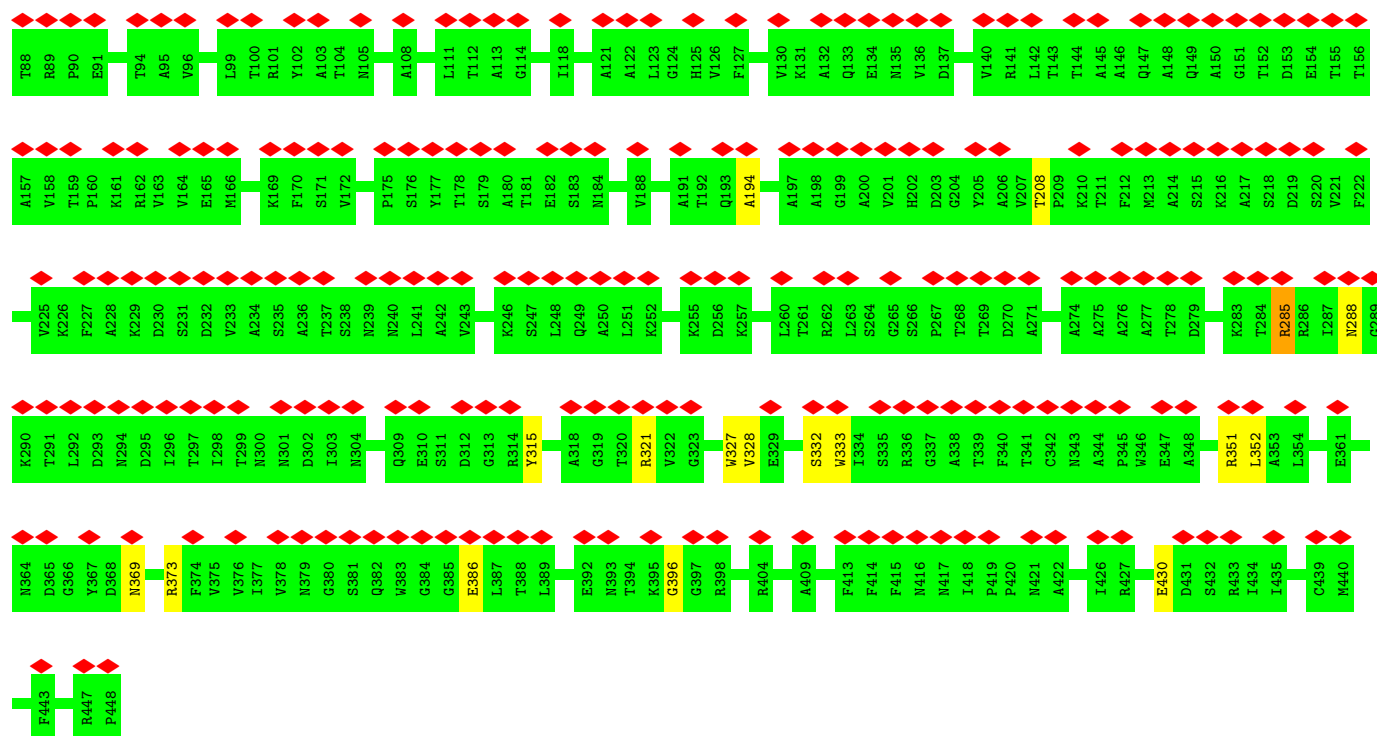


• Molecule 12: Gp12 short tail fibers



• Molecule 12: Gp12 short tail fibers

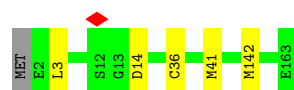




- Molecule 13: Tail tube protein



- Molecule 13: Tail tube protein



- Molecule 13: Tail tube protein

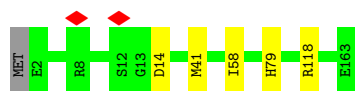


- Molecule 13: Tail tube protein

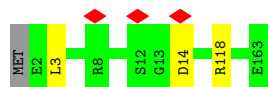




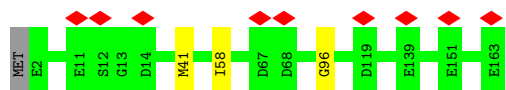
- Molecule 13: Tail tube protein



- Molecule 13: Tail tube protein



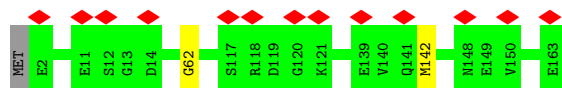
- Molecule 13: Tail tube protein



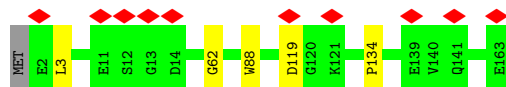
- Molecule 13: Tail tube protein



- Molecule 13: Tail tube protein

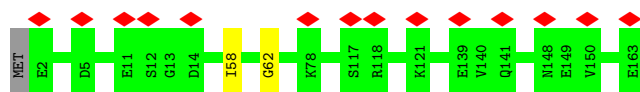


- Molecule 13: Tail tube protein

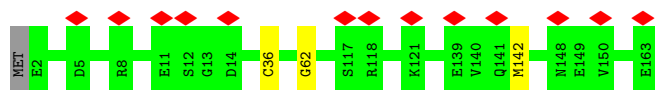


- Molecule 13: Tail tube protein





- Molecule 13: Tail tube protein



- Molecule 14: IraD/Gp25-like domain-containing protein



- Molecule 14: IraD/Gp25-like domain-containing protein



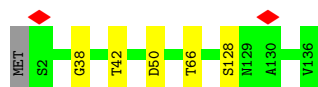
- Molecule 14: IraD/Gp25-like domain-containing protein



- Molecule 14: IraD/Gp25-like domain-containing protein

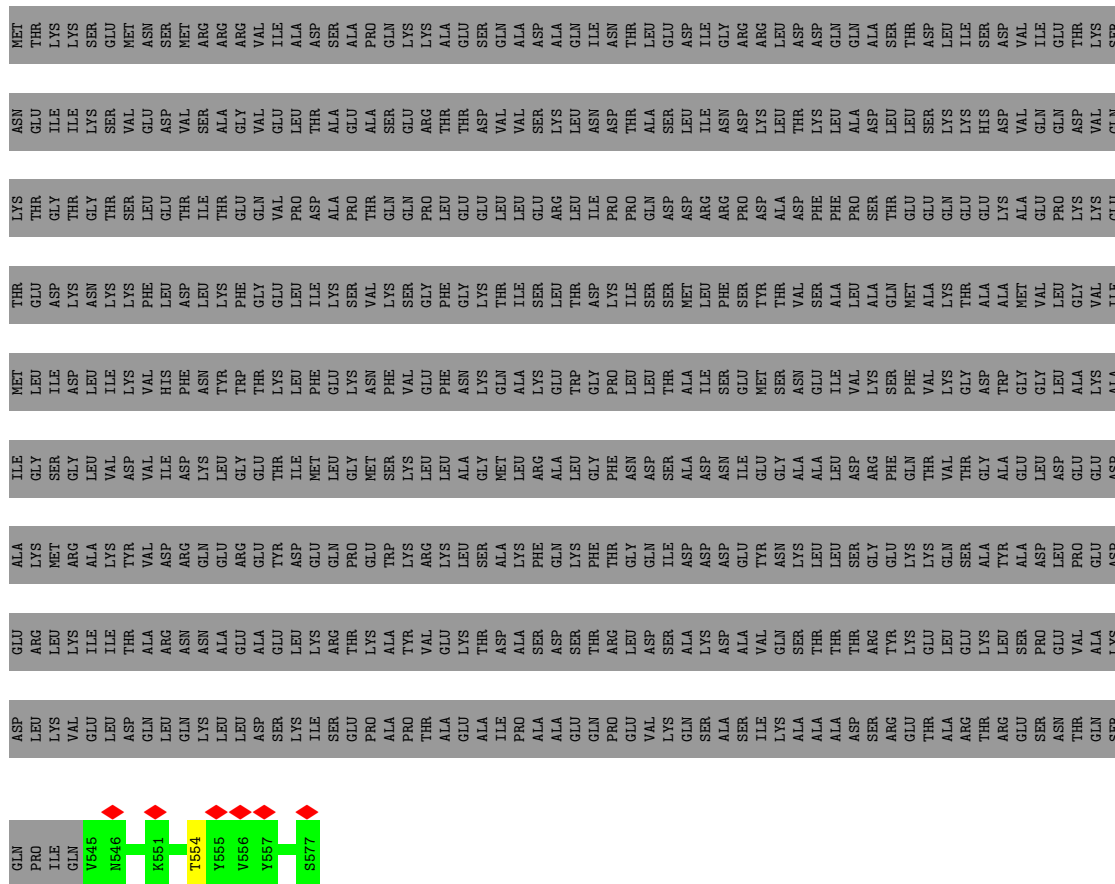


- Molecule 14: IraD/Gp25-like domain-containing protein

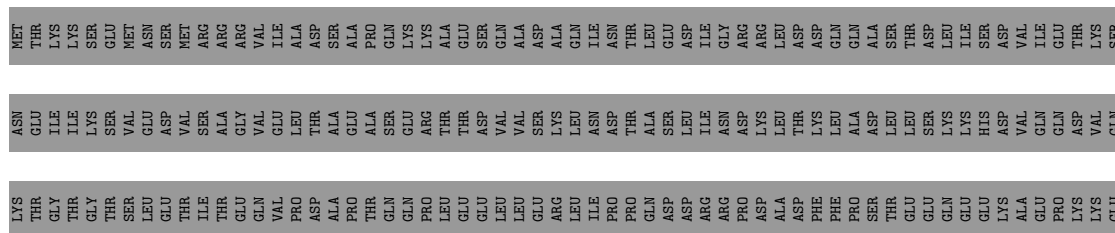




- Molecule 16: Baseplate hub subunit tail length determinator



- Molecule 16: Baseplate hub subunit tail length determinator





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	34528	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	83505	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.317	Depositor
Minimum map value	-1.951	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	691.416, 691.416, 691.416	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AM	0.56	0/5307	1.00	3/7218 (0.0%)
1	AN	0.57	0/5307	1.02	3/7218 (0.0%)
1	AO	0.56	0/5307	1.01	6/7218 (0.1%)
1	AP	0.57	0/5307	1.02	3/7218 (0.0%)
1	AQ	0.56	0/5307	1.02	4/7218 (0.1%)
1	AR	0.57	0/5307	1.01	3/7218 (0.0%)
1	AS	0.57	0/5260	1.03	4/7154 (0.1%)
1	AT	0.56	0/5239	1.03	5/7125 (0.1%)
1	AU	0.57	0/5260	1.03	5/7154 (0.1%)
1	AV	0.57	0/5239	1.04	8/7125 (0.1%)
1	AW	0.57	0/5260	1.02	3/7154 (0.0%)
1	AX	0.56	0/5239	1.04	5/7125 (0.1%)
2	BK	0.62	0/2370	1.15	3/3220 (0.1%)
2	BL	0.62	0/1828	1.07	1/2480 (0.0%)
2	BM	0.62	0/2370	1.15	5/3220 (0.2%)
2	BN	0.61	0/1828	1.07	1/2480 (0.0%)
2	BO	0.62	0/2370	1.14	6/3220 (0.2%)
2	BP	0.62	0/1828	1.08	3/2480 (0.1%)
3	BQ	0.56	0/1757	1.02	2/2383 (0.1%)
3	BR	0.57	0/1757	1.07	3/2383 (0.1%)
3	BS	0.56	0/1757	1.03	2/2383 (0.1%)
3	BT	0.57	0/1757	1.06	0/2383
3	BU	0.57	0/1757	1.04	2/2383 (0.1%)
3	BV	0.56	0/1757	1.04	2/2383 (0.1%)
4	AG	0.54	0/1794	0.99	2/2435 (0.1%)
4	AH	0.54	0/1794	0.99	1/2435 (0.0%)
4	AI	0.54	0/1794	1.00	0/2435
4	AJ	0.55	0/1794	0.97	0/2435
4	AK	0.54	0/1794	0.99	1/2435 (0.0%)
4	AL	0.54	0/1794	0.98	0/2435
5	BB	0.60	0/4441	1.08	5/6025 (0.1%)
5	BC	0.59	0/4441	1.07	7/6025 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	BD	0.59	0/4441	1.07	4/6025 (0.1%)
6	BA	0.75	0/721	1.15	1/982 (0.1%)
7	A0	0.65	0/8656	1.09	9/11738 (0.1%)
7	A1	0.65	0/8656	1.09	9/11738 (0.1%)
7	A2	0.65	0/8656	1.09	9/11738 (0.1%)
7	A3	0.65	0/8656	1.09	9/11738 (0.1%)
7	AY	0.65	0/8656	1.09	9/11738 (0.1%)
7	AZ	0.65	0/8656	1.09	9/11738 (0.1%)
8	A4	0.58	0/2743	1.06	3/3730 (0.1%)
8	A5	0.59	0/2743	1.06	4/3730 (0.1%)
8	A6	0.58	0/2743	1.06	5/3730 (0.1%)
8	A7	0.59	0/2743	1.05	4/3730 (0.1%)
8	A8	0.58	0/2743	1.05	4/3730 (0.1%)
8	A9	0.58	0/2743	1.03	1/3730 (0.0%)
8	Aa	0.67	0/2707	1.13	3/3682 (0.1%)
8	Ab	0.67	0/2707	1.13	3/3682 (0.1%)
8	Ac	0.67	0/2707	1.13	3/3682 (0.1%)
8	Ad	0.67	0/2707	1.13	3/3682 (0.1%)
8	Ae	0.67	0/2707	1.13	3/3682 (0.1%)
8	Af	0.67	0/2707	1.14	3/3682 (0.1%)
9	LA	0.73	0/2304	1.07	3/3114 (0.1%)
9	LB	0.72	0/2304	1.07	0/3114
9	LC	0.71	0/2304	1.03	0/3114
9	LD	0.73	0/2304	1.07	3/3114 (0.1%)
9	LE	0.72	0/2304	1.07	0/3114
9	LF	0.71	0/2304	1.03	0/3114
9	LG	0.73	0/2304	1.07	3/3114 (0.1%)
9	LH	0.72	0/2304	1.07	0/3114
9	LI	0.71	0/2304	1.03	0/3114
9	LJ	0.73	0/2304	1.07	3/3114 (0.1%)
9	LK	0.72	0/2304	1.07	0/3114
9	LL	0.71	0/2304	1.03	1/3114 (0.0%)
9	LM	0.73	0/2304	1.07	3/3114 (0.1%)
9	LN	0.72	0/2304	1.07	0/3114
9	LO	0.71	0/2304	1.03	0/3114
9	LP	0.73	0/2304	1.07	3/3114 (0.1%)
9	LQ	0.72	0/2304	1.07	0/3114
9	LR	0.71	0/2304	1.03	0/3114
10	FA	0.56	0/4789	0.99	3/6512 (0.0%)
10	FB	0.58	0/4789	0.98	6/6512 (0.1%)
10	FC	0.57	0/4789	0.99	2/6512 (0.0%)
10	FJ	0.56	0/4789	0.99	3/6512 (0.0%)
10	FK	0.58	0/4789	0.98	6/6512 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
10	FL	0.57	0/4789	0.99	2/6512 (0.0%)
10	FS	0.56	0/4789	0.99	3/6512 (0.0%)
10	FT	0.58	0/4789	0.98	6/6512 (0.1%)
10	FU	0.57	0/4789	0.99	2/6512 (0.0%)
10	Fb	0.56	0/4789	0.99	3/6512 (0.0%)
10	Fc	0.58	0/4789	0.98	6/6512 (0.1%)
10	Fd	0.57	0/4789	0.99	2/6512 (0.0%)
10	Fk	0.56	0/4789	0.99	3/6512 (0.0%)
10	Fl	0.58	0/4789	0.98	6/6512 (0.1%)
10	Fm	0.57	0/4789	0.99	2/6512 (0.0%)
10	Ft	0.56	0/4789	0.99	3/6512 (0.0%)
10	Fu	0.58	0/4789	0.98	6/6512 (0.1%)
10	Fv	0.57	0/4789	0.99	2/6512 (0.0%)
11	FD	0.62	0/1761	0.98	1/2397 (0.0%)
11	FE	0.60	0/1761	1.00	1/2397 (0.0%)
11	FF	0.61	0/1761	1.00	2/2397 (0.1%)
11	FM	0.62	0/1761	0.98	1/2397 (0.0%)
11	FN	0.60	0/1761	1.00	1/2397 (0.0%)
11	FO	0.61	0/1761	1.00	2/2397 (0.1%)
11	FV	0.62	0/1761	0.98	1/2397 (0.0%)
11	FW	0.60	0/1761	1.00	1/2397 (0.0%)
11	FX	0.61	0/1761	1.00	2/2397 (0.1%)
11	Fe	0.62	0/1761	0.98	1/2397 (0.0%)
11	Ff	0.60	0/1761	1.00	1/2397 (0.0%)
11	Fg	0.61	0/1761	1.00	2/2397 (0.1%)
11	Fn	0.62	0/1761	0.98	1/2397 (0.0%)
11	Fo	0.60	0/1761	1.00	1/2397 (0.0%)
11	Fp	0.61	0/1761	1.00	2/2397 (0.1%)
11	Fw	0.62	0/1761	0.98	1/2397 (0.0%)
11	Fx	0.60	0/1761	1.00	1/2397 (0.0%)
11	Fy	0.61	0/1761	1.00	2/2397 (0.1%)
12	F1	0.62	0/3426	1.04	0/4675
12	F2	0.61	0/3440	1.06	4/4694 (0.1%)
12	FG	0.61	0/3435	1.05	1/4687 (0.0%)
12	FH	0.62	0/3426	1.04	0/4675
12	FI	0.61	0/3440	1.06	4/4694 (0.1%)
12	FP	0.61	0/3435	1.05	1/4687 (0.0%)
12	FQ	0.62	0/3426	1.04	0/4675
12	FR	0.61	0/3440	1.06	4/4694 (0.1%)
12	FY	0.61	0/3435	1.05	1/4687 (0.0%)
12	FZ	0.62	0/3426	1.04	0/4675
12	Fa	0.61	0/3440	1.06	4/4694 (0.1%)
12	Fh	0.61	0/3435	1.05	1/4687 (0.0%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
12	Fi	0.62	0/3426	1.04	0/4675
12	Fj	0.61	0/3440	1.06	4/4694 (0.1%)
12	Fq	0.61	0/3435	1.05	1/4687 (0.0%)
12	Fr	0.62	0/3426	1.04	0/4675
12	Fs	0.61	0/3440	1.06	4/4694 (0.1%)
12	Fz	0.61	0/3435	1.05	1/4687 (0.0%)
13	B1	0.55	0/1339	0.99	1/1821 (0.1%)
13	B2	0.55	0/1339	0.99	1/1821 (0.1%)
13	B3	0.60	0/1339	1.03	0/1821
13	B4	0.60	0/1339	1.04	1/1821 (0.1%)
13	B5	0.59	0/1339	1.05	0/1821
13	B6	0.60	0/1339	1.05	1/1821 (0.1%)
13	B7	0.59	0/1339	1.03	0/1821
13	B8	0.60	0/1339	1.07	2/1821 (0.1%)
13	BW	0.55	0/1339	0.98	1/1821 (0.1%)
13	BX	0.56	0/1339	1.00	3/1821 (0.2%)
13	BY	0.55	0/1339	0.99	1/1821 (0.1%)
13	BZ	0.55	0/1339	1.02	3/1821 (0.2%)
14	AA	0.56	0/1084	1.10	1/1470 (0.1%)
14	AB	0.56	0/1084	1.11	1/1470 (0.1%)
14	AC	0.57	0/1084	1.11	1/1470 (0.1%)
14	AD	0.56	0/1084	1.14	0/1470
14	AE	0.56	0/1084	1.11	2/1470 (0.1%)
14	AF	0.57	0/1084	1.12	1/1470 (0.1%)
15	BE	0.58	0/3125	1.05	2/4232 (0.0%)
15	BF	0.58	0/3125	1.04	1/4232 (0.0%)
15	BG	0.58	0/3125	1.06	3/4232 (0.1%)
16	BH	0.66	0/246	1.14	0/334
16	BI	0.66	0/246	1.12	0/334
16	BJ	0.63	0/246	1.10	0/334
All	All	0.61	0/449782	1.04	361/611230 (0.1%)

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
2	BM	0	1
7	A0	0	2
7	A1	0	2
7	A2	0	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
7	A3	0	2
7	AY	0	2
7	AZ	0	3
8	A6	0	1
10	FA	0	2
10	FC	0	1
10	FJ	0	2
10	FL	0	1
10	FS	0	2
10	FU	0	1
10	Fb	0	2
10	Fd	0	1
10	Fk	0	2
10	Fm	0	1
10	Ft	0	2
10	Fv	0	1
11	FF	0	1
11	FO	0	1
11	FX	0	1
11	Fg	0	1
11	Fp	0	1
11	Fy	0	1
12	F1	0	1
12	FH	0	1
12	FQ	0	1
12	FZ	0	1
12	Fi	0	1
12	Fr	0	1
15	BE	0	1
15	BF	0	1
15	BG	0	1
All	All	0	49

There are no bond length outliers.

The worst 5 of 361 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BM	200	ARG	NE-CZ-NH1	-8.21	113.29	121.50
15	BG	326	ASP	CA-CB-CG	7.91	120.51	112.60
2	BK	200	ARG	NE-CZ-NH1	-7.66	113.84	121.50
2	BO	200	ARG	NE-CZ-NH1	-7.59	113.91	121.50
10	Fu	357	GLN	CB-CG-CD	7.27	124.97	112.60

There are no chirality outliers.

5 of 49 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A2	427	ARG	Sidechain
7	A2	447	ALA	Peptide
7	AY	427	ARG	Sidechain
7	AY	447	ALA	Peptide
2	BM	264	SER	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	AM	5191	0	5061	12	0
1	AN	5191	0	5061	22	0
1	AO	5191	0	5061	14	0
1	AP	5191	0	5061	17	0
1	AQ	5191	0	5061	14	0
1	AR	5191	0	5061	21	0
1	AS	5145	0	5008	12	0
1	AT	5125	0	4993	10	0
1	AU	5145	0	5008	4	0
1	AV	5125	0	4993	14	0
1	AW	5145	0	5008	11	0
1	AX	5125	0	4993	13	0
2	BK	2323	0	2255	6	0
2	BL	1790	0	1747	3	0
2	BM	2323	0	2255	5	0
2	BN	1790	0	1747	4	0
2	BO	2323	0	2255	5	0
2	BP	1790	0	1747	2	0
3	BQ	1719	0	1662	8	0
3	BR	1719	0	1662	8	0
3	BS	1719	0	1662	3	0
3	BT	1719	0	1662	8	0
3	BU	1719	0	1662	5	0
3	BV	1719	0	1662	4	0
4	AG	1747	0	1652	12	0
4	AH	1747	0	1652	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AI	1747	0	1652	14	0
4	AJ	1747	0	1652	15	0
4	AK	1747	0	1652	14	0
4	AL	1747	0	1652	11	0
5	BB	4354	0	4218	6	0
5	BC	4354	0	4218	3	0
5	BD	4354	0	4218	3	0
6	BA	706	0	700	0	0
7	A0	8438	0	8098	119	0
7	A1	8438	0	8098	108	0
7	A2	8438	0	8098	109	0
7	A3	8438	0	8098	111	0
7	AY	8438	0	8098	117	0
7	AZ	8438	0	8098	105	0
8	A4	2669	0	2557	44	0
8	A5	2669	0	2557	45	0
8	A6	2669	0	2557	36	0
8	A7	2669	0	2557	38	0
8	A8	2669	0	2557	37	0
8	A9	2669	0	2557	40	0
8	Aa	2633	0	2518	26	0
8	Ab	2633	0	2518	30	0
8	Ac	2633	0	2518	30	0
8	Ad	2633	0	2518	27	0
8	Ae	2633	0	2518	31	0
8	Af	2633	0	2518	40	0
9	LA	2270	0	2236	2	0
9	LB	2270	0	2236	2	0
9	LC	2270	0	2236	2	0
9	LD	2270	0	2236	3	0
9	LE	2270	0	2236	2	0
9	LF	2270	0	2236	2	0
9	LG	2270	0	2236	3	0
9	LH	2270	0	2236	2	0
9	LI	2270	0	2236	2	0
9	LJ	2270	0	2236	3	0
9	LK	2270	0	2236	2	0
9	LL	2270	0	2236	2	0
9	LM	2270	0	2236	7	0
9	LN	2270	0	2236	4	0
9	LO	2270	0	2236	4	0
9	LP	2270	0	2236	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	LQ	2270	0	2236	2	0
9	LR	2270	0	2236	2	0
10	FA	4696	0	4547	29	0
10	FB	4696	0	4548	16	0
10	FC	4696	0	4547	19	0
10	FJ	4696	0	4548	32	0
10	FK	4696	0	4548	15	0
10	FL	4696	0	4547	21	0
10	FS	4696	0	4547	35	0
10	FT	4696	0	4548	14	0
10	FU	4696	0	4547	17	0
10	Fb	4696	0	4548	33	0
10	Fc	4696	0	4548	15	0
10	Fd	4696	0	4547	27	0
10	Fk	4696	0	4548	37	0
10	Fl	4696	0	4548	15	0
10	Fm	4696	0	4547	15	0
10	Ft	4696	0	4548	34	0
10	Fu	4696	0	4548	14	0
10	Fv	4696	0	4547	25	0
11	FD	1722	0	1676	1	0
11	FE	1722	0	1676	0	0
11	FF	1722	0	1676	2	0
11	FM	1722	0	1676	1	0
11	FN	1722	0	1676	0	0
11	FO	1722	0	1676	2	0
11	FV	1722	0	1676	1	0
11	FW	1722	0	1676	0	0
11	FX	1722	0	1676	2	0
11	Fe	1722	0	1676	1	0
11	Ff	1722	0	1676	0	0
11	Fg	1722	0	1676	2	0
11	Fn	1722	0	1676	1	0
11	Fo	1722	0	1676	0	0
11	Fp	1722	0	1676	2	0
11	Fw	1722	0	1676	1	0
11	Fx	1722	0	1676	0	0
11	Fy	1722	0	1676	2	0
12	F1	3362	0	3297	15	0
12	F2	3376	0	3317	10	0
12	FG	3371	0	3312	11	0
12	FH	3362	0	3297	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	FI	3376	0	3317	16	0
12	FP	3371	0	3312	10	0
12	FQ	3362	0	3297	14	0
12	FR	3376	0	3317	11	0
12	FY	3371	0	3312	11	0
12	FZ	3362	0	3297	17	0
12	Fa	3376	0	3317	13	0
12	Fh	3371	0	3312	9	0
12	Fi	3362	0	3297	14	0
12	Fj	3376	0	3317	10	0
12	Fq	3371	0	3312	10	0
12	Fr	3362	0	3297	20	0
12	Fs	3376	0	3317	16	0
12	Fz	3371	0	3312	10	0
13	B1	1305	0	1235	4	0
13	B2	1305	0	1235	2	0
13	B3	1305	0	1235	3	0
13	B4	1305	0	1235	3	0
13	B5	1305	0	1235	2	0
13	B6	1305	0	1235	3	0
13	B7	1305	0	1235	2	0
13	B8	1305	0	1235	2	0
13	BW	1305	0	1235	3	0
13	BX	1305	0	1235	3	0
13	BY	1305	0	1235	5	0
13	BZ	1305	0	1235	6	0
14	AA	1069	0	1069	2	0
14	AB	1069	0	1069	2	0
14	AC	1069	0	1069	7	0
14	AD	1069	0	1069	5	0
14	AE	1069	0	1069	2	0
14	AF	1069	0	1069	4	0
15	BE	3055	0	2962	10	0
15	BF	3055	0	2962	8	0
15	BG	3055	0	2962	7	0
16	BH	242	0	239	0	0
16	BI	242	0	239	0	0
16	BJ	242	0	239	0	0
17	BB	1	0	0	0	0
18	FA	1	0	0	0	0
18	FJ	1	0	0	0	0
18	FS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Fb	1	0	0	0	0
18	Fk	1	0	0	0	0
18	Ft	1	0	0	0	0
19	FB	1	0	0	0	0
19	FG	1	0	0	0	0
19	FK	1	0	0	0	0
19	FT	1	0	0	0	0
19	Fc	1	0	0	0	0
19	Fl	1	0	0	0	0
All	All	440315	0	427316	1308	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 2.

The worst 5 of 1308 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:906:MET:HE1	8:A9:27:LYS:CD	1.54	1.37
7:AZ:469:SER:OG	8:Af:62:GLY:HA3	1.14	1.28
7:AY:483:ASP:OD1	8:Ac:72:GLU:HG2	1.30	1.27
7:A2:906:MET:HE1	8:A5:27:LYS:CD	1.63	1.26
7:A2:1028:VAL:CG2	8:A5:14:ILE:HG22	1.67	1.24

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	AM	652/655 (100%)	624 (96%)	28 (4%)	0	100	100
1	AN	652/655 (100%)	622 (95%)	30 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AO	652/655 (100%)	630 (97%)	22 (3%)	0	100	100
1	AP	652/655 (100%)	625 (96%)	27 (4%)	0	100	100
1	AQ	652/655 (100%)	630 (97%)	21 (3%)	1 (0%)	44	71
1	AR	652/655 (100%)	624 (96%)	28 (4%)	0	100	100
1	AS	646/655 (99%)	610 (94%)	36 (6%)	0	100	100
1	AT	644/655 (98%)	623 (97%)	21 (3%)	0	100	100
1	AU	646/655 (99%)	616 (95%)	30 (5%)	0	100	100
1	AV	644/655 (98%)	616 (96%)	28 (4%)	0	100	100
1	AW	646/655 (99%)	616 (95%)	30 (5%)	0	100	100
1	AX	644/655 (98%)	614 (95%)	30 (5%)	0	100	100
2	BK	297/350 (85%)	273 (92%)	24 (8%)	0	100	100
2	BL	217/350 (62%)	200 (92%)	16 (7%)	1 (0%)	25	53
2	BM	297/350 (85%)	276 (93%)	21 (7%)	0	100	100
2	BN	217/350 (62%)	200 (92%)	16 (7%)	1 (0%)	25	53
2	BO	297/350 (85%)	275 (93%)	22 (7%)	0	100	100
2	BP	217/350 (62%)	198 (91%)	18 (8%)	1 (0%)	25	53
3	BQ	216/308 (70%)	208 (96%)	8 (4%)	0	100	100
3	BR	216/308 (70%)	207 (96%)	8 (4%)	1 (0%)	25	53
3	BS	216/308 (70%)	206 (95%)	10 (5%)	0	100	100
3	BT	216/308 (70%)	211 (98%)	4 (2%)	1 (0%)	25	53
3	BU	216/308 (70%)	207 (96%)	8 (4%)	1 (0%)	25	53
3	BV	216/308 (70%)	210 (97%)	6 (3%)	0	100	100
4	AG	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
4	AH	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
4	AI	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
4	AJ	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
4	AK	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
4	AL	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
5	BB	560/576 (97%)	533 (95%)	27 (5%)	0	100	100
5	BC	560/576 (97%)	533 (95%)	27 (5%)	0	100	100
5	BD	560/576 (97%)	529 (94%)	31 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BA	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
7	A0	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
7	A1	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
7	A2	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
7	A3	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
7	AY	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
7	AZ	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
8	A4	332/341 (97%)	308 (93%)	24 (7%)	0	100	100
8	A5	332/341 (97%)	308 (93%)	24 (7%)	0	100	100
8	A6	332/341 (97%)	310 (93%)	22 (7%)	0	100	100
8	A7	332/341 (97%)	318 (96%)	14 (4%)	0	100	100
8	A8	332/341 (97%)	311 (94%)	21 (6%)	0	100	100
8	A9	332/341 (97%)	313 (94%)	19 (6%)	0	100	100
8	Aa	327/341 (96%)	306 (94%)	21 (6%)	0	100	100
8	Ab	327/341 (96%)	306 (94%)	21 (6%)	0	100	100
8	Ac	327/341 (96%)	306 (94%)	21 (6%)	0	100	100
8	Ad	327/341 (96%)	306 (94%)	21 (6%)	0	100	100
8	Ae	327/341 (96%)	306 (94%)	21 (6%)	0	100	100
8	Af	327/341 (96%)	307 (94%)	20 (6%)	0	100	100
9	LA	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LB	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LC	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
9	LD	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LE	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LF	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
9	LG	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LH	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LI	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
9	LJ	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LK	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LL	301/303 (99%)	290 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	LM	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LN	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LO	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
9	LP	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LQ	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LR	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
10	FA	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	FB	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	FC	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
10	FJ	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	FK	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	FL	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
10	FS	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	FT	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	FU	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
10	Fb	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	Fc	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	Fd	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
10	Fk	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	Fl	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	Fm	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
10	Ft	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	Fu	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	Fv	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
11	FD	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	FE	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	FF	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	FM	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	FN	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	FO	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	FV	220/223 (99%)	211 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	FW	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	FX	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	Fe	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	Ff	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	Fg	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	Fn	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	Fo	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	Fp	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	Fw	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	Fx	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	Fy	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
12	F1	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	F2	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	FG	444/448 (99%)	430 (97%)	14 (3%)	0	100	100
12	FH	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	FI	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	FP	444/448 (99%)	430 (97%)	14 (3%)	0	100	100
12	FQ	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	FR	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	FY	444/448 (99%)	430 (97%)	14 (3%)	0	100	100
12	FZ	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	Fa	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	Fh	444/448 (99%)	430 (97%)	14 (3%)	0	100	100
12	Fi	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	Fj	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	Fq	444/448 (99%)	430 (97%)	14 (3%)	0	100	100
12	Fr	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	Fs	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	Fz	444/448 (99%)	429 (97%)	15 (3%)	0	100	100
13	B1	160/163 (98%)	154 (96%)	6 (4%)	0	100	100
13	B2	160/163 (98%)	154 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	B3	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
13	B4	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
13	B5	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
13	B6	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
13	B7	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
13	B8	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
13	BW	160/163 (98%)	154 (96%)	6 (4%)	0	100	100
13	BX	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
13	BY	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
13	BZ	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
14	AA	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
14	AB	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
14	AC	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
14	AD	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
14	AE	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
14	AF	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
15	BE	377/380 (99%)	363 (96%)	14 (4%)	0	100	100
15	BF	377/380 (99%)	360 (96%)	17 (4%)	0	100	100
15	BG	377/380 (99%)	362 (96%)	15 (4%)	0	100	100
16	BH	31/577 (5%)	27 (87%)	4 (13%)	0	100	100
16	BI	31/577 (5%)	30 (97%)	1 (3%)	0	100	100
16	BJ	31/577 (5%)	27 (87%)	4 (13%)	0	100	100
All	All	55991/59290 (94%)	53339 (95%)	2645 (5%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BN	297	GLY
2	BL	297	GLY
2	BP	297	GLY
3	BR	145	ALA
3	BT	145	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AM	570/571 (100%)	562 (99%)	8 (1%)	62	78
1	AN	570/571 (100%)	563 (99%)	7 (1%)	67	80
1	AO	570/571 (100%)	563 (99%)	7 (1%)	67	80
1	AP	570/571 (100%)	561 (98%)	9 (2%)	58	75
1	AQ	570/571 (100%)	561 (98%)	9 (2%)	58	75
1	AR	570/571 (100%)	563 (99%)	7 (1%)	67	80
1	AS	565/571 (99%)	561 (99%)	4 (1%)	81	89
1	AT	563/571 (99%)	558 (99%)	5 (1%)	75	87
1	AU	565/571 (99%)	560 (99%)	5 (1%)	75	87
1	AV	563/571 (99%)	555 (99%)	8 (1%)	62	78
1	AW	565/571 (99%)	562 (100%)	3 (0%)	86	92
1	AX	563/571 (99%)	554 (98%)	9 (2%)	58	75
2	BK	257/297 (86%)	253 (98%)	4 (2%)	58	75
2	BL	199/297 (67%)	198 (100%)	1 (0%)	86	92
2	BM	257/297 (86%)	250 (97%)	7 (3%)	40	64
2	BN	199/297 (67%)	197 (99%)	2 (1%)	73	84
2	BO	257/297 (86%)	253 (98%)	4 (2%)	58	75
2	BP	199/297 (67%)	196 (98%)	3 (2%)	60	76
3	BQ	187/256 (73%)	184 (98%)	3 (2%)	58	75
3	BR	187/256 (73%)	187 (100%)	0	100	100
3	BS	187/256 (73%)	184 (98%)	3 (2%)	58	75
3	BT	187/256 (73%)	187 (100%)	0	100	100
3	BU	187/256 (73%)	183 (98%)	4 (2%)	48	69
3	BV	187/256 (73%)	185 (99%)	2 (1%)	70	82
4	AG	184/184 (100%)	184 (100%)	0	100	100
4	AH	184/184 (100%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AI	184/184 (100%)	183 (100%)	1 (0%)	86	92
4	AJ	184/184 (100%)	184 (100%)	0	100	100
4	AK	184/184 (100%)	182 (99%)	2 (1%)	70	82
4	AL	184/184 (100%)	184 (100%)	0	100	100
5	BB	474/484 (98%)	467 (98%)	7 (2%)	60	76
5	BC	474/484 (98%)	467 (98%)	7 (2%)	60	76
5	BD	474/484 (98%)	468 (99%)	6 (1%)	65	79
6	BA	80/80 (100%)	80 (100%)	0	100	100
7	A0	923/924 (100%)	916 (99%)	7 (1%)	79	88
7	A1	923/924 (100%)	916 (99%)	7 (1%)	79	88
7	A2	923/924 (100%)	915 (99%)	8 (1%)	75	87
7	A3	923/924 (100%)	916 (99%)	7 (1%)	79	88
7	AY	923/924 (100%)	915 (99%)	8 (1%)	75	87
7	AZ	923/924 (100%)	915 (99%)	8 (1%)	75	87
8	A4	293/299 (98%)	292 (100%)	1 (0%)	91	95
8	A5	293/299 (98%)	288 (98%)	5 (2%)	56	74
8	A6	293/299 (98%)	290 (99%)	3 (1%)	73	84
8	A7	293/299 (98%)	288 (98%)	5 (2%)	56	74
8	A8	293/299 (98%)	287 (98%)	6 (2%)	50	71
8	A9	293/299 (98%)	289 (99%)	4 (1%)	62	78
8	Aa	288/299 (96%)	283 (98%)	5 (2%)	56	74
8	Ab	288/299 (96%)	283 (98%)	5 (2%)	56	74
8	Ac	288/299 (96%)	283 (98%)	5 (2%)	56	74
8	Ad	288/299 (96%)	283 (98%)	5 (2%)	56	74
8	Ae	288/299 (96%)	283 (98%)	5 (2%)	56	74
8	Af	288/299 (96%)	283 (98%)	5 (2%)	56	74
9	LA	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LB	245/245 (100%)	245 (100%)	0	100	100
9	LC	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LD	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LE	245/245 (100%)	245 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	LF	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LG	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LH	245/245 (100%)	245 (100%)	0	100	100
9	LI	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LJ	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LK	245/245 (100%)	245 (100%)	0	100	100
9	LL	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LM	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LN	245/245 (100%)	245 (100%)	0	100	100
9	LO	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LP	245/245 (100%)	244 (100%)	1 (0%)	89	94
9	LQ	245/245 (100%)	245 (100%)	0	100	100
9	LR	245/245 (100%)	244 (100%)	1 (0%)	89	94
10	FA	509/509 (100%)	503 (99%)	6 (1%)	67	80
10	FB	509/509 (100%)	505 (99%)	4 (1%)	79	88
10	FC	509/509 (100%)	507 (100%)	2 (0%)	89	94
10	FJ	509/509 (100%)	503 (99%)	6 (1%)	67	80
10	FK	509/509 (100%)	504 (99%)	5 (1%)	73	84
10	FL	509/509 (100%)	506 (99%)	3 (1%)	84	91
10	FS	509/509 (100%)	503 (99%)	6 (1%)	67	80
10	FT	509/509 (100%)	504 (99%)	5 (1%)	73	84
10	FU	509/509 (100%)	507 (100%)	2 (0%)	89	94
10	Fb	509/509 (100%)	503 (99%)	6 (1%)	67	80
10	Fc	509/509 (100%)	504 (99%)	5 (1%)	73	84
10	Fd	509/509 (100%)	506 (99%)	3 (1%)	84	91
10	Fk	509/509 (100%)	503 (99%)	6 (1%)	67	80
10	Fl	509/509 (100%)	504 (99%)	5 (1%)	73	84
10	Fm	509/509 (100%)	507 (100%)	2 (0%)	89	94
10	Ft	509/509 (100%)	503 (99%)	6 (1%)	67	80
10	Fu	509/509 (100%)	505 (99%)	4 (1%)	79	88
10	Fv	509/509 (100%)	506 (99%)	3 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	FD	183/184 (100%)	181 (99%)	2 (1%)	70	82
11	FE	183/184 (100%)	182 (100%)	1 (0%)	86	92
11	FF	183/184 (100%)	180 (98%)	3 (2%)	58	75
11	FM	183/184 (100%)	181 (99%)	2 (1%)	70	82
11	FN	183/184 (100%)	182 (100%)	1 (0%)	86	92
11	FO	183/184 (100%)	180 (98%)	3 (2%)	58	75
11	FV	183/184 (100%)	181 (99%)	2 (1%)	70	82
11	FW	183/184 (100%)	182 (100%)	1 (0%)	86	92
11	FX	183/184 (100%)	180 (98%)	3 (2%)	58	75
11	Fe	183/184 (100%)	181 (99%)	2 (1%)	70	82
11	Ff	183/184 (100%)	182 (100%)	1 (0%)	86	92
11	Fg	183/184 (100%)	180 (98%)	3 (2%)	58	75
11	Fn	183/184 (100%)	181 (99%)	2 (1%)	70	82
11	Fo	183/184 (100%)	182 (100%)	1 (0%)	86	92
11	Fp	183/184 (100%)	180 (98%)	3 (2%)	58	75
11	Fw	183/184 (100%)	181 (99%)	2 (1%)	70	82
11	Fx	183/184 (100%)	182 (100%)	1 (0%)	86	92
11	Fy	183/184 (100%)	180 (98%)	3 (2%)	58	75
12	F1	357/361 (99%)	352 (99%)	5 (1%)	62	78
12	F2	360/361 (100%)	354 (98%)	6 (2%)	56	74
12	FG	360/361 (100%)	357 (99%)	3 (1%)	79	88
12	FH	357/361 (99%)	352 (99%)	5 (1%)	62	78
12	FI	360/361 (100%)	354 (98%)	6 (2%)	56	74
12	FP	360/361 (100%)	357 (99%)	3 (1%)	79	88
12	FQ	357/361 (99%)	352 (99%)	5 (1%)	62	78
12	FR	360/361 (100%)	354 (98%)	6 (2%)	56	74
12	FY	360/361 (100%)	357 (99%)	3 (1%)	79	88
12	FZ	357/361 (99%)	352 (99%)	5 (1%)	62	78
12	Fa	360/361 (100%)	354 (98%)	6 (2%)	56	74
12	Fh	360/361 (100%)	357 (99%)	3 (1%)	79	88
12	Fi	357/361 (99%)	352 (99%)	5 (1%)	62	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Fj	360/361 (100%)	354 (98%)	6 (2%)	56	74
12	Fq	360/361 (100%)	357 (99%)	3 (1%)	79	88
12	Fr	357/361 (99%)	352 (99%)	5 (1%)	62	78
12	Fs	360/361 (100%)	354 (98%)	6 (2%)	56	74
12	Fz	360/361 (100%)	357 (99%)	3 (1%)	79	88
13	B1	138/139 (99%)	138 (100%)	0	100	100
13	B2	138/139 (99%)	138 (100%)	0	100	100
13	B3	138/139 (99%)	138 (100%)	0	100	100
13	B4	138/139 (99%)	138 (100%)	0	100	100
13	B5	138/139 (99%)	138 (100%)	0	100	100
13	B6	138/139 (99%)	138 (100%)	0	100	100
13	B7	138/139 (99%)	138 (100%)	0	100	100
13	B8	138/139 (99%)	138 (100%)	0	100	100
13	BW	138/139 (99%)	138 (100%)	0	100	100
13	BX	138/139 (99%)	138 (100%)	0	100	100
13	BY	138/139 (99%)	138 (100%)	0	100	100
13	BZ	138/139 (99%)	138 (100%)	0	100	100
14	AA	125/126 (99%)	124 (99%)	1 (1%)	79	88
14	AB	125/126 (99%)	123 (98%)	2 (2%)	58	75
14	AC	125/126 (99%)	124 (99%)	1 (1%)	79	88
14	AD	125/126 (99%)	124 (99%)	1 (1%)	79	88
14	AE	125/126 (99%)	124 (99%)	1 (1%)	79	88
14	AF	125/126 (99%)	124 (99%)	1 (1%)	79	88
15	BE	333/334 (100%)	328 (98%)	5 (2%)	60	76
15	BF	333/334 (100%)	328 (98%)	5 (2%)	60	76
15	BG	333/334 (100%)	329 (99%)	4 (1%)	67	80
16	BH	27/497 (5%)	26 (96%)	1 (4%)	29	55
16	BI	27/497 (5%)	26 (96%)	1 (4%)	29	55
16	BJ	27/497 (5%)	27 (100%)	0	100	100
All	All	47738/50237 (95%)	47268 (99%)	470 (1%)	71	84

5 of 470 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	A8	341	PHE
12	F1	285	ARG
10	FU	214	ASP
12	F2	260	LEU
12	Fa	411	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 645 such sidechains are listed below:

Mol	Chain	Res	Type
11	Fx	34	ASN
12	Fs	446	ASN
12	FG	357	ASN
11	Fx	14	ASN
12	FY	125	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

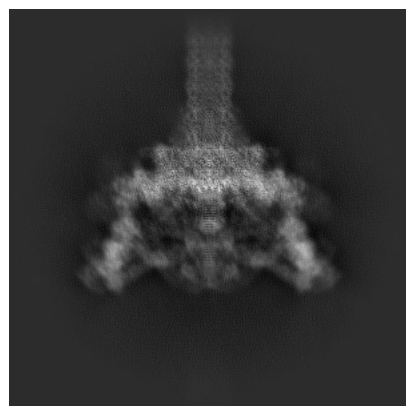
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50187. These allow visual inspection of the internal detail of the map and identification of artifacts.

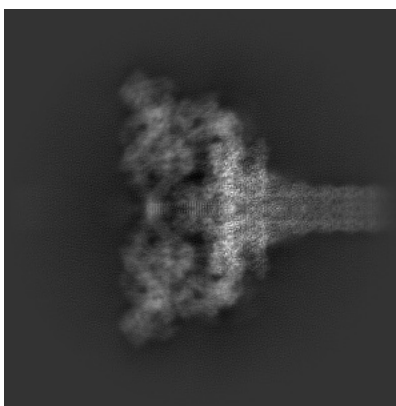
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

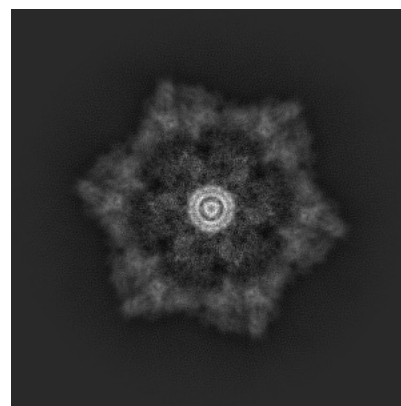
#### 6.1.1 Primary map



X

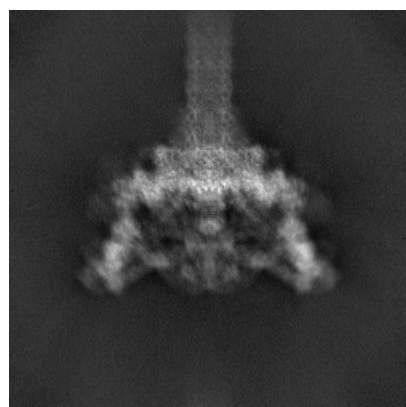


Y

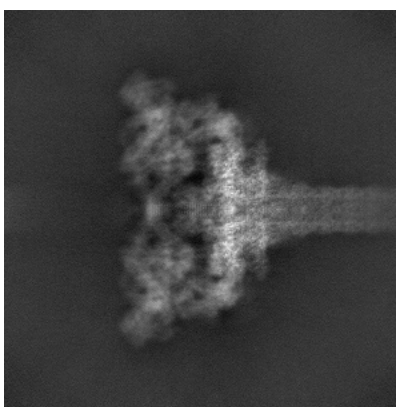


Z

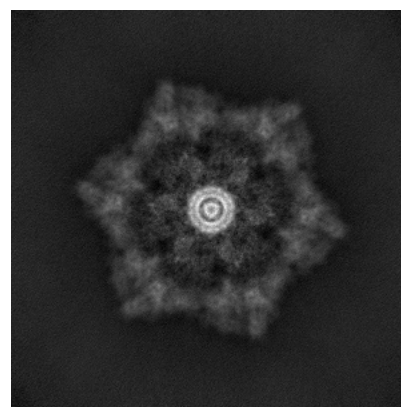
#### 6.1.2 Raw map



X



Y

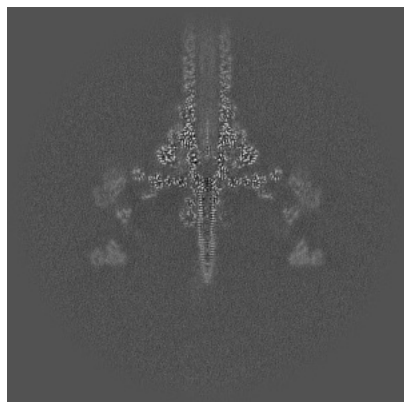


Z

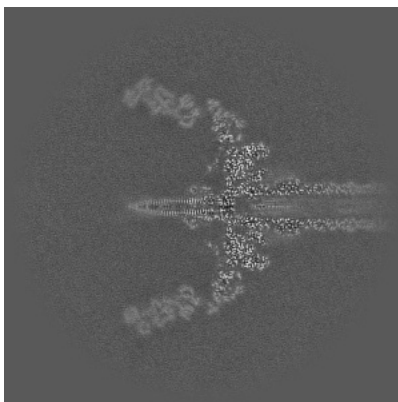
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

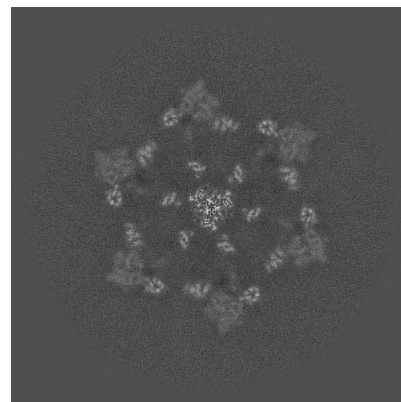
### 6.2.1 Primary map



X Index: 324

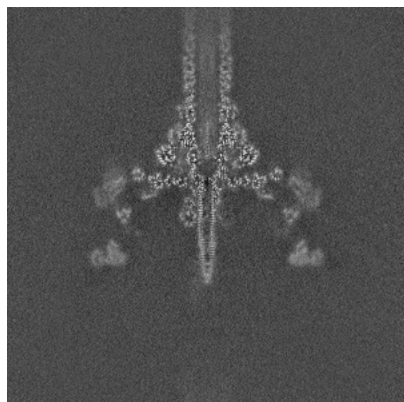


Y Index: 324

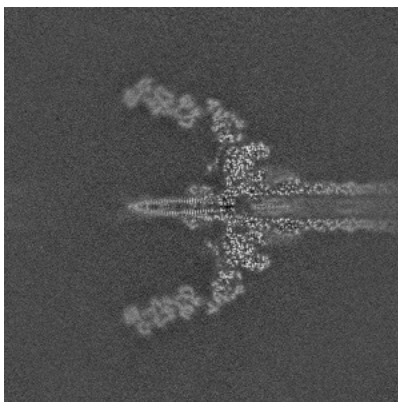


Z Index: 324

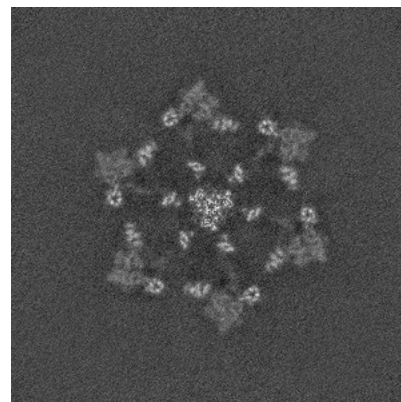
### 6.2.2 Raw map



X Index: 324



Y Index: 324

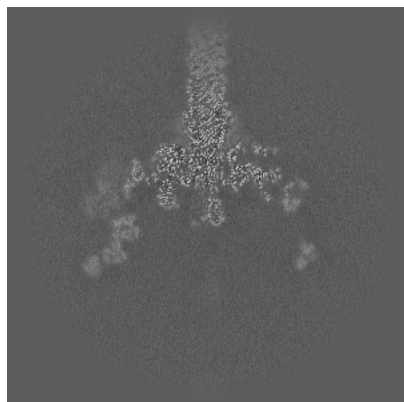


Z Index: 324

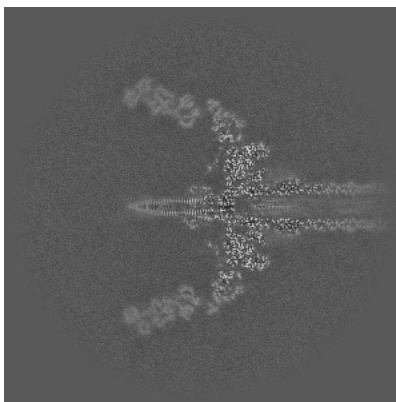
The images above show central slices of the map in three orthogonal directions.

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

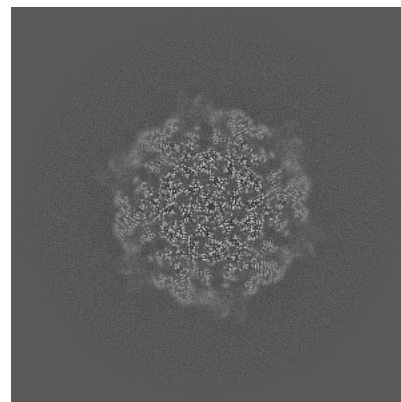
### 6.3.1 Primary map



X Index: 346

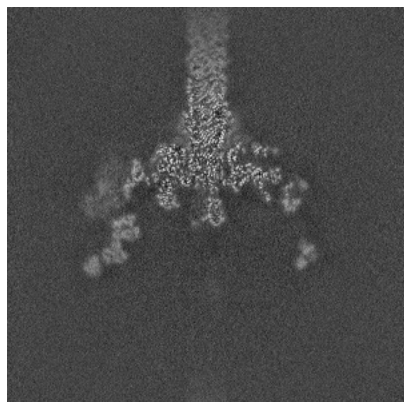


Y Index: 324

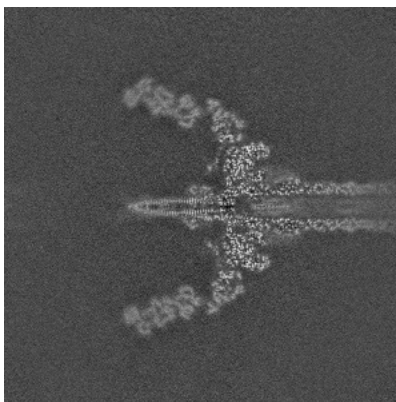


Z Index: 366

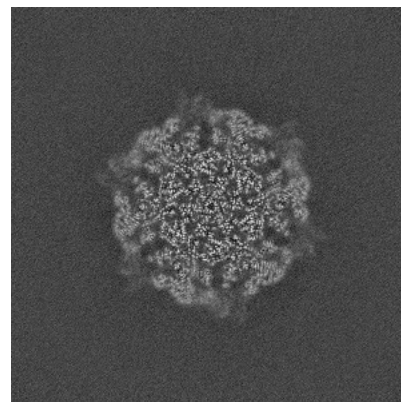
### 6.3.2 Raw map



X Index: 346



Y Index: 324



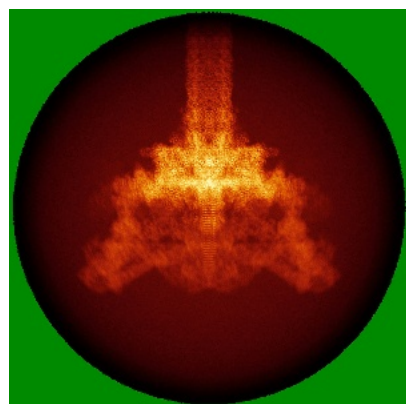
Z Index: 366

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

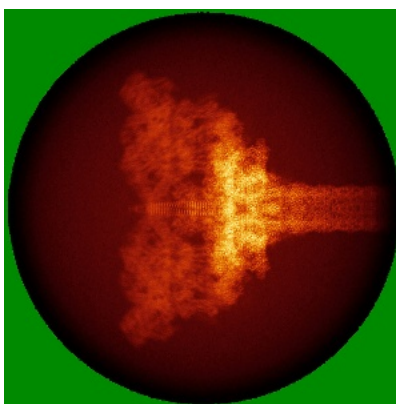


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

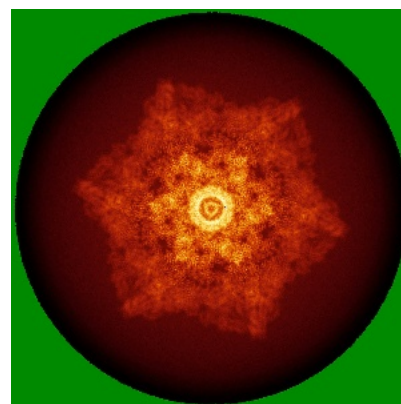
### 6.4.1 Primary map



X

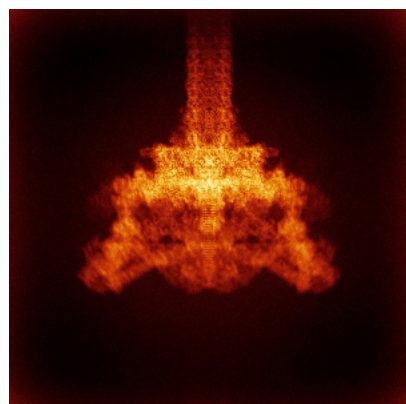


Y

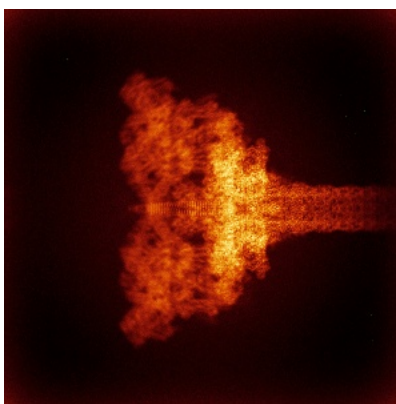


Z

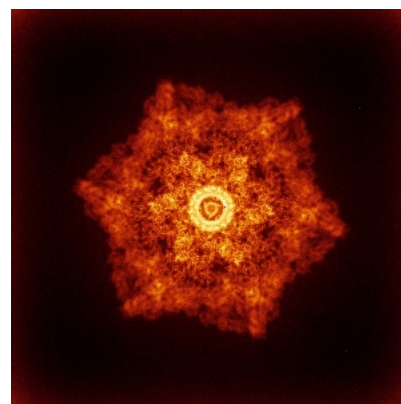
### 6.4.2 Raw map



X



Y

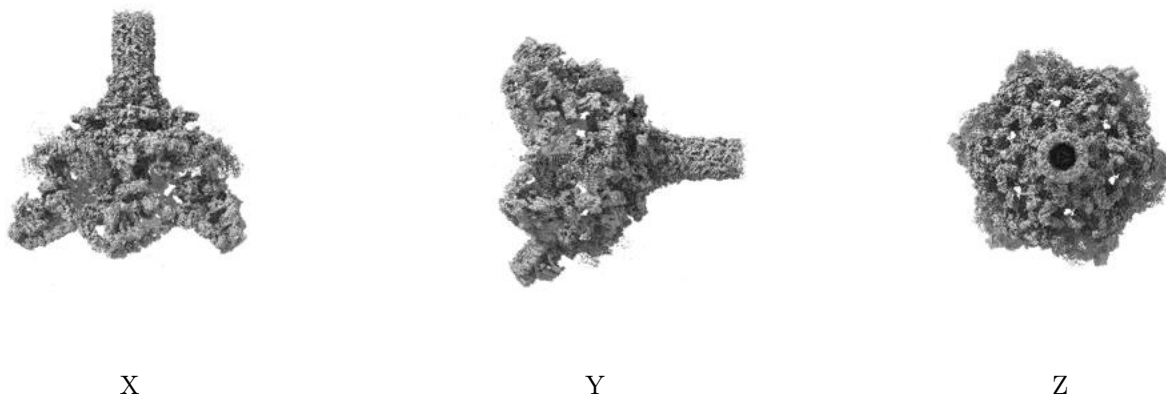


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

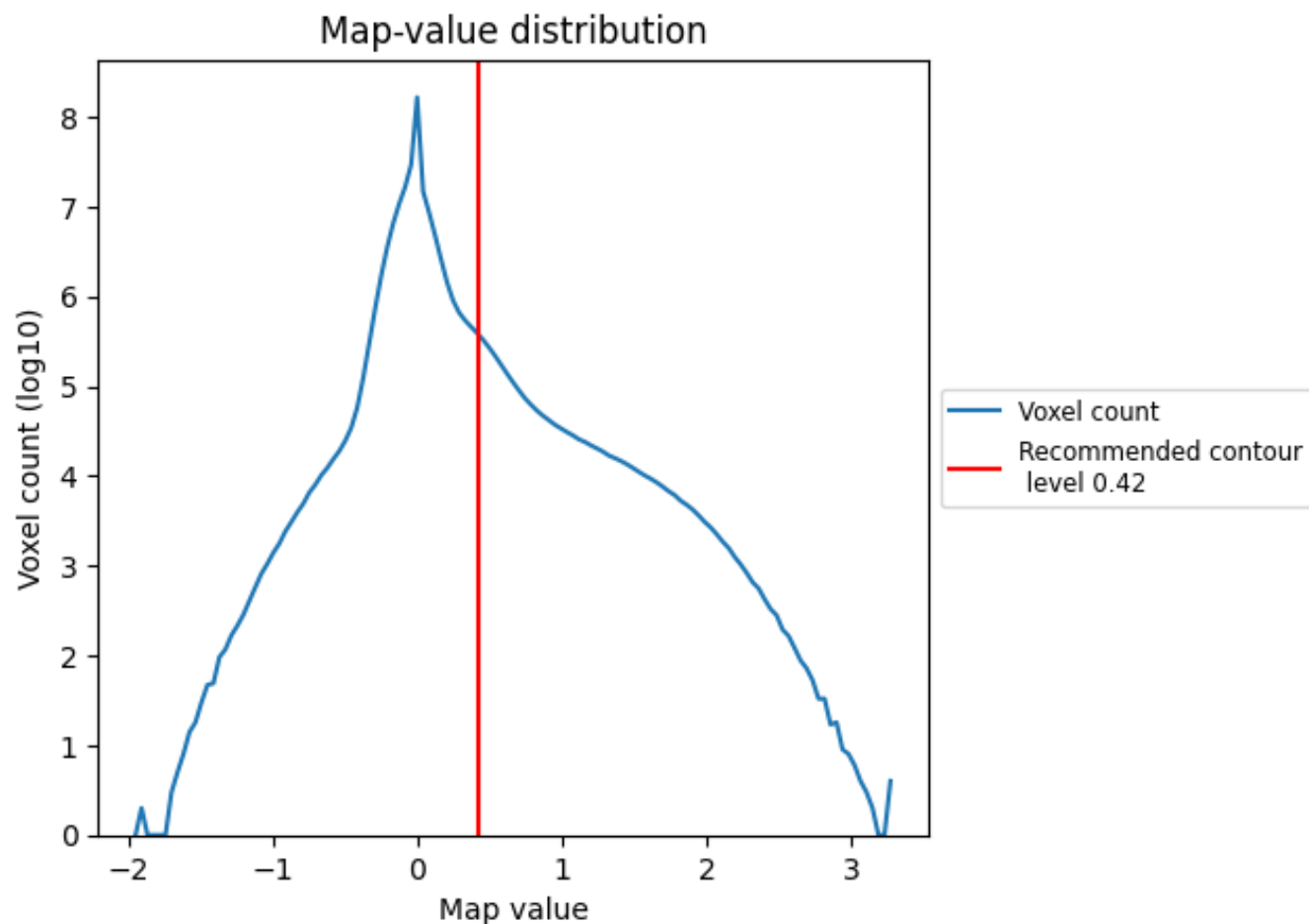
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

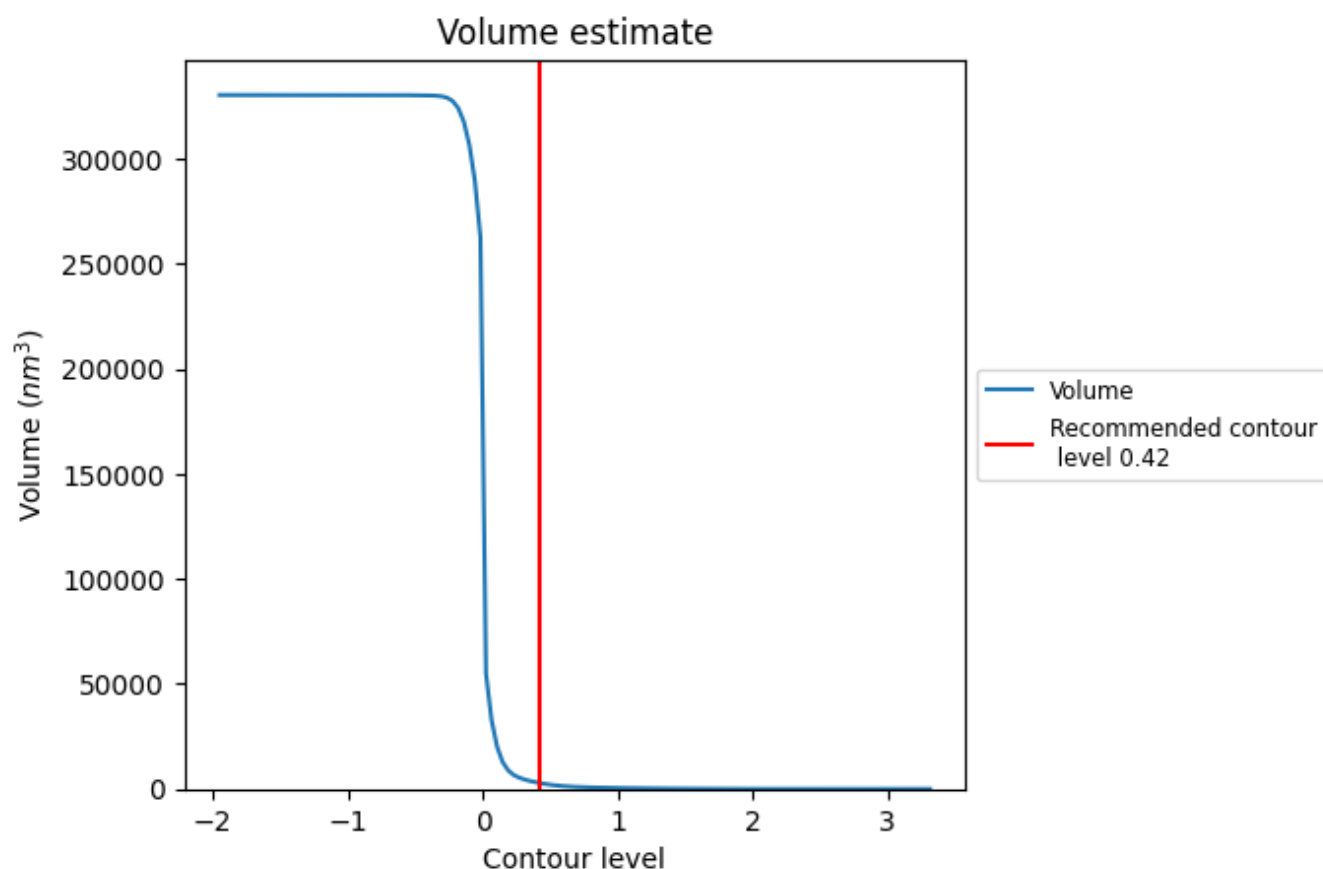
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

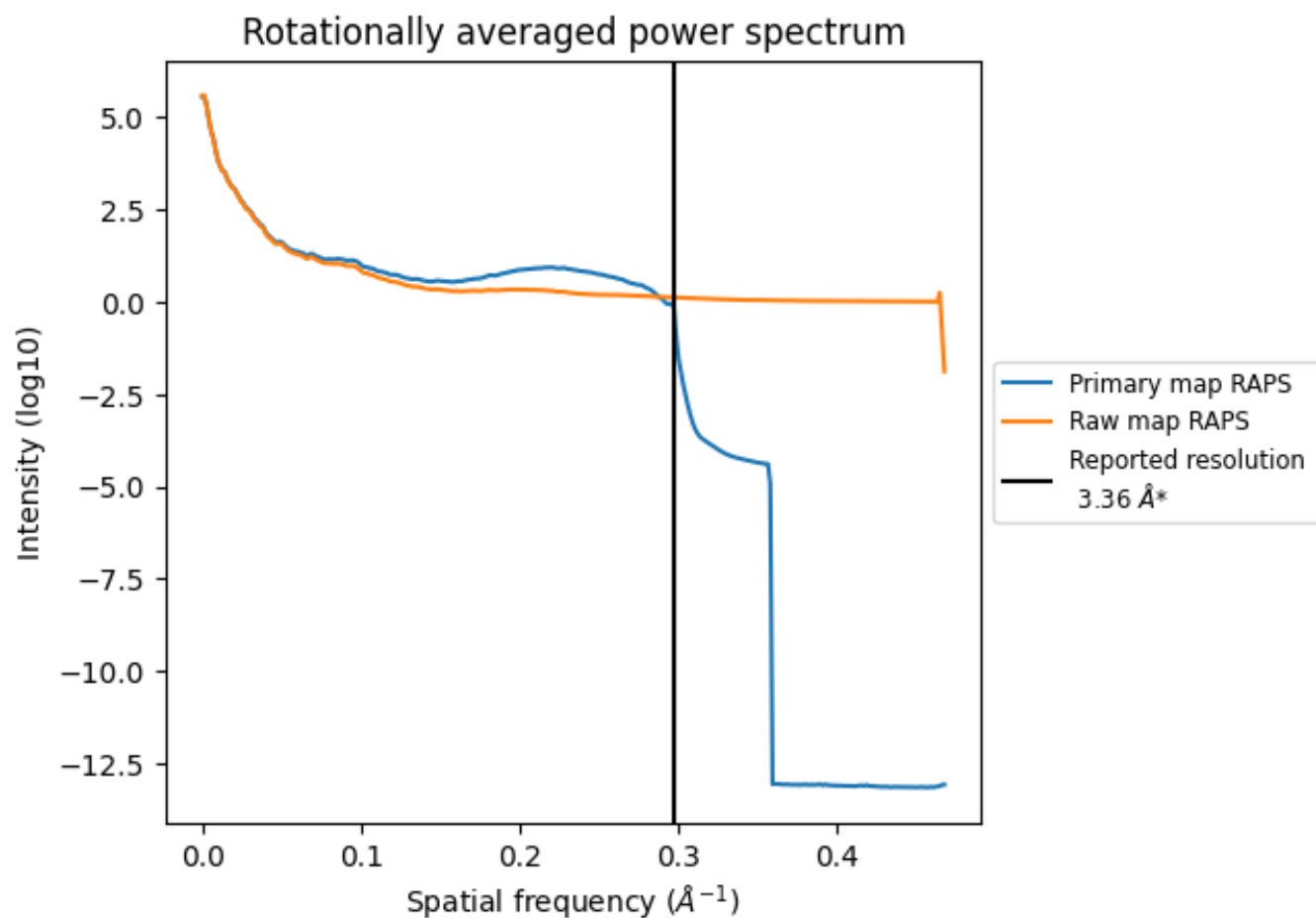
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2851  $\text{nm}^3$ ; this corresponds to an approximate mass of 2576 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

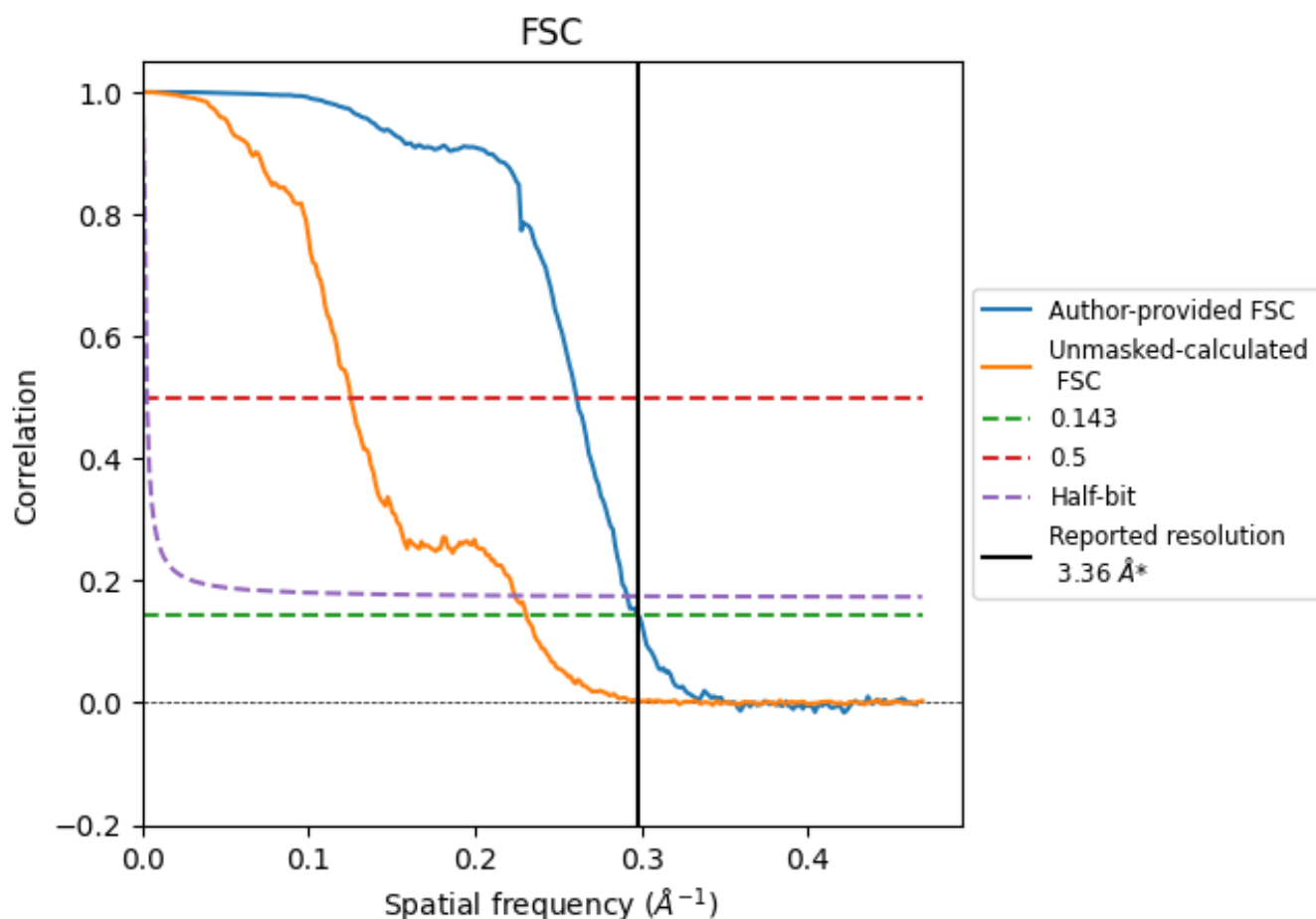


\*Reported resolution corresponds to spatial frequency of 0.298 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.298 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

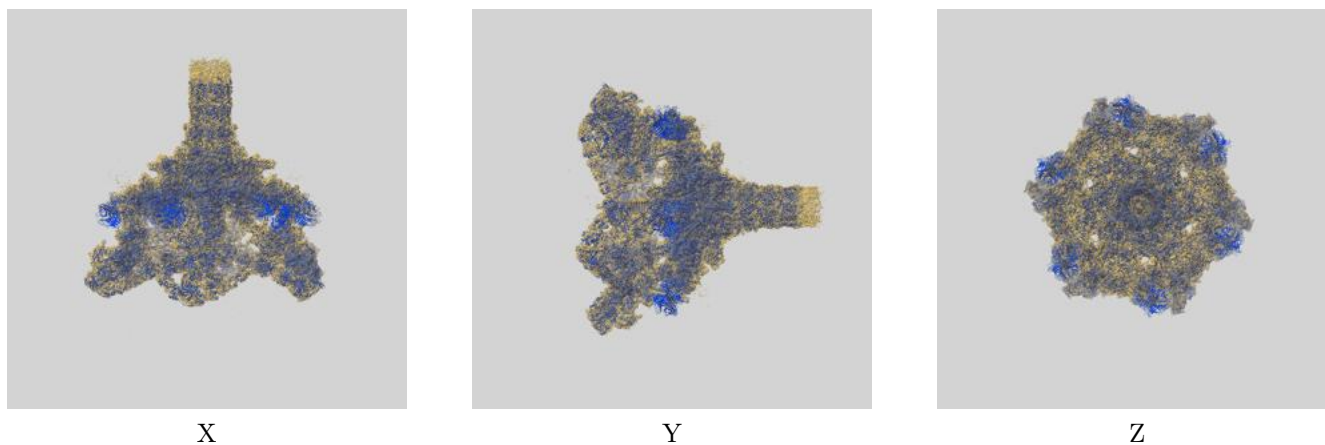
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.35	3.83	3.43
Unmasked-calculated*	4.33	7.98	4.47

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.33 differs from the reported value 3.36 by more than 10 %

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

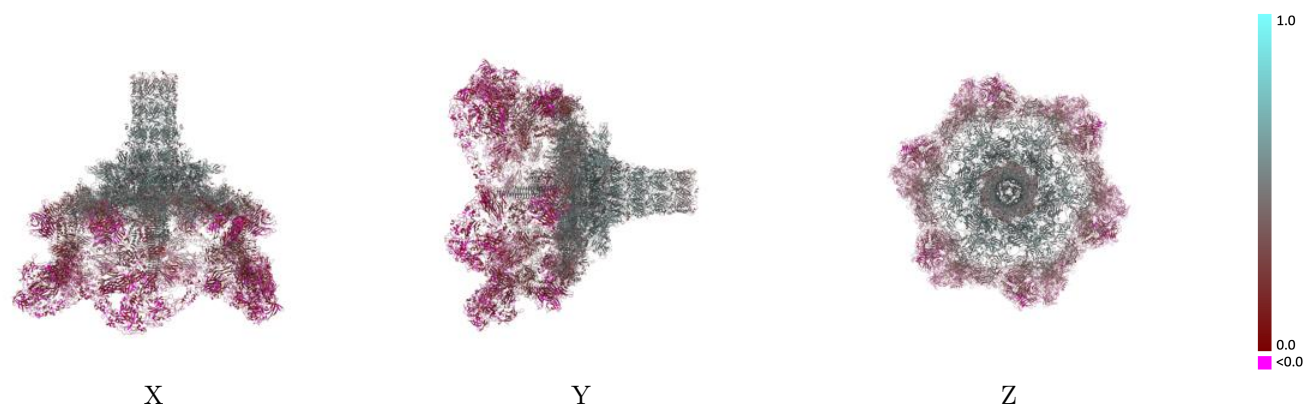
This section contains information regarding the fit between EMDB map EMD-50187 and PDB model 9F4B. Per-residue inclusion information can be found in section [3](#) on page [20](#).

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



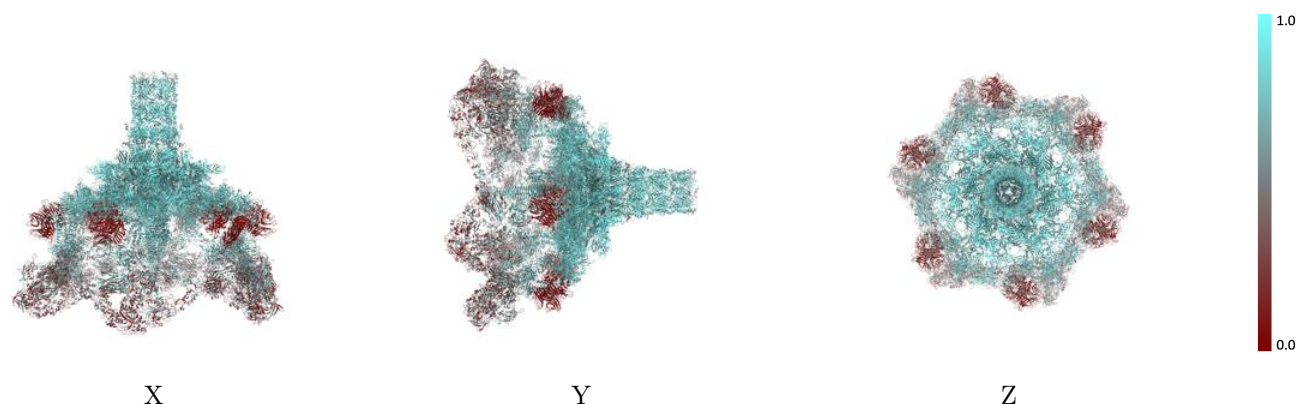
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



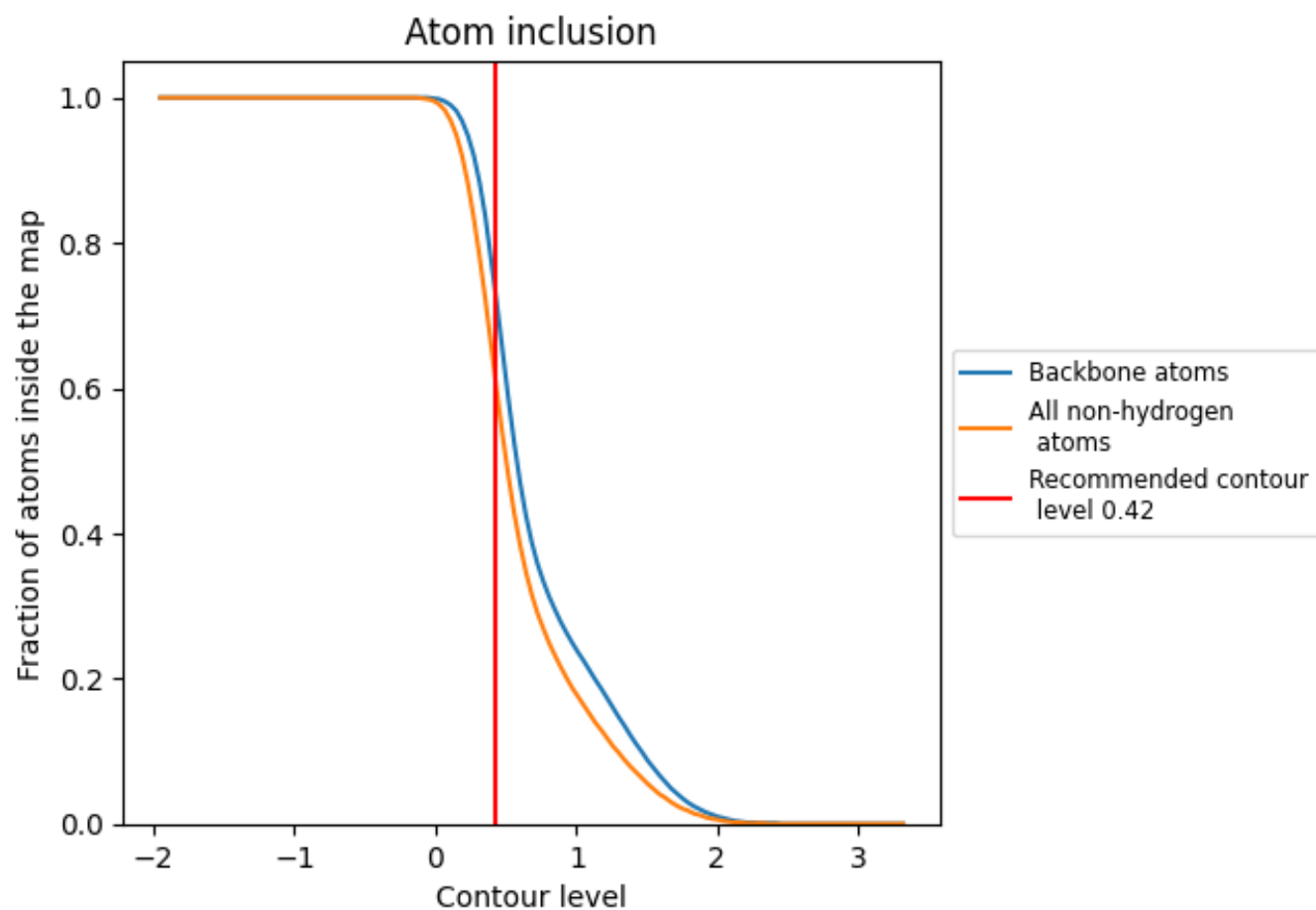
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.42).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 74% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6190	 0.3210
A0	 0.7760	 0.4120
A1	 0.7710	 0.4230
A2	 0.7690	 0.4220
A3	 0.7770	 0.4110
A4	 0.8480	 0.4860
A5	 0.8400	 0.4800
A6	 0.8500	 0.4850
A7	 0.8440	 0.4790
A8	 0.8450	 0.4870
A9	 0.8430	 0.4800
AA	 0.8640	 0.5080
AB	 0.8660	 0.5090
AC	 0.8660	 0.5090
AD	 0.8700	 0.5090
AE	 0.8650	 0.5080
AF	 0.8710	 0.5080
AG	 0.8810	 0.5230
AH	 0.8730	 0.5200
AI	 0.8800	 0.5200
AJ	 0.8750	 0.5210
AK	 0.8820	 0.5220
AL	 0.8730	 0.5210
AM	 0.8520	 0.5160
AN	 0.8670	 0.5150
AO	 0.8520	 0.5160
AP	 0.8680	 0.5150
AQ	 0.8540	 0.5170
AR	 0.8680	 0.5160
AS	 0.8690	 0.5100
AT	 0.8680	 0.5080
AU	 0.8670	 0.5090
AV	 0.8650	 0.5070
AW	 0.8640	 0.5090
AX	 0.8670	 0.5070























































































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Chain	Atom inclusion	Q-score
AY	 0.7790	 0.4080
AZ	 0.7720	 0.4240
Aa	 0.7850	 0.4080
Ab	 0.7800	 0.4070
Ac	 0.7870	 0.4060
Ad	 0.7790	 0.4070
Ae	 0.7870	 0.4060
Af	 0.7780	 0.4060
B1	 0.8300	 0.4960
B2	 0.8300	 0.4950
B3	 0.7230	 0.4190
B4	 0.7200	 0.4180
B5	 0.6980	 0.4150
B6	 0.7250	 0.4200
B7	 0.7030	 0.4150
B8	 0.6970	 0.4180
BA	 0.6770	 0.2750
BB	 0.8170	 0.5010
BC	 0.8160	 0.4990
BD	 0.8160	 0.5000
BE	 0.8650	 0.5310
BF	 0.8640	 0.5300
BG	 0.8640	 0.5290
BH	 0.6340	 0.4500
BI	 0.6010	 0.4360
BJ	 0.6220	 0.4420
BK	 0.7490	 0.4690
BL	 0.7880	 0.4940
BM	 0.7500	 0.4740
BN	 0.7850	 0.4920
BO	 0.7480	 0.4740
BP	 0.7840	 0.4930
BQ	 0.8530	 0.5110
BR	 0.8570	 0.5150
BS	 0.8630	 0.5120
BT	 0.8610	 0.5160
BU	 0.8620	 0.5120
BV	 0.8660	 0.5180
BW	 0.8350	 0.4930
BX	 0.8330	 0.4920
BY	 0.8260	 0.4950
BZ	 0.8350	 0.4940





























































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Chain	Atom inclusion	Q-score
F1	 0.3670	 0.1210
F2	 0.3850	 0.1210
FA	 0.5800	 0.2210
FB	 0.5780	 0.2040
FC	 0.5820	 0.2190
FD	 0.3610	 0.1250
FE	 0.3590	 0.1250
FF	 0.4000	 0.1190
FG	 0.4250	 0.1210
FH	 0.4180	 0.1270
FI	 0.4220	 0.1160
FJ	 0.5760	 0.2150
FK	 0.5500	 0.2090
FL	 0.5710	 0.2050
FM	 0.3780	 0.1230
FN	 0.3710	 0.1050
FO	 0.3500	 0.1040
FP	 0.4000	 0.1460
FQ	 0.3650	 0.1200
FR	 0.3780	 0.1190
FS	 0.5770	 0.2230
FT	 0.5770	 0.2060
FU	 0.5830	 0.2200
FV	 0.3620	 0.1250
FW	 0.3580	 0.1230
FX	 0.4100	 0.1220
FY	 0.4250	 0.1230
FZ	 0.4220	 0.1260
Fa	 0.4260	 0.1180
Fb	 0.5790	 0.2180
Fc	 0.5490	 0.2110
Fd	 0.5760	 0.2070
Fe	 0.3850	 0.1220
Ff	 0.3750	 0.1040
Fg	 0.3580	 0.1080
Fh	 0.3990	 0.1490
Fi	 0.3640	 0.1200
Fj	 0.3780	 0.1190
Fk	 0.5720	 0.2210
Fl	 0.5740	 0.2040
Fm	 0.5760	 0.2190
Fn	 0.3590	 0.1240

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Chain	Atom inclusion	Q-score
Fo	 0.3590	 0.1260
Fp	 0.4010	 0.1220
Fq	 0.4240	 0.1190
Fr	 0.4210	 0.1270
Fs	 0.4240	 0.1170
Ft	 0.5800	 0.2160
Fu	 0.5480	 0.2090
Fv	 0.5740	 0.2080
Fw	 0.3870	 0.1270
Fx	 0.3690	 0.1020
Fy	 0.3600	 0.1050
Fz	 0.4010	 0.1470
LA	 0.0950	 0.1360
LB	 0.1730	 0.1680
LC	 0.1160	 0.1400
LD	 0.1080	 0.1610
LE	 0.1810	 0.1650
LF	 0.1140	 0.1480
LG	 0.0940	 0.1370
LH	 0.1790	 0.1670
LI	 0.1170	 0.1410
LJ	 0.1070	 0.1610
LK	 0.1820	 0.1670
LL	 0.1150	 0.1510
LM	 0.0920	 0.1340
LN	 0.1710	 0.1650
LO	 0.1140	 0.1410
LP	 0.1070	 0.1610
LQ	 0.1840	 0.1680
LR	 0.1170	 0.1500