



# wwPDB EM Validation Summary Report ⓘ

Aug 15, 2024 – 03:58 PM EDT

PDB ID : 8T8O  
EMDB ID : EMD-41100  
Title : CCW Flagellar Switch Complex - FliF, FliG, FliM, and FliN forming 34-mer C-ring from Salmonella  
Authors : Singh, P.K.; Iverson, T.M.  
Deposited on : 2023-06-22  
Resolution : 4.00 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](mailto: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>.

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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

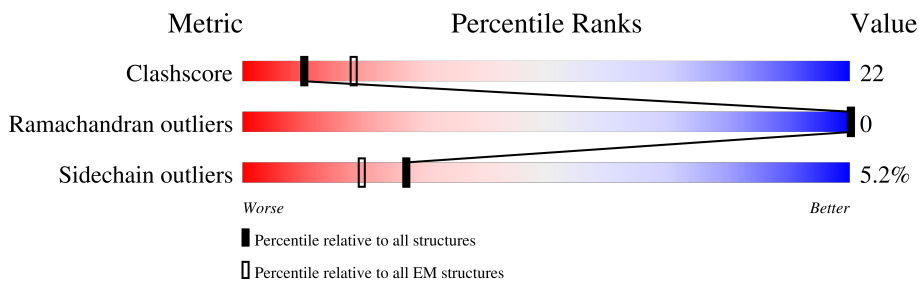
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	47	49% 100%
1	BC	47	49% 100%
1	BF	47	51% 100%
1	DB	47	49% 100%
1	DE	47	51% 100%
1	F	47	49% 100%
1	FA	47	49% 100%
1	FD	47	51% 100%

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Mol	Chain	Length	Quality of chain	
1	FG	47	49%	100%
1	HC	47	51%	98%
1	HF	47	51%	100%
1	I	47	49%	100%
1	JB	47	49%	100%
1	JE	47	51%	100%
1	LA	47	49%	100%
1	LD	47	51%	100%
1	LG	47	49%	98%
1	NC	47	51%	100%
1	NF	47	49%	98%
1	PB	47	49%	98%
1	PE	47	51%	98%
1	RA	47	49%	100%
1	RD	47	51%	98%
1	RG	47	49%	100%
1	S	47	49%	100%
1	TC	47	51%	100%
1	TF	47	49%	100%
1	VB	47	49%	100%
1	VE	47	51%	100%
1	XA	47	49%	98%
1	XD	47	51%	96%
1	Z	47	49%	98%
1	ZC	47	51%	100%

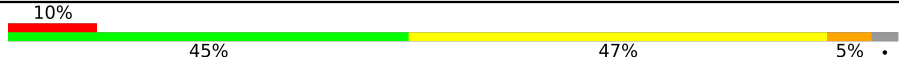
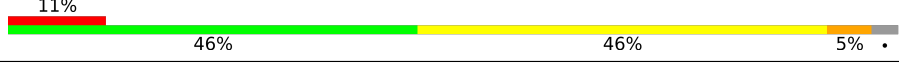
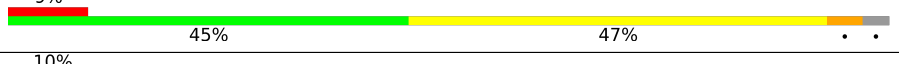
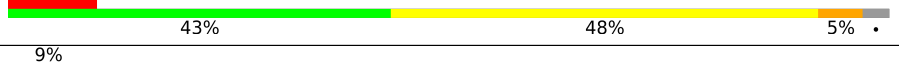

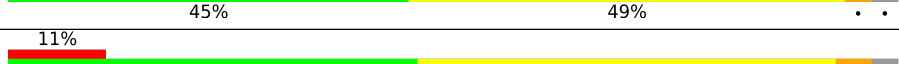


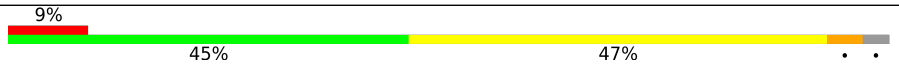


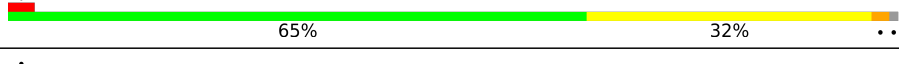
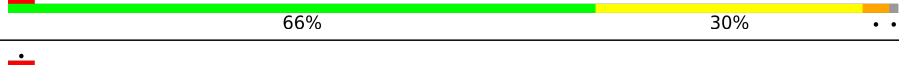

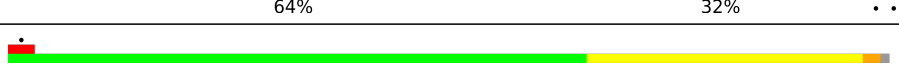










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Mol	Chain	Length	Quality of chain	
1	ZF	47	49%	100%
2	AA	331	9%	44% 48% 5%
2	AD	331	9%	47% 45% 5%
2	AG	331	10%	45% 47%
2	B	331	9%	49% 44%
2	CC	331	9%	46% 46% 5%
2	CF	331	10%	45% 47%
2	EB	331	9%	47% 47%
2	EE	331	10%	47% 44% 5%
2	G	331	10%	47% 45%
2	GA	331	10%	47% 45%
2	GD	331	9%	46% 46% 5%
2	GG	331	10%	48% 45%
2	IC	331	10%	45% 47% 5%
2	IF	331	10%	44% 48% 5%
2	J	331	10%	45% 47% 5%
2	KB	331	9%	45% 47% 5%
2	KE	331	9%	48% 45%
2	MA	331	10%	49% 44%
2	MD	331	10%	44% 48%
2	MG	331	10%	47% 45% 5%
2	OC	331	9%	49% 43% 5%
2	OF	331	10%	41% 49% 6%
2	QB	331	10%	44% 48%
2	QE	331	10%	46% 48%




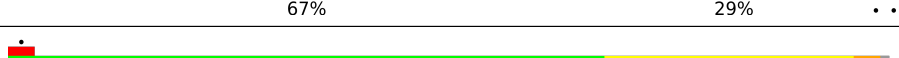
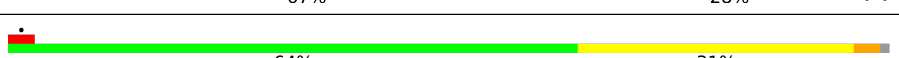
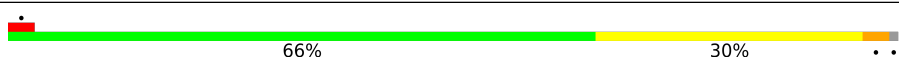
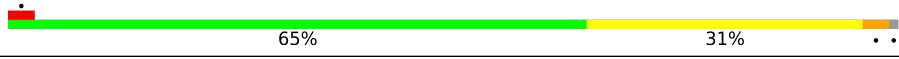
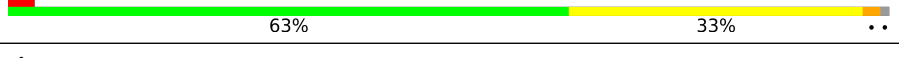
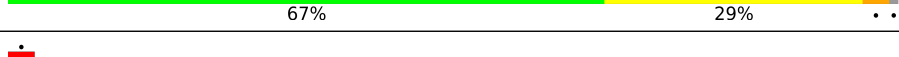

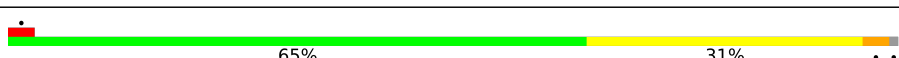



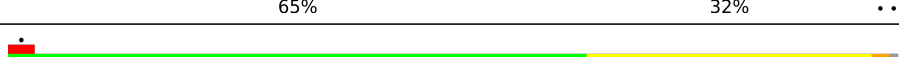









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Mol	Chain	Length	Quality of chain
2	SA	331	
2	SD	331	
2	SG	331	
2	T	331	
2	UC	331	
2	UF	331	
2	WB	331	
2	WE	331	
2	YA	331	
2	YD	331	
3	BA	300	
3	BD	300	
3	BG	300	
3	C	300	
3	DC	300	
3	DF	300	
3	FB	300	
3	FE	300	
3	HA	300	
3	HD	300	
3	HG	300	
3	JC	300	
3	JF	300	
3	K	300	
3	LB	300	

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Mol	Chain	Length	Quality of chain
3	LE	300	 64% 32% ..
3	M	300	 65% 31% ..
3	NA	300	 63% 33% ..
3	ND	300	 67% 29% ..
3	NG	300	 67% 28% ..
3	PC	300	 64% 31% ..
3	PF	300	 66% 30% ..
3	RB	300	 65% 31% ..
3	RE	300	 63% 33% ..
3	TA	300	 67% 29% ..
3	TD	300	 65% 30% ..
3	TG	300	 64% 33% ..
3	V	300	 65% 31% ..
3	VC	300	 64% 32% ..
3	VF	300	 64% 31% ..
3	XB	300	 62% 34% ..
3	XE	300	 65% 32% ..
3	ZA	300	 65% 32% ..
3	ZD	300	 65% 31% ..
4	AB	137	 61% 7% 32%
4	AC	137	 53% 45%
4	AE	137	 5% 62% 6% 32%
4	AF	137	 5% 51% 45%
4	BB	137	 58% 42%
4	BE	137	57% 42%













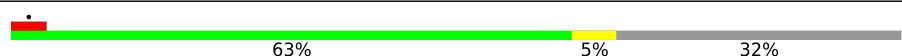
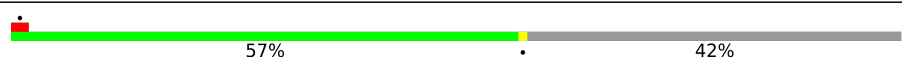
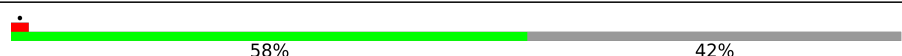

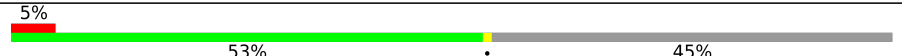
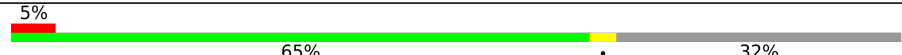
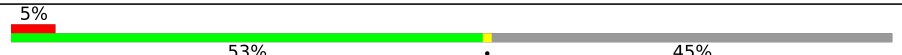
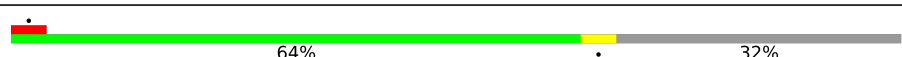
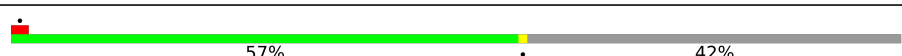




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Mol	Chain	Length	Quality of chain
4	CA	137	64% 32%
4	CB	137	53% 45%
4	CD	137	64% 32%
4	CE	137	53% 45%
4	CG	137	63% 5% 32%
4	D	137	64% 32%
4	DA	137	58% 42%
4	DD	137	58% 42%
4	DG	137	58% 42%
4	E	137	58% 42%
4	EA	137	52% 45%
4	EC	137	63% 5% 32%
4	ED	137	54% 45%
4	EF	137	64% 32%
4	EG	137	54% 45%
4	FC	137	58% 42%
4	FF	137	58% 42%
4	GB	137	63% 5% 32%
4	GC	137	54% 45%
4	GE	137	64% 32%
4	GF	137	54% 45%
4	H	137	53% 45%
4	HB	137	58% 42%
4	HE	137	57% 42%
4	IA	137	64% 32%

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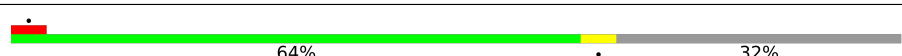
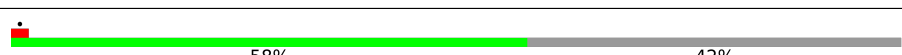
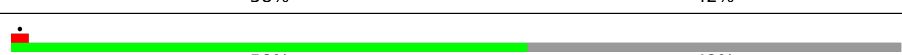

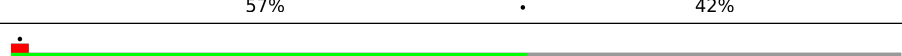
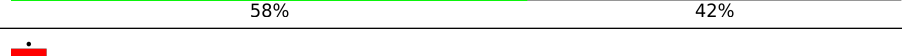



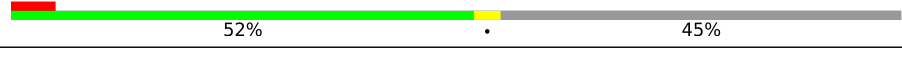
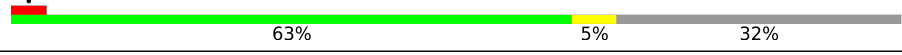



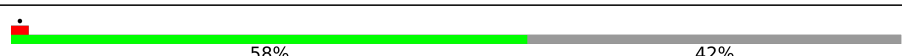
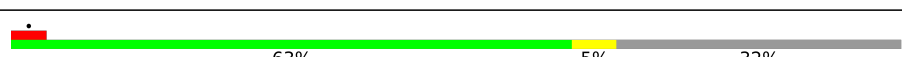






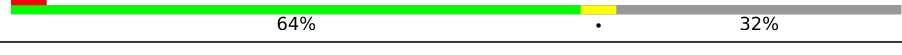
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Mol	Chain	Length	Quality of chain
4	IB	137	 53% 45%
4	ID	137	 63% 32%
4	IE	137	 53% 45%
4	IG	137	 64% 32%
4	JA	137	 58% 42%
4	JD	137	 58% 42%
4	JG	137	 57% 42%
4	KA	137	 53% 45%
4	KC	137	 64% 32%
4	KD	137	 54% 45%
4	KF	137	 64% 32%
4	KG	137	 53% 45%
4	L	137	 63% 32%
4	LC	137	 57% 42%
4	LF	137	 58% 42%
4	MB	137	 63% 32%
4	MC	137	 53% 45%
4	ME	137	 65% 32%
4	MF	137	 53% 45%
4	N	137	 64% 32%
4	NB	137	 57% 42%
4	NE	137	 56% 42%
4	O	137	 57% 42%
4	OA	137	 65% 32%
4	OB	137	 51% 45%

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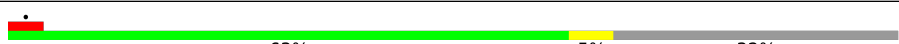
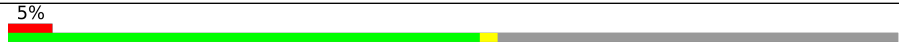

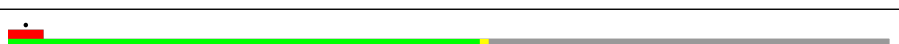

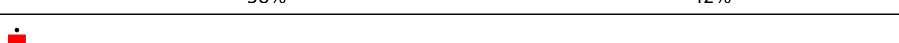
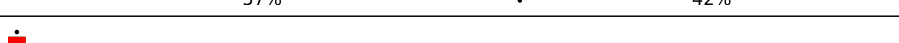
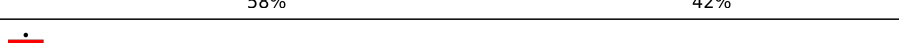
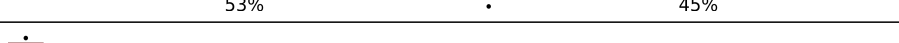
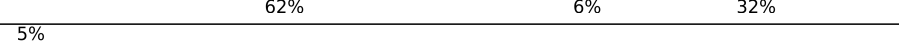






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Mol	Chain	Length	Quality of chain
4	OD	137	 64% 32%
4	OE	137	 53% 45%
4	OG	137	 64% 32%
4	P	137	 58% 42%
4	PA	137	 58% 42%
4	PD	137	 57% 42%
4	PG	137	 58% 42%
4	Q	137	 53% 45%
4	QA	137	 53% 45%
4	QC	137	 63% 5% 32%
4	QD	137	 52% 45%
4	QF	137	 63% 5% 32%
4	QG	137	 53% 45%
4	R	137	 51% 45%
4	RC	137	 58% 42%
4	RF	137	 58% 42%
4	SB	137	 63% 5% 32%
4	SC	137	 52% 45%
4	SE	137	 63% 5% 32%
4	SF	137	 53% 45%
4	TB	137	 58% 42%
4	TE	137	 58% 42%
4	UA	137	 64% 32%
4	UB	137	 52% 45%
4	UD	137	 64% 32%

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Mol	Chain	Length	Quality of chain
4	UE	137	
4	UG	137	
4	VA	137	
4	VD	137	
4	VG	137	
4	W	137	
4	WA	137	
4	WC	137	
4	WD	137	
4	WF	137	
4	WG	137	
4	X	137	
4	XC	137	
4	XF	137	
4	Y	137	
4	YB	137	
4	YC	137	
4	YE	137	
4	YF	137	
4	ZB	137	
4	ZE	137	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 205020 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
			Total	C	N	O		
1	F	47	234	140	47	47	0	0
1	A	47	234	140	47	47	0	0
1	I	47	234	140	47	47	0	0
1	S	47	234	140	47	47	0	0
1	Z	47	234	140	47	47	0	0
1	FA	47	234	140	47	47	0	0
1	LA	47	234	140	47	47	0	0
1	RA	47	234	140	47	47	0	0
1	XA	47	234	140	47	47	0	0
1	DB	47	234	140	47	47	0	0
1	JB	47	234	140	47	47	0	0
1	PB	47	234	140	47	47	0	0
1	VB	47	234	140	47	47	0	0
1	BC	47	234	140	47	47	0	0
1	HC	47	234	140	47	47	0	0
1	NC	47	234	140	47	47	0	0
1	TC	47	234	140	47	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	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	B	320	Total 2496	C 1552	N 443	O 492	S 9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	T	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	AA	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	GA	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	MA	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	SA	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	YA	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	EB	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	KB	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	QB	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	WB	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	CC	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	IC	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	OC	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	UC	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	AD	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	GD	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	MD	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	SD	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	YD	320	Total 2496	C 1552	N 443	O 492	S 9	0	0
2	EE	320	Total 2496	C 1552	N 443	O 492	S 9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	KE	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		
2	QE	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		
2	WE	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		
2	CF	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		
2	IF	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		
2	OF	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		
2	UF	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		
2	AG	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		
2	GG	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		
2	MG	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		
2	SG	320	Total	C	N	O	S	0	0
			2496	1552	443	492	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	C	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	K	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	V	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	BA	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	HA	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	NA	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	TA	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	ZA	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	FB	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	LB	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	RB	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	XB	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	DC	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	JC	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	PC	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	VC	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	BD	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	HD	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	ND	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	TD	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	ZD	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	FE	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	LE	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	RE	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	XE	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	DF	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	JF	296	Total 2086	C 1314	N 383	O 384	S 5	0	0
3	PF	296	Total 2086	C 1314	N 383	O 384	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	VF	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	BG	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	HG	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	NG	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		
3	TG	296	Total	C	N	O	S	0	0
			2086	1314	383	384	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	N	93	Total	C	N	O	0	0
			456	270	93	93		
4	P	79	Total	C	N	O	0	0
			389	230	79	80		
4	Q	75	Total	C	N	O	0	0
			369	218	75	76		
4	D	93	Total	C	N	O	0	0
			456	270	93	93		
4	E	79	Total	C	N	O	0	0
			389	230	79	80		
4	H	75	Total	C	N	O	0	0
			369	218	75	76		
4	L	93	Total	C	N	O	0	0
			456	270	93	93		
4	O	79	Total	C	N	O	0	0
			389	230	79	80		
4	R	75	Total	C	N	O	0	0
			369	218	75	76		
4	W	93	Total	C	N	O	0	0
			456	270	93	93		
4	X	79	Total	C	N	O	0	0
			389	230	79	80		
4	Y	75	Total	C	N	O	0	0
			369	218	75	76		
4	CA	93	Total	C	N	O	0	0
			456	270	93	93		
4	DA	79	Total	C	N	O	0	0
			389	230	79	80		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	EA	75	Total	C	N	O	0	0
			369	218	75	76		
4	IA	93	Total	C	N	O	0	0
			456	270	93	93		
4	JA	79	Total	C	N	O	0	0
			389	230	79	80		
4	KA	75	Total	C	N	O	0	0
			369	218	75	76		
4	OA	93	Total	C	N	O	0	0
			456	270	93	93		
4	PA	79	Total	C	N	O	0	0
			389	230	79	80		
4	QA	75	Total	C	N	O	0	0
			369	218	75	76		
4	UA	93	Total	C	N	O	0	0
			456	270	93	93		
4	VA	79	Total	C	N	O	0	0
			389	230	79	80		
4	WA	75	Total	C	N	O	0	0
			369	218	75	76		
4	AB	93	Total	C	N	O	0	0
			456	270	93	93		
4	BB	79	Total	C	N	O	0	0
			389	230	79	80		
4	CB	75	Total	C	N	O	0	0
			369	218	75	76		
4	GB	93	Total	C	N	O	0	0
			456	270	93	93		
4	HB	79	Total	C	N	O	0	0
			389	230	79	80		
4	IB	75	Total	C	N	O	0	0
			369	218	75	76		
4	MB	93	Total	C	N	O	0	0
			456	270	93	93		
4	NB	79	Total	C	N	O	0	0
			389	230	79	80		
4	OB	75	Total	C	N	O	0	0
			369	218	75	76		
4	SB	93	Total	C	N	O	0	0
			456	270	93	93		
4	TB	79	Total	C	N	O	0	0
			389	230	79	80		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	UB	75	Total	C	N	O	0	0
			369	218	75	76		
4	YB	93	Total	C	N	O	0	0
			456	270	93	93		
4	ZB	79	Total	C	N	O	0	0
			389	230	79	80		
4	AC	75	Total	C	N	O	0	0
			369	218	75	76		
4	EC	93	Total	C	N	O	0	0
			456	270	93	93		
4	FC	79	Total	C	N	O	0	0
			389	230	79	80		
4	GC	75	Total	C	N	O	0	0
			369	218	75	76		
4	KC	93	Total	C	N	O	0	0
			456	270	93	93		
4	LC	79	Total	C	N	O	0	0
			389	230	79	80		
4	MC	75	Total	C	N	O	0	0
			369	218	75	76		
4	QC	93	Total	C	N	O	0	0
			456	270	93	93		
4	RC	79	Total	C	N	O	0	0
			389	230	79	80		
4	SC	75	Total	C	N	O	0	0
			369	218	75	76		
4	WC	93	Total	C	N	O	0	0
			456	270	93	93		
4	XC	79	Total	C	N	O	0	0
			389	230	79	80		
4	YC	75	Total	C	N	O	0	0
			369	218	75	76		
4	CD	93	Total	C	N	O	0	0
			456	270	93	93		
4	DD	79	Total	C	N	O	0	0
			389	230	79	80		
4	ED	75	Total	C	N	O	0	0
			369	218	75	76		
4	ID	93	Total	C	N	O	0	0
			456	270	93	93		
4	JD	79	Total	C	N	O	0	0
			389	230	79	80		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	KD	75	Total 369	C 218	N 75	O 76	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 369	C 218	N 75	O 76	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 369	C 218	N 75	O 76	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 369	C 218	N 75	O 76	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 369	C 218	N 75	O 76	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 369	C 218	N 75	O 76	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 369	C 218	N 75	O 76	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	C	N	O	0	0
			369	218	75	76		
4	EF	93	Total	C	N	O	0	0
			456	270	93	93		
4	FF	79	Total	C	N	O	0	0
			389	230	79	80		
4	GF	75	Total	C	N	O	0	0
			369	218	75	76		
4	KF	93	Total	C	N	O	0	0
			456	270	93	93		
4	LF	79	Total	C	N	O	0	0
			389	230	79	80		
4	MF	75	Total	C	N	O	0	0
			369	218	75	76		
4	QF	93	Total	C	N	O	0	0
			456	270	93	93		
4	RF	79	Total	C	N	O	0	0
			389	230	79	80		
4	SF	75	Total	C	N	O	0	0
			369	218	75	76		
4	WF	93	Total	C	N	O	0	0
			456	270	93	93		
4	XF	79	Total	C	N	O	0	0
			389	230	79	80		
4	YF	75	Total	C	N	O	0	0
			369	218	75	76		
4	CG	93	Total	C	N	O	0	0
			456	270	93	93		
4	DG	79	Total	C	N	O	0	0
			389	230	79	80		
4	EG	75	Total	C	N	O	0	0
			369	218	75	76		
4	IG	93	Total	C	N	O	0	0
			456	270	93	93		
4	JG	79	Total	C	N	O	0	0
			389	230	79	80		
4	KG	75	Total	C	N	O	0	0
			369	218	75	76		
4	OG	93	Total	C	N	O	0	0
			456	270	93	93		
4	PG	79	Total	C	N	O	0	0
			389	230	79	80		

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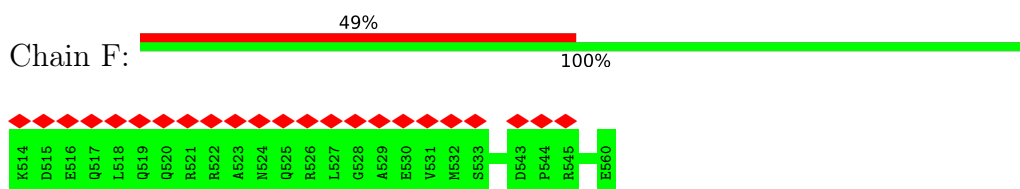
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>AltConf</b>	<b>Trace</b>
4	QG	75	Total 369	C 218	N 75	O 76	0	0
4	UG	93	Total 456	C 270	N 93	O 93	0	0
4	VG	79	Total 389	C 230	N 79	O 80	0	0
4	WG	75	Total 369	C 218	N 75	O 76	0	0

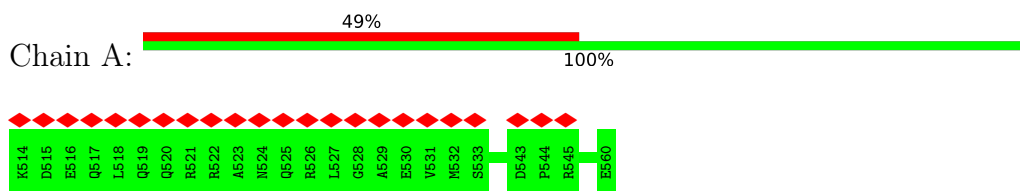
### 3 Residue-property plots [i](#)

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.

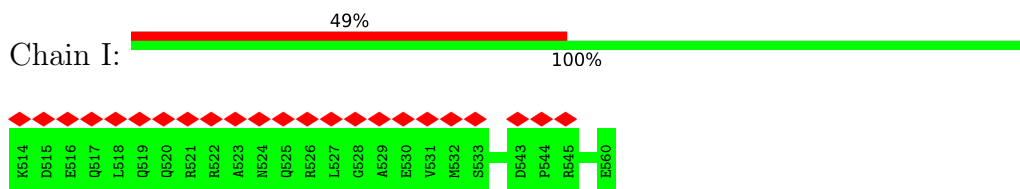
- Molecule 1: Flagellar M-ring protein



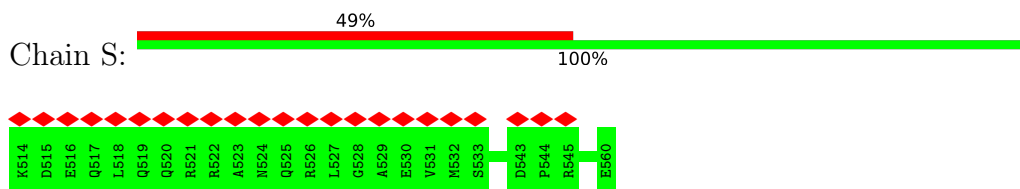
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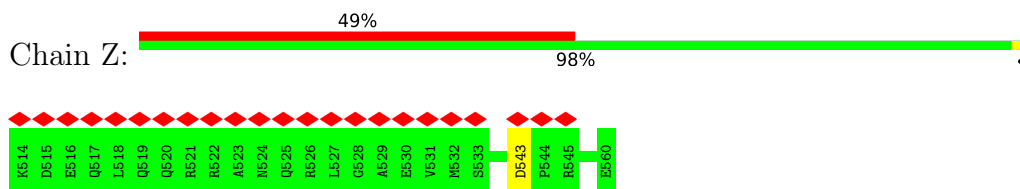
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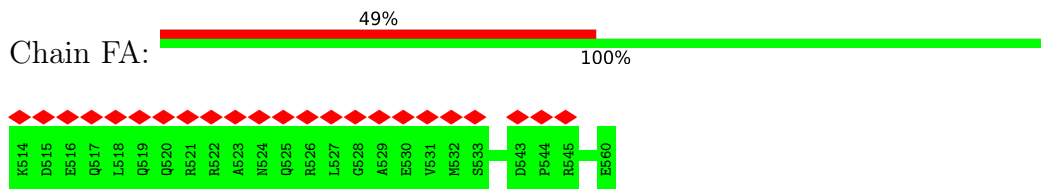
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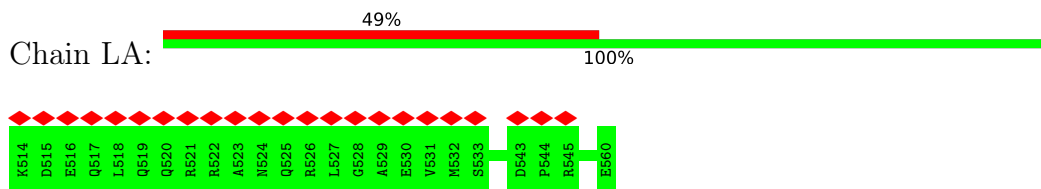
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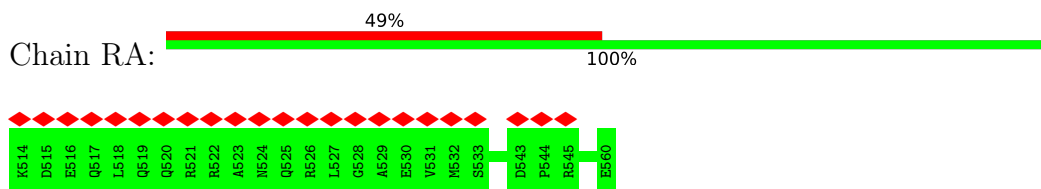
• Molecule 1: Flagellar M-ring protein



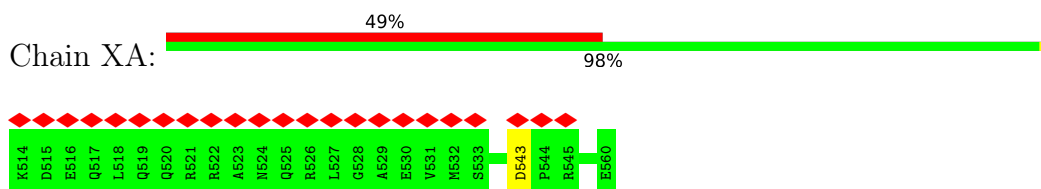
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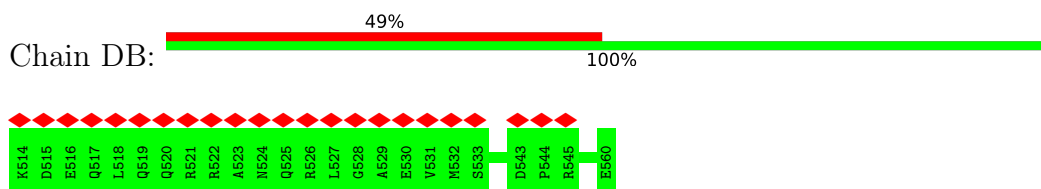
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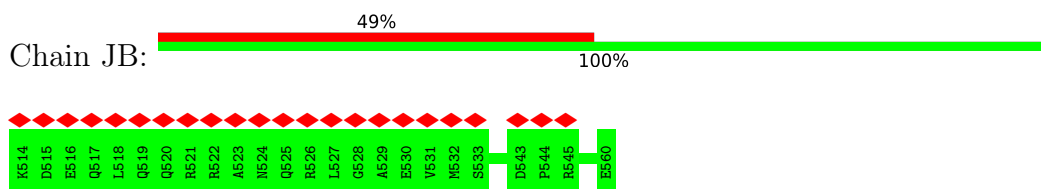
• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein





• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein



• Molecule 1: Flagellar M-ring protein

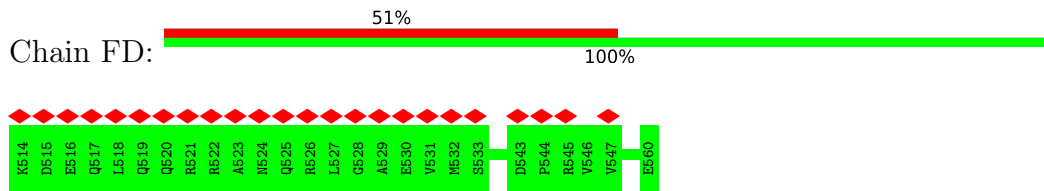


• Molecule 1: Flagellar M-ring protein

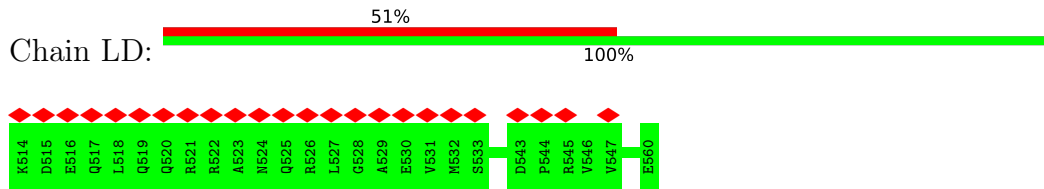


• Molecule 1: Flagellar M-ring protein

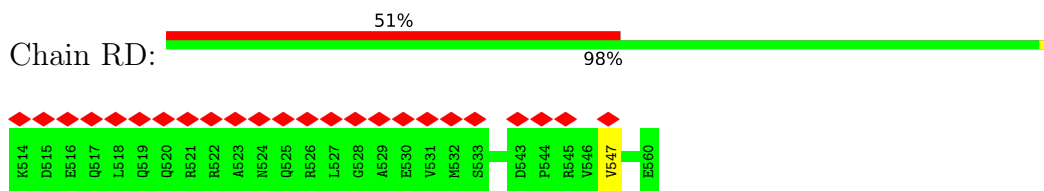




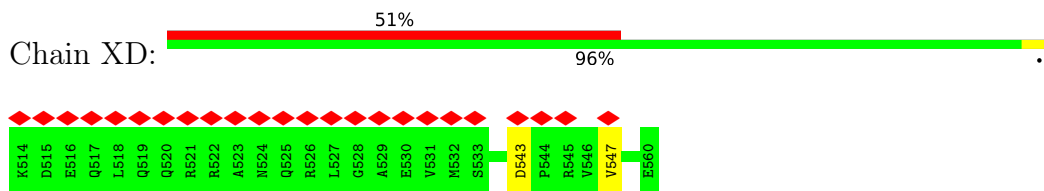
- Molecule 1: Flagellar M-ring protein



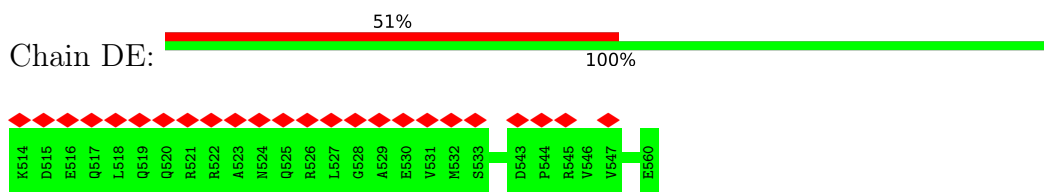
- Molecule 1: Flagellar M-ring protein



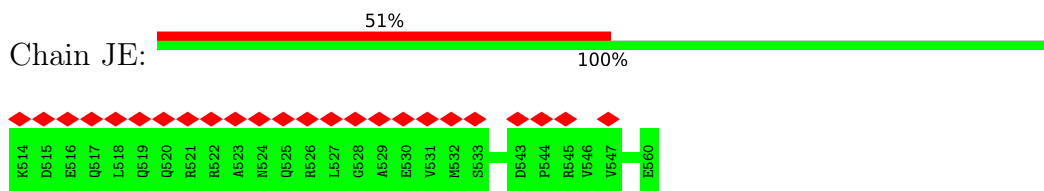
- Molecule 1: Flagellar M-ring protein



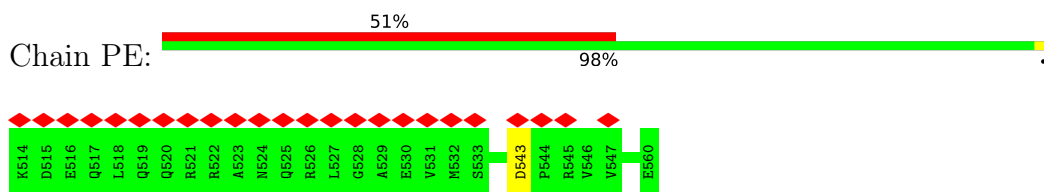
- Molecule 1: Flagellar M-ring protein



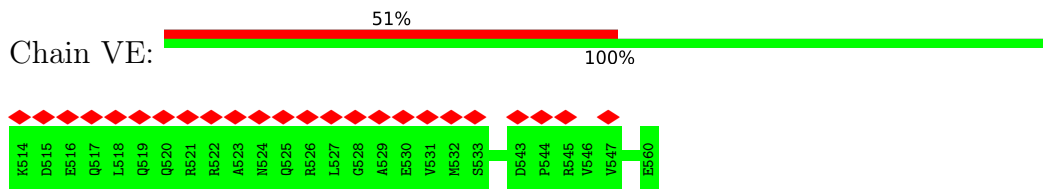
- Molecule 1: Flagellar M-ring protein



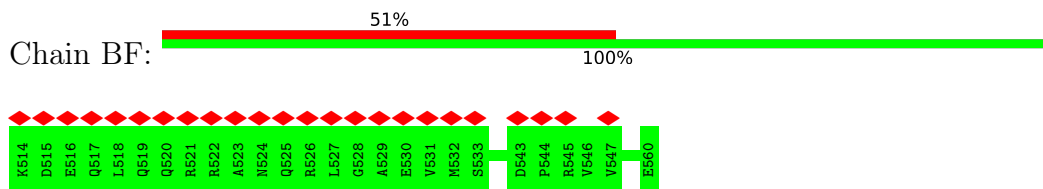
- Molecule 1: Flagellar M-ring protein



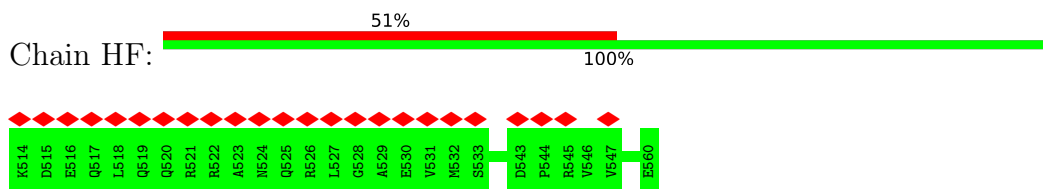
• Molecule 1: Flagellar M-ring protein



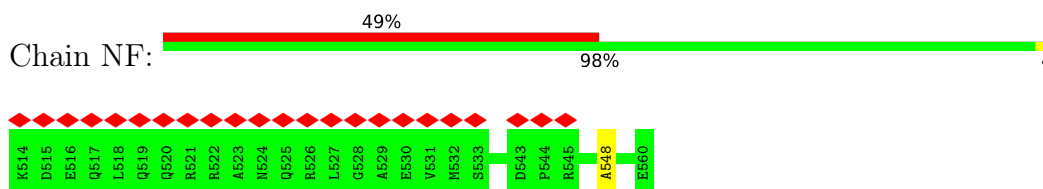
• Molecule 1: Flagellar M-ring protein



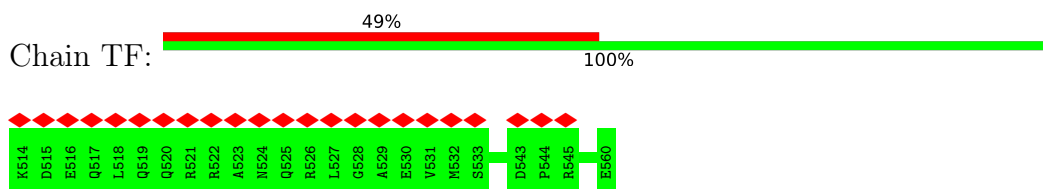
• Molecule 1: Flagellar M-ring protein



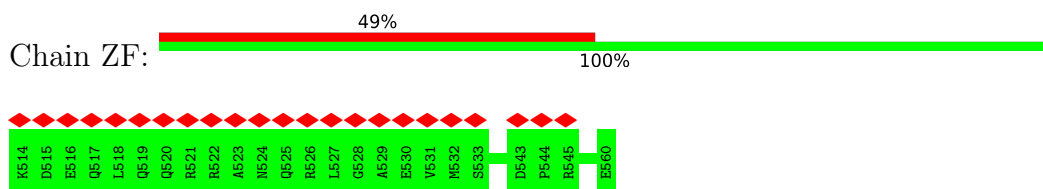
• Molecule 1: Flagellar M-ring protein



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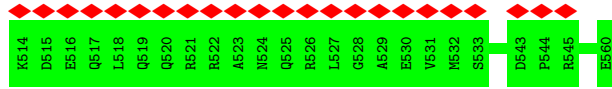


• Molecule 1: Flagellar M-ring protein

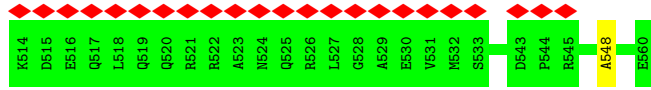


• Molecule 1: Flagellar M-ring protein

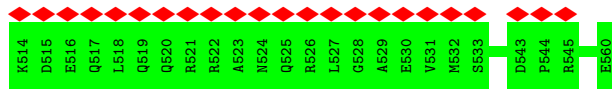




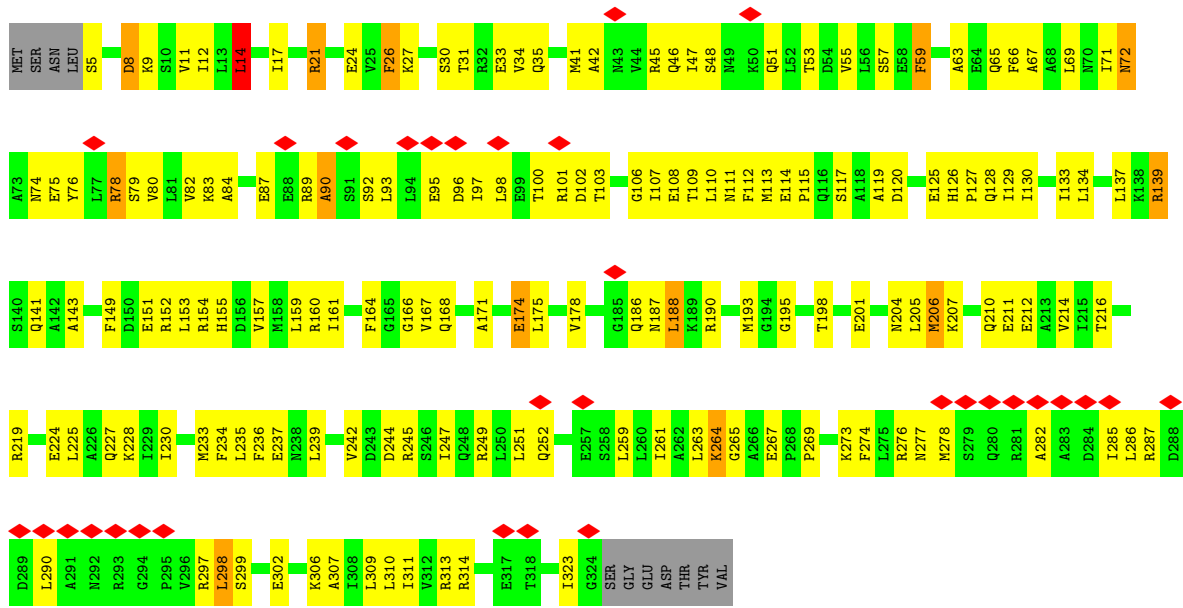
• Molecule 1: Flagellar M-ring protein



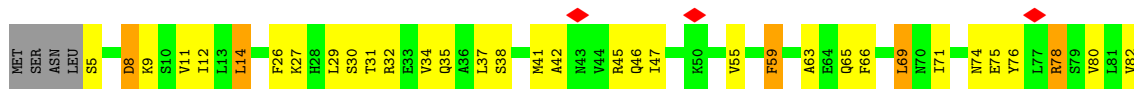
• Molecule 1: Flagellar M-ring protein

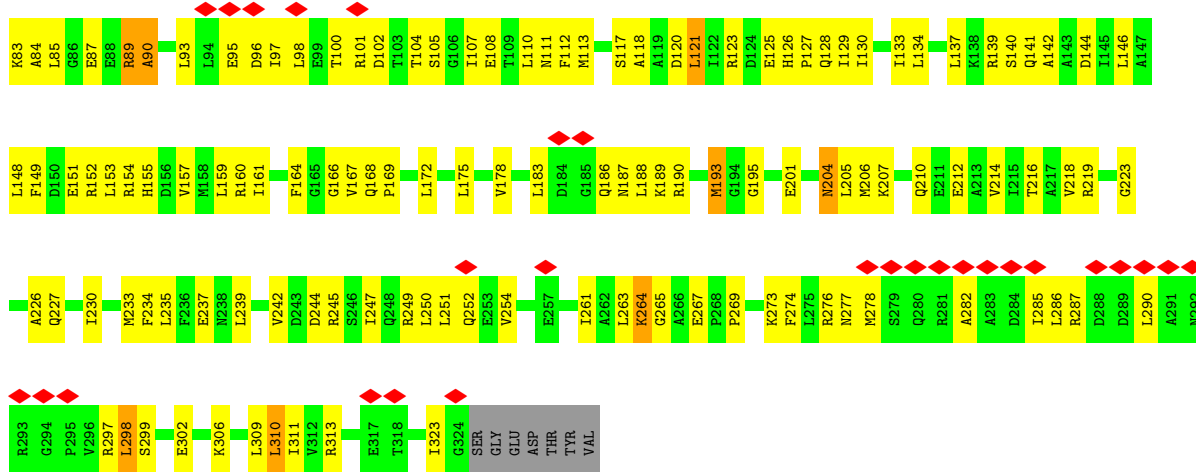


• Molecule 2: Flagellar motor switch protein FliG

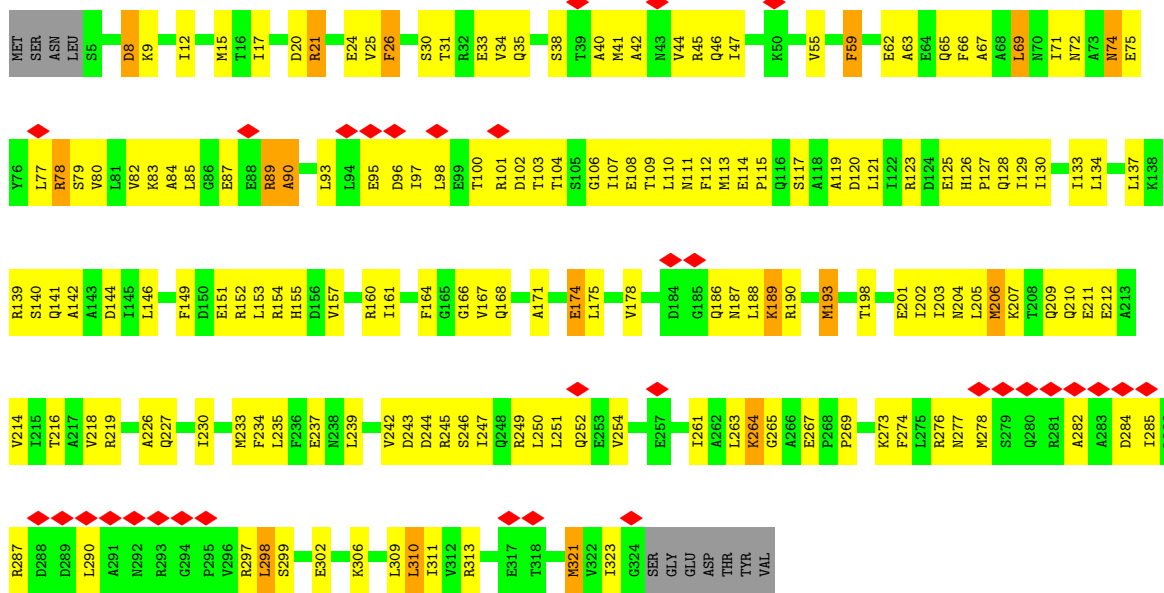


• Molecule 2: Flagellar motor switch protein FliG

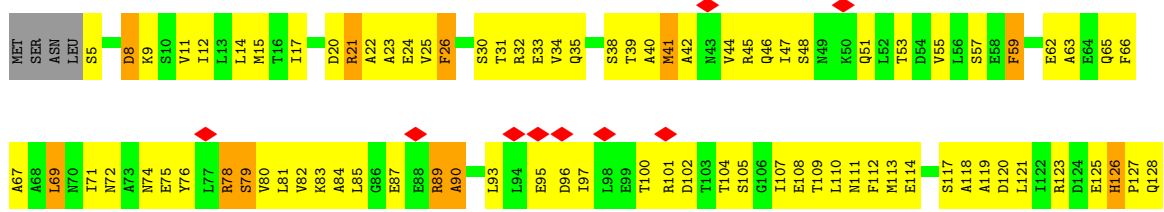


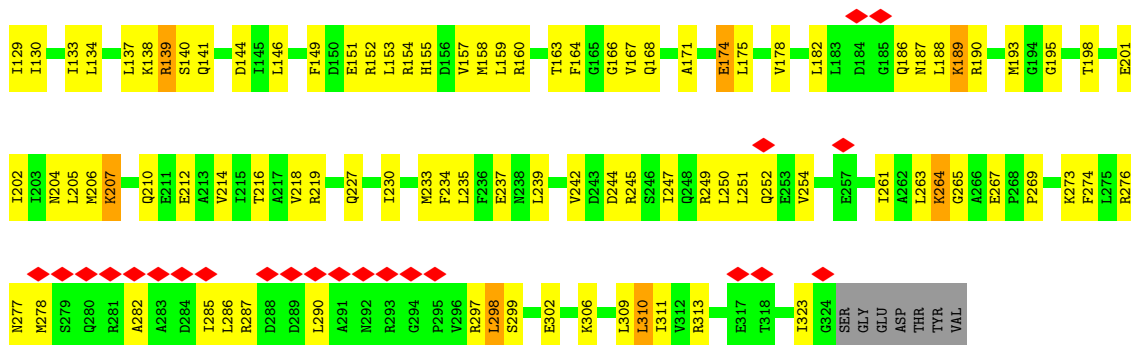


• Molecule 2: Flagellar motor switch protein FlIG

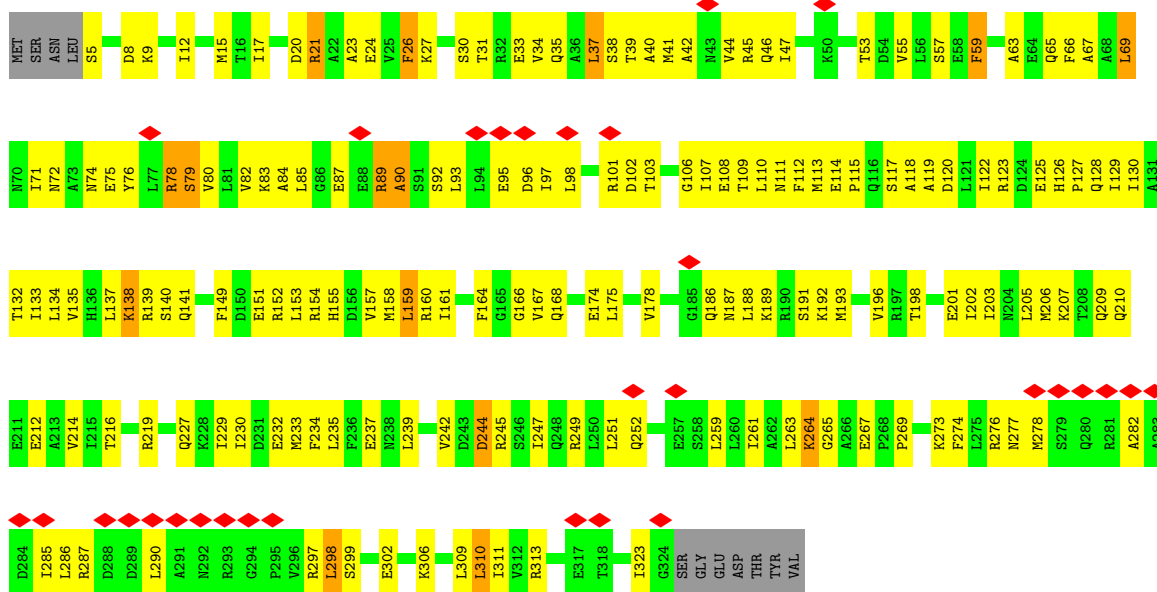


• Molecule 2: Flagellar motor switch protein FlIG

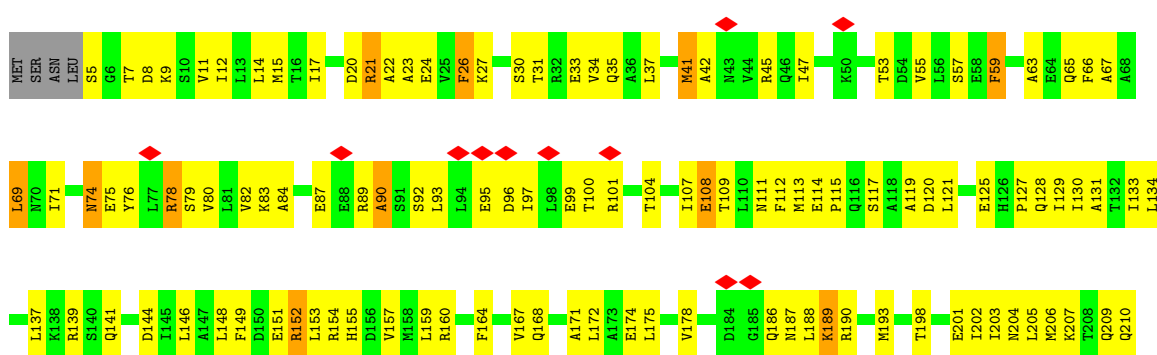


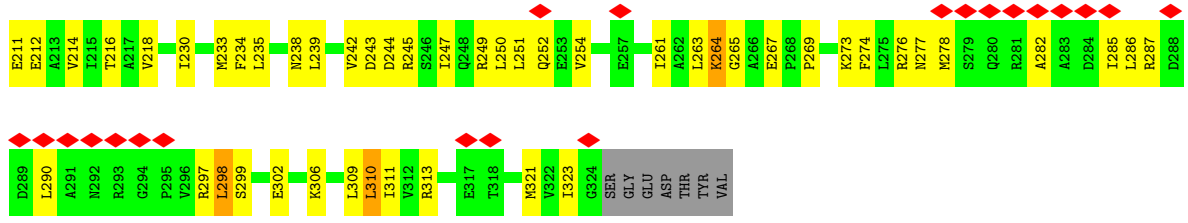


• Molecule 2: Flagellar motor switch protein FliG

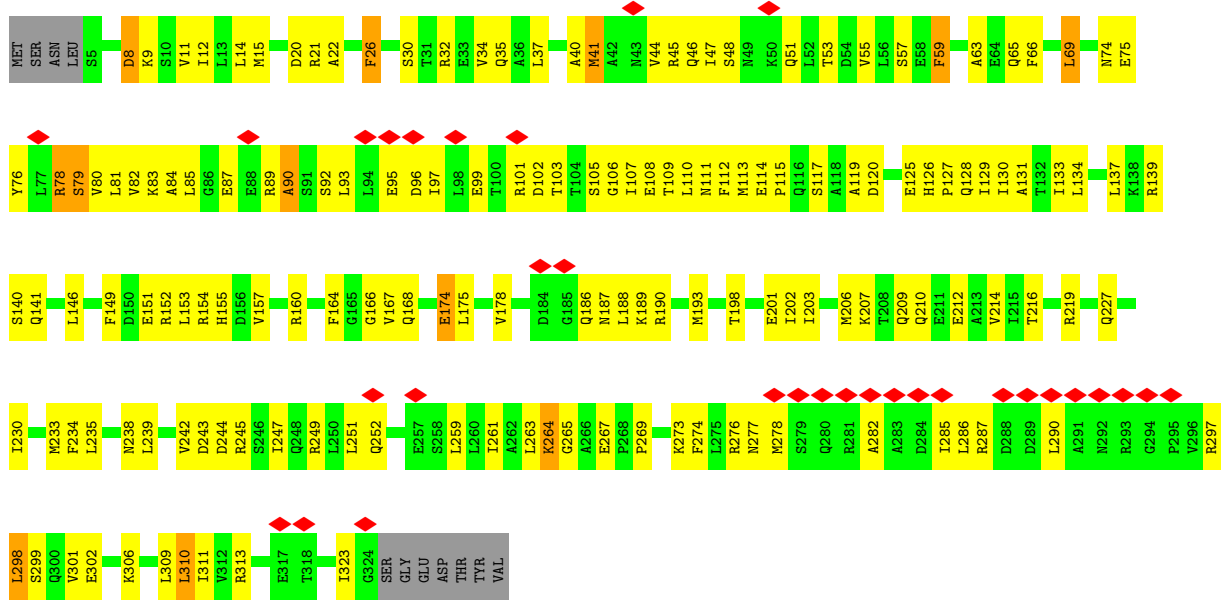


• Molecule 2: Flagellar motor switch protein FliG

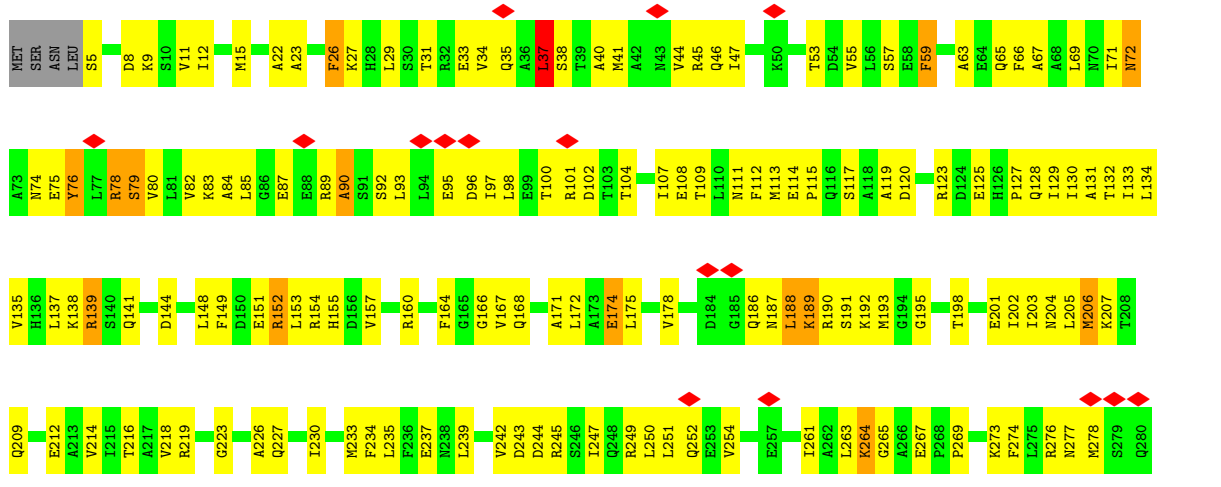


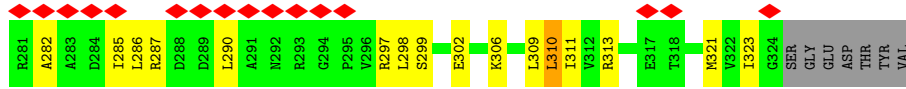


• Molecule 2: Flagellar motor switch protein FliG

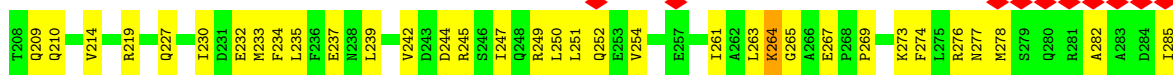
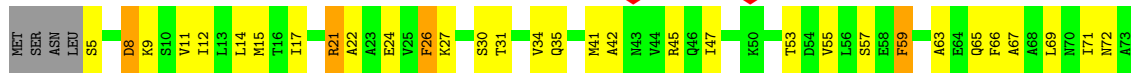


• Molecule 2: Flagellar motor switch protein FliG

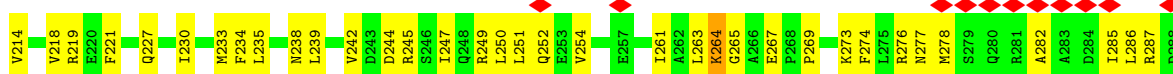
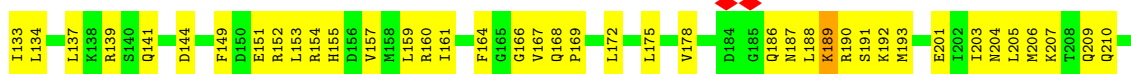
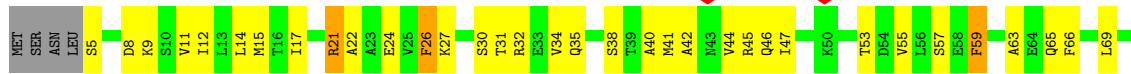




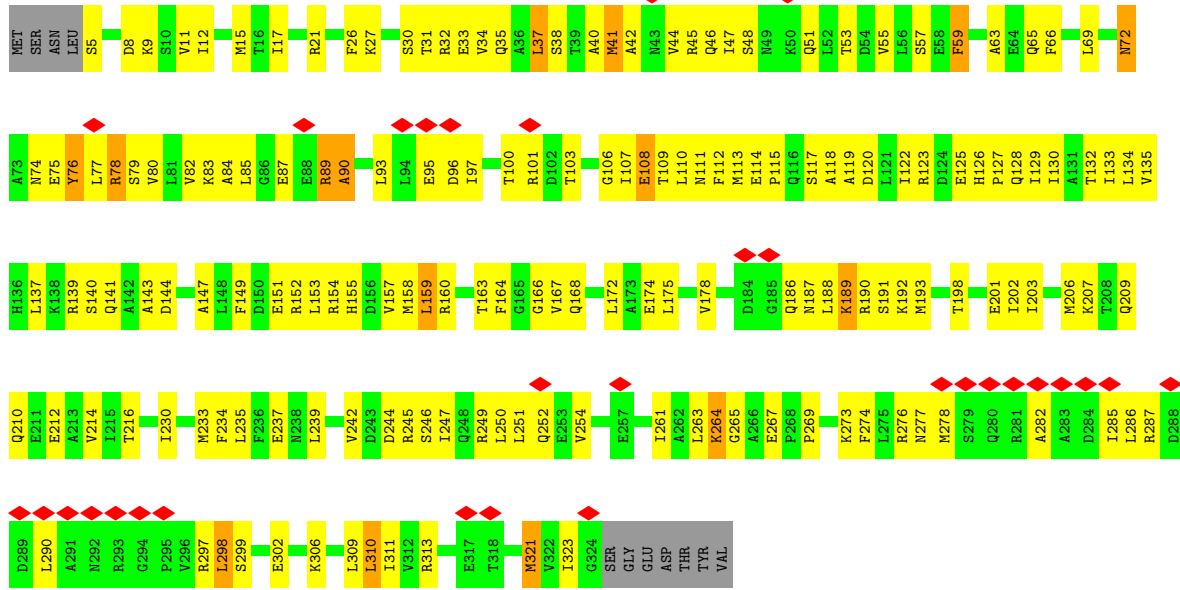
• Molecule 2: Flagellar motor switch protein FliG



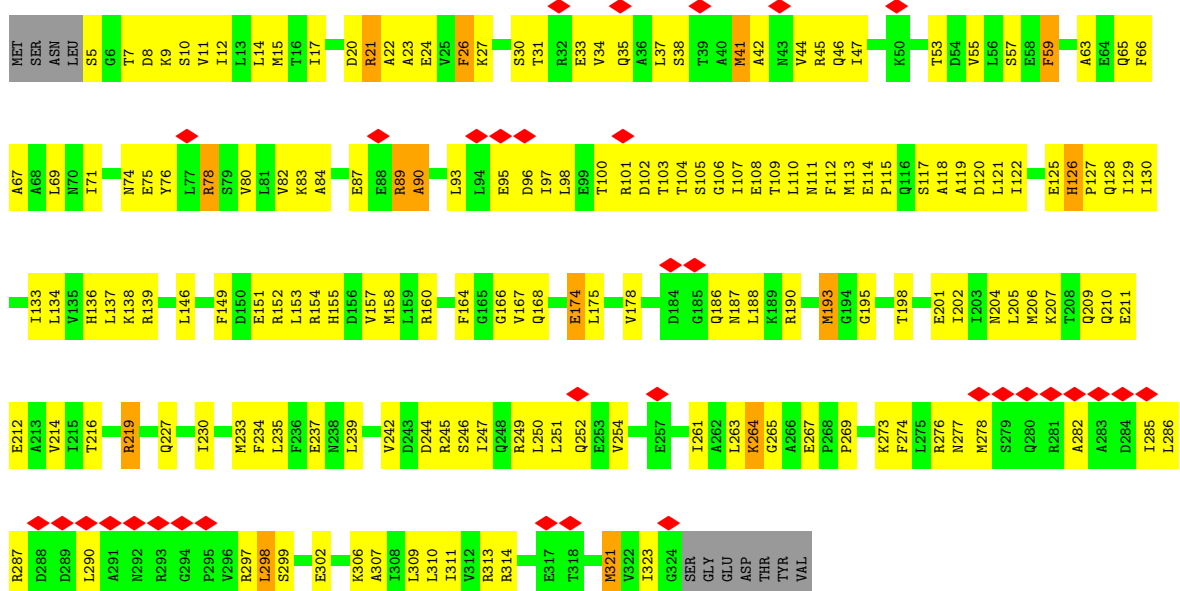
• Molecule 2: Flagellar motor switch protein FliG



• Molecule 2: Flagellar motor switch protein FliG



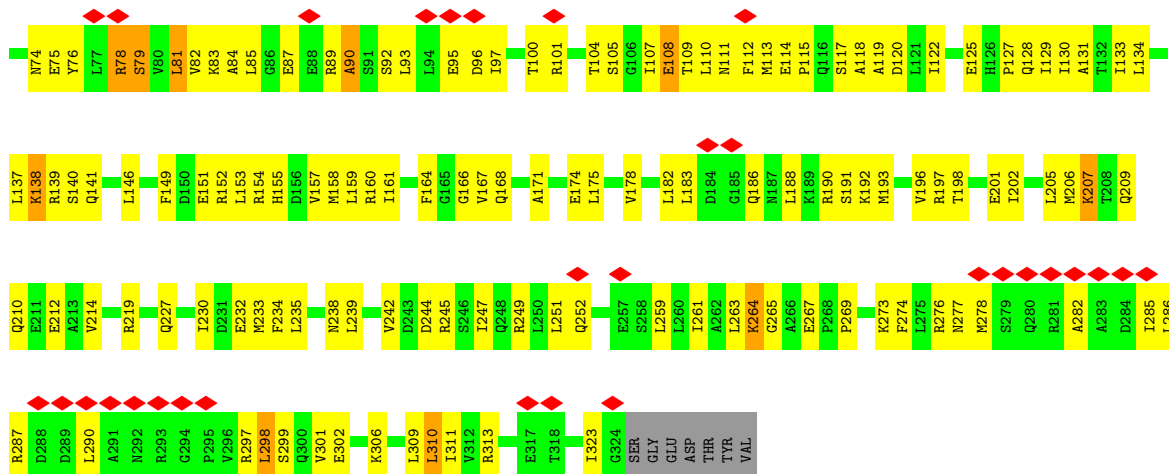
• Molecule 2: Flagellar motor switch protein FliG



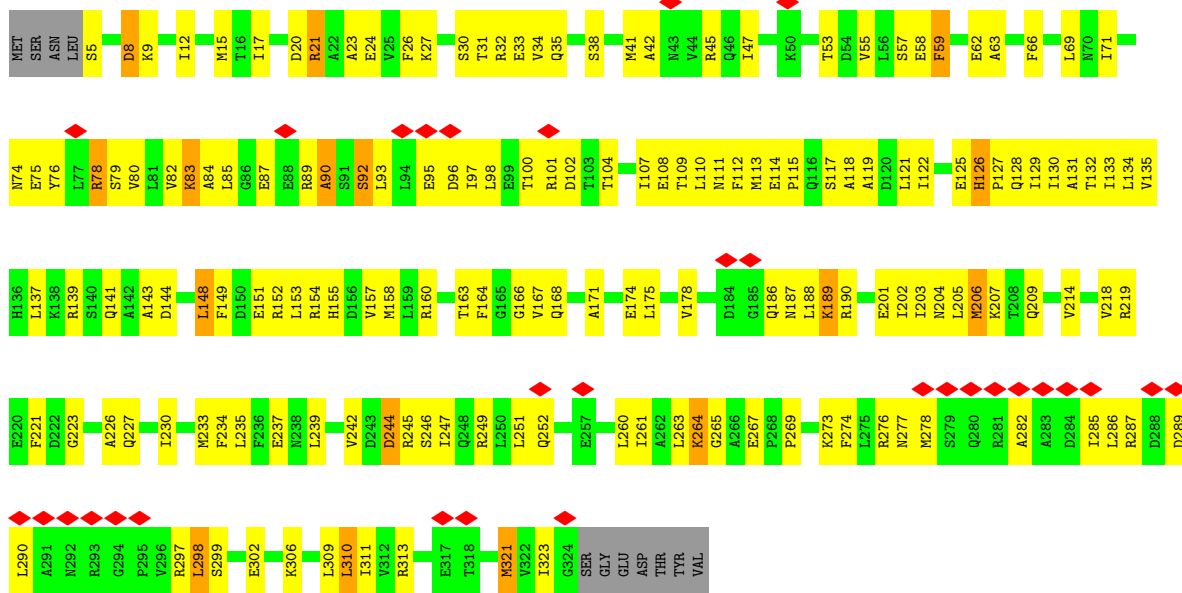
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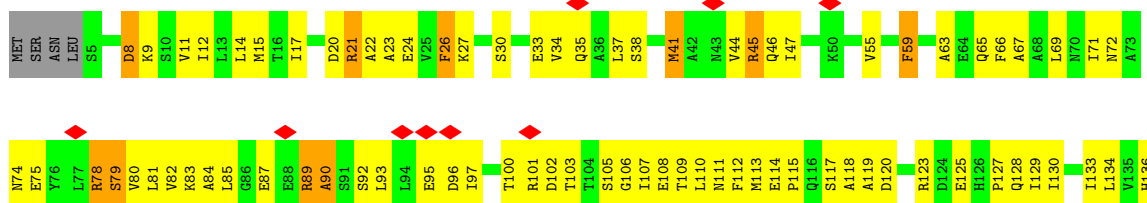
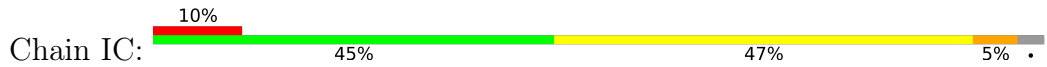


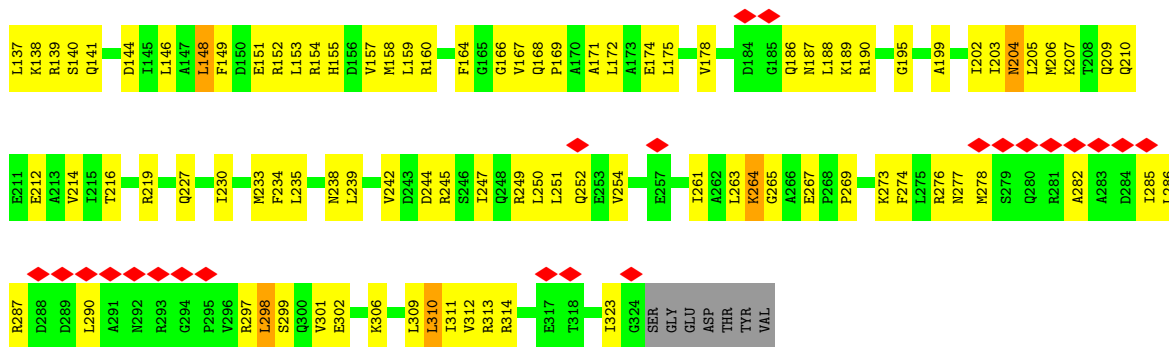


• Molecule 2: Flagellar motor switch protein Flig

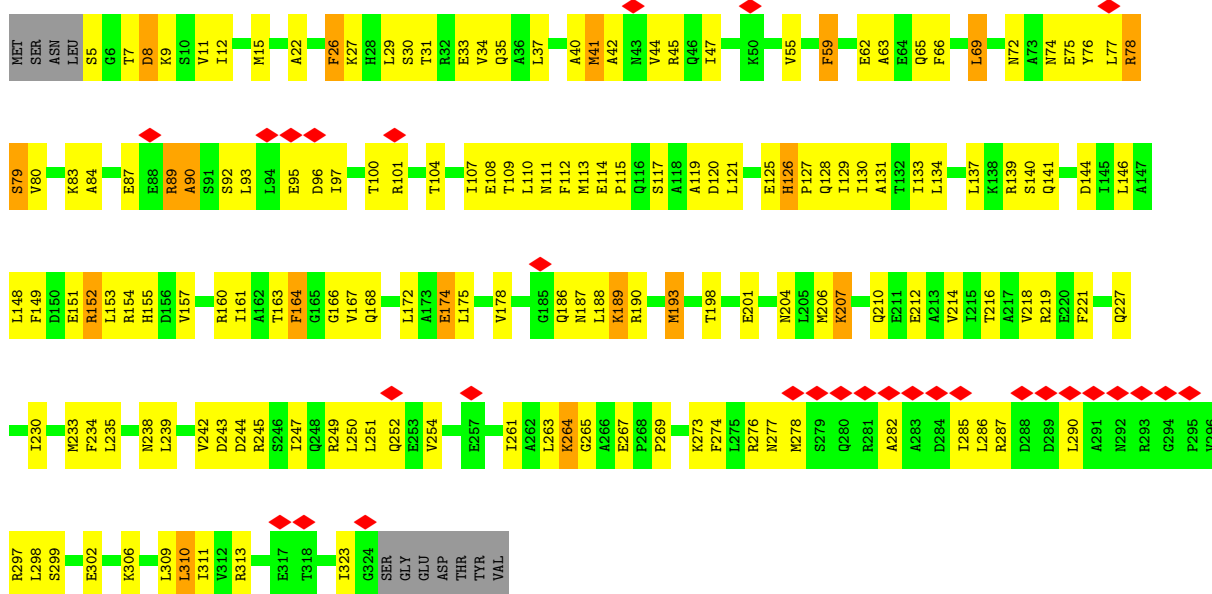


• Molecule 2: Flagellar motor switch protein Flig

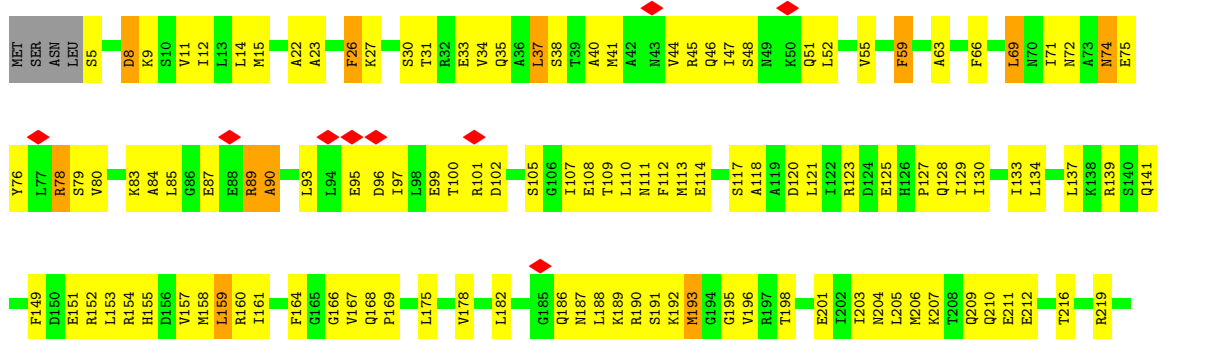


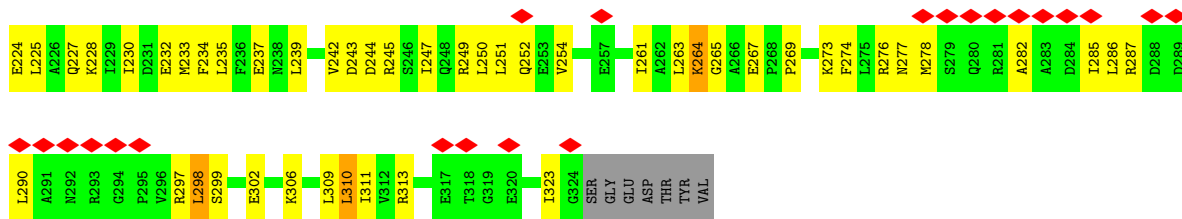


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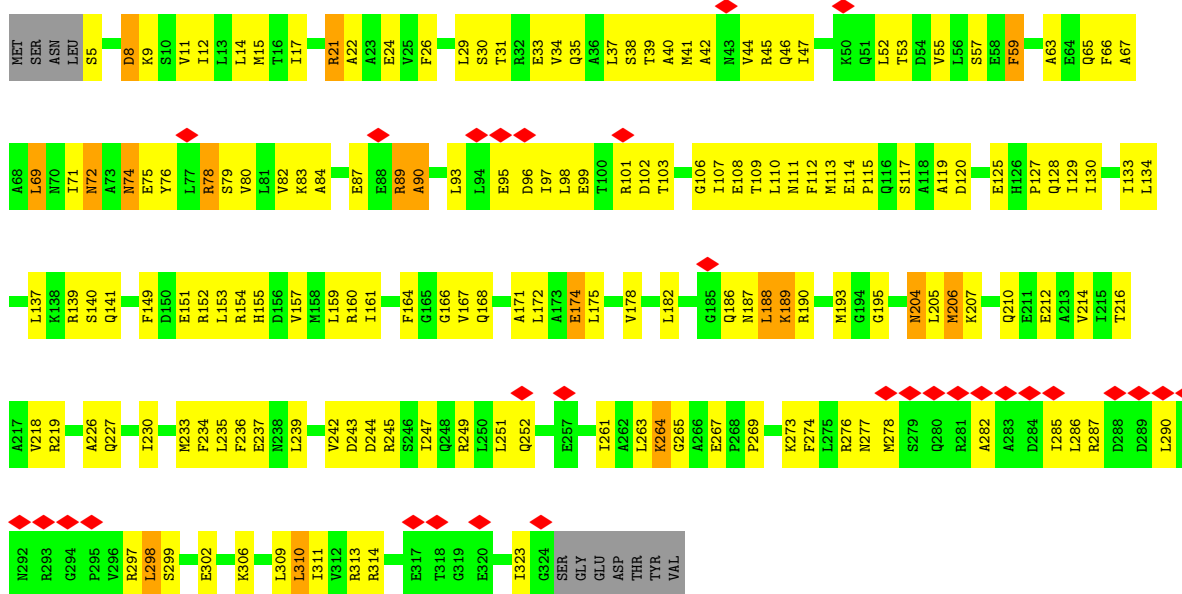


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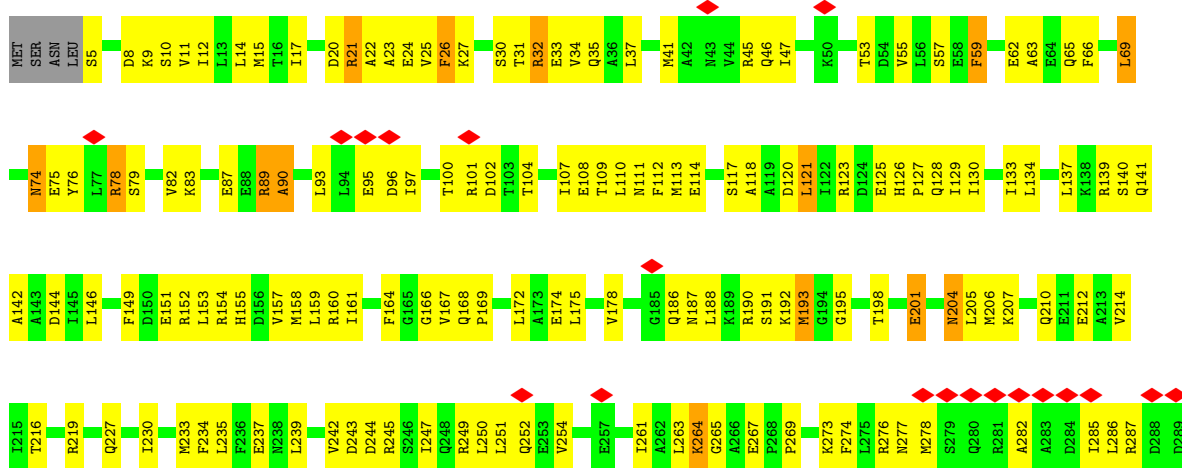




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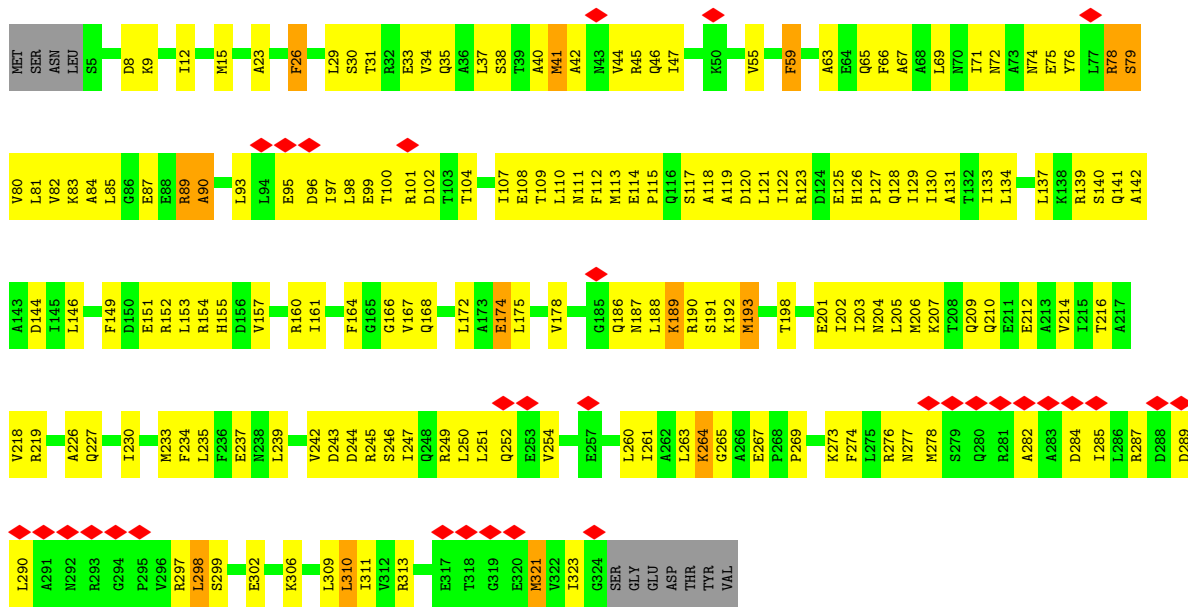


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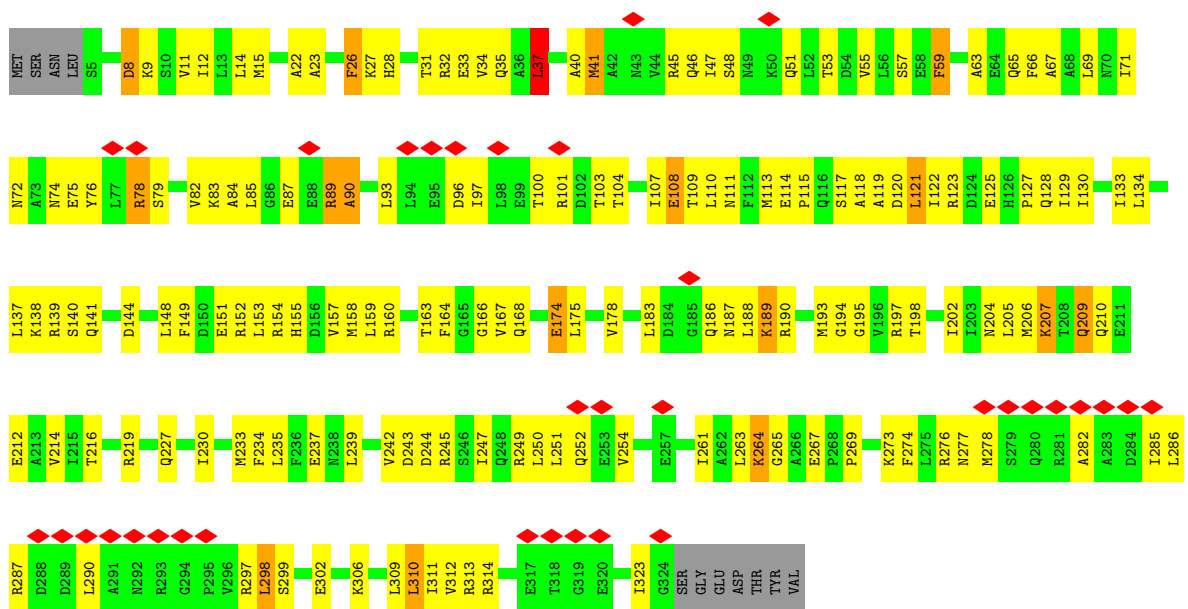




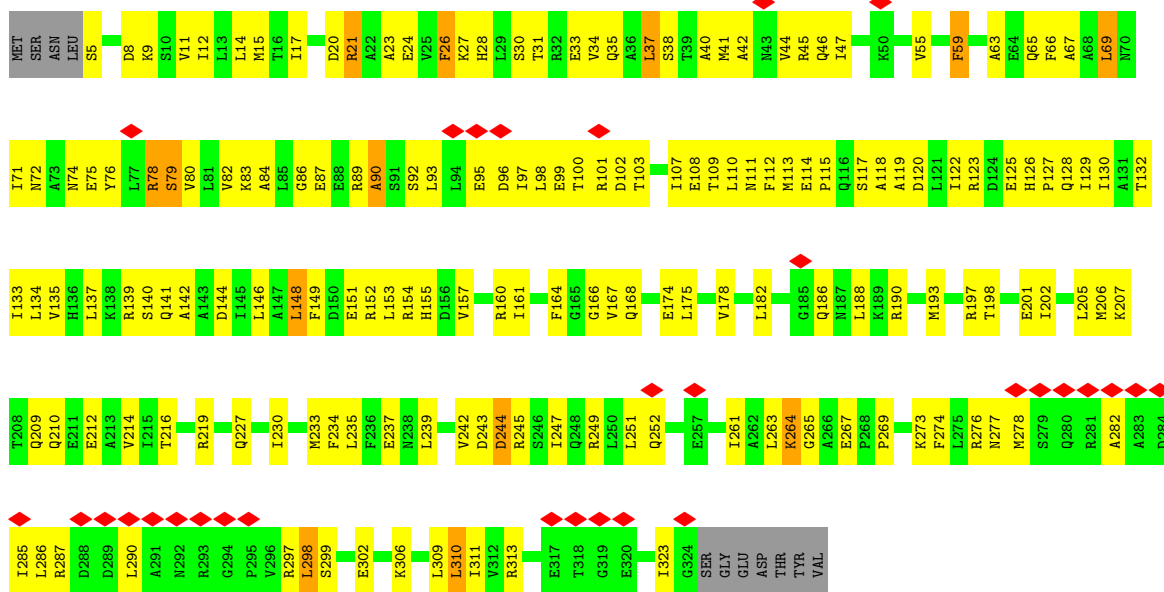
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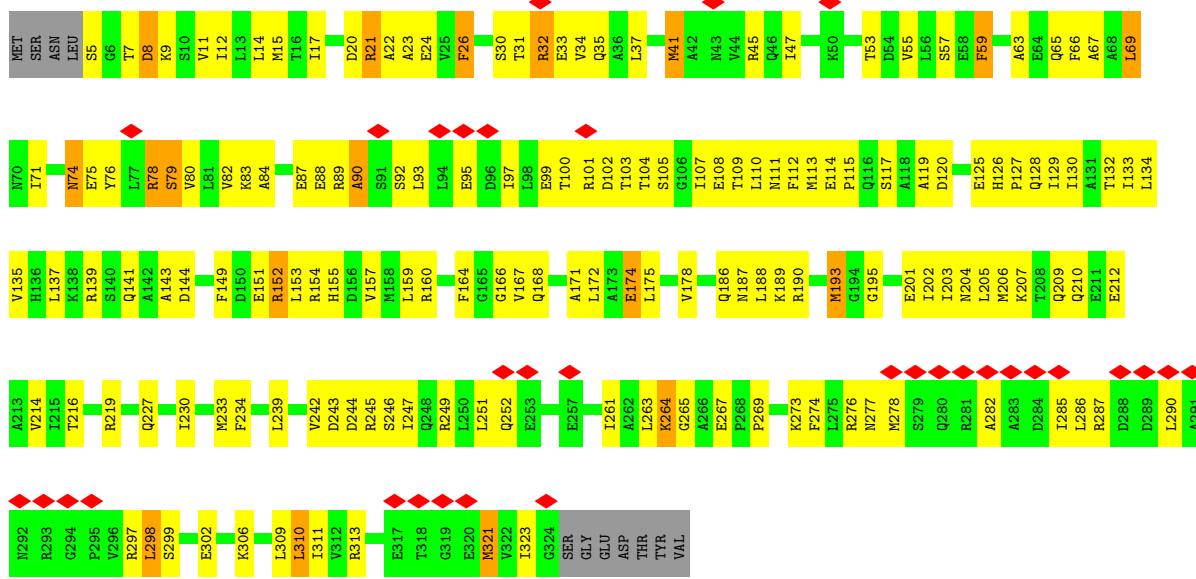
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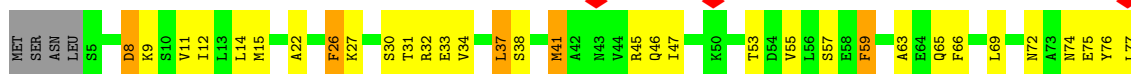
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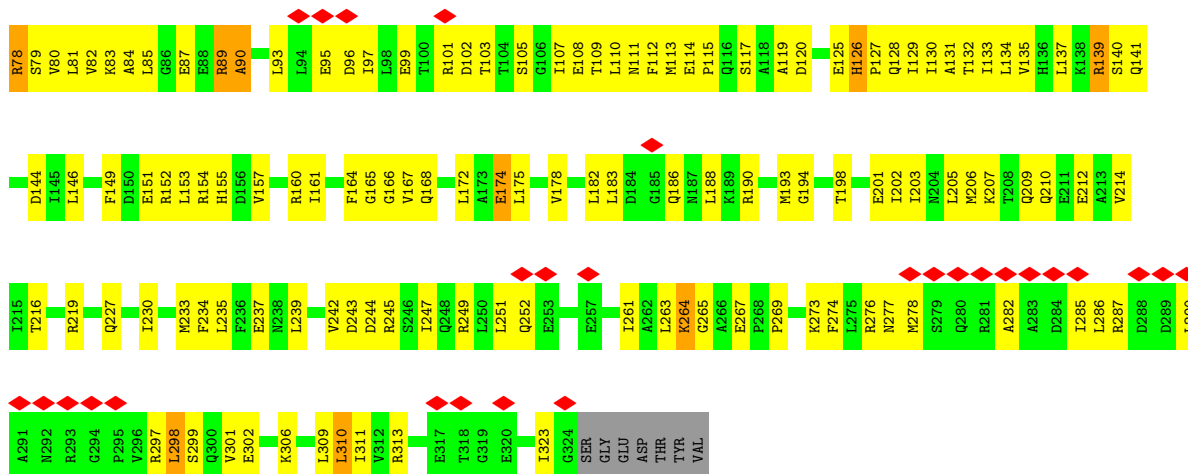


• Molecule 2: Flagellar motor switch protein FliG

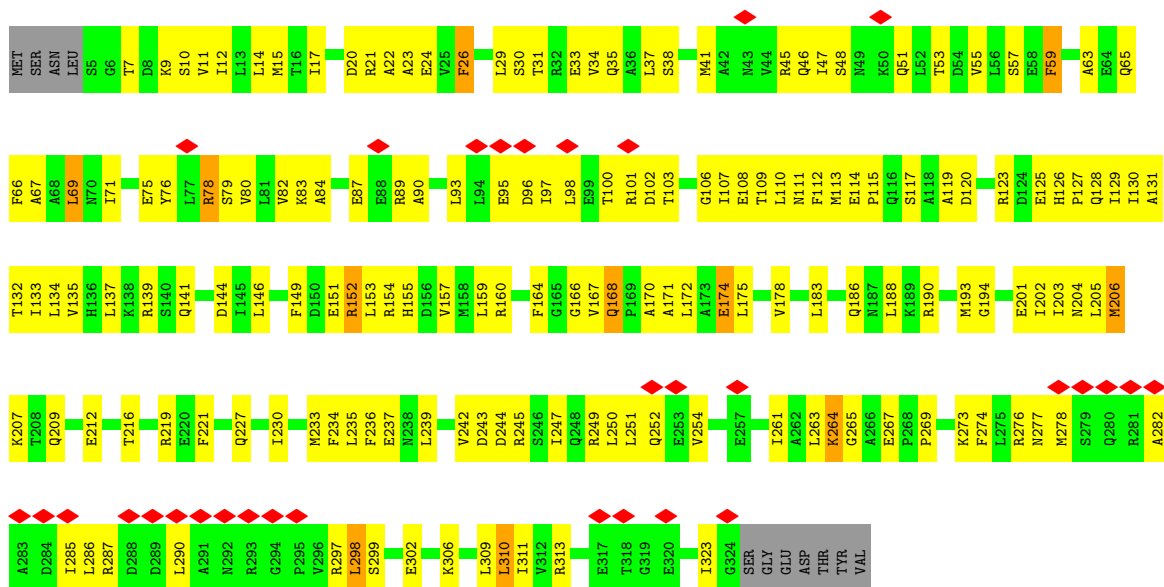


• Molecule 2: Flagellar motor switch protein FliG

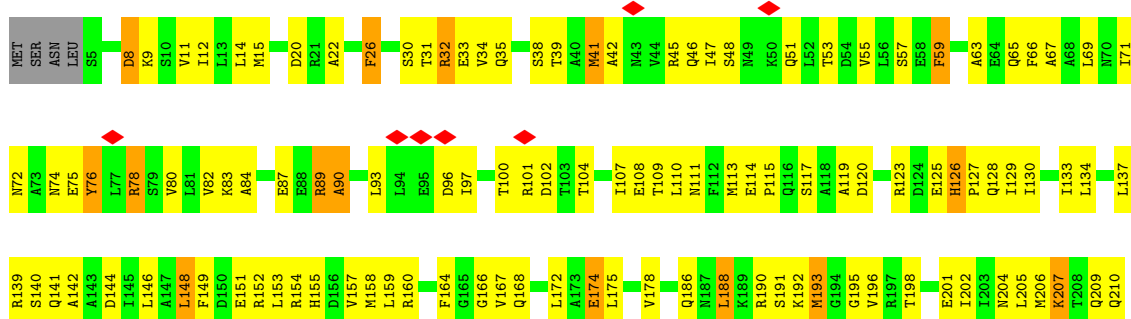


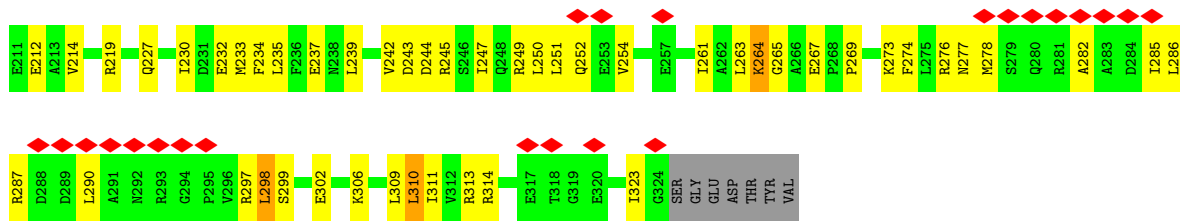


• Molecule 2: Flagellar motor switch protein FlIG

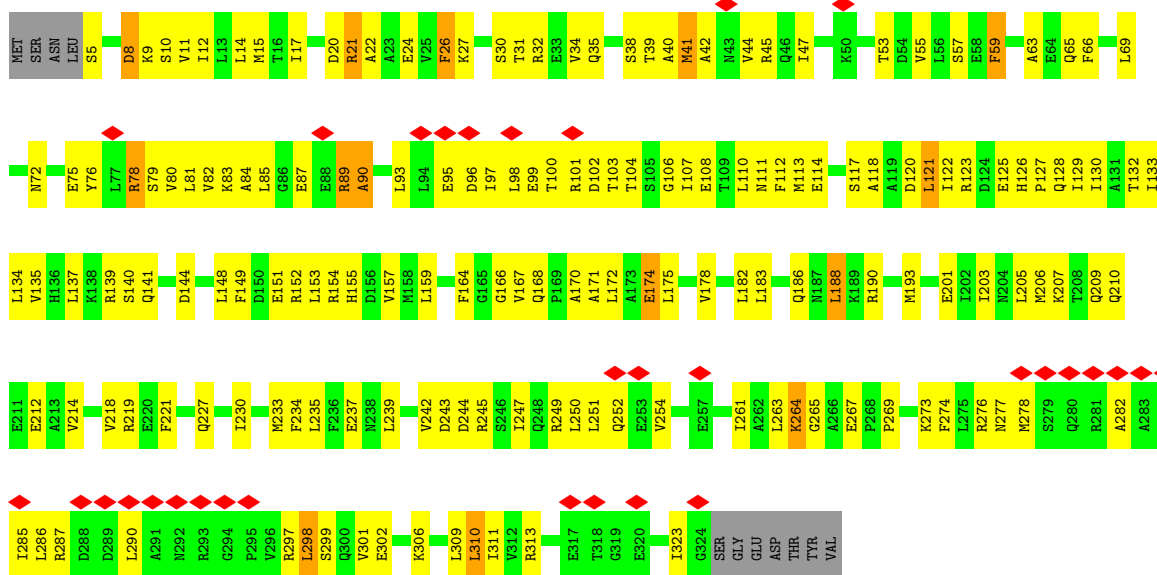


• Molecule 2: Flagellar motor switch protein FlIG

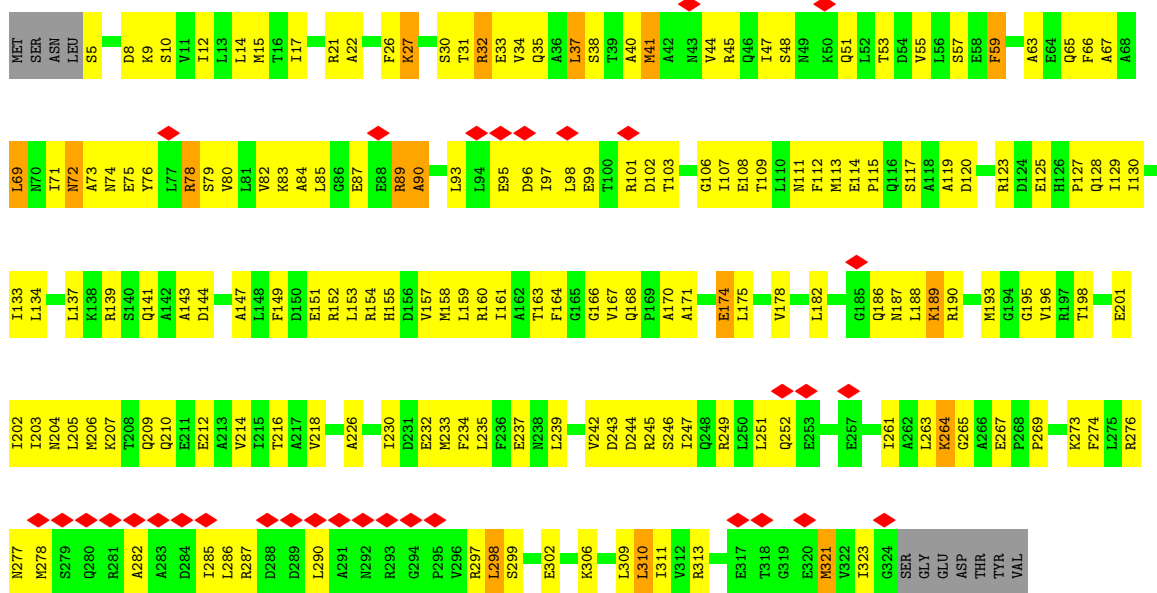
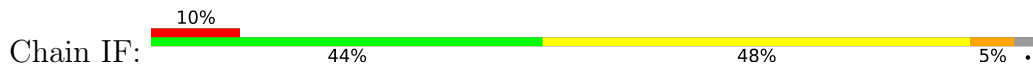




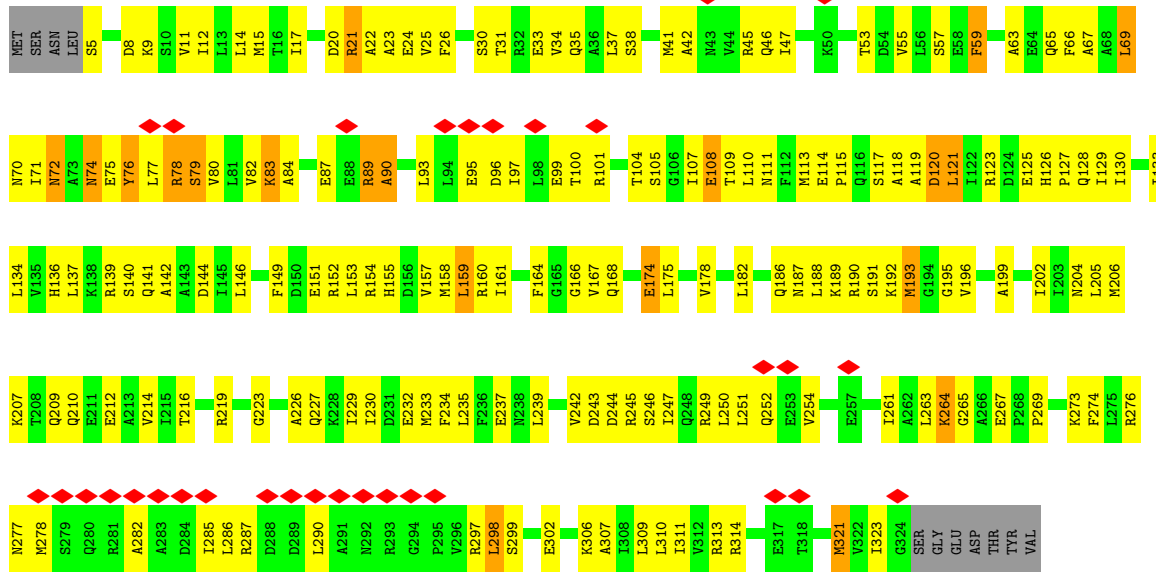
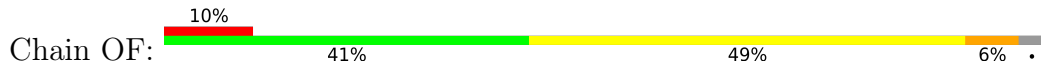
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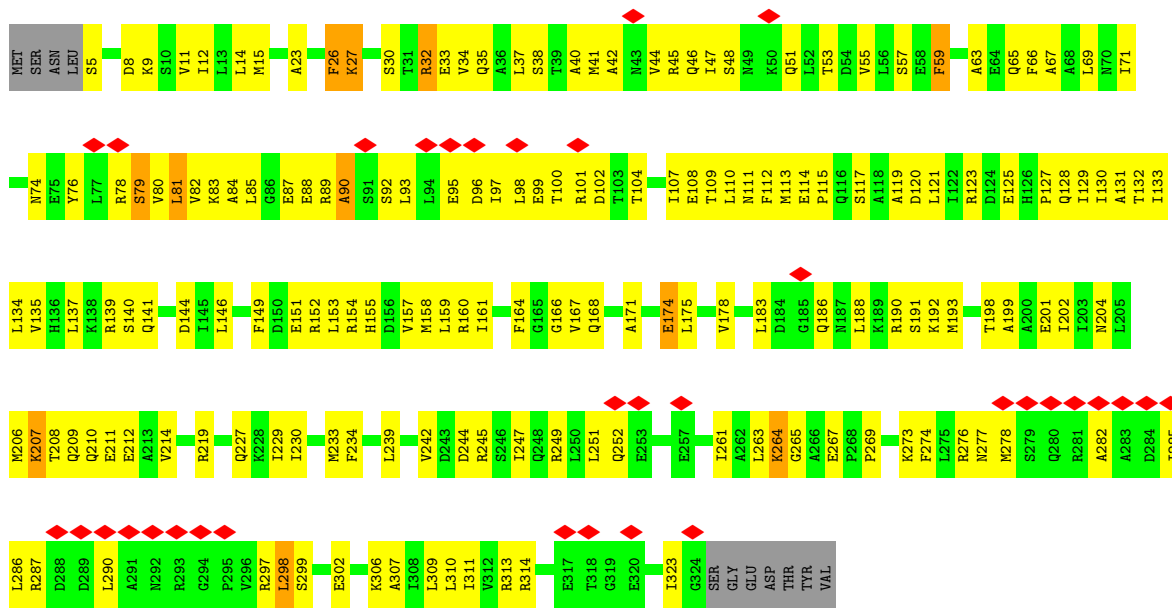
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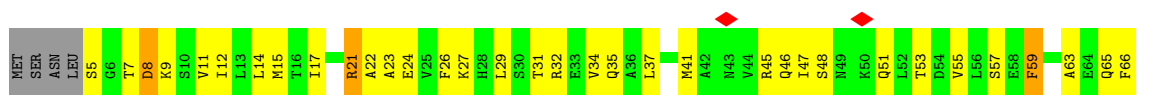
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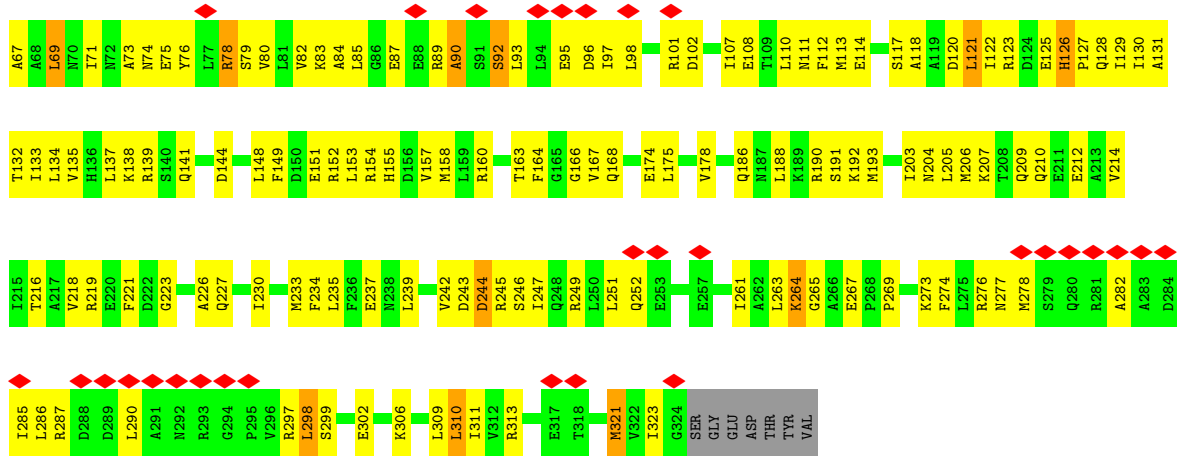
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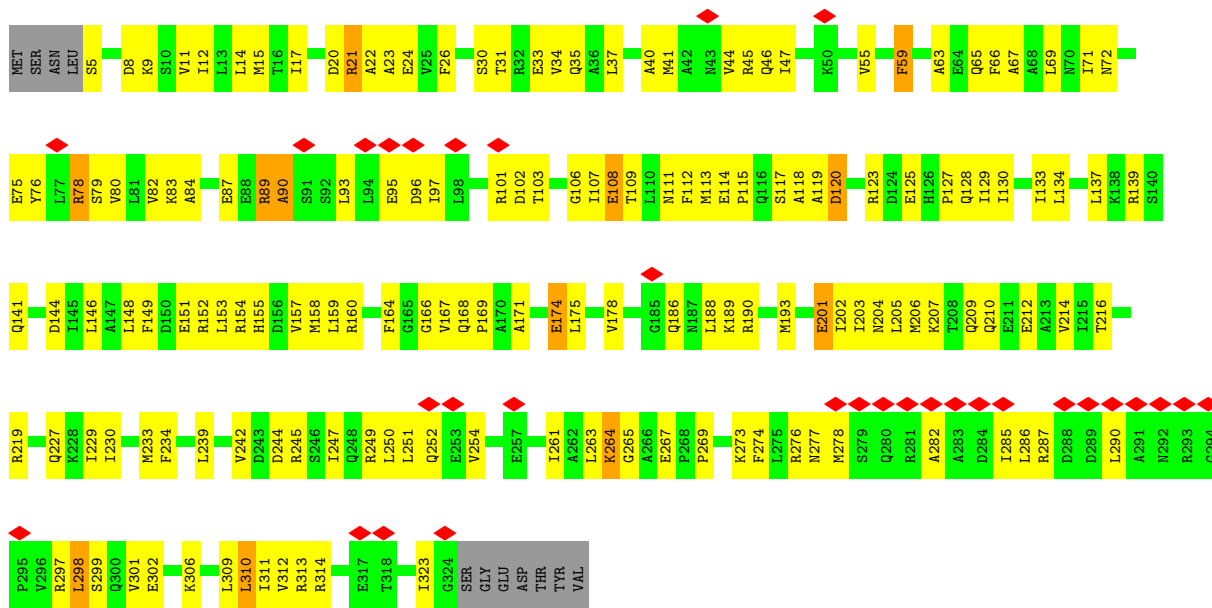
• Molecule 2: Flagellar motor switch protein FlIG



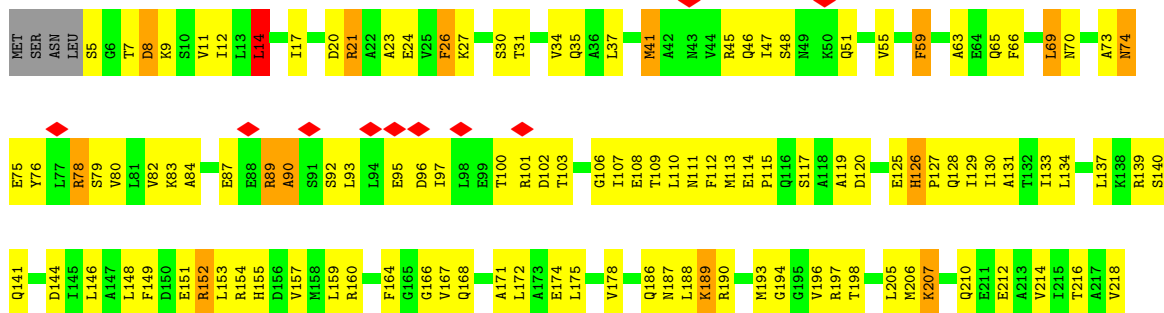


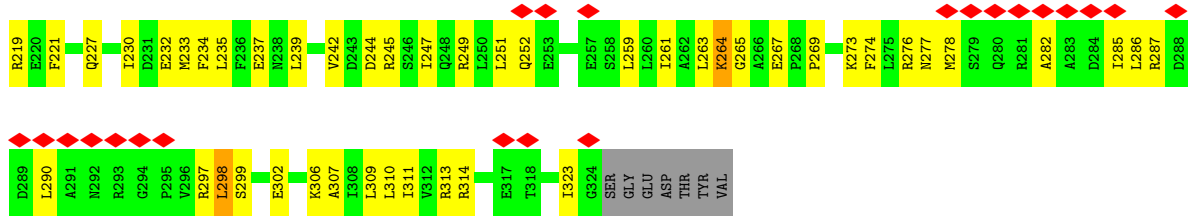


• Molecule 2: Flagellar motor switch protein FliG

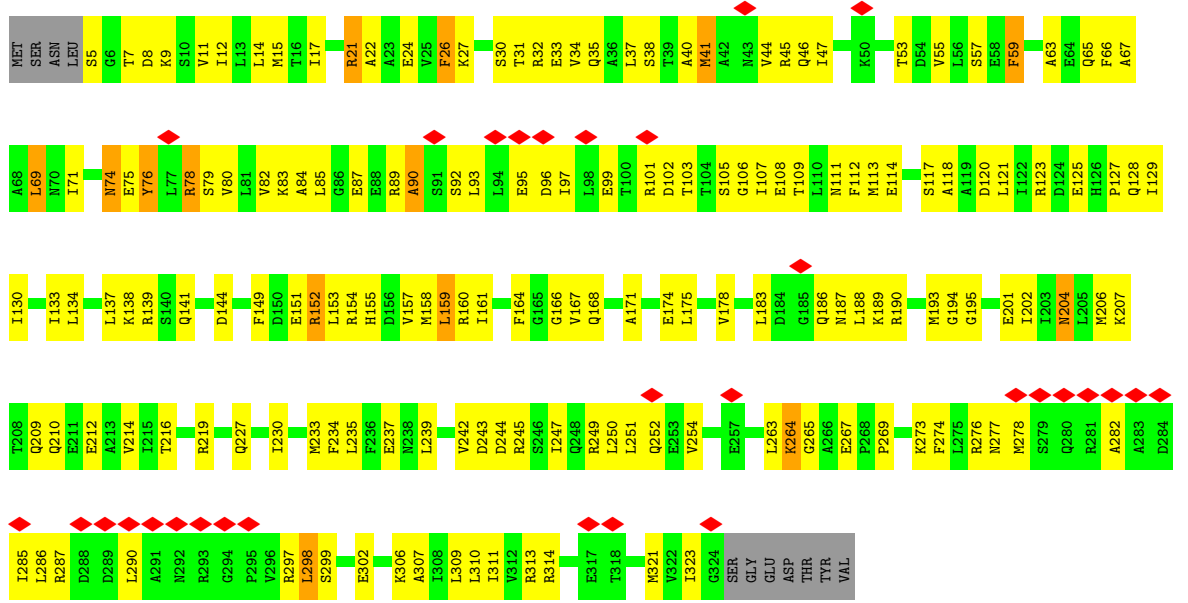


• Molecule 2: Flagellar motor switch protein FliG

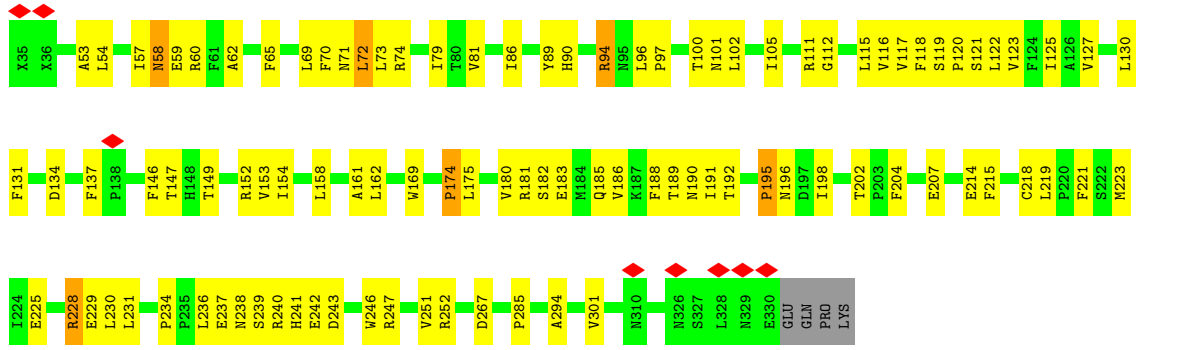




• Molecule 2: Flagellar motor switch protein FliG

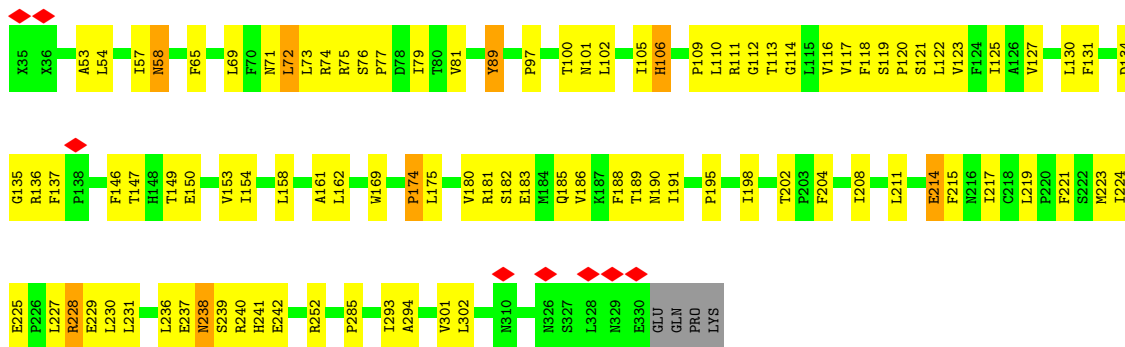


• Molecule 3: FliM, Flagellar motor switch protein FliM

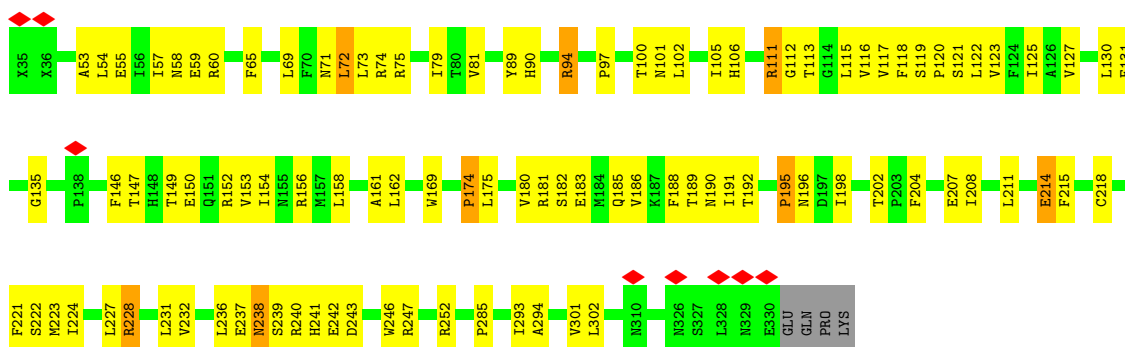


• Molecule 3: FliM, Flagellar motor switch protein FliM

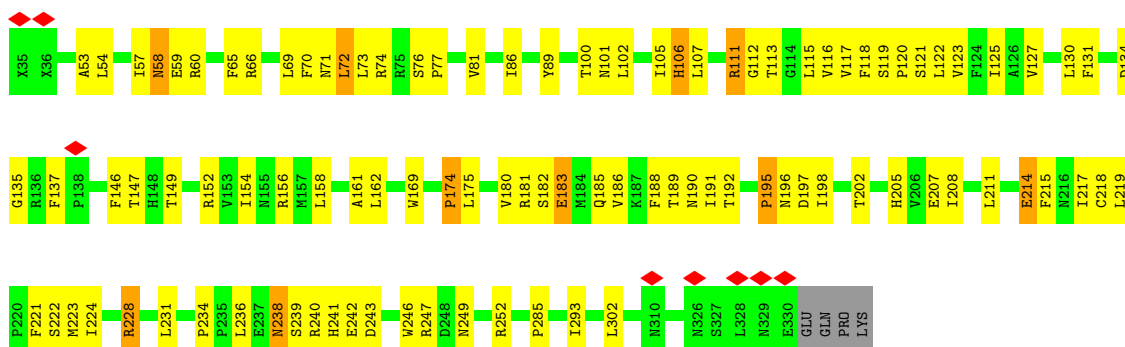




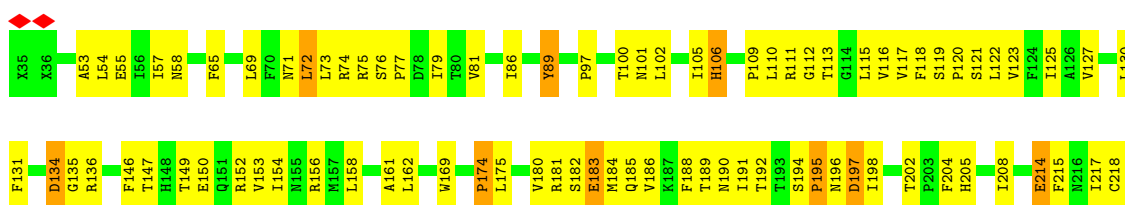
• Molecule 3: FliM, Flagellar motor switch protein FliM

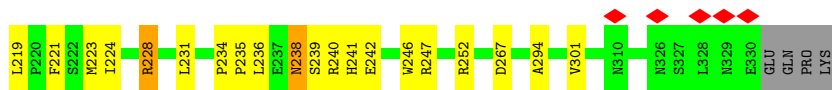


• Molecule 3: FliM, Flagellar motor switch protein FliM



• Molecule 3: FliM, Flagellar motor switch protein FliM

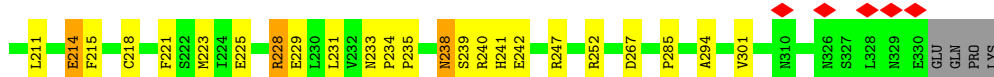




• Molecule 3: FliM,Flagellar motor switch protein FliM



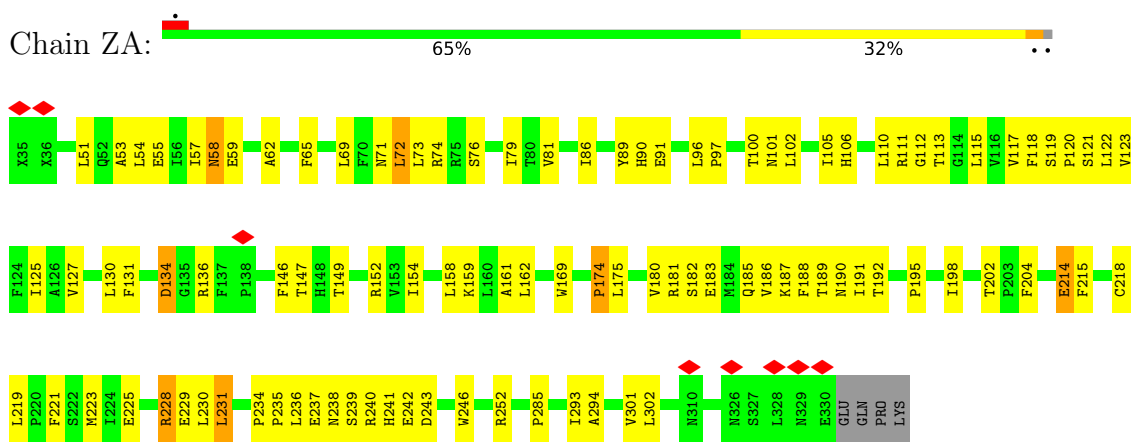
• Molecule 3: FliM,Flagellar motor switch protein FliM



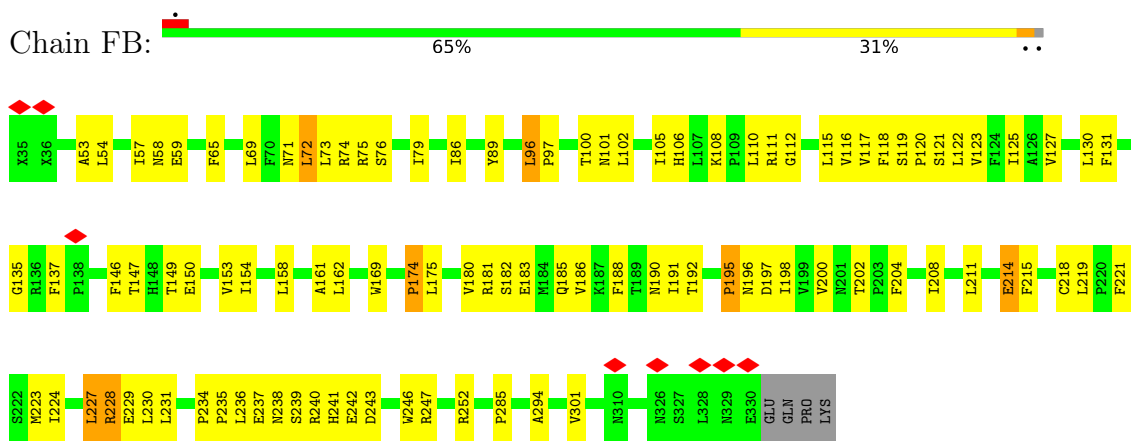
• Molecule 3: FliM,Flagellar motor switch protein FliM



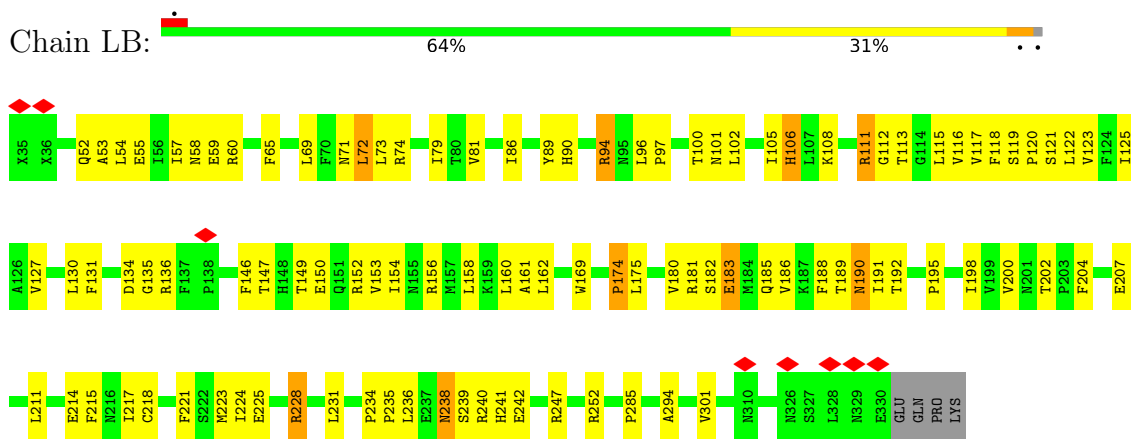
• Molecule 3: FliM,Flagellar motor switch protein FliM



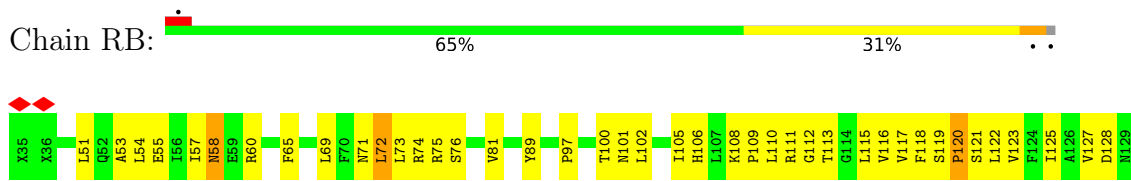
• Molecule 3: FlIM,Flagellar motor switch protein FlIM

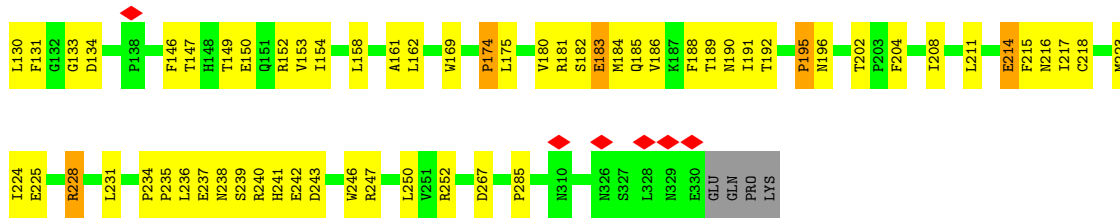


• Molecule 3: FlIM,Flagellar motor switch protein FlIM

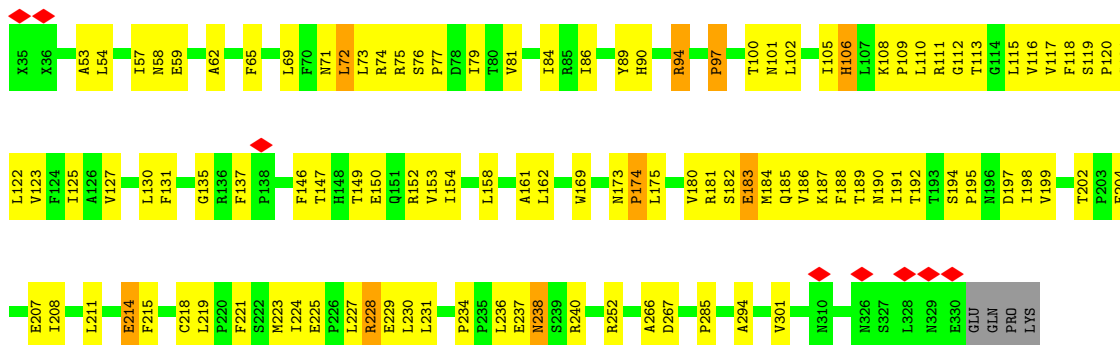


• Molecule 3: FlIM,Flagellar motor switch protein FlIM

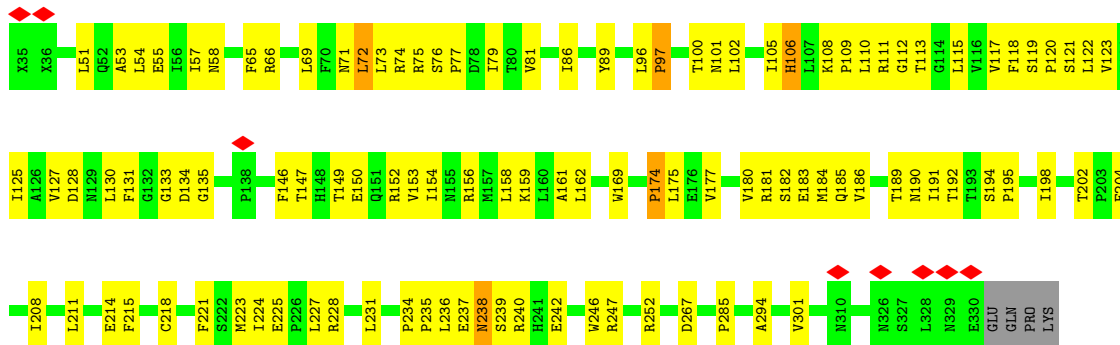




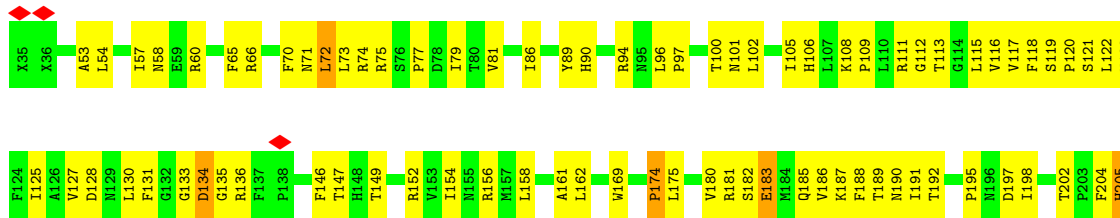
• Molecule 3: FliM,Flagellar motor switch protein FliM

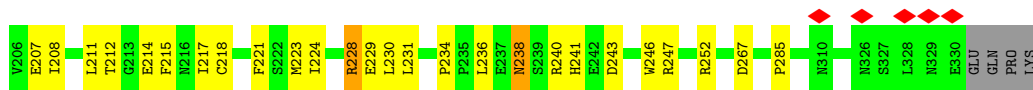


• Molecule 3: FliM,Flagellar motor switch protein FliM

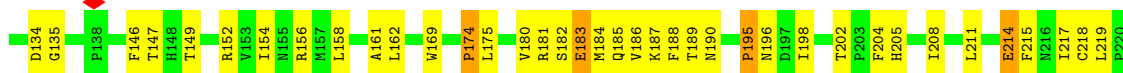
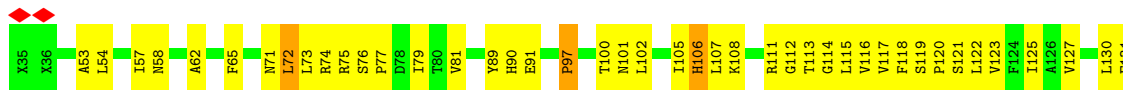


• Molecule 3: FliM,Flagellar motor switch protein FliM

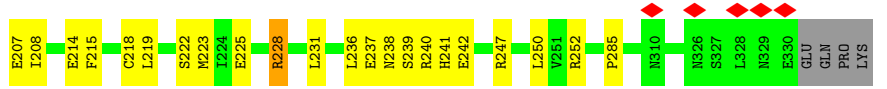
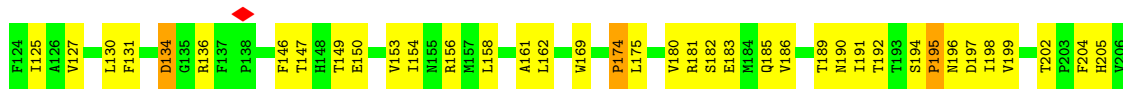
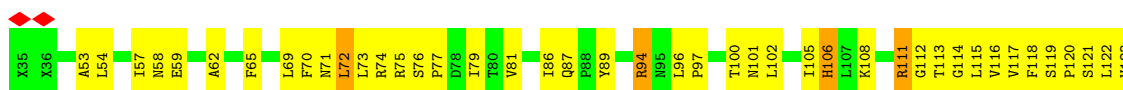




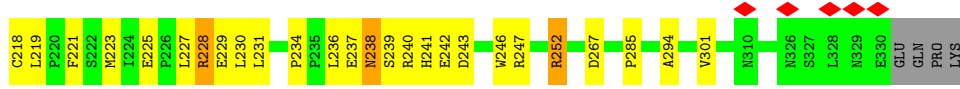
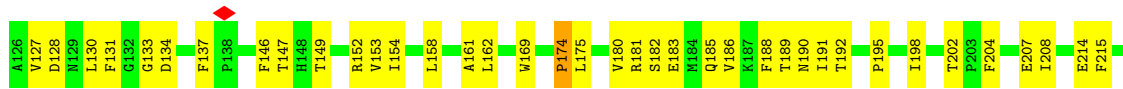
• Molecule 3: FliM,Flagellar motor switch protein FliM



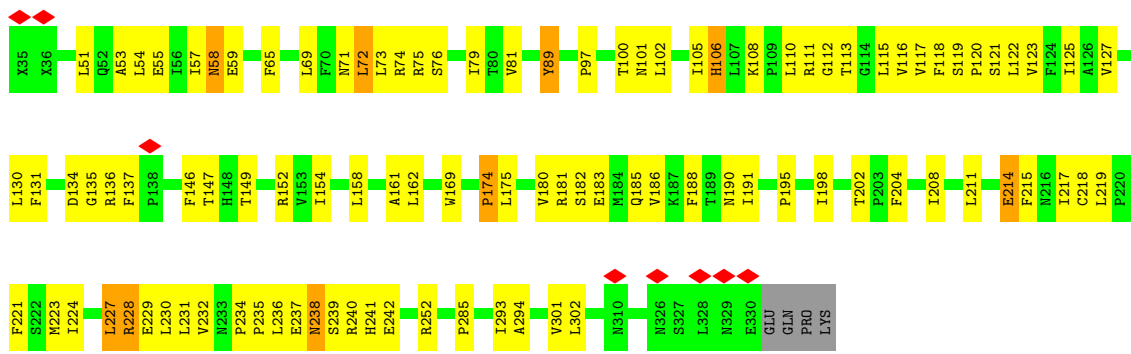
• Molecule 3: FliM,Flagellar motor switch protein FliM



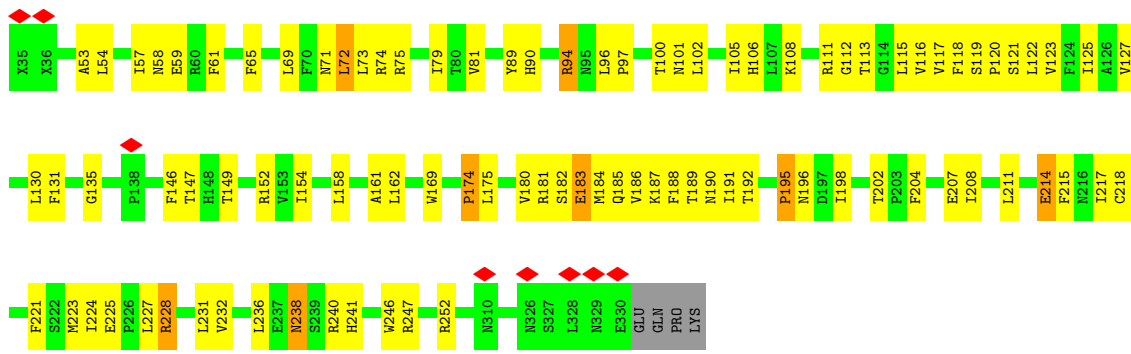
• Molecule 3: FliM,Flagellar motor switch protein FliM



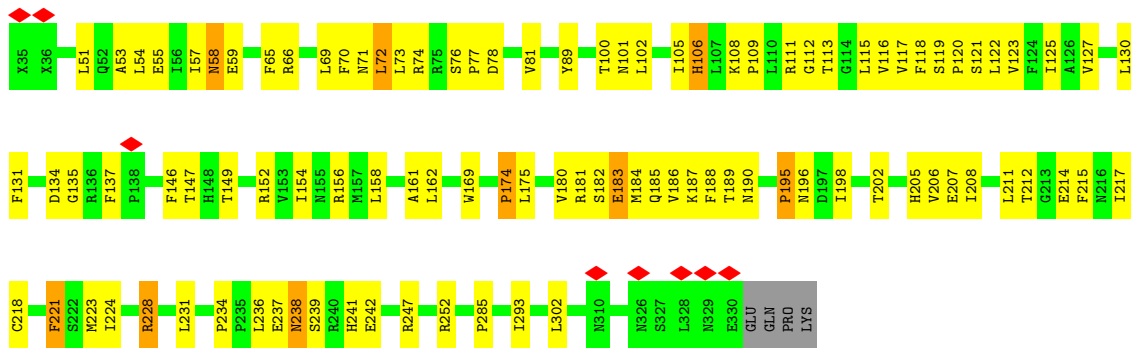
• Molecule 3: FliM,Flagellar motor switch protein FliM



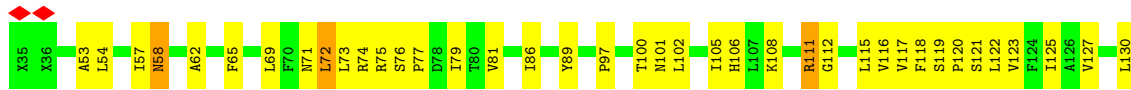
• Molecule 3: FlIM,Flagellar motor switch protein FlIM



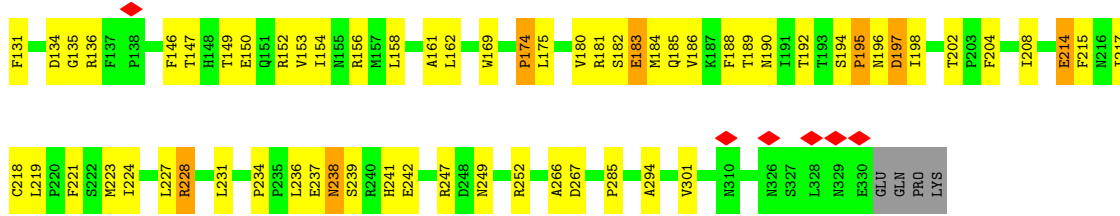
• Molecule 3: FlIM,Flagellar motor switch protein FlIM



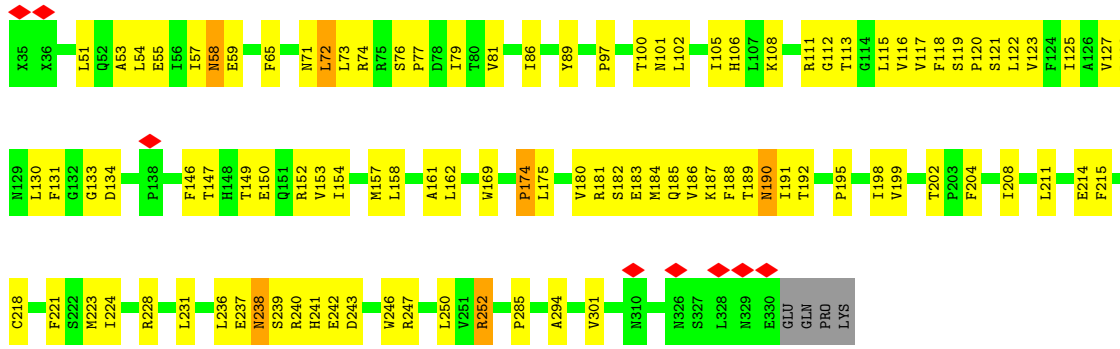
• Molecule 3: FlIM,Flagellar motor switch protein FlIM



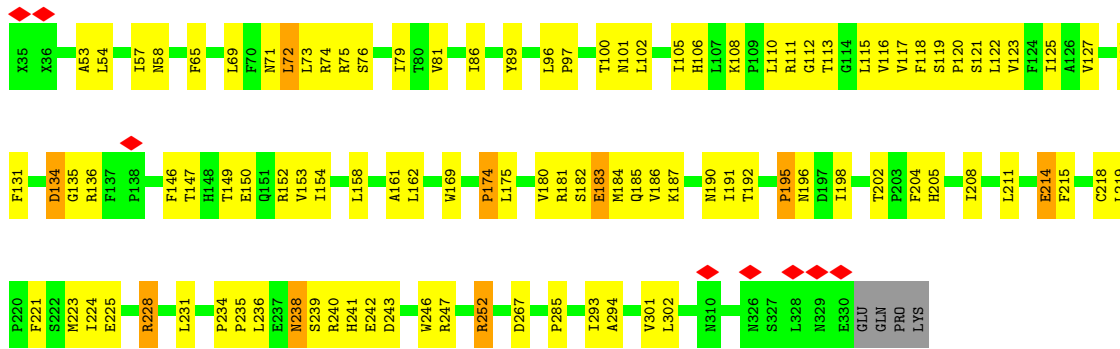




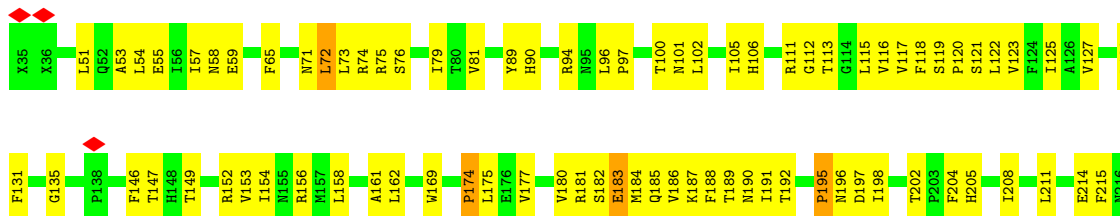
• Molecule 3: FliM,Flagellar motor switch protein FliM



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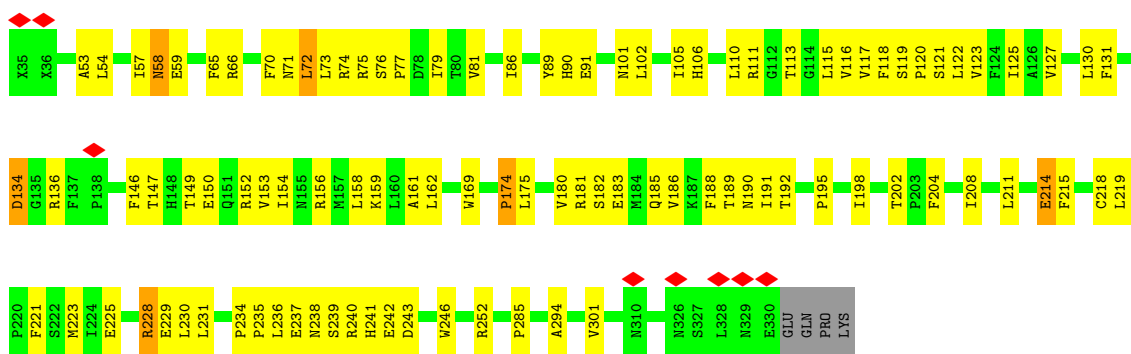


• Molecule 3: FliM,Flagellar motor switch protein FliM

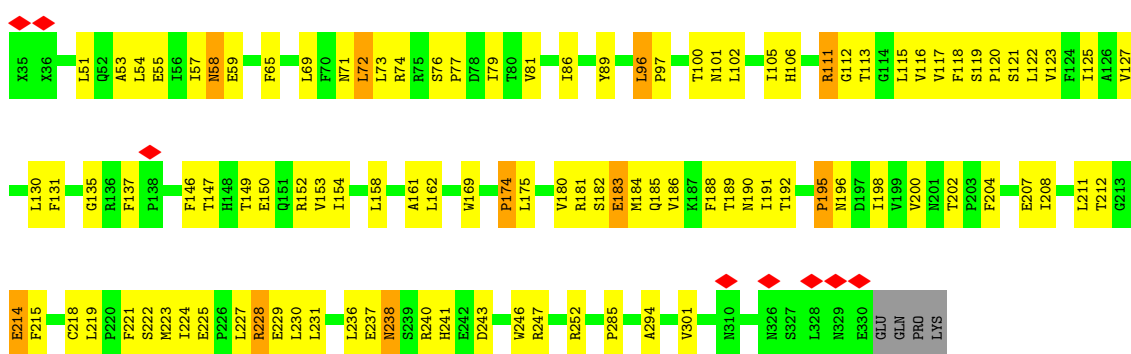




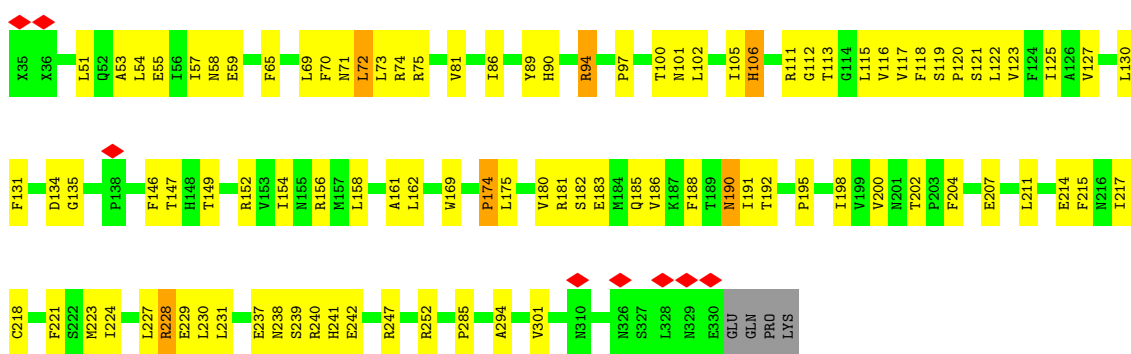
• Molecule 3: FliM,Flagellar motor switch protein FliM



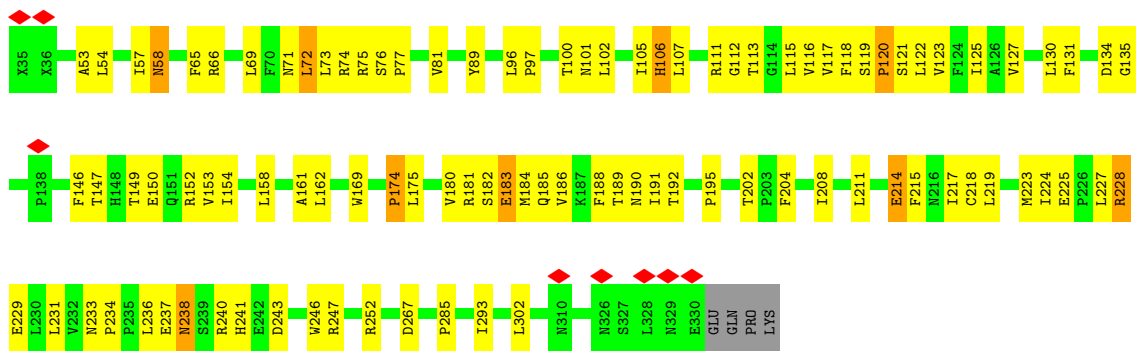
• Molecule 3: FliM,Flagellar motor switch protein FliM



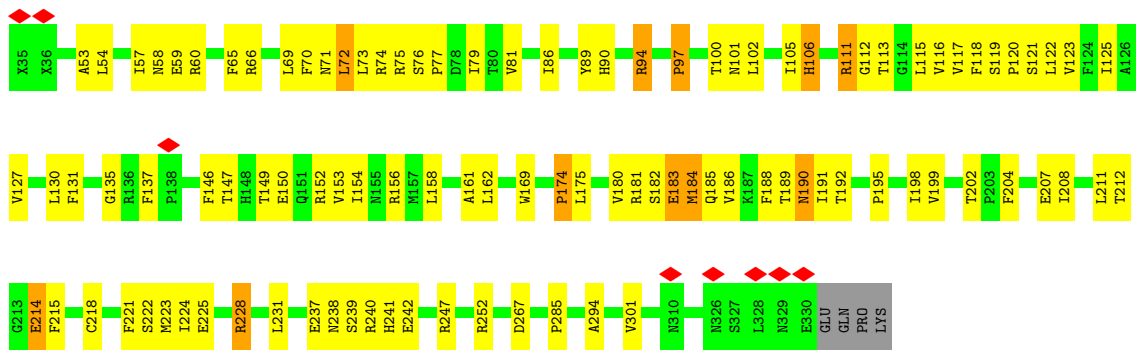
• Molecule 3: FliM,Flagellar motor switch protein FliM



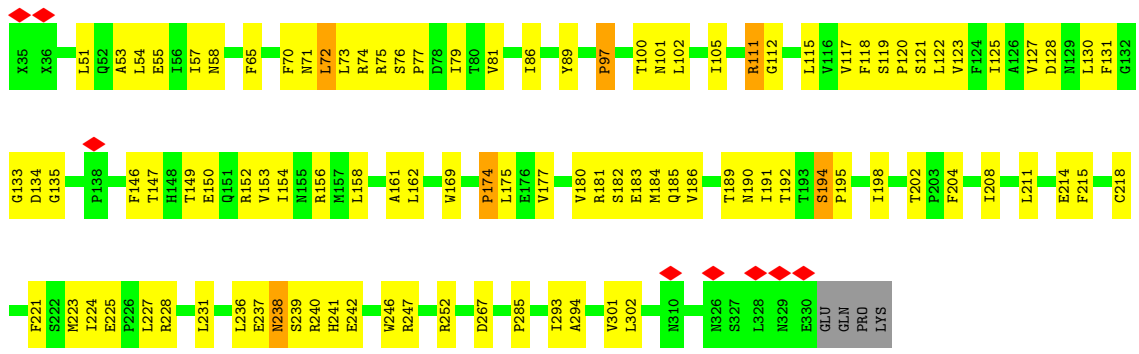
• Molecule 3: FliM,Flagellar motor switch protein FliM



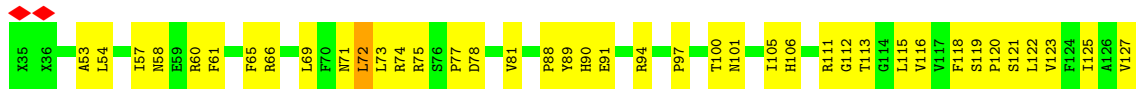
• Molecule 3: FliM,Flagellar motor switch protein FliM

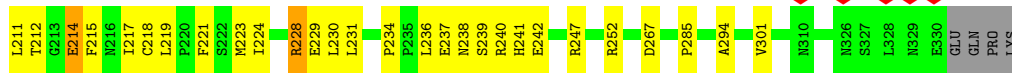


• Molecule 3: FliM,Flagellar motor switch protein FliM

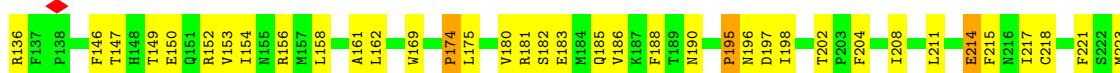
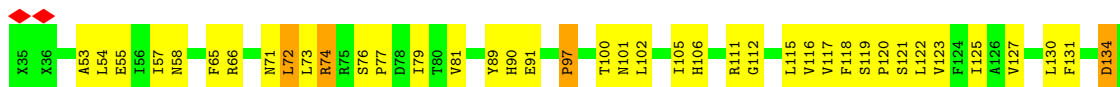


• Molecule 3: FliM,Flagellar motor switch protein FliM

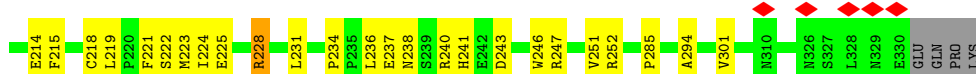
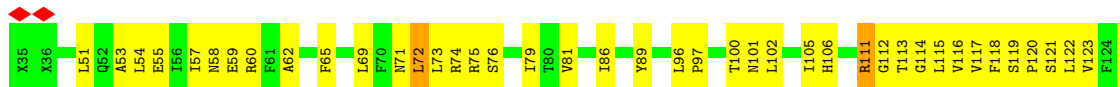




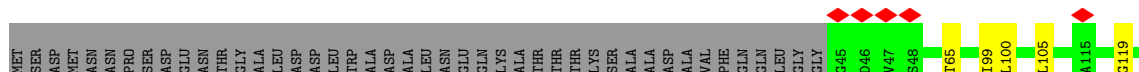
• Molecule 3: FliM,Flagellar motor switch protein FliM



• Molecule 3: FliM,Flagellar motor switch protein FliM

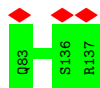
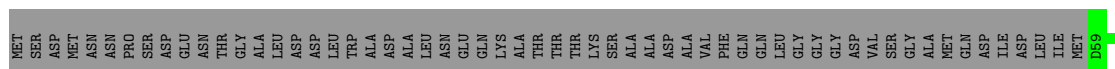


• Molecule 4: Flagellar motor switch protein FliN

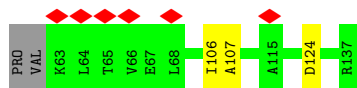
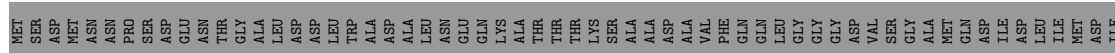


• Molecule 4: Flagellar motor switch protein FliN

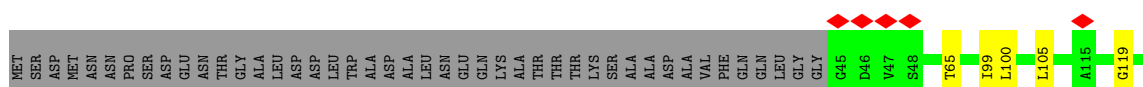




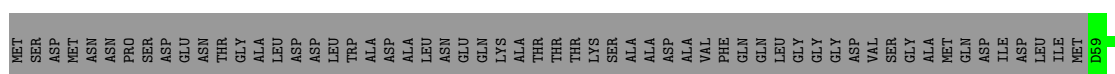
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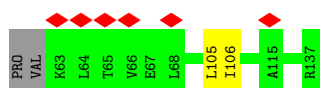
• Molecule 4: Flagellar motor switch protein FliN



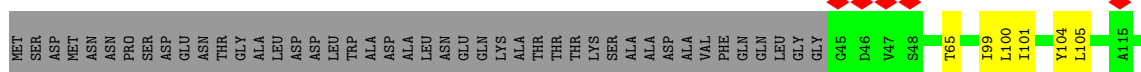
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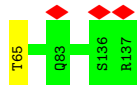
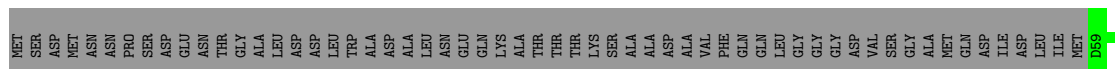
• Molecule 4: Flagellar motor switch protein FliN



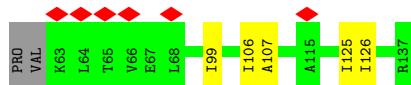
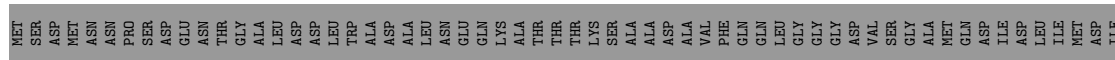
• Molecule 4: Flagellar motor switch protein FliN



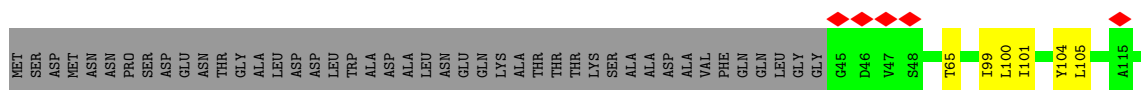
• Molecule 4: Flagellar motor switch protein FliN



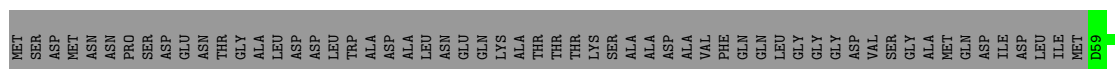
• Molecule 4: Flagellar motor switch protein FliN



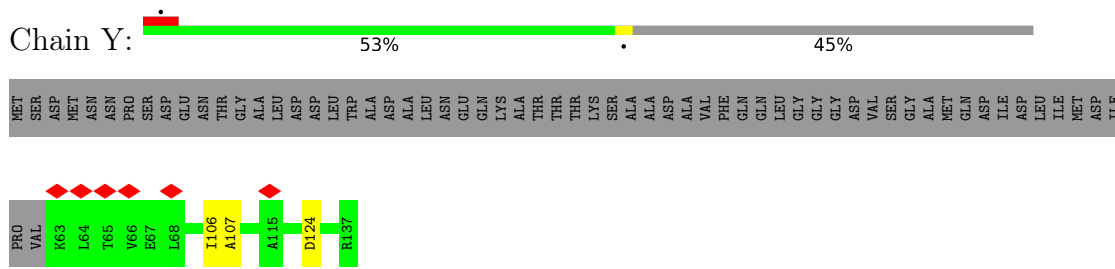
• Molecule 4: Flagellar motor switch protein FliN



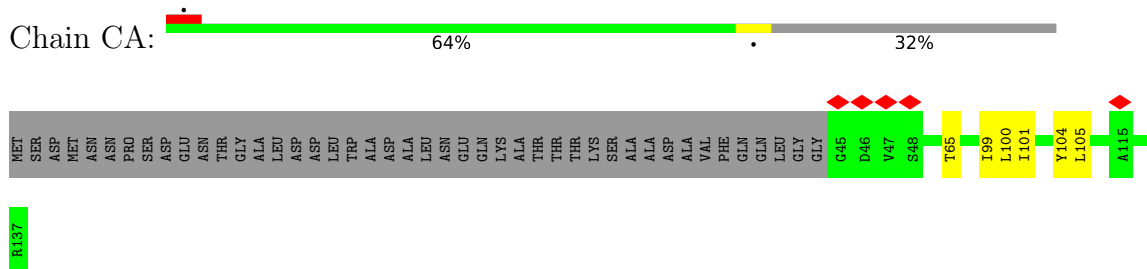
• Molecule 4: Flagellar motor switch protein FliN



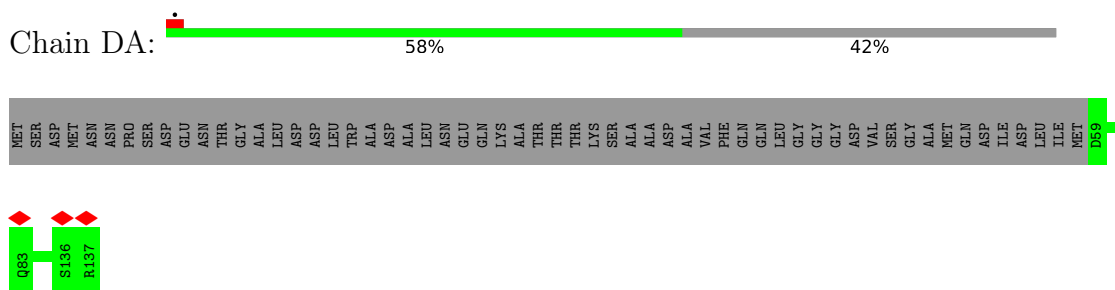
• Molecule 4: Flagellar motor switch protein FliN



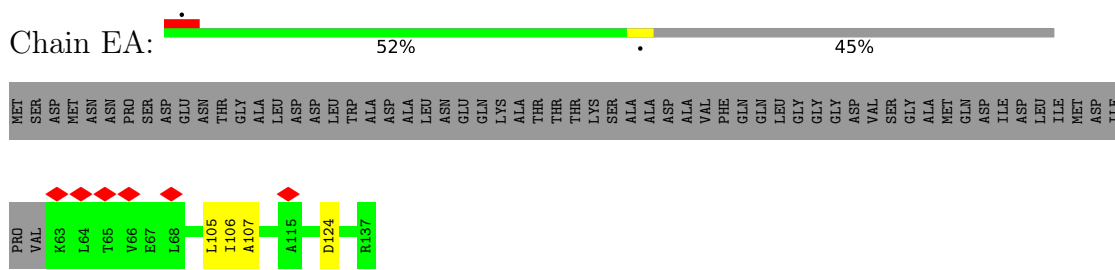
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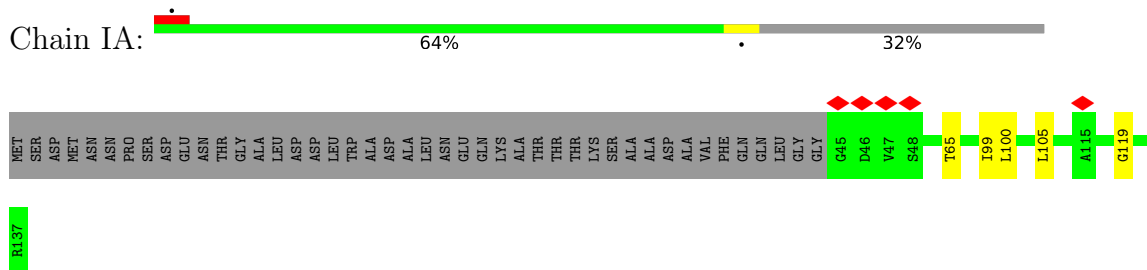
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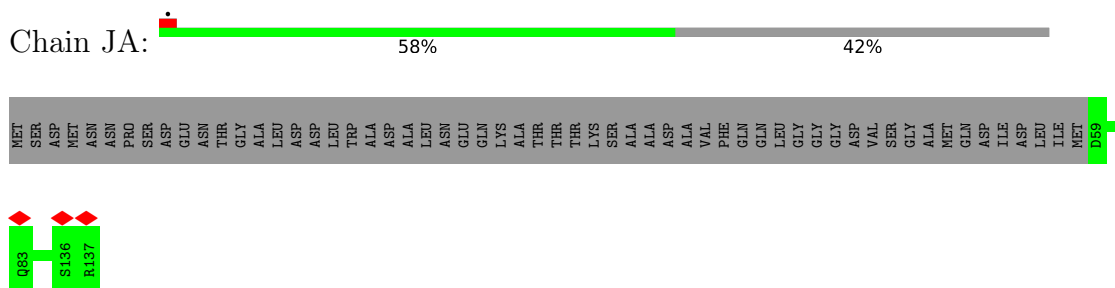
• Molecule 4: Flagellar motor switch protein FliN



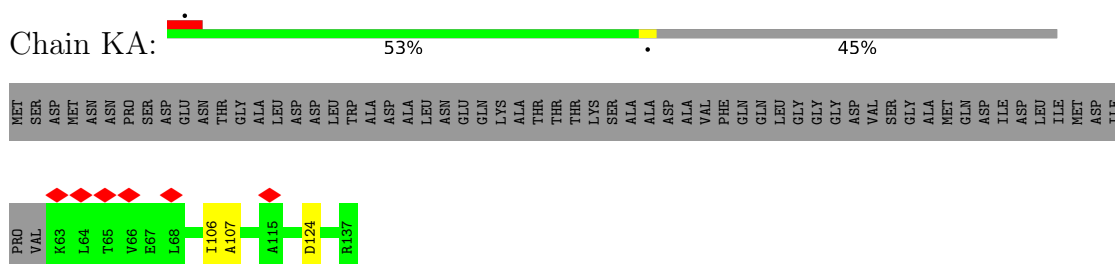
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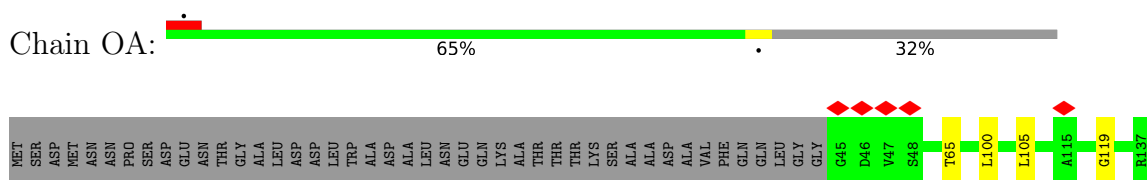
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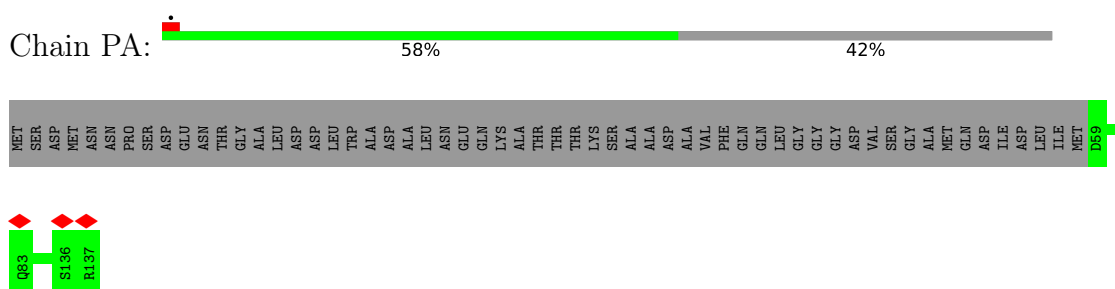
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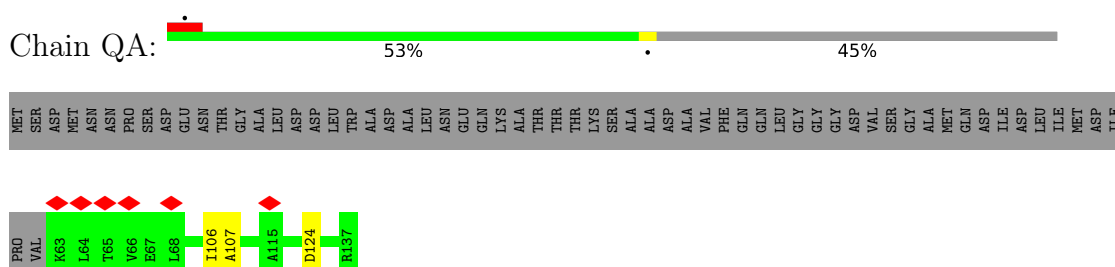
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



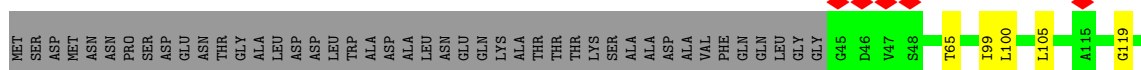
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• Molecule 4: Flagellar motor switch protein FliN



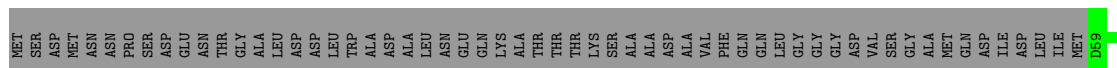
Chain UA:  64% 32%



 R137

- Molecule 4: Flagellar motor switch protein FliN

Chain VA:  58% 42%



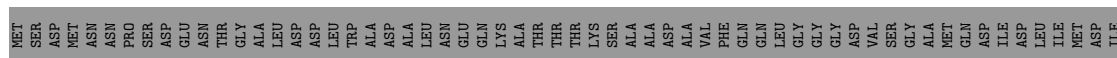
 Q83


 S136


 R137


- Molecule 4: Flagellar motor switch protein FliN


Chain WA:  53% 45%





 PRO


 K63


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 T65


 V66


 E67


 L68

 I106

 A107

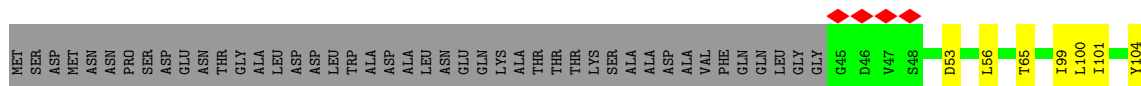
 A115


 D124

 R137

- Molecule 4: Flagellar motor switch protein FliN

Chain AB:  61% 7% 32%



 L105

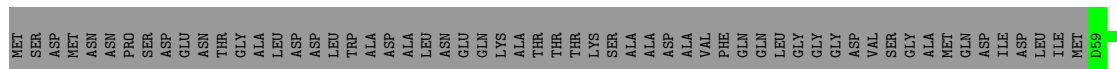
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 G119

 R137

- Molecule 4: Flagellar motor switch protein FliN

Chain BB:  58% 42%

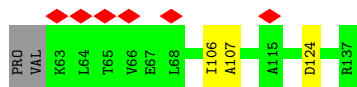
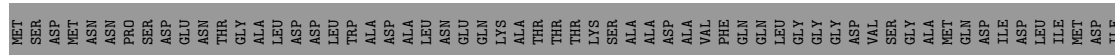


 Q83

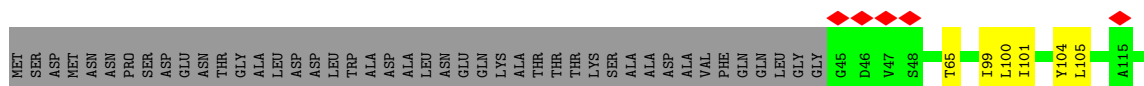
 S136

 R137

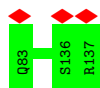
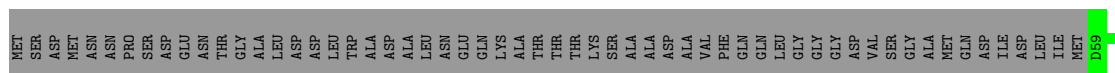
• Molecule 4: Flagellar motor switch protein FliN



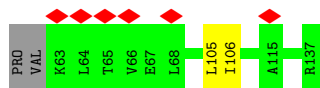
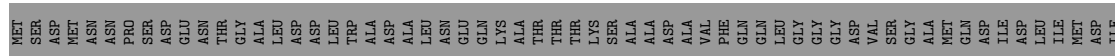
• Molecule 4: Flagellar motor switch protein FliN



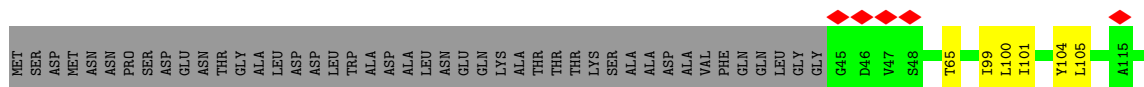
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

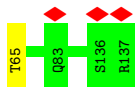
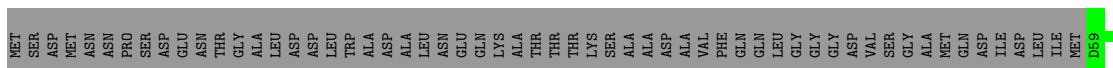


• Molecule 4: Flagellar motor switch protein FliN

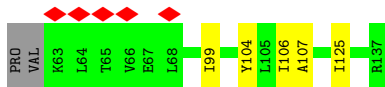
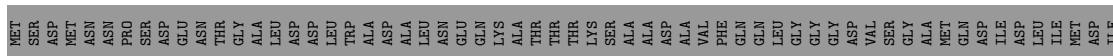




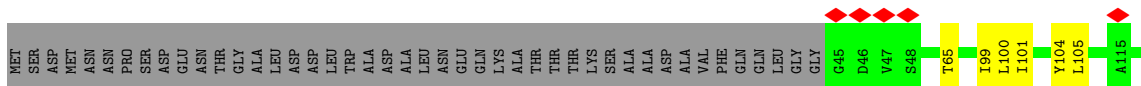
- Molecule 4: Flagellar motor switch protein FliN



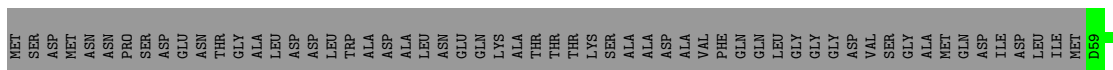
- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN

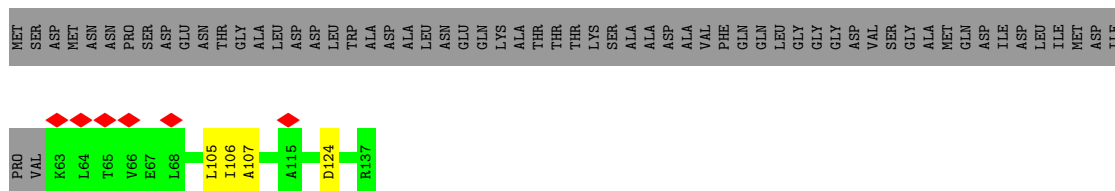


- Molecule 4: Flagellar motor switch protein FliN

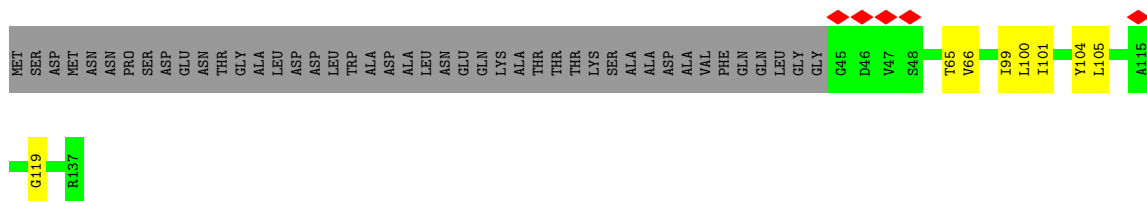


- Molecule 4: Flagellar motor switch protein FliN

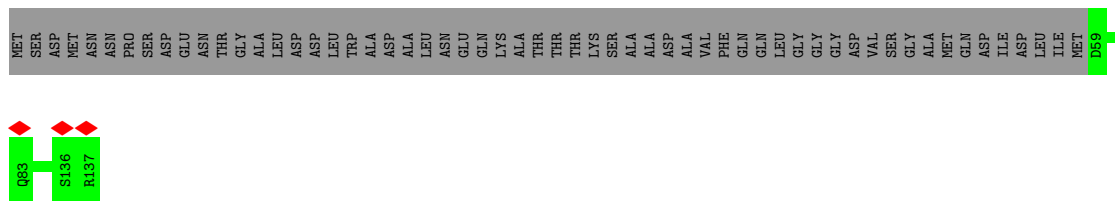




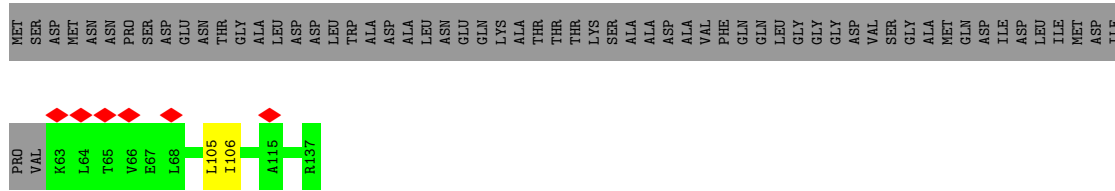
• Molecule 4: Flagellar motor switch protein FliN



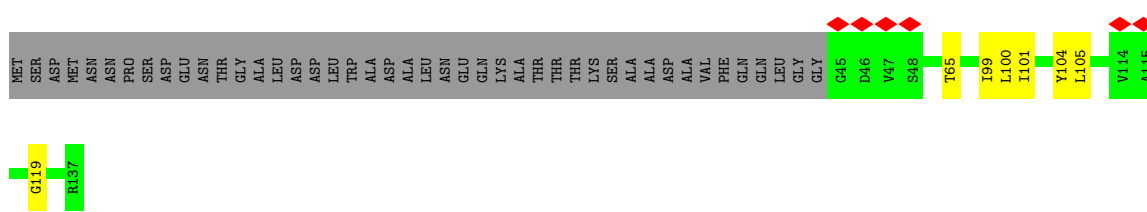
• Molecule 4: Flagellar motor switch protein FliN



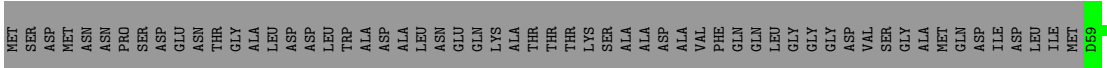
• Molecule 4: Flagellar motor switch protein FliN



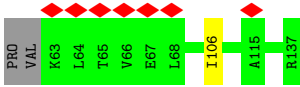
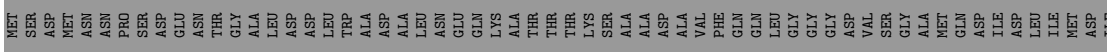
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



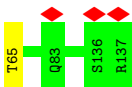
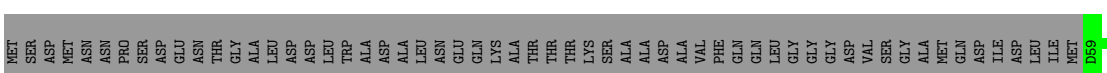
- Molecule 4: Flagellar motor switch protein FliN



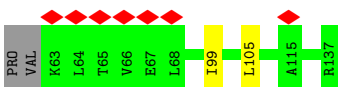
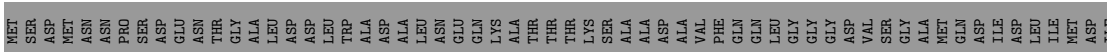
- Molecule 4: Flagellar motor switch protein FliN



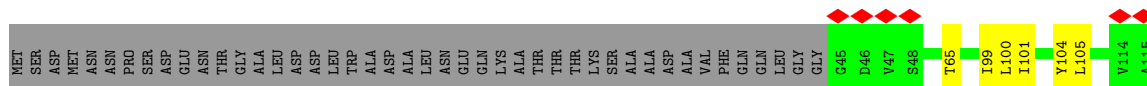
- Molecule 4: Flagellar motor switch protein FliN



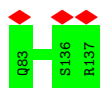
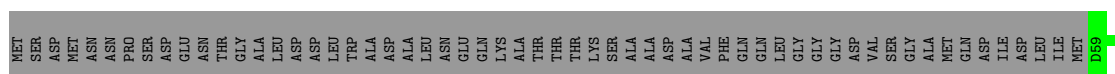
- Molecule 4: Flagellar motor switch protein FliN



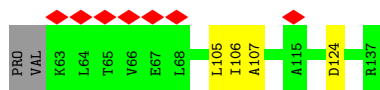
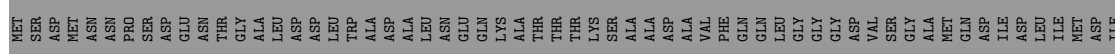
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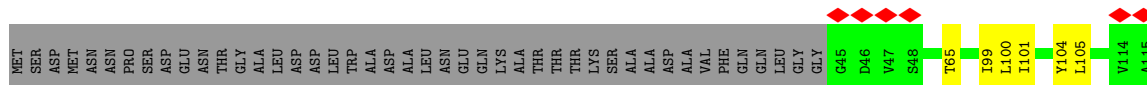
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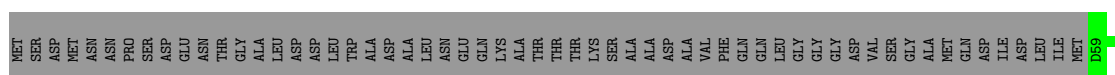
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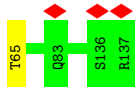


• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

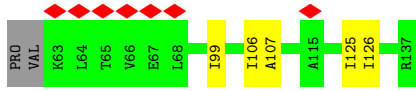




• Molecule 4: Flagellar motor switch protein FliN



MET	SER	ASP	ASP	ASN	ASN	PRO	SER	ASP	GLU	THR	THR	GLY	ALA	LEU	ASP	ASP	LEU	TRP	ALA	ASP	LEU	LEU	ALA	LEU	ASN	GLU	GLN	LYS	THR	THR	THR	THR	LYS	SER	SER	ALA	ALA	ALA	ASP	ASP	ALA	VAL	PHE	GLN	GLN	LEU	GLY	GLY	GLY	ASP	VAL	SER	SER	GLY	GLY	ALA	ALA	MET	GLN	ASP	ASP	ILE	ILE	ASP	LEU	ILE	MET	ASP	ASP	ILE
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• Molecule 4: Flagellar motor switch protein FliN



MET	SER	ASP	MET	ASN	ASN	PRO	SER	SER	ASP	GLU	ASN	ASN	THR	GLY	ALA	LEU	ASP	ASP	LEU	TRP	ALA	ASP	LEU	LEU	ASN	GLU	GLN	LYS	THR	THR	THR	THR	LYS	SER	SER	ALA	ALA	ALA	ASP	ASP	ALA	VAL	PHE	GLN	GLN	LEU	LEU	GLY	GLY	G45	D46	V47	S48	T65	I99	L100	L105	L106	V114	A115	G119
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• Molecule 4: Flagellar motor switch protein FliN



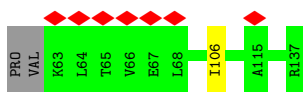
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• Molecule 4: Flagellar motor switch protein FliN

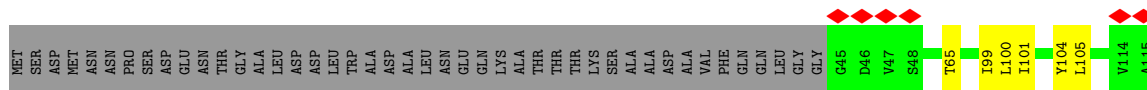


MET	SER	ASP	ASP	ASN	ASN	PRO	SER	SER	ASP	GLU	ASN	ASN	THR	GLY	ALA	LEU	ASP	ASP	LEU	TRP	ALA	ASP	LEU	LEU	ASN	GLU	GLN	LYS	THR	THR	THR	THR	LYS	SER	SER	ALA	ALA	ALA	ASP	ASP	ALA	VAL	PHE	GLN	GLN	LEU	LEU	GLY	GLY	GLY	ASP	VAL	SER	SER	GLY	GLY	ALA	ALA	MET	GLN	ASP	ASP	ILE	ILE	ASP	LEU	ILE	MET	ASP	ASP	ILE
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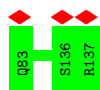
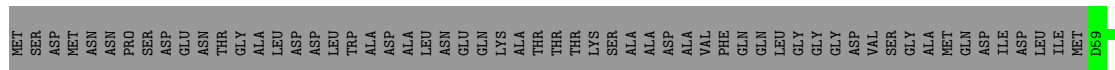


• Molecule 4: Flagellar motor switch protein FliN

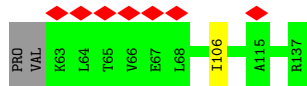
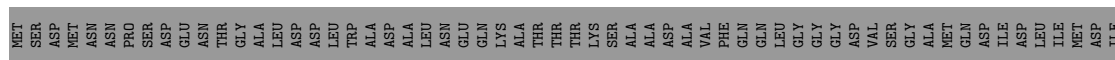




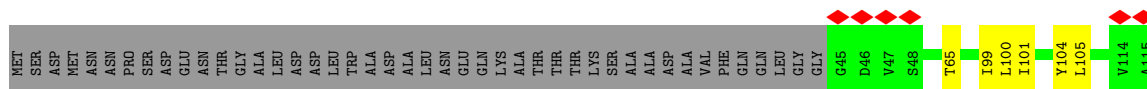
- Molecule 4: Flagellar motor switch protein FliN



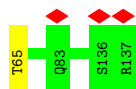
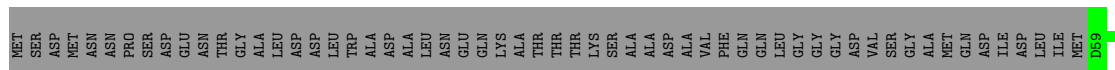
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- Molecule 4: Flagellar motor switch protein FliN

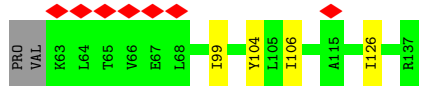


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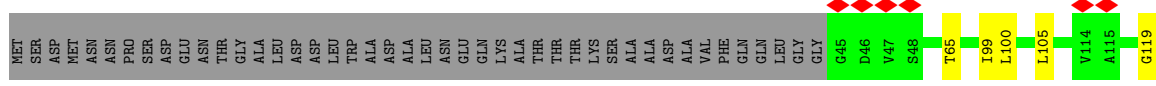


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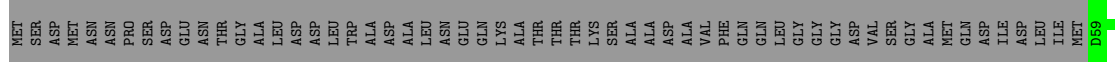




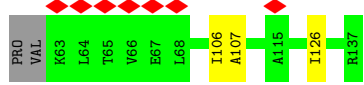
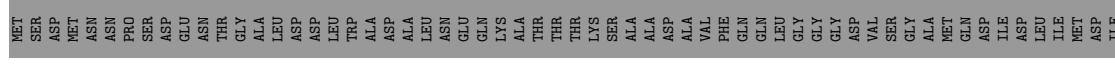
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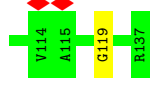
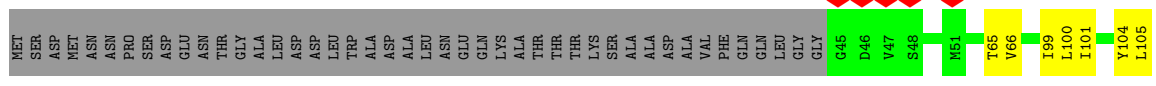
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• Molecule 4: Flagellar motor switch protein FliN



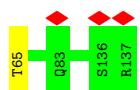
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● Molecule 4: Flagellar motor switch protein FliN



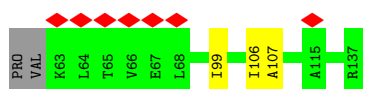
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● Molecule 4: Flagellar motor switch protein FliN



MET	SER	ASP	MET	ASN	ASN	PRO	SER	ASP	ASP	GLU	THR	GLY	ALA	LEU	LEU	LEU	ASP	ASP	TRP	ALA	ASP	LEU	LEU	GLU	GLN	LYS	ALA	ALA	ALA	ASP	ASP	VAL	VAL	PHE	GLN	GLN	LEU	LEU	GLY	GLY	GLY	ASP	VAL	SER	GLY	ALA	MET	GLN	ASP	ILE	ASP	LEU	ILE	MET	ASP	ILE
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● Molecule 4: Flagellar motor switch protein FliN



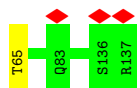
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● Molecule 4: Flagellar motor switch protein FliN



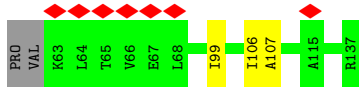
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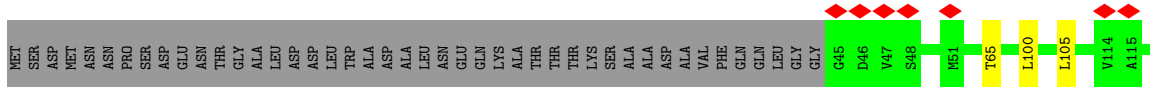
● Molecule 4: Flagellar motor switch protein FliN



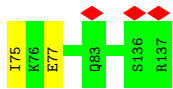
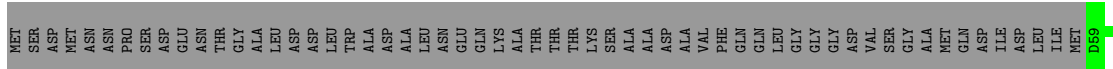
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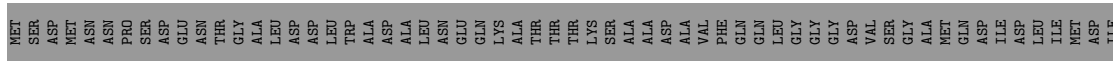
• Molecule 4: Flagellar motor switch protein FliN



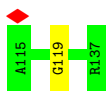
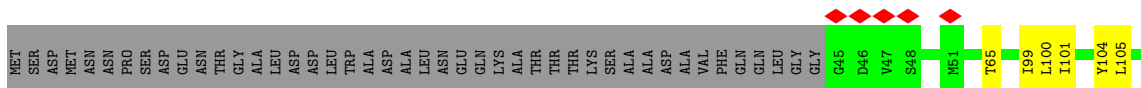
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

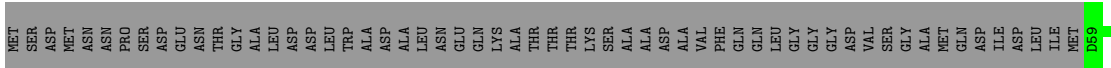


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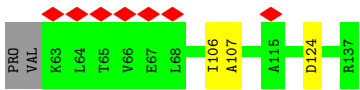


• Molecule 4: Flagellar motor switch protein FliN

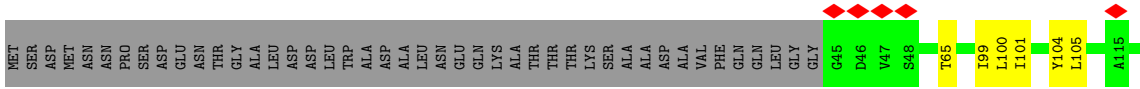




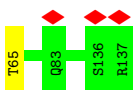
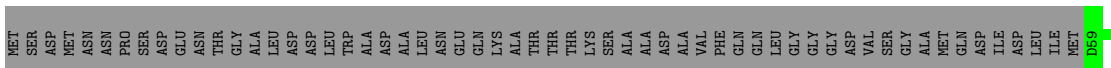
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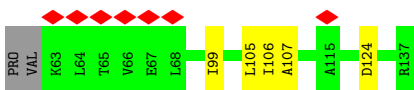
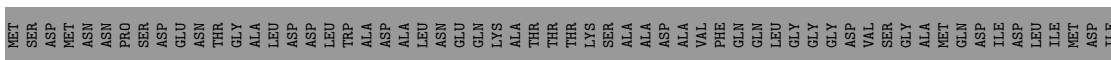
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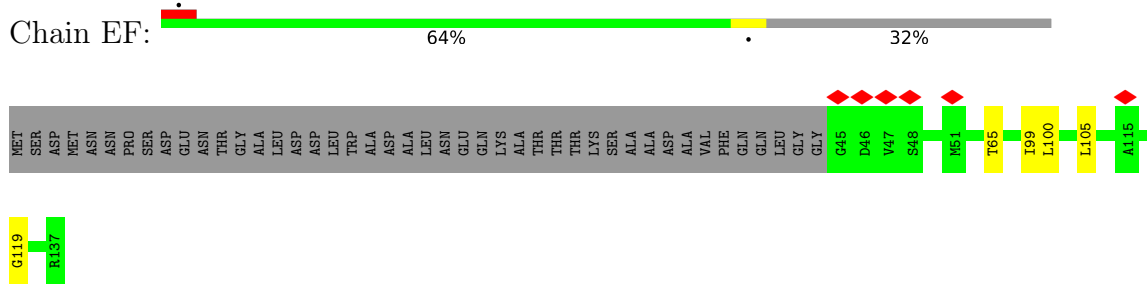
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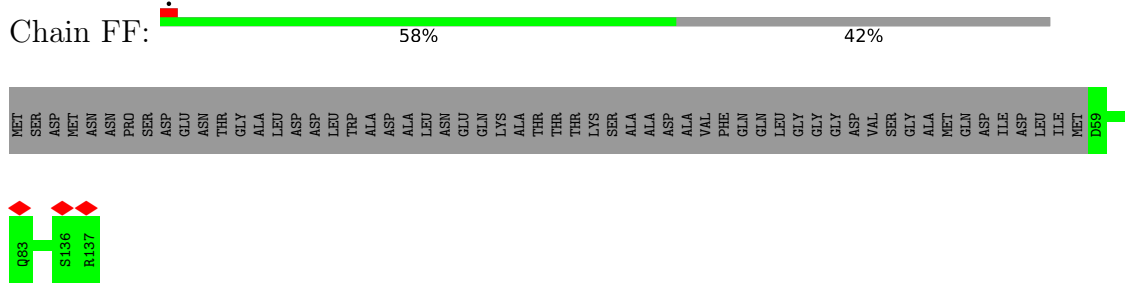
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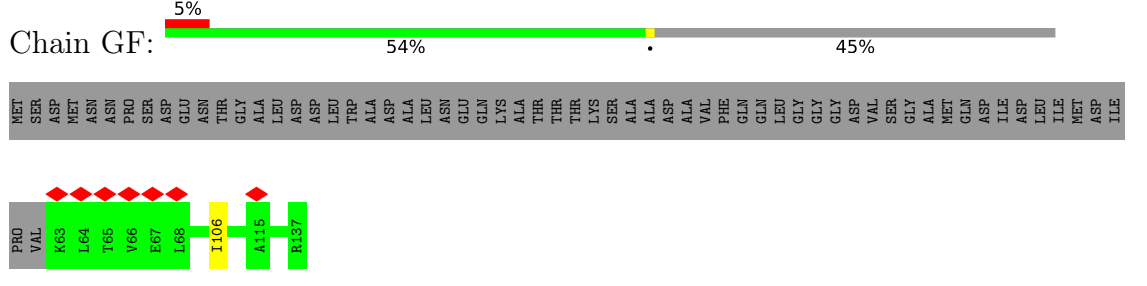
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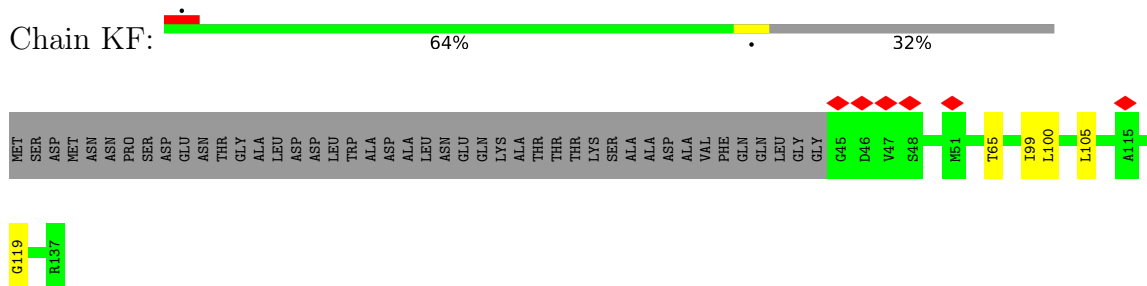
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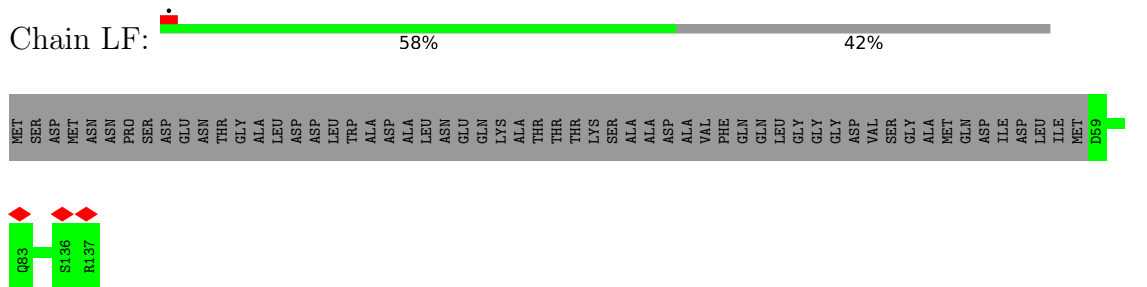
• Molecule 4: Flagellar motor switch protein FliN



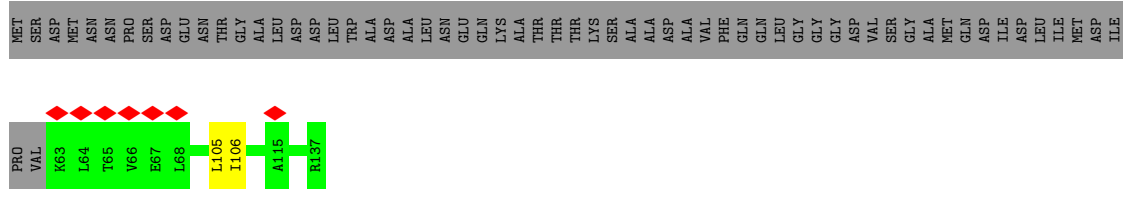
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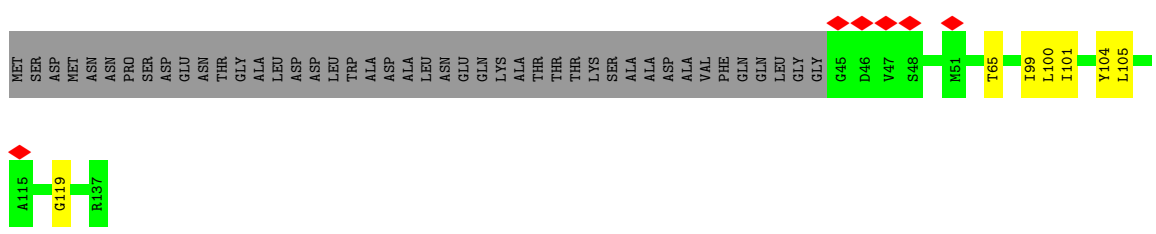
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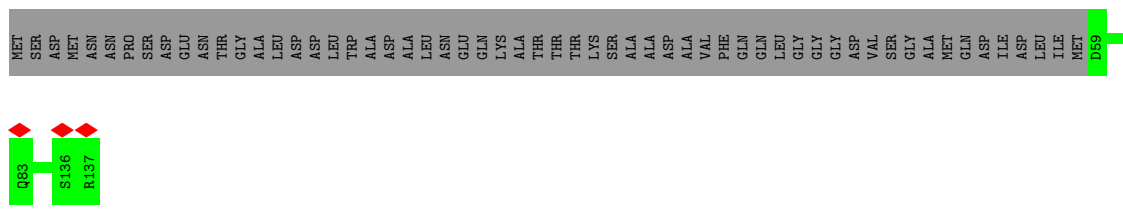
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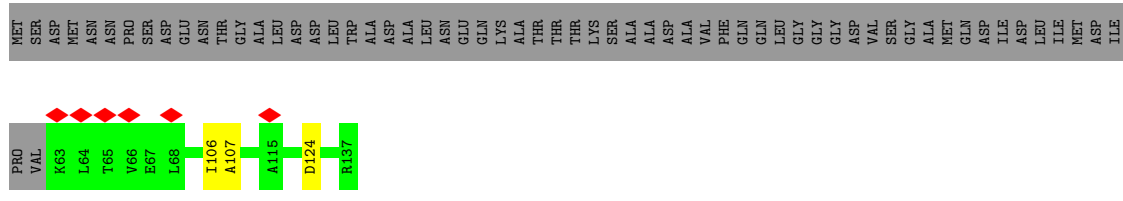
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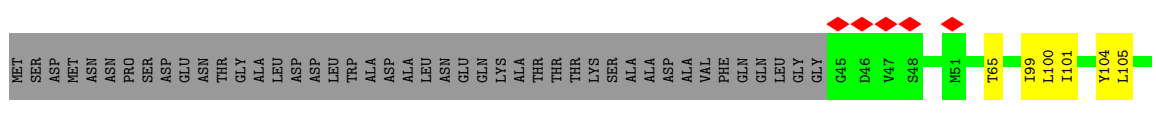
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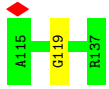


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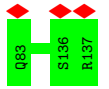
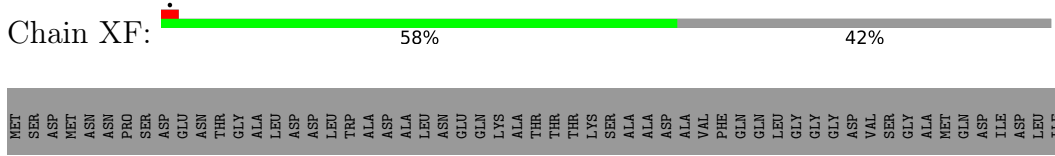


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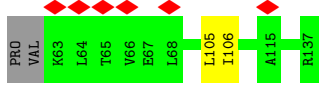
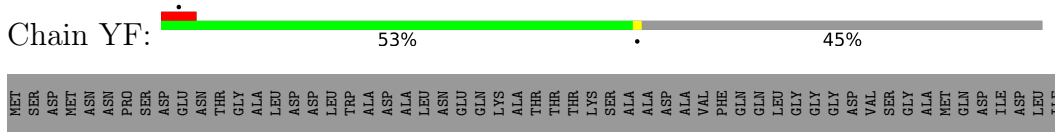




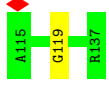
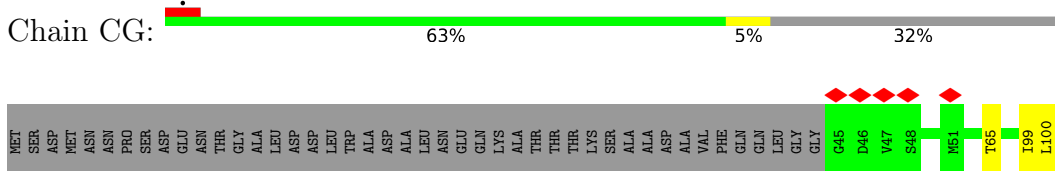
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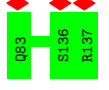
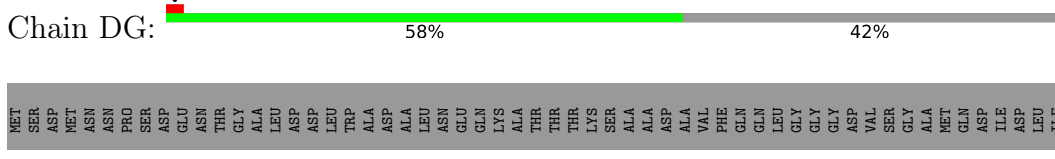
• Molecule 4: Flagellar motor switch protein FliN



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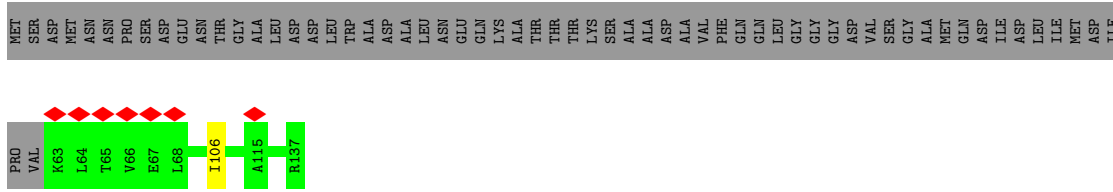


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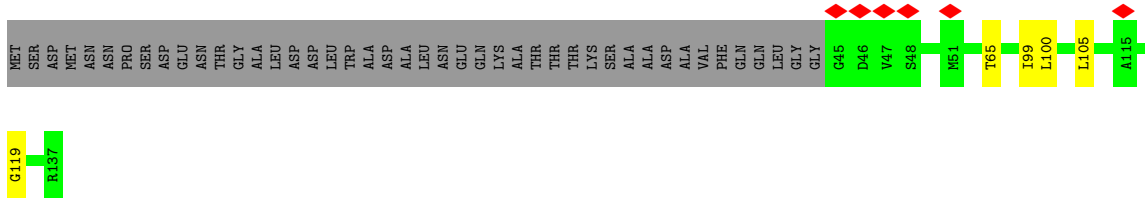


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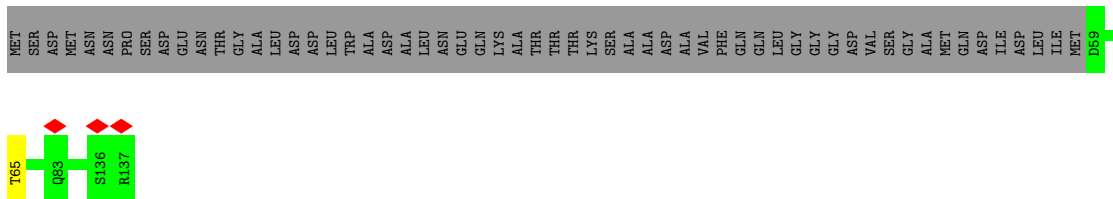




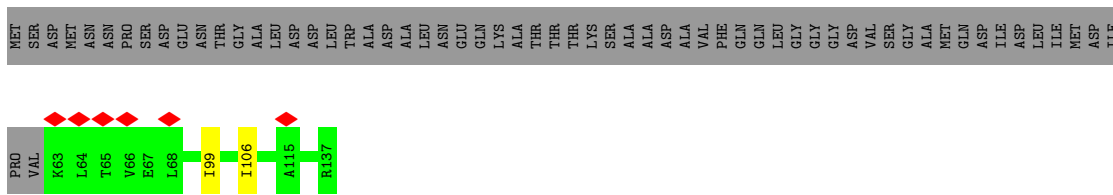
- Molecule 4: Flagellar motor switch protein FliN



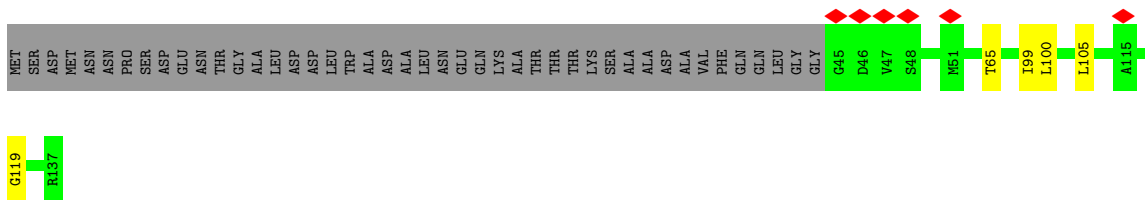
- Molecule 4: Flagellar motor switch protein FliN



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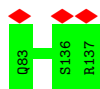
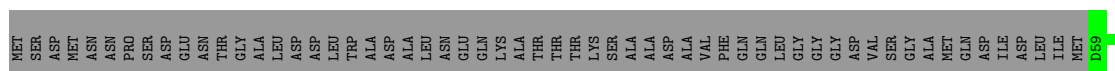


- Molecule 4: Flagellar motor switch protein FliN

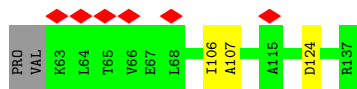


- Molecule 4: Flagellar motor switch protein FliN

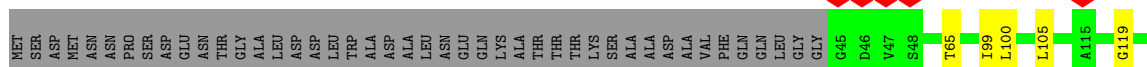




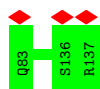
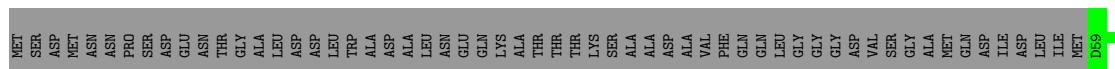
• Molecule 4: Flagellar motor switch protein FliN



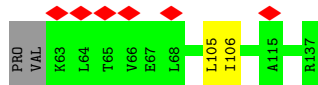
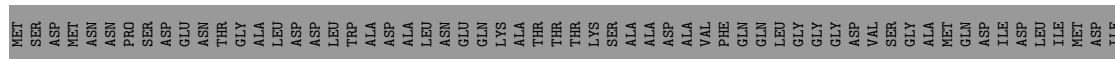
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	51268	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 ( $e^-/\text{\AA}^2$ )	51.557	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	0.483	Depositor
Minimum map value	-0.133	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.147	Depositor
Map size ( $\text{\AA}$ )	1046.784, 1046.784, 1046.784	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.363, 1.363, 1.363	Depositor

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.22	0/233	0.35	0/324
1	BC	0.22	0/233	0.34	0/324
1	BF	0.22	0/233	0.34	0/324
1	DB	0.22	0/233	0.34	0/324
1	DE	0.22	0/233	0.34	0/324
1	F	0.22	0/233	0.34	0/324
1	FA	0.22	0/233	0.35	0/324
1	FD	0.22	0/233	0.34	0/324
1	FG	0.22	0/233	0.34	0/324
1	HC	0.22	0/233	0.34	0/324
1	HF	0.22	0/233	0.35	0/324
1	I	0.22	0/233	0.35	0/324
1	JB	0.22	0/233	0.34	0/324
1	JE	0.22	0/233	0.35	0/324
1	LA	0.22	0/233	0.35	0/324
1	LD	0.22	0/233	0.35	0/324
1	LG	0.22	0/233	0.35	0/324
1	NC	0.22	0/233	0.35	0/324
1	NF	0.22	0/233	0.35	0/324
1	PB	0.22	0/233	0.34	0/324
1	PE	0.22	0/233	0.34	0/324
1	RA	0.22	0/233	0.34	0/324
1	RD	0.22	0/233	0.35	0/324
1	RG	0.22	0/233	0.34	0/324
1	S	0.22	0/233	0.35	0/324
1	TC	0.22	0/233	0.34	0/324
1	TF	0.22	0/233	0.34	0/324
1	VB	0.22	0/233	0.34	0/324
1	VE	0.22	0/233	0.34	0/324
1	XA	0.22	0/233	0.35	0/324
1	XD	0.22	0/233	0.36	0/324
1	Z	0.22	0/233	0.34	0/324
1	ZC	0.22	0/233	0.34	0/324
1	ZF	0.22	0/233	0.34	0/324

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	AA	0.30	0/2516	0.65	3/3393 (0.1%)
2	AD	0.29	0/2516	0.64	2/3393 (0.1%)
2	AG	0.30	0/2516	0.65	3/3393 (0.1%)
2	B	0.30	0/2516	0.64	3/3393 (0.1%)
2	CC	0.31	0/2516	0.66	3/3393 (0.1%)
2	CF	0.30	0/2516	0.66	6/3393 (0.2%)
2	EB	0.30	0/2516	0.66	2/3393 (0.1%)
2	EE	0.29	0/2516	0.64	2/3393 (0.1%)
2	G	0.30	0/2516	0.65	2/3393 (0.1%)
2	GA	0.29	0/2516	0.62	1/3393 (0.0%)
2	GD	0.29	0/2516	0.62	1/3393 (0.0%)
2	GG	0.29	0/2516	0.64	1/3393 (0.0%)
2	IC	0.29	0/2516	0.65	2/3393 (0.1%)
2	IF	0.30	0/2516	0.65	2/3393 (0.1%)
2	J	0.29	0/2516	0.63	2/3393 (0.1%)
2	KB	0.30	0/2516	0.66	3/3393 (0.1%)
2	KE	0.29	0/2516	0.64	2/3393 (0.1%)
2	MA	0.29	0/2516	0.64	2/3393 (0.1%)
2	MD	0.29	0/2516	0.64	2/3393 (0.1%)
2	MG	0.28	0/2516	0.63	2/3393 (0.1%)
2	OC	0.28	0/2516	0.63	2/3393 (0.1%)
2	OF	0.30	0/2516	0.65	2/3393 (0.1%)
2	QB	0.30	0/2516	0.63	0/3393
2	QE	0.29	0/2516	0.62	1/3393 (0.0%)
2	SA	0.30	0/2516	0.63	2/3393 (0.1%)
2	SD	0.29	0/2516	0.63	4/3393 (0.1%)
2	SG	0.28	0/2516	0.65	1/3393 (0.0%)
2	T	0.30	0/2516	0.65	3/3393 (0.1%)
2	UC	0.30	0/2516	0.66	3/3393 (0.1%)
2	UF	0.28	0/2516	0.60	0/3393
2	WB	0.30	0/2516	0.63	3/3393 (0.1%)
2	WE	0.29	0/2516	0.63	4/3393 (0.1%)
2	YA	0.30	0/2516	0.63	2/3393 (0.1%)
2	YD	0.31	0/2516	0.63	2/3393 (0.1%)
3	BA	0.42	0/2043	0.73	4/2790 (0.1%)
3	BD	0.47	2/2043 (0.1%)	0.73	4/2790 (0.1%)
3	BG	0.52	3/2043 (0.1%)	0.81	7/2790 (0.3%)
3	C	0.44	2/2043 (0.1%)	0.75	4/2790 (0.1%)
3	DC	0.53	3/2043 (0.1%)	0.82	7/2790 (0.3%)
3	DF	0.44	1/2043 (0.0%)	0.74	5/2790 (0.2%)
3	FB	0.44	1/2043 (0.0%)	0.74	5/2790 (0.2%)
3	FE	0.45	1/2043 (0.0%)	0.77	4/2790 (0.1%)
3	HA	0.46	2/2043 (0.1%)	0.76	4/2790 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	HD	0.45	1/2043 (0.0%)	0.75	4/2790 (0.1%)
3	HG	0.53	3/2043 (0.1%)	0.78	6/2790 (0.2%)
3	JC	0.52	4/2043 (0.2%)	0.79	6/2790 (0.2%)
3	JF	0.46	2/2043 (0.1%)	0.75	4/2790 (0.1%)
3	K	0.44	1/2043 (0.0%)	0.73	4/2790 (0.1%)
3	LB	0.46	2/2043 (0.1%)	0.75	4/2790 (0.1%)
3	LE	0.40	0/2043	0.72	3/2790 (0.1%)
3	M	0.47	2/2043 (0.1%)	0.76	5/2790 (0.2%)
3	NA	0.40	0/2043	0.72	3/2790 (0.1%)
3	ND	0.44	1/2043 (0.0%)	0.73	4/2790 (0.1%)
3	NG	0.46	2/2043 (0.1%)	0.77	5/2790 (0.2%)
3	PC	0.46	2/2043 (0.1%)	0.76	5/2790 (0.2%)
3	PF	0.47	2/2043 (0.1%)	0.77	6/2790 (0.2%)
3	RB	0.46	2/2043 (0.1%)	0.78	6/2790 (0.2%)
3	RE	0.43	1/2043 (0.0%)	0.72	3/2790 (0.1%)
3	TA	0.43	1/2043 (0.0%)	0.72	3/2790 (0.1%)
3	TD	0.38	0/2043	0.70	2/2790 (0.1%)
3	TG	0.45	1/2043 (0.0%)	0.74	5/2790 (0.2%)
3	V	0.39	0/2043	0.70	2/2790 (0.1%)
3	VC	0.44	1/2043 (0.0%)	0.74	4/2790 (0.1%)
3	VF	0.47	2/2043 (0.1%)	0.77	6/2790 (0.2%)
3	XB	0.48	2/2043 (0.1%)	0.77	6/2790 (0.2%)
3	XE	0.47	2/2043 (0.1%)	0.75	4/2790 (0.1%)
3	ZA	0.48	2/2043 (0.1%)	0.76	5/2790 (0.2%)
3	ZD	0.42	0/2043	0.73	4/2790 (0.1%)
4	AB	0.25	0/455	0.47	0/630
4	AC	0.27	0/368	0.47	0/508
4	AE	0.25	0/455	0.47	0/630
4	AF	0.26	0/368	0.47	0/508
4	BB	0.27	0/388	0.49	0/536
4	BE	0.26	0/388	0.49	0/536
4	CA	0.25	0/455	0.47	0/630
4	CB	0.26	0/368	0.47	0/508
4	CD	0.25	0/455	0.47	0/630
4	CE	0.26	0/368	0.46	0/508
4	CG	0.25	0/455	0.47	0/630
4	D	0.25	0/455	0.47	0/630
4	DA	0.26	0/388	0.49	0/536
4	DD	0.26	0/388	0.50	0/536
4	DG	0.26	0/388	0.50	0/536
4	E	0.26	0/388	0.50	0/536
4	EA	0.27	0/368	0.47	0/508
4	EC	0.25	0/455	0.47	0/630

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	ED	0.27	0/368	0.47	0/508
4	EF	0.25	0/455	0.47	0/630
4	EG	0.27	0/368	0.47	0/508
4	FC	0.27	0/388	0.51	0/536
4	FF	0.27	0/388	0.49	0/536
4	GB	0.25	0/455	0.47	0/630
4	GC	0.27	0/368	0.47	0/508
4	GE	0.25	0/455	0.47	0/630
4	GF	0.27	0/368	0.47	0/508
4	H	0.27	0/368	0.47	0/508
4	HB	0.26	0/388	0.49	0/536
4	HE	0.27	0/388	0.50	0/536
4	IA	0.25	0/455	0.47	0/630
4	IB	0.27	0/368	0.48	0/508
4	ID	0.25	0/455	0.47	0/630
4	IE	0.26	0/368	0.45	0/508
4	IG	0.25	0/455	0.47	0/630
4	JA	0.26	0/388	0.49	0/536
4	JD	0.26	0/388	0.49	0/536
4	JG	0.26	0/388	0.49	0/536
4	KA	0.26	0/368	0.46	0/508
4	KC	0.25	0/455	0.47	0/630
4	KD	0.27	0/368	0.47	0/508
4	KF	0.25	0/455	0.47	0/630
4	KG	0.27	0/368	0.47	0/508
4	L	0.25	0/455	0.47	0/630
4	LC	0.26	0/388	0.49	0/536
4	LF	0.26	0/388	0.50	0/536
4	MB	0.25	0/455	0.47	0/630
4	MC	0.27	0/368	0.46	0/508
4	ME	0.25	0/455	0.47	0/630
4	MF	0.26	0/368	0.47	0/508
4	N	0.25	0/455	0.47	0/630
4	NB	0.26	0/388	0.49	0/536
4	NE	0.26	0/388	0.49	0/536
4	O	0.26	0/388	0.49	0/536
4	OA	0.25	0/455	0.47	0/630
4	OB	0.26	0/368	0.45	0/508
4	OD	0.25	0/455	0.47	0/630
4	OE	0.27	0/368	0.47	0/508
4	OG	0.25	0/455	0.47	0/630
4	P	0.26	0/388	0.51	0/536
4	PA	0.27	0/388	0.50	0/536

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	PD	0.26	0/388	0.49	0/536
4	PG	0.27	0/388	0.50	0/536
4	Q	0.27	0/368	0.47	0/508
4	QA	0.27	0/368	0.47	0/508
4	QC	0.25	0/455	0.47	0/630
4	QD	0.26	0/368	0.46	0/508
4	QF	0.25	0/455	0.47	0/630
4	QG	0.27	0/368	0.47	0/508
4	R	0.26	0/368	0.46	0/508
4	RC	0.27	0/388	0.50	0/536
4	RF	0.26	0/388	0.49	0/536
4	SB	0.25	0/455	0.47	0/630
4	SC	0.27	0/368	0.47	0/508
4	SE	0.25	0/455	0.47	0/630
4	SF	0.27	0/368	0.47	0/508
4	TB	0.27	0/388	0.49	0/536
4	TE	0.26	0/388	0.50	0/536
4	UA	0.25	0/455	0.47	0/630
4	UB	0.27	0/368	0.47	0/508
4	UD	0.25	0/455	0.47	0/630
4	UE	0.27	0/368	0.47	0/508
4	UG	0.25	0/455	0.47	0/630
4	VA	0.27	0/388	0.50	0/536
4	VD	0.26	0/388	0.49	0/536
4	VG	0.26	0/388	0.50	0/536
4	W	0.25	0/455	0.47	0/630
4	WA	0.27	0/368	0.47	0/508
4	WC	0.25	0/455	0.47	0/630
4	WD	0.26	0/368	0.46	0/508
4	WF	0.25	0/455	0.47	0/630
4	WG	0.27	0/368	0.47	0/508
4	X	0.27	0/388	0.49	0/536
4	XC	0.27	0/388	0.51	0/536
4	XF	0.26	0/388	0.49	0/536
4	Y	0.27	0/368	0.47	0/508
4	YB	0.25	0/455	0.47	0/630
4	YC	0.26	0/368	0.46	0/508
4	YE	0.25	0/455	0.47	0/630
4	YF	0.27	0/368	0.47	0/508
4	ZB	0.26	0/388	0.49	0/536
4	ZE	0.27	0/388	0.49	0/536
All	All	0.35	51/204102 (0.0%)	0.64	228/278154 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AA	0	1
2	AD	0	1
2	AG	0	1
2	B	0	1
2	CC	0	1
2	CF	0	1
2	EB	0	1
2	EE	0	1
2	G	0	2
2	GA	0	1
2	GD	0	1
2	GG	0	1
2	IC	0	1
2	IF	0	1
2	J	0	1
2	KB	0	1
2	KE	0	1
2	MA	0	1
2	MD	0	1
2	MG	0	1
2	OC	0	1
2	OF	0	1
2	QB	0	1
2	QE	0	1
2	SA	0	2
2	SD	0	1
2	SG	0	1
2	T	0	2
2	UC	0	1
2	UF	0	1
2	WB	0	1
2	WE	0	1
2	YA	0	1
2	YD	0	1
All	All	0	37

The worst 5 of 51 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DC	174	PRO	CG-CD	-10.95	1.14	1.50
3	HG	195	PRO	CG-CD	-10.51	1.16	1.50
3	BD	174	PRO	CG-CD	-10.23	1.16	1.50
3	BG	174	PRO	CG-CD	-10.20	1.17	1.50
3	M	174	PRO	CG-CD	-9.84	1.18	1.50

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DC	174	PRO	N-CD-CG	-12.15	84.98	103.20
3	FE	195	PRO	CA-N-CD	-11.99	94.71	111.50
3	HA	195	PRO	CA-N-CD	-11.96	94.76	111.50
3	LB	195	PRO	CA-N-CD	-11.92	94.81	111.50
3	JC	195	PRO	CA-N-CD	-11.88	94.87	111.50

There are no chirality outliers.

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	90	ALA	Peptide
2	G	139	ARG	Sidechain
2	G	90	ALA	Peptide
2	J	90	ALA	Peptide
2	T	90	ALA	Peptide

## 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	0	0
1	BC	234	0	102	0	0
1	BF	234	0	102	0	0
1	DB	234	0	102	0	0
1	DE	234	0	102	0	0
1	F	234	0	102	0	0
1	FA	234	0	102	0	0
1	FD	234	0	102	0	0
1	FG	234	0	102	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	HC	234	0	102	1	0
1	HF	234	0	102	0	0
1	I	234	0	102	0	0
1	JB	234	0	102	0	0
1	JE	234	0	102	0	0
1	LA	234	0	102	0	0
1	LD	234	0	102	0	0
1	LG	234	0	102	1	0
1	NC	234	0	102	0	0
1	NF	234	0	102	1	0
1	PB	234	0	102	1	0
1	PE	234	0	102	1	0
1	RA	234	0	102	0	0
1	RD	234	0	102	2	0
1	RG	234	0	102	0	0
1	S	234	0	102	0	0
1	TC	234	0	102	0	0
1	TF	234	0	102	0	0
1	VB	234	0	102	0	0
1	VE	234	0	102	0	0
1	XA	234	0	102	1	0
1	XD	234	0	102	2	0
1	Z	234	0	102	1	0
1	ZC	234	0	102	0	0
1	ZF	234	0	102	0	0
2	AA	2496	0	2546	176	0
2	AD	2496	0	2546	169	0
2	AG	2496	0	2546	185	0
2	B	2496	0	2546	175	0
2	CC	2496	0	2546	186	0
2	CF	2496	0	2546	185	0
2	EB	2496	0	2546	177	0
2	EE	2496	0	2546	161	0
2	G	2496	0	2546	182	0
2	GA	2496	0	2546	164	0
2	GD	2496	0	2546	181	0
2	GG	2496	0	2546	168	0
2	IC	2496	0	2546	181	0
2	IF	2496	0	2546	194	0
2	J	2496	0	2546	175	0
2	KB	2496	0	2546	183	0
2	KE	2496	0	2546	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	MA	2496	0	2546	178	0
2	MD	2496	0	2546	180	0
2	MG	2496	0	2546	171	0
2	OC	2496	0	2546	166	0
2	OF	2496	0	2546	209	0
2	QB	2496	0	2546	189	0
2	QE	2496	0	2546	170	0
2	SA	2496	0	2546	181	0
2	SD	2496	0	2546	182	0
2	SG	2496	0	2546	190	0
2	T	2496	0	2546	195	0
2	UC	2496	0	2546	179	0
2	UF	2496	0	2546	188	0
2	WB	2496	0	2546	183	0
2	WE	2496	0	2546	179	0
2	YA	2496	0	2546	182	0
2	YD	2496	0	2546	175	0
3	BA	2086	0	1798	101	0
3	BD	2086	0	1797	99	0
3	BG	2086	0	1799	99	0
3	C	2086	0	1798	99	0
3	DC	2086	0	1799	102	0
3	DF	2086	0	1798	95	0
3	FB	2086	0	1798	93	0
3	FE	2086	0	1798	97	0
3	HA	2086	0	1798	86	0
3	HD	2086	0	1798	97	0
3	HG	2086	0	1798	96	0
3	JC	2086	0	1799	100	0
3	JF	2086	0	1798	81	0
3	K	2086	0	1798	96	0
3	LB	2086	0	1798	95	0
3	LE	2086	0	1798	95	0
3	M	2086	0	1798	95	0
3	NA	2086	0	1798	99	0
3	ND	2086	0	1798	87	0
3	NG	2086	0	1798	84	0
3	PC	2086	0	1798	95	0
3	PF	2086	0	1798	97	0
3	RB	2086	0	1798	102	0
3	RE	2086	0	1799	92	0
3	TA	2086	0	1799	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	TD	2086	0	1799	89	0
3	TG	2086	0	1799	104	0
3	V	2086	0	1799	93	0
3	VC	2086	0	1797	97	0
3	VF	2086	0	1798	96	0
3	XB	2086	0	1798	114	0
3	XE	2086	0	1799	93	0
3	ZA	2086	0	1799	96	0
3	ZD	2086	0	1798	96	0
4	AB	456	0	206	5	0
4	AC	369	0	166	2	0
4	AE	456	0	206	6	0
4	AF	369	0	166	4	0
4	BB	389	0	173	0	0
4	BE	389	0	173	1	0
4	CA	456	0	206	4	0
4	CB	369	0	166	2	0
4	CD	456	0	206	4	0
4	CE	369	0	166	6	0
4	CG	456	0	206	5	0
4	D	456	0	206	3	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	369	0	166	3	0
4	EC	456	0	206	5	0
4	ED	369	0	166	1	0
4	EF	456	0	206	3	0
4	EG	369	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	369	0	166	1	0
4	GE	456	0	206	3	0
4	GF	369	0	166	2	0
4	H	369	0	166	2	0
4	HB	389	0	173	0	0
4	HE	389	0	173	1	0
4	IA	456	0	206	4	0
4	IB	369	0	166	2	0
4	ID	456	0	206	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	IE	369	0	166	5	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	1	0
4	KA	369	0	166	2	0
4	KC	456	0	206	4	0
4	KD	369	0	166	1	0
4	KF	456	0	206	3	0
4	KG	369	0	166	2	0
4	L	456	0	206	4	0
4	LC	389	0	173	1	0
4	LF	389	0	173	0	0
4	MB	456	0	206	4	0
4	MC	369	0	166	2	0
4	ME	456	0	206	3	0
4	MF	369	0	166	2	0
4	N	456	0	206	4	0
4	NB	389	0	173	1	0
4	NE	389	0	173	1	0
4	O	389	0	173	1	0
4	OA	456	0	206	3	0
4	OB	369	0	166	8	0
4	OD	456	0	206	3	0
4	OE	369	0	166	3	0
4	OG	456	0	206	3	0
4	P	389	0	173	0	0
4	PA	389	0	173	0	0
4	PD	389	0	173	1	0
4	PG	389	0	173	0	0
4	Q	369	0	166	2	0
4	QA	369	0	166	2	0
4	QC	456	0	206	5	0
4	QD	369	0	166	6	0
4	QF	456	0	206	5	0
4	QG	369	0	166	2	0
4	R	369	0	166	8	0
4	RC	389	0	173	0	0
4	RF	389	0	173	0	0
4	SB	456	0	206	5	0
4	SC	369	0	166	3	0
4	SE	456	0	206	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	SF	369	0	166	2	0
4	TB	389	0	173	0	0
4	TE	389	0	173	0	0
4	UA	456	0	206	3	0
4	UB	369	0	166	3	0
4	UD	456	0	206	3	0
4	UE	369	0	166	2	0
4	UG	456	0	206	3	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	369	0	166	2	0
4	WC	456	0	206	4	0
4	WD	369	0	166	6	0
4	WF	456	0	206	5	0
4	WG	369	0	166	2	0
4	X	389	0	173	0	0
4	XC	389	0	173	1	0
4	XF	389	0	173	0	0
4	Y	369	0	166	2	0
4	YB	456	0	206	6	0
4	YC	369	0	166	8	0
4	YE	456	0	206	4	0
4	YF	369	0	166	2	0
4	ZB	389	0	173	0	0
4	ZE	389	0	173	1	0
All	All	205020	0	169702	8071	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 22.

The worst 5 of 8071 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:WB:83:LYS:HE3	2:CC:23:ALA:HA	1.33	1.10
2:YD:186:GLN:HE22	3:FE:71:ASN:HA	1.18	1.04
2:WB:89:ARG:HG2	2:WB:90:ALA:H	1.23	1.02
2:QB:80:VAL:HA	2:QB:83:LYS:HD3	1.39	1.01
2:IC:80:VAL:HA	2:IC:83:LYS:HD3	1.43	0.99

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	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	BC	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	BF	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	DB	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	DE	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	F	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	FA	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	FD	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	FG	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	HC	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	HF	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	I	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	JB	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	JE	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	LA	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	LD	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	LG	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	NC	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	NF	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	PB	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	PE	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	RA	45/47 (96%)	44 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	RD	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	RG	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	S	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	TC	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	TF	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	VB	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	VE	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	XA	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	XD	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	Z	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	ZC	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	ZF	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
2	AA	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	AD	318/331 (96%)	307 (96%)	11 (4%)	0	100	100
2	AG	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	B	318/331 (96%)	311 (98%)	7 (2%)	0	100	100
2	CC	318/331 (96%)	310 (98%)	8 (2%)	0	100	100
2	CF	318/331 (96%)	308 (97%)	10 (3%)	0	100	100
2	EB	318/331 (96%)	310 (98%)	8 (2%)	0	100	100
2	EE	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	G	318/331 (96%)	310 (98%)	8 (2%)	0	100	100
2	GA	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	GD	318/331 (96%)	310 (98%)	8 (2%)	0	100	100
2	GG	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	IC	318/331 (96%)	310 (98%)	8 (2%)	0	100	100
2	IF	318/331 (96%)	307 (96%)	11 (4%)	0	100	100
2	J	318/331 (96%)	308 (97%)	10 (3%)	0	100	100
2	KB	318/331 (96%)	308 (97%)	10 (3%)	0	100	100
2	KE	318/331 (96%)	306 (96%)	12 (4%)	0	100	100
2	MA	318/331 (96%)	310 (98%)	8 (2%)	0	100	100
2	MD	318/331 (96%)	305 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	MG	318/331 (96%)	312 (98%)	6 (2%)	0	100	100
2	OC	318/331 (96%)	311 (98%)	7 (2%)	0	100	100
2	OF	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	QB	318/331 (96%)	308 (97%)	10 (3%)	0	100	100
2	QE	318/331 (96%)	310 (98%)	8 (2%)	0	100	100
2	SA	318/331 (96%)	308 (97%)	10 (3%)	0	100	100
2	SD	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	SG	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	T	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	UC	318/331 (96%)	308 (97%)	10 (3%)	0	100	100
2	UF	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	WB	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	WE	318/331 (96%)	308 (97%)	10 (3%)	0	100	100
2	YA	318/331 (96%)	309 (97%)	9 (3%)	0	100	100
2	YD	318/331 (96%)	308 (97%)	10 (3%)	0	100	100
3	BA	279/300 (93%)	260 (93%)	19 (7%)	0	100	100
3	BD	279/300 (93%)	261 (94%)	18 (6%)	0	100	100
3	BG	279/300 (93%)	262 (94%)	17 (6%)	0	100	100
3	C	279/300 (93%)	260 (93%)	19 (7%)	0	100	100
3	DC	279/300 (93%)	263 (94%)	16 (6%)	0	100	100
3	DF	279/300 (93%)	262 (94%)	17 (6%)	0	100	100
3	FB	279/300 (93%)	261 (94%)	18 (6%)	0	100	100
3	FE	279/300 (93%)	258 (92%)	21 (8%)	0	100	100
3	HA	279/300 (93%)	260 (93%)	19 (7%)	0	100	100
3	HD	279/300 (93%)	260 (93%)	19 (7%)	0	100	100
3	HG	279/300 (93%)	257 (92%)	22 (8%)	0	100	100
3	JC	279/300 (93%)	262 (94%)	17 (6%)	0	100	100
3	JF	279/300 (93%)	259 (93%)	20 (7%)	0	100	100
3	K	279/300 (93%)	262 (94%)	17 (6%)	0	100	100
3	LB	279/300 (93%)	261 (94%)	18 (6%)	0	100	100
3	LE	279/300 (93%)	261 (94%)	18 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	279/300 (93%)	262 (94%)	17 (6%)	0	100	100
3	NA	279/300 (93%)	261 (94%)	18 (6%)	0	100	100
3	ND	279/300 (93%)	260 (93%)	19 (7%)	0	100	100
3	NG	279/300 (93%)	261 (94%)	18 (6%)	0	100	100
3	PC	279/300 (93%)	259 (93%)	20 (7%)	0	100	100
3	PF	279/300 (93%)	264 (95%)	15 (5%)	0	100	100
3	RB	279/300 (93%)	261 (94%)	18 (6%)	0	100	100
3	RE	279/300 (93%)	262 (94%)	17 (6%)	0	100	100
3	TA	279/300 (93%)	263 (94%)	16 (6%)	0	100	100
3	TD	279/300 (93%)	258 (92%)	21 (8%)	0	100	100
3	TG	279/300 (93%)	261 (94%)	18 (6%)	0	100	100
3	V	279/300 (93%)	260 (93%)	19 (7%)	0	100	100
3	VC	279/300 (93%)	260 (93%)	19 (7%)	0	100	100
3	VF	279/300 (93%)	259 (93%)	20 (7%)	0	100	100
3	XB	279/300 (93%)	257 (92%)	22 (8%)	0	100	100
3	XE	279/300 (93%)	260 (93%)	19 (7%)	0	100	100
3	ZA	279/300 (93%)	259 (93%)	20 (7%)	0	100	100
3	ZD	279/300 (93%)	259 (93%)	20 (7%)	0	100	100
4	AB	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	AC	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	AE	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	AF	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	BB	77/137 (56%)	67 (87%)	10 (13%)	0	100	100
4	BE	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	CA	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	CB	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	CD	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	CE	73/137 (53%)	68 (93%)	5 (7%)	0	100	100
4	CG	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	D	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	DA	77/137 (56%)	68 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	DD	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	DG	77/137 (56%)	70 (91%)	7 (9%)	0	100	100
4	E	77/137 (56%)	68 (88%)	9 (12%)	0	100	100
4	EA	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	EC	91/137 (66%)	88 (97%)	3 (3%)	0	100	100
4	ED	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	EF	91/137 (66%)	91 (100%)	0	0	100	100
4	EG	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	FC	77/137 (56%)	70 (91%)	7 (9%)	0	100	100
4	FF	77/137 (56%)	67 (87%)	10 (13%)	0	100	100
4	GB	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	GC	73/137 (53%)	69 (94%)	4 (6%)	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%)	67 (87%)	10 (13%)	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%)	69 (94%)	4 (6%)	0	100	100
4	ID	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	IE	73/137 (53%)	67 (92%)	6 (8%)	0	100	100
4	IG	91/137 (66%)	89 (98%)	2 (2%)	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%)	66 (86%)	11 (14%)	0	100	100
4	KA	73/137 (53%)	68 (93%)	5 (7%)	0	100	100
4	KC	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	KD	73/137 (53%)	70 (96%)	3 (4%)	0	100	100
4	KF	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	KG	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	L	91/137 (66%)	89 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LC	77/137 (56%)	67 (87%)	10 (13%)	0	100	100
4	LF	77/137 (56%)	67 (87%)	10 (13%)	0	100	100
4	MB	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	MC	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	ME	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	MF	73/137 (53%)	68 (93%)	5 (7%)	0	100	100
4	N	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	NB	77/137 (56%)	68 (88%)	9 (12%)	0	100	100
4	NE	77/137 (56%)	68 (88%)	9 (12%)	0	100	100
4	O	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	OA	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	OB	73/137 (53%)	68 (93%)	5 (7%)	0	100	100
4	OD	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	OE	73/137 (53%)	69 (94%)	4 (6%)	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%)	67 (87%)	10 (13%)	0	100	100
4	PD	77/137 (56%)	66 (86%)	11 (14%)	0	100	100
4	PG	77/137 (56%)	68 (88%)	9 (12%)	0	100	100
4	Q	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	QA	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	QC	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	QD	73/137 (53%)	67 (92%)	6 (8%)	0	100	100
4	QF	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	QG	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	R	73/137 (53%)	68 (93%)	5 (7%)	0	100	100
4	RC	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	RF	77/137 (56%)	68 (88%)	9 (12%)	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%)	89 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	SF	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	TB	77/137 (56%)	69 (90%)	8 (10%)	0	100	100
4	TE	77/137 (56%)	70 (91%)	7 (9%)	0	100	100
4	UA	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	UB	73/137 (53%)	68 (93%)	5 (7%)	0	100	100
4	UD	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	UE	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	UG	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	VA	77/137 (56%)	70 (91%)	7 (9%)	0	100	100
4	VD	77/137 (56%)	68 (88%)	9 (12%)	0	100	100
4	VG	77/137 (56%)	66 (86%)	11 (14%)	0	100	100
4	W	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	WA	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	WC	91/137 (66%)	90 (99%)	1 (1%)	0	100	100
4	WD	73/137 (53%)	67 (92%)	6 (8%)	0	100	100
4	WF	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	WG	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	X	77/137 (56%)	67 (87%)	10 (13%)	0	100	100
4	XC	77/137 (56%)	67 (87%)	10 (13%)	0	100	100
4	XF	77/137 (56%)	68 (88%)	9 (12%)	0	100	100
4	Y	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	YB	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	YC	73/137 (53%)	68 (93%)	5 (7%)	0	100	100
4	YE	91/137 (66%)	89 (98%)	2 (2%)	0	100	100
4	YF	73/137 (53%)	69 (94%)	4 (6%)	0	100	100
4	ZB	77/137 (56%)	68 (88%)	9 (12%)	0	100	100
4	ZE	77/137 (56%)	67 (87%)	10 (13%)	0	100	100
All	All	30022/37026 (81%)	28539 (95%)	1483 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	271/282 (96%)	256 (94%)	15 (6%)	21	50
2	AD	271/282 (96%)	255 (94%)	16 (6%)	19	48
2	AG	271/282 (96%)	258 (95%)	13 (5%)	25	53
2	B	271/282 (96%)	260 (96%)	11 (4%)	30	57
2	CC	271/282 (96%)	258 (95%)	13 (5%)	25	53
2	CF	271/282 (96%)	259 (96%)	12 (4%)	28	55
2	EB	271/282 (96%)	259 (96%)	12 (4%)	28	55
2	EE	271/282 (96%)	255 (94%)	16 (6%)	19	48
2	G	271/282 (96%)	257 (95%)	14 (5%)	23	51
2	GA	271/282 (96%)	256 (94%)	15 (6%)	21	50
2	GD	271/282 (96%)	257 (95%)	14 (5%)	23	51
2	GG	271/282 (96%)	258 (95%)	13 (5%)	25	53
2	IC	271/282 (96%)	256 (94%)	15 (6%)	21	50
2	IF	271/282 (96%)	257 (95%)	14 (5%)	23	51
2	J	271/282 (96%)	256 (94%)	15 (6%)	21	50
2	KB	271/282 (96%)	258 (95%)	13 (5%)	25	53
2	KE	271/282 (96%)	259 (96%)	12 (4%)	28	55
2	MA	271/282 (96%)	258 (95%)	13 (5%)	25	53
2	MD	271/282 (96%)	259 (96%)	12 (4%)	28	55
2	MG	271/282 (96%)	255 (94%)	16 (6%)	19	48
2	OC	271/282 (96%)	254 (94%)	17 (6%)	18	46
2	OF	271/282 (96%)	253 (93%)	18 (7%)	16	45
2	QB	271/282 (96%)	257 (95%)	14 (5%)	23	51
2	QE	271/282 (96%)	258 (95%)	13 (5%)	25	53
2	SA	271/282 (96%)	255 (94%)	16 (6%)	19	48
2	SD	271/282 (96%)	255 (94%)	16 (6%)	19	48

*Continued on next page...*

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SG	271/282 (96%)	258 (95%)	13 (5%)	25	53
2	T	271/282 (96%)	255 (94%)	16 (6%)	19	48
2	UC	271/282 (96%)	259 (96%)	12 (4%)	28	55
2	UF	271/282 (96%)	258 (95%)	13 (5%)	25	53
2	WB	271/282 (96%)	255 (94%)	16 (6%)	19	48
2	WE	271/282 (96%)	258 (95%)	13 (5%)	25	53
2	YA	271/282 (96%)	255 (94%)	16 (6%)	19	48
2	YD	271/282 (96%)	256 (94%)	15 (6%)	21	50
3	BA	177/257 (69%)	166 (94%)	11 (6%)	18	46
3	BD	177/257 (69%)	168 (95%)	9 (5%)	24	52
3	BG	177/257 (69%)	170 (96%)	7 (4%)	31	57
3	C	177/257 (69%)	169 (96%)	8 (4%)	27	55
3	DC	177/257 (69%)	170 (96%)	7 (4%)	31	57
3	DF	177/257 (69%)	168 (95%)	9 (5%)	24	52
3	FB	177/257 (69%)	168 (95%)	9 (5%)	24	52
3	FE	177/257 (69%)	169 (96%)	8 (4%)	27	55
3	HA	177/257 (69%)	169 (96%)	8 (4%)	27	55
3	HD	177/257 (69%)	169 (96%)	8 (4%)	27	55
3	HG	177/257 (69%)	168 (95%)	9 (5%)	24	52
3	JC	177/257 (69%)	167 (94%)	10 (6%)	21	49
3	JF	177/257 (69%)	168 (95%)	9 (5%)	24	52
3	K	177/257 (69%)	168 (95%)	9 (5%)	24	52
3	LB	177/257 (69%)	166 (94%)	11 (6%)	18	46
3	LE	177/257 (69%)	167 (94%)	10 (6%)	21	49
3	M	177/257 (69%)	170 (96%)	7 (4%)	31	57
3	NA	177/257 (69%)	167 (94%)	10 (6%)	21	49
3	ND	177/257 (69%)	169 (96%)	8 (4%)	27	55
3	NG	177/257 (69%)	165 (93%)	12 (7%)	16	44
3	PC	177/257 (69%)	167 (94%)	10 (6%)	21	49
3	PF	177/257 (69%)	166 (94%)	11 (6%)	18	46
3	RB	177/257 (69%)	170 (96%)	7 (4%)	31	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	RE	177/257 (69%)	167 (94%)	10 (6%)	21	49
3	TA	177/257 (69%)	168 (95%)	9 (5%)	24	52
3	TD	177/257 (69%)	165 (93%)	12 (7%)	16	44
3	TG	177/257 (69%)	170 (96%)	7 (4%)	31	57
3	V	177/257 (69%)	164 (93%)	13 (7%)	14	42
3	VC	177/257 (69%)	168 (95%)	9 (5%)	24	52
3	VF	177/257 (69%)	165 (93%)	12 (7%)	16	44
3	XB	177/257 (69%)	169 (96%)	8 (4%)	27	55
3	XE	177/257 (69%)	170 (96%)	7 (4%)	31	57
3	ZA	177/257 (69%)	170 (96%)	7 (4%)	31	57
3	ZD	177/257 (69%)	165 (93%)	12 (7%)	16	44
All	All	15232/18326 (83%)	14437 (95%)	795 (5%)	27	51

5 of 795 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SD	26	PHE
2	QE	206	MET
2	SD	209	GLN
3	ND	238	ASN
2	EE	32	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
2	OF	72	ASN
3	PF	106	HIS
2	SG	141	GLN
3	RB	190	ASN
3	RB	106	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

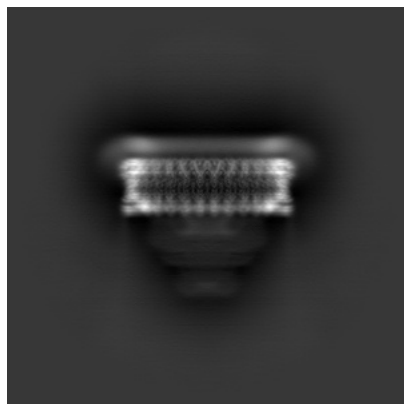
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41100. These allow visual inspection of the internal detail of the map and identification of artifacts.

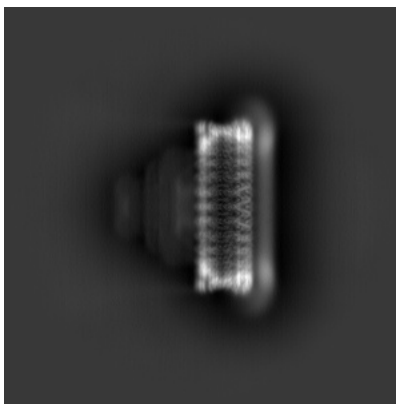
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

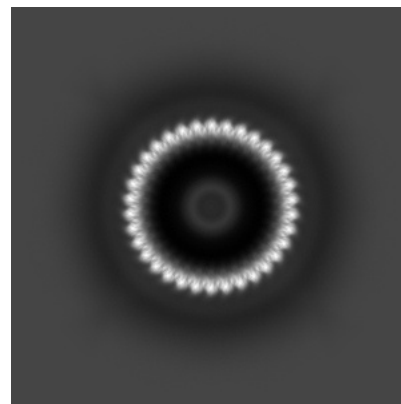
#### 6.1.1 Primary map



X

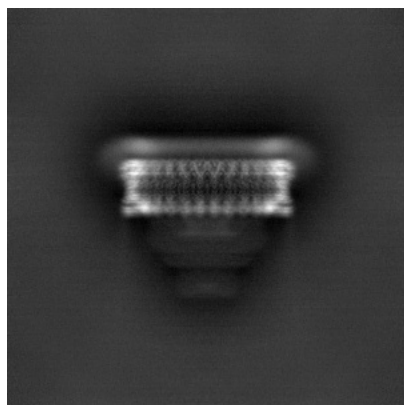


Y

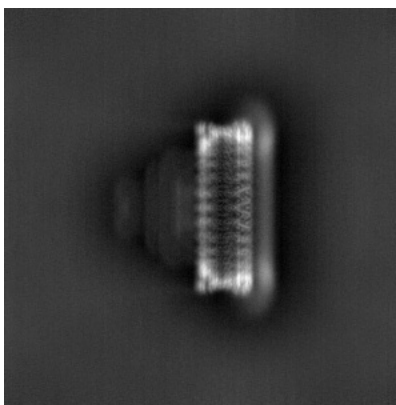


Z

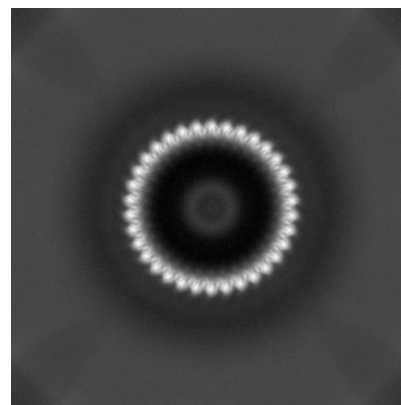
#### 6.1.2 Raw map



X



Y

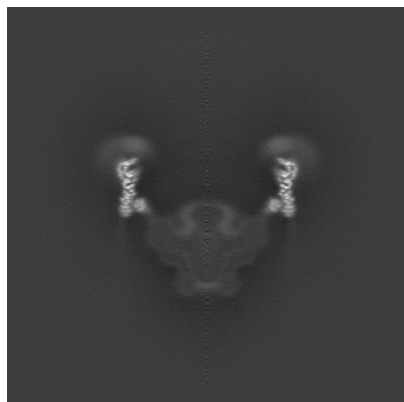


Z

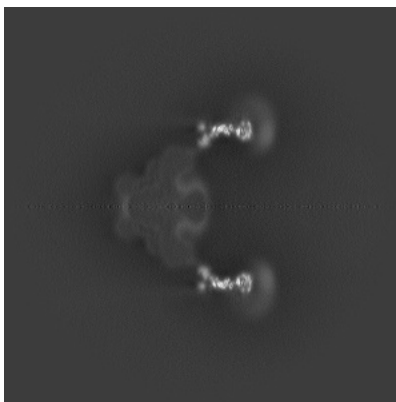
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

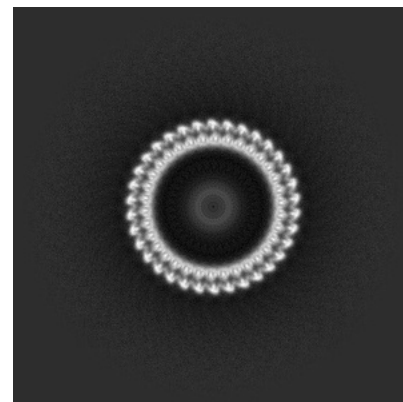
### 6.2.1 Primary map



X Index: 384

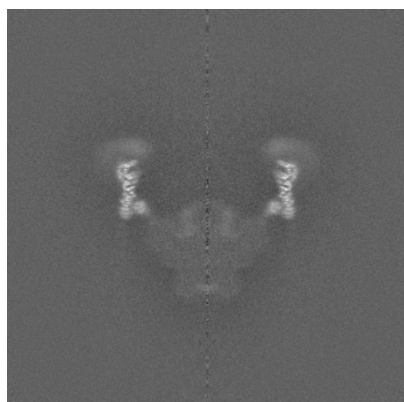


Y Index: 384

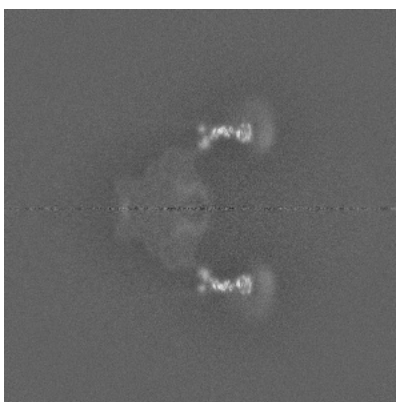


Z Index: 384

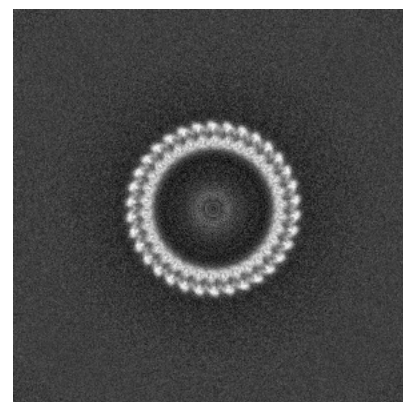
### 6.2.2 Raw map



X Index: 384



Y Index: 384

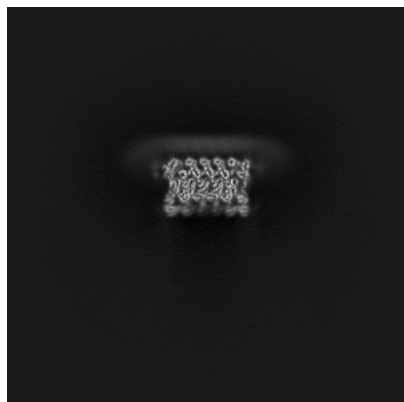


Z Index: 384

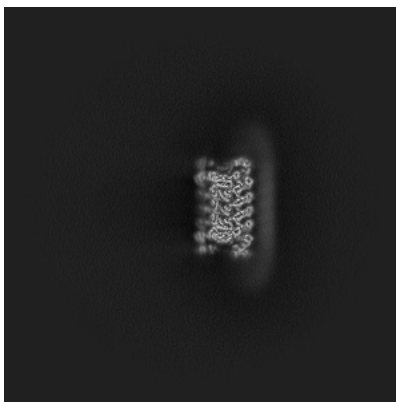
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

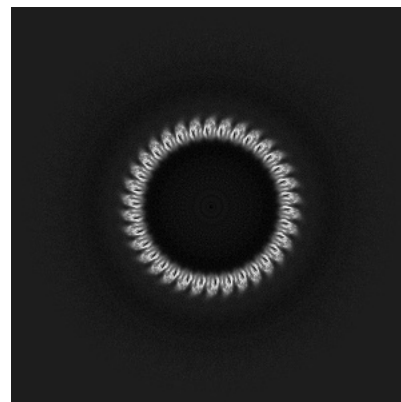
### 6.3.1 Primary map



X Index: 241

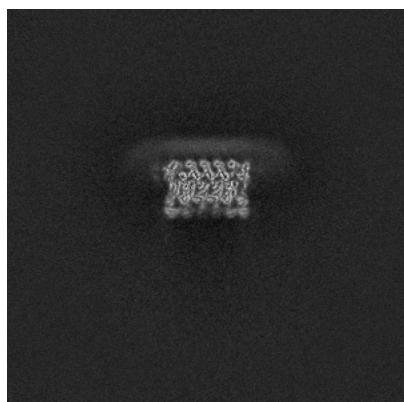


Y Index: 242

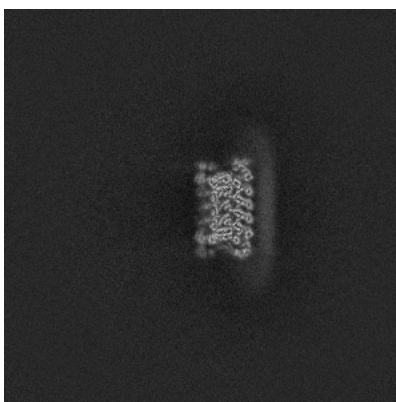


Z Index: 449

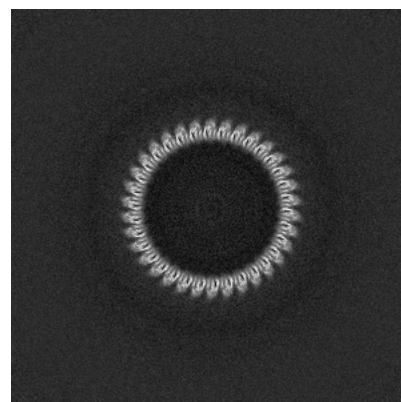
### 6.3.2 Raw map



X Index: 241



Y Index: 526

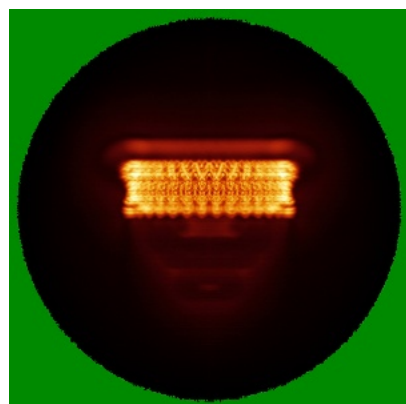


Z Index: 449

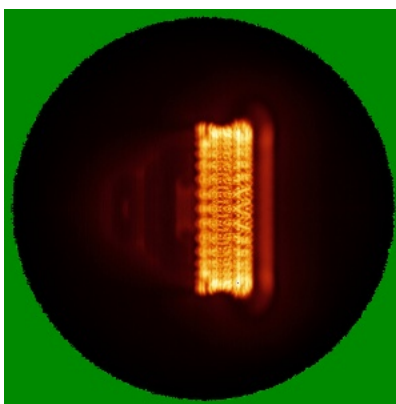
The images above show the largest variance slices of the map in three orthogonal directions.

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

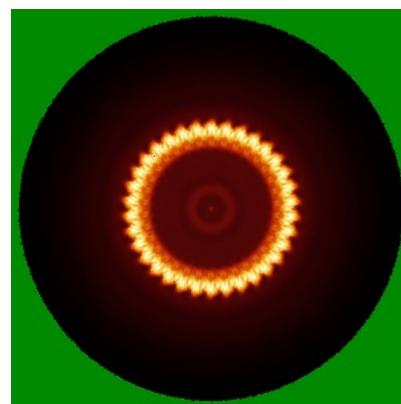
### 6.4.1 Primary map



X

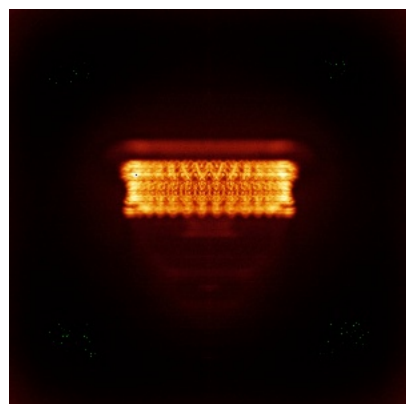


Y

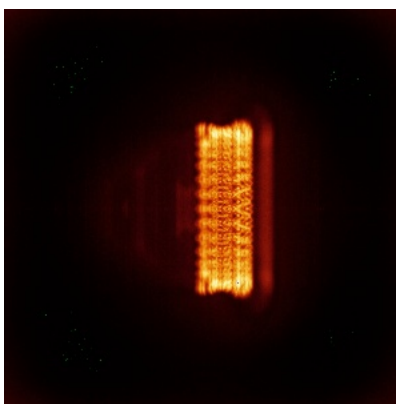


Z

### 6.4.2 Raw map



X



Y



Z

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

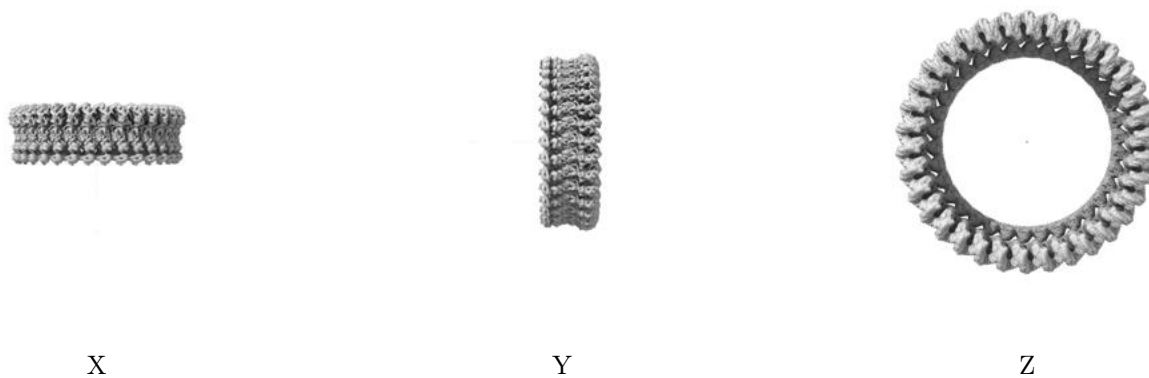
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.147. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

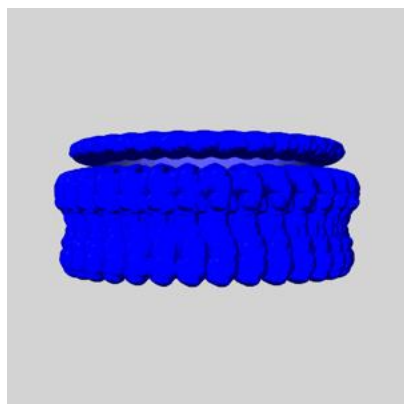
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

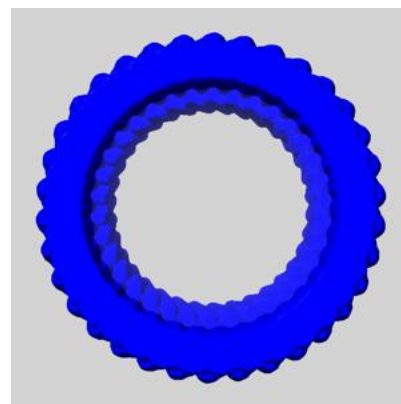
### 6.6.1 emd\_41100\_msk\_1.map [i](#)



X



Y



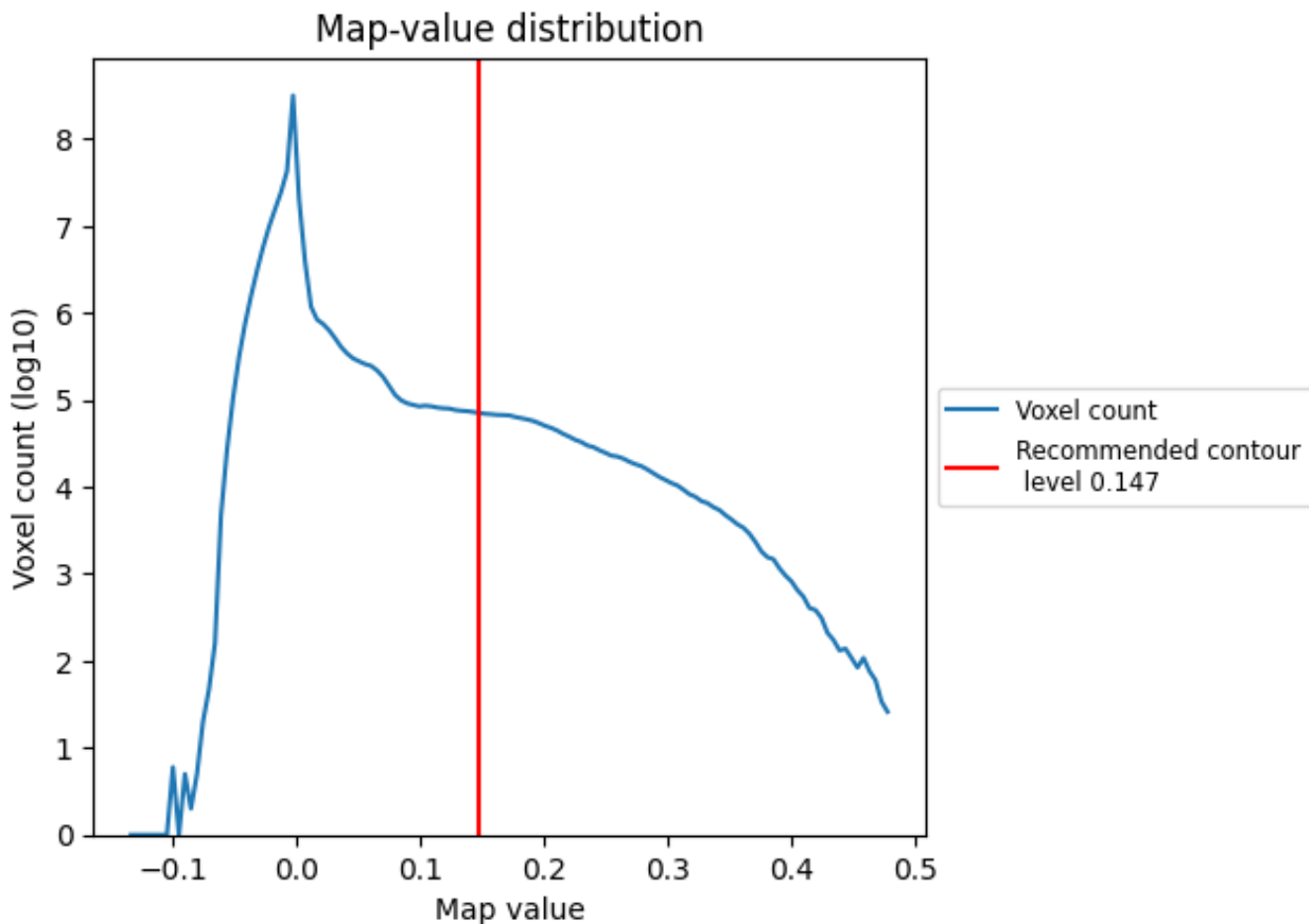
Z



## 7 Map analysis [i](#)

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

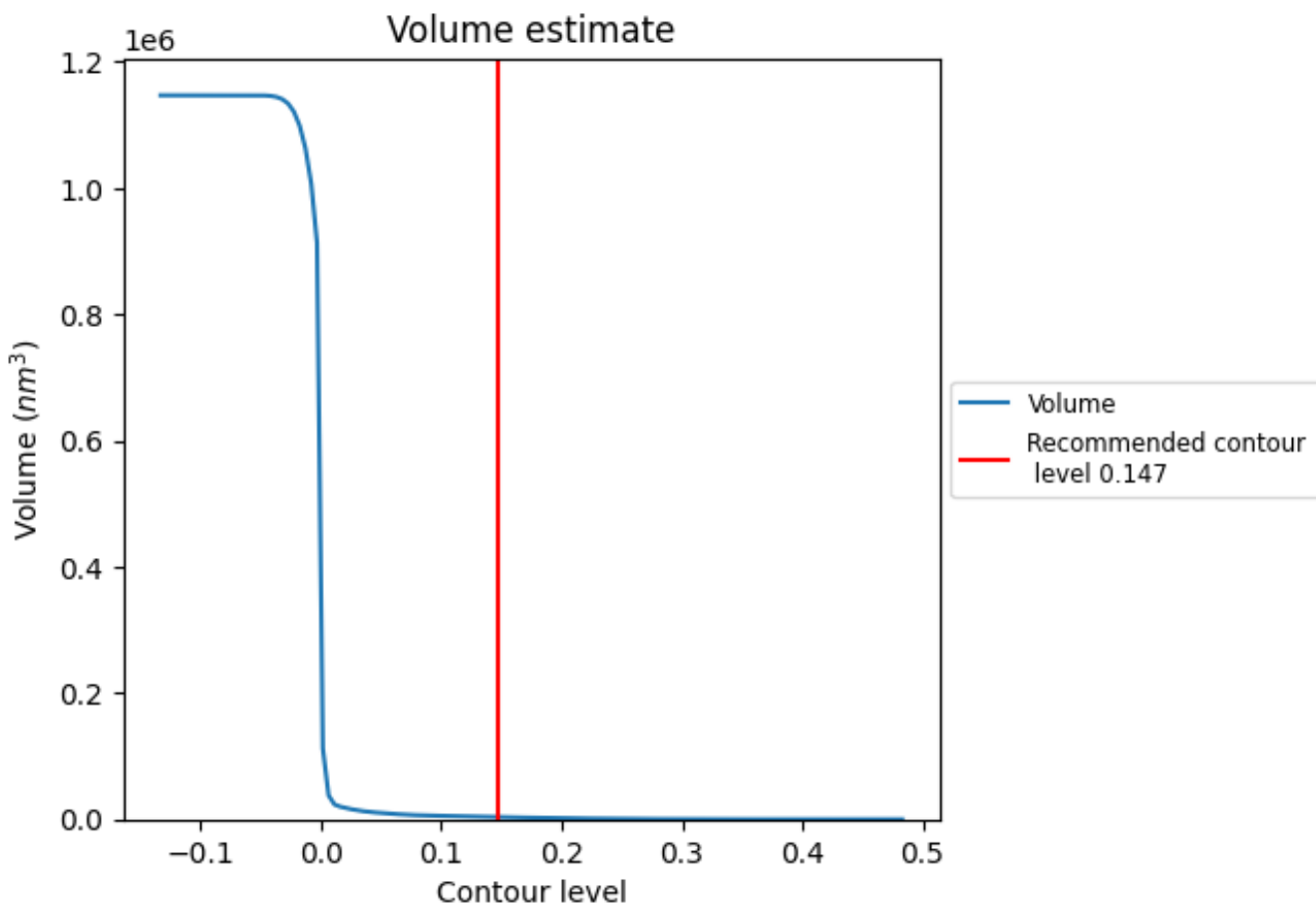
### 7.1 Map-value distribution [i](#)



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



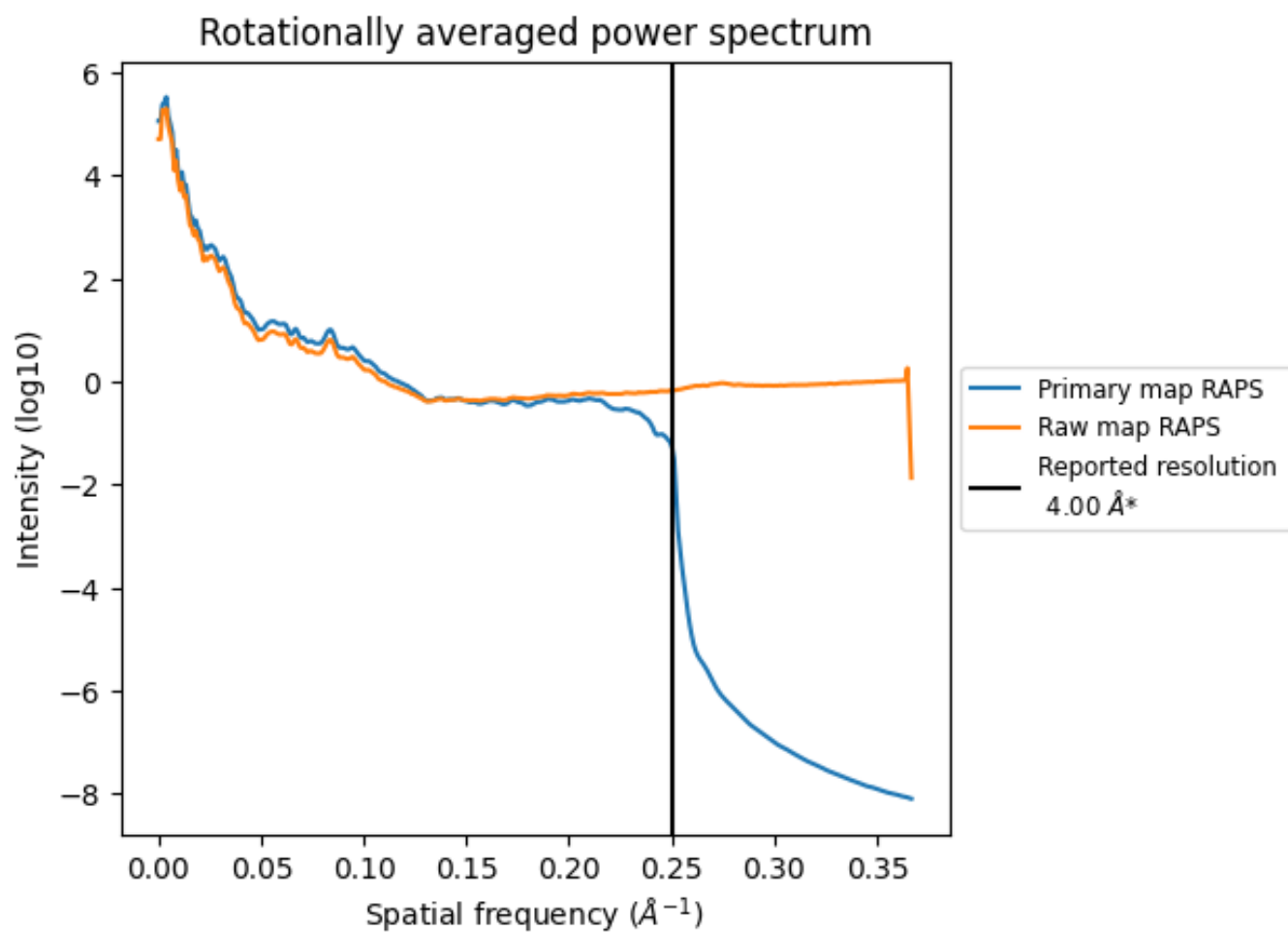
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $3549 \text{ nm}^3$ ; this corresponds to an approximate mass of 3206 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](#)

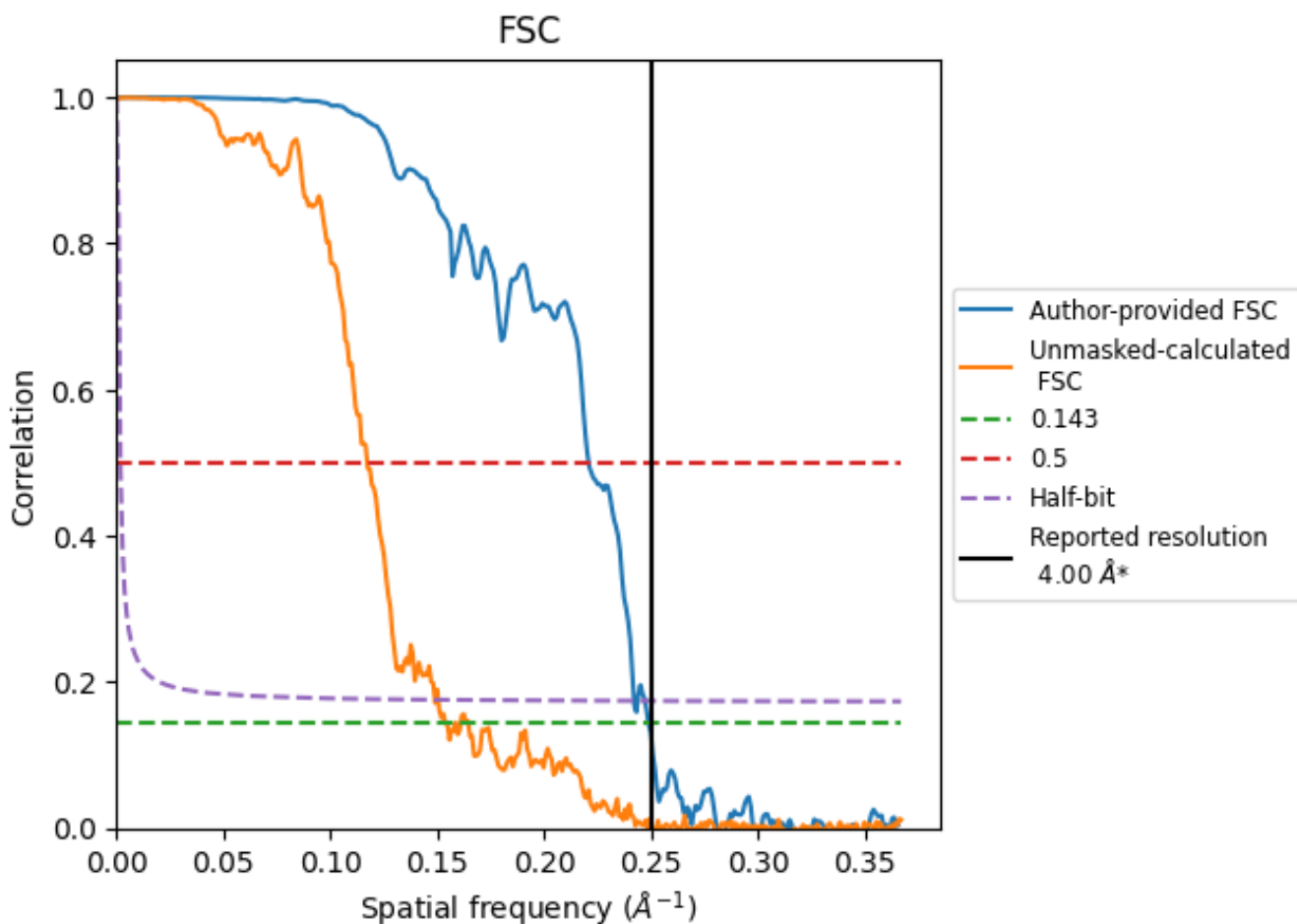


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 8.2 Resolution estimates

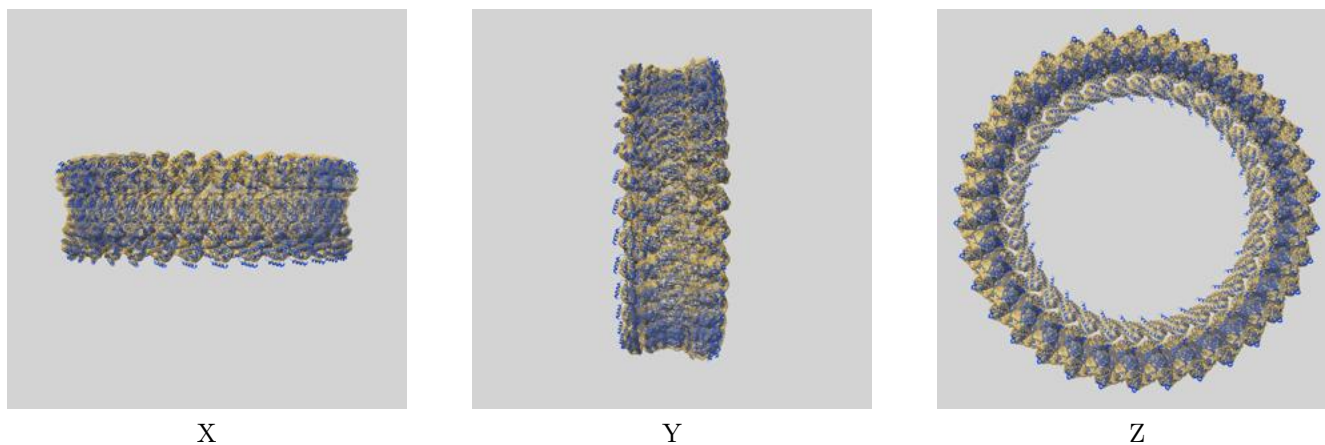
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.02	4.53	4.13
Unmasked-calculated*	6.50	8.53	6.72

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.50 differs from the reported value 4.0 by more than 10 %

## 9 Map-model fit [i](#)

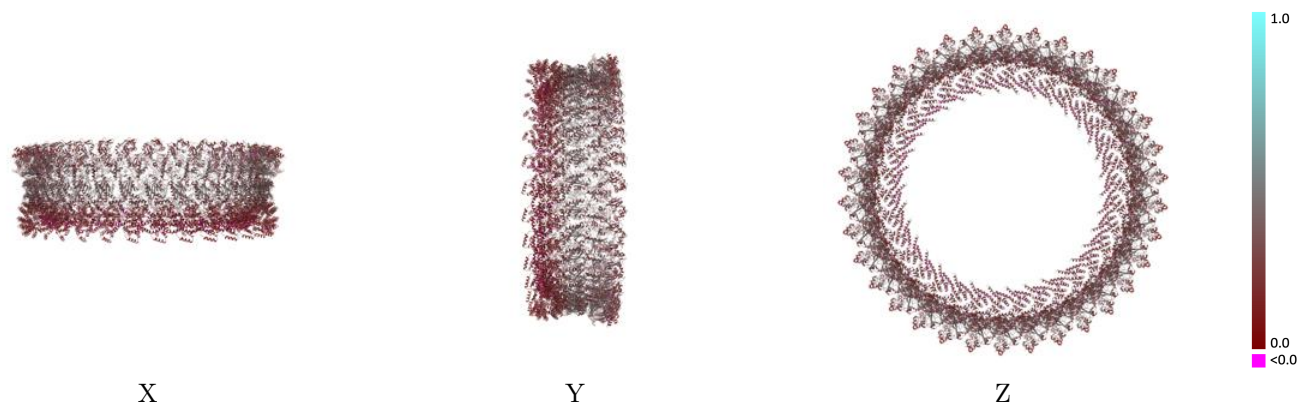
This section contains information regarding the fit between EMDB map EMD-41100 and PDB model 8T8O. Per-residue inclusion information can be found in section 3 on page 22.

### 9.1 Map-model overlay [i](#)



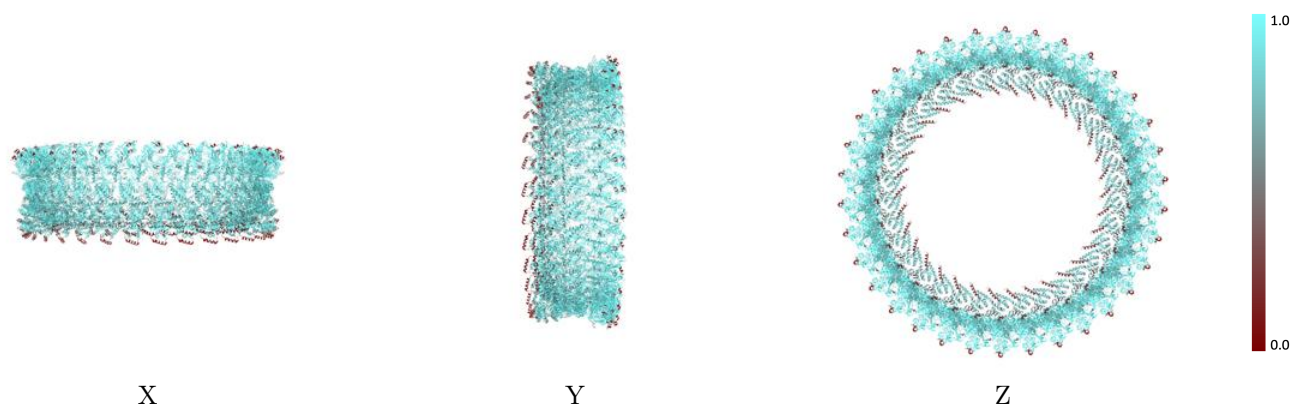
The images above show the 3D surface view of the map at the recommended contour level 0.147 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



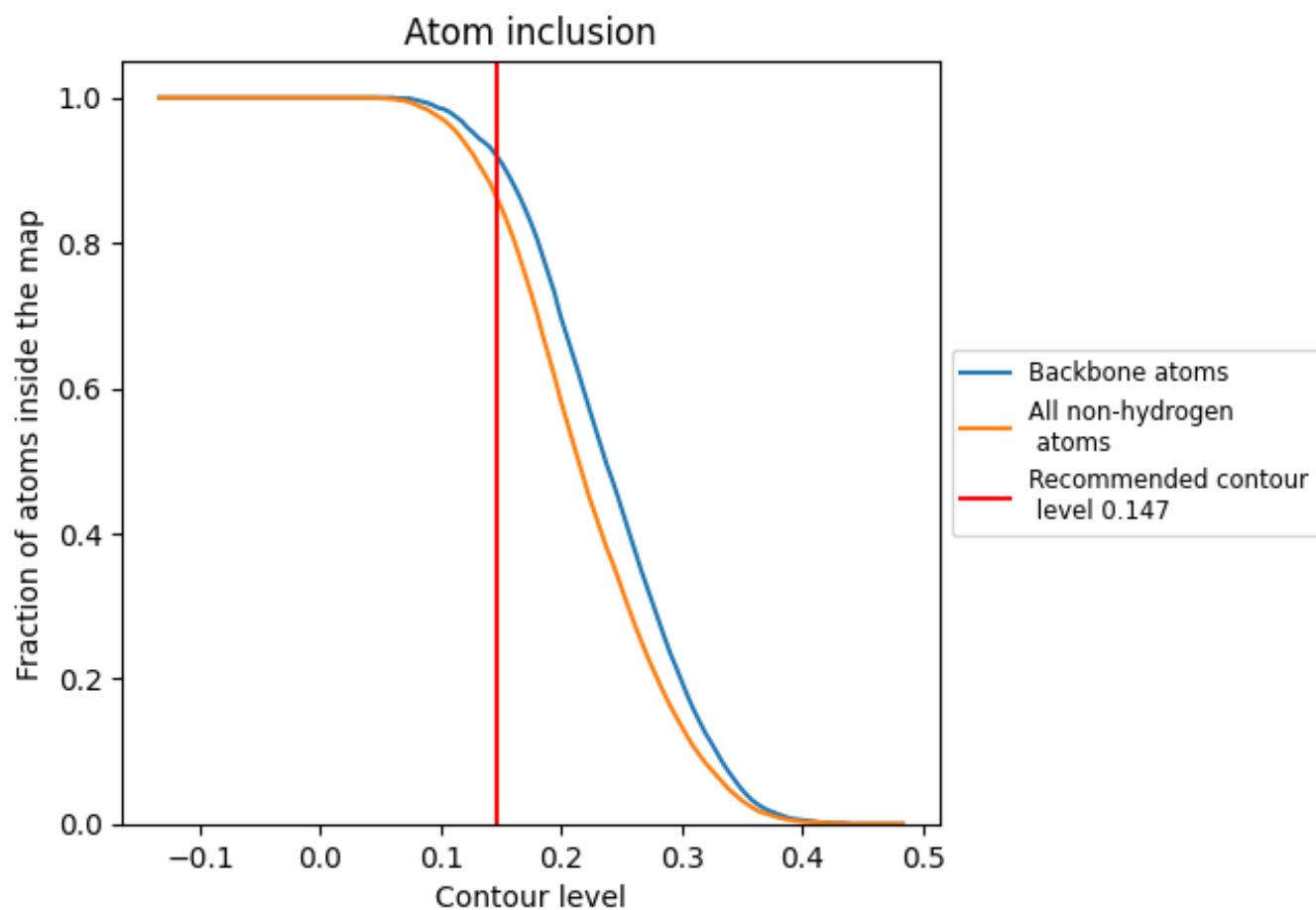
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.147).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.147) and Q-score for the entire model and for each chain.





















































































Chain	Atom inclusion	Q-score
All	 0.8600	 0.2720
A	 0.4960	 0.1610
AA	 0.8160	 0.1970
AB	 0.9230	 0.3140
AC	 0.9190	 0.3650
AD	 0.8140	 0.1950
AE	 0.9120	 0.3140
AF	 0.9050	 0.3600
AG	 0.8120	 0.1960
B	 0.8120	 0.1970
BA	 0.9220	 0.3430
BB	 0.9510	 0.3260
BC	 0.4790	 0.1520
BD	 0.9160	 0.3400
BE	 0.9490	 0.3260
BF	 0.4830	 0.1540
BG	 0.9190	 0.3420
C	 0.9250	 0.3410
CA	 0.9230	 0.3130
CB	 0.9130	 0.3630
CC	 0.8150	 0.1950
CD	 0.9190	 0.3140
CE	 0.9000	 0.3580
CF	 0.8090	 0.1950
CG	 0.9170	 0.3100
D	 0.9250	 0.3140
DA	 0.9560	 0.3220
DB	 0.4910	 0.1550
DC	 0.9180	 0.3380
DD	 0.9490	 0.3270
DE	 0.4830	 0.1530
DF	 0.9200	 0.3450
DG	 0.9540	 0.3200
E	 0.9590	 0.3230
EA	 0.9050	 0.3640



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































































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Chain	Atom inclusion	Q-score
EB	 0.8150	 0.1970
EC	 0.9190	 0.3170
ED	 0.9080	 0.3630
EE	 0.8150	 0.1950
EF	 0.9170	 0.3130
EG	 0.9020	 0.3570
F	 0.5000	 0.1610
FA	 0.4960	 0.1560
FB	 0.9240	 0.3430
FC	 0.9460	 0.3260
FD	 0.4790	 0.1490
FE	 0.9150	 0.3410
FF	 0.9510	 0.3230
FG	 0.4910	 0.1630
G	 0.8150	 0.1970
GA	 0.8190	 0.1970
GB	 0.9210	 0.3140
GC	 0.9080	 0.3640
GD	 0.8120	 0.1930
GE	 0.9140	 0.3130
GF	 0.9020	 0.3620
GG	 0.8100	 0.1960
H	 0.9050	 0.3600
HA	 0.9230	 0.3430
HB	 0.9540	 0.3260
HC	 0.4700	 0.1550
HD	 0.9150	 0.3400
HE	 0.9460	 0.3250
HF	 0.4830	 0.1540
HG	 0.9190	 0.3410
I	 0.5000	 0.1600
IA	 0.9230	 0.3130
IB	 0.9130	 0.3640
IC	 0.8160	 0.1970
ID	 0.9140	 0.3150
IE	 0.9000	 0.3570
IF	 0.8120	 0.1960
IG	 0.9170	 0.3110
J	 0.8130	 0.1980
JA	 0.9590	 0.3260
JB	 0.4910	 0.1520
JC	 0.9180	 0.3390





















































































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Chain	Atom inclusion	Q-score
JD	 0.9490	 0.3270
JE	 0.4790	 0.1530
JF	 0.9190	 0.3430
JG	 0.9560	 0.3180
K	 0.9230	 0.3410
KA	 0.9050	 0.3590
KB	 0.8140	 0.1980
KC	 0.9190	 0.3140
KD	 0.9080	 0.3620
KE	 0.8130	 0.1940
KF	 0.9170	 0.3170
KG	 0.9050	 0.3550
L	 0.9250	 0.3140
LA	 0.4960	 0.1550
LB	 0.9220	 0.3420
LC	 0.9430	 0.3200
LD	 0.4790	 0.1540
LE	 0.9170	 0.3400
LF	 0.9540	 0.3230
LG	 0.4960	 0.1610
M	 0.9220	 0.3390
MA	 0.8160	 0.1960
MB	 0.9250	 0.3140
MC	 0.9110	 0.3610
MD	 0.8120	 0.1940
ME	 0.9140	 0.3130
MF	 0.9050	 0.3630
MG	 0.8130	 0.1970
N	 0.9190	 0.3110
NA	 0.9220	 0.3420
NB	 0.9510	 0.3260
NC	 0.4700	 0.1550
ND	 0.9150	 0.3400
NE	 0.9510	 0.3270
NF	 0.4870	 0.1580
NG	 0.9210	 0.3440
O	 0.9540	 0.3220
OA	 0.9230	 0.3130
OB	 0.9160	 0.3560
OC	 0.8100	 0.1950
OD	 0.9140	 0.3160
OE	 0.9020	 0.3610





















































































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Chain	Atom inclusion	Q-score
OF	 0.8120	 0.1980
OG	 0.9170	 0.3120
P	 0.9560	 0.3240
PA	 0.9560	 0.3250
PB	 0.4830	 0.1520
PC	 0.9180	 0.3410
PD	 0.9460	 0.3260
PE	 0.4830	 0.1530
PF	 0.9220	 0.3440
PG	 0.9540	 0.3230
Q	 0.9050	 0.3580
QA	 0.9050	 0.3620
QB	 0.8100	 0.1970
QC	 0.9140	 0.3150
QD	 0.9050	 0.3540
QE	 0.8090	 0.1950
QF	 0.9170	 0.3150
QG	 0.9050	 0.3570
R	 0.9080	 0.3500
RA	 0.4960	 0.1560
RB	 0.9220	 0.3410
RC	 0.9460	 0.3250
RD	 0.4660	 0.1530
RE	 0.9200	 0.3420
RF	 0.9510	 0.3220
RG	 0.5000	 0.1610
S	 0.5000	 0.1560
SA	 0.8160	 0.1960
SB	 0.9230	 0.3160
SC	 0.9130	 0.3610
SD	 0.8090	 0.1950
SE	 0.9170	 0.3140
SF	 0.9080	 0.3560
SG	 0.8150	 0.1950
T	 0.8120	 0.1970
TA	 0.9200	 0.3430
TB	 0.9460	 0.3250
TC	 0.4740	 0.1550
TD	 0.9150	 0.3400
TE	 0.9540	 0.3250
TF	 0.4870	 0.1620
TG	 0.9190	 0.3410





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Chain	Atom inclusion	Q-score
UA	 0.9230	 0.3140
UB	 0.9110	 0.3620
UC	 0.8100	 0.1940
UD	 0.9140	 0.3170
UE	 0.9050	 0.3610
UF	 0.8100	 0.1950
UG	 0.9230	 0.3110
V	 0.9220	 0.3420
VA	 0.9560	 0.3260
VB	 0.4790	 0.1530
VC	 0.9140	 0.3400
VD	 0.9490	 0.3230
VE	 0.4830	 0.1530
VF	 0.9210	 0.3410
VG	 0.9560	 0.3270
W	 0.9230	 0.3110
WA	 0.9130	 0.3630
WB	 0.8110	 0.1960
WC	 0.9190	 0.3140
WD	 0.9000	 0.3510
WE	 0.8060	 0.1950
WF	 0.9140	 0.3100
WG	 0.9050	 0.3550
X	 0.9590	 0.3210
XA	 0.4960	 0.1560
XB	 0.9230	 0.3390
XC	 0.9460	 0.3280
XD	 0.4700	 0.1550
XE	 0.9210	 0.3420
XF	 0.9560	 0.3240
Y	 0.9050	 0.3620
YA	 0.8120	 0.1980
YB	 0.9210	 0.3120
YC	 0.9130	 0.3510
YD	 0.8140	 0.1970
YE	 0.9190	 0.3130
YF	 0.9050	 0.3560
Z	 0.5000	 0.1560
ZA	 0.9220	 0.3430
ZB	 0.9490	 0.3250
ZC	 0.4660	 0.1520
ZD	 0.9170	 0.3410

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Chain	Atom inclusion	Q-score
ZE	 0.9510	 0.3260
ZF	 0.4910	 0.1590