



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 05:27 PM EST

PDB ID : 6PWB
EMDB ID : EMD-20504
Title : Rigid body fitting of flagellin FlaB, and flagellar coiling proteins, FcpA and FcpB, into a 10 Angstrom structure of the asymmetric flagellar filament purified from *Leptospira biflexa* Patoc WT cells resolved via subtomogram averaging
Authors : Gibson, K.H.; Sindelar, C.V.; Trajtenberg, F.; Buschiazzi, A.; San Martin, F.; Mechaly, A.
Deposited on : 2019-07-22
Resolution : 9.83 Å (reported)
Based on initial models : 5WJT, 6NQZ, 6NQW

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

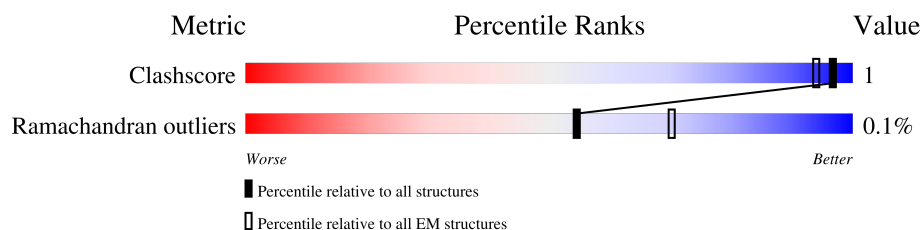
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.83 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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	AG	265	<div> <div>84%</div> <div>99%</div> </div>
1	AH	265	<div> <div>82%</div> <div>99%</div> </div>
1	AI	265	<div> <div>79%</div> <div>100%</div> </div>
1	AR	265	<div> <div>81%</div> <div>98%</div> </div>
1	BA	265	<div> <div>76%</div> <div>97%</div> </div>
1	BB	265	<div> <div>61%</div> <div>99%</div> </div>
1	BC	265	<div> <div>66%</div> <div>98%</div> </div>
1	BD	265	<div> <div>79%</div> <div>98%</div> </div>
1	BL	265	<div> <div>84%</div> <div>99%</div> </div>

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Mol	Chain	Length	Quality of chain
1	BM	265	61% 99% .
1	BS	265	83% 98% .
1	BT	265	93% 99% .
1	BU	265	86% 98% .
1	BV	265	75% 98% .
1	BW	265	56% 98% .
1	BX	265	66% 98% .
1	BY	265	79% 98% .
1	CG	265	78% 98% .
1	CH	265	56% 98% .
1	CL	265	95% 98% .
1	CM	265	58% 98% .
1	CN	265	57% 99% .
1	CO	265	79% 100% .
1	CP	265	79% 98% .
1	CQ	265	77% 98% .
1	CR	265	55% 99% .
1	CS	265	62% 98% .
1	CT	265	78% 98% .
1	DB	265	77% 98% .
1	DC	265	55% 99% .
1	DG	265	79% 97% .
1	DH	265	49% 98% .
1	DI	265	37% 98% .
1	DJ	265	70% 99% .

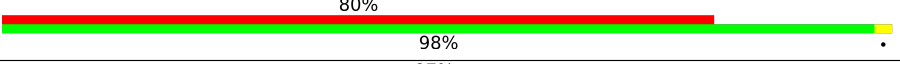
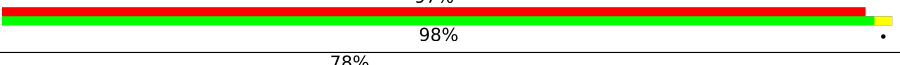
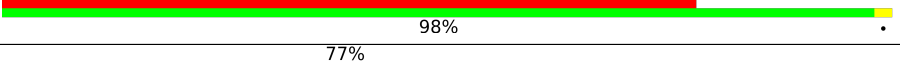
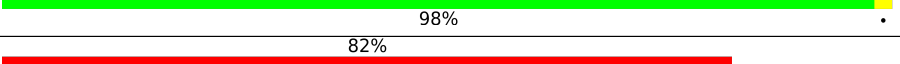
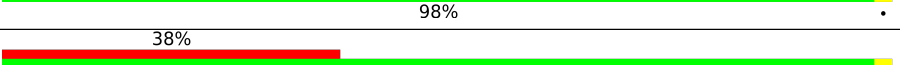
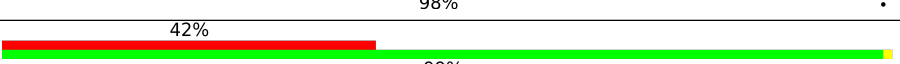
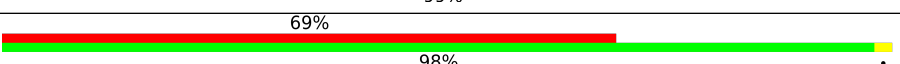
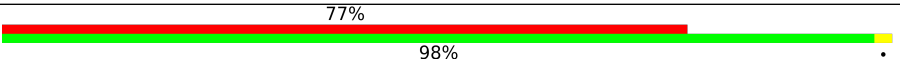
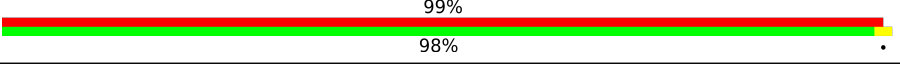
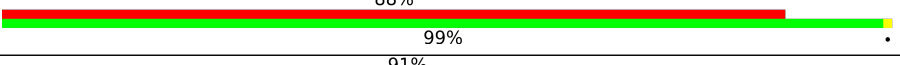
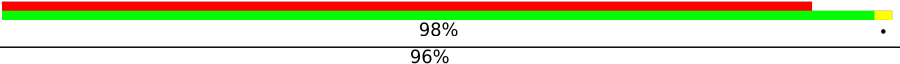
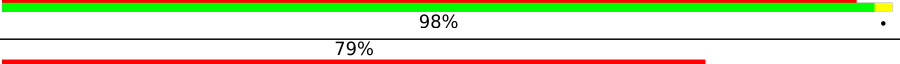
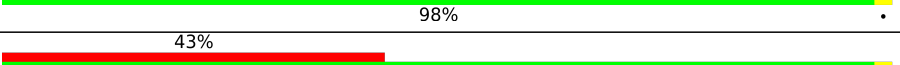
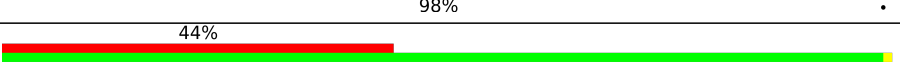
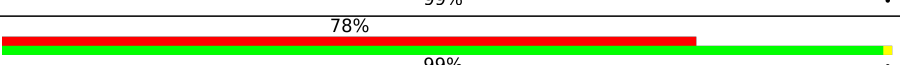
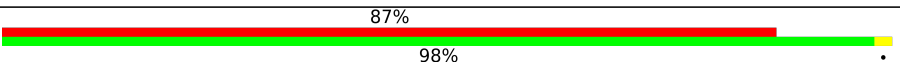
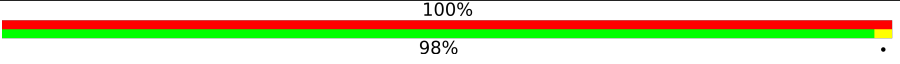
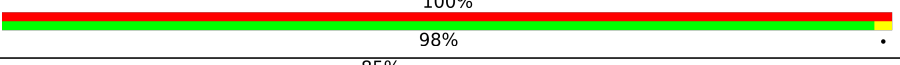
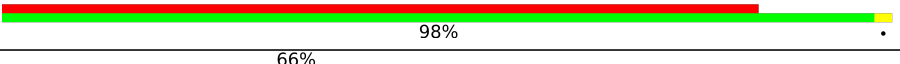
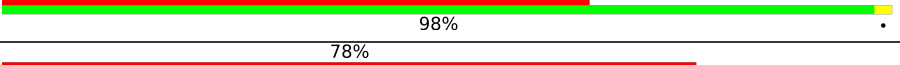
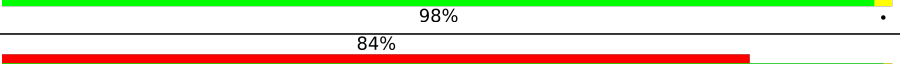
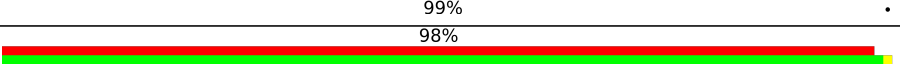
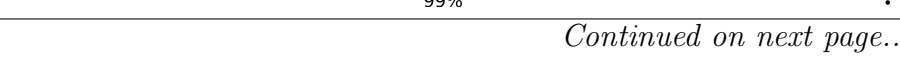


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Mol	Chain	Length	Quality of chain
1	DK	265	77% 98%
1	DL	265	77% 97%
1	DM	265	56% 98%
1	DN	265	65% 98%
1	DO	265	81% 98%
1	DW	265	75% 98%
1	DX	265	57% 98%
1	EB	265	85% 97%
1	EC	265	45% 98%
1	ED	265	38% 99%
1	EE	265	69% 99%
1	EF	265	75% 98%
1	EG	265	78% 97%
1	EH	265	55% 98%
1	EI	265	68% 98%
1	EJ	265	89% 98%
1	ER	265	74% 98%
1	ES	265	57% 98%
1	EW	265	82% 98%
1	EX	265	43% 98%
1	EY	265	37% 99%
1	EZ	265	68% 98%
1	FA	265	75% 98%
1	FB	265	80% 98%
1	FC	265	66% 98%

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Mol	Chain	Length	Quality of chain
1	FD	265	80% 
1	FE	265	97% 
1	FM	265	78% 
1	FN	265	77% 
1	FR	265	82% 
1	FS	265	38% 
1	FT	265	42% 
1	FU	265	69% 
1	FV	265	77% 
1	FW	265	99% 
1	FX	265	88% 
1	GH	265	91% 
1	GI	265	96% 
1	GM	265	79% 
1	GN	265	43% 
1	GO	265	44% 
1	GP	265	78% 
1	GQ	265	87% 
1	GR	265	100% 
1	HC	265	100% 
1	HH	265	85% 
1	HI	265	66% 
1	HJ	265	78% 
1	HK	265	84% 
1	HL	265	98% 

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Mol	Chain	Length	Quality of chain
2	AL	237	59% 100%
2	AM	237	39% 100%
2	AU	237	93% 99%
2	BE	237	41% 100%
2	BF	237	41% 100%
2	BG	237	53% 100%
2	BH	237	33% 100%
2	BN	237	58% 100%
2	BP	237	43% 100%
2	BZ	237	33% 99%
2	CA	237	40% 100%
2	CB	237	52% 100%
2	CC	237	32% 100%
2	CI	237	24% 100%
2	CK	237	46% 100%
2	CU	237	34% 100%
2	CV	237	38% 100%
2	CW	237	51% 100%
2	CX	237	37% 100%
2	DD	237	26% 100%
2	DF	237	44% 100%
2	DP	237	37% 100%
2	DQ	237	42% 100%
2	DR	237	46% 100%
2	DS	237	36% 100%

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Mol	Chain	Length	Quality of chain
2	DY	237	24% 100%
2	EA	237	43% 100%
2	EK	237	39% 99%
2	EL	237	44% 100%
2	EM	237	49% 100%
2	EN	237	40% 100%
2	ET	237	26% 100%
2	EV	237	47% 100%
2	FF	237	46% 100%
2	FG	237	44% 100%
2	FH	237	80% 100%
2	FI	237	95% 100%
2	FO	237	26% 100%
2	FQ	237	50% 100%
2	GA	237	87% 100%
2	GB	237	98% 100%
2	GC	237	100% 100%
2	GJ	237	39% 100%
2	GL	237	100% 100%
2	GV	237	100% 100%
2	GW	237	100% 100%
2	HE	237	100% 100%
3	AO	221	79% 83% 17%
3	BI	221	18% 83% 17%
3	BJ	221	19% 83% 17%

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Mol	Chain	Length	Quality of chain		
3	BK	221	43%	83%	17%
3	BO	221	10%	83%	17%
3	CD	221	8%	83%	17%
3	CE	221	17%	83%	17%
3	CF	221	12%	83%	17%
3	CJ	221	10%	83%	17%
3	CY	221	9%	83%	17%
3	CZ	221	17%	83%	17%
3	DA	221	10%	83%	17%
3	DE	221	11%	83%	17%
3	DT	221	8%	83%	17%
3	DU	221	18%	83%	17%
3	DV	221	14%	83%	17%
3	DZ	221	12%	83%	17%
3	EO	221	10%	83%	17%
3	EP	221	21%	83%	17%
3	EQ	221	13%	83%	17%
3	EU	221	10%	83%	17%
3	FJ	221	10%	83%	17%
3	FK	221	29%	83%	17%
3	FL	221	14%	83%	17%
3	FP	221	14%	83%	17%
3	GE	221	60%	83%	17%
3	GF	221	83%	83%	17%
3	GG	221	25%	83%	17%

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Mol	Chain	Length	Quality of chain	
3	GK	221	77%	
			83%	17%
3	GZ	221	83%	
			83%	17%
3	HB	221	83%	
			83%	17%
3	HF	221	83%	
			83%	17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 157148 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 Flagellin B1 (FlaB1).

Mol	Chain	Residues	Atoms				AltConf	Trace
1	AG	265	Total	C	N	O	0	0
			1060	530	265	265		
1	AH	265	Total	C	N	O	0	0
			1060	530	265	265		
1	AI	265	Total	C	N	O	0	0
			1060	530	265	265		
1	AR	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BA	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BB	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BC	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BD	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BL	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BM	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CG	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CH	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BS	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BT	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BU	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BV	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BW	265	Total	C	N	O	0	0
			1060	530	265	265		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	BX	265	Total	C	N	O	0	0
			1060	530	265	265		
1	BY	265	Total	C	N	O	0	0
			1060	530	265	265		
1	DB	265	Total	C	N	O	0	0
			1060	530	265	265		
1	DC	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CL	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CM	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CN	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CO	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CP	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CQ	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CR	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CS	265	Total	C	N	O	0	0
			1060	530	265	265		
1	CT	265	Total	C	N	O	0	0
			1060	530	265	265		
1	DG	265	Total	C	N	O	0	0
			1060	530	265	265		
1	DH	265	Total	C	N	O	0	0
			1060	530	265	265		
1	DI	265	Total	C	N	O	0	0
			1060	530	265	265		
1	DJ	265	Total	C	N	O	0	0
			1060	530	265	265		
1	DK	265	Total	C	N	O	0	0
			1060	530	265	265		
1	DL	265	Total	C	N	O	0	0
			1060	530	265	265		
1	DM	265	Total	C	N	O	0	0
			1060	530	265	265		
1	DN	265	Total	C	N	O	0	0
			1060	530	265	265		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	DO	265	Total 1060	C 530	N 265	O 265	0	0
1	DW	265	Total 1060	C 530	N 265	O 265	0	0
1	DX	265	Total 1060	C 530	N 265	O 265	0	0
1	EB	265	Total 1060	C 530	N 265	O 265	0	0
1	EC	265	Total 1060	C 530	N 265	O 265	0	0
1	ED	265	Total 1060	C 530	N 265	O 265	0	0
1	EE	265	Total 1060	C 530	N 265	O 265	0	0
1	EF	265	Total 1060	C 530	N 265	O 265	0	0
1	EG	265	Total 1060	C 530	N 265	O 265	0	0
1	EH	265	Total 1060	C 530	N 265	O 265	0	0
1	EI	265	Total 1060	C 530	N 265	O 265	0	0
1	EJ	265	Total 1060	C 530	N 265	O 265	0	0
1	ER	265	Total 1060	C 530	N 265	O 265	0	0
1	ES	265	Total 1060	C 530	N 265	O 265	0	0
1	FA	265	Total 1060	C 530	N 265	O 265	0	0
1	FB	265	Total 1060	C 530	N 265	O 265	0	0
1	FC	265	Total 1060	C 530	N 265	O 265	0	0
1	FD	265	Total 1060	C 530	N 265	O 265	0	0
1	FE	265	Total 1060	C 530	N 265	O 265	0	0
1	FM	265	Total 1060	C 530	N 265	O 265	0	0
1	FN	265	Total 1060	C 530	N 265	O 265	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	EW	265	Total 1060	C 530	N 265	O 265	0	0
1	EX	265	Total 1060	C 530	N 265	O 265	0	0
1	EY	265	Total 1060	C 530	N 265	O 265	0	0
1	EZ	265	Total 1060	C 530	N 265	O 265	0	0
1	GH	265	Total 1060	C 530	N 265	O 265	0	0
1	GI	265	Total 1060	C 530	N 265	O 265	0	0
1	FR	265	Total 1060	C 530	N 265	O 265	0	0
1	FS	265	Total 1060	C 530	N 265	O 265	0	0
1	FT	265	Total 1060	C 530	N 265	O 265	0	0
1	FU	265	Total 1060	C 530	N 265	O 265	0	0
1	FV	265	Total 1060	C 530	N 265	O 265	0	0
1	FW	265	Total 1060	C 530	N 265	O 265	0	0
1	FX	265	Total 1060	C 530	N 265	O 265	0	0
1	HC	265	Total 1060	C 530	N 265	O 265	0	0
1	GM	265	Total 1060	C 530	N 265	O 265	0	0
1	GN	265	Total 1060	C 530	N 265	O 265	0	0
1	GO	265	Total 1060	C 530	N 265	O 265	0	0
1	GP	265	Total 1060	C 530	N 265	O 265	0	0
1	GQ	265	Total 1060	C 530	N 265	O 265	0	0
1	GR	265	Total 1060	C 530	N 265	O 265	0	0
1	HH	265	Total 1060	C 530	N 265	O 265	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	HI	265	Total	C	N	O	0	0
			1060	530	265	265		
1	HJ	265	Total	C	N	O	0	0
			1060	530	265	265		
1	HK	265	Total	C	N	O	0	0
			1060	530	265	265		
1	HL	265	Total	C	N	O	0	0
			1060	530	265	265		

- Molecule 2 is a protein called Flagellar coiling protein A (FcpA).

Mol	Chain	Residues	Atoms				AltConf	Trace
2	AL	237	Total	C	N	O	0	0
			948	474	237	237		
2	AM	237	Total	C	N	O	0	0
			948	474	237	237		
2	AU	237	Total	C	N	O	0	0
			948	474	237	237		
2	BE	237	Total	C	N	O	0	0
			948	474	237	237		
2	BF	237	Total	C	N	O	0	0
			948	474	237	237		
2	BG	237	Total	C	N	O	0	0
			948	474	237	237		
2	BH	237	Total	C	N	O	0	0
			948	474	237	237		
2	BN	237	Total	C	N	O	0	0
			948	474	237	237		
2	BP	237	Total	C	N	O	0	0
			948	474	237	237		
2	CA	237	Total	C	N	O	0	0
			948	474	237	237		
2	CB	237	Total	C	N	O	0	0
			948	474	237	237		
2	CC	237	Total	C	N	O	0	0
			948	474	237	237		
2	CI	237	Total	C	N	O	0	0
			948	474	237	237		
2	CK	237	Total	C	N	O	0	0
			948	474	237	237		
2	BZ	237	Total	C	N	O	0	0
			948	474	237	237		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	DD	237	Total 948	C 474	N 237	O 237	0	0
2	DF	237	Total 948	C 474	N 237	O 237	0	0
2	CU	237	Total 948	C 474	N 237	O 237	0	0
2	CV	237	Total 948	C 474	N 237	O 237	0	0
2	CW	237	Total 948	C 474	N 237	O 237	0	0
2	CX	237	Total 948	C 474	N 237	O 237	0	0
2	EA	237	Total 948	C 474	N 237	O 237	0	0
2	DP	237	Total 948	C 474	N 237	O 237	0	0
2	DQ	237	Total 948	C 474	N 237	O 237	0	0
2	DR	237	Total 948	C 474	N 237	O 237	0	0
2	DS	237	Total 948	C 474	N 237	O 237	0	0
2	DY	237	Total 948	C 474	N 237	O 237	0	0
2	EK	237	Total 948	C 474	N 237	O 237	0	0
2	EL	237	Total 948	C 474	N 237	O 237	0	0
2	EM	237	Total 948	C 474	N 237	O 237	0	0
2	EN	237	Total 948	C 474	N 237	O 237	0	0
2	ET	237	Total 948	C 474	N 237	O 237	0	0
2	EV	237	Total 948	C 474	N 237	O 237	0	0
2	FF	237	Total 948	C 474	N 237	O 237	0	0
2	FG	237	Total 948	C 474	N 237	O 237	0	0
2	FH	237	Total 948	C 474	N 237	O 237	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	FI	237	Total	C	N	O	0	0
			948	474	237	237		
2	FO	237	Total	C	N	O	0	0
			948	474	237	237		
2	FQ	237	Total	C	N	O	0	0
			948	474	237	237		
2	GA	237	Total	C	N	O	0	0
			948	474	237	237		
2	GB	237	Total	C	N	O	0	0
			948	474	237	237		
2	GC	237	Total	C	N	O	0	0
			948	474	237	237		
2	GJ	237	Total	C	N	O	0	0
			948	474	237	237		
2	GL	237	Total	C	N	O	0	0
			948	474	237	237		
2	HE	237	Total	C	N	O	0	0
			948	474	237	237		
2	GV	237	Total	C	N	O	0	0
			948	474	237	237		
2	GW	237	Total	C	N	O	0	0
			948	474	237	237		

- Molecule 3 is a protein called Flagellar coiling protein B (FcpB).

Mol	Chain	Residues	Atoms				AltConf	Trace
3	AO	184	Total	C	N	O	0	0
			736	368	184	184		
3	BI	184	Total	C	N	O	0	0
			736	368	184	184		
3	BJ	184	Total	C	N	O	0	0
			736	368	184	184		
3	BK	184	Total	C	N	O	0	0
			736	368	184	184		
3	BO	184	Total	C	N	O	0	0
			736	368	184	184		
3	CD	184	Total	C	N	O	0	0
			736	368	184	184		
3	CE	184	Total	C	N	O	0	0
			736	368	184	184		
3	CF	184	Total	C	N	O	0	0
			736	368	184	184		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	CJ	184	Total 736	C 368	N 184	O 184	0	0
3	DA	184	Total 736	C 368	N 184	O 184	0	0
3	DE	184	Total 736	C 368	N 184	O 184	0	0
3	CY	184	Total 736	C 368	N 184	O 184	0	0
3	CZ	184	Total 736	C 368	N 184	O 184	0	0
3	DT	184	Total 736	C 368	N 184	O 184	0	0
3	DU	184	Total 736	C 368	N 184	O 184	0	0
3	DV	184	Total 736	C 368	N 184	O 184	0	0
3	DZ	184	Total 736	C 368	N 184	O 184	0	0
3	EO	184	Total 736	C 368	N 184	O 184	0	0
3	EP	184	Total 736	C 368	N 184	O 184	0	0
3	EQ	184	Total 736	C 368	N 184	O 184	0	0
3	EU	184	Total 736	C 368	N 184	O 184	0	0
3	FJ	184	Total 736	C 368	N 184	O 184	0	0
3	FK	184	Total 736	C 368	N 184	O 184	0	0
3	FL	184	Total 736	C 368	N 184	O 184	0	0
3	FP	184	Total 736	C 368	N 184	O 184	0	0
3	GE	184	Total 736	C 368	N 184	O 184	0	0
3	GF	184	Total 736	C 368	N 184	O 184	0	0
3	GG	184	Total 736	C 368	N 184	O 184	0	0
3	GK	184	Total 736	C 368	N 184	O 184	0	0

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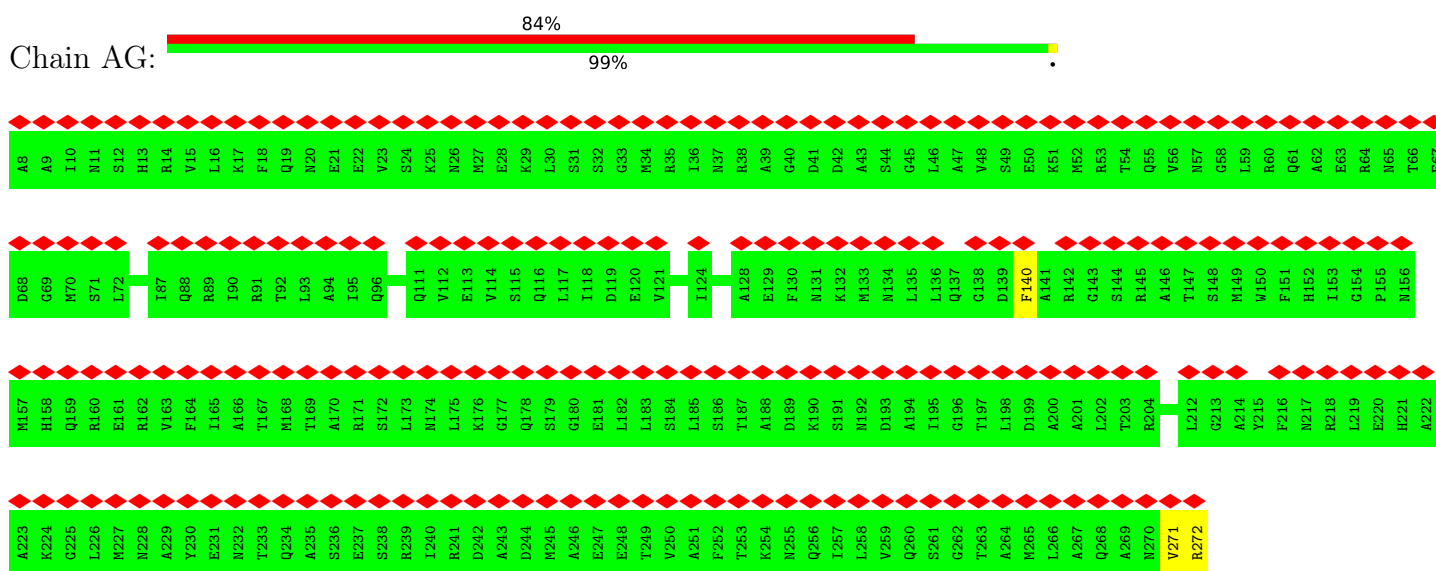
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Mol	Chain	Residues	Atoms				AltConf	Trace
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3	HF	184	Total 736	C 368	N 184	O 184	0	0
3	GZ	184	Total 736	C 368	N 184	O 184	0	0

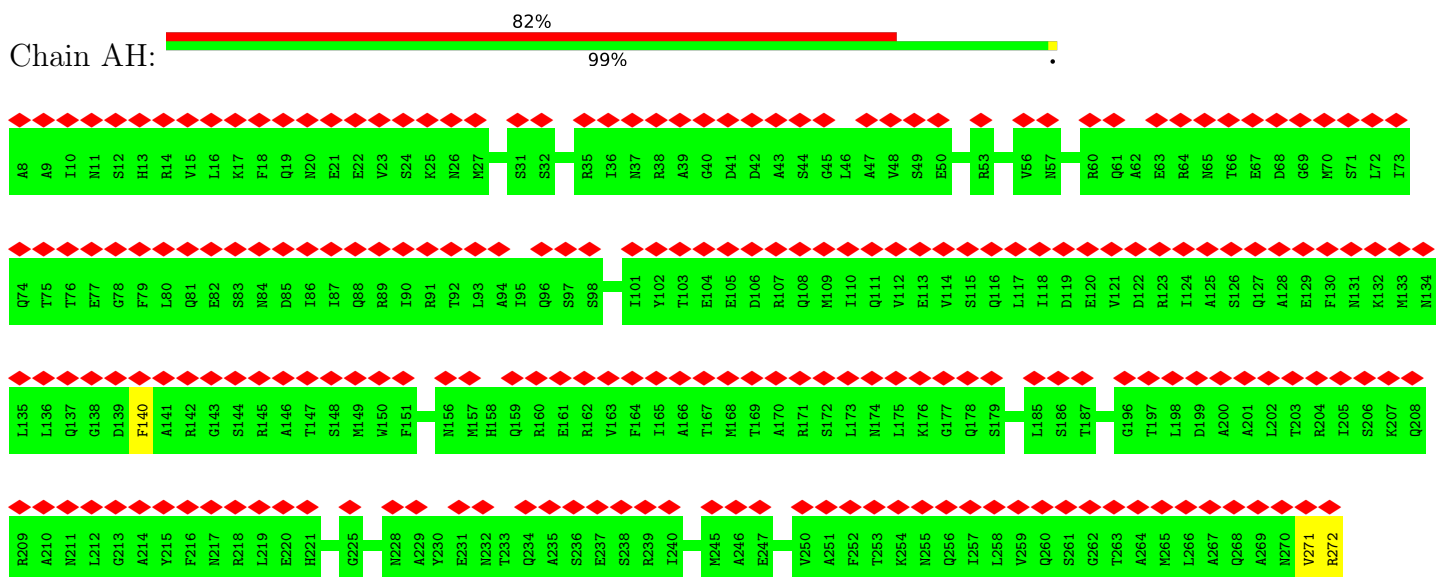
3 Residue-property plots

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.

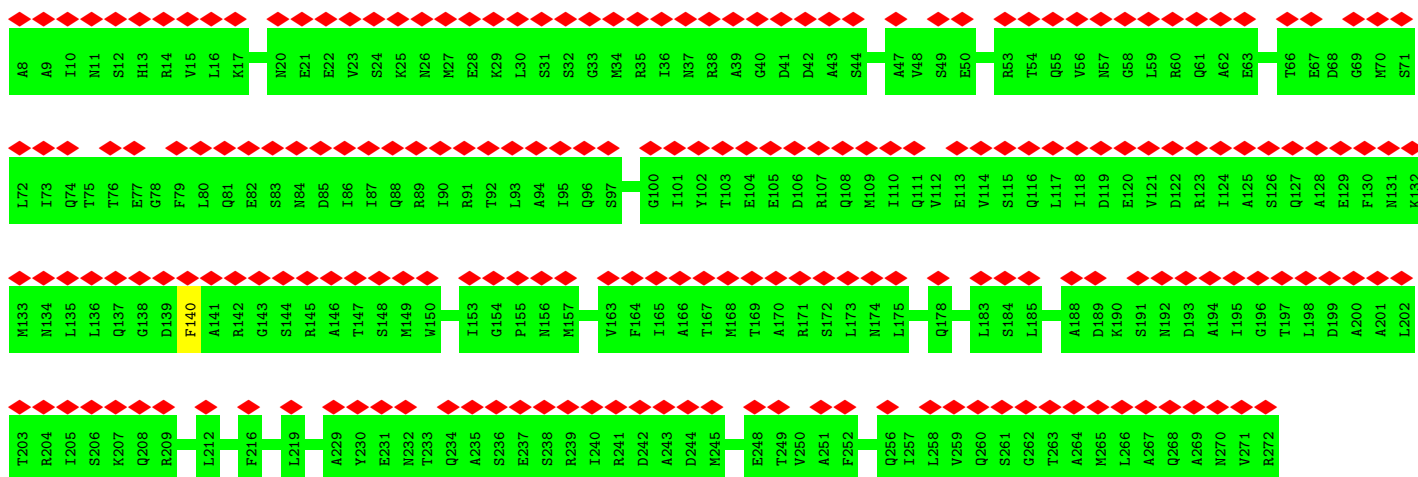
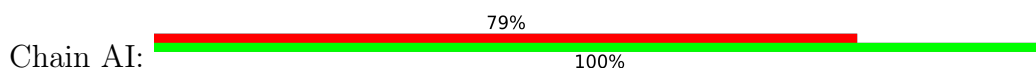
• Molecule 1: Flagellin B1 (FlaB1)



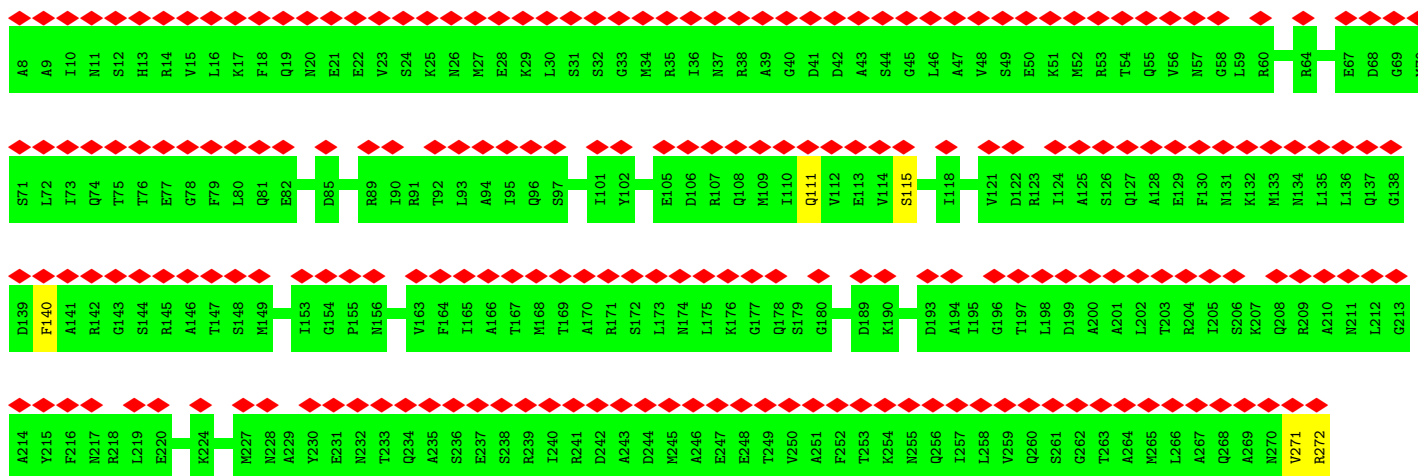
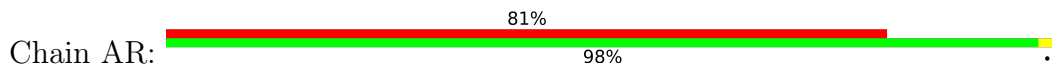
• Molecule 1: Flagellin B1 (FlaB1)



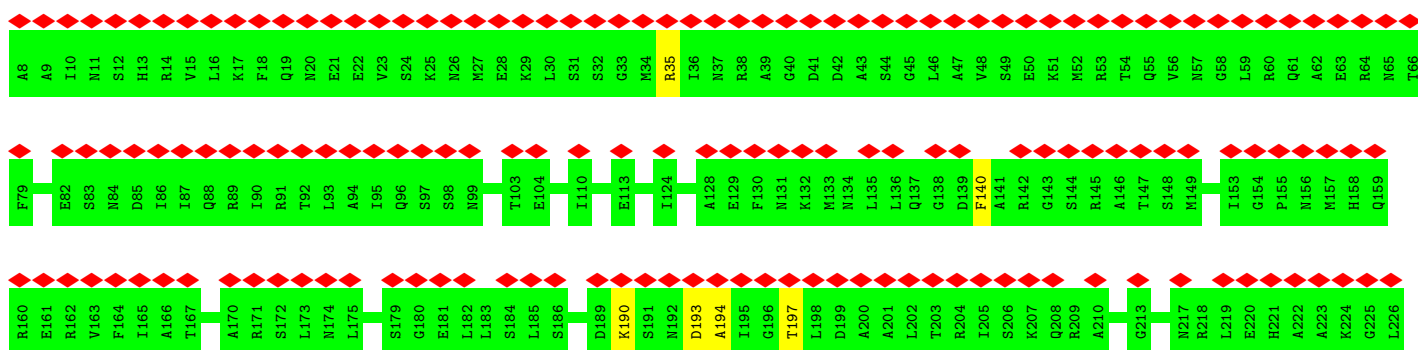
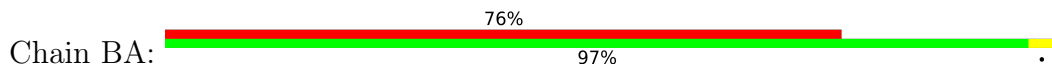
• Molecule 1: Flagellin B1 (FlaB1)

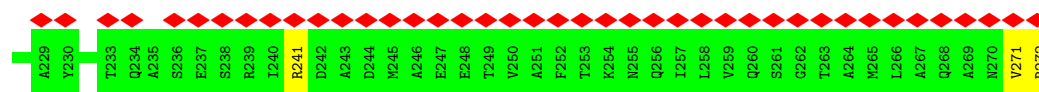


• Molecule 1: Flagellin B1 (FlaB1)

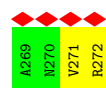
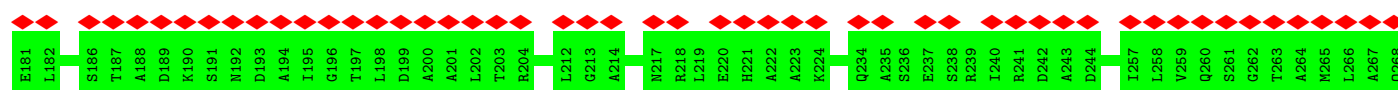
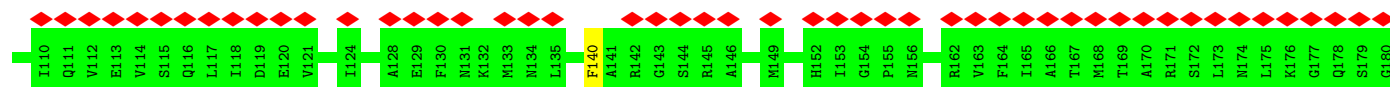
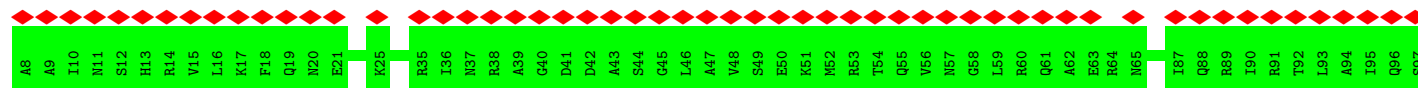


• Molecule 1: Flagellin B1 (FlaB1)

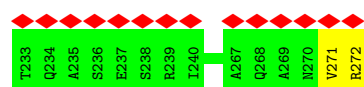
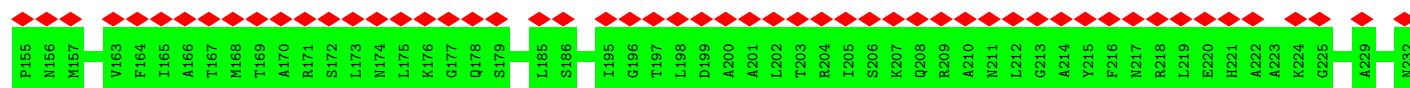
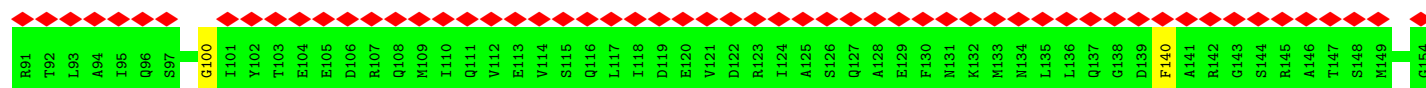
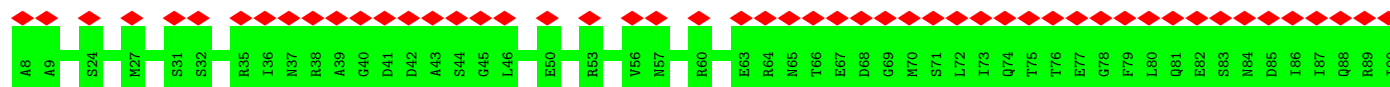




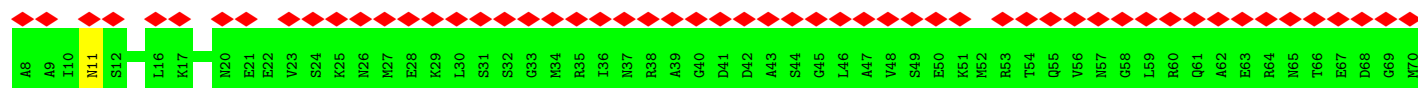
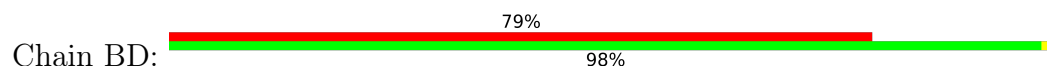
• Molecule 1: Flagellin B1 (FlaB1)

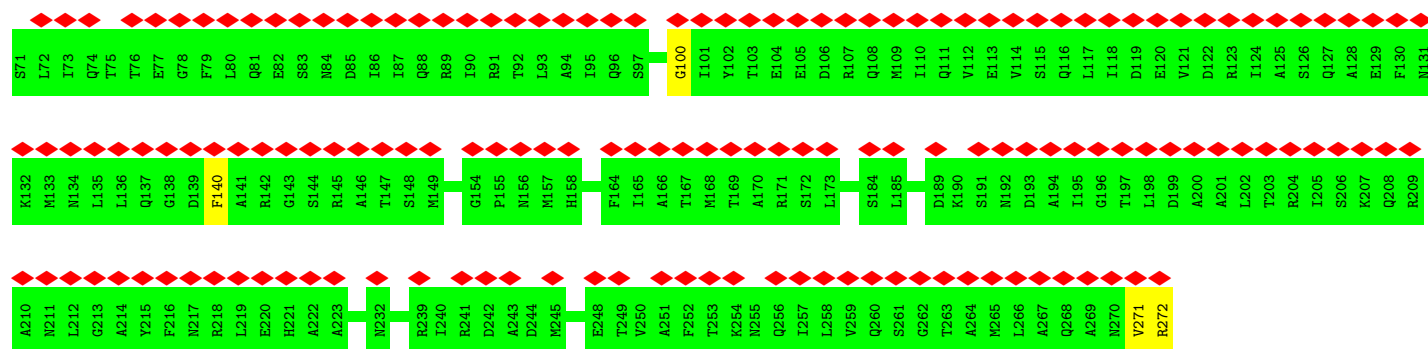


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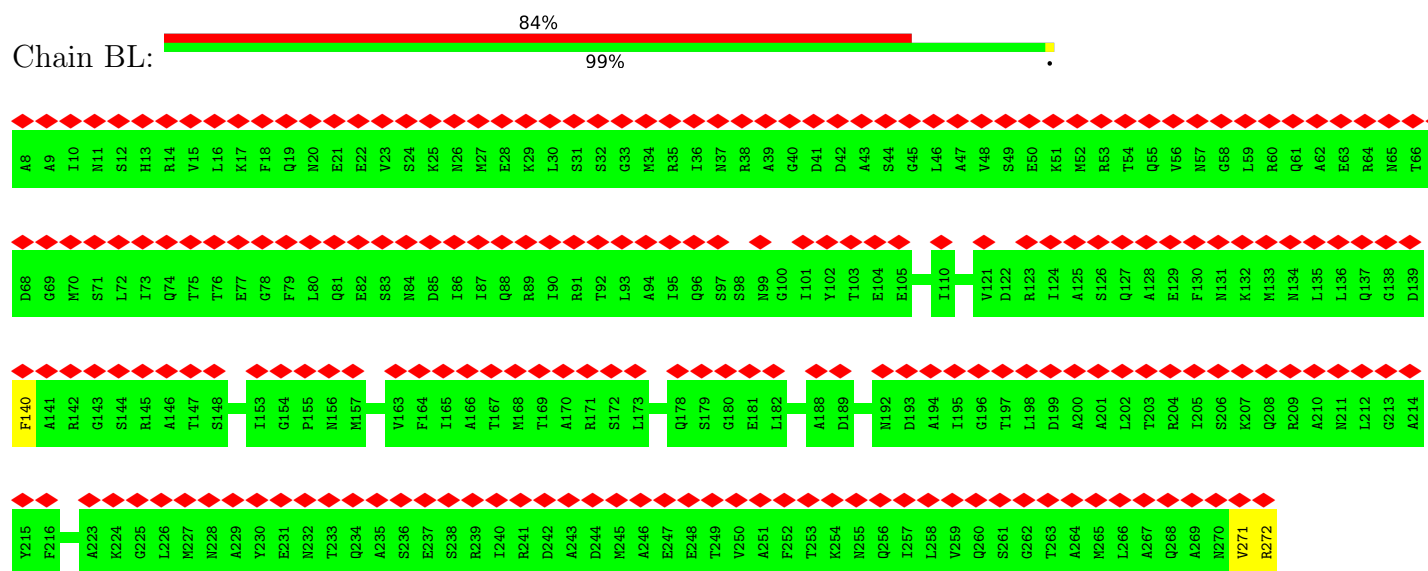


• Molecule 1: Flagellin B1 (FlaB1)

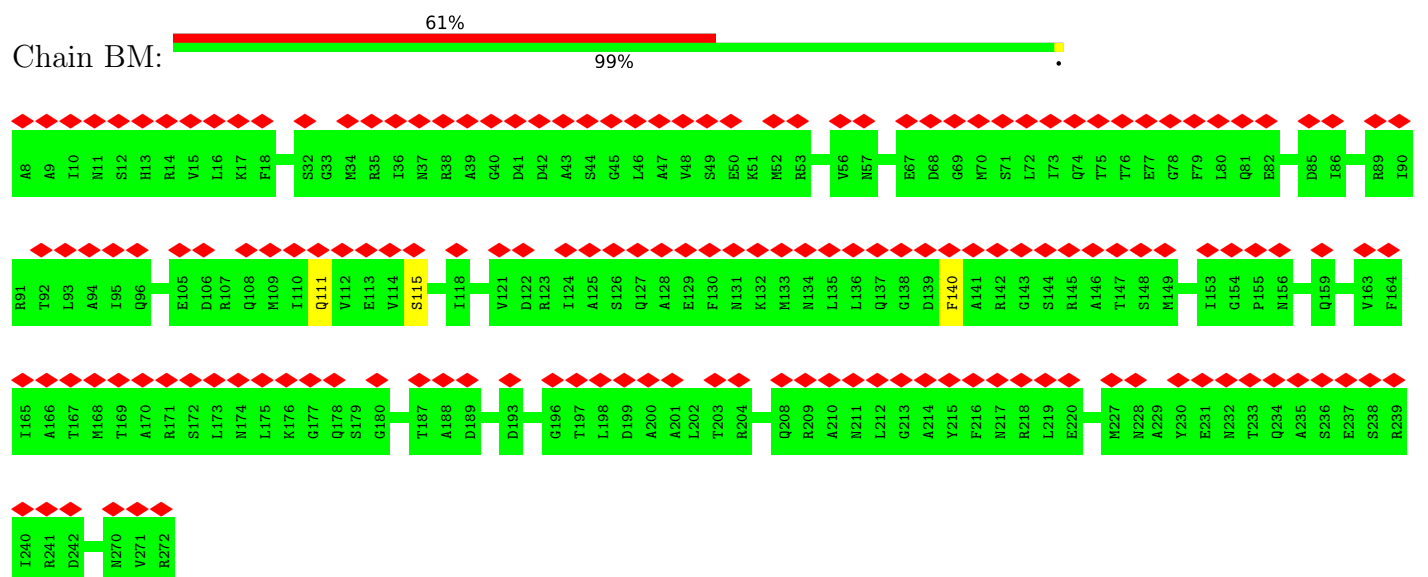




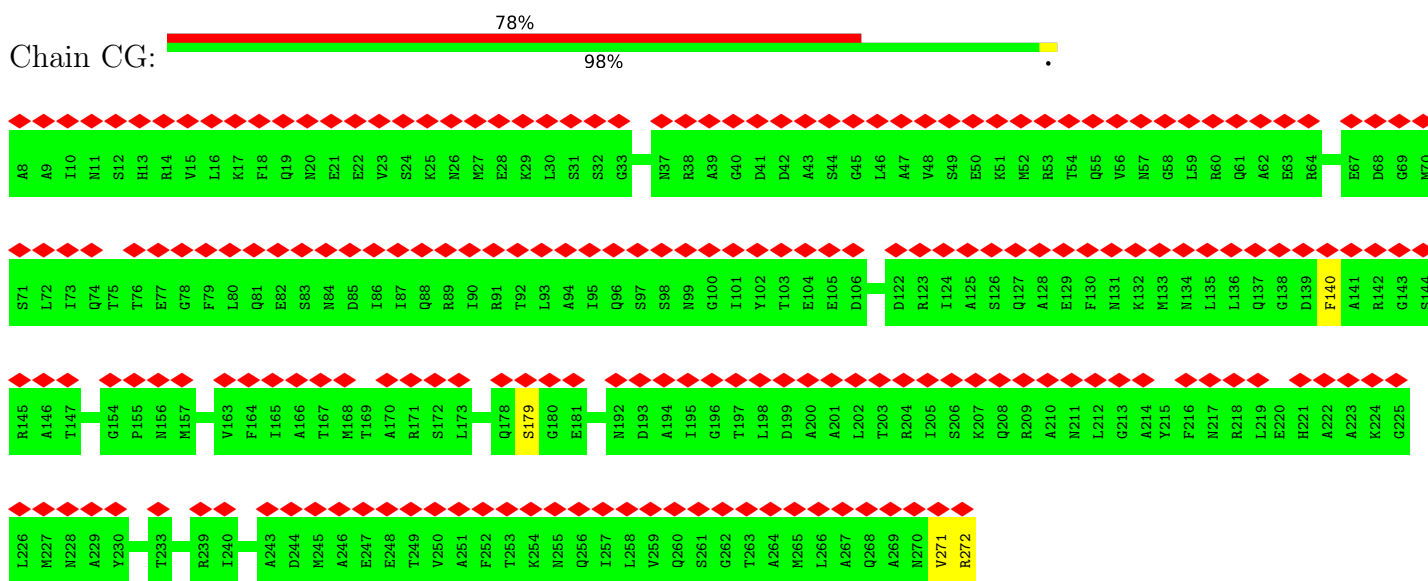
• Molecule 1: Flagellin B1 (FlaB1)



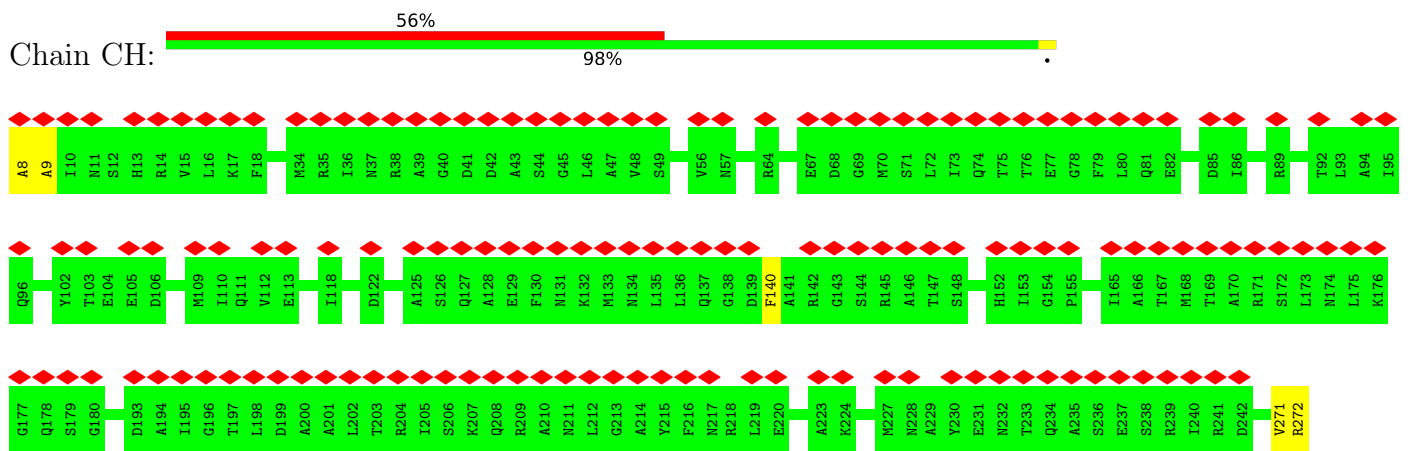
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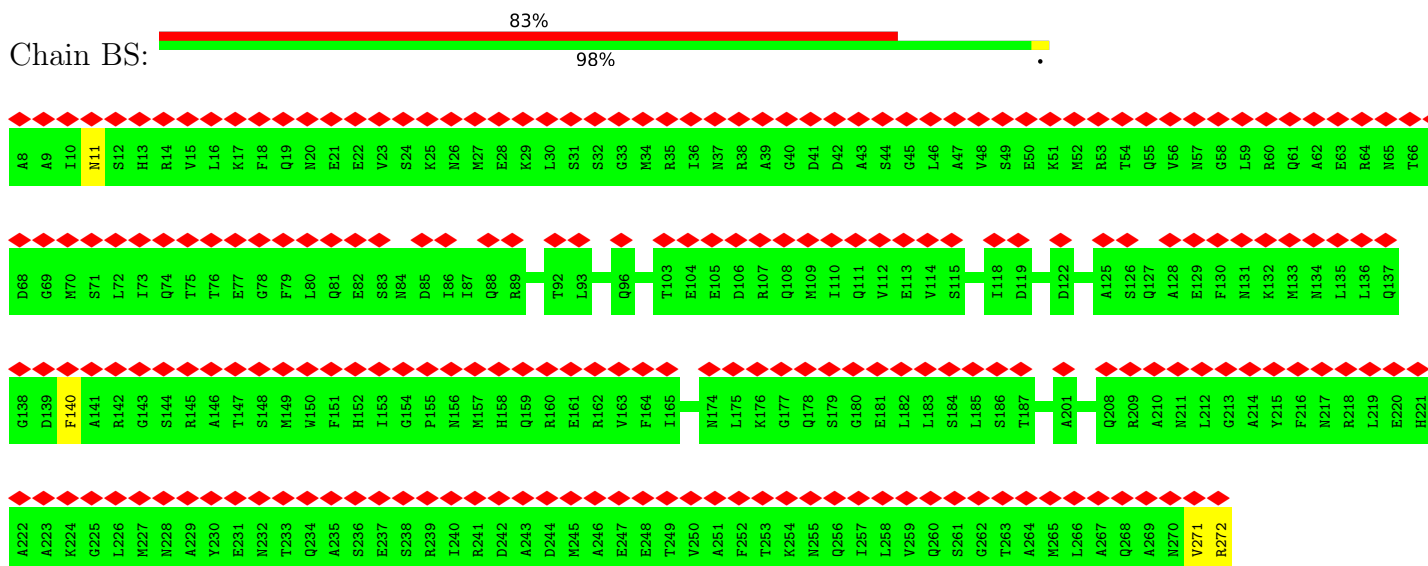
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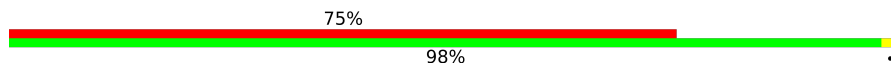


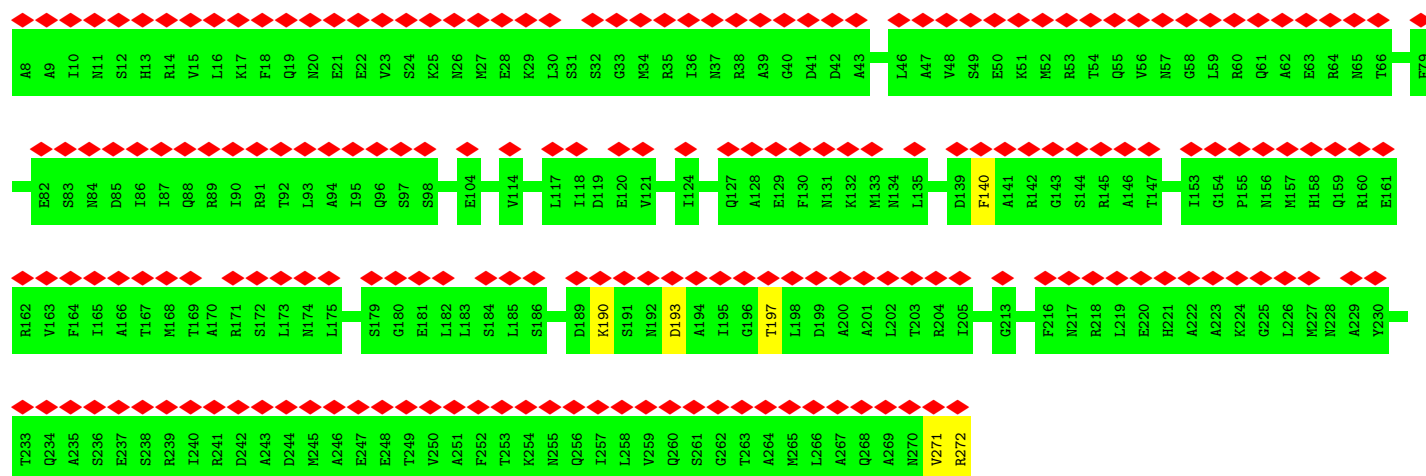
• Molecule 1: Flagellin B1 (FlaB1)



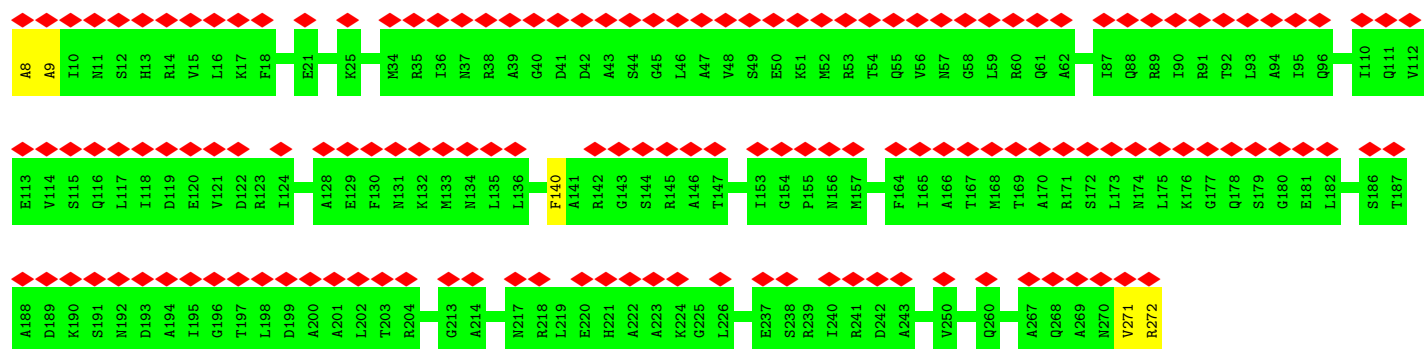
• Molecule 1: Flagellin B1 (FlaB1)







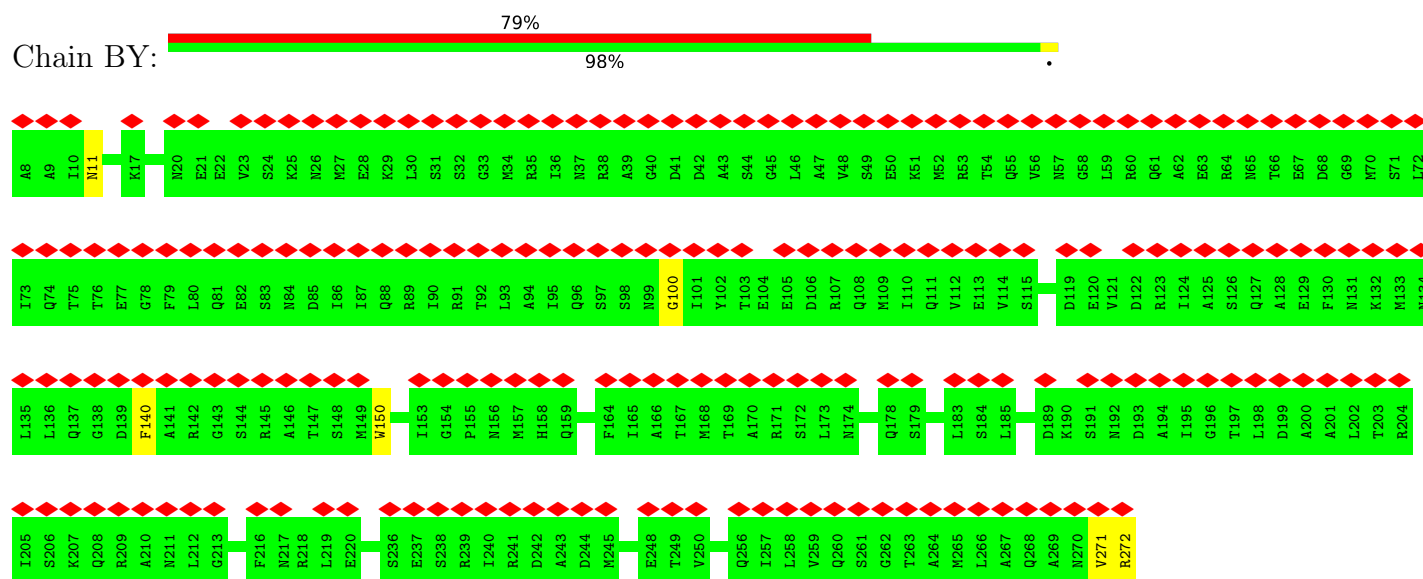
• Molecule 1: Flagellin B1 (FlaB1)



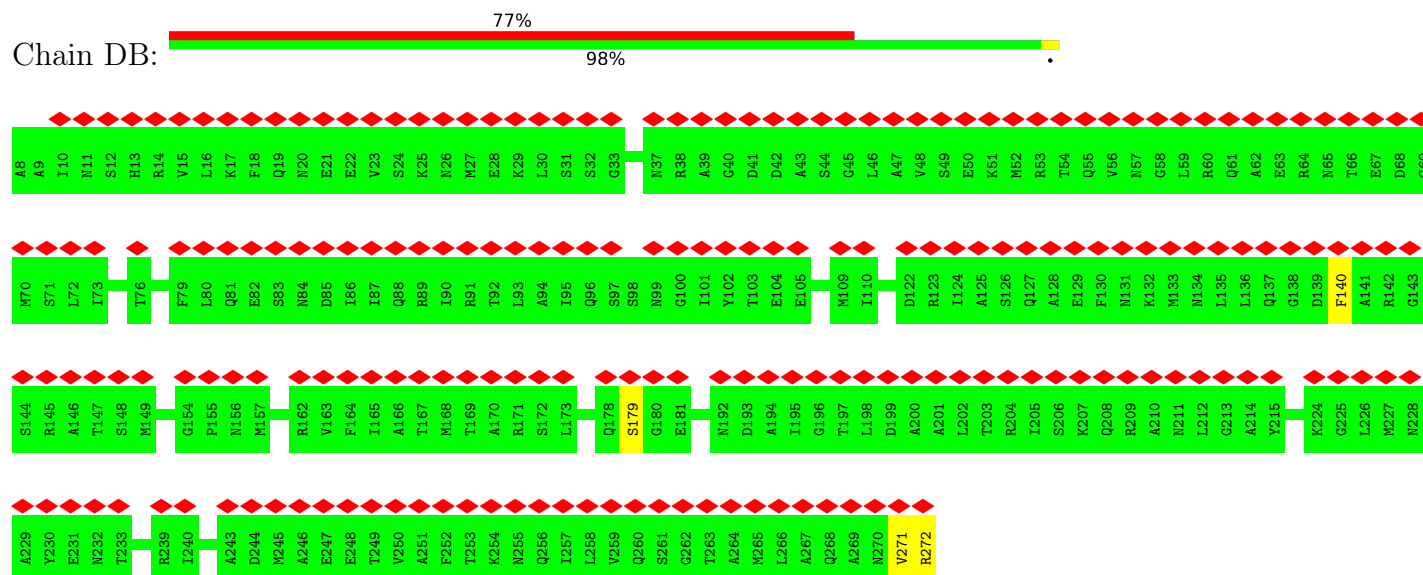
• Molecule 1: Flagellin B1 (FlaB1)



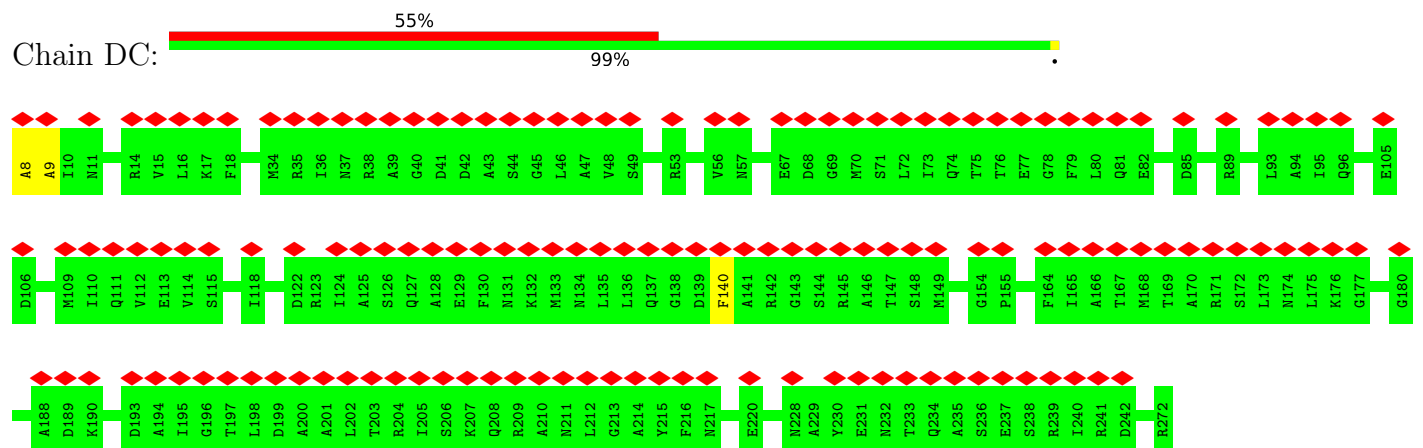
• Molecule 1: Flagellin B1 (FlaB1)



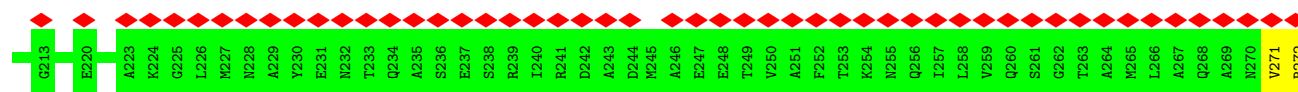
• Molecule 1: Flagellin B1 (FlaB1)



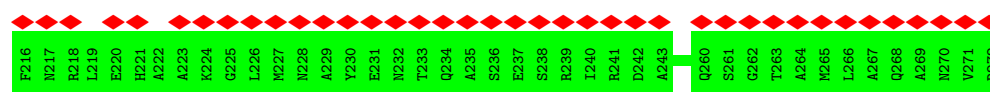
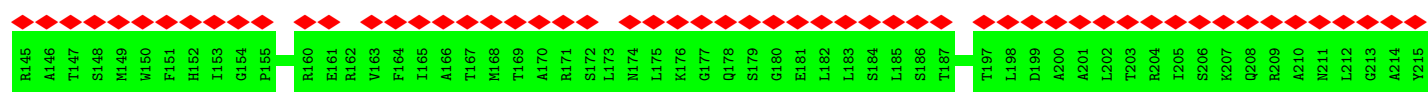
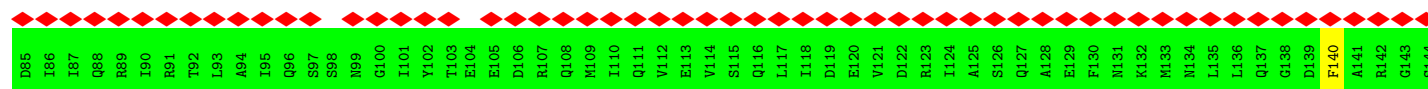
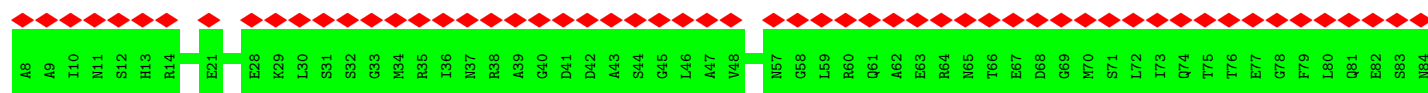
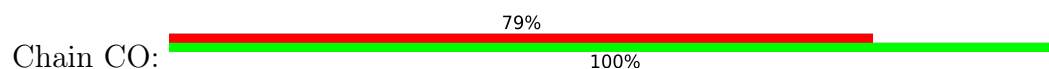
• Molecule 1: Flagellin B1 (FlaB1)



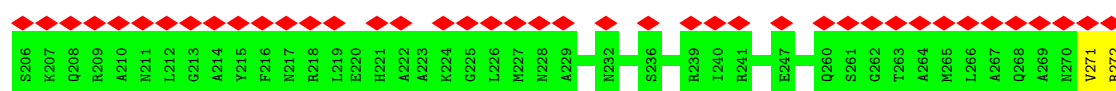
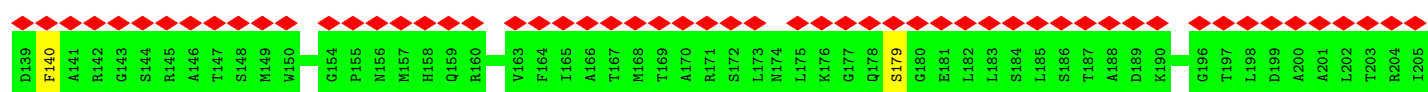
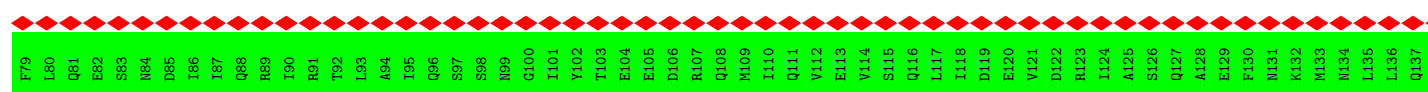
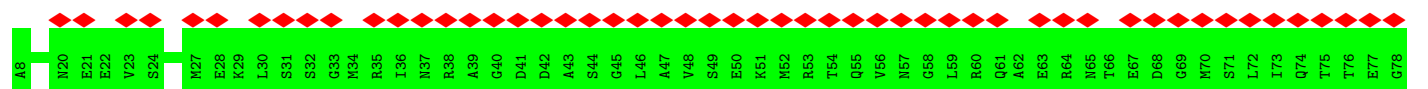
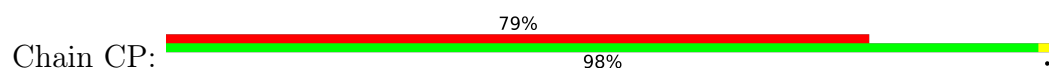
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S71	A9
L72	I10
I73	N11
Q74	S12
T75	H13
T76	R14
E77	V15
G78	L16
F79	K17
L80	F18
Q81	I19
E82	N20
D85	E21
I86	E22
R89	V23
T92	K25
Q96	N26
T103	M27
E104	E28
D106	K29
R107	L30
E113	S31
L117	S32
I118	G33
D119	M34
E120	R35
V121	I36
A128	N37
E129	R38
F130	A39
N131	G40
K132	D41
F140	D42
T169	A43
N174	S44
L175	G45
K176	L46
S179	S49
G180	M52
E181	R53
L182	T54
L183	Q55
S184	V56
L185	N57
S186	G58
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	D68
	G69



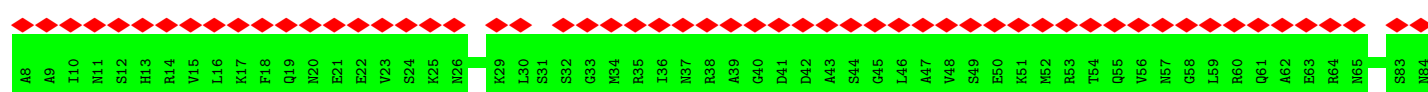
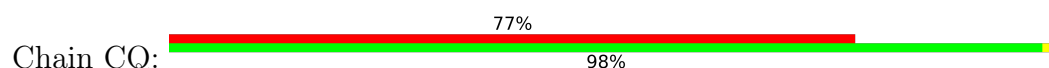
• Molecule 1: Flagellin B1 (FlaB1)

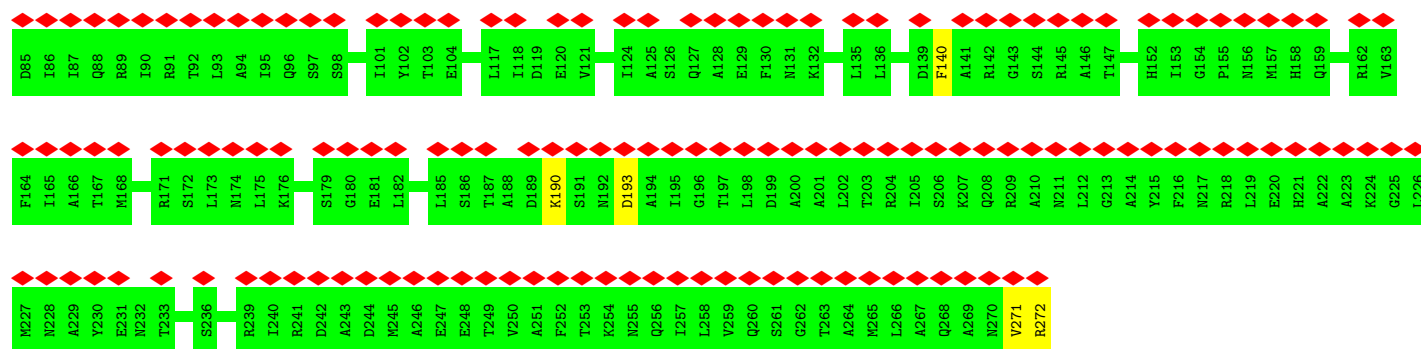


• Molecule 1: Flagellin B1 (FlaB1)

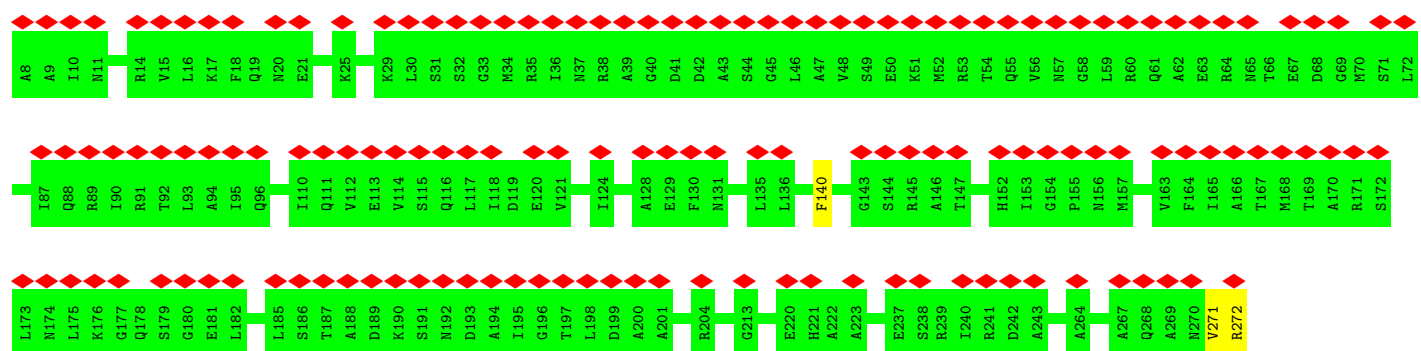


• Molecule 1: Flagellin B1 (FlaB1)

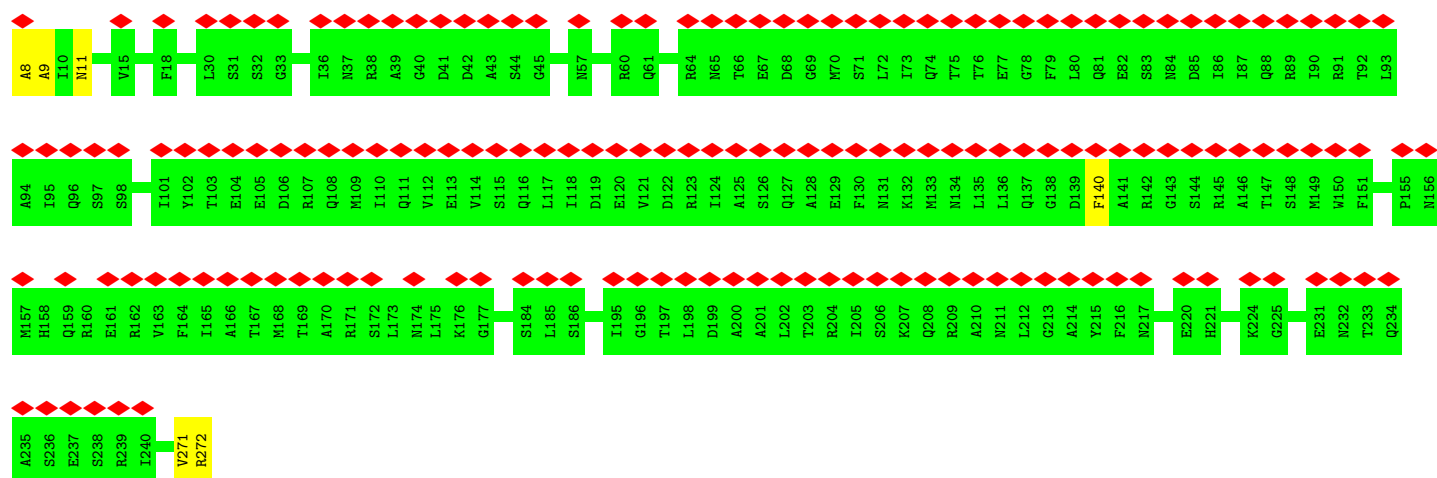




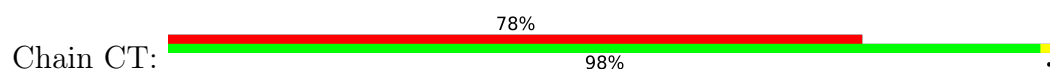
• Molecule 1: Flagellin B1 (FlaB1)

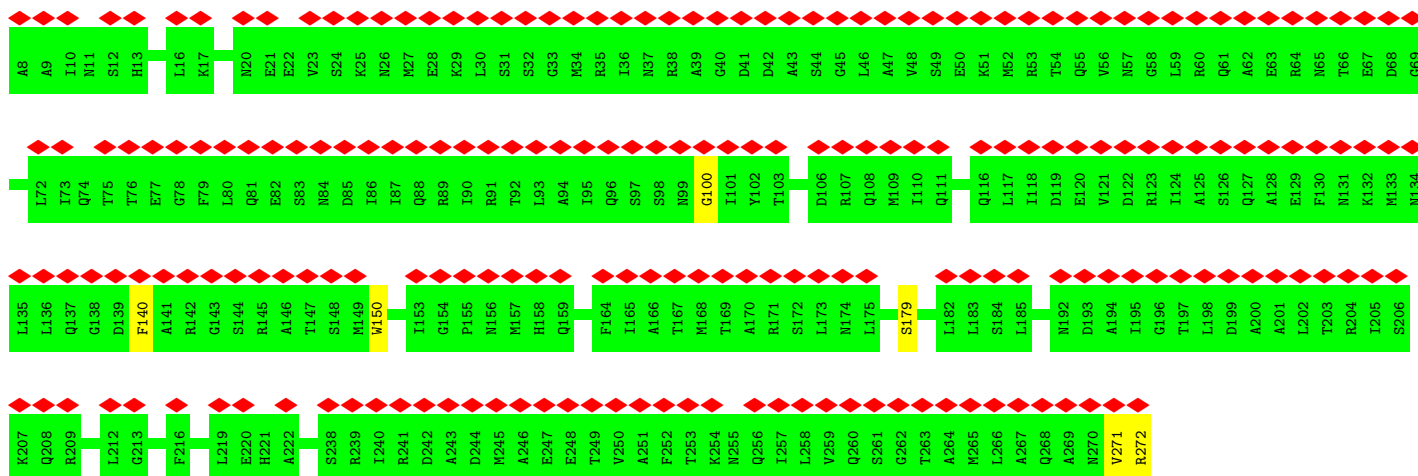


• Molecule 1: Flagellin B1 (FlaB1)

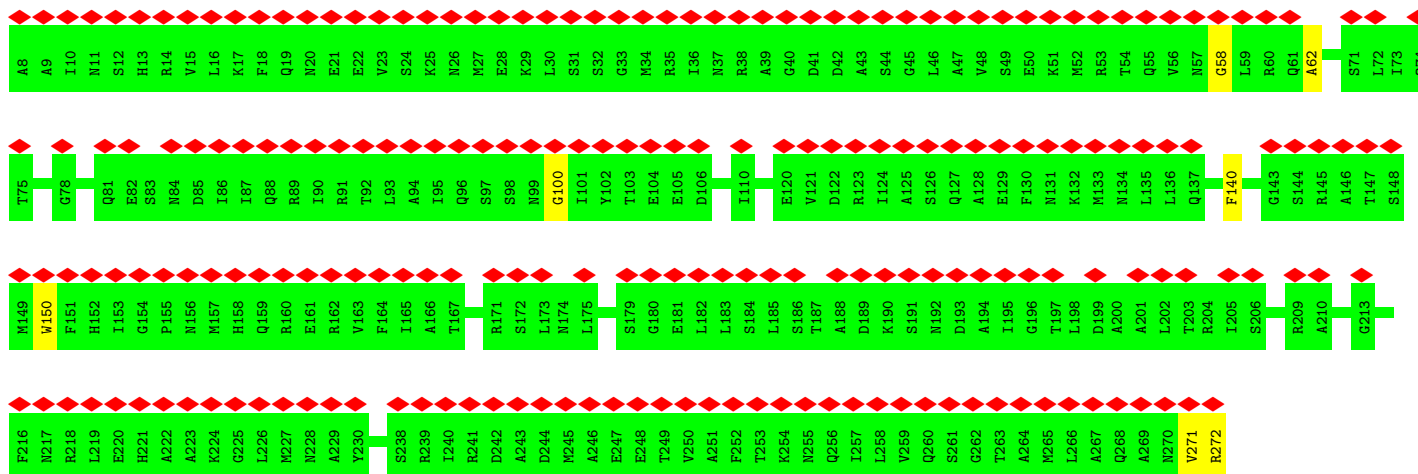
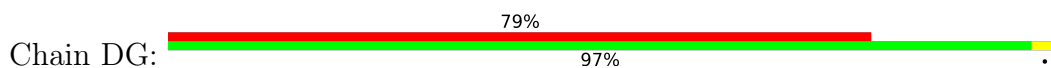


• Molecule 1: Flagellin B1 (FlaB1)

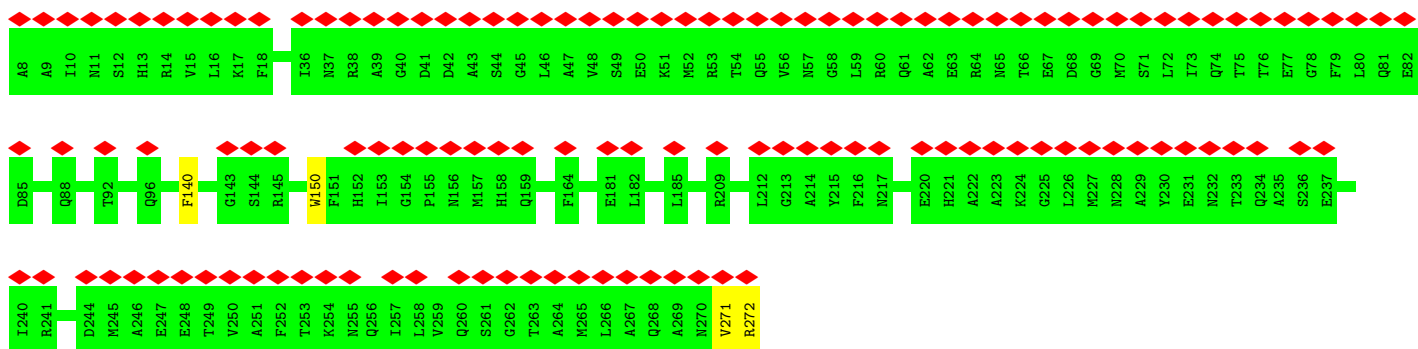




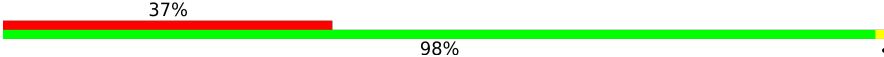
• Molecule 1: Flagellin B1 (FlaB1)

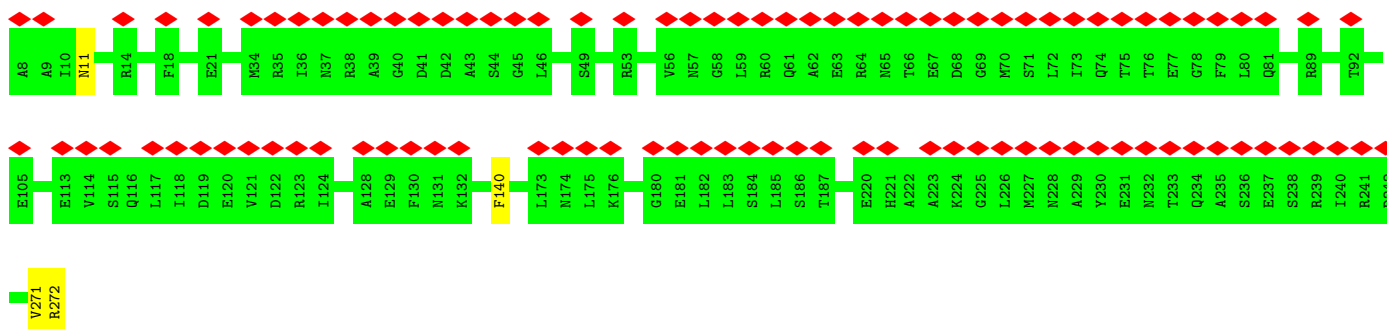


• Molecule 1: Flagellin B1 (FlaB1)

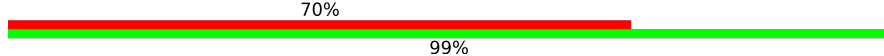


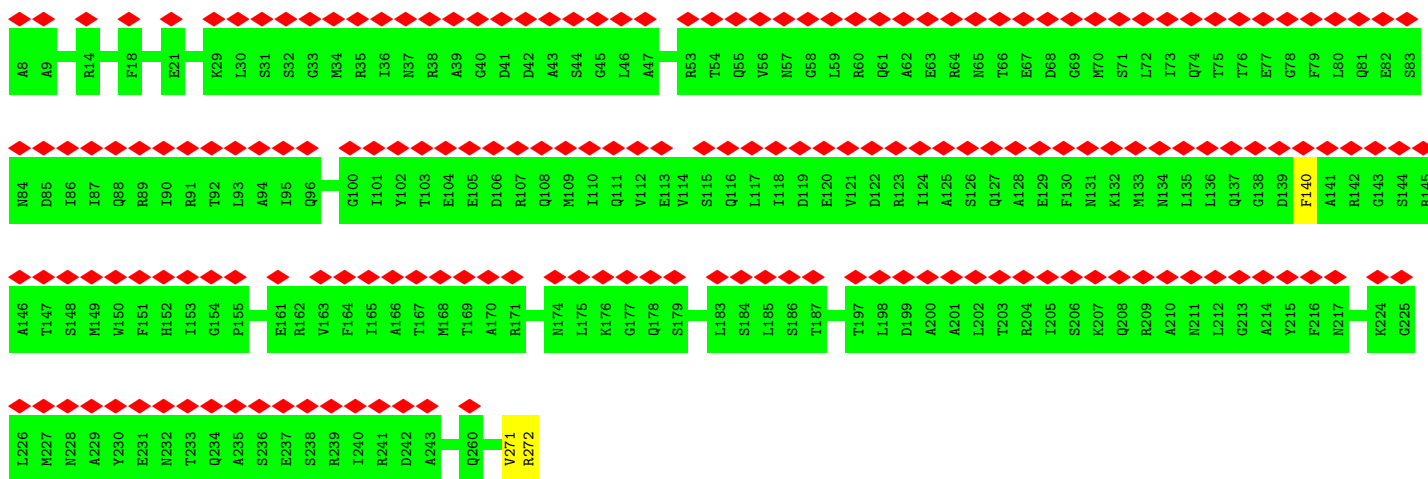
• Molecule 1: Flagellin B1 (FlaB1)

Chain DI:  37% 98%

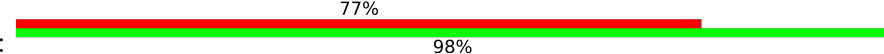


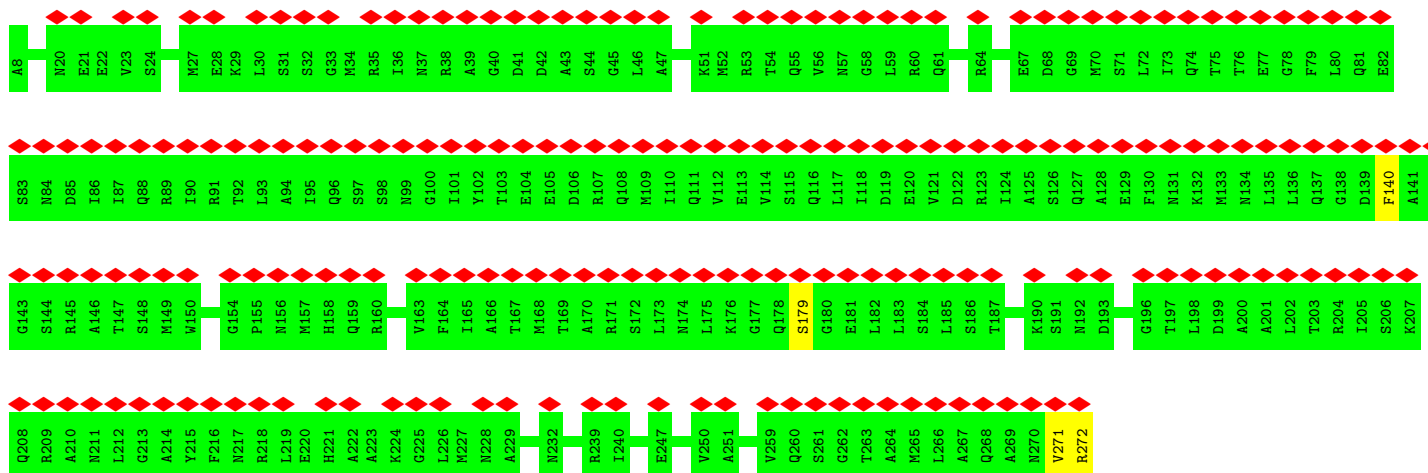
• Molecule 1: Flagellin B1 (FlaB1)

Chain DJ:  70% 99%

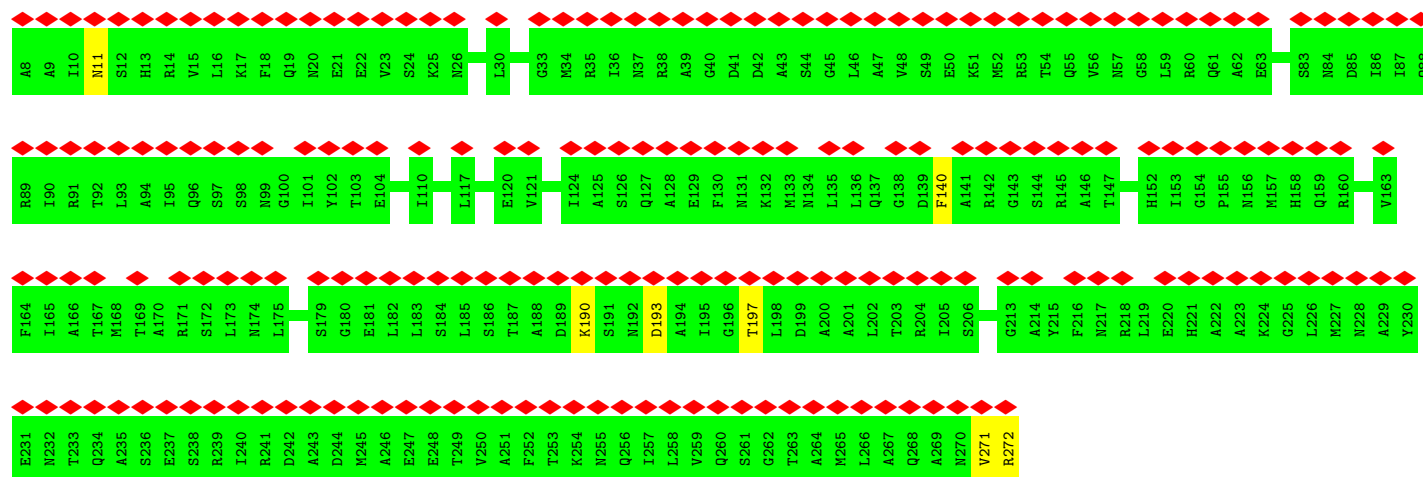
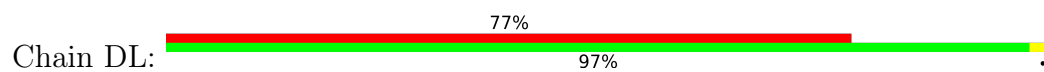


• Molecule 1: Flagellin B1 (FlaB1)

Chain DK:  77% 98%



• Molecule 1: Flagellin B1 (FlaB1)



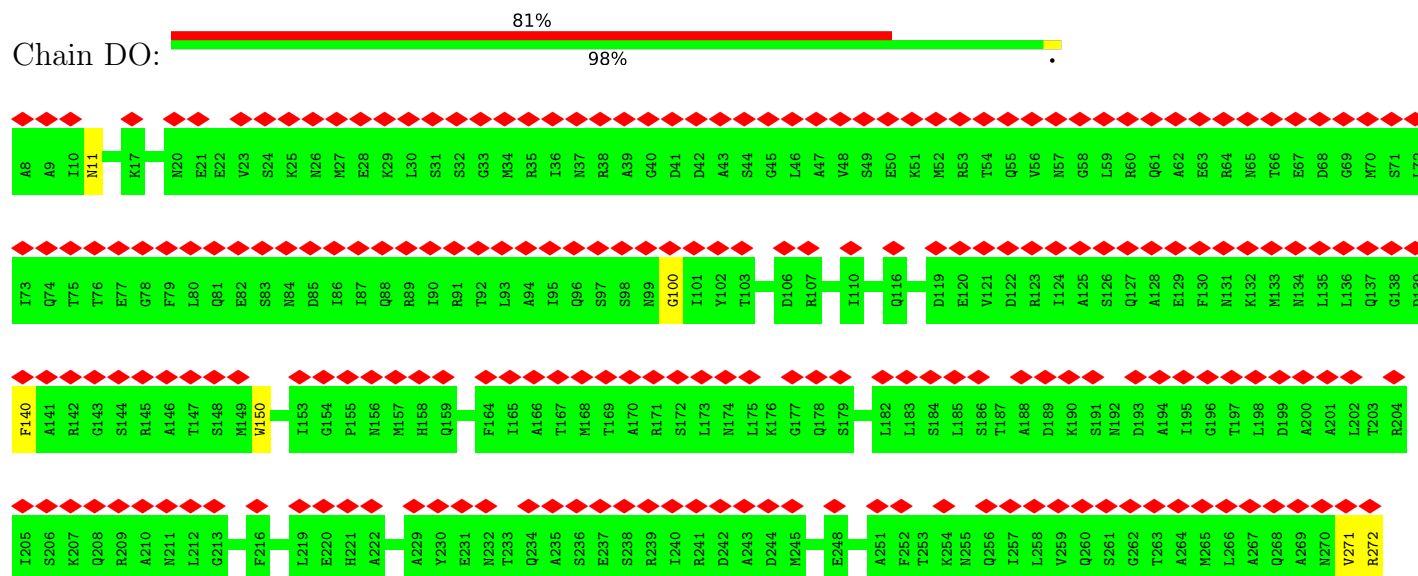
• Molecule 1: Flagellin B1 (FlaB1)



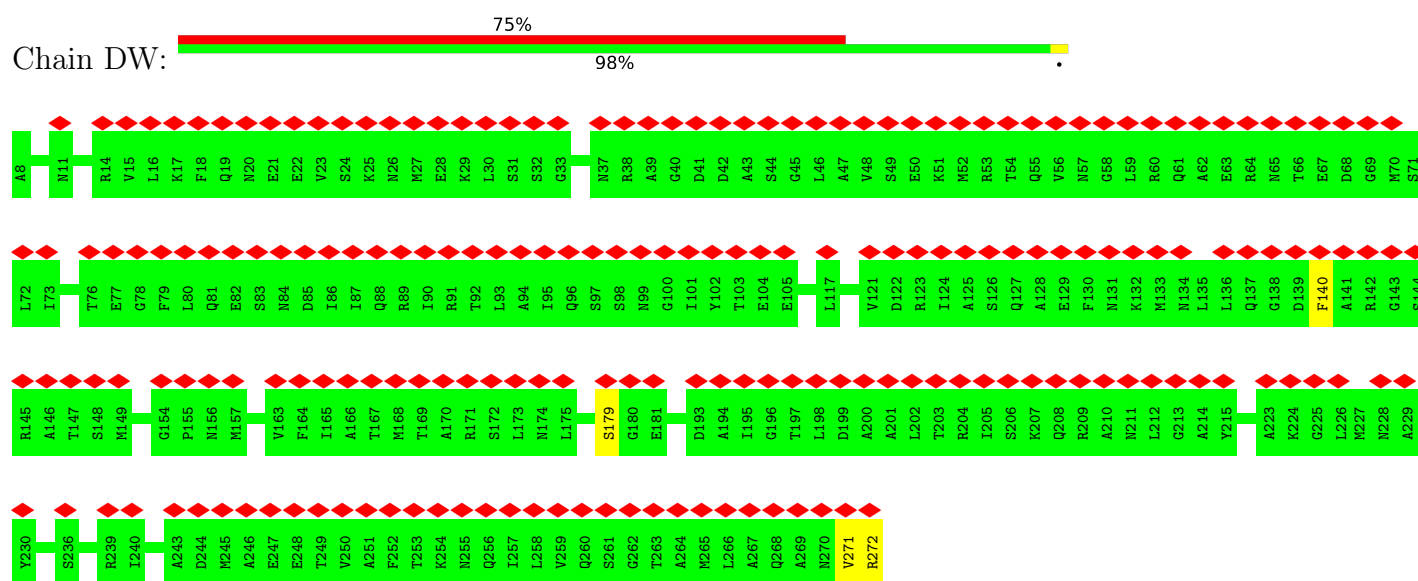
• Molecule 1: Flagellin B1 (FlaB1)



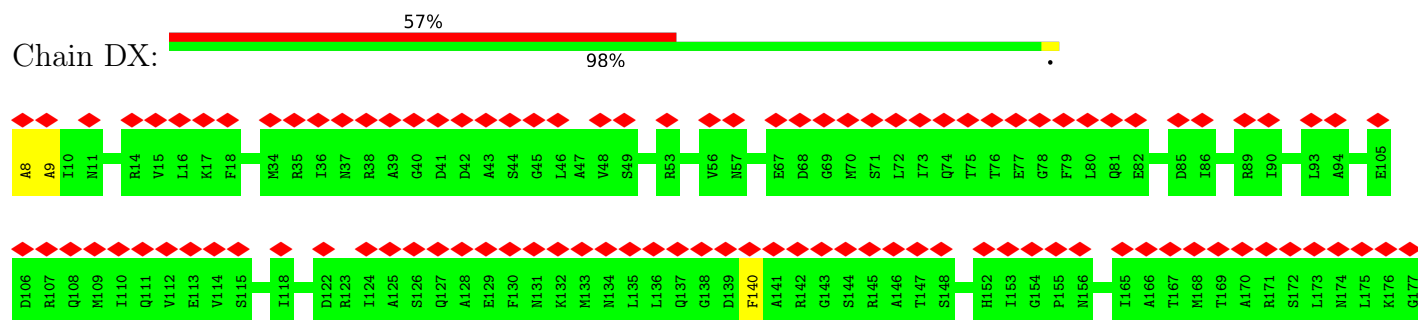
- Molecule 1: Flagellin B1 (FlaB1)

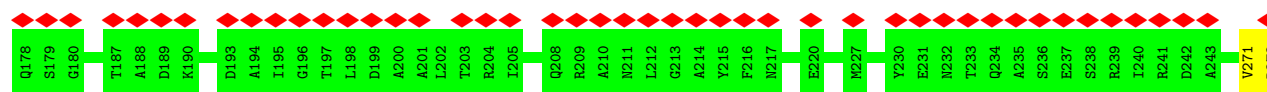


- Molecule 1: Flagellin B1 (FlaB1)



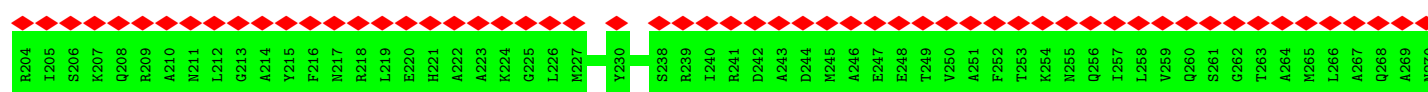
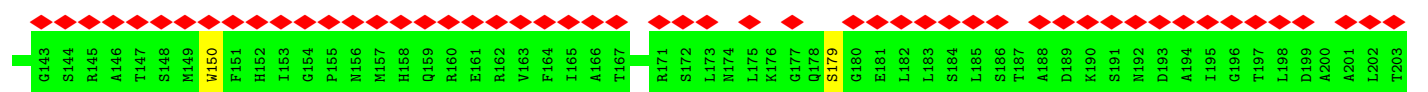
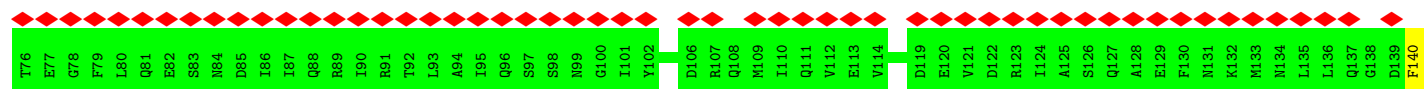
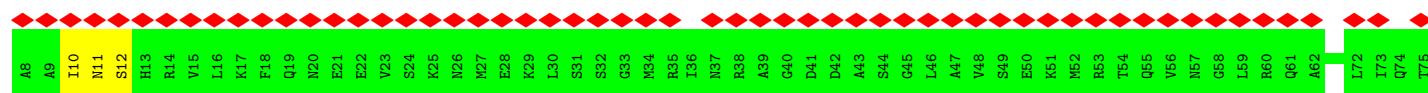
- Molecule 1: Flagellin B1 (FlaB1)





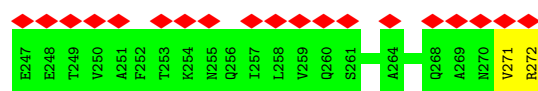
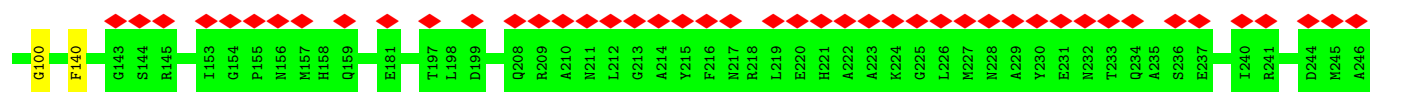
• Molecule 1: Flagellin B1 (FlaB1)

Chain EB: 85% 97%



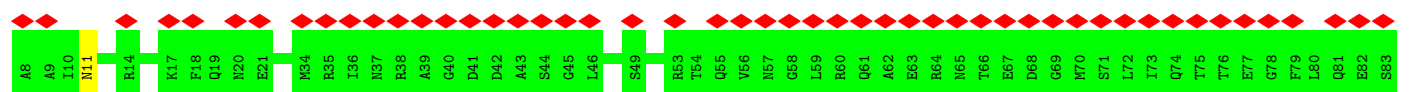
• Molecule 1: Flagellin B1 (FlaB1)

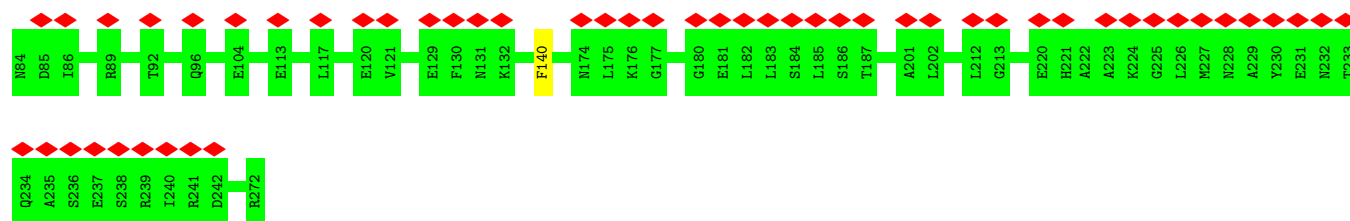
Chain EC: 45% 98%



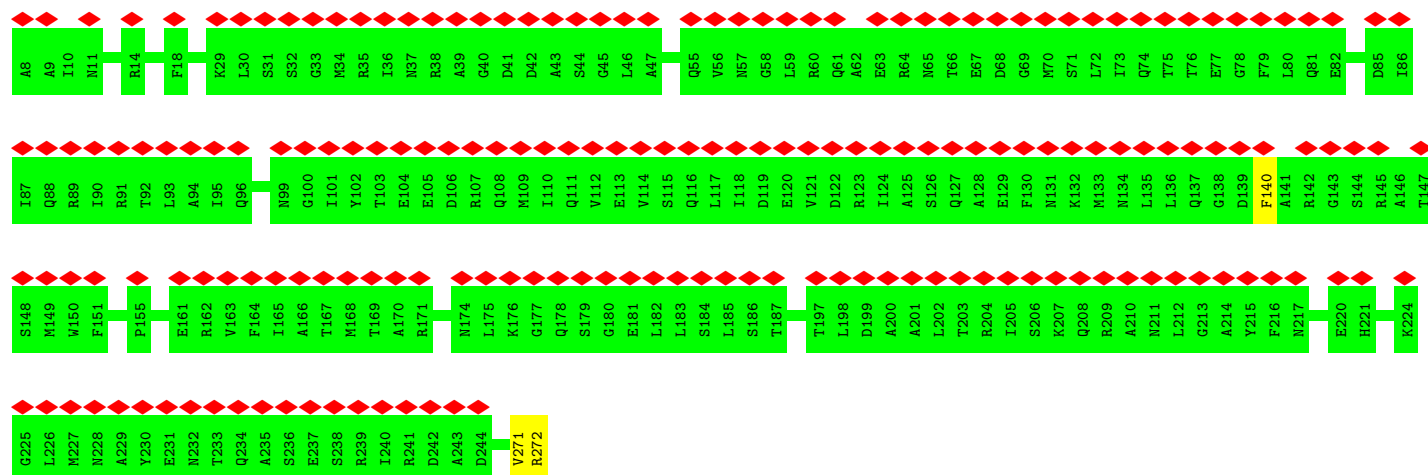
• Molecule 1: Flagellin B1 (FlaB1)

Chain ED: 38% 99%

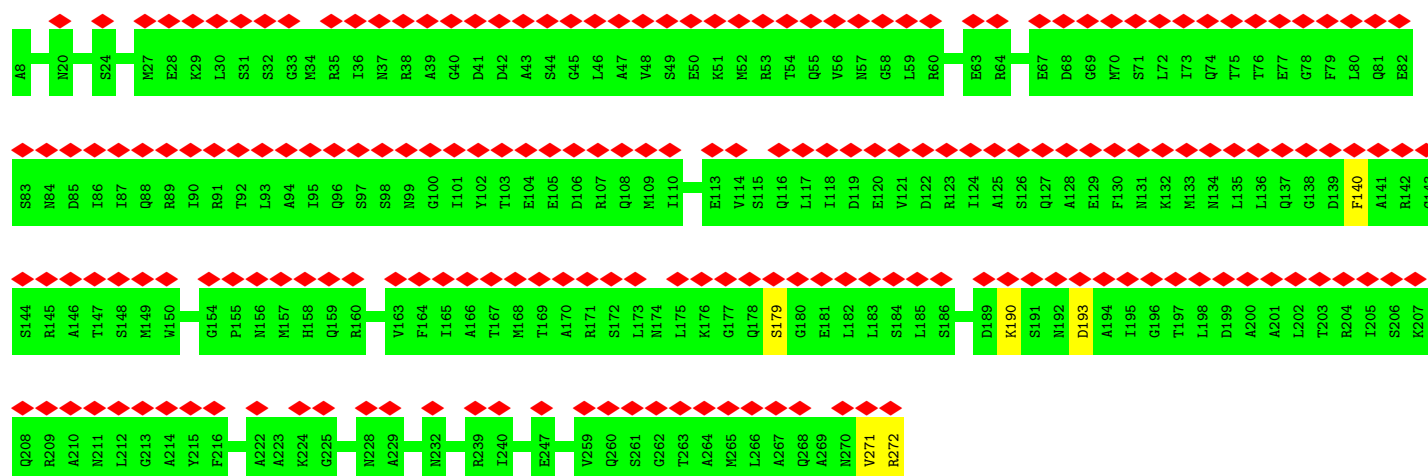
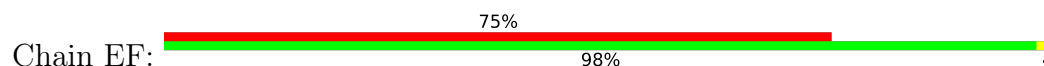




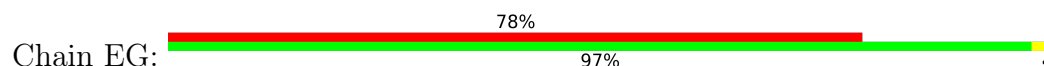
• Molecule 1: Flagellin B1 (FlaB1)

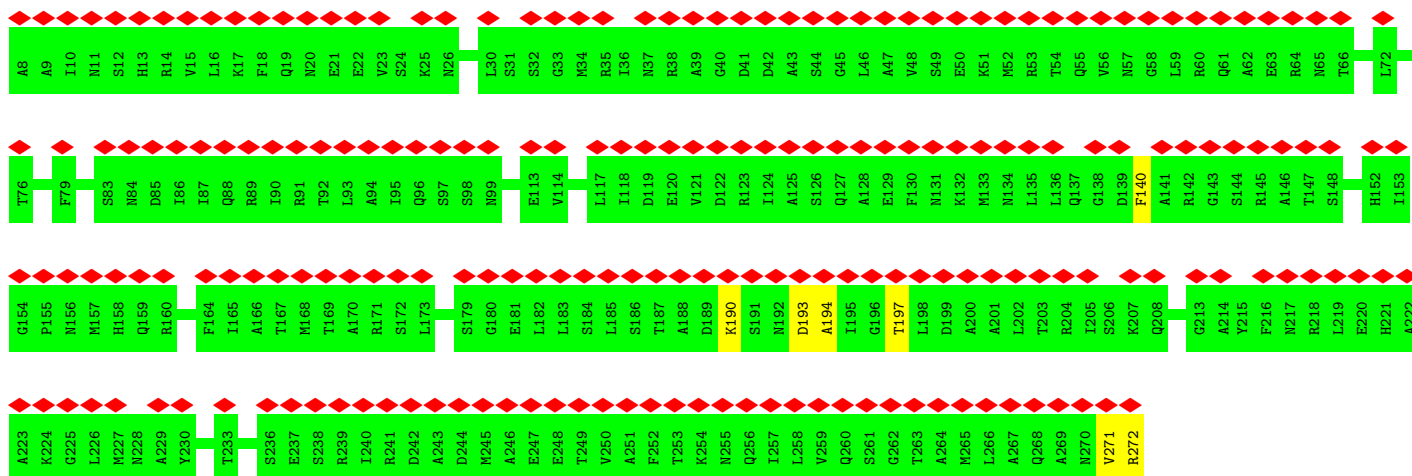


• Molecule 1: Flagellin B1 (FlaB1)

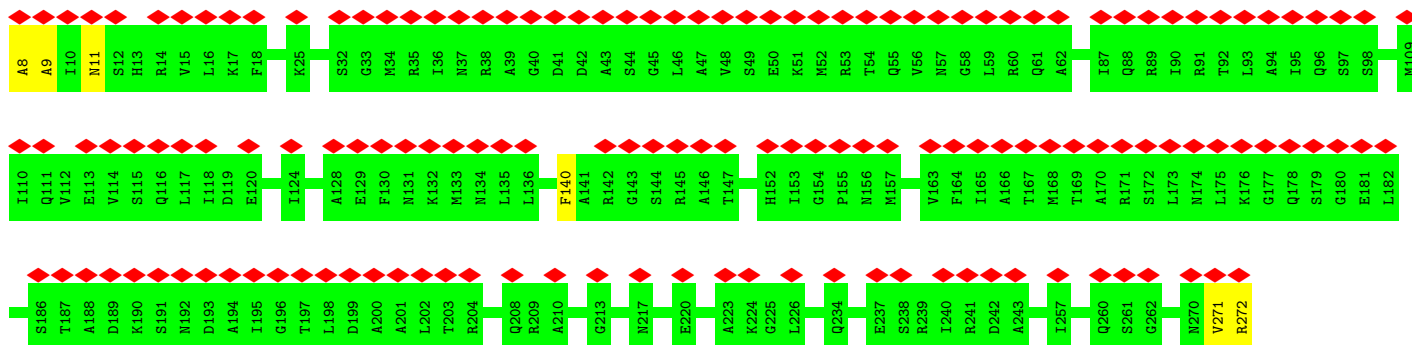


• Molecule 1: Flagellin B1 (FlaB1)

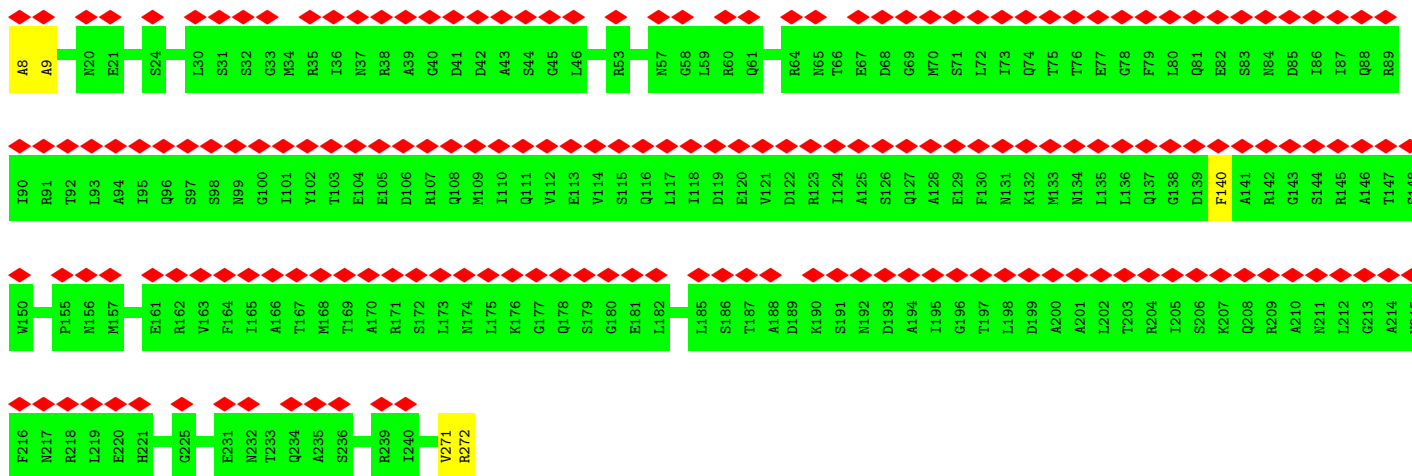




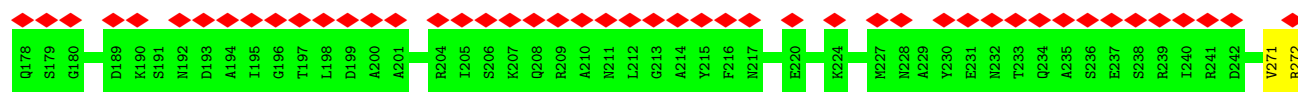
• Molecule 1: Flagellin B1 (FlaB1)



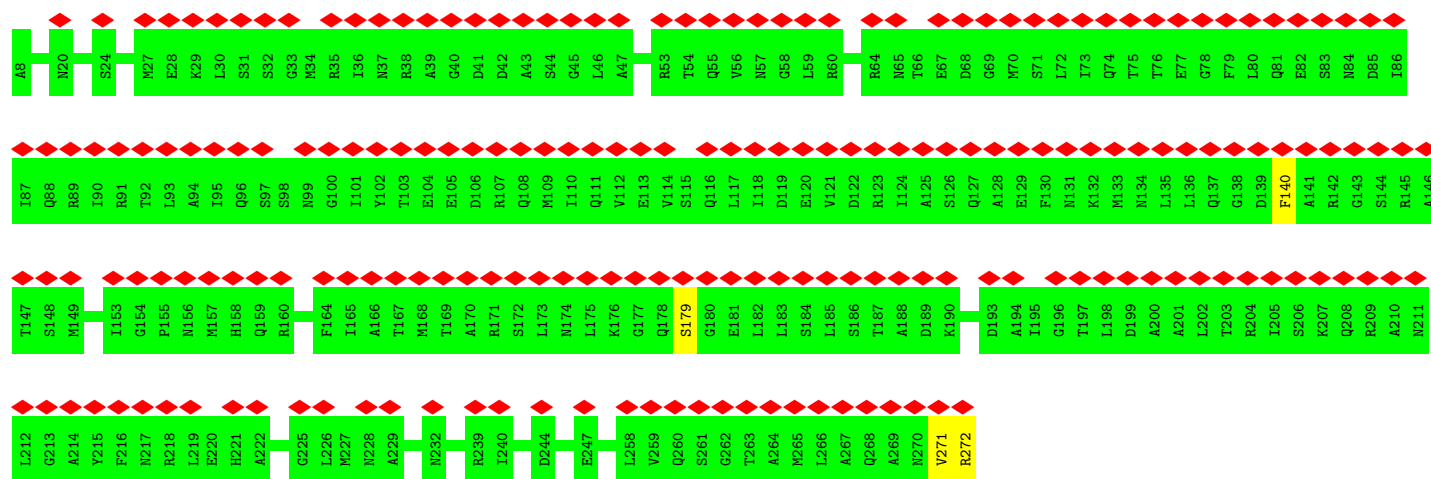
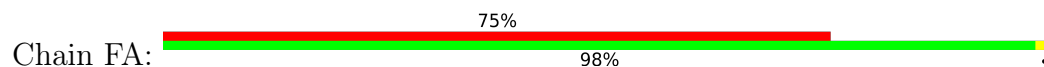
• Molecule 1: Flagellin B1 (FlaB1)



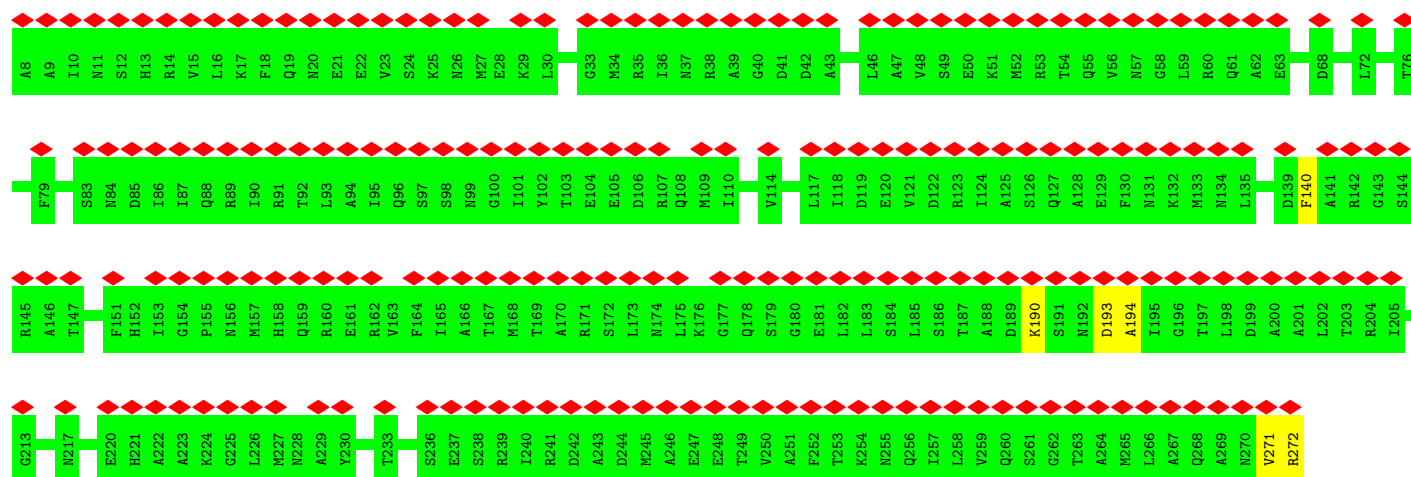




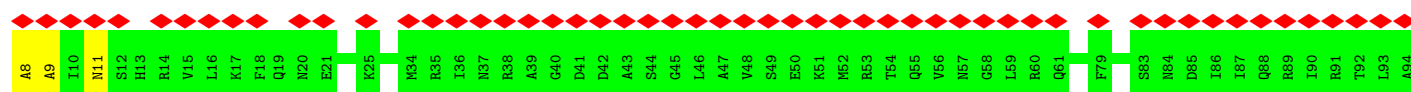
• Molecule 1: Flagellin B1 (FlaB1)

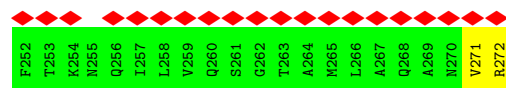


• Molecule 1: Flagellin B1 (FlaB1)

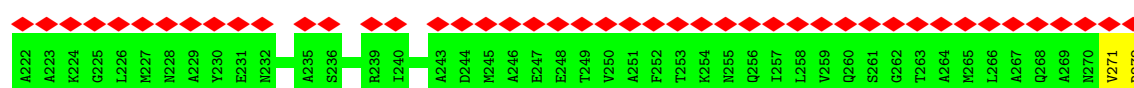
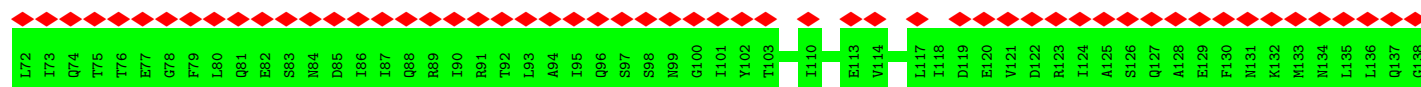
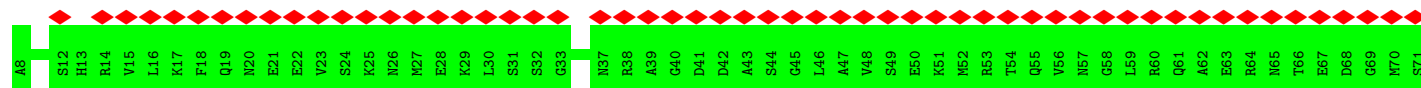
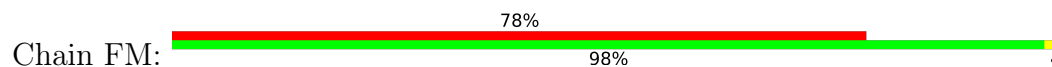


• Molecule 1: Flagellin B1 (FlaB1)

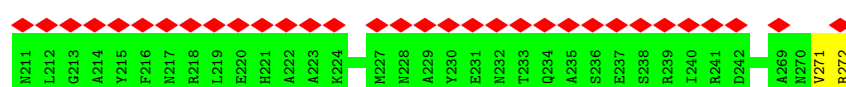
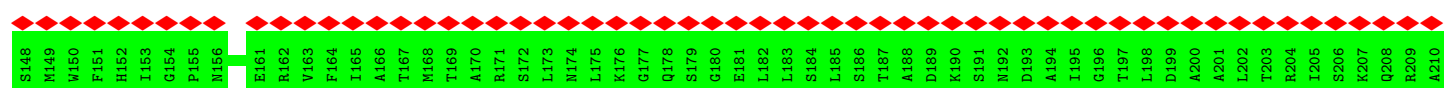
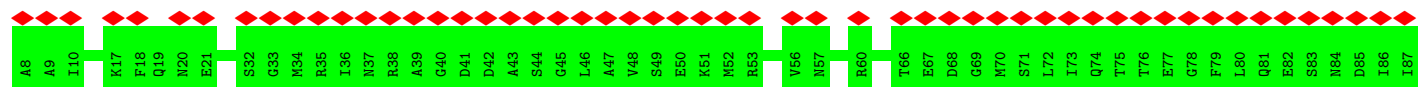
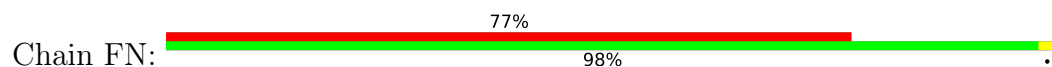




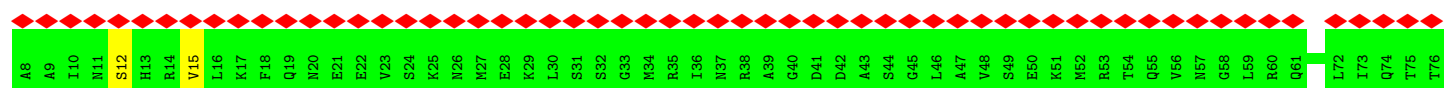
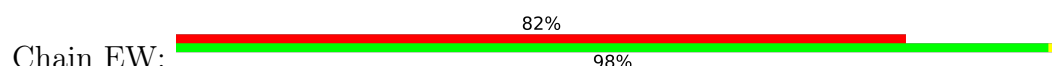
• Molecule 1: Flagellin B1 (FlaB1)

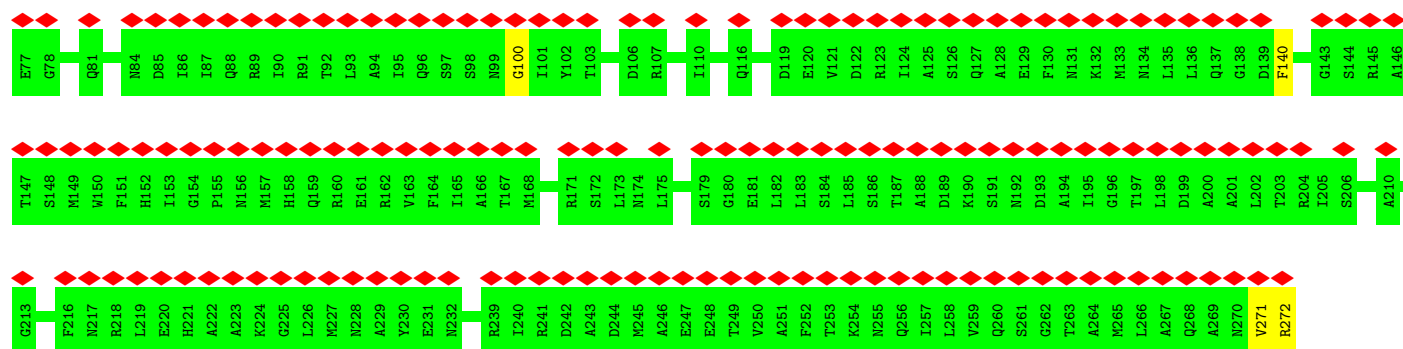


• Molecule 1: Flagellin B1 (FlaB1)



• Molecule 1: Flagellin B1 (FlaB1)





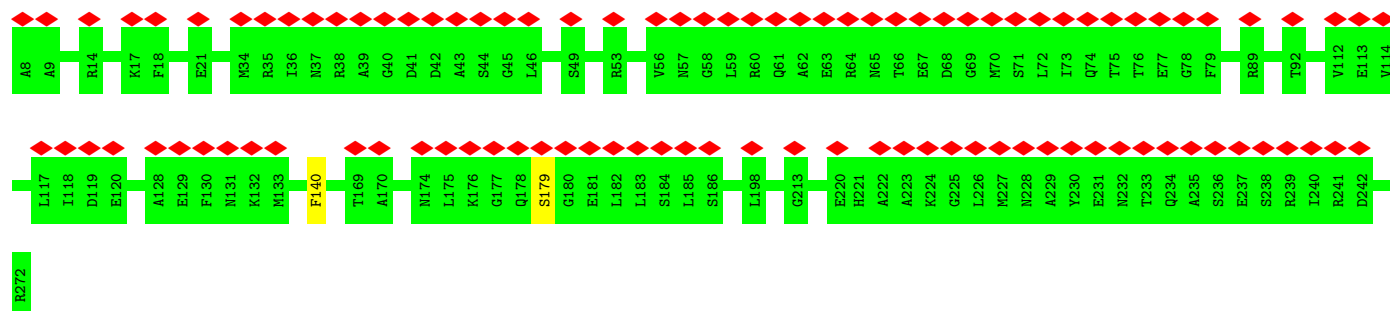
• Molecule 1: Flagellin B1 (FlaB1)

Chain EX: 43% 98%



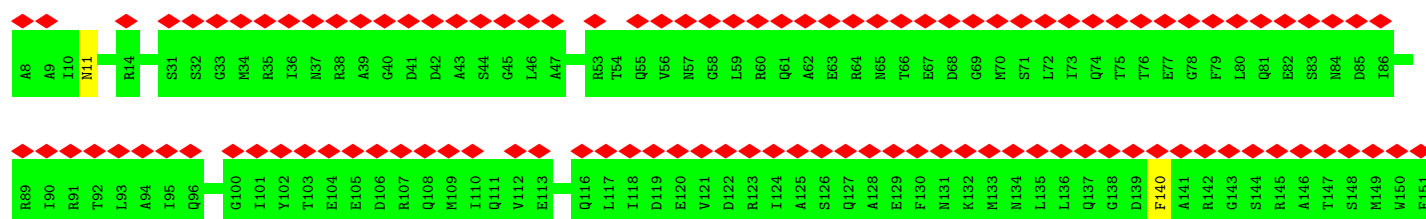
• Molecule 1: Flagellin B1 (FlaB1)

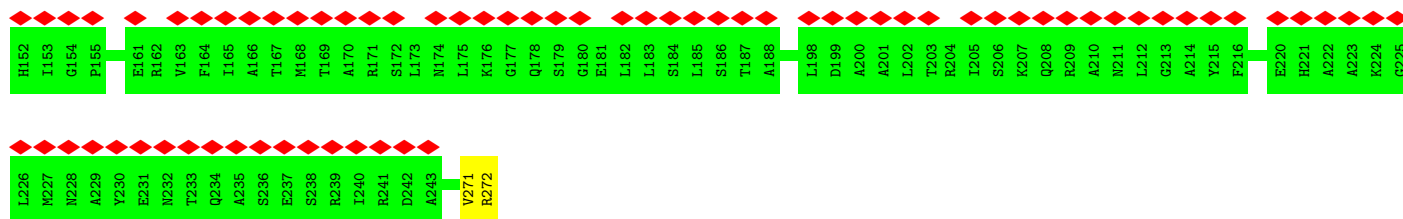
Chain EY: 37% 99%



• Molecule 1: Flagellin B1 (FlaB1)

Chain EZ: 68% 98%

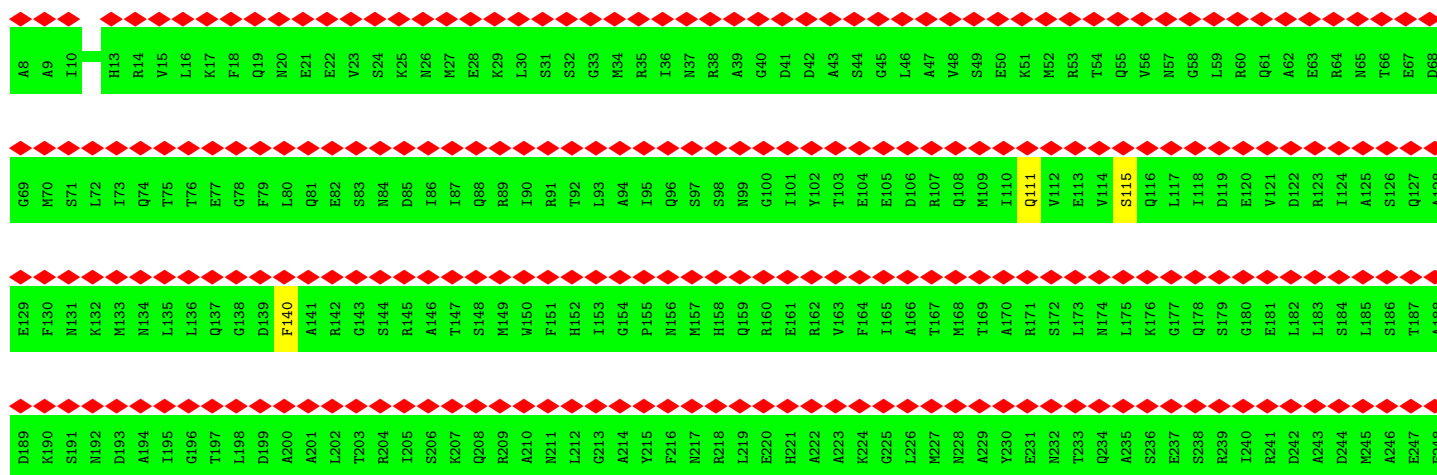


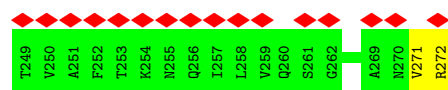


• Molecule 1: Flagellin B1 (FlaB1)

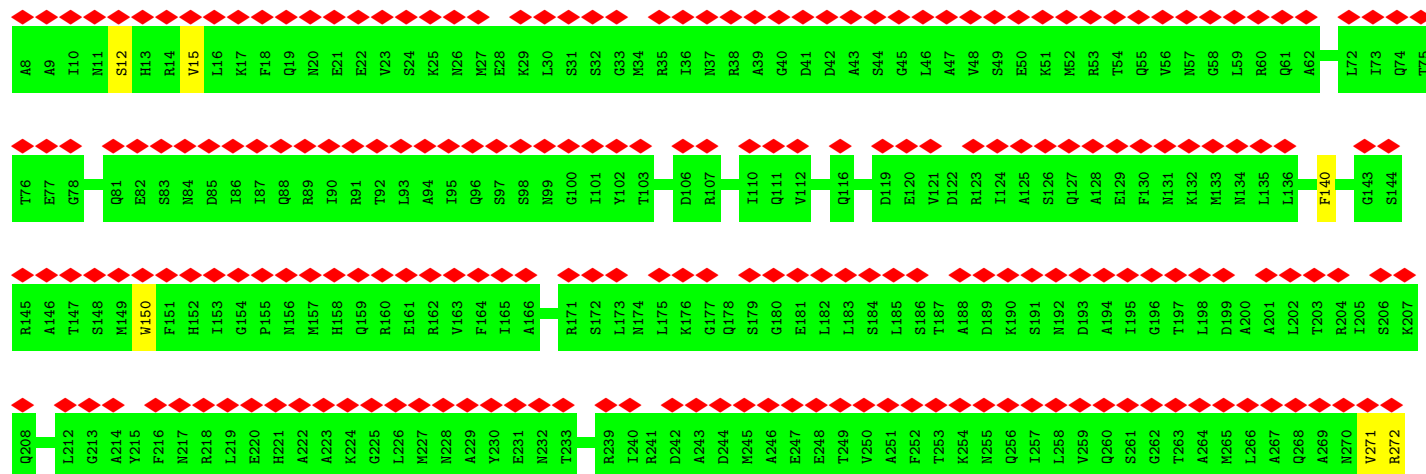
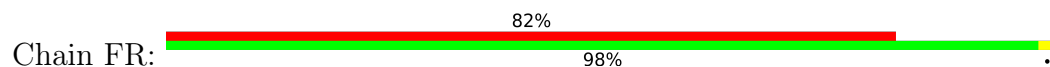


• Molecule 1: Flagellin B1 (FlaB1)

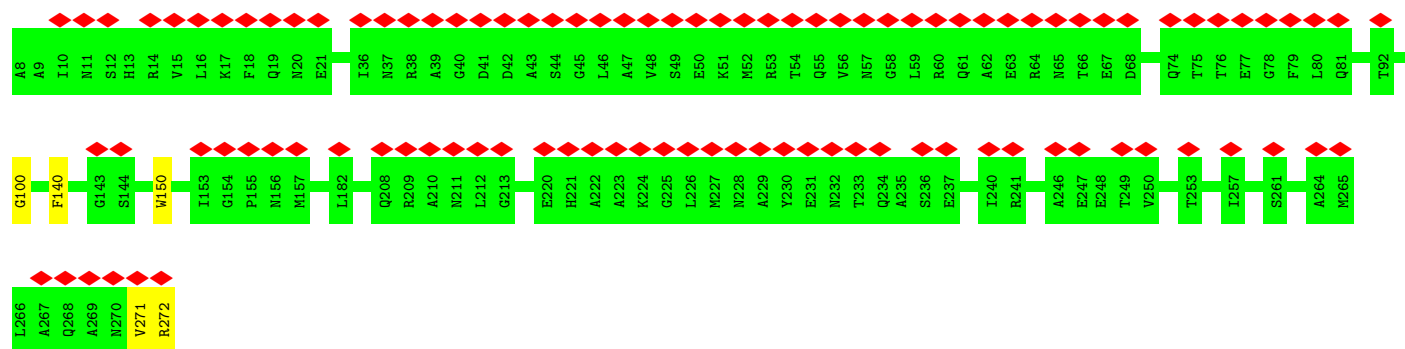
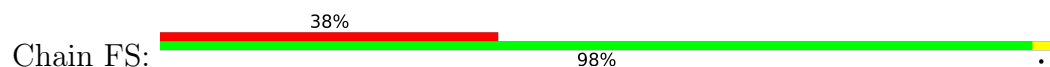




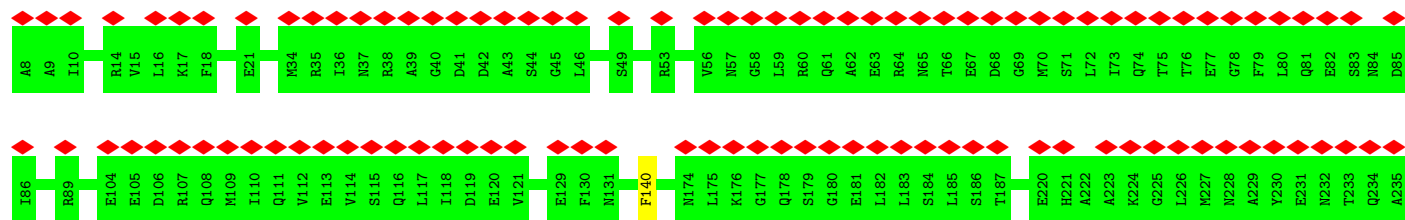
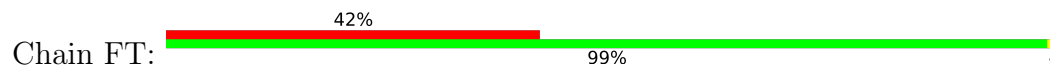
• Molecule 1: Flagellin B1 (FlaB1)

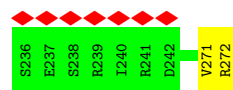


• Molecule 1: Flagellin B1 (FlaB1)

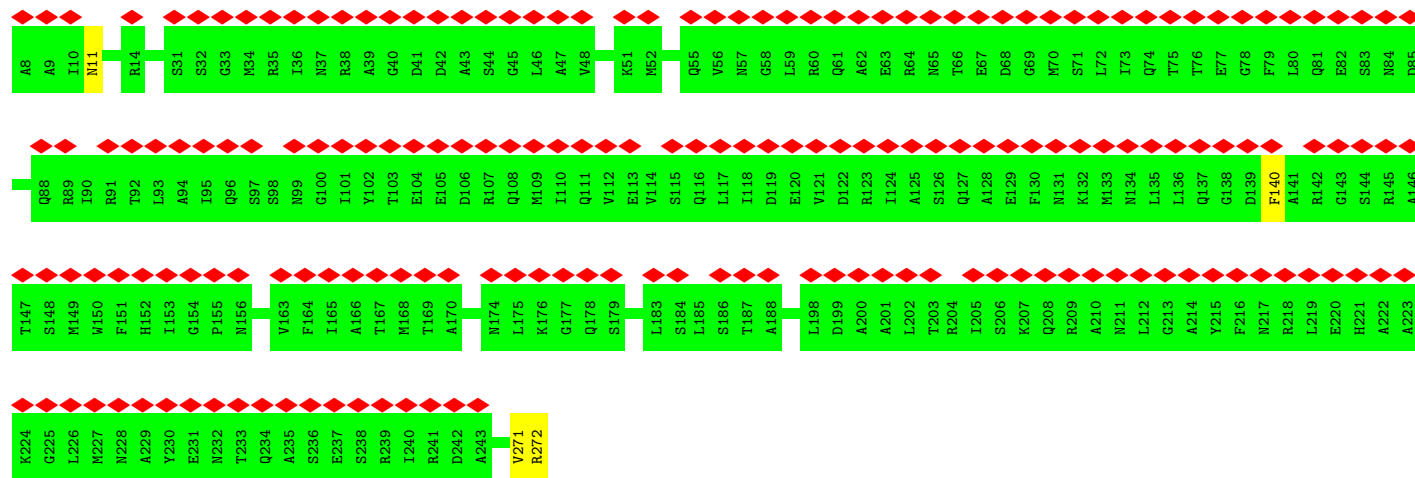


• Molecule 1: Flagellin B1 (FlaB1)

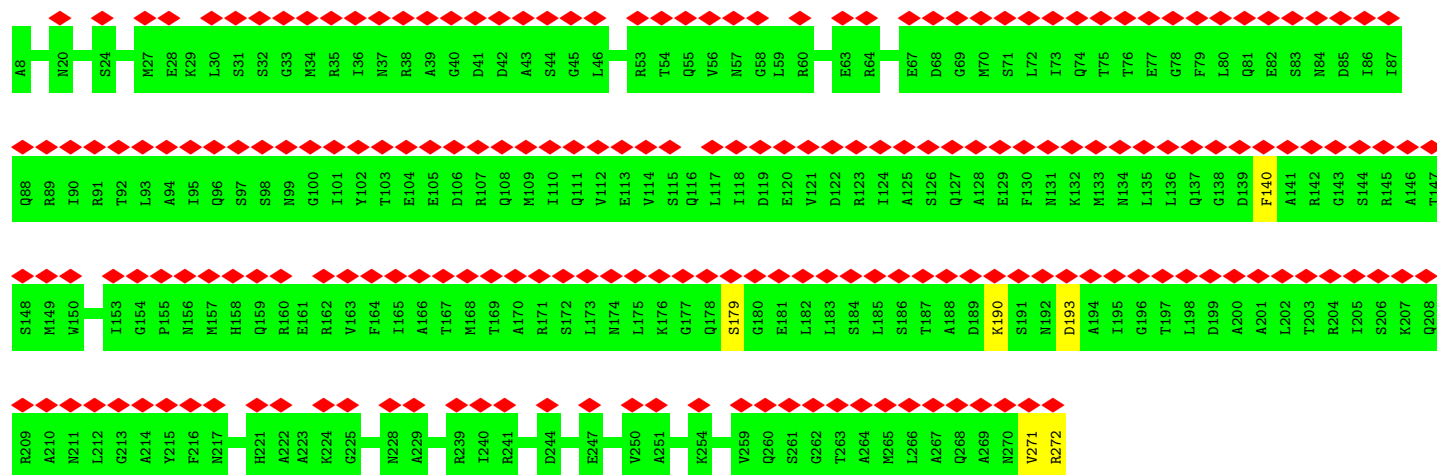
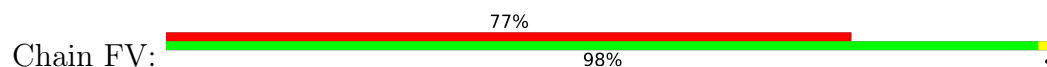




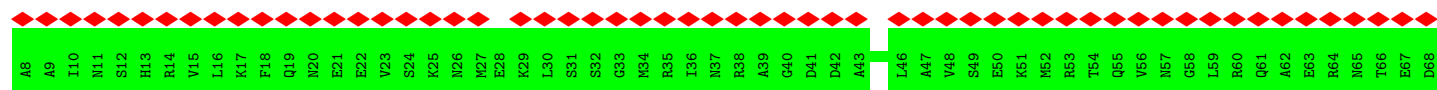
• Molecule 1: Flagellin B1 (FlaB1)



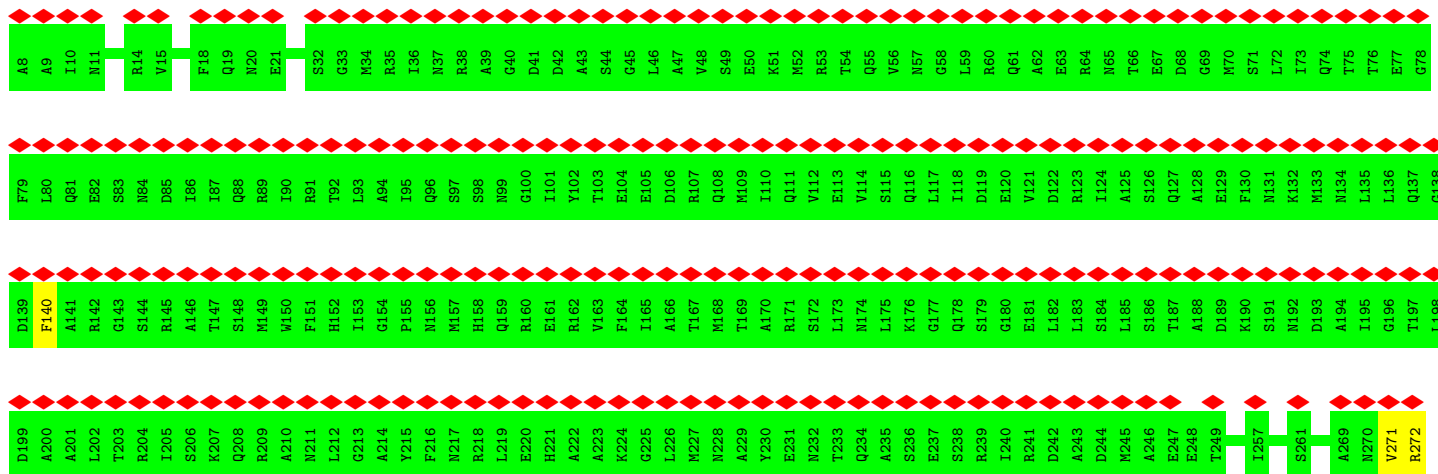
• Molecule 1: Flagellin B1 (FlaB1)



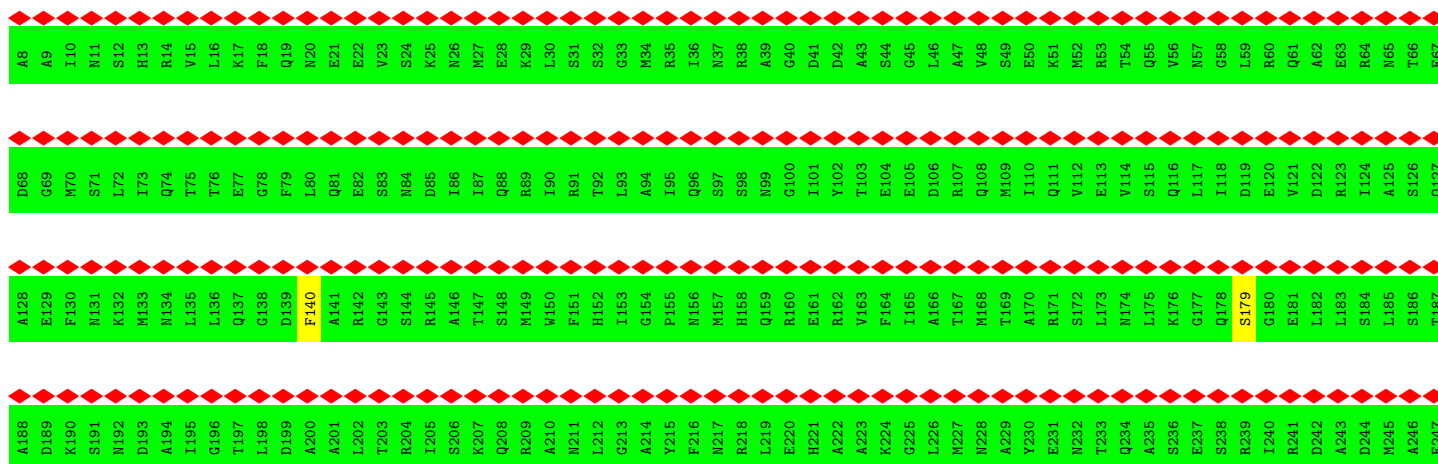
• Molecule 1: Flagellin B1 (FlaB1)

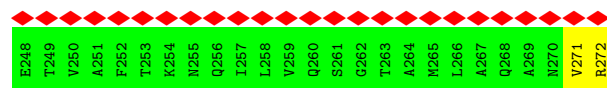


- Molecule 1: Flagellin B1 (FlaB1)

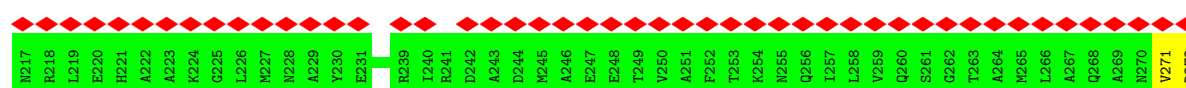
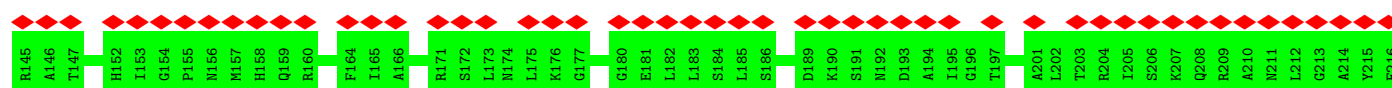
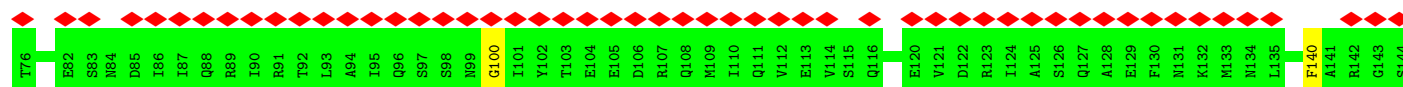
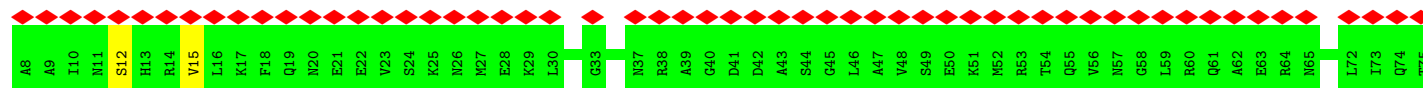
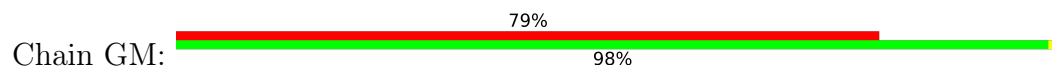


- Molecule 1: Flagellin B1 (FlaB1)

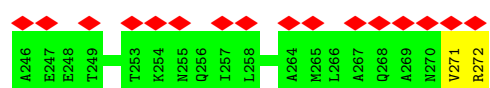
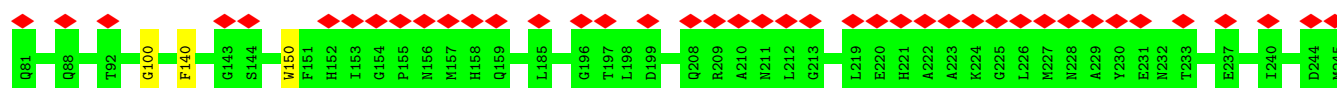
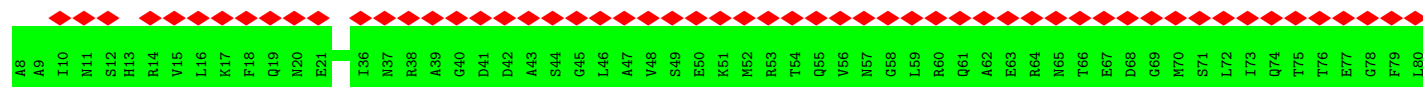
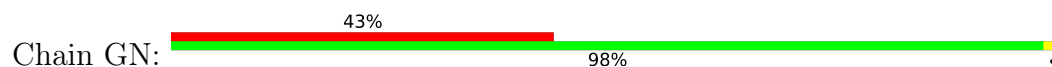




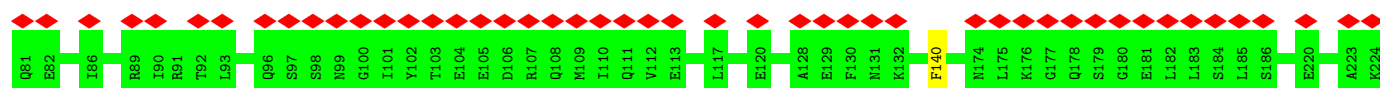
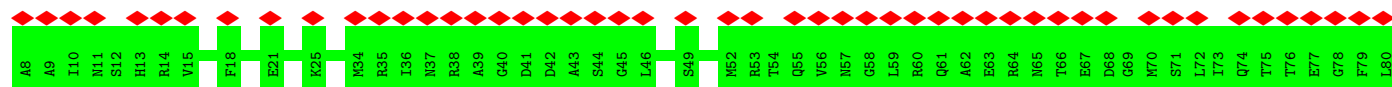
• Molecule 1: Flagellin B1 (FlaB1)

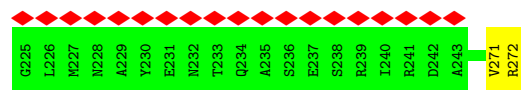


• Molecule 1: Flagellin B1 (FlaB1)

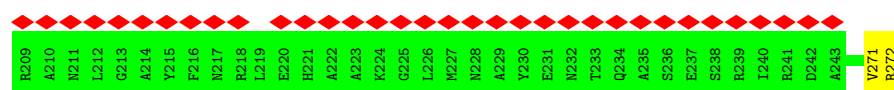
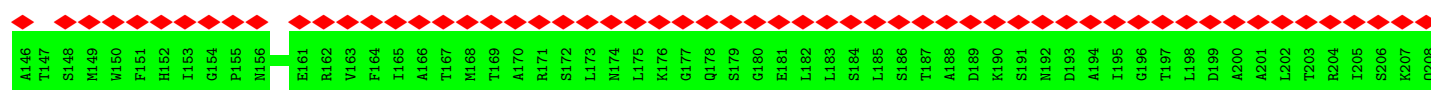
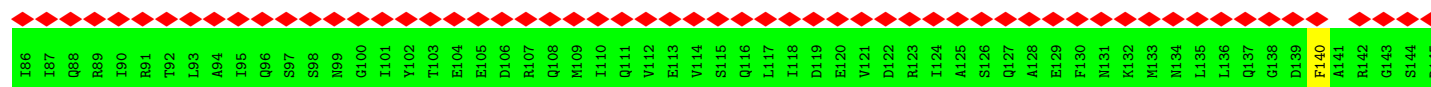
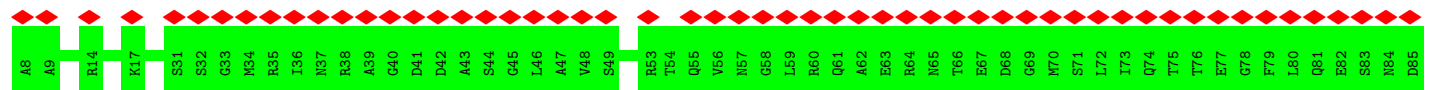
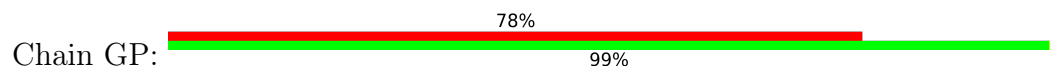


• Molecule 1: Flagellin B1 (FlaB1)

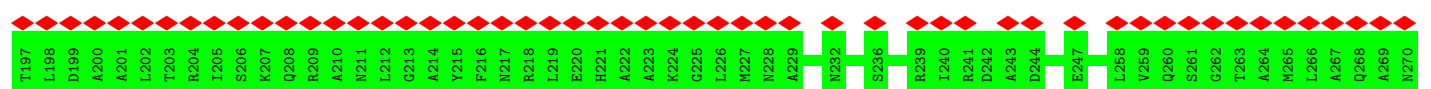
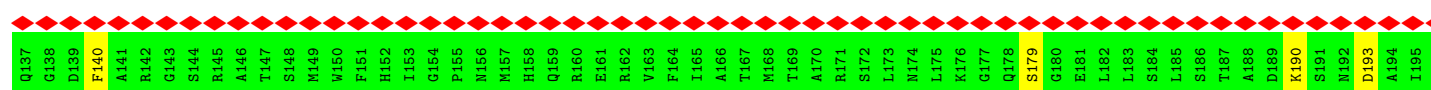
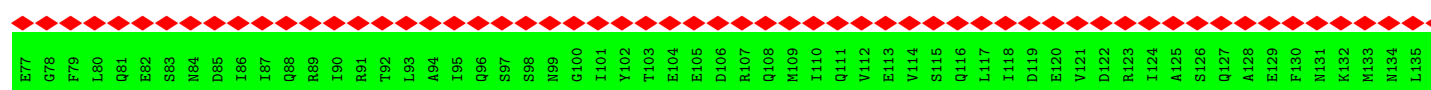
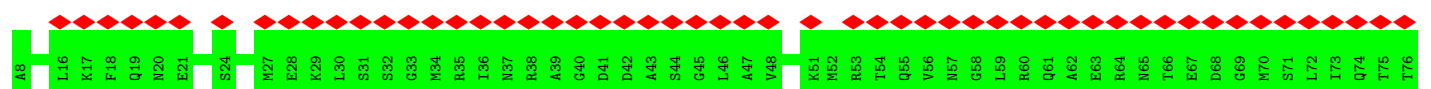
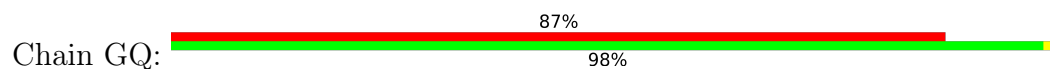




• Molecule 1: Flagellin B1 (FlaB1)

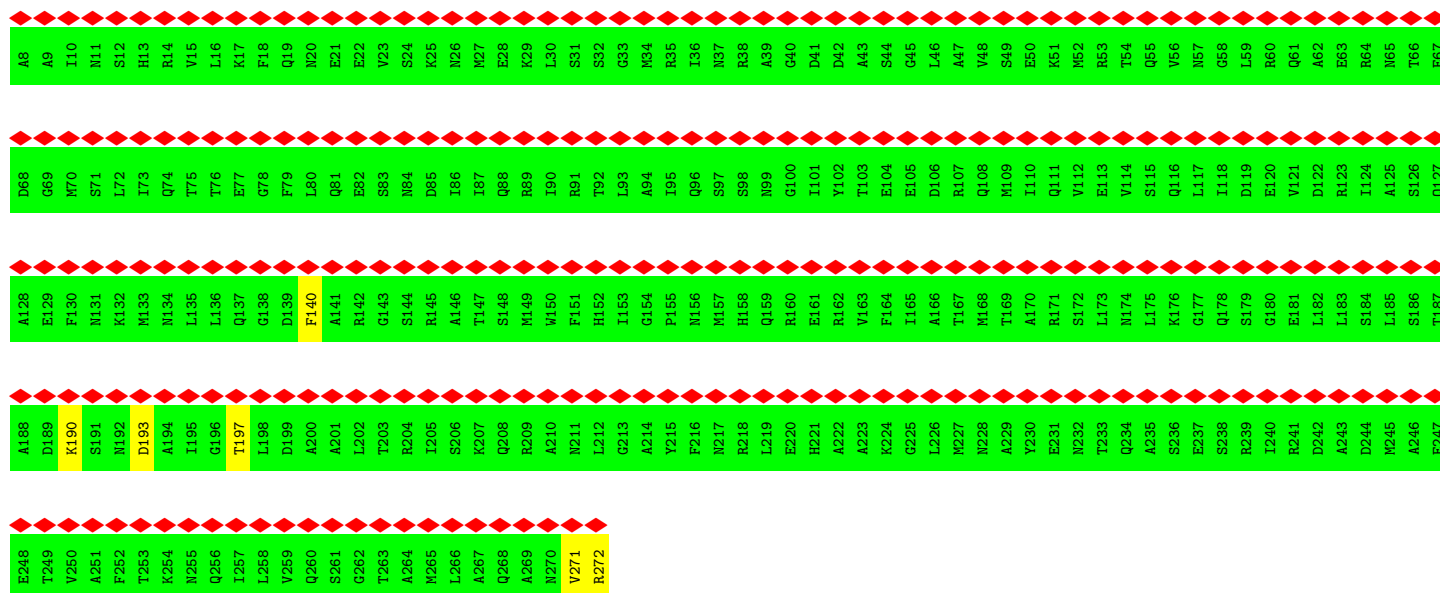


• Molecule 1: Flagellin B1 (FlaB1)

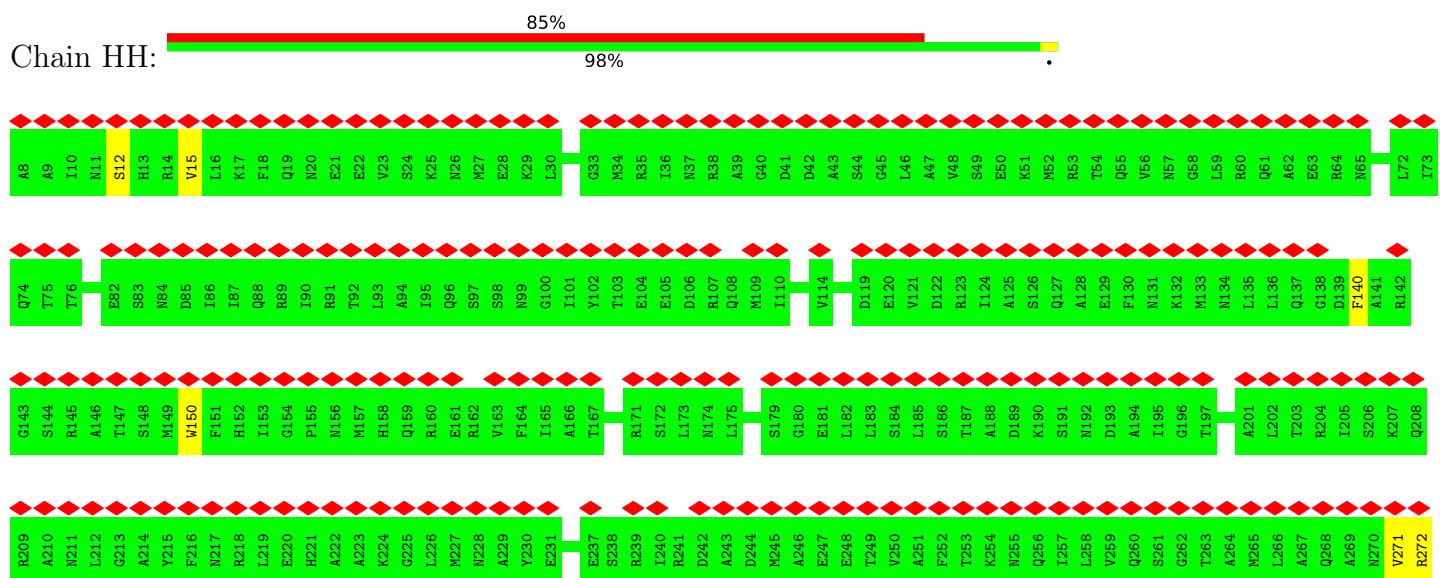


• Molecule 1: Flagellin B1 (FlaB1)

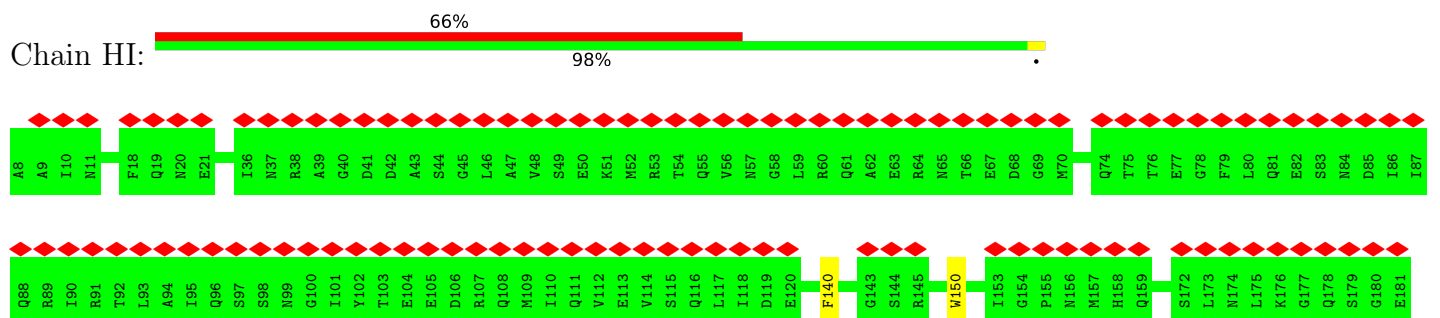


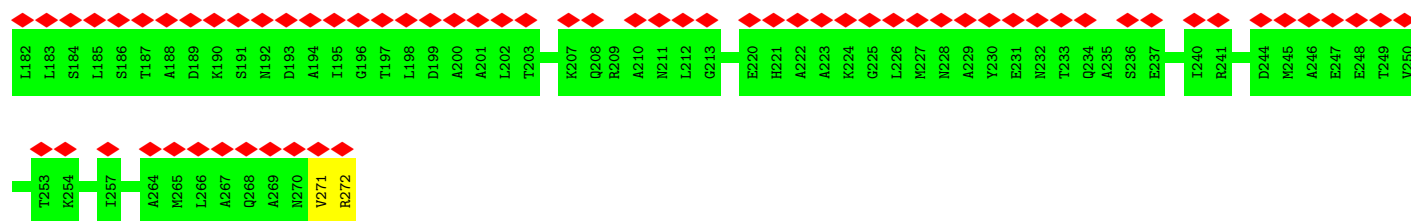


• Molecule 1: Flagellin B1 (FlaB1)

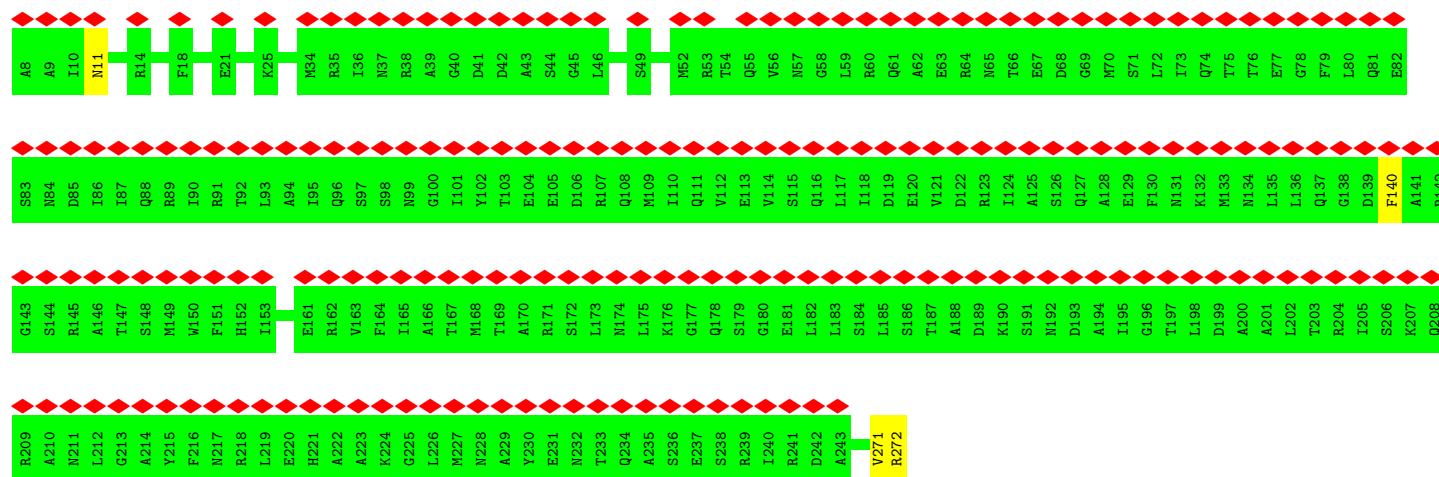
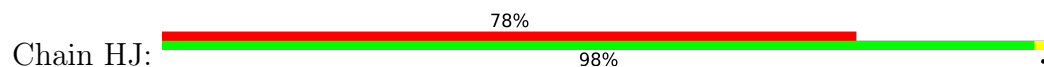


• Molecule 1: Flagellin B1 (FlaB1)

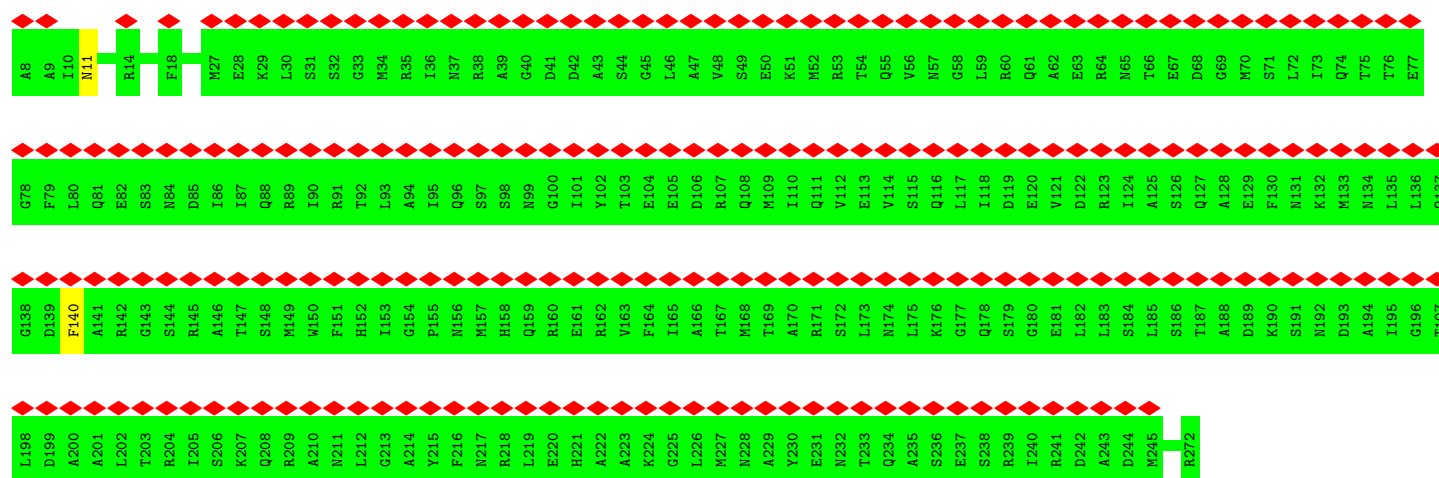
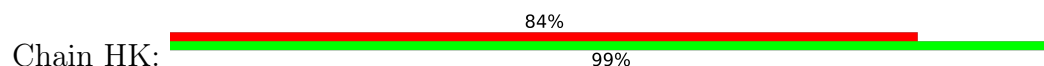




• Molecule 1: Flagellin B1 (FlaB1)

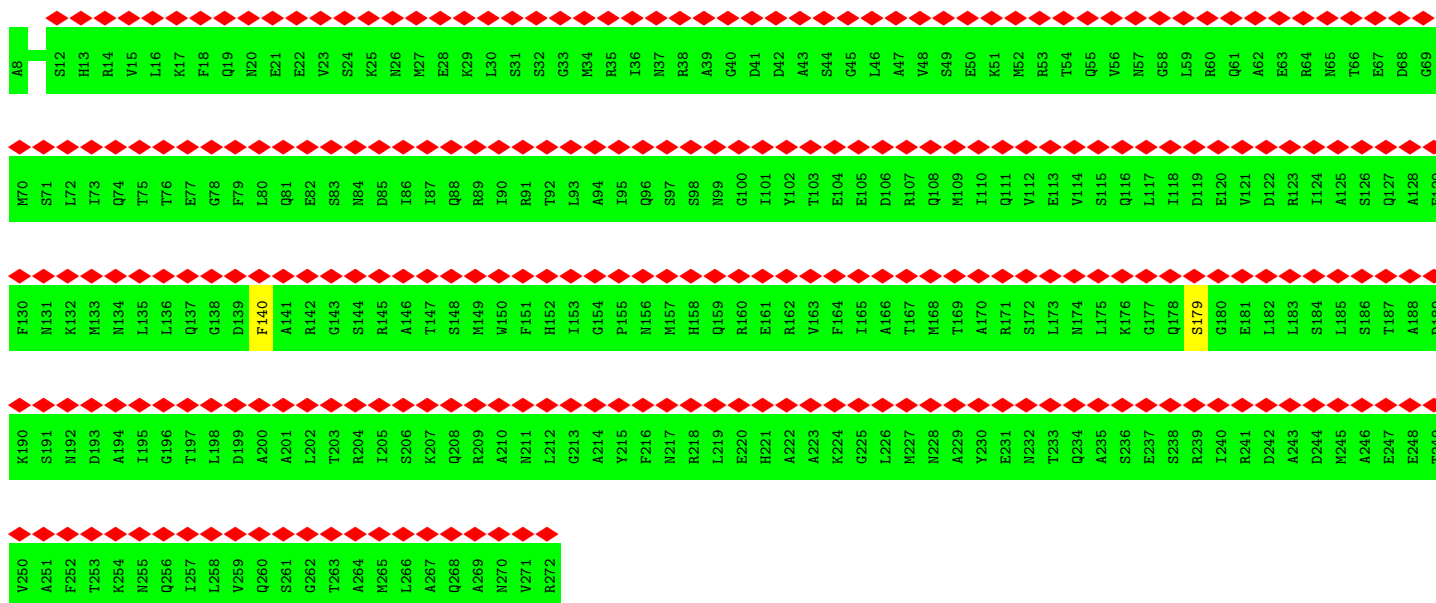


• Molecule 1: Flagellin B1 (FlaB1)

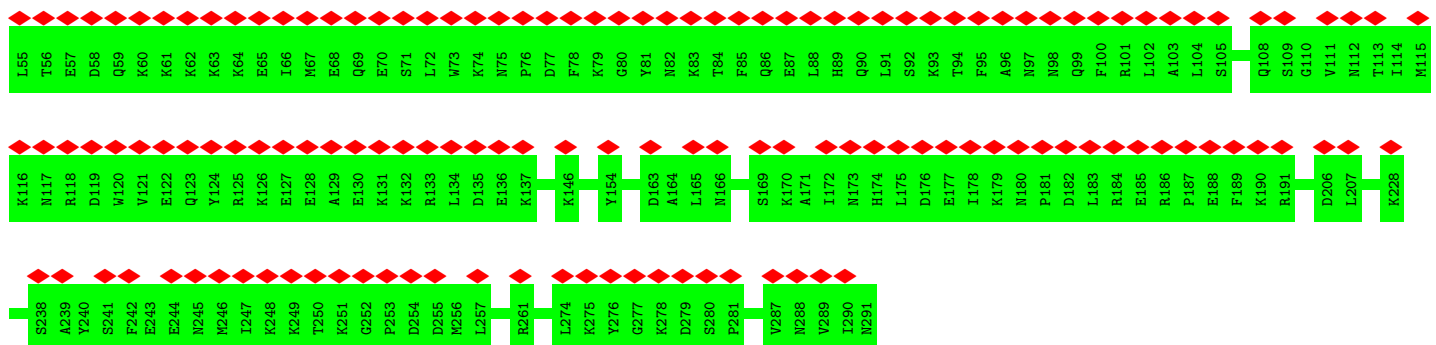


• Molecule 1: Flagellin B1 (FlaB1)

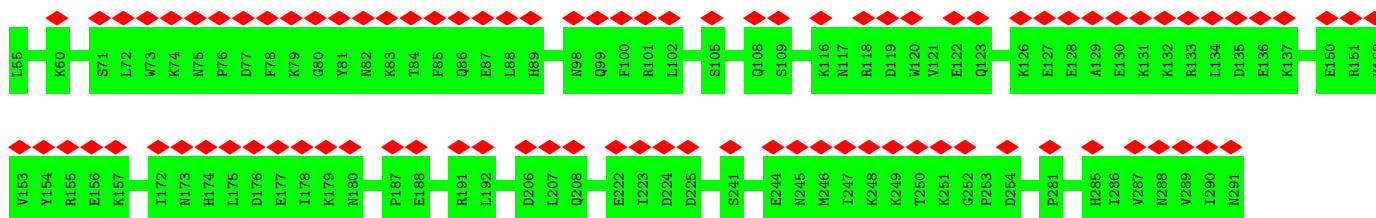




- Molecule 2: Flagellar coiling protein A (FcpA)

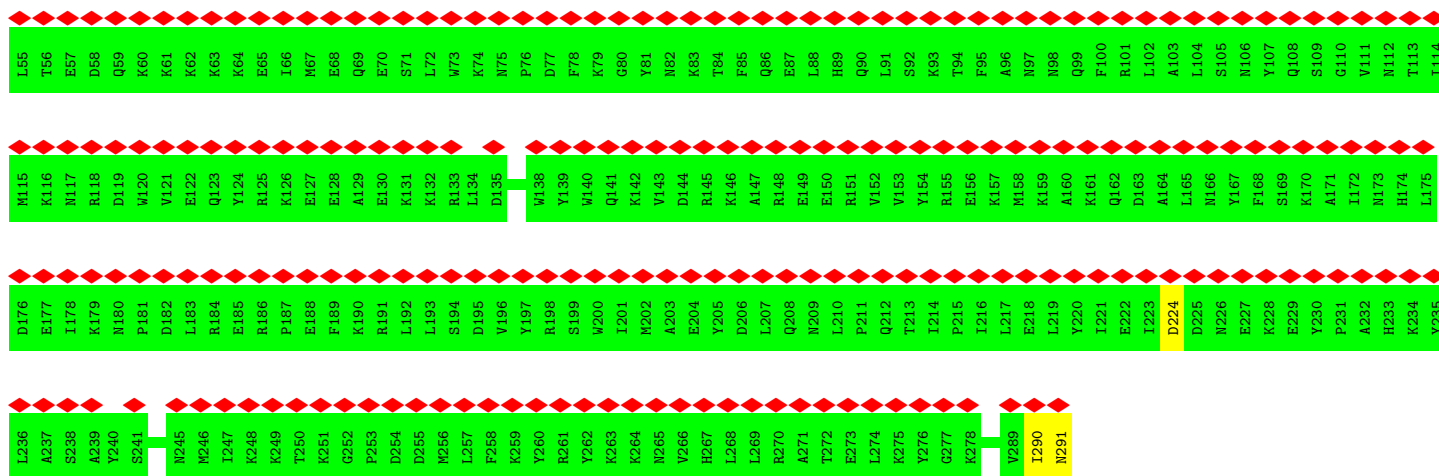


- Molecule 2: Flagellar coiling protein A (FcpA)

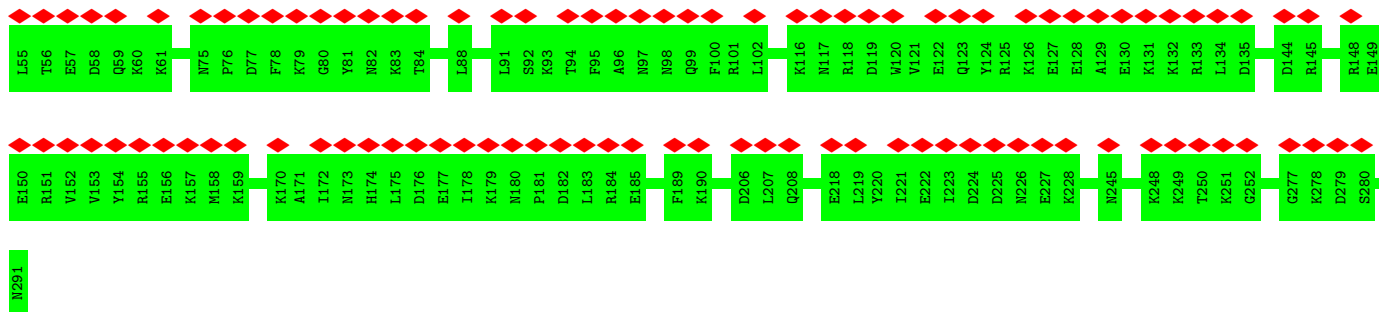
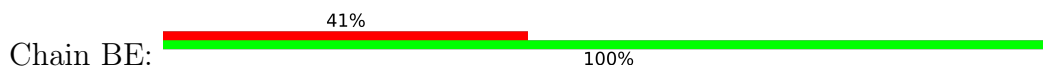


- Molecule 2: Flagellar coiling protein A (FcpA)

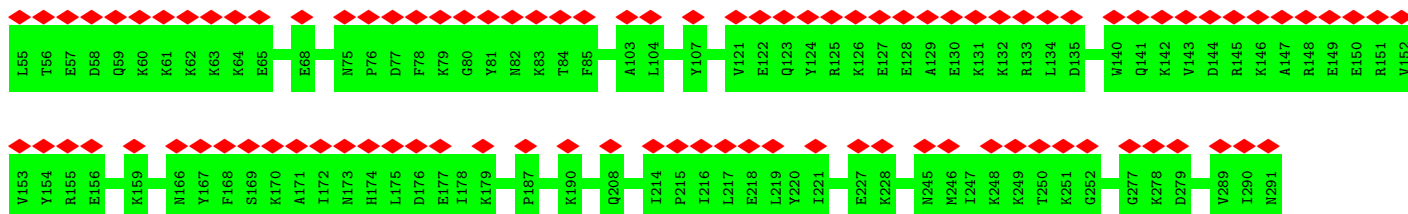
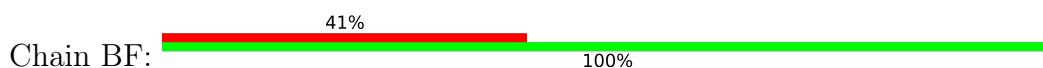




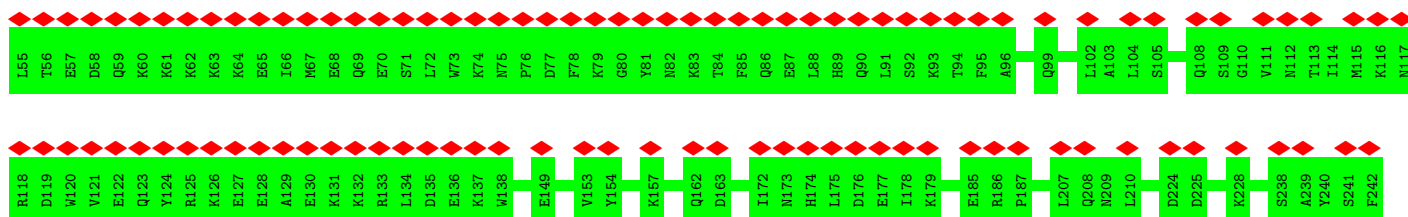
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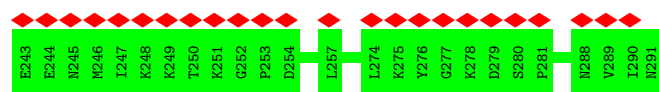


• Molecule 2: Flagellar coiling protein A (FcpA)

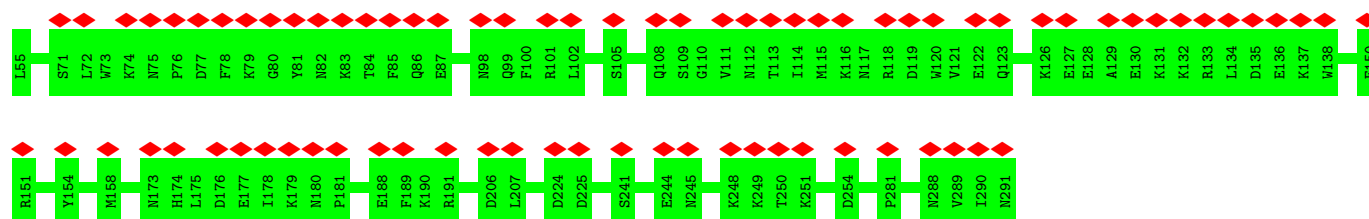


• Molecule 2: Flagellar coiling protein A (FcpA)

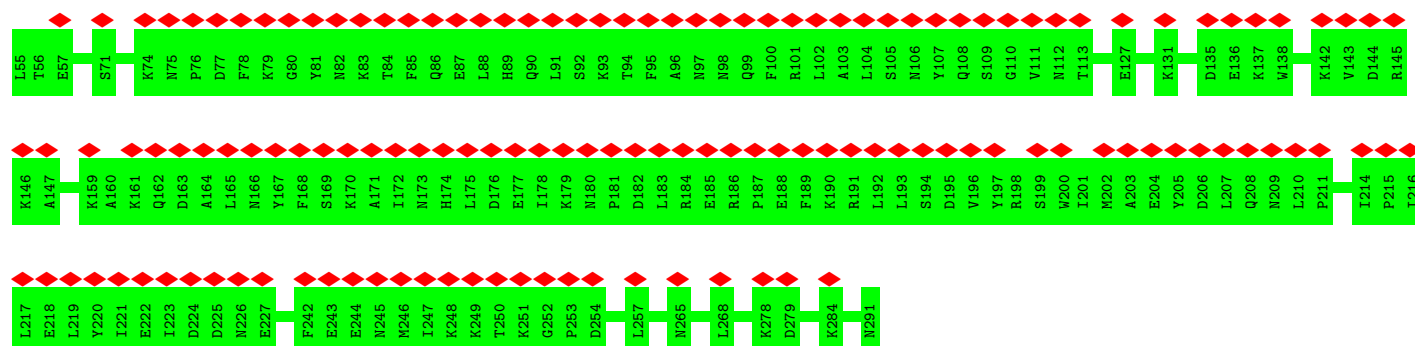




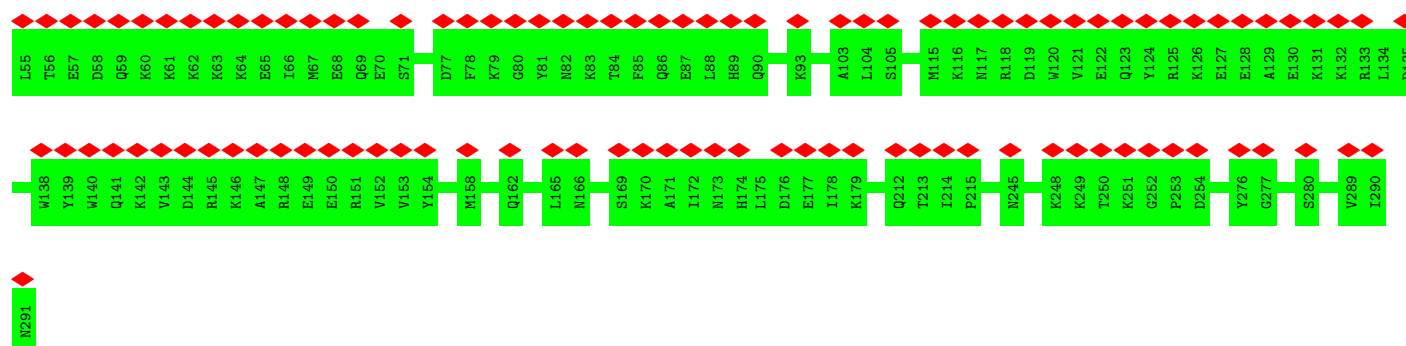
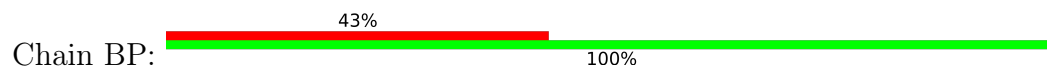
• Molecule 2: Flagellar coiling protein A (FcpA)



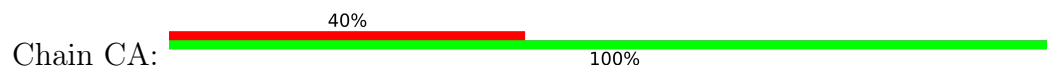
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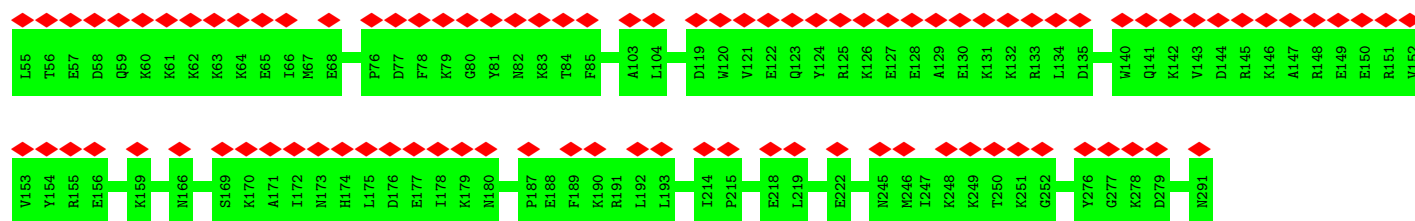


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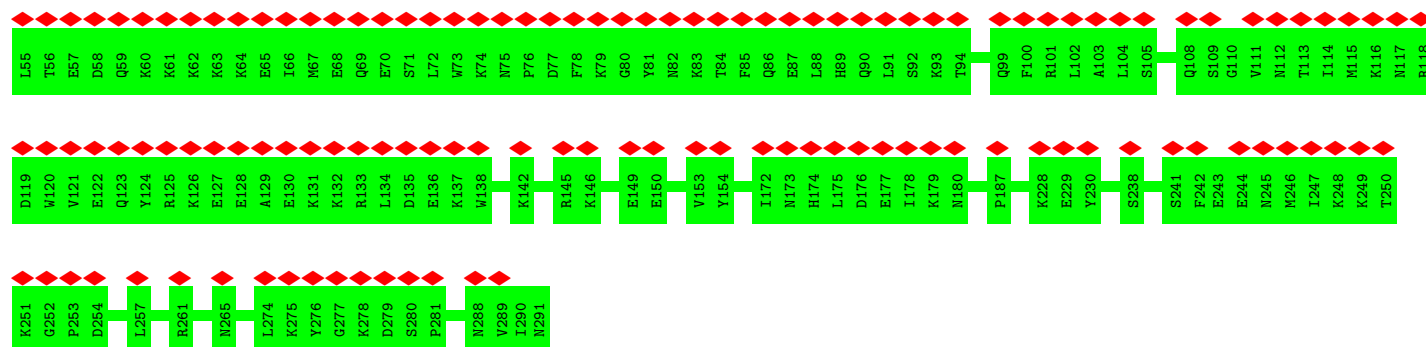


• Molecule 2: Flagellar coiling protein A (FcpA)

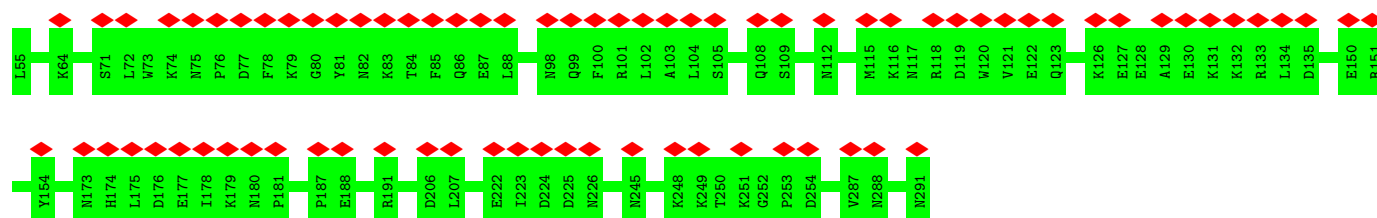




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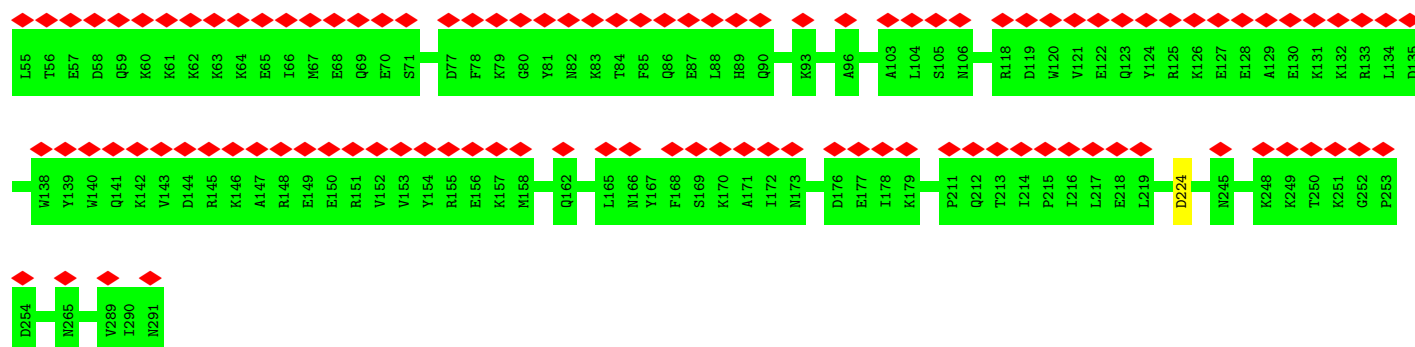


• Molecule 2: Flagellar coiling protein A (FcpA)



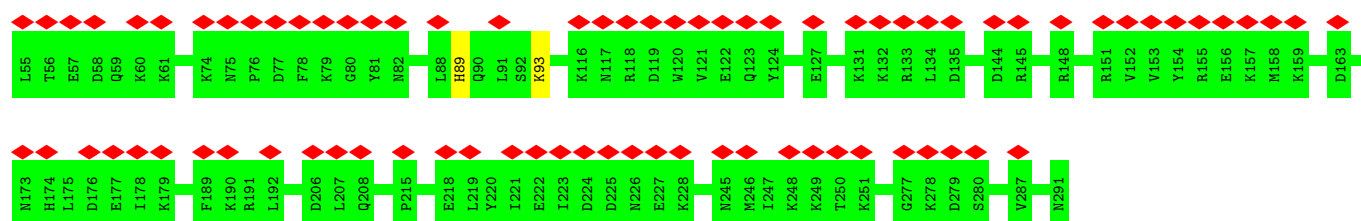
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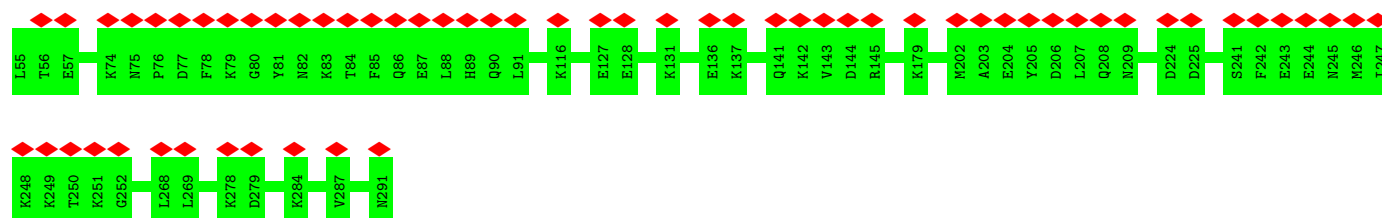
• Molecule 2: Flagellar coiling protein A (FcpA)

Chain BZ: 33% 99%



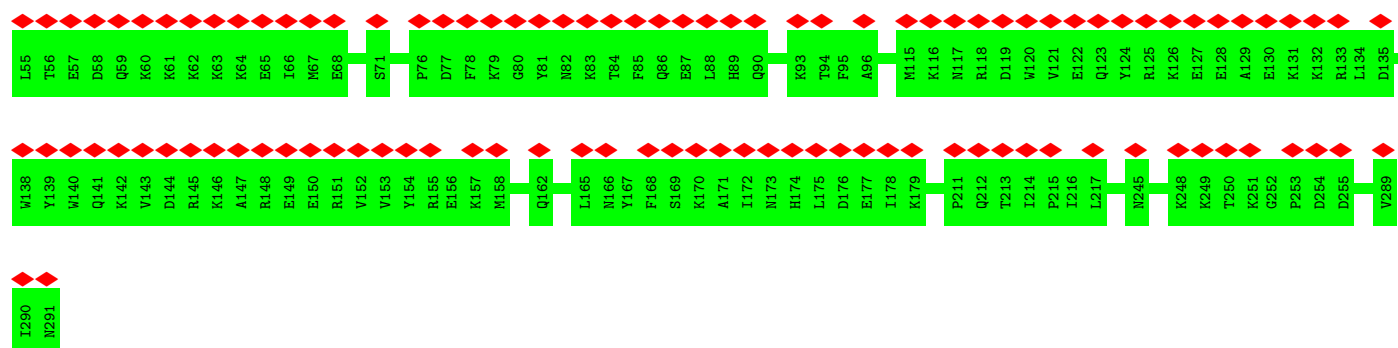
• Molecule 2: Flagellar coiling protein A (FcpA)

Chain DD: 26% 100%

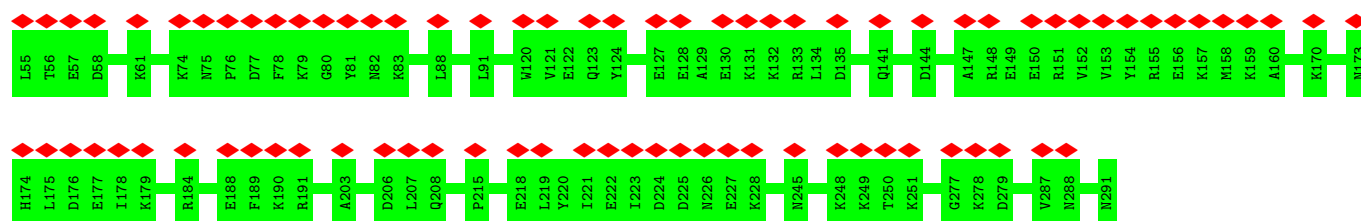


• Molecule 2: Flagellar coiling protein A (FcpA)

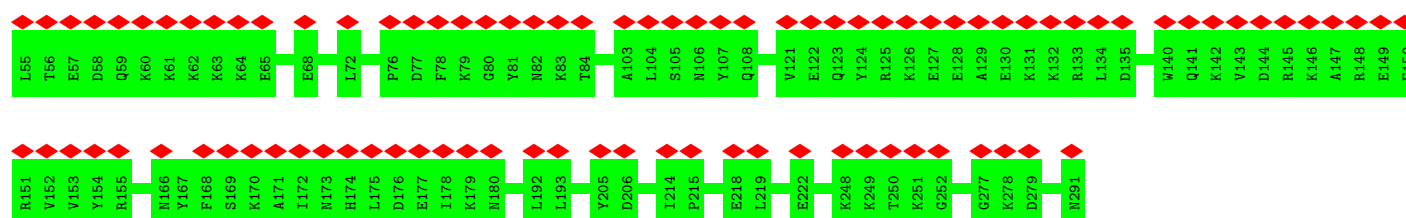
Chain DF: 44% 100%



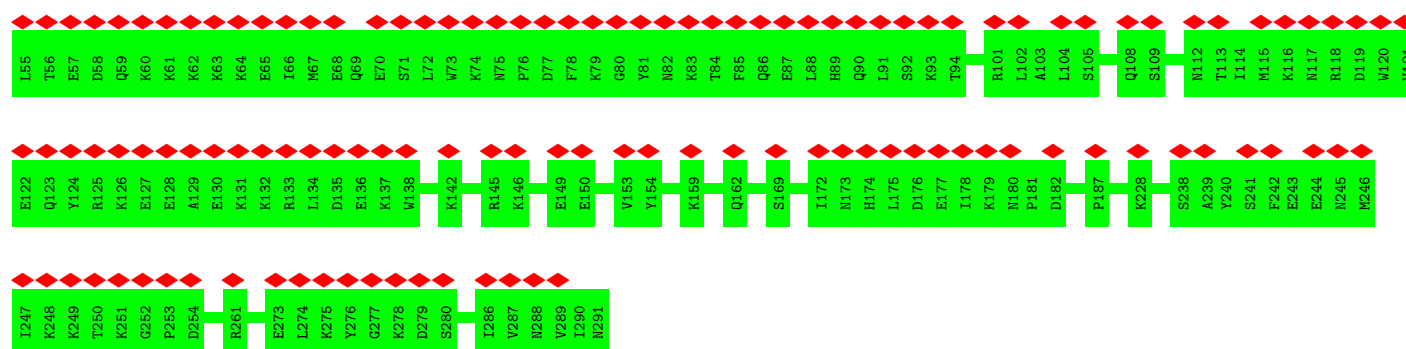
• Molecule 2: Flagellar coiling protein A (FcpA)



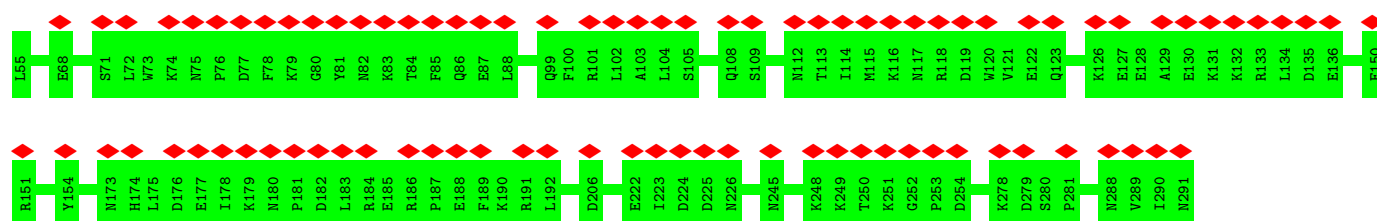
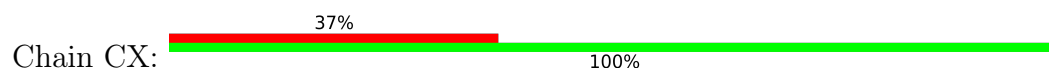
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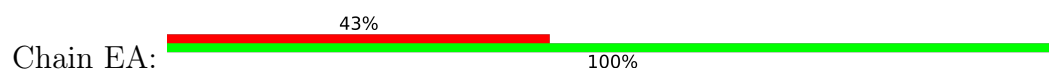
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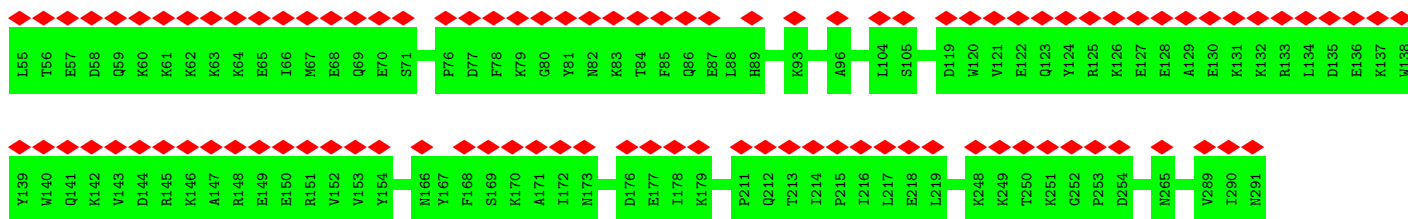


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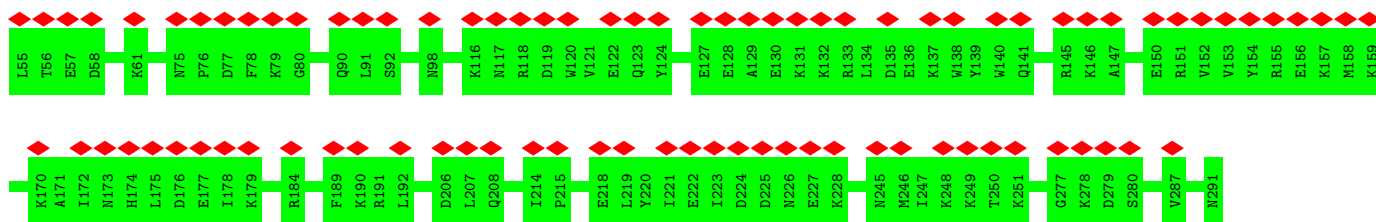
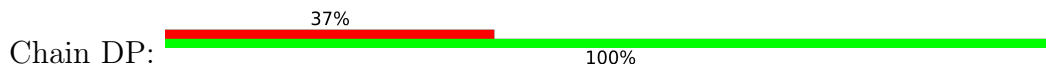


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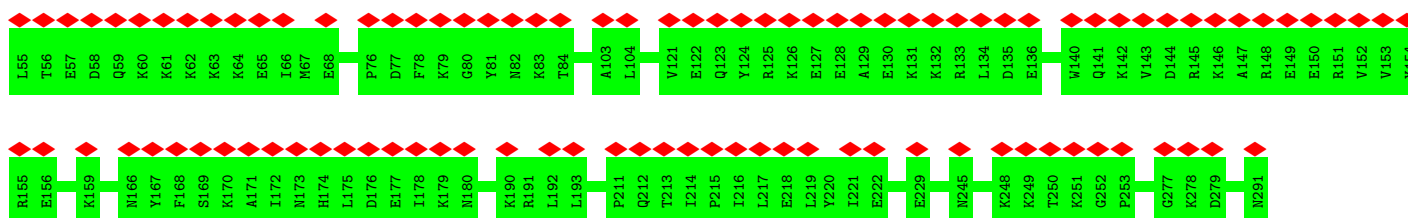
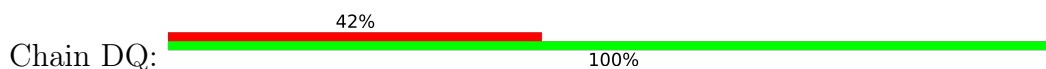




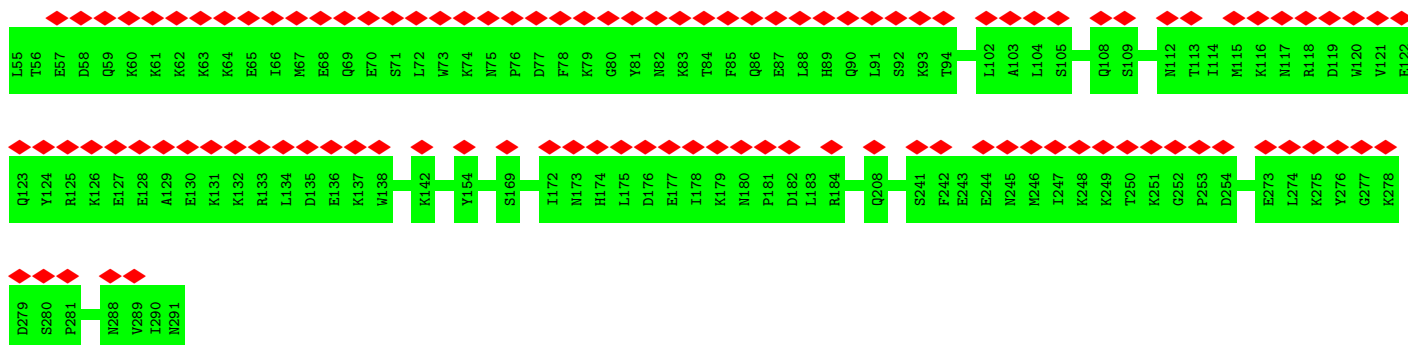
• Molecule 2: Flagellar coiling protein A (FcpA)



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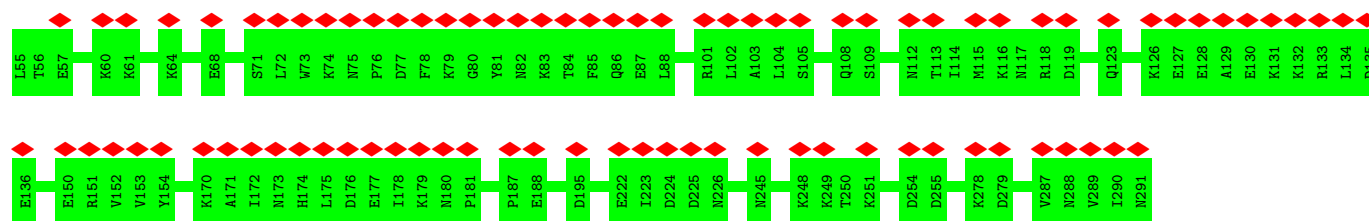


• Molecule 2: Flagellar coiling protein A (FcpA)

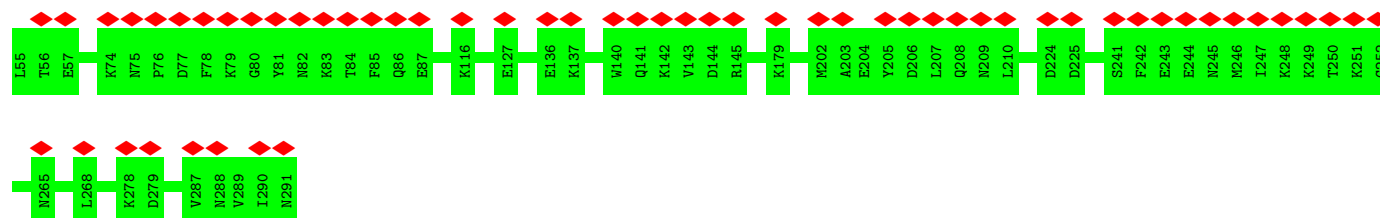


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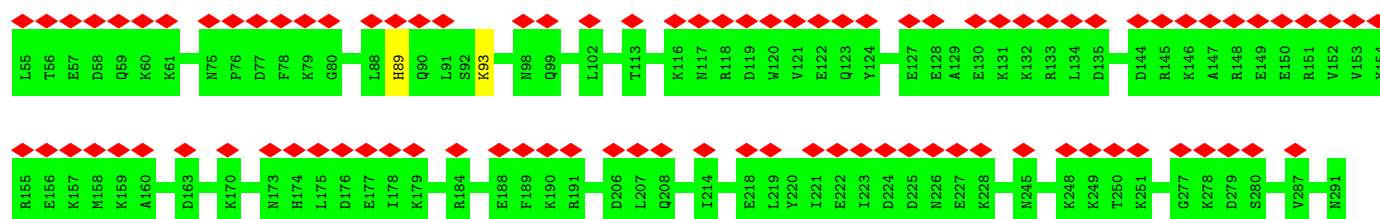




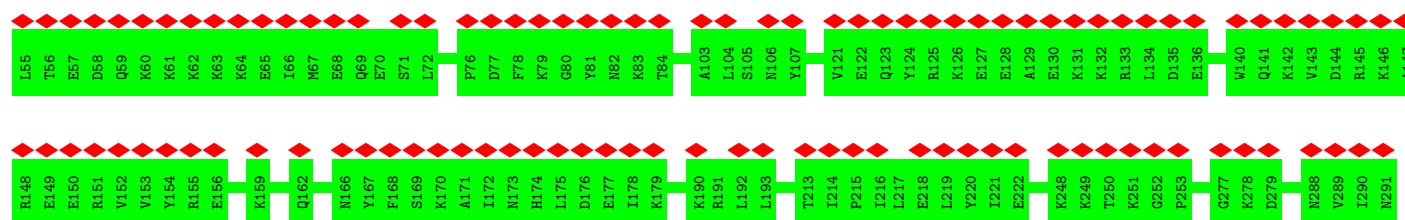
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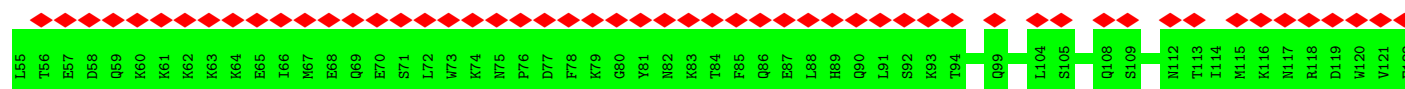
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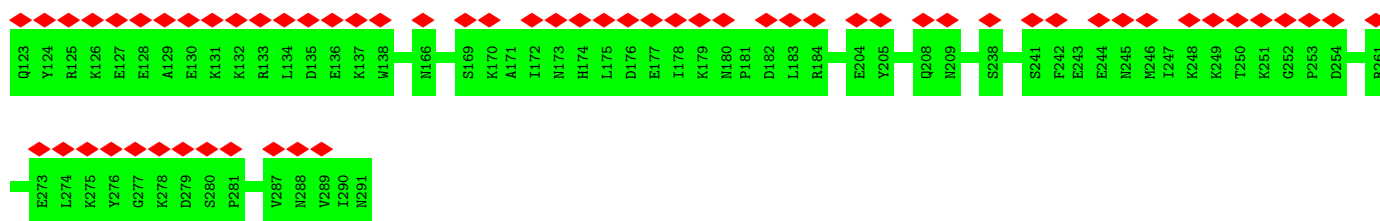


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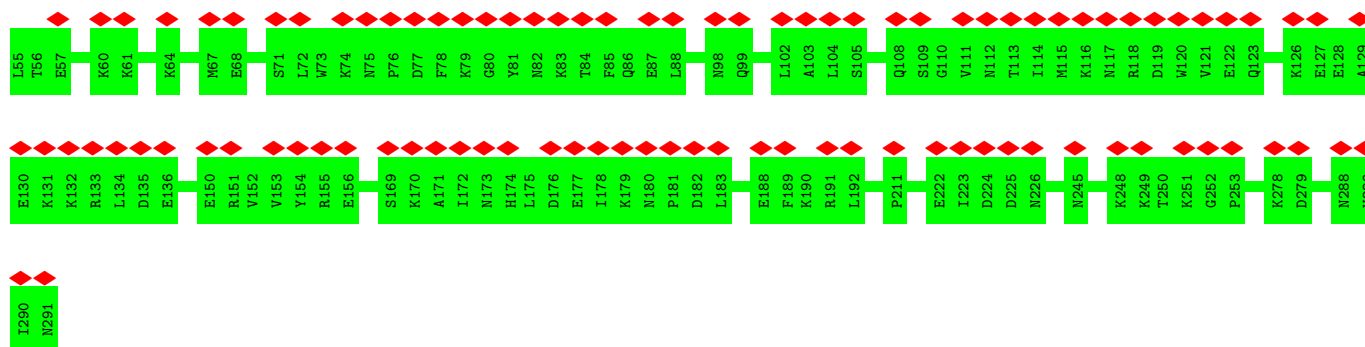
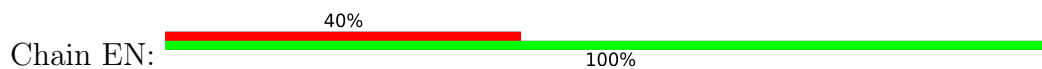


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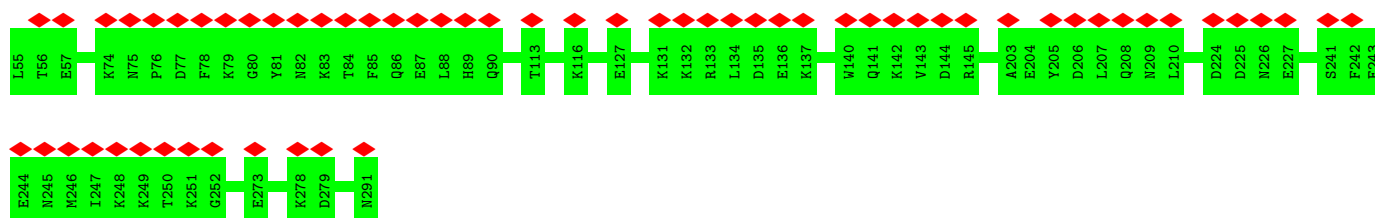




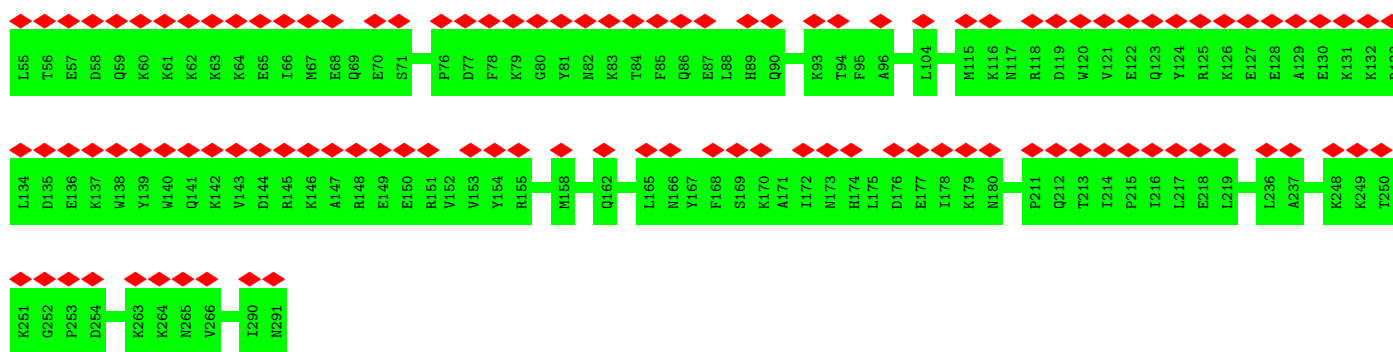
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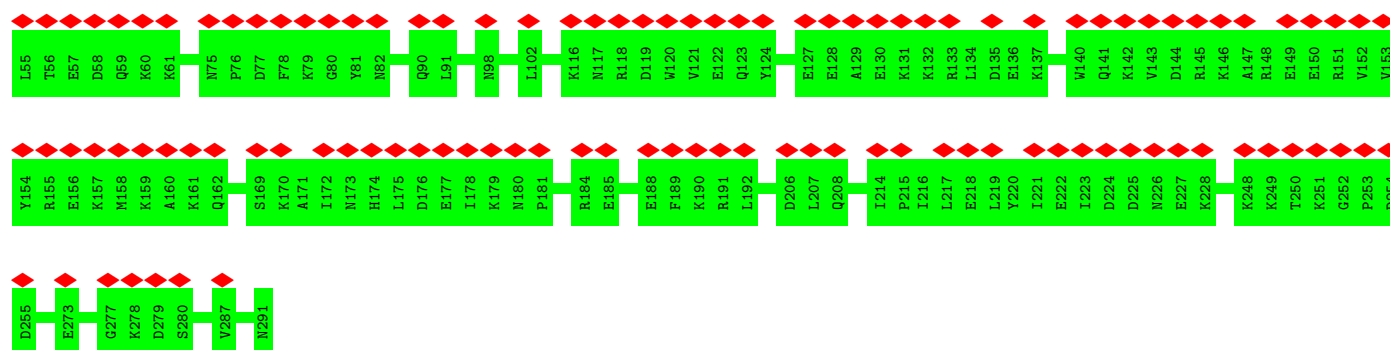
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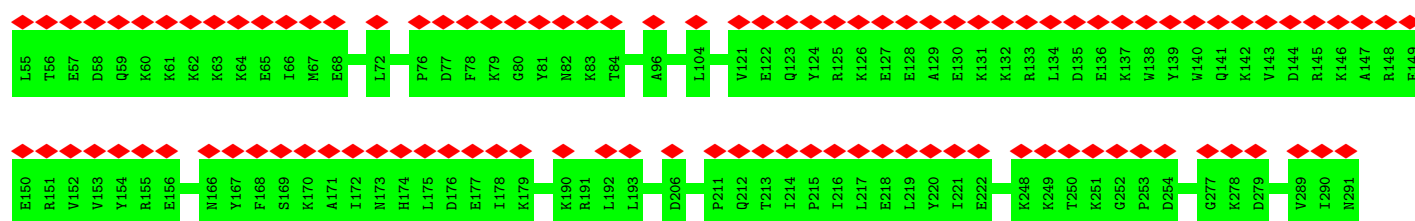
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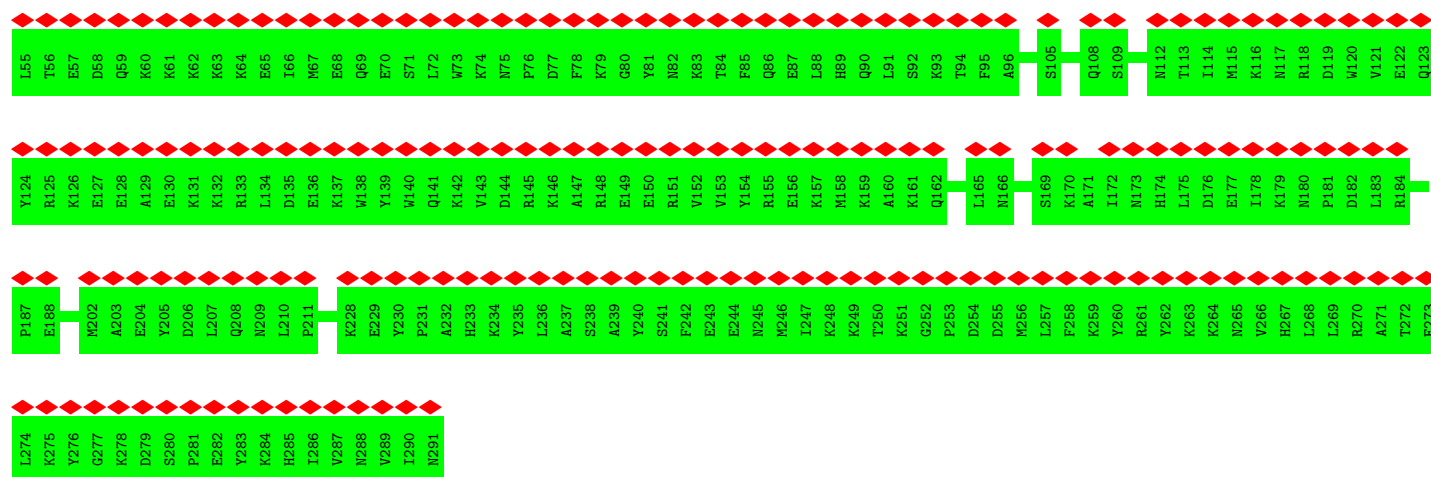
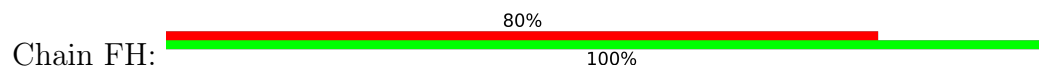
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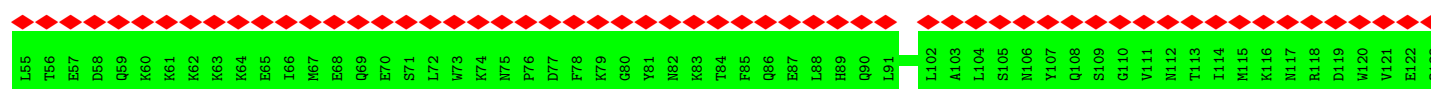
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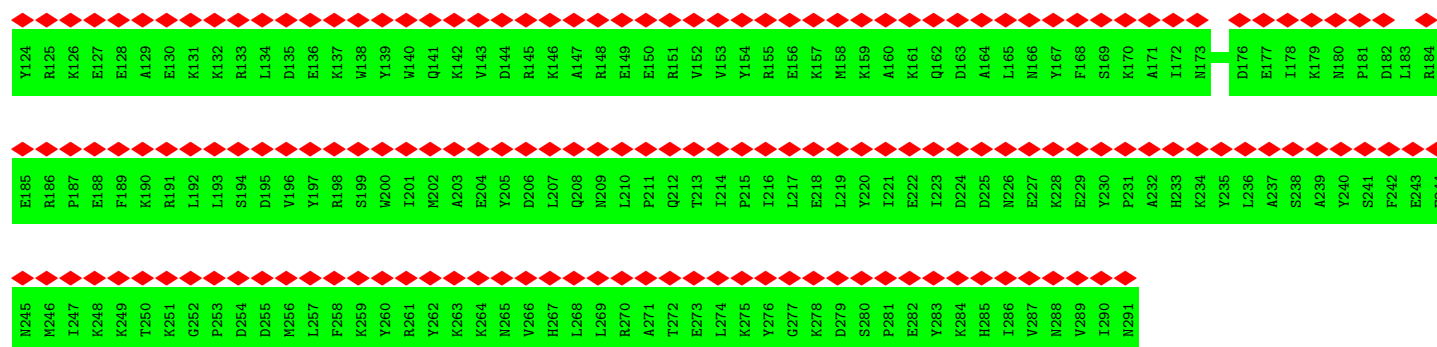


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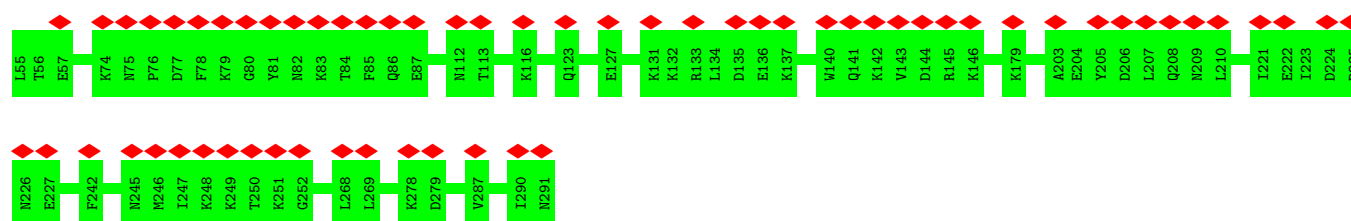


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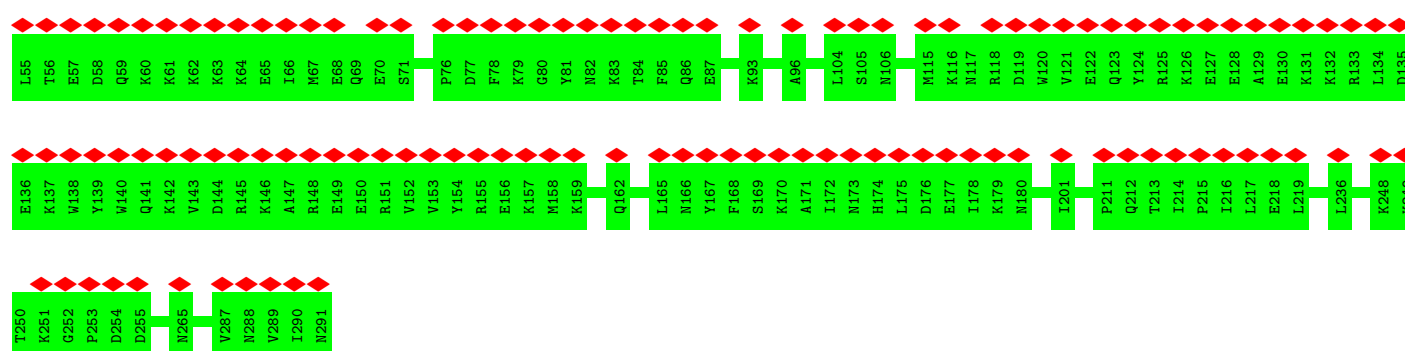




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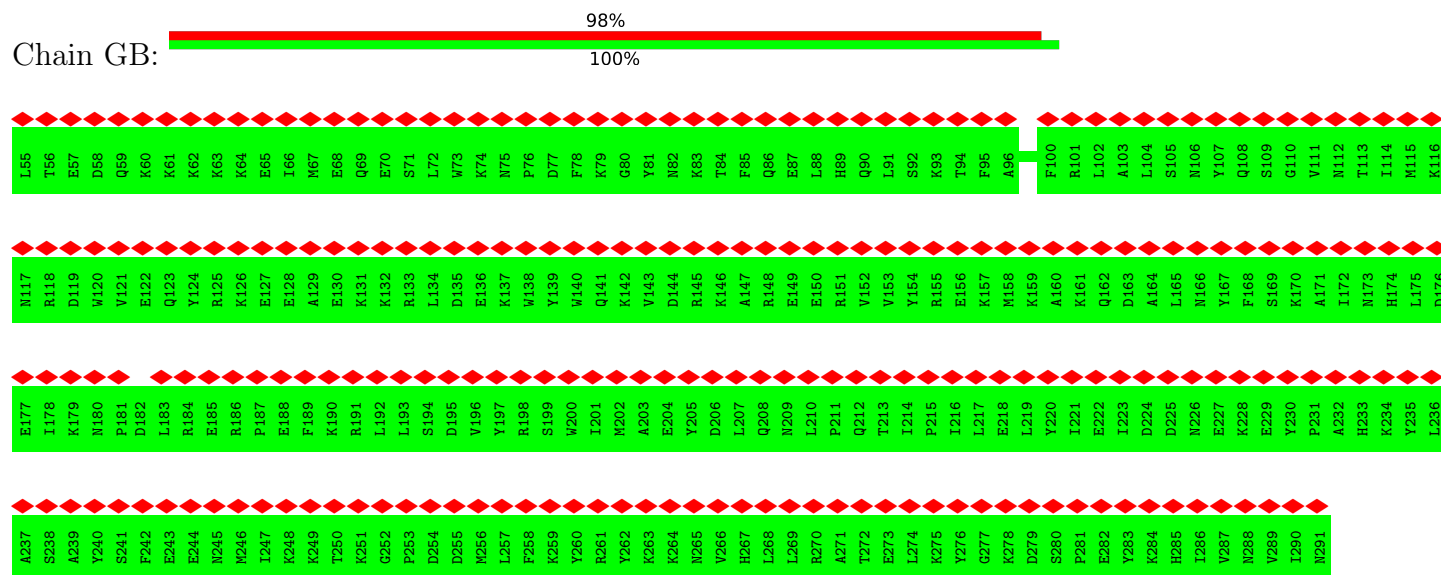


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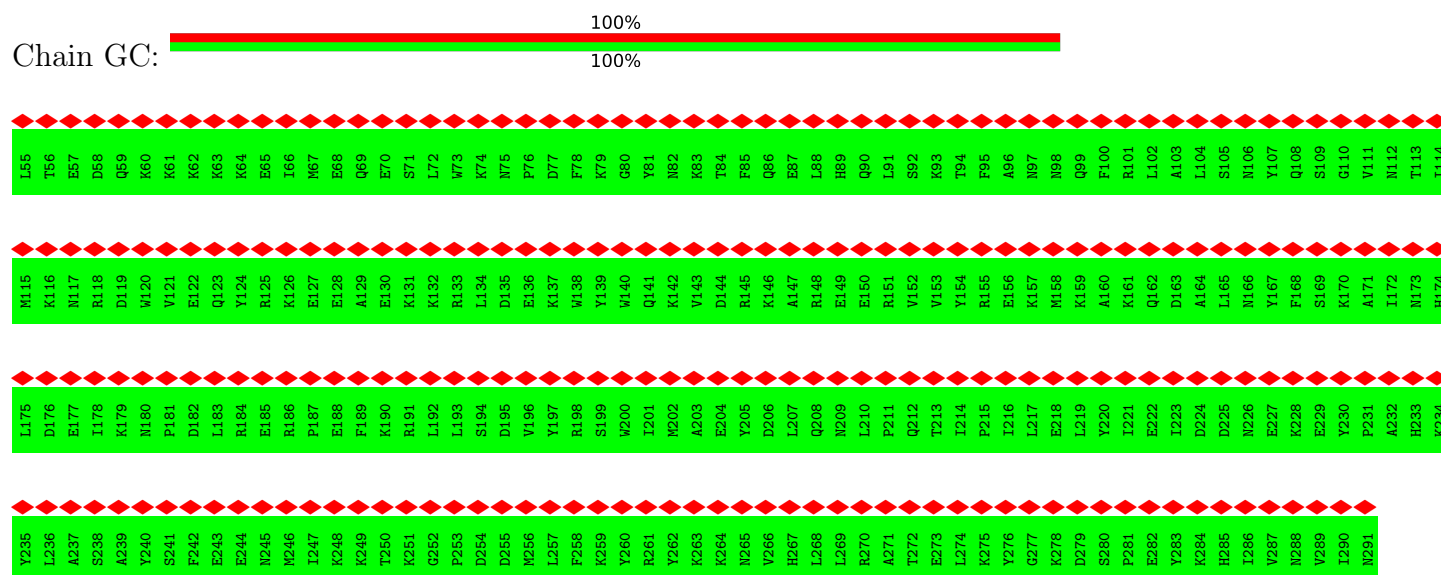




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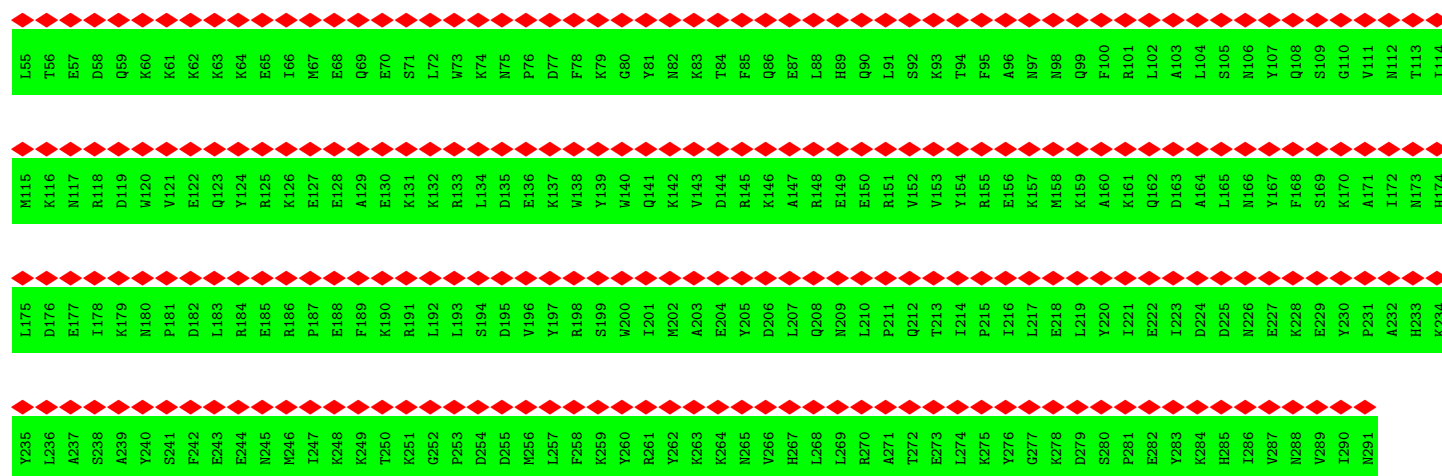
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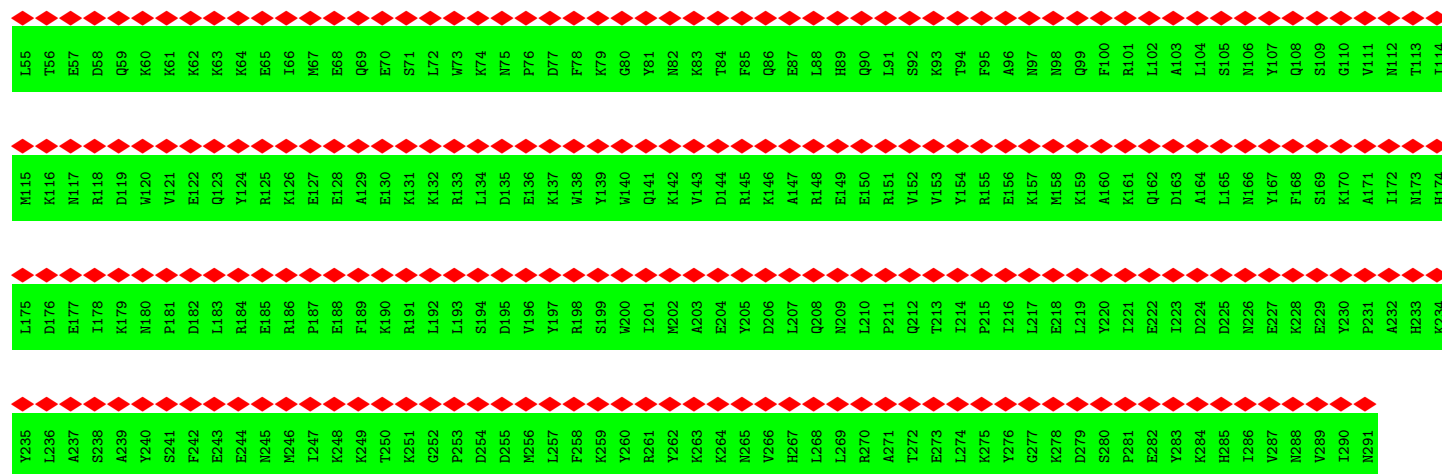
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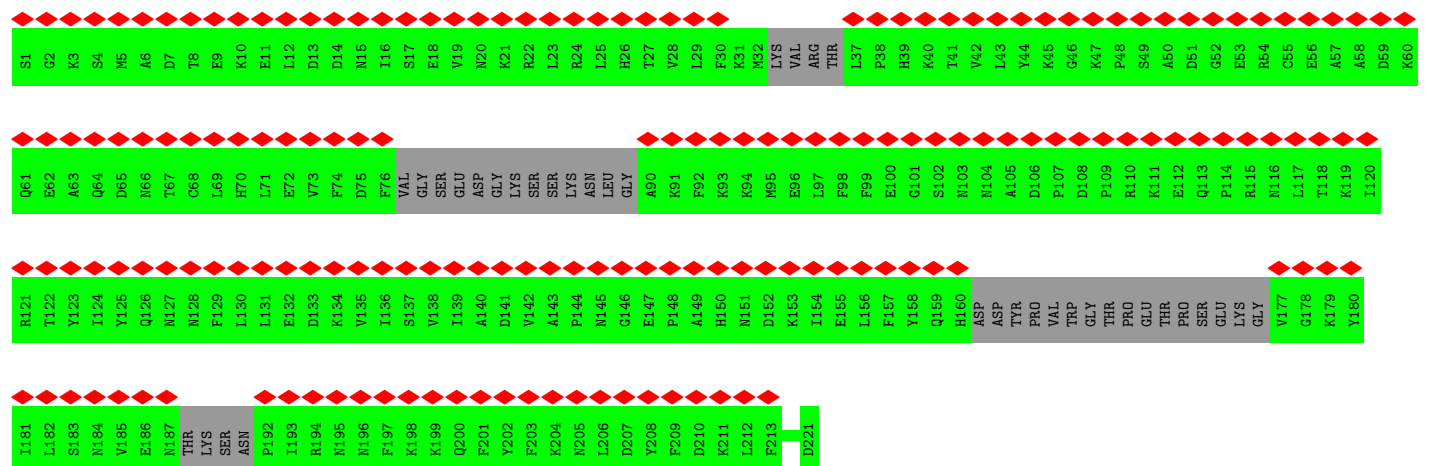
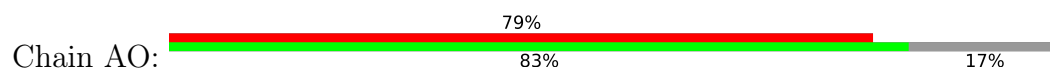





• Molecule 2: Flagellar coiling protein A (FcpA)

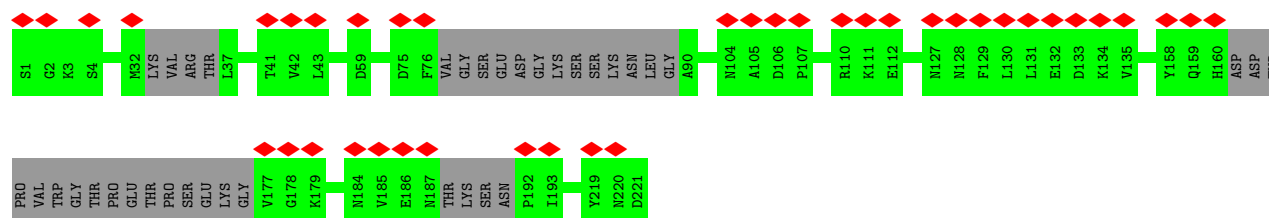


• Molecule 3: Flagellar coiling protein B (FcpB)




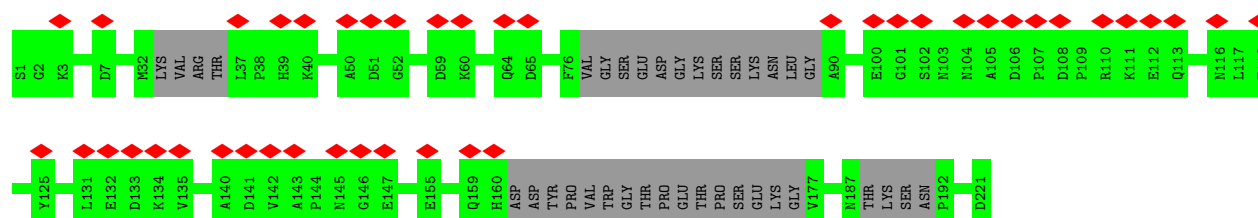
- Molecule 3: Flagellar coiling protein B (FcpB)

Chain BI: 




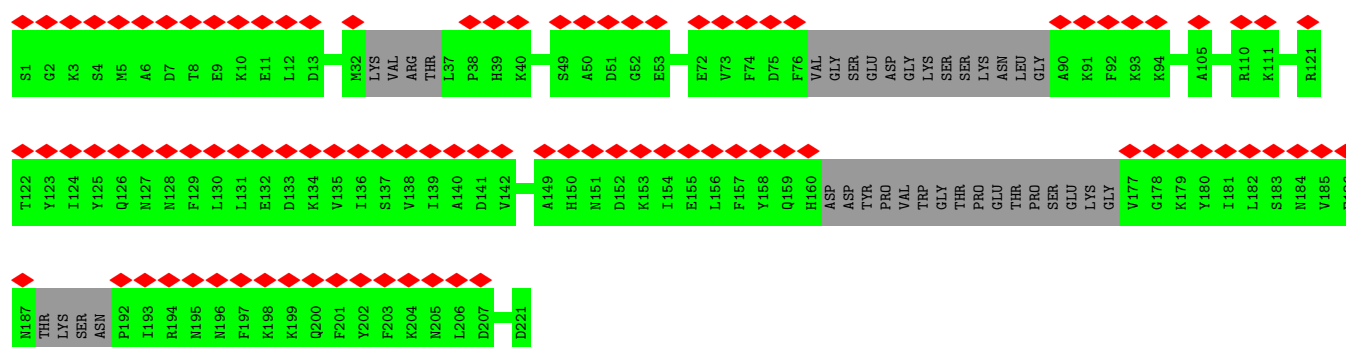
- Molecule 3: Flagellar coiling protein B (FcpB)

Chain BJ: 




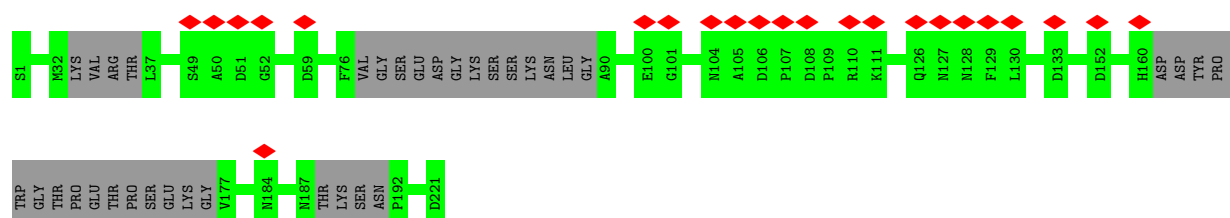
- Molecule 3: Flagellar coiling protein B (FcpB)

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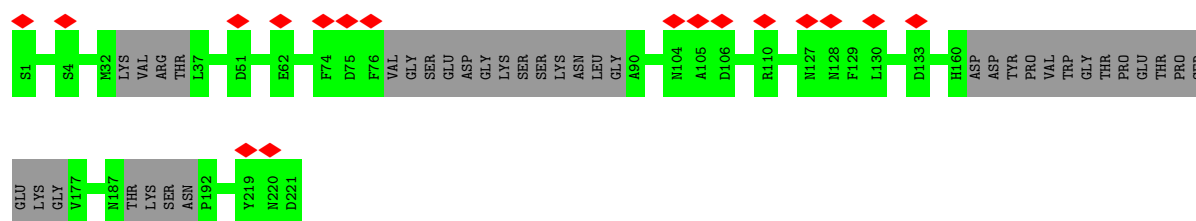
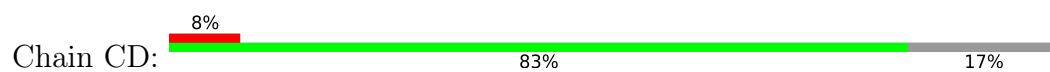


- Molecule 3: Flagellar coiling protein B (FcpB)

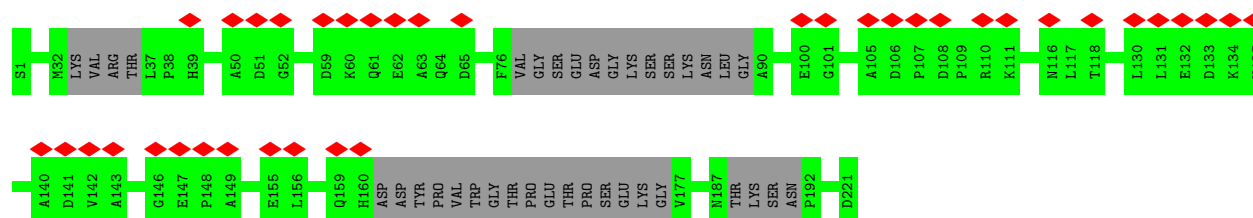
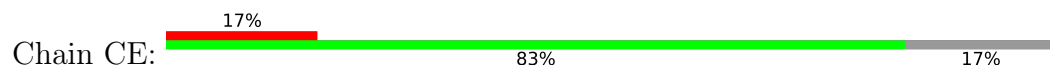
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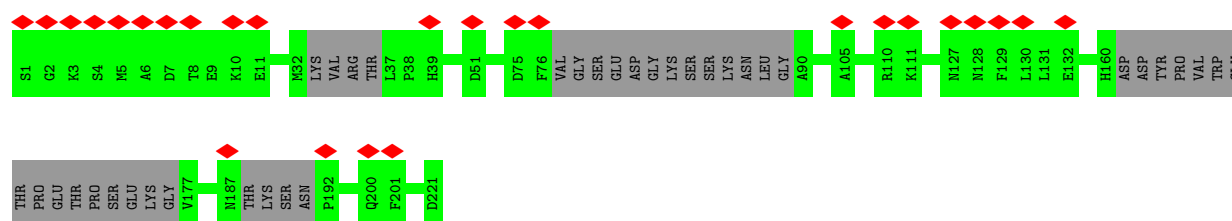
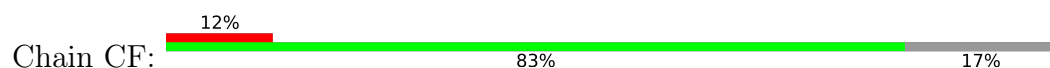
- Molecule 3: Flagellar coiling protein B (FcpB)



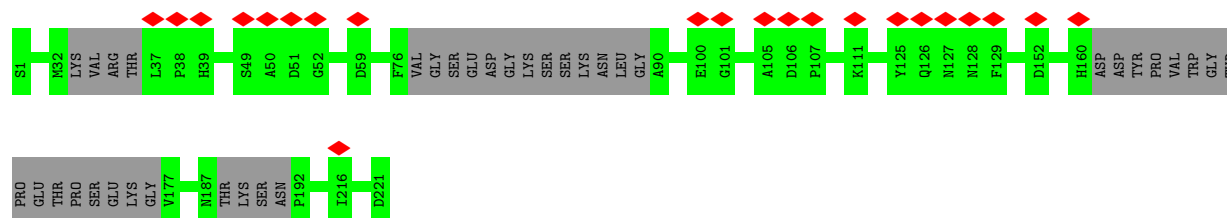
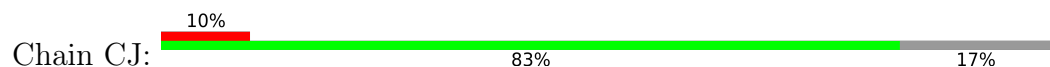
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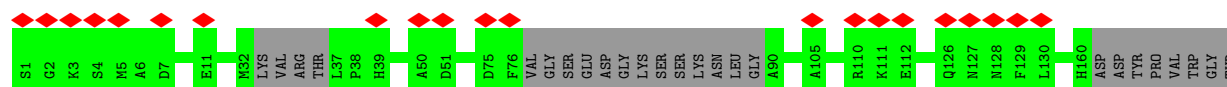
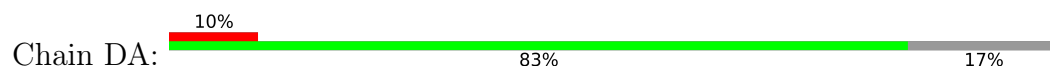
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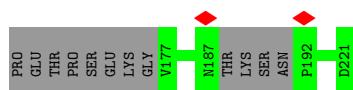


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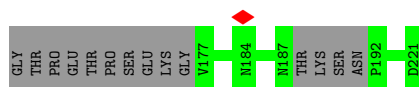
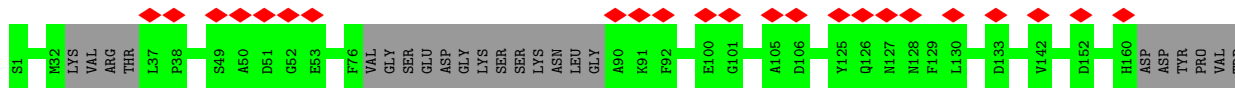
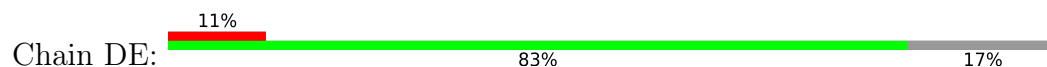


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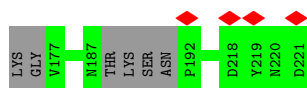
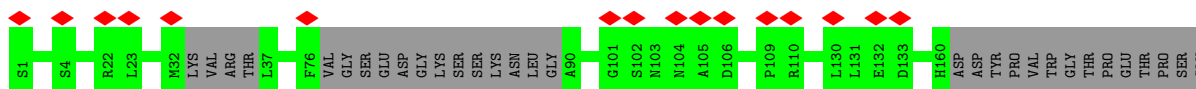
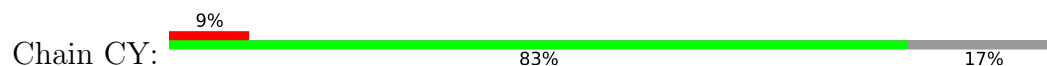




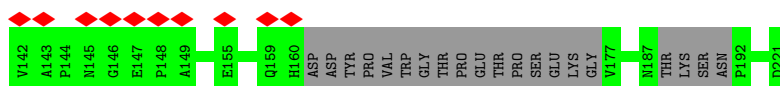
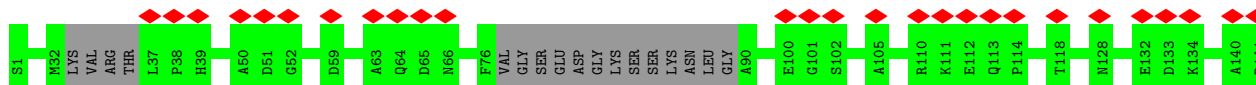
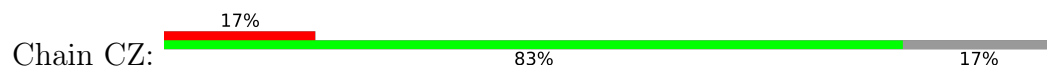
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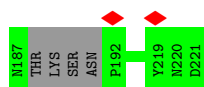
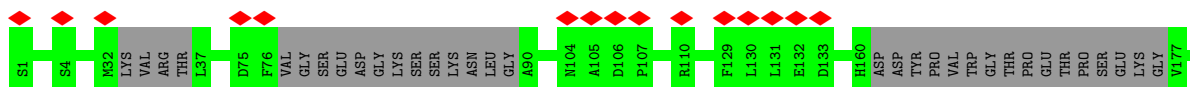
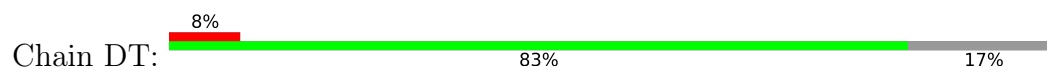
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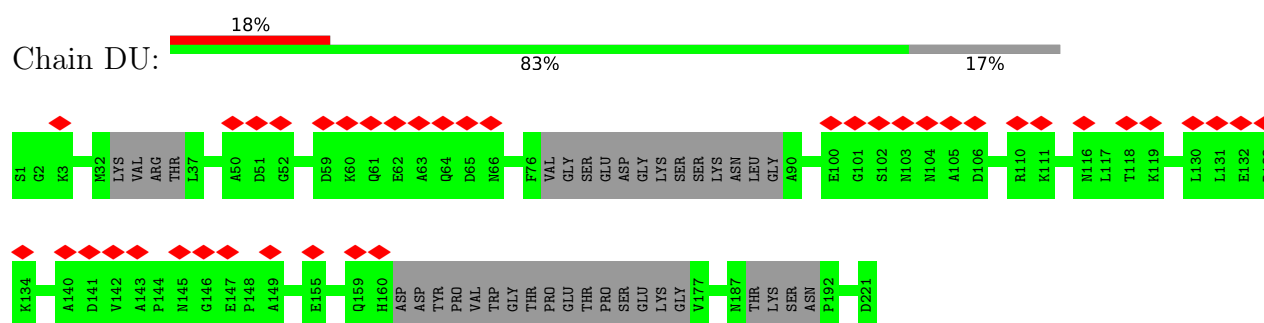
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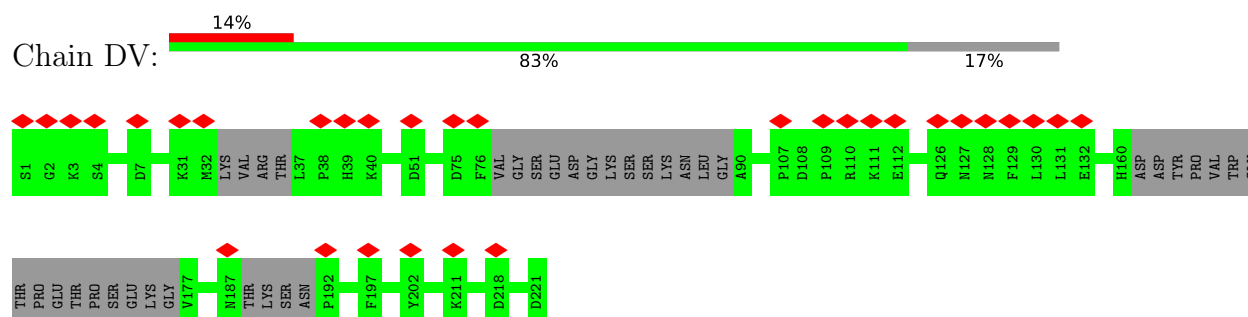
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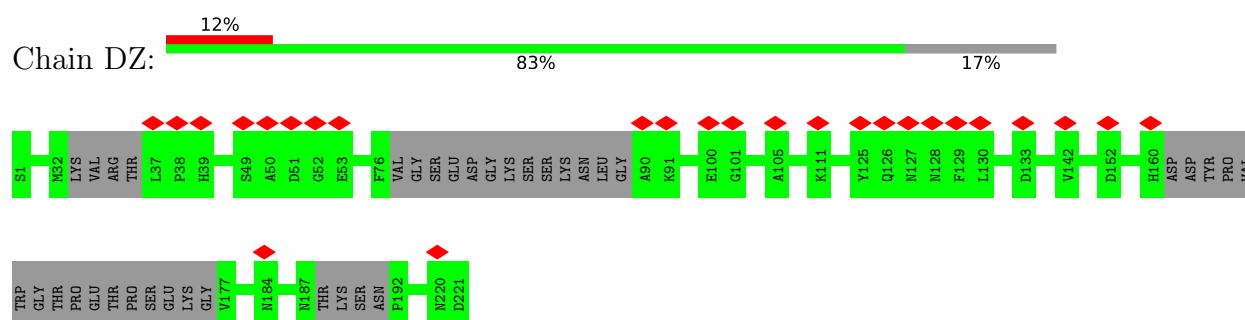
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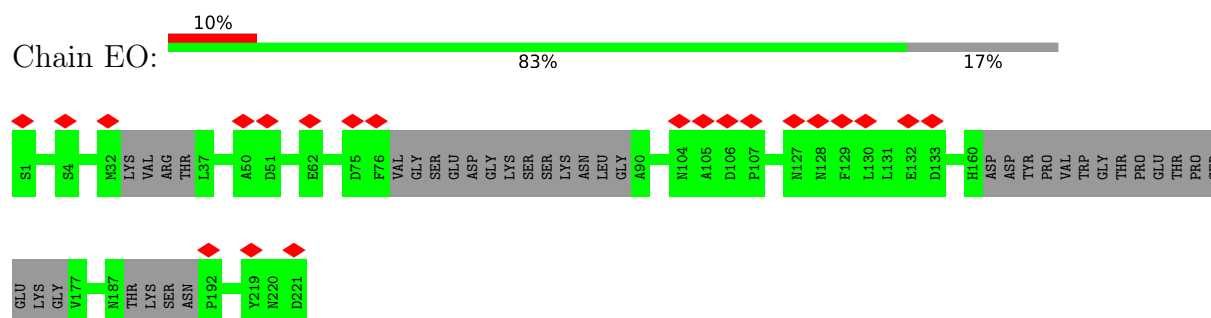
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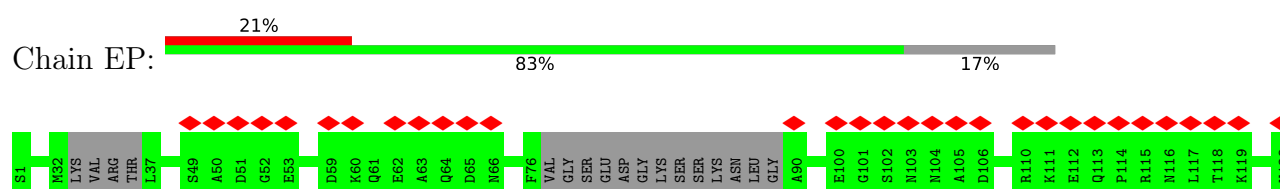
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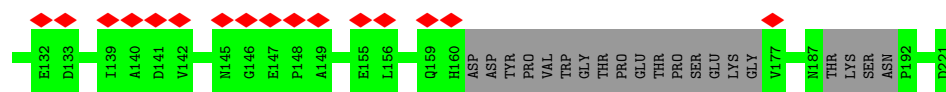


- Molecule 3: Flagellar coiling protein B (FcpB)

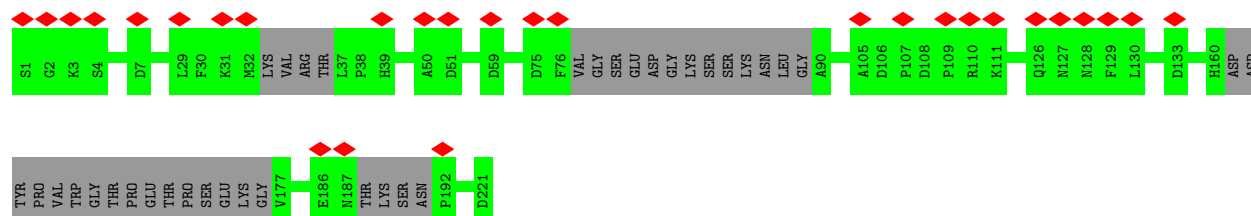
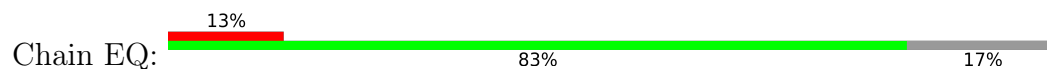


- Molecule 3: Flagellar coiling protein B (FcpB)

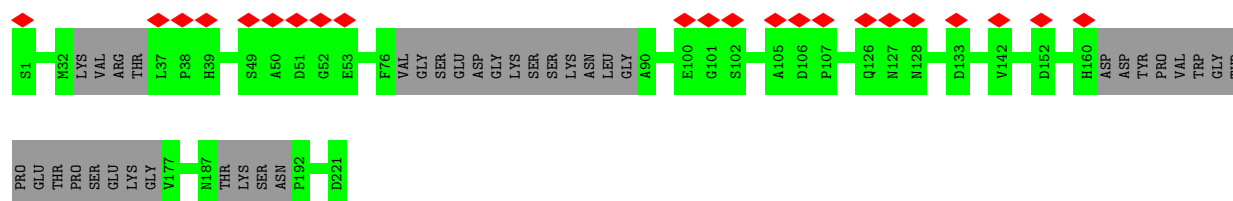
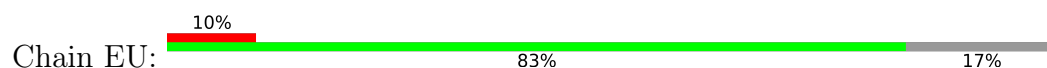




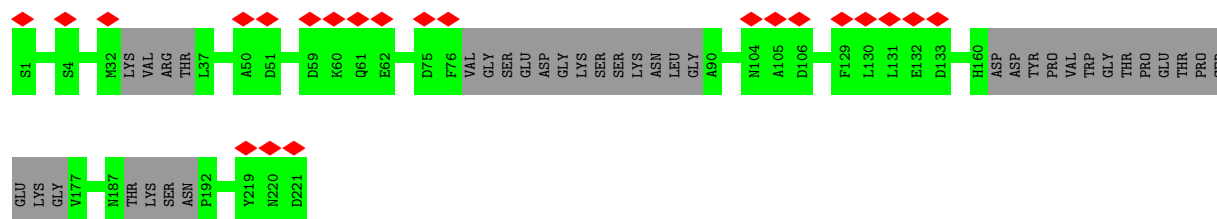
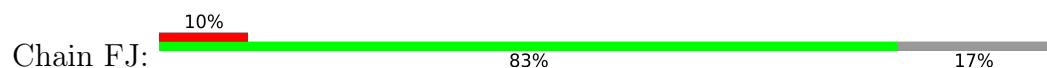
• Molecule 3: Flagellar coiling protein B (FcpB)



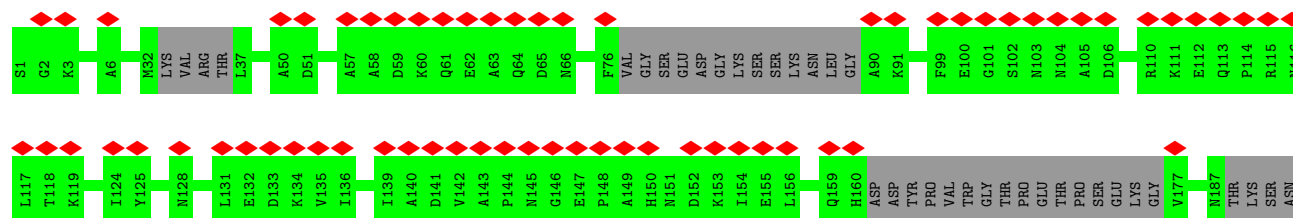
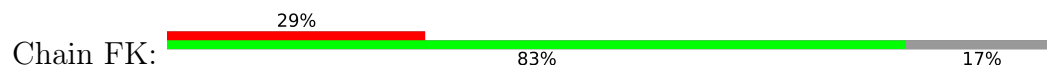
• Molecule 3: Flagellar coiling protein B (FcpB)



• Molecule 3: Flagellar coiling protein B (FcpB)

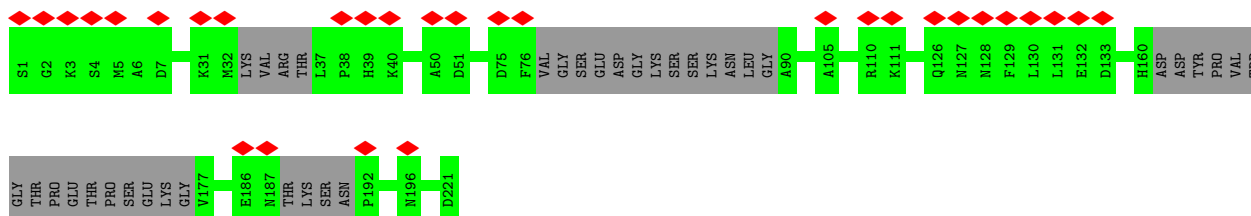
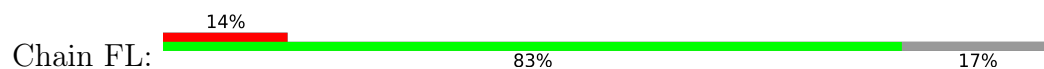


• Molecule 3: Flagellar coiling protein B (FcpB)

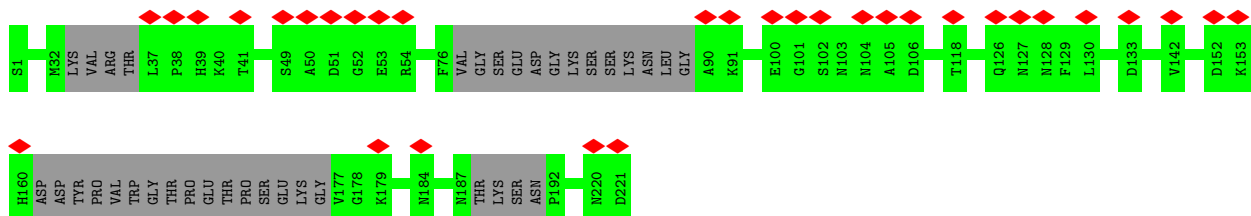
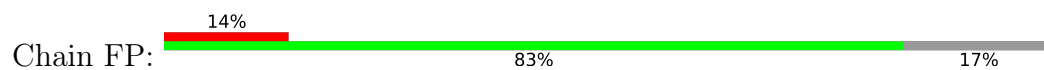




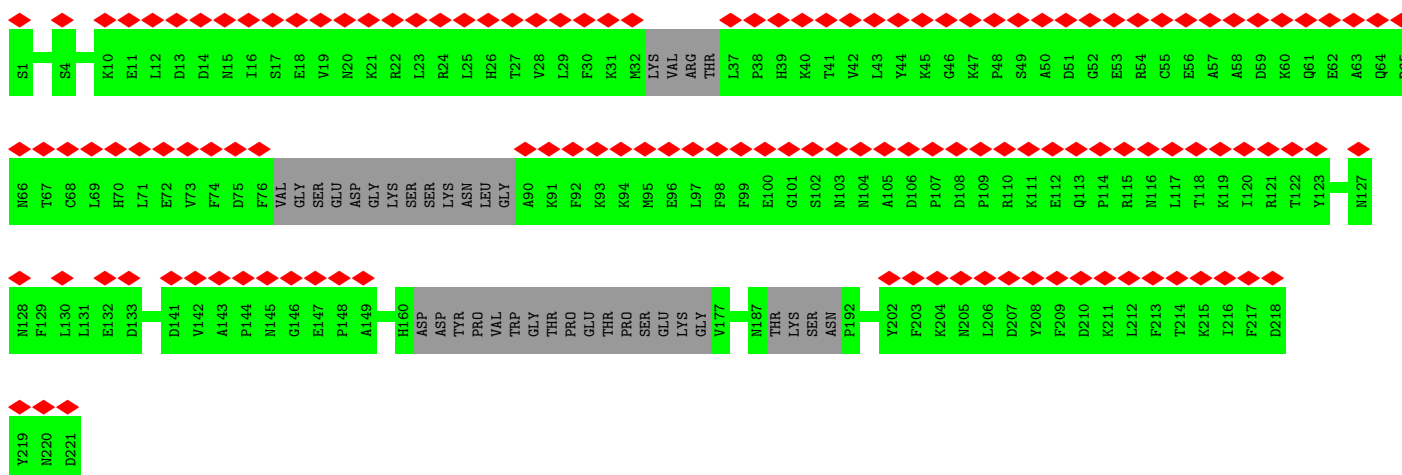
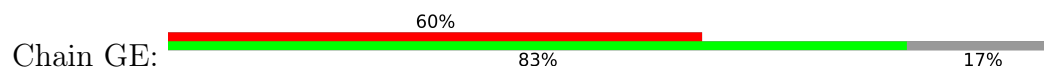
- Molecule 3: Flagellar coiling protein B (FcpB)



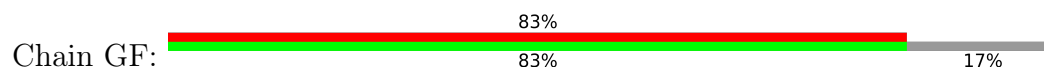
- Molecule 3: Flagellar coiling protein B (FcpB)

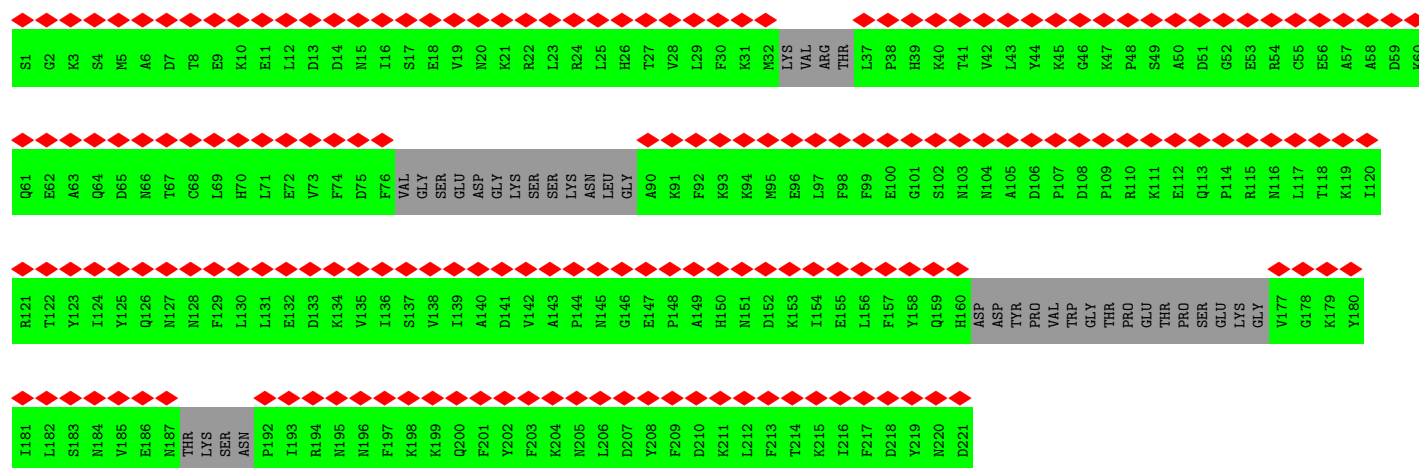


- Molecule 3: Flagellar coiling protein B (FcpB)

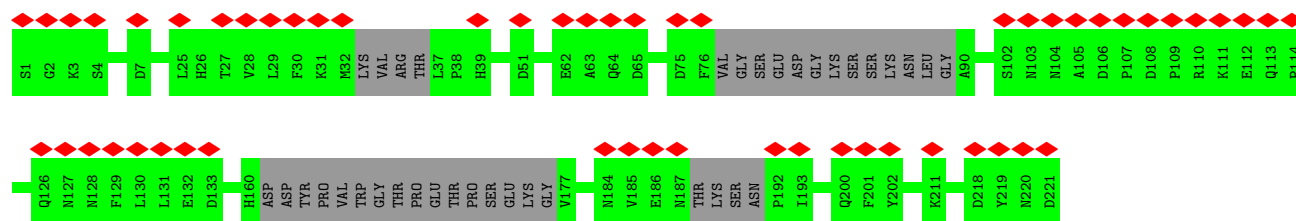
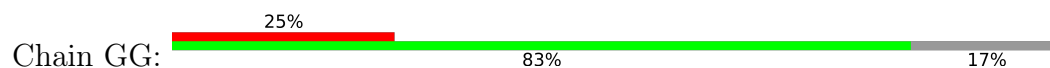


- Molecule 3: Flagellar coiling protein B (FcpB)

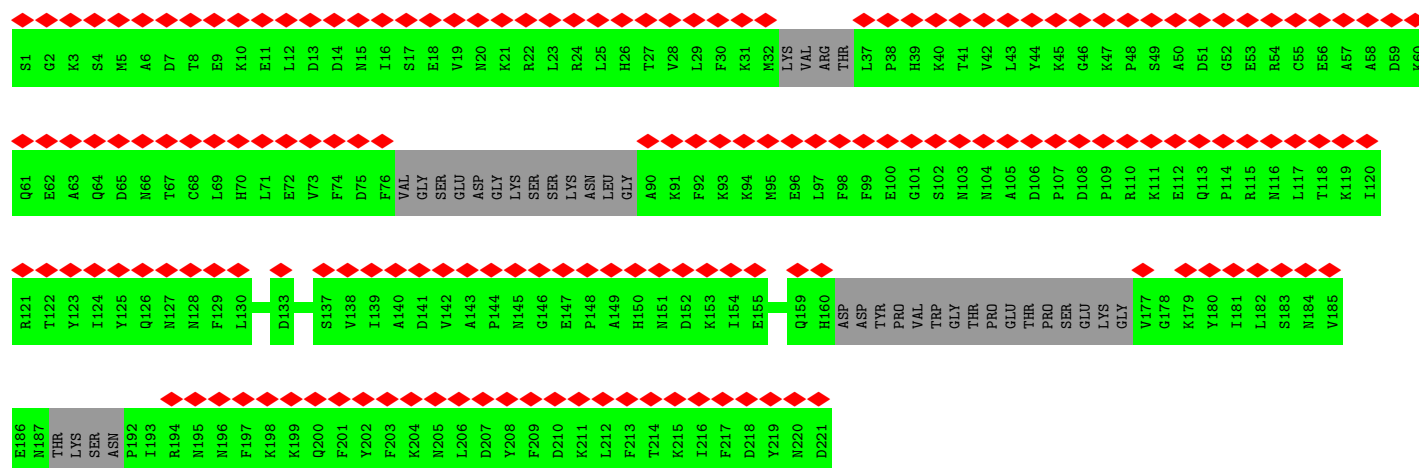
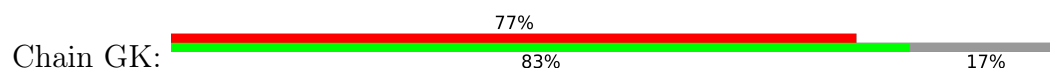




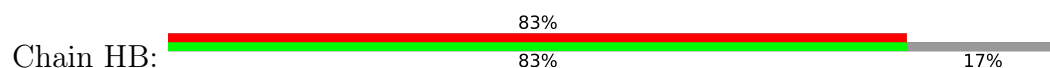
• Molecule 3: Flagellar coiling protein B (FcpB)

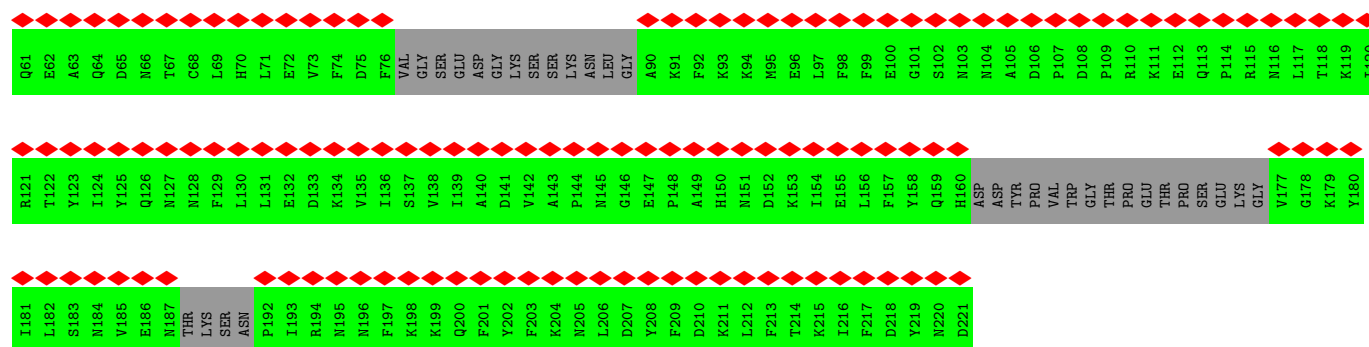


• Molecule 3: Flagellar coiling protein B (FcpB)

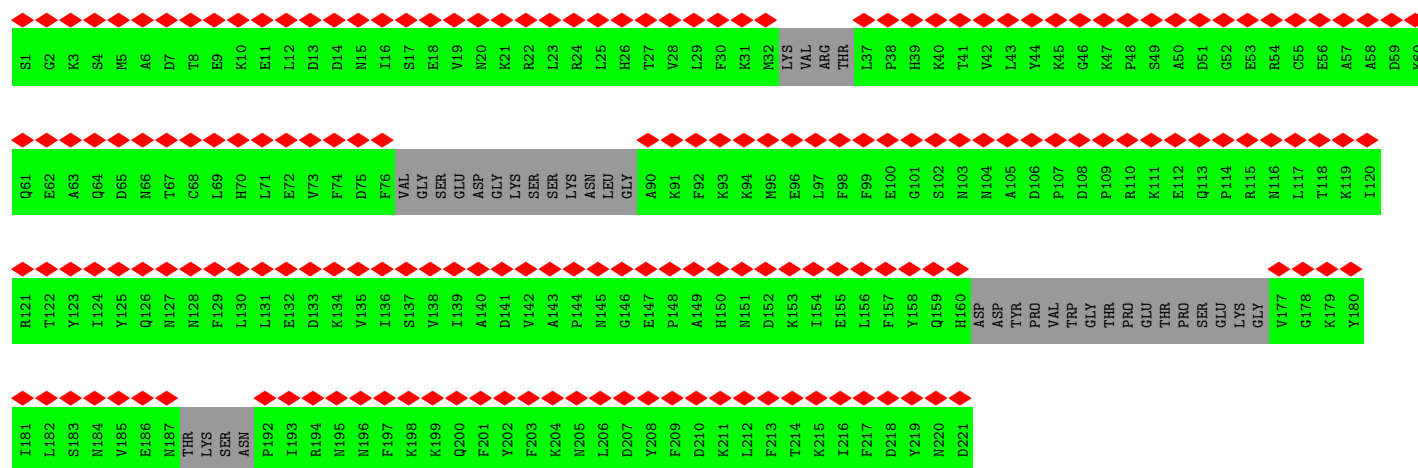
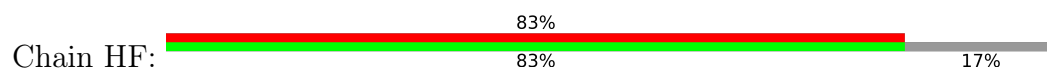


• Molecule 3: Flagellar coiling protein B (FcpB)

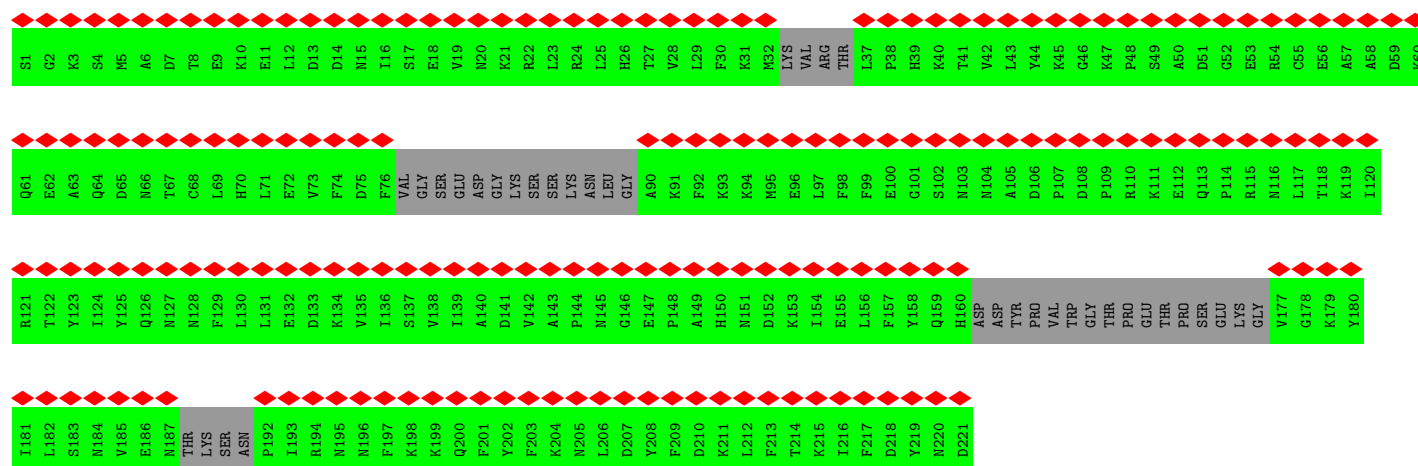
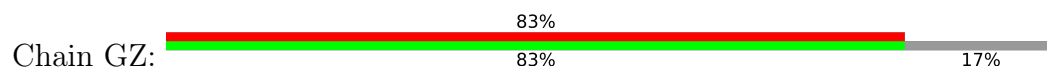




• Molecule 3: Flagellar coiling protein B (FcpB)



• Molecule 3: Flagellar coiling protein B (FcpB)



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	10581	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation was initially done in IMOD.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.7	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	19230	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.010	Depositor
Minimum map value	-3.804	Depositor
Average map value	0.158	Depositor
Map value standard deviation	0.895	Depositor
Recommended contour level	3.15	Depositor
Map size (\AA)	499.96802, 499.96802, 499.96802	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.604, 2.604, 2.604	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	AG	0.40	0/1059	0.67	0/1322
1	AH	0.40	0/1059	0.67	0/1322
1	AI	0.40	0/1059	0.67	0/1322
1	AR	0.40	0/1059	0.67	0/1322
1	BA	0.40	0/1059	0.67	0/1322
1	BB	0.40	0/1059	0.67	0/1322
1	BC	0.40	0/1059	0.67	0/1322
1	BD	0.40	0/1059	0.67	0/1322
1	BL	0.40	0/1059	0.67	0/1322
1	BM	0.40	0/1059	0.67	0/1322
1	BS	0.40	0/1059	0.67	0/1322
1	BT	0.40	0/1059	0.67	0/1322
1	BU	0.40	0/1059	0.67	0/1322
1	BV	0.41	0/1059	0.67	0/1322
1	BW	0.40	0/1059	0.67	0/1322
1	BX	0.40	0/1059	0.67	0/1322
1	BY	0.40	0/1059	0.67	0/1322
1	CG	0.41	0/1059	0.67	0/1322
1	CH	0.40	0/1059	0.67	0/1322
1	CL	0.40	0/1059	0.67	0/1322
1	CM	0.40	0/1059	0.67	0/1322
1	CN	0.40	0/1059	0.67	0/1322
1	CO	0.40	0/1059	0.67	0/1322
1	CP	0.40	0/1059	0.67	0/1322
1	CQ	0.41	0/1059	0.67	0/1322
1	CR	0.40	0/1059	0.67	0/1322
1	CS	0.40	0/1059	0.67	0/1322
1	CT	0.40	0/1059	0.67	0/1322
1	DB	0.40	0/1059	0.67	0/1322
1	DC	0.40	0/1059	0.67	0/1322
1	DG	0.40	0/1059	0.67	0/1322
1	DH	0.40	0/1059	0.67	0/1322
1	DI	0.40	0/1059	0.67	0/1322
1	DJ	0.40	0/1059	0.67	0/1322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	DK	0.40	0/1059	0.67	0/1322
1	DL	0.40	0/1059	0.67	0/1322
1	DM	0.40	0/1059	0.67	0/1322
1	DN	0.40	0/1059	0.67	0/1322
1	DO	0.40	0/1059	0.67	0/1322
1	DW	0.40	0/1059	0.67	0/1322
1	DX	0.40	0/1059	0.67	0/1322
1	EB	0.40	0/1059	0.67	0/1322
1	EC	0.40	0/1059	0.67	0/1322
1	ED	0.40	0/1059	0.67	0/1322
1	EE	0.40	0/1059	0.67	0/1322
1	EF	0.40	0/1059	0.67	0/1322
1	EG	0.40	0/1059	0.67	0/1322
1	EH	0.40	0/1059	0.67	0/1322
1	EI	0.41	0/1059	0.67	0/1322
1	EJ	0.40	0/1059	0.67	0/1322
1	ER	0.41	0/1059	0.67	0/1322
1	ES	0.40	0/1059	0.67	0/1322
1	EW	0.41	0/1059	0.67	0/1322
1	EX	0.40	0/1059	0.67	0/1322
1	EY	0.40	0/1059	0.67	0/1322
1	EZ	0.40	0/1059	0.67	0/1322
1	FA	0.40	0/1059	0.67	0/1322
1	FB	0.40	0/1059	0.67	0/1322
1	FC	0.40	0/1059	0.67	0/1322
1	FD	0.40	0/1059	0.67	0/1322
1	FE	0.40	0/1059	0.67	0/1322
1	FM	0.41	0/1059	0.67	0/1322
1	FN	0.40	0/1059	0.67	0/1322
1	FR	0.40	0/1059	0.67	0/1322
1	FS	0.41	0/1059	0.67	0/1322
1	FT	0.40	0/1059	0.67	0/1322
1	FU	0.40	0/1059	0.67	0/1322
1	FV	0.40	0/1059	0.67	0/1322
1	FW	0.40	0/1059	0.67	0/1322
1	FX	0.40	0/1059	0.67	0/1322
1	GH	0.40	0/1059	0.67	0/1322
1	GI	0.40	0/1059	0.67	0/1322
1	GM	0.40	0/1059	0.67	0/1322
1	GN	0.40	0/1059	0.67	0/1322
1	GO	0.40	0/1059	0.67	0/1322
1	GP	0.40	0/1059	0.67	0/1322
1	GQ	0.40	0/1059	0.67	0/1322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GR	0.41	0/1059	0.67	0/1322
1	HC	0.40	0/1059	0.67	0/1322
1	HH	0.40	0/1059	0.67	0/1322
1	HI	0.40	0/1059	0.67	0/1322
1	HJ	0.40	0/1059	0.67	0/1322
1	HK	0.40	0/1059	0.67	0/1322
1	HL	0.40	0/1059	0.67	0/1322
2	AL	0.57	0/947	0.55	0/1182
2	AM	0.57	0/947	0.55	0/1182
2	AU	0.57	0/947	0.55	0/1182
2	BE	0.57	0/947	0.55	0/1182
2	BF	0.57	0/947	0.55	0/1182
2	BG	0.57	0/947	0.55	0/1182
2	BH	0.57	0/947	0.55	0/1182
2	BN	0.57	0/947	0.55	0/1182
2	BP	0.57	0/947	0.55	0/1182
2	BZ	0.57	0/947	0.55	0/1182
2	CA	0.57	0/947	0.55	0/1182
2	CB	0.57	0/947	0.55	0/1182
2	CC	0.57	0/947	0.55	0/1182
2	CI	0.57	0/947	0.55	0/1182
2	CK	0.57	0/947	0.55	0/1182
2	CU	0.57	0/947	0.55	0/1182
2	CV	0.57	0/947	0.55	0/1182
2	CW	0.57	0/947	0.55	0/1182
2	CX	0.57	0/947	0.55	0/1182
2	DD	0.57	0/947	0.55	0/1182
2	DF	0.57	0/947	0.55	0/1182
2	DP	0.57	0/947	0.55	0/1182
2	DQ	0.57	0/947	0.55	0/1182
2	DR	0.57	0/947	0.55	0/1182
2	DS	0.57	0/947	0.55	0/1182
2	DY	0.57	0/947	0.55	0/1182
2	EA	0.57	0/947	0.55	0/1182
2	EK	0.57	0/947	0.55	0/1182
2	EL	0.57	0/947	0.55	0/1182
2	EM	0.57	0/947	0.55	0/1182
2	EN	0.57	0/947	0.55	0/1182
2	ET	0.57	0/947	0.55	0/1182
2	EV	0.57	0/947	0.55	0/1182
2	FF	0.57	0/947	0.55	0/1182
2	FG	0.57	0/947	0.55	0/1182
2	FH	0.57	0/947	0.55	0/1182

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	FI	0.57	0/947	0.55	0/1182
2	FO	0.57	0/947	0.55	0/1182
2	FQ	0.57	0/947	0.55	0/1182
2	GA	0.57	0/947	0.55	0/1182
2	GB	0.57	0/947	0.55	0/1182
2	GC	0.57	0/947	0.55	0/1182
2	GJ	0.57	0/947	0.55	0/1182
2	GL	0.57	0/947	0.55	0/1182
2	GV	0.57	0/947	0.55	0/1182
2	GW	0.58	0/947	0.55	0/1182
2	HE	0.57	0/947	0.55	0/1182
3	AO	0.47	0/731	0.73	0/905
3	BI	0.47	0/731	0.73	0/905
3	BJ	0.46	0/731	0.73	0/905
3	BK	0.47	0/731	0.73	0/905
3	BO	0.47	0/731	0.73	0/905
3	CD	0.46	0/731	0.73	0/905
3	CE	0.46	0/731	0.73	0/905
3	CF	0.46	0/731	0.73	0/905
3	CJ	0.47	0/731	0.73	0/905
3	CY	0.47	0/731	0.73	0/905
3	CZ	0.46	0/731	0.73	0/905
3	DA	0.46	0/731	0.73	0/905
3	DE	0.47	0/731	0.73	0/905
3	DT	0.47	0/731	0.73	0/905
3	DU	0.46	0/731	0.73	0/905
3	DV	0.47	0/731	0.73	0/905
3	DZ	0.46	0/731	0.73	0/905
3	EO	0.47	0/731	0.73	0/905
3	EP	0.46	0/731	0.73	0/905
3	EQ	0.46	0/731	0.73	0/905
3	EU	0.46	0/731	0.73	0/905
3	FJ	0.47	0/731	0.73	0/905
3	FK	0.46	0/731	0.73	0/905
3	FL	0.47	0/731	0.73	0/905
3	FP	0.47	0/731	0.73	0/905
3	GE	0.47	0/731	0.73	0/905
3	GF	0.46	0/731	0.73	0/905
3	GG	0.46	0/731	0.73	0/905
3	GK	0.46	0/731	0.73	0/905
3	GZ	0.46	0/731	0.73	0/905
3	HB	0.46	0/731	0.73	0/905
3	HF	0.46	0/731	0.73	0/905

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.47	0/156857	0.65	0/195562

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AG	0	2
1	AH	0	2
1	AI	0	2
1	AR	0	2
1	BA	0	2
1	BB	0	2
1	BC	0	2
1	BD	0	1
1	BL	0	2
1	BM	0	2
1	BS	0	2
1	BT	0	2
1	BU	0	2
1	BV	0	2
1	BW	0	2
1	BX	0	2
1	BY	0	1
1	CG	0	2
1	CH	0	2
1	CL	0	2
1	CM	0	2
1	CN	0	2
1	CO	0	2
1	CP	0	2
1	CQ	0	2
1	CR	0	2
1	CS	0	2
1	CT	0	2
1	DB	0	2
1	DC	0	2
1	DG	0	2
1	DH	0	2
1	DI	0	2
1	DJ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	DK	0	2
1	DL	0	2
1	DM	0	2
1	DN	0	2
1	DO	0	2
1	DW	0	2
1	DX	0	2
1	EB	0	2
1	EC	0	2
1	ED	0	2
1	EE	0	2
1	EF	0	2
1	EG	0	2
1	EH	0	2
1	EI	0	2
1	EJ	0	2
1	ER	0	2
1	ES	0	2
1	EW	0	2
1	EX	0	2
1	EY	0	2
1	EZ	0	2
1	FA	0	2
1	FB	0	2
1	FC	0	2
1	FD	0	2
1	FE	0	2
1	FM	0	2
1	FN	0	2
1	FR	0	2
1	FS	0	2
1	FT	0	2
1	FU	0	2
1	FV	0	2
1	FW	0	2
1	FX	0	2
1	GH	0	2
1	GI	0	2
1	GM	0	2
1	GN	0	2
1	GO	0	2
1	GP	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	GQ	0	2
1	GR	0	2
1	HC	0	2
1	HH	0	2
1	HI	0	2
1	HJ	0	2
1	HK	0	2
1	HL	0	2
All	All	0	166

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (166) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AG	140	PHE	Mainchain,Peptide
1	AH	140	PHE	Mainchain,Peptide
1	AI	140	PHE	Mainchain,Peptide
1	AR	140	PHE	Mainchain,Peptide
1	BA	140	PHE	Mainchain,Peptide
1	BB	140	PHE	Mainchain,Peptide
1	BC	140	PHE	Mainchain,Peptide
1	BD	140	PHE	Mainchain
1	BL	140	PHE	Mainchain,Peptide
1	BM	140	PHE	Mainchain,Peptide
1	BS	140	PHE	Mainchain,Peptide
1	BT	140	PHE	Mainchain,Peptide
1	BU	140	PHE	Mainchain,Peptide
1	BV	140	PHE	Mainchain,Peptide
1	BW	140	PHE	Mainchain,Peptide
1	BX	140	PHE	Mainchain,Peptide
1	BY	140	PHE	Mainchain
1	CG	140	PHE	Mainchain,Peptide
1	CH	140	PHE	Mainchain,Peptide
1	CL	140	PHE	Mainchain,Peptide
1	CM	140	PHE	Mainchain,Peptide
1	CN	140	PHE	Mainchain,Peptide
1	CO	140	PHE	Mainchain,Peptide
1	CP	140	PHE	Mainchain,Peptide
1	CQ	140	PHE	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	CR	140	PHE	Mainchain,Peptide
1	CS	140	PHE	Mainchain,Peptide
1	CT	140	PHE	Mainchain,Peptide
1	DB	140	PHE	Mainchain,Peptide
1	DC	140	PHE	Mainchain,Peptide
1	DG	140	PHE	Mainchain,Peptide
1	DH	140	PHE	Mainchain,Peptide
1	DI	140	PHE	Mainchain,Peptide
1	DJ	140	PHE	Mainchain,Peptide
1	DK	140	PHE	Mainchain,Peptide
1	DL	140	PHE	Mainchain,Peptide
1	DM	140	PHE	Mainchain,Peptide
1	DN	140	PHE	Mainchain,Peptide
1	DO	140	PHE	Mainchain,Peptide
1	DW	140	PHE	Mainchain,Peptide
1	DX	140	PHE	Mainchain,Peptide
1	EB	140	PHE	Mainchain,Peptide
1	EC	140	PHE	Mainchain,Peptide
1	ED	140	PHE	Mainchain,Peptide
1	EE	140	PHE	Mainchain,Peptide
1	EF	140	PHE	Mainchain,Peptide
1	EG	140	PHE	Mainchain,Peptide
1	EH	140	PHE	Mainchain,Peptide
1	EI	140	PHE	Mainchain,Peptide
1	EJ	140	PHE	Mainchain,Peptide
1	ER	140	PHE	Mainchain,Peptide
1	ES	140	PHE	Mainchain,Peptide
1	EW	140	PHE	Mainchain,Peptide
1	EX	140	PHE	Mainchain,Peptide
1	EY	140	PHE	Mainchain,Peptide
1	EZ	140	PHE	Mainchain,Peptide
1	FA	140	PHE	Mainchain,Peptide
1	FB	140	PHE	Mainchain,Peptide
1	FC	140	PHE	Mainchain,Peptide
1	FD	140	PHE	Mainchain,Peptide
1	FE	140	PHE	Mainchain,Peptide
1	FM	140	PHE	Mainchain,Peptide
1	FN	140	PHE	Mainchain,Peptide
1	FR	140	PHE	Mainchain,Peptide
1	FS	140	PHE	Mainchain,Peptide
1	FT	140	PHE	Mainchain,Peptide
1	FU	140	PHE	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	FV	140	PHE	Mainchain,Peptide
1	FW	140	PHE	Mainchain,Peptide
1	FX	140	PHE	Mainchain,Peptide
1	GH	140	PHE	Mainchain,Peptide
1	GI	140	PHE	Mainchain,Peptide
1	GM	140	PHE	Mainchain,Peptide
1	GN	140	PHE	Mainchain,Peptide
1	GO	140	PHE	Mainchain,Peptide
1	GP	140	PHE	Mainchain,Peptide
1	GQ	140	PHE	Mainchain,Peptide
1	GR	140	PHE	Mainchain,Peptide
1	HC	140	PHE	Mainchain,Peptide
1	HH	140	PHE	Mainchain,Peptide
1	HI	140	PHE	Mainchain,Peptide
1	HJ	140	PHE	Mainchain,Peptide
1	HK	140	PHE	Mainchain,Peptide
1	HL	140	PHE	Mainchain,Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AG	1060	0	295	1	0
1	AH	1060	0	295	1	0
1	AI	1060	0	295	0	0
1	AR	1060	0	295	2	0
1	BA	1060	0	295	4	0
1	BB	1060	0	295	1	0
1	BC	1060	0	295	2	0
1	BD	1060	0	295	2	0
1	BL	1060	0	295	1	0
1	BM	1060	0	295	1	0
1	BS	1060	0	295	1	0
1	BT	1060	0	295	0	0
1	BU	1060	0	295	1	0
1	BV	1060	0	295	3	0
1	BW	1060	0	295	2	0
1	BX	1060	0	295	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BY	1060	0	295	4	0
1	CG	1060	0	295	1	0
1	CH	1060	0	295	2	0
1	CL	1060	0	295	2	0
1	CM	1060	0	295	2	0
1	CN	1060	0	295	1	0
1	CO	1060	0	295	0	0
1	CP	1060	0	295	1	0
1	CQ	1060	0	295	2	0
1	CR	1060	0	295	1	0
1	CS	1060	0	295	2	0
1	CT	1060	0	295	4	0
1	DB	1060	0	295	1	0
1	DC	1060	0	295	1	0
1	DG	1060	0	295	4	0
1	DH	1060	0	295	2	0
1	DI	1060	0	295	1	0
1	DJ	1060	0	295	1	0
1	DK	1060	0	295	1	0
1	DL	1060	0	295	3	0
1	DM	1060	0	295	1	0
1	DN	1060	0	295	2	0
1	DO	1060	0	295	3	0
1	DW	1060	0	295	1	0
1	DX	1060	0	295	2	0
1	EB	1060	0	295	4	0
1	EC	1060	0	295	2	0
1	ED	1060	0	295	0	0
1	EE	1060	0	295	1	0
1	EF	1060	0	295	2	0
1	EG	1060	0	295	4	0
1	EH	1060	0	295	2	0
1	EI	1060	0	295	2	0
1	EJ	1060	0	295	5	0
1	ER	1060	0	295	1	0
1	ES	1060	0	295	2	0
1	EW	1060	0	295	4	0
1	EX	1060	0	295	3	0
1	EY	1060	0	295	0	0
1	EZ	1060	0	295	1	0
1	FA	1060	0	295	1	0
1	FB	1060	0	295	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FC	1060	0	295	2	0
1	FD	1060	0	295	2	0
1	FE	1060	0	295	4	0
1	FM	1060	0	295	2	0
1	FN	1060	0	295	2	0
1	FR	1060	0	295	4	0
1	FS	1060	0	295	3	0
1	FT	1060	0	295	1	0
1	FU	1060	0	295	1	0
1	FV	1060	0	295	2	0
1	FW	1060	0	295	3	0
1	FX	1060	0	295	1	0
1	GH	1060	0	295	1	0
1	GI	1060	0	295	2	0
1	GM	1060	0	295	4	0
1	GN	1060	0	295	3	0
1	GO	1060	0	295	1	0
1	GP	1060	0	295	1	0
1	GQ	1060	0	295	1	0
1	GR	1060	0	295	3	0
1	HC	1060	0	295	1	0
1	HH	1060	0	295	4	0
1	HI	1060	0	295	2	0
1	HJ	1060	0	295	1	0
1	HK	1060	0	295	0	0
1	HL	1060	0	295	0	0
2	AL	948	0	236	0	0
2	AM	948	0	236	0	0
2	AU	948	0	236	1	0
2	BE	948	0	236	0	0
2	BF	948	0	236	0	0
2	BG	948	0	236	0	0
2	BH	948	0	236	0	0
2	BN	948	0	236	0	0
2	BP	948	0	236	0	0
2	BZ	948	0	236	1	0
2	CA	948	0	236	0	0
2	CB	948	0	236	0	0
2	CC	948	0	236	0	0
2	CI	948	0	236	0	0
2	CK	948	0	236	0	0
2	CU	948	0	236	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CV	948	0	236	0	0
2	CW	948	0	236	0	0
2	CX	948	0	236	0	0
2	DD	948	0	236	0	0
2	DF	948	0	236	0	0
2	DP	948	0	236	0	0
2	DQ	948	0	236	0	0
2	DR	948	0	236	0	0
2	DS	948	0	236	0	0
2	DY	948	0	236	0	0
2	EA	948	0	236	0	0
2	EK	948	0	236	1	0
2	EL	948	0	236	0	0
2	EM	948	0	236	0	0
2	EN	948	0	236	0	0
2	ET	948	0	236	0	0
2	EV	948	0	236	0	0
2	FF	948	0	236	0	0
2	FG	948	0	236	0	0
2	FH	948	0	236	0	0
2	FI	948	0	236	0	0
2	FO	948	0	236	0	0
2	FQ	948	0	236	0	0
2	GA	948	0	236	0	0
2	GB	948	0	236	0	0
2	GC	948	0	236	0	0
2	GJ	948	0	236	0	0
2	GL	948	0	236	0	0
2	GV	948	0	236	0	0
2	GW	948	0	236	0	0
2	HE	948	0	236	0	0
3	AO	736	0	187	0	0
3	BI	736	0	187	0	0
3	BJ	736	0	187	0	0
3	BK	736	0	187	0	0
3	BO	736	0	187	0	0
3	CD	736	0	187	0	0
3	CE	736	0	187	0	0
3	CF	736	0	187	0	0
3	CJ	736	0	187	0	0
3	CY	736	0	187	0	0
3	CZ	736	0	187	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	DA	736	0	187	0	0
3	DE	736	0	187	0	0
3	DT	736	0	187	0	0
3	DU	736	0	187	0	0
3	DV	736	0	187	0	0
3	DZ	736	0	187	0	0
3	EO	736	0	187	0	0
3	EP	736	0	187	0	0
3	EQ	736	0	187	0	0
3	EU	736	0	187	0	0
3	FJ	736	0	187	0	0
3	FK	736	0	187	0	0
3	FL	736	0	187	0	0
3	FP	736	0	187	0	0
3	GE	736	0	187	0	0
3	GF	736	0	187	0	0
3	GG	736	0	187	0	0
3	GK	736	0	187	0	0
3	GZ	736	0	187	0	0
3	HB	736	0	187	0	0
3	HF	736	0	187	0	0
All	All	157148	0	41856	140	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 (140) 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:GM:100:GLY:HA3	1:HH:150:TRP:O	1.99	0.62
1:BY:100:GLY:CA	1:CT:150:TRP:O	2.48	0.61
1:FR:12:SER:O	1:FR:15:VAL:N	2.36	0.58
1:EJ:100:GLY:CA	1:FE:150:TRP:O	2.53	0.56
1:HH:12:SER:O	1:HH:15:VAL:N	2.38	0.56
1:DO:100:GLY:CA	1:EJ:150:TRP:O	2.56	0.54
1:DG:58:GLY:O	1:DG:62:ALA:N	2.36	0.53
1:EW:12:SER:O	1:EW:15:VAL:N	2.40	0.53
1:BD:100:GLY:CA	1:BY:150:TRP:O	2.57	0.53
2:EK:89:HIS:O	2:EK:93:LYS:N	2.35	0.52
1:BY:100:GLY:HA3	1:CT:150:TRP:O	2.10	0.51
1:GM:12:SER:O	1:GM:15:VAL:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CT:100:GLY:CA	1:DO:150:TRP:O	2.60	0.50
1:CL:100:GLY:HA3	1:DG:150:TRP:O	2.12	0.49
1:EB:10:ILE:O	1:EB:12:SER:N	2.44	0.49
1:BA:193:ASP:O	1:BA:197:THR:N	2.41	0.48
1:EX:100:GLY:HA3	1:FS:150:TRP:O	2.14	0.48
1:DG:100:GLY:HA3	1:EB:150:TRP:O	2.14	0.47
1:GM:100:GLY:CA	1:HH:150:TRP:O	2.61	0.47
2:BZ:89:HIS:O	2:BZ:93:LYS:N	2.40	0.47
1:EG:190:LYS:O	1:EG:193:ASP:N	2.47	0.47
1:ES:111:GLN:O	1:ES:115:SER:N	2.44	0.47
1:GN:100:GLY:HA3	1:HI:150:TRP:O	2.14	0.47
1:FW:193:ASP:O	1:FW:197:THR:N	2.38	0.47
1:FD:8:ALA:O	1:FD:9:ALA:C	2.54	0.46
1:EW:100:GLY:HA3	1:FR:150:TRP:O	2.16	0.46
1:BA:190:LYS:O	1:BA:194:ALA:N	2.39	0.46
1:EC:100:GLY:HA3	1:EX:150:TRP:O	2.16	0.46
1:FN:111:GLN:O	1:FN:115:SER:N	2.42	0.45
1:BM:111:GLN:O	1:BM:115:SER:N	2.45	0.45
1:DL:190:LYS:O	1:DL:193:ASP:N	2.49	0.45
1:EI:8:ALA:O	1:EI:9:ALA:C	2.53	0.45
1:AR:111:GLN:O	1:AR:115:SER:N	2.43	0.45
1:BV:190:LYS:O	1:BV:193:ASP:N	2.49	0.45
1:EJ:100:GLY:C	1:FE:150:TRP:O	2.55	0.45
1:DL:193:ASP:O	1:DL:197:THR:N	2.39	0.45
1:FW:190:LYS:O	1:FW:193:ASP:N	2.50	0.44
1:EB:10:ILE:C	1:EB:12:SER:H	2.20	0.44
1:EG:193:ASP:O	1:EG:197:THR:N	2.39	0.44
1:CH:8:ALA:O	1:CH:9:ALA:C	2.56	0.44
1:GR:193:ASP:O	1:GR:197:THR:N	2.43	0.44
2:AU:290:ILE:O	2:AU:291:ASN:C	2.56	0.43
1:GI:111:GLN:O	1:GI:115:SER:N	2.45	0.43
1:FS:100:GLY:HA3	1:GN:150:TRP:O	2.19	0.43
1:BW:8:ALA:O	1:BW:9:ALA:C	2.55	0.42
1:BC:100:GLY:C	1:BX:150:TRP:O	2.56	0.42
1:BA:35:ARG:N	1:BA:241:ARG:O	2.52	0.42
1:DC:8:ALA:O	1:DC:9:ALA:C	2.57	0.42
1:GQ:190:LYS:O	1:GQ:193:ASP:N	2.53	0.42
1:EH:8:ALA:O	1:EH:9:ALA:C	2.57	0.42
1:FC:8:ALA:O	1:FC:9:ALA:C	2.56	0.42
1:FB:190:LYS:O	1:FB:193:ASP:N	2.53	0.42
1:CS:8:ALA:O	1:CS:9:ALA:C	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DX:8:ALA:O	1:DX:9:ALA:C	2.57	0.42
1:EJ:10:ILE:O	1:EJ:12:SER:N	2.53	0.42
1:CM:100:GLY:HA3	1:DH:150:TRP:O	2.20	0.41
1:CT:271:VAL:O	1:CT:272:ARG:C	2.59	0.41
1:DO:271:VAL:O	1:DO:272:ARG:C	2.59	0.41
1:CS:271:VAL:O	1:CS:272:ARG:C	2.58	0.41
1:GR:190:LYS:O	1:GR:193:ASP:N	2.53	0.41
1:AH:271:VAL:O	1:AH:272:ARG:C	2.59	0.41
1:CL:271:VAL:O	1:CL:272:ARG:C	2.59	0.41
1:DN:271:VAL:O	1:DN:272:ARG:C	2.59	0.41
1:FV:190:LYS:O	1:FV:193:ASP:N	2.54	0.41
1:BY:271:VAL:O	1:BY:272:ARG:C	2.59	0.41
1:EF:190:LYS:O	1:EF:193:ASP:N	2.54	0.41
1:FB:271:VAL:O	1:FB:272:ARG:C	2.59	0.41
1:GI:271:VAL:O	1:GI:272:ARG:C	2.59	0.41
1:GN:271:VAL:O	1:GN:272:ARG:C	2.59	0.41
1:HI:271:VAL:O	1:HI:272:ARG:C	2.59	0.41
1:CG:271:VAL:O	1:CG:272:ARG:C	2.59	0.41
1:BV:271:VAL:O	1:BV:272:ARG:C	2.59	0.41
1:DW:271:VAL:O	1:DW:272:ARG:C	2.59	0.41
1:EC:271:VAL:O	1:EC:272:ARG:C	2.59	0.41
1:ER:271:VAL:O	1:ER:272:ARG:C	2.59	0.41
1:EZ:271:VAL:O	1:EZ:272:ARG:C	2.59	0.41
1:FT:271:VAL:O	1:FT:272:ARG:C	2.59	0.41
1:GO:271:VAL:O	1:GO:272:ARG:C	2.59	0.41
1:BV:193:ASP:O	1:BV:197:THR:N	2.40	0.41
1:DB:271:VAL:O	1:DB:272:ARG:C	2.59	0.41
1:DG:271:VAL:O	1:DG:272:ARG:C	2.59	0.41
1:GR:271:VAL:O	1:GR:272:ARG:C	2.59	0.41
1:CM:271:VAL:O	1:CM:272:ARG:C	2.59	0.41
1:CN:271:VAL:O	1:CN:272:ARG:C	2.59	0.41
1:CQ:271:VAL:O	1:CQ:272:ARG:C	2.59	0.41
1:DH:271:VAL:O	1:DH:272:ARG:C	2.59	0.41
1:EB:271:VAL:O	1:EB:272:ARG:C	2.59	0.41
1:FC:271:VAL:O	1:FC:272:ARG:C	2.59	0.41
1:EX:271:VAL:O	1:EX:272:ARG:C	2.59	0.41
1:FS:271:VAL:O	1:FS:272:ARG:C	2.59	0.41
1:FX:271:VAL:O	1:FX:272:ARG:C	2.59	0.41
1:AG:271:VAL:O	1:AG:272:ARG:C	2.59	0.41
1:BL:271:VAL:O	1:BL:272:ARG:C	2.59	0.41
1:BW:271:VAL:O	1:BW:272:ARG:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BX:271:VAL:O	1:BX:272:ARG:C	2.59	0.41
1:CQ:190:LYS:O	1:CQ:193:ASP:N	2.53	0.41
1:DM:271:VAL:O	1:DM:272:ARG:C	2.59	0.41
1:EG:271:VAL:O	1:EG:272:ARG:C	2.59	0.41
1:EI:271:VAL:O	1:EI:272:ARG:C	2.59	0.41
1:FB:190:LYS:O	1:FB:194:ALA:N	2.41	0.41
1:FM:271:VAL:O	1:FM:272:ARG:C	2.59	0.41
1:GH:271:VAL:O	1:GH:272:ARG:C	2.59	0.41
1:FR:271:VAL:O	1:FR:272:ARG:C	2.59	0.41
1:FW:271:VAL:O	1:FW:272:ARG:C	2.59	0.41
1:GM:271:VAL:O	1:GM:272:ARG:C	2.59	0.41
1:HJ:271:VAL:O	1:HJ:272:ARG:C	2.59	0.41
1:DI:271:VAL:O	1:DI:272:ARG:C	2.59	0.41
1:EF:271:VAL:O	1:EF:272:ARG:C	2.60	0.41
1:ES:271:VAL:O	1:ES:272:ARG:C	2.60	0.41
1:FA:271:VAL:O	1:FA:272:ARG:C	2.60	0.41
1:FM:189:ASP:O	1:FM:190:LYS:C	2.59	0.41
1:FN:271:VAL:O	1:FN:272:ARG:C	2.59	0.41
1:BA:271:VAL:O	1:BA:272:ARG:C	2.59	0.40
1:BC:271:VAL:O	1:BC:272:ARG:C	2.59	0.40
1:CH:271:VAL:O	1:CH:272:ARG:C	2.59	0.40
1:DK:271:VAL:O	1:DK:272:ARG:C	2.60	0.40
1:EH:271:VAL:O	1:EH:272:ARG:C	2.59	0.40
1:FE:271:VAL:O	1:FE:272:ARG:C	2.59	0.40
1:FV:271:VAL:O	1:FV:272:ARG:C	2.60	0.40
1:HC:271:VAL:O	1:HC:272:ARG:C	2.59	0.40
1:DJ:271:VAL:O	1:DJ:272:ARG:C	2.59	0.40
1:EG:190:LYS:O	1:EG:194:ALA:N	2.45	0.40
1:EJ:100:GLY:HA3	1:FE:150:TRP:O	2.20	0.40
1:FD:271:VAL:O	1:FD:272:ARG:C	2.58	0.40
1:BB:271:VAL:O	1:BB:272:ARG:C	2.59	0.40
1:BS:271:VAL:O	1:BS:272:ARG:C	2.59	0.40
1:BU:271:VAL:O	1:BU:272:ARG:C	2.60	0.40
1:DL:271:VAL:O	1:DL:272:ARG:C	2.59	0.40
1:DX:271:VAL:O	1:DX:272:ARG:C	2.59	0.40
1:AR:271:VAL:O	1:AR:272:ARG:C	2.59	0.40
1:BD:271:VAL:O	1:BD:272:ARG:C	2.59	0.40
1:CP:271:VAL:O	1:CP:272:ARG:C	2.60	0.40
1:CR:271:VAL:O	1:CR:272:ARG:C	2.59	0.40
1:DN:8:ALA:O	1:DN:9:ALA:C	2.57	0.40
1:EE:271:VAL:O	1:EE:272:ARG:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EW:271:VAL:O	1:EW:272:ARG:C	2.59	0.40
1:HH:271:VAL:O	1:HH:272:ARG:C	2.59	0.40
1:EW:100:GLY:CA	1:FR:150:TRP:O	2.70	0.40
1:FU:271:VAL:O	1:FU:272:ARG:C	2.60	0.40
1:GP:271:VAL:O	1:GP:272:ARG:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AG	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	AH	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	AI	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	AR	263/265 (99%)	254 (97%)	9 (3%)	0	100	100
1	BA	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	BB	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	BC	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	BD	263/265 (99%)	253 (96%)	9 (3%)	1 (0%)	34	72
1	BL	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	BM	263/265 (99%)	253 (96%)	10 (4%)	0	100	100
1	BS	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	BT	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	BU	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	BV	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	BW	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	BX	263/265 (99%)	249 (95%)	13 (5%)	1 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BY	263/265 (99%)	253 (96%)	9 (3%)	1 (0%)	34	72
1	CG	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	CH	263/265 (99%)	253 (96%)	10 (4%)	0	100	100
1	CL	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	CM	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	CN	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	CO	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	CP	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	CQ	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	CR	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	CS	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	CT	263/265 (99%)	253 (96%)	9 (3%)	1 (0%)	34	72
1	DB	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	DC	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	DG	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	DH	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	DI	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	DJ	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	DK	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	DL	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	DM	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	DN	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	DO	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	DW	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	DX	263/265 (99%)	253 (96%)	10 (4%)	0	100	100
1	EB	263/265 (99%)	251 (95%)	10 (4%)	2 (1%)	19	60
1	EC	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	ED	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	EE	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	EF	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	EG	263/265 (99%)	252 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EH	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	EI	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	EJ	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	ER	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	ES	263/265 (99%)	253 (96%)	10 (4%)	0	100	100
1	EW	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	EX	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	EY	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	EZ	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	FA	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	FB	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	FC	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	FD	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	FE	263/265 (99%)	253 (96%)	8 (3%)	2 (1%)	19	60
1	FM	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	FN	263/265 (99%)	253 (96%)	10 (4%)	0	100	100
1	FR	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	FS	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	FT	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	FU	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	FV	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	FW	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	FX	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	GH	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	GI	263/265 (99%)	253 (96%)	10 (4%)	0	100	100
1	GM	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	GN	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	GO	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	GP	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	GQ	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
1	GR	263/265 (99%)	250 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	HC	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	HH	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	HI	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	HJ	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	HK	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	34	72
1	HL	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	34	72
2	AL	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	AM	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	AU	235/237 (99%)	232 (99%)	2 (1%)	1 (0%)	34	72
2	BE	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	BF	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	BG	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	BH	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	BN	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	BP	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	BZ	235/237 (99%)	231 (98%)	4 (2%)	0	100	100
2	CA	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	CB	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	CC	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	CI	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	CK	235/237 (99%)	232 (99%)	2 (1%)	1 (0%)	34	72
2	CU	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	CV	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	CW	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	CX	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	DD	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	DF	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	DP	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	DQ	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	DR	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	DS	235/237 (99%)	233 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	DY	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	EA	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	EK	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	EL	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	EM	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	EN	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	ET	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	EV	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	FF	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	FG	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	FH	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	FI	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	FO	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	FQ	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	GA	235/237 (99%)	231 (98%)	4 (2%)	0	100	100
2	GB	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	GC	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	GJ	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	GL	235/237 (99%)	232 (99%)	2 (1%)	1 (0%)	34	72
2	GV	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
2	GW	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
2	HE	235/237 (99%)	233 (99%)	2 (1%)	0	100	100
3	AO	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	BI	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	BJ	174/221 (79%)	170 (98%)	4 (2%)	0	100	100
3	BK	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	BO	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	CD	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	CE	174/221 (79%)	170 (98%)	4 (2%)	0	100	100
3	CF	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	CJ	174/221 (79%)	171 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CY	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	CZ	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	DA	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	DE	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	DT	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	DU	174/221 (79%)	170 (98%)	4 (2%)	0	100	100
3	DV	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	DZ	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	EO	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	EP	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	EQ	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	EU	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	FJ	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	FK	174/221 (79%)	170 (98%)	4 (2%)	0	100	100
3	FL	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	FP	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	GE	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	GF	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	GG	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	GK	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	GZ	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	HB	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
3	HF	174/221 (79%)	171 (98%)	3 (2%)	0	100	100
All	All	38705/40471 (96%)	37532 (97%)	1131 (3%)	42 (0%)	54	86

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	EB	11	ASN
1	BU	179	SER
1	DK	179	SER
1	EJ	11	ASN
1	FV	179	SER
1	GQ	179	SER

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Mol	Chain	Res	Type
1	BD	11	ASN
1	CG	179	SER
1	DB	179	SER
1	CP	179	SER
1	DM	11	ASN
1	DW	179	SER
1	EF	179	SER
1	ER	179	SER
1	FA	179	SER
1	FM	179	SER
1	GH	179	SER
1	FU	11	ASN
1	HC	179	SER
1	HL	179	SER
2	AU	224	ASP
2	CK	224	ASP
1	BS	11	ASN
1	BT	11	ASN
1	BX	11	ASN
1	BY	11	ASN
1	CS	11	ASN
1	DL	11	ASN
1	DO	11	ASN
1	ED	11	ASN
1	EH	11	ASN
1	FC	11	ASN
1	FE	11	ASN
1	HJ	11	ASN
1	HK	11	ASN
1	CT	179	SER
1	DI	11	ASN
1	EB	179	SER
1	FE	179	SER
1	EY	179	SER
1	EZ	11	ASN
2	GL	224	ASP

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides 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.

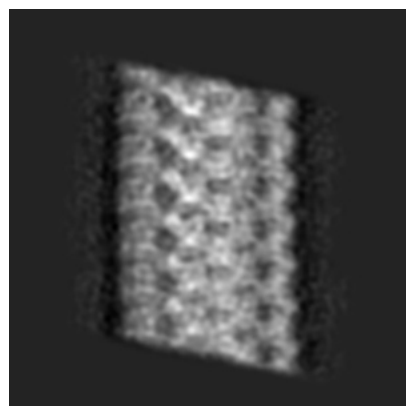
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20504. These allow visual inspection of the internal detail of the map and identification of artifacts.

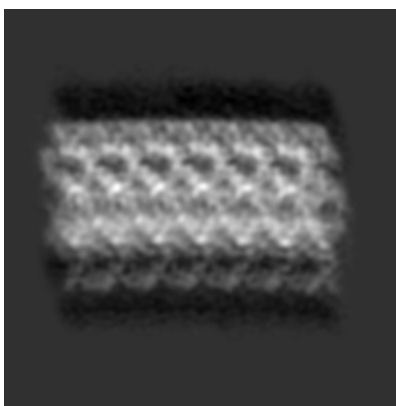
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

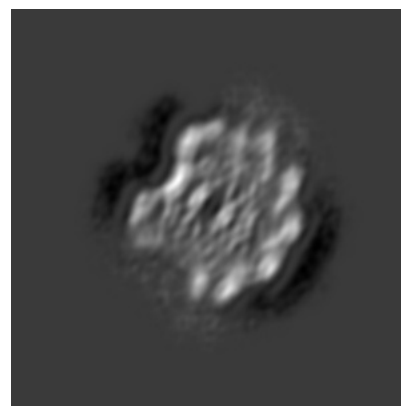
6.1.1 Primary map



X

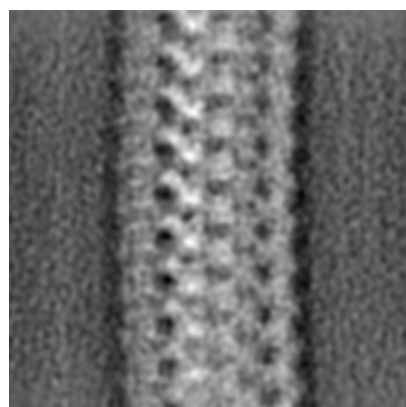


Y

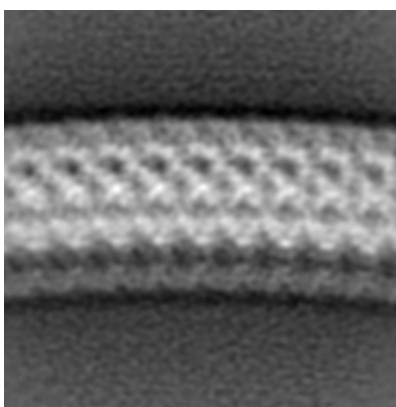


Z

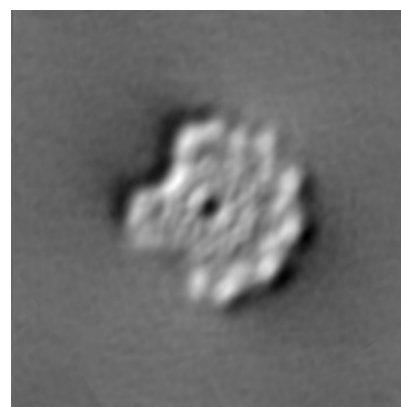
6.1.2 Raw map



X



Y

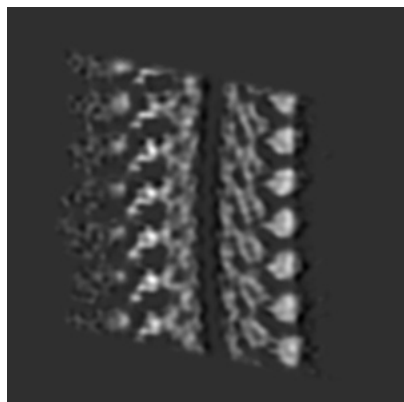


Z

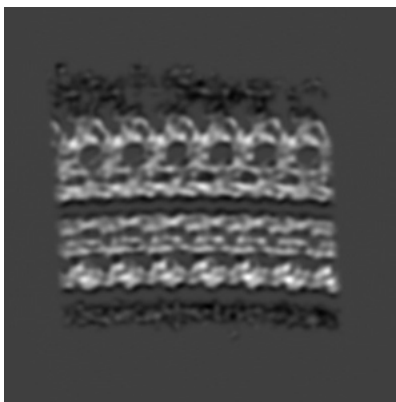
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

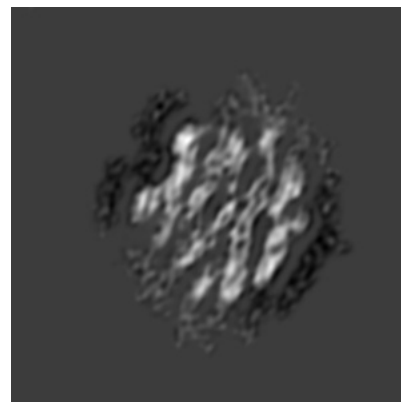
6.2.1 Primary map



X Index: 96



Y Index: 96

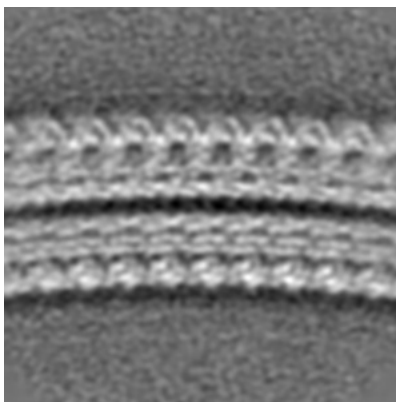


Z Index: 96

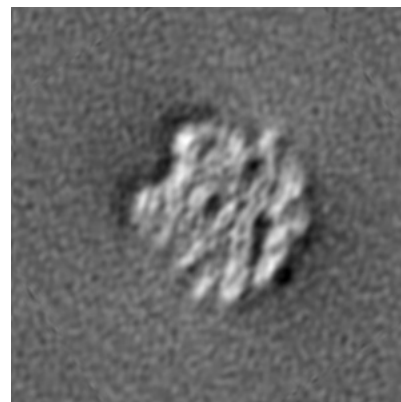
6.2.2 Raw map



X Index: 96



Y Index: 96

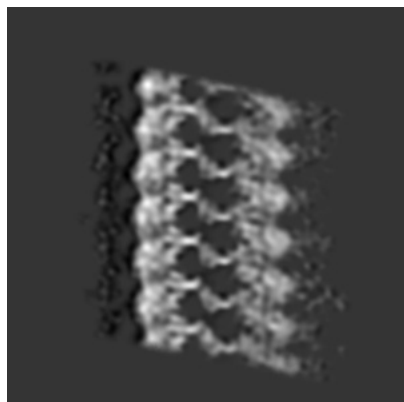


Z Index: 96

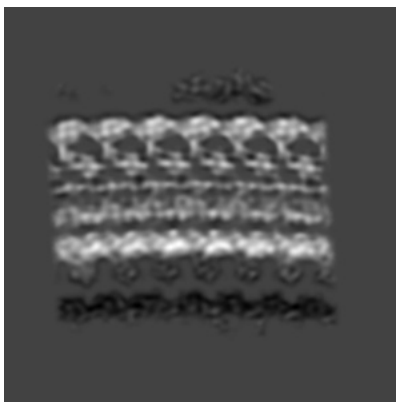
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

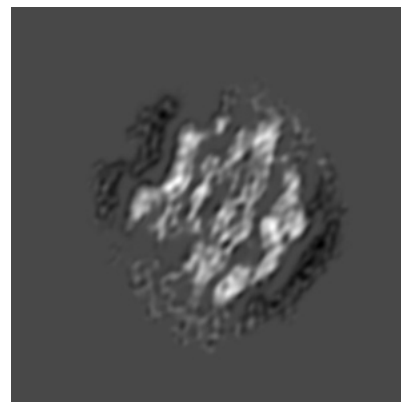
6.3.1 Primary map



X Index: 124



Y Index: 106

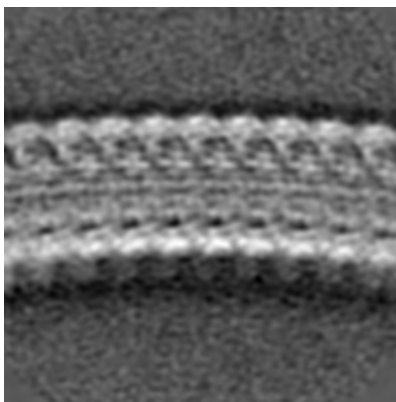


Z Index: 100

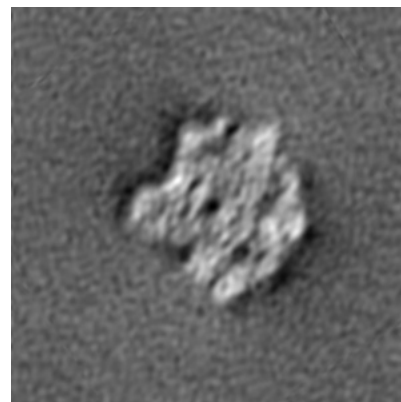
6.3.2 Raw map



X Index: 123



Y Index: 107

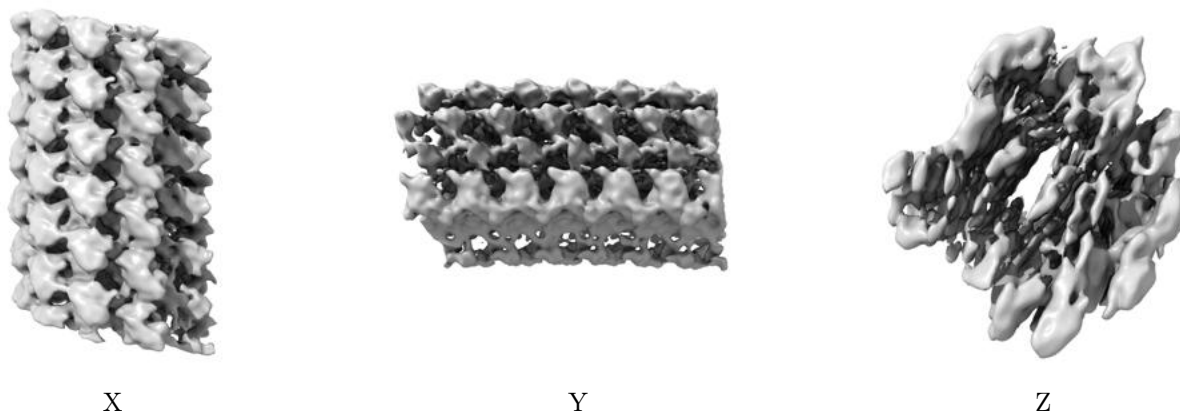


Z Index: 101

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

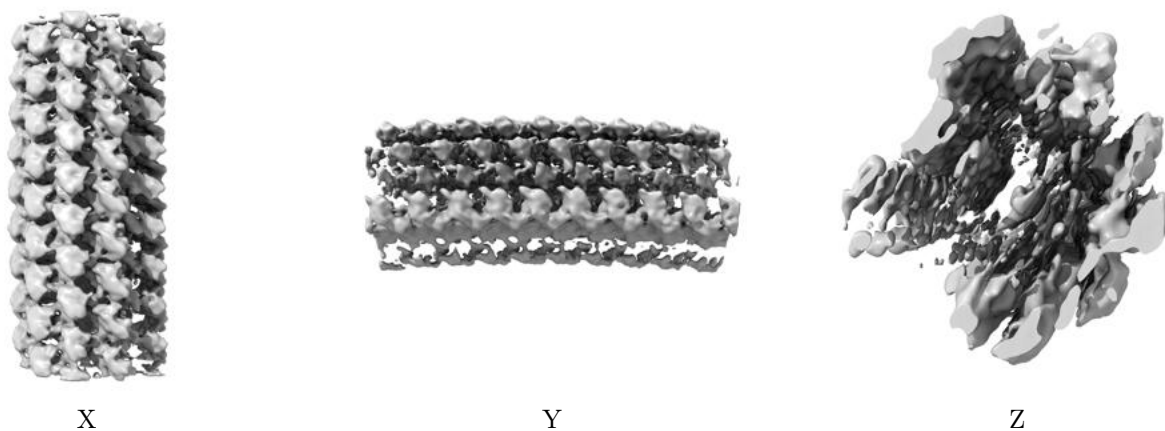
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

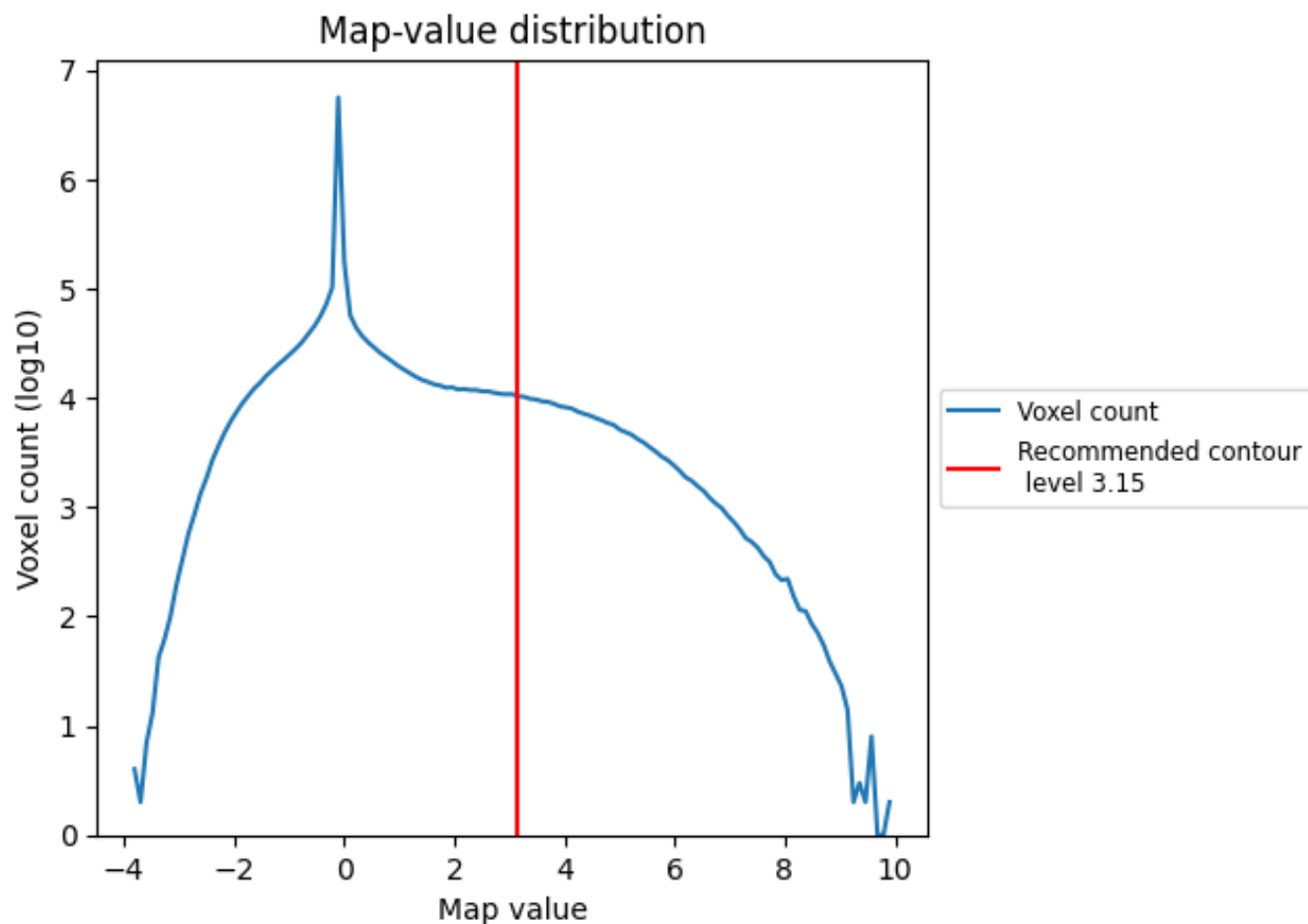
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

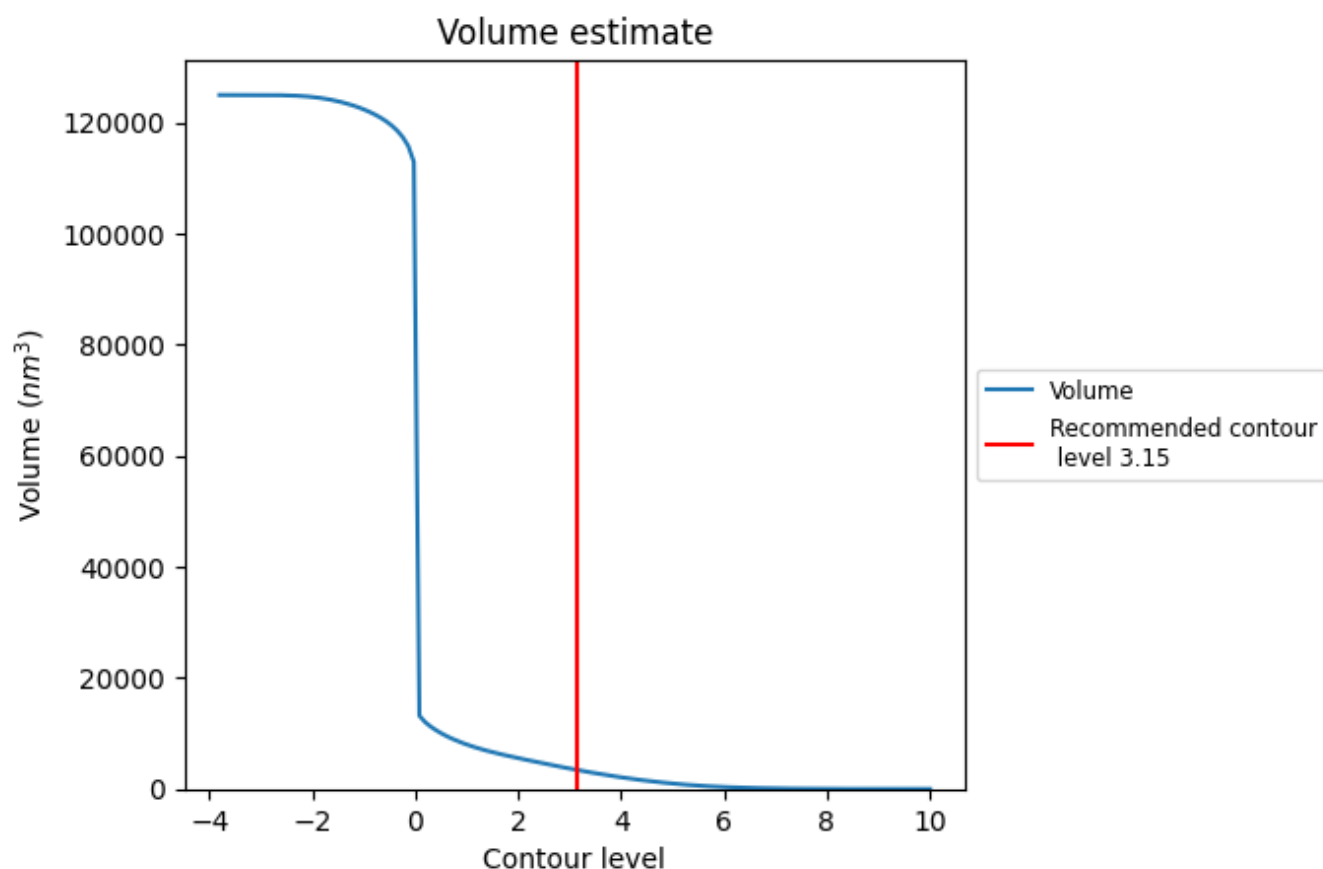
This section contains the results of statistical analysis of the map.

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.

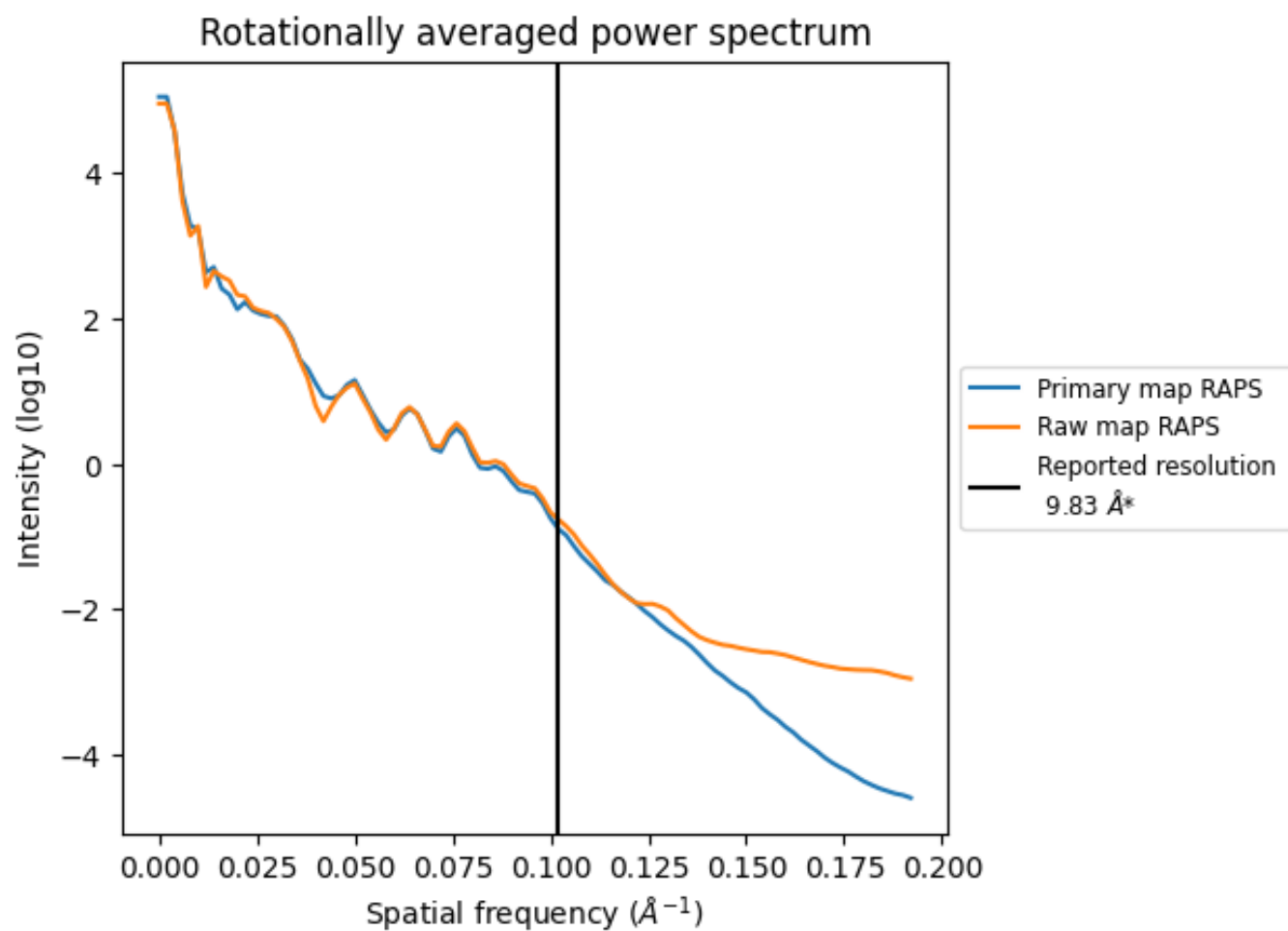
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3419 nm³; this corresponds to an approximate mass of 3088 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 [i](#)

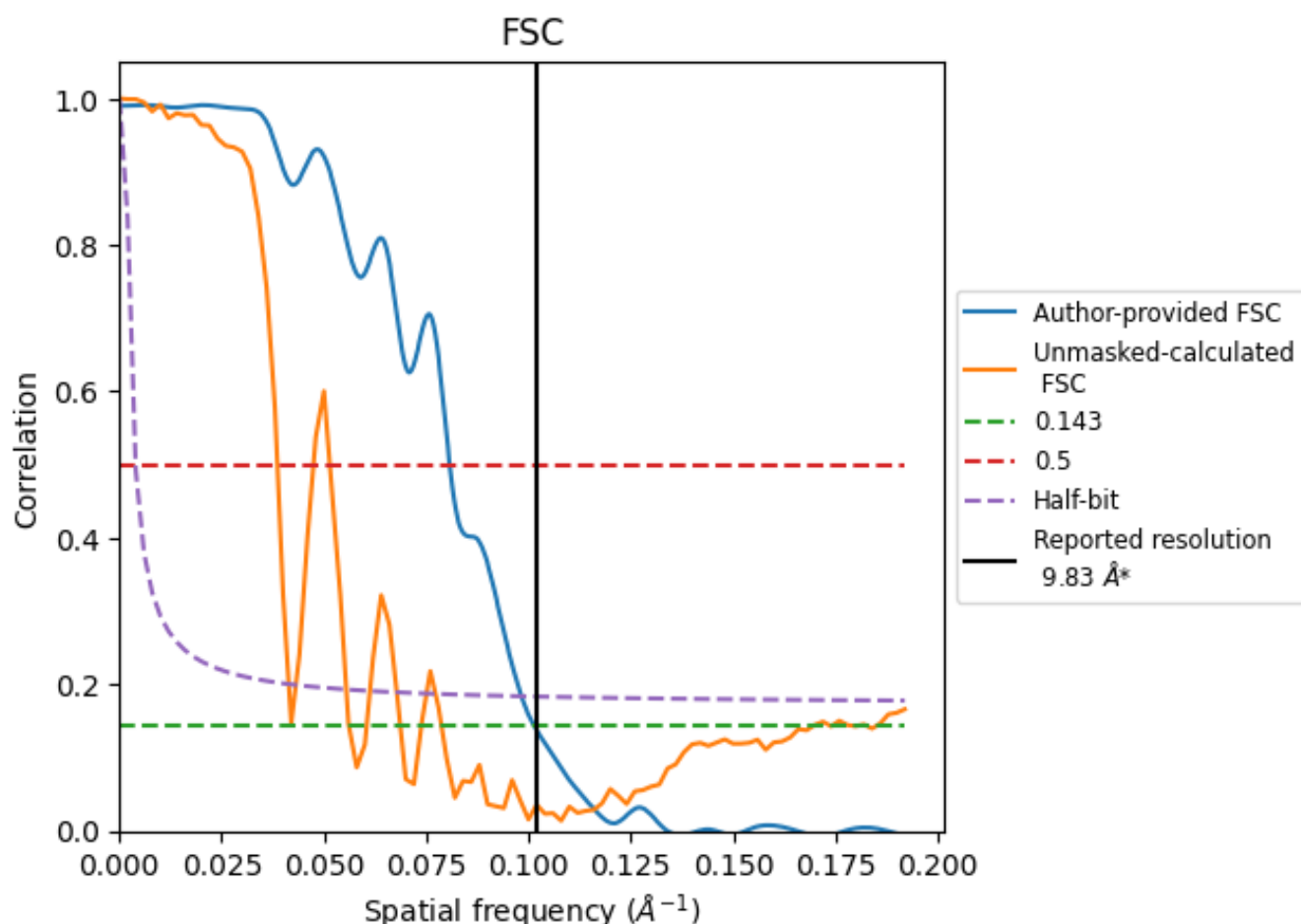


*Reported resolution corresponds to spatial frequency of 0.102 Å⁻¹

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 0.102 Å⁻¹

8.2 Resolution estimates [i](#)

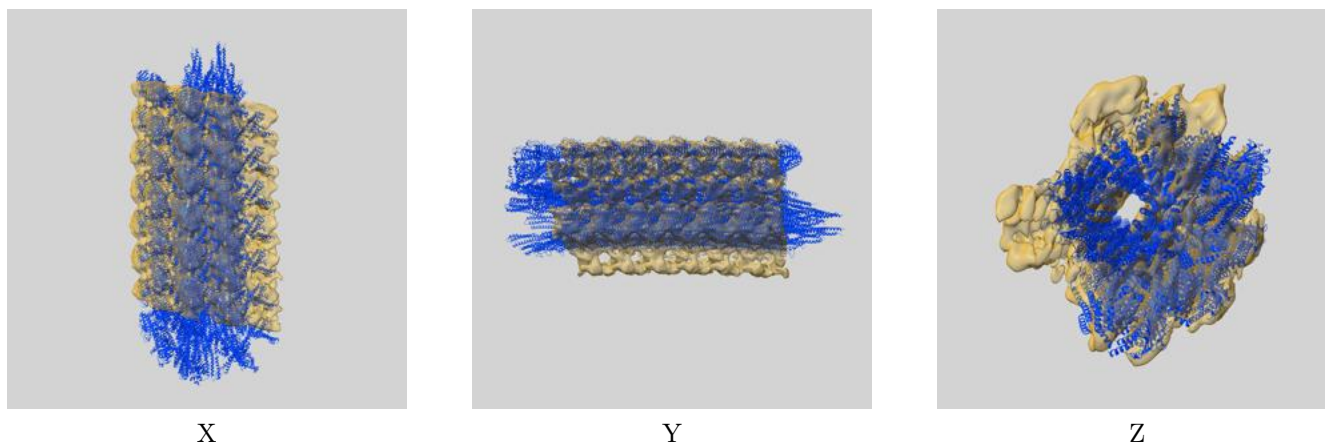
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.83	-	-
Author-provided FSC curve	9.86	12.39	10.11
Unmasked-calculated*	17.83	25.91	24.15

*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 17.83 differs from the reported value 9.83 by more than 10 %

9 Map-model fit [i](#)

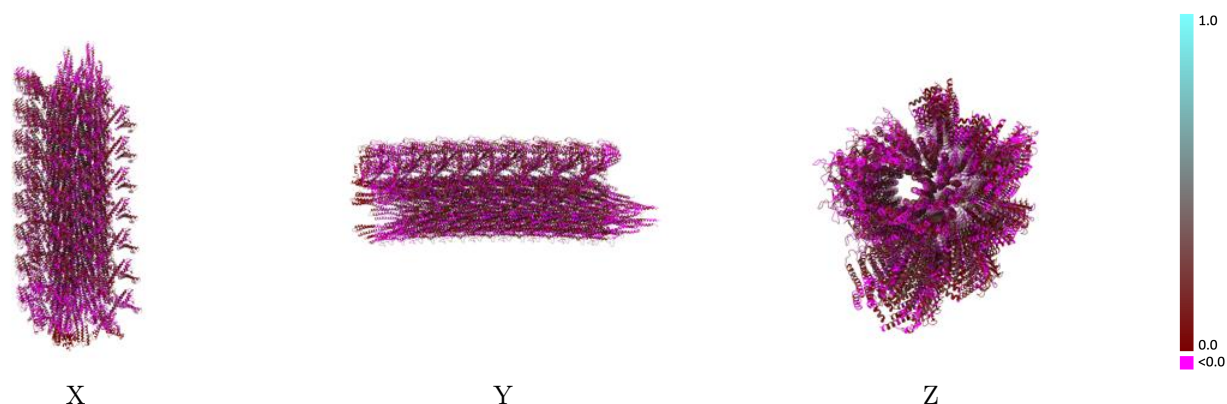
This section contains information regarding the fit between EMDB map EMD-20504 and PDB model 6PWB. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



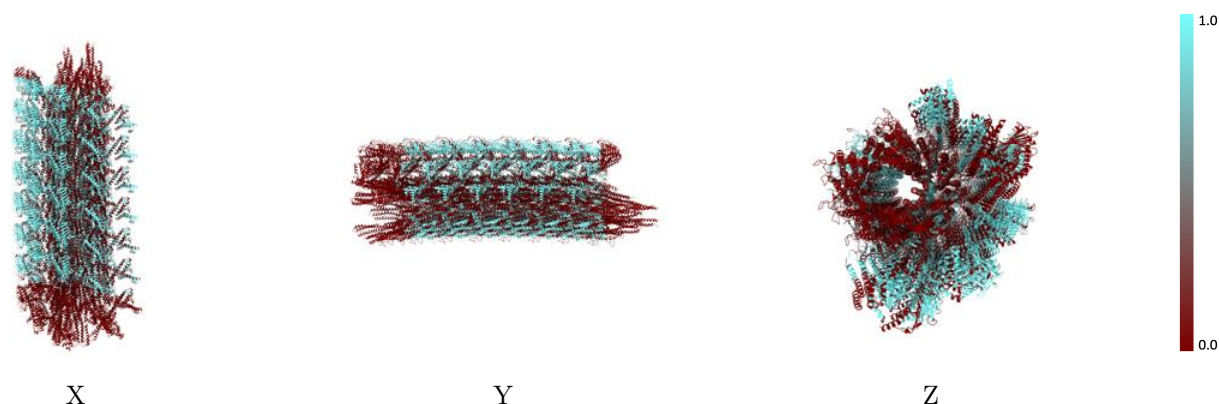
The images above show the 3D surface view of the map at the recommended contour level 3.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



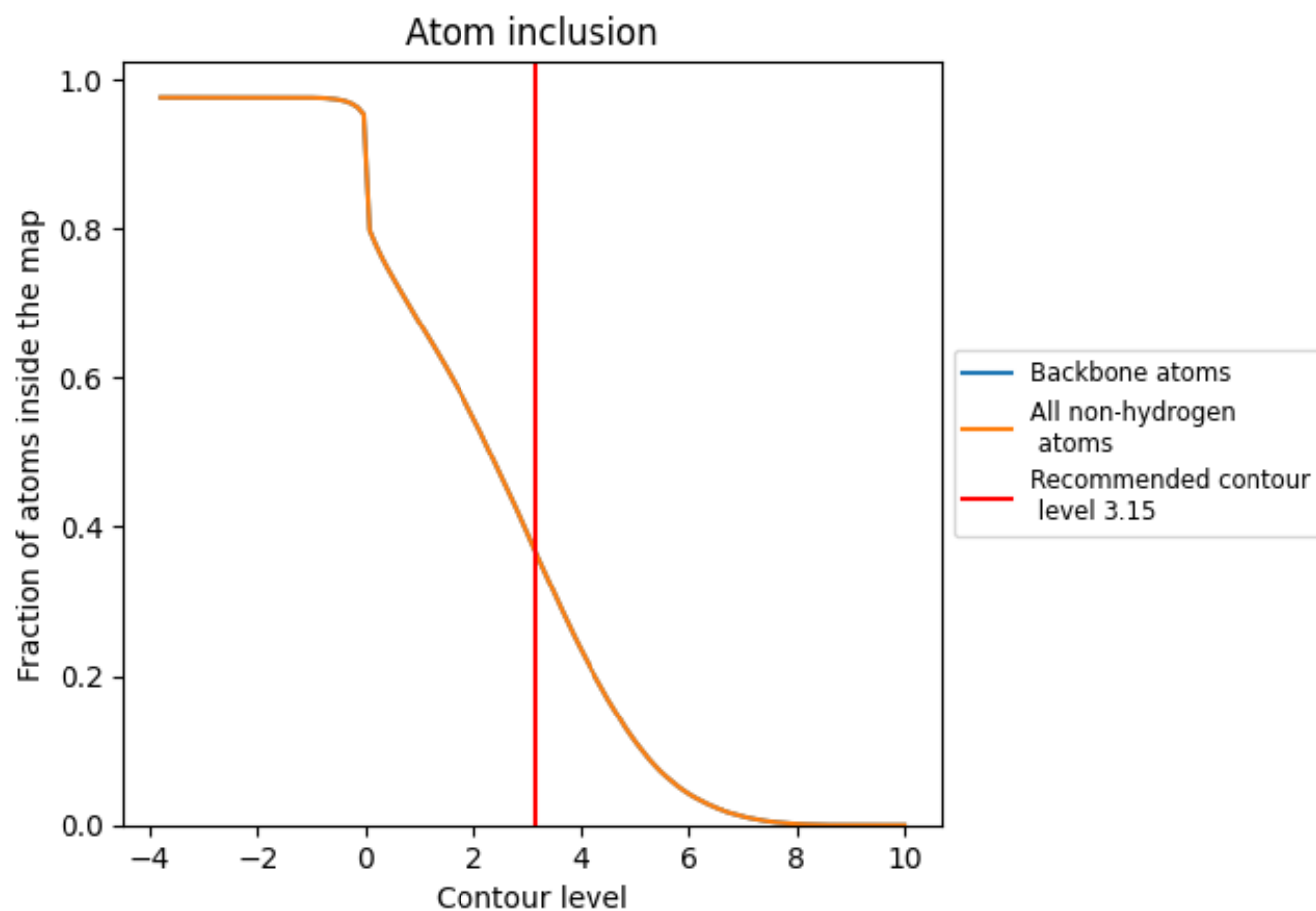
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.15).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 37% of all backbone atoms, 37% 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 (3.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3672	 0.0590
AG	 0.1462	 0.0390
AH	 0.1642	 0.0170
AI	 0.1698	 0.0890
AL	 0.3703	 0.0240
AM	 0.5939	 0.0850
AO	 0.0543	 0.0100
AR	 0.1623	 0.0500
AU	 0.0612	 0.0280
BA	 0.2274	 0.0710
BB	 0.3509	 0.0890
BC	 0.3123	 0.0500
BD	 0.1830	 0.0740
BE	 0.5432	 0.0990
BF	 0.5306	 0.0800
BG	 0.4283	 0.0360
BH	 0.6361	 0.0880
BI	 0.7568	 0.0990
BJ	 0.7364	 0.0920
BK	 0.4592	 0.0540
BL	 0.1462	 0.0500
BM	 0.3717	 0.0740
BN	 0.3861	 0.0820
BO	 0.8505	 0.0820
BP	 0.5116	 0.0530
BS	 0.1528	 -0.0020
BT	 0.0623	 0.0300
BU	 0.1245	 0.0380
BV	 0.2198	 0.0750
BW	 0.4123	 0.0900
BX	 0.3292	 0.0370
BY	 0.1774	 0.0750
BZ	 0.6150	 0.1060
CA	 0.5591	 0.0800
CB	 0.4462	 0.0400























































































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Chain	Atom inclusion	Q-score
CC	 0.6477	 0.0940
CD	 0.8954	 0.1280
CE	 0.7595	 0.1140
CF	 0.8315	 0.1090
CG	 0.2057	 0.0800
CH	 0.3981	 0.0570
CI	 0.7321	 0.1200
CJ	 0.8533	 0.0790
CK	 0.5264	 0.0430
CL	 0.0453	 0.0270
CM	 0.4009	 0.0500
CN	 0.4009	 0.0360
CO	 0.1821	 0.0530
CP	 0.1849	 0.0510
CQ	 0.2113	 0.0570
CR	 0.4189	 0.1020
CS	 0.3500	 0.0400
CT	 0.1887	 0.0780
CU	 0.5981	 0.0840
CV	 0.5791	 0.0900
CW	 0.4557	 0.0500
CX	 0.6097	 0.0970
CY	 0.8736	 0.1280
CZ	 0.7649	 0.1200
DA	 0.8438	 0.1080
DB	 0.2047	 0.0930
DC	 0.4179	 0.0610
DD	 0.7110	 0.1150
DE	 0.8397	 0.0750
DF	 0.5380	 0.0500
DG	 0.1887	 0.0540
DH	 0.4943	 0.0510
DI	 0.5877	 0.0500
DJ	 0.2670	 0.0610
DK	 0.2085	 0.0580
DL	 0.2160	 0.0670
DM	 0.4038	 0.0940
DN	 0.3292	 0.0560
DO	 0.1566	 0.0740
DP	 0.5791	 0.0880
DQ	 0.5570	 0.0830
DR	 0.5084	 0.0600





















































































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Chain	Atom inclusion	Q-score
DS	 0.6150	 0.0990
DT	 0.8859	 0.1260
DU	 0.7337	 0.1130
DV	 0.8166	 0.1190
DW	 0.2264	 0.0990
DX	 0.3953	 0.0660
DY	 0.7363	 0.1200
DZ	 0.8329	 0.0810
EA	 0.5475	 0.0580
EB	 0.1528	 0.0460
EC	 0.5104	 0.0480
ED	 0.5736	 0.0600
EE	 0.2849	 0.0560
EF	 0.2264	 0.0740
EG	 0.2019	 0.0610
EH	 0.4085	 0.0890
EI	 0.2991	 0.0440
EJ	 0.1019	 0.0430
EK	 0.5675	 0.0680
EL	 0.5380	 0.0730
EM	 0.4694	 0.0480
EN	 0.5707	 0.0930
EO	 0.8587	 0.1180
EP	 0.7201	 0.1080
EQ	 0.8220	 0.1140
ER	 0.2264	 0.0900
ES	 0.3840	 0.0800
ET	 0.7046	 0.1110
EU	 0.8329	 0.0690
EV	 0.4947	 0.0400
EW	 0.1632	 0.0490
EX	 0.5472	 0.0510
EY	 0.6019	 0.0530
EZ	 0.2934	 0.0670
FA	 0.2236	 0.0590
FB	 0.1726	 0.0710
FC	 0.2943	 0.0620
FD	 0.1840	 0.0390
FE	 0.0255	 0.0180
FF	 0.5084	 0.0530
FG	 0.5253	 0.0780
FH	 0.1983	 0.0200







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Chain	Atom inclusion	Q-score
FI	 0.0517	 0.0260
FJ	 0.8573	 0.1030
FK	 0.6168	 0.0820
FL	 0.8234	 0.1230
FM	 0.2009	 0.0800
FN	 0.2113	 0.0310
FO	 0.7068	 0.1170
FP	 0.7935	 0.0840
FQ	 0.4979	 0.0490
FR	 0.1528	 0.0420
FS	 0.5745	 0.0740
FT	 0.5557	 0.0530
FU	 0.2774	 0.0500
FV	 0.2151	 0.0570
FW	 0.0113	 0.0230
FX	 0.1075	 0.0050
GA	 0.1160	 -0.0160
GB	 0.0137	 0.0070
GC	 0.0000	 -0.0140
GE	 0.2622	 0.0330
GF	 0.0000	 -0.0020
GG	 0.6793	 0.1010
GH	 0.0811	 0.0430
GI	 0.0387	 -0.0110
GJ	 0.5770	 0.0940
GK	 0.0557	 -0.0090
GL	 0.0000	 -0.0160
GM	 0.1821	 0.0600
GN	 0.5623	 0.0770
GO	 0.5396	 0.0490
GP	 0.2085	 0.0230
GQ	 0.1255	 0.0300
GR	 0.0000	 -0.0060
GV	 0.0000	 0.0120
GW	 0.0000	 -0.0070
GZ	 0.0000	 0.0260
HB	 0.0000	 -0.0120
HC	 0.0009	 0.0020
HE	 0.0000	 0.0020
HF	 0.0000	 -0.0050
HH	 0.1358	 0.0590
HI	 0.3142	 0.0500

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Chain	Atom inclusion	Q-score
HJ	 0.2142	 -0.0160
HK	 0.1491	 0.0120
HL	 0.0123	 0.0200