wwPDB EM Validation Summary Report (i)

May 11, 2024 – 04:00 PM EDT

PDB ID	:	8UPL
EMDB ID	:	EMD-42451
Title	:	Cryo-EM structure of a Clockwise locked form of the Salmonella enterica Typhimurium flagellar C-ring, with C34 symmetry applied
Authors	:	Johnson, S.; Deme, J.C.; Lea, S.M.
Deposited on	:	2023-10-22
Resolution	:	5.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

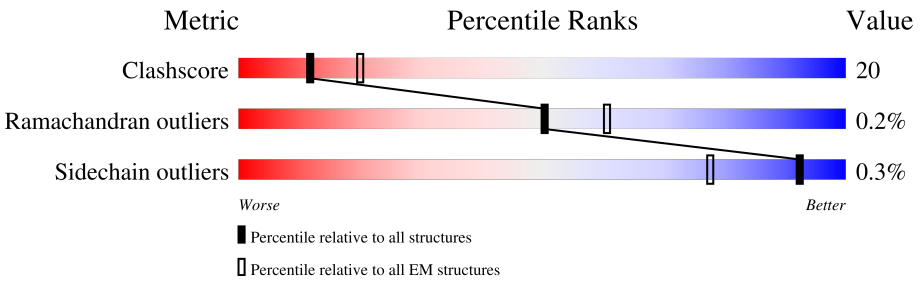
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 5.40 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	560	92%
1	A2	560	92%
1	A3	560	5% 92%
1	A4	560	92%
1	A5	560	92%
1	A6	560	92%
1	A7	560	92%
1	A8	560	92%

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Mol	Chain	Length	Quality of chain
1	A9	560	92%
1	AA	560	92%
1	AB	560	92%
1	AC	560	92%
1	AD	560	92%
1	AE	560	92%
1	AF	560	92%
1	AG	560	92%
1	AH	560	92%
1	AI	560	92%
1	AJ	560	92%
1	AK	560	92%
1	AL	560	92%
1	AM	560	92%
1	AN	560	92%
1	AO	560	5% 92%
1	AP	560	92%
1	AQ	560	92%
1	AR	560	92%
1	AS	560	92%
1	AT	560	92%
1	AU	560	92%
1	AV	560	92%
1	AW	560	92%
1	AX	560	92%

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Mol	Chain	Length	Quality of chain
1	AY	560	92%
2	B1	328	17% 62% 38%
2	B2	328	17% 63% 37%
2	B3	328	18% 63% 37%
2	B4	328	18% 60% 40%
2	B5	328	18% 61% 39%
2	B6	328	18% 62% 38%
2	B7	328	18% 64% 36%
2	B8	328	18% 62% 38%
2	B9	328	18% 63% 37%
2	BA	328	17% 63% 37%
2	BB	328	18% 63% 37%
2	BC	328	18% 63% 37%
2	BD	328	18% 63% 37%
2	BE	328	17% 62% 38%
2	BF	328	18% 63% 37%
2	BG	328	18% 62% 38%
2	BH	328	18% 65% 35%
2	BI	328	18% 62% 38%
2	BJ	328	18% 64% 36%
2	BK	328	18% 63% 37%
2	BL	328	17% 62% 38%
2	BM	328	18% 61% 39%
2	BN	328	18% 63% 37%
2	BO	328	18% 63% 37%

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Mol	Chain	Length	Quality of chain
2	BP	328	18% 63% 37%
2	BQ	328	18% 63% 37%
2	BR	328	18% 63% 37%
2	BS	328	18% 62% 38%
2	BT	328	18% 63% 37%
2	BU	328	18% 62% 38%
2	BV	328	18% 62% 38%
2	BW	328	18% 63% 36%
2	BX	328	18% 63% 37%
2	BY	328	18% 62% 38%
3	C1	334	51% 34% 14%
3	C2	334	53% 33% 14%
3	C3	334	54% 32% 14%
3	C4	334	52% 34% 14%
3	C5	334	54% 32% 14%
3	C6	334	55% 31% 14%
3	C7	334	52% 34% 14%
3	C8	334	52% 34% 14%
3	C9	334	53% 33% 14%
3	CA	334	53% 33% 14%
3	CB	334	53% 33% 14%
3	CC	334	51% 34% 14%
3	CD	334	52% 34% 14%
3	CE	334	52% 34% 14%
3	CF	334	53% 33% 14%

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Mol	Chain	Length	Quality of chain
3	CG	334	51% 34% 14%
3	CH	334	52% 34% 14%
3	CI	334	52% 34% 14%
3	CJ	334	52% 34% 14%
3	CK	334	53% 33% 14%
3	CL	334	52% 34% 14%
3	CM	334	54% 32% 14%
3	CN	334	53% 33% 14%
3	CO	334	52% 34% 14%
3	CP	334	52% 34% 14%
3	CQ	334	54% 32% 14%
3	CR	334	53% 33% 14%
3	CS	334	52% 34% 14%
3	CT	334	52% 34% 14%
3	CU	334	51% 34% 14%
3	CV	334	51% 35% 14%
3	CW	334	54% 31% 14%
3	CX	334	52% 34% 14%
3	CY	334	53% 33% 14%
4	D1	137	32% 28% 39%
4	D2	137	31% 30% 39%
4	D3	137	31% 30% 39%
4	D4	137	31% 28% 39%
4	D5	137	34% 27% 39%
4	D6	137	34% 27% 39%

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Mol	Chain	Length	Quality of chain
4	D7	137	35% 26% 39%
4	D8	137	32% 28% 39%
4	D9	137	32% 28% 39%
4	DA	137	33% 28% 39%
4	DB	137	31% 29% 39%
4	DC	137	32% 28% 39%
4	DD	137	38% 23% 39%
4	DE	137	31% 30% 39%
4	DF	137	31% 30% 39%
4	DG	137	33% 28% 39%
4	DH	137	31% 29% 39%
4	DI	137	33% 28% 39%
4	DJ	137	35% 26% 39%
4	DK	137	31% 29% 39%
4	DL	137	33% 27% 39%
4	DM	137	37% 23% 39%
4	DN	137	31% 29% 39%
4	DO	137	34% 26% 39%
4	DP	137	32% 28% 39%
4	DQ	137	32% 28% 39%
4	DR	137	34% 26% 39%
4	DS	137	32% 28% 39%
4	DT	137	33% 28% 39%
4	DU	137	37% 23% 39%
4	DV	137	33% 28% 39%

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Mol	Chain	Length	Quality of chain
4	DW	137	31% 29% 39%
4	DX	137	34% 26% 39%
4	DY	137	29% 31% 39%
4	E1	137	28% 28% 42%
4	E2	137	31% 26% 42%
4	E3	137	26% 31% 42%
4	E4	137	31% 26% 42%
4	E5	137	28% 28% 42%
4	E6	137	30% 26% 42%
4	E7	137	29% 27% 42%
4	E8	137	28% 28% 42%
4	E9	137	29% 28% 42%
4	EA	137	30% 27% 42%
4	EB	137	28% 28% 42%
4	EC	137	28% 28% 42%
4	ED	137	29% 28% 42%
4	EE	137	29% 26% 42%
4	EF	137	29% 27% 42%
4	EG	137	26% 31% 42%
4	EH	137	29% 27% 42%
4	EI	137	28% 28% 42%
4	EJ	137	31% 26% 42%
4	EK	137	29% 27% 42%
4	EL	137	31% 26% 42%
4	EM	137	29% 28% 42%

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Mol	Chain	Length	Quality of chain
4	EN	137	31% 26% • 42%
4	EO	137	31% 26% • 42%
4	EP	137	29% 28% • 42%
4	EQ	137	28% 28% • 42%
4	ER	137	26% 30% • 42%
4	ES	137	29% 27% • 42%
4	ET	137	28% 28% • 42%
4	EU	137	31% 26% • 42%
4	EV	137	26% 31% • 42%
4	EW	137	31% 26% • 42%
4	EX	137	31% 26% • 42%
4	EY	137	28% 29% • 42%
4	F1	137	• 28% 34% 38%
4	F2	137	• 33% 29% 38%
4	F3	137	• 33% 28% • 38%
4	F4	137	• 34% 28% 38%
4	F5	137	• 31% 31% 38%
4	F6	137	• 33% 29% 38%
4	F7	137	• 28% 34% • 38%
4	F8	137	• 30% 31% • 38%
4	F9	137	• 31% 30% • 38%
4	FA	137	• 30% 32% 38%
4	FB	137	• 31% 31% • 38%
4	FC	137	• 25% 36% • 38%
4	FD	137	• 28% 33% • 38%

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Mol	Chain	Length	Quality of chain
4	FE	137	30% 31% 38%
4	FF	137	31% 30% 38%
4	FG	137	28% 34% 38%
4	FH	137	30% 32% 38%
4	FI	137	31% 31% 38%
4	FJ	137	31% 31% 38%
4	FK	137	32% 29% 38%
4	FL	137	32% 30% 38%
4	FM	137	30% 32% 38%
4	FN	137	33% 29% 38%
4	FO	137	29% 32% 38%
4	FP	137	31% 31% 38%
4	FQ	137	30% 31% 38%
4	FR	137	28% 34% 38%
4	FS	137	31% 31% 38%
4	FT	137	30% 32% 38%
4	FU	137	30% 32% 38%
4	FV	137	32% 30% 38%
4	FW	137	34% 28% 38%
4	FX	137	31% 30% 38%
4	FY	137	34% 27% 38%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 243644 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	S		
1	A1	44	367	218	77	69	3	0	0
1	A2	44	367	218	77	69	3	0	0
1	A3	44	367	218	77	69	3	0	0
1	A4	44	367	218	77	69	3	0	0
1	A5	44	367	218	77	69	3	0	0
1	A6	44	367	218	77	69	3	0	0
1	A7	44	367	218	77	69	3	0	0
1	A8	44	367	218	77	69	3	0	0
1	A9	44	367	218	77	69	3	0	0
1	AA	44	367	218	77	69	3	0	0
1	AB	44	367	218	77	69	3	0	0
1	AC	44	367	218	77	69	3	0	0
1	AD	44	367	218	77	69	3	0	0
1	AE	44	367	218	77	69	3	0	0
1	AF	44	367	218	77	69	3	0	0
1	AG	44	367	218	77	69	3	0	0
1	AH	44	367	218	77	69	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AI	44	367	218	77	69	3	0	0
1	AJ	44	367	218	77	69	3	0	0
1	AK	44	367	218	77	69	3	0	0
1	AL	44	367	218	77	69	3	0	0
1	AM	44	367	218	77	69	3	0	0
1	AN	44	367	218	77	69	3	0	0
1	AO	44	367	218	77	69	3	0	0
1	AP	44	367	218	77	69	3	0	0
1	AQ	44	367	218	77	69	3	0	0
1	AR	44	367	218	77	69	3	0	0
1	AS	44	367	218	77	69	3	0	0
1	AT	44	367	218	77	69	3	0	0
1	AU	44	367	218	77	69	3	0	0
1	AV	44	367	218	77	69	3	0	0
1	AW	44	367	218	77	69	3	0	0
1	AX	44	367	218	77	69	3	0	0
1	AY	44	367	218	77	69	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B1	328	2566	1594	452	510	10	0	0
2	B2	328	2566	1594	452	510	10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B3	328	2566	1594	452	510	10	0	0
2	B4	328	2566	1594	452	510	10	0	0
2	B5	328	2566	1594	452	510	10	0	0
2	B6	328	2566	1594	452	510	10	0	0
2	B7	328	2566	1594	452	510	10	0	0
2	B8	328	2566	1594	452	510	10	0	0
2	B9	328	2566	1594	452	510	10	0	0
2	BA	328	2566	1594	452	510	10	0	0
2	BB	328	2566	1594	452	510	10	0	0
2	BC	328	2566	1594	452	510	10	0	0
2	BD	328	2566	1594	452	510	10	0	0
2	BE	328	2566	1594	452	510	10	0	0
2	BF	328	2566	1594	452	510	10	0	0
2	BG	328	2566	1594	452	510	10	0	0
2	BH	328	2566	1594	452	510	10	0	0
2	BI	328	2566	1594	452	510	10	0	0
2	BJ	328	2566	1594	452	510	10	0	0
2	BK	328	2566	1594	452	510	10	0	0
2	BL	328	2566	1594	452	510	10	0	0
2	BM	328	2566	1594	452	510	10	0	0
2	BN	328	2566	1594	452	510	10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BO	328	2566	1594	452	510	10	0	0
2	BP	328	2566	1594	452	510	10	0	0
2	BQ	328	2566	1594	452	510	10	0	0
2	BR	328	2566	1594	452	510	10	0	0
2	BS	328	2566	1594	452	510	10	0	0
2	BT	328	2566	1594	452	510	10	0	0
2	BU	328	2566	1594	452	510	10	0	0
2	BV	328	2566	1594	452	510	10	0	0
2	BW	328	2566	1594	452	510	10	0	0
2	BX	328	2566	1594	452	510	10	0	0
2	BY	328	2566	1594	452	510	10	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	?	-	PRO	deletion	UNP P0A1J9
B1	?	-	ALA	deletion	UNP P0A1J9
B1	?	-	ALA	deletion	UNP P0A1J9
B2	?	-	PRO	deletion	UNP P0A1J9
B2	?	-	ALA	deletion	UNP P0A1J9
B2	?	-	ALA	deletion	UNP P0A1J9
B3	?	-	PRO	deletion	UNP P0A1J9
B3	?	-	ALA	deletion	UNP P0A1J9
B3	?	-	ALA	deletion	UNP P0A1J9
B4	?	-	PRO	deletion	UNP P0A1J9
B4	?	-	ALA	deletion	UNP P0A1J9
B4	?	-	ALA	deletion	UNP P0A1J9
B5	?	-	PRO	deletion	UNP P0A1J9
B5	?	-	ALA	deletion	UNP P0A1J9
B5	?	-	ALA	deletion	UNP P0A1J9
B6	?	-	PRO	deletion	UNP P0A1J9
B6	?	-	ALA	deletion	UNP P0A1J9

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Chain	Residue	Modelled	Actual	Comment	Reference
B6	?	-	ALA	deletion	UNP P0A1J9
B7	?	-	PRO	deletion	UNP P0A1J9
B7	?	-	ALA	deletion	UNP P0A1J9
B7	?	-	ALA	deletion	UNP P0A1J9
B8	?	-	PRO	deletion	UNP P0A1J9
B8	?	-	ALA	deletion	UNP P0A1J9
B8	?	-	ALA	deletion	UNP P0A1J9
B9	?	-	PRO	deletion	UNP P0A1J9
B9	?	-	ALA	deletion	UNP P0A1J9
B9	?	-	ALA	deletion	UNP P0A1J9
BA	?	-	PRO	deletion	UNP P0A1J9
BA	?	-	ALA	deletion	UNP P0A1J9
BA	?	-	ALA	deletion	UNP P0A1J9
BB	?	-	PRO	deletion	UNP P0A1J9
BB	?	-	ALA	deletion	UNP P0A1J9
BB	?	-	ALA	deletion	UNP P0A1J9
BC	?	-	PRO	deletion	UNP P0A1J9
BC	?	-	ALA	deletion	UNP P0A1J9
BC	?	-	ALA	deletion	UNP P0A1J9
BD	?	-	PRO	deletion	UNP P0A1J9
BD	?	-	ALA	deletion	UNP P0A1J9
BD	?	-	ALA	deletion	UNP P0A1J9
BE	?	-	PRO	deletion	UNP P0A1J9
BE	?	-	ALA	deletion	UNP P0A1J9
BE	?	-	ALA	deletion	UNP P0A1J9
BF	?	-	PRO	deletion	UNP P0A1J9
BF	?	-	ALA	deletion	UNP P0A1J9
BF	?	-	ALA	deletion	UNP P0A1J9
BG	?	-	PRO	deletion	UNP P0A1J9
BG	?	-	ALA	deletion	UNP P0A1J9
BG	?	-	ALA	deletion	UNP P0A1J9
BH	?	-	PRO	deletion	UNP P0A1J9
BH	?	-	ALA	deletion	UNP P0A1J9
BH	?	-	ALA	deletion	UNP P0A1J9
BI	?	-	PRO	deletion	UNP P0A1J9
BI	?	-	ALA	deletion	UNP P0A1J9
BI	?	-	ALA	deletion	UNP P0A1J9
BJ	?	-	PRO	deletion	UNP P0A1J9
BJ	?	-	ALA	deletion	UNP P0A1J9
BJ	?	-	ALA	deletion	UNP P0A1J9
BK	?	-	PRO	deletion	UNP P0A1J9
BK	?	-	ALA	deletion	UNP P0A1J9

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Chain	Residue	Modelled	Actual	Comment	Reference
BK	?	-	ALA	deletion	UNP P0A1J9
BL	?	-	PRO	deletion	UNP P0A1J9
BL	?	-	ALA	deletion	UNP P0A1J9
BL	?	-	ALA	deletion	UNP P0A1J9
BM	?	-	PRO	deletion	UNP P0A1J9
BM	?	-	ALA	deletion	UNP P0A1J9
BM	?	-	ALA	deletion	UNP P0A1J9
BN	?	-	PRO	deletion	UNP P0A1J9
BN	?	-	ALA	deletion	UNP P0A1J9
BN	?	-	ALA	deletion	UNP P0A1J9
BO	?	-	PRO	deletion	UNP P0A1J9
BO	?	-	ALA	deletion	UNP P0A1J9
BO	?	-	ALA	deletion	UNP P0A1J9
BP	?	-	PRO	deletion	UNP P0A1J9
BP	?	-	ALA	deletion	UNP P0A1J9
BP	?	-	ALA	deletion	UNP P0A1J9
BQ	?	-	PRO	deletion	UNP P0A1J9
BQ	?	-	ALA	deletion	UNP P0A1J9
BQ	?	-	ALA	deletion	UNP P0A1J9
BR	?	-	PRO	deletion	UNP P0A1J9
BR	?	-	ALA	deletion	UNP P0A1J9
BR	?	-	ALA	deletion	UNP P0A1J9
BS	?	-	PRO	deletion	UNP P0A1J9
BS	?	-	ALA	deletion	UNP P0A1J9
BS	?	-	ALA	deletion	UNP P0A1J9
BT	?	-	PRO	deletion	UNP P0A1J9
BT	?	-	ALA	deletion	UNP P0A1J9
BT	?	-	ALA	deletion	UNP P0A1J9
BU	?	-	PRO	deletion	UNP P0A1J9
BU	?	-	ALA	deletion	UNP P0A1J9
BU	?	-	ALA	deletion	UNP P0A1J9
BV	?	-	PRO	deletion	UNP P0A1J9
BV	?	-	ALA	deletion	UNP P0A1J9
BV	?	-	ALA	deletion	UNP P0A1J9
BW	?	-	PRO	deletion	UNP P0A1J9
BW	?	-	ALA	deletion	UNP P0A1J9
BW	?	-	ALA	deletion	UNP P0A1J9
BX	?	-	PRO	deletion	UNP P0A1J9
BX	?	-	ALA	deletion	UNP P0A1J9
BX	?	-	ALA	deletion	UNP P0A1J9
BY	?	-	PRO	deletion	UNP P0A1J9
BY	?	-	ALA	deletion	UNP P0A1J9

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Chain	Residue	Modelled	Actual	Comment	Reference
BY	?	-	ALA	deletion	UNP P0A1J9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C1	287	2325	1482	421	417	5	0	0
3	C2	287	2325	1482	421	417	5	0	0
3	C3	287	2325	1482	421	417	5	0	0
3	C4	287	2325	1482	421	417	5	0	0
3	C5	287	2325	1482	421	417	5	0	0
3	C6	287	2325	1482	421	417	5	0	0
3	C7	287	2325	1482	421	417	5	0	0
3	C8	287	2325	1482	421	417	5	0	0
3	C9	287	2325	1482	421	417	5	0	0
3	CA	287	2325	1482	421	417	5	0	0
3	CB	287	2325	1482	421	417	5	0	0
3	CC	287	2325	1482	421	417	5	0	0
3	CD	287	2325	1482	421	417	5	0	0
3	CE	287	2325	1482	421	417	5	0	0
3	CF	287	2325	1482	421	417	5	0	0
3	CG	287	2325	1482	421	417	5	0	0
3	CH	287	2325	1482	421	417	5	0	0
3	CI	287	2325	1482	421	417	5	0	0
3	CJ	287	2325	1482	421	417	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CK	287	2325	1482	421	417	5	0	0
3	CL	287	2325	1482	421	417	5	0	0
3	CM	287	2325	1482	421	417	5	0	0
3	CN	287	2325	1482	421	417	5	0	0
3	CO	287	2325	1482	421	417	5	0	0
3	CP	287	2325	1482	421	417	5	0	0
3	CQ	287	2325	1482	421	417	5	0	0
3	CR	287	2325	1482	421	417	5	0	0
3	CS	287	2325	1482	421	417	5	0	0
3	CT	287	2325	1482	421	417	5	0	0
3	CU	287	2325	1482	421	417	5	0	0
3	CV	287	2325	1482	421	417	5	0	0
3	CW	287	2325	1482	421	417	5	0	0
3	CX	287	2325	1482	421	417	5	0	0
3	CY	287	2325	1482	421	417	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D1	83	643	407	113	120	3	0	0
4	E1	79	609	388	106	112	3	0	0
4	F1	85	656	416	113	124	3	0	0
4	D2	83	643	407	113	120	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E2	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	F2	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	D3	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	E3	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	F3	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	D4	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	E4	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	F4	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	D5	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	E5	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	F5	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	D6	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	E6	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	F6	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	D7	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	E7	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	F7	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	D8	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	E8	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	F8	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	D9	83	643	407	113	120	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E9	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	F9	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DA	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EA	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FA	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DB	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EB	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FB	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DC	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EC	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FC	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DD	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	ED	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FD	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DE	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EE	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FE	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DF	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EF	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FF	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DG	83	643	407	113	120	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	EG	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FG	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DH	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EH	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FH	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DI	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EI	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FI	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DJ	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EJ	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FJ	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DK	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EK	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FK	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DL	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EL	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FL	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DM	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EM	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FM	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DN	83	643	407	113	120	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	EN	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FN	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DO	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EO	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FO	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DP	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EP	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FP	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DQ	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EQ	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FQ	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DR	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	ER	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FR	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DS	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	ES	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FS	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DT	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	ET	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FT	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DU	83	643	407	113	120	3	0	0

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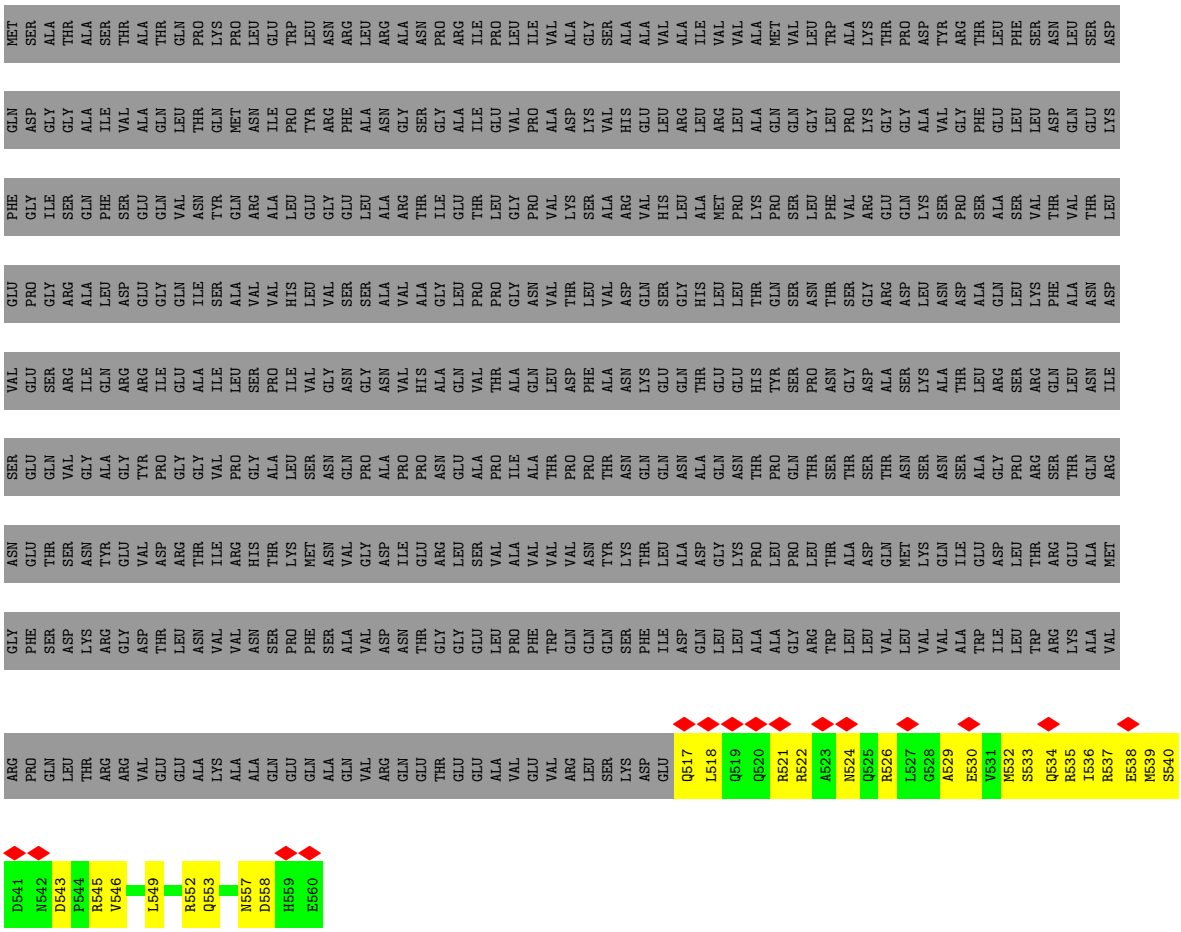
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	EU	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FU	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DV	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EV	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FV	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DW	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EW	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FW	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DX	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EX	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FX	85	656	416	113	124	3	0	0
			Total	C	N	O	S		
4	DY	83	643	407	113	120	3	0	0
			Total	C	N	O	S		
4	EY	79	609	388	106	112	3	0	0
			Total	C	N	O	S		
4	FY	85	656	416	113	124	3	0	0

3 Residue-property plots (i)

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

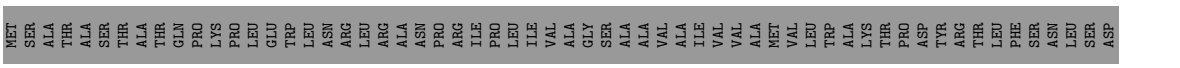
- Molecule 1: Flagellar M-ring protein

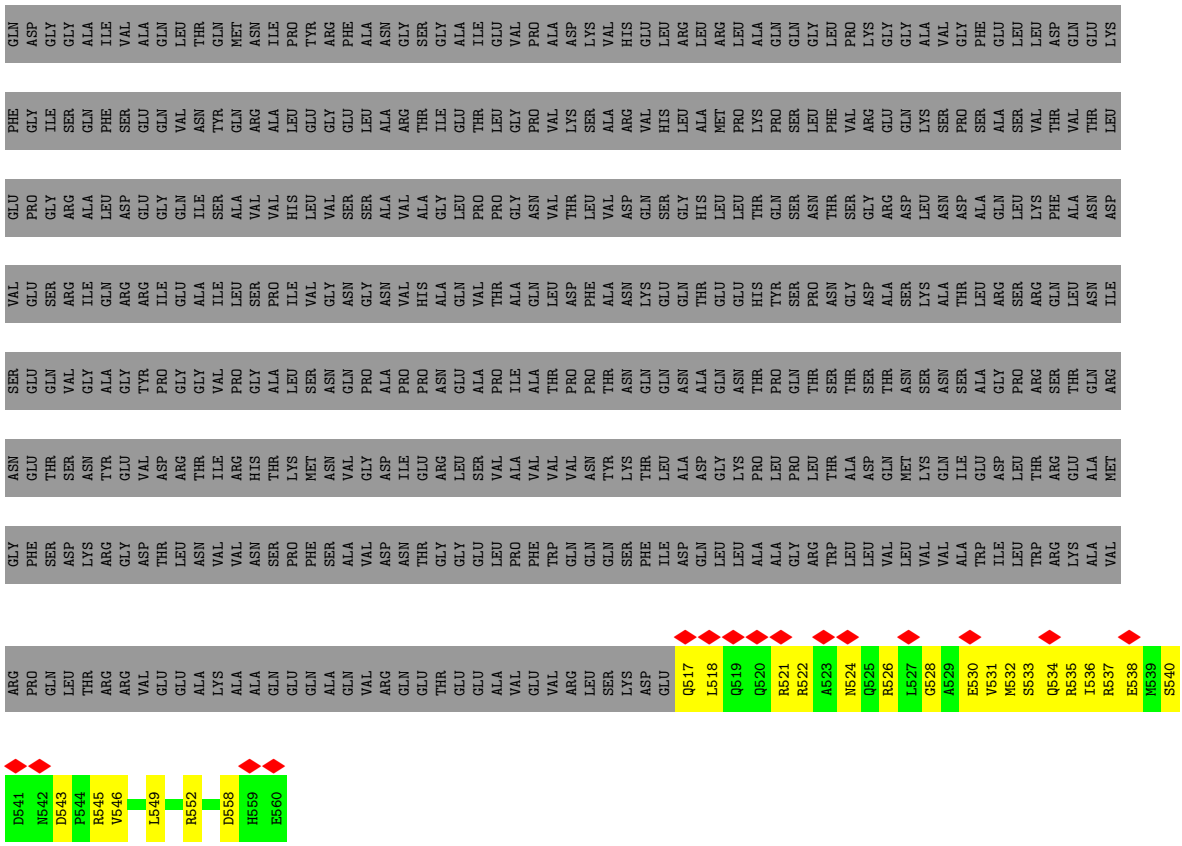
Chain A1: 92%



- Molecule 1: Flagellar M-ring protein

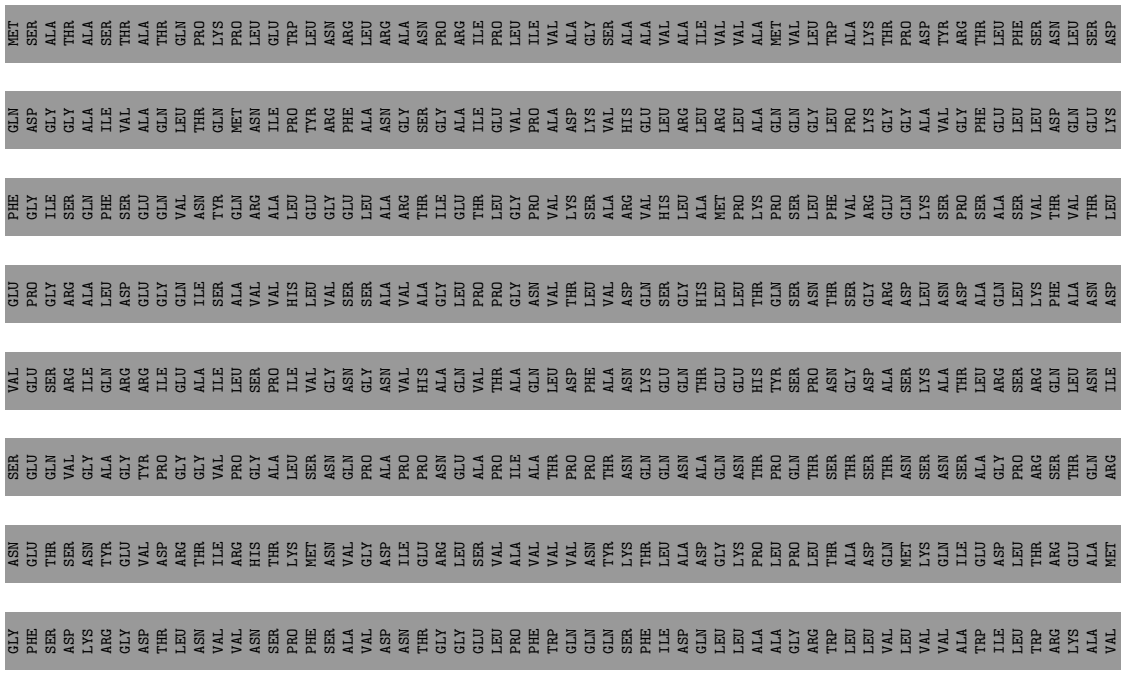
Chain A2: 92%

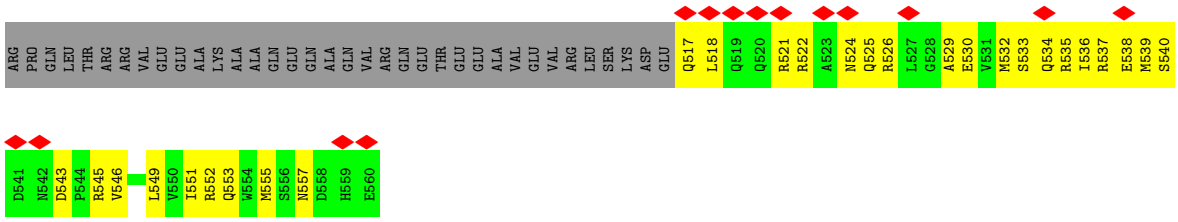




• Molecule 1: Flagellar M-ring protein

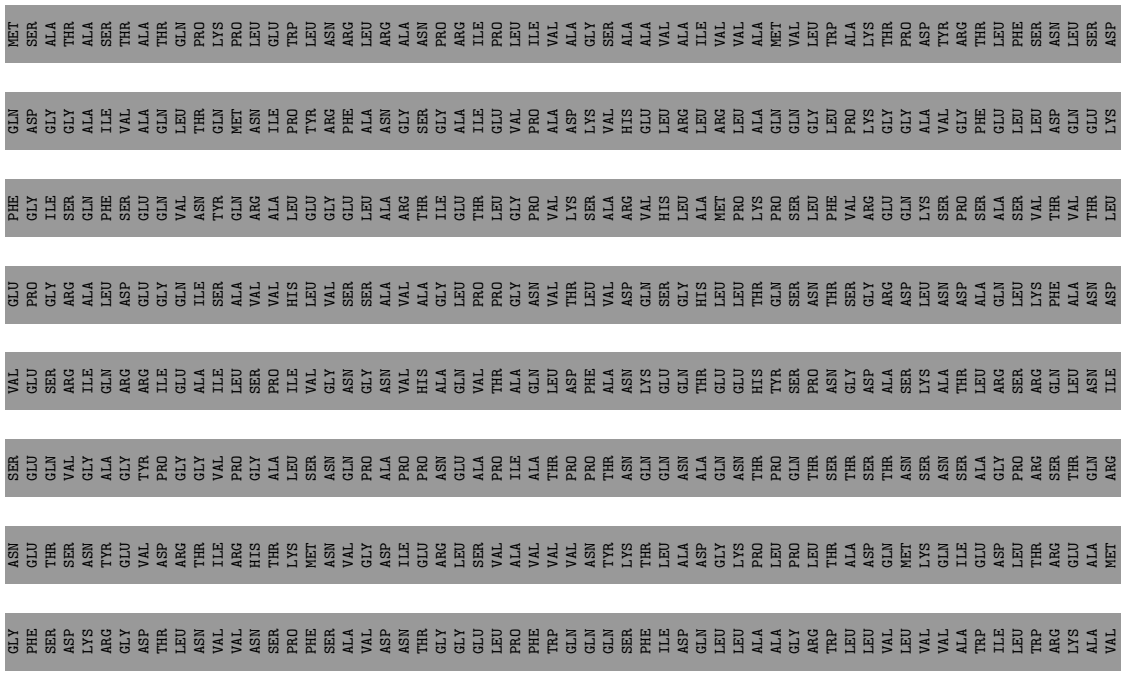
Chain A3: 5% 92%

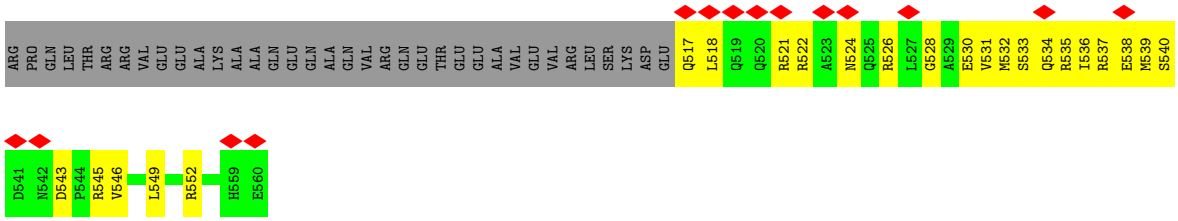




• Molecule 1: Flagellar M-ring protein

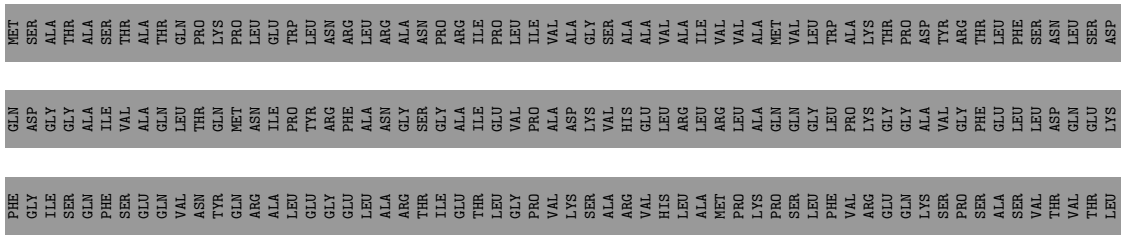
Chain A4: 92%

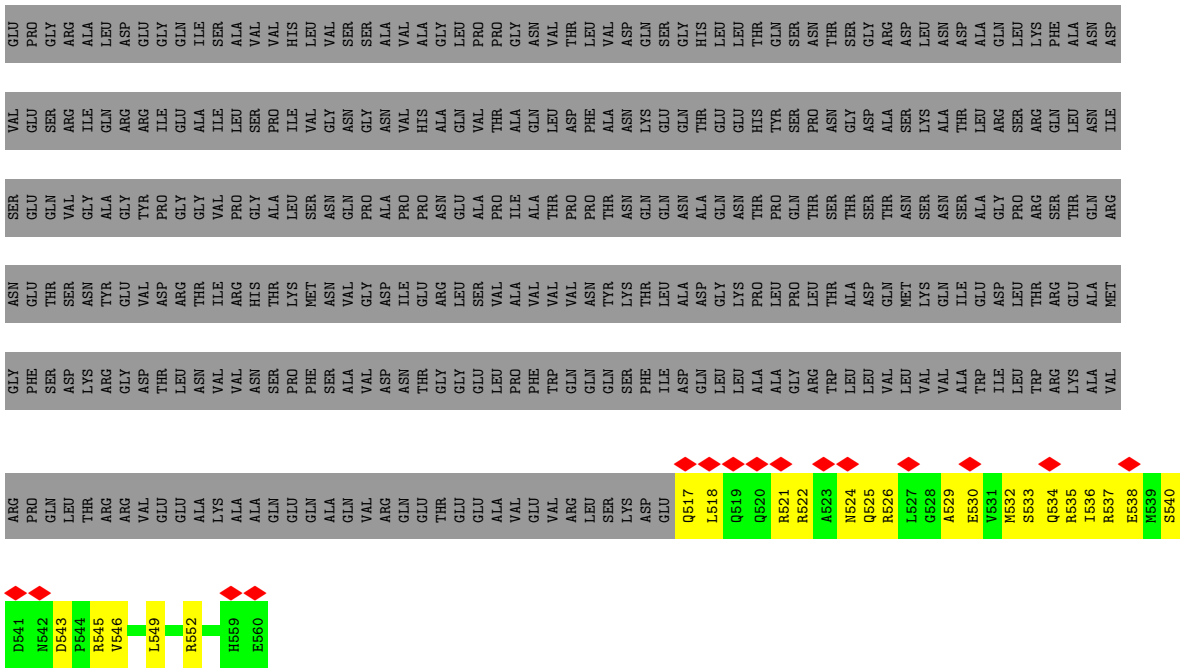




• Molecule 1: Flagellar M-ring protein

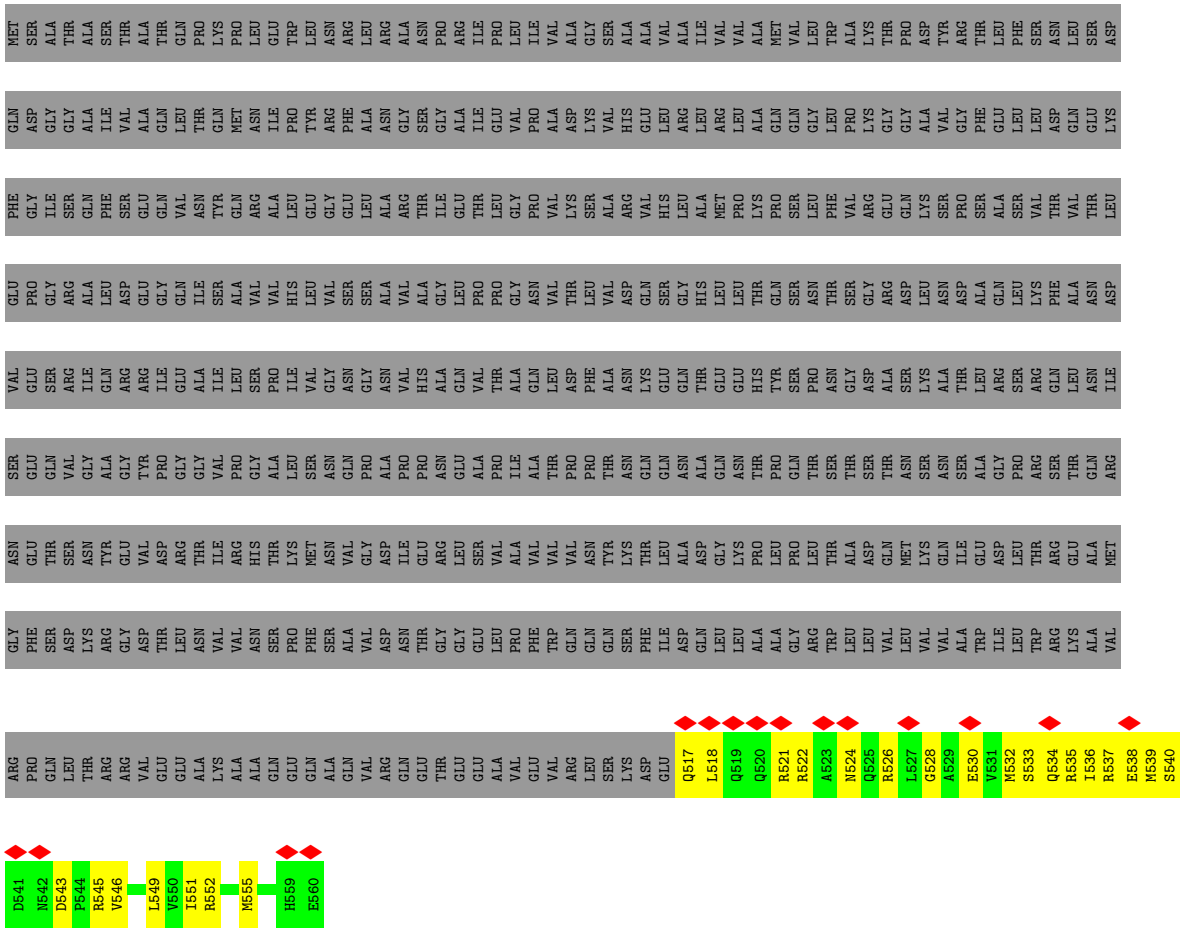
Chain A5: 92%





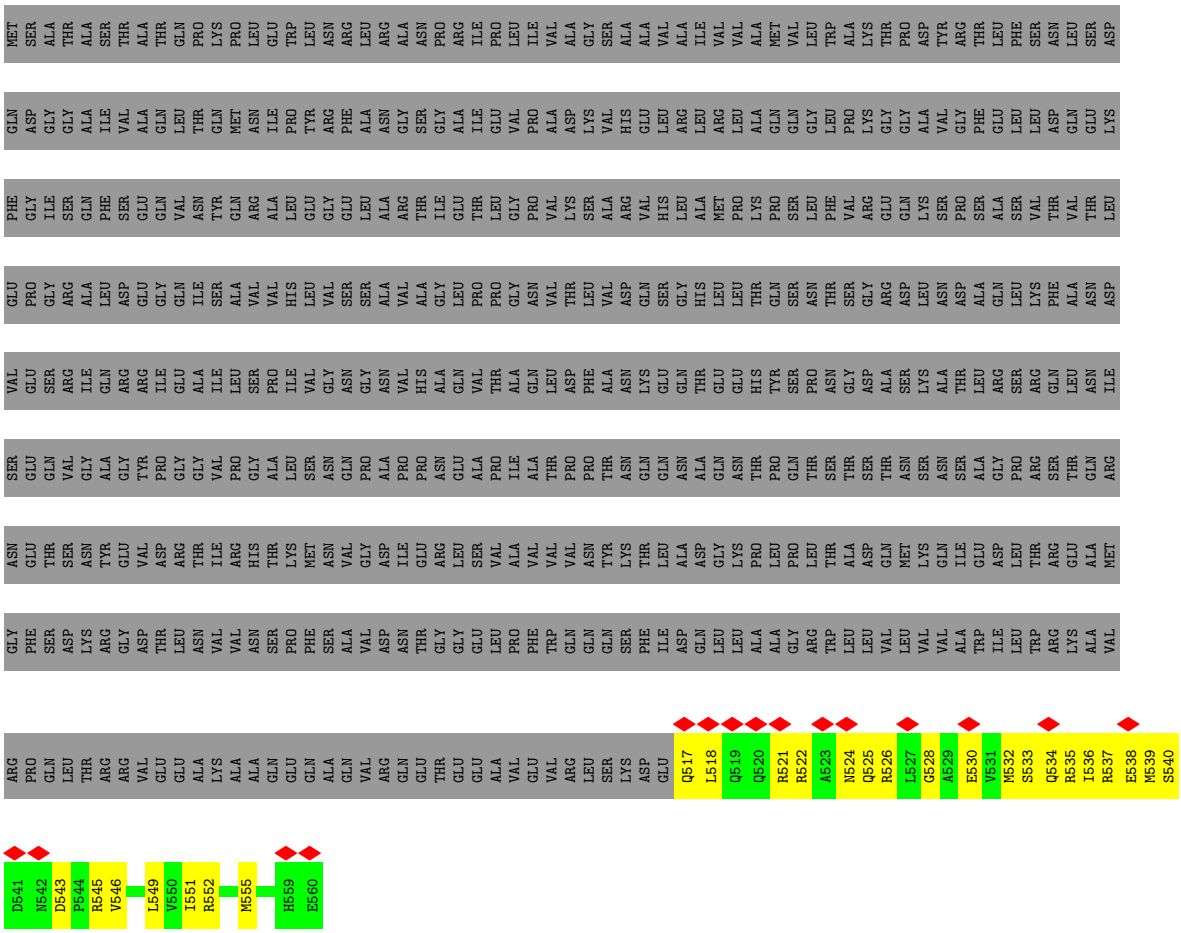
• Molecule 1: Flagellar M-ring protein

Chain A6: 92%



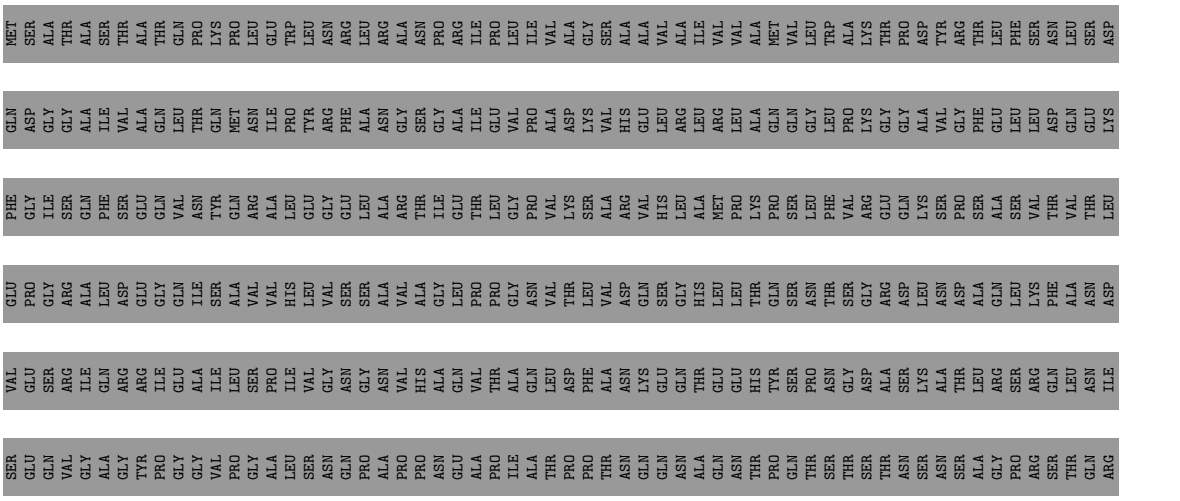
- Molecule 1: Flagellar M-ring protein

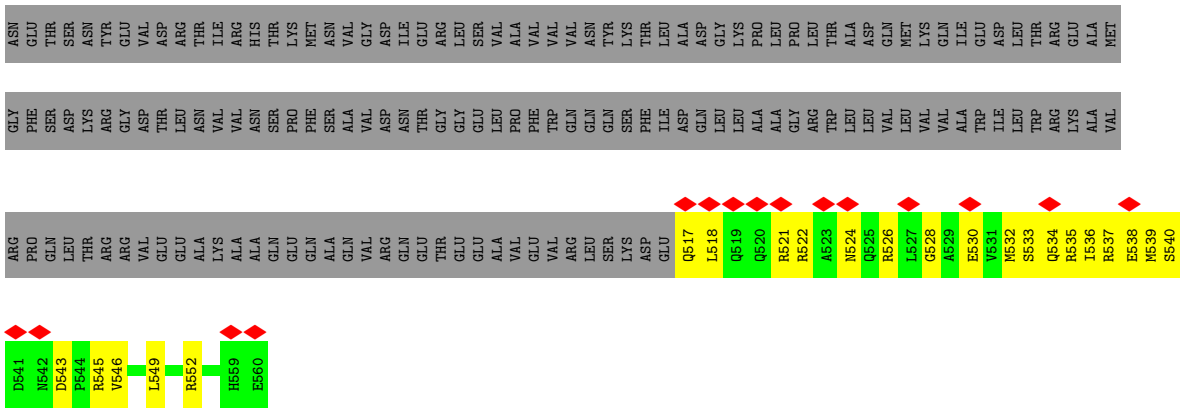
Chain A7: 92%



- Molecule 1: Flagellar M-ring protein

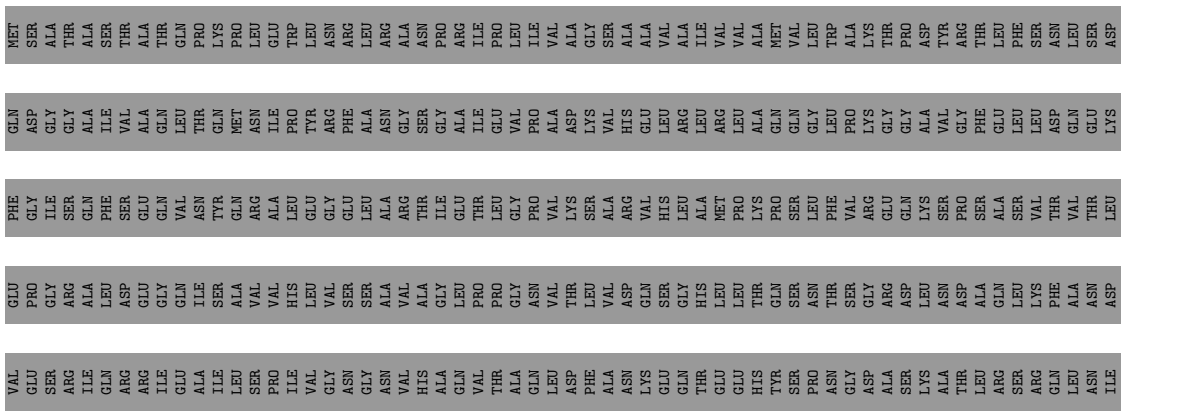
Chain A8: 92%





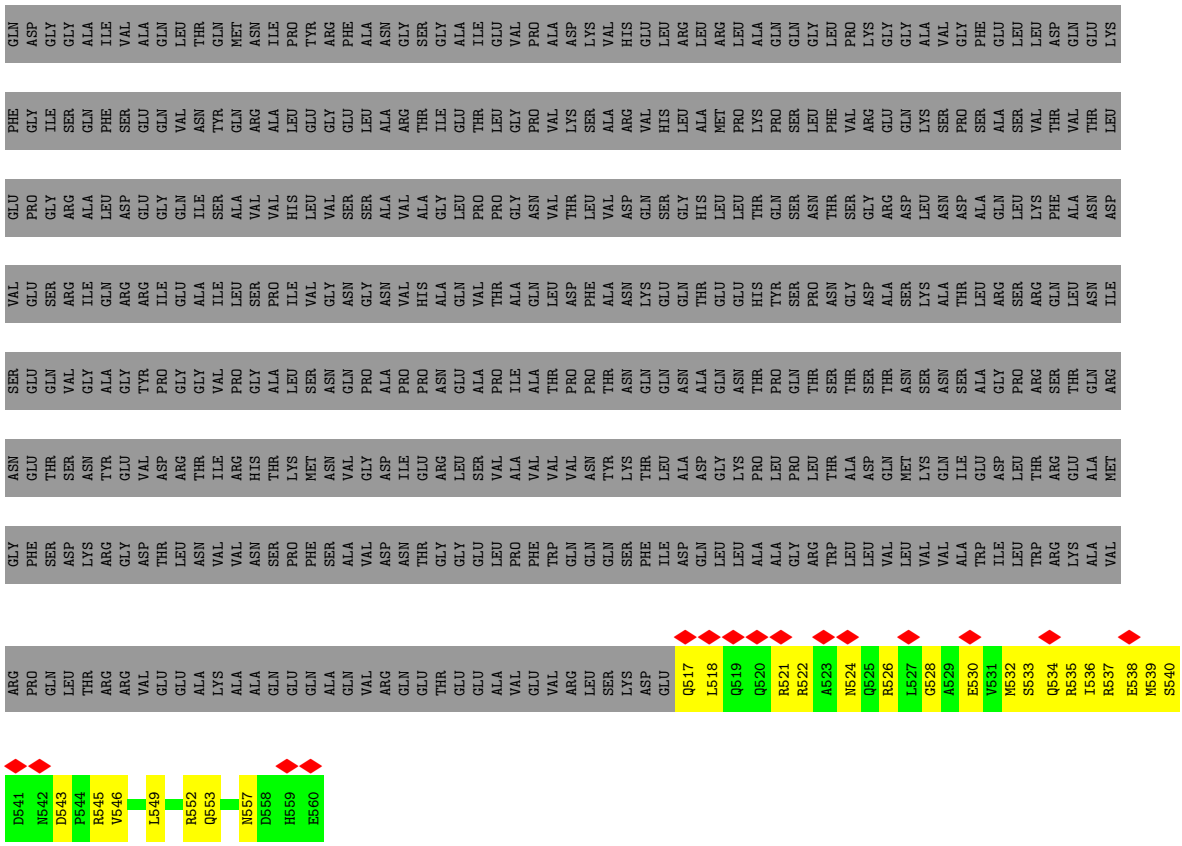
- Molecule 1: Flagellar M-ring protein

Chain A9: 92%



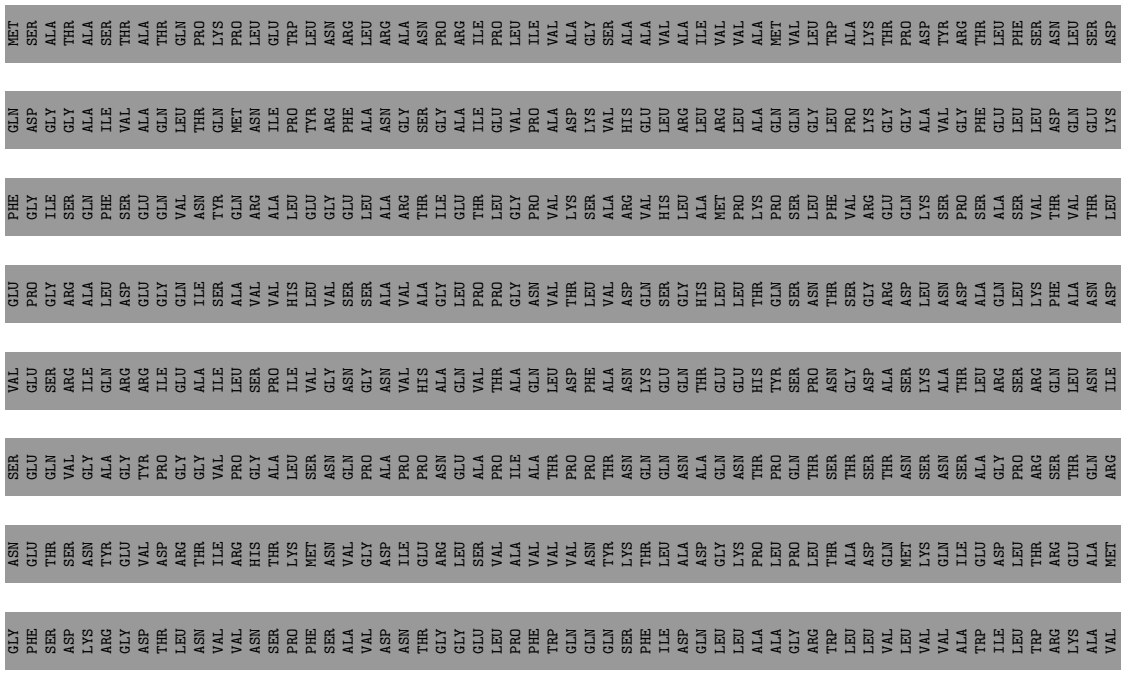
- Molecule 1: Flagellar M-ring protein

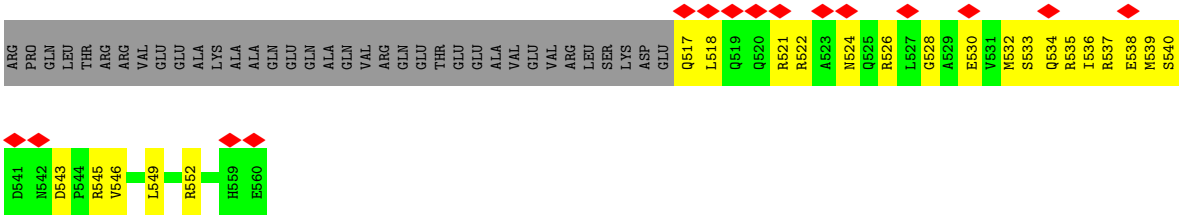
Chain AA: 92%



- Molecule 1: Flagellar M-ring protein

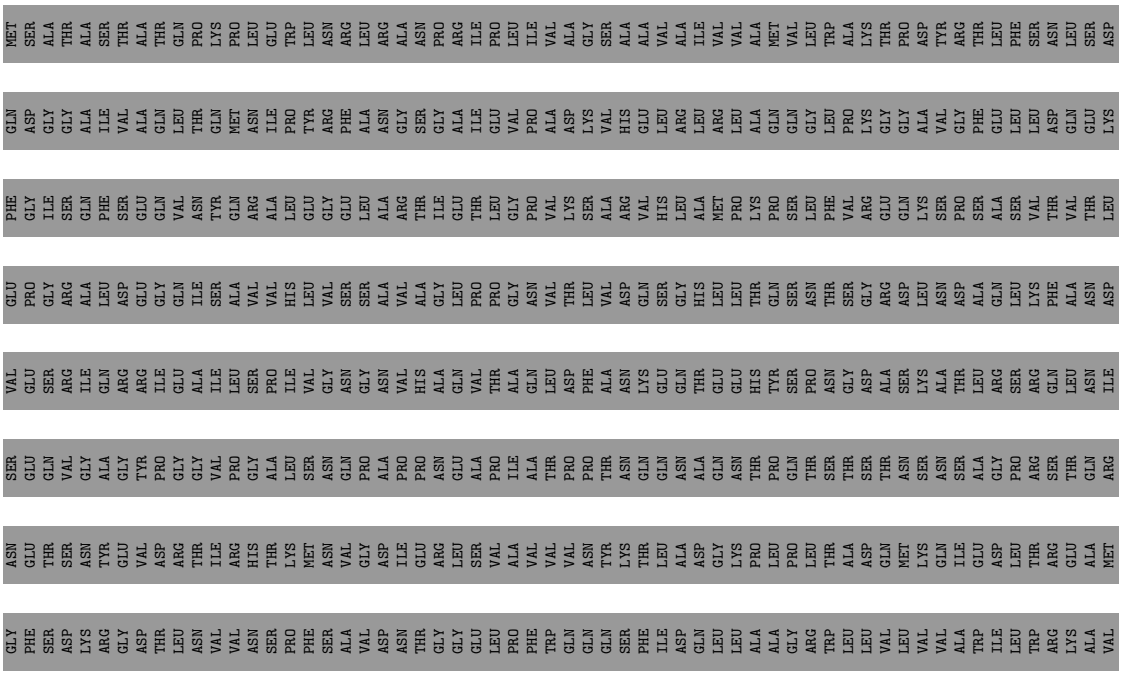
Chain AB: 92%





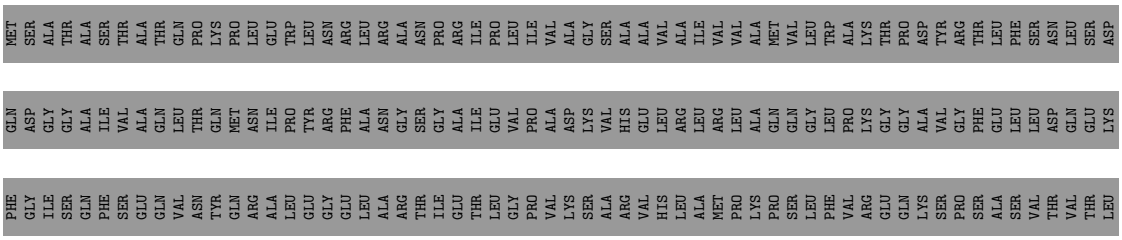
• Molecule 1: Flagellar M-ring protein

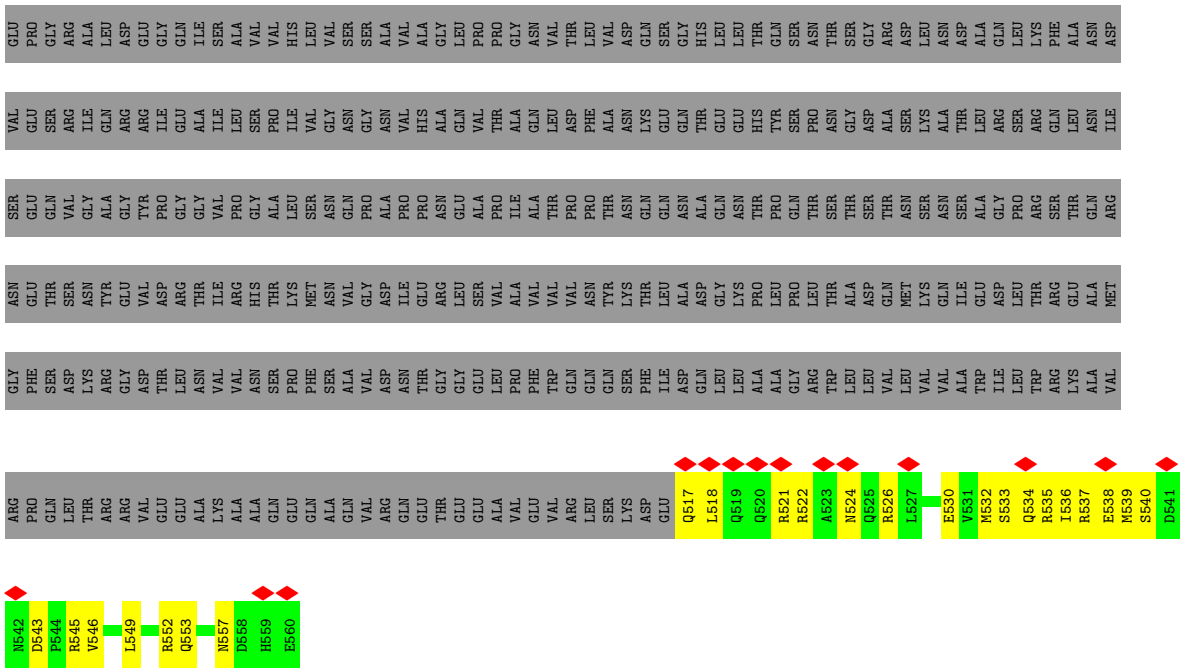
Chain AC: 92%



• Molecule 1: Flagellar M-ring protein

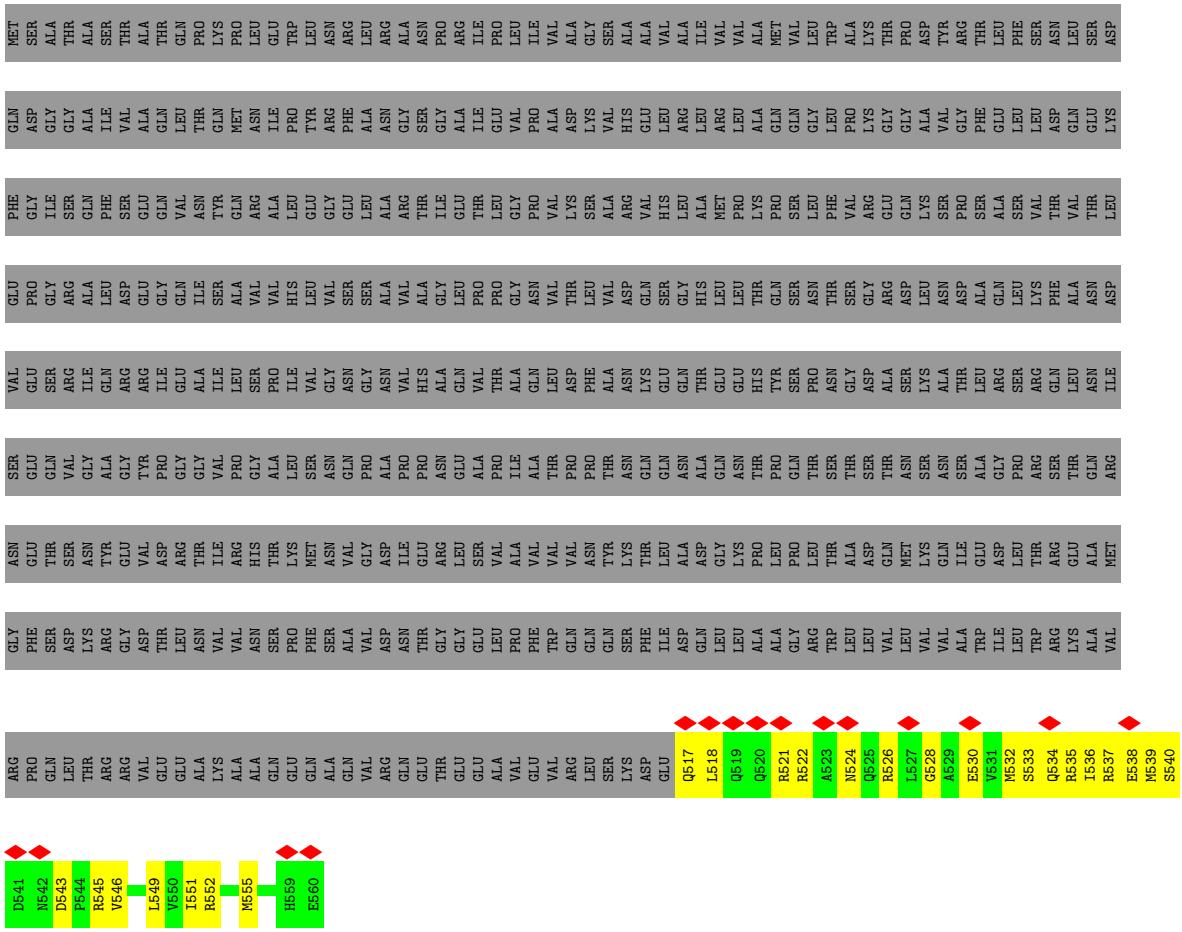
Chain AD: 92%





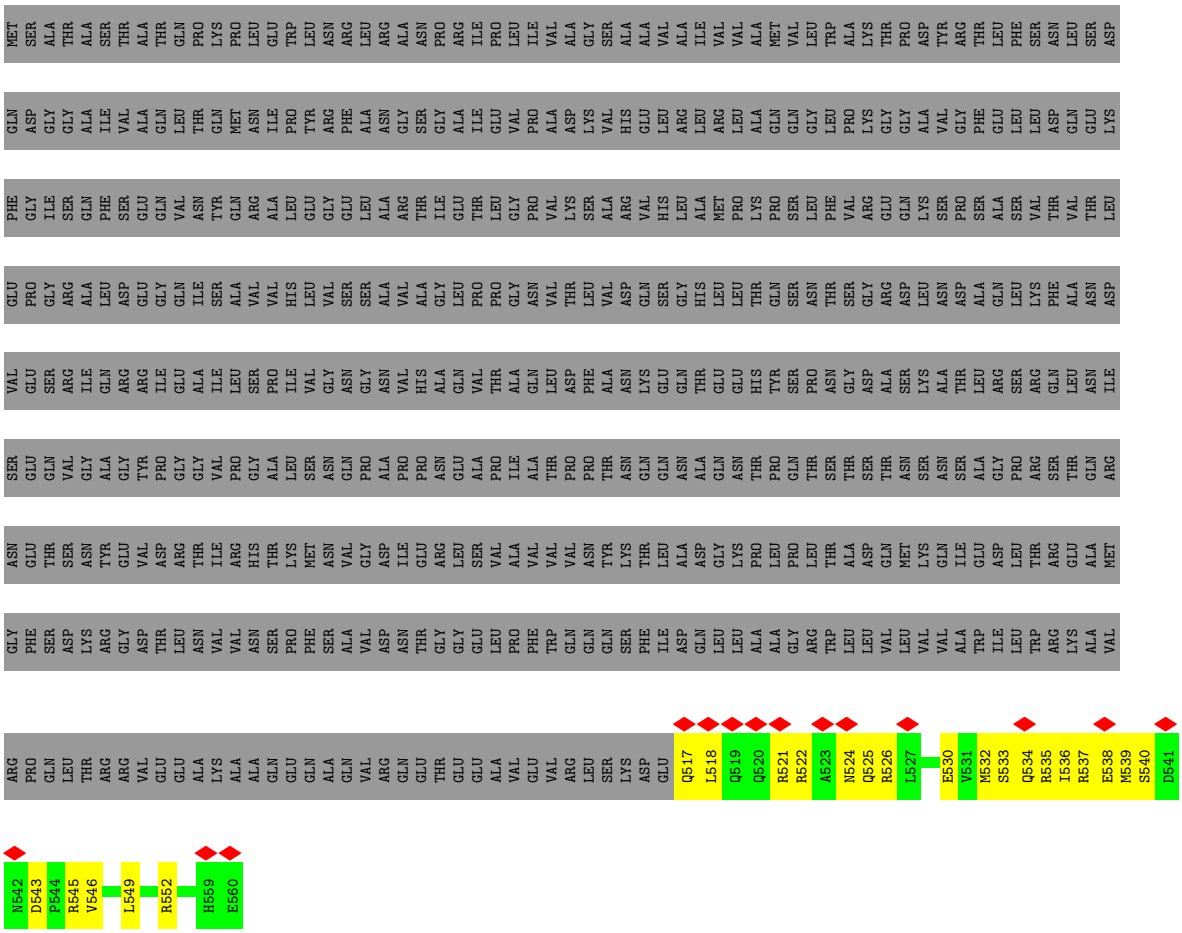
• Molecule 1: Flagellar M-ring protein

Chain AE: 92%



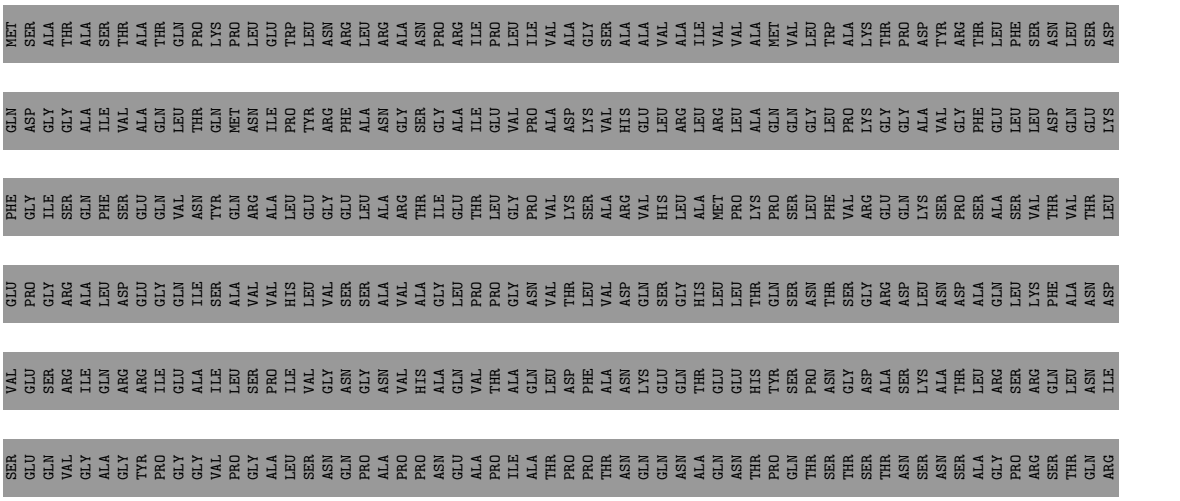
- Molecule 1: Flagellar M-ring protein

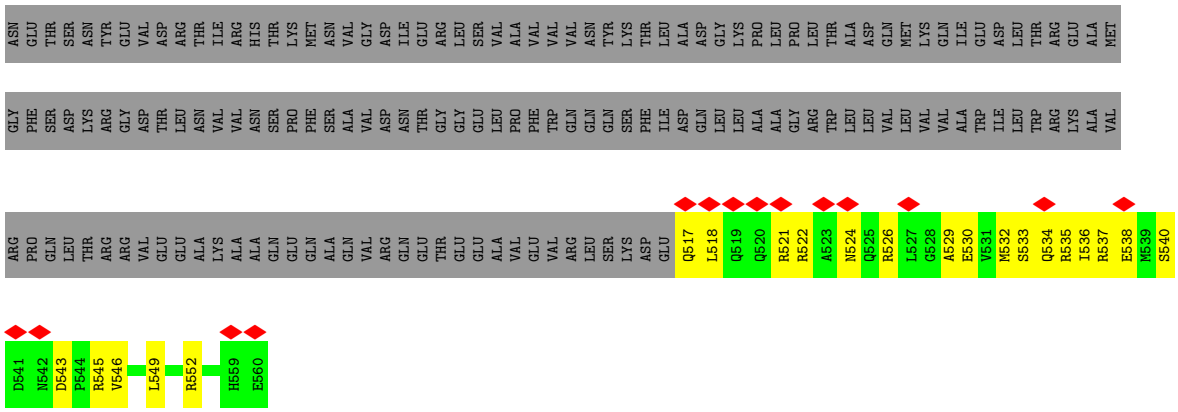
Chain AF: 92%



- Molecule 1: Flagellar M-ring protein

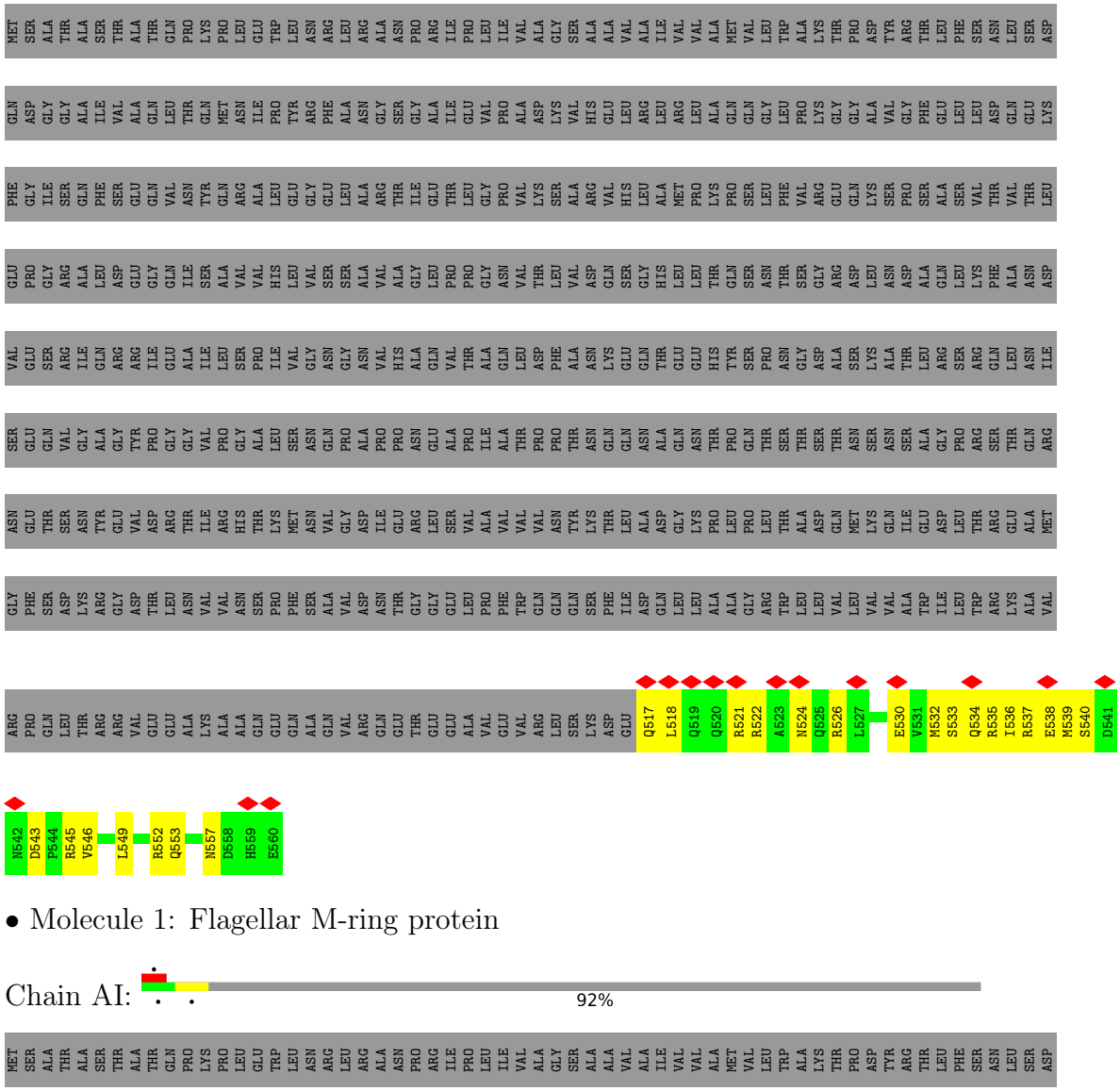
Chain AG: 92%





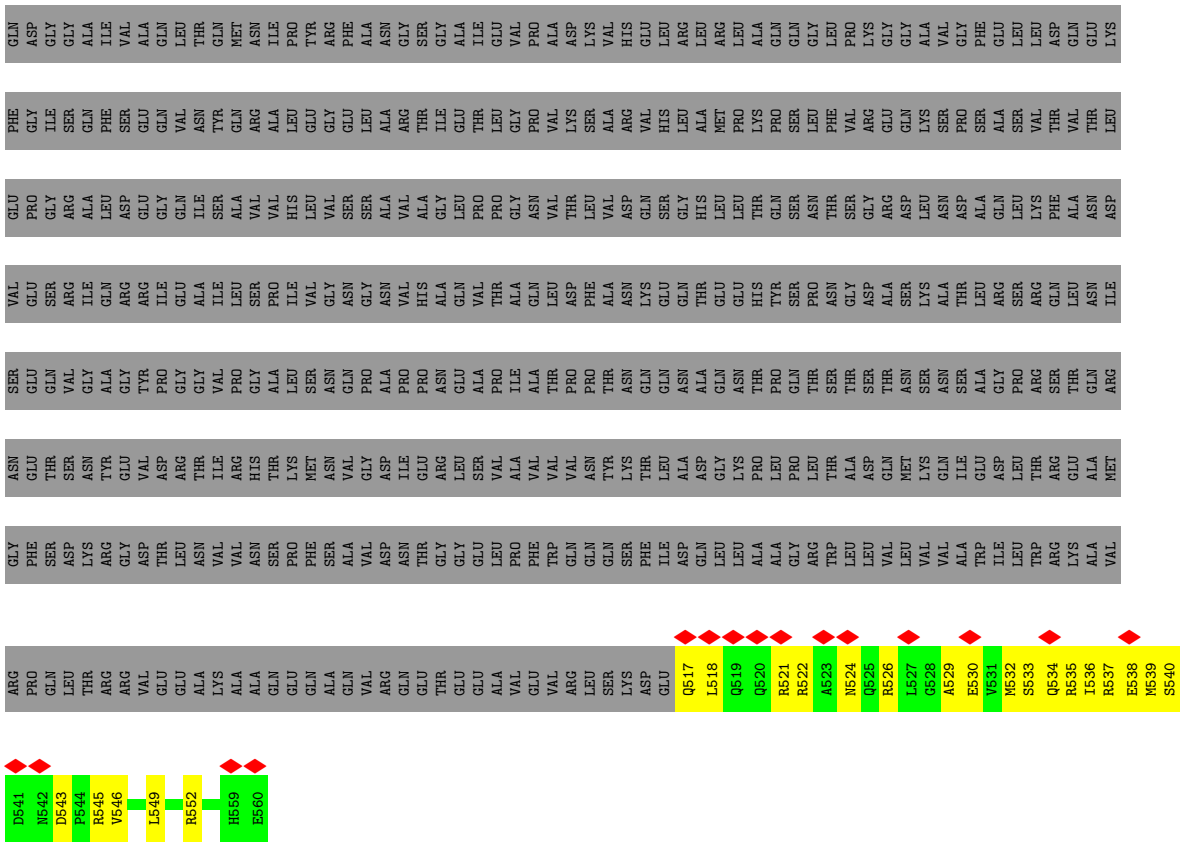
• Molecule 1: Flagellar M-ring protein

Chain AH: 92%



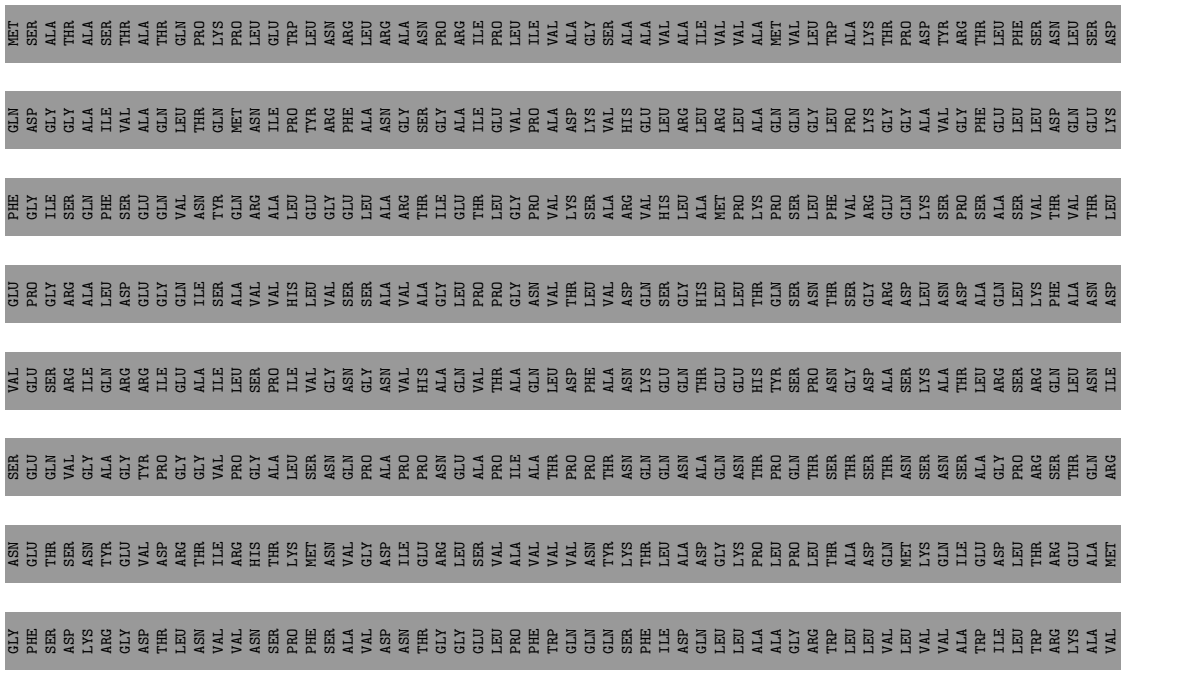
• Molecule 1: Flagellar M-ring protein

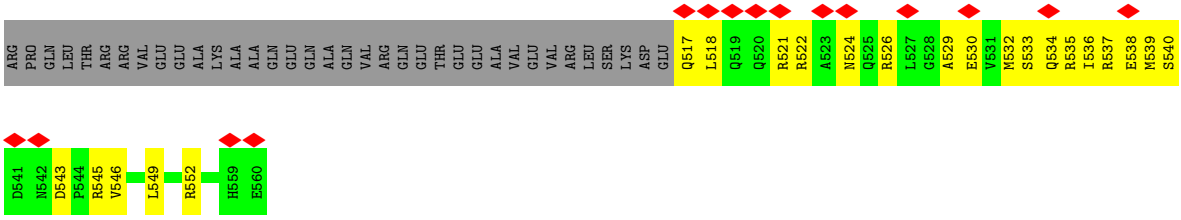
Chain AI: 92%



- Molecule 1: Flagellar M-ring protein

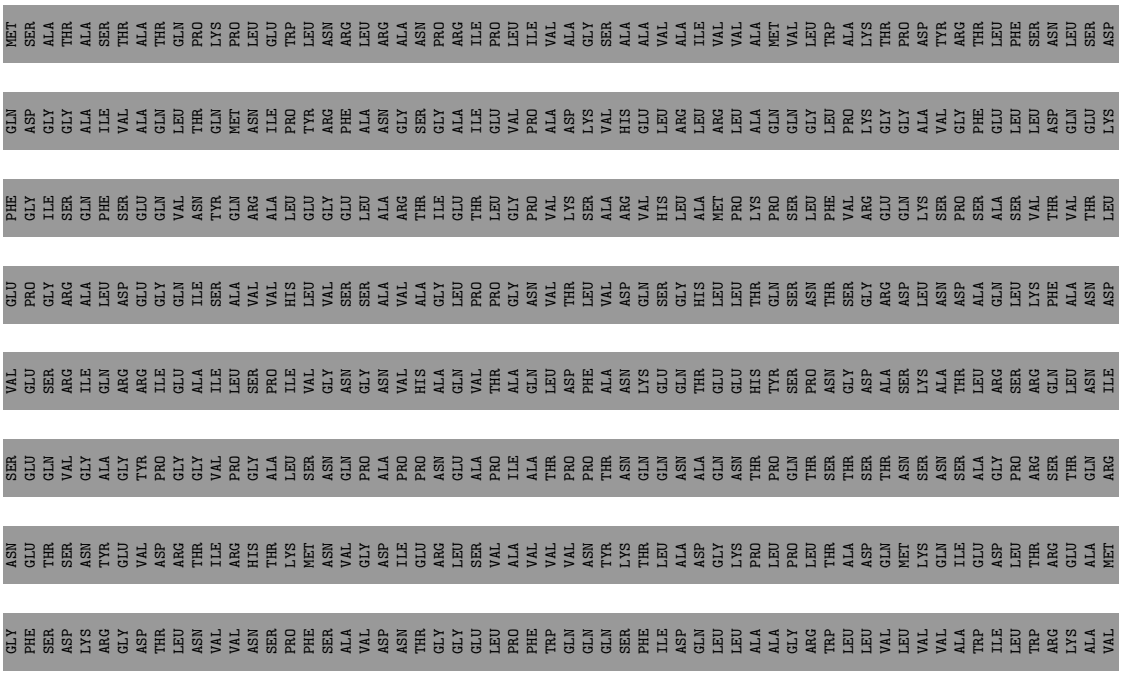
Chain AJ: 92%





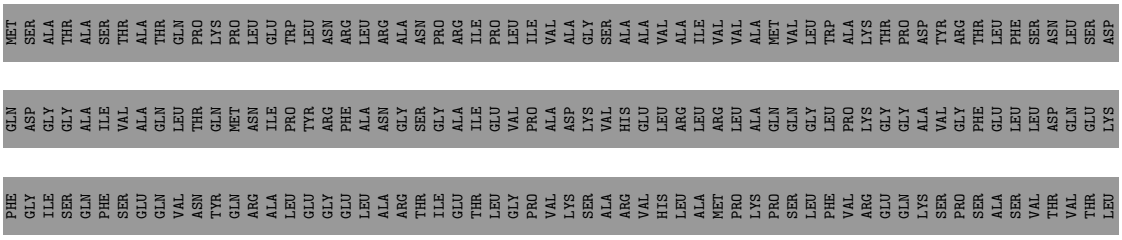
• Molecule 1: Flagellar M-ring protein

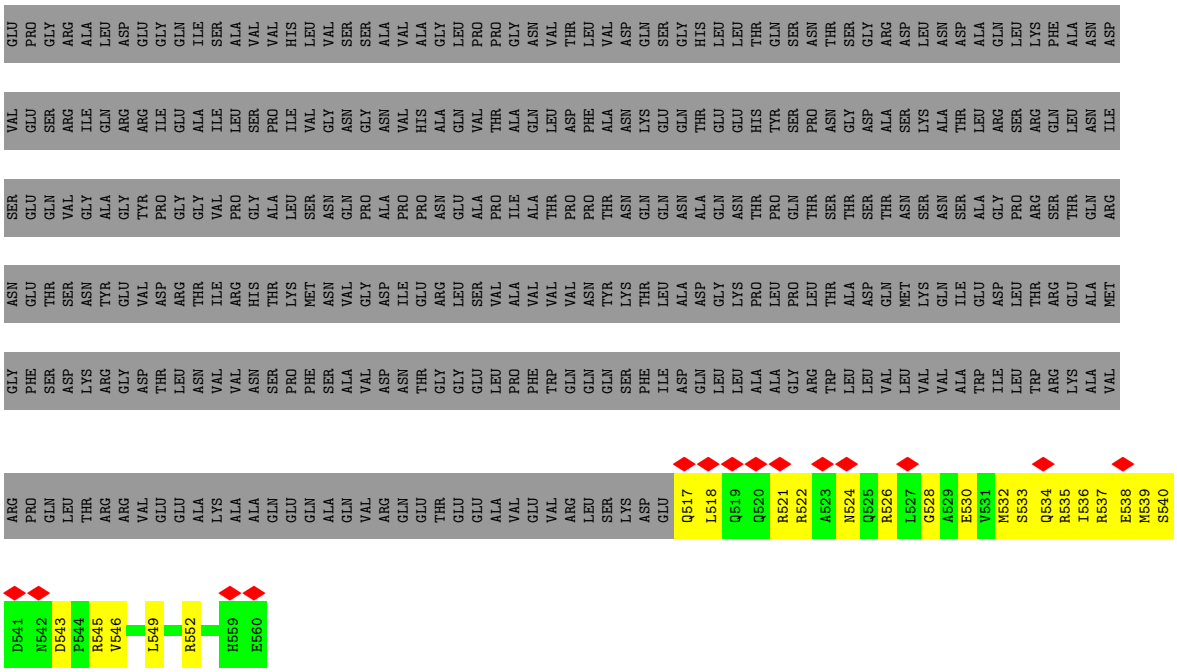
Chain AK: 92%



• Molecule 1: Flagellar M-ring protein

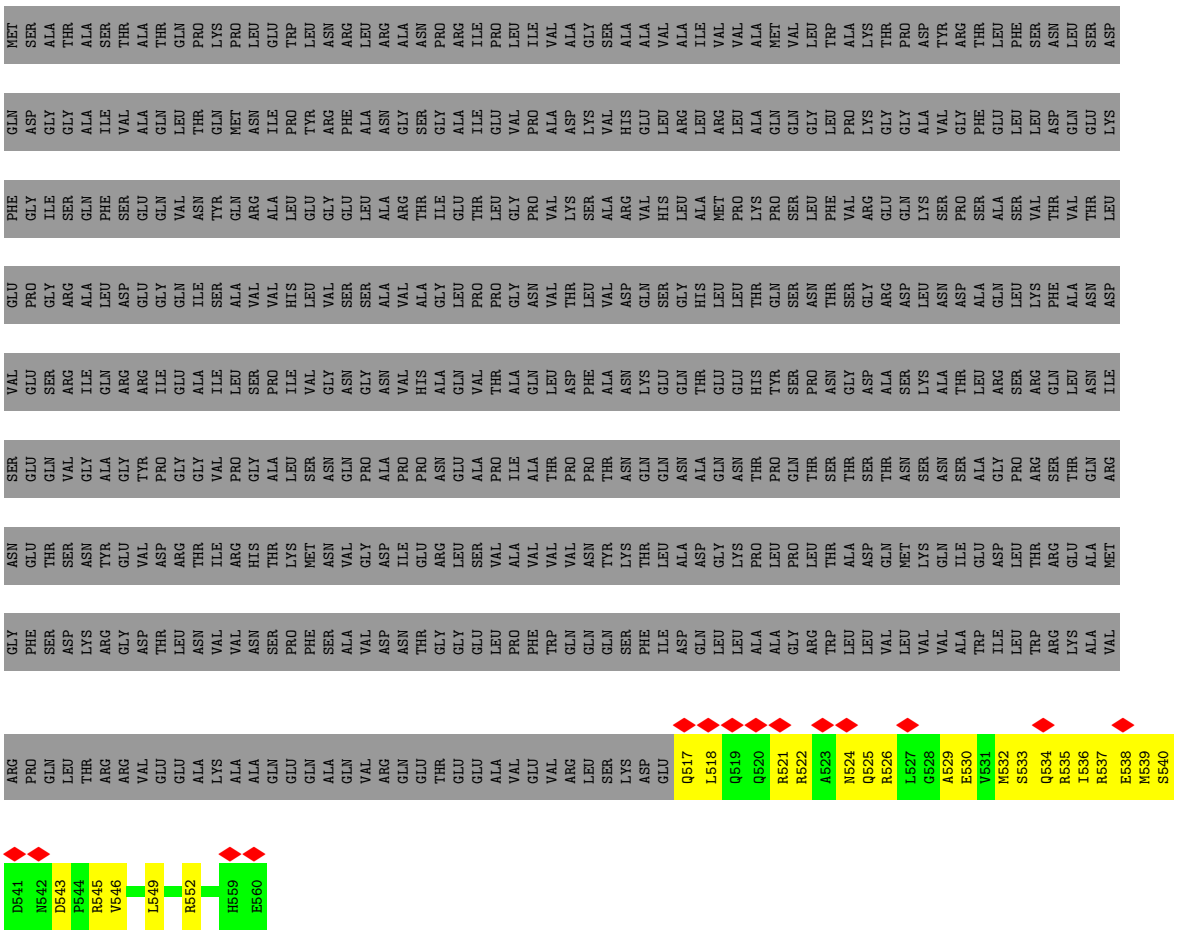
Chain AL: 92%





• Molecule 1: Flagellar M-ring protein

Chain AM: 92%



- Molecule 1: Flagellar M-ring protein

Chain AN: 92%

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

GLN ASP GLY GLY ALA ILE VAL ALA GLN LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ASN GLY SER GLY ALA ILE GLU VAL PRO ALA ASP LYS VAL HIS GLU LEU ARG LEU ARG LEU ALA GLN GLN GLY LEU PRO LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU ASP GLN GLU LYS

PHE GLY ILE SER GLN PHE SER GLU GLN VAL ASN TYR GLN ARG ALA LEU GLU GLY GLU LEU ALA ARG THR ILE GLU THR LEU GLY PRO VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO LYS PRO SER LEU PHE VAL ARG GLU GLN LYS SER PRO SER ALA SER VAL THR VAL THR LEU

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU ASN ASP LEU LYS PHE ALA ASN ASP

VAL GLU SER ARG ILE GLN ARG ARG ILE GLU ALA ILE LEU SER PRO ILE VAL GLY ASN GLY ASN VAL HIS ALA GLN VAL THR ALA GLN LEU ASP PHE ALA ASN LYS GLU GLN THR GLU GLU HIS TYR SER PRO ASN GLY ASP ALA SER LYS ALA THR LEU ARG SER ARG GLN LEU LEU ASN ILE

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLY GLN GLN ASN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG

ASN GLU THR SER ASN TYR GLU VAL ASP ARG THR ILE ARG HIS THR LYS MET ASN VAL GLY ASP ILE GLU ARG LEU SER VAL ALA ALA VAL VAL VAL ASN TYR LYS THR LEU ALA ASP GLY LYS PRO LEU PRO LEU THR ALA ASP GLN MET LYS GLN ILE GLU ASP LEU THR ARG GLU ALA MET

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

ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU Q517 L518 Q519 Q520 R521 R522 A523 N524 Q525 R526 L527 G528 A529 E530 V531 M532 S533 Q534 R535 T536 R537 E538 M539 S540

D541 N542 D543 P544 R545 V546 L549 R552 Q553 N557 D558 H559 E560

- Molecule 1: Flagellar M-ring protein

Chain AO: 5% 92%

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

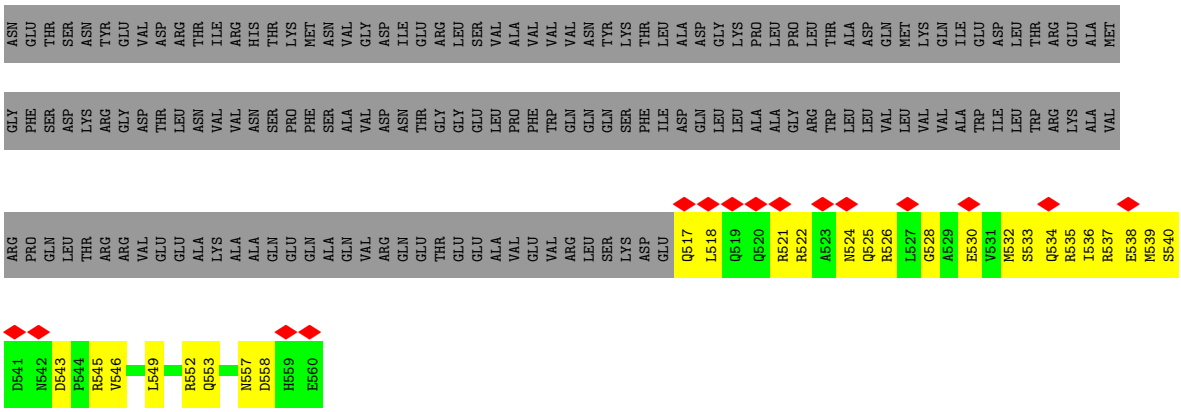
GLN ASP GLY GLY ALA ILE VAL ALA GLN LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ASN GLY SER GLY ALA ILE GLU VAL PRO ALA ASP LYS VAL HIS GLU LEU ARG LEU ARG LEU ALA GLN GLN GLY LEU PRO LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU ASP GLN GLU LYS

PHE GLY ILE SER GLN PHE SER GLU GLN VAL ASN TYR GLN ARG ALA LEU GLU GLY GLU LEU ALA ARG THR ILE GLU THR LEU GLY PRO VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO LYS PRO SER LEU PHE VAL ARG GLU GLN LYS SER PRO SER ALA SER VAL THR VAL THR LEU

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU ASN ASP LEU LYS PHE ALA ASN ASP

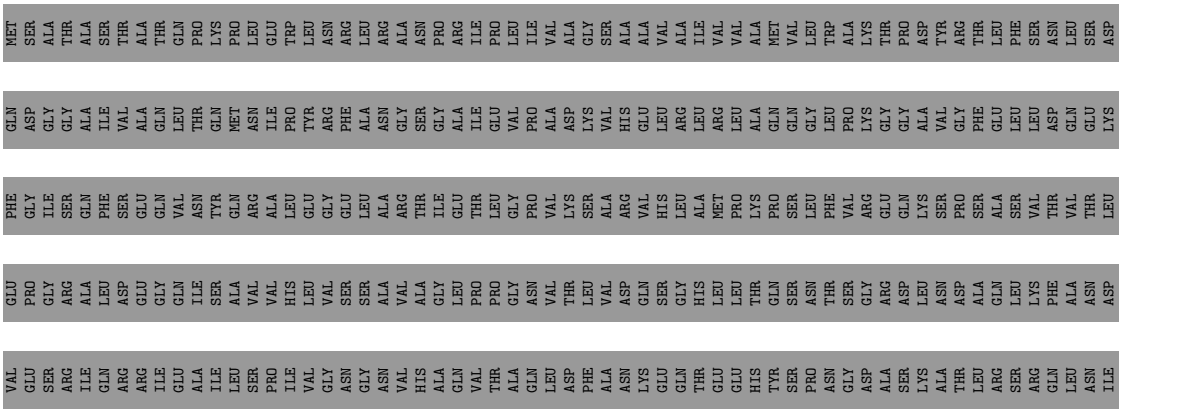
VAL GLU SER ARG ILE GLN ARG ARG ILE GLU ALA ILE LEU SER PRO ILE VAL GLY ASN GLY ASN VAL HIS ALA GLN VAL THR ALA GLN LEU ASP PHE ALA ASN LYS GLU GLN THR GLU GLU HIS TYR SER PRO ASN GLY ASP ALA SER LYS ALA THR LEU ARG SER ARG GLN LEU LEU ASN ILE

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLY GLN GLN ASN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG



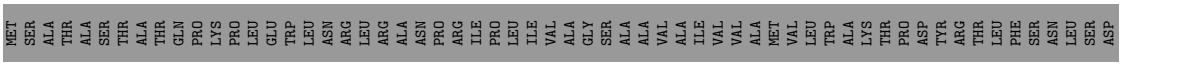
- Molecule 1: Flagellar M-ring protein

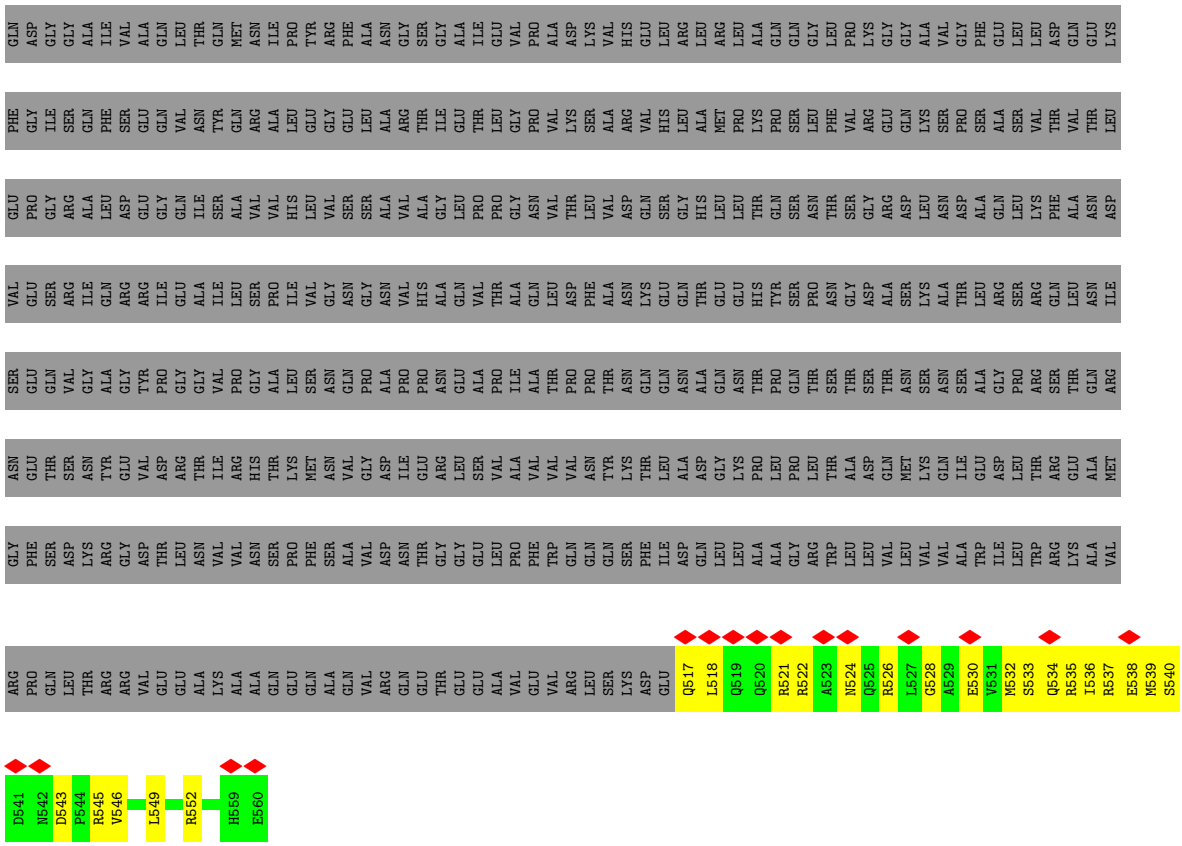
Chain AP: 92%



- Molecule 1: Flagellar M-ring protein

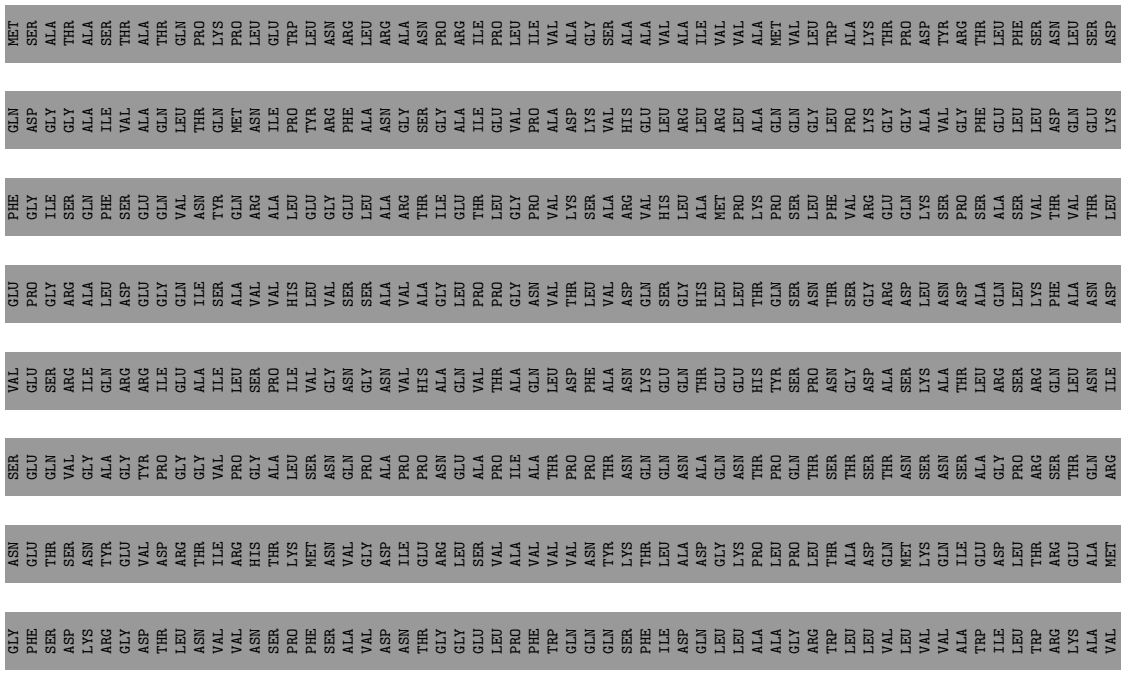
Chain AQ: 92%

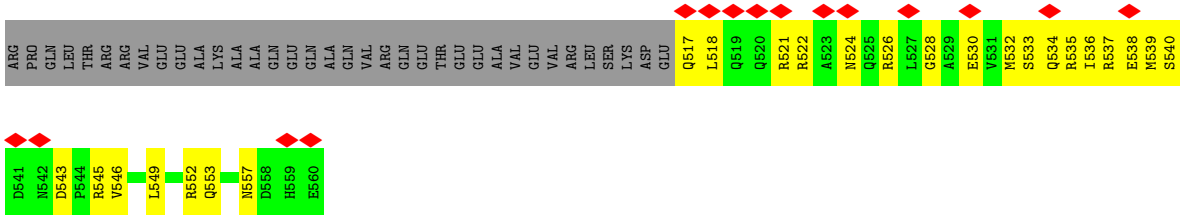




• Molecule 1: Flagellar M-ring protein

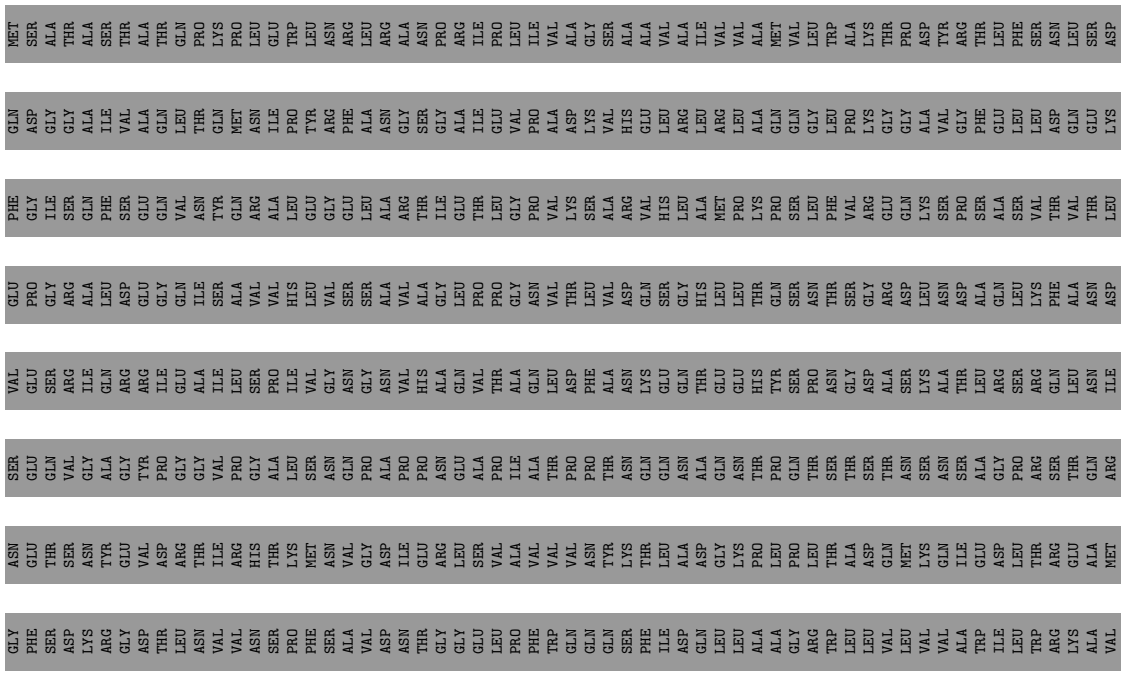
Chain AR: 92%





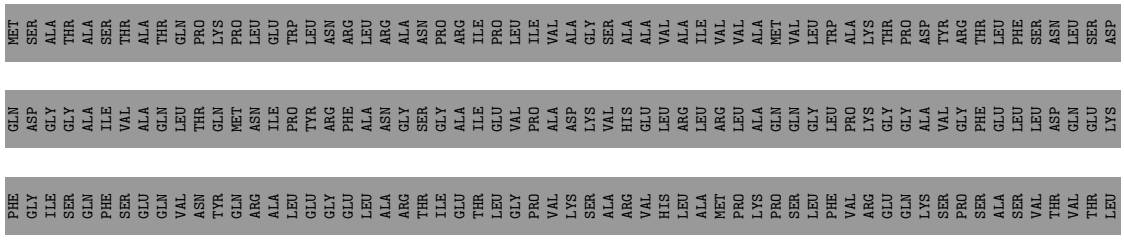
• Molecule 1: Flagellar M-ring protein

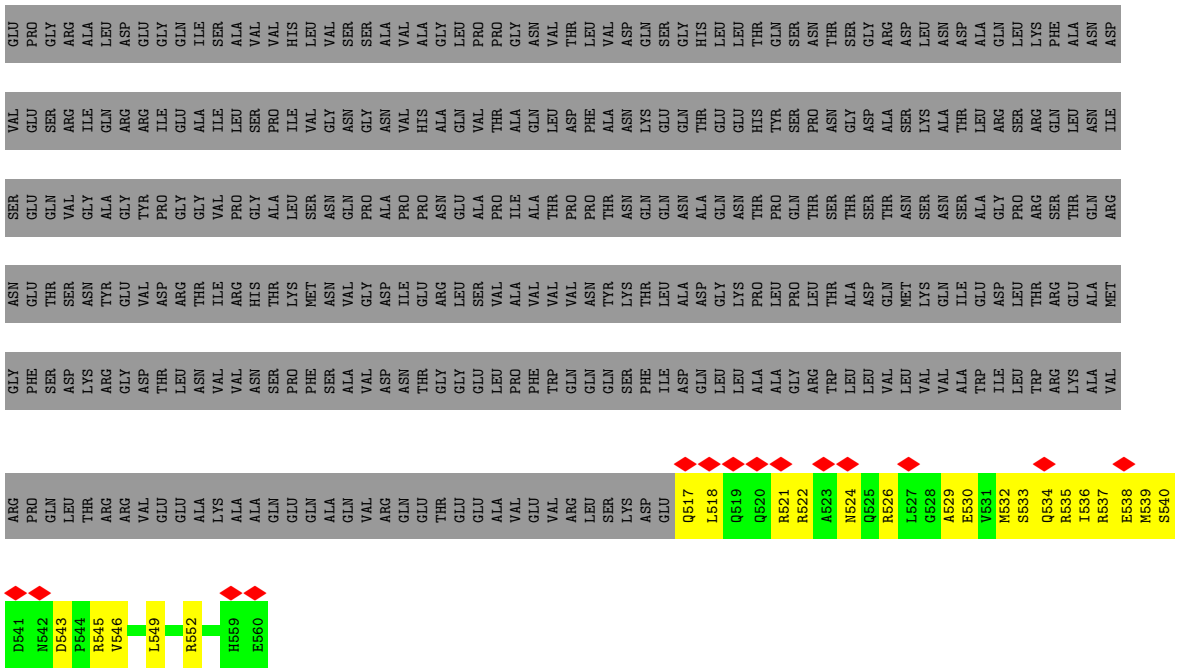
Chain AS: 92%



• Molecule 1: Flagellar M-ring protein

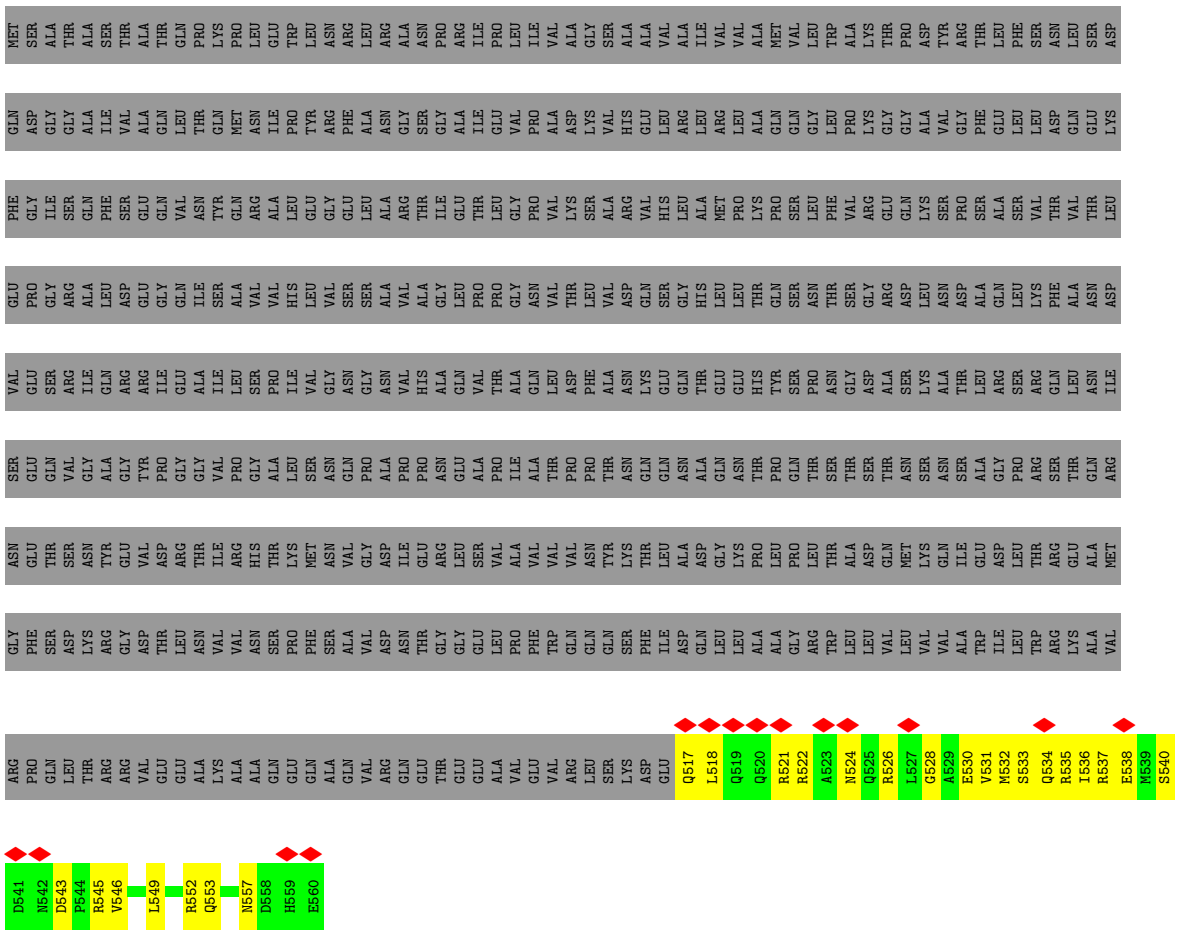
Chain AT: 92%





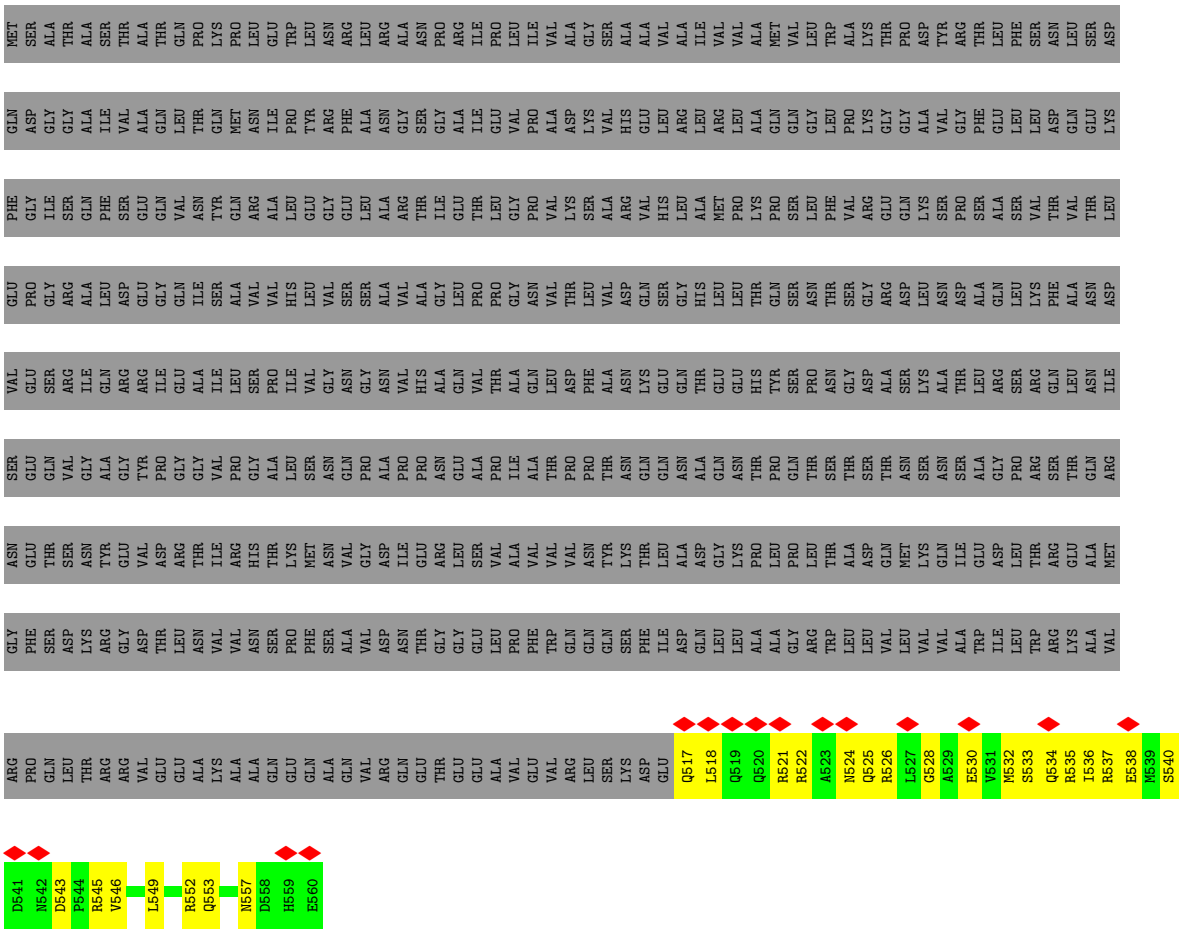
• Molecule 1: Flagellar M-ring protein

Chain AU: 92%



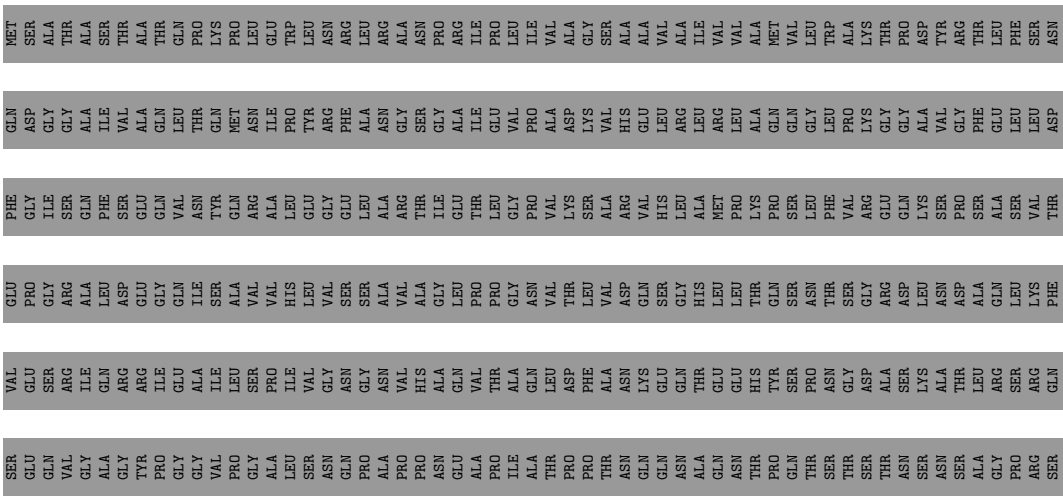
- Molecule 1: Flagellar M-ring protein

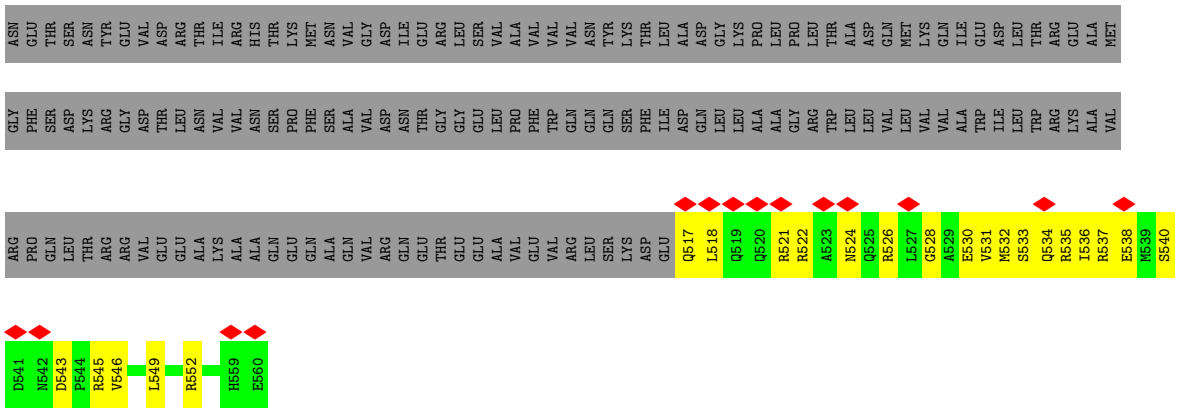
Chain AV: 92%



- Molecule 1: Flagellar M-ring protein

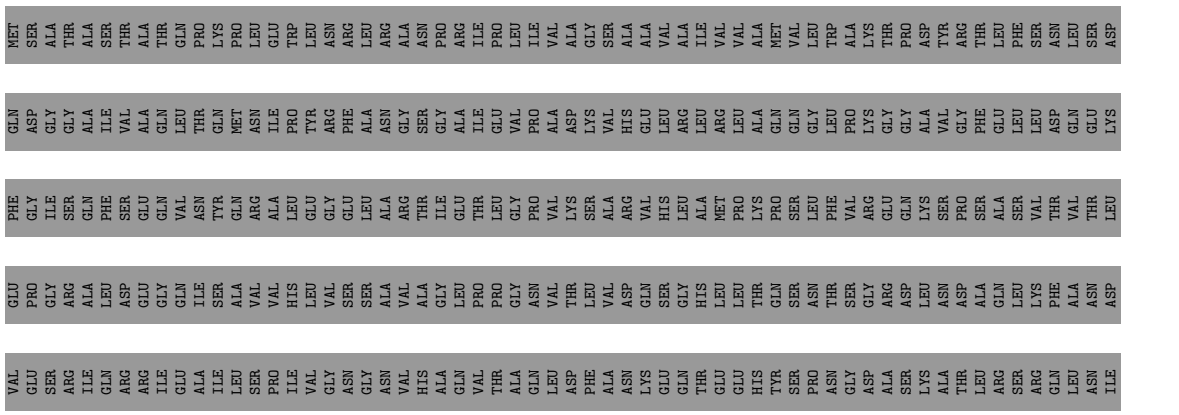
Chain AW: 92%





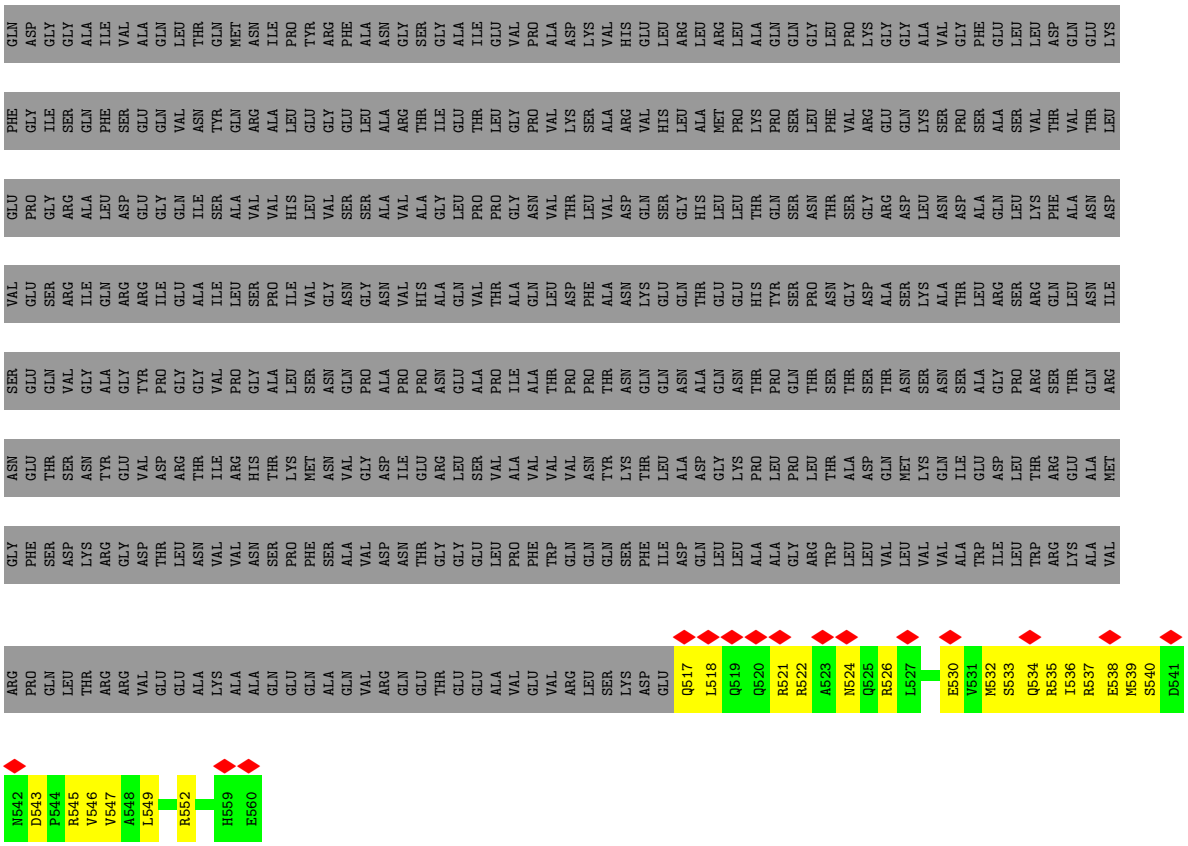
- Molecule 1: Flagellar M-ring protein

Chain AX: 92%



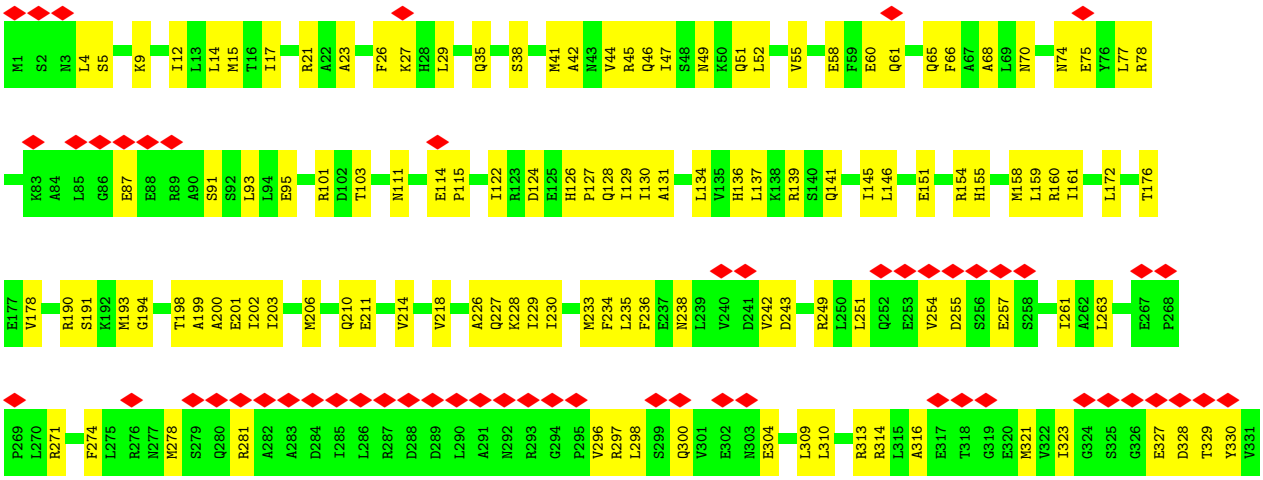
- Molecule 1: Flagellar M-ring protein

Chain AY: 92%



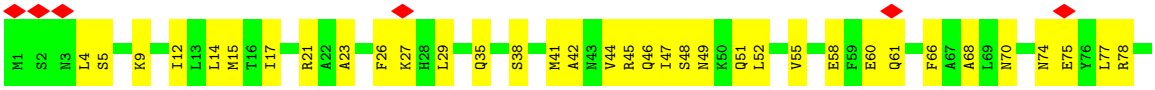
• Molecule 2: Flagellar motor switch protein FliG

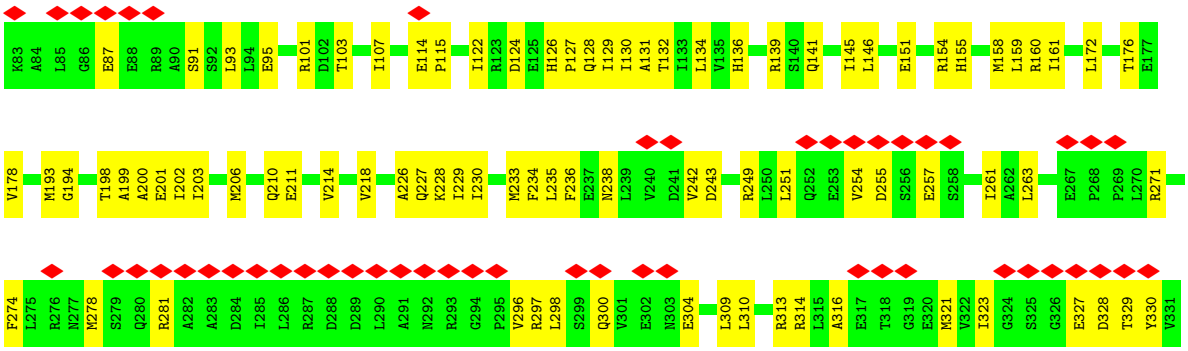
Chain B1:



• Molecule 2: Flagellar motor switch protein FliG

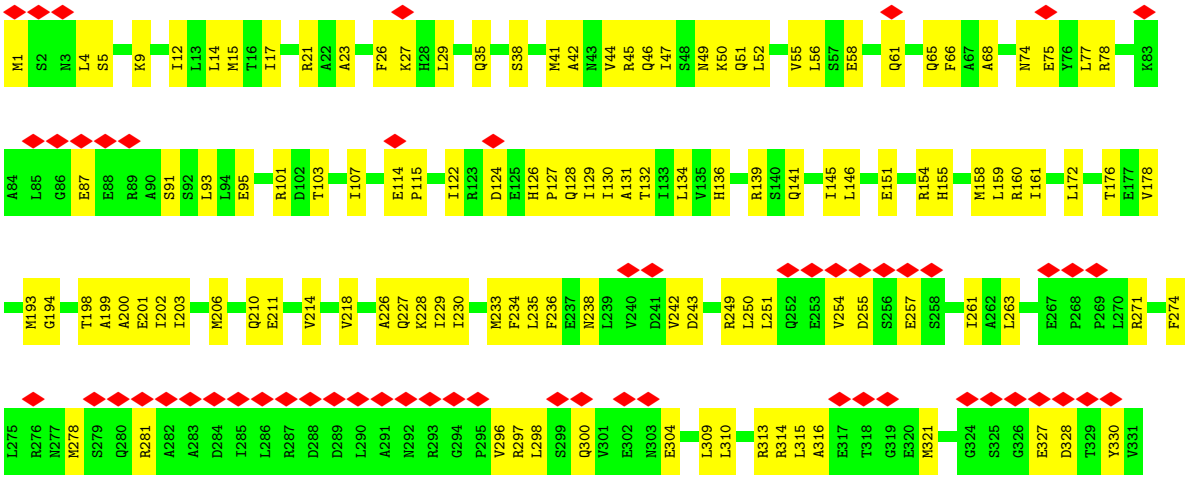
Chain B2:





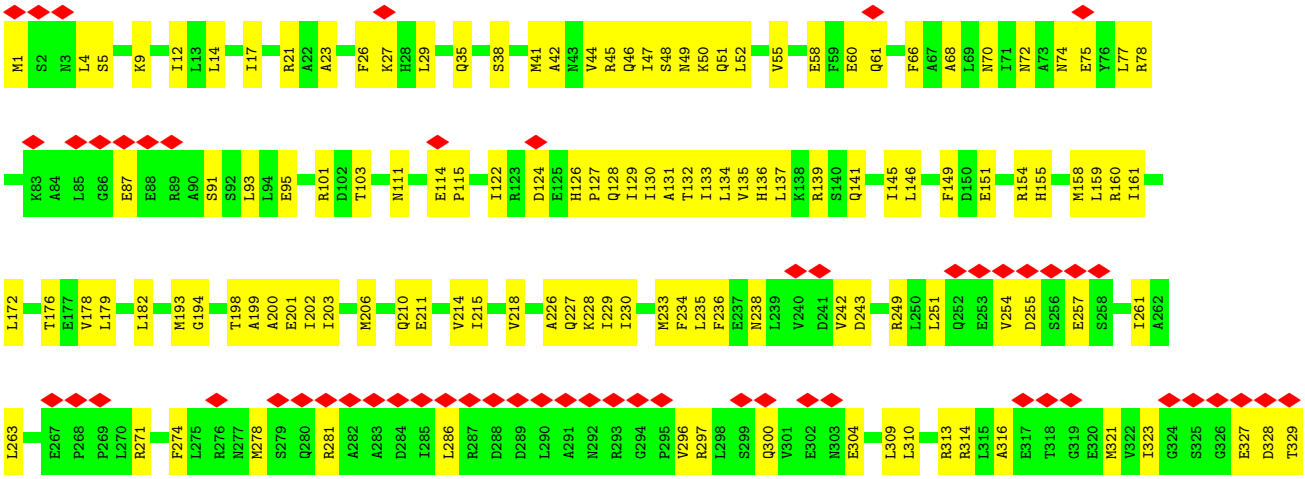
• Molecule 2: Flagellar motor switch protein FliG

Chain B3:



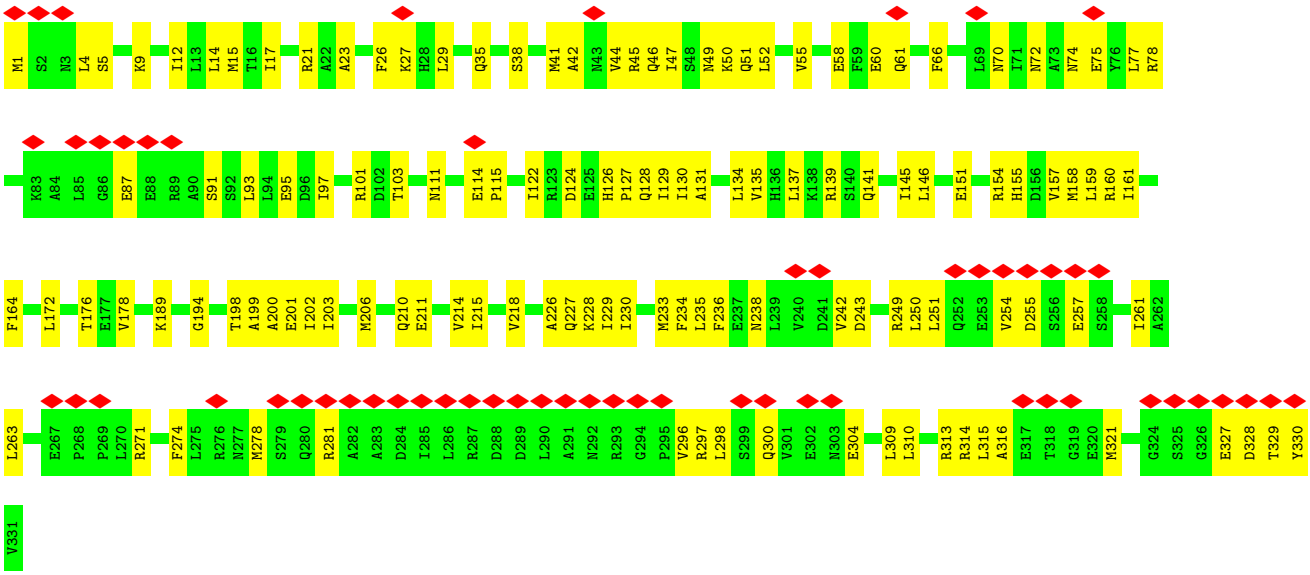
• Molecule 2: Flagellar motor switch protein FliG

Chain B4:



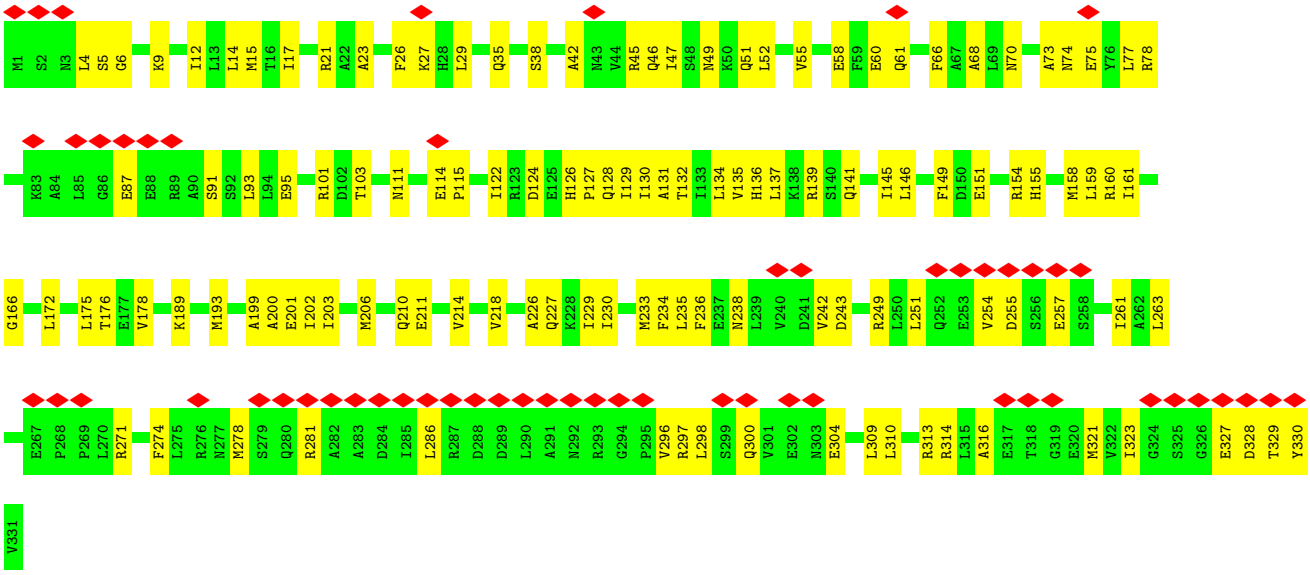
• Molecule 2: Flagellar motor switch protein FliG

Chain B5:



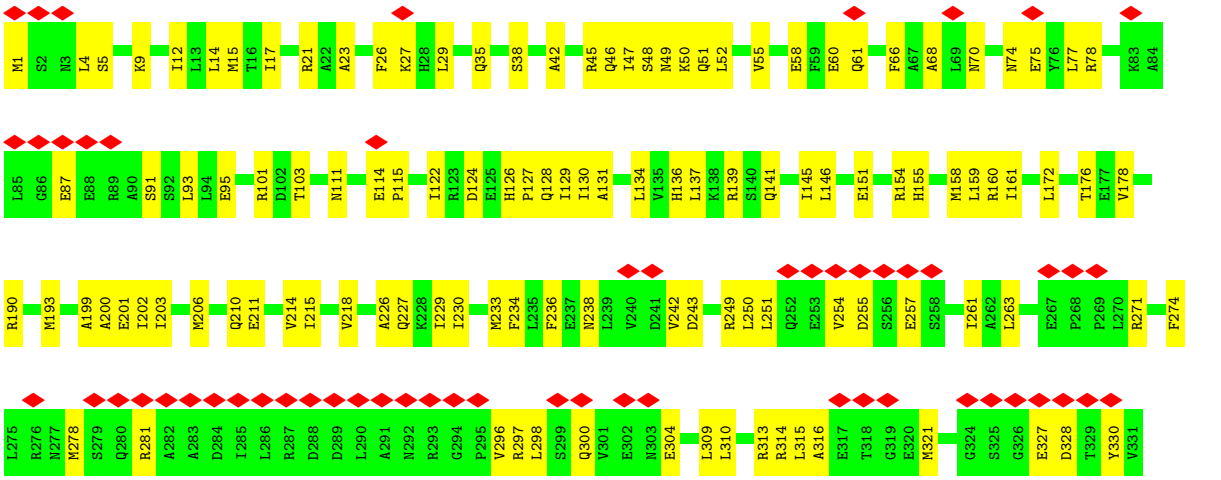
• Molecule 2: Flagellar motor switch protein FliG

Chain B6:



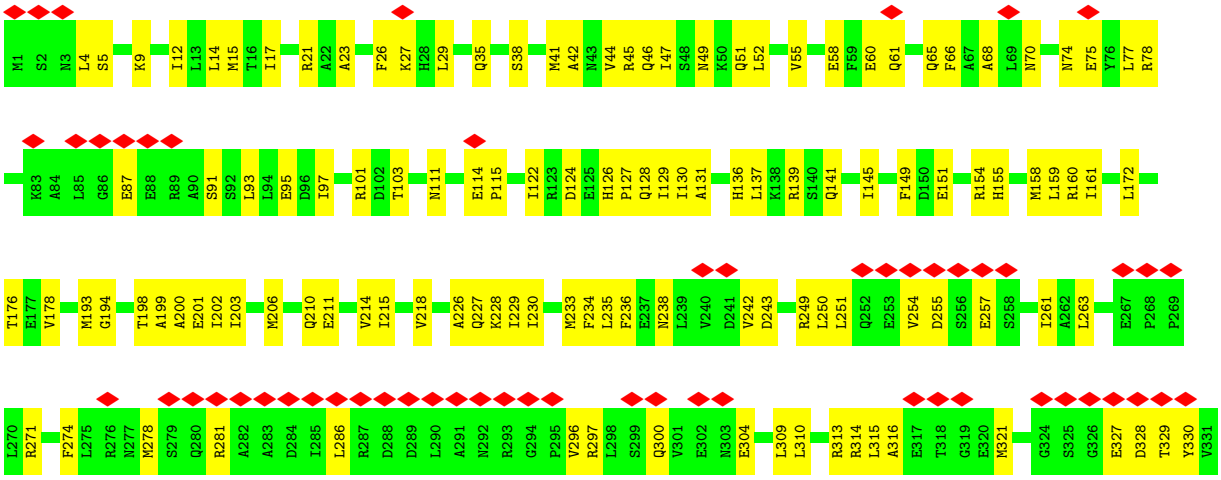
• Molecule 2: Flagellar motor switch protein FliG

Chain B7:



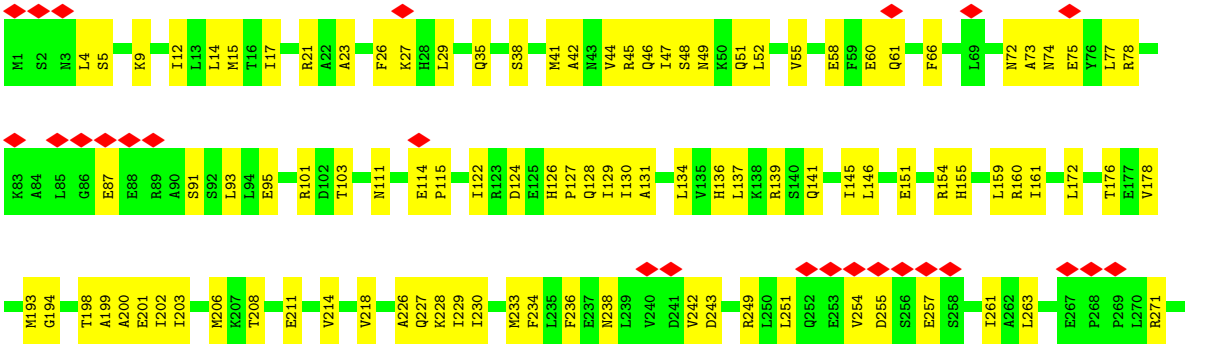
• Molecule 2: Flagellar motor switch protein FliG

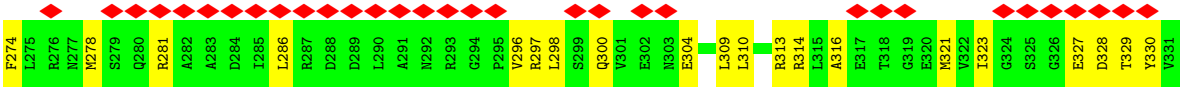
Chain B8:



• Molecule 2: Flagellar motor switch protein FliG

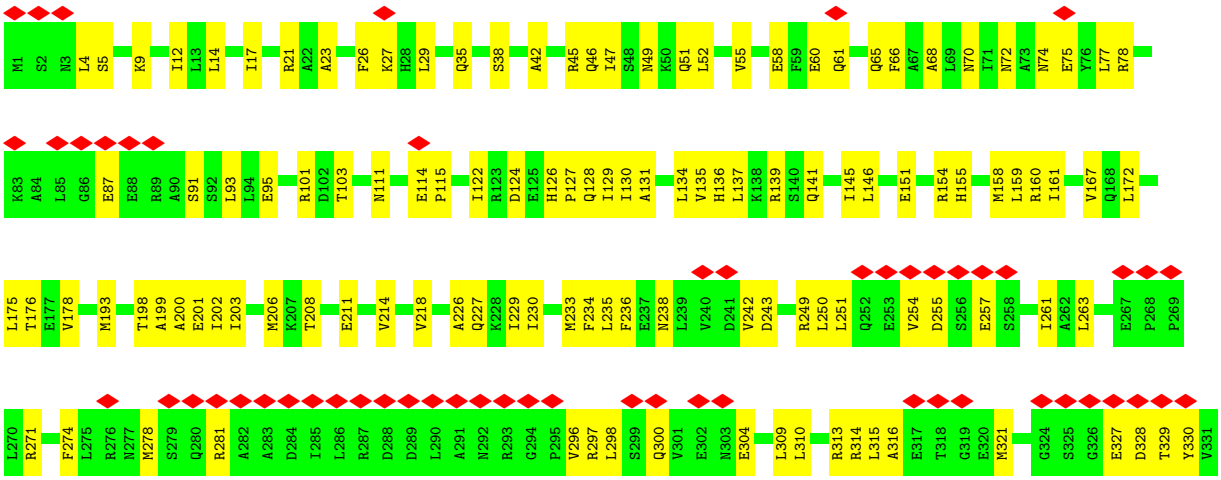
Chain B9:





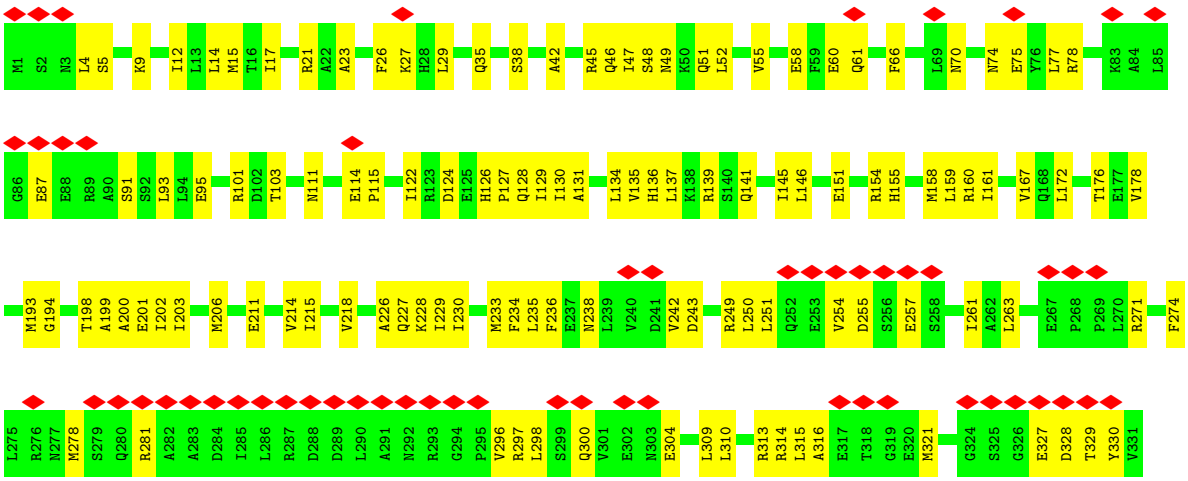
• Molecule 2: Flagellar motor switch protein FliG

Chain BA:



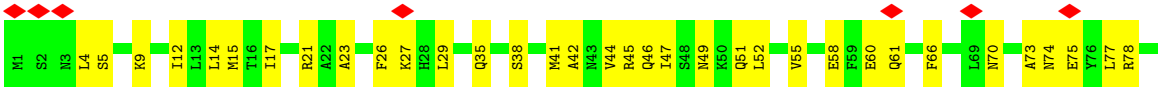
• Molecule 2: Flagellar motor switch protein FliG

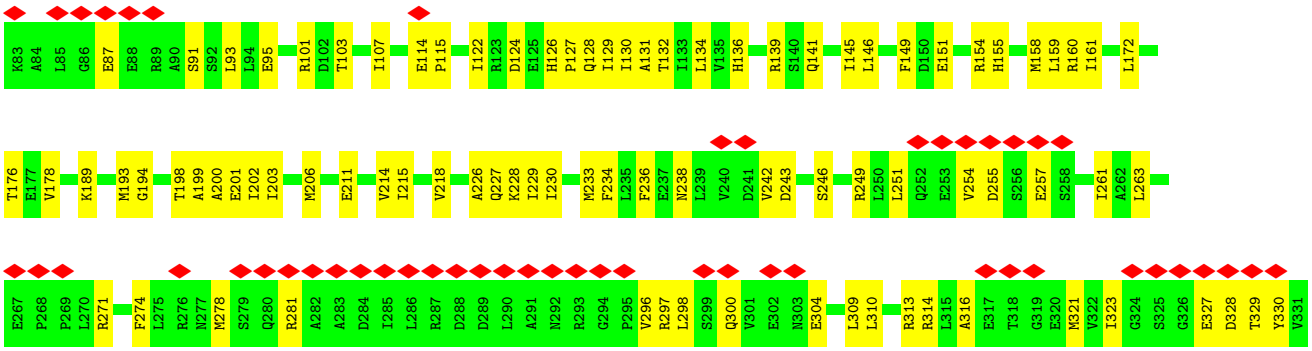
Chain BB:



• Molecule 2: Flagellar motor switch protein FliG

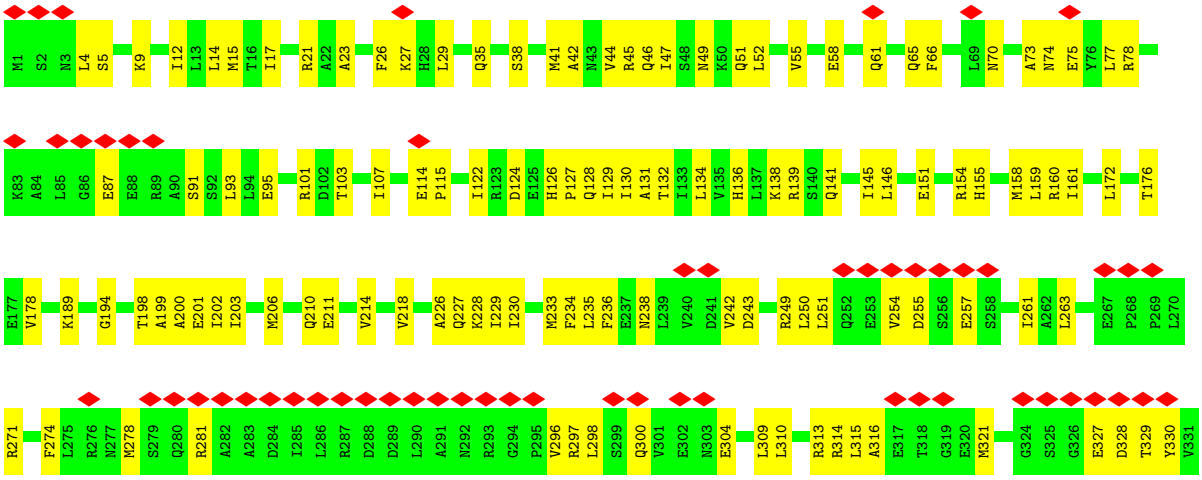
Chain BC:





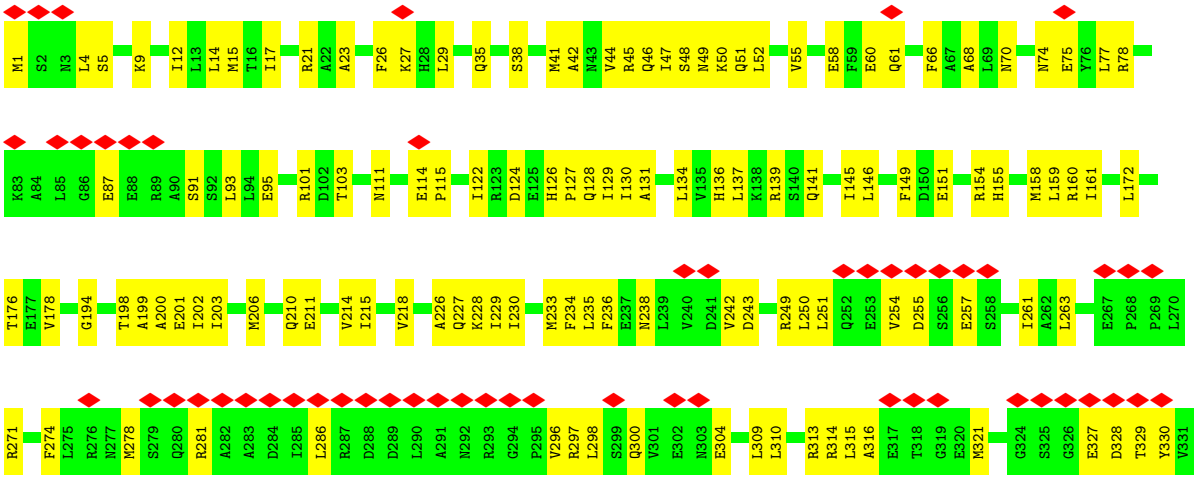
• Molecule 2: Flagellar motor switch protein FliG

Chain BD:



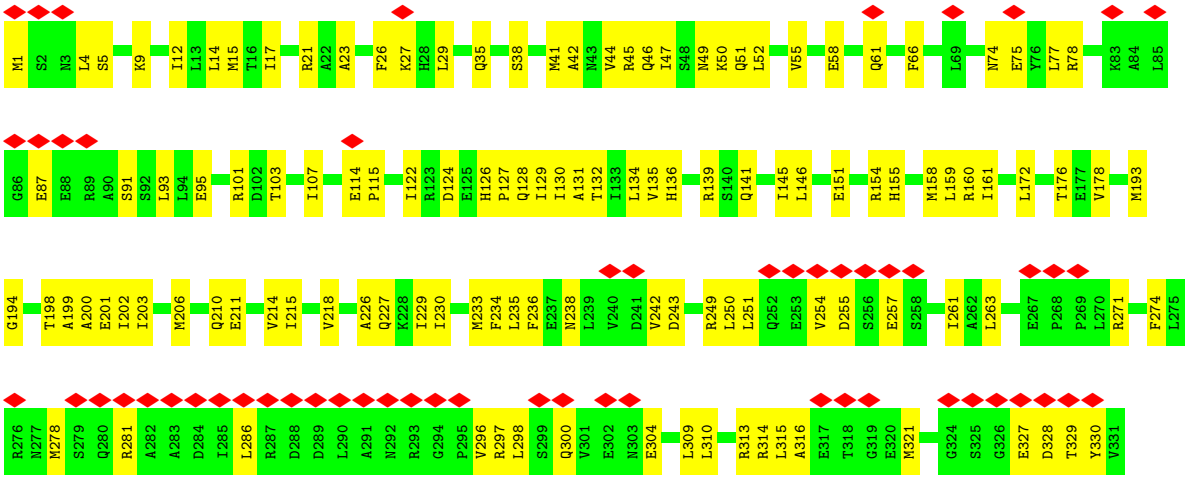
• Molecule 2: Flagellar motor switch protein FliG

Chain BE:



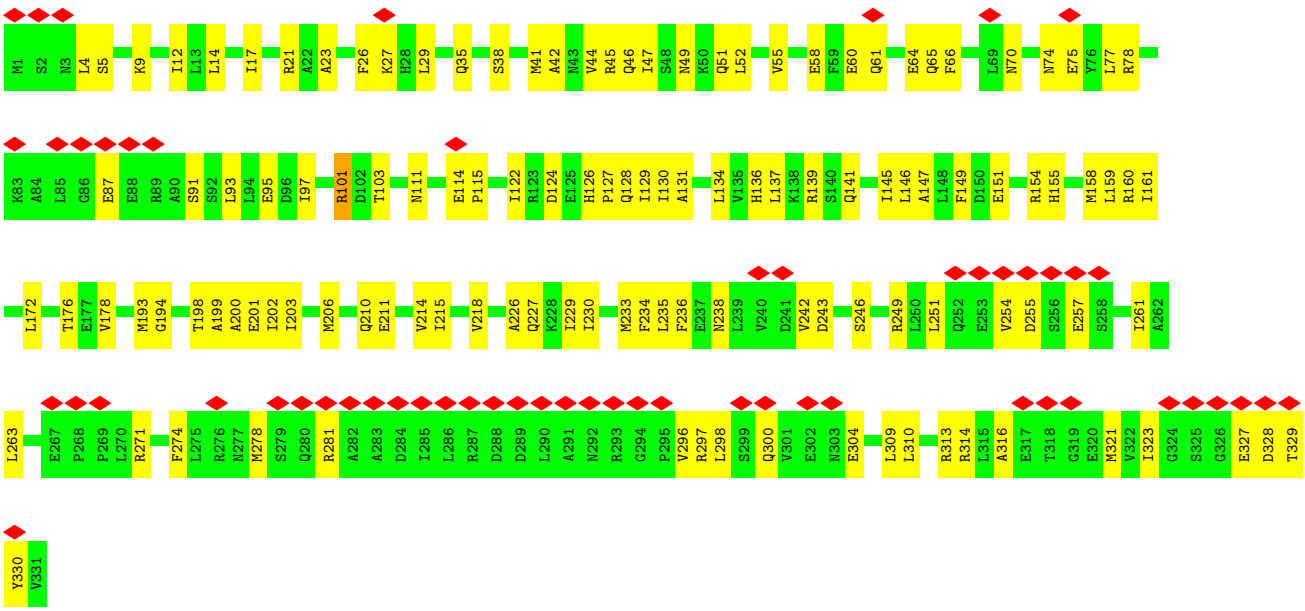
• Molecule 2: Flagellar motor switch protein FliG

Chain BF:



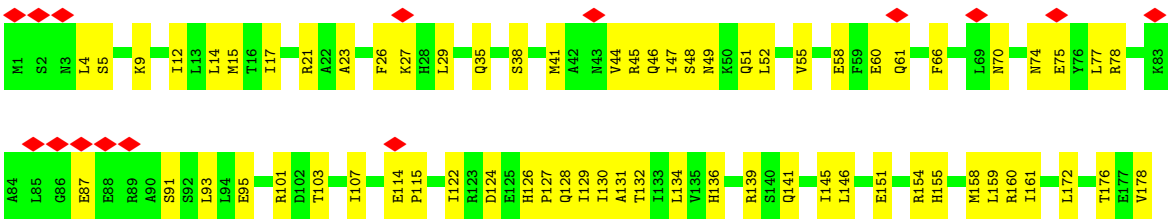
- Molecule 2: Flagellar motor switch protein FliG

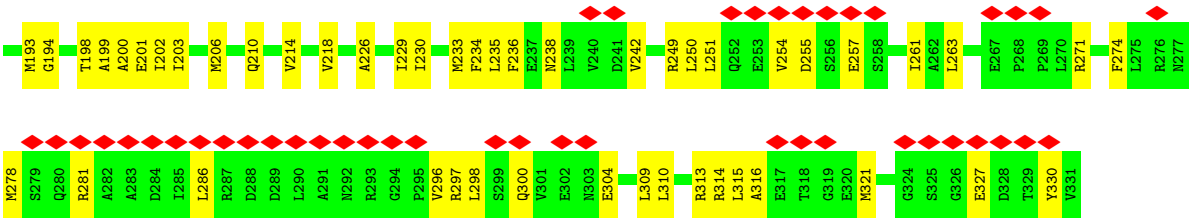
Chain BG:



- Molecule 2: Flagellar motor switch protein FliG

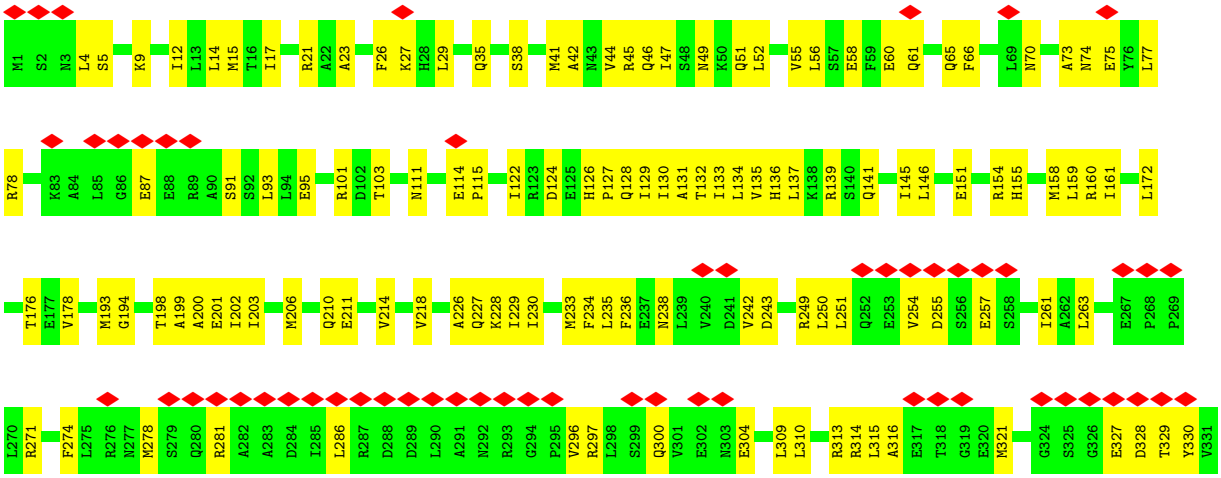
Chain BH:





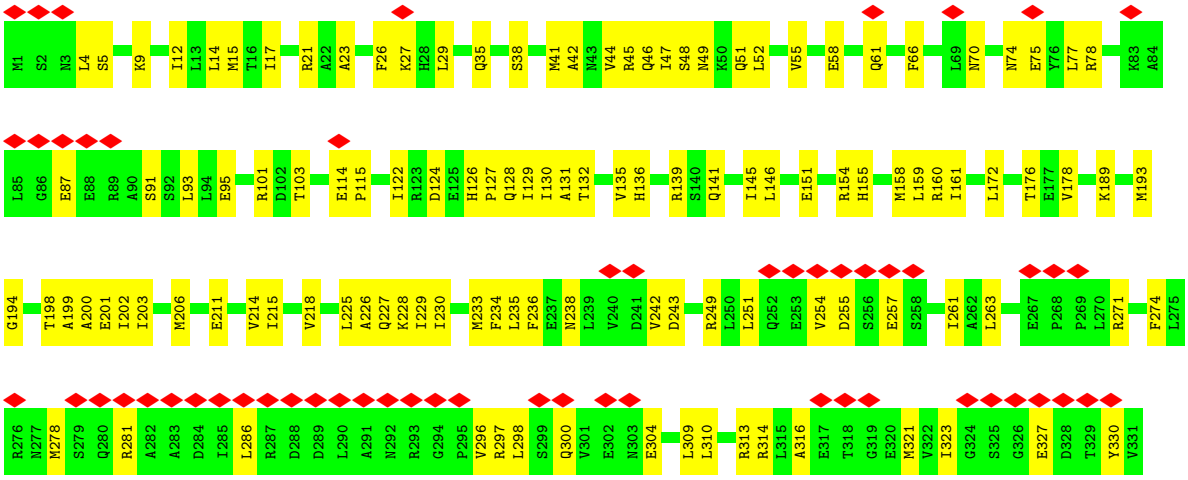
• Molecule 2: Flagellar motor switch protein FliG

Chain BI:



• Molecule 2: Flagellar motor switch protein FliG

Chain BJ:



• Molecule 2: Flagellar motor switch protein FliG

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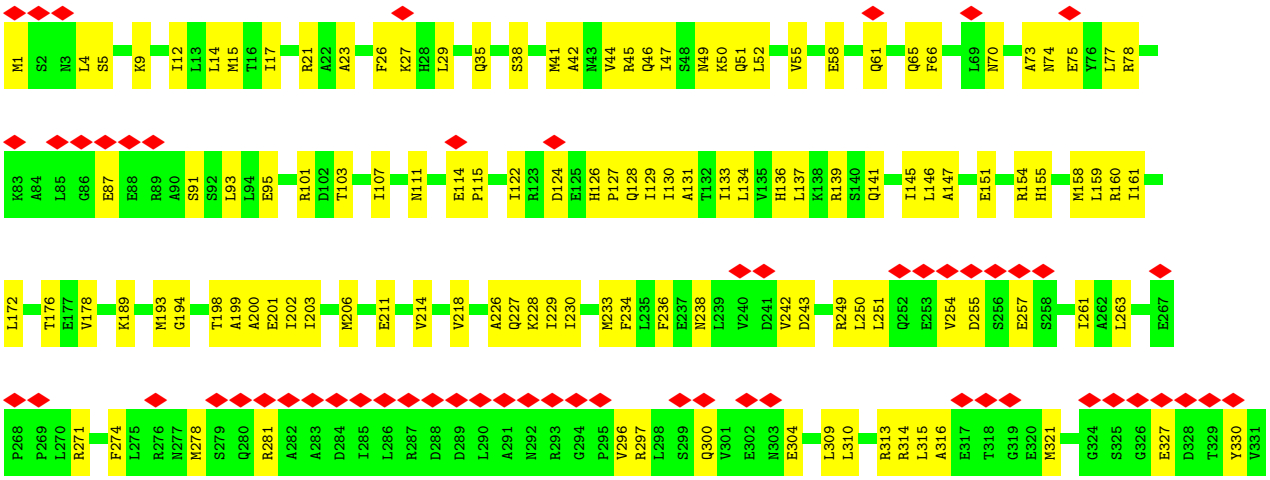
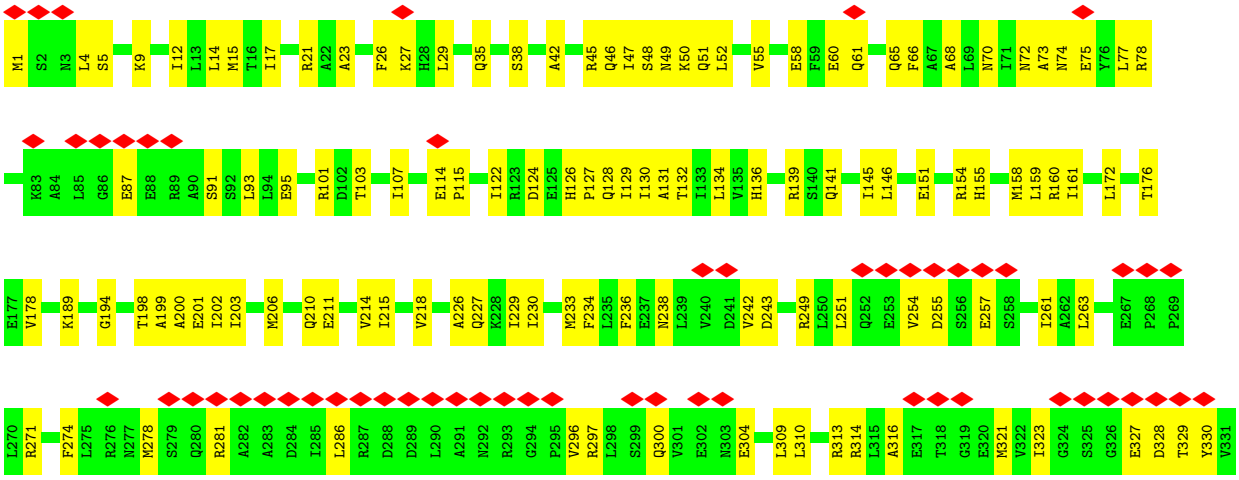


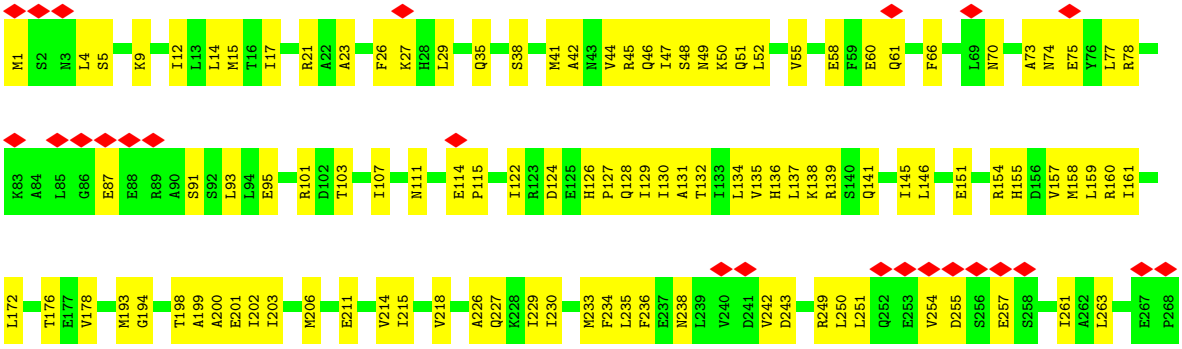
- Molecule 2: Flagellar motor switch protein FliG

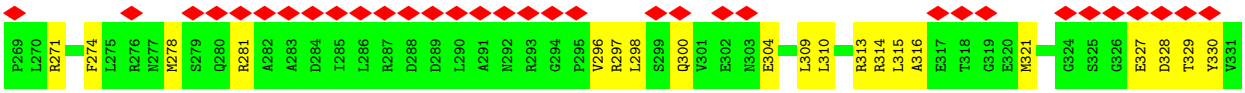
Chain BL:



- Molecule 2: Flagellar motor switch protein FliG

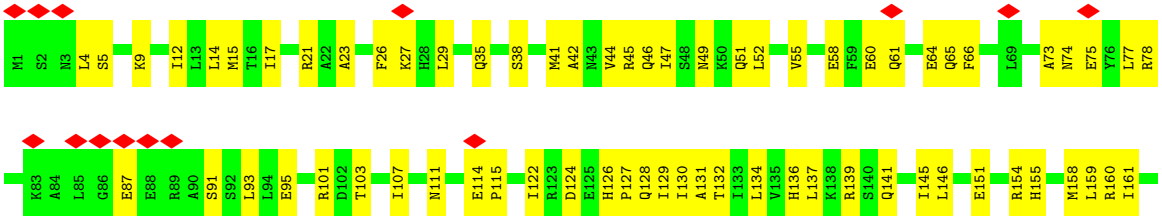
Chain BM:





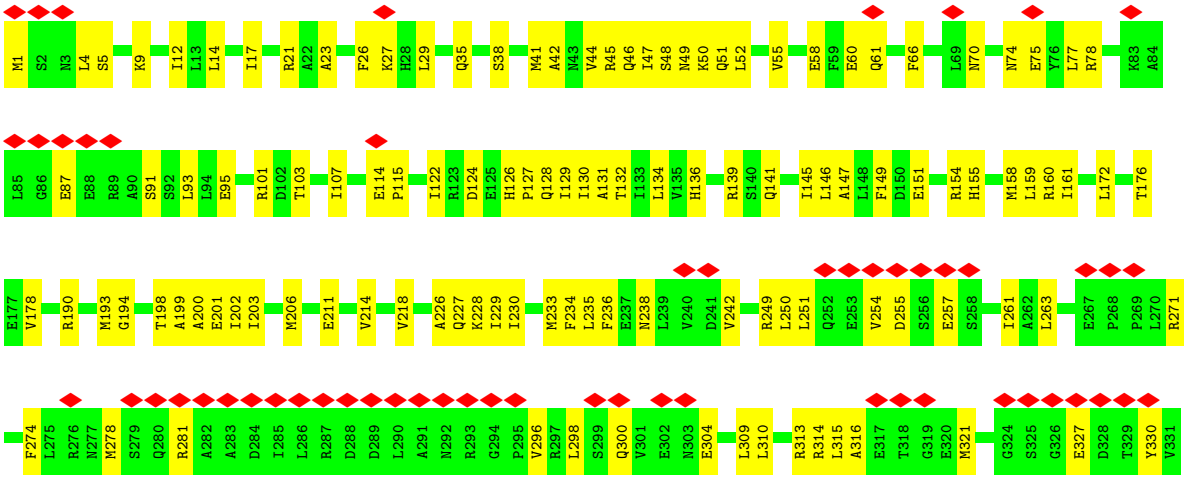
• Molecule 2: Flagellar motor switch protein FliG

Chain BN:



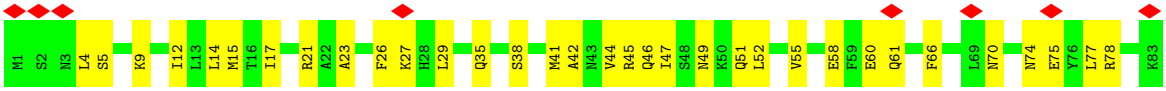
• Molecule 2: Flagellar motor switch protein FliG

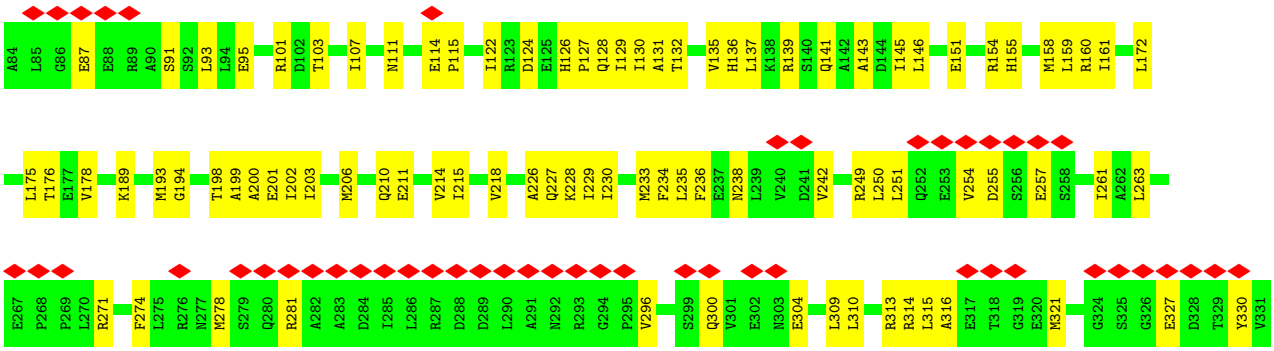
Chain BO:



• Molecule 2: Flagellar motor switch protein FliG

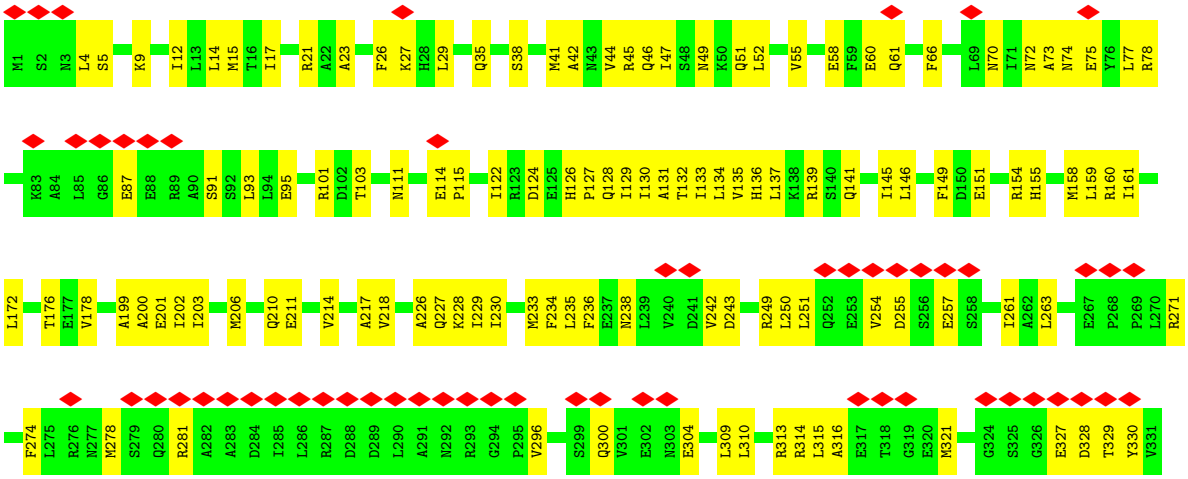
Chain BP:





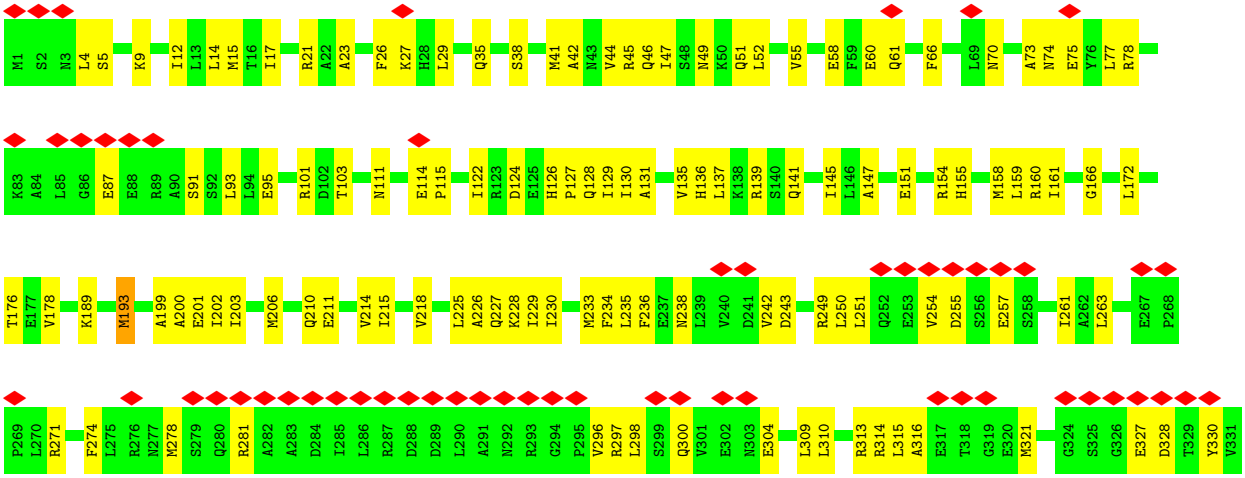
- Molecule 2: Flagellar motor switch protein FliG

Chain BQ:



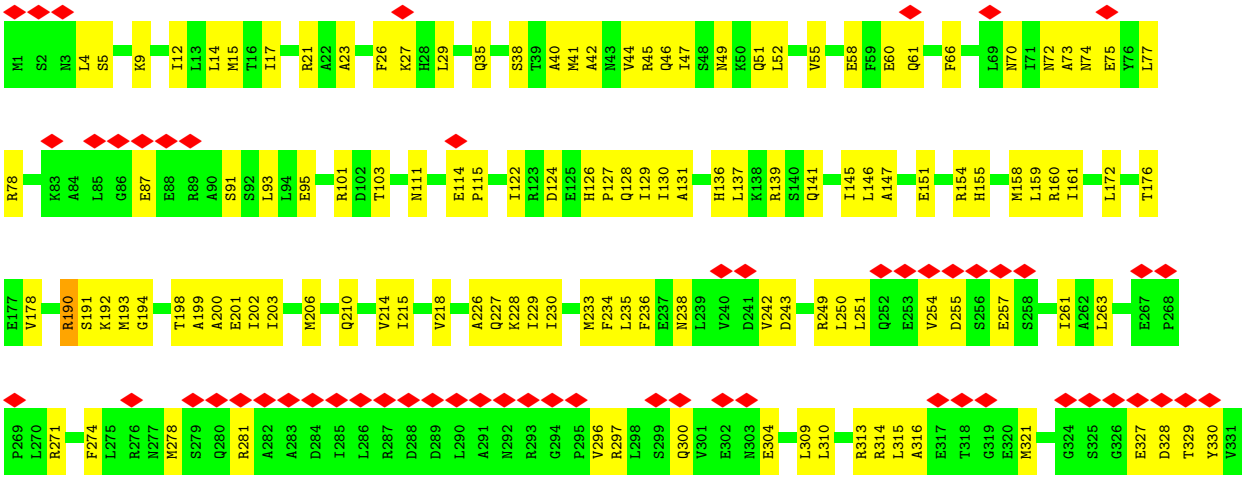
- Molecule 2: Flagellar motor switch protein FliG

Chain BR:



- Molecule 2: Flagellar motor switch protein FliG

Chain BS:



- Molecule 2: Flagellar motor switch protein FliG

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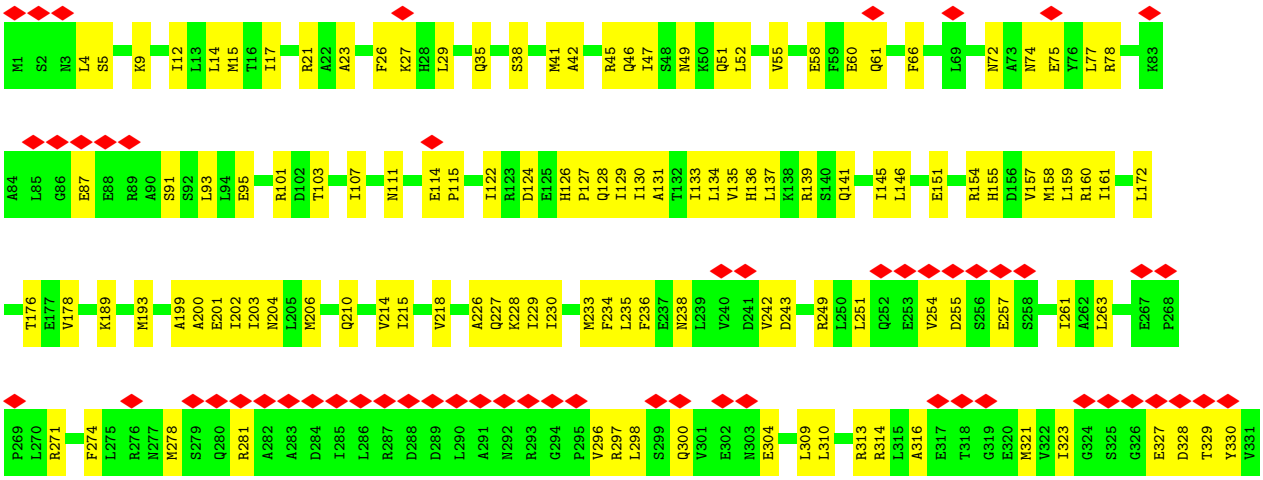

- Molecule 2: Flagellar motor switch protein FliG

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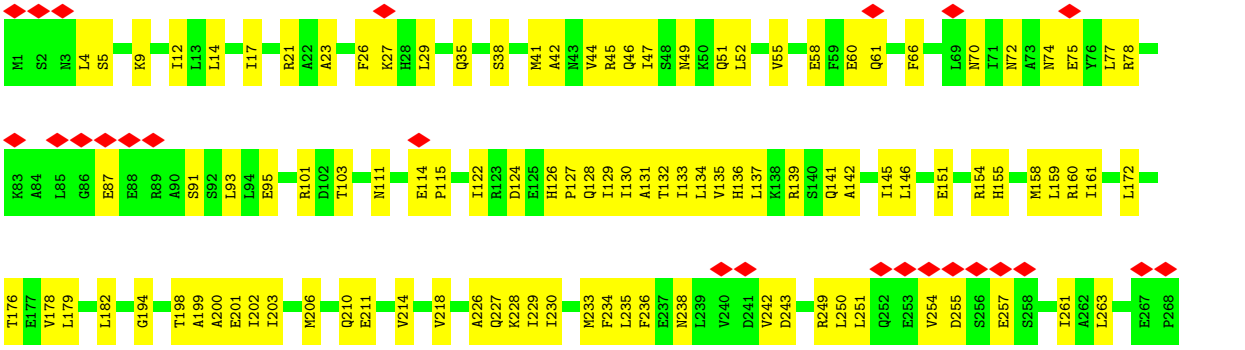

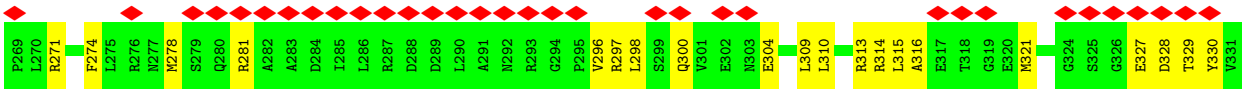

• Molecule 2: Flagellar motor switch protein FliG

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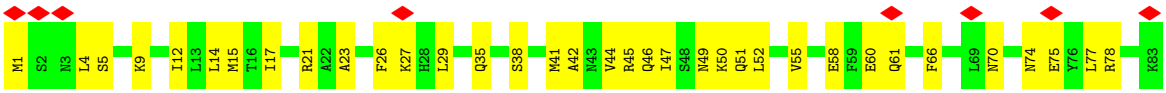
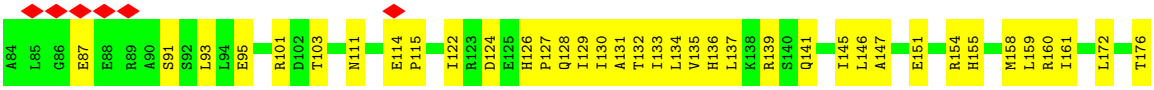
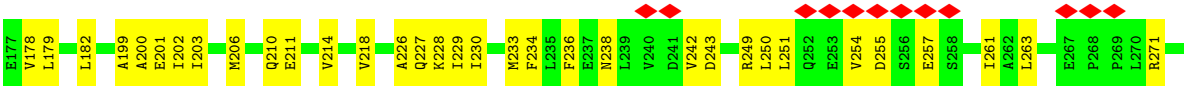
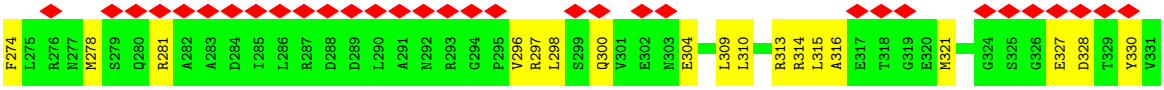


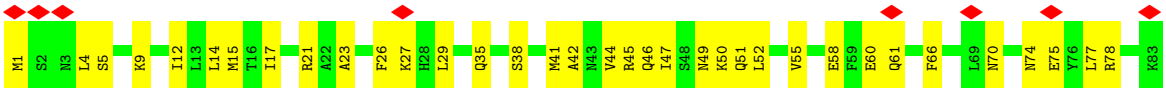


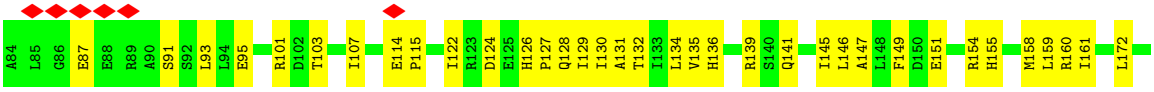


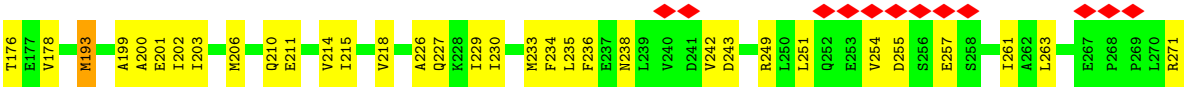


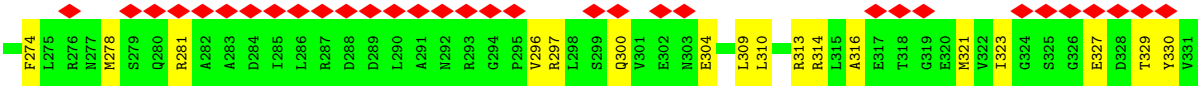
• Molecule 2: Flagellar motor switch protein FliG

Chain BW:



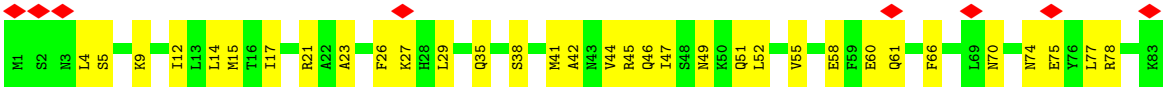


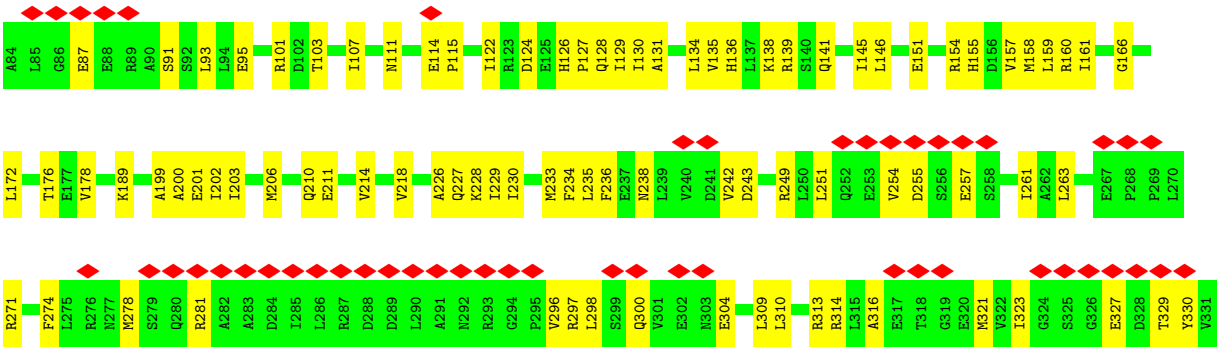




• Molecule 2: Flagellar motor switch protein FliG

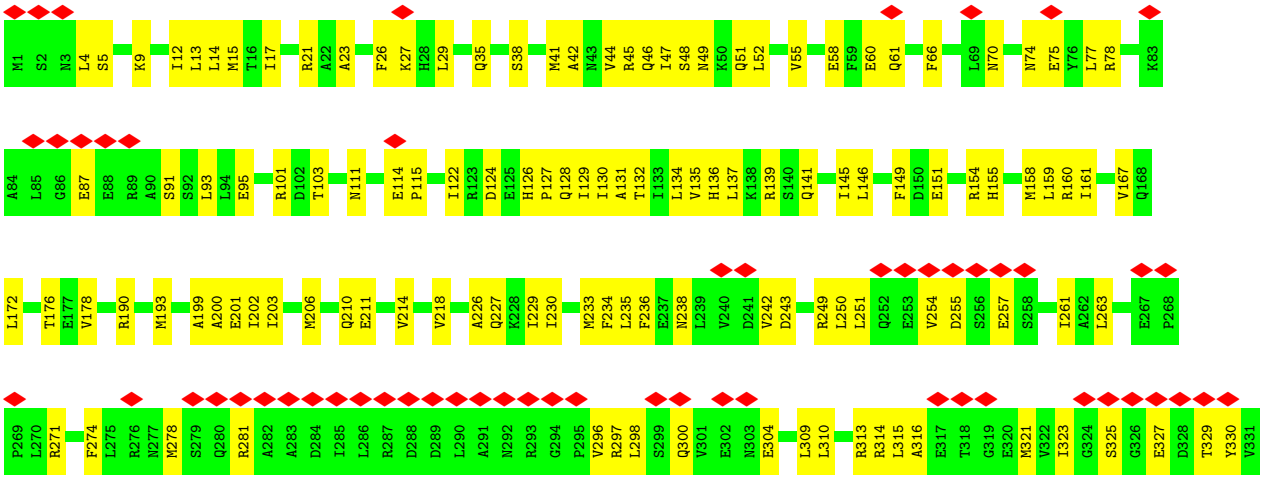
Chain BX:





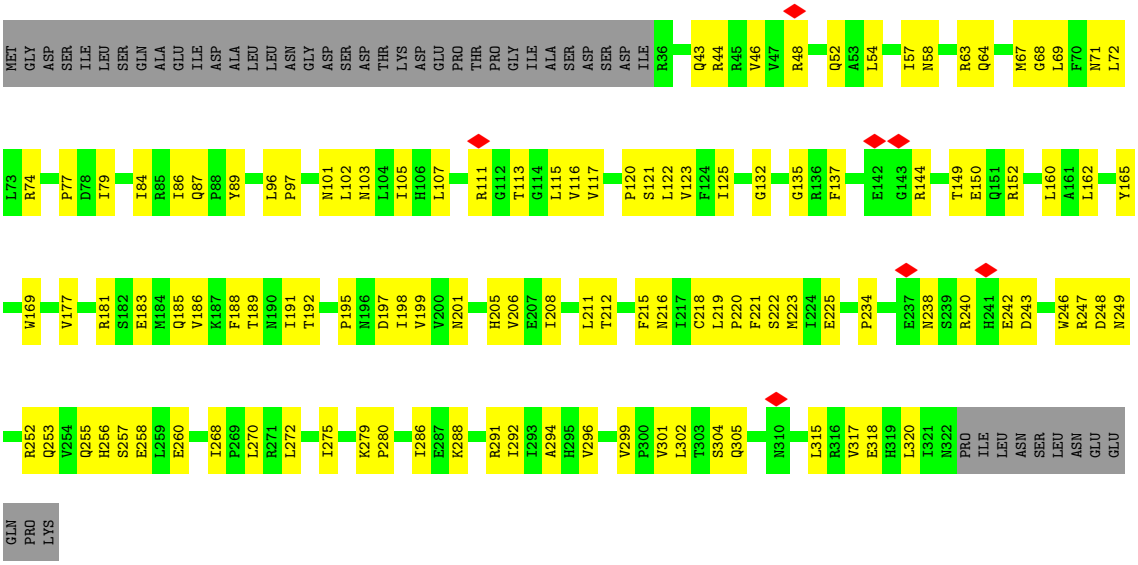
• Molecule 2: Flagellar motor switch protein FliG

Chain BY:



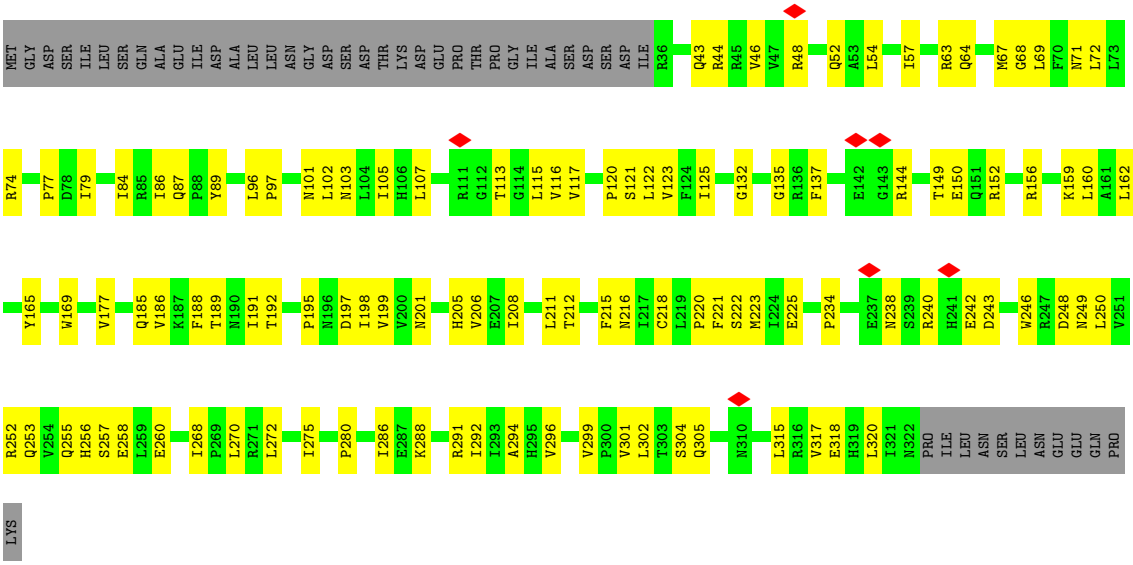
• Molecule 3: Flagellar motor switch protein FliM

Chain C1:



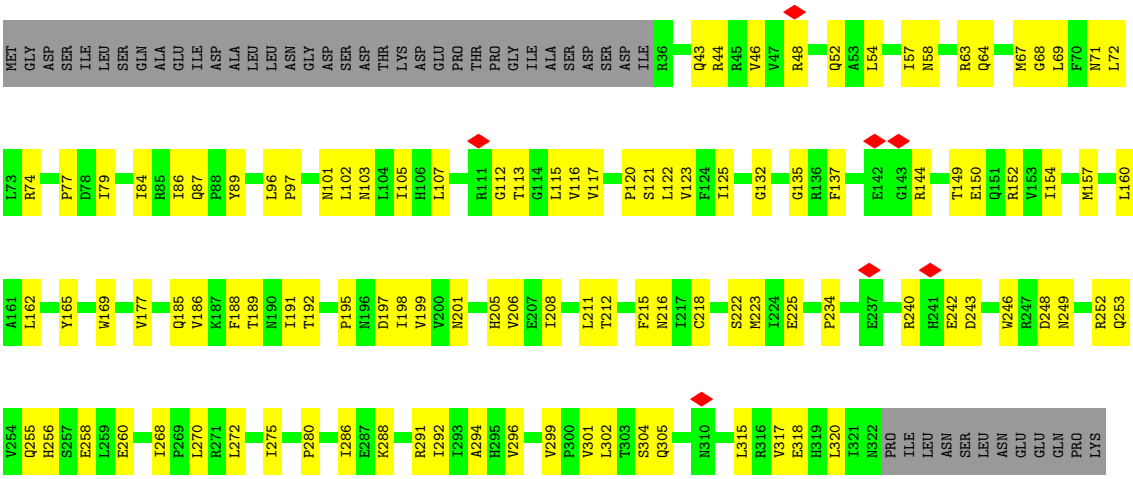
• Molecule 3: Flagellar motor switch protein FliM

Chain C2: 53% 33% 14%



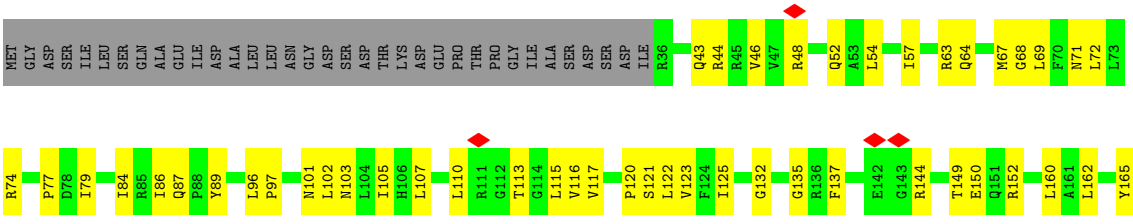
• Molecule 3: Flagellar motor switch protein FliM

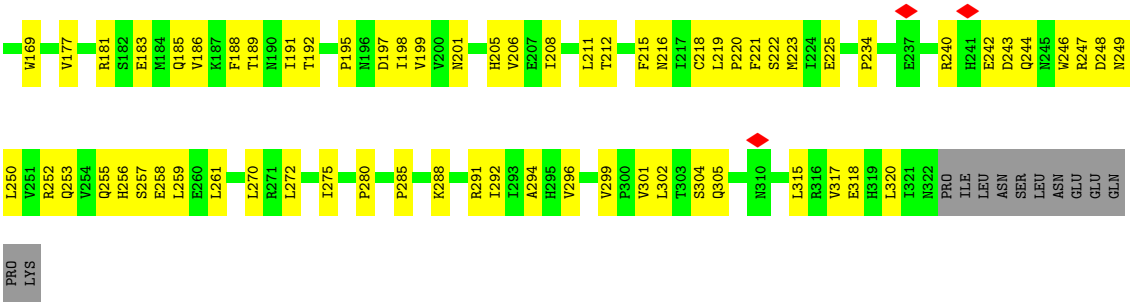
Chain C3: 54% 32% 14%



• Molecule 3: Flagellar motor switch protein FliM

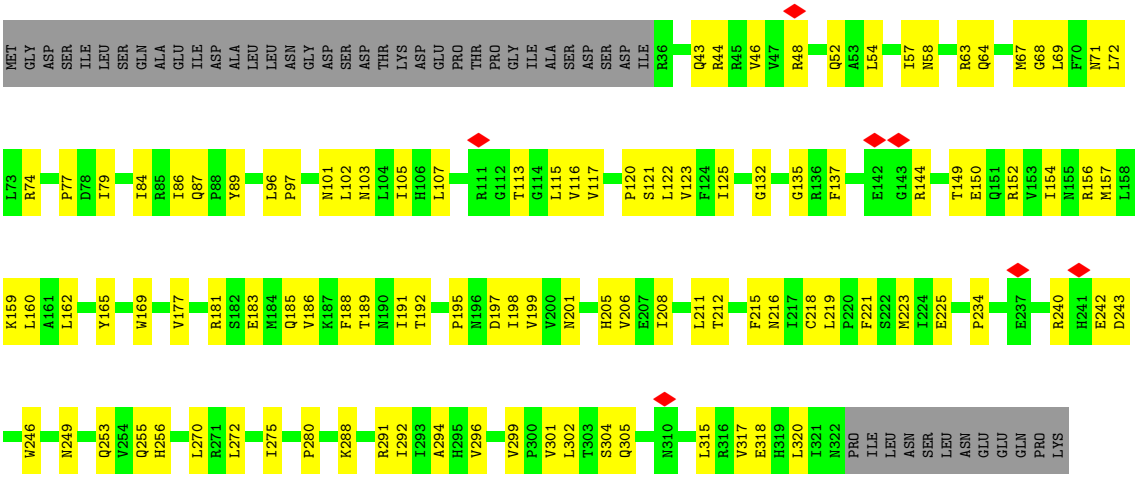
Chain C4: 52% 34% 14%





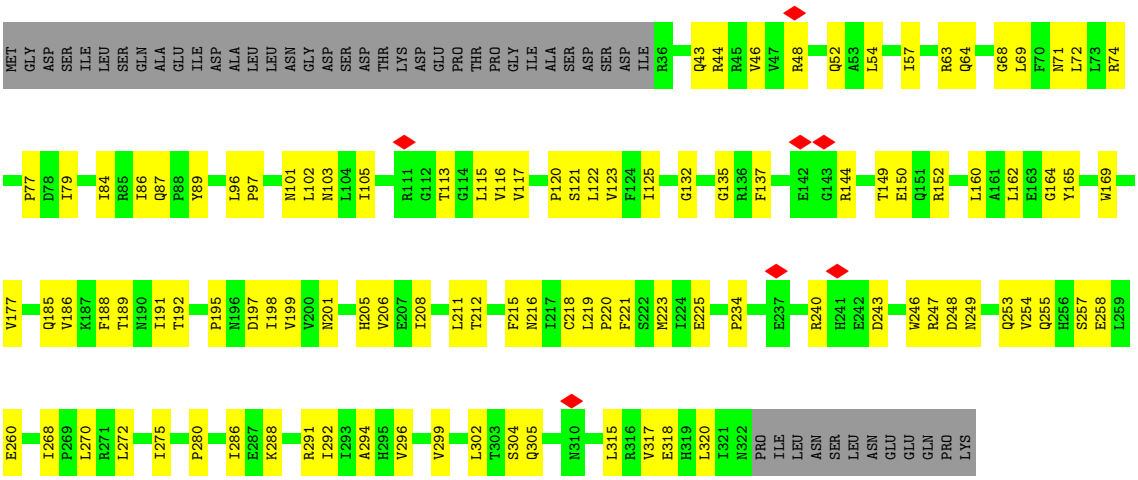
• Molecule 3: Flagellar motor switch protein FliM

Chain C5:



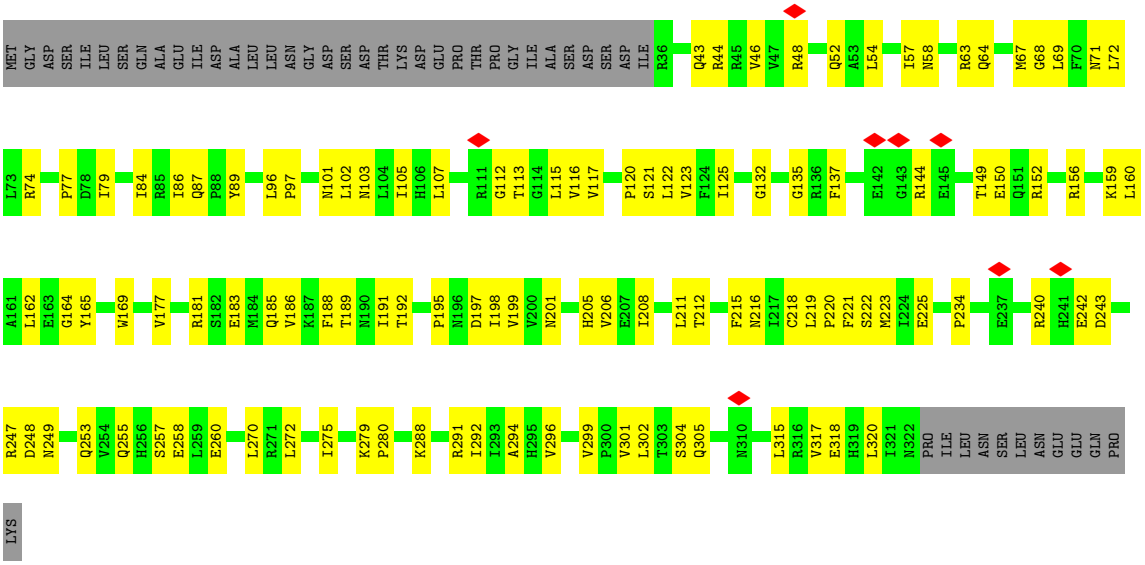
• Molecule 3: Flagellar motor switch protein FliM

Chain C6:



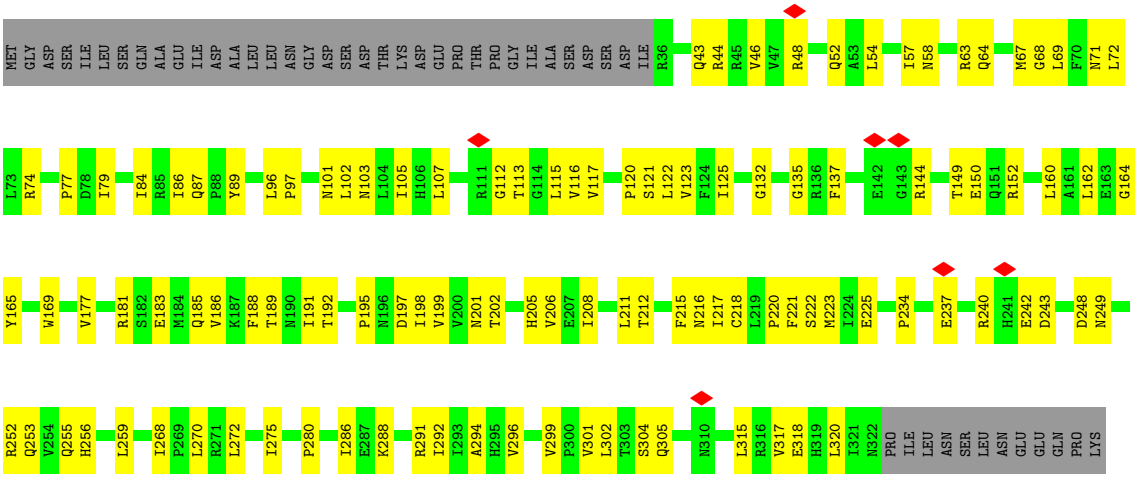
• Molecule 3: Flagellar motor switch protein FliM

Chain C7:



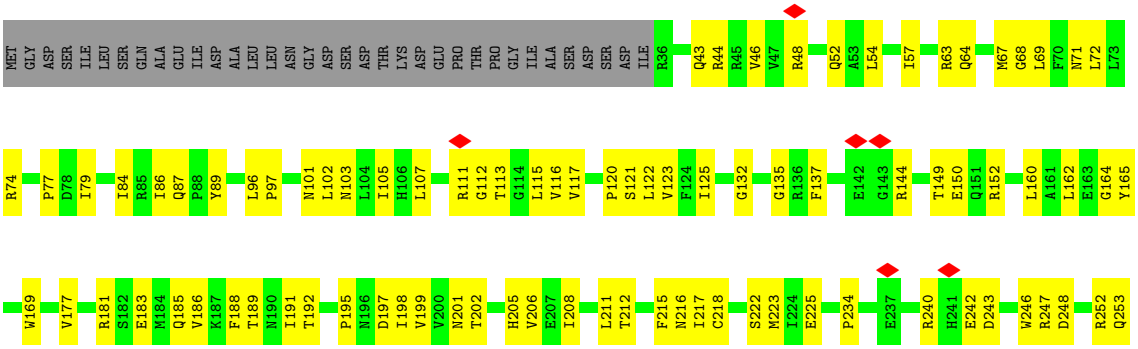
- Molecule 3: Flagellar motor switch protein FliM

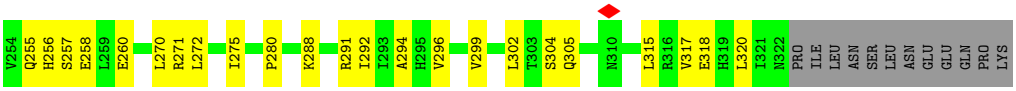
Chain C8:



- Molecule 3: Flagellar motor switch protein FliM

Chain C9:





• Molecule 3: Flagellar motor switch protein FliM

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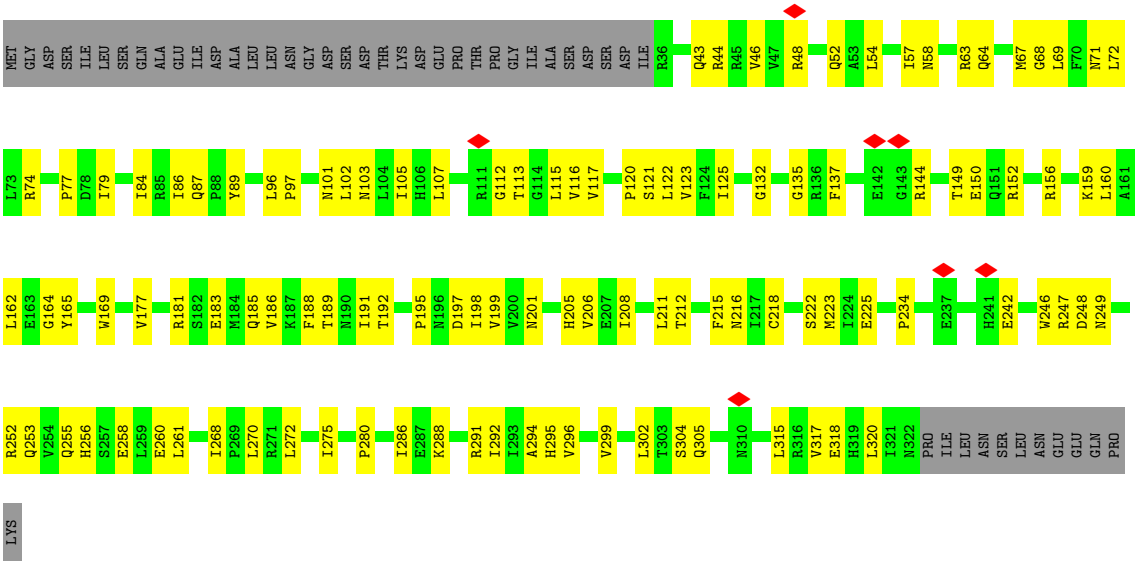
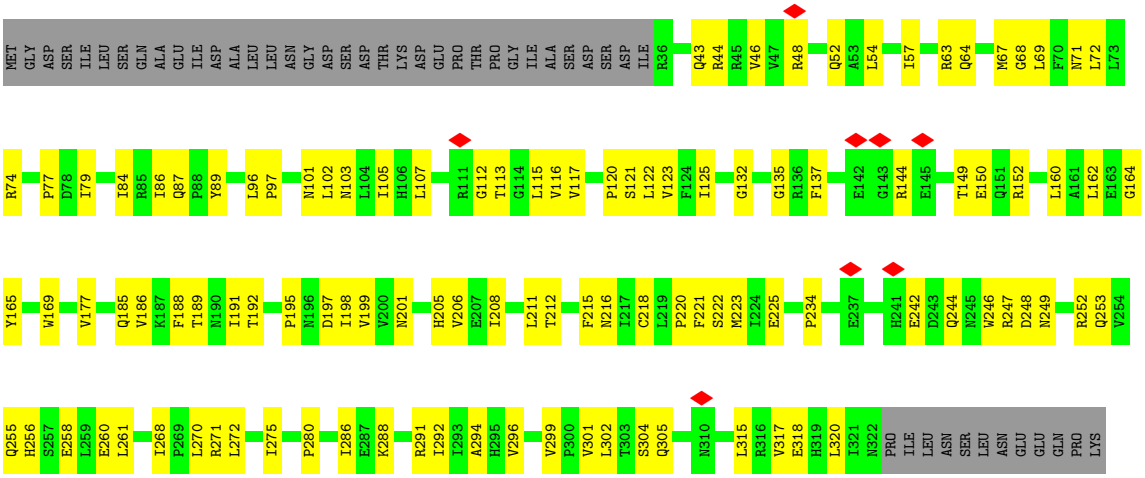


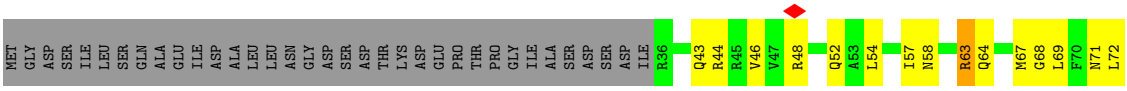
• Molecule 3: Flagellar motor switch protein FliM

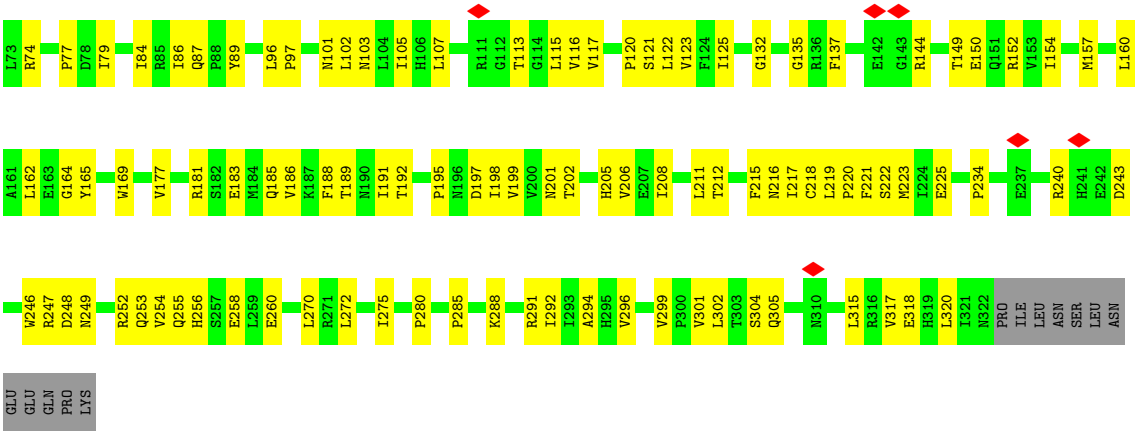
Chain CB:



• Molecule 3: Flagellar motor switch protein FliM

Chain CC:





- Molecule 3: Flagellar motor switch protein FliM

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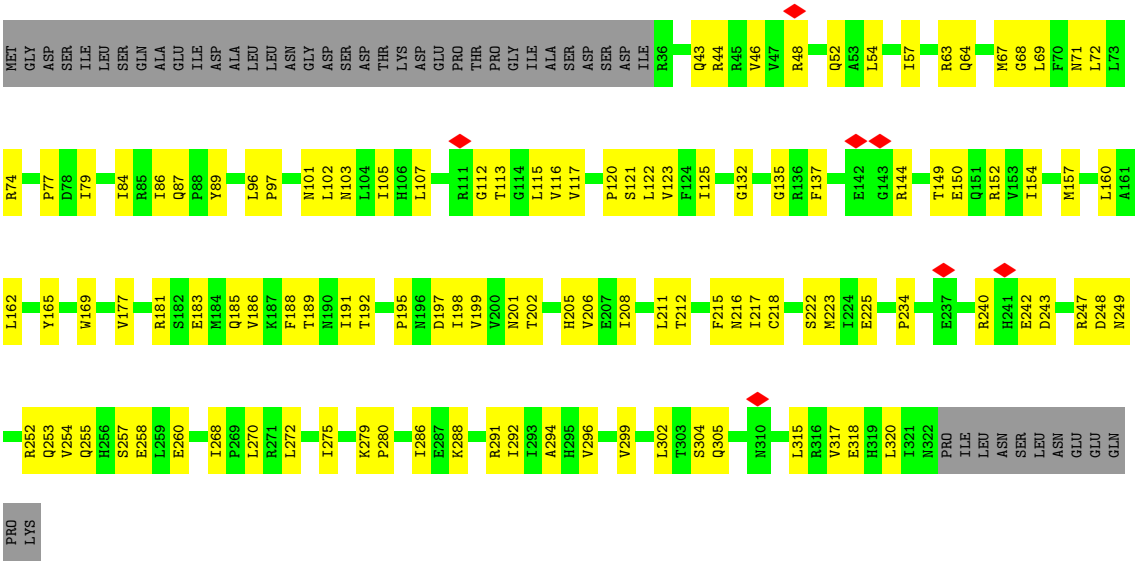
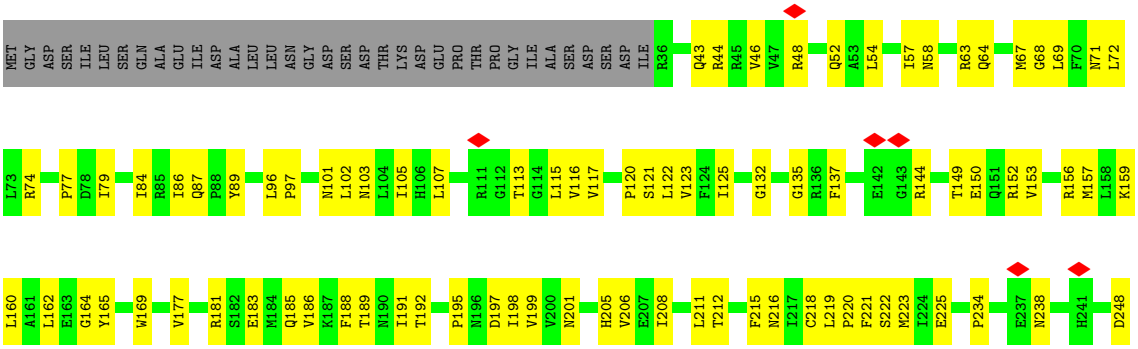
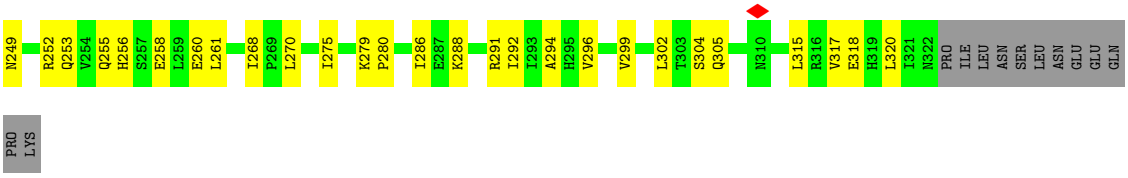


- Molecule 3: Flagellar motor switch protein FliM

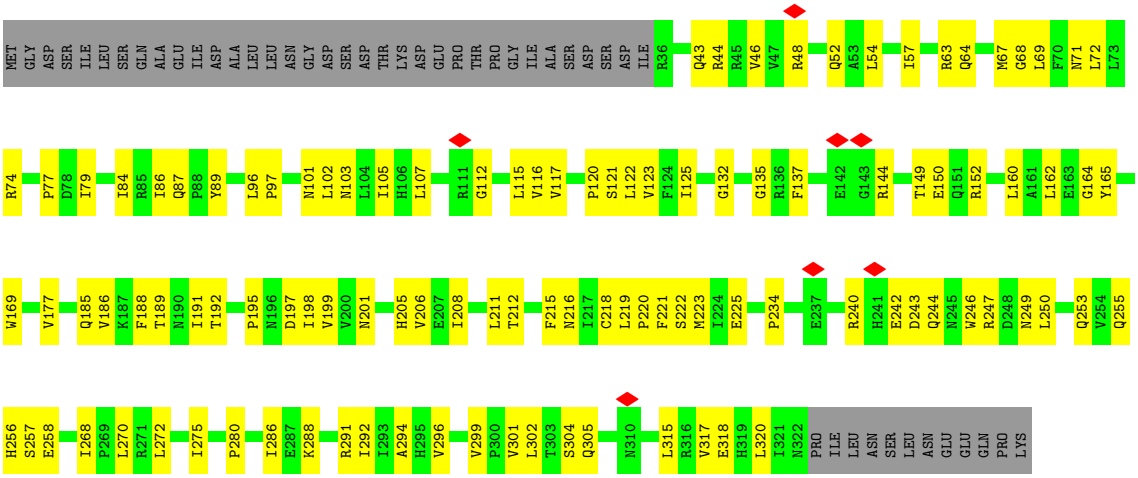
Chain CE:





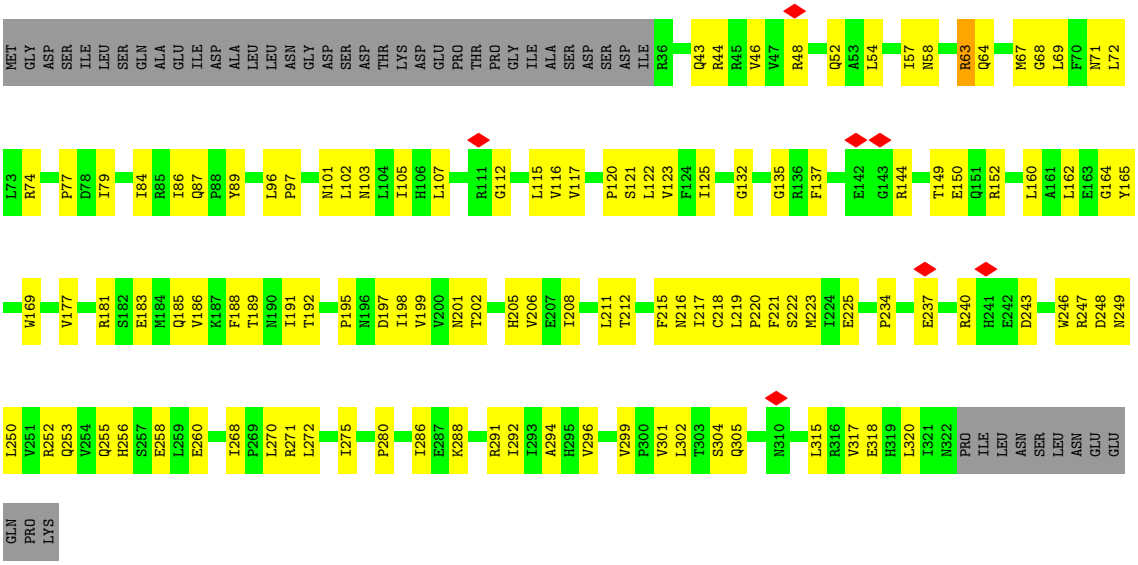
• Molecule 3: Flagellar motor switch protein FliM

Chain CF:



• Molecule 3: Flagellar motor switch protein FliM

Chain CG:



• Molecule 3: Flagellar motor switch protein FliM

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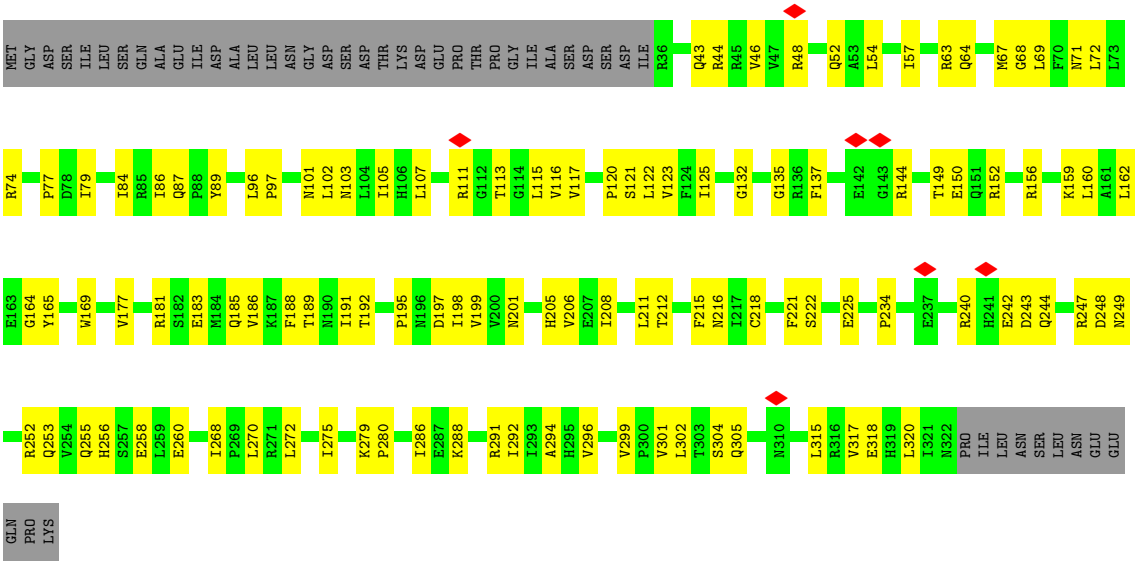

• Molecule 3: Flagellar motor switch protein FliM

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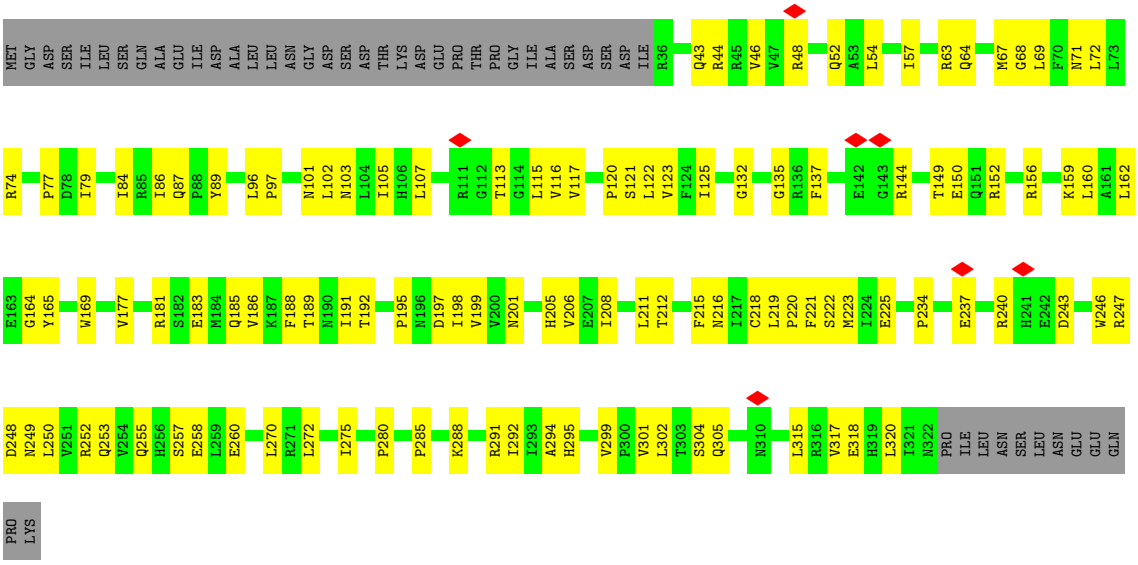
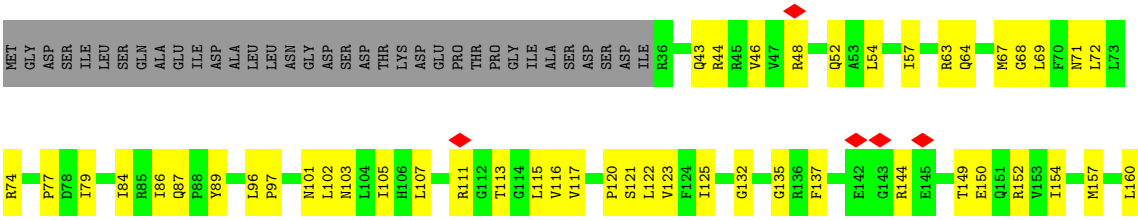
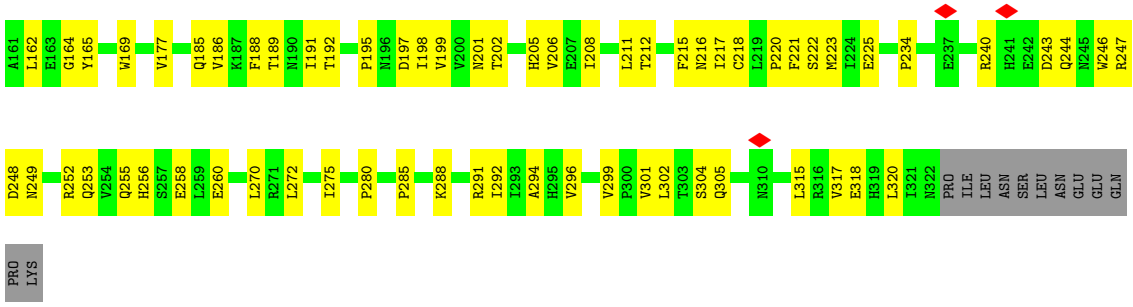


• Molecule 3: Flagellar motor switch protein FliM

Chain CJ:





• Molecule 3: Flagellar motor switch protein FliM

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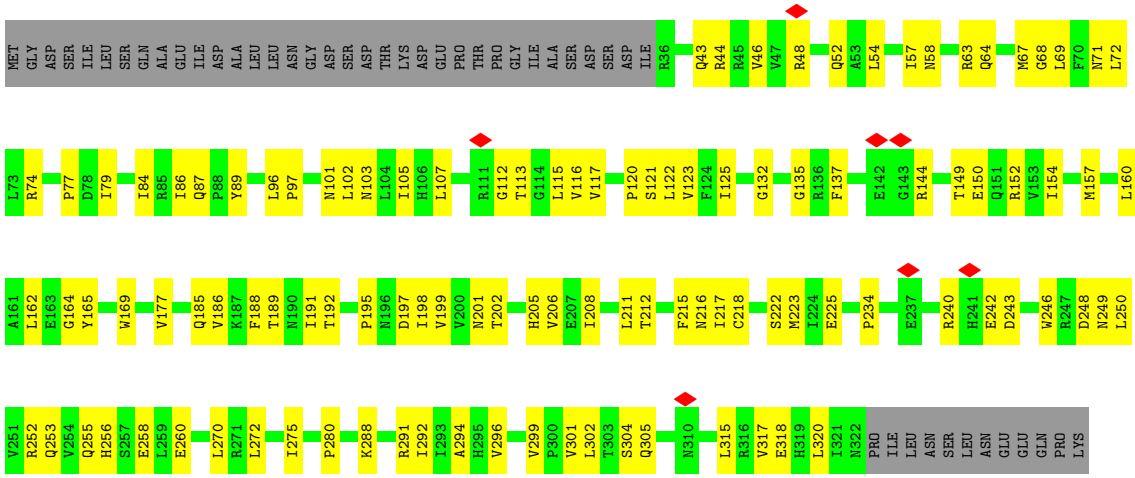

• Molecule 3: Flagellar motor switch protein FliM

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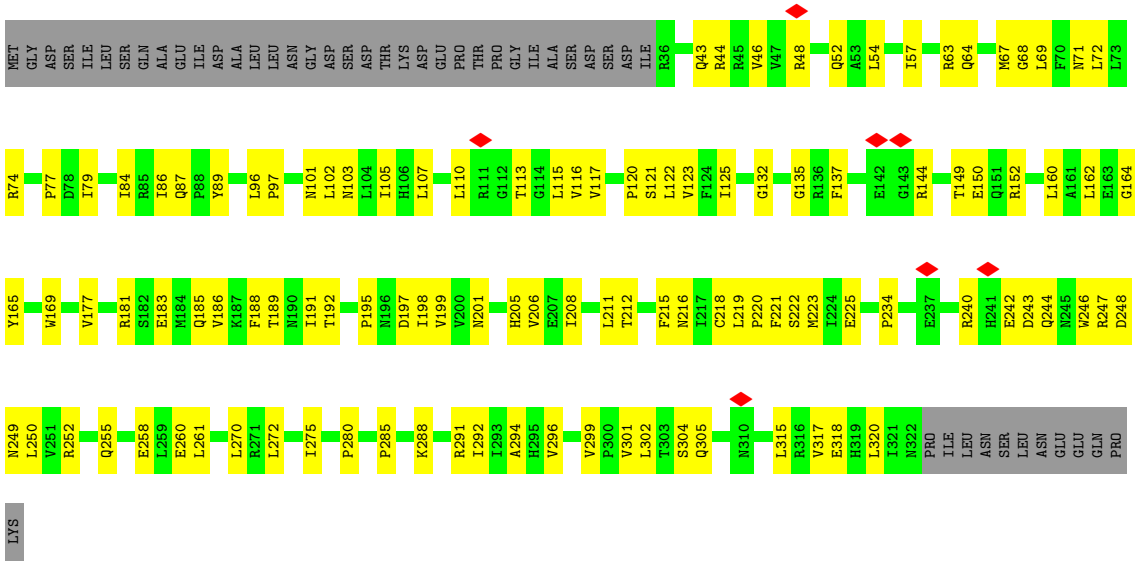

• Molecule 3: Flagellar motor switch protein FliM

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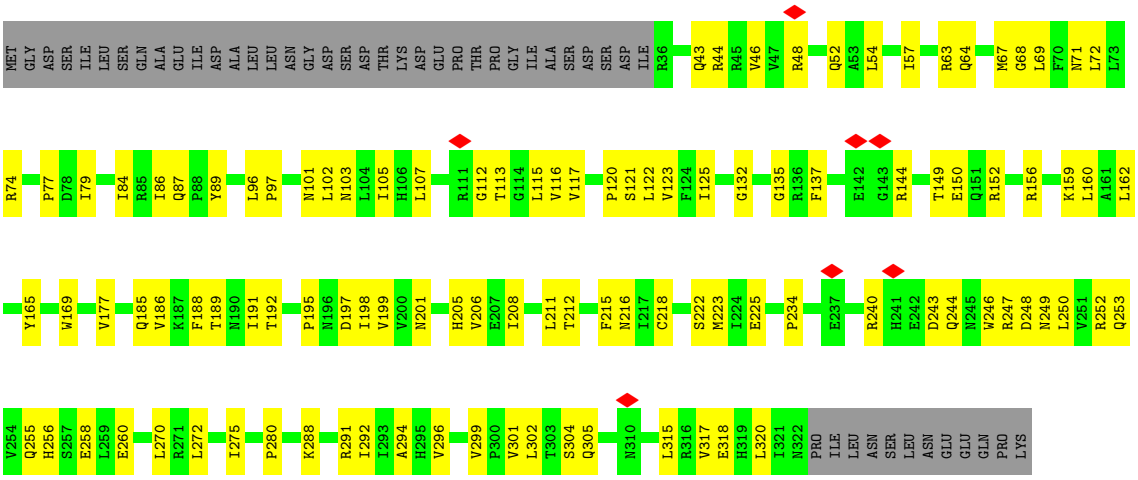

• Molecule 3: Flagellar motor switch protein FliM

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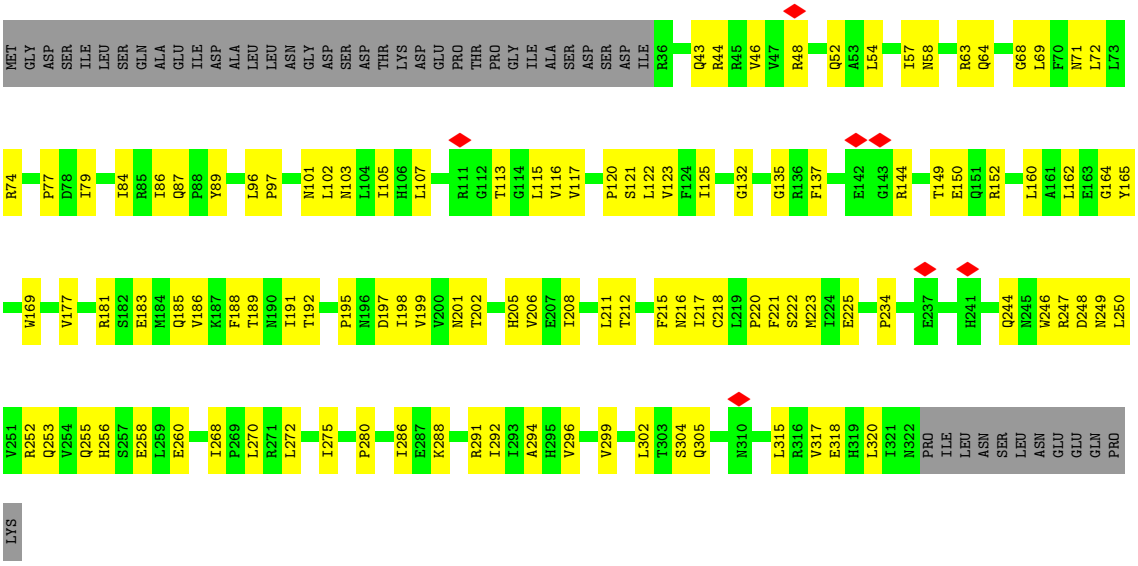
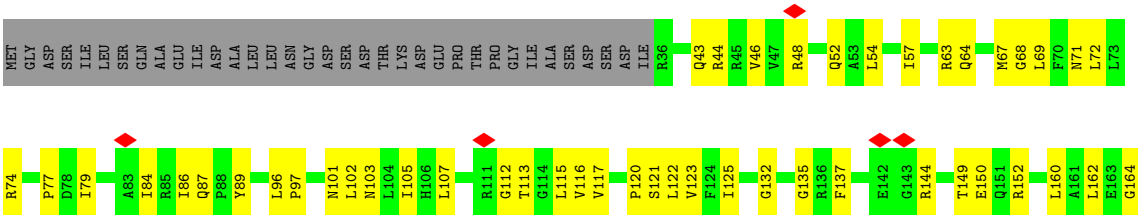
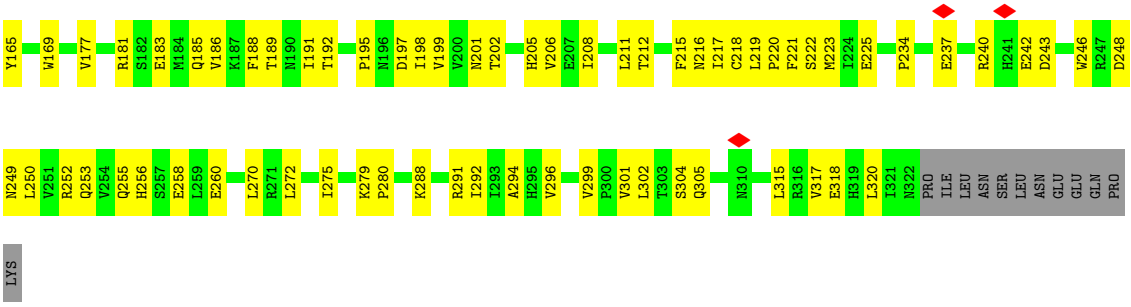


• Molecule 3: Flagellar motor switch protein FliM

Chain CO:





• Molecule 3: Flagellar motor switch protein FliM

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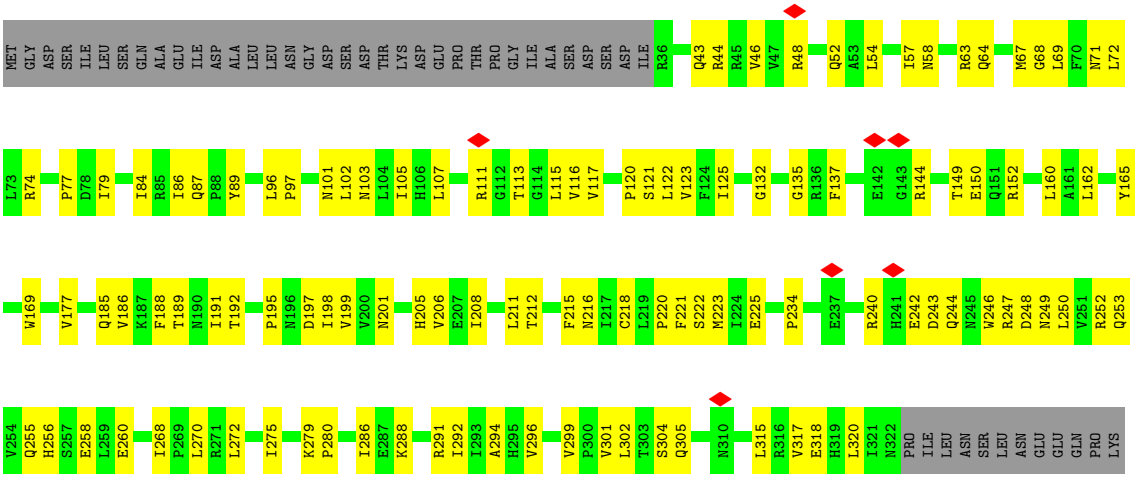
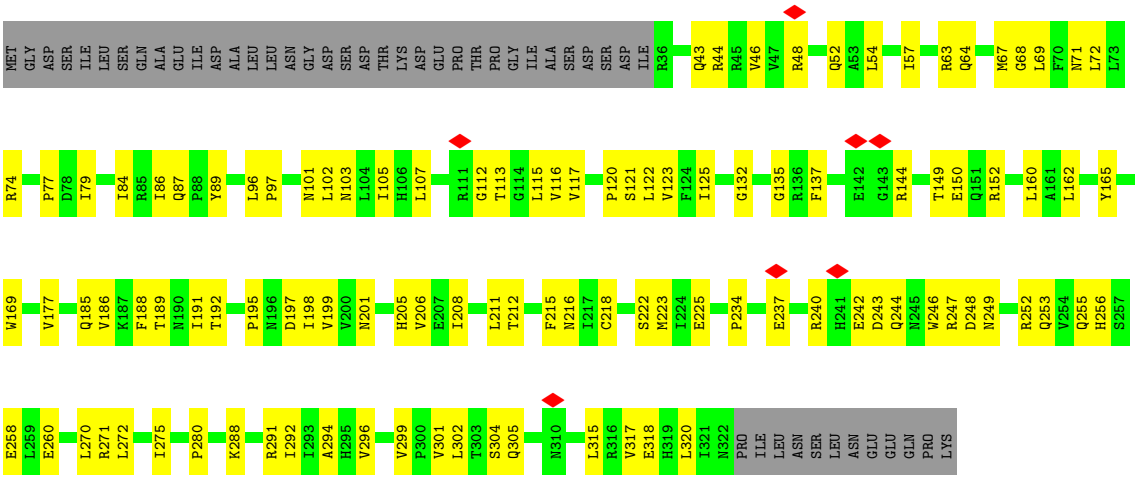


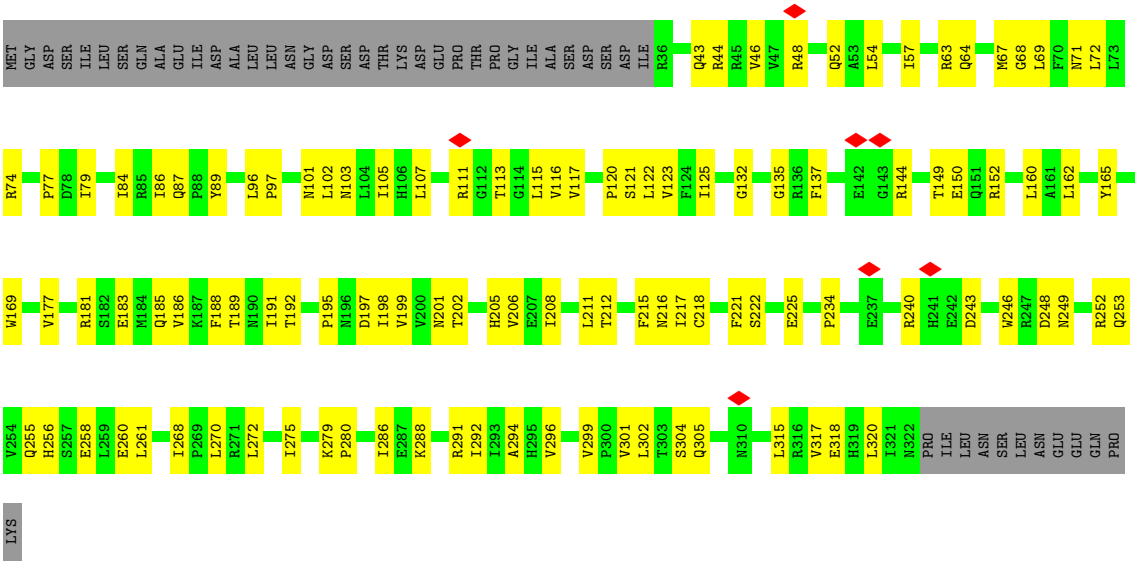
• Molecule 3: Flagellar motor switch protein FliM

Chain CQ:



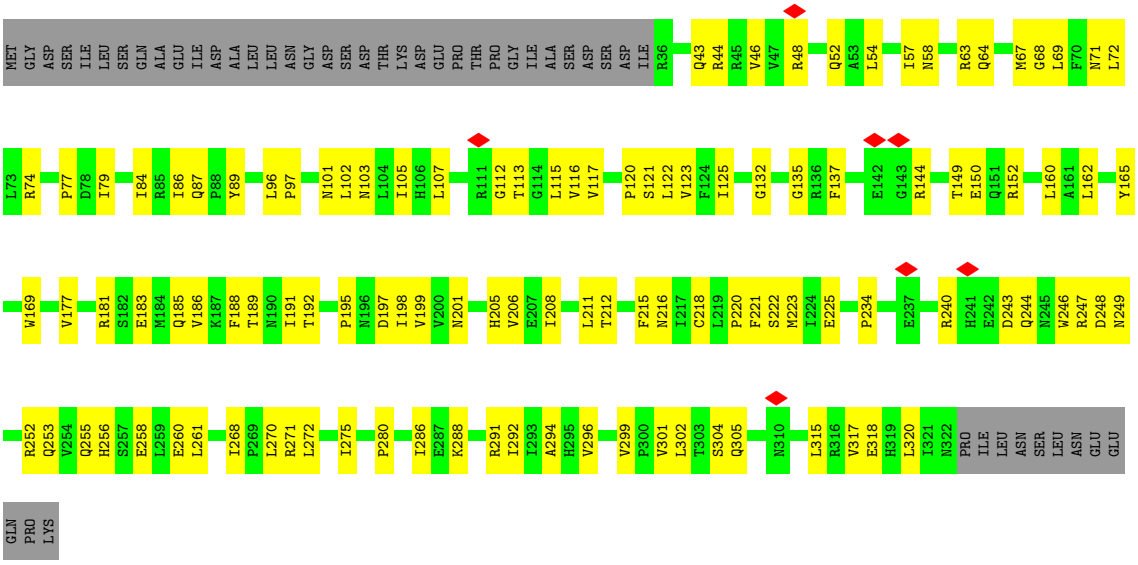
• Molecule 3: Flagellar motor switch protein FliM

Chain CR:



• Molecule 3: Flagellar motor switch protein FliM

Chain CS:



• Molecule 3: Flagellar motor switch protein FliM

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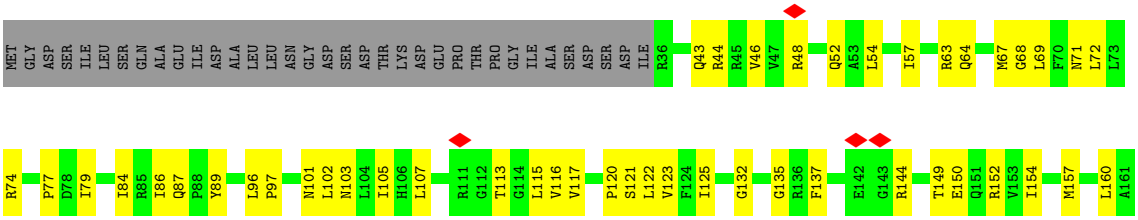
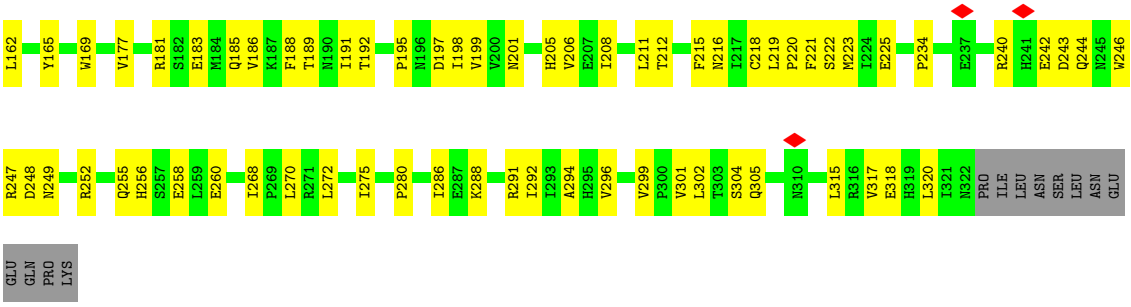
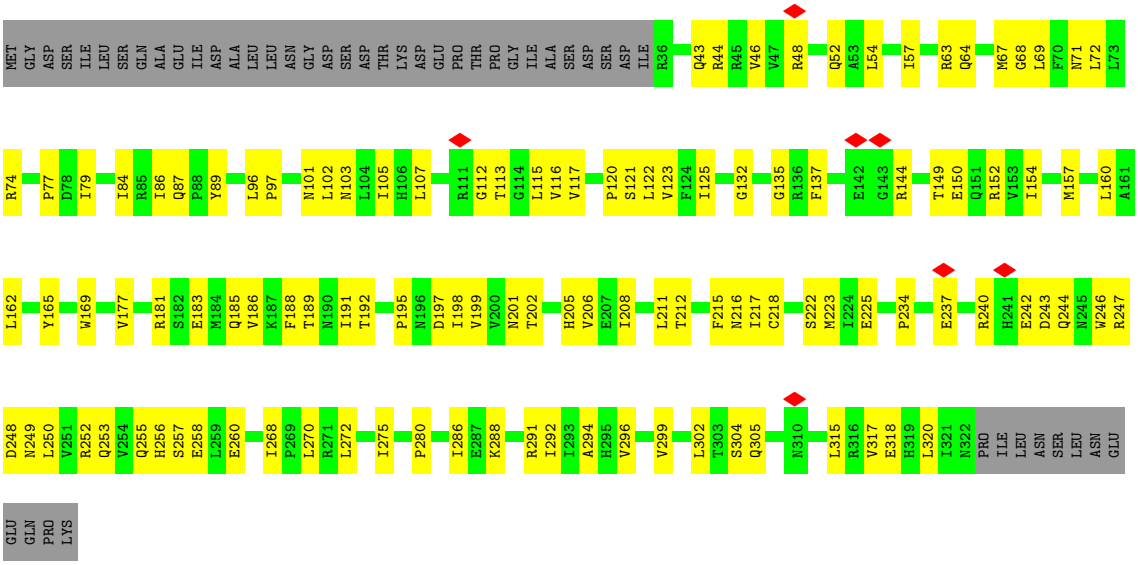




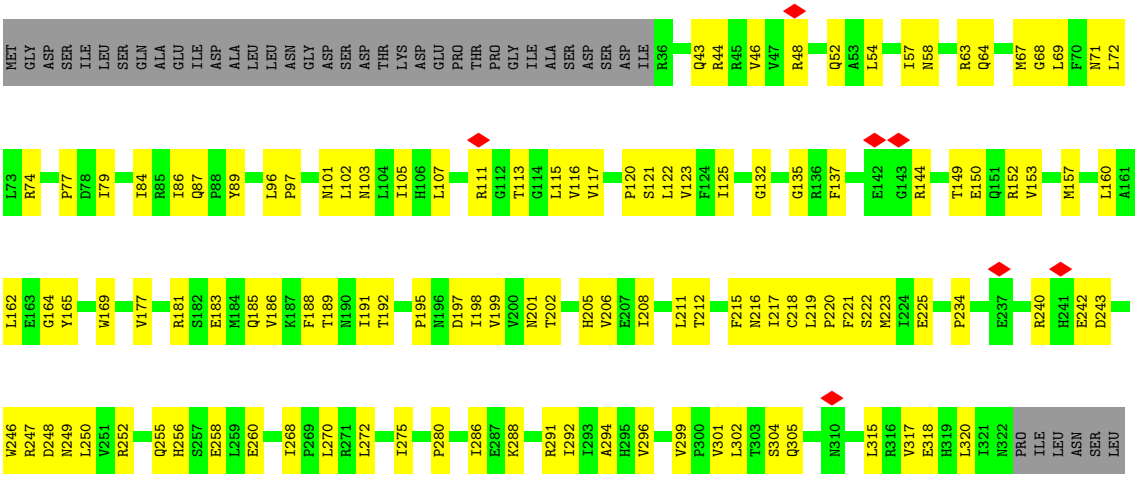
• Molecule 3: Flagellar motor switch protein FliM

Chain CU:



• Molecule 3: Flagellar motor switch protein FliM

Chain CV:



ASN GLU GLU GLN PRO LYS

• Molecule 3: Flagellar motor switch protein FliM

Chain CW: 54% 31% 14%

MET GLY ASP SER ILE LEU SER GLN ALA GLU ILE ASP ALA LEU LEU ASN GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER ASP ILE R36 Q43 R44 R45 V46 V47 R48 Q52 A53 L54 I57 R63 Q64 M67 G68 L69 F70 N71 L72 L73

R74 P77 D78 I79 A83 I84 R85 I86 Q87 P88 Y89 L96 P97 N101 L102 N103 L104 I105 H106 L107 R111 G112 L115 V116 V117 P120 S121 L122 V123 F124 I125 G132 G135 R136 F137 E142 G143 R144 T149 E150 Q151 R152 L160 A161 L162 Y165

W169 V177 Q185 V186 K187 F188 T189 N190 I191 T192 P195 N196 D197 I198 V199 V200 N201 H205 V206 E207 I208 L211 T212 F215 N216 I217 C218 L219 P220 F221 S222 M223 I224 E225 P234 E237 R240 H241 E242 D243 W246 N249 L250 Q253 V254 Q255 H256 S257

E258 L259 E260 I268 P269 L270 R271 L272 I275 P280 I286 E287 K288 R291 I292 I293 A294 H295 V296 V299 P300 V301 L302 T303 S304 Q305 N310 L315 R316 V317 E318 H319 L320 I321 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU GLN PRO LYS

• Molecule 3: Flagellar motor switch protein FliM

Chain CX: 52% 34% 14%

MET GLY ASP SER ILE LEU SER GLN ALA GLU ILE ASP ALA LEU LEU ASN GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER ASP ILE R36 Q43 R44 R45 V46 V47 R48 Q52 A53 L54 I57 N58 R63 Q64 M67 G68 L69 F70 N71 L72

L73 R74 P77 D78 I79 I84 R85 I86 Q87 P88 Y89 L96 P97 N101 L102 N103 L104 I105 H106 L107 R111 G112 T113 G114 L115 V116 V117 P120 S121 L122 V123 F124 I125 G132 G135 R136 F137 E142 G143 R144 T149 E150 Q151 R152 L160 A161 L162 E163 G164

Y165 W169 V177 Q185 V186 K187 F188 T189 N190 I191 T192 P195 N196 D197 I198 V199 V200 N201 H205 V206 E207 I208 L211 T212 F215 N216 I217 C218 L219 P220 F221 S222 M223 I224 E225 P234 E237 N238 S239 R240 H241 E242 D243 W246 R247 D248 N249 L250 V251 R252

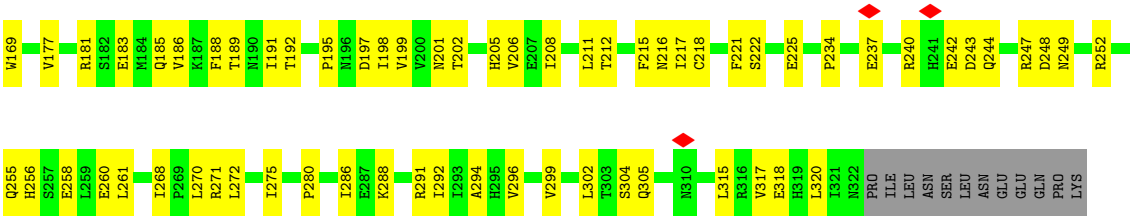
Q253 V254 Q255 H256 S257 E258 L259 E260 I268 P269 L270 R271 L272 I275 P280 I286 E287 K288 R291 I292 I293 A294 H295 V296 V299 P300 V301 L302 T303 S304 Q305 N310 L315 R316 V317 E318 H319 L320 I321 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU GLN PRO LYS

• Molecule 3: Flagellar motor switch protein FliM

Chain CY: 53% 33% 14%

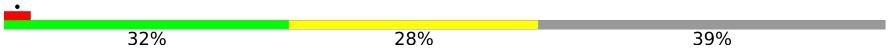
MET GLY ASP SER ILE LEU SER GLN ALA GLU ILE ASP ALA LEU LEU ASN GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER ASP ILE R36 Q43 R44 R45 V46 V47 R48 Q52 A53 L54 I57 R63 Q64 G68 L69 F70 N71 L72 L73 R74

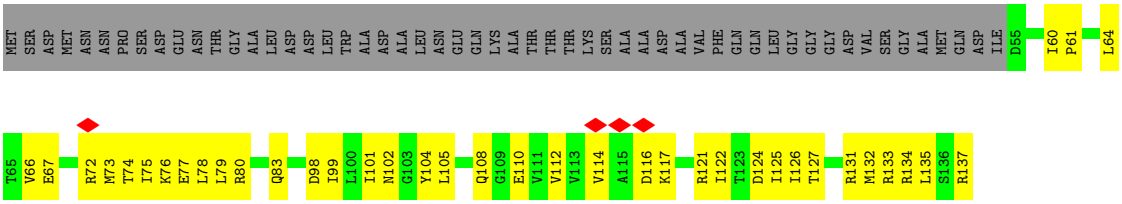
P77 D78 I79 I84 R85 I86 Q87 P88 Y89 L96 P97 N101 L102 N103 L104 I105 H106 L107 R111 G112 T113 G114 L115 V116 V117 P120 S121 L122 V123 F124 I125 G132 G135 R136 F137 E142 G143 R144 T149 E150 Q151 R152 L160 A161 L162 E163 G164 Y165



• Molecule 4: Flagellar motor switch protein FliN

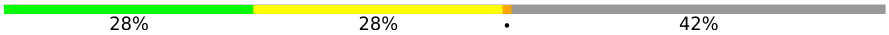
Chain D1:

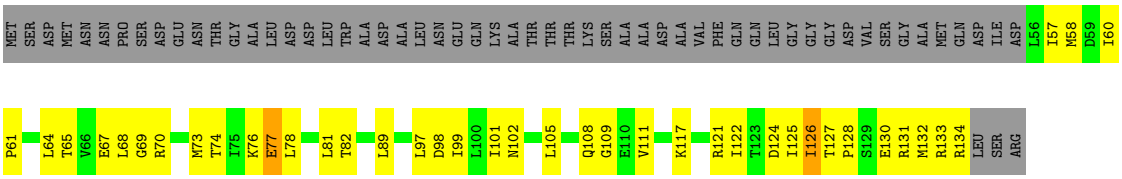




• Molecule 4: Flagellar motor switch protein FliN

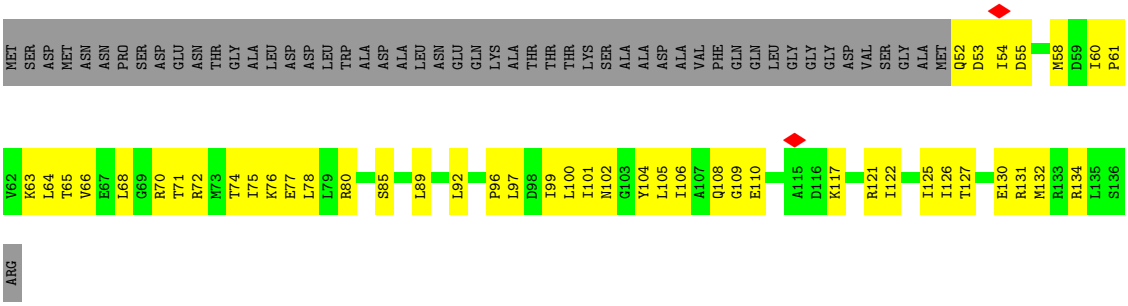
Chain E1:





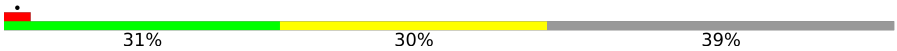
• Molecule 4: Flagellar motor switch protein FliN

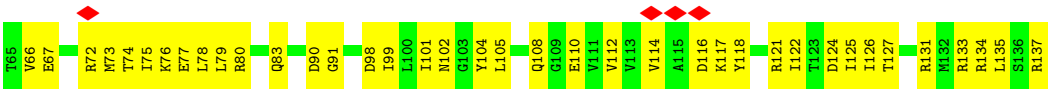
Chain F1:



• Molecule 4: Flagellar motor switch protein FliN

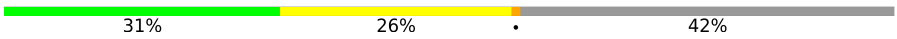
Chain D2:

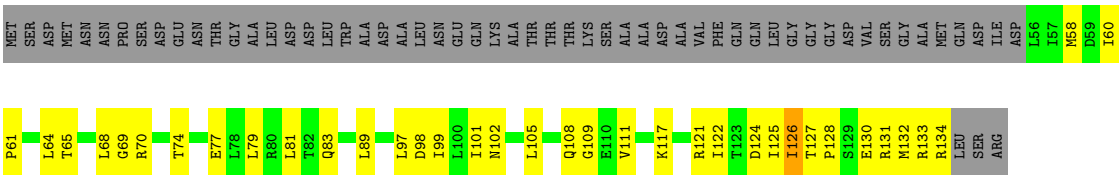




• Molecule 4: Flagellar motor switch protein FliN

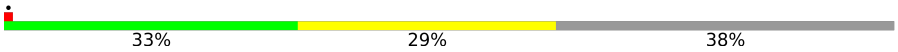
Chain E2:

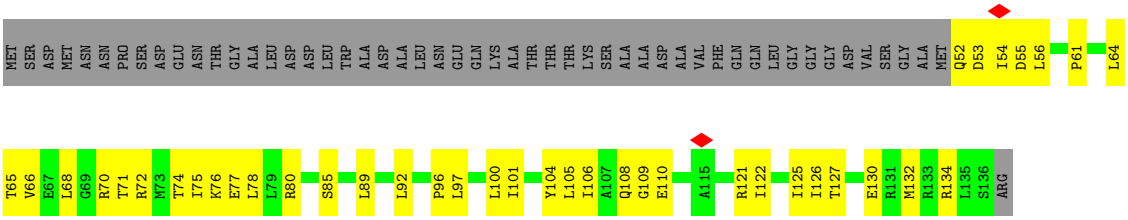




• Molecule 4: Flagellar motor switch protein FliN

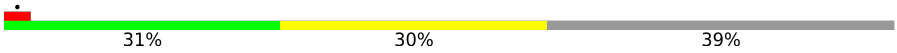
Chain F2:

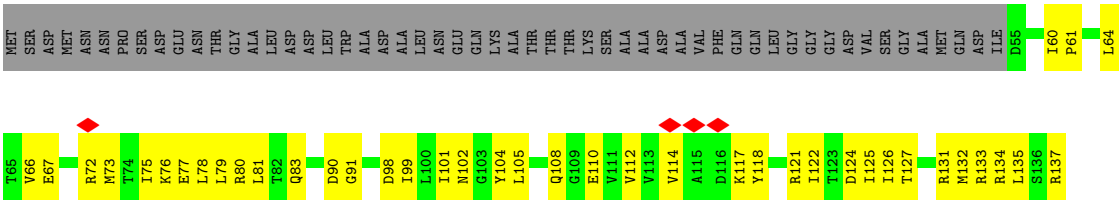




• Molecule 4: Flagellar motor switch protein FliN

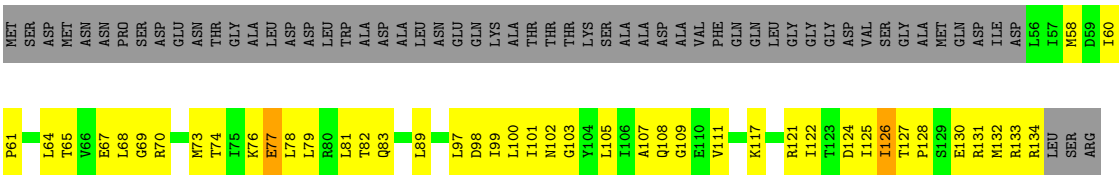
Chain D3:





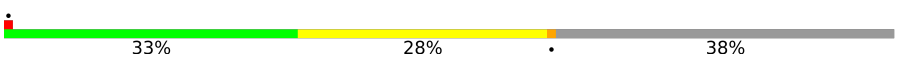
• Molecule 4: Flagellar motor switch protein FliN

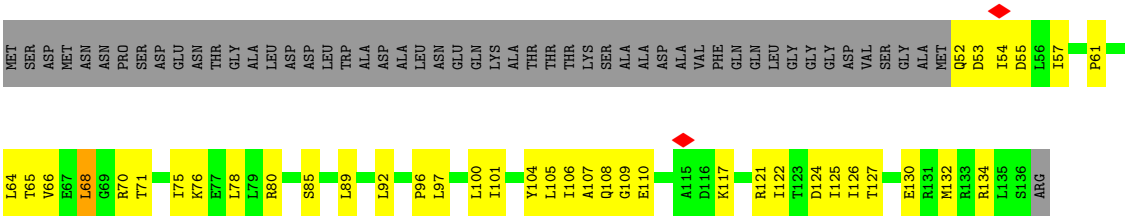
Chain E3:



• Molecule 4: Flagellar motor switch protein FliN

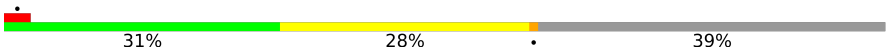
Chain F3:

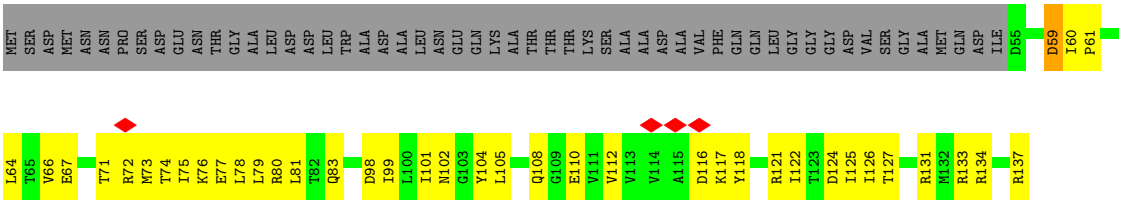




• Molecule 4: Flagellar motor switch protein FliN

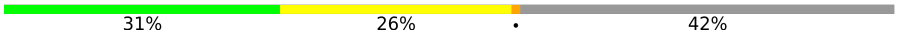
Chain D4:

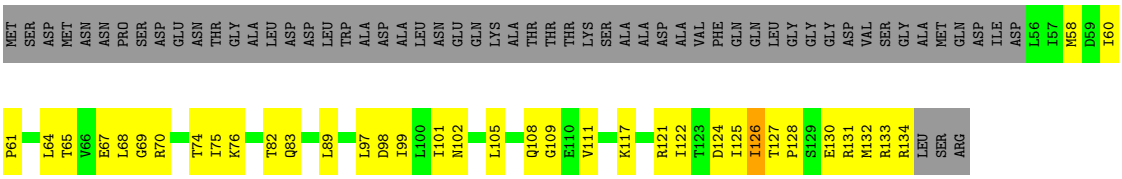




• Molecule 4: Flagellar motor switch protein FliN

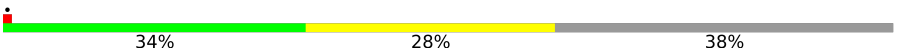
Chain E4:

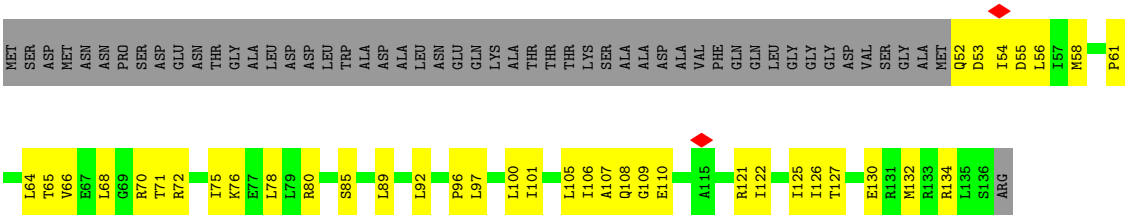




• Molecule 4: Flagellar motor switch protein FliN

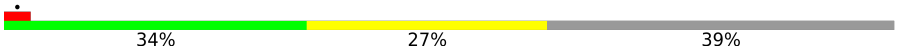
Chain F4:

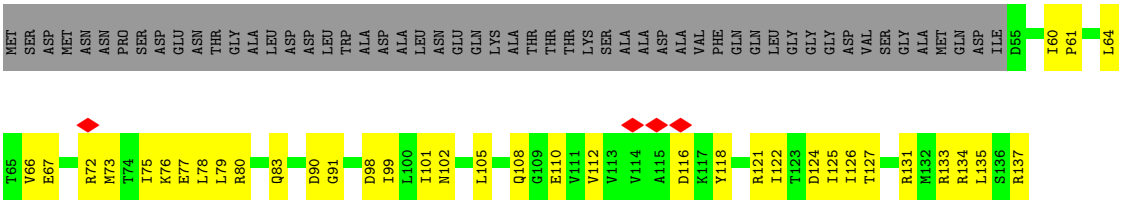




• Molecule 4: Flagellar motor switch protein FliN

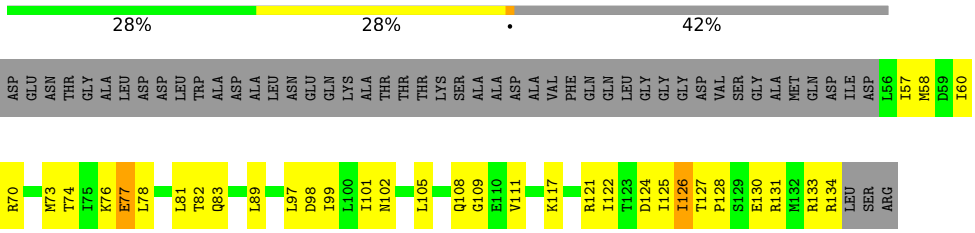
Chain D5:





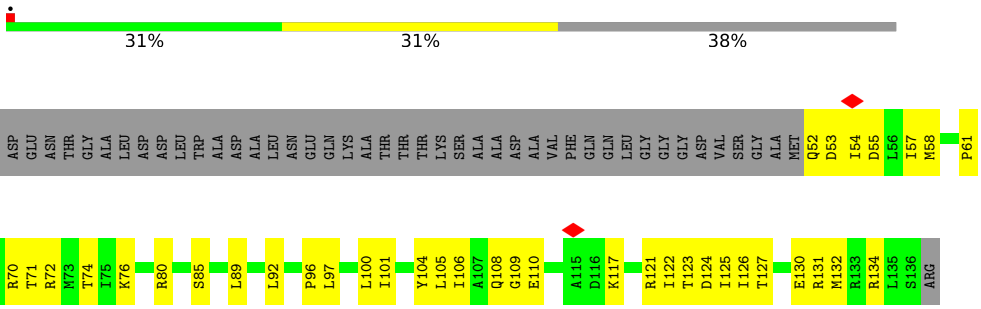
• Molecule 4: Flagellar motor switch protein FliN

Chain E5:



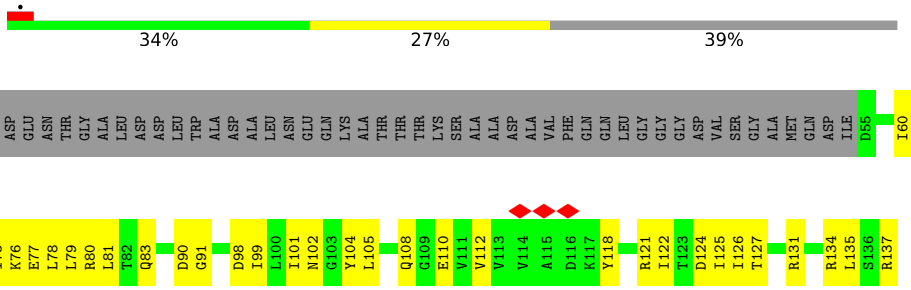
• Molecule 4: Flagellar motor switch protein FliN

Chain F5:



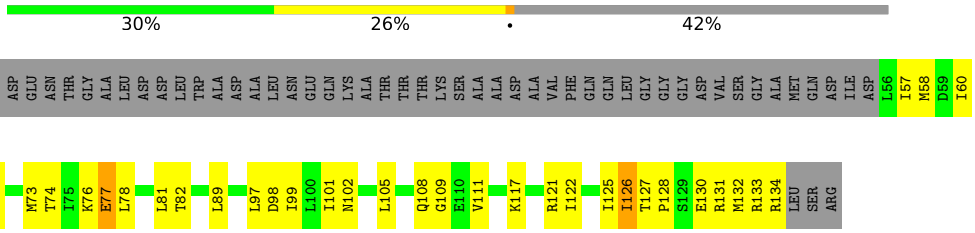
• Molecule 4: Flagellar motor switch protein FliN

Chain D6:



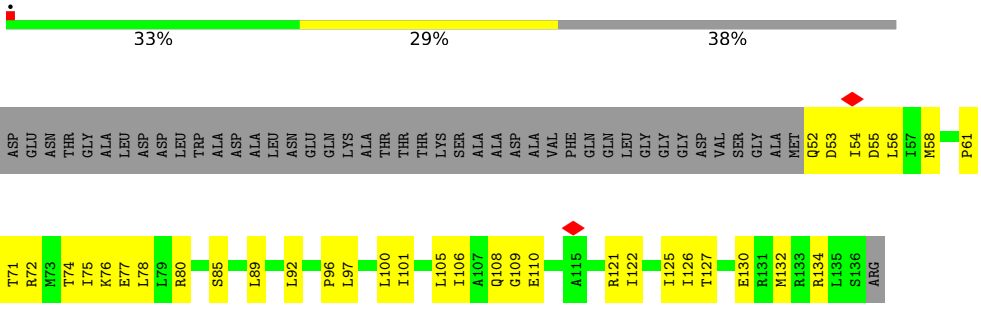
• Molecule 4: Flagellar motor switch protein FliN

Chain E6:



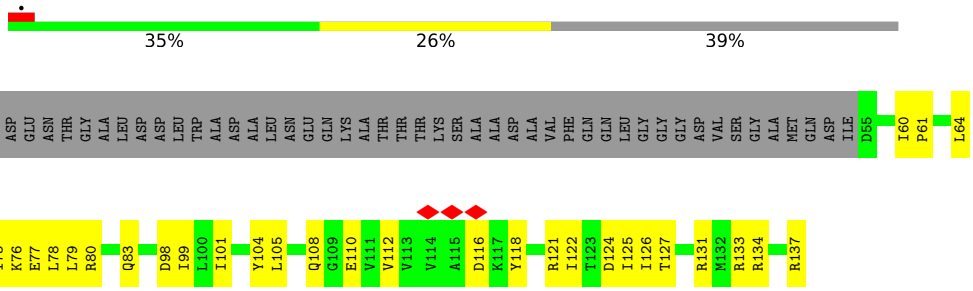
• Molecule 4: Flagellar motor switch protein FliN

Chain F6:



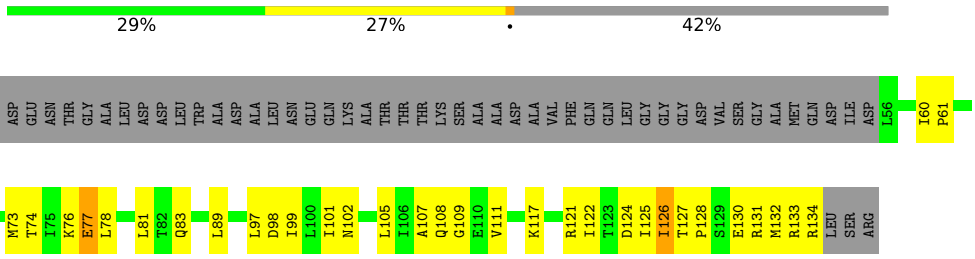
• Molecule 4: Flagellar motor switch protein FliN

Chain D7:



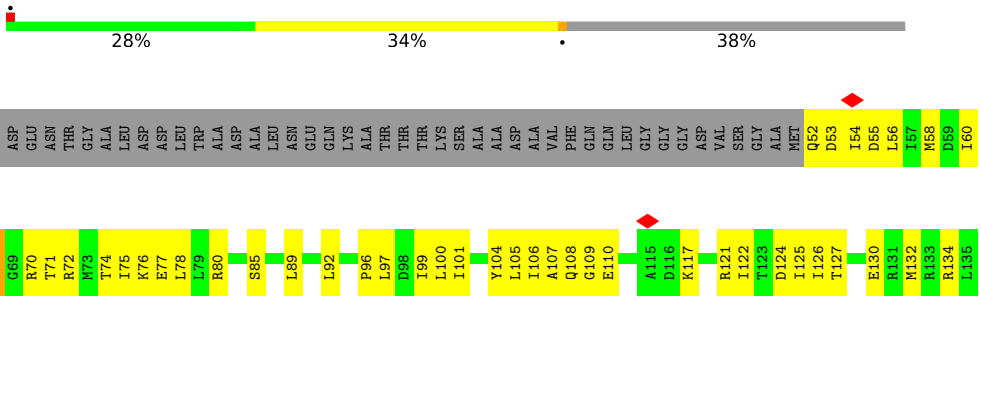
• Molecule 4: Flagellar motor switch protein FliN

Chain E7:



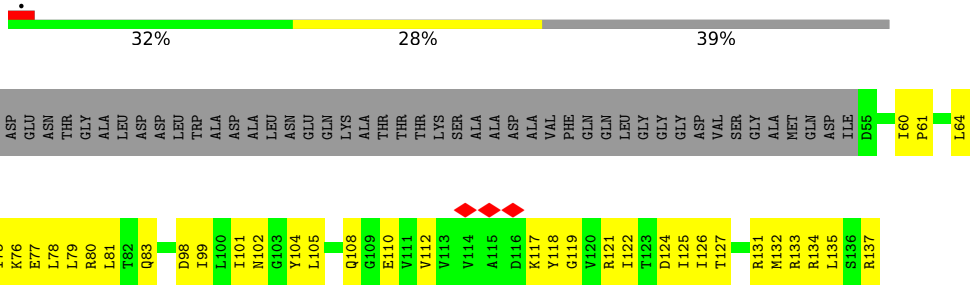
• Molecule 4: Flagellar motor switch protein FliN

Chain F7:



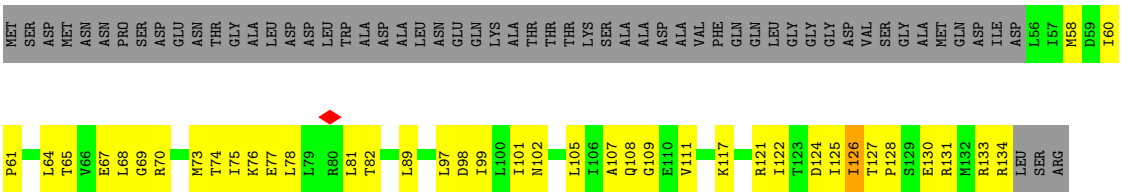
• Molecule 4: Flagellar motor switch protein FliN

Chain D8:



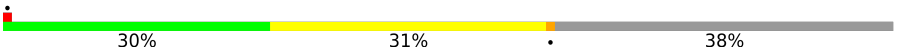
• Molecule 4: Flagellar motor switch protein FliN

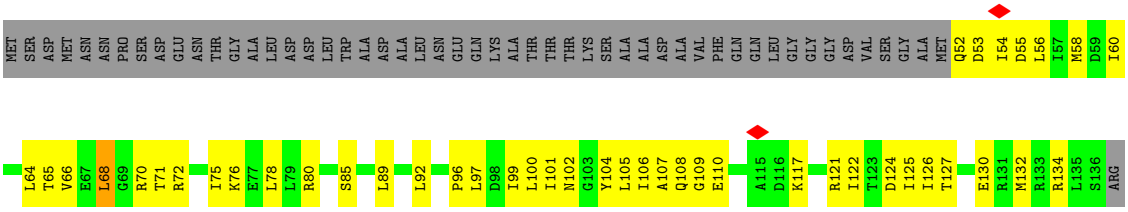
Chain E8:



• Molecule 4: Flagellar motor switch protein FliN

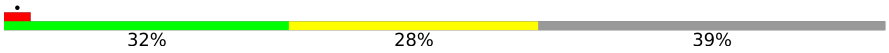
Chain F8:

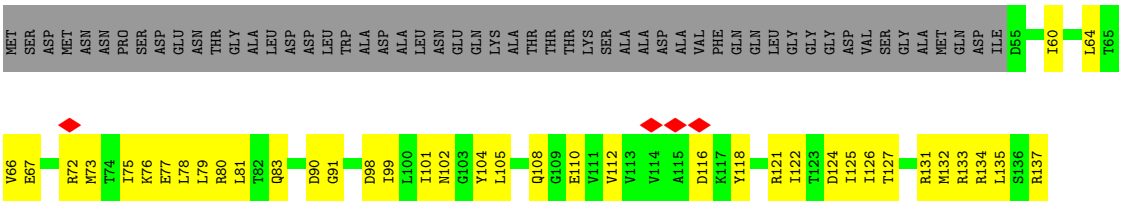




• Molecule 4: Flagellar motor switch protein FliN

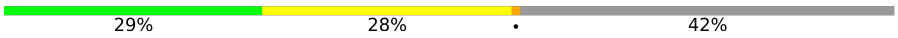
Chain D9:

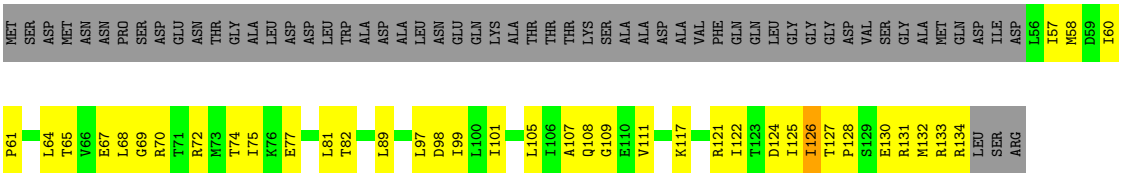




• Molecule 4: Flagellar motor switch protein FliN

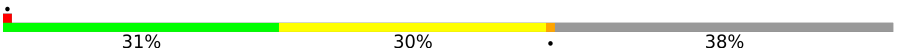
Chain E9:

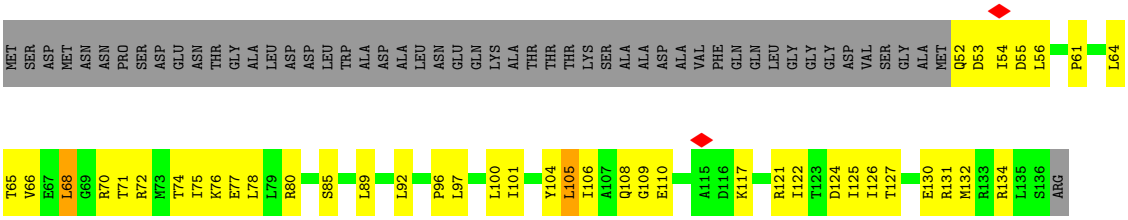




• Molecule 4: Flagellar motor switch protein FliN

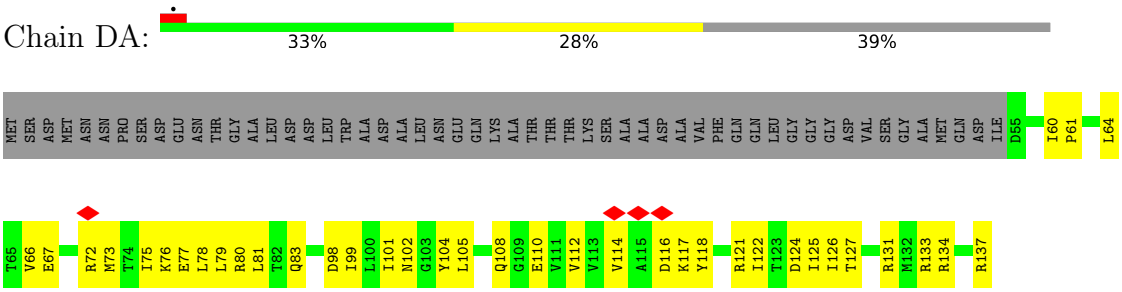
Chain F9:





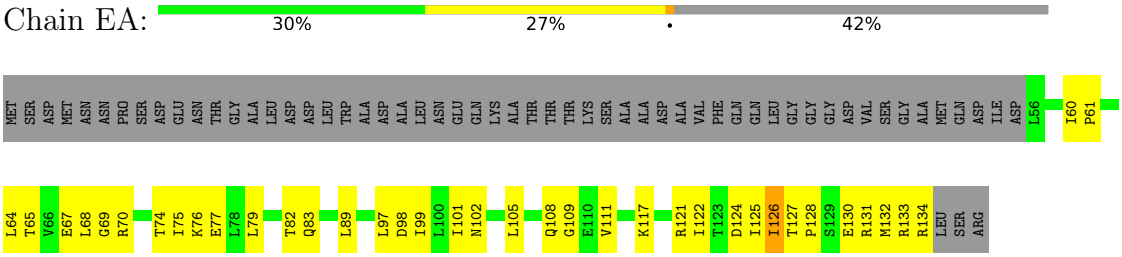
• Molecule 4: Flagellar motor switch protein FliN

Chain DA:



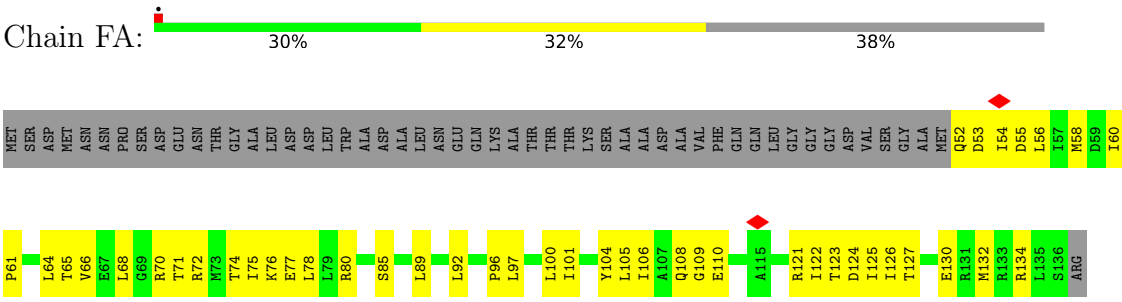
- Molecule 4: Flagellar motor switch protein FliN

Chain EA:



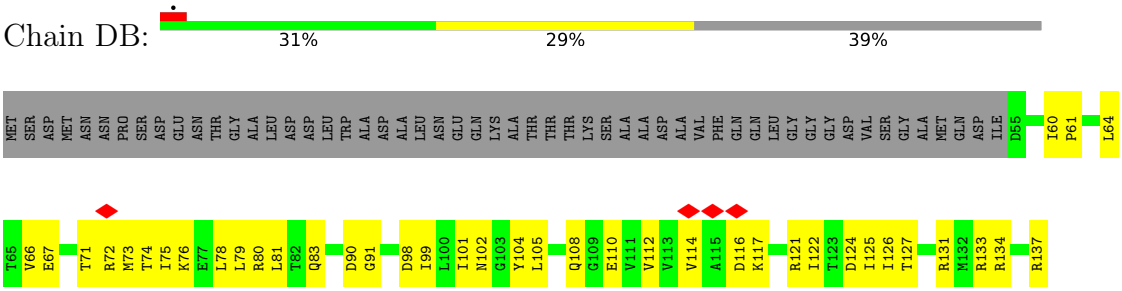
- Molecule 4: Flagellar motor switch protein FliN

Chain FA:



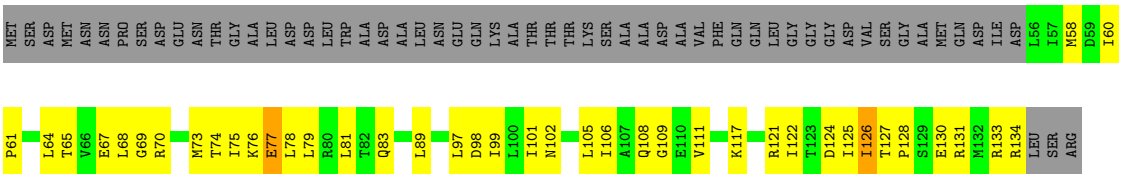
- Molecule 4: Flagellar motor switch protein FliN

Chain DB:



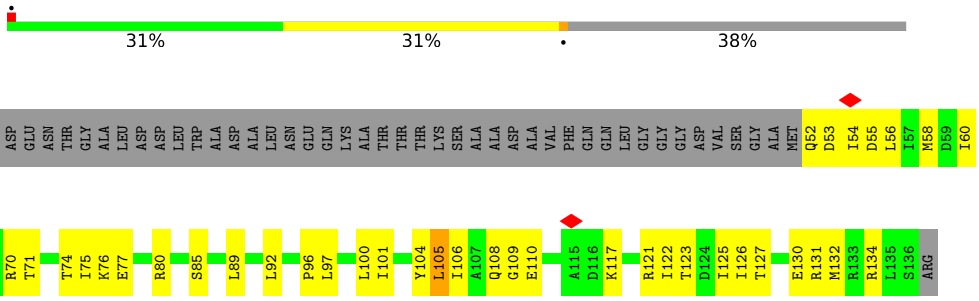
- Molecule 4: Flagellar motor switch protein FliN

Chain EB:



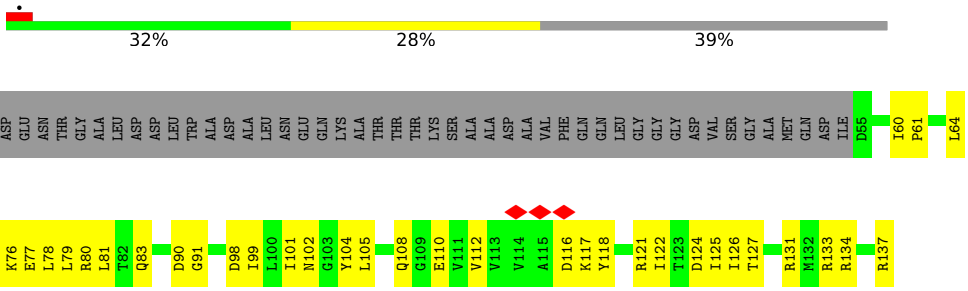
• Molecule 4: Flagellar motor switch protein FliN

Chain FB:



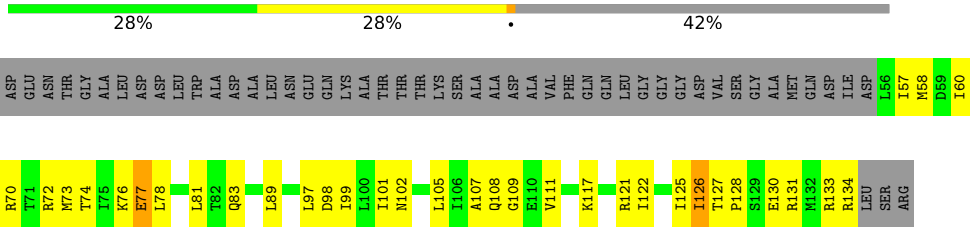
• Molecule 4: Flagellar motor switch protein FliN

Chain DC:



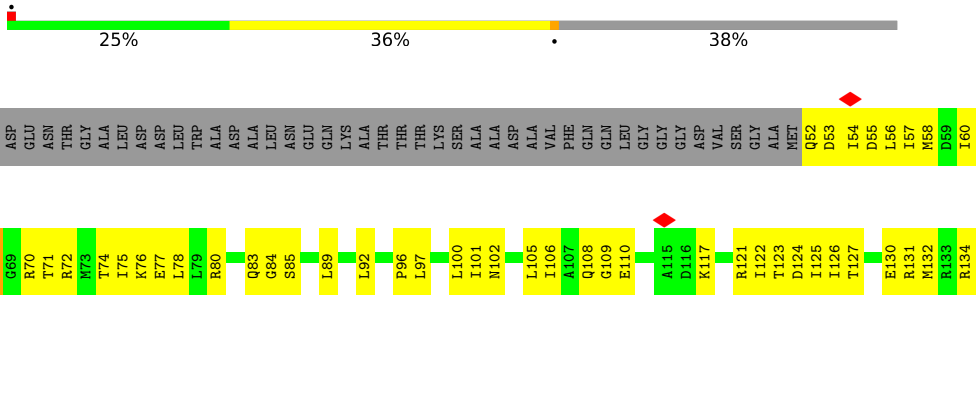
• Molecule 4: Flagellar motor switch protein FliN

Chain EC:



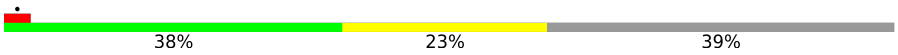
• Molecule 4: Flagellar motor switch protein FliN

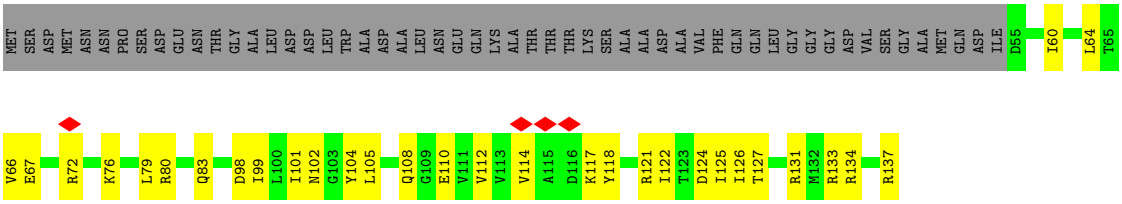
Chain FC:



• Molecule 4: Flagellar motor switch protein FliN

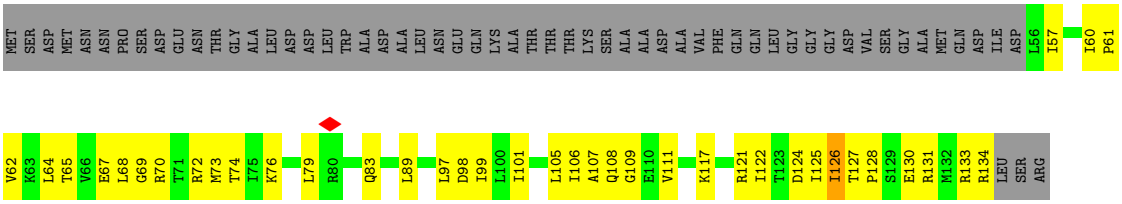
Chain DD:





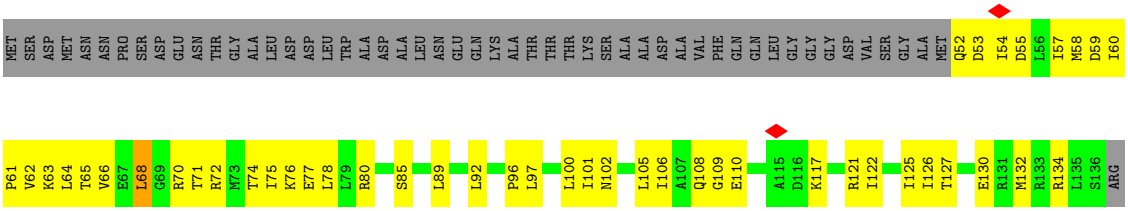
• Molecule 4: Flagellar motor switch protein FliN

Chain ED:



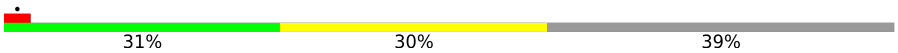
• Molecule 4: Flagellar motor switch protein FliN

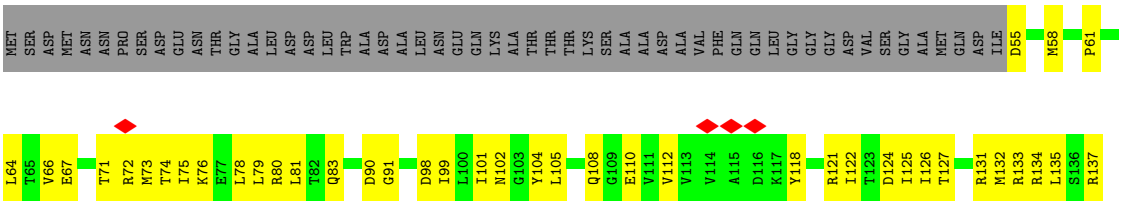
Chain FD:



• Molecule 4: Flagellar motor switch protein FliN

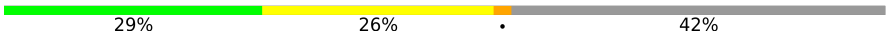
Chain DE:

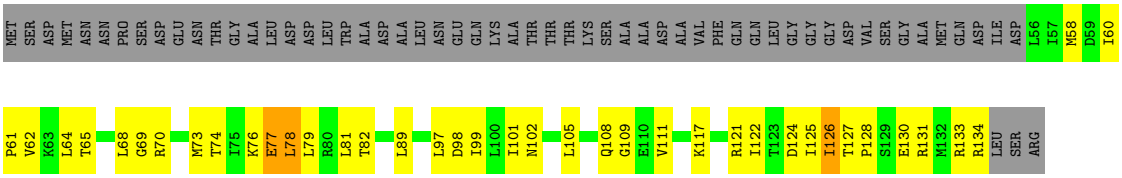




• Molecule 4: Flagellar motor switch protein FliN

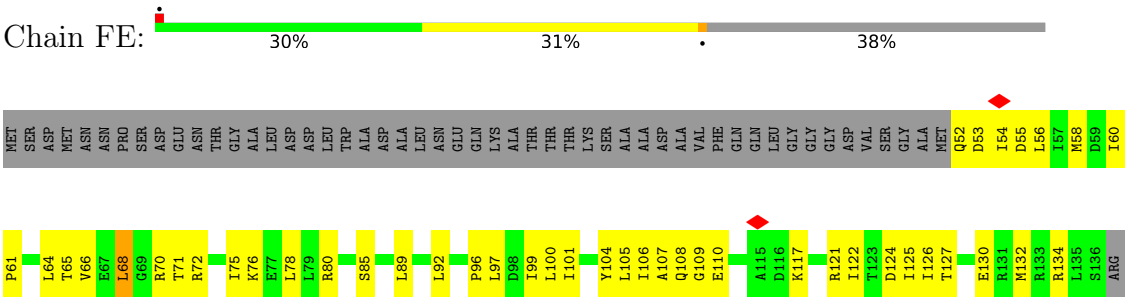
Chain EE:





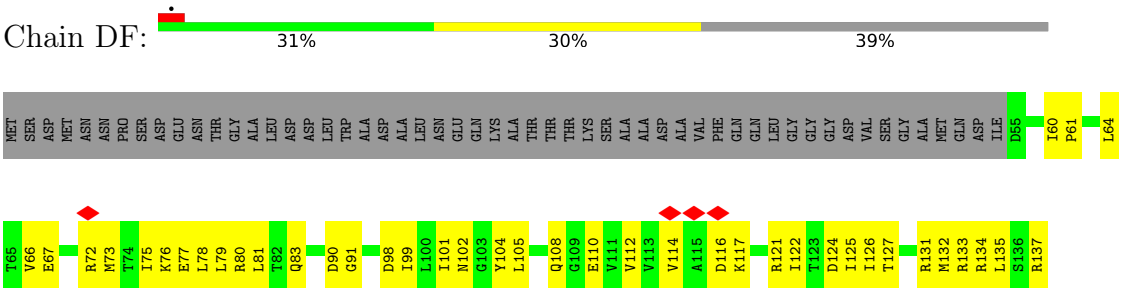
• Molecule 4: Flagellar motor switch protein FliN

Chain FE:



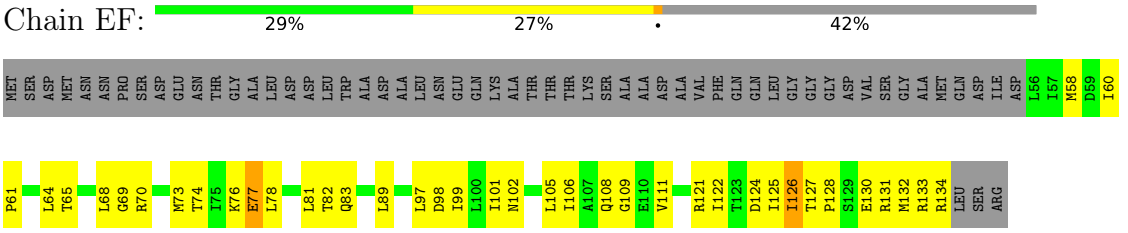
- Molecule 4: Flagellar motor switch protein FliN

Chain DF:



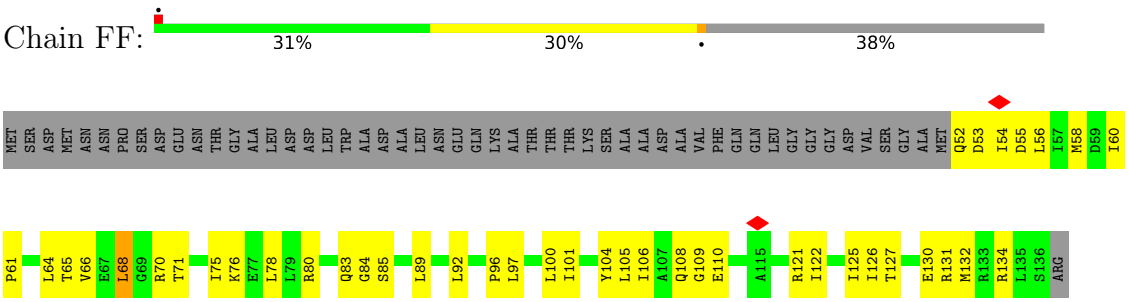
- Molecule 4: Flagellar motor switch protein FliN

Chain EF:



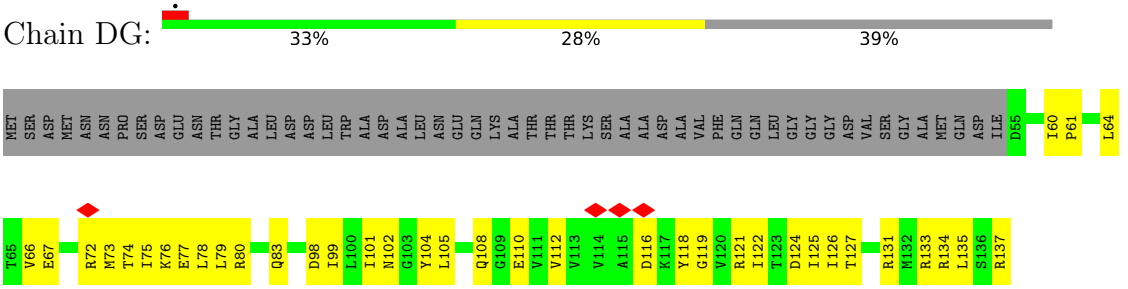
- Molecule 4: Flagellar motor switch protein FliN

Chain FF:



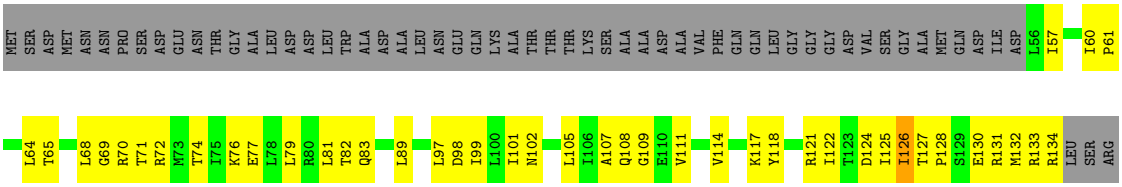
- Molecule 4: Flagellar motor switch protein FliN

Chain DG:



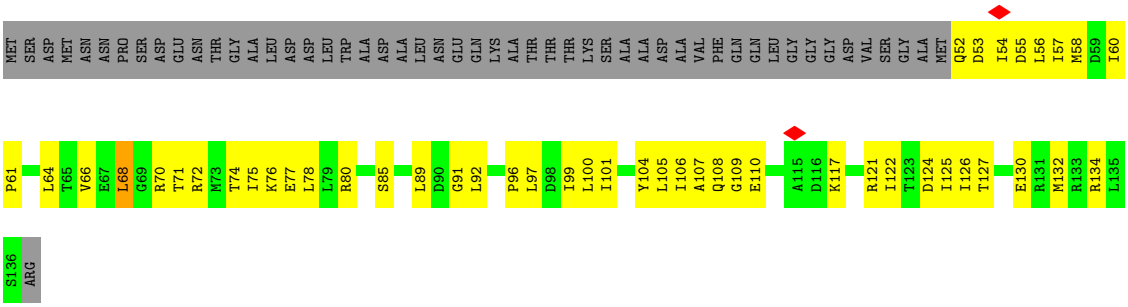
• Molecule 4: Flagellar motor switch protein FliN

Chain EG: 26% 31% • 42%



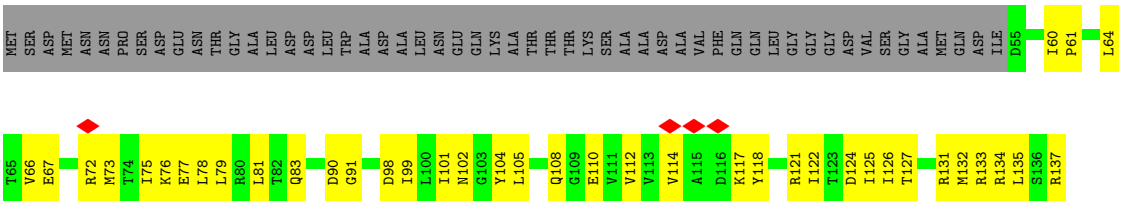
• Molecule 4: Flagellar motor switch protein FliN

Chain FG: 28% 34% • 38%



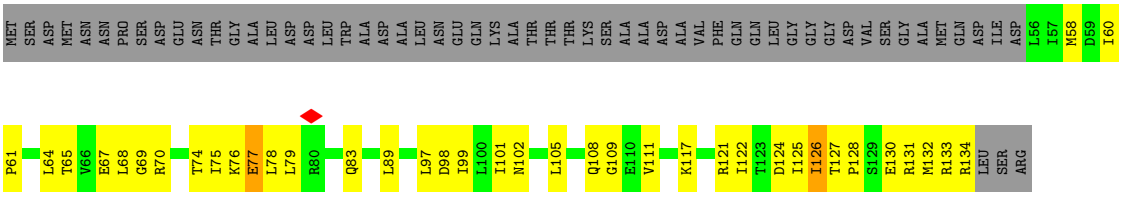
• Molecule 4: Flagellar motor switch protein FliN

Chain DH: 31% 29% 39%



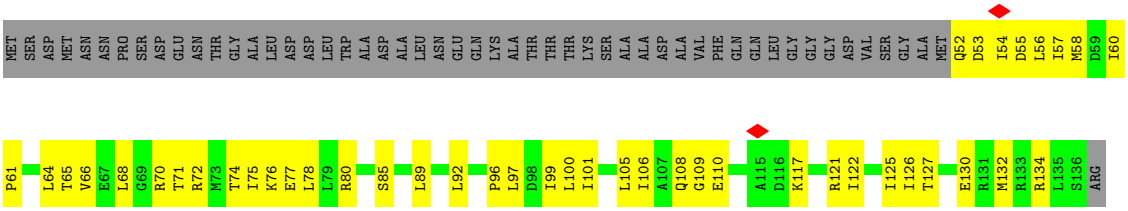
• Molecule 4: Flagellar motor switch protein FliN

Chain EH: 29% 27% • 42%



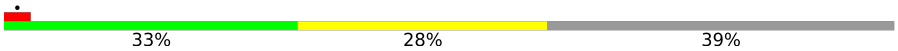
• Molecule 4: Flagellar motor switch protein FliN

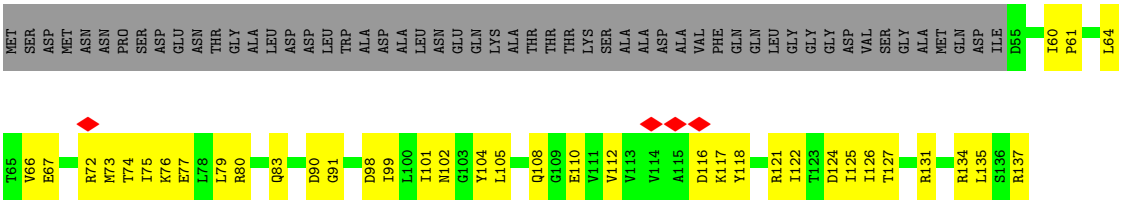
Chain FH: 30% 32% 38%



• Molecule 4: Flagellar motor switch protein FliN

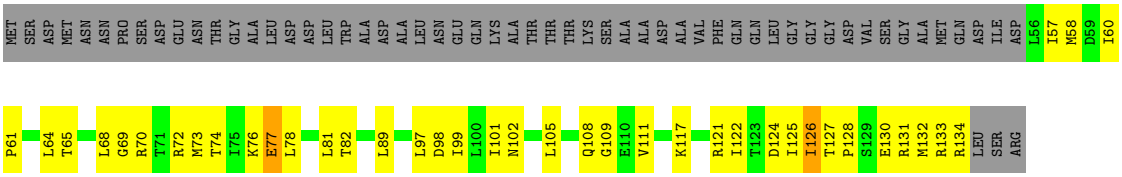
Chain DI:





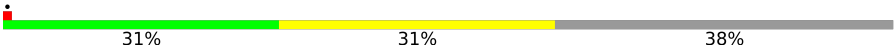
• Molecule 4: Flagellar motor switch protein FliN

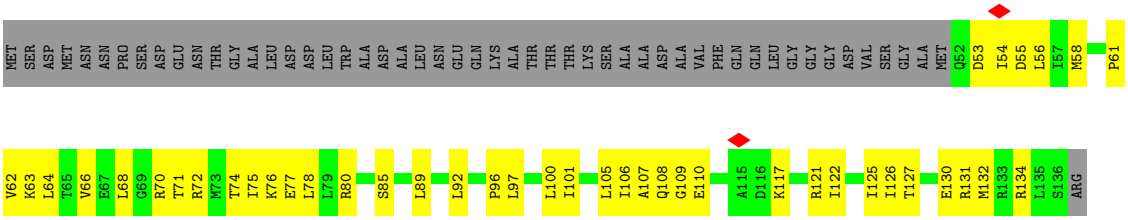
Chain EI:



• Molecule 4: Flagellar motor switch protein FliN

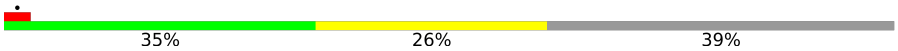
Chain FI:

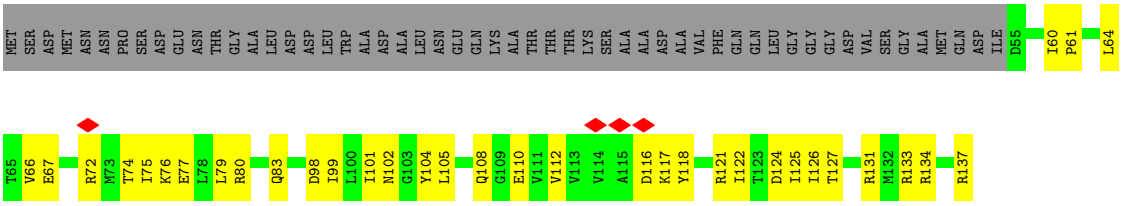




• Molecule 4: Flagellar motor switch protein FliN

Chain DJ:





• Molecule 4: Flagellar motor switch protein FliN

Chain EJ: 31% 26% • 42%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA MET GLN ASP ILE ASP L56 I60 P61

L64 T65 V66 E67 L68 G69 R70 M73 T74 I75 K76 E77 L78 L79 R80 L89 L97 D98 I99 L100 I101 N102 L105 Q108 G109 E110 V111 K117 R121 I122 T123 D124 I125 I126 T127 P128 S129 E130 R131 M132 R133 R134 LEU SER ARG

• Molecule 4: Flagellar motor switch protein FliN

Chain FJ: 31% 31% 38%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA MET Q52 D53 I54 D55 L56 I57 M58 P61

L64 T65 V66 E67 L68 G69 R70 T71 R72 M73 T74 I75 K76 E77 L78 L79 R80 S85 L89 L92 P96 L97 D98 I99 L100 I101 Y104 L105 I106 A107 Q108 G109 E110 A115 R121 I122 I125 I126 T127 E130 R131 M132 R133 R134 L135 S136 ARG

• Molecule 4: Flagellar motor switch protein FliN

Chain DK: 31% 29% 39%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA MET GLN ASP ILE D55 I60 P61 L64

T65 V66 E67 R72 M73 T74 I75 K76 E77 L78 L79 R80 L81 T82 Q83 D90 G91 D98 I99 L100 I101 N102 G103 Y104 L105 Q108 G109 E110 V111 V112 V113 V114 A115 D116 K117 Y118 R121 I122 T123 D124 I125 I126 T127 R131 M132 R133 R134 L135 S136 R137

• Molecule 4: Flagellar motor switch protein FliN

Chain EK: 29% 27% • 42%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA MET GLN ASP ILE ASP L56 I57 M58 D59 I60

P61 L64 T65 L68 G69 R70 M73 T74 I75 K76 E77 L78 L81 L89 L97 D98 I99 L100 I101 N102 G103 Y104 L105 I106 A107 Q108 G109 E110 V111 K117 R121 I122 I125 I126 T127 P128 S129 E130 R131 M132 R133 R134 LEU SER ARG

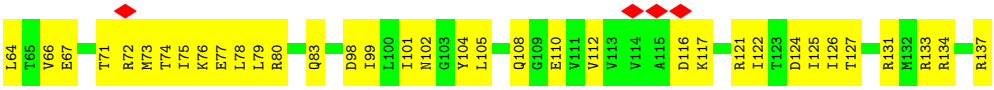
• Molecule 4: Flagellar motor switch protein FliN

Chain FK: 32% 29% • 38%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA MET Q52 D53 I54 D55 L56 I57 M58 P61

• Molecule 4: Flagellar motor switch protein FliN

Chain DL: 33% 27% 39%

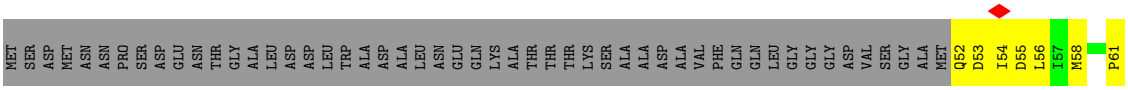


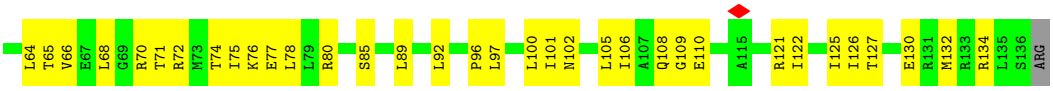
• Molecule 4: Flagellar motor switch protein FliN

Chain EL: 31% 26% 42%

• Molecule 4: Flagellar motor switch protein FliN

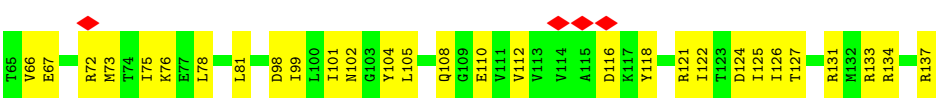
Chain FL: 32% 30% 38%





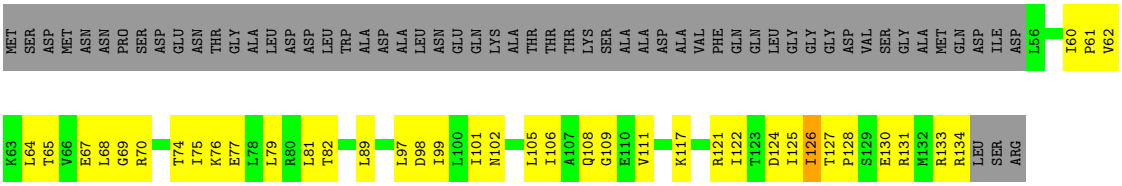
• Molecule 4: Flagellar motor switch protein FliN

Chain DM: 37% 23% 39%



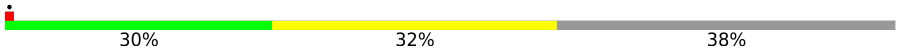
• Molecule 4: Flagellar motor switch protein FliN

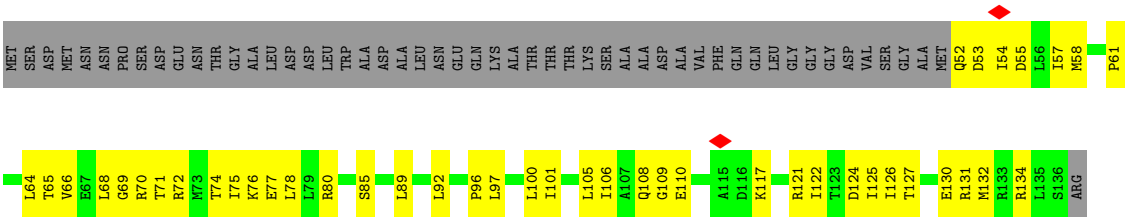
Chain EM: 29% 28% 42%



• Molecule 4: Flagellar motor switch protein FliN

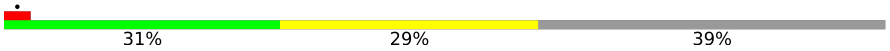
Chain FM:

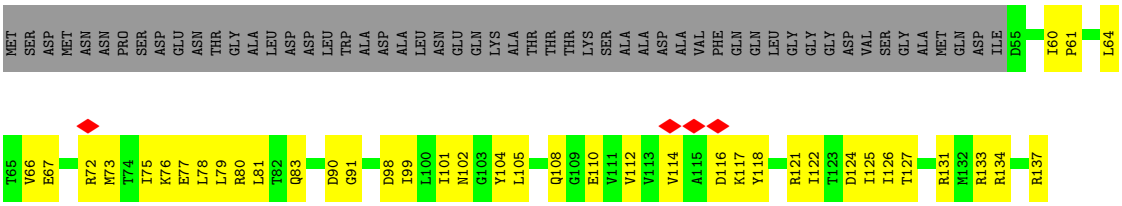




• Molecule 4: Flagellar motor switch protein FliN

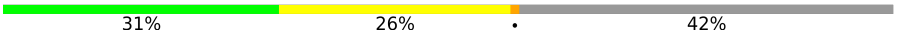
Chain DN:

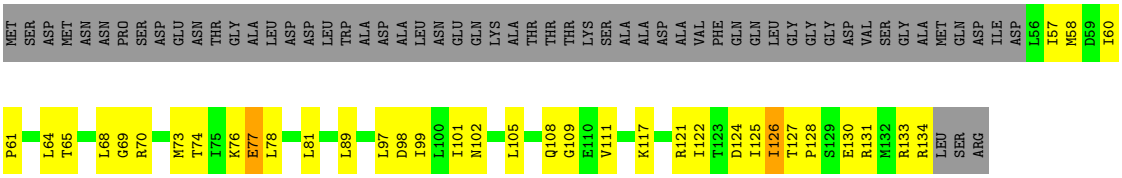




• Molecule 4: Flagellar motor switch protein FliN

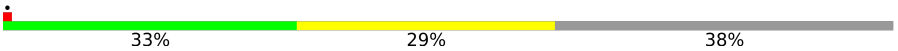
Chain EN:

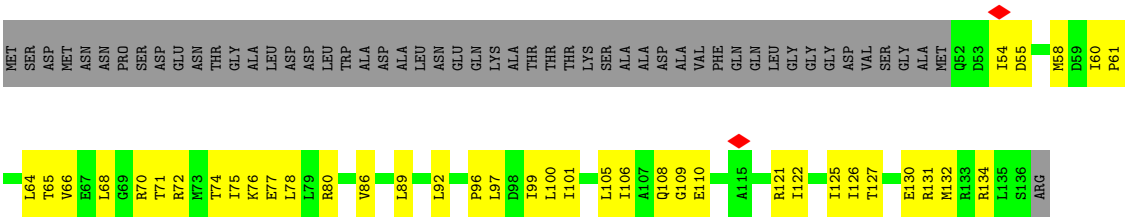




• Molecule 4: Flagellar motor switch protein FliN

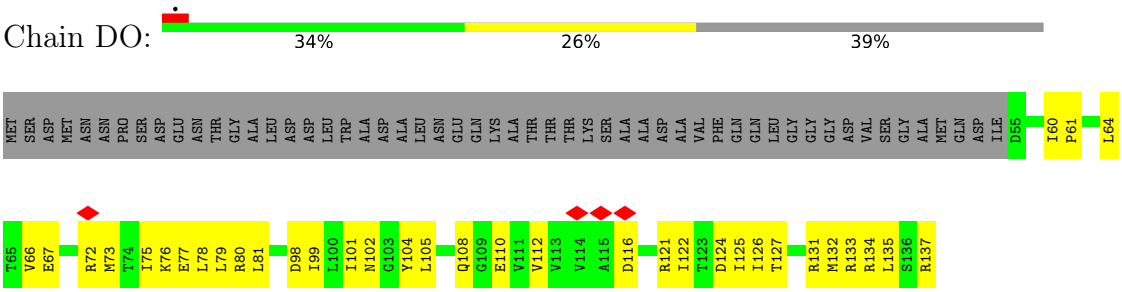
Chain FN:





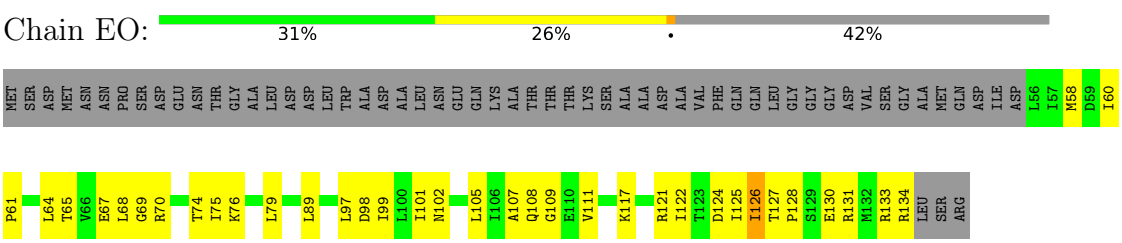
• Molecule 4: Flagellar motor switch protein FliN

Chain DO:



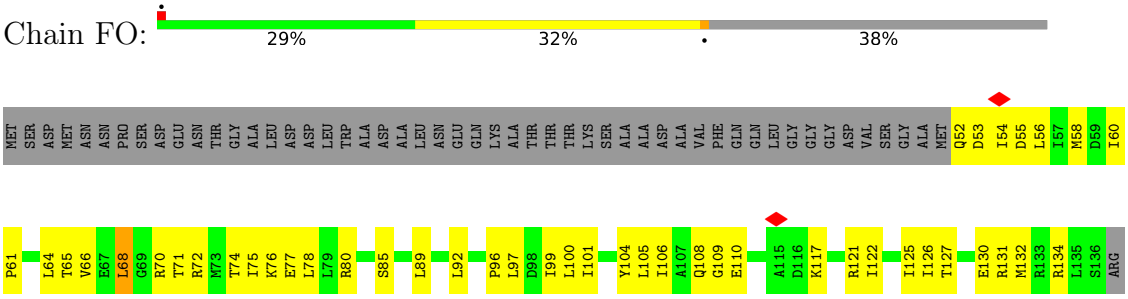
• Molecule 4: Flagellar motor switch protein FliN

Chain EO:



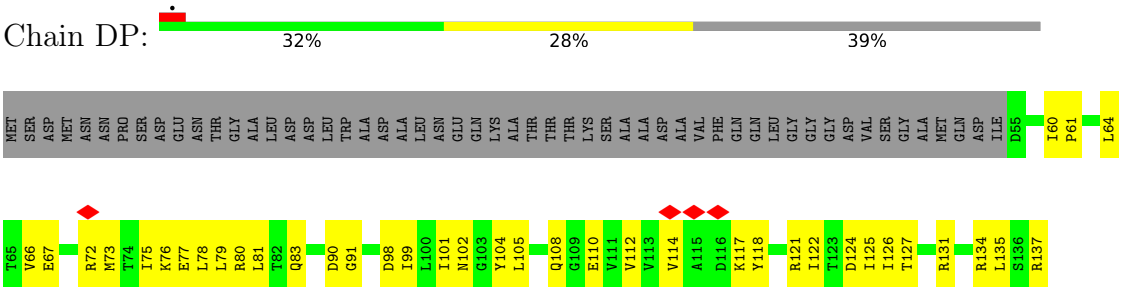
• Molecule 4: Flagellar motor switch protein FliN

Chain FO:



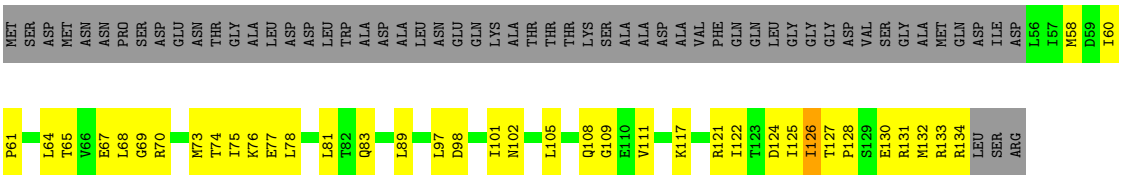
• Molecule 4: Flagellar motor switch protein FliN

Chain DP:



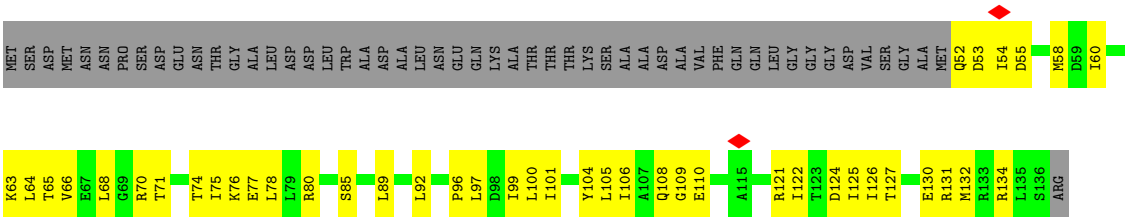
• Molecule 4: Flagellar motor switch protein FliN

Chain EP:



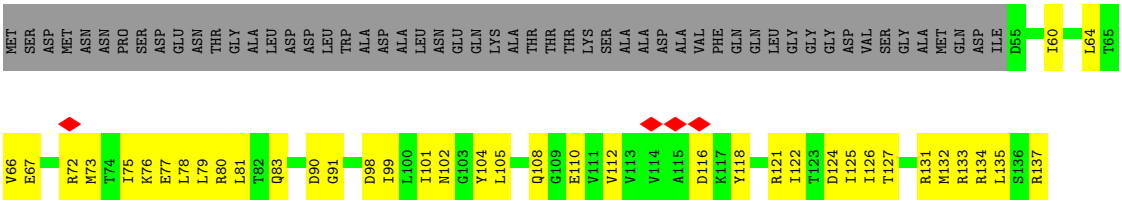
• Molecule 4: Flagellar motor switch protein FliN

Chain FP: 31% 31% 38%



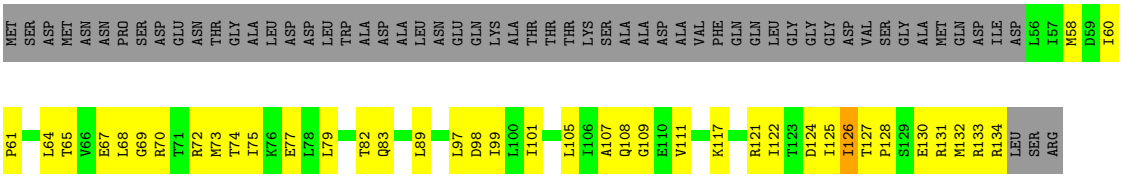
- Molecule 4: Flagellar motor switch protein FliN

Chain DQ: 32% 28% 39%



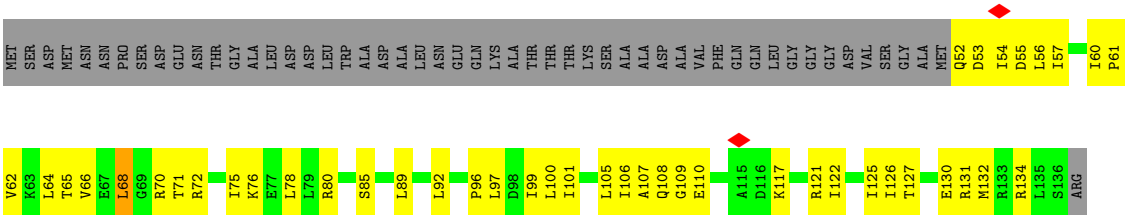
- Molecule 4: Flagellar motor switch protein FliN

Chain EQ: 28% 28% 42%



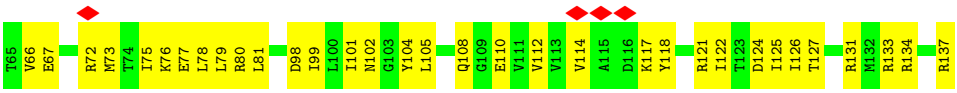
- Molecule 4: Flagellar motor switch protein FliN

Chain FQ: 30% 31% 38%



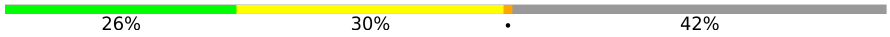
- Molecule 4: Flagellar motor switch protein FliN

Chain DR: 34% 26% 39%



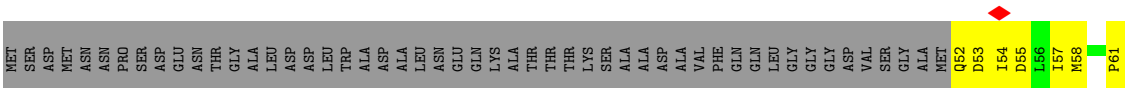
• Molecule 4: Flagellar motor switch protein FliN

Chain ER:



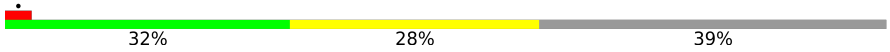
• Molecule 4: Flagellar motor switch protein FliN

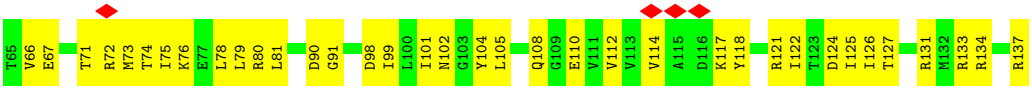
Chain FR:



• Molecule 4: Flagellar motor switch protein FliN

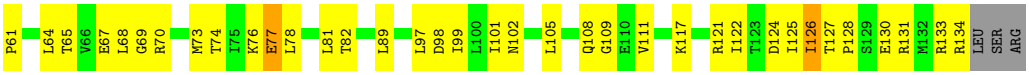
Chain DS:





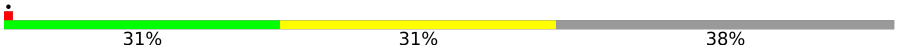
• Molecule 4: Flagellar motor switch protein FliN

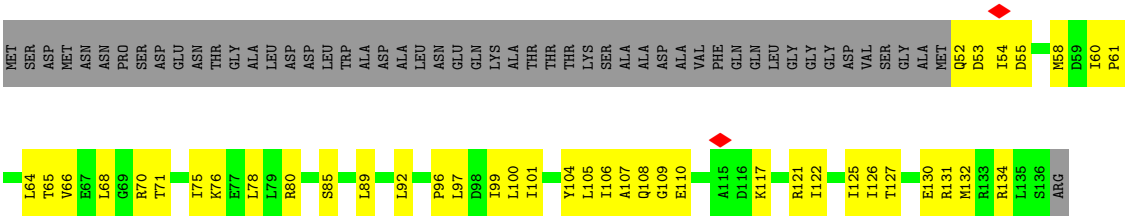
Chain ES:



• Molecule 4: Flagellar motor switch protein FliN

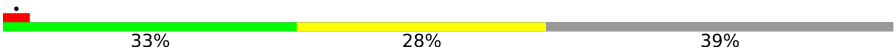
Chain FS:

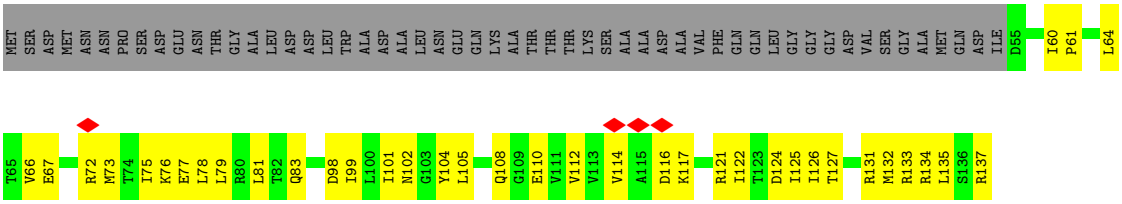




• Molecule 4: Flagellar motor switch protein FliN

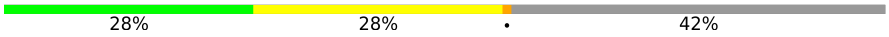
Chain DT:

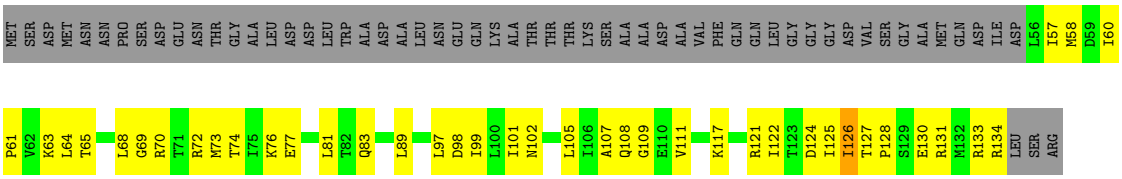




• Molecule 4: Flagellar motor switch protein FliN

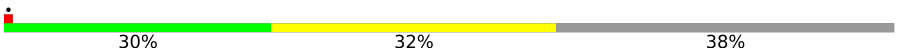
Chain ET:

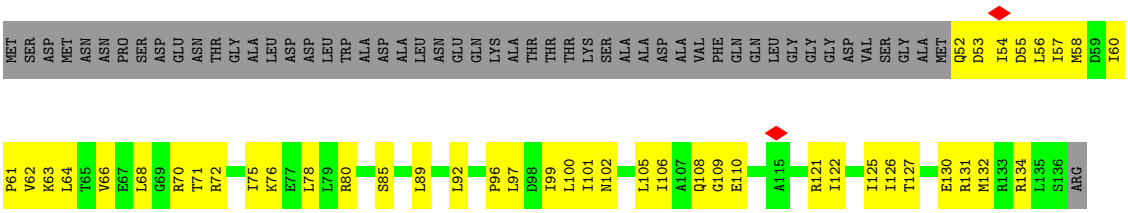




• Molecule 4: Flagellar motor switch protein FliN

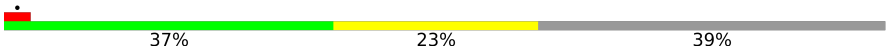
Chain FT:

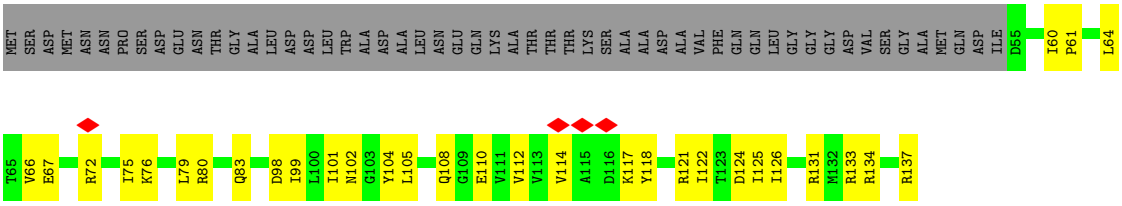




• Molecule 4: Flagellar motor switch protein FliN

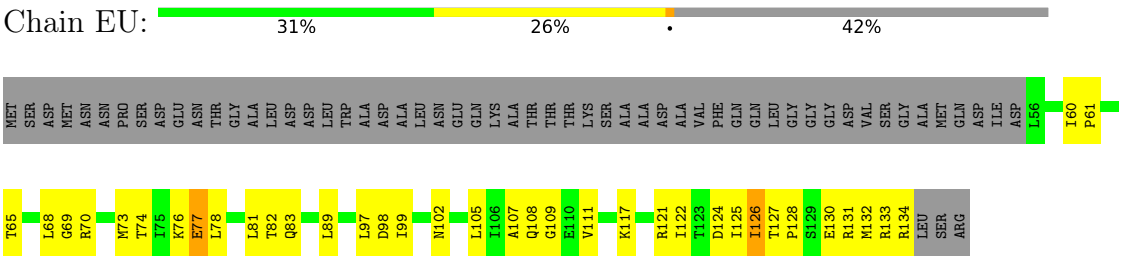
Chain DU:





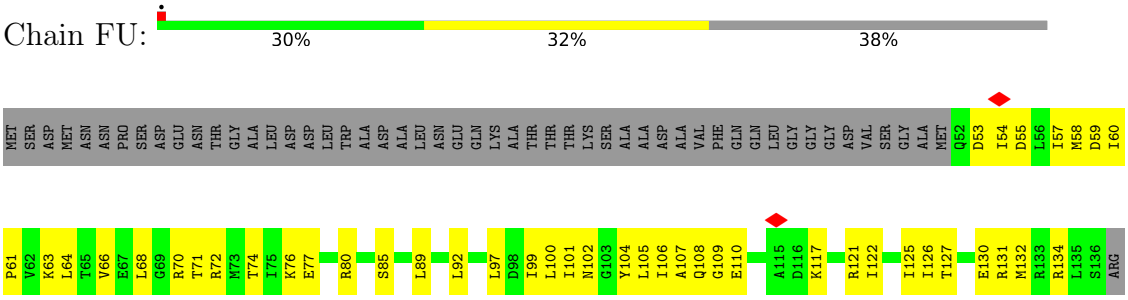
• Molecule 4: Flagellar motor switch protein FliN

Chain EU:



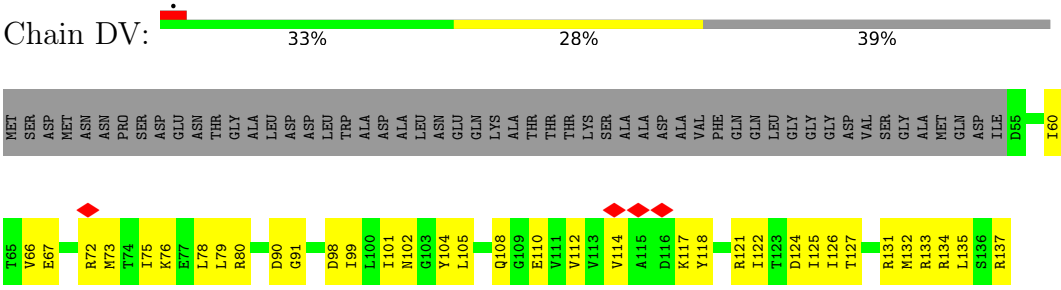
• Molecule 4: Flagellar motor switch protein FliN

Chain FU:



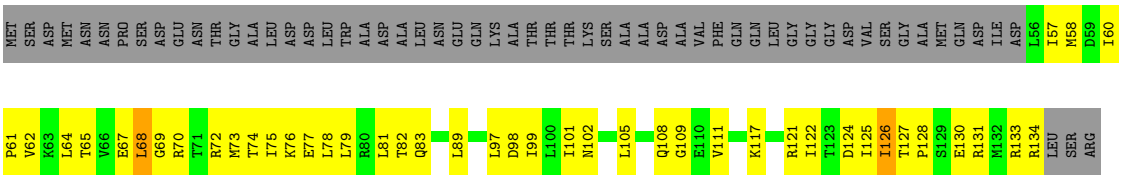
• Molecule 4: Flagellar motor switch protein FliN

Chain DV:



• Molecule 4: Flagellar motor switch protein FliN

Chain EV:



• Molecule 4: Flagellar motor switch protein FliN

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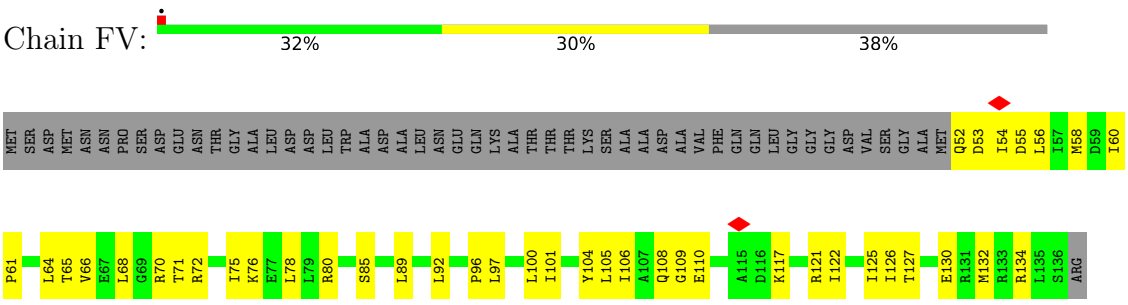
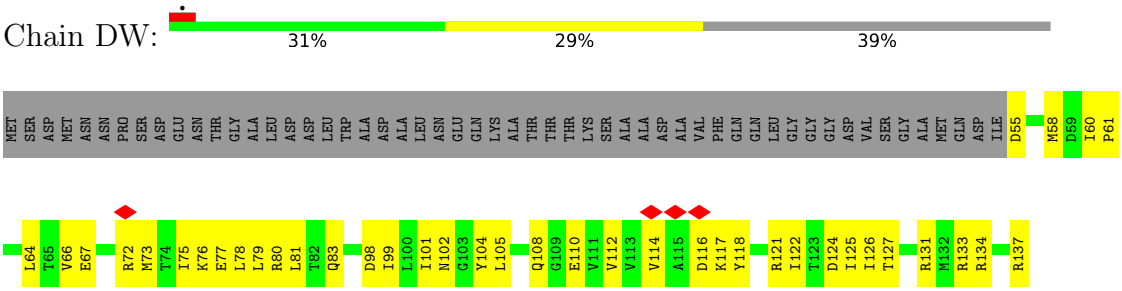


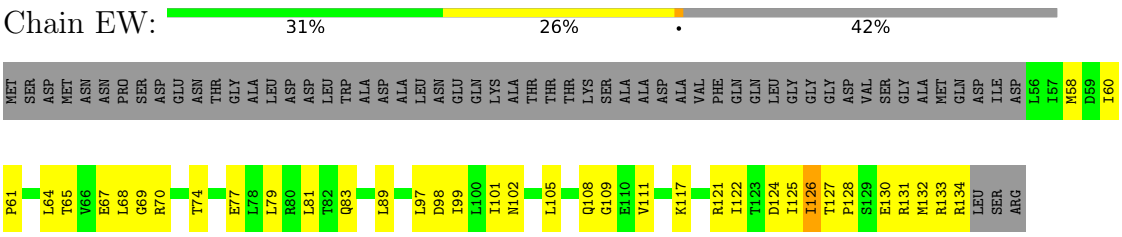
• Molecule 4: Flagellar motor switch protein FliN

Chain DW:



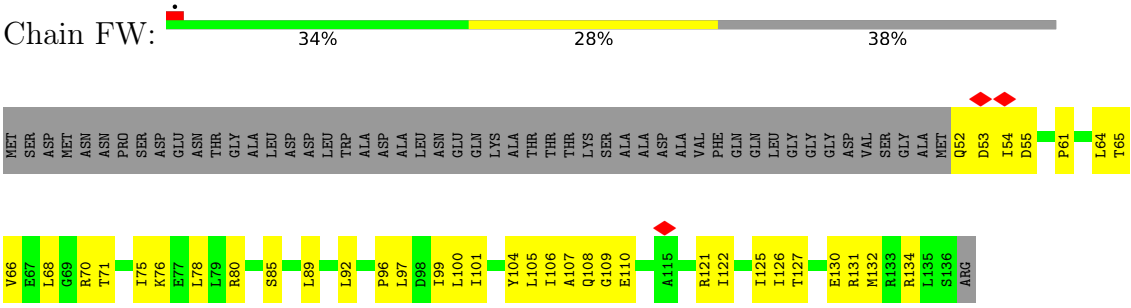
• Molecule 4: Flagellar motor switch protein FliN

Chain EW:



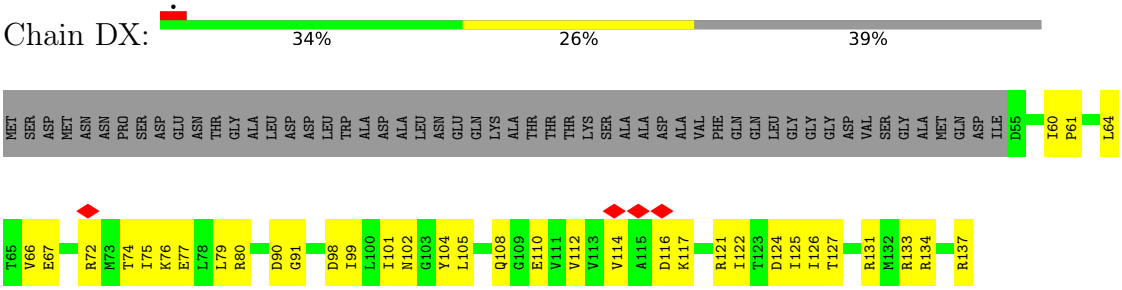
• Molecule 4: Flagellar motor switch protein FliN

Chain FW:



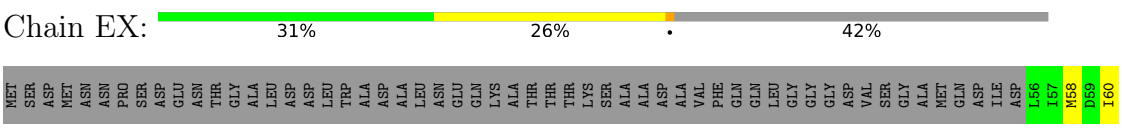
• Molecule 4: Flagellar motor switch protein FliN

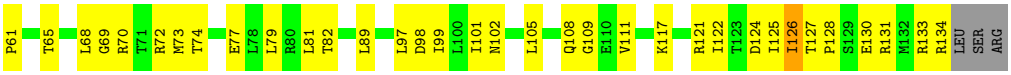
Chain DX:



• Molecule 4: Flagellar motor switch protein FliN

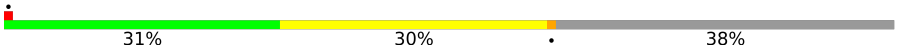
Chain EX:

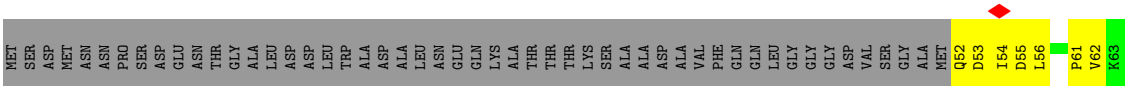


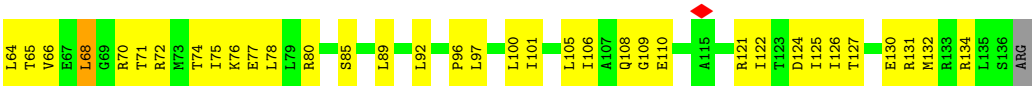


• Molecule 4: Flagellar motor switch protein FliN

Chain FX:

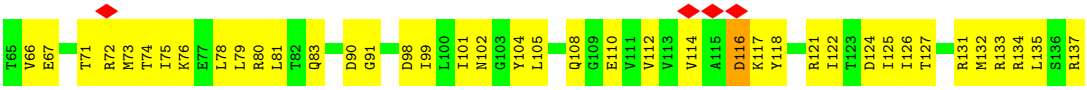






• Molecule 4: Flagellar motor switch protein FliN

Chain DY:

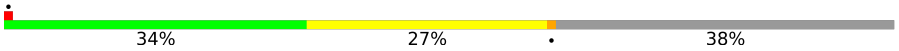


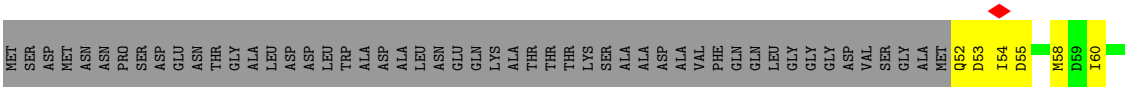
• Molecule 4: Flagellar motor switch protein FliN

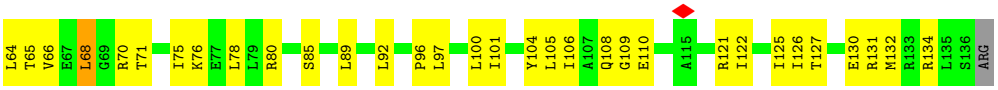
Chain EY:

• Molecule 4: Flagellar motor switch protein FliN

Chain FY:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19363	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.271	Depositor
Minimum map value	-0.262	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	851.968, 851.968, 851.968	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.664, 1.664, 1.664	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A1	0.24	0/370	0.58	0/494
1	A2	0.22	0/370	0.57	0/494
1	A3	0.24	0/370	0.58	0/494
1	A4	0.23	0/370	0.57	0/494
1	A5	0.23	0/370	0.57	0/494
1	A6	0.23	0/370	0.58	0/494
1	A7	0.22	0/370	0.56	0/494
1	A8	0.23	0/370	0.57	0/494
1	A9	0.24	0/370	0.58	0/494
1	AA	0.23	0/370	0.58	0/494
1	AB	0.23	0/370	0.57	0/494
1	AC	0.24	0/370	0.58	0/494
1	AD	0.23	0/370	0.58	0/494
1	AE	0.22	0/370	0.57	0/494
1	AF	0.22	0/370	0.56	0/494
1	AG	0.22	0/370	0.56	0/494
1	AH	0.24	0/370	0.59	0/494
1	AI	0.23	0/370	0.57	0/494
1	AJ	0.23	0/370	0.57	0/494
1	AK	0.24	0/370	0.58	0/494
1	AL	0.23	0/370	0.56	0/494
1	AM	0.23	0/370	0.57	0/494
1	AN	0.24	0/370	0.58	0/494
1	AO	0.22	0/370	0.57	0/494
1	AP	0.23	0/370	0.58	0/494
1	AQ	0.22	0/370	0.57	0/494
1	AR	0.23	0/370	0.58	0/494
1	AS	0.23	0/370	0.57	0/494
1	AT	0.22	0/370	0.56	0/494
1	AU	0.23	0/370	0.58	0/494
1	AV	0.24	0/370	0.57	0/494
1	AW	0.23	0/370	0.57	0/494
1	AX	0.23	0/370	0.56	0/494
1	AY	0.23	0/370	0.58	0/494

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	B1	0.25	0/2586	0.52	0/3485
2	B2	0.25	0/2586	0.52	0/3485
2	B3	0.25	0/2586	0.52	0/3485
2	B4	0.25	0/2586	0.53	0/3485
2	B5	0.25	0/2586	0.53	0/3485
2	B6	0.25	0/2586	0.52	0/3485
2	B7	0.25	0/2586	0.52	0/3485
2	B8	0.25	0/2586	0.52	0/3485
2	B9	0.25	0/2586	0.52	0/3485
2	BA	0.25	0/2586	0.52	0/3485
2	BB	0.25	0/2586	0.52	0/3485
2	BC	0.25	0/2586	0.52	0/3485
2	BD	0.25	0/2586	0.52	0/3485
2	BE	0.25	0/2586	0.52	0/3485
2	BF	0.25	0/2586	0.52	0/3485
2	BG	0.25	0/2586	0.53	0/3485
2	BH	0.25	0/2586	0.52	0/3485
2	BI	0.25	0/2586	0.53	0/3485
2	BJ	0.25	0/2586	0.52	0/3485
2	BK	0.24	0/2586	0.52	0/3485
2	BL	0.25	0/2586	0.52	0/3485
2	BM	0.25	0/2586	0.52	0/3485
2	BN	0.25	0/2586	0.53	0/3485
2	BO	0.24	0/2586	0.52	0/3485
2	BP	0.25	0/2586	0.52	0/3485
2	BQ	0.24	0/2586	0.53	0/3485
2	BR	0.25	0/2586	0.54	1/3485 (0.0%)
2	BS	0.25	0/2586	0.53	0/3485
2	BT	0.25	0/2586	0.52	0/3485
2	BU	0.25	0/2586	0.53	0/3485
2	BV	0.25	0/2586	0.53	0/3485
2	BW	0.25	0/2586	0.54	1/3485 (0.0%)
2	BX	0.25	0/2586	0.53	0/3485
2	BY	0.25	0/2586	0.53	0/3485
3	C1	0.26	0/2377	0.55	0/3233
3	C2	0.26	0/2377	0.55	0/3233
3	C3	0.26	0/2377	0.56	0/3233
3	C4	0.26	0/2377	0.56	0/3233
3	C5	0.26	0/2377	0.56	0/3233
3	C6	0.26	0/2377	0.55	0/3233
3	C7	0.26	0/2377	0.56	0/3233
3	C8	0.26	0/2377	0.55	0/3233
3	C9	0.26	0/2377	0.56	0/3233

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	CA	0.27	0/2377	0.57	0/3233
3	CB	0.27	0/2377	0.56	0/3233
3	CC	0.26	0/2377	0.56	0/3233
3	CD	0.26	0/2377	0.56	0/3233
3	CE	0.26	0/2377	0.56	0/3233
3	CF	0.26	0/2377	0.55	0/3233
3	CG	0.26	0/2377	0.55	0/3233
3	CH	0.26	0/2377	0.55	0/3233
3	CI	0.26	0/2377	0.56	0/3233
3	CJ	0.26	0/2377	0.57	0/3233
3	CK	0.26	0/2377	0.56	0/3233
3	CL	0.26	0/2377	0.56	0/3233
3	CM	0.26	0/2377	0.56	0/3233
3	CN	0.26	0/2377	0.55	0/3233
3	CO	0.26	0/2377	0.55	0/3233
3	CP	0.26	0/2377	0.55	0/3233
3	CQ	0.26	0/2377	0.56	0/3233
3	CR	0.26	0/2377	0.55	0/3233
3	CS	0.26	0/2377	0.55	0/3233
3	CT	0.26	0/2377	0.57	0/3233
3	CU	0.26	0/2377	0.56	0/3233
3	CV	0.26	0/2377	0.56	0/3233
3	CW	0.26	0/2377	0.55	0/3233
3	CX	0.26	0/2377	0.55	0/3233
3	CY	0.26	0/2377	0.55	0/3233
4	D1	0.26	0/647	0.66	0/873
4	D2	0.25	0/647	0.65	0/873
4	D3	0.27	0/647	0.65	0/873
4	D4	0.28	0/647	0.74	1/873 (0.1%)
4	D5	0.27	0/647	0.67	0/873
4	D6	0.26	0/647	0.67	0/873
4	D7	0.30	0/647	0.70	0/873
4	D8	0.27	0/647	0.66	0/873
4	D9	0.27	0/647	0.66	0/873
4	DA	0.27	0/647	0.67	0/873
4	DB	0.27	0/647	0.69	0/873
4	DC	0.26	0/647	0.68	0/873
4	DD	0.25	0/647	0.66	0/873
4	DE	0.27	0/647	0.71	0/873
4	DF	0.27	0/647	0.67	0/873
4	DG	0.25	0/647	0.68	0/873
4	DH	0.27	0/647	0.69	0/873
4	DI	0.25	0/647	0.65	0/873

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	DJ	0.26	0/647	0.67	0/873
4	DK	0.27	0/647	0.66	0/873
4	DL	0.27	0/647	0.74	1/873 (0.1%)
4	DM	0.27	0/647	0.70	0/873
4	DN	0.27	0/647	0.69	0/873
4	DO	0.28	0/647	0.67	0/873
4	DP	0.27	0/647	0.65	0/873
4	DQ	0.27	0/647	0.66	0/873
4	DR	0.27	0/647	0.67	0/873
4	DS	0.27	0/647	0.70	0/873
4	DT	0.27	0/647	0.68	0/873
4	DU	0.25	0/647	0.66	0/873
4	DV	0.26	0/647	0.65	0/873
4	DW	0.26	0/647	0.68	0/873
4	DX	0.25	0/647	0.66	0/873
4	DY	0.28	0/647	0.72	1/873 (0.1%)
4	E1	0.26	0/613	0.66	0/829
4	E2	0.25	0/613	0.67	0/829
4	E3	0.26	0/613	0.69	0/829
4	E4	0.23	0/613	0.63	0/829
4	E5	0.26	0/613	0.66	0/829
4	E6	0.26	0/613	0.68	0/829
4	E7	0.26	0/613	0.68	0/829
4	E8	0.24	0/613	0.64	0/829
4	E9	0.24	0/613	0.65	0/829
4	EA	0.26	0/613	0.68	0/829
4	EB	0.27	0/613	0.67	0/829
4	EC	0.27	0/613	0.68	0/829
4	ED	0.25	0/613	0.69	0/829
4	EE	0.26	0/613	0.68	1/829 (0.1%)
4	EF	0.26	0/613	0.67	0/829
4	EG	0.25	0/613	0.68	0/829
4	EH	0.26	0/613	0.69	0/829
4	EI	0.26	0/613	0.66	0/829
4	EJ	0.26	0/613	0.68	0/829
4	EK	0.26	0/613	0.68	0/829
4	EL	0.23	0/613	0.63	0/829
4	EM	0.24	0/613	0.63	0/829
4	EN	0.26	0/613	0.68	0/829
4	EO	0.24	0/613	0.65	0/829
4	EP	0.23	0/613	0.65	0/829
4	EQ	0.27	0/613	0.68	0/829
4	ER	0.27	0/613	0.67	0/829

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	ES	0.26	0/613	0.66	0/829
4	ET	0.25	0/613	0.67	0/829
4	EU	0.27	0/613	0.68	0/829
4	EV	0.30	0/613	0.69	1/829 (0.1%)
4	EW	0.24	0/613	0.63	0/829
4	EX	0.24	0/613	0.69	0/829
4	EY	0.25	0/613	0.64	0/829
4	F1	0.25	0/660	0.66	0/893
4	F2	0.25	0/660	0.63	0/893
4	F3	0.25	0/660	0.63	1/893 (0.1%)
4	F4	0.25	0/660	0.64	0/893
4	F5	0.26	0/660	0.63	0/893
4	F6	0.25	0/660	0.65	0/893
4	F7	0.25	0/660	0.64	1/893 (0.1%)
4	F8	0.26	0/660	0.67	1/893 (0.1%)
4	F9	0.27	0/660	0.68	2/893 (0.2%)
4	FA	0.25	0/660	0.66	0/893
4	FB	0.27	0/660	0.68	1/893 (0.1%)
4	FC	0.25	0/660	0.65	1/893 (0.1%)
4	FD	0.26	0/660	0.67	2/893 (0.2%)
4	FE	0.26	0/660	0.65	1/893 (0.1%)
4	FF	0.25	0/660	0.66	1/893 (0.1%)
4	FG	0.26	0/660	0.66	1/893 (0.1%)
4	FH	0.25	0/660	0.67	0/893
4	FI	0.25	0/660	0.64	0/893
4	FJ	0.26	0/660	0.65	0/893
4	FK	0.25	0/660	0.63	1/893 (0.1%)
4	FL	0.25	0/660	0.65	0/893
4	FM	0.26	0/660	0.66	0/893
4	FN	0.26	0/660	0.64	0/893
4	FO	0.25	0/660	0.66	1/893 (0.1%)
4	FP	0.25	0/660	0.66	0/893
4	FQ	0.25	0/660	0.64	1/893 (0.1%)
4	FR	0.25	0/660	0.67	0/893
4	FS	0.25	0/660	0.65	0/893
4	FT	0.25	0/660	0.65	0/893
4	FU	0.29	0/660	0.68	1/893 (0.1%)
4	FV	0.26	0/660	0.64	0/893
4	FW	0.25	0/660	0.66	0/893
4	FX	0.26	0/660	0.65	1/893 (0.1%)
4	FY	0.25	0/660	0.65	1/893 (0.1%)
All	All	0.25	0/246602	0.58	25/333438 (0.0%)

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
3	CC	0	1
3	CG	0	1
3	CY	0	1
4	E1	0	1
4	E3	0	1
4	E5	0	1
4	E6	0	1
4	E7	0	1
4	EA	0	1
4	EB	0	1
4	EC	0	1
4	EE	0	1
4	EF	0	1
4	EH	0	1
4	EI	0	1
4	EK	0	1
4	EN	0	1
4	ER	0	1
4	ES	0	1
4	EU	0	1
All	All	0	20

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BR	193	MET	CA-CB-CG	7.27	125.66	113.30
2	BW	193	MET	CA-CB-CG	7.21	125.56	113.30
4	FB	105	LEU	CA-CB-CG	5.84	128.74	115.30
4	F9	105	LEU	CA-CB-CG	5.78	128.58	115.30
4	FU	59	ASP	CB-CG-OD2	5.31	123.08	118.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E1	77	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	E3	77	GLU	Peptide
4	E5	77	GLU	Peptide
4	E6	77	GLU	Peptide
4	E7	77	GLU	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	A1	367	0	361	26	0
1	A2	367	0	361	25	0
1	A3	367	0	361	27	0
1	A4	367	0	361	25	0
1	A5	367	0	361	24	0
1	A6	367	0	361	24	0
1	A7	367	0	361	24	0
1	A8	367	0	361	23	0
1	A9	367	0	361	25	0
1	AA	367	0	361	24	0
1	AB	367	0	361	25	0
1	AC	367	0	361	23	0
1	AD	367	0	361	23	0
1	AE	367	0	361	26	0
1	AF	367	0	361	21	0
1	AG	367	0	361	20	0
1	AH	367	0	361	30	0
1	AI	367	0	361	25	0
1	AJ	367	0	361	21	0
1	AK	367	0	361	23	0
1	AL	367	0	361	23	0
1	AM	367	0	361	22	0
1	AN	367	0	361	25	0
1	AO	367	0	361	27	0
1	AP	367	0	361	26	0
1	AQ	367	0	361	23	0
1	AR	367	0	361	24	0
1	AS	367	0	361	24	0
1	AT	367	0	361	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AU	367	0	361	24	0
1	AV	367	0	361	26	0
1	AW	367	0	361	23	0
1	AX	367	0	361	22	0
1	AY	367	0	361	24	0
2	B1	2566	0	2615	125	0
2	B2	2566	0	2615	125	0
2	B3	2566	0	2615	121	0
2	B4	2566	0	2615	132	0
2	B5	2566	0	2615	121	0
2	B6	2566	0	2615	124	0
2	B7	2566	0	2615	122	0
2	B8	2566	0	2615	120	0
2	B9	2566	0	2615	115	0
2	BA	2566	0	2615	119	0
2	BB	2566	0	2615	118	0
2	BC	2566	0	2615	120	0
2	BD	2566	0	2615	121	0
2	BE	2566	0	2615	122	0
2	BF	2566	0	2615	120	0
2	BG	2566	0	2615	120	0
2	BH	2566	0	2615	116	0
2	BI	2566	0	2615	128	0
2	BJ	2566	0	2615	127	0
2	BK	2566	0	2615	121	0
2	BL	2566	0	2615	119	0
2	BM	2566	0	2615	125	0
2	BN	2566	0	2615	119	0
2	BO	2566	0	2615	119	0
2	BP	2566	0	2615	119	0
2	BQ	2566	0	2615	125	0
2	BR	2566	0	2615	117	0
2	BS	2566	0	2615	120	0
2	BT	2566	0	2615	126	0
2	BU	2566	0	2615	123	0
2	BV	2566	0	2615	121	0
2	BW	2566	0	2615	119	0
2	BX	2566	0	2615	124	0
2	BY	2566	0	2615	131	0
3	C1	2325	0	2354	96	0
3	C2	2325	0	2354	93	0
3	C3	2325	0	2354	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C4	2325	0	2354	92	0
3	C5	2325	0	2354	86	0
3	C6	2325	0	2354	86	0
3	C7	2325	0	2354	94	0
3	C8	2325	0	2354	95	0
3	C9	2325	0	2354	91	0
3	CA	2325	0	2354	96	0
3	CB	2325	0	2354	94	0
3	CC	2325	0	2354	90	0
3	CD	2325	0	2354	92	0
3	CE	2325	0	2354	94	0
3	CF	2325	0	2354	94	0
3	CG	2325	0	2354	99	0
3	CH	2325	0	2354	85	0
3	CI	2325	0	2354	96	0
3	CJ	2325	0	2354	86	0
3	CK	2325	0	2354	88	0
3	CL	2325	0	2354	90	0
3	CM	2325	0	2354	81	0
3	CN	2325	0	2354	90	0
3	CO	2325	0	2354	91	0
3	CP	2325	0	2354	93	0
3	CQ	2325	0	2354	88	0
3	CR	2325	0	2354	85	0
3	CS	2325	0	2354	92	0
3	CT	2325	0	2354	88	0
3	CU	2325	0	2354	89	0
3	CV	2325	0	2354	90	0
3	CW	2325	0	2354	88	0
3	CX	2325	0	2354	92	0
3	CY	2325	0	2354	84	0
4	D1	643	0	694	36	0
4	D2	643	0	694	38	0
4	D3	643	0	694	36	0
4	D4	643	0	694	39	0
4	D5	643	0	694	32	0
4	D6	643	0	694	37	0
4	D7	643	0	694	33	0
4	D8	643	0	694	36	0
4	D9	643	0	694	36	0
4	DA	643	0	694	42	0
4	DB	643	0	694	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	DC	643	0	694	37	0
4	DD	643	0	694	29	0
4	DE	643	0	694	38	0
4	DF	643	0	694	41	0
4	DG	643	0	694	40	0
4	DH	643	0	694	37	0
4	DI	643	0	694	35	0
4	DJ	643	0	694	37	0
4	DK	643	0	694	39	0
4	DL	643	0	694	36	0
4	DM	643	0	694	31	0
4	DN	643	0	694	39	0
4	DO	643	0	694	35	0
4	DP	643	0	694	34	0
4	DQ	643	0	694	37	0
4	DR	643	0	694	35	0
4	DS	643	0	694	38	0
4	DT	643	0	694	35	0
4	DU	643	0	694	29	0
4	DV	643	0	694	34	0
4	DW	643	0	694	39	0
4	DX	643	0	694	35	0
4	DY	643	0	694	43	0
4	E1	609	0	661	42	0
4	E2	609	0	661	40	0
4	E3	609	0	661	42	0
4	E4	609	0	661	35	0
4	E5	609	0	661	41	0
4	E6	609	0	661	39	0
4	E7	609	0	661	42	0
4	E8	609	0	661	38	0
4	E9	609	0	661	41	0
4	EA	609	0	661	39	0
4	EB	609	0	661	39	0
4	EC	609	0	661	44	0
4	ED	609	0	661	43	0
4	EE	609	0	661	42	0
4	EF	609	0	661	40	0
4	EG	609	0	661	47	0
4	EH	609	0	661	44	0
4	EI	609	0	661	41	0
4	EJ	609	0	661	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	EK	609	0	661	41	0
4	EL	609	0	661	39	0
4	EM	609	0	661	41	0
4	EN	609	0	661	37	0
4	EO	609	0	661	40	0
4	EP	609	0	661	37	0
4	EQ	609	0	661	40	0
4	ER	609	0	661	47	0
4	ES	609	0	661	38	0
4	ET	609	0	661	42	0
4	EU	609	0	661	39	0
4	EV	609	0	661	46	0
4	EW	609	0	661	34	0
4	EX	609	0	661	38	0
4	EY	609	0	661	42	0
4	F1	656	0	704	43	0
4	F2	656	0	704	41	0
4	F3	656	0	704	42	0
4	F4	656	0	704	40	0
4	F5	656	0	704	47	0
4	F6	656	0	704	43	0
4	F7	656	0	704	54	0
4	F8	656	0	704	52	0
4	F9	656	0	704	51	0
4	FA	656	0	704	47	0
4	FB	656	0	704	51	0
4	FC	656	0	704	51	0
4	FD	656	0	704	46	0
4	FE	656	0	704	51	0
4	FF	656	0	704	38	0
4	FG	656	0	704	51	0
4	FH	656	0	704	48	0
4	FI	656	0	704	42	0
4	FJ	656	0	704	46	0
4	FK	656	0	704	40	0
4	FL	656	0	704	42	0
4	FM	656	0	704	45	0
4	FN	656	0	704	40	0
4	FO	656	0	704	47	0
4	FP	656	0	704	44	0
4	FQ	656	0	704	46	0
4	FR	656	0	704	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	FS	656	0	704	41	0
4	FT	656	0	704	45	0
4	FU	656	0	704	40	0
4	FV	656	0	704	44	0
4	FW	656	0	704	37	0
4	FX	656	0	704	43	0
4	FY	656	0	704	43	0
All	All	243644	0	251226	9691	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 20.

The worst 5 of 9691 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)
4:ES:73:MET:HE1	4:ES:78:LEU:HG	1.44	1.00
4:E5:73:MET:HE1	4:E5:78:LEU:HG	1.44	0.98
4:EN:73:MET:HE1	4:EN:78:LEU:HG	1.45	0.96
4:EG:72:ARG:HH12	4:FG:61:PRO:HB2	1.32	0.94
4:ER:73:MET:HE1	4:ER:78:LEU:HG	1.49	0.93

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	A1	42/560 (8%)	42 (100%)	0	0	100	100
1	A2	42/560 (8%)	42 (100%)	0	0	100	100
1	A3	42/560 (8%)	42 (100%)	0	0	100	100
1	A4	42/560 (8%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A5	42/560 (8%)	42 (100%)	0	0	100	100
1	A6	42/560 (8%)	42 (100%)	0	0	100	100
1	A7	42/560 (8%)	42 (100%)	0	0	100	100
1	A8	42/560 (8%)	42 (100%)	0	0	100	100
1	A9	42/560 (8%)	42 (100%)	0	0	100	100
1	AA	42/560 (8%)	42 (100%)	0	0	100	100
1	AB	42/560 (8%)	42 (100%)	0	0	100	100
1	AC	42/560 (8%)	42 (100%)	0	0	100	100
1	AD	42/560 (8%)	42 (100%)	0	0	100	100
1	AE	42/560 (8%)	42 (100%)	0	0	100	100
1	AF	42/560 (8%)	42 (100%)	0	0	100	100
1	AG	42/560 (8%)	42 (100%)	0	0	100	100
1	AH	42/560 (8%)	42 (100%)	0	0	100	100
1	AI	42/560 (8%)	42 (100%)	0	0	100	100
1	AJ	42/560 (8%)	42 (100%)	0	0	100	100
1	AK	42/560 (8%)	42 (100%)	0	0	100	100
1	AL	42/560 (8%)	42 (100%)	0	0	100	100
1	AM	42/560 (8%)	42 (100%)	0	0	100	100
1	AN	42/560 (8%)	42 (100%)	0	0	100	100
1	AO	42/560 (8%)	42 (100%)	0	0	100	100
1	AP	42/560 (8%)	42 (100%)	0	0	100	100
1	AQ	42/560 (8%)	42 (100%)	0	0	100	100
1	AR	42/560 (8%)	42 (100%)	0	0	100	100
1	AS	42/560 (8%)	42 (100%)	0	0	100	100
1	AT	42/560 (8%)	42 (100%)	0	0	100	100
1	AU	42/560 (8%)	42 (100%)	0	0	100	100
1	AV	42/560 (8%)	42 (100%)	0	0	100	100
1	AW	42/560 (8%)	42 (100%)	0	0	100	100
1	AX	42/560 (8%)	42 (100%)	0	0	100	100
1	AY	42/560 (8%)	42 (100%)	0	0	100	100
2	B1	326/328 (99%)	313 (96%)	12 (4%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B2	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	41	76
2	B3	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	41	76
2	B4	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	41	76
2	B5	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	41	76
2	B6	326/328 (99%)	312 (96%)	13 (4%)	1 (0%)	41	76
2	B7	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	41	76
2	B8	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	41	76
2	B9	326/328 (99%)	313 (96%)	12 (4%)	1 (0%)	41	76
2	BA	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	41	76
2	BB	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	41	76
2	BC	326/328 (99%)	313 (96%)	12 (4%)	1 (0%)	41	76
2	BD	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	41	76
2	BE	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	41	76
2	BF	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	41	76
2	BG	326/328 (99%)	313 (96%)	12 (4%)	1 (0%)	41	76
2	BH	326/328 (99%)	316 (97%)	10 (3%)	0	100	100
2	BI	326/328 (99%)	316 (97%)	9 (3%)	1 (0%)	41	76
2	BJ	326/328 (99%)	313 (96%)	13 (4%)	0	100	100
2	BK	326/328 (99%)	313 (96%)	13 (4%)	0	100	100
2	BL	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	41	76
2	BM	326/328 (99%)	316 (97%)	9 (3%)	1 (0%)	41	76
2	BN	326/328 (99%)	313 (96%)	12 (4%)	1 (0%)	41	76
2	BO	326/328 (99%)	316 (97%)	10 (3%)	0	100	100
2	BP	326/328 (99%)	316 (97%)	10 (3%)	0	100	100
2	BQ	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	41	76
2	BR	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	41	76
2	BS	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	41	76
2	BT	326/328 (99%)	312 (96%)	13 (4%)	1 (0%)	41	76
2	BU	326/328 (99%)	316 (97%)	9 (3%)	1 (0%)	41	76
2	BV	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	41	76
2	BW	326/328 (99%)	314 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BX	326/328 (99%)	311 (95%)	15 (5%)	0	100	100
2	BY	326/328 (99%)	313 (96%)	13 (4%)	0	100	100
3	C1	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	C2	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	C3	285/334 (85%)	275 (96%)	10 (4%)	0	100	100
3	C4	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	C5	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	C6	285/334 (85%)	275 (96%)	10 (4%)	0	100	100
3	C7	285/334 (85%)	275 (96%)	10 (4%)	0	100	100
3	C8	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	C9	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	CA	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	CB	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	CC	285/334 (85%)	275 (96%)	10 (4%)	0	100	100
3	CD	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	CE	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	CF	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	CG	285/334 (85%)	275 (96%)	10 (4%)	0	100	100
3	CH	285/334 (85%)	275 (96%)	10 (4%)	0	100	100
3	CI	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	CJ	285/334 (85%)	277 (97%)	8 (3%)	0	100	100
3	CK	285/334 (85%)	275 (96%)	10 (4%)	0	100	100
3	CL	285/334 (85%)	275 (96%)	10 (4%)	0	100	100
3	CM	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	CN	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	CO	285/334 (85%)	277 (97%)	8 (3%)	0	100	100
3	CP	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	CQ	285/334 (85%)	277 (97%)	8 (3%)	0	100	100
3	CR	285/334 (85%)	277 (97%)	8 (3%)	0	100	100
3	CS	285/334 (85%)	277 (97%)	8 (3%)	0	100	100
3	CT	285/334 (85%)	275 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CU	285/334 (85%)	274 (96%)	11 (4%)	0	100	100
3	CV	285/334 (85%)	277 (97%)	8 (3%)	0	100	100
3	CW	285/334 (85%)	275 (96%)	10 (4%)	0	100	100
3	CX	285/334 (85%)	276 (97%)	9 (3%)	0	100	100
3	CY	285/334 (85%)	277 (97%)	8 (3%)	0	100	100
4	D1	81/137 (59%)	74 (91%)	7 (9%)	0	100	100
4	D2	81/137 (59%)	74 (91%)	7 (9%)	0	100	100
4	D3	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	D4	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	D5	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	D6	81/137 (59%)	74 (91%)	7 (9%)	0	100	100
4	D7	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	D8	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	D9	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DA	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	DB	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DC	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	DD	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DE	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DF	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	DG	81/137 (59%)	74 (91%)	7 (9%)	0	100	100
4	DH	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DI	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	DJ	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DK	81/137 (59%)	77 (95%)	4 (5%)	0	100	100
4	DL	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DM	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	DN	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DO	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	DP	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	DQ	81/137 (59%)	75 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	DR	81/137 (59%)	77 (95%)	4 (5%)	0	100	100
4	DS	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DT	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	DU	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DV	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	DW	81/137 (59%)	76 (94%)	5 (6%)	0	100	100
4	DX	81/137 (59%)	74 (91%)	7 (9%)	0	100	100
4	DY	81/137 (59%)	75 (93%)	6 (7%)	0	100	100
4	E1	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	E2	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	E3	77/137 (56%)	70 (91%)	6 (8%)	1 (1%)	12	48
4	E4	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	E5	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	12	48
4	E6	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	E7	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	12	48
4	E8	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	E9	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	EA	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	12	48
4	EB	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	EC	77/137 (56%)	69 (90%)	7 (9%)	1 (1%)	12	48
4	ED	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	12	48
4	EE	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	EF	77/137 (56%)	70 (91%)	6 (8%)	1 (1%)	12	48
4	EG	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	12	48
4	EH	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	EI	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	EJ	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	EK	77/137 (56%)	70 (91%)	6 (8%)	1 (1%)	12	48
4	EL	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	EM	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	12	48
4	EN	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	EO	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	12	48
4	EP	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	12	48
4	EQ	77/137 (56%)	69 (90%)	7 (9%)	1 (1%)	12	48
4	ER	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	ES	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	12	48
4	ET	77/137 (56%)	70 (91%)	6 (8%)	1 (1%)	12	48
4	EU	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	EV	77/137 (56%)	70 (91%)	6 (8%)	1 (1%)	12	48
4	EW	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	12	48
4	EX	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	12	48
4	EY	77/137 (56%)	73 (95%)	3 (4%)	1 (1%)	12	48
4	F1	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	F2	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	F3	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
4	F4	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
4	F5	83/137 (61%)	75 (90%)	8 (10%)	0	100	100
4	F6	83/137 (61%)	78 (94%)	5 (6%)	0	100	100
4	F7	83/137 (61%)	75 (90%)	8 (10%)	0	100	100
4	F8	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
4	F9	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FA	83/137 (61%)	75 (90%)	8 (10%)	0	100	100
4	FB	83/137 (61%)	75 (90%)	8 (10%)	0	100	100
4	FC	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
4	FD	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FE	83/137 (61%)	75 (90%)	8 (10%)	0	100	100
4	FF	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FG	83/137 (61%)	74 (89%)	9 (11%)	0	100	100
4	FH	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
4	FI	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FJ	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
4	FK	83/137 (61%)	75 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	FL	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
4	FM	83/137 (61%)	75 (90%)	8 (10%)	0	100	100
4	FN	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FO	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FP	83/137 (61%)	77 (93%)	6 (7%)	0	100	100
4	FQ	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FR	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FS	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FT	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FU	83/137 (61%)	75 (90%)	8 (10%)	0	100	100
4	FV	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
4	FW	83/137 (61%)	75 (90%)	8 (10%)	0	100	100
4	FX	83/137 (61%)	78 (94%)	5 (6%)	0	100	100
4	FY	83/137 (61%)	76 (92%)	7 (8%)	0	100	100
All	All	30396/55522 (55%)	29041 (96%)	1295 (4%)	60 (0%)	50	81

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E1	126	ILE
4	E2	126	ILE
4	E3	126	ILE
4	E4	126	ILE
4	E5	126	ILE

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	
1	A1	40/467 (9%)	40 (100%)	0	100	100
1	A2	40/467 (9%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A3	40/467 (9%)	40 (100%)	0	100	100
1	A4	40/467 (9%)	40 (100%)	0	100	100
1	A5	40/467 (9%)	40 (100%)	0	100	100
1	A6	40/467 (9%)	40 (100%)	0	100	100
1	A7	40/467 (9%)	40 (100%)	0	100	100
1	A8	40/467 (9%)	40 (100%)	0	100	100
1	A9	40/467 (9%)	40 (100%)	0	100	100
1	AA	40/467 (9%)	40 (100%)	0	100	100
1	AB	40/467 (9%)	40 (100%)	0	100	100
1	AC	40/467 (9%)	40 (100%)	0	100	100
1	AD	40/467 (9%)	40 (100%)	0	100	100
1	AE	40/467 (9%)	40 (100%)	0	100	100
1	AF	40/467 (9%)	40 (100%)	0	100	100
1	AG	40/467 (9%)	40 (100%)	0	100	100
1	AH	40/467 (9%)	40 (100%)	0	100	100
1	AI	40/467 (9%)	40 (100%)	0	100	100
1	AJ	40/467 (9%)	40 (100%)	0	100	100
1	AK	40/467 (9%)	40 (100%)	0	100	100
1	AL	40/467 (9%)	40 (100%)	0	100	100
1	AM	40/467 (9%)	40 (100%)	0	100	100
1	AN	40/467 (9%)	40 (100%)	0	100	100
1	AO	40/467 (9%)	40 (100%)	0	100	100
1	AP	40/467 (9%)	40 (100%)	0	100	100
1	AQ	40/467 (9%)	40 (100%)	0	100	100
1	AR	40/467 (9%)	40 (100%)	0	100	100
1	AS	40/467 (9%)	40 (100%)	0	100	100
1	AT	40/467 (9%)	40 (100%)	0	100	100
1	AU	40/467 (9%)	40 (100%)	0	100	100
1	AV	40/467 (9%)	40 (100%)	0	100	100
1	AW	40/467 (9%)	40 (100%)	0	100	100
1	AX	40/467 (9%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AY	40/467 (9%)	40 (100%)	0	100	100
2	B1	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	B2	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	B3	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	B4	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	B5	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	B6	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	B7	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	B8	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	B9	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BA	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BB	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BC	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BD	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BE	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BF	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BG	281/281 (100%)	279 (99%)	2 (1%)	84	90
2	BH	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BI	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BJ	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BK	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BL	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BM	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BN	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BO	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BP	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BQ	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BR	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BS	281/281 (100%)	279 (99%)	2 (1%)	84	90
2	BT	281/281 (100%)	279 (99%)	2 (1%)	84	90
2	BU	281/281 (100%)	280 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BV	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BW	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BX	281/281 (100%)	280 (100%)	1 (0%)	91	94
2	BY	281/281 (100%)	280 (100%)	1 (0%)	91	94
3	C1	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	C2	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	C3	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	C4	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	C5	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	C6	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	C7	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	C8	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	C9	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CA	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CB	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CC	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CD	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CE	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CF	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CG	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CH	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CI	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CJ	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CK	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CL	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CM	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CN	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CO	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CP	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CQ	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CR	260/301 (86%)	259 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CS	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CT	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CU	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CV	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CW	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CX	260/301 (86%)	259 (100%)	1 (0%)	91	94
3	CY	260/301 (86%)	259 (100%)	1 (0%)	91	94
4	D1	72/113 (64%)	72 (100%)	0	100	100
4	D2	72/113 (64%)	72 (100%)	0	100	100
4	D3	72/113 (64%)	72 (100%)	0	100	100
4	D4	72/113 (64%)	72 (100%)	0	100	100
4	D5	72/113 (64%)	72 (100%)	0	100	100
4	D6	72/113 (64%)	72 (100%)	0	100	100
4	D7	72/113 (64%)	72 (100%)	0	100	100
4	D8	72/113 (64%)	72 (100%)	0	100	100
4	D9	72/113 (64%)	72 (100%)	0	100	100
4	DA	72/113 (64%)	72 (100%)	0	100	100
4	DB	72/113 (64%)	72 (100%)	0	100	100
4	DC	72/113 (64%)	72 (100%)	0	100	100
4	DD	72/113 (64%)	72 (100%)	0	100	100
4	DE	72/113 (64%)	72 (100%)	0	100	100
4	DF	72/113 (64%)	72 (100%)	0	100	100
4	DG	72/113 (64%)	72 (100%)	0	100	100
4	DH	72/113 (64%)	72 (100%)	0	100	100
4	DI	72/113 (64%)	72 (100%)	0	100	100
4	DJ	72/113 (64%)	72 (100%)	0	100	100
4	DK	72/113 (64%)	72 (100%)	0	100	100
4	DL	72/113 (64%)	72 (100%)	0	100	100
4	DM	72/113 (64%)	72 (100%)	0	100	100
4	DN	72/113 (64%)	72 (100%)	0	100	100
4	DO	72/113 (64%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	DP	72/113 (64%)	72 (100%)	0	100	100
4	DQ	72/113 (64%)	72 (100%)	0	100	100
4	DR	72/113 (64%)	72 (100%)	0	100	100
4	DS	72/113 (64%)	72 (100%)	0	100	100
4	DT	72/113 (64%)	72 (100%)	0	100	100
4	DU	72/113 (64%)	72 (100%)	0	100	100
4	DV	72/113 (64%)	72 (100%)	0	100	100
4	DW	72/113 (64%)	72 (100%)	0	100	100
4	DX	72/113 (64%)	72 (100%)	0	100	100
4	DY	72/113 (64%)	72 (100%)	0	100	100
4	E1	68/113 (60%)	68 (100%)	0	100	100
4	E2	68/113 (60%)	68 (100%)	0	100	100
4	E3	68/113 (60%)	68 (100%)	0	100	100
4	E4	68/113 (60%)	68 (100%)	0	100	100
4	E5	68/113 (60%)	68 (100%)	0	100	100
4	E6	68/113 (60%)	68 (100%)	0	100	100
4	E7	68/113 (60%)	68 (100%)	0	100	100
4	E8	68/113 (60%)	68 (100%)	0	100	100
4	E9	68/113 (60%)	68 (100%)	0	100	100
4	EA	68/113 (60%)	68 (100%)	0	100	100
4	EB	68/113 (60%)	68 (100%)	0	100	100
4	EC	68/113 (60%)	68 (100%)	0	100	100
4	ED	68/113 (60%)	68 (100%)	0	100	100
4	EE	68/113 (60%)	68 (100%)	0	100	100
4	EF	68/113 (60%)	68 (100%)	0	100	100
4	EG	68/113 (60%)	68 (100%)	0	100	100
4	EH	68/113 (60%)	68 (100%)	0	100	100
4	EI	68/113 (60%)	68 (100%)	0	100	100
4	EJ	68/113 (60%)	68 (100%)	0	100	100
4	EK	68/113 (60%)	68 (100%)	0	100	100
4	EL	68/113 (60%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	EM	68/113 (60%)	68 (100%)	0	100	100
4	EN	68/113 (60%)	68 (100%)	0	100	100
4	EO	68/113 (60%)	68 (100%)	0	100	100
4	EP	68/113 (60%)	68 (100%)	0	100	100
4	EQ	68/113 (60%)	68 (100%)	0	100	100
4	ER	68/113 (60%)	68 (100%)	0	100	100
4	ES	68/113 (60%)	68 (100%)	0	100	100
4	ET	68/113 (60%)	68 (100%)	0	100	100
4	EU	68/113 (60%)	68 (100%)	0	100	100
4	EV	68/113 (60%)	68 (100%)	0	100	100
4	EW	68/113 (60%)	68 (100%)	0	100	100
4	EX	68/113 (60%)	68 (100%)	0	100	100
4	EY	68/113 (60%)	68 (100%)	0	100	100
4	F1	74/113 (66%)	74 (100%)	0	100	100
4	F2	74/113 (66%)	74 (100%)	0	100	100
4	F3	74/113 (66%)	74 (100%)	0	100	100
4	F4	74/113 (66%)	74 (100%)	0	100	100
4	F5	74/113 (66%)	74 (100%)	0	100	100
4	F6	74/113 (66%)	74 (100%)	0	100	100
4	F7	74/113 (66%)	74 (100%)	0	100	100
4	F8	74/113 (66%)	74 (100%)	0	100	100
4	F9	74/113 (66%)	74 (100%)	0	100	100
4	FA	74/113 (66%)	74 (100%)	0	100	100
4	FB	74/113 (66%)	74 (100%)	0	100	100
4	FC	74/113 (66%)	74 (100%)	0	100	100
4	FD	74/113 (66%)	74 (100%)	0	100	100
4	FE	74/113 (66%)	74 (100%)	0	100	100
4	FF	74/113 (66%)	74 (100%)	0	100	100
4	FG	74/113 (66%)	74 (100%)	0	100	100
4	FH	74/113 (66%)	74 (100%)	0	100	100
4	FI	74/113 (66%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	FJ	74/113 (66%)	74 (100%)	0	100	100
4	FK	74/113 (66%)	74 (100%)	0	100	100
4	FL	74/113 (66%)	74 (100%)	0	100	100
4	FM	74/113 (66%)	74 (100%)	0	100	100
4	FN	74/113 (66%)	74 (100%)	0	100	100
4	FO	74/113 (66%)	74 (100%)	0	100	100
4	FP	74/113 (66%)	74 (100%)	0	100	100
4	FQ	74/113 (66%)	74 (100%)	0	100	100
4	FR	74/113 (66%)	74 (100%)	0	100	100
4	FS	74/113 (66%)	74 (100%)	0	100	100
4	FT	74/113 (66%)	74 (100%)	0	100	100
4	FU	74/113 (66%)	74 (100%)	0	100	100
4	FV	74/113 (66%)	74 (100%)	0	100	100
4	FW	74/113 (66%)	74 (100%)	0	100	100
4	FX	74/113 (66%)	74 (100%)	0	100	100
4	FY	74/113 (66%)	74 (100%)	0	100	100
All	All	27030/47192 (57%)	26959 (100%)	71 (0%)	92	95

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CS	44	ARG
2	BT	281	ARG
2	BW	281	ARG
2	BD	281	ARG
3	CC	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 408 such sidechains are listed below:

Mol	Chain	Res	Type
3	CK	64	GLN
3	CP	87	GLN
2	BY	128	GLN
2	BL	46	GLN
3	CN	58	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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)

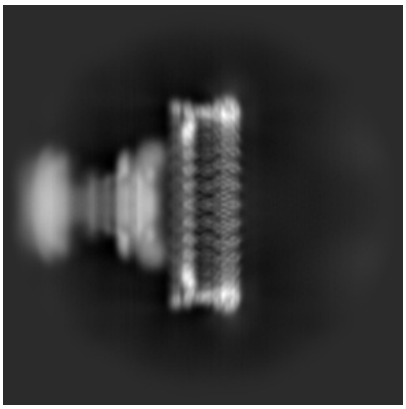
This section contains visualisations of the EMDB entry EMD-42451. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

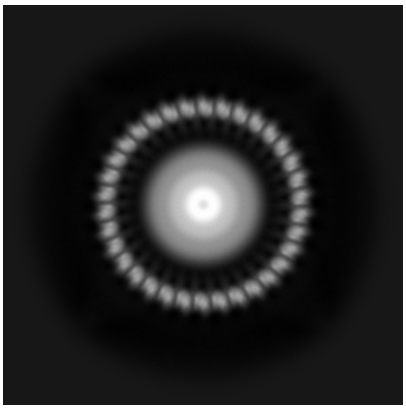
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

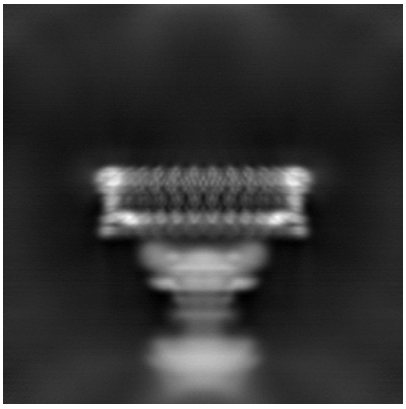


Y

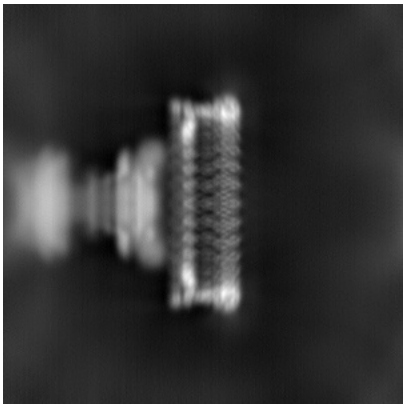


Z

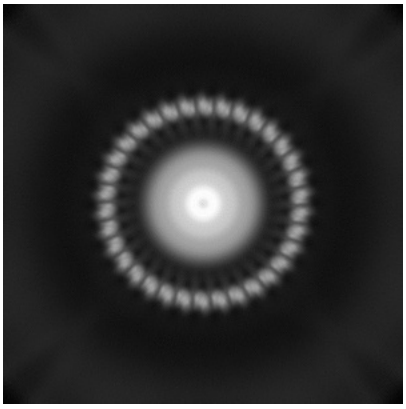
6.1.2 Raw map



X



Y

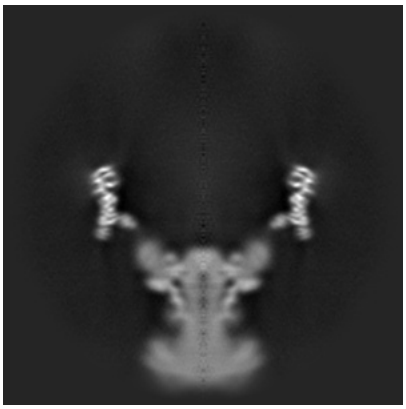


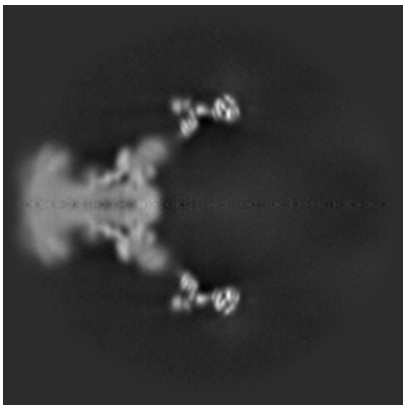
Z

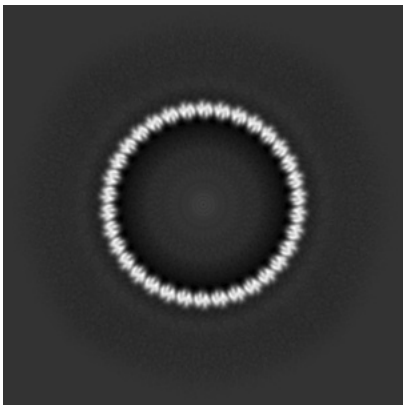
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

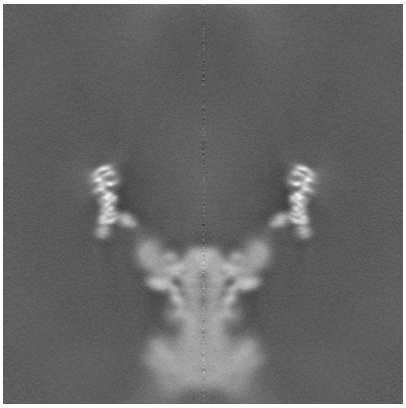
6.2.1 Primary map

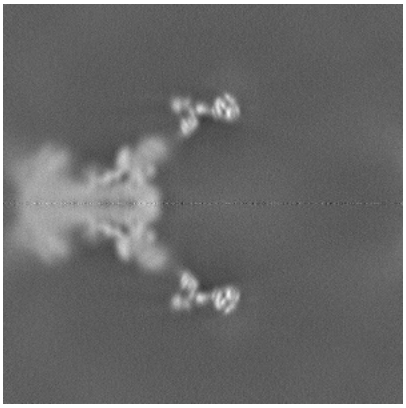

X Index: 256

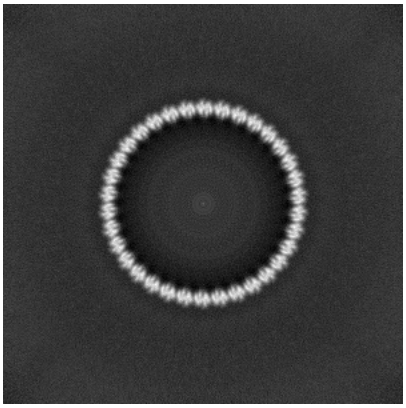

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

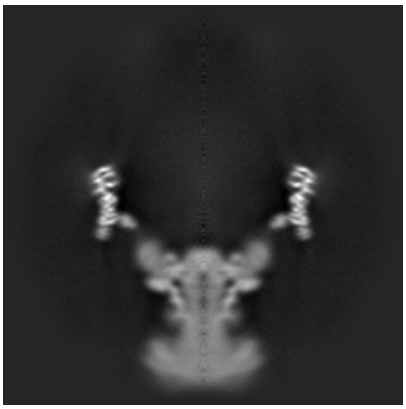

Y Index: 256


Z Index: 256

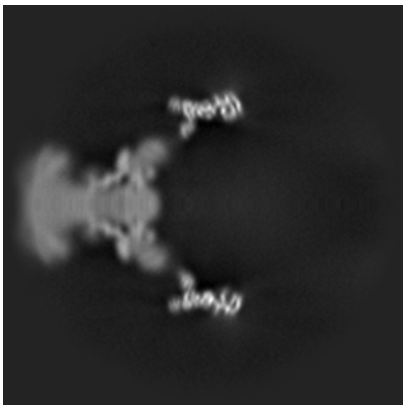
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

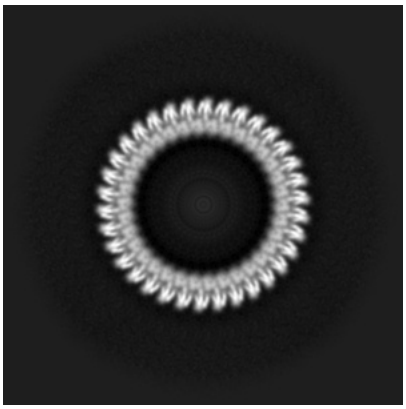
6.3.1 Primary map



X Index: 256

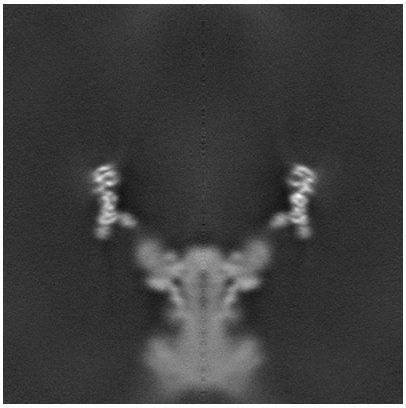


Y Index: 244

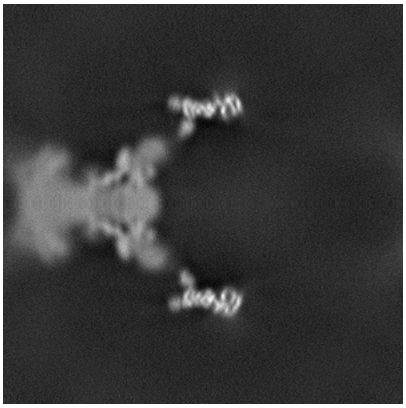


Z Index: 239

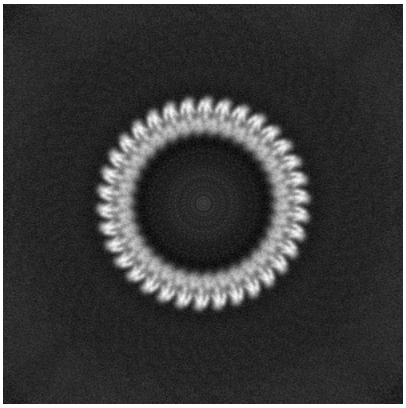
6.3.2 Raw map



X Index: 255



Y Index: 267

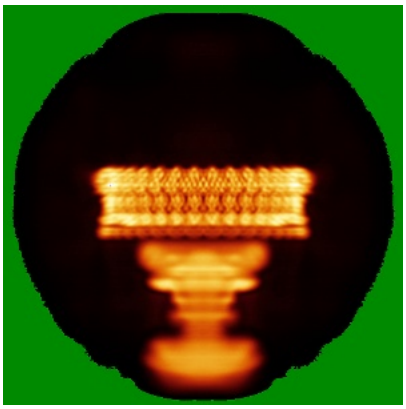


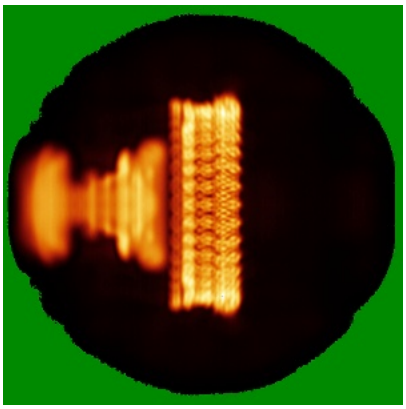
Z Index: 239

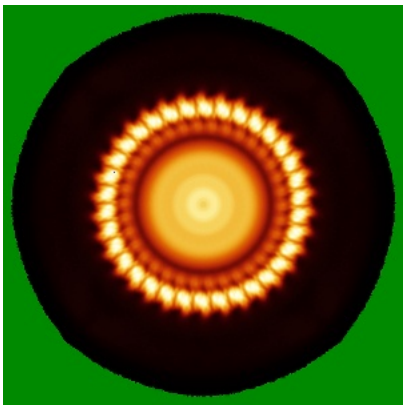
The images above show the largest variance slices of the map in three orthogonal directions.

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

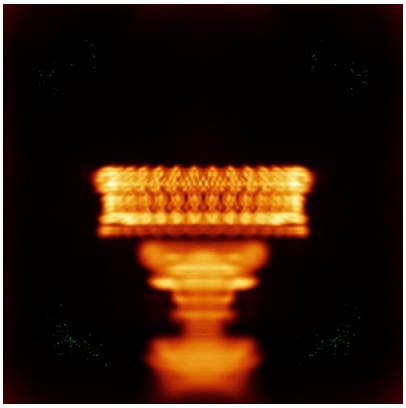
6.4.1 Primary map

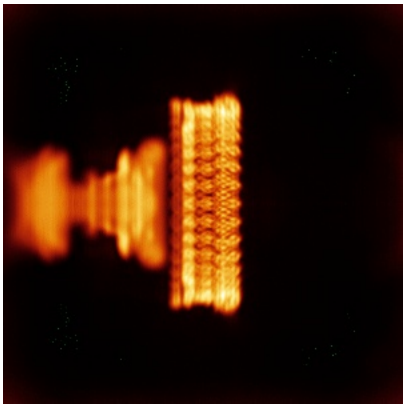

X

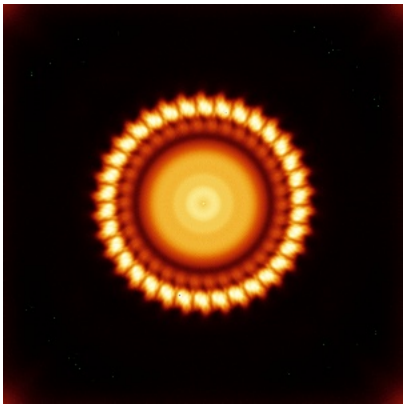

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

6.6 Mask visualisation (i)

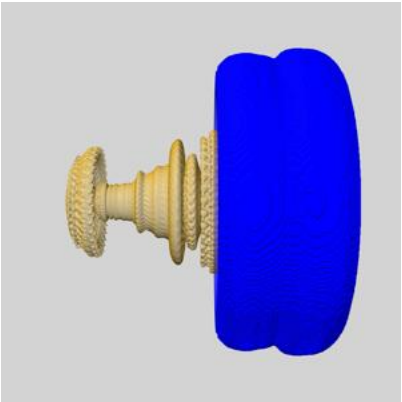
This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

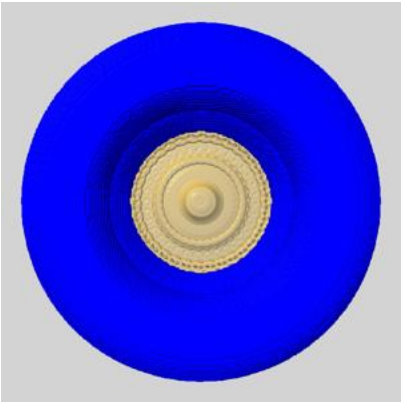
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1 emd_42451_msk_1.map (i)

X



Y

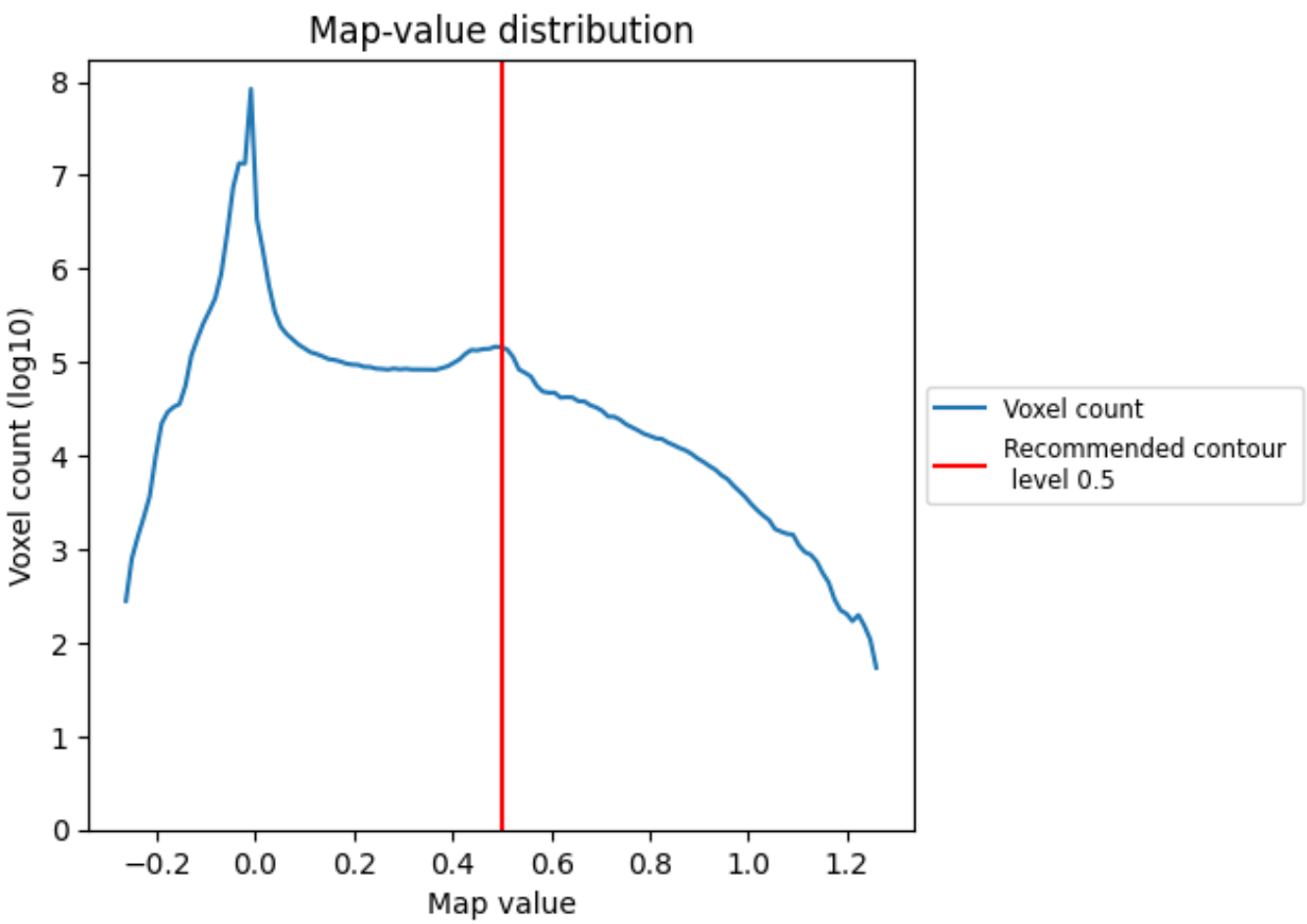


Z

7 Map analysis (i)

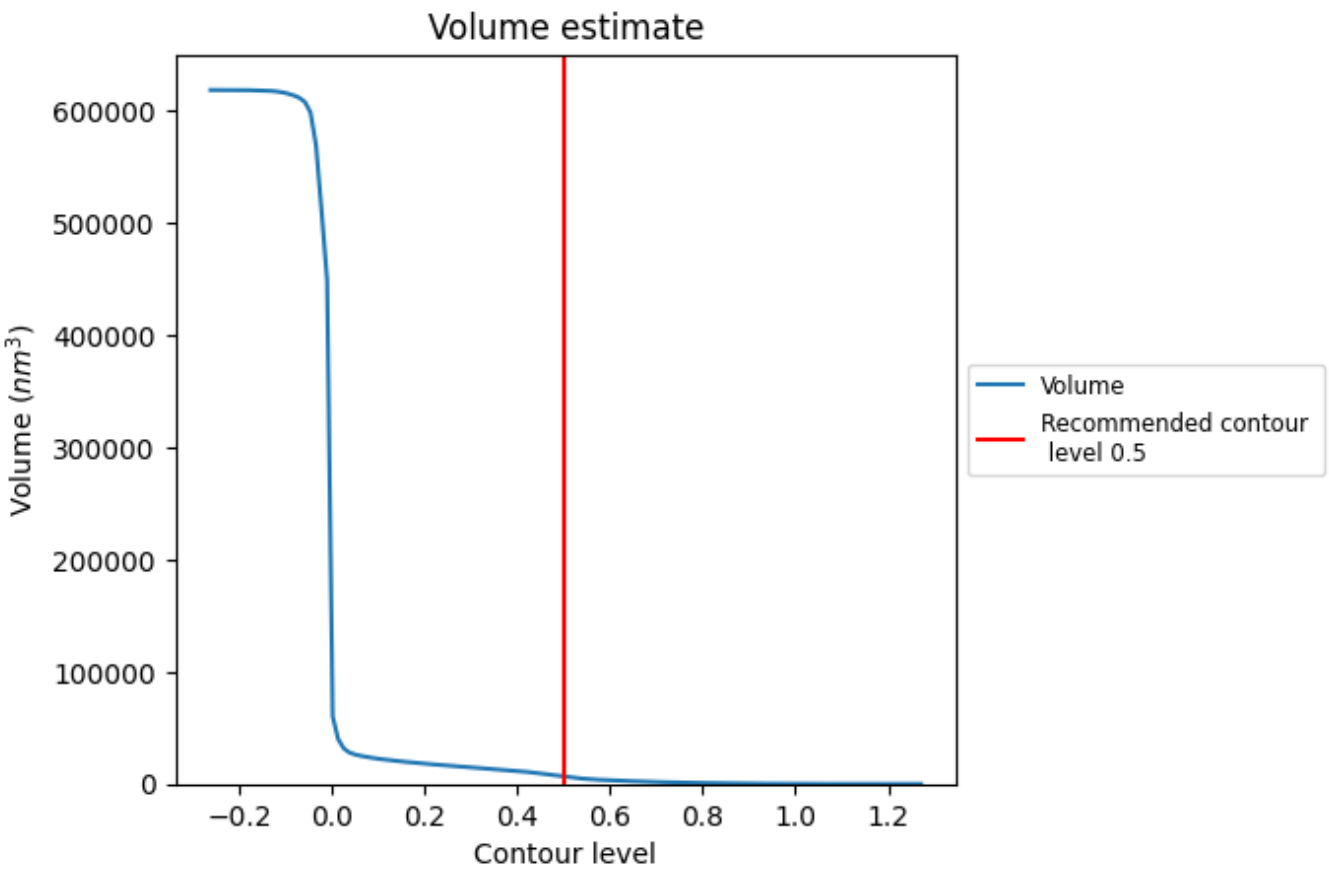
This section contains the results of statistical analysis of the map.

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.

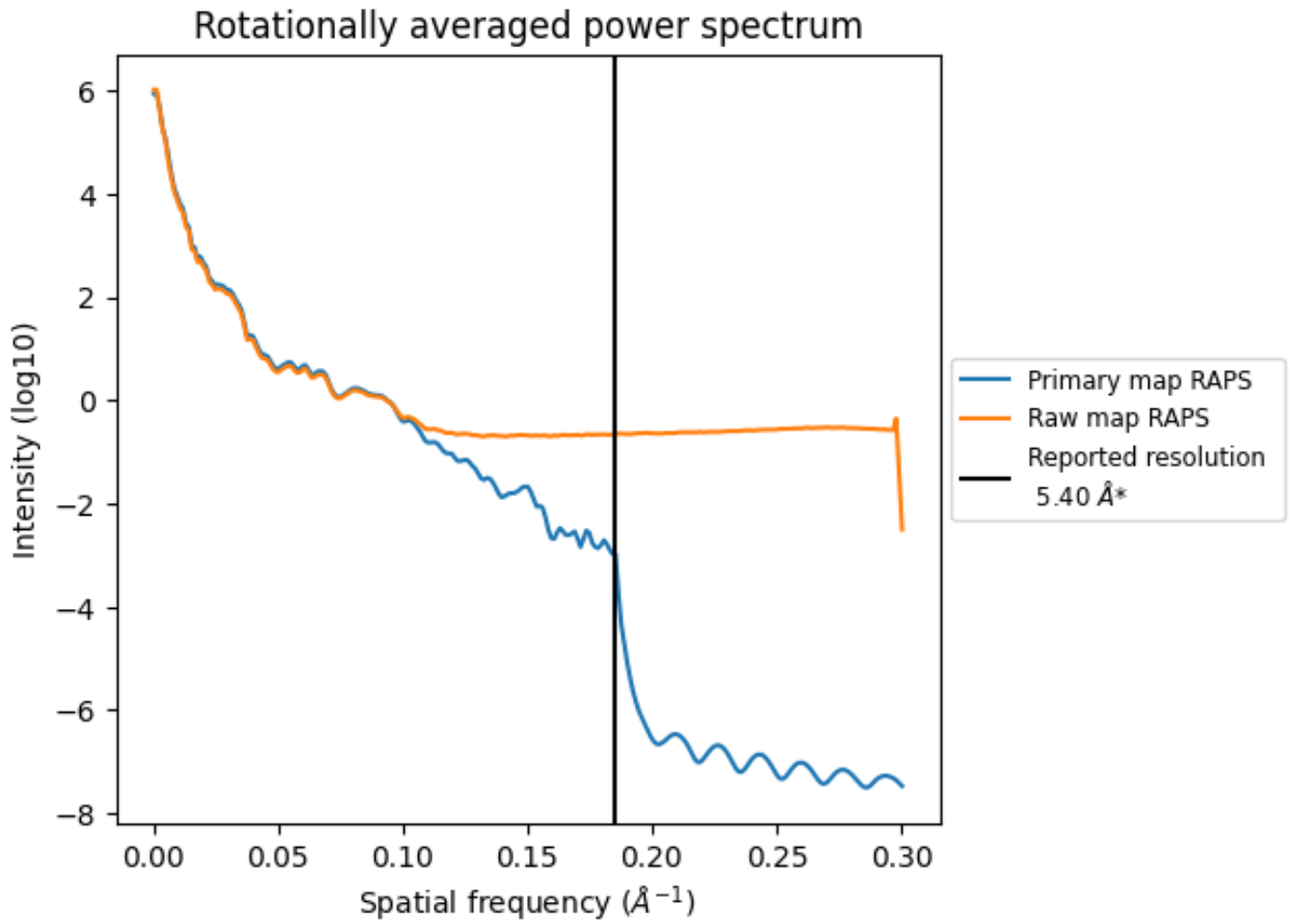
7.2 Volume estimate (i)



The volume at the recommended contour level is 6675 nm^3; this corresponds to an approximate mass of 6030 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)

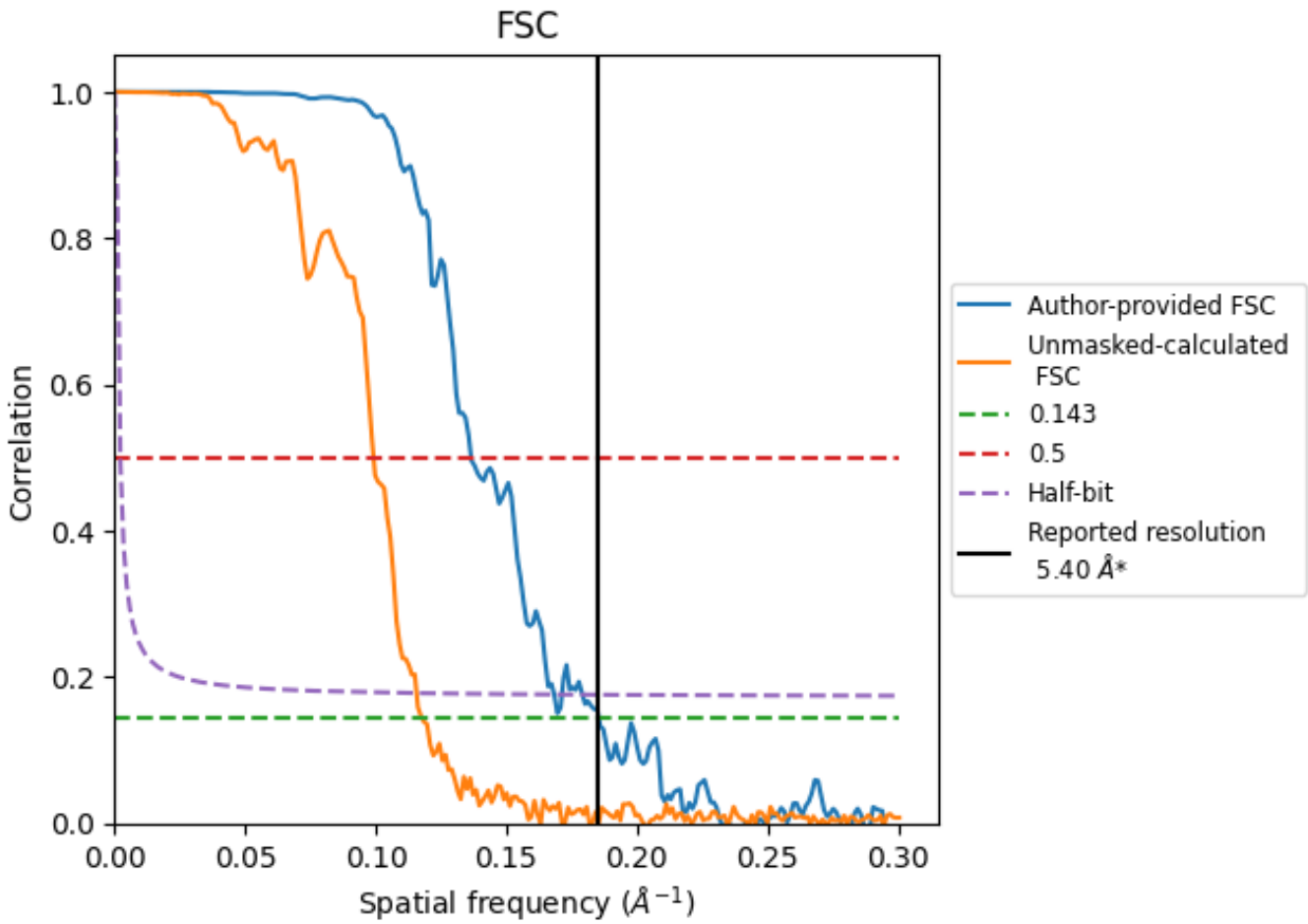


*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.185 Å^{-1}

8.2 Resolution estimates (i)

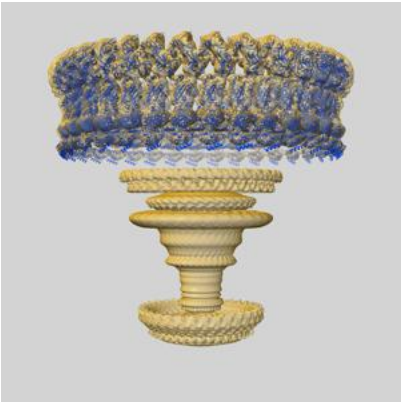
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	5.39	7.32	5.94
Unmasked-calculated*	8.49	10.08	8.64

*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 8.49 differs from the reported value 5.4 by more than 10 %

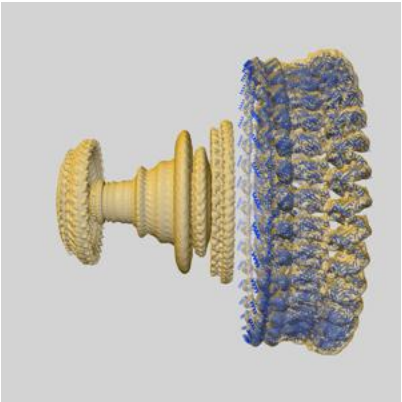
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-42451 and PDB model 8UPL. Per-residue inclusion information can be found in section 3 on page 24.

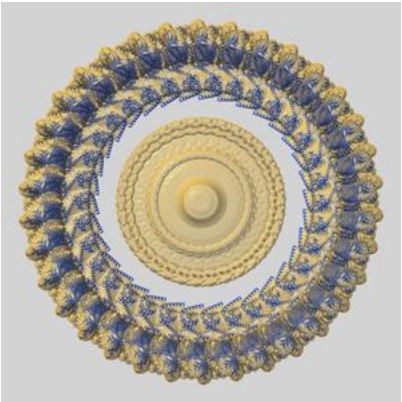
9.1 Map-model overlay (i)



X



Y



Z

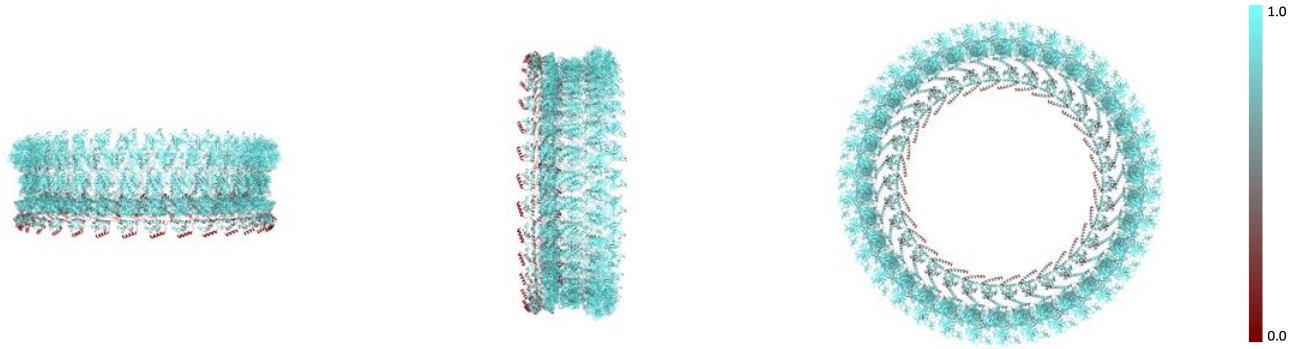
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

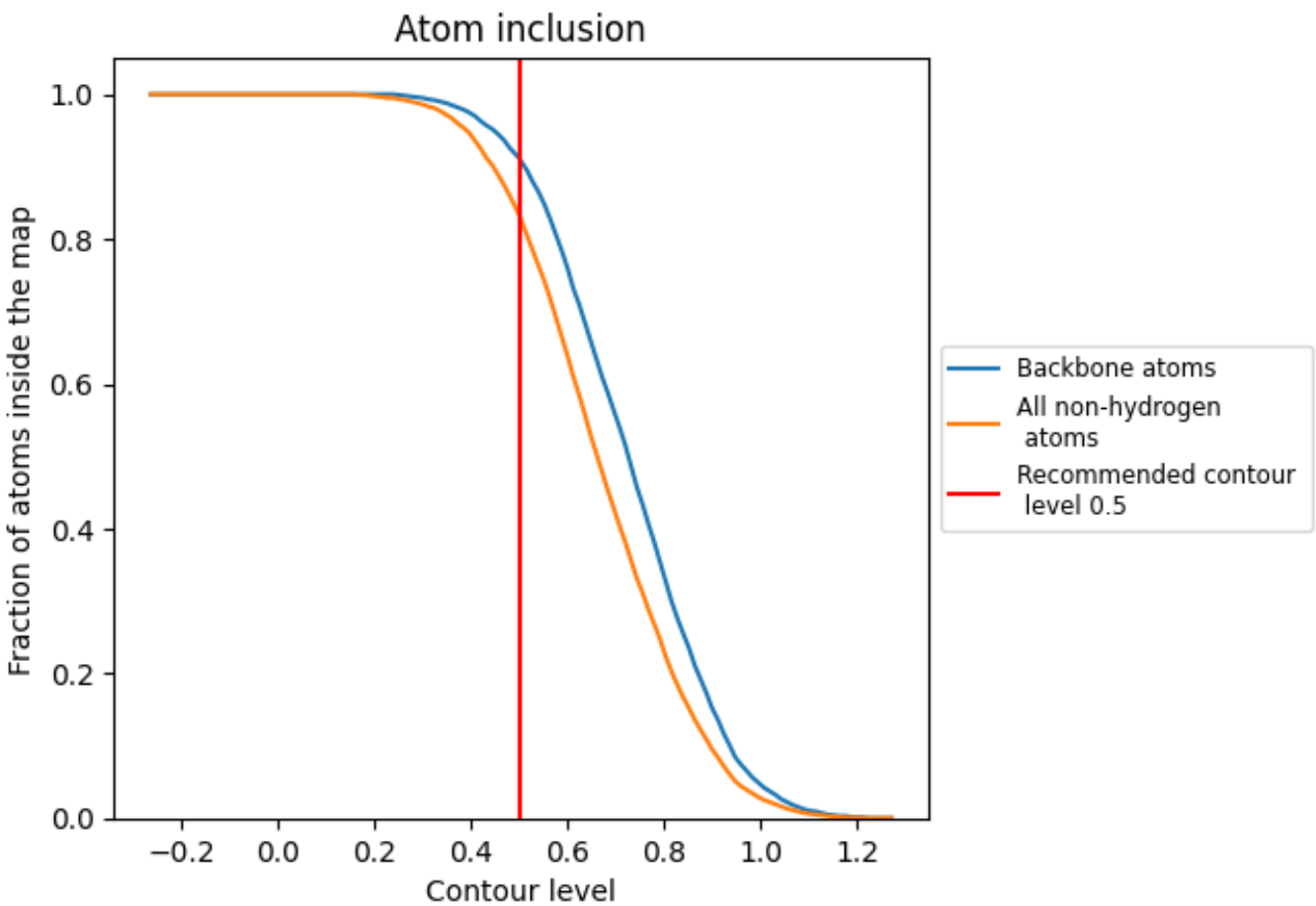
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8340	0.1500
A1	0.6020	0.1430
A2	0.6050	0.1370
A3	0.6080	0.1420
A4	0.6080	0.1400
A5	0.5990	0.1420
A6	0.5940	0.1380
A7	0.5940	0.1390
A8	0.5970	0.1380
A9	0.5990	0.1410
AA	0.6020	0.1380
AB	0.5970	0.1350
AC	0.6080	0.1350
AD	0.6080	0.1370
AE	0.5990	0.1340
AF	0.6080	0.1350
AG	0.6050	0.1340
AH	0.5940	0.1340
AI	0.6020	0.1300
AJ	0.6050	0.1350
AK	0.6080	0.1370
AL	0.5990	0.1370
AM	0.6020	0.1340
AN	0.6020	0.1300
AO	0.5990	0.1380
AP	0.5970	0.1370
AQ	0.5990	0.1370
AR	0.6020	0.1390
AS	0.6050	0.1400
AT	0.6050	0.1400
AU	0.6080	0.1420
AV	0.5990	0.1370
AW	0.6080	0.1400
AX	0.6020	0.1440
AY	0.5990	0.1440

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Chain	Atom inclusion	Q-score
B1	0.7470	0.1400
B2	0.7460	0.1400
B3	0.7410	0.1390
B4	0.7430	0.1400
B5	0.7460	0.1400
B6	0.7480	0.1390
B7	0.7440	0.1390
B8	0.7430	0.1400
B9	0.7460	0.1390
BA	0.7490	0.1390
BB	0.7440	0.1400
BC	0.7420	0.1400
BD	0.7460	0.1390
BE	0.7480	0.1380
BF	0.7440	0.1400
BG	0.7440	0.1400
BH	0.7420	0.1410
BI	0.7460	0.1400
BJ	0.7460	0.1390
BK	0.7440	0.1400
BL	0.7430	0.1390
BM	0.7470	0.1400
BN	0.7470	0.1400
BO	0.7440	0.1400
BP	0.7410	0.1400
BQ	0.7460	0.1400
BR	0.7480	0.1390
BS	0.7440	0.1390
BT	0.7430	0.1410
BU	0.7450	0.1390
BV	0.7470	0.1400
BW	0.7450	0.1400
BX	0.7420	0.1400
BY	0.7430	0.1390
C1	0.8960	0.1540
C2	0.8940	0.1550
C3	0.8950	0.1550
C4	0.8940	0.1540
C5	0.8960	0.1550
C6	0.8960	0.1560
C7	0.8950	0.1550
C8	0.8960	0.1560

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Chain	Atom inclusion	Q-score
C9	0.8960	0.1550
CA	0.8970	0.1560
CB	0.8950	0.1560
CC	0.8940	0.1540
CD	0.8960	0.1530
CE	0.8950	0.1550
CF	0.8960	0.1550
CG	0.8950	0.1540
CH	0.8960	0.1550
CI	0.8980	0.1550
CJ	0.8940	0.1570
CK	0.8940	0.1560
CL	0.8950	0.1550
CM	0.8980	0.1550
CN	0.8960	0.1550
CO	0.8930	0.1560
CP	0.8920	0.1560
CQ	0.8970	0.1540
CR	0.8950	0.1550
CS	0.8940	0.1550
CT	0.8960	0.1550
CU	0.8980	0.1560
CV	0.8950	0.1540
CW	0.8960	0.1550
CX	0.8930	0.1540
CY	0.8970	0.1560
D1	0.9150	0.1640
D2	0.9090	0.1650
D3	0.9100	0.1650
D4	0.9200	0.1680
D5	0.9200	0.1650
D6	0.9180	0.1680
D7	0.9150	0.1630
D8	0.9200	0.1650
D9	0.9200	0.1630
DA	0.9100	0.1630
DB	0.9140	0.1650
DC	0.9150	0.1640
DD	0.9070	0.1620
DE	0.9140	0.1650
DF	0.9100	0.1620
DG	0.9070	0.1620

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Chain	Atom inclusion	Q-score
DH	0.9120	0.1630
DI	0.9170	0.1640
DJ	0.9180	0.1640
DK	0.9200	0.1650
DL	0.9180	0.1660
DM	0.9180	0.1670
DN	0.9120	0.1670
DO	0.9150	0.1620
DP	0.9120	0.1640
DQ	0.9180	0.1660
DR	0.9120	0.1670
DS	0.9120	0.1660
DT	0.9120	0.1670
DU	0.9060	0.1650
DV	0.9090	0.1630
DW	0.9090	0.1650
DX	0.9070	0.1670
DY	0.9140	0.1670
E1	0.9390	0.1550
E2	0.9410	0.1570
E3	0.9360	0.1550
E4	0.9390	0.1540
E5	0.9390	0.1530
E6	0.9380	0.1540
E7	0.9380	0.1560
E8	0.9360	0.1550
E9	0.9380	0.1550
EA	0.9430	0.1530
EB	0.9380	0.1560
EC	0.9410	0.1560
ED	0.9380	0.1590
EE	0.9390	0.1550
EF	0.9360	0.1570
EG	0.9360	0.1590
EH	0.9360	0.1580
EI	0.9390	0.1560
EJ	0.9360	0.1550
EK	0.9360	0.1600
EL	0.9390	0.1590
EM	0.9410	0.1580
EN	0.9390	0.1570
EO	0.9380	0.1610

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Chain	Atom inclusion	Q-score
EP	0.9340	0.1610
EQ	0.9390	0.1610
ER	0.9430	0.1590
ES	0.9390	0.1590
ET	0.9390	0.1600
EU	0.9410	0.1630
EV	0.9430	0.1600
EW	0.9320	0.1580
EX	0.9380	0.1590
EY	0.9410	0.1600
F1	0.9170	0.1570
F2	0.9220	0.1600
F3	0.9200	0.1580
F4	0.9190	0.1620
F5	0.9220	0.1590
F6	0.9160	0.1580
F7	0.9230	0.1600
F8	0.9190	0.1560
F9	0.9140	0.1570
FA	0.9170	0.1590
FB	0.9140	0.1580
FC	0.9200	0.1610
FD	0.9220	0.1590
FE	0.9170	0.1600
FF	0.9230	0.1600
FG	0.9120	0.1570
FH	0.9190	0.1570
FI	0.9230	0.1570
FJ	0.9160	0.1550
FK	0.9200	0.1540
FL	0.9160	0.1580
FM	0.9170	0.1550
FN	0.9250	0.1560
FO	0.9170	0.1540
FP	0.9160	0.1530
FQ	0.9120	0.1530
FR	0.9160	0.1540
FS	0.9160	0.1520
FT	0.9160	0.1530
FU	0.9170	0.1560
FV	0.9160	0.1580
FW	0.9140	0.1540

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Chain	Atom inclusion	Q-score
FX	0.9120	0.1530
FY	0.9200	0.1550