wwPDB EM Validation Summary Report

Aug 15, 2024 – 02:26 PM EDT

PDB ID	:	8VKQ
EMDB ID	:	EMD-43327
Title	:	CW Flagellar Switch Complex - FliF, FliG, FliM, and FliN forming the C-ring from Salmonella
Authors	:	Singh, P.K.; Iverson, T.M.
Deposited on	:	2024-01-09
Resolution	:	4.60 Å(reported)

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

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

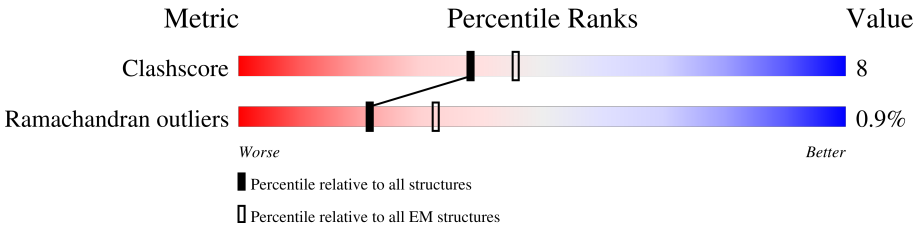
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	A	560	6% 8% · 92%
1	BC	560	6% 8% · 92%
1	BF	560	6% 8% · 92%
1	DB	560	6% 8% · 92%
1	DE	560	6% 8% · 92%
1	F	560	6% 8% · 92%
1	FA	560	6% 8% · 92%
1	FD	560	6% 8% · 92%
1	FG	560	6% 8% · 92%

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Mol	Chain	Length	Quality of chain
1	HC	560	6% 8% 92%
1	HF	560	6% 8% 92%
1	I	560	6% 8% 92%
1	JB	560	6% 8% 92%
1	JE	560	6% 8% 92%
1	LA	560	6% 8% 92%
1	LD	560	6% 8% 92%
1	LG	560	6% 8% 92%
1	NC	560	6% 8% 92%
1	NF	560	6% 8% 92%
1	PB	560	6% 8% 92%
1	PE	560	6% 8% 92%
1	RA	560	6% 8% 92%
1	RD	560	6% 8% 92%
1	RG	560	6% 8% 92%
1	S	560	6% 8% 92%
1	TC	560	6% 8% 92%
1	TF	560	6% 8% 92%
1	VB	560	6% 8% 92%
1	VE	560	6% 8% 92%
1	XA	560	6% 8% 92%
1	XD	560	6% 8% 92%
1	Z	560	6% 8% 92%
1	ZC	560	6% 8% 92%
1	ZF	560	6% 8% 92%

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Mol	Chain	Length	Quality of chain
2	AA	331	11% 85% 10% 5%
2	AD	331	15% 86% 9% 5%
2	AG	331	9% 85% 9% 5%
2	B	331	11% 85% 9% 5%
2	CC	331	14% 86% 9% 5%
2	CF	331	11% 85% 9% 5%
2	EB	331	12% 85% 9% 5%
2	EE	331	13% 85% 9% 5%
2	G	331	11% 85% 9% 5%
2	GA	331	10% 85% 9% 5%
2	GD	331	15% 85% 10% 5%
2	GG	331	9% 85% 9% 5%
2	IC	331	14% 86% 9% 5%
2	IF	331	10% 85% 9% 5%
2	J	331	11% 85% 9% 5%
2	KB	331	12% 86% 9% 5%
2	KE	331	12% 86% 9% 5%
2	MA	331	11% 87% 8% 5%
2	MD	331	15% 86% 8% 5%
2	MG	331	9% 85% 9% 5%
2	OC	331	14% 85% 9% 5%
2	OF	331	10% 85% 10% 5%
2	QB	331	13% 85% 9% 5%
2	QE	331	12% 85% 10% 5%
2	SA	331	11% 86% 9% 5%

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Mol	Chain	Length	Quality of chain
2	SD	331	14% 85% 9% 5%
2	SG	331	10% 86% 8% 5%
2	T	331	11% 86% 8% 5%
2	UC	331	15% 86% 8% 5%
2	UF	331	9% 85% 9% 5%
2	WB	331	13% 86% 9% 5%
2	WE	331	12% 86% 9% 5%
2	YA	331	12% 86% 9% 5%
2	YD	331	13% 85% 9% 5%
3	BA	291	92% 5%
3	BD	291	7% 92% 5%
3	BG	291	92% 5%
3	C	291	92% 5%
3	DC	291	6% 92% 5%
3	DF	291	92% 5%
3	FB	291	5% 92% 5%
3	FE	291	92% 5%
3	HA	291	92% 5%
3	HD	291	6% 92% 5%
3	HG	291	92% 5%
3	JC	291	7% 92% 5%
3	JF	291	92% 5%
3	K	291	92% 5%
3	LB	291	6% 92% 5%
3	LE	291	92% 5%

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Mol	Chain	Length	Quality of chain
3	M	291	92% 5%
3	NA	291	5% 92% 5%
3	ND	291	6% 92% 5%
3	NG	291	92% 5%
3	PC	291	7% 92% 5%
3	PF	291	92% 5%
3	RB	291	7% 92% 5%
3	RE	291	92% 5%
3	TA	291	5% 92% 5%
3	TD	291	5% 92% 5%
3	TG	291	92% 5%
3	V	291	92% 5%
3	VC	291	7% 92% 5%
3	VF	291	92% 5%
3	XB	291	6% 92% 5%
3	XE	291	92% 5%
3	ZA	291	5% 92% 5%
3	ZD	291	5% 92% 5%
4	AB	137	7% 64% 32%
4	AC	137	53% 45%
4	AE	137	65% 32%
4	AF	137	53% 45%
4	BB	137	58% 42%
4	BE	137	58% 42%
4	CA	137	7% 64% 32%

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Mol	Chain	Length	Quality of chain
4	CB	137	53% 45%
4	CD	137	5% 64% 32%
4	CE	137	53% 45%
4	CG	137	65% 32%
4	D	137	5% 64% 32%
4	DA	137	58% 42%
4	DD	137	58% 42%
4	DG	137	58% 42%
4	E	137	58% 42%
4	EA	137	53% 45%
4	EC	137	5% 64% 32%
4	ED	137	53% 45%
4	EF	137	64% 32%
4	EG	137	53% 45%
4	FC	137	58% 42%
4	FF	137	58% 42%
4	GB	137	6% 64% 32%
4	GC	137	53% 45%
4	GE	137	64% 32%
4	GF	137	53% 45%
4	H	137	53% 45%
4	HB	137	58% 42%
4	HE	137	58% 42%
4	IA	137	7% 64% 32%
4	IB	137	53% 45%

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Mol	Chain	Length	Quality of chain
4	ID	137	5% 64% 32%
4	IE	137	53% 45%
4	IG	137	64% 32%
4	JA	137	58% 42%
4	JD	137	58% 42%
4	JG	137	58% 42%
4	KA	137	53% 45%
4	KC	137	5% 64% 32%
4	KD	137	53% 45%
4	KF	137	64% 32%
4	KG	137	53% 45%
4	L	137	5% 64% 32%
4	LC	137	58% 42%
4	LF	137	58% 42%
4	MB	137	5% 64% 32%
4	MC	137	53% 45%
4	ME	137	64% 32%
4	MF	137	53% 45%
4	N	137	5% 65% 32%
4	NB	137	58% 42%
4	NE	137	58% 42%
4	O	137	58% 42%
4	OA	137	7% 64% 32%
4	OB	137	53% 45%
4	OD	137	64% 32%

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Mol	Chain	Length	Quality of chain
4	OE	137	53% 45%
4	OG	137	5% 64% 32%
4	P	137	58% 42%
4	PA	137	58% 42%
4	PD	137	58% 42%
4	PG	137	58% 42%
4	Q	137	53% 45%
4	QA	137	53% 45%
4	QC	137	5% 64% 32%
4	QD	137	53% 45%
4	QF	137	64% 32%
4	QG	137	53% 45%
4	R	137	53% 45%
4	RC	137	58% 42%
4	RF	137	58% 42%
4	SB	137	5% 64% 32%
4	SC	137	53% 45%
4	SE	137	64% 32%
4	SF	137	53% 45%
4	TB	137	58% 42%
4	TE	137	58% 42%
4	UA	137	7% 64% 32%
4	UB	137	53% 45%
4	UD	137	65% 32%
4	UE	137	53% 45%

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Mol	Chain	Length	Quality of chain
4	UG	137	5% 64% 32%
4	VA	137	58% 42%
4	VD	137	58% 42%
4	VG	137	58% 42%
4	W	137	5% 64% 32%
4	WA	137	53% 45%
4	WC	137	5% 64% 32%
4	WD	137	53% 45%
4	WF	137	65% 32%
4	WG	137	53% 45%
4	X	137	58% 42%
4	XC	137	58% 42%
4	XF	137	58% 42%
4	Y	137	53% 45%
4	YB	137	6% 64% 32%
4	YC	137	53% 45%
4	YE	137	65% 32%
4	YF	137	53% 45%
4	ZB	137	58% 42%
4	ZE	137	58% 42%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 150314 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 Flagellar M-ring protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	F	47	Total 234	C 140	N 47	O 47	0	0
1	A	47	Total 234	C 140	N 47	O 47	0	0
1	I	47	Total 234	C 140	N 47	O 47	0	0
1	S	47	Total 234	C 140	N 47	O 47	0	0
1	Z	47	Total 234	C 140	N 47	O 47	0	0
1	FA	47	Total 234	C 140	N 47	O 47	0	0
1	LA	47	Total 234	C 140	N 47	O 47	0	0
1	RA	47	Total 234	C 140	N 47	O 47	0	0
1	XA	47	Total 234	C 140	N 47	O 47	0	0
1	DB	47	Total 234	C 140	N 47	O 47	0	0
1	JB	47	Total 234	C 140	N 47	O 47	0	0
1	PB	47	Total 234	C 140	N 47	O 47	0	0
1	VB	47	Total 234	C 140	N 47	O 47	0	0
1	BC	47	Total 234	C 140	N 47	O 47	0	0
1	HC	47	Total 234	C 140	N 47	O 47	0	0
1	NC	47	Total 234	C 140	N 47	O 47	0	0
1	TC	47	Total 234	C 140	N 47	O 47	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	ZC	47	Total 234	C 140	N 47	O 47	0	0
1	FD	47	Total 234	C 140	N 47	O 47	0	0
1	LD	47	Total 234	C 140	N 47	O 47	0	0
1	RD	47	Total 234	C 140	N 47	O 47	0	0
1	XD	47	Total 234	C 140	N 47	O 47	0	0
1	DE	47	Total 234	C 140	N 47	O 47	0	0
1	JE	47	Total 234	C 140	N 47	O 47	0	0
1	PE	47	Total 234	C 140	N 47	O 47	0	0
1	VE	47	Total 234	C 140	N 47	O 47	0	0
1	BF	47	Total 234	C 140	N 47	O 47	0	0
1	HF	47	Total 234	C 140	N 47	O 47	0	0
1	NF	47	Total 234	C 140	N 47	O 47	0	0
1	TF	47	Total 234	C 140	N 47	O 47	0	0
1	ZF	47	Total 234	C 140	N 47	O 47	0	0
1	FG	47	Total 234	C 140	N 47	O 47	0	0
1	LG	47	Total 234	C 140	N 47	O 47	0	0
1	RG	47	Total 234	C 140	N 47	O 47	0	0

- Molecule 2 is a protein called Flagellar motor switch protein FliG.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	314	Total 1554	C 926	N 314	O 314	0	0
2	B	314	Total 1554	C 926	N 314	O 314	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	314	Total 1554	C 926	N 314	O 314	0	0
2	T	314	Total 1554	C 926	N 314	O 314	0	0
2	AA	314	Total 1554	C 926	N 314	O 314	0	0
2	GA	314	Total 1554	C 926	N 314	O 314	0	0
2	MA	314	Total 1554	C 926	N 314	O 314	0	0
2	SA	314	Total 1554	C 926	N 314	O 314	0	0
2	YA	314	Total 1554	C 926	N 314	O 314	0	0
2	EB	314	Total 1554	C 926	N 314	O 314	0	0
2	KB	314	Total 1554	C 926	N 314	O 314	0	0
2	QB	314	Total 1554	C 926	N 314	O 314	0	0
2	WB	314	Total 1554	C 926	N 314	O 314	0	0
2	CC	314	Total 1554	C 926	N 314	O 314	0	0
2	IC	314	Total 1554	C 926	N 314	O 314	0	0
2	OC	314	Total 1554	C 926	N 314	O 314	0	0
2	UC	314	Total 1554	C 926	N 314	O 314	0	0
2	AD	314	Total 1554	C 926	N 314	O 314	0	0
2	GD	314	Total 1554	C 926	N 314	O 314	0	0
2	MD	314	Total 1554	C 926	N 314	O 314	0	0
2	SD	314	Total 1554	C 926	N 314	O 314	0	0
2	YD	314	Total 1554	C 926	N 314	O 314	0	0
2	EE	314	Total 1554	C 926	N 314	O 314	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	KE	314	Total 1554	C 926	N 314	O 314	0	0
2	QE	314	Total 1554	C 926	N 314	O 314	0	0
2	WE	314	Total 1554	C 926	N 314	O 314	0	0
2	CF	314	Total 1554	C 926	N 314	O 314	0	0
2	IF	314	Total 1554	C 926	N 314	O 314	0	0
2	OF	314	Total 1554	C 926	N 314	O 314	0	0
2	UF	314	Total 1554	C 926	N 314	O 314	0	0
2	AG	314	Total 1554	C 926	N 314	O 314	0	0
2	GG	314	Total 1554	C 926	N 314	O 314	0	0
2	MG	314	Total 1554	C 926	N 314	O 314	0	0
2	SG	314	Total 1554	C 926	N 314	O 314	0	0

- Molecule 3 is a protein called Flagellar motor switch protein FliM.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	M	287	Total 1420	C 846	N 287	O 287	0	0
3	C	287	Total 1420	C 846	N 287	O 287	0	0
3	K	287	Total 1420	C 846	N 287	O 287	0	0
3	V	287	Total 1420	C 846	N 287	O 287	0	0
3	BA	287	Total 1420	C 846	N 287	O 287	0	0
3	HA	287	Total 1420	C 846	N 287	O 287	0	0
3	NA	287	Total 1420	C 846	N 287	O 287	0	0
3	TA	287	Total 1420	C 846	N 287	O 287	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	ZA	287	Total 1420	C 846	N 287	O 287	0	0
3	FB	287	Total 1420	C 846	N 287	O 287	0	0
3	LB	287	Total 1420	C 846	N 287	O 287	0	0
3	RB	287	Total 1420	C 846	N 287	O 287	0	0
3	XB	287	Total 1420	C 846	N 287	O 287	0	0
3	DC	287	Total 1420	C 846	N 287	O 287	0	0
3	JC	287	Total 1420	C 846	N 287	O 287	0	0
3	PC	287	Total 1420	C 846	N 287	O 287	0	0
3	VC	287	Total 1420	C 846	N 287	O 287	0	0
3	BD	287	Total 1420	C 846	N 287	O 287	0	0
3	HD	287	Total 1420	C 846	N 287	O 287	0	0
3	ND	287	Total 1420	C 846	N 287	O 287	0	0
3	TD	287	Total 1420	C 846	N 287	O 287	0	0
3	ZD	287	Total 1420	C 846	N 287	O 287	0	0
3	FE	287	Total 1420	C 846	N 287	O 287	0	0
3	LE	287	Total 1420	C 846	N 287	O 287	0	0
3	RE	287	Total 1420	C 846	N 287	O 287	0	0
3	XE	287	Total 1420	C 846	N 287	O 287	0	0
3	DF	287	Total 1420	C 846	N 287	O 287	0	0
3	JF	287	Total 1420	C 846	N 287	O 287	0	0
3	PF	287	Total 1420	C 846	N 287	O 287	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	VF	287	Total 1420	C 846	N 287	O 287	0	0
3	BG	287	Total 1420	C 846	N 287	O 287	0	0
3	HG	287	Total 1420	C 846	N 287	O 287	0	0
3	NG	287	Total 1420	C 846	N 287	O 287	0	0
3	TG	287	Total 1420	C 846	N 287	O 287	0	0

- Molecule 4 is a protein called Flagellar motor switch protein FliN.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	N	93	Total 456	C 270	N 93	O 93	0	0
4	P	79	Total 389	C 230	N 79	O 80	0	0
4	Q	75	Total 368	C 218	N 75	O 75	0	0
4	D	93	Total 456	C 270	N 93	O 93	0	0
4	E	79	Total 389	C 230	N 79	O 80	0	0
4	H	75	Total 368	C 218	N 75	O 75	0	0
4	L	93	Total 456	C 270	N 93	O 93	0	0
4	O	79	Total 389	C 230	N 79	O 80	0	0
4	R	75	Total 368	C 218	N 75	O 75	0	0
4	W	93	Total 456	C 270	N 93	O 93	0	0
4	X	79	Total 389	C 230	N 79	O 80	0	0
4	Y	75	Total 368	C 218	N 75	O 75	0	0
4	CA	93	Total 456	C 270	N 93	O 93	0	0
4	DA	79	Total 389	C 230	N 79	O 80	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	EA	75	Total 368	C 218	N 75	O 75	0	0
4	IA	93	Total 456	C 270	N 93	O 93	0	0
4	JA	79	Total 389	C 230	N 79	O 80	0	0
4	KA	75	Total 368	C 218	N 75	O 75	0	0
4	OA	93	Total 456	C 270	N 93	O 93	0	0
4	PA	79	Total 389	C 230	N 79	O 80	0	0
4	QA	75	Total 368	C 218	N 75	O 75	0	0
4	UA	93	Total 456	C 270	N 93	O 93	0	0
4	VA	79	Total 389	C 230	N 79	O 80	0	0
4	WA	75	Total 368	C 218	N 75	O 75	0	0
4	AB	93	Total 456	C 270	N 93	O 93	0	0
4	BB	79	Total 389	C 230	N 79	O 80	0	0
4	CB	75	Total 368	C 218	N 75	O 75	0	0
4	GB	93	Total 456	C 270	N 93	O 93	0	0
4	HB	79	Total 389	C 230	N 79	O 80	0	0
4	IB	75	Total 368	C 218	N 75	O 75	0	0
4	MB	93	Total 456	C 270	N 93	O 93	0	0
4	NB	79	Total 389	C 230	N 79	O 80	0	0
4	OB	75	Total 368	C 218	N 75	O 75	0	0
4	SB	93	Total 456	C 270	N 93	O 93	0	0
4	TB	79	Total 389	C 230	N 79	O 80	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	UB	75	Total 368	C 218	N 75	O 75	0	0
4	YB	93	Total 456	C 270	N 93	O 93	0	0
4	ZB	79	Total 389	C 230	N 79	O 80	0	0
4	AC	75	Total 368	C 218	N 75	O 75	0	0
4	EC	93	Total 456	C 270	N 93	O 93	0	0
4	FC	79	Total 389	C 230	N 79	O 80	0	0
4	GC	75	Total 368	C 218	N 75	O 75	0	0
4	KC	93	Total 456	C 270	N 93	O 93	0	0
4	LC	79	Total 389	C 230	N 79	O 80	0	0
4	MC	75	Total 368	C 218	N 75	O 75	0	0
4	QC	93	Total 456	C 270	N 93	O 93	0	0
4	RC	79	Total 389	C 230	N 79	O 80	0	0
4	SC	75	Total 368	C 218	N 75	O 75	0	0
4	WC	93	Total 456	C 270	N 93	O 93	0	0
4	XC	79	Total 389	C 230	N 79	O 80	0	0
4	YC	75	Total 368	C 218	N 75	O 75	0	0
4	CD	93	Total 456	C 270	N 93	O 93	0	0
4	DD	79	Total 389	C 230	N 79	O 80	0	0
4	ED	75	Total 368	C 218	N 75	O 75	0	0
4	ID	93	Total 456	C 270	N 93	O 93	0	0
4	JD	79	Total 389	C 230	N 79	O 80	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	KD	75	Total 368	C 218	N 75	O 75	0	0
4	OD	93	Total 456	C 270	N 93	O 93	0	0
4	PD	79	Total 389	C 230	N 79	O 80	0	0
4	QD	75	Total 368	C 218	N 75	O 75	0	0
4	UD	93	Total 456	C 270	N 93	O 93	0	0
4	VD	79	Total 389	C 230	N 79	O 80	0	0
4	WD	75	Total 368	C 218	N 75	O 75	0	0
4	AE	93	Total 456	C 270	N 93	O 93	0	0
4	BE	79	Total 389	C 230	N 79	O 80	0	0
4	CE	75	Total 368	C 218	N 75	O 75	0	0
4	GE	93	Total 456	C 270	N 93	O 93	0	0
4	HE	79	Total 389	C 230	N 79	O 80	0	0
4	IE	75	Total 368	C 218	N 75	O 75	0	0
4	ME	93	Total 456	C 270	N 93	O 93	0	0
4	NE	79	Total 389	C 230	N 79	O 80	0	0
4	OE	75	Total 368	C 218	N 75	O 75	0	0
4	SE	93	Total 456	C 270	N 93	O 93	0	0
4	TE	79	Total 389	C 230	N 79	O 80	0	0
4	UE	75	Total 368	C 218	N 75	O 75	0	0
4	YE	93	Total 456	C 270	N 93	O 93	0	0
4	ZE	79	Total 389	C 230	N 79	O 80	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	AF	75	Total 368	C 218	N 75	O 75	0	0
4	EF	93	Total 456	C 270	N 93	O 93	0	0
4	FF	79	Total 389	C 230	N 79	O 80	0	0
4	GF	75	Total 368	C 218	N 75	O 75	0	0
4	KF	93	Total 456	C 270	N 93	O 93	0	0
4	LF	79	Total 389	C 230	N 79	O 80	0	0
4	MF	75	Total 368	C 218	N 75	O 75	0	0
4	QF	93	Total 456	C 270	N 93	O 93	0	0
4	RF	79	Total 389	C 230	N 79	O 80	0	0
4	SF	75	Total 368	C 218	N 75	O 75	0	0
4	WF	93	Total 456	C 270	N 93	O 93	0	0
4	XF	79	Total 389	C 230	N 79	O 80	0	0
4	YF	75	Total 368	C 218	N 75	O 75	0	0
4	CG	93	Total 456	C 270	N 93	O 93	0	0
4	DG	79	Total 389	C 230	N 79	O 80	0	0
4	EG	75	Total 368	C 218	N 75	O 75	0	0
4	IG	93	Total 456	C 270	N 93	O 93	0	0
4	JG	79	Total 389	C 230	N 79	O 80	0	0
4	KG	75	Total 368	C 218	N 75	O 75	0	0
4	OG	93	Total 456	C 270	N 93	O 93	0	0
4	PG	79	Total 389	C 230	N 79	O 80	0	0

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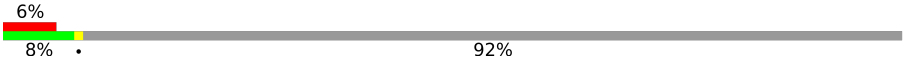
Mol	Chain	Residues	Atoms				AltConf	Trace
4	QG	75	Total 368	C 218	N 75	O 75	0	0
4	UG	93	Total 456	C 270	N 93	O 93	0	0
4	VG	79	Total 389	C 230	N 79	O 80	0	0
4	WG	75	Total 368	C 218	N 75	O 75	0	0

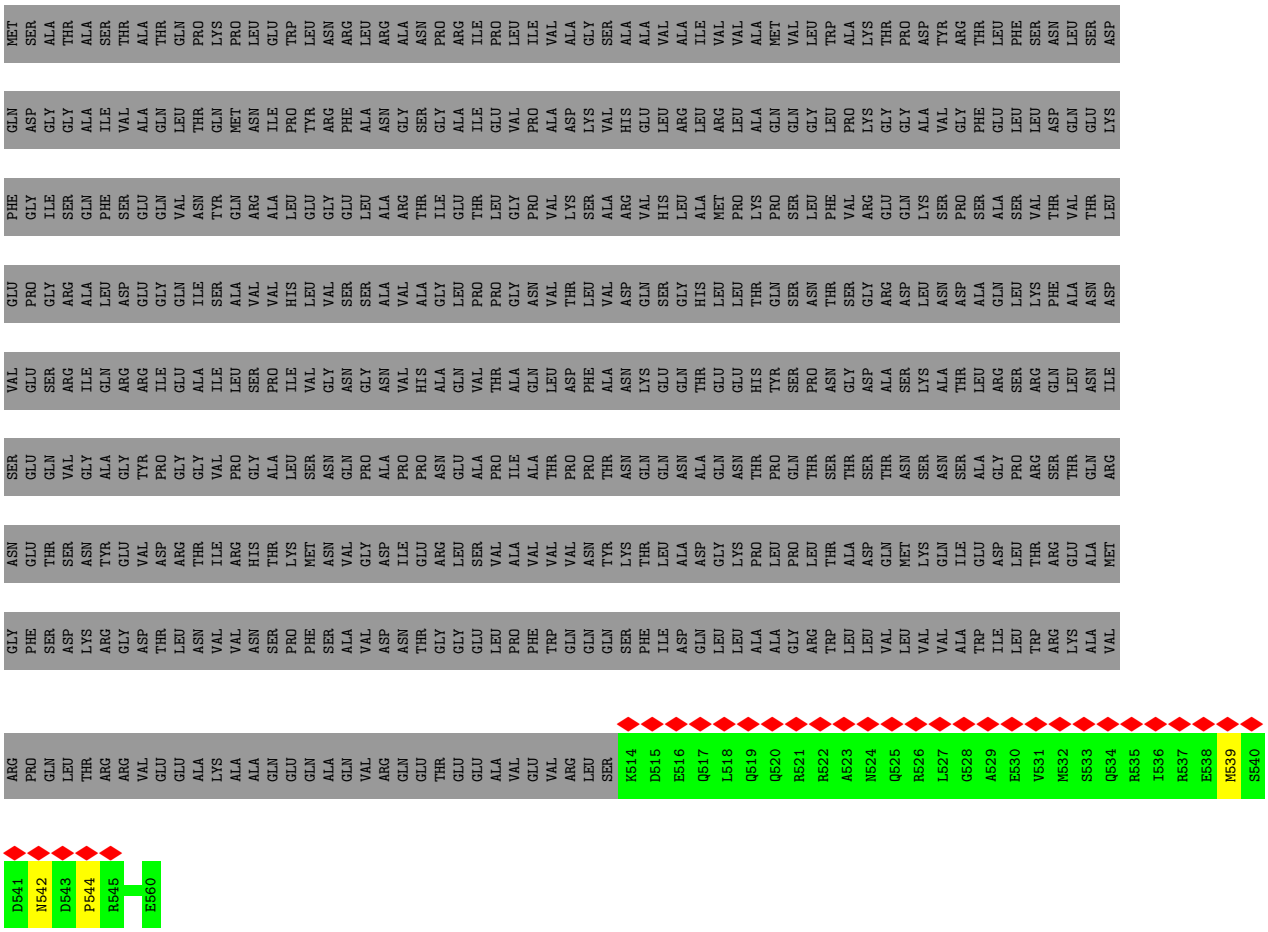
3 Residue-property plots (i)

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

• Molecule 1: Flagellar M-ring protein

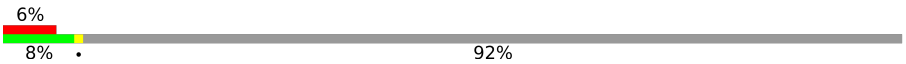
Chain F:

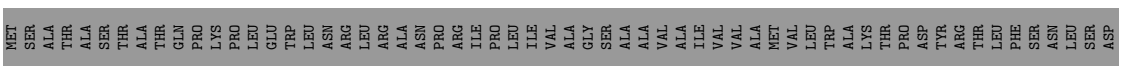


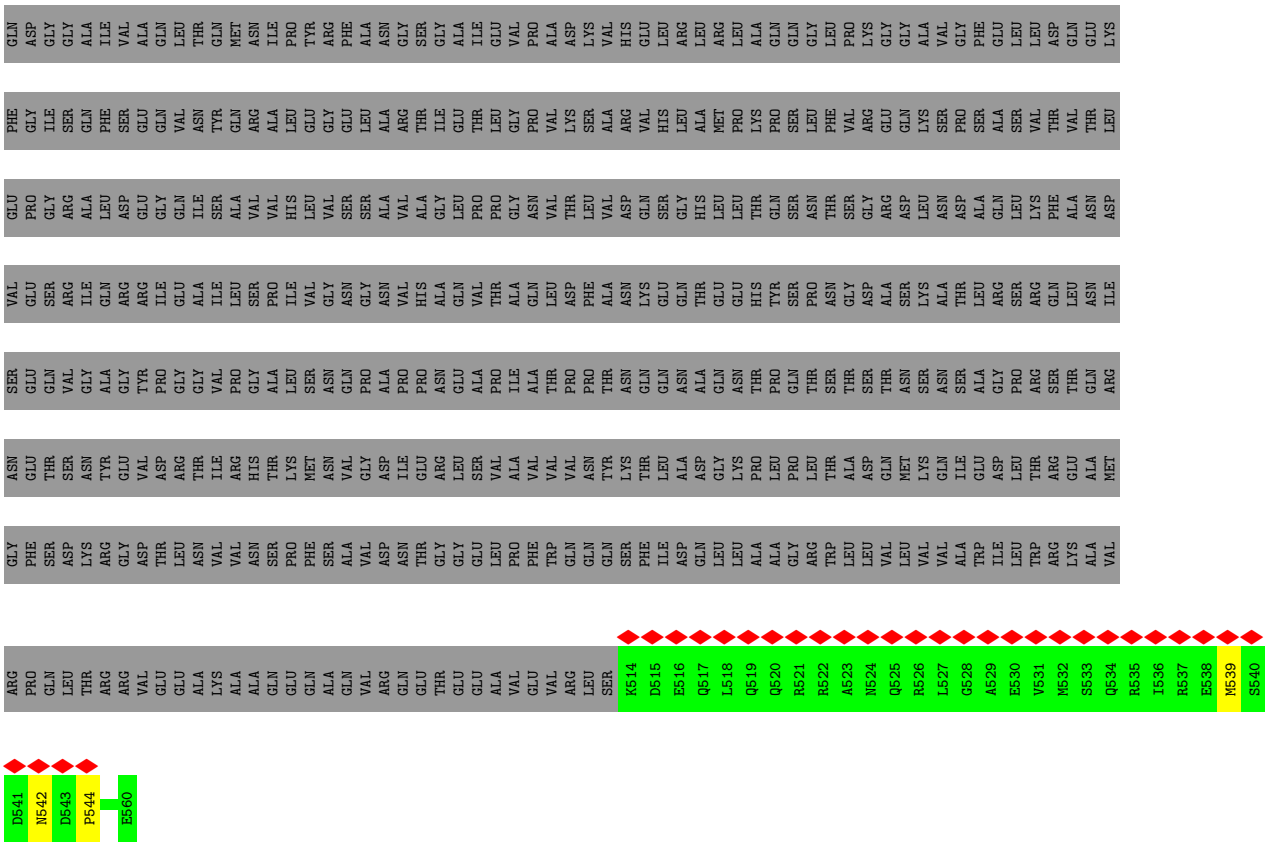


• Molecule 1: Flagellar M-ring protein

Chain A:

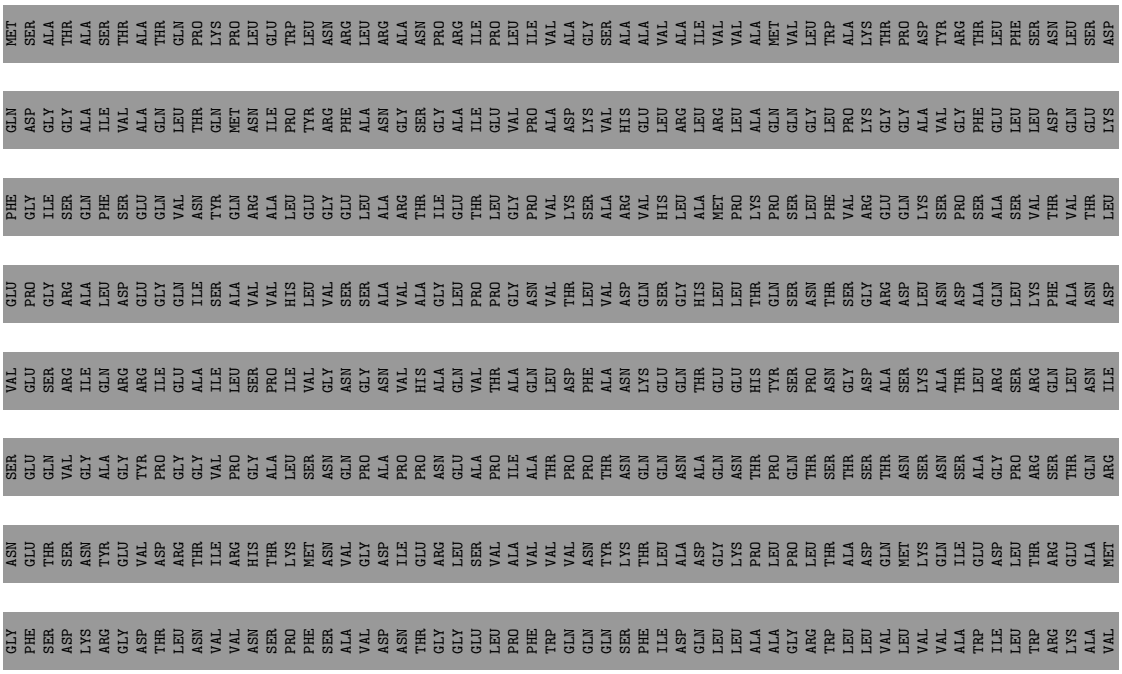


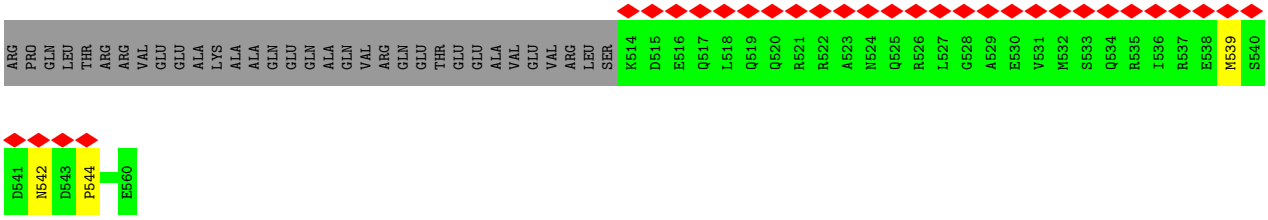




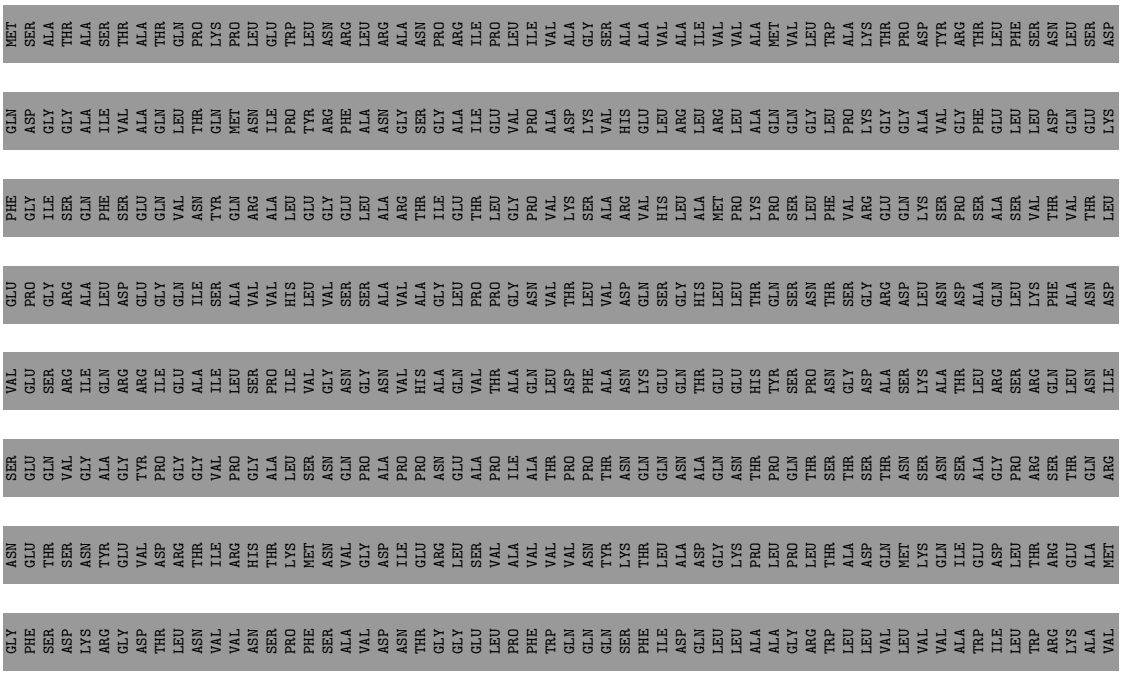
- Molecule 1: Flagellar M-ring protein

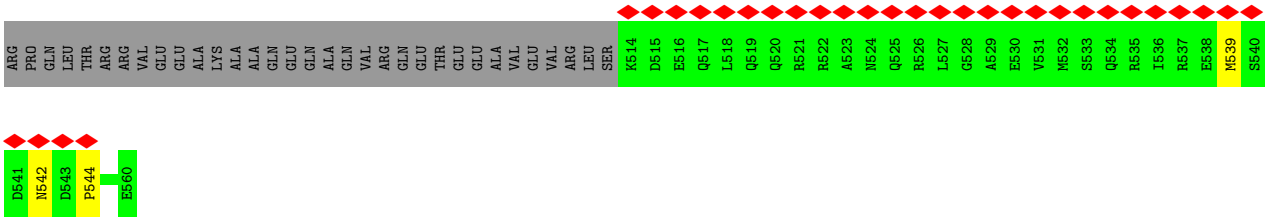
Chain I:



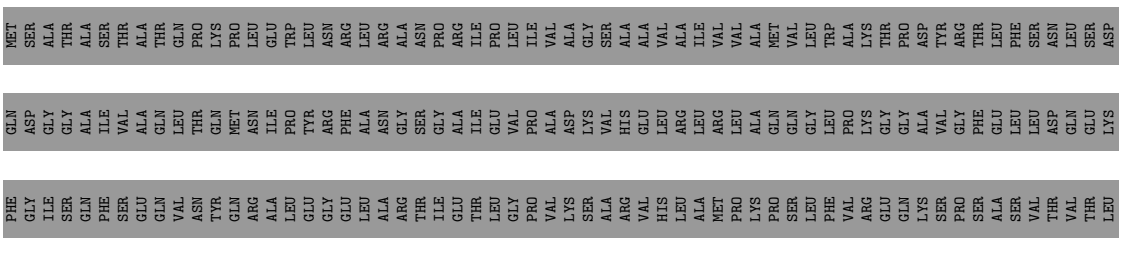


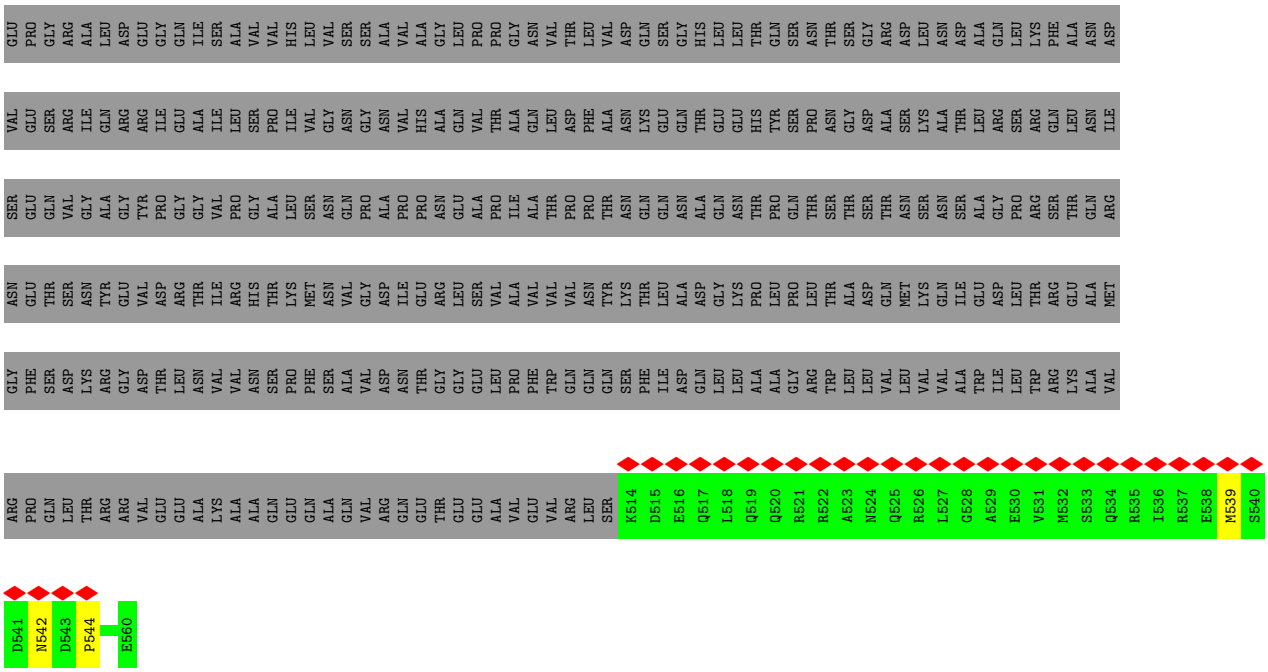
• Molecule 1: Flagellar M-ring protein



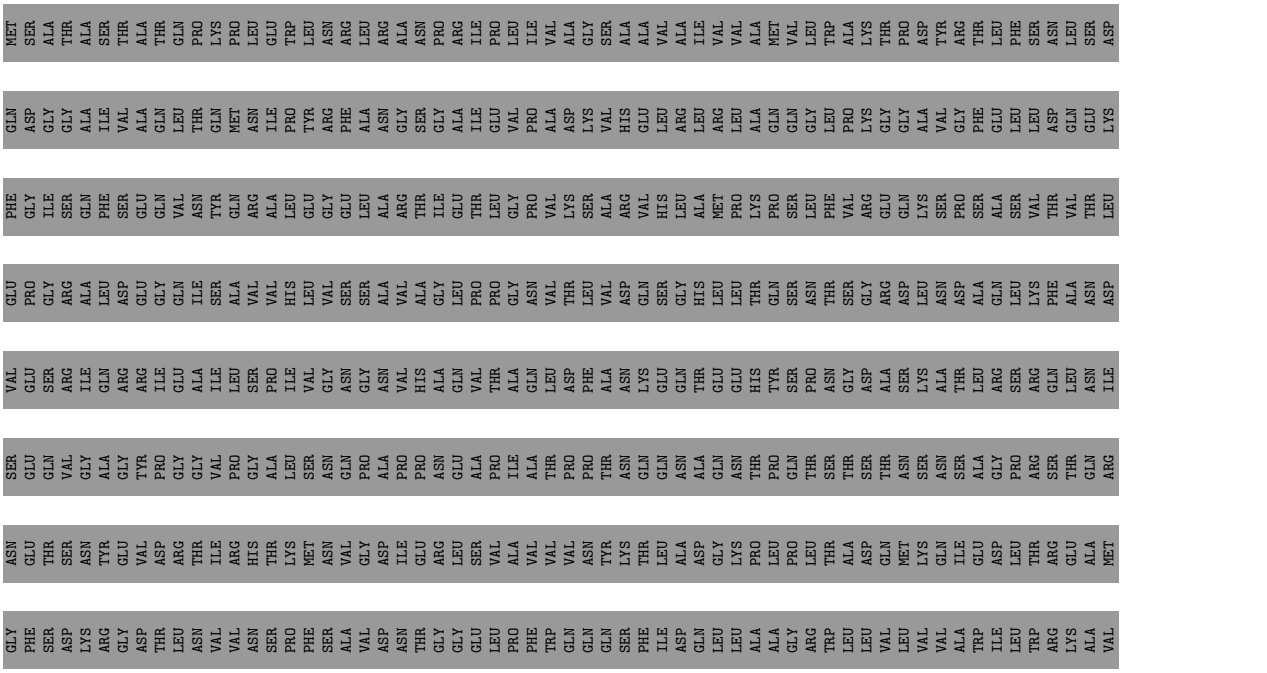


• Molecule 1: Flagellar M-ring protein



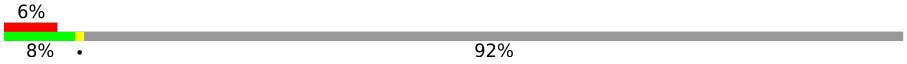


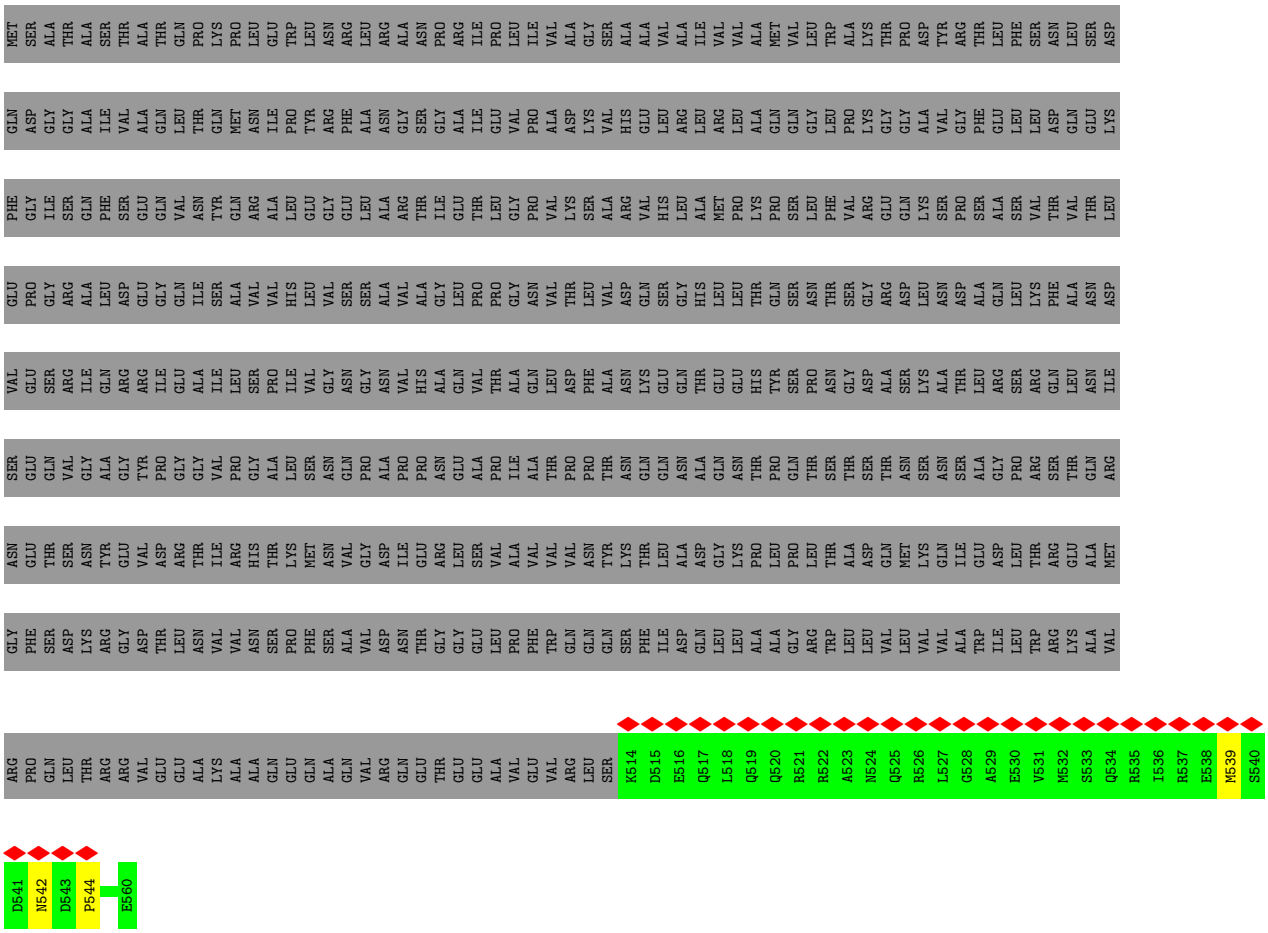
• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein

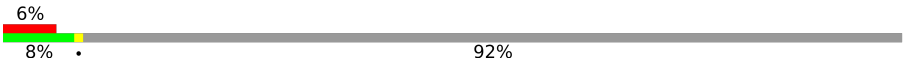
Chain LA:

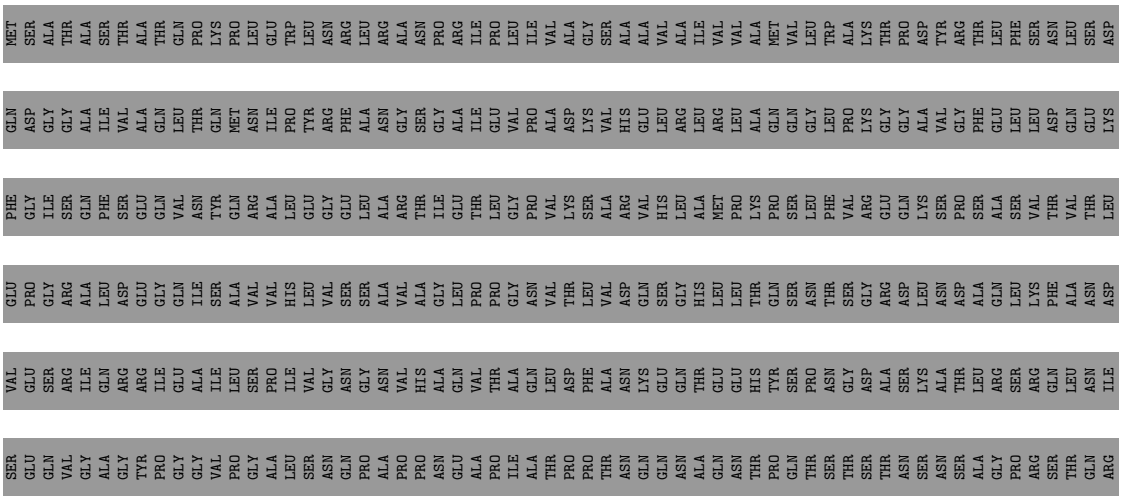


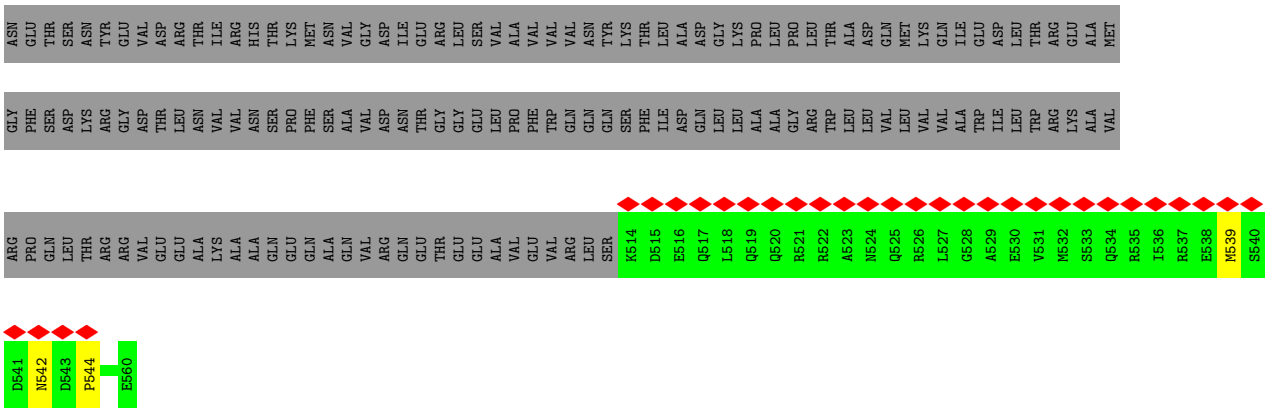


• Molecule 1: Flagellar M-ring protein

Chain RA:

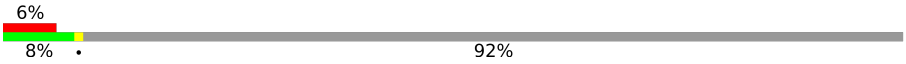


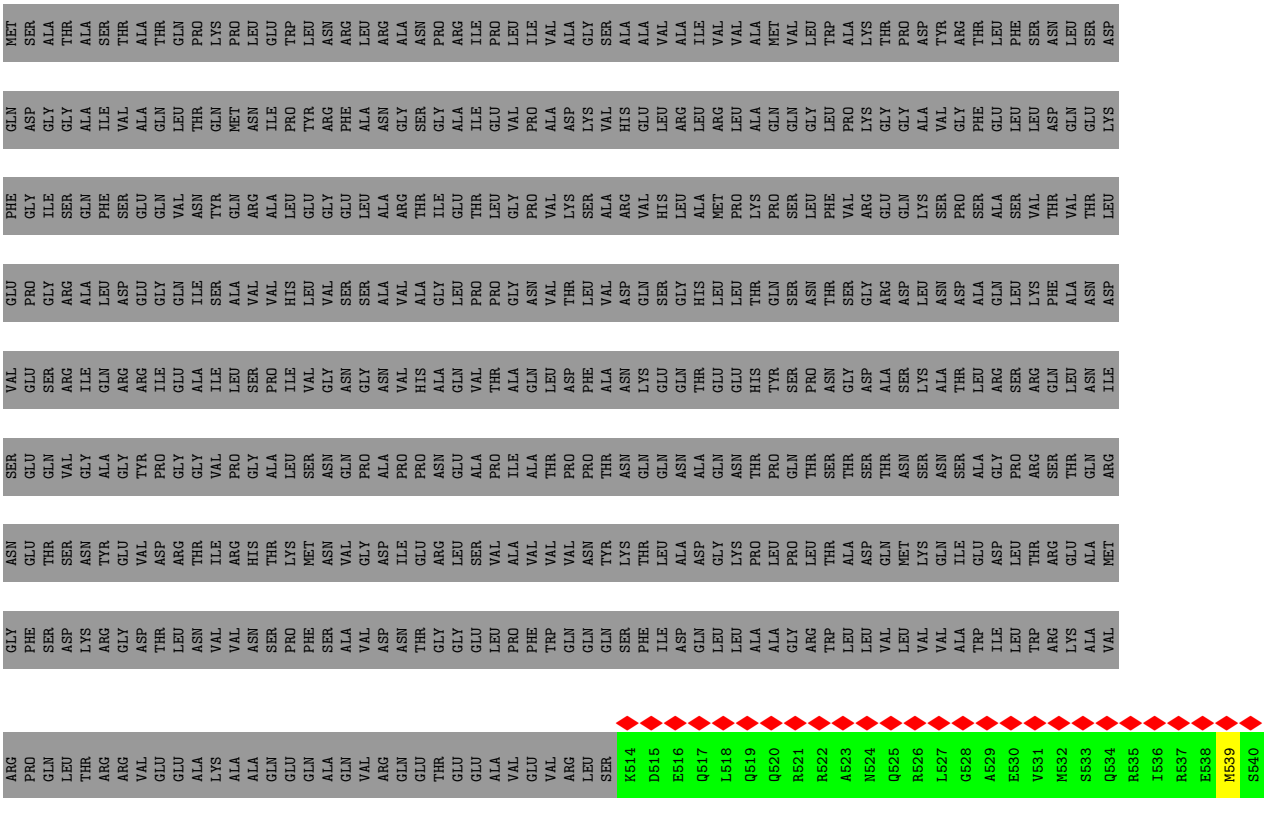




• Molecule 1: Flagellar M-ring protein

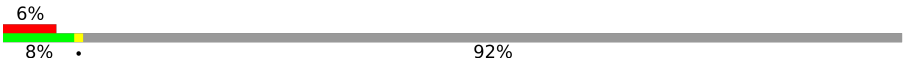
Chain XA:

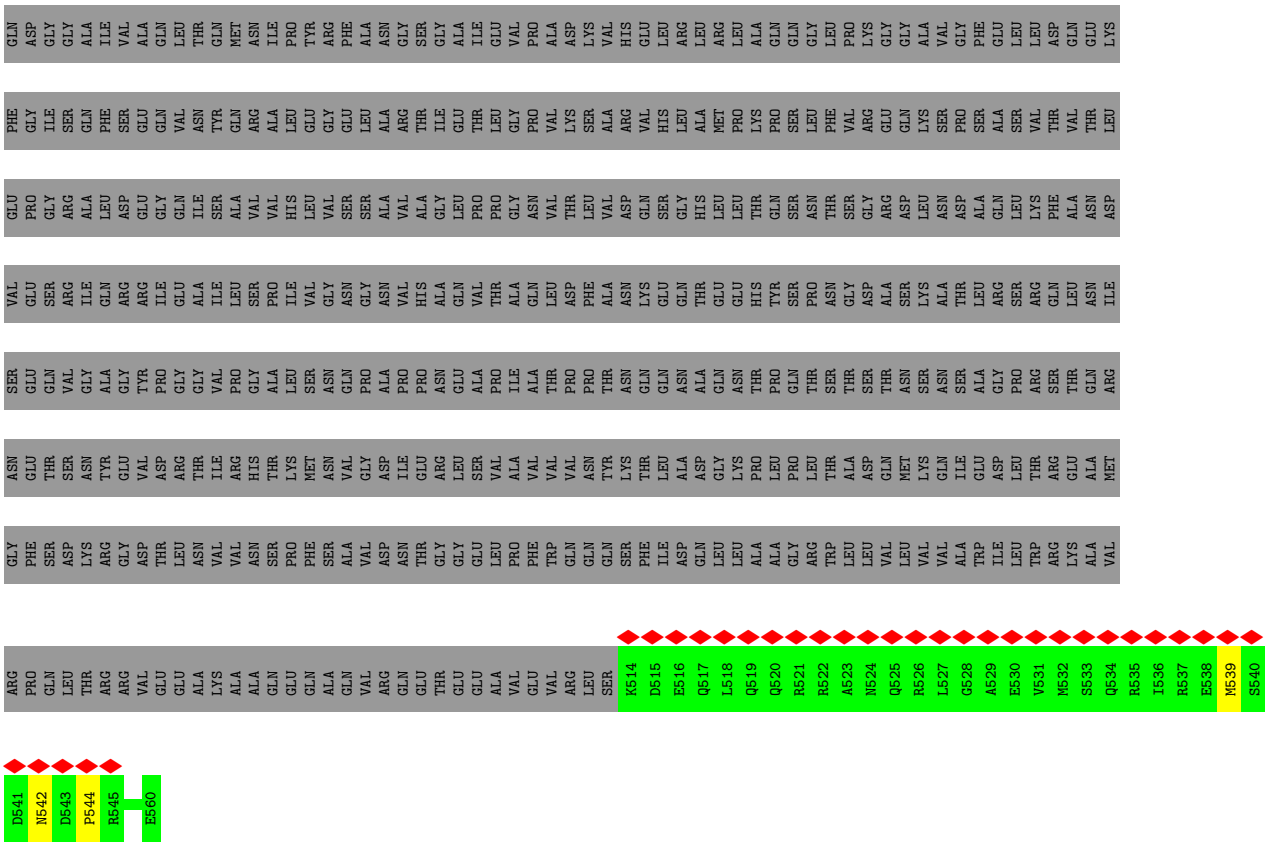




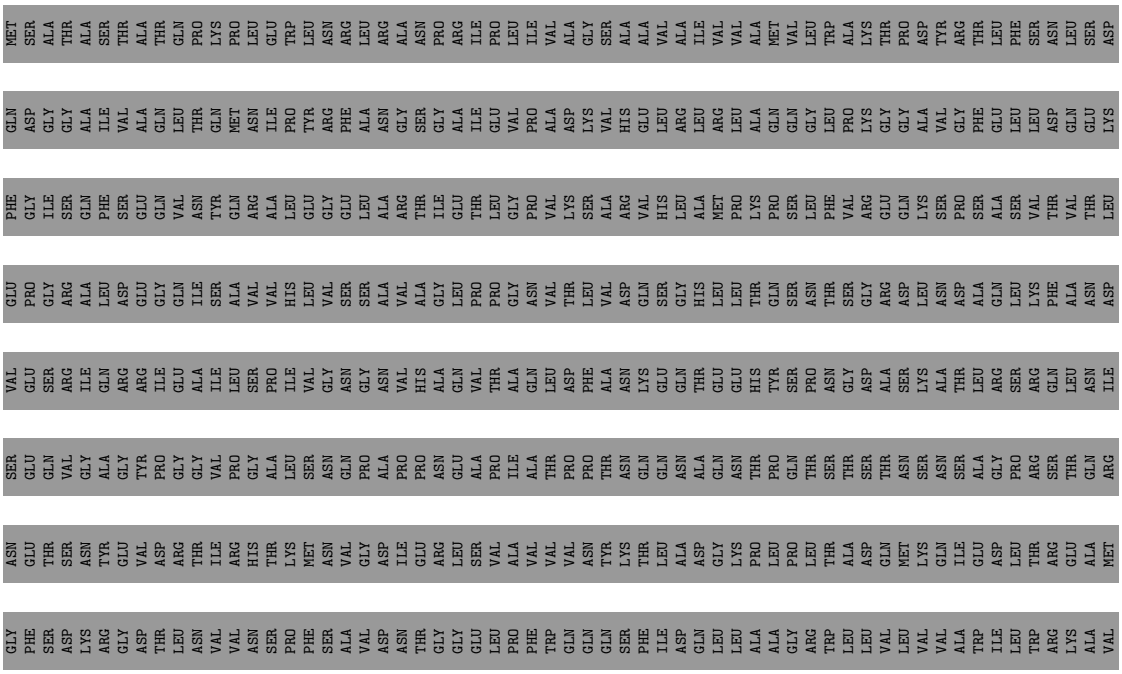
• Molecule 1: Flagellar M-ring protein

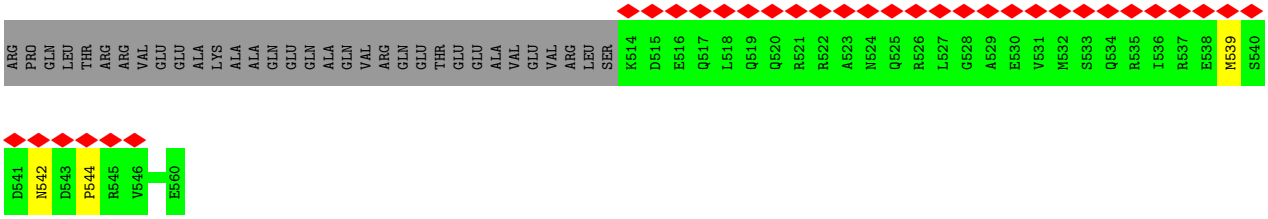
Chain DB:





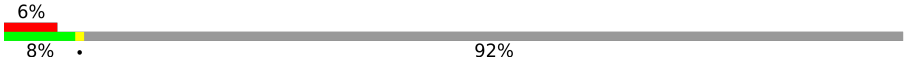
• Molecule 1: Flagellar M-ring protein

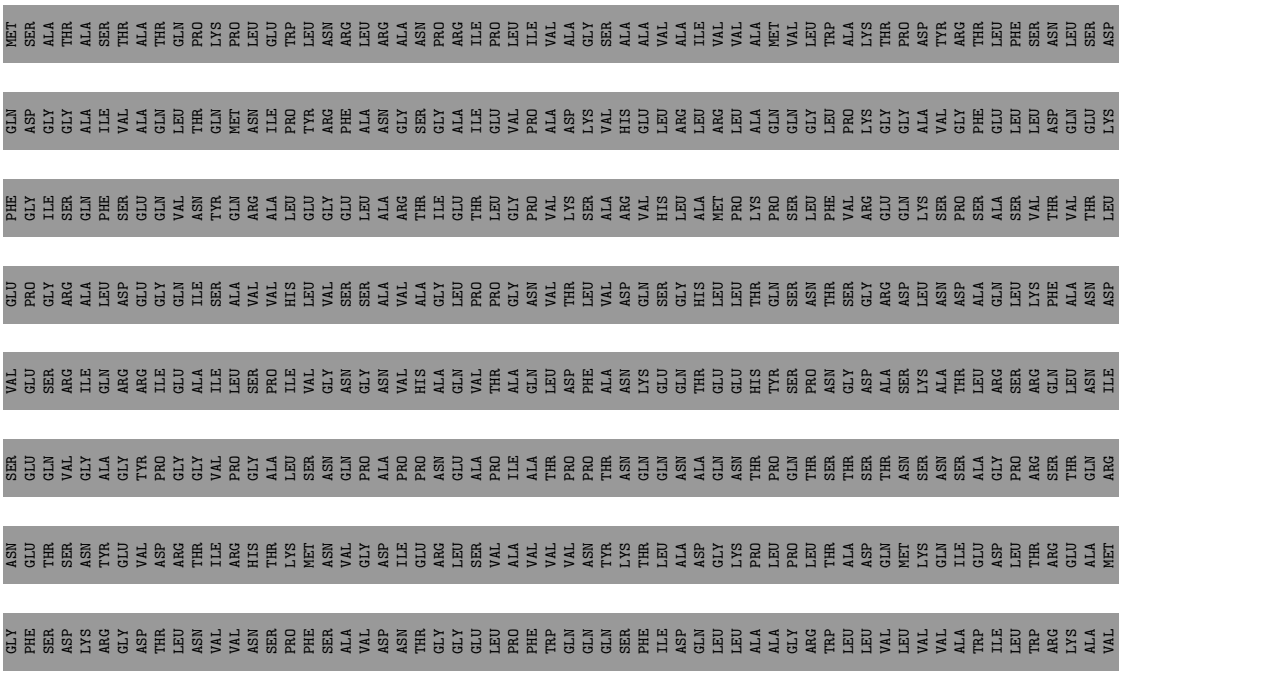


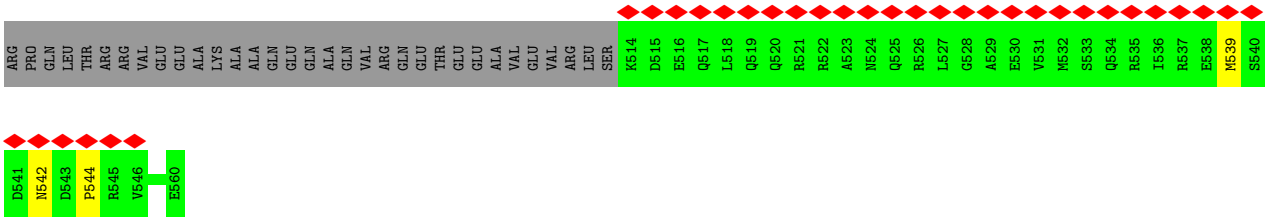


• Molecule 1: Flagellar M-ring protein

Chain PB:

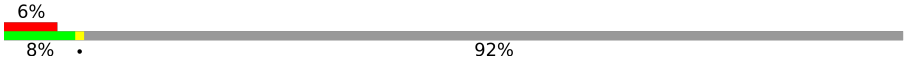


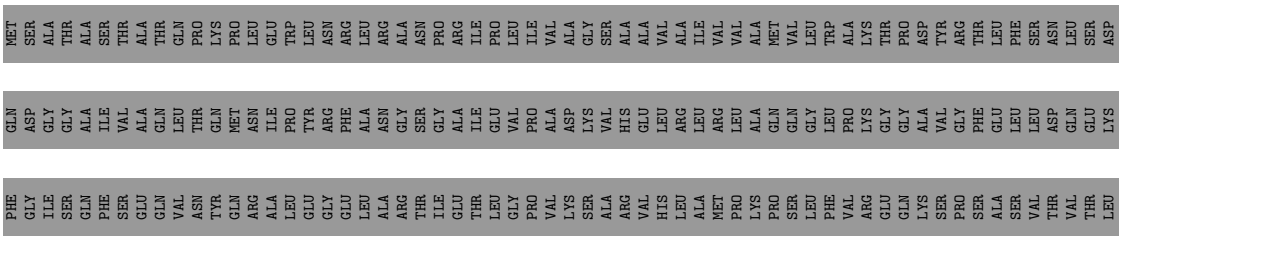


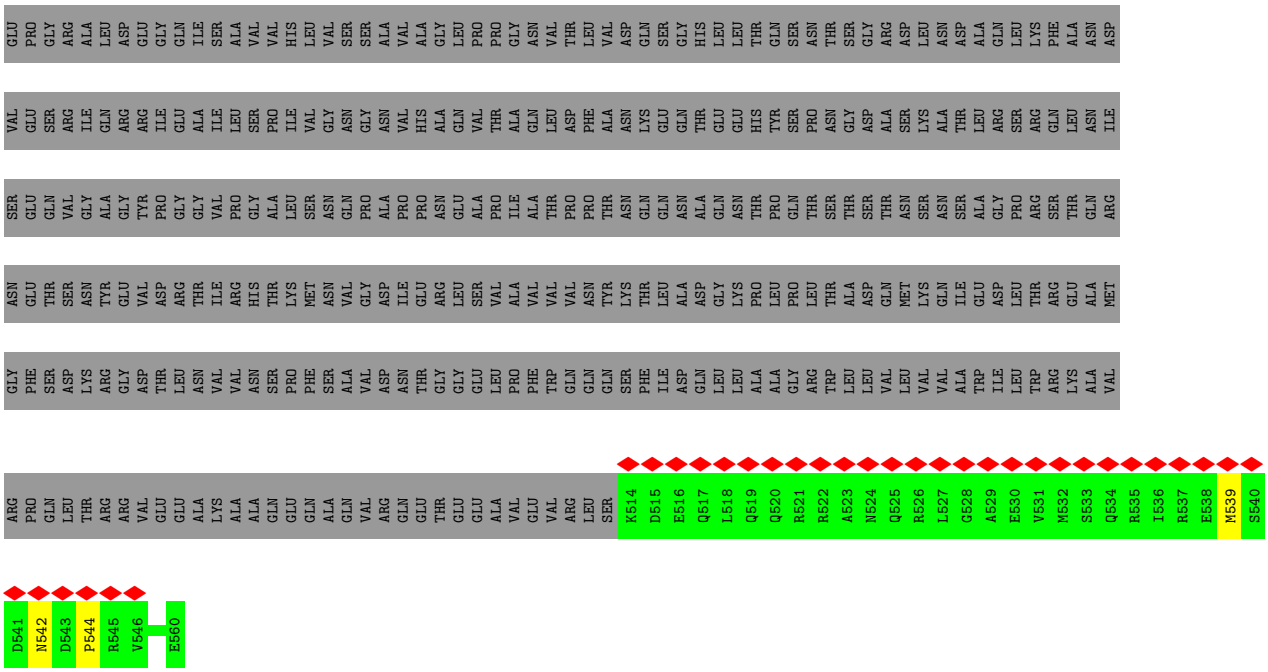


• Molecule 1: Flagellar M-ring protein

Chain VB:

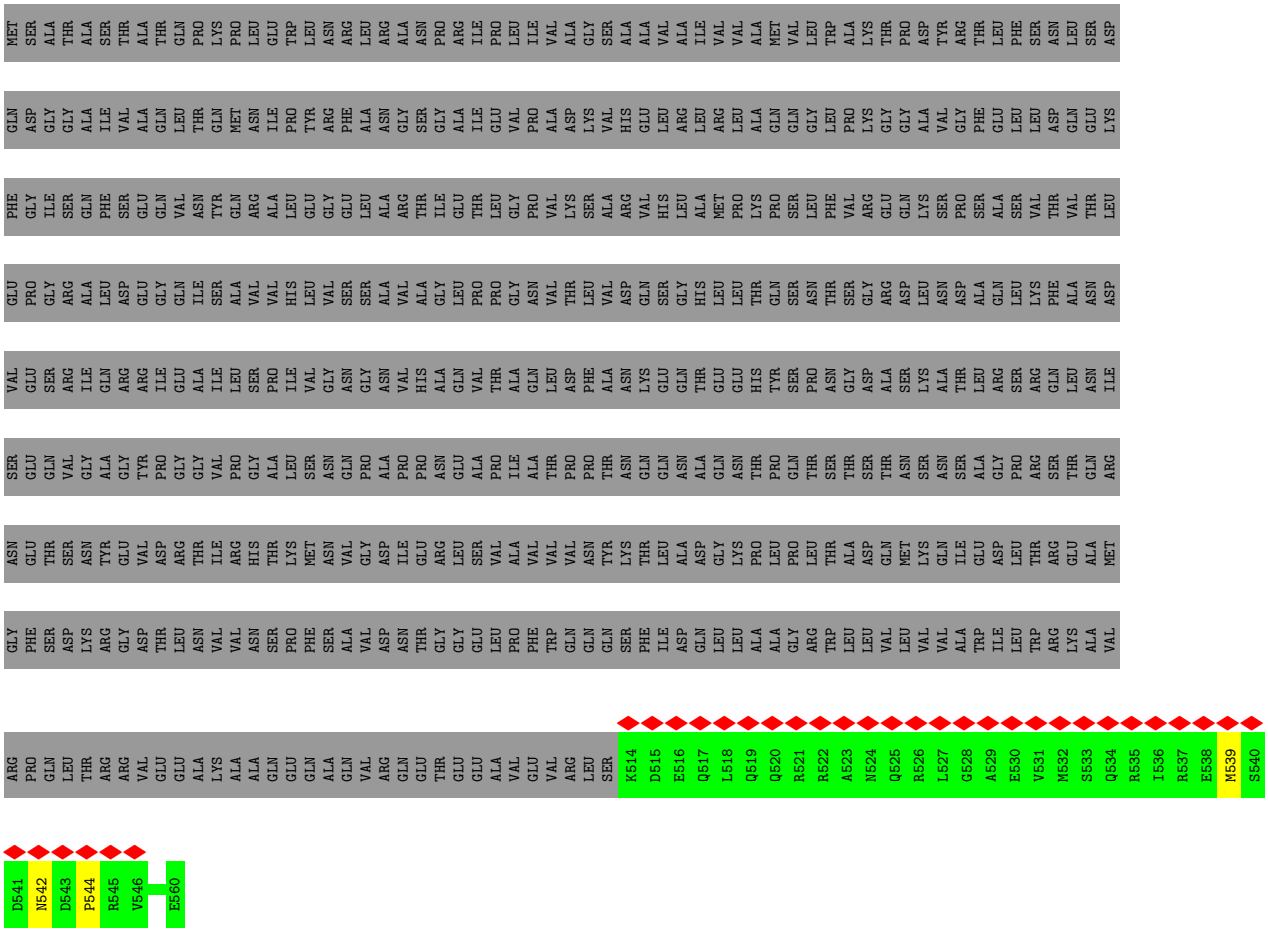






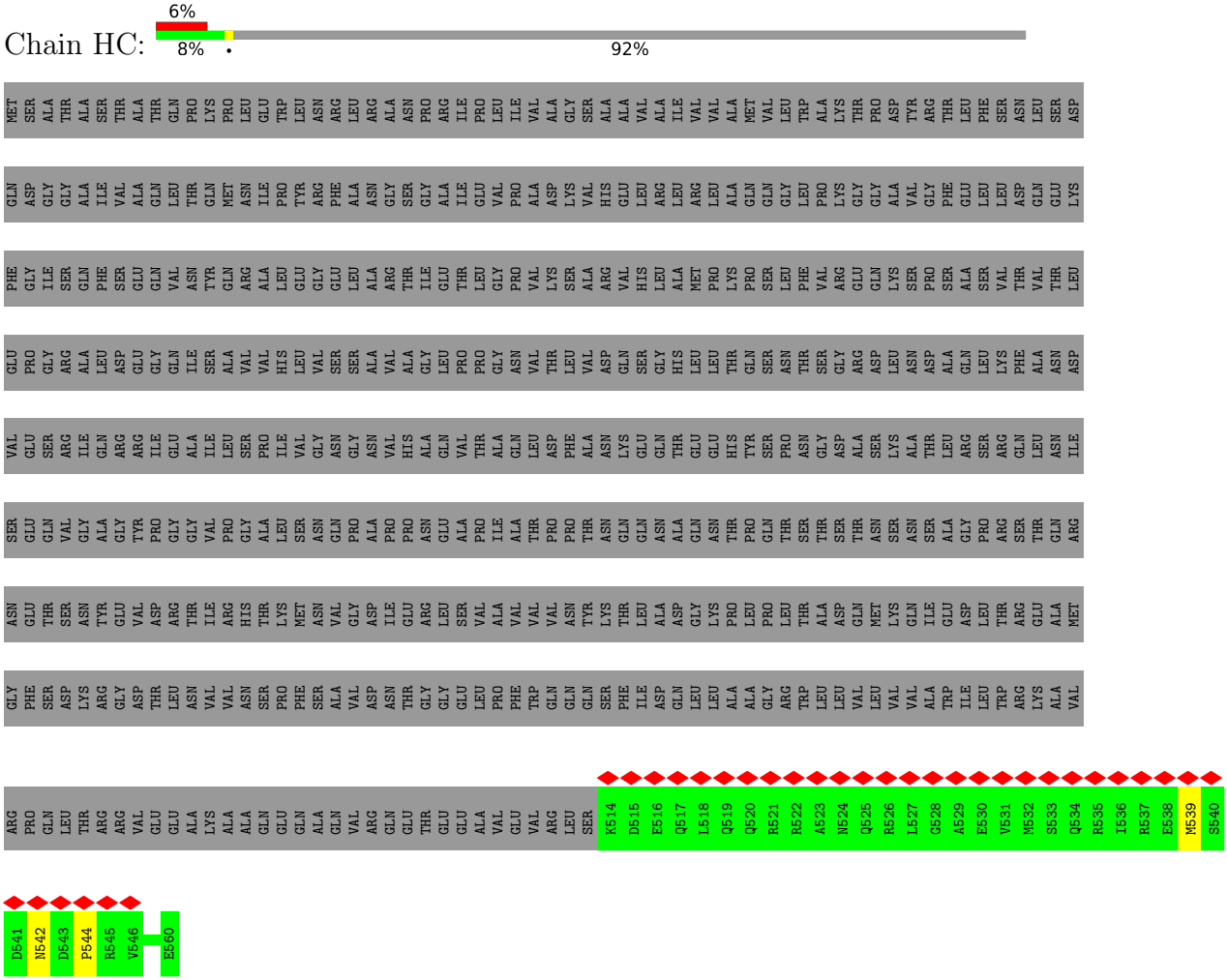
• Molecule 1: Flagellar M-ring protein

Chain BC: 6% 8% 92%



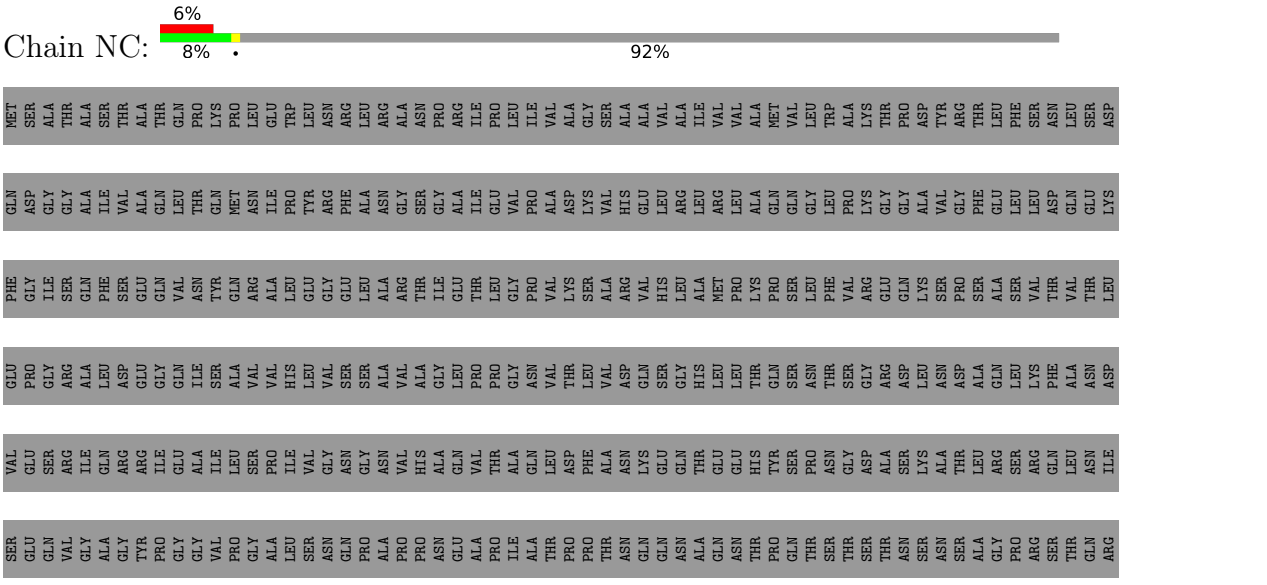
• Molecule 1: Flagellar M-ring protein

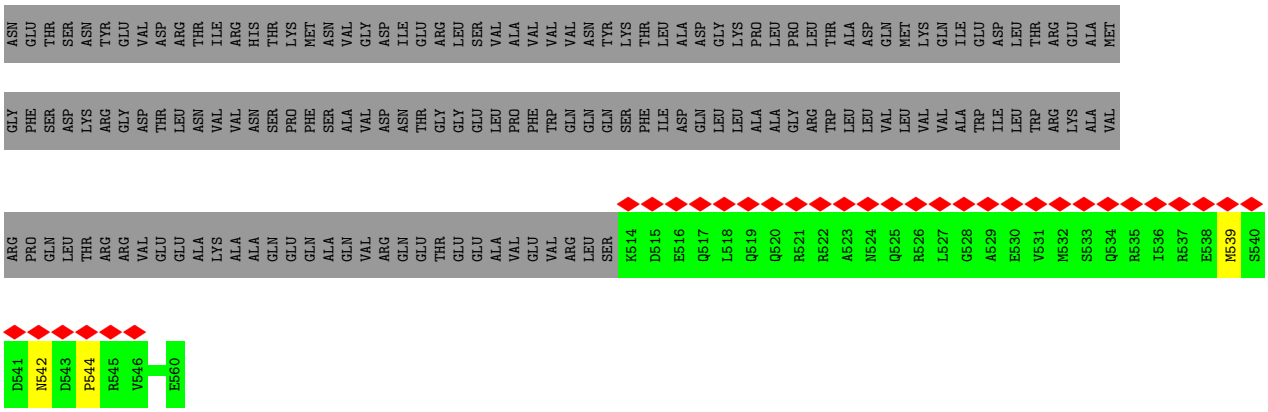
Chain HC:



• Molecule 1: Flagellar M-ring protein

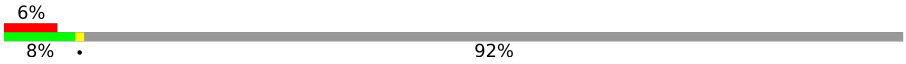
Chain NC:

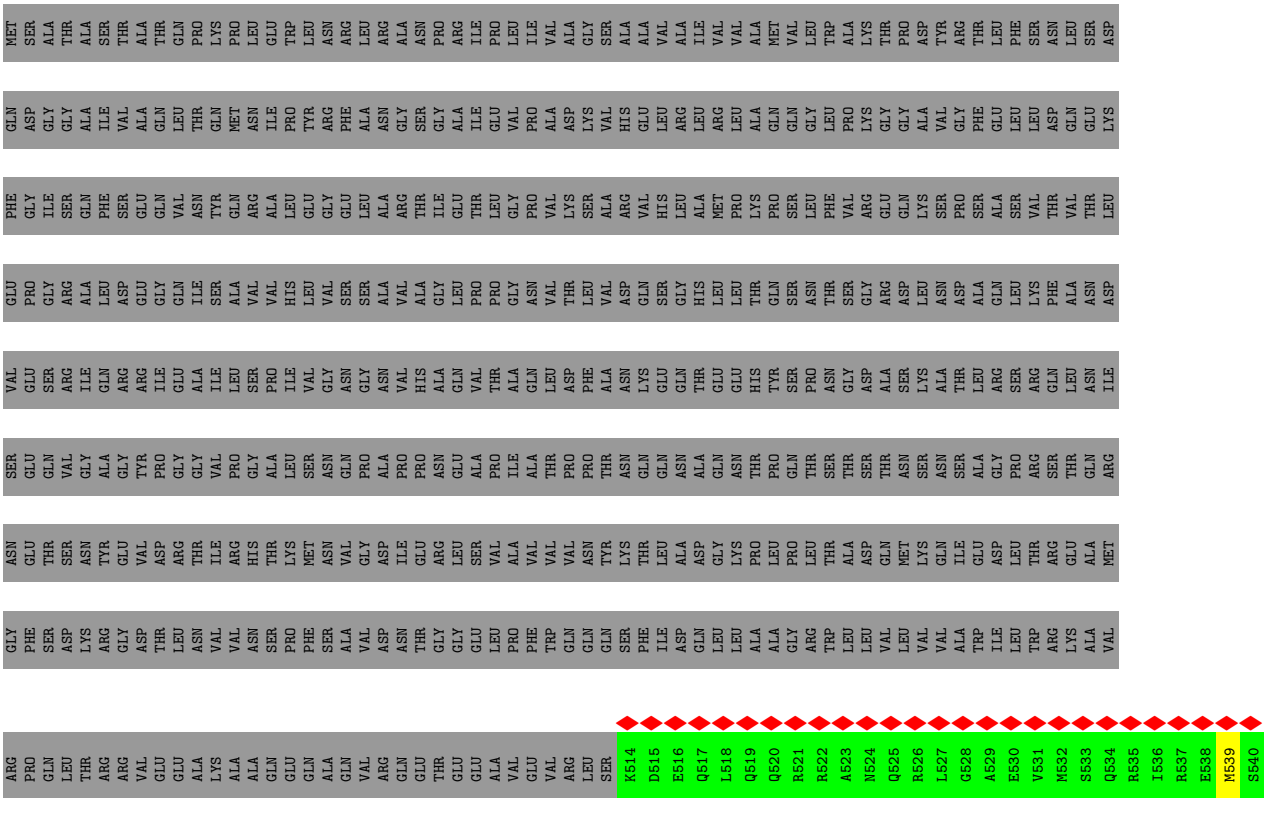




• Molecule 1: Flagellar M-ring protein

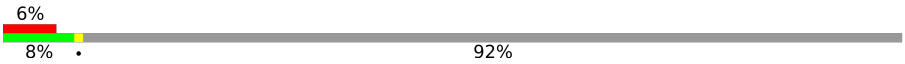
Chain TC:

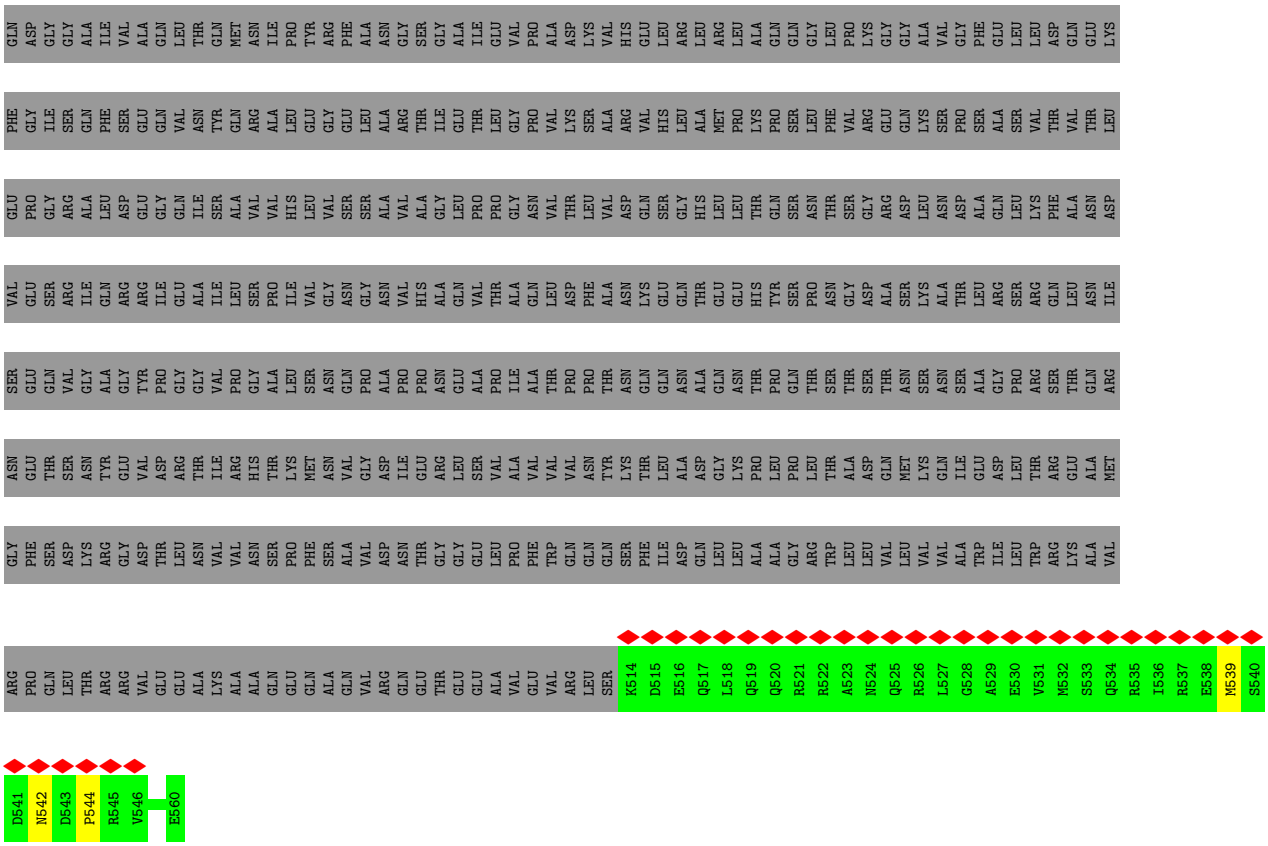




• Molecule 1: Flagellar M-ring protein

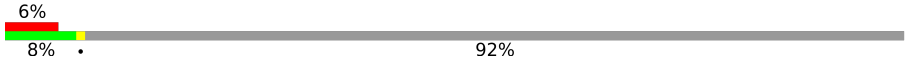
Chain ZC:

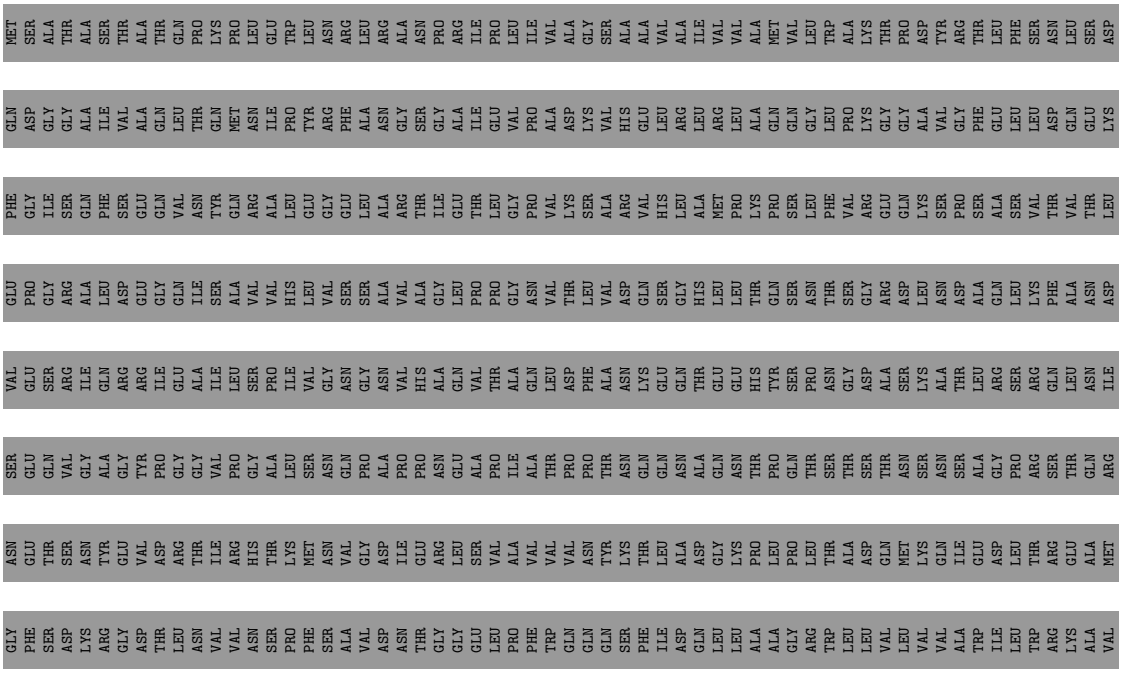


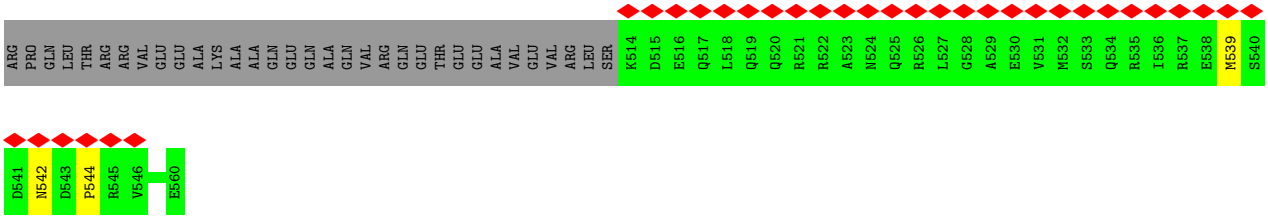


- Molecule 1: Flagellar M-ring protein

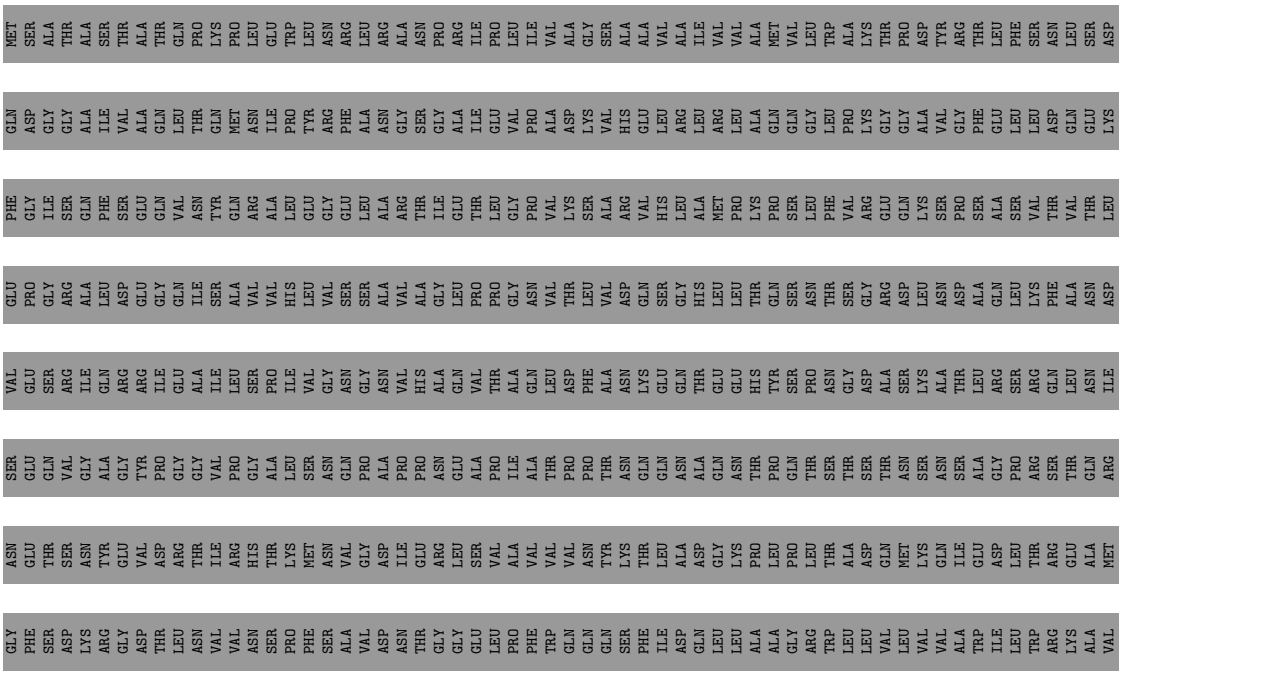
Chain FD:

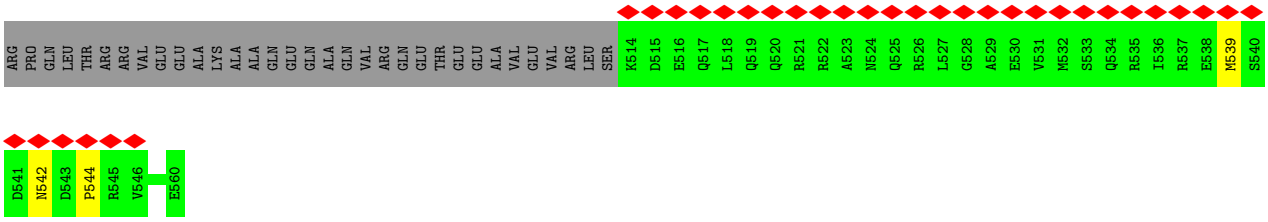




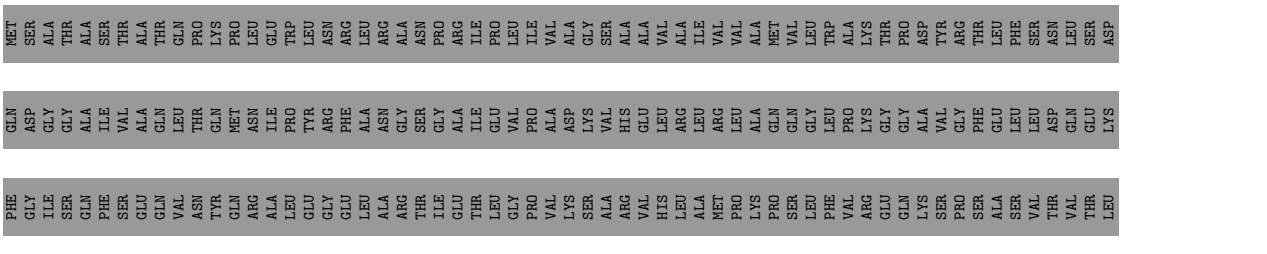


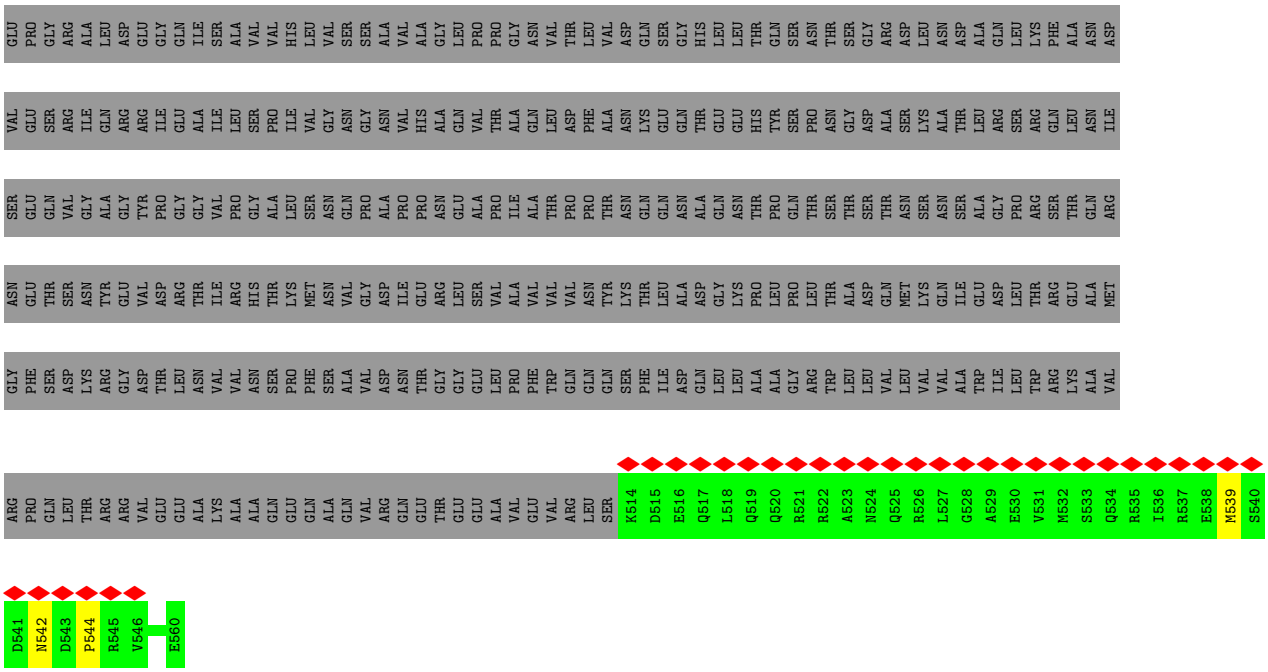
• Molecule 1: Flagellar M-ring protein





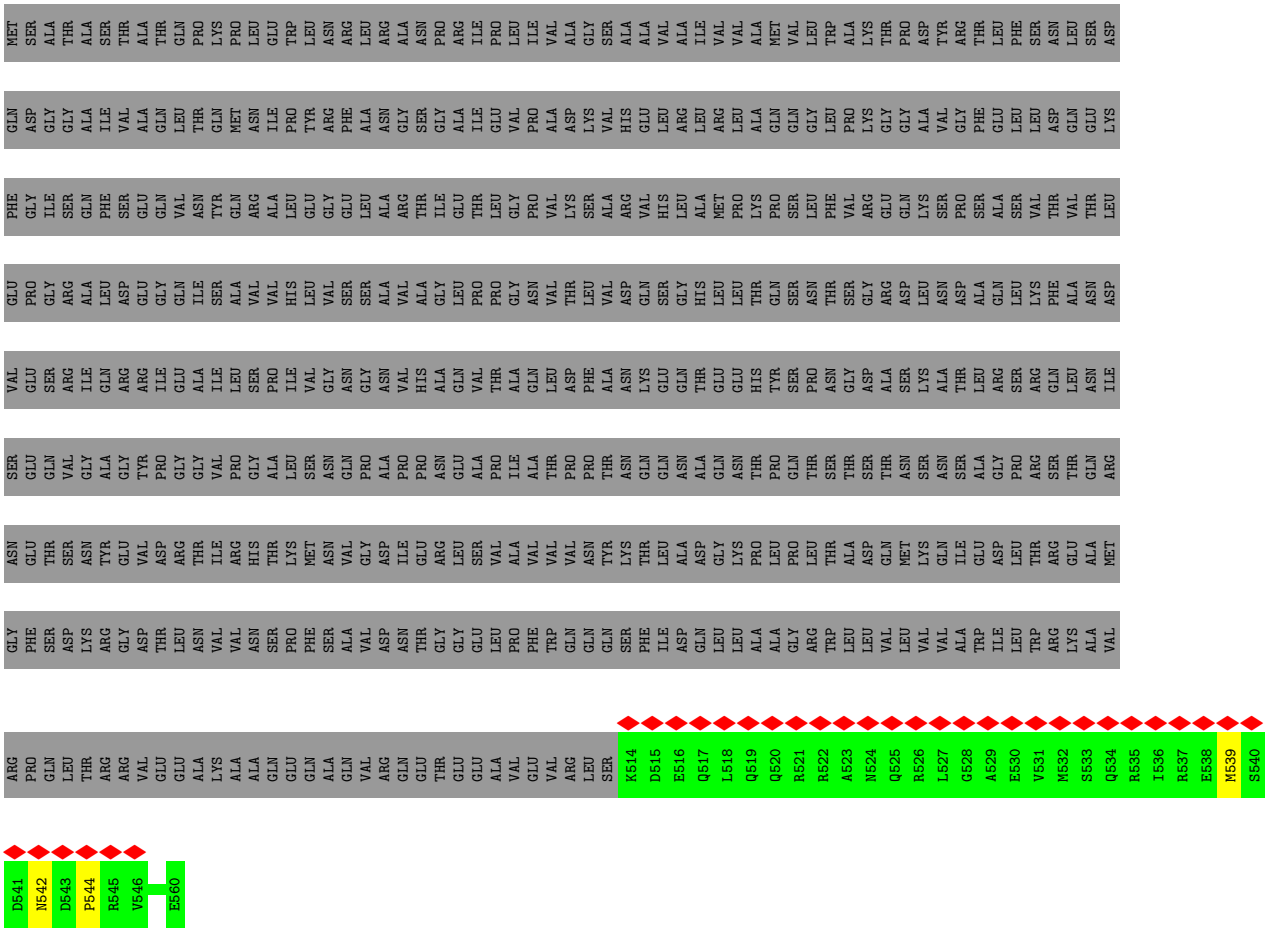
• Molecule 1: Flagellar M-ring protein





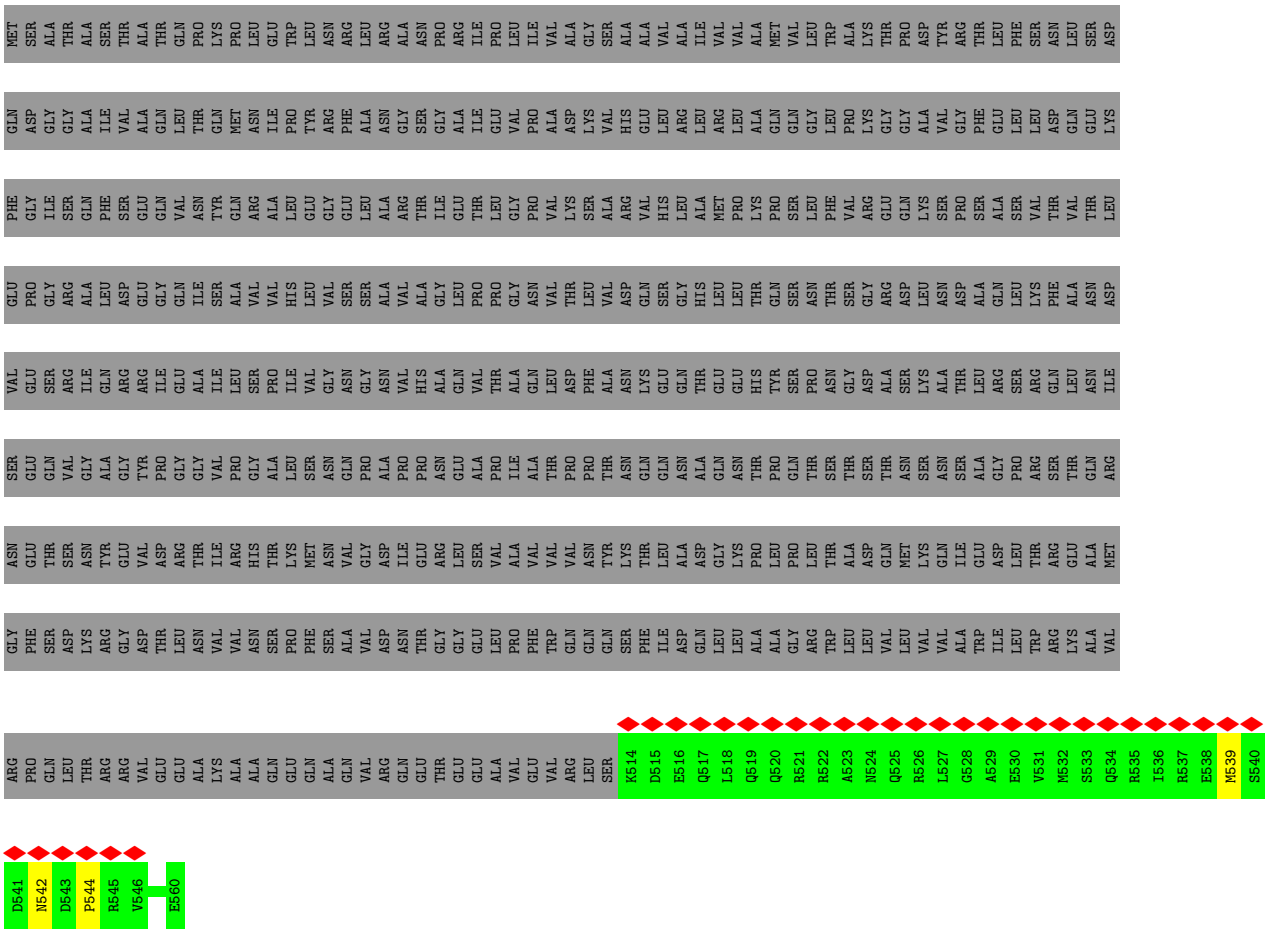
• Molecule 1: Flagellar M-ring protein

Chain XD: 6% 8% 92%



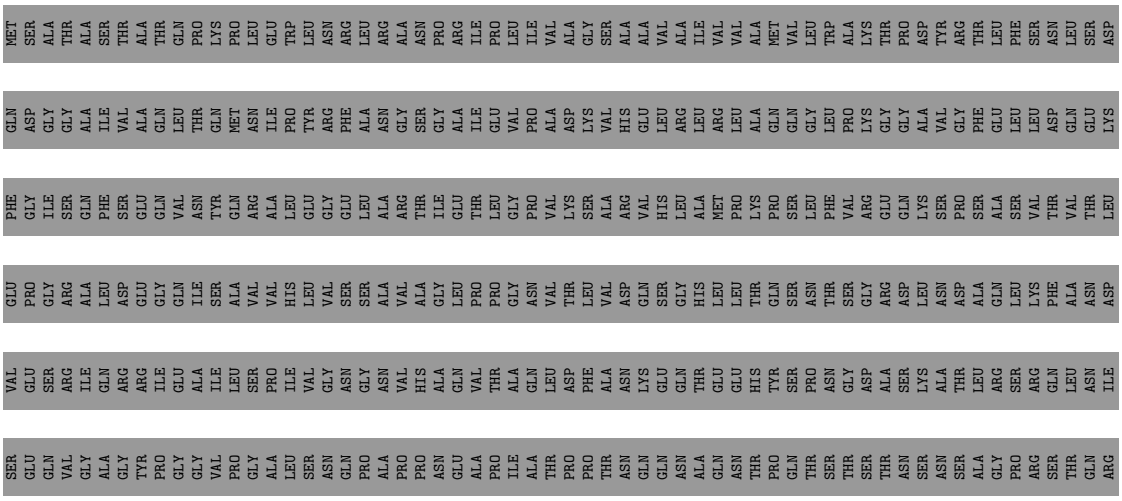
• Molecule 1: Flagellar M-ring protein

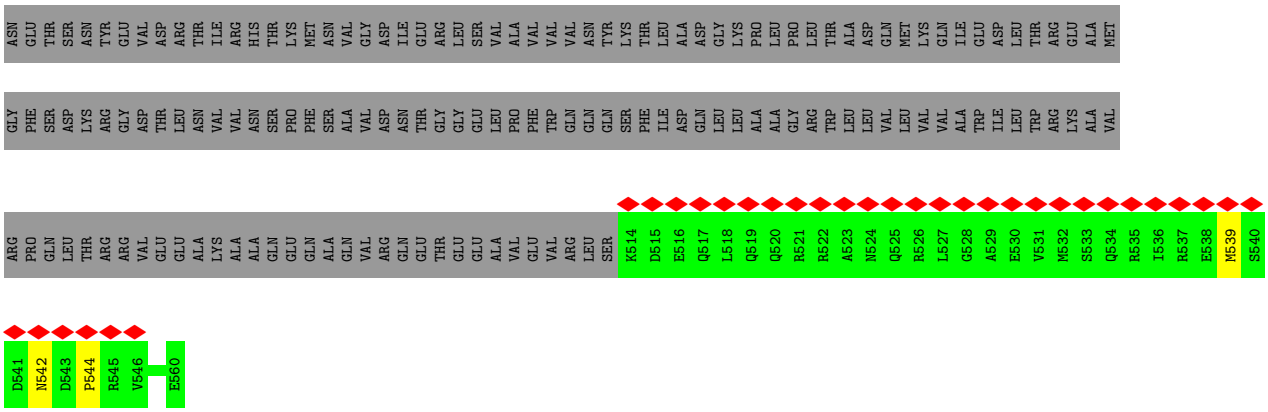
Chain DE:



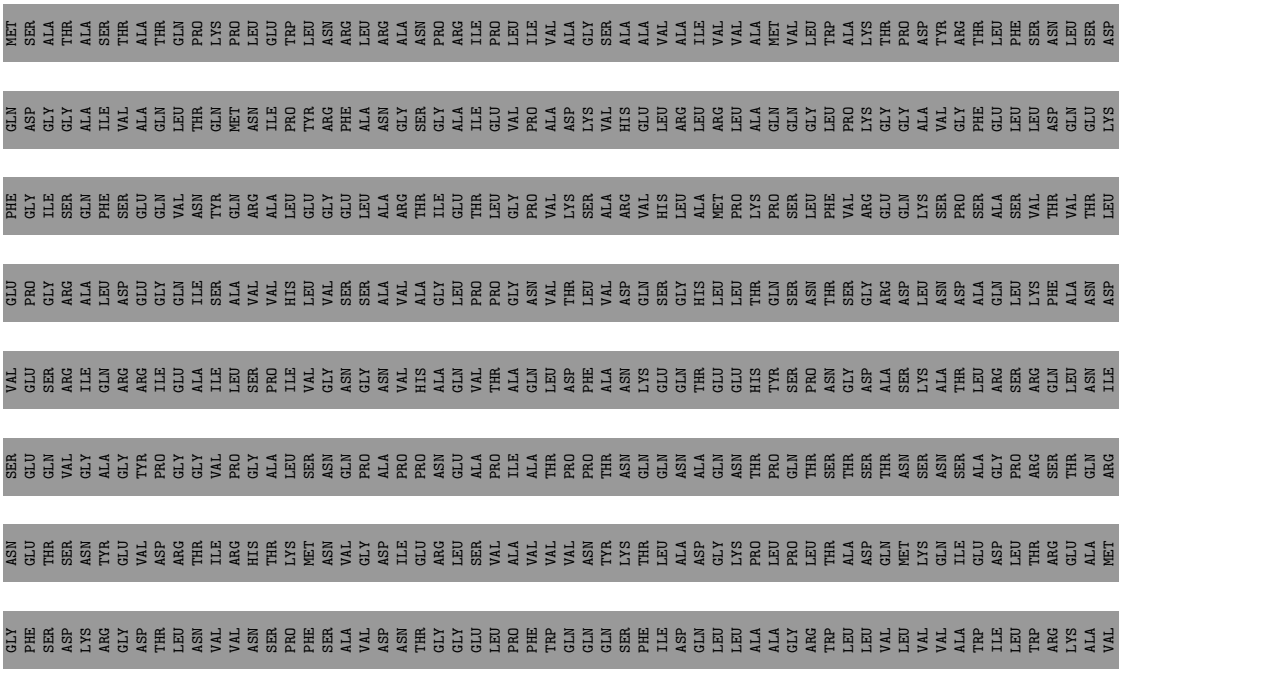
• Molecule 1: Flagellar M-ring protein

Chain JE:

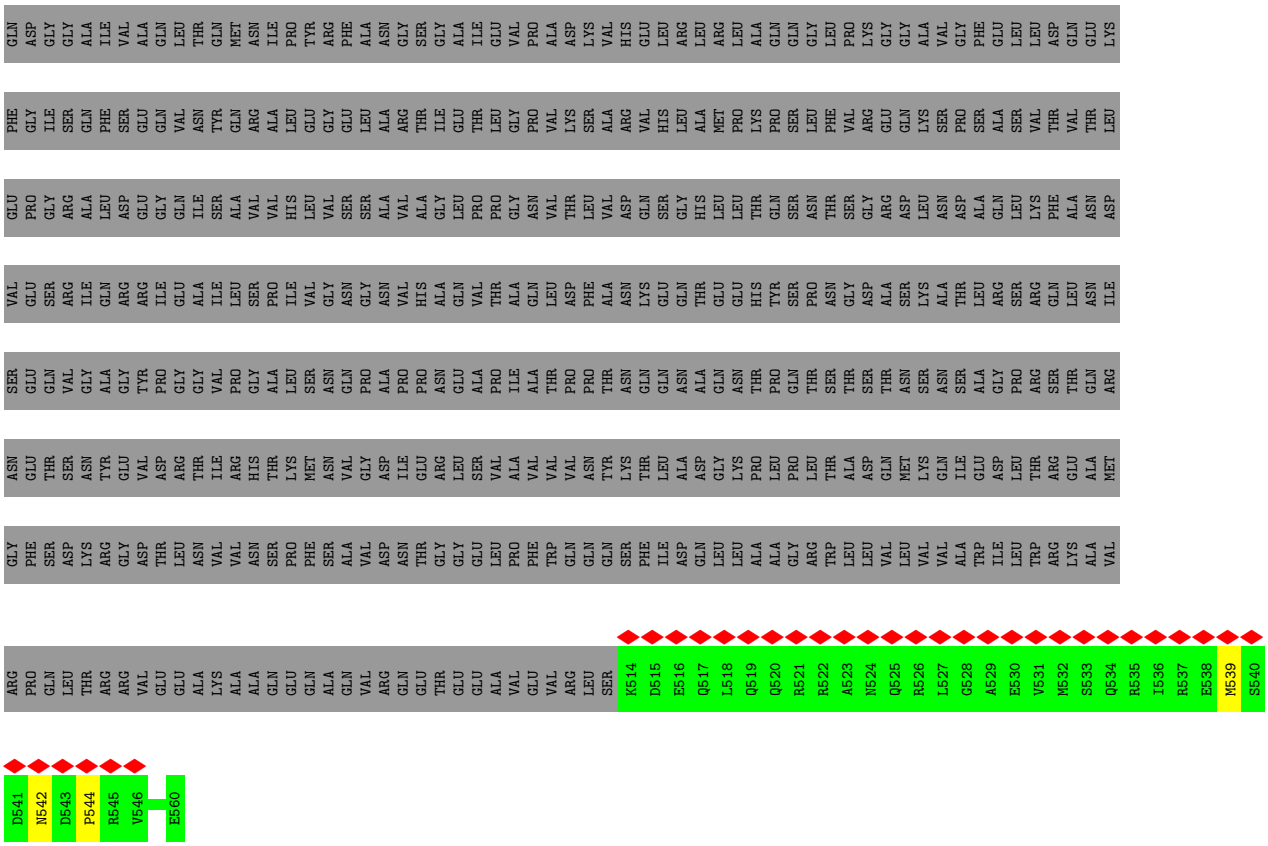




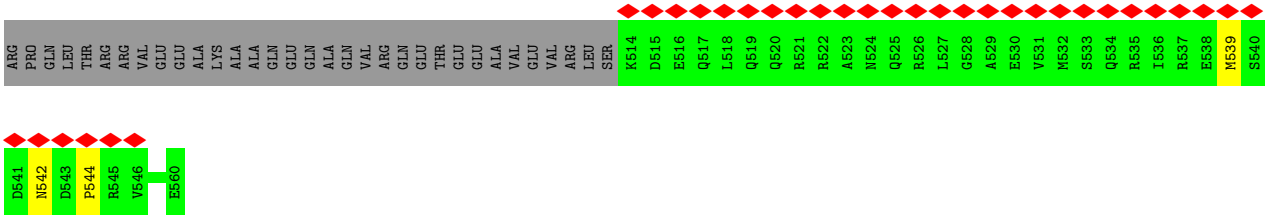
• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein

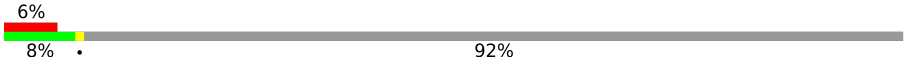


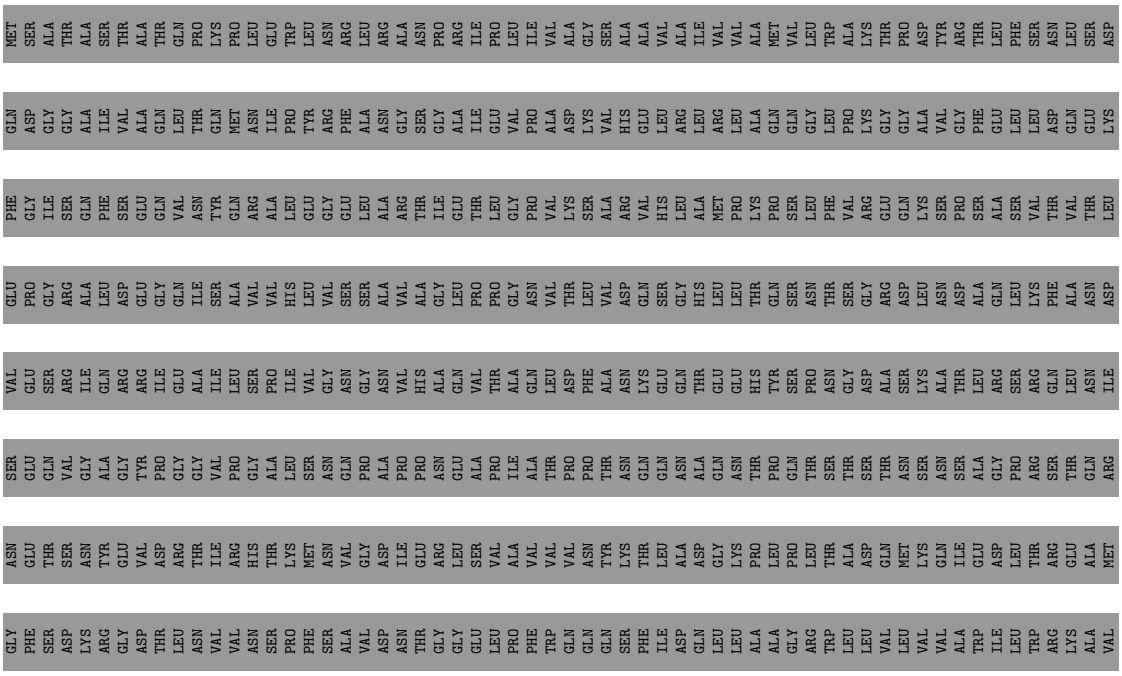
• Molecule 1: Flagellar M-ring protein

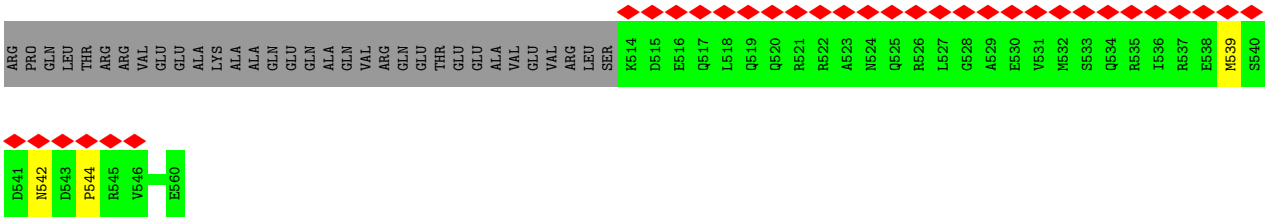


• Molecule 1: Flagellar M-ring protein

Chain HF:

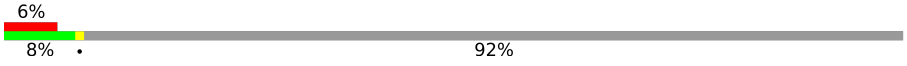


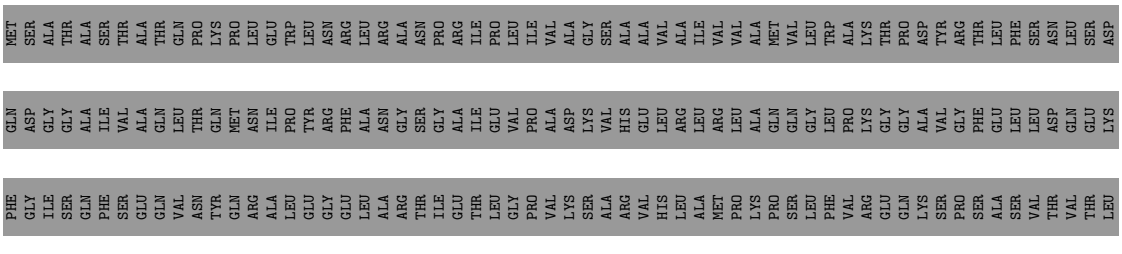


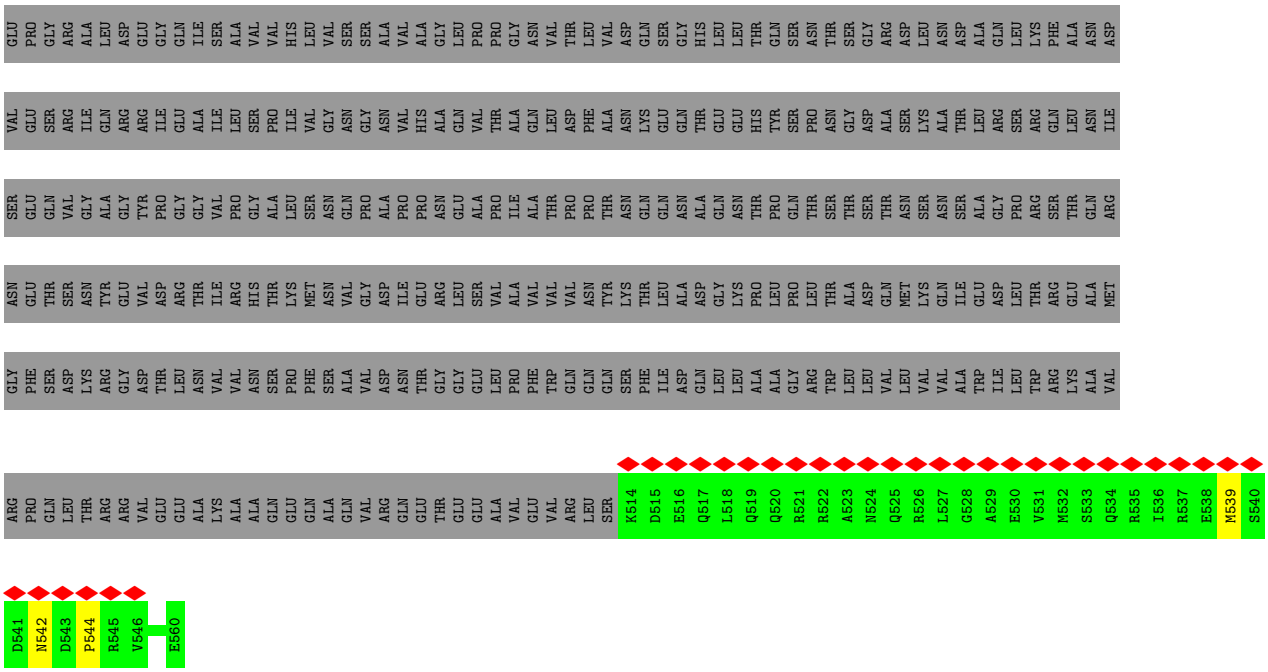


• Molecule 1: Flagellar M-ring protein

Chain NF:

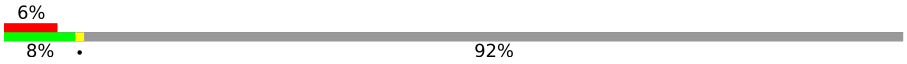


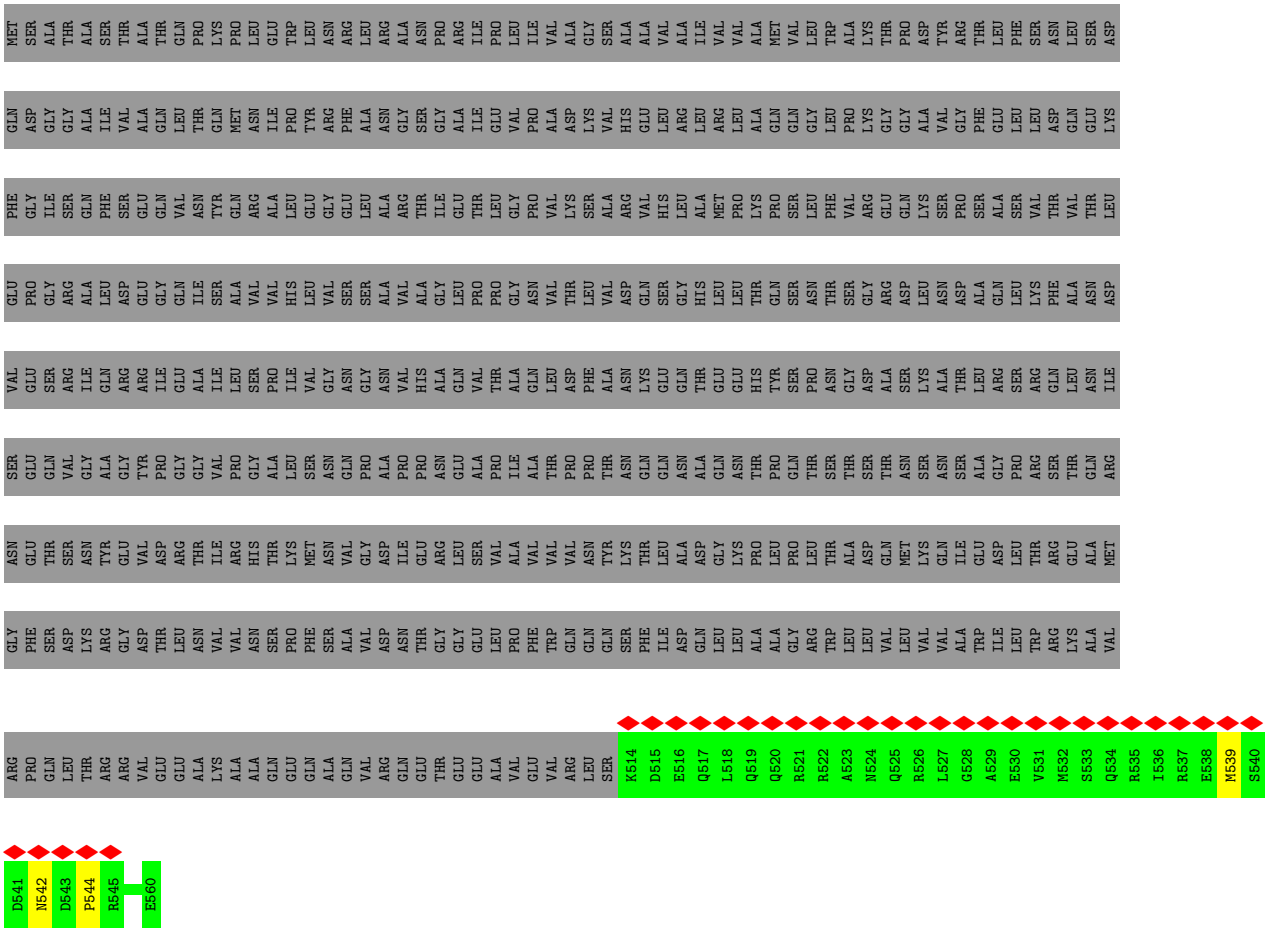




• Molecule 1: Flagellar M-ring protein

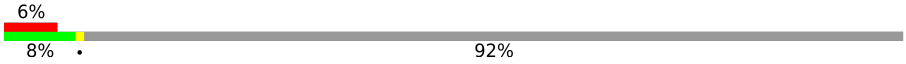
Chain TF:

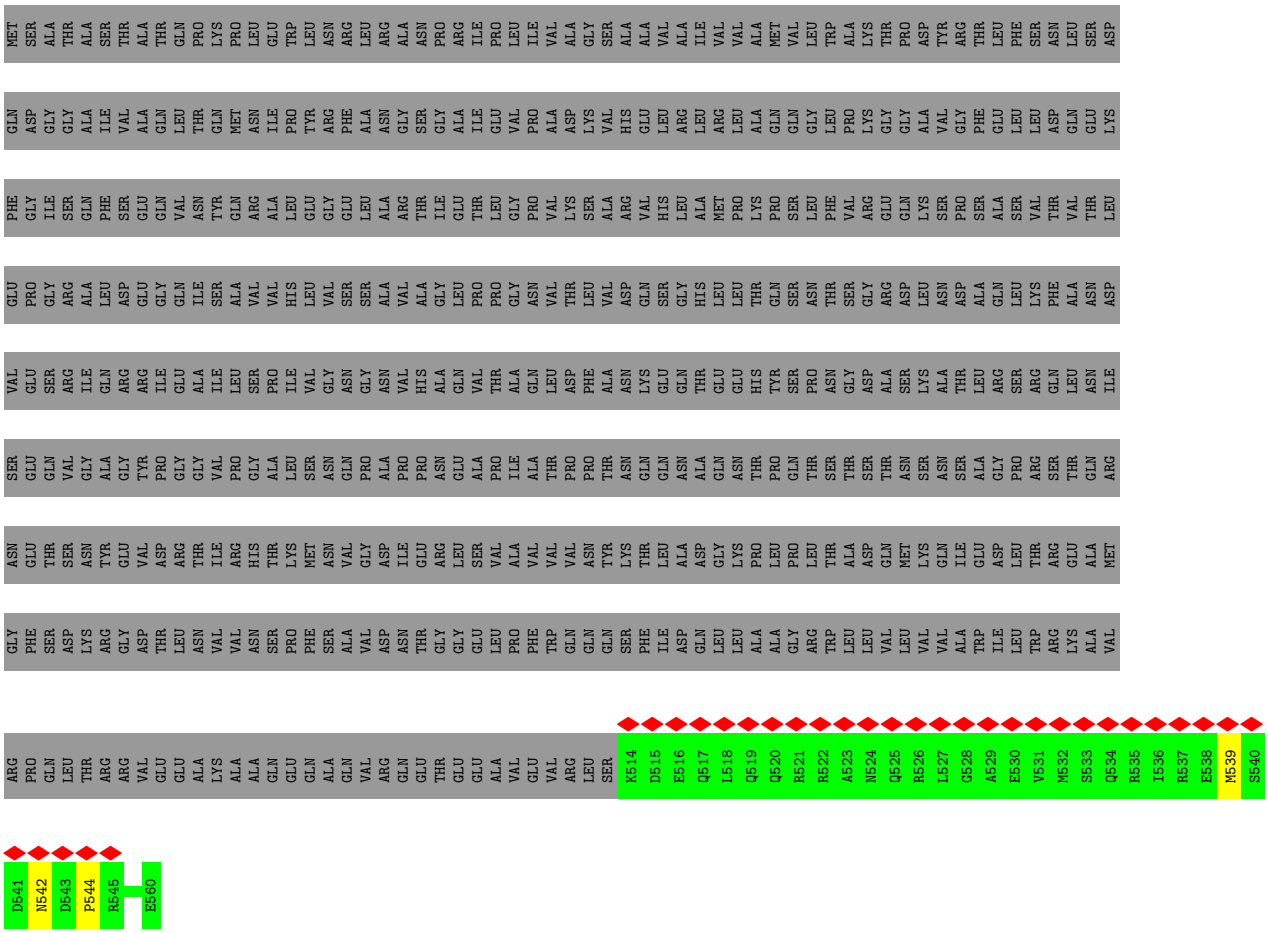




• Molecule 1: Flagellar M-ring protein

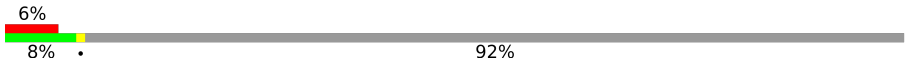
Chain ZF:

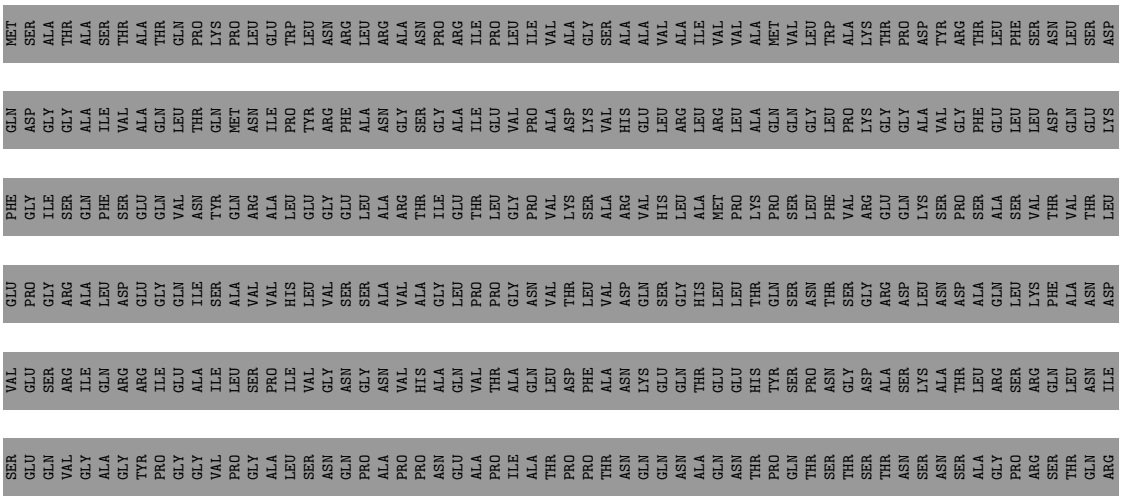


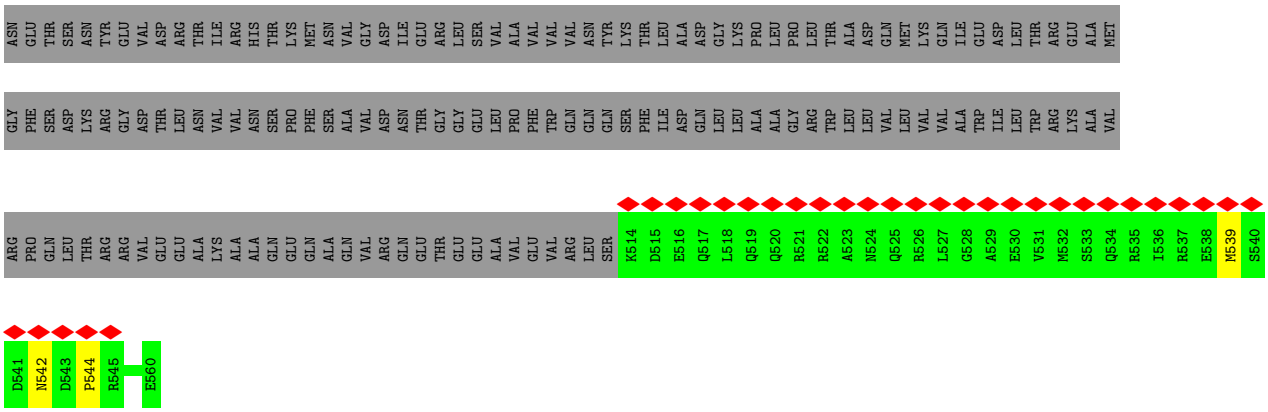


• Molecule 1: Flagellar M-ring protein

Chain FG:

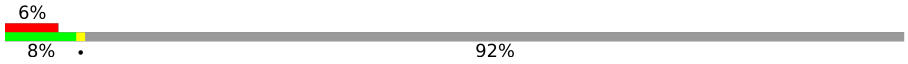


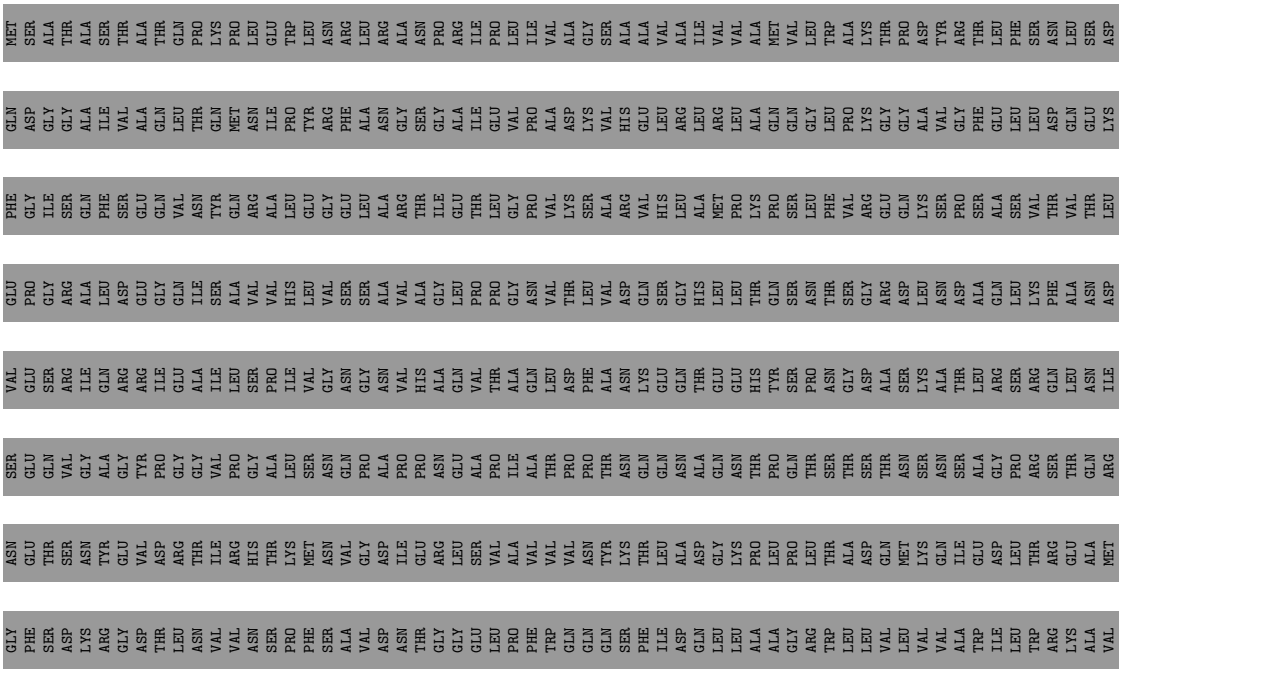




• Molecule 1: Flagellar M-ring protein

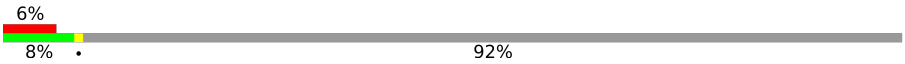
Chain LG:

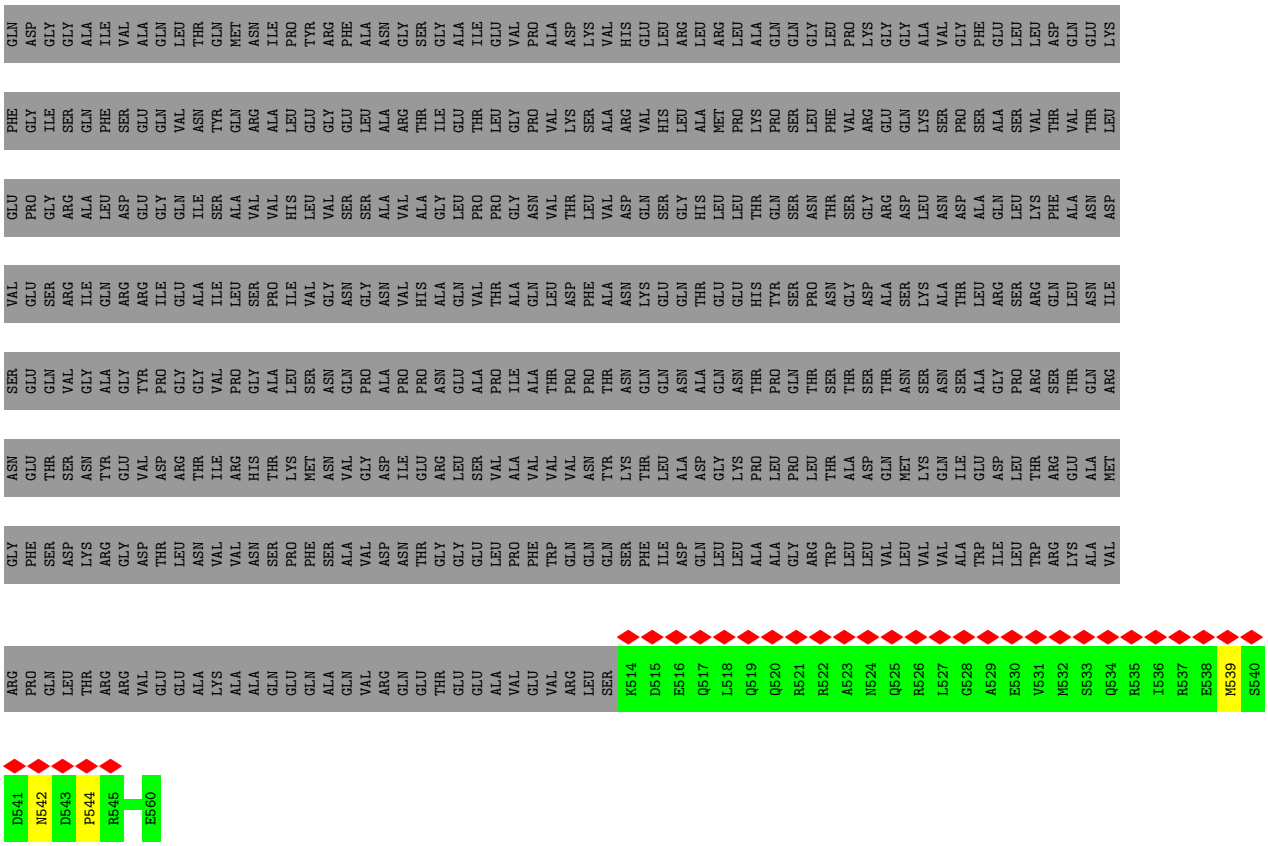




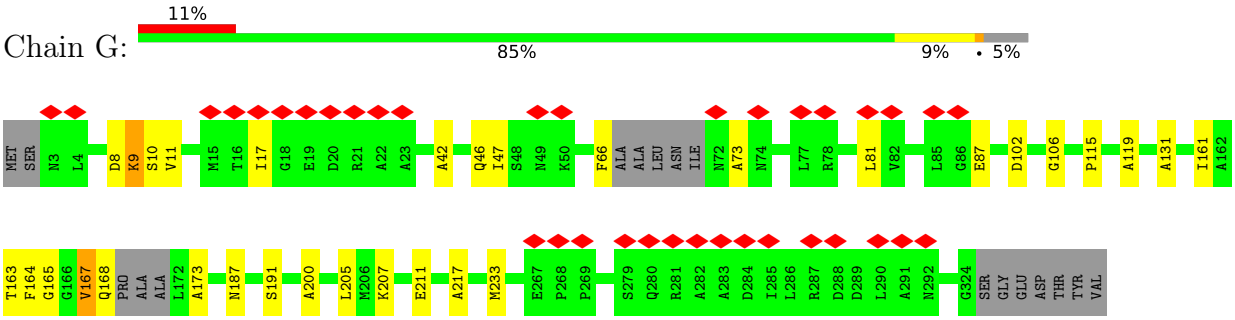
• Molecule 1: Flagellar M-ring protein

Chain RG:

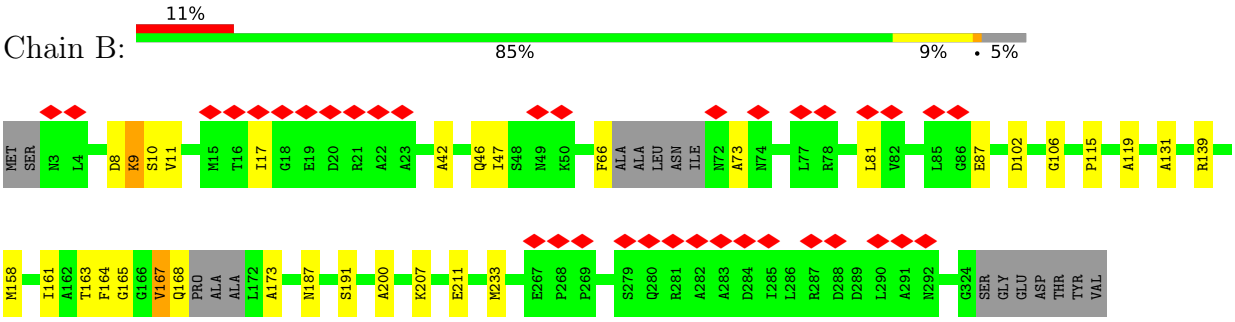




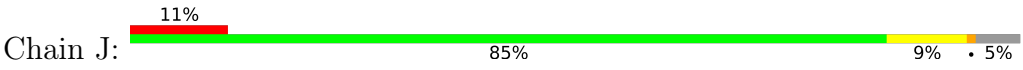
• Molecule 2: Flagellar motor switch protein FliG

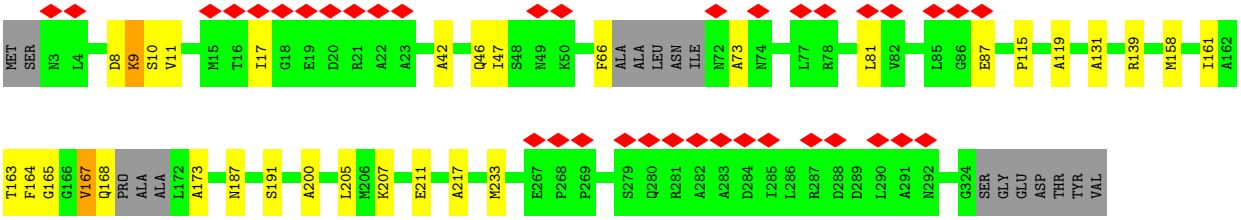


• Molecule 2: Flagellar motor switch protein FliG



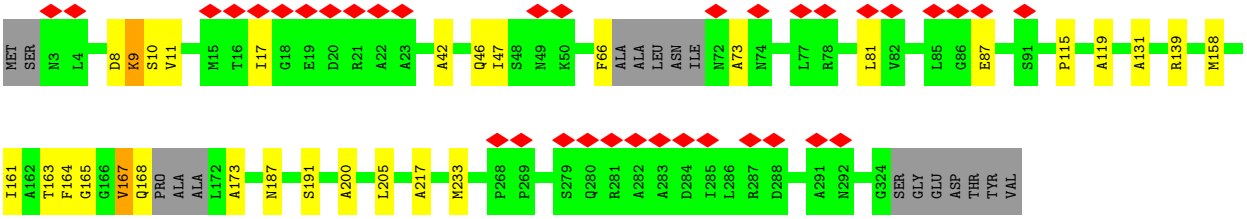
• Molecule 2: Flagellar motor switch protein FliG





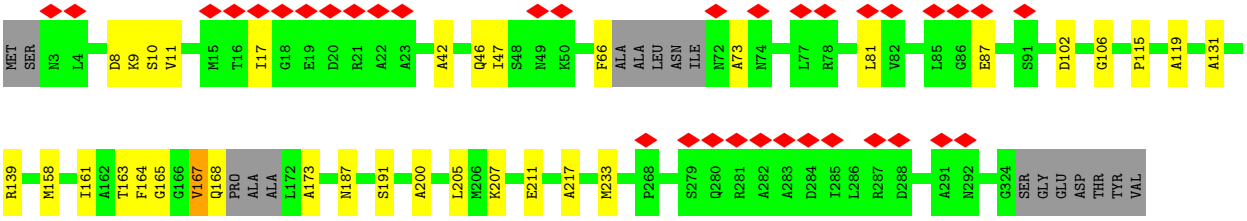
• Molecule 2: Flagellar motor switch protein FliG

Chain T:



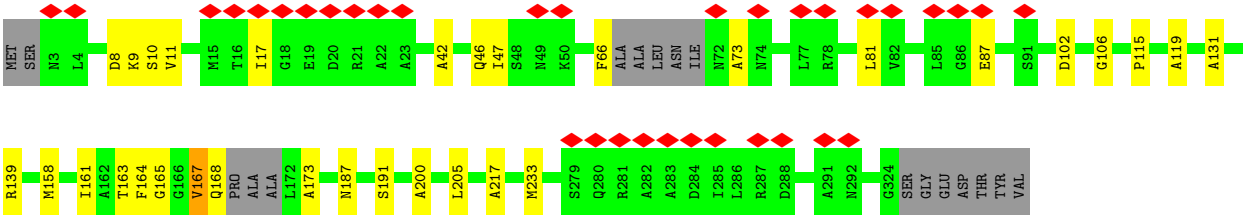
• Molecule 2: Flagellar motor switch protein FliG

Chain AA:



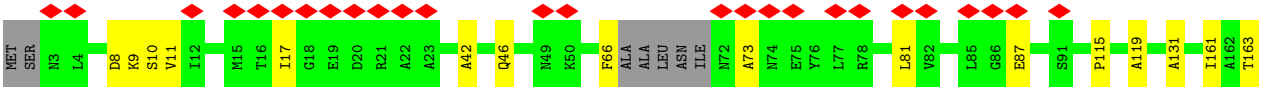
• Molecule 2: Flagellar motor switch protein FliG

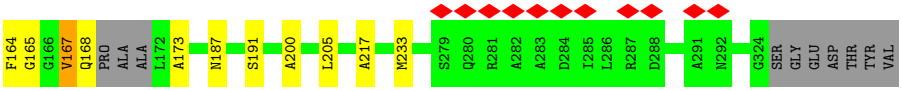
Chain GA:



• Molecule 2: Flagellar motor switch protein FliG

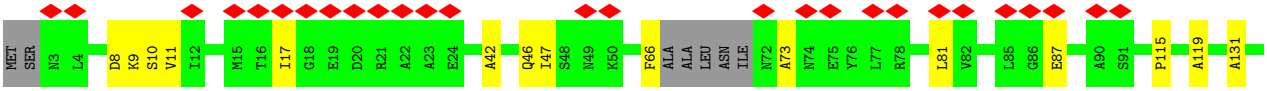
Chain MA:

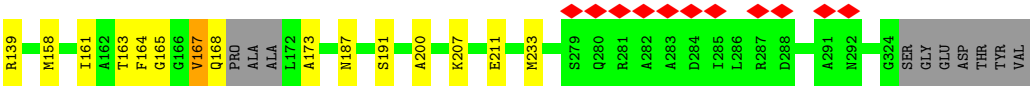




• Molecule 2: Flagellar motor switch protein FliG

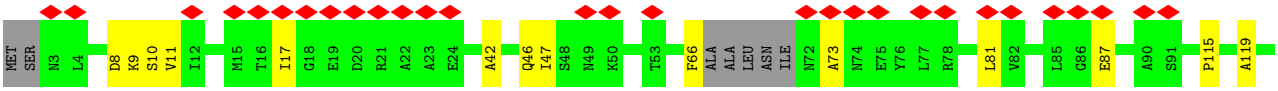
Chain SA:





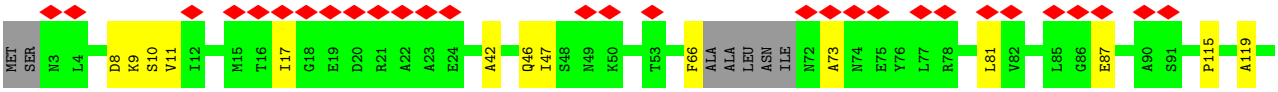
• Molecule 2: Flagellar motor switch protein FliG

Chain YA:



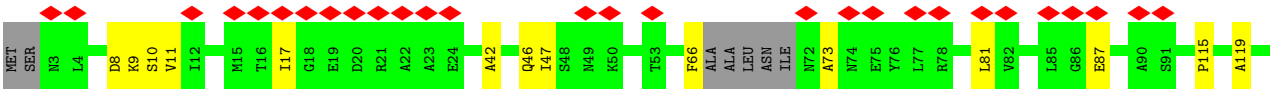
• Molecule 2: Flagellar motor switch protein FliG

Chain EB:



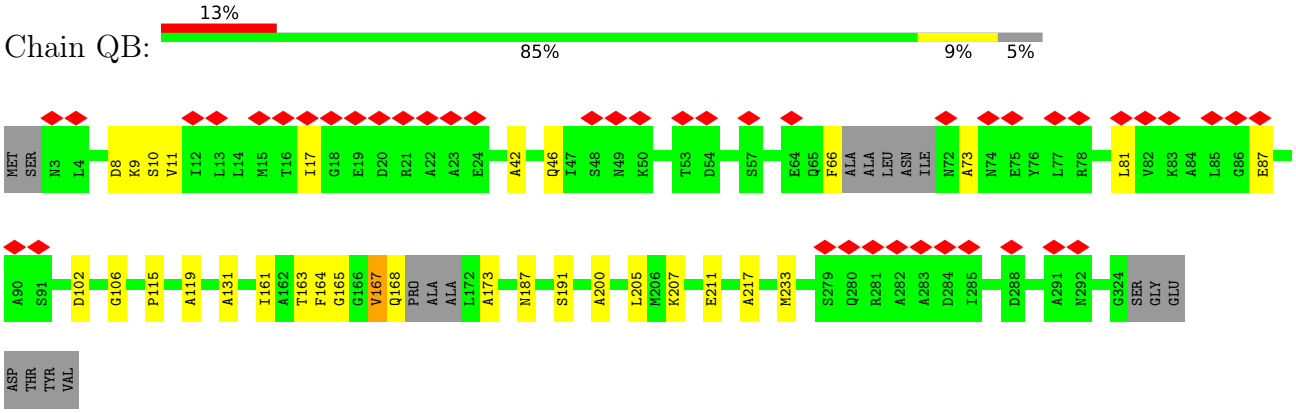
• Molecule 2: Flagellar motor switch protein FliG

Chain KB:



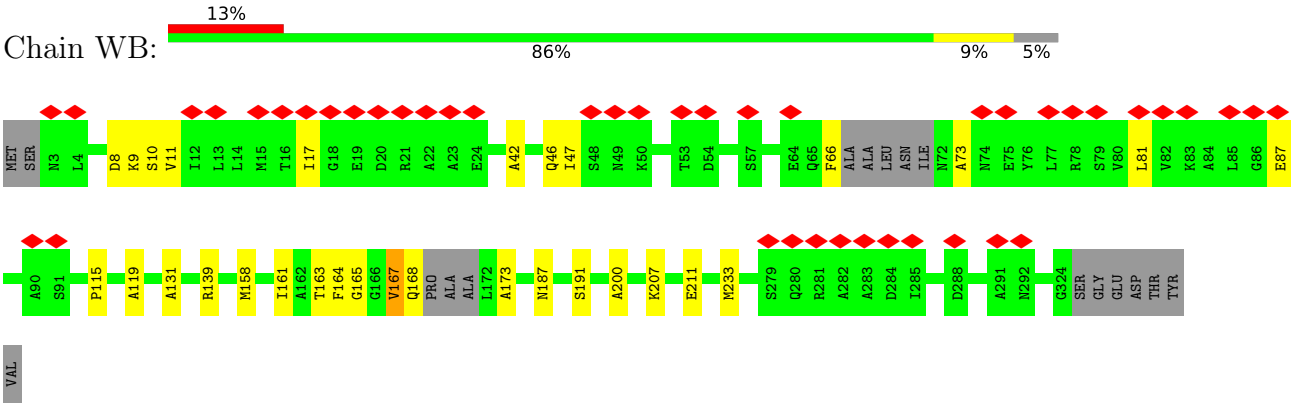
• Molecule 2: Flagellar motor switch protein FliG

Chain QB:



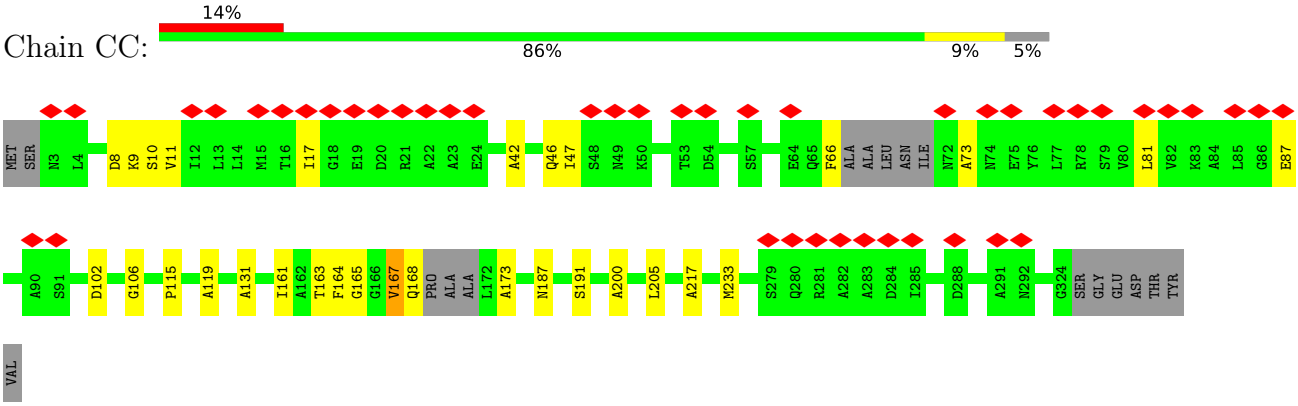
• Molecule 2: Flagellar motor switch protein FliG

Chain WB:



• Molecule 2: Flagellar motor switch protein FliG

Chain CC:



• Molecule 2: Flagellar motor switch protein FliG

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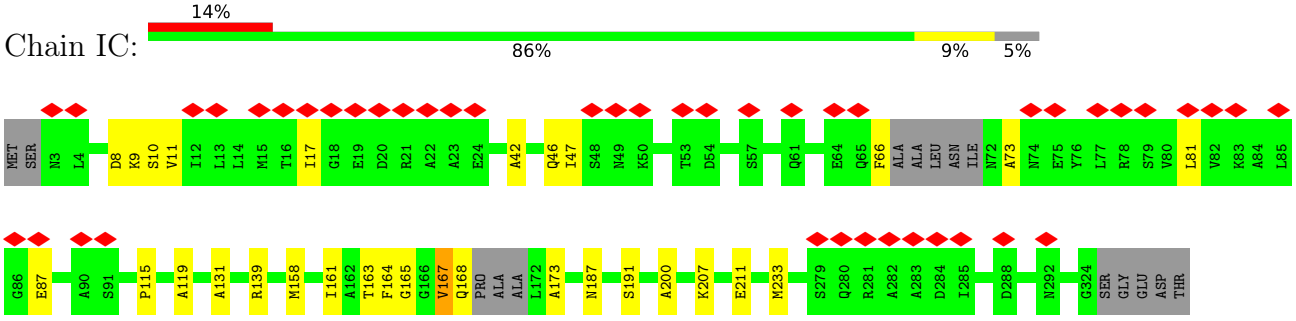
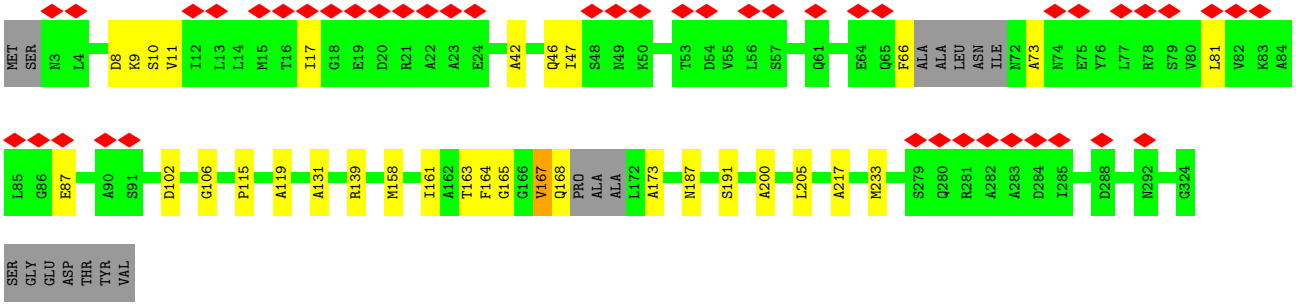


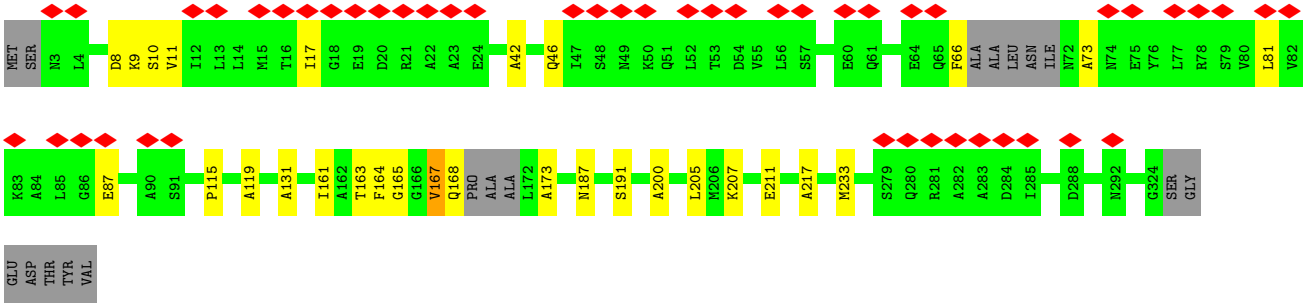
• Molecule 2: Flagellar motor switch protein FliG

Chain OC:



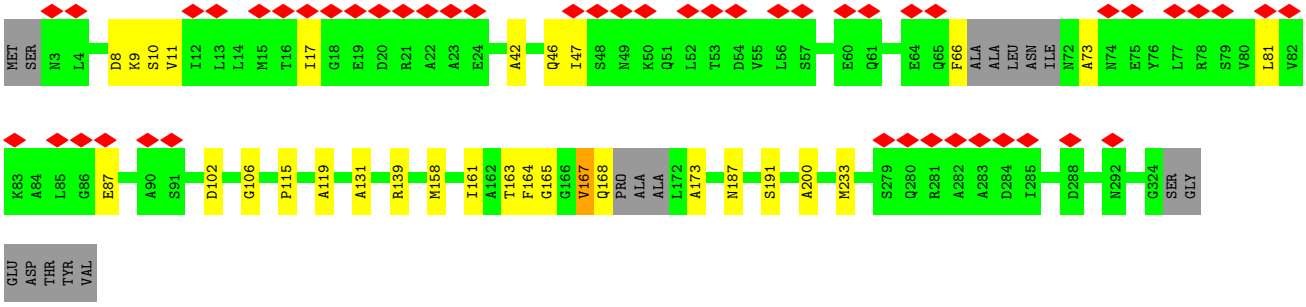
• Molecule 2: Flagellar motor switch protein FliG

Chain UC:



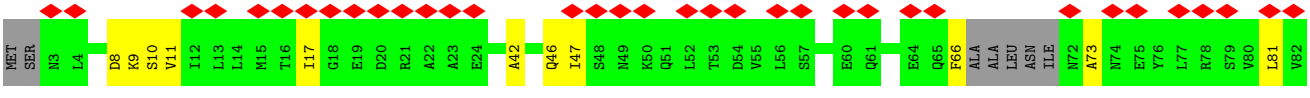
• Molecule 2: Flagellar motor switch protein FliG

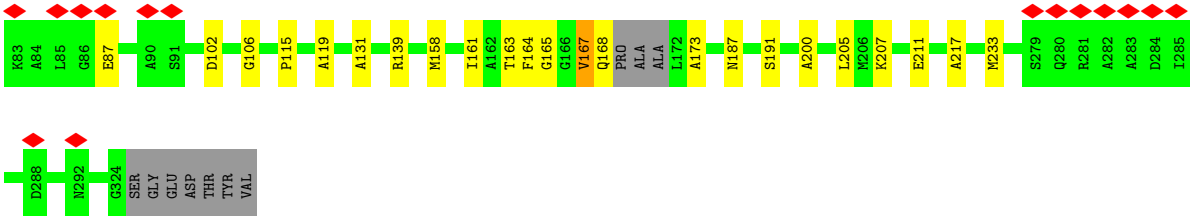
Chain AD:



• Molecule 2: Flagellar motor switch protein FliG

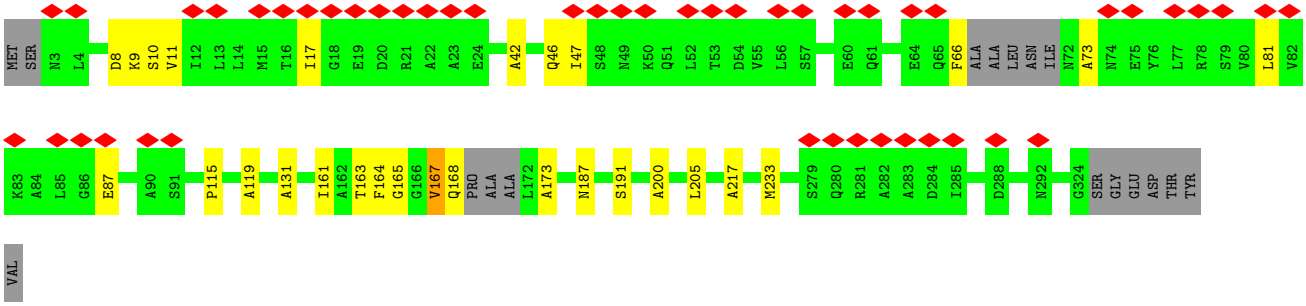
Chain GD:





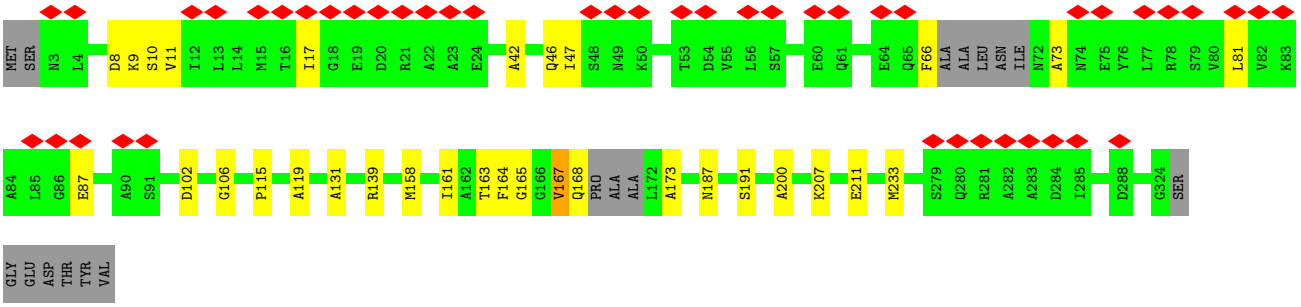
• Molecule 2: Flagellar motor switch protein FliG

Chain MD:



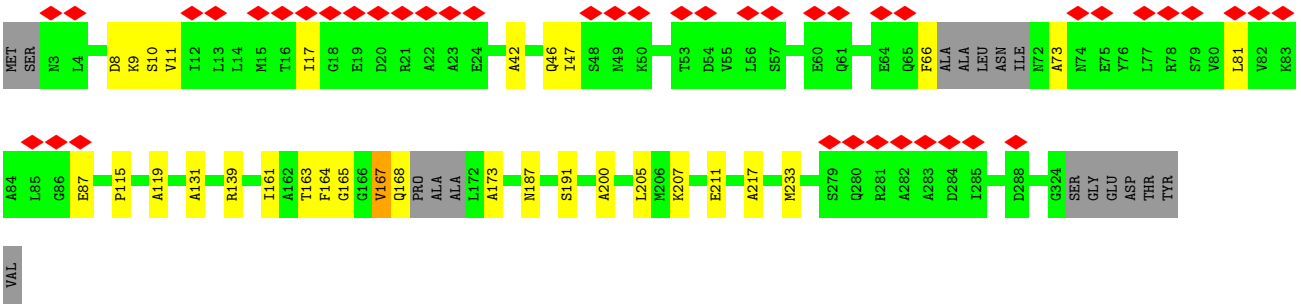
• Molecule 2: Flagellar motor switch protein FliG

Chain SD:



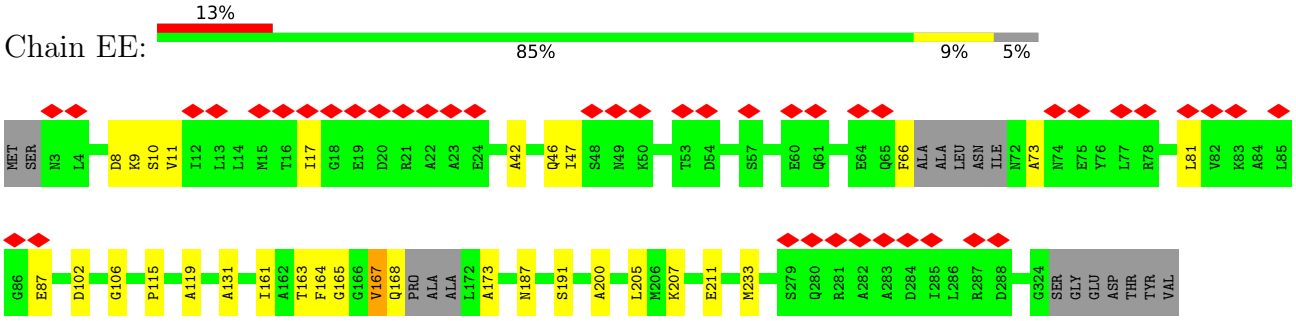
• Molecule 2: Flagellar motor switch protein FliG

Chain YD:



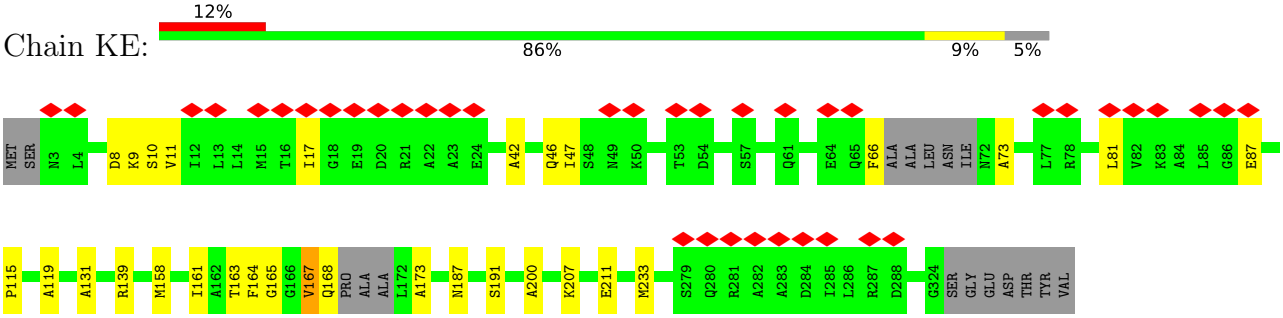
• Molecule 2: Flagellar motor switch protein FliG

Chain EE:



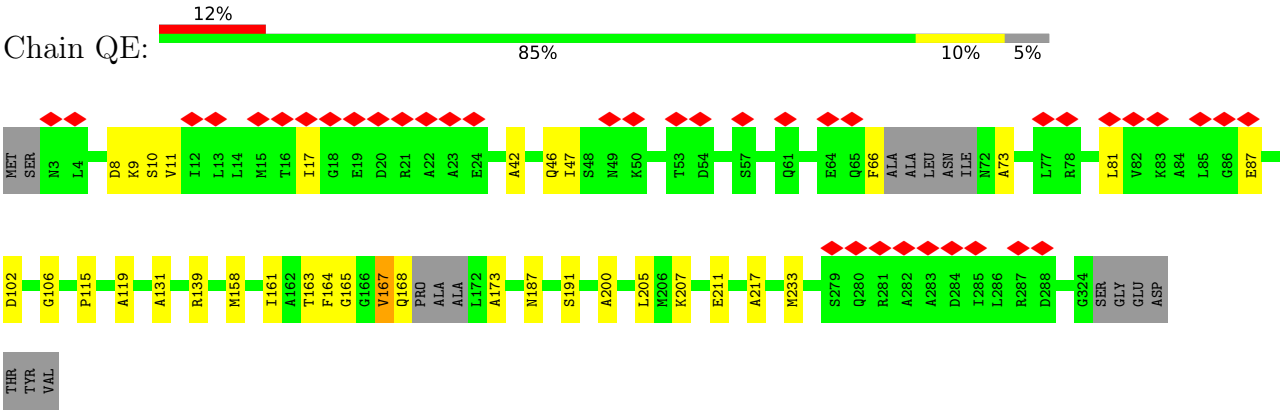
• Molecule 2: Flagellar motor switch protein FliG

Chain KE:



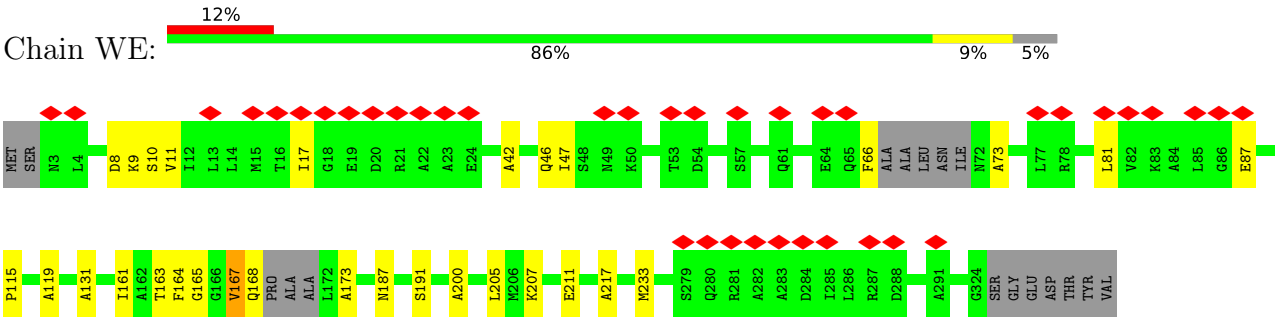
• Molecule 2: Flagellar motor switch protein FliG

Chain QE:



• Molecule 2: Flagellar motor switch protein FliG

Chain WE:



• Molecule 2: Flagellar motor switch protein FliG

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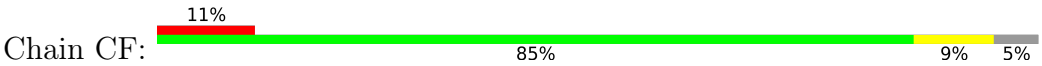
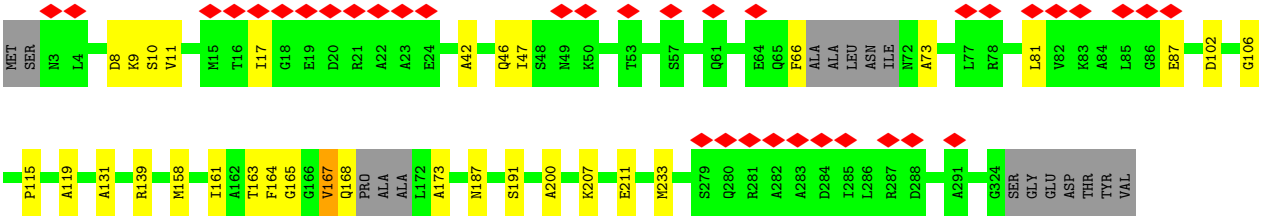
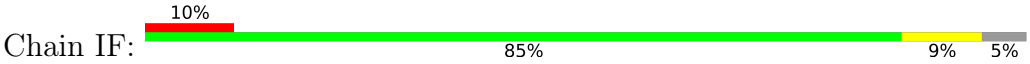
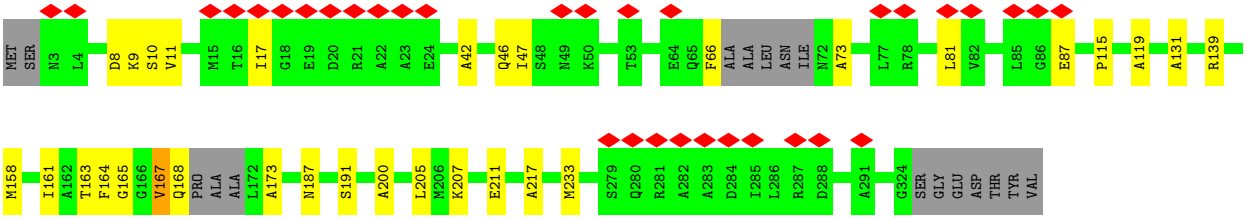


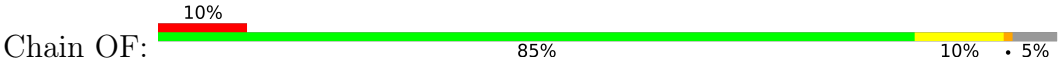


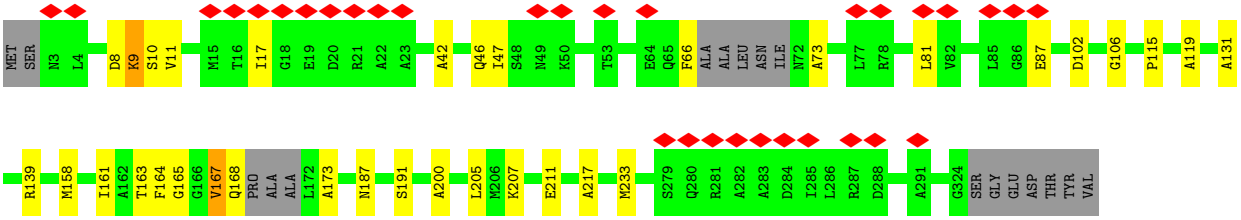
• Molecule 2: Flagellar motor switch protein FliG



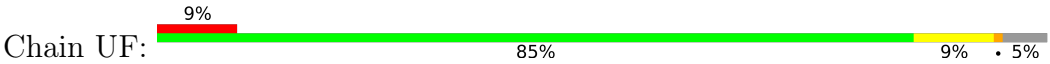


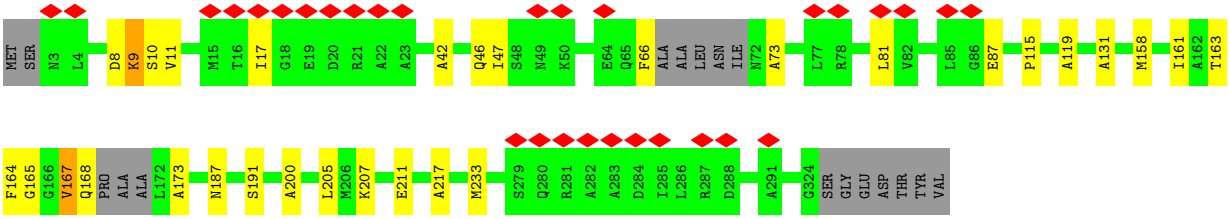
• Molecule 2: Flagellar motor switch protein FliG



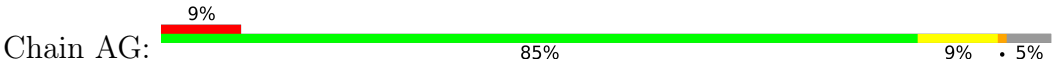


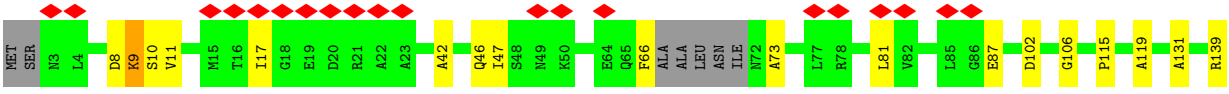
• Molecule 2: Flagellar motor switch protein FliG

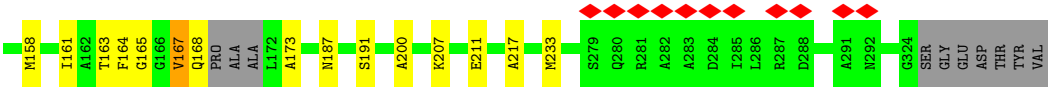




• Molecule 2: Flagellar motor switch protein FliG

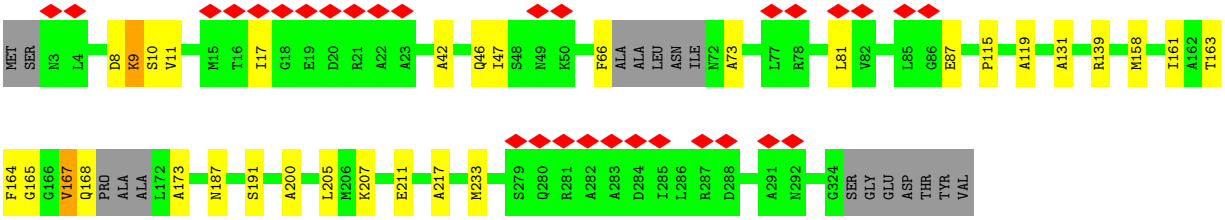






• Molecule 2: Flagellar motor switch protein FliG

Chain GG:



• Molecule 2: Flagellar motor switch protein FliG

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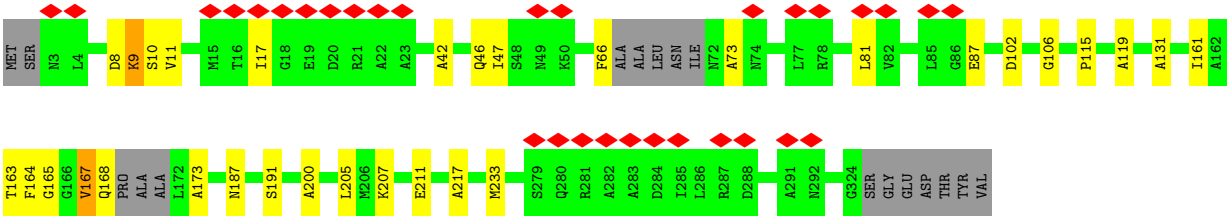

• Molecule 2: Flagellar motor switch protein FliG

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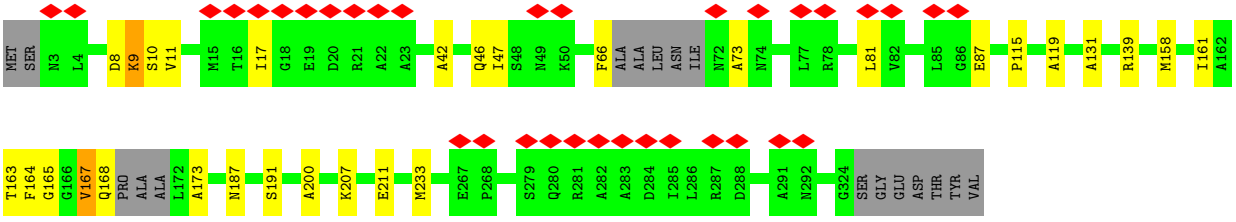
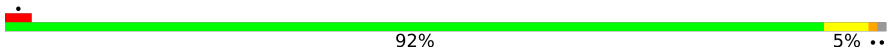


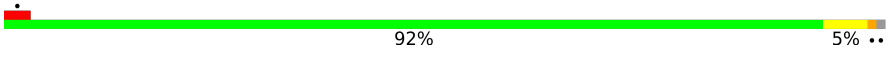
• Molecule 3: Flagellar motor switch protein FliM

Chain M:



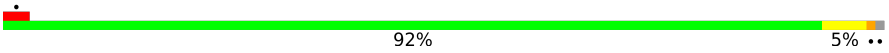
• Molecule 3: Flagellar motor switch protein FliM

Chain C:



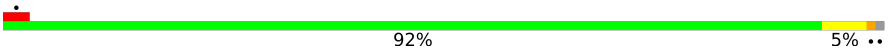
• Molecule 3: Flagellar motor switch protein FliM

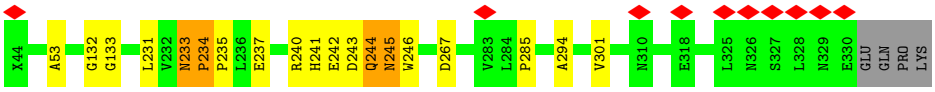
Chain K:



• Molecule 3: Flagellar motor switch protein FliM

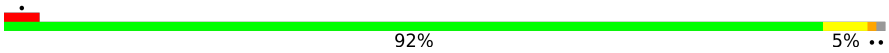
Chain V:

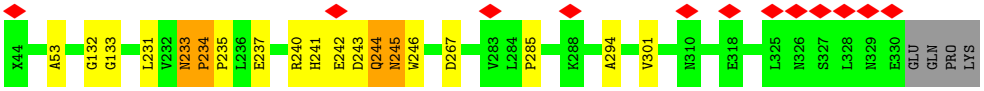




• Molecule 3: Flagellar motor switch protein FliM

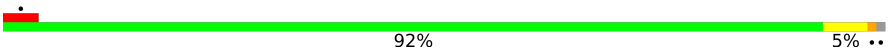
Chain BA:

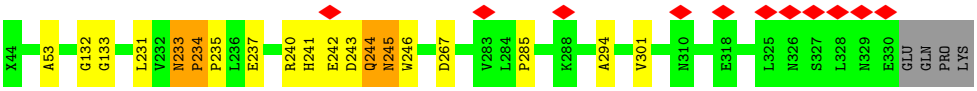




• Molecule 3: Flagellar motor switch protein FliM

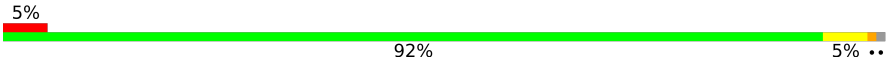
Chain HA:

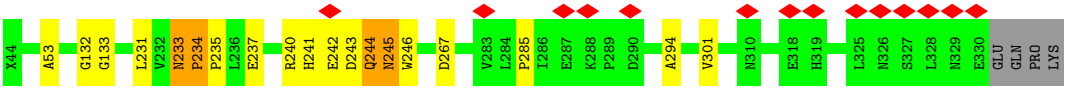




• Molecule 3: Flagellar motor switch protein FliM

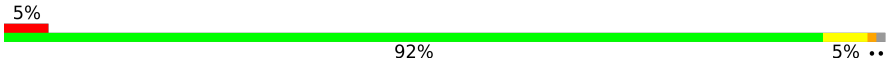
Chain NA:

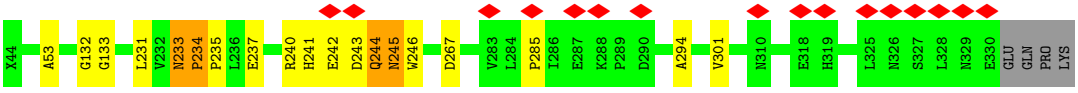




• Molecule 3: Flagellar motor switch protein FliM

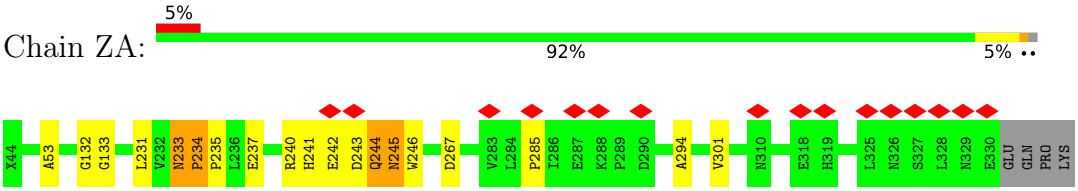
Chain TA:





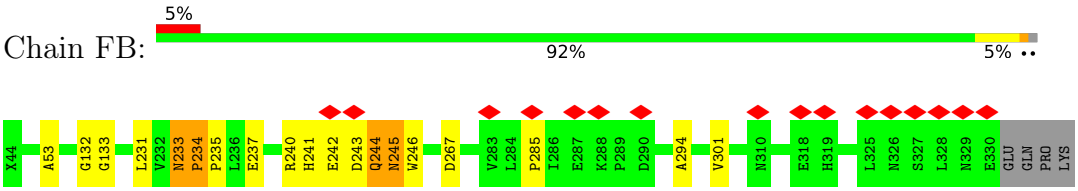
• Molecule 3: Flagellar motor switch protein FliM

Chain ZA:



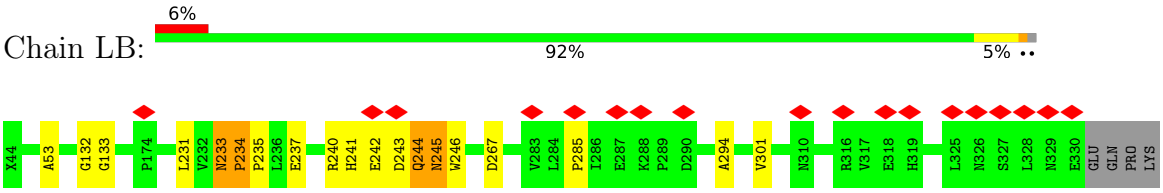
• Molecule 3: Flagellar motor switch protein FliM

Chain FB:



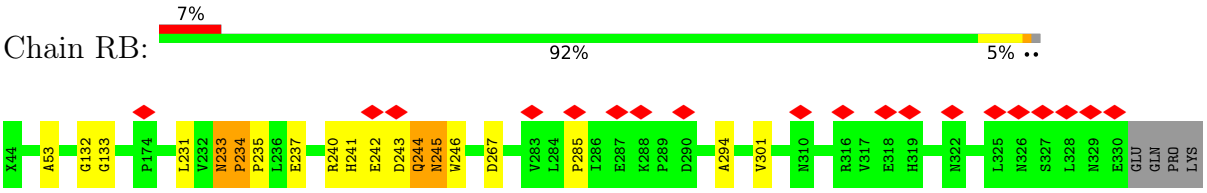
• Molecule 3: Flagellar motor switch protein FliM

Chain LB:



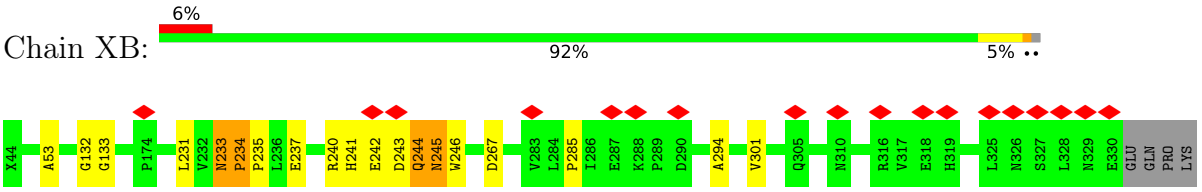
• Molecule 3: Flagellar motor switch protein FliM

Chain RB:



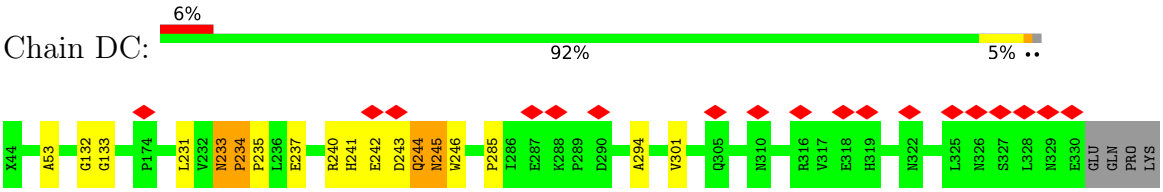
• Molecule 3: Flagellar motor switch protein FliM

Chain XB:



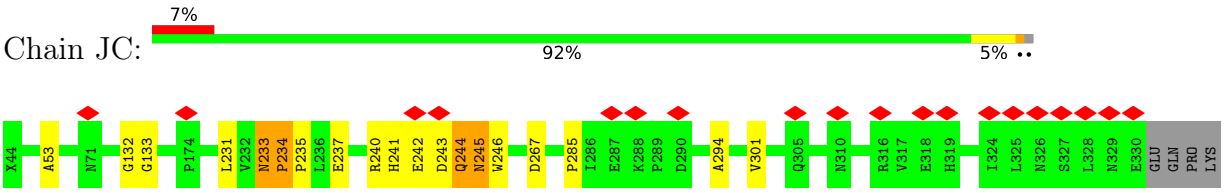
• Molecule 3: Flagellar motor switch protein FliM

Chain DC:



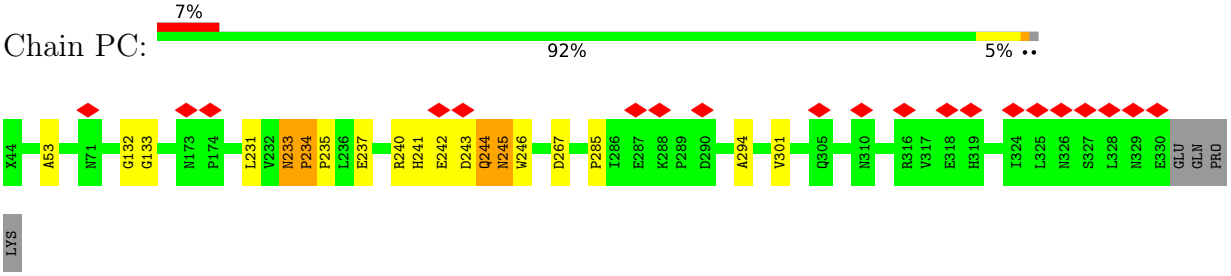
• Molecule 3: Flagellar motor switch protein FliM

Chain JC:



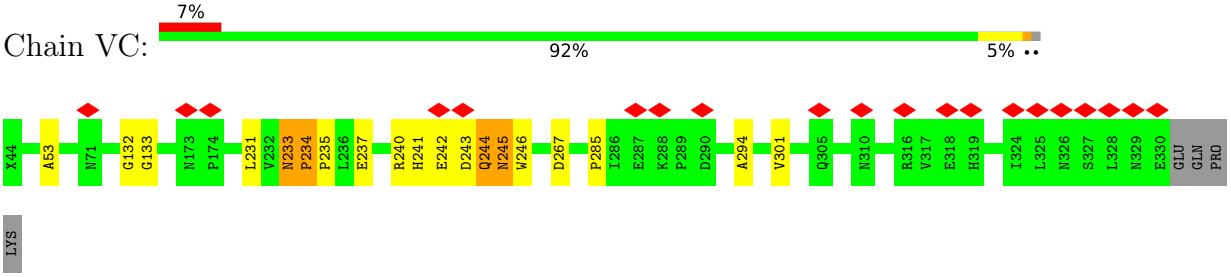
• Molecule 3: Flagellar motor switch protein FliM

Chain PC:



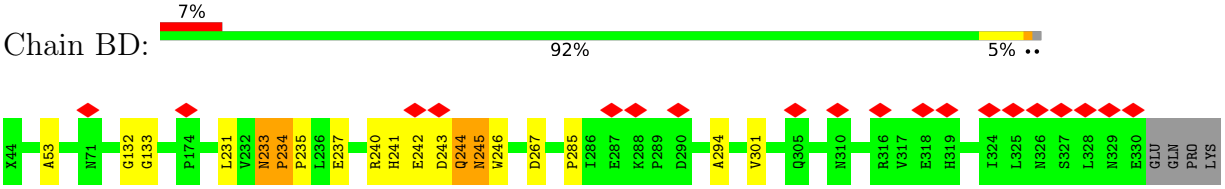
• Molecule 3: Flagellar motor switch protein FliM

Chain VC:



• Molecule 3: Flagellar motor switch protein FliM

Chain BD:



• Molecule 3: Flagellar motor switch protein FliM

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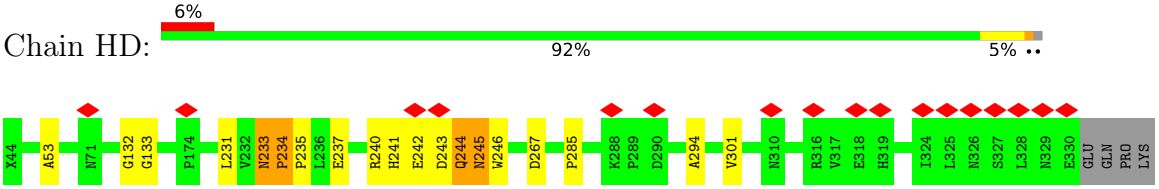
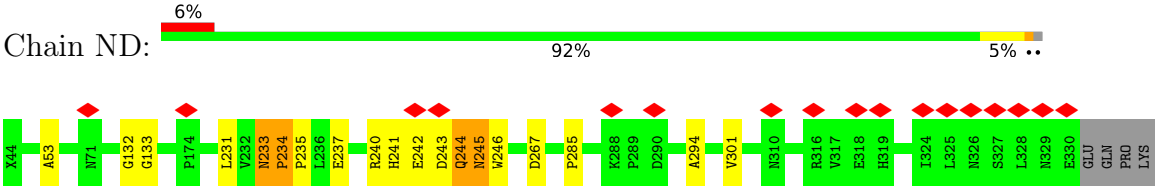


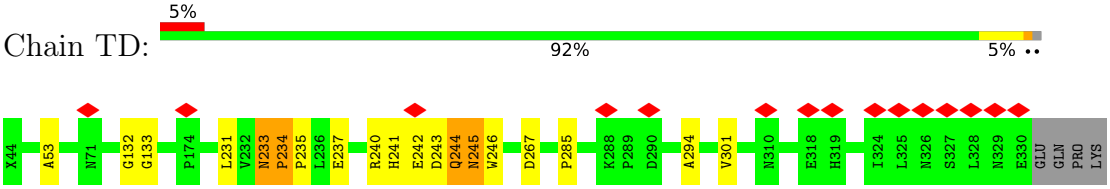
• Molecule 3: Flagellar motor switch protein FliM

Chain ND:



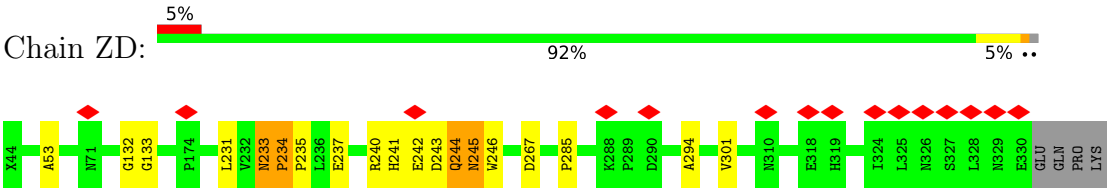
• Molecule 3: Flagellar motor switch protein FliM

Chain TD:



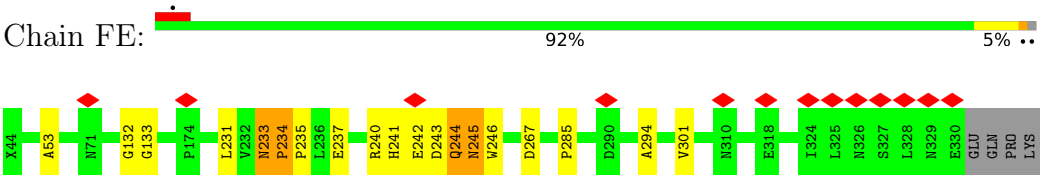
• Molecule 3: Flagellar motor switch protein FliM

Chain ZD:



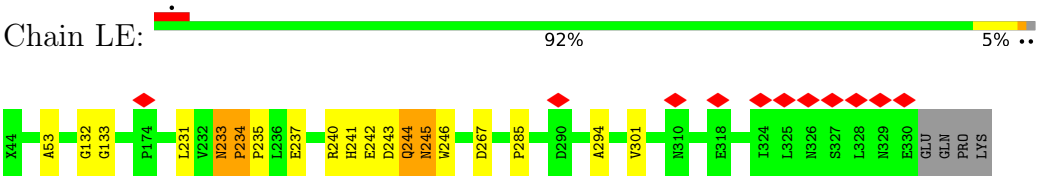
• Molecule 3: Flagellar motor switch protein FliM

Chain FE:



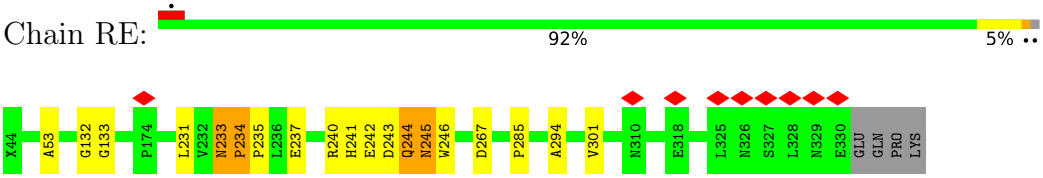
• Molecule 3: Flagellar motor switch protein FliM

Chain LE:



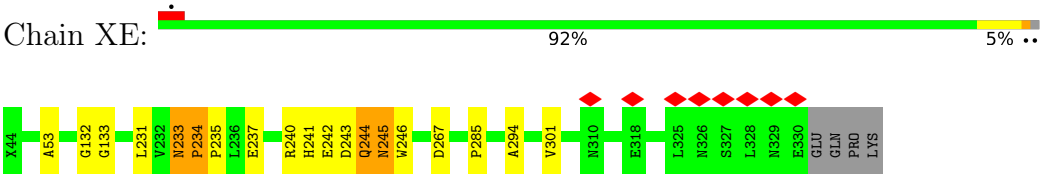
• Molecule 3: Flagellar motor switch protein FliM

Chain RE:



• Molecule 3: Flagellar motor switch protein FliM

Chain XE:



• Molecule 3: Flagellar motor switch protein FliM

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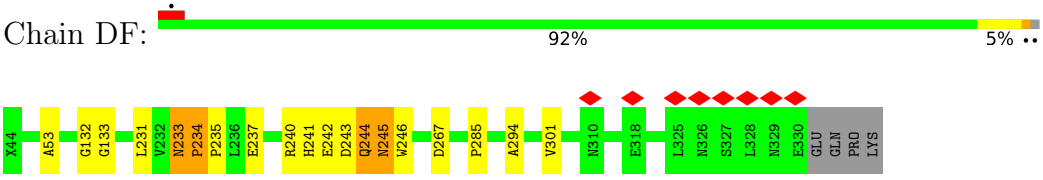
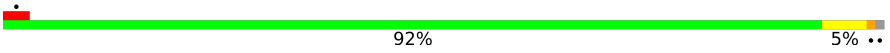
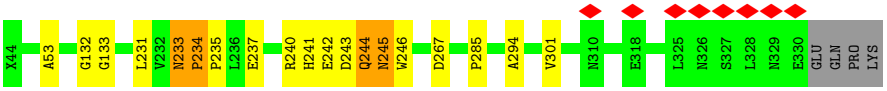


• Molecule 3: Flagellar motor switch protein FliM

Chain JF:





• Molecule 3: Flagellar motor switch protein FliM

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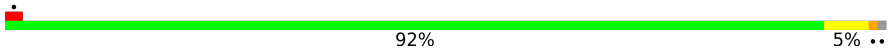
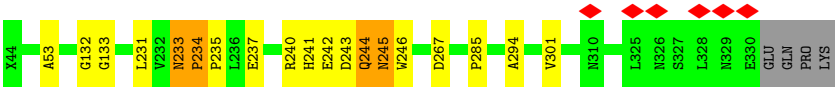
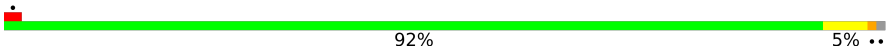
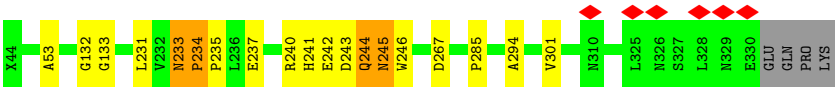




• Molecule 3: Flagellar motor switch protein FliM

Chain VF:





• Molecule 3: Flagellar motor switch protein FliM

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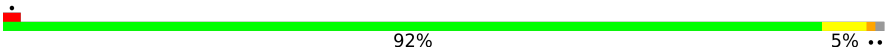
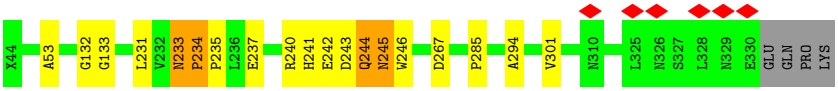
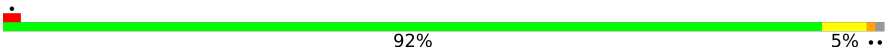




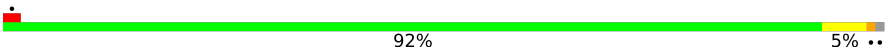
• Molecule 3: Flagellar motor switch protein FliM

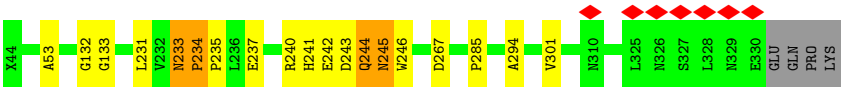
Chain HG:



• Molecule 3: Flagellar motor switch protein FliM

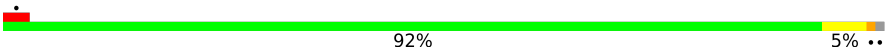
Chain NG:





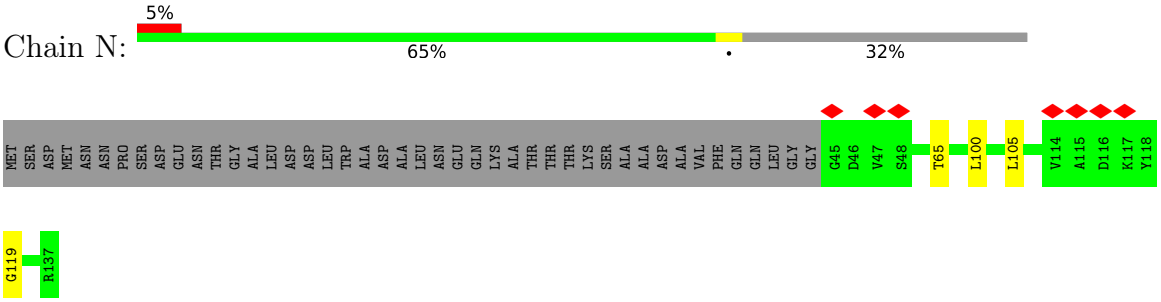
• Molecule 3: Flagellar motor switch protein FliM

Chain TG:



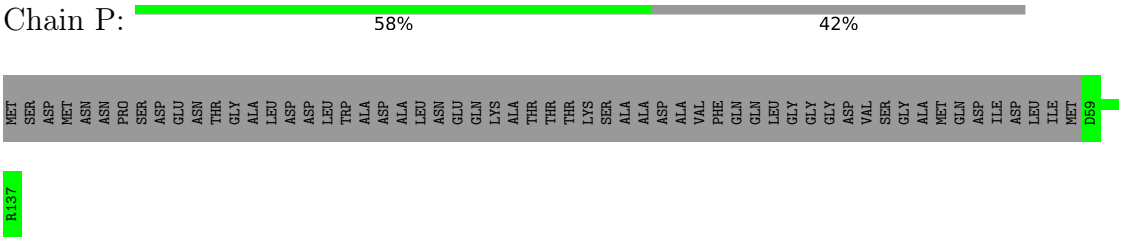
• Molecule 4: Flagellar motor switch protein FliN

Chain N:



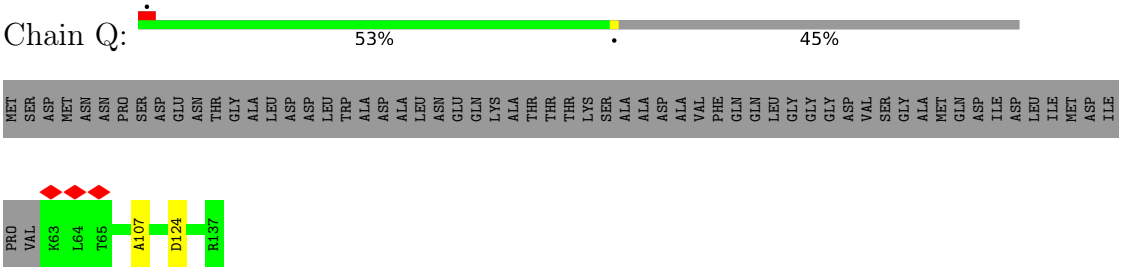
• Molecule 4: Flagellar motor switch protein FliN

Chain P:



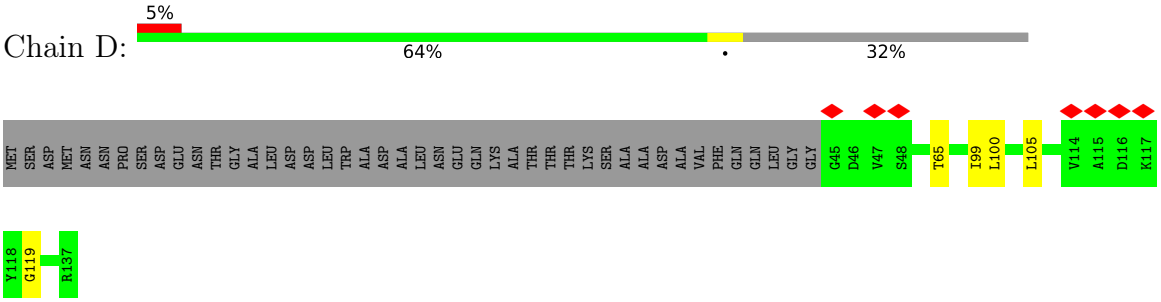
• Molecule 4: Flagellar motor switch protein FliN

Chain Q:



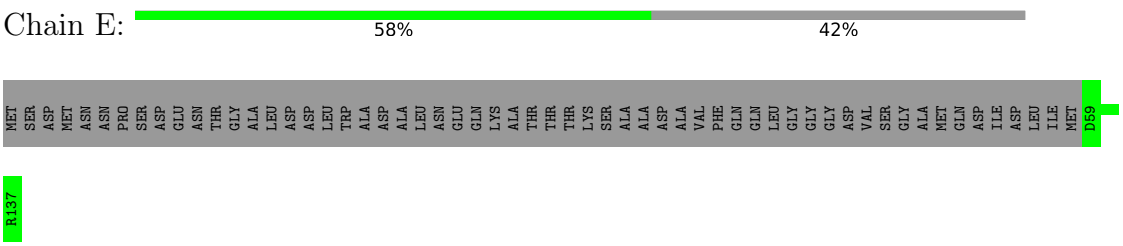
• Molecule 4: Flagellar motor switch protein FliN

Chain D:



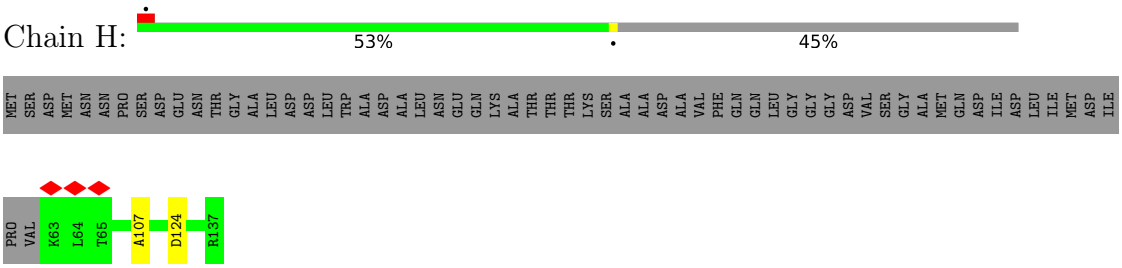
• Molecule 4: Flagellar motor switch protein FliN

Chain E:



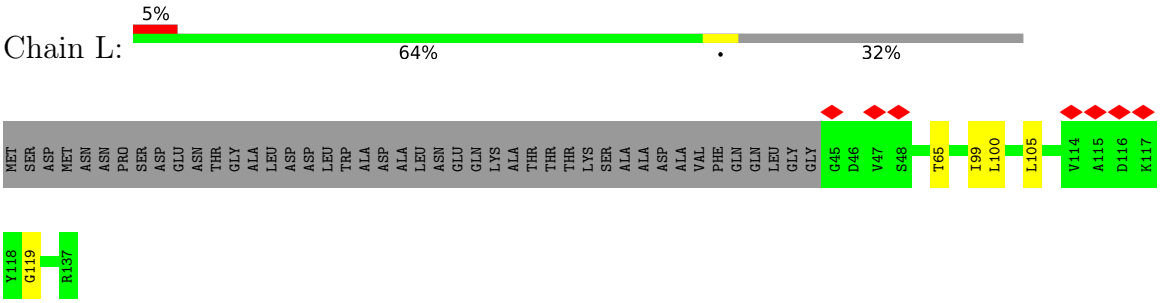
• Molecule 4: Flagellar motor switch protein FliN

Chain H:



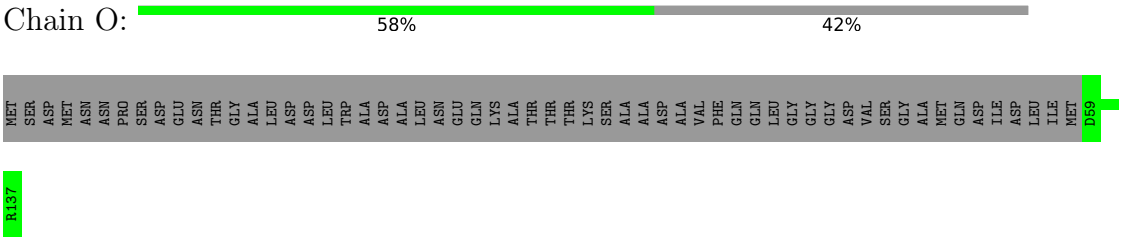
• Molecule 4: Flagellar motor switch protein FliN

Chain L:



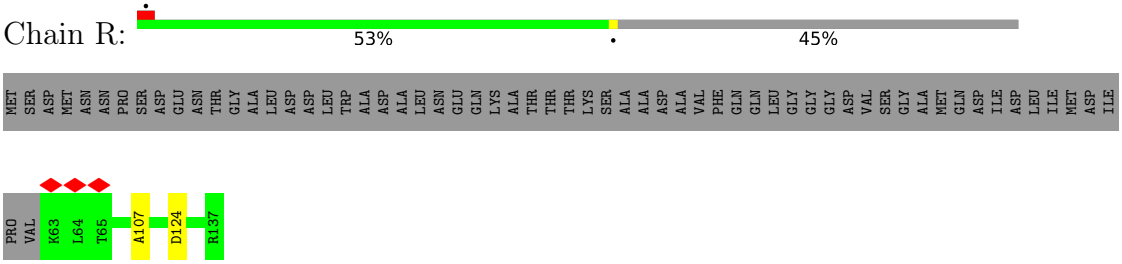
• Molecule 4: Flagellar motor switch protein FliN

Chain O:



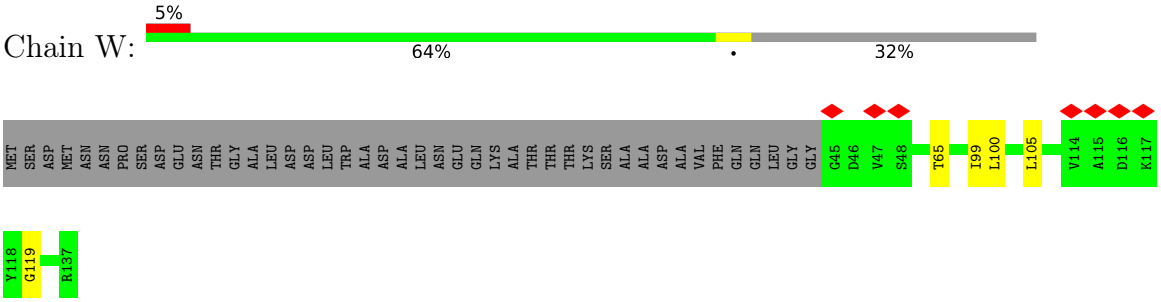
• Molecule 4: Flagellar motor switch protein FliN

Chain R:



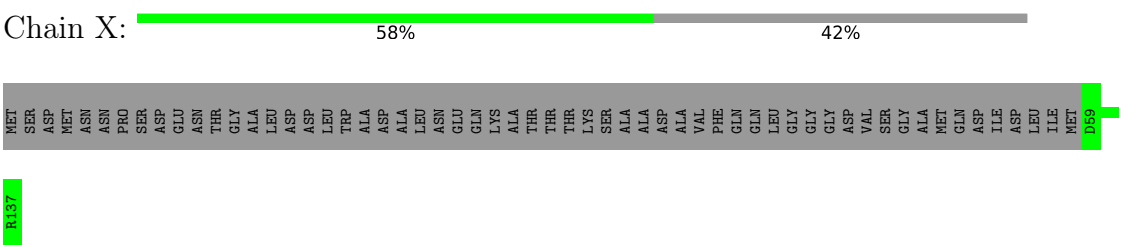
• Molecule 4: Flagellar motor switch protein FliN

Chain W:



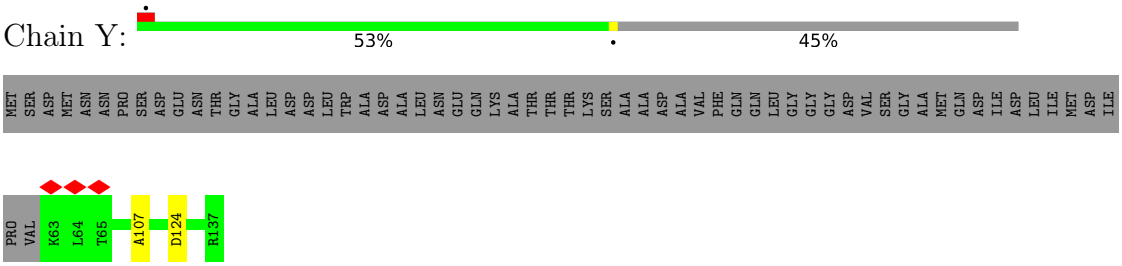
• Molecule 4: Flagellar motor switch protein FliN

Chain X:



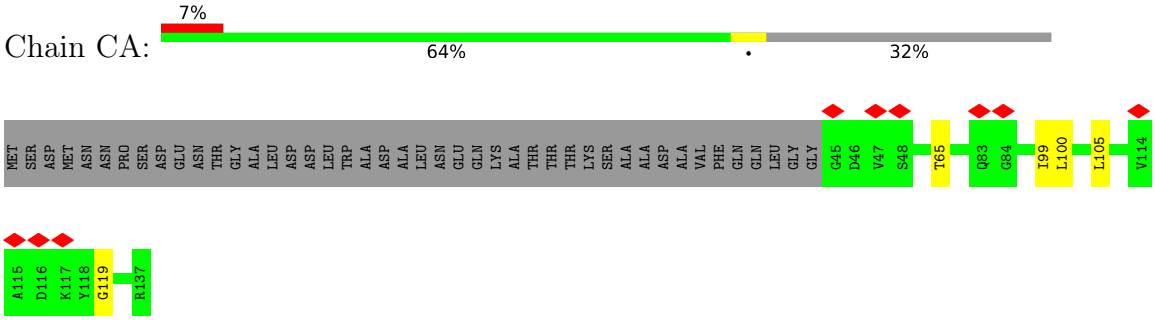
• Molecule 4: Flagellar motor switch protein FliN

Chain Y:



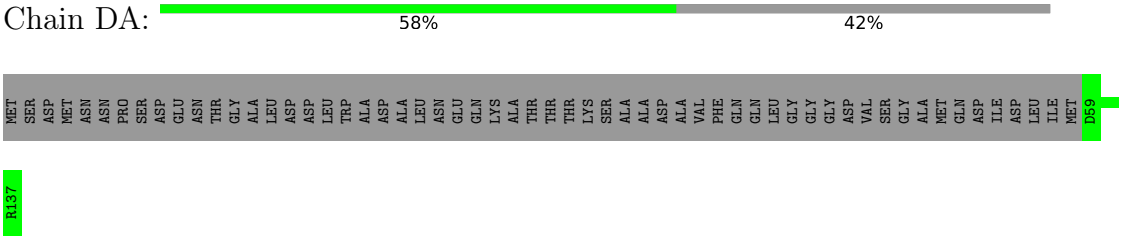
• Molecule 4: Flagellar motor switch protein FliN

Chain CA:



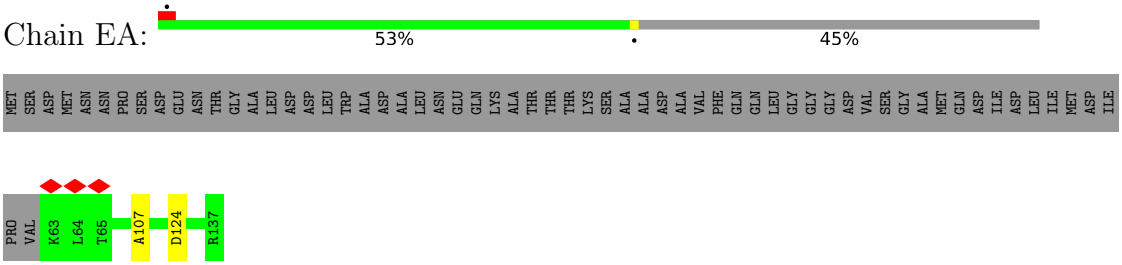
• Molecule 4: Flagellar motor switch protein FliN

Chain DA:



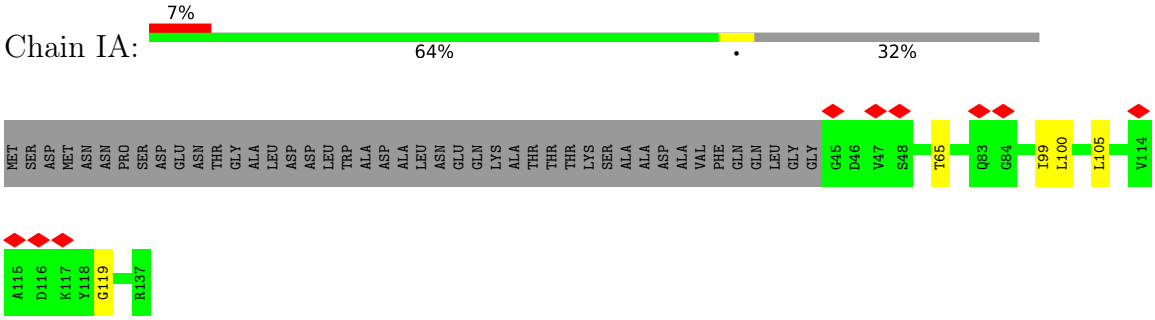
• Molecule 4: Flagellar motor switch protein FliN

Chain EA:



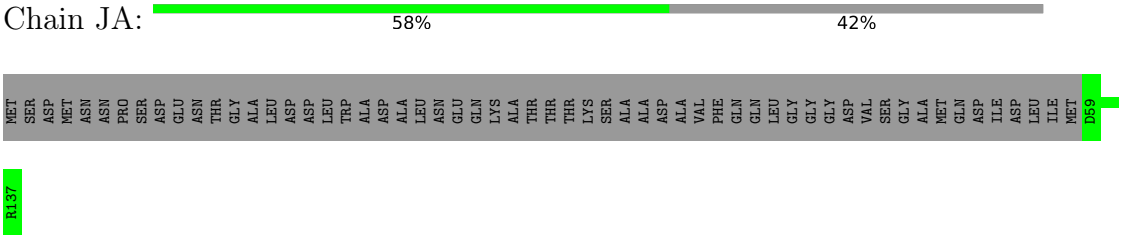
• Molecule 4: Flagellar motor switch protein FliN

Chain IA:



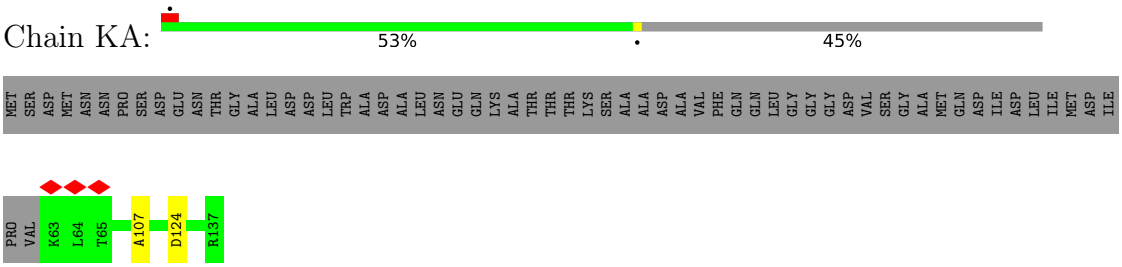
• Molecule 4: Flagellar motor switch protein FliN

Chain JA:



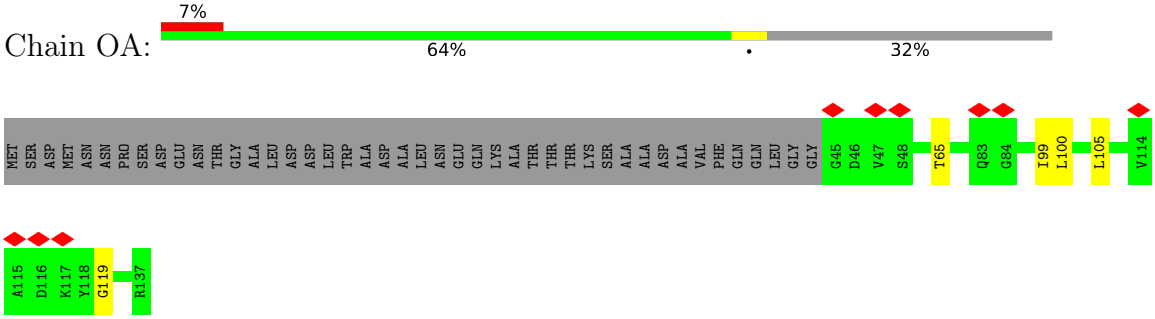
• Molecule 4: Flagellar motor switch protein FliN

Chain KA:



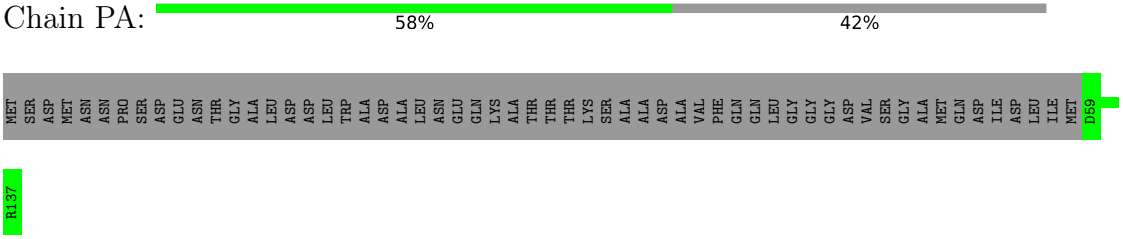
• Molecule 4: Flagellar motor switch protein FliN

Chain OA:



• Molecule 4: Flagellar motor switch protein FliN

Chain PA:



• Molecule 4: Flagellar motor switch protein FliN

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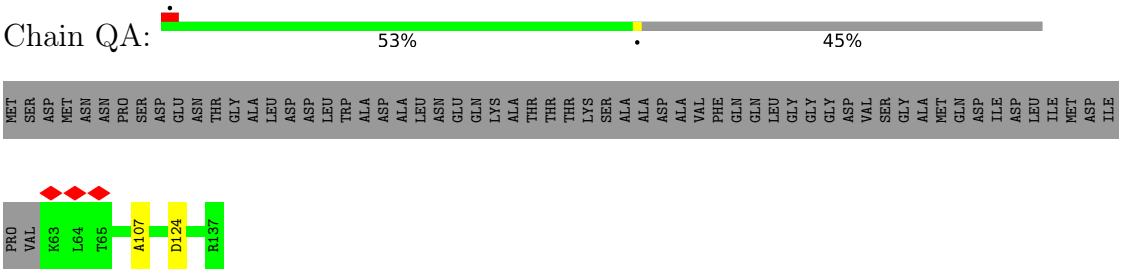
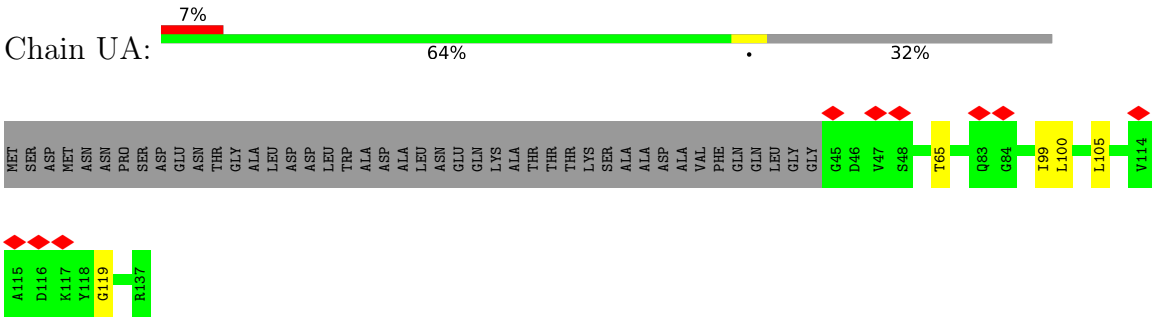


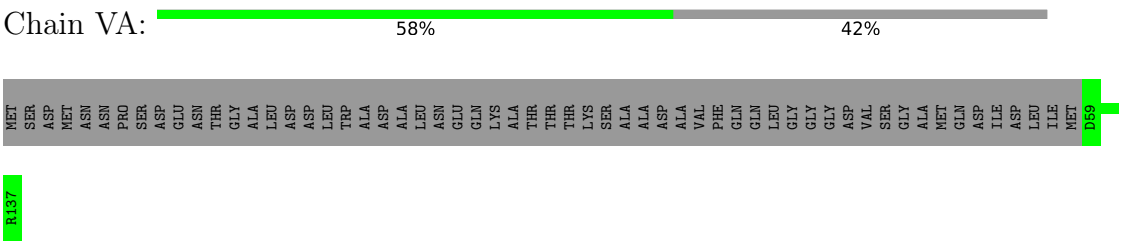
• Molecule 4: Flagellar motor switch protein FliN

Chain UA:



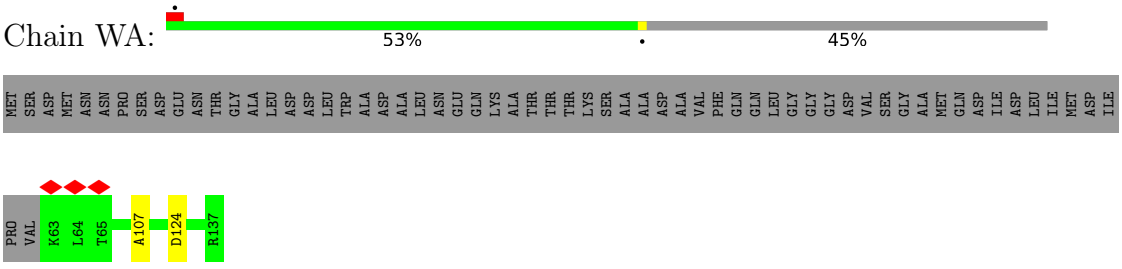
• Molecule 4: Flagellar motor switch protein FliN

Chain VA:



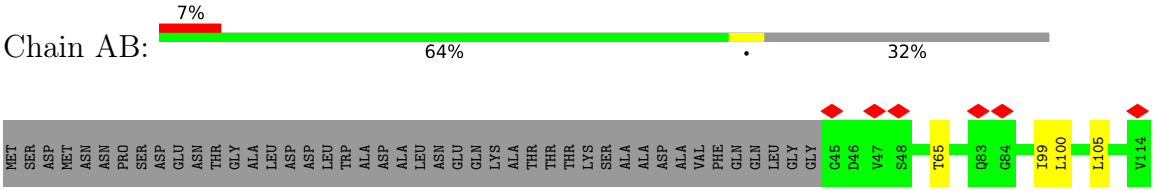
• Molecule 4: Flagellar motor switch protein FliN

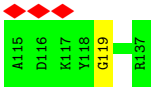
Chain WA:



• Molecule 4: Flagellar motor switch protein FliN

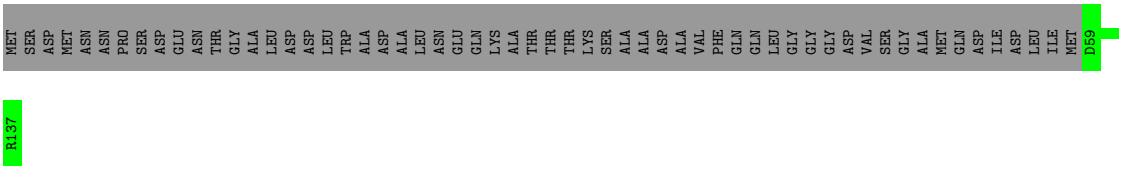
Chain AB:





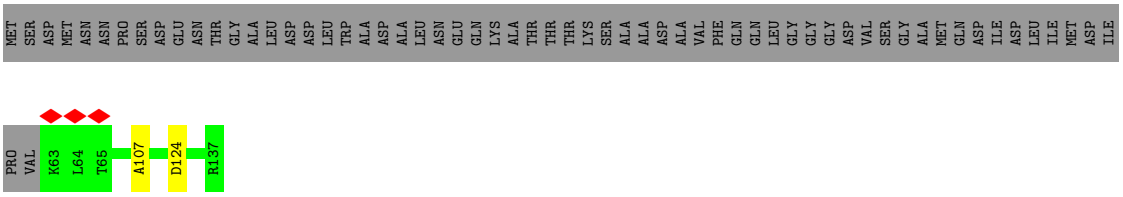
• Molecule 4: Flagellar motor switch protein FliN

Chain BB:



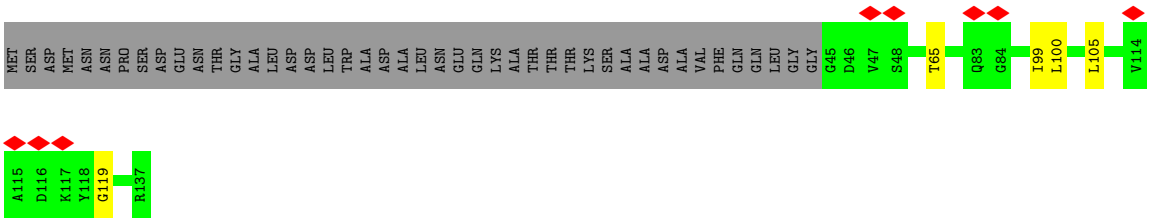
• Molecule 4: Flagellar motor switch protein FliN

Chain CB:



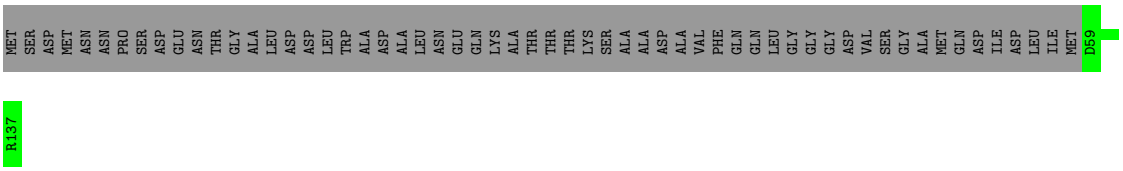
• Molecule 4: Flagellar motor switch protein FliN

Chain GB:



• Molecule 4: Flagellar motor switch protein FliN

Chain HB:



• Molecule 4: Flagellar motor switch protein FliN

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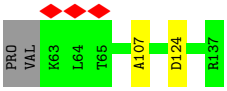
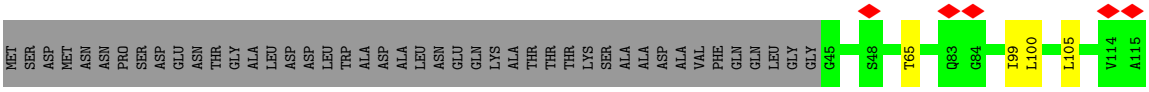
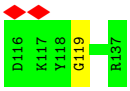


• Molecule 4: Flagellar motor switch protein FliN

Chain MB:





• Molecule 4: Flagellar motor switch protein FliN

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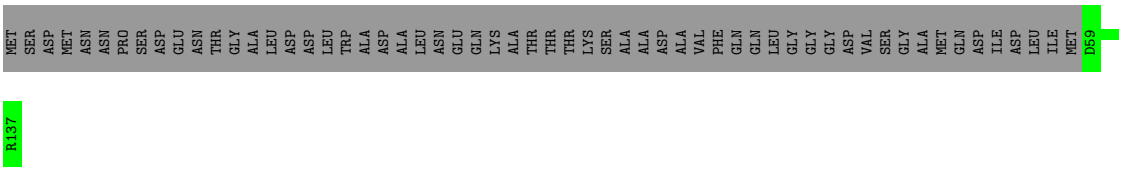
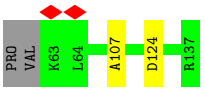


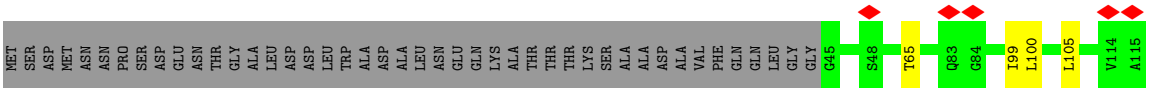
• Molecule 4: Flagellar motor switch protein FliN

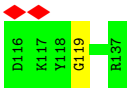
Chain OB:



• Molecule 4: Flagellar motor switch protein FliN

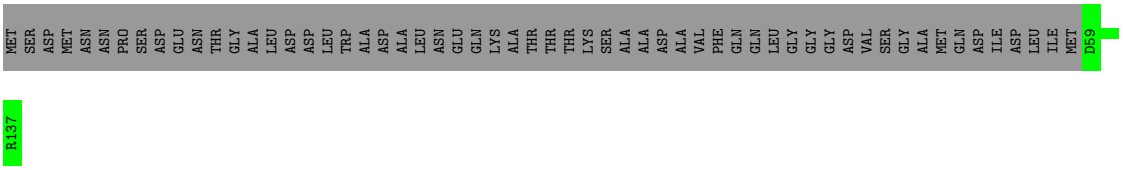
Chain SB:





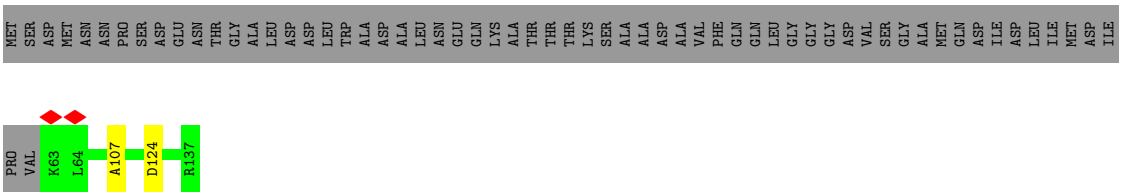
• Molecule 4: Flagellar motor switch protein FliN

Chain TB:



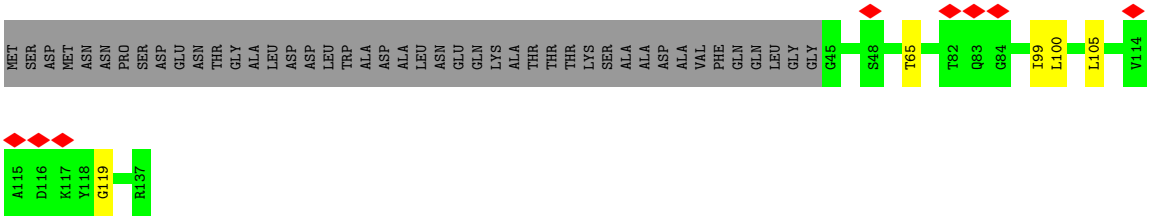
• Molecule 4: Flagellar motor switch protein FliN

Chain UB:



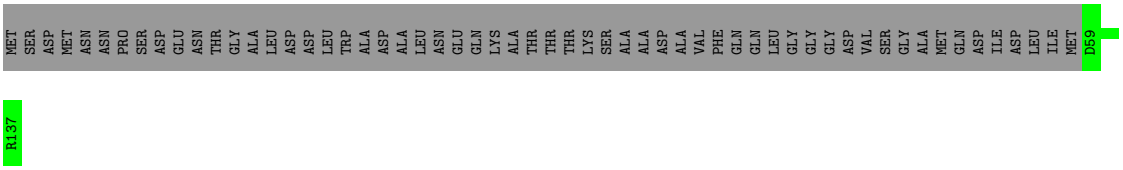
• Molecule 4: Flagellar motor switch protein FliN

Chain YB:



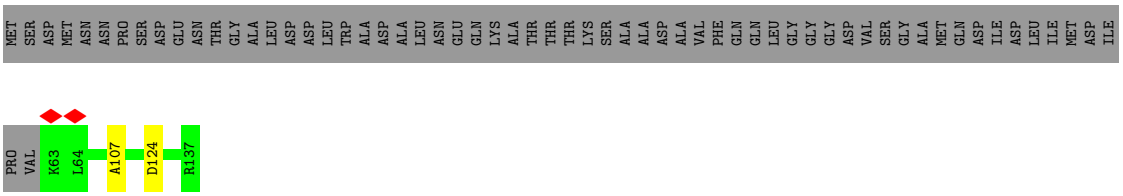
• Molecule 4: Flagellar motor switch protein FliN

Chain ZB:



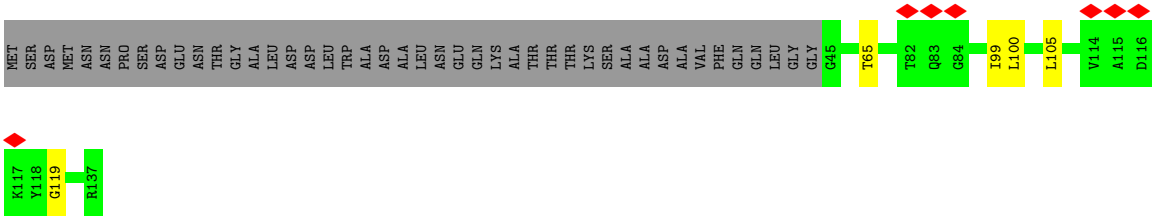
• Molecule 4: Flagellar motor switch protein FliN

Chain AC:



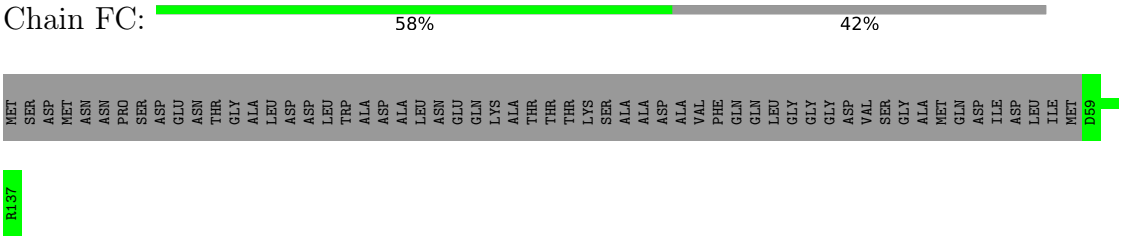
• Molecule 4: Flagellar motor switch protein FliN

Chain EC:



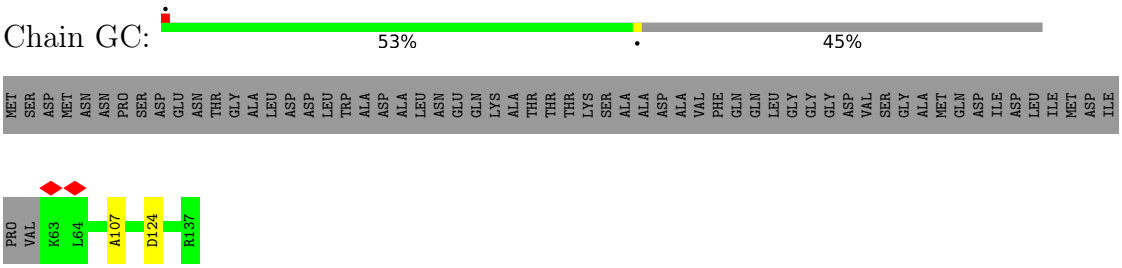
• Molecule 4: Flagellar motor switch protein FliN

Chain FC:



• Molecule 4: Flagellar motor switch protein FliN

Chain GC:



• Molecule 4: Flagellar motor switch protein FliN

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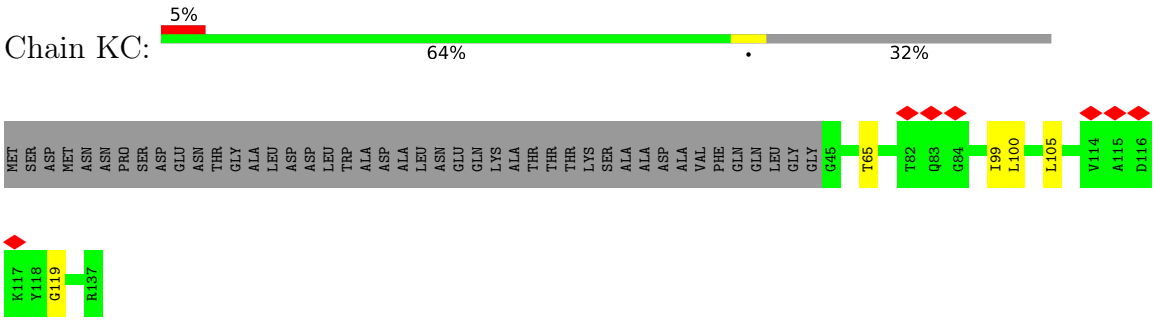
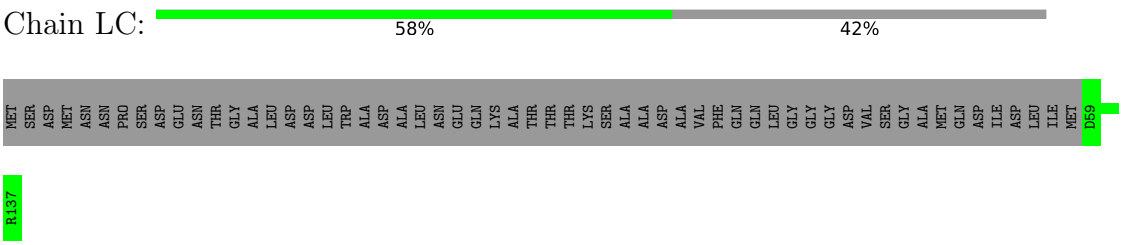


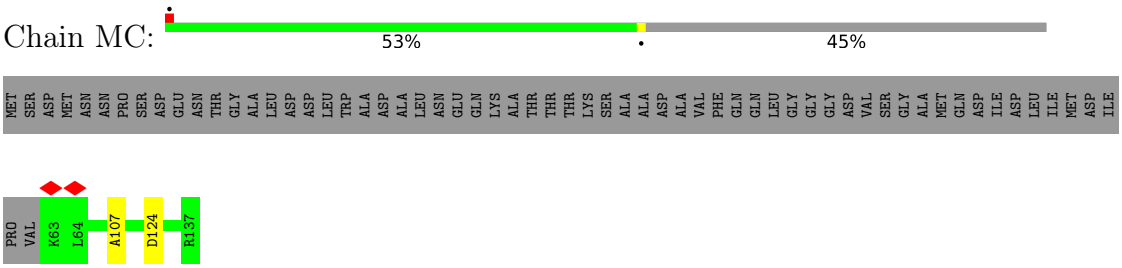
• Molecule 4: Flagellar motor switch protein FliN

Chain LC:



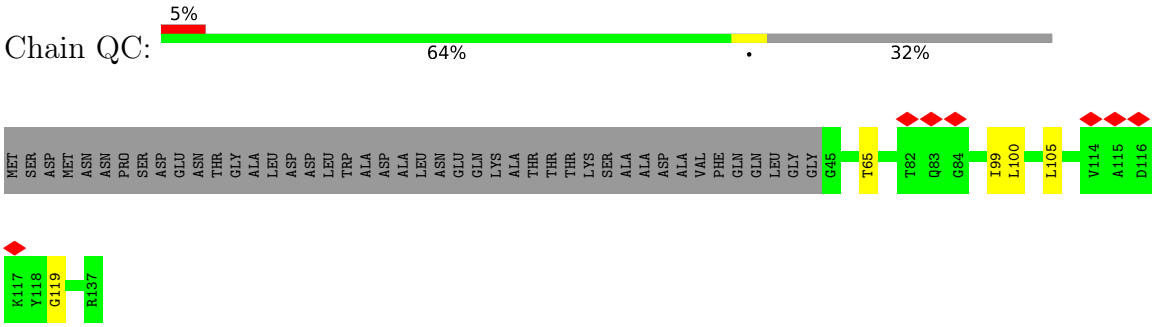
• Molecule 4: Flagellar motor switch protein FliN

Chain MC:



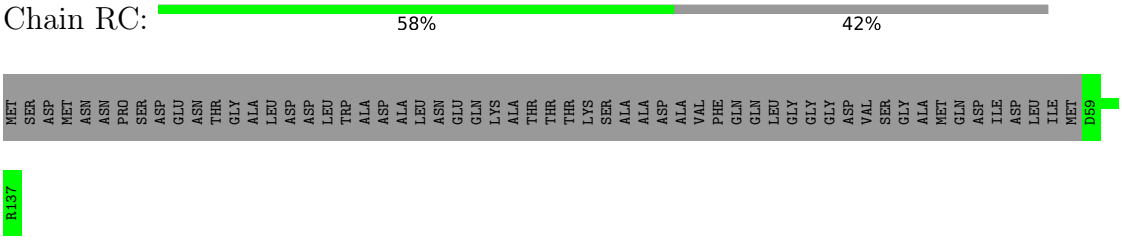
• Molecule 4: Flagellar motor switch protein FliN

Chain QC:



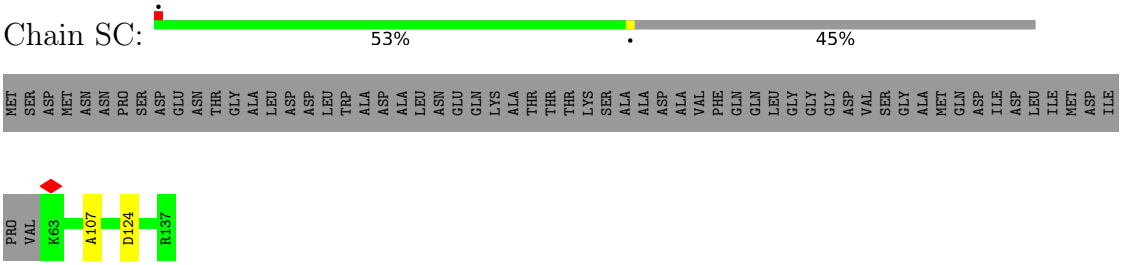
• Molecule 4: Flagellar motor switch protein FliN

Chain RC:



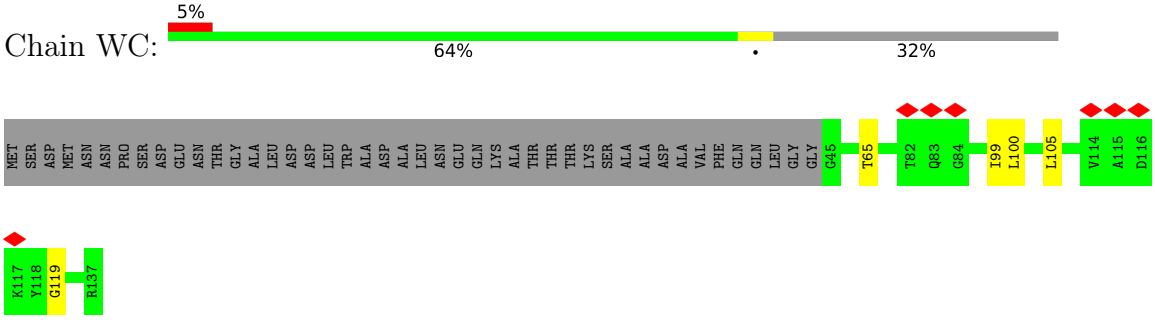
• Molecule 4: Flagellar motor switch protein FliN

Chain SC:



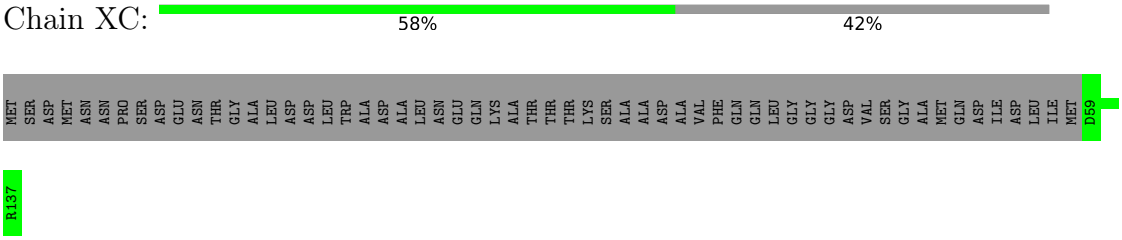
• Molecule 4: Flagellar motor switch protein FliN

Chain WC:



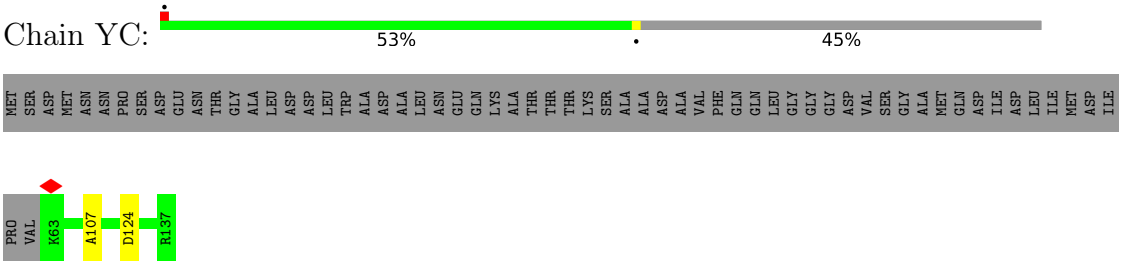
• Molecule 4: Flagellar motor switch protein FliN

Chain XC:



• Molecule 4: Flagellar motor switch protein FliN

Chain YC:



• Molecule 4: Flagellar motor switch protein FliN

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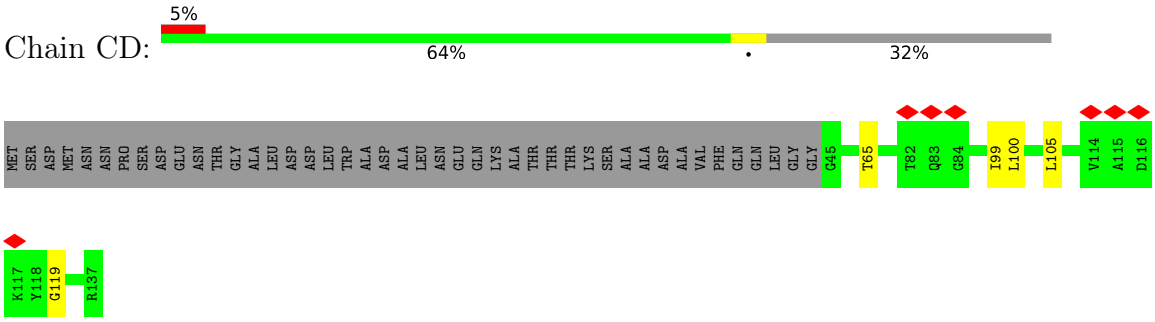
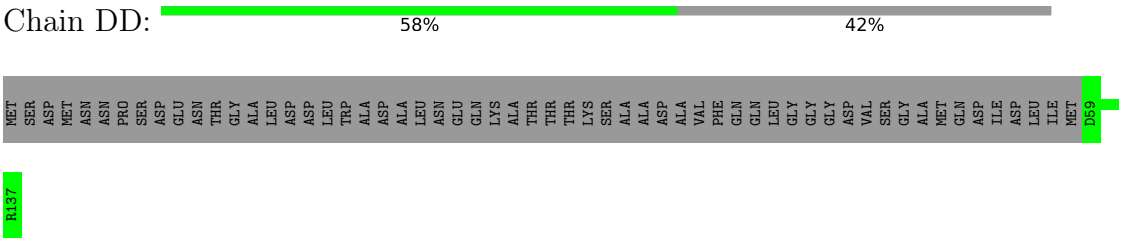


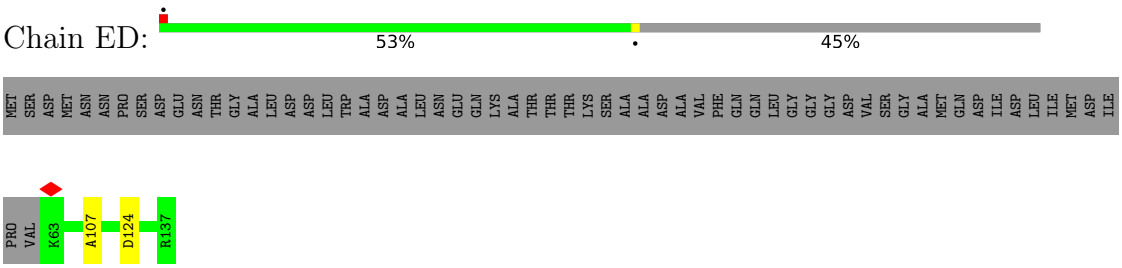
• Molecule 4: Flagellar motor switch protein FliN

Chain DD:



• Molecule 4: Flagellar motor switch protein FliN

Chain ED:



• Molecule 4: Flagellar motor switch protein FliN

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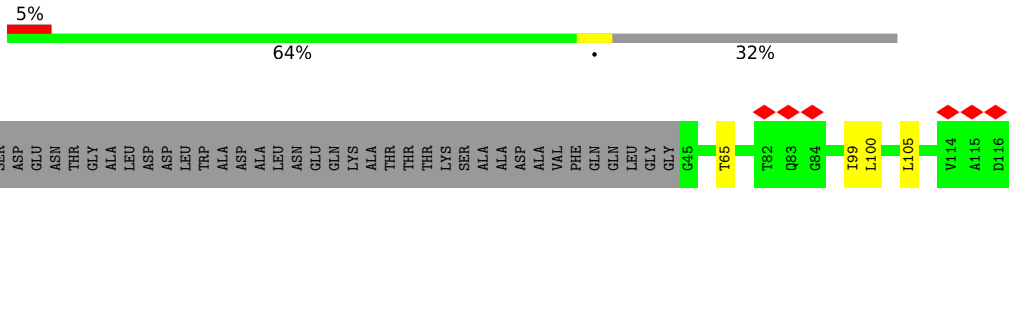

• Molecule 4: Flagellar motor switch protein FliN

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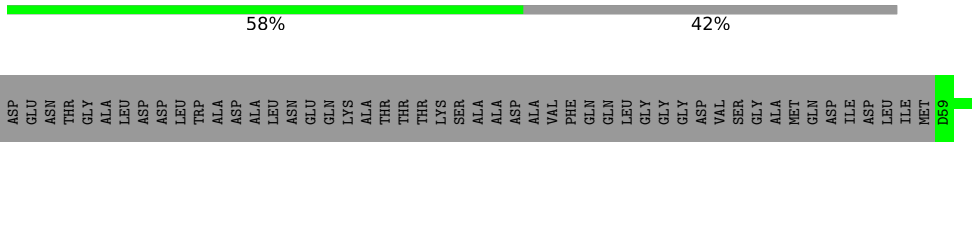
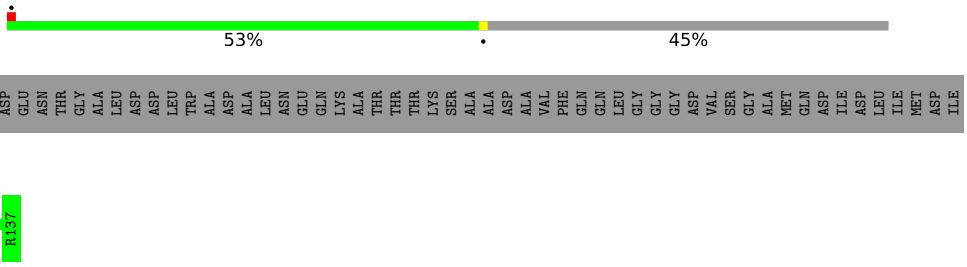


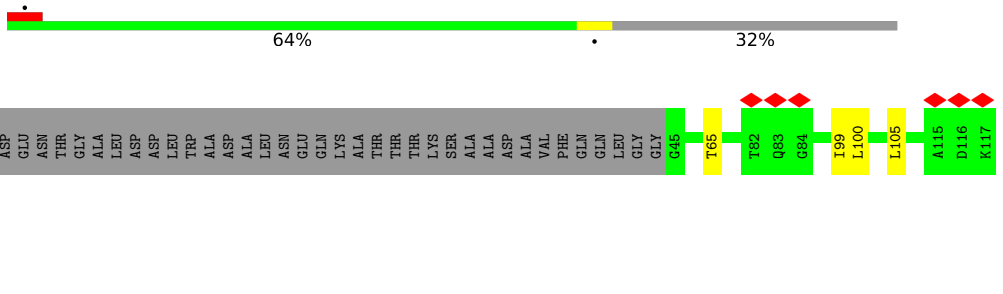
• Molecule 4: Flagellar motor switch protein FliN

Chain KD:



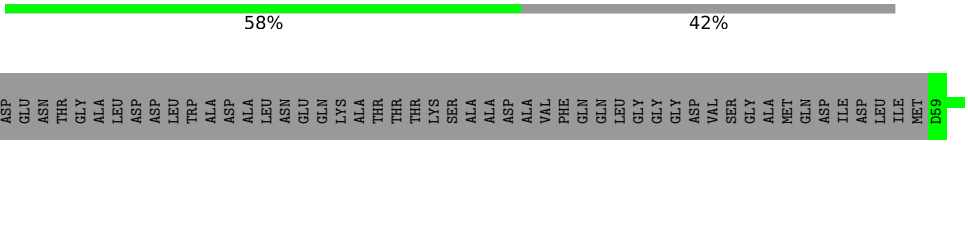
• Molecule 4: Flagellar motor switch protein FliN

Chain OD:



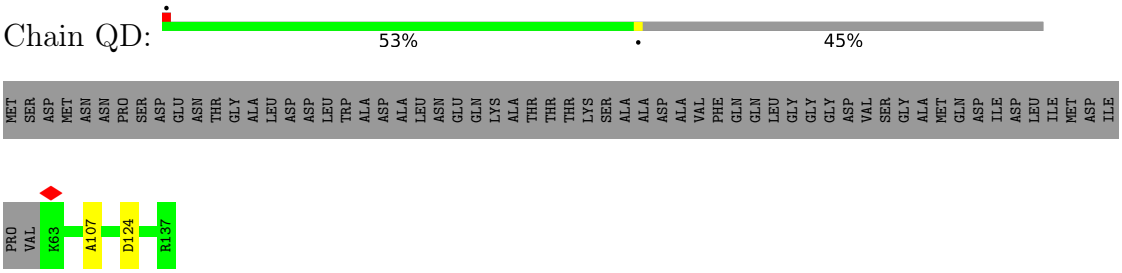
• Molecule 4: Flagellar motor switch protein FliN

Chain PD:



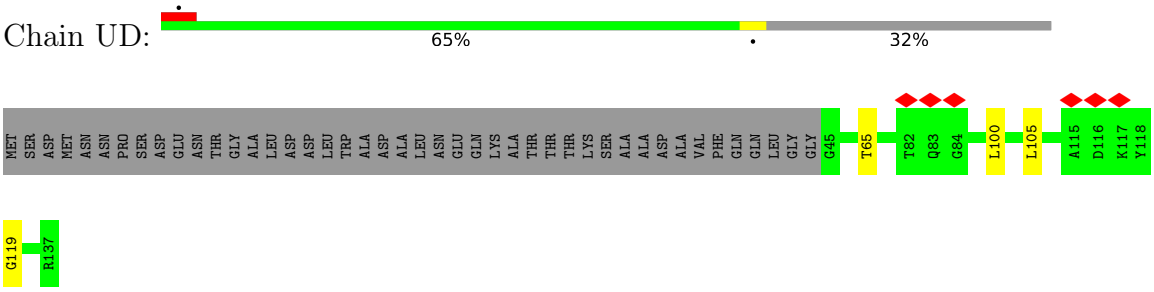
• Molecule 4: Flagellar motor switch protein FliN

Chain QD:



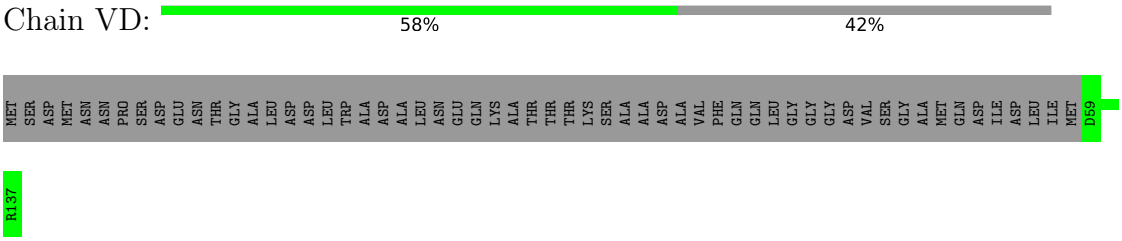
• Molecule 4: Flagellar motor switch protein FliN

Chain UD:



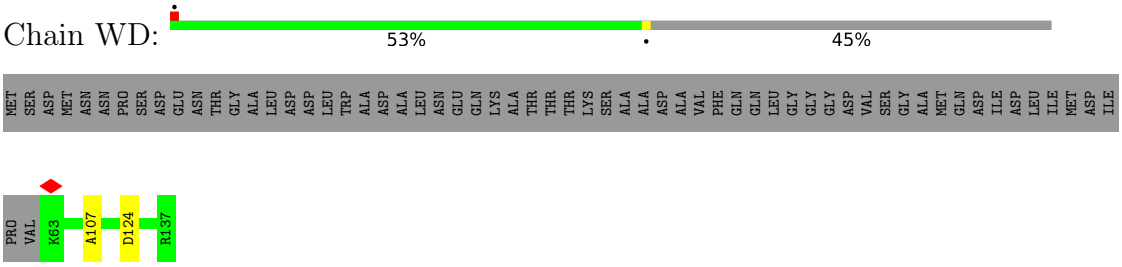
• Molecule 4: Flagellar motor switch protein FliN

Chain VD:



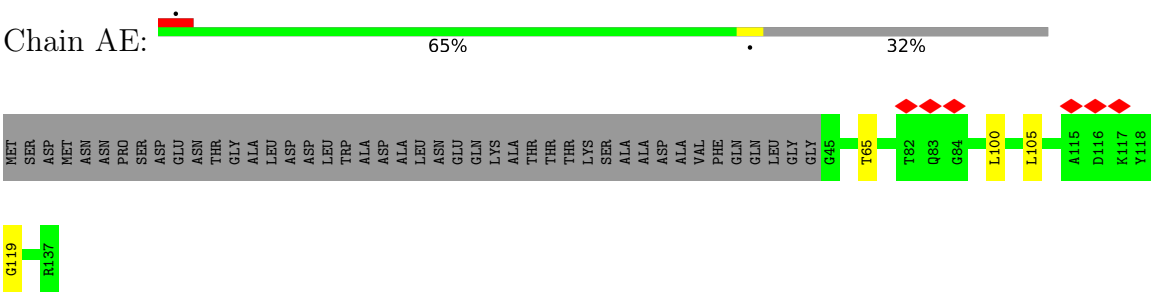
• Molecule 4: Flagellar motor switch protein FliN

Chain WD:



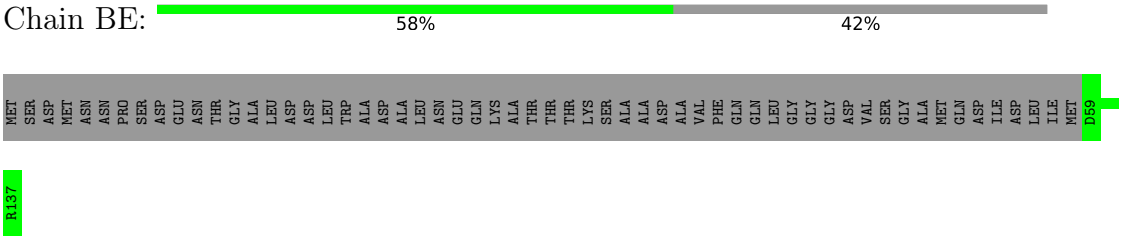
• Molecule 4: Flagellar motor switch protein FliN

Chain AE:



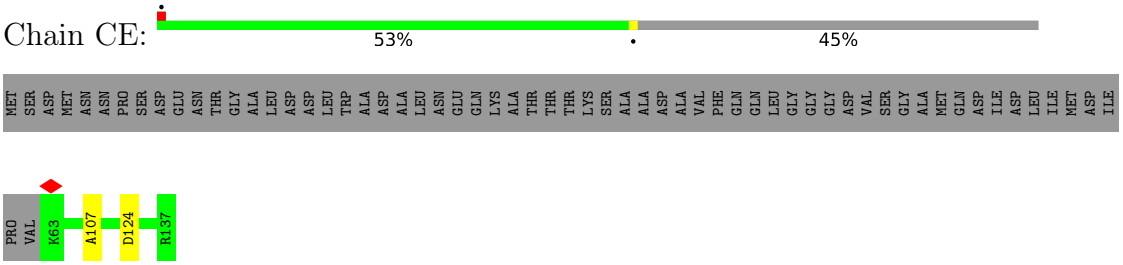
• Molecule 4: Flagellar motor switch protein FliN

Chain BE:



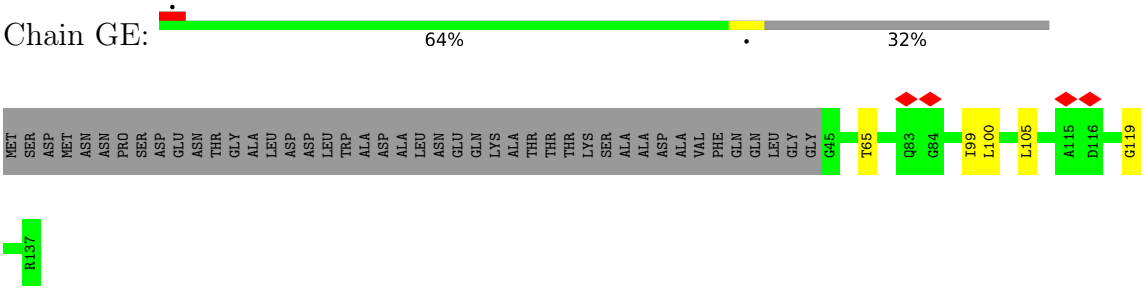
• Molecule 4: Flagellar motor switch protein FliN

Chain CE:



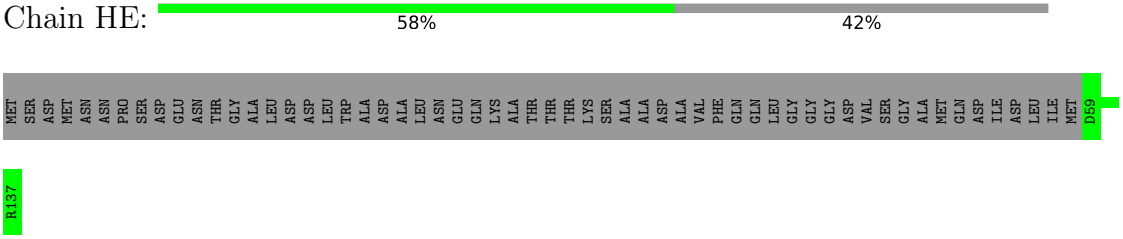
• Molecule 4: Flagellar motor switch protein FliN

Chain GE:



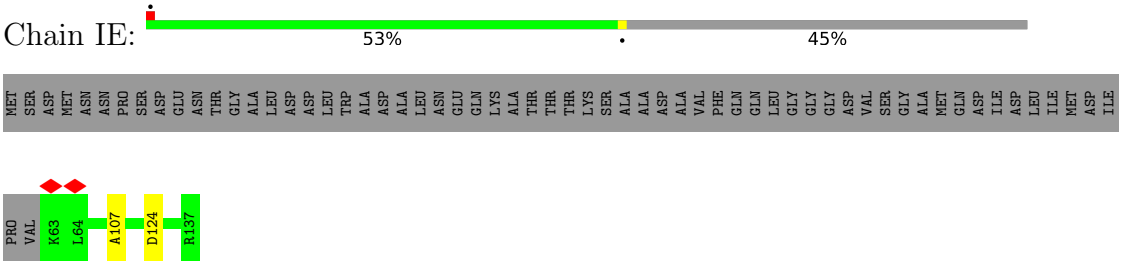
• Molecule 4: Flagellar motor switch protein FliN

Chain HE:



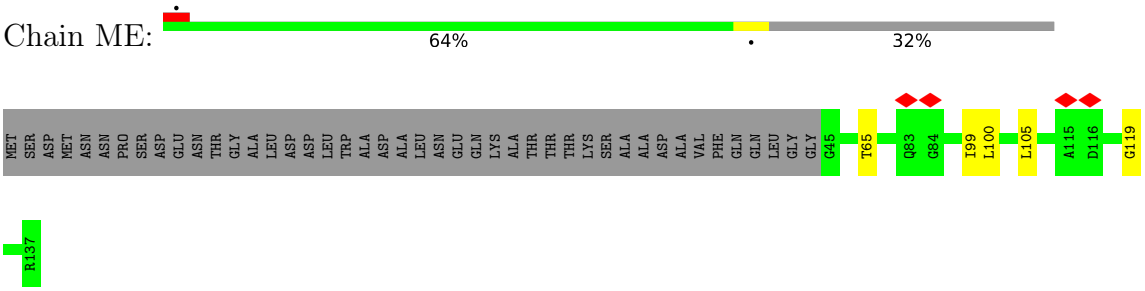
• Molecule 4: Flagellar motor switch protein FliN

Chain IE:



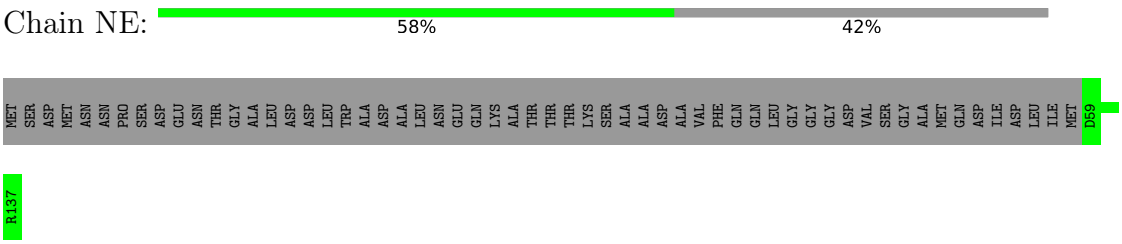
• Molecule 4: Flagellar motor switch protein FliN

Chain ME:



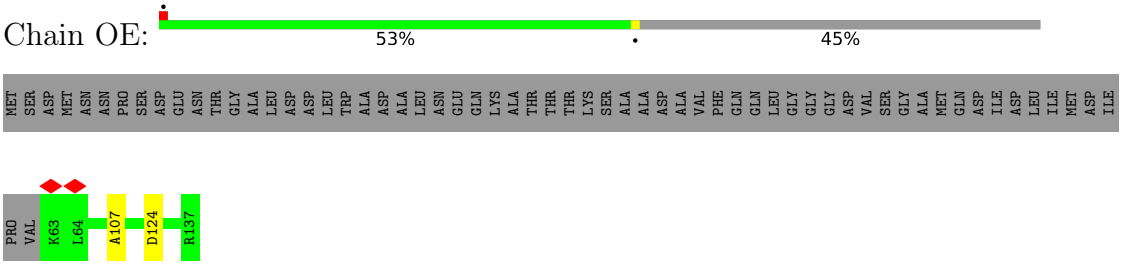
• Molecule 4: Flagellar motor switch protein FliN

Chain NE:



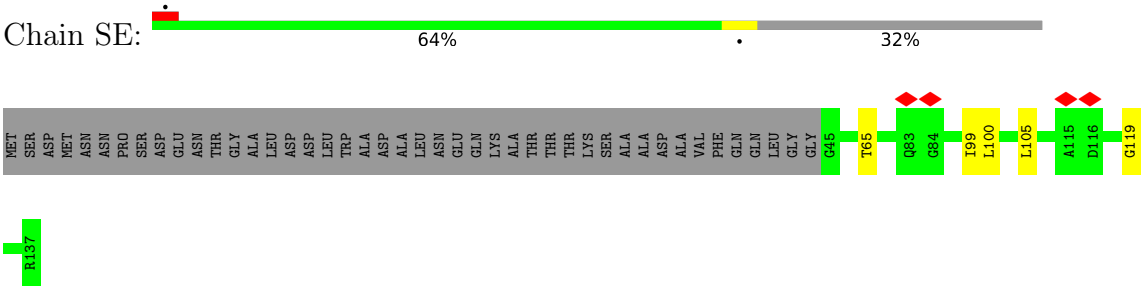
• Molecule 4: Flagellar motor switch protein FliN

Chain OE:



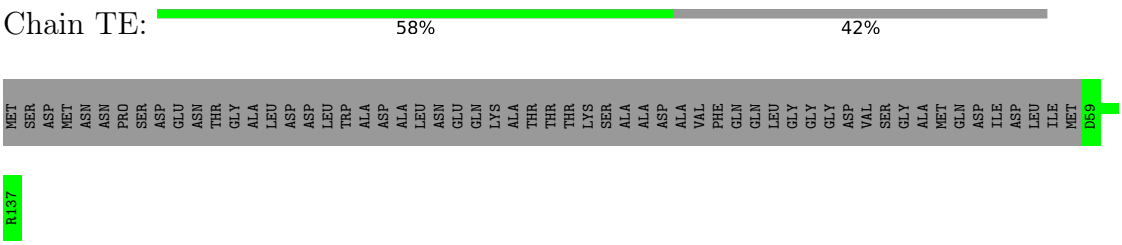
• Molecule 4: Flagellar motor switch protein FliN

Chain SE:



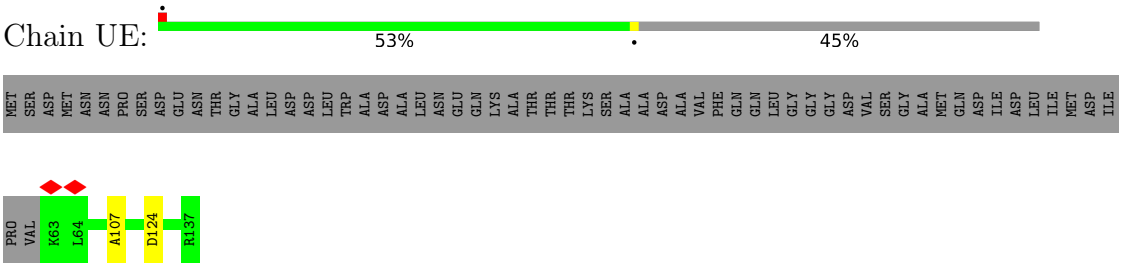
• Molecule 4: Flagellar motor switch protein FliN

Chain TE:



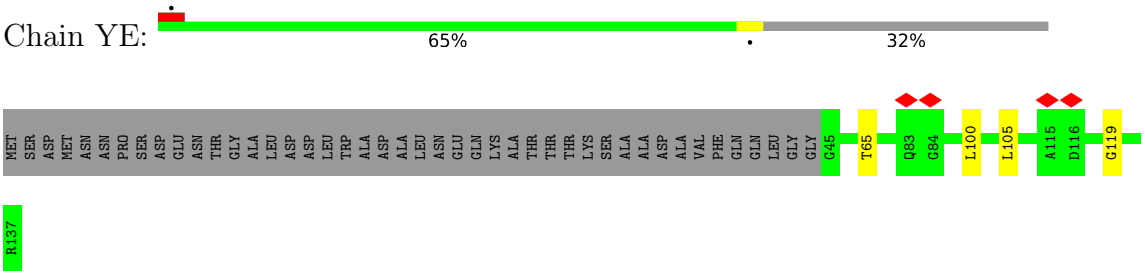
• Molecule 4: Flagellar motor switch protein FliN

Chain UE:



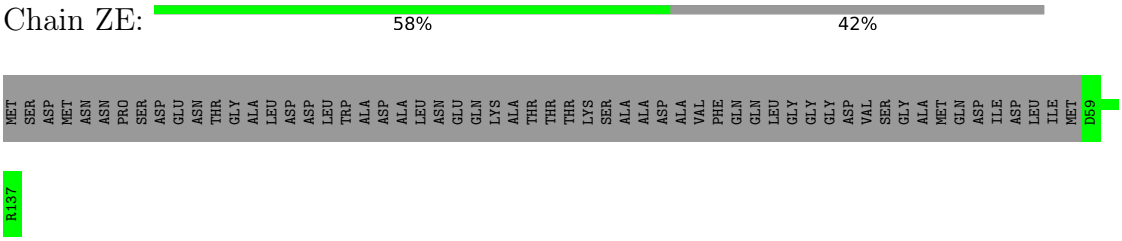
• Molecule 4: Flagellar motor switch protein FliN

Chain YE:



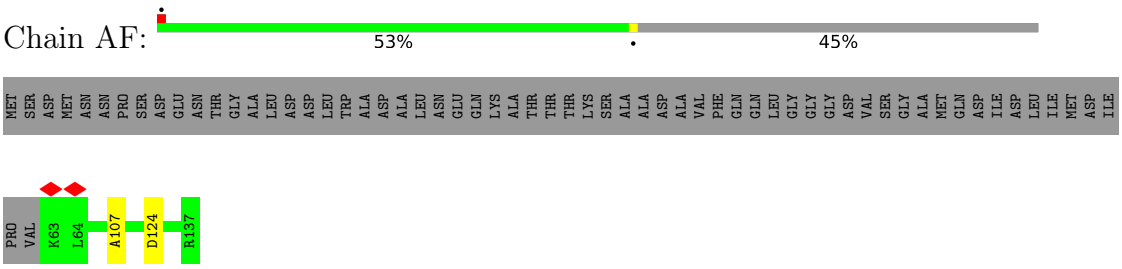
• Molecule 4: Flagellar motor switch protein FliN

Chain ZE:



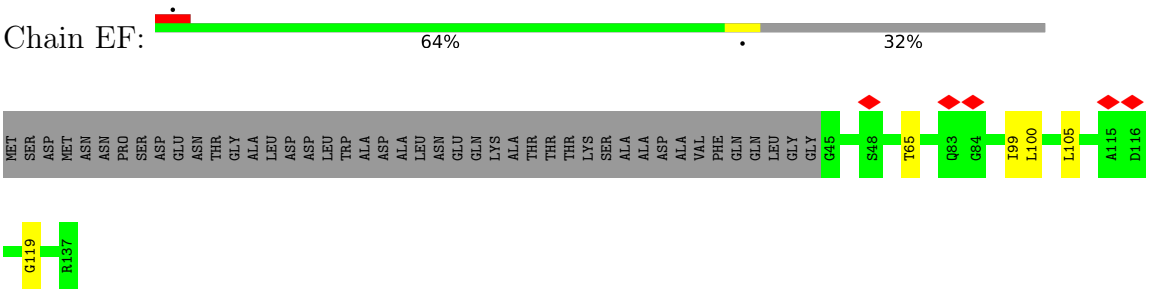
• Molecule 4: Flagellar motor switch protein FliN

Chain AF:



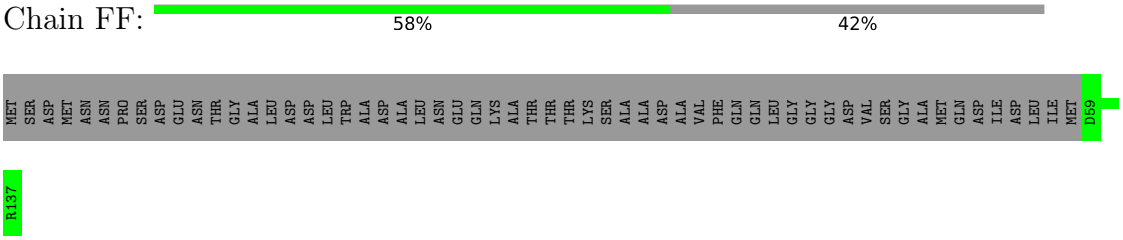
• Molecule 4: Flagellar motor switch protein FliN

Chain EF:



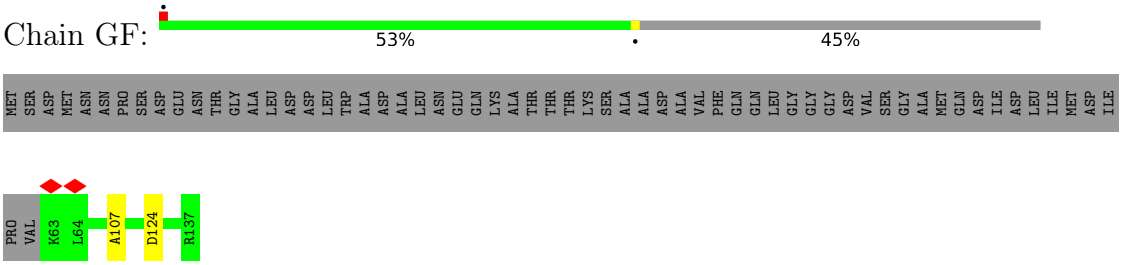
• Molecule 4: Flagellar motor switch protein FliN

Chain FF:



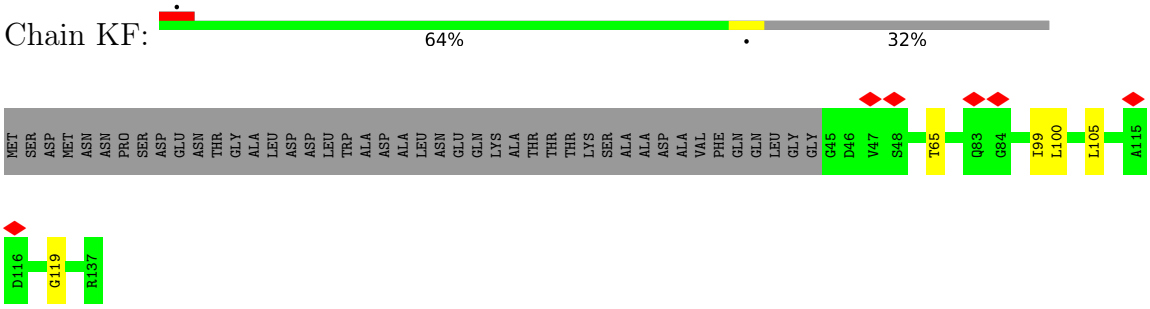
• Molecule 4: Flagellar motor switch protein FliN

Chain GF:



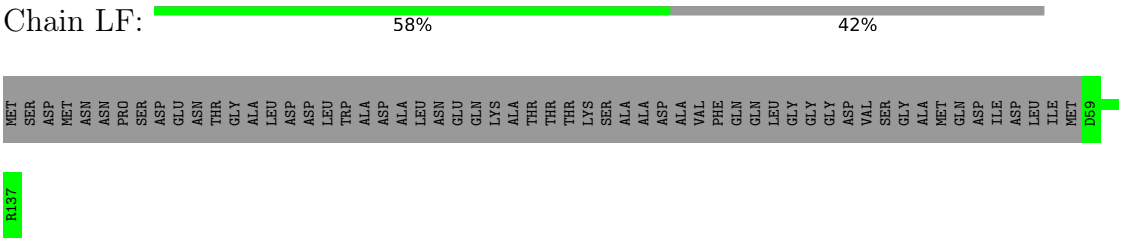
• Molecule 4: Flagellar motor switch protein FliN

Chain KF:



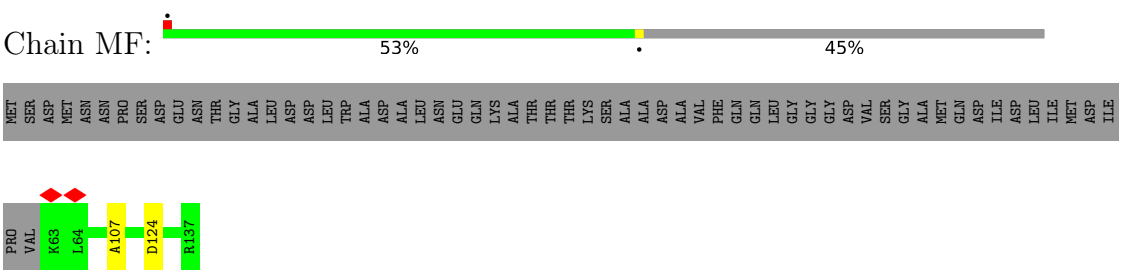
• Molecule 4: Flagellar motor switch protein FliN

Chain LF:



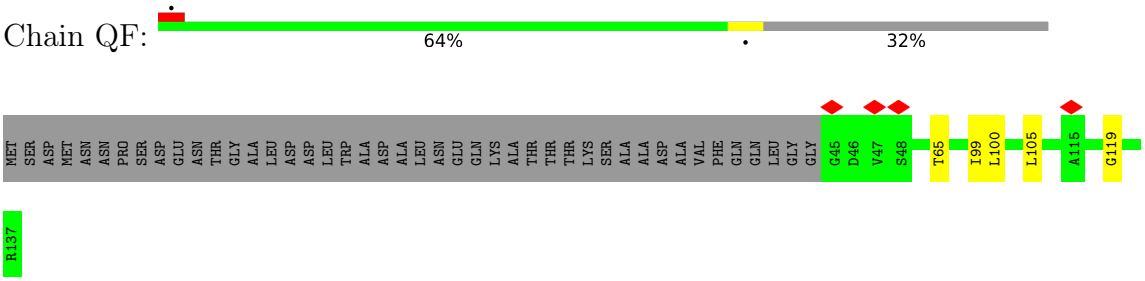
• Molecule 4: Flagellar motor switch protein FliN

Chain MF:



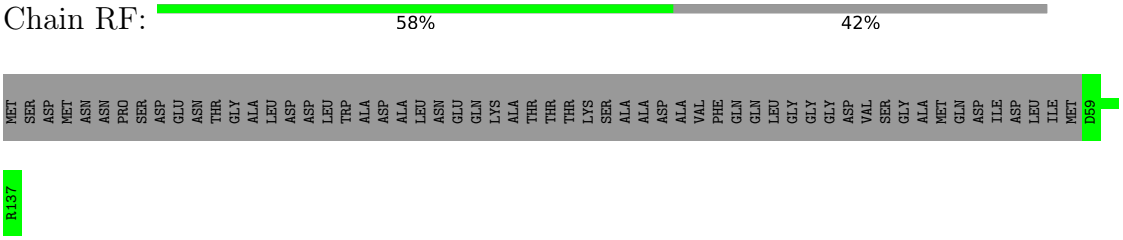
• Molecule 4: Flagellar motor switch protein FliN

Chain QF:



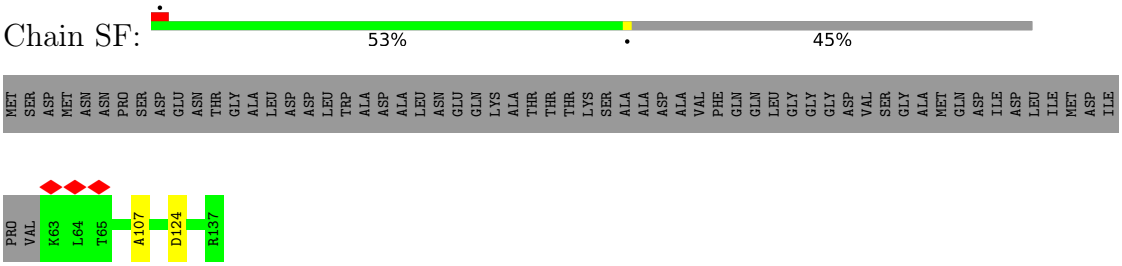
• Molecule 4: Flagellar motor switch protein FliN

Chain RF:



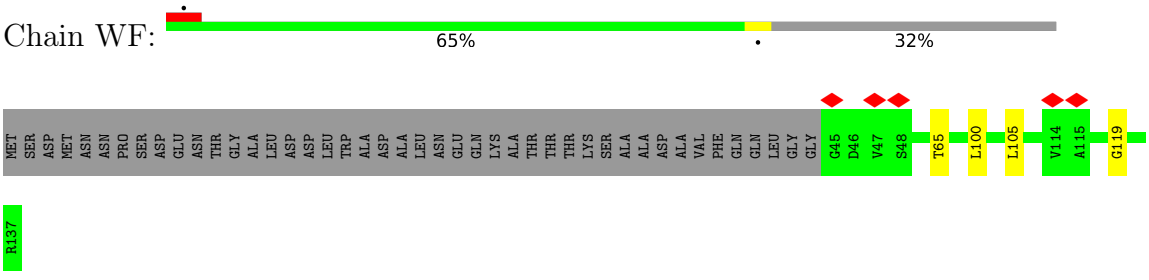
• Molecule 4: Flagellar motor switch protein FliN

Chain SF:



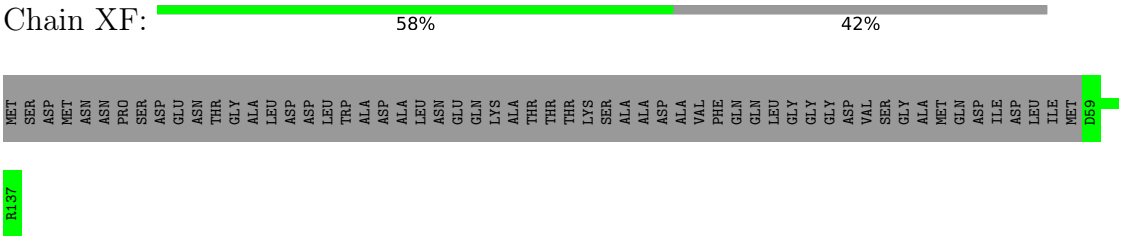
• Molecule 4: Flagellar motor switch protein FliN

Chain WF:



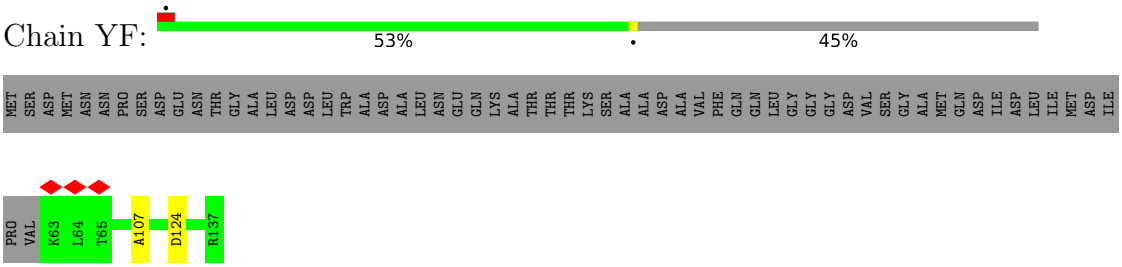
• Molecule 4: Flagellar motor switch protein FliN

Chain XF:



• Molecule 4: Flagellar motor switch protein FliN

Chain YF:



• Molecule 4: Flagellar motor switch protein FliN

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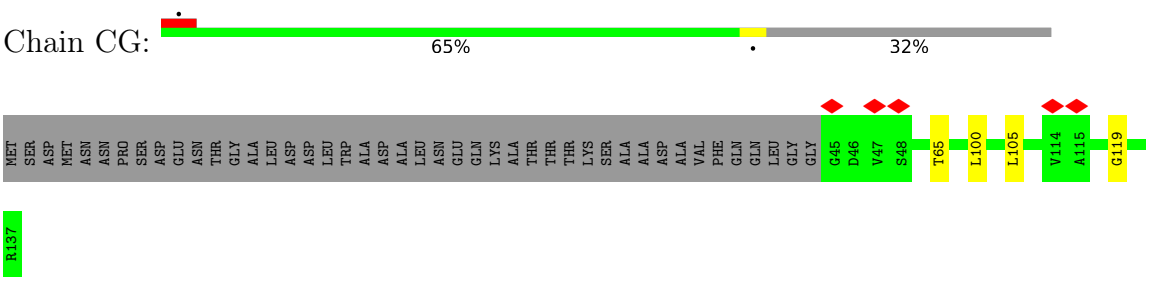
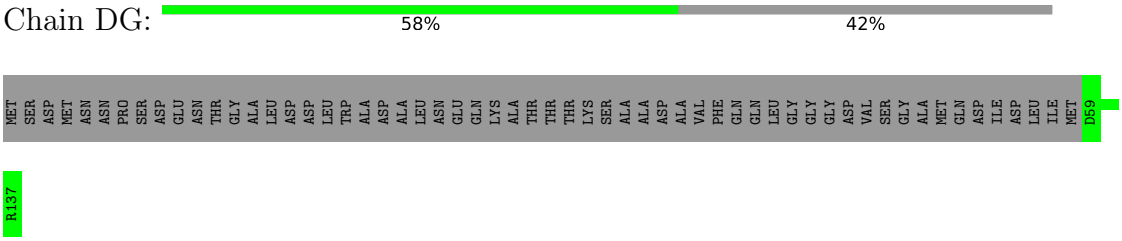


• Molecule 4: Flagellar motor switch protein FliN

Chain DG:



• Molecule 4: Flagellar motor switch protein FliN

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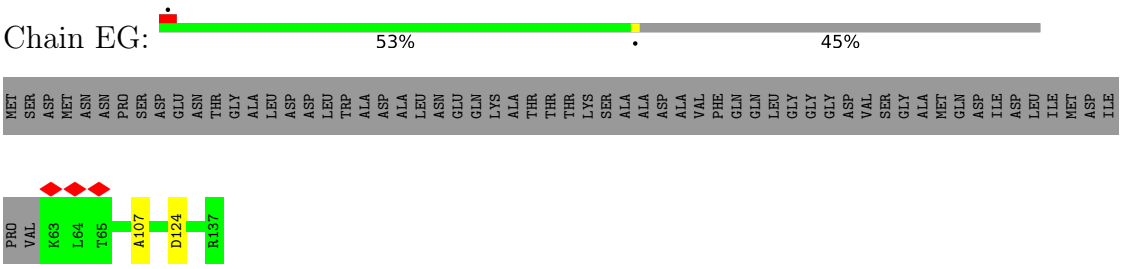
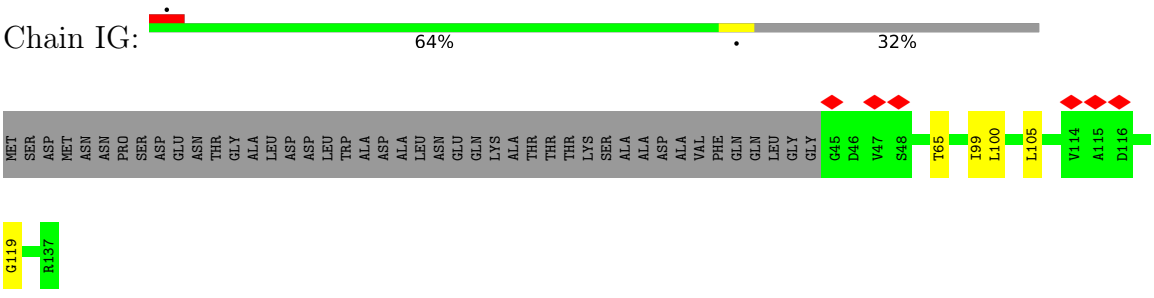


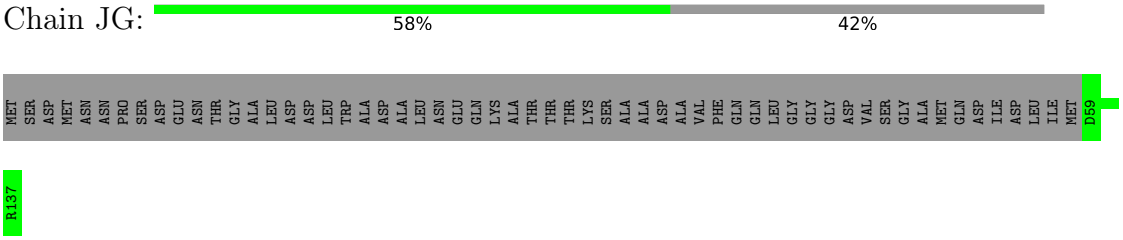
• Molecule 4: Flagellar motor switch protein FliN

Chain IG:



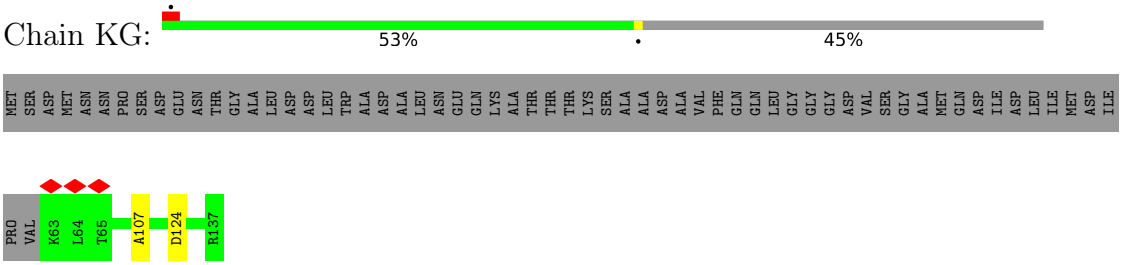
• Molecule 4: Flagellar motor switch protein FliN

Chain JG:



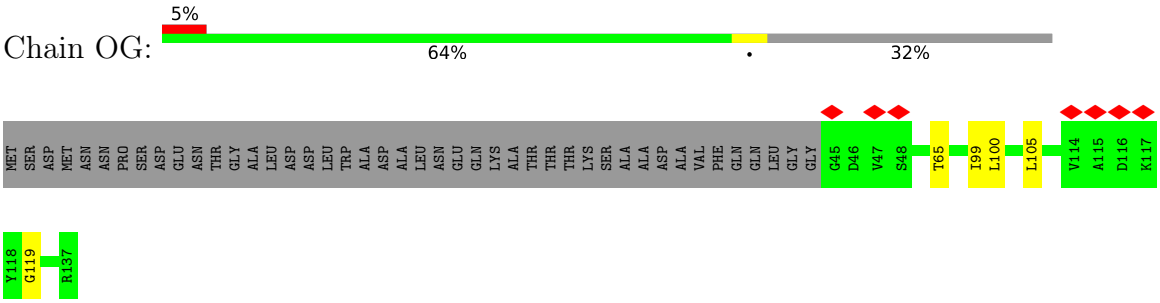
• Molecule 4: Flagellar motor switch protein FliN

Chain KG:



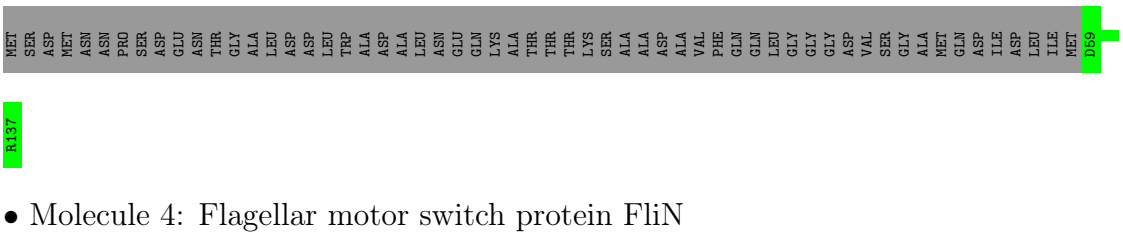
• Molecule 4: Flagellar motor switch protein FliN

Chain OG:



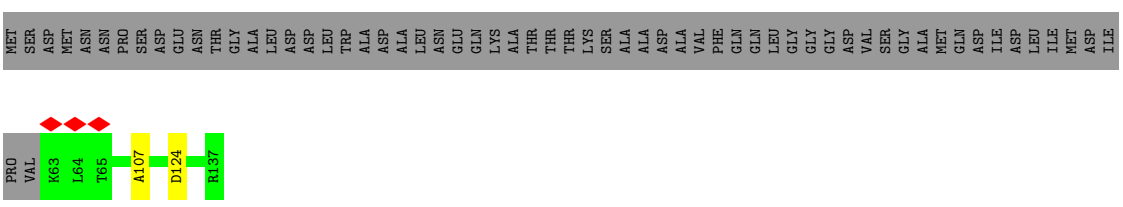
• Molecule 4: Flagellar motor switch protein FliN

Chain PG:



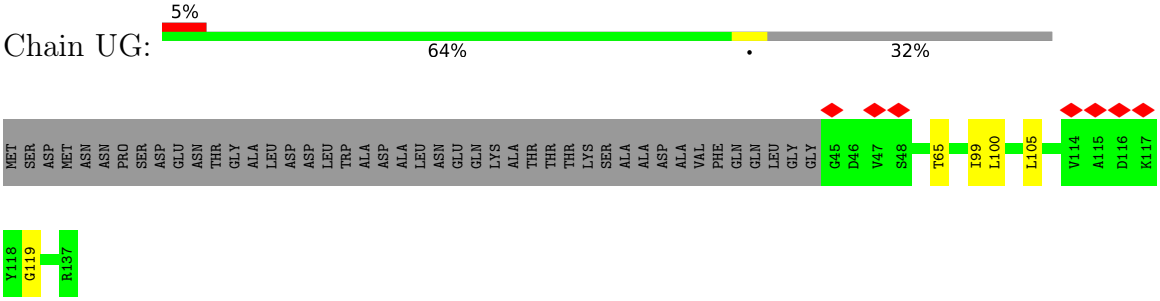
• Molecule 4: Flagellar motor switch protein FliN

Chain QG:



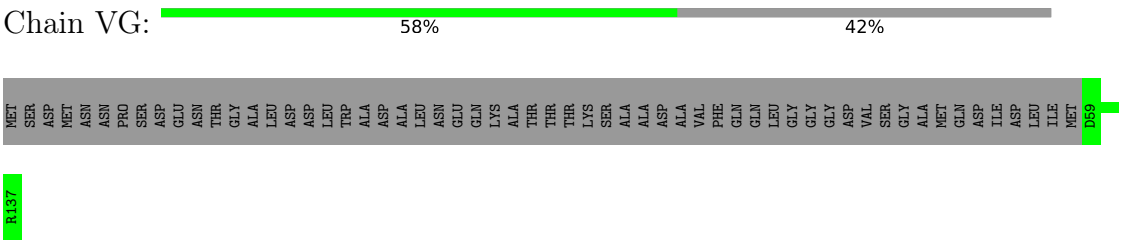
• Molecule 4: Flagellar motor switch protein FliN

Chain UG:



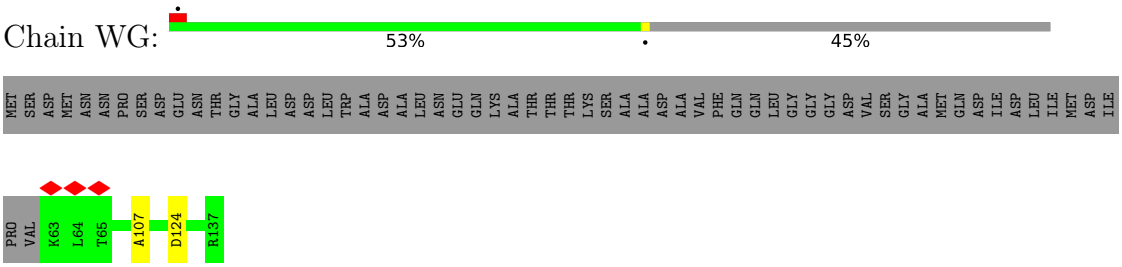
• Molecule 4: Flagellar motor switch protein FliN

Chain VG:



• Molecule 4: Flagellar motor switch protein FliN

Chain WG:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7201	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56.323	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.376	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.151	Depositor
Map size (Å)	1049.6, 1049.6, 1049.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.05, 2.05, 2.05	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	A	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	BC	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	BF	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	DB	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	DE	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	F	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	FA	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	FD	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	FG	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	HC	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	HF	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	I	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	JB	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	JE	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	LA	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	LD	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	LG	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	NC	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	NF	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	PB	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	PE	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	RA	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	RD	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	RG	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	S	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	TC	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	TF	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	VB	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	VE	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	XA	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	XD	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	Z	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	ZC	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)
1	ZF	0.81	1/233 (0.4%)	0.74	2/324 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	AA	0.52	0/1551	0.63	0/2157
2	AD	0.53	0/1551	0.63	0/2157
2	AG	0.53	0/1551	0.63	0/2157
2	B	0.53	0/1551	0.63	0/2157
2	CC	0.53	0/1551	0.63	0/2157
2	CF	0.53	0/1551	0.63	0/2157
2	EB	0.53	0/1551	0.63	0/2157
2	EE	0.53	0/1551	0.63	0/2157
2	G	0.53	0/1551	0.63	0/2157
2	GA	0.53	0/1551	0.63	0/2157
2	GD	0.52	0/1551	0.63	0/2157
2	GG	0.53	0/1551	0.63	0/2157
2	IC	0.53	0/1551	0.63	0/2157
2	IF	0.53	0/1551	0.63	0/2157
2	J	0.53	0/1551	0.63	0/2157
2	KB	0.53	0/1551	0.63	0/2157
2	KE	0.53	0/1551	0.63	0/2157
2	MA	0.52	0/1551	0.63	0/2157
2	MD	0.52	0/1551	0.63	0/2157
2	MG	0.53	0/1551	0.63	0/2157
2	OC	0.53	0/1551	0.63	0/2157
2	OF	0.53	0/1551	0.63	0/2157
2	QB	0.53	0/1551	0.63	0/2157
2	QE	0.53	0/1551	0.63	0/2157
2	SA	0.53	0/1551	0.63	0/2157
2	SD	0.53	0/1551	0.63	0/2157
2	SG	0.52	0/1551	0.63	0/2157
2	T	0.53	0/1551	0.63	0/2157
2	UC	0.52	0/1551	0.63	0/2157
2	UF	0.53	0/1551	0.63	0/2157
2	WB	0.53	0/1551	0.63	0/2157
2	WE	0.53	0/1551	0.63	0/2157
2	YA	0.53	0/1551	0.63	0/2157
2	YD	0.53	0/1551	0.63	0/2157
3	BA	0.38	0/1384	0.59	0/1927
3	BD	0.38	0/1384	0.59	0/1927
3	BG	0.38	0/1384	0.59	0/1927
3	C	0.38	0/1384	0.59	0/1927
3	DC	0.38	0/1384	0.59	0/1927
3	DF	0.38	0/1384	0.59	0/1927
3	FB	0.38	0/1384	0.59	0/1927
3	FE	0.38	0/1384	0.59	0/1927
3	HA	0.38	0/1384	0.59	0/1927

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
3	HD	0.38	0/1384	0.59	0/1927
3	HG	0.38	0/1384	0.59	0/1927
3	JC	0.38	0/1384	0.59	0/1927
3	JF	0.38	0/1384	0.59	0/1927
3	K	0.38	0/1384	0.59	0/1927
3	LB	0.38	0/1384	0.59	0/1927
3	LE	0.38	0/1384	0.59	0/1927
3	M	0.38	0/1384	0.59	0/1927
3	NA	0.38	0/1384	0.59	0/1927
3	ND	0.38	0/1384	0.59	0/1927
3	NG	0.38	0/1384	0.59	0/1927
3	PC	0.38	0/1384	0.59	0/1927
3	PF	0.38	0/1384	0.59	0/1927
3	RB	0.38	0/1384	0.59	0/1927
3	RE	0.38	0/1384	0.59	0/1927
3	TA	0.38	0/1384	0.59	0/1927
3	TD	0.38	0/1384	0.59	0/1927
3	TG	0.38	0/1384	0.59	0/1927
3	V	0.38	0/1384	0.59	0/1927
3	VC	0.38	0/1384	0.59	0/1927
3	VF	0.38	0/1384	0.59	0/1927
3	XB	0.38	0/1384	0.59	0/1927
3	XE	0.38	0/1384	0.59	0/1927
3	ZA	0.38	0/1384	0.59	0/1927
3	ZD	0.38	0/1384	0.59	0/1927
4	AB	0.42	0/455	0.52	0/630
4	AC	0.47	0/367	0.56	0/508
4	AE	0.42	0/455	0.52	0/630
4	AF	0.47	0/367	0.56	0/508
4	BB	0.41	0/388	0.56	0/536
4	BE	0.41	0/388	0.56	0/536
4	CA	0.42	0/455	0.52	0/630
4	CB	0.47	0/367	0.56	0/508
4	CD	0.42	0/455	0.52	0/630
4	CE	0.47	0/367	0.56	0/508
4	CG	0.42	0/455	0.52	0/630
4	D	0.42	0/455	0.52	0/630
4	DA	0.41	0/388	0.56	0/536
4	DD	0.41	0/388	0.56	0/536
4	DG	0.41	0/388	0.56	0/536
4	E	0.41	0/388	0.56	0/536
4	EA	0.47	0/367	0.56	0/508
4	EC	0.42	0/455	0.52	0/630

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
4	ED	0.47	0/367	0.56	0/508
4	EF	0.42	0/455	0.52	0/630
4	EG	0.47	0/367	0.56	0/508
4	FC	0.41	0/388	0.56	0/536
4	FF	0.41	0/388	0.56	0/536
4	GB	0.42	0/455	0.52	0/630
4	GC	0.47	0/367	0.56	0/508
4	GE	0.42	0/455	0.52	0/630
4	GF	0.47	0/367	0.56	0/508
4	H	0.47	0/367	0.56	0/508
4	HB	0.41	0/388	0.56	0/536
4	HE	0.41	0/388	0.56	0/536
4	IA	0.42	0/455	0.52	0/630
4	IB	0.47	0/367	0.56	0/508
4	ID	0.42	0/455	0.52	0/630
4	IE	0.47	0/367	0.56	0/508
4	IG	0.42	0/455	0.52	0/630
4	JA	0.41	0/388	0.56	0/536
4	JD	0.41	0/388	0.56	0/536
4	JG	0.41	0/388	0.56	0/536
4	KA	0.47	0/367	0.56	0/508
4	KC	0.42	0/455	0.52	0/630
4	KD	0.47	0/367	0.56	0/508
4	KF	0.42	0/455	0.52	0/630
4	KG	0.47	0/367	0.56	0/508
4	L	0.42	0/455	0.52	0/630
4	LC	0.41	0/388	0.56	0/536
4	LF	0.41	0/388	0.56	0/536
4	MB	0.42	0/455	0.52	0/630
4	MC	0.47	0/367	0.56	0/508
4	ME	0.42	0/455	0.52	0/630
4	MF	0.47	0/367	0.56	0/508
4	N	0.42	0/455	0.52	0/630
4	NB	0.41	0/388	0.56	0/536
4	NE	0.41	0/388	0.56	0/536
4	O	0.41	0/388	0.56	0/536
4	OA	0.42	0/455	0.52	0/630
4	OB	0.47	0/367	0.56	0/508
4	OD	0.42	0/455	0.52	0/630
4	OE	0.47	0/367	0.56	0/508
4	OG	0.42	0/455	0.52	0/630
4	P	0.41	0/388	0.56	0/536
4	PA	0.41	0/388	0.56	0/536

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
4	PD	0.41	0/388	0.56	0/536
4	PG	0.41	0/388	0.56	0/536
4	Q	0.47	0/367	0.56	0/508
4	QA	0.47	0/367	0.56	0/508
4	QC	0.42	0/455	0.52	0/630
4	QD	0.47	0/367	0.56	0/508
4	QF	0.42	0/455	0.52	0/630
4	QG	0.47	0/367	0.56	0/508
4	R	0.47	0/367	0.56	0/508
4	RC	0.41	0/388	0.56	0/536
4	RF	0.41	0/388	0.56	0/536
4	SB	0.42	0/455	0.52	0/630
4	SC	0.47	0/367	0.56	0/508
4	SE	0.42	0/455	0.52	0/630
4	SF	0.47	0/367	0.56	0/508
4	TB	0.41	0/388	0.56	0/536
4	TE	0.41	0/388	0.56	0/536
4	UA	0.42	0/455	0.52	0/630
4	UB	0.47	0/367	0.56	0/508
4	UD	0.42	0/455	0.52	0/630
4	UE	0.47	0/367	0.56	0/508
4	UG	0.42	0/455	0.52	0/630
4	VA	0.41	0/388	0.56	0/536
4	VD	0.41	0/388	0.56	0/536
4	VG	0.41	0/388	0.56	0/536
4	W	0.42	0/455	0.52	0/630
4	WA	0.47	0/367	0.56	0/508
4	WC	0.42	0/455	0.52	0/630
4	WD	0.47	0/367	0.56	0/508
4	WF	0.42	0/455	0.52	0/630
4	WG	0.47	0/367	0.56	0/508
4	X	0.41	0/388	0.56	0/536
4	XC	0.41	0/388	0.56	0/536
4	XF	0.41	0/388	0.56	0/536
4	Y	0.47	0/367	0.56	0/508
4	YB	0.42	0/455	0.52	0/630
4	YC	0.47	0/367	0.56	0/508
4	YE	0.42	0/455	0.52	0/630
4	YF	0.47	0/367	0.56	0/508
4	ZB	0.41	0/388	0.56	0/536
4	ZE	0.41	0/388	0.56	0/536
All	All	0.48	34/148852 (0.0%)	0.60	68/206788 (0.0%)

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	HC	544	PRO	C-N	10.90	1.59	1.34
1	FG	544	PRO	C-N	10.90	1.59	1.34
1	DB	544	PRO	C-N	10.90	1.59	1.34
1	NC	544	PRO	C-N	10.90	1.59	1.34
1	RG	544	PRO	C-N	10.89	1.59	1.34

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	FD	544	PRO	O-C-N	8.80	136.78	122.70
1	I	544	PRO	O-C-N	8.79	136.76	122.70
1	BF	544	PRO	O-C-N	8.79	136.76	122.70
1	HF	544	PRO	O-C-N	8.78	136.75	122.70
1	LD	544	PRO	O-C-N	8.78	136.75	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	A	234	0	102	4	0
1	BC	234	0	102	4	0
1	BF	234	0	102	4	0
1	DB	234	0	102	4	0
1	DE	234	0	102	4	0
1	F	234	0	102	4	0
1	FA	234	0	102	5	0
1	FD	234	0	102	4	0
1	FG	234	0	102	4	0
1	HC	234	0	102	4	0
1	HF	234	0	102	4	0
1	I	234	0	102	5	0
1	JB	234	0	102	4	0
1	JE	234	0	102	4	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	LA	234	0	102	4	0
1	LD	234	0	102	4	0
1	LG	234	0	102	5	0
1	NC	234	0	102	4	0
1	NF	234	0	102	5	0
1	PB	234	0	102	4	0
1	PE	234	0	102	4	0
1	RA	234	0	102	4	0
1	RD	234	0	102	4	0
1	RG	234	0	102	4	0
1	S	234	0	102	4	0
1	TC	234	0	102	4	0
1	TF	234	0	102	4	0
1	VB	234	0	102	4	0
1	VE	234	0	102	4	0
1	XA	234	0	102	4	0
1	XD	234	0	102	4	0
1	Z	234	0	102	4	0
1	ZC	234	0	102	4	0
1	ZF	234	0	102	4	0
2	AA	1554	0	723	54	0
2	AD	1554	0	723	51	0
2	AG	1554	0	723	54	0
2	B	1554	0	723	53	0
2	CC	1554	0	723	51	0
2	CF	1554	0	723	52	0
2	EB	1554	0	723	52	0
2	EE	1554	0	723	51	0
2	G	1554	0	723	53	0
2	GA	1554	0	723	48	0
2	GD	1554	0	723	54	0
2	GG	1554	0	723	54	0
2	IC	1554	0	723	51	0
2	IF	1554	0	723	53	0
2	J	1554	0	723	55	0
2	KB	1554	0	723	46	0
2	KE	1554	0	723	45	0
2	MA	1554	0	723	44	0
2	MD	1554	0	723	50	0
2	MG	1554	0	723	54	0
2	OC	1554	0	723	46	0
2	OF	1554	0	723	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	QB	1554	0	723	46	0
2	QE	1554	0	723	48	0
2	SA	1554	0	723	51	0
2	SD	1554	0	723	52	0
2	SG	1554	0	723	52	0
2	T	1554	0	723	53	0
2	UC	1554	0	723	44	0
2	UF	1554	0	723	53	0
2	WB	1554	0	723	51	0
2	WE	1554	0	723	51	0
2	YA	1554	0	723	51	0
2	YD	1554	0	723	52	0
3	BA	1420	0	604	17	0
3	BD	1420	0	604	17	0
3	BG	1420	0	604	17	0
3	C	1420	0	604	17	0
3	DC	1420	0	604	16	0
3	DF	1420	0	604	17	0
3	FB	1420	0	604	17	0
3	FE	1420	0	604	17	0
3	HA	1420	0	604	17	0
3	HD	1420	0	604	17	0
3	HG	1420	0	604	17	0
3	JC	1420	0	604	17	0
3	JF	1420	0	604	17	0
3	K	1420	0	604	17	0
3	LB	1420	0	604	17	0
3	LE	1420	0	604	17	0
3	M	1420	0	604	17	0
3	NA	1420	0	604	17	0
3	ND	1420	0	604	17	0
3	NG	1420	0	604	17	0
3	PC	1420	0	604	17	0
3	PF	1420	0	604	17	0
3	RB	1420	0	604	17	0
3	RE	1420	0	604	17	0
3	TA	1420	0	604	17	0
3	TD	1420	0	604	17	0
3	TG	1420	0	604	17	0
3	V	1420	0	604	17	0
3	VC	1420	0	604	17	0
3	VF	1420	0	604	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	XB	1420	0	604	17	0
3	XE	1420	0	604	17	0
3	ZA	1420	0	604	17	0
3	ZD	1420	0	604	17	0
4	AB	456	0	206	4	0
4	AC	368	0	166	1	0
4	AE	456	0	206	3	0
4	AF	368	0	166	1	0
4	BB	389	0	173	0	0
4	BE	389	0	173	0	0
4	CA	456	0	206	4	0
4	CB	368	0	166	1	0
4	CD	456	0	206	4	0
4	CE	368	0	166	1	0
4	CG	456	0	206	3	0
4	D	456	0	206	4	0
4	DA	389	0	173	0	0
4	DD	389	0	173	0	0
4	DG	389	0	173	0	0
4	E	389	0	173	0	0
4	EA	368	0	166	1	0
4	EC	456	0	206	3	0
4	ED	368	0	166	1	0
4	EF	456	0	206	4	0
4	EG	368	0	166	1	0
4	FC	389	0	173	0	0
4	FF	389	0	173	0	0
4	GB	456	0	206	4	0
4	GC	368	0	166	1	0
4	GE	456	0	206	4	0
4	GF	368	0	166	1	0
4	H	368	0	166	1	0
4	HB	389	0	173	0	0
4	HE	389	0	173	0	0
4	IA	456	0	206	4	0
4	IB	368	0	166	1	0
4	ID	456	0	206	4	0
4	IE	368	0	166	1	0
4	IG	456	0	206	4	0
4	JA	389	0	173	0	0
4	JD	389	0	173	0	0
4	JG	389	0	173	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	KA	368	0	166	1	0
4	KC	456	0	206	4	0
4	KD	368	0	166	1	0
4	KF	456	0	206	4	0
4	KG	368	0	166	1	0
4	L	456	0	206	4	0
4	LC	389	0	173	0	0
4	LF	389	0	173	0	0
4	MB	456	0	206	4	0
4	MC	368	0	166	1	0
4	ME	456	0	206	4	0
4	MF	368	0	166	1	0
4	N	456	0	206	3	0
4	NB	389	0	173	0	0
4	NE	389	0	173	0	0
4	O	389	0	173	0	0
4	OA	456	0	206	4	0
4	OB	368	0	166	1	0
4	OD	456	0	206	4	0
4	OE	368	0	166	1	0
4	OG	456	0	206	4	0
4	P	389	0	173	0	0
4	PA	389	0	173	0	0
4	PD	389	0	173	0	0
4	PG	389	0	173	0	0
4	Q	368	0	166	1	0
4	QA	368	0	166	1	0
4	QC	456	0	206	4	0
4	QD	368	0	166	1	0
4	QF	456	0	206	4	0
4	QG	368	0	166	1	0
4	R	368	0	166	1	0
4	RC	389	0	173	0	0
4	RF	389	0	173	0	0
4	SB	456	0	206	4	0
4	SC	368	0	166	1	0
4	SE	456	0	206	4	0
4	SF	368	0	166	1	0
4	TB	389	0	173	0	0
4	TE	389	0	173	0	0
4	UA	456	0	206	4	0
4	UB	368	0	166	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	UD	456	0	206	3	0
4	UE	368	0	166	1	0
4	UG	456	0	206	4	0
4	VA	389	0	173	0	0
4	VD	389	0	173	0	0
4	VG	389	0	173	0	0
4	W	456	0	206	4	0
4	WA	368	0	166	1	0
4	WC	456	0	206	4	0
4	WD	368	0	166	1	0
4	WF	456	0	206	3	0
4	WG	368	0	166	1	0
4	X	389	0	173	0	0
4	XC	389	0	173	0	0
4	XF	389	0	173	0	0
4	Y	368	0	166	1	0
4	YB	456	0	206	4	0
4	YC	368	0	166	1	0
4	YE	456	0	206	3	0
4	YF	368	0	166	1	0
4	ZB	389	0	173	0	0
4	ZE	389	0	173	0	0
All	All	150314	0	67116	1736	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 8.

The worst 5 of 1736 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)
2:AD:66:PHE:O	2:GD:46:GLN:CA	1.63	1.46
2:AD:66:PHE:O	2:GD:46:GLN:CB	1.64	1.45
2:T:66:PHE:O	2:AA:46:GLN:CA	1.64	1.44
2:G:46:GLN:CB	2:SG:66:PHE:O	1.65	1.44
2:OF:66:PHE:O	2:UF:46:GLN:CB	1.65	1.44

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	A	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	BC	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	BF	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	DB	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	DE	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	F	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	FA	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	FD	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	FG	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	HC	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	HF	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	I	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	JB	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	JE	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	LA	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	LD	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	LG	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	NC	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	NF	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	PB	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	PE	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	RA	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	RD	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	RG	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	S	45/560 (8%)	44 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	TC	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	TF	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	VB	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	VE	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	XA	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	XD	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	Z	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	ZC	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
1	ZF	45/560 (8%)	44 (98%)	1 (2%)	0	100	100
2	AA	308/331 (93%)	295 (96%)	10 (3%)	3 (1%)	15	54
2	AD	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	AG	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	B	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	CC	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	CF	308/331 (93%)	295 (96%)	10 (3%)	3 (1%)	15	54
2	EB	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	EE	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	G	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	GA	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	GD	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	GG	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	IC	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	IF	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	J	308/331 (93%)	295 (96%)	10 (3%)	3 (1%)	15	54
2	KB	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	KE	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	MA	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	MD	308/331 (93%)	295 (96%)	10 (3%)	3 (1%)	15	54
2	MG	308/331 (93%)	295 (96%)	10 (3%)	3 (1%)	15	54
2	OC	308/331 (93%)	295 (96%)	10 (3%)	3 (1%)	15	54
2	OF	308/331 (93%)	295 (96%)	10 (3%)	3 (1%)	15	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	QE	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	SA	308/331 (93%)	295 (96%)	10 (3%)	3 (1%)	15	54
2	SD	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	SG	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	T	308/331 (93%)	295 (96%)	10 (3%)	3 (1%)	15	54
2	UC	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	UF	308/331 (93%)	295 (96%)	10 (3%)	3 (1%)	15	54
2	WB	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	WE	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	YA	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
2	YD	308/331 (93%)	294 (96%)	11 (4%)	3 (1%)	15	54
3	BA	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	BD	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	BG	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	C	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	DC	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	DF	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	FB	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	FE	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	HA	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	HD	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	HG	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	JC	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	JF	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	K	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	LB	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	LE	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	M	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	NA	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	ND	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	NG	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	PC	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	PF	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	RB	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	RE	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	TA	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	TD	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	TG	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	V	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	VC	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	VF	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	XB	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	XE	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	ZA	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
3	ZD	279/291 (96%)	249 (89%)	25 (9%)	5 (2%)	8	42
4	AB	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	AC	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	AE	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	AF	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	BB	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	BE	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	CA	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	CB	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	CD	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	CE	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	CG	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	D	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	DA	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	DD	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	DG	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	E	77/137 (56%)	69 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	EA	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	EC	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	ED	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	EF	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	EG	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	FC	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	FF	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	GB	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	GC	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	GE	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	GF	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	H	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	HB	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	HE	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	IA	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	IB	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	ID	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	IE	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	IG	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	JA	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	JD	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	JG	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	KA	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	KC	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	KD	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	KF	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	KG	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	L	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	LC	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	LF	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	MB	91/137 (66%)	90 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	MC	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	ME	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	MF	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	N	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	NB	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	NE	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	O	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	OA	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	OB	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	OD	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	OE	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	OG	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	P	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	PA	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	PD	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	PG	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	Q	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	QA	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	QC	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	QD	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	QF	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	QG	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	R	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	RC	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	RF	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	SB	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	SC	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	SE	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	SF	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	TB	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	TE	77/137 (56%)	69 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	UA	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	UB	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	UD	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	UE	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	UG	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	VA	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	VD	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	VG	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	W	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	WA	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	WC	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	WD	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	WF	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	WG	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	X	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	XC	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	XF	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	Y	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	YB	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	YC	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	YE	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	YF	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	ZB	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	ZE	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
All	All	29682/54162 (55%)	27754 (94%)	1656 (6%)	272 (1%)	21	56

5 of 272 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	9	LYS
2	G	167	VAL
3	M	234	PRO
3	M	237	GLU
2	B	9	LYS

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

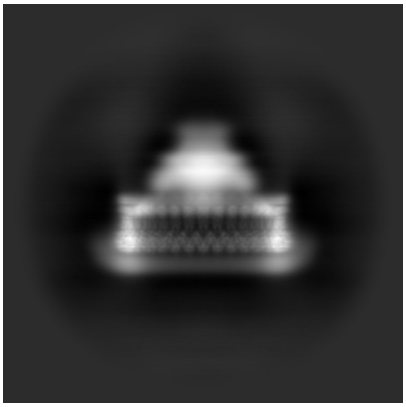
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43327. These allow visual inspection of the internal detail of the map and identification of artifacts.

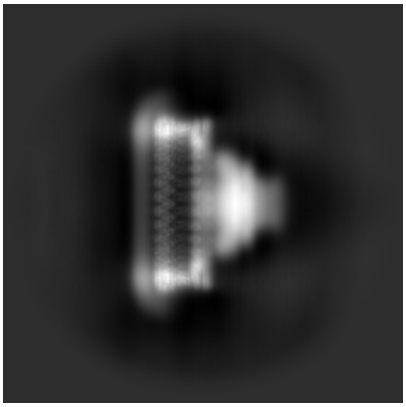
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

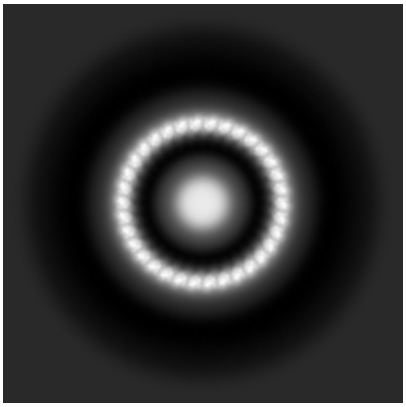
6.1.1 Primary map



X



Y

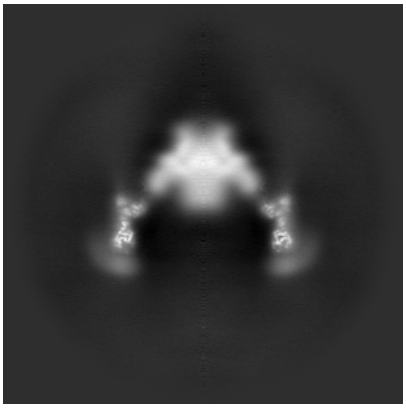


Z

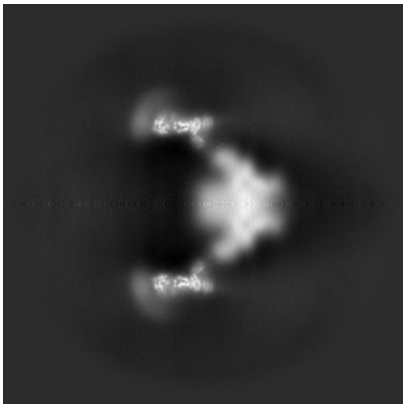
The images above show the map projected in three orthogonal directions.

6.2 Central slices

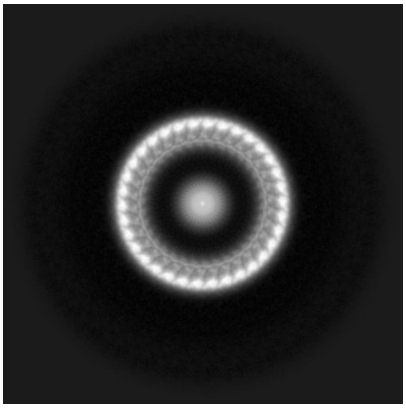
6.2.1 Primary map



X Index: 256



Y Index: 256

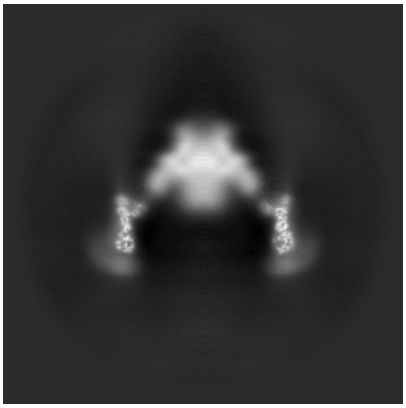


Z Index: 256

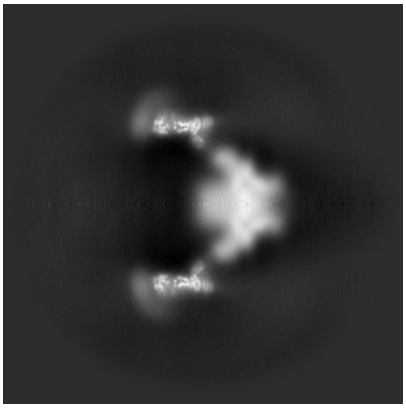
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

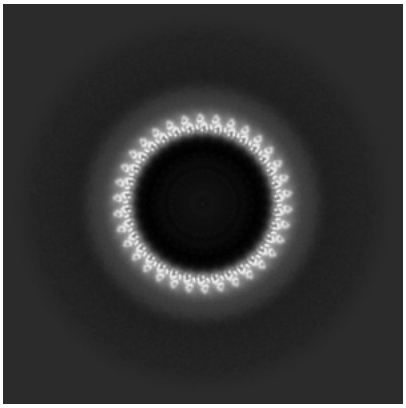
6.3.1 Primary map



X Index: 250



Y Index: 256

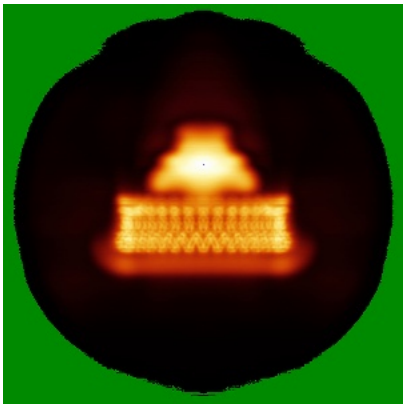


Z Index: 211

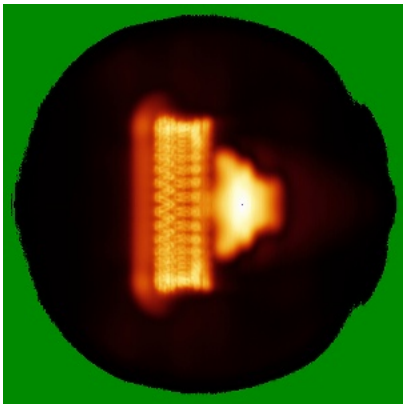
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

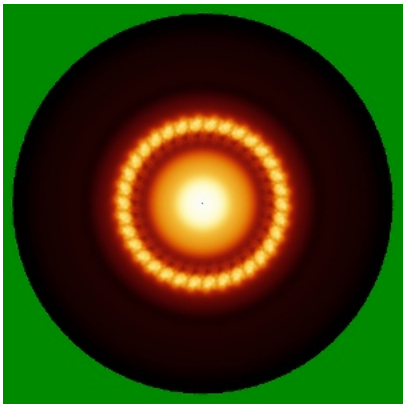
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.151. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

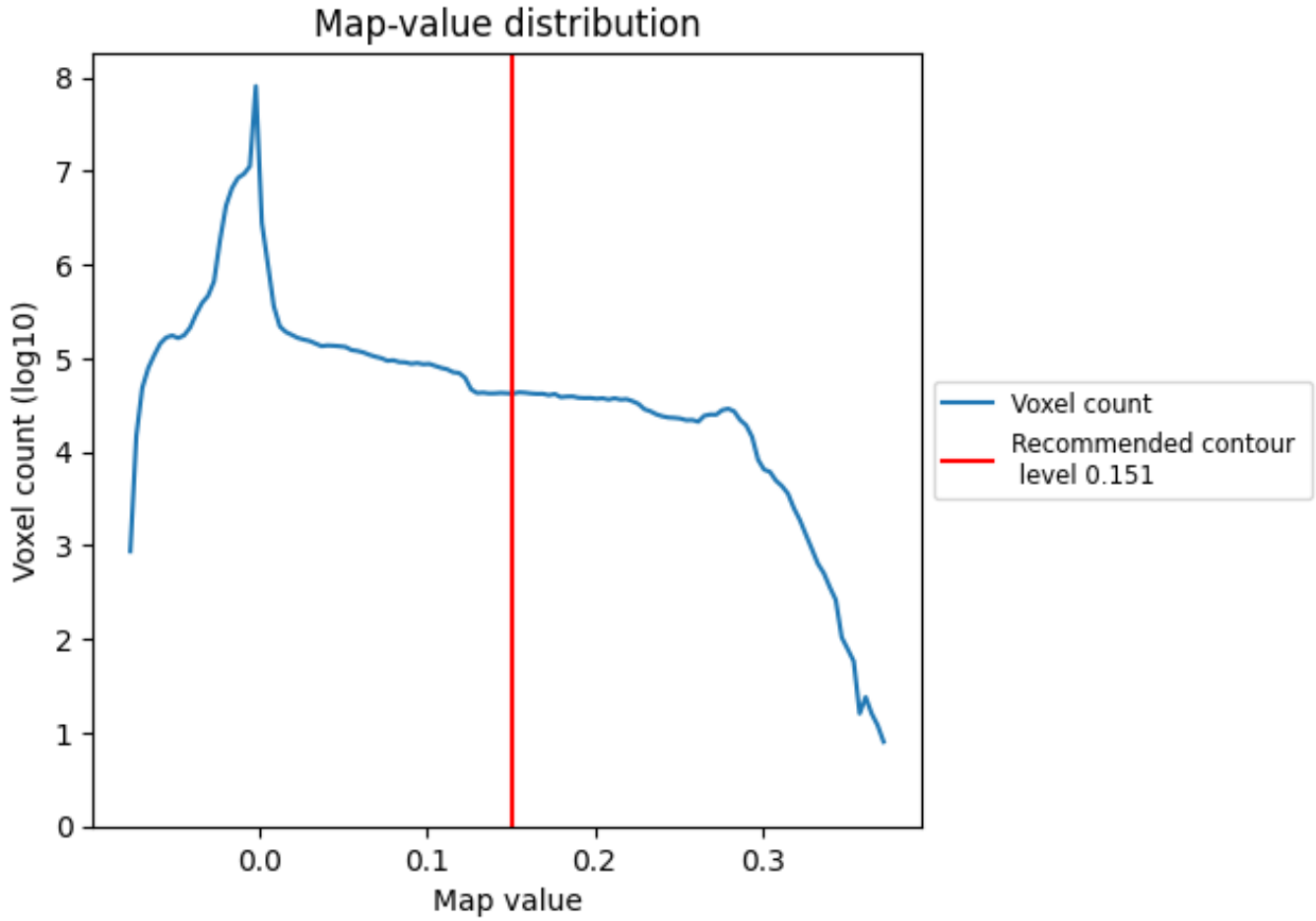
6.6 Mask visualisation (i)

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

7 Map analysis

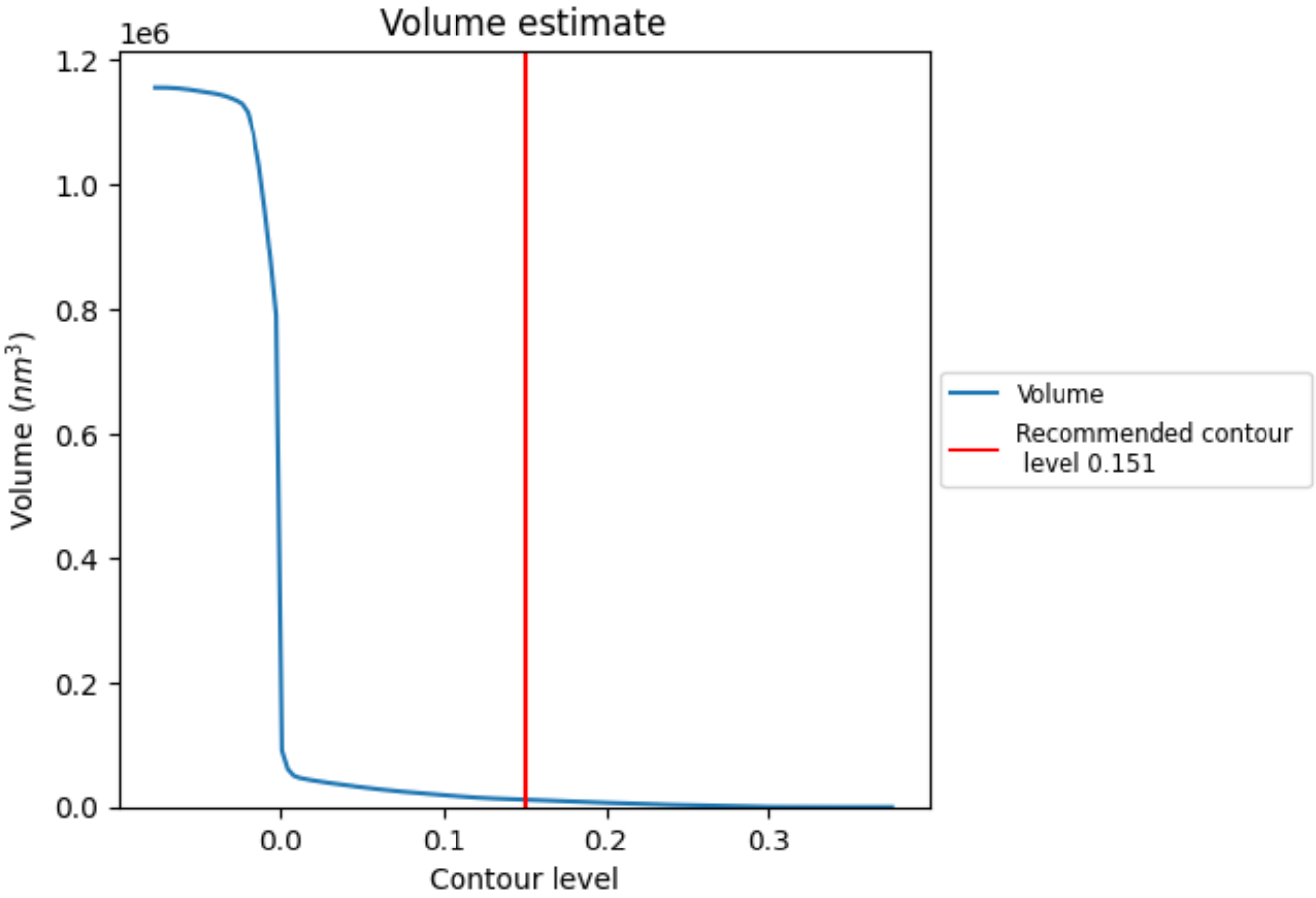
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

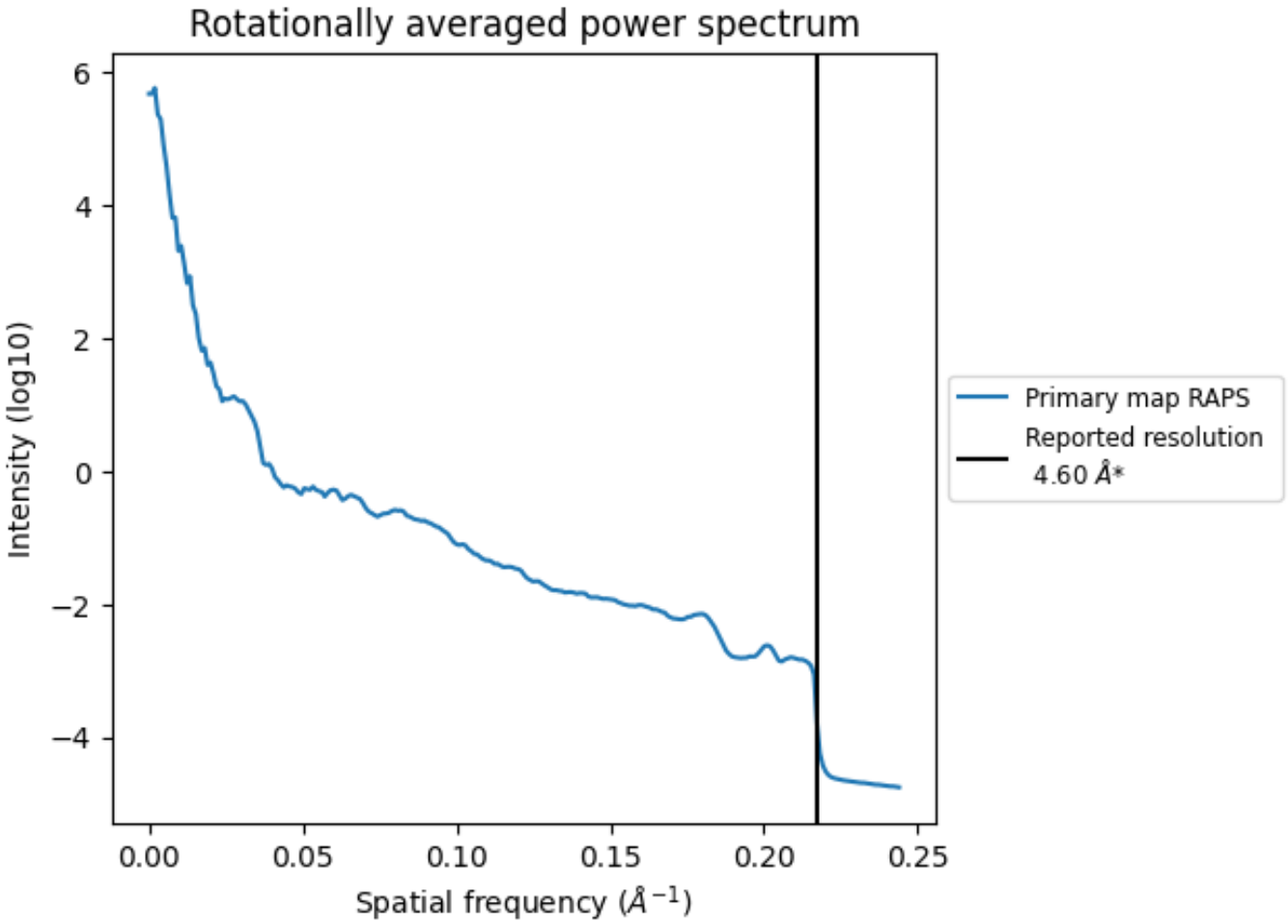
7.2 Volume estimate (i)



The volume at the recommended contour level is 11612 nm^3; this corresponds to an approximate mass of 10489 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

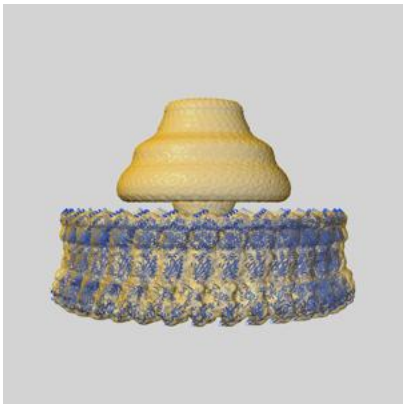
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

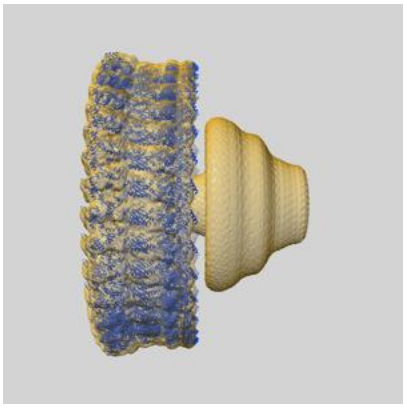
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43327 and PDB model 8VKQ. Per-residue inclusion information can be found in section 3 on page 22.

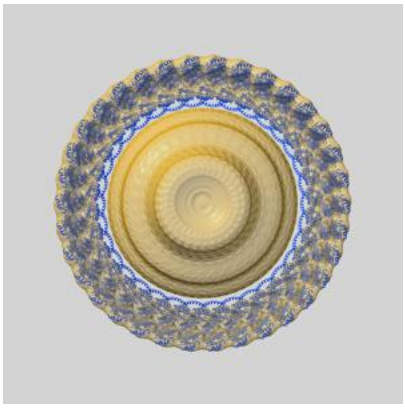
9.1 Map-model overlay



X



Y



Z

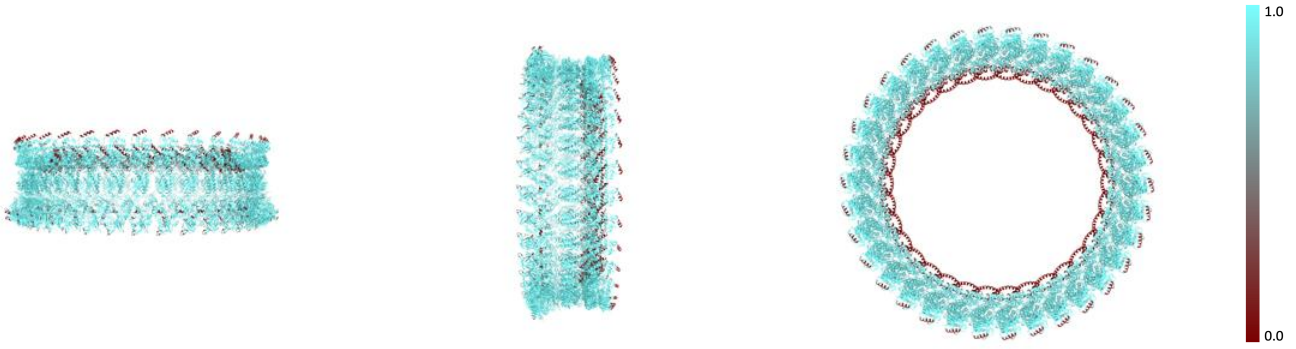
The images above show the 3D surface view of the map at the recommended contour level 0.151 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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.

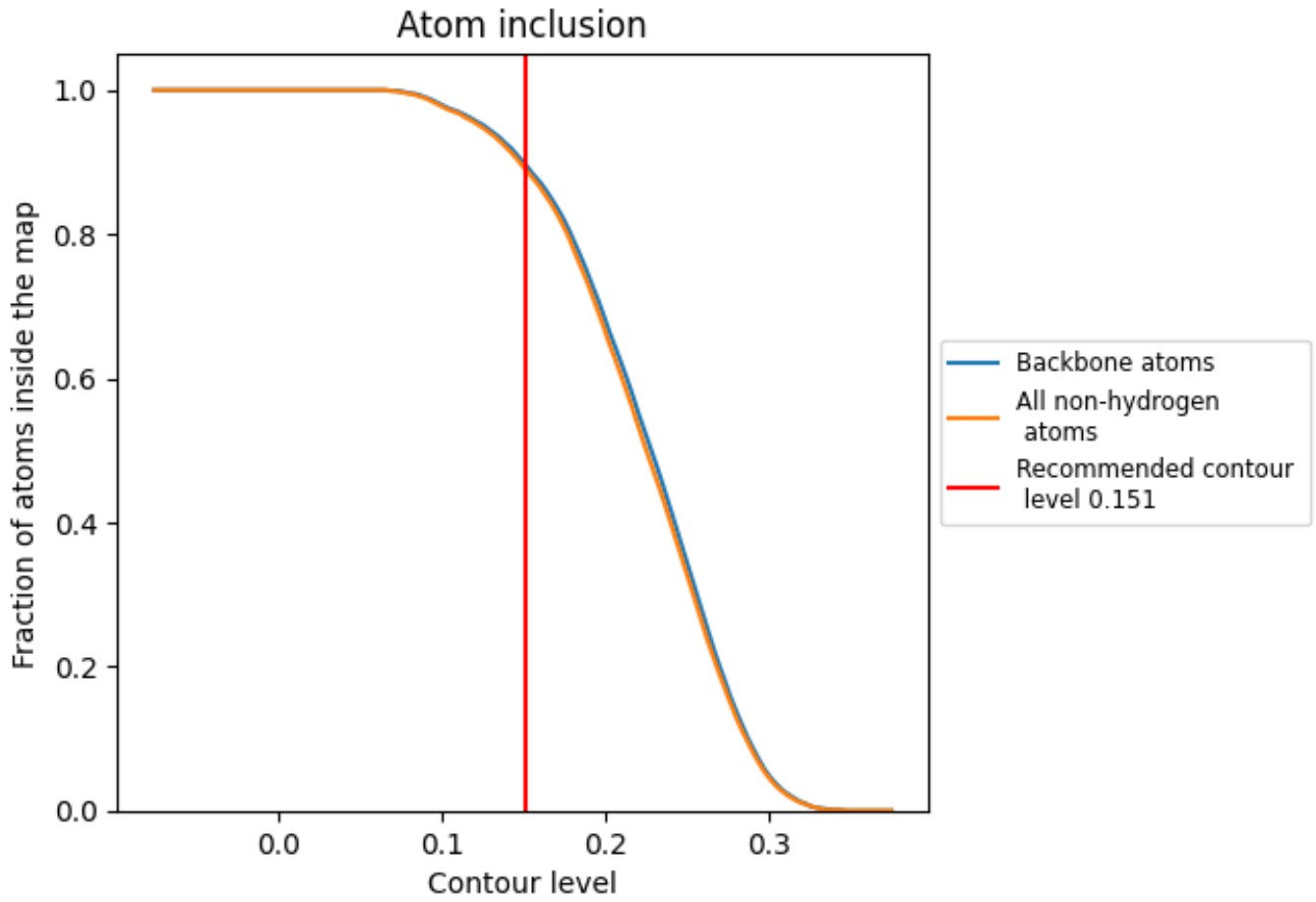
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.151).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.151) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.1440
A	0.3420	0.1360
AA	0.8790	0.1270
AB	0.8950	0.1190
AC	0.9670	0.1120
AD	0.8480	0.1010
AE	0.9280	0.1830
AF	0.9760	0.2150
AG	0.8980	0.1630
B	0.8890	0.1480
BA	0.9560	0.0970
BB	1.0000	0.1490
BC	0.3120	0.1400
BD	0.9140	0.1190
BE	1.0000	0.1650
BF	0.3030	0.1360
BG	0.9750	0.1920
C	0.9650	0.1340
CA	0.9060	0.1460
CB	0.9650	0.1410
CC	0.8510	0.0990
CD	0.9230	0.1520
CE	0.9840	0.1770
CF	0.8890	0.1580
CG	0.9410	0.2080
D	0.9170	0.1690
DA	1.0000	0.2070
DB	0.3210	0.1400
DC	0.9110	0.0960
DD	1.0000	0.1290
DE	0.2990	0.1300
DF	0.9660	0.1920
DG	1.0000	0.2450
E	1.0000	0.2380
EA	0.9650	0.2040

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Chain	Atom inclusion	Q-score
EB	0.8650	0.1030
EC	0.9120	0.1240
ED	0.9810	0.1350
EE	0.8660	0.1310
EF	0.9430	0.2120
EG	0.9650	0.2460
F	0.3380	0.1340
FA	0.3420	0.1370
FB	0.9250	0.0810
FC	0.9970	0.1250
FD	0.2990	0.1350
FE	0.9440	0.1600
FF	1.0000	0.2060
FG	0.3250	0.1370
G	0.8890	0.1510
GA	0.8780	0.1200
GB	0.9100	0.1170
GC	0.9730	0.1160
GD	0.8450	0.1070
GE	0.9320	0.1930
GF	0.9730	0.2190
GG	0.8960	0.1620
H	0.9650	0.2430
HA	0.9510	0.0940
HB	1.0000	0.1420
HC	0.3120	0.1390
HD	0.9180	0.1280
HE	1.0000	0.1730
HF	0.3030	0.1350
HG	0.9750	0.1820
I	0.3420	0.1390
IA	0.9010	0.1380
IB	0.9650	0.1310
IC	0.8510	0.0990
ID	0.9250	0.1610
IE	0.9780	0.1880
IF	0.8910	0.1610
IG	0.9320	0.1980
J	0.8830	0.1390
JA	1.0000	0.1920
JB	0.3160	0.1300
JC	0.9100	0.1010

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Chain	Atom inclusion	Q-score
JD	1.0000	0.1330
JE	0.2990	0.1350
JF	0.9710	0.1940
JG	1.0000	0.2460
K	0.9630	0.1190
KA	0.9620	0.1910
KB	0.8640	0.1010
KC	0.9190	0.1290
KD	0.9840	0.1480
KE	0.8750	0.1400
KF	0.9430	0.2140
KG	0.9650	0.2460
L	0.9170	0.1590
LA	0.3380	0.1310
LB	0.9210	0.0850
LC	1.0000	0.1220
LD	0.2990	0.1340
LE	0.9510	0.1730
LF	1.0000	0.2230
LG	0.3290	0.1350
M	0.9670	0.1460
MA	0.8710	0.1150
MB	0.9140	0.1200
MC	0.9780	0.1230
MD	0.8480	0.1120
ME	0.9360	0.2010
MF	0.9700	0.2350
MG	0.8960	0.1610
N	0.9170	0.1820
NA	0.9420	0.0870
NB	1.0000	0.1340
NC	0.3080	0.1450
ND	0.9220	0.1350
NE	1.0000	0.1860
NF	0.3080	0.1330
NG	0.9750	0.1720
O	1.0000	0.2290
OA	0.9030	0.1350
OB	0.9670	0.1300
OC	0.8480	0.1000
OD	0.9280	0.1670
OE	0.9780	0.1980

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Chain	Atom inclusion	Q-score
OF	0.8960	0.1650
OG	0.9210	0.1930
P	1.0000	0.2450
PA	1.0000	0.1750
PB	0.3160	0.1380
PC	0.9100	0.1120
PD	1.0000	0.1400
PE	0.2990	0.1370
PF	0.9730	0.1960
PG	1.0000	0.2550
Q	0.9620	0.2470
QA	0.9620	0.1690
QB	0.8550	0.0970
QC	0.9170	0.1380
QD	0.9860	0.1520
QE	0.8760	0.1440
QF	0.9410	0.2110
QG	0.9650	0.2440
R	0.9650	0.2290
RA	0.3330	0.1320
RB	0.9150	0.0810
RC	1.0000	0.1240
RD	0.2990	0.1350
RE	0.9570	0.1840
RF	1.0000	0.2290
RG	0.3380	0.1340
S	0.3420	0.1390
SA	0.8690	0.1100
SB	0.9170	0.1130
SC	0.9810	0.1250
SD	0.8520	0.1180
SE	0.9410	0.2050
SF	0.9650	0.2410
SG	0.8920	0.1560
T	0.8820	0.1330
TA	0.9350	0.0800
TB	1.0000	0.1270
TC	0.3030	0.1380
TD	0.9320	0.1440
TE	1.0000	0.1910
TF	0.3120	0.1400
TG	0.9710	0.1600

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Chain	Atom inclusion	Q-score
UA	0.8950	0.1240
UB	0.9670	0.1120
UC	0.8460	0.0970
UD	0.9250	0.1710
UE	0.9780	0.2030
UF	0.8970	0.1640
UG	0.9170	0.1870
V	0.9610	0.1090
VA	1.0000	0.1670
VB	0.3120	0.1380
VC	0.9100	0.1120
VD	1.0000	0.1540
VE	0.3030	0.1350
VF	0.9730	0.1960
VG	1.0000	0.2490
W	0.9120	0.1530
WA	0.9650	0.1550
WB	0.8520	0.0970
WC	0.9210	0.1420
WD	0.9860	0.1680
WE	0.8820	0.1520
WF	0.9390	0.2080
WG	0.9620	0.2470
X	1.0000	0.2150
XA	0.3290	0.1310
XB	0.9150	0.0890
XC	1.0000	0.1230
XD	0.2950	0.1340
XE	0.9620	0.1870
XF	1.0000	0.2400
Y	0.9650	0.2180
YA	0.8660	0.1060
YB	0.9120	0.1200
YC	0.9810	0.1270
YD	0.8610	0.1250
YE	0.9430	0.2070
YF	0.9650	0.2360
Z	0.3420	0.1350
ZA	0.9300	0.0770
ZB	0.9970	0.1260
ZC	0.3030	0.1380
ZD	0.9370	0.1530

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Chain	Atom inclusion	Q-score
ZE	1.0000	0.1990
ZF	0.3160	0.1390