



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 06:10 PM UTC

PDB ID : 6PWB / pdb_00006pwb
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 : 6NQW, 6NQZ, 5WJT

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

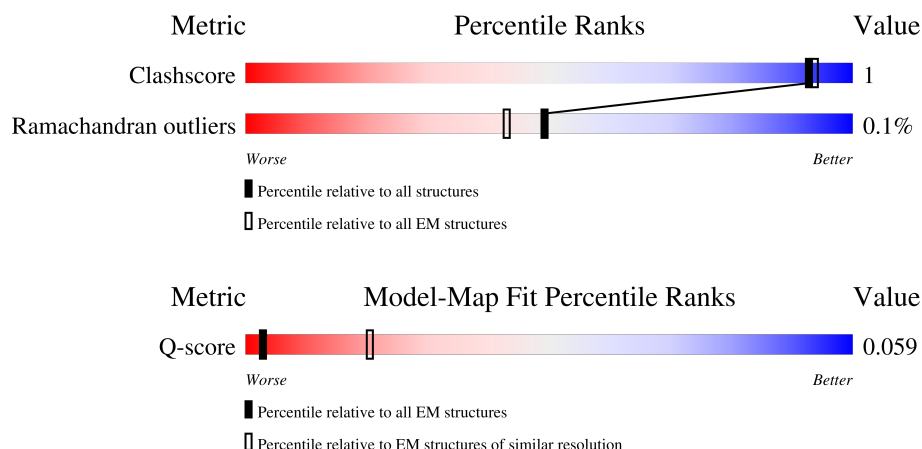
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	143 (9.40 - 10.31)

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	84% 95% .
1	AH	265	82% 97% .
1	AI	265	79% 97% .
1	AR	265	81% 95% .

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Mol	Chain	Length	Quality of chain
1	BA	265	76% 93% 6%
1	BB	265	61% 96% .
1	BC	265	66% 95% 5%
1	BD	265	79% 95% .
1	BL	265	84% 95% 5%
1	BM	265	61% 95% 5%
1	BS	265	83% 97% .
1	BT	265	93% 95% 5%
1	BU	265	86% 95% 5% .
1	BV	265	75% 94% 5%
1	BW	265	56% 95% .
1	BX	265	66% 94% 5%
1	BY	265	79% 95% 5%
1	CG	265	78% 95% 5% .
1	CH	265	56% 95% .
1	CL	265	95% 96% .
1	CM	265	58% 95% 5%
1	CN	265	57% 96% .
1	CO	265	79% 95% .
1	CP	265	79% 97% .
1	CQ	265	77% 95% 5%
1	CR	265	55% 95% .
1	CS	265	62% 95% 5%
1	CT	265	78% 95% 5%
1	DB	265	77% 95% . .

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Mol	Chain	Length	Quality of chain
1	DC	265	55% 95% .
1	DG	265	79% 94% 6%
1	DH	265	49% 96% .
1	DI	265	37% 97% .
1	DJ	265	70% 95% .
1	DK	265	77% 96% .
1	DL	265	77% 95% 5%
1	DM	265	56% 95% 5%
1	DN	265	65% 95% .
1	DO	265	81% 96% .
1	DW	265	75% 95% ..
1	DX	265	57% 96% .
1	EB	265	85% 95% 5% .
1	EC	265	45% 96% .
1	ED	265	38% 96% .
1	EE	265	69% 95% .
1	EF	265	75% 95% 5%
1	EG	265	78% 94% 6%
1	EH	265	55% 95% 5%
1	EI	265	68% 95% .
1	EJ	265	89% 94% 5%
1	ER	265	74% 95% ..
1	ES	265	57% 95% 5%
1	EW	265	82% 95% 5%
1	EX	265	43% 95% .

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Mol	Chain	Length	Quality of chain
1	EY	265	37% 96% • •
1	EZ	265	68% 96% •
1	FA	265	75% 96% •
1	FB	265	80% 95% 5%
1	FC	265	66% 95% 5%
1	FD	265	80% 95% •
1	FE	265	97% 95% • •
1	FM	265	78% 95% • •
1	FN	265	77% 95% •
1	FR	265	82% 95% 5%
1	FS	265	38% 95% •
1	FT	265	42% 96% •
1	FU	265	69% 96% •
1	FV	265	77% 95% 5%
1	FW	265	99% 94% 5%
1	FX	265	88% 95% •
1	GH	265	91% 94% 5% •
1	GI	265	96% 95% •
1	GM	265	79% 95% 5%
1	GN	265	43% 95% •
1	GO	265	44% 96% •
1	GP	265	78% 96% •
1	GQ	265	87% 94% 6%
1	GR	265	100% 94% 5%
1	HC	265	100% 94% 5% •

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Mol	Chain	Length	Quality of chain
1	HH	265	85% 95% 5%
1	HI	265	66% 96% •
1	HJ	265	78% 97% •
1	HK	265	84% 96% •
1	HL	265	98% 97% •
2	AL	237	59% 100%
2	AM	237	39% 100%
2	AU	237	93% 98% •
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% 99% •
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%

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Mol	Chain	Length	Quality of chain
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%
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% 98%
2	GV	237	100% 100%

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Mol	Chain	Length	Quality of chain
2	GW	237	100%
2	HE	237	100%
3	AO	221	79% 81%
3	BI	221	18% 81%
3	BJ	221	19% 81%
3	BK	221	43% 81%
3	BO	221	10% 81%
3	CD	221	8% 81%
3	CE	221	17% 81%
3	CF	221	12% 81%
3	CJ	221	10% 81%
3	CY	221	9% 81%
3	CZ	221	17% 81%
3	DA	221	10% 81%
3	DE	221	11% 81%
3	DT	221	8% 81%
3	DU	221	18% 81%
3	DV	221	14% 81%
3	DZ	221	12% 81%
3	EO	221	10% 81%
3	EP	221	21% 81%
3	EQ	221	13% 81%
3	EU	221	10% 81%
3	FJ	221	10% 81%
3	FK	221	29% 81%

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Mol	Chain	Length	Quality of chain
3	FL	221	 14% 81% 17%
3	FP	221	 14% 81% 17%
3	GE	221	 60% 81% 17%
3	GF	221	 83% 81% 17%
3	GG	221	 25% 81% 17%
3	GK	221	 77% 81% 17%
3	GZ	221	 83% 81% 17%
3	HB	221	 83% 81% 17%
3	HF	221	 83% 80% 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	C	N	O	0	0
			1060	530	265	265		
1	EX	265	Total	C	N	O	0	0
			1060	530	265	265		
1	EY	265	Total	C	N	O	0	0
			1060	530	265	265		
1	EZ	265	Total	C	N	O	0	0
			1060	530	265	265		
1	GH	265	Total	C	N	O	0	0
			1060	530	265	265		
1	GI	265	Total	C	N	O	0	0
			1060	530	265	265		
1	FR	265	Total	C	N	O	0	0
			1060	530	265	265		
1	FS	265	Total	C	N	O	0	0
			1060	530	265	265		
1	FT	265	Total	C	N	O	0	0
			1060	530	265	265		
1	FU	265	Total	C	N	O	0	0
			1060	530	265	265		
1	FV	265	Total	C	N	O	0	0
			1060	530	265	265		
1	FW	265	Total	C	N	O	0	0
			1060	530	265	265		
1	FX	265	Total	C	N	O	0	0
			1060	530	265	265		
1	HC	265	Total	C	N	O	0	0
			1060	530	265	265		
1	GM	265	Total	C	N	O	0	0
			1060	530	265	265		
1	GN	265	Total	C	N	O	0	0
			1060	530	265	265		
1	GO	265	Total	C	N	O	0	0
			1060	530	265	265		
1	GP	265	Total	C	N	O	0	0
			1060	530	265	265		
1	GQ	265	Total	C	N	O	0	0
			1060	530	265	265		
1	GR	265	Total	C	N	O	0	0
			1060	530	265	265		
1	HH	265	Total	C	N	O	0	0
			1060	530	265	265		

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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

Continued on next page...

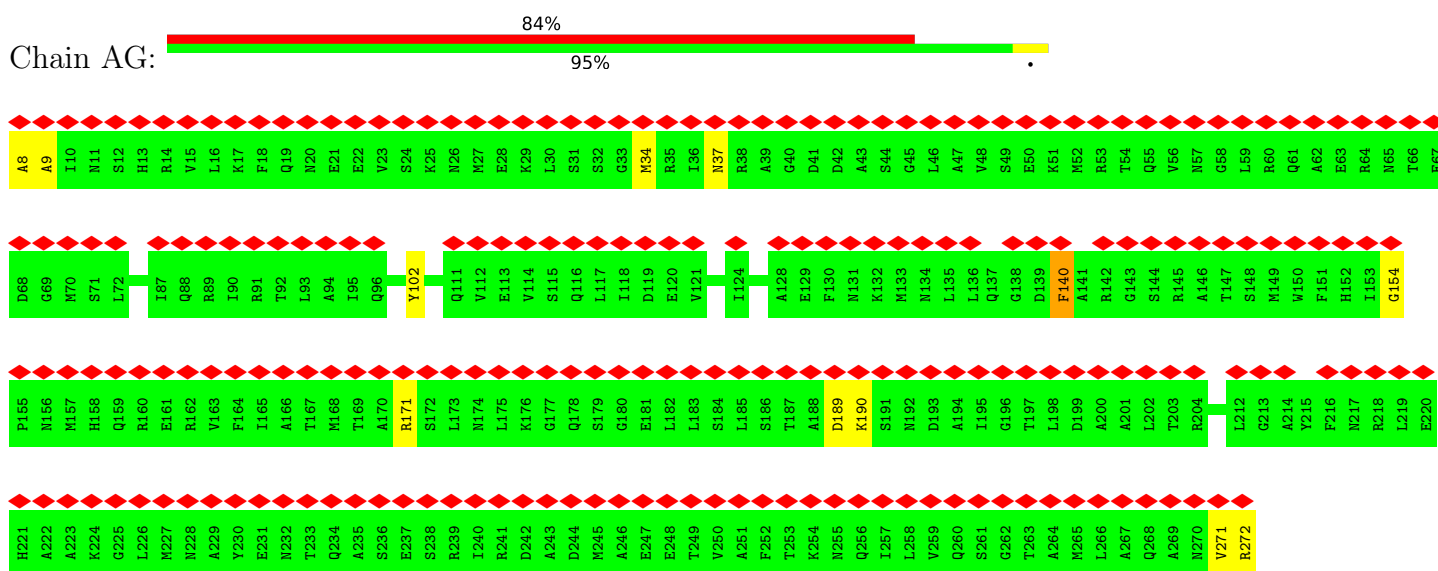
Continued from previous page...

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

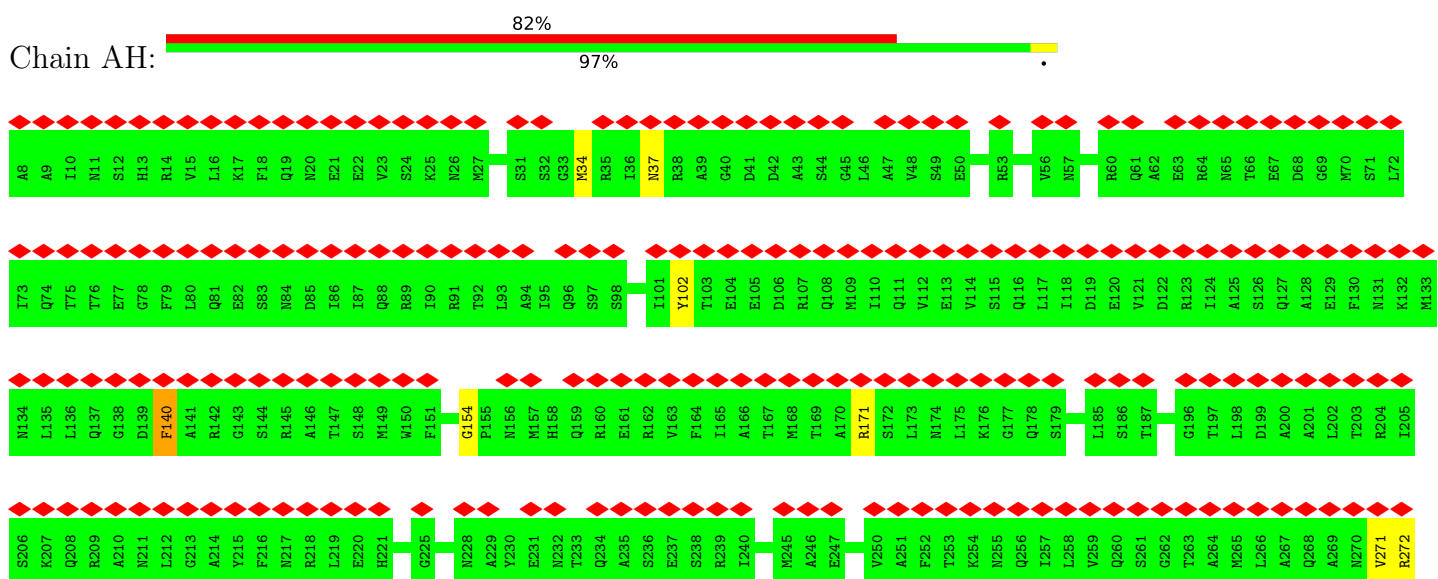
3 Residue-property plots

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)



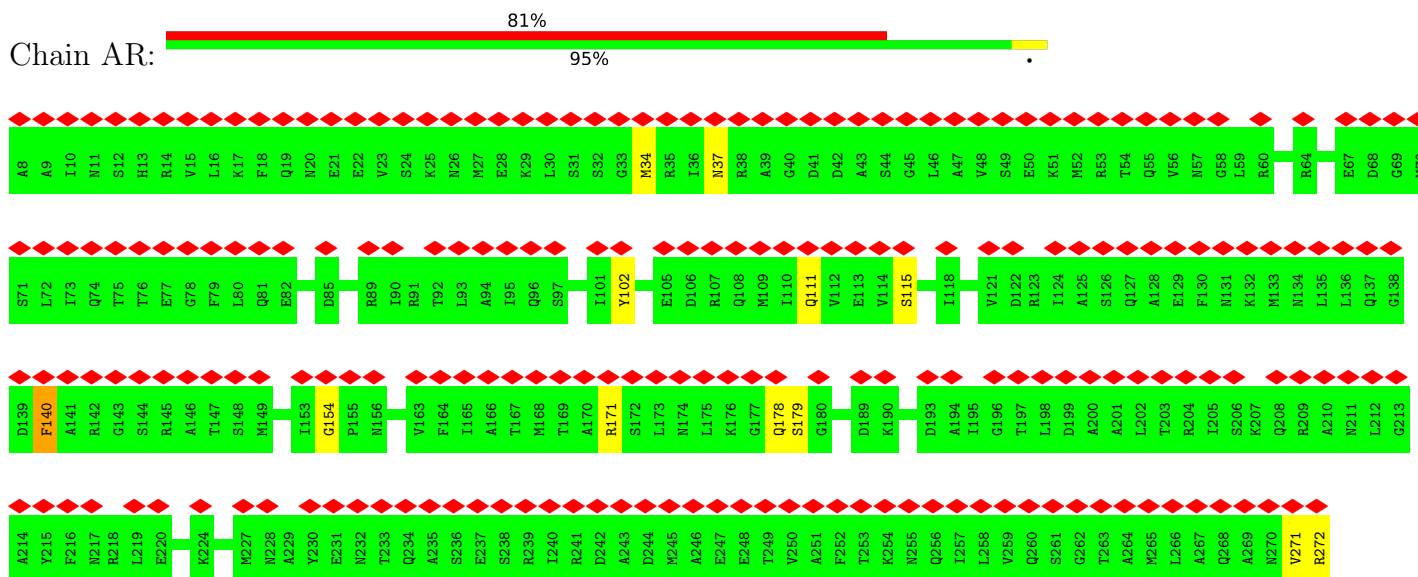
• Molecule 1: Flagellin B1 (FlaB1)



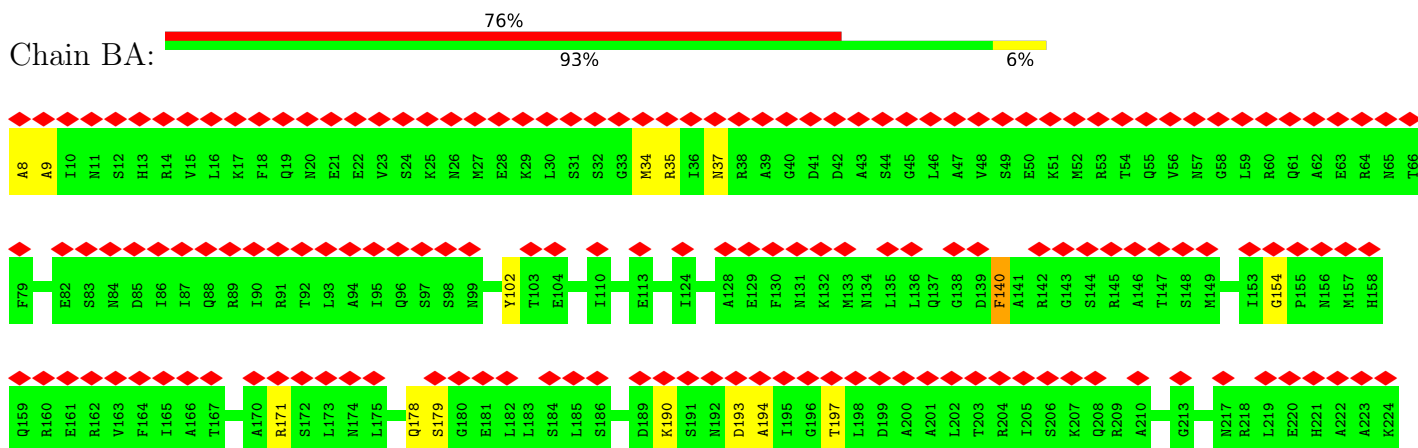
• Molecule 1: Flagellin B1 (FlaB1)

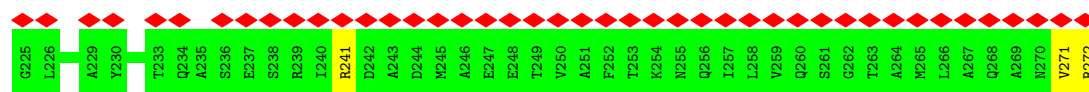


• Molecule 1: Flagellin B1 (FlaB1)

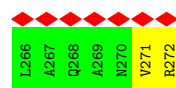
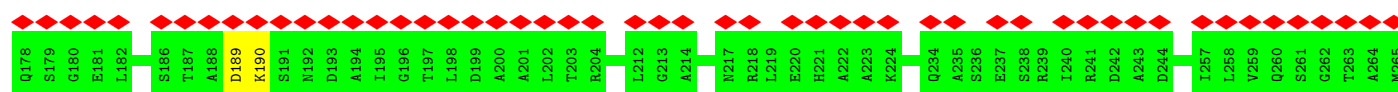
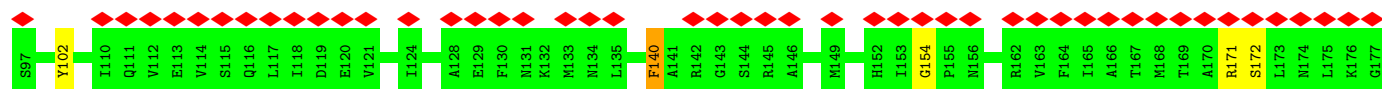
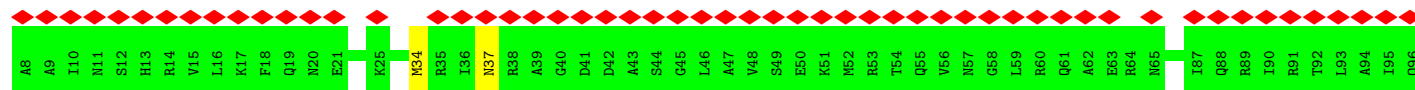


• Molecule 1: Flagellin B1 (FlaB1)

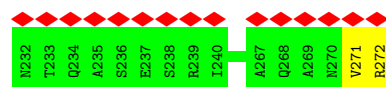
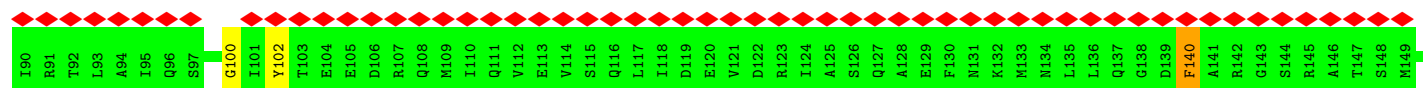
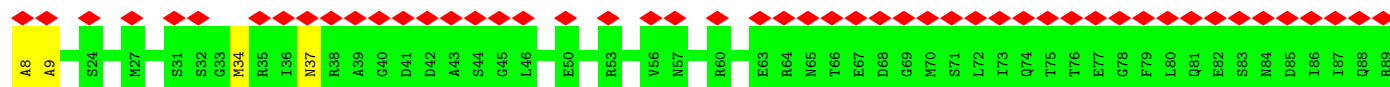




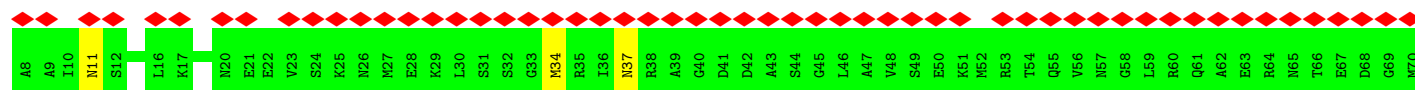
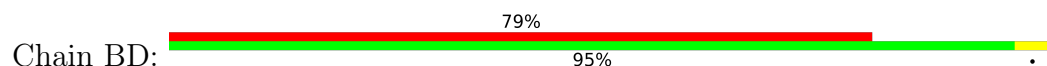
• Molecule 1: Flagellin B1 (FlaB1)

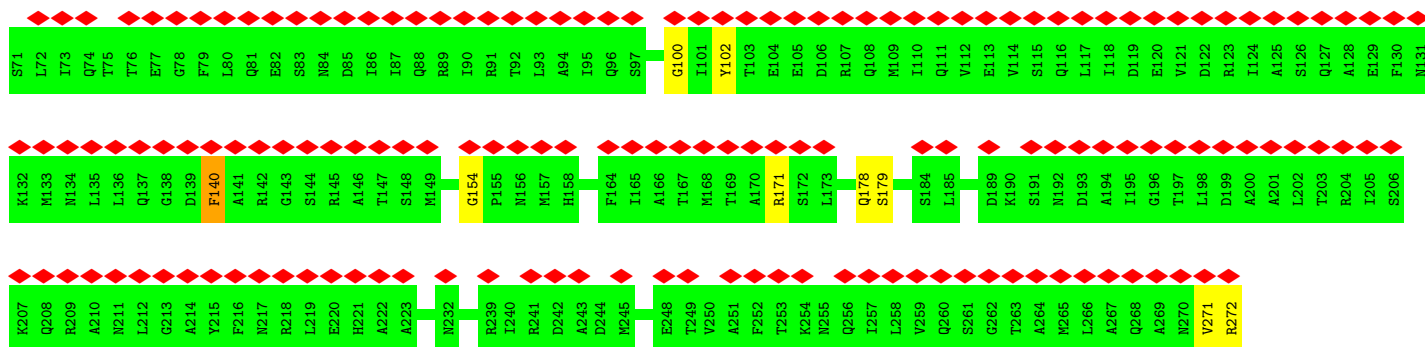


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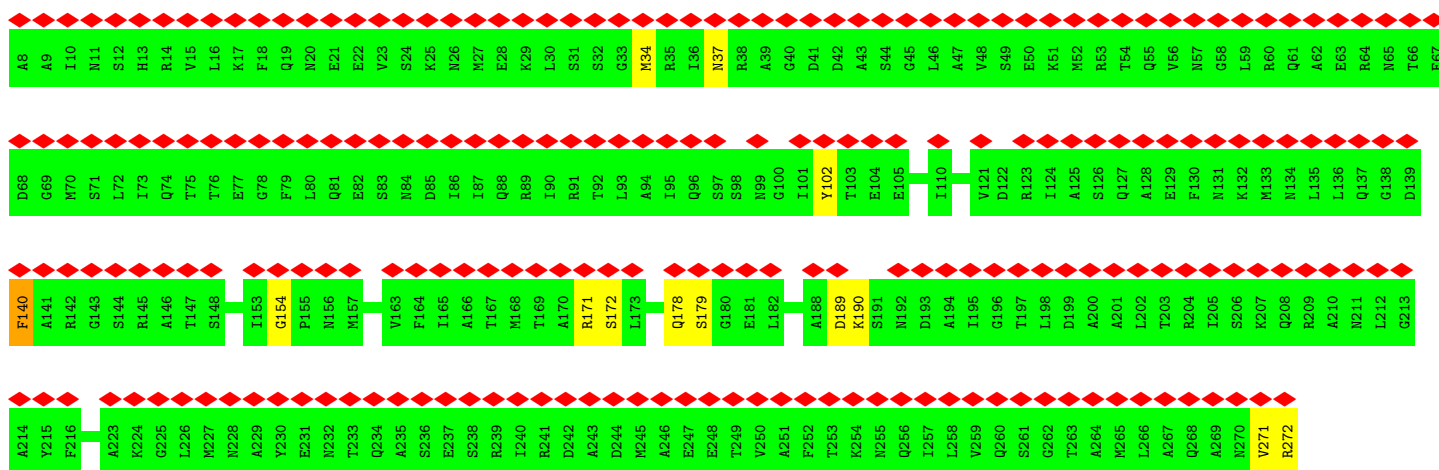
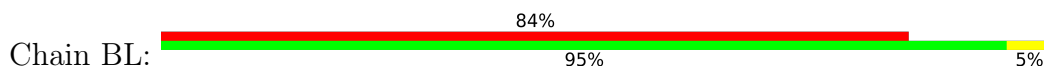


• Molecule 1: Flagellin B1 (FlaB1)

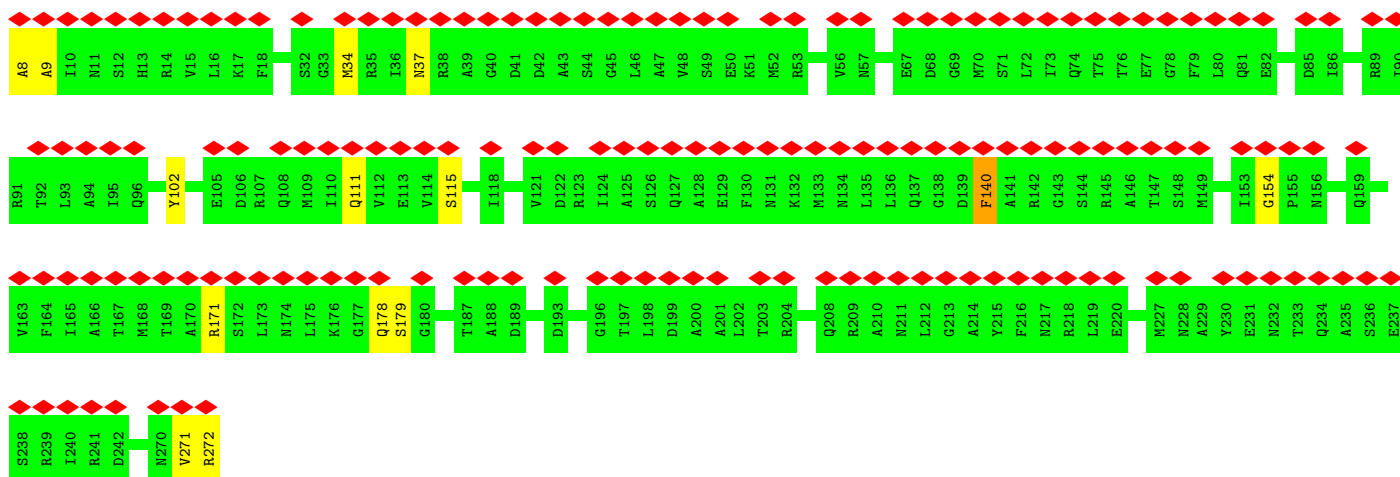




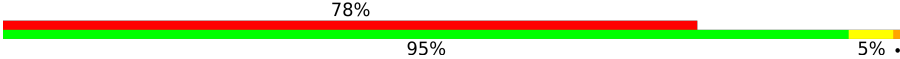
• Molecule 1: Flagellin B1 (FlaB1)

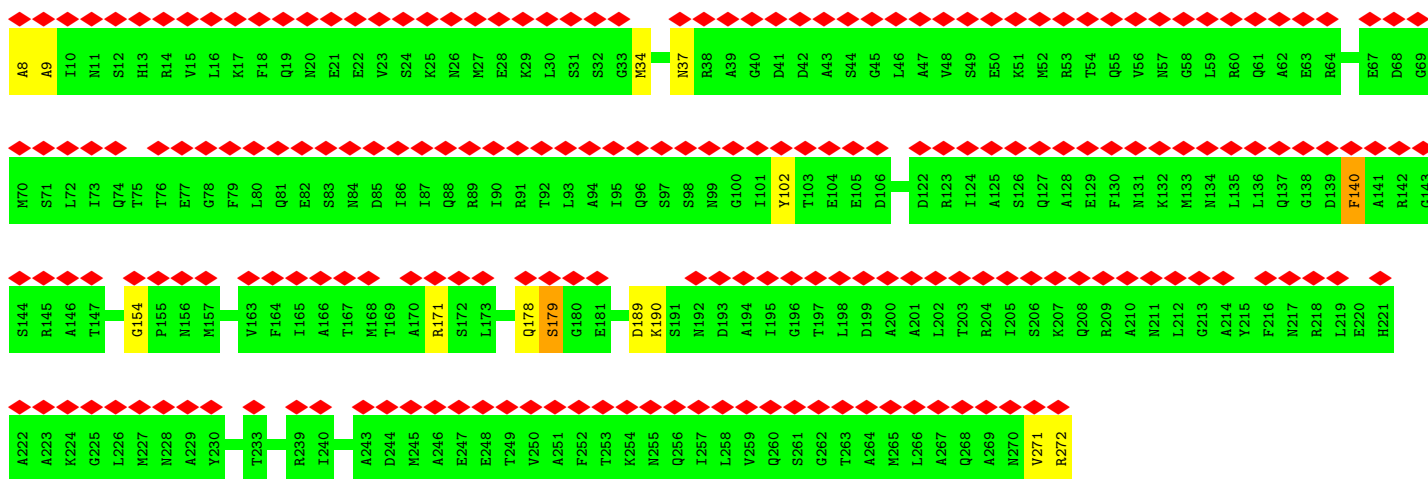


• Molecule 1: Flagellin B1 (FlaB1)

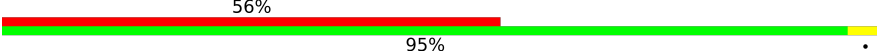


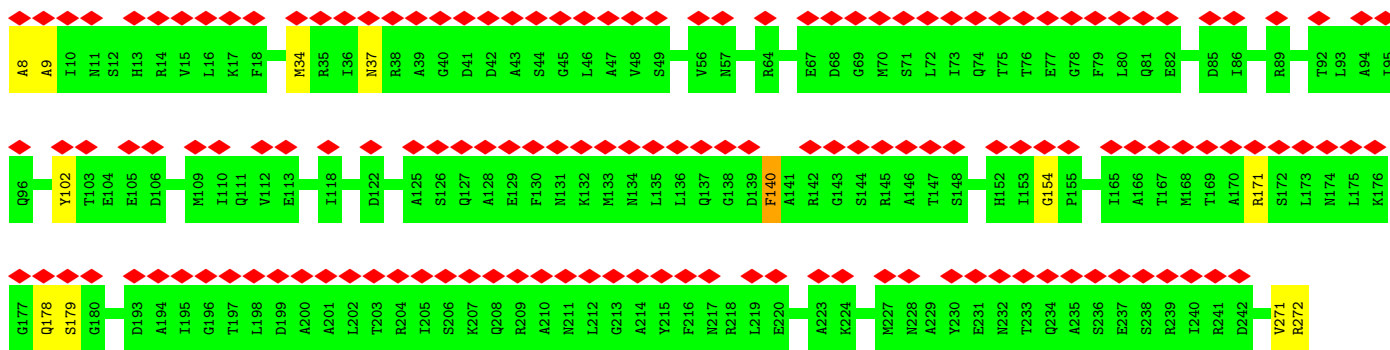
• Molecule 1: Flagellin B1 (FlaB1)

Chain CG: 

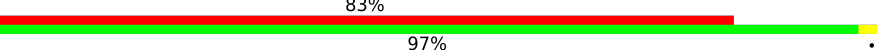


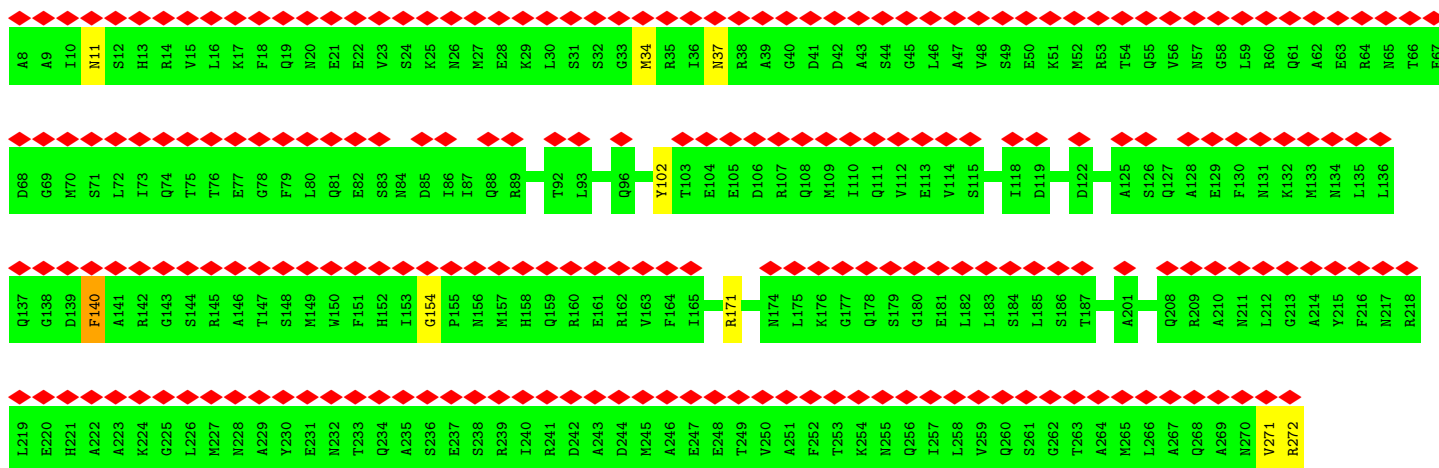
• Molecule 1: Flagellin B1 (FlaB1)

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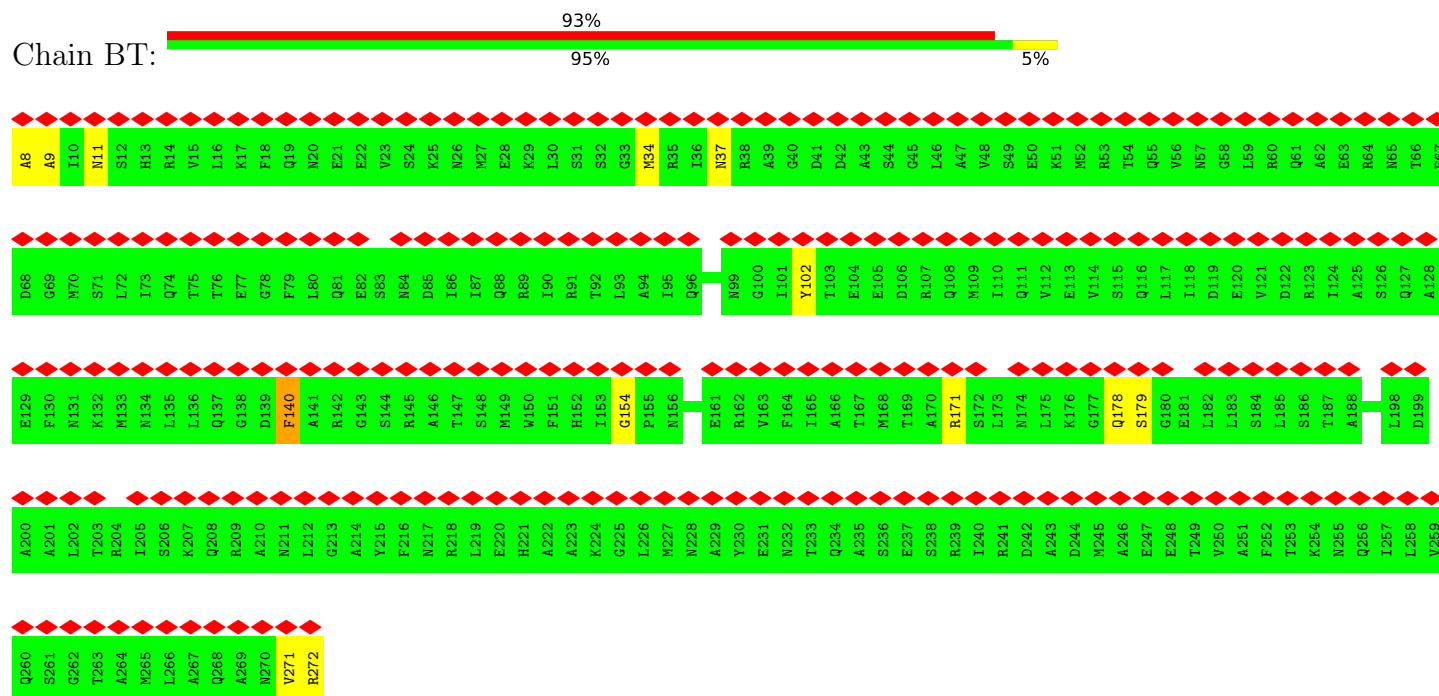
• Molecule 1: Flagellin B1 (FlaB1)

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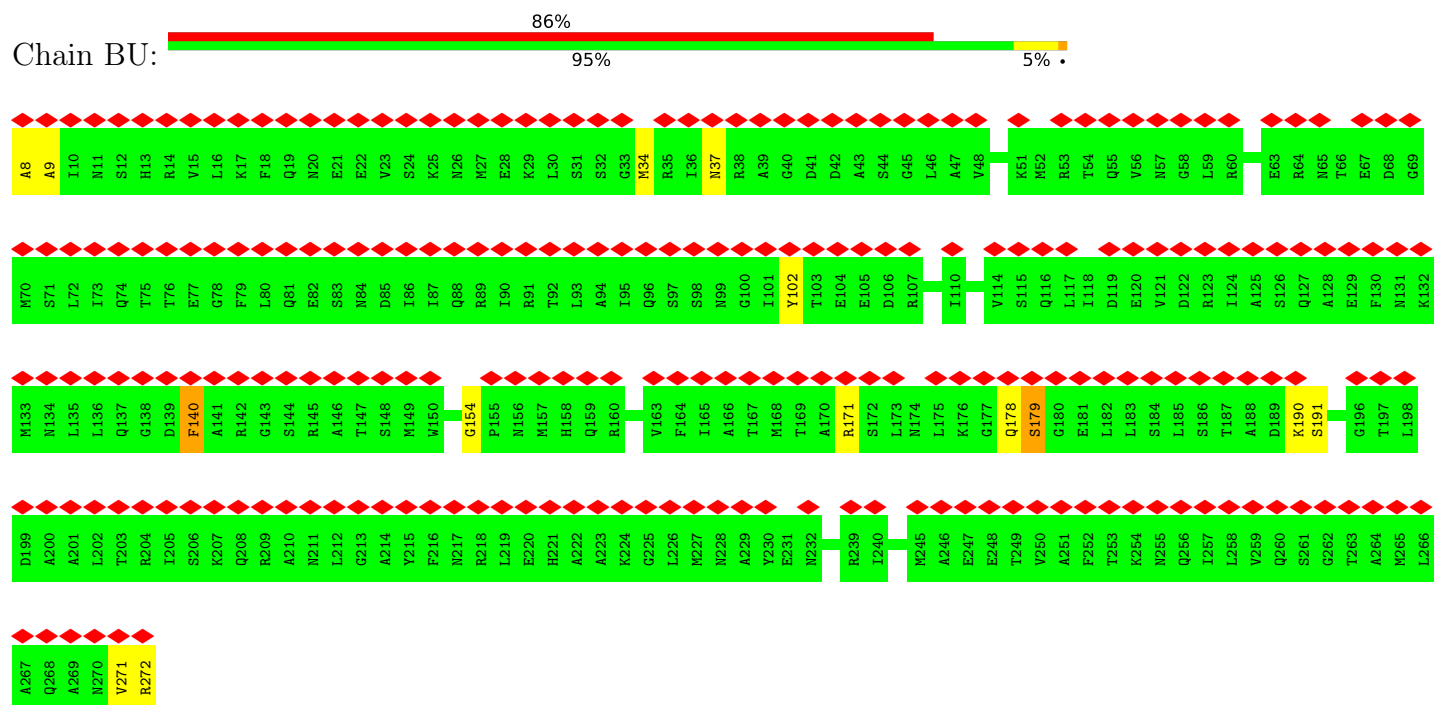
- Molecule 1: Flagellin B1 (FlaB1)

Chain BT:



- Molecule 1: Flagellin B1 (FlaB1)

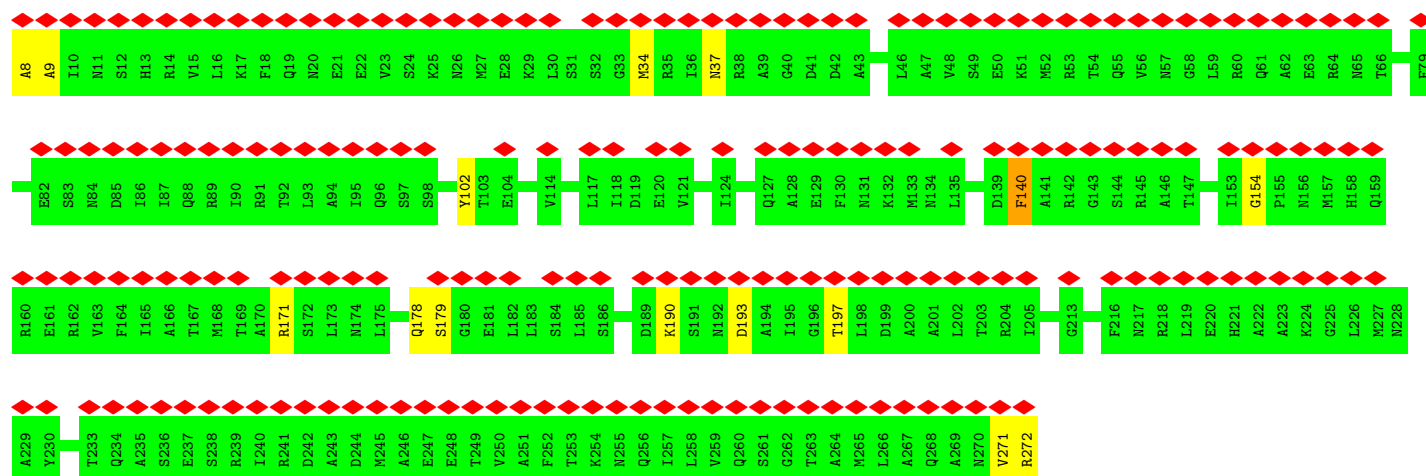
Chain BU:



- Molecule 1: Flagellin B1 (FlaB1)

Chain BV:

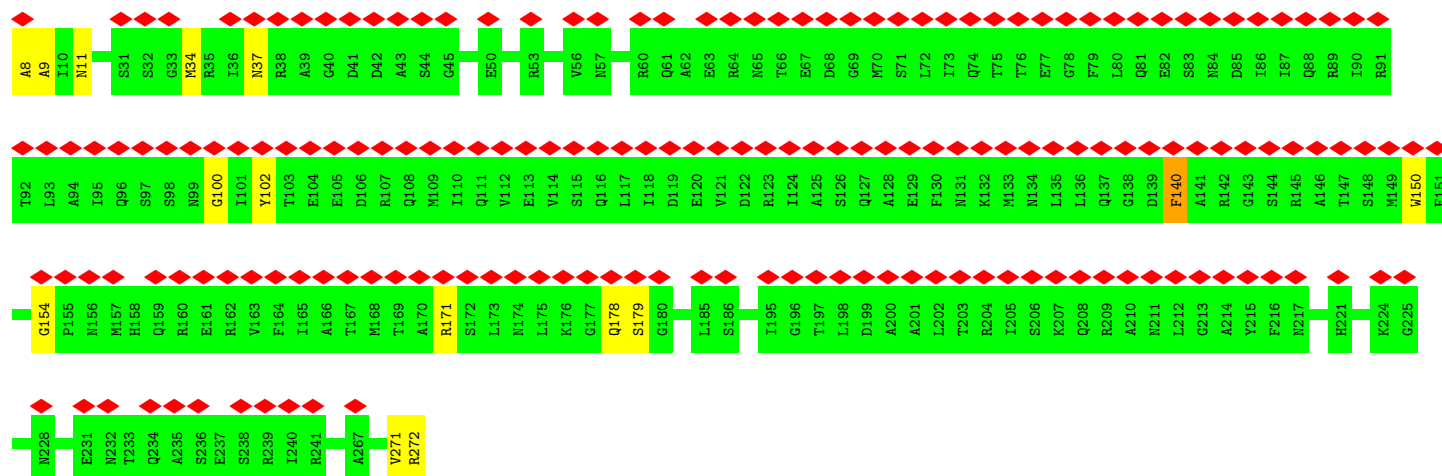




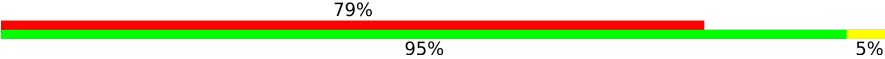
• Molecule 1: Flagellin B1 (FlaB1)

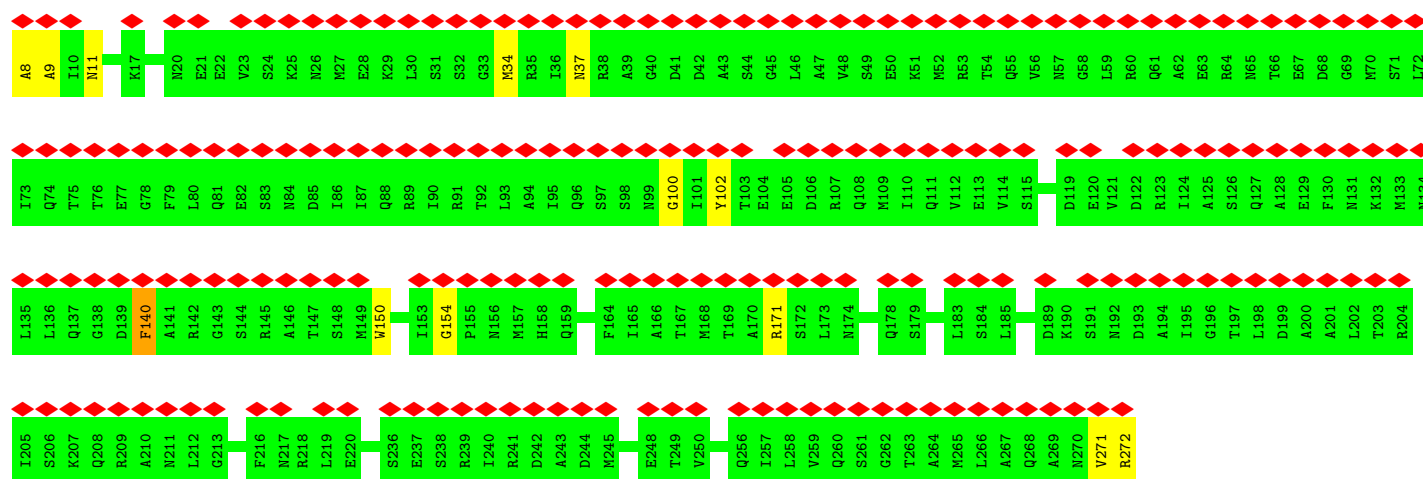


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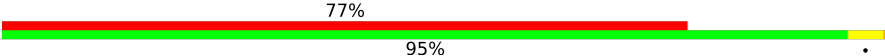


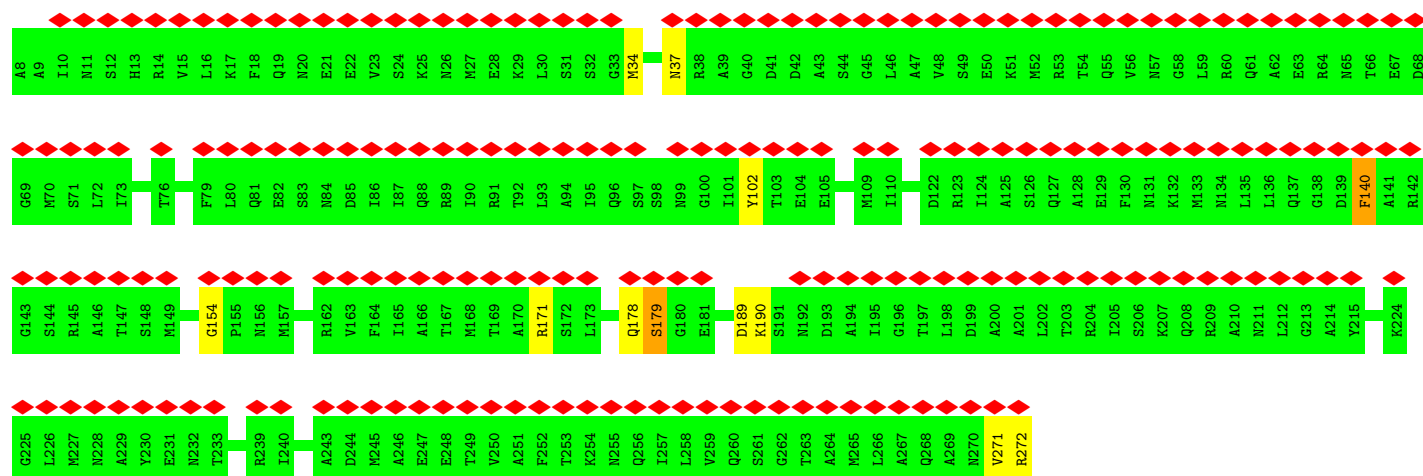
• Molecule 1: Flagellin B1 (FlaB1)

Chain BY: 

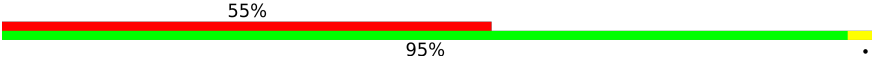


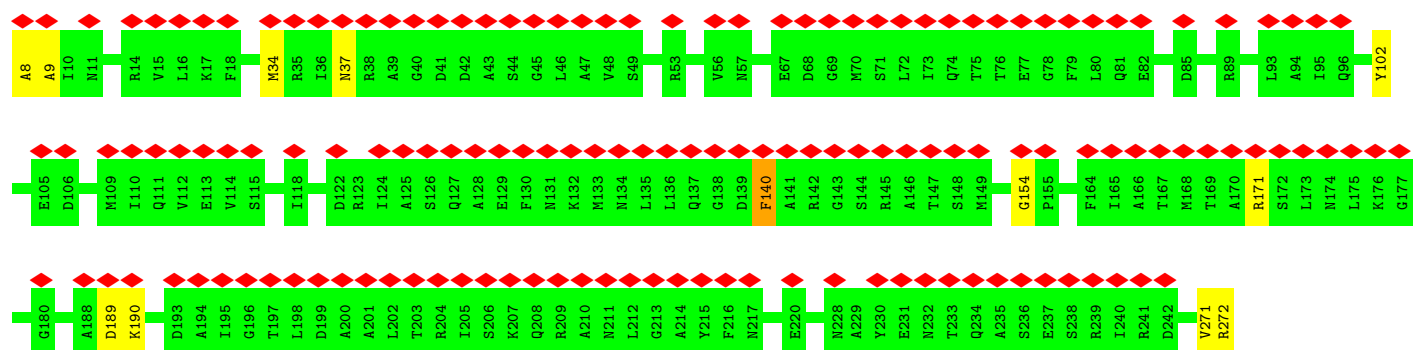
• Molecule 1: Flagellin B1 (FlaB1)

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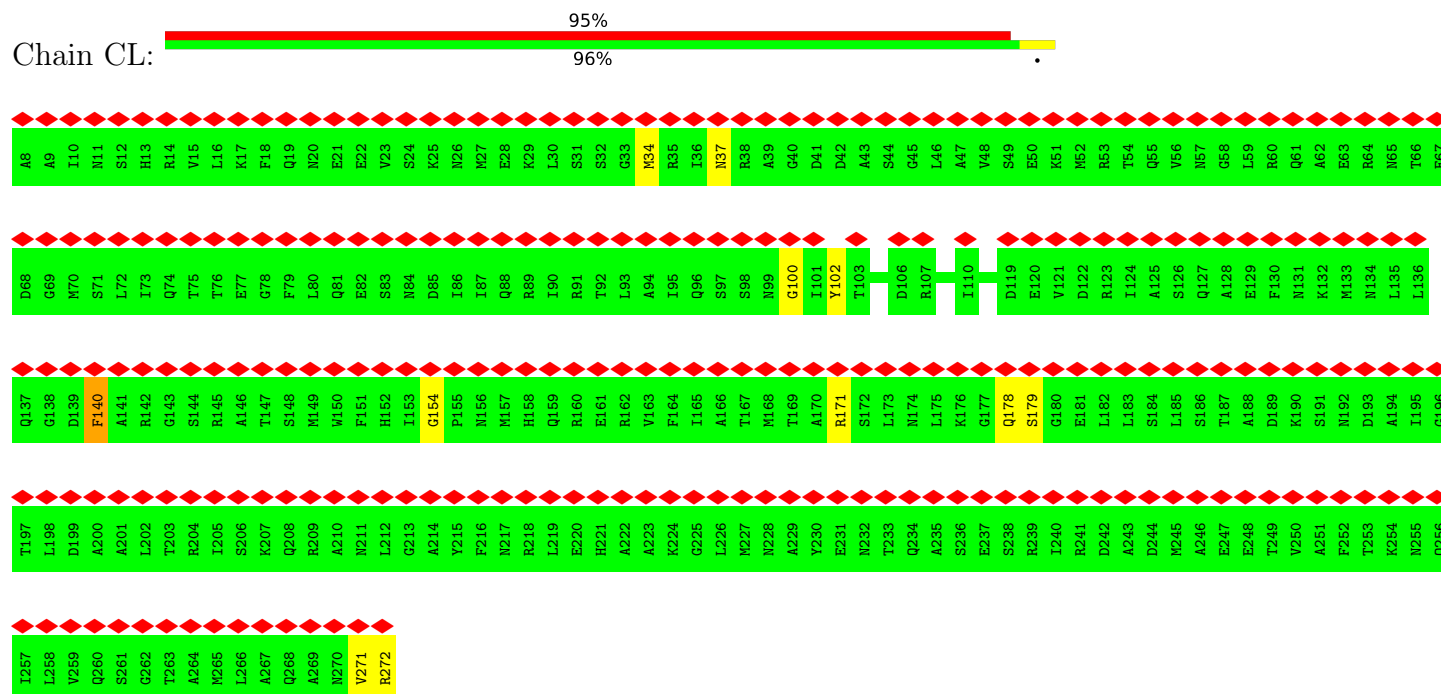


• Molecule 1: Flagellin B1 (FlaB1)

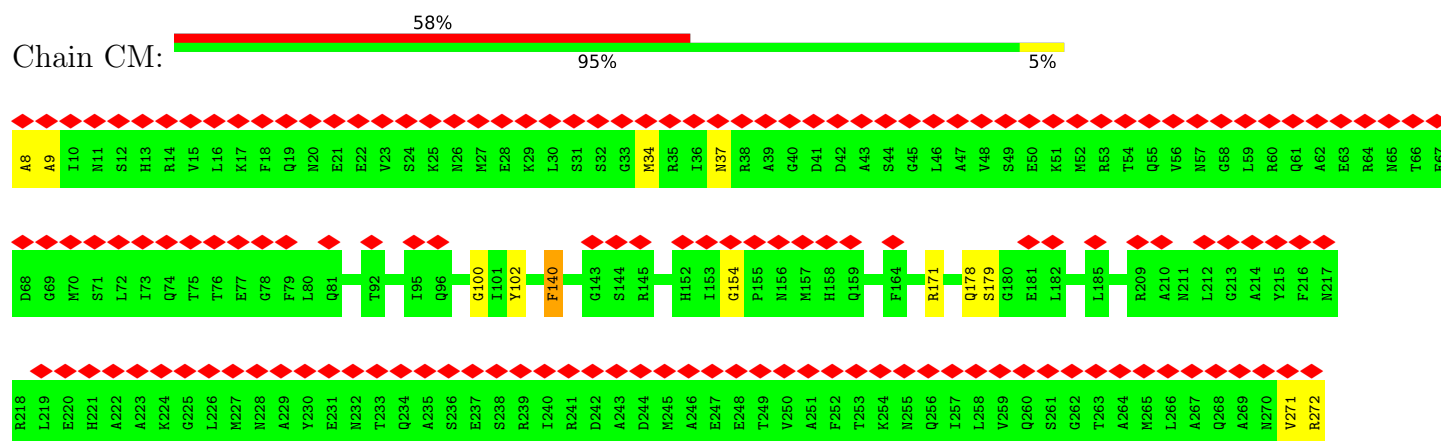
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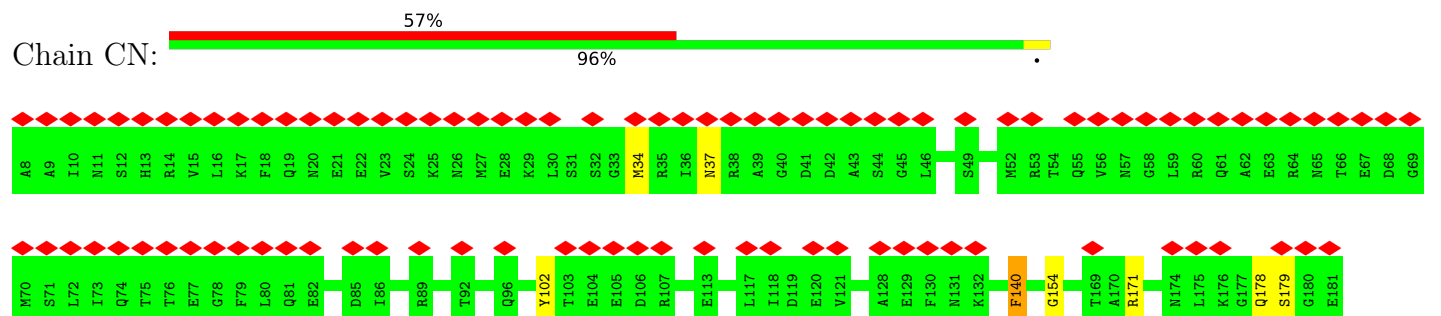
● Molecule 1: Flagellin B1 (FlaB1)

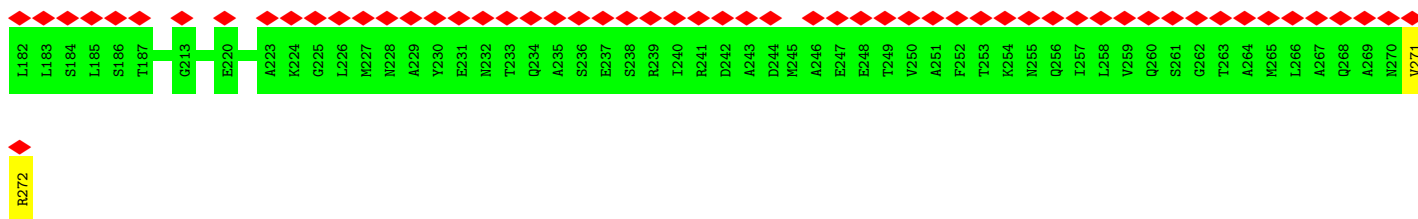


● Molecule 1: Flagellin B1 (FlaB1)

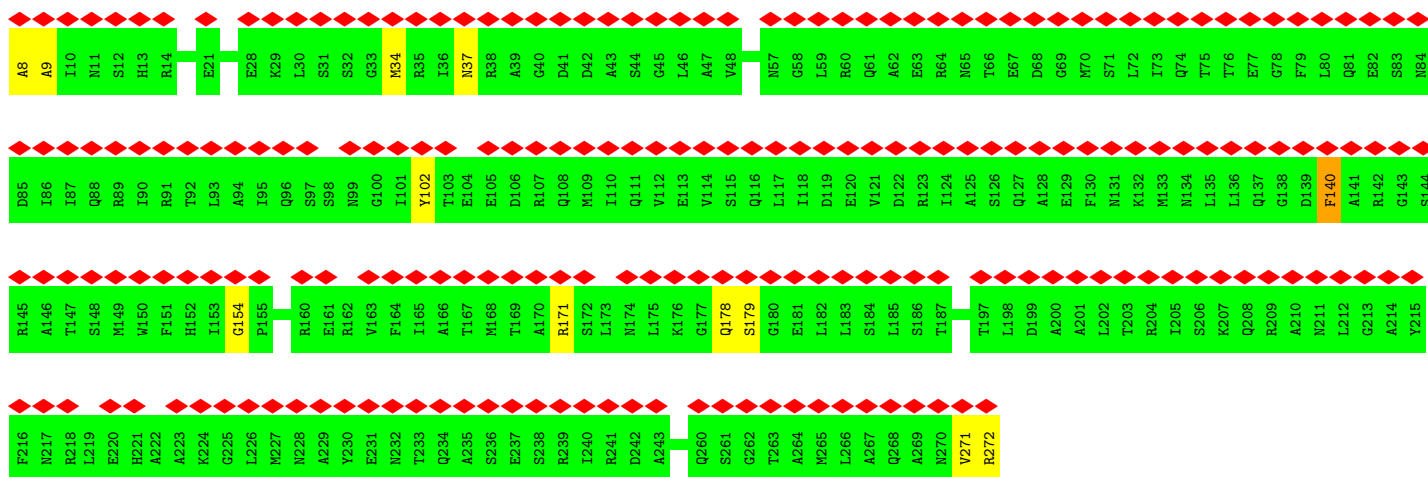
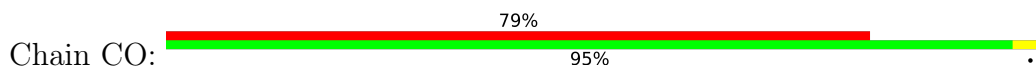


● Molecule 1: Flagellin B1 (FlaB1)

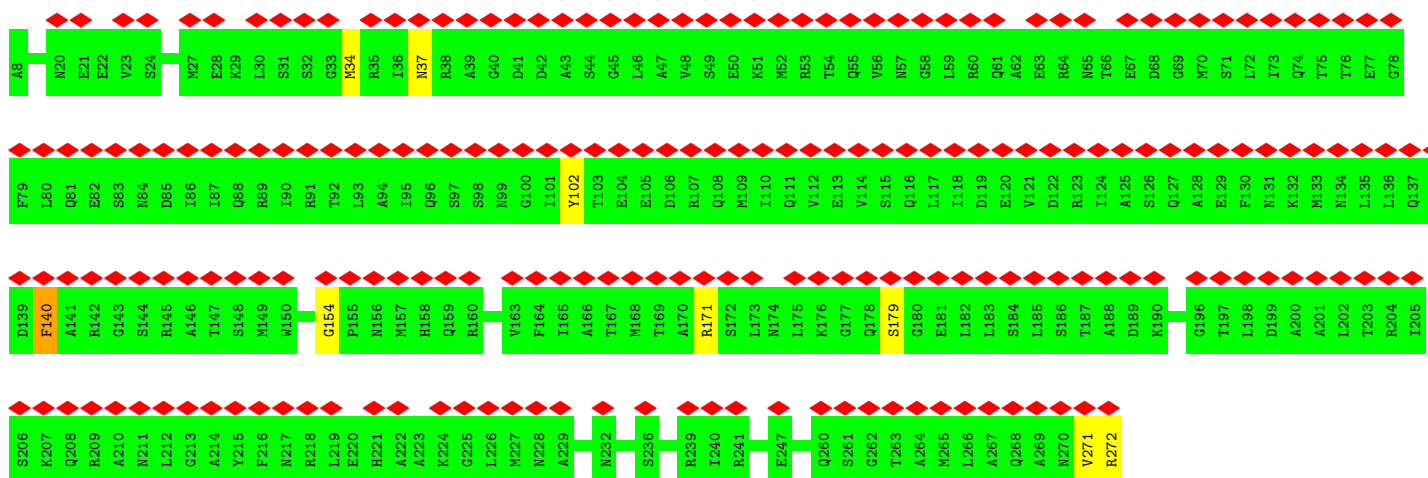
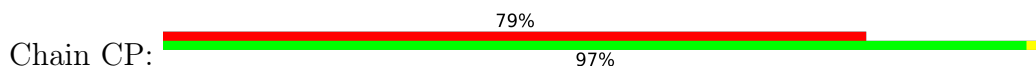




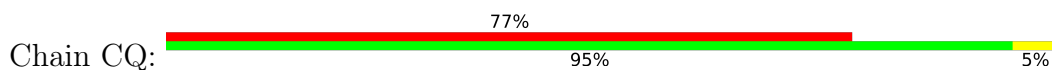
• Molecule 1: Flagellin B1 (FlaB1)

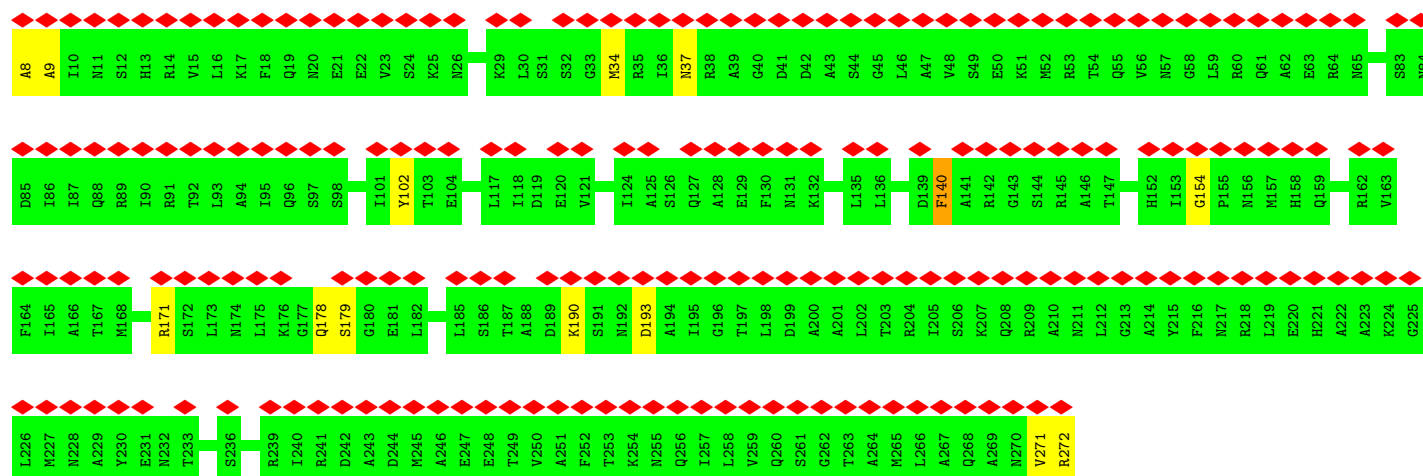


• Molecule 1: Flagellin B1 (FlaB1)



• Molecule 1: Flagellin B1 (FlaB1)

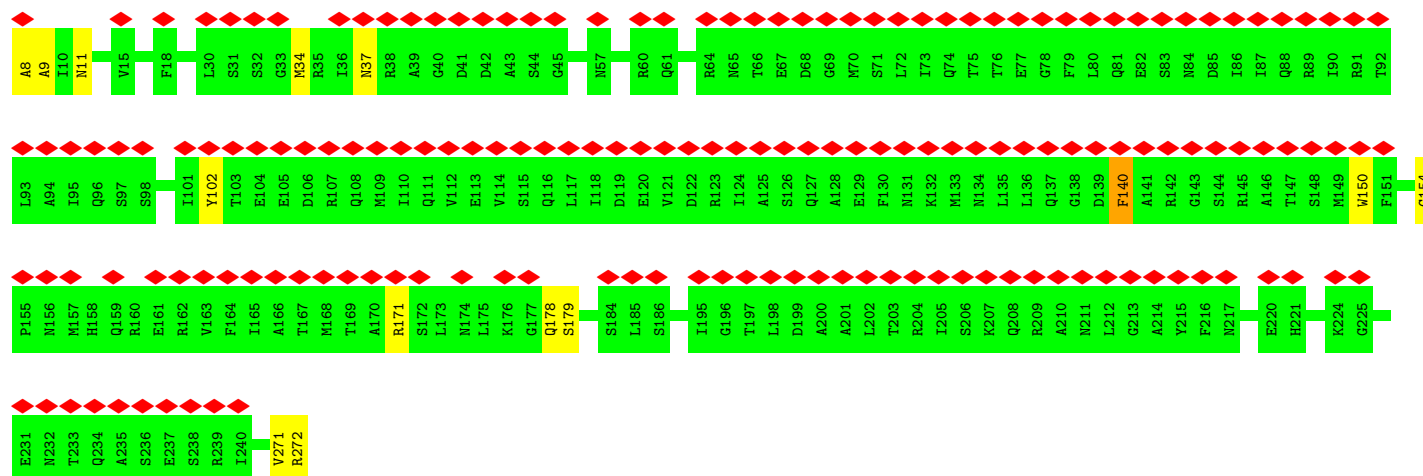




• Molecule 1: Flagellin B1 (FlaB1)



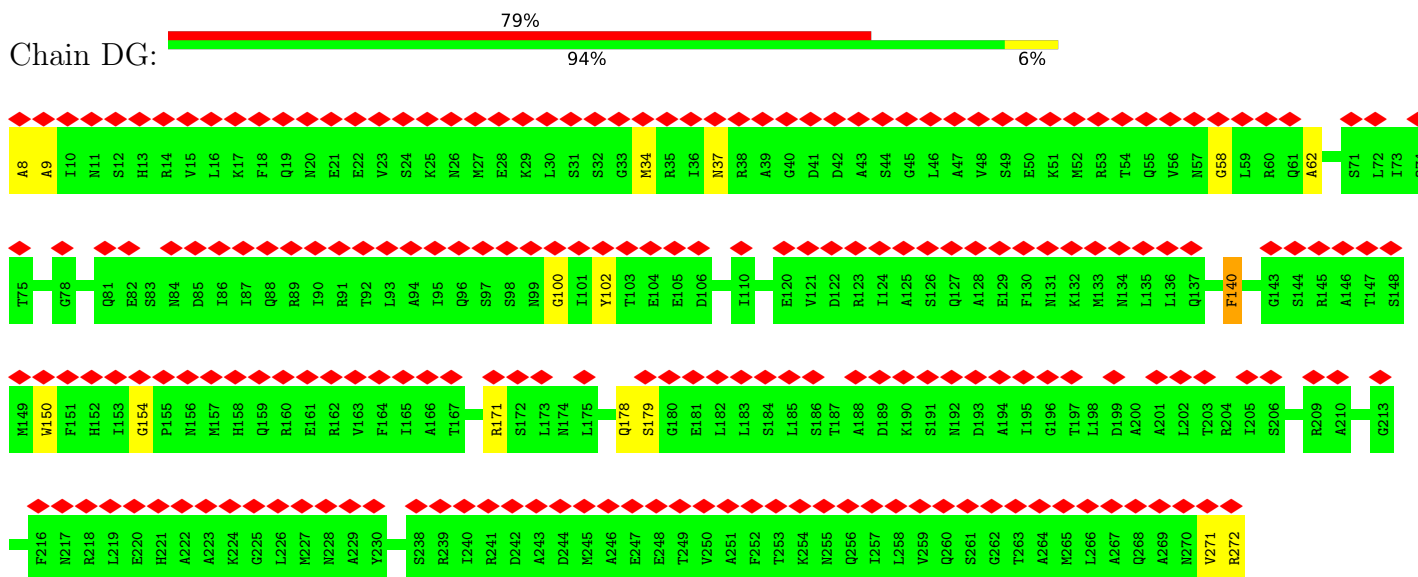
• Molecule 1: Flagellin B1 (FlaB1)



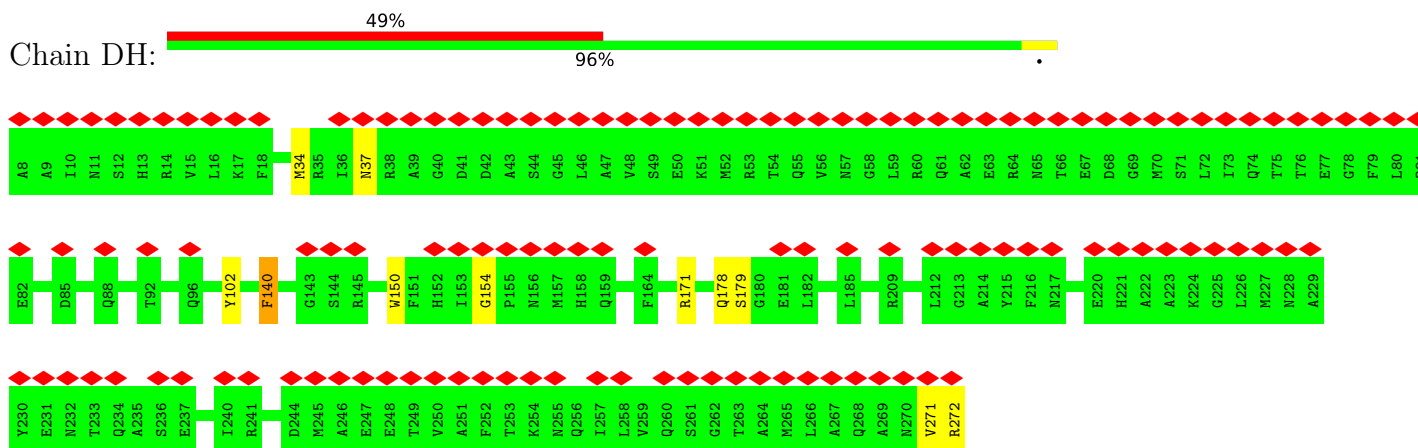
• Molecule 1: Flagellin B1 (FlaB1)



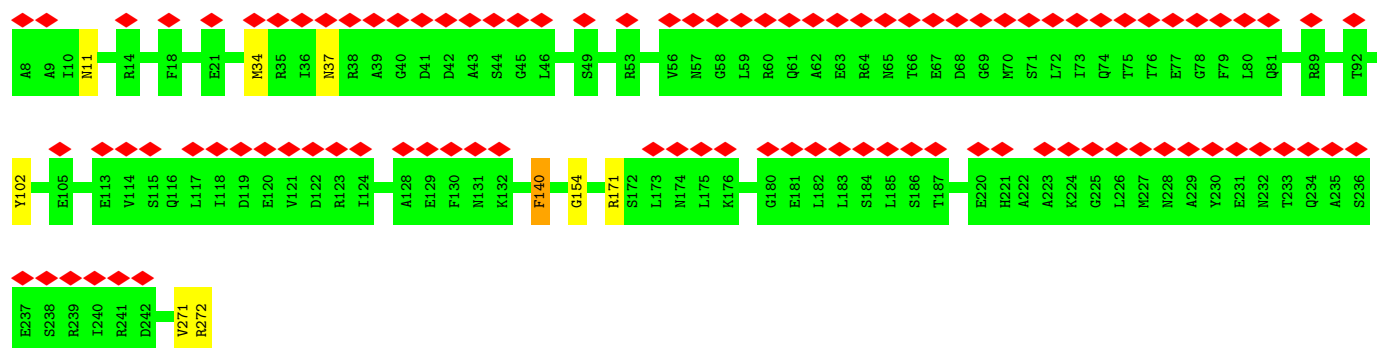
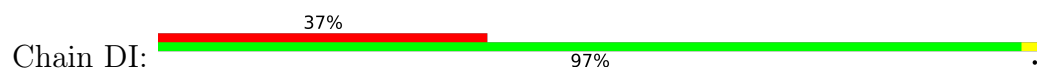
• Molecule 1: Flagellin B1 (FlaB1)



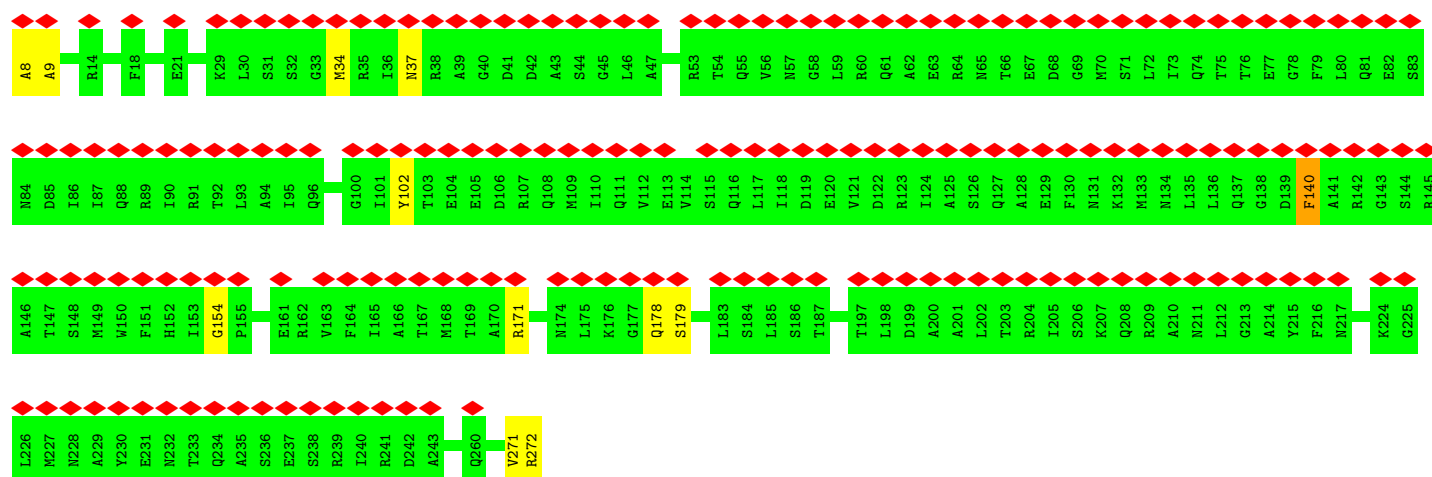
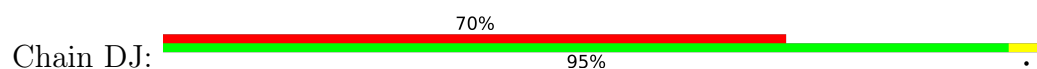
• Molecule 1: Flagellin B1 (FlaB1)



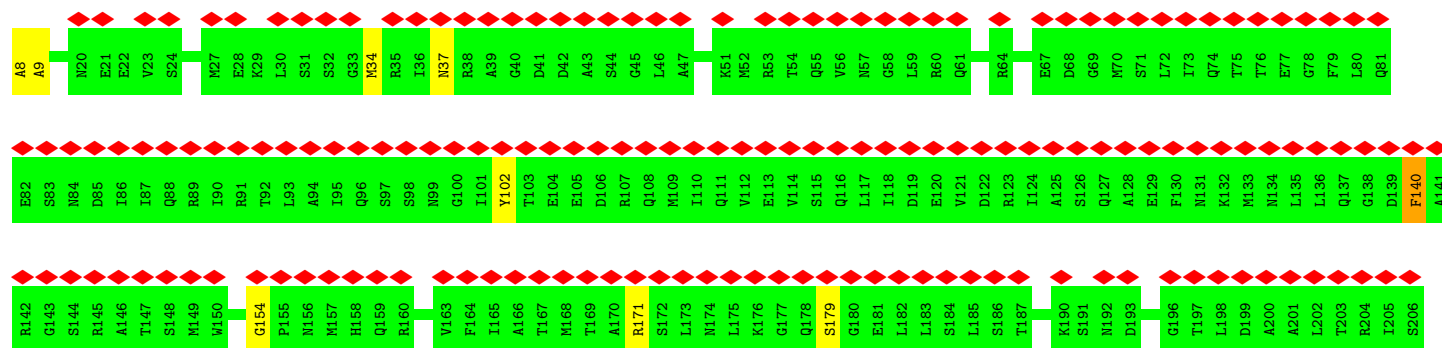
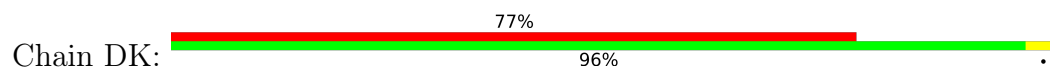
- Molecule 1: Flagellin B1 (FlaB1)

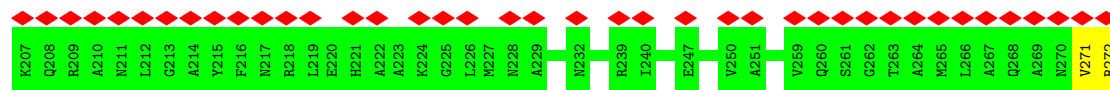


- Molecule 1: Flagellin B1 (FlaB1)

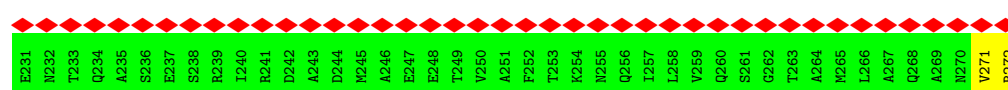
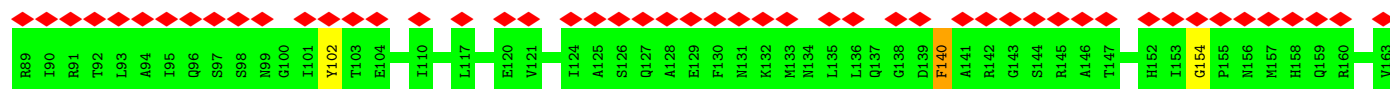
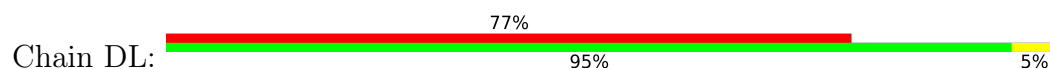


- Molecule 1: Flagellin B1 (FlaB1)

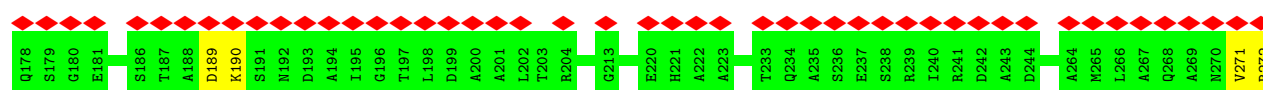
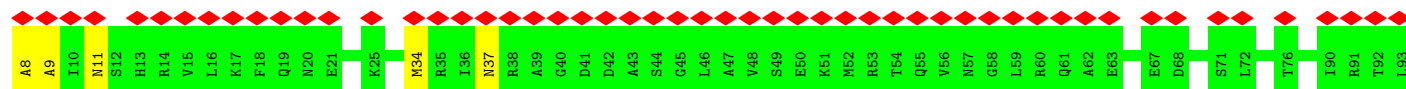




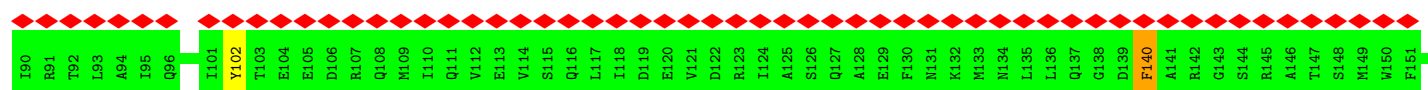
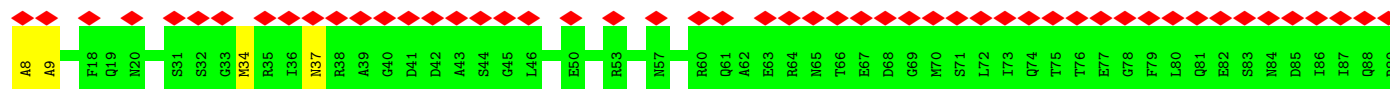
• Molecule 1: Flagellin B1 (FlaB1)

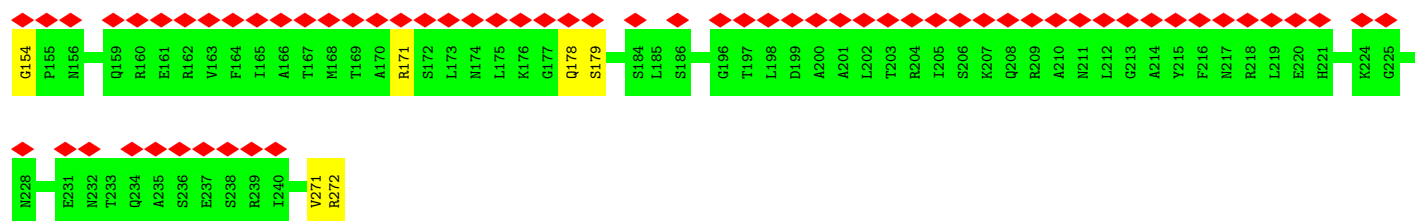


• Molecule 1: Flagellin B1 (FlaB1)

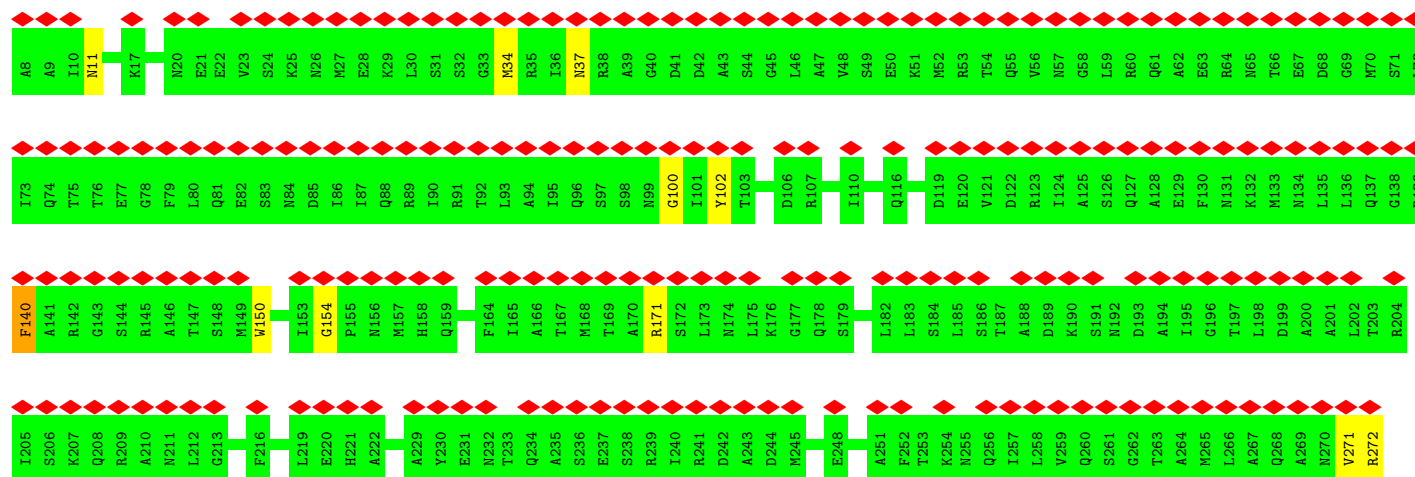
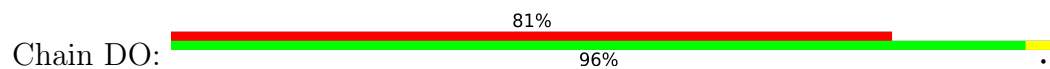


• Molecule 1: Flagellin B1 (FlaB1)

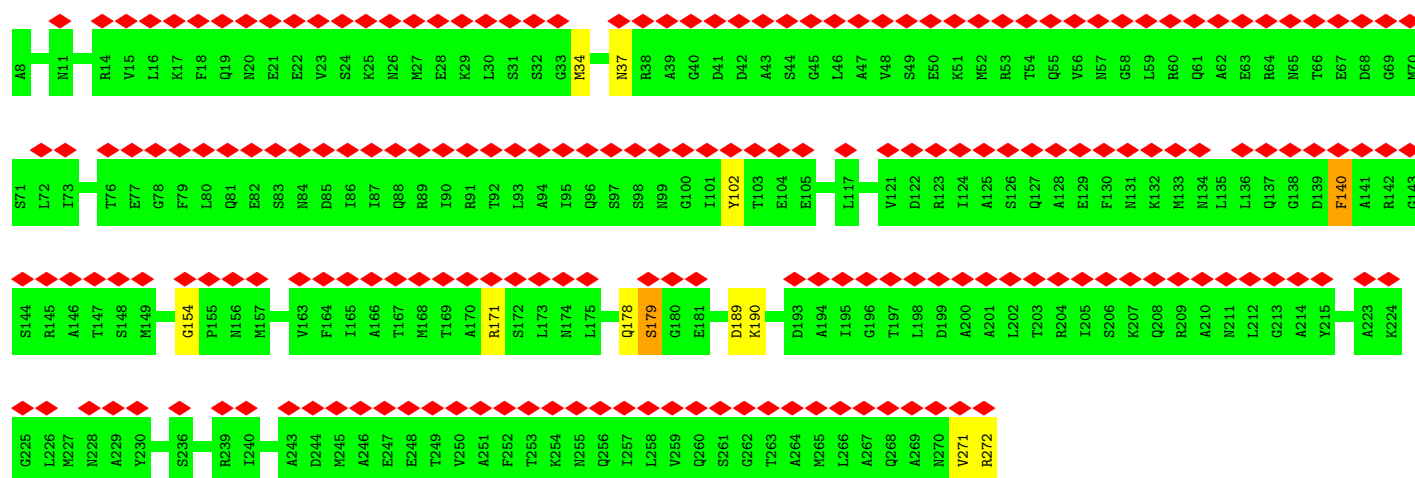
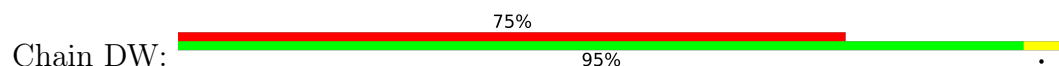




• Molecule 1: Flagellin B1 (FlaB1)

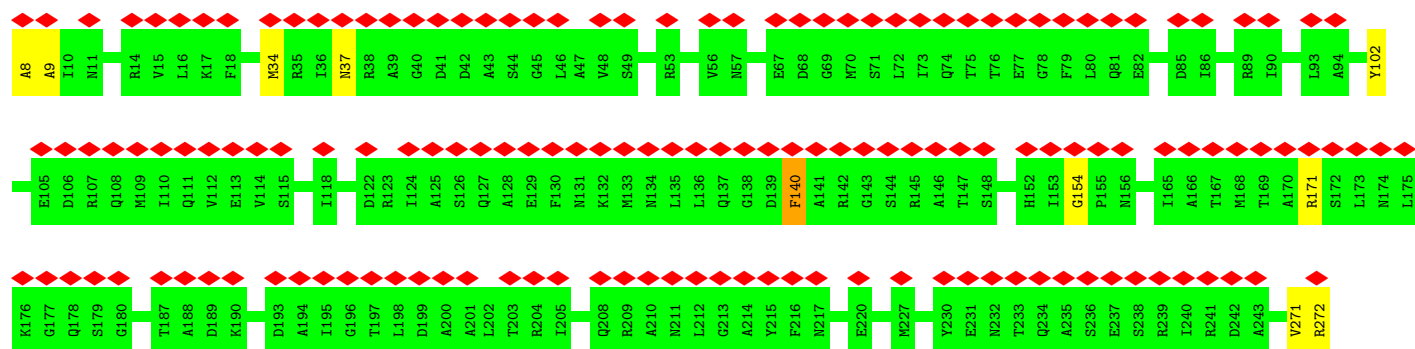


• Molecule 1: Flagellin B1 (FlaB1)

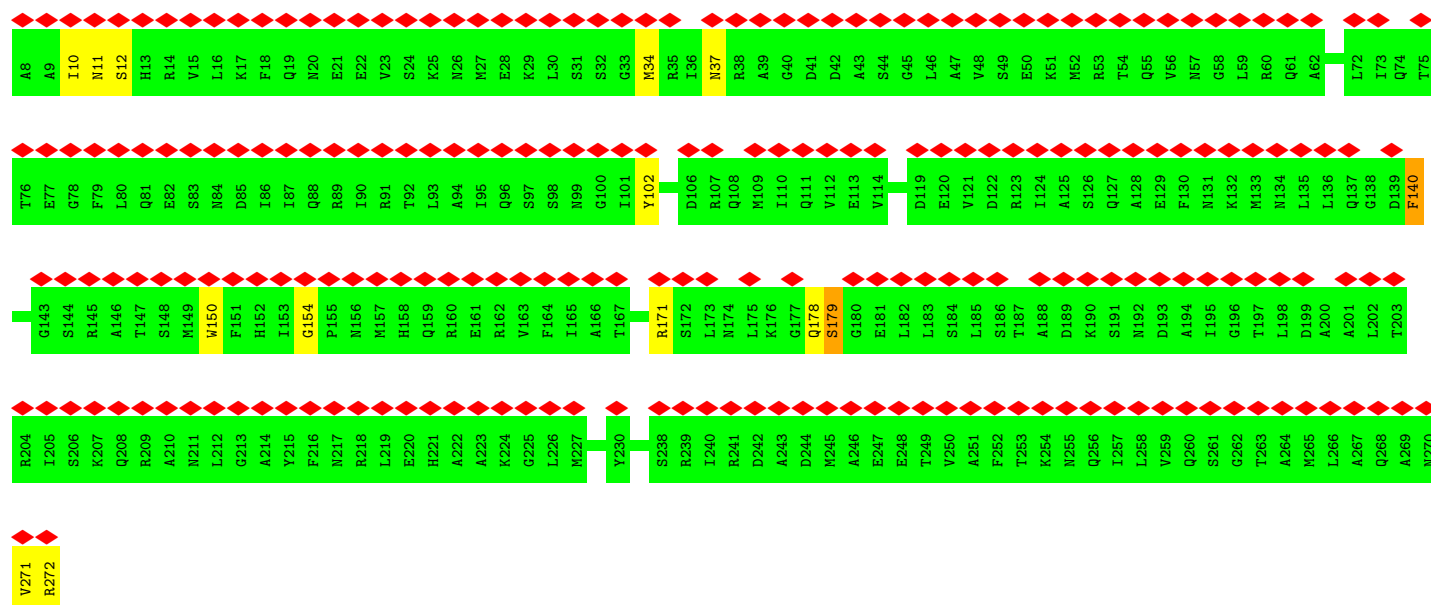
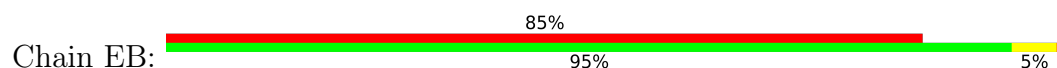


• Molecule 1: Flagellin B1 (FlaB1)

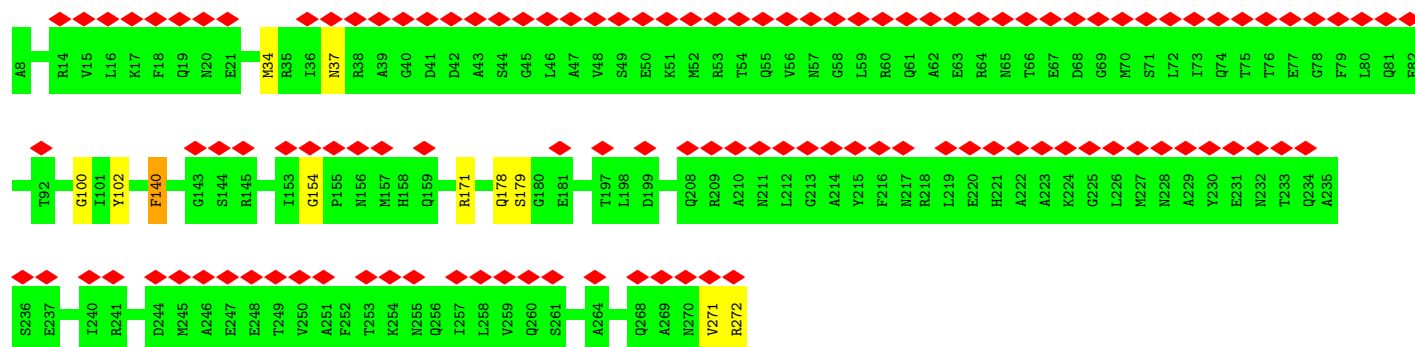




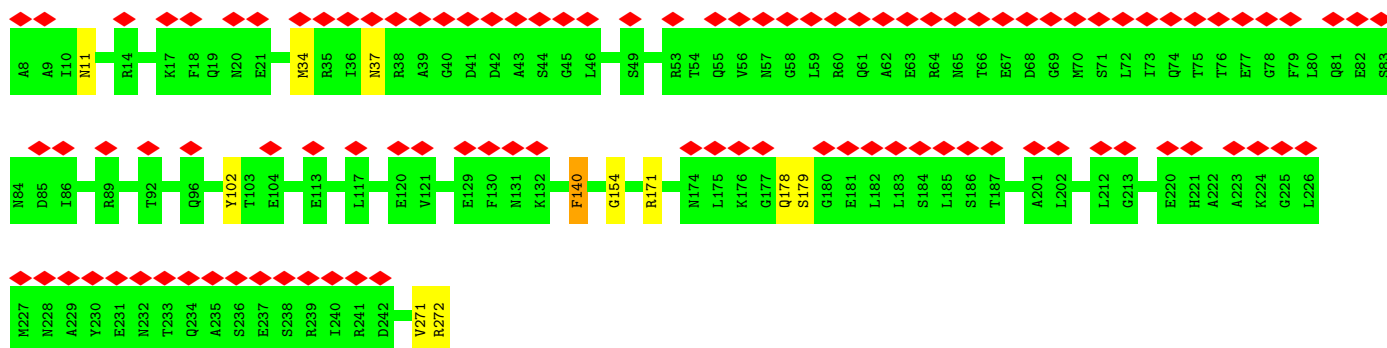
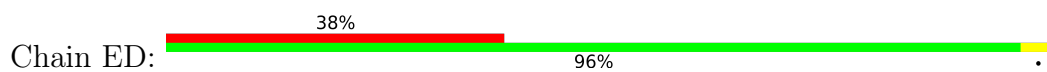
• Molecule 1: Flagellin B1 (FlaB1)



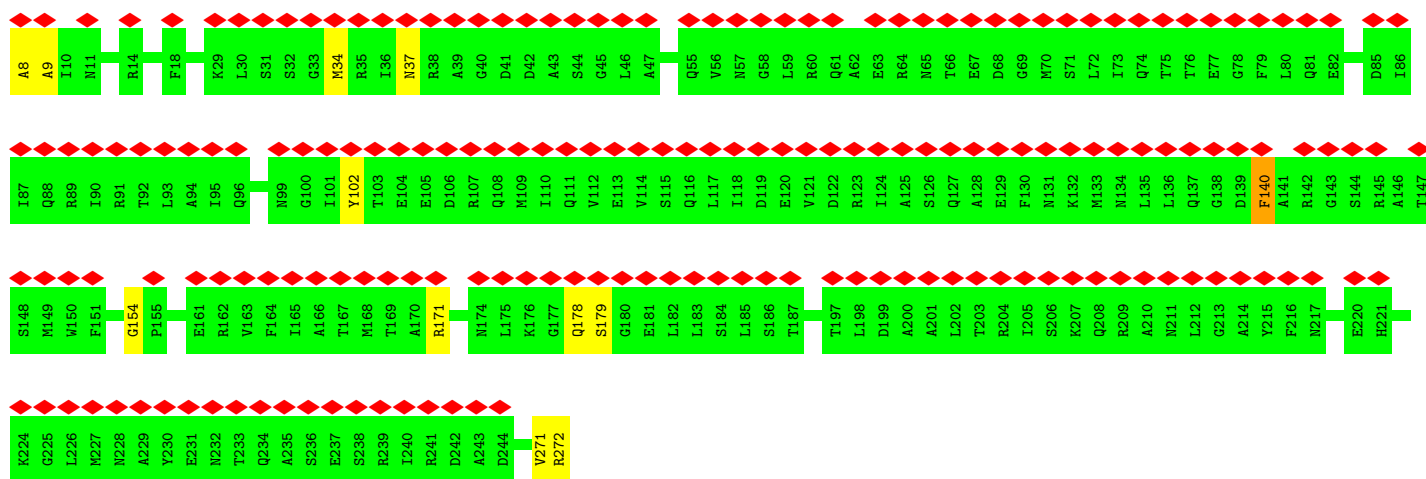
• Molecule 1: Flagellin B1 (FlaB1)



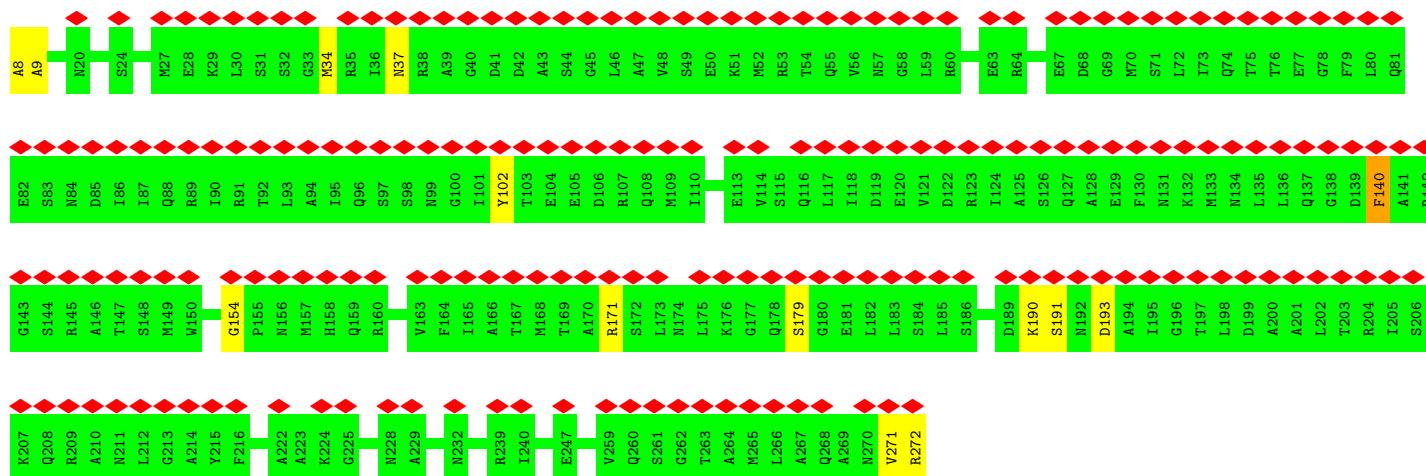
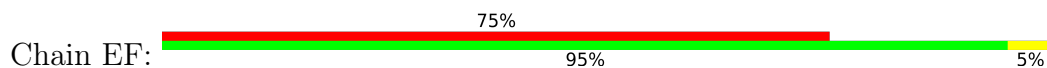
• Molecule 1: Flagellin B1 (FlaB1)



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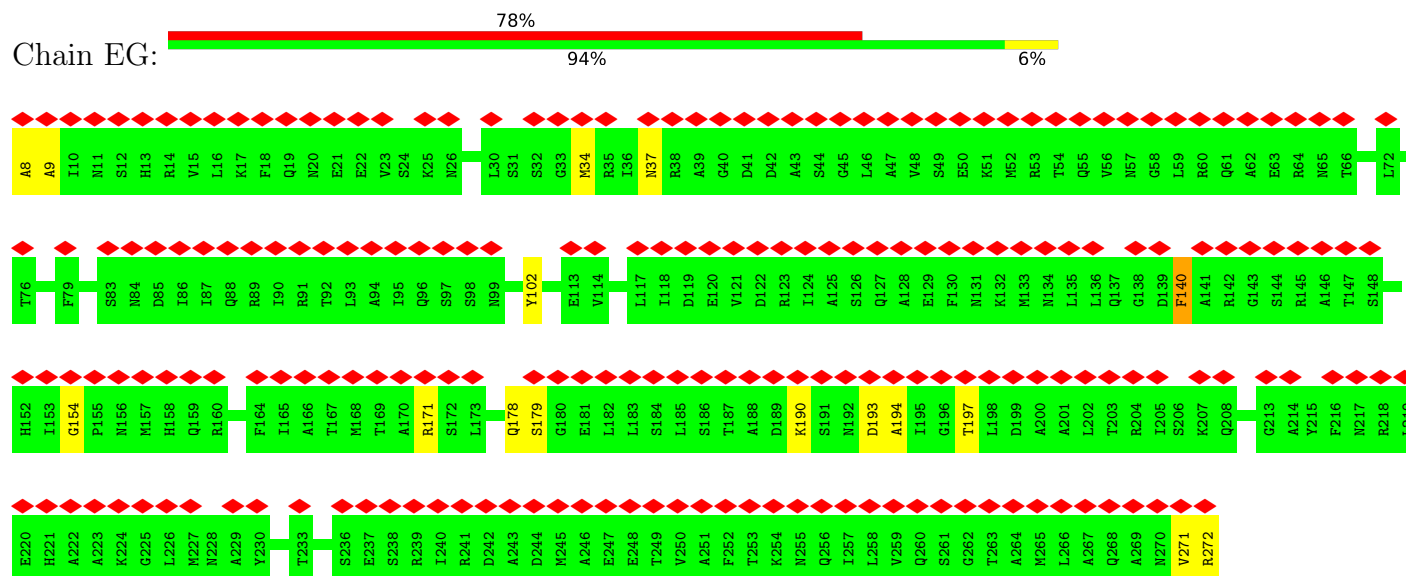


• Molecule 1: Flagellin B1 (FlaB1)



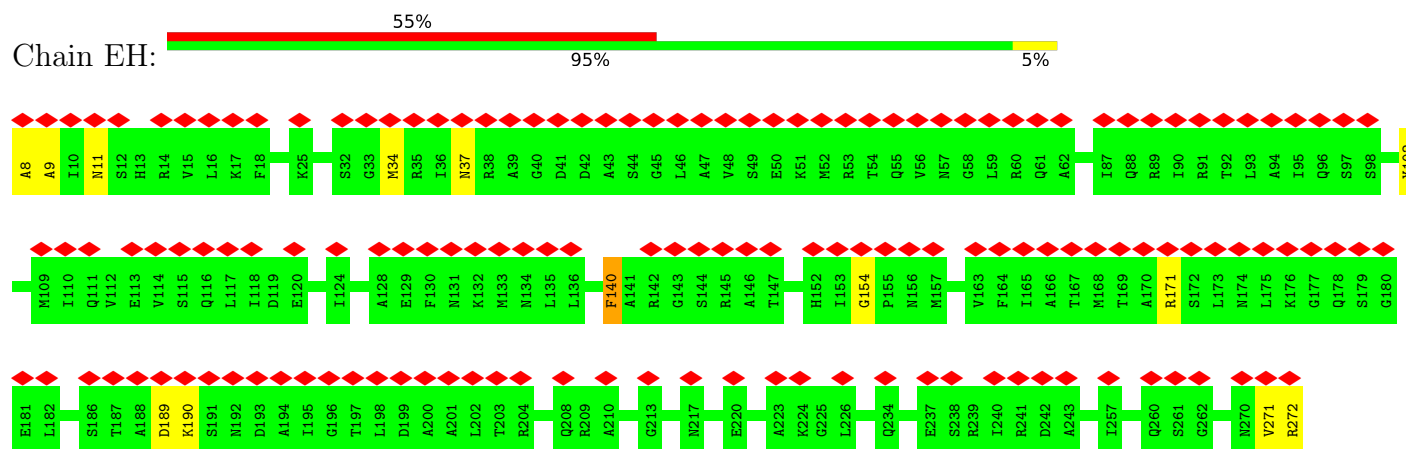
● Molecule 1: Flagellin B1 (FlaB1)

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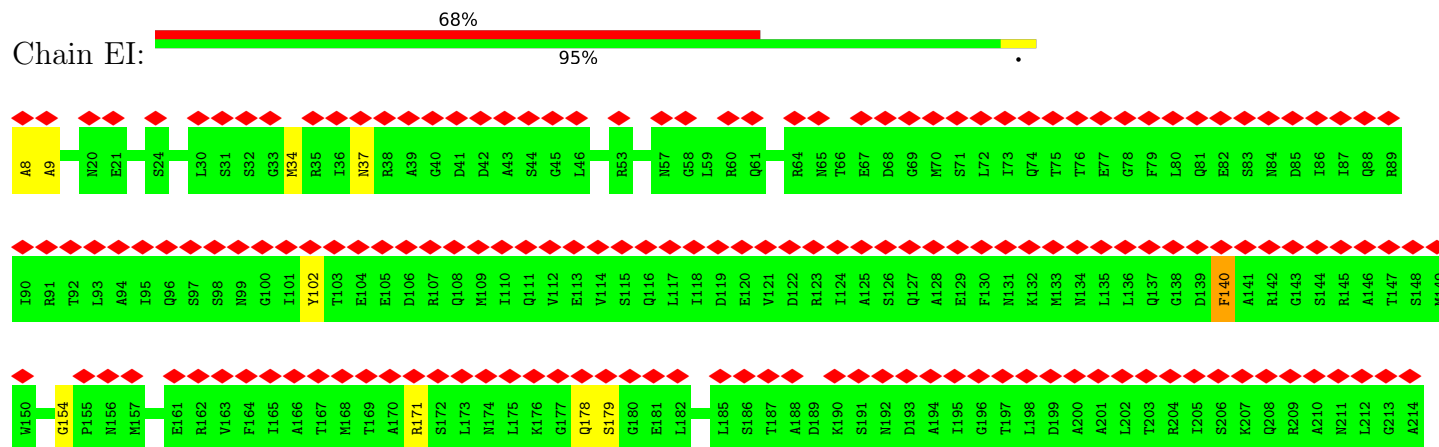
● Molecule 1: Flagellin B1 (FlaB1)

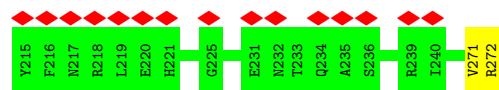
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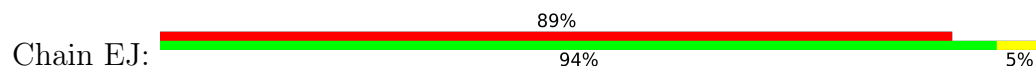
● Molecule 1: Flagellin B1 (FlaB1)

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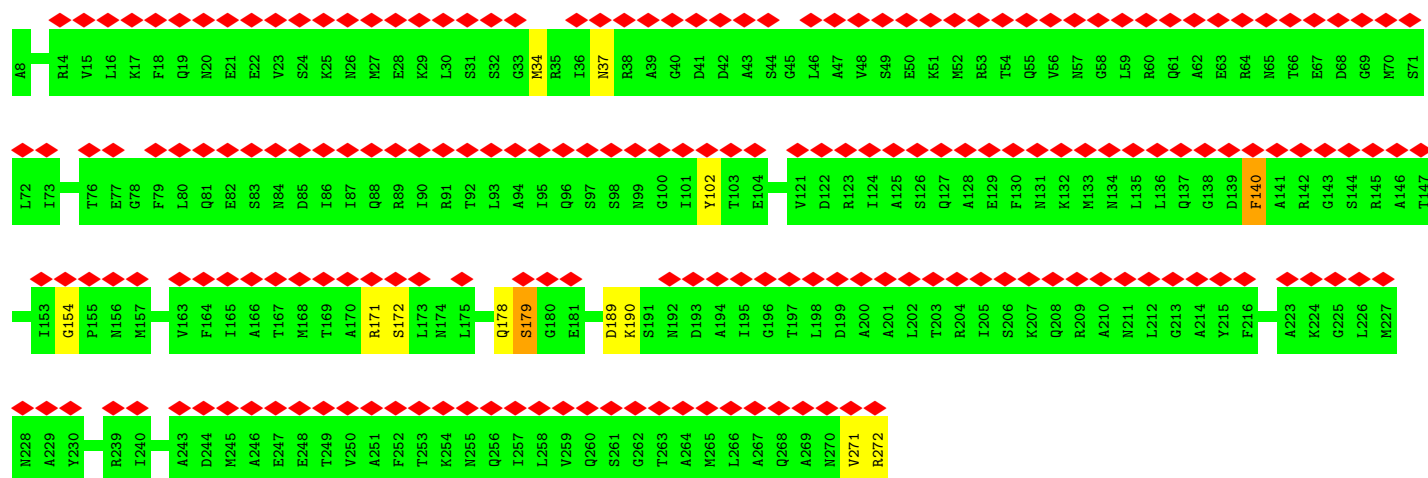
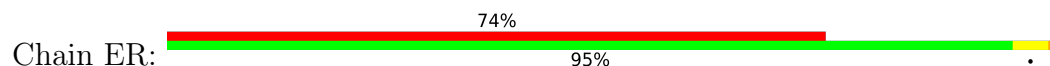




• Molecule 1: Flagellin B1 (FlaB1)

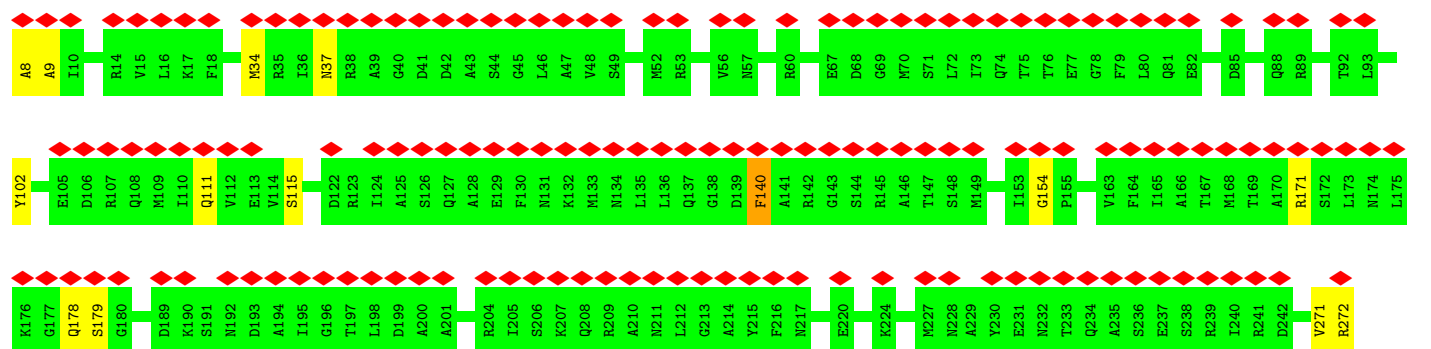


• Molecule 1: Flagellin B1 (FlaB1)

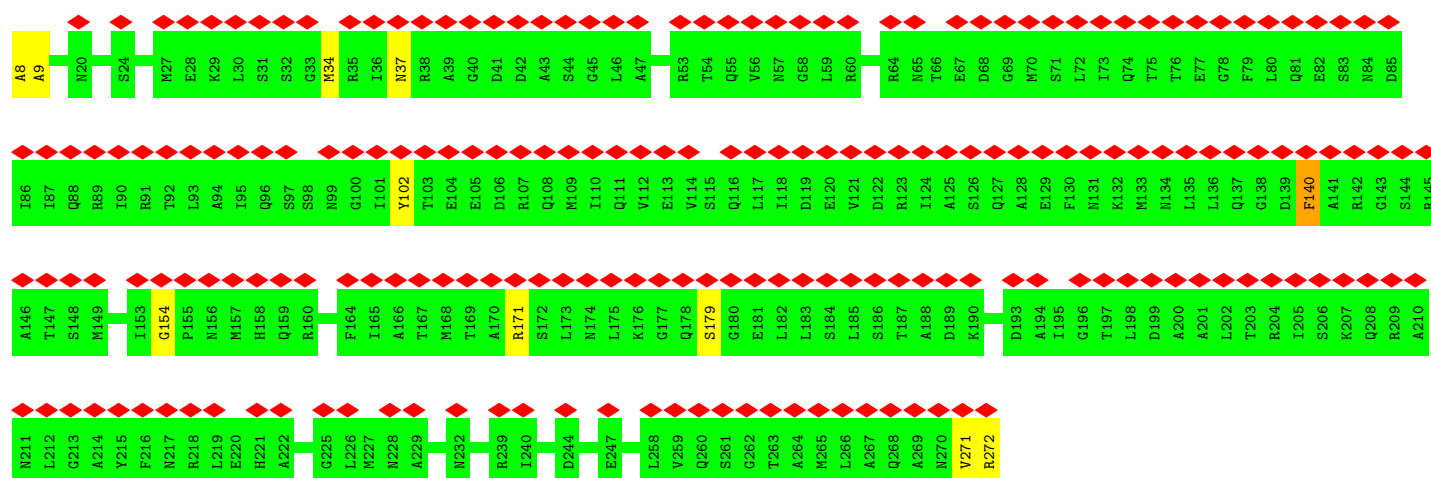
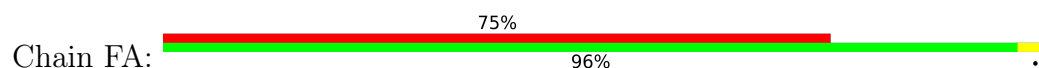


• Molecule 1: Flagellin B1 (FlaB1)

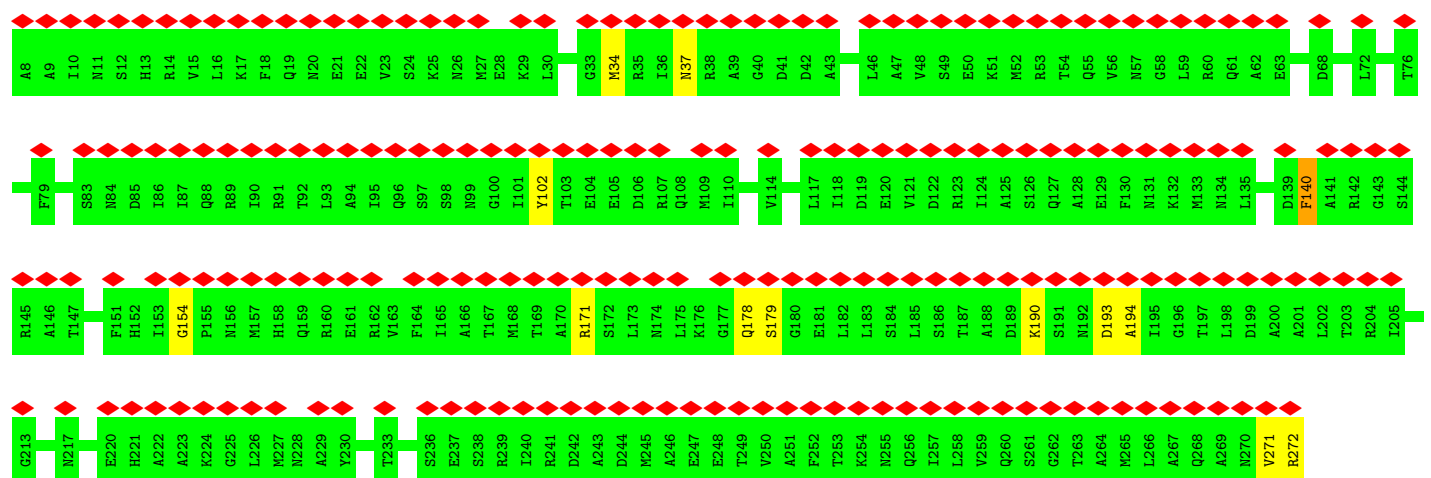




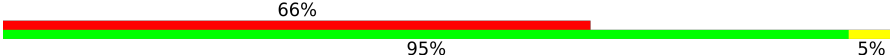
• Molecule 1: Flagellin B1 (FlaB1)

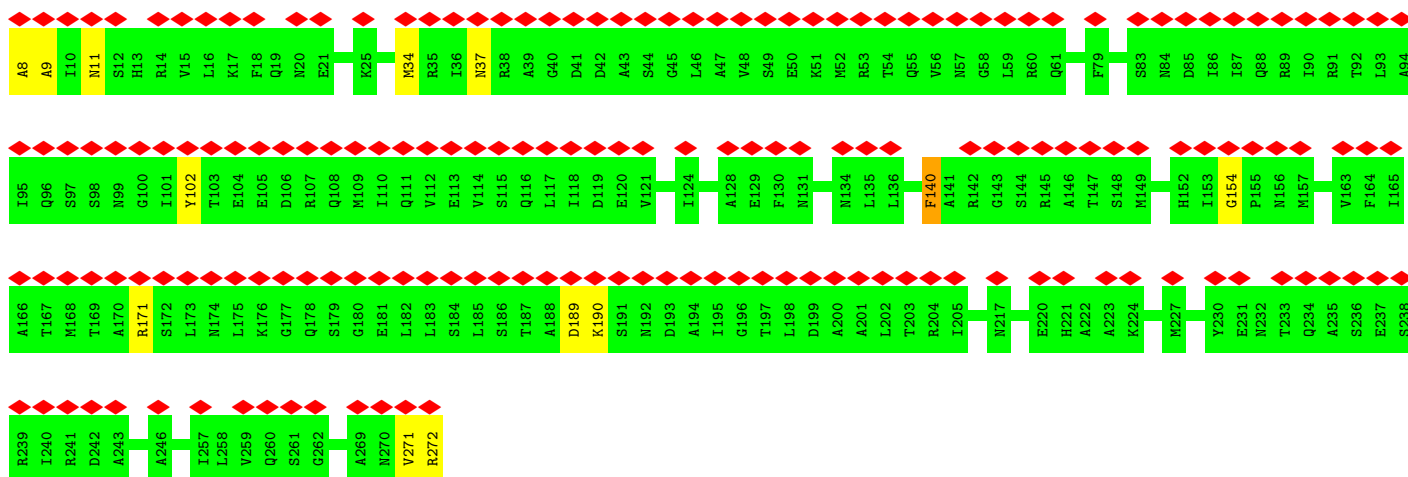


• Molecule 1: Flagellin B1 (FlaB1)

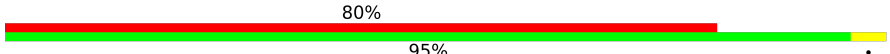


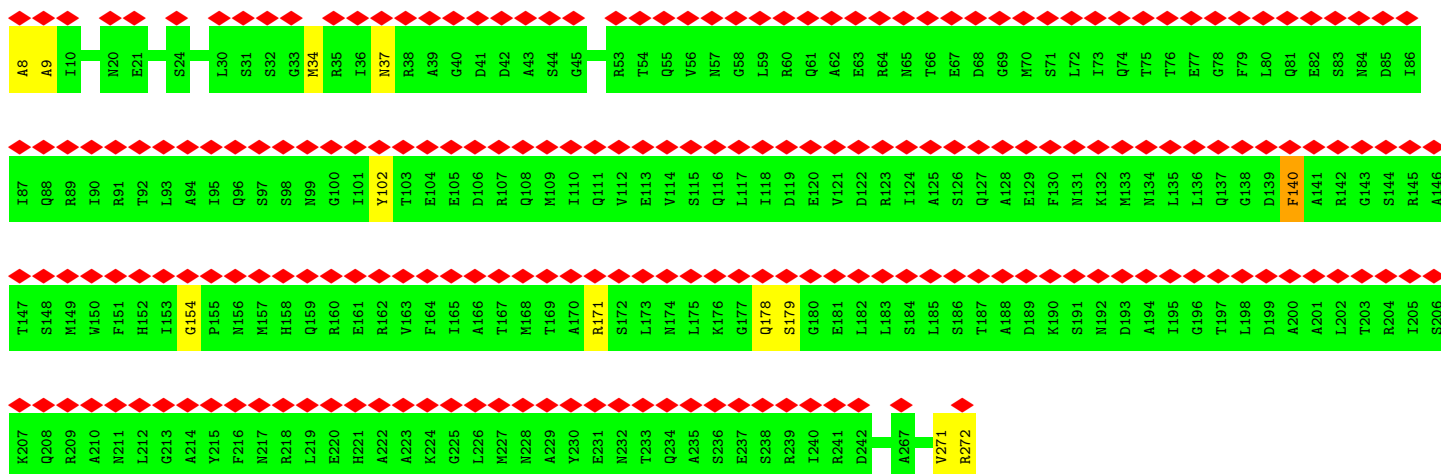
• Molecule 1: Flagellin B1 (FlaB1)

Chain FC: 

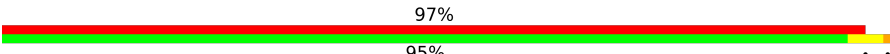


• Molecule 1: Flagellin B1 (FlaB1)

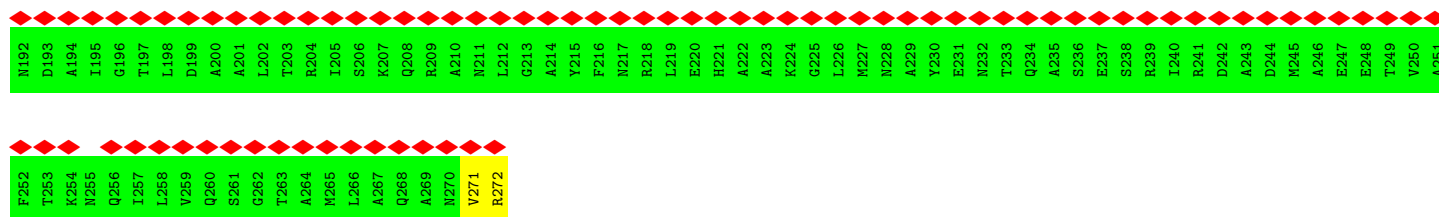
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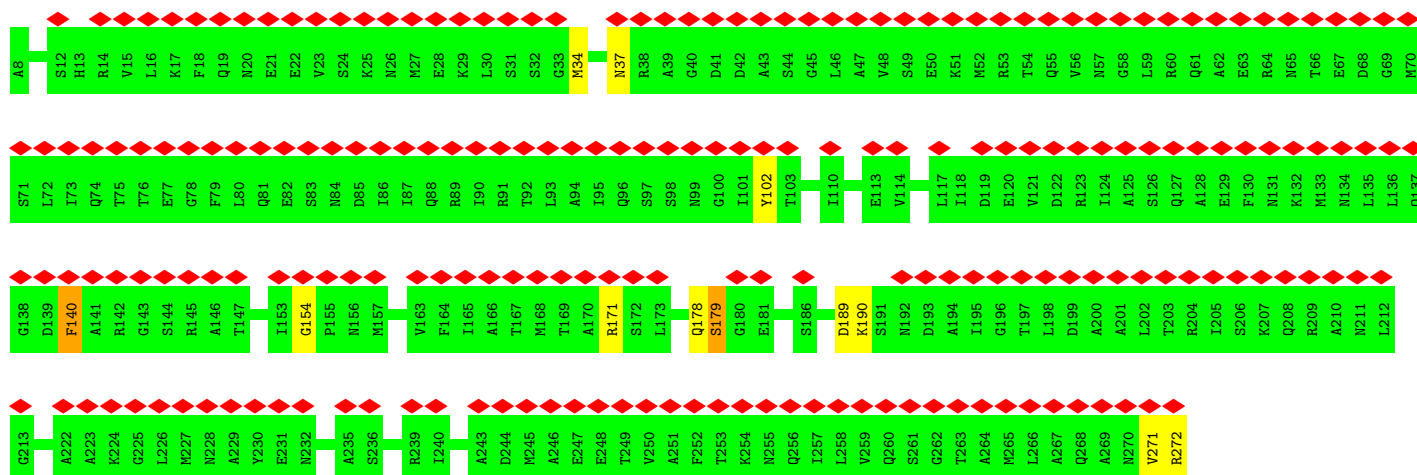
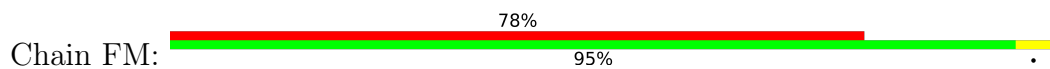
• Molecule 1: Flagellin B1 (FlaB1)

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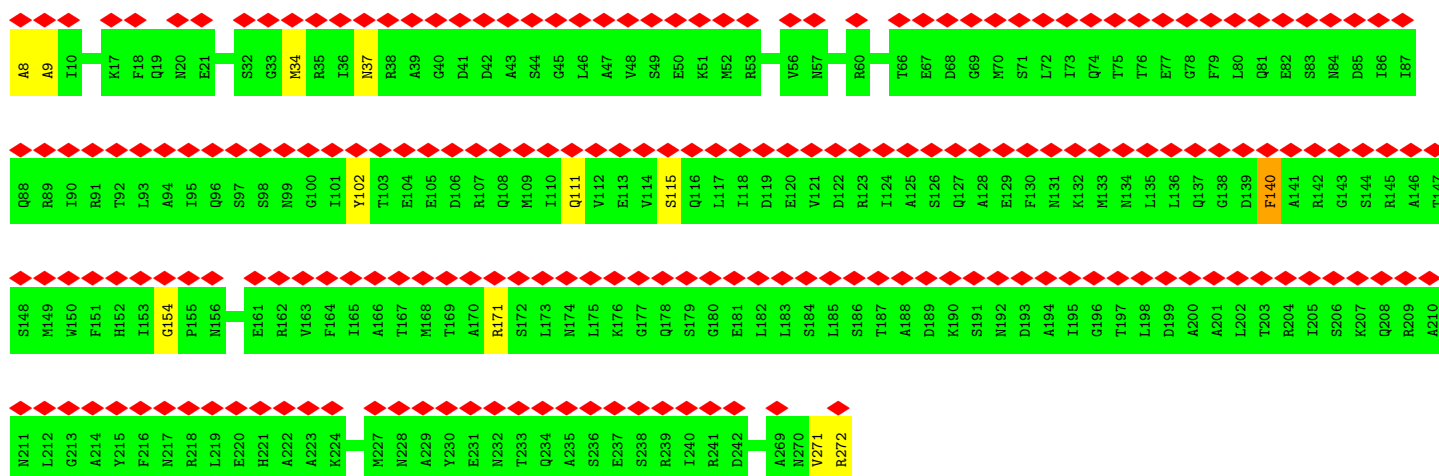
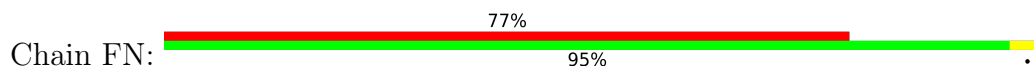




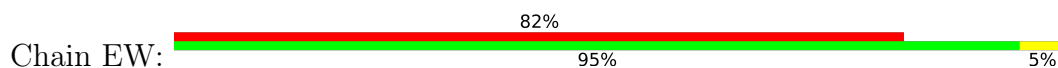
• Molecule 1: Flagellin B1 (FlaB1)

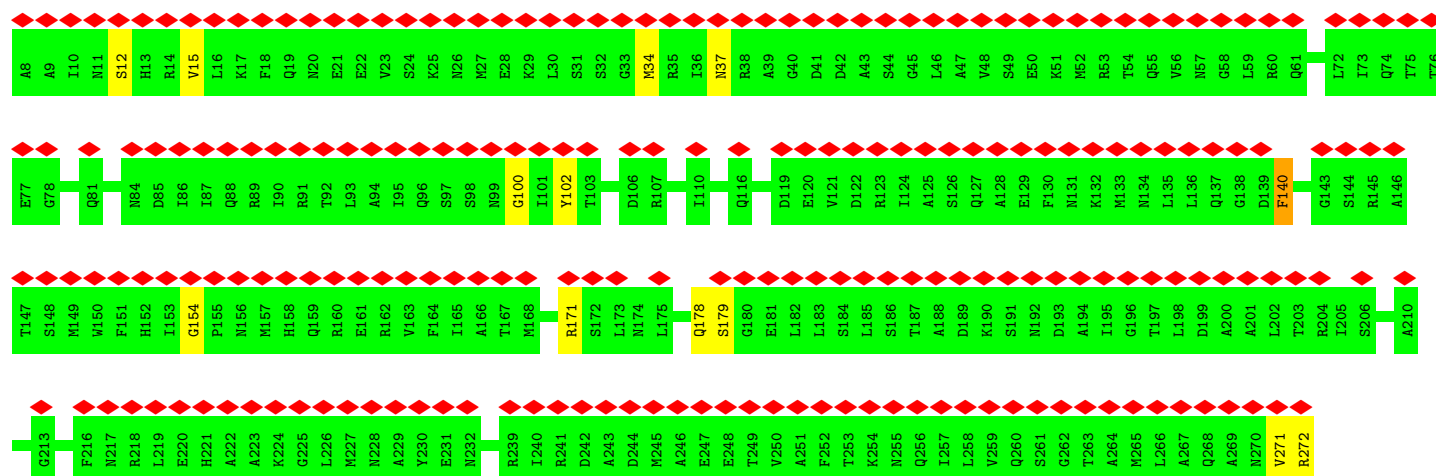


• Molecule 1: Flagellin B1 (FlaB1)

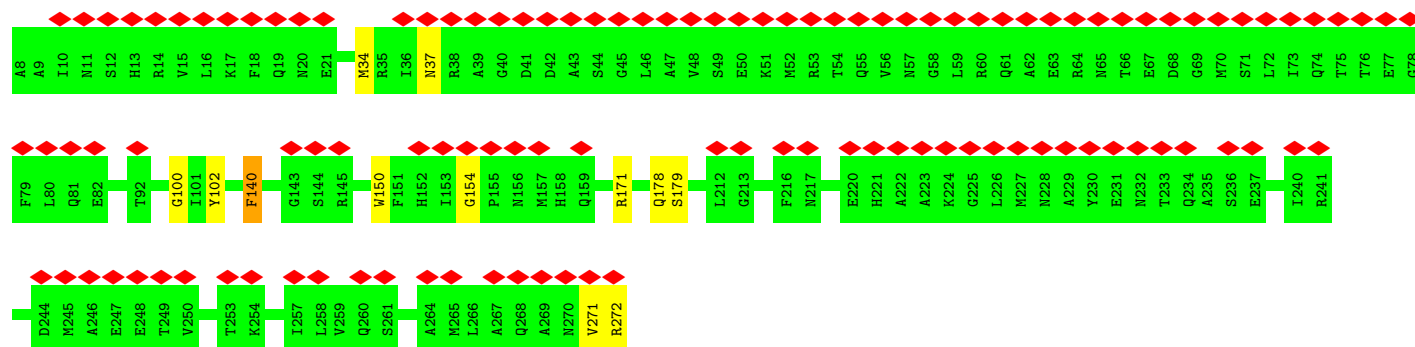


• Molecule 1: Flagellin B1 (FlaB1)

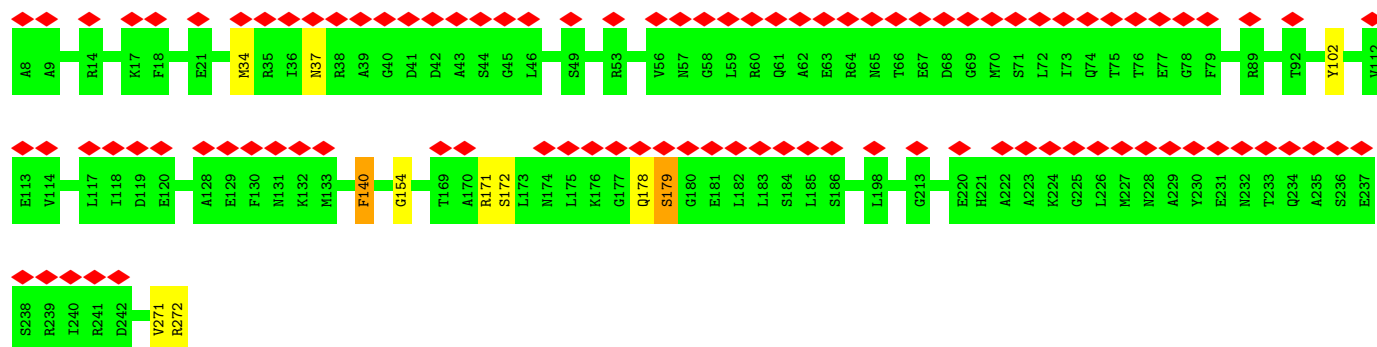
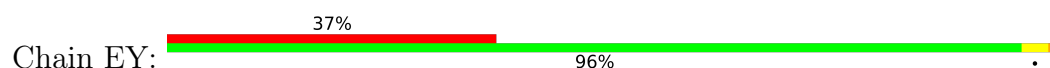




• Molecule 1: Flagellin B1 (FlaB1)

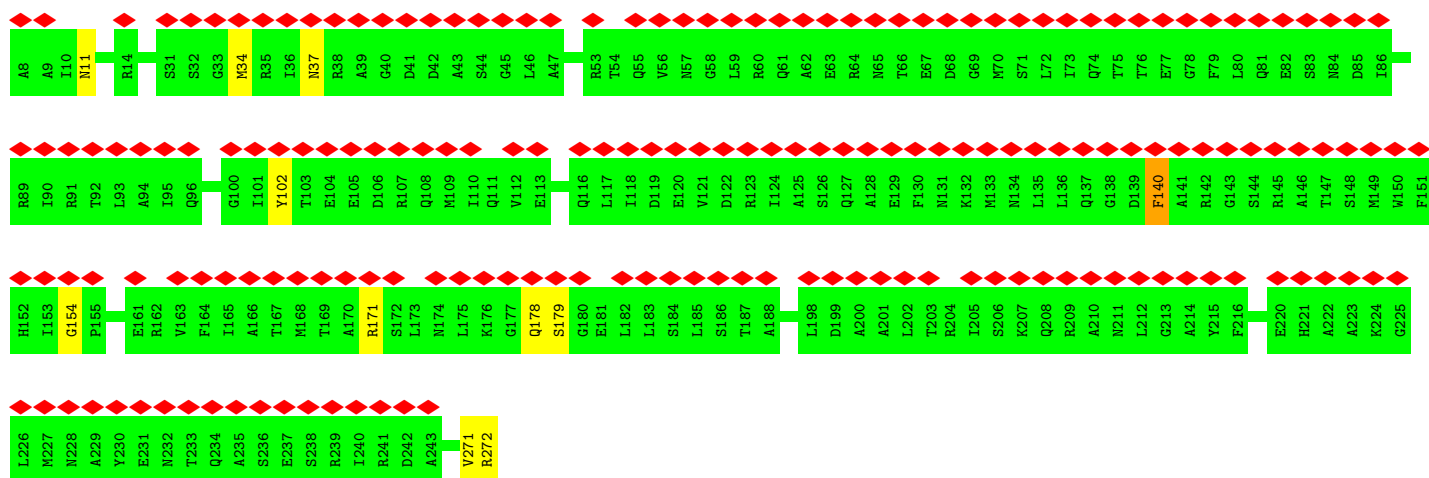


• Molecule 1: Flagellin B1 (FlaB1)



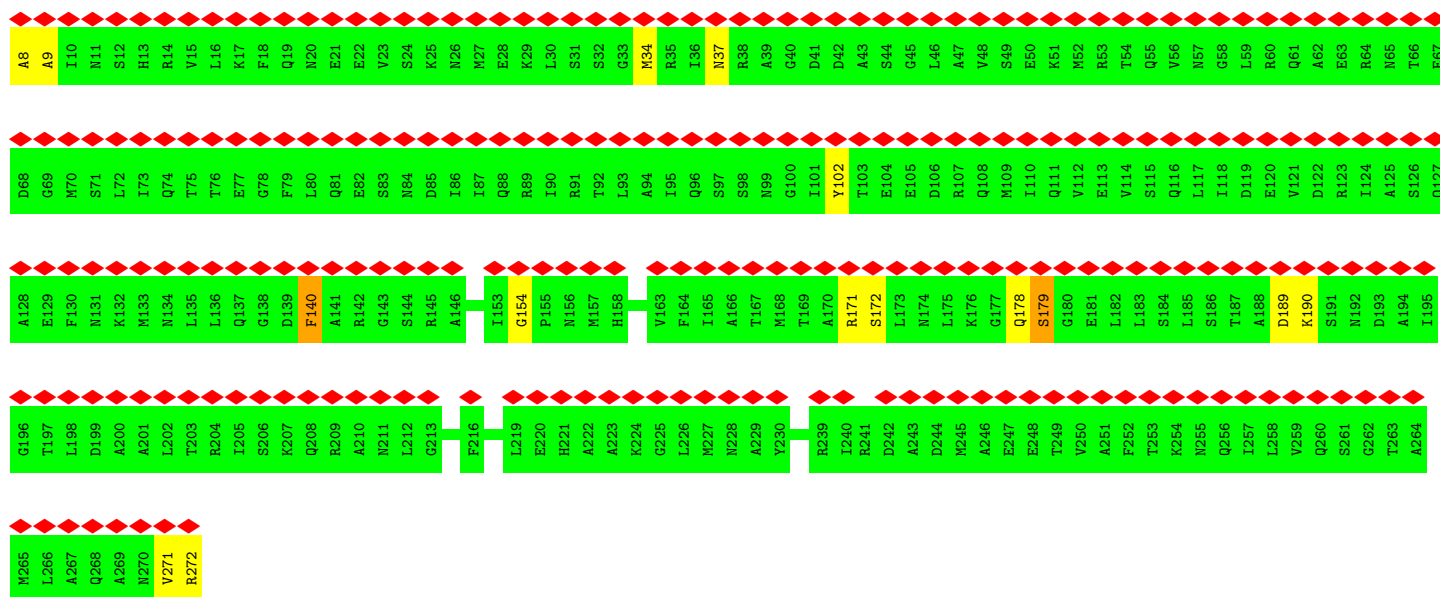
• Molecule 1: Flagellin B1 (FlaB1)





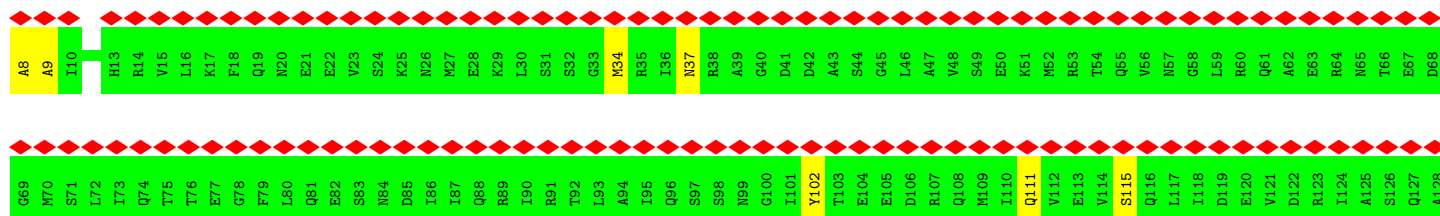
• Molecule 1: Flagellin B1 (FlaB1)

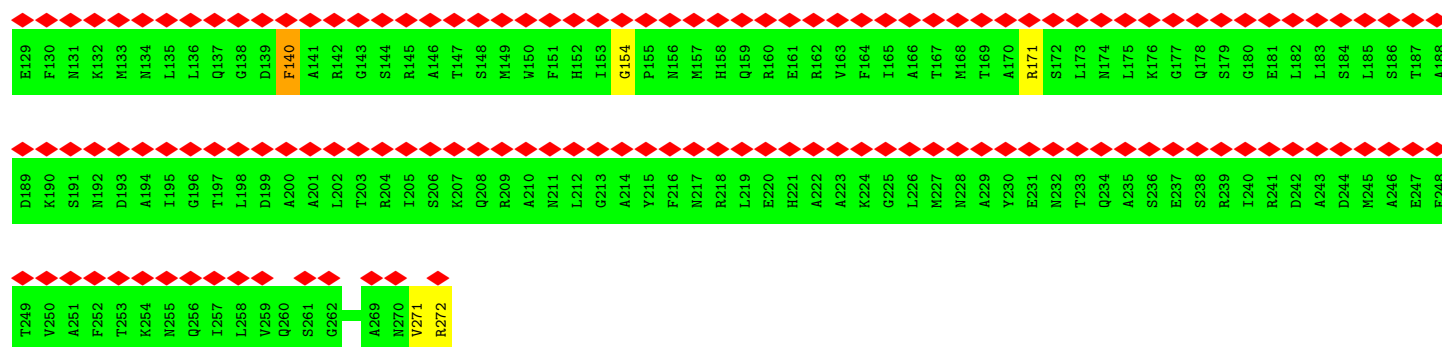
Chain GH: 91% 94% 5% .



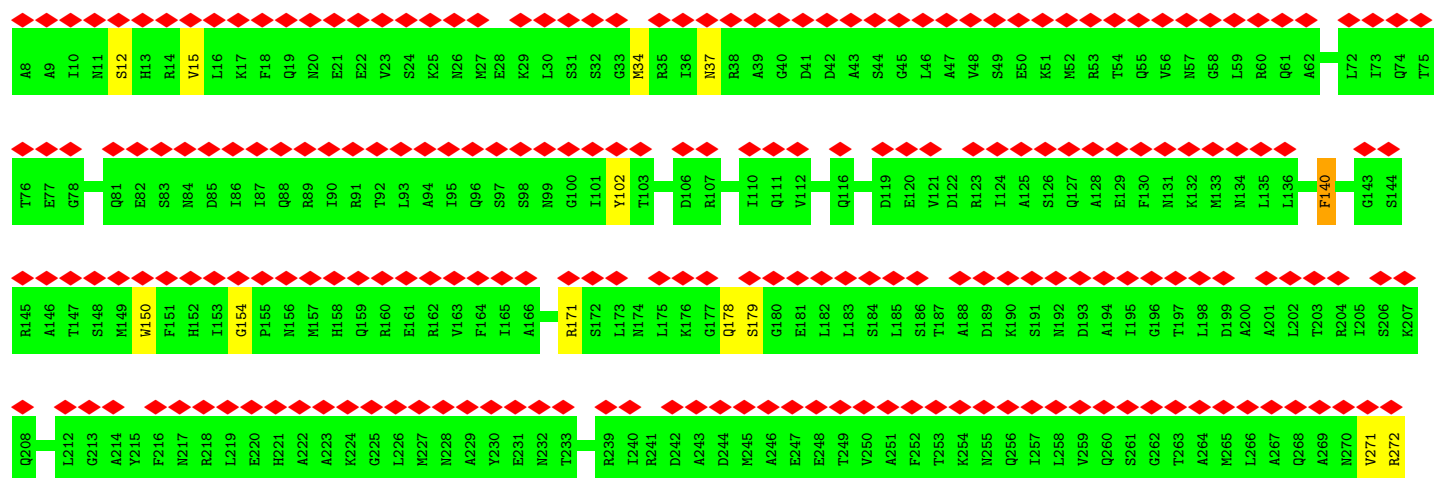
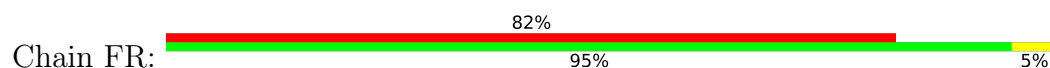
• Molecule 1: Flagellin B1 (FlaB1)

Chain GI: 96% 95% .





• Molecule 1: Flagellin B1 (FlaB1)

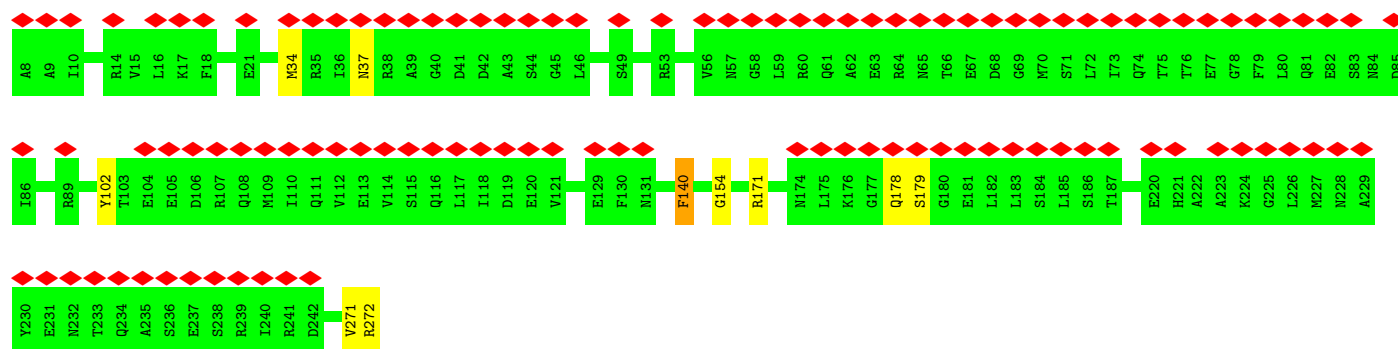


• Molecule 1: Flagellin B1 (FlaB1)

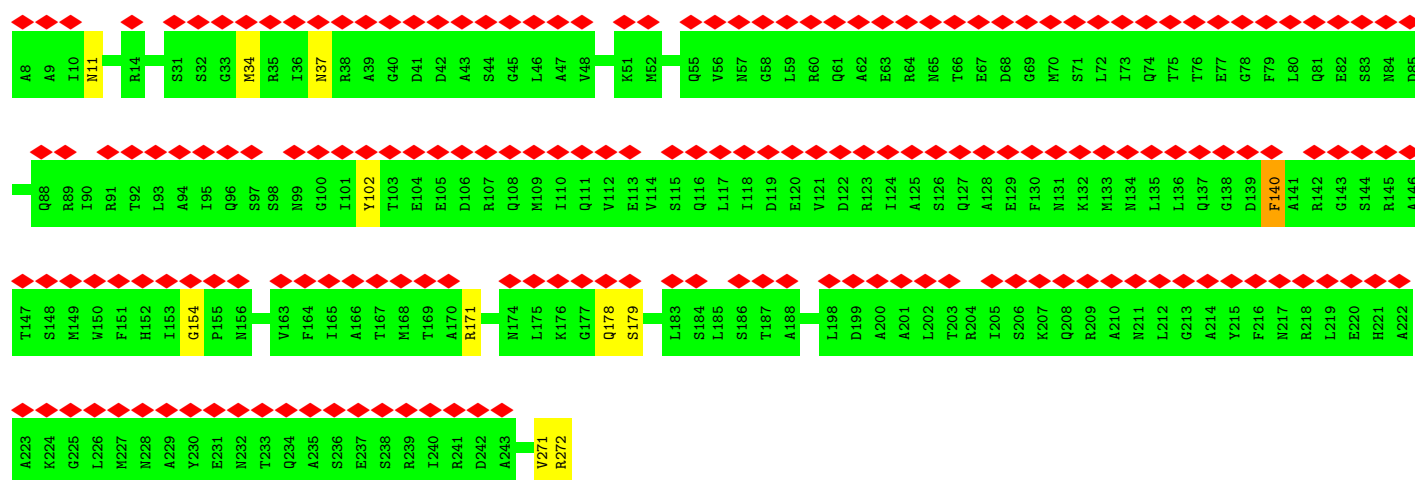


• Molecule 1: Flagellin B1 (FlaB1)

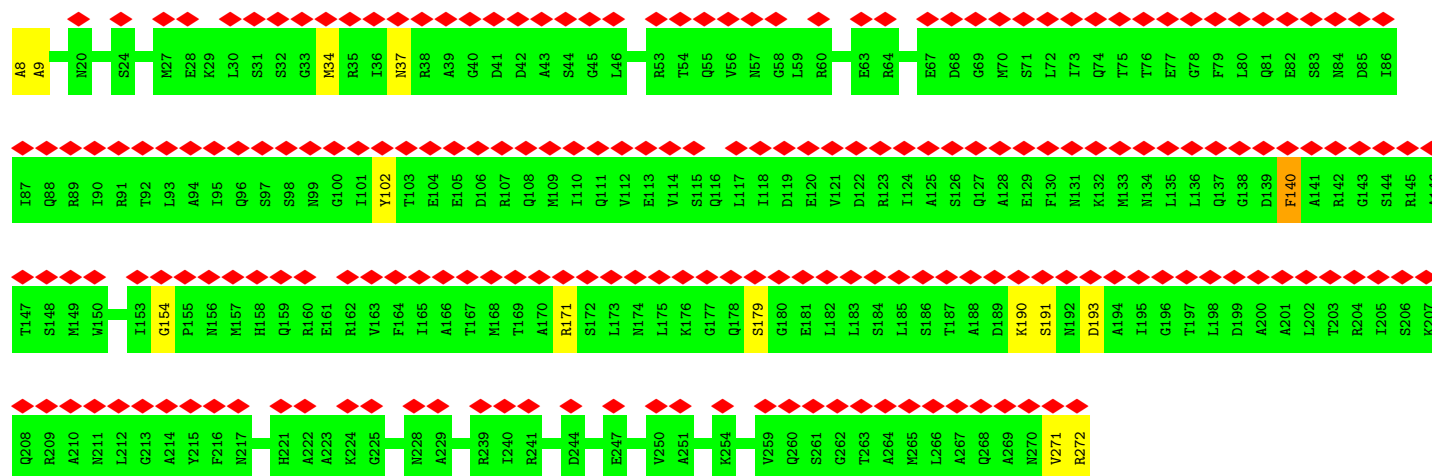
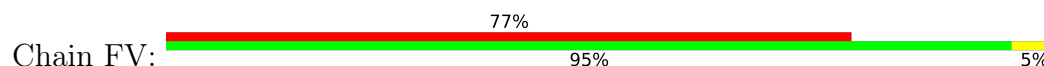




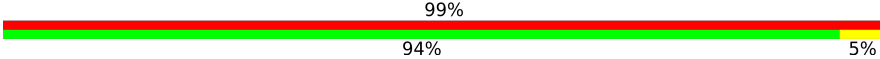
• Molecule 1: Flagellin B1 (FlaB1)

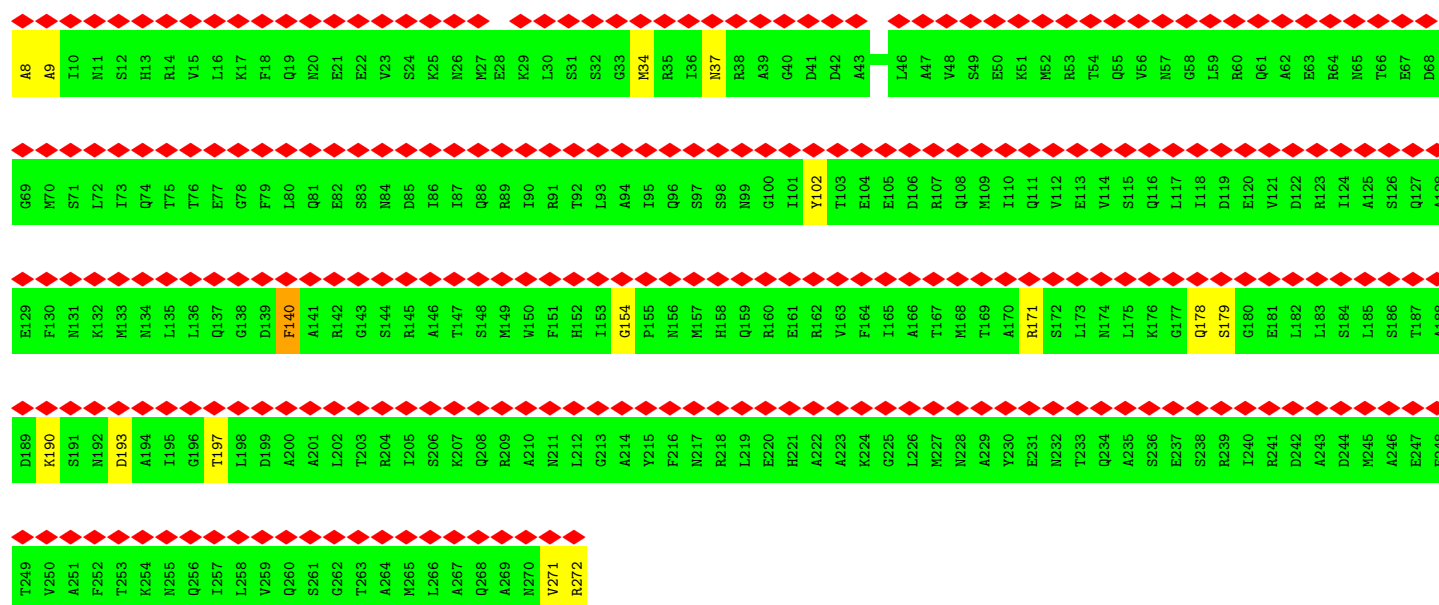


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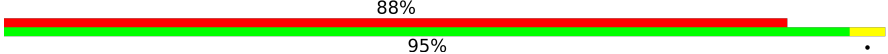


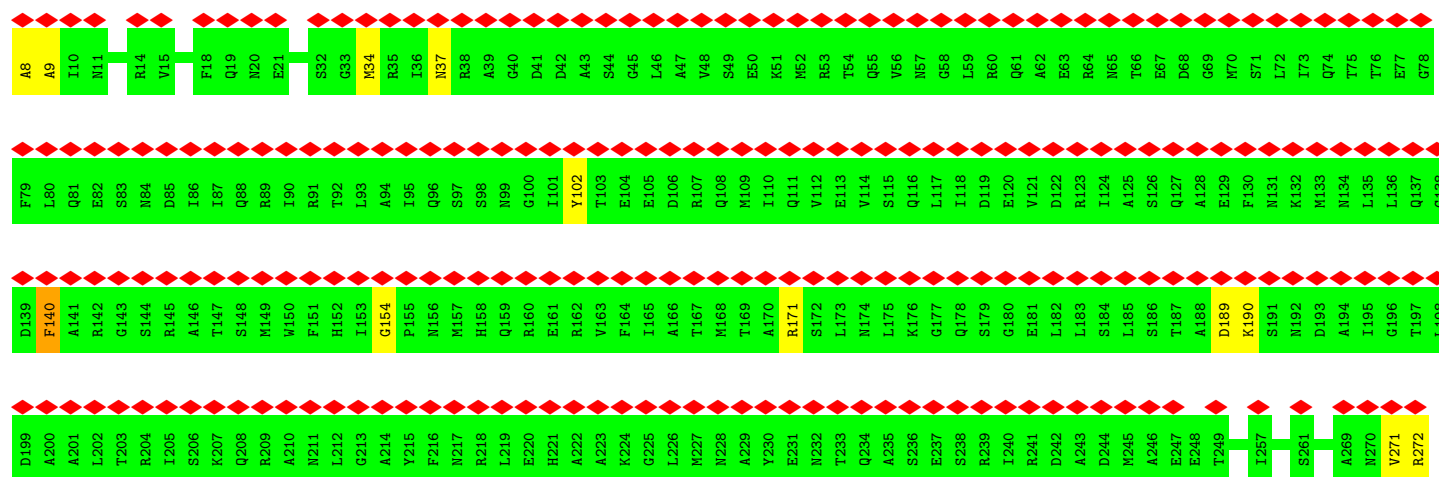
• Molecule 1: Flagellin B1 (FlaB1)

Chain FW: 

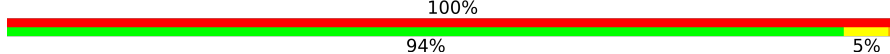


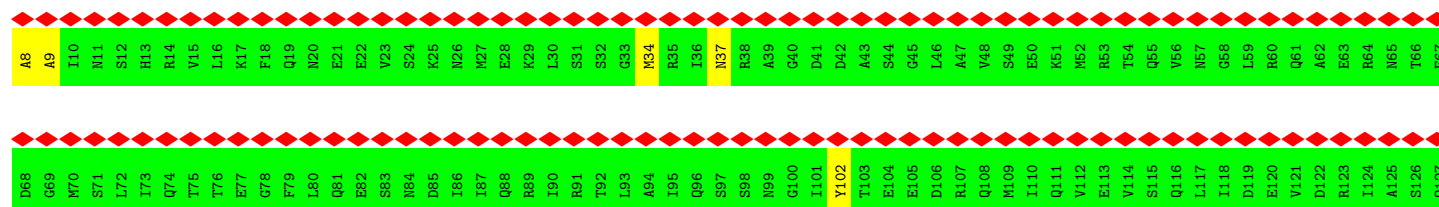
• Molecule 1: Flagellin B1 (FlaB1)

Chain FX: 



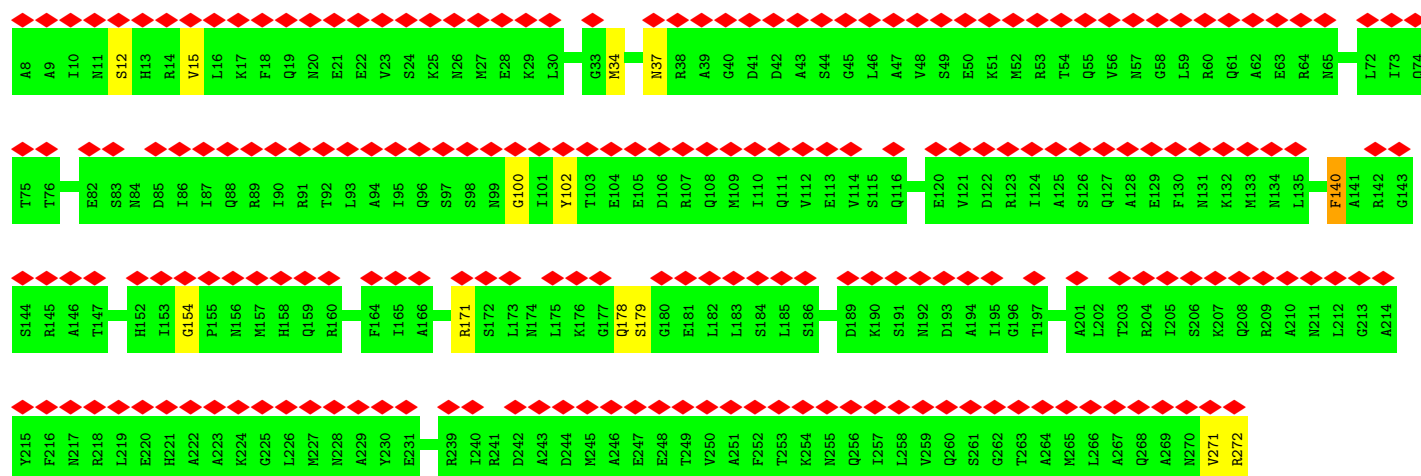
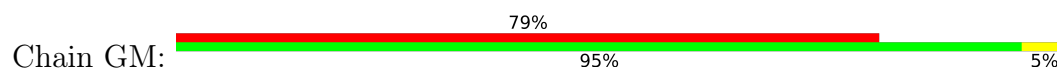
• Molecule 1: Flagellin B1 (FlaB1)

Chain HC: 

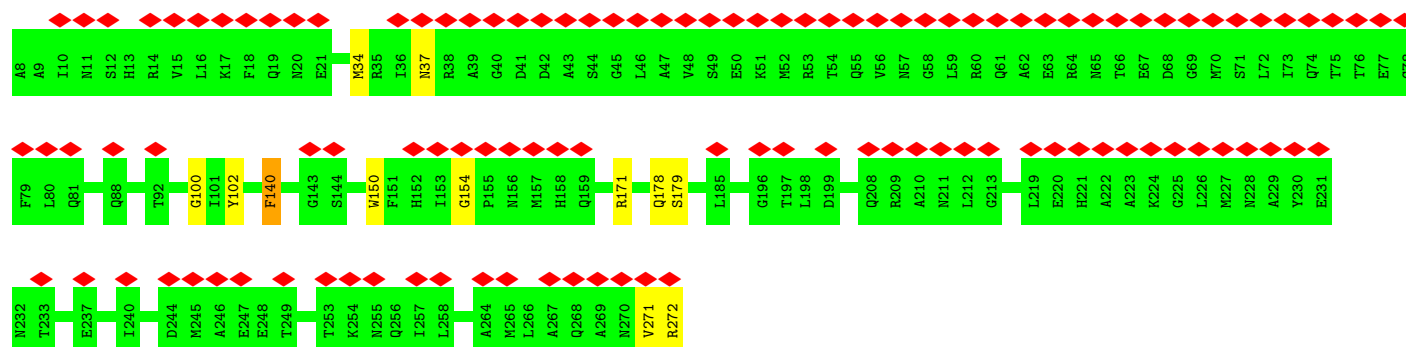




• Molecule 1: Flagellin B1 (FlaB1)

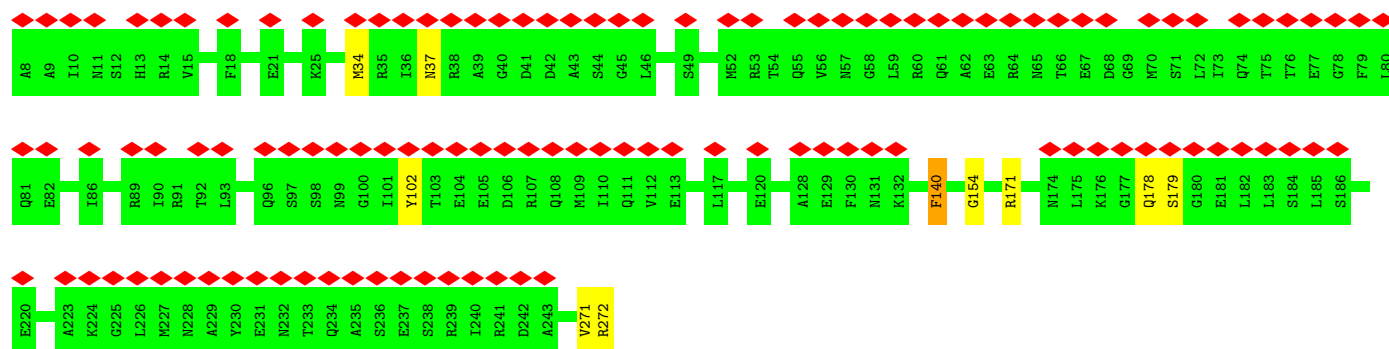


• Molecule 1: Flagellin B1 (FlaB1)

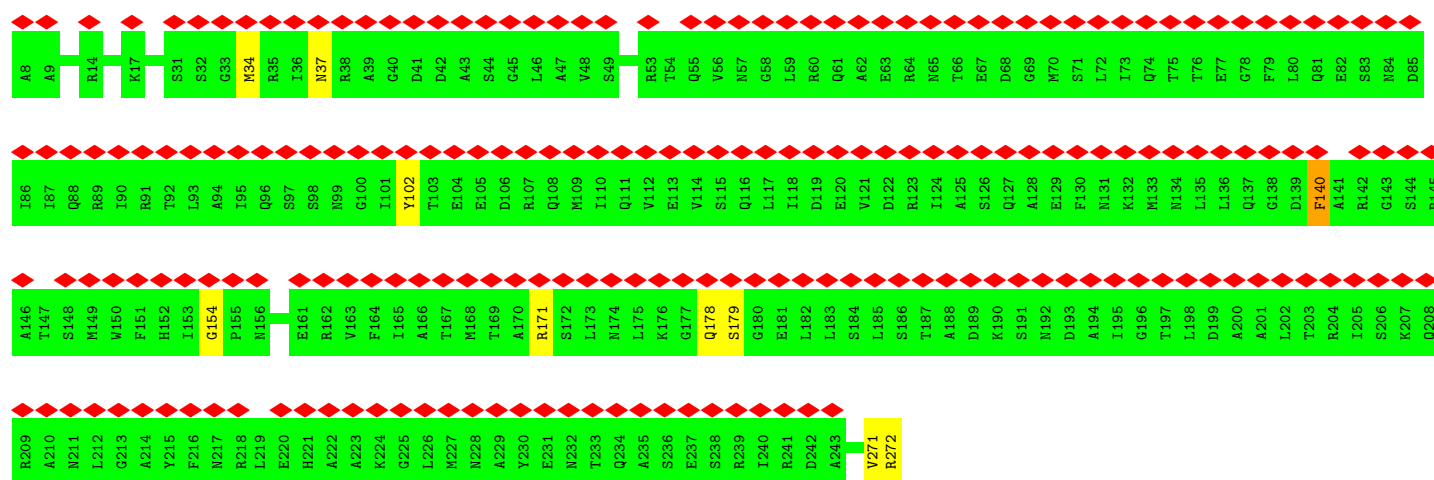
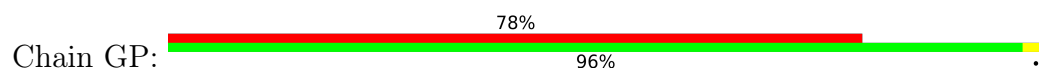


• Molecule 1: Flagellin B1 (FlaB1)

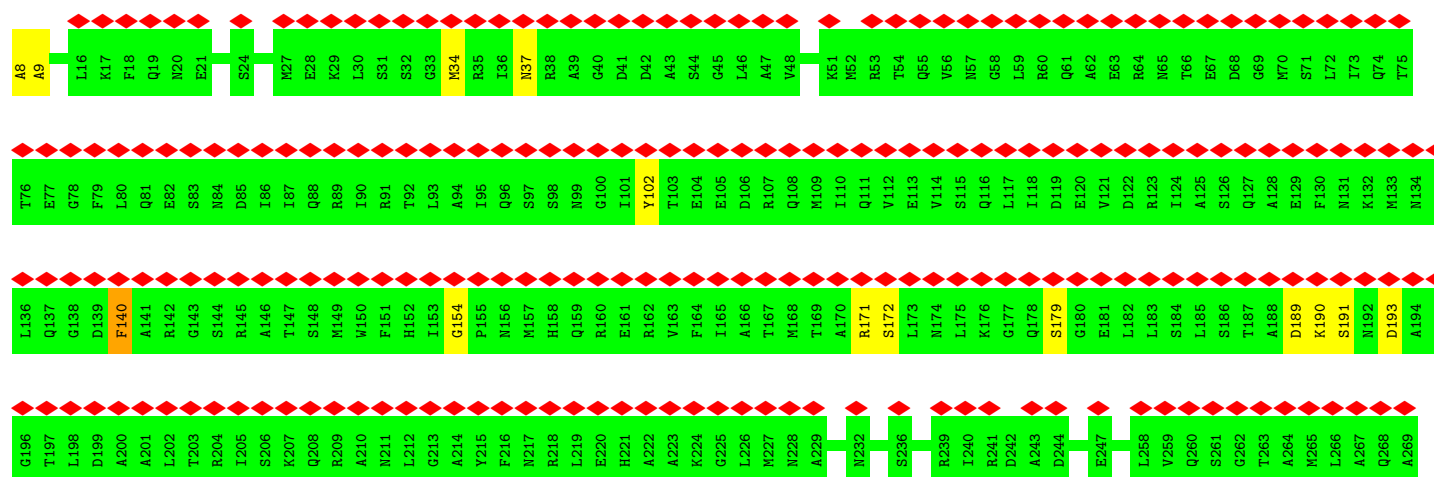




• Molecule 1: Flagellin B1 (FlaB1)

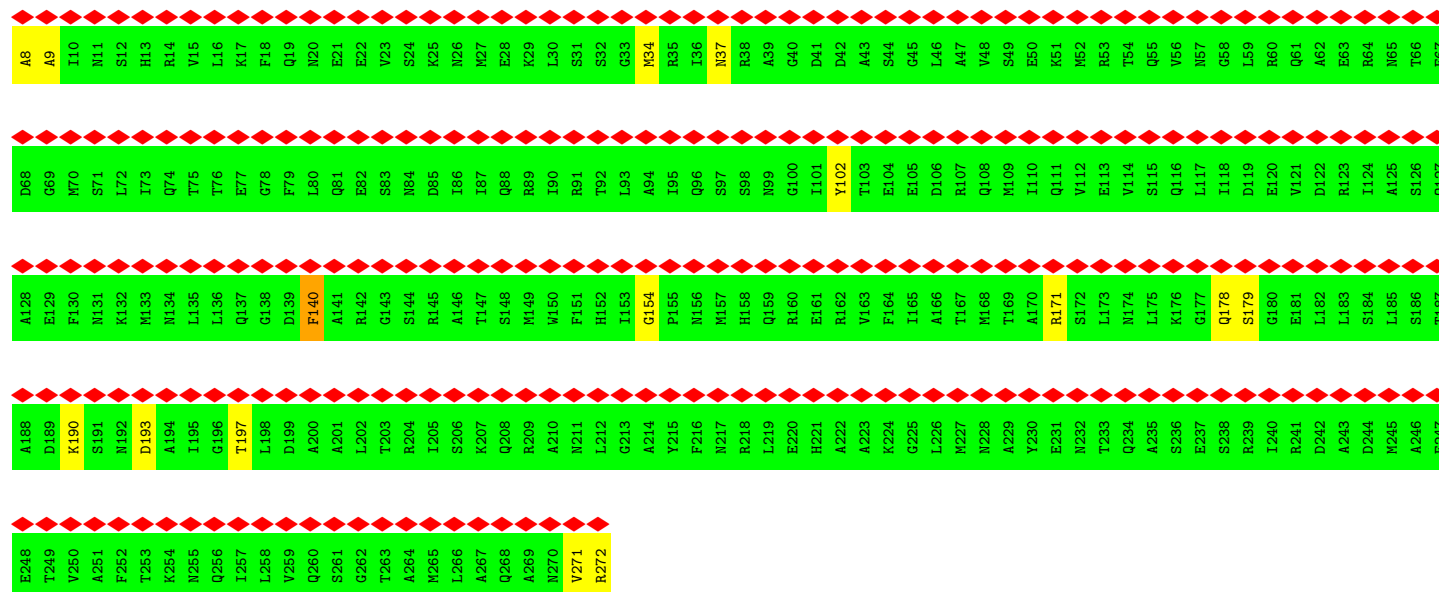


• Molecule 1: Flagellin B1 (FlaB1)

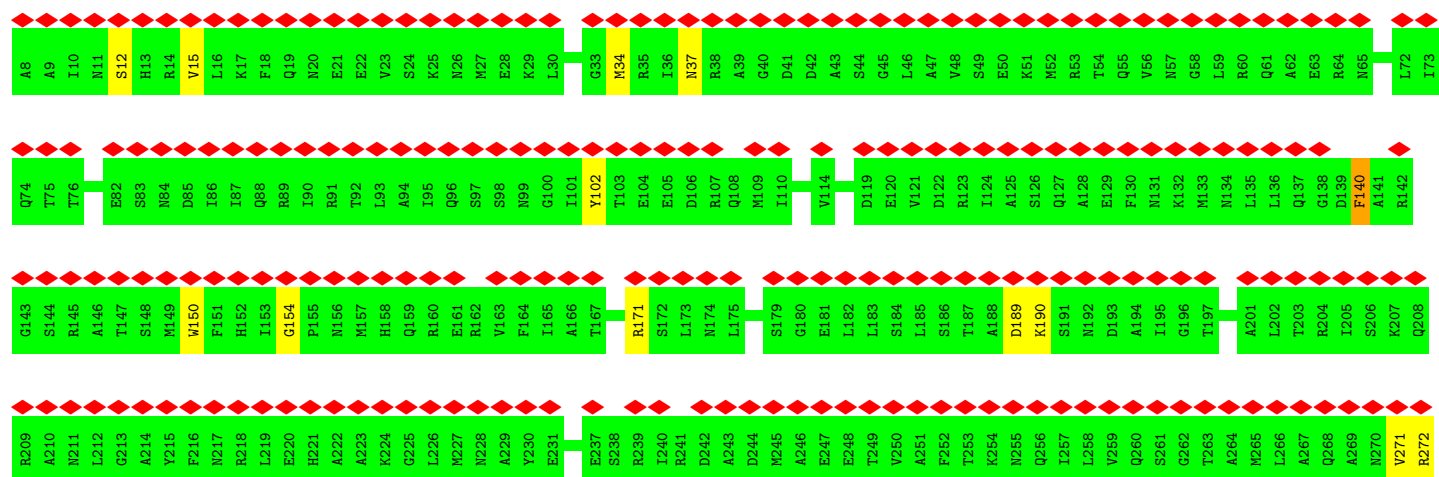
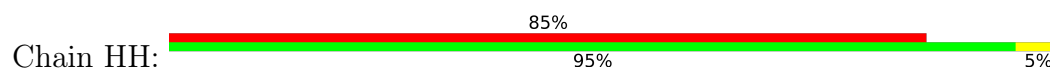




• Molecule 1: Flagellin B1 (FlaB1)

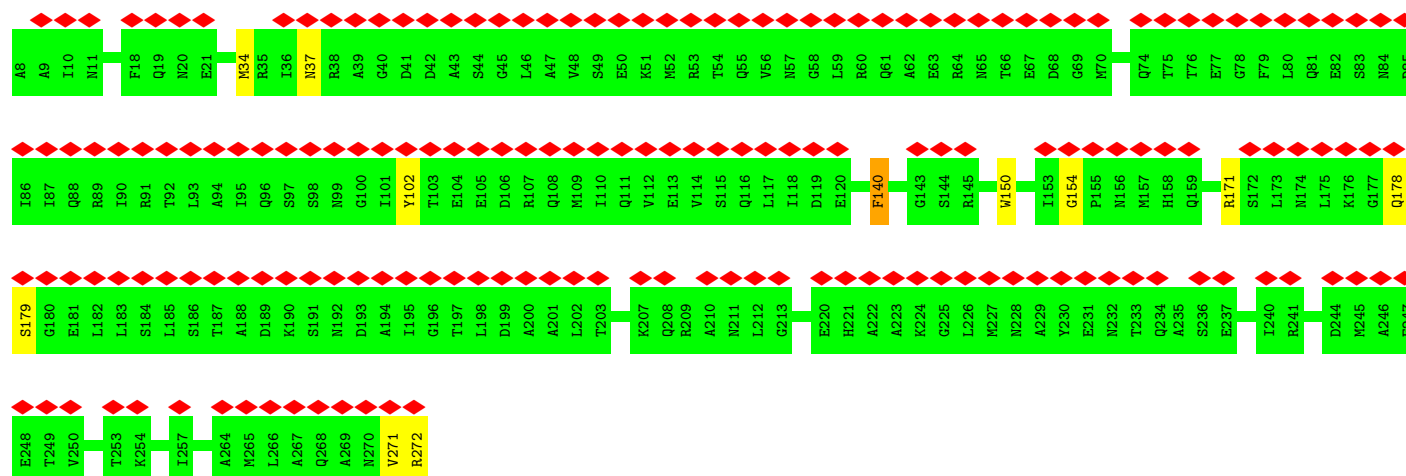


• Molecule 1: Flagellin B1 (FlaB1)

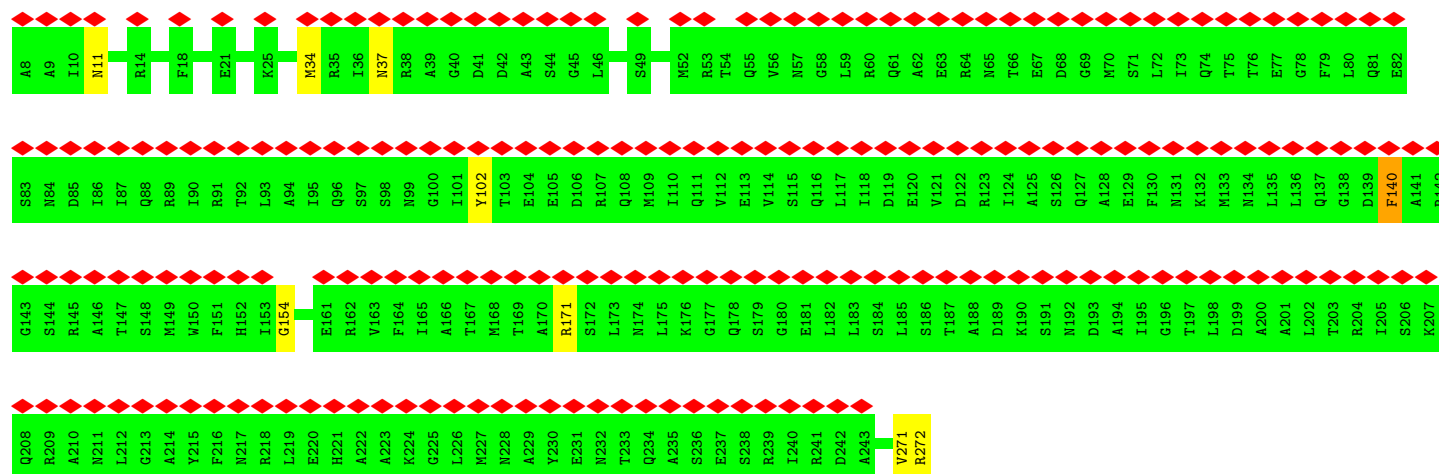
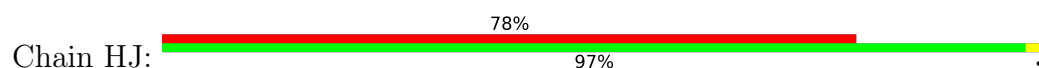


• Molecule 1: Flagellin B1 (FlaB1)

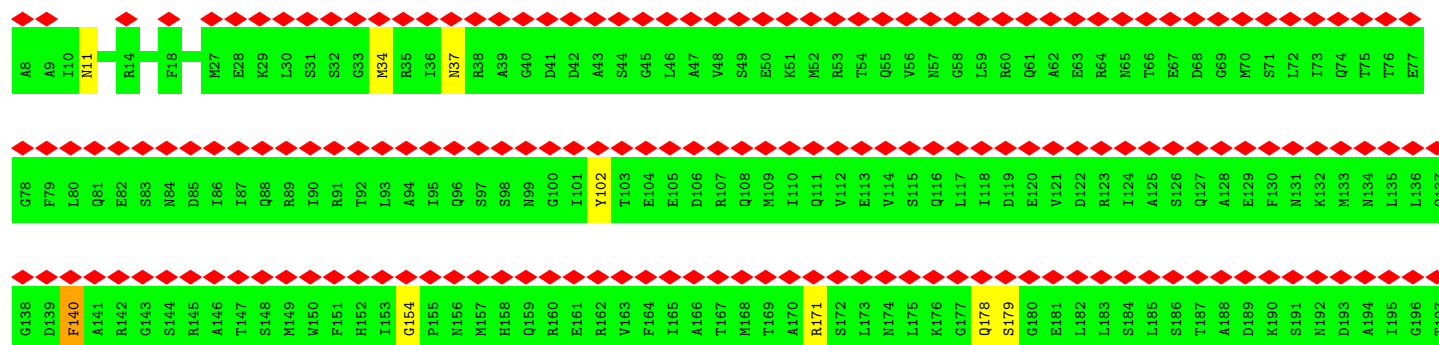
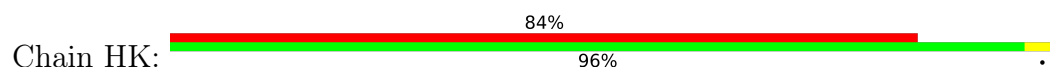


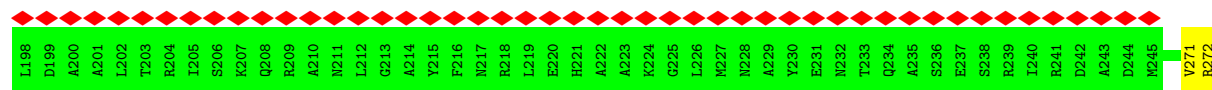


• Molecule 1: Flagellin B1 (FlaB1)

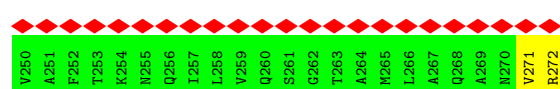
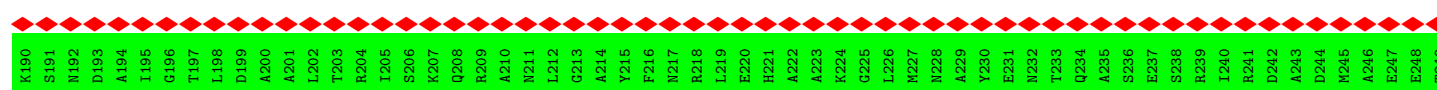
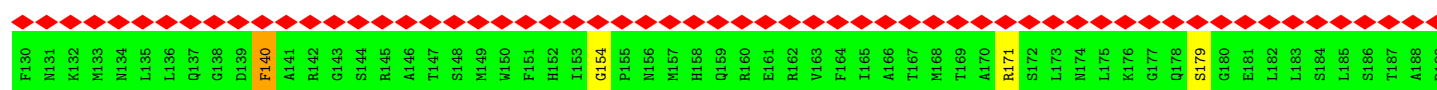
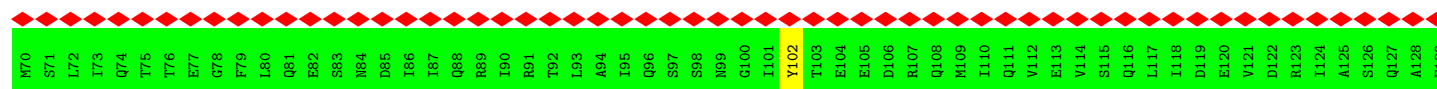
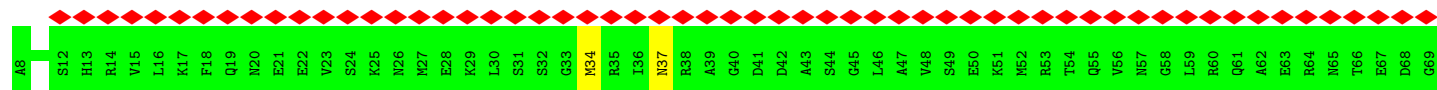


• Molecule 1: Flagellin B1 (FlaB1)

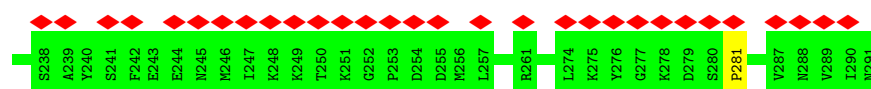
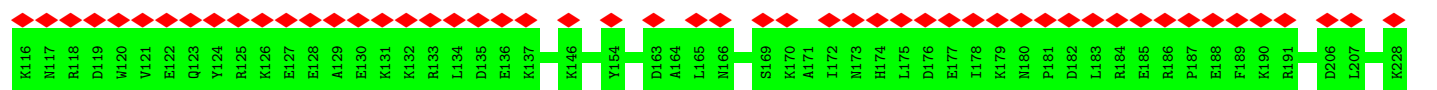
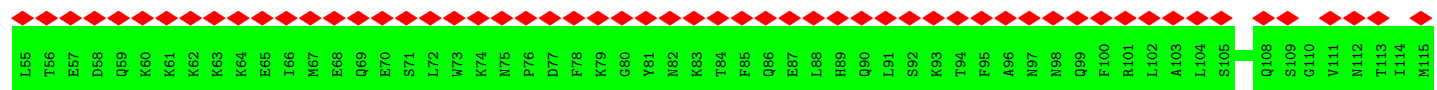




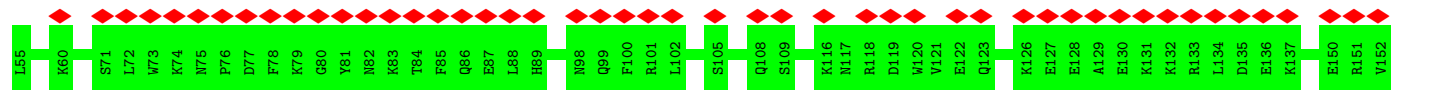
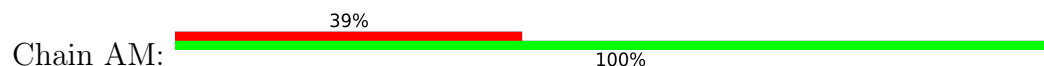
• Molecule 1: Flagellin B1 (FlaB1)

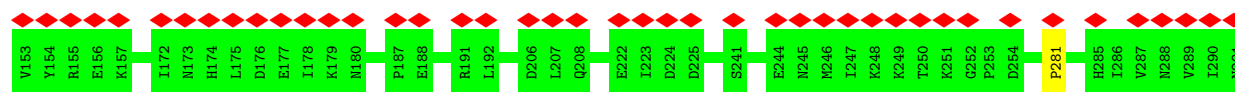


• Molecule 2: Flagellar coiling protein A (FcpA)

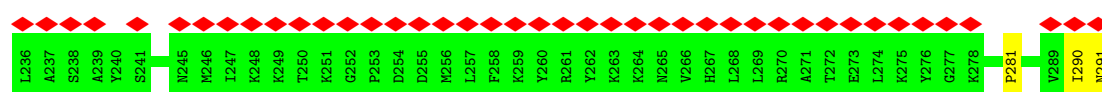
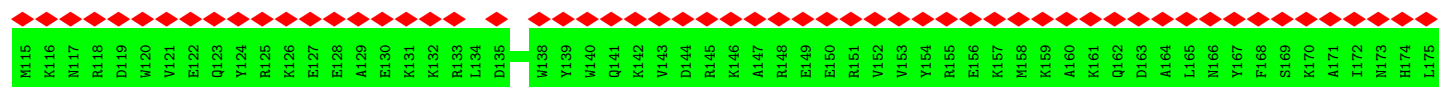
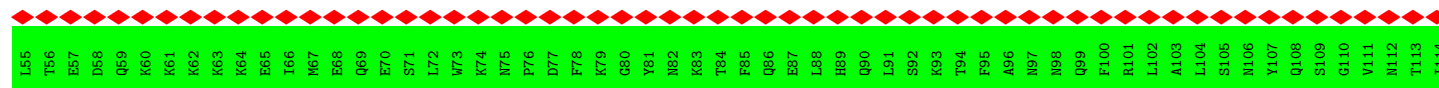


• Molecule 2: Flagellar coiling protein A (FcpA)

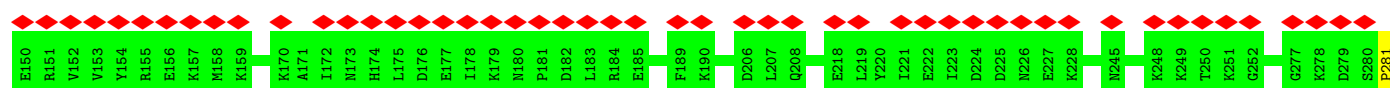
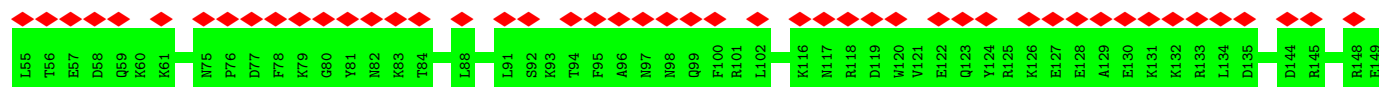
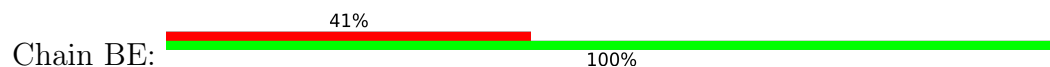




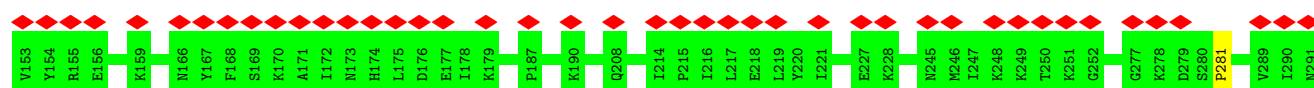
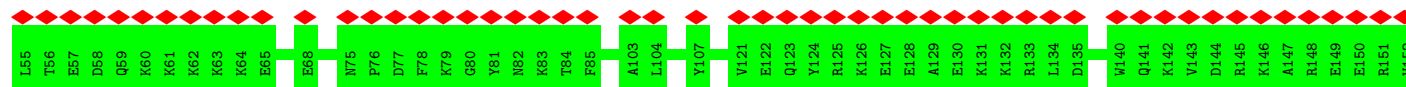
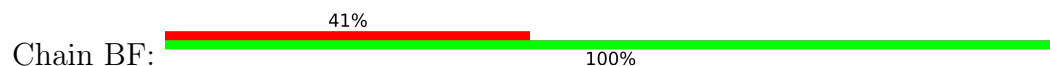
• Molecule 2: Flagellar coiling protein A (FcpA)



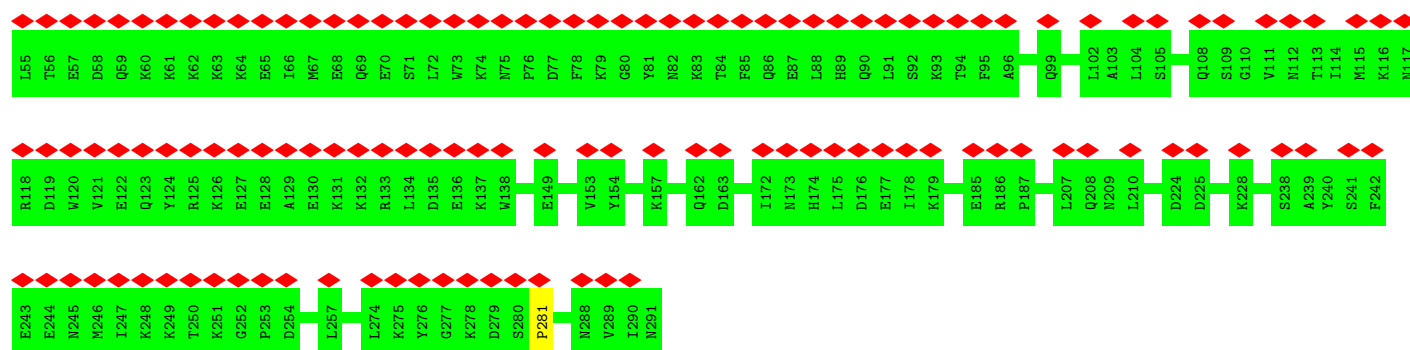
• Molecule 2: Flagellar coiling protein A (FcpA)



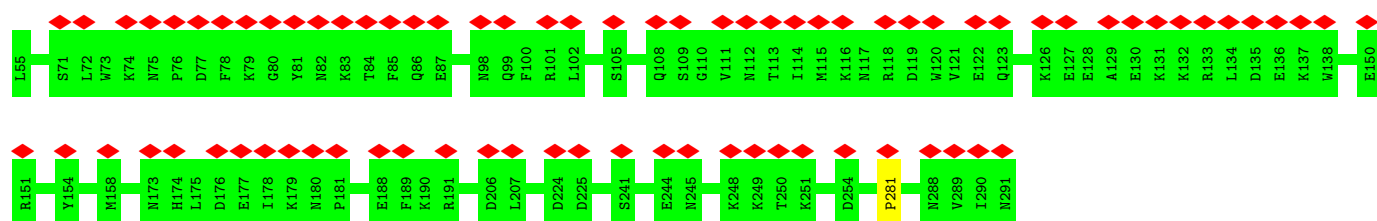
• Molecule 2: Flagellar coiling protein A (FcpA)



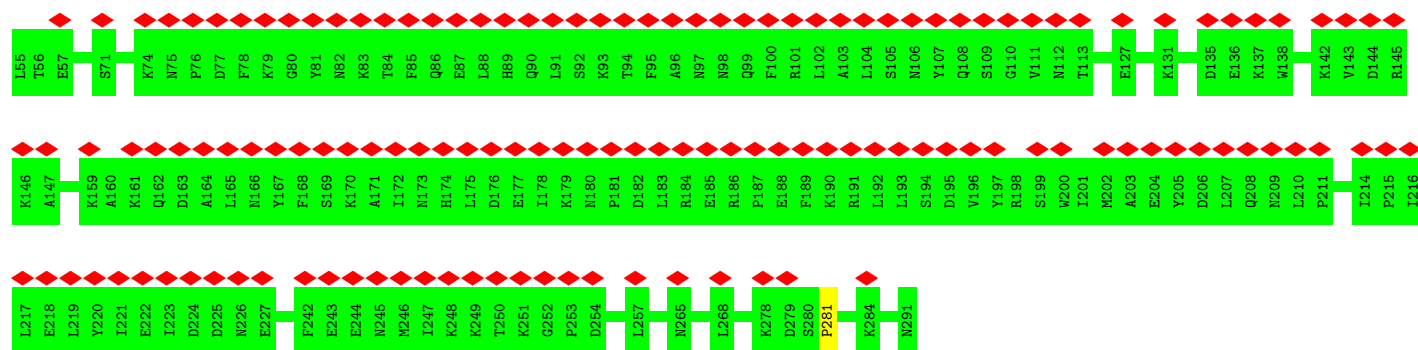
• Molecule 2: Flagellar coiling protein A (FcpA)



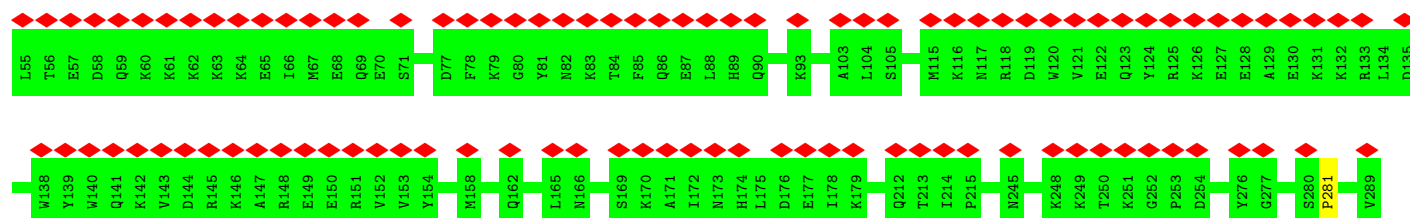
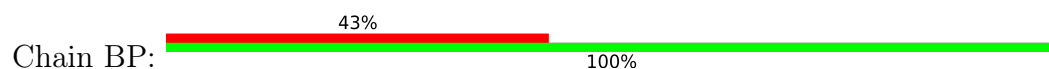
• Molecule 2: Flagellar coiling protein A (FcpA)



• Molecule 2: Flagellar coiling protein A (FcpA)

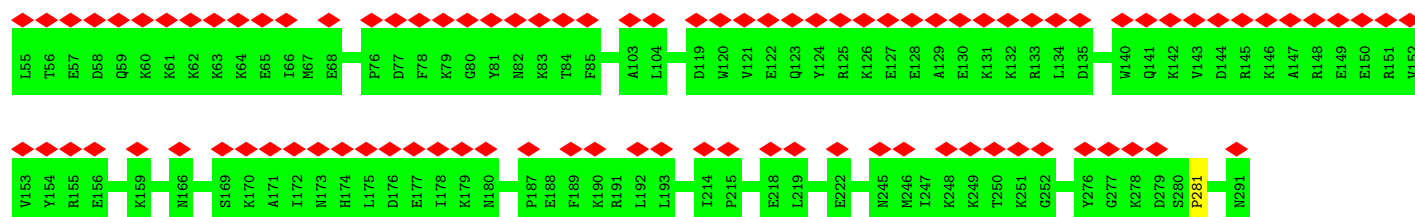


• Molecule 2: Flagellar coiling protein A (FcpA)

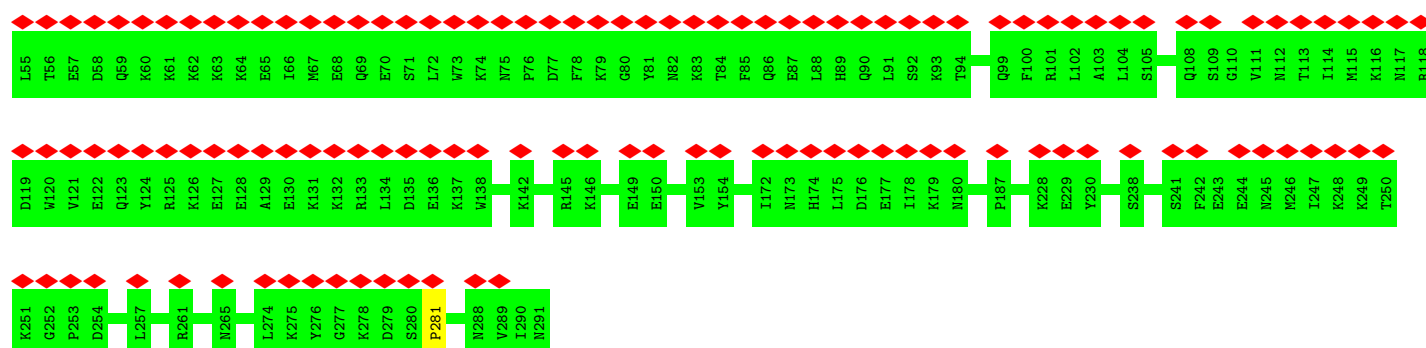




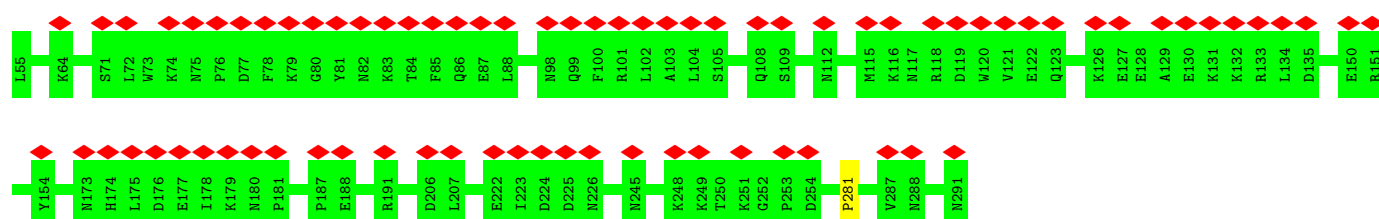
• Molecule 2: Flagellar coiling protein A (FcpA)



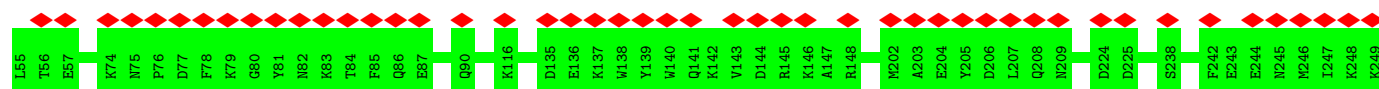
• Molecule 2: Flagellar coiling protein A (FcpA)

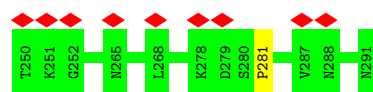


• Molecule 2: Flagellar coiling protein A (FcpA)



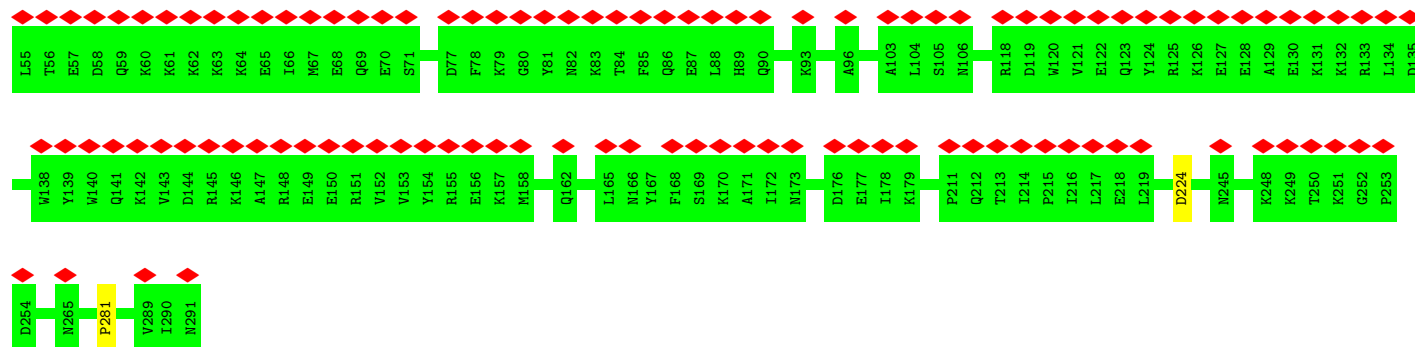
• Molecule 2: Flagellar coiling protein A (FcpA)





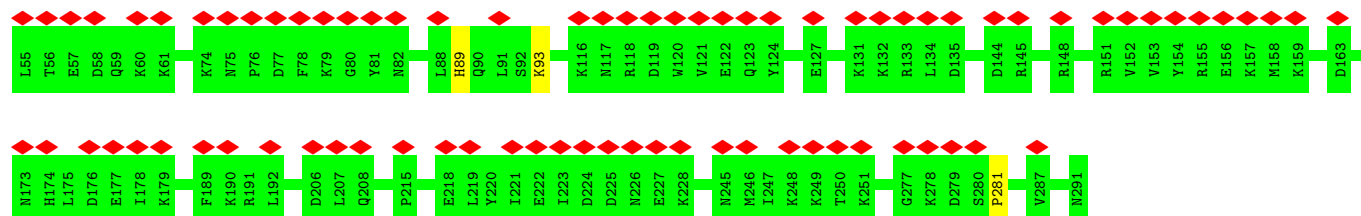
• Molecule 2: Flagellar coiling protein A (FcpA)

Chain CK: 46% 99%



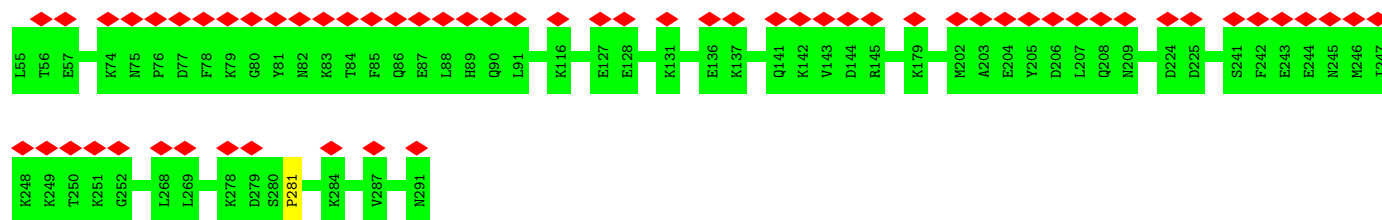
• Molecule 2: Flagellar coiling protein A (FcpA)

Chain BZ: 33% 99%



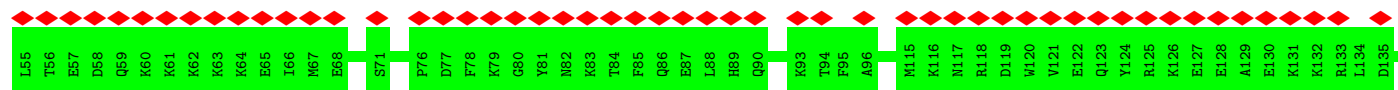
• Molecule 2: Flagellar coiling protein A (FcpA)

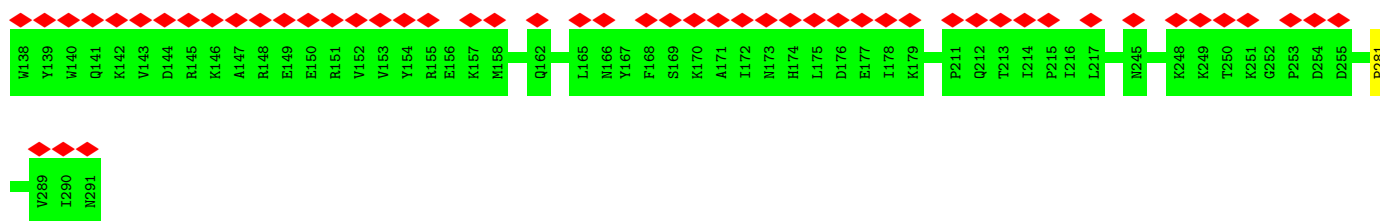
Chain DD: 26% 100%



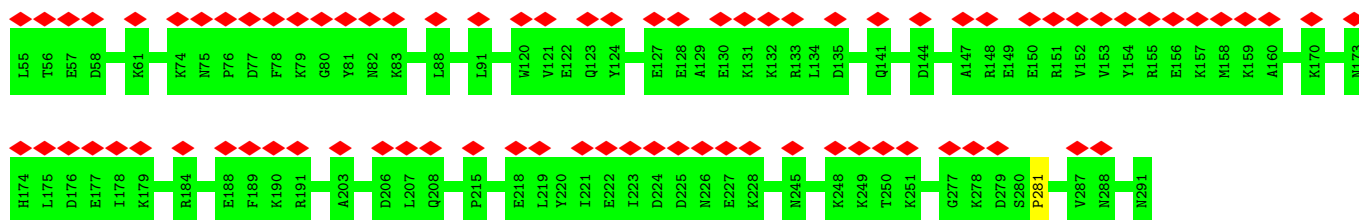
• Molecule 2: Flagellar coiling protein A (FcpA)

Chain DF: 44% 100%

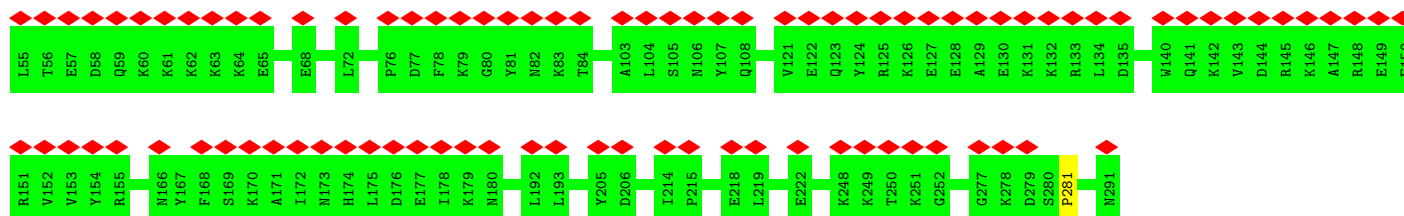




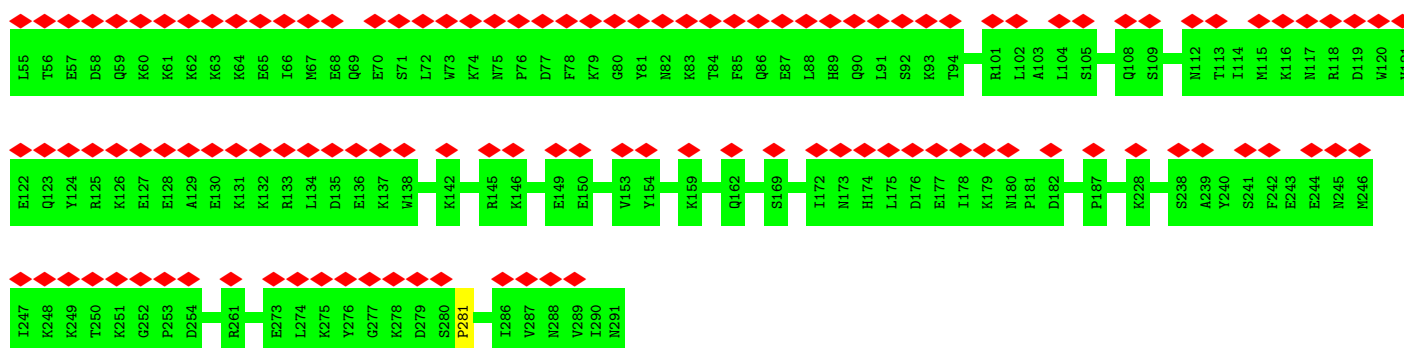
• Molecule 2: Flagellar coiling protein A (FcpA)



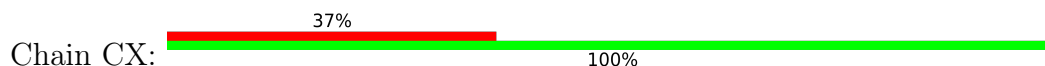
• Molecule 2: Flagellar coiling protein A (FcpA)

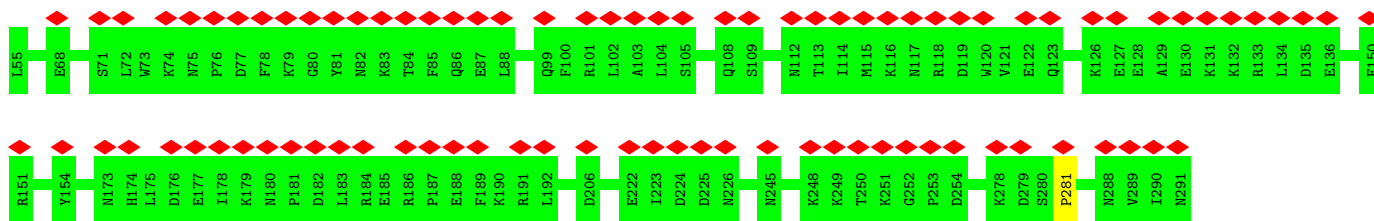


• Molecule 2: Flagellar coiling protein A (FcpA)

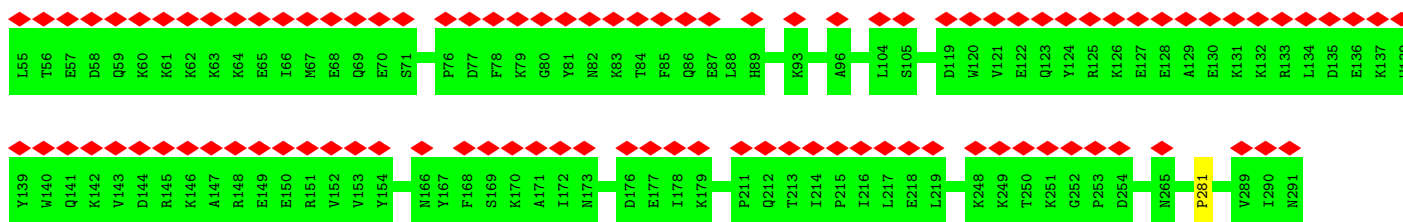
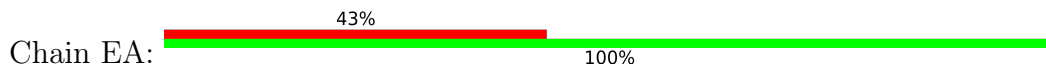


• Molecule 2: Flagellar coiling protein A (FcpA)

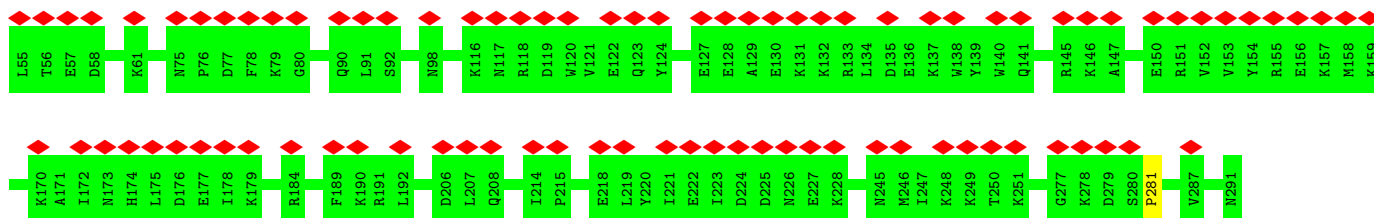
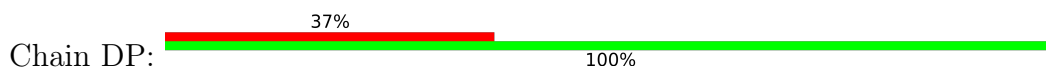




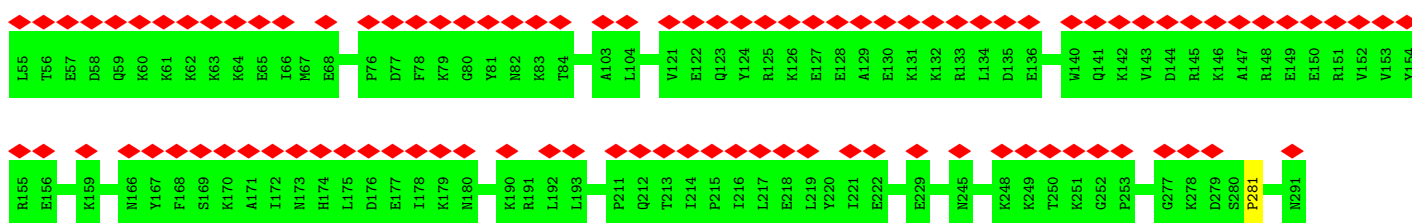
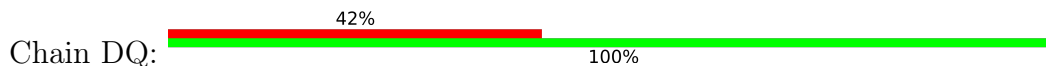
• Molecule 2: Flagellar coiling protein A (FcpA)



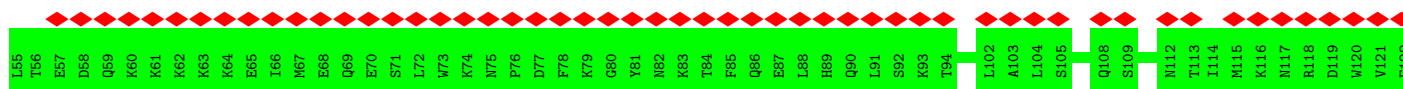
• Molecule 2: Flagellar coiling protein A (FcpA)



• Molecule 2: Flagellar coiling protein A (FcpA)

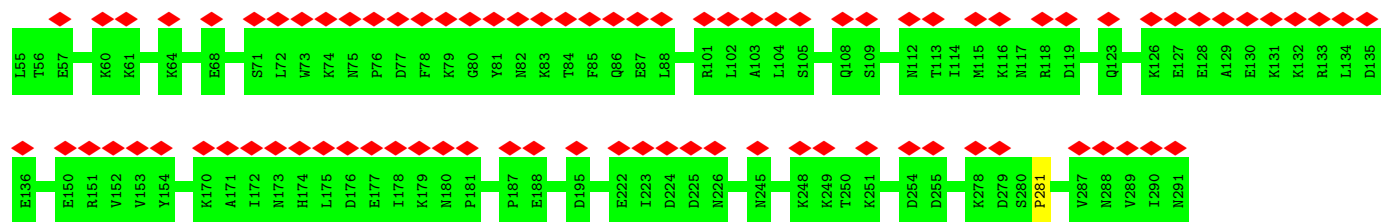


• Molecule 2: Flagellar coiling protein A (FcpA)

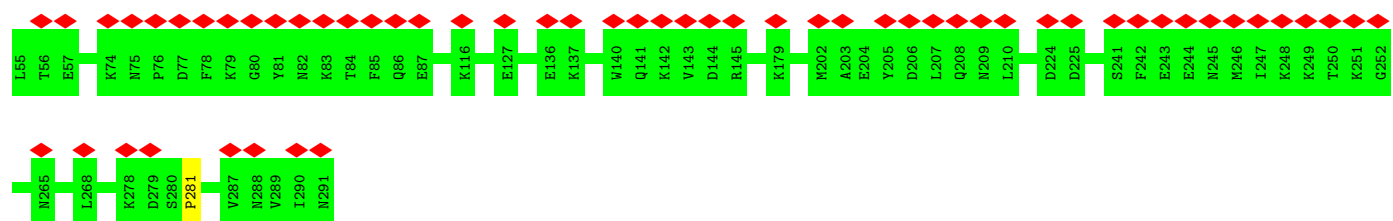




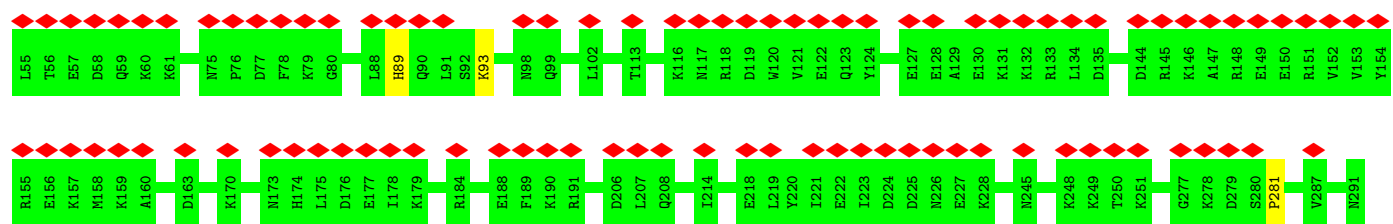
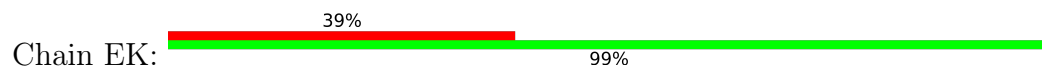
• Molecule 2: Flagellar coiling protein A (FcpA)



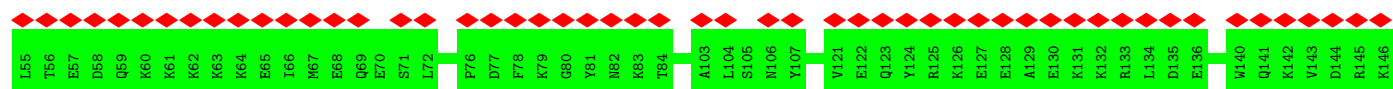
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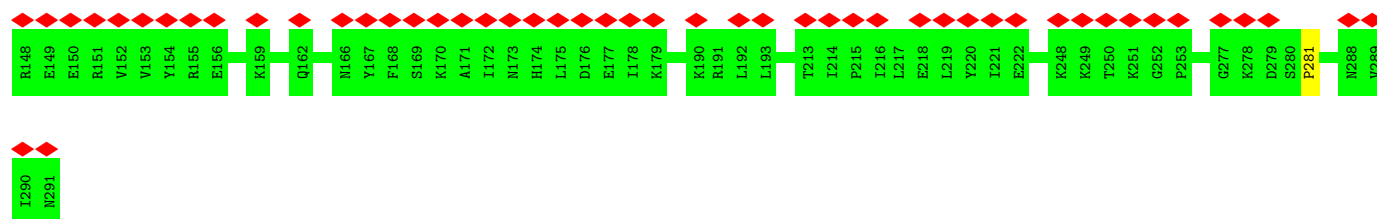


• Molecule 2: Flagellar coiling protein A (FcpA)

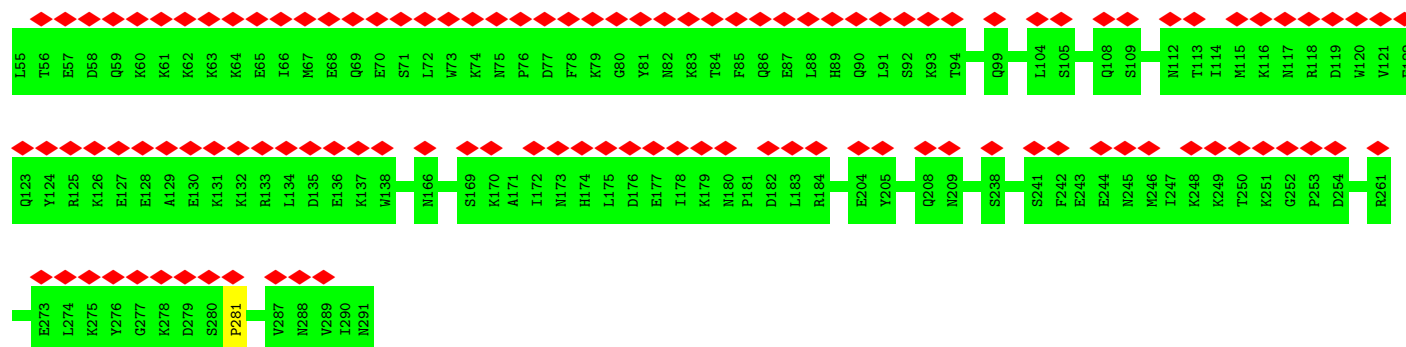


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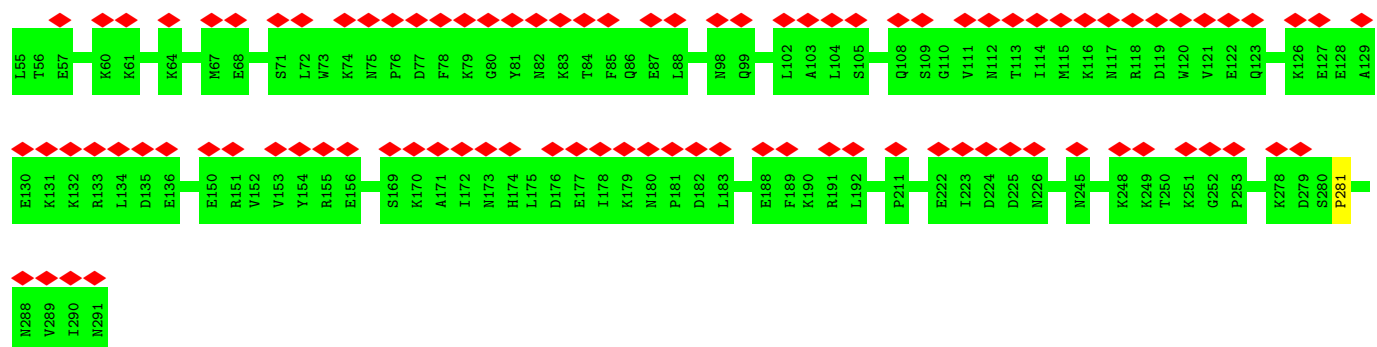
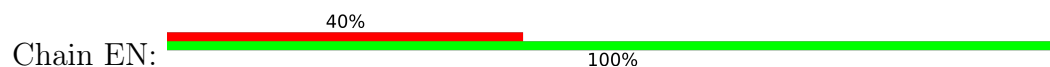




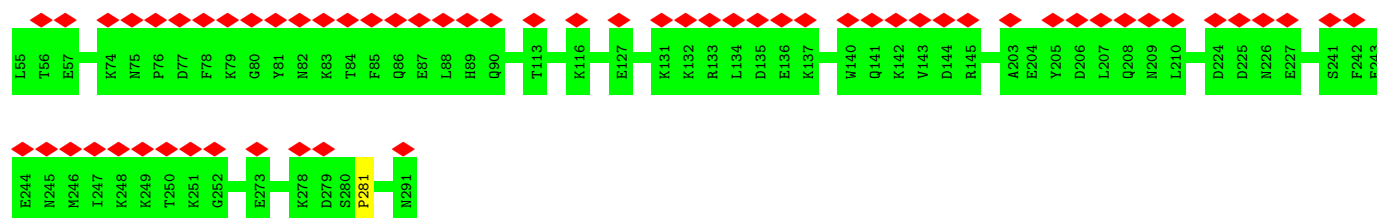
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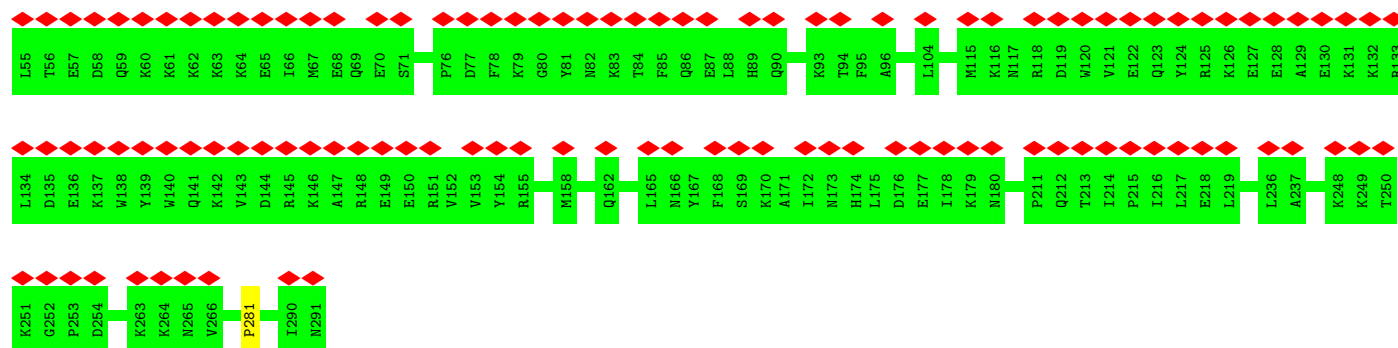
• Molecule 2: Flagellar coiling protein A (FcpA)



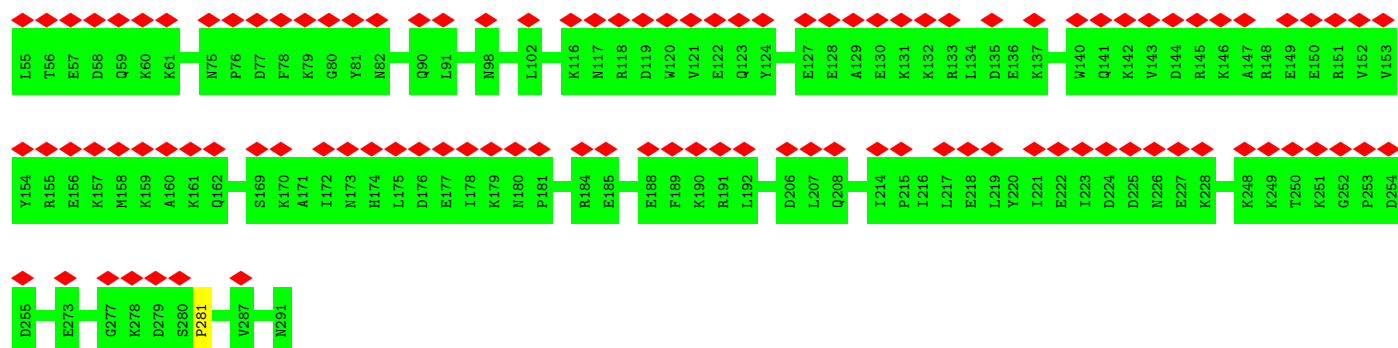
• Molecule 2: Flagellar coiling protein A (FcpA)



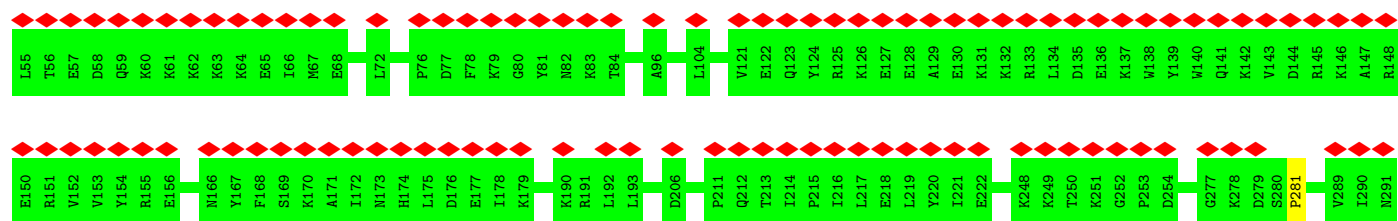
• Molecule 2: Flagellar coiling protein A (FcpA)



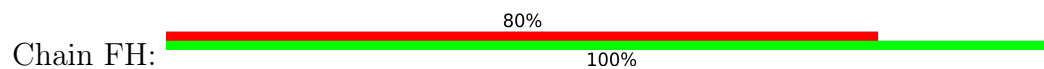
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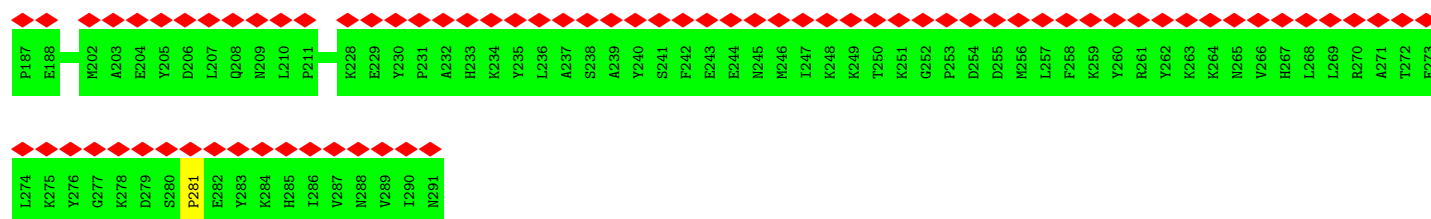


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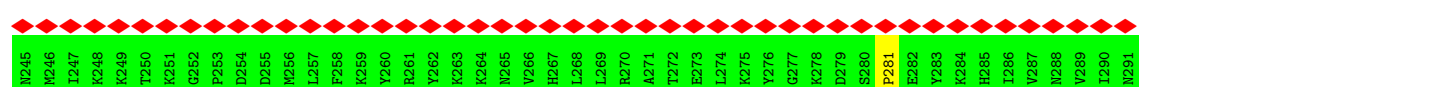
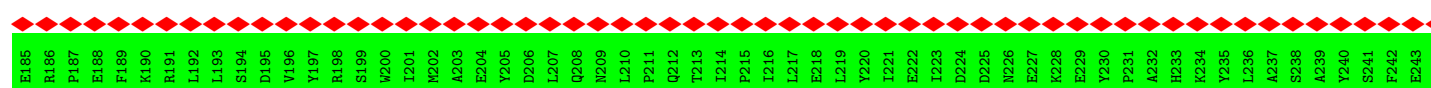
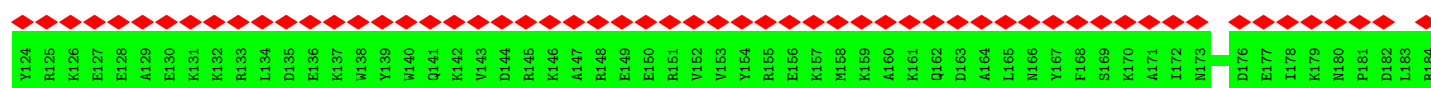
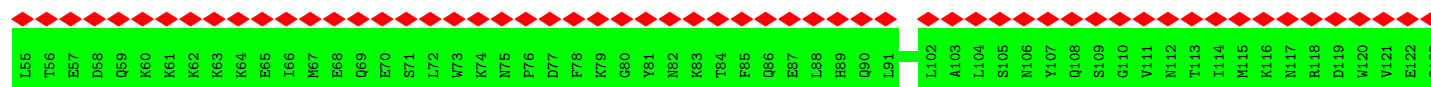


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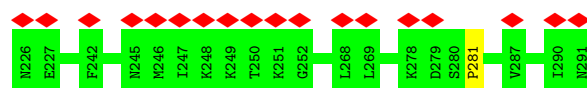
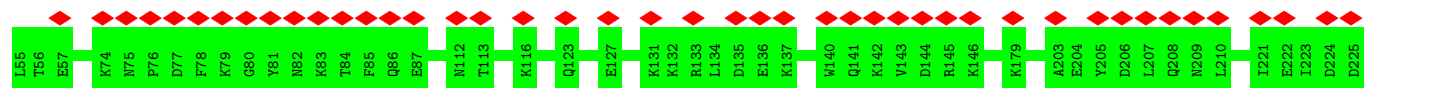




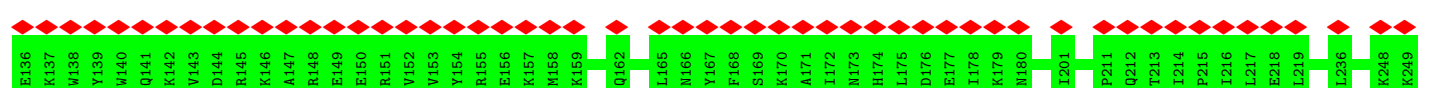
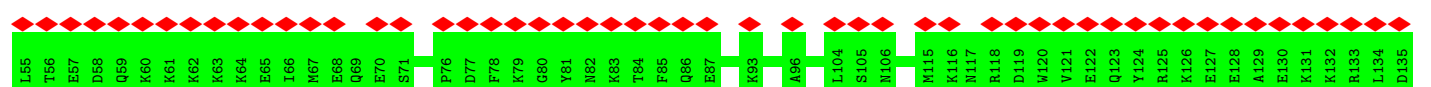
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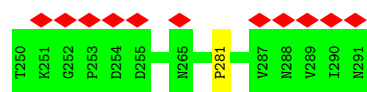


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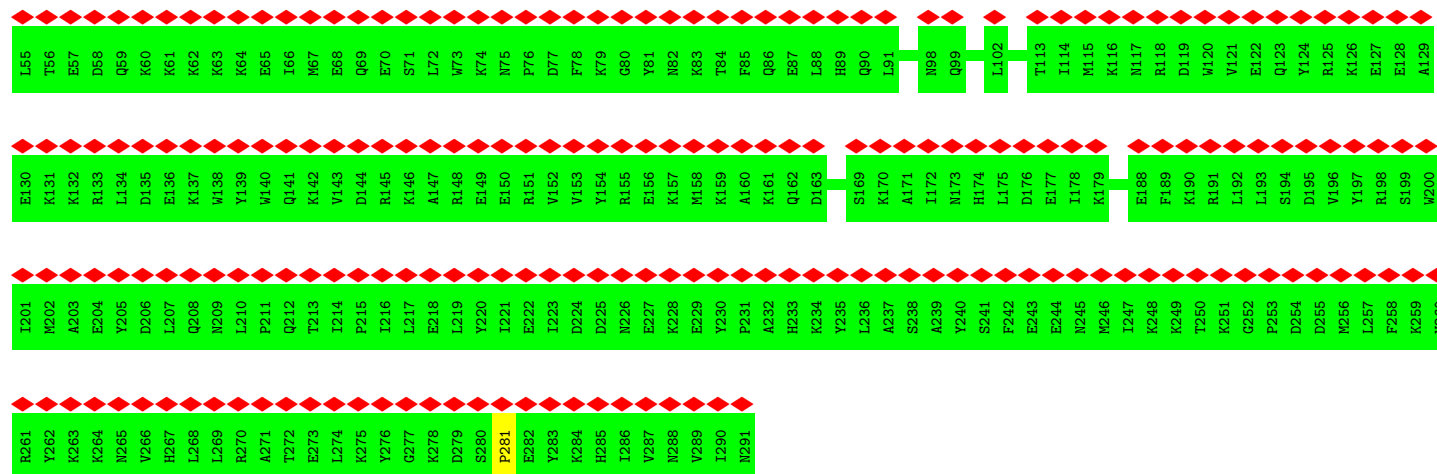


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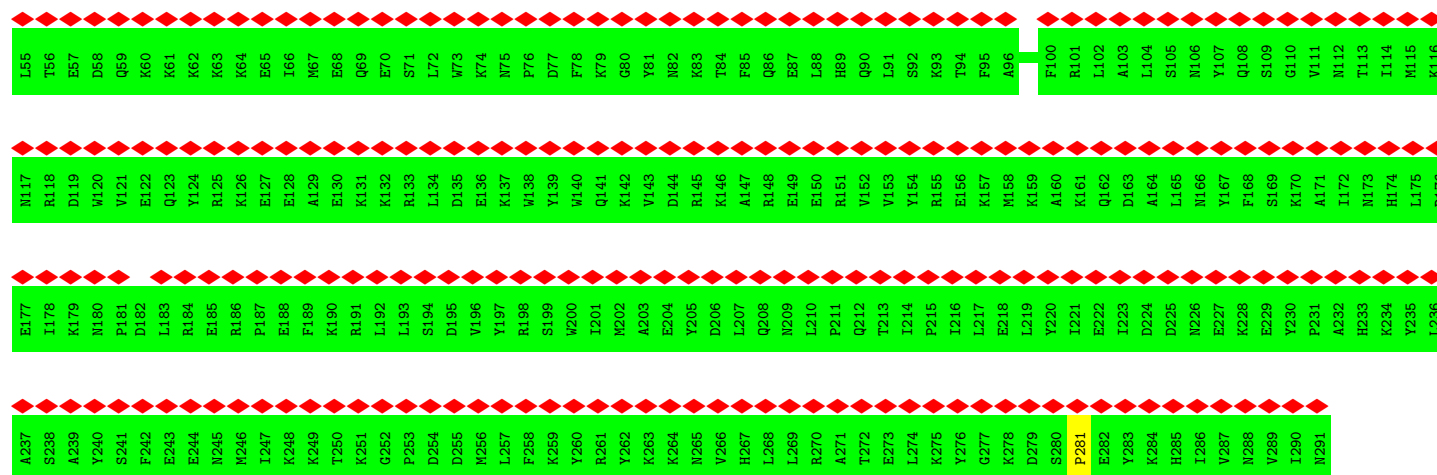




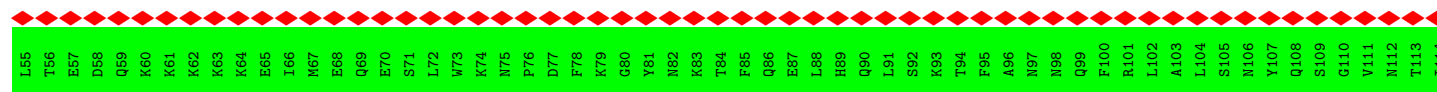
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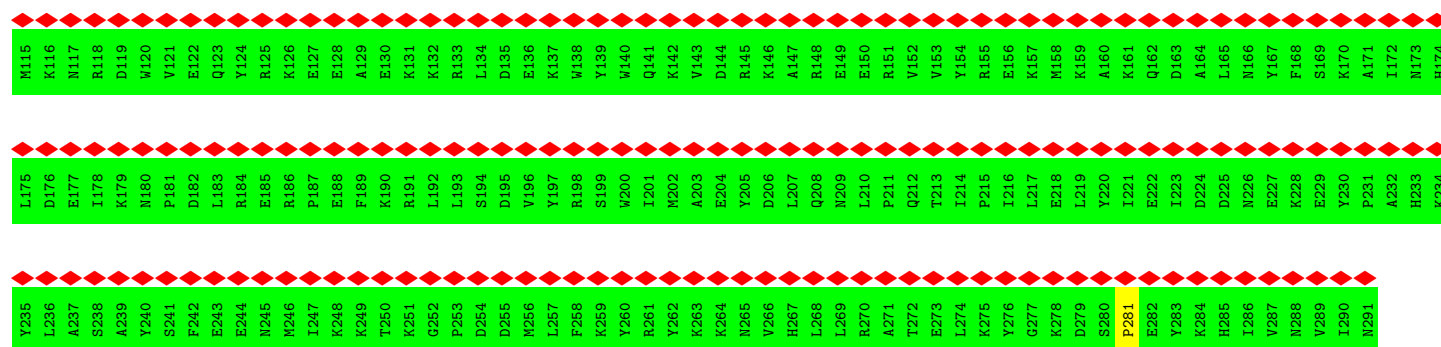


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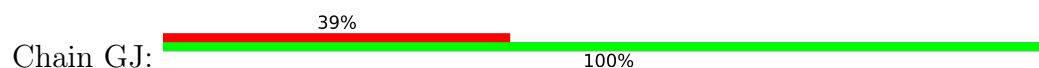


• Molecule 2: Flagellar coiling protein A (FcpA)





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• Molecule 2: Flagellar coiling protein A (FcpA)



Y235	L236	A237	S238	A239	Y240	S241	F242	E243	E244	N245	M246	I247	K248	K249	T250	K251	G252	P253	D254	D255	M256	L257	F258	K259	Y260	R261	Y262	K263	K264	N265	V266	H267	L268	L269	R270	A271	T272	E273	L274	K275	Y276	G277	K278	D279	S280	P281	E282	Y283	K284	H285	I286	V287	N288	V289	I290	N291			
L176	D176	E177	I178	K179	N180	P181	D182	L183	R184	E185	R186	P187	E188	F189	K190	R191	L192	L193	S194	D195	V196	Y197	R198	S199	W200	I201	M202	A203	E204	Y205	D206	L207	Q208	N209	L210	P211	Q212	T213	I214	P215	I216	L217	E218	L219	Y220	I221	E222	I223	D224	D225	N226	E227	K228	E229	I230	P231	A232	H233	K234
M115	K116	N117	R118	D119	W120	V121	E122	Q123	Y124	R125	K126	E127	E128	A129	E130	K131	K132	R133	L134	D135	E136	K137	W138	Y139	W140	Q141	K142	V143	D144	R145	K146	A147	R148	E149	E150	R151	V152	V153	Y154	R155	E156	K157	M158	K159	A160	K161	Q162	D163	A164	L165	N166	Y167	F168	S169	K170	A171	I172	N173	H174

• Molecule 2: Flagellar coiling protein A (FcpA)



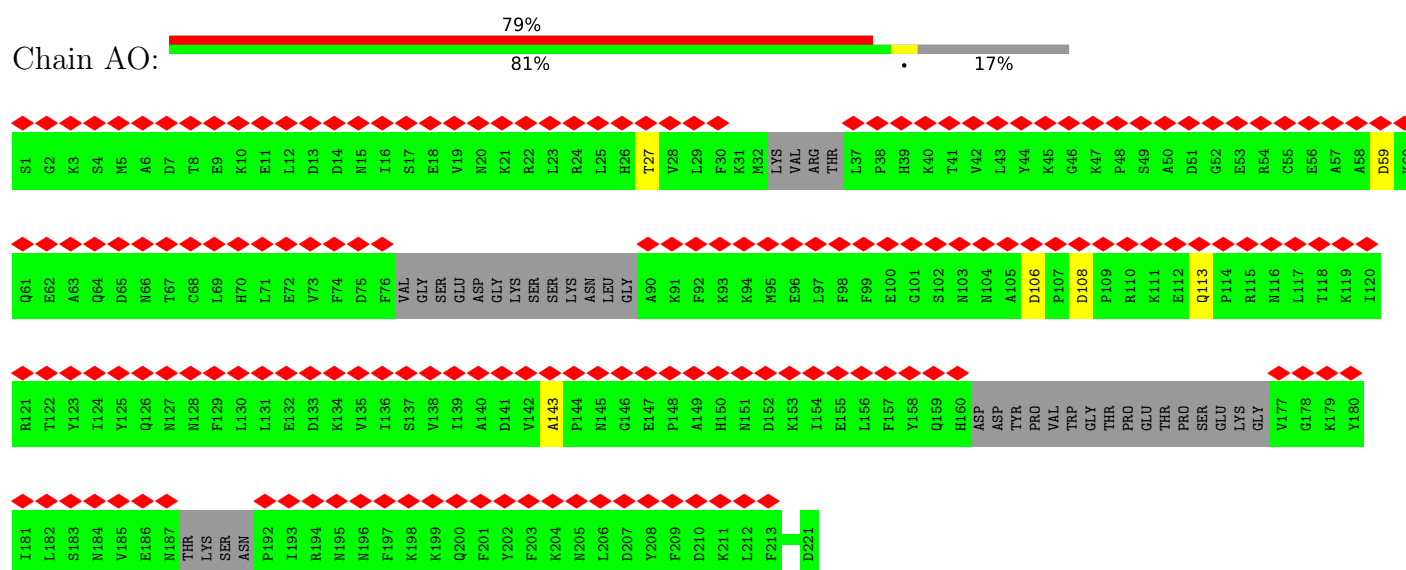
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• Molecule 2: Flagellar coiling protein A (FcpA)

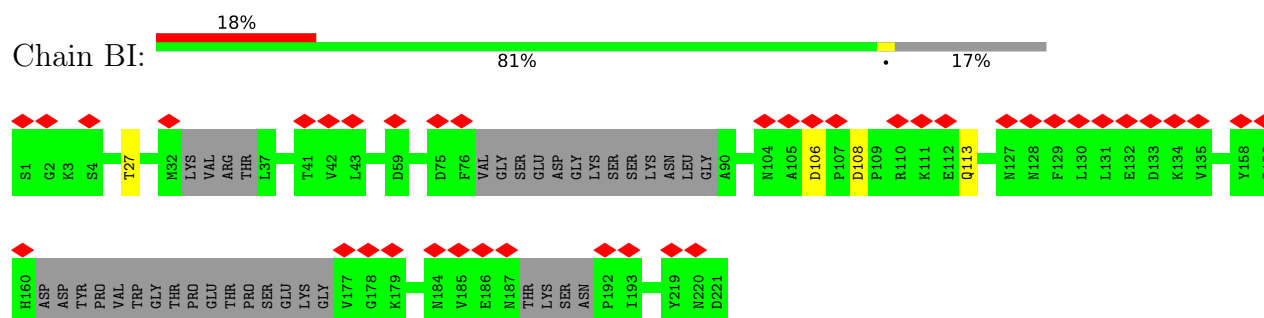


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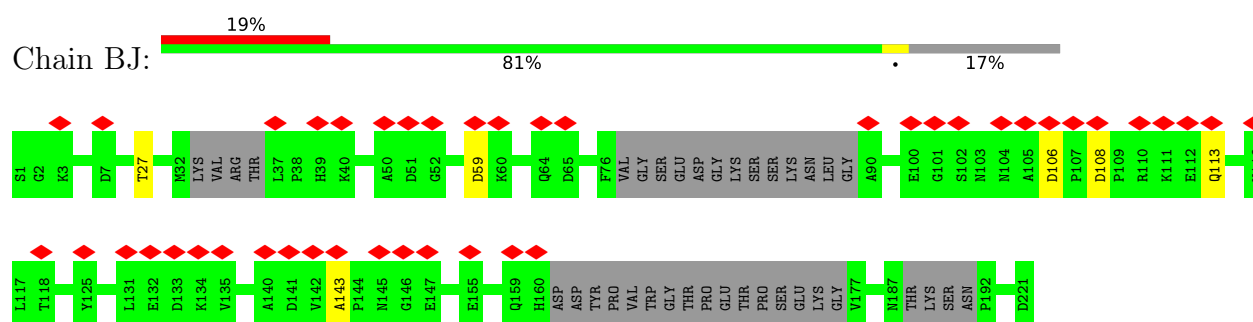
• Molecule 3: Flagellar coiling protein B (FcpB)



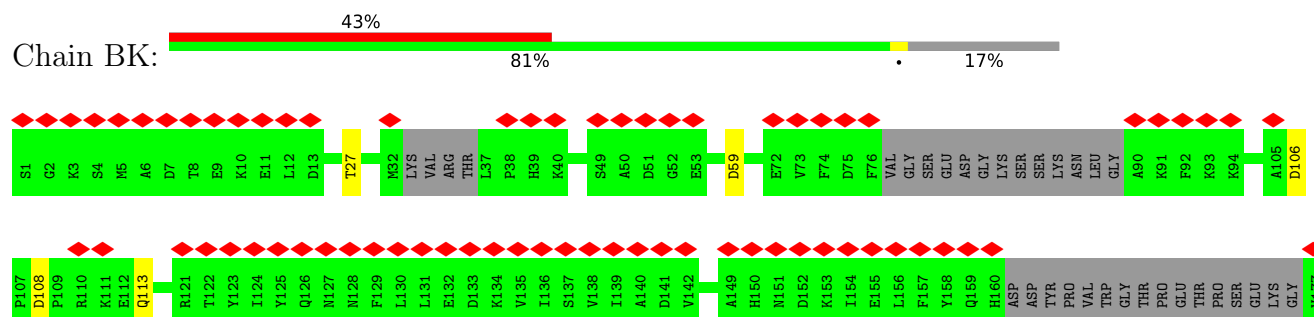
• Molecule 3: Flagellar coiling protein B (FcpB)

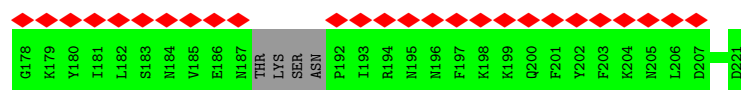


• Molecule 3: Flagellar coiling protein B (FcpB)

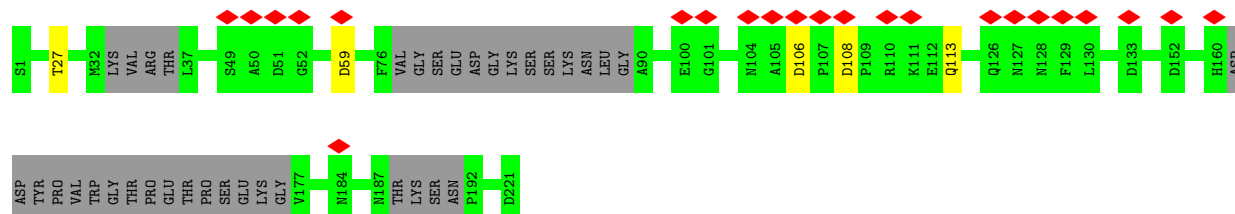
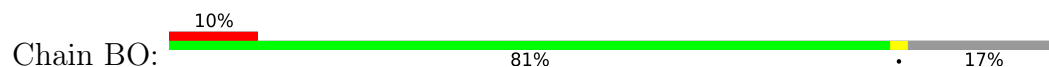


• Molecule 3: Flagellar coiling protein B (FcpB)

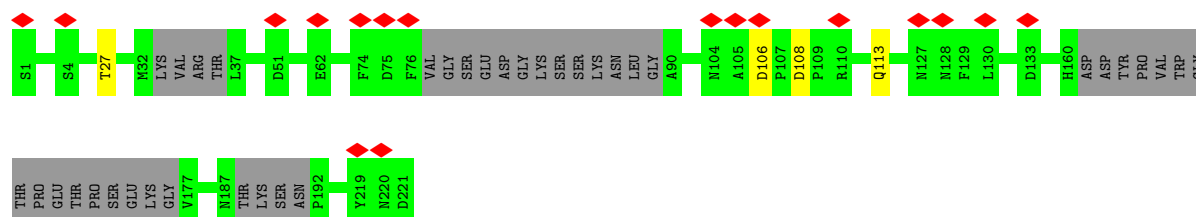
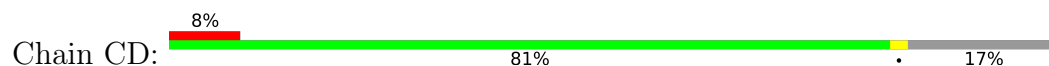




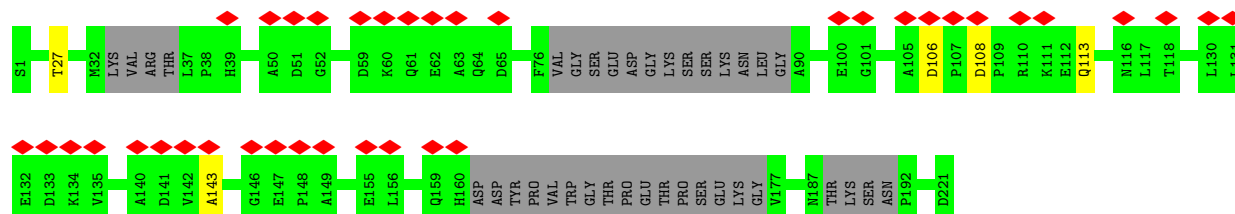
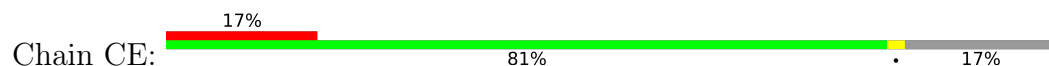
• Molecule 3: Flagellar coiling protein B (FcpB)



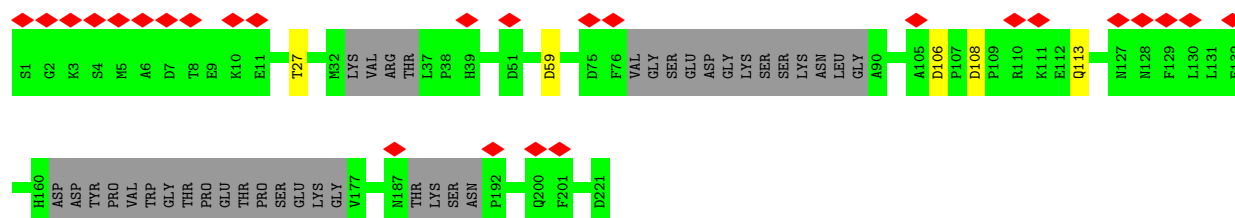
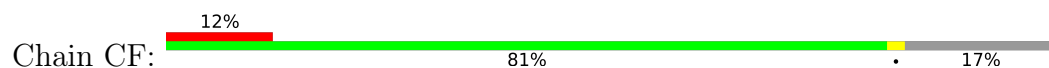
• Molecule 3: Flagellar coiling protein B (FcpB)



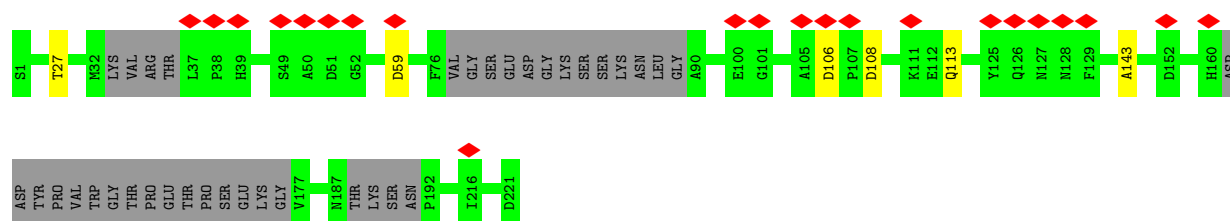
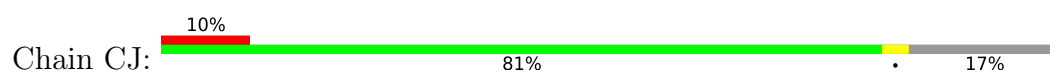
• Molecule 3: Flagellar coiling protein B (FcpB)



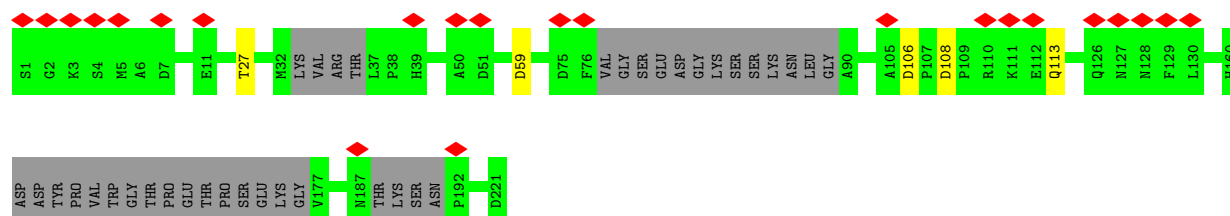
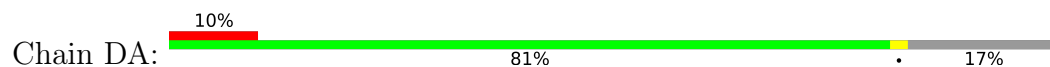
• Molecule 3: Flagellar coiling protein B (FcpB)



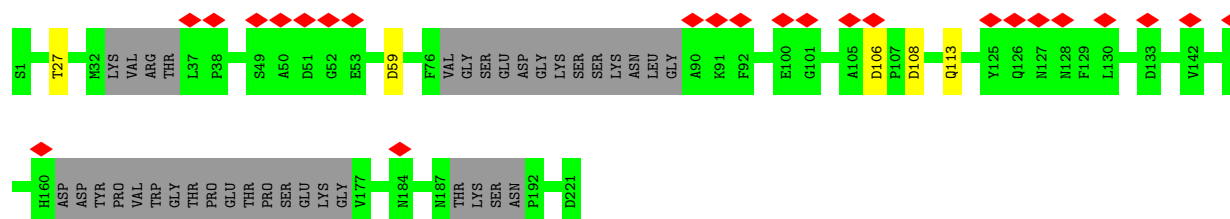
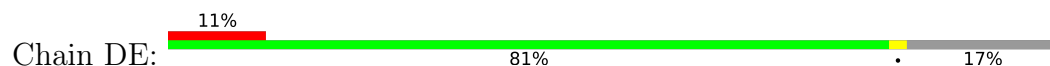
• Molecule 3: Flagellar coiling protein B (FcpB)



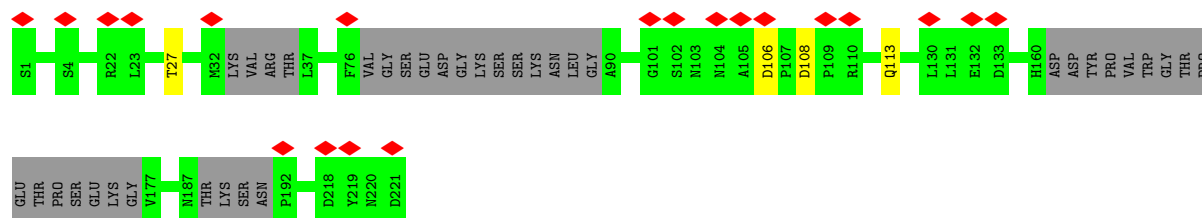
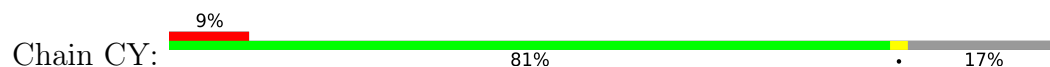
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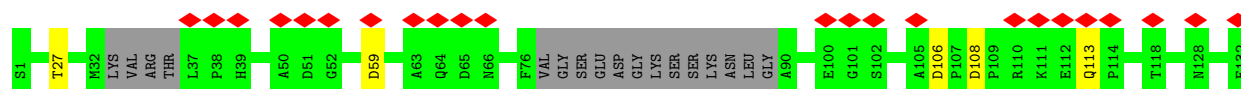
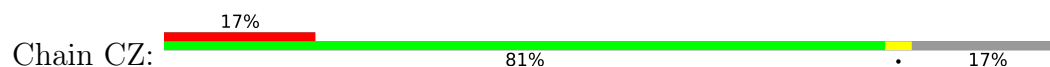
• Molecule 3: Flagellar coiling protein B (FcpB)

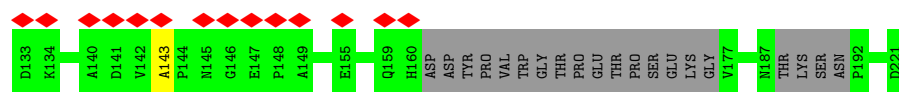


• Molecule 3: Flagellar coiling protein B (FcpB)

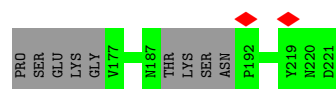
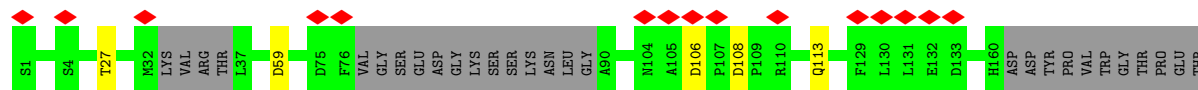
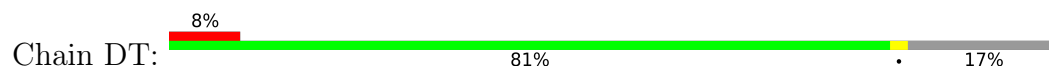


• Molecule 3: Flagellar coiling protein B (FcpB)

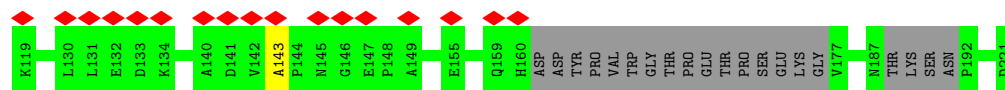
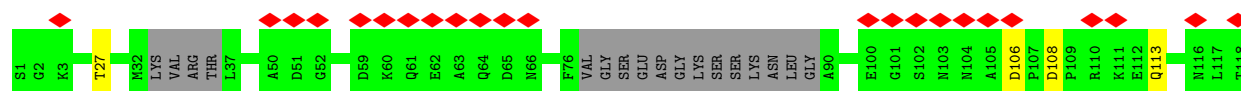
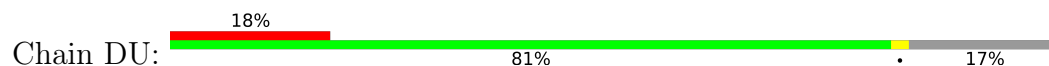




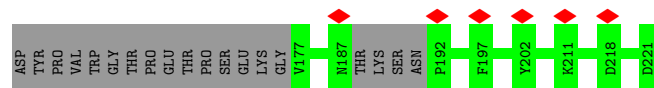
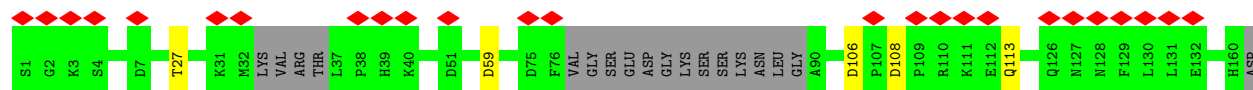
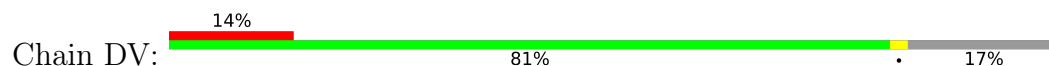
- Molecule 3: Flagellar coiling protein B (FcpB)



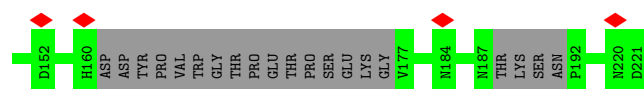
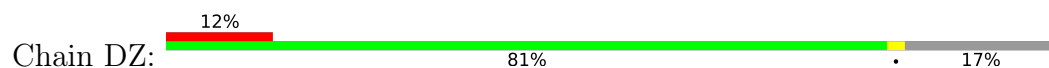
- Molecule 3: Flagellar coiling protein B (FcpB)



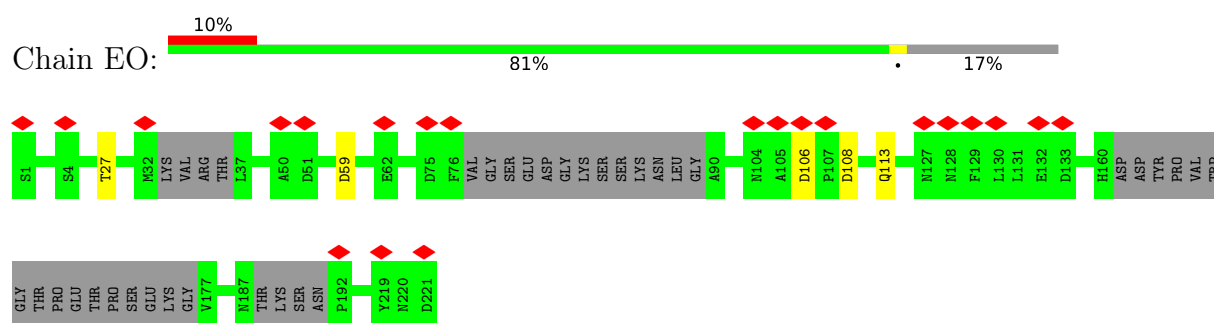
- Molecule 3: Flagellar coiling protein B (FcpB)



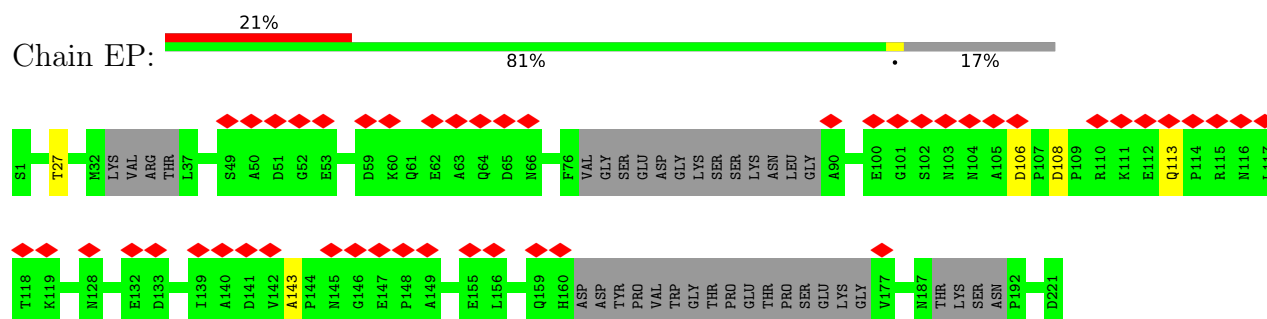
- Molecule 3: Flagellar coiling protein B (FcpB)



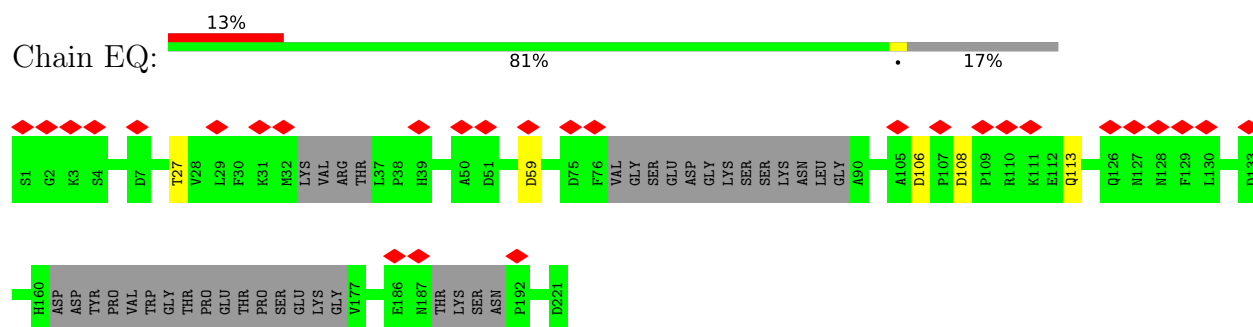
- Molecule 3: Flagellar coiling protein B (FcpB)



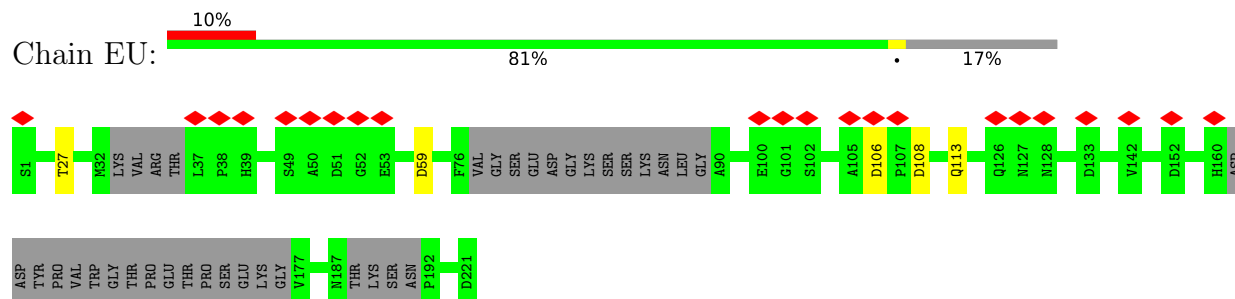
- Molecule 3: Flagellar coiling protein B (FcpB)



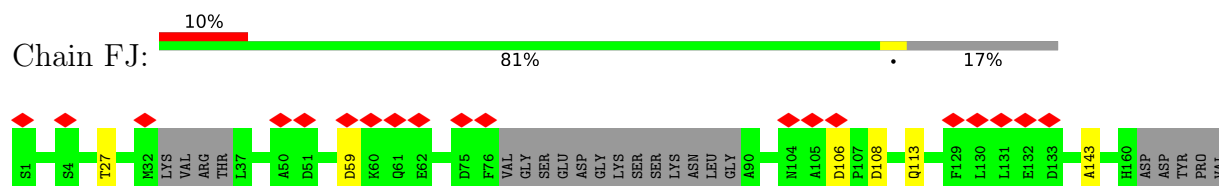
- Molecule 3: Flagellar coiling protein B (FcpB)



- Molecule 3: Flagellar coiling protein B (FcpB)

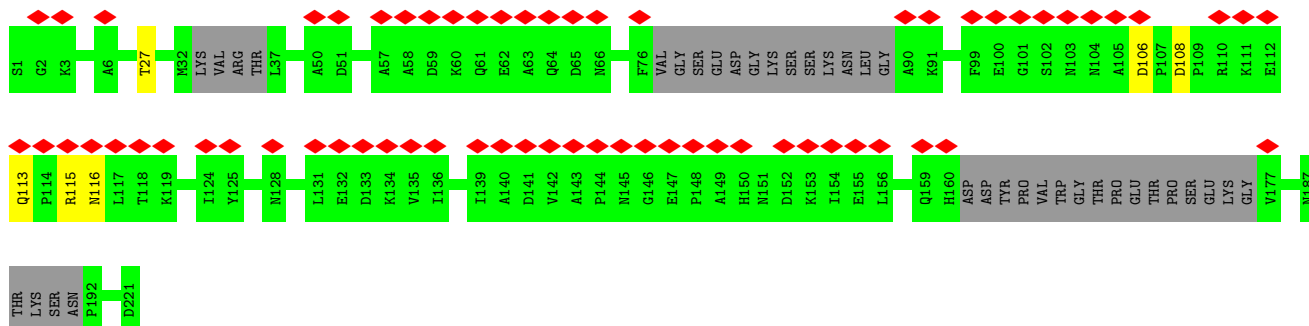
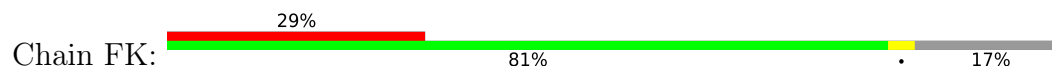


- Molecule 3: Flagellar coiling protein B (FcpB)

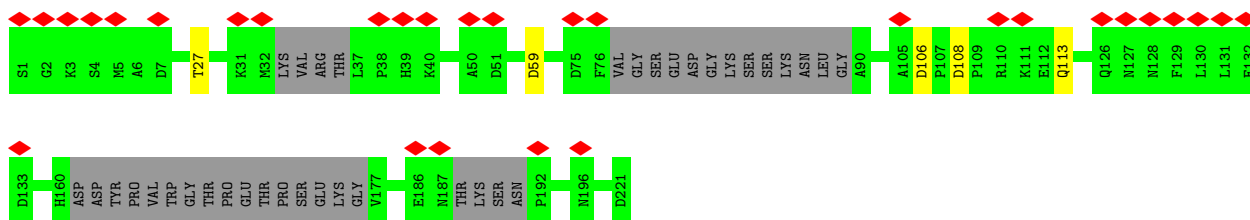
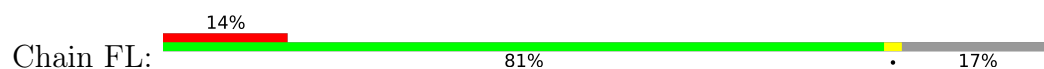




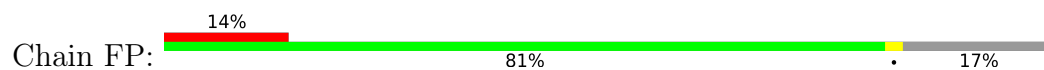
• Molecule 3: Flagellar coiling protein B (FcpB)



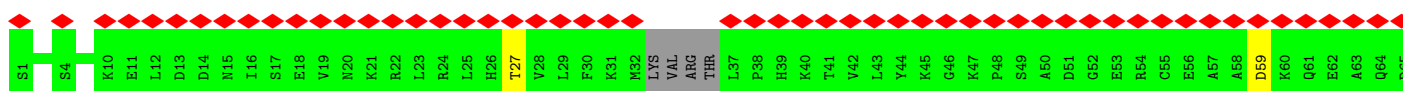
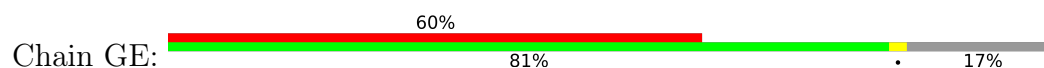
• Molecule 3: Flagellar coiling protein B (FcpB)

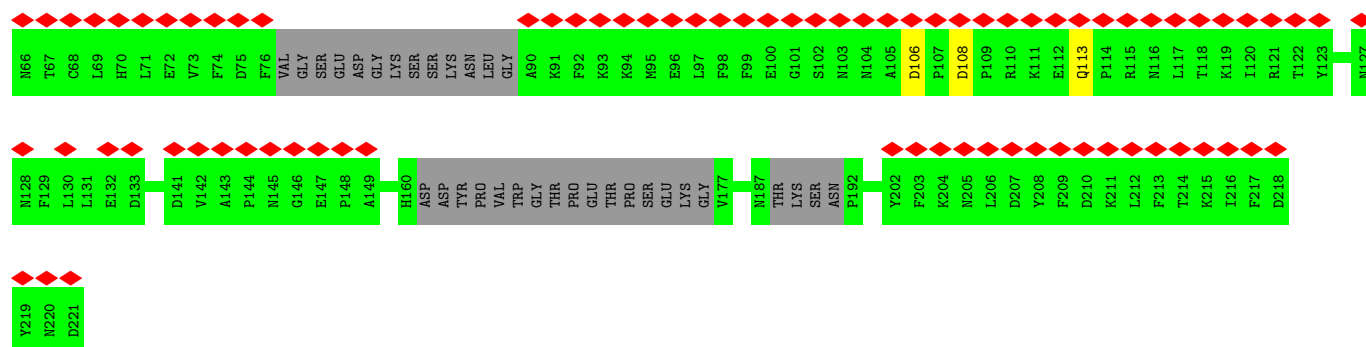


• Molecule 3: Flagellar coiling protein B (FcpB)

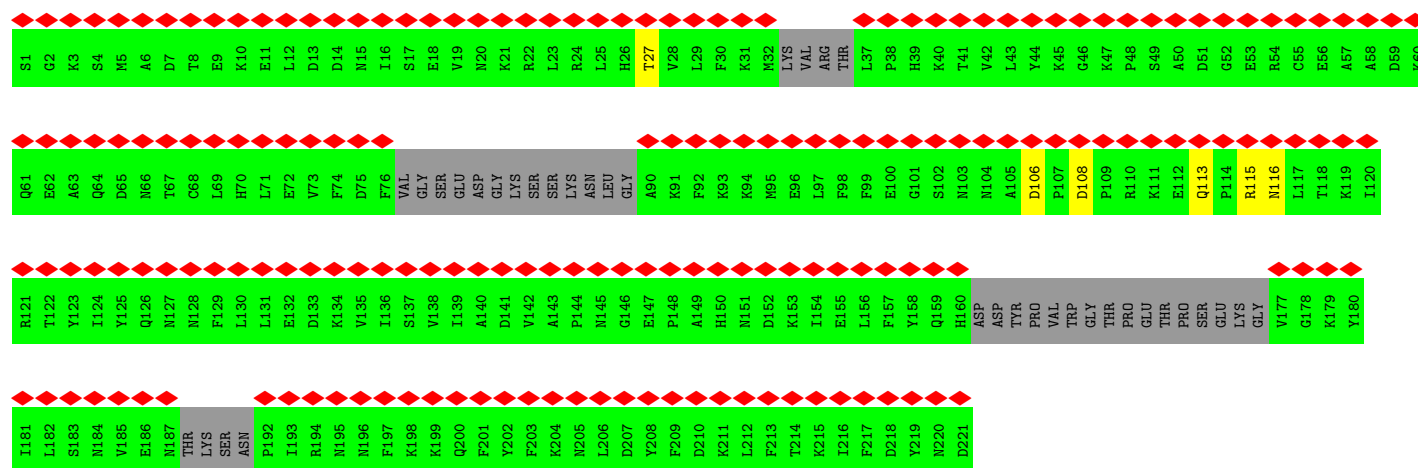


• Molecule 3: Flagellar coiling protein B (FcpB)

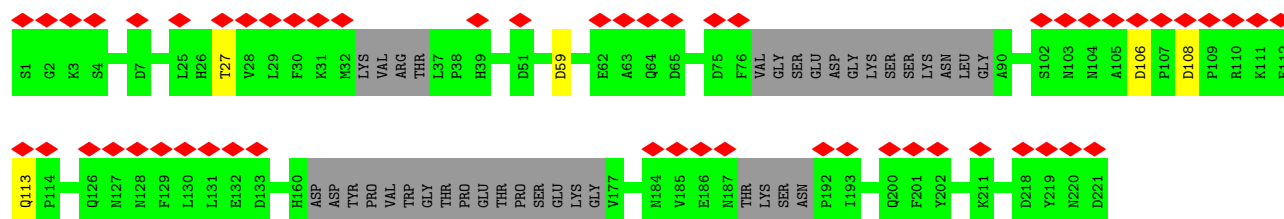




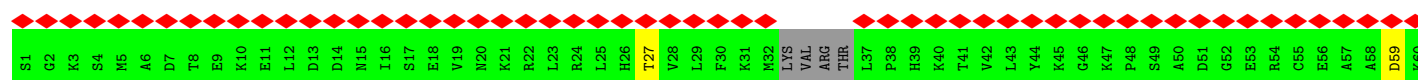
Chain GF:

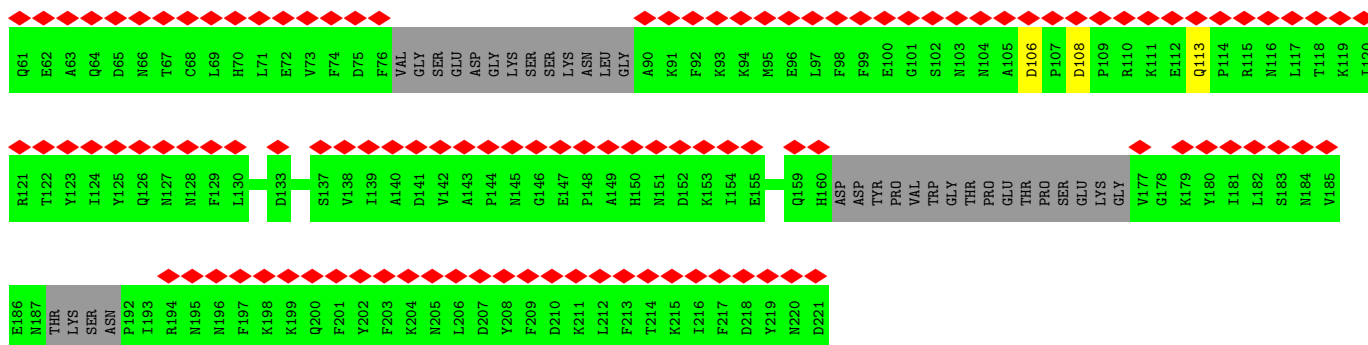


Chain GG:

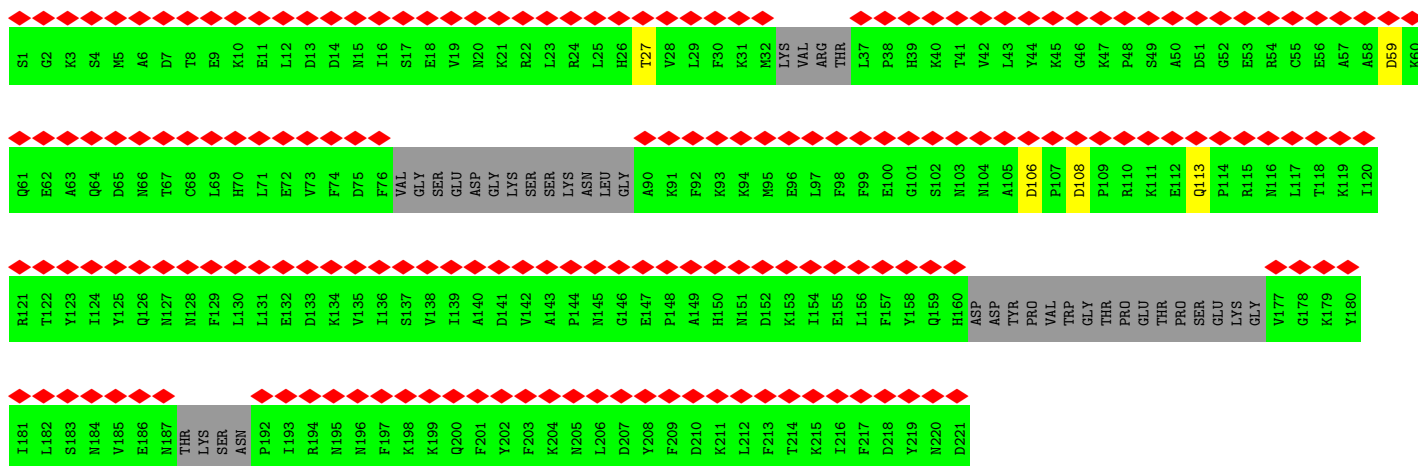
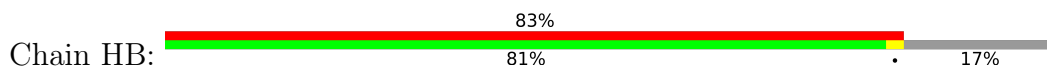


Chain GK:

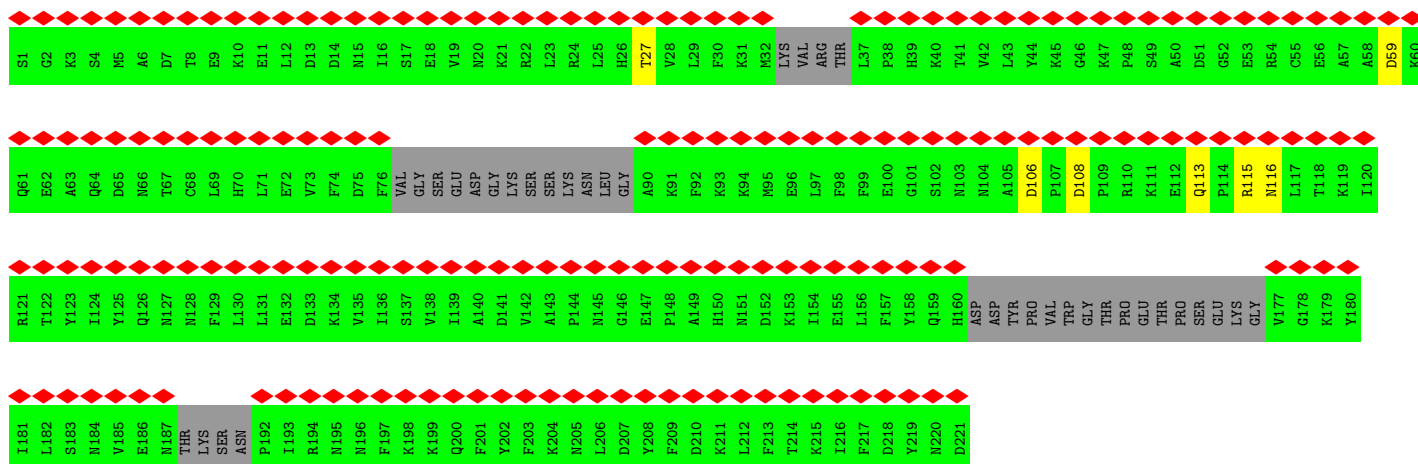
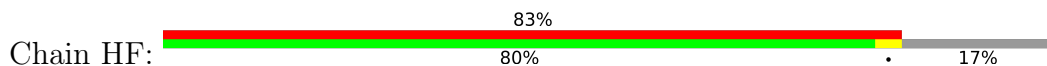




• Molecule 3: Flagellar coiling protein B (FcpB)



• Molecule 3: Flagellar coiling protein B (FcpB)



• Molecule 3: Flagellar coiling protein B (FcpB)

I181	L181	R121	Q61	S1
L182	L182	T122	E62	G2
S183	K3	Y123	A63	K3
M184	L124	I124	Q64	S4
L185	V185	Q125	D65	M5
E186	Q126	N127	N66	A6
T187	N128	T127	T67	D7
LYS	F129	N128	C68	T8
ASW	L130	F129	L69	E9
P192	L131	L130	H70	K10
I193	E132	L131	L71	E11
R194	D133	E132	E72	L12
N195	K134	D133	W73	D13
N196	V135	K134	F74	D14
F197	I136	V135	D75	M15
K198	S137	I136	F76	I16
K199	V138	S137	VAL	S17
Q200	I139	V138	GLY	S17
F201	A140	I139	SER	E18
Y202	D141	I140	GLU	E18
F203	V142	A140	ASP	V19
K204	A143	D141	GLY	N20
N205	P144	V142	LYS	K21
L206	N145	A143	SER	R22
D207	G146	P144	SER	R22
Y208	E147	N145	LYS	L23
F209	P148	G146	ASN	R24
D210	A149	E147	LEU	L25
K211	H150	P148	GLY	H26
L212	N151	F149	A90	T27
F213	D152	A149	K91	V28
T214	K153	H150	F92	L29
K215	I154	N151	K93	L29
L216	E155	D152	X94	F30
F217	L156	K153	N95	K31
D218	F157	I154	E96	M32
Y219	Y158	E155	L97	LYS
N220	Q159	L156	F98	ARG
D221	H160	F157	F99	THR
	ASP	L156	E100	L37
	TYR	F157	G101	P38
	PRO	Y158	S102	H39
	VAL	Q159	N103	K40
	TRP	H160	E112	T41
	GLY	ASP	Q113	V42
	THR	TYR	P114	L43
	GLU	PRO	R115	L44
	THR	VAL	N116	G45
	PRO	TRP	L117	G46
	SER	GLY	T118	K47
	LYS	THR	K119	P48
	GLY	GLU	E119	S49
	V177	THR		A50
	G178	SER		D51
	K179	GLU		G52
	Y180	LYS		E53
		GLY		R54
				C55
				E56
				A57
				A58
				D59
				K60

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 ($\text{\AA}$)	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 ($\text{\AA}$)	2.604, 2.604, 2.604	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.67	0/1059	1.32	8/1322 (0.6%)
1	AH	0.67	0/1059	1.32	8/1322 (0.6%)
1	AI	0.67	0/1059	1.31	7/1322 (0.5%)
1	AR	0.67	0/1059	1.31	8/1322 (0.6%)
1	BA	0.67	0/1059	1.31	8/1322 (0.6%)
1	BB	0.67	0/1059	1.32	10/1322 (0.8%)
1	BC	0.67	0/1059	1.32	8/1322 (0.6%)
1	BD	0.67	0/1059	1.31	8/1322 (0.6%)
1	BL	0.67	0/1059	1.32	10/1322 (0.8%)
1	BM	0.67	0/1059	1.31	8/1322 (0.6%)
1	BS	0.67	0/1059	1.31	8/1322 (0.6%)
1	BT	0.67	0/1059	1.31	8/1322 (0.6%)
1	BU	0.67	0/1059	1.31	8/1322 (0.6%)
1	BV	0.67	0/1059	1.32	8/1322 (0.6%)
1	BW	0.67	0/1059	1.31	8/1322 (0.6%)
1	BX	0.67	0/1059	1.32	8/1322 (0.6%)
1	BY	0.68	0/1059	1.32	8/1322 (0.6%)
1	CG	0.67	0/1059	1.31	8/1322 (0.6%)
1	CH	0.67	0/1059	1.31	8/1322 (0.6%)
1	CL	0.67	0/1059	1.31	8/1322 (0.6%)
1	CM	0.67	0/1059	1.31	8/1322 (0.6%)
1	CN	0.67	0/1059	1.31	8/1322 (0.6%)
1	CO	0.67	0/1059	1.31	8/1322 (0.6%)
1	CP	0.67	0/1059	1.31	8/1322 (0.6%)
1	CQ	0.68	0/1059	1.32	8/1322 (0.6%)
1	CR	0.67	0/1059	1.31	8/1322 (0.6%)
1	CS	0.67	0/1059	1.32	8/1322 (0.6%)
1	CT	0.67	0/1059	1.32	8/1322 (0.6%)
1	DB	0.67	0/1059	1.31	8/1322 (0.6%)
1	DC	0.67	0/1059	1.31	8/1322 (0.6%)
1	DG	0.67	0/1059	1.31	8/1322 (0.6%)
1	DH	0.67	0/1059	1.32	8/1322 (0.6%)
1	DI	0.67	0/1059	1.31	8/1322 (0.6%)
1	DJ	0.67	0/1059	1.31	8/1322 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	DK	0.67	0/1059	1.31	8/1322 (0.6%)
1	DL	0.67	0/1059	1.32	8/1322 (0.6%)
1	DM	0.67	0/1059	1.31	10/1322 (0.8%)
1	DN	0.67	0/1059	1.32	8/1322 (0.6%)
1	DO	0.67	0/1059	1.32	8/1322 (0.6%)
1	DW	0.67	0/1059	1.31	8/1322 (0.6%)
1	DX	0.67	0/1059	1.31	8/1322 (0.6%)
1	EB	0.67	0/1059	1.30	8/1322 (0.6%)
1	EC	0.67	0/1059	1.31	8/1322 (0.6%)
1	ED	0.67	0/1059	1.30	8/1322 (0.6%)
1	EE	0.67	0/1059	1.31	8/1322 (0.6%)
1	EF	0.67	0/1059	1.31	8/1322 (0.6%)
1	EG	0.67	0/1059	1.32	8/1322 (0.6%)
1	EH	0.67	0/1059	1.31	8/1322 (0.6%)
1	EI	0.67	0/1059	1.32	8/1322 (0.6%)
1	EJ	0.67	0/1059	1.30	8/1322 (0.6%)
1	ER	0.67	0/1059	1.31	10/1322 (0.8%)
1	ES	0.67	0/1059	1.31	8/1322 (0.6%)
1	EW	0.67	0/1059	1.31	8/1322 (0.6%)
1	EX	0.67	0/1059	1.31	8/1322 (0.6%)
1	EY	0.67	0/1059	1.31	10/1322 (0.8%)
1	EZ	0.67	0/1059	1.31	8/1322 (0.6%)
1	FA	0.67	0/1059	1.31	8/1322 (0.6%)
1	FB	0.67	0/1059	1.32	8/1322 (0.6%)
1	FC	0.67	0/1059	1.32	8/1322 (0.6%)
1	FD	0.67	0/1059	1.32	8/1322 (0.6%)
1	FE	0.67	0/1059	1.31	8/1322 (0.6%)
1	FM	0.67	0/1059	1.31	8/1322 (0.6%)
1	FN	0.67	0/1059	1.31	8/1322 (0.6%)
1	FR	0.67	0/1059	1.31	8/1322 (0.6%)
1	FS	0.68	0/1059	1.31	8/1322 (0.6%)
1	FT	0.67	0/1059	1.30	8/1322 (0.6%)
1	FU	0.67	0/1059	1.32	8/1322 (0.6%)
1	FV	0.67	0/1059	1.30	8/1322 (0.6%)
1	FW	0.67	0/1059	1.32	8/1322 (0.6%)
1	FX	0.67	0/1059	1.31	8/1322 (0.6%)
1	GH	0.67	0/1059	1.32	10/1322 (0.8%)
1	GI	0.67	0/1059	1.31	8/1322 (0.6%)
1	GM	0.67	0/1059	1.31	8/1322 (0.6%)
1	GN	0.67	0/1059	1.32	8/1322 (0.6%)
1	GO	0.67	0/1059	1.31	8/1322 (0.6%)
1	GP	0.67	0/1059	1.31	8/1322 (0.6%)
1	GQ	0.67	0/1059	1.31	10/1322 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GR	0.67	0/1059	1.32	8/1322 (0.6%)
1	HC	0.67	0/1059	1.32	10/1322 (0.8%)
1	HH	0.67	0/1059	1.30	8/1322 (0.6%)
1	HI	0.67	0/1059	1.32	8/1322 (0.6%)
1	HJ	0.67	0/1059	1.31	8/1322 (0.6%)
1	HK	0.67	0/1059	1.32	8/1322 (0.6%)
1	HL	0.67	0/1059	1.31	8/1322 (0.6%)
2	AL	1.07	0/947	1.46	2/1182 (0.2%)
2	AM	1.07	0/947	1.46	2/1182 (0.2%)
2	AU	1.06	0/947	1.45	2/1182 (0.2%)
2	BE	1.06	0/947	1.45	2/1182 (0.2%)
2	BF	1.07	0/947	1.46	2/1182 (0.2%)
2	BG	1.06	0/947	1.46	2/1182 (0.2%)
2	BH	1.07	0/947	1.46	2/1182 (0.2%)
2	BN	1.07	0/947	1.46	2/1182 (0.2%)
2	BP	1.07	0/947	1.45	2/1182 (0.2%)
2	BZ	1.07	0/947	1.45	2/1182 (0.2%)
2	CA	1.07	0/947	1.46	2/1182 (0.2%)
2	CB	1.06	0/947	1.46	2/1182 (0.2%)
2	CC	1.07	0/947	1.46	2/1182 (0.2%)
2	CI	1.07	0/947	1.46	2/1182 (0.2%)
2	CK	1.07	0/947	1.45	2/1182 (0.2%)
2	CU	1.07	0/947	1.44	2/1182 (0.2%)
2	CV	1.07	0/947	1.46	2/1182 (0.2%)
2	CW	1.07	0/947	1.46	2/1182 (0.2%)
2	CX	1.06	0/947	1.46	2/1182 (0.2%)
2	DD	1.07	0/947	1.46	2/1182 (0.2%)
2	DF	1.06	0/947	1.45	2/1182 (0.2%)
2	DP	1.07	0/947	1.45	2/1182 (0.2%)
2	DQ	1.07	0/947	1.45	2/1182 (0.2%)
2	DR	1.07	0/947	1.45	2/1182 (0.2%)
2	DS	1.07	0/947	1.46	2/1182 (0.2%)
2	DY	1.07	0/947	1.46	2/1182 (0.2%)
2	EA	1.07	0/947	1.45	2/1182 (0.2%)
2	EK	1.06	0/947	1.45	2/1182 (0.2%)
2	EL	1.06	0/947	1.46	2/1182 (0.2%)
2	EM	1.07	0/947	1.46	2/1182 (0.2%)
2	EN	1.07	0/947	1.46	2/1182 (0.2%)
2	ET	1.07	0/947	1.46	2/1182 (0.2%)
2	EV	1.07	0/947	1.45	2/1182 (0.2%)
2	FF	1.07	0/947	1.45	2/1182 (0.2%)
2	FG	1.07	0/947	1.46	2/1182 (0.2%)
2	FH	1.06	0/947	1.46	2/1182 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	FI	1.07	0/947	1.46	2/1182 (0.2%)
2	FO	1.07	0/947	1.46	2/1182 (0.2%)
2	FQ	1.07	0/947	1.45	2/1182 (0.2%)
2	GA	1.07	0/947	1.45	2/1182 (0.2%)
2	GB	1.07	0/947	1.46	2/1182 (0.2%)
2	GC	1.06	0/947	1.45	2/1182 (0.2%)
2	GJ	1.06	0/947	1.46	2/1182 (0.2%)
2	GL	1.07	0/947	1.44	2/1182 (0.2%)
2	GV	1.07	0/947	1.45	2/1182 (0.2%)
2	GW	1.07	0/947	1.46	2/1182 (0.2%)
2	HE	1.07	0/947	1.45	2/1182 (0.2%)
3	AO	0.72	0/731	1.46	10/905 (1.1%)
3	BI	0.72	0/731	1.46	7/905 (0.8%)
3	BJ	0.72	0/731	1.46	10/905 (1.1%)
3	BK	0.73	0/731	1.46	8/905 (0.9%)
3	BO	0.72	0/731	1.46	8/905 (0.9%)
3	CD	0.72	0/731	1.46	7/905 (0.8%)
3	CE	0.72	0/731	1.46	9/905 (1.0%)
3	CF	0.72	0/731	1.46	8/905 (0.9%)
3	CJ	0.72	0/731	1.46	10/905 (1.1%)
3	CY	0.72	0/731	1.46	7/905 (0.8%)
3	CZ	0.72	0/731	1.46	10/905 (1.1%)
3	DA	0.72	0/731	1.46	8/905 (0.9%)
3	DE	0.72	0/731	1.46	8/905 (0.9%)
3	DT	0.72	0/731	1.46	8/905 (0.9%)
3	DU	0.72	0/731	1.46	9/905 (1.0%)
3	DV	0.72	0/731	1.46	8/905 (0.9%)
3	DZ	0.72	0/731	1.45	8/905 (0.9%)
3	EO	0.72	0/731	1.46	8/905 (0.9%)
3	EP	0.72	0/731	1.45	9/905 (1.0%)
3	EQ	0.72	0/731	1.46	8/905 (0.9%)
3	EU	0.72	0/731	1.46	8/905 (0.9%)
3	FJ	0.72	0/731	1.46	10/905 (1.1%)
3	FK	0.72	0/731	1.46	7/905 (0.8%)
3	FL	0.73	0/731	1.46	8/905 (0.9%)
3	FP	0.72	0/731	1.46	8/905 (0.9%)
3	GE	0.72	0/731	1.46	8/905 (0.9%)
3	GF	0.72	0/731	1.45	7/905 (0.8%)
3	GG	0.72	0/731	1.46	8/905 (0.9%)
3	GK	0.72	0/731	1.46	8/905 (0.9%)
3	GZ	0.72	0/731	1.46	10/905 (1.1%)
3	HB	0.72	0/731	1.46	8/905 (0.9%)
3	HF	0.72	0/731	1.46	8/905 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.81	0/156857	1.38	1047/195562 (0.5%)

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.

All (1047) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	EP	27	THR	N-CA-C	-9.33	102.28	114.31
3	DU	27	THR	N-CA-C	-9.31	102.30	114.31
3	CE	27	THR	N-CA-C	-9.31	102.30	114.31
3	HF	27	THR	N-CA-C	-9.30	102.31	114.31
3	EO	27	THR	N-CA-C	-9.30	102.31	114.31
3	HB	27	THR	N-CA-C	-9.29	102.32	114.31
3	GG	27	THR	N-CA-C	-9.29	102.33	114.31
3	EQ	27	THR	N-CA-C	-9.28	102.33	114.31
3	CJ	27	THR	N-CA-C	-9.28	102.34	114.31
3	BJ	27	THR	N-CA-C	-9.28	102.34	114.31
3	DA	27	THR	N-CA-C	-9.26	102.36	114.31
3	CD	27	THR	N-CA-C	-9.26	102.37	114.31
3	FK	27	THR	N-CA-C	-9.26	102.37	114.31
3	CZ	27	THR	N-CA-C	-9.25	102.37	114.31
3	FJ	27	THR	N-CA-C	-9.25	102.38	114.31
3	CY	27	THR	N-CA-C	-9.25	102.38	114.31
3	DZ	27	THR	N-CA-C	-9.25	102.38	114.31
3	FL	27	THR	N-CA-C	-9.24	102.38	114.31
3	AO	27	THR	N-CA-C	-9.24	102.39	114.31
3	DV	27	THR	N-CA-C	-9.24	102.39	114.31
3	BK	27	THR	N-CA-C	-9.23	102.40	114.31
3	DE	27	THR	N-CA-C	-9.22	102.42	114.31
3	EU	27	THR	N-CA-C	-9.22	102.42	114.31
3	GK	27	THR	N-CA-C	-9.22	102.42	114.31
3	GZ	27	THR	N-CA-C	-9.22	102.42	114.31
3	CF	27	THR	N-CA-C	-9.21	102.43	114.31
3	FP	27	THR	N-CA-C	-9.21	102.42	114.31
3	GF	27	THR	N-CA-C	-9.21	102.42	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DT	27	THR	N-CA-C	-9.21	102.43	114.31
3	BO	27	THR	N-CA-C	-9.21	102.44	114.31
3	GE	27	THR	N-CA-C	-9.21	102.44	114.31
3	BI	27	THR	N-CA-C	-9.18	102.47	114.31
1	BD	37	ASN	N-CA-C	-8.15	103.86	113.88
1	ES	37	ASN	N-CA-C	-8.11	103.91	113.88
1	AH	154	GLY	CA-C-N	8.09	127.73	119.56
1	AH	154	GLY	C-N-CA	8.09	127.73	119.56
1	AI	37	ASN	N-CA-C	-8.09	103.93	113.88
1	CT	37	ASN	N-CA-C	-8.09	103.93	113.88
1	BC	154	GLY	CA-C-N	8.07	127.71	119.56
1	BC	154	GLY	C-N-CA	8.07	127.71	119.56
1	BY	37	ASN	N-CA-C	-8.07	103.95	113.88
1	DO	37	ASN	N-CA-C	-8.06	103.97	113.88
1	DX	37	ASN	N-CA-C	-8.05	103.97	113.88
1	EY	37	ASN	N-CA-C	-8.05	103.97	113.88
1	CS	154	GLY	CA-C-N	8.05	127.69	119.56
1	CS	154	GLY	C-N-CA	8.05	127.69	119.56
1	EG	154	GLY	CA-C-N	8.04	127.68	119.56
1	EG	154	GLY	C-N-CA	8.04	127.68	119.56
1	EJ	37	ASN	N-CA-C	-8.04	104.00	113.88
1	FT	37	ASN	N-CA-C	-8.04	104.00	113.88
1	DJ	154	GLY	CA-C-N	8.03	127.67	119.56
1	DJ	154	GLY	C-N-CA	8.03	127.67	119.56
1	BX	154	GLY	CA-C-N	8.02	127.66	119.56
1	BX	154	GLY	C-N-CA	8.02	127.66	119.56
1	DI	37	ASN	N-CA-C	-8.02	104.02	113.88
1	BT	154	GLY	CA-C-N	8.01	127.64	119.56
1	BT	154	GLY	C-N-CA	8.01	127.64	119.56
1	BA	154	GLY	CA-C-N	8.00	127.64	119.56
1	BA	154	GLY	C-N-CA	8.00	127.64	119.56
1	CO	154	GLY	CA-C-N	8.00	127.64	119.56
1	CO	154	GLY	C-N-CA	8.00	127.64	119.56
1	BS	154	GLY	CA-C-N	8.00	127.72	119.64
1	BS	154	GLY	C-N-CA	8.00	127.72	119.64
1	DO	154	GLY	CA-C-N	7.99	127.63	119.56
1	DO	154	GLY	C-N-CA	7.99	127.63	119.56
1	HC	154	GLY	CA-C-N	7.99	127.63	119.56
1	HC	154	GLY	C-N-CA	7.99	127.63	119.56
1	FN	154	GLY	CA-C-N	7.98	127.62	119.56
1	FN	154	GLY	C-N-CA	7.98	127.62	119.56
1	AI	154	GLY	CA-C-N	7.97	127.61	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AI	154	GLY	C-N-CA	7.97	127.61	119.56
1	FD	154	GLY	CA-C-N	7.97	127.61	119.56
1	FD	154	GLY	C-N-CA	7.97	127.61	119.56
1	AG	154	GLY	CA-C-N	7.97	127.61	119.56
1	AG	154	GLY	C-N-CA	7.97	127.61	119.56
1	EI	154	GLY	CA-C-N	7.97	127.61	119.56
1	EI	154	GLY	C-N-CA	7.97	127.61	119.56
1	CR	154	GLY	CA-C-N	7.96	127.60	119.56
1	CR	154	GLY	C-N-CA	7.96	127.60	119.56
1	FE	154	GLY	CA-C-N	7.96	127.60	119.56
1	FE	154	GLY	C-N-CA	7.96	127.60	119.56
1	EC	154	GLY	CA-C-N	7.96	127.59	119.56
1	EC	154	GLY	C-N-CA	7.96	127.59	119.56
1	GP	154	GLY	CA-C-N	7.95	127.59	119.56
1	GP	154	GLY	C-N-CA	7.95	127.59	119.56
1	DL	154	GLY	CA-C-N	7.95	127.59	119.56
1	DL	154	GLY	C-N-CA	7.95	127.59	119.56
1	GR	154	GLY	CA-C-N	7.95	127.59	119.56
1	GR	154	GLY	C-N-CA	7.95	127.59	119.56
1	BL	154	GLY	CA-C-N	7.95	127.59	119.56
1	BL	154	GLY	C-N-CA	7.95	127.59	119.56
1	DI	154	GLY	CA-C-N	7.95	127.59	119.56
1	DI	154	GLY	C-N-CA	7.95	127.59	119.56
1	EX	154	GLY	CA-C-N	7.95	127.59	119.56
1	EX	154	GLY	C-N-CA	7.95	127.59	119.56
1	CH	154	GLY	CA-C-N	7.94	127.58	119.56
1	CH	154	GLY	C-N-CA	7.94	127.58	119.56
1	FW	154	GLY	CA-C-N	7.94	127.58	119.56
1	FW	154	GLY	C-N-CA	7.94	127.58	119.56
1	EE	154	GLY	CA-C-N	7.94	127.58	119.56
1	EE	154	GLY	C-N-CA	7.94	127.58	119.56
1	HK	154	GLY	CA-C-N	7.94	127.58	119.56
1	HK	154	GLY	C-N-CA	7.94	127.58	119.56
1	DN	154	GLY	CA-C-N	7.94	127.58	119.56
1	DN	154	GLY	C-N-CA	7.94	127.58	119.56
1	BY	154	GLY	CA-C-N	7.93	127.57	119.56
1	BY	154	GLY	C-N-CA	7.93	127.57	119.56
1	EF	154	GLY	CA-C-N	7.92	127.56	119.56
1	EF	154	GLY	C-N-CA	7.92	127.56	119.56
1	CG	154	GLY	CA-C-N	7.92	127.56	119.56
1	CG	154	GLY	C-N-CA	7.92	127.56	119.56
1	DM	154	GLY	CA-C-N	7.92	127.55	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DM	154	GLY	C-N-CA	7.92	127.55	119.56
1	BW	154	GLY	CA-C-N	7.91	127.55	119.56
1	BW	154	GLY	C-N-CA	7.91	127.55	119.56
1	DW	154	GLY	CA-C-N	7.91	127.55	119.56
1	DW	154	GLY	C-N-CA	7.91	127.55	119.56
1	FU	154	GLY	CA-C-N	7.91	127.55	119.56
1	FU	154	GLY	C-N-CA	7.91	127.55	119.56
1	GN	154	GLY	CA-C-N	7.91	127.55	119.56
1	GN	154	GLY	C-N-CA	7.91	127.55	119.56
1	FX	154	GLY	CA-C-N	7.91	127.55	119.56
1	FX	154	GLY	C-N-CA	7.91	127.55	119.56
1	BD	154	GLY	CA-C-N	7.90	127.54	119.56
1	BD	154	GLY	C-N-CA	7.90	127.54	119.56
1	CT	154	GLY	CA-C-N	7.90	127.54	119.56
1	CT	154	GLY	C-N-CA	7.90	127.54	119.56
1	EZ	154	GLY	CA-C-N	7.90	127.54	119.56
1	EZ	154	GLY	C-N-CA	7.90	127.54	119.56
1	HI	154	GLY	CA-C-N	7.90	127.54	119.56
1	HI	154	GLY	C-N-CA	7.90	127.54	119.56
1	CP	154	GLY	CA-C-N	7.90	127.54	119.56
1	CP	154	GLY	C-N-CA	7.90	127.54	119.56
1	EJ	154	GLY	CA-C-N	7.90	127.54	119.56
1	EJ	154	GLY	C-N-CA	7.90	127.54	119.56
1	EH	154	GLY	CA-C-N	7.90	127.54	119.56
1	EH	154	GLY	C-N-CA	7.90	127.54	119.56
1	FC	154	GLY	CA-C-N	7.90	127.54	119.56
1	FC	154	GLY	C-N-CA	7.90	127.54	119.56
1	CQ	154	GLY	CA-C-N	7.89	127.53	119.56
1	CQ	154	GLY	C-N-CA	7.89	127.53	119.56
1	DH	154	GLY	CA-C-N	7.89	127.53	119.56
1	DH	154	GLY	C-N-CA	7.89	127.53	119.56
1	CN	154	GLY	CA-C-N	7.89	127.53	119.56
1	CN	154	GLY	C-N-CA	7.89	127.53	119.56
1	GO	154	GLY	CA-C-N	7.89	127.53	119.56
1	GO	154	GLY	C-N-CA	7.89	127.53	119.56
1	FM	154	GLY	CA-C-N	7.88	127.52	119.56
1	FM	154	GLY	C-N-CA	7.88	127.52	119.56
1	DB	154	GLY	CA-C-N	7.88	127.52	119.56
1	DB	154	GLY	C-N-CA	7.88	127.52	119.56
1	BV	154	GLY	CA-C-N	7.88	127.52	119.56
1	BV	154	GLY	C-N-CA	7.88	127.52	119.56
1	AR	154	GLY	CA-C-N	7.87	127.51	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	154	GLY	C-N-CA	7.87	127.51	119.56
1	DK	154	GLY	CA-C-N	7.87	127.51	119.56
1	DK	154	GLY	C-N-CA	7.87	127.51	119.56
1	ES	154	GLY	CA-C-N	7.87	127.51	119.56
1	ES	154	GLY	C-N-CA	7.87	127.51	119.56
1	GI	154	GLY	CA-C-N	7.87	127.51	119.56
1	GI	154	GLY	C-N-CA	7.87	127.51	119.56
1	HL	154	GLY	CA-C-N	7.87	127.51	119.56
1	HL	154	GLY	C-N-CA	7.87	127.51	119.56
1	BB	154	GLY	CA-C-N	7.87	127.51	119.56
1	BB	154	GLY	C-N-CA	7.87	127.51	119.56
1	GH	154	GLY	CA-C-N	7.86	127.50	119.56
1	GH	154	GLY	C-N-CA	7.86	127.50	119.56
1	BM	154	GLY	CA-C-N	7.86	127.49	119.56
1	BM	154	GLY	C-N-CA	7.86	127.49	119.56
1	FB	154	GLY	CA-C-N	7.85	127.49	119.56
1	FB	154	GLY	C-N-CA	7.85	127.49	119.56
1	FS	154	GLY	CA-C-N	7.85	127.48	119.56
1	FS	154	GLY	C-N-CA	7.85	127.48	119.56
1	HJ	154	GLY	CA-C-N	7.84	127.56	119.64
1	HJ	154	GLY	C-N-CA	7.84	127.56	119.64
1	ER	154	GLY	CA-C-N	7.83	127.47	119.56
1	ER	154	GLY	C-N-CA	7.83	127.47	119.56
1	DC	154	GLY	CA-C-N	7.81	127.45	119.56
1	DC	154	GLY	C-N-CA	7.81	127.45	119.56
1	DX	154	GLY	CA-C-N	7.80	127.44	119.56
1	DX	154	GLY	C-N-CA	7.80	127.44	119.56
1	CM	154	GLY	CA-C-N	7.79	127.43	119.56
1	CM	154	GLY	C-N-CA	7.79	127.43	119.56
1	FA	154	GLY	CA-C-N	7.78	127.42	119.56
1	FA	154	GLY	C-N-CA	7.78	127.42	119.56
1	GM	37	ASN	N-CA-C	-7.67	103.89	113.55
1	BB	37	ASN	N-CA-C	-7.66	103.90	113.55
1	DW	37	ASN	N-CA-C	-7.65	103.91	113.55
1	FE	37	ASN	N-CA-C	-7.64	103.92	113.55
1	FC	37	ASN	N-CA-C	-7.64	103.92	113.55
1	GR	37	ASN	N-CA-C	-7.64	103.92	113.55
1	FM	37	ASN	N-CA-C	-7.64	103.92	113.55
1	EH	37	ASN	N-CA-C	-7.64	103.93	113.55
1	FR	37	ASN	N-CA-C	-7.64	103.93	113.55
1	CR	37	ASN	N-CA-C	-7.63	103.93	113.55
1	DN	37	ASN	N-CA-C	-7.63	103.93	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FB	37	ASN	N-CA-C	-7.63	103.94	113.55
1	HK	37	ASN	N-CA-C	-7.63	103.94	113.55
1	FX	37	ASN	N-CA-C	-7.62	103.94	113.55
1	BC	37	ASN	N-CA-C	-7.62	103.95	113.55
1	EG	37	ASN	N-CA-C	-7.62	103.94	113.55
1	FN	37	ASN	N-CA-C	-7.62	103.95	113.55
1	GI	37	ASN	N-CA-C	-7.62	103.95	113.55
1	AH	37	ASN	N-CA-C	-7.61	103.96	113.55
1	CG	37	ASN	N-CA-C	-7.61	103.96	113.55
1	BX	37	ASN	N-CA-C	-7.61	103.96	113.55
1	BV	37	ASN	N-CA-C	-7.61	103.97	113.55
1	CL	37	ASN	N-CA-C	-7.60	103.97	113.55
1	CN	37	ASN	N-CA-C	-7.60	103.97	113.55
1	DL	37	ASN	N-CA-C	-7.60	103.97	113.55
1	EI	37	ASN	N-CA-C	-7.60	103.97	113.55
1	EW	37	ASN	N-CA-C	-7.60	103.97	113.55
1	DC	37	ASN	N-CA-C	-7.60	103.97	113.55
1	ER	37	ASN	N-CA-C	-7.60	103.97	113.55
1	DB	37	ASN	N-CA-C	-7.60	103.98	113.55
1	EB	37	ASN	N-CA-C	-7.60	103.98	113.55
1	EZ	37	ASN	N-CA-C	-7.59	103.98	113.55
1	CP	37	ASN	N-CA-C	-7.59	103.98	113.55
1	HC	37	ASN	N-CA-C	-7.59	103.98	113.55
1	DM	37	ASN	N-CA-C	-7.59	103.99	113.55
1	FD	37	ASN	N-CA-C	-7.59	103.99	113.55
1	DJ	37	ASN	N-CA-C	-7.59	103.99	113.55
1	GO	37	ASN	N-CA-C	-7.58	103.99	113.55
1	EE	37	ASN	N-CA-C	-7.58	103.99	113.55
1	FU	37	ASN	N-CA-C	-7.58	104.00	113.55
1	GH	37	ASN	N-CA-C	-7.58	104.00	113.55
1	CH	37	ASN	N-CA-C	-7.58	104.00	113.55
1	BL	37	ASN	N-CA-C	-7.58	104.00	113.55
1	BW	37	ASN	N-CA-C	-7.58	104.00	113.55
1	GQ	37	ASN	N-CA-C	-7.58	104.00	113.55
1	BU	37	ASN	N-CA-C	-7.57	104.01	113.55
1	CO	37	ASN	N-CA-C	-7.57	104.01	113.55
1	BA	37	ASN	N-CA-C	-7.57	104.01	113.55
1	DK	37	ASN	N-CA-C	-7.57	104.01	113.55
1	EC	37	ASN	N-CA-C	-7.57	104.01	113.55
1	GP	37	ASN	N-CA-C	-7.57	104.01	113.55
1	AR	37	ASN	N-CA-C	-7.57	104.02	113.55
1	FW	37	ASN	N-CA-C	-7.57	104.02	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HH	37	ASN	N-CA-C	-7.57	104.02	113.55
1	FA	37	ASN	N-CA-C	-7.56	104.02	113.55
1	HL	37	ASN	N-CA-C	-7.56	104.03	113.55
1	ED	37	ASN	N-CA-C	-7.56	104.03	113.55
1	DG	37	ASN	N-CA-C	-7.55	104.04	113.55
1	HJ	37	ASN	N-CA-C	-7.55	104.04	113.55
1	BT	37	ASN	N-CA-C	-7.55	104.04	113.55
1	AG	37	ASN	N-CA-C	-7.54	104.05	113.55
1	BS	37	ASN	N-CA-C	-7.54	104.05	113.55
1	CS	37	ASN	N-CA-C	-7.53	104.06	113.55
1	BM	37	ASN	N-CA-C	-7.53	104.06	113.55
1	CQ	37	ASN	N-CA-C	-7.52	104.07	113.55
1	EF	37	ASN	N-CA-C	-7.52	104.08	113.55
1	FV	37	ASN	N-CA-C	-7.51	104.08	113.55
1	ED	154	GLY	CA-C-N	7.44	127.60	119.87
1	ED	154	GLY	C-N-CA	7.44	127.60	119.87
1	EY	154	GLY	CA-C-N	7.43	127.60	119.87
1	EY	154	GLY	C-N-CA	7.43	127.60	119.87
1	BU	154	GLY	CA-C-N	7.41	127.58	119.87
1	BU	154	GLY	C-N-CA	7.41	127.58	119.87
1	EW	154	GLY	CA-C-N	7.38	127.54	119.87
1	EW	154	GLY	C-N-CA	7.38	127.54	119.87
1	FV	154	GLY	CA-C-N	7.37	127.53	119.87
1	FV	154	GLY	C-N-CA	7.37	127.53	119.87
1	CL	154	GLY	CA-C-N	7.36	127.53	119.87
1	CL	154	GLY	C-N-CA	7.36	127.53	119.87
1	FT	154	GLY	CA-C-N	7.35	127.52	119.87
1	FT	154	GLY	C-N-CA	7.35	127.52	119.87
1	EB	154	GLY	CA-C-N	7.34	127.50	119.87
1	EB	154	GLY	C-N-CA	7.34	127.50	119.87
1	DG	154	GLY	CA-C-N	7.33	127.50	119.87
1	DG	154	GLY	C-N-CA	7.33	127.50	119.87
1	DH	37	ASN	N-CA-C	-7.31	103.98	113.12
1	CM	37	ASN	N-CA-C	-7.28	104.02	113.12
1	FR	154	GLY	CA-C-N	7.28	127.44	119.87
1	FR	154	GLY	C-N-CA	7.28	127.44	119.87
1	GM	154	GLY	CA-C-N	7.28	127.44	119.87
1	GM	154	GLY	C-N-CA	7.28	127.44	119.87
1	EX	37	ASN	N-CA-C	-7.27	104.03	113.12
1	HI	37	ASN	N-CA-C	-7.27	104.03	113.12
1	GQ	154	GLY	CA-C-N	7.24	127.40	119.87
1	GQ	154	GLY	C-N-CA	7.24	127.40	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GN	37	ASN	N-CA-C	-7.24	104.07	113.12
1	FS	37	ASN	N-CA-C	-7.22	104.09	113.12
1	HH	154	GLY	CA-C-N	6.90	127.50	120.04
1	HH	154	GLY	C-N-CA	6.90	127.50	120.04
3	BO	106	ASP	CA-C-N	6.82	126.97	119.87
3	BO	106	ASP	C-N-CA	6.82	126.97	119.87
3	DV	106	ASP	CA-C-N	6.77	126.91	119.87
3	DV	106	ASP	C-N-CA	6.77	126.91	119.87
3	FL	106	ASP	CA-C-N	6.76	126.90	119.87
3	FL	106	ASP	C-N-CA	6.76	126.90	119.87
3	FK	106	ASP	CA-C-N	6.76	126.90	119.87
3	FK	106	ASP	C-N-CA	6.76	126.90	119.87
3	FP	106	ASP	CA-C-N	6.74	126.88	119.87
3	FP	106	ASP	C-N-CA	6.74	126.88	119.87
3	FJ	106	ASP	CA-C-N	6.73	126.87	119.87
3	FJ	106	ASP	C-N-CA	6.73	126.87	119.87
3	EU	106	ASP	CA-C-N	6.71	126.85	119.87
3	EU	106	ASP	C-N-CA	6.71	126.85	119.87
3	DE	106	ASP	CA-C-N	6.70	126.84	119.87
3	DE	106	ASP	C-N-CA	6.70	126.84	119.87
3	CE	106	ASP	CA-C-N	6.70	126.83	119.87
3	CE	106	ASP	C-N-CA	6.70	126.83	119.87
3	DZ	106	ASP	CA-C-N	6.70	126.83	119.87
3	DZ	106	ASP	C-N-CA	6.70	126.83	119.87
3	CZ	106	ASP	CA-C-N	6.69	126.83	119.87
3	CZ	106	ASP	C-N-CA	6.69	126.83	119.87
3	CD	106	ASP	CA-C-N	6.68	126.82	119.87
3	CD	106	ASP	C-N-CA	6.68	126.82	119.87
3	HF	106	ASP	CA-C-N	6.68	126.82	119.87
3	HF	106	ASP	C-N-CA	6.68	126.82	119.87
3	GK	106	ASP	CA-C-N	6.68	126.81	119.87
3	GK	106	ASP	C-N-CA	6.68	126.81	119.87
3	DT	106	ASP	CA-C-N	6.67	126.81	119.87
3	DT	106	ASP	C-N-CA	6.67	126.81	119.87
3	CY	106	ASP	CA-C-N	6.67	126.81	119.87
3	CY	106	ASP	C-N-CA	6.67	126.81	119.87
3	HB	106	ASP	CA-C-N	6.67	126.80	119.87
3	HB	106	ASP	C-N-CA	6.67	126.80	119.87
3	GG	106	ASP	CA-C-N	6.66	126.80	119.87
3	GG	106	ASP	C-N-CA	6.66	126.80	119.87
3	DU	106	ASP	CA-C-N	6.65	126.79	119.87
3	DU	106	ASP	C-N-CA	6.65	126.79	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BK	106	ASP	CA-C-N	6.65	126.79	119.87
3	BK	106	ASP	C-N-CA	6.65	126.79	119.87
3	GZ	106	ASP	CA-C-N	6.64	126.78	119.87
3	GZ	106	ASP	C-N-CA	6.64	126.78	119.87
3	AO	106	ASP	CA-C-N	6.64	126.78	119.87
3	AO	106	ASP	C-N-CA	6.64	126.78	119.87
3	CF	106	ASP	CA-C-N	6.64	126.78	119.87
3	CF	106	ASP	C-N-CA	6.64	126.78	119.87
3	CJ	106	ASP	CA-C-N	6.64	126.78	119.87
3	CJ	106	ASP	C-N-CA	6.64	126.78	119.87
3	DA	106	ASP	CA-C-N	6.63	126.77	119.87
3	DA	106	ASP	C-N-CA	6.63	126.77	119.87
3	BJ	106	ASP	CA-C-N	6.61	126.75	119.87
3	BJ	106	ASP	C-N-CA	6.61	126.75	119.87
3	EQ	106	ASP	CA-C-N	6.61	126.75	119.87
3	EQ	106	ASP	C-N-CA	6.61	126.75	119.87
3	EO	106	ASP	CA-C-N	6.60	126.73	119.87
3	EO	106	ASP	C-N-CA	6.60	126.73	119.87
3	EP	106	ASP	CA-C-N	6.59	126.73	119.87
3	EP	106	ASP	C-N-CA	6.59	126.73	119.87
3	GE	106	ASP	CA-C-N	6.58	126.71	119.87
3	GE	106	ASP	C-N-CA	6.58	126.71	119.87
3	GF	106	ASP	CA-C-N	6.56	126.69	119.87
3	GF	106	ASP	C-N-CA	6.56	126.69	119.87
3	BI	106	ASP	CA-C-N	6.55	126.69	119.87
3	BI	106	ASP	C-N-CA	6.55	126.69	119.87
1	BS	171	ARG	N-CA-C	-6.39	106.06	114.31
1	CS	171	ARG	N-CA-C	-6.39	106.07	114.31
1	FD	171	ARG	N-CA-C	-6.39	106.07	114.31
1	BU	171	ARG	N-CA-C	-6.38	106.08	114.31
1	ES	171	ARG	N-CA-C	-6.38	106.09	114.31
1	FS	171	ARG	N-CA-C	-6.36	106.10	114.31
1	BX	171	ARG	N-CA-C	-6.36	106.10	114.31
1	AI	171	ARG	N-CA-C	-6.36	106.11	114.31
1	FB	171	ARG	N-CA-C	-6.36	106.11	114.31
1	DI	171	ARG	N-CA-C	-6.35	106.12	114.31
1	AH	171	ARG	N-CA-C	-6.35	106.12	114.31
1	CN	171	ARG	N-CA-C	-6.35	106.12	114.31
1	DM	171	ARG	N-CA-C	-6.35	106.12	114.31
1	FM	171	ARG	N-CA-C	-6.35	106.12	114.31
1	EF	171	ARG	N-CA-C	-6.35	106.12	114.31
1	BC	171	ARG	N-CA-C	-6.35	106.12	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CT	171	ARG	N-CA-C	-6.34	106.12	114.31
1	EJ	171	ARG	N-CA-C	-6.34	106.12	114.31
1	FA	171	ARG	N-CA-C	-6.34	106.13	114.31
1	FV	171	ARG	N-CA-C	-6.34	106.13	114.31
1	BB	171	ARG	N-CA-C	-6.34	106.13	114.31
1	EB	171	ARG	N-CA-C	-6.34	106.13	114.31
1	FX	171	ARG	N-CA-C	-6.34	106.13	114.31
1	HJ	171	ARG	N-CA-C	-6.34	106.13	114.31
1	FC	171	ARG	N-CA-C	-6.34	106.13	114.31
1	CP	171	ARG	N-CA-C	-6.34	106.14	114.31
1	DX	171	ARG	N-CA-C	-6.34	106.14	114.31
1	GO	171	ARG	N-CA-C	-6.34	106.14	114.31
1	ER	171	ARG	N-CA-C	-6.33	106.14	114.31
1	GR	171	ARG	N-CA-C	-6.33	106.14	114.31
1	DK	171	ARG	N-CA-C	-6.33	106.14	114.31
1	EX	171	ARG	N-CA-C	-6.33	106.15	114.31
1	CG	171	ARG	N-CA-C	-6.32	106.15	114.31
1	EI	171	ARG	N-CA-C	-6.32	106.15	114.31
1	FN	171	ARG	N-CA-C	-6.32	106.15	114.31
1	HH	171	ARG	N-CA-C	-6.32	106.15	114.31
1	DG	171	ARG	N-CA-C	-6.32	106.15	114.31
1	HL	171	ARG	N-CA-C	-6.32	106.16	114.31
1	EC	171	ARG	N-CA-C	-6.31	106.17	114.31
1	BW	171	ARG	N-CA-C	-6.31	106.17	114.31
1	DN	171	ARG	N-CA-C	-6.31	106.17	114.31
1	BD	171	ARG	N-CA-C	-6.31	106.17	114.31
1	FW	171	ARG	N-CA-C	-6.31	106.17	114.31
1	HC	171	ARG	N-CA-C	-6.31	106.17	114.31
1	CM	171	ARG	N-CA-C	-6.31	106.17	114.31
1	FE	171	ARG	N-CA-C	-6.31	106.17	114.31
1	FT	171	ARG	N-CA-C	-6.31	106.17	114.31
1	DL	171	ARG	N-CA-C	-6.30	106.18	114.31
1	GH	171	ARG	N-CA-C	-6.30	106.18	114.31
1	AG	171	ARG	N-CA-C	-6.30	106.18	114.31
1	AR	171	ARG	N-CA-C	-6.30	106.18	114.31
1	DO	171	ARG	N-CA-C	-6.30	106.19	114.31
1	EG	171	ARG	N-CA-C	-6.30	106.19	114.31
1	FR	171	ARG	N-CA-C	-6.30	106.19	114.31
1	BM	171	ARG	N-CA-C	-6.29	106.19	114.31
1	DC	171	ARG	N-CA-C	-6.29	106.19	114.31
1	DW	171	ARG	N-CA-C	-6.29	106.19	114.31
1	GQ	171	ARG	N-CA-C	-6.29	106.19	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	HI	171	ARG	N-CA-C	-6.29	106.19	114.31
1	EY	171	ARG	N-CA-C	-6.29	106.19	114.31
1	BA	171	ARG	N-CA-C	-6.29	106.20	114.31
1	DB	171	ARG	N-CA-C	-6.29	106.20	114.31
1	DJ	171	ARG	N-CA-C	-6.29	106.20	114.31
1	CR	171	ARG	N-CA-C	-6.29	106.20	114.31
1	EW	171	ARG	N-CA-C	-6.29	106.20	114.31
1	CH	171	ARG	N-CA-C	-6.28	106.21	114.31
1	CQ	171	ARG	N-CA-C	-6.28	106.21	114.31
1	ED	171	ARG	N-CA-C	-6.28	106.21	114.31
1	FU	171	ARG	N-CA-C	-6.28	106.21	114.31
1	EH	171	ARG	N-CA-C	-6.28	106.21	114.31
1	DH	171	ARG	N-CA-C	-6.28	106.21	114.31
1	GM	171	ARG	N-CA-C	-6.28	106.22	114.31
1	GN	171	ARG	N-CA-C	-6.28	106.21	114.31
1	BY	171	ARG	N-CA-C	-6.27	106.22	114.31
1	GI	171	ARG	N-CA-C	-6.27	106.22	114.31
1	BL	171	ARG	N-CA-C	-6.26	106.23	114.31
1	CL	171	ARG	N-CA-C	-6.26	106.23	114.31
1	BT	171	ARG	N-CA-C	-6.25	106.25	114.31
1	EZ	171	ARG	N-CA-C	-6.25	106.25	114.31
1	CO	171	ARG	N-CA-C	-6.24	106.26	114.31
1	EE	171	ARG	N-CA-C	-6.24	106.26	114.31
1	GP	171	ARG	N-CA-C	-6.22	106.28	114.31
1	BV	171	ARG	N-CA-C	-6.22	106.29	114.31
1	HK	171	ARG	N-CA-C	-6.22	106.29	114.31
3	GG	108	ASP	CA-C-N	6.17	125.80	119.56
3	GG	108	ASP	C-N-CA	6.17	125.80	119.56
1	FB	140	PHE	CA-C-O	-6.17	113.70	120.24
1	FE	140	PHE	CA-C-O	-6.17	113.70	120.36
3	BK	108	ASP	CA-C-N	6.15	125.78	119.56
3	BK	108	ASP	C-N-CA	6.15	125.78	119.56
1	BV	140	PHE	CA-C-O	-6.15	113.72	120.24
1	BY	140	PHE	CA-C-O	-6.15	113.72	120.36
1	BM	140	PHE	CA-C-O	-6.14	113.73	120.24
1	CS	140	PHE	CA-C-O	-6.14	113.73	120.30
1	CT	140	PHE	CA-C-O	-6.14	113.73	120.36
1	FW	140	PHE	CA-C-O	-6.13	113.74	120.24
1	BX	140	PHE	CA-C-O	-6.13	113.74	120.36
1	DO	140	PHE	CA-C-O	-6.12	113.75	120.36
1	GI	140	PHE	CA-C-O	-6.12	113.76	120.24
1	EG	140	PHE	CA-C-O	-6.11	113.76	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GE	108	ASP	CA-C-N	6.11	125.73	119.56
3	GE	108	ASP	C-N-CA	6.11	125.73	119.56
1	GR	140	PHE	CA-C-O	-6.11	113.76	120.24
1	EJ	140	PHE	CA-C-O	-6.11	113.76	120.36
3	FK	108	ASP	CA-C-N	6.11	125.73	119.56
3	FK	108	ASP	C-N-CA	6.11	125.73	119.56
1	CQ	140	PHE	CA-C-O	-6.11	113.77	120.24
1	BA	140	PHE	CA-C-O	-6.11	113.77	120.24
1	DC	140	PHE	CA-C-O	-6.11	113.77	120.24
3	DA	108	ASP	CA-C-N	6.11	125.73	119.56
3	DA	108	ASP	C-N-CA	6.11	125.73	119.56
1	EI	140	PHE	CA-C-O	-6.11	113.77	120.30
3	FP	108	ASP	CA-C-N	6.11	125.73	119.56
3	FP	108	ASP	C-N-CA	6.11	125.73	119.56
3	EQ	108	ASP	CA-C-N	6.10	125.73	119.56
3	EQ	108	ASP	C-N-CA	6.10	125.73	119.56
3	AO	108	ASP	CA-C-N	6.10	125.72	119.56
3	AO	108	ASP	C-N-CA	6.10	125.72	119.56
3	HF	108	ASP	CA-C-N	6.10	125.72	119.56
3	HF	108	ASP	C-N-CA	6.10	125.72	119.56
3	CD	108	ASP	CA-C-N	6.10	125.72	119.56
3	CD	108	ASP	C-N-CA	6.10	125.72	119.56
1	CH	140	PHE	CA-C-O	-6.09	113.78	120.24
3	CY	108	ASP	CA-C-N	6.09	125.71	119.56
3	CY	108	ASP	C-N-CA	6.09	125.71	119.56
1	DL	140	PHE	CA-C-O	-6.09	113.79	120.24
1	BD	140	PHE	CA-C-O	-6.08	113.79	120.30
1	ES	140	PHE	CA-C-O	-6.08	113.80	120.24
1	FN	140	PHE	CA-C-O	-6.08	113.80	120.24
3	FJ	108	ASP	CA-C-N	6.07	125.69	119.56
3	FJ	108	ASP	C-N-CA	6.07	125.69	119.56
1	DN	140	PHE	CA-C-O	-6.07	113.81	120.36
3	GZ	108	ASP	CA-C-N	6.05	125.67	119.56
3	GZ	108	ASP	C-N-CA	6.05	125.67	119.56
1	AH	140	PHE	CA-C-O	-6.05	113.82	120.30
3	CF	108	ASP	CA-C-N	6.05	125.67	119.56
3	CF	108	ASP	C-N-CA	6.05	125.67	119.56
3	DE	108	ASP	CA-C-N	6.05	125.67	119.56
3	DE	108	ASP	C-N-CA	6.05	125.67	119.56
1	AR	140	PHE	CA-C-O	-6.05	113.83	120.24
3	BJ	108	ASP	CA-C-N	6.05	125.67	119.56
3	BJ	108	ASP	C-N-CA	6.05	125.67	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BC	140	PHE	CA-C-O	-6.04	113.83	120.30
1	EC	140	PHE	CA-C-O	-6.04	113.61	120.32
3	HB	108	ASP	CA-C-N	6.04	125.66	119.56
3	HB	108	ASP	C-N-CA	6.04	125.66	119.56
1	AI	140	PHE	CA-C-O	-6.03	113.85	120.30
3	CZ	108	ASP	CA-C-N	6.03	125.65	119.56
3	CZ	108	ASP	C-N-CA	6.03	125.65	119.56
3	DV	108	ASP	CA-C-N	6.03	125.65	119.56
3	DV	108	ASP	C-N-CA	6.03	125.65	119.56
3	CJ	108	ASP	CA-C-N	6.02	125.64	119.56
3	CJ	108	ASP	C-N-CA	6.02	125.64	119.56
1	FD	140	PHE	CA-C-O	-6.02	113.86	120.36
3	GF	108	ASP	CA-C-N	6.01	125.64	119.56
3	GF	108	ASP	C-N-CA	6.01	125.64	119.56
3	DZ	108	ASP	CA-C-N	6.01	125.63	119.56
3	DZ	108	ASP	C-N-CA	6.01	125.63	119.56
3	EO	108	ASP	CA-C-N	6.01	125.63	119.56
3	EO	108	ASP	C-N-CA	6.01	125.63	119.56
3	EU	108	ASP	CA-C-N	6.01	125.63	119.56
3	EU	108	ASP	C-N-CA	6.01	125.63	119.56
1	DX	140	PHE	CA-C-O	-6.00	113.88	120.24
3	GK	108	ASP	CA-C-N	5.99	125.61	119.56
3	GK	108	ASP	C-N-CA	5.99	125.61	119.56
1	DH	140	PHE	CA-C-O	-5.98	113.68	120.32
1	GQ	140	PHE	CA-C-O	-5.98	113.68	120.32
1	FV	140	PHE	CA-C-O	-5.98	113.68	120.32
3	GG	113	GLN	CA-C-N	5.98	125.95	120.03
3	GG	113	GLN	C-N-CA	5.98	125.95	120.03
3	BO	108	ASP	CA-C-N	5.97	125.59	119.56
3	BO	108	ASP	C-N-CA	5.97	125.59	119.56
3	DU	108	ASP	CA-C-N	5.97	125.59	119.56
3	DU	108	ASP	C-N-CA	5.97	125.59	119.56
3	EP	108	ASP	CA-C-N	5.97	125.59	119.56
3	EP	108	ASP	C-N-CA	5.97	125.59	119.56
3	BI	108	ASP	CA-C-N	5.96	125.58	119.56
3	BI	108	ASP	C-N-CA	5.96	125.58	119.56
3	DT	108	ASP	CA-C-N	5.96	125.58	119.56
3	DT	108	ASP	C-N-CA	5.96	125.58	119.56
3	FL	108	ASP	CA-C-N	5.96	125.58	119.56
3	FL	108	ASP	C-N-CA	5.96	125.58	119.56
1	GH	140	PHE	CA-C-O	-5.96	113.70	120.32
1	BB	140	PHE	CA-C-O	-5.96	113.71	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CO	140	PHE	CA-C-O	-5.95	113.71	120.32
1	HC	140	PHE	CA-C-O	-5.95	113.72	120.32
3	BK	113	GLN	CA-C-N	5.95	125.92	120.03
3	BK	113	GLN	C-N-CA	5.95	125.92	120.03
3	CJ	113	GLN	CA-C-N	5.94	125.91	120.03
3	CJ	113	GLN	C-N-CA	5.94	125.91	120.03
3	HB	113	GLN	CA-C-N	5.94	125.92	120.03
3	HB	113	GLN	C-N-CA	5.94	125.92	120.03
3	CD	113	GLN	CA-C-N	5.94	125.91	120.03
3	CD	113	GLN	C-N-CA	5.94	125.91	120.03
3	GF	113	GLN	CA-C-N	5.94	125.91	120.03
3	GF	113	GLN	C-N-CA	5.94	125.91	120.03
1	HH	140	PHE	CA-C-O	-5.94	113.73	120.32
1	BU	140	PHE	CA-C-O	-5.94	113.73	120.32
1	DM	140	PHE	CA-C-O	-5.93	113.73	120.32
3	BI	113	GLN	CA-C-N	5.93	125.90	120.03
3	BI	113	GLN	C-N-CA	5.93	125.90	120.03
3	CE	108	ASP	CA-C-N	5.93	125.55	119.56
3	CE	108	ASP	C-N-CA	5.93	125.55	119.56
1	DW	140	PHE	CA-C-O	-5.93	113.73	120.32
1	GP	140	PHE	CA-C-O	-5.93	113.73	120.32
1	DB	140	PHE	CA-C-O	-5.93	113.74	120.32
3	DZ	113	GLN	CA-C-N	5.93	125.90	120.03
3	DZ	113	GLN	C-N-CA	5.93	125.90	120.03
1	ER	140	PHE	CA-C-O	-5.93	113.74	120.32
3	FP	113	GLN	CA-C-N	5.92	125.89	120.03
3	FP	113	GLN	C-N-CA	5.92	125.89	120.03
1	FX	140	PHE	CA-C-O	-5.92	113.74	120.32
3	CE	113	GLN	CA-C-N	5.92	125.89	120.03
3	CE	113	GLN	C-N-CA	5.92	125.89	120.03
3	DE	113	GLN	CA-C-N	5.92	125.89	120.03
3	DE	113	GLN	C-N-CA	5.92	125.89	120.03
1	EZ	140	PHE	CA-C-O	-5.92	113.75	120.32
3	CZ	113	GLN	CA-C-N	5.91	125.88	120.03
3	CZ	113	GLN	C-N-CA	5.91	125.88	120.03
1	DG	140	PHE	CA-C-O	-5.91	113.75	120.32
1	EH	140	PHE	CA-C-O	-5.91	113.76	120.32
3	FK	113	GLN	CA-C-N	5.91	125.88	120.03
3	FK	113	GLN	C-N-CA	5.91	125.88	120.03
3	HF	113	GLN	CA-C-N	5.91	125.88	120.03
3	HF	113	GLN	C-N-CA	5.91	125.88	120.03
1	HL	140	PHE	CA-C-O	-5.91	113.76	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	EO	113	GLN	CA-C-N	5.91	125.88	120.03
3	EO	113	GLN	C-N-CA	5.91	125.88	120.03
1	EX	140	PHE	CA-C-O	-5.91	113.76	120.32
1	EE	140	PHE	CA-C-O	-5.91	113.76	120.32
1	GM	140	PHE	CA-C-O	-5.91	113.76	120.32
1	GO	140	PHE	CA-C-O	-5.91	113.76	120.32
1	ED	140	PHE	CA-C-O	-5.90	113.77	120.32
1	CN	140	PHE	CA-C-O	-5.90	113.77	120.32
3	GK	113	GLN	CA-C-N	5.90	125.87	120.03
3	GK	113	GLN	C-N-CA	5.90	125.87	120.03
1	CG	140	PHE	CA-C-O	-5.90	113.78	120.32
3	CF	113	GLN	CA-C-N	5.89	125.86	120.03
3	CF	113	GLN	C-N-CA	5.89	125.86	120.03
3	FJ	113	GLN	CA-C-N	5.89	125.86	120.03
3	FJ	113	GLN	C-N-CA	5.89	125.86	120.03
1	FM	140	PHE	CA-C-O	-5.89	113.78	120.32
1	FR	140	PHE	CA-C-O	-5.89	113.78	120.32
1	BS	140	PHE	CA-C-O	-5.88	113.79	120.32
1	DJ	140	PHE	CA-C-O	-5.88	113.79	120.32
3	DV	113	GLN	CA-C-N	5.88	125.85	120.03
3	DV	113	GLN	C-N-CA	5.88	125.85	120.03
3	GZ	113	GLN	CA-C-N	5.88	125.85	120.03
3	GZ	113	GLN	C-N-CA	5.88	125.85	120.03
1	BL	140	PHE	CA-C-O	-5.87	113.80	120.32
1	CL	140	PHE	CA-C-O	-5.87	113.80	120.32
1	CM	140	PHE	CA-C-O	-5.87	113.80	120.32
1	DK	140	PHE	CA-C-O	-5.87	113.80	120.32
1	HJ	140	PHE	CA-C-O	-5.87	113.80	120.32
1	BW	140	PHE	CA-C-O	-5.86	113.81	120.32
1	CP	140	PHE	CA-C-O	-5.86	113.81	120.32
3	DU	113	GLN	CA-C-N	5.86	125.83	120.03
3	DU	113	GLN	C-N-CA	5.86	125.83	120.03
3	FL	113	GLN	CA-C-N	5.86	125.83	120.03
3	FL	113	GLN	C-N-CA	5.86	125.83	120.03
1	EW	140	PHE	CA-C-O	-5.86	113.81	120.32
1	EF	140	PHE	CA-C-O	-5.86	113.82	120.32
1	FU	140	PHE	CA-C-O	-5.85	113.82	120.32
1	HI	140	PHE	CA-C-O	-5.85	113.83	120.32
1	EY	140	PHE	CA-C-O	-5.85	113.83	120.32
3	DA	113	GLN	CA-C-N	5.84	125.82	120.03
3	DA	113	GLN	C-N-CA	5.84	125.82	120.03
3	AO	113	GLN	CA-C-N	5.84	125.81	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AO	113	GLN	C-N-CA	5.84	125.81	120.03
3	BJ	113	GLN	CA-C-N	5.84	125.81	120.03
3	BJ	113	GLN	C-N-CA	5.84	125.81	120.03
3	EQ	113	GLN	CA-C-N	5.84	125.81	120.03
3	EQ	113	GLN	C-N-CA	5.84	125.81	120.03
1	FA	140	PHE	CA-C-O	-5.84	113.84	120.32
1	HK	140	PHE	CA-C-O	-5.84	113.84	120.32
3	GE	113	GLN	CA-C-N	5.83	125.80	120.03
3	GE	113	GLN	C-N-CA	5.83	125.80	120.03
1	EB	140	PHE	CA-C-O	-5.82	113.86	120.32
1	DI	140	PHE	CA-C-O	-5.82	113.86	120.32
1	FS	140	PHE	CA-C-O	-5.82	113.86	120.32
1	FT	140	PHE	CA-C-O	-5.82	113.86	120.32
1	BT	140	PHE	CA-C-O	-5.81	113.87	120.32
1	AG	140	PHE	CA-C-O	-5.81	113.87	120.32
1	FC	140	PHE	CA-C-O	-5.79	113.89	120.32
1	GN	140	PHE	CA-C-O	-5.79	113.89	120.32
1	CR	140	PHE	CA-C-O	-5.79	113.90	120.32
3	EP	113	GLN	CA-C-N	5.79	125.76	120.03
3	EP	113	GLN	C-N-CA	5.79	125.76	120.03
3	BO	113	GLN	CA-C-N	5.78	125.76	120.03
3	BO	113	GLN	C-N-CA	5.78	125.76	120.03
3	CY	113	GLN	CA-C-N	5.78	125.76	120.03
3	CY	113	GLN	C-N-CA	5.78	125.76	120.03
3	EU	113	GLN	CA-C-N	5.76	125.73	120.03
3	EU	113	GLN	C-N-CA	5.76	125.73	120.03
3	DT	113	GLN	CA-C-N	5.73	125.70	120.03
3	DT	113	GLN	C-N-CA	5.73	125.70	120.03
2	FQ	281	PRO	CA-C-N	5.59	127.71	120.44
2	FQ	281	PRO	C-N-CA	5.59	127.71	120.44
1	GR	34	MET	N-CA-C	5.39	118.19	109.40
1	EI	34	MET	N-CA-C	5.39	118.18	109.40
1	FV	34	MET	N-CA-C	5.38	118.23	109.24
2	BP	281	PRO	CA-C-N	5.38	127.76	120.44
2	BP	281	PRO	C-N-CA	5.38	127.76	120.44
1	BB	34	MET	N-CA-C	5.38	118.17	109.40
1	FR	140	PHE	O-C-N	-5.37	117.03	123.31
1	FC	34	MET	N-CA-C	5.37	118.15	109.40
1	BW	34	MET	N-CA-C	5.37	118.14	109.40
1	HL	34	MET	N-CA-C	5.37	118.15	109.40
1	FA	34	MET	N-CA-C	5.36	118.14	109.40
1	GR	102	TYR	N-CA-C	-5.36	101.23	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FB	34	MET	N-CA-C	5.36	118.14	109.40
1	BM	34	MET	N-CA-C	5.36	118.14	109.40
1	BY	34	MET	N-CA-C	5.36	118.13	109.40
1	CQ	34	MET	N-CA-C	5.36	118.13	109.40
1	GM	34	MET	N-CA-C	5.36	118.13	109.40
1	FR	34	MET	N-CA-C	5.35	118.12	109.40
1	BV	34	MET	N-CA-C	5.35	118.12	109.40
1	CT	34	MET	N-CA-C	5.35	118.12	109.40
1	EY	34	MET	N-CA-C	5.35	118.12	109.40
1	FU	34	MET	N-CA-C	5.35	118.12	109.40
1	FX	34	MET	N-CA-C	5.35	118.12	109.40
1	CO	34	MET	N-CA-C	5.35	118.11	109.40
1	EJ	34	MET	N-CA-C	5.34	118.11	109.40
1	FM	34	MET	N-CA-C	5.34	118.11	109.40
1	BS	140	PHE	O-C-N	-5.34	117.06	123.31
1	BU	34	MET	N-CA-C	5.34	118.11	109.40
1	DB	34	MET	N-CA-C	5.34	118.11	109.40
1	CH	34	MET	N-CA-C	5.34	118.10	109.40
1	FA	102	TYR	N-CA-C	-5.34	101.08	109.25
1	BD	34	MET	N-CA-C	5.34	118.10	109.40
1	DL	34	MET	N-CA-C	5.34	118.10	109.40
1	EB	140	PHE	O-C-N	-5.34	117.06	123.31
1	FA	140	PHE	O-C-N	-5.34	117.07	123.31
1	GN	140	PHE	O-C-N	-5.34	117.06	123.31
2	GV	281	PRO	CA-C-N	5.34	127.70	120.44
2	GV	281	PRO	C-N-CA	5.34	127.70	120.44
1	DJ	140	PHE	O-C-N	-5.33	117.07	123.31
1	AG	34	MET	N-CA-C	5.33	118.09	109.40
1	AG	140	PHE	O-C-N	-5.33	117.07	123.31
1	BD	140	PHE	O-C-N	-5.33	117.08	123.27
1	DX	34	MET	N-CA-C	5.33	118.09	109.40
2	EV	281	PRO	CA-C-N	5.33	127.69	120.44
2	EV	281	PRO	C-N-CA	5.33	127.69	120.44
1	BS	34	MET	N-CA-C	5.33	118.14	109.24
1	HK	34	MET	N-CA-C	5.33	118.09	109.40
1	FD	34	MET	N-CA-C	5.33	118.14	109.24
1	GO	34	MET	N-CA-C	5.33	118.14	109.24
1	AR	34	MET	N-CA-C	5.33	118.08	109.40
1	EX	34	MET	N-CA-C	5.33	118.08	109.40
1	AI	140	PHE	O-C-N	-5.32	117.09	123.27
1	CR	34	MET	N-CA-C	5.32	118.08	109.40
1	DO	34	MET	N-CA-C	5.32	118.08	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	FS	34	MET	N-CA-C	5.32	118.08	109.40
1	HL	140	PHE	O-C-N	-5.32	117.08	123.31
1	BL	34	MET	N-CA-C	5.32	118.07	109.40
1	DN	34	MET	N-CA-C	5.32	118.07	109.40
1	AI	34	MET	N-CA-C	5.32	118.07	109.40
1	DC	34	MET	N-CA-C	5.32	118.07	109.40
2	DF	281	PRO	CA-C-N	5.32	127.67	120.44
2	DF	281	PRO	C-N-CA	5.32	127.67	120.44
2	EA	281	PRO	CA-C-N	5.32	127.67	120.44
2	EA	281	PRO	C-N-CA	5.32	127.67	120.44
1	GQ	34	MET	N-CA-C	5.32	118.07	109.40
1	HI	34	MET	N-CA-C	5.32	118.07	109.40
1	BC	34	MET	N-CA-C	5.32	118.12	109.24
1	CM	140	PHE	O-C-N	-5.32	117.09	123.31
1	CR	140	PHE	O-C-N	-5.32	117.09	123.31
1	EW	34	MET	N-CA-C	5.32	118.06	109.40
1	FT	34	MET	N-CA-C	5.32	118.11	109.24
1	FT	140	PHE	O-C-N	-5.32	117.09	123.31
1	BX	34	MET	N-CA-C	5.31	118.11	109.24
1	DK	34	MET	N-CA-C	5.31	118.06	109.40
1	ER	102	TYR	N-CA-C	-5.31	101.12	109.25
1	GH	34	MET	N-CA-C	5.31	118.06	109.40
1	HC	34	MET	N-CA-C	5.31	118.06	109.40
1	GN	34	MET	N-CA-C	5.31	118.06	109.40
1	DW	102	TYR	N-CA-C	-5.31	101.12	109.25
1	EE	34	MET	N-CA-C	5.31	118.11	109.24
1	EF	140	PHE	O-C-N	-5.31	117.10	123.31
1	BT	34	MET	N-CA-C	5.31	118.06	109.40
1	DH	34	MET	N-CA-C	5.31	118.05	109.40
1	DJ	34	MET	N-CA-C	5.31	118.06	109.40
1	DW	34	MET	N-CA-C	5.31	118.06	109.40
1	ES	34	MET	N-CA-C	5.31	118.06	109.40
1	EY	140	PHE	O-C-N	-5.31	117.10	123.31
1	EZ	34	MET	N-CA-C	5.31	118.11	109.24
1	BA	34	MET	N-CA-C	5.31	118.10	109.24
1	BW	140	PHE	O-C-N	-5.31	117.10	123.31
1	CN	34	MET	N-CA-C	5.31	118.10	109.24
1	CP	34	MET	N-CA-C	5.31	118.05	109.40
1	GP	34	MET	N-CA-C	5.31	118.05	109.40
1	HJ	34	MET	N-CA-C	5.31	118.11	109.24
1	AH	34	MET	N-CA-C	5.30	118.10	109.24
1	DG	34	MET	N-CA-C	5.30	118.10	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EF	34	MET	N-CA-C	5.30	118.05	109.40
1	EG	34	MET	N-CA-C	5.30	118.05	109.40
1	FE	34	MET	N-CA-C	5.30	118.05	109.40
1	CS	34	MET	N-CA-C	5.30	118.10	109.24
1	DG	140	PHE	O-C-N	-5.30	117.11	123.31
1	ED	34	MET	N-CA-C	5.30	118.09	109.24
1	DI	34	MET	N-CA-C	5.30	118.09	109.24
1	ER	34	MET	N-CA-C	5.30	118.03	109.40
1	AR	140	PHE	O-C-N	-5.30	117.07	123.27
1	CP	140	PHE	O-C-N	-5.30	117.11	123.31
1	FN	34	MET	N-CA-C	5.30	118.03	109.40
1	EX	102	TYR	N-CA-C	-5.30	101.15	109.25
1	FC	102	TYR	N-CA-C	-5.29	101.15	109.25
2	GL	281	PRO	CA-C-N	5.29	127.64	120.44
2	GL	281	PRO	C-N-CA	5.29	127.64	120.44
1	CG	34	MET	N-CA-C	5.29	118.03	109.40
1	FW	34	MET	N-CA-C	5.29	118.03	109.40
1	HJ	140	PHE	O-C-N	-5.29	117.12	123.31
1	BC	140	PHE	O-C-N	-5.29	117.13	123.27
1	FM	102	TYR	N-CA-C	-5.29	101.16	109.25
1	GQ	102	TYR	N-CA-C	-5.29	101.16	109.25
2	AU	281	PRO	CA-C-N	5.29	127.63	120.44
2	AU	281	PRO	C-N-CA	5.29	127.63	120.44
1	CM	34	MET	N-CA-C	5.29	118.02	109.40
1	BT	140	PHE	O-C-N	-5.28	117.13	123.31
1	GI	34	MET	N-CA-C	5.28	118.01	109.40
1	FU	140	PHE	O-C-N	-5.28	117.13	123.31
1	CH	102	TYR	N-CA-C	-5.28	101.17	109.25
1	DL	102	TYR	N-CA-C	-5.28	101.17	109.25
1	DK	102	TYR	N-CA-C	-5.28	101.17	109.25
1	EH	34	MET	N-CA-C	5.28	118.00	109.40
1	BB	140	PHE	O-C-N	-5.28	117.14	123.31
1	AG	102	TYR	N-CA-C	-5.28	101.18	109.25
2	BN	281	PRO	CA-C-N	5.28	127.78	120.29
2	BN	281	PRO	C-N-CA	5.28	127.78	120.29
1	DC	102	TYR	N-CA-C	-5.27	101.18	109.25
1	FC	140	PHE	O-C-N	-5.27	117.14	123.31
1	FX	140	PHE	O-C-N	-5.27	117.14	123.31
1	BA	102	TYR	N-CA-C	-5.27	101.18	109.25
1	BM	102	TYR	N-CA-C	-5.27	101.18	109.25
1	CQ	102	TYR	N-CA-C	-5.27	101.18	109.25
1	EC	34	MET	N-CA-C	5.27	118.00	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ED	102	TYR	N-CA-C	-5.27	101.18	109.25
1	CL	34	MET	N-CA-C	5.27	117.99	109.40
1	EG	140	PHE	O-C-N	-5.27	117.10	123.27
1	FD	102	TYR	N-CA-C	-5.27	101.19	109.25
1	FT	102	TYR	N-CA-C	-5.27	101.19	109.25
1	EB	34	MET	N-CA-C	5.27	118.03	109.24
1	GI	140	PHE	O-C-N	-5.27	117.11	123.27
1	GM	140	PHE	O-C-N	-5.27	117.15	123.31
1	GQ	172	SER	CA-C-N	-5.27	114.14	121.99
1	GQ	172	SER	C-N-CA	-5.27	114.14	121.99
1	CM	102	TYR	N-CA-C	-5.27	101.19	109.25
1	BY	102	TYR	N-CA-C	-5.26	101.19	109.25
1	CR	102	TYR	N-CA-C	-5.26	101.20	109.25
1	CS	102	TYR	N-CA-C	-5.26	101.20	109.25
1	FN	102	TYR	N-CA-C	-5.26	101.20	109.25
1	FW	140	PHE	O-C-N	-5.26	117.11	123.27
1	CT	102	TYR	N-CA-C	-5.26	101.20	109.25
1	FN	140	PHE	O-C-N	-5.26	117.12	123.27
1	HH	140	PHE	O-C-N	-5.26	117.16	123.31
1	BC	102	TYR	N-CA-C	-5.26	101.20	109.25
1	CL	140	PHE	O-C-N	-5.26	117.16	123.31
1	DX	140	PHE	O-C-N	-5.26	117.12	123.27
1	GH	172	SER	CA-C-N	-5.26	114.16	121.99
1	GH	172	SER	C-N-CA	-5.26	114.16	121.99
1	FS	102	TYR	N-CA-C	-5.26	101.21	109.25
1	EE	140	PHE	O-C-N	-5.26	117.16	123.31
1	EX	140	PHE	O-C-N	-5.26	117.16	123.31
1	GI	102	TYR	N-CA-C	-5.26	101.21	109.25
1	HC	102	TYR	N-CA-C	-5.26	101.21	109.25
1	HC	172	SER	CA-C-N	-5.26	114.16	121.99
1	HC	172	SER	C-N-CA	-5.26	114.16	121.99
1	BU	102	TYR	N-CA-C	-5.25	101.21	109.25
1	BV	102	TYR	N-CA-C	-5.25	101.21	109.25
1	CP	102	TYR	N-CA-C	-5.25	101.21	109.25
1	FS	140	PHE	O-C-N	-5.25	117.16	123.31
1	GN	102	TYR	N-CA-C	-5.25	101.21	109.25
1	HK	140	PHE	O-C-N	-5.25	117.17	123.31
1	BA	140	PHE	O-C-N	-5.25	117.13	123.27
1	EG	102	TYR	N-CA-C	-5.25	101.22	109.25
1	EW	140	PHE	O-C-N	-5.25	117.17	123.31
1	GO	140	PHE	O-C-N	-5.25	117.17	123.31
1	GP	140	PHE	O-C-N	-5.25	117.17	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BL	140	PHE	O-C-N	-5.25	117.17	123.31
2	CK	281	PRO	CA-C-N	5.25	127.58	120.44
2	CK	281	PRO	C-N-CA	5.25	127.58	120.44
1	DX	102	TYR	N-CA-C	-5.25	101.22	109.25
1	GP	102	TYR	N-CA-C	-5.25	101.22	109.25
1	CG	102	TYR	N-CA-C	-5.25	101.22	109.25
1	AH	140	PHE	O-C-N	-5.24	117.19	123.27
1	ES	102	TYR	N-CA-C	-5.24	101.23	109.25
1	FR	102	TYR	N-CA-C	-5.24	101.23	109.25
1	FV	140	PHE	O-C-N	-5.24	117.17	123.31
1	FW	102	TYR	N-CA-C	-5.24	101.23	109.25
1	HI	102	TYR	N-CA-C	-5.24	101.23	109.25
1	EB	102	TYR	N-CA-C	-5.24	101.23	109.25
1	EC	102	TYR	N-CA-C	-5.24	101.23	109.25
2	EN	281	PRO	CA-C-N	5.24	127.73	120.29
2	EN	281	PRO	C-N-CA	5.24	127.73	120.29
1	HL	102	TYR	N-CA-C	-5.24	101.23	109.25
1	AR	102	TYR	N-CA-C	-5.24	101.23	109.25
1	CG	140	PHE	O-C-N	-5.24	117.18	123.31
1	EJ	102	TYR	N-CA-C	-5.24	101.23	109.25
1	FM	140	PHE	O-C-N	-5.24	117.18	123.31
1	GM	102	TYR	N-CA-C	-5.24	101.23	109.25
1	HH	102	TYR	N-CA-C	-5.24	101.23	109.25
1	GH	102	TYR	N-CA-C	-5.24	101.24	109.25
1	FU	102	TYR	N-CA-C	-5.24	101.23	109.25
1	CN	102	TYR	N-CA-C	-5.24	101.24	109.25
1	DM	34	MET	N-CA-C	5.24	117.94	109.40
1	HJ	102	TYR	N-CA-C	-5.24	101.24	109.25
1	BX	102	TYR	N-CA-C	-5.24	101.24	109.25
1	CO	102	TYR	N-CA-C	-5.24	101.24	109.25
2	DR	281	PRO	CA-C-N	5.24	127.72	120.29
2	DR	281	PRO	C-N-CA	5.24	127.72	120.29
1	HH	34	MET	N-CA-C	5.24	117.98	109.24
1	BL	102	TYR	N-CA-C	-5.23	101.24	109.25
1	DN	102	TYR	N-CA-C	-5.23	101.24	109.25
1	HI	140	PHE	O-C-N	-5.23	117.19	123.31
1	BW	102	TYR	N-CA-C	-5.23	101.24	109.25
1	GR	140	PHE	O-C-N	-5.23	117.15	123.27
1	ER	140	PHE	O-C-N	-5.23	117.19	123.31
1	ER	172	SER	CA-C-N	-5.23	114.20	121.99
1	ER	172	SER	C-N-CA	-5.23	114.20	121.99
1	DC	140	PHE	O-C-N	-5.23	117.15	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CQ	140	PHE	O-C-N	-5.23	117.15	123.27
1	DO	102	TYR	N-CA-C	-5.23	101.25	109.25
1	CN	140	PHE	O-C-N	-5.22	117.20	123.31
1	DG	102	TYR	N-CA-C	-5.22	101.26	109.25
1	DM	102	TYR	N-CA-C	-5.22	101.25	109.25
1	EZ	102	TYR	N-CA-C	-5.22	101.25	109.25
2	GJ	281	PRO	CA-C-N	5.22	127.71	120.29
2	GJ	281	PRO	C-N-CA	5.22	127.71	120.29
1	DI	140	PHE	O-C-N	-5.22	117.20	123.31
1	EC	140	PHE	O-C-N	-5.22	117.20	123.31
1	AH	102	TYR	N-CA-C	-5.22	101.26	109.25
1	DI	102	TYR	N-CA-C	-5.22	101.27	109.25
1	ED	140	PHE	O-C-N	-5.22	117.20	123.31
1	FX	102	TYR	N-CA-C	-5.22	101.26	109.25
1	DK	140	PHE	O-C-N	-5.22	117.20	123.31
1	DH	102	TYR	N-CA-C	-5.22	101.27	109.25
1	DJ	102	TYR	N-CA-C	-5.22	101.27	109.25
1	DL	140	PHE	O-C-N	-5.22	117.17	123.27
1	EE	102	TYR	N-CA-C	-5.22	101.27	109.25
1	EI	140	PHE	O-C-N	-5.22	117.22	123.27
1	EY	102	TYR	N-CA-C	-5.22	101.27	109.25
1	BS	102	TYR	N-CA-C	-5.21	101.27	109.25
1	CL	102	TYR	N-CA-C	-5.21	101.27	109.25
1	EF	102	TYR	N-CA-C	-5.21	101.27	109.25
1	EH	102	TYR	N-CA-C	-5.21	101.27	109.25
1	EH	140	PHE	O-C-N	-5.21	117.21	123.31
1	FB	102	TYR	N-CA-C	-5.21	101.28	109.25
1	FD	140	PHE	O-C-N	-5.21	117.10	123.30
1	GQ	140	PHE	O-C-N	-5.21	117.21	123.31
1	BB	102	TYR	N-CA-C	-5.21	101.28	109.25
1	FE	102	TYR	N-CA-C	-5.21	101.28	109.25
1	FV	102	TYR	N-CA-C	-5.21	101.28	109.25
1	GO	102	TYR	N-CA-C	-5.21	101.28	109.25
1	DB	102	TYR	N-CA-C	-5.21	101.28	109.25
2	DQ	281	PRO	CA-C-N	5.21	127.68	120.29
2	DQ	281	PRO	C-N-CA	5.21	127.68	120.29
1	FB	140	PHE	O-C-N	-5.21	117.18	123.27
2	BF	281	PRO	CA-C-N	5.20	127.68	120.29
2	BF	281	PRO	C-N-CA	5.20	127.68	120.29
2	GW	281	PRO	CA-C-N	5.20	127.68	120.29
2	GW	281	PRO	C-N-CA	5.20	127.68	120.29
2	FO	281	PRO	CA-C-N	5.20	127.67	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	FO	281	PRO	C-N-CA	5.20	127.67	120.29
1	BD	102	TYR	N-CA-C	-5.20	101.30	109.25
1	EZ	140	PHE	O-C-N	-5.20	117.23	123.31
2	BE	281	PRO	CA-C-N	5.20	127.67	120.29
2	BE	281	PRO	C-N-CA	5.20	127.67	120.29
2	CA	281	PRO	CA-C-N	5.20	127.67	120.29
2	CA	281	PRO	C-N-CA	5.20	127.67	120.29
1	EJ	140	PHE	O-C-N	-5.20	117.12	123.30
1	FE	140	PHE	O-C-N	-5.20	117.12	123.30
1	HK	102	TYR	N-CA-C	-5.20	101.30	109.25
2	DD	281	PRO	CA-C-N	5.19	127.67	120.29
2	DD	281	PRO	C-N-CA	5.19	127.67	120.29
1	EI	102	TYR	N-CA-C	-5.19	101.30	109.25
1	GH	140	PHE	O-C-N	-5.19	117.24	123.31
2	EK	281	PRO	CA-C-N	5.19	127.66	120.29
2	EK	281	PRO	C-N-CA	5.19	127.66	120.29
1	ES	140	PHE	O-C-N	-5.19	117.20	123.27
1	CO	140	PHE	O-C-N	-5.19	117.24	123.31
1	BT	102	TYR	N-CA-C	-5.19	101.31	109.25
2	BZ	281	PRO	CA-C-N	5.19	127.66	120.29
2	BZ	281	PRO	C-N-CA	5.19	127.66	120.29
1	CS	140	PHE	O-C-N	-5.19	117.25	123.27
2	DY	281	PRO	CA-C-N	5.19	127.66	120.29
2	DY	281	PRO	C-N-CA	5.19	127.66	120.29
1	DB	140	PHE	O-C-N	-5.19	117.24	123.31
1	DM	140	PHE	O-C-N	-5.18	117.25	123.31
2	DP	281	PRO	CA-C-N	5.18	127.65	120.29
2	DP	281	PRO	C-N-CA	5.18	127.65	120.29
1	EW	102	TYR	N-CA-C	-5.18	101.32	109.25
1	CH	140	PHE	O-C-N	-5.18	117.21	123.27
2	GB	281	PRO	CA-C-N	5.18	127.64	120.29
2	GB	281	PRO	C-N-CA	5.18	127.64	120.29
2	GA	281	PRO	CA-C-N	5.17	127.64	120.29
2	GA	281	PRO	C-N-CA	5.17	127.64	120.29
2	EL	281	PRO	CA-C-N	5.17	127.64	120.29
2	EL	281	PRO	C-N-CA	5.17	127.64	120.29
1	BV	140	PHE	O-C-N	-5.17	117.22	123.27
2	FF	281	PRO	CA-C-N	5.17	127.64	120.29
2	FF	281	PRO	C-N-CA	5.17	127.64	120.29
1	BL	172	SER	CA-C-N	-5.17	114.29	121.99
1	BL	172	SER	C-N-CA	-5.17	114.29	121.99
2	CI	281	PRO	CA-C-N	5.17	127.63	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CI	281	PRO	C-N-CA	5.17	127.63	120.29
1	DH	140	PHE	O-C-N	-5.17	117.26	123.31
2	CB	281	PRO	CA-C-N	5.16	127.62	120.29
2	CB	281	PRO	C-N-CA	5.16	127.62	120.29
2	BH	281	PRO	CA-C-N	5.16	127.61	120.29
2	BH	281	PRO	C-N-CA	5.16	127.61	120.29
2	CW	281	PRO	CA-C-N	5.16	127.62	120.29
2	CW	281	PRO	C-N-CA	5.16	127.62	120.29
2	CX	281	PRO	CA-C-N	5.16	127.61	120.29
2	CX	281	PRO	C-N-CA	5.16	127.61	120.29
1	CT	140	PHE	O-C-N	-5.16	117.17	123.30
1	BX	140	PHE	O-C-N	-5.15	117.17	123.30
1	HC	140	PHE	O-C-N	-5.15	117.28	123.31
2	FH	281	PRO	CA-C-N	5.15	127.60	120.29
2	FH	281	PRO	C-N-CA	5.15	127.60	120.29
2	HE	281	PRO	CA-C-N	5.15	127.60	120.29
2	HE	281	PRO	C-N-CA	5.15	127.60	120.29
1	DW	140	PHE	O-C-N	-5.15	117.29	123.31
2	DS	281	PRO	CA-C-N	5.14	127.59	120.29
2	DS	281	PRO	C-N-CA	5.14	127.59	120.29
2	CU	281	PRO	CA-C-N	5.14	127.59	120.29
2	CU	281	PRO	C-N-CA	5.14	127.59	120.29
1	BM	140	PHE	O-C-N	-5.14	117.25	123.27
2	AL	281	PRO	CA-C-N	5.13	127.58	120.29
2	AL	281	PRO	C-N-CA	5.13	127.58	120.29
3	CJ	59	ASP	N-CA-C	-5.13	105.86	111.82
1	BY	140	PHE	O-C-N	-5.13	117.19	123.30
2	ET	281	PRO	CA-C-N	5.13	127.58	120.29
2	ET	281	PRO	C-N-CA	5.13	127.58	120.29
1	DO	140	PHE	O-C-N	-5.13	117.20	123.30
2	FI	281	PRO	CA-C-N	5.13	127.57	120.29
2	FI	281	PRO	C-N-CA	5.13	127.57	120.29
2	CV	281	PRO	CA-C-N	5.12	127.56	120.29
2	CV	281	PRO	C-N-CA	5.12	127.56	120.29
3	EO	59	ASP	N-CA-C	-5.11	105.89	111.82
1	BU	140	PHE	O-C-N	-5.11	117.33	123.31
2	GC	281	PRO	CA-C-N	5.11	127.54	120.29
2	GC	281	PRO	C-N-CA	5.11	127.54	120.29
3	DE	59	ASP	N-CA-C	-5.10	105.90	111.82
3	BJ	59	ASP	N-CA-C	-5.10	105.90	111.82
3	FJ	143	ALA	CA-C-N	5.10	124.76	119.56
3	FJ	143	ALA	C-N-CA	5.10	124.76	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AM	281	PRO	CA-C-N	5.10	127.53	120.29
2	AM	281	PRO	C-N-CA	5.10	127.53	120.29
2	BG	281	PRO	CA-C-N	5.09	127.53	120.29
2	BG	281	PRO	C-N-CA	5.09	127.53	120.29
2	CC	281	PRO	CA-C-N	5.09	127.52	120.29
2	CC	281	PRO	C-N-CA	5.09	127.52	120.29
2	EM	281	PRO	CA-C-N	5.09	127.52	120.29
2	EM	281	PRO	C-N-CA	5.09	127.52	120.29
2	FG	281	PRO	CA-C-N	5.09	127.52	120.29
2	FG	281	PRO	C-N-CA	5.09	127.52	120.29
3	AO	143	ALA	CA-C-N	5.09	124.70	119.56
3	AO	143	ALA	C-N-CA	5.09	124.70	119.56
3	DV	59	ASP	N-CA-C	-5.08	105.93	111.82
3	FJ	59	ASP	N-CA-C	-5.08	105.93	111.82
3	DA	59	ASP	N-CA-C	-5.08	105.93	111.82
3	CF	59	ASP	N-CA-C	-5.07	105.94	111.82
3	DT	59	ASP	N-CA-C	-5.06	105.95	111.82
3	FL	59	ASP	N-CA-C	-5.06	105.95	111.82
3	BO	59	ASP	N-CA-C	-5.06	105.95	111.82
3	BJ	143	ALA	CA-C-N	5.05	124.66	119.56
3	BJ	143	ALA	C-N-CA	5.05	124.66	119.56
1	DN	140	PHE	O-C-N	-5.05	117.29	123.30
3	EQ	59	ASP	N-CA-C	-5.05	105.96	111.82
3	FP	59	ASP	N-CA-C	-5.05	105.97	111.82
3	BK	59	ASP	N-CA-C	-5.05	105.97	111.82
1	DM	172	SER	CA-C-N	-5.04	114.00	122.17
1	DM	172	SER	C-N-CA	-5.04	114.00	122.17
3	DU	143	ALA	CA-C-N	5.04	124.65	119.56
3	DU	143	ALA	C-N-CA	5.04	124.65	119.56
3	HF	59	ASP	N-CA-C	-5.04	105.97	111.82
3	AO	59	ASP	N-CA-C	-5.04	105.97	111.82
3	GG	59	ASP	N-CA-C	-5.04	105.97	111.82
3	HB	59	ASP	N-CA-C	-5.04	105.98	111.82
3	GZ	143	ALA	CA-C-N	5.04	124.70	119.56
3	GZ	143	ALA	C-N-CA	5.04	124.70	119.56
3	EU	59	ASP	N-CA-C	-5.04	105.98	111.82
3	GK	59	ASP	N-CA-C	-5.03	105.99	111.82
3	EP	143	ALA	CA-C-N	5.03	124.69	119.56
3	EP	143	ALA	C-N-CA	5.03	124.69	119.56
1	EY	172	SER	CA-C-N	-5.02	114.03	122.17
1	EY	172	SER	C-N-CA	-5.02	114.03	122.17
3	DZ	59	ASP	N-CA-C	-5.01	106.00	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CJ	143	ALA	CA-C-N	5.01	124.67	119.56
3	CJ	143	ALA	C-N-CA	5.01	124.67	119.56
3	CZ	59	ASP	N-CA-C	-5.01	105.92	112.23
3	GE	59	ASP	N-CA-C	-5.01	106.01	111.82
3	GZ	59	ASP	N-CA-C	-5.01	105.92	112.23
3	CE	143	ALA	CA-C-N	5.01	124.67	119.56
3	CE	143	ALA	C-N-CA	5.01	124.67	119.56
3	CZ	143	ALA	CA-C-N	5.00	124.61	119.56
3	CZ	143	ALA	C-N-CA	5.00	124.61	119.56
1	BB	172	SER	CA-C-N	-5.00	114.07	122.17
1	BB	172	SER	C-N-CA	-5.00	114.07	122.17

There are no chirality outliers.

All (166) planarity outliers are listed below:

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

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

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

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	3	0
1	AH	1060	0	295	1	0
1	AI	1060	0	295	1	0
1	AR	1060	0	295	3	0
1	BA	1060	0	295	6	0
1	BB	1060	0	295	2	0
1	BC	1060	0	295	4	0
1	BD	1060	0	295	4	0
1	BL	1060	0	295	3	0
1	BM	1060	0	295	4	0
1	BS	1060	0	295	1	0
1	BT	1060	0	295	3	0
1	BU	1060	0	295	4	0
1	BV	1060	0	295	5	0
1	BW	1060	0	295	3	0
1	BX	1060	0	295	5	0
1	BY	1060	0	295	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CG	1060	0	295	4	0
1	CH	1060	0	295	3	0
1	CL	1060	0	295	3	0
1	CM	1060	0	295	4	0
1	CN	1060	0	295	2	0
1	CO	1060	0	295	3	0
1	CP	1060	0	295	1	0
1	CQ	1060	0	295	4	0
1	CR	1060	0	295	3	0
1	CS	1060	0	295	4	0
1	CT	1060	0	295	7	0
1	DB	1060	0	295	3	0
1	DC	1060	0	295	3	0
1	DG	1060	0	295	6	0
1	DH	1060	0	295	3	0
1	DI	1060	0	295	1	0
1	DJ	1060	0	295	3	0
1	DK	1060	0	295	2	0
1	DL	1060	0	295	4	0
1	DM	1060	0	295	3	0
1	DN	1060	0	295	3	0
1	DO	1060	0	295	4	0
1	DW	1060	0	295	3	0
1	DX	1060	0	295	2	0
1	EB	1060	0	295	5	0
1	EC	1060	0	295	3	0
1	ED	1060	0	295	2	0
1	EE	1060	0	295	3	0
1	EF	1060	0	295	4	0
1	EG	1060	0	295	6	0
1	EH	1060	0	295	3	0
1	EI	1060	0	295	3	0
1	EJ	1060	0	295	7	0
1	ER	1060	0	295	3	0
1	ES	1060	0	295	4	0
1	EW	1060	0	295	5	0
1	EX	1060	0	295	4	0
1	EY	1060	0	295	2	0
1	EZ	1060	0	295	2	0
1	FA	1060	0	295	2	0
1	FB	1060	0	295	4	0
1	FC	1060	0	295	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FD	1060	0	295	3	0
1	FE	1060	0	295	5	0
1	FM	1060	0	295	3	0
1	FN	1060	0	295	3	0
1	FR	1060	0	295	5	0
1	FS	1060	0	295	4	0
1	FT	1060	0	295	2	0
1	FU	1060	0	295	2	0
1	FV	1060	0	295	4	0
1	FW	1060	0	295	5	0
1	FX	1060	0	295	3	0
1	GH	1060	0	295	4	0
1	GI	1060	0	295	3	0
1	GM	1060	0	295	5	0
1	GN	1060	0	295	4	0
1	GO	1060	0	295	2	0
1	GP	1060	0	295	2	0
1	GQ	1060	0	295	5	0
1	GR	1060	0	295	5	0
1	HC	1060	0	295	4	0
1	HH	1060	0	295	5	0
1	HI	1060	0	295	3	0
1	HJ	1060	0	295	1	0
1	HK	1060	0	295	2	0
1	HL	1060	0	295	1	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
2	CV	948	0	236	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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
3	DA	736	0	187	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	1	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	1	0
All	All	157148	0	41856	270	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 (270) 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:FD:8:ALA:O	1:FD:9:ALA:C	2.54	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:EB:10:ILE:C	1:EB:12:SER:H	2.20	0.50
1:CT:100:GLY:CA	1:DO:150:TRP:O	2.60	0.50
1:EJ:100:GLY:C	1:FE:150:TRP:O	2.55	0.49
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:CH:8:ALA:O	1:CH:9:ALA:C	2.56	0.48
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
2:AU:290:ILE:O	2:AU:291:ASN:C	2.56	0.47
1:DG:100:GLY:HA3	1:EB:150:TRP:O	2.14	0.47
1:BW:8:ALA:O	1:BW:9:ALA:C	2.55	0.47
1:GM:100:GLY:CA	1:HH:150:TRP:O	2.61	0.47
1:BC:100:GLY:C	1:BX:150:TRP:O	2.56	0.47
2:BZ:89:HIS:O	2:BZ:93:LYS:N	2.40	0.47
1:DC:8:ALA:O	1:DC:9:ALA:C	2.57	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:FC:8:ALA:O	1:FC:9:ALA:C	2.56	0.47
1:GN:100:GLY:HA3	1:HI:150:TRP:O	2.14	0.47
1:EH:8:ALA:O	1:EH:9:ALA:C	2.57	0.47
1:FW:193:ASP:O	1:FW:197:THR:N	2.38	0.47
1:CS:8:ALA:O	1:CS:9:ALA:C	2.55	0.47
1:DX:8:ALA:O	1:DX:9:ALA:C	2.57	0.46
1:EI:8:ALA:O	1:EI:9:ALA:C	2.53	0.46
1:CT:271:VAL:O	1:CT:272:ARG:C	2.59	0.46
1:DO:271:VAL:O	1:DO:272:ARG:C	2.59	0.46
1:EW:100:GLY:HA3	1:FR:150:TRP:O	2.16	0.46
1:CS:271:VAL:O	1:CS:272:ARG:C	2.58	0.46
1:AH:271:VAL:O	1:AH:272:ARG:C	2.59	0.46
1:DN:271:VAL:O	1:DN:272:ARG:C	2.59	0.46
1:BY:271:VAL:O	1:BY:272:ARG:C	2.59	0.46
1:GI:271:VAL:O	1:GI:272:ARG:C	2.59	0.46
1:GN:271:VAL:O	1:GN:272:ARG:C	2.59	0.46
1:HI:271:VAL:O	1:HI:272:ARG:C	2.59	0.46
1:BA:190:LYS:O	1:BA:194:ALA:N	2.39	0.46
1:CG:271:VAL:O	1:CG:272:ARG:C	2.59	0.46
1:DB:271:VAL:O	1:DB:272:ARG:C	2.59	0.46
1:EC:271:VAL:O	1:EC:272:ARG:C	2.59	0.46
1:FD:271:VAL:O	1:FD:272:ARG:C	2.58	0.46
1:EZ:271:VAL:O	1:EZ:272:ARG:C	2.59	0.46
1:CM:271:VAL:O	1:CM:272:ARG:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CN:271:VAL:O	1:CN:272:ARG:C	2.59	0.46
1:DH:271:VAL:O	1:DH:272:ARG:C	2.59	0.46
1:EB:271:VAL:O	1:EB:272:ARG:C	2.59	0.46
1:EC:100:GLY:HA3	1:EX:150:TRP:O	2.16	0.46
1:EX:271:VAL:O	1:EX:272:ARG:C	2.59	0.46
1:FS:271:VAL:O	1:FS:272:ARG:C	2.59	0.46
1:FX:271:VAL:O	1:FX:272:ARG:C	2.59	0.46
1:EI:271:VAL:O	1:EI:272:ARG:C	2.59	0.45
1:FN:111:GLN:O	1:FN:115:SER:N	2.42	0.45
1:FR:271:VAL:O	1:FR:272:ARG:C	2.59	0.45
1:GM:271:VAL:O	1:GM:272:ARG:C	2.59	0.45
1:BL:271:VAL:O	1:BL:272:ARG:C	2.59	0.45
1:DG:271:VAL:O	1:DG:272:ARG:C	2.59	0.45
1:AG:271:VAL:O	1:AG:272:ARG:C	2.59	0.45
1:BM:111:GLN:O	1:BM:115:SER:N	2.45	0.45
1:BX:271:VAL:O	1:BX:272:ARG:C	2.59	0.45
1:CL:271:VAL:O	1:CL:272:ARG:C	2.59	0.45
1:DI:271:VAL:O	1:DI:272:ARG:C	2.59	0.45
1:DL:190:LYS:O	1:DL:193:ASP:N	2.49	0.45
1:FM:189:ASP:O	1:FM:190:LYS:C	2.59	0.45
1:FN:271:VAL:O	1:FN:272:ARG:C	2.59	0.45
1:FW:271:VAL:O	1:FW:272:ARG:C	2.59	0.45
1:BC:271:VAL:O	1:BC:272:ARG:C	2.59	0.45
1:CH:271:VAL:O	1:CH:272:ARG:C	2.59	0.45
1:DK:271:VAL:O	1:DK:272:ARG:C	2.60	0.45
1:EH:271:VAL:O	1:EH:272:ARG:C	2.59	0.45
1:FC:271:VAL:O	1:FC:272:ARG:C	2.59	0.45
1:FE:271:VAL:O	1:FE:272:ARG:C	2.59	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:DJ:271:VAL:O	1:DJ:272:ARG:C	2.59	0.45
1:ES:271:VAL:O	1:ES:272:ARG:C	2.60	0.45
1:HC:271:VAL:O	1:HC:272:ARG:C	2.59	0.45
1:BB:271:VAL:O	1:BB:272:ARG:C	2.59	0.45
1:BU:271:VAL:O	1:BU:272:ARG:C	2.60	0.45
1:DM:271:VAL:O	1:DM:272:ARG:C	2.59	0.45
1:DX:271:VAL:O	1:DX:272:ARG:C	2.59	0.45
1:AR:271:VAL:O	1:AR:272:ARG:C	2.59	0.45
1:BD:271:VAL:O	1:BD:272:ARG:C	2.59	0.45
1:BV:271:VAL:O	1:BV:272:ARG:C	2.59	0.45
1:CP:271:VAL:O	1:CP:272:ARG:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DN:8:ALA:O	1:DN:9:ALA:C	2.57	0.45
1:DW:271:VAL:O	1:DW:272:ARG:C	2.59	0.45
1:EE:271:VAL:O	1:EE:272:ARG:C	2.60	0.45
1:FB:271:VAL:O	1:FB:272:ARG:C	2.59	0.45
1:EW:271:VAL:O	1:EW:272:ARG:C	2.59	0.45
1:GR:271:VAL:O	1:GR:272:ARG:C	2.59	0.45
1:EF:271:VAL:O	1:EF:272:ARG:C	2.60	0.45
1:FU:271:VAL:O	1:FU:272:ARG:C	2.60	0.45
1:BD:100:GLY:C	1:BY:150:TRP:O	2.60	0.45
1:DL:193:ASP:O	1:DL:197:THR:N	2.39	0.45
1:FA:271:VAL:O	1:FA:272:ARG:C	2.60	0.45
1:EY:271:VAL:O	1:EY:272:ARG:C	2.59	0.45
1:GP:271:VAL:O	1:GP:272:ARG:C	2.60	0.45
1:BS:271:VAL:O	1:BS:272:ARG:C	2.59	0.45
1:EG:271:VAL:O	1:EG:272:ARG:C	2.59	0.45
1:ER:271:VAL:O	1:ER:272:ARG:C	2.59	0.45
1:GH:178:GLN:O	1:GH:179:SER:C	2.60	0.45
1:FV:271:VAL:O	1:FV:272:ARG:C	2.60	0.45
1:GQ:271:VAL:O	1:GQ:272:ARG:C	2.60	0.45
1:BA:271:VAL:O	1:BA:272:ARG:C	2.59	0.44
1:ED:271:VAL:O	1:ED:272:ARG:C	2.59	0.44
1:EJ:271:VAL:O	1:EJ:272:ARG:C	2.59	0.44
1:FT:271:VAL:O	1:FT:272:ARG:C	2.59	0.44
1:FW:190:LYS:O	1:FW:193:ASP:N	2.50	0.44
1:GO:271:VAL:O	1:GO:272:ARG:C	2.59	0.44
1:BM:271:VAL:O	1:BM:272:ARG:C	2.59	0.44
1:CO:271:VAL:O	1:CO:272:ARG:C	2.60	0.44
1:CQ:271:VAL:O	1:CQ:272:ARG:C	2.59	0.44
1:HJ:271:VAL:O	1:HJ:272:ARG:C	2.59	0.44
1:HL:271:VAL:O	1:HL:272:ARG:C	2.60	0.44
1:BW:271:VAL:O	1:BW:272:ARG:C	2.59	0.44
1:FM:271:VAL:O	1:FM:272:ARG:C	2.59	0.44
1:DB:189:ASP:O	1:DB:190:LYS:C	2.59	0.44
1:CR:271:VAL:O	1:CR:272:ARG:C	2.59	0.44
1:DL:8:ALA:O	1:DL:9:ALA:C	2.58	0.44
1:EG:193:ASP:O	1:EG:197:THR:N	2.39	0.44
1:BA:8:ALA:O	1:BA:9:ALA:C	2.59	0.44
1:BT:271:VAL:O	1:BT:272:ARG:C	2.60	0.44
1:DC:271:VAL:O	1:DC:272:ARG:C	2.59	0.44
1:DL:271:VAL:O	1:DL:272:ARG:C	2.59	0.44
1:GH:271:VAL:O	1:GH:272:ARG:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HH:271:VAL:O	1:HH:272:ARG:C	2.59	0.44
1:AI:271:VAL:O	1:AI:272:ARG:C	2.59	0.44
1:BV:8:ALA:O	1:BV:9:ALA:C	2.61	0.44
1:GR:193:ASP:O	1:GR:197:THR:N	2.43	0.44
1:HK:271:VAL:O	1:HK:272:ARG:C	2.60	0.44
1:CG:178:GLN:O	1:CG:179:SER:C	2.60	0.44
1:BX:8:ALA:O	1:BX:9:ALA:C	2.59	0.43
1:DW:178:GLN:O	1:DW:179:SER:C	2.61	0.43
1:ER:178:GLN:O	1:ER:179:SER:C	2.61	0.43
1:FM:178:GLN:O	1:FM:179:SER:C	2.61	0.43
1:CQ:8:ALA:O	1:CQ:9:ALA:C	2.59	0.43
1:FX:8:ALA:O	1:FX:9:ALA:C	2.59	0.43
1:HC:178:GLN:O	1:HC:179:SER:C	2.61	0.43
1:CG:189:ASP:O	1:CG:190:LYS:C	2.61	0.43
1:BC:8:ALA:O	1:BC:9:ALA:C	2.60	0.43
1:GI:111:GLN:O	1:GI:115:SER:N	2.45	0.43
1:EB:178:GLN:O	1:EB:179:SER:C	2.62	0.43
1:FS:100:GLY:HA3	1:GN:150:TRP:O	2.19	0.43
1:DB:178:GLN:O	1:DB:179:SER:C	2.61	0.43
1:DG:8:ALA:O	1:DG:9:ALA:C	2.61	0.43
1:CQ:178:GLN:O	1:CQ:179:SER:C	2.62	0.43
1:EE:8:ALA:O	1:EE:9:ALA:C	2.61	0.43
1:EG:8:ALA:O	1:EG:9:ALA:C	2.59	0.43
1:HC:189:ASP:O	1:HC:190:LYS:C	2.60	0.43
1:EY:178:GLN:O	1:EY:179:SER:C	2.62	0.43
1:BX:178:GLN:O	1:BX:179:SER:C	2.62	0.42
1:ER:189:ASP:O	1:ER:190:LYS:C	2.61	0.42
1:DJ:8:ALA:O	1:DJ:9:ALA:C	2.62	0.42
1:FE:178:GLN:O	1:FE:179:SER:C	2.63	0.42
1:BA:35:ARG:N	1:BA:241:ARG:O	2.52	0.42
1:CR:189:ASP:O	1:CR:190:LYS:C	2.62	0.42
1:GH:189:ASP:O	1:GH:190:LYS:C	2.60	0.42
1:GM:178:GLN:O	1:GM:179:SER:C	2.63	0.42
1:GQ:190:LYS:O	1:GQ:193:ASP:N	2.53	0.42
1:CL:178:GLN:O	1:CL:179:SER:C	2.63	0.42
1:CR:8:ALA:O	1:CR:9:ALA:C	2.58	0.42
1:DG:178:GLN:O	1:DG:179:SER:C	2.63	0.42
1:DW:189:ASP:O	1:DW:190:LYS:C	2.61	0.42
1:FV:8:ALA:O	1:FV:9:ALA:C	2.61	0.42
1:BT:8:ALA:O	1:BT:9:ALA:C	2.60	0.42
1:CT:8:ALA:O	1:CT:9:ALA:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DM:8:ALA:O	1:DM:9:ALA:C	2.58	0.42
1:EH:189:ASP:O	1:EH:190:LYS:C	2.63	0.42
1:FS:178:GLN:O	1:FS:179:SER:C	2.63	0.42
1:GN:178:GLN:O	1:GN:179:SER:C	2.63	0.42
1:BL:189:ASP:O	1:BL:190:LYS:C	2.62	0.42
1:FB:178:GLN:O	1:FB:179:SER:C	2.63	0.42
1:FB:190:LYS:O	1:FB:193:ASP:N	2.53	0.42
1:BW:189:ASP:O	1:BW:190:LYS:C	2.63	0.42
1:BB:189:ASP:O	1:BB:190:LYS:C	2.63	0.42
1:EC:178:GLN:O	1:EC:179:SER:C	2.62	0.42
1:EJ:10:ILE:O	1:EJ:12:SER:N	2.53	0.42
1:EX:178:GLN:O	1:EX:179:SER:C	2.63	0.42
1:AR:178:GLN:O	1:AR:179:SER:C	2.62	0.42
1:BA:178:GLN:O	1:BA:179:SER:C	2.63	0.42
1:BC:178:GLN:O	1:BC:179:SER:C	2.62	0.42
1:CG:8:ALA:O	1:CG:9:ALA:C	2.62	0.42
1:CM:178:GLN:O	1:CM:179:SER:C	2.63	0.42
1:DJ:178:GLN:O	1:DJ:179:SER:C	2.63	0.41
1:DM:189:ASP:O	1:DM:190:LYS:C	2.63	0.41
1:FD:178:GLN:O	1:FD:179:SER:C	2.63	0.41
1:FW:178:GLN:O	1:FW:179:SER:C	2.63	0.41
1:FX:189:ASP:O	1:FX:190:LYS:C	2.61	0.41
1:BM:178:GLN:O	1:BM:179:SER:C	2.62	0.41
1:CM:100:GLY:HA3	1:DH:150:TRP:O	2.20	0.41
1:CO:8:ALA:O	1:CO:9:ALA:C	2.62	0.41
1:DH:178:GLN:O	1:DH:179:SER:C	2.63	0.41
1:ES:8:ALA:O	1:ES:9:ALA:C	2.61	0.41
1:ES:178:GLN:O	1:ES:179:SER:C	2.63	0.41
1:GI:8:ALA:O	1:GI:9:ALA:C	2.59	0.41
1:BY:100:GLY:C	1:CT:150:TRP:O	2.63	0.41
1:GR:190:LYS:O	1:GR:193:ASP:N	2.53	0.41
1:HI:178:GLN:O	1:HI:179:SER:C	2.63	0.41
1:AG:189:ASP:O	1:AG:190:LYS:C	2.63	0.41
1:BD:178:GLN:O	1:BD:179:SER:C	2.62	0.41
1:BY:8:ALA:O	1:BY:9:ALA:C	2.62	0.41
1:DN:178:GLN:O	1:DN:179:SER:C	2.63	0.41
1:FA:8:ALA:O	1:FA:9:ALA:C	2.62	0.41
1:FV:190:LYS:O	1:FV:191:SER:C	2.64	0.41
1:FV:190:LYS:O	1:FV:193:ASP:N	2.54	0.41
1:HC:8:ALA:O	1:HC:9:ALA:C	2.62	0.41
1:GR:178:GLN:O	1:GR:179:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CH:178:GLN:O	1:CH:179:SER:C	2.63	0.41
1:CT:100:GLY:C	1:DO:150:TRP:O	2.63	0.41
1:EF:190:LYS:O	1:EF:193:ASP:N	2.54	0.41
1:GR:8:ALA:O	1:GR:9:ALA:C	2.59	0.41
1:BT:178:GLN:O	1:BT:179:SER:C	2.64	0.41
1:GQ:8:ALA:O	1:GQ:9:ALA:C	2.64	0.41
1:BV:193:ASP:O	1:BV:197:THR:N	2.40	0.41
1:CS:178:GLN:O	1:CS:179:SER:C	2.63	0.41
1:EF:190:LYS:O	1:EF:191:SER:C	2.64	0.41
1:EG:178:GLN:O	1:EG:179:SER:C	2.63	0.41
1:EI:178:GLN:O	1:EI:179:SER:C	2.63	0.41
1:EW:178:GLN:O	1:EW:179:SER:C	2.63	0.41
1:FW:8:ALA:O	1:FW:9:ALA:C	2.61	0.41
1:BU:190:LYS:O	1:BU:191:SER:C	2.64	0.41
1:EE:178:GLN:O	1:EE:179:SER:C	2.64	0.41
1:FR:178:GLN:O	1:FR:179:SER:C	2.63	0.41
1:GQ:189:ASP:O	1:GQ:190:LYS:C	2.64	0.41
1:CO:178:GLN:O	1:CO:179:SER:C	2.64	0.41
1:CQ:190:LYS:O	1:CQ:193:ASP:N	2.53	0.41
1:EF:8:ALA:O	1:EF:9:ALA:C	2.61	0.41
1:EJ:178:GLN:O	1:EJ:179:SER:C	2.64	0.41
1:FB:190:LYS:O	1:FB:194:ALA:N	2.41	0.41
1:FC:189:ASP:O	1:FC:190:LYS:C	2.62	0.41
1:FN:8:ALA:O	1:FN:9:ALA:C	2.60	0.41
1:GP:178:GLN:O	1:GP:179:SER:C	2.64	0.41
1:GQ:190:LYS:O	1:GQ:191:SER:C	2.64	0.41
1:HK:178:GLN:O	1:HK:179:SER:C	2.63	0.41
1:BL:178:GLN:O	1:BL:179:SER:C	2.64	0.41
1:CM:8:ALA:O	1:CM:9:ALA:C	2.63	0.41
1:FT:178:GLN:O	1:FT:179:SER:C	2.64	0.41
1:DC:189:ASP:O	1:DC:190:LYS:C	2.64	0.40
3:FK:115:ARG:O	3:FK:116:ASN:C	2.64	0.40
1:GH:8:ALA:O	1:GH:9:ALA:C	2.62	0.40
1:FU:178:GLN:O	1:FU:179:SER:C	2.63	0.40
1:GO:178:GLN:O	1:GO:179:SER:C	2.63	0.40
1:CN:178:GLN:O	1:CN:179:SER:C	2.63	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:EZ:178:GLN:O	1:EZ:179:SER:C	2.64	0.40
2:GL:290:ILE:O	2:GL:291:ASN:C	2.65	0.40
1:AG:8:ALA:O	1:AG:9:ALA:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BM:8:ALA:O	1:BM:9:ALA:C	2.61	0.40
1:BX:100:GLY:C	1:CS:150:TRP:O	2.64	0.40
1:BU:8:ALA:O	1:BU:9:ALA:C	2.63	0.40
1:BU:178:GLN:O	1:BU:179:SER:C	2.65	0.40
1:BV:178:GLN:O	1:BV:179:SER:C	2.64	0.40
1:DK:8:ALA:O	1:DK:9:ALA:C	2.61	0.40
1:ED:178:GLN:O	1:ED:179:SER:C	2.64	0.40
1:EW:100:GLY:CA	1:FR:150:TRP:O	2.70	0.40
3:GF:115:ARG:O	3:GF:116:ASN:C	2.64	0.40
3:HF:115:ARG:O	3:HF:116:ASN:C	2.65	0.40
1:HH:189:ASP:O	1:HH:190:LYS:C	2.65	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%)	30	67
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%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BT	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
1	BU	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	30	67
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%)	30	67
1	BY	263/265 (99%)	253 (96%)	9 (3%)	1 (0%)	30	67
1	CG	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
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%)	30	67
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%)	30	67
1	CT	263/265 (99%)	253 (96%)	9 (3%)	1 (0%)	30	67
1	DB	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
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%)	30	67
1	DJ	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	DK	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	30	67
1	DL	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
1	DM	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
1	DN	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	DO	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	30	67
1	DW	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
1	DX	263/265 (99%)	253 (96%)	10 (4%)	0	100	100
1	EB	263/265 (99%)	251 (95%)	10 (4%)	2 (1%)	16	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EC	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	ED	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	30	67
1	EE	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	EF	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	30	67
1	EG	263/265 (99%)	252 (96%)	11 (4%)	0	100	100
1	EH	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
1	EI	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	EJ	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	30	67
1	ER	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
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%)	30	67
1	EZ	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
1	FA	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	30	67
1	FB	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	FC	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
1	FD	263/265 (99%)	251 (95%)	12 (5%)	0	100	100
1	FE	263/265 (99%)	253 (96%)	8 (3%)	2 (1%)	16	54
1	FM	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
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%)	30	67
1	FV	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	30	67
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%)	30	67
1	GI	263/265 (99%)	253 (96%)	10 (4%)	0	100	100
1	GM	263/265 (99%)	252 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	30	67
1	GR	263/265 (99%)	250 (95%)	13 (5%)	0	100	100
1	HC	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
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%)	30	67
1	HK	263/265 (99%)	251 (95%)	11 (4%)	1 (0%)	30	67
1	HL	263/265 (99%)	252 (96%)	10 (4%)	1 (0%)	30	67
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%)	30	67
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%)	30	67
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	30	67
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	49	83

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
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 [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

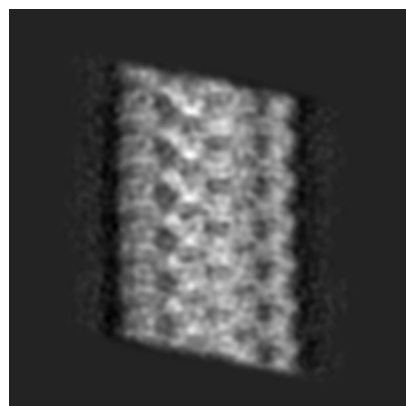
6 Map visualisation [i](#)

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

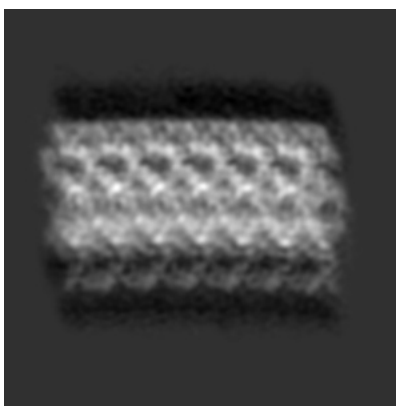
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

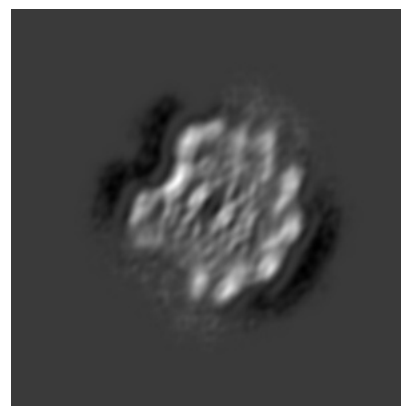
6.1.1 Primary map



X

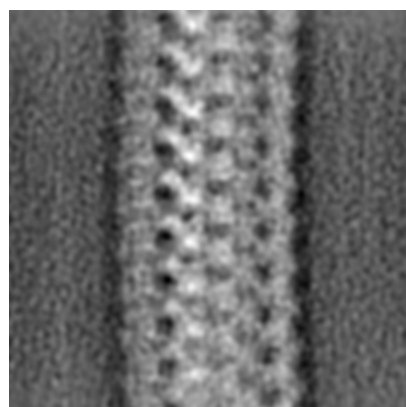


Y

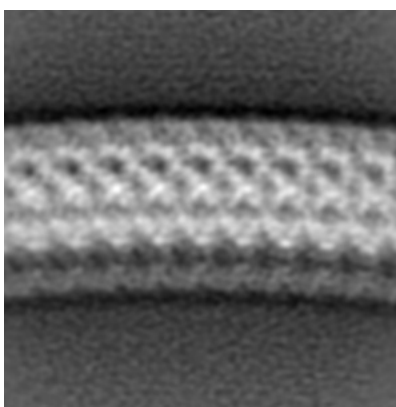


Z

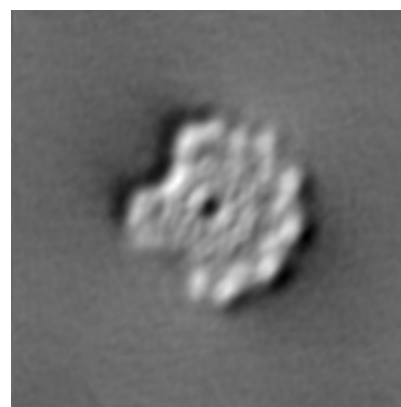
6.1.2 Raw map



X



Y

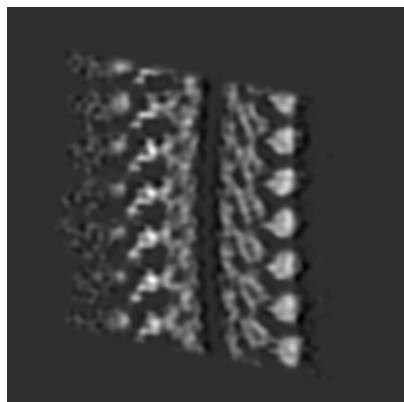


Z

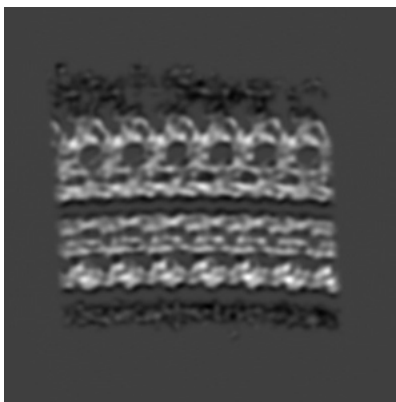
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

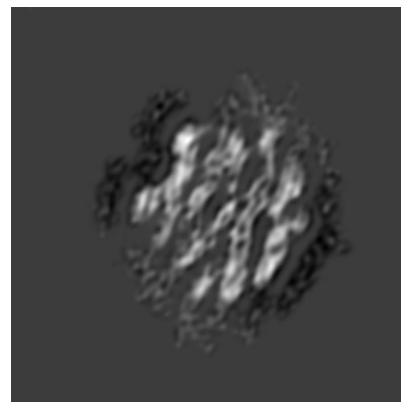
6.2.1 Primary map



X Index: 96

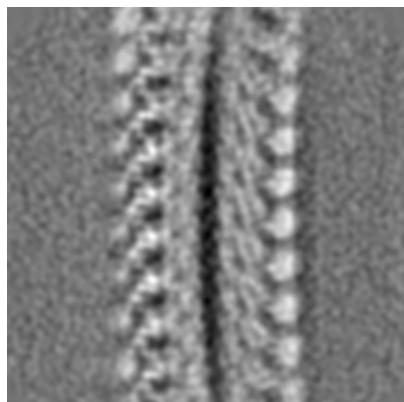


Y Index: 96

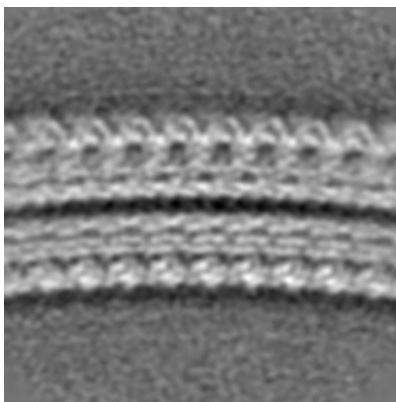


Z Index: 96

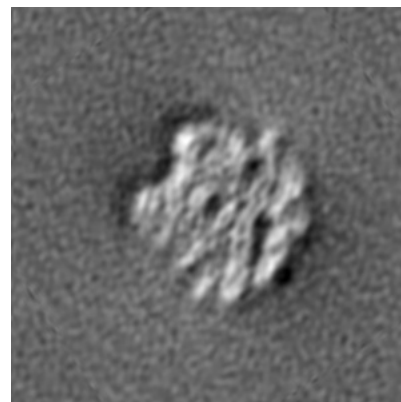
6.2.2 Raw map



X Index: 96



Y Index: 96

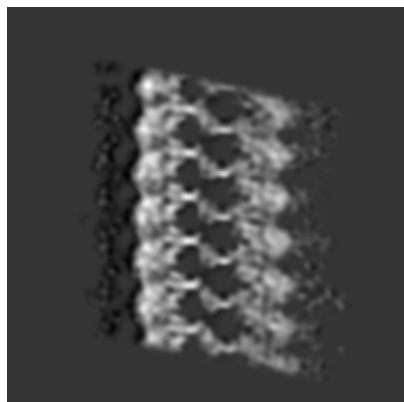


Z Index: 96

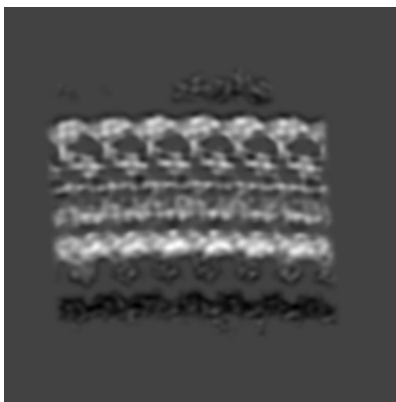
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

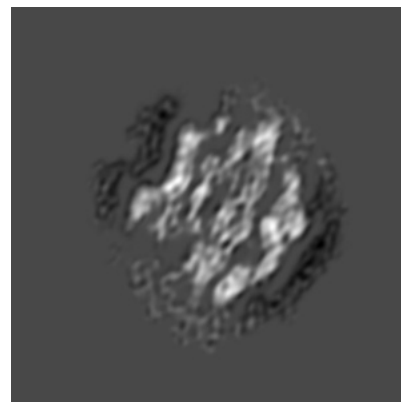
6.3.1 Primary map



X Index: 124



Y Index: 106

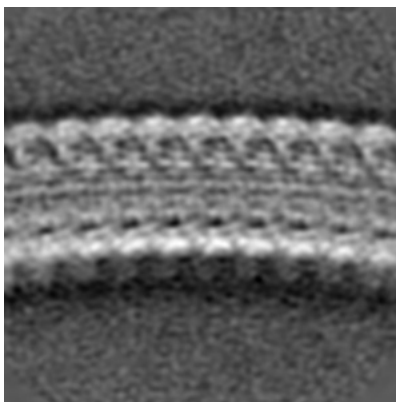


Z Index: 100

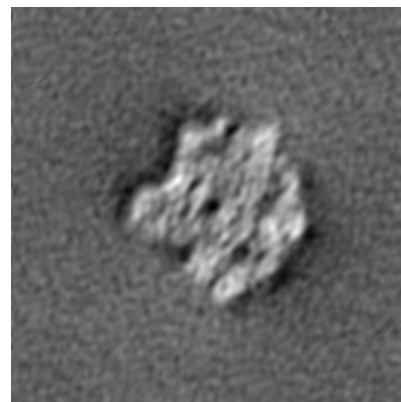
6.3.2 Raw map



X Index: 123



Y Index: 107

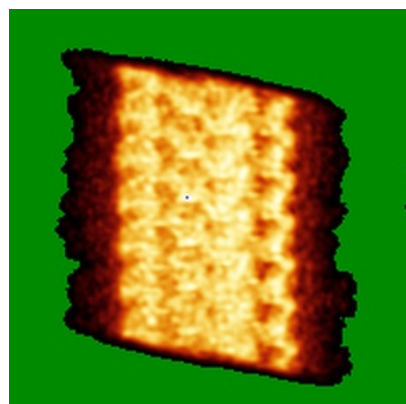


Z Index: 101

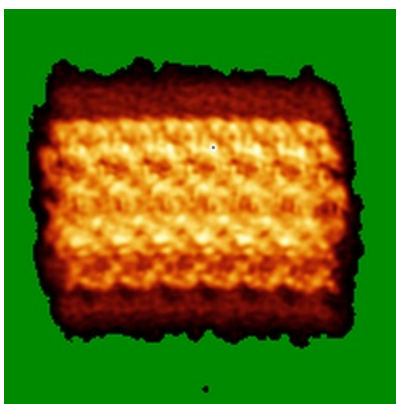
The images above show the largest variance slices of the map in three orthogonal directions.

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

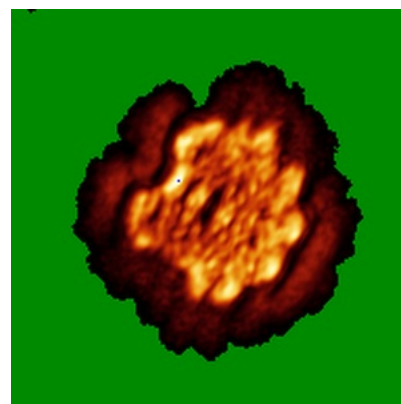
6.4.1 Primary map



X

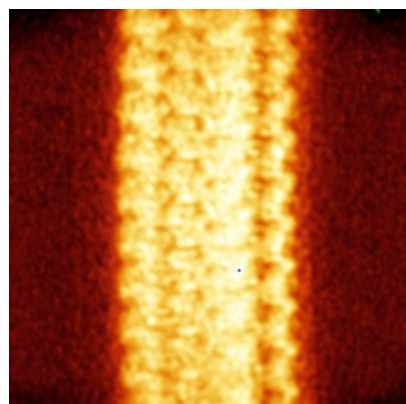


Y

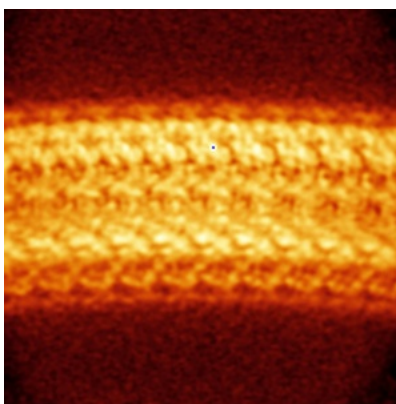


Z

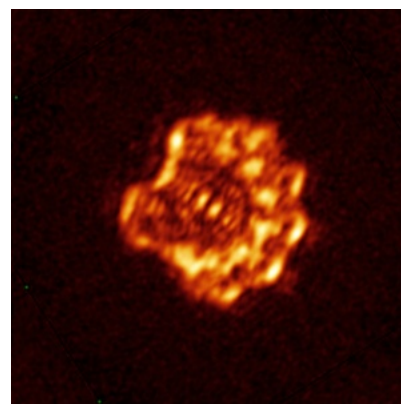
6.4.2 Raw map



X



Y

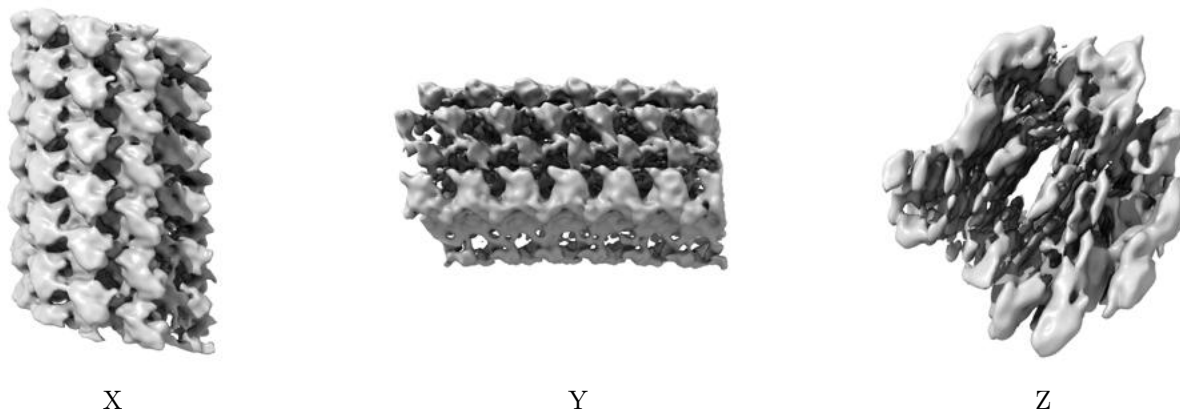


Z

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

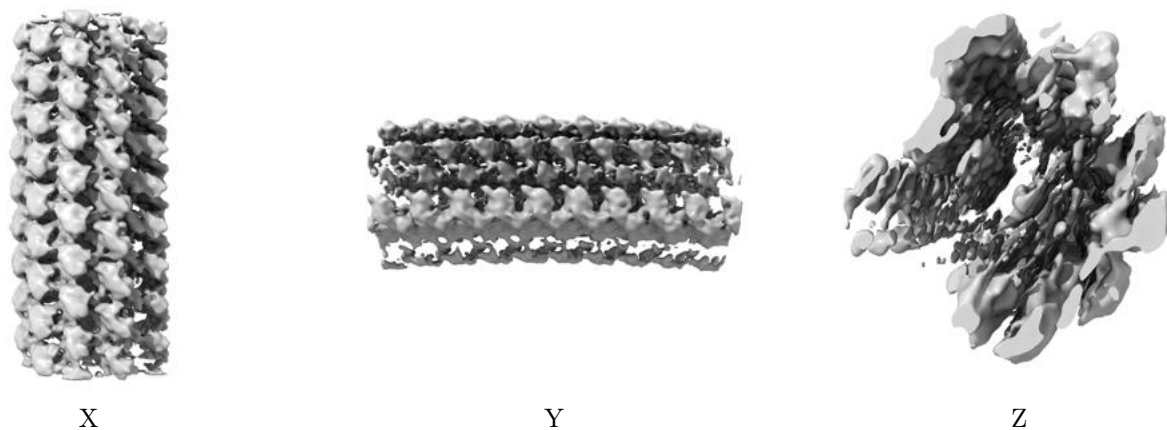
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

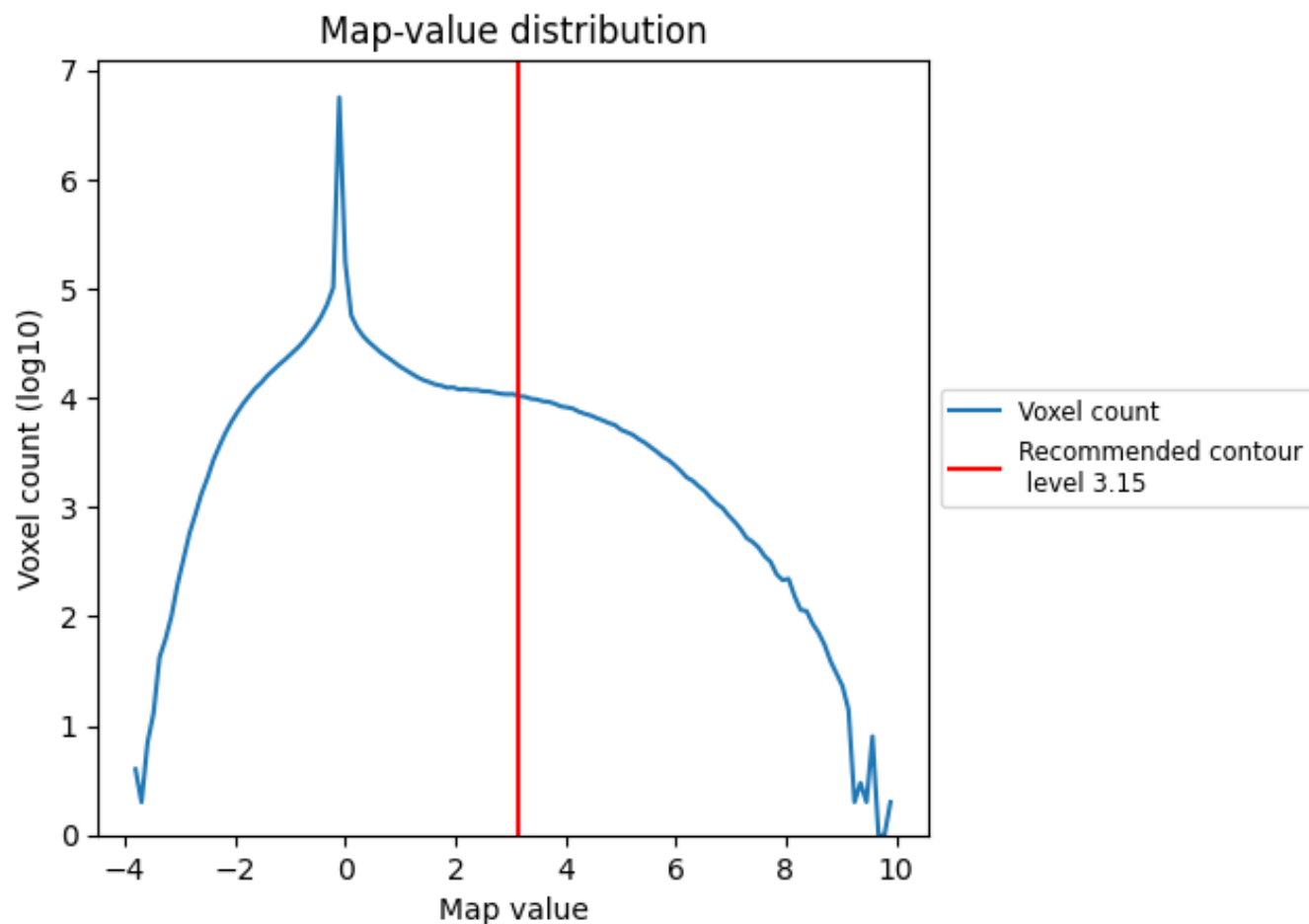
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

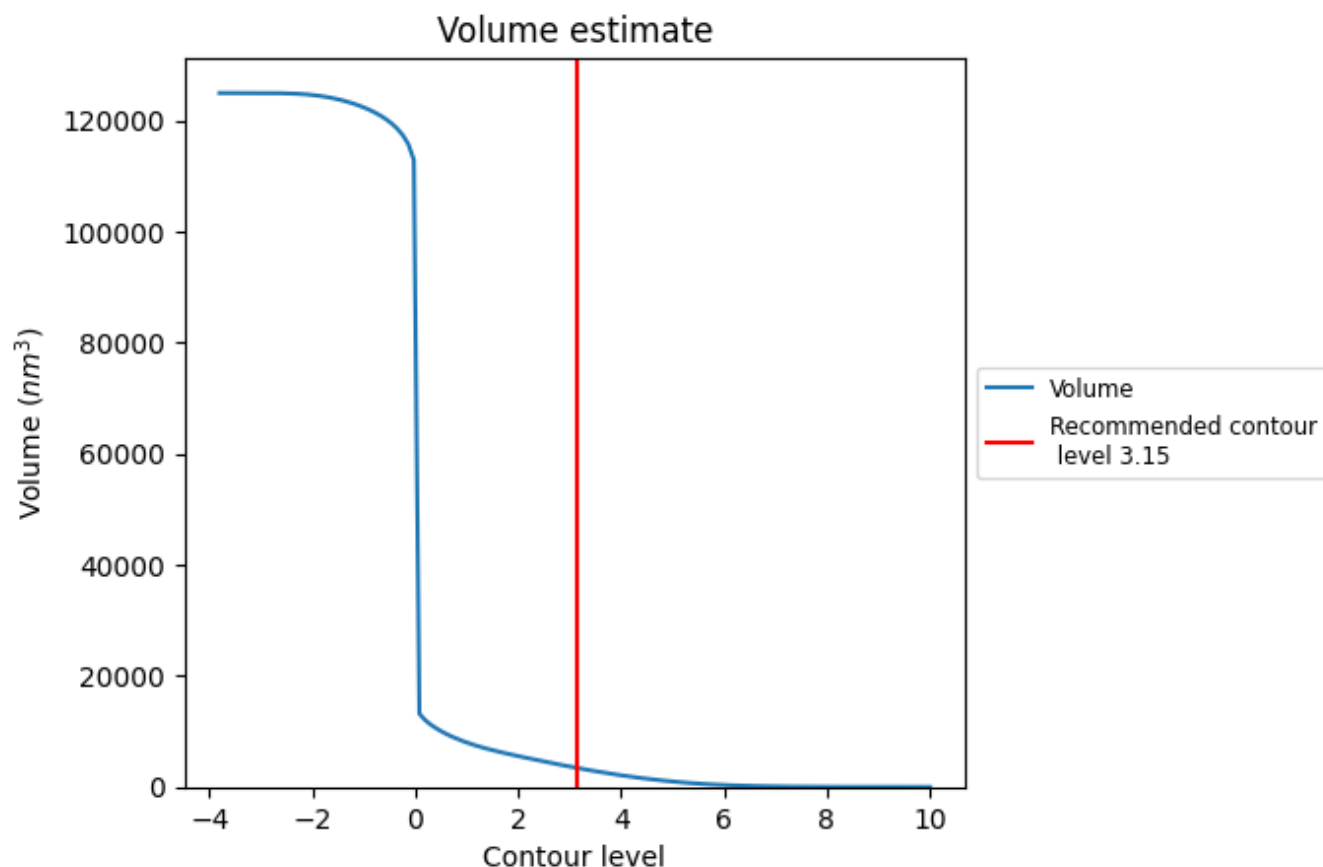
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

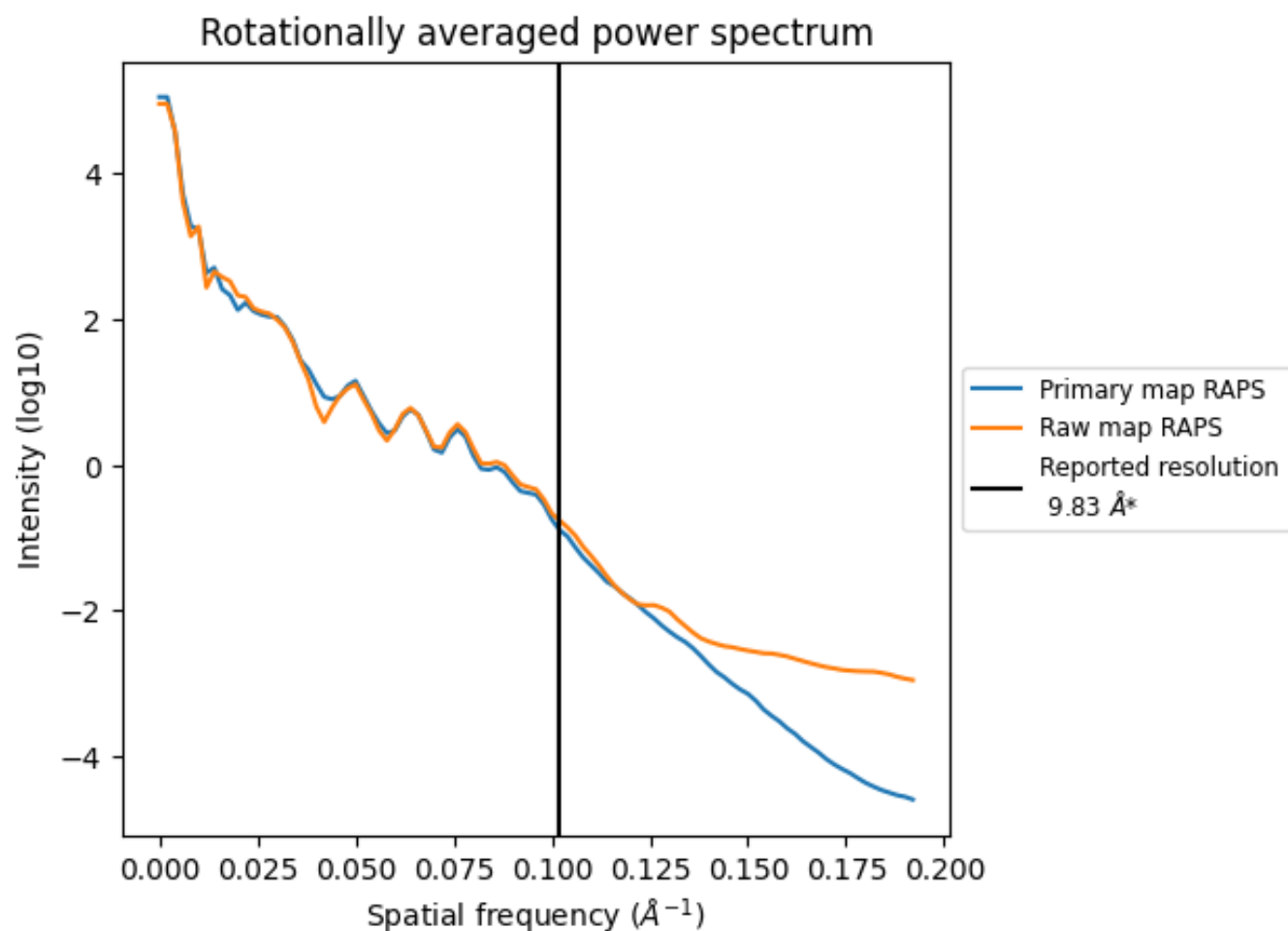
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

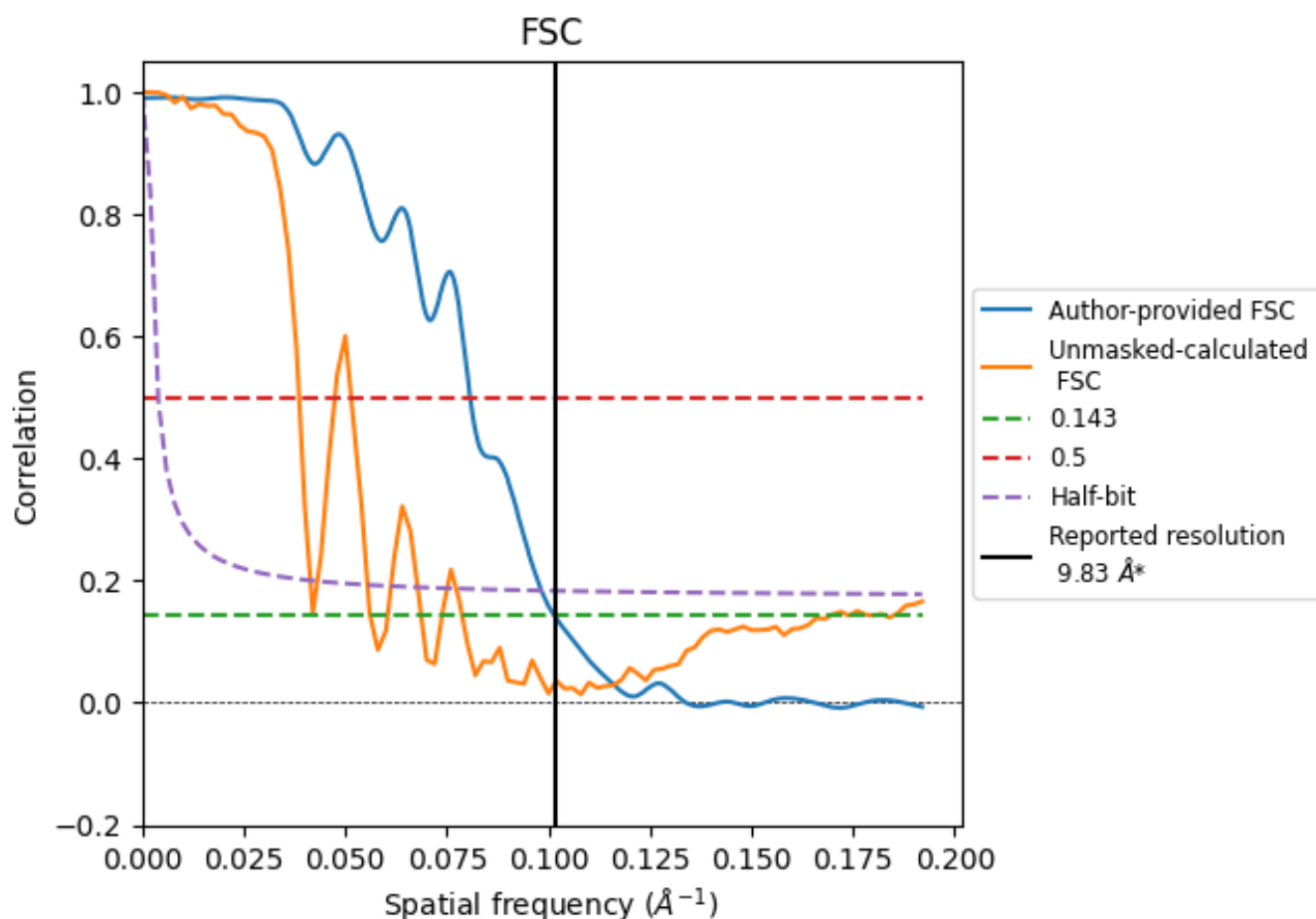


*Reported resolution corresponds to spatial frequency of 0.102 Å⁻¹

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

8.2 Resolution estimates [i](#)

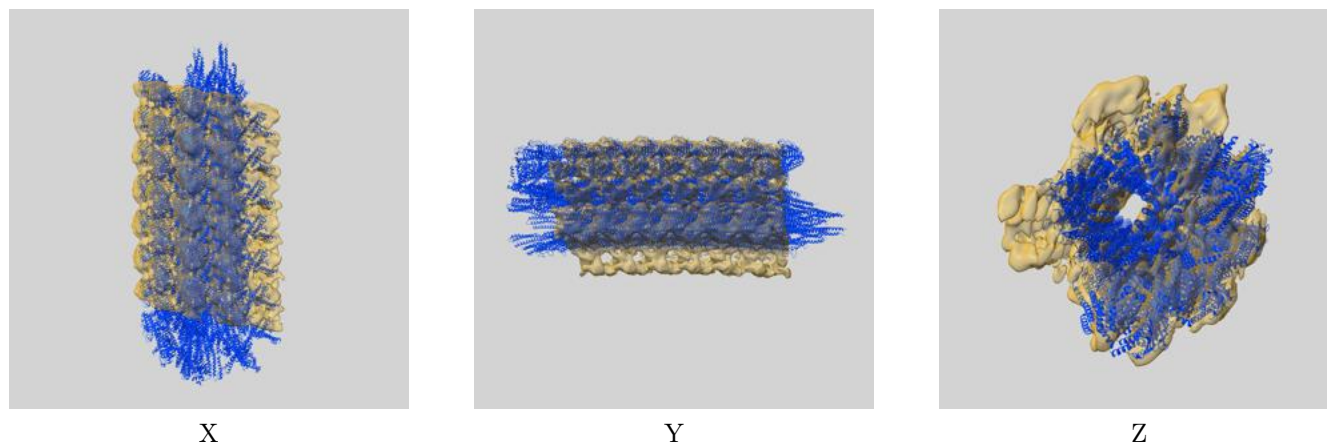
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.83	-	-
Author-provided FSC curve	9.86	12.39	10.11
Unmasked-calculated*	17.83	25.91	24.15

*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](#)

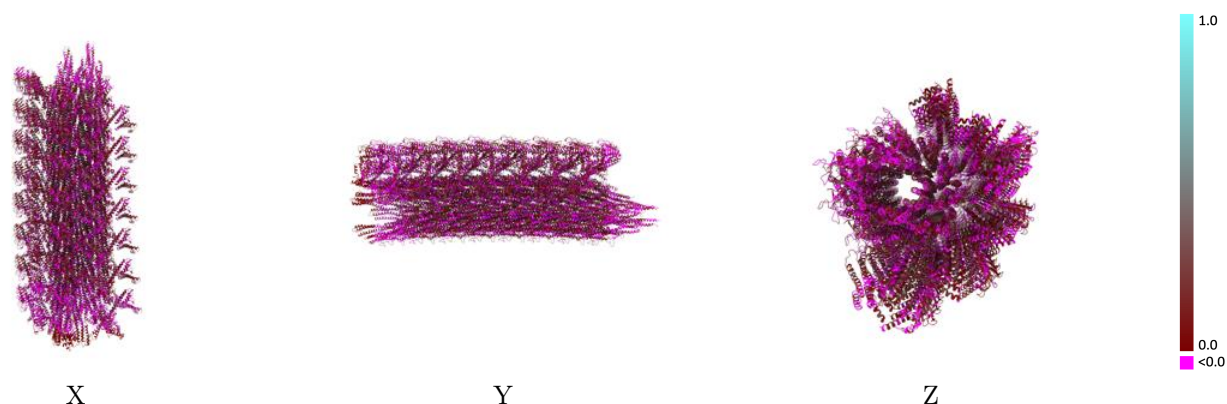
This section contains information regarding the fit between EMDB map EMD-20504 and PDB model 6PWB. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



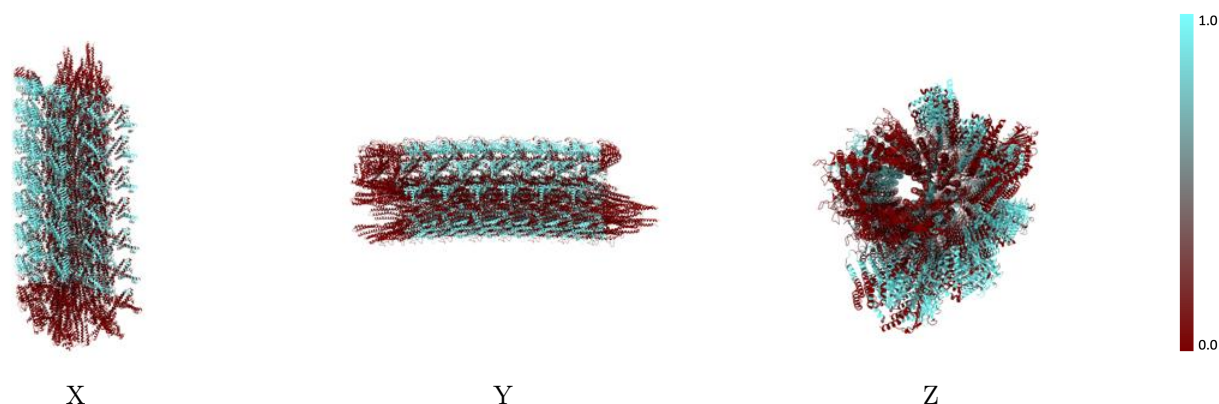
The images above show the 3D surface view of the map at the recommended contour level 3.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



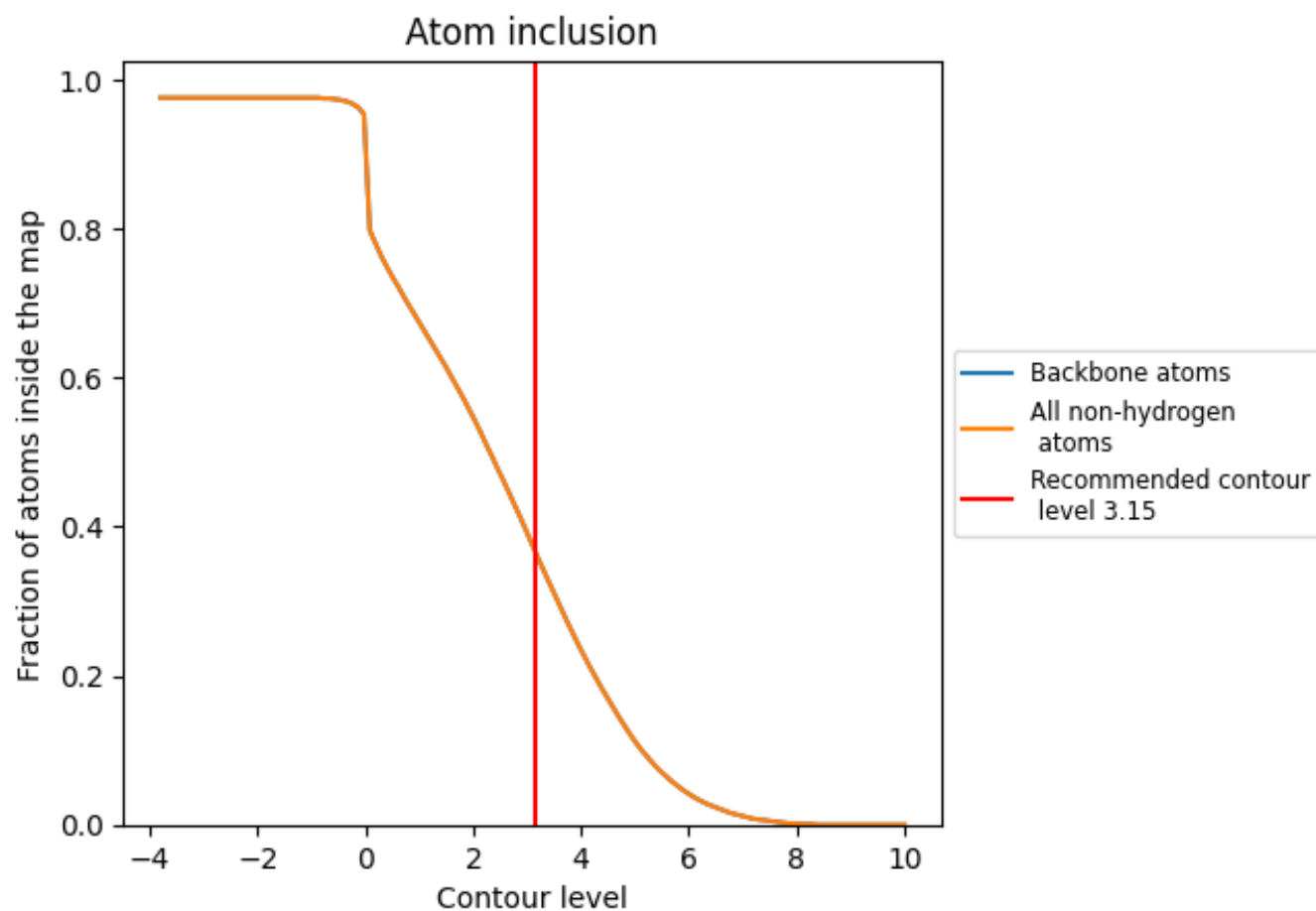
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.3670	 0.0590
AG	 0.1460	 0.0390
AH	 0.1640	 0.0170
AI	 0.1700	 0.0890
AL	 0.3700	 0.0240
AM	 0.5940	 0.0850
AO	 0.0540	 0.0100
AR	 0.1620	 0.0500
AU	 0.0610	 0.0280
BA	 0.2270	 0.0710
BB	 0.3510	 0.0890
BC	 0.3120	 0.0500
BD	 0.1830	 0.0740
BE	 0.5430	 0.0990
BF	 0.5310	 0.0800
BG	 0.4280	 0.0360
BH	 0.6360	 0.0880
BI	 0.7570	 0.0990
BJ	 0.7360	 0.0920
BK	 0.4590	 0.0540
BL	 0.1460	 0.0500
BM	 0.3720	 0.0740
BN	 0.3860	 0.0820
BO	 0.8510	 0.0820
BP	 0.5120	 0.0530
BS	 0.1530	 -0.0020
BT	 0.0620	 0.0300
BU	 0.1240	 0.0380
BV	 0.2200	 0.0750
BW	 0.4120	 0.0900
BX	 0.3290	 0.0370
BY	 0.1770	 0.0750
BZ	 0.6150	 0.1060
CA	 0.5590	 0.0800
CB	 0.4460	 0.0400



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Chain	Atom inclusion	Q-score
CC	 0.6480	 0.0940
CD	 0.8950	 0.1280
CE	 0.7590	 0.1140
CF	 0.8320	 0.1090
CG	 0.2060	 0.0800
CH	 0.3980	 0.0570
CI	 0.7320	 0.1200
CJ	 0.8530	 0.0790
CK	 0.5260	 0.0430
CL	 0.0450	 0.0270
CM	 0.4010	 0.0500
CN	 0.4010	 0.0360
CO	 0.1820	 0.0530
CP	 0.1850	 0.0510
CQ	 0.2110	 0.0570
CR	 0.4190	 0.1020
CS	 0.3500	 0.0400
CT	 0.1890	 0.0780
CU	 0.5980	 0.0840
CV	 0.5790	 0.0900
CW	 0.4560	 0.0500
CX	 0.6100	 0.0970
CY	 0.8740	 0.1280
CZ	 0.7650	 0.1200
DA	 0.8440	 0.1080
DB	 0.2050	 0.0930
DC	 0.4180	 0.0610
DD	 0.7110	 0.1150
DE	 0.8400	 0.0750
DF	 0.5380	 0.0500
DG	 0.1890	 0.0540
DH	 0.4940	 0.0510
DI	 0.5880	 0.0500
DJ	 0.2670	 0.0610
DK	 0.2080	 0.0580
DL	 0.2160	 0.0670
DM	 0.4040	 0.0940
DN	 0.3290	 0.0560
DO	 0.1570	 0.0740
DP	 0.5790	 0.0880
DQ	 0.5570	 0.0830
DR	 0.5080	 0.0600

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Chain	Atom inclusion	Q-score
DS	 0.6150	 0.0990
DT	 0.8860	 0.1260
DU	 0.7340	 0.1130
DV	 0.8170	 0.1190
DW	 0.2260	 0.0990
DX	 0.3950	 0.0660
DY	 0.7360	 0.1200
DZ	 0.8330	 0.0810
EA	 0.5470	 0.0580
EB	 0.1530	 0.0460
EC	 0.5100	 0.0480
ED	 0.5740	 0.0600
EE	 0.2850	 0.0560
EF	 0.2260	 0.0740
EG	 0.2020	 0.0610
EH	 0.4080	 0.0890
EI	 0.2990	 0.0440
EJ	 0.1020	 0.0430
EK	 0.5680	 0.0680
EL	 0.5380	 0.0730
EM	 0.4690	 0.0480
EN	 0.5710	 0.0930
EO	 0.8590	 0.1180
EP	 0.7200	 0.1080
EQ	 0.8220	 0.1140
ER	 0.2260	 0.0900
ES	 0.3840	 0.0800
ET	 0.7050	 0.1110
EU	 0.8330	 0.0690
EV	 0.4950	 0.0400
EW	 0.1630	 0.0490
EX	 0.5470	 0.0510
EY	 0.6020	 0.0530
EZ	 0.2930	 0.0670
FA	 0.2240	 0.0590
FB	 0.1730	 0.0710
FC	 0.2940	 0.0620
FD	 0.1840	 0.0380
FE	 0.0250	 0.0170
FF	 0.5080	 0.0530
FG	 0.5250	 0.0780
FH	 0.1980	 0.0200

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Chain	Atom inclusion	Q-score
FI	 0.0520	 0.0260
FJ	 0.8570	 0.1030
FK	 0.6170	 0.0820
FL	 0.8230	 0.1230
FM	 0.2010	 0.0800
FN	 0.2110	 0.0310
FO	 0.7070	 0.1170
FP	 0.7930	 0.0840
FQ	 0.4980	 0.0490
FR	 0.1530	 0.0420
FS	 0.5750	 0.0740
FT	 0.5560	 0.0530
FU	 0.2770	 0.0500
FV	 0.2150	 0.0570
FW	 0.0110	 0.0230
FX	 0.1070	 0.0040
GA	 0.1160	 -0.0160
GB	 0.0140	 0.0070
GC	 0.0000	 -0.0140
GE	 0.2620	 0.0330
GF	 0.0000	 -0.0020
GG	 0.6790	 0.1010
GH	 0.0810	 0.0430
GI	 0.0390	 -0.0110
GJ	 0.5770	 0.0940
GK	 0.0560	 -0.0090
GL	 0.0000	 -0.0160
GM	 0.1820	 0.0600
GN	 0.5620	 0.0770
GO	 0.5400	 0.0490
GP	 0.2080	 0.0230
GQ	 0.1260	 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	 0.0010	 0.0020
HE	 0.0000	 0.0020
HF	 0.0000	 -0.0050
HH	 0.1360	 0.0590
HI	 0.3140	 0.0500

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Chain	Atom inclusion	Q-score
HJ	 0.2140	 -0.0160
HK	 0.1490	 0.0120
HL	 0.0120	 0.0200