



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 09:24 PM UTC

PDB ID : 9EV2 / pdb_00009ev2
EMDB ID : EMD-19992
Title : Tail tube and extended tail sheath tube of Klebsiella phage KP1 variant vB_Kpn_Lilla1
Authors : Orlova, E.V.; Isupov, M.N.
Deposited on : 2024-03-28
Resolution : 3.80 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:

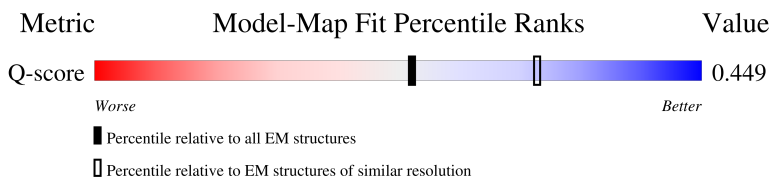
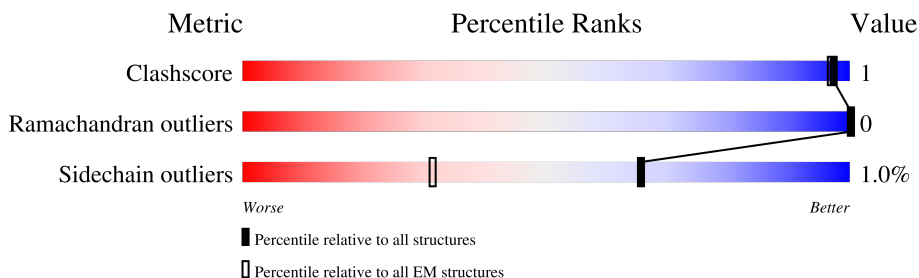
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.80 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	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	S1	656	84% 98% .
1	S2	656	84% 97% .
1	SA	656	87% 97% .
1	SB	656	88% 97% .

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Mol	Chain	Length	Quality of chain
1	SC	656	87% 97%
1	SD	656	87% 97%
1	SE	656	88% 97%
1	SF	656	87% 97%
1	SG	656	83% 97%
1	SH	656	81% 97%
1	SI	656	81% 97%
1	SJ	656	82% 97%
1	SK	656	81% 97%
1	SL	656	81% 97%
1	SM	656	81% 97%
1	SN	656	82% 97%
1	SO	656	82% 97%
1	SP	656	81% 97%
1	SQ	656	82% 97%
1	SR	656	82% 97%
1	SS	656	82% 97%
1	ST	656	81% 97%
1	SU	656	81% 97%
1	SV	656	82% 97%
1	SW	656	81% 97%
1	SX	656	81% 97%
1	SY	656	81% 97%
1	SZ	656	82% 97%
1	Sa	656	81% 97%

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Mol	Chain	Length	Quality of chain
1	Sb	656	81% 97% .
1	Sc	656	82% 97% .
1	Sd	656	81% 97% .
1	Se	656	82% 97% .
1	Sf	656	82% 97% .
1	Sg	656	82% 97% .
1	Sh	656	82% 97% .
1	Si	656	82% 97% .
1	Sj	656	82% 97% .
1	Sk	656	83% 97% .
1	Sl	656	82% 97% .
1	Sm	656	82% 97% .
1	Sn	656	83% 97% .
1	So	656	82% 97% .
1	Sp	656	82% 97% .
1	Sq	656	82% 97% .
1	Sr	656	81% 97% .
1	Ss	656	81% 97% .
1	St	656	82% 97% .
1	Su	656	81% 97% .
1	Sv	656	82% 97% .
1	Sw	656	84% 97% .
1	Sx	656	84% 98% .
1	Sy	656	84% 97% .
1	Sz	656	84% 97% .

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Mol	Chain	Length	Quality of chain
2	T1	163	44% 96% ..
2	T2	163	44% 97% ..
2	TA	163	61% 97% ..
2	TB	163	62% 97% ..
2	TC	163	62% 97% ..
2	TD	163	61% 97% ..
2	TE	163	62% 97% ..
2	TF	163	61% 97% ..
2	TG	163	43% 96% ..
2	TH	163	44% 95% ..
2	TI	163	43% 95% ..
2	TJ	163	43% 96% ..
2	TK	163	44% 96% ..
2	TL	163	43% 96% ..
2	TM	163	43% 96% ..
2	TN	163	42% 96% ..
2	TO	163	44% 96% ..
2	TP	163	43% 96% ..
2	TQ	163	42% 96% ..
2	TR	163	44% 96% ..
2	TS	163	39% 96% ..
2	TT	163	42% 96% ..
2	TU	163	43% 96% ..
2	TV	163	40% 96% ..
2	TW	163	42% 96% ..

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Mol	Chain	Length	Quality of chain	
2	TX	163	43%	96%
2	TY	163	42%	96%
2	TZ	163	43%	96%
2	Ta	163	41%	96%
2	Tb	163	42%	96%
2	Tc	163	43%	96%
2	Td	163	41%	96%
2	Te	163	43%	96%
2	Tf	163	43%	96%
2	Tg	163	42%	96%
2	Th	163	44%	96%
2	Ti	163	43%	96%
2	Tj	163	42%	96%
2	Tk	163	42%	96%
2	Tl	163	43%	96%
2	Tm	163	41%	95%
2	Tn	163	42%	96%
2	To	163	43%	96%
2	Tp	163	42%	95%
2	Tq	163	43%	96%
2	Tr	163	40%	95%
2	Ts	163	43%	95%
2	Tt	163	42%	96%
2	Tu	163	40%	96%
2	Tv	163	43%	96%

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Mol	Chain	Length	Quality of chain
2	Tw	163	43% 97% ..
2	Tx	163	44% 96% ..
2	Ty	163	44% 97% ..
2	Tz	163	42% 96% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 342468 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 Tail sheath protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S1	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	S2	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SA	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SB	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SC	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SD	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SE	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SF	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SG	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SH	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SI	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SJ	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SK	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SL	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SM	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SN	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	SO	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Sk	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sl	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sm	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sn	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	So	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sp	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sq	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sr	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Ss	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	St	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Su	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sv	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sw	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sx	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sy	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		
1	Sz	655	Total	C	N	O	S	0	0
			5037	3170	856	995	16		

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S1	482	ILE	VAL	conflict	UNP A0A2K9V5S7
S2	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
SQ	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SR	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SS	482	ILE	VAL	conflict	UNP A0A2K9V5S7
ST	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SU	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SV	482	ILE	VAL	conflict	UNP A0A2K9V5S7
SW	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
Sq	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sr	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Ss	482	ILE	VAL	conflict	UNP A0A2K9V5S7
St	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Su	482	ILE	VAL	conflict	UNP A0A2K9V5S7

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Chain	Residue	Modelled	Actual	Comment	Reference
Sv	482	ILE	VAL	conflict	UNP A0A2K9V5S7
Sw	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

- Molecule 2 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T1	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	T2	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TA	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TB	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TC	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TD	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TE	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TF	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TG	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TH	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TI	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TJ	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TK	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TL	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TM	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TN	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TO	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	TP	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TQ	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TR	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TS	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TT	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TU	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TV	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TW	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TX	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TY	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	TZ	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Ta	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tb	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tc	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Td	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Te	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tf	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tg	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Th	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Ti	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tj	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		

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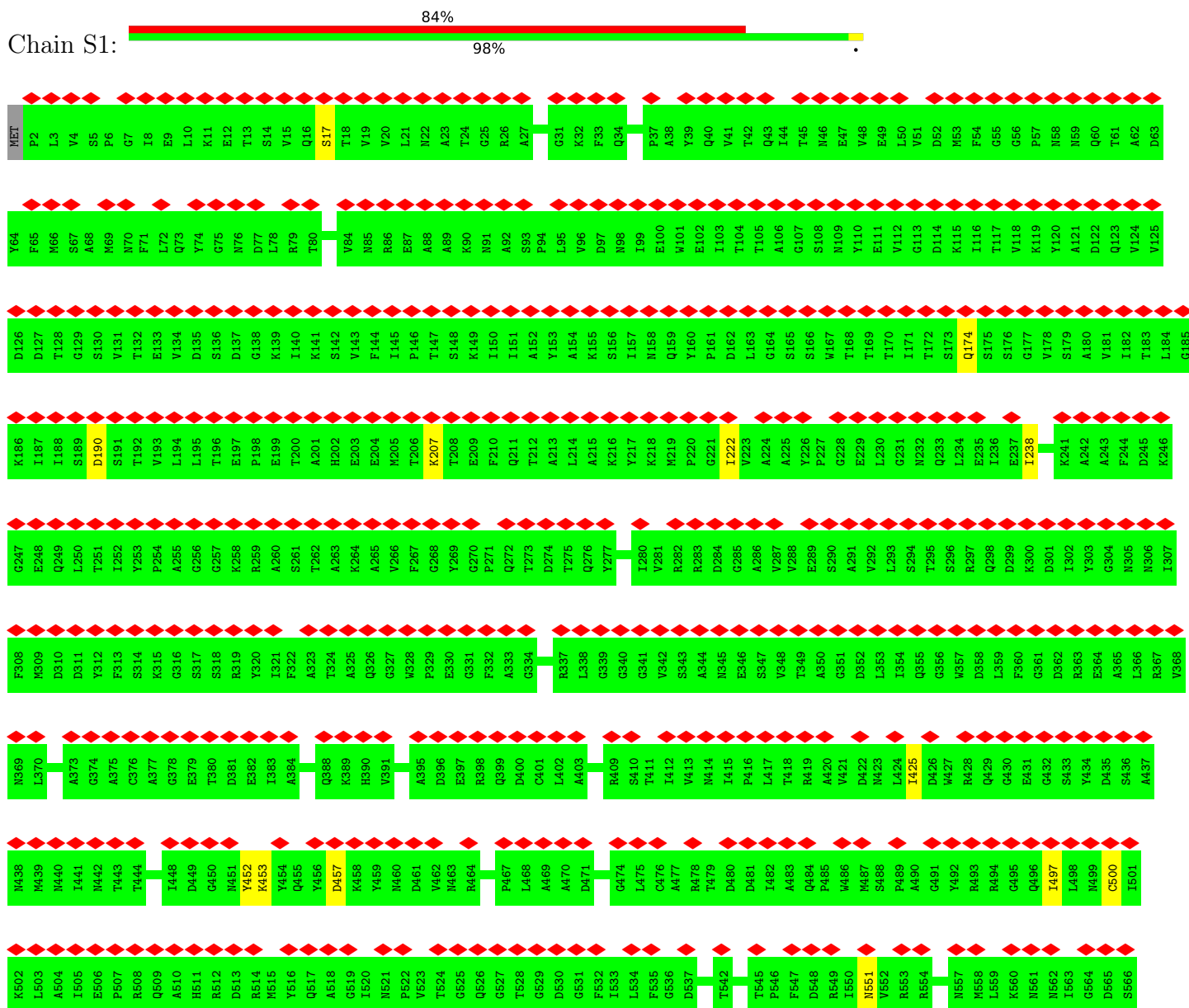
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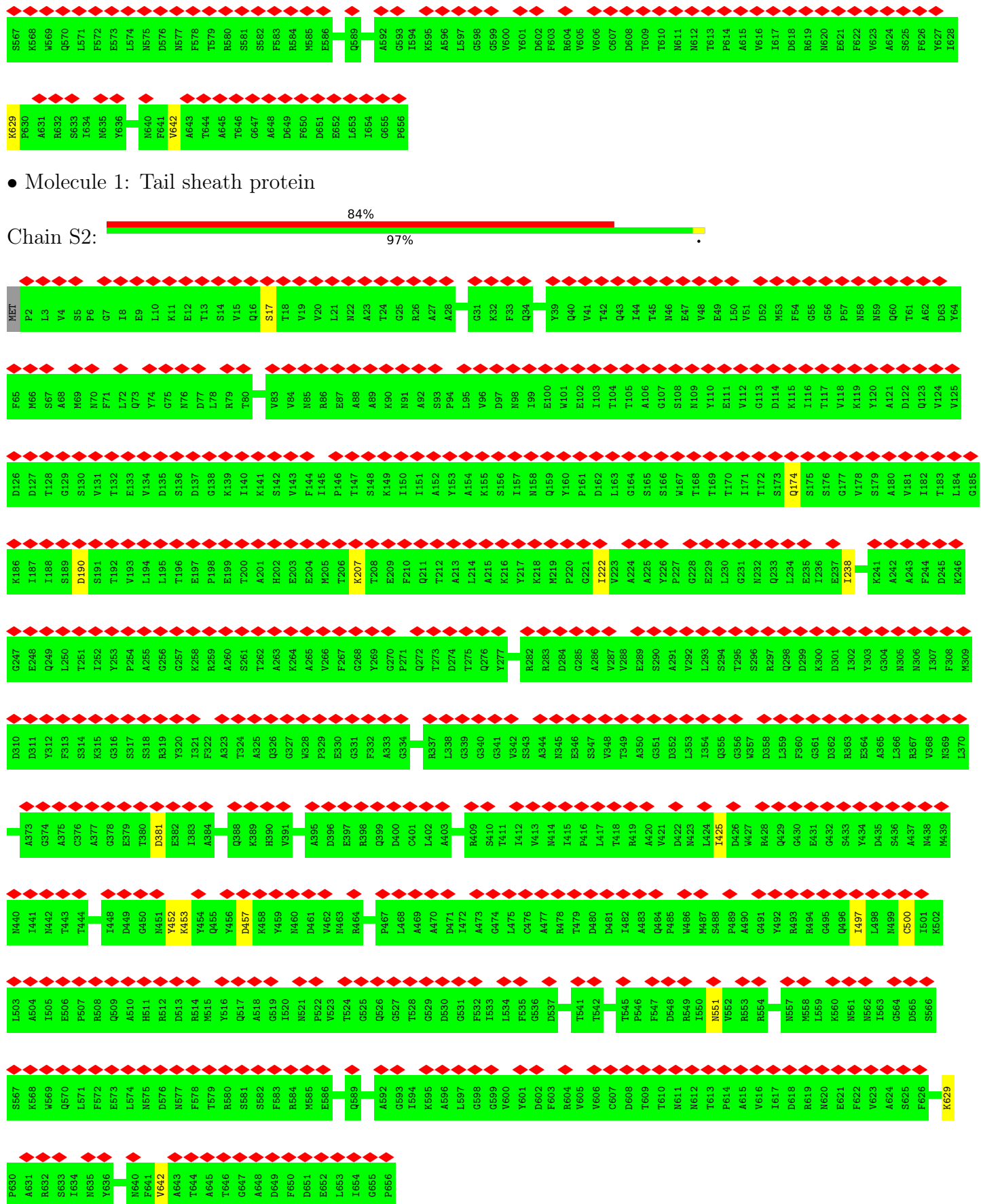
Mol	Chain	Residues	Atoms					AltConf	Trace
2	Tk	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tl	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tm	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tn	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	To	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tp	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tq	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tr	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Ts	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tt	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tu	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tv	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tw	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tx	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Ty	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
2	Tz	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		

3 Residue-property plots

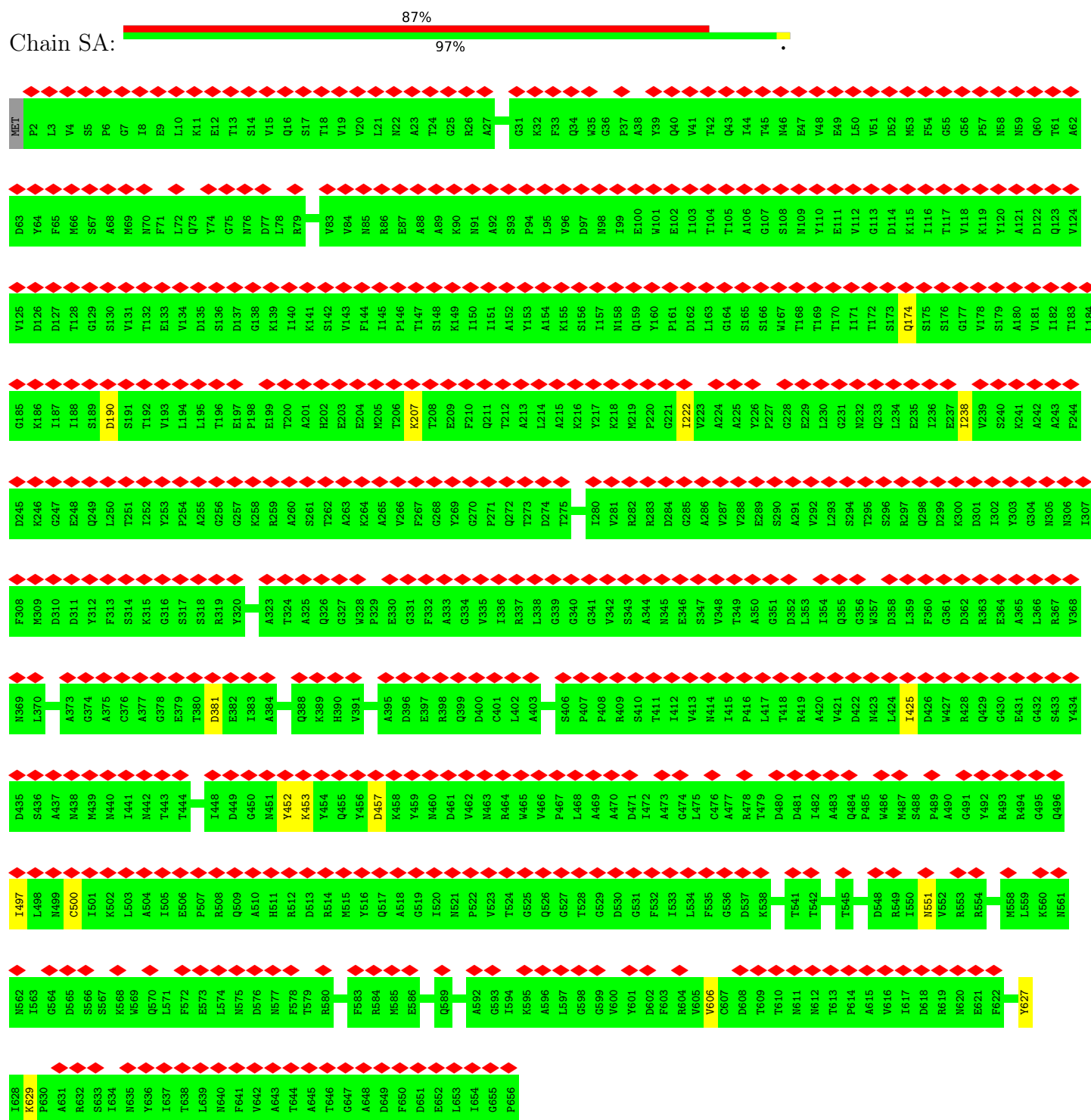
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

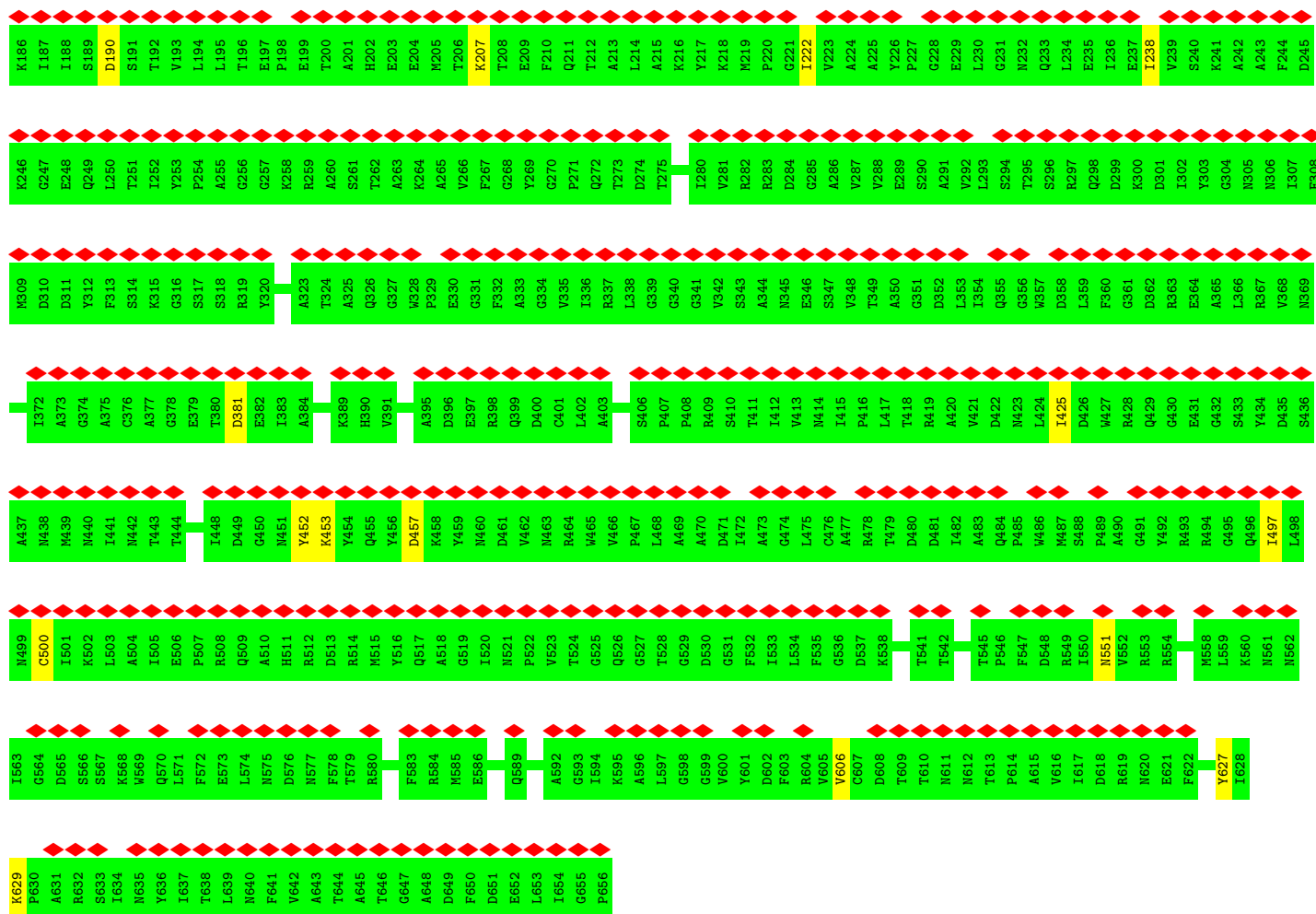
- Molecule 1: Tail sheath protein



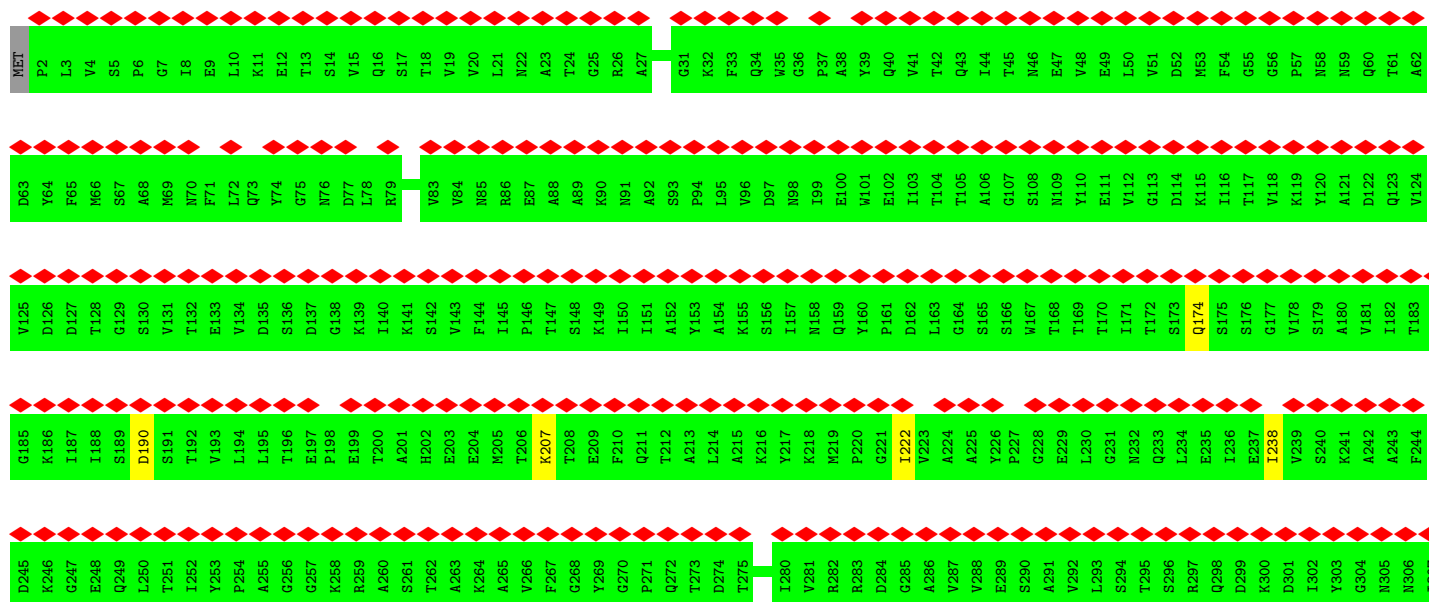


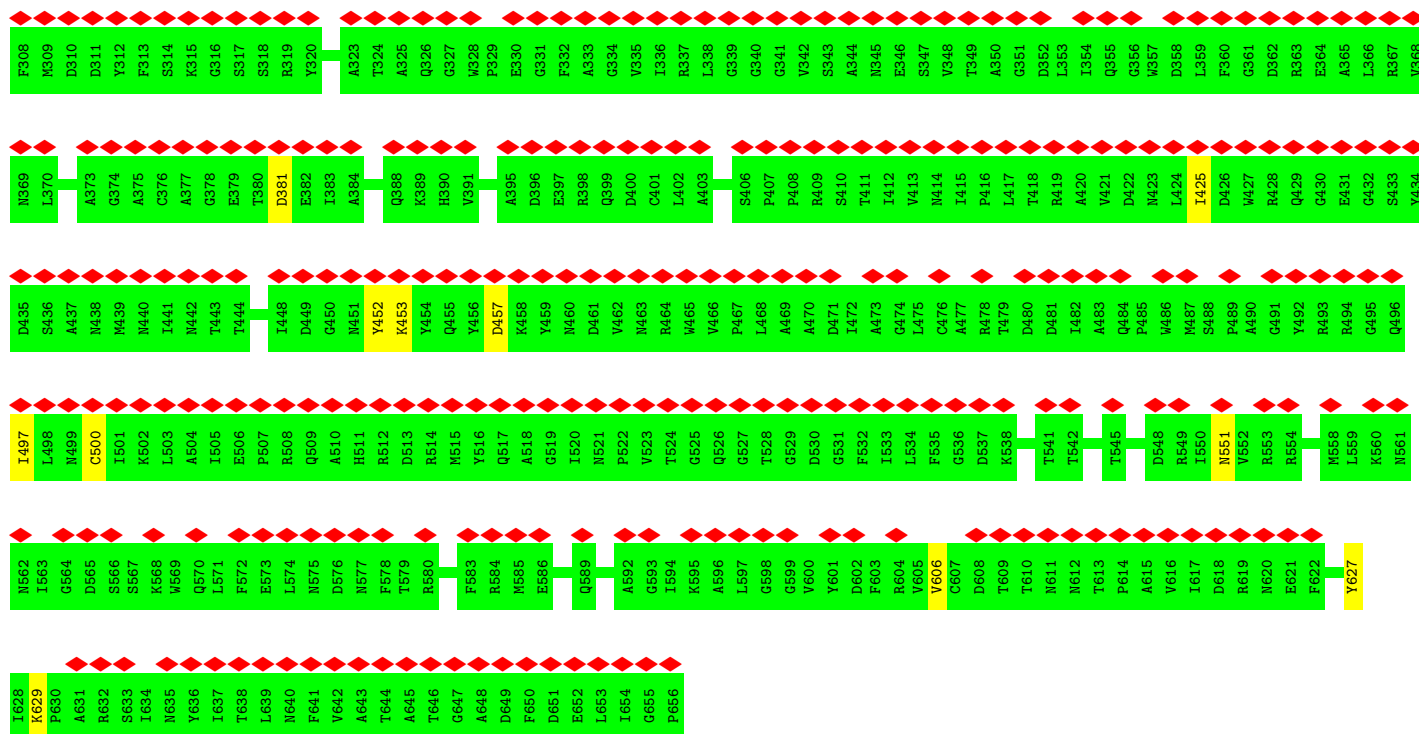
• Molecule 1: Tail sheath protein



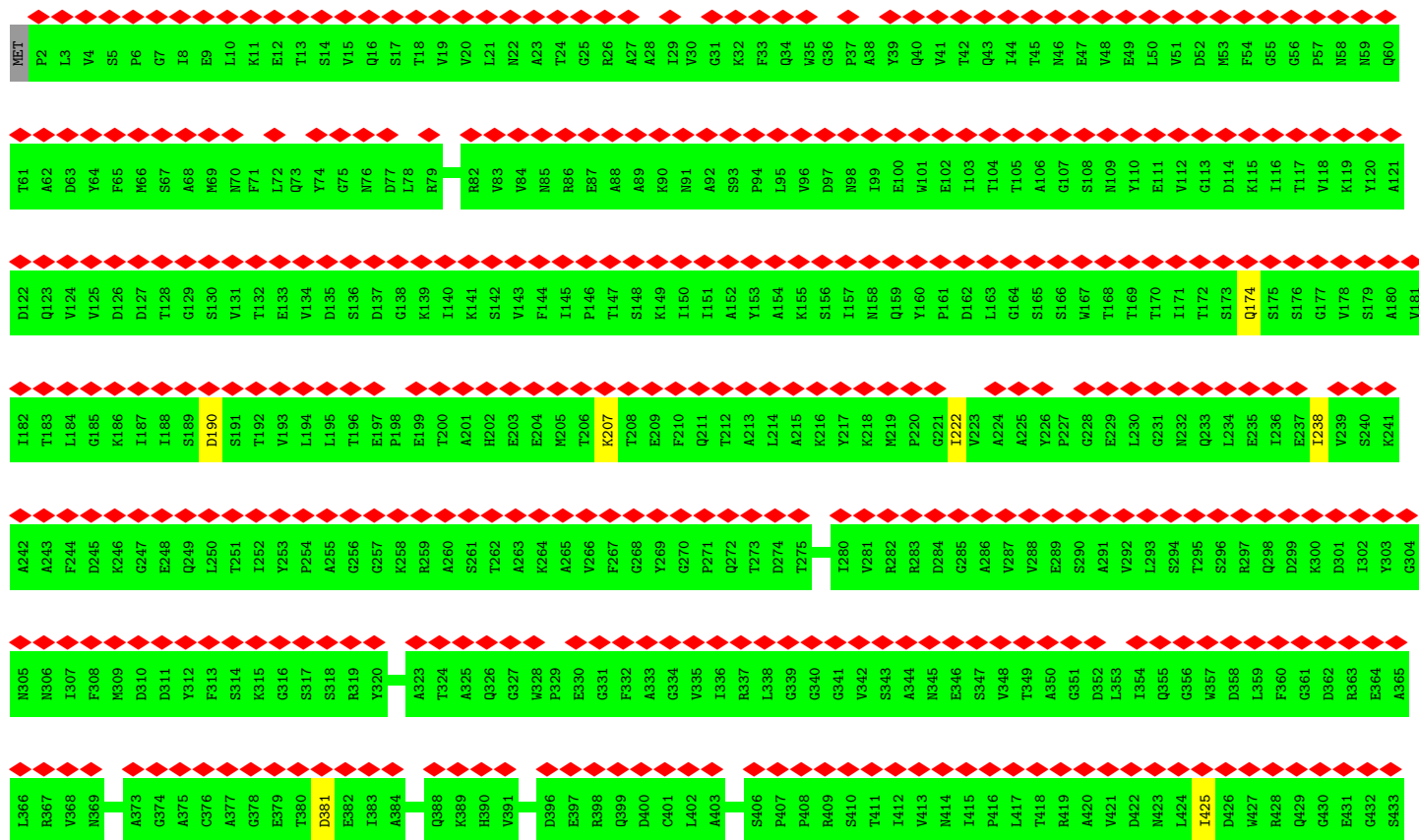


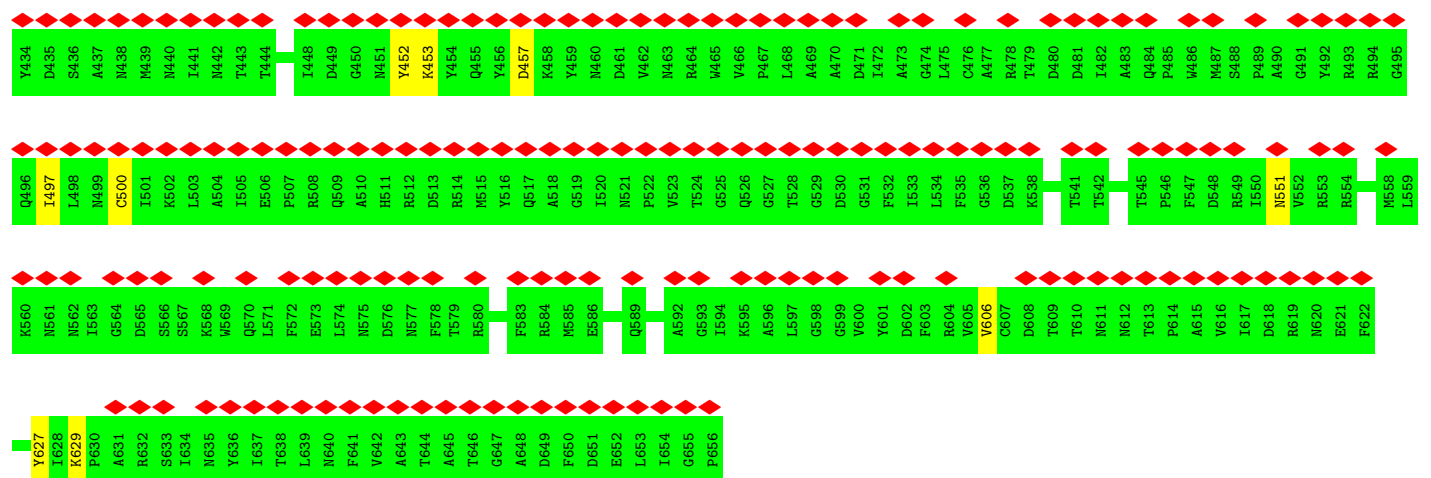
• Molecule 1: Tail sheath protein



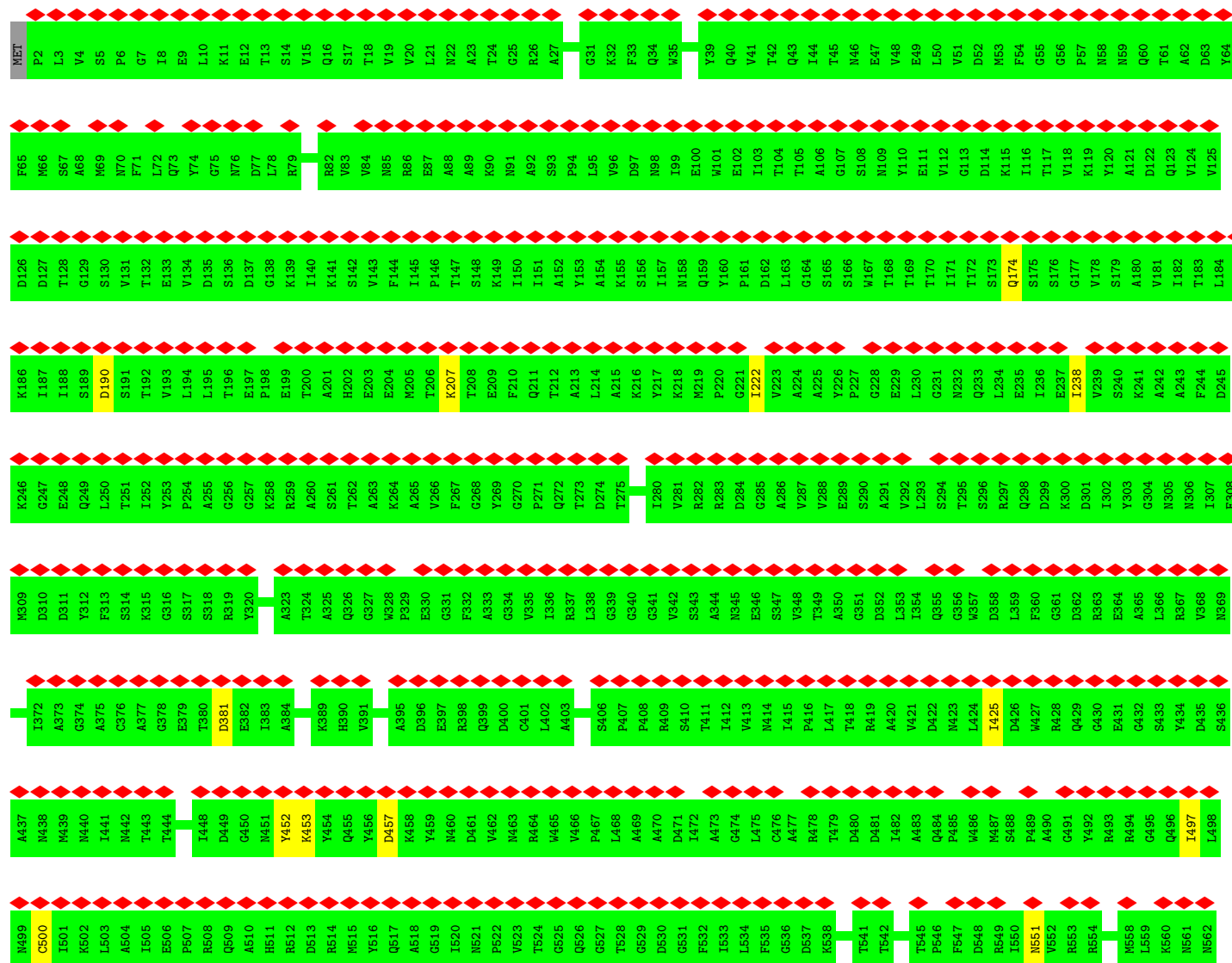


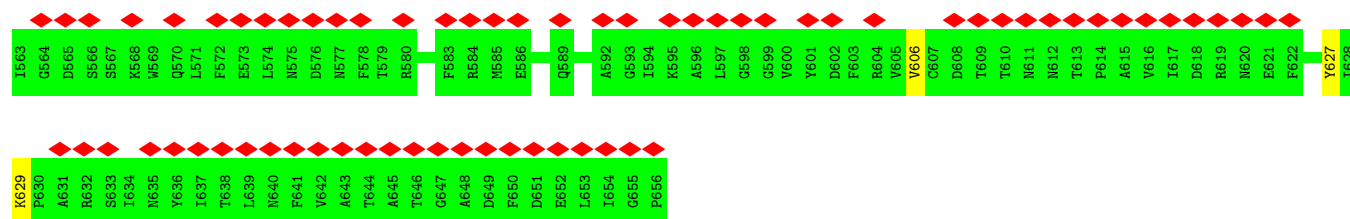
• Molecule 1: Tail sheath protein



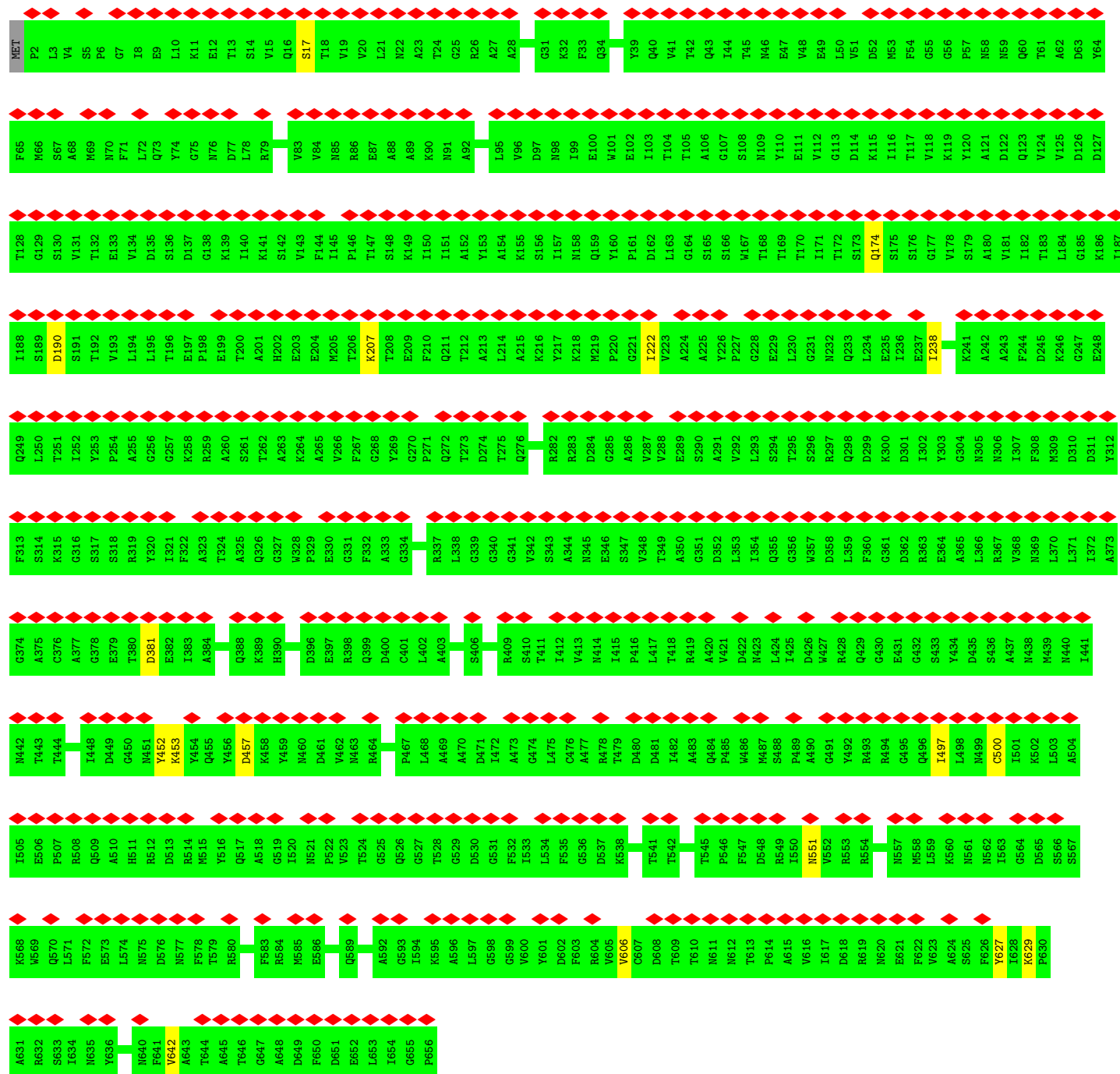
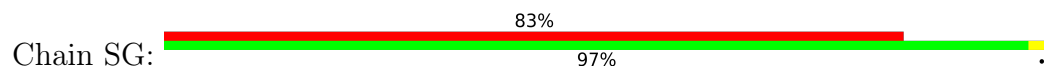


• Molecule 1: Tail sheath protein



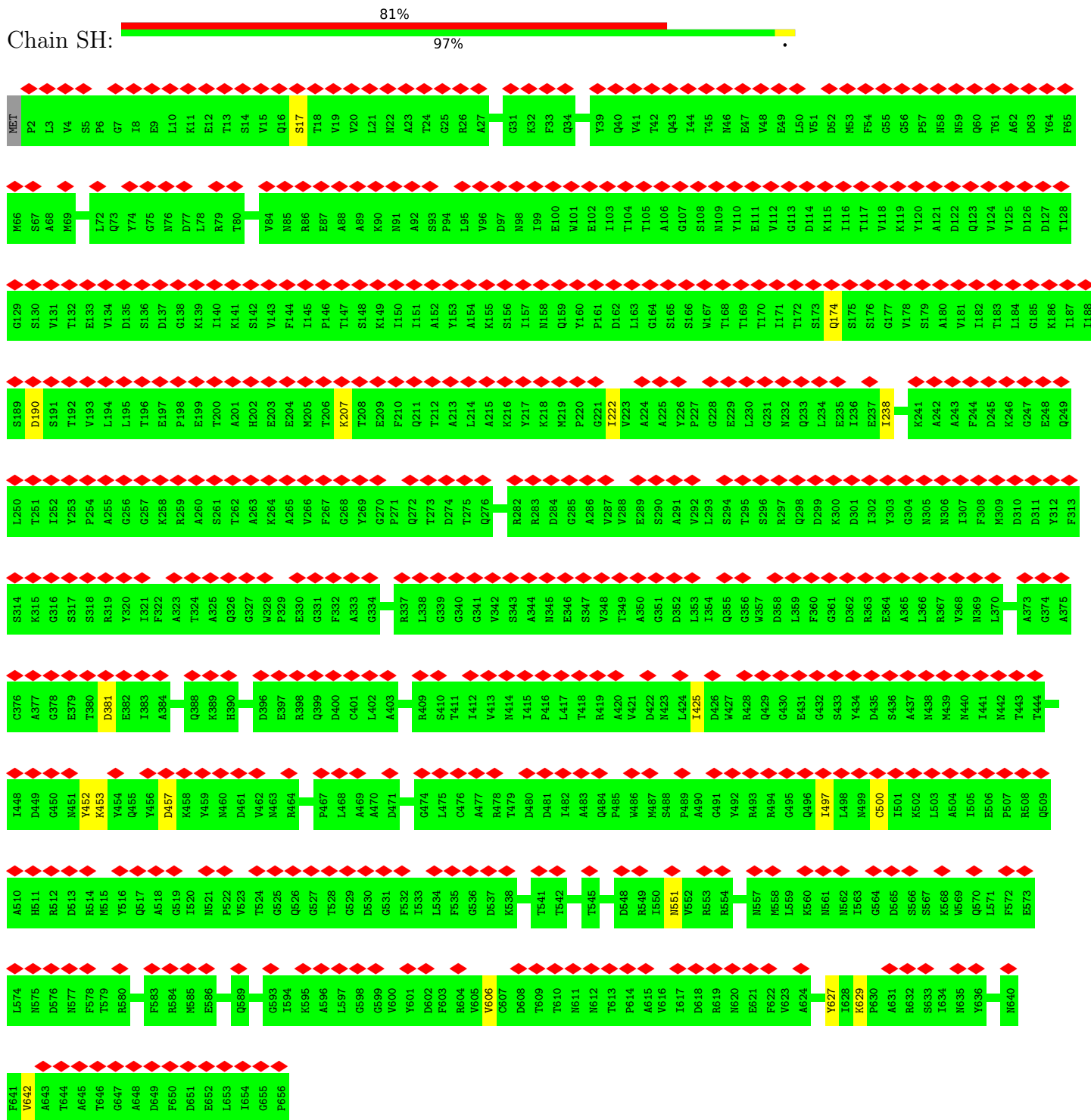


• Molecule 1: Tail sheath protein



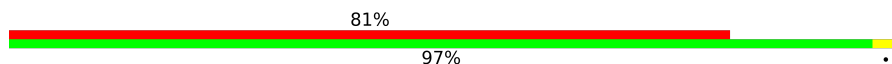
- Molecule 1: Tail sheath protein

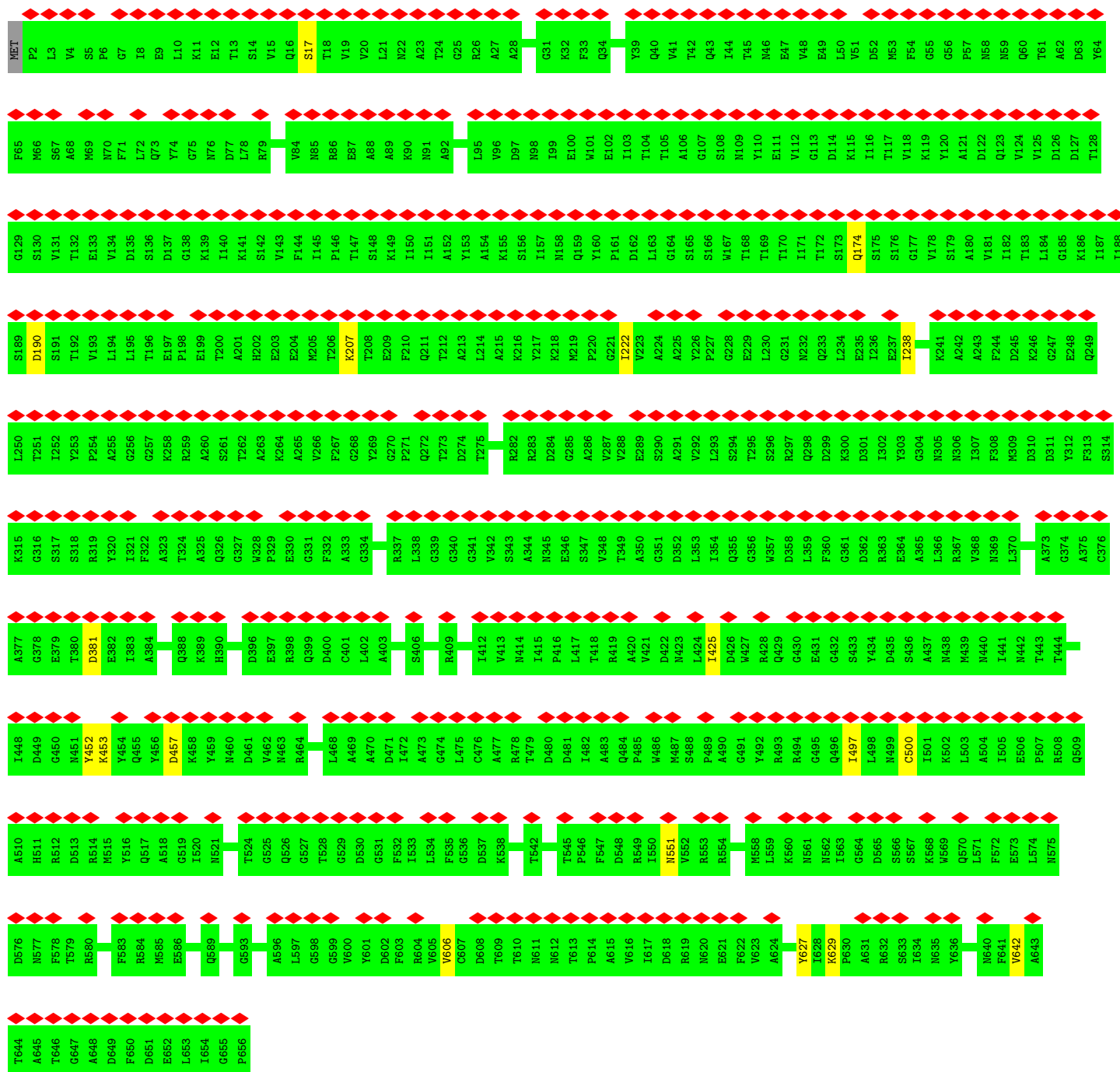
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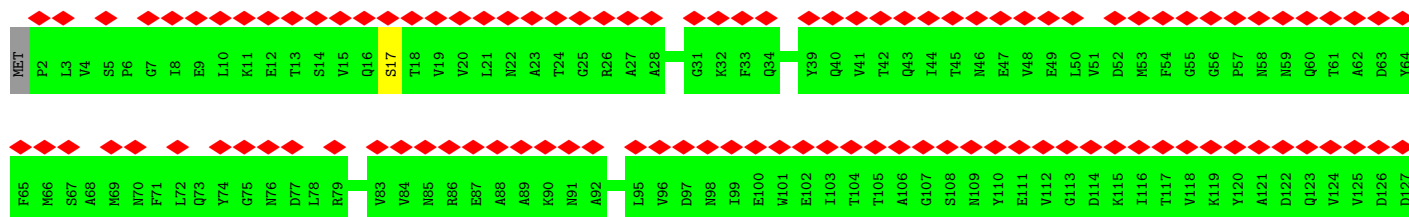
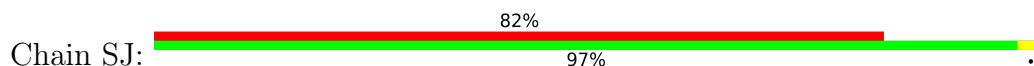
- Molecule 1: Tail sheath protein

Chain SI:





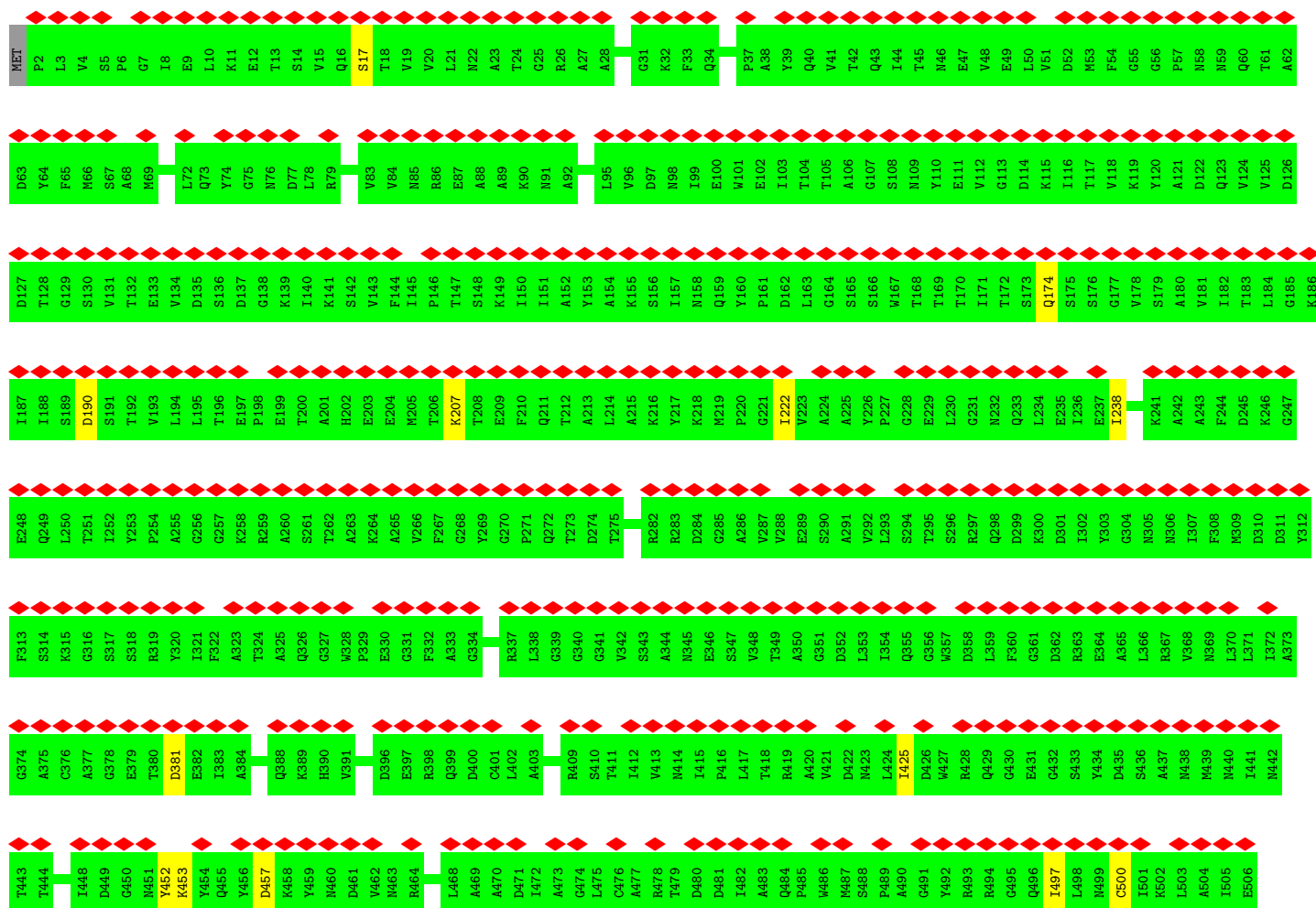
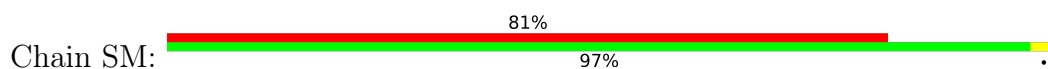
• Molecule 1: Tail sheath protein

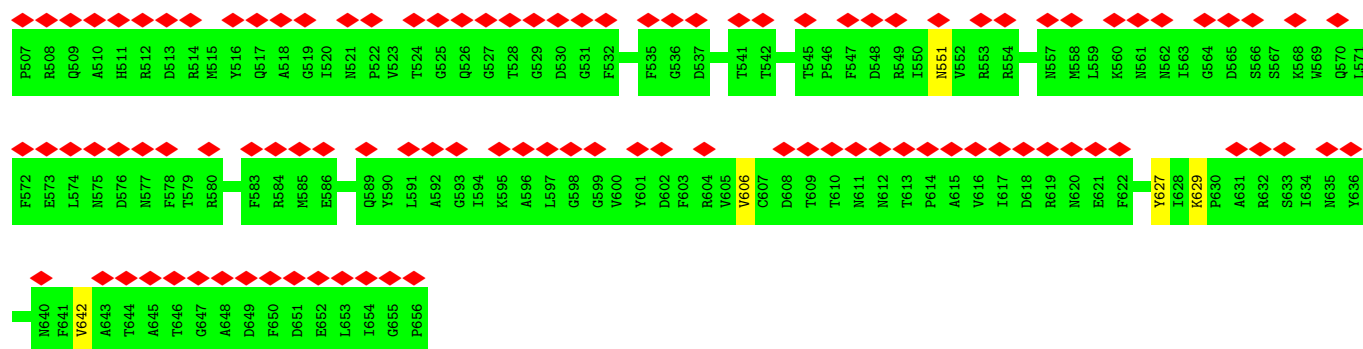




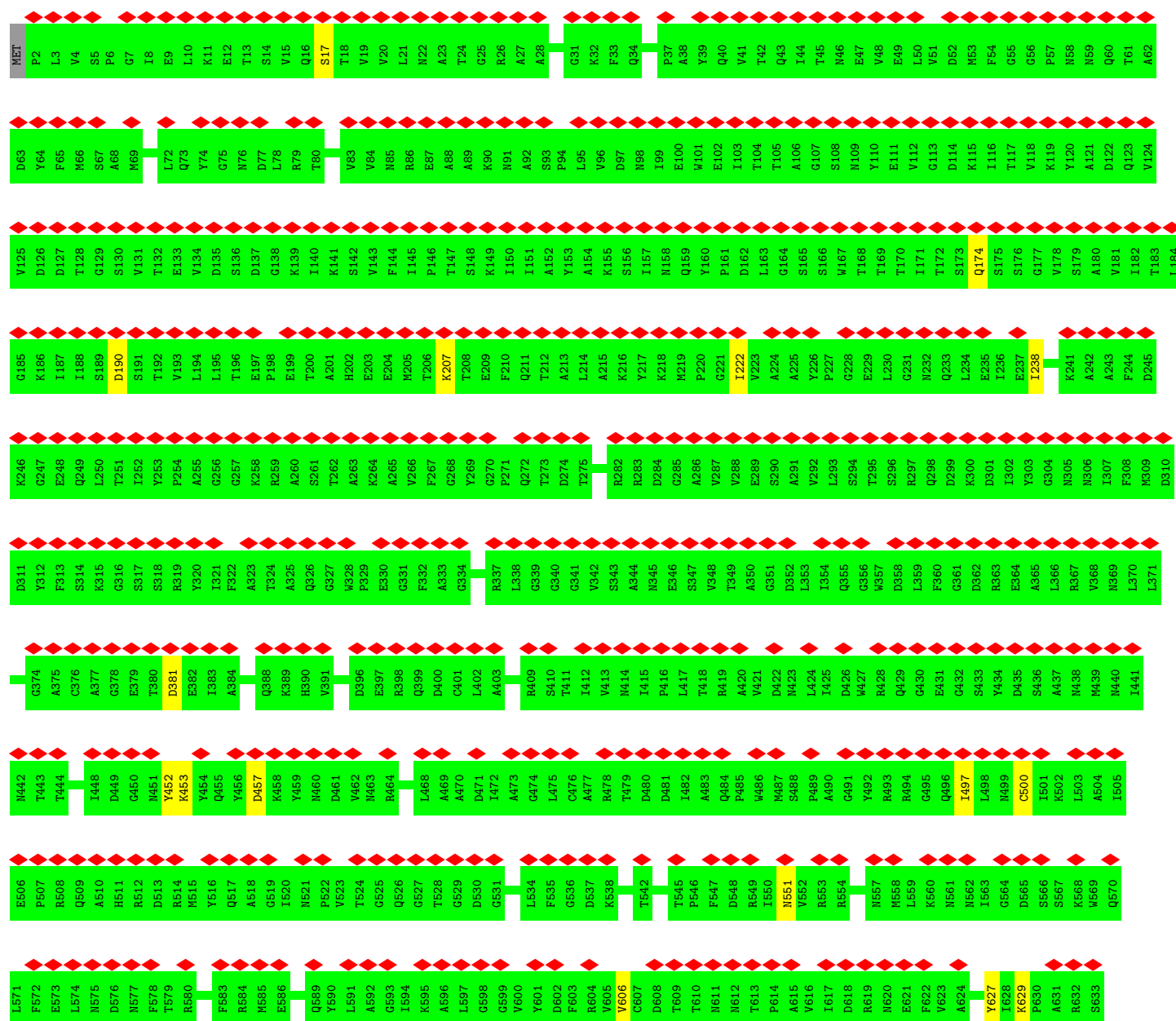
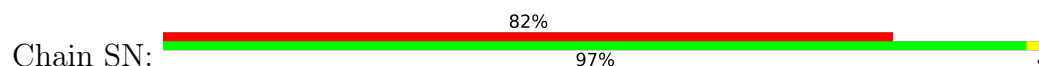


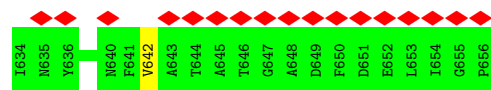
• Molecule 1: Tail sheath protein



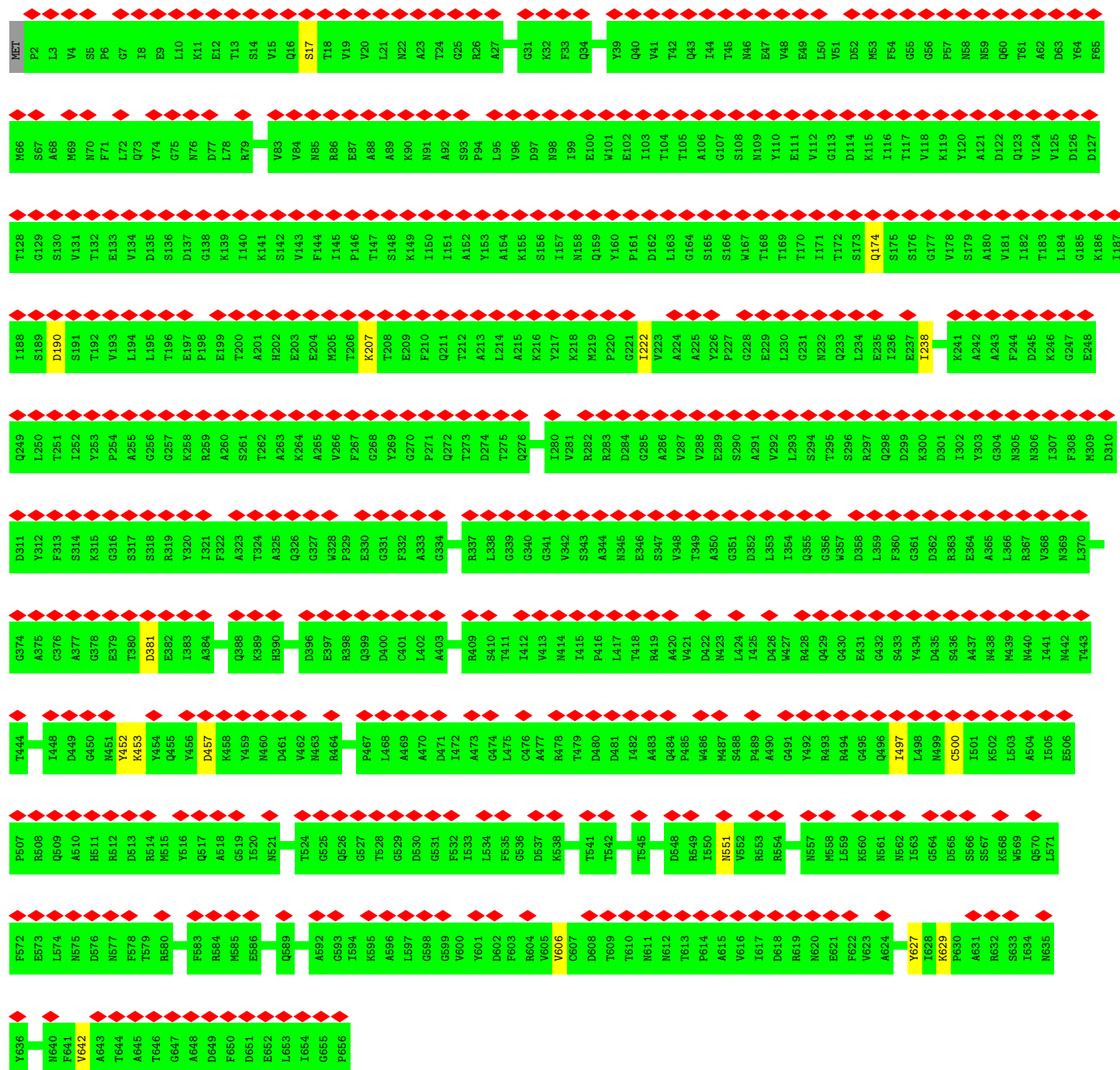
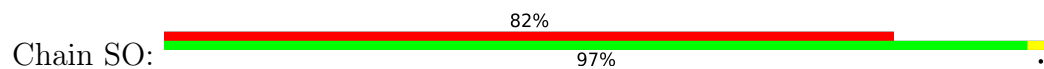


• Molecule 1: Tail sheath protein

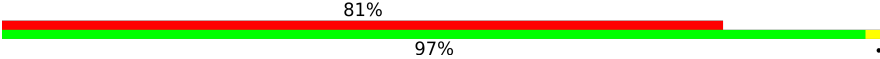


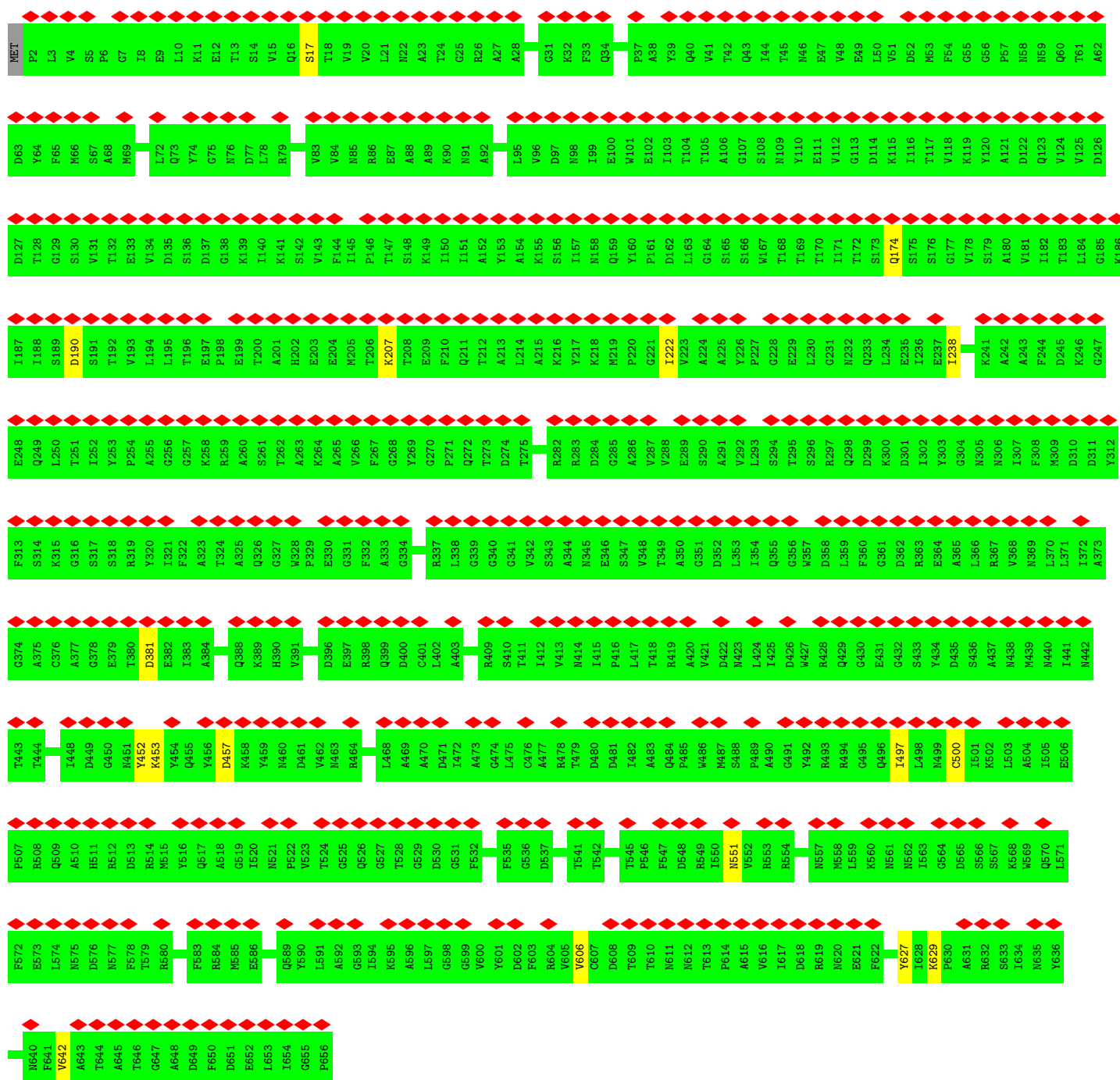


• Molecule 1: Tail sheath protein

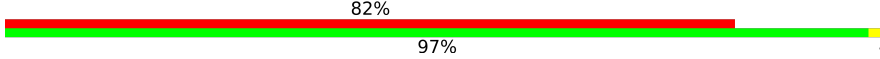


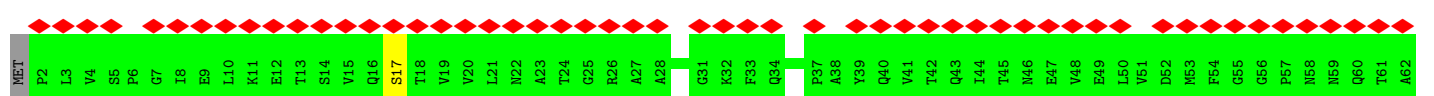
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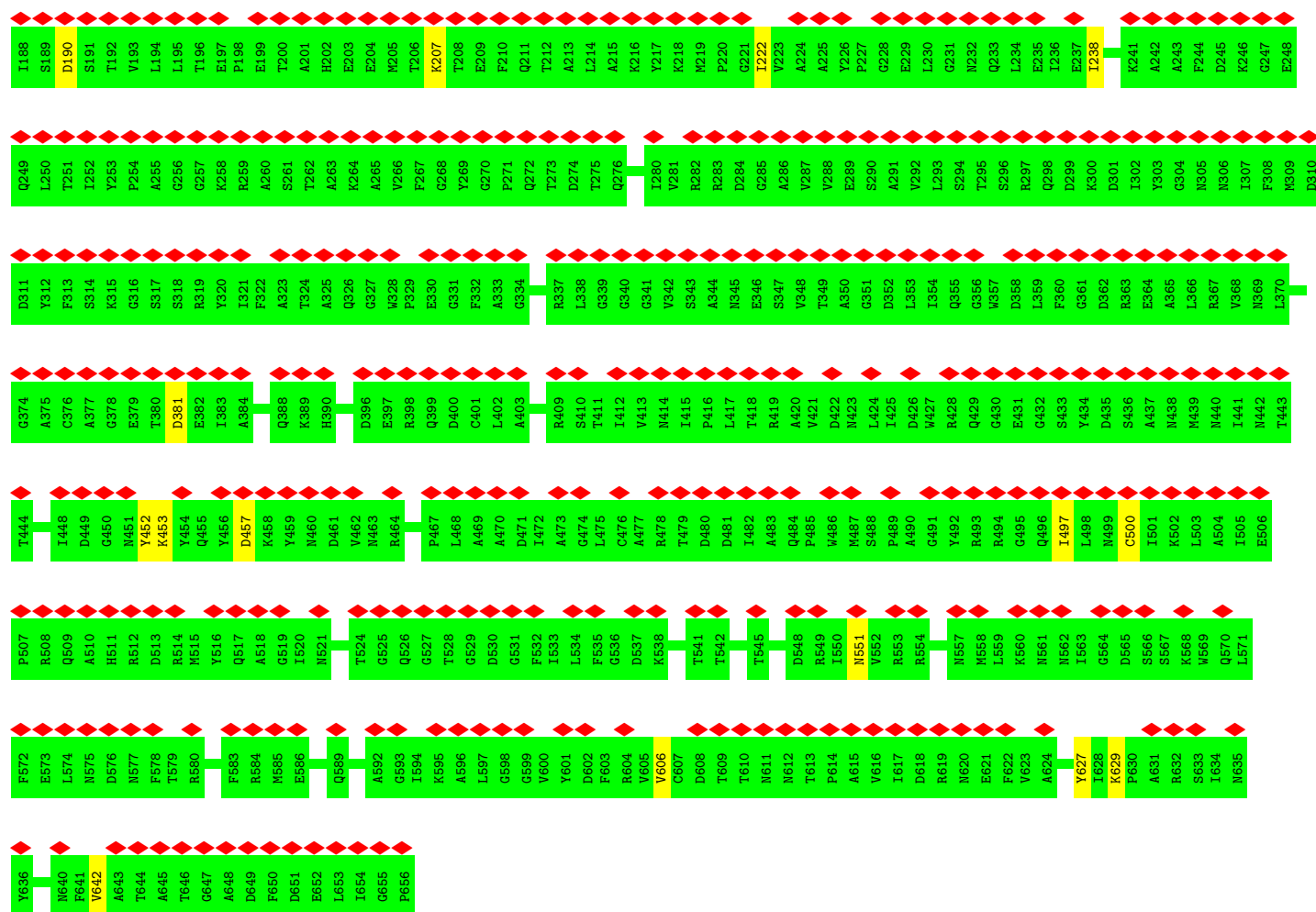
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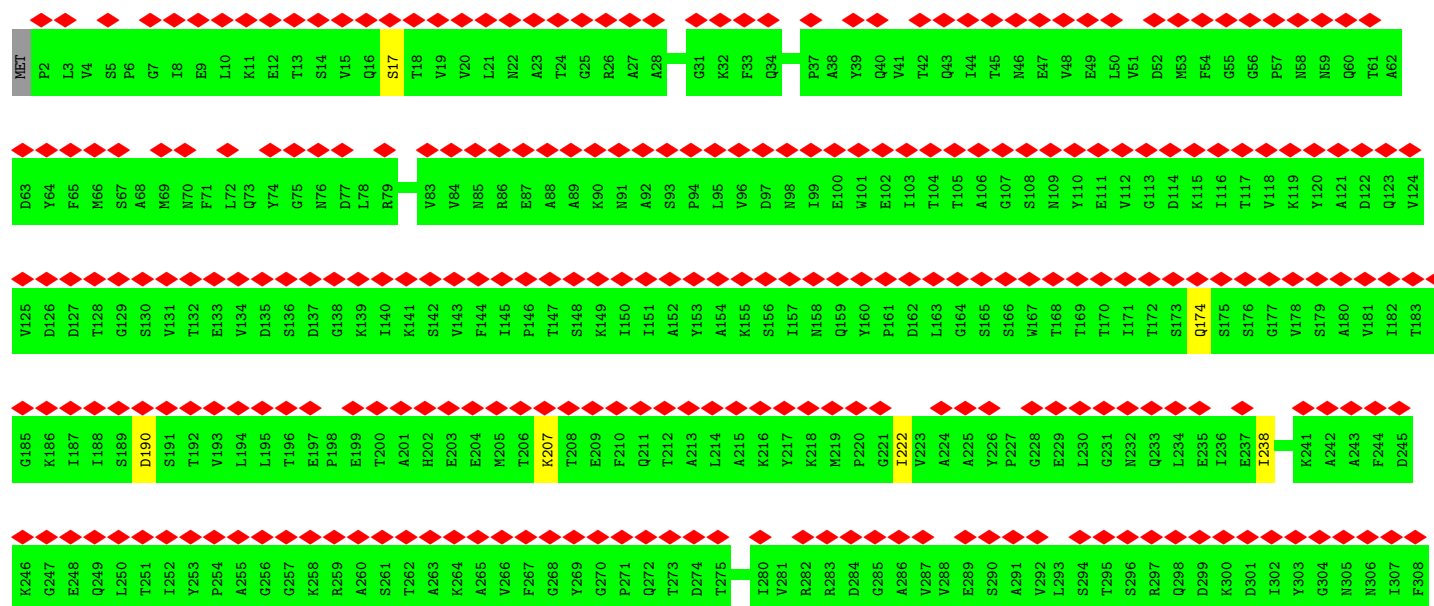
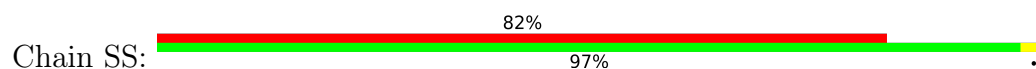
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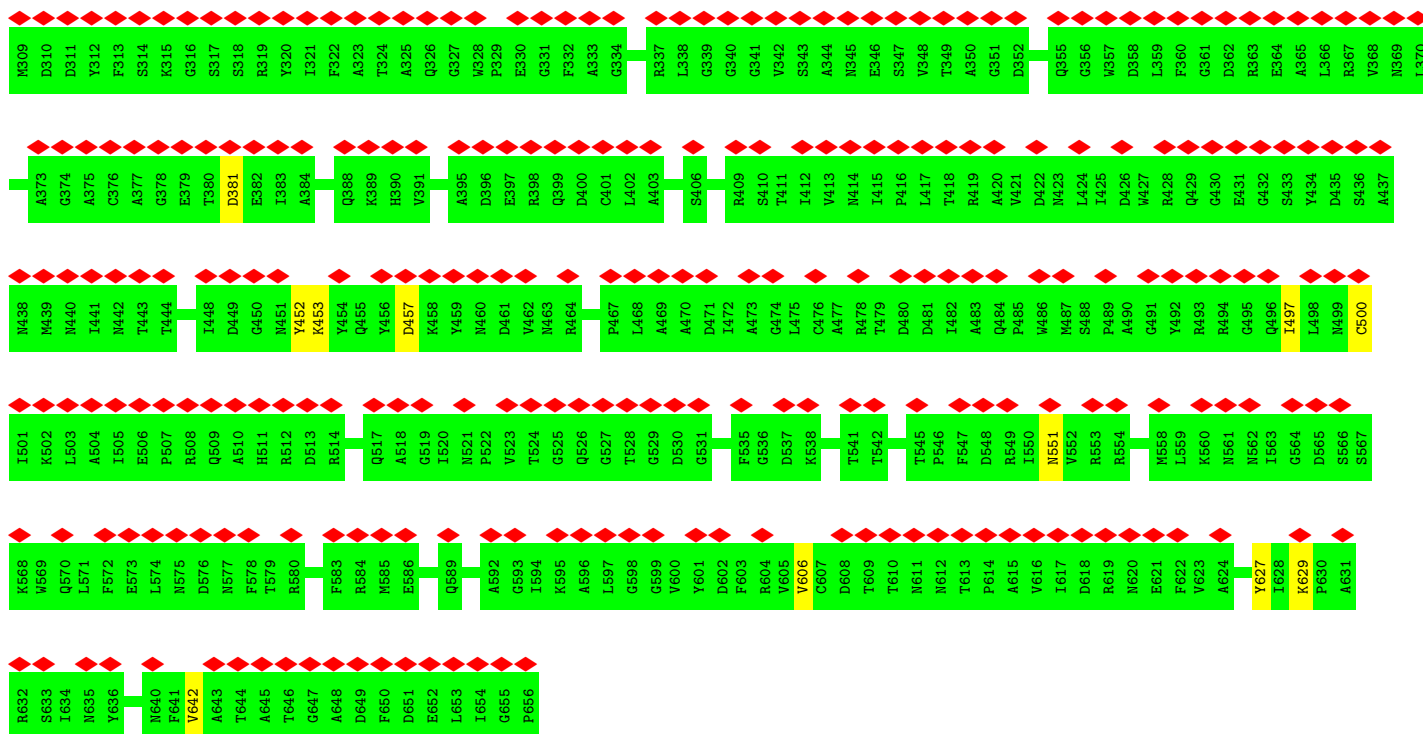
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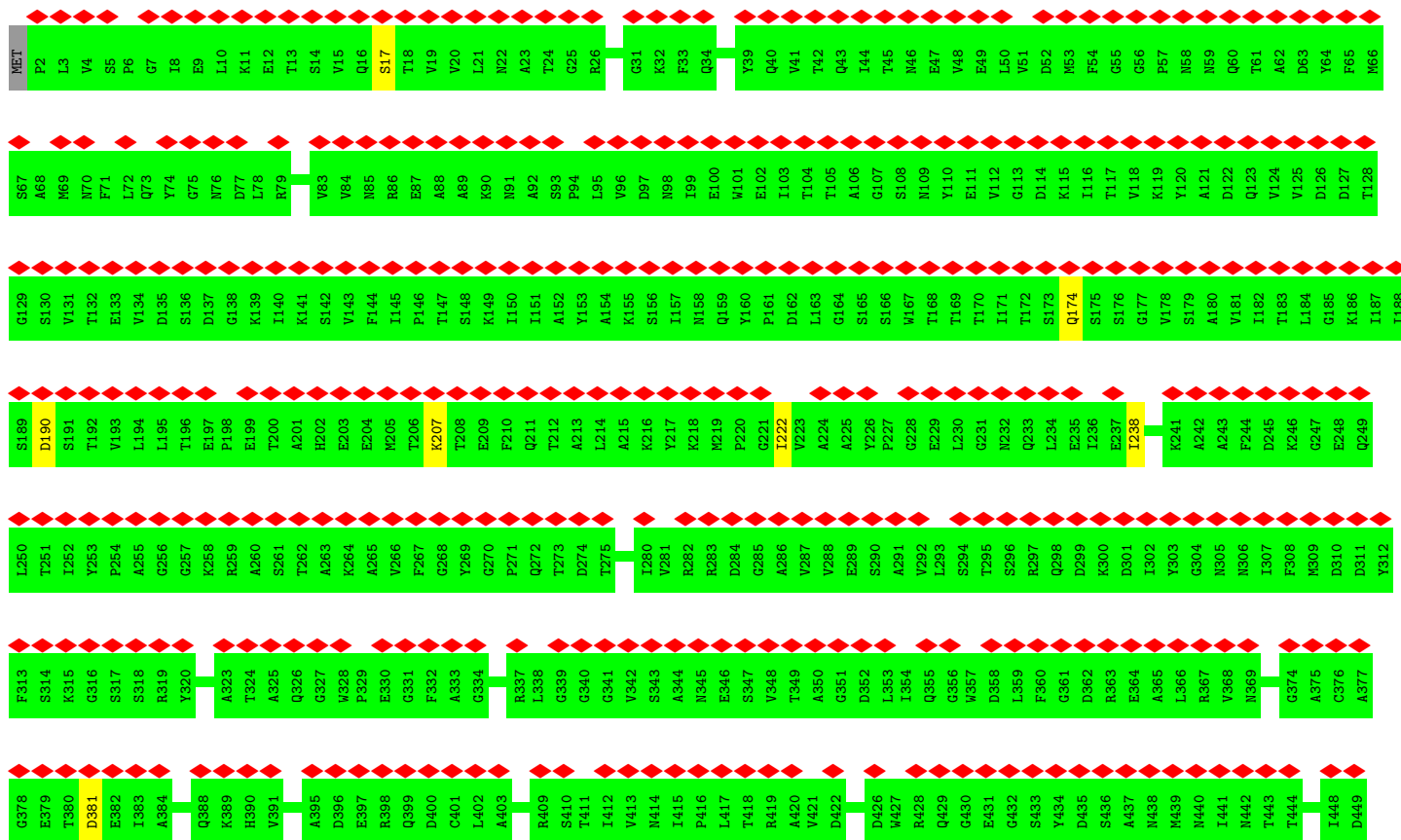
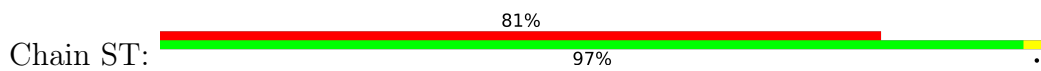


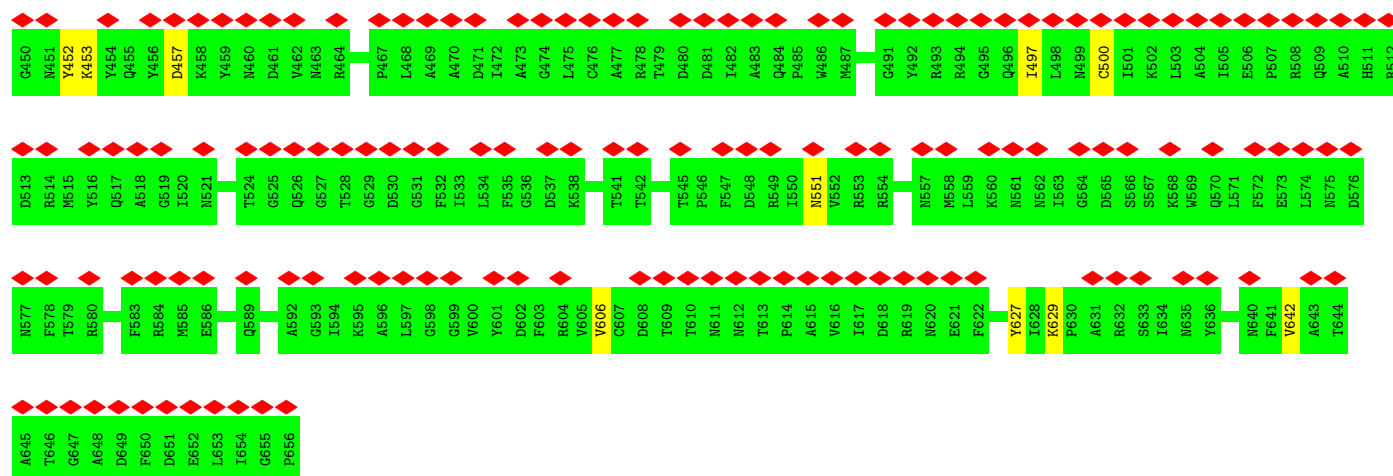
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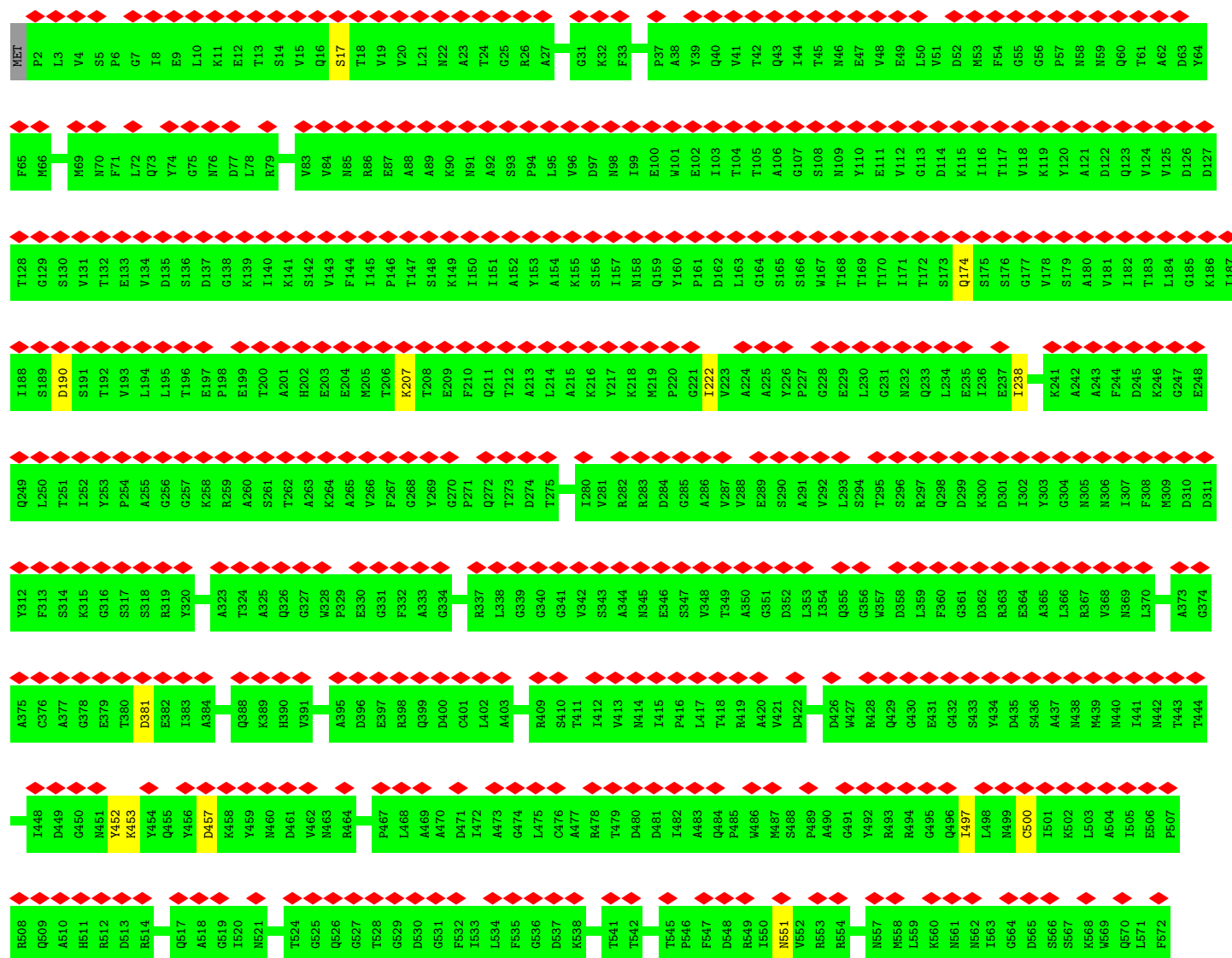
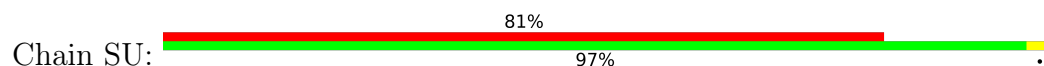


• Molecule 1: Tail sheath protein

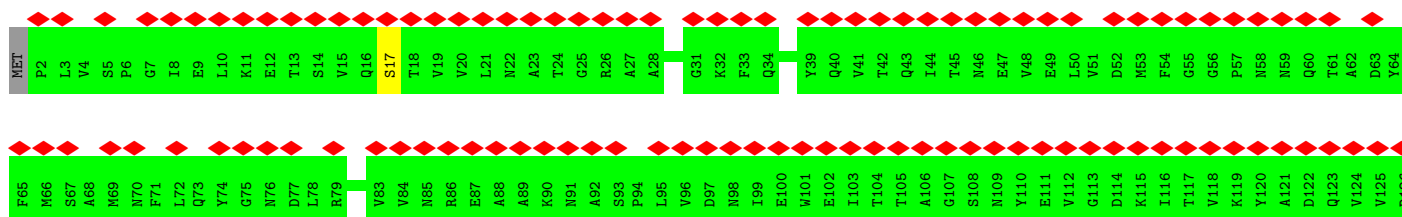


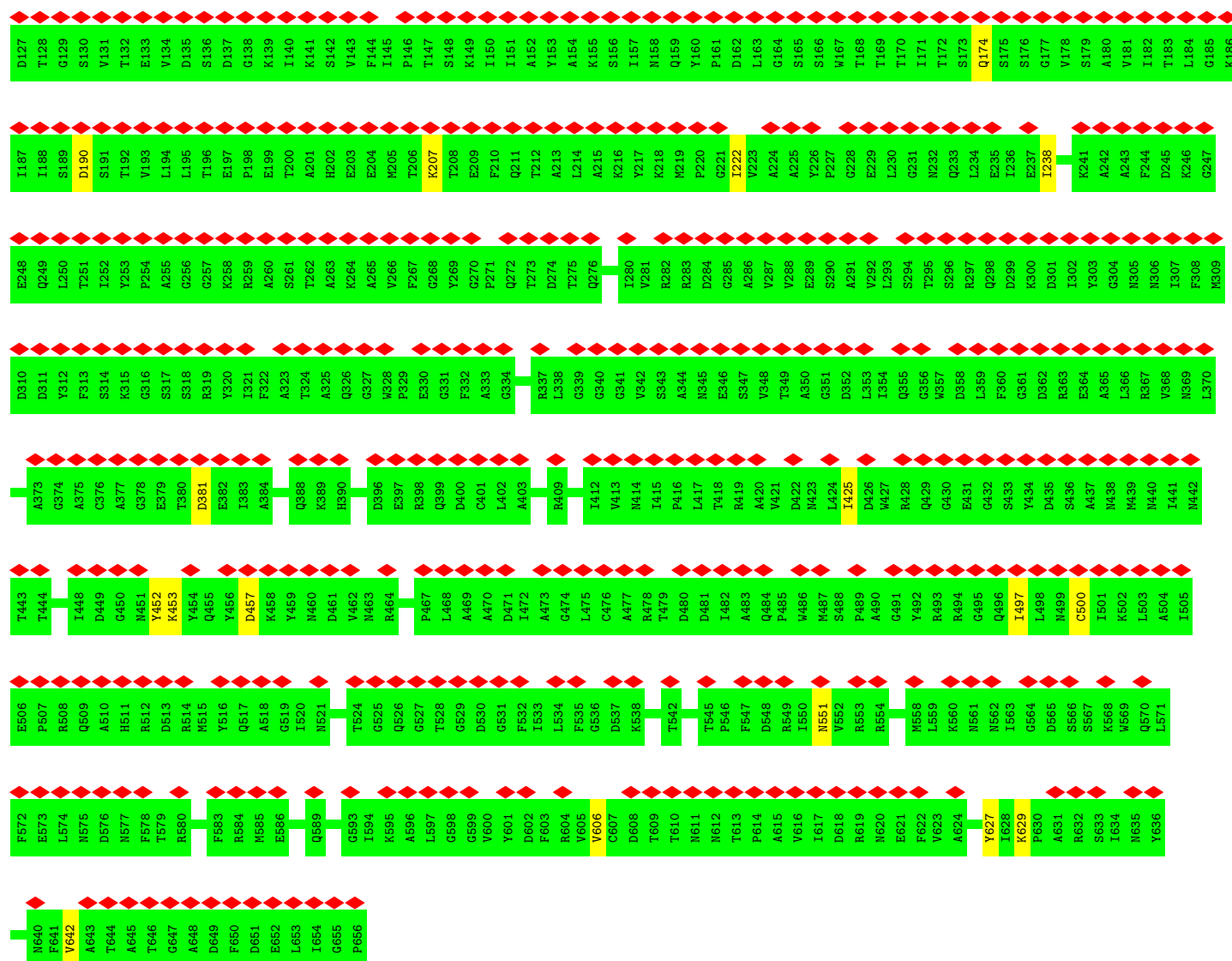


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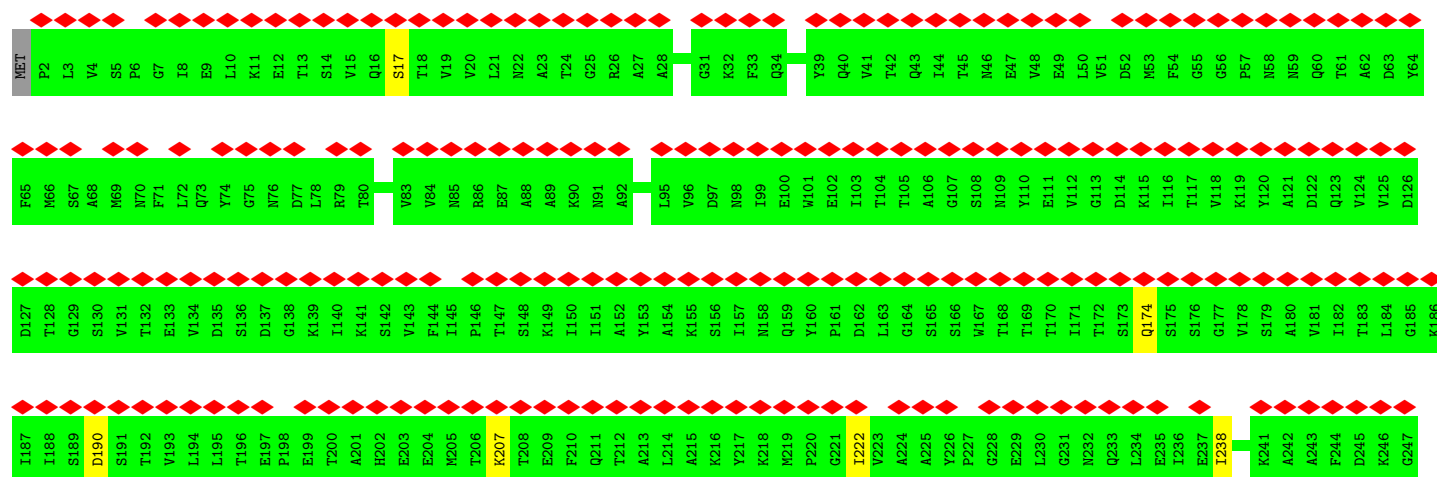
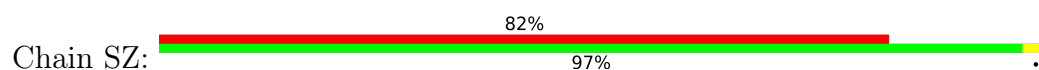


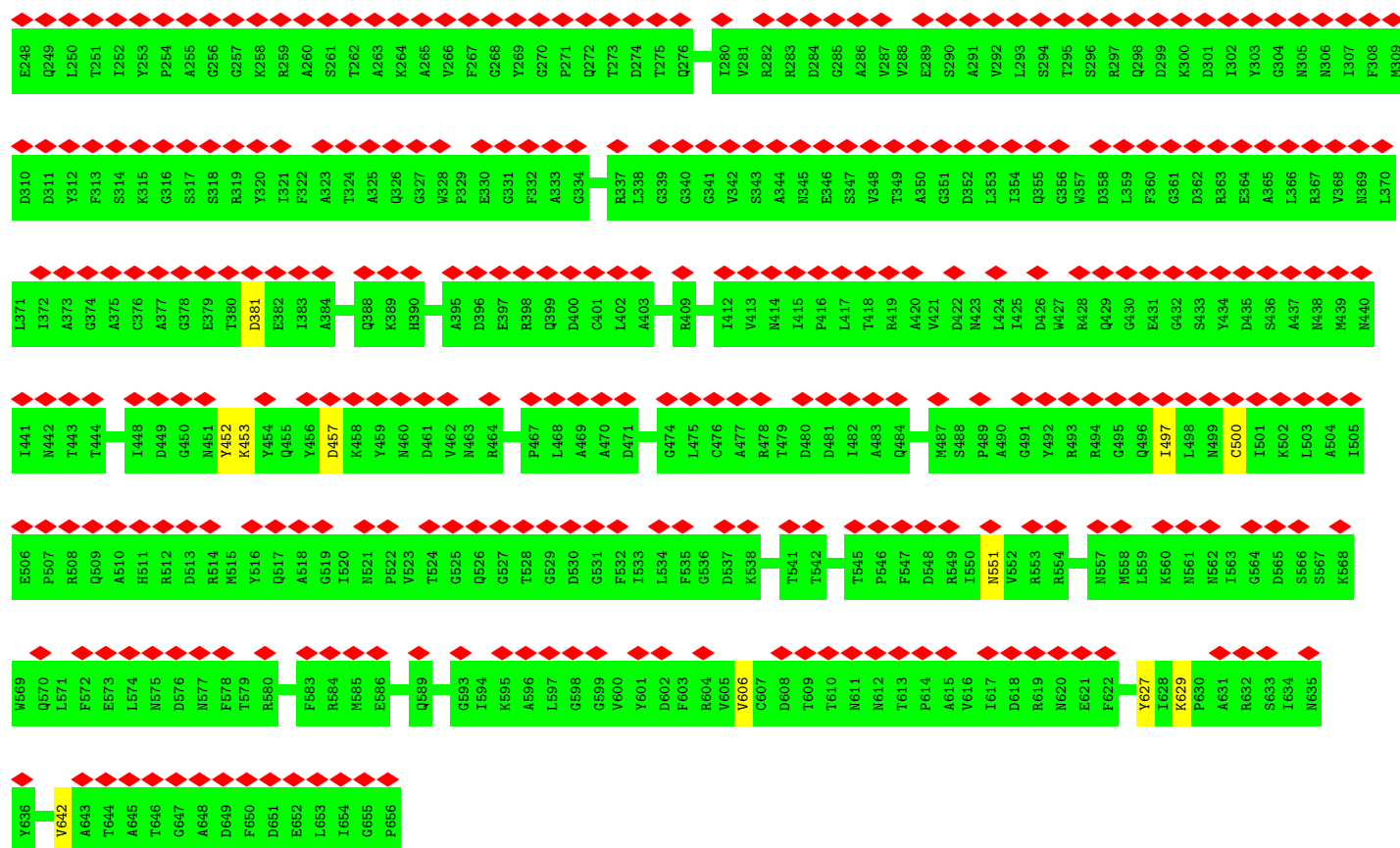




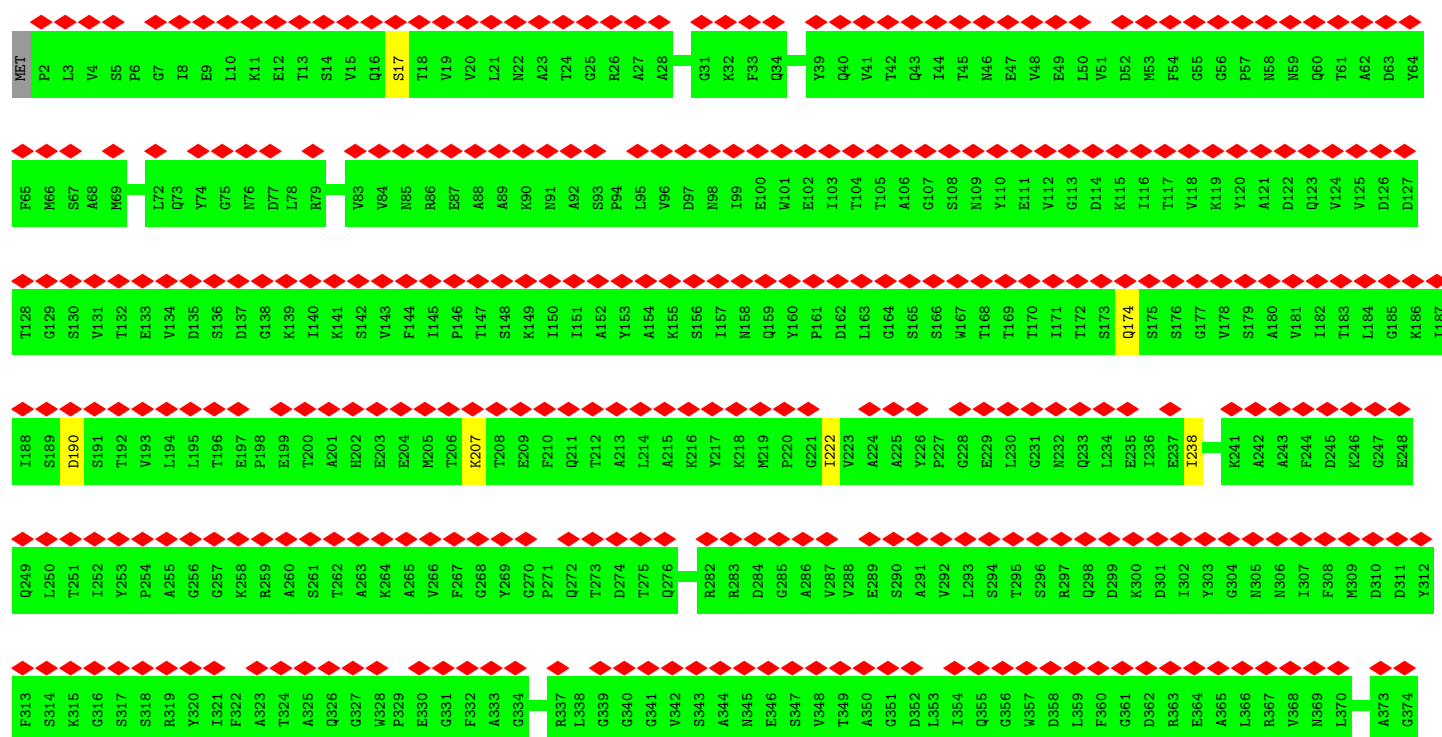
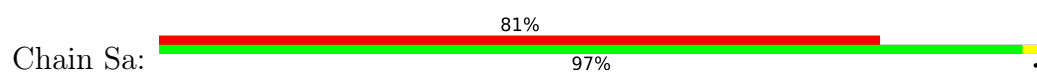


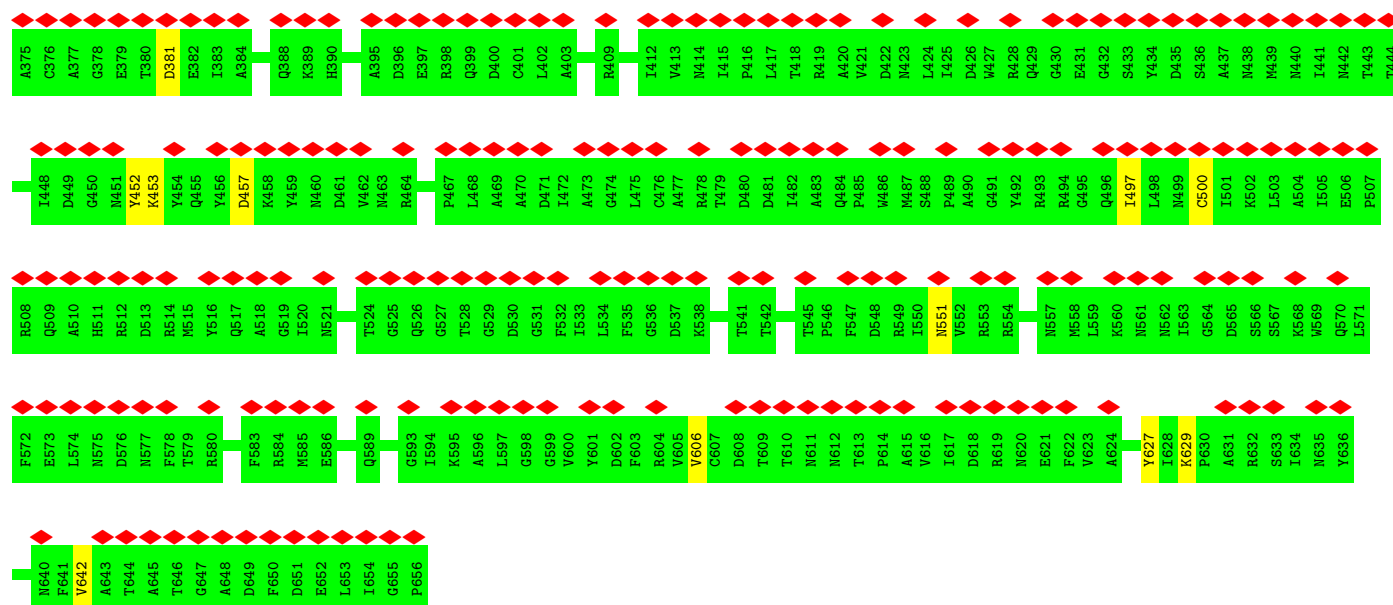
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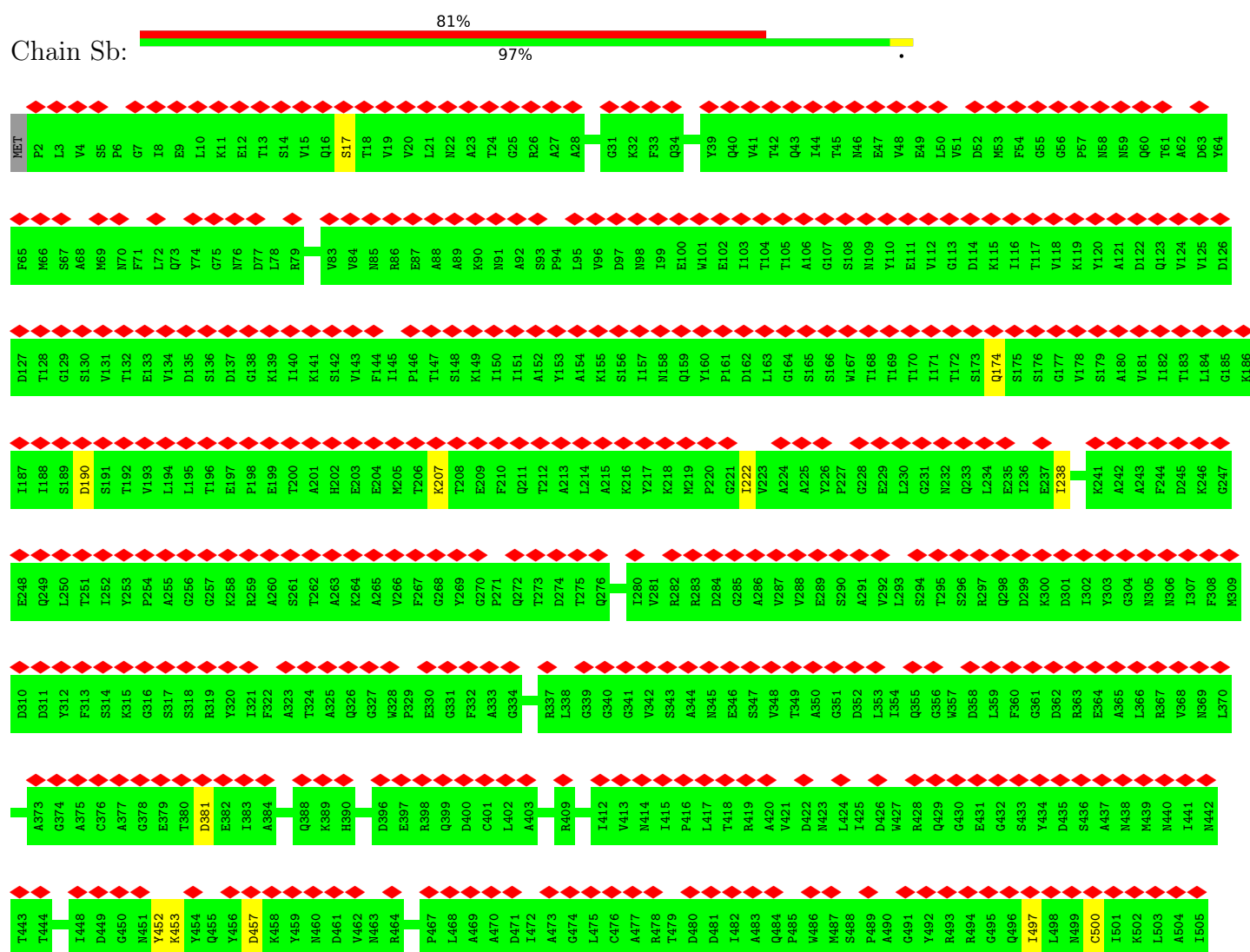


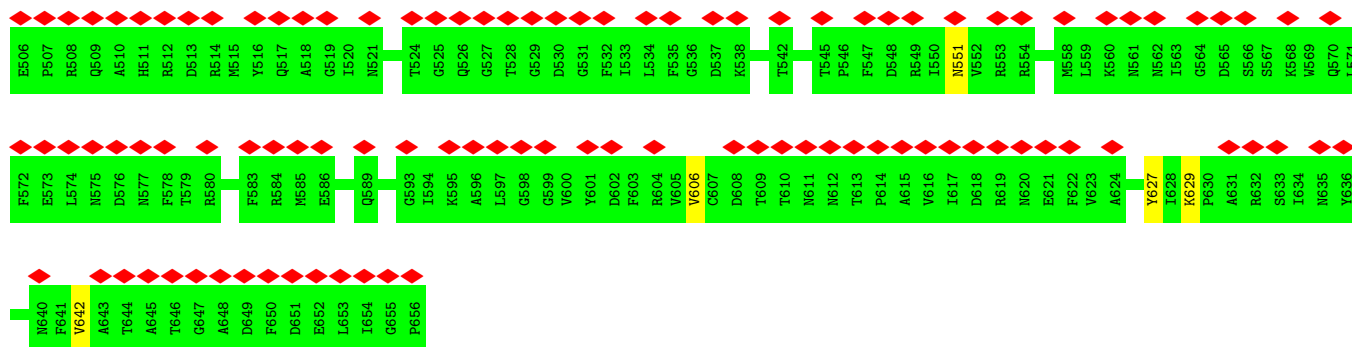
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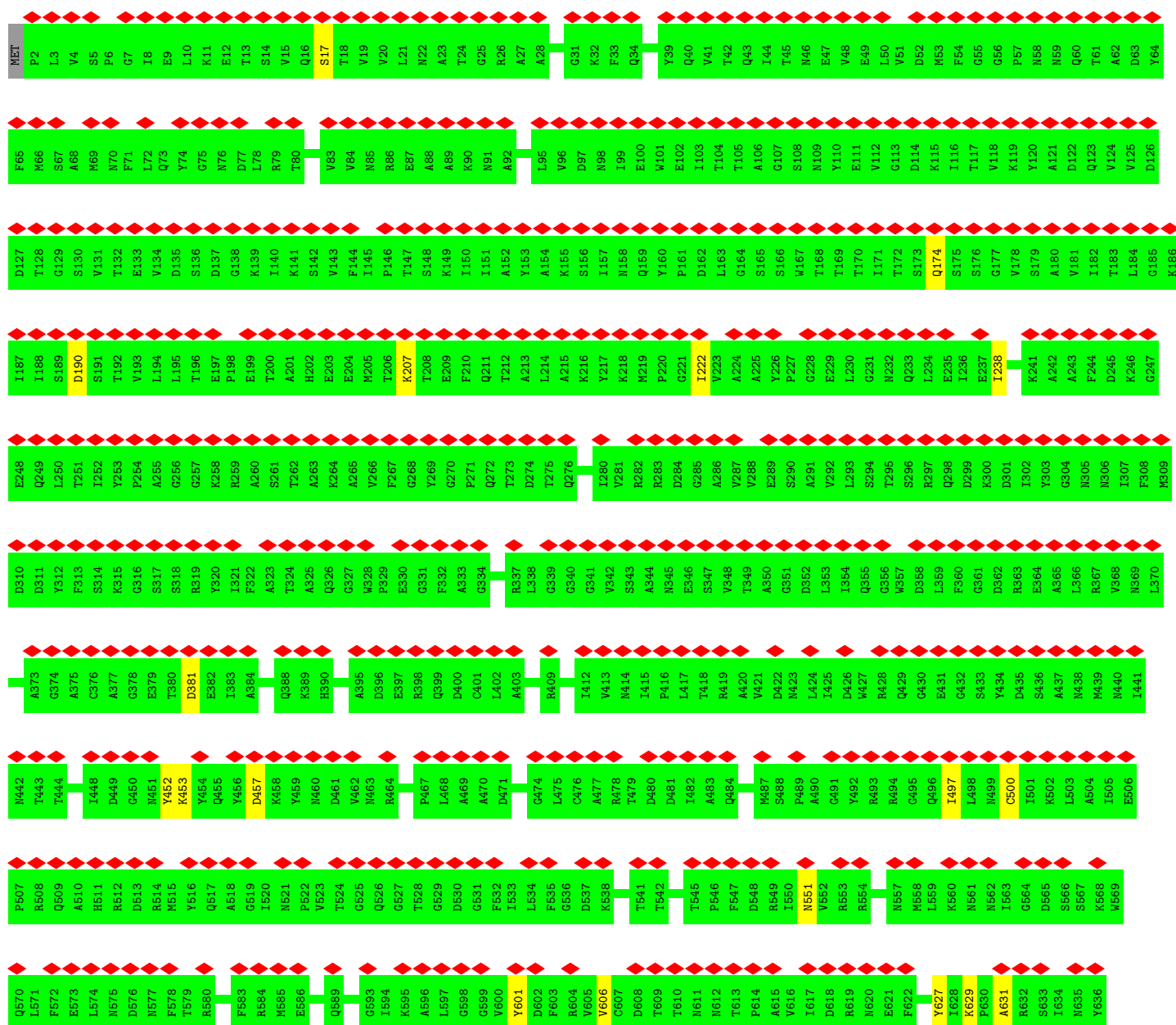
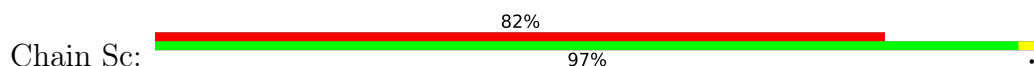


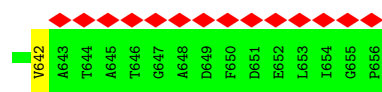
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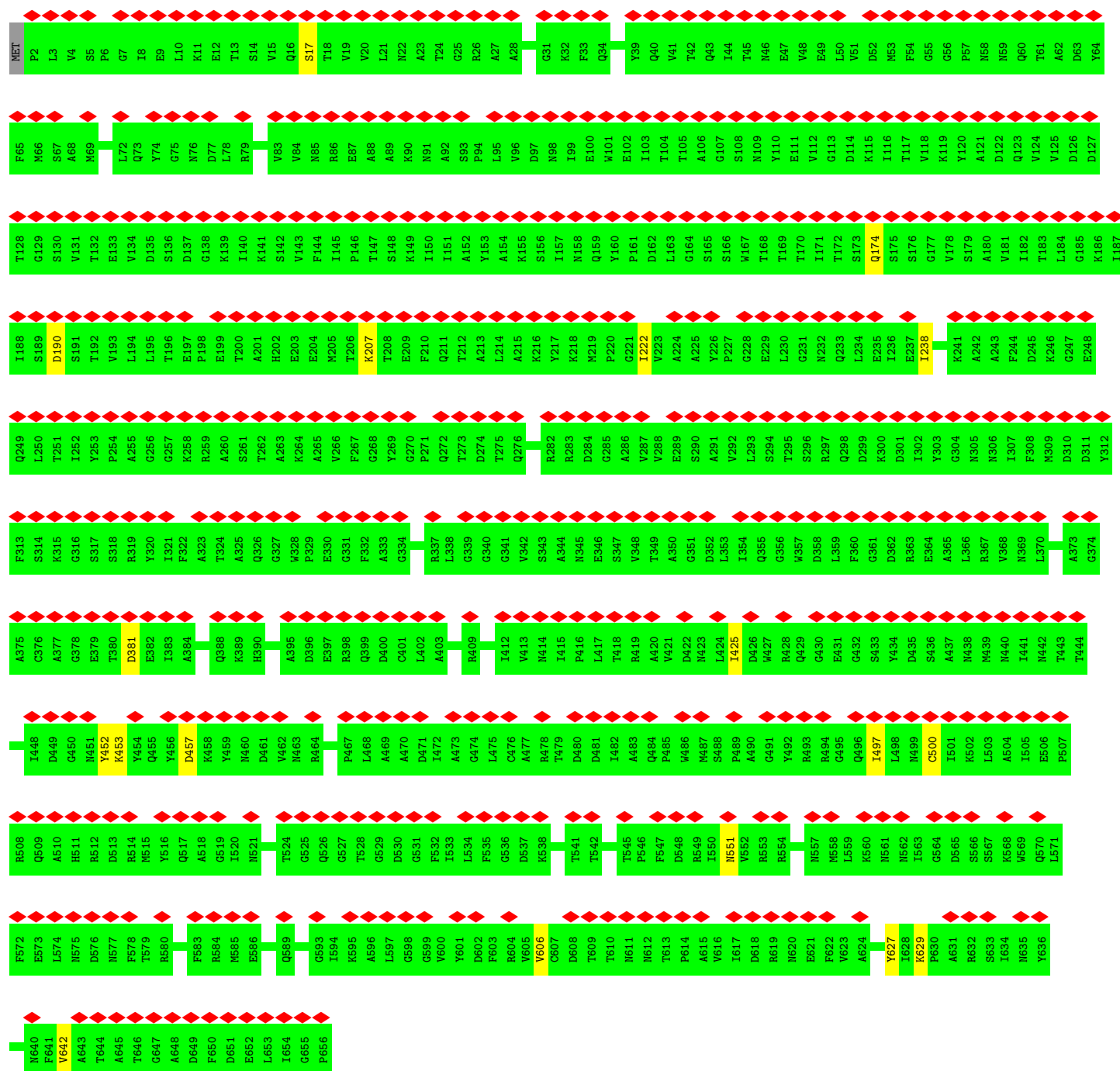
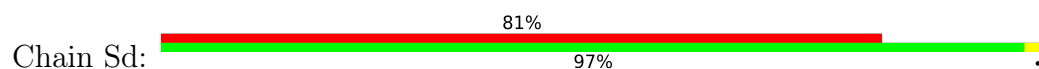


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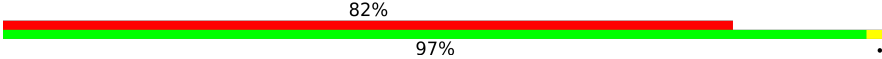


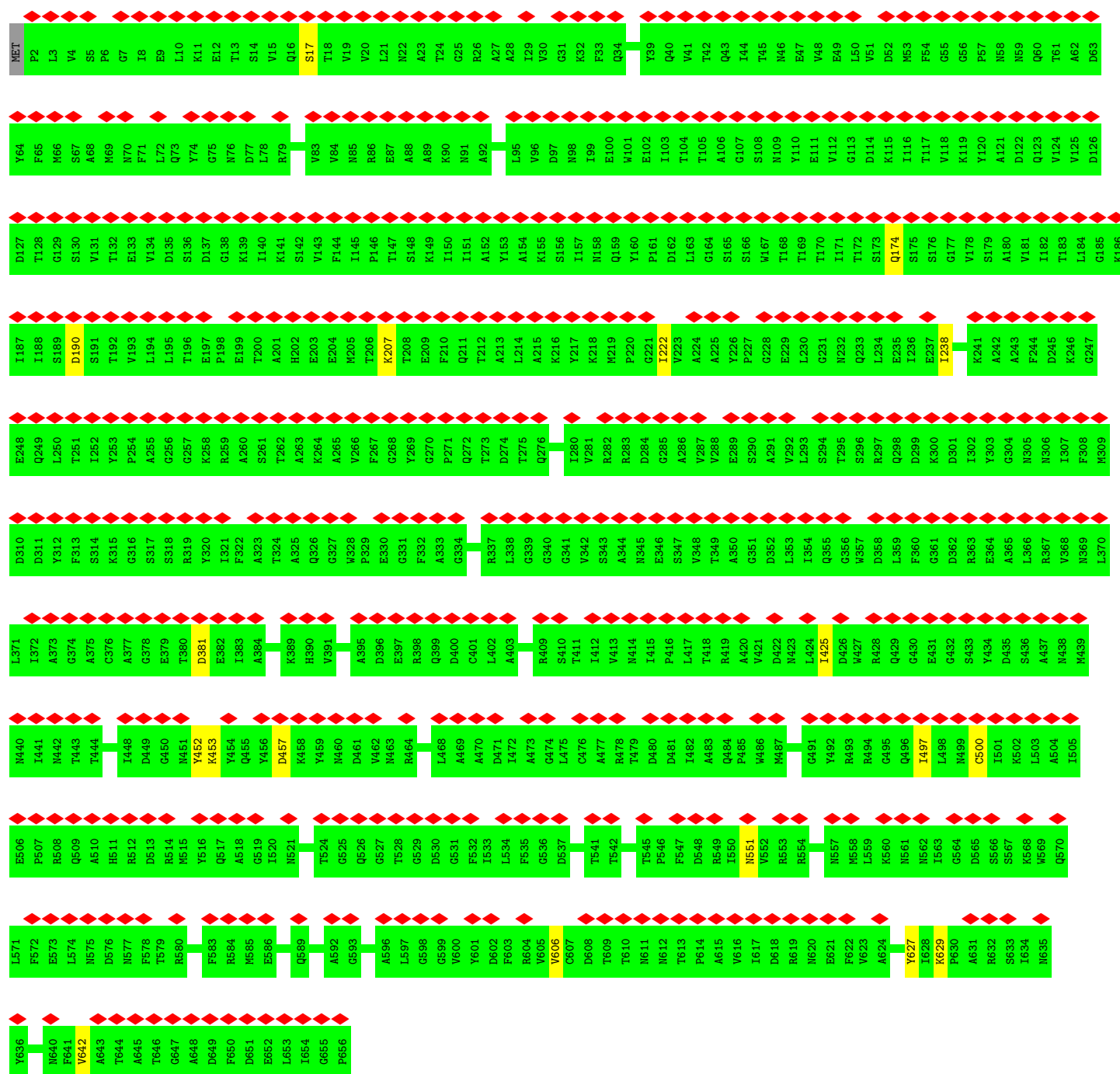


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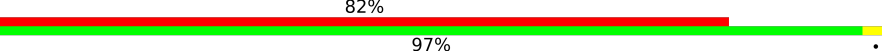


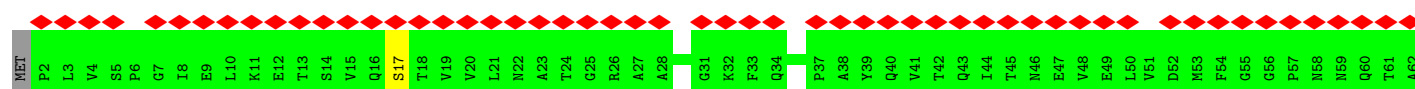
• Molecule 1: Tail sheath protein

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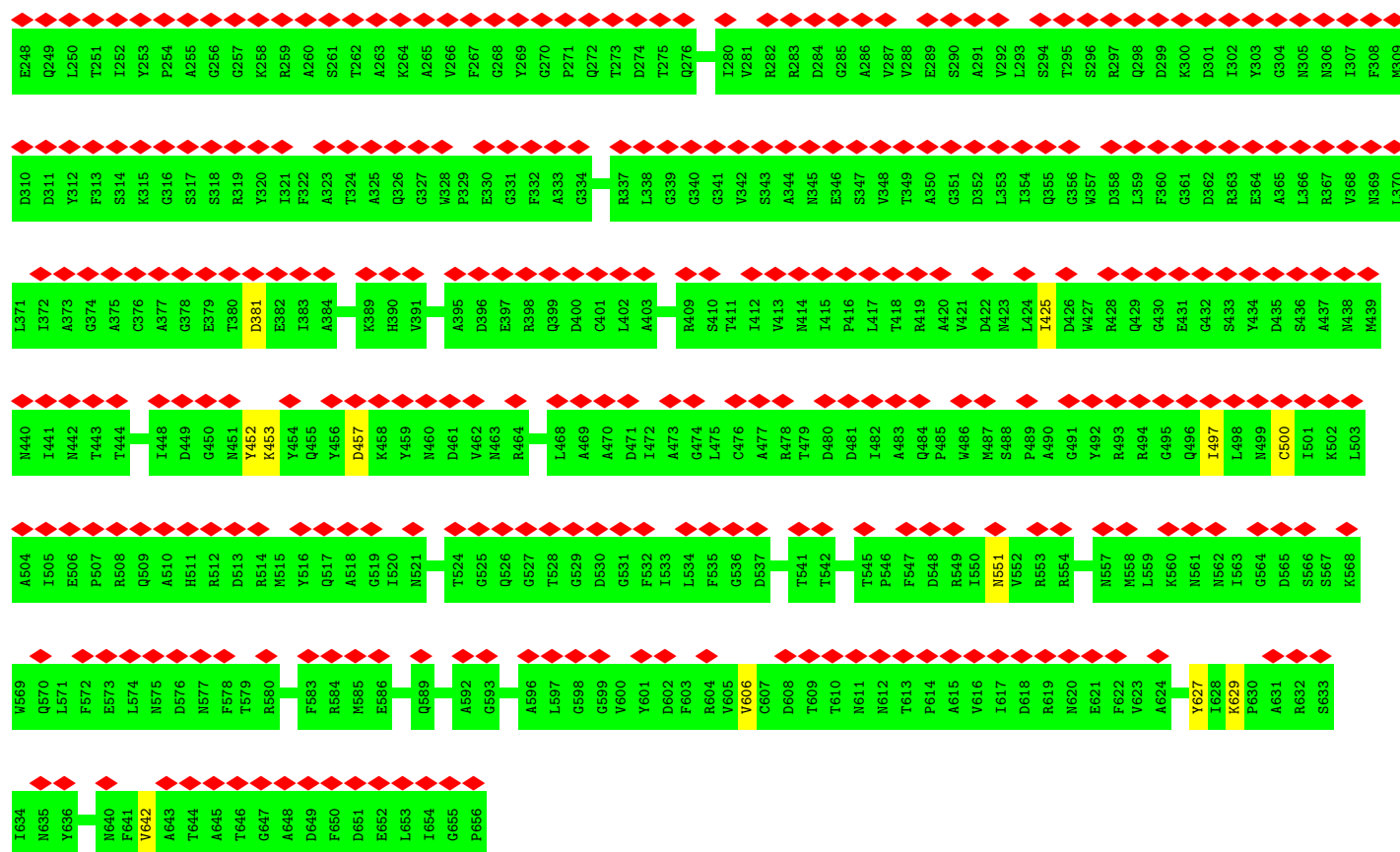
• Molecule 1: Tail sheath protein

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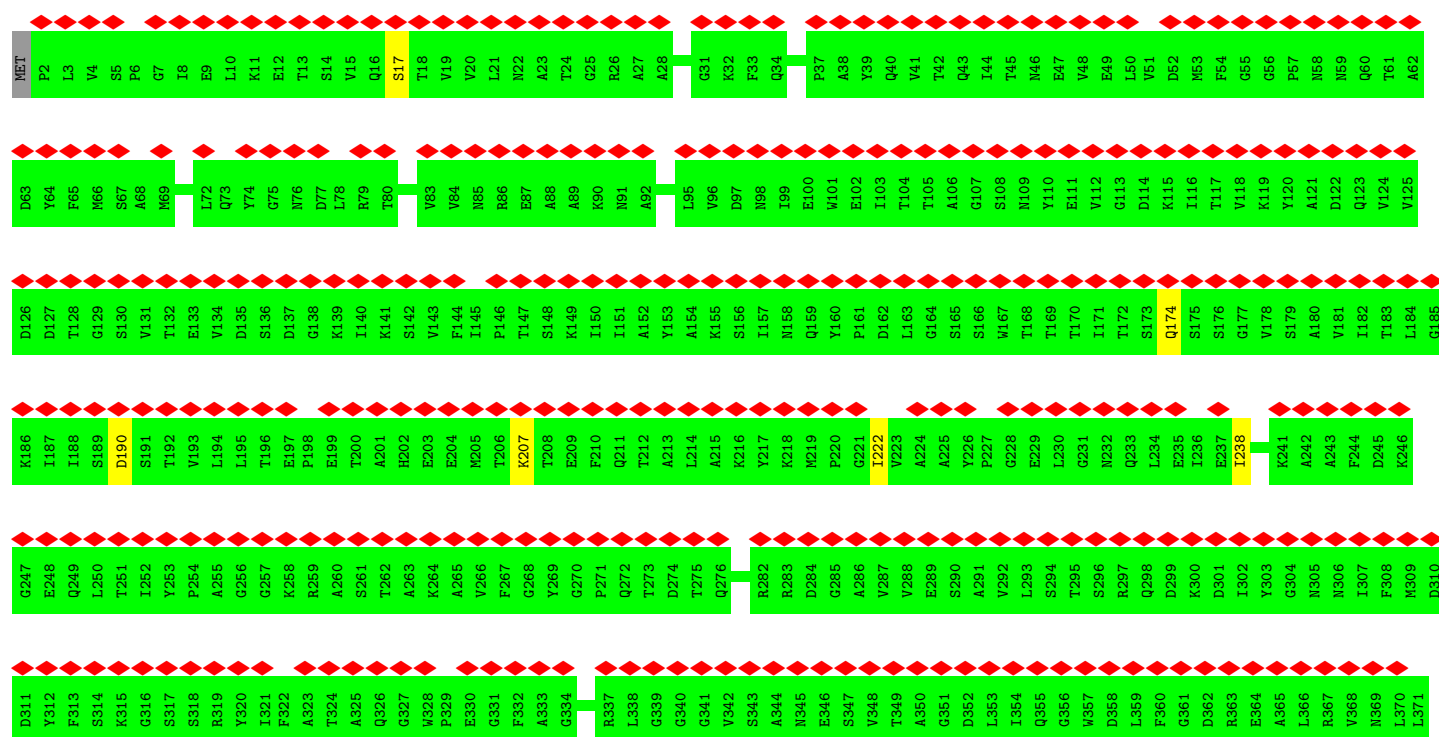
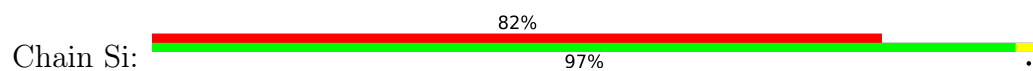


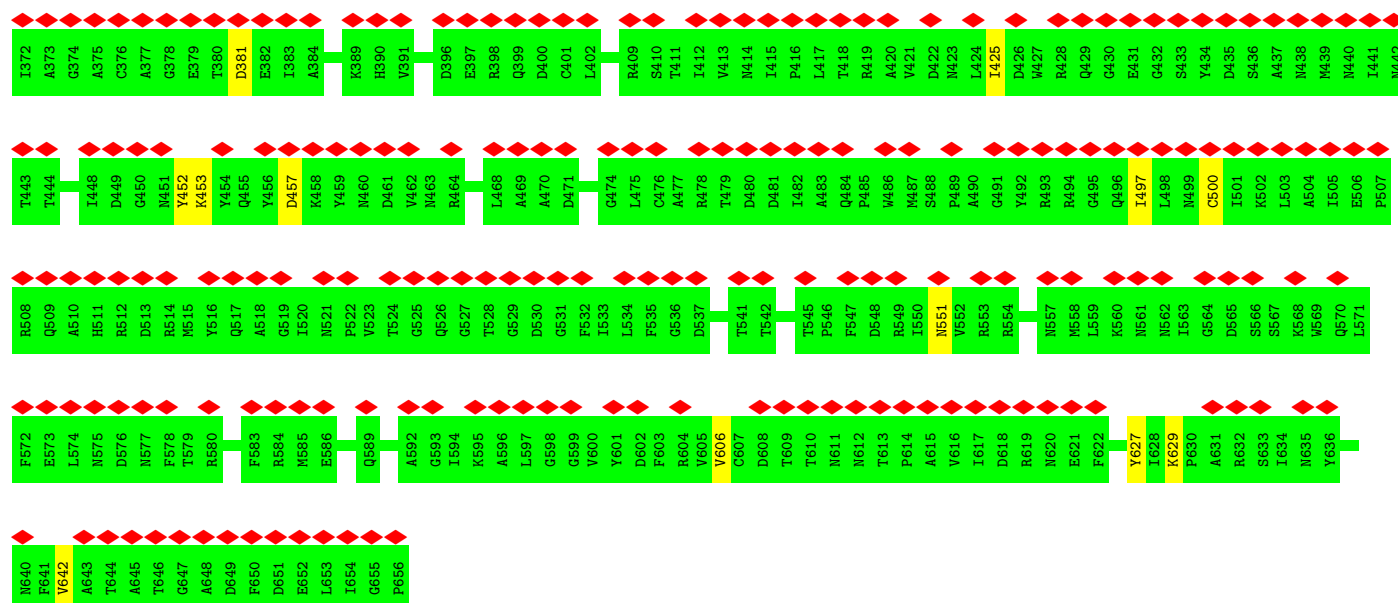


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P2	L3	V4	S5	P6	G7	I8	E9	L10	K11	E12	T13	S14	V15	Q16	S17	T18	V19	Z20	L21	N22	A23	T24	G25	R26	A27	A28		G31	K32	F33	Q34		Y39	Q40	V41	T42	Q43	I44	T45	N46	E47	V48	E49	L50	V51	D52	M53	F54	G55	P56	F57	N58	Q60	T61	A62	D63	V64

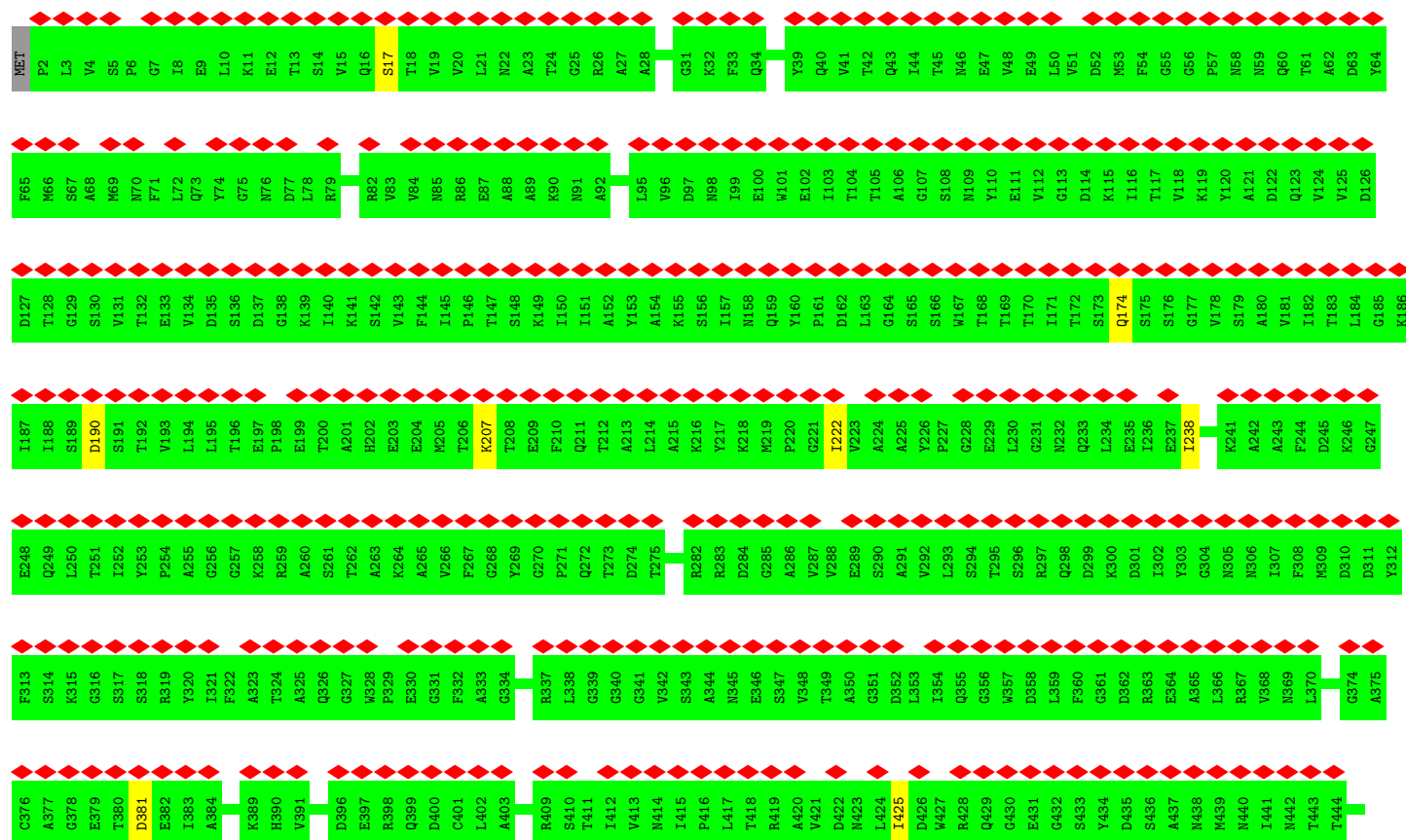
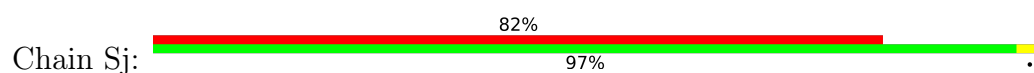


• Molecule 1: Tail sheath protein

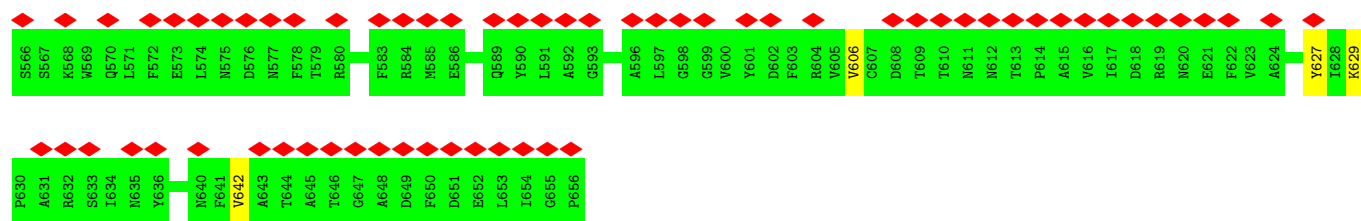




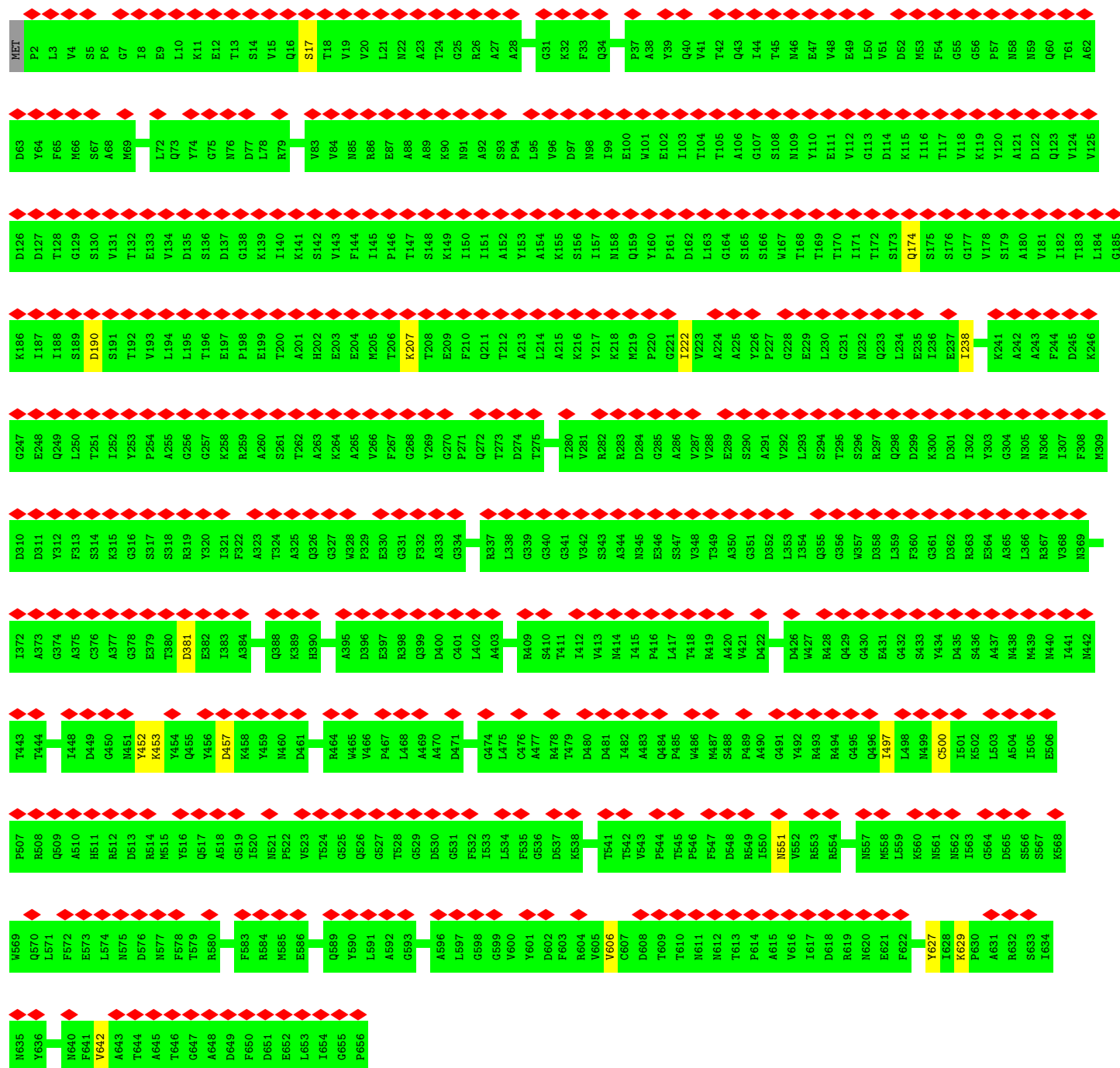
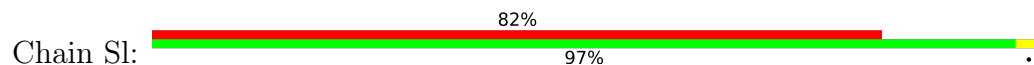
• Molecule 1: Tail sheath protein





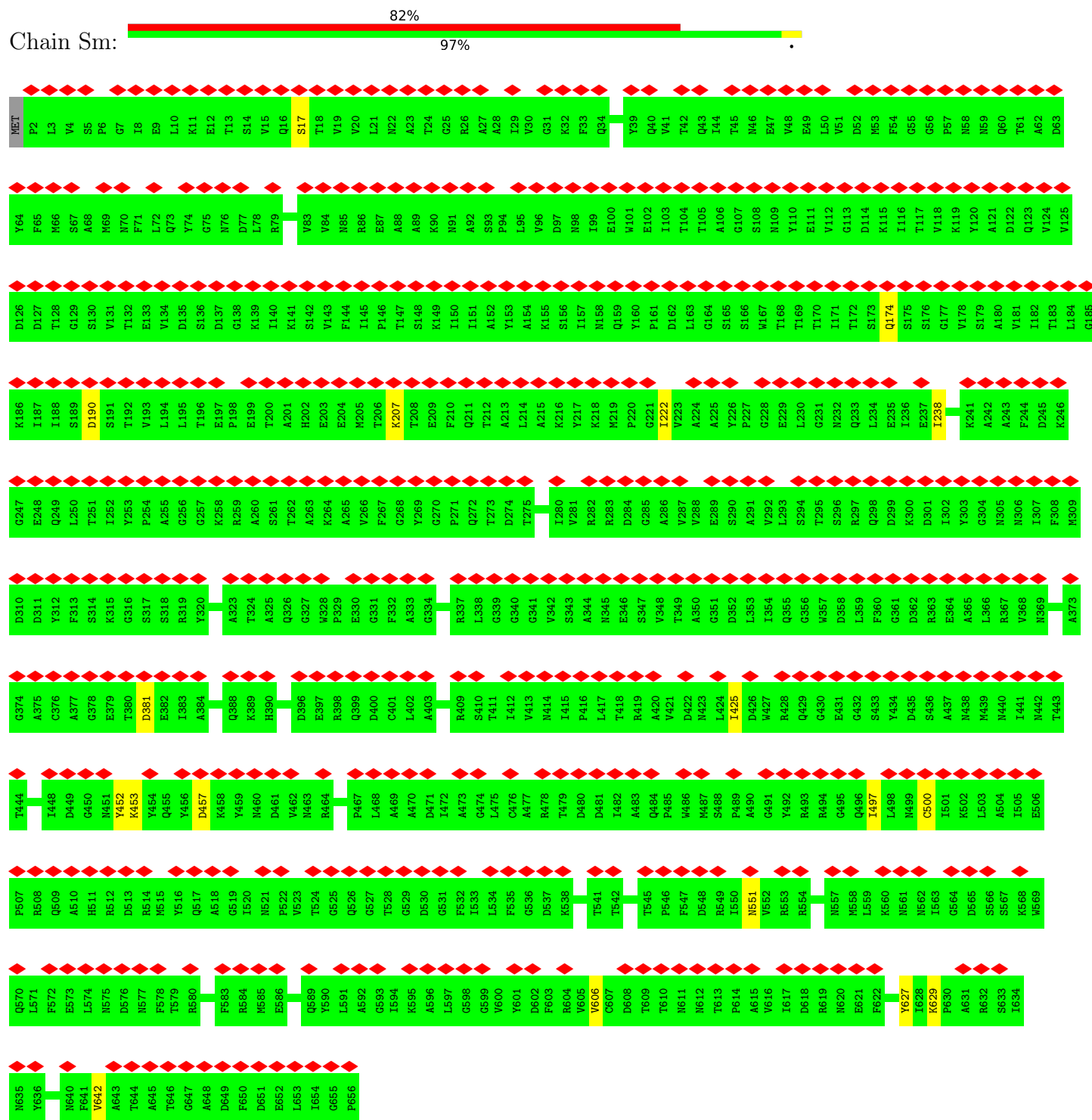


• Molecule 1: Tail sheath protein



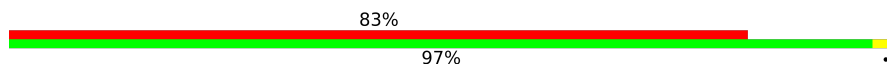
● Molecule 1: Tail sheath protein

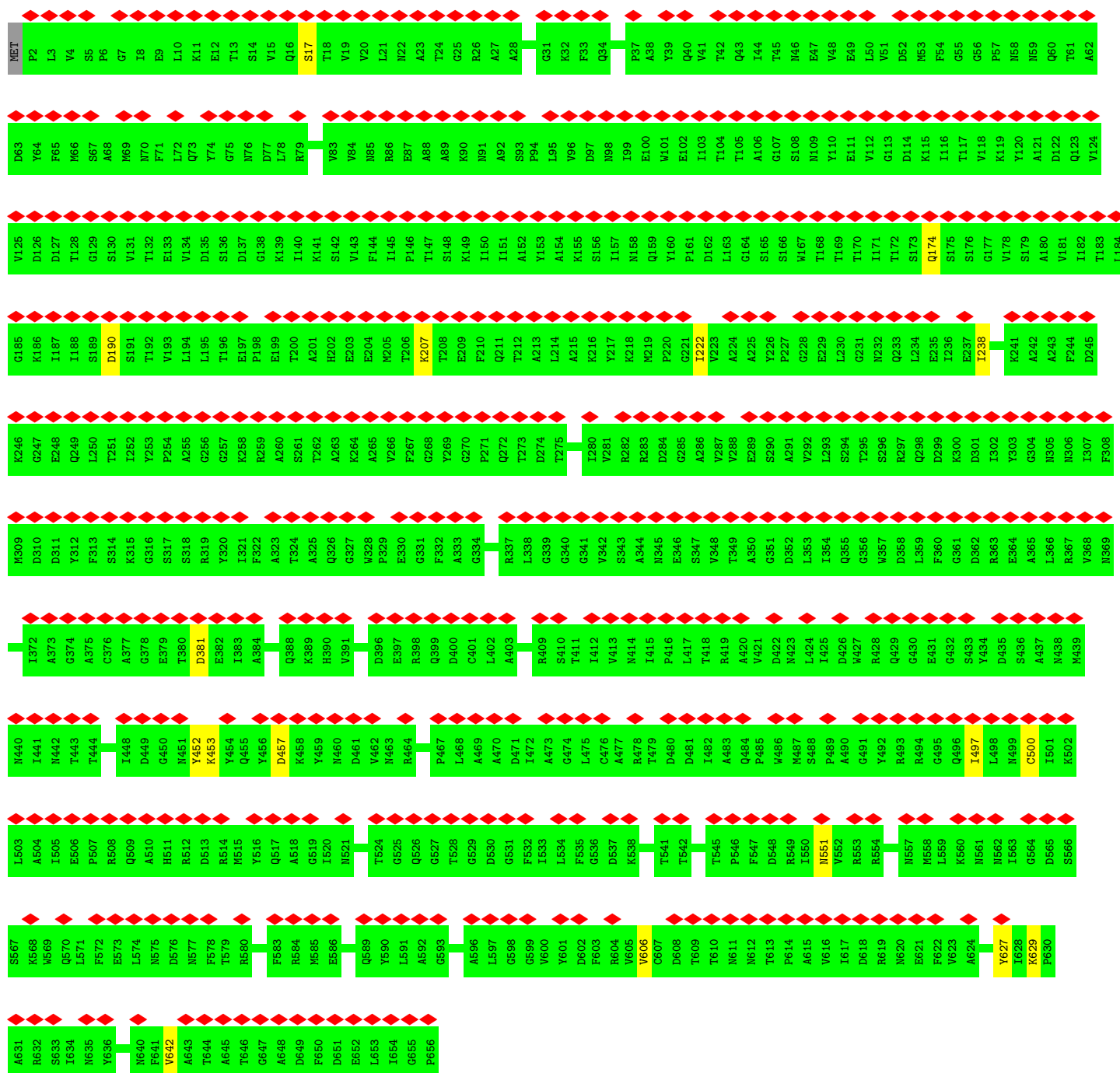
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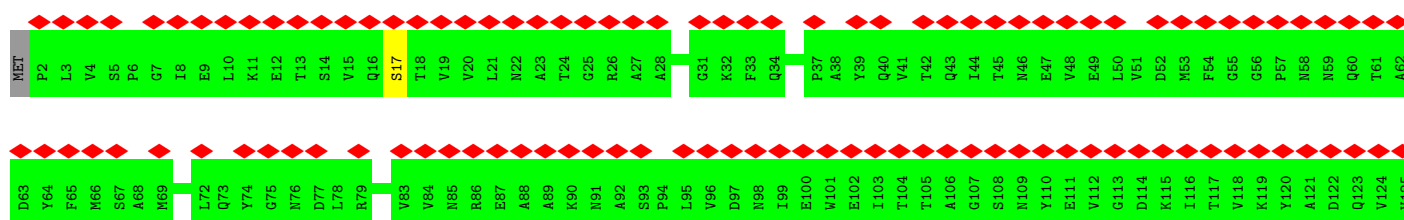
● Molecule 1: Tail sheath protein

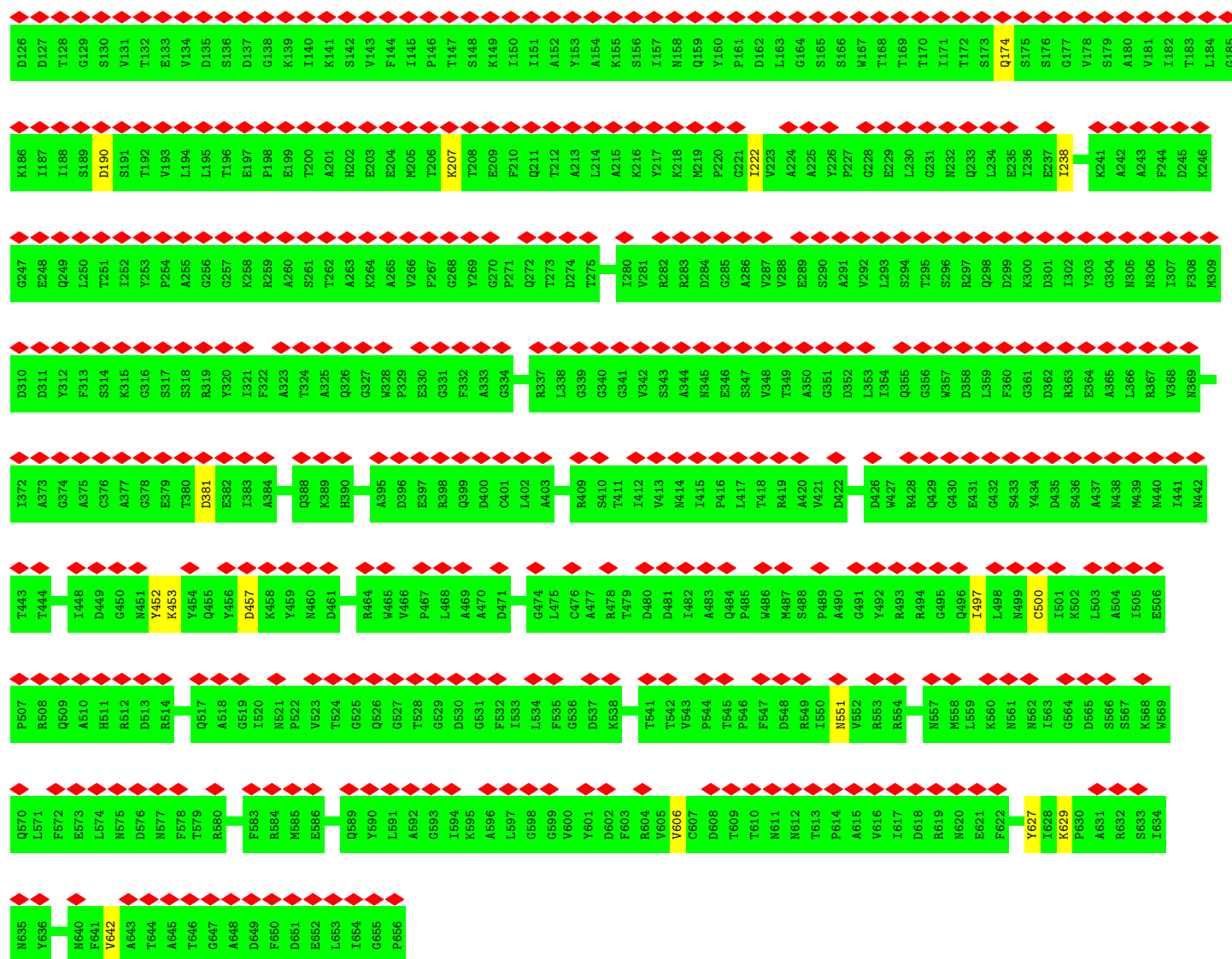
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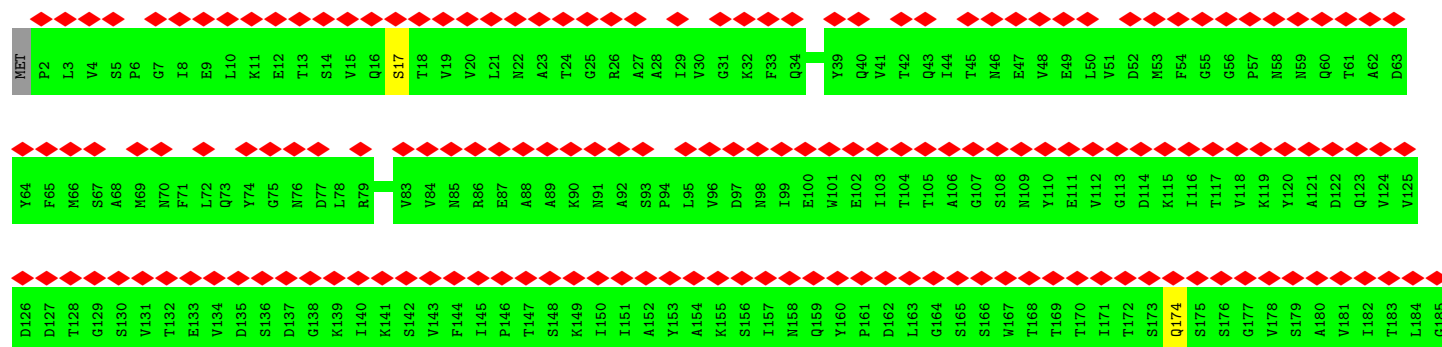
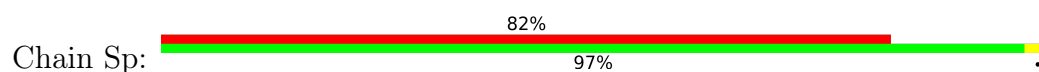


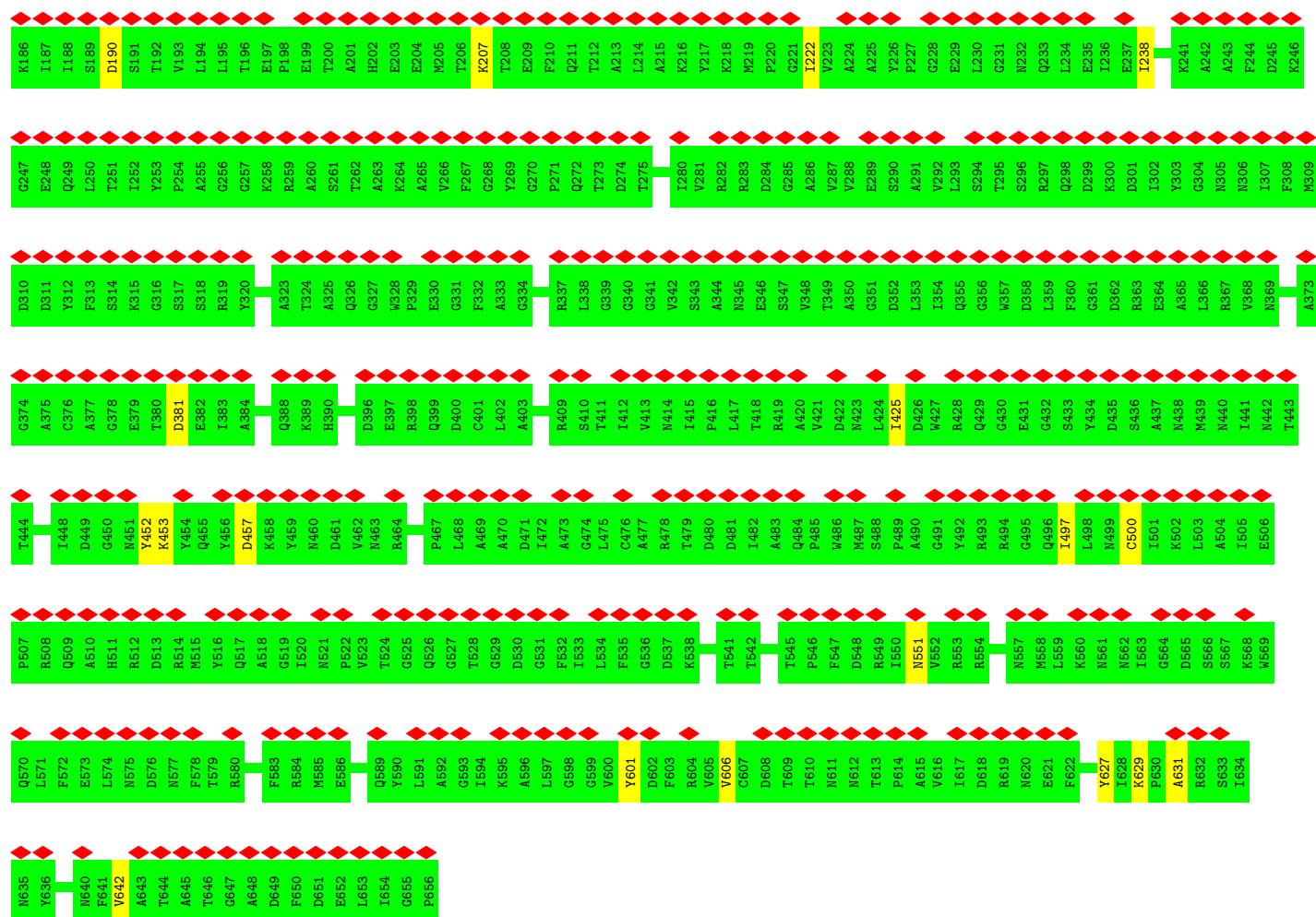
• Molecule 1: Tail sheath protein



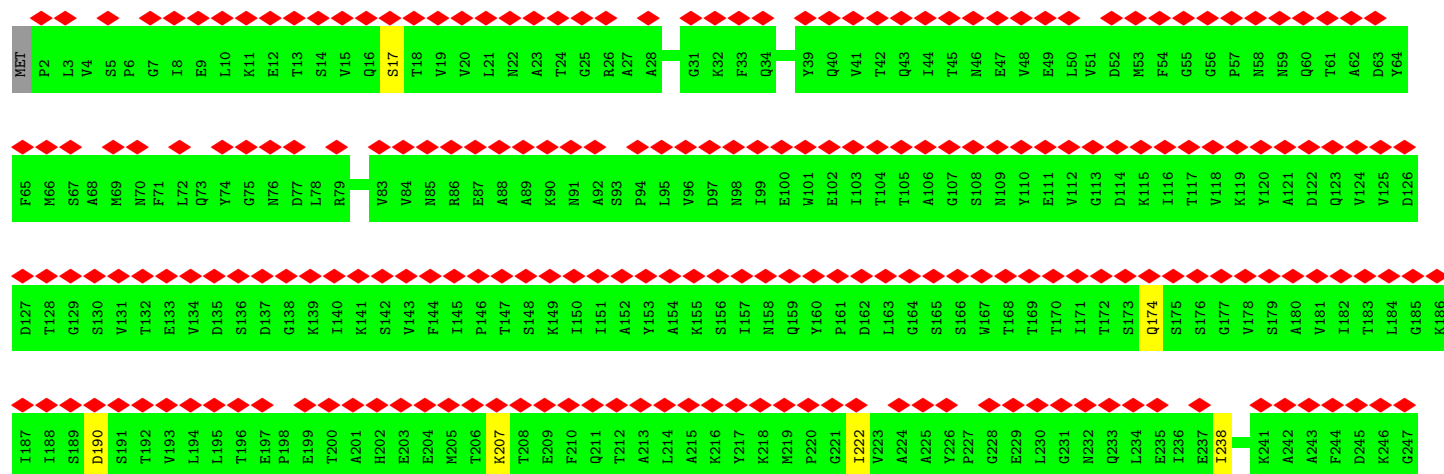
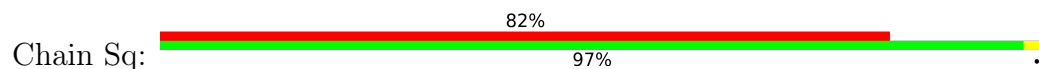


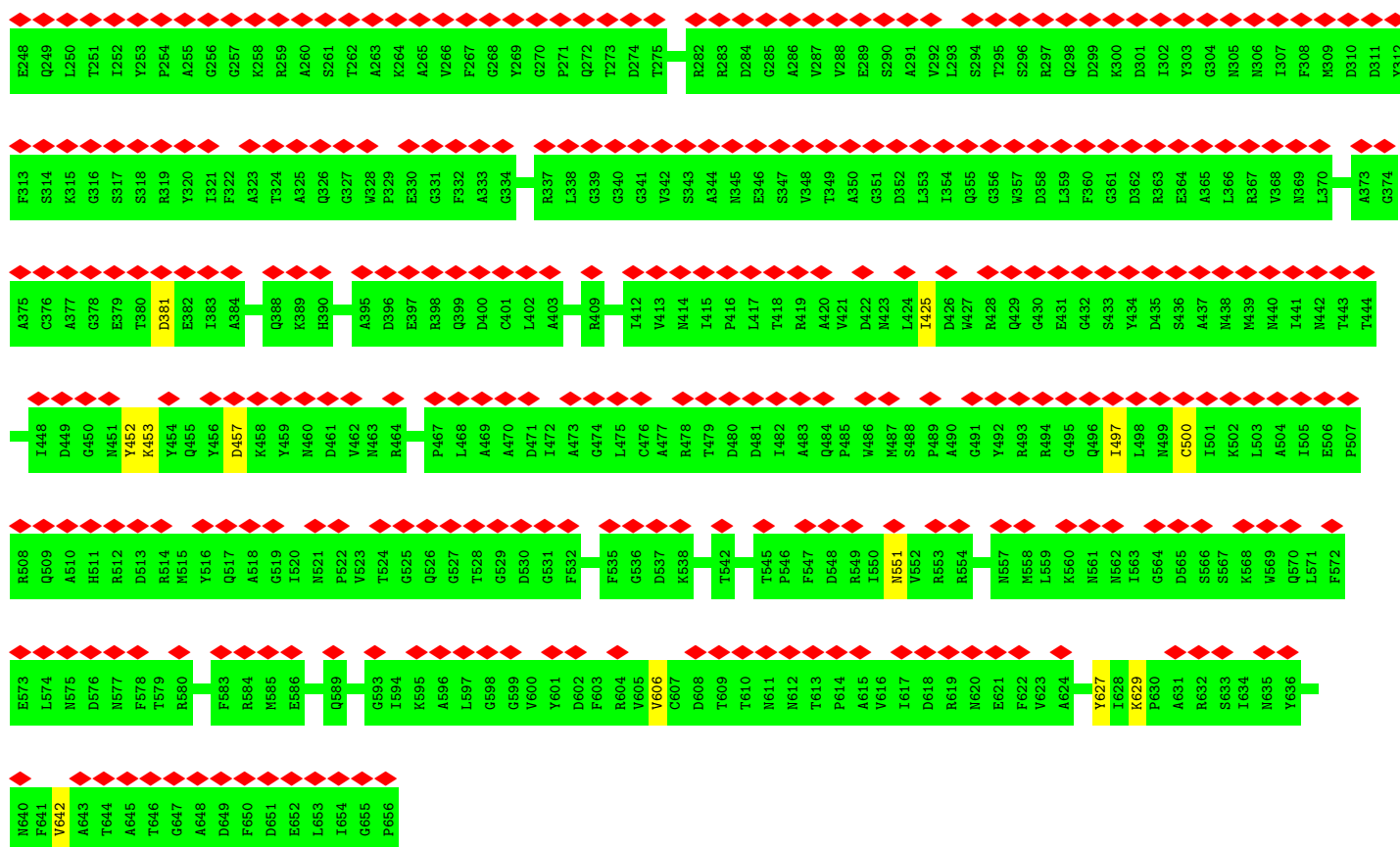
● Molecule 1: Tail sheath protein



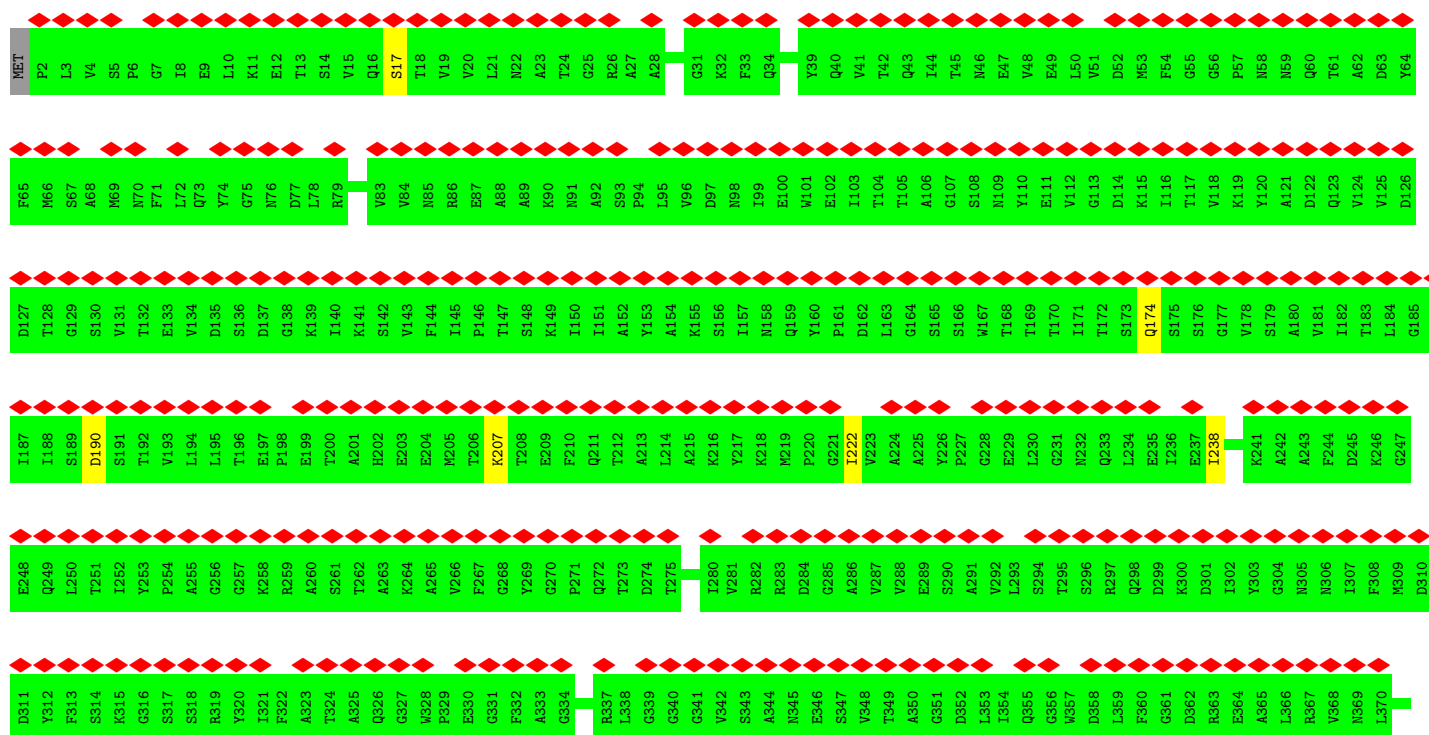
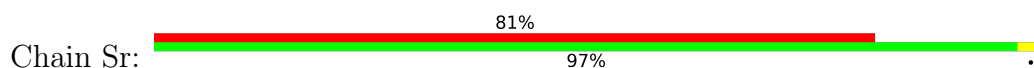


• Molecule 1: Tail sheath protein



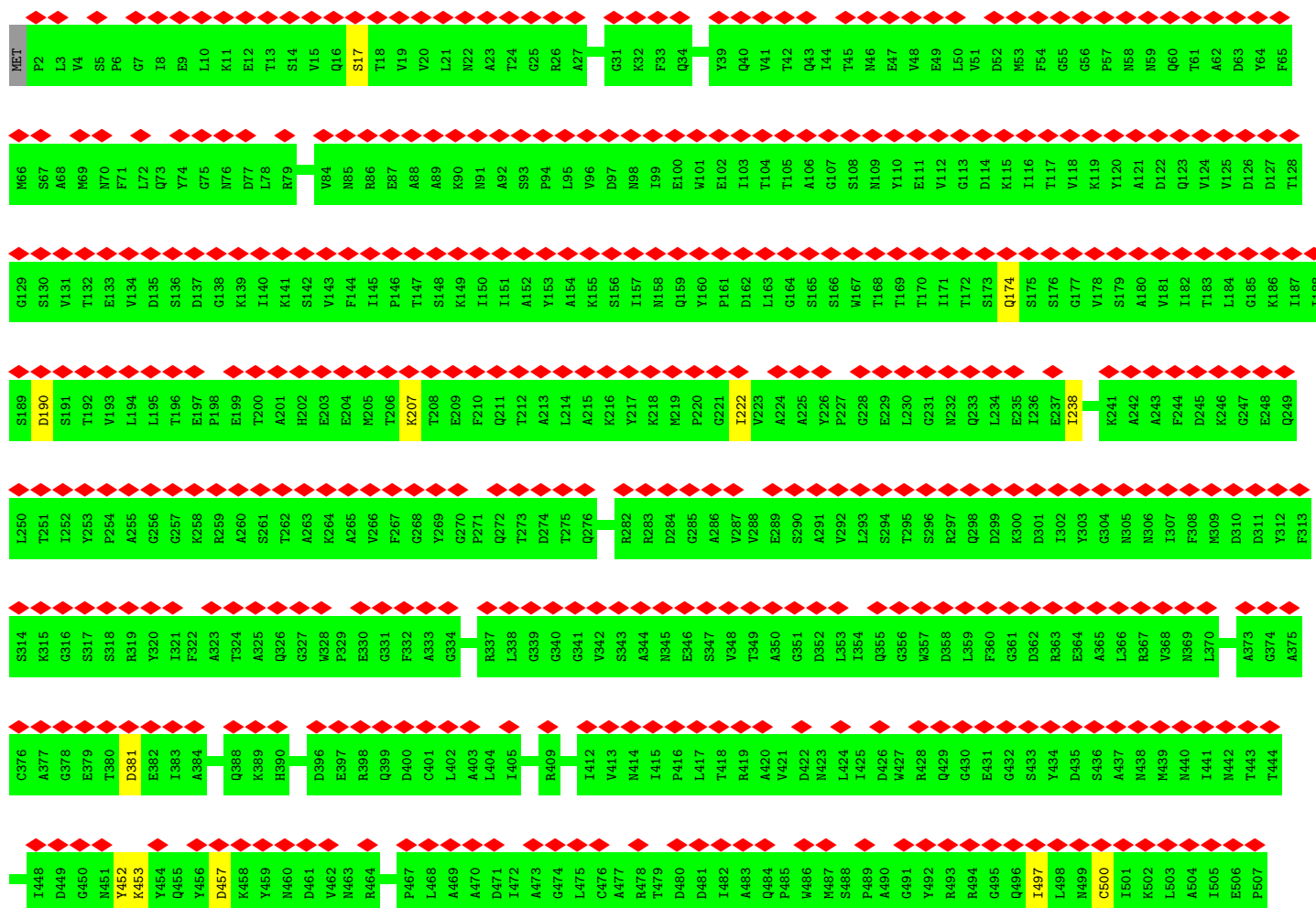
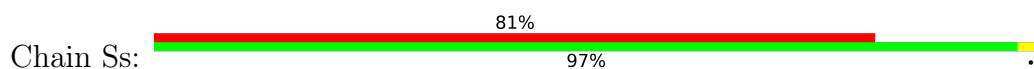


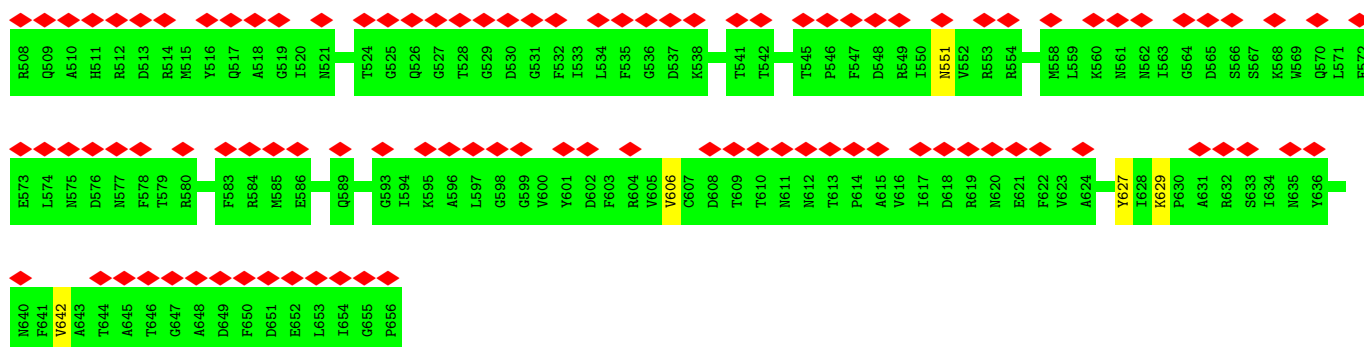
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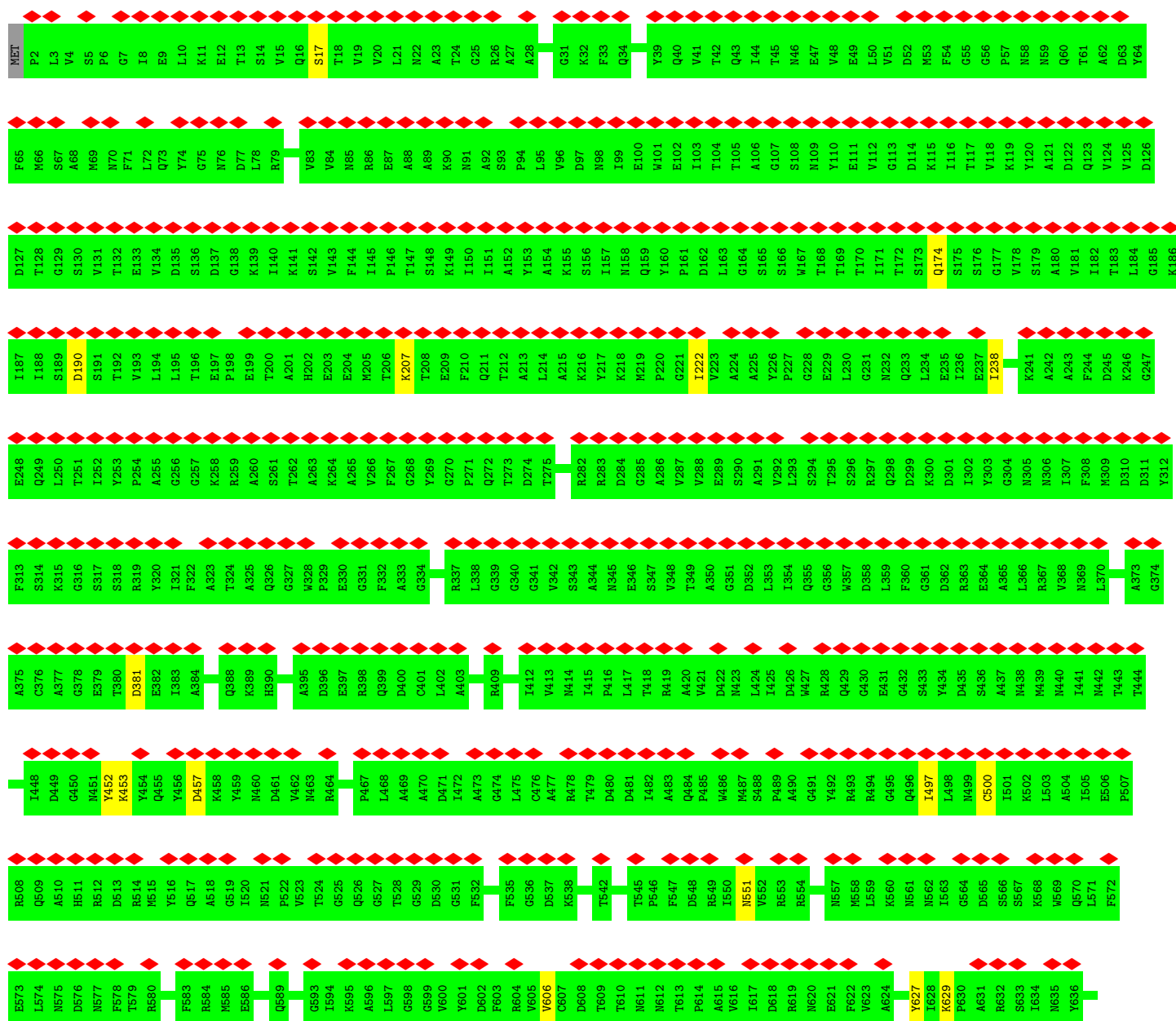
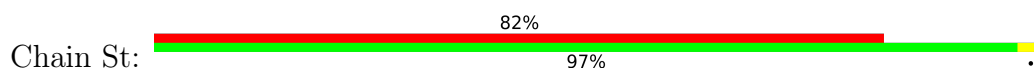


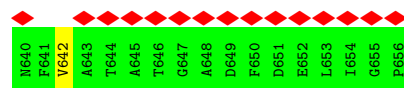
• Molecule 1: Tail sheath protein



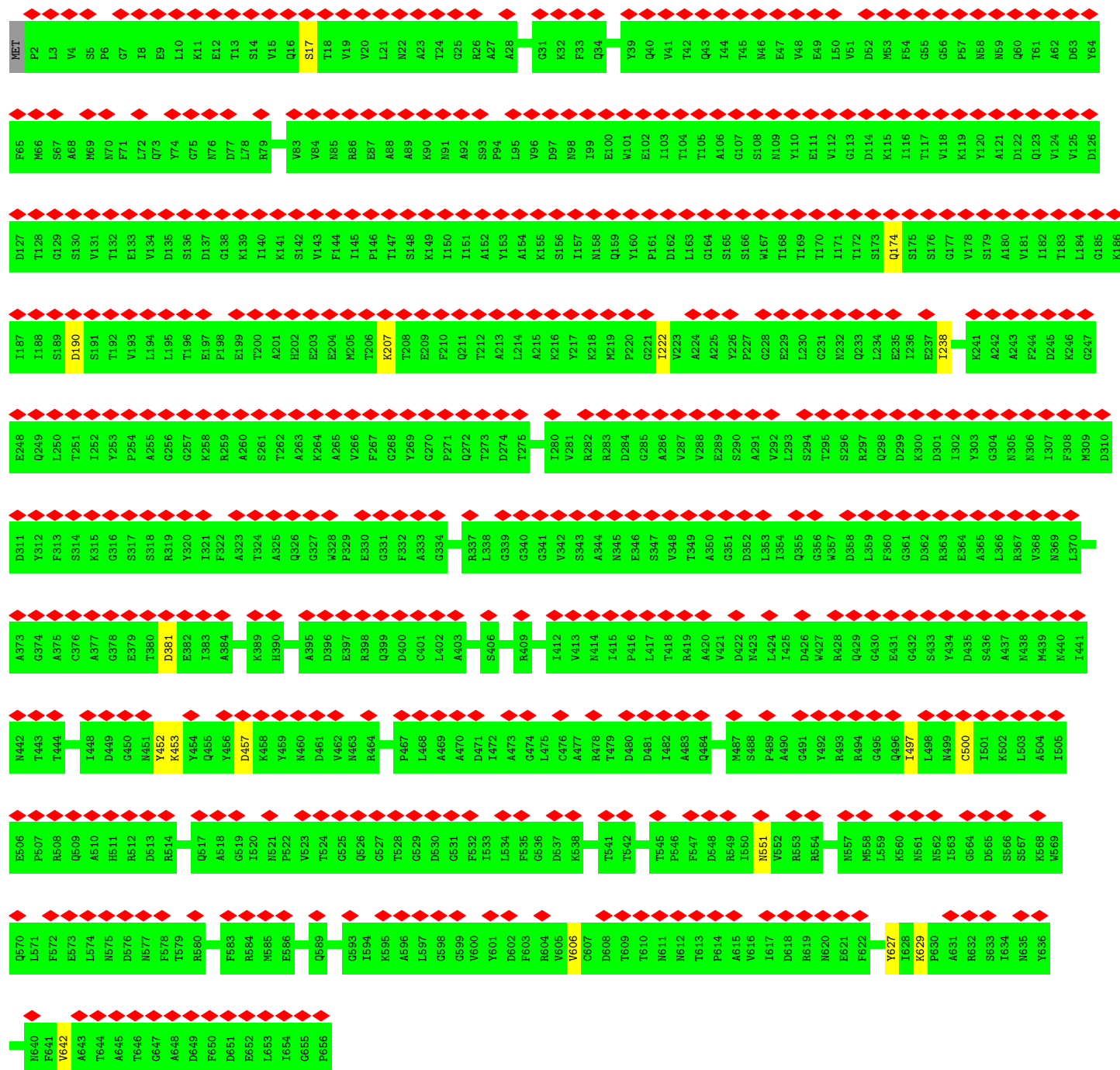
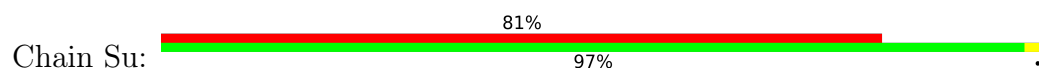


• Molecule 1: Tail sheath protein



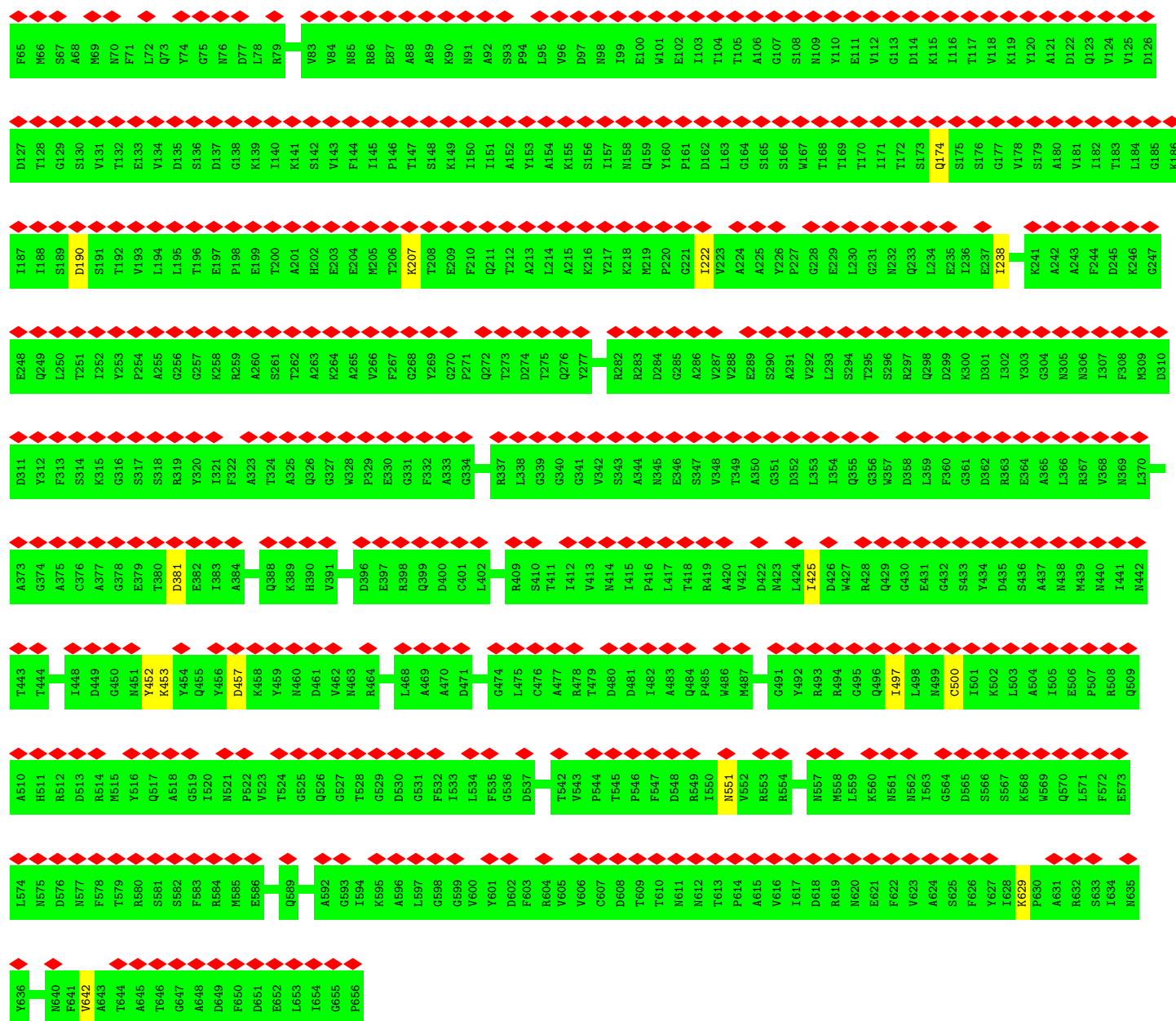


• Molecule 1: Tail sheath protein

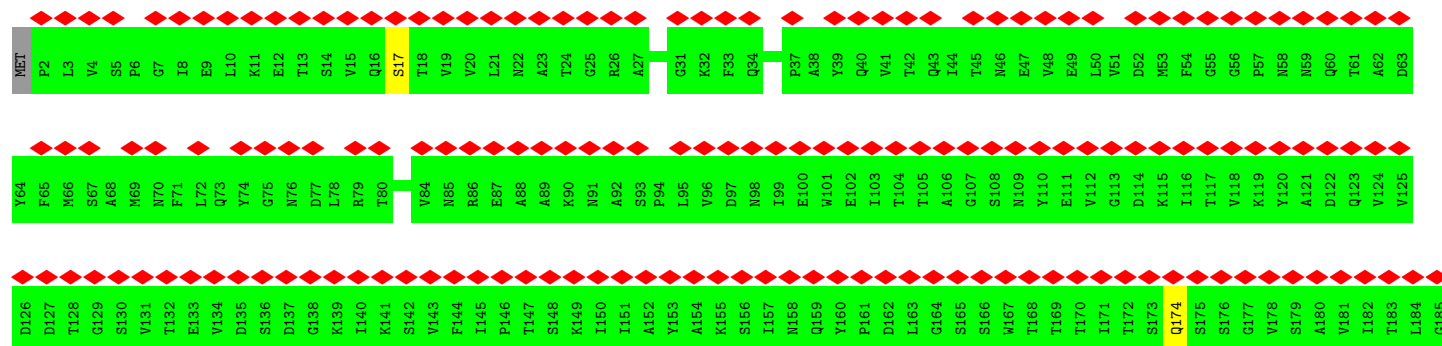
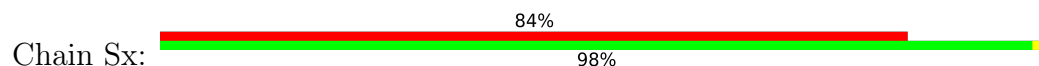


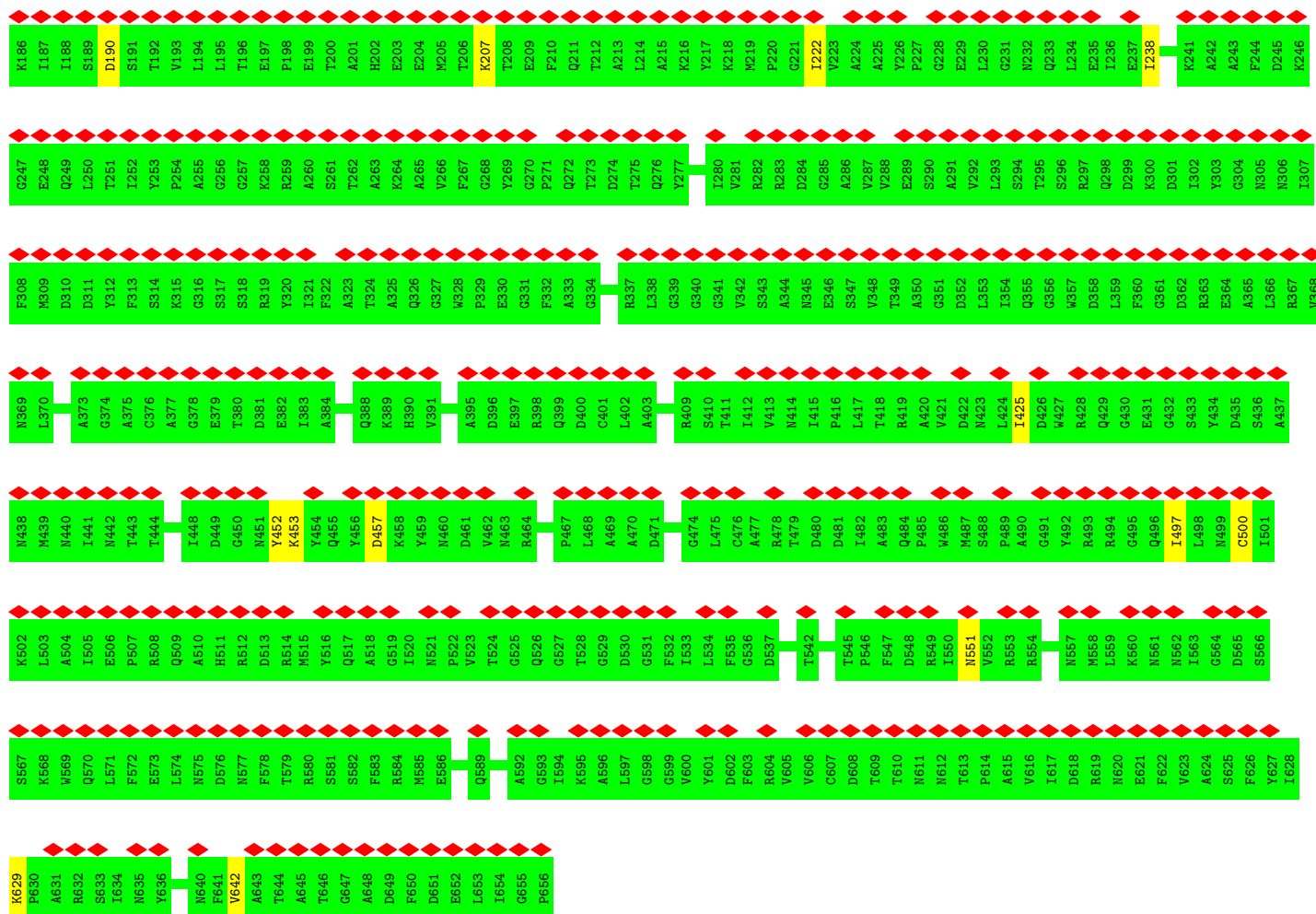
• Molecule 1: Tail sheath protein



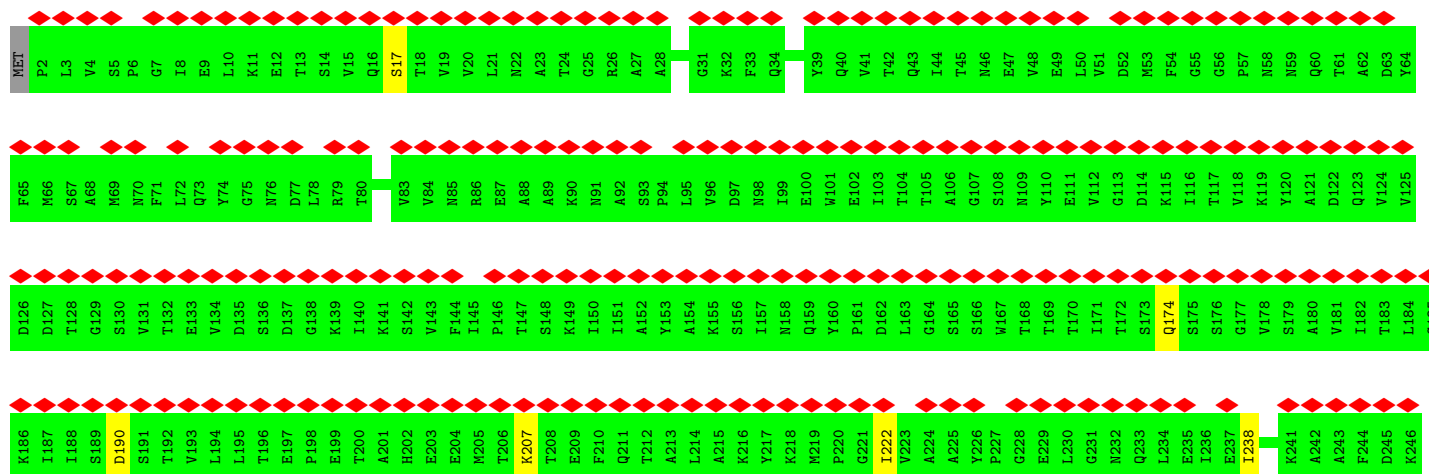
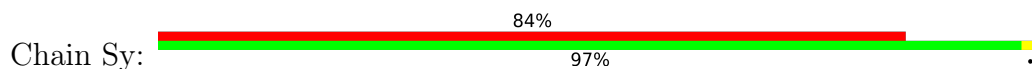


• Molecule 1: Tail sheath protein

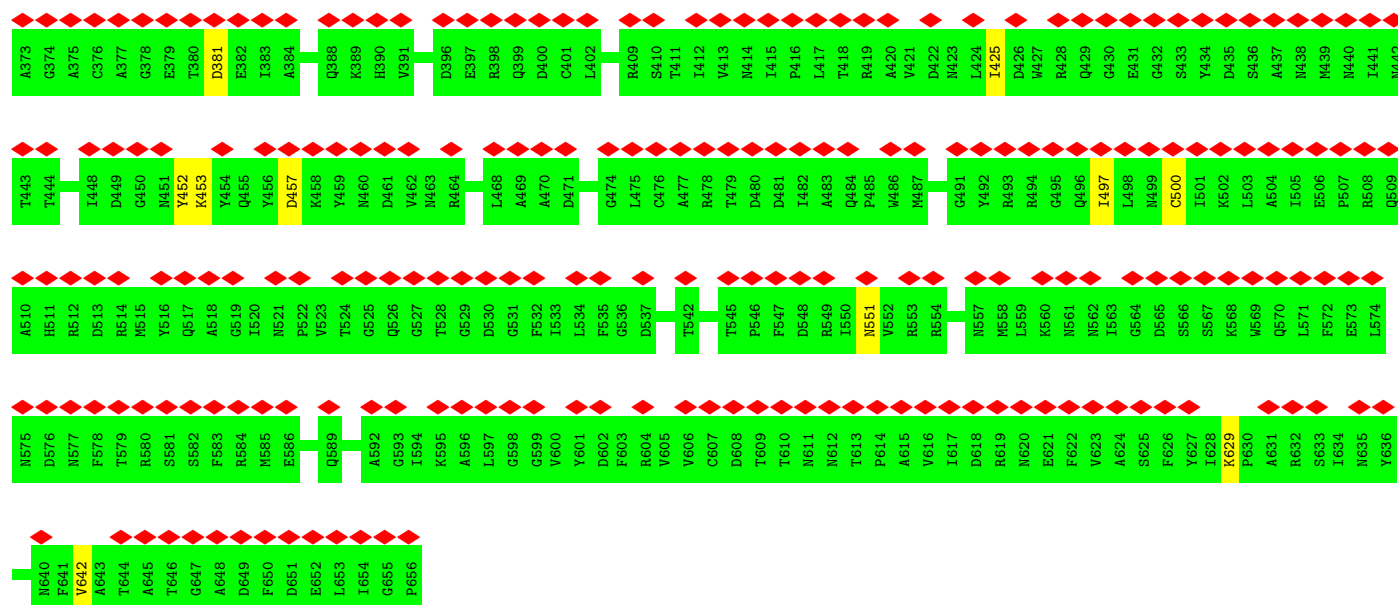




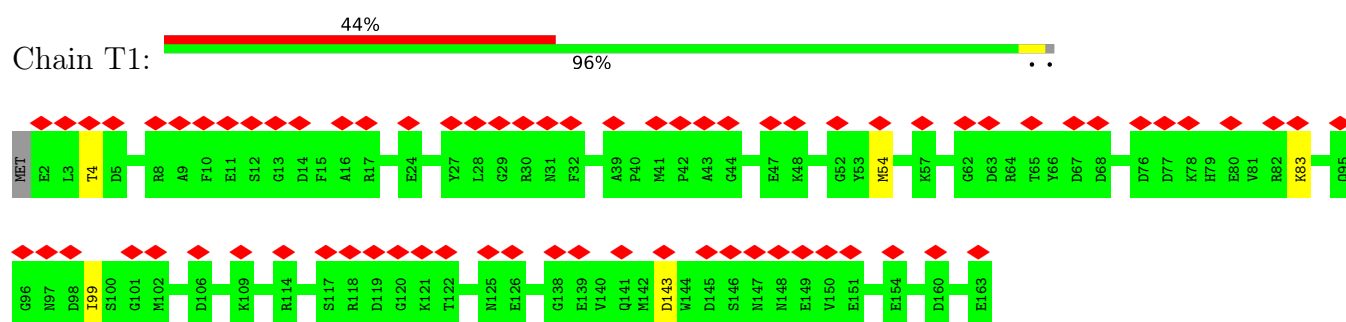
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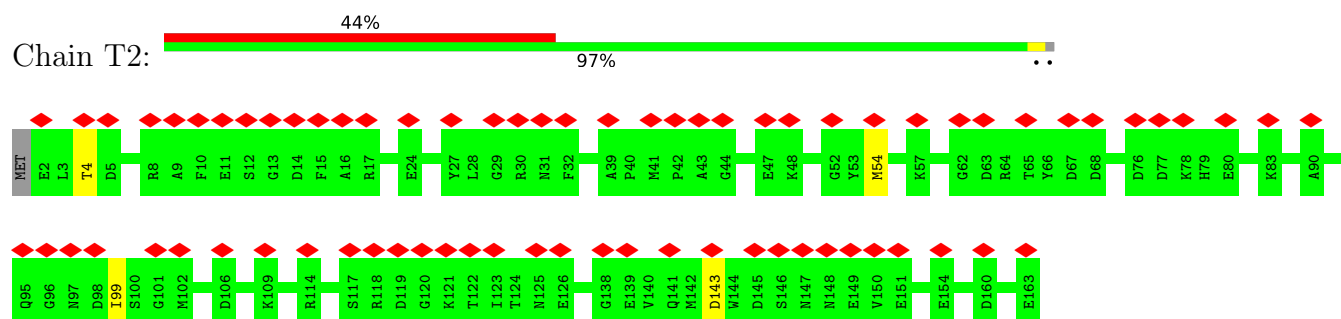




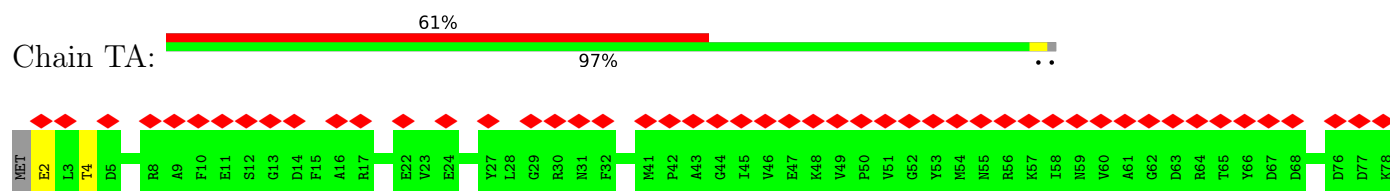
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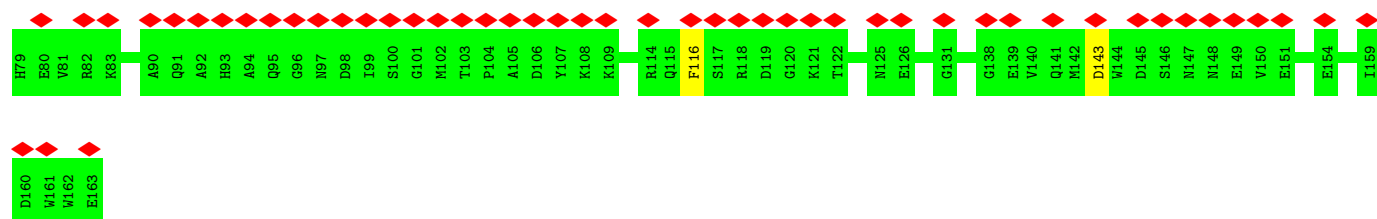


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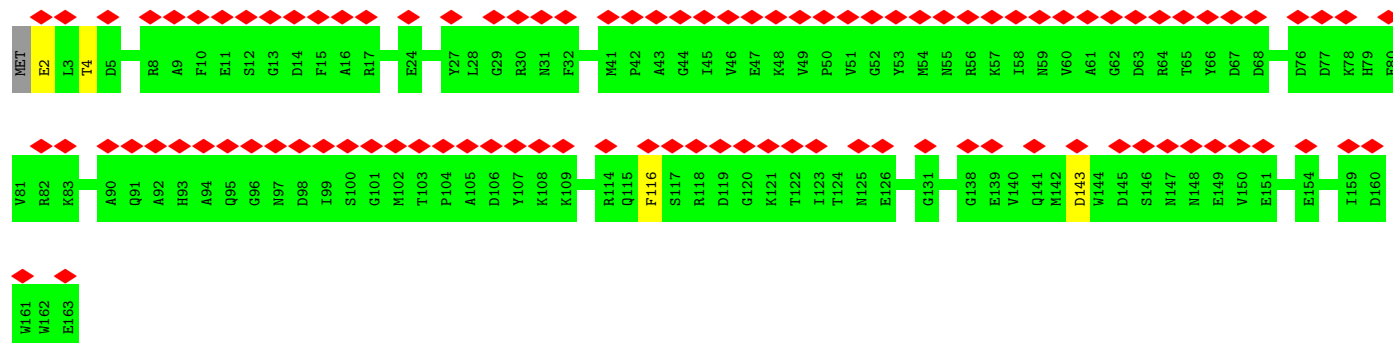
- Molecule 2: Tail tube protein





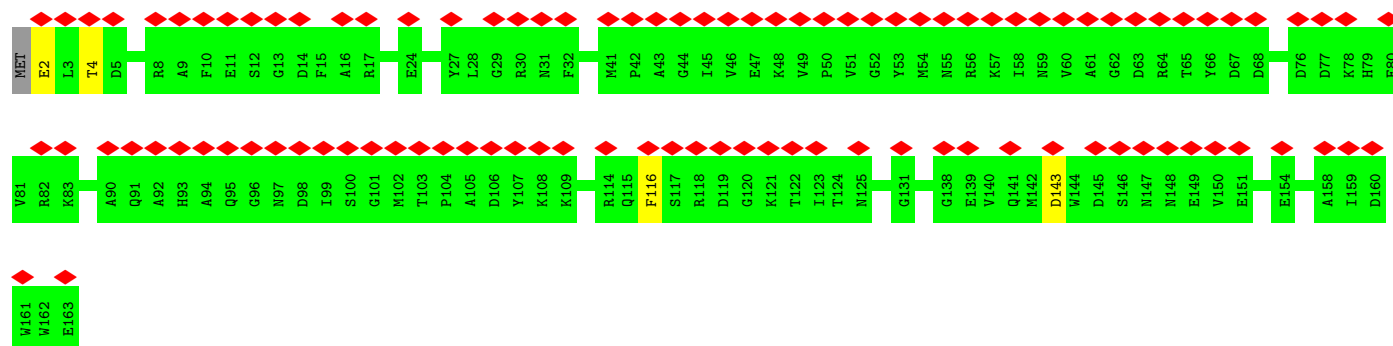
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Chain TB: 62% 97%



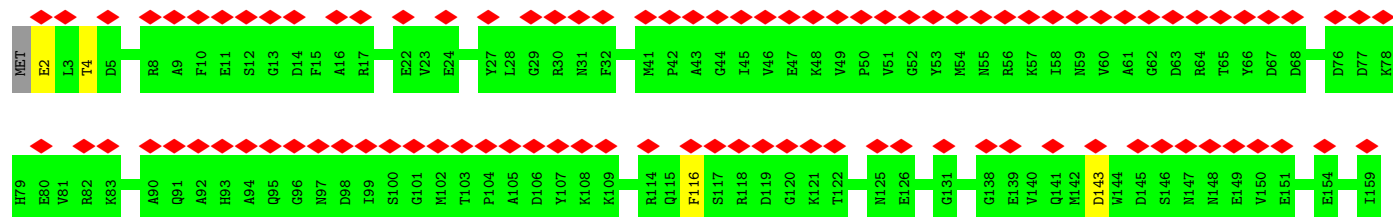
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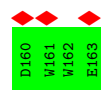
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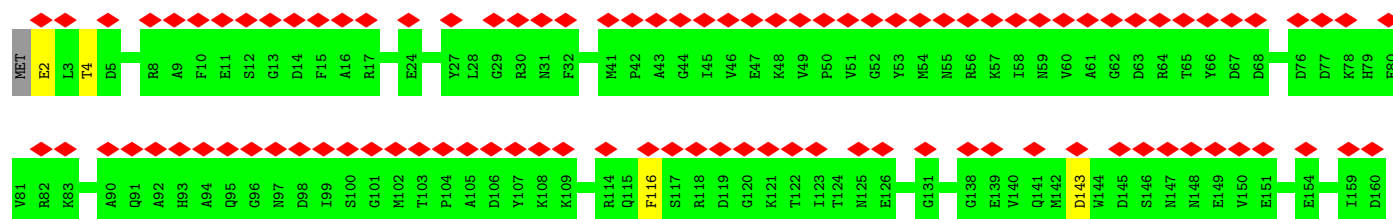
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Chain TD: 61% 97%

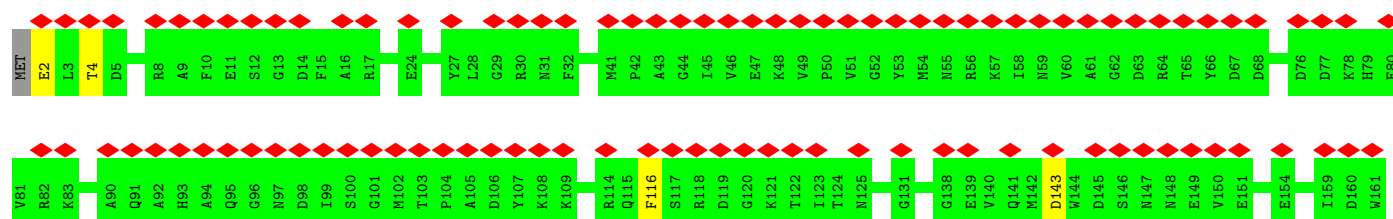




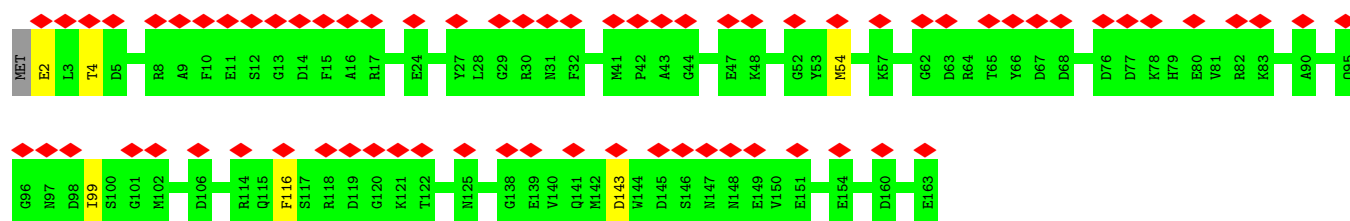
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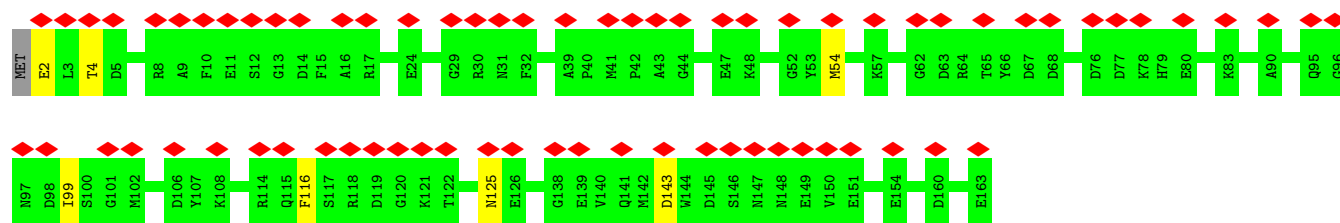


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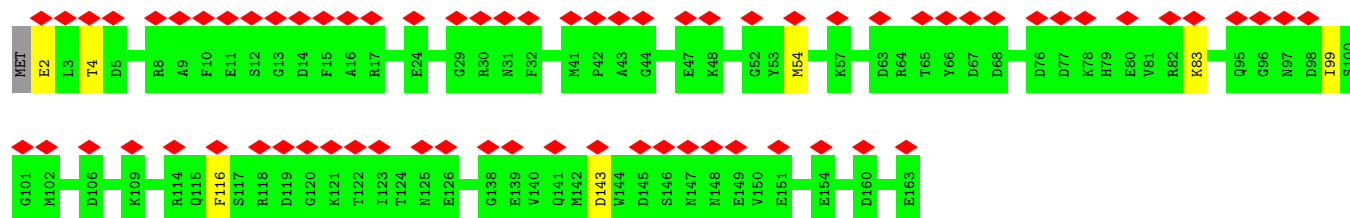


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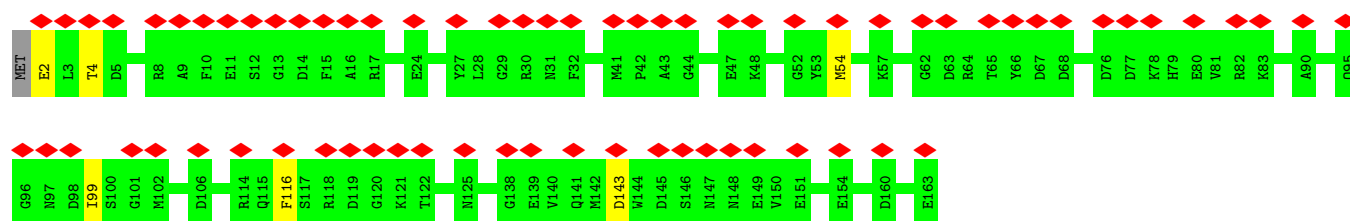
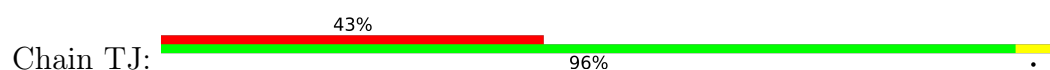




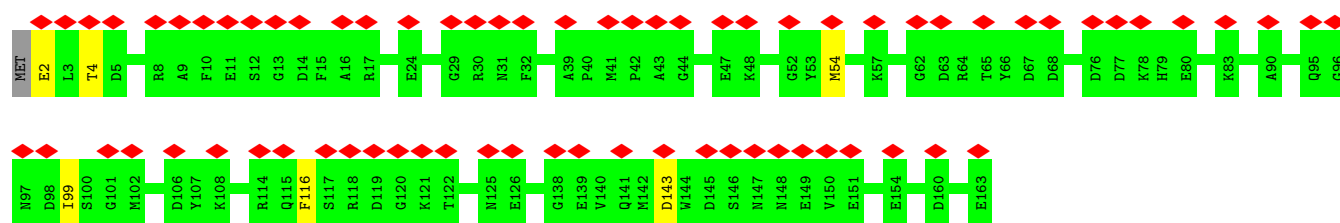
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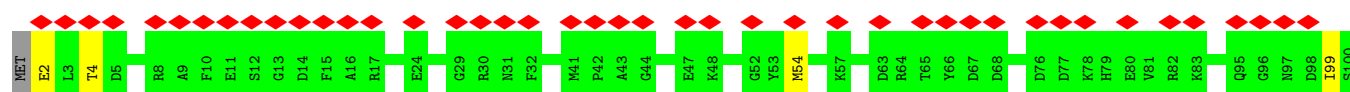
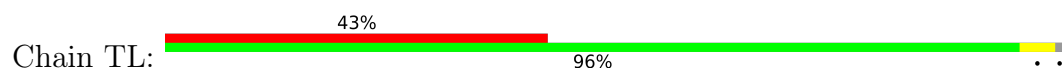
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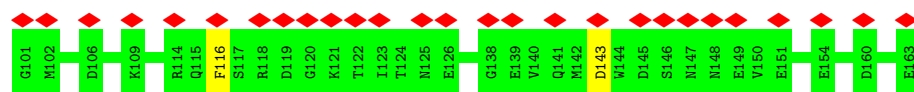


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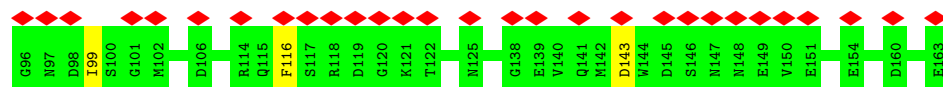
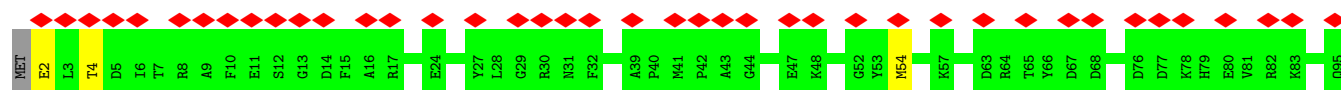


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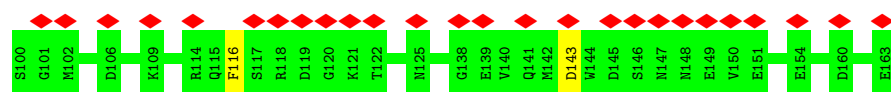
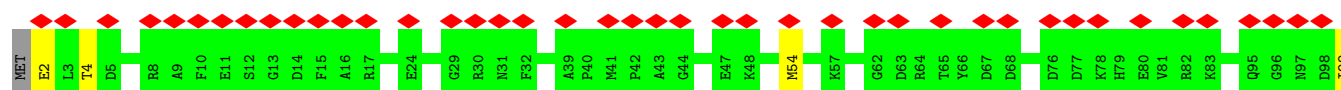
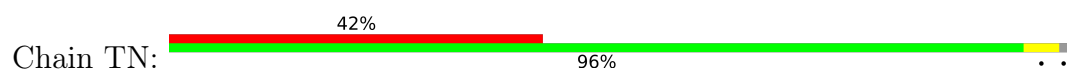




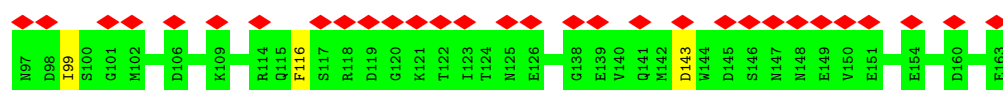
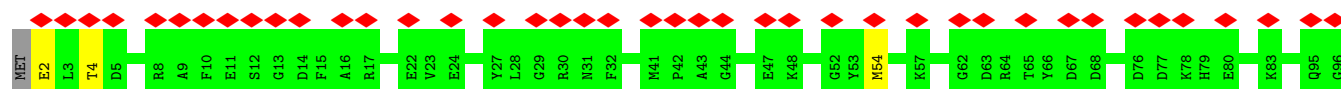
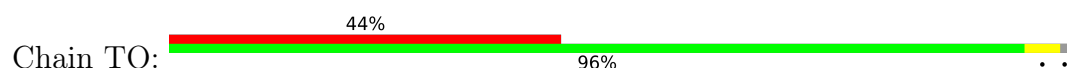
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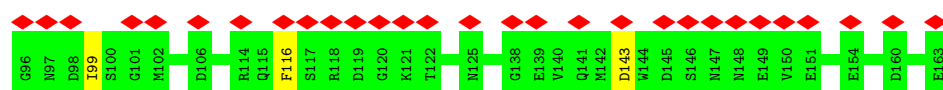
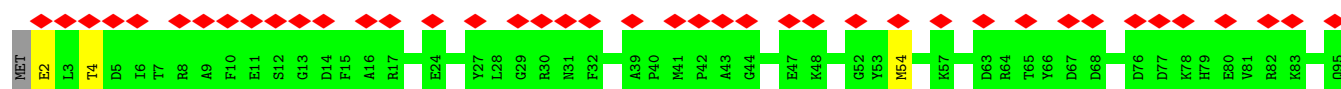
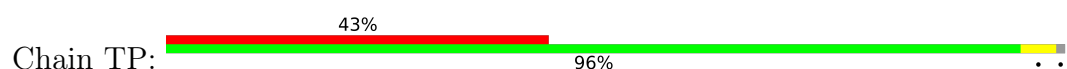
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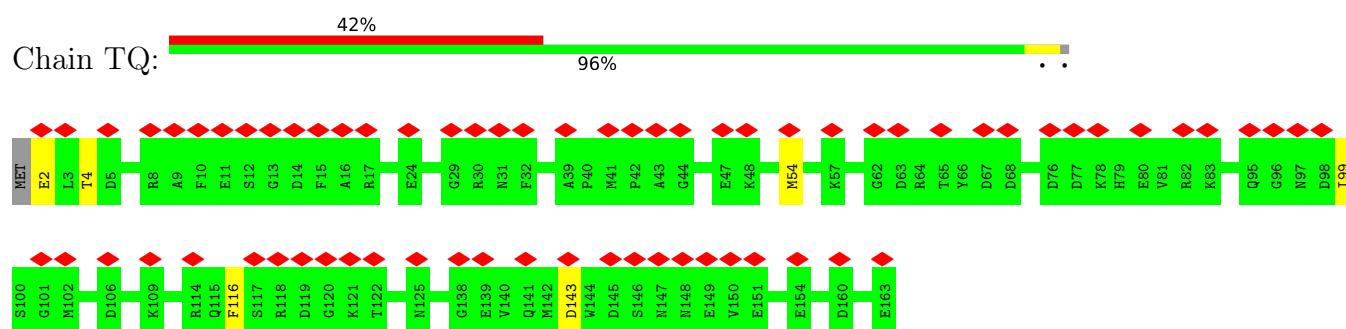
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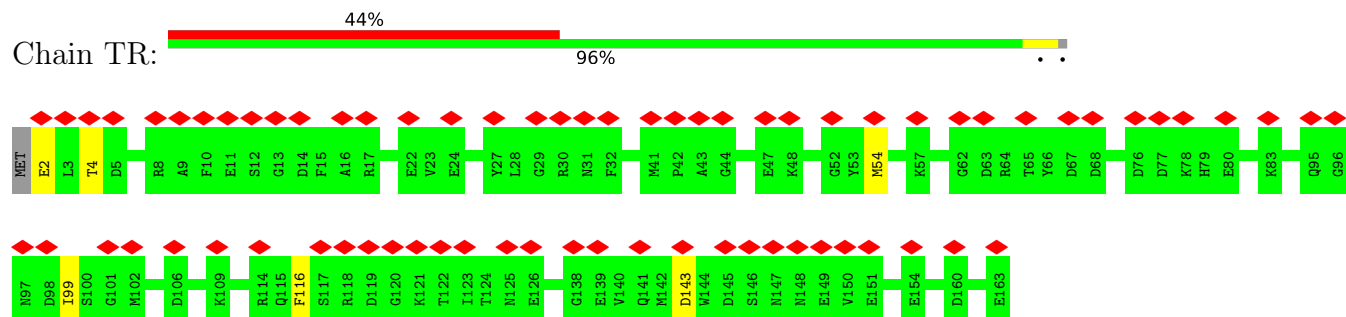
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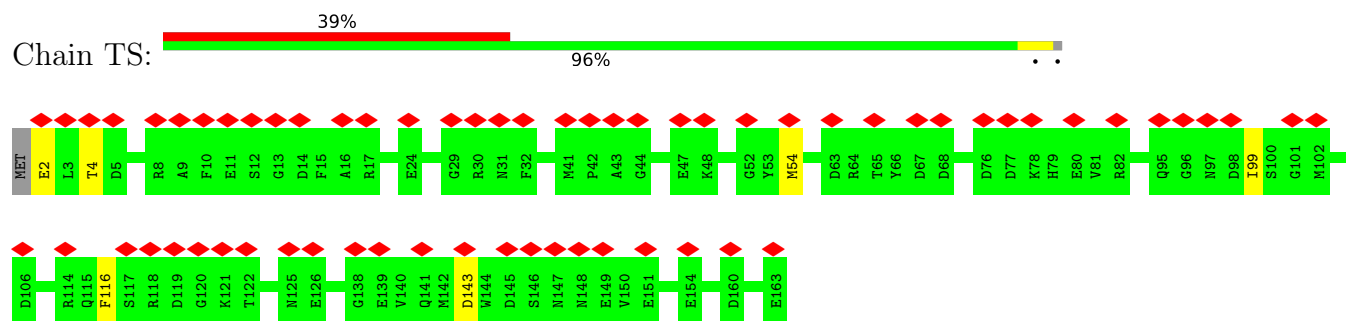
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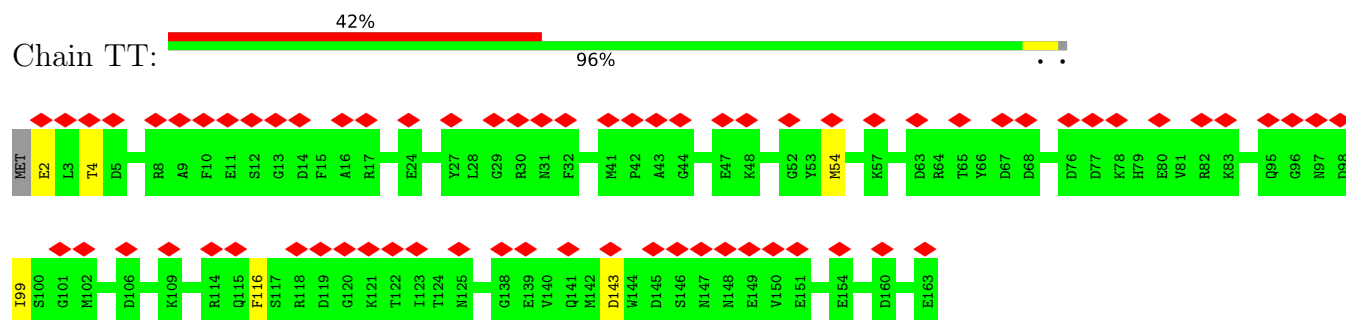
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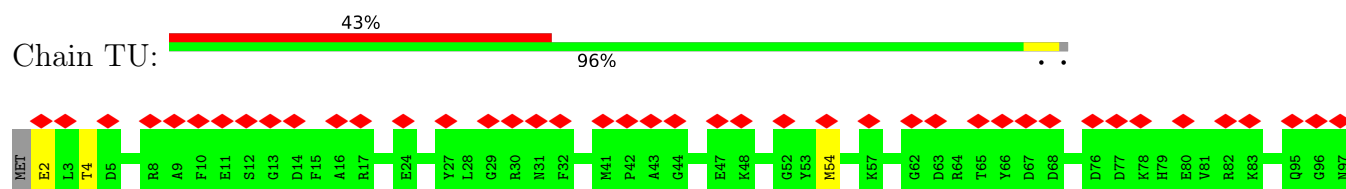
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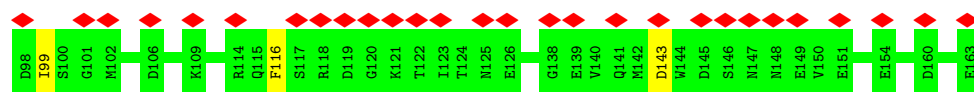


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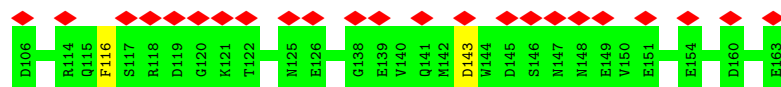
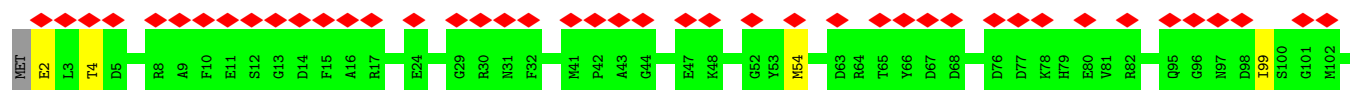
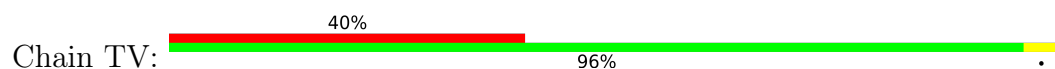


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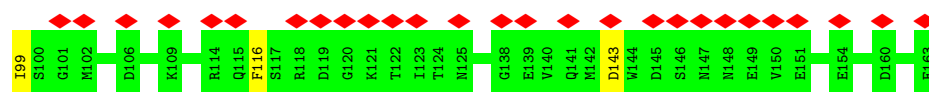
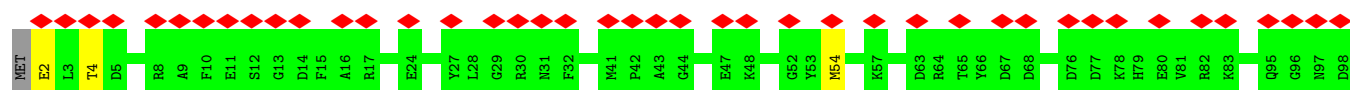
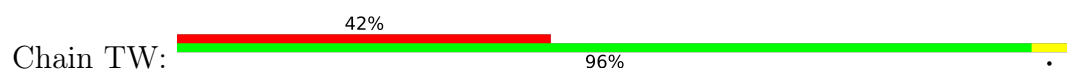




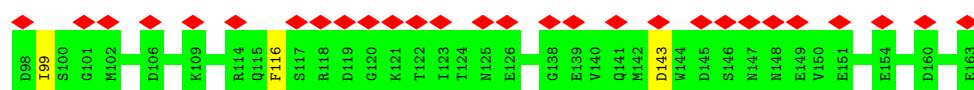
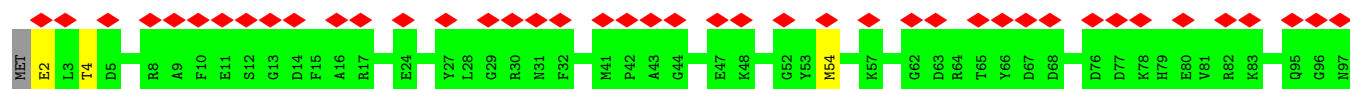
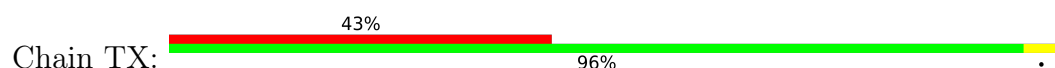
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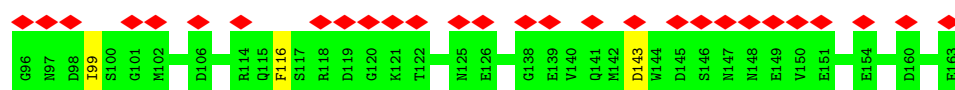
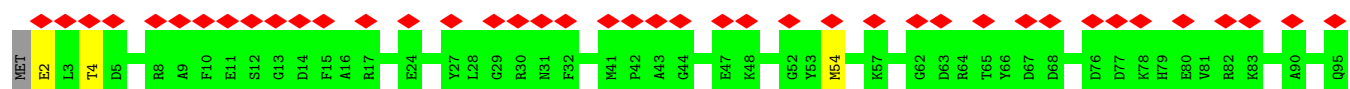
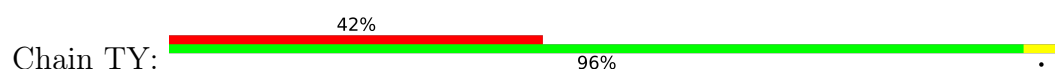
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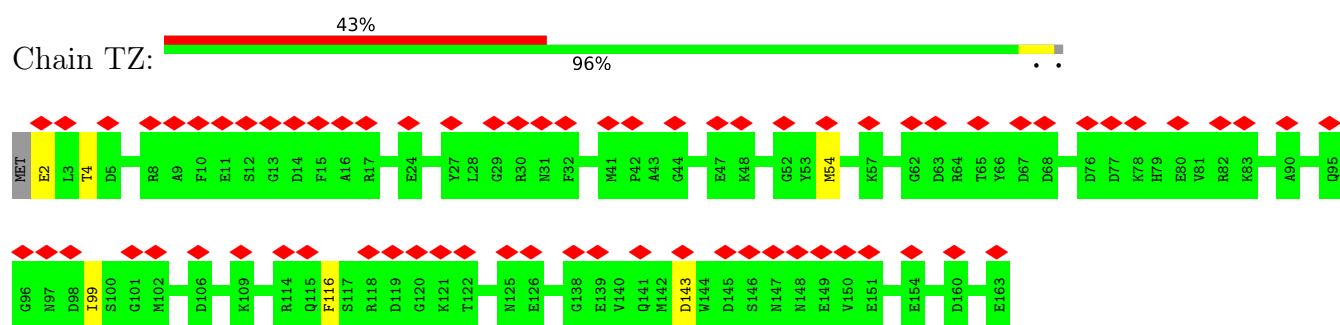
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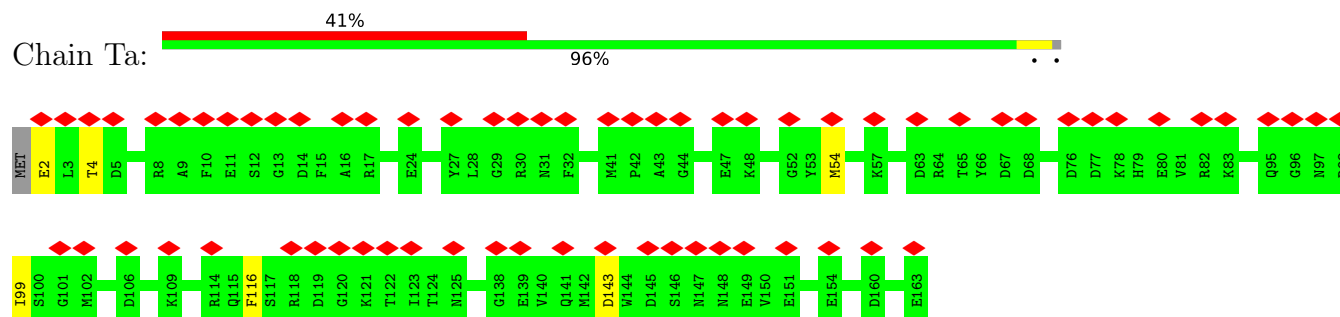
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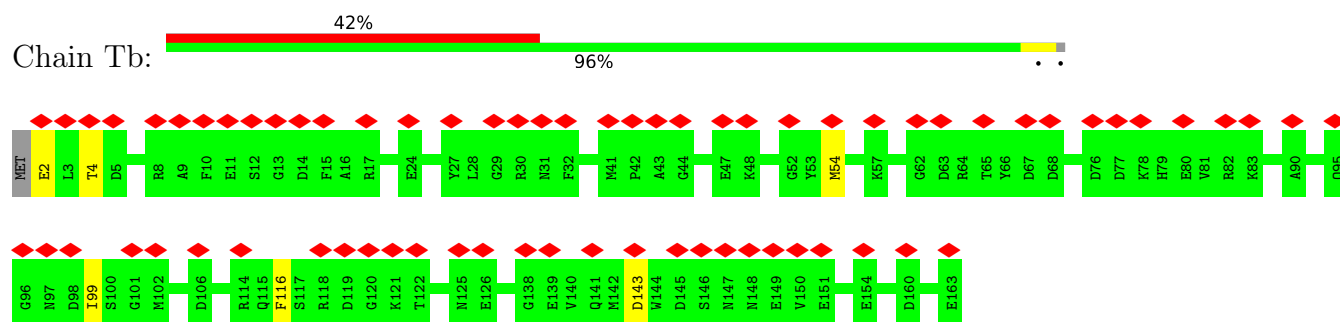
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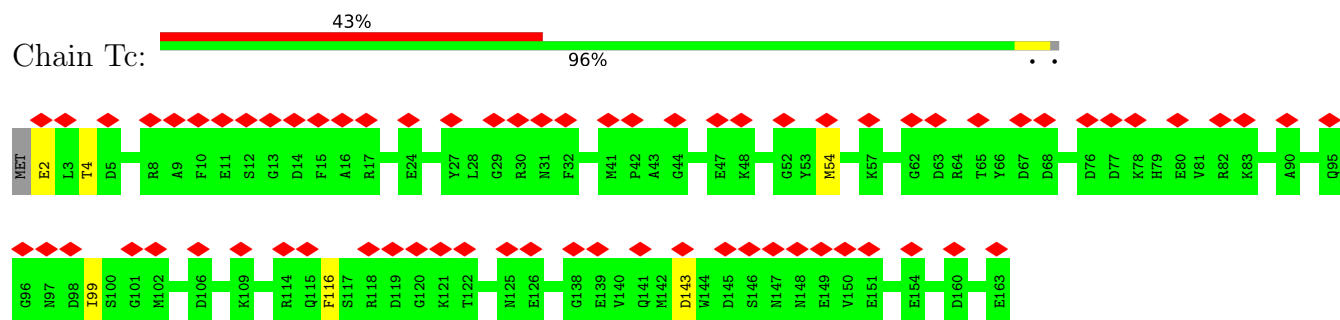
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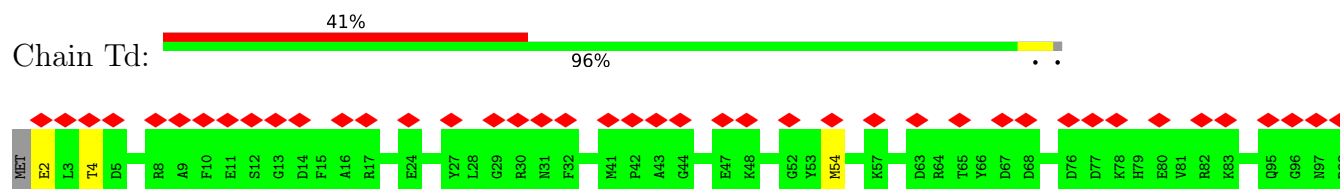
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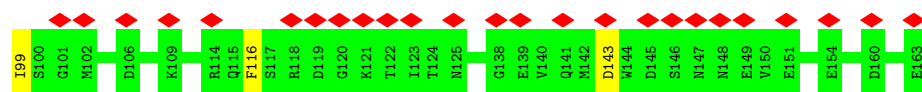


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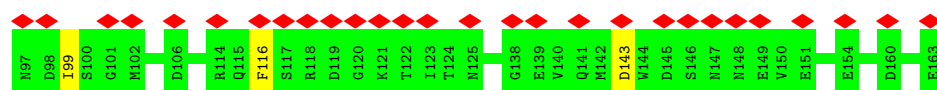
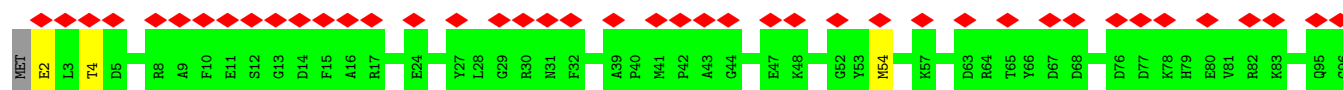
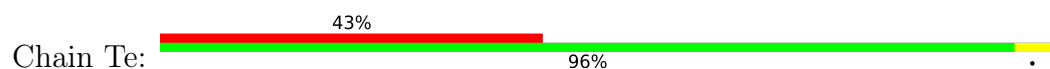


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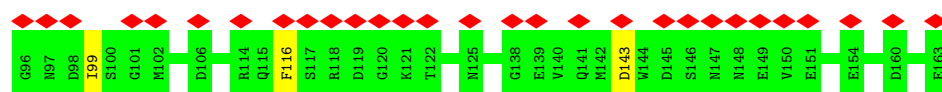
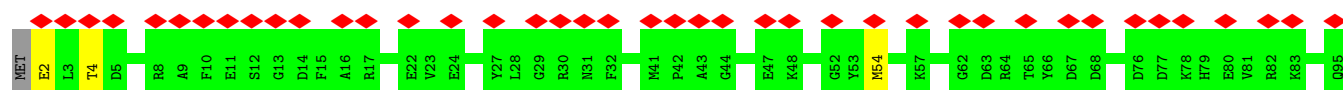
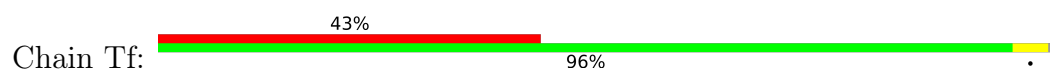




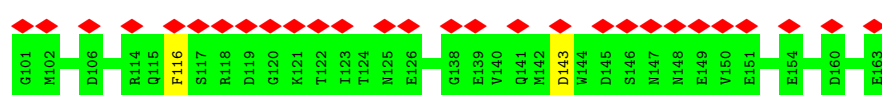
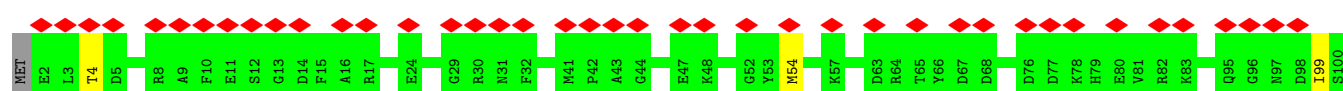
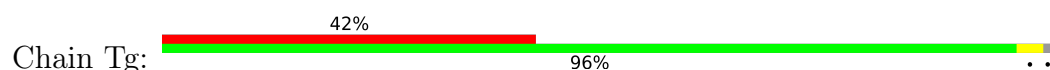
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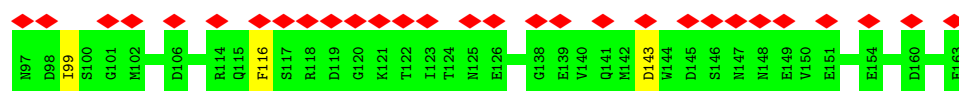
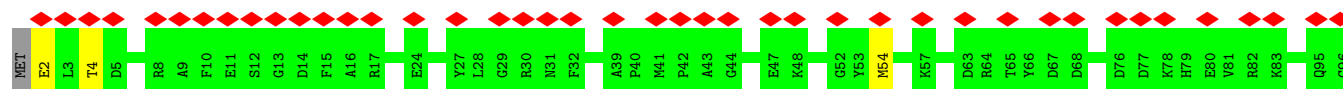
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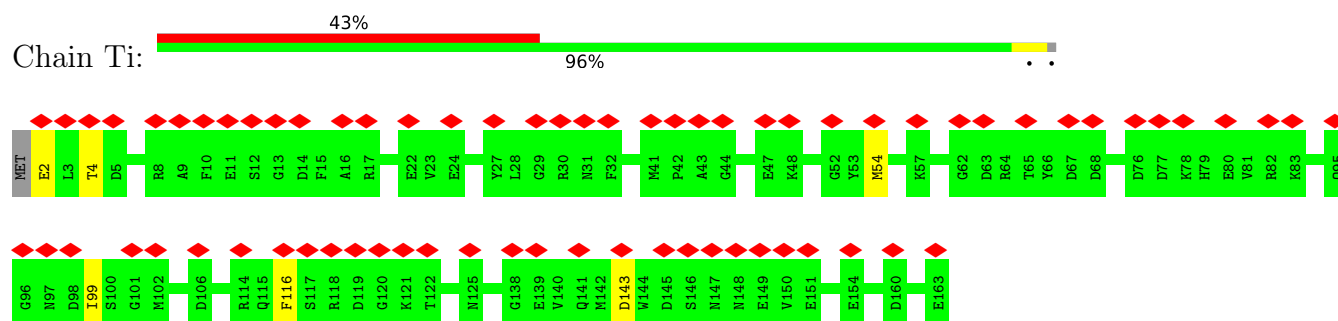
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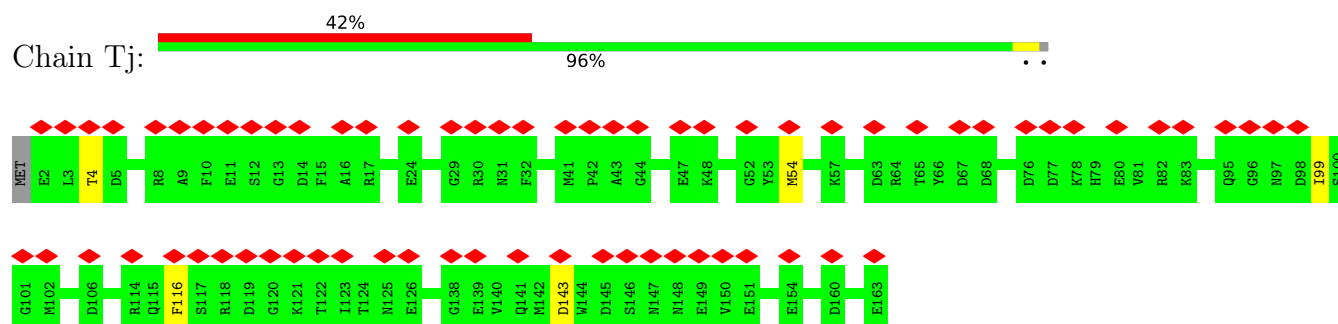
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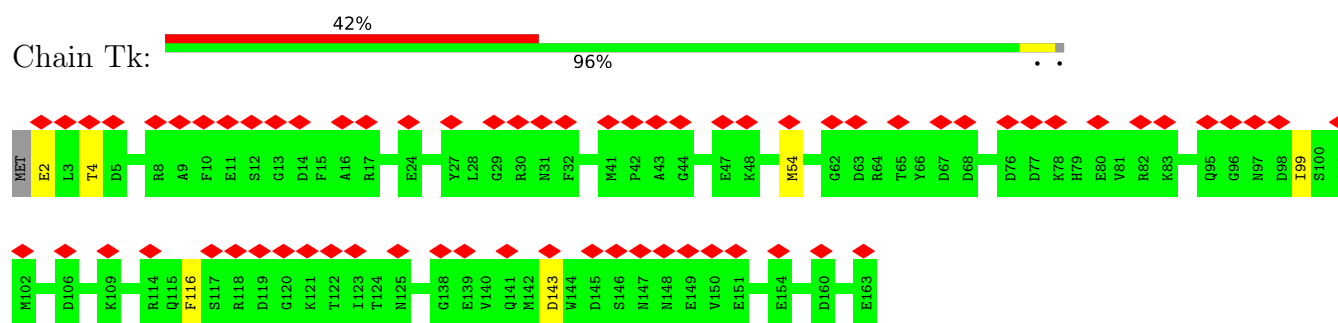
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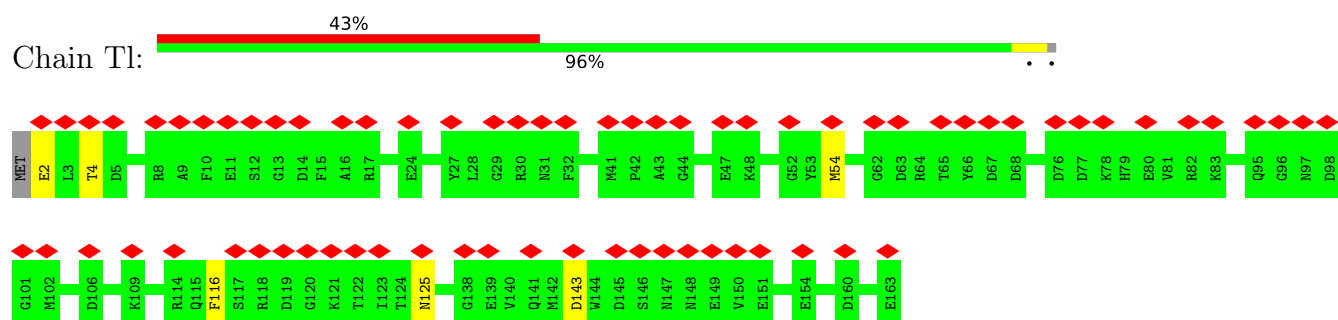
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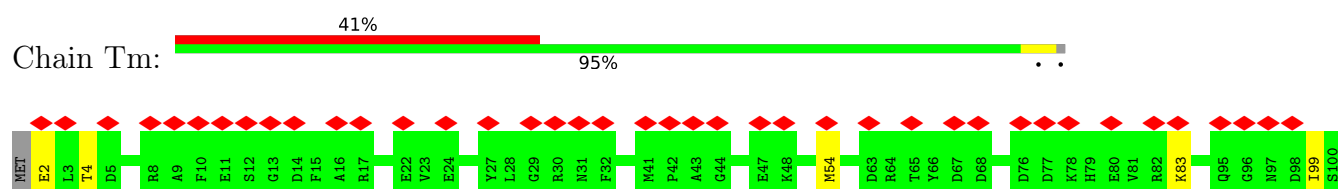
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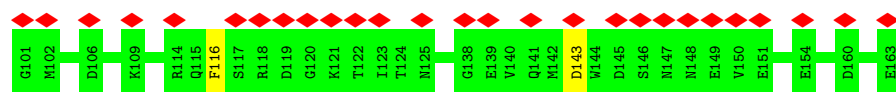


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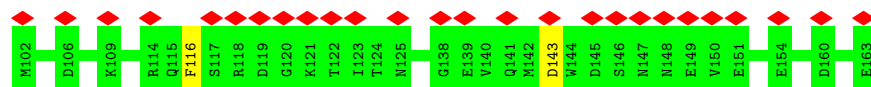
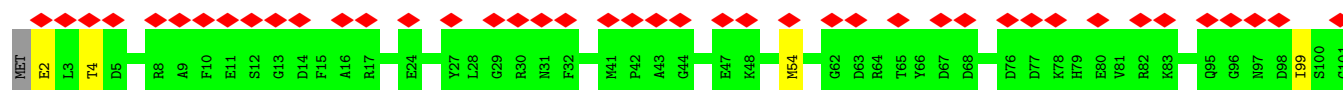
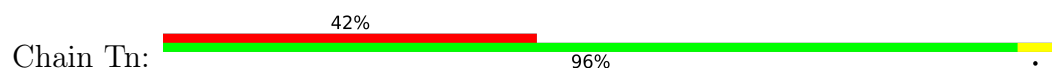


- Molecule 2: Tail tube protein

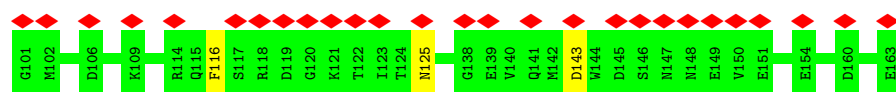
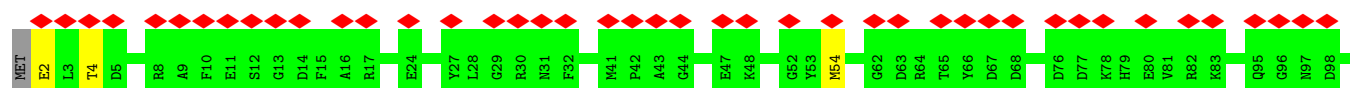
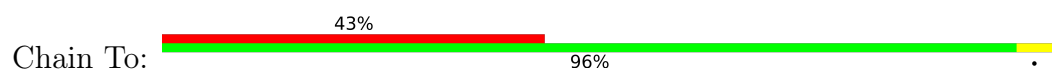




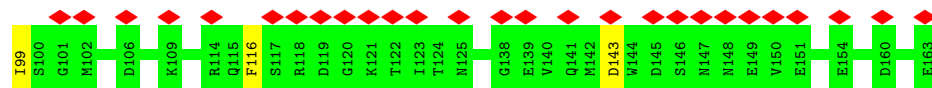
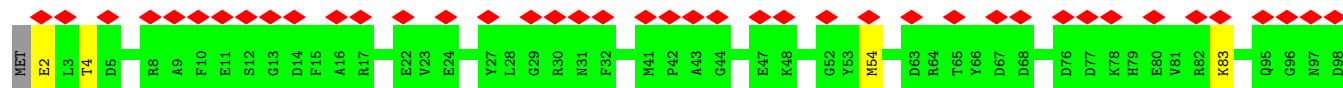
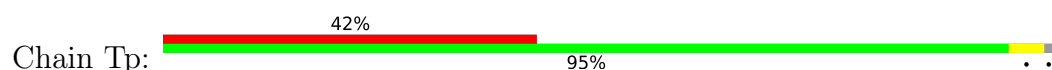
- Molecule 2: Tail tube protein



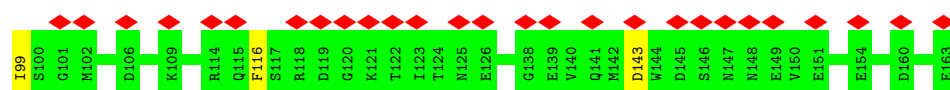
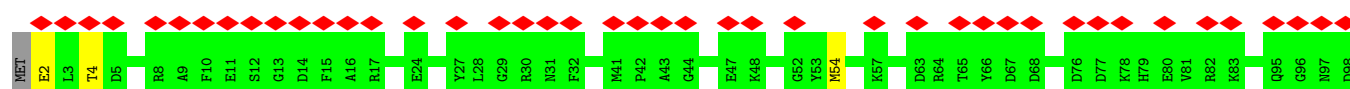
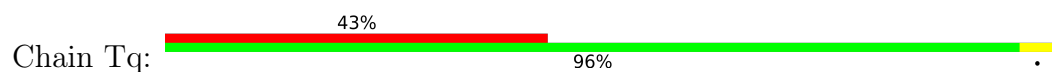
- Molecule 2: Tail tube protein



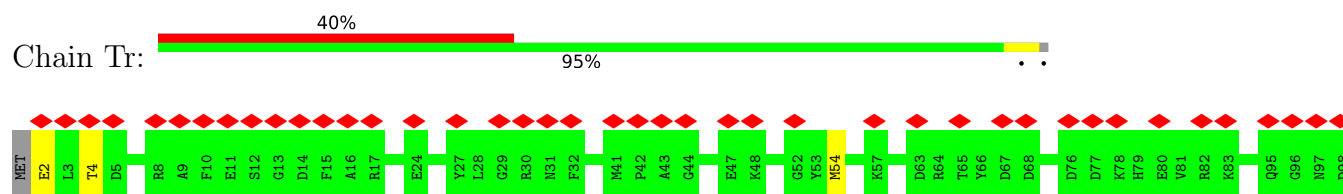
- Molecule 2: Tail tube protein



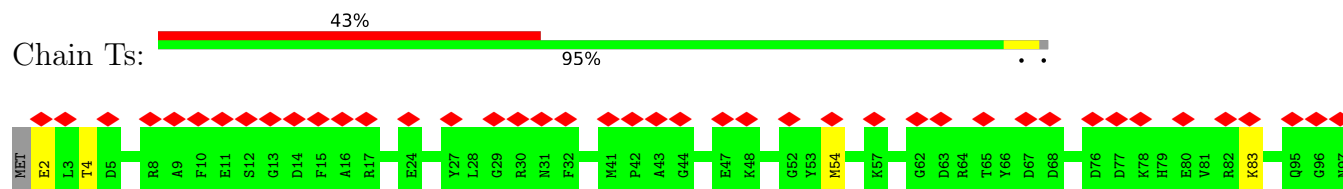
- Molecule 2: Tail tube protein



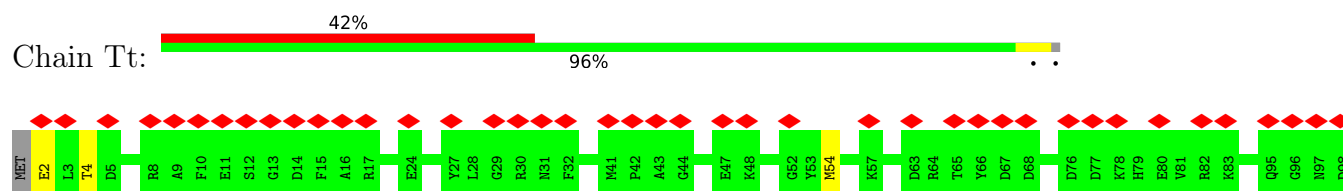
- Molecule 2: Tail tube protein



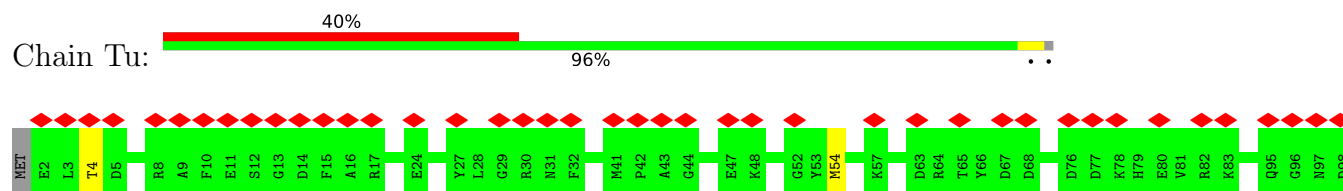
- Molecule 2: Tail tube protein



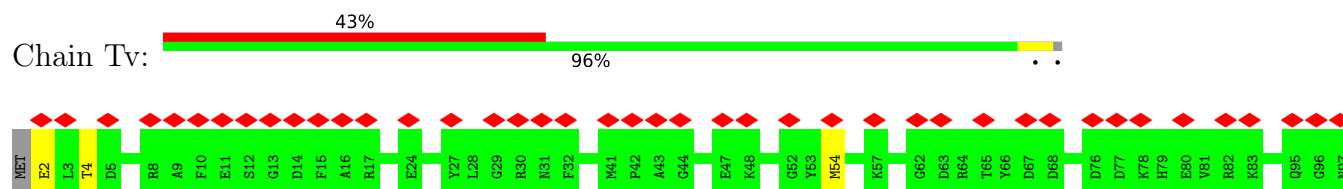
- Molecule 2: Tail tube protein

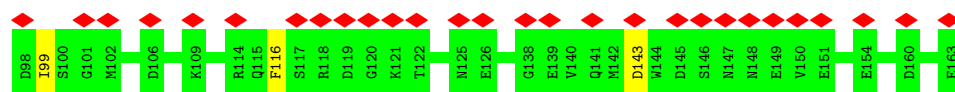


- Molecule 2: Tail tube protein

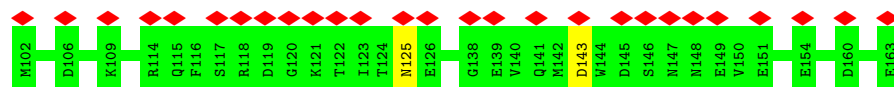
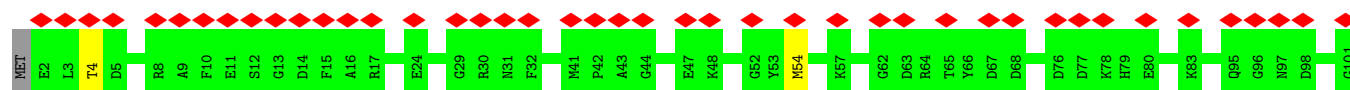


- Molecule 2: Tail tube protein

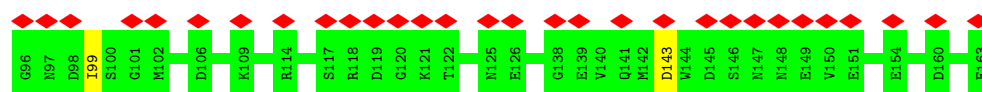
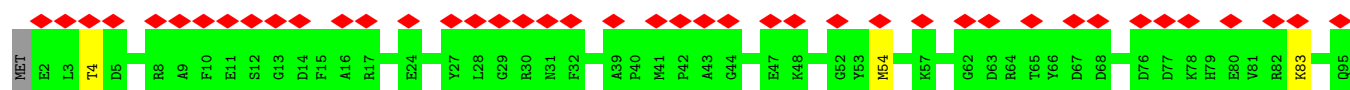
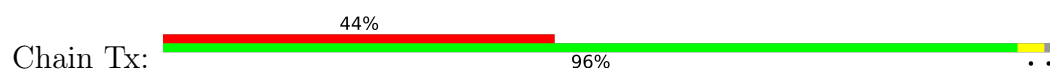




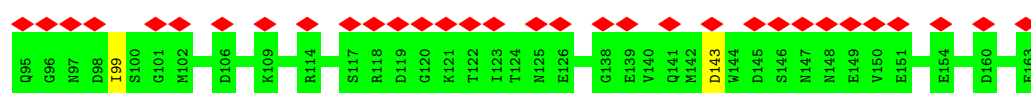
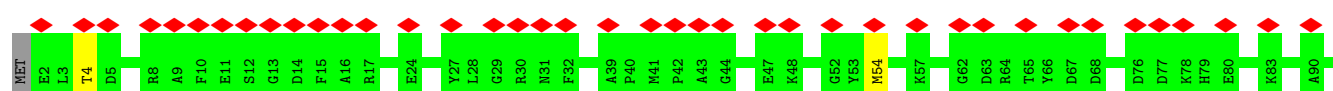
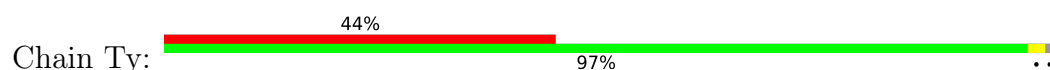
- Molecule 2: Tail tube protein



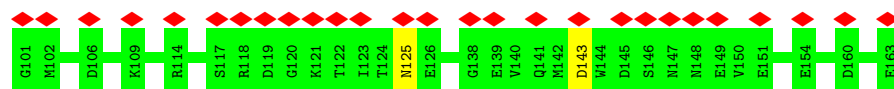
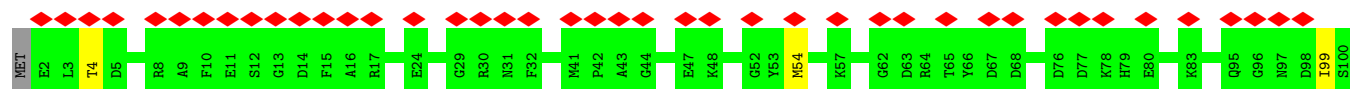
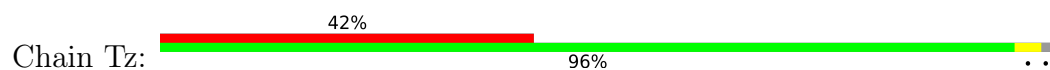
- Molecule 2: Tail tube protein



- Molecule 2: Tail tube protein



- Molecule 2: Tail tube protein



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=16.93°, rise=40.22 Å, axial sym=C6	Depositor
Number of segments used	7017	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 ($e^-/\text{Å}^2$)	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	0.868	Depositor
Minimum map value	-0.402	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.34	Depositor
Map size (Å)	426.80002, 426.80002, 426.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

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	S1	0.58	0/5135	1.06	3/6983 (0.0%)
1	S2	0.58	0/5135	1.06	3/6983 (0.0%)
1	SA	0.59	0/5135	1.07	3/6983 (0.0%)
1	SB	0.59	0/5135	1.07	3/6983 (0.0%)
1	SC	0.59	0/5135	1.07	3/6983 (0.0%)
1	SD	0.59	0/5135	1.07	3/6983 (0.0%)
1	SE	0.59	0/5135	1.07	3/6983 (0.0%)
1	SF	0.59	0/5135	1.07	3/6983 (0.0%)
1	SG	0.58	0/5135	1.06	3/6983 (0.0%)
1	SH	0.58	0/5135	1.06	3/6983 (0.0%)
1	SI	0.58	0/5135	1.06	3/6983 (0.0%)
1	SJ	0.58	0/5135	1.06	3/6983 (0.0%)
1	SK	0.58	0/5135	1.06	3/6983 (0.0%)
1	SL	0.58	0/5135	1.06	3/6983 (0.0%)
1	SM	0.58	0/5135	1.06	3/6983 (0.0%)
1	SN	0.58	0/5135	1.06	3/6983 (0.0%)
1	SO	0.58	0/5135	1.06	3/6983 (0.0%)
1	SP	0.58	0/5135	1.06	3/6983 (0.0%)
1	SQ	0.58	0/5135	1.06	3/6983 (0.0%)
1	SR	0.58	0/5135	1.06	3/6983 (0.0%)
1	SS	0.58	0/5135	1.06	3/6983 (0.0%)
1	ST	0.58	0/5135	1.06	3/6983 (0.0%)
1	SU	0.58	0/5135	1.06	3/6983 (0.0%)
1	SV	0.58	0/5135	1.06	3/6983 (0.0%)
1	SW	0.58	0/5135	1.06	3/6983 (0.0%)
1	SX	0.58	0/5135	1.06	3/6983 (0.0%)
1	SY	0.58	0/5135	1.06	3/6983 (0.0%)
1	SZ	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sa	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sb	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sc	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sd	0.58	0/5135	1.06	3/6983 (0.0%)
1	Se	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sf	0.58	0/5135	1.06	3/6983 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Sg	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sh	0.58	0/5135	1.06	3/6983 (0.0%)
1	Si	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sj	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sk	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sl	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sm	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sn	0.58	0/5135	1.06	3/6983 (0.0%)
1	So	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sp	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sq	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sr	0.58	0/5135	1.06	3/6983 (0.0%)
1	Ss	0.58	0/5135	1.06	3/6983 (0.0%)
1	St	0.58	0/5135	1.06	3/6983 (0.0%)
1	Su	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sv	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sw	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sx	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sy	0.58	0/5135	1.06	3/6983 (0.0%)
1	Sz	0.58	0/5135	1.06	3/6983 (0.0%)
2	T1	0.55	0/1339	0.95	1/1821 (0.1%)
2	T2	0.55	0/1339	0.95	1/1821 (0.1%)
2	TA	0.54	0/1339	0.94	1/1821 (0.1%)
2	TB	0.54	0/1339	0.94	1/1821 (0.1%)
2	TC	0.54	0/1339	0.94	1/1821 (0.1%)
2	TD	0.54	0/1339	0.94	1/1821 (0.1%)
2	TE	0.54	0/1339	0.94	1/1821 (0.1%)
2	TF	0.54	0/1339	0.94	1/1821 (0.1%)
2	TG	0.54	0/1339	0.94	1/1821 (0.1%)
2	TH	0.55	0/1339	0.94	1/1821 (0.1%)
2	TI	0.54	0/1339	0.94	1/1821 (0.1%)
2	TJ	0.54	0/1339	0.94	1/1821 (0.1%)
2	TK	0.55	0/1339	0.94	1/1821 (0.1%)
2	TL	0.55	0/1339	0.94	1/1821 (0.1%)
2	TM	0.54	0/1339	0.94	1/1821 (0.1%)
2	TN	0.55	0/1339	0.94	1/1821 (0.1%)
2	TO	0.54	0/1339	0.94	1/1821 (0.1%)
2	TP	0.54	0/1339	0.94	1/1821 (0.1%)
2	TQ	0.55	0/1339	0.94	1/1821 (0.1%)
2	TR	0.54	0/1339	0.94	1/1821 (0.1%)
2	TS	0.54	0/1339	0.94	1/1821 (0.1%)
2	TT	0.54	0/1339	0.94	1/1821 (0.1%)
2	TU	0.54	0/1339	0.94	1/1821 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	TV	0.55	0/1339	0.94	1/1821 (0.1%)
2	TW	0.54	0/1339	0.94	1/1821 (0.1%)
2	TX	0.54	0/1339	0.94	1/1821 (0.1%)
2	TY	0.54	0/1339	0.94	1/1821 (0.1%)
2	TZ	0.54	0/1339	0.94	1/1821 (0.1%)
2	Ta	0.55	0/1339	0.94	1/1821 (0.1%)
2	Tb	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tc	0.54	0/1339	0.94	1/1821 (0.1%)
2	Td	0.55	0/1339	0.94	1/1821 (0.1%)
2	Te	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tf	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tg	0.55	0/1339	0.94	1/1821 (0.1%)
2	Th	0.54	0/1339	0.94	1/1821 (0.1%)
2	Ti	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tj	0.55	0/1339	0.94	1/1821 (0.1%)
2	Tk	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tl	0.55	0/1339	0.94	1/1821 (0.1%)
2	Tm	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tn	0.54	0/1339	0.94	1/1821 (0.1%)
2	To	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tp	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tq	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tr	0.55	0/1339	0.94	1/1821 (0.1%)
2	Ts	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tt	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tu	0.55	0/1339	0.94	1/1821 (0.1%)
2	Tv	0.54	0/1339	0.94	1/1821 (0.1%)
2	Tw	0.55	0/1339	0.95	1/1821 (0.1%)
2	Tx	0.55	0/1339	0.95	1/1821 (0.1%)
2	Ty	0.55	0/1339	0.95	1/1821 (0.1%)
2	Tz	0.55	0/1339	0.95	1/1821 (0.1%)
All	All	0.57	0/349596	1.04	216/475416 (0.0%)

There are no bond length outliers.

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	St	190	ASP	CA-CB-CG	6.36	118.96	112.60
1	Sk	190	ASP	CA-CB-CG	6.35	118.95	112.60
1	SO	190	ASP	CA-CB-CG	6.35	118.95	112.60
1	Sh	190	ASP	CA-CB-CG	6.35	118.95	112.60
1	Sd	190	ASP	CA-CB-CG	6.34	118.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	SR	190	ASP	CA-CB-CG	6.34	118.94	112.60
1	Sn	190	ASP	CA-CB-CG	6.34	118.94	112.60
1	SU	190	ASP	CA-CB-CG	6.33	118.94	112.60
1	SY	190	ASP	CA-CB-CG	6.33	118.93	112.60
1	SE	190	ASP	CA-CB-CG	6.32	118.92	112.60
1	S1	190	ASP	CA-CB-CG	6.31	118.91	112.60
1	Se	190	ASP	CA-CB-CG	6.31	118.91	112.60
1	SK	190	ASP	CA-CB-CG	6.31	118.91	112.60
1	SX	190	ASP	CA-CB-CG	6.31	118.91	112.60
1	Sw	190	ASP	CA-CB-CG	6.30	118.90	112.60
1	SL	190	ASP	CA-CB-CG	6.30	118.90	112.60
1	Sq	190	ASP	CA-CB-CG	6.30	118.90	112.60
1	Sb	190	ASP	CA-CB-CG	6.29	118.89	112.60
1	Sa	190	ASP	CA-CB-CG	6.29	118.89	112.60
1	SB	190	ASP	CA-CB-CG	6.29	118.89	112.60
1	Sx	190	ASP	CA-CB-CG	6.29	118.89	112.60
1	SC	190	ASP	CA-CB-CG	6.29	118.89	112.60
1	Sj	190	ASP	CA-CB-CG	6.29	118.89	112.60
1	SH	190	ASP	CA-CB-CG	6.26	118.86	112.60
1	SI	190	ASP	CA-CB-CG	6.26	118.86	112.60
1	Sg	190	ASP	CA-CB-CG	6.26	118.86	112.60
1	SV	190	ASP	CA-CB-CG	6.25	118.85	112.60
1	Su	190	ASP	CA-CB-CG	6.25	118.85	112.60
1	Sl	190	ASP	CA-CB-CG	6.24	118.84	112.60
1	SQ	190	ASP	CA-CB-CG	6.23	118.83	112.60
1	SJ	190	ASP	CA-CB-CG	6.23	118.83	112.60
1	Sr	190	ASP	CA-CB-CG	6.23	118.83	112.60
1	SF	190	ASP	CA-CB-CG	6.22	118.82	112.60
1	Sz	190	ASP	CA-CB-CG	6.22	118.82	112.60
1	SS	190	ASP	CA-CB-CG	6.22	118.82	112.60
1	SZ	190	ASP	CA-CB-CG	6.21	118.81	112.60
1	SP	190	ASP	CA-CB-CG	6.21	118.81	112.60
1	Sf	190	ASP	CA-CB-CG	6.21	118.81	112.60
1	Si	190	ASP	CA-CB-CG	6.21	118.81	112.60
1	SW	190	ASP	CA-CB-CG	6.20	118.80	112.60
1	ST	190	ASP	CA-CB-CG	6.20	118.80	112.60
1	SN	190	ASP	CA-CB-CG	6.20	118.80	112.60
1	Sm	190	ASP	CA-CB-CG	6.20	118.80	112.60
1	SD	190	ASP	CA-CB-CG	6.20	118.80	112.60
1	SM	190	ASP	CA-CB-CG	6.20	118.80	112.60
1	So	190	ASP	CA-CB-CG	6.20	118.80	112.60
1	SG	190	ASP	CA-CB-CG	6.19	118.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	190	ASP	CA-CB-CG	6.17	118.77	112.60
1	Sp	190	ASP	CA-CB-CG	6.16	118.76	112.60
1	Sc	190	ASP	CA-CB-CG	6.15	118.75	112.60
1	Ss	190	ASP	CA-CB-CG	6.15	118.75	112.60
1	Sv	190	ASP	CA-CB-CG	6.15	118.75	112.60
1	SA	190	ASP	CA-CB-CG	6.14	118.74	112.60
1	Sy	190	ASP	CA-CB-CG	6.14	118.74	112.60
1	So	457	ASP	CA-CB-CG	6.04	118.64	112.60
1	Sl	457	ASP	CA-CB-CG	6.04	118.64	112.60
1	SN	457	ASP	CA-CB-CG	6.03	118.63	112.60
1	SW	457	ASP	CA-CB-CG	6.02	118.62	112.60
1	Sm	457	ASP	CA-CB-CG	6.02	118.62	112.60
1	SQ	457	ASP	CA-CB-CG	6.02	118.62	112.60
1	ST	457	ASP	CA-CB-CG	6.01	118.61	112.60
1	SV	457	ASP	CA-CB-CG	6.01	118.61	112.60
1	SK	457	ASP	CA-CB-CG	6.01	118.61	112.60
1	Sc	457	ASP	CA-CB-CG	6.01	118.61	112.60
1	Sp	457	ASP	CA-CB-CG	6.01	118.61	112.60
1	Sr	457	ASP	CA-CB-CG	6.00	118.61	112.60
1	SH	457	ASP	CA-CB-CG	6.00	118.60	112.60
1	SJ	457	ASP	CA-CB-CG	6.00	118.60	112.60
1	Sf	457	ASP	CA-CB-CG	6.00	118.60	112.60
1	Ss	457	ASP	CA-CB-CG	6.00	118.60	112.60
1	Sg	457	ASP	CA-CB-CG	5.98	118.58	112.60
1	Sv	457	ASP	CA-CB-CG	5.98	118.58	112.60
1	SG	457	ASP	CA-CB-CG	5.98	118.58	112.60
1	SZ	457	ASP	CA-CB-CG	5.97	118.57	112.60
1	Su	457	ASP	CA-CB-CG	5.97	118.57	112.60
1	SY	457	ASP	CA-CB-CG	5.97	118.57	112.60
1	SS	457	ASP	CA-CB-CG	5.97	118.57	112.60
1	Sa	457	ASP	CA-CB-CG	5.97	118.57	112.60
1	Sk	457	ASP	CA-CB-CG	5.97	118.57	112.60
1	Sb	457	ASP	CA-CB-CG	5.97	118.57	112.60
1	Si	457	ASP	CA-CB-CG	5.97	118.57	112.60
1	SP	457	ASP	CA-CB-CG	5.96	118.56	112.60
1	SL	457	ASP	CA-CB-CG	5.96	118.56	112.60
1	SI	457	ASP	CA-CB-CG	5.95	118.55	112.60
1	Sd	457	ASP	CA-CB-CG	5.95	118.55	112.60
1	Sj	457	ASP	CA-CB-CG	5.95	118.55	112.60
1	SU	457	ASP	CA-CB-CG	5.95	118.55	112.60
1	SM	457	ASP	CA-CB-CG	5.95	118.55	112.60
1	SO	457	ASP	CA-CB-CG	5.95	118.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Sn	457	ASP	CA-CB-CG	5.95	118.55	112.60
1	SX	457	ASP	CA-CB-CG	5.94	118.54	112.60
1	Se	457	ASP	CA-CB-CG	5.94	118.54	112.60
1	Sx	457	ASP	CA-CB-CG	5.94	118.54	112.60
1	Sh	457	ASP	CA-CB-CG	5.93	118.53	112.60
1	Sq	457	ASP	CA-CB-CG	5.93	118.53	112.60
1	Sw	457	ASP	CA-CB-CG	5.93	118.53	112.60
1	Sy	457	ASP	CA-CB-CG	5.93	118.53	112.60
1	Sr	629	LYS	CB-CA-C	5.93	116.75	110.17
1	SC	629	LYS	CB-CA-C	5.92	116.74	110.17
1	St	457	ASP	CA-CB-CG	5.92	118.52	112.60
1	S2	457	ASP	CA-CB-CG	5.91	118.51	112.60
1	S1	457	ASP	CA-CB-CG	5.91	118.51	112.60
1	SR	457	ASP	CA-CB-CG	5.91	118.51	112.60
1	Sk	629	LYS	CB-CA-C	5.91	116.73	110.17
1	Sz	457	ASP	CA-CB-CG	5.91	118.51	112.60
1	Su	629	LYS	CB-CA-C	5.91	116.73	110.17
1	Sq	629	LYS	CB-CA-C	5.90	116.72	110.17
1	SF	629	LYS	CB-CA-C	5.90	116.72	110.17
1	St	629	LYS	CB-CA-C	5.90	116.72	110.17
1	SI	629	LYS	CB-CA-C	5.89	116.71	110.17
1	SI	629	LYS	CB-CA-C	5.89	116.71	110.17
1	So	629	LYS	CB-CA-C	5.89	116.71	110.17
1	Sn	629	LYS	CB-CA-C	5.88	116.70	110.17
1	Si	629	LYS	CB-CA-C	5.88	116.70	110.17
1	SL	629	LYS	CB-CA-C	5.87	116.68	110.17
1	SD	629	LYS	CB-CA-C	5.85	116.66	110.17
1	SV	629	LYS	CB-CA-C	5.85	116.66	110.17
1	Se	629	LYS	CB-CA-C	5.85	116.66	110.17
1	Sv	629	LYS	CB-CA-C	5.84	116.66	110.17
1	Sf	629	LYS	CB-CA-C	5.84	116.65	110.17
1	SY	629	LYS	CB-CA-C	5.84	116.65	110.17
1	Sh	629	LYS	CB-CA-C	5.84	116.65	110.17
1	SB	629	LYS	CB-CA-C	5.83	116.65	110.17
1	SD	457	ASP	CA-CB-CG	5.83	118.44	112.60
1	SM	629	LYS	CB-CA-C	5.83	116.64	110.17
1	Sb	629	LYS	CB-CA-C	5.83	116.64	110.17
1	Ss	629	LYS	CB-CA-C	5.83	116.64	110.17
1	SE	629	LYS	CB-CA-C	5.83	116.64	110.17
1	Sm	629	LYS	CB-CA-C	5.83	116.64	110.17
1	SA	629	LYS	CB-CA-C	5.82	116.63	110.17
1	SG	629	LYS	CB-CA-C	5.82	116.63	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	SR	629	LYS	CB-CA-C	5.82	116.63	110.17
1	SX	629	LYS	CB-CA-C	5.81	116.62	110.17
1	SO	629	LYS	CB-CA-C	5.81	116.62	110.17
1	SZ	629	LYS	CB-CA-C	5.80	116.61	110.17
1	SS	629	LYS	CB-CA-C	5.80	116.61	110.17
1	ST	629	LYS	CB-CA-C	5.80	116.60	110.17
1	SU	629	LYS	CB-CA-C	5.80	116.61	110.17
1	SA	457	ASP	CA-CB-CG	5.79	118.39	112.60
1	SC	457	ASP	CA-CB-CG	5.79	118.39	112.60
1	SJ	629	LYS	CB-CA-C	5.79	116.60	110.17
1	SB	457	ASP	CA-CB-CG	5.79	118.39	112.60
1	SF	457	ASP	CA-CB-CG	5.79	118.39	112.60
1	SH	629	LYS	CB-CA-C	5.78	116.59	110.17
1	SE	457	ASP	CA-CB-CG	5.78	118.38	112.60
1	SP	629	LYS	CB-CA-C	5.78	116.59	110.17
1	Sy	629	LYS	CB-CA-C	5.78	116.58	110.17
1	S2	629	LYS	CB-CA-C	5.78	116.58	110.17
1	SW	629	LYS	CB-CA-C	5.77	116.58	110.17
1	Sj	629	LYS	CB-CA-C	5.77	116.58	110.17
1	Sg	629	LYS	CB-CA-C	5.77	116.58	110.17
1	S1	629	LYS	CB-CA-C	5.77	116.57	110.17
1	Sx	629	LYS	CB-CA-C	5.77	116.57	110.17
1	Sp	629	LYS	CB-CA-C	5.77	116.57	110.17
1	Sa	629	LYS	CB-CA-C	5.76	116.56	110.17
1	Sc	629	LYS	CB-CA-C	5.75	116.56	110.17
1	SK	629	LYS	CB-CA-C	5.75	116.55	110.17
1	SN	629	LYS	CB-CA-C	5.73	116.53	110.17
1	SQ	629	LYS	CB-CA-C	5.72	116.52	110.17
1	Sd	629	LYS	CB-CA-C	5.72	116.51	110.17
1	Sz	629	LYS	CB-CA-C	5.71	116.51	110.17
1	Sw	629	LYS	CB-CA-C	5.67	116.46	110.17
2	TX	143	ASP	CA-CB-CG	5.56	118.16	112.60
2	TG	143	ASP	CA-CB-CG	5.55	118.15	112.60
2	TJ	143	ASP	CA-CB-CG	5.55	118.15	112.60
2	TB	143	ASP	CA-CB-CG	5.54	118.14	112.60
2	TU	143	ASP	CA-CB-CG	5.53	118.13	112.60
2	Ti	143	ASP	CA-CB-CG	5.52	118.12	112.60
2	Tf	143	ASP	CA-CB-CG	5.51	118.11	112.60
2	Tk	143	ASP	CA-CB-CG	5.50	118.11	112.60
2	TK	143	ASP	CA-CB-CG	5.50	118.10	112.60
2	TZ	143	ASP	CA-CB-CG	5.49	118.09	112.60
2	Tc	143	ASP	CA-CB-CG	5.47	118.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Tq	143	ASP	CA-CB-CG	5.47	118.07	112.60
2	TE	143	ASP	CA-CB-CG	5.46	118.06	112.60
2	TA	143	ASP	CA-CB-CG	5.46	118.06	112.60
2	TD	143	ASP	CA-CB-CG	5.46	118.06	112.60
2	TR	143	ASP	CA-CB-CG	5.46	118.06	112.60
2	Tv	143	ASP	CA-CB-CG	5.46	118.06	112.60
2	TM	143	ASP	CA-CB-CG	5.45	118.05	112.60
2	Te	143	ASP	CA-CB-CG	5.45	118.05	112.60
2	TP	143	ASP	CA-CB-CG	5.44	118.04	112.60
2	Tt	143	ASP	CA-CB-CG	5.44	118.04	112.60
2	TV	143	ASP	CA-CB-CG	5.44	118.04	112.60
2	Ta	143	ASP	CA-CB-CG	5.44	118.04	112.60
2	Tl	143	ASP	CA-CB-CG	5.44	118.04	112.60
2	TC	143	ASP	CA-CB-CG	5.43	118.03	112.60
2	TO	143	ASP	CA-CB-CG	5.42	118.02	112.60
2	TF	143	ASP	CA-CB-CG	5.42	118.02	112.60
2	TH	143	ASP	CA-CB-CG	5.42	118.02	112.60
2	Ty	143	ASP	CA-CB-CG	5.42	118.02	112.60
2	T2	143	ASP	CA-CB-CG	5.41	118.01	112.60
2	Td	143	ASP	CA-CB-CG	5.41	118.01	112.60
2	Tn	143	ASP	CA-CB-CG	5.40	118.00	112.60
2	Tw	143	ASP	CA-CB-CG	5.40	118.00	112.60
2	TI	143	ASP	CA-CB-CG	5.39	117.99	112.60
2	To	143	ASP	CA-CB-CG	5.37	117.97	112.60
2	Tl	143	ASP	CA-CB-CG	5.37	117.97	112.60
2	Tg	143	ASP	CA-CB-CG	5.37	117.97	112.60
2	Ts	143	ASP	CA-CB-CG	5.37	117.97	112.60
2	Th	143	ASP	CA-CB-CG	5.37	117.97	112.60
2	TS	143	ASP	CA-CB-CG	5.37	117.97	112.60
2	TT	143	ASP	CA-CB-CG	5.37	117.97	112.60
2	Tz	143	ASP	CA-CB-CG	5.37	117.97	112.60
2	TL	143	ASP	CA-CB-CG	5.37	117.97	112.60
2	TQ	143	ASP	CA-CB-CG	5.37	117.97	112.60
2	TW	143	ASP	CA-CB-CG	5.36	117.96	112.60
2	TN	143	ASP	CA-CB-CG	5.36	117.96	112.60
2	Tj	143	ASP	CA-CB-CG	5.36	117.96	112.60
2	TY	143	ASP	CA-CB-CG	5.35	117.95	112.60
2	Tx	143	ASP	CA-CB-CG	5.35	117.95	112.60
2	Tu	143	ASP	CA-CB-CG	5.35	117.95	112.60
2	Tp	143	ASP	CA-CB-CG	5.34	117.94	112.60
2	Tb	143	ASP	CA-CB-CG	5.34	117.94	112.60
2	Tr	143	ASP	CA-CB-CG	5.33	117.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Tm	143	ASP	CA-CB-CG	5.32	117.92	112.60

There are no chirality outliers.

There are no planarity outliers.

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	S1	5037	0	4931	5	0
1	S2	5037	0	4931	5	0
1	SA	5037	0	4931	5	0
1	SB	5037	0	4931	6	0
1	SC	5037	0	4931	5	0
1	SD	5037	0	4931	5	0
1	SE	5037	0	4931	6	0
1	SF	5037	0	4931	5	0
1	SG	5037	0	4931	7	0
1	SH	5037	0	4931	8	0
1	SI	5037	0	4931	7	0
1	SJ	5037	0	4931	7	0
1	SK	5037	0	4931	8	0
1	SL	5037	0	4931	7	0
1	SM	5037	0	4931	7	0
1	SN	5037	0	4931	7	0
1	SO	5037	0	4931	7	0
1	SP	5037	0	4931	7	0
1	SQ	5037	0	4931	7	0
1	SR	5037	0	4931	7	0
1	SS	5037	0	4931	7	0
1	ST	5037	0	4931	7	0
1	SU	5037	0	4931	8	0
1	SV	5037	0	4931	7	0
1	SW	5037	0	4931	7	0
1	SX	5037	0	4931	8	0
1	SY	5037	0	4931	7	0
1	SZ	5037	0	4931	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Sa	5037	0	4931	8	0
1	Sb	5037	0	4931	7	0
1	Sc	5037	0	4931	8	0
1	Sd	5037	0	4931	9	0
1	Se	5037	0	4931	7	0
1	Sf	5037	0	4931	10	0
1	Sg	5037	0	4931	7	0
1	Sh	5037	0	4931	7	0
1	Si	5037	0	4931	9	0
1	Sj	5037	0	4931	8	0
1	Sk	5037	0	4931	8	0
1	Sl	5037	0	4931	9	0
1	Sm	5037	0	4931	7	0
1	Sn	5037	0	4931	7	0
1	So	5037	0	4931	9	0
1	Sp	5037	0	4931	8	0
1	Sq	5037	0	4931	9	0
1	Sr	5037	0	4931	7	0
1	Ss	5037	0	4931	7	0
1	St	5037	0	4931	8	0
1	Su	5037	0	4931	7	0
1	Sv	5037	0	4931	7	0
1	Sw	5037	0	4931	6	0
1	Sx	5037	0	4931	5	0
1	Sy	5037	0	4931	5	0
1	Sz	5037	0	4931	6	0
2	T1	1305	0	1235	3	0
2	T2	1305	0	1235	2	0
2	TA	1305	0	1235	2	0
2	TB	1305	0	1235	2	0
2	TC	1305	0	1235	2	0
2	TD	1305	0	1235	2	0
2	TE	1305	0	1235	2	0
2	TF	1305	0	1235	2	0
2	TG	1305	0	1235	4	0
2	TH	1305	0	1235	5	0
2	TI	1305	0	1235	5	0
2	TJ	1305	0	1235	4	0
2	TK	1305	0	1235	4	0
2	TL	1305	0	1235	4	0
2	TM	1305	0	1235	4	0
2	TN	1305	0	1235	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	TO	1305	0	1235	4	0
2	TP	1305	0	1235	4	0
2	TQ	1305	0	1235	4	0
2	TR	1305	0	1235	4	0
2	TS	1305	0	1235	4	0
2	TT	1305	0	1235	4	0
2	TU	1305	0	1235	4	0
2	TV	1305	0	1235	4	0
2	TW	1305	0	1235	4	0
2	TX	1305	0	1235	4	0
2	TY	1305	0	1235	4	0
2	TZ	1305	0	1235	4	0
2	Ta	1305	0	1235	4	0
2	Tb	1305	0	1235	4	0
2	Tc	1305	0	1235	4	0
2	Td	1305	0	1235	4	0
2	Te	1305	0	1235	4	0
2	Tf	1305	0	1235	4	0
2	Tg	1305	0	1235	3	0
2	Th	1305	0	1235	4	0
2	Ti	1305	0	1235	4	0
2	Tj	1305	0	1235	3	0
2	Tk	1305	0	1235	4	0
2	Tl	1305	0	1235	4	0
2	Tm	1305	0	1235	5	0
2	Tn	1305	0	1235	4	0
2	To	1305	0	1235	4	0
2	Tp	1305	0	1235	5	0
2	Tq	1305	0	1235	4	0
2	Tr	1305	0	1235	5	0
2	Ts	1305	0	1235	5	0
2	Tt	1305	0	1235	4	0
2	Tu	1305	0	1235	3	0
2	Tv	1305	0	1235	4	0
2	Tw	1305	0	1235	2	0
2	Tx	1305	0	1235	3	0
2	Ty	1305	0	1235	2	0
2	Tz	1305	0	1235	3	0
All	All	342468	0	332964	372	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 (372) 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)
1:SB:627:TYR:CD2	1:SH:642:VAL:HG21	2.46	0.51
1:Sf:627:TYR:CD2	1:Sl:642:VAL:HG21	2.46	0.50
1:SE:627:TYR:CD2	1:SK:642:VAL:HG21	2.46	0.50
1:Si:627:TYR:CD2	1:So:642:VAL:HG21	2.46	0.50
1:SX:627:TYR:CD2	1:Sd:642:VAL:HG21	2.47	0.50
1:SU:627:TYR:CD2	1:Sa:642:VAL:HG21	2.47	0.49
1:SA:627:TYR:CD2	1:SG:642:VAL:HG21	2.47	0.49
1:Sc:627:TYR:CD2	1:Si:642:VAL:HG21	2.48	0.49
1:So:627:TYR:CD2	1:Su:642:VAL:HG21	2.48	0.49
1:Sa:627:TYR:CD2	1:Sg:642:VAL:HG21	2.47	0.49
1:Sn:627:TYR:CD2	1:St:642:VAL:HG21	2.47	0.49
1:Sh:627:TYR:CD2	1:Sn:642:VAL:HG21	2.48	0.49
1:Sk:627:TYR:CD2	1:Sq:642:VAL:HG21	2.47	0.49
1:Se:627:TYR:CD2	1:Sk:642:VAL:HG21	2.48	0.49
1:SD:627:TYR:CD2	1:SJ:642:VAL:HG21	2.47	0.49
1:St:627:TYR:CD2	1:Sz:642:VAL:HG21	2.48	0.49
1:Sd:627:TYR:CD2	1:Sj:642:VAL:HG21	2.48	0.48
1:Sg:627:TYR:CD2	1:Sm:642:VAL:HG21	2.48	0.48
1:SP:627:TYR:CD2	1:SV:642:VAL:HG21	2.48	0.48
1:SC:627:TYR:CD2	1:SI:642:VAL:HG21	2.48	0.48
1:SO:627:TYR:CD2	1:SU:642:VAL:HG21	2.49	0.48
1:SF:627:TYR:CD2	1:SL:642:VAL:HG21	2.48	0.48
2:TE:2:GLU:HG3	2:TG:99:ILE:HD12	1.96	0.48
1:Sb:627:TYR:CD2	1:Sh:642:VAL:HG21	2.49	0.48
1:SZ:627:TYR:CD2	1:Sf:642:VAL:HG21	2.48	0.48
1:Sj:627:TYR:CD2	1:Sp:642:VAL:HG21	2.48	0.48
1:Sl:627:TYR:CD2	1:Sr:642:VAL:HG21	2.48	0.48
1:SW:627:TYR:CD2	1:Sc:642:VAL:HG21	2.49	0.48
1:SS:627:TYR:CD2	1:SY:642:VAL:HG21	2.49	0.47
1:SY:627:TYR:CD2	1:Se:642:VAL:HG21	2.49	0.47
1:Sp:627:TYR:CD2	1:Sv:642:VAL:HG21	2.50	0.47
1:Sq:627:TYR:CD2	1:Sw:642:VAL:HG21	2.48	0.47
1:SJ:627:TYR:CD2	1:SP:642:VAL:HG21	2.50	0.47
1:ST:627:TYR:CD2	1:SZ:642:VAL:HG21	2.49	0.47
1:SV:627:TYR:CD2	1:Sb:642:VAL:HG21	2.49	0.47
1:SM:627:TYR:CD2	1:SS:642:VAL:HG21	2.49	0.47
1:SR:627:TYR:CD2	1:SX:642:VAL:HG21	2.49	0.47
1:SK:627:TYR:CD2	1:SQ:642:VAL:HG21	2.50	0.47
1:SC:453:LYS:HE3	1:SC:500:CYS:SG	2.55	0.47
1:SM:453:LYS:HE3	1:SM:500:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ss:627:TYR:CD2	1:Sy:642:VAL:HG21	2.50	0.47
1:S2:642:VAL:HG21	1:Sv:627:TYR:CD2	2.50	0.47
1:SB:453:LYS:HE3	1:SB:500:CYS:SG	2.55	0.47
1:SS:453:LYS:HE3	1:SS:500:CYS:SG	2.55	0.47
1:SX:453:LYS:HE3	1:SX:500:CYS:SG	2.55	0.47
1:Sm:627:TYR:CD2	1:Ss:642:VAL:HG21	2.49	0.47
2:TB:2:GLU:HG3	2:TJ:99:ILE:HD12	1.96	0.47
1:SF:453:LYS:HE3	1:SF:500:CYS:SG	2.55	0.47
1:SG:627:TYR:CD2	1:SM:642:VAL:HG21	2.50	0.47
1:Sd:453:LYS:HE3	1:Sd:500:CYS:SG	2.55	0.47
1:S1:642:VAL:HG21	1:Su:627:TYR:CD2	2.50	0.46
1:SK:453:LYS:HE3	1:SK:500:CYS:SG	2.55	0.46
1:SN:627:TYR:CD2	1:ST:642:VAL:HG21	2.50	0.46
1:SP:453:LYS:HE3	1:SP:500:CYS:SG	2.55	0.46
1:Sg:453:LYS:HE3	1:Sg:500:CYS:SG	2.55	0.46
1:So:453:LYS:HE3	1:So:500:CYS:SG	2.56	0.46
1:Su:453:LYS:HE3	1:Su:500:CYS:SG	2.56	0.46
1:SD:453:LYS:HE3	1:SD:500:CYS:SG	2.56	0.46
1:SI:453:LYS:HE3	1:SI:500:CYS:SG	2.56	0.46
1:Sk:453:LYS:HE3	1:Sk:500:CYS:SG	2.56	0.46
1:St:453:LYS:HE3	1:St:500:CYS:SG	2.56	0.46
1:SJ:453:LYS:HE3	1:SJ:500:CYS:SG	2.56	0.46
1:SL:453:LYS:HE3	1:SL:500:CYS:SG	2.56	0.46
1:SN:453:LYS:HE3	1:SN:500:CYS:SG	2.55	0.46
1:SZ:453:LYS:HE3	1:SZ:500:CYS:SG	2.56	0.46
1:Sa:453:LYS:HE3	1:Sa:500:CYS:SG	2.55	0.46
1:Se:453:LYS:HE3	1:Se:500:CYS:SG	2.56	0.46
1:Sf:453:LYS:HE3	1:Sf:500:CYS:SG	2.56	0.46
1:Si:453:LYS:HE3	1:Si:500:CYS:SG	2.55	0.46
1:Sn:453:LYS:HE3	1:Sn:500:CYS:SG	2.56	0.46
1:Ss:453:LYS:HE3	1:Ss:500:CYS:SG	2.56	0.46
1:SH:453:LYS:HE3	1:SH:500:CYS:SG	2.56	0.46
1:SO:453:LYS:HE3	1:SO:500:CYS:SG	2.55	0.46
1:Sh:453:LYS:HE3	1:Sh:500:CYS:SG	2.56	0.46
1:Sm:453:LYS:HE3	1:Sm:500:CYS:SG	2.56	0.46
1:Sr:453:LYS:HE3	1:Sr:500:CYS:SG	2.56	0.46
1:SQ:453:LYS:HE3	1:SQ:500:CYS:SG	2.56	0.46
1:Sv:453:LYS:HE3	1:Sv:500:CYS:SG	2.56	0.46
1:Sw:453:LYS:HE3	1:Sw:500:CYS:SG	2.56	0.46
1:Sp:453:LYS:HE3	1:Sp:500:CYS:SG	2.56	0.46
1:SF:497:ILE:HG22	1:SF:497:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SV:453:LYS:HE3	1:SV:500:CYS:SG	2.55	0.46
1:Sb:453:LYS:HE3	1:Sb:500:CYS:SG	2.55	0.46
1:Sx:453:LYS:HE3	1:Sx:500:CYS:SG	2.56	0.46
1:Sz:453:LYS:HE3	1:Sz:500:CYS:SG	2.56	0.46
1:S1:453:LYS:HE3	1:S1:500:CYS:SG	2.56	0.46
1:SA:453:LYS:HE3	1:SA:500:CYS:SG	2.56	0.46
1:SE:453:LYS:HE3	1:SE:500:CYS:SG	2.55	0.46
1:SH:627:TYR:CD2	1:SN:642:VAL:HG21	2.50	0.46
1:Sc:453:LYS:HE3	1:Sc:500:CYS:SG	2.56	0.46
2:TD:2:GLU:HG3	2:TL:99:ILE:HD12	1.98	0.46
1:SQ:627:TYR:CD2	1:SW:642:VAL:HG21	2.51	0.46
1:SU:453:LYS:HE3	1:SU:500:CYS:SG	2.55	0.46
1:Sr:627:TYR:CD2	1:Sx:642:VAL:HG21	2.50	0.46
1:S2:453:LYS:HE3	1:S2:500:CYS:SG	2.56	0.45
1:SD:497:ILE:O	1:SD:497:ILE:HG22	2.16	0.45
1:SL:627:TYR:CD2	1:SR:642:VAL:HG21	2.51	0.45
1:SR:453:LYS:HE3	1:SR:500:CYS:SG	2.56	0.45
1:Sj:453:LYS:HE3	1:Sj:500:CYS:SG	2.55	0.45
1:Sj:497:ILE:HG22	1:Sj:497:ILE:O	2.17	0.45
1:SG:453:LYS:HE3	1:SG:500:CYS:SG	2.56	0.45
1:SY:453:LYS:HE3	1:SY:500:CYS:SG	2.55	0.45
1:Sq:453:LYS:HE3	1:Sq:500:CYS:SG	2.56	0.45
1:Sr:497:ILE:O	1:Sr:497:ILE:HG22	2.17	0.45
1:SE:497:ILE:O	1:SE:497:ILE:HG22	2.16	0.45
1:SW:453:LYS:HE3	1:SW:500:CYS:SG	2.56	0.45
1:Sv:497:ILE:O	1:Sv:497:ILE:HG22	2.17	0.45
1:Sw:497:ILE:HG22	1:Sw:497:ILE:O	2.17	0.45
2:TG:2:GLU:HG3	2:TO:99:ILE:HD12	1.99	0.45
1:SI:627:TYR:CD2	1:SO:642:VAL:HG21	2.51	0.45
1:Sk:497:ILE:HG22	1:Sk:497:ILE:O	2.17	0.45
2:Tc:116:PHE:CD2	2:Th:54:MET:HE1	2.52	0.45
2:Tk:116:PHE:CD2	2:Tv:54:MET:HE1	2.52	0.45
1:ST:453:LYS:HE3	1:ST:500:CYS:SG	2.56	0.45
1:Sx:497:ILE:HG22	1:Sx:497:ILE:O	2.17	0.45
2:TA:2:GLU:HG3	2:TI:99:ILE:HD12	1.98	0.45
2:TJ:2:GLU:HG3	2:TR:99:ILE:HD12	1.99	0.45
2:Tk:2:GLU:HG3	2:Ts:99:ILE:HD12	1.99	0.45
1:SQ:497:ILE:O	1:SQ:497:ILE:HG22	2.17	0.45
1:SR:497:ILE:HG22	1:SR:497:ILE:O	2.17	0.45
1:SY:497:ILE:O	1:SY:497:ILE:HG22	2.17	0.45
1:Se:497:ILE:O	1:Se:497:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Sl:453:LYS:HE3	1:Sl:500:CYS:SG	2.56	0.45
2:Tn:116:PHE:CD2	2:Ts:54:MET:HE1	2.51	0.45
1:SX:497:ILE:HG22	1:SX:497:ILE:O	2.17	0.45
1:Sc:497:ILE:HG22	1:Sc:497:ILE:O	2.17	0.45
1:Sd:497:ILE:HG22	1:Sd:497:ILE:O	2.17	0.45
1:So:497:ILE:HG22	1:So:497:ILE:O	2.17	0.45
1:Sv:606:VAL:HG11	1:Sw:17:SER:HB3	1.98	0.45
2:TK:2:GLU:HG3	2:TM:99:ILE:HD12	1.99	0.45
2:Td:2:GLU:HG3	2:Tf:99:ILE:HD12	1.99	0.45
1:SK:497:ILE:HG22	1:SK:497:ILE:O	2.17	0.45
1:Sf:497:ILE:O	1:Sf:497:ILE:HG22	2.17	0.45
1:Sq:606:VAL:HG11	1:Sx:17:SER:HB3	1.99	0.45
2:Tl:2:GLU:HG3	2:Tt:99:ILE:HD12	1.99	0.45
1:SV:497:ILE:HG22	1:SV:497:ILE:O	2.17	0.45
1:Si:497:ILE:O	1:Si:497:ILE:HG22	2.17	0.45
2:Tp:116:PHE:CD2	2:Tu:54:MET:HE1	2.52	0.45
1:S1:17:SER:HB3	1:St:606:VAL:HG11	1.99	0.45
1:SC:497:ILE:HG22	1:SC:497:ILE:O	2.16	0.45
1:SL:497:ILE:O	1:SL:497:ILE:HG22	2.17	0.45
1:SS:497:ILE:HG22	1:SS:497:ILE:O	2.17	0.45
1:Sh:497:ILE:HG22	1:Sh:497:ILE:O	2.16	0.45
1:Sy:453:LYS:HE3	1:Sy:500:CYS:SG	2.56	0.45
2:T1:54:MET:HE1	2:Tv:116:PHE:CD2	2.53	0.45
1:SP:497:ILE:HG22	1:SP:497:ILE:O	2.17	0.44
1:Sq:497:ILE:O	1:Sq:497:ILE:HG22	2.17	0.44
1:Sy:497:ILE:O	1:Sy:497:ILE:HG22	2.17	0.44
2:TL:2:GLU:HG3	2:TN:99:ILE:HD12	1.99	0.44
2:TM:2:GLU:HG3	2:TU:99:ILE:HD12	1.99	0.44
2:Tc:2:GLU:HG3	2:Te:99:ILE:HD12	1.99	0.44
2:Ti:116:PHE:CD2	2:Tn:54:MET:HE1	2.53	0.44
1:SW:497:ILE:HG22	1:SW:497:ILE:O	2.17	0.44
2:To:2:GLU:HG3	2:Tq:99:ILE:HD12	1.99	0.44
2:Tr:116:PHE:CD2	2:Tw:54:MET:HE1	2.53	0.44
2:Tu:116:PHE:CD2	2:Tz:54:MET:HE1	2.53	0.44
1:S1:497:ILE:O	1:S1:497:ILE:HG22	2.17	0.44
1:SB:497:ILE:HG22	1:SB:497:ILE:O	2.16	0.44
1:SJ:497:ILE:HG22	1:SJ:497:ILE:O	2.17	0.44
1:SM:497:ILE:O	1:SM:497:ILE:HG22	2.17	0.44
1:Sz:497:ILE:O	1:Sz:497:ILE:HG22	2.17	0.44
2:TS:116:PHE:CD2	2:Td:54:MET:HE1	2.52	0.44
2:TZ:116:PHE:CD2	2:Te:54:MET:HE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:St:497:ILE:HG22	1:St:497:ILE:O	2.16	0.44
2:TH:2:GLU:HG3	2:TP:99:ILE:HD12	1.99	0.44
1:SA:497:ILE:O	1:SA:497:ILE:HG22	2.16	0.44
1:SG:497:ILE:HG22	1:SG:497:ILE:O	2.17	0.44
2:T2:54:MET:HE1	2:Tq:116:PHE:CD2	2.53	0.44
2:TO:116:PHE:CD2	2:TT:54:MET:HE1	2.53	0.44
2:TP:2:GLU:HG3	2:TX:99:ILE:HD12	2.00	0.44
2:TW:2:GLU:HG3	2:TY:99:ILE:HD12	2.00	0.44
2:TZ:2:GLU:HG3	2:Th:99:ILE:HD12	1.99	0.44
2:Tf:116:PHE:CD2	2:Tk:54:MET:HE1	2.53	0.44
1:S2:497:ILE:HG22	1:S2:497:ILE:O	2.17	0.44
1:SU:606:VAL:HG11	1:Sb:17:SER:HB3	1.99	0.44
1:Sl:497:ILE:HG22	1:Sl:497:ILE:O	2.17	0.44
1:Sm:497:ILE:O	1:Sm:497:ILE:HG22	2.17	0.44
1:Ss:606:VAL:HG11	1:Sz:17:SER:HB3	1.98	0.44
2:Tm:116:PHE:CD2	2:Tr:54:MET:HE1	2.52	0.44
2:Ts:116:PHE:CD2	2:Tx:54:MET:HE1	2.52	0.44
1:S2:17:SER:HB3	1:Su:606:VAL:HG11	2.00	0.44
1:SH:497:ILE:HG22	1:SH:497:ILE:O	2.17	0.44
1:SU:497:ILE:O	1:SU:497:ILE:HG22	2.17	0.44
1:SX:606:VAL:HG11	1:SY:17:SER:HB3	1.99	0.44
2:TC:116:PHE:CD2	2:TH:54:MET:HE1	2.53	0.44
2:TI:2:GLU:HG3	2:TQ:99:ILE:HD12	1.99	0.44
2:TU:116:PHE:CD2	2:TZ:54:MET:HE1	2.53	0.44
2:TY:116:PHE:CD2	2:Tj:54:MET:HE1	2.53	0.44
2:To:116:PHE:CD2	2:Tt:54:MET:HE1	2.53	0.44
1:ST:497:ILE:HG22	1:ST:497:ILE:O	2.17	0.44
1:Sn:497:ILE:HG22	1:Sn:497:ILE:O	2.17	0.44
1:Sp:497:ILE:HG22	1:Sp:497:ILE:O	2.17	0.44
1:Ss:497:ILE:HG22	1:Ss:497:ILE:O	2.17	0.44
2:TF:116:PHE:CD2	2:TK:54:MET:HE1	2.53	0.44
2:Ta:116:PHE:CD2	2:Tf:54:MET:HE1	2.53	0.44
1:SI:497:ILE:O	1:SI:497:ILE:HG22	2.17	0.44
1:SN:497:ILE:HG22	1:SN:497:ILE:O	2.17	0.44
1:SO:497:ILE:HG22	1:SO:497:ILE:O	2.17	0.44
1:SZ:497:ILE:HG22	1:SZ:497:ILE:O	2.17	0.44
1:Sa:497:ILE:O	1:Sa:497:ILE:HG22	2.17	0.44
2:Th:2:GLU:HG3	2:Tv:99:ILE:HD12	1.99	0.44
1:Sb:497:ILE:HG22	1:Sb:497:ILE:O	2.17	0.43
1:Sf:606:VAL:HG11	1:Sm:17:SER:HB3	1.99	0.43
2:TT:116:PHE:CD2	2:TY:54:MET:HE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:TX:2:GLU:HG3	2:TZ:99:ILE:HD12	2.00	0.43
2:Tb:116:PHE:CD2	2:Tg:54:MET:HE1	2.53	0.43
2:Th:116:PHE:CD2	2:Tm:54:MET:HE1	2.53	0.43
1:Sd:606:VAL:HG11	1:Se:17:SER:HB3	1.99	0.43
1:Sk:606:VAL:HG11	1:Sr:17:SER:HB3	2.00	0.43
1:Sn:606:VAL:HG11	1:Su:17:SER:HB3	1.99	0.43
2:TT:2:GLU:HG3	2:Tb:99:ILE:HD12	2.00	0.43
2:TX:116:PHE:CD2	2:Tc:54:MET:HE1	2.53	0.43
2:Ta:2:GLU:HG3	2:Ti:99:ILE:HD12	1.99	0.43
2:Tl:116:PHE:CD2	2:Tq:54:MET:HE1	2.53	0.43
2:Tt:116:PHE:CD2	2:Ty:54:MET:HE1	2.53	0.43
1:SB:606:VAL:HG11	1:SI:17:SER:HB3	2.00	0.43
1:Sl:606:VAL:HG11	1:Ss:17:SER:HB3	1.99	0.43
1:Su:497:ILE:O	1:Su:497:ILE:HG22	2.17	0.43
2:TA:116:PHE:CD2	2:TL:54:MET:HE1	2.54	0.43
2:TR:116:PHE:CD2	2:TW:54:MET:HE1	2.53	0.43
1:Sg:497:ILE:HG22	1:Sg:497:ILE:O	2.17	0.43
2:TR:2:GLU:HG3	2:TT:99:ILE:HD12	2.00	0.43
2:Tp:2:GLU:HG3	2:Tr:99:ILE:HD12	2.00	0.43
1:Sc:606:VAL:HG11	1:Sj:17:SER:HB3	1.99	0.43
2:Td:116:PHE:CD2	2:Ti:54:MET:HE1	2.53	0.43
2:Tg:116:PHE:CD2	2:Tl:54:MET:HE1	2.54	0.43
2:TG:116:PHE:CD2	2:TR:54:MET:HE1	2.54	0.43
2:TP:116:PHE:CD2	2:TU:54:MET:HE1	2.54	0.43
2:Tq:2:GLU:HG3	2:Ty:99:ILE:HD12	2.01	0.43
1:SO:606:VAL:HG11	1:SV:17:SER:HB3	2.00	0.43
1:Sg:606:VAL:HG11	1:Sn:17:SER:HB3	2.00	0.43
1:Si:606:VAL:HG11	1:Sp:17:SER:HB3	1.99	0.43
2:TW:116:PHE:CD2	2:Tb:54:MET:HE1	2.53	0.43
1:SE:606:VAL:HG11	1:SL:17:SER:HB3	2.00	0.43
1:Sh:606:VAL:HG11	1:So:17:SER:HB3	2.01	0.43
1:So:606:VAL:HG11	1:Sv:17:SER:HB3	2.00	0.43
2:TS:2:GLU:HG3	2:Ta:99:ILE:HD12	2.01	0.43
2:TU:2:GLU:HG3	2:Tc:99:ILE:HD12	2.00	0.43
1:Sr:606:VAL:HG11	1:Sy:17:SER:HB3	2.00	0.43
2:TO:2:GLU:HG3	2:TW:99:ILE:HD12	2.00	0.43
2:Tj:116:PHE:CD2	2:To:54:MET:HE1	2.53	0.43
1:SP:606:VAL:HG11	1:SW:17:SER:HB3	2.00	0.43
1:SZ:606:VAL:HG11	1:Sg:17:SER:HB3	2.00	0.43
1:Se:606:VAL:HG11	1:Sl:17:SER:HB3	2.00	0.43
2:TF:2:GLU:HG3	2:TH:99:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Sp:606:VAL:HG11	1:Sq:17:SER:HB3	2.00	0.42
2:TL:116:PHE:CD2	2:TQ:54:MET:HE1	2.54	0.42
2:To:125:ASN:OD1	2:Tp:83:LYS:HE3	2.18	0.42
2:Tv:2:GLU:HG3	2:Tx:99:ILE:HD12	2.01	0.42
1:SR:222:ILE:HD12	1:SR:238:ILE:HD11	2.02	0.42
1:ST:606:VAL:HG11	1:Sa:17:SER:HB3	2.01	0.42
1:Sb:606:VAL:HG11	1:Si:17:SER:HB3	2.01	0.42
1:Sj:606:VAL:HG11	1:Sk:17:SER:HB3	2.01	0.42
2:T1:99:ILE:HD12	2:Ts:2:GLU:HG3	2.01	0.42
2:TM:116:PHE:CD2	2:TX:54:MET:HE1	2.53	0.42
1:SG:606:VAL:HG11	1:SN:17:SER:HB3	2.00	0.42
1:SI:222:ILE:HD12	1:SI:238:ILE:HD11	2.02	0.42
1:SL:222:ILE:HD12	1:SL:238:ILE:HD11	2.02	0.42
1:SO:222:ILE:HD12	1:SO:238:ILE:HD11	2.02	0.42
1:Sa:606:VAL:HG11	1:Sh:17:SER:HB3	2.00	0.42
1:Sm:606:VAL:HG11	1:St:17:SER:HB3	2.01	0.42
2:TJ:116:PHE:CD2	2:TO:54:MET:HE1	2.54	0.42
2:TQ:116:PHE:CD2	2:TV:54:MET:HE1	2.54	0.42
2:TV:116:PHE:CD2	2:Ta:54:MET:HE1	2.54	0.42
1:SJ:606:VAL:HG11	1:SQ:17:SER:HB3	2.00	0.42
1:SM:222:ILE:HD12	1:SM:238:ILE:HD11	2.02	0.42
1:SS:222:ILE:HD12	1:SS:238:ILE:HD11	2.02	0.42
2:TI:116:PHE:CD2	2:TN:54:MET:HE1	2.54	0.42
2:Te:116:PHE:CD2	2:Tp:54:MET:HE1	2.53	0.42
1:SG:222:ILE:HD12	1:SG:238:ILE:HD11	2.01	0.42
1:SJ:222:ILE:HD12	1:SJ:238:ILE:HD11	2.01	0.42
1:SP:222:ILE:HD12	1:SP:238:ILE:HD11	2.02	0.42
1:SW:606:VAL:HG11	1:Sd:17:SER:HB3	2.00	0.42
1:SY:606:VAL:HG11	1:Sf:17:SER:HB3	2.01	0.42
2:Tm:2:GLU:HG3	2:Tu:99:ILE:HD12	2.00	0.42
1:SH:606:VAL:HG11	1:SO:17:SER:HB3	2.01	0.42
1:SL:606:VAL:HG11	1:SM:17:SER:HB3	2.01	0.42
2:TB:116:PHE:CD2	2:TG:54:MET:HE1	2.55	0.42
2:TV:2:GLU:HG3	2:Td:99:ILE:HD12	2.01	0.42
2:Tl:125:ASN:OD1	2:Tm:83:LYS:HE3	2.19	0.42
1:SK:222:ILE:HD12	1:SK:238:ILE:HD11	2.02	0.42
1:SY:222:ILE:HD12	1:SY:238:ILE:HD11	2.02	0.42
1:SK:606:VAL:HG11	1:SR:17:SER:HB3	2.01	0.42
1:ST:222:ILE:HD12	1:ST:238:ILE:HD11	2.02	0.42
1:SV:222:ILE:HD12	1:SV:238:ILE:HD11	2.02	0.42
1:Sb:222:ILE:HD12	1:Sb:238:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:TD:116:PHE:CD2	2:TI:54:MET:HE1	2.54	0.42
1:SR:606:VAL:HG11	1:SS:17:SER:HB3	2.02	0.42
1:SZ:222:ILE:HD12	1:SZ:238:ILE:HD11	2.02	0.42
1:Sh:222:ILE:HD12	1:Sh:238:ILE:HD11	2.02	0.42
2:T2:99:ILE:HD12	2:Tt:2:GLU:HG3	2.01	0.42
2:TN:116:PHE:CD2	2:TS:54:MET:HE1	2.55	0.42
1:SQ:222:ILE:HD12	1:SQ:238:ILE:HD11	2.02	0.42
1:SW:222:ILE:HD12	1:SW:238:ILE:HD11	2.02	0.42
1:Sc:222:ILE:HD12	1:Sc:238:ILE:HD11	2.02	0.42
2:TC:2:GLU:HG3	2:TK:99:ILE:HD12	2.01	0.42
1:SC:606:VAL:HG11	1:SJ:17:SER:HB3	2.01	0.41
1:SF:606:VAL:HG11	1:SG:17:SER:HB3	2.01	0.41
1:SN:222:ILE:HD12	1:SN:238:ILE:HD11	2.02	0.41
1:Sa:222:ILE:HD12	1:Sa:238:ILE:HD11	2.02	0.41
2:TK:116:PHE:CD2	2:TP:54:MET:HE1	2.55	0.41
2:TY:2:GLU:HG3	2:Tg:99:ILE:HD12	2.02	0.41
1:SU:222:ILE:HD12	1:SU:238:ILE:HD11	2.02	0.41
1:Se:222:ILE:HD12	1:Se:238:ILE:HD11	2.02	0.41
1:Sk:222:ILE:HD12	1:Sk:238:ILE:HD11	2.03	0.41
1:Sn:222:ILE:HD12	1:Sn:238:ILE:HD11	2.03	0.41
2:Te:2:GLU:HG3	2:Tm:99:ILE:HD12	2.03	0.41
1:SA:606:VAL:HG11	1:SH:17:SER:HB3	2.01	0.41
1:SE:222:ILE:HD12	1:SE:238:ILE:HD11	2.03	0.41
1:SH:222:ILE:HD12	1:SH:238:ILE:HD11	2.02	0.41
1:SX:222:ILE:HD12	1:SX:238:ILE:HD11	2.02	0.41
1:Sd:222:ILE:HD12	1:Sd:238:ILE:HD11	2.02	0.41
1:SM:606:VAL:HG11	1:ST:17:SER:HB3	2.01	0.41
1:SQ:606:VAL:HG11	1:SX:17:SER:HB3	2.02	0.41
1:Sg:222:ILE:HD12	1:Sg:238:ILE:HD11	2.03	0.41
1:Sj:222:ILE:HD12	1:Sj:238:ILE:HD11	2.03	0.41
2:TQ:2:GLU:HG3	2:TS:99:ILE:HD12	2.03	0.41
1:Su:222:ILE:HD12	1:Su:238:ILE:HD11	2.03	0.41
1:Sx:222:ILE:HD12	1:Sx:238:ILE:HD11	2.03	0.41
2:TH:116:PHE:CD2	2:TM:54:MET:HE1	2.55	0.41
1:SI:606:VAL:HG11	1:SP:17:SER:HB3	2.01	0.41
1:SN:606:VAL:HG11	1:SU:17:SER:HB3	2.01	0.41
1:SS:606:VAL:HG11	1:SZ:17:SER:HB3	2.02	0.41
1:Sr:222:ILE:HD12	1:Sr:238:ILE:HD11	2.03	0.41
1:St:222:ILE:HD12	1:St:238:ILE:HD11	2.03	0.41
1:SD:606:VAL:HG11	1:SK:17:SER:HB3	2.02	0.41
1:Sl:222:ILE:HD12	1:Sl:238:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:So:222:ILE:HD12	1:So:238:ILE:HD11	2.03	0.41
1:Sp:222:ILE:HD12	1:Sp:238:ILE:HD11	2.03	0.41
1:Sq:222:ILE:HD12	1:Sq:238:ILE:HD11	2.03	0.41
1:Sy:222:ILE:HD12	1:Sy:238:ILE:HD11	2.03	0.41
2:T1:83:LYS:HE3	2:Tz:125:ASN:OD1	2.20	0.41
1:S1:222:ILE:HD12	1:S1:238:ILE:HD11	2.03	0.41
1:SB:222:ILE:HD12	1:SB:238:ILE:HD11	2.03	0.41
1:Si:627:TYR:CE2	1:So:642:VAL:HG21	2.56	0.41
1:Ss:222:ILE:HD12	1:Ss:238:ILE:HD11	2.03	0.41
2:Tr:2:GLU:HG3	2:Tz:99:ILE:HD12	2.03	0.41
1:S2:222:ILE:HD12	1:S2:238:ILE:HD11	2.03	0.41
1:SA:222:ILE:HD12	1:SA:238:ILE:HD11	2.03	0.41
1:SC:222:ILE:HD12	1:SC:238:ILE:HD11	2.03	0.41
1:SD:222:ILE:HD12	1:SD:238:ILE:HD11	2.03	0.41
1:Sf:222:ILE:HD12	1:Sf:238:ILE:HD11	2.03	0.41
1:Sf:627:TYR:CE2	1:Sl:642:VAL:HG21	2.56	0.41
1:Sm:222:ILE:HD12	1:Sm:238:ILE:HD11	2.03	0.41
1:Sq:627:TYR:CD2	1:Sw:642:VAL:CG2	3.04	0.41
1:Sz:222:ILE:HD12	1:Sz:238:ILE:HD11	2.03	0.41
2:TE:116:PHE:CD2	2:TJ:54:MET:HE1	2.55	0.41
2:TN:2:GLU:HG3	2:TV:99:ILE:HD12	2.02	0.41
2:Tf:2:GLU:HG3	2:Th:99:ILE:HD12	2.03	0.41
2:Ti:2:GLU:HG3	2:Tk:99:ILE:HD12	2.03	0.41
2:Tw:125:ASN:OD1	2:Tx:83:LYS:HE3	2.20	0.41
1:SV:606:VAL:HG11	1:Sc:17:SER:HB3	2.01	0.41
1:Sf:627:TYR:CD2	1:Sl:642:VAL:CG2	3.04	0.41
1:Si:222:ILE:HD12	1:Si:238:ILE:HD11	2.03	0.41
1:Sv:222:ILE:HD12	1:Sv:238:ILE:HD11	2.03	0.41
1:Sw:222:ILE:HD12	1:Sw:238:ILE:HD11	2.03	0.41
1:SX:627:TYR:CD2	1:Sd:642:VAL:CG2	3.05	0.40
1:SE:627:TYR:CD2	1:SK:642:VAL:CG2	3.05	0.40
1:Sc:601:TYR:CE2	1:Sc:631:ALA:HA	2.57	0.40
2:TH:125:ASN:OD1	2:TI:83:LYS:HE3	2.22	0.40
2:Tr:125:ASN:OD1	2:Ts:83:LYS:HE3	2.21	0.40
1:SB:627:TYR:CD2	1:SH:642:VAL:CG2	3.05	0.40
1:SF:222:ILE:HD12	1:SF:238:ILE:HD11	2.03	0.40
1:Si:627:TYR:CD2	1:So:642:VAL:CG2	3.04	0.40
2:Tb:2:GLU:HG3	2:Tj:99:ILE:HD12	2.02	0.40
1:Sp:601:TYR:CE2	1:Sp:631:ALA:HA	2.57	0.40
1:SU:627:TYR:CD2	1:Sa:642:VAL:CG2	3.05	0.40
1:SZ:627:TYR:CD2	1:Sf:642:VAL:CG2	3.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Sd:627:TYR:CD2	1:Sj:642:VAL:CG2	3.05	0.40
1:Sk:627:TYR:CD2	1:Sq:642:VAL:CG2	3.05	0.40
1:St:627:TYR:CD2	1:Sz:642:VAL:CG2	3.04	0.40
2:Th:2:GLU:HG3	2:Tp:99:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S1	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	S2	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	SA	653/656 (100%)	621 (95%)	32 (5%)	0	100	100
1	SB	653/656 (100%)	620 (95%)	33 (5%)	0	100	100
1	SC	653/656 (100%)	621 (95%)	32 (5%)	0	100	100
1	SD	653/656 (100%)	621 (95%)	32 (5%)	0	100	100
1	SE	653/656 (100%)	621 (95%)	32 (5%)	0	100	100
1	SF	653/656 (100%)	621 (95%)	32 (5%)	0	100	100
1	SG	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SH	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	SI	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SJ	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SK	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SL	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SM	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	SN	653/656 (100%)	618 (95%)	35 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SO	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SP	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SQ	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SR	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	SS	653/656 (100%)	620 (95%)	33 (5%)	0	100	100
1	ST	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SU	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	SV	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	SW	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SX	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	SY	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	SZ	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sa	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sb	653/656 (100%)	620 (95%)	33 (5%)	0	100	100
1	Sc	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sd	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	Se	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	Sf	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sg	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sh	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Si	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	Sj	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	Sk	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sl	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sm	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	Sn	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	So	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	Sp	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sq	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	Sr	653/656 (100%)	620 (95%)	33 (5%)	0	100	100
1	Ss	653/656 (100%)	619 (95%)	34 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	St	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Su	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	Sv	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sw	653/656 (100%)	619 (95%)	34 (5%)	0	100	100
1	Sx	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sy	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
1	Sz	653/656 (100%)	618 (95%)	35 (5%)	0	100	100
2	T1	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	T2	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TA	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TB	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TC	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TD	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TE	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TF	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TG	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TH	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	TI	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TJ	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TK	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	TL	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TM	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TN	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	TO	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TP	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	TQ	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TR	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TS	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TT	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	TU	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TV	160/163 (98%)	151 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	TW	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TX	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	TY	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	TZ	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Ta	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Tb	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Tc	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Td	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Te	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Tf	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Tg	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Th	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Ti	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Tj	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Tk	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Tl	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Tm	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Tn	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	To	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Tp	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Tq	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Tr	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Ts	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Tt	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Tu	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Tv	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Tw	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Tx	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
2	Ty	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
2	Tz	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
All	All	43902/44226 (99%)	41583 (95%)	2319 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S1	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	S2	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SA	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SB	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SC	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SD	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SE	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SF	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SG	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SH	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SI	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SJ	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SK	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SL	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SM	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SN	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SO	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SP	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SQ	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SR	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SS	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	ST	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SU	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SV	539/540 (100%)	534 (99%)	5 (1%)	70	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SW	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SX	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	SY	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	SZ	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sa	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sb	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sc	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sd	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Se	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Sf	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sg	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Sh	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Si	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Sj	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Sk	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sl	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sm	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Sn	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	So	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sp	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Sq	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Sr	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Ss	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	St	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Su	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sv	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sw	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Sx	539/540 (100%)	534 (99%)	5 (1%)	70	74
1	Sy	539/540 (100%)	533 (99%)	6 (1%)	65	73
1	Sz	539/540 (100%)	533 (99%)	6 (1%)	65	73
2	T1	138/139 (99%)	137 (99%)	1 (1%)	76	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	T2	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TA	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TB	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TC	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TD	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TE	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TF	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TG	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TH	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TI	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TJ	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TK	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TL	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TM	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TN	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TO	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TP	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TQ	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TR	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TS	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TT	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TU	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TV	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TW	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TX	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TY	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	TZ	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	Ta	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	Tb	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	Tc	138/139 (99%)	137 (99%)	1 (1%)	76	77	
2	Td	138/139 (99%)	137 (99%)	1 (1%)	76	77	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Te	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tf	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tg	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Th	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Ti	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tj	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tk	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tl	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tm	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tn	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	To	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tp	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tq	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tr	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Ts	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tt	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tu	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tv	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tw	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tx	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Ty	138/139 (99%)	137 (99%)	1 (1%)	76	77
2	Tz	138/139 (99%)	137 (99%)	1 (1%)	76	77
All	All	36558/36666 (100%)	36209 (99%)	349 (1%)	65	74

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S1	174	GLN
1	S1	207	LYS
1	S1	425	ILE
1	S1	452	TYR
1	S1	551	ASN
1	S2	174	GLN
1	S2	207	LYS

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Mol	Chain	Res	Type
1	S2	381	ASP
1	S2	425	ILE
1	S2	452	TYR
1	S2	551	ASN
1	SA	174	GLN
1	SA	207	LYS
1	SA	381	ASP
1	SA	425	ILE
1	SA	452	TYR
1	SA	551	ASN
1	SB	174	GLN
1	SB	207	LYS
1	SB	381	ASP
1	SB	425	ILE
1	SB	452	TYR
1	SB	551	ASN
1	SC	174	GLN
1	SC	207	LYS
1	SC	381	ASP
1	SC	425	ILE
1	SC	452	TYR
1	SC	551	ASN
1	SD	174	GLN
1	SD	207	LYS
1	SD	381	ASP
1	SD	425	ILE
1	SD	452	TYR
1	SD	551	ASN
1	SE	174	GLN
1	SE	207	LYS
1	SE	381	ASP
1	SE	425	ILE
1	SE	452	TYR
1	SE	551	ASN
1	SF	174	GLN
1	SF	207	LYS
1	SF	381	ASP
1	SF	425	ILE
1	SF	452	TYR
1	SF	551	ASN
1	SG	174	GLN
1	SG	207	LYS

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Mol	Chain	Res	Type
1	SG	381	ASP
1	SG	452	TYR
1	SG	551	ASN
1	SH	174	GLN
1	SH	207	LYS
1	SH	381	ASP
1	SH	425	ILE
1	SH	452	TYR
1	SH	551	ASN
1	SI	174	GLN
1	SI	207	LYS
1	SI	381	ASP
1	SI	425	ILE
1	SI	452	TYR
1	SI	551	ASN
1	SJ	174	GLN
1	SJ	207	LYS
1	SJ	381	ASP
1	SJ	452	TYR
1	SJ	551	ASN
1	SK	174	GLN
1	SK	207	LYS
1	SK	381	ASP
1	SK	425	ILE
1	SK	452	TYR
1	SK	551	ASN
1	SL	174	GLN
1	SL	207	LYS
1	SL	381	ASP
1	SL	452	TYR
1	SL	551	ASN
1	SM	174	GLN
1	SM	207	LYS
1	SM	381	ASP
1	SM	425	ILE
1	SM	452	TYR
1	SM	551	ASN
1	SN	174	GLN
1	SN	207	LYS
1	SN	381	ASP
1	SN	452	TYR
1	SN	551	ASN

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Mol	Chain	Res	Type
1	SO	174	GLN
1	SO	207	LYS
1	SO	381	ASP
1	SO	452	TYR
1	SO	551	ASN
1	SP	174	GLN
1	SP	207	LYS
1	SP	381	ASP
1	SP	452	TYR
1	SP	551	ASN
1	SQ	174	GLN
1	SQ	207	LYS
1	SQ	381	ASP
1	SQ	452	TYR
1	SQ	551	ASN
1	SR	174	GLN
1	SR	207	LYS
1	SR	381	ASP
1	SR	452	TYR
1	SR	551	ASN
1	SS	174	GLN
1	SS	207	LYS
1	SS	381	ASP
1	SS	452	TYR
1	SS	551	ASN
1	ST	174	GLN
1	ST	207	LYS
1	ST	381	ASP
1	ST	452	TYR
1	ST	551	ASN
1	SU	174	GLN
1	SU	207	LYS
1	SU	381	ASP
1	SU	452	TYR
1	SU	551	ASN
1	SV	174	GLN
1	SV	207	LYS
1	SV	381	ASP
1	SV	452	TYR
1	SV	551	ASN
1	SW	174	GLN
1	SW	207	LYS

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Mol	Chain	Res	Type
1	SW	381	ASP
1	SW	452	TYR
1	SW	551	ASN
1	SX	174	GLN
1	SX	207	LYS
1	SX	381	ASP
1	SX	452	TYR
1	SX	551	ASN
1	SY	174	GLN
1	SY	207	LYS
1	SY	381	ASP
1	SY	425	ILE
1	SY	452	TYR
1	SY	551	ASN
1	SZ	174	GLN
1	SZ	207	LYS
1	SZ	381	ASP
1	SZ	452	TYR
1	SZ	551	ASN
1	Sa	174	GLN
1	Sa	207	LYS
1	Sa	381	ASP
1	Sa	452	TYR
1	Sa	551	ASN
1	Sb	174	GLN
1	Sb	207	LYS
1	Sb	381	ASP
1	Sb	452	TYR
1	Sb	551	ASN
1	Sc	174	GLN
1	Sc	207	LYS
1	Sc	381	ASP
1	Sc	452	TYR
1	Sc	551	ASN
1	Sd	174	GLN
1	Sd	207	LYS
1	Sd	381	ASP
1	Sd	425	ILE
1	Sd	452	TYR
1	Sd	551	ASN
1	Se	174	GLN
1	Se	207	LYS

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Mol	Chain	Res	Type
1	Se	381	ASP
1	Se	425	ILE
1	Se	452	TYR
1	Se	551	ASN
1	Sf	174	GLN
1	Sf	207	LYS
1	Sf	381	ASP
1	Sf	452	TYR
1	Sf	551	ASN
1	Sg	174	GLN
1	Sg	207	LYS
1	Sg	381	ASP
1	Sg	425	ILE
1	Sg	452	TYR
1	Sg	551	ASN
1	Sh	174	GLN
1	Sh	207	LYS
1	Sh	381	ASP
1	Sh	425	ILE
1	Sh	452	TYR
1	Sh	551	ASN
1	Si	174	GLN
1	Si	207	LYS
1	Si	381	ASP
1	Si	425	ILE
1	Si	452	TYR
1	Si	551	ASN
1	Sj	174	GLN
1	Sj	207	LYS
1	Sj	381	ASP
1	Sj	425	ILE
1	Sj	452	TYR
1	Sj	551	ASN
1	Sk	174	GLN
1	Sk	207	LYS
1	Sk	381	ASP
1	Sk	452	TYR
1	Sk	551	ASN
1	Sl	174	GLN
1	Sl	207	LYS
1	Sl	381	ASP
1	Sl	452	TYR

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Mol	Chain	Res	Type
1	Sl	551	ASN
1	Sm	174	GLN
1	Sm	207	LYS
1	Sm	381	ASP
1	Sm	425	ILE
1	Sm	452	TYR
1	Sm	551	ASN
1	Sn	174	GLN
1	Sn	207	LYS
1	Sn	381	ASP
1	Sn	452	TYR
1	Sn	551	ASN
1	So	174	GLN
1	So	207	LYS
1	So	381	ASP
1	So	452	TYR
1	So	551	ASN
1	Sp	174	GLN
1	Sp	207	LYS
1	Sp	381	ASP
1	Sp	425	ILE
1	Sp	452	TYR
1	Sp	551	ASN
1	Sq	174	GLN
1	Sq	207	LYS
1	Sq	381	ASP
1	Sq	425	ILE
1	Sq	452	TYR
1	Sq	551	ASN
1	Sr	174	GLN
1	Sr	207	LYS
1	Sr	381	ASP
1	Sr	425	ILE
1	Sr	452	TYR
1	Sr	551	ASN
1	Ss	174	GLN
1	Ss	207	LYS
1	Ss	381	ASP
1	Ss	452	TYR
1	Ss	551	ASN
1	St	174	GLN
1	St	207	LYS

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Mol	Chain	Res	Type
1	St	381	ASP
1	St	452	TYR
1	St	551	ASN
1	Su	174	GLN
1	Su	207	LYS
1	Su	381	ASP
1	Su	452	TYR
1	Su	551	ASN
1	Sv	174	GLN
1	Sv	207	LYS
1	Sv	381	ASP
1	Sv	452	TYR
1	Sv	551	ASN
1	Sw	174	GLN
1	Sw	207	LYS
1	Sw	381	ASP
1	Sw	425	ILE
1	Sw	452	TYR
1	Sw	551	ASN
1	Sx	174	GLN
1	Sx	207	LYS
1	Sx	425	ILE
1	Sx	452	TYR
1	Sx	551	ASN
1	Sy	174	GLN
1	Sy	207	LYS
1	Sy	381	ASP
1	Sy	425	ILE
1	Sy	452	TYR
1	Sy	551	ASN
1	Sz	174	GLN
1	Sz	207	LYS
1	Sz	381	ASP
1	Sz	425	ILE
1	Sz	452	TYR
1	Sz	551	ASN
2	T1	4	THR
2	T2	4	THR
2	TA	4	THR
2	TB	4	THR
2	TC	4	THR
2	TD	4	THR

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Mol	Chain	Res	Type
2	TE	4	THR
2	TF	4	THR
2	TG	4	THR
2	TH	4	THR
2	TI	4	THR
2	TJ	4	THR
2	TK	4	THR
2	TL	4	THR
2	TM	4	THR
2	TN	4	THR
2	TO	4	THR
2	TP	4	THR
2	TQ	4	THR
2	TR	4	THR
2	TS	4	THR
2	TT	4	THR
2	TU	4	THR
2	TV	4	THR
2	TW	4	THR
2	TX	4	THR
2	TY	4	THR
2	TZ	4	THR
2	Ta	4	THR
2	Tb	4	THR
2	Tc	4	THR
2	Td	4	THR
2	Te	4	THR
2	Tf	4	THR
2	Tg	4	THR
2	Th	4	THR
2	Ti	4	THR
2	Tj	4	THR
2	Tk	4	THR
2	Tl	4	THR
2	Tm	4	THR
2	Tn	4	THR
2	To	4	THR
2	Tp	4	THR
2	Tq	4	THR
2	Tr	4	THR
2	Ts	4	THR
2	Tt	4	THR

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Mol	Chain	Res	Type
2	Tu	4	THR
2	Tv	4	THR
2	Tw	4	THR
2	Tx	4	THR
2	Ty	4	THR
2	Tz	4	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (411) such sidechains are listed below:

Mol	Chain	Res	Type
1	S1	34	GLN
1	S1	211	GLN
1	S1	249	GLN
1	S1	423	ASN
1	S1	517	GLN
1	S1	551	ASN
1	S1	589	GLN
1	S1	640	ASN
1	S2	34	GLN
1	S2	211	GLN
1	S2	249	GLN
1	S2	423	ASN
1	S2	517	GLN
1	S2	551	ASN
1	S2	589	GLN
1	S2	640	ASN
1	SA	34	GLN
1	SA	211	GLN
1	SA	249	GLN
1	SA	423	ASN
1	SA	551	ASN
1	SA	589	GLN
1	SA	640	ASN
1	SB	34	GLN
1	SB	211	GLN
1	SB	249	GLN
1	SB	423	ASN
1	SB	551	ASN
1	SB	640	ASN
1	SC	34	GLN
1	SC	211	GLN
1	SC	249	GLN

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Mol	Chain	Res	Type
1	SC	423	ASN
1	SC	551	ASN
1	SC	589	GLN
1	SC	640	ASN
1	SD	34	GLN
1	SD	211	GLN
1	SD	249	GLN
1	SD	551	ASN
1	SD	589	GLN
1	SD	640	ASN
1	SE	34	GLN
1	SE	211	GLN
1	SE	249	GLN
1	SE	551	ASN
1	SE	589	GLN
1	SE	640	ASN
1	SF	34	GLN
1	SF	211	GLN
1	SF	249	GLN
1	SF	423	ASN
1	SF	551	ASN
1	SF	589	GLN
1	SF	640	ASN
1	SG	34	GLN
1	SG	211	GLN
1	SG	249	GLN
1	SG	423	ASN
1	SG	551	ASN
1	SG	589	GLN
1	SG	640	ASN
1	SH	34	GLN
1	SH	211	GLN
1	SH	249	GLN
1	SH	517	GLN
1	SH	551	ASN
1	SH	589	GLN
1	SH	640	ASN
1	SI	34	GLN
1	SI	211	GLN
1	SI	249	GLN
1	SI	272	GLN
1	SI	423	ASN

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Mol	Chain	Res	Type
1	SI	551	ASN
1	SI	589	GLN
1	SI	640	ASN
1	SJ	34	GLN
1	SJ	211	GLN
1	SJ	249	GLN
1	SJ	423	ASN
1	SJ	517	GLN
1	SJ	551	ASN
1	SJ	589	GLN
1	SK	34	GLN
1	SK	211	GLN
1	SK	249	GLN
1	SK	423	ASN
1	SK	551	ASN
1	SL	34	GLN
1	SL	211	GLN
1	SL	249	GLN
1	SL	423	ASN
1	SL	551	ASN
1	SL	589	GLN
1	SM	34	GLN
1	SM	211	GLN
1	SM	249	GLN
1	SM	423	ASN
1	SM	463	ASN
1	SM	551	ASN
1	SM	589	GLN
1	SM	640	ASN
1	SN	34	GLN
1	SN	211	GLN
1	SN	249	GLN
1	SN	423	ASN
1	SN	551	ASN
1	SN	589	GLN
1	SN	640	ASN
1	SO	34	GLN
1	SO	211	GLN
1	SO	249	GLN
1	SO	423	ASN
1	SO	551	ASN
1	SO	640	ASN

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Mol	Chain	Res	Type
1	SP	34	GLN
1	SP	211	GLN
1	SP	249	GLN
1	SP	272	GLN
1	SP	423	ASN
1	SP	551	ASN
1	SP	589	GLN
1	SP	640	ASN
1	SQ	34	GLN
1	SQ	211	GLN
1	SQ	249	GLN
1	SQ	423	ASN
1	SQ	589	GLN
1	SQ	640	ASN
1	SR	34	GLN
1	SR	211	GLN
1	SR	249	GLN
1	SR	423	ASN
1	SR	551	ASN
1	SR	589	GLN
1	SR	640	ASN
1	SS	34	GLN
1	SS	211	GLN
1	SS	249	GLN
1	SS	272	GLN
1	SS	423	ASN
1	SS	551	ASN
1	SS	589	GLN
1	SS	640	ASN
1	ST	34	GLN
1	ST	211	GLN
1	ST	249	GLN
1	ST	551	ASN
1	ST	589	GLN
1	ST	640	ASN
1	SU	34	GLN
1	SU	211	GLN
1	SU	249	GLN
1	SU	272	GLN
1	SU	551	ASN
1	SU	589	GLN
1	SU	640	ASN

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Mol	Chain	Res	Type
1	SV	34	GLN
1	SV	211	GLN
1	SV	249	GLN
1	SV	551	ASN
1	SV	589	GLN
1	SV	640	ASN
1	SW	34	GLN
1	SW	211	GLN
1	SW	249	GLN
1	SW	423	ASN
1	SW	551	ASN
1	SW	589	GLN
1	SW	640	ASN
1	SX	34	GLN
1	SX	211	GLN
1	SX	249	GLN
1	SX	272	GLN
1	SX	551	ASN
1	SX	589	GLN
1	SX	640	ASN
1	SY	34	GLN
1	SY	211	GLN
1	SY	249	GLN
1	SY	423	ASN
1	SY	551	ASN
1	SY	589	GLN
1	SY	640	ASN
1	SZ	34	GLN
1	SZ	211	GLN
1	SZ	249	GLN
1	SZ	423	ASN
1	SZ	551	ASN
1	SZ	589	GLN
1	SZ	640	ASN
1	Sa	34	GLN
1	Sa	211	GLN
1	Sa	249	GLN
1	Sa	423	ASN
1	Sa	551	ASN
1	Sa	589	GLN
1	Sa	640	ASN
1	Sb	34	GLN

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Mol	Chain	Res	Type
1	Sb	211	GLN
1	Sb	249	GLN
1	Sb	272	GLN
1	Sb	551	ASN
1	Sb	589	GLN
1	Sb	640	ASN
1	Sc	34	GLN
1	Sc	211	GLN
1	Sc	249	GLN
1	Sc	423	ASN
1	Sc	551	ASN
1	Sc	589	GLN
1	Sd	34	GLN
1	Sd	211	GLN
1	Sd	249	GLN
1	Sd	423	ASN
1	Sd	551	ASN
1	Sd	589	GLN
1	Sd	640	ASN
1	Se	34	GLN
1	Se	211	GLN
1	Se	249	GLN
1	Se	423	ASN
1	Se	551	ASN
1	Se	589	GLN
1	Se	640	ASN
1	Sf	34	GLN
1	Sf	211	GLN
1	Sf	249	GLN
1	Sf	423	ASN
1	Sf	551	ASN
1	Sf	589	GLN
1	Sf	640	ASN
1	Sg	34	GLN
1	Sg	211	GLN
1	Sg	249	GLN
1	Sg	551	ASN
1	Sg	589	GLN
1	Sg	640	ASN
1	Sh	34	GLN
1	Sh	211	GLN
1	Sh	249	GLN

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Mol	Chain	Res	Type
1	Sh	551	ASN
1	Sh	589	GLN
1	Sh	640	ASN
1	Si	34	GLN
1	Si	211	GLN
1	Si	249	GLN
1	Si	423	ASN
1	Si	551	ASN
1	Si	589	GLN
1	Si	640	ASN
1	Sj	34	GLN
1	Sj	211	GLN
1	Sj	249	GLN
1	Sj	423	ASN
1	Sj	551	ASN
1	Sj	589	GLN
1	Sj	640	ASN
1	Sk	34	GLN
1	Sk	211	GLN
1	Sk	249	GLN
1	Sk	551	ASN
1	Sk	589	GLN
1	Sk	640	ASN
1	Sl	34	GLN
1	Sl	211	GLN
1	Sl	249	GLN
1	Sl	517	GLN
1	Sl	551	ASN
1	Sl	589	GLN
1	Sm	34	GLN
1	Sm	211	GLN
1	Sm	249	GLN
1	Sm	423	ASN
1	Sm	551	ASN
1	Sm	589	GLN
1	Sm	640	ASN
1	Sn	34	GLN
1	Sn	211	GLN
1	Sn	249	GLN
1	Sn	272	GLN
1	Sn	551	ASN
1	Sn	589	GLN

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Mol	Chain	Res	Type
1	So	34	GLN
1	So	211	GLN
1	So	249	GLN
1	So	517	GLN
1	So	551	ASN
1	So	589	GLN
1	So	640	ASN
1	Sp	34	GLN
1	Sp	211	GLN
1	Sp	249	GLN
1	Sp	551	ASN
1	Sp	589	GLN
1	Sp	640	ASN
1	Sq	34	GLN
1	Sq	211	GLN
1	Sq	249	GLN
1	Sq	551	ASN
1	Sq	589	GLN
1	Sr	34	GLN
1	Sr	211	GLN
1	Sr	249	GLN
1	Sr	517	GLN
1	Sr	551	ASN
1	Sr	589	GLN
1	Sr	640	ASN
1	Ss	34	GLN
1	Ss	211	GLN
1	Ss	249	GLN
1	Ss	423	ASN
1	Ss	551	ASN
1	St	34	GLN
1	St	211	GLN
1	St	249	GLN
1	St	272	GLN
1	St	423	ASN
1	St	551	ASN
1	St	589	GLN
1	St	640	ASN
1	Su	34	GLN
1	Su	211	GLN
1	Su	249	GLN
1	Su	551	ASN

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Mol	Chain	Res	Type
1	Su	589	GLN
1	Su	640	ASN
1	Sv	34	GLN
1	Sv	211	GLN
1	Sv	249	GLN
1	Sv	423	ASN
1	Sv	551	ASN
1	Sv	589	GLN
1	Sv	640	ASN
1	Sw	34	GLN
1	Sw	211	GLN
1	Sw	249	GLN
1	Sw	517	GLN
1	Sw	551	ASN
1	Sw	589	GLN
1	Sw	640	ASN
1	Sx	34	GLN
1	Sx	211	GLN
1	Sx	249	GLN
1	Sx	517	GLN
1	Sx	551	ASN
1	Sx	589	GLN
1	Sy	34	GLN
1	Sy	211	GLN
1	Sy	249	GLN
1	Sy	423	ASN
1	Sy	517	GLN
1	Sy	551	ASN
1	Sy	589	GLN
1	Sy	640	ASN
1	Sz	34	GLN
1	Sz	211	GLN
1	Sz	249	GLN
1	Sz	423	ASN
1	Sz	517	GLN
1	Sz	551	ASN
1	Sz	589	GLN
1	Sz	640	ASN
2	T1	97	ASN
2	T2	97	ASN
2	TG	97	ASN
2	TH	97	ASN

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Mol	Chain	Res	Type
2	TI	97	ASN
2	TK	97	ASN
2	TL	97	ASN
2	TM	97	ASN
2	TN	97	ASN
2	TO	97	ASN
2	TP	97	ASN
2	TQ	97	ASN
2	TR	97	ASN
2	TS	97	ASN
2	TT	97	ASN
2	TU	97	ASN
2	TV	97	ASN
2	TW	97	ASN
2	TX	97	ASN
2	TY	97	ASN
2	TZ	97	ASN
2	Ta	97	ASN
2	Tb	97	ASN
2	Tc	97	ASN
2	Td	97	ASN
2	Te	97	ASN
2	Tf	97	ASN
2	Tg	97	ASN
2	Th	97	ASN
2	Ti	97	ASN
2	Tj	97	ASN
2	Tk	97	ASN
2	Tl	97	ASN
2	Tm	97	ASN
2	Tn	97	ASN
2	To	97	ASN
2	Tp	97	ASN
2	Tq	97	ASN
2	Tr	97	ASN
2	Ts	97	ASN
2	Tt	97	ASN
2	Tu	97	ASN
2	Tv	97	ASN
2	Tw	97	ASN
2	Tx	97	ASN
2	Ty	97	ASN

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Mol	Chain	Res	Type
2	Tz	97	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

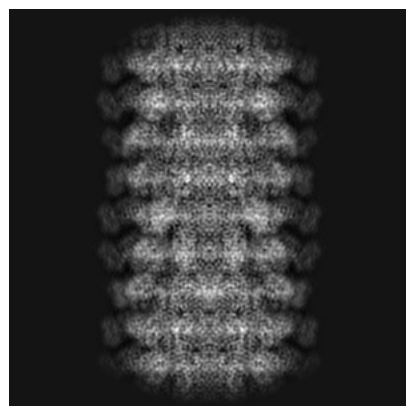
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19992. These allow visual inspection of the internal detail of the map and identification of artifacts.

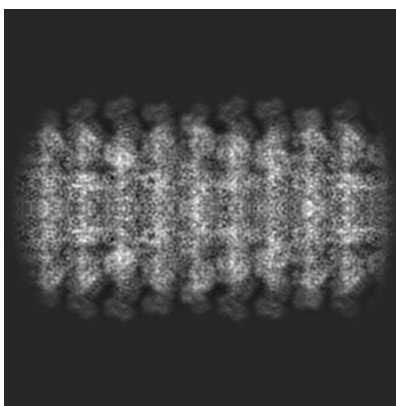
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

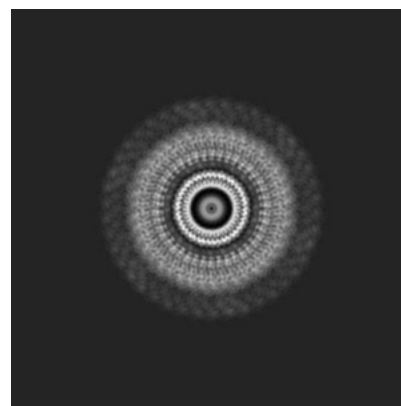
6.1.1 Primary map



X

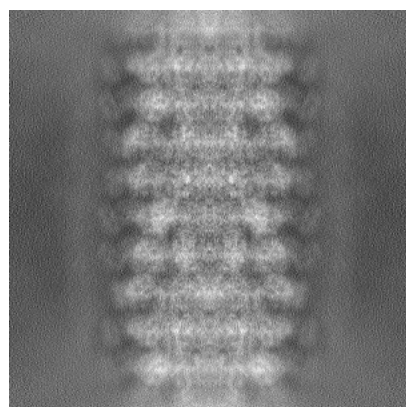


Y

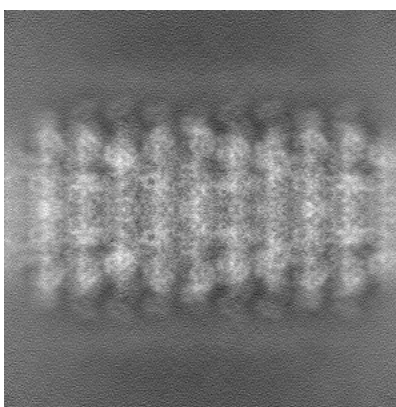


Z

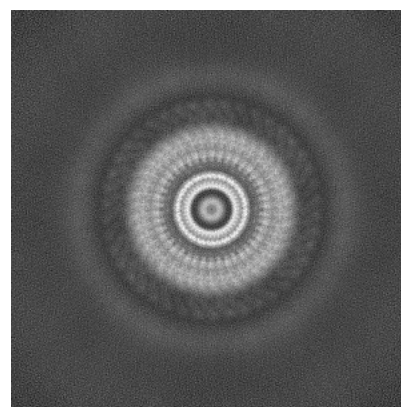
6.1.2 Raw map



X



Y

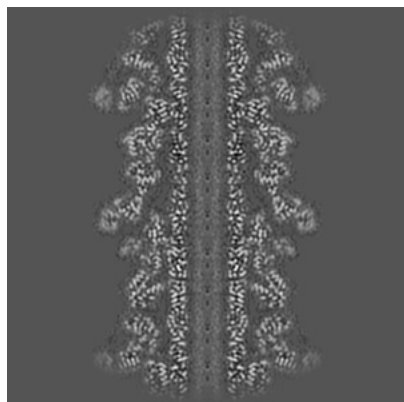


Z

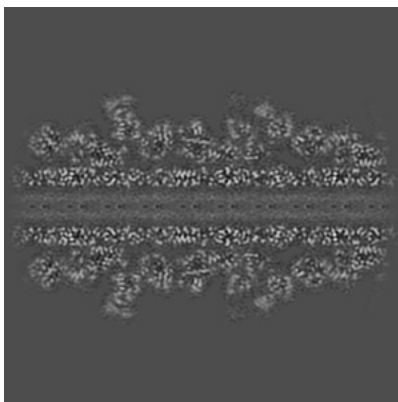
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

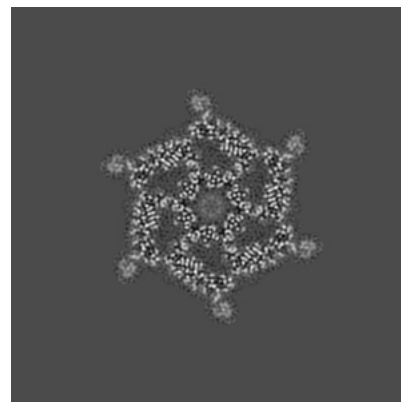
6.2.1 Primary map



X Index: 200

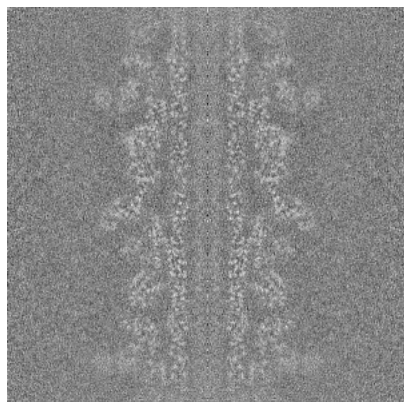


Y Index: 200

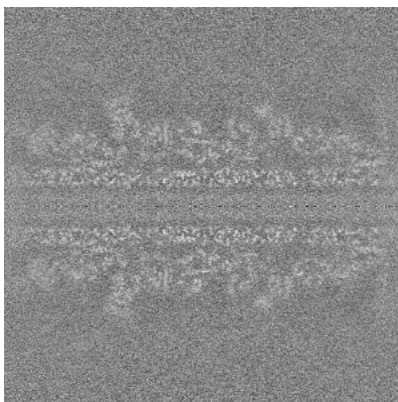


Z Index: 200

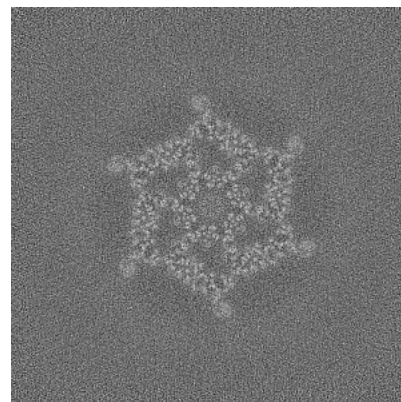
6.2.2 Raw map



X Index: 200



Y Index: 200

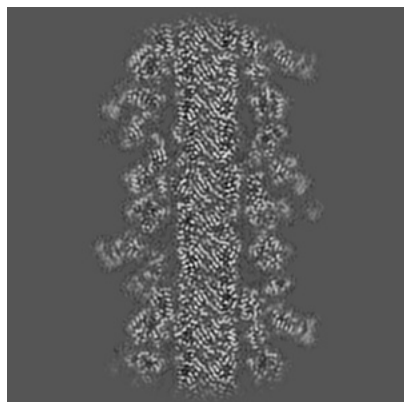


Z Index: 200

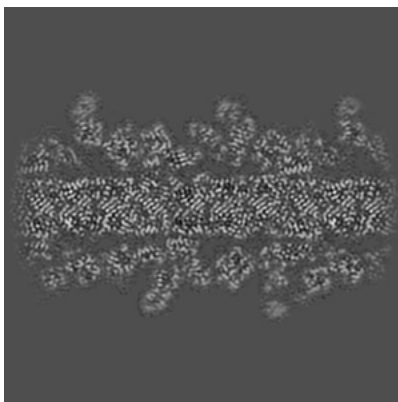
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

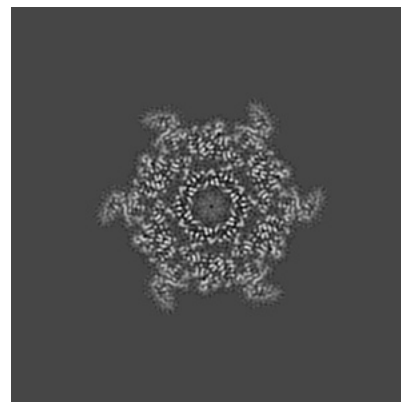
6.3.1 Primary map



X Index: 178

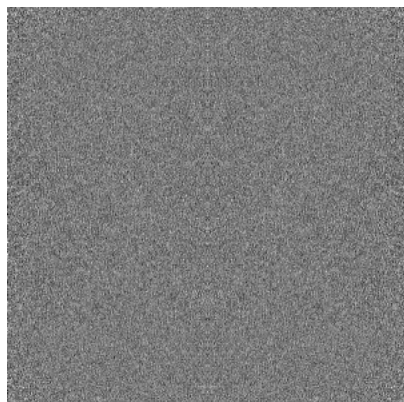


Y Index: 176

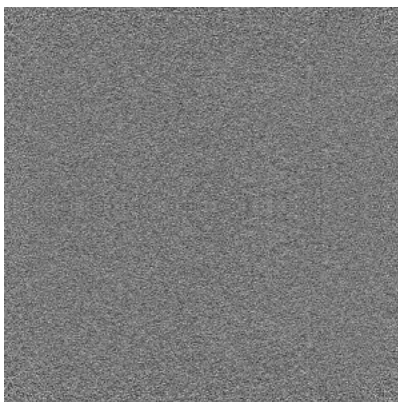


Z Index: 115

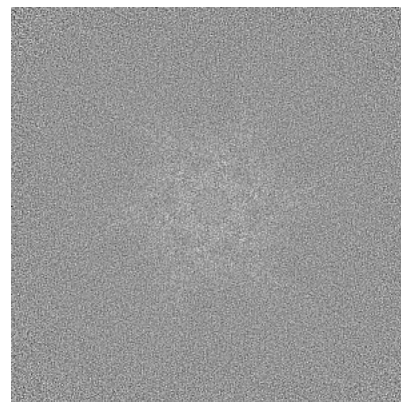
6.3.2 Raw map



X Index: 0



Y Index: 0

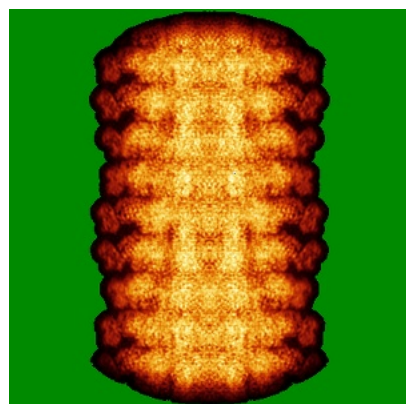


Z Index: 0

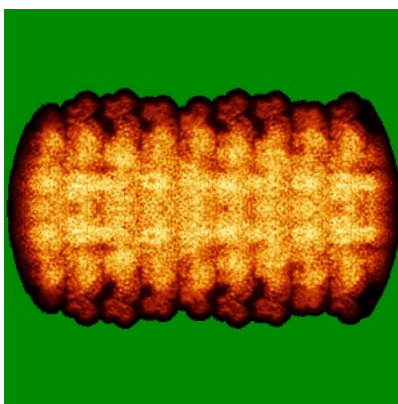
The images above show the largest variance slices of the map in three orthogonal directions.

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

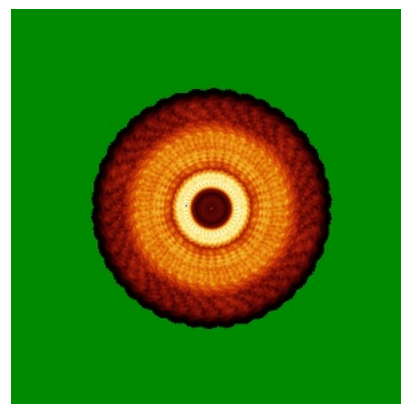
6.4.1 Primary map



X

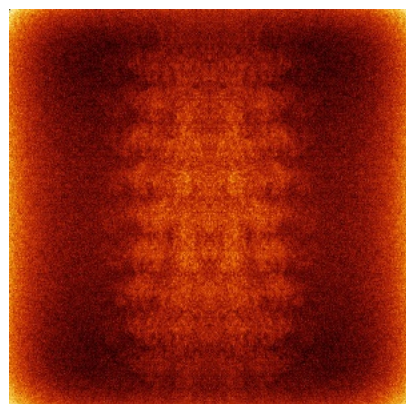


Y

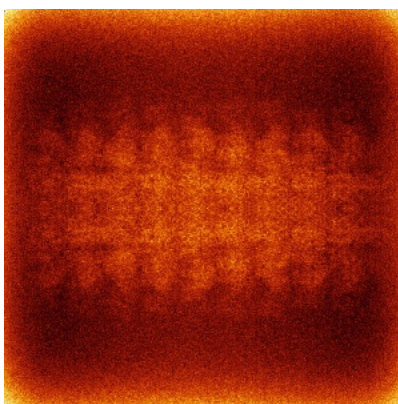


Z

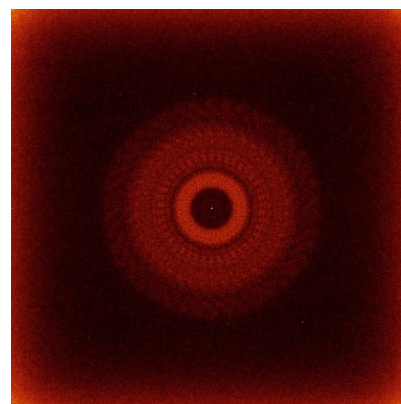
6.4.2 Raw map



X



Y

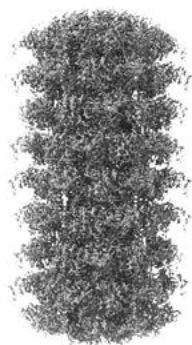


Z

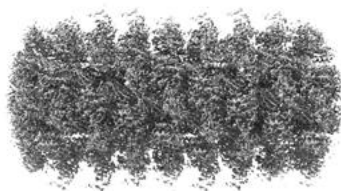
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

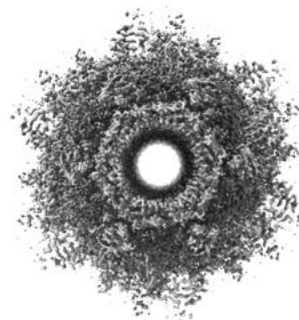
6.5.1 Primary map



X



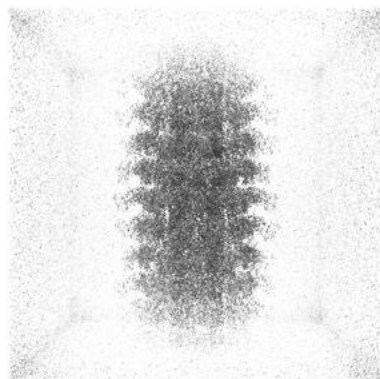
Y



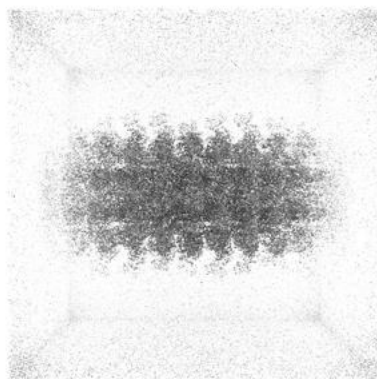
Z

The images above show the 3D surface view of the map at the recommended contour level 0.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

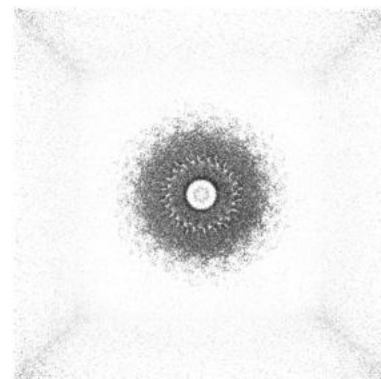
6.5.2 Raw map



X



Y



Z

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.

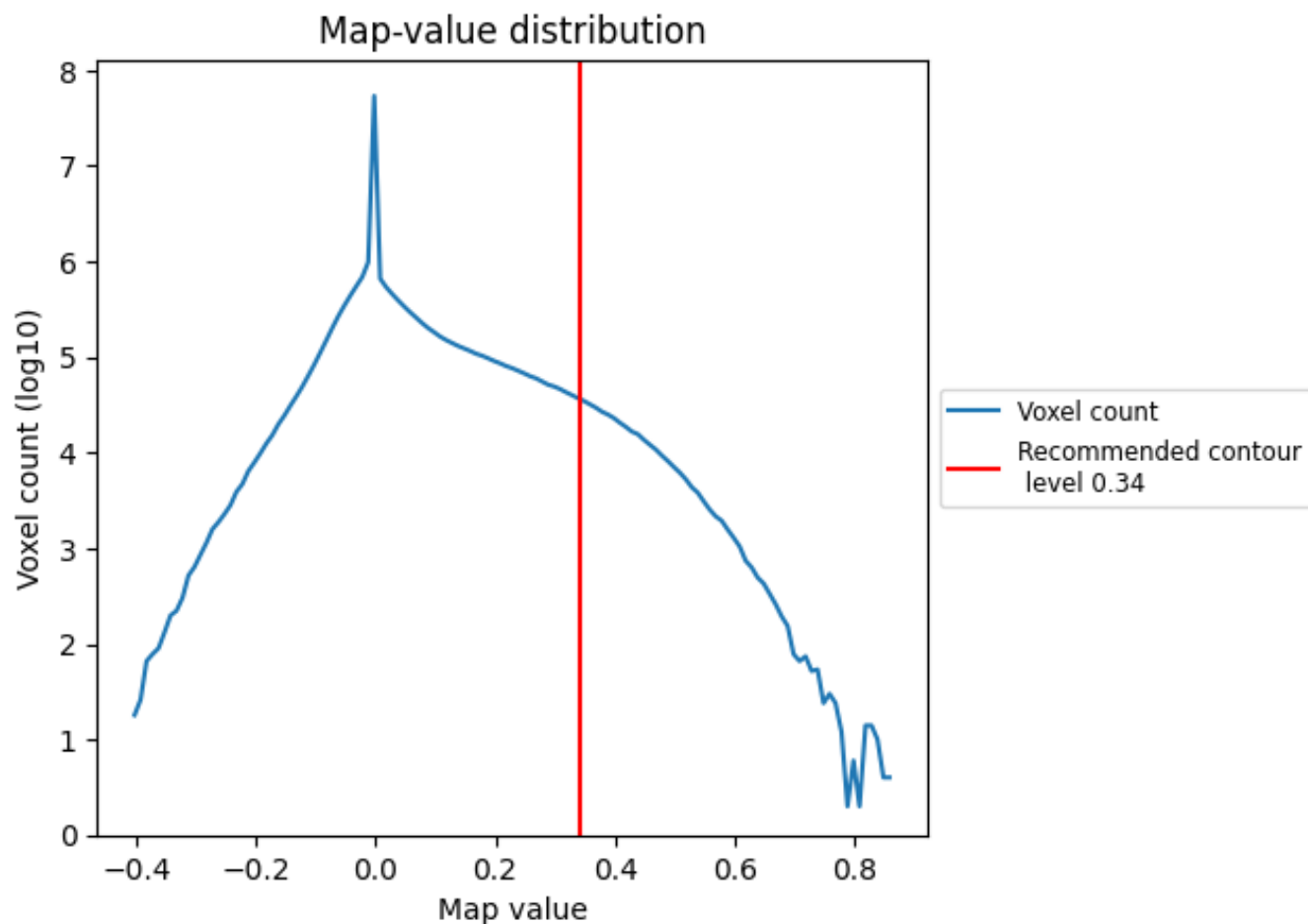
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

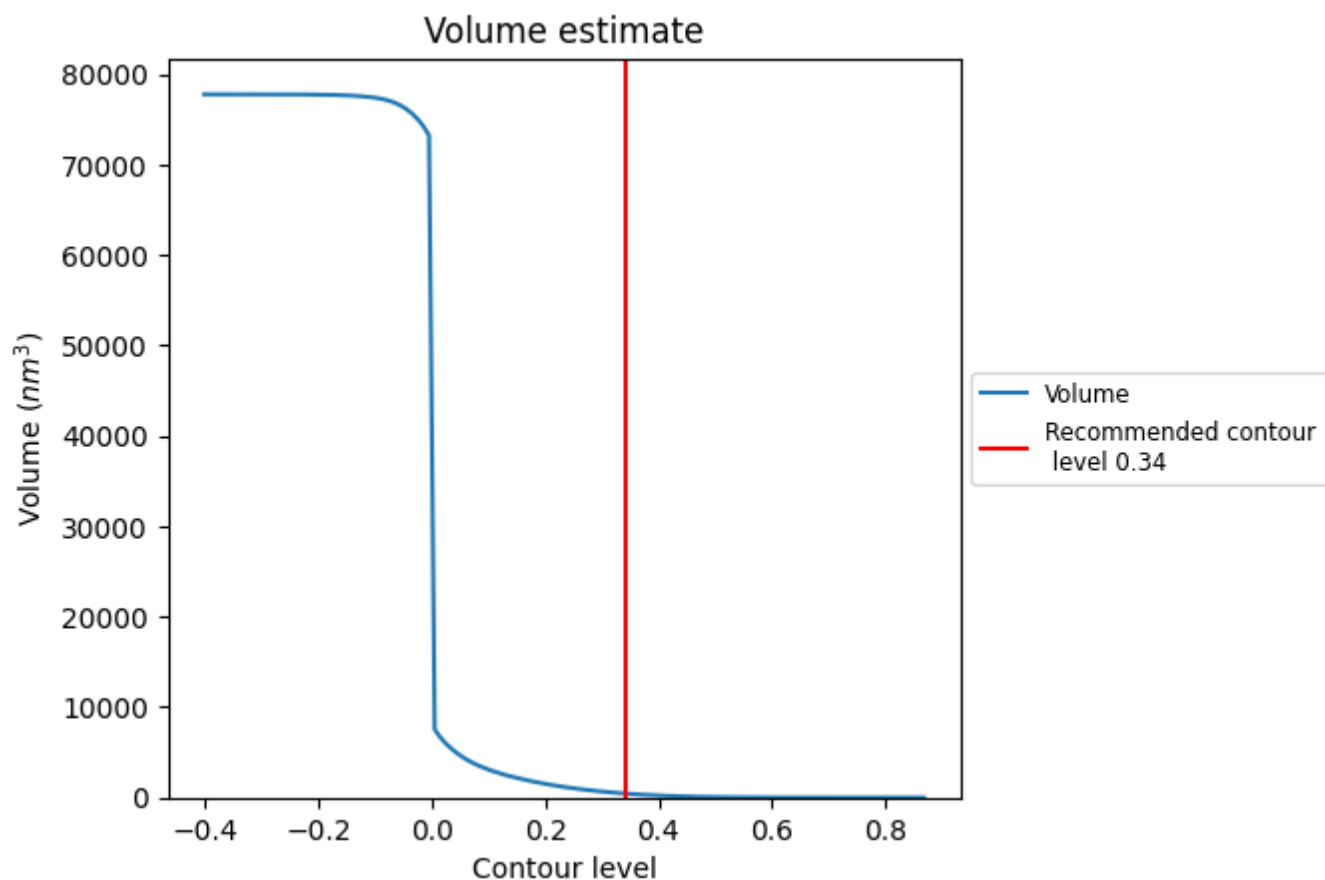
This section contains the results of statistical analysis of the map.

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.

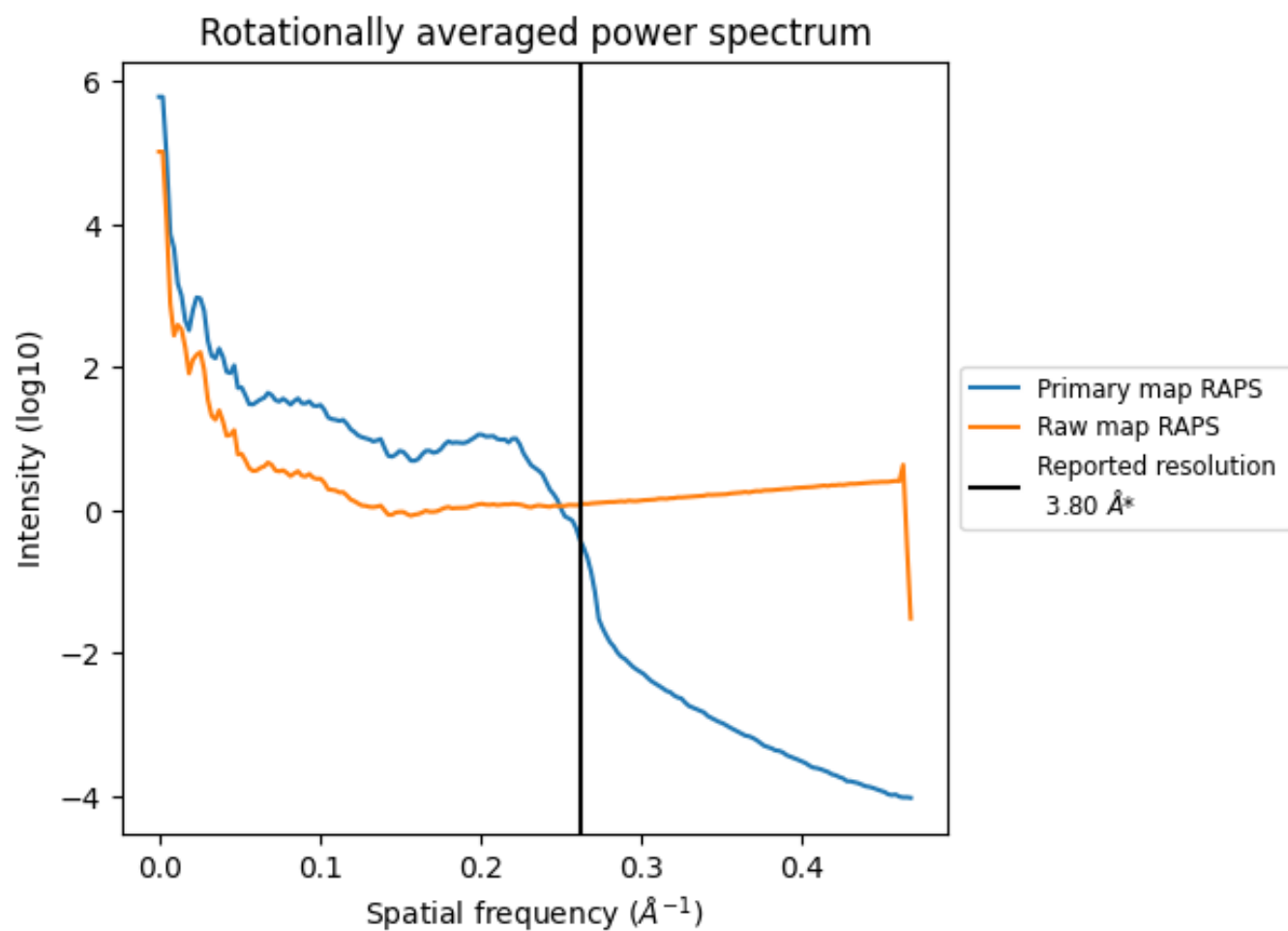
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 451 nm³; this corresponds to an approximate mass of 407 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 ⓘ

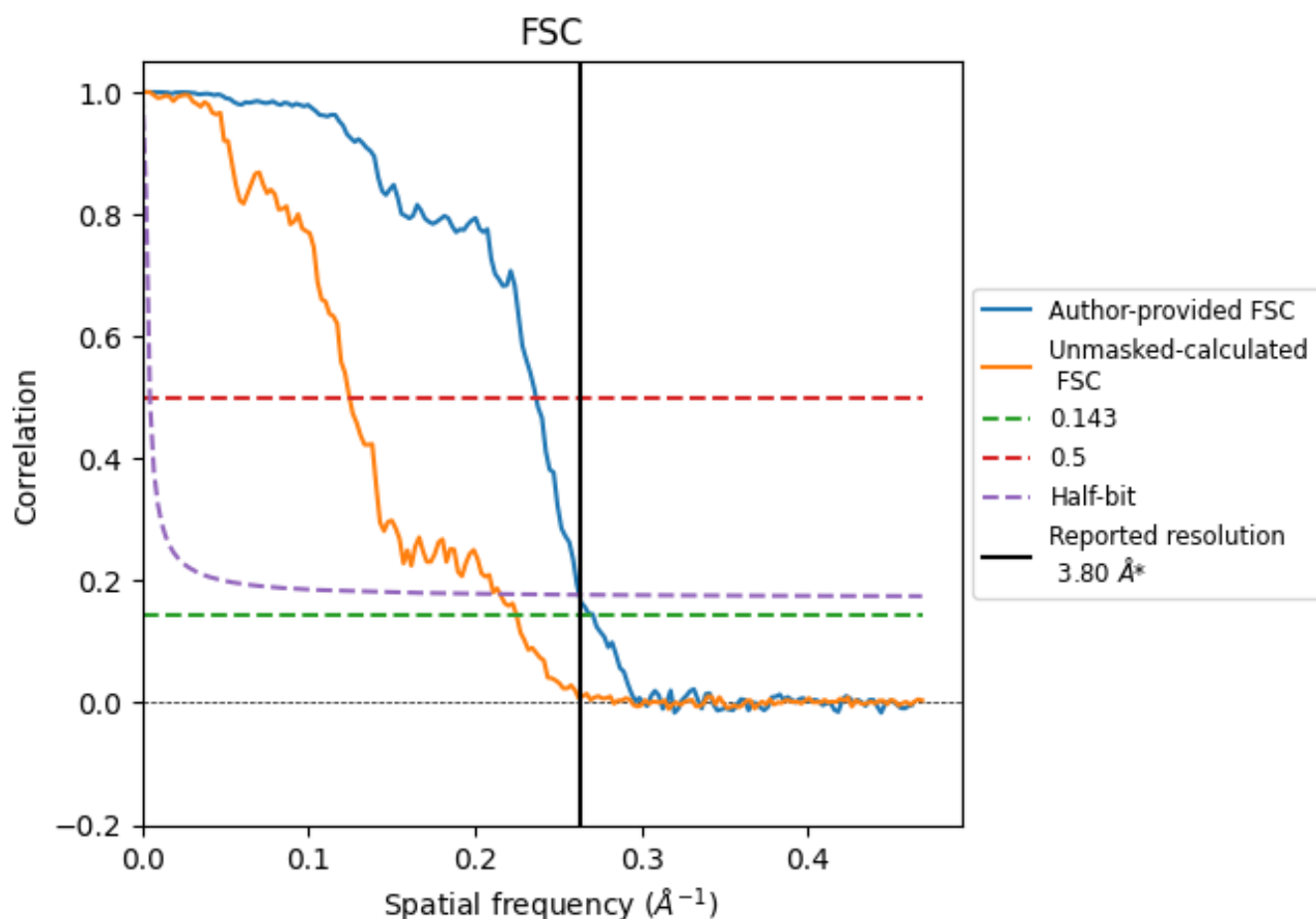


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

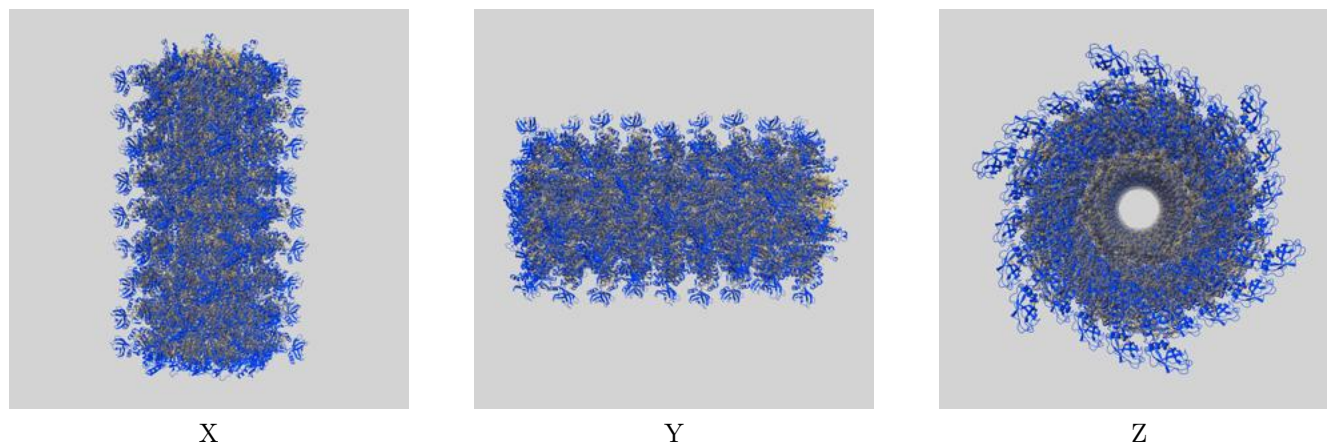
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.69	4.23	3.81
Unmasked-calculated*	4.44	8.03	4.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

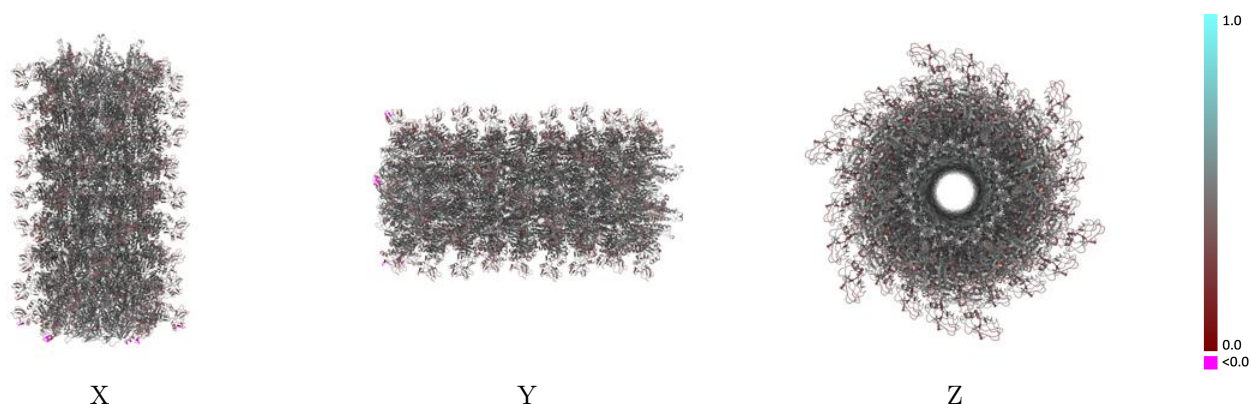
This section contains information regarding the fit between EMDB map EMD-19992 and PDB model 9EV2. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



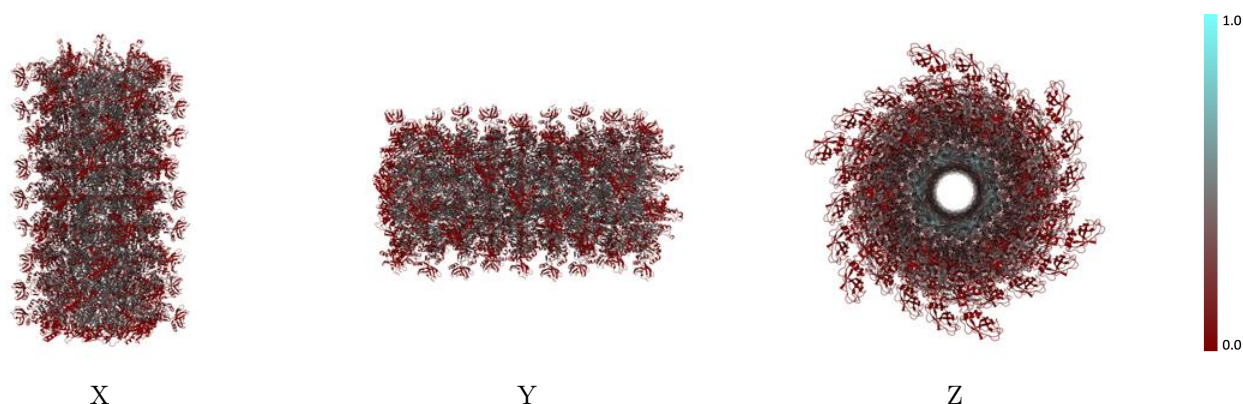
The images above show the 3D surface view of the map at the recommended contour level 0.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



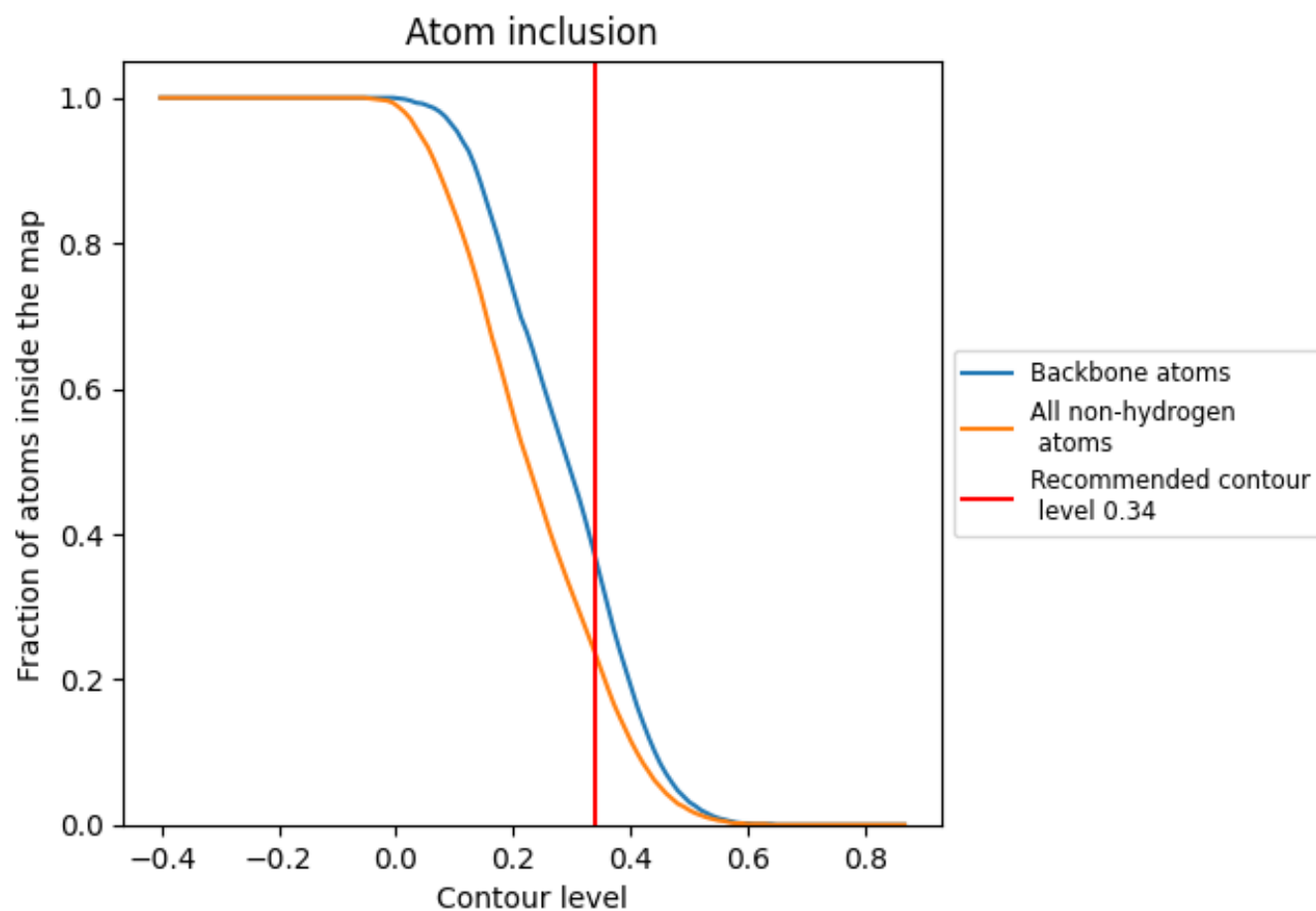
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.34).

9.4 Atom inclusion [i](#)



At the recommended contour level, 37% of all backbone atoms, 24% 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 (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2350	 0.4490
S1	 0.1740	 0.4380
S2	 0.1730	 0.4390
SA	 0.1370	 0.4270
SB	 0.1350	 0.4270
SC	 0.1360	 0.4270
SD	 0.1370	 0.4270
SE	 0.1350	 0.4280
SF	 0.1360	 0.4270
SG	 0.2010	 0.4400
SH	 0.2010	 0.4390
SI	 0.2040	 0.4400
SJ	 0.2010	 0.4400
SK	 0.2000	 0.4400
SL	 0.2040	 0.4410
SM	 0.2030	 0.4400
SN	 0.2030	 0.4400
SO	 0.2040	 0.4400
SP	 0.2030	 0.4400
SQ	 0.2030	 0.4400
SR	 0.2040	 0.4410
SS	 0.2030	 0.4410
ST	 0.2020	 0.4400
SU	 0.2030	 0.4400
SV	 0.2030	 0.4410
SW	 0.2030	 0.4400
SX	 0.2030	 0.4410
SY	 0.2040	 0.4400
SZ	 0.2020	 0.4400
Sa	 0.2030	 0.4390
Sb	 0.2030	 0.4390
Sc	 0.2020	 0.4400
Sd	 0.2030	 0.4410
Se	 0.2030	 0.4410
Sf	 0.2030	 0.4400



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Chain	Atom inclusion	Q-score
Sg	 0.2020	 0.4400
Sh	 0.2020	 0.4390
Si	 0.2030	 0.4400
Sj	 0.2020	 0.4410
Sk	 0.2010	 0.4410
Sl	 0.2000	 0.4400
Sm	 0.2040	 0.4390
Sn	 0.2010	 0.4400
So	 0.2000	 0.4400
Sp	 0.2040	 0.4410
Sq	 0.2030	 0.4410
Sr	 0.2010	 0.4390
Ss	 0.2000	 0.4400
St	 0.2030	 0.4390
Su	 0.2020	 0.4390
Sv	 0.2000	 0.4400
Sw	 0.1740	 0.4390
Sx	 0.1740	 0.4390
Sy	 0.1730	 0.4380
Sz	 0.1740	 0.4380
T1	 0.4200	 0.4890
T2	 0.4160	 0.4910
TA	 0.2940	 0.4890
TB	 0.2950	 0.4870
TC	 0.2950	 0.4890
TD	 0.2940	 0.4890
TE	 0.2950	 0.4890
TF	 0.2950	 0.4890
TG	 0.4160	 0.4880
TH	 0.4160	 0.4880
TI	 0.4150	 0.4890
TJ	 0.4160	 0.4910
TK	 0.4160	 0.4890
TL	 0.4150	 0.4900
TM	 0.4200	 0.4890
TN	 0.4180	 0.4880
TO	 0.4180	 0.4900
TP	 0.4210	 0.4900
TQ	 0.4190	 0.4890
TR	 0.4180	 0.4900
TS	 0.4180	 0.4900
TT	 0.4130	 0.4900

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Chain	Atom inclusion	Q-score
TU	 0.4190	 0.4900
TV	 0.4180	 0.4910
TW	 0.4130	 0.4900
TX	 0.4190	 0.4920
TY	 0.4200	 0.4900
TZ	 0.4170	 0.4880
Ta	 0.4190	 0.4880
Tb	 0.4210	 0.4890
Tc	 0.4180	 0.4910
Td	 0.4190	 0.4900
Te	 0.4260	 0.4890
Tf	 0.4180	 0.4890
Tg	 0.4150	 0.4870
Th	 0.4250	 0.4880
Ti	 0.4170	 0.4910
Tj	 0.4160	 0.4880
Tk	 0.4180	 0.4920
Tl	 0.4160	 0.4890
Tm	 0.4200	 0.4900
Tn	 0.4180	 0.4900
To	 0.4150	 0.4900
Tp	 0.4190	 0.4900
Tq	 0.4160	 0.4910
Tr	 0.4250	 0.4910
Ts	 0.4170	 0.4890
Tt	 0.4170	 0.4890
Tu	 0.4260	 0.4900
Tv	 0.4170	 0.4890
Tw	 0.4150	 0.4900
Tx	 0.4200	 0.4900
Ty	 0.4160	 0.4880
Tz	 0.4160	 0.4880