



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:25 PM UTC

PDB ID : 9F4A / pdb_00009f4a
EMDB ID : EMD-50186
Title : Interface between baseplate cup and extended tail tube/sheath of Klebsiella phage KP1 variant vB_Kpn_Lilla1
Authors : Orlova, E.V.; Isupov, M.N.
Deposited on : 2024-04-26
Resolution : 3.95 Å(reported)

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

We welcome your comments at 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>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

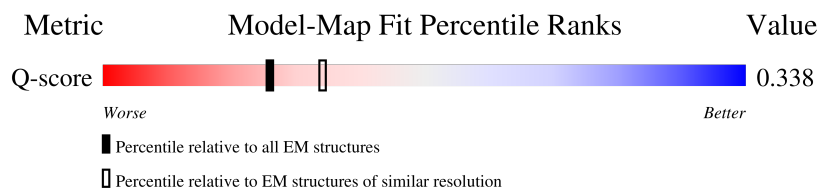
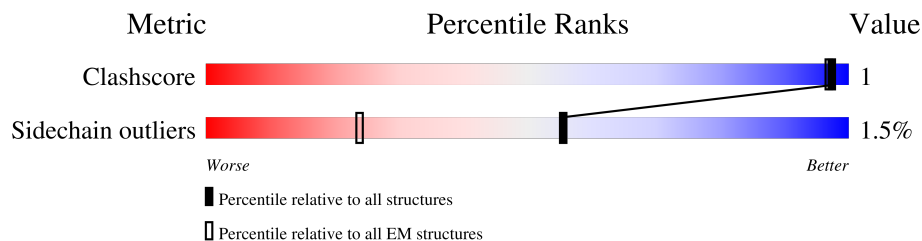
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.95 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7707 (3.45 - 4.45)

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 ≥ 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	LS	1281	48% 46% 52%
1	LT	1281	48% 46% 52%
1	LU	1281	48% 46% 52%
1	LV	1281	48% 46% 52%
1	LW	1281	48% 47% 52%

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Mol	Chain	Length	Quality of chain
1	LX	1281	48% 46% 52%
1	LY	1281	48% 46% 52%
1	LZ	1281	48% 47% 52%
1	La	1281	48% 46% 52%
1	Lb	1281	48% 46% 52%
1	Lc	1281	48% 46% 52%
1	Ld	1281	48% 47% 52%
1	Le	1281	48% 46% 52%
1	Lf	1281	48% 46% 52%
1	Lg	1281	48% 46% 52%
1	Lh	1281	48% 46% 52%
1	Li	1281	48% 46% 52%
1	Lj	1281	48% 46% 52%
2	BK	350	47% 95%
2	BL	350	28% 76% 21%
2	BM	350	46% 94% 5%
2	BN	350	27% 75% 21%
2	BO	350	45% 95%
2	BP	350	27% 74% 5% 21%
3	BQ	308	19% 90% 5%
3	BR	308	18% 90% 5%
3	BS	308	19% 91% 5%
3	BT	308	19% 90% 5%
3	BU	308	19% 90% 5%
3	BV	308	18% 91% 5%

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Mol	Chain	Length	Quality of chain
4	AM	655	12% 97%
4	AN	655	11% 97%
4	AO	655	12% 96%
4	AP	655	11% 97%
4	AQ	655	10% 97%
4	AR	655	11% 97%
4	AS	655	15% 97%
4	AT	655	13% 96%
4	AU	655	15% 96%
4	AV	655	14% 95%
4	AW	655	15% 97%
4	AX	655	14% 95%
5	A0	1032	47% 96%
5	A1	1032	45% 96%
5	A2	1032	46% 96%
5	A3	1032	46% 96%
5	AY	1032	45% 96%
5	AZ	1032	46% 96%
6	A4	341	40% 94%
6	A5	341	40% 94%
6	A6	341	40% 94%
6	A7	341	39% 94%
6	A8	341	39% 94%
6	A9	341	40% 95%
6	Aa	341	55% 92%

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Mol	Chain	Length	Quality of chain
6	Ab	341	52% 93% .
6	Ac	341	54% 92% .
6	Ad	341	54% 92% .
6	Ae	341	55% 93% .
6	Af	341	52% 93% .
7	LA	303	93% 96% .
7	LB	303	95% 97% .
7	LC	303	96% 98% .
7	LD	303	93% 97% .
7	LE	303	97% 97% .
7	LF	303	97% 97% .
7	LG	303	93% 96% .
7	LH	303	97% 97% .
7	LI	303	96% 98% .
7	LJ	303	93% 97% .
7	LK	303	96% 98% .
7	LL	303	96% 97% .
7	LM	303	93% 97% .
7	LN	303	97% 96% .
7	LO	303	97% 97% .
7	LP	303	94% 97% .
7	LQ	303	96% 97% .
7	LR	303	97% 97% .
8	FA	607	9% 10% 89%
8	FB	607	9% 10% 89%

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Mol	Chain	Length	Quality of chain
8	FC	607	8% 10% 89%
8	FJ	607	9% 10% 89%
8	FK	607	9% 10% 89%
8	FL	607	9% 10% 89%
8	FS	607	9% 10% 89%
8	FT	607	10% 10% 89%
8	FU	607	9% 10% 89%
8	Fb	607	9% 10% 89%
8	Fc	607	9% 10% 89%
8	Fd	607	8% 10% 89%
8	Fk	607	9% 10% 89%
8	Fl	607	10% 10% 89%
8	Fm	607	9% 10% 89%
8	Ft	607	9% 10% 89%
8	Fu	607	10% 10% 89%
8	Fv	607	9% 10% 89%
9	SA	656	16% 95%
9	SB	656	17% 95%
9	SC	656	16% 96%
9	SD	656	17% 96%
9	SE	656	16% 96%
9	SF	656	17% 96%
9	SG	656	11% 95%
9	SH	656	11% 96%
9	SI	656	11% 95%

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Mol	Chain	Length	Quality of chain
9	SJ	656	11% 96% .
9	SK	656	11% 96% .
9	SL	656	11% 95% .
9	SM	656	11% 96% .
9	SN	656	12% 97% .
9	SO	656	13% 96% .
9	SP	656	12% 96% .
9	SQ	656	12% 98% .
9	SR	656	12% 96% .
9	SS	656	13% 97% .
9	ST	656	14% 97% .
9	SU	656	13% 98% .
9	SV	656	13% 97% .
9	SW	656	14% 97% .
9	SX	656	13% 98% .
9	SY	656	16% 98% .
9	SZ	656	17% 98% ..
9	Sa	656	16% 98% .
9	Sb	656	16% 98% .
9	Sc	656	17% 98% .
9	Sd	656	16% 99% .
9	Se	656	20% 97% .
9	Sf	656	19% 97% .
9	Sg	656	19% 97% .
9	Sh	656	20% 97% .

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Mol	Chain	Length	Quality of chain
9	Si	656	
9	Sj	656	
9	Sk	656	
9	Sl	656	
9	Sm	656	
9	Sn	656	
9	So	656	
9	Sp	656	
10	TM	163	
10	TN	163	
10	TO	163	
10	TP	163	
10	TQ	163	
10	TR	163	
10	TS	163	
10	TT	163	
10	TU	163	
10	TV	163	
10	TW	163	
10	TX	163	
10	TY	163	
10	TZ	163	
10	Ta	163	
10	Tb	163	
10	Tc	163	

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Mol	Chain	Length	Quality of chain
10	Td	163	6% 95% ..
10	Te	163	12% 95% ..
10	Tf	163	12% 94% 5% .
10	Tg	163	12% 94% 5% .
10	Th	163	11% 96% ..
10	Ti	163	12% 92% 7% .
10	Tj	163	12% 93% 7% .
10	Tk	163	12% 95% ..
10	Tl	163	14% 93% 7% .
10	Tm	163	12% 95% ..
10	Tn	163	12% 94% 5% .
10	To	163	13% 93% 7% .
10	Tp	163	13% 95% ..
10	Tq	163	85% 98% ..
10	Tr	163	84% 98% ..
10	Ts	163	85% 98% ..
10	Tt	163	85% 98% ..
10	Tu	163	85% 97% ..
10	Tv	163	85% 98% ..
11	AA	136	27% 91% 5% ..
11	AB	136	27% 94% ..
11	AC	136	26% 90% 5% ..
11	AD	136	28% 93% ..
11	AE	136	28% 93% ..
11	AF	136	27% 91% 6% .

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Mol	Chain	Length	Quality of chain
12	BE	380	43% 93% 6%
12	BF	380	43% 95% 5%
12	BG	380	43% 94% 5%
13	AG	212	15% 98% .
13	AH	212	13% 96% .
13	AI	212	13% 99% .
13	AJ	212	15% 98% .
13	AK	212	12% 99% .
13	AL	212	14% 97% .
14	BB	576	57% 93% 5% .
14	BC	576	57% 93% 5% .
14	BD	576	57% 93% 5% .

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 605128 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 Long tail fiber proximal subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Le	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	Lf	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	Lg	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	Lh	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	Li	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	Lj	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	LS	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	LT	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	LU	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	LV	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	LW	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	LX	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	LY	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	LZ	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	La	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	Lb	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		
1	Lc	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ld	617	Total	C	N	O	S	0	0
			4752	2963	834	947	8		

There are 306 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Le	217	SER	ALA	conflict	UNP A0A5B9NKG2
Le	278	ILE	VAL	conflict	UNP A0A5B9NKG2
Le	328	THR	ALA	conflict	UNP A0A5B9NKG2
Le	369	GLY	ASP	conflict	UNP A0A5B9NKG2
Le	413	GLU	GLY	conflict	UNP A0A5B9NKG2
Le	419	GLU	ASP	conflict	UNP A0A5B9NKG2
Le	422	THR	SER	conflict	UNP A0A5B9NKG2
Le	429	ILE	VAL	conflict	UNP A0A5B9NKG2
Le	467	ALA	PRO	conflict	UNP A0A5B9NKG2
Le	535	SER	THR	conflict	UNP A0A5B9NKG2
Le	567	VAL	ILE	conflict	UNP A0A5B9NKG2
Le	580	ASN	ALA	conflict	UNP A0A5B9NKG2
Le	727	GLY	ASP	conflict	UNP A0A5B9NKG2
Le	964	SER	THR	conflict	UNP A0A5B9NKG2
Le	973	PRO	THR	conflict	UNP A0A5B9NKG2
Le	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
Le	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
Lf	217	SER	ALA	conflict	UNP A0A5B9NKG2
Lf	278	ILE	VAL	conflict	UNP A0A5B9NKG2
Lf	328	THR	ALA	conflict	UNP A0A5B9NKG2
Lf	369	GLY	ASP	conflict	UNP A0A5B9NKG2
Lf	413	GLU	GLY	conflict	UNP A0A5B9NKG2
Lf	419	GLU	ASP	conflict	UNP A0A5B9NKG2
Lf	422	THR	SER	conflict	UNP A0A5B9NKG2
Lf	429	ILE	VAL	conflict	UNP A0A5B9NKG2
Lf	467	ALA	PRO	conflict	UNP A0A5B9NKG2
Lf	535	SER	THR	conflict	UNP A0A5B9NKG2
Lf	567	VAL	ILE	conflict	UNP A0A5B9NKG2
Lf	580	ASN	ALA	conflict	UNP A0A5B9NKG2
Lf	727	GLY	ASP	conflict	UNP A0A5B9NKG2
Lf	964	SER	THR	conflict	UNP A0A5B9NKG2
Lf	973	PRO	THR	conflict	UNP A0A5B9NKG2
Lf	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
Lf	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
Lg	217	SER	ALA	conflict	UNP A0A5B9NKG2
Lg	278	ILE	VAL	conflict	UNP A0A5B9NKG2

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Chain	Residue	Modelled	Actual	Comment	Reference
Lg	328	THR	ALA	conflict	UNP A0A5B9NKG2
Lg	369	GLY	ASP	conflict	UNP A0A5B9NKG2
Lg	413	GLU	GLY	conflict	UNP A0A5B9NKG2
Lg	419	GLU	ASP	conflict	UNP A0A5B9NKG2
Lg	422	THR	SER	conflict	UNP A0A5B9NKG2
Lg	429	ILE	VAL	conflict	UNP A0A5B9NKG2
Lg	467	ALA	PRO	conflict	UNP A0A5B9NKG2
Lg	535	SER	THR	conflict	UNP A0A5B9NKG2
Lg	567	VAL	ILE	conflict	UNP A0A5B9NKG2
Lg	580	ASN	ALA	conflict	UNP A0A5B9NKG2
Lg	727	GLY	ASP	conflict	UNP A0A5B9NKG2
Lg	964	SER	THR	conflict	UNP A0A5B9NKG2
Lg	973	PRO	THR	conflict	UNP A0A5B9NKG2
Lg	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
Lg	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
Lh	217	SER	ALA	conflict	UNP A0A5B9NKG2
Lh	278	ILE	VAL	conflict	UNP A0A5B9NKG2
Lh	328	THR	ALA	conflict	UNP A0A5B9NKG2
Lh	369	GLY	ASP	conflict	UNP A0A5B9NKG2
Lh	413	GLU	GLY	conflict	UNP A0A5B9NKG2
Lh	419	GLU	ASP	conflict	UNP A0A5B9NKG2
Lh	422	THR	SER	conflict	UNP A0A5B9NKG2
Lh	429	ILE	VAL	conflict	UNP A0A5B9NKG2
Lh	467	ALA	PRO	conflict	UNP A0A5B9NKG2
Lh	535	SER	THR	conflict	UNP A0A5B9NKG2
Lh	567	VAL	ILE	conflict	UNP A0A5B9NKG2
Lh	580	ASN	ALA	conflict	UNP A0A5B9NKG2
Lh	727	GLY	ASP	conflict	UNP A0A5B9NKG2
Lh	964	SER	THR	conflict	UNP A0A5B9NKG2
Lh	973	PRO	THR	conflict	UNP A0A5B9NKG2
Lh	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
Lh	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
Li	217	SER	ALA	conflict	UNP A0A5B9NKG2
Li	278	ILE	VAL	conflict	UNP A0A5B9NKG2
Li	328	THR	ALA	conflict	UNP A0A5B9NKG2
Li	369	GLY	ASP	conflict	UNP A0A5B9NKG2
Li	413	GLU	GLY	conflict	UNP A0A5B9NKG2
Li	419	GLU	ASP	conflict	UNP A0A5B9NKG2
Li	422	THR	SER	conflict	UNP A0A5B9NKG2
Li	429	ILE	VAL	conflict	UNP A0A5B9NKG2
Li	467	ALA	PRO	conflict	UNP A0A5B9NKG2
Li	535	SER	THR	conflict	UNP A0A5B9NKG2

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Chain	Residue	Modelled	Actual	Comment	Reference
Li	567	VAL	ILE	conflict	UNP A0A5B9NKG2
Li	580	ASN	ALA	conflict	UNP A0A5B9NKG2
Li	727	GLY	ASP	conflict	UNP A0A5B9NKG2
Li	964	SER	THR	conflict	UNP A0A5B9NKG2
Li	973	PRO	THR	conflict	UNP A0A5B9NKG2
Li	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
Li	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
Lj	217	SER	ALA	conflict	UNP A0A5B9NKG2
Lj	278	ILE	VAL	conflict	UNP A0A5B9NKG2
Lj	328	THR	ALA	conflict	UNP A0A5B9NKG2
Lj	369	GLY	ASP	conflict	UNP A0A5B9NKG2
Lj	413	GLU	GLY	conflict	UNP A0A5B9NKG2
Lj	419	GLU	ASP	conflict	UNP A0A5B9NKG2
Lj	422	THR	SER	conflict	UNP A0A5B9NKG2
Lj	429	ILE	VAL	conflict	UNP A0A5B9NKG2
Lj	467	ALA	PRO	conflict	UNP A0A5B9NKG2
Lj	535	SER	THR	conflict	UNP A0A5B9NKG2
Lj	567	VAL	ILE	conflict	UNP A0A5B9NKG2
Lj	580	ASN	ALA	conflict	UNP A0A5B9NKG2
Lj	727	GLY	ASP	conflict	UNP A0A5B9NKG2
Lj	964	SER	THR	conflict	UNP A0A5B9NKG2
Lj	973	PRO	THR	conflict	UNP A0A5B9NKG2
Lj	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
Lj	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
LS	217	SER	ALA	conflict	UNP A0A5B9NKG2
LS	278	ILE	VAL	conflict	UNP A0A5B9NKG2
LS	328	THR	ALA	conflict	UNP A0A5B9NKG2
LS	369	GLY	ASP	conflict	UNP A0A5B9NKG2
LS	413	GLU	GLY	conflict	UNP A0A5B9NKG2
LS	419	GLU	ASP	conflict	UNP A0A5B9NKG2
LS	422	THR	SER	conflict	UNP A0A5B9NKG2
LS	429	ILE	VAL	conflict	UNP A0A5B9NKG2
LS	467	ALA	PRO	conflict	UNP A0A5B9NKG2
LS	535	SER	THR	conflict	UNP A0A5B9NKG2
LS	567	VAL	ILE	conflict	UNP A0A5B9NKG2
LS	580	ASN	ALA	conflict	UNP A0A5B9NKG2
LS	727	GLY	ASP	conflict	UNP A0A5B9NKG2
LS	964	SER	THR	conflict	UNP A0A5B9NKG2
LS	973	PRO	THR	conflict	UNP A0A5B9NKG2
LS	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
LS	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
LT	217	SER	ALA	conflict	UNP A0A5B9NKG2

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Chain	Residue	Modelled	Actual	Comment	Reference
LT	278	ILE	VAL	conflict	UNP A0A5B9NKG2
LT	328	THR	ALA	conflict	UNP A0A5B9NKG2
LT	369	GLY	ASP	conflict	UNP A0A5B9NKG2
LT	413	GLU	GLY	conflict	UNP A0A5B9NKG2
LT	419	GLU	ASP	conflict	UNP A0A5B9NKG2
LT	422	THR	SER	conflict	UNP A0A5B9NKG2
LT	429	ILE	VAL	conflict	UNP A0A5B9NKG2
LT	467	ALA	PRO	conflict	UNP A0A5B9NKG2
LT	535	SER	THR	conflict	UNP A0A5B9NKG2
LT	567	VAL	ILE	conflict	UNP A0A5B9NKG2
LT	580	ASN	ALA	conflict	UNP A0A5B9NKG2
LT	727	GLY	ASP	conflict	UNP A0A5B9NKG2
LT	964	SER	THR	conflict	UNP A0A5B9NKG2
LT	973	PRO	THR	conflict	UNP A0A5B9NKG2
LT	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
LT	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
LU	217	SER	ALA	conflict	UNP A0A5B9NKG2
LU	278	ILE	VAL	conflict	UNP A0A5B9NKG2
LU	328	THR	ALA	conflict	UNP A0A5B9NKG2
LU	369	GLY	ASP	conflict	UNP A0A5B9NKG2
LU	413	GLU	GLY	conflict	UNP A0A5B9NKG2
LU	419	GLU	ASP	conflict	UNP A0A5B9NKG2
LU	422	THR	SER	conflict	UNP A0A5B9NKG2
LU	429	ILE	VAL	conflict	UNP A0A5B9NKG2
LU	467	ALA	PRO	conflict	UNP A0A5B9NKG2
LU	535	SER	THR	conflict	UNP A0A5B9NKG2
LU	567	VAL	ILE	conflict	UNP A0A5B9NKG2
LU	580	ASN	ALA	conflict	UNP A0A5B9NKG2
LU	727	GLY	ASP	conflict	UNP A0A5B9NKG2
LU	964	SER	THR	conflict	UNP A0A5B9NKG2
LU	973	PRO	THR	conflict	UNP A0A5B9NKG2
LU	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
LU	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
LV	217	SER	ALA	conflict	UNP A0A5B9NKG2
LV	278	ILE	VAL	conflict	UNP A0A5B9NKG2
LV	328	THR	ALA	conflict	UNP A0A5B9NKG2
LV	369	GLY	ASP	conflict	UNP A0A5B9NKG2
LV	413	GLU	GLY	conflict	UNP A0A5B9NKG2
LV	419	GLU	ASP	conflict	UNP A0A5B9NKG2
LV	422	THR	SER	conflict	UNP A0A5B9NKG2
LV	429	ILE	VAL	conflict	UNP A0A5B9NKG2
LV	467	ALA	PRO	conflict	UNP A0A5B9NKG2

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Chain	Residue	Modelled	Actual	Comment	Reference
LV	535	SER	THR	conflict	UNP A0A5B9NKG2
LV	567	VAL	ILE	conflict	UNP A0A5B9NKG2
LV	580	ASN	ALA	conflict	UNP A0A5B9NKG2
LV	727	GLY	ASP	conflict	UNP A0A5B9NKG2
LV	964	SER	THR	conflict	UNP A0A5B9NKG2
LV	973	PRO	THR	conflict	UNP A0A5B9NKG2
LV	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
LV	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
LW	217	SER	ALA	conflict	UNP A0A5B9NKG2
LW	278	ILE	VAL	conflict	UNP A0A5B9NKG2
LW	328	THR	ALA	conflict	UNP A0A5B9NKG2
LW	369	GLY	ASP	conflict	UNP A0A5B9NKG2
LW	413	GLU	GLY	conflict	UNP A0A5B9NKG2
LW	419	GLU	ASP	conflict	UNP A0A5B9NKG2
LW	422	THR	SER	conflict	UNP A0A5B9NKG2
LW	429	ILE	VAL	conflict	UNP A0A5B9NKG2
LW	467	ALA	PRO	conflict	UNP A0A5B9NKG2
LW	535	SER	THR	conflict	UNP A0A5B9NKG2
LW	567	VAL	ILE	conflict	UNP A0A5B9NKG2
LW	580	ASN	ALA	conflict	UNP A0A5B9NKG2
LW	727	GLY	ASP	conflict	UNP A0A5B9NKG2
LW	964	SER	THR	conflict	UNP A0A5B9NKG2
LW	973	PRO	THR	conflict	UNP A0A5B9NKG2
LW	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
LW	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
LX	217	SER	ALA	conflict	UNP A0A5B9NKG2
LX	278	ILE	VAL	conflict	UNP A0A5B9NKG2
LX	328	THR	ALA	conflict	UNP A0A5B9NKG2
LX	369	GLY	ASP	conflict	UNP A0A5B9NKG2
LX	413	GLU	GLY	conflict	UNP A0A5B9NKG2
LX	419	GLU	ASP	conflict	UNP A0A5B9NKG2
LX	422	THR	SER	conflict	UNP A0A5B9NKG2
LX	429	ILE	VAL	conflict	UNP A0A5B9NKG2
LX	467	ALA	PRO	conflict	UNP A0A5B9NKG2
LX	535	SER	THR	conflict	UNP A0A5B9NKG2
LX	567	VAL	ILE	conflict	UNP A0A5B9NKG2
LX	580	ASN	ALA	conflict	UNP A0A5B9NKG2
LX	727	GLY	ASP	conflict	UNP A0A5B9NKG2
LX	964	SER	THR	conflict	UNP A0A5B9NKG2
LX	973	PRO	THR	conflict	UNP A0A5B9NKG2
LX	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
LX	1180	ILE	VAL	conflict	UNP A0A5B9NKG2

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Chain	Residue	Modelled	Actual	Comment	Reference
LY	217	SER	ALA	conflict	UNP A0A5B9NKG2
LY	278	ILE	VAL	conflict	UNP A0A5B9NKG2
LY	328	THR	ALA	conflict	UNP A0A5B9NKG2
LY	369	GLY	ASP	conflict	UNP A0A5B9NKG2
LY	413	GLU	GLY	conflict	UNP A0A5B9NKG2
LY	419	GLU	ASP	conflict	UNP A0A5B9NKG2
LY	422	THR	SER	conflict	UNP A0A5B9NKG2
LY	429	ILE	VAL	conflict	UNP A0A5B9NKG2
LY	467	ALA	PRO	conflict	UNP A0A5B9NKG2
LY	535	SER	THR	conflict	UNP A0A5B9NKG2
LY	567	VAL	ILE	conflict	UNP A0A5B9NKG2
LY	580	ASN	ALA	conflict	UNP A0A5B9NKG2
LY	727	GLY	ASP	conflict	UNP A0A5B9NKG2
LY	964	SER	THR	conflict	UNP A0A5B9NKG2
LY	973	PRO	THR	conflict	UNP A0A5B9NKG2
LY	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
LY	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
LZ	217	SER	ALA	conflict	UNP A0A5B9NKG2
LZ	278	ILE	VAL	conflict	UNP A0A5B9NKG2
LZ	328	THR	ALA	conflict	UNP A0A5B9NKG2
LZ	369	GLY	ASP	conflict	UNP A0A5B9NKG2
LZ	413	GLU	GLY	conflict	UNP A0A5B9NKG2
LZ	419	GLU	ASP	conflict	UNP A0A5B9NKG2
LZ	422	THR	SER	conflict	UNP A0A5B9NKG2
LZ	429	ILE	VAL	conflict	UNP A0A5B9NKG2
LZ	467	ALA	PRO	conflict	UNP A0A5B9NKG2
LZ	535	SER	THR	conflict	UNP A0A5B9NKG2
LZ	567	VAL	ILE	conflict	UNP A0A5B9NKG2
LZ	580	ASN	ALA	conflict	UNP A0A5B9NKG2
LZ	727	GLY	ASP	conflict	UNP A0A5B9NKG2
LZ	964	SER	THR	conflict	UNP A0A5B9NKG2
LZ	973	PRO	THR	conflict	UNP A0A5B9NKG2
LZ	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
LZ	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
La	217	SER	ALA	conflict	UNP A0A5B9NKG2
La	278	ILE	VAL	conflict	UNP A0A5B9NKG2
La	328	THR	ALA	conflict	UNP A0A5B9NKG2
La	369	GLY	ASP	conflict	UNP A0A5B9NKG2
La	413	GLU	GLY	conflict	UNP A0A5B9NKG2
La	419	GLU	ASP	conflict	UNP A0A5B9NKG2
La	422	THR	SER	conflict	UNP A0A5B9NKG2
La	429	ILE	VAL	conflict	UNP A0A5B9NKG2

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Chain	Residue	Modelled	Actual	Comment	Reference
La	467	ALA	PRO	conflict	UNP A0A5B9NKG2
La	535	SER	THR	conflict	UNP A0A5B9NKG2
La	567	VAL	ILE	conflict	UNP A0A5B9NKG2
La	580	ASN	ALA	conflict	UNP A0A5B9NKG2
La	727	GLY	ASP	conflict	UNP A0A5B9NKG2
La	964	SER	THR	conflict	UNP A0A5B9NKG2
La	973	PRO	THR	conflict	UNP A0A5B9NKG2
La	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
La	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
Lb	217	SER	ALA	conflict	UNP A0A5B9NKG2
Lb	278	ILE	VAL	conflict	UNP A0A5B9NKG2
Lb	328	THR	ALA	conflict	UNP A0A5B9NKG2
Lb	369	GLY	ASP	conflict	UNP A0A5B9NKG2
Lb	413	GLU	GLY	conflict	UNP A0A5B9NKG2
Lb	419	GLU	ASP	conflict	UNP A0A5B9NKG2
Lb	422	THR	SER	conflict	UNP A0A5B9NKG2
Lb	429	ILE	VAL	conflict	UNP A0A5B9NKG2
Lb	467	ALA	PRO	conflict	UNP A0A5B9NKG2
Lb	535	SER	THR	conflict	UNP A0A5B9NKG2
Lb	567	VAL	ILE	conflict	UNP A0A5B9NKG2
Lb	580	ASN	ALA	conflict	UNP A0A5B9NKG2
Lb	727	GLY	ASP	conflict	UNP A0A5B9NKG2
Lb	964	SER	THR	conflict	UNP A0A5B9NKG2
Lb	973	PRO	THR	conflict	UNP A0A5B9NKG2
Lb	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
Lb	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
Lc	217	SER	ALA	conflict	UNP A0A5B9NKG2
Lc	278	ILE	VAL	conflict	UNP A0A5B9NKG2
Lc	328	THR	ALA	conflict	UNP A0A5B9NKG2
Lc	369	GLY	ASP	conflict	UNP A0A5B9NKG2
Lc	413	GLU	GLY	conflict	UNP A0A5B9NKG2
Lc	419	GLU	ASP	conflict	UNP A0A5B9NKG2
Lc	422	THR	SER	conflict	UNP A0A5B9NKG2
Lc	429	ILE	VAL	conflict	UNP A0A5B9NKG2
Lc	467	ALA	PRO	conflict	UNP A0A5B9NKG2
Lc	535	SER	THR	conflict	UNP A0A5B9NKG2
Lc	567	VAL	ILE	conflict	UNP A0A5B9NKG2
Lc	580	ASN	ALA	conflict	UNP A0A5B9NKG2
Lc	727	GLY	ASP	conflict	UNP A0A5B9NKG2
Lc	964	SER	THR	conflict	UNP A0A5B9NKG2
Lc	973	PRO	THR	conflict	UNP A0A5B9NKG2
Lc	1141	LYS	GLN	conflict	UNP A0A5B9NKG2

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Chain	Residue	Modelled	Actual	Comment	Reference
Lc	1180	ILE	VAL	conflict	UNP A0A5B9NKG2
Ld	217	SER	ALA	conflict	UNP A0A5B9NKG2
Ld	278	ILE	VAL	conflict	UNP A0A5B9NKG2
Ld	328	THR	ALA	conflict	UNP A0A5B9NKG2
Ld	369	GLY	ASP	conflict	UNP A0A5B9NKG2
Ld	413	GLU	GLY	conflict	UNP A0A5B9NKG2
Ld	419	GLU	ASP	conflict	UNP A0A5B9NKG2
Ld	422	THR	SER	conflict	UNP A0A5B9NKG2
Ld	429	ILE	VAL	conflict	UNP A0A5B9NKG2
Ld	467	ALA	PRO	conflict	UNP A0A5B9NKG2
Ld	535	SER	THR	conflict	UNP A0A5B9NKG2
Ld	567	VAL	ILE	conflict	UNP A0A5B9NKG2
Ld	580	ASN	ALA	conflict	UNP A0A5B9NKG2
Ld	727	GLY	ASP	conflict	UNP A0A5B9NKG2
Ld	964	SER	THR	conflict	UNP A0A5B9NKG2
Ld	973	PRO	THR	conflict	UNP A0A5B9NKG2
Ld	1141	LYS	GLN	conflict	UNP A0A5B9NKG2
Ld	1180	ILE	VAL	conflict	UNP A0A5B9NKG2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BM	347	Total	C	N	O	S	0	0
			2664	1664	459	533	8		
2	BK	347	Total	C	N	O	S	0	0
			2664	1664	459	533	8		
2	BO	347	Total	C	N	O	S	0	0
			2664	1664	459	533	8		
2	BP	277	Total	C	N	O	S	0	0
			2180	1373	377	424	6		
2	BL	277	Total	C	N	O	S	0	0
			2180	1373	377	424	6		
2	BN	277	Total	C	N	O	S	0	0
			2180	1373	377	424	6		

- Molecule 3 is a protein called Baseplate subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BQ	295	Total	C	N	O	S	0	0
			2263	1426	385	436	16		
3	BV	295	Total	C	N	O	S	0	0
			2263	1426	385	436	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	BS	295	Total	C	N	O	S	0	0
			2263	1426	385	436	16		
3	BR	295	Total	C	N	O	S	0	0
			2263	1426	385	436	16		
3	BT	295	Total	C	N	O	S	0	0
			2263	1426	385	436	16		
3	BU	295	Total	C	N	O	S	0	0
			2263	1426	385	436	16		

- Molecule 4 is a protein called Baseplate wedge protein gp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AX	646	Total	C	N	O	S	0	0
			5125	3252	853	1009	11		
4	AW	648	Total	C	N	O	S	0	0
			5145	3265	856	1013	11		
4	AT	646	Total	C	N	O	S	0	0
			5125	3252	853	1009	11		
4	AS	648	Total	C	N	O	S	0	0
			5145	3265	856	1013	11		
4	AV	646	Total	C	N	O	S	0	0
			5125	3252	853	1009	11		
4	AU	648	Total	C	N	O	S	0	0
			5145	3265	856	1013	11		
4	AR	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
4	AQ	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
4	AN	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
4	AM	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
4	AP	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
4	AO	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		

- Molecule 5 is a protein called Baseplate wedge protein gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AY	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	AZ	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
5	A0	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
5	A1	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
5	A2	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
5	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
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
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
A2	530	ALA	SER	conflict	UNP A0A2K9V5T9
A2	532	HIS	ASN	conflict	UNP A0A2K9V5T9
A2	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 6 is a protein called Baseplate wedge subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A4	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
6	A9	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
6	A6	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		

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

- Molecule 7 is a protein called Baseplate wedge tail fiber connector.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LN	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LO	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LM	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LQ	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LR	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LP	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LB	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LC	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LA	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LE	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	LF	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LD	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LH	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LI	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LG	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LK	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LL	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
7	LJ	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		

- Molecule 8 is a protein called Baseplate wedge protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	FA	66	Total	C	N	O	S	0	0
			499	311	85	101	2		
8	FB	66	Total	C	N	O	S	0	0
			499	311	85	101	2		
8	FC	66	Total	C	N	O	S	0	0
			499	311	85	101	2		
8	FJ	66	Total	C	N	O	S	0	0
			499	311	85	101	2		
8	FK	66	Total	C	N	O	S	0	0
			499	311	85	101	2		
8	FL	66	Total	C	N	O	S	0	0
			499	311	85	101	2		
8	FS	66	Total	C	N	O	S	0	0
			499	311	85	101	2		
8	FT	66	Total	C	N	O	S	0	0
			499	311	85	101	2		
8	FU	66	Total	C	N	O	S	0	0
			499	311	85	101	2		
8	Fb	66	Total	C	N	O	S	0	0
			499	311	85	101	2		
8	Fc	66	Total	C	N	O	S	0	0
			499	311	85	101	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	Fd	66	Total 499	C 311	N 85	O 101	S 2	0	0
8	Fk	66	Total 499	C 311	N 85	O 101	S 2	0	0
8	Fl	66	Total 499	C 311	N 85	O 101	S 2	0	0
8	Fm	66	Total 499	C 311	N 85	O 101	S 2	0	0
8	Ft	66	Total 499	C 311	N 85	O 101	S 2	0	0
8	Fu	66	Total 499	C 311	N 85	O 101	S 2	0	0
8	Fv	66	Total 499	C 311	N 85	O 101	S 2	0	0

- Molecule 9 is a protein called Tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SA	649	Total 4993	C 3142	N 850	O 985	S 16	0	0
9	SB	649	Total 4993	C 3142	N 850	O 985	S 16	0	0
9	SC	649	Total 4993	C 3142	N 850	O 985	S 16	0	0
9	SD	649	Total 4993	C 3142	N 850	O 985	S 16	0	0
9	SE	649	Total 4993	C 3142	N 850	O 985	S 16	0	0
9	SF	649	Total 4993	C 3142	N 850	O 985	S 16	0	0
9	SK	655	Total 5037	C 3170	N 856	O 995	S 16	0	0
9	SG	655	Total 5037	C 3170	N 856	O 995	S 16	0	0
9	SL	655	Total 5037	C 3170	N 856	O 995	S 16	0	0
9	SH	655	Total 5037	C 3170	N 856	O 995	S 16	0	0
9	SI	655	Total 5037	C 3170	N 856	O 995	S 16	0	0
9	SJ	655	Total 5037	C 3170	N 856	O 995	S 16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	SQ	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SP	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SM	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SN	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SO	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SR	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SW	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SS	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	ST	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SU	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SV	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SX	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SY	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	SZ	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sa	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sb	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sc	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sd	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Se	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sf	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sg	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	Sh	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Si	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sj	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sk	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sl	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sm	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sn	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	So	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
9	Sp	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SA	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SB	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SC	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SD	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SE	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SF	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SK	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SG	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SL	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SH	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SI	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SJ	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SQ	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SP	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SM	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SN	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SO	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SR	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SW	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SS	482	ILE	VAL	conflict	UNP A0A2K9V5S7
ST	482	ILE	VAL	conflict	UNP A0A2K9V5S7

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Chain	Residue	Modelled	Actual	Comment	Reference
SU	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SV	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SX	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SY	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SZ	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sa	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sb	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sc	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sd	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Se	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sf	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sg	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sh	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Si	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sj	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sk	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sl	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sm	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sn	482	ILE	VAL	conflict	UNP A0A2K9V5S7
So	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sp	482	ILE	VAL	conflict	UNP A0A2K9V5S7

- Molecule 10 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	TM	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TN	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TO	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TP	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TQ	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TR	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TW	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TS	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TT	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	TU	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TV	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TX	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TY	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	TZ	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Ta	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tb	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tc	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Td	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Te	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tf	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tg	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Th	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Ti	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tj	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tk	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tl	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tm	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tn	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	To	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tp	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	Tq	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tr	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Ts	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tt	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tu	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
10	Tv	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		

- Molecule 11 is a protein called IraD/Gp25-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	132	Total	C	N	O	S	0	0
			1044	648	183	209	4		
11	AB	132	Total	C	N	O	S	0	0
			1044	648	183	209	4		
11	AD	132	Total	C	N	O	S	0	0
			1044	648	183	209	4		
11	AC	132	Total	C	N	O	S	0	0
			1044	648	183	209	4		
11	AE	132	Total	C	N	O	S	0	0
			1044	648	183	209	4		
11	AF	132	Total	C	N	O	S	0	0
			1044	648	183	209	4		

- Molecule 12 is a protein called Putative baseplate hub subunit.

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

- Molecule 13 is a protein called Baseplate wedge subunit.

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

- Molecule 14 is a protein called Baseplate central spike protein.

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

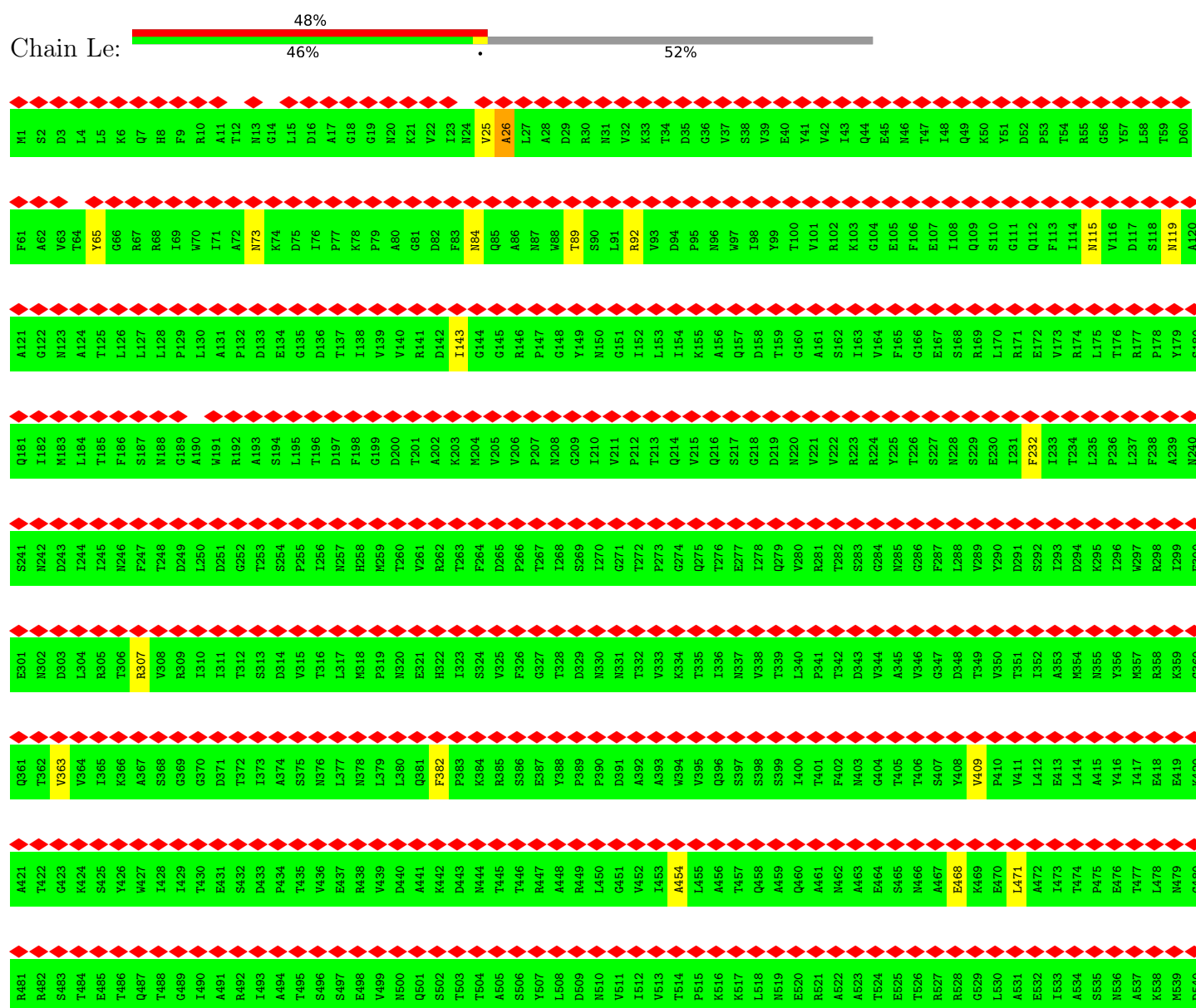
- Molecule 15 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

3 Residue-property plots

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: Long tail fiber proximal subunit





GLY
PRO
VAL
LYS
ILE
TRP
PRO
ASP
ARG
PRO
ASN
GLN
THR
LEU
LYS
PHE
GLU
TRP
VAL
GLY
ASP

- Molecule 1: Long tail fiber proximal subunit



F61	A62	T63	V64	Y65	G66	R67	R68	I69	W70	I71	A72	N73	K74	D75	I76	P77	K78	F79	A80	G81	D82	F83	N84	Q85	A86	N87	W88	T89	S90	L91	R92	V93	D94	P95	P96	W97	I98	Y99	T100	V101	R102	K103	G104	E105	F106	E107	I108	Q109	S110	G111	Q112	F113	I114	N115	V116	D117	S118	N119	A120
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A121	G122	M123	A124	T125	L126	L127	L128	P129	L130	A131	P132	D133	E134	G135	D136	T137	I138	V139	V140	D142	I143	G144	G145	R146	P147	G148	Y149	M150	G151	I152	L153	I154	K155	A156	Q157	D158	T159	G160	A161	S162	I163	V164	F165	G166	E167	S168	R169	L170	R171	E172	V173	R174	L175	T176	R177	P178	Y179	S180
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Q181	I182	M183	L184	T185	F186	S187	M188	G189	A190	W191	R192	R193	S194	L195	T196	D197	F198	G199	D200	T201	D202	A203	M204	V205	V206	P207	N208	G209	T210	V211	P212	T213	Q214	V215	Q216	S217	G218	D219	N220	V221	V222	A223	R224	Y225	T226	S227	N228	S229	E230	T231	F232	T233	T234	L235	L236	L237	F238	A239	M240
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S241	N242	D243	L244	T245	N246	F247	T248	D249	L250	D251	G252	T253	S254	P255	L256	N257	H258	M259	T260	R262	T263	F264	D265	P266	T267	L268	S269	L270	G271	T272	T273	G274	G275	T276	E277	L278	Q279	V280	R281	T282	S283	G284	N285	G286	F287	L288	V289	Y290	D291	S292	L293	D294	K295	L296	W297	R298	L299	F300
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E301	N302	D303	L304	R305	T306	R307	V308	R309	I310	I311	T312	S313	D314	V315	T316	L317	M318	P319	N320	E321	H322	I323	S324	V325	F326	G327	T328	D329	N330	N331	T332	V333	K334	T335	I336	N337	V338	L339	L340	P341	T342	D343	V344	A345	V346	G347	D348	T349	V350	T351	I352	A353	M354	N355	V356	M357	R358	K359	G360
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Q361	T362	V363	V364	V365	K366	A367	S368	G369	G370	D371	T372	L373	A374	S375	N376	L377	N378	L380	Q381	F382	P383	K384	S386	E387	Y388	P389	D391	A392	A393	W394	V395	Q396	S397	S398	S399	I400	T401	F402	N403	G404	T405	T406	S407	Y408	V409	P410	V411	L412	E413	L414	A415	Y416	I417	E418	E419	K420
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A421	T422	G423	K424	S425	Y426	W427	I428	L429	T430	E431	S432	D433	P434	T435	V436	E437	R438	V439	D440	A441	K442	D443	N444	T445	T446	R447	A448	R449	L450	G451	V452	I453	A454	L455	A456	T457	Q458	A459	Q460	A461	N462	A463	E464	S465	N466	A467	E468	K469	E470	L471	A472	I473	T474	P475	E476	T477	L478	N479	C480
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R481	R482	R483	T484	E485	T486	T487	T488	G489	I490	A491	R492	I493	A494	T495	S496	S497	E498	V499	N500	Q501	S502	T503	T504	A505	S506	Y507	L508	D509	N510	V511	F512	V513	T514	P515	K516	K517	L518	N519	F520	R521	A522	A523	T524	E525	T526	R527	R528	G529	L530	A531	F532	T533	A534	S535	N536	A537	K538	D540
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A541	G542	T543	D544	D545	F546	T547	T548	V549	T550	P551	K552	K553	L554	L555	V556	V557	T558	T559	S560	D601	S562	S563	L564	S565	V566	V567	Q568	L569	V570	K571	T572	G573	G574	A575	P576	N577	T578	T579	N580	D601	S582	S583	S584	A585	G586	T587	G588	T589	F590	D601	H592	S593	D594	V595	K596	N597	A598	V599	T600
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P601	K602	T603	L604	R605	E606	Y607	K608	A609	T610	V611	M612	Q613	S614	G615	I616	TRP	LEU	ALA	ASP	SER	GLU	VAL	ARG	ASN	GLY	THR	PRO	ALA	SER	SER	SER	ASN	ILE	PRO	THR	VAL	VAL	THR	PRO	PRO	GLU	ALA	ALA	LEU	HIS	LYS	LYS	VAL	ALA	ALA	THR	ASP	GLY	GLY	ALA	ILE	GLY	LEU	ILE	ILE	GLN	ILE	ALA
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THR	GLN	THR	THR	VAL	GLU	ASN	ALA	ALA	GLY	GLY	VAL	THR	ASN	LYS	ALA	VAL	THR	THR	PRO	LYS	THR	LEU	ASN	ASP	ARG	THR	ALA	THR	THR	ASN	ASP	ARG	THR	GLY	ILE	ALA	ALA	ARG	PHE	ALA	THR	THR	PRO	PRO	GLY	GLN	GLY	GLU	PHE	GLU	GLU	ALA	ALA	GLY	THR	SER	SER	THR	THR	VAL	MET	VAL	ASN	PRO	PRO	LYS	LEU	LEU	PHE
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[illegible]

- Molecule 1: Long tail fiber proximal subunit



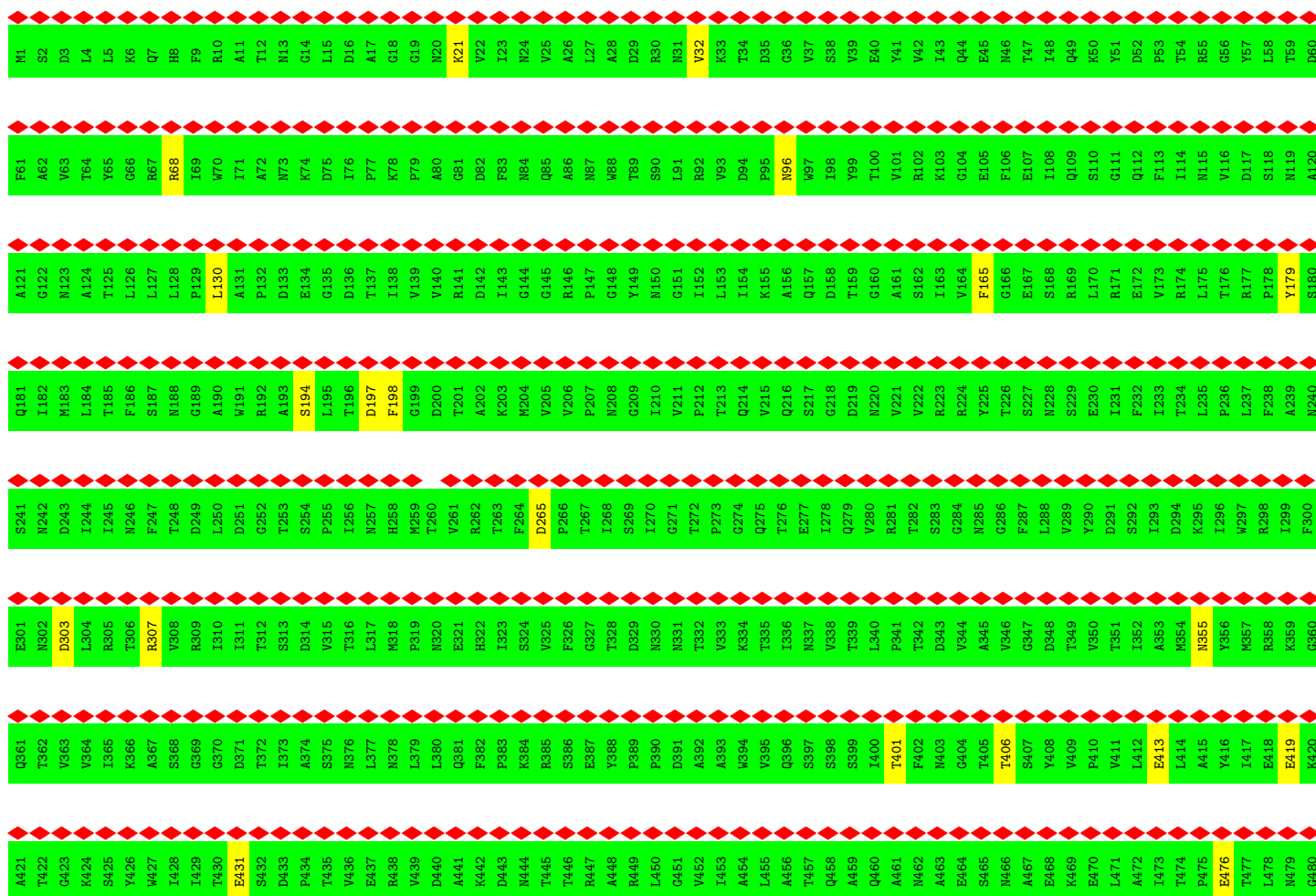
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N302	N242	I182	G122	A62	S2
D303	D243	M183	G123	V63	D3
L304	L244	L184	A124	T64	L4
R305	T245	T185	T125	Y65	L5
T306	N246	F186	L126	G66	K6
R307	T247	S187	L127	R67	Q7
V308	T248	N188	L128	R68	H8
R309	D249	G189	P129	I69	F9
I310	L250	A190	L130	W70	R10
I311	D251	W191	A131	I71	A11
T312	G252	W192	P132	A72	T12
S313	T253	A193	D133	N73	M13
D314	S254	S194	E134	K74	G14
V315	P255	L195	G135	D75	L15
T316	T256	T196	D136	I76	D16
L317	N257	D197	T137	F77	A17
M318	H258	F198	I138	K78	G18
P319	M259	G199	V139	F79	G19
N320	T260	D200	V140	A80	N20
E321	V261	T201	R141	G81	K21
H322	R262	A202	D142	D82	V22
I323	T263	K203	I143	F83	T23
S324	F264	M204	G144	N84	N24
V325	D265	V205	G145	K85	V25
F326	P266	V206	R146	A86	A26
G327	T267	P207	P147	N87	L27
T328	T268	N208	G148	W88	A28
D329	S269	G209	Y149	T89	D29
N330	L270	I210	N150	S90	R30
N331	G271	V211	G151	L91	N31
T332	T272	P212	I152	R92	V32
V333	P273	T213	L153	V93	K33
K334	G274	Q214	I154	D94	T34
T335	Q275	V215	K155	P95	D35
I336	T276	Q216	A156	N96	G36
N337	E277	S217	Q157	W97	V37
V338	L278	G218	D158	I98	S38
T339	Q279	D219	T159	Y99	V39
L340	N280	N220	G160	T100	E40
P341	R281	V221	A161	V101	Y41
T342	T282	V222	S162	R102	V42
D343	S283	R223	I163	K103	I43
V344	G284	R224	V164	G104	O44
A345	N285	Y225	F165	E105	E45
V346	G286	T226	G166	F106	N46
G347	F287	S227	E167	E107	T47
D348	L288	N228	S168	I108	I48
T349	V289	S229	R169	Q109	Q49
V350	Y290	E230	L170	S110	K50
T351	D291	I231	R171	G111	Y51
I352	S292	F232	E172	Q112	D52
A353	T293	I233	V173	F113	P53
M354	D294	T234	R174	I114	T54
N355	K295	L235	R175	N115	R55
Y356	T296	P236	T176	V116	G56
M357	W297	L237	R177	D117	Y57
R358	R298	F238	P178	S118	L58
K359	T299	A239	Y179	N119	T59
T360	F300	N240	G180	A120	D60





GLY	ALA	LYS	TYR	GLY	ARG	THR
PRO	ASP	GLY	ALA	ASP	ASP	PRO
VAL	LYS	LEU	ARG	ALA	GLY	ASP
LYS	PHE	ARG	LEU	ILE	SER	LYS
TRP	ALA	TYR	ASP	GLY	GLY	ALA
PRO	HIS	MET	GLY	GLY	ARG	ARG
ASP	ARG	VAL	ARG	THR	ILE	ARG
PRO	VAL	PRO	TYR	VAL	ILE	ILE
PRO	TRP	ILE	VAL	MET	TYR	TYR
ASN	MET	ARG	LYS	VAL	ALA	ALA
GLN	ARG	THR	LYS	LYS	GLY	GLN
THR	ILE	PRO	ALA	ASP	PRO	THR
LEU	TYR	ILE	GLY	VAL	GLN	ILE
LYS	ASN	ASP	ASP	GLN	THR	THR
PHE	ASN	PRO	THR	MET	ALA	GLY
GLU	ASN	ALA	MET	LEU	SER	ALA
TRP	LEU	ASN	THR	ALA	ALA	TRP
VAL	ASN	PRO	GLY	VAL	GLY	SER
GLY	LYS	SER	ASN	GLU	THR	PHE
ASP	PHE	THR	LEU	GLY	THR	GLN
	ASP	LEU	ASN	LEU	LYS	GLN
	ASP	VAL	ILE	ASN	ILE	ASP
	THR	VAL	ASN	SER	ARG	THR
	MET	THR	ASN	ILE	VAL	SER
	ARG	GLY	SER	PHE	LYS	PHE
	VAL	TYR	ALA	GLY	ASN	SER
	PHE	GLU	ILE	ALA	GLY	ASN
	THR	THR	VAL	GLN	THR	ASN
	SER	LYS	ILE	SER	GLY	ILE
	THR	THR	THR	GLN	THR	SER
	ALA	ALA	GLY	SER	THR	VAL
	THR	ALA	THR	SER	THR	GLN
	PRO	THR	SER	ALA	ALA	ASN
	ILE	THR	VAL	ARG	ALA	ASN
	GLY	ILE	PRO	THR	THR	ASN
	ALA	GLY	THR	ALA	PHE	GLY
	PRO	VAL	ASN	ASP	GLY	GLY
	SER	THR	ASN	THR	GLY	GLU
	SER	THR	THR	THR	ASN	VAL
	VAL	ASN	ILE	GLN	GLU	VAL
	LYS	LEU	VAL	GLN	VAL	LYS
	SER	THR	THR	THR	PRO	THR
	THR	THR	TRP	GLY	ASN	THR
	LEU	THR	ALA	SER	VAL	GLY
	GLU	PRO	GLU	TYR	THR	ASN
	VAL	TYR	ILE	PRO	THR	VAL
	LEU	PRO	LYS	ILE	LYS	HIS
	THR	THR	THR	THR	THR	THR
	GLY	GLY	THR	THR	THR	ARG
	ASP	THR	LEU	ASN	SER	GLN

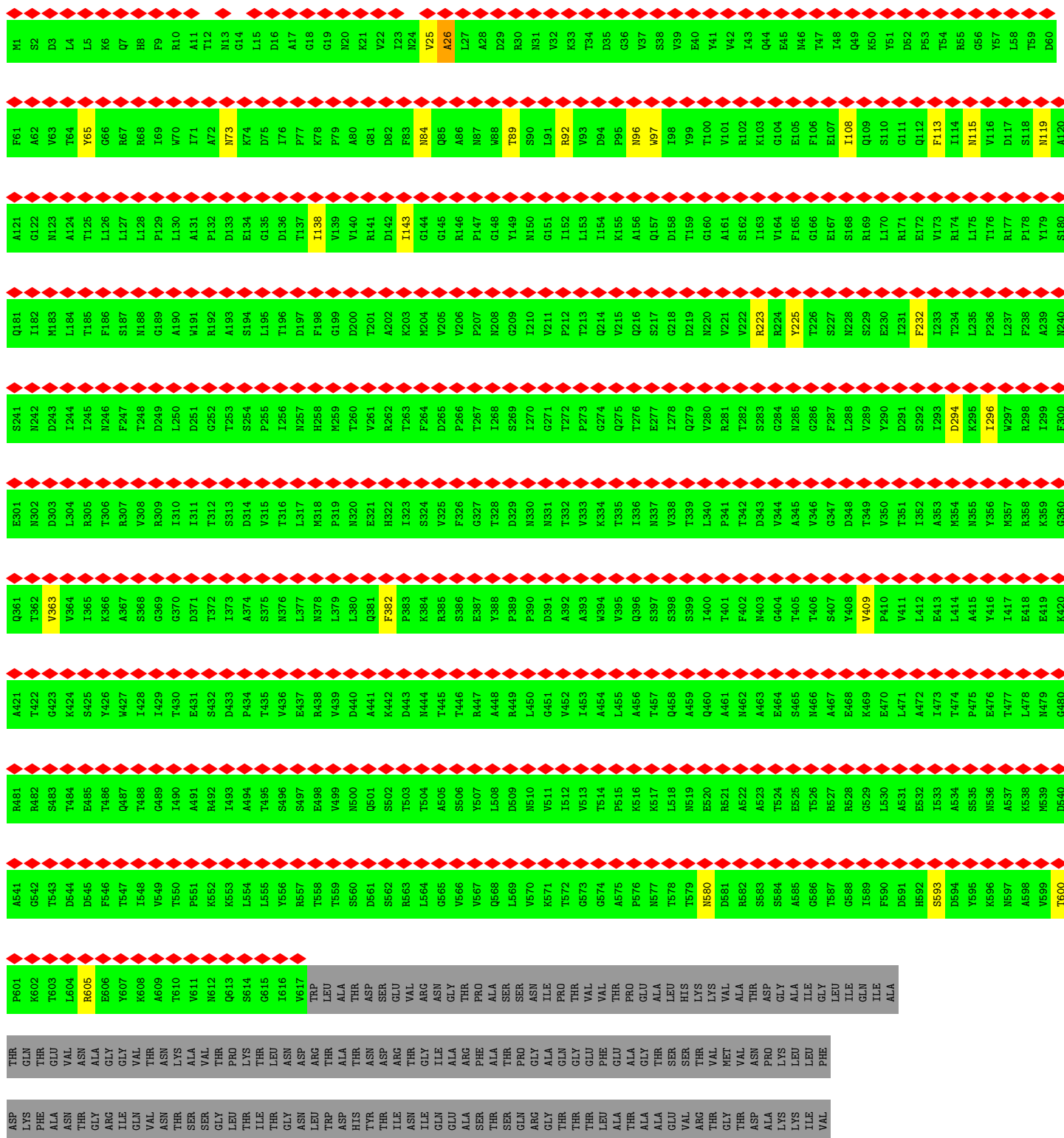
- Molecule 1: Long tail fiber proximal subunit











[illegible]

- Molecule 1: Long tail fiber proximal subunit



E301	Q361	E301	S241	Q181	A121	F61	M1
	T362	N302	N242	I182	G122	A62	S2
	V363	L303	D243	M183	D243	W63	D3
	V364	L304	I244	L184	A124	T64	I4
	L365	R305	I245	L185	T125	W65	L5
	K366	T306	N246	F186	L126	G66	K6
	A367	R307	F247	S187	L127	B67	Q7
	S368	V308	T248	N188	L128	B68	H8
	G369	R309	D249	G189	P129	T69	F9
	G370	I310	L250	A190	L130	W70	R10
H322	D371	I311	D251	W191	A131	I71	A11
	T372	T312	G252	R192	P132	A72	T12
	L373	S313	T253	A193	D133	W73	N13
	A374	D314	S254	S194	E134	K74	G14
	S375	V315	P255	L195	G135	D75	L15
	N376	T316	I256	T196	D136	I76	D16
	L377	L317	N257	D197	T137	P77	A17
	N378	M318	H258	F198	I138	K78	G18
	L379	P319	M259	G199	V139	P79	G19
	L380	N320	T260	D200	V140	A80	N20
F382	Q381	E321	V261	T201	R141	C81	K21
	F382	H322	R262	A202	D142	D82	V22
	P383	I323	T263	K203	I143	F83	T23
	K384	S324	F264	W204	G144	N84	N24
	R385	V325	D265	V205	G145	C85	V25
	S386	F326	P266	V206	R146	A86	A26
	E387	G327	T267	P207	P147	N87	L27
	L388	T328	I268	N208	G148	N88	A28
	P389	D329	S269	G209	Y149	T89	D29
	P390	N330	I270	T210	N150	S90	R30
I400	D391	N331	G271	V211	G151	L91	N31
	A392	T332	T272	P212	I152	R92	V32
	A393	V333	T273	T213	L153	W93	K33
	W394	K334	G274	Q214	I154	D94	T34
	V395	T335	Q275	V215	K155	P95	D35
	Q396	I336	T276	Q216	A156	N96	D36
	S397	N337	E277	S217	Q157	W97	G36
	S398	V338	L278	C218	D158	I98	S38
	S399	T339	Q279	D219	T159	Y99	V39
	I400	L340	V280	N220	G160	T100	E40
Y401	F401	P341	R281	V221	A161	V101	E41
	F402	T342	T282	V222	S162	R102	W42
	M403	D343	S283	R223	I163	K103	I43
	G404	V344	G284	R224	V164	G104	Q44
	T405	A345	N285	Y225	F165	E105	E45
	T406	V346	G286	T226	G166	F106	M46
	S407	G347	F287	S227	E167	E107	T47
	Y408	D348	L288	N228	S168	I108	I48
	V409	T349	T289	S229	R169	Q109	Q49
	P410	V350	Y290	E230	L170	S110	K50
Y411	V411	T351	D291	I231	R171	G111	V51
	L412	S352	S292	F232	E172	Q112	D52
	E413	A353	I293	I233	V173	F113	P53
	L414	M354	D294	T234	R174	I114	T54
	A415	N355	K295	L235	L175	N115	R55
	Y416	V356	I296	P236	T176	V116	G56
	I417	M357	W297	L237	R177	D117	V57
	E418	R358	R298	F238	P178	S118	L58
	E419	K359	I299	A239	Y179	N119	T59
	I420	C360	T300	W240	F180	A120	T60

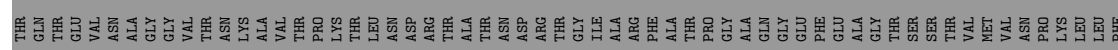
ARG	ASP	THR	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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LYS	TYR	GLY	ARG	THR	VAL	THR	ASP	THR	P601	A541	R481	A421	Q361	E301	S241	Q181
GLY	ALA	ASN	ASP	PRO	ARG	ALA	LYS	GLN	K602	G542	R482	T422	T362	N302	N242	I182
LEU	ARG	ALA	GLY	THR	LEU	ALA	THR	THR	T603	T543	S483	G423	V363	D303	D243	M183
GLY	THR	VAL	THR	TYR	THR	LEU	ASN	VAL	L604	D544	T484	K424	V364	L304	I244	L184
MET	GLY	GLY	ASP	ALA	GLY	ALA	GLY	GLY	R605	D545	E485	S425	I365	R305	I245	T185
VAL	THR	THR	GLY	ARG	GLY	GLY	ILE	GLY	E606	F546	T486	Y426	K366	T306	N246	F186
ILE	ARG	THR	ILE	ASP	THR	THR	ILE	THR	Y607	T547	Q487	W427	A367	R307	F247	S187
THR	VAL	THR	THR	ILE	THR	THR	GLN	VAL	K608	I548	T488	I428	S368	V308	T248	N188
ARG	ALA	GLY	VAL	ALA	THR	THR	VAL	THR	A609	V549	G489	I429	G369	R309	D249	G189
GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASN	ASN	T610	T550	L490	T430	G370	I310	L250	A190
ASN	ASP	ASN	ASP	ALA	THR	THR	THR	ALA	V611	P651	A491	E431	D371	I311	D251	W191
ASP	THR	THR	THR	THR	THR	THR	THR	THR	N612	K552	R492	S432	T372	T312	G252	R192
THR	THR	THR	THR	THR	THR	THR	THR	THR	Q613	K553	I493	D433	I373	S313	T253	A193
THR	THR	THR	THR	THR	THR	THR	THR	THR	S614	L554	A494	P434	A374	D314	S254	S194
THR	THR	THR	THR	THR	THR	THR	THR	THR	G615	L555	T495	T435	S375	V315	P255	L195
THR	THR	THR	THR	THR	THR	THR	THR	THR	I616	V556	S496	W436	N376	T316	I256	T196
THR	THR	THR	THR	THR	THR	THR	THR	THR	V617	R557	S497	E437	L377	L317	N257	F197
THR	THR	THR	THR	THR	THR	THR	THR	THR	TRP	T558	E498	R438	N378	M318	H258	D198
THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU	T559	V499	W439	L379	P319	M259	G199
THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	V560	N500	D440	L380	N320	T260	D200
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	S561	Q501	A441	Q381	E321	V261	T201
THR	THR	THR	THR	THR	THR	THR	THR	THR	ASP	D562	S502	K442	F382	H322	R262	A202
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	S563	T503	D443	P383	I323	T263	K203
THR	THR	THR	THR	THR	THR	THR	THR	THR	VAL	R663	T504	M444	K384	S324	F264	M204
THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	L564	T505	T445	R385	V325	D265	V205
THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN	G565	A506	T446	S386	F326	P266	V206
THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	V566	S506	T447	E387	G327	T267	P207
THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	G568	L508	A448	P388	T328	I268	N208
THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	L569	D509	R449	P389	D329	S269	G209
THR	THR	THR	THR	THR	THR	THR	THR	THR	SER	V570	N510	L450	P390	N330	I270	I210
THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN	K571	V511	G451	D391	N331	G271	V211
THR	THR	THR	THR	THR	THR	THR	THR	THR	ILE	T572	I512	W452	A392	T332	T272	P212
THR	THR	THR	THR	THR	THR	THR	THR	THR	PRO	G573	V513	I453	A393	V333	P273	T213
THR	THR	THR	THR	THR	THR	THR	THR	THR	VAL	G574	T514	W394	G274	K334	G274	Q214
THR	THR	THR	THR	THR	THR	THR	THR	THR	VAL	A575	P515	I454	V395	T335	Q275	V215
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	A576	K516	L455	Q396	I336	Q216	V216
THR	THR	THR	THR	THR	THR	THR	THR	THR	PRO	P576	K516	A456	Q396	I336	Q216	V216
THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	N577	K517	T457	S397	I337	E277	S217
THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	T578	L518	Q458	S398	V338	E278	G218
THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU	T579	N519	A459	S399	T339	D219	G219
THR	THR	THR	THR	THR	THR	THR	THR	THR	LYS	V580	E520	Q460	I400	L340	V280	N220
THR	THR	THR	THR	THR	THR	THR	THR	THR	LYS	N581	R521	A461	T401	P341	R281	V221
THR	THR	THR	THR	THR	THR	THR	THR	THR	VAL	D582	A522	W462	F402	T342	T282	V222
THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	R583	A523	A463	M403	D343	S283	R223
THR	THR	THR	THR	THR	THR	THR	THR	THR	ASP	S584	T524	E464	G404	V344	G284	R224
THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	A585	E525	S465	T405	A345	N285	Y225
THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	T526	T526	W466	T406	V346	G286	T226
THR	THR	THR	THR	THR	THR	THR	THR	THR	ILE	R527	R528	A467	S407	G347	F287	S227
THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	V528	G529	E468	W408	L288	L288	N228
THR	THR	THR	THR	THR	THR	THR	THR	THR	LEU	V529	V529	K469	W409	T349	V289	S229
THR	THR	THR	THR	THR	THR	THR	THR	THR	ILE	L530	L530	E470	P410	V290	E230	E230
THR	THR	THR	THR	THR	THR	THR	THR	THR	ILE	A531	A531	L471	V411	T291	D291	I231
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	H532	E532	A472	L412	S292	S292	F232
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	I533	I533	I473	E413	I293	I293	I233
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	A534	A534	T474	L414	D294	T234	T234
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F475	S535	F475	A415	N355	N235	L235
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	N536	N536	E476	Y416	I296	P236	P236
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	K537	K537	T477	I417	W297	W297	F238
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	A538	A538	L478	E418	R298	R298	F238
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	V539	V539	M479	E419	K359	I299	A239
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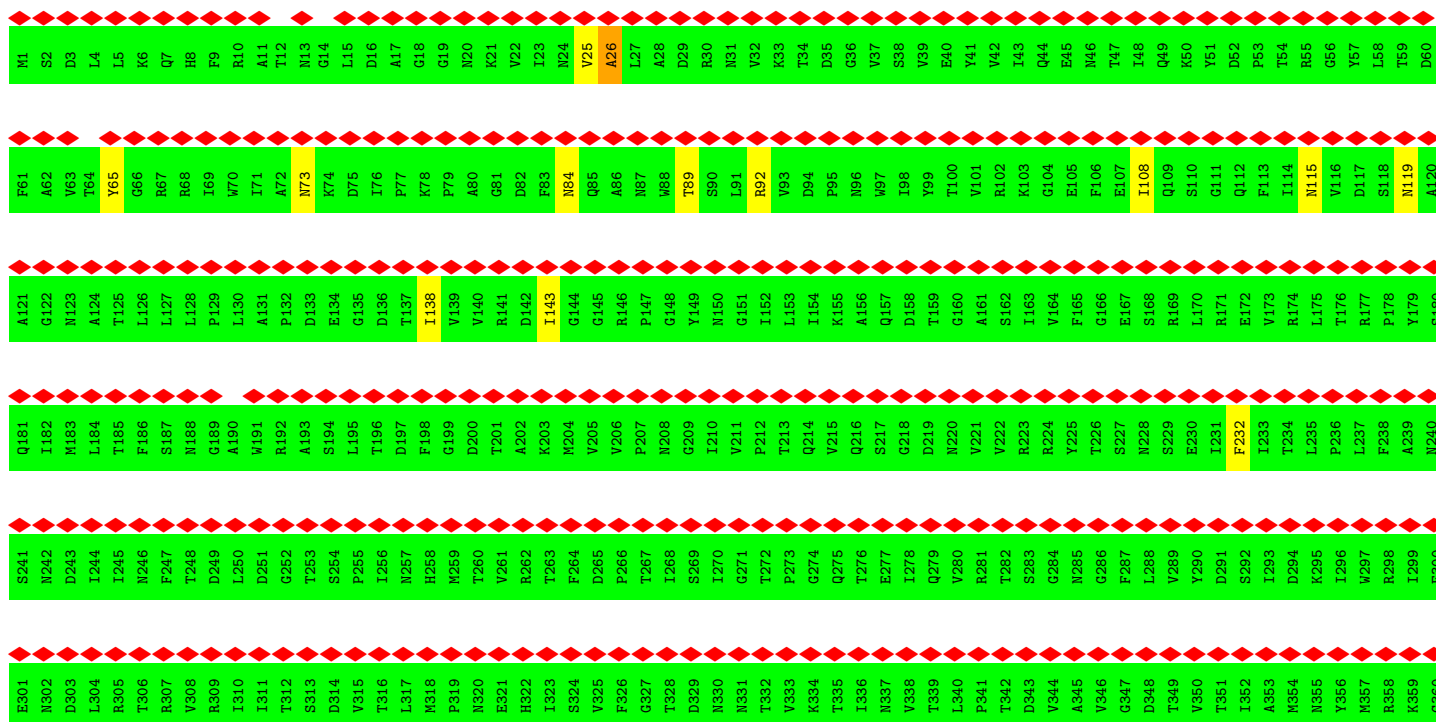
GLY PRO VAL LYS ILE TRP PRO ASP ARG PRO ASN GLN THR LEU LYS PHE GLU TRP VAL GLY ASP

Chain La: 48% 46% 52%



[illegible]

- Molecule 1: Long tail fiber proximal subunit







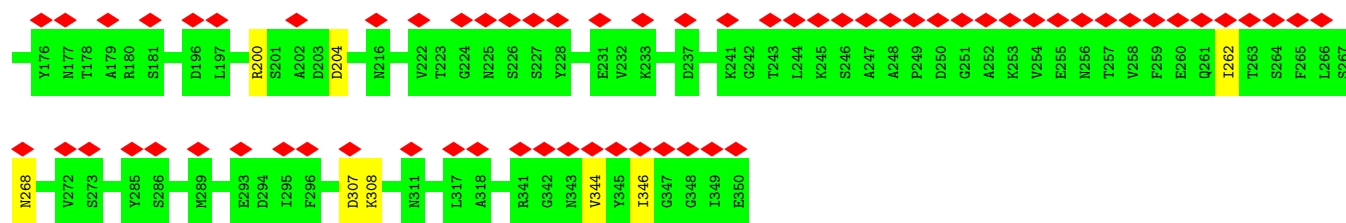
[illegible]

- Molecule 1: Long tail fiber proximal subunit

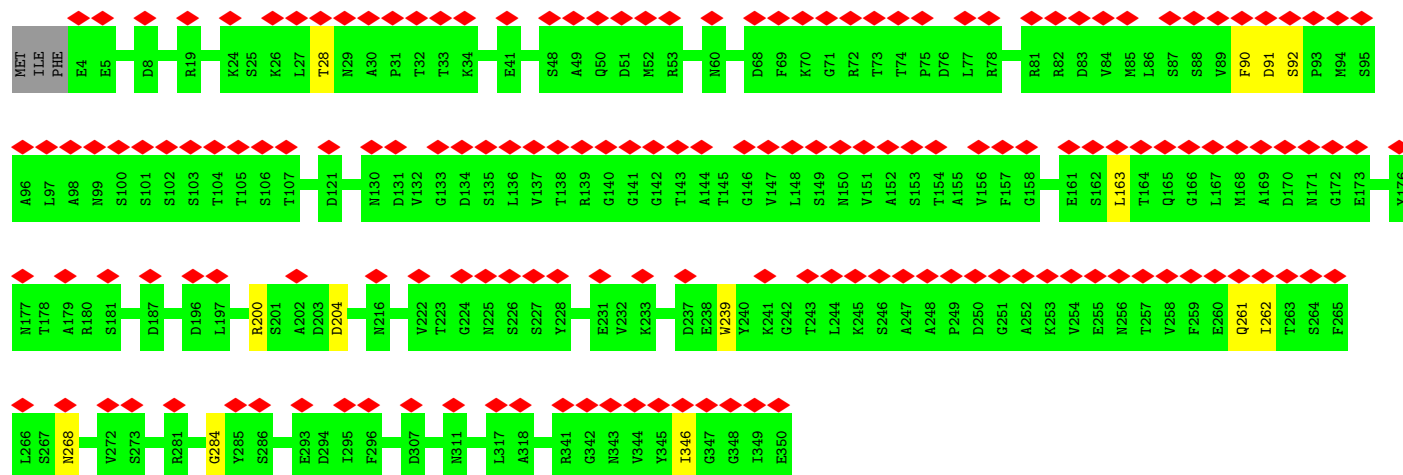


A421	T422	G423	K424	S425	Y426	W427	L428	L429	T430	E431	S432	D433	P434	T435	V436	E437	R438	V439	D440	A441	K442	D443	N444	T445	T446	R447	A448	R449	L450	G451	A452	I453	A454	L455	A456	T457	Q458	A459	Q460	A461	N462	A463	E464	S465	N466	A467	E468	K469	E470	L471	A472	I473	T474	P475	E476	T477	L478	N479	D480
Q361	T362	V363	V364	I365	K366	A367	S368	G369	G370	D371	T372	I373	A374	S375	N376	L377	N378	L379	L380	Q381	F382	K383	K384	K385	S386	E387	X388	P389	P390	D391	A392	A393	W394	V395	Q396	Q397	S398	S399	A400	T401	F402	N403	A404	T405	T406	S407	Y408	V409	P410	V411	L412	E413	L414	A415	Y416	L417	E418	E419	K420
E301	N302	D303	L304	R305	T306	R307	V308	R309	T310	T311	T312	S313	D314	V315	T316	L317	N318	P319	N320	E321	R322	L323	S324	V325	F326	G327	T328	D329	N330	N331	T332	V333	K334	T335	T336	N337	V338	T339	L340	P341	T342	A343	V344	A345	V346	G347	D348	T349	V350	T351	L352	A353	K354	N355	V356	N357	K358	K359	G360
S241	N242	D243	I244	I245	N246	F247	T248	D249	L250	D251	G252	T253	S254	T255	I256	N257	H258	M259	T260	V261	R262	T263	F264	D265	P266	T267	L268	S269	I270	G271	T272	P273	G274	Q275	T276	E277	L278	Q279	V280	R281	T282	S283	G284	N285	G286	F287	L288	V289	V290	D291	S292	T293	D294	K295	T296	W297	R298	I299	F300
Q181	I182	M183	L184	T185	F186	N187	N188	G189	A190	W191	R192	A193	S194	T195	T196	D197	F198	G199	D200	T201	A202	K203	M204	V205	V206	P207	N208	G209	I210	V211	P212	T213	L214	V215	Q216	S217	G218	D219	N220	V221	V222	R223	R224	Y225	T226	S227	N228	S229	E230	I231	F232	T233	T234	L235	P236	L237	F238	A239	N240
A121	G122	A123	A124	T125	L126	L127	L128	P129	L130	A131	P132	D133	E134	G135	D136	T137	I138	V139	V140	R141	D142	K213	G144	Q145	R146	P147	G148	Y149	N150	G151	I152	L153	I154	K155	A156	Q157	D158	T159	G160	A161	S162	K163	V164	F165	G166	E167	L168	R169	L170	R171	E172	V173	R174	L175	T176	R177	P178	Y179	S180
F61	A62	V63	T64	V65	G66	R67	R68	T69	W70	I71	A72	N73	K74	D75	I76	P77	K78	P79	A80	G81	D82	F83	N84	Q85	A86	N87	W88	T89	S90	R91	L92	V93	D94	P95	N96	Q97	I98	V99	T100	V101	R102	K103	G104	E105	F106	E107	I108	Q109	S110	G111	Q112	F113	I114	M115	G116	D117	S118	M119	A120

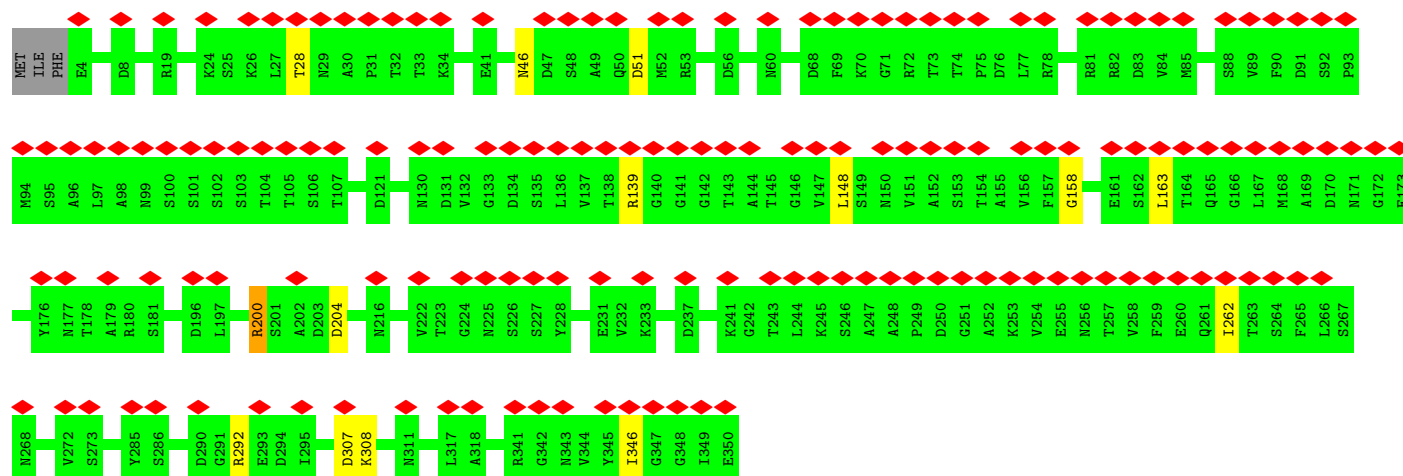




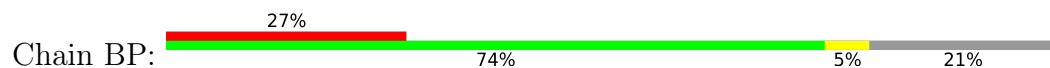
• Molecule 2: Baseplate tail tube cap

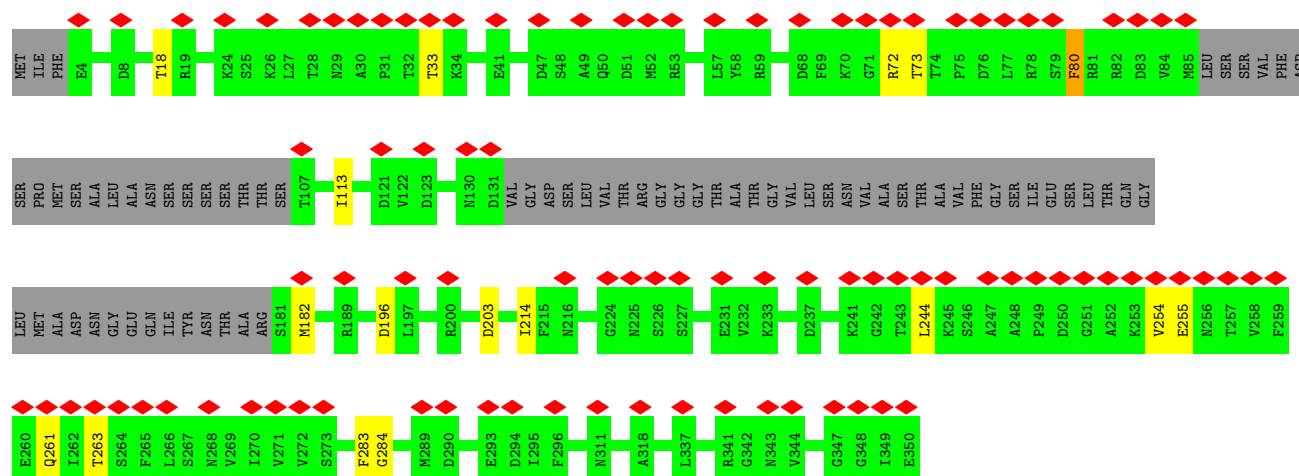


• Molecule 2: Baseplate tail tube cap

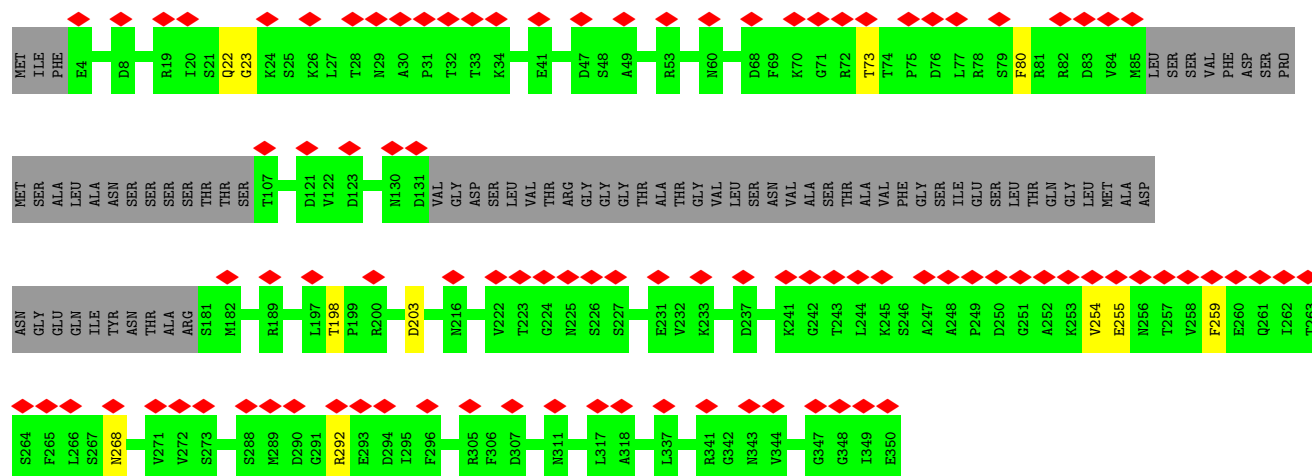
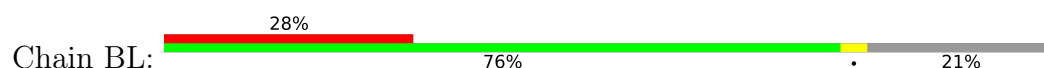


• Molecule 2: Baseplate tail tube cap

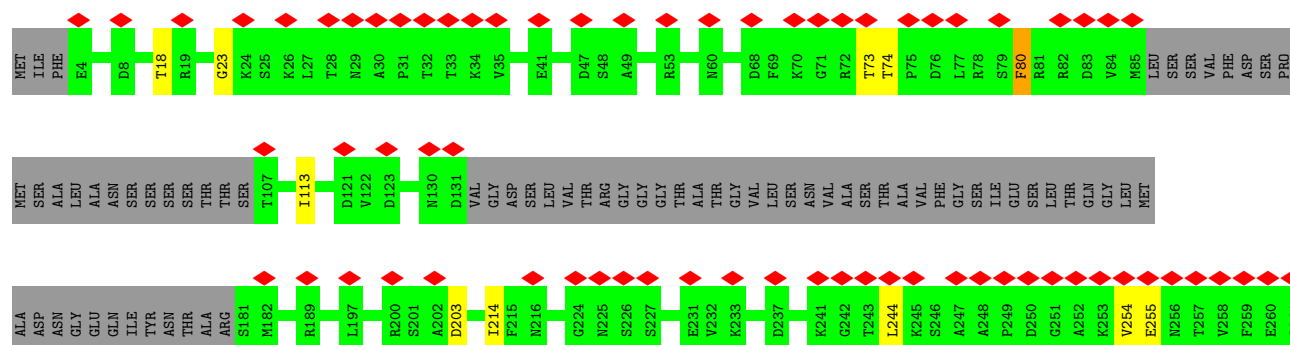
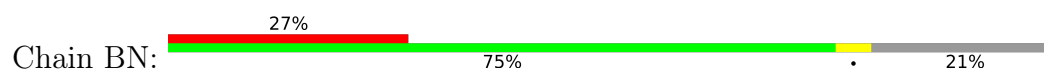


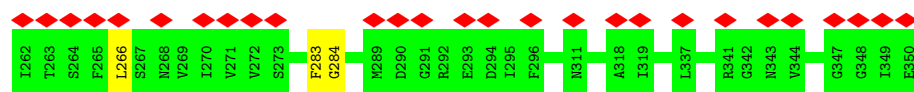


• Molecule 2: Baseplate tail tube cap

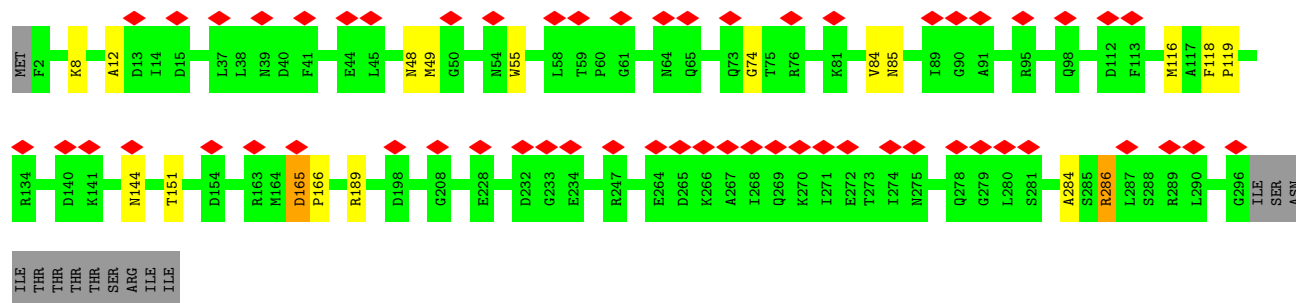
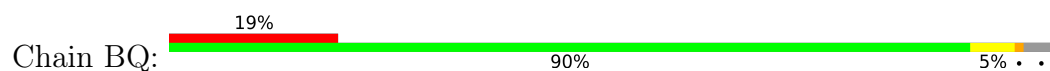


• Molecule 2: Baseplate tail tube cap

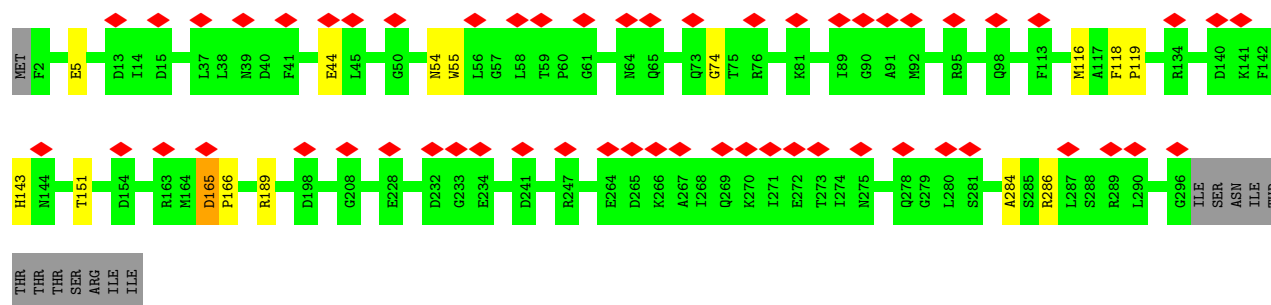
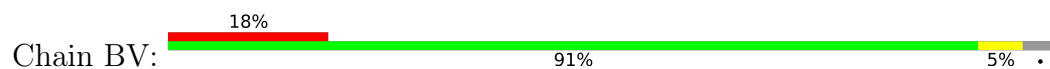




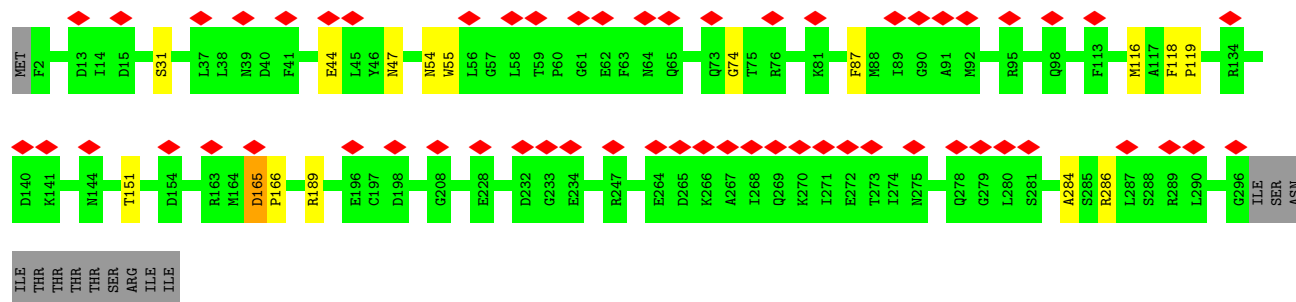
- Molecule 3: Baseplate subunit



- Molecule 3: Baseplate subunit

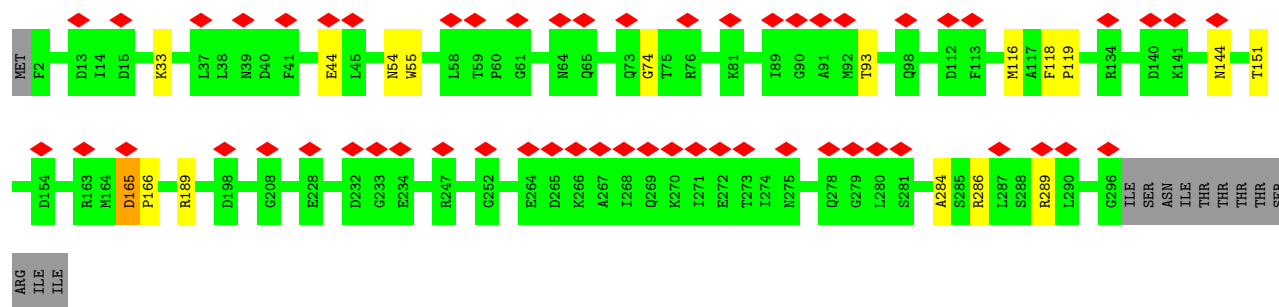


- Molecule 3: Baseplate subunit

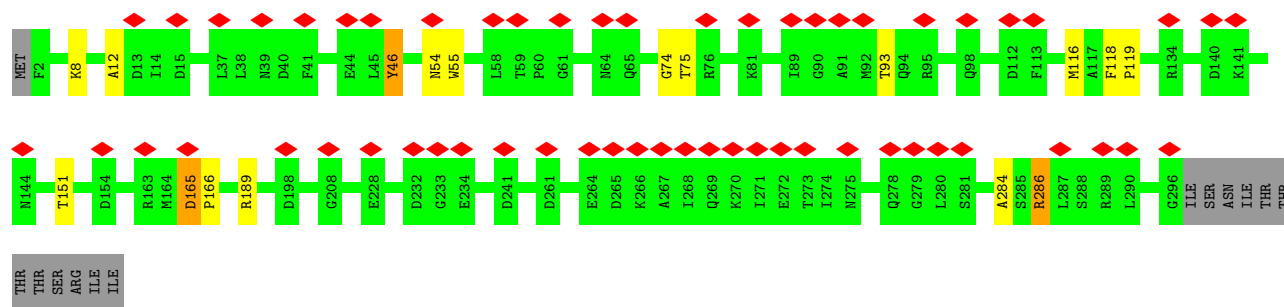
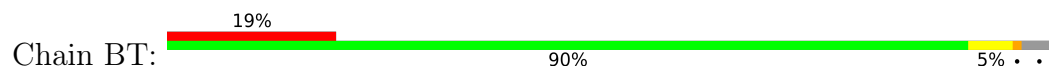


- Molecule 3: Baseplate subunit

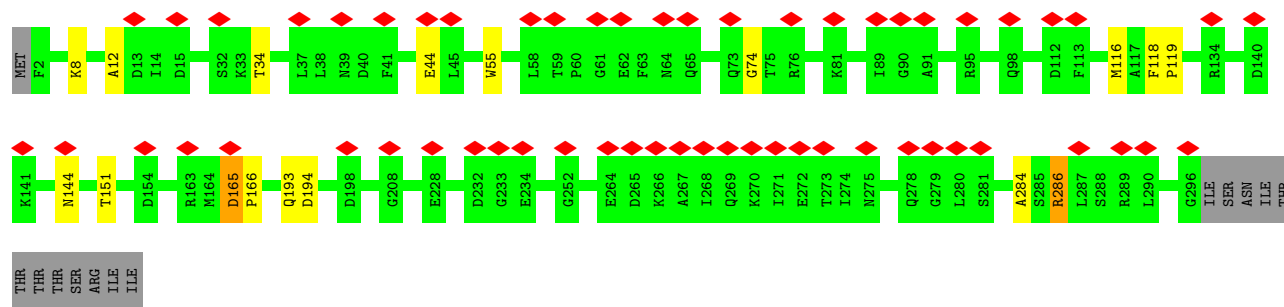




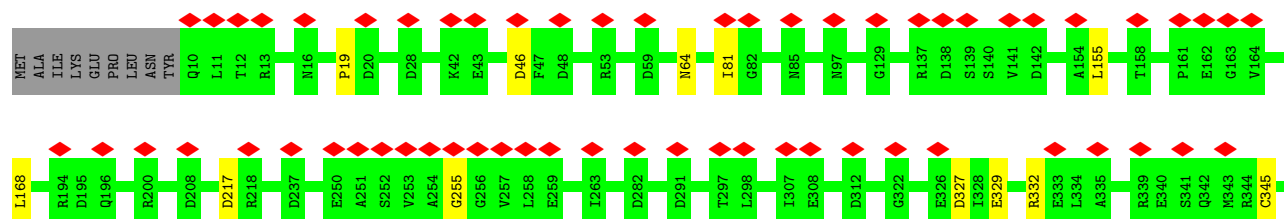
• Molecule 3: Baseplate subunit

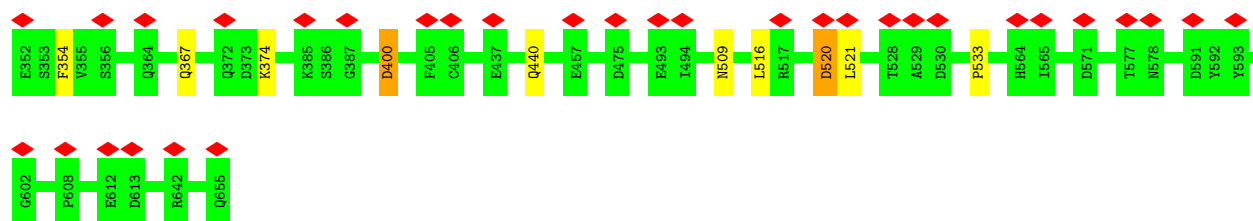


• Molecule 3: Baseplate subunit



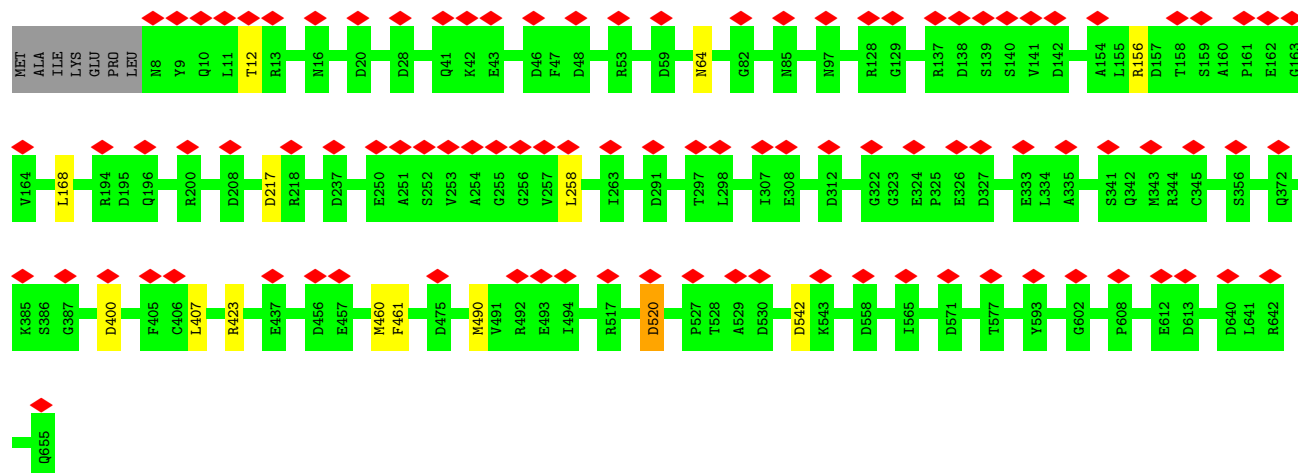
• Molecule 4: Baseplate wedge protein gp6





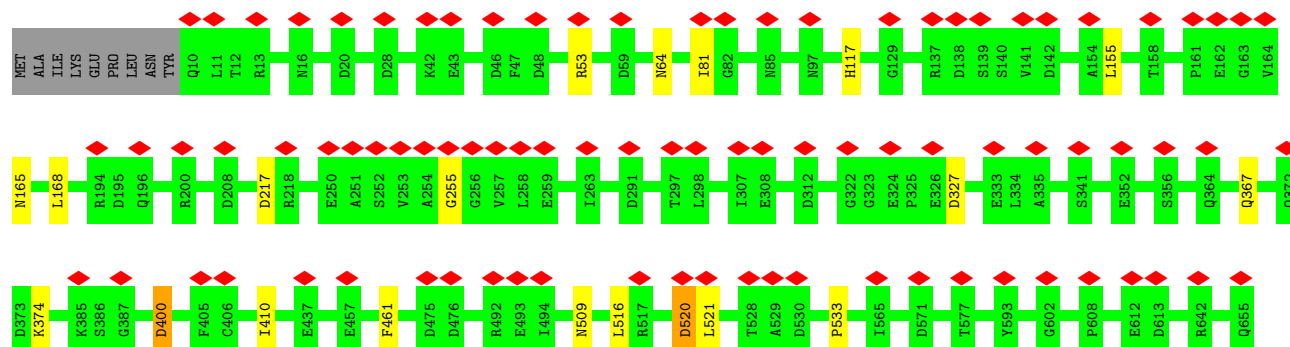
• Molecule 4: Baseplate wedge protein gp6

Chain AW: 15% 97%



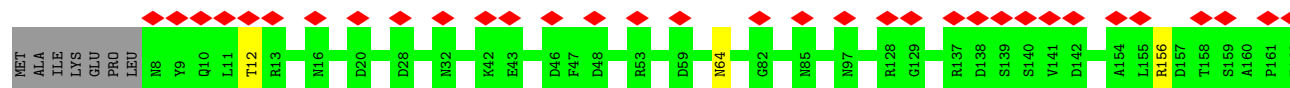
• Molecule 4: Baseplate wedge protein gp6

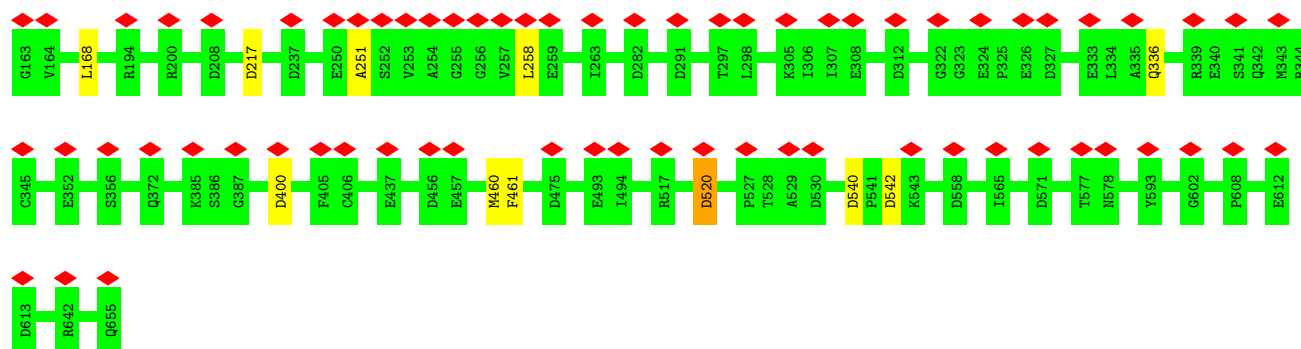
Chain AT: 13% 96%



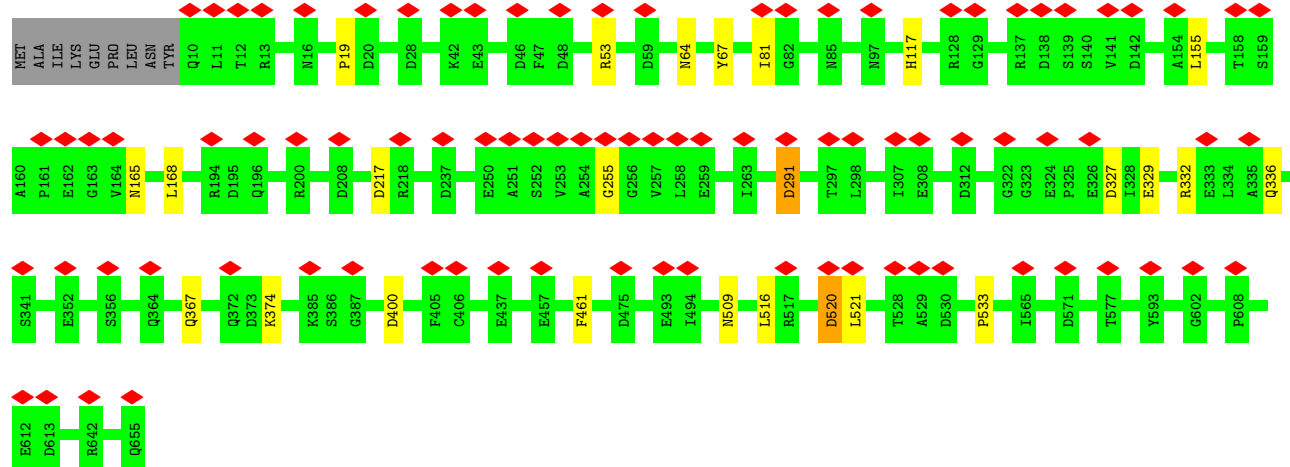
• Molecule 4: Baseplate wedge protein gp6

Chain AS: 15% 97%

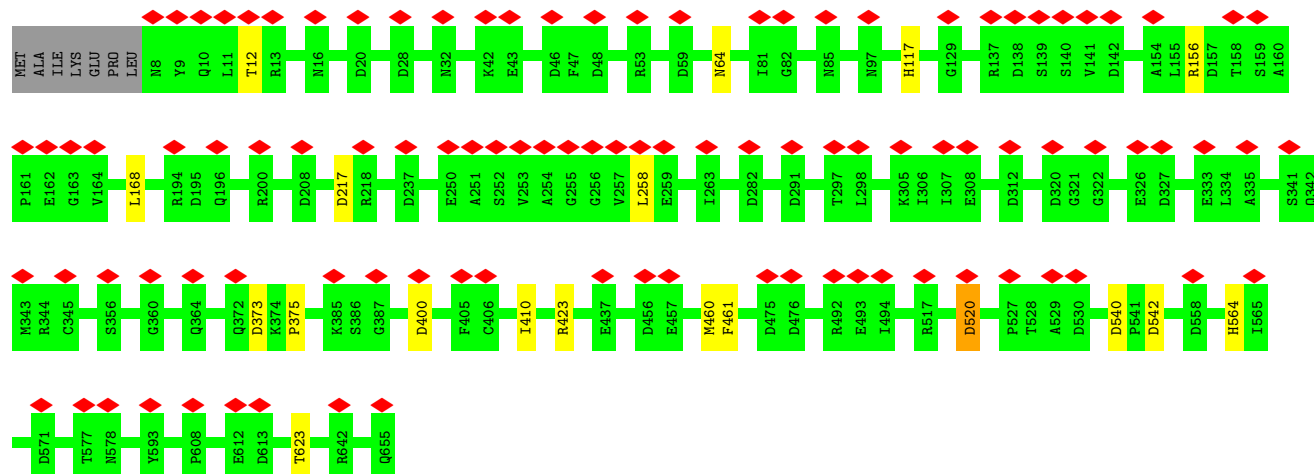




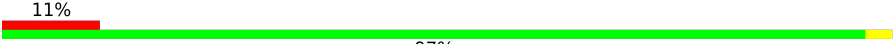
• Molecule 4: Baseplate wedge protein gp6

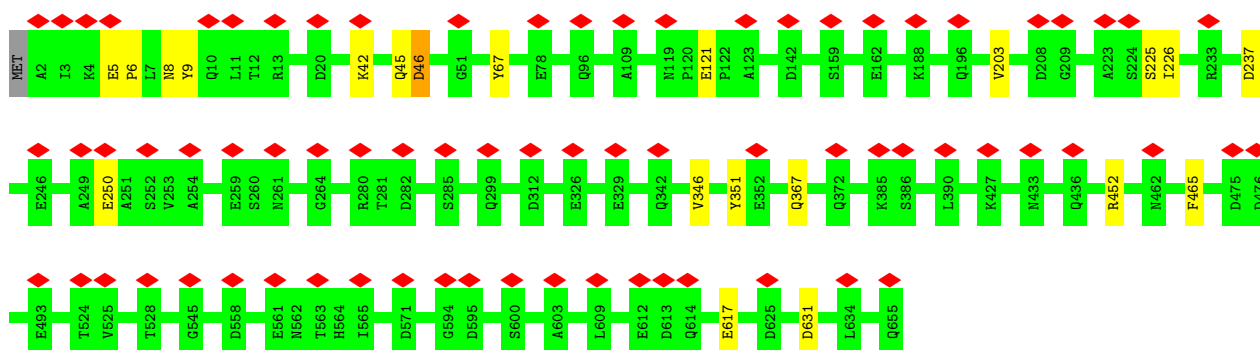


• Molecule 4: Baseplate wedge protein gp6

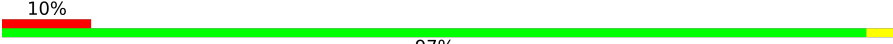


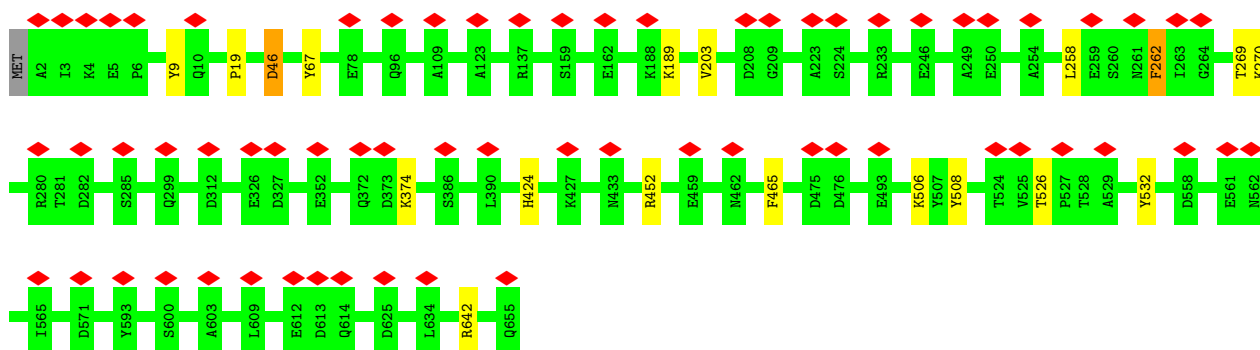
• Molecule 4: Baseplate wedge protein gp6

Chain AR:  11% 97%

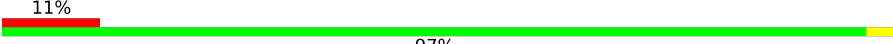


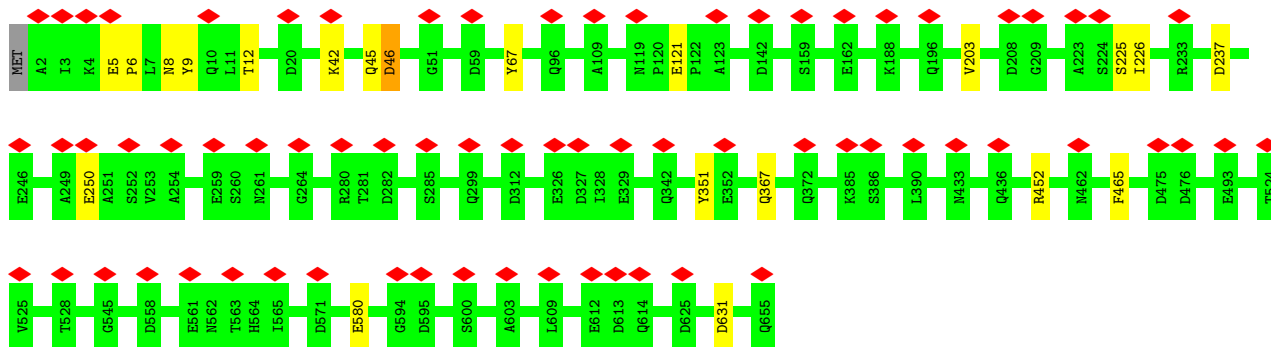
• Molecule 4: Baseplate wedge protein gp6

Chain AQ:  10% 97%

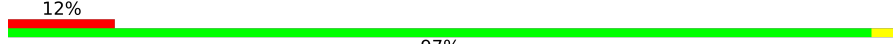


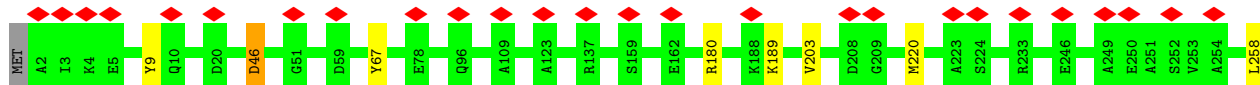
• Molecule 4: Baseplate wedge protein gp6

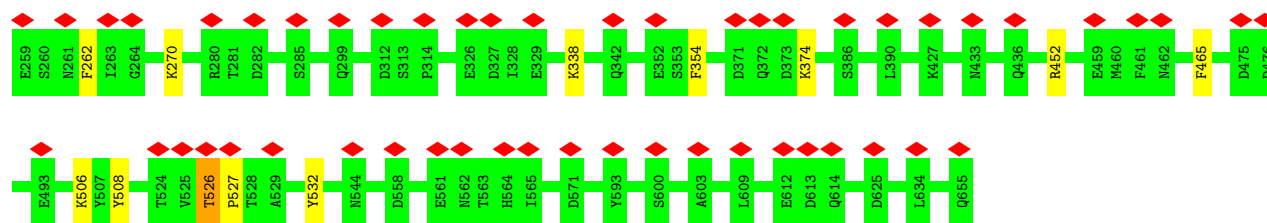
Chain AN:  11% 97%



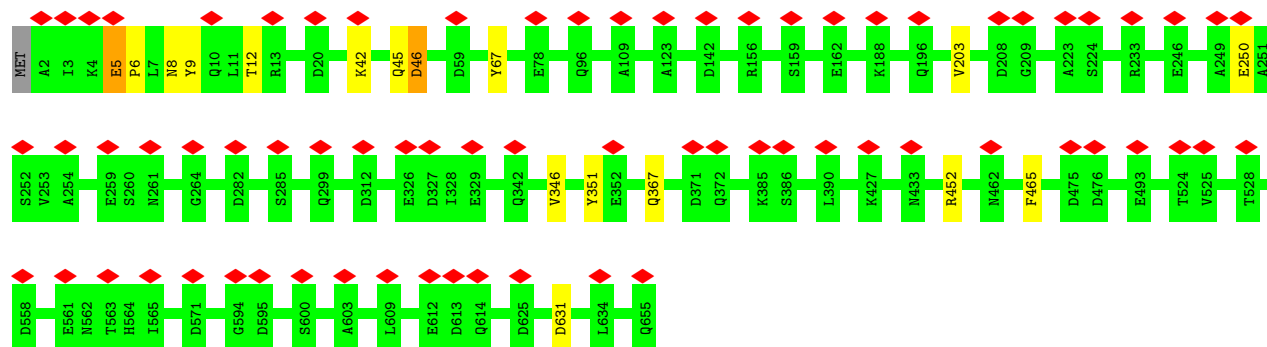
• Molecule 4: Baseplate wedge protein gp6

Chain AM:  12% 97%

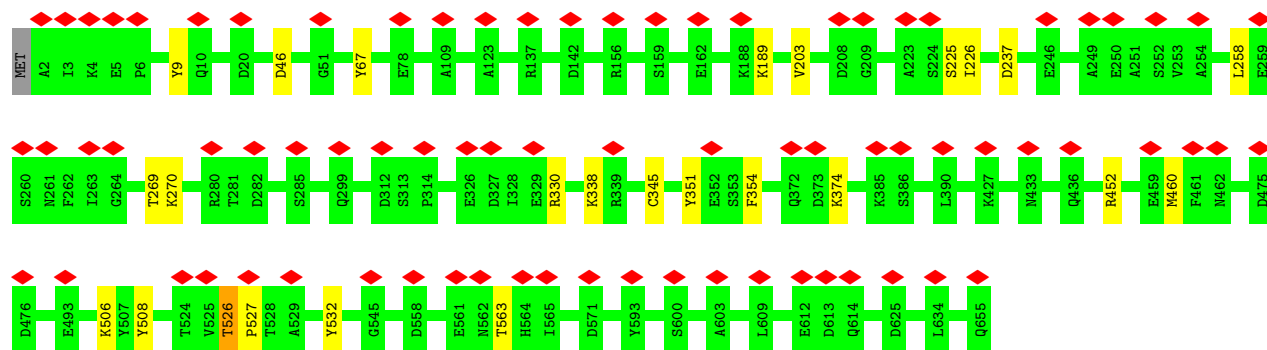




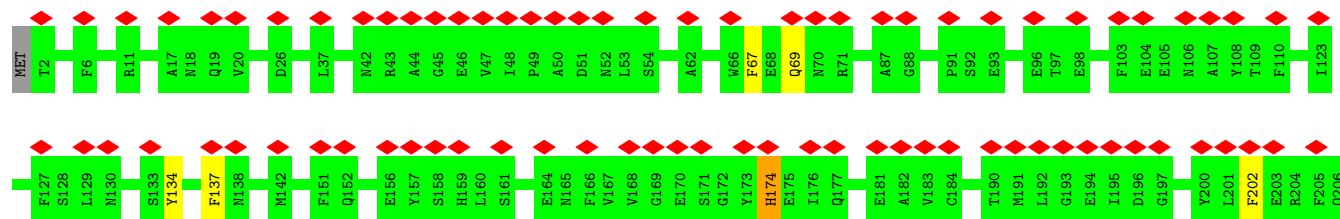
• Molecule 4: Baseplate wedge protein gp6

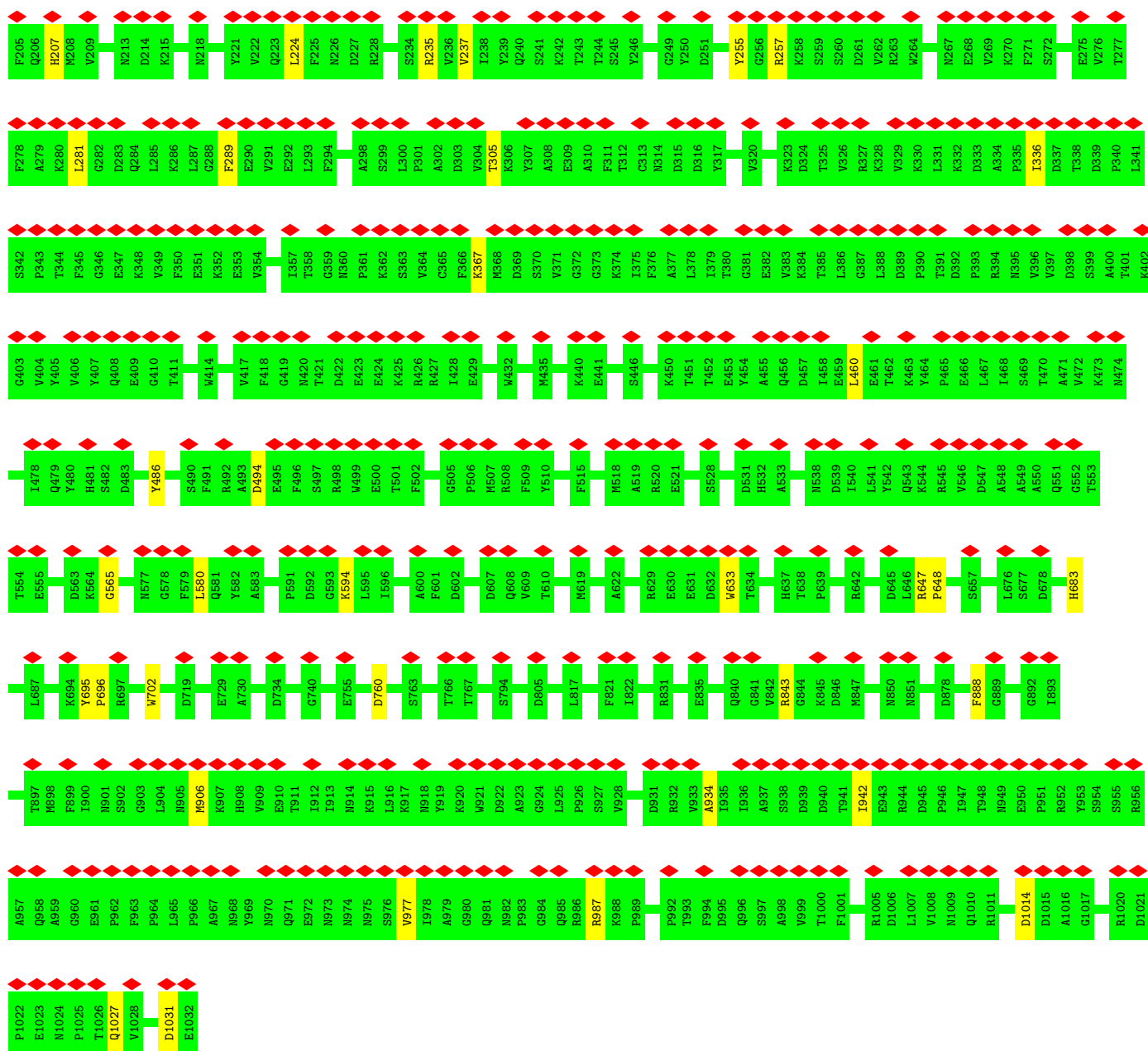


• Molecule 4: Baseplate wedge protein gp6



• Molecule 5: Baseplate wedge protein gp7

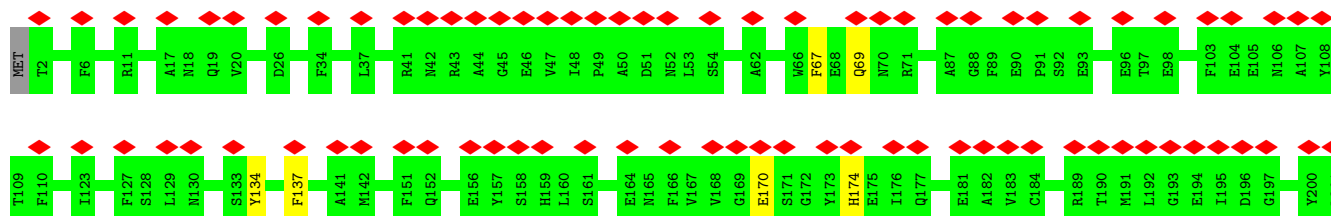


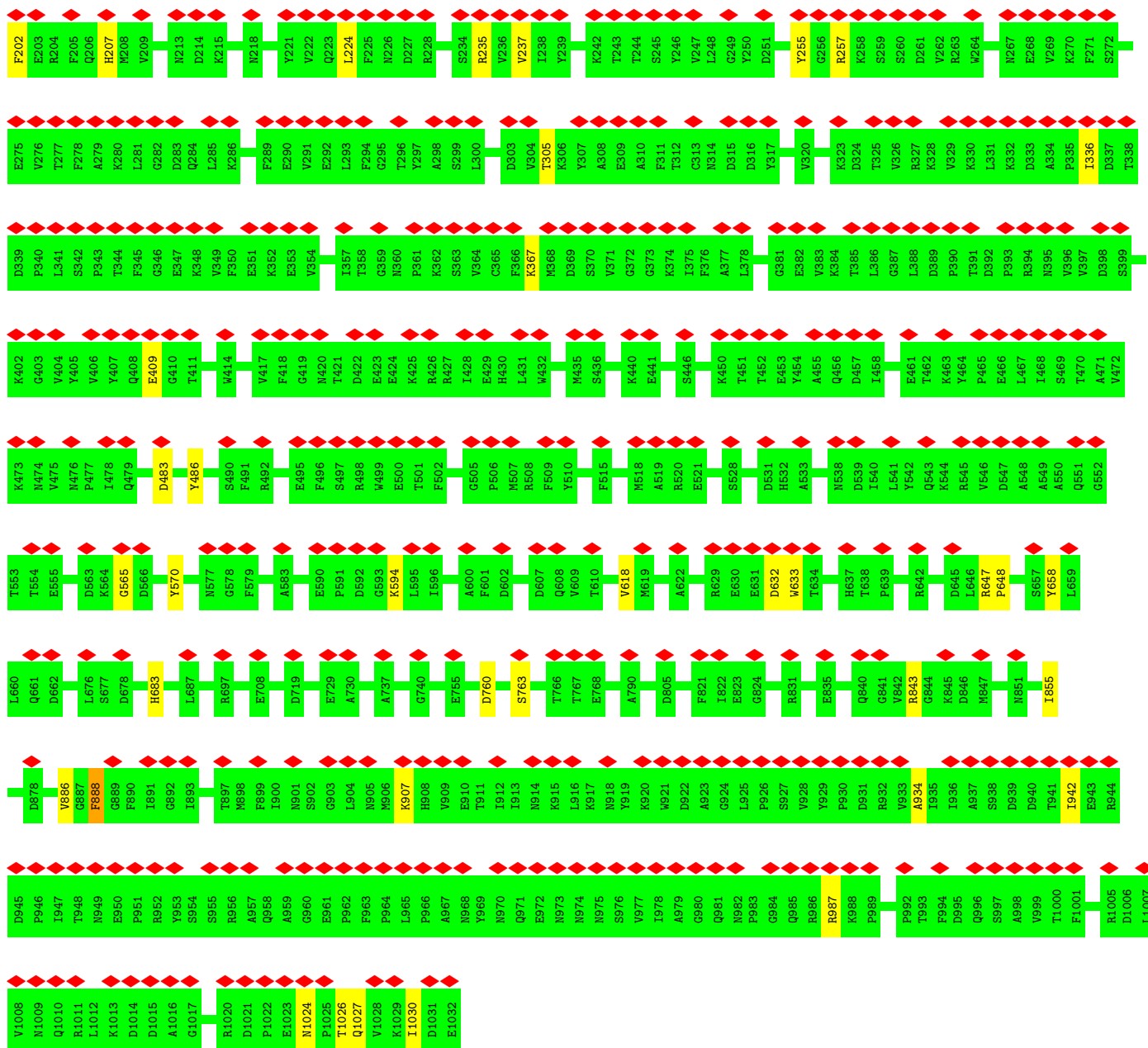


• Molecule 5: Baseplate wedge protein gp7



Chain A0:

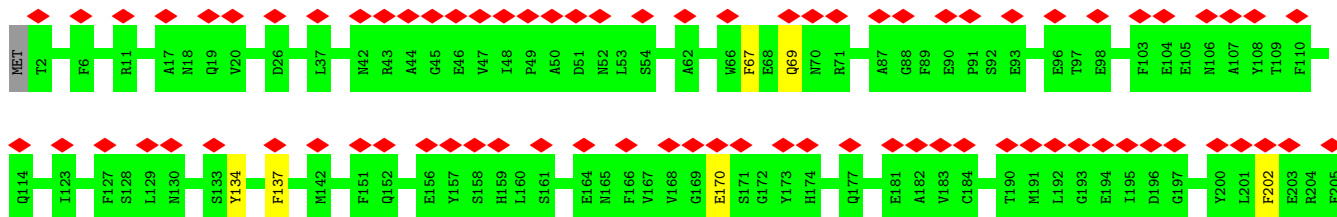


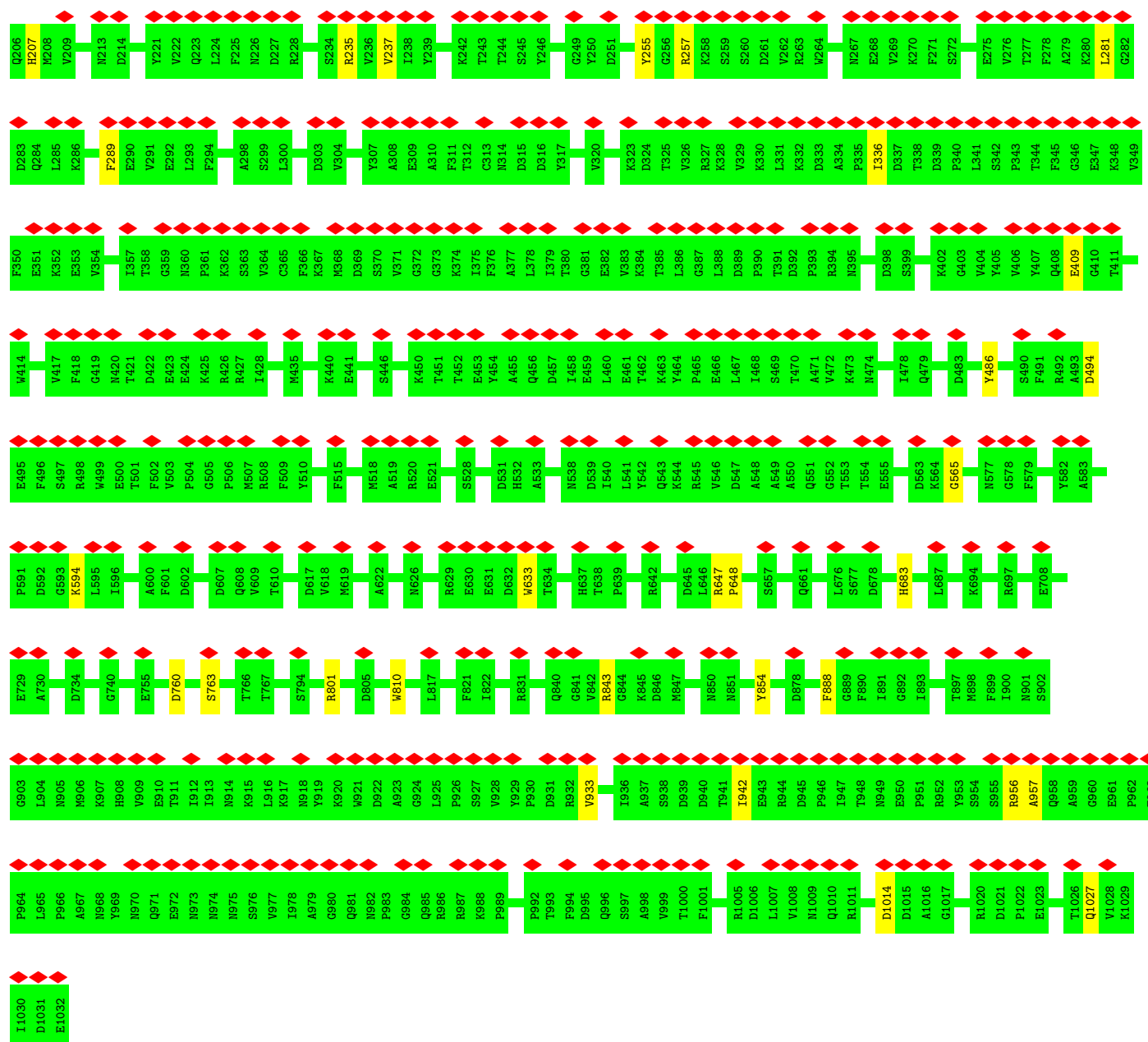


• Molecule 5: Baseplate wedge protein gp7

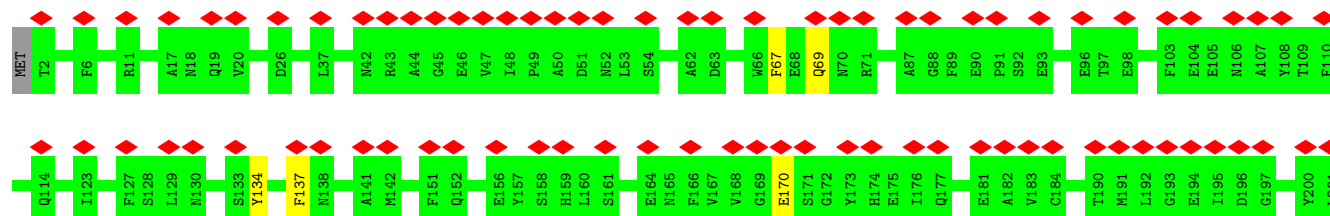


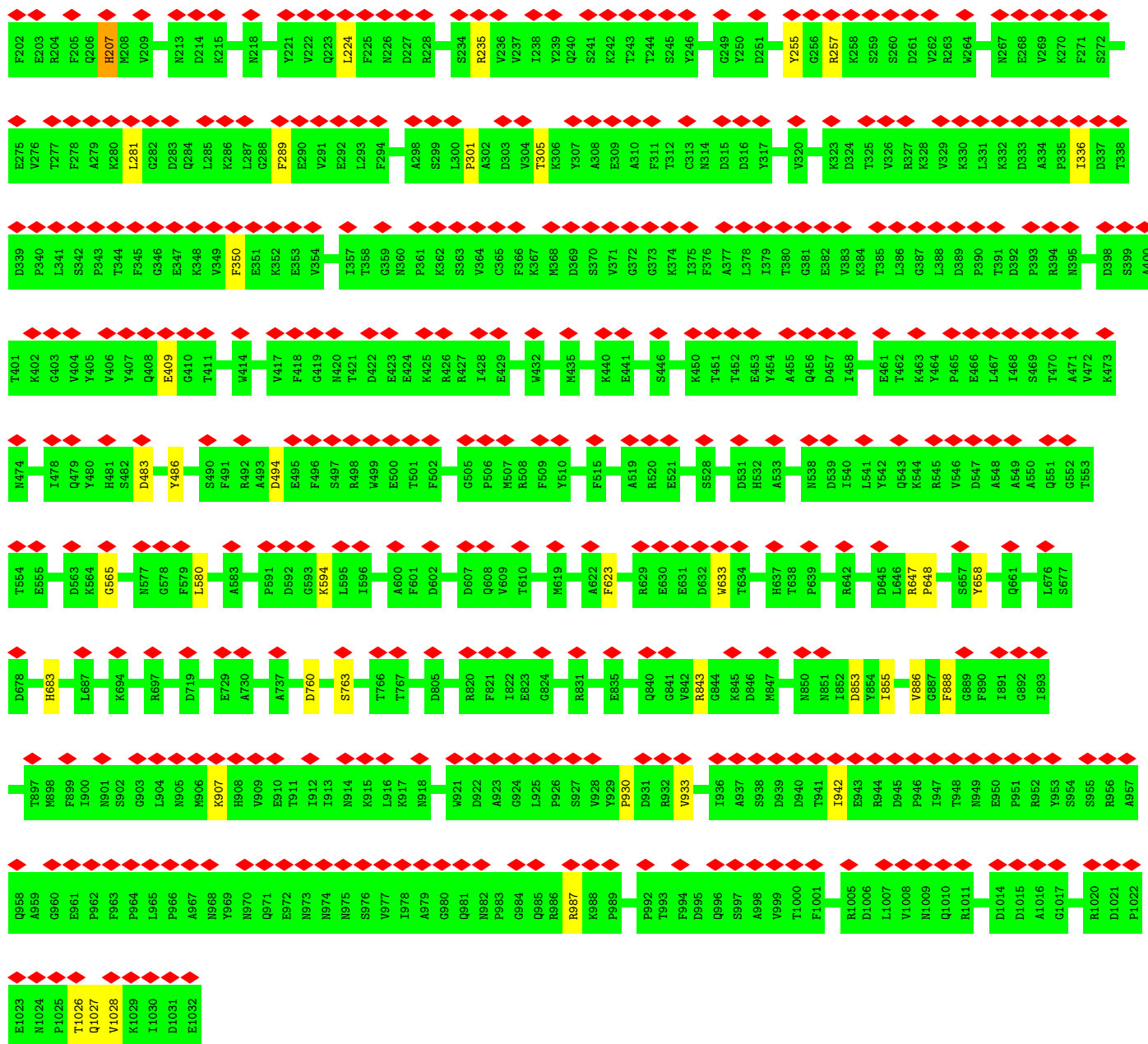
Chain A1:





• Molecule 5: Baseplate wedge protein gp7

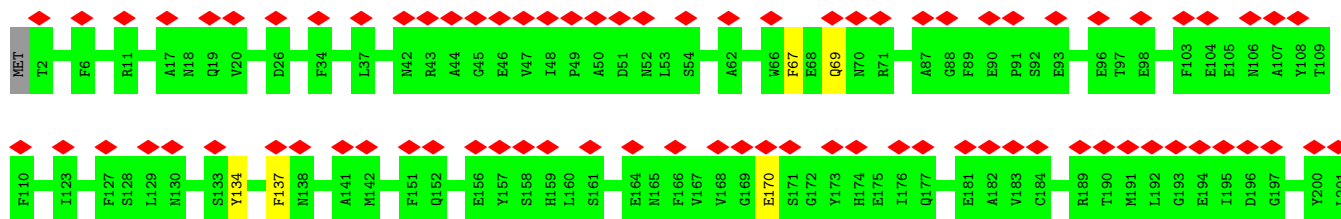


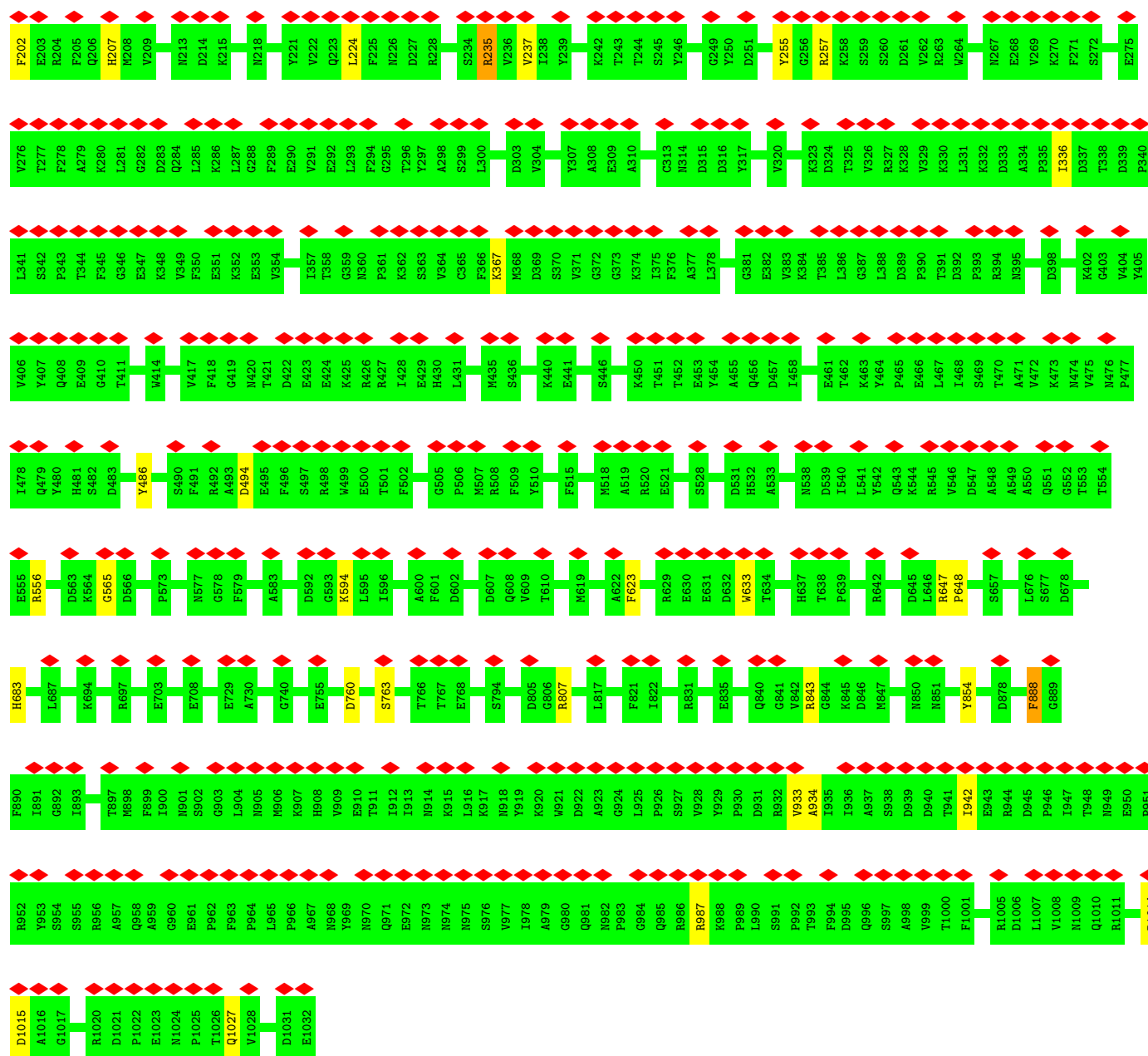


• Molecule 5: Baseplate wedge protein gp7

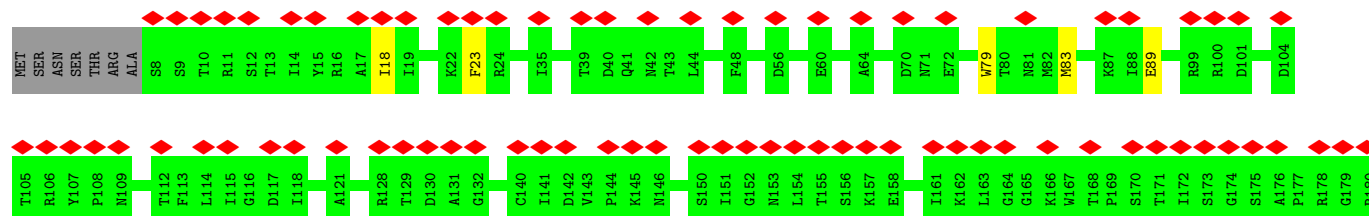
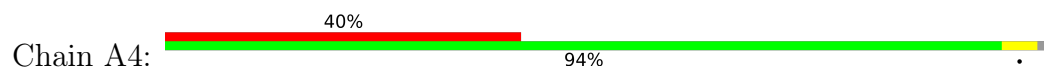


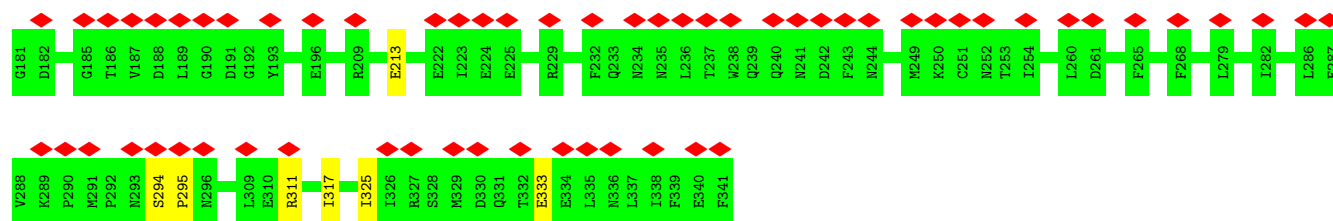
Chain A3:





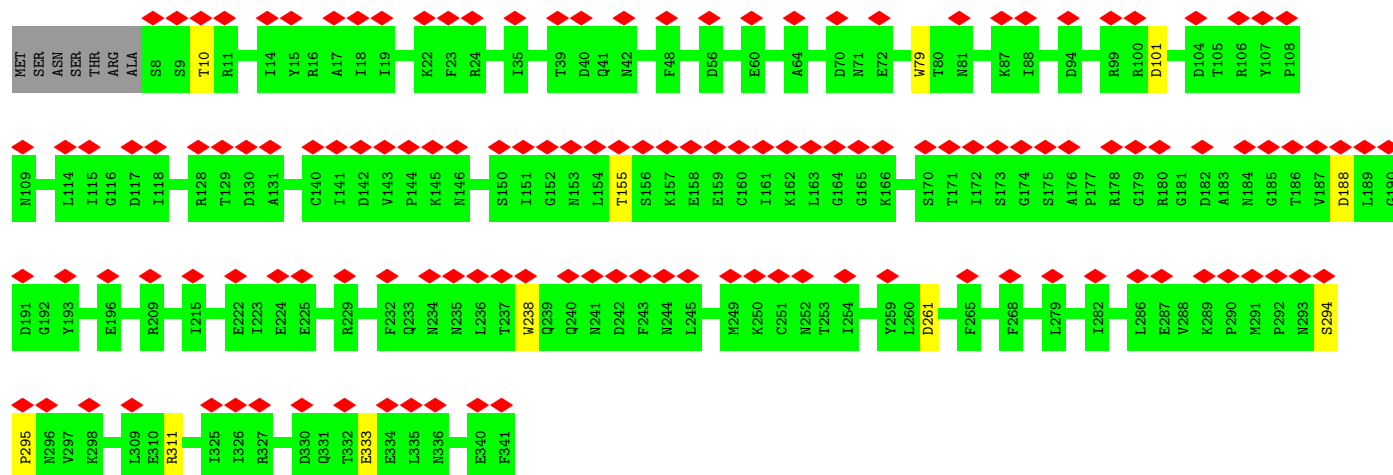
• Molecule 6: Baseplate wedge subunit





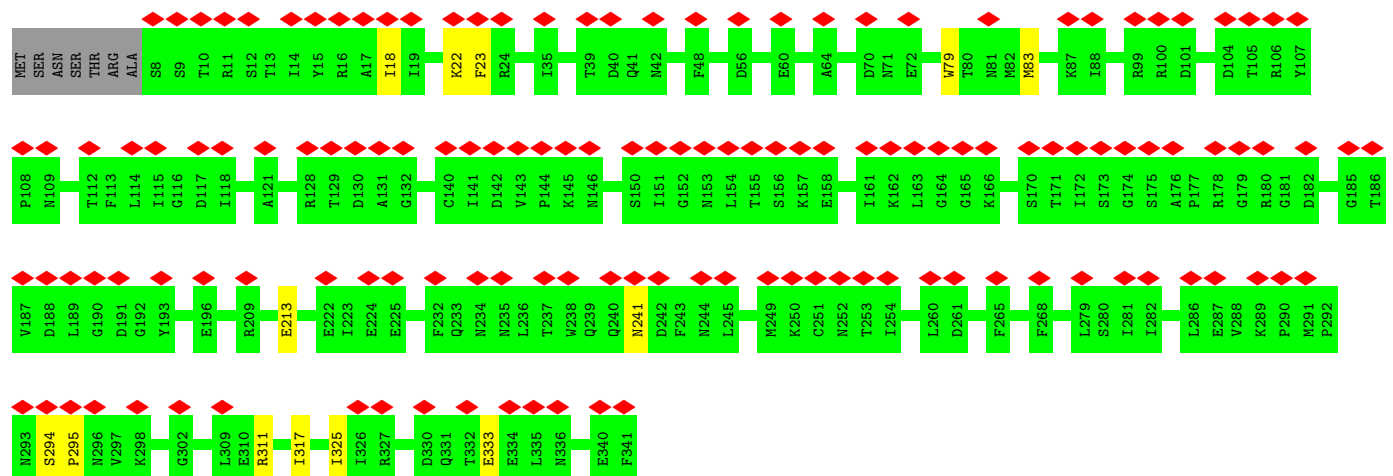
• Molecule 6: Baseplate wedge subunit

Chain A9: 40% 95%



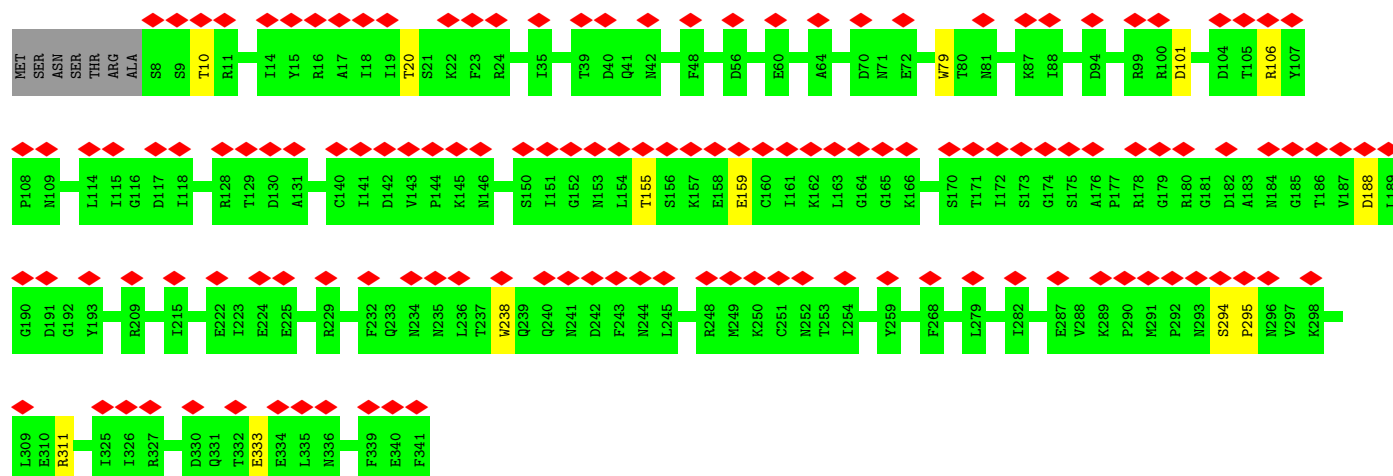
• Molecule 6: Baseplate wedge subunit

Chain A6: 40% 94%



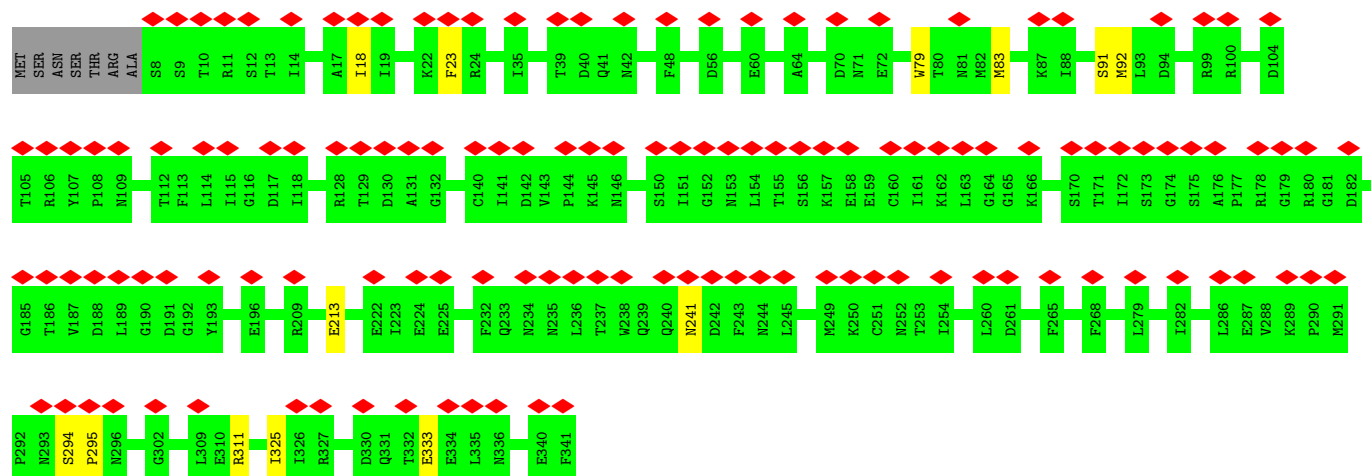
• Molecule 6: Baseplate wedge subunit

Chain A5: 40% 94%



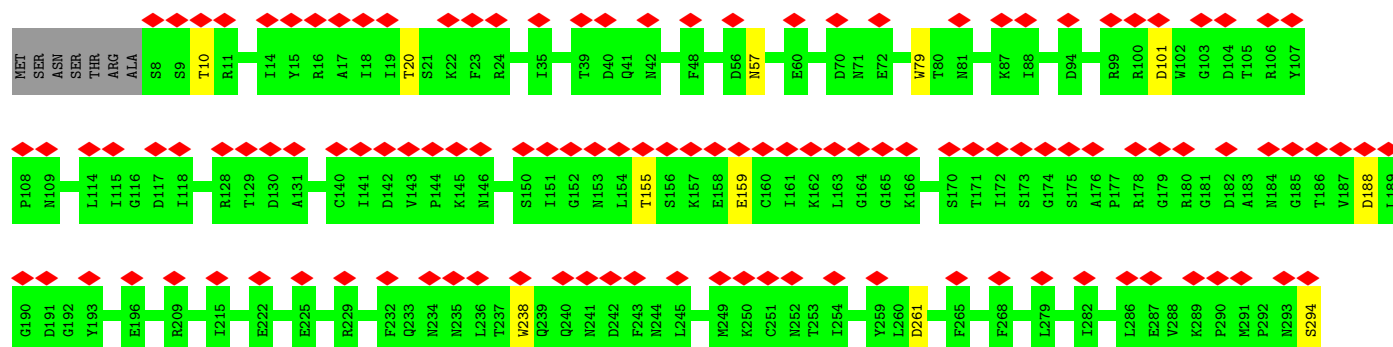
• Molecule 6: Baseplate wedge subunit

Chain A8: 39% 94%

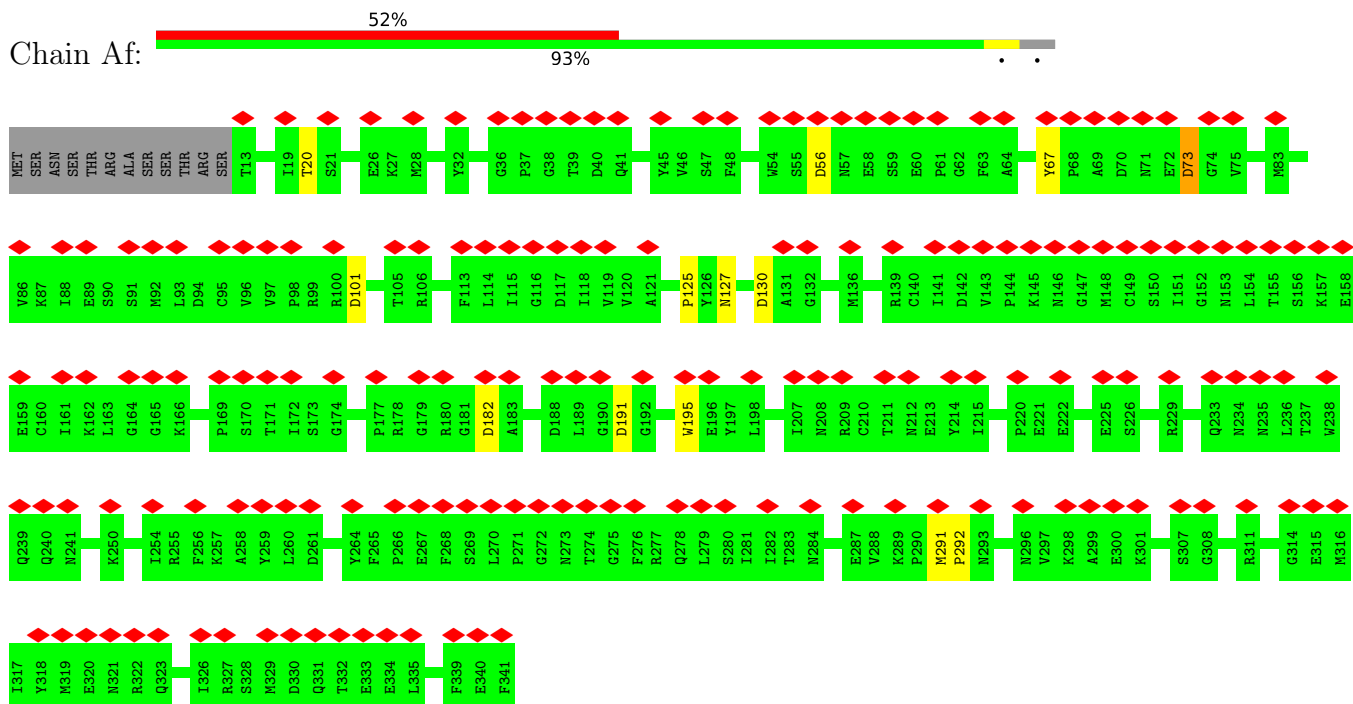


• Molecule 6: Baseplate wedge subunit

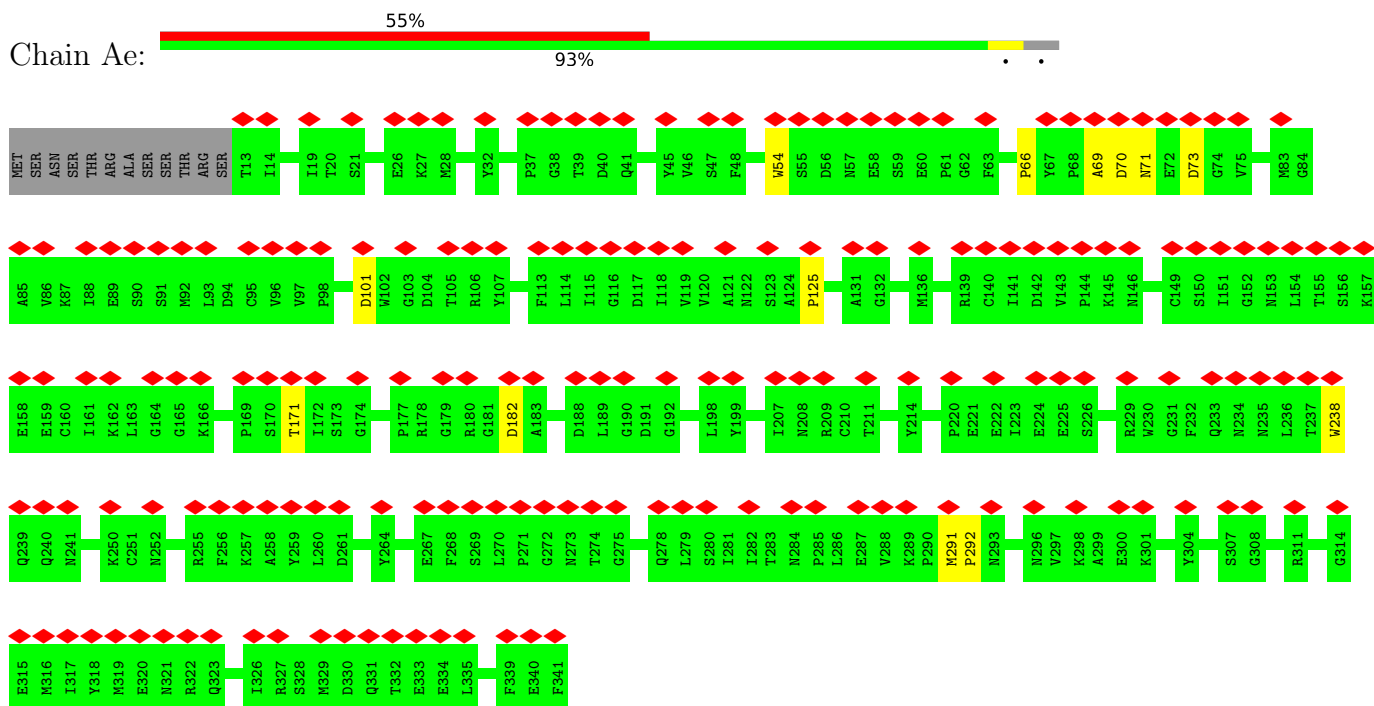
Chain A7: 39% 94%



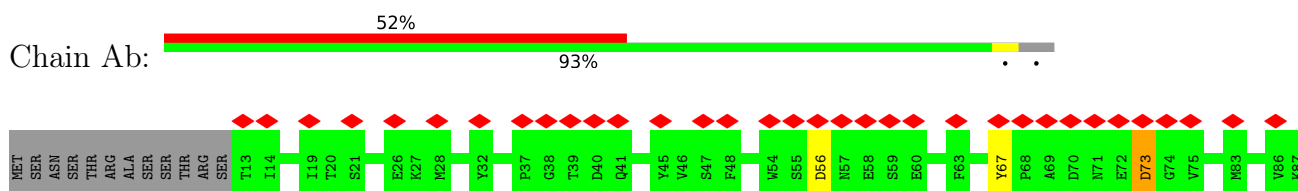


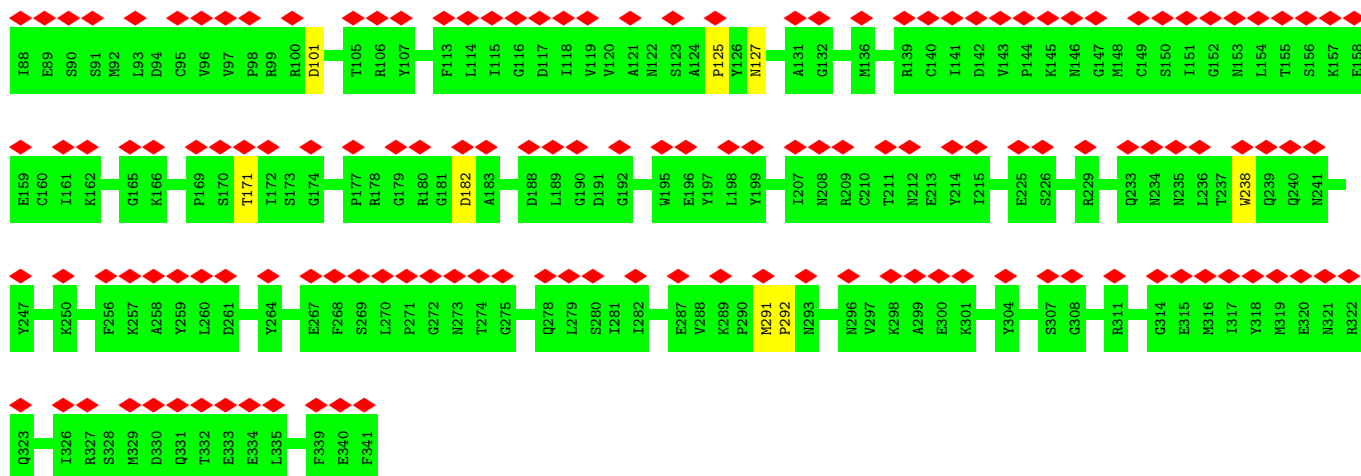


- Molecule 6: Baseplate wedge subunit

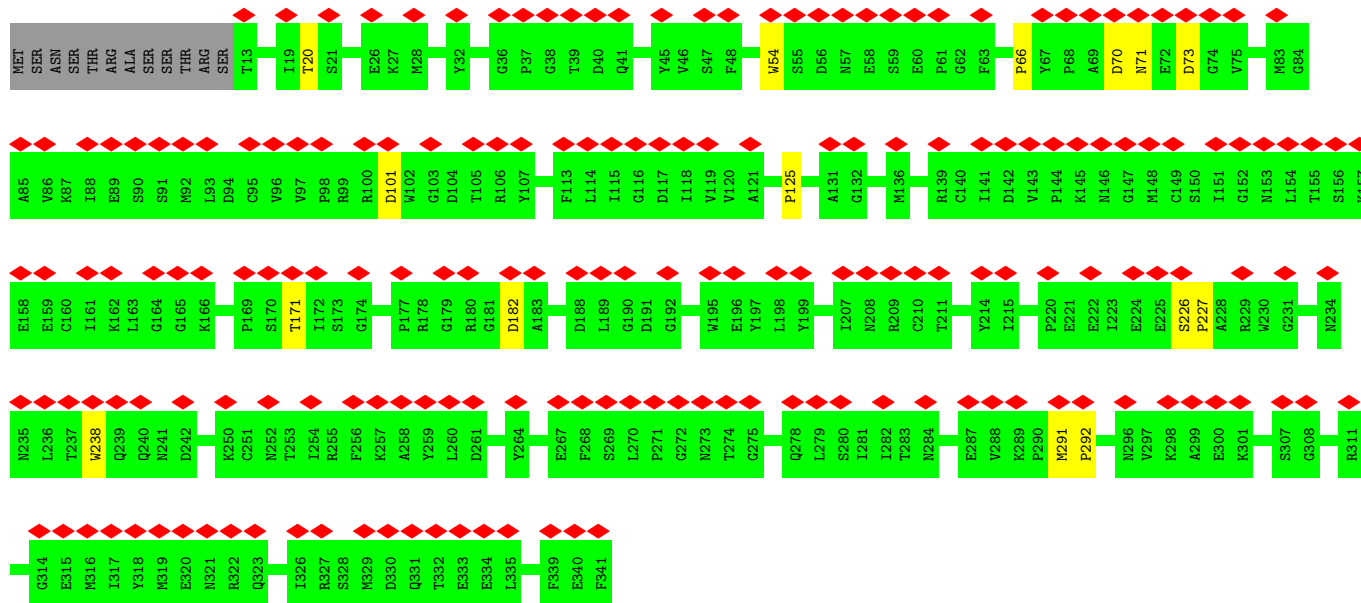


- Molecule 6: Baseplate wedge subunit

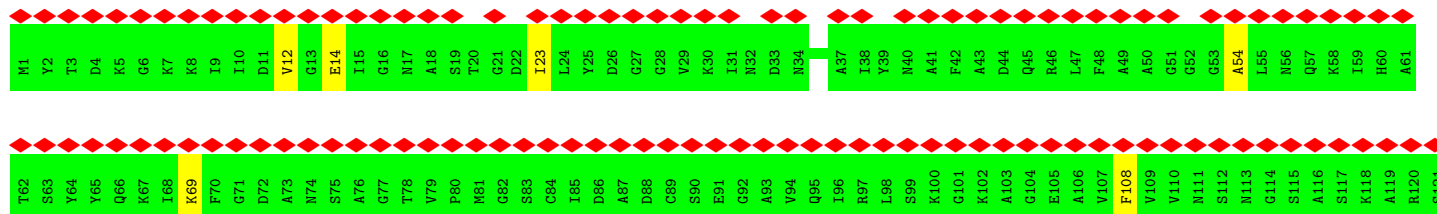


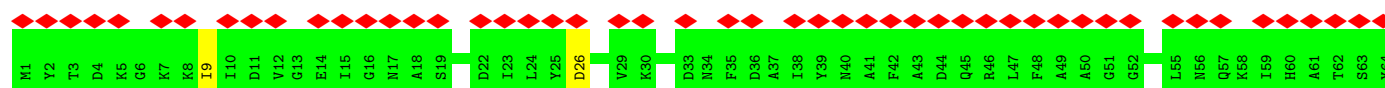


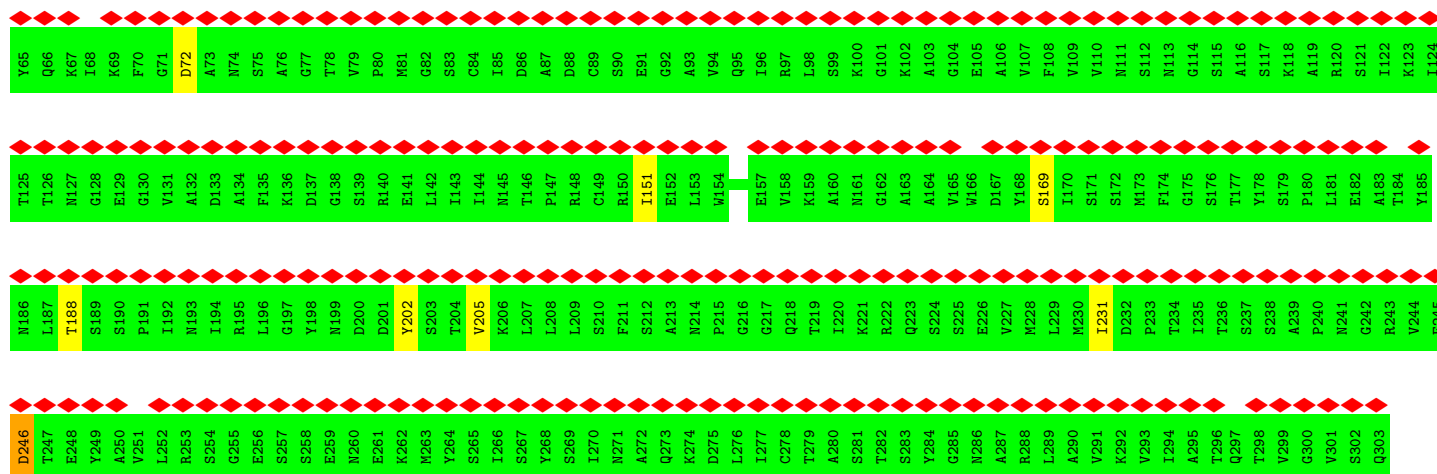
• Molecule 6: Baseplate wedge subunit



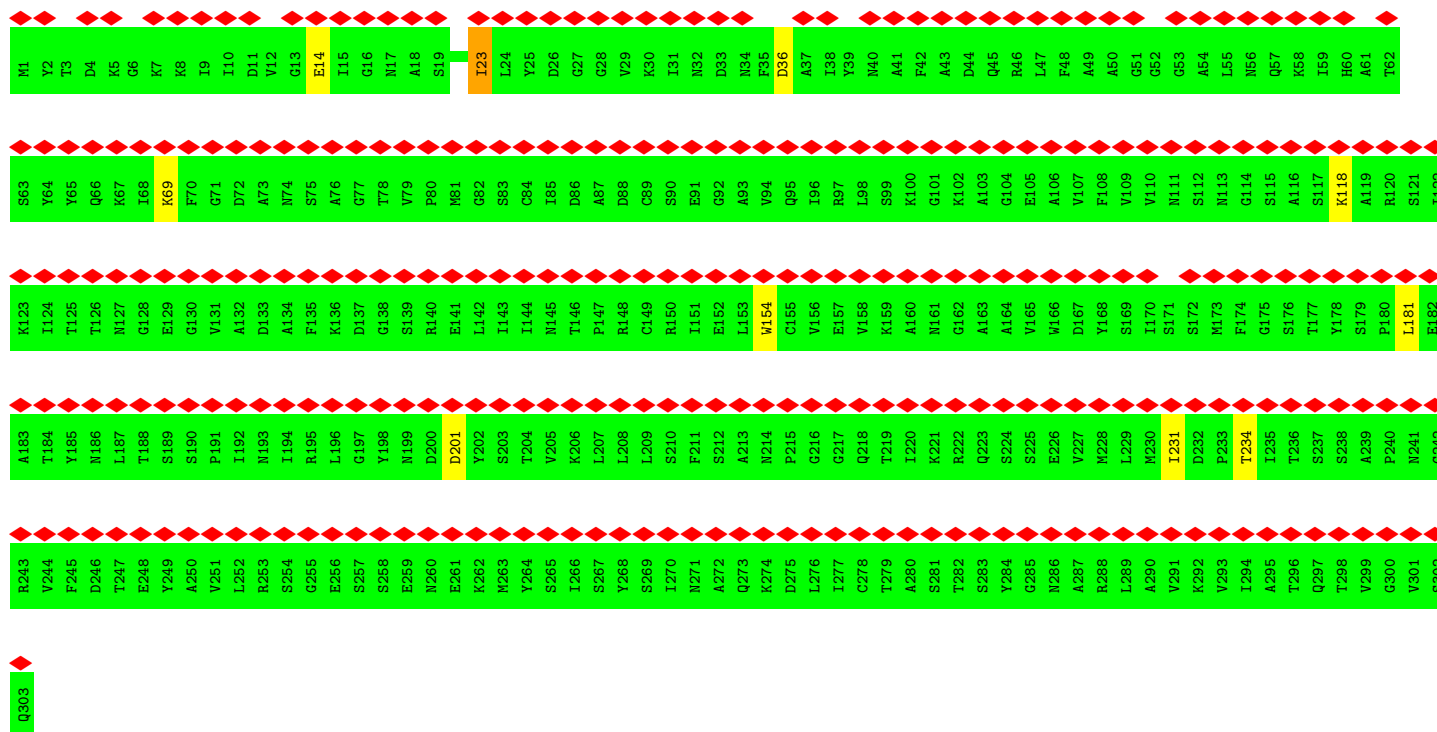
• Molecule 7: Baseplate wedge tail fiber connector



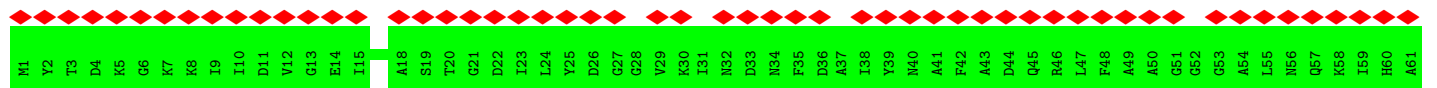


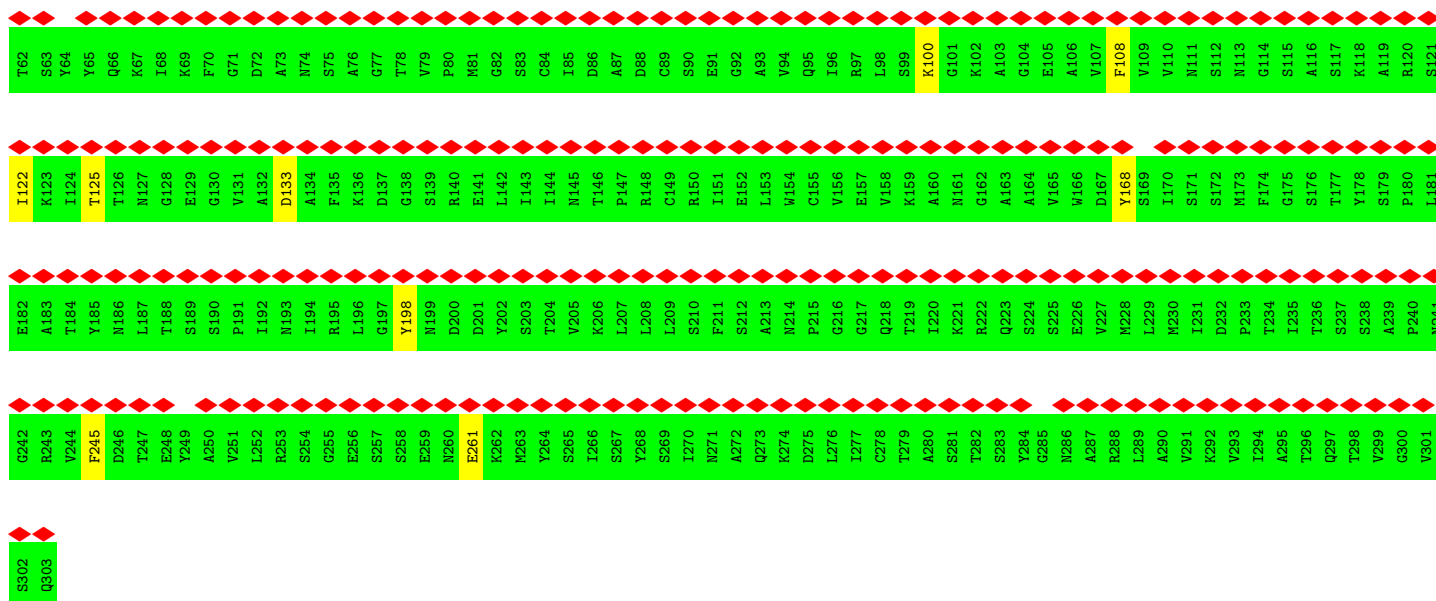


• Molecule 7: Baseplate wedge tail fiber connector

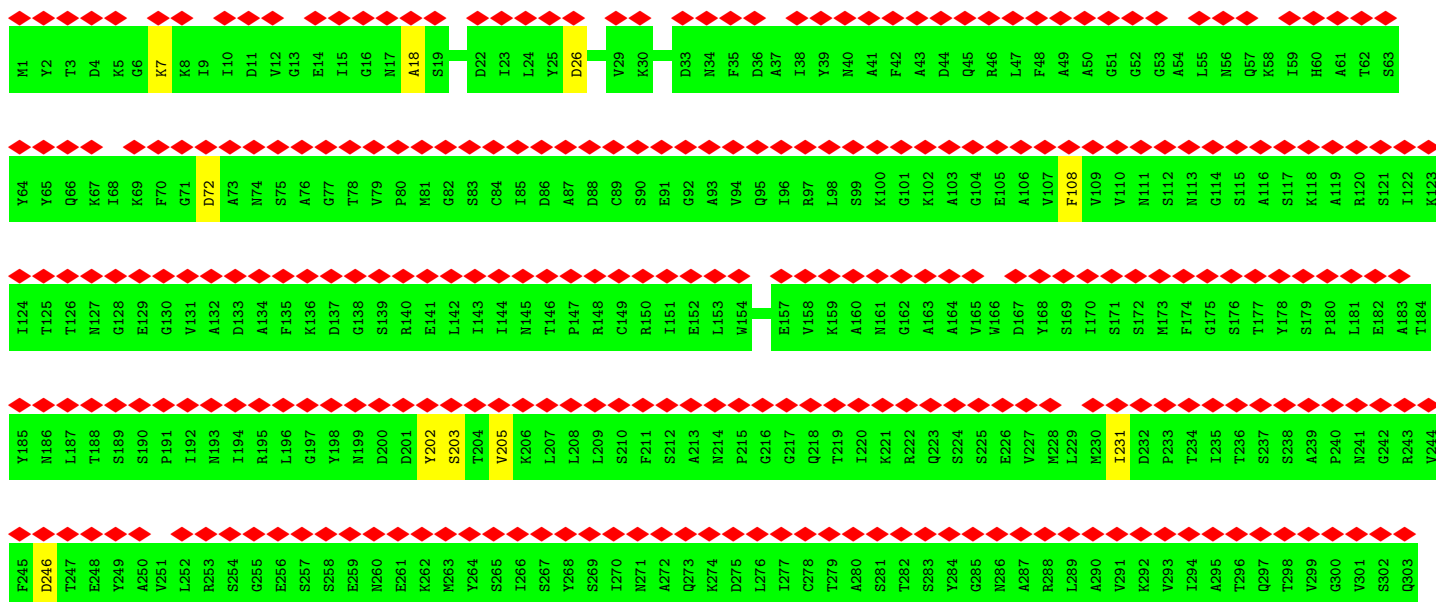


• Molecule 7: Baseplate wedge tail fiber connector

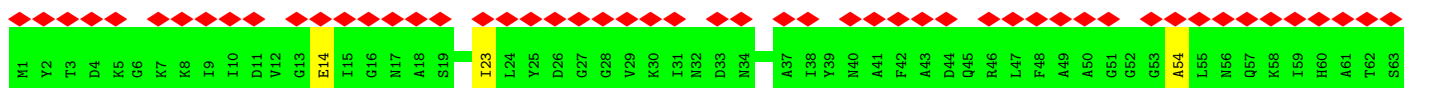




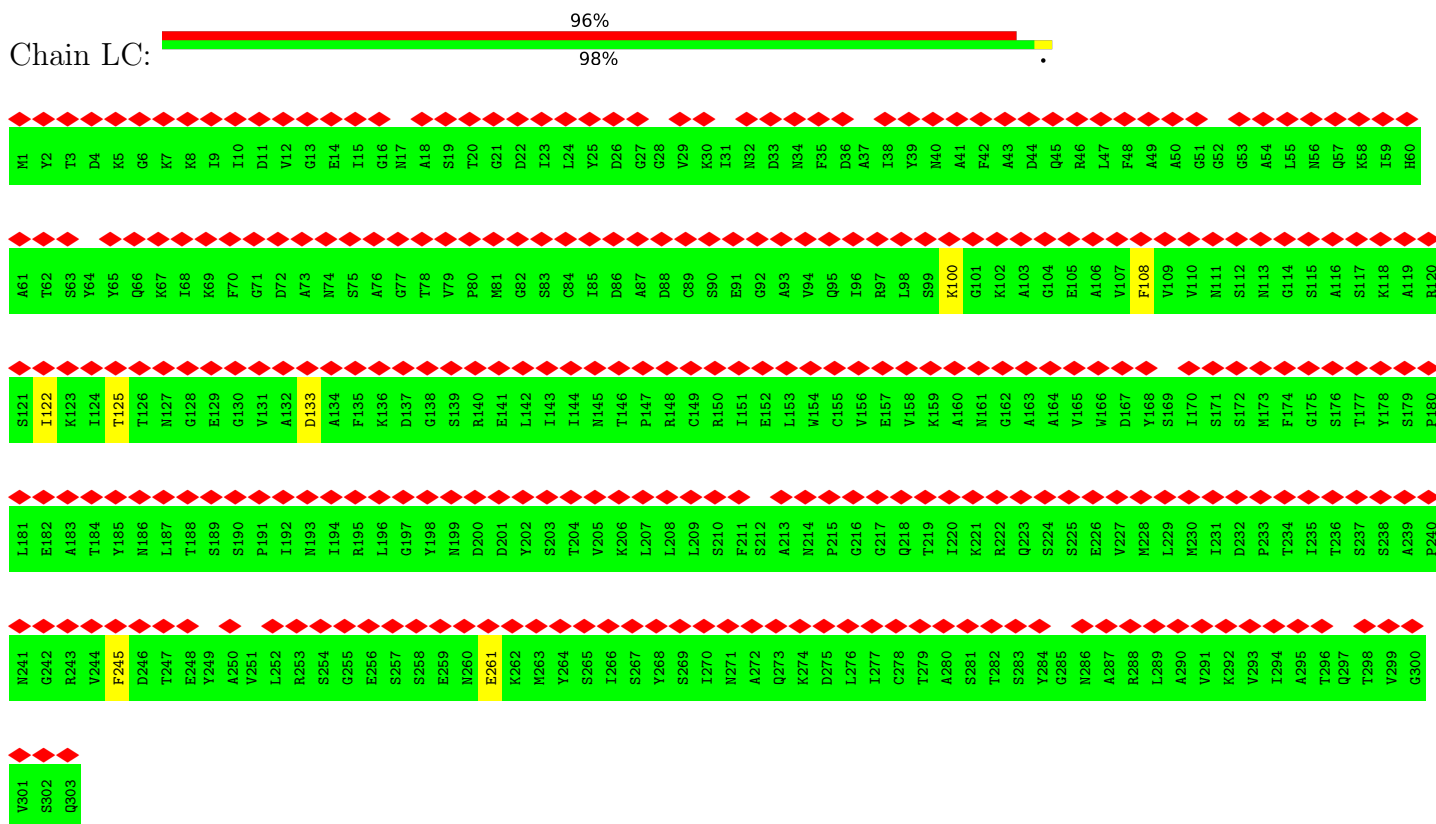
- Molecule 7: Baseplate wedge tail fiber connector



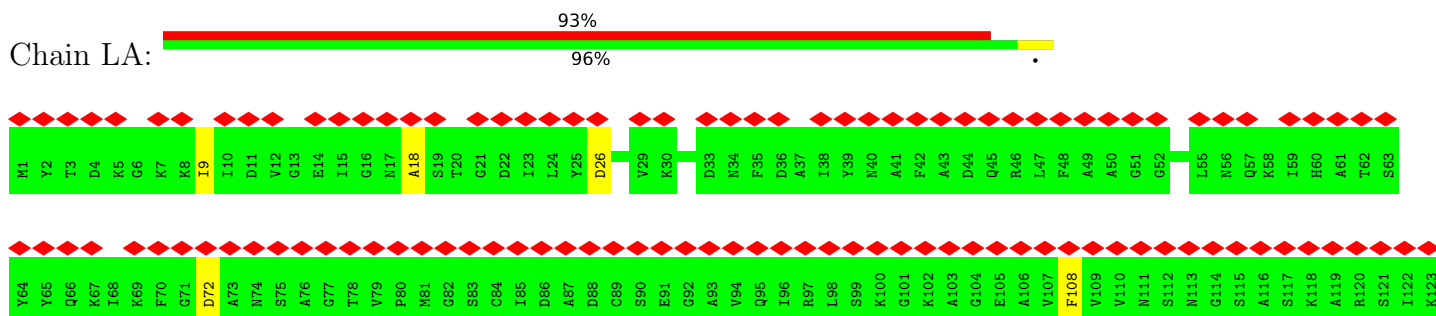
- Molecule 7: Baseplate wedge tail fiber connector

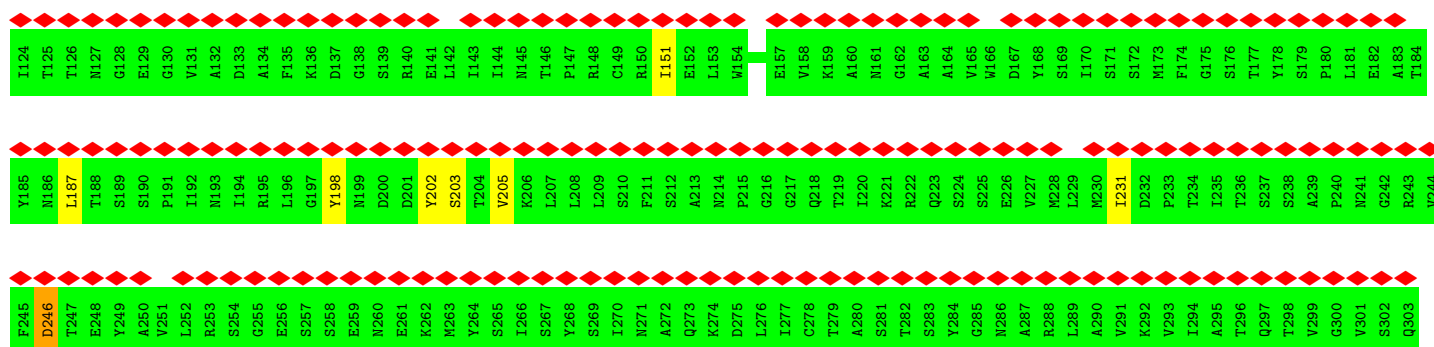


- Molecule 7: Baseplate wedge tail fiber connector

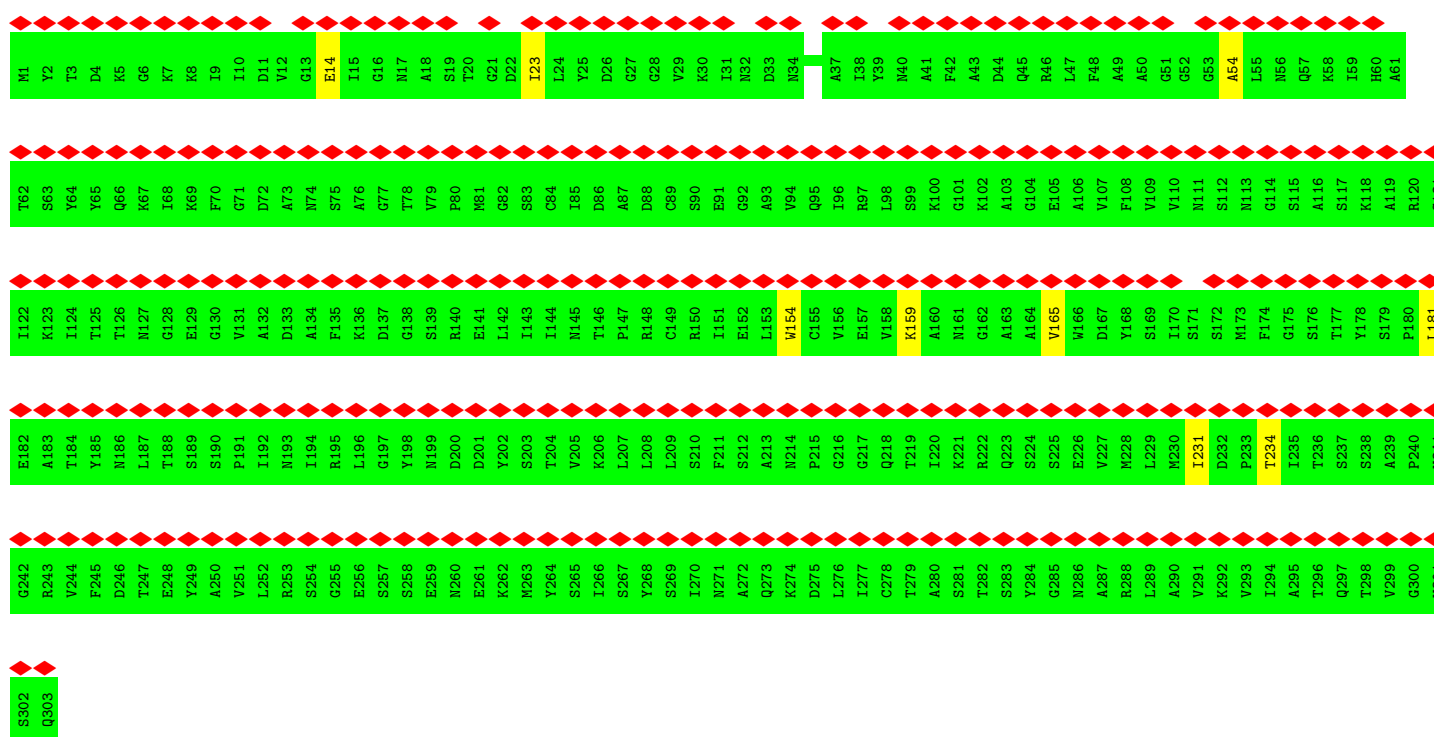


- Molecule 7: Baseplate wedge tail fiber connector



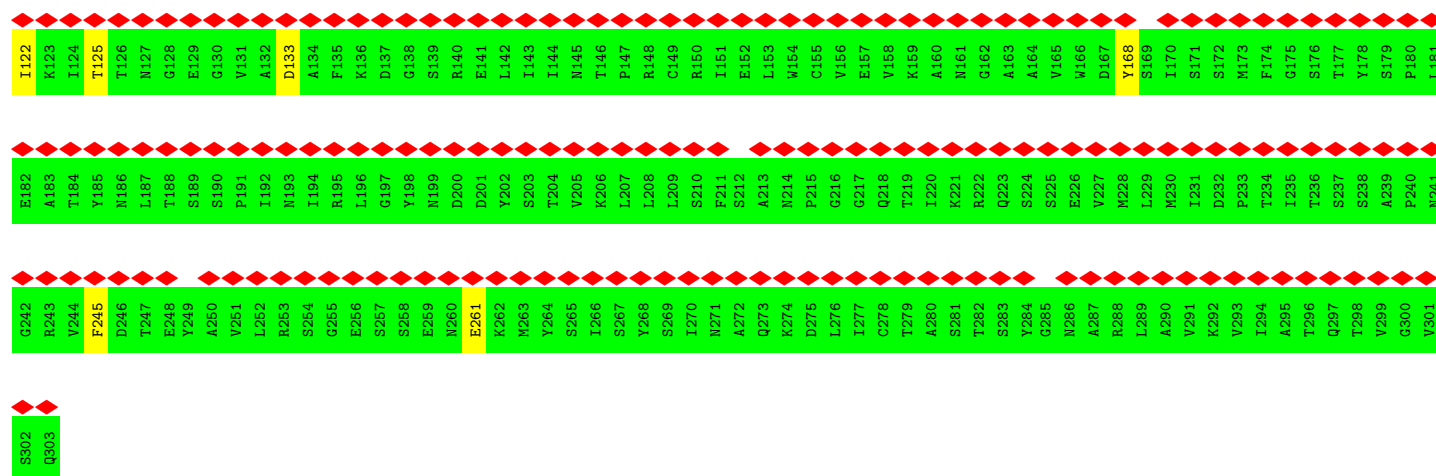


• Molecule 7: Baseplate wedge tail fiber connector

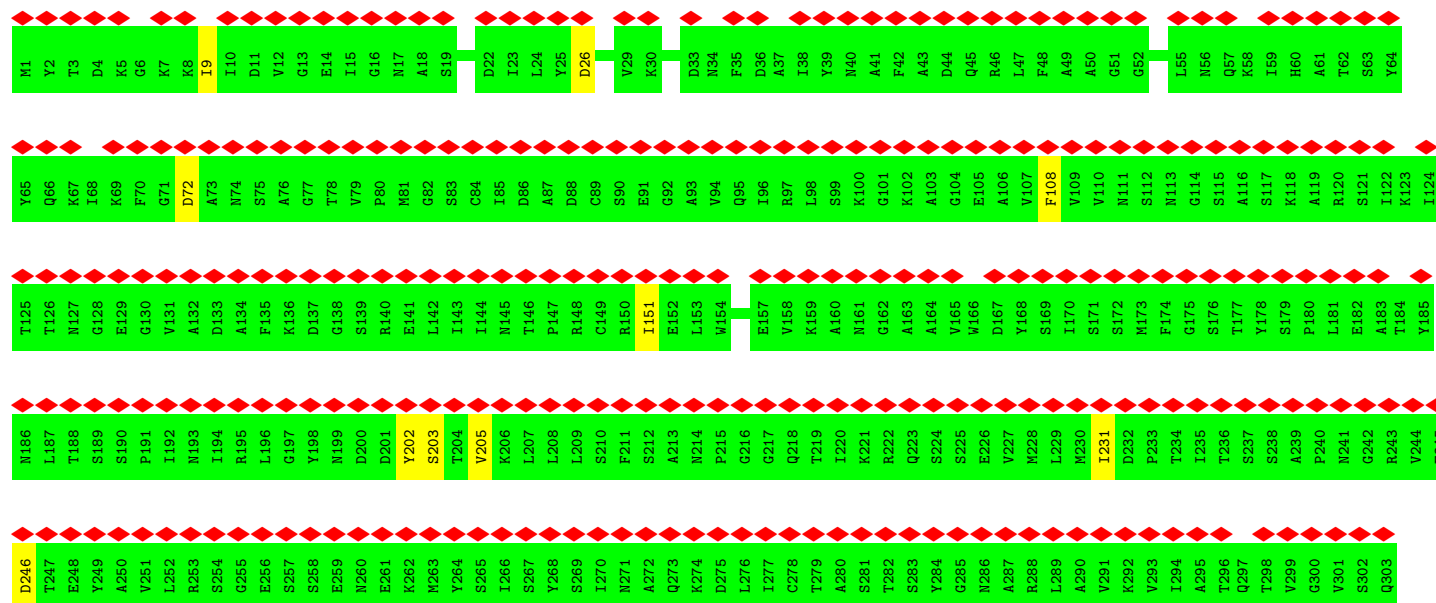


• Molecule 7: Baseplate wedge tail fiber connector

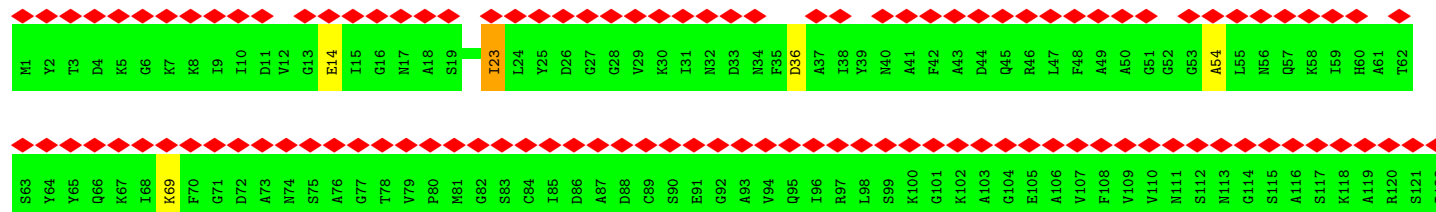


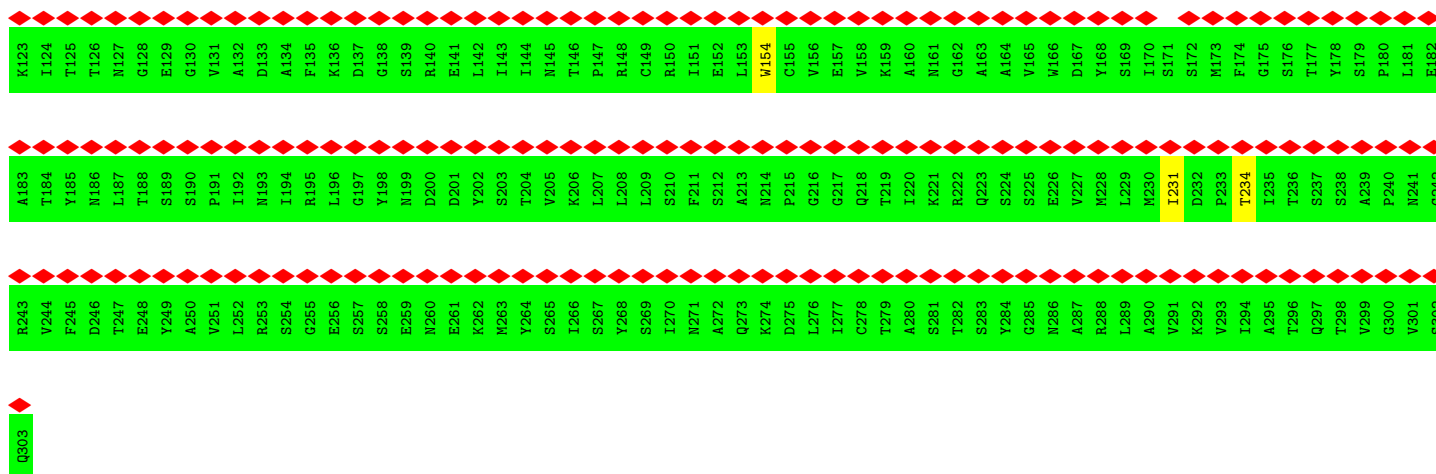


- Molecule 7: Baseplate wedge tail fiber connector

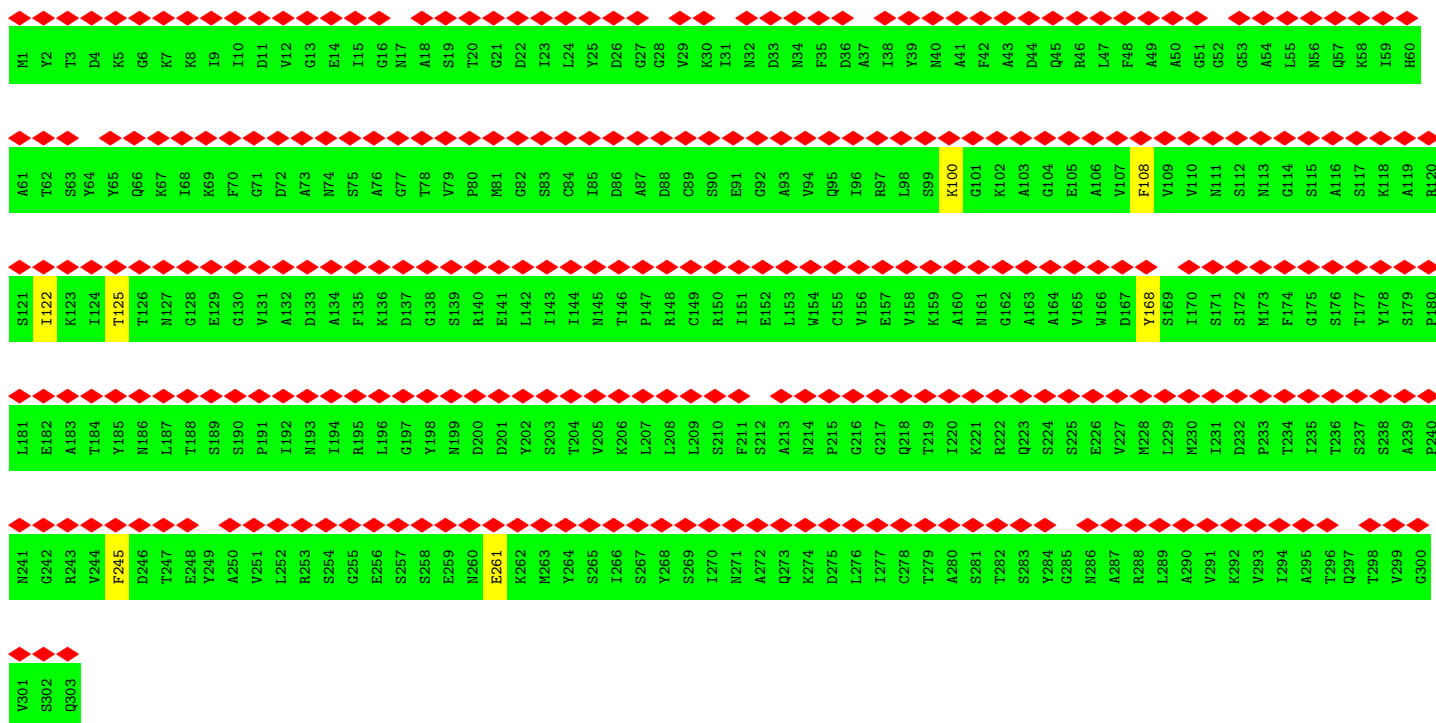


- Molecule 7: Baseplate wedge tail fiber connector

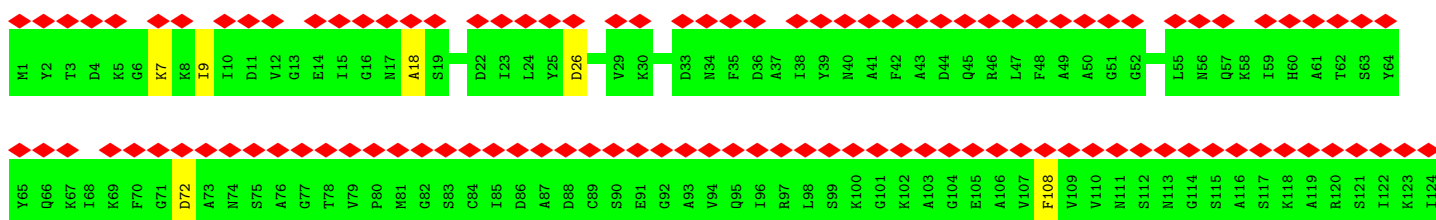


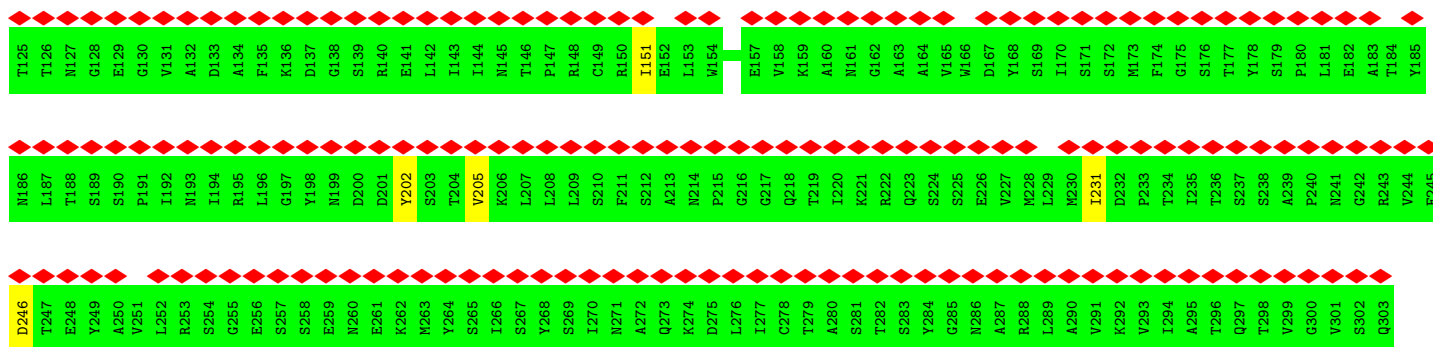


- Molecule 7: Baseplate wedge tail fiber connector

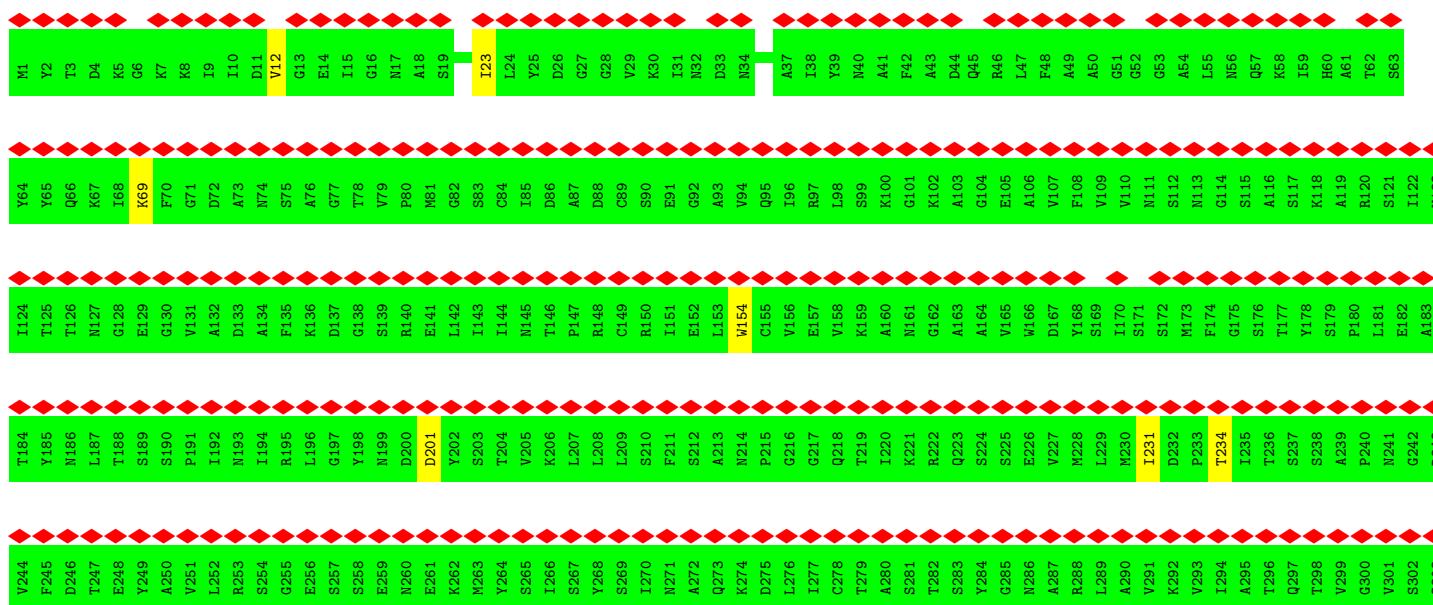


- Molecule 7: Baseplate wedge tail fiber connector

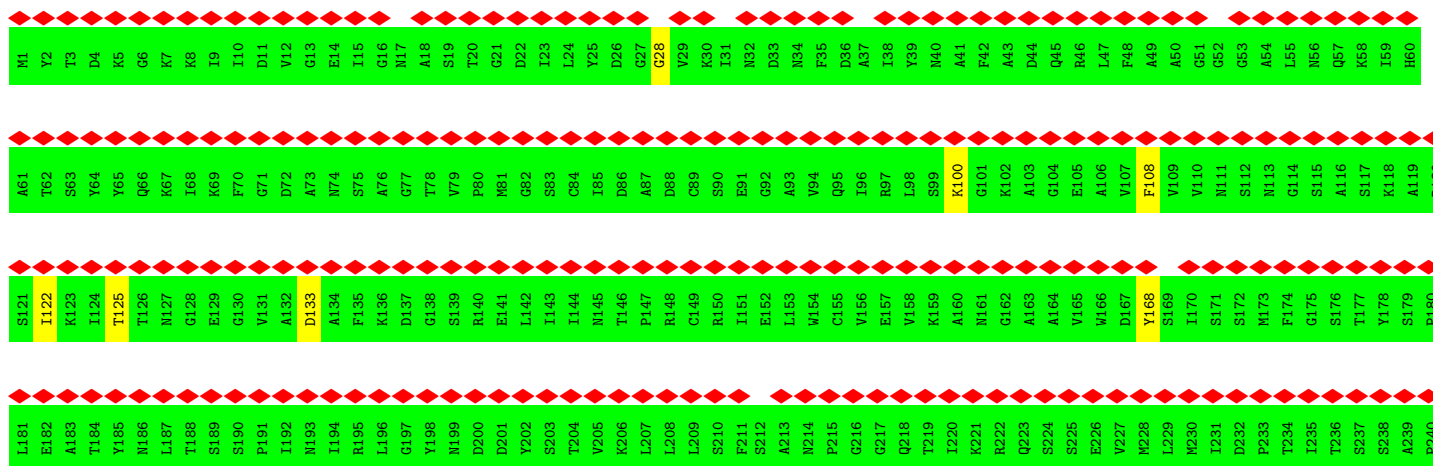




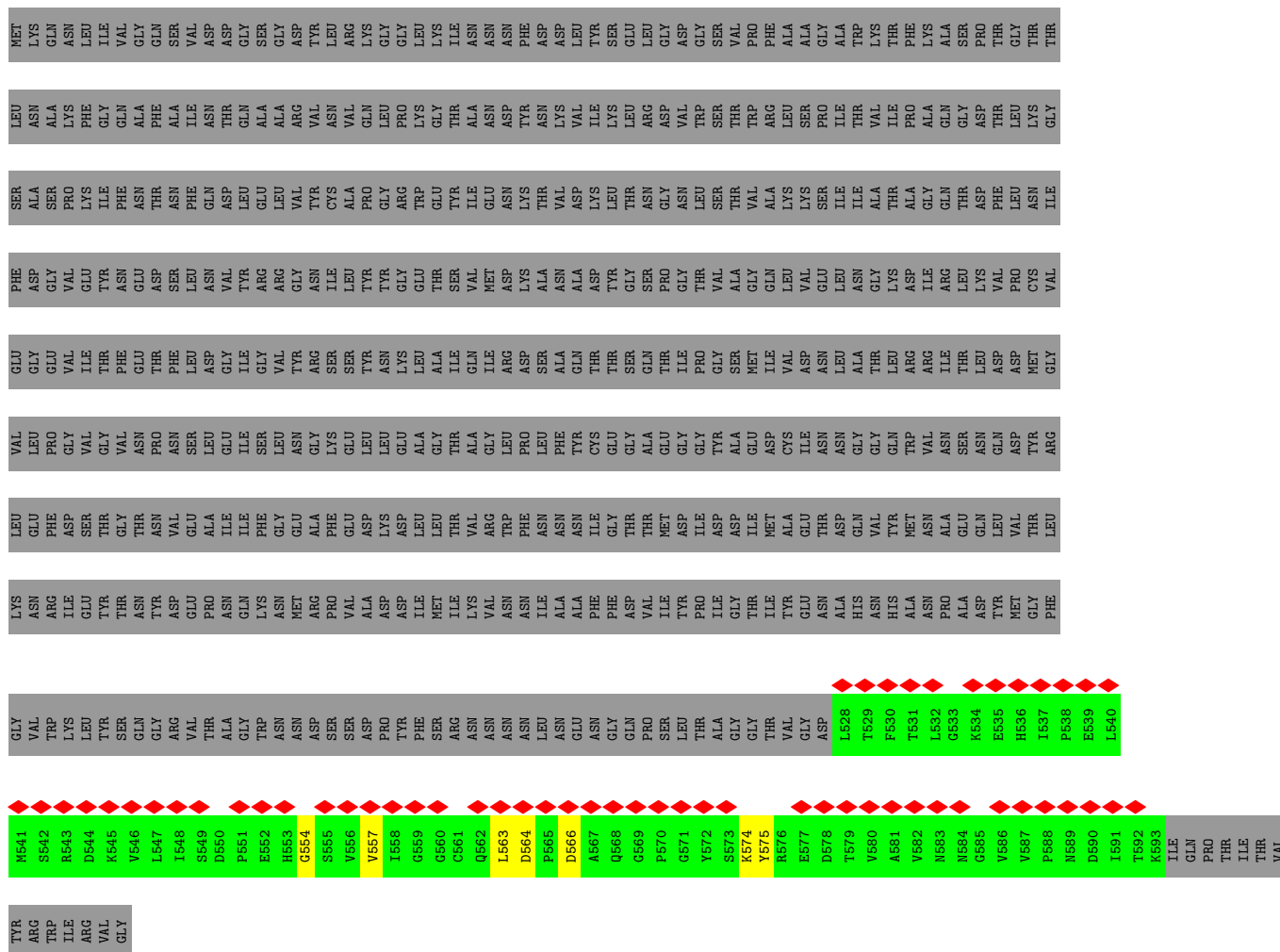
• Molecule 7: Baseplate wedge tail fiber connector



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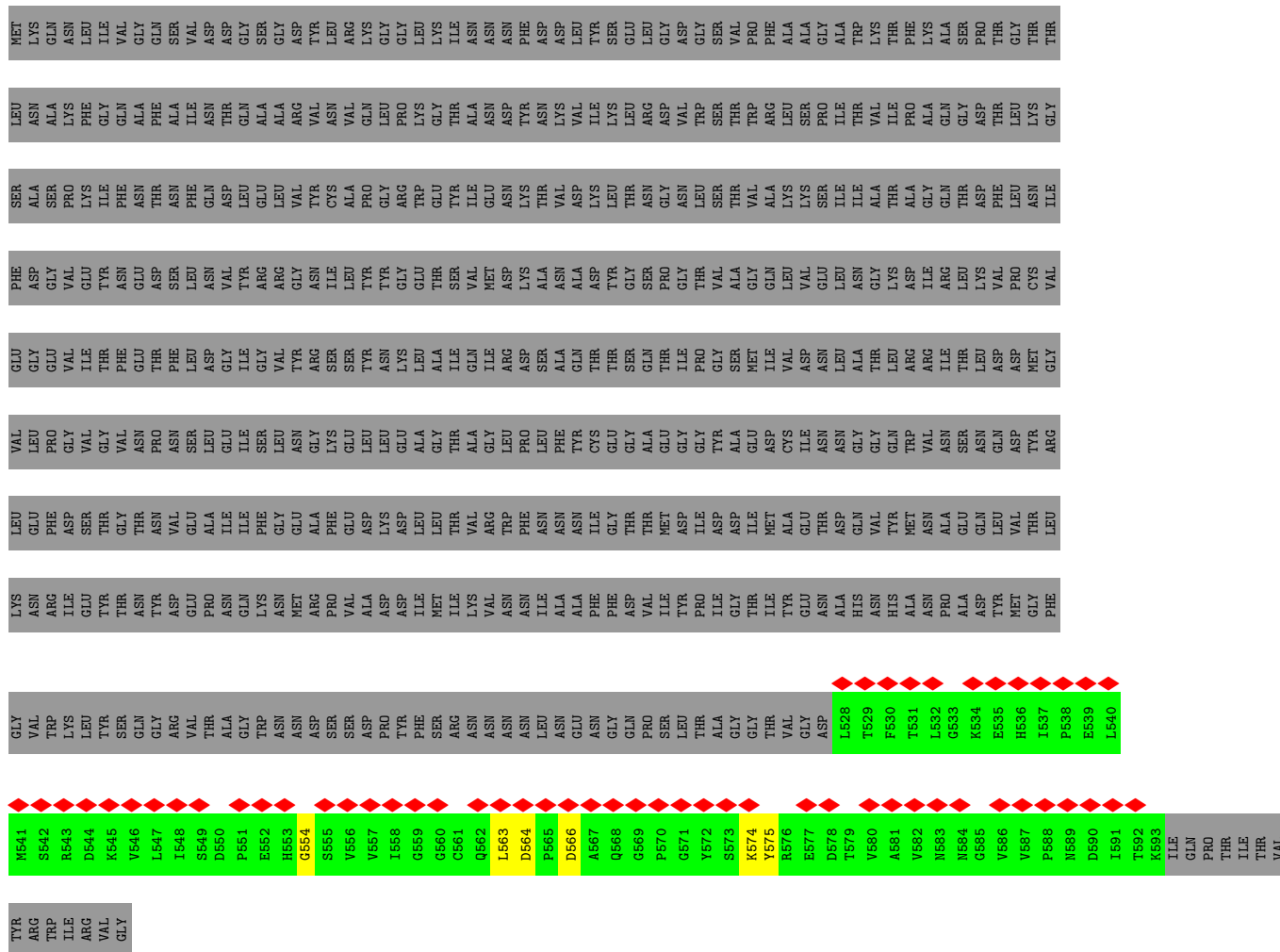
- Molecule 8: Baseplate wedge protein gp10



- Molecule 8: Baseplate wedge protein gp10



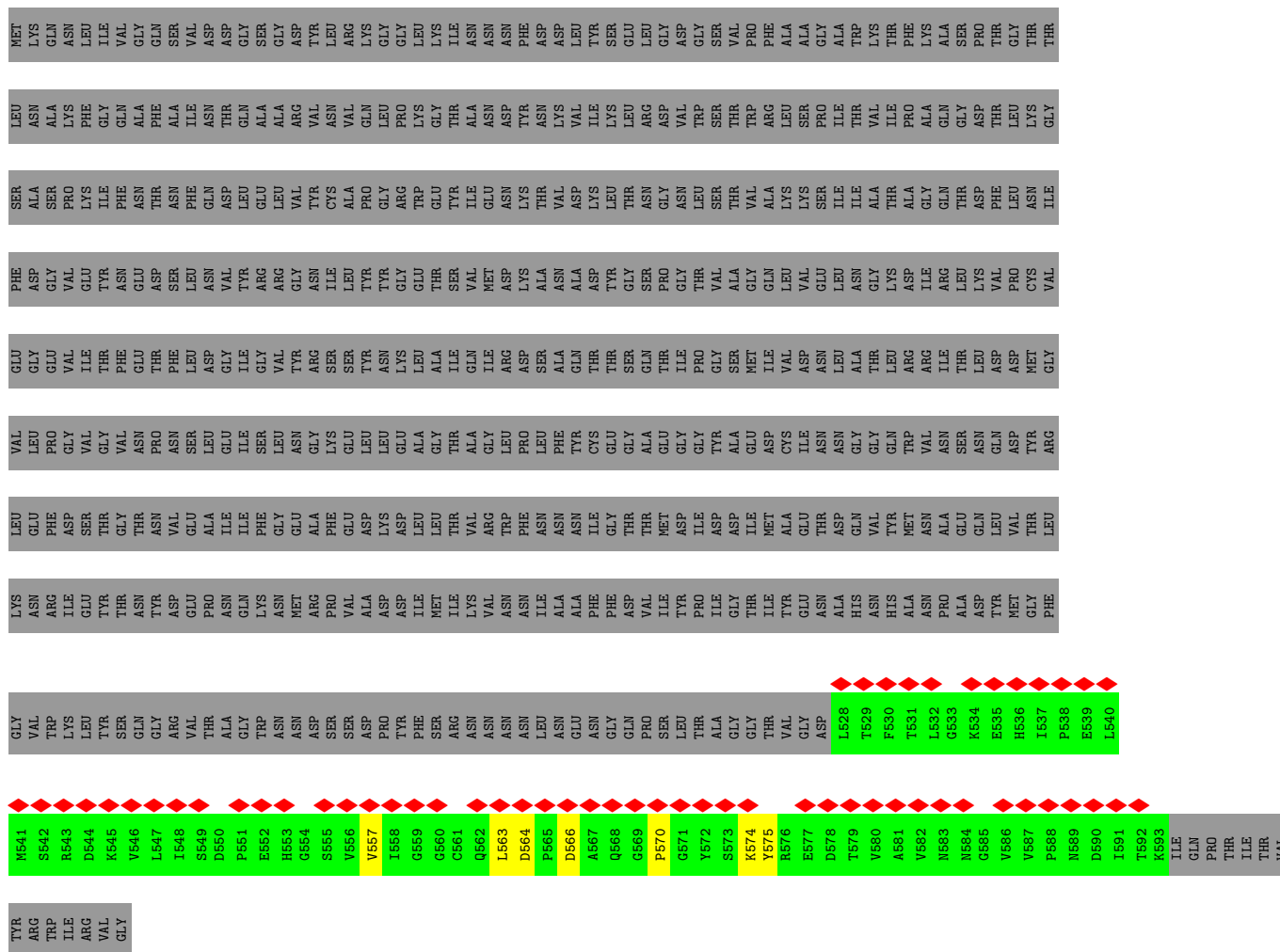
- Molecule 8: Baseplate wedge protein gp10



- Molecule 8: Baseplate wedge protein gp10

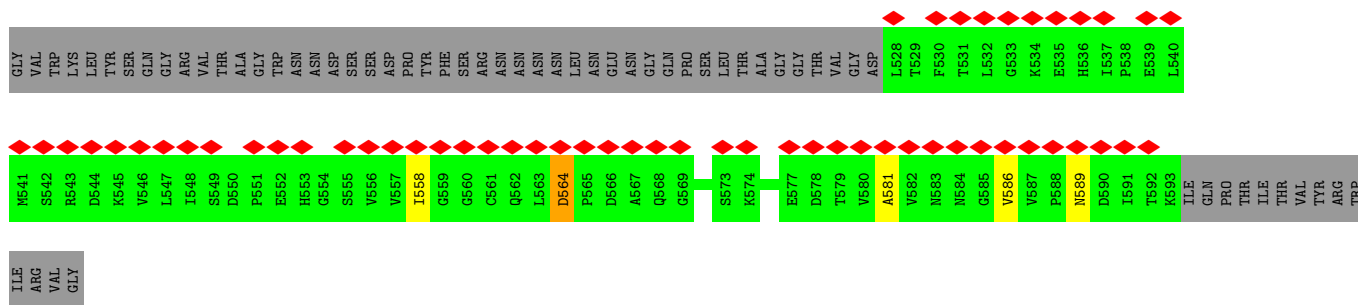


- Molecule 8: Baseplate wedge protein gp10

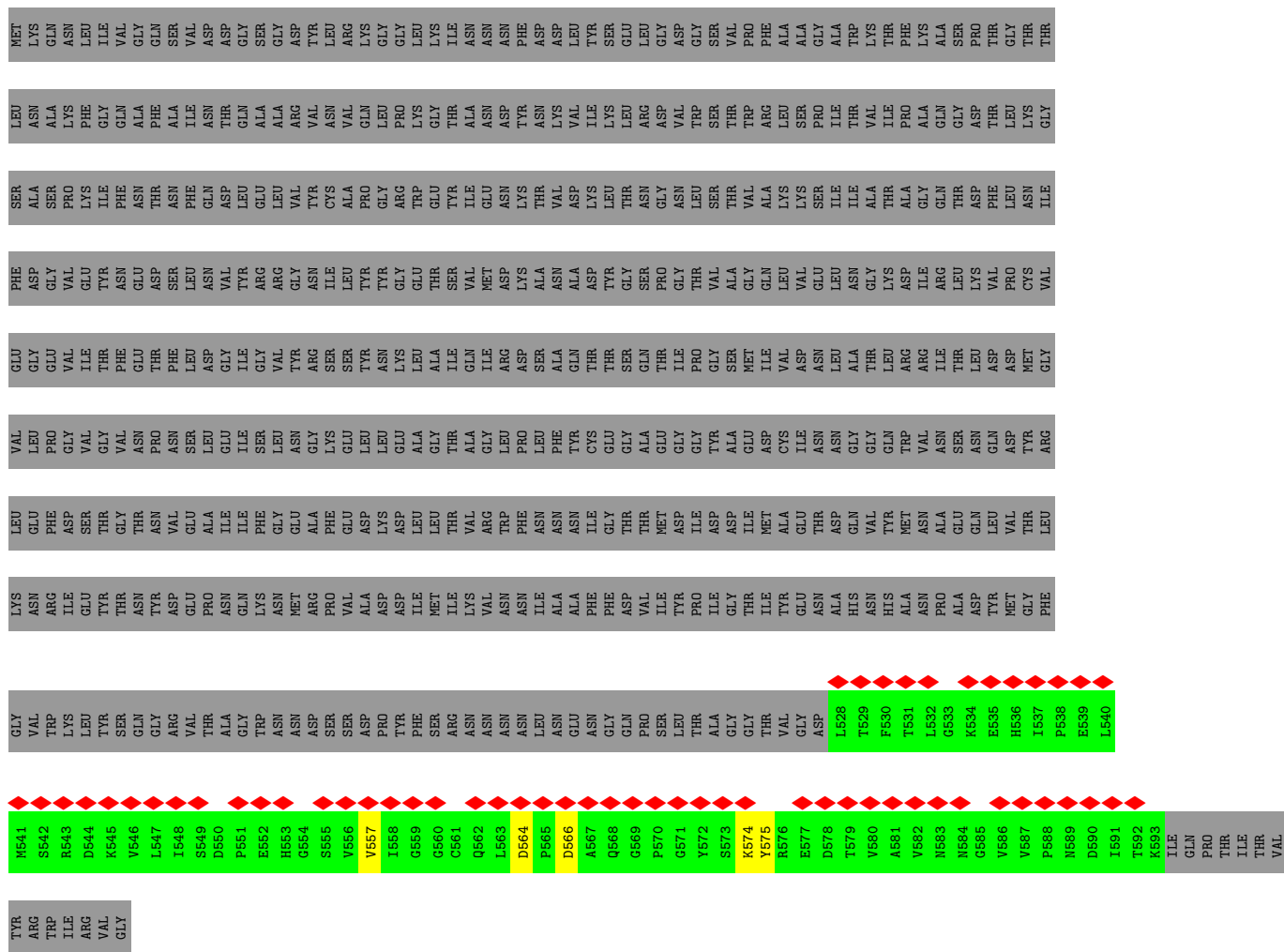


- Molecule 8: Baseplate wedge protein gp10

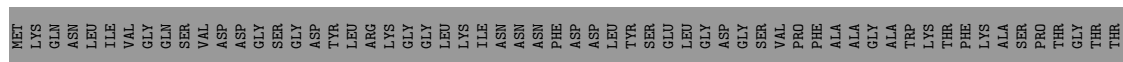




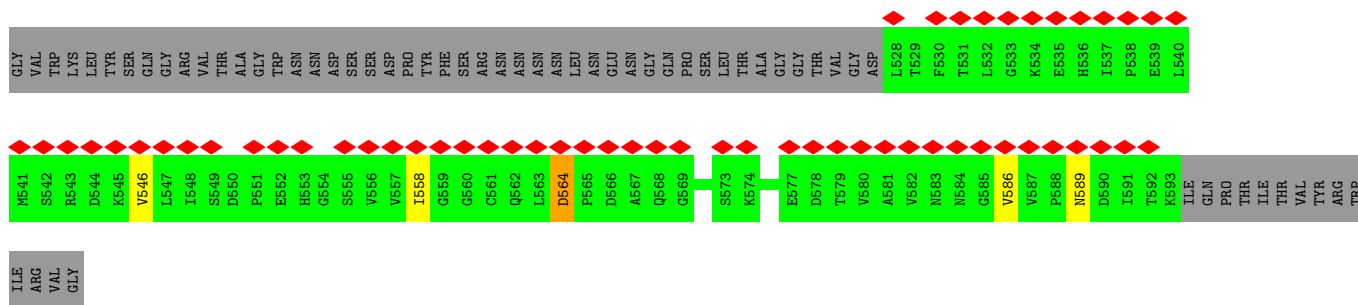
- Molecule 8: Baseplate wedge protein gp10



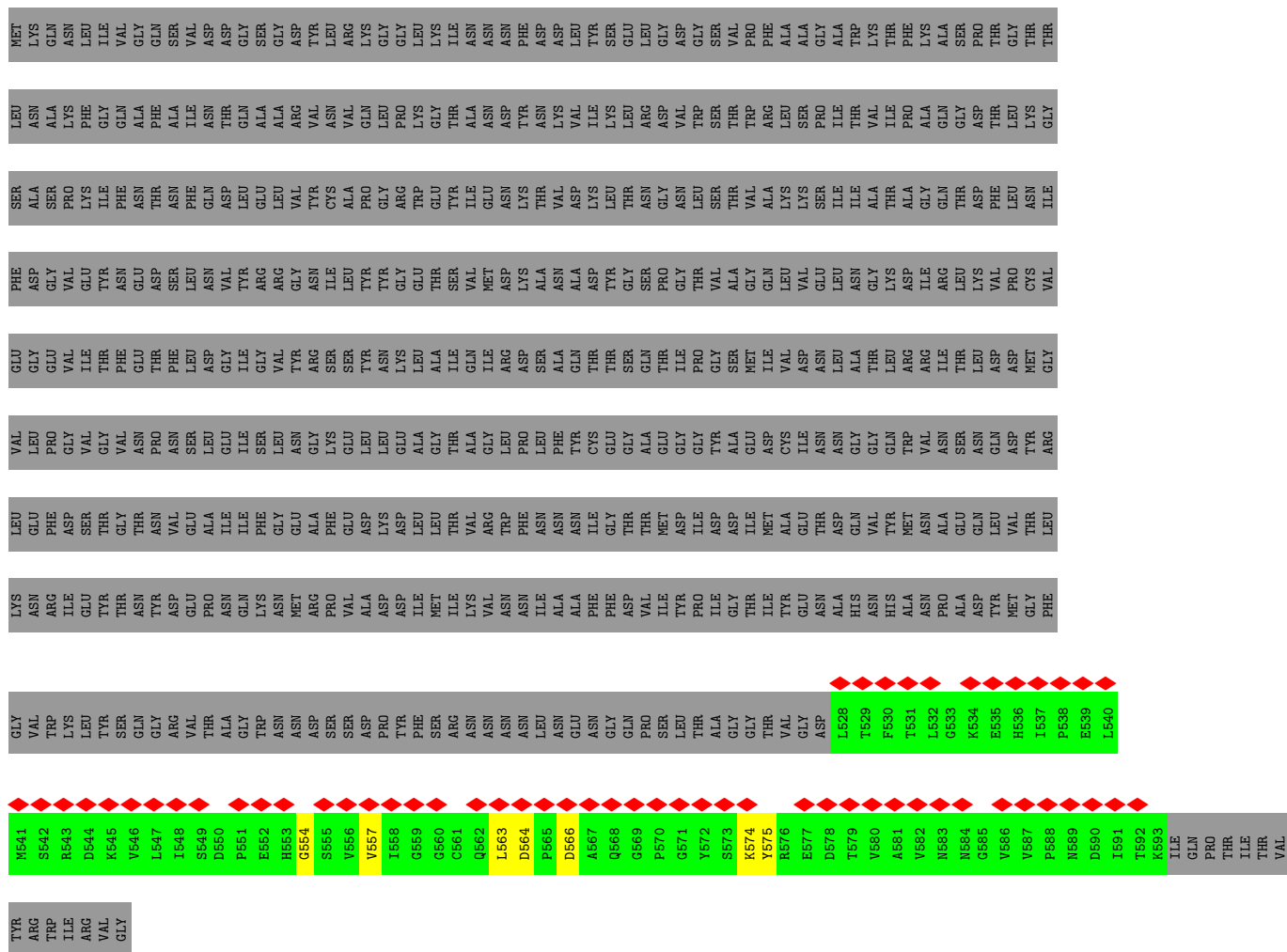
- Molecule 8: Baseplate wedge protein gp10





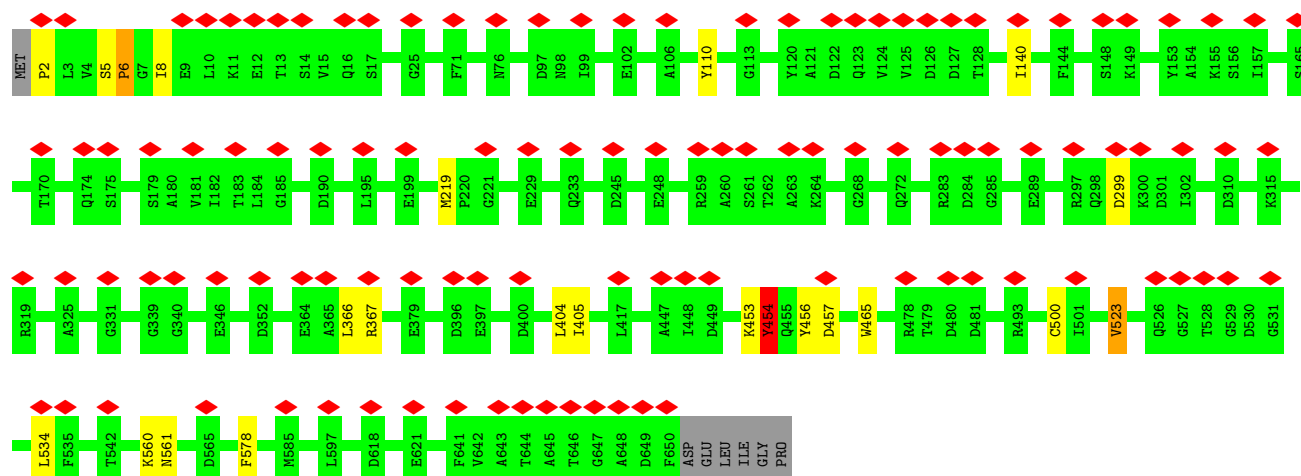


- Molecule 8: Baseplate wedge protein gp10

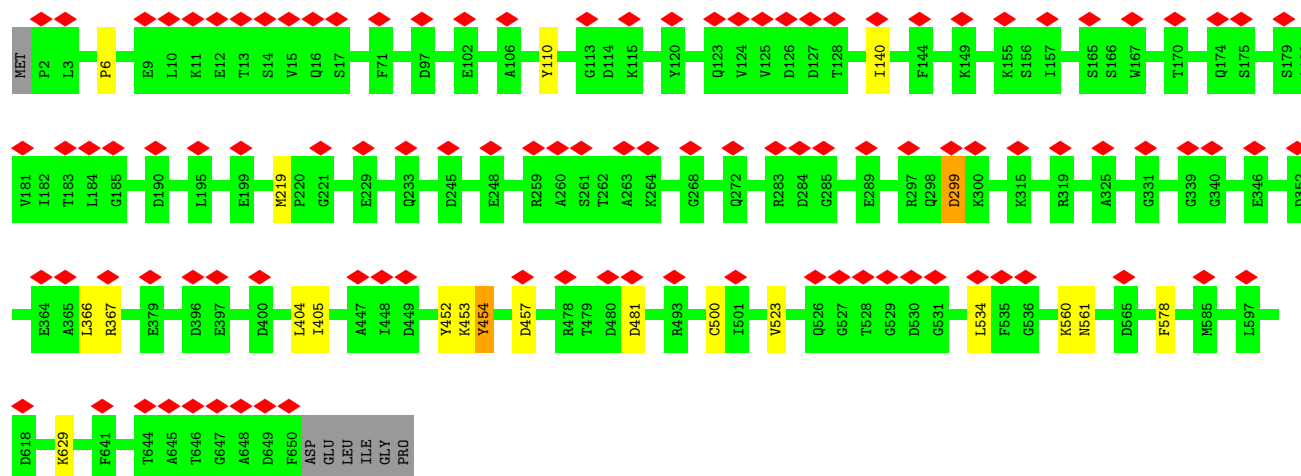


- Molecule 8: Baseplate wedge protein gp10

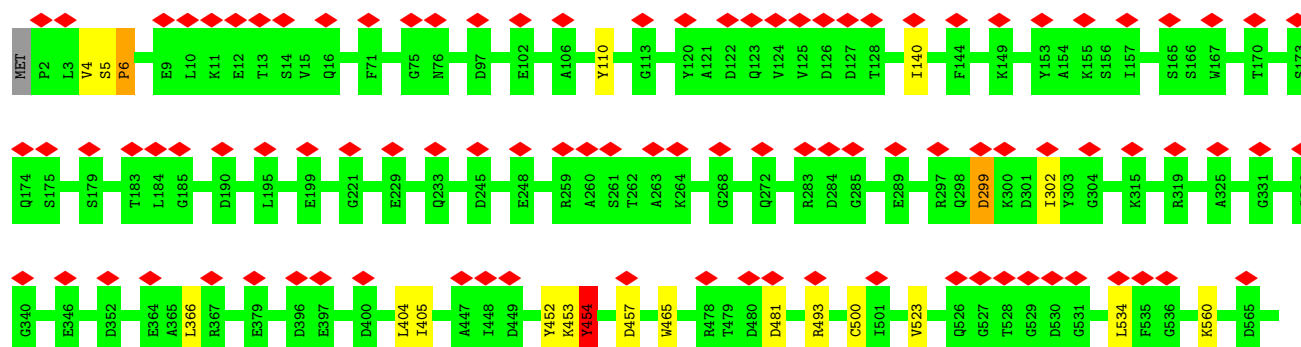


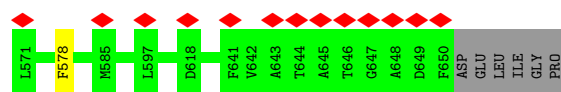


• Molecule 9: Tail sheath protein

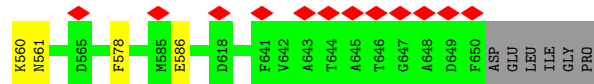
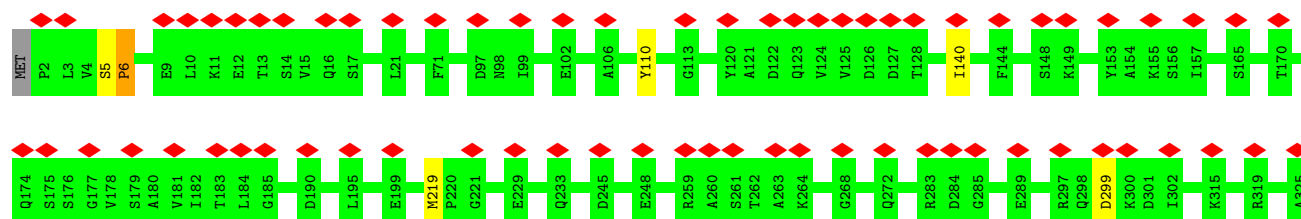


• Molecule 9: Tail sheath protein

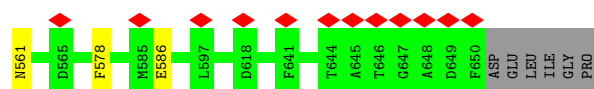
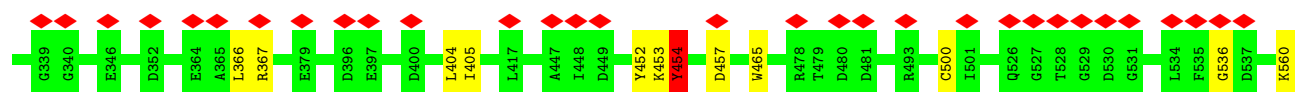
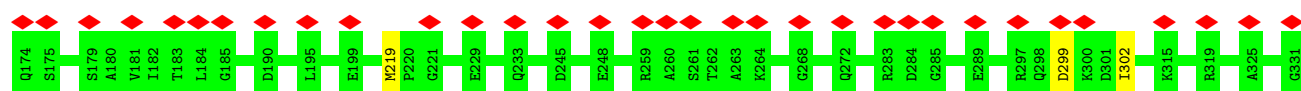
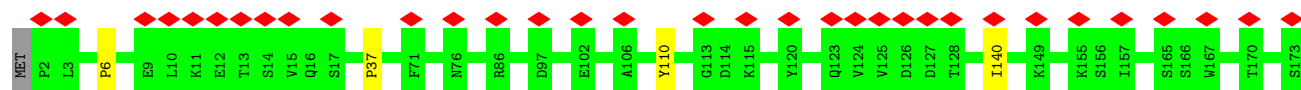




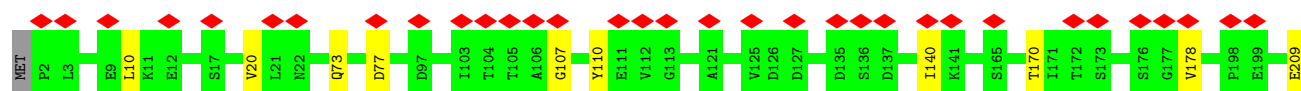
• Molecule 9: Tail sheath protein

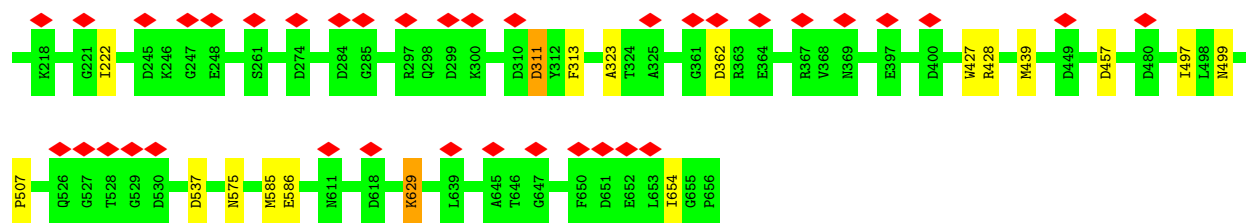


• Molecule 9: Tail sheath protein

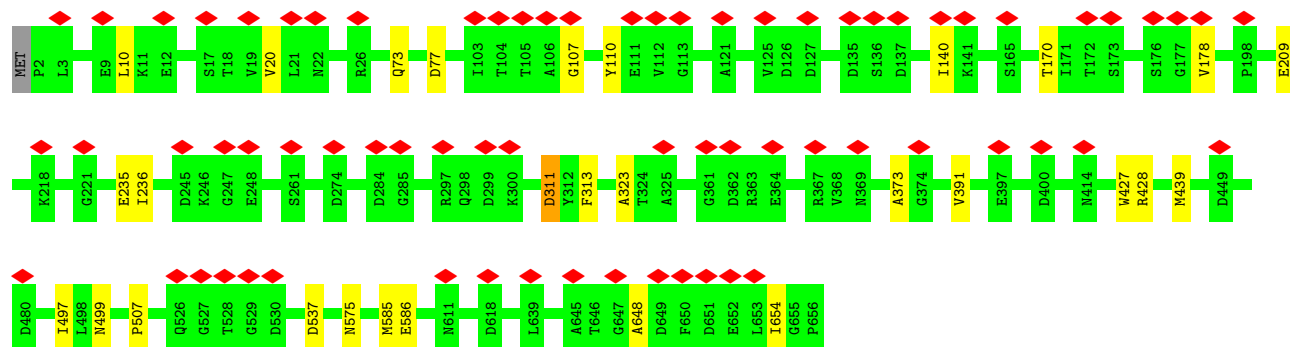


• Molecule 9: Tail sheath protein

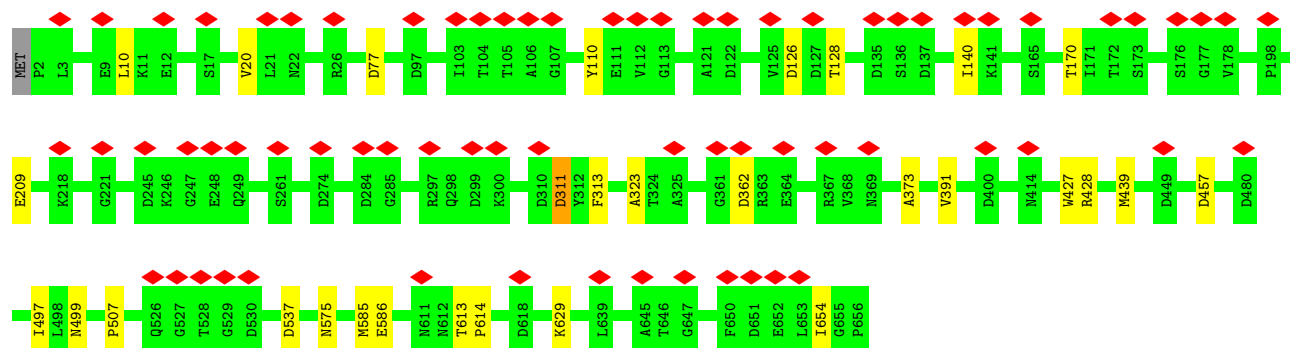




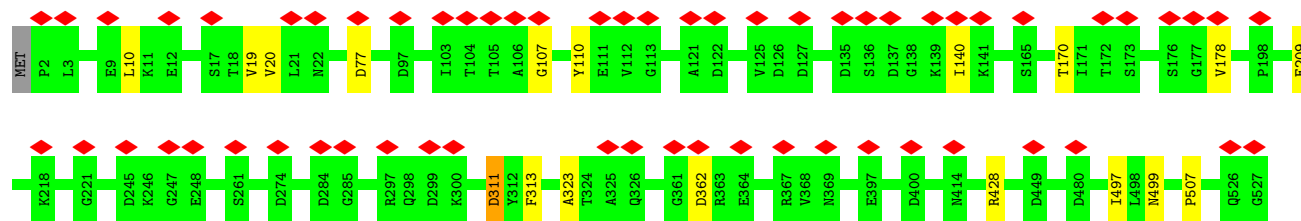
• Molecule 9: Tail sheath protein

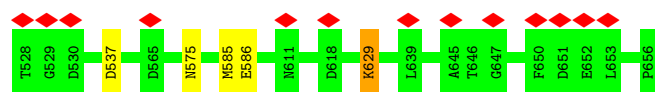


• Molecule 9: Tail sheath protein

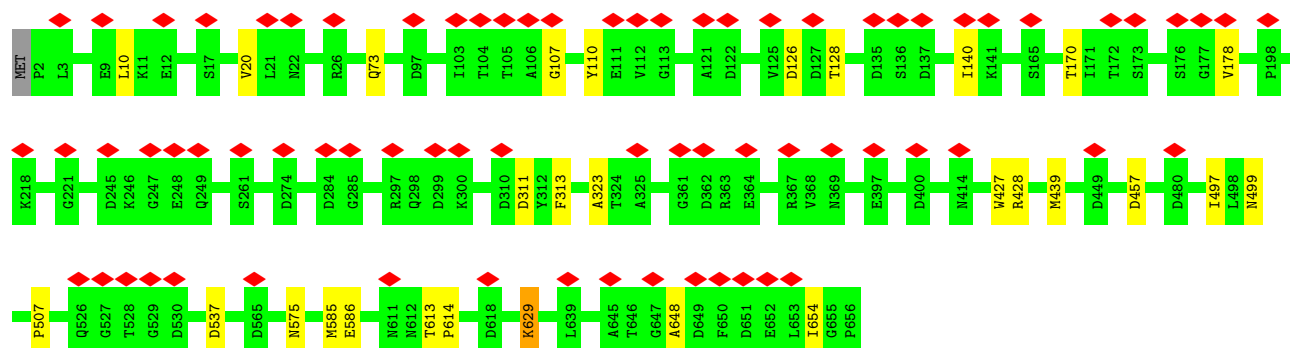


• Molecule 9: Tail sheath protein

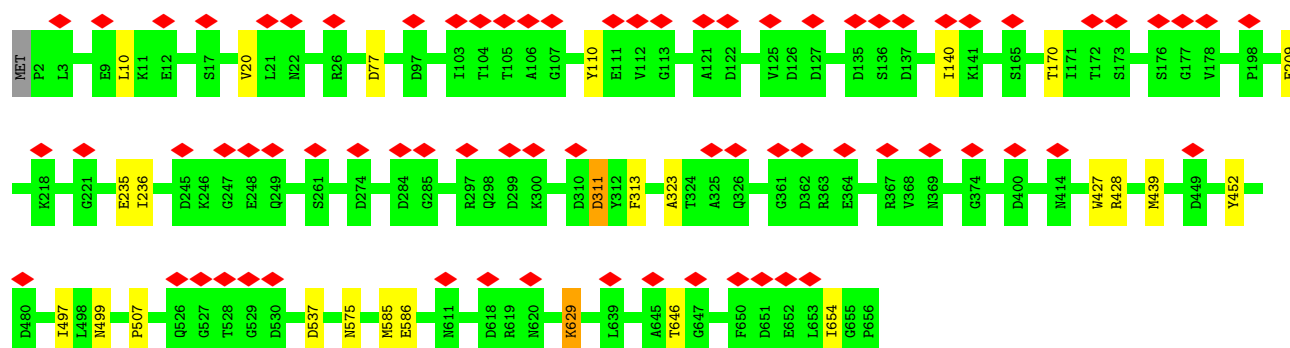




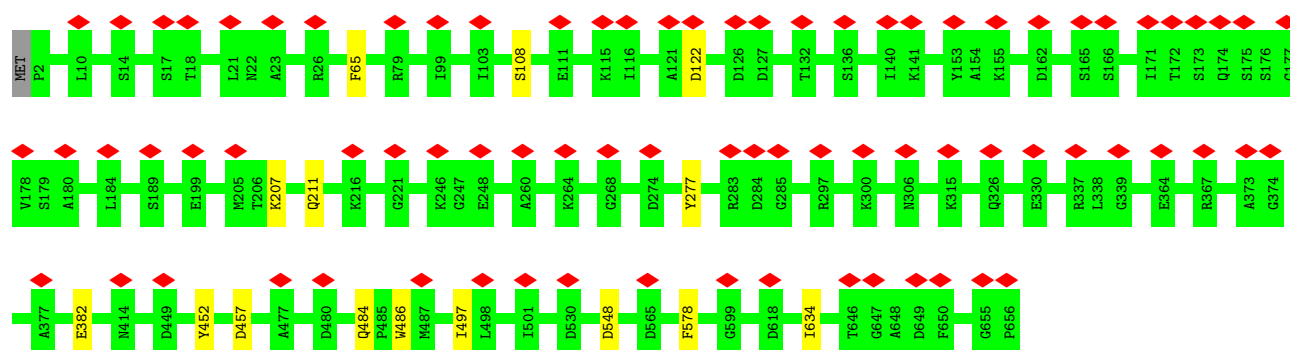
- Molecule 9: Tail sheath protein



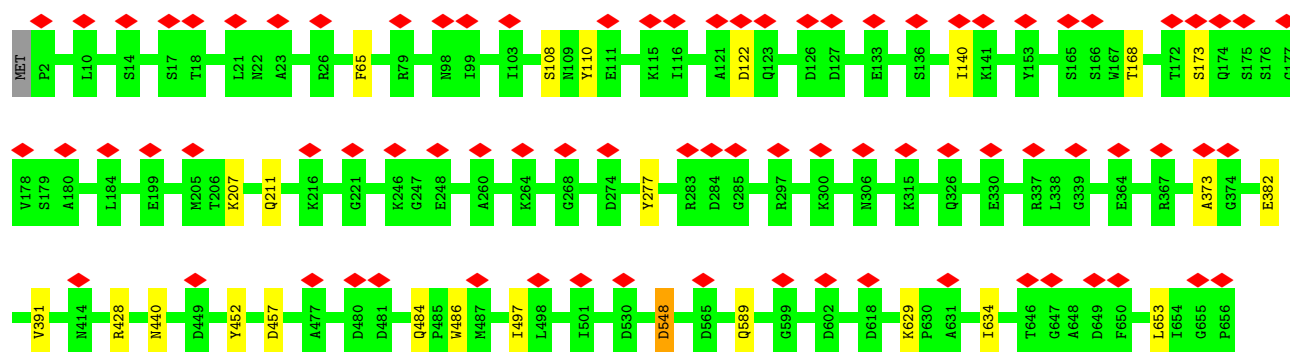
- Molecule 9: Tail sheath protein



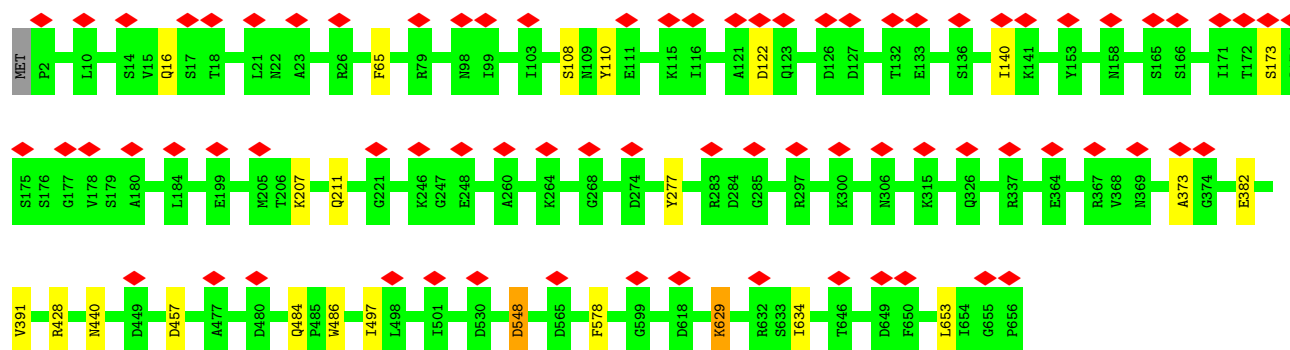
- Molecule 9: Tail sheath protein



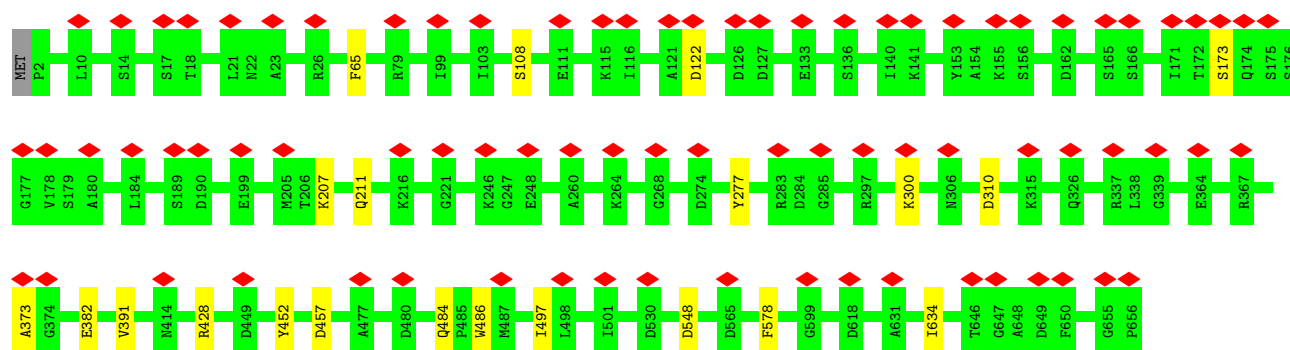
- Molecule 9: Tail sheath protein



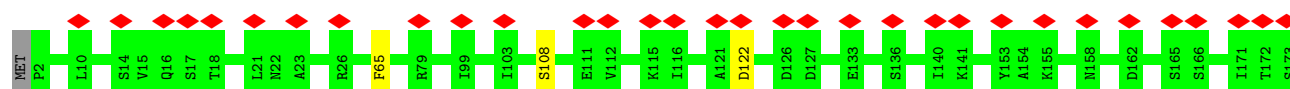
• Molecule 9: Tail sheath protein

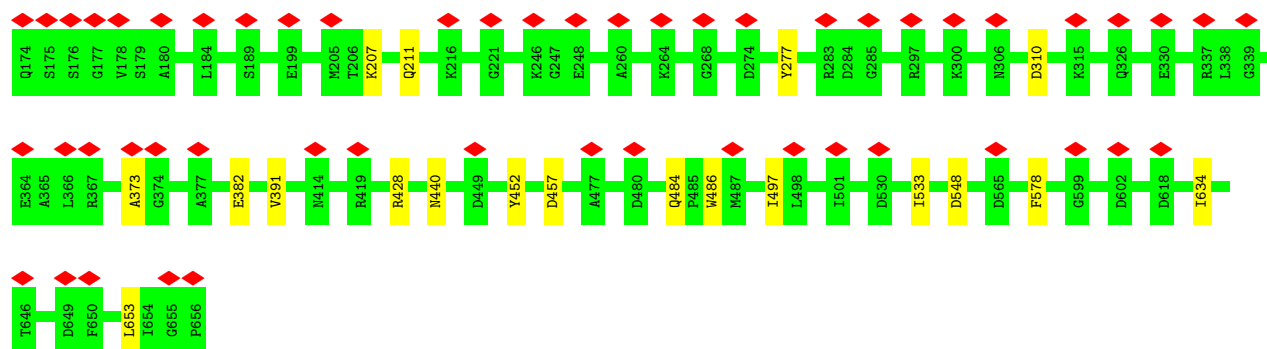


• Molecule 9: Tail sheath protein



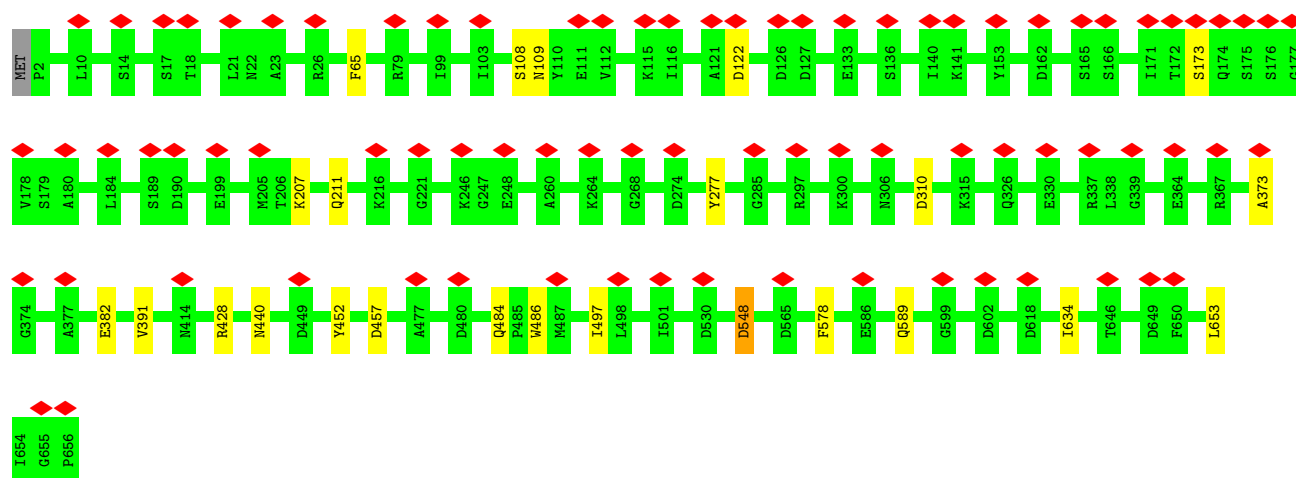
• Molecule 9: Tail sheath protein





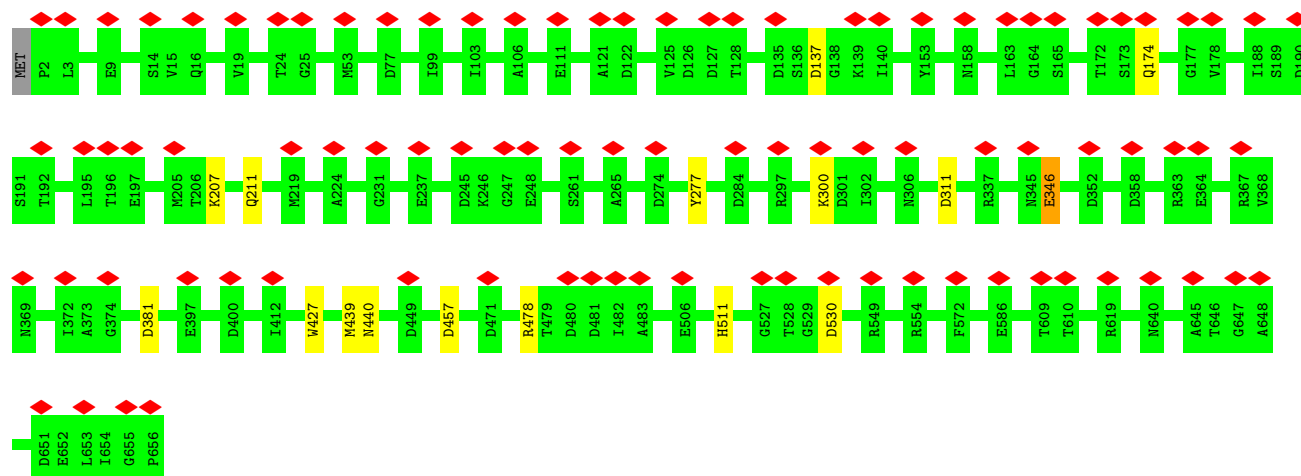
- Molecule 9: Tail sheath protein

Chain SR: 12% 96%

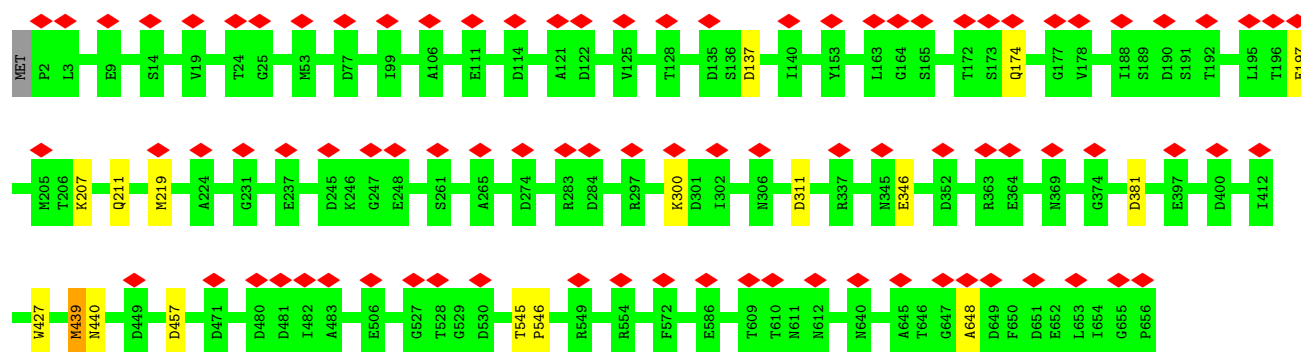


- Molecule 9: Tail sheath protein

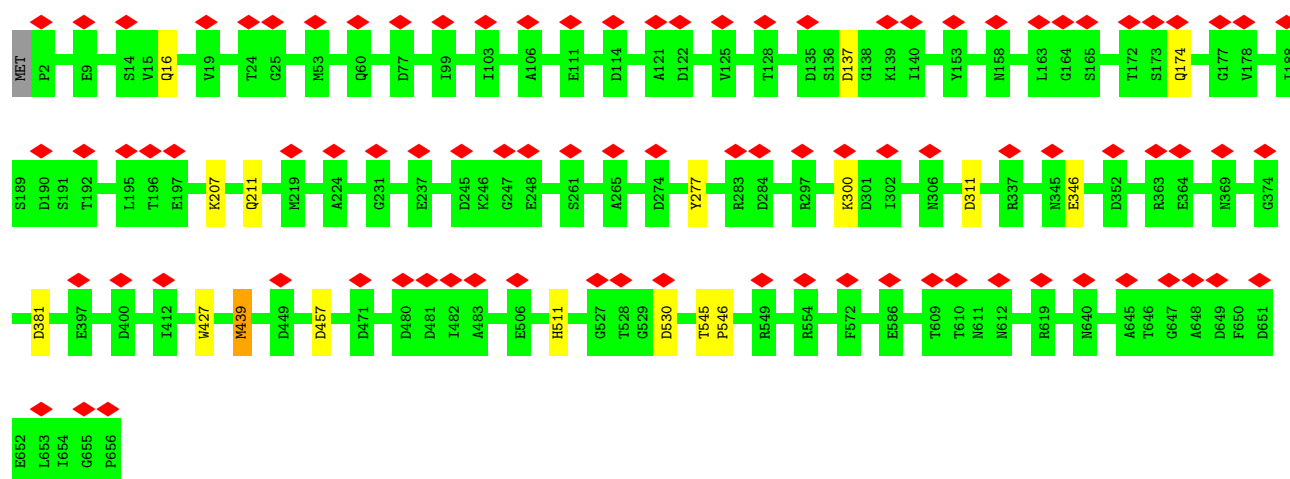
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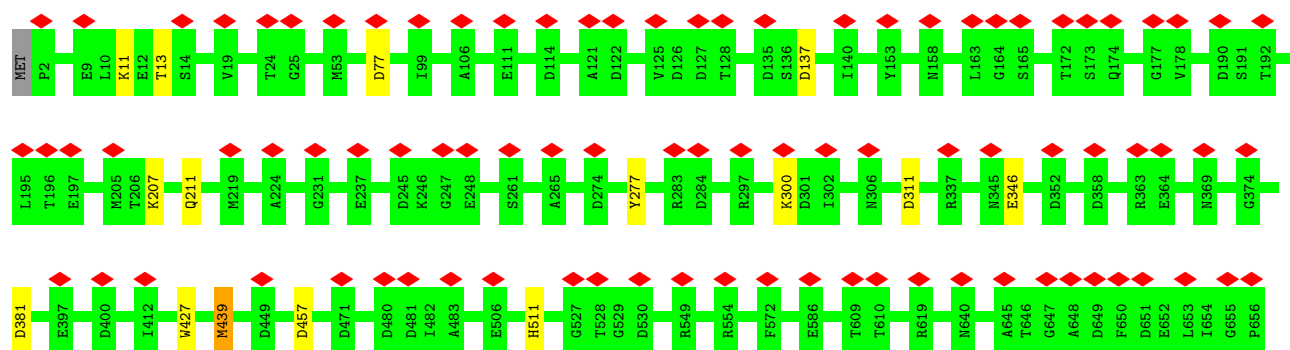
- Molecule 9: Tail sheath protein



• Molecule 9: Tail sheath protein

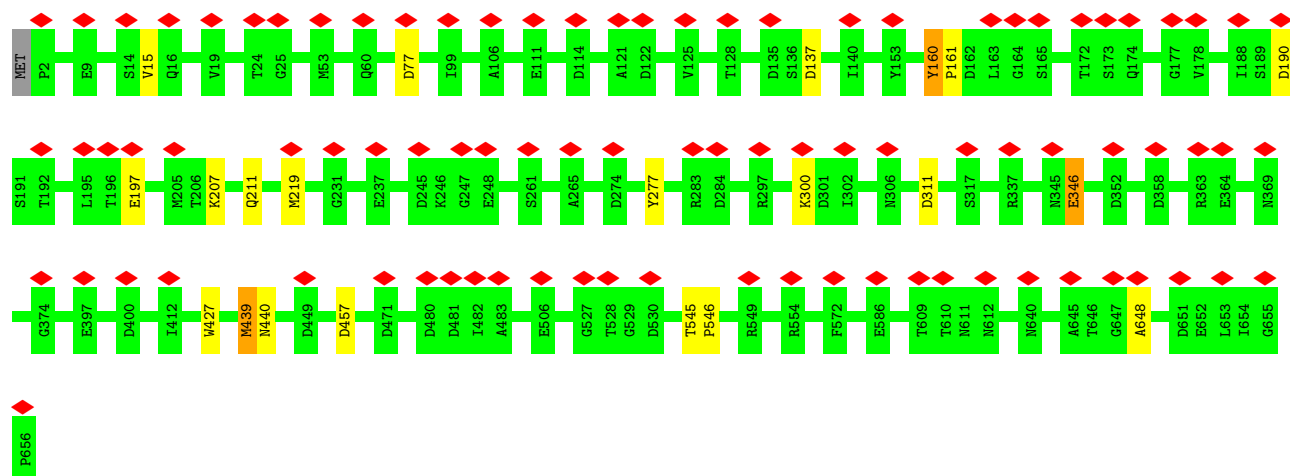


• Molecule 9: Tail sheath protein

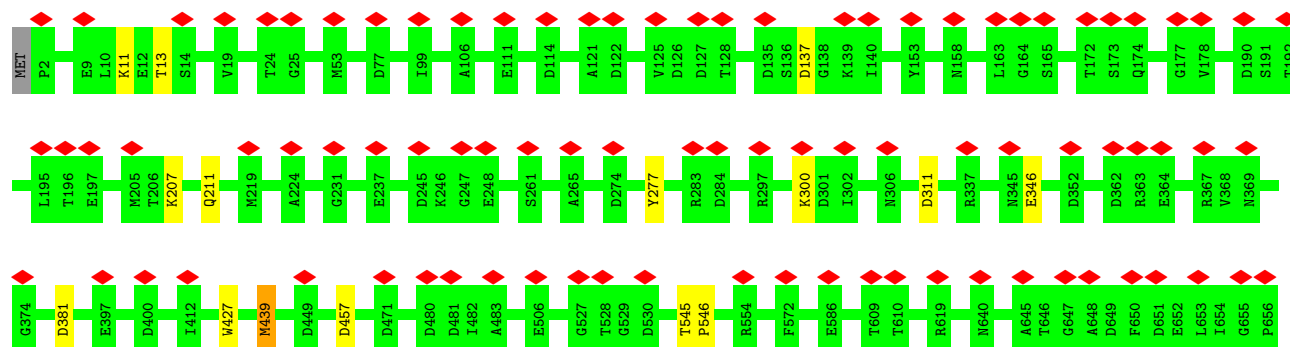


• Molecule 9: Tail sheath protein

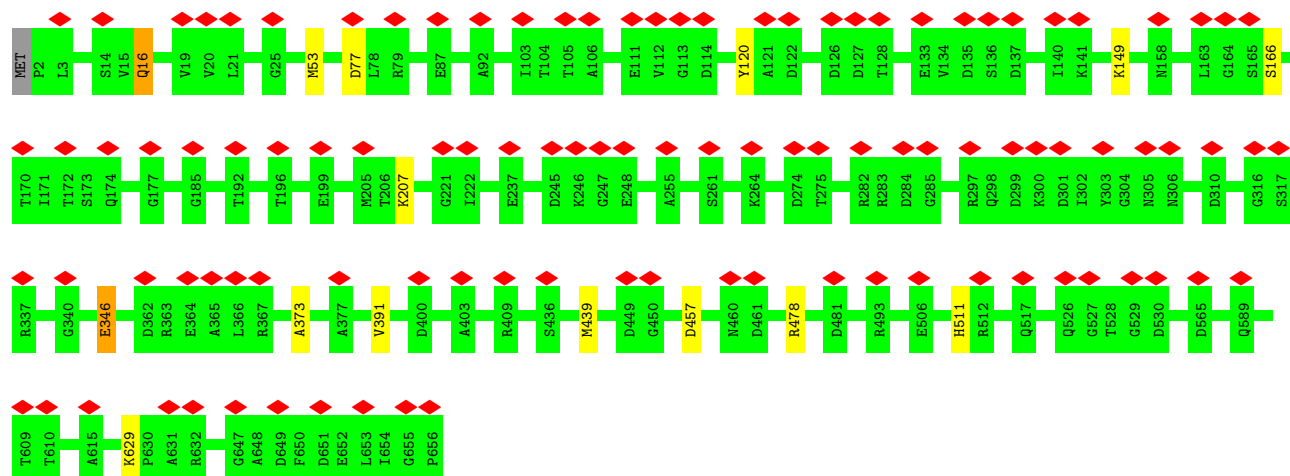




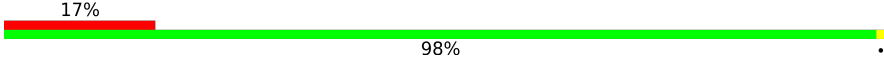
- Molecule 9: Tail sheath protein

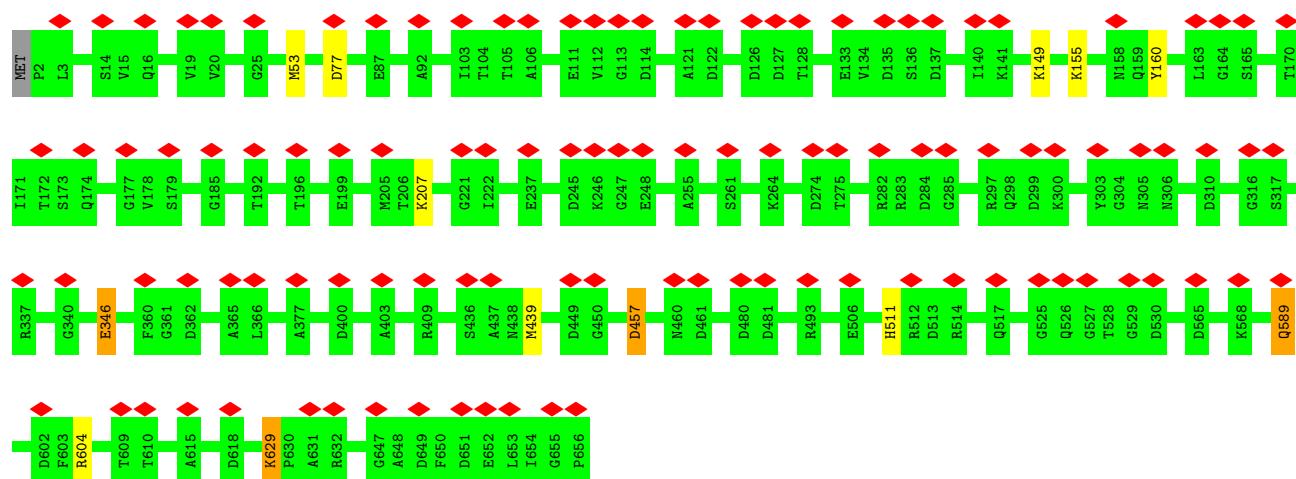


- Molecule 9: Tail sheath protein

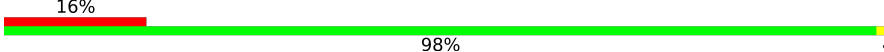


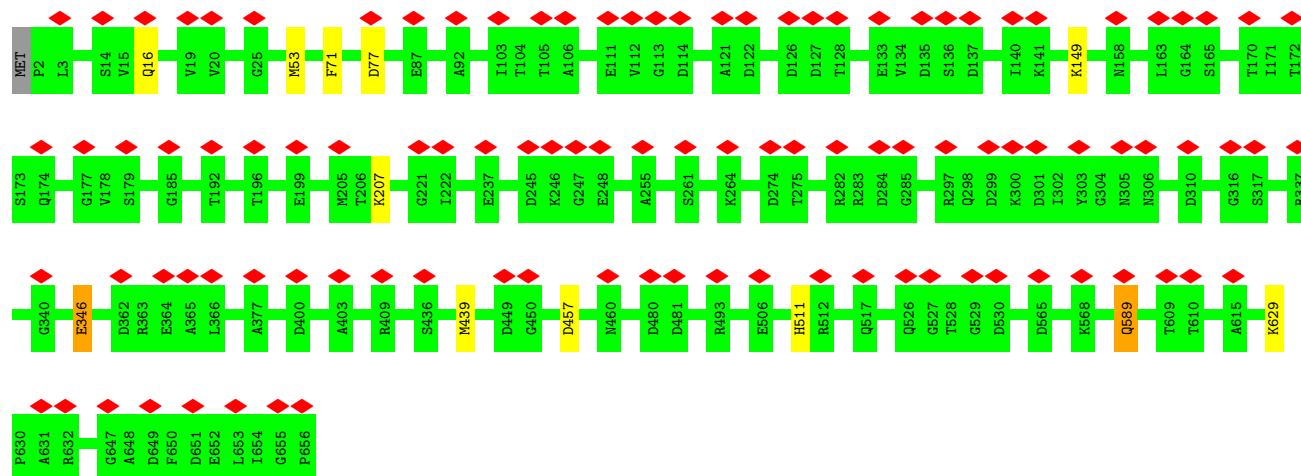
- Molecule 9: Tail sheath protein

Chain SZ:  17% 98% ..

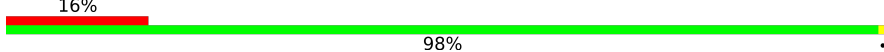


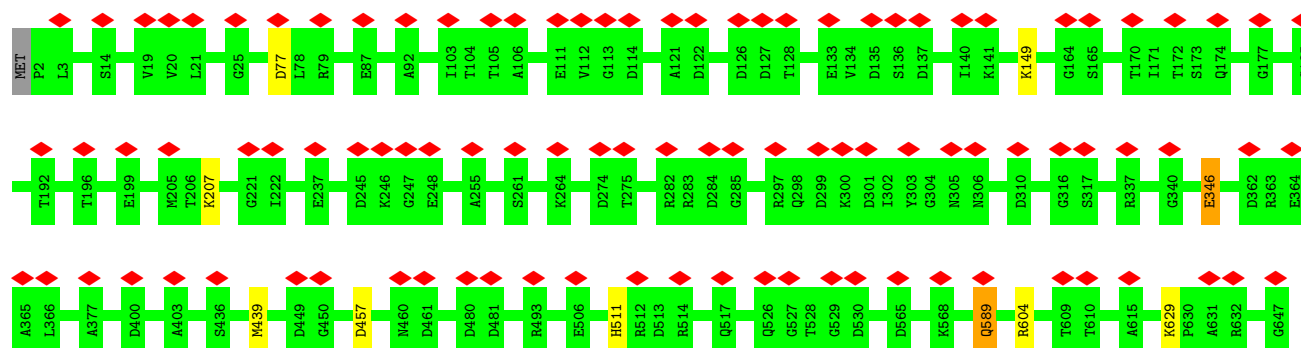
• Molecule 9: Tail sheath protein

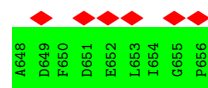
Chain Sa:  16% 98% .



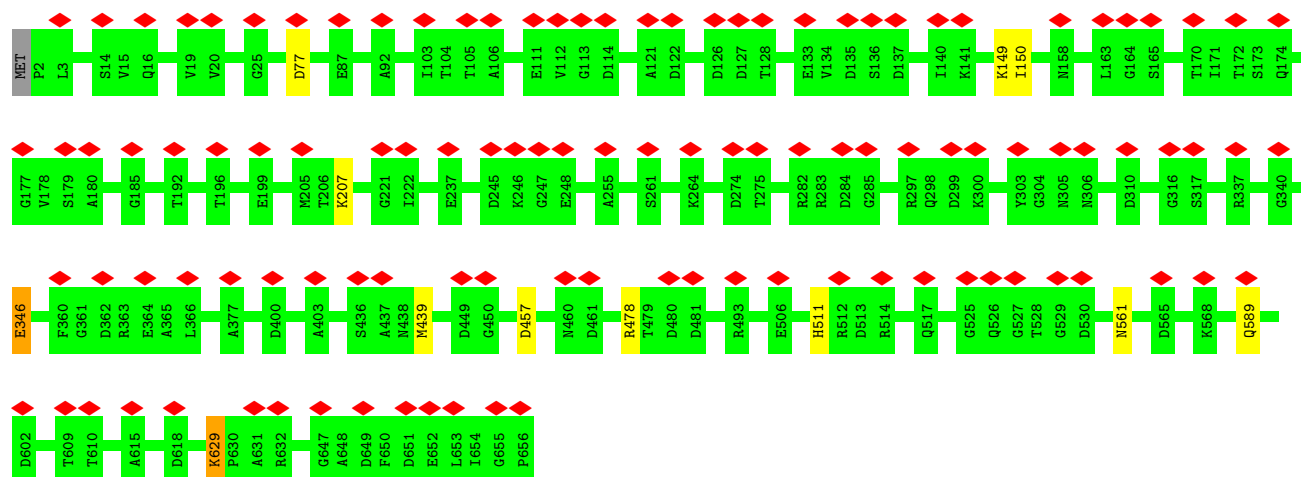
• Molecule 9: Tail sheath protein

Chain Sb:  16% 98% .

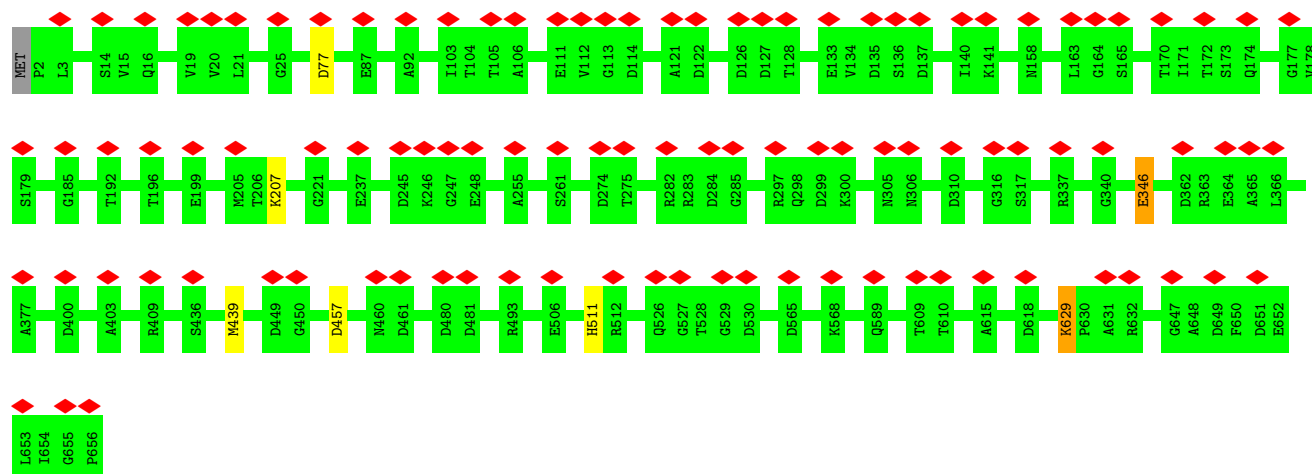




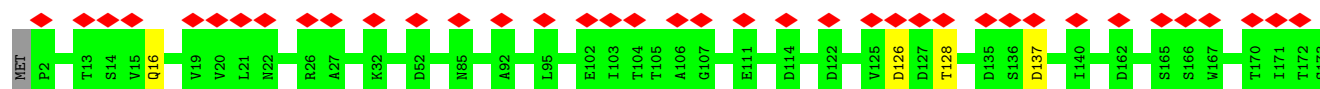
• Molecule 9: Tail sheath protein

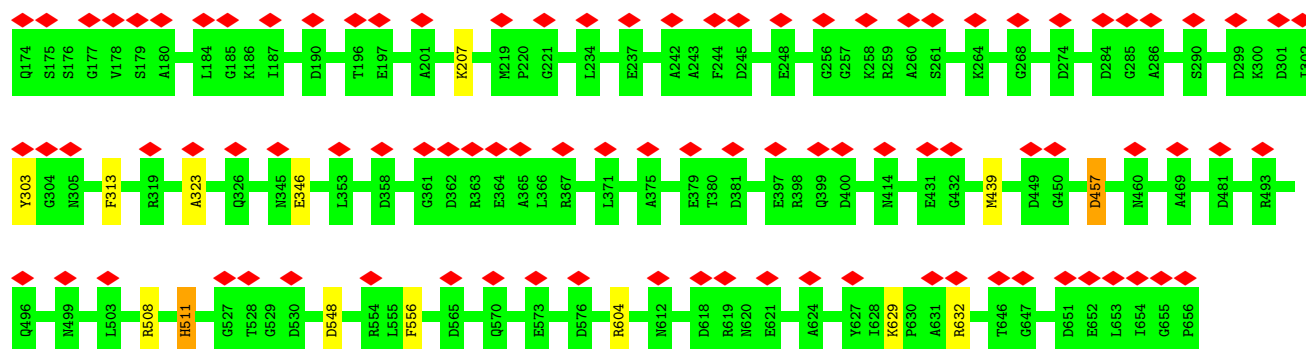


• Molecule 9: Tail sheath protein

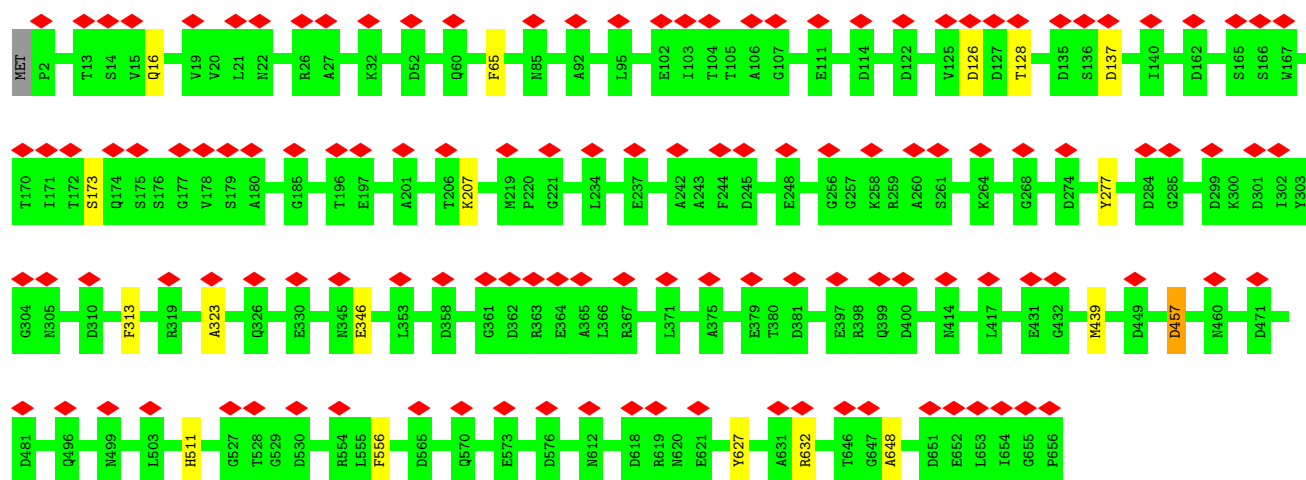


• Molecule 9: Tail sheath protein

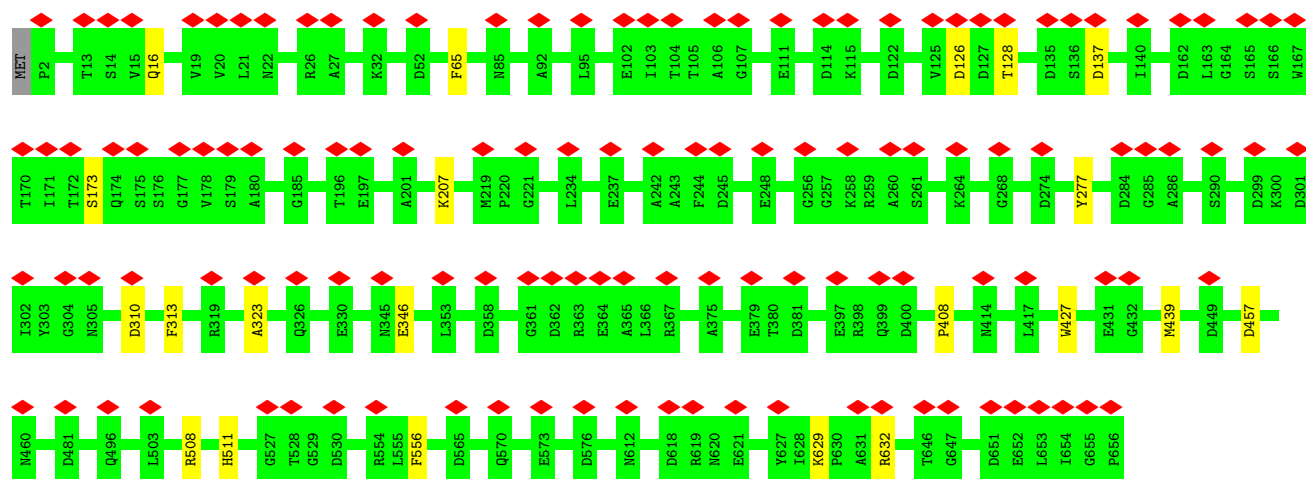




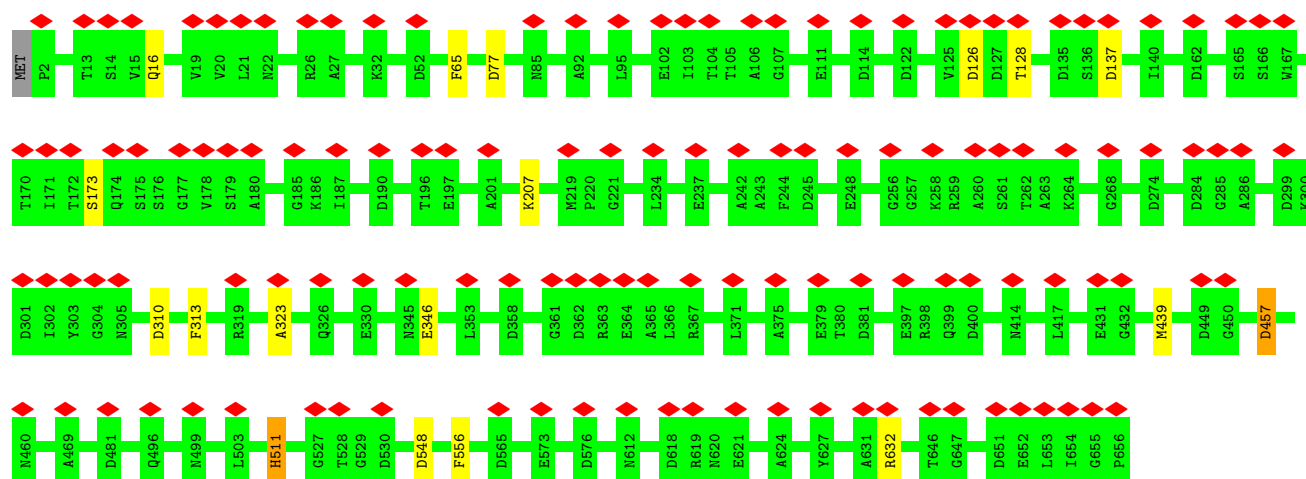
• Molecule 9: Tail sheath protein



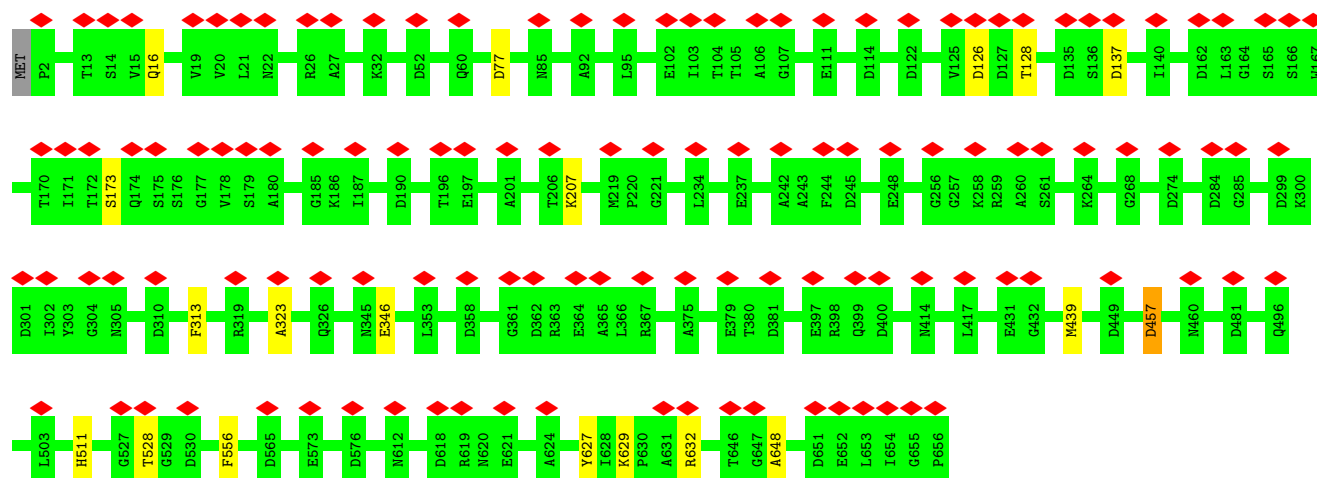
• Molecule 9: Tail sheath protein



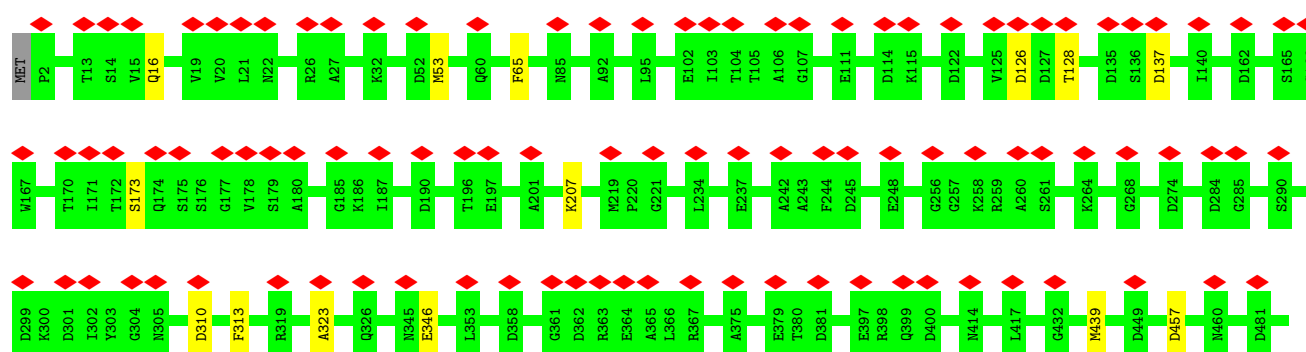
• Molecule 9: Tail sheath protein

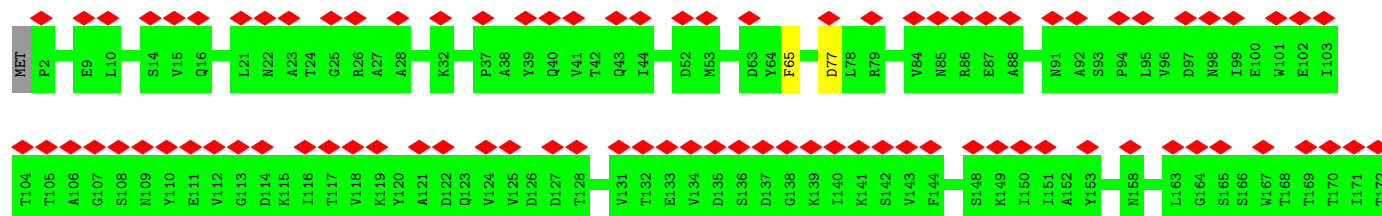


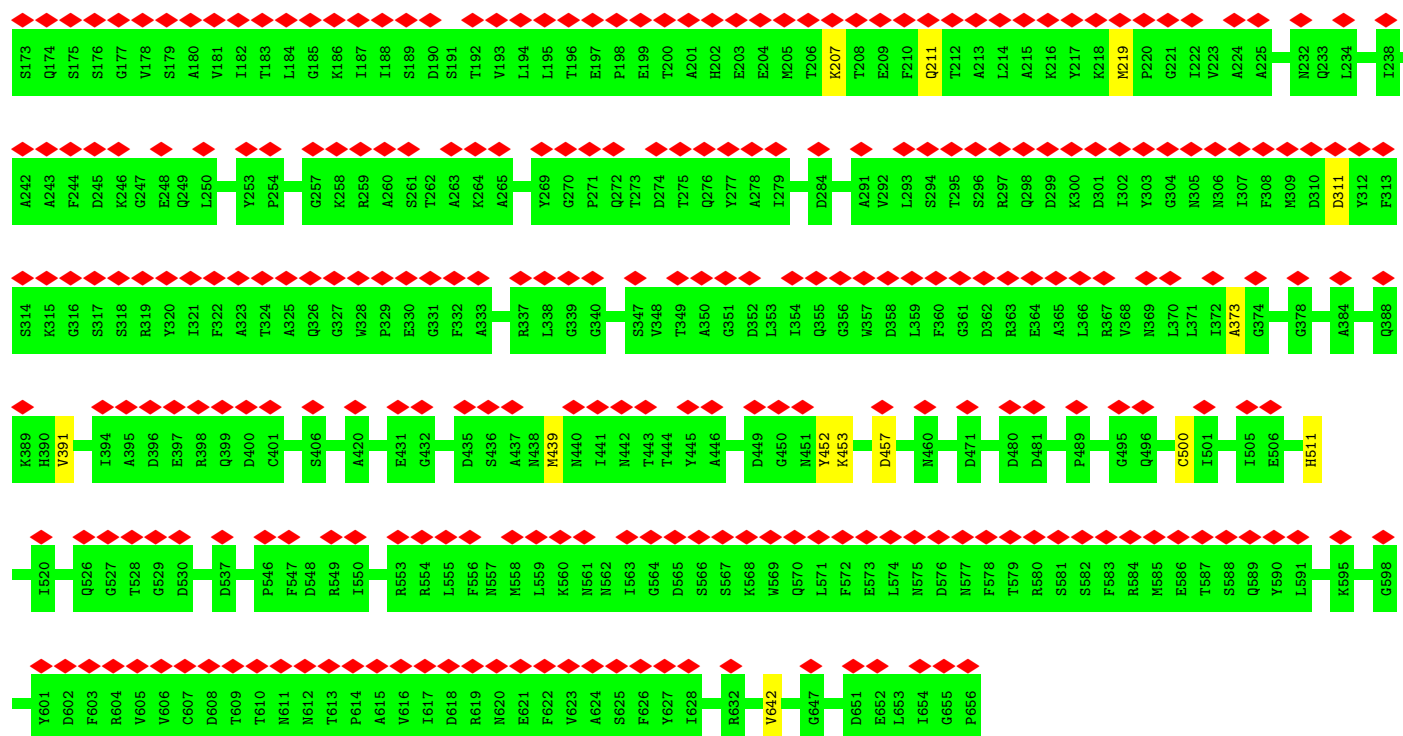
• Molecule 9: Tail sheath protein



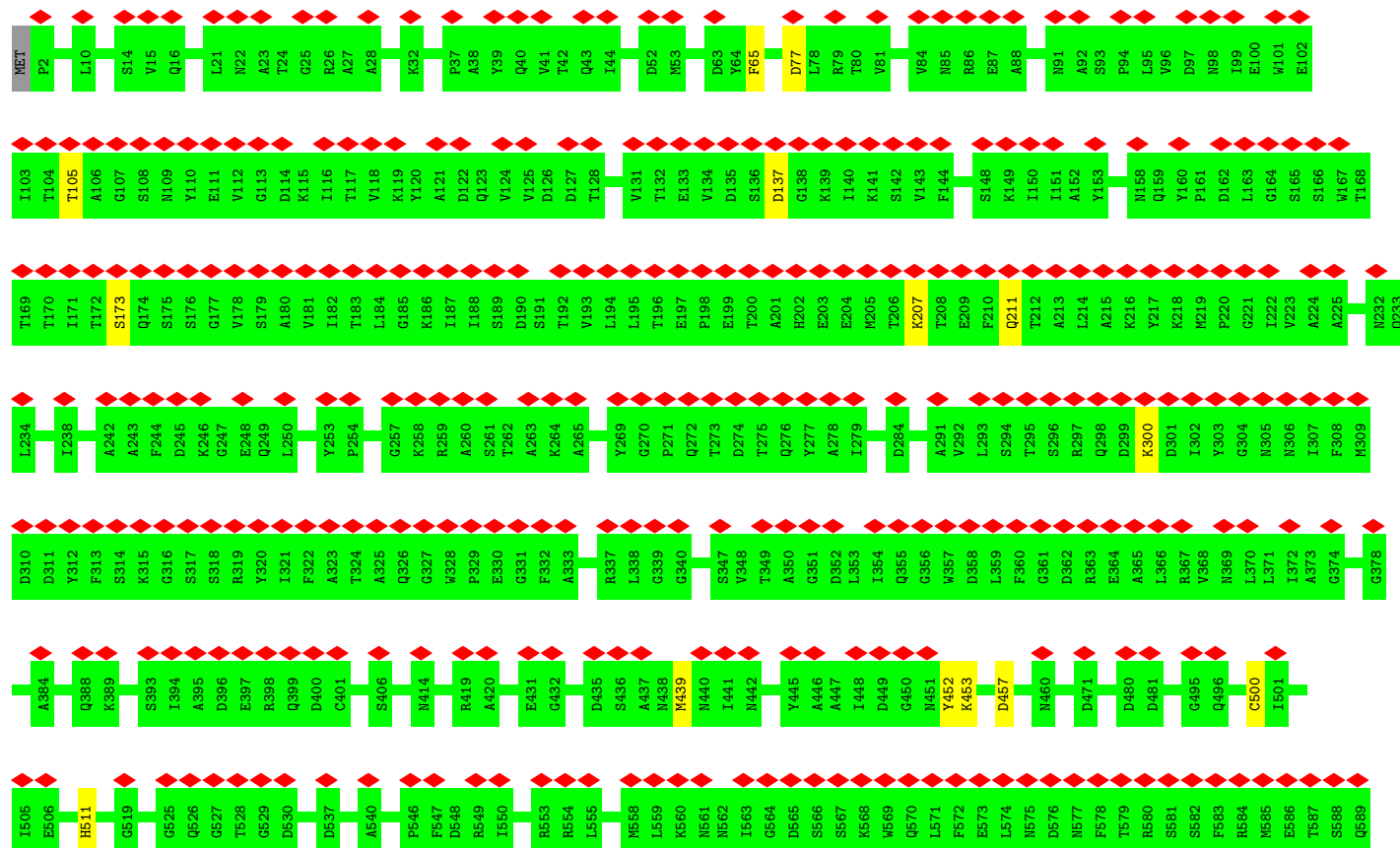
• Molecule 9: Tail sheath protein

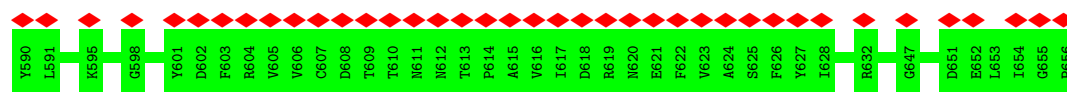






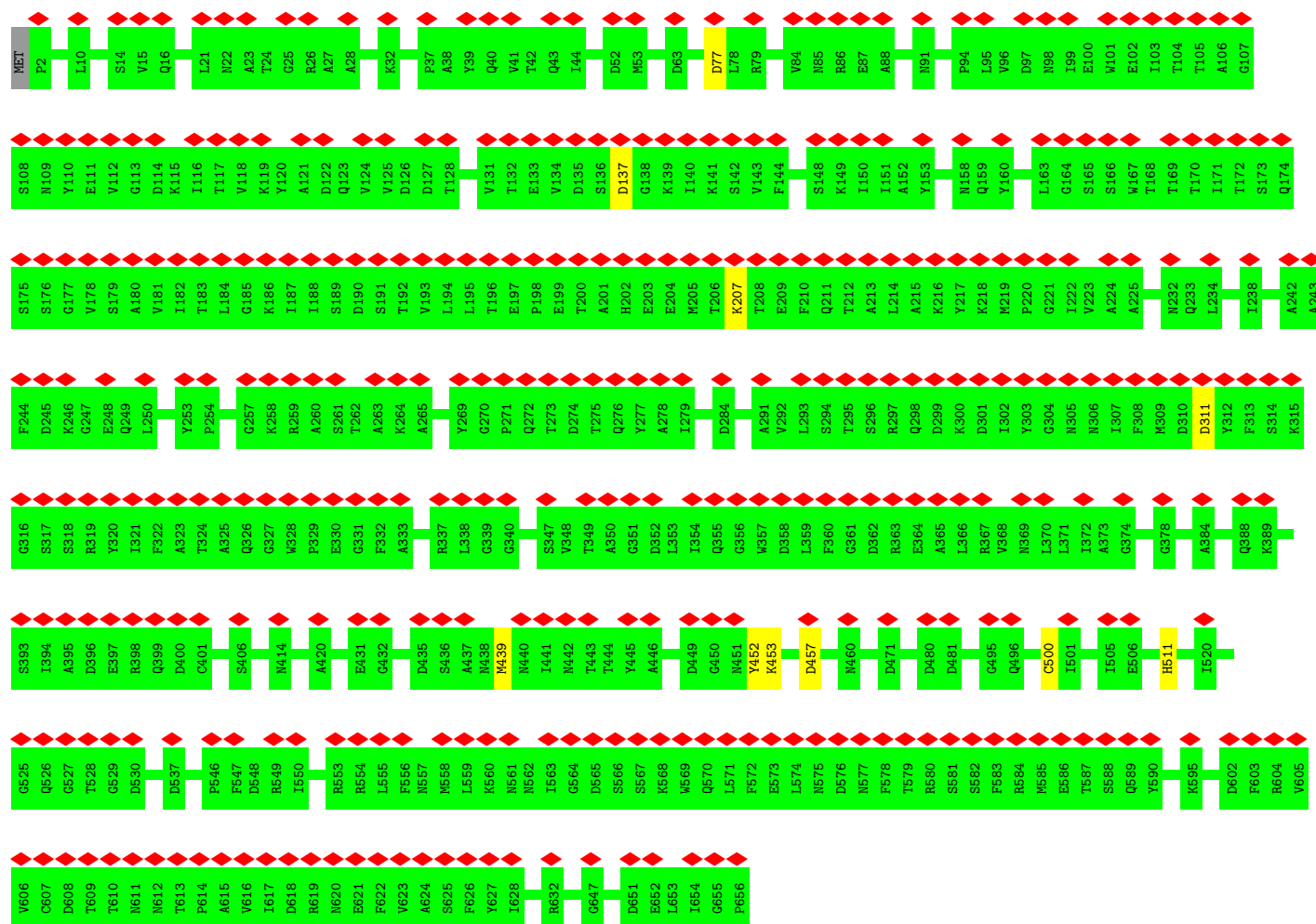
• Molecule 9: Tail sheath protein





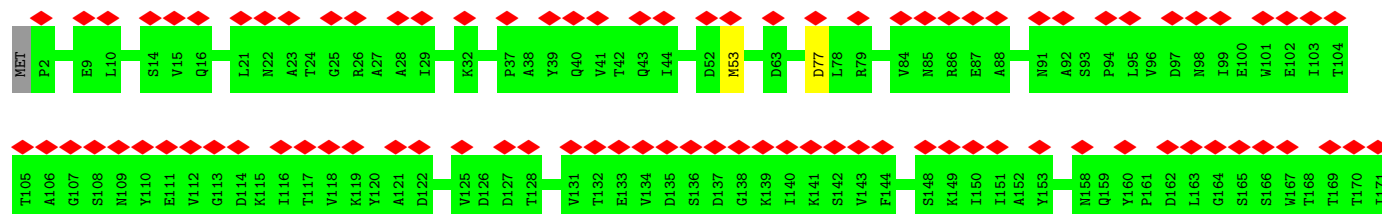
• Molecule 9: Tail sheath protein

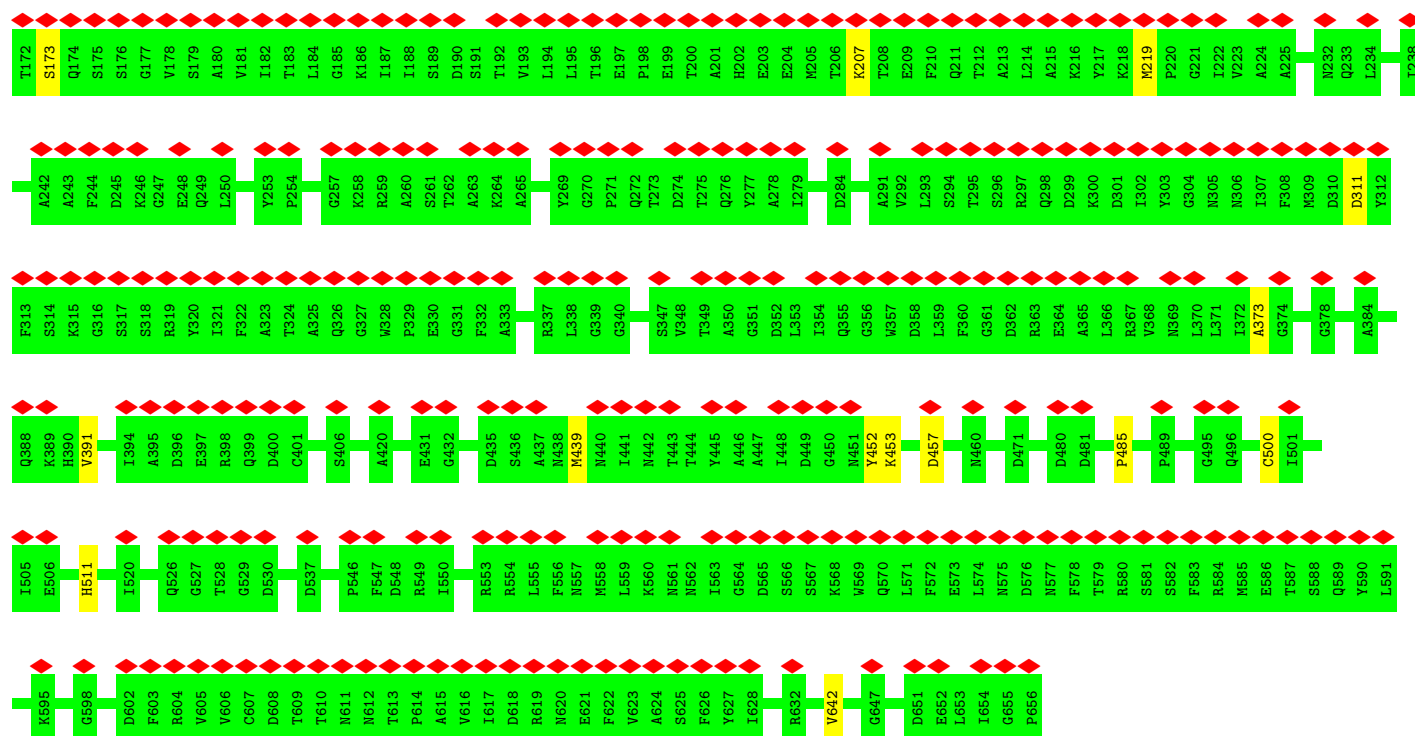
Chain Sn: 55% 98%



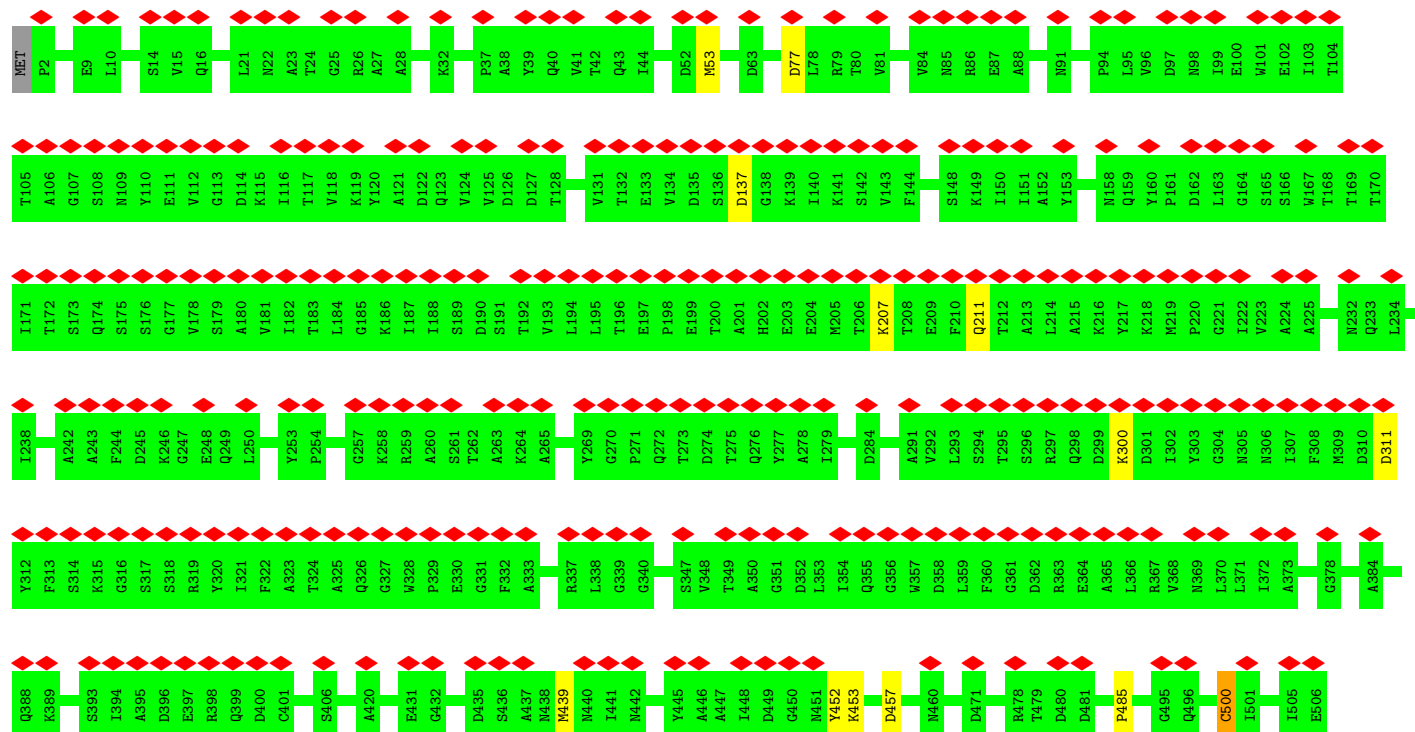
• Molecule 9: Tail sheath protein

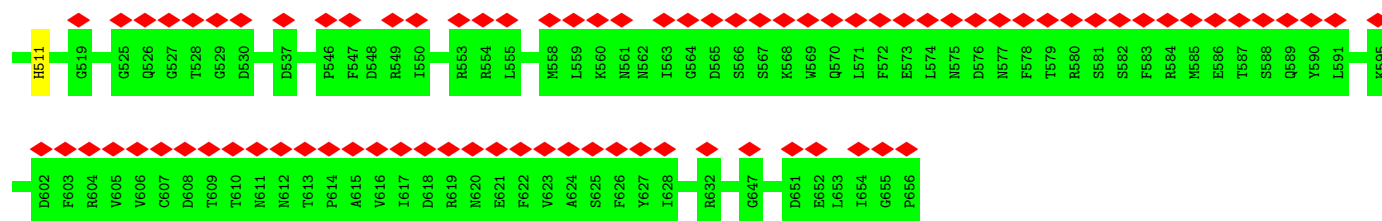
Chain So: 56% 97%



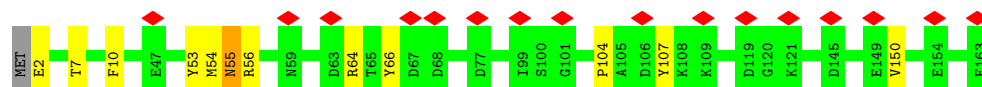


• Molecule 9: Tail sheath protein

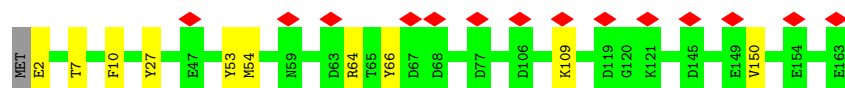




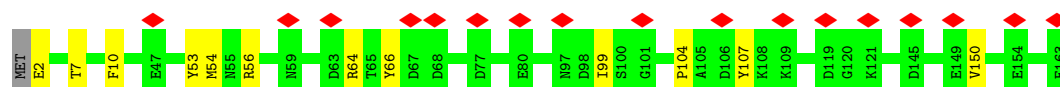
• Molecule 10: Tail tube protein



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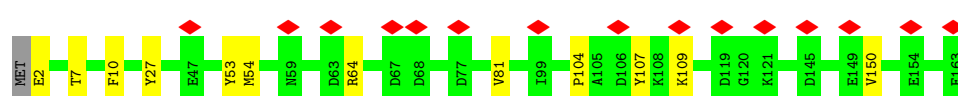
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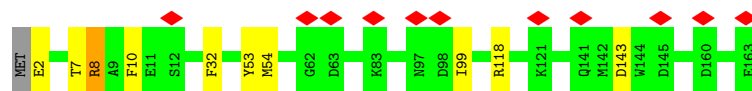


• Molecule 10: Tail tube protein

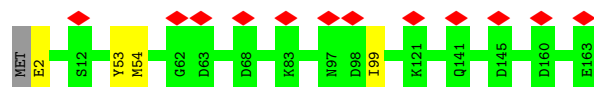




- Molecule 10: Tail tube protein



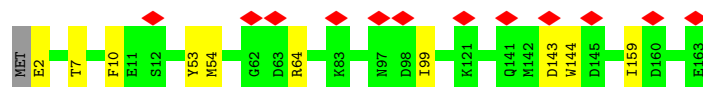
- Molecule 10: Tail tube protein



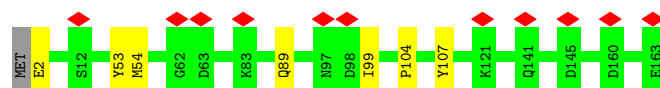
- Molecule 10: Tail tube protein



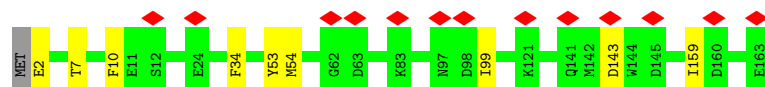
- Molecule 10: Tail tube protein



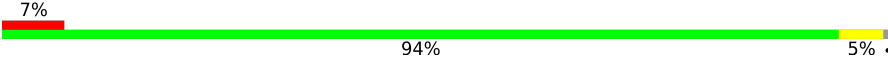
- Molecule 10: Tail tube protein

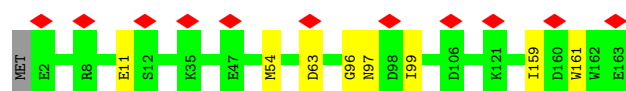


- Molecule 10: Tail tube protein

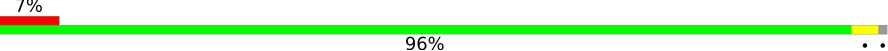


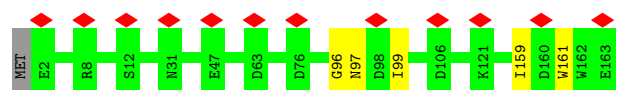
- Molecule 10: Tail tube protein

Chain TY: 

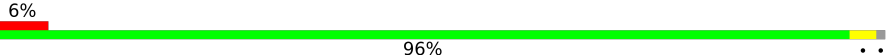


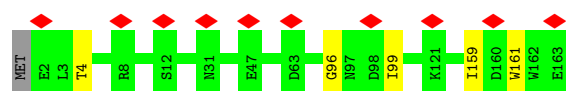
- Molecule 10: Tail tube protein

Chain TZ: 

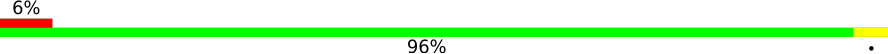


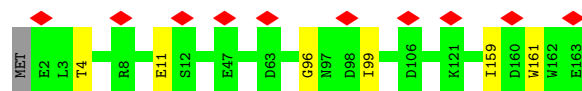
- Molecule 10: Tail tube protein

Chain Ta: 

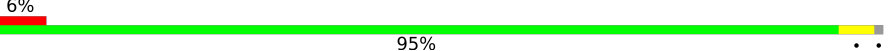


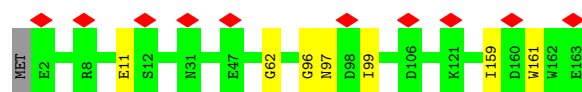
- Molecule 10: Tail tube protein

Chain Tb: 

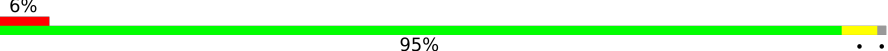


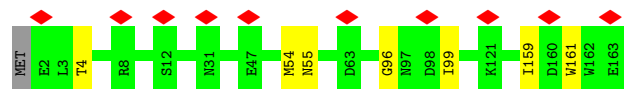
- Molecule 10: Tail tube protein

Chain Tc: 

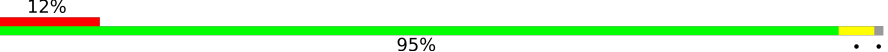


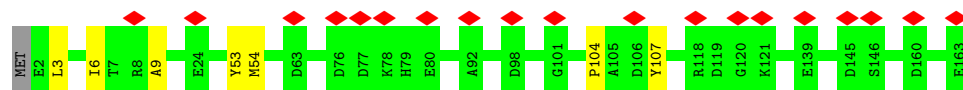
- Molecule 10: Tail tube protein

Chain Td: 

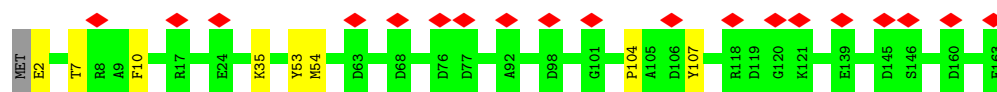
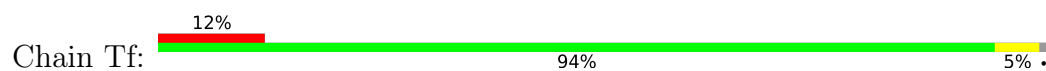


- Molecule 10: Tail tube protein

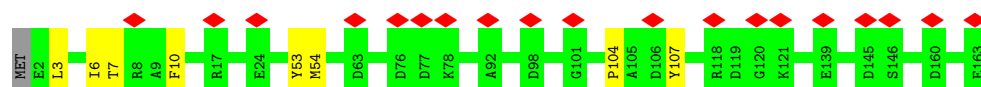
Chain Te: 



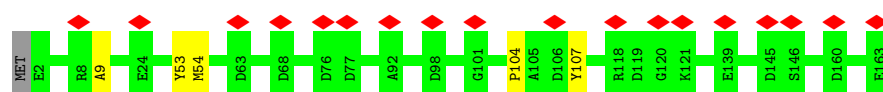
• Molecule 10: Tail tube protein



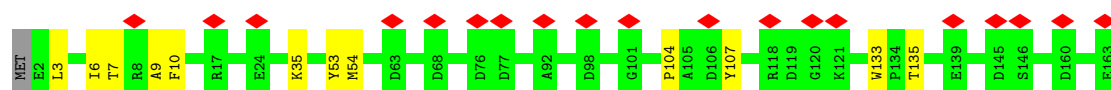
• Molecule 10: Tail tube protein



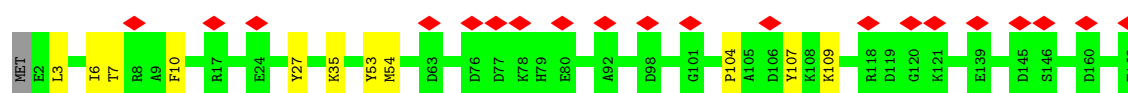
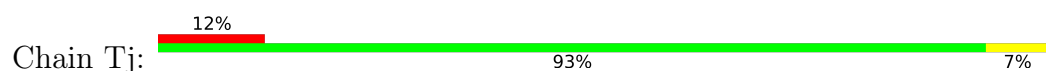
• Molecule 10: Tail tube protein



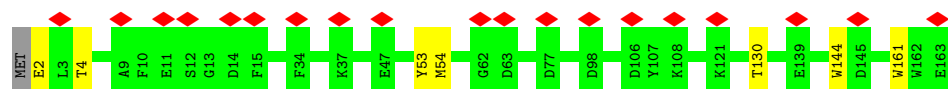
• Molecule 10: Tail tube protein



• Molecule 10: Tail tube protein

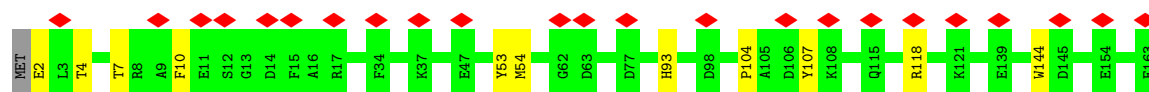


• Molecule 10: Tail tube protein

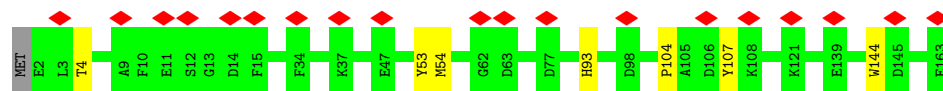


• Molecule 10: Tail tube protein

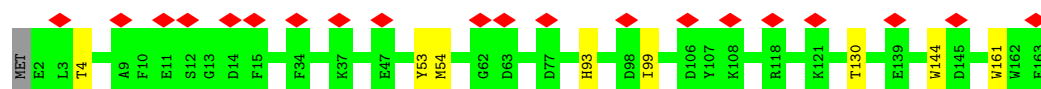




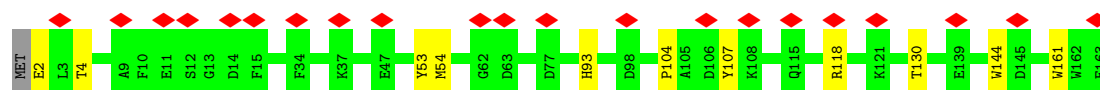
- Molecule 10: Tail tube protein



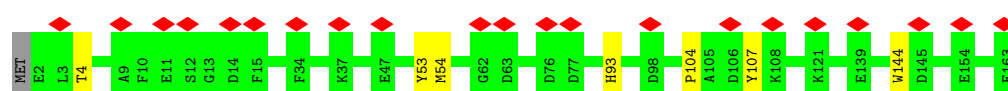
- Molecule 10: Tail tube protein



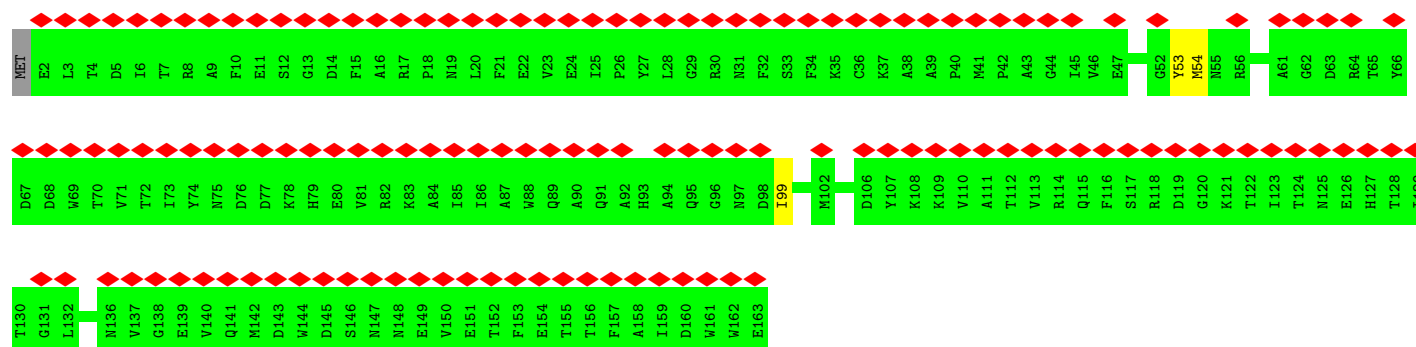
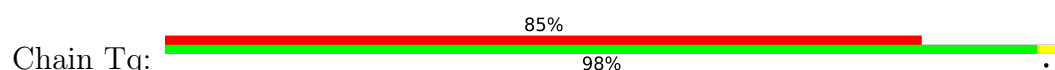
- Molecule 10: Tail tube protein



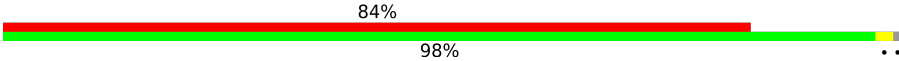
- Molecule 10: Tail tube protein

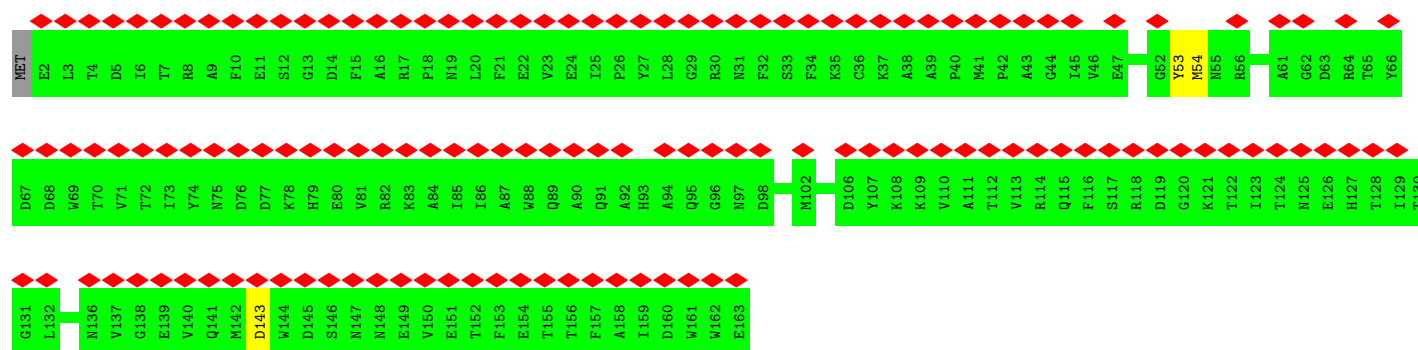


- Molecule 10: Tail tube protein

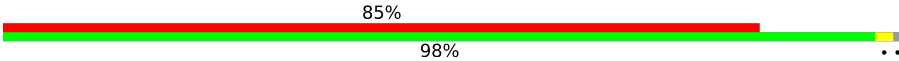


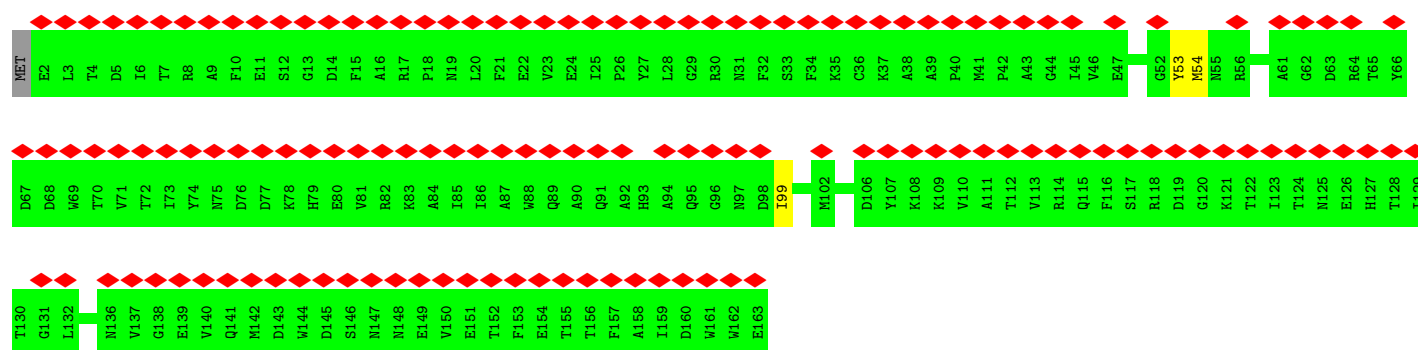
- Molecule 10: Tail tube protein

Chain Tr: 

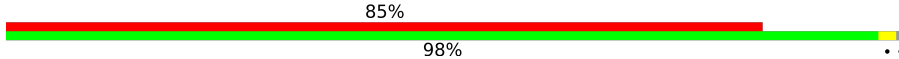


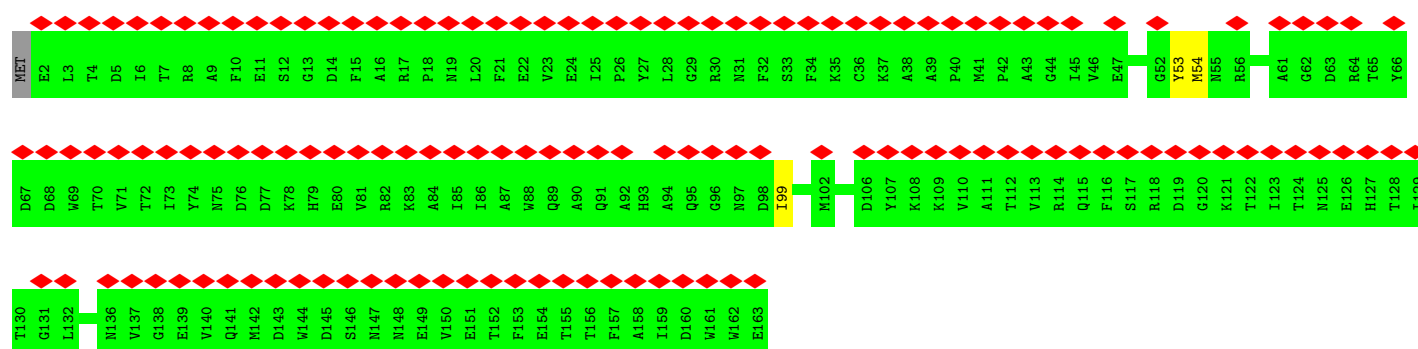
• Molecule 10: Tail tube protein

Chain Ts: 

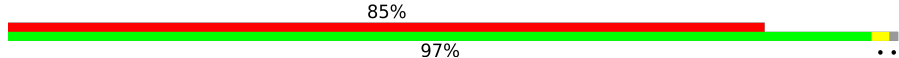


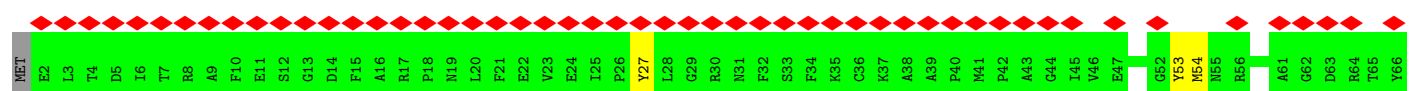
• Molecule 10: Tail tube protein

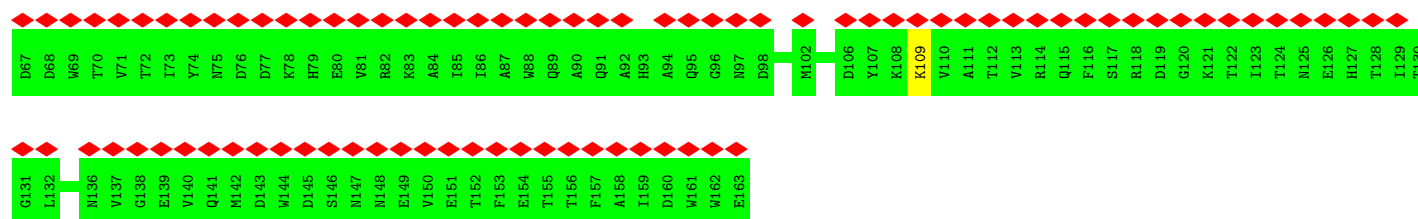
Chain Tt: 



• Molecule 10: Tail tube protein

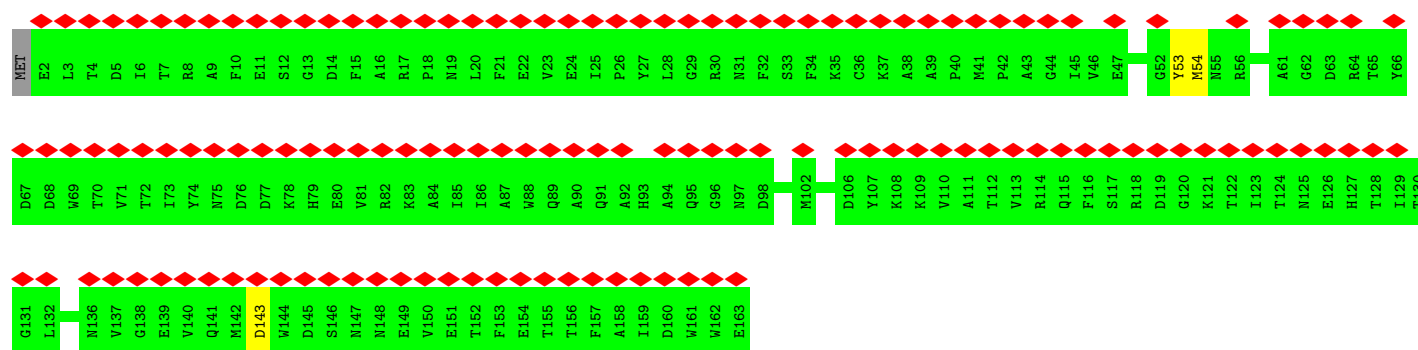
Chain Tu: 





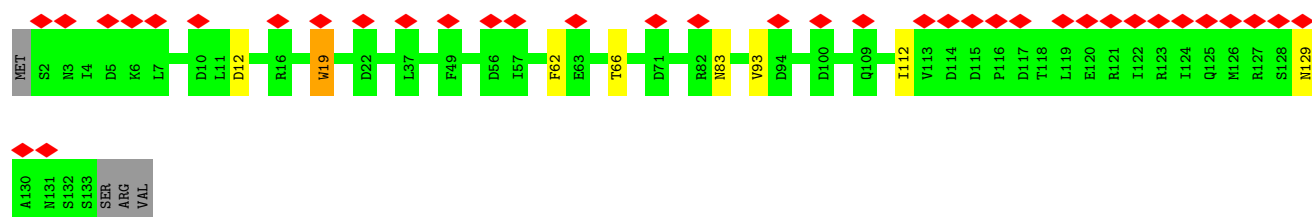
• Molecule 10: Tail tube protein

Chain Tv: 85% 98%



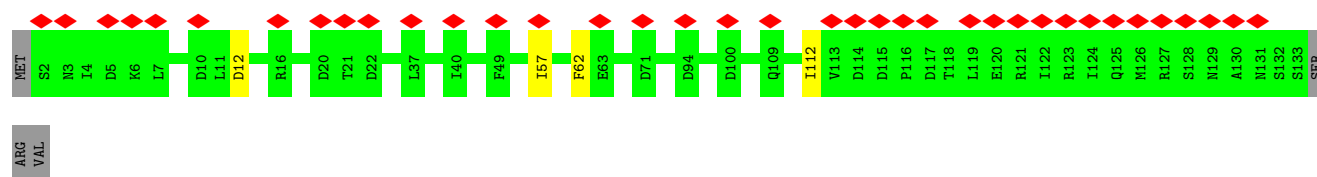
• Molecule 11: IraD/Gp25-like domain-containing protein

Chain AA: 27% 91% 5%



• Molecule 11: IraD/Gp25-like domain-containing protein

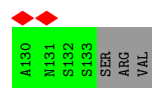
Chain AB: 27% 94%



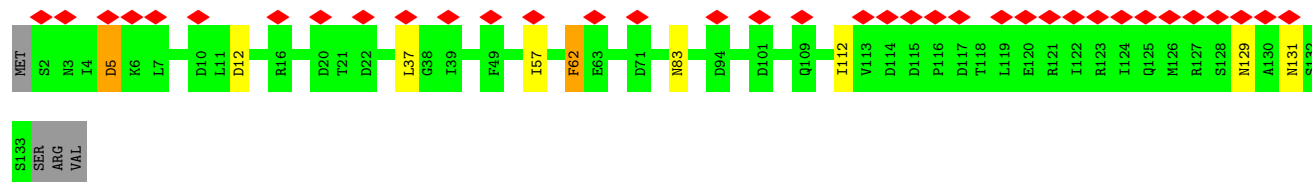
• Molecule 11: IraD/Gp25-like domain-containing protein

Chain AD: 28% 93%

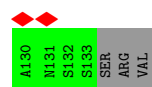




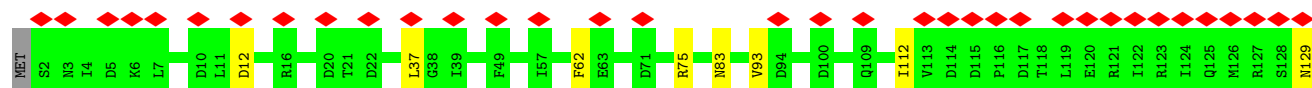
- Molecule 11: IraD/Gp25-like domain-containing protein



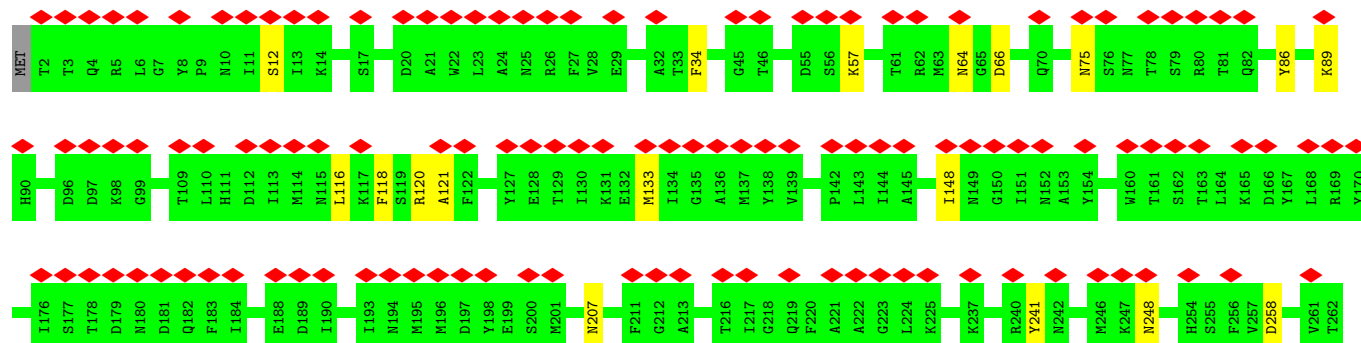
- Molecule 11: IraD/Gp25-like domain-containing protein

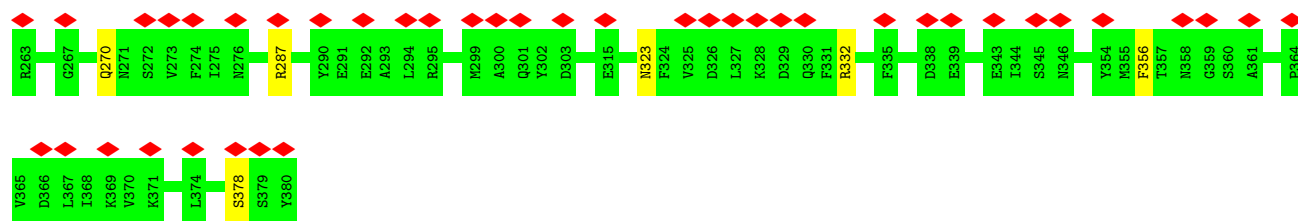


- Molecule 11: IraD/Gp25-like domain-containing protein

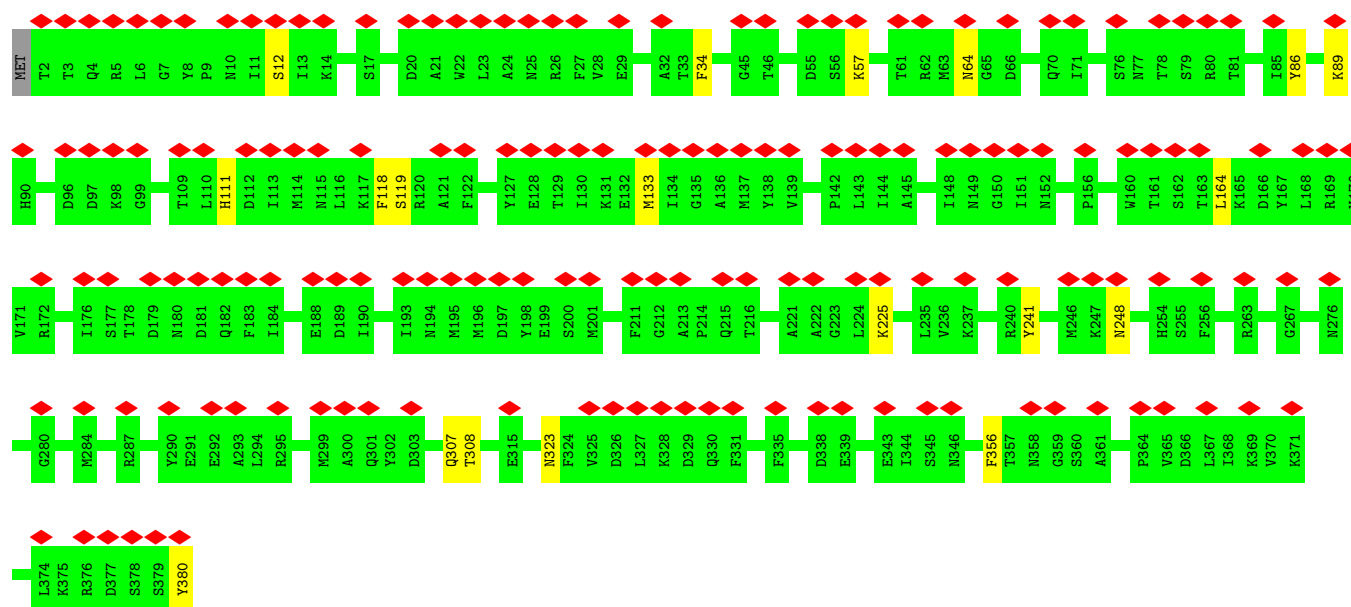
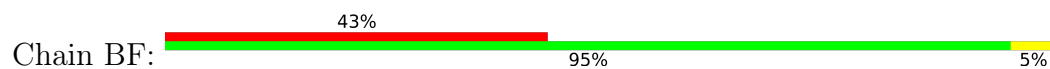


- Molecule 12: Putative baseplate hub subunit

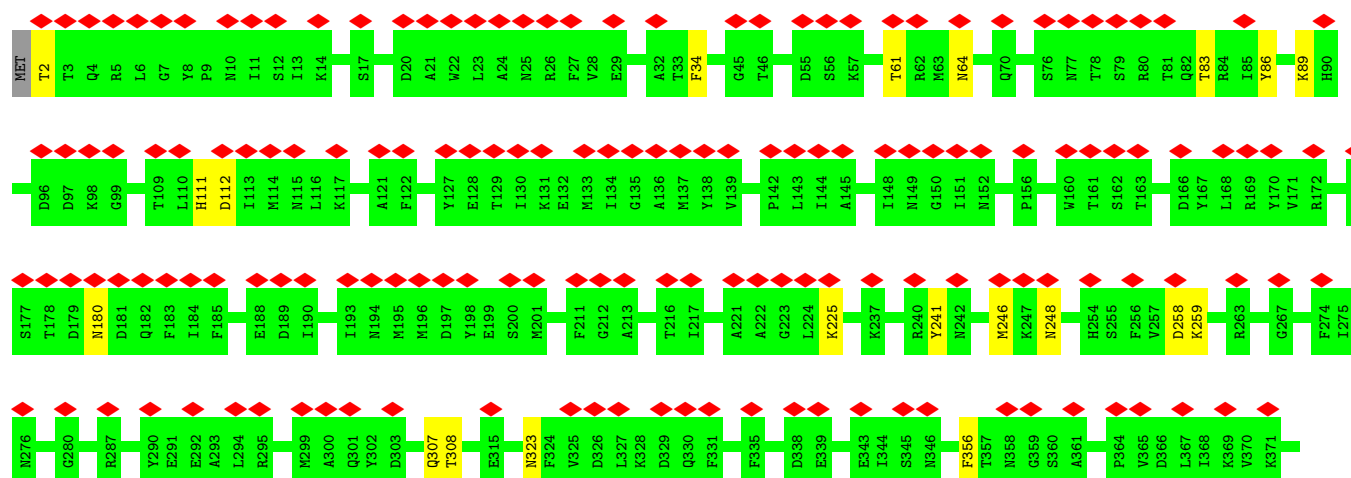
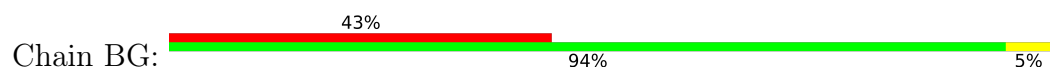


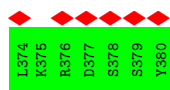


• Molecule 12: Putative baseplate hub subunit

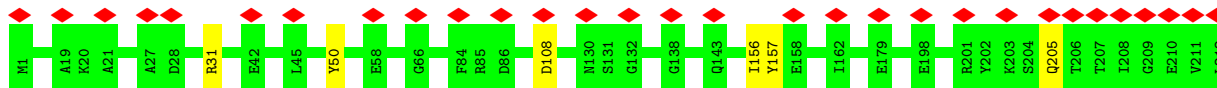


• Molecule 12: Putative baseplate hub subunit

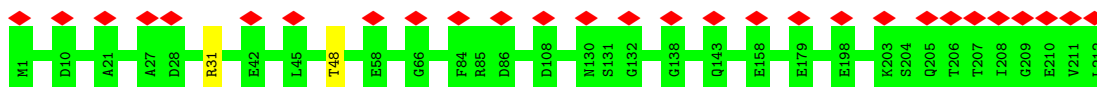




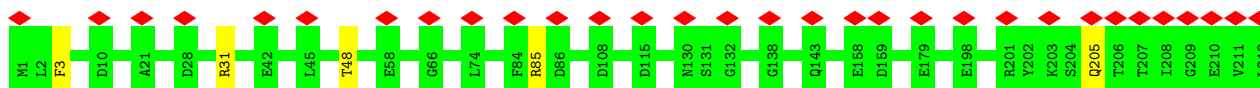
- Molecule 13: Baseplate wedge subunit



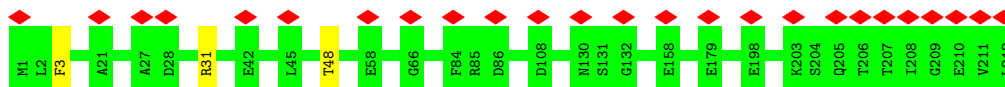
- Molecule 13: Baseplate wedge subunit



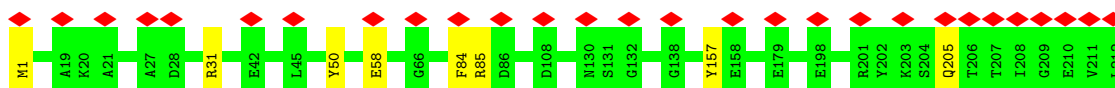
- Molecule 13: Baseplate wedge subunit



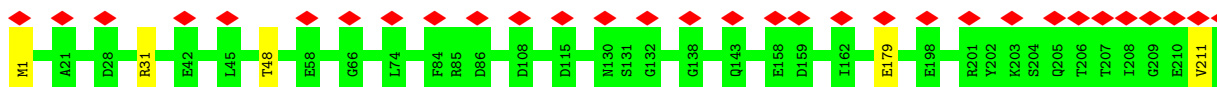
- Molecule 13: Baseplate wedge subunit



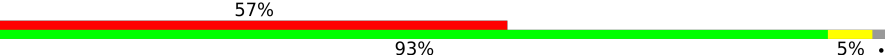
- Molecule 13: Baseplate wedge subunit

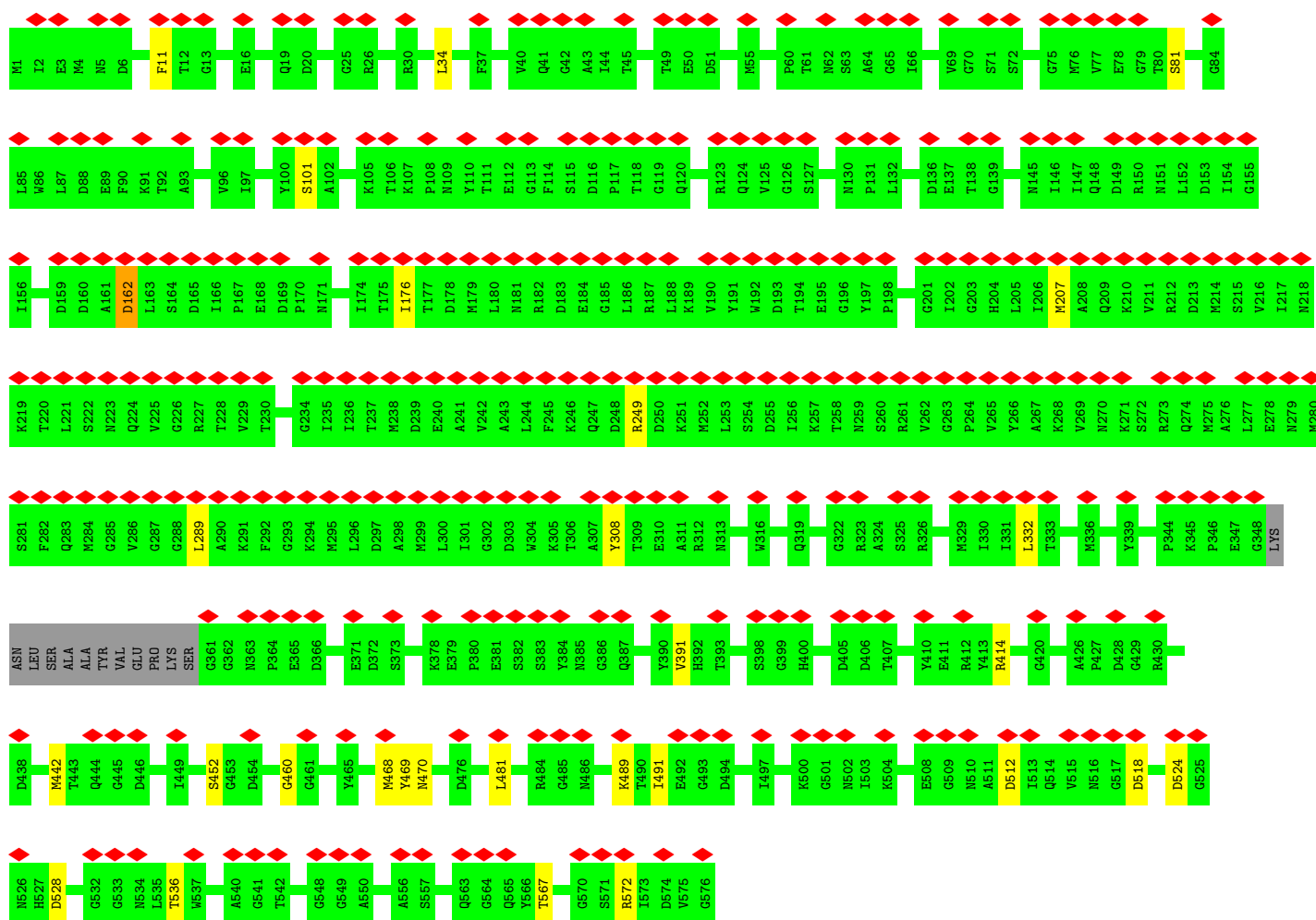


- Molecule 13: Baseplate wedge subunit

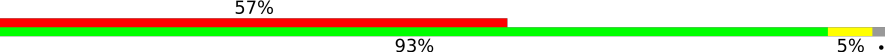


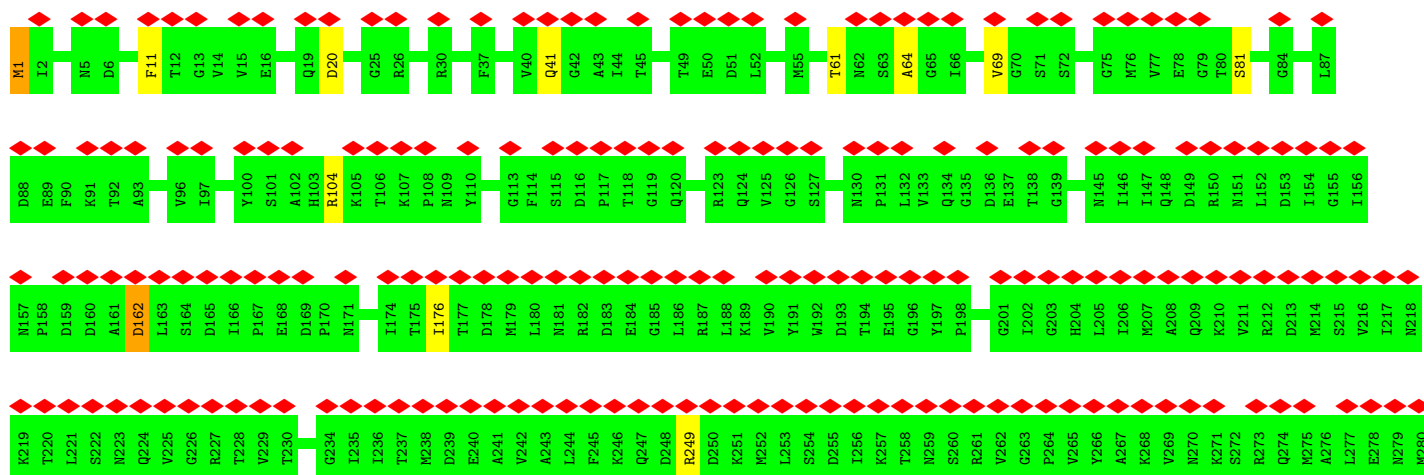
- Molecule 14: Baseplate central spike protein

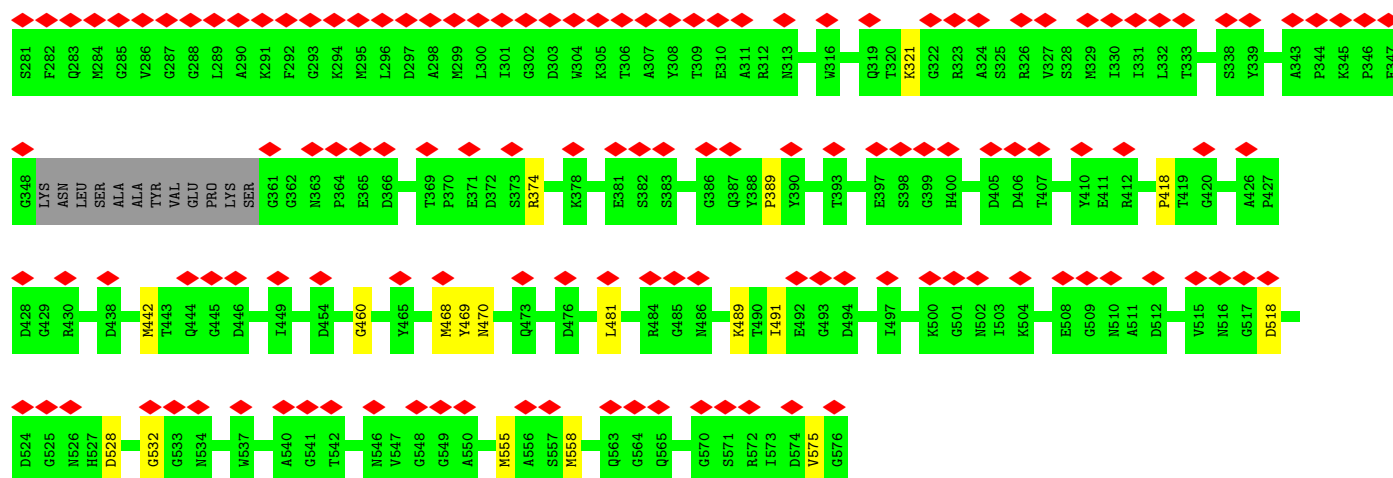
Chain BB: 



• Molecule 14: Baseplate central spike protein

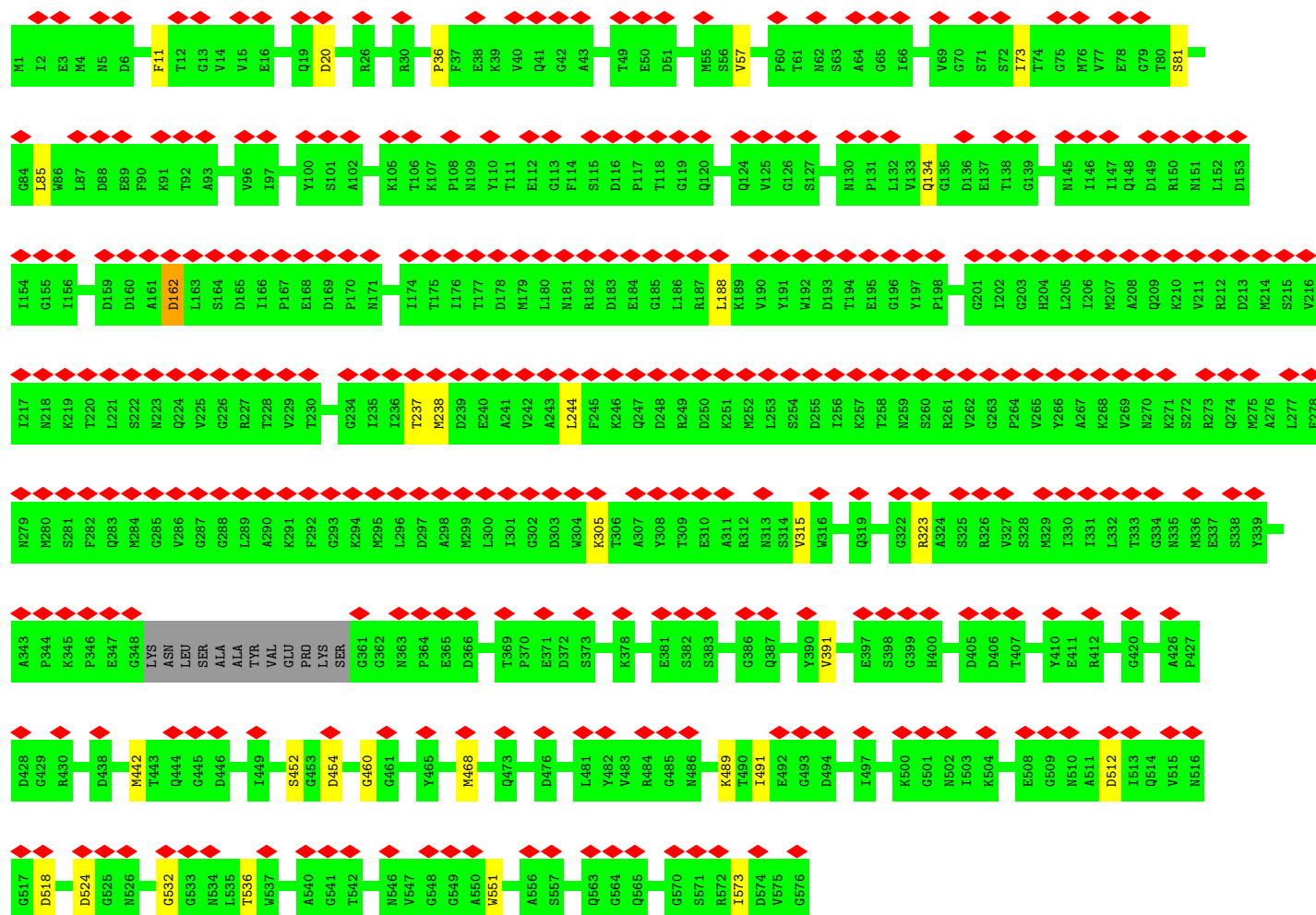
Chain BC: 





• Molecule 14: Baseplate central spike protein

Chain BD: 57% 93% 5% •



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	2415	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	0.544	Depositor
Minimum map value	-0.295	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.16	Depositor
Map size ($\text{\AA}$)	546.304, 546.304, 546.304	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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

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	LS	0.71	0/4832	1.21	8/6581 (0.1%)
1	LT	0.74	0/4832	1.27	14/6581 (0.2%)
1	LU	0.71	0/4832	1.23	5/6581 (0.1%)
1	LV	0.71	0/4832	1.21	7/6581 (0.1%)
1	LW	0.74	0/4832	1.28	10/6581 (0.2%)
1	LX	0.71	0/4832	1.23	6/6581 (0.1%)
1	LY	0.72	0/4832	1.21	6/6581 (0.1%)
1	LZ	0.74	0/4832	1.28	10/6581 (0.2%)
1	La	0.71	0/4832	1.22	7/6581 (0.1%)
1	Lb	0.72	0/4832	1.21	8/6581 (0.1%)
1	Lc	0.74	0/4832	1.27	11/6581 (0.2%)
1	Ld	0.71	0/4832	1.23	3/6581 (0.0%)
1	Le	0.71	0/4832	1.21	8/6581 (0.1%)
1	Lf	0.74	0/4832	1.28	11/6581 (0.2%)
1	Lg	0.71	0/4832	1.23	5/6581 (0.1%)
1	Lh	0.72	0/4832	1.21	6/6581 (0.1%)
1	Li	0.74	0/4832	1.28	9/6581 (0.1%)
1	Lj	0.71	0/4832	1.23	6/6581 (0.1%)
2	BK	0.64	0/2714	1.21	11/3681 (0.3%)
2	BL	0.61	0/2224	1.11	3/3011 (0.1%)
2	BM	0.64	0/2714	1.21	7/3681 (0.2%)
2	BN	0.61	0/2224	1.11	1/3011 (0.0%)
2	BO	0.64	0/2714	1.19	7/3681 (0.2%)
2	BP	0.62	0/2224	1.13	2/3011 (0.1%)
3	BQ	0.60	0/2309	1.10	4/3130 (0.1%)
3	BR	0.60	0/2309	1.10	3/3130 (0.1%)
3	BS	0.60	0/2309	1.11	5/3130 (0.2%)
3	BT	0.60	0/2309	1.09	4/3130 (0.1%)
3	BU	0.60	0/2309	1.09	3/3130 (0.1%)
3	BV	0.61	0/2309	1.09	4/3130 (0.1%)
4	AM	0.55	0/5307	1.02	3/7218 (0.0%)
4	AN	0.55	0/5307	1.01	3/7218 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	AO	0.56	0/5307	1.02	2/7218 (0.0%)
4	AP	0.55	0/5307	1.02	4/7218 (0.1%)
4	AQ	0.55	0/5307	1.02	4/7218 (0.1%)
4	AR	0.55	0/5307	1.02	2/7218 (0.0%)
4	AS	0.55	0/5260	1.03	6/7154 (0.1%)
4	AT	0.56	0/5239	1.05	8/7125 (0.1%)
4	AU	0.56	0/5260	1.02	6/7154 (0.1%)
4	AV	0.56	0/5239	1.05	9/7125 (0.1%)
4	AW	0.56	0/5260	1.03	5/7154 (0.1%)
4	AX	0.56	0/5239	1.04	7/7125 (0.1%)
5	A0	0.61	0/8656	1.12	11/11738 (0.1%)
5	A1	0.60	0/8656	1.11	10/11738 (0.1%)
5	A2	0.61	0/8656	1.12	15/11738 (0.1%)
5	A3	0.60	0/8656	1.12	12/11738 (0.1%)
5	AY	0.61	0/8656	1.12	13/11738 (0.1%)
5	AZ	0.60	0/8656	1.12	9/11738 (0.1%)
6	A4	0.60	0/2743	1.11	1/3730 (0.0%)
6	A5	0.61	0/2743	1.11	5/3730 (0.1%)
6	A6	0.61	0/2743	1.12	1/3730 (0.0%)
6	A7	0.61	0/2743	1.11	8/3730 (0.2%)
6	A8	0.61	0/2743	1.11	1/3730 (0.0%)
6	A9	0.61	0/2743	1.11	3/3730 (0.1%)
6	Aa	0.63	0/2707	1.17	4/3682 (0.1%)
6	Ab	0.63	0/2707	1.18	6/3682 (0.2%)
6	Ac	0.63	0/2707	1.17	5/3682 (0.1%)
6	Ad	0.64	0/2707	1.18	7/3682 (0.2%)
6	Ae	0.63	0/2707	1.19	6/3682 (0.2%)
6	Af	0.64	0/2707	1.18	8/3682 (0.2%)
7	LA	0.68	0/2304	1.12	3/3114 (0.1%)
7	LB	0.69	0/2304	1.12	2/3114 (0.1%)
7	LC	0.68	0/2304	1.16	4/3114 (0.1%)
7	LD	0.68	0/2304	1.12	2/3114 (0.1%)
7	LE	0.69	0/2304	1.12	0/3114
7	LF	0.68	0/2304	1.16	4/3114 (0.1%)
7	LG	0.67	0/2304	1.11	2/3114 (0.1%)
7	LH	0.68	0/2304	1.12	1/3114 (0.0%)
7	LI	0.67	0/2304	1.16	3/3114 (0.1%)
7	LJ	0.68	0/2304	1.12	3/3114 (0.1%)
7	LK	0.68	0/2304	1.11	2/3114 (0.1%)
7	LL	0.68	0/2304	1.16	4/3114 (0.1%)
7	LM	0.67	0/2304	1.12	2/3114 (0.1%)
7	LN	0.68	0/2304	1.12	2/3114 (0.1%)
7	LO	0.68	0/2304	1.16	4/3114 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	LP	0.67	0/2304	1.12	2/3114 (0.1%)
7	LQ	0.68	0/2304	1.12	2/3114 (0.1%)
7	LR	0.67	0/2304	1.15	4/3114 (0.1%)
8	FA	0.72	0/508	1.29	2/690 (0.3%)
8	FB	0.75	0/508	1.34	6/690 (0.9%)
8	FC	0.75	0/508	1.27	1/690 (0.1%)
8	FJ	0.72	0/508	1.28	2/690 (0.3%)
8	FK	0.75	0/508	1.36	6/690 (0.9%)
8	FL	0.74	0/508	1.28	2/690 (0.3%)
8	FS	0.71	0/508	1.26	1/690 (0.1%)
8	FT	0.76	0/508	1.38	6/690 (0.9%)
8	FU	0.75	0/508	1.26	0/690
8	Fb	0.71	0/508	1.28	1/690 (0.1%)
8	Fc	0.75	0/508	1.33	6/690 (0.9%)
8	Fd	0.75	0/508	1.25	2/690 (0.3%)
8	Fk	0.72	0/508	1.29	1/690 (0.1%)
8	Fl	0.74	0/508	1.30	2/690 (0.3%)
8	Fm	0.73	0/508	1.24	1/690 (0.1%)
8	Ft	0.71	0/508	1.27	2/690 (0.3%)
8	Fu	0.75	0/508	1.35	6/690 (0.9%)
8	Fv	0.73	0/508	1.25	1/690 (0.1%)
9	SA	0.58	0/5090	1.08	4/6921 (0.1%)
9	SB	0.57	0/5090	1.08	5/6921 (0.1%)
9	SC	0.58	0/5090	1.08	5/6921 (0.1%)
9	SD	0.57	0/5090	1.08	6/6921 (0.1%)
9	SE	0.57	0/5090	1.08	4/6921 (0.1%)
9	SF	0.57	0/5090	1.08	5/6921 (0.1%)
9	SG	0.57	0/5135	1.08	5/6983 (0.1%)
9	SH	0.57	0/5135	1.07	7/6983 (0.1%)
9	SI	0.57	0/5135	1.07	5/6983 (0.1%)
9	SJ	0.57	0/5135	1.07	6/6983 (0.1%)
9	SK	0.57	0/5135	1.07	8/6983 (0.1%)
9	SL	0.57	0/5135	1.08	7/6983 (0.1%)
9	SM	0.57	0/5135	1.08	4/6983 (0.1%)
9	SN	0.57	0/5135	1.08	3/6983 (0.0%)
9	SO	0.57	0/5135	1.08	3/6983 (0.0%)
9	SP	0.57	0/5135	1.08	4/6983 (0.1%)
9	SQ	0.57	0/5135	1.08	1/6983 (0.0%)
9	SR	0.57	0/5135	1.08	5/6983 (0.1%)
9	SS	0.58	0/5135	1.09	7/6983 (0.1%)
9	ST	0.57	0/5135	1.08	5/6983 (0.1%)
9	SU	0.58	0/5135	1.08	5/6983 (0.1%)
9	SV	0.58	0/5135	1.08	8/6983 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	SW	0.57	0/5135	1.08	6/6983 (0.1%)
9	SX	0.58	0/5135	1.07	4/6983 (0.1%)
9	SY	0.57	0/5135	1.05	3/6983 (0.0%)
9	SZ	0.57	0/5135	1.05	3/6983 (0.0%)
9	Sa	0.56	0/5135	1.05	4/6983 (0.1%)
9	Sb	0.57	0/5135	1.05	3/6983 (0.0%)
9	Sc	0.56	0/5135	1.06	3/6983 (0.0%)
9	Sd	0.57	0/5135	1.05	3/6983 (0.0%)
9	Se	0.56	0/5135	1.07	5/6983 (0.1%)
9	Sf	0.57	0/5135	1.07	5/6983 (0.1%)
9	Sg	0.57	0/5135	1.06	7/6983 (0.1%)
9	Sh	0.56	0/5135	1.07	8/6983 (0.1%)
9	Si	0.56	0/5135	1.07	7/6983 (0.1%)
9	Sj	0.56	0/5135	1.06	7/6983 (0.1%)
9	Sk	0.59	0/5135	1.11	7/6983 (0.1%)
9	Sl	0.59	0/5135	1.11	3/6983 (0.0%)
9	Sm	0.59	0/5135	1.10	5/6983 (0.1%)
9	Sn	0.59	0/5135	1.10	4/6983 (0.1%)
9	So	0.59	0/5135	1.10	6/6983 (0.1%)
9	Sp	0.59	0/5135	1.10	5/6983 (0.1%)
10	TM	0.60	0/1339	0.99	2/1821 (0.1%)
10	TN	0.59	0/1339	0.97	0/1821
10	TO	0.60	0/1339	1.00	1/1821 (0.1%)
10	TP	0.59	0/1339	0.99	0/1821
10	TQ	0.59	0/1339	0.98	0/1821
10	TR	0.59	0/1339	0.98	1/1821 (0.1%)
10	TS	0.58	0/1339	0.98	0/1821
10	TT	0.58	0/1339	0.99	2/1821 (0.1%)
10	TU	0.58	0/1339	0.99	1/1821 (0.1%)
10	TV	0.58	0/1339	0.98	0/1821
10	TW	0.68	2/1339 (0.1%)	1.00	3/1821 (0.2%)
10	TX	0.58	0/1339	0.99	1/1821 (0.1%)
10	TY	0.57	0/1339	0.99	0/1821
10	TZ	0.57	0/1339	0.99	0/1821
10	Ta	0.57	0/1339	0.99	0/1821
10	Tb	0.56	0/1339	0.98	0/1821
10	Tc	0.56	0/1339	0.99	0/1821
10	Td	0.56	0/1339	0.99	0/1821
10	Te	0.56	0/1339	0.96	0/1821
10	Tf	0.56	0/1339	0.96	0/1821
10	Tg	0.56	0/1339	0.98	0/1821
10	Th	0.56	0/1339	0.96	0/1821
10	Ti	0.56	0/1339	0.96	0/1821

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	Tj	0.56	0/1339	0.97	0/1821
10	Tk	0.52	0/1339	0.95	0/1821
10	Tl	0.52	0/1339	0.95	0/1821
10	Tm	0.52	0/1339	0.95	0/1821
10	Tn	0.52	0/1339	0.95	0/1821
10	To	0.52	0/1339	0.94	0/1821
10	Tp	0.52	0/1339	0.95	0/1821
10	Tq	0.60	0/1339	1.05	0/1821
10	Tr	0.61	0/1339	1.05	1/1821 (0.1%)
10	Ts	0.61	0/1339	1.04	0/1821
10	Tt	0.60	0/1339	1.04	0/1821
10	Tu	0.61	0/1339	1.04	0/1821
10	Tv	0.61	0/1339	1.03	1/1821 (0.1%)
11	AA	0.58	0/1059	1.15	5/1438 (0.3%)
11	AB	0.57	0/1059	1.13	2/1438 (0.1%)
11	AC	0.57	0/1059	1.16	4/1438 (0.3%)
11	AD	0.57	0/1059	1.13	3/1438 (0.2%)
11	AE	0.57	0/1059	1.16	4/1438 (0.3%)
11	AF	0.58	0/1059	1.17	5/1438 (0.3%)
12	BE	0.62	0/3125	1.21	7/4232 (0.2%)
12	BF	0.62	0/3125	1.18	5/4232 (0.1%)
12	BG	0.63	0/3125	1.20	6/4232 (0.1%)
13	AG	0.53	0/1794	1.00	1/2435 (0.0%)
13	AH	0.53	0/1794	0.98	1/2435 (0.0%)
13	AI	0.53	0/1794	0.99	0/2435
13	AJ	0.53	0/1794	0.98	1/2435 (0.0%)
13	AK	0.53	0/1794	0.98	0/2435
13	AL	0.53	0/1794	0.97	0/2435
14	BB	0.64	0/4441	1.19	5/6025 (0.1%)
14	BC	0.64	0/4441	1.16	6/6025 (0.1%)
14	BD	0.64	0/4441	1.17	5/6025 (0.1%)
All	All	0.61	2/617655 (0.0%)	1.11	755/839310 (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
1	LS	0	3
1	LU	0	2
1	LV	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	LX	0	2
1	LY	0	5
1	LZ	0	1
1	La	0	2
1	Lb	0	3
1	Ld	0	1
1	Le	0	5
1	Lf	0	1
1	Lg	0	2
1	Lh	0	4
1	Lj	0	1
2	BM	0	1
2	BO	0	2
2	BP	0	1
3	BQ	0	1
3	BR	0	1
3	BS	0	2
3	BT	0	2
3	BU	0	1
3	BV	0	1
4	AM	0	1
4	AO	0	1
4	AQ	0	1
4	AS	0	1
5	A0	0	4
5	A1	0	2
5	A2	0	4
5	A3	0	3
5	AY	0	2
5	AZ	0	5
7	LE	0	1
7	LQ	0	1
8	FC	0	1
8	FL	0	1
8	FU	0	1
8	Fd	0	1
8	Fm	0	1
8	Fv	0	1
9	SM	0	1
9	SN	0	1
9	SO	0	1
9	SP	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	SQ	0	1
9	SR	0	2
9	ST	0	1
9	SU	0	1
9	SV	0	1
9	SW	0	1
9	SX	0	1
9	Se	0	1
9	Sf	0	2
9	Sg	0	2
9	Sh	0	1
9	Si	0	1
All	All	0	100

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	TW	8	ARG	CD-NE	9.59	1.59	1.46
10	TW	8	ARG	NE-CZ	7.99	1.41	1.33

All (755) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	SA	6	PRO	CB-CA-C	-8.81	99.44	110.98
2	BK	200	ARG	NE-CZ-NH1	-7.98	113.52	121.50
8	Fb	564	ASP	CA-CB-CG	7.70	120.30	112.60
8	FA	564	ASP	CA-CB-CG	7.67	120.27	112.60
12	BE	34	PHE	CA-CB-CG	7.59	121.39	113.80
8	Fk	564	ASP	CA-CB-CG	7.55	120.15	112.60
2	BM	200	ARG	NE-CZ-NH1	-7.48	114.02	121.50
11	AF	62	PHE	CA-CB-CG	-7.44	106.36	113.80
8	Ft	564	ASP	CA-CB-CG	7.36	119.96	112.60
4	AS	400	ASP	CA-CB-CG	7.30	119.91	112.60
12	BG	34	PHE	CA-CB-CG	7.30	121.10	113.80
4	AP	46	ASP	CA-CB-CG	7.28	119.88	112.60
2	BP	80	PHE	CA-CB-CG	-7.28	106.52	113.80
8	FS	564	ASP	CA-CB-CG	7.25	119.85	112.60
9	SC	299	ASP	CA-CB-CG	7.24	119.84	112.60
12	BF	34	PHE	CA-CB-CG	7.24	121.04	113.80
11	AB	62	PHE	CA-CB-CG	-7.16	106.64	113.80
11	AE	62	PHE	CA-CB-CG	-7.12	106.68	113.80
8	FJ	564	ASP	CA-CB-CG	7.09	119.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	SA	299	ASP	CA-CB-CG	7.08	119.68	112.60
4	AS	520	ASP	CA-CB-CG	7.04	119.64	112.60
4	AW	520	ASP	CA-CB-CG	7.03	119.63	112.60
1	LW	136	ASP	CA-CB-CG	7.02	119.62	112.60
4	AU	400	ASP	CA-CB-CG	7.02	119.62	112.60
1	LZ	136	ASP	CA-CB-CG	6.98	119.58	112.60
2	BO	200	ARG	NE-CZ-NH1	-6.98	114.52	121.50
9	SD	299	ASP	CA-CB-CG	6.98	119.58	112.60
9	SD	6	PRO	CB-CA-C	-6.96	101.86	110.98
4	AV	400	ASP	CA-CB-CG	6.93	119.53	112.60
1	Lb	25	VAL	CA-C-N	6.90	130.63	120.90
1	Lb	25	VAL	C-N-CA	6.90	130.63	120.90
9	Sa	629	LYS	CB-CA-C	6.89	117.36	110.33
1	Lf	136	ASP	CA-CB-CG	6.89	119.49	112.60
4	AV	520	ASP	CA-CB-CG	6.89	119.49	112.60
11	AC	62	PHE	CA-CB-CG	-6.86	106.94	113.80
9	SU	457	ASP	CA-CB-CG	6.84	119.44	112.60
1	LT	136	ASP	CA-CB-CG	6.83	119.43	112.60
9	SV	190	ASP	CA-CB-CG	6.83	119.43	112.60
9	ST	457	ASP	CA-CB-CG	6.83	119.43	112.60
1	Lh	25	VAL	CA-C-N	6.82	130.52	120.90
1	Lh	25	VAL	C-N-CA	6.82	130.52	120.90
9	SS	457	ASP	CA-CB-CG	6.81	119.41	112.60
4	AX	520	ASP	CA-CB-CG	6.81	119.41	112.60
4	AU	520	ASP	CA-CB-CG	6.81	119.41	112.60
9	SE	299	ASP	CA-CB-CG	6.79	119.39	112.60
1	Li	136	ASP	CA-CB-CG	6.79	119.39	112.60
4	AT	520	ASP	CA-CB-CG	6.78	119.38	112.60
7	LI	108	PHE	CA-CB-CG	6.78	120.58	113.80
7	LO	108	PHE	CA-CB-CG	6.77	120.57	113.80
1	Lf	287	PHE	CA-CB-CG	6.76	120.56	113.80
9	SV	457	ASP	CA-CB-CG	6.76	119.36	112.60
9	SF	299	ASP	CA-CB-CG	6.75	119.35	112.60
9	SW	457	ASP	CA-CB-CG	6.75	119.35	112.60
4	AX	400	ASP	CA-CB-CG	6.72	119.32	112.60
9	SJ	311	ASP	CA-CB-CG	6.70	119.30	112.60
1	LV	25	VAL	CA-C-N	6.70	130.35	120.90
1	LV	25	VAL	C-N-CA	6.70	130.35	120.90
1	Lc	136	ASP	CA-CB-CG	6.69	119.29	112.60
9	SI	77	ASP	CA-CB-CG	6.69	119.29	112.60
9	SE	6	PRO	CB-CA-C	-6.69	102.22	110.98
7	LR	108	PHE	CA-CB-CG	6.68	120.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BR	165	ASP	CA-CB-CG	6.68	119.28	112.60
9	SB	299	ASP	CA-CB-CG	6.67	119.28	112.60
4	AW	400	ASP	CA-CB-CG	6.67	119.27	112.60
3	BV	165	ASP	CA-CB-CG	6.67	119.27	112.60
4	AN	46	ASP	CA-CB-CG	6.66	119.26	112.60
4	AM	46	ASP	CA-CB-CG	6.65	119.25	112.60
1	LZ	287	PHE	CA-CB-CG	6.64	120.44	113.80
9	Sn	77	ASP	CA-CB-CG	6.64	119.24	112.60
9	Sc	629	LYS	CB-CA-C	6.63	117.10	110.33
9	SX	457	ASP	CA-CB-CG	6.59	119.19	112.60
1	Li	287	PHE	CA-CB-CG	6.58	120.38	113.80
2	BK	200	ARG	NE-CZ-NH2	6.57	125.11	119.20
4	AV	255	GLY	CA-C-N	6.56	126.33	120.10
4	AV	255	GLY	C-N-CA	6.56	126.33	120.10
2	BK	200	ARG	CG-CD-NE	-6.55	97.58	112.00
9	SZ	629	LYS	CB-CA-C	6.55	117.01	110.33
2	BM	200	ARG	CG-CD-NE	-6.55	97.59	112.00
7	LL	108	PHE	CA-CB-CG	6.55	120.35	113.80
6	Ae	101	ASP	CA-CB-CG	6.53	119.13	112.60
1	Lc	287	PHE	CA-CB-CG	6.53	120.33	113.80
1	LU	510	ASN	CA-CB-CG	6.52	119.12	112.60
9	Sp	77	ASP	CA-CB-CG	6.51	119.11	112.60
5	A0	137	PHE	CA-CB-CG	6.50	120.30	113.80
3	BS	165	ASP	CA-CB-CG	6.49	119.09	112.60
9	Sk	77	ASP	CA-CB-CG	6.49	119.09	112.60
11	AA	62	PHE	CA-CB-CG	-6.48	107.32	113.80
1	LZ	322	HIS	CA-CB-CG	6.47	120.27	113.80
9	SP	457	ASP	CA-CB-CG	6.47	119.07	112.60
9	SL	311	ASP	CA-CB-CG	6.46	119.06	112.60
9	SF	6	PRO	CB-CA-C	-6.46	102.52	110.98
9	SZ	457	ASP	CA-CB-CG	6.46	119.06	112.60
4	AT	255	GLY	CA-C-N	6.45	126.23	120.10
4	AT	255	GLY	C-N-CA	6.45	126.23	120.10
9	SA	481	ASP	CA-CB-CG	6.45	119.05	112.60
4	AT	400	ASP	CA-CB-CG	6.44	119.04	112.60
9	Sd	629	LYS	CB-CA-C	6.44	116.90	110.33
5	A2	137	PHE	CA-CB-CG	6.43	120.23	113.80
5	A1	137	PHE	CA-CB-CG	6.42	120.22	113.80
1	Le	25	VAL	CA-C-N	6.41	129.94	120.90
1	Le	25	VAL	C-N-CA	6.41	129.94	120.90
4	AR	46	ASP	CA-CB-CG	6.41	119.01	112.60
6	Ac	101	ASP	CA-CB-CG	6.41	119.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	SO	457	ASP	CA-CB-CG	6.41	119.01	112.60
3	BT	165	ASP	CA-CB-CG	6.40	119.00	112.60
9	Sc	77	ASP	CA-CB-CG	6.39	118.99	112.60
4	AS	64	ASN	CA-CB-CG	-6.38	106.22	112.60
9	SC	6	PRO	CB-CA-C	-6.38	102.63	110.98
9	SG	311	ASP	CA-CB-CG	6.37	118.97	112.60
2	BM	200	ARG	NE-CZ-NH2	6.35	124.91	119.20
3	BQ	165	ASP	CA-CB-CG	6.35	118.95	112.60
1	LT	287	PHE	CA-CB-CG	6.33	120.13	113.80
8	FT	566	ASP	CA-CB-CG	6.33	118.93	112.60
9	So	77	ASP	CA-CB-CG	6.32	118.92	112.60
9	SH	311	ASP	CA-CB-CG	6.31	118.91	112.60
11	AF	75	ARG	NE-CZ-NH1	-6.30	115.20	121.50
9	Si	457	ASP	CA-CB-CG	6.30	118.90	112.60
3	BU	165	ASP	CA-CB-CG	6.29	118.89	112.60
4	AX	64	ASN	CA-CB-CG	-6.28	106.32	112.60
9	SB	6	PRO	CB-CA-C	-6.27	102.77	110.98
8	FK	566	ASP	CA-CB-CG	6.27	118.87	112.60
1	Lj	510	ASN	CA-CB-CG	6.26	118.86	112.60
5	A3	137	PHE	CA-CB-CG	6.25	120.05	113.80
1	LX	510	ASN	CA-CB-CG	6.25	118.85	112.60
9	Se	457	ASP	CA-CB-CG	6.25	118.84	112.60
9	Sj	629	LYS	CB-CA-C	6.24	117.10	110.17
9	Sb	77	ASP	CA-CB-CG	6.24	118.84	112.60
9	Sm	77	ASP	CA-CB-CG	6.23	118.83	112.60
14	BC	518	ASP	CA-CB-CG	6.23	118.83	112.60
9	Sd	457	ASP	CA-CB-CG	6.21	118.81	112.60
1	LY	25	VAL	CA-C-N	6.21	129.66	120.90
1	LY	25	VAL	C-N-CA	6.21	129.66	120.90
2	BO	200	ARG	CG-CD-NE	-6.20	98.36	112.00
1	LS	25	VAL	CA-C-N	6.19	129.63	120.90
1	LS	25	VAL	C-N-CA	6.19	129.63	120.90
9	Sa	457	ASP	CA-CB-CG	6.18	118.78	112.60
5	A0	486	TYR	CB-CA-C	6.18	121.61	112.09
5	AZ	137	PHE	CA-CB-CG	6.18	119.98	113.80
1	LW	607	TYR	CA-CB-CG	6.18	125.02	113.90
9	Sc	457	ASP	CA-CB-CG	6.17	118.77	112.60
9	Sb	629	LYS	CB-CA-C	6.17	116.62	110.33
14	BD	162	ASP	CA-CB-CG	6.17	118.77	112.60
9	SM	457	ASP	CA-CB-CG	6.16	118.76	112.60
9	Sf	556	PHE	CA-CB-CG	-6.16	107.64	113.80
6	A5	101	ASP	CA-CB-CG	6.16	118.76	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	LW	287	PHE	CA-CB-CG	6.16	119.96	113.80
9	SE	481	ASP	CA-CB-CG	6.16	118.76	112.60
9	Sk	457	ASP	CA-CB-CG	6.15	118.75	112.60
4	AQ	46	ASP	CA-CB-CG	6.14	118.74	112.60
1	Ld	510	ASN	CA-CB-CG	6.12	118.72	112.60
7	LF	108	PHE	CA-CB-CG	6.12	119.92	113.80
1	LT	322	HIS	CA-CB-CG	6.12	119.92	113.80
9	SQ	457	ASP	CA-CB-CG	6.12	118.72	112.60
9	SC	481	ASP	CA-CB-CG	6.10	118.70	112.60
12	BE	270	GLN	N-CA-C	6.10	118.01	111.36
9	So	457	ASP	CA-CB-CG	6.09	118.69	112.60
14	BC	162	ASP	CA-CB-CG	6.09	118.69	112.60
9	SY	457	ASP	CA-CB-CG	6.09	118.69	112.60
1	LW	113	PHE	CA-CB-CG	6.09	119.89	113.80
4	AW	461	PHE	N-CA-C	6.09	118.71	111.71
1	Lg	510	ASN	CA-CB-CG	6.08	118.68	112.60
9	Sm	457	ASP	CA-CB-CG	6.08	118.68	112.60
12	BG	356	PHE	CA-CB-CG	6.08	119.88	113.80
9	Sh	457	ASP	CA-CB-CG	6.07	118.67	112.60
12	BG	248	ASN	CA-CB-CG	6.06	118.66	112.60
1	Lc	607	TYR	CA-CB-CG	6.06	124.80	113.90
9	Sb	457	ASP	CA-CB-CG	6.05	118.65	112.60
9	SR	457	ASP	CA-CB-CG	6.05	118.65	112.60
1	Lg	546	PHE	CA-CB-CG	6.05	119.85	113.80
7	LD	72	ASP	CA-CB-CG	6.05	118.65	112.60
4	AO	374	LYS	O-C-N	-6.05	118.75	121.53
12	BG	258	ASP	CA-CB-CG	6.05	118.65	112.60
6	Aa	101	ASP	CA-CB-CG	6.03	118.63	112.60
9	SN	457	ASP	CA-CB-CG	6.03	118.63	112.60
1	Li	607	TYR	CA-CB-CG	6.03	124.75	113.90
7	LA	72	ASP	CA-CB-CG	6.02	118.62	112.60
9	SY	77	ASP	CA-CB-CG	6.02	118.62	112.60
9	Sn	457	ASP	CA-CB-CG	6.02	118.62	112.60
2	BP	196	ASP	CA-CB-CG	6.01	118.61	112.60
1	LZ	113	PHE	CA-CB-CG	6.01	119.81	113.80
4	AV	64	ASN	CA-CB-CG	-6.01	106.59	112.60
7	LC	108	PHE	CA-CB-CG	6.01	119.81	113.80
9	SY	629	LYS	CB-CA-C	6.01	116.46	110.33
9	SK	311	ASP	CA-CB-CG	6.00	118.60	112.60
4	AT	64	ASN	CA-CB-CG	-6.00	106.60	112.60
5	AY	137	PHE	CA-CB-CG	5.99	119.79	113.80
7	LJ	72	ASP	CA-CB-CG	5.99	118.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Lf	322	HIS	CA-CB-CG	5.98	119.78	113.80
7	LR	100	LYS	CA-C-N	5.98	125.78	120.10
7	LR	100	LYS	C-N-CA	5.98	125.78	120.10
4	AX	255	GLY	CA-C-N	5.97	125.65	119.92
4	AX	255	GLY	C-N-CA	5.97	125.65	119.92
9	Se	629	LYS	CB-CA-C	5.97	116.80	110.17
8	Fl	566	ASP	CA-CB-CG	5.97	118.57	112.60
4	AU	461	PHE	N-CA-C	5.96	118.57	111.71
10	TW	8	ARG	CG-CD-NE	-5.96	98.88	112.00
1	LT	607	TYR	CA-CB-CG	5.96	124.63	113.90
6	Ab	101	ASP	CA-CB-CG	5.96	118.56	112.60
9	Sh	556	PHE	CA-CB-CG	-5.95	107.85	113.80
3	BS	118	PHE	CA-CB-CG	5.94	119.74	113.80
9	SZ	77	ASP	CA-CB-CG	5.94	118.54	112.60
3	BQ	118	PHE	CA-CB-CG	5.94	119.74	113.80
7	LL	100	LYS	CA-C-N	5.94	125.74	120.10
7	LL	100	LYS	C-N-CA	5.94	125.74	120.10
9	Sf	457	ASP	CA-CB-CG	5.94	118.54	112.60
6	Ae	70	ASP	CA-CB-CG	5.93	118.53	112.60
8	FK	564	ASP	CA-CB-CG	5.93	118.53	112.60
6	A7	101	ASP	CA-CB-CG	5.92	118.52	112.60
7	LI	100	LYS	CA-C-N	5.92	125.73	120.10
7	LI	100	LYS	C-N-CA	5.92	125.73	120.10
7	LJ	108	PHE	CA-CB-CG	5.92	119.72	113.80
1	La	510	ASN	CA-CB-CG	5.92	118.52	112.60
5	A0	1026	THR	CB-CA-C	5.92	120.61	111.02
9	Sa	77	ASP	CA-CB-CG	5.91	118.51	112.60
5	A0	633	TRP	N-CA-C	5.91	117.53	111.14
8	Fc	564	ASP	CA-CB-CG	5.91	118.51	112.60
8	Fl	564	ASP	CA-CB-CG	5.91	118.51	112.60
9	Sj	457	ASP	CA-CB-CG	5.91	118.51	112.60
9	SU	311	ASP	CA-CB-CG	5.90	118.50	112.60
6	Ac	70	ASP	CA-CB-CG	5.90	118.50	112.60
4	AS	461	PHE	N-CA-C	5.90	118.50	111.71
6	A9	101	ASP	CA-CB-CG	5.90	118.50	112.60
8	FB	566	ASP	CA-CB-CG	5.89	118.49	112.60
1	Lf	113	PHE	CA-CB-CG	5.89	119.69	113.80
4	AM	262	PHE	CA-CB-CG	5.89	119.69	113.80
6	Ab	125	PRO	N-CA-C	5.89	124.60	112.47
6	Ad	101	ASP	CA-CB-CG	5.88	118.47	112.60
4	AU	64	ASN	CA-CB-CG	-5.87	106.73	112.60
9	Sl	457	ASP	CA-CB-CG	5.87	118.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Li	322	HIS	CA-CB-CG	5.86	119.66	113.80
14	BB	11	PHE	CA-CB-CG	5.86	119.66	113.80
9	So	173	SER	CA-C-N	5.86	128.41	120.38
9	So	173	SER	C-N-CA	5.86	128.41	120.38
9	Sd	77	ASP	CA-CB-CG	5.86	118.46	112.60
1	Lc	113	PHE	CA-CB-CG	5.86	119.66	113.80
9	SS	311	ASP	CA-CB-CG	5.86	118.46	112.60
3	BU	118	PHE	CA-CB-CG	5.86	119.66	113.80
6	Af	101	ASP	CA-CB-CG	5.85	118.45	112.60
3	BT	118	PHE	CA-CB-CG	5.85	119.65	113.80
11	AF	12	ASP	CA-CB-CG	5.85	118.45	112.60
1	Lb	84	ASN	CA-C-N	5.85	128.11	120.28
1	Lb	84	ASN	C-N-CA	5.85	128.11	120.28
1	Lj	546	PHE	CA-CB-CG	5.84	119.64	113.80
2	BM	268	ASN	CA-CB-CG	5.84	118.44	112.60
9	Se	556	PHE	CA-CB-CG	-5.84	107.96	113.80
11	AC	12	ASP	CA-CB-CG	5.84	118.44	112.60
1	LS	382	PHE	CA-CB-CG	5.84	119.64	113.80
14	BB	518	ASP	CA-CB-CG	5.84	118.44	112.60
1	Ld	546	PHE	CA-CB-CG	5.84	119.64	113.80
9	Sp	457	ASP	CA-CB-CG	5.84	118.44	112.60
1	LU	546	PHE	CA-CB-CG	5.83	119.63	113.80
8	Fm	544	ASP	CA-CB-CG	5.83	118.43	112.60
9	SC	457	ASP	CA-CB-CG	5.83	118.43	112.60
9	Sg	556	PHE	CA-CB-CG	-5.83	107.97	113.80
2	BO	307	ASP	CA-CB-CG	5.83	118.43	112.60
9	SV	311	ASP	CA-CB-CG	5.83	118.43	112.60
9	Sg	457	ASP	CA-CB-CG	5.83	118.43	112.60
9	Sj	556	PHE	CA-CB-CG	-5.83	107.97	113.80
7	LP	108	PHE	CA-CB-CG	5.82	119.62	113.80
1	Lb	545	ASP	CA-CB-CG	5.82	118.42	112.60
5	A2	486	TYR	CB-CA-C	5.81	121.04	112.09
7	LD	108	PHE	CA-CB-CG	5.80	119.60	113.80
5	A2	633	TRP	N-CA-C	5.80	117.41	111.14
8	FT	564	ASP	CA-CB-CG	5.80	118.40	112.60
5	AY	486	TYR	CB-CA-C	5.79	121.01	112.09
7	LF	100	LYS	CA-C-N	5.79	125.60	120.10
7	LF	100	LYS	C-N-CA	5.79	125.60	120.10
1	LV	382	PHE	CA-CB-CG	5.78	119.58	113.80
7	LO	100	LYS	CA-C-N	5.78	125.59	120.10
7	LO	100	LYS	C-N-CA	5.78	125.59	120.10
9	Sg	629	LYS	CB-CA-C	5.78	116.58	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BF	356	PHE	CA-CB-CG	5.77	119.57	113.80
7	LM	72	ASP	CA-CB-CG	5.77	118.37	112.60
2	BK	92	SER	CA-C-N	5.77	125.77	119.89
2	BK	92	SER	C-N-CA	5.77	125.77	119.89
6	Ad	182	ASP	CA-CB-CG	5.76	118.36	112.60
9	SF	457	ASP	CA-CB-CG	5.76	118.36	112.60
11	AF	75	ARG	CG-CD-NE	5.76	124.67	112.00
9	Si	556	PHE	CA-CB-CG	-5.75	108.05	113.80
8	FL	588	PRO	N-CA-C	5.75	120.26	111.11
1	Lf	607	TYR	CA-CB-CG	5.75	124.25	113.90
2	BK	284	GLY	CA-C-N	5.75	129.88	120.63
2	BK	284	GLY	C-N-CA	5.75	129.88	120.63
11	AD	12	ASP	CA-CB-CG	5.73	118.33	112.60
9	SD	457	ASP	CA-CB-CG	5.73	118.33	112.60
6	Af	125	PRO	N-CA-C	5.72	124.25	112.47
6	Ab	182	ASP	CA-CB-CG	5.71	118.31	112.60
9	ST	137	ASP	CA-CB-CG	5.71	118.31	112.60
2	BN	80	PHE	CA-CB-CG	-5.71	108.09	113.80
9	SA	457	ASP	CA-CB-CG	5.71	118.31	112.60
1	LZ	607	TYR	CA-CB-CG	5.71	124.18	113.90
2	BO	200	ARG	NE-CZ-NH2	5.71	124.34	119.20
7	LA	108	PHE	CA-CB-CG	5.71	119.51	113.80
2	BO	51	ASP	CA-CB-CG	5.69	118.29	112.60
6	Ae	182	ASP	CA-CB-CG	5.69	118.29	112.60
1	Le	382	PHE	CA-CB-CG	5.68	119.48	113.80
6	A4	23	PHE	CA-CB-CG	5.68	119.48	113.80
8	FL	544	ASP	CA-CB-CG	5.68	118.28	112.60
1	Le	84	ASN	CA-C-N	5.68	127.89	120.28
1	Le	84	ASN	C-N-CA	5.68	127.89	120.28
4	AO	46	ASP	CA-CB-CG	5.68	118.28	112.60
1	LW	322	HIS	CA-CB-CG	5.67	119.47	113.80
6	Ad	125	PRO	N-CA-C	5.67	124.16	112.47
6	Ab	73	ASP	CA-CB-CG	5.67	118.27	112.60
12	BE	356	PHE	CA-CB-CG	5.66	119.46	113.80
1	LZ	33	LYS	CA-C-N	5.66	128.65	120.38
1	LZ	33	LYS	C-N-CA	5.66	128.65	120.38
5	AZ	987	ARG	NE-CZ-NH2	5.66	124.30	119.20
1	LW	251	ASP	CA-CB-CG	5.66	118.26	112.60
12	BF	248	ASN	CA-CB-CG	5.66	118.26	112.60
6	Aa	182	ASP	CA-CB-CG	5.65	118.25	112.60
9	SU	381	ASP	CA-CB-CG	5.64	118.24	112.60
1	Lf	251	ASP	CA-CB-CG	5.63	118.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AX	327	ASP	CA-CB-CG	5.62	118.22	112.60
9	SI	629	LYS	CB-CA-C	5.62	115.50	110.44
9	Sf	137	ASP	CA-CB-CG	5.62	118.22	112.60
9	Sn	311	ASP	CA-CB-CG	5.61	118.21	112.60
1	Lc	322	HIS	CA-CB-CG	5.61	119.41	113.80
3	BV	118	PHE	CA-CB-CG	5.60	119.40	113.80
4	AQ	374	LYS	CB-CA-C	5.60	115.18	111.20
7	LG	72	ASP	CA-CB-CG	5.60	118.20	112.60
9	Sh	77	ASP	CA-CB-CG	5.60	118.20	112.60
5	A1	683	HIS	CA-CB-CG	-5.59	108.20	113.80
8	FC	588	PRO	N-CA-C	5.59	120.01	111.34
1	LT	33	LYS	CA-C-N	5.59	128.54	120.38
1	LT	33	LYS	C-N-CA	5.59	128.54	120.38
1	Li	343	ASP	CA-CB-CG	5.59	118.19	112.60
3	BR	118	PHE	CA-CB-CG	5.59	119.39	113.80
6	A9	188	ASP	CA-CB-CG	5.59	118.19	112.60
8	FB	564	ASP	CA-CB-CG	5.58	118.19	112.60
9	Si	137	ASP	CA-CB-CG	5.58	118.18	112.60
1	La	546	PHE	CA-CB-CG	5.58	119.38	113.80
4	AT	117	HIS	CA-CB-CG	5.57	119.37	113.80
6	Ac	182	ASP	CA-CB-CG	5.57	118.17	112.60
1	Li	251	ASP	CA-CB-CG	5.57	118.17	112.60
1	Lc	33	LYS	CA-C-N	5.57	128.51	120.38
1	Lc	33	LYS	C-N-CA	5.57	128.51	120.38
11	AE	12	ASP	CA-CB-CG	5.57	118.17	112.60
6	Ac	125	PRO	N-CA-C	5.56	123.92	112.47
6	Aa	125	PRO	N-CA-C	5.55	123.91	112.47
7	LG	108	PHE	CA-CB-CG	5.55	119.36	113.80
9	SW	381	ASP	CA-CB-CG	5.55	118.15	112.60
9	Sl	311	ASP	CA-CB-CG	5.55	118.15	112.60
6	A9	261	ASP	CA-CB-CG	5.55	118.15	112.60
6	Af	182	ASP	CA-CB-CG	5.55	118.15	112.60
7	LF	133	ASP	CA-CB-CG	5.54	118.14	112.60
6	Ae	125	PRO	N-CA-C	5.54	123.89	112.47
5	A3	987	ARG	NE-CZ-NH2	5.54	124.18	119.20
7	LP	72	ASP	CA-CB-CG	5.53	118.13	112.60
9	SX	311	ASP	CA-CB-CG	5.53	118.13	112.60
11	AC	83	ASN	CA-CB-CG	5.52	118.12	112.60
2	BM	204	ASP	CA-CB-CG	5.52	118.12	112.60
5	A2	1026	THR	CB-CA-C	5.52	120.05	110.72
1	Lh	84	ASN	CA-C-N	5.52	127.67	120.28
1	Lh	84	ASN	C-N-CA	5.52	127.67	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Ad	73	ASP	CA-CB-CG	5.52	118.12	112.60
7	LH	69	LYS	CB-CA-C	5.50	121.38	110.42
9	SU	137	ASP	CA-CB-CG	5.50	118.11	112.60
5	A2	987	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	LY	84	ASN	CA-C-N	5.50	127.65	120.28
1	LY	84	ASN	C-N-CA	5.50	127.65	120.28
9	Si	629	LYS	CB-CA-C	5.50	116.27	110.17
9	Sh	137	ASP	CA-CB-CG	5.50	118.09	112.60
5	AY	683	HIS	CA-CB-CG	-5.49	108.31	113.80
1	Lh	382	PHE	CA-CB-CG	5.49	119.28	113.80
1	Li	113	PHE	CA-CB-CG	5.48	119.28	113.80
2	BK	268	ASN	CA-CB-CG	5.48	118.08	112.60
1	Lc	251	ASP	CA-CB-CG	5.48	118.08	112.60
9	Sp	311	ASP	CA-CB-CG	5.48	118.08	112.60
1	LX	197	ASP	CA-CB-CG	5.47	118.07	112.60
1	LS	84	ASN	CA-C-N	5.47	127.61	120.28
1	LS	84	ASN	C-N-CA	5.47	127.61	120.28
1	LW	106	PHE	CA-CB-CG	5.47	119.27	113.80
5	AY	483	ASP	CA-CB-CG	5.47	118.07	112.60
9	SB	457	ASP	CA-CB-CG	5.46	118.06	112.60
14	BB	162	ASP	CA-CB-CG	5.46	118.06	112.60
1	Lj	165	PHE	CA-CB-CG	5.46	119.26	113.80
1	Lh	545	ASP	CA-CB-CG	5.46	118.06	112.60
4	AT	327	ASP	CA-CB-CG	5.45	118.05	112.60
3	BU	286	ARG	NE-CZ-NH1	-5.45	116.05	121.50
5	AY	494	ASP	CA-C-N	5.45	127.85	120.38
5	AY	494	ASP	C-N-CA	5.45	127.85	120.38
7	LK	69	LYS	CB-CA-C	5.45	121.27	110.42
8	Fc	566	ASP	CA-CB-CG	5.45	118.05	112.60
8	Fu	564	ASP	CA-CB-CG	5.45	118.05	112.60
4	AV	327	ASP	CA-CB-CG	5.45	118.05	112.60
3	BS	47	ASN	CA-CB-CG	-5.44	107.16	112.60
11	AB	12	ASP	CA-CB-CG	5.44	118.04	112.60
5	AY	289	PHE	CA-CB-CG	5.44	119.24	113.80
9	SJ	537	ASP	CA-CB-CG	5.44	118.04	112.60
6	Af	127	ASN	CA-CB-CG	5.44	118.04	112.60
9	Si	173	SER	CA-C-N	5.43	128.31	120.38
9	Si	173	SER	C-N-CA	5.43	128.31	120.38
10	TT	32	PHE	CA-CB-CG	-5.43	108.37	113.80
1	Li	232	PHE	CA-CB-CG	5.43	119.23	113.80
9	SE	457	ASP	CA-CB-CG	5.43	118.03	112.60
6	Af	73	ASP	CA-CB-CG	5.43	118.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	LX	546	PHE	CA-CB-CG	5.43	119.23	113.80
5	AZ	494	ASP	CA-C-N	5.43	127.81	120.38
5	AZ	494	ASP	C-N-CA	5.43	127.81	120.38
9	SL	362	ASP	CA-CB-CG	5.43	118.03	112.60
9	SW	137	ASP	CA-CB-CG	5.42	118.03	112.60
9	Sj	137	ASP	CA-CB-CG	5.42	118.02	112.60
12	BE	66	ASP	CA-CB-CG	5.42	118.02	112.60
5	A3	235	ARG	CA-C-N	5.42	126.74	121.65
5	A3	235	ARG	C-N-CA	5.42	126.74	121.65
9	Sk	485	PRO	N-CA-C	5.42	120.97	113.98
13	AH	85	ARG	CG-CD-NE	5.41	123.91	112.00
7	LQ	69	LYS	CB-CA-C	5.41	121.19	110.42
9	SG	537	ASP	CA-CB-CG	5.41	118.01	112.60
9	SH	537	ASP	CA-CB-CG	5.41	118.01	112.60
1	LY	382	PHE	CA-CB-CG	5.40	119.20	113.80
4	AQ	262	PHE	CA-CB-CG	5.40	119.20	113.80
7	LC	100	LYS	CA-C-N	5.40	125.23	120.10
7	LC	100	LYS	C-N-CA	5.40	125.23	120.10
9	SR	548	ASP	CA-CB-CG	5.40	118.00	112.60
12	BG	112	ASP	CA-CB-CG	5.40	118.00	112.60
4	AM	374	LYS	CB-CA-C	5.40	115.03	111.20
11	AD	62	PHE	CA-CB-CG	-5.40	108.40	113.80
2	BK	261	GLN	CA-C-N	5.39	128.13	120.53
2	BK	261	GLN	C-N-CA	5.39	128.13	120.53
5	AY	1026	THR	CB-CA-C	5.39	119.28	110.17
1	LT	150	ASN	CA-C-N	5.39	125.09	119.92
1	LT	150	ASN	C-N-CA	5.39	125.09	119.92
1	Lf	343	ASP	CA-CB-CG	5.38	117.98	112.60
9	SM	548	ASP	CA-CB-CG	5.38	117.98	112.60
9	Sh	310	ASP	CA-CB-CG	5.38	117.98	112.60
1	LV	84	ASN	CA-C-N	5.38	127.49	120.28
1	LV	84	ASN	C-N-CA	5.38	127.49	120.28
8	Fu	563	LEU	CA-C-N	5.38	130.72	124.21
8	Fu	563	LEU	C-N-CA	5.38	130.72	124.21
1	LS	545	ASP	CA-CB-CG	5.37	117.97	112.60
7	LB	69	LYS	CB-CA-C	5.37	121.11	110.42
9	SH	629	LYS	CB-CA-C	5.37	115.81	110.33
11	AC	5	ASP	CA-CB-CG	5.37	117.97	112.60
1	LY	545	ASP	CA-CB-CG	5.37	117.97	112.60
5	A0	683	HIS	CA-CB-CG	-5.36	108.44	113.80
1	Lf	440	ASP	CA-CB-CG	5.36	117.96	112.60
5	A1	494	ASP	CA-C-N	5.36	127.72	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A1	494	ASP	C-N-CA	5.36	127.72	120.38
1	Lb	382	PHE	CA-CB-CG	5.36	119.16	113.80
11	AA	66	THR	CB-CA-C	-5.36	103.15	110.22
3	BS	87	PHE	CA-CB-CG	-5.35	108.45	113.80
9	SL	537	ASP	CA-CB-CG	5.35	117.95	112.60
4	AW	64	ASN	CA-CB-CG	-5.35	107.25	112.60
5	A2	289	PHE	CA-CB-CG	5.35	119.15	113.80
9	SS	137	ASP	CA-CB-CG	5.35	117.95	112.60
9	Sm	137	ASP	CA-CB-CG	5.35	117.95	112.60
8	FT	570	PRO	N-CA-C	5.34	120.87	113.98
9	ST	381	ASP	CA-CB-CG	5.34	117.94	112.60
4	AU	540	ASP	CA-CB-CG	5.34	117.94	112.60
2	BK	204	ASP	CA-CB-CG	5.34	117.94	112.60
9	SC	454	TYR	CB-CA-C	5.34	119.47	109.71
9	SJ	629	LYS	CB-CA-C	5.34	115.77	110.33
9	SX	381	ASP	CA-CB-CG	5.33	117.93	112.60
9	SI	537	ASP	CA-CB-CG	5.33	117.93	112.60
5	A2	683	HIS	CA-CB-CG	-5.32	108.48	113.80
11	AA	19	TRP	CA-CB-CG	5.32	123.72	113.60
5	A3	760	ASP	CA-CB-CG	5.32	117.92	112.60
8	Fu	566	ASP	CA-CB-CG	5.32	117.92	112.60
9	Sp	137	ASP	CA-CB-CG	5.32	117.92	112.60
4	AV	117	HIS	CA-CB-CG	5.31	119.11	113.80
7	LO	133	ASP	CA-CB-CG	5.31	117.91	112.60
5	A1	1014	ASP	CA-CB-CG	5.31	117.91	112.60
6	A5	188	ASP	CA-CB-CG	5.31	117.91	112.60
7	LN	69	LYS	CB-CA-C	5.31	120.99	110.42
9	So	311	ASP	CA-CB-CG	5.31	117.91	112.60
2	BL	80	PHE	CA-CB-CG	-5.30	108.50	113.80
1	LT	106	PHE	CA-CB-CG	5.30	119.10	113.80
4	AP	631	ASP	CA-CB-CG	5.30	117.90	112.60
7	LL	133	ASP	CA-CB-CG	5.30	117.90	112.60
6	A7	159	GLU	CA-C-N	5.30	127.83	120.63
6	A7	159	GLU	C-N-CA	5.30	127.83	120.63
12	BE	248	ASN	CA-CB-CG	5.30	117.90	112.60
1	Le	545	ASP	CA-CB-CG	5.29	117.89	112.60
1	LX	198	PHE	CA-CB-CG	5.29	119.09	113.80
6	Ab	56	ASP	CA-CB-CG	5.29	117.89	112.60
3	BQ	286	ARG	NE-CZ-NH1	-5.29	116.21	121.50
5	A3	486	TYR	CB-CA-C	5.29	119.83	112.11
8	Fd	544	ASP	CA-CB-CG	5.29	117.89	112.60
9	SK	77	ASP	CA-CB-CG	5.29	117.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BM	307	ASP	CA-CB-CG	5.28	117.88	112.60
8	Fc	554	GLY	CA-C-N	5.28	127.89	120.28
8	Fc	554	GLY	C-N-CA	5.28	127.89	120.28
7	LA	246	ASP	CA-CB-CG	5.28	117.88	112.60
1	La	165	PHE	CA-CB-CG	5.28	119.08	113.80
14	BB	512	ASP	CA-CB-CG	5.28	117.88	112.60
9	SO	440	ASN	CA-CB-CG	5.27	117.87	112.60
9	SD	4	VAL	CB-CA-C	5.27	116.19	111.71
8	Fd	588	PRO	N-CA-C	5.26	119.50	111.34
9	SP	548	ASP	CA-CB-CG	5.26	117.86	112.60
12	BG	258	ASP	CB-CA-C	5.26	118.78	111.51
5	AZ	289	PHE	CA-CB-CG	5.26	119.06	113.80
1	Li	440	ASP	CA-CB-CG	5.26	117.86	112.60
14	BB	528	ASP	CA-CB-CG	5.26	117.86	112.60
1	Lc	242	ASN	CA-CB-CG	5.26	117.86	112.60
9	SK	362	ASP	CA-CB-CG	5.26	117.86	112.60
9	Sp	485	PRO	N-CA-C	5.26	120.76	113.98
7	LQ	201	ASP	CA-CB-CG	5.25	117.86	112.60
8	FK	554	GLY	CA-C-N	5.25	127.84	120.28
8	FK	554	GLY	C-N-CA	5.25	127.84	120.28
9	SH	77	ASP	CA-CB-CG	5.25	117.85	112.60
1	Lc	440	ASP	CA-CB-CG	5.25	117.85	112.60
4	AP	12	THR	CB-CA-C	5.25	118.65	110.67
5	A0	760	ASP	CA-CB-CG	5.25	117.85	112.60
6	Aa	70	ASP	CA-CB-CG	5.25	117.85	112.60
1	LU	198	PHE	CA-CB-CG	5.25	119.05	113.80
5	A2	760	ASP	CA-CB-CG	5.25	117.84	112.60
1	LT	113	PHE	CA-CB-CG	5.24	119.04	113.80
2	BL	268	ASN	CA-CB-CG	5.24	117.84	112.60
1	Lf	242	ASN	CA-CB-CG	5.24	117.84	112.60
13	AJ	179	GLU	CB-CG-CD	5.24	121.51	112.60
5	AZ	760	ASP	CA-CB-CG	5.24	117.84	112.60
8	FB	563	LEU	CA-C-N	5.24	130.54	124.21
8	FB	563	LEU	C-N-CA	5.24	130.54	124.21
1	LV	96	ASN	CA-CB-CG	5.23	117.83	112.60
5	A1	760	ASP	CA-CB-CG	5.23	117.83	112.60
6	Ac	56	ASP	CA-CB-CG	5.23	117.83	112.60
9	Sh	173	SER	CA-C-N	5.23	128.02	120.38
9	Sh	173	SER	C-N-CA	5.23	128.02	120.38
7	LK	201	ASP	CA-CB-CG	5.23	117.83	112.60
8	FT	563	LEU	CA-C-N	5.23	130.54	124.21
8	FT	563	LEU	C-N-CA	5.23	130.54	124.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Lb	468	GLU	CA-C-N	5.23	128.26	120.31
1	Lb	468	GLU	C-N-CA	5.23	128.26	120.31
9	Se	511	HIS	CA-CB-CG	5.23	119.03	113.80
11	AA	83	ASN	CA-CB-CG	5.23	117.83	112.60
3	BV	189	ARG	CD-NE-CZ	5.23	131.72	124.40
5	A0	987	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	La	253	THR	CA-C-N	5.22	127.47	120.58
1	La	253	THR	C-N-CA	5.22	127.47	120.58
6	A8	23	PHE	CA-CB-CG	5.22	119.02	113.80
5	A1	289	PHE	CA-CB-CG	5.22	119.02	113.80
9	SD	454	TYR	CB-CA-C	5.22	119.15	109.70
1	LU	197	ASP	CA-CB-CG	5.22	117.82	112.60
9	SL	77	ASP	CA-CB-CG	5.22	117.82	112.60
9	SI	457	ASP	CA-CB-CG	5.22	117.82	112.60
11	AF	83	ASN	CA-CB-CG	5.22	117.82	112.60
1	LU	165	PHE	CA-CB-CG	5.22	119.02	113.80
1	LW	440	ASP	CA-CB-CG	5.22	117.82	112.60
3	BQ	189	ARG	NE-CZ-NH1	-5.22	116.28	121.50
9	SW	440	ASN	CA-CB-CG	5.22	117.82	112.60
5	A2	483	ASP	CA-CB-CG	5.21	117.81	112.60
14	BC	11	PHE	CA-CB-CG	5.21	119.01	113.80
1	LS	457	THR	N-CA-C	5.21	113.05	108.78
1	LX	165	PHE	CA-CB-CG	5.21	119.01	113.80
9	SH	507	PRO	CA-C-N	5.21	128.48	120.82
9	SH	507	PRO	C-N-CA	5.21	128.48	120.82
10	TX	143	ASP	CA-CB-CG	5.21	117.81	112.60
11	AE	83	ASN	CA-CB-CG	5.21	117.81	112.60
9	SB	454	TYR	CB-CA-C	5.21	119.24	109.71
9	Sm	173	SER	CA-C-N	5.21	127.98	120.38
9	Sm	173	SER	C-N-CA	5.21	127.98	120.38
6	Ad	130	ASP	CA-CB-CG	5.20	117.80	112.60
9	SK	507	PRO	CA-C-N	5.20	128.47	120.82
9	SK	507	PRO	C-N-CA	5.20	128.47	120.82
4	AW	542	ASP	CA-CB-CG	5.20	117.80	112.60
6	Ad	191	ASP	CA-CB-CG	5.20	117.80	112.60
9	SM	440	ASN	CA-CB-CG	5.20	117.80	112.60
9	ST	311	ASP	CA-CB-CG	5.20	117.80	112.60
2	BO	204	ASP	CA-CB-CG	5.20	117.80	112.60
6	A7	188	ASP	CA-CB-CG	5.20	117.80	112.60
5	A3	494	ASP	CA-C-N	5.20	127.50	120.38
5	A3	494	ASP	C-N-CA	5.20	127.50	120.38
10	TW	32	PHE	CA-CB-CG	-5.20	108.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BM	90	PHE	CA-CB-CG	5.19	118.99	113.80
1	Lc	106	PHE	CA-CB-CG	5.19	118.99	113.80
9	SP	440	ASN	CA-CB-CG	5.19	117.79	112.60
5	A3	1014	ASP	CA-CB-CG	5.19	117.79	112.60
6	A7	261	ASP	CA-CB-CG	5.19	117.79	112.60
9	SK	537	ASP	CA-CB-CG	5.19	117.79	112.60
9	SJ	77	ASP	CA-CB-CG	5.19	117.79	112.60
9	Sk	311	ASP	CA-CB-CG	5.19	117.79	112.60
9	SH	362	ASP	CA-CB-CG	5.18	117.78	112.60
9	SW	530	ASP	CA-CB-CG	5.18	117.78	112.60
9	ST	530	ASP	CA-CB-CG	5.18	117.78	112.60
14	BD	11	PHE	CA-CB-CG	5.18	118.98	113.80
1	Lj	198	PHE	CA-CB-CG	5.18	118.98	113.80
9	SL	457	ASP	CA-CB-CG	5.18	117.78	112.60
6	Ad	339	PHE	CA-CB-CG	5.17	118.97	113.80
9	Sj	173	SER	CA-C-N	5.17	127.73	120.28
9	Sj	173	SER	C-N-CA	5.17	127.73	120.28
5	AY	409	GLU	CA-C-N	5.17	125.82	120.03
5	AY	409	GLU	C-N-CA	5.17	125.82	120.03
9	SN	173	SER	N-CA-C	5.17	115.07	108.24
4	AU	542	ASP	CA-CB-CG	5.17	117.77	112.60
7	LB	201	ASP	CA-CB-CG	5.17	117.77	112.60
1	Lf	33	LYS	CA-C-N	5.17	127.72	120.28
1	Lf	33	LYS	C-N-CA	5.17	127.72	120.28
9	SG	77	ASP	CA-CB-CG	5.17	117.77	112.60
5	A3	556	ARG	NE-CZ-NH2	5.16	123.85	119.20
6	A7	57	ASN	CA-C-N	5.16	127.92	120.38
6	A7	57	ASN	C-N-CA	5.16	127.92	120.38
11	AE	5	ASP	CA-CB-CG	5.16	117.76	112.60
9	SL	507	PRO	CA-C-N	5.16	128.41	120.82
9	SL	507	PRO	C-N-CA	5.16	128.41	120.82
13	AG	85	ARG	CG-CD-NE	5.16	123.36	112.00
14	BC	418	PRO	N-CA-C	5.16	120.62	113.65
3	BT	286	ARG	NE-CZ-NH1	-5.16	116.34	121.50
9	SF	454	TYR	CB-CA-C	5.16	119.15	109.71
9	SJ	507	PRO	CA-C-N	5.16	128.40	120.82
9	SJ	507	PRO	C-N-CA	5.16	128.40	120.82
9	SG	507	PRO	CA-C-N	5.16	128.40	120.82
9	SG	507	PRO	C-N-CA	5.16	128.40	120.82
4	AR	631	ASP	CA-CB-CG	5.15	117.75	112.60
9	SI	507	PRO	CA-C-N	5.15	128.40	120.82
9	SI	507	PRO	C-N-CA	5.15	128.40	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	SV	440	ASN	CA-CB-CG	5.15	117.75	112.60
1	LT	440	ASP	CA-CB-CG	5.15	117.75	112.60
1	LZ	224	ARG	CB-CG-CD	5.15	123.14	111.30
10	TO	56	ARG	CG-CD-NE	-5.15	100.67	112.00
10	Tr	143	ASP	CA-CB-CG	5.15	117.75	112.60
14	BD	20	ASP	CA-CB-CG	5.14	117.74	112.60
10	TU	143	ASP	CA-CB-CG	5.14	117.74	112.60
14	BC	20	ASP	CA-CB-CG	5.14	117.74	112.60
7	LN	108	PHE	CA-CB-CG	5.13	118.94	113.80
4	AV	291	ASP	CA-CB-CG	5.13	117.73	112.60
5	AZ	683	HIS	CA-CB-CG	-5.13	108.67	113.80
9	SM	173	SER	N-CA-C	5.13	115.02	108.24
1	Lg	253	THR	CA-C-N	5.13	127.35	120.58
1	Lg	253	THR	C-N-CA	5.13	127.35	120.58
5	A0	409	GLU	CA-C-N	5.13	125.78	120.03
5	A0	409	GLU	C-N-CA	5.13	125.78	120.03
9	SS	381	ASP	CA-CB-CG	5.13	117.73	112.60
9	SS	197	GLU	CA-C-N	5.13	125.42	119.47
9	SS	197	GLU	C-N-CA	5.13	125.42	119.47
5	A0	1024	ASN	CA-CB-CG	5.13	117.73	112.60
9	SP	173	SER	N-CA-C	5.13	115.01	108.24
9	SK	629	LYS	CB-CA-C	5.13	115.56	110.33
2	BL	259	PHE	N-CA-C	5.12	116.59	108.96
9	SV	137	ASP	CA-CB-CG	5.12	117.72	112.60
9	Sn	137	ASP	CA-CB-CG	5.12	117.72	112.60
9	So	485	PRO	N-CA-C	5.12	120.58	113.98
7	LM	246	ASP	CA-CB-CG	5.12	117.72	112.60
9	Se	137	ASP	CA-CB-CG	5.12	117.72	112.60
9	SR	440	ASN	CA-CB-CG	5.12	117.72	112.60
7	LR	133	ASP	CA-CB-CG	5.11	117.71	112.60
9	SR	173	SER	N-CA-C	5.11	114.99	108.24
6	A5	159	GLU	CA-C-N	5.11	127.58	120.63
6	A5	159	GLU	C-N-CA	5.11	127.58	120.63
9	SD	481	ASP	CA-CB-CG	5.11	117.71	112.60
8	Fc	563	LEU	CA-C-N	5.11	130.39	124.21
8	Fc	563	LEU	C-N-CA	5.11	130.39	124.21
8	Fu	554	GLY	CA-C-N	5.11	127.64	120.28
8	Fu	554	GLY	C-N-CA	5.11	127.64	120.28
9	SU	77	ASP	CA-CB-CG	5.11	117.71	112.60
8	FJ	589	ASN	CB-CA-C	5.11	118.76	109.62
9	Sg	310	ASP	CA-CB-CG	5.11	117.71	112.60
9	Sk	173	SER	CA-C-N	5.11	127.84	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Sk	173	SER	C-N-CA	5.11	127.84	120.38
1	LZ	251	ASP	CA-CB-CG	5.11	117.71	112.60
5	AZ	1014	ASP	CA-CB-CG	5.10	117.70	112.60
8	Fv	588	PRO	N-CA-C	5.10	119.32	111.21
10	TM	55	ASN	CA-CB-CG	-5.10	107.50	112.60
1	Lj	197	ASP	CA-CB-CG	5.10	117.70	112.60
10	TT	143	ASP	CA-CB-CG	5.10	117.70	112.60
1	LV	294	ASP	CA-CB-CG	5.10	117.70	112.60
10	TR	56	ARG	CG-CD-NE	-5.10	100.79	112.00
3	BV	5	GLU	CB-CA-C	-5.09	102.02	110.68
4	AV	461	PHE	N-CA-C	5.09	117.57	111.71
4	AN	12	THR	CB-CA-C	5.09	118.41	110.67
6	A5	20	THR	CB-CA-C	5.09	118.14	109.53
4	AT	461	PHE	N-CA-C	5.09	117.57	111.71
6	A6	23	PHE	CA-CB-CG	5.09	118.89	113.80
6	Ae	69	ALA	CA-C-N	5.09	127.61	120.28
6	Ae	69	ALA	C-N-CA	5.09	127.61	120.28
8	FB	554	GLY	CA-C-N	5.09	127.61	120.28
8	FB	554	GLY	C-N-CA	5.09	127.61	120.28
9	SV	197	GLU	CA-C-N	5.09	125.38	119.47
9	SV	197	GLU	C-N-CA	5.09	125.38	119.47
11	AD	83	ASN	CA-CB-CG	5.09	117.69	112.60
12	BF	164	LEU	CA-C-N	5.09	127.36	120.38
12	BF	164	LEU	C-N-CA	5.09	127.36	120.38
3	BT	189	ARG	CD-NE-CZ	5.09	131.53	124.40
11	AA	12	ASP	CA-CB-CG	5.09	117.69	112.60
9	Sf	173	SER	CA-C-N	5.09	127.81	120.38
9	Sf	173	SER	C-N-CA	5.09	127.81	120.38
9	Sh	511	HIS	CA-CB-CG	5.09	118.89	113.80
5	AZ	486	TYR	CB-CA-C	5.09	119.54	112.11
9	SB	2	PRO	CA-N-CD	-5.09	104.88	112.00
1	LW	232	PHE	CA-CB-CG	5.08	118.89	113.80
8	FK	563	LEU	CA-C-N	5.08	130.36	124.21
8	FK	563	LEU	C-N-CA	5.08	130.36	124.21
9	Sj	310	ASP	CA-CB-CG	5.08	117.69	112.60
14	BC	528	ASP	CA-CB-CG	5.08	117.69	112.60
9	SF	37	PRO	CB-CA-C	-5.08	104.91	111.46
9	Sg	137	ASP	CA-CB-CG	5.08	117.68	112.60
4	AS	542	ASP	CA-CB-CG	5.08	117.68	112.60
9	SW	311	ASP	CA-CB-CG	5.08	117.67	112.60
5	A3	683	HIS	CA-CB-CG	-5.07	108.73	113.80
5	A2	494	ASP	CA-C-N	5.07	127.33	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A2	494	ASP	C-N-CA	5.07	127.33	120.38
10	TM	56	ARG	CG-CD-NE	-5.07	100.85	112.00
5	A0	483	ASP	CA-CB-CG	5.07	117.67	112.60
4	AN	631	ASP	CA-CB-CG	5.06	117.66	112.60
6	Af	56	ASP	CA-CB-CG	5.06	117.66	112.60
9	SO	310	ASP	CA-CB-CG	5.06	117.66	112.60
1	LT	232	PHE	CA-CB-CG	5.06	118.86	113.80
9	SV	77	ASP	CA-CB-CG	5.06	117.66	112.60
14	BD	518	ASP	CA-CB-CG	5.05	117.65	112.60
9	Sa	71	PHE	CA-CB-CG	-5.05	108.75	113.80
9	Sg	173	SER	CA-C-N	5.05	127.55	120.28
9	Sg	173	SER	C-N-CA	5.05	127.55	120.28
9	Sk	137	ASP	CA-CB-CG	5.05	117.65	112.60
2	BO	158	GLY	N-CA-C	5.04	117.84	110.63
4	AQ	642	ARG	CG-CD-NE	-5.04	100.90	112.00
4	AX	46	ASP	CA-CB-CG	5.04	117.64	112.60
1	Lj	265	ASP	CA-CB-CG	5.04	117.64	112.60
4	AP	5	GLU	CB-CA-C	5.04	116.70	109.09
6	Af	130	ASP	CA-CB-CG	5.04	117.64	112.60
8	FT	564	ASP	CB-CA-C	5.04	114.78	111.20
5	A1	409	GLU	CA-C-N	5.04	125.67	120.03
5	A1	409	GLU	C-N-CA	5.04	125.67	120.03
10	TW	143	ASP	CA-CB-CG	5.04	117.64	112.60
3	BS	189	ARG	NE-CZ-NH1	-5.04	116.46	121.50
5	A2	409	GLU	CA-C-N	5.04	125.67	120.03
5	A2	409	GLU	C-N-CA	5.04	125.67	120.03
5	AY	633	TRP	N-CA-C	5.04	116.62	111.03
1	Le	468	GLU	CA-C-N	5.03	127.96	120.31
1	Le	468	GLU	C-N-CA	5.03	127.96	120.31
1	La	449	ARG	NE-CZ-NH2	5.03	123.73	119.20
9	SK	457	ASP	CA-CB-CG	5.03	117.63	112.60
9	SS	440	ASN	CA-CB-CG	5.03	117.63	112.60
7	LC	133	ASP	CA-CB-CG	5.03	117.63	112.60
10	Tv	143	ASP	CA-CB-CG	5.03	117.63	112.60
1	LZ	440	ASP	CA-CB-CG	5.03	117.63	112.60
9	SN	310	ASP	CA-CB-CG	5.03	117.63	112.60
5	A1	486	TYR	CB-CA-C	5.03	119.45	112.11
9	SR	310	ASP	CA-CB-CG	5.03	117.63	112.60
1	Lg	198	PHE	CA-CB-CG	5.03	118.83	113.80
5	A2	853	ASP	CA-C-N	5.03	127.72	120.38
5	A2	853	ASP	C-N-CA	5.03	127.72	120.38
1	LX	561	ASP	CA-CB-CG	5.02	117.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Af	191	ASP	CA-CB-CG	5.02	117.62	112.60
8	FA	589	ASN	CB-CA-C	5.02	118.61	109.62
9	SX	137	ASP	CA-CB-CG	5.02	117.62	112.60
1	La	265	ASP	CA-CB-CG	5.02	117.62	112.60
5	A3	1015	ASP	CA-CB-CG	5.02	117.62	112.60
6	A7	20	THR	CB-CA-C	5.02	117.81	109.53
1	LW	242	ASN	CA-CB-CG	5.01	117.61	112.60
5	AY	987	ARG	NE-CZ-NH2	5.01	123.71	119.20
4	AS	540	ASP	CA-CB-CG	5.01	117.61	112.60
1	LT	419	GLU	CA-C-N	5.01	126.99	120.28
1	LT	419	GLU	C-N-CA	5.01	126.99	120.28
9	Si	77	ASP	CA-CB-CG	5.01	117.61	112.60
1	Ld	197	ASP	CA-CB-CG	5.01	117.61	112.60
5	AY	515	PHE	CA-CB-CG	5.01	118.81	113.80
6	Ab	127	ASN	CA-CB-CG	5.01	117.61	112.60
1	LS	294	ASP	CA-CB-CG	5.00	117.60	112.60
14	BD	512	ASP	CA-CB-CG	5.00	117.60	112.60
3	BR	189	ARG	CD-NE-CZ	5.00	131.40	124.40
7	LJ	246	ASP	CA-CB-CG	5.00	117.60	112.60
8	Ft	589	ASN	CB-CA-C	5.00	118.57	109.62
12	BE	75	ASN	CA-C-N	5.00	128.68	120.63
12	BE	75	ASN	C-N-CA	5.00	128.68	120.63

There are no chirality outliers.

All (100) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A0	305	THR	Peptide
5	A0	69	GLN	Peptide
5	A0	907	LYS	Peptide
5	A0	934	ALA	Peptide
5	A1	633	TRP	Peptide
5	A1	69	GLN	Peptide
5	A2	305	THR	Peptide
5	A2	69	GLN	Peptide
5	A2	907	LYS	Peptide
5	A2	930	PRO	Peptide
5	A3	633	TRP	Peptide
5	A3	69	GLN	Peptide
5	A3	934	ALA	Peptide
4	AM	532	TYR	Sidechain
4	AO	532	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	AQ	532	TYR	Sidechain
4	AS	251	ALA	Peptide
5	AY	69	GLN	Peptide
5	AY	930	PRO	Peptide
5	AZ	305	THR	Peptide
5	AZ	633	TRP	Peptide
5	AZ	69	GLN	Peptide
5	AZ	934	ALA	Peptide
5	AZ	977	VAL	Peptide
2	BM	93	PRO	Peptide
2	BO	148	LEU	Peptide
2	BO	292	ARG	Peptide
2	BP	72	ARG	Peptide
3	BQ	74	GLY	Peptide
3	BR	74	GLY	Peptide
3	BS	31	SER	Peptide
3	BS	74	GLY	Peptide
3	BT	46	TYR	Peptide
3	BT	74	GLY	Peptide
3	BU	74	GLY	Peptide
3	BV	74	GLY	Peptide
8	FC	552	GLU	Peptide
8	FL	552	GLU	Peptide
8	FU	552	GLU	Peptide
8	Fd	552	GLU	Peptide
8	Fm	552	GLU	Peptide
8	Fv	552	GLU	Peptide
7	LE	181	LEU	Peptide
7	LQ	181	LEU	Peptide
1	LS	26	ALA	Peptide
1	LS	605	ARG	Peptide
1	LS	92	ARG	Peptide
1	LU	28	ALA	Peptide
1	LU	508	LEU	Peptide
1	LV	26	ALA	Peptide
1	LV	593	SER	Peptide
1	LV	605	ARG	Peptide
1	LV	92	ARG	Peptide
1	LX	28	ALA	Peptide
1	LX	508	LEU	Peptide
1	LY	26	ALA	Peptide
1	LY	307	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	LY	593	SER	Peptide
1	LY	605	ARG	Peptide
1	LY	92	ARG	Peptide
1	LZ	236	PRO	Peptide
1	La	28	ALA	Peptide
1	La	508	LEU	Peptide
1	Lb	26	ALA	Peptide
1	Lb	605	ARG	Peptide
1	Lb	92	ARG	Peptide
1	Ld	28	ALA	Peptide
1	Le	26	ALA	Peptide
1	Le	307	ARG	Peptide
1	Le	593	SER	Peptide
1	Le	605	ARG	Peptide
1	Le	92	ARG	Peptide
1	Lf	247	PHE	Sidechain
1	Lg	28	ALA	Peptide
1	Lg	508	LEU	Peptide
1	Lh	26	ALA	Peptide
1	Lh	593	SER	Peptide
1	Lh	605	ARG	Peptide
1	Lh	92	ARG	Peptide
1	Lj	508	LEU	Peptide
9	SM	277	TYR	Sidechain
9	SN	277	TYR	Sidechain
9	SO	277	TYR	Sidechain
9	SP	168	THR	Peptide
9	SP	277	TYR	Sidechain
9	SQ	277	TYR	Sidechain
9	SR	109	ASN	Peptide
9	SR	277	TYR	Sidechain
9	ST	277	TYR	Sidechain
9	SU	277	TYR	Sidechain
9	SV	277	TYR	Sidechain
9	SW	277	TYR	Sidechain
9	SX	277	TYR	Sidechain
9	Se	632	ARG	Peptide
9	Sf	277	TYR	Sidechain
9	Sf	632	ARG	Peptide
9	Sg	277	TYR	Sidechain
9	Sg	632	ARG	Peptide
9	Sh	632	ARG	Peptide

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Mol	Chain	Res	Type	Group
9	Si	632	ARG	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	LS	4752	0	4730	5	0
1	LT	4752	0	4730	5	0
1	LU	4752	0	4730	3	0
1	LV	4752	0	4730	6	0
1	LW	4752	0	4730	4	0
1	LX	4752	0	4730	5	0
1	LY	4752	0	4730	7	0
1	LZ	4752	0	4730	3	0
1	La	4752	0	4730	4	0
1	Lb	4752	0	4730	5	0
1	Lc	4752	0	4730	4	0
1	Ld	4752	0	4730	4	0
1	Le	4752	0	4730	4	0
1	Lf	4752	0	4730	4	0
1	Lg	4752	0	4730	5	0
1	Lh	4752	0	4730	6	0
1	Li	4752	0	4730	5	0
1	Lj	4752	0	4730	4	0
2	BK	2664	0	2609	3	0
2	BL	2180	0	2138	7	0
2	BM	2664	0	2609	5	0
2	BN	2180	0	2138	7	0
2	BO	2664	0	2609	2	0
2	BP	2180	0	2138	11	0
3	BQ	2263	0	2203	9	0
3	BR	2263	0	2203	8	0
3	BS	2263	0	2203	7	0
3	BT	2263	0	2203	7	0
3	BU	2263	0	2203	8	0
3	BV	2263	0	2203	8	0
4	AM	5191	0	5061	5	0
4	AN	5191	0	5061	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AO	5191	0	5061	7	0
4	AP	5191	0	5061	3	0
4	AQ	5191	0	5061	3	0
4	AR	5191	0	5061	5	0
4	AS	5145	0	5008	1	0
4	AT	5125	0	4993	6	0
4	AU	5145	0	5008	3	0
4	AV	5125	0	4993	8	0
4	AW	5145	0	5008	0	0
4	AX	5125	0	4993	8	0
5	A0	8438	0	8098	13	0
5	A1	8438	0	8098	8	0
5	A2	8438	0	8098	11	0
5	A3	8438	0	8098	8	0
5	AY	8438	0	8098	14	0
5	AZ	8438	0	8098	10	0
6	A4	2669	0	2557	4	0
6	A5	2669	0	2557	3	0
6	A6	2669	0	2557	5	0
6	A7	2669	0	2557	4	0
6	A8	2669	0	2557	4	0
6	A9	2669	0	2557	3	0
6	Aa	2633	0	2522	5	0
6	Ab	2633	0	2522	3	0
6	Ac	2633	0	2522	5	0
6	Ad	2633	0	2522	7	0
6	Ae	2633	0	2522	4	0
6	Af	2633	0	2522	4	0
7	LA	2270	0	2236	3	0
7	LB	2270	0	2236	2	0
7	LC	2270	0	2236	1	0
7	LD	2270	0	2236	2	0
7	LE	2270	0	2236	2	0
7	LF	2270	0	2236	1	0
7	LG	2270	0	2236	4	0
7	LH	2270	0	2236	3	0
7	LI	2270	0	2236	1	0
7	LJ	2270	0	2236	2	0
7	LK	2270	0	2236	1	0
7	LL	2270	0	2236	2	0
7	LM	2270	0	2236	2	0
7	LN	2270	0	2236	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	LO	2270	0	2236	2	0
7	LP	2270	0	2236	4	0
7	LQ	2270	0	2236	4	0
7	LR	2270	0	2236	2	0
8	FA	499	0	490	1	0
8	FB	499	0	490	2	0
8	FC	499	0	490	3	0
8	FJ	499	0	490	0	0
8	FK	499	0	490	1	0
8	FL	499	0	490	0	0
8	FS	499	0	490	0	0
8	FT	499	0	490	2	0
8	FU	499	0	490	1	0
8	Fb	499	0	490	0	0
8	Fc	499	0	490	2	0
8	Fd	499	0	490	1	0
8	Fk	499	0	490	1	0
8	Fl	499	0	490	2	0
8	Fm	499	0	490	3	0
8	Ft	499	0	490	0	0
8	Fu	499	0	490	2	0
8	Fv	499	0	490	1	0
9	SA	4993	0	4889	13	0
9	SB	4993	0	4889	13	0
9	SC	4993	0	4889	8	0
9	SD	4993	0	4889	9	0
9	SE	4993	0	4889	9	0
9	SF	4993	0	4889	10	0
9	SG	5037	0	4931	11	0
9	SH	5037	0	4931	7	0
9	SI	5037	0	4931	10	0
9	SJ	5037	0	4931	9	0
9	SK	5037	0	4931	9	0
9	SL	5037	0	4931	10	0
9	SM	5037	0	4931	11	0
9	SN	5037	0	4931	8	0
9	SO	5037	0	4931	9	0
9	SP	5037	0	4931	10	0
9	SQ	5037	0	4931	6	0
9	SR	5037	0	4931	9	0
9	SS	5037	0	4931	4	0
9	ST	5037	0	4931	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	SU	5037	0	4931	2	0
9	SV	5037	0	4931	7	0
9	SW	5037	0	4931	2	0
9	SX	5037	0	4931	4	0
9	SY	5037	0	4931	4	0
9	SZ	5037	0	4931	4	0
9	Sa	5037	0	4931	3	0
9	Sb	5037	0	4931	2	0
9	Sc	5037	0	4931	3	0
9	Sd	5037	0	4931	2	0
9	Se	5037	0	4931	3	0
9	Sf	5037	0	4931	6	0
9	Sg	5037	0	4931	4	0
9	Sh	5037	0	4931	3	0
9	Si	5037	0	4931	6	0
9	Sj	5037	0	4931	5	0
9	Sk	5037	0	4931	4	0
9	Sl	5037	0	4931	7	0
9	Sm	5037	0	4931	3	0
9	Sn	5037	0	4931	2	0
9	So	5037	0	4931	7	0
9	Sp	5037	0	4931	3	0
10	TM	1305	0	1235	9	0
10	TN	1305	0	1235	6	0
10	TO	1305	0	1235	9	0
10	TP	1305	0	1235	10	0
10	TQ	1305	0	1235	7	0
10	TR	1305	0	1235	7	0
10	TS	1305	0	1235	5	0
10	TT	1305	0	1235	6	0
10	TU	1305	0	1235	9	0
10	TV	1305	0	1235	7	0
10	TW	1305	0	1235	7	0
10	TX	1305	0	1235	8	0
10	TY	1305	0	1235	7	0
10	TZ	1305	0	1235	5	0
10	Ta	1305	0	1235	4	0
10	Tb	1305	0	1235	4	0
10	Tc	1305	0	1235	6	0
10	Td	1305	0	1235	7	0
10	Te	1305	0	1235	4	0
10	Tf	1305	0	1235	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Tg	1305	0	1235	4	0
10	Th	1305	0	1235	3	0
10	Ti	1305	0	1235	7	0
10	Tj	1305	0	1235	6	0
10	Tk	1305	0	1235	4	0
10	Tl	1305	0	1235	5	0
10	Tm	1305	0	1235	3	0
10	Tn	1305	0	1235	4	0
10	To	1305	0	1235	5	0
10	Tp	1305	0	1235	3	0
10	Tq	1305	0	1235	3	0
10	Tr	1305	0	1235	2	0
10	Ts	1305	0	1235	3	0
10	Tt	1305	0	1235	3	0
10	Tu	1305	0	1235	3	0
10	Tv	1305	0	1235	2	0
11	AA	1044	0	1042	1	0
11	AB	1044	0	1042	4	0
11	AC	1044	0	1042	7	0
11	AD	1044	0	1042	1	0
11	AE	1044	0	1042	1	0
11	AF	1044	0	1042	1	0
12	BE	3055	0	2962	9	0
12	BF	3055	0	2962	7	0
12	BG	3055	0	2962	7	0
13	AG	1747	0	1652	0	0
13	AH	1747	0	1652	3	0
13	AI	1747	0	1652	0	0
13	AJ	1747	0	1652	3	0
13	AK	1747	0	1652	0	0
13	AL	1747	0	1652	2	0
14	BB	4354	0	4218	7	0
14	BC	4354	0	4218	15	0
14	BD	4354	0	4218	15	0
15	BB	1	0	0	0	0
All	All	605128	0	590112	710	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 1.

All (710) 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)
12:BG:246:MET:HE1	14:BC:1:MET:HE1	1.56	0.86
10:TP:2:GLU:CG	10:TX:99:ILE:HD12	2.14	0.77
5:A3:235:ARG:NH2	6:Ad:291:MET:HE1	2.01	0.74
10:TM:2:GLU:CG	10:TU:99:ILE:HD12	2.18	0.74
5:A0:235:ARG:NH2	6:Ae:291:MET:HE1	2.03	0.73
12:BG:246:MET:CE	14:BC:1:MET:HE1	2.20	0.71
10:TU:2:GLU:HG3	10:Tc:99:ILE:HD12	1.74	0.70
3:BV:116:MET:HE2	3:BU:284:ALA:HB3	1.73	0.69
2:BM:262:ILE:HD12	2:BM:262:ILE:H	1.60	0.67
4:AR:346:VAL:O	5:AY:886:VAL:HG23	1.96	0.66
6:A8:18:ILE:HD12	6:Ab:67:TYR:CZ	2.32	0.65
6:A4:18:ILE:HD12	6:Ad:67:TYR:CZ	2.33	0.64
10:TX:2:GLU:HG3	10:TZ:99:ILE:HD12	1.80	0.64
10:TP:55:ASN:HB3	10:TR:99:ILE:HD13	1.81	0.62
10:TP:2:GLU:HG3	10:TX:99:ILE:HD12	1.82	0.62
10:To:144:TRP:CD1	10:Ts:54:MET:HA	2.35	0.61
10:Tp:144:TRP:CD1	10:Tt:54:MET:HA	2.37	0.60
10:TM:2:GLU:HG3	10:TU:99:ILE:HD12	1.84	0.60
1:Lb:108:ILE:HD12	1:Lb:138:ILE:HD13	1.83	0.59
9:SA:8:ILE:HG21	11:AC:57:ILE:CD1	2.33	0.59
7:LN:159:LYS:HE2	7:LN:165:VAL:HG22	1.85	0.59
10:TM:55:ASN:HB3	10:TO:99:ILE:HD13	1.83	0.59
9:Sd:629:LYS:NZ	9:Sj:648:ALA:O	2.32	0.58
4:AX:155:LEU:H	4:AX:155:LEU:HD23	1.69	0.58
4:AV:155:LEU:HD23	4:AV:155:LEU:H	1.67	0.58
14:BC:61:THR:HG21	14:BD:57:VAL:HG13	1.86	0.57
9:SA:8:ILE:HG21	11:AC:57:ILE:HD12	1.85	0.57
2:BL:73:THR:HG21	12:BF:57:LYS:HE3	1.86	0.57
9:SX:427:TRP:CZ2	9:SX:439:MET:HG3	2.40	0.57
10:TU:2:GLU:CG	10:Tc:99:ILE:HD12	2.33	0.57
2:BP:73:THR:HG21	12:BE:57:LYS:HE3	1.87	0.57
2:BL:254:VAL:HG12	2:BL:255:GLU:H	1.70	0.57
4:AT:155:LEU:HD23	4:AT:155:LEU:H	1.70	0.57
10:Tl:144:TRP:CD1	10:Tv:54:MET:HA	2.39	0.57
10:Tk:144:TRP:CD1	10:Tu:54:MET:HA	2.40	0.57
5:AY:235:ARG:NH2	6:Ac:291:MET:HE1	2.19	0.56
14:BC:558:MET:HE1	14:BD:551:TRP:CD2	2.41	0.56
10:Tn:144:TRP:CD1	10:Tr:54:MET:HA	2.41	0.56
10:TN:2:GLU:CG	10:TV:99:ILE:HD12	2.35	0.56
9:ST:427:TRP:CZ2	9:ST:439:MET:HG3	2.41	0.56
10:TO:2:GLU:HG3	10:TW:99:ILE:HD12	1.88	0.56
12:BE:89:LYS:HE3	12:BF:241:TYR:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BP:263:THR:HG23	12:BF:225:LYS:HD3	1.88	0.55
5:A1:134:TYR:CE1	5:A1:594:LYS:HE3	2.41	0.55
7:LE:159:LYS:HE2	7:LE:165:VAL:HG22	1.87	0.55
8:Fc:574:LYS:C	8:Fc:575:TYR:CD1	2.84	0.55
11:AD:112:ILE:H	11:AD:112:ILE:HD12	1.72	0.55
12:BF:89:LYS:HE3	12:BG:241:TYR:CD1	2.42	0.55
2:BO:262:ILE:HD12	2:BO:262:ILE:H	1.70	0.55
2:BP:80:PHE:CE1	13:AJ:1:MET:HE3	2.41	0.55
3:BV:286:ARG:CA	3:BV:286:ARG:HE	2.20	0.55
10:Tm:144:TRP:CD1	10:Tq:54:MET:HA	2.41	0.55
9:SA:629:LYS:NZ	9:SG:648:ALA:O	2.40	0.55
3:BS:286:ARG:HE	3:BS:286:ARG:CA	2.20	0.55
8:FK:574:LYS:C	8:FK:575:TYR:CD1	2.85	0.55
10:TO:2:GLU:CG	10:TW:99:ILE:HD12	2.37	0.55
8:FT:574:LYS:C	8:FT:575:TYR:CD1	2.86	0.54
9:SS:427:TRP:CZ2	9:SS:439:MET:HG3	2.42	0.54
9:SU:427:TRP:CZ2	9:SU:439:MET:HG3	2.42	0.54
9:SW:427:TRP:CZ2	9:SW:439:MET:HG3	2.42	0.54
9:Sf:627:TYR:CD2	9:Sl:642:VAL:HG11	2.42	0.54
8:Fl:574:LYS:C	8:Fl:575:TYR:CD1	2.85	0.54
10:TM:2:GLU:HG2	10:TU:99:ILE:HD12	1.90	0.54
3:BQ:284:ALA:HB3	3:BR:116:MET:HE2	1.89	0.54
3:BT:286:ARG:HE	3:BT:286:ARG:C	2.16	0.54
3:BQ:286:ARG:HE	3:BQ:286:ARG:C	2.16	0.53
3:BU:286:ARG:HE	3:BU:286:ARG:C	2.16	0.53
8:FB:574:LYS:C	8:FB:575:TYR:CD1	2.86	0.53
10:TQ:2:GLU:CG	10:TS:99:ILE:HD12	2.37	0.53
11:AC:112:ILE:HD12	11:AC:112:ILE:H	1.73	0.53
2:BN:254:VAL:HG12	2:BN:255:GLU:H	1.73	0.53
8:Fu:574:LYS:C	8:Fu:575:TYR:CD1	2.86	0.53
5:A1:235:ARG:NH2	6:Ab:291:MET:HE1	2.23	0.53
9:SC:453:LYS:HE3	9:SC:500:CYS:SG	2.48	0.53
10:TP:2:GLU:HG2	10:TX:99:ILE:HD12	1.89	0.53
3:BV:286:ARG:HE	3:BV:286:ARG:HA	1.74	0.53
9:SV:427:TRP:CZ2	9:SV:439:MET:HG3	2.43	0.53
9:SV:160:TYR:CD2	9:SV:161:PRO:HD3	2.44	0.52
9:Sf:313:PHE:CE2	9:Sf:323:ALA:HB3	2.45	0.52
9:SH:575:ASN:HB2	9:SN:634:ILE:HD11	1.92	0.52
9:Si:313:PHE:CE2	9:Si:323:ALA:HB3	2.45	0.52
10:Tk:53:TYR:CG	10:Tk:54:MET:N	2.77	0.52
3:BR:286:ARG:CA	3:BR:286:ARG:HE	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A6:18:ILE:HD12	6:Af:67:TYR:CZ	2.45	0.52
10:Th:53:TYR:CG	10:Th:54:MET:N	2.78	0.52
9:SA:453:LYS:HE3	9:SA:500:CYS:SG	2.50	0.52
10:Tj:104:PRO:HA	10:Tj:107:TYR:CE2	2.46	0.51
3:BS:286:ARG:HE	3:BS:286:ARG:HA	1.75	0.51
5:A0:235:ARG:HH22	6:Ae:291:MET:HE1	1.71	0.51
10:TR:53:TYR:CG	10:TR:54:MET:N	2.78	0.51
10:Tn:53:TYR:CG	10:Tn:54:MET:N	2.78	0.51
3:BR:286:ARG:HE	3:BR:286:ARG:C	2.19	0.51
4:AX:440:GLN:CD	4:AX:440:GLN:H	2.18	0.51
4:AR:351:TYR:HD2	5:AY:886:VAL:HG21	1.76	0.51
1:LV:108:ILE:HD12	1:LV:138:ILE:HD13	1.93	0.51
10:TN:2:GLU:HG3	10:TV:99:ILE:HD12	1.92	0.51
10:TP:53:TYR:CG	10:TP:54:MET:N	2.79	0.51
9:Sj:313:PHE:CE2	9:Sj:323:ALA:HB3	2.46	0.51
10:TR:2:GLU:CG	10:TT:99:ILE:HD12	2.41	0.51
5:A3:235:ARG:HH22	6:Ad:291:MET:HE1	1.73	0.50
9:SL:575:ASN:HB2	9:SR:634:ILE:HD11	1.92	0.50
3:BS:284:ALA:HB3	3:BT:116:MET:HE2	1.93	0.50
10:Tp:53:TYR:CG	10:Tp:54:MET:N	2.78	0.50
10:TX:2:GLU:CG	10:TZ:99:ILE:HD12	2.39	0.50
2:BM:47:ASP:HB2	2:BM:57:LEU:HD21	1.92	0.50
10:TQ:53:TYR:CG	10:TQ:54:MET:N	2.79	0.50
4:AR:351:TYR:CD2	5:AY:886:VAL:HG21	2.46	0.50
6:A7:79:TRP:CE3	6:A7:311:ARG:HA	2.47	0.50
9:SF:560:LYS:HE3	9:SG:10:LEU:HD13	1.93	0.50
10:TM:53:TYR:CG	10:TM:54:MET:N	2.78	0.50
9:SK:313:PHE:CE2	9:SK:323:ALA:HB3	2.47	0.50
9:SR:484:GLN:HB2	9:SR:486:TRP:CH2	2.47	0.50
9:Sg:313:PHE:CE2	9:Sg:323:ALA:HB3	2.47	0.50
10:TQ:27:TYR:CD1	10:TQ:109:LYS:HE3	2.47	0.50
10:Te:104:PRO:HA	10:Te:107:TYR:CE2	2.47	0.50
4:AP:346:VAL:O	5:A2:886:VAL:HG23	2.12	0.50
11:AB:112:ILE:HD12	11:AB:112:ILE:H	1.76	0.50
4:AV:67:TYR:HB3	13:AH:84:PHE:CZ	2.46	0.50
10:Tl:53:TYR:CG	10:Tl:54:MET:N	2.77	0.50
9:SA:560:LYS:HE3	9:SH:10:LEU:HD13	1.94	0.49
10:Ti:53:TYR:CG	10:Ti:54:MET:N	2.80	0.49
10:Tm:53:TYR:CG	10:Tm:54:MET:N	2.79	0.49
4:AP:351:TYR:CD2	5:A2:886:VAL:HG21	2.47	0.49
10:Tf:104:PRO:HA	10:Tf:107:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Tg:104:PRO:HA	10:Tg:107:TYR:CE2	2.47	0.49
1:LV:26:ALA:HB2	1:LX:21:LYS:HA	1.94	0.49
2:BP:33:THR:HB	9:SD:493:ARG:HH21	1.78	0.49
9:SA:8:ILE:CG2	11:AC:57:ILE:HD12	2.42	0.49
9:SO:484:GLN:HB2	9:SO:486:TRP:CH2	2.47	0.49
4:AN:351:TYR:CD2	5:A0:886:VAL:HG21	2.47	0.49
1:LS:115:ASN:HB3	1:LS:143:ILE:HD13	1.94	0.49
6:Af:291:MET:SD	6:Af:292:PRO:HD2	2.53	0.49
9:SM:484:GLN:HB2	9:SM:486:TRP:CH2	2.47	0.49
3:BT:284:ALA:HB3	3:BU:116:MET:HE2	1.94	0.49
9:SF:536:GLY:CA	11:AC:62:PHE:CZ	2.95	0.49
9:Sn:453:LYS:HE3	9:Sn:500:CYS:SG	2.52	0.49
10:Tg:53:TYR:CG	10:Tg:54:MET:N	2.80	0.49
5:A2:134:TYR:CE1	5:A2:594:LYS:HE3	2.48	0.49
6:A5:294:SER:HB2	6:A5:295:PRO:HD2	1.95	0.49
9:SI:575:ASN:HB2	9:SO:634:ILE:HD11	1.95	0.49
9:So:453:LYS:HE3	9:So:500:CYS:SG	2.53	0.48
10:TM:55:ASN:CB	10:TO:99:ILE:HD13	2.42	0.48
10:Ti:104:PRO:HA	10:Ti:107:TYR:CE2	2.48	0.48
10:Tj:53:TYR:CG	10:Tj:54:MET:N	2.79	0.48
14:BD:489:LYS:HD3	14:BD:491:ILE:HD11	1.95	0.48
4:AV:155:LEU:H	4:AV:155:LEU:CD2	2.26	0.48
9:SD:110:TYR:CD2	9:SD:140:ILE:HD11	2.48	0.48
9:SP:382:GLU:CD	9:SP:382:GLU:H	2.21	0.48
9:SM:653:LEU:HD23	9:SM:653:LEU:H	1.77	0.48
10:Th:104:PRO:HA	10:Th:107:TYR:CE2	2.48	0.48
12:BE:241:TYR:CD2	12:BG:89:LYS:HE3	2.48	0.48
5:AZ:134:TYR:CE1	5:AZ:594:LYS:HE3	2.49	0.48
9:SC:560:LYS:HE3	9:SJ:10:LEU:HD13	1.95	0.48
9:SN:484:GLN:HB2	9:SN:486:TRP:CH2	2.48	0.48
10:TQ:2:GLU:HG3	10:TS:99:ILE:HD12	1.96	0.48
1:Lb:115:ASN:HB3	1:Lb:143:ILE:HD13	1.96	0.48
5:AZ:906:MET:HE3	6:Ac:341:PHE:HA	1.95	0.48
1:Li:5:LEU:HD23	7:LR:245:PHE:HA	1.94	0.48
9:SF:453:LYS:HE3	9:SF:500:CYS:SG	2.52	0.48
3:BT:286:ARG:HE	3:BT:286:ARG:CA	2.27	0.48
9:SQ:484:GLN:HB2	9:SQ:486:TRP:CH2	2.48	0.48
12:BE:241:TYR:CG	12:BG:89:LYS:HE3	2.48	0.48
3:BT:119:PRO:HA	9:SB:578:PHE:CZ	2.49	0.48
4:AT:155:LEU:H	4:AT:155:LEU:CD2	2.27	0.48
9:SE:453:LYS:HE3	9:SE:500:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SH:313:PHE:CE2	9:SH:323:ALA:HB3	2.48	0.48
9:SM:382:GLU:CD	9:SM:382:GLU:H	2.22	0.48
6:A5:79:TRP:CE3	6:A5:311:ARG:HA	2.48	0.48
5:A1:67:PHE:CZ	5:A1:565:GLY:HA3	2.49	0.48
7:LQ:118:LYS:HZ1	7:LR:198:TYR:HB2	1.79	0.48
9:SD:404:LEU:C	9:SD:405:ILE:HD12	2.39	0.48
9:SE:367:ARG:HG3	9:SE:561:ASN:HD21	1.79	0.48
10:TU:53:TYR:CG	10:TU:54:MET:N	2.82	0.48
2:BK:262:ILE:HD12	2:BK:262:ILE:H	1.78	0.47
9:SH:497:ILE:HG22	9:SH:497:ILE:O	2.14	0.47
9:SZ:589:GLN:HE21	9:SZ:589:GLN:HA	1.79	0.47
9:Se:313:PHE:CE2	9:Se:323:ALA:HB3	2.49	0.47
10:Tc:161:TRP:CD1	10:Td:96:GLY:HA2	2.49	0.47
1:LY:26:ALA:HB2	1:La:21:LYS:HA	1.96	0.47
9:Sh:313:PHE:CE2	9:Sh:323:ALA:HB3	2.48	0.47
10:TN:53:TYR:CG	10:TN:54:MET:N	2.78	0.47
10:TX:53:TYR:CG	10:TX:54:MET:N	2.82	0.47
10:To:53:TYR:CG	10:To:54:MET:N	2.77	0.47
1:LT:5:LEU:HD23	7:LC:245:PHE:HA	1.94	0.47
3:BV:119:PRO:HA	9:SD:578:PHE:CZ	2.49	0.47
9:SB:453:LYS:HE3	9:SB:500:CYS:SG	2.54	0.47
9:SF:404:LEU:C	9:SF:405:ILE:HD12	2.38	0.47
9:SG:497:ILE:HG22	9:SG:497:ILE:O	2.14	0.47
9:Si:627:TYR:CD2	9:So:642:VAL:HG11	2.49	0.47
4:AX:155:LEU:H	4:AX:155:LEU:CD2	2.25	0.47
5:AY:134:TYR:CE1	5:AY:594:LYS:HE3	2.49	0.47
5:A3:134:TYR:CE1	5:A3:594:LYS:HE3	2.49	0.47
9:SK:575:ASN:HB2	9:SQ:634:ILE:HD11	1.97	0.47
9:SE:454:TYR:HB2	9:SE:465:TRP:CE3	2.50	0.47
9:SL:613:THR:OG1	9:SL:614:PRO:HD2	2.14	0.47
9:SM:629:LYS:NZ	9:SS:648:ALA:O	2.47	0.47
10:TN:27:TYR:CD1	10:TN:109:LYS:HE3	2.49	0.47
14:BB:308:TYR:CD1	14:BB:332:LEU:HD21	2.50	0.47
14:BC:489:LYS:HD3	14:BC:491:ILE:HD11	1.97	0.47
1:Lc:411:VAL:HG22	1:Ld:431:GLU:HG3	1.96	0.47
2:BK:90:PHE:CG	2:BK:91:ASP:N	2.82	0.47
2:BN:113:ILE:HD11	2:BN:214:ILE:HG21	1.97	0.47
5:A0:134:TYR:CE1	5:A0:594:LYS:HE3	2.50	0.47
5:A2:235:ARG:NH2	6:Aa:291:MET:HE1	2.29	0.47
7:LH:36:ASP:HA	7:LG:7:LYS:HZ1	1.79	0.47
8:FB:557:VAL:HG12	8:FC:574:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SD:453:LYS:HE3	9:SD:500:CYS:SG	2.54	0.47
9:SG:313:PHE:CE2	9:SG:323:ALA:HB3	2.49	0.47
9:SI:497:ILE:O	9:SI:497:ILE:HG22	2.15	0.47
9:SN:382:GLU:H	9:SN:382:GLU:CD	2.23	0.47
9:Sm:453:LYS:CE	9:Sm:500:CYS:SG	3.03	0.47
10:TM:64:ARG:HD3	10:TM:66:TYR:CZ	2.50	0.47
10:TO:53:TYR:CG	10:TO:54:MET:N	2.79	0.47
1:LW:5:LEU:HD23	7:LF:245:PHE:HA	1.97	0.47
6:A8:79:TRP:CE3	6:A8:311:ARG:HA	2.50	0.47
1:LY:108:ILE:HD12	1:LY:138:ILE:HD13	1.97	0.47
2:BP:254:VAL:HG12	2:BP:255:GLU:H	1.79	0.47
3:BS:116:MET:HE2	3:BR:284:ALA:HB3	1.96	0.47
14:BB:460:GLY:HA2	14:BD:468:MET:HE2	1.96	0.47
6:A9:79:TRP:CE3	6:A9:311:ARG:HA	2.50	0.47
9:SG:575:ASN:HB2	9:SM:634:ILE:HD11	1.96	0.47
9:SI:313:PHE:CE2	9:SI:323:ALA:HB3	2.49	0.47
9:Sn:453:LYS:CE	9:Sn:500:CYS:SG	3.03	0.47
1:Lf:5:LEU:HD23	7:LO:245:PHE:HA	1.97	0.46
1:LT:68:ARG:HH12	1:LU:96:ASN:HB2	1.80	0.46
10:TT:2:GLU:HG3	10:Tb:99:ILE:HD12	1.98	0.46
10:TY:96:GLY:HA2	10:Td:161:TRP:CD1	2.50	0.46
14:BC:575:VAL:HG13	14:BD:573:ILE:HD13	1.97	0.46
1:LS:65:TYR:CD2	1:LS:65:TYR:C	2.94	0.46
9:SL:497:ILE:O	9:SL:497:ILE:HG22	2.15	0.46
11:AE:112:ILE:HD12	11:AE:112:ILE:H	1.81	0.46
10:TP:7:THR:HA	10:TP:10:PHE:CE1	2.51	0.46
9:SA:404:LEU:C	9:SA:405:ILE:HD12	2.40	0.46
9:SC:629:LYS:NZ	9:SI:648:ALA:O	2.48	0.46
9:Sa:346:GLU:CD	9:Sa:346:GLU:H	2.24	0.46
10:TR:2:GLU:HG3	10:TT:99:ILE:HD12	1.98	0.46
1:LS:108:ILE:HD12	1:LS:138:ILE:HD13	1.97	0.46
5:AZ:460:LEU:HD11	5:A0:1030:ILE:HG23	1.98	0.46
10:Tv:53:TYR:CG	10:Tv:54:MET:N	2.84	0.46
4:AT:374:LYS:HE2	5:A0:855:ILE:O	2.15	0.46
9:SA:5:SER:HB2	9:SA:6:PRO:HD2	1.97	0.46
9:SB:560:LYS:HE3	9:SI:10:LEU:HD13	1.97	0.46
9:SX:11:LYS:HE2	9:SX:13:THR:HG22	1.98	0.46
9:Sf:627:TYR:HA	9:Sl:642:VAL:HB	1.98	0.46
10:TV:2:GLU:CG	10:Td:99:ILE:HD12	2.46	0.46
14:BB:468:MET:HE2	14:BC:460:GLY:HA2	1.98	0.46
1:Lb:26:ALA:HB2	1:Ld:21:LYS:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BL:254:VAL:CG1	2:BL:255:GLU:H	2.27	0.46
4:AS:336:GLN:HB3	4:AM:220:MET:HE1	1.97	0.46
9:SA:110:TYR:CD2	9:SA:140:ILE:HD11	2.51	0.46
9:SC:110:TYR:CD2	9:SC:140:ILE:HD11	2.51	0.46
9:SK:110:TYR:CD1	9:SK:140:ILE:HD11	2.51	0.46
9:SH:110:TYR:CG	9:SH:140:ILE:HD11	2.50	0.46
10:TW:8:ARG:HD2	10:TX:34:PHE:CE2	2.51	0.46
9:SB:404:LEU:C	9:SB:405:ILE:HD12	2.41	0.46
9:SK:107:GLY:HA2	9:SK:178:VAL:HG13	1.97	0.46
10:TS:2:GLU:HG3	10:Ta:99:ILE:HD12	1.98	0.46
10:TT:53:TYR:CG	10:TT:54:MET:N	2.83	0.46
10:Ts:53:TYR:CG	10:Ts:54:MET:N	2.84	0.46
14:BB:489:LYS:HD3	14:BB:491:ILE:HD11	1.98	0.46
14:BC:64:ALA:HB3	14:BC:69:VAL:HG12	1.98	0.46
2:BP:80:PHE:CZ	13:AJ:1:MET:HE3	2.51	0.46
3:BQ:286:ARG:HE	3:BQ:286:ARG:CA	2.29	0.46
9:SA:367:ARG:HG3	9:SA:561:ASN:HD21	1.81	0.46
9:SP:484:GLN:HB2	9:SP:486:TRP:CH2	2.51	0.46
9:Si:627:TYR:HA	9:So:642:VAL:HB	1.97	0.46
9:Sm:453:LYS:HE3	9:Sm:500:CYS:SG	2.56	0.46
12:BE:258:ASP:CG	12:BE:287:ARG:HH11	2.24	0.46
14:BC:555:MET:HG2	14:BD:551:TRP:HB2	1.97	0.46
9:SD:454:TYR:HB2	9:SD:465:TRP:CE3	2.51	0.46
9:SK:497:ILE:HG22	9:SK:497:ILE:O	2.16	0.46
9:SJ:575:ASN:HB2	9:SP:634:ILE:HD11	1.96	0.46
1:Lf:68:ARG:HH12	1:Lg:96:ASN:HB2	1.81	0.45
2:BO:200:ARG:HD2	3:BV:143:HIS:CD2	2.51	0.45
9:SC:404:LEU:C	9:SC:405:ILE:HD12	2.42	0.45
9:SR:653:LEU:H	9:SR:653:LEU:HD23	1.82	0.45
9:SJ:497:ILE:HG22	9:SJ:497:ILE:O	2.17	0.45
9:SM:497:ILE:O	9:SM:497:ILE:HG22	2.16	0.45
9:Sl:453:LYS:HE3	9:Sl:500:CYS:SG	2.56	0.45
10:TW:53:TYR:CG	10:TW:54:MET:N	2.83	0.45
10:To:104:PRO:HA	10:To:107:TYR:CZ	2.51	0.45
1:LV:115:ASN:HB3	1:LV:143:ILE:HD13	1.97	0.45
2:BL:23:GLY:HA2	13:AL:50:TYR:CG	2.51	0.45
4:AV:374:LYS:HE2	5:A2:855:ILE:O	2.17	0.45
9:SV:15:VAL:O	9:SV:15:VAL:HG13	2.16	0.45
10:Tf:53:TYR:CG	10:Tf:54:MET:N	2.79	0.45
1:LV:65:TYR:CD2	1:LV:65:TYR:C	2.94	0.45
1:LZ:5:LEU:HD23	7:LI:245:PHE:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BR:119:PRO:HA	9:SF:578:PHE:CZ	2.52	0.45
4:AO:225:SER:C	4:AO:226:ILE:HG13	2.41	0.45
5:AY:202:PHE:CD1	5:AY:237:VAL:HG11	2.51	0.45
9:SF:110:TYR:CD2	9:SF:140:ILE:HD11	2.51	0.45
9:SJ:313:PHE:CE2	9:SJ:323:ALA:HB3	2.52	0.45
10:TW:2:GLU:HG3	10:TY:99:ILE:HD12	1.99	0.45
1:LW:68:ARG:HH12	1:LX:96:ASN:HB2	1.81	0.45
4:AP:5:GLU:HG2	4:AP:6:PRO:HD2	1.99	0.45
5:A3:202:PHE:CD1	5:A3:237:VAL:HG11	2.51	0.45
9:SF:536:GLY:HA2	11:AC:62:PHE:CZ	2.51	0.45
9:SO:382:GLU:CD	9:SO:382:GLU:H	2.23	0.45
9:SR:497:ILE:HG22	9:SR:497:ILE:O	2.17	0.45
9:Sd:346:GLU:H	9:Sd:346:GLU:CD	2.25	0.45
5:A2:67:PHE:CZ	5:A2:565:GLY:HA3	2.52	0.45
9:SR:382:GLU:H	9:SR:382:GLU:CD	2.23	0.45
10:Ta:161:TRP:CD1	10:Tb:96:GLY:HA2	2.52	0.45
1:Le:454:ALA:HB3	1:Le:471:LEU:CD2	2.47	0.45
3:BR:33:LYS:HD2	3:BR:33:LYS:O	2.16	0.45
6:Ad:276:PHE:CZ	6:Ad:325:ILE:HD13	2.51	0.45
9:SD:5:SER:HB2	9:SD:6:PRO:HD2	1.99	0.45
9:SL:313:PHE:CE2	9:SL:323:ALA:HB3	2.52	0.45
12:BF:119:SER:HB3	14:BD:36:PRO:HD3	1.98	0.45
10:TU:144:TRP:CD1	10:TY:54:MET:HA	2.51	0.45
1:Le:26:ALA:HB2	1:Lg:21:LYS:HA	1.99	0.45
2:BN:80:PHE:HE1	13:AH:1:MET:HE2	1.82	0.45
3:BT:8:LYS:HA	3:BT:12:ALA:HB3	1.98	0.45
6:A8:92:MET:HA	6:A8:92:MET:HE3	1.98	0.45
7:LJ:202:TYR:CD2	7:LJ:205:VAL:CG2	3.00	0.45
9:So:453:LYS:CE	9:So:500:CYS:SG	3.05	0.45
10:Tt:53:TYR:CG	10:Tt:54:MET:N	2.84	0.45
4:AX:19:PRO:HG3	4:AQ:269:THR:HG21	1.99	0.45
5:AY:487:HIS:HD2	6:Ac:312:GLN:OE1	1.99	0.45
5:A0:647:ARG:N	5:A0:648:PRO:CD	2.80	0.45
9:SB:5:SER:HB2	9:SB:6:PRO:HD2	1.98	0.45
9:SE:404:LEU:C	9:SE:405:ILE:HD12	2.41	0.45
9:SI:613:THR:OG1	9:SI:614:PRO:HD2	2.16	0.45
9:SY:346:GLU:CD	9:SY:346:GLU:H	2.25	0.45
9:Sp:453:LYS:CE	9:Sp:500:CYS:SG	3.05	0.45
14:BC:61:THR:HG21	14:BD:57:VAL:CG1	2.47	0.45
1:Le:115:ASN:HB3	1:Le:143:ILE:HD13	1.98	0.44
1:LW:411:VAL:HG22	1:LX:431:GLU:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LZ:411:VAL:HG22	1:La:431:GLU:HG3	1.98	0.44
3:BU:119:PRO:HA	9:SC:578:PHE:CZ	2.51	0.44
6:Ad:325:ILE:HD12	6:Ad:325:ILE:N	2.32	0.44
9:SE:110:TYR:CD2	9:SE:140:ILE:HD11	2.52	0.44
9:SK:427:TRP:CZ2	9:SK:439:MET:HG3	2.52	0.44
9:SA:454:TYR:HB2	9:SA:465:TRP:CE3	2.52	0.44
9:SO:497:ILE:HG22	9:SO:497:ILE:O	2.17	0.44
10:TO:7:THR:HA	10:TO:10:PHE:CE1	2.53	0.44
1:LY:115:ASN:HB3	1:LY:143:ILE:HD13	1.99	0.44
5:AY:67:PHE:CZ	5:AY:565:GLY:HA3	2.52	0.44
5:A0:202:PHE:CD1	5:A0:237:VAL:HG11	2.52	0.44
7:LQ:23:ILE:HD13	7:LQ:23:ILE:H	1.82	0.44
9:SG:110:TYR:CG	9:SG:140:ILE:HD11	2.52	0.44
9:Sl:453:LYS:CE	9:Sl:500:CYS:SG	3.05	0.44
1:Lh:115:ASN:HB3	1:Lh:143:ILE:HD13	1.98	0.44
1:Lb:65:TYR:CD2	1:Lb:65:TYR:C	2.95	0.44
9:SJ:110:TYR:CG	9:SJ:140:ILE:HD11	2.53	0.44
9:SP:653:LEU:HD23	9:SP:653:LEU:H	1.83	0.44
2:BP:254:VAL:CG1	2:BP:255:GLU:H	2.31	0.44
3:BQ:116:MET:HE2	3:BV:284:ALA:HB3	1.98	0.44
5:AY:281:LEU:HD21	7:LG:18:ALA:HA	2.00	0.44
9:SF:536:GLY:HA3	11:AC:62:PHE:CZ	2.52	0.44
9:SQ:497:ILE:O	9:SQ:497:ILE:HG22	2.18	0.44
6:A8:294:SER:HB2	6:A8:295:PRO:HD2	1.99	0.44
9:SB:454:TYR:HB2	9:SB:465:TRP:CE3	2.53	0.44
9:SQ:382:GLU:CD	9:SQ:382:GLU:H	2.23	0.44
10:Tr:53:TYR:CG	10:Tr:54:MET:N	2.84	0.44
12:BF:118:PHE:CE2	12:BF:133:MET:SD	3.11	0.44
1:LU:303:ASP:CG	1:LU:307:ARG:HH22	2.26	0.44
10:TR:104:PRO:HA	10:TR:107:TYR:CE2	2.53	0.44
10:TS:53:TYR:CG	10:TS:54:MET:N	2.84	0.44
10:TT:144:TRP:CD1	10:Td:54:MET:HA	2.53	0.44
10:Tq:53:TYR:CG	10:Tq:54:MET:N	2.86	0.44
14:BD:188:LEU:HD21	14:BD:238:MET:HG3	1.98	0.44
1:Lh:108:ILE:HD12	1:Lh:138:ILE:HD13	2.00	0.44
3:BQ:119:PRO:HA	9:SE:578:PHE:CZ	2.53	0.44
4:AO:345:CYS:HB3	4:AO:351:TYR:CE1	2.53	0.44
6:A6:22:LYS:HB2	6:A6:22:LYS:HE2	1.69	0.44
9:SE:560:LYS:HE3	9:SL:10:LEU:HD13	1.99	0.44
10:TO:104:PRO:HA	10:TO:107:TYR:CE2	2.53	0.44
1:Le:65:TYR:CD2	1:Le:65:TYR:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BL:254:VAL:HG12	2:BL:255:GLU:N	2.31	0.44
2:BN:254:VAL:HG12	2:BN:255:GLU:N	2.32	0.44
4:AR:5:GLU:HG2	4:AR:6:PRO:HD2	2.00	0.44
5:A1:647:ARG:N	5:A1:648:PRO:CD	2.81	0.44
5:A3:647:ARG:N	5:A3:648:PRO:CD	2.81	0.44
7:LQ:36:ASP:HA	7:LP:7:LYS:HZ1	1.82	0.44
9:SN:373:ALA:HB2	9:SN:391:VAL:HG11	1.99	0.44
10:TW:118:ARG:NH1	10:Tc:62:GLY:O	2.51	0.44
1:Li:411:VAL:HG22	1:Lj:431:GLU:HG3	2.00	0.43
2:BN:254:VAL:CG1	2:BN:255:GLU:H	2.30	0.43
5:AY:647:ARG:N	5:AY:648:PRO:CD	2.81	0.43
6:A6:79:TRP:CE3	6:A6:311:ARG:HA	2.53	0.43
7:LP:202:TYR:CD2	7:LP:205:VAL:CG2	3.00	0.43
9:SZ:346:GLU:CD	9:SZ:346:GLU:H	2.25	0.43
9:Sk:453:LYS:HE3	9:Sk:500:CYS:SG	2.58	0.43
4:AQ:19:PRO:HD3	5:AZ:702:TRP:CE3	2.53	0.43
4:AM:180:ARG:HH12	13:AJ:211:VAL:HA	1.82	0.43
5:AZ:235:ARG:NH2	6:Af:291:MET:HE1	2.33	0.43
7:LN:54:ALA:HB2	7:LM:9:ILE:HD12	2.00	0.43
8:Fu:557:VAL:HG12	8:Fv:574:LYS:HG2	2.00	0.43
10:TY:63:ASP:CG	10:Td:55:ASN:HD21	2.26	0.43
10:Tf:2:GLU:HG3	10:Tn:99:ILE:HD12	2.00	0.43
1:LS:454:ALA:HB3	1:LS:471:LEU:CD2	2.48	0.43
4:AU:564:HIS:CE1	5:A3:807:ARG:HG2	2.54	0.43
5:A1:281:LEU:HD21	7:LP:18:ALA:HA	2.00	0.43
5:A3:67:PHE:CZ	5:A3:565:GLY:HA3	2.53	0.43
6:A4:79:TRP:CE3	6:A4:311:ARG:HA	2.54	0.43
7:LD:202:TYR:CD2	7:LD:205:VAL:CG2	3.02	0.43
3:BS:286:ARG:HE	3:BS:286:ARG:C	2.27	0.43
5:A0:67:PHE:CZ	5:A0:565:GLY:HA3	2.54	0.43
6:A6:294:SER:HB2	6:A6:295:PRO:HD2	2.00	0.43
6:A7:238:TRP:CZ3	6:Aa:292:PRO:HG2	2.53	0.43
7:LG:202:TYR:CD2	7:LG:205:VAL:CG2	3.00	0.43
9:SN:497:ILE:HG22	9:SN:497:ILE:O	2.17	0.43
10:TZ:161:TRP:CD1	10:Ta:96:GLY:HA2	2.54	0.43
1:La:303:ASP:CG	1:La:307:ARG:HH22	2.26	0.43
1:Lc:37:VAL:HG22	1:Lc:38:SER:H	1.84	0.43
3:BV:165:ASP:HB3	3:BV:166:PRO:HD2	2.00	0.43
3:BV:286:ARG:HE	3:BV:286:ARG:C	2.27	0.43
3:BR:165:ASP:HB3	3:BR:166:PRO:HD2	2.00	0.43
6:Ac:54:TRP:CZ3	6:Ac:66:PRO:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SP:373:ALA:HB2	9:SP:391:VAL:HG11	1.99	0.43
9:Sk:453:LYS:CE	9:Sk:500:CYS:SG	3.06	0.43
10:Tu:53:TYR:CG	10:Tu:54:MET:N	2.85	0.43
1:Lj:303:ASP:CG	1:Lj:307:ARG:HH22	2.27	0.43
2:BK:239:TRP:CE3	2:BL:292:ARG:HD2	2.54	0.43
4:AX:374:LYS:HE2	5:AY:855:ILE:O	2.18	0.43
4:AV:19:PRO:HG3	4:AO:269:THR:HG21	1.99	0.43
9:SD:560:LYS:HE3	9:SK:10:LEU:HD13	2.00	0.43
9:SM:578:PHE:C	9:SM:578:PHE:CD1	2.97	0.43
10:TR:7:THR:HA	10:TR:10:PHE:CE1	2.53	0.43
10:Tg:7:THR:HA	10:Tg:10:PHE:CE2	2.54	0.43
1:LT:411:VAL:HG22	1:LU:431:GLU:HG3	1.99	0.43
1:LT:531:ALA:CB	1:LT:548:ILE:HD11	2.49	0.43
5:A0:570:TYR:CE2	5:A0:618:VAL:HG22	2.54	0.43
8:Fc:557:VAL:HG12	8:Fd:574:LYS:HG2	2.01	0.43
9:SK:110:TYR:CG	9:SK:140:ILE:HD11	2.54	0.43
10:TM:7:THR:HA	10:TM:10:PHE:CE1	2.53	0.43
10:TV:2:GLU:HG3	10:Td:99:ILE:HD12	2.01	0.43
1:Lf:411:VAL:HG22	1:Lg:431:GLU:HG3	2.01	0.43
1:LY:454:ALA:HB3	1:LY:471:LEU:CD2	2.49	0.43
5:A2:647:ARG:N	5:A2:648:PRO:CD	2.82	0.43
6:Ad:291:MET:SD	6:Ad:292:PRO:HD2	2.59	0.43
9:SX:11:LYS:HE2	9:SX:13:THR:CG2	2.49	0.43
9:Sb:589:GLN:HE21	9:Sb:589:GLN:HA	1.84	0.43
10:Tu:27:TYR:CD1	10:Tu:109:LYS:HE3	2.53	0.43
2:BP:113:ILE:HD11	2:BP:214:ILE:HG21	2.00	0.43
5:AZ:67:PHE:CZ	5:AZ:565:GLY:HA3	2.53	0.43
9:SS:219:MET:HE2	9:SS:219:MET:HA	2.01	0.43
9:SS:545:THR:HB	9:SS:546:PRO:HD2	2.01	0.43
9:Sc:629:LYS:NZ	9:Si:648:ALA:O	2.37	0.43
9:Sl:373:ALA:HB2	9:Sl:391:VAL:HG11	2.01	0.43
10:Tl:104:PRO:HA	10:Tl:107:TYR:CZ	2.54	0.43
1:Lh:26:ALA:HB2	1:Lj:21:LYS:HA	2.00	0.43
1:Lb:454:ALA:HB3	1:Lb:471:LEU:CD2	2.48	0.43
5:AZ:647:ARG:N	5:AZ:648:PRO:CD	2.81	0.43
9:Sg:126:ASP:CG	9:Sg:128:THR:H	2.26	0.43
9:Sk:373:ALA:HB2	9:Sk:391:VAL:HG11	2.01	0.43
9:So:219:MET:HE2	9:So:219:MET:HA	2.00	0.43
9:So:373:ALA:HB2	9:So:391:VAL:HG11	2.01	0.43
10:Tj:3:LEU:O	10:Tj:6:ILE:HG22	2.19	0.43
4:AN:5:GLU:HG2	4:AN:6:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AO:526:THR:HB	4:AO:527:PRO:HD2	2.00	0.42
5:A1:801:ARG:HG2	5:A1:810:TRP:CZ3	2.54	0.42
6:A7:294:SER:HB2	6:A7:295:PRO:HD2	2.01	0.42
9:SI:427:TRP:CZ2	9:SI:439:MET:HG3	2.54	0.42
9:SJ:427:TRP:CZ2	9:SJ:439:MET:HG3	2.54	0.42
9:SY:373:ALA:HB2	9:SY:391:VAL:HG11	2.01	0.42
9:Sf:126:ASP:CG	9:Sf:128:THR:H	2.27	0.42
14:BC:468:MET:HE2	14:BD:460:GLY:HA2	2.00	0.42
7:LA:202:TYR:CD2	7:LA:205:VAL:CG2	3.02	0.42
9:SF:454:TYR:HB2	9:SF:465:TRP:CE3	2.54	0.42
9:SN:65:PHE:CD1	9:SN:65:PHE:C	2.98	0.42
9:SZ:155:LYS:HD3	9:SZ:160:TYR:CG	2.54	0.42
9:Sa:589:GLN:HA	9:Sa:589:GLN:HE21	1.84	0.42
12:BG:259:LYS:HD3	14:BD:81:SER:OG	2.18	0.42
14:BB:469:TYR:CG	14:BB:470:ASN:N	2.87	0.42
1:Li:68:ARG:HH12	1:Lj:96:ASN:HB2	1.85	0.42
1:LX:303:ASP:CG	1:LX:307:ARG:HH22	2.27	0.42
4:AM:338:LYS:HE2	4:AM:354:PHE:CE1	2.54	0.42
9:SG:107:GLY:HA2	9:SG:178:VAL:HG13	2.00	0.42
9:SL:110:TYR:CG	9:SL:140:ILE:HD11	2.53	0.42
9:SO:653:LEU:HD23	9:SO:653:LEU:H	1.85	0.42
9:Sb:346:GLU:CD	9:Sb:346:GLU:H	2.27	0.42
9:Sj:126:ASP:CG	9:Sj:128:THR:H	2.27	0.42
12:BE:120:ARG:HG2	12:BE:121:ALA:N	2.35	0.42
2:BN:23:GLY:HA2	13:AH:50:TYR:CG	2.54	0.42
3:BU:286:ARG:HE	3:BU:286:ARG:CA	2.32	0.42
9:Si:627:TYR:CE2	9:So:642:VAL:HG11	2.54	0.42
10:TN:7:THR:HA	10:TN:10:PHE:CE1	2.55	0.42
10:TW:7:THR:HA	10:TW:10:PHE:CE1	2.54	0.42
4:AU:373:ASP:C	4:AU:375:PRO:HD3	2.45	0.42
5:A2:207:HIS:CG	8:Fm:562:GLN:HE22	2.37	0.42
6:Ae:54:TRP:CZ3	6:Ae:66:PRO:HD2	2.54	0.42
7:LB:81:MET:HE2	7:LB:102:LYS:H	1.84	0.42
9:SG:235:GLU:C	9:SG:236:ILE:HD12	2.43	0.42
9:SV:219:MET:HA	9:SV:219:MET:HE2	2.00	0.42
9:Se:303:TYR:CE1	9:Sj:546:PRO:HB3	2.55	0.42
10:TQ:104:PRO:HA	10:TQ:107:TYR:CE2	2.54	0.42
2:BP:261:GLN:OE1	12:BF:225:LYS:HE2	2.19	0.42
4:AQ:506:LYS:HE3	4:AQ:508:TYR:CE1	2.55	0.42
6:A9:294:SER:HB2	6:A9:295:PRO:HD2	2.00	0.42
9:SH:110:TYR:CD1	9:SH:140:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SU:11:LYS:HE2	9:SU:13:THR:HG22	2.00	0.42
10:TY:161:TRP:CD1	10:TZ:96:GLY:HA2	2.55	0.42
12:BE:118:PHE:CE2	12:BE:133:MET:SD	3.13	0.42
6:A4:294:SER:HB2	6:A4:295:PRO:HD2	2.02	0.42
10:TU:64:ARG:NH2	10:TV:89:GLN:OE1	2.53	0.42
10:Te:53:TYR:CG	10:Te:54:MET:N	2.80	0.42
14:BB:101:SER:HB2	14:BD:73:ILE:HD11	2.02	0.42
2:BM:46:ASN:C	2:BM:46:ASN:HD22	2.28	0.42
2:BP:283:PHE:CG	2:BP:284:GLY:N	2.88	0.42
4:AV:53:ARG:HD3	5:A2:658:TYR:CD2	2.55	0.42
4:AN:351:TYR:CE2	5:A0:886:VAL:HG21	2.55	0.42
9:SI:107:GLY:HA2	9:SI:178:VAL:HG13	2.02	0.42
9:SY:16:GLN:CD	9:SY:16:GLN:H	2.28	0.42
10:Tb:161:TRP:CD1	10:Tc:96:GLY:HA2	2.54	0.42
3:BS:119:PRO:HA	9:SA:578:PHE:CZ	2.55	0.42
6:A9:238:TRP:CZ3	6:Ac:292:PRO:HG2	2.55	0.42
7:LN:12:VAL:CG1	7:LO:28:GLY:HA3	2.50	0.42
7:LE:54:ALA:HB2	7:LD:9:ILE:HD12	2.01	0.42
9:SP:65:PHE:CD1	9:SP:65:PHE:C	2.97	0.42
9:Sp:453:LYS:HE2	9:Sp:500:CYS:SG	2.60	0.42
10:Tg:3:LEU:O	10:Tg:6:ILE:HG22	2.20	0.42
10:To:2:GLU:HG3	10:Tq:99:ILE:HD12	2.02	0.42
1:Lh:223:ARG:HD2	1:Lh:225:TYR:CE2	2.55	0.42
2:BM:69:PHE:O	12:BG:2:THR:HA	2.20	0.42
2:BM:344:VAL:O	2:BM:344:VAL:HG22	2.20	0.42
5:A2:301:PRO:HD3	5:A2:350:PHE:CZ	2.55	0.42
8:Fk:581:ALA:HB2	8:Fm:541:MET:HE3	2.02	0.42
9:SM:428:ARG:HD3	9:SM:428:ARG:C	2.45	0.42
9:Sc:346:GLU:CD	9:Sc:346:GLU:H	2.28	0.42
9:Sp:453:LYS:HE3	9:Sp:500:CYS:SG	2.60	0.42
1:Lh:65:TYR:CD2	1:Lh:65:TYR:C	2.97	0.41
2:BP:254:VAL:HG12	2:BP:255:GLU:N	2.34	0.41
3:BR:286:ARG:HE	3:BR:286:ARG:HA	1.85	0.41
4:AR:225:SER:C	4:AR:226:ILE:HG13	2.45	0.41
4:AO:506:LYS:HE3	4:AO:508:TYR:CE1	2.55	0.41
9:SG:427:TRP:CZ2	9:SG:439:MET:HG3	2.54	0.41
10:TQ:7:THR:HA	10:TQ:10:PHE:CE1	2.55	0.41
10:TS:2:GLU:CG	10:Ta:99:ILE:HD12	2.50	0.41
10:Ti:9:ALA:O	10:Tj:35:LYS:HE2	2.20	0.41
13:AL:108:ASP:HA	13:AL:156:ILE:HD12	2.02	0.41
1:Lg:303:ASP:CG	1:Lg:307:ARG:HH22	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LT:37:VAL:HG22	1:LT:38:SER:H	1.85	0.41
6:Ab:291:MET:SD	6:Ab:292:PRO:HD2	2.60	0.41
9:SB:523:VAL:HG22	9:SB:534:LEU:HA	2.01	0.41
9:SR:428:ARG:C	9:SR:428:ARG:HD3	2.46	0.41
10:Ti:7:THR:HA	10:Ti:10:PHE:CE1	2.55	0.41
10:Tj:7:THR:HA	10:Tj:10:PHE:CE1	2.55	0.41
1:LV:97:TRP:CE3	1:LV:113:PHE:HB3	2.55	0.41
3:BQ:8:LYS:HA	3:BQ:12:ALA:HB3	2.01	0.41
5:AY:207:HIS:CG	8:FC:562:GLN:HE22	2.38	0.41
5:A1:202:PHE:CD1	5:A1:237:VAL:HG11	2.55	0.41
9:SI:126:ASP:CG	9:SI:128:THR:H	2.29	0.41
9:SP:428:ARG:HD3	9:SP:428:ARG:C	2.45	0.41
9:SO:65:PHE:CD1	9:SO:65:PHE:C	2.97	0.41
9:SO:578:PHE:CD1	9:SO:578:PHE:C	2.99	0.41
10:TN:64:ARG:HD3	10:TN:66:TYR:CZ	2.55	0.41
10:Tl:2:GLU:HG3	10:Tt:99:ILE:HD12	2.02	0.41
14:BC:469:TYR:CG	14:BC:470:ASN:N	2.87	0.41
2:BN:283:PHE:CG	2:BN:284:GLY:N	2.88	0.41
6:A6:317:ILE:C	6:Af:20:THR:HG22	2.45	0.41
8:Fl:557:VAL:HG12	8:Fm:574:LYS:HG2	2.02	0.41
9:SM:65:PHE:CD1	9:SM:65:PHE:C	2.98	0.41
9:SR:65:PHE:CD1	9:SR:65:PHE:C	2.98	0.41
9:SV:346:GLU:CD	9:SV:346:GLU:H	2.28	0.41
9:Sc:150:ILE:HD12	9:Sc:150:ILE:H	1.85	0.41
9:Se:126:ASP:CG	9:Se:128:THR:H	2.27	0.41
9:Sg:65:PHE:CD1	9:Sg:65:PHE:C	2.98	0.41
10:Ti:133:TRP:CH2	10:Ti:135:THR:HG22	2.55	0.41
12:BE:332:ARG:HH21	12:BE:332:ARG:HB2	1.86	0.41
1:Lf:37:VAL:HG22	1:Lf:38:SER:H	1.86	0.41
1:Lc:5:LEU:HD23	7:LL:245:PHE:HA	2.02	0.41
3:BT:165:ASP:HB3	3:BT:166:PRO:HD2	2.02	0.41
3:BU:165:ASP:HB3	3:BU:166:PRO:HD2	2.01	0.41
3:BU:193:GLN:O	3:BU:194:ASP:HB2	2.20	0.41
4:AM:526:THR:HB	4:AM:527:PRO:HD2	2.01	0.41
9:SL:427:TRP:CZ2	9:SL:439:MET:HG3	2.55	0.41
9:SJ:110:TYR:CD1	9:SJ:140:ILE:HD11	2.56	0.41
9:SP:497:ILE:HG22	9:SP:497:ILE:O	2.19	0.41
9:SR:578:PHE:CD1	9:SR:578:PHE:C	2.99	0.41
9:Sh:65:PHE:CD1	9:Sh:65:PHE:C	2.98	0.41
9:Si:126:ASP:CG	9:Si:128:THR:H	2.28	0.41
10:TV:53:TYR:CG	10:TV:54:MET:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Tk:2:GLU:HG3	10:Ts:99:ILE:HD12	2.03	0.41
1:LV:223:ARG:HD2	1:LV:225:TYR:CE2	2.56	0.41
1:LW:37:VAL:HG22	1:LW:38:SER:H	1.85	0.41
1:LY:65:TYR:CD2	1:LY:65:TYR:C	2.97	0.41
5:AZ:202:PHE:CD1	5:AZ:237:VAL:HG11	2.55	0.41
6:Aa:226:SER:N	6:Aa:227:PRO:HD3	2.34	0.41
7:LM:202:TYR:CD2	7:LM:205:VAL:CG2	3.03	0.41
9:SB:8:ILE:CD1	11:AB:57:ILE:HD11	2.51	0.41
9:SO:373:ALA:HB2	9:SO:391:VAL:HG11	2.02	0.41
9:Sa:16:GLN:H	9:Sa:16:GLN:CD	2.28	0.41
9:Sg:408:PRO:HD3	9:Sg:427:TRP:CZ2	2.56	0.41
10:TX:7:THR:HA	10:TX:10:PHE:CE1	2.55	0.41
10:To:130:THR:HG21	10:To:161:TRP:CZ2	2.56	0.41
11:AF:112:ILE:HD12	11:AF:112:ILE:H	1.85	0.41
14:BB:524:ASP:O	14:BD:532:GLY:HA3	2.20	0.41
3:BQ:49:MET:HE2	9:SJ:646:THR:HG22	2.03	0.41
3:BU:8:LYS:HA	3:BU:12:ALA:HB3	2.03	0.41
5:AY:570:TYR:CE2	5:AY:618:VAL:HG22	2.56	0.41
5:AZ:281:LEU:HD21	7:LJ:18:ALA:HA	2.03	0.41
9:SB:8:ILE:HG12	11:AB:57:ILE:CD1	2.51	0.41
9:SB:367:ARG:HG3	9:SB:561:ASN:HD21	1.85	0.41
9:SE:5:SER:HB2	9:SE:6:PRO:HD2	2.01	0.41
9:ST:545:THR:HB	9:ST:546:PRO:HD2	2.02	0.41
9:Sf:65:PHE:CD1	9:Sf:65:PHE:C	2.99	0.41
9:Sj:65:PHE:CD1	9:Sj:65:PHE:C	2.98	0.41
10:TM:104:PRO:HA	10:TM:107:TYR:CE2	2.55	0.41
10:TP:27:TYR:CD1	10:TP:109:LYS:HE3	2.56	0.41
10:TY:97:ASN:ND2	10:Td:161:TRP:CH2	2.88	0.41
10:Te:3:LEU:O	10:Te:6:ILE:HG22	2.21	0.41
10:Th:9:ALA:O	10:Ti:35:LYS:HE2	2.21	0.41
10:Tm:104:PRO:HA	10:Tm:107:TYR:CZ	2.55	0.41
1:LX:589:ILE:C	1:LX:589:ILE:HD12	2.46	0.41
4:AT:53:ARG:HD3	5:A0:658:TYR:CD2	2.56	0.41
9:SC:523:VAL:HG22	9:SC:534:LEU:HA	2.02	0.41
9:SN:428:ARG:HD3	9:SN:428:ARG:C	2.46	0.41
9:SO:428:ARG:HD3	9:SO:428:ARG:C	2.45	0.41
9:SZ:629:LYS:NZ	9:Sf:648:ALA:O	2.37	0.41
10:Tb:161:TRP:CH2	10:Tc:97:ASN:ND2	2.88	0.41
1:Lh:454:ALA:HB3	1:Lh:471:LEU:CD2	2.50	0.41
1:LY:97:TRP:CE3	1:LY:113:PHE:HB3	2.56	0.41
4:AX:521:LEU:O	4:AX:533:PRO:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AT:410:ILE:HD11	5:A0:888:PHE:CZ	2.55	0.41
4:AV:329:GLU:CD	4:AV:332:ARG:HH22	2.29	0.41
4:AO:330:ARG:HA	4:AO:460:MET:HE1	2.03	0.41
5:AY:174:HIS:CD2	5:AY:174:HIS:H	2.36	0.41
6:A4:317:ILE:C	6:Ad:20:THR:HG22	2.45	0.41
7:LQ:36:ASP:HA	7:LP:7:LYS:NZ	2.34	0.41
9:SB:110:TYR:CD2	9:SB:140:ILE:HD11	2.56	0.41
9:SD:523:VAL:HG22	9:SD:534:LEU:HA	2.02	0.41
9:SF:367:ARG:HG3	9:SF:561:ASN:HD21	1.86	0.41
9:SK:222:ILE:HG12	9:SK:323:ALA:HB2	2.02	0.41
9:SH:107:GLY:HA2	9:SH:178:VAL:HG13	2.03	0.41
9:SI:110:TYR:CG	9:SI:140:ILE:HD11	2.56	0.41
9:SJ:235:GLU:C	9:SJ:236:ILE:HD12	2.46	0.41
9:SP:110:TYR:CD2	9:SP:140:ILE:HD11	2.56	0.41
9:SM:373:ALA:HB2	9:SM:391:VAL:HG11	2.02	0.41
9:SR:373:ALA:HB2	9:SR:391:VAL:HG11	2.03	0.41
9:Sh:126:ASP:CG	9:Sh:128:THR:H	2.28	0.41
10:Tl:7:THR:HA	10:Tl:10:PHE:CE1	2.56	0.41
10:Tn:130:THR:HG21	10:Tn:161:TRP:CZ2	2.56	0.41
11:AA:112:ILE:H	11:AA:112:ILE:HD12	1.86	0.41
14:BC:176:ILE:H	14:BC:176:ILE:HG13	1.71	0.41
1:LS:97:TRP:CE3	1:LS:113:PHE:HB3	2.56	0.41
4:AX:345:CYS:HB3	4:AX:354:PHE:CE2	2.55	0.41
4:AU:410:ILE:HD11	5:A3:888:PHE:CZ	2.56	0.41
6:A5:238:TRP:CZ3	6:Ae:292:PRO:HG2	2.56	0.41
7:LB:54:ALA:HB2	7:LA:9:ILE:HD12	2.02	0.41
7:LK:12:VAL:CG1	7:LL:28:GLY:HA3	2.51	0.41
9:SC:367:ARG:HG3	9:SC:561:ASN:HD21	1.85	0.41
9:SE:523:VAL:HG22	9:SE:534:LEU:HA	2.03	0.41
9:SL:373:ALA:HB2	9:SL:391:VAL:HG11	2.03	0.41
9:SN:578:PHE:CD1	9:SN:578:PHE:C	2.99	0.41
10:TO:64:ARG:HD3	10:TO:66:TYR:CZ	2.56	0.41
10:TP:144:TRP:CD1	10:TT:54:MET:HA	2.55	0.41
10:Tp:104:PRO:HA	10:Tp:107:TYR:CZ	2.55	0.41
1:LZ:262:ARG:HE	1:LZ:277:GLU:CD	2.29	0.40
3:BQ:84:VAL:C	3:BQ:85:ASN:HD22	2.29	0.40
4:AM:506:LYS:HE3	4:AM:508:TYR:CE1	2.56	0.40
9:SG:373:ALA:HB2	9:SG:391:VAL:HG11	2.03	0.40
9:SP:629:LYS:NZ	9:SV:648:ALA:O	2.53	0.40
9:Sl:65:PHE:CD1	9:Sl:65:PHE:C	2.99	0.40
9:Sm:65:PHE:CD1	9:Sm:65:PHE:C	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:TQ:64:ARG:H	10:TR:93:HIS:CE1	2.38	0.40
10:TU:7:THR:HA	10:TU:10:PHE:CE1	2.56	0.40
1:Lg:198:PHE:CD1	1:Lg:198:PHE:C	2.99	0.40
1:Li:37:VAL:HG22	1:Li:38:SER:H	1.86	0.40
1:Lc:262:ARG:HE	1:Lc:277:GLU:CD	2.28	0.40
4:AN:225:SER:C	4:AN:226:ILE:HG13	2.46	0.40
5:A2:281:LEU:HD21	7:LA:18:ALA:HA	2.03	0.40
8:FT:557:VAL:HG12	8:FU:574:LYS:HG2	2.03	0.40
9:SA:523:VAL:HG22	9:SA:534:LEU:HA	2.03	0.40
9:SM:110:TYR:CD2	9:SM:140:ILE:HD11	2.56	0.40
9:SW:346:GLU:CD	9:SW:346:GLU:H	2.29	0.40
10:TO:64:ARG:H	10:TP:93:HIS:CE1	2.38	0.40
10:TV:104:PRO:HA	10:TV:107:TYR:CZ	2.57	0.40
10:TY:161:TRP:CH2	10:TZ:97:ASN:ND2	2.89	0.40
14:BC:321:LYS:HE2	14:BD:454:ASP:OD2	2.21	0.40
1:LY:410:PRO:HA	1:LY:434:PRO:HA	2.04	0.40
4:AV:521:LEU:O	4:AV:533:PRO:HA	2.21	0.40
5:AZ:695:TYR:HA	5:AZ:696:PRO:HD3	1.95	0.40
7:LH:23:ILE:HD13	7:LH:23:ILE:H	1.85	0.40
7:LH:54:ALA:HB2	7:LG:9:ILE:HD12	2.04	0.40
9:SQ:65:PHE:CD1	9:SQ:65:PHE:C	2.98	0.40
9:SV:545:THR:HB	9:SV:546:PRO:HD2	2.03	0.40
9:SX:545:THR:HB	9:SX:546:PRO:HD2	2.03	0.40
9:SY:120:TYR:CE1	9:SY:166:SER:HB3	2.56	0.40
9:Sl:219:MET:HE2	9:Sl:219:MET:HA	2.03	0.40
10:Tf:7:THR:HA	10:Tf:10:PHE:CE1	2.57	0.40
10:Ti:3:LEU:O	10:Ti:6:ILE:HG22	2.21	0.40
10:Tj:27:TYR:CE1	10:Tj:109:LYS:HE3	2.57	0.40
1:Li:262:ARG:HE	1:Li:277:GLU:CD	2.29	0.40
1:La:589:ILE:HD12	1:La:589:ILE:C	2.46	0.40
4:AX:329:GLU:CD	4:AX:332:ARG:HH22	2.28	0.40
4:AT:521:LEU:O	4:AT:533:PRO:HA	2.21	0.40
4:AO:338:LYS:HE2	4:AO:354:PHE:CE1	2.57	0.40
5:A1:956:ARG:HG2	5:A1:957:ALA:H	1.87	0.40
6:A7:317:ILE:C	6:Aa:20:THR:HG22	2.46	0.40
6:Aa:54:TRP:CZ3	6:Aa:66:PRO:HD2	2.56	0.40
8:FA:547:LEU:HD21	8:FC:575:TYR:CE1	2.56	0.40
9:SB:8:ILE:HG12	11:AB:57:ILE:HD11	2.03	0.40
9:SL:110:TYR:CD1	9:SL:140:ILE:HD11	2.57	0.40
10:Te:9:ALA:O	10:Tf:35:LYS:HE2	2.20	0.40
12:BE:332:ARG:HB2	12:BE:332:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ld:303:ASP:CG	1:Ld:307:ARG:HH22	2.29	0.40
1:Ld:589:ILE:HD12	1:Ld:589:ILE:C	2.46	0.40
2:BL:22:GLN:HB3	9:SB:456:TYR:CE1	2.57	0.40
3:BQ:165:ASP:HB3	3:BQ:166:PRO:HD2	2.03	0.40
3:BS:165:ASP:HB3	3:BS:166:PRO:HD2	2.03	0.40
9:SG:110:TYR:CD1	9:SG:140:ILE:HD11	2.56	0.40
9:SL:126:ASP:CG	9:SL:128:THR:H	2.30	0.40
9:SQ:578:PHE:CD1	9:SQ:578:PHE:C	2.99	0.40
9:Sk:98:ASN:HA	9:Sk:147:THR:HG21	2.04	0.40
10:TP:104:PRO:HA	10:TP:107:TYR:CE2	2.56	0.40
10:Tk:130:THR:HG21	10:Tk:161:TRP:CZ2	2.56	0.40
14:BC:532:GLY:HA3	14:BD:524:ASP:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LS	525/1065 (49%)	518 (99%)	7 (1%)	61	72
1	LT	525/1065 (49%)	518 (99%)	7 (1%)	61	72
1	LU	525/1065 (49%)	511 (97%)	14 (3%)	39	60
1	LV	525/1065 (49%)	516 (98%)	9 (2%)	53	68
1	LW	525/1065 (49%)	519 (99%)	6 (1%)	65	74
1	LX	525/1065 (49%)	512 (98%)	13 (2%)	42	62
1	LY	525/1065 (49%)	517 (98%)	8 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	LZ	525/1065 (49%)	518 (99%)	7 (1%)	61	72
1	La	525/1065 (49%)	513 (98%)	12 (2%)	44	64
1	Lb	525/1065 (49%)	518 (99%)	7 (1%)	61	72
1	Lc	525/1065 (49%)	518 (99%)	7 (1%)	61	72
1	Ld	525/1065 (49%)	513 (98%)	12 (2%)	44	64
1	Le	525/1065 (49%)	517 (98%)	8 (2%)	57	70
1	Lf	525/1065 (49%)	516 (98%)	9 (2%)	53	68
1	Lg	525/1065 (49%)	511 (97%)	14 (3%)	39	60
1	Lh	525/1065 (49%)	516 (98%)	9 (2%)	53	68
1	Li	525/1065 (49%)	517 (98%)	8 (2%)	57	70
1	Lj	525/1065 (49%)	511 (97%)	14 (3%)	39	60
2	BK	294/297 (99%)	291 (99%)	3 (1%)	68	76
2	BL	239/297 (80%)	237 (99%)	2 (1%)	73	77
2	BM	294/297 (99%)	287 (98%)	7 (2%)	43	63
2	BN	239/297 (80%)	233 (98%)	6 (2%)	42	62
2	BO	294/297 (99%)	288 (98%)	6 (2%)	48	66
2	BP	239/297 (80%)	235 (98%)	4 (2%)	53	68
3	BQ	243/256 (95%)	239 (98%)	4 (2%)	55	69
3	BR	243/256 (95%)	236 (97%)	7 (3%)	37	58
3	BS	243/256 (95%)	239 (98%)	4 (2%)	55	69
3	BT	243/256 (95%)	237 (98%)	6 (2%)	42	62
3	BU	243/256 (95%)	238 (98%)	5 (2%)	47	65
3	BV	243/256 (95%)	239 (98%)	4 (2%)	55	69
4	AM	570/571 (100%)	560 (98%)	10 (2%)	51	67
4	AN	570/571 (100%)	556 (98%)	14 (2%)	42	62
4	AO	570/571 (100%)	560 (98%)	10 (2%)	51	67
4	AP	570/571 (100%)	559 (98%)	11 (2%)	50	67
4	AQ	570/571 (100%)	558 (98%)	12 (2%)	47	65
4	AR	570/571 (100%)	556 (98%)	14 (2%)	42	62
4	AS	565/571 (99%)	558 (99%)	7 (1%)	63	73
4	AT	563/571 (99%)	554 (98%)	9 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AU	565/571 (99%)	555 (98%)	10 (2%)	51	67
4	AV	563/571 (99%)	553 (98%)	10 (2%)	51	67
4	AW	565/571 (99%)	555 (98%)	10 (2%)	51	67
4	AX	563/571 (99%)	555 (99%)	8 (1%)	59	71
5	A0	923/924 (100%)	909 (98%)	14 (2%)	57	70
5	A1	923/924 (100%)	911 (99%)	12 (1%)	61	72
5	A2	923/924 (100%)	908 (98%)	15 (2%)	55	69
5	A3	923/924 (100%)	908 (98%)	15 (2%)	55	69
5	AY	923/924 (100%)	912 (99%)	11 (1%)	63	73
5	AZ	923/924 (100%)	910 (99%)	13 (1%)	59	71
6	A4	293/299 (98%)	288 (98%)	5 (2%)	53	68
6	A5	293/299 (98%)	289 (99%)	4 (1%)	59	71
6	A6	293/299 (98%)	288 (98%)	5 (2%)	53	68
6	A7	293/299 (98%)	290 (99%)	3 (1%)	68	76
6	A8	293/299 (98%)	287 (98%)	6 (2%)	48	66
6	A9	293/299 (98%)	290 (99%)	3 (1%)	68	76
6	Aa	288/299 (96%)	284 (99%)	4 (1%)	59	71
6	Ab	288/299 (96%)	285 (99%)	3 (1%)	68	76
6	Ac	288/299 (96%)	284 (99%)	4 (1%)	59	71
6	Ad	288/299 (96%)	285 (99%)	3 (1%)	68	76
6	Ae	288/299 (96%)	284 (99%)	4 (1%)	59	71
6	Af	288/299 (96%)	286 (99%)	2 (1%)	76	79
7	LA	245/245 (100%)	238 (97%)	7 (3%)	37	58
7	LB	245/245 (100%)	240 (98%)	5 (2%)	48	66
7	LC	245/245 (100%)	242 (99%)	3 (1%)	63	73
7	LD	245/245 (100%)	240 (98%)	5 (2%)	48	66
7	LE	245/245 (100%)	240 (98%)	5 (2%)	48	66
7	LF	245/245 (100%)	241 (98%)	4 (2%)	55	69
7	LG	245/245 (100%)	241 (98%)	4 (2%)	55	69
7	LH	245/245 (100%)	240 (98%)	5 (2%)	48	66
7	LI	245/245 (100%)	241 (98%)	4 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	LJ	245/245 (100%)	240 (98%)	5 (2%)	48	66
7	LK	245/245 (100%)	241 (98%)	4 (2%)	55	69
7	LL	245/245 (100%)	241 (98%)	4 (2%)	55	69
7	LM	245/245 (100%)	239 (98%)	6 (2%)	43	63
7	LN	245/245 (100%)	240 (98%)	5 (2%)	48	66
7	LO	245/245 (100%)	241 (98%)	4 (2%)	55	69
7	LP	245/245 (100%)	241 (98%)	4 (2%)	55	69
7	LQ	245/245 (100%)	240 (98%)	5 (2%)	48	66
7	LR	245/245 (100%)	241 (98%)	4 (2%)	55	69
8	FA	57/509 (11%)	54 (95%)	3 (5%)	20	45
8	FB	57/509 (11%)	57 (100%)	0	100	100
8	FC	57/509 (11%)	55 (96%)	2 (4%)	32	54
8	FJ	57/509 (11%)	54 (95%)	3 (5%)	20	45
8	FK	57/509 (11%)	57 (100%)	0	100	100
8	FL	57/509 (11%)	55 (96%)	2 (4%)	32	54
8	FS	57/509 (11%)	54 (95%)	3 (5%)	20	45
8	FT	57/509 (11%)	57 (100%)	0	100	100
8	FU	57/509 (11%)	55 (96%)	2 (4%)	32	54
8	Fb	57/509 (11%)	53 (93%)	4 (7%)	14	39
8	Fc	57/509 (11%)	57 (100%)	0	100	100
8	Fd	57/509 (11%)	55 (96%)	2 (4%)	32	54
8	Fk	57/509 (11%)	53 (93%)	4 (7%)	14	39
8	Fl	57/509 (11%)	57 (100%)	0	100	100
8	Fm	57/509 (11%)	54 (95%)	3 (5%)	20	45
8	Ft	57/509 (11%)	53 (93%)	4 (7%)	14	39
8	Fu	57/509 (11%)	57 (100%)	0	100	100
8	Fv	57/509 (11%)	55 (96%)	2 (4%)	32	54
9	SA	534/540 (99%)	529 (99%)	5 (1%)	70	76
9	SB	534/540 (99%)	530 (99%)	4 (1%)	76	79
9	SC	534/540 (99%)	529 (99%)	5 (1%)	70	76
9	SD	534/540 (99%)	529 (99%)	5 (1%)	70	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	SE	534/540 (99%)	531 (99%)	3 (1%)	78	81
9	SF	534/540 (99%)	528 (99%)	6 (1%)	65	74
9	SG	539/540 (100%)	529 (98%)	10 (2%)	50	67
9	SH	539/540 (100%)	529 (98%)	10 (2%)	50	67
9	SI	539/540 (100%)	529 (98%)	10 (2%)	50	67
9	SJ	539/540 (100%)	528 (98%)	11 (2%)	48	66
9	SK	539/540 (100%)	528 (98%)	11 (2%)	48	66
9	SL	539/540 (100%)	529 (98%)	10 (2%)	50	67
9	SM	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	SN	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	SO	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	SP	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	SQ	539/540 (100%)	533 (99%)	6 (1%)	65	74
9	SR	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	SS	539/540 (100%)	533 (99%)	6 (1%)	65	74
9	ST	539/540 (100%)	531 (98%)	8 (2%)	57	70
9	SU	539/540 (100%)	533 (99%)	6 (1%)	65	74
9	SV	539/540 (100%)	533 (99%)	6 (1%)	65	74
9	SW	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	SX	539/540 (100%)	534 (99%)	5 (1%)	70	76
9	SY	539/540 (100%)	531 (98%)	8 (2%)	57	70
9	SZ	539/540 (100%)	530 (98%)	9 (2%)	53	68
9	Sa	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	Sb	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	Sc	539/540 (100%)	531 (98%)	8 (2%)	57	70
9	Sd	539/540 (100%)	535 (99%)	4 (1%)	76	79
9	Se	539/540 (100%)	530 (98%)	9 (2%)	53	68
9	Sf	539/540 (100%)	533 (99%)	6 (1%)	65	74
9	Sg	539/540 (100%)	533 (99%)	6 (1%)	65	74
9	Sh	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	Si	539/540 (100%)	532 (99%)	7 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Sj	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	Sk	539/540 (100%)	534 (99%)	5 (1%)	70	76
9	Sl	539/540 (100%)	534 (99%)	5 (1%)	70	76
9	Sm	539/540 (100%)	532 (99%)	7 (1%)	61	72
9	Sn	539/540 (100%)	535 (99%)	4 (1%)	76	79
9	So	539/540 (100%)	534 (99%)	5 (1%)	70	76
9	Sp	539/540 (100%)	531 (98%)	8 (2%)	57	70
10	TM	138/139 (99%)	137 (99%)	1 (1%)	76	79
10	TN	138/139 (99%)	137 (99%)	1 (1%)	76	79
10	TO	138/139 (99%)	137 (99%)	1 (1%)	76	79
10	TP	138/139 (99%)	138 (100%)	0	100	100
10	TQ	138/139 (99%)	136 (99%)	2 (1%)	59	71
10	TR	138/139 (99%)	138 (100%)	0	100	100
10	TS	138/139 (99%)	138 (100%)	0	100	100
10	TT	138/139 (99%)	138 (100%)	0	100	100
10	TU	138/139 (99%)	137 (99%)	1 (1%)	76	79
10	TV	138/139 (99%)	138 (100%)	0	100	100
10	TW	138/139 (99%)	138 (100%)	0	100	100
10	TX	138/139 (99%)	137 (99%)	1 (1%)	76	79
10	TY	138/139 (99%)	136 (99%)	2 (1%)	59	71
10	TZ	138/139 (99%)	137 (99%)	1 (1%)	76	79
10	Ta	138/139 (99%)	136 (99%)	2 (1%)	59	71
10	Tb	138/139 (99%)	135 (98%)	3 (2%)	45	64
10	Tc	138/139 (99%)	136 (99%)	2 (1%)	59	71
10	Td	138/139 (99%)	136 (99%)	2 (1%)	59	71
10	Te	138/139 (99%)	138 (100%)	0	100	100
10	Tf	138/139 (99%)	138 (100%)	0	100	100
10	Tg	138/139 (99%)	138 (100%)	0	100	100
10	Th	138/139 (99%)	138 (100%)	0	100	100
10	Ti	138/139 (99%)	138 (100%)	0	100	100
10	Tj	138/139 (99%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	Tk	138/139 (99%)	137 (99%)	1 (1%)	76	79
10	Tl	138/139 (99%)	135 (98%)	3 (2%)	45	64
10	Tm	138/139 (99%)	136 (99%)	2 (1%)	59	71
10	Tn	138/139 (99%)	136 (99%)	2 (1%)	59	71
10	To	138/139 (99%)	135 (98%)	3 (2%)	45	64
10	Tp	138/139 (99%)	136 (99%)	2 (1%)	59	71
10	Tq	138/139 (99%)	138 (100%)	0	100	100
10	Tr	138/139 (99%)	138 (100%)	0	100	100
10	Ts	138/139 (99%)	138 (100%)	0	100	100
10	Tt	138/139 (99%)	138 (100%)	0	100	100
10	Tu	138/139 (99%)	138 (100%)	0	100	100
10	Tv	138/139 (99%)	138 (100%)	0	100	100
11	AA	122/126 (97%)	119 (98%)	3 (2%)	42	62
11	AB	122/126 (97%)	122 (100%)	0	100	100
11	AC	122/126 (97%)	118 (97%)	4 (3%)	33	56
11	AD	122/126 (97%)	120 (98%)	2 (2%)	55	69
11	AE	122/126 (97%)	121 (99%)	1 (1%)	73	77
11	AF	122/126 (97%)	119 (98%)	3 (2%)	42	62
12	BE	333/334 (100%)	325 (98%)	8 (2%)	43	63
12	BF	333/334 (100%)	325 (98%)	8 (2%)	43	63
12	BG	333/334 (100%)	323 (97%)	10 (3%)	36	57
13	AG	184/184 (100%)	180 (98%)	4 (2%)	45	64
13	AH	184/184 (100%)	180 (98%)	4 (2%)	45	64
13	AI	184/184 (100%)	182 (99%)	2 (1%)	65	74
13	AJ	184/184 (100%)	182 (99%)	2 (1%)	65	74
13	AK	184/184 (100%)	181 (98%)	3 (2%)	55	69
13	AL	184/184 (100%)	181 (98%)	3 (2%)	55	69
14	BB	474/484 (98%)	459 (97%)	15 (3%)	34	56
14	BC	474/484 (98%)	464 (98%)	10 (2%)	47	65
14	BD	474/484 (98%)	462 (98%)	12 (2%)	42	62
All	All	65604/84042 (78%)	64593 (98%)	1011 (2%)	55	70

All (1011) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Le	73	ASN
1	Le	89	THR
1	Le	119	ASN
1	Le	232	PHE
1	Le	363	VAL
1	Le	409	VAL
1	Le	579	THR
1	Le	600	THR
1	Lf	32	VAL
1	Lf	67	ARG
1	Lf	244	ILE
1	Lf	290	TYR
1	Lf	299	ILE
1	Lf	340	LEU
1	Lf	400	ILE
1	Lf	416	TYR
1	Lf	474	THR
1	Lg	32	VAL
1	Lg	68	ARG
1	Lg	130	LEU
1	Lg	179	TYR
1	Lg	194	SER
1	Lg	355	ASN
1	Lg	401	THR
1	Lg	406	THR
1	Lg	413	GLU
1	Lg	476	GLU
1	Lg	487	GLN
1	Lg	521	ARG
1	Lg	607	TYR
1	Lg	616	ILE
1	Lh	73	ASN
1	Lh	89	THR
1	Lh	119	ASN
1	Lh	232	PHE
1	Lh	287	PHE
1	Lh	296	ILE
1	Lh	363	VAL
1	Lh	409	VAL
1	Lh	600	THR
1	Li	32	VAL
1	Li	67	ARG

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Mol	Chain	Res	Type
1	Li	244	ILE
1	Li	290	TYR
1	Li	299	ILE
1	Li	400	ILE
1	Li	416	TYR
1	Li	474	THR
1	Lj	32	VAL
1	Lj	68	ARG
1	Lj	130	LEU
1	Lj	179	TYR
1	Lj	194	SER
1	Lj	355	ASN
1	Lj	401	THR
1	Lj	406	THR
1	Lj	413	GLU
1	Lj	419	GLU
1	Lj	476	GLU
1	Lj	487	GLN
1	Lj	521	ARG
1	Lj	607	TYR
1	LS	73	ASN
1	LS	89	THR
1	LS	119	ASN
1	LS	232	PHE
1	LS	363	VAL
1	LS	409	VAL
1	LS	600	THR
1	LT	32	VAL
1	LT	67	ARG
1	LT	290	TYR
1	LT	299	ILE
1	LT	400	ILE
1	LT	416	TYR
1	LT	474	THR
1	LU	32	VAL
1	LU	68	ARG
1	LU	130	LEU
1	LU	179	TYR
1	LU	194	SER
1	LU	355	ASN
1	LU	372	THR
1	LU	401	THR

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Mol	Chain	Res	Type
1	LU	406	THR
1	LU	413	GLU
1	LU	476	GLU
1	LU	487	GLN
1	LU	607	TYR
1	LU	616	ILE
1	LV	73	ASN
1	LV	89	THR
1	LV	119	ASN
1	LV	232	PHE
1	LV	296	ILE
1	LV	363	VAL
1	LV	409	VAL
1	LV	580	ASN
1	LV	600	THR
1	LW	67	ARG
1	LW	290	TYR
1	LW	299	ILE
1	LW	400	ILE
1	LW	416	TYR
1	LW	474	THR
1	LX	32	VAL
1	LX	68	ARG
1	LX	130	LEU
1	LX	179	TYR
1	LX	194	SER
1	LX	355	ASN
1	LX	401	THR
1	LX	406	THR
1	LX	413	GLU
1	LX	476	GLU
1	LX	487	GLN
1	LX	607	TYR
1	LX	616	ILE
1	LY	73	ASN
1	LY	89	THR
1	LY	119	ASN
1	LY	232	PHE
1	LY	363	VAL
1	LY	409	VAL
1	LY	580	ASN
1	LY	600	THR

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Mol	Chain	Res	Type
1	LZ	32	VAL
1	LZ	67	ARG
1	LZ	244	ILE
1	LZ	299	ILE
1	LZ	400	ILE
1	LZ	416	TYR
1	LZ	474	THR
1	La	32	VAL
1	La	68	ARG
1	La	179	TYR
1	La	194	SER
1	La	349	THR
1	La	355	ASN
1	La	401	THR
1	La	406	THR
1	La	413	GLU
1	La	476	GLU
1	La	487	GLN
1	La	607	TYR
1	Lb	73	ASN
1	Lb	89	THR
1	Lb	119	ASN
1	Lb	232	PHE
1	Lb	363	VAL
1	Lb	409	VAL
1	Lb	600	THR
1	Lc	5	LEU
1	Lc	67	ARG
1	Lc	244	ILE
1	Lc	290	TYR
1	Lc	299	ILE
1	Lc	400	ILE
1	Lc	416	TYR
1	Ld	32	VAL
1	Ld	68	ARG
1	Ld	130	LEU
1	Ld	179	TYR
1	Ld	194	SER
1	Ld	355	ASN
1	Ld	401	THR
1	Ld	406	THR
1	Ld	413	GLU

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Mol	Chain	Res	Type
1	Ld	476	GLU
1	Ld	487	GLN
1	Ld	607	TYR
2	BM	28	THR
2	BM	46	ASN
2	BM	54	VAL
2	BM	139	ARG
2	BM	164	THR
2	BM	308	LYS
2	BM	346	ILE
2	BK	28	THR
2	BK	163	LEU
2	BK	346	ILE
2	BO	28	THR
2	BO	46	ASN
2	BO	139	ARG
2	BO	163	LEU
2	BO	308	LYS
2	BO	346	ILE
2	BP	18	THR
2	BP	182	MET
2	BP	203	ASP
2	BP	244	LEU
2	BL	198	THR
2	BL	203	ASP
2	BN	18	THR
2	BN	73	THR
2	BN	74	THR
2	BN	203	ASP
2	BN	244	LEU
2	BN	266	LEU
3	BQ	48	ASN
3	BQ	55	TRP
3	BQ	144	ASN
3	BQ	151	THR
3	BV	44	GLU
3	BV	54	ASN
3	BV	55	TRP
3	BV	151	THR
3	BS	44	GLU
3	BS	54	ASN
3	BS	55	TRP

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Mol	Chain	Res	Type
3	BS	151	THR
3	BR	44	GLU
3	BR	54	ASN
3	BR	55	TRP
3	BR	93	THR
3	BR	144	ASN
3	BR	151	THR
3	BR	289	ARG
3	BT	46	TYR
3	BT	54	ASN
3	BT	55	TRP
3	BT	75	THR
3	BT	93	THR
3	BT	151	THR
3	BU	34	THR
3	BU	44	GLU
3	BU	55	TRP
3	BU	144	ASN
3	BU	151	THR
4	AX	81	ILE
4	AX	168	LEU
4	AX	217	ASP
4	AX	367	GLN
4	AX	400	ASP
4	AX	509	ASN
4	AX	516	LEU
4	AX	520	ASP
4	AW	12	THR
4	AW	156	ARG
4	AW	168	LEU
4	AW	217	ASP
4	AW	258	LEU
4	AW	407	LEU
4	AW	423	ARG
4	AW	460	MET
4	AW	490	MET
4	AW	520	ASP
4	AT	81	ILE
4	AT	165	ASN
4	AT	168	LEU
4	AT	217	ASP
4	AT	367	GLN

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Mol	Chain	Res	Type
4	AT	400	ASP
4	AT	509	ASN
4	AT	516	LEU
4	AT	520	ASP
4	AS	12	THR
4	AS	156	ARG
4	AS	168	LEU
4	AS	217	ASP
4	AS	258	LEU
4	AS	460	MET
4	AS	520	ASP
4	AV	81	ILE
4	AV	165	ASN
4	AV	168	LEU
4	AV	217	ASP
4	AV	291	ASP
4	AV	336	GLN
4	AV	367	GLN
4	AV	509	ASN
4	AV	516	LEU
4	AV	520	ASP
4	AU	12	THR
4	AU	117	HIS
4	AU	156	ARG
4	AU	168	LEU
4	AU	217	ASP
4	AU	258	LEU
4	AU	423	ARG
4	AU	460	MET
4	AU	520	ASP
4	AU	623	THR
4	AR	8	ASN
4	AR	9	TYR
4	AR	42	LYS
4	AR	45	GLN
4	AR	46	ASP
4	AR	67	TYR
4	AR	121	GLU
4	AR	203	VAL
4	AR	237	ASP
4	AR	250	GLU
4	AR	367	GLN

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Mol	Chain	Res	Type
4	AR	452	ARG
4	AR	465	PHE
4	AR	617	GLU
4	AQ	9	TYR
4	AQ	46	ASP
4	AQ	67	TYR
4	AQ	189	LYS
4	AQ	203	VAL
4	AQ	258	LEU
4	AQ	262	PHE
4	AQ	270	LYS
4	AQ	424	HIS
4	AQ	452	ARG
4	AQ	465	PHE
4	AQ	526	THR
4	AN	8	ASN
4	AN	9	TYR
4	AN	42	LYS
4	AN	45	GLN
4	AN	46	ASP
4	AN	67	TYR
4	AN	121	GLU
4	AN	203	VAL
4	AN	237	ASP
4	AN	250	GLU
4	AN	367	GLN
4	AN	452	ARG
4	AN	465	PHE
4	AN	580	GLU
4	AM	9	TYR
4	AM	46	ASP
4	AM	67	TYR
4	AM	189	LYS
4	AM	203	VAL
4	AM	258	LEU
4	AM	270	LYS
4	AM	452	ARG
4	AM	465	PHE
4	AM	526	THR
4	AP	8	ASN
4	AP	9	TYR
4	AP	42	LYS

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Mol	Chain	Res	Type
4	AP	45	GLN
4	AP	46	ASP
4	AP	67	TYR
4	AP	203	VAL
4	AP	250	GLU
4	AP	367	GLN
4	AP	452	ARG
4	AP	465	PHE
4	AO	9	TYR
4	AO	67	TYR
4	AO	189	LYS
4	AO	203	VAL
4	AO	237	ASP
4	AO	258	LEU
4	AO	270	LYS
4	AO	452	ARG
4	AO	526	THR
4	AO	563	THR
5	AY	174	HIS
5	AY	207	HIS
5	AY	224	LEU
5	AY	255	TYR
5	AY	257	ARG
5	AY	580	LEU
5	AY	623	PHE
5	AY	843	ARG
5	AY	888	PHE
5	AY	933	VAL
5	AY	942	ILE
5	AZ	170	GLU
5	AZ	207	HIS
5	AZ	224	LEU
5	AZ	255	TYR
5	AZ	257	ARG
5	AZ	336	ILE
5	AZ	367	LYS
5	AZ	580	LEU
5	AZ	843	ARG
5	AZ	888	PHE
5	AZ	942	ILE
5	AZ	1027	GLN
5	AZ	1031	ASP

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Mol	Chain	Res	Type
5	A0	170	GLU
5	A0	174	HIS
5	A0	207	HIS
5	A0	224	LEU
5	A0	255	TYR
5	A0	257	ARG
5	A0	336	ILE
5	A0	367	LYS
5	A0	632	ASP
5	A0	763	SER
5	A0	843	ARG
5	A0	888	PHE
5	A0	942	ILE
5	A0	1027	GLN
5	A1	170	GLU
5	A1	207	HIS
5	A1	255	TYR
5	A1	257	ARG
5	A1	336	ILE
5	A1	763	SER
5	A1	843	ARG
5	A1	854	TYR
5	A1	888	PHE
5	A1	933	VAL
5	A1	942	ILE
5	A1	1027	GLN
5	A2	170	GLU
5	A2	207	HIS
5	A2	224	LEU
5	A2	255	TYR
5	A2	257	ARG
5	A2	336	ILE
5	A2	580	LEU
5	A2	623	PHE
5	A2	763	SER
5	A2	843	ARG
5	A2	888	PHE
5	A2	933	VAL
5	A2	942	ILE
5	A2	1027	GLN
5	A2	1028	VAL
5	A3	170	GLU

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Mol	Chain	Res	Type
5	A3	207	HIS
5	A3	224	LEU
5	A3	255	TYR
5	A3	257	ARG
5	A3	336	ILE
5	A3	367	LYS
5	A3	623	PHE
5	A3	763	SER
5	A3	843	ARG
5	A3	854	TYR
5	A3	888	PHE
5	A3	933	VAL
5	A3	942	ILE
5	A3	1027	GLN
6	A4	83	MET
6	A4	89	GLU
6	A4	213	GLU
6	A4	325	ILE
6	A4	333	GLU
6	A9	10	THR
6	A9	155	THR
6	A9	333	GLU
6	A6	83	MET
6	A6	213	GLU
6	A6	241	ASN
6	A6	325	ILE
6	A6	333	GLU
6	A5	10	THR
6	A5	106	ARG
6	A5	155	THR
6	A5	333	GLU
6	A8	83	MET
6	A8	91	SER
6	A8	213	GLU
6	A8	241	ASN
6	A8	325	ILE
6	A8	333	GLU
6	A7	10	THR
6	A7	155	THR
6	A7	333	GLU
6	Ad	73	ASP
6	Ad	171	THR

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Mol	Chain	Res	Type
6	Ad	238	TRP
6	Ac	20	THR
6	Ac	71	ASN
6	Ac	73	ASP
6	Ac	171	THR
6	Af	73	ASP
6	Af	195	TRP
6	Ae	71	ASN
6	Ae	73	ASP
6	Ae	171	THR
6	Ae	238	TRP
6	Ab	73	ASP
6	Ab	171	THR
6	Ab	238	TRP
6	Aa	71	ASN
6	Aa	73	ASP
6	Aa	171	THR
6	Aa	238	TRP
7	LN	14	GLU
7	LN	23	ILE
7	LN	154	TRP
7	LN	231	ILE
7	LN	234	THR
7	LO	122	ILE
7	LO	125	THR
7	LO	168	TYR
7	LO	261	GLU
7	LM	26	ASP
7	LM	151	ILE
7	LM	169	SER
7	LM	188	THR
7	LM	231	ILE
7	LM	246	ASP
7	LQ	14	GLU
7	LQ	23	ILE
7	LQ	154	TRP
7	LQ	231	ILE
7	LQ	234	THR
7	LR	122	ILE
7	LR	125	THR
7	LR	168	TYR
7	LR	261	GLU

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Mol	Chain	Res	Type
7	LP	26	ASP
7	LP	203	SER
7	LP	231	ILE
7	LP	246	ASP
7	LB	14	GLU
7	LB	23	ILE
7	LB	154	TRP
7	LB	231	ILE
7	LB	234	THR
7	LC	122	ILE
7	LC	125	THR
7	LC	261	GLU
7	LA	26	ASP
7	LA	151	ILE
7	LA	187	LEU
7	LA	198	TYR
7	LA	203	SER
7	LA	231	ILE
7	LA	246	ASP
7	LE	14	GLU
7	LE	23	ILE
7	LE	154	TRP
7	LE	231	ILE
7	LE	234	THR
7	LF	122	ILE
7	LF	125	THR
7	LF	168	TYR
7	LF	261	GLU
7	LD	26	ASP
7	LD	151	ILE
7	LD	203	SER
7	LD	231	ILE
7	LD	246	ASP
7	LH	14	GLU
7	LH	23	ILE
7	LH	154	TRP
7	LH	231	ILE
7	LH	234	THR
7	LI	122	ILE
7	LI	125	THR
7	LI	168	TYR
7	LI	261	GLU

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Mol	Chain	Res	Type
7	LG	26	ASP
7	LG	151	ILE
7	LG	231	ILE
7	LG	246	ASP
7	LK	23	ILE
7	LK	154	TRP
7	LK	231	ILE
7	LK	234	THR
7	LL	122	ILE
7	LL	125	THR
7	LL	168	TYR
7	LL	261	GLU
7	LJ	26	ASP
7	LJ	169	SER
7	LJ	198	TYR
7	LJ	231	ILE
7	LJ	246	ASP
8	FA	558	ILE
8	FA	564	ASP
8	FA	586	VAL
8	FC	531	THR
8	FC	545	LYS
8	FJ	558	ILE
8	FJ	564	ASP
8	FJ	586	VAL
8	FL	531	THR
8	FL	545	LYS
8	FS	558	ILE
8	FS	564	ASP
8	FS	586	VAL
8	FU	531	THR
8	FU	545	LYS
8	Fb	546	VAL
8	Fb	558	ILE
8	Fb	564	ASP
8	Fb	586	VAL
8	Fd	531	THR
8	Fd	545	LYS
8	Fk	558	ILE
8	Fk	564	ASP
8	Fk	586	VAL
8	Fk	589	ASN

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Mol	Chain	Res	Type
8	Fm	531	THR
8	Fm	545	LYS
8	Fm	584	ASN
8	Ft	546	VAL
8	Ft	558	ILE
8	Ft	564	ASP
8	Ft	586	VAL
8	Fv	531	THR
8	Fv	545	LYS
9	SA	219	MET
9	SA	299	ASP
9	SA	366	LEU
9	SA	452	TYR
9	SA	573	GLU
9	SB	219	MET
9	SB	366	LEU
9	SB	454	TYR
9	SB	523	VAL
9	SC	219	MET
9	SC	299	ASP
9	SC	366	LEU
9	SC	452	TYR
9	SC	454	TYR
9	SD	299	ASP
9	SD	302	ILE
9	SD	366	LEU
9	SD	452	TYR
9	SD	454	TYR
9	SE	219	MET
9	SE	366	LEU
9	SE	586	GLU
9	SF	219	MET
9	SF	302	ILE
9	SF	366	LEU
9	SF	452	TYR
9	SF	454	TYR
9	SF	586	GLU
9	SK	20	VAL
9	SK	73	GLN
9	SK	170	THR
9	SK	209	GLU
9	SK	311	ASP

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Mol	Chain	Res	Type
9	SK	428	ARG
9	SK	499	ASN
9	SK	585	MET
9	SK	586	GLU
9	SK	629	LYS
9	SK	654	ILE
9	SG	20	VAL
9	SG	73	GLN
9	SG	170	THR
9	SG	209	GLU
9	SG	311	ASP
9	SG	428	ARG
9	SG	499	ASN
9	SG	585	MET
9	SG	586	GLU
9	SG	654	ILE
9	SL	20	VAL
9	SL	170	THR
9	SL	209	GLU
9	SL	311	ASP
9	SL	428	ARG
9	SL	499	ASN
9	SL	585	MET
9	SL	586	GLU
9	SL	629	LYS
9	SL	654	ILE
9	SH	19	VAL
9	SH	20	VAL
9	SH	170	THR
9	SH	209	GLU
9	SH	311	ASP
9	SH	428	ARG
9	SH	499	ASN
9	SH	585	MET
9	SH	586	GLU
9	SH	629	LYS
9	SI	20	VAL
9	SI	73	GLN
9	SI	170	THR
9	SI	311	ASP
9	SI	428	ARG
9	SI	499	ASN

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Mol	Chain	Res	Type
9	SI	585	MET
9	SI	586	GLU
9	SI	629	LYS
9	SI	654	ILE
9	SJ	20	VAL
9	SJ	170	THR
9	SJ	209	GLU
9	SJ	311	ASP
9	SJ	428	ARG
9	SJ	452	TYR
9	SJ	499	ASN
9	SJ	585	MET
9	SJ	586	GLU
9	SJ	629	LYS
9	SJ	654	ILE
9	SQ	108	SER
9	SQ	122	ASP
9	SQ	207	LYS
9	SQ	211	GLN
9	SQ	452	TYR
9	SQ	548	ASP
9	SP	108	SER
9	SP	122	ASP
9	SP	207	LYS
9	SP	211	GLN
9	SP	452	TYR
9	SP	548	ASP
9	SP	589	GLN
9	SM	16	GLN
9	SM	108	SER
9	SM	122	ASP
9	SM	207	LYS
9	SM	211	GLN
9	SM	548	ASP
9	SM	629	LYS
9	SN	108	SER
9	SN	122	ASP
9	SN	207	LYS
9	SN	211	GLN
9	SN	300	LYS
9	SN	452	TYR
9	SN	548	ASP

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Mol	Chain	Res	Type
9	SO	108	SER
9	SO	122	ASP
9	SO	207	LYS
9	SO	211	GLN
9	SO	452	TYR
9	SO	533	ILE
9	SO	548	ASP
9	SR	108	SER
9	SR	122	ASP
9	SR	207	LYS
9	SR	211	GLN
9	SR	452	TYR
9	SR	548	ASP
9	SR	589	GLN
9	SW	174	GLN
9	SW	207	LYS
9	SW	211	GLN
9	SW	300	LYS
9	SW	346	GLU
9	SW	478	ARG
9	SW	511	HIS
9	SS	174	GLN
9	SS	207	LYS
9	SS	211	GLN
9	SS	300	LYS
9	SS	346	GLU
9	SS	439	MET
9	ST	16	GLN
9	ST	174	GLN
9	ST	207	LYS
9	ST	211	GLN
9	ST	300	LYS
9	ST	346	GLU
9	ST	439	MET
9	ST	511	HIS
9	SU	207	LYS
9	SU	211	GLN
9	SU	300	LYS
9	SU	346	GLU
9	SU	439	MET
9	SU	511	HIS
9	SV	160	TYR

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Mol	Chain	Res	Type
9	SV	207	LYS
9	SV	211	GLN
9	SV	300	LYS
9	SV	346	GLU
9	SV	439	MET
9	SX	207	LYS
9	SX	211	GLN
9	SX	300	LYS
9	SX	346	GLU
9	SX	439	MET
9	SY	16	GLN
9	SY	53	MET
9	SY	149	LYS
9	SY	207	LYS
9	SY	346	GLU
9	SY	439	MET
9	SY	478	ARG
9	SY	511	HIS
9	SZ	53	MET
9	SZ	149	LYS
9	SZ	207	LYS
9	SZ	346	GLU
9	SZ	439	MET
9	SZ	457	ASP
9	SZ	511	HIS
9	SZ	589	GLN
9	SZ	604	ARG
9	Sa	53	MET
9	Sa	149	LYS
9	Sa	207	LYS
9	Sa	346	GLU
9	Sa	439	MET
9	Sa	511	HIS
9	Sa	589	GLN
9	Sb	149	LYS
9	Sb	207	LYS
9	Sb	346	GLU
9	Sb	439	MET
9	Sb	511	HIS
9	Sb	589	GLN
9	Sb	604	ARG
9	Sc	149	LYS

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Mol	Chain	Res	Type
9	Sc	207	LYS
9	Sc	346	GLU
9	Sc	439	MET
9	Sc	478	ARG
9	Sc	511	HIS
9	Sc	561	ASN
9	Sc	589	GLN
9	Sd	207	LYS
9	Sd	346	GLU
9	Sd	439	MET
9	Sd	511	HIS
9	Se	16	GLN
9	Se	207	LYS
9	Se	346	GLU
9	Se	439	MET
9	Se	457	ASP
9	Se	508	ARG
9	Se	511	HIS
9	Se	548	ASP
9	Se	604	ARG
9	Sf	16	GLN
9	Sf	207	LYS
9	Sf	346	GLU
9	Sf	439	MET
9	Sf	457	ASP
9	Sf	511	HIS
9	Sg	16	GLN
9	Sg	207	LYS
9	Sg	346	GLU
9	Sg	439	MET
9	Sg	508	ARG
9	Sg	511	HIS
9	Sh	16	GLN
9	Sh	207	LYS
9	Sh	346	GLU
9	Sh	439	MET
9	Sh	457	ASP
9	Sh	511	HIS
9	Sh	548	ASP
9	Si	16	GLN
9	Si	207	LYS
9	Si	346	GLU

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Mol	Chain	Res	Type
9	Si	439	MET
9	Si	457	ASP
9	Si	511	HIS
9	Si	528	THR
9	Sj	16	GLN
9	Sj	53	MET
9	Sj	207	LYS
9	Sj	346	GLU
9	Sj	439	MET
9	Sj	511	HIS
9	Sj	551	ASN
9	Sk	207	LYS
9	Sk	439	MET
9	Sk	452	TYR
9	Sk	457	ASP
9	Sk	500	CYS
9	Sl	207	LYS
9	Sl	211	GLN
9	Sl	439	MET
9	Sl	452	TYR
9	Sl	511	HIS
9	Sm	105	THR
9	Sm	207	LYS
9	Sm	211	GLN
9	Sm	300	LYS
9	Sm	439	MET
9	Sm	452	TYR
9	Sm	511	HIS
9	Sn	207	LYS
9	Sn	439	MET
9	Sn	452	TYR
9	Sn	511	HIS
9	So	53	MET
9	So	207	LYS
9	So	439	MET
9	So	452	TYR
9	So	511	HIS
9	Sp	53	MET
9	Sp	207	LYS
9	Sp	211	GLN
9	Sp	300	LYS
9	Sp	439	MET

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Mol	Chain	Res	Type
9	Sp	452	TYR
9	Sp	500	CYS
9	Sp	511	HIS
10	TM	150	VAL
10	TN	150	VAL
10	TO	150	VAL
10	TQ	81	VAL
10	TQ	150	VAL
10	TU	159	ILE
10	TX	159	ILE
10	TY	11	GLU
10	TY	159	ILE
10	TZ	159	ILE
10	Ta	4	THR
10	Ta	159	ILE
10	Tb	4	THR
10	Tb	11	GLU
10	Tb	159	ILE
10	Tc	11	GLU
10	Tc	159	ILE
10	Td	4	THR
10	Td	159	ILE
10	Tk	4	THR
10	Tl	4	THR
10	Tl	93	HIS
10	Tl	118	ARG
10	Tm	4	THR
10	Tm	93	HIS
10	Tn	4	THR
10	Tn	93	HIS
10	To	4	THR
10	To	93	HIS
10	To	118	ARG
10	Tp	4	THR
10	Tp	93	HIS
11	AA	19	TRP
11	AA	93	VAL
11	AA	129	ASN
11	AD	17	LEU
11	AD	129	ASN
11	AC	5	ASP
11	AC	37	LEU

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Mol	Chain	Res	Type
11	AC	129	ASN
11	AC	131	ASN
11	AE	129	ASN
11	AF	37	LEU
11	AF	93	VAL
11	AF	129	ASN
12	BE	12	SER
12	BE	64	ASN
12	BE	86	TYR
12	BE	116	LEU
12	BE	148	ILE
12	BE	207	ASN
12	BE	323	ASN
12	BE	378	SER
12	BF	12	SER
12	BF	64	ASN
12	BF	86	TYR
12	BF	111	HIS
12	BF	307	GLN
12	BF	308	THR
12	BF	323	ASN
12	BF	380	TYR
12	BG	61	THR
12	BG	64	ASN
12	BG	83	THR
12	BG	86	TYR
12	BG	111	HIS
12	BG	180	ASN
12	BG	225	LYS
12	BG	307	GLN
12	BG	308	THR
12	BG	323	ASN
13	AL	31	ARG
13	AL	157	TYR
13	AL	205	GLN
13	AI	31	ARG
13	AI	48	THR
13	AG	3	PHE
13	AG	31	ARG
13	AG	48	THR
13	AG	205	GLN
13	AK	3	PHE

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Mol	Chain	Res	Type
13	AK	31	ARG
13	AK	48	THR
13	AH	31	ARG
13	AH	58	GLU
13	AH	157	TYR
13	AH	205	GLN
13	AJ	31	ARG
13	AJ	48	THR
14	BB	34	LEU
14	BB	81	SER
14	BB	162	ASP
14	BB	176	ILE
14	BB	207	MET
14	BB	249	ARG
14	BB	289	LEU
14	BB	391	VAL
14	BB	414	ARG
14	BB	442	MET
14	BB	452	SER
14	BB	481	LEU
14	BB	536	THR
14	BB	567	THR
14	BB	572	ARG
14	BC	1	MET
14	BC	41	GLN
14	BC	81	SER
14	BC	104	ARG
14	BC	162	ASP
14	BC	249	ARG
14	BC	374	ARG
14	BC	389	PRO
14	BC	442	MET
14	BC	481	LEU
14	BD	85	LEU
14	BD	134	GLN
14	BD	162	ASP
14	BD	237	THR
14	BD	244	LEU
14	BD	305	LYS
14	BD	315	VAL
14	BD	323	ARG
14	BD	391	VAL

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Mol	Chain	Res	Type
14	BD	442	MET
14	BD	452	SER
14	BD	536	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (693) such sidechains are listed below:

Mol	Chain	Res	Type
1	Le	44	GLN
1	Le	285	ASN
1	Le	302	ASN
1	Le	487	GLN
1	Le	519	ASN
1	Le	597	ASN
1	Lf	181	GLN
1	Lf	220	ASN
1	Lf	246	ASN
1	Lf	403	ASN
1	Lf	597	ASN
1	Lg	85	GLN
1	Lg	337	ASN
1	Lg	381	GLN
1	Lg	462	ASN
1	Lg	536	ASN
1	Lg	597	ASN
1	Lh	44	GLN
1	Lh	279	GLN
1	Lh	285	ASN
1	Lh	302	ASN
1	Lh	378	ASN
1	Lh	487	GLN
1	Lh	519	ASN
1	Lh	597	ASN
1	Li	157	GLN
1	Li	181	GLN
1	Li	220	ASN
1	Li	242	ASN
1	Li	246	ASN
1	Li	403	ASN
1	Li	597	ASN
1	Lj	381	GLN
1	Lj	462	ASN
1	Lj	536	ASN

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Mol	Chain	Res	Type
1	Lj	597	ASN
1	LS	44	GLN
1	LS	242	ASN
1	LS	279	GLN
1	LS	285	ASN
1	LS	302	ASN
1	LS	487	GLN
1	LS	519	ASN
1	LS	597	ASN
1	LT	157	GLN
1	LT	181	GLN
1	LT	220	ASN
1	LT	242	ASN
1	LT	246	ASN
1	LT	597	ASN
1	LU	381	GLN
1	LU	462	ASN
1	LU	536	ASN
1	LU	597	ASN
1	LV	44	GLN
1	LV	242	ASN
1	LV	285	ASN
1	LV	302	ASN
1	LV	361	GLN
1	LV	487	GLN
1	LV	519	ASN
1	LW	157	GLN
1	LW	181	GLN
1	LW	220	ASN
1	LW	242	ASN
1	LW	246	ASN
1	LW	403	ASN
1	LW	597	ASN
1	LX	381	GLN
1	LX	462	ASN
1	LX	597	ASN
1	LY	302	ASN
1	LY	361	GLN
1	LY	487	GLN
1	LY	519	ASN
1	LY	597	ASN
1	LY	612	ASN

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Mol	Chain	Res	Type
1	LZ	181	GLN
1	LZ	220	ASN
1	LZ	242	ASN
1	LZ	246	ASN
1	LZ	597	ASN
1	La	381	GLN
1	La	462	ASN
1	La	536	ASN
1	La	597	ASN
1	Lb	44	GLN
1	Lb	240	ASN
1	Lb	285	ASN
1	Lb	302	ASN
1	Lb	519	ASN
1	Lb	597	ASN
1	Lc	181	GLN
1	Lc	220	ASN
1	Lc	246	ASN
1	Lc	403	ASN
1	Lc	597	ASN
1	Ld	228	ASN
1	Ld	240	ASN
1	Ld	257	ASN
1	Ld	337	ASN
1	Ld	381	GLN
1	Ld	462	ASN
1	Ld	536	ASN
1	Ld	597	ASN
2	BM	46	ASN
2	BM	127	HIS
2	BM	268	ASN
2	BM	343	ASN
2	BK	46	ASN
2	BK	112	ASN
2	BK	127	HIS
2	BK	268	ASN
2	BO	127	HIS
2	BO	177	ASN
2	BO	302	GLN
2	BP	22	GLN
2	BP	127	HIS
2	BP	268	ASN

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Mol	Chain	Res	Type
2	BP	300	GLN
2	BP	340	ASN
2	BL	207	GLN
2	BL	268	ASN
2	BL	300	GLN
2	BL	340	ASN
2	BL	343	ASN
2	BN	22	GLN
2	BN	50	GLN
2	BN	300	GLN
2	BN	340	ASN
2	BN	343	ASN
3	BQ	133	ASN
3	BS	35	GLN
3	BS	77	GLN
3	BS	85	ASN
3	BS	115	ASN
3	BS	179	ASN
3	BR	77	GLN
3	BR	85	ASN
3	BR	115	ASN
3	BR	133	ASN
3	BR	179	ASN
3	BT	77	GLN
3	BT	115	ASN
3	BU	64	ASN
3	BU	85	ASN
3	BU	115	ASN
4	AX	33	GLN
4	AX	45	GLN
4	AX	92	GLN
4	AX	96	GLN
4	AX	399	GLN
4	AX	451	ASN
4	AX	462	ASN
4	AW	10	GLN
4	AW	45	GLN
4	AW	95	GLN
4	AW	261	ASN
4	AW	464	ASN
4	AW	564	HIS
4	AW	624	GLN

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Mol	Chain	Res	Type
4	AW	655	GLN
4	AT	45	GLN
4	AT	55	ASN
4	AT	97	ASN
4	AT	451	ASN
4	AT	462	ASN
4	AT	548	ASN
4	AS	10	GLN
4	AS	45	GLN
4	AS	55	ASN
4	AS	261	ASN
4	AS	464	ASN
4	AS	564	HIS
4	AS	655	GLN
4	AV	36	ASN
4	AV	45	GLN
4	AV	462	ASN
4	AU	10	GLN
4	AU	16	ASN
4	AU	45	GLN
4	AU	95	GLN
4	AU	261	ASN
4	AU	451	ASN
4	AU	464	ASN
4	AU	564	HIS
4	AU	655	GLN
4	AR	10	GLN
4	AR	64	ASN
4	AR	165	ASN
4	AR	182	GLN
4	AR	273	GLN
4	AR	389	GLN
4	AR	425	ASN
4	AR	464	ASN
4	AR	548	ASN
4	AR	655	GLN
4	AQ	64	ASN
4	AQ	92	GLN
4	AQ	97	ASN
4	AQ	172	ASN
4	AQ	273	GLN
4	AQ	614	GLN

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Mol	Chain	Res	Type
4	AN	8	ASN
4	AN	64	ASN
4	AN	145	ASN
4	AN	182	GLN
4	AN	425	ASN
4	AN	464	ASN
4	AN	548	ASN
4	AM	92	GLN
4	AM	172	ASN
4	AM	372	GLN
4	AM	496	ASN
4	AM	614	GLN
4	AM	639	ASN
4	AP	8	ASN
4	AP	64	ASN
4	AP	119	ASN
4	AP	182	GLN
4	AP	202	GLN
4	AP	389	GLN
4	AP	425	ASN
4	AP	464	ASN
4	AP	548	ASN
4	AP	655	GLN
4	AO	64	ASN
4	AO	92	GLN
4	AO	97	ASN
4	AO	172	ASN
4	AO	273	GLN
4	AO	496	ASN
4	AO	614	GLN
5	AY	21	ASN
5	AY	206	GLN
5	AY	267	ASN
5	AY	408	GLN
5	AY	476	ASN
5	AY	487	HIS
5	AY	577	ASN
5	AY	627	GLN
5	AY	664	ASN
5	AY	825	GLN
5	AY	851	ASN
5	AY	905	ASN

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Mol	Chain	Res	Type
5	AY	981	GLN
5	AY	1018	ASN
5	AZ	21	ASN
5	AZ	174	HIS
5	AZ	207	HIS
5	AZ	267	ASN
5	AZ	408	GLN
5	AZ	487	HIS
5	AZ	577	ASN
5	AZ	627	GLN
5	AZ	664	ASN
5	AZ	905	ASN
5	AZ	981	GLN
5	A0	21	ASN
5	A0	218	ASN
5	A0	267	ASN
5	A0	408	GLN
5	A0	474	ASN
5	A0	476	ASN
5	A0	487	HIS
5	A0	627	GLN
5	A0	664	ASN
5	A0	689	ASN
5	A0	905	ASN
5	A0	981	GLN
5	A0	1018	ASN
5	A1	21	ASN
5	A1	174	HIS
5	A1	206	GLN
5	A1	207	HIS
5	A1	220	GLN
5	A1	267	ASN
5	A1	408	GLN
5	A1	476	ASN
5	A1	481	HIS
5	A1	487	HIS
5	A1	627	GLN
5	A1	664	ASN
5	A1	689	ASN
5	A1	825	GLN
5	A1	905	ASN
5	A1	908	HIS

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Mol	Chain	Res	Type
5	A1	981	GLN
5	A1	1018	ASN
5	A2	206	GLN
5	A2	207	HIS
5	A2	267	ASN
5	A2	430	HIS
5	A2	476	ASN
5	A2	487	HIS
5	A2	577	ASN
5	A2	627	GLN
5	A2	905	ASN
5	A2	975	ASN
5	A2	981	GLN
5	A2	1010	GLN
5	A2	1018	ASN
5	A3	21	ASN
5	A3	83	GLN
5	A3	174	HIS
5	A3	267	ASN
5	A3	408	GLN
5	A3	476	ASN
5	A3	487	HIS
5	A3	627	GLN
5	A3	664	ASN
5	A3	825	GLN
5	A3	905	ASN
5	A3	981	GLN
6	A4	81	ASN
6	A4	321	ASN
6	A9	81	ASN
6	A9	278	GLN
6	A9	321	ASN
6	A9	323	GLN
6	A9	336	ASN
6	A6	81	ASN
6	A6	321	ASN
6	A5	81	ASN
6	A5	278	GLN
6	A5	321	ASN
6	A5	323	GLN
6	A5	336	ASN
6	A8	81	ASN

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Mol	Chain	Res	Type
6	A8	278	GLN
6	A7	81	ASN
6	A7	278	GLN
6	A7	321	ASN
6	A7	323	GLN
6	A7	336	ASN
6	Ad	240	GLN
6	Ac	109	ASN
6	Af	109	ASN
6	Af	240	GLN
6	Ab	109	ASN
6	Aa	239	GLN
7	LN	186	ASN
7	LN	297	GLN
7	LO	145	ASN
7	LO	241	ASN
7	LM	40	ASN
7	LM	57	GLN
7	LM	145	ASN
7	LM	186	ASN
7	LR	145	ASN
7	LR	241	ASN
7	LP	40	ASN
7	LP	57	GLN
7	LP	95	GLN
7	LP	145	ASN
7	LP	186	ASN
7	LB	95	GLN
7	LB	186	ASN
7	LB	297	GLN
7	LC	95	GLN
7	LC	241	ASN
7	LA	40	ASN
7	LA	57	GLN
7	LA	95	GLN
7	LA	145	ASN
7	LA	186	ASN
7	LA	218	GLN
7	LE	186	ASN
7	LE	297	GLN
7	LF	145	ASN
7	LF	241	ASN

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Mol	Chain	Res	Type
7	LD	40	ASN
7	LD	57	GLN
7	LD	145	ASN
7	LD	186	ASN
7	LH	297	GLN
7	LI	145	ASN
7	LI	241	ASN
7	LG	40	ASN
7	LG	57	GLN
7	LG	95	GLN
7	LG	145	ASN
7	LG	186	ASN
7	LG	218	GLN
7	LK	186	ASN
7	LK	297	GLN
7	LL	145	ASN
7	LL	241	ASN
7	LJ	40	ASN
7	LJ	56	ASN
7	LJ	57	GLN
7	LJ	145	ASN
7	LJ	186	ASN
7	LJ	218	GLN
8	FA	553	HIS
8	FJ	553	HIS
8	FL	562	GLN
8	FS	553	HIS
8	Fb	553	HIS
8	Fb	583	ASN
8	Fd	562	GLN
8	Fk	553	HIS
8	Fm	562	GLN
9	SA	34	GLN
9	SA	345	ASN
9	SA	499	ASN
9	SB	34	GLN
9	SB	345	ASN
9	SB	429	GLN
9	SB	499	ASN
9	SC	34	GLN
9	SC	345	ASN
9	SC	355	GLN

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Mol	Chain	Res	Type
9	SC	429	GLN
9	SC	499	ASN
9	SD	34	GLN
9	SD	305	ASN
9	SD	345	ASN
9	SD	355	GLN
9	SD	429	GLN
9	SE	34	GLN
9	SE	305	ASN
9	SE	345	ASN
9	SE	355	GLN
9	SE	429	GLN
9	SE	499	ASN
9	SF	34	GLN
9	SF	305	ASN
9	SF	345	ASN
9	SF	499	ASN
9	SK	16	GLN
9	SK	34	GLN
9	SK	43	GLN
9	SK	570	GLN
9	SK	589	GLN
9	SG	16	GLN
9	SG	34	GLN
9	SG	43	GLN
9	SG	570	GLN
9	SG	589	GLN
9	SL	16	GLN
9	SL	34	GLN
9	SL	326	GLN
9	SL	570	GLN
9	SL	589	GLN
9	SH	34	GLN
9	SH	43	GLN
9	SH	570	GLN
9	SH	589	GLN
9	SI	16	GLN
9	SI	34	GLN
9	SI	43	GLN
9	SI	249	GLN
9	SI	326	GLN
9	SI	570	GLN

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Mol	Chain	Res	Type
9	SI	589	GLN
9	SI	640	ASN
9	SJ	16	GLN
9	SJ	34	GLN
9	SJ	43	GLN
9	SJ	249	GLN
9	SJ	326	GLN
9	SJ	570	GLN
9	SJ	589	GLN
9	SJ	640	ASN
9	SQ	463	ASN
9	SQ	551	ASN
9	SQ	570	GLN
9	SQ	589	GLN
9	SP	463	ASN
9	SP	570	GLN
9	SP	589	GLN
9	SM	463	ASN
9	SM	551	ASN
9	SM	570	GLN
9	SM	589	GLN
9	SN	463	ASN
9	SN	551	ASN
9	SN	570	GLN
9	SN	589	GLN
9	SO	463	ASN
9	SO	551	ASN
9	SO	570	GLN
9	SO	589	GLN
9	SR	463	ASN
9	SR	551	ASN
9	SR	570	GLN
9	SR	589	GLN
9	SW	34	GLN
9	SW	463	ASN
9	SW	484	GLN
9	SS	463	ASN
9	SS	570	GLN
9	ST	34	GLN
9	ST	40	GLN
9	ST	272	GLN
9	ST	463	ASN

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Mol	Chain	Res	Type
9	SU	34	GLN
9	SU	233	GLN
9	SU	463	ASN
9	SV	34	GLN
9	SV	463	ASN
9	SX	34	GLN
9	SX	272	GLN
9	SX	463	ASN
9	SY	34	GLN
9	SY	423	ASN
9	SY	484	GLN
9	SY	589	GLN
9	SZ	34	GLN
9	SZ	484	GLN
9	SZ	570	GLN
9	SZ	589	GLN
9	SZ	640	ASN
9	Sa	34	GLN
9	Sa	484	GLN
9	Sa	570	GLN
9	Sa	589	GLN
9	Sb	34	GLN
9	Sb	484	GLN
9	Sb	570	GLN
9	Sb	589	GLN
9	Sc	34	GLN
9	Sc	484	GLN
9	Sc	561	ASN
9	Sc	570	GLN
9	Sc	589	GLN
9	Sd	34	GLN
9	Sd	423	ASN
9	Sd	484	GLN
9	Sd	570	GLN
9	Sd	589	GLN
9	Sd	640	ASN
9	Se	60	GLN
9	Se	73	GLN
9	Se	463	ASN
9	Se	499	ASN
9	Se	551	ASN
9	Sf	34	GLN

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Mol	Chain	Res	Type
9	Sf	73	GLN
9	Sf	272	GLN
9	Sf	463	ASN
9	Sf	499	ASN
9	Sf	551	ASN
9	Sf	570	GLN
9	Sg	34	GLN
9	Sg	73	GLN
9	Sg	298	GLN
9	Sg	463	ASN
9	Sg	499	ASN
9	Sg	551	ASN
9	Sh	34	GLN
9	Sh	40	GLN
9	Sh	60	GLN
9	Sh	73	GLN
9	Sh	463	ASN
9	Sh	499	ASN
9	Sh	551	ASN
9	Sh	570	GLN
9	Si	34	GLN
9	Si	73	GLN
9	Si	272	GLN
9	Si	463	ASN
9	Si	499	ASN
9	Si	551	ASN
9	Sj	34	GLN
9	Sj	73	GLN
9	Sj	249	GLN
9	Sj	298	GLN
9	Sj	463	ASN
9	Sj	499	ASN
9	Sj	551	ASN
9	Sj	570	GLN
9	Sk	59	ASN
9	Sk	70	ASN
9	Sk	73	GLN
9	Sk	272	GLN
9	Sk	440	ASN
9	Sk	455	GLN
9	Sk	463	ASN
9	Sk	499	ASN

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Mol	Chain	Res	Type
9	Sl	70	ASN
9	Sl	73	GLN
9	Sl	202	HIS
9	Sl	455	GLN
9	Sl	463	ASN
9	Sl	499	ASN
9	Sm	40	GLN
9	Sm	59	ASN
9	Sm	70	ASN
9	Sm	73	GLN
9	Sm	272	GLN
9	Sm	440	ASN
9	Sm	455	GLN
9	Sm	463	ASN
9	Sm	499	ASN
9	Sn	34	GLN
9	Sn	59	ASN
9	Sn	70	ASN
9	Sn	73	GLN
9	Sn	272	GLN
9	Sn	455	GLN
9	Sn	463	ASN
9	Sn	499	ASN
9	So	40	GLN
9	So	59	ASN
9	So	70	ASN
9	So	73	GLN
9	So	440	ASN
9	So	455	GLN
9	So	463	ASN
9	So	499	ASN
9	Sp	59	ASN
9	Sp	70	ASN
9	Sp	73	GLN
9	Sp	272	GLN
9	Sp	455	GLN
9	Sp	463	ASN
9	Sp	499	ASN
10	TZ	55	ASN
10	Tb	59	ASN
10	Tc	55	ASN
10	Td	55	ASN

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Mol	Chain	Res	Type
10	Te	89	GLN
10	Tf	89	GLN
10	Tj	89	GLN
10	Tk	59	ASN
10	Tk	89	GLN
10	Tl	59	ASN
10	Tl	89	GLN
10	Tm	59	ASN
10	Tm	97	ASN
10	Tn	59	ASN
10	To	59	ASN
10	Tp	59	ASN
10	Tp	89	GLN
10	Tp	125	ASN
10	Tq	125	ASN
10	Tr	125	ASN
10	Ts	125	ASN
10	Tt	125	ASN
10	Tu	125	ASN
10	Tv	125	ASN
11	AA	129	ASN
11	AA	131	ASN
11	AB	129	ASN
11	AD	102	ASN
11	AD	129	ASN
11	AD	131	ASN
11	AE	129	ASN
11	AE	131	ASN
11	AF	131	ASN
12	BE	52	GLN
12	BE	182	GLN
12	BE	352	ASN
12	BF	52	GLN
12	BF	352	ASN
12	BG	4	GLN
12	BG	10	ASN
12	BG	52	GLN
12	BG	77	ASN
12	BG	194	ASN
12	BG	352	ASN
13	AL	99	GLN
13	AL	113	HIS

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Mol	Chain	Res	Type
13	AL	119	ASN
13	AL	130	ASN
13	AL	141	ASN
13	AI	43	ASN
13	AI	47	GLN
13	AI	119	ASN
13	AI	143	GLN
13	AG	119	ASN
13	AG	171	ASN
13	AK	113	HIS
13	AK	119	ASN
13	AH	113	HIS
13	AH	119	ASN
13	AJ	113	HIS
13	AJ	117	ASN
13	AJ	119	ASN
13	AJ	141	ASN
13	AJ	143	GLN
14	BB	120	GLN
14	BB	157	ASN
14	BB	232	ASN
14	BB	444	GLN
14	BB	448	ASN
14	BB	462	ASN
14	BB	479	ASN
14	BC	448	ASN
14	BC	479	ASN
14	BD	448	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

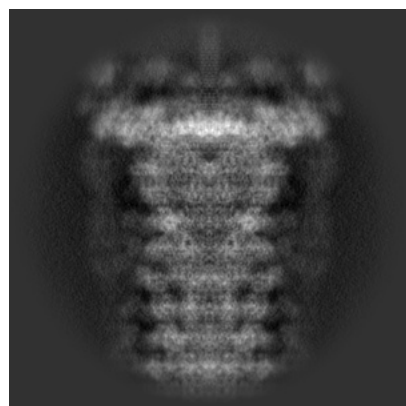
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50186. These allow visual inspection of the internal detail of the map and identification of artifacts.

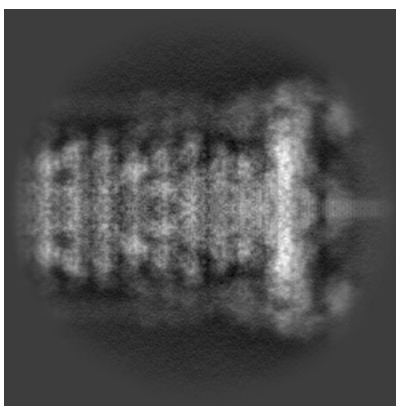
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

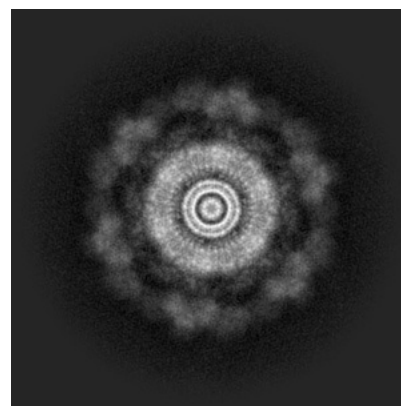
6.1.1 Primary map



X

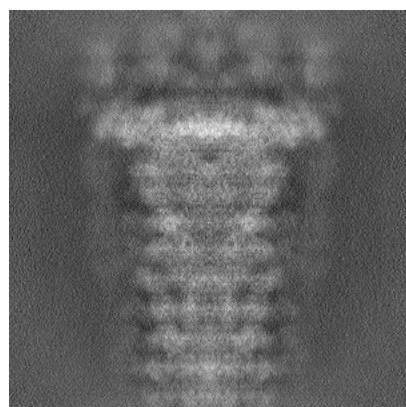


Y

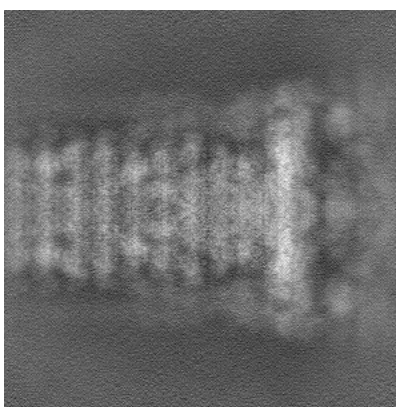


Z

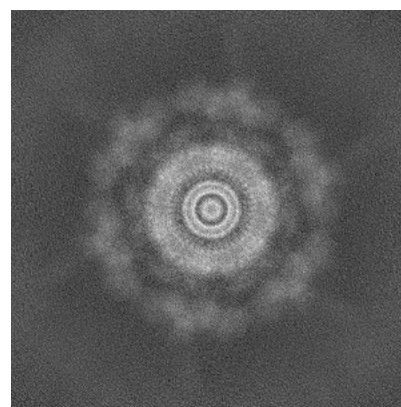
6.1.2 Raw map



X



Y

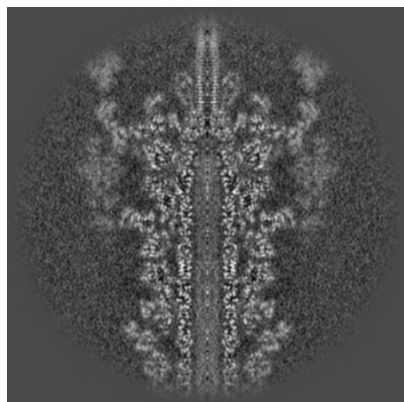


Z

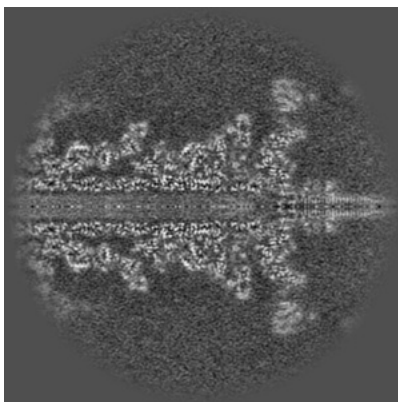
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

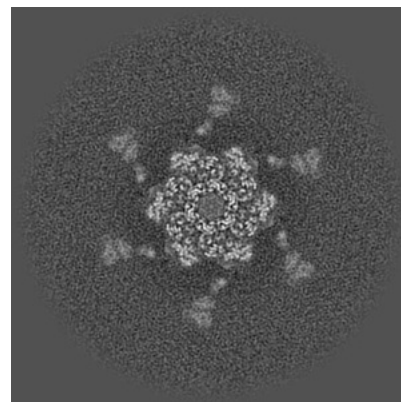
6.2.1 Primary map



X Index: 256

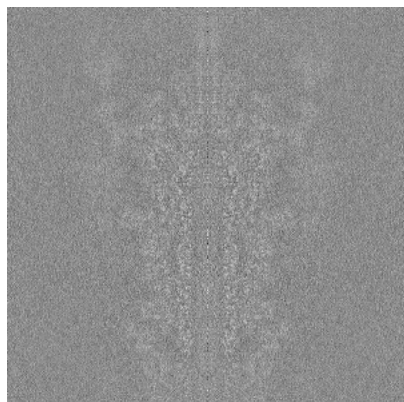


Y Index: 256

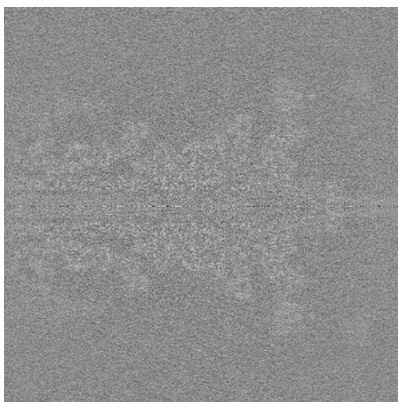


Z Index: 256

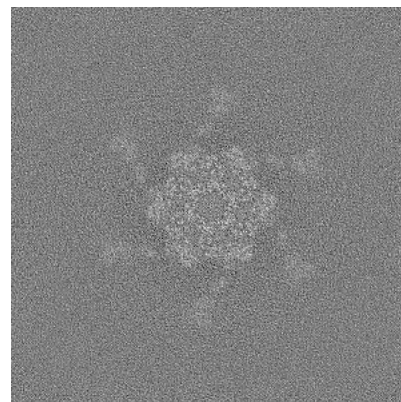
6.2.2 Raw map



X Index: 256



Y Index: 256

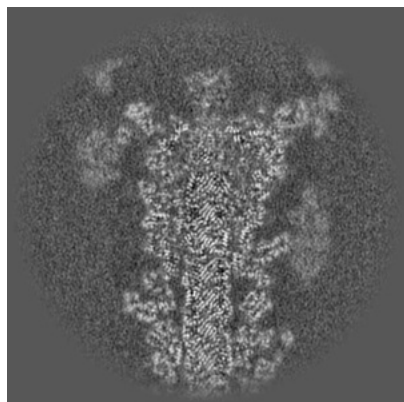


Z Index: 256

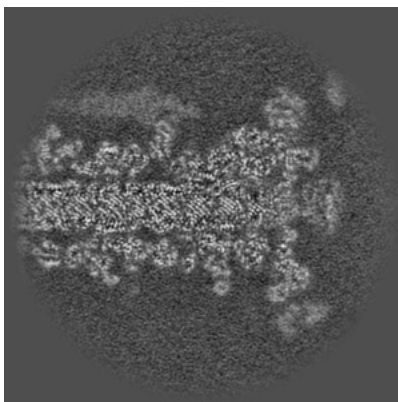
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

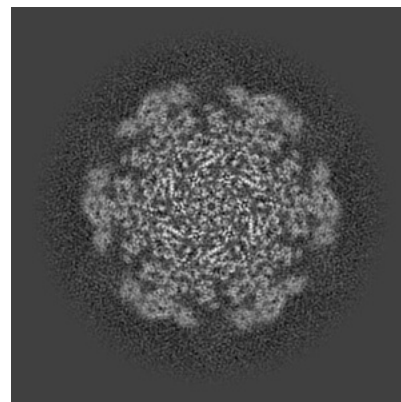
6.3.1 Primary map



X Index: 279

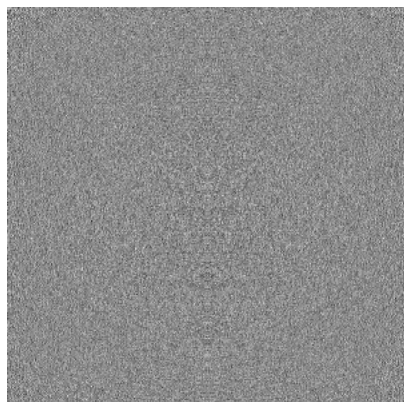


Y Index: 278

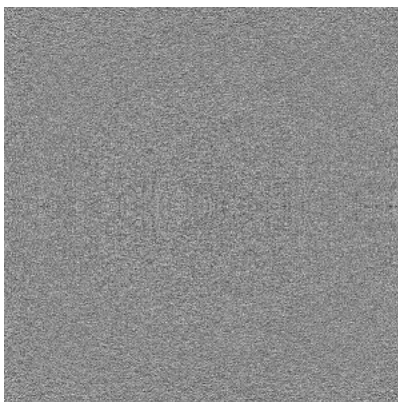


Z Index: 356

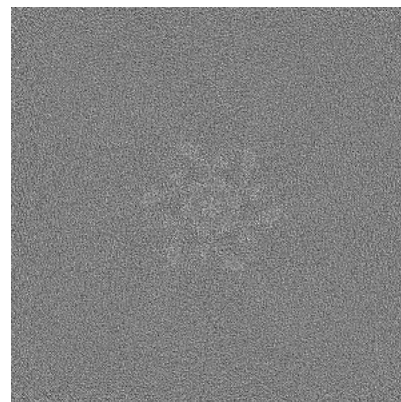
6.3.2 Raw map



X Index: 0



Y Index: 0

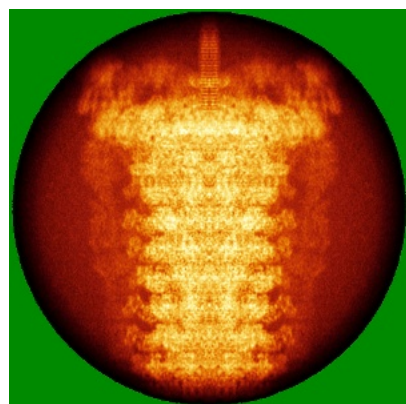


Z Index: 0

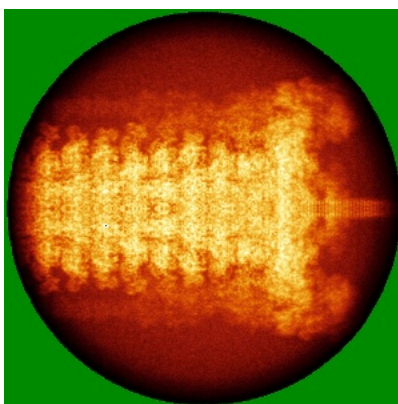
The images above show the largest variance slices of the map in three orthogonal directions.

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

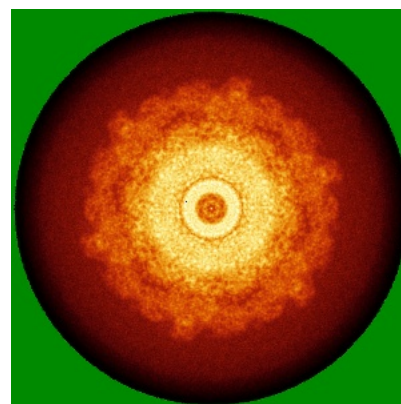
6.4.1 Primary map



X

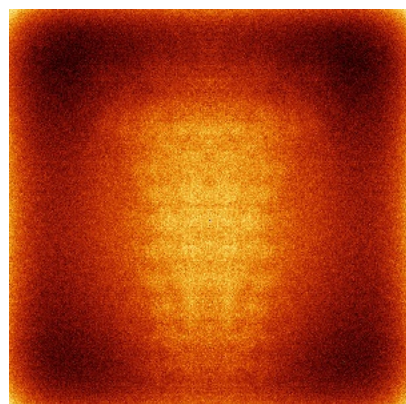


Y

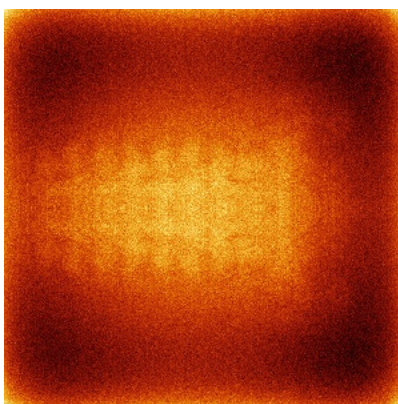


Z

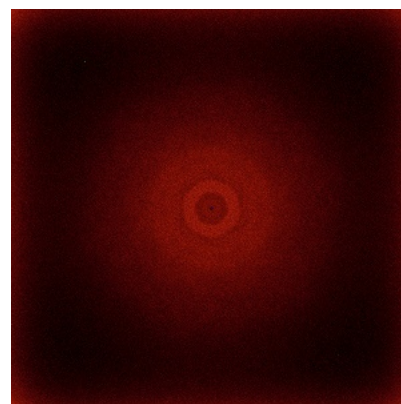
6.4.2 Raw map



X



Y

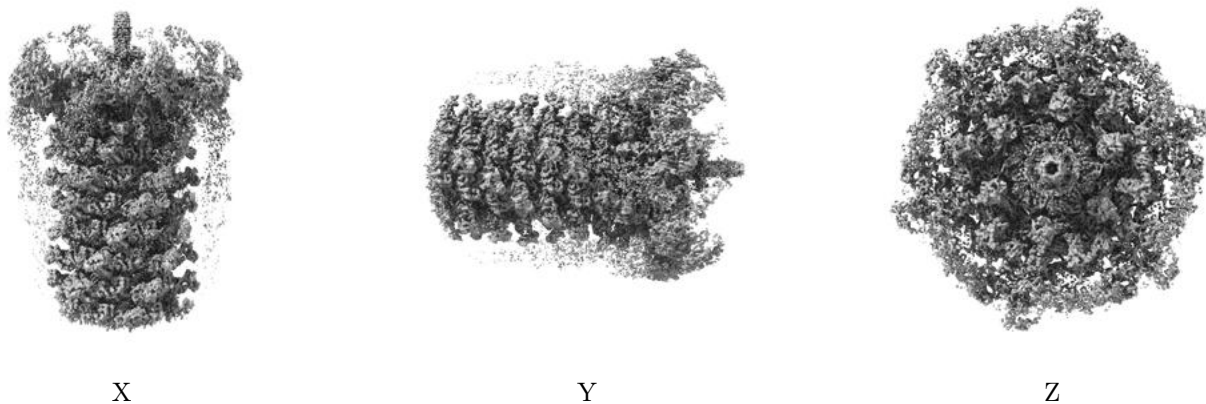


Z

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.

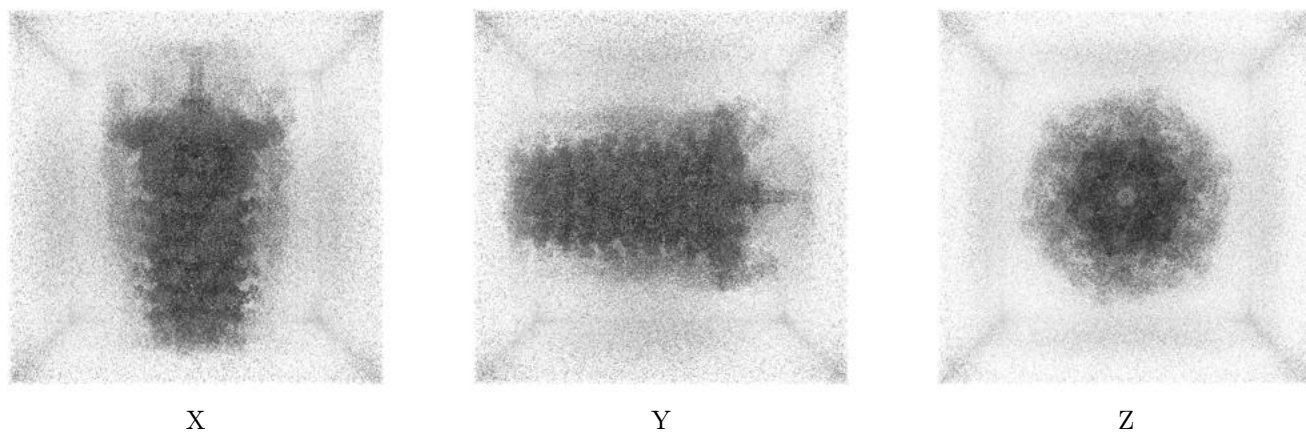
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

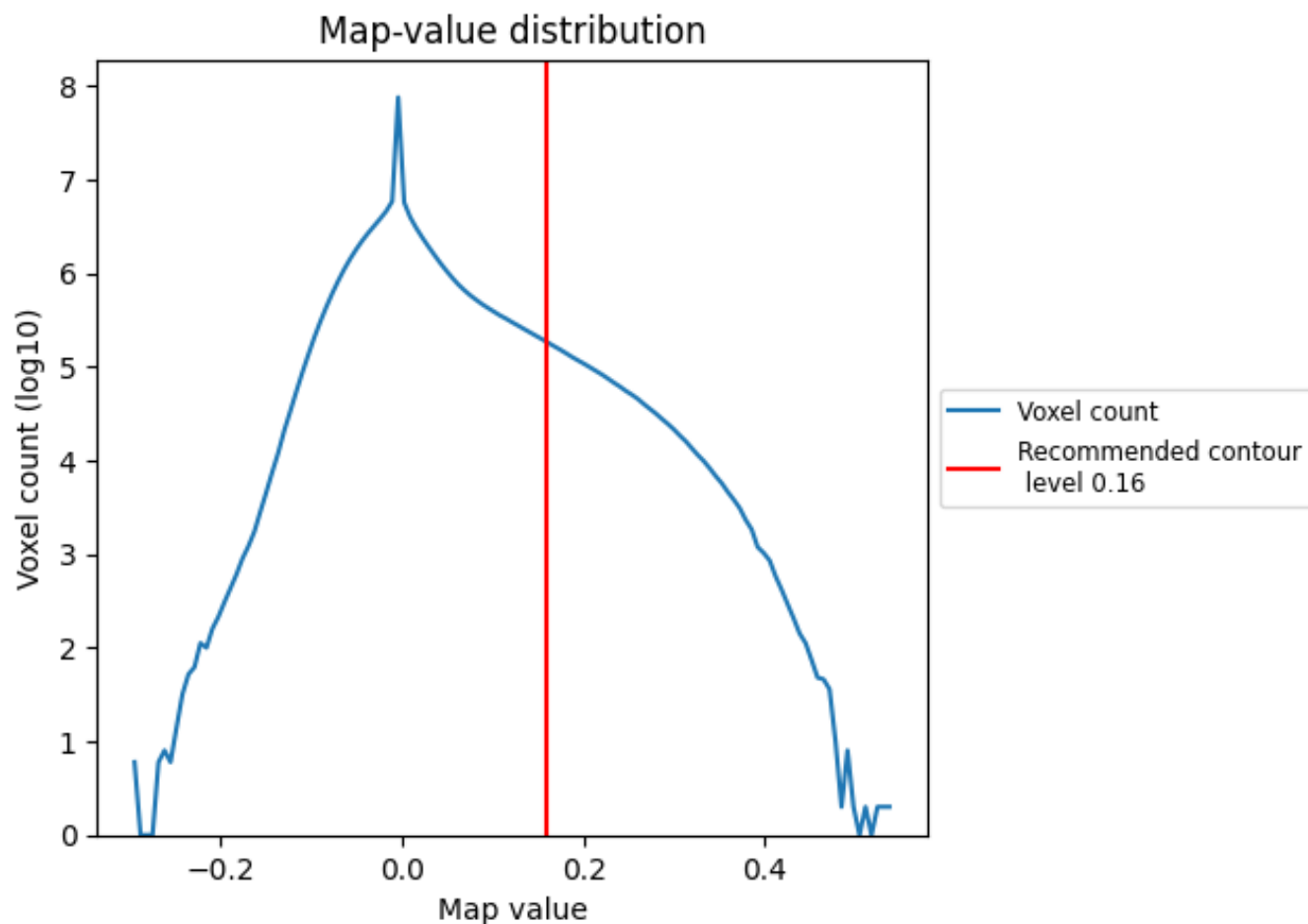
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

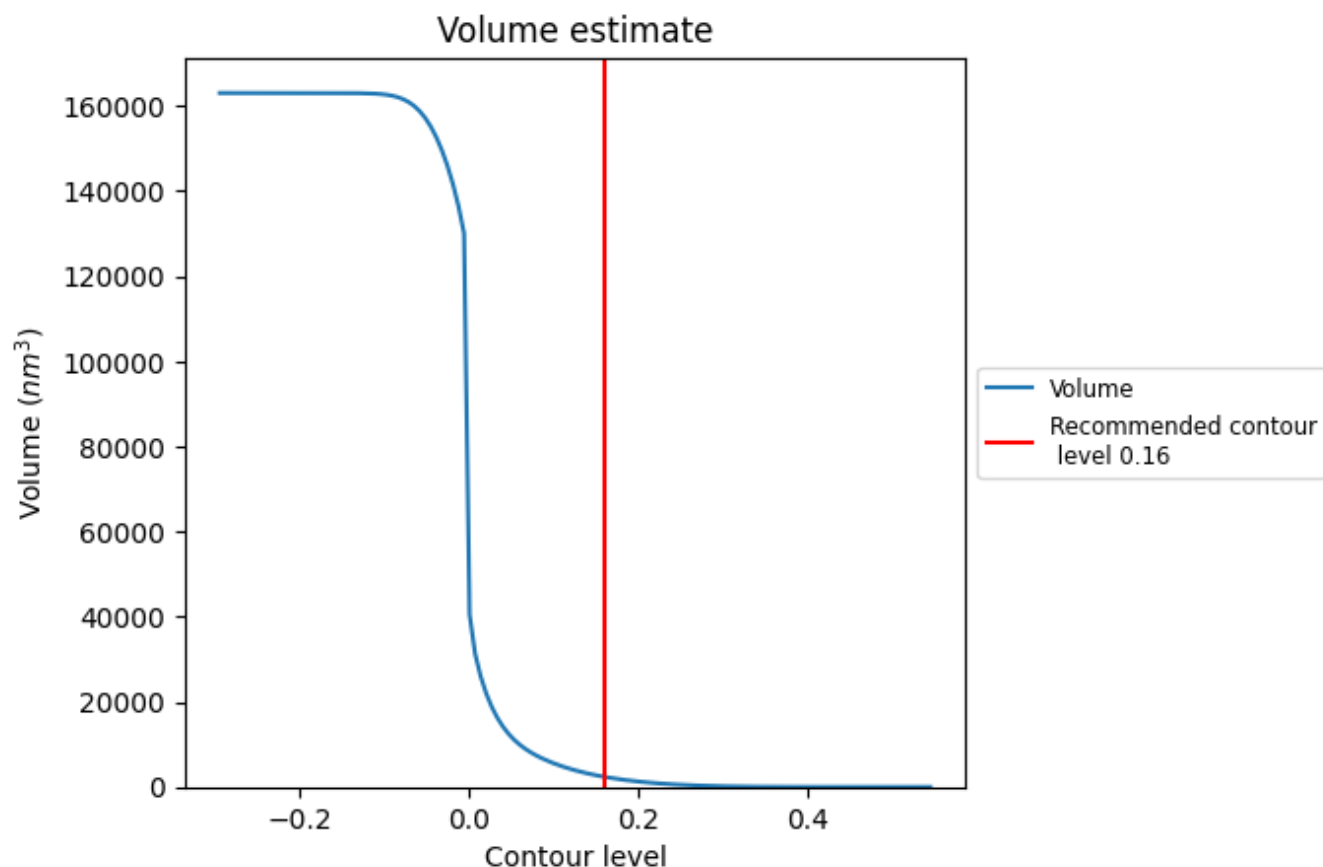
This section contains the results of statistical analysis of the map.

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.

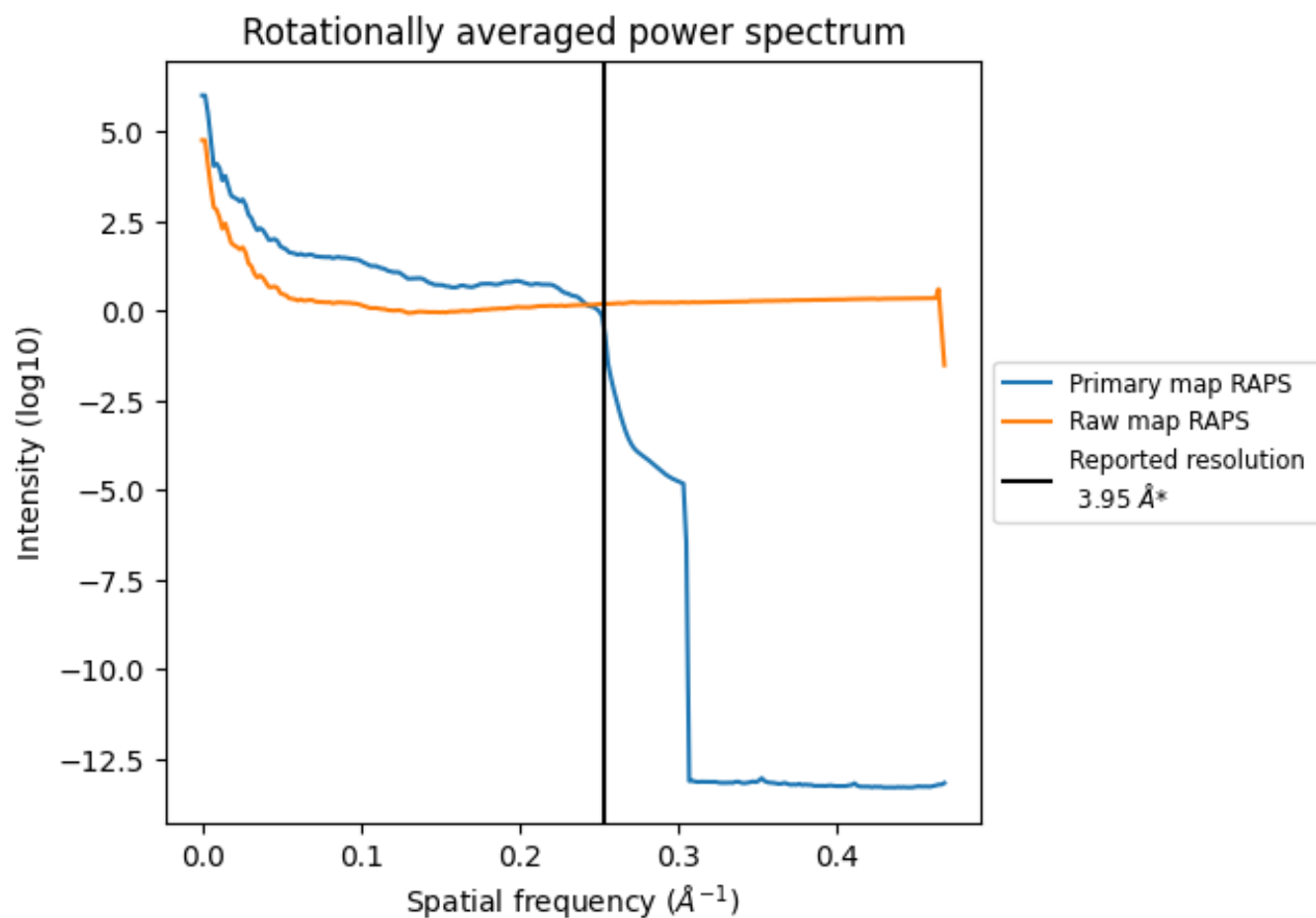
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2352 nm³; this corresponds to an approximate mass of 2125 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 ⓘ

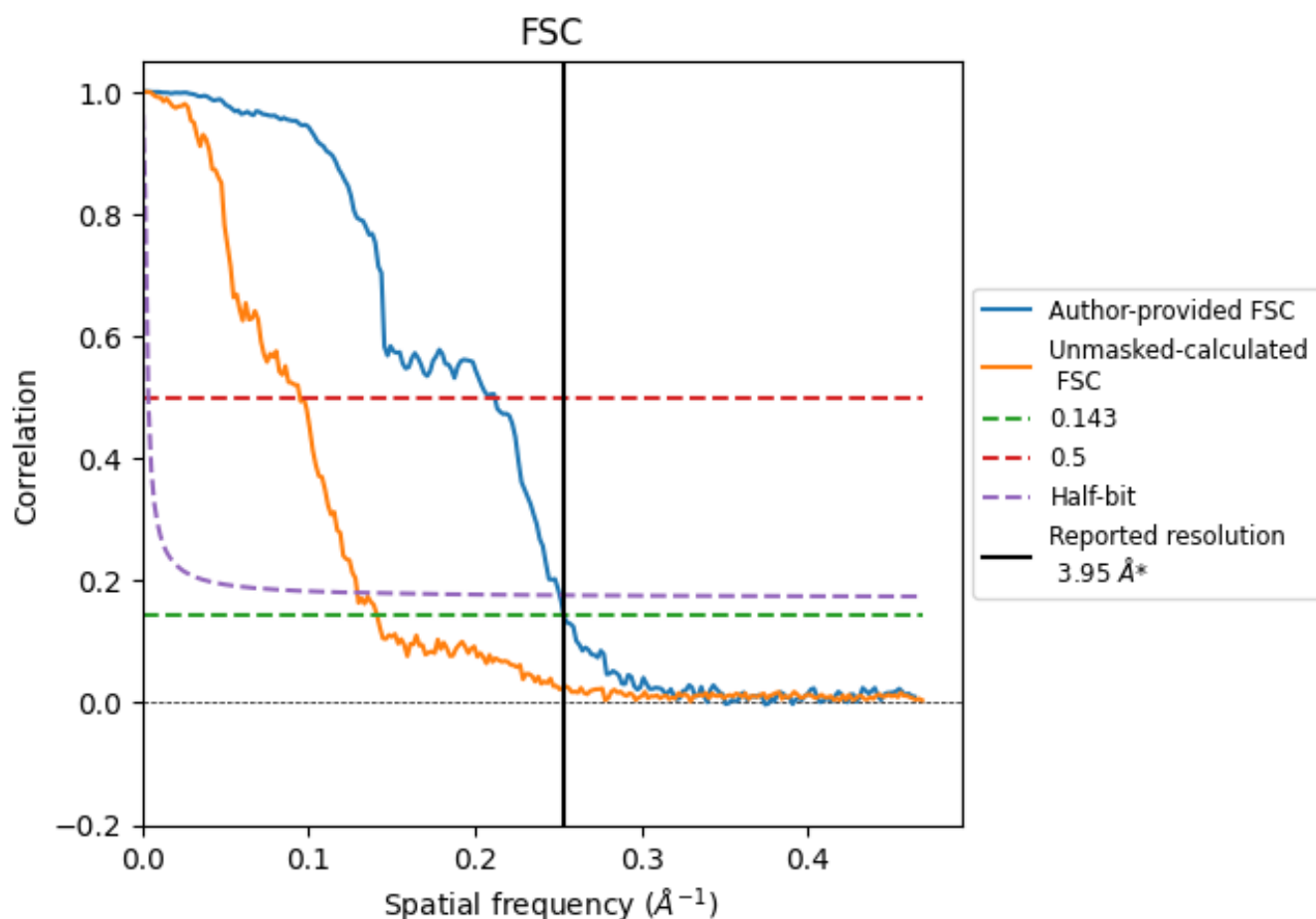


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

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 $0.253 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

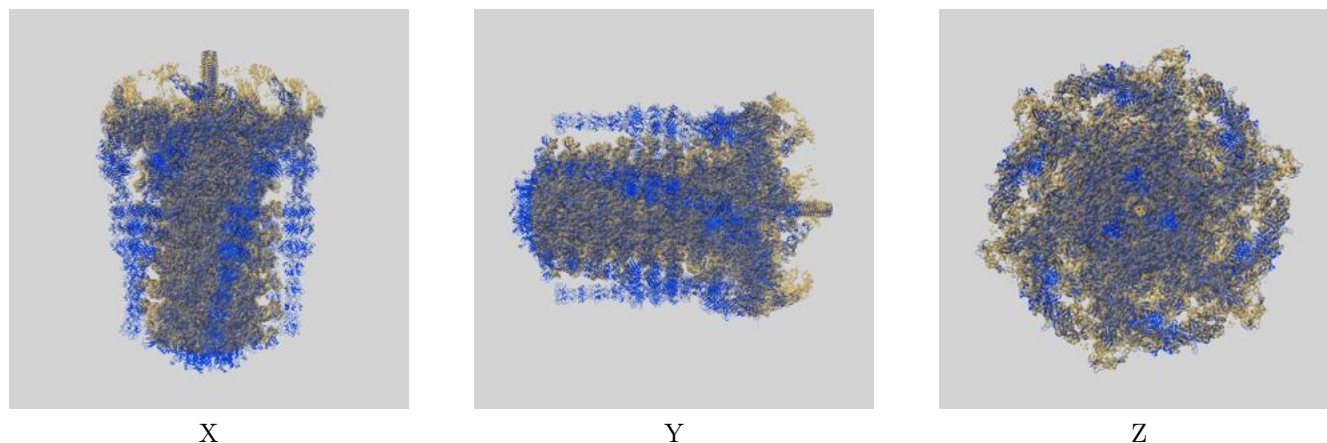
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	3.95	4.72	3.99
Unmasked-calculated*	7.09	10.56	7.74

*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 7.09 differs from the reported value 3.95 by more than 10 %

9 Map-model fit [i](#)

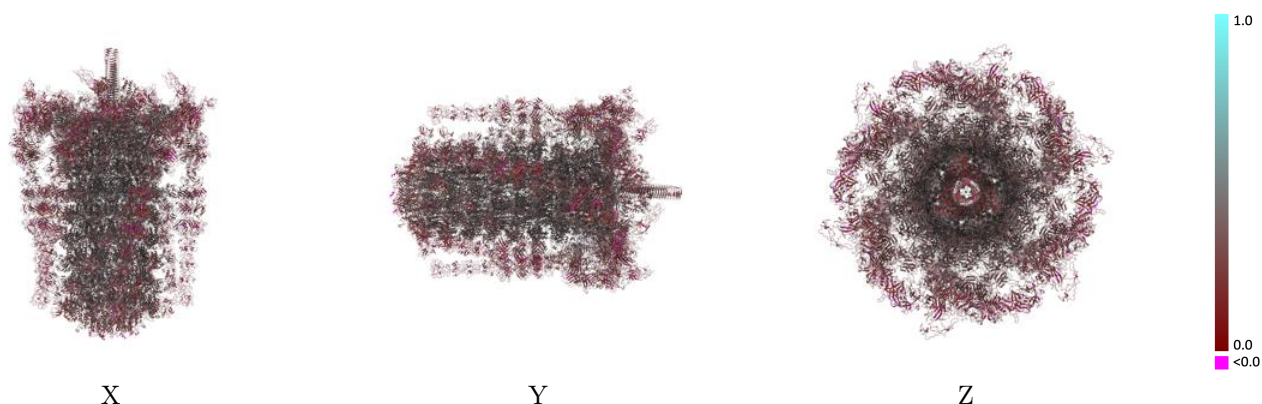
This section contains information regarding the fit between EMDB map EMD-50186 and PDB model 9F4A. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



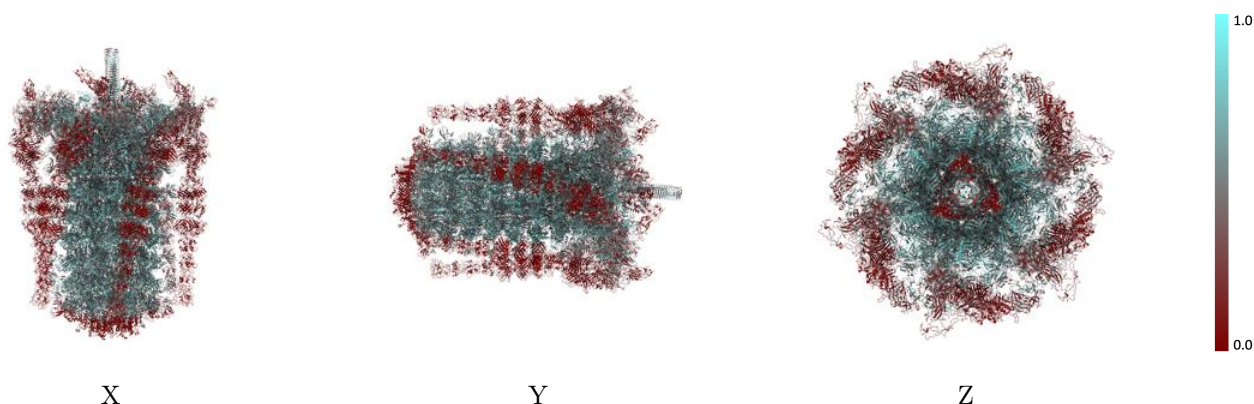
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



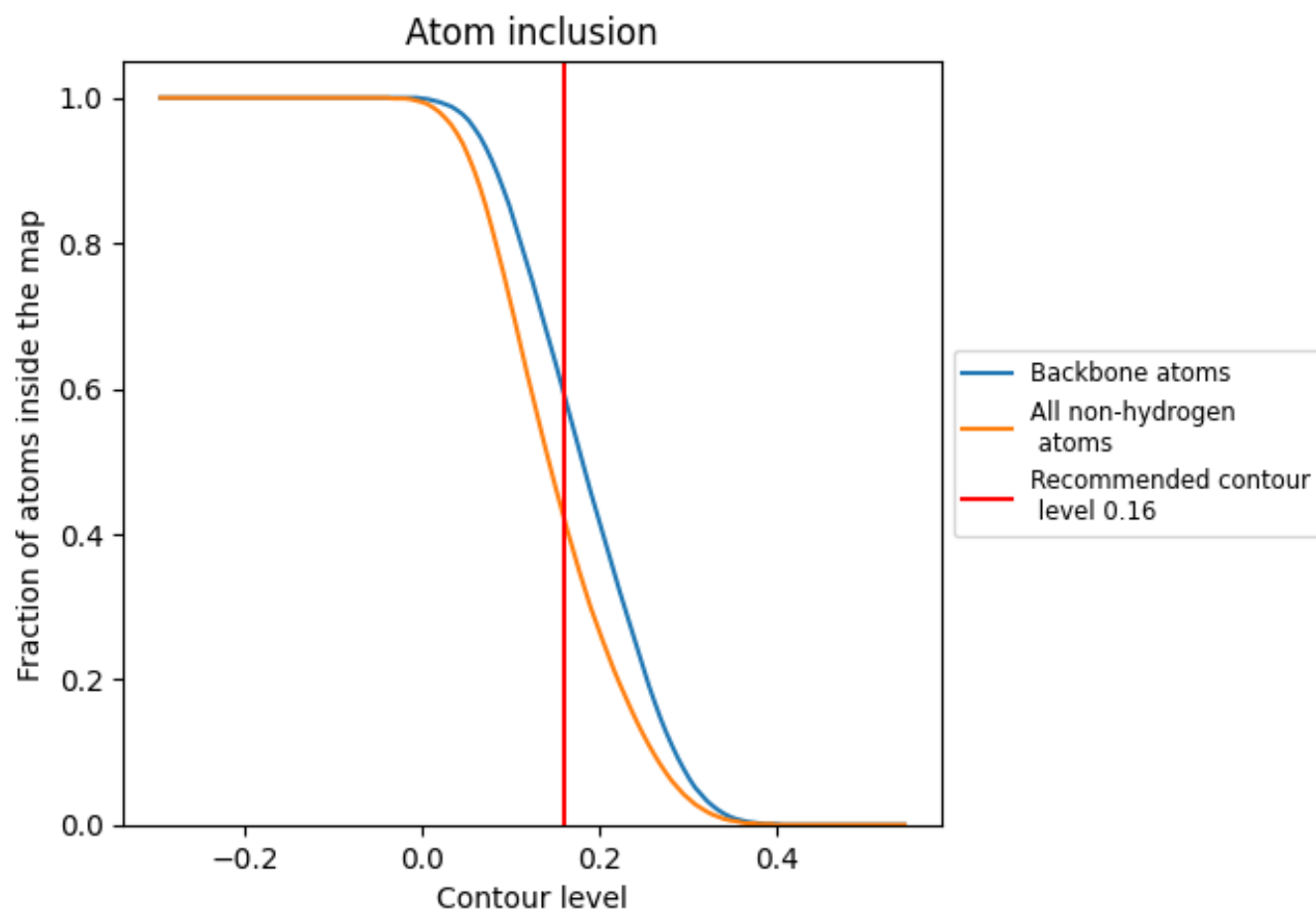
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 42% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4220	 0.3380
A0	 0.4220	 0.2960
A1	 0.4250	 0.2950
A2	 0.4270	 0.2950
A3	 0.4200	 0.2950
A4	 0.4580	 0.3220
A5	 0.4560	 0.3200
A6	 0.4630	 0.3220
A7	 0.4600	 0.3210
A8	 0.4620	 0.3200
A9	 0.4670	 0.3200
AA	 0.4760	 0.3900
AB	 0.4730	 0.3910
AC	 0.4740	 0.3920
AD	 0.4740	 0.3910
AE	 0.4700	 0.3910
AF	 0.4740	 0.3970
AG	 0.5890	 0.4020
AH	 0.5870	 0.4020
AI	 0.5890	 0.4010
AJ	 0.5890	 0.3990
AK	 0.5890	 0.3960
AL	 0.5870	 0.4010
AM	 0.6240	 0.3900
AN	 0.6280	 0.3900
AO	 0.6250	 0.3890
AP	 0.6270	 0.3910
AQ	 0.6270	 0.3900
AR	 0.6290	 0.3890
AS	 0.5990	 0.3760
AT	 0.6050	 0.3790
AU	 0.6000	 0.3770
AV	 0.6070	 0.3780
AW	 0.6030	 0.3770
AX	 0.6030	 0.3790



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Chain	Atom inclusion	Q-score
AY	0.4240	0.2960
AZ	0.4280	0.2960
Aa	0.3770	0.2560
Ab	0.3810	0.2550
Ac	0.3800	0.2520
Ad	0.3720	0.2510
Ae	0.3730	0.2520
Af	0.3760	0.2530
BB	0.3640	0.3020
BC	0.3600	0.3010
BD	0.3600	0.3000
BE	0.4220	0.3580
BF	0.4260	0.3590
BG	0.4230	0.3600
BK	0.4090	0.3770
BL	0.4670	0.3840
BM	0.4090	0.3740
BN	0.4680	0.3860
BO	0.4070	0.3720
BP	0.4690	0.3860
BQ	0.5340	0.4280
BR	0.5290	0.4300
BS	0.5330	0.4300
BT	0.5310	0.4300
BU	0.5310	0.4310
BV	0.5330	0.4280
FA	0.1640	0.2180
FB	0.1580	0.2200
FC	0.1800	0.2390
FJ	0.1540	0.2200
FK	0.1680	0.2180
FL	0.1740	0.2340
FS	0.1540	0.2180
FT	0.1540	0.2190
FU	0.1760	0.2370
Fb	0.1680	0.2240
Fc	0.1640	0.2200
Fd	0.1850	0.2400
Fk	0.1600	0.2210
Fl	0.1680	0.2210
Fm	0.1700	0.2390
Ft	0.1500	0.2220

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Chain	Atom inclusion	Q-score
Fu	 0.1540	 0.2180
Fv	 0.1780	 0.2350
LA	 0.0870	 0.2620
LB	 0.0650	 0.2510
LC	 0.0630	 0.2530
LD	 0.0890	 0.2620
LE	 0.0600	 0.2500
LF	 0.0610	 0.2540
LG	 0.0870	 0.2610
LH	 0.0630	 0.2530
LI	 0.0620	 0.2530
LJ	 0.0880	 0.2630
LK	 0.0660	 0.2510
LL	 0.0610	 0.2520
LM	 0.0840	 0.2630
LN	 0.0570	 0.2520
LO	 0.0600	 0.2540
LP	 0.0890	 0.2620
LQ	 0.0620	 0.2520
LR	 0.0610	 0.2540
LS	 0.0130	 0.2710
LT	 0.0120	 0.2410
LU	 0.0220	 0.2630
LV	 0.0130	 0.2730
LW	 0.0120	 0.2410
LX	 0.0230	 0.2620
LY	 0.0130	 0.2710
LZ	 0.0120	 0.2390
La	 0.0260	 0.2600
Lb	 0.0130	 0.2710
Lc	 0.0130	 0.2380
Ld	 0.0220	 0.2620
Le	 0.0150	 0.2710
Lf	 0.0130	 0.2400
Lg	 0.0230	 0.2620
Lh	 0.0130	 0.2690
Li	 0.0120	 0.2400
Lj	 0.0250	 0.2610
SA	 0.5870	 0.4010
SB	 0.5870	 0.4010
SC	 0.5900	 0.4010
SD	 0.5880	 0.4010

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Chain	Atom inclusion	Q-score
SE	 0.5860	 0.4010
SF	 0.5860	 0.4010
SG	 0.6340	 0.3990
SH	 0.6340	 0.3990
SI	 0.6300	 0.3990
SJ	 0.6320	 0.3990
SK	 0.6330	 0.3980
SL	 0.6320	 0.3980
SM	 0.6200	 0.3850
SN	 0.6190	 0.3850
SO	 0.6160	 0.3850
SP	 0.6190	 0.3850
SQ	 0.6190	 0.3840
SR	 0.6180	 0.3850
SS	 0.6100	 0.3800
ST	 0.6090	 0.3790
SU	 0.6110	 0.3790
SV	 0.6130	 0.3800
SW	 0.6110	 0.3800
SX	 0.6110	 0.3800
SY	 0.5940	 0.3600
SZ	 0.5930	 0.3600
Sa	 0.5950	 0.3590
Sb	 0.5970	 0.3610
Sc	 0.5910	 0.3600
Sd	 0.5950	 0.3610
Se	 0.5670	 0.3440
Sf	 0.5730	 0.3430
Sg	 0.5710	 0.3440
Sh	 0.5700	 0.3430
Si	 0.5730	 0.3440
Sj	 0.5700	 0.3440
Sk	 0.3440	 0.3000
Sl	 0.3440	 0.3000
Sm	 0.3430	 0.3000
Sn	 0.3450	 0.3000
So	 0.3420	 0.3010
Sp	 0.3440	 0.3000
TM	 0.6350	 0.4510
TN	 0.6400	 0.4490
TO	 0.6350	 0.4480
TP	 0.6410	 0.4500

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Chain	Atom inclusion	Q-score
TQ	 0.6420	 0.4500
TR	 0.6320	 0.4490
TS	 0.6450	 0.4420
TT	 0.6440	 0.4430
TU	 0.6520	 0.4440
TV	 0.6480	 0.4440
TW	 0.6470	 0.4450
TX	 0.6490	 0.4430
TY	 0.6500	 0.4440
TZ	 0.6470	 0.4420
Ta	 0.6500	 0.4440
Tb	 0.6560	 0.4460
Tc	 0.6500	 0.4440
Td	 0.6530	 0.4440
Te	 0.6340	 0.4360
Tf	 0.6310	 0.4370
Tg	 0.6290	 0.4370
Th	 0.6310	 0.4360
Ti	 0.6270	 0.4350
Tj	 0.6310	 0.4350
Tk	 0.6170	 0.4040
Tl	 0.6190	 0.4030
Tm	 0.6190	 0.4050
Tn	 0.6210	 0.4050
To	 0.6200	 0.4030
Tp	 0.6150	 0.4060
Tq	 0.1420	 0.2930
Tr	 0.1430	 0.2900
Ts	 0.1450	 0.2900
Tt	 0.1420	 0.2900
Tu	 0.1420	 0.2920
Tv	 0.1450	 0.2920