



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 07:29 PM UTC

PDB ID : 8UPL / pdb_00008upl
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 ⓘ symbol.

The types of validation reports are described at

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

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

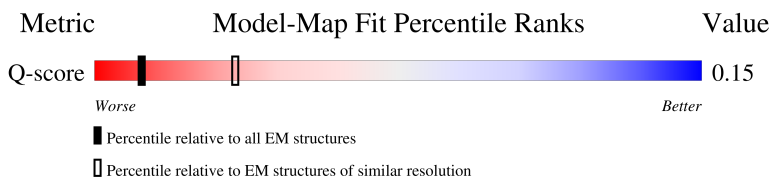
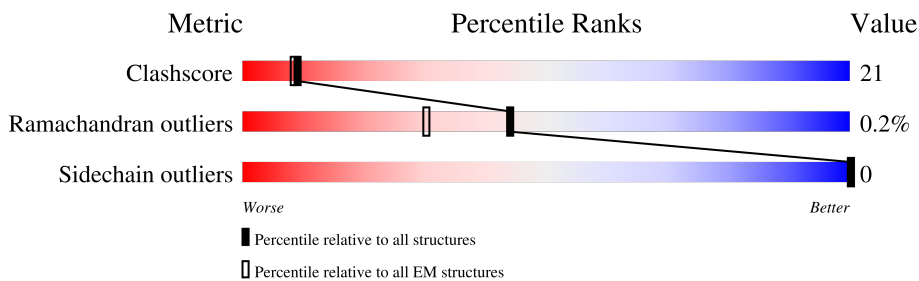
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	538 (4.90 - 5.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	560	92%
1	A2	560	92%
1	A3	560	92%
1	A4	560	92%

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Mol	Chain	Length	Quality of chain
1	A5	560	92%
1	A6	560	92%
1	A7	560	92%
1	A8	560	92%
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	92%
1	AP	560	92%
1	AQ	560	92%
1	AR	560	92%
1	AS	560	92%
1	AT	560	92%

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Mol	Chain	Length	Quality of chain
1	AU	560	92%
1	AV	560	92%
1	AW	560	92%
1	AX	560	92%
1	AY	560	92%
2	B1	328	17% 61% 39%
2	B2	328	17% 62% 38%
2	B3	328	18% 62% 38%
2	B4	328	18% 59% 41%
2	B5	328	18% 61% 39%
2	B6	328	18% 62% 38%
2	B7	328	18% 62% 38%
2	B8	328	18% 62% 38%
2	B9	328	18% 61% 38%
2	BA	328	17% 61% 39%
2	BB	328	18% 62% 38%
2	BC	328	18% 62% 38%
2	BD	328	18% 61% 39%
2	BE	328	17% 61% 39%
2	BF	328	18% 62% 38%
2	BG	328	18% 61% 39%
2	BH	328	18% 63% 37%
2	BI	328	18% 60% 40%
2	BJ	328	18% 62% 38%
2	BK	328	18% 62% 38%


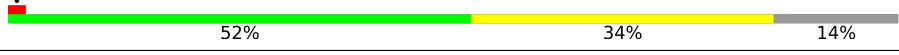

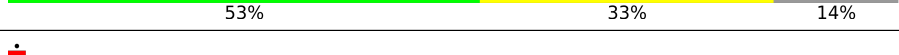




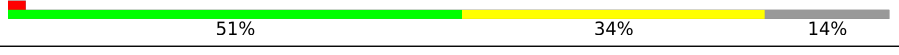





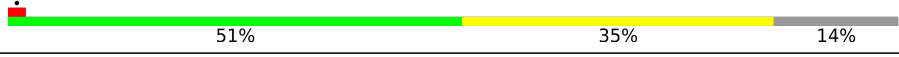





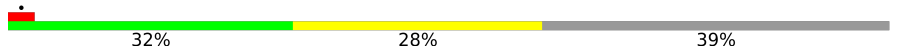
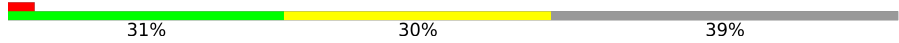



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Mol	Chain	Length	Quality of chain			
2	BL	328	17%	62%	38%	
2	BM	328	18%	60%	40%	
2	BN	328	18%	62%	38%	
2	BO	328	18%	63%	37%	
2	BP	328	18%	63%	37%	
2	BQ	328	18%	62%	38%	
2	BR	328	18%	62%	38%	
2	BS	328	18%	61%	39%	
2	BT	328	18%	63%	37%	
2	BU	328	18%	61%	39%	
2	BV	328	18%	62%	38%	
2	BW	328	18%	62%	38%	
2	BX	328	18%	62%	38%	
2	BY	328	18%	61%	39%	
3	C1	334	•	51%	35%	14%
3	C2	334	•	53%	33%	14%
3	C3	334	•	53%	33%	14%
3	C4	334	•	51%	35%	14%
3	C5	334	•	54%	32%	14%
3	C6	334	•	54%	32%	14%
3	C7	334	•	52%	34%	14%
3	C8	334	•	52%	34%	14%
3	C9	334	•	52%	34%	14%
3	CA	334	•	52%	34%	14%
3	CB	334	•	52%	34%	14%

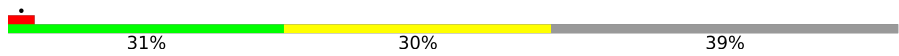
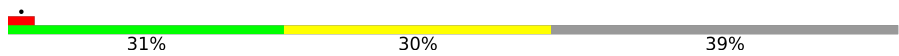
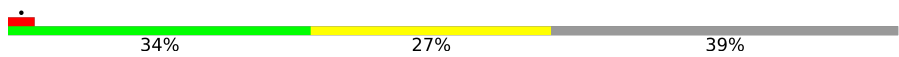
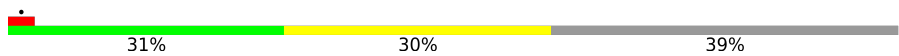
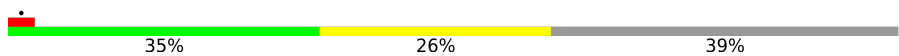
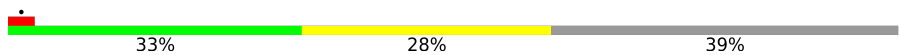
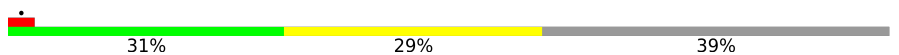
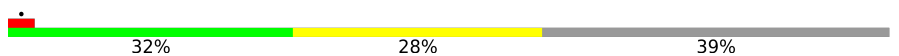
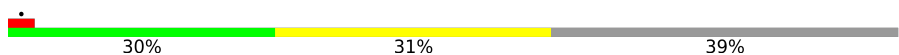
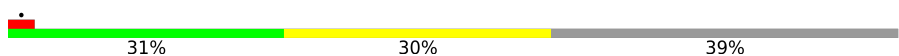
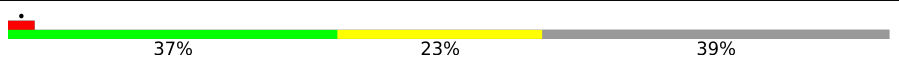
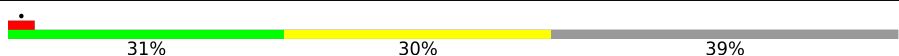
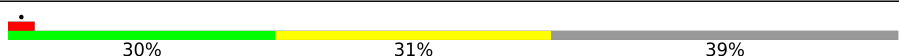
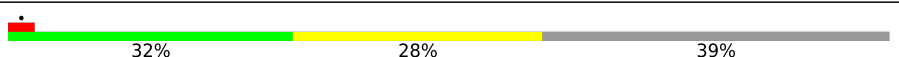
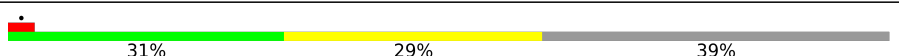
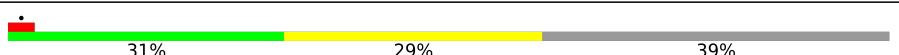
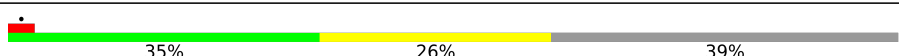
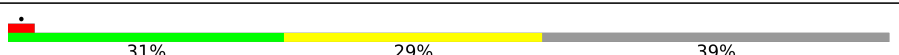
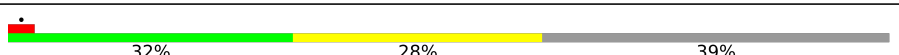
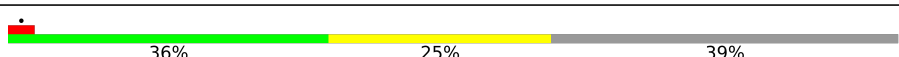
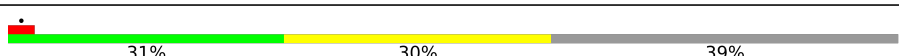
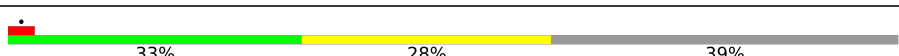
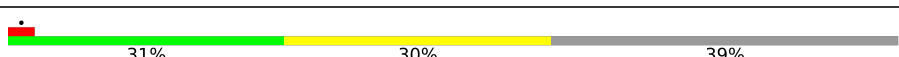
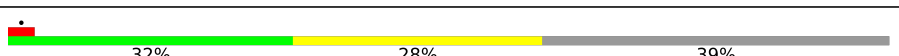
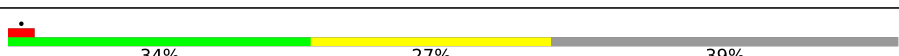
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Mol	Chain	Length	Quality of chain
3	CC	334	 50% 35% 14%
3	CD	334	 52% 34% 14%
3	CE	334	 52% 34% 14%
3	CF	334	 53% 33% 14%
3	CG	334	 51% 35% 14%
3	CH	334	 52% 34% 14%
3	CI	334	 51% 34% 14%
3	CJ	334	 52% 34% 14%
3	CK	334	 53% 33% 14%
3	CL	334	 51% 34% 14%
3	CM	334	 53% 33% 14%
3	CN	334	 52% 34% 14%
3	CO	334	 51% 35% 14%
3	CP	334	 52% 34% 14%
3	CQ	334	 53% 33% 14%
3	CR	334	 53% 33% 14%
3	CS	334	 51% 35% 14%
3	CT	334	 51% 35% 14%
3	CU	334	 51% 35% 14%
3	CV	334	 51% 35% 14%
3	CW	334	 54% 32% 14%
3	CX	334	 51% 34% 14%
3	CY	334	 52% 33% 14%
4	D1	137	 32% 28% 39%
4	D2	137	 31% 30% 39%

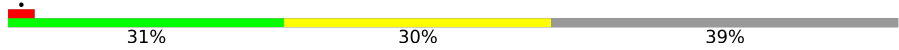
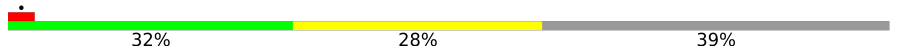
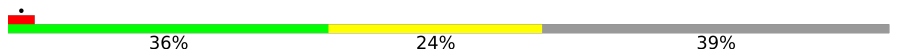
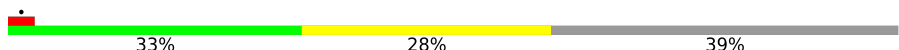
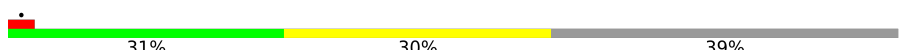
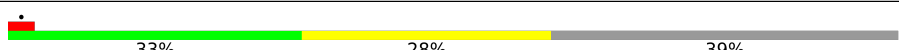
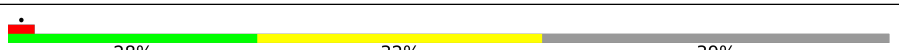
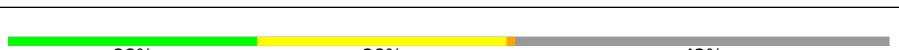
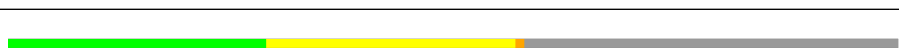
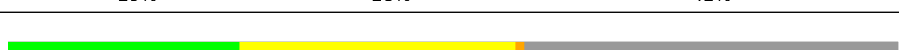
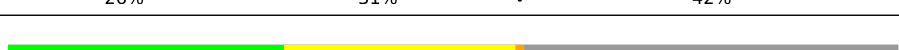
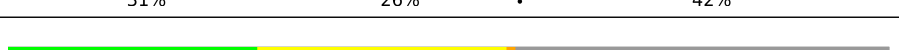

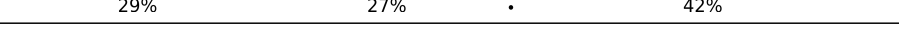
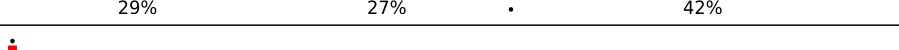
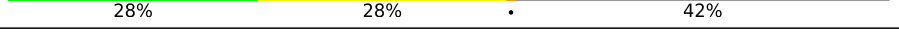


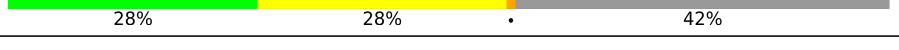



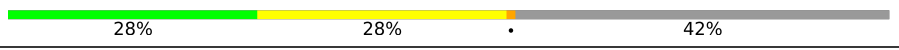


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Mol	Chain	Length	Quality of chain
4	D3	137	 31% 30% 39%
4	D4	137	 31% 30% 39%
4	D5	137	 34% 27% 39%
4	D6	137	 31% 30% 39%
4	D7	137	 35% 26% 39%
4	D8	137	 33% 28% 39%
4	D9	137	 31% 29% 39%
4	DA	137	 32% 28% 39%
4	DB	137	 30% 31% 39%
4	DC	137	 31% 30% 39%
4	DD	137	 37% 23% 39%
4	DE	137	 31% 30% 39%
4	DF	137	 30% 31% 39%
4	DG	137	 32% 28% 39%
4	DH	137	 31% 29% 39%
4	DI	137	 31% 29% 39%
4	DJ	137	 35% 26% 39%
4	DK	137	 31% 29% 39%
4	DL	137	 32% 28% 39%
4	DM	137	 36% 25% 39%
4	DN	137	 31% 30% 39%
4	DO	137	 33% 28% 39%
4	DP	137	 31% 30% 39%
4	DQ	137	 32% 28% 39%
4	DR	137	 34% 27% 39%

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Mol	Chain	Length	Quality of chain
4	DS	137	
4	DT	137	
4	DU	137	
4	DV	137	
4	DW	137	
4	DX	137	
4	DY	137	
4	E1	137	
4	E2	137	
4	E3	137	
4	E4	137	
4	E5	137	
4	E6	137	
4	E7	137	
4	E8	137	
4	E9	137	
4	EA	137	
4	EB	137	
4	EC	137	
4	ED	137	
4	EE	137	
4	EF	137	
4	EG	137	
4	EH	137	
4	EI	137	

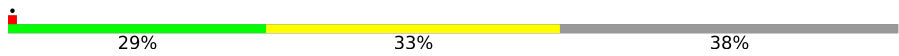
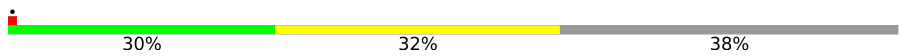

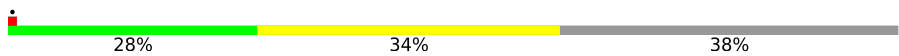
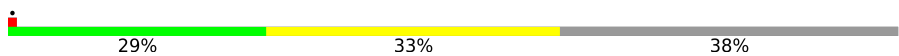
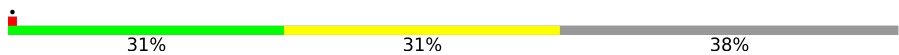

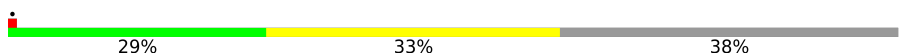
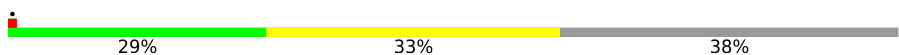
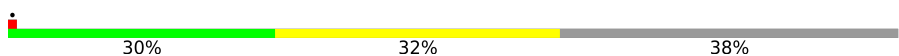
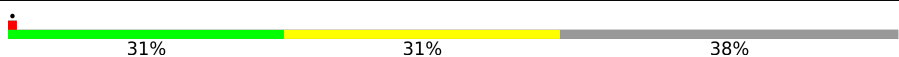
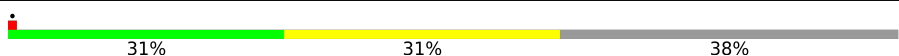
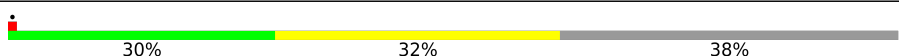
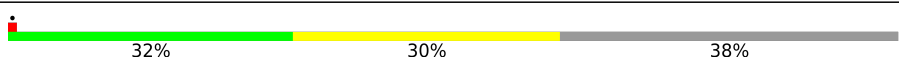
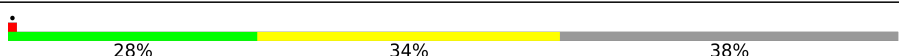
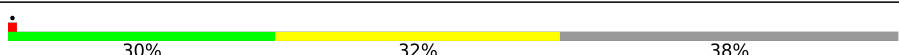
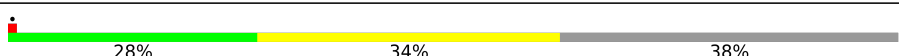
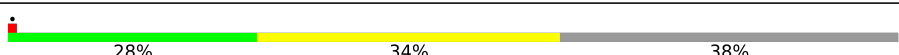
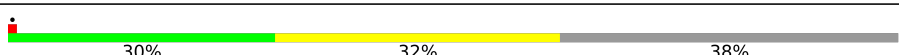
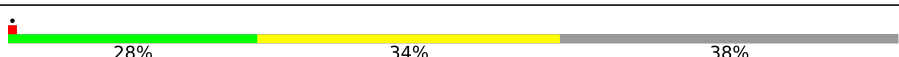
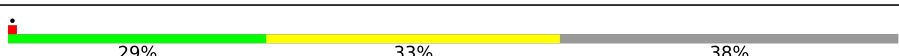
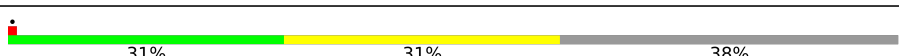
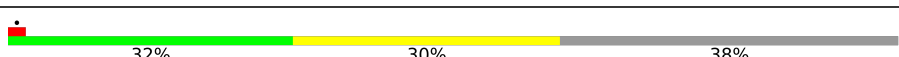
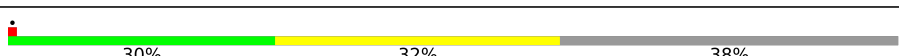
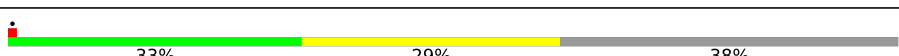
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Mol	Chain	Length	Quality of chain
4	EJ	137	30% 27% 42%
4	EK	137	28% 28% 42%
4	EL	137	30% 27% 42%
4	EM	137	29% 28% 42%
4	EN	137	30% 26% 42%
4	EO	137	31% 26% 42%
4	EP	137	29% 28% 42%
4	EQ	137	28% 29% 42%
4	ER	137	26% 31% 42%
4	ES	137	28% 28% 42%
4	ET	137	27% 30% 42%
4	EU	137	30% 26% 42%
4	EV	137	26% 31% 42%
4	EW	137	31% 26% 42%
4	EX	137	30% 27% 42%
4	EY	137	28% 29% 42%
4	F1	137	28% 34% 38%
4	F2	137	31% 31% 38%
4	F3	137	31% 31% 38%
4	F4	137	33% 29% 38%
4	F5	137	30% 32% 38%
4	F6	137	32% 30% 38%
4	F7	137	27% 35% 38%
4	F8	137	29% 33% 38%
4	F9	137	29% 33% 38%

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Mol	Chain	Length	Quality of chain
4	FA	137	
4	FB	137	
4	FC	137	
4	FD	137	
4	FE	137	
4	FF	137	
4	FG	137	
4	FH	137	
4	FI	137	
4	FJ	137	
4	FK	137	
4	FL	137	
4	FM	137	
4	FN	137	
4	FO	137	
4	FP	137	
4	FQ	137	
4	FR	137	
4	FS	137	
4	FT	137	
4	FU	137	
4	FV	137	
4	FW	137	
4	FX	137	
4	FY	137	

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	83	Total 643	C 407	N 113	O 120	S 3	0	0
4	E1	79	Total 609	C 388	N 106	O 112	S 3	0	0
4	F1	85	Total 656	C 416	N 113	O 124	S 3	0	0
4	D2	83	Total 643	C 407	N 113	O 120	S 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
4	F2	85	656	416	113	124	3	0	0
4	D3	83	643	407	113	120	3	0	0
4	E3	79	609	388	106	112	3	0	0
4	F3	85	656	416	113	124	3	0	0
4	D4	83	643	407	113	120	3	0	0
4	E4	79	609	388	106	112	3	0	0
4	F4	85	656	416	113	124	3	0	0
4	D5	83	643	407	113	120	3	0	0
4	E5	79	609	388	106	112	3	0	0
4	F5	85	656	416	113	124	3	0	0
4	D6	83	643	407	113	120	3	0	0
4	E6	79	609	388	106	112	3	0	0
4	F6	85	656	416	113	124	3	0	0
4	D7	83	643	407	113	120	3	0	0
4	E7	79	609	388	106	112	3	0	0
4	F7	85	656	416	113	124	3	0	0
4	D8	83	643	407	113	120	3	0	0
4	E8	79	609	388	106	112	3	0	0
4	F8	85	656	416	113	124	3	0	0
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
4	F9	85	656	416	113	124	3	0	0
4	DA	83	643	407	113	120	3	0	0
4	EA	79	609	388	106	112	3	0	0
4	FA	85	656	416	113	124	3	0	0
4	DB	83	643	407	113	120	3	0	0
4	EB	79	609	388	106	112	3	0	0
4	FB	85	656	416	113	124	3	0	0
4	DC	83	643	407	113	120	3	0	0
4	EC	79	609	388	106	112	3	0	0
4	FC	85	656	416	113	124	3	0	0
4	DD	83	643	407	113	120	3	0	0
4	ED	79	609	388	106	112	3	0	0
4	FD	85	656	416	113	124	3	0	0
4	DE	83	643	407	113	120	3	0	0
4	EE	79	609	388	106	112	3	0	0
4	FE	85	656	416	113	124	3	0	0
4	DF	83	643	407	113	120	3	0	0
4	EF	79	609	388	106	112	3	0	0
4	FF	85	656	416	113	124	3	0	0
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
4	FG	85	656	416	113	124	3	0	0
4	DH	83	643	407	113	120	3	0	0
4	EH	79	609	388	106	112	3	0	0
4	FH	85	656	416	113	124	3	0	0
4	DI	83	643	407	113	120	3	0	0
4	EI	79	609	388	106	112	3	0	0
4	FI	85	656	416	113	124	3	0	0
4	DJ	83	643	407	113	120	3	0	0
4	EJ	79	609	388	106	112	3	0	0
4	FJ	85	656	416	113	124	3	0	0
4	DK	83	643	407	113	120	3	0	0
4	EK	79	609	388	106	112	3	0	0
4	FK	85	656	416	113	124	3	0	0
4	DL	83	643	407	113	120	3	0	0
4	EL	79	609	388	106	112	3	0	0
4	FL	85	656	416	113	124	3	0	0
4	DM	83	643	407	113	120	3	0	0
4	EM	79	609	388	106	112	3	0	0
4	FM	85	656	416	113	124	3	0	0
4	DN	83	643	407	113	120	3	0	0

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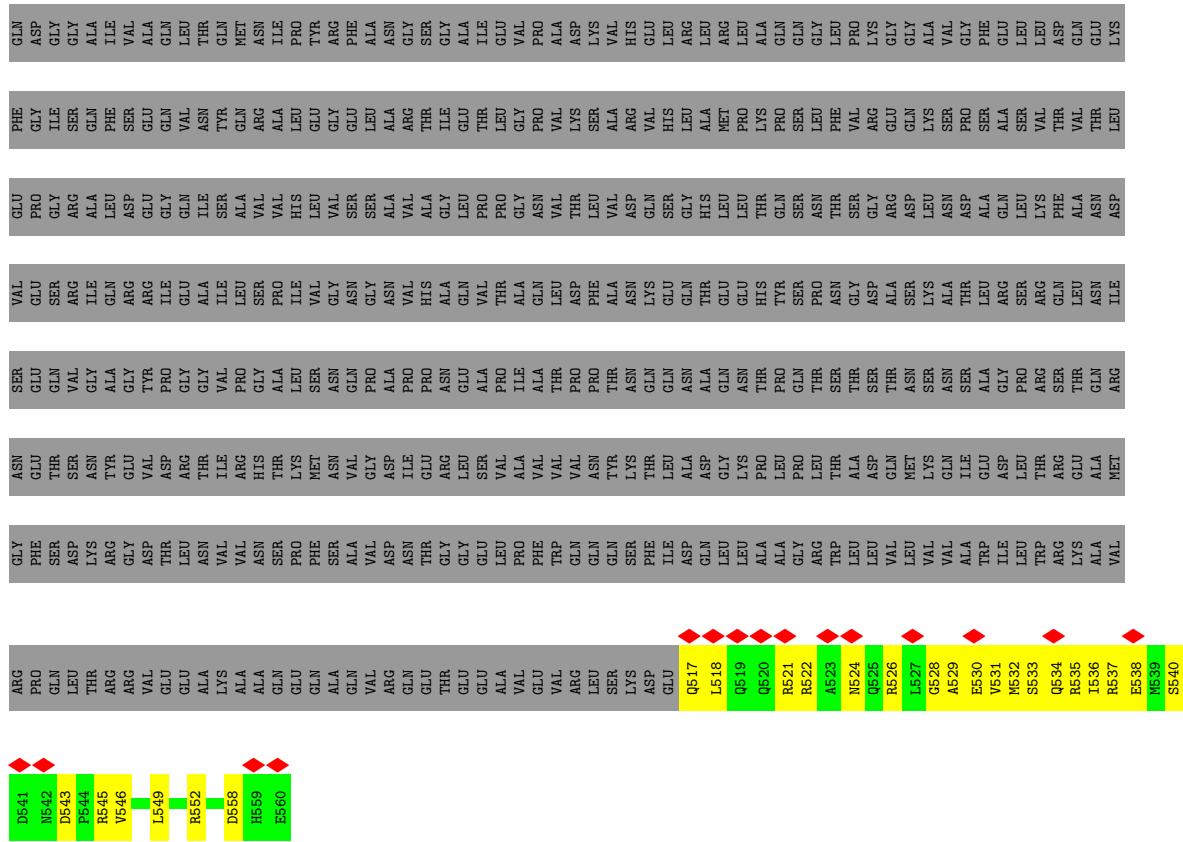
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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4	FN	85	656	416	113	124	3	0	0
4	DO	83	643	407	113	120	3	0	0
4	EO	79	609	388	106	112	3	0	0
4	FO	85	656	416	113	124	3	0	0
4	DP	83	643	407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

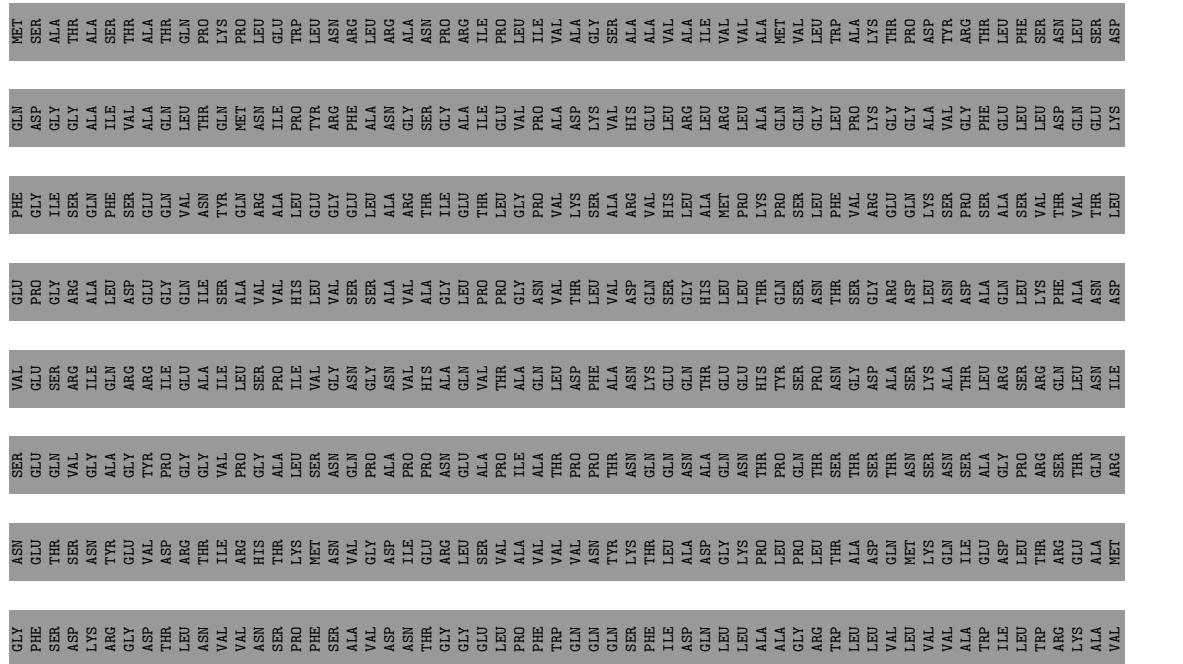
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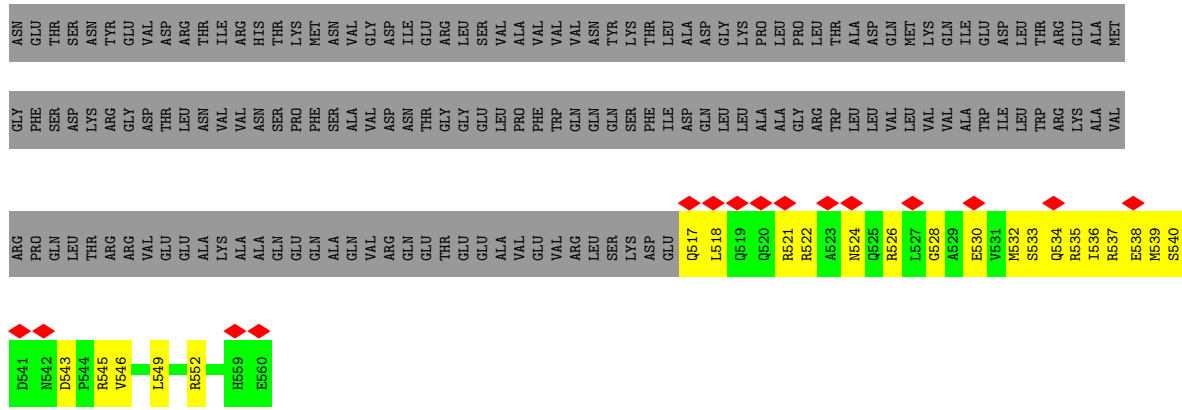
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Mol	Chain	Residues	Atoms					AltConf	Trace
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			609	388	106	112	3		
4	FU	85	Total	C	N	O	S	0	0
			656	416	113	124	3		
4	DV	83	Total	C	N	O	S	0	0
			643	407	113	120	3		
4	EV	79	Total	C	N	O	S	0	0
			609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



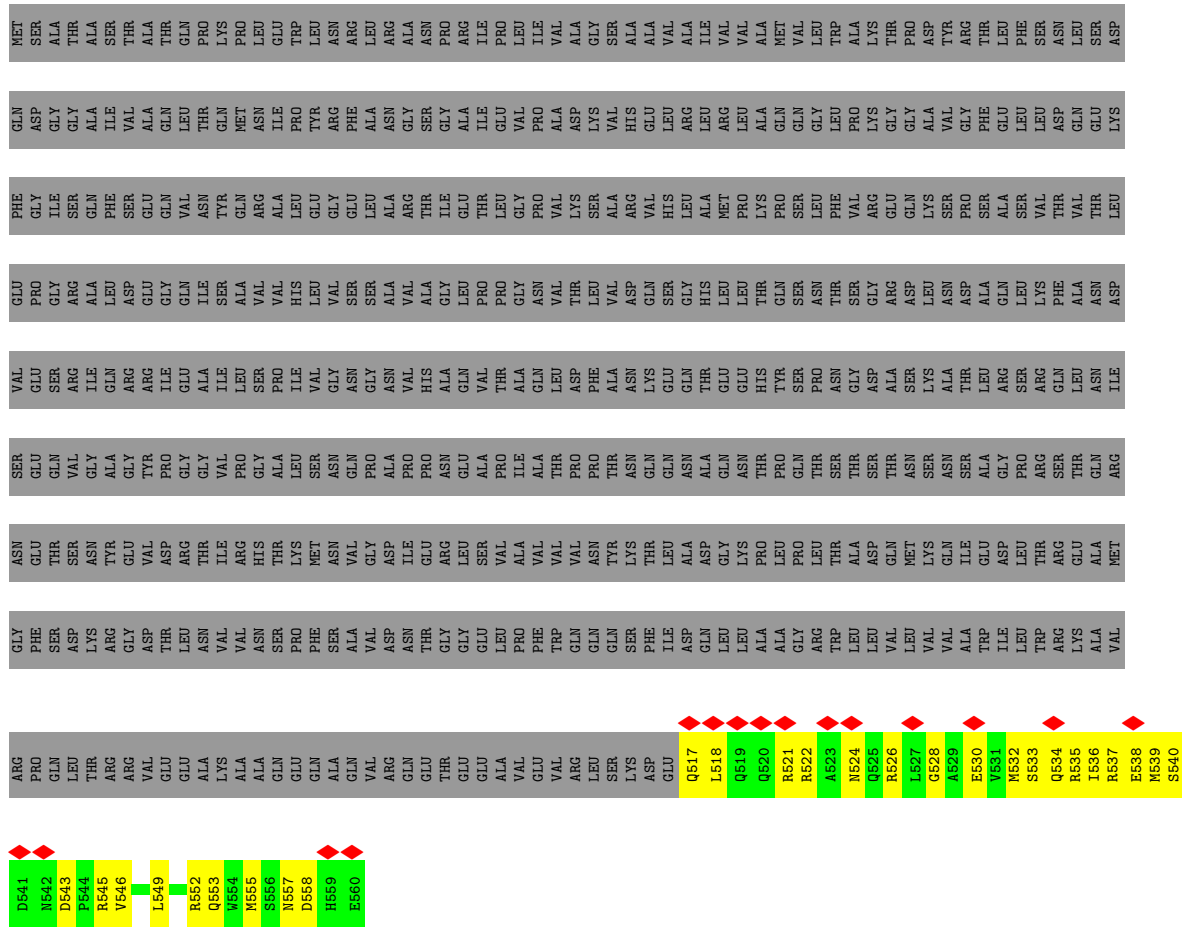
● Molecule 1: Flagellar M-ring protein





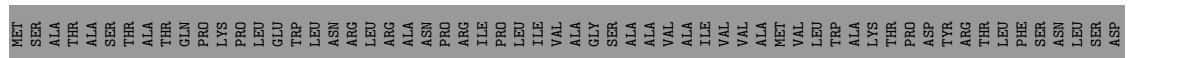
• Molecule 1: Flagellar M-ring protein

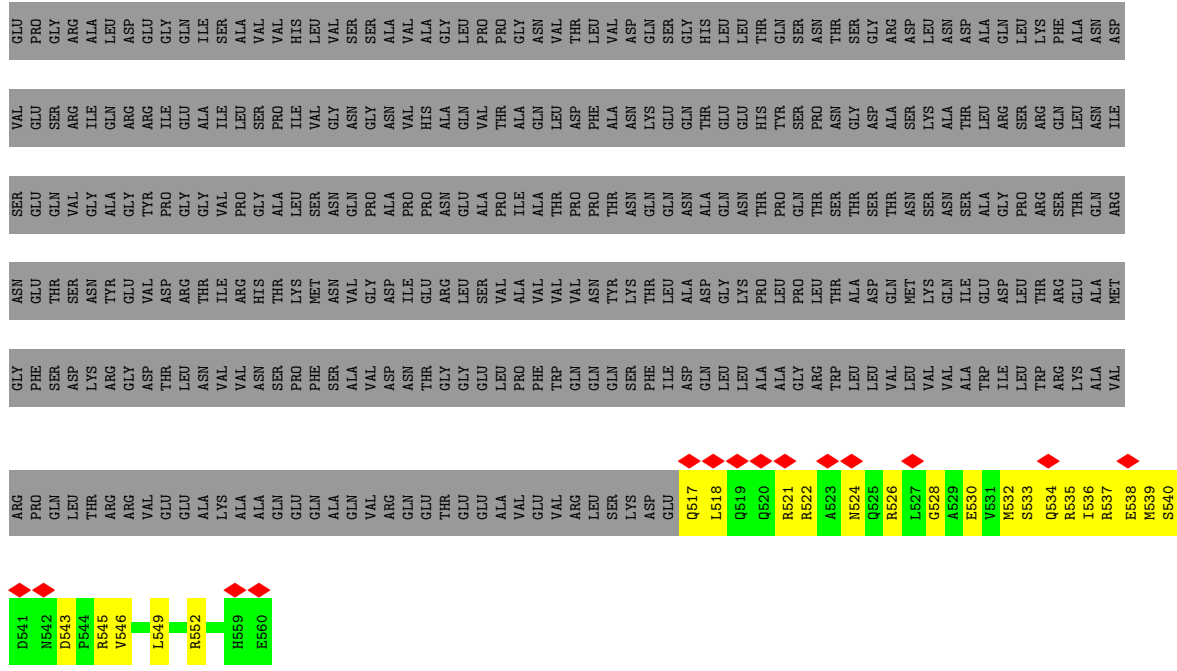
Chain A9: 92%



• Molecule 1: Flagellar M-ring protein

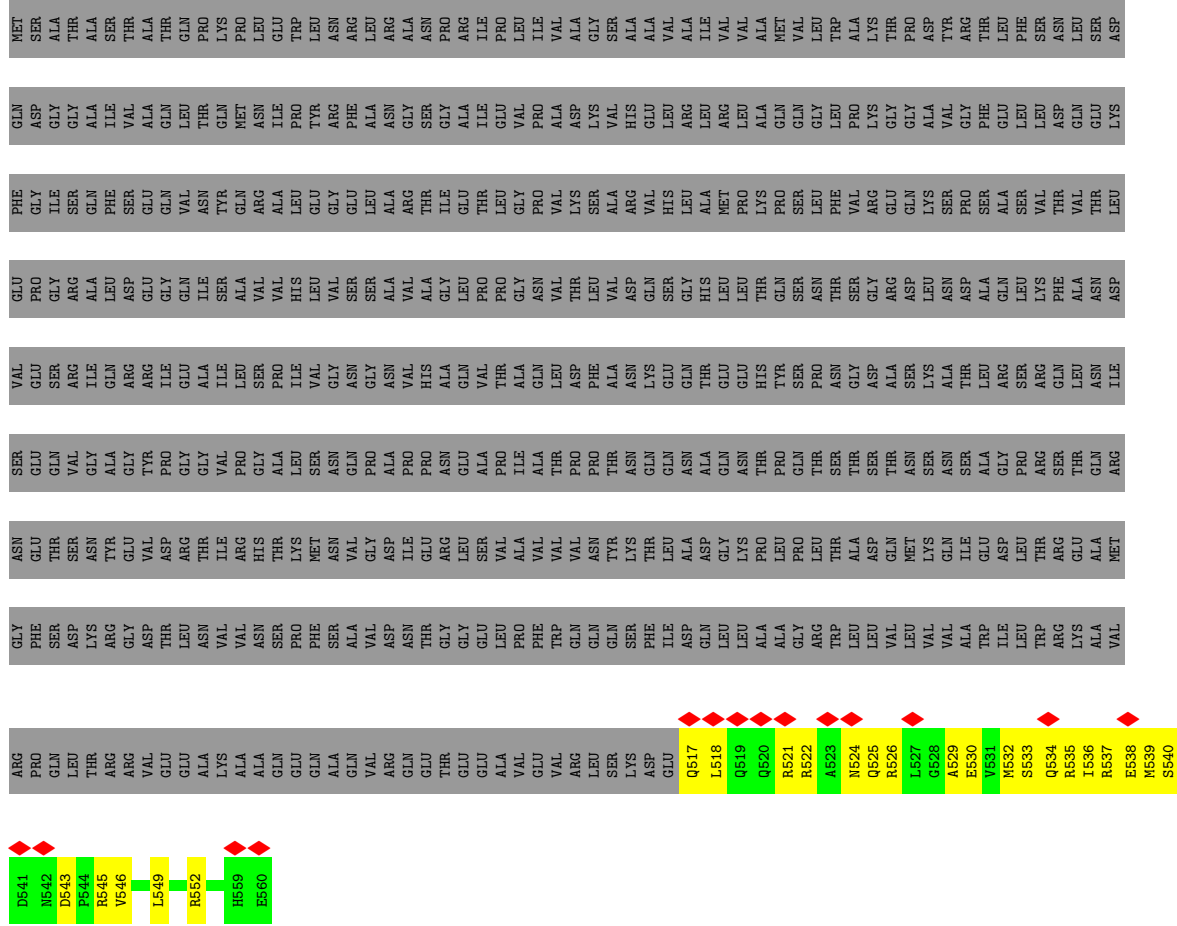
Chain AA: 92%

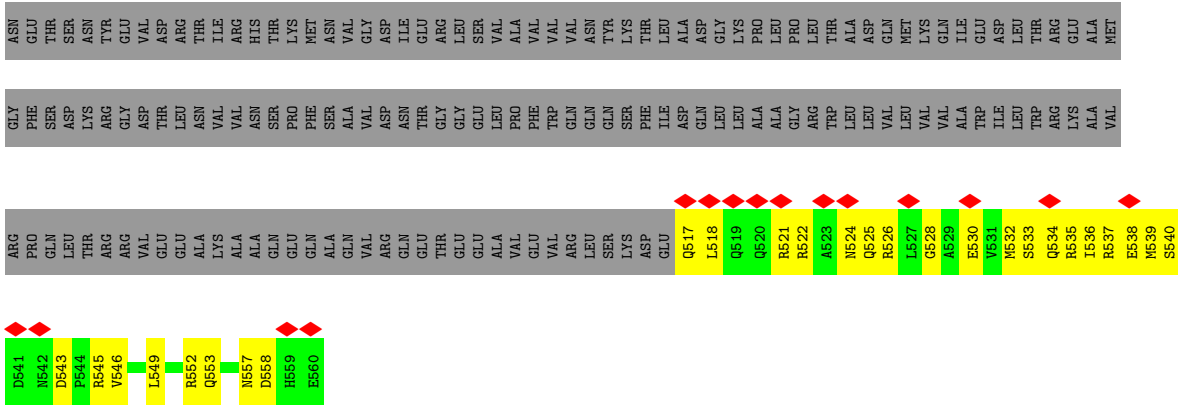




• Molecule 1: Flagellar M-ring protein

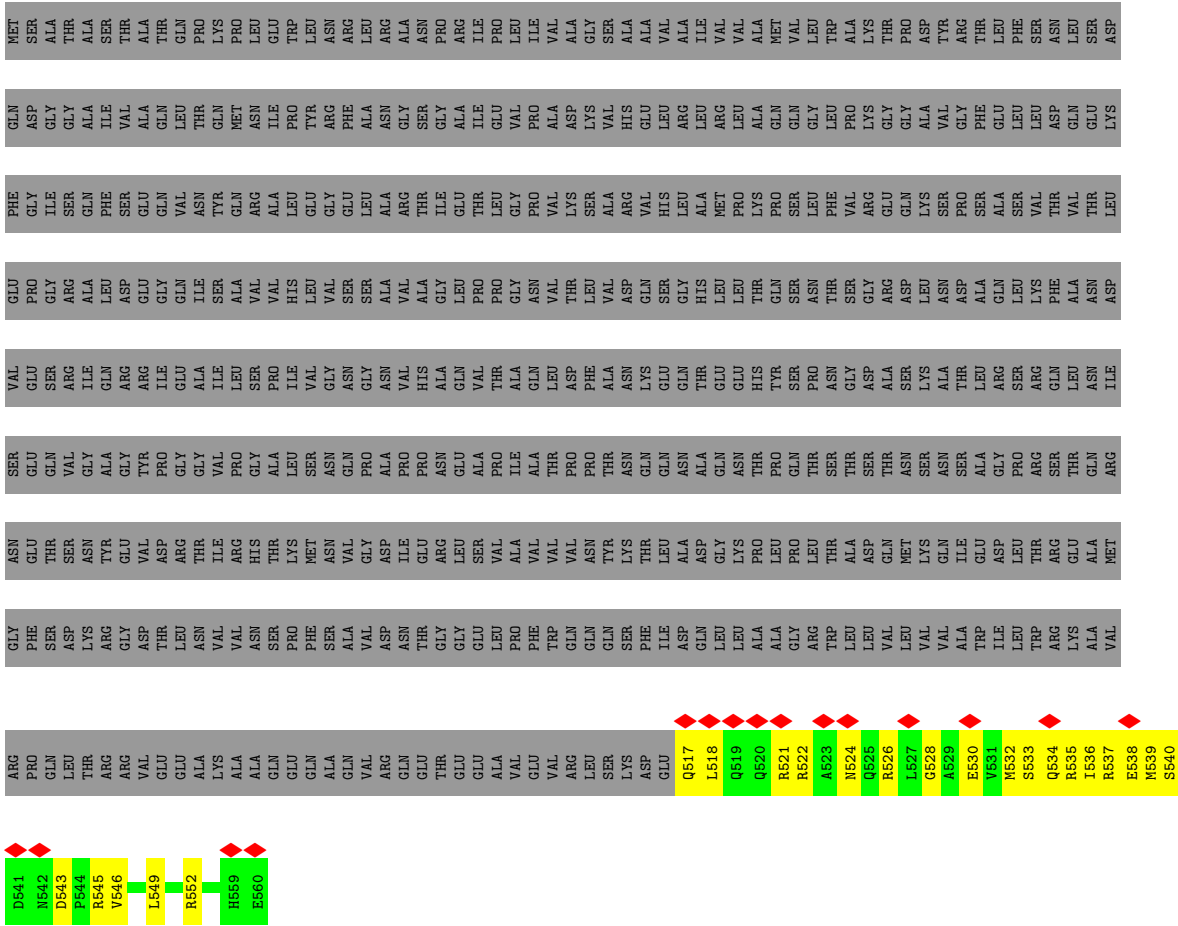
Chain AM: 92%





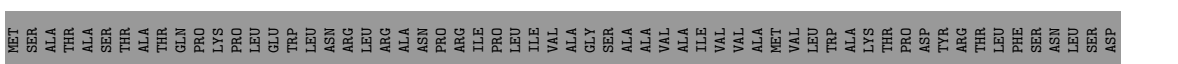
• Molecule 1: Flagellar M-ring protein

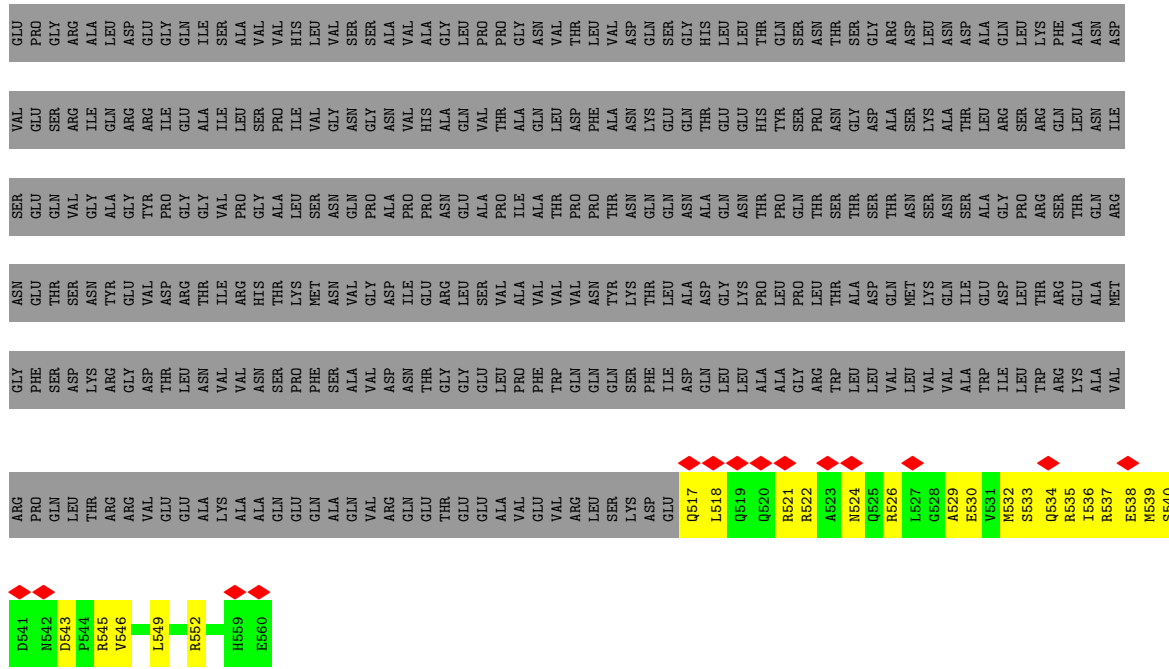
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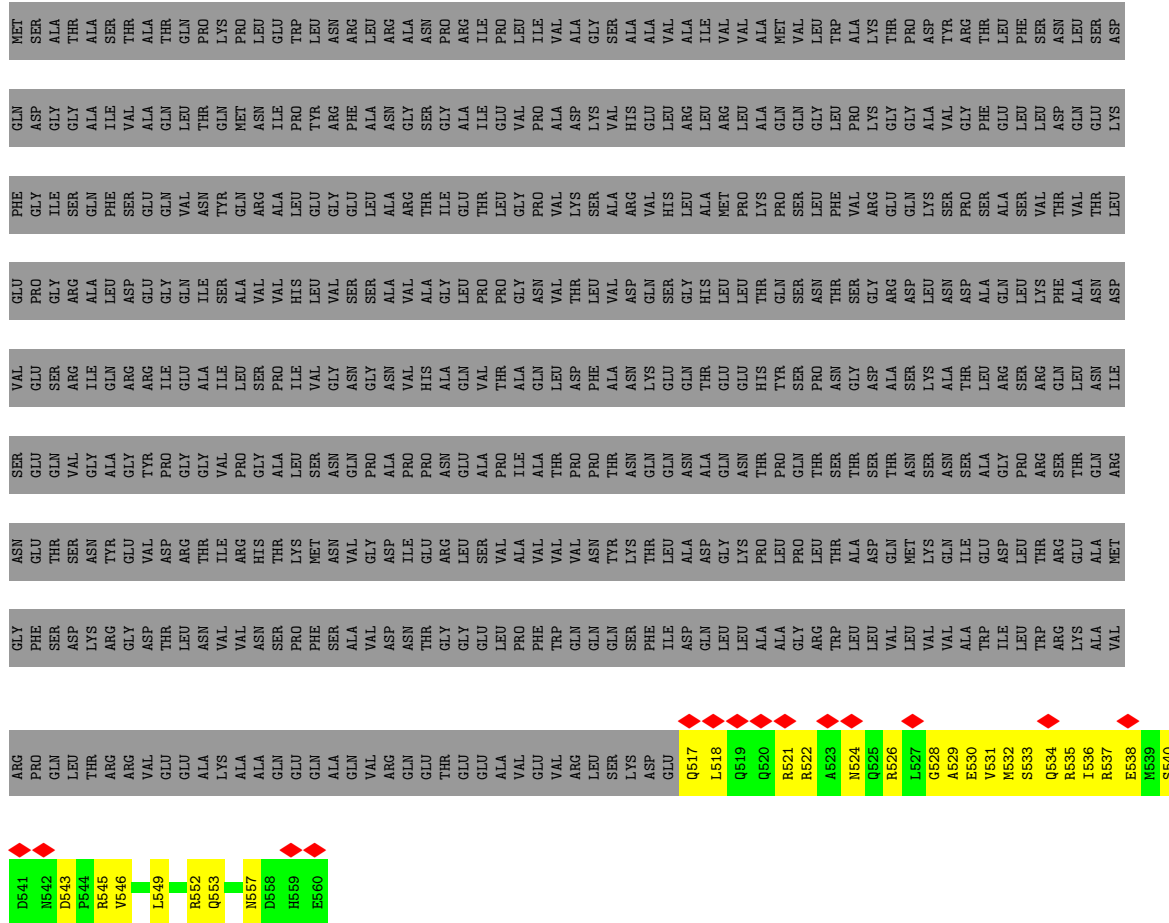
• Molecule 1: Flagellar M-ring protein

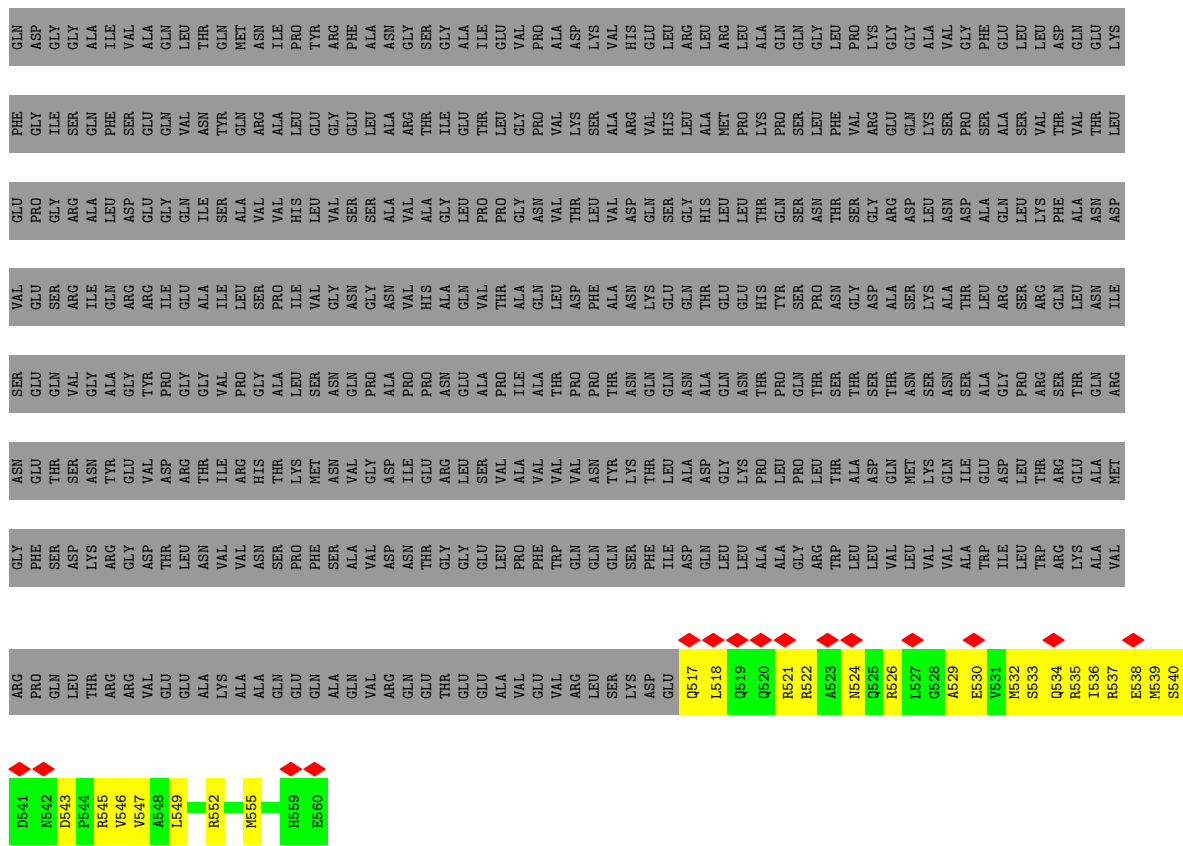
Chain AQ: 92%



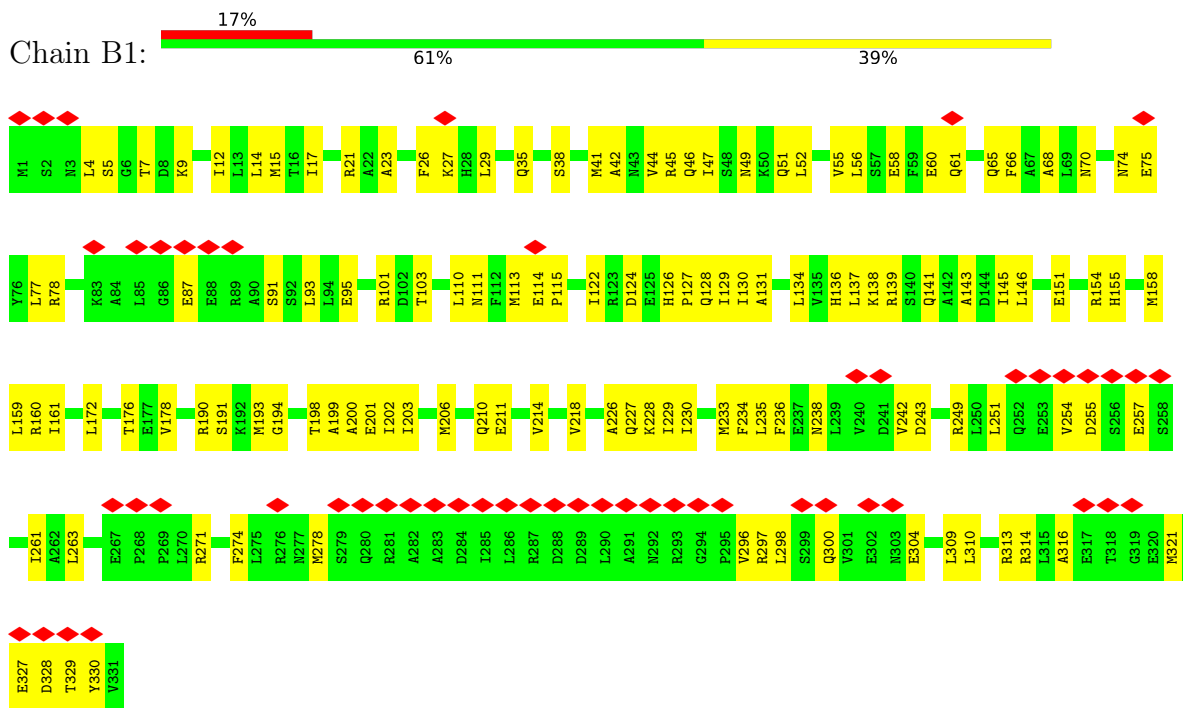


● Molecule 1: Flagellar M-ring protein



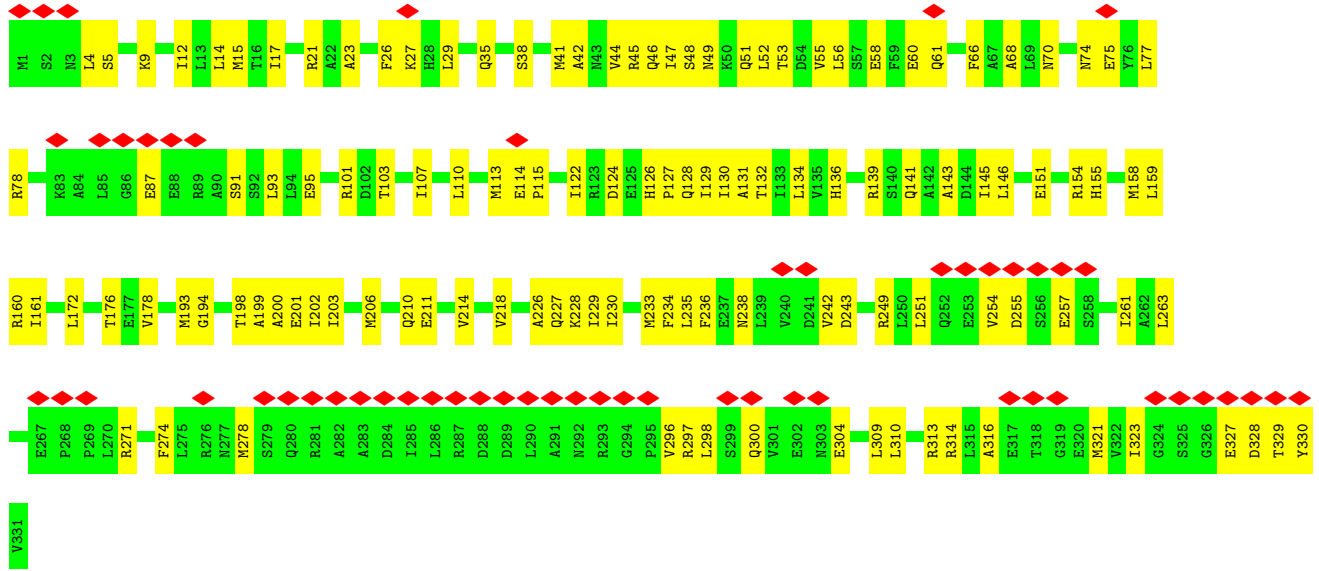


• Molecule 2: Flagellar motor switch protein FliG



• Molecule 2: Flagellar motor switch protein FliG

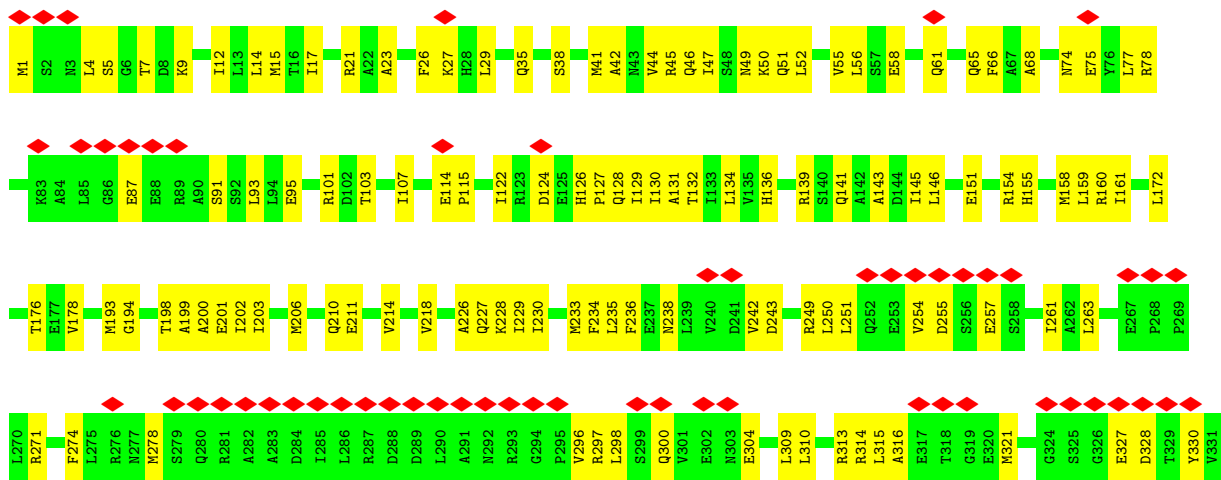




• Molecule 2: Flagellar motor switch protein FliG



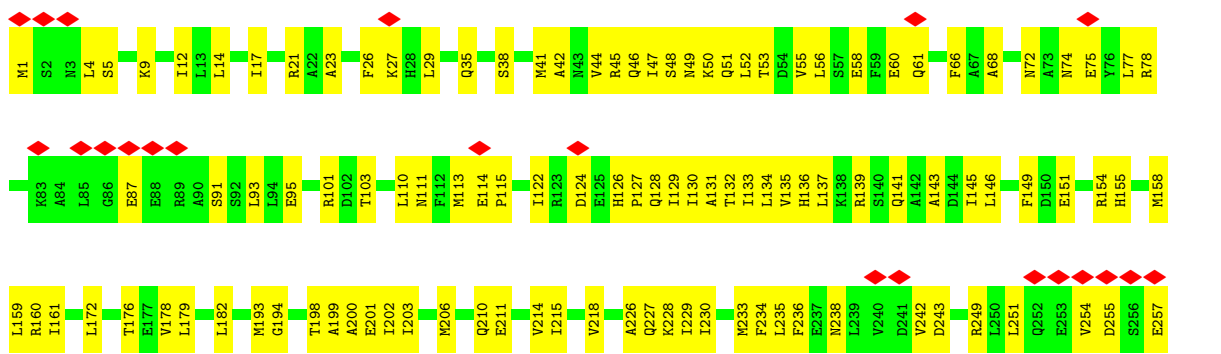
Chain B3:



• Molecule 2: Flagellar motor switch protein FliG

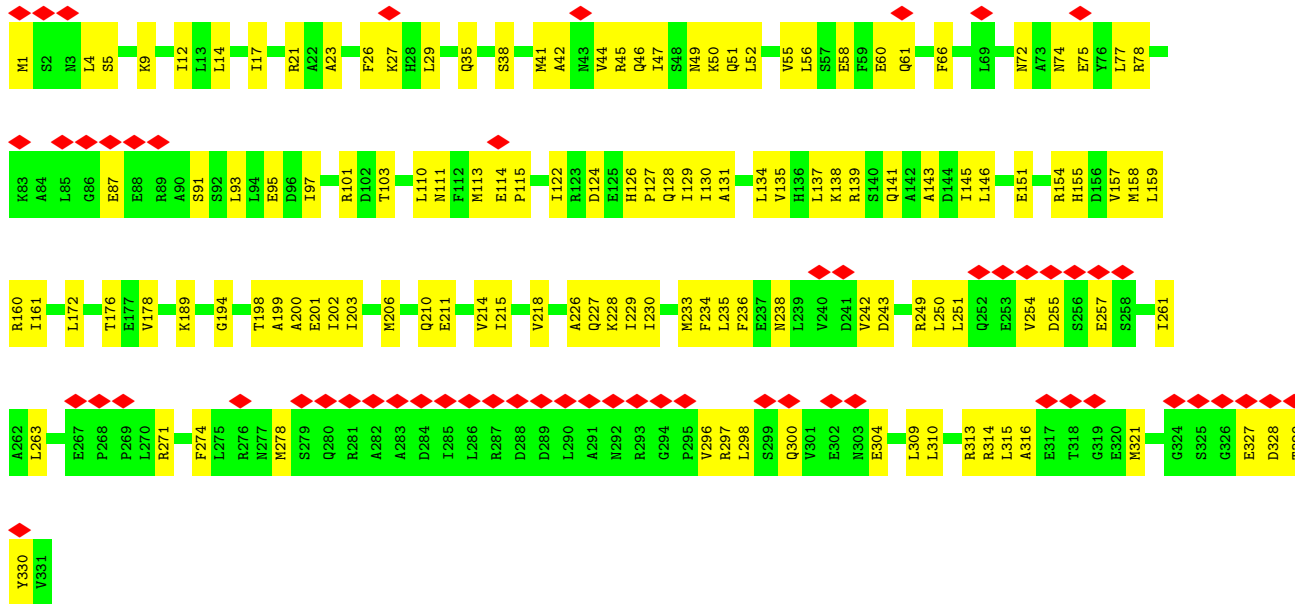


Chain B4:

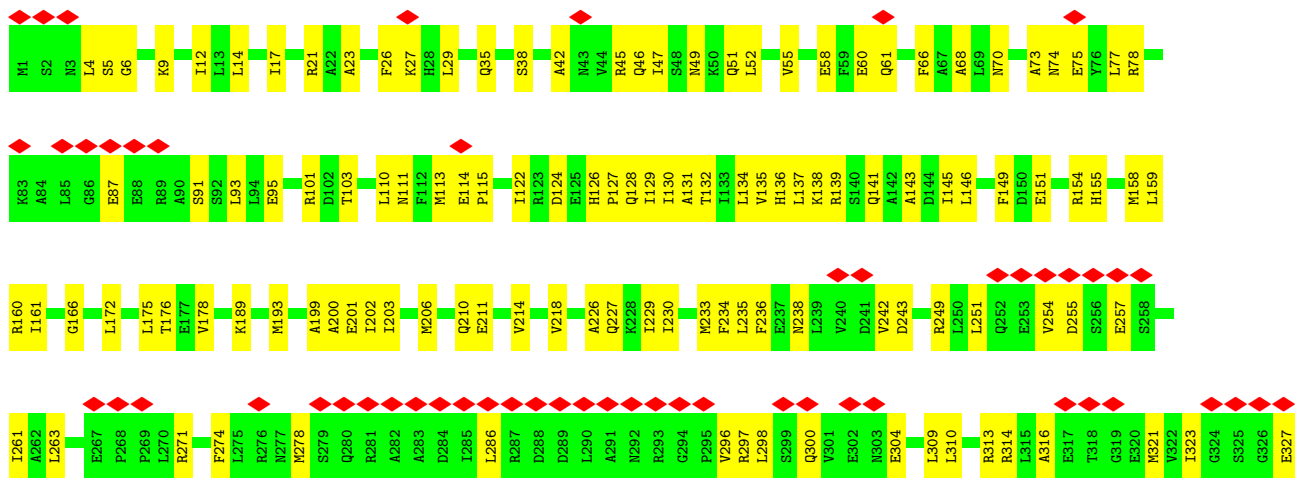


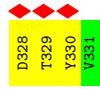


• Molecule 2: Flagellar motor switch protein FliG

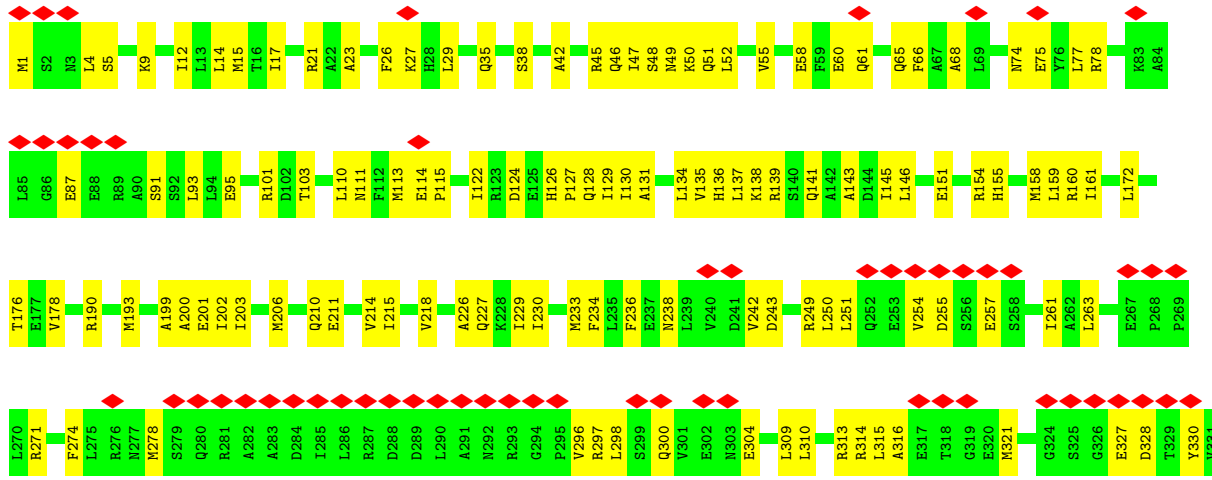


• Molecule 2: Flagellar motor switch protein FliG

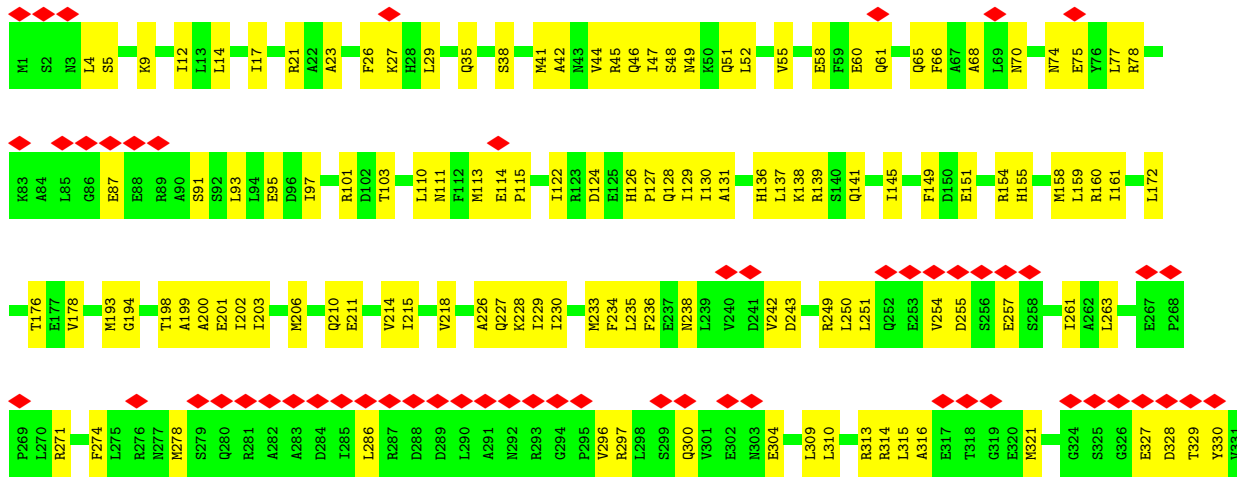




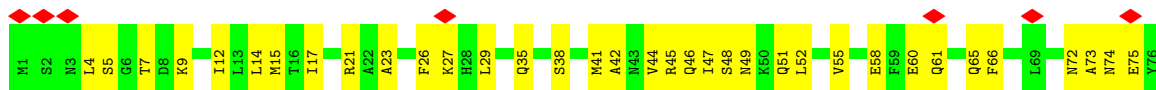
• Molecule 2: Flagellar motor switch protein FliG

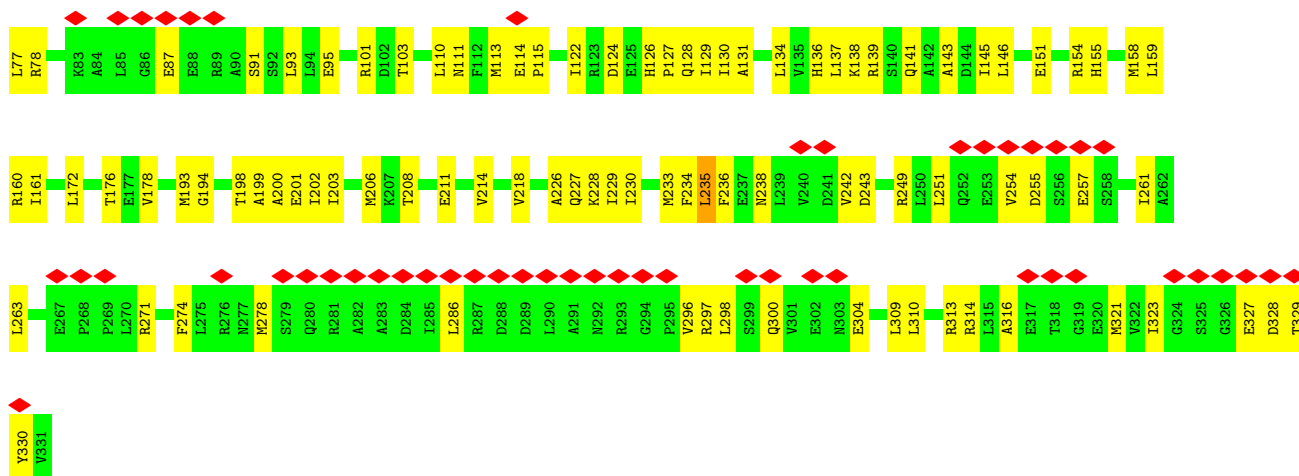


• Molecule 2: Flagellar motor switch protein FliG

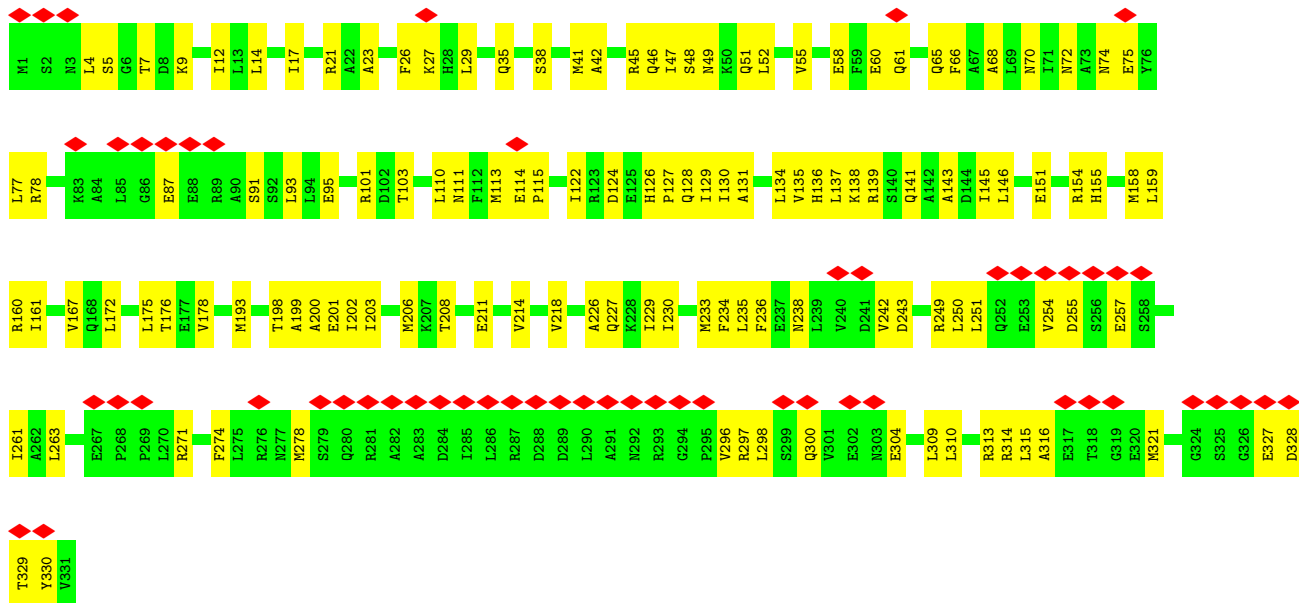


• Molecule 2: Flagellar motor switch protein FliG

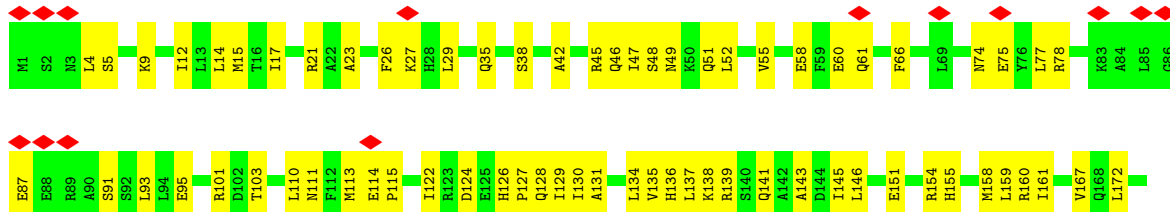


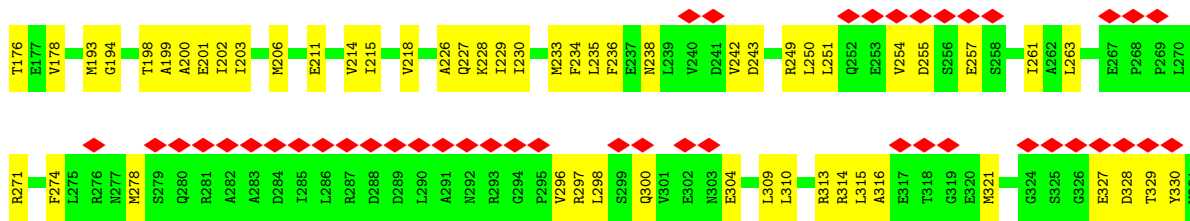


• Molecule 2: Flagellar motor switch protein FlIG

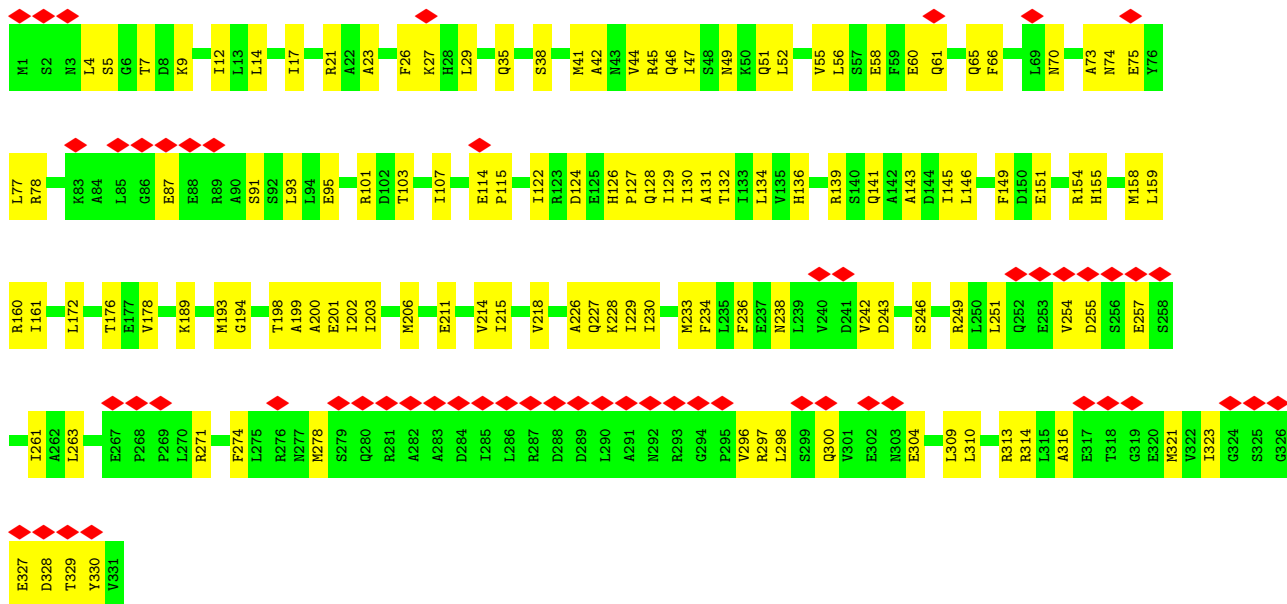


• Molecule 2: Flagellar motor switch protein FlIG

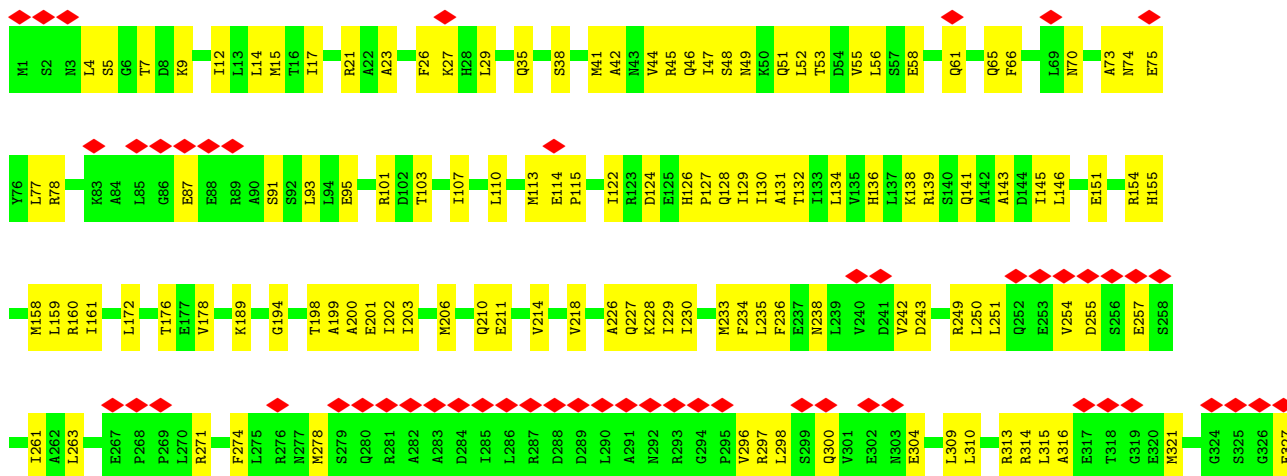




• Molecule 2: Flagellar motor switch protein FlhG

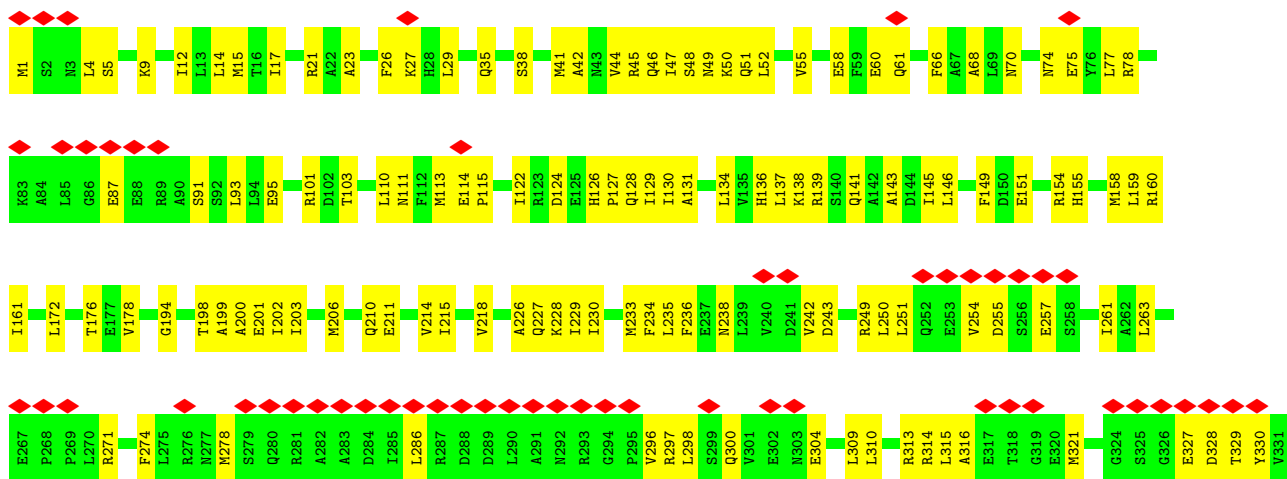


• Molecule 2: Flagellar motor switch protein FlhG

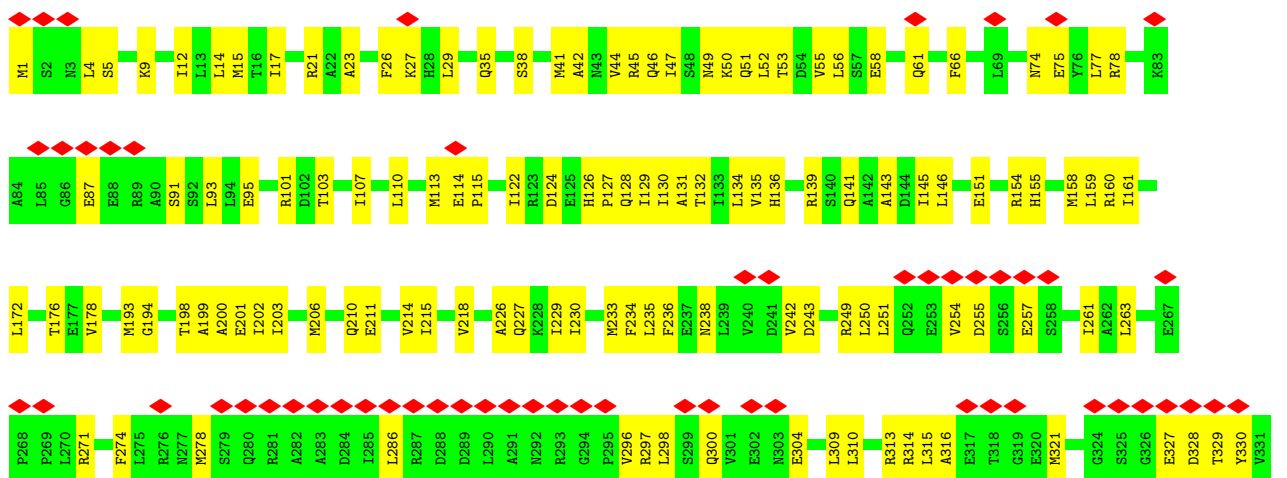




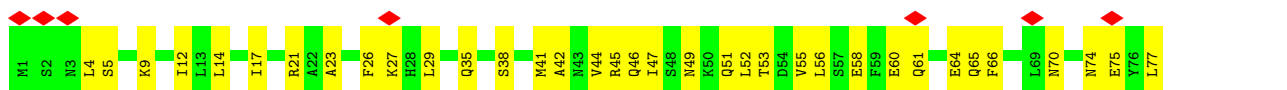
• Molecule 2: Flagellar motor switch protein FlIG

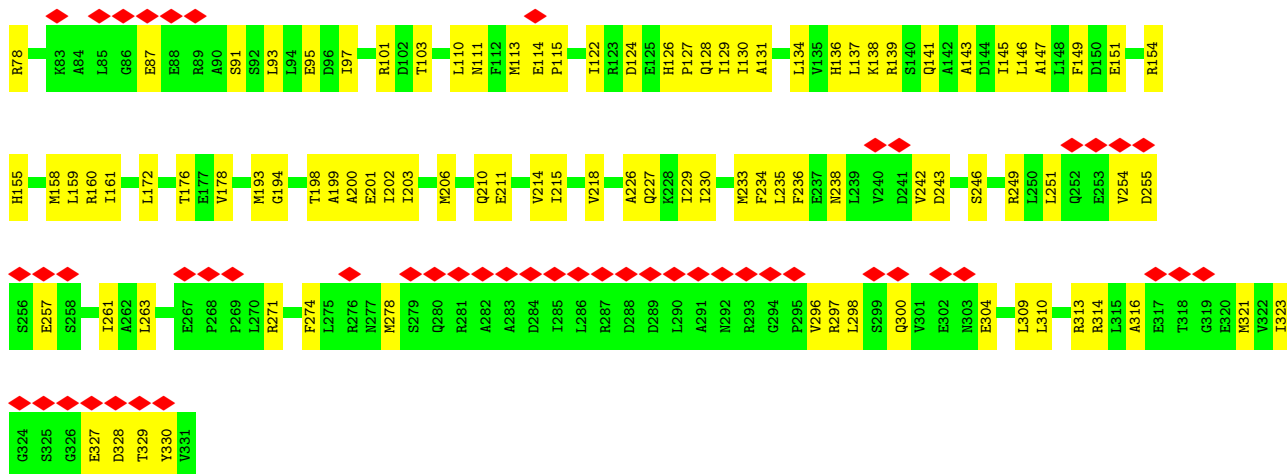


• Molecule 2: Flagellar motor switch protein FlIG

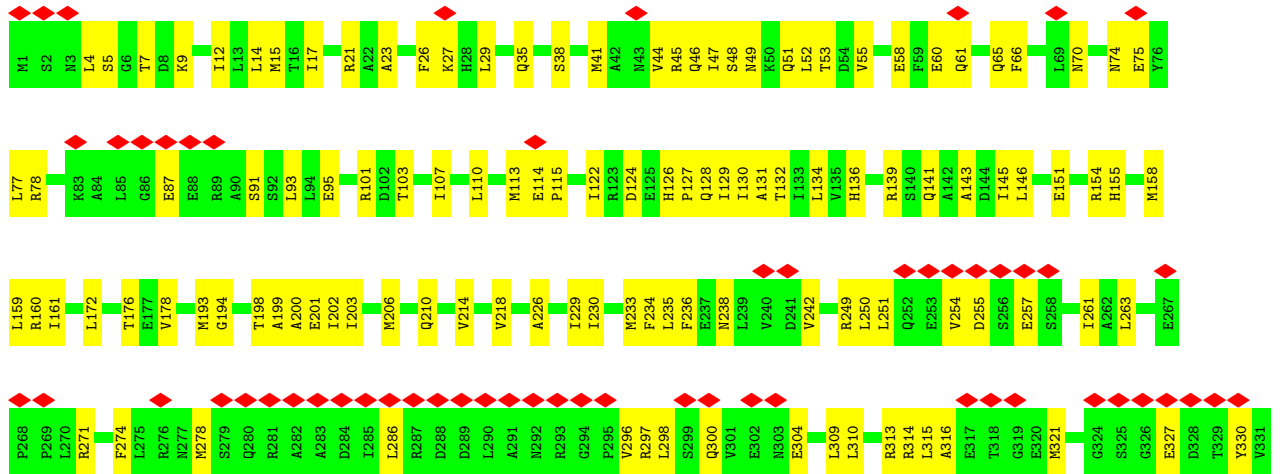


• Molecule 2: Flagellar motor switch protein FlIG

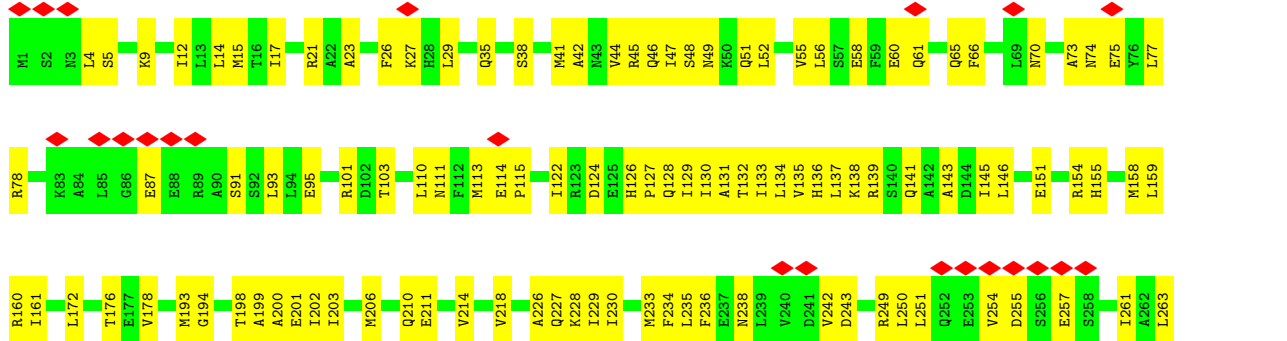


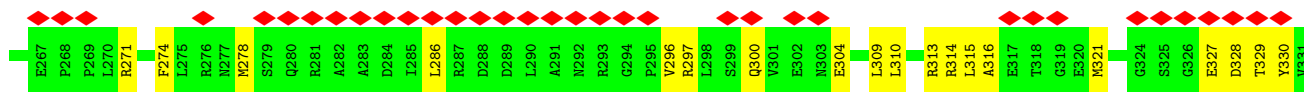


• Molecule 2: Flagellar motor switch protein FlIG

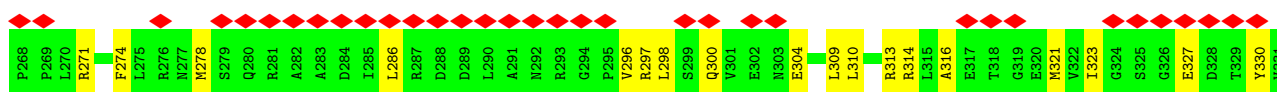
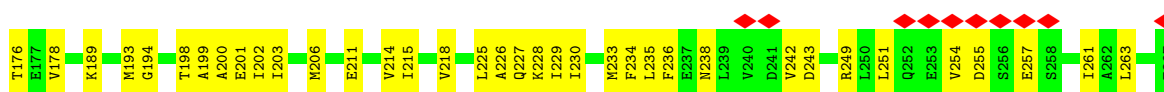


• Molecule 2: Flagellar motor switch protein FlIG

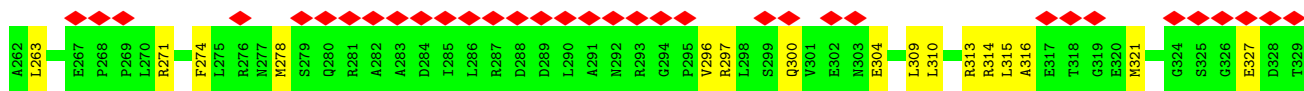
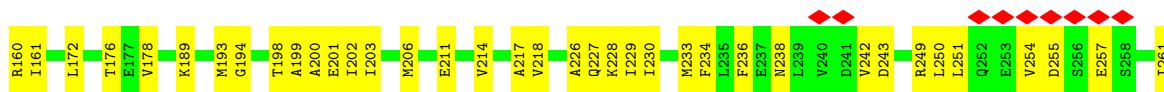
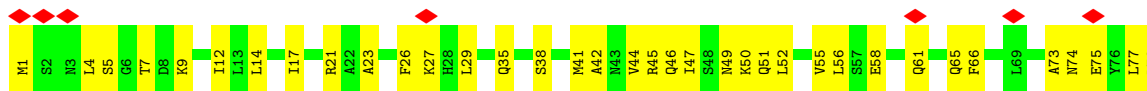




• Molecule 2: Flagellar motor switch protein FliG

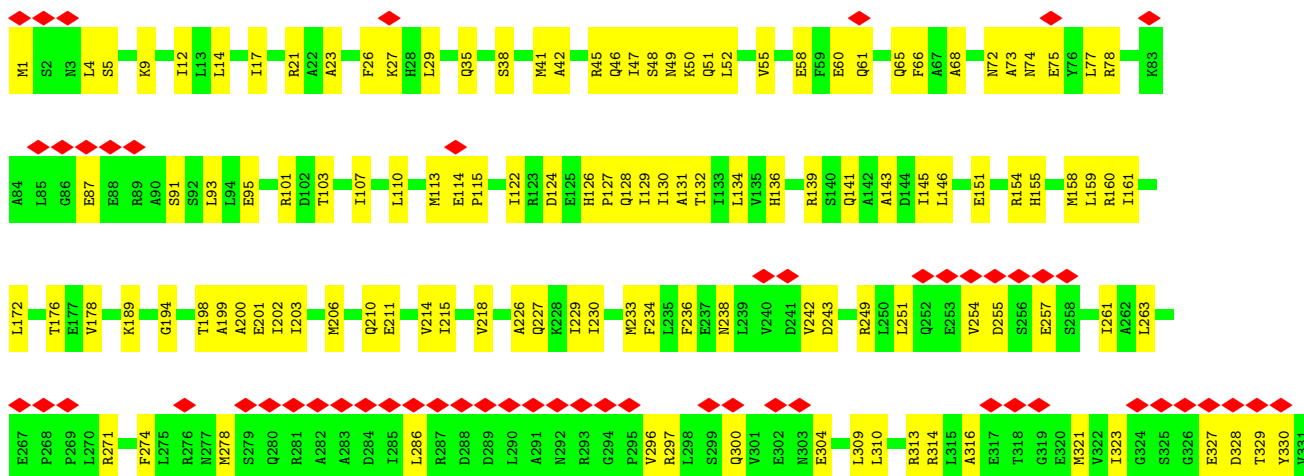


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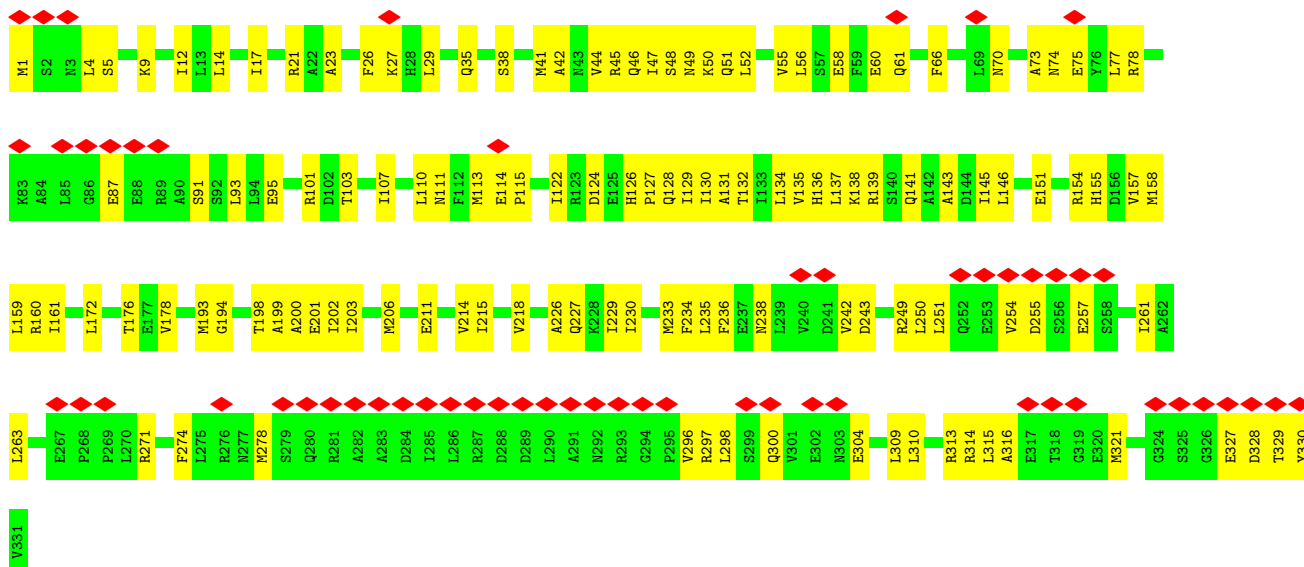


• Molecule 2: Flagellar motor switch protein FliG

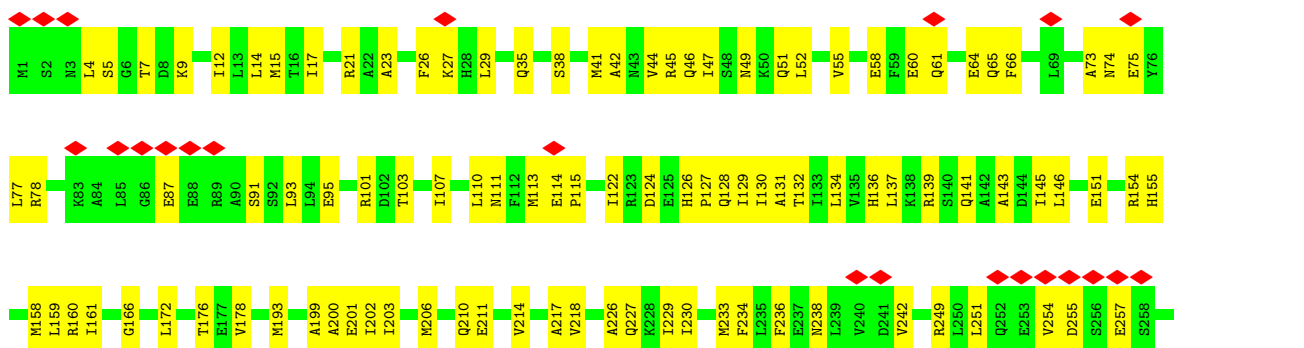




• Molecule 2: Flagellar motor switch protein Flig

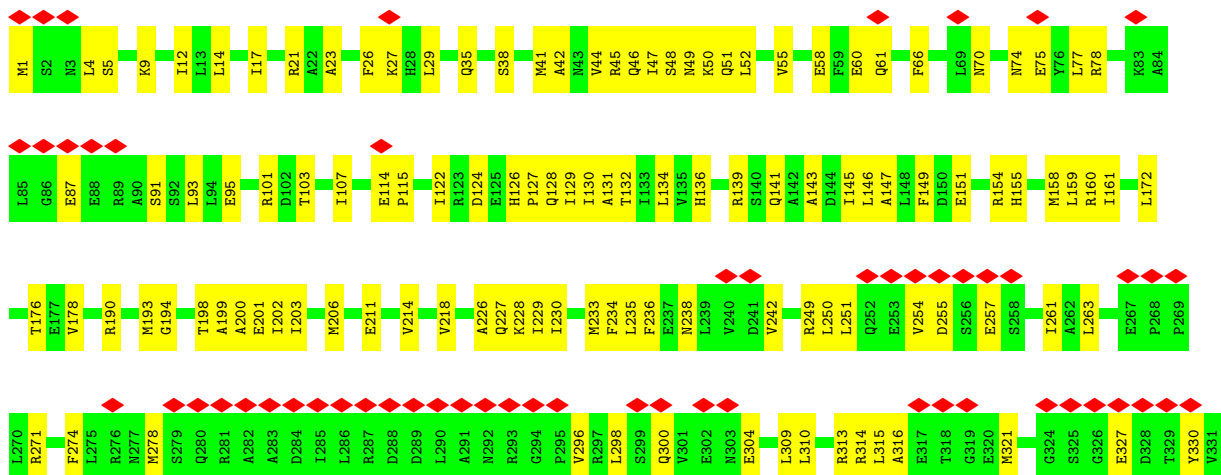


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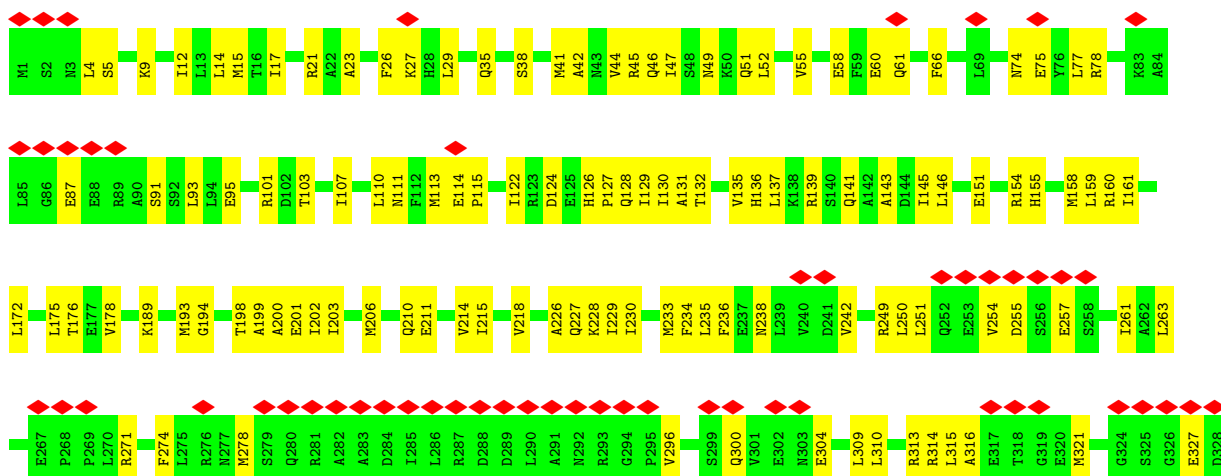




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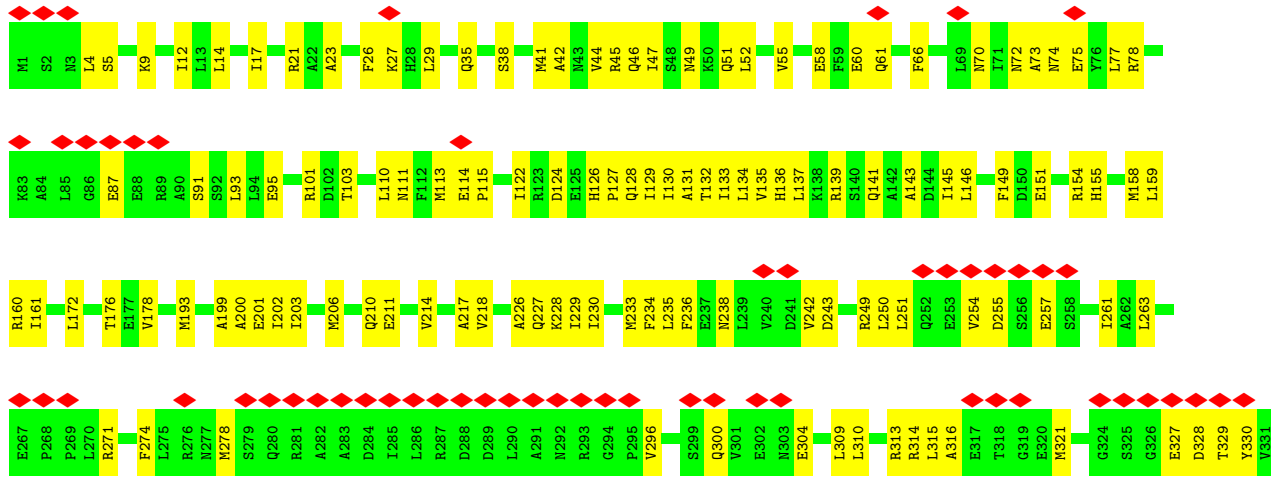


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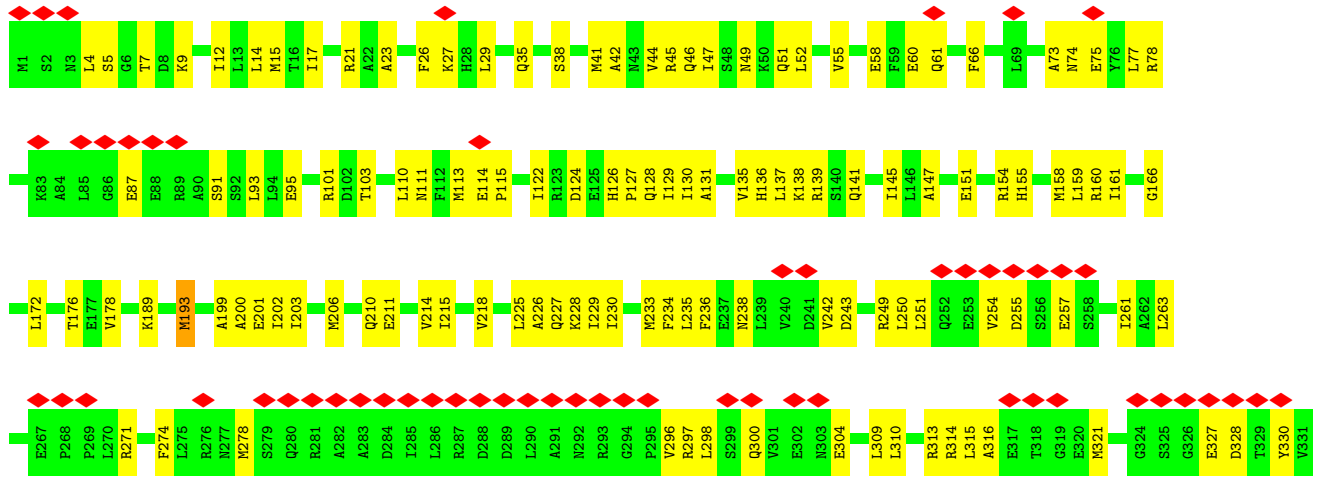


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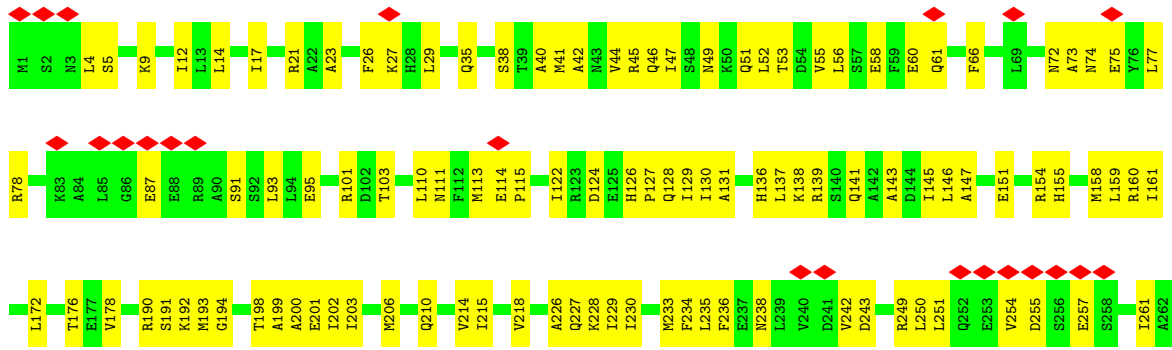


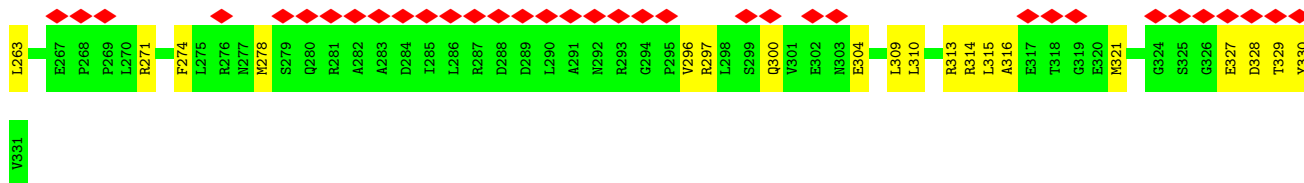


• Molecule 2: Flagellar motor switch protein FlIG

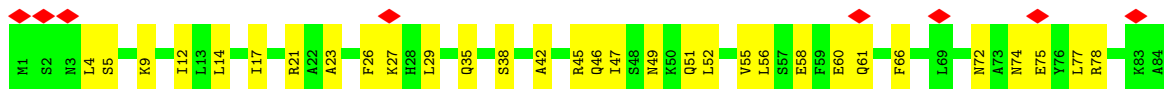


• Molecule 2: Flagellar motor switch protein FlIG

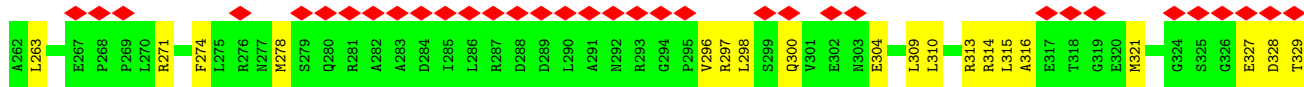
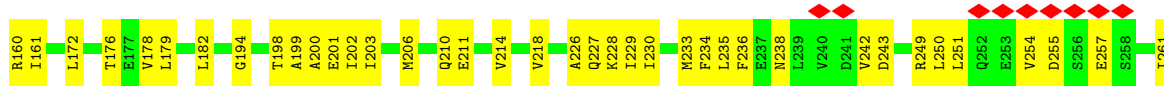




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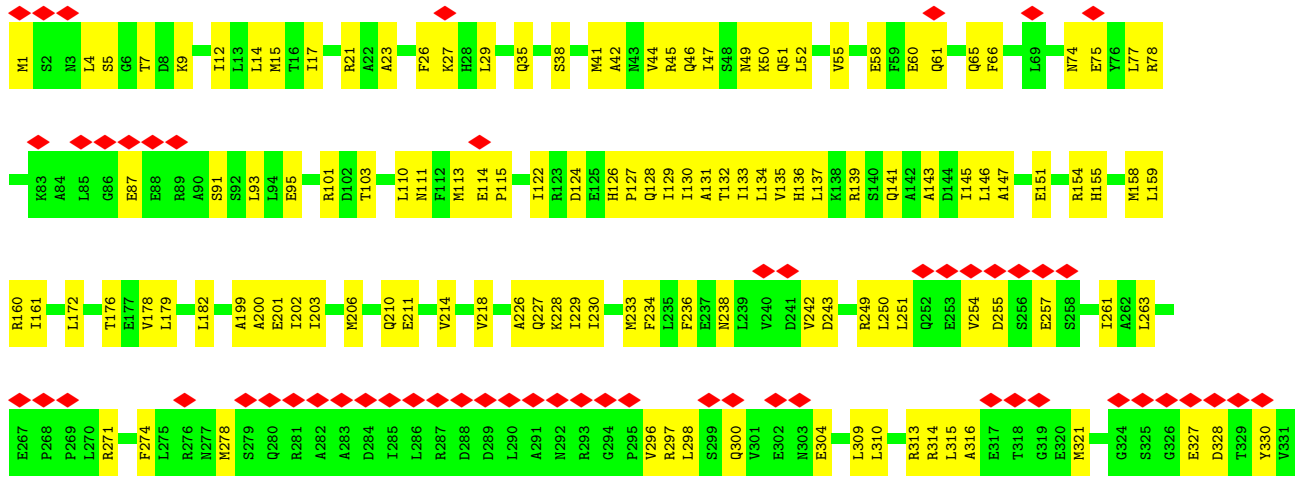


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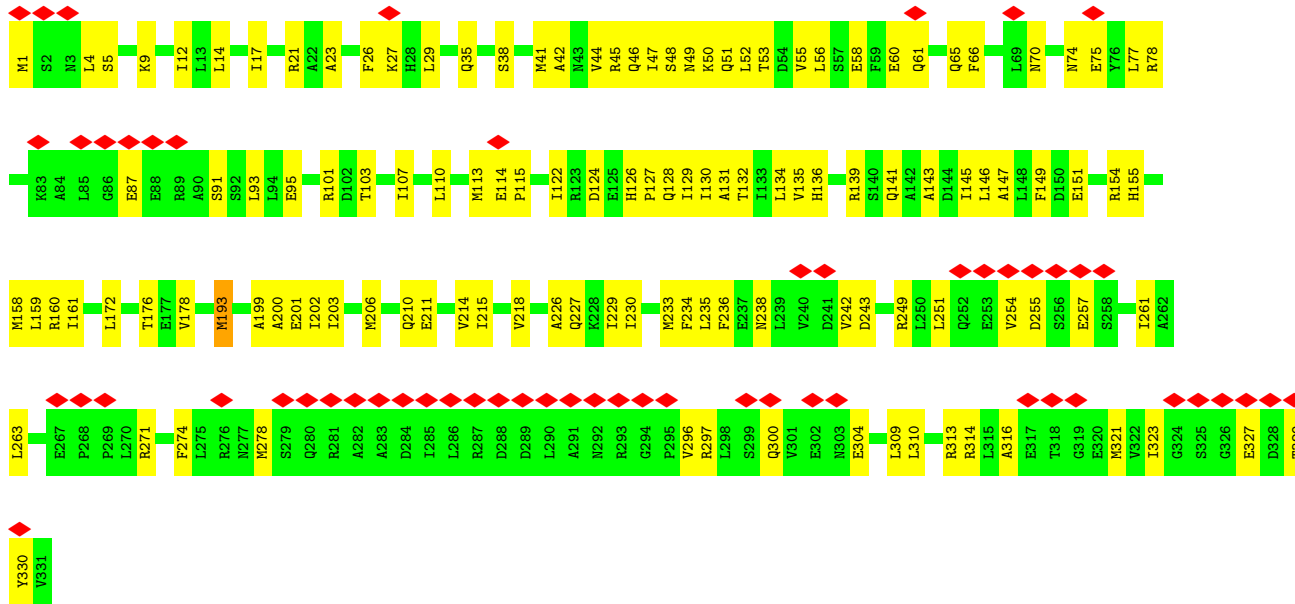


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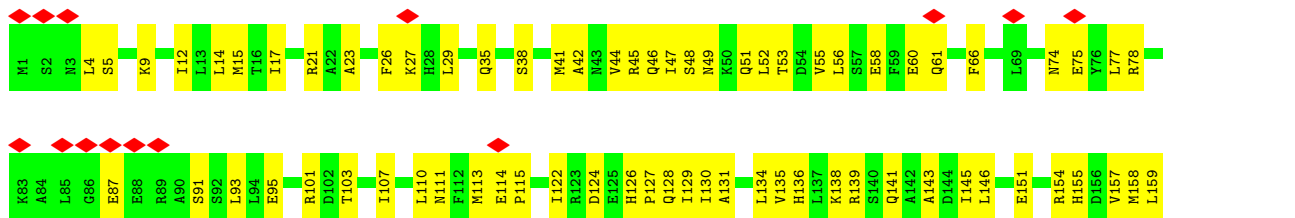


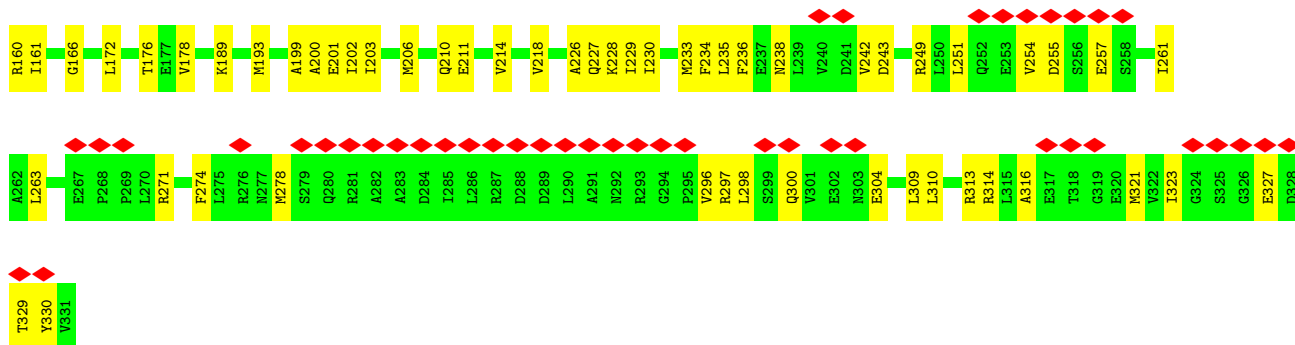


• Molecule 2: Flagellar motor switch protein FlhG

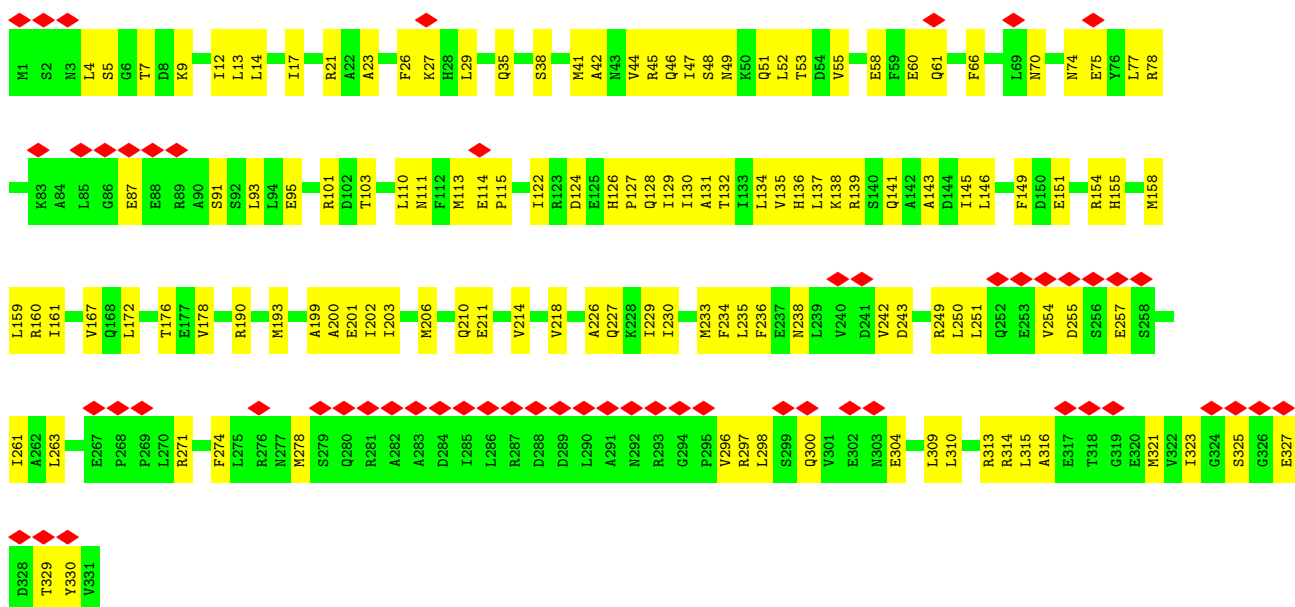


• Molecule 2: Flagellar motor switch protein FlhG

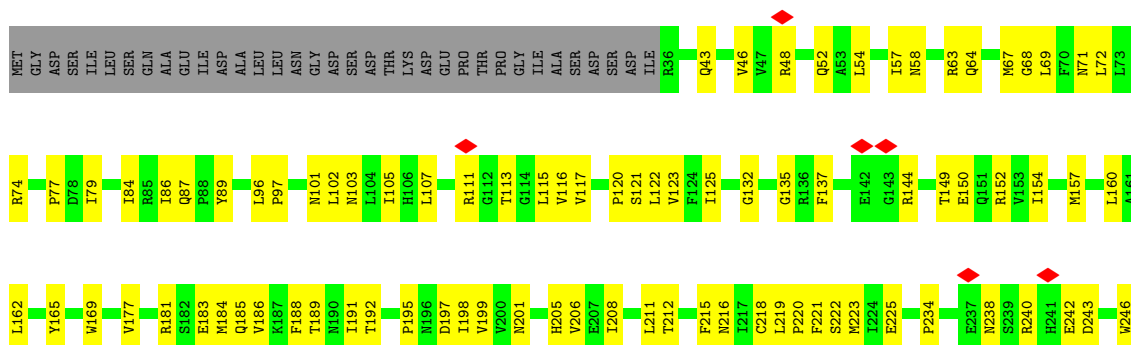


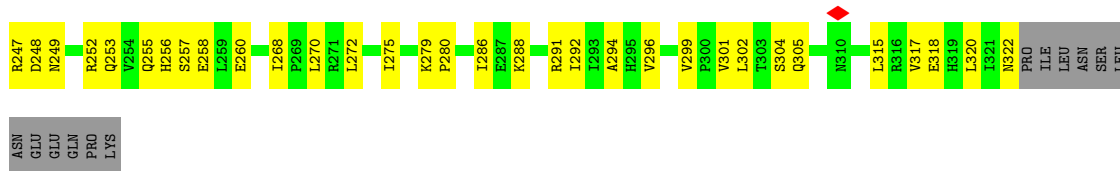


• Molecule 2: Flagellar motor switch protein FliG

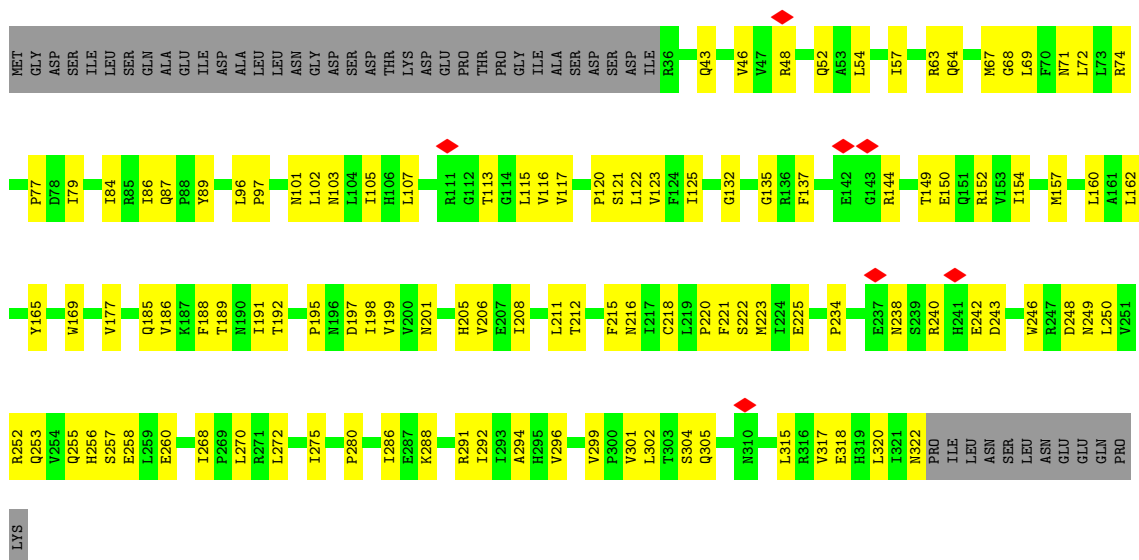


• Molecule 3: Flagellar motor switch protein FliM

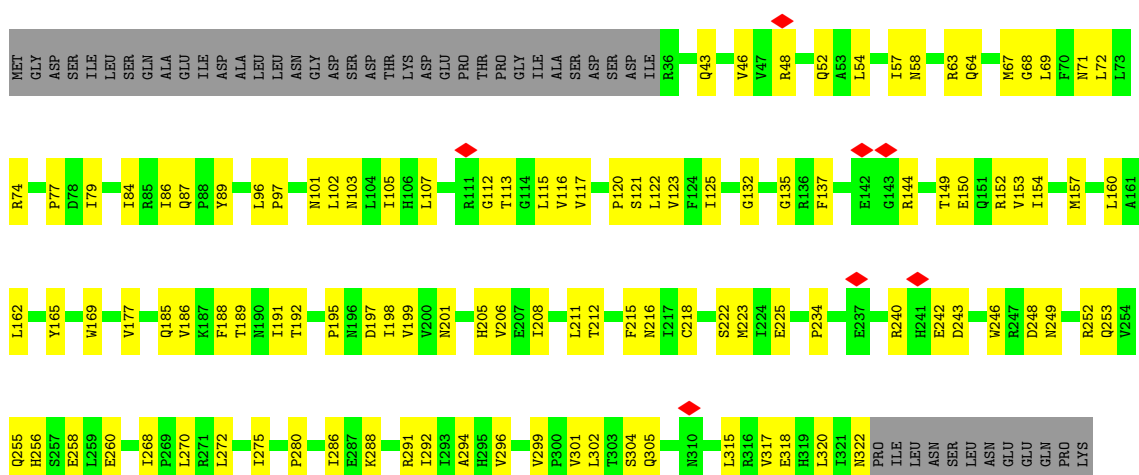




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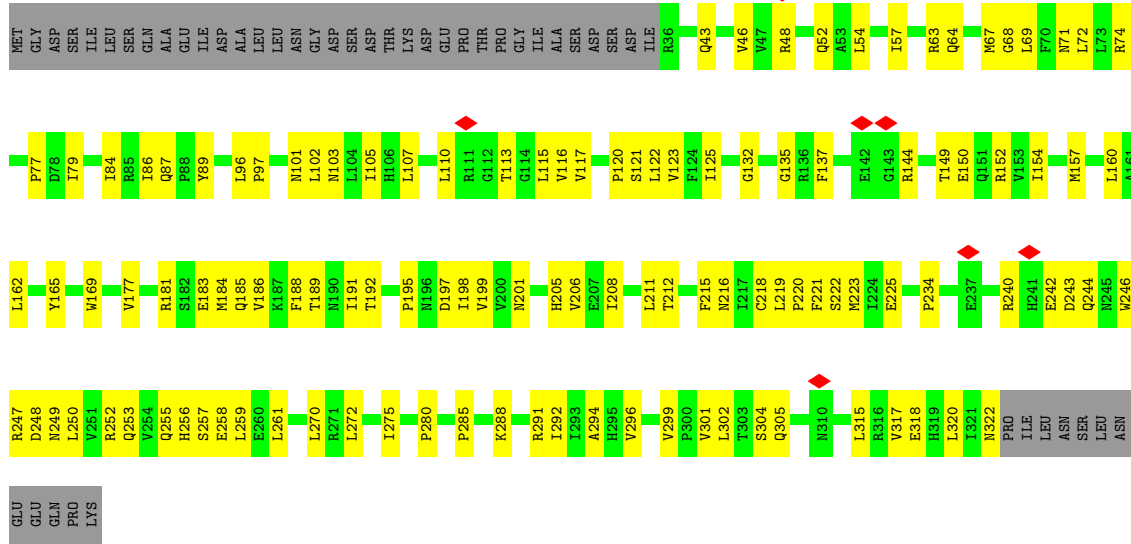


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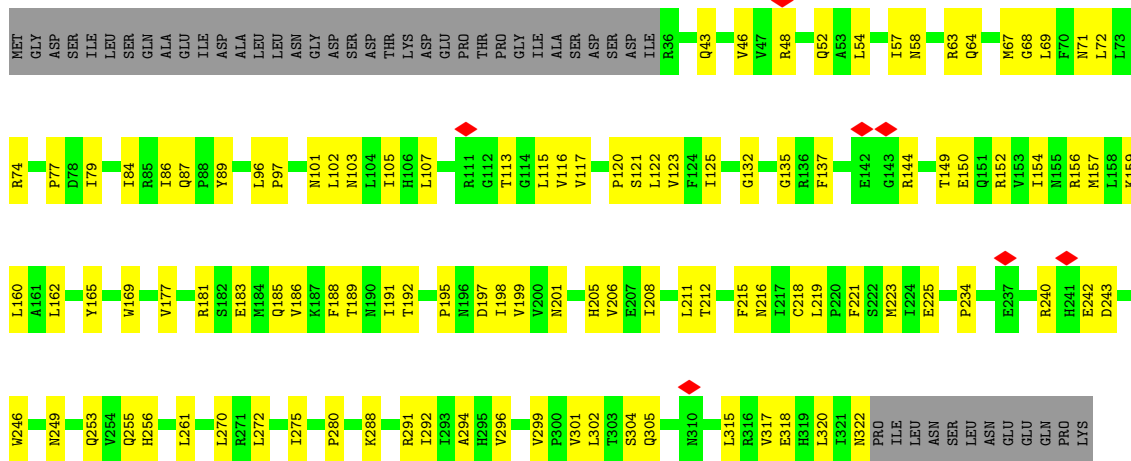


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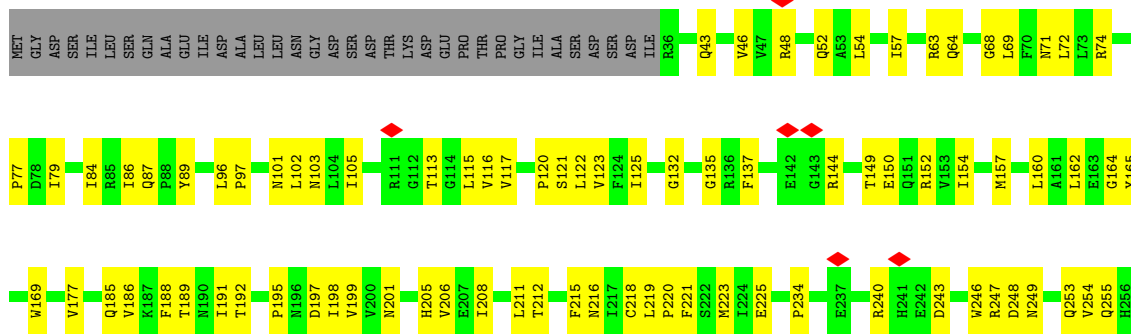


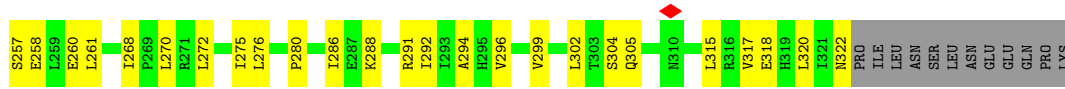


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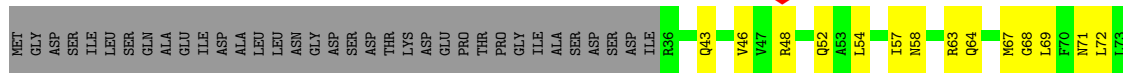


• Molecule 3: Flagellar motor switch protein FliM



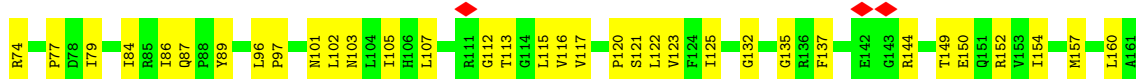
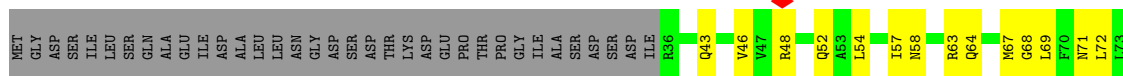


• Molecule 3: Flagellar motor switch protein FliM



GLN
PRO
LYS

• Molecule 3: Flagellar motor switch protein FliM



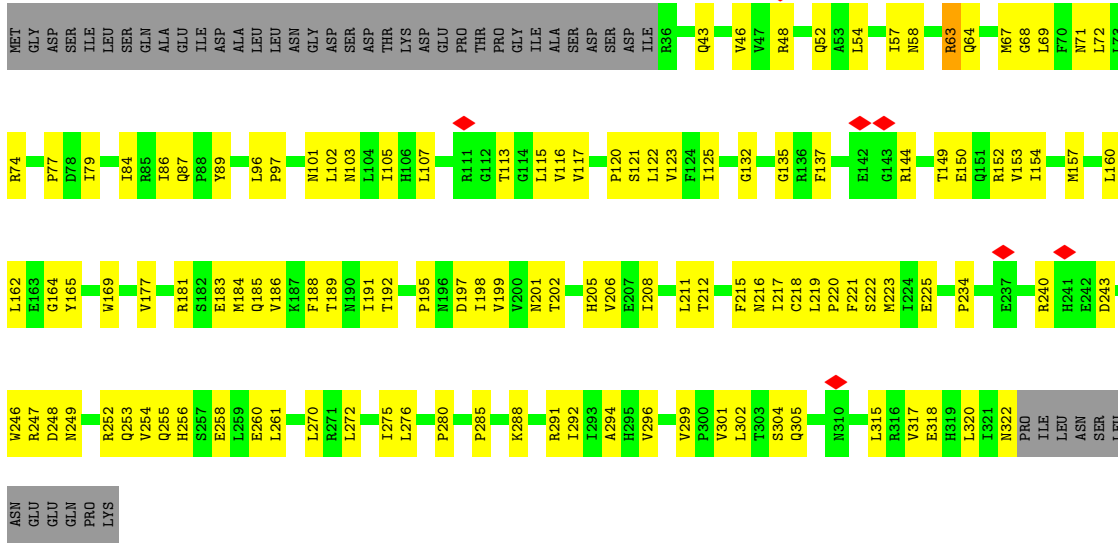
PRO
LYS

• Molecule 3: Flagellar motor switch protein FliM

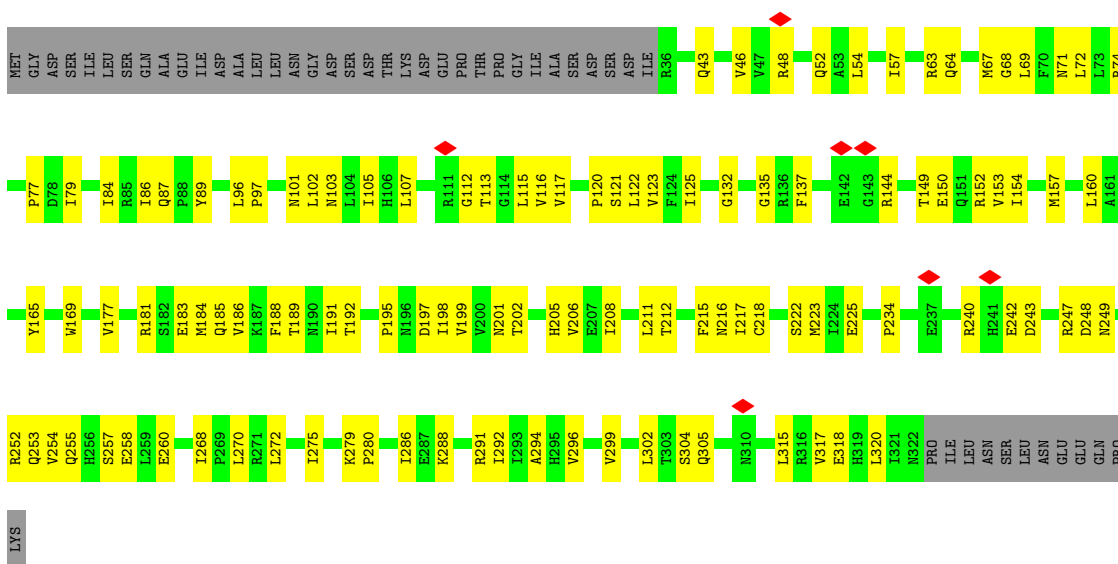




● Molecule 3: Flagellar motor switch protein FliM



● Molecule 3: Flagellar motor switch protein FliM

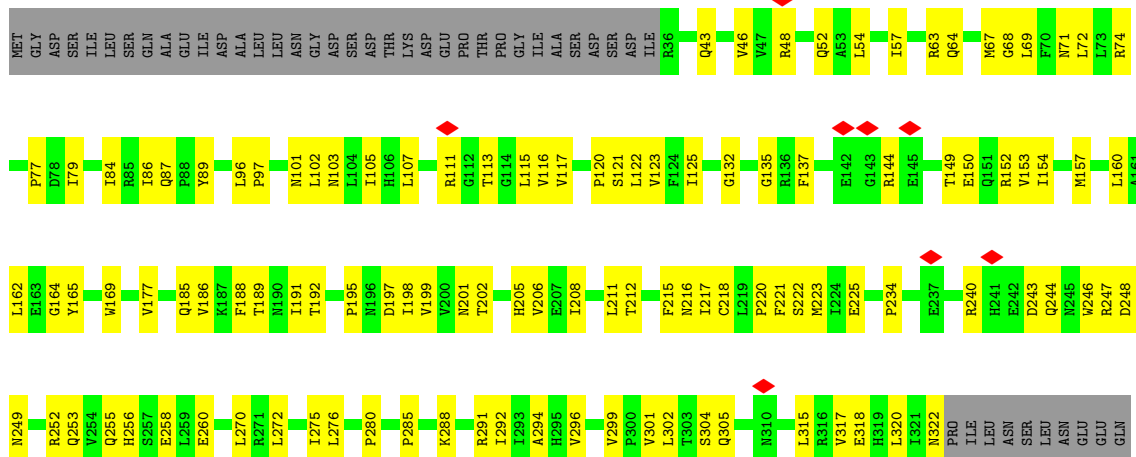


● Molecule 3: Flagellar motor switch protein FliM

GLU
GLN
PRO
LYS

• Molecule 3: Flagellar motor switch protein FliM

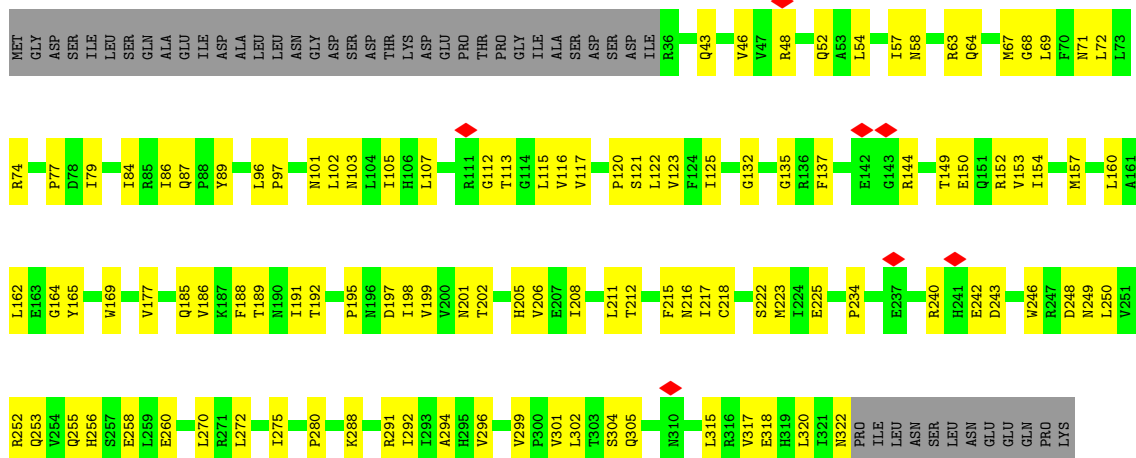
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PRO
LYS

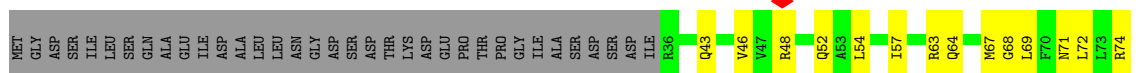
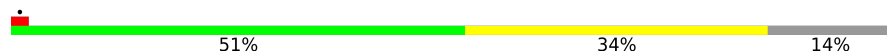
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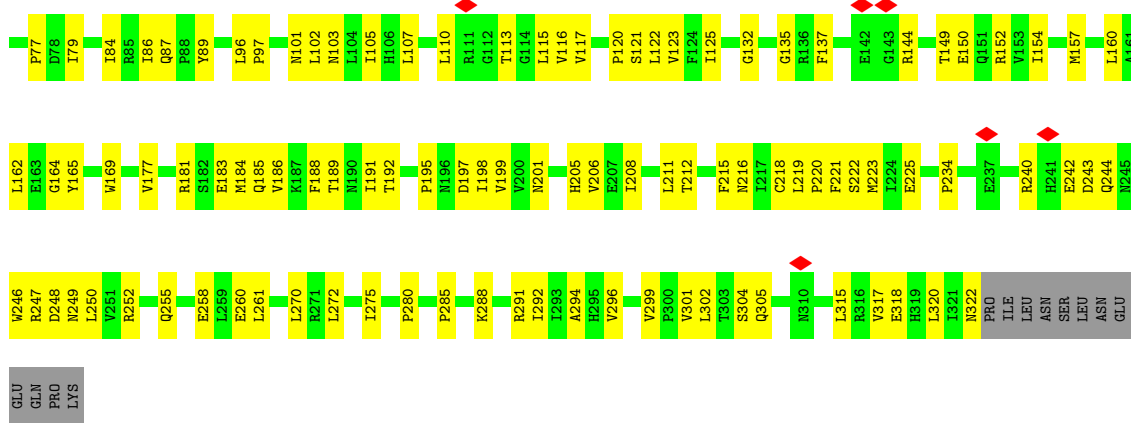
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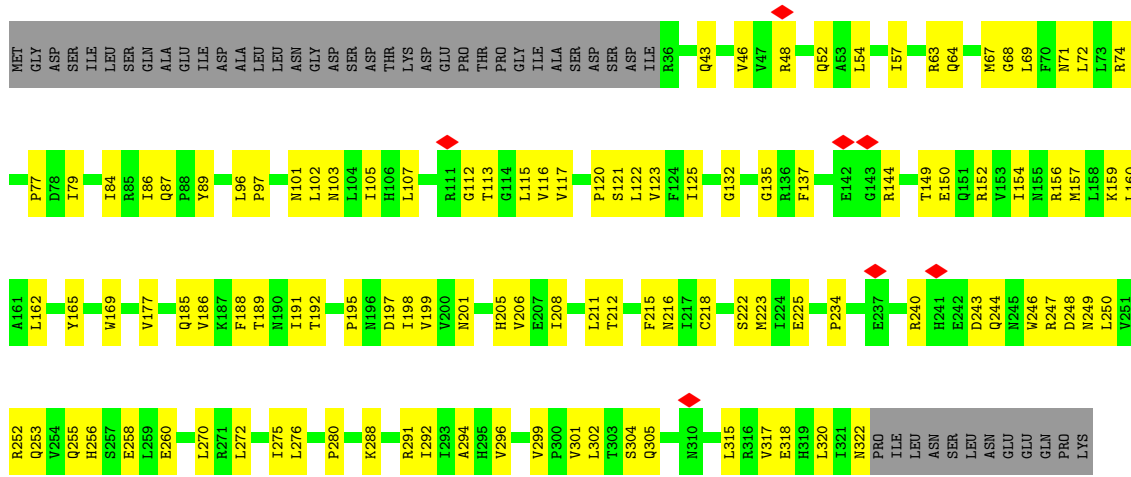
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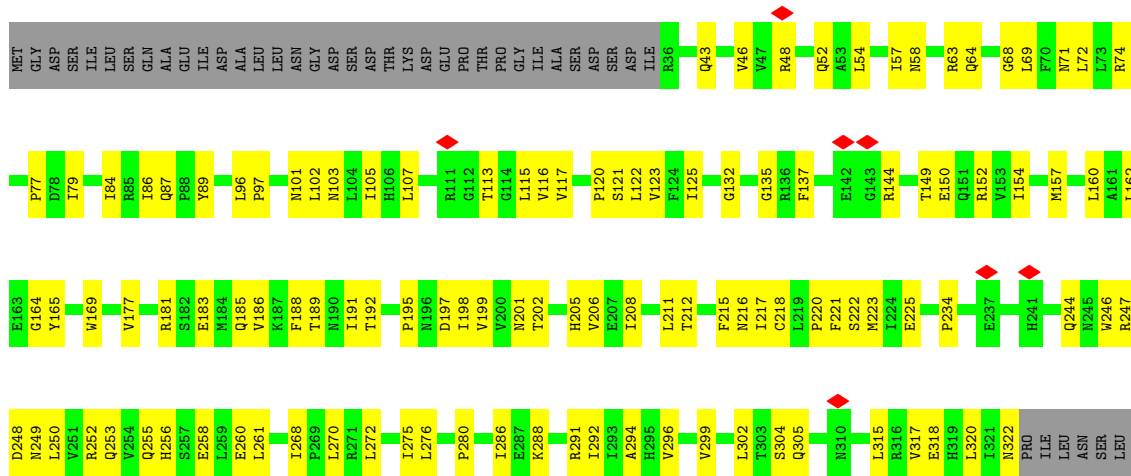




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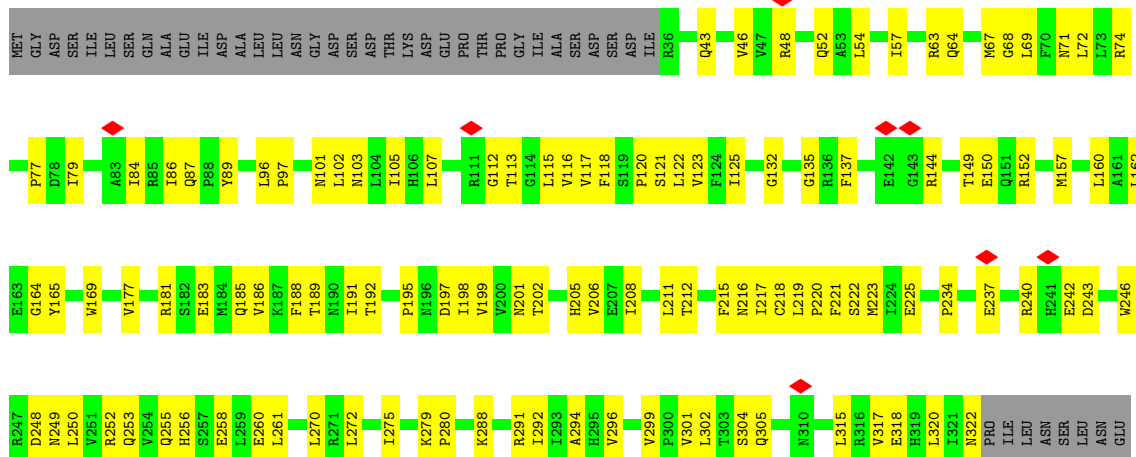
• Molecule 3: Flagellar motor switch protein FlIM



ASN
GLU
GLU
GLN
GLN
PRO
PRO
LYS

• Molecule 3: Flagellar motor switch protein FliM

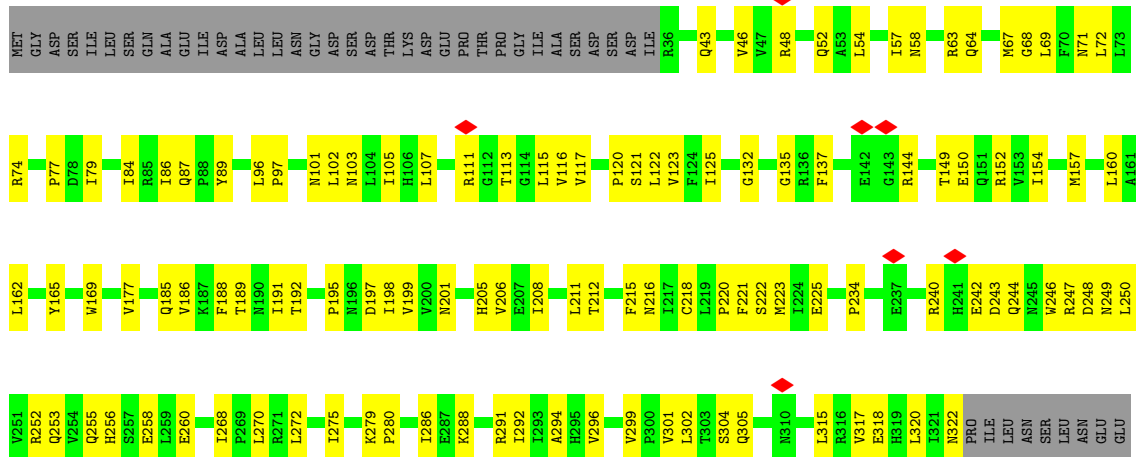
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GLU
GLN
PRO
LYS

• Molecule 3: Flagellar motor switch protein FliM

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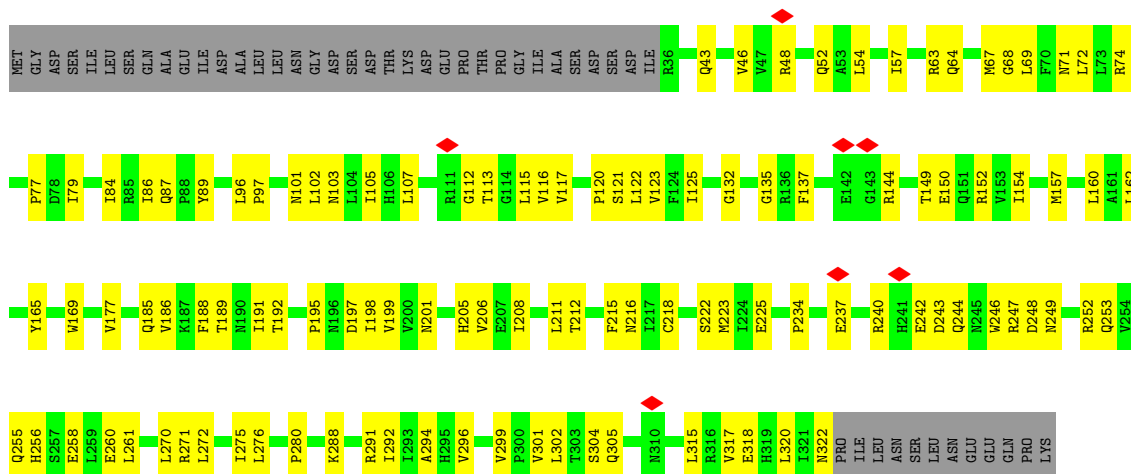


GLN
PRO
LYS

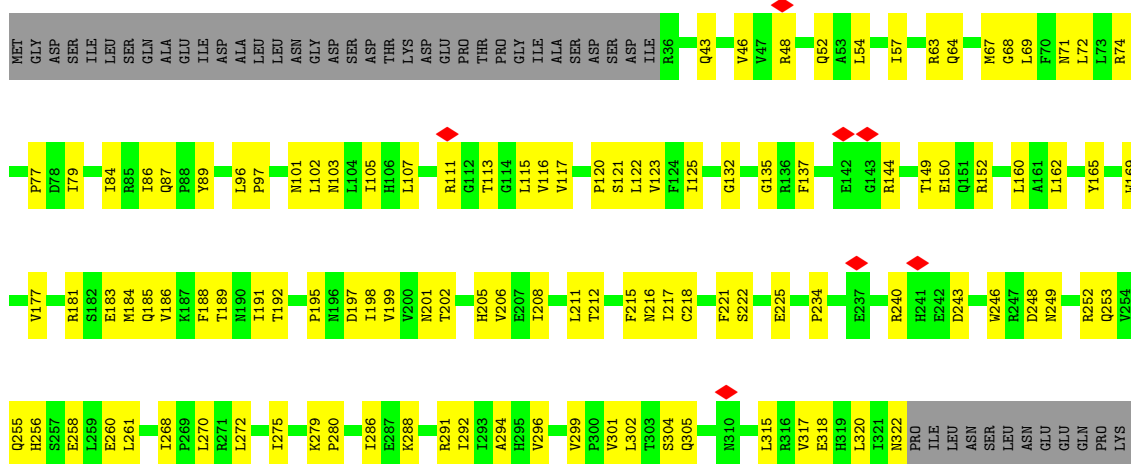
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Chain CQ:



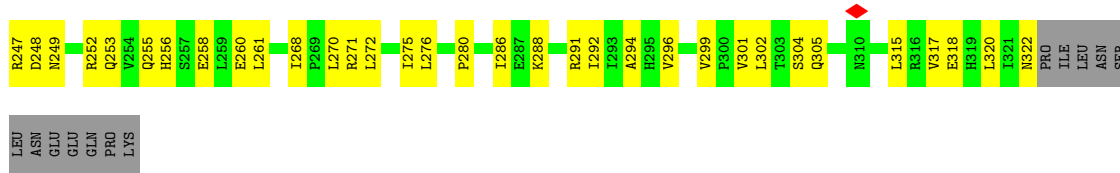


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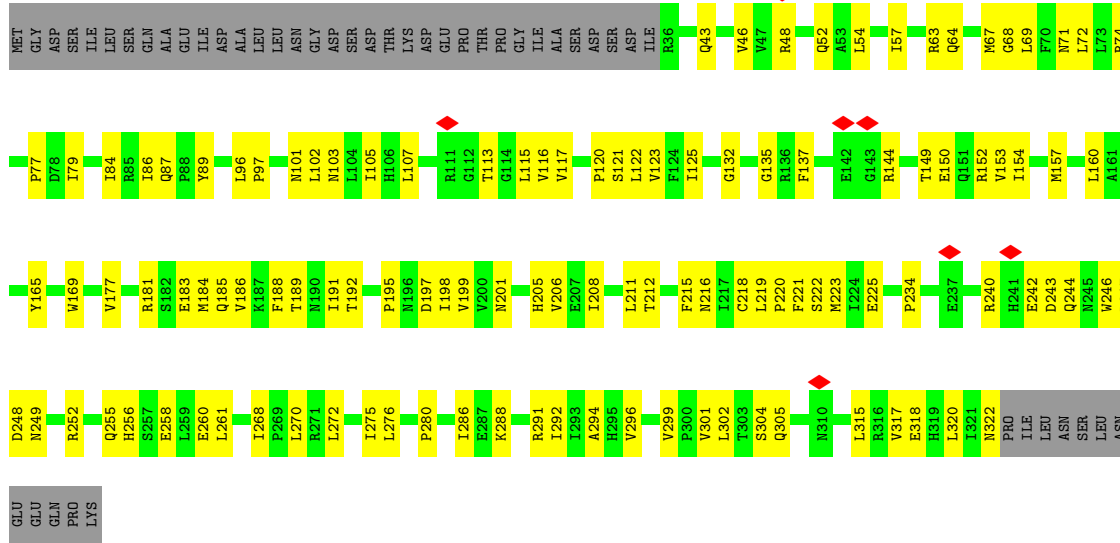


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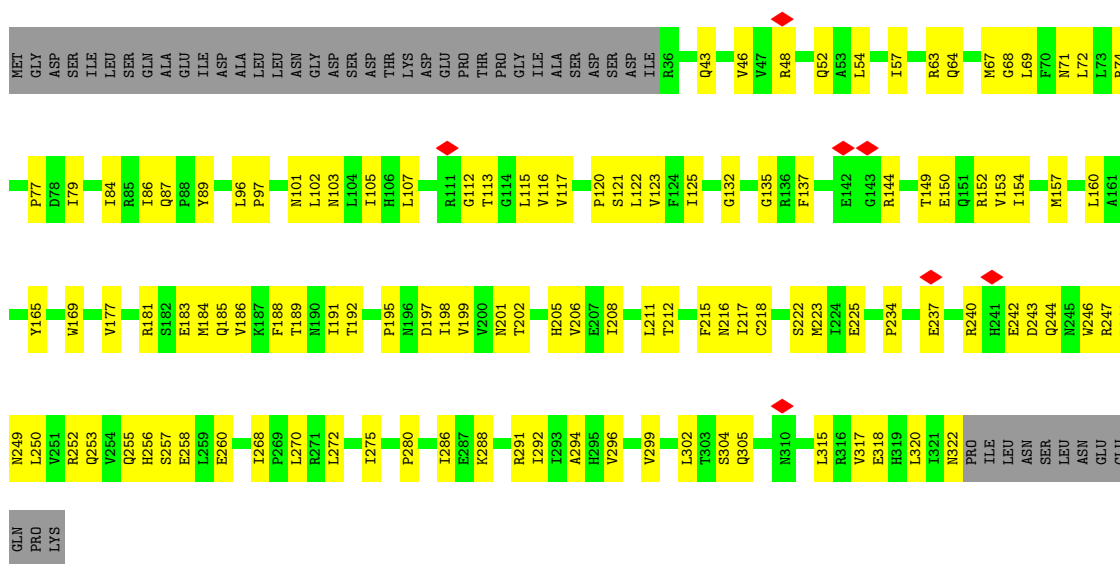




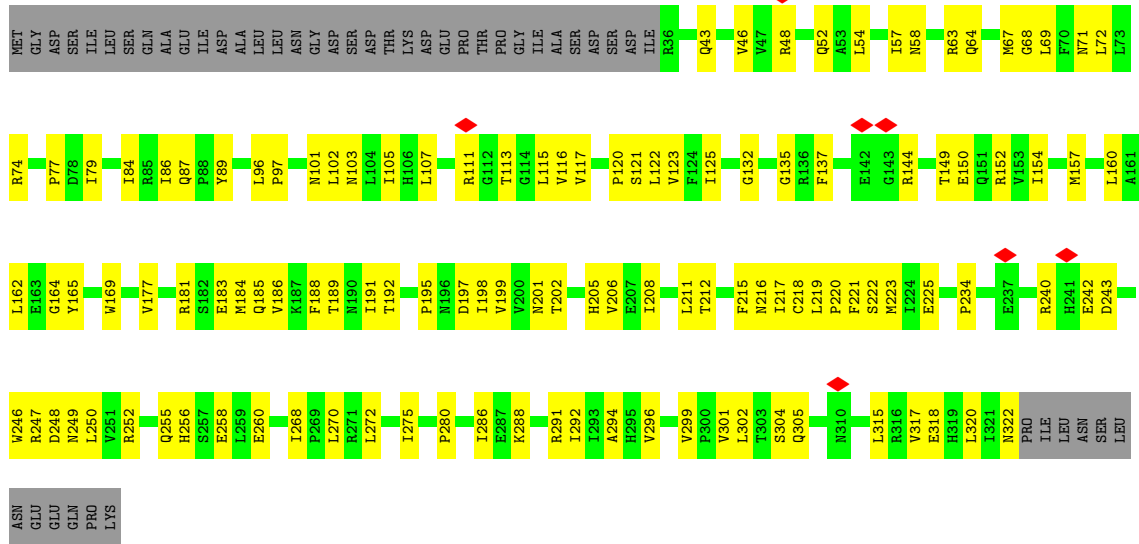
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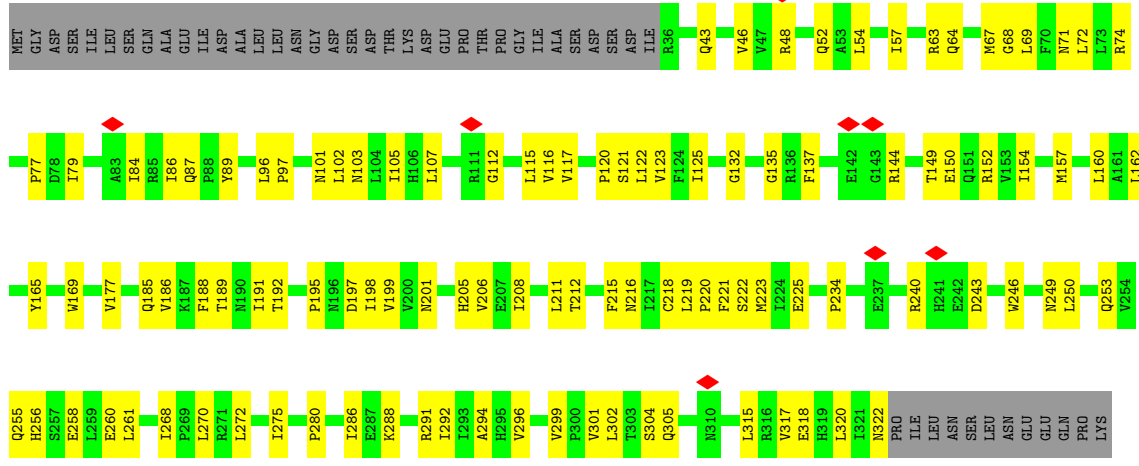
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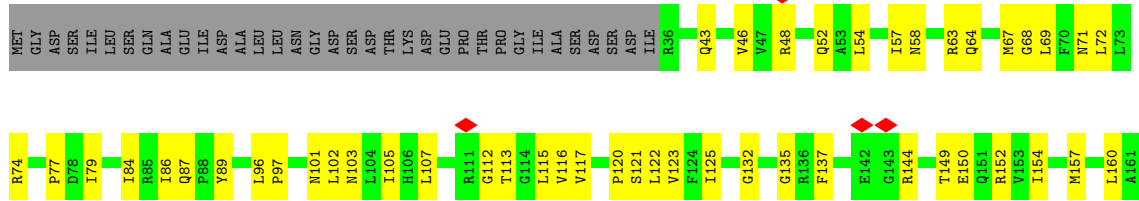
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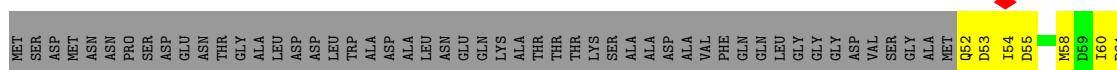
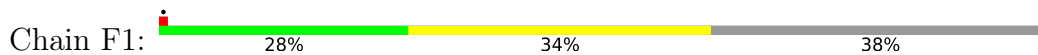


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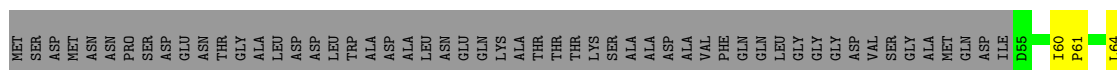
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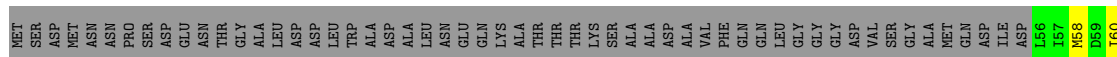
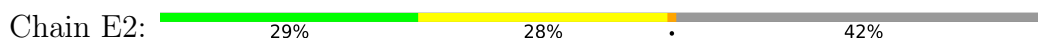


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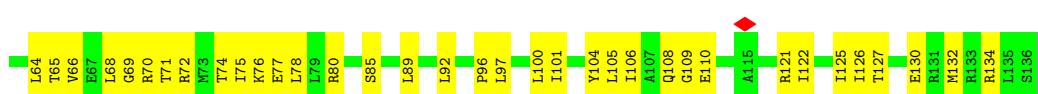
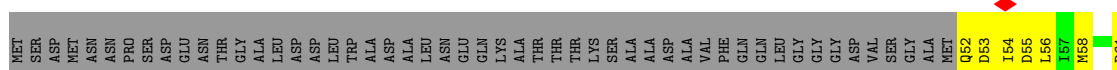
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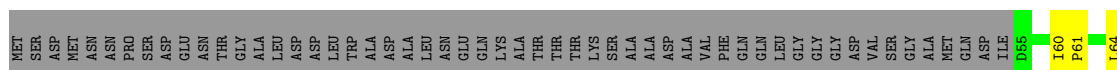
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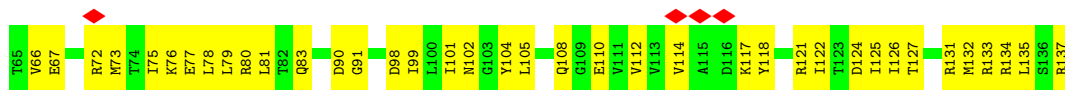


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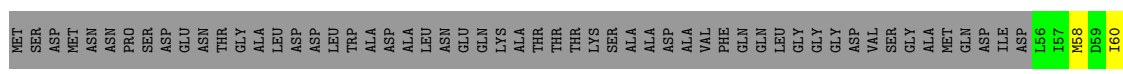
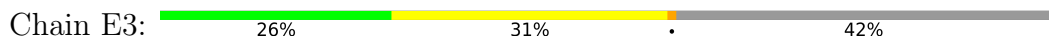


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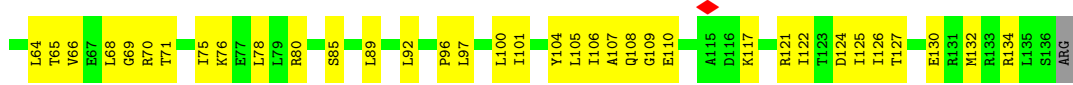
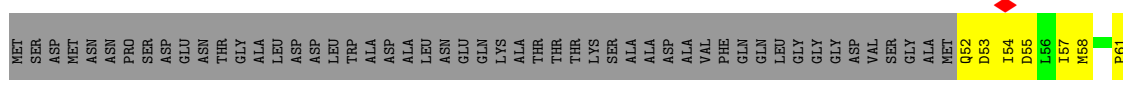




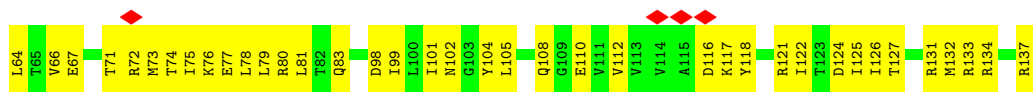
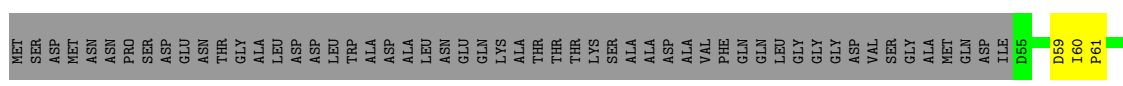
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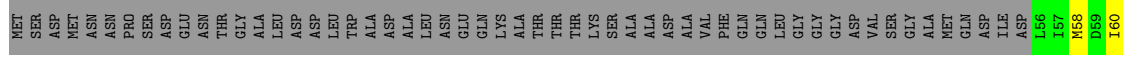
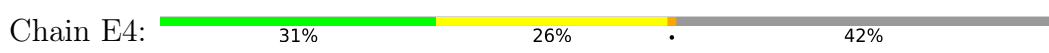
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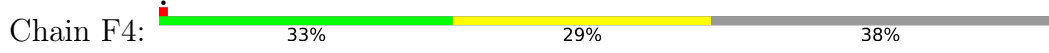
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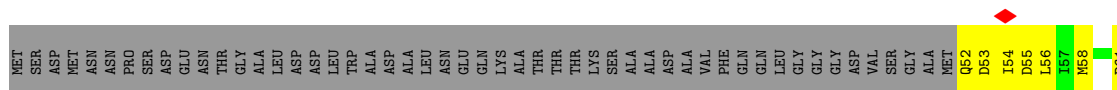


• Molecule 4: Flagellar motor switch protein FliN

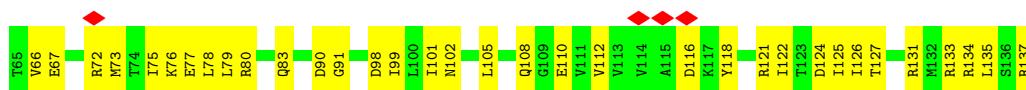
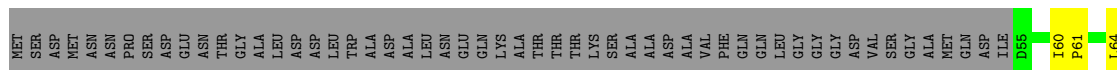
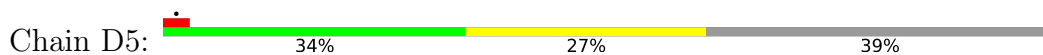


• Molecule 4: Flagellar motor switch protein FliN

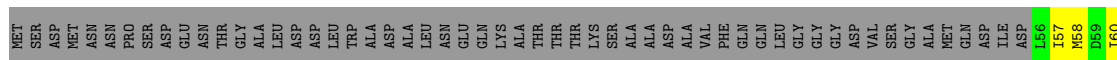
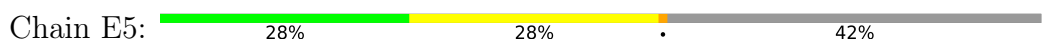




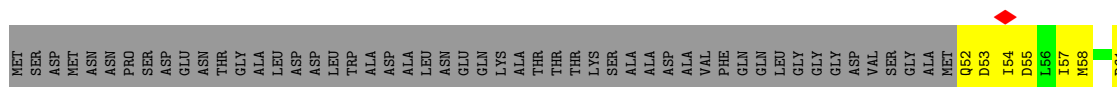
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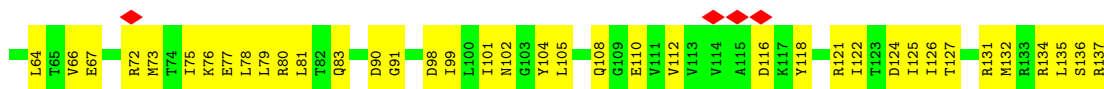
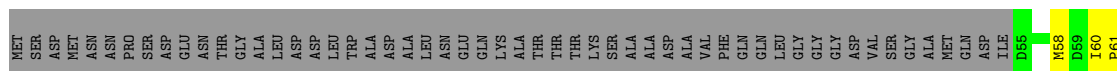
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

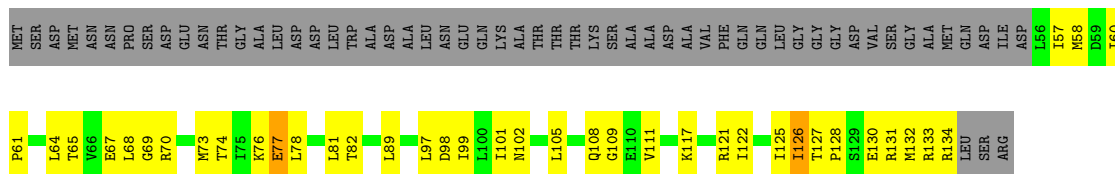


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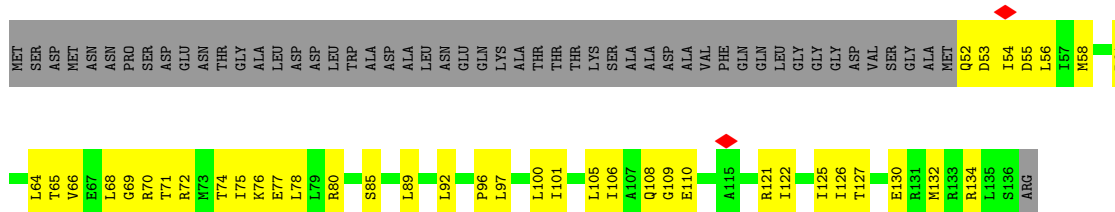
• Molecule 4: Flagellar motor switch protein FliN

Chain E6: 29% 27% 42%



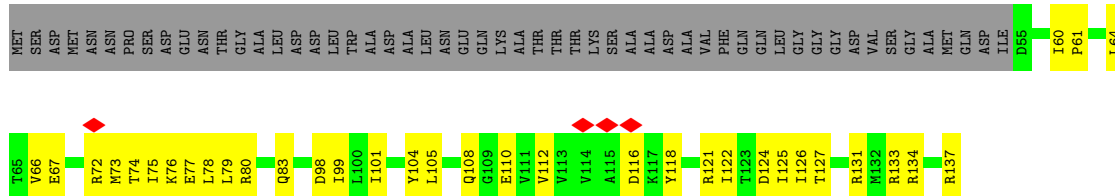
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Chain F6: 32% 30% 38%



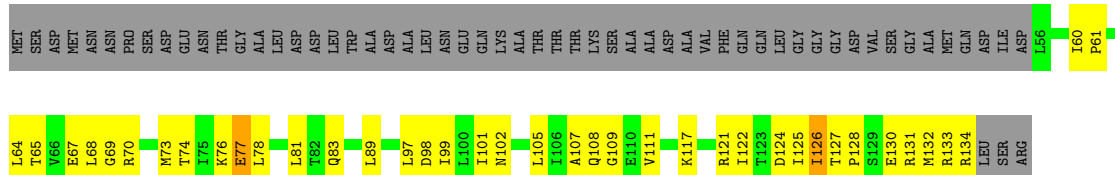
• Molecule 4: Flagellar motor switch protein FliN

Chain D7: 35% 26% 39%



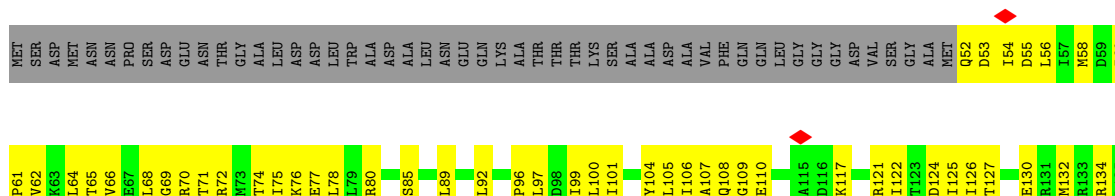
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Chain E7: 29% 27% 42%



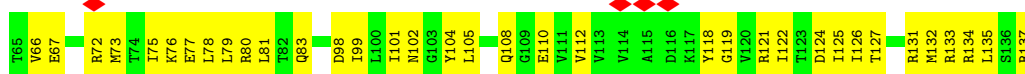
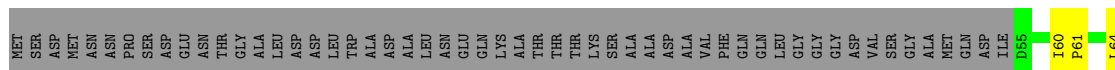
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Chain F7: 27% 35% 38%

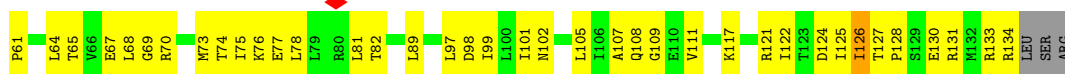
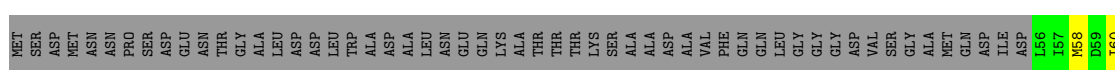
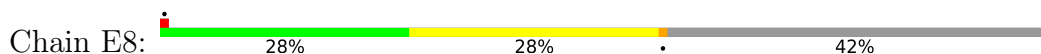


S136
ARG

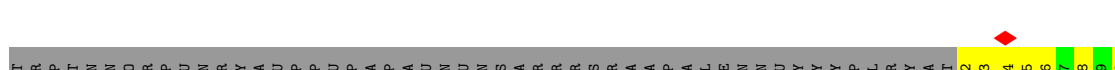
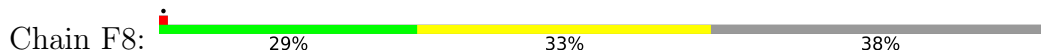
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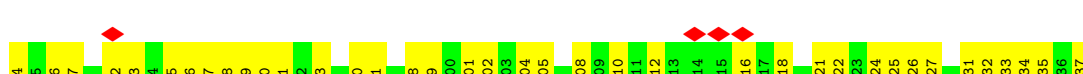
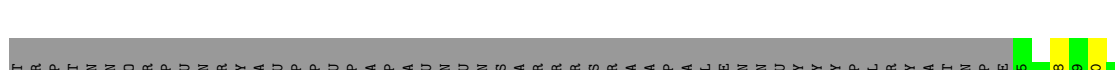
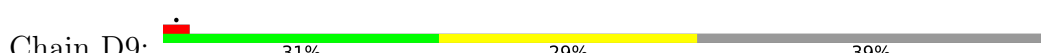
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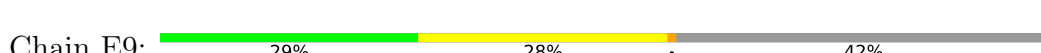
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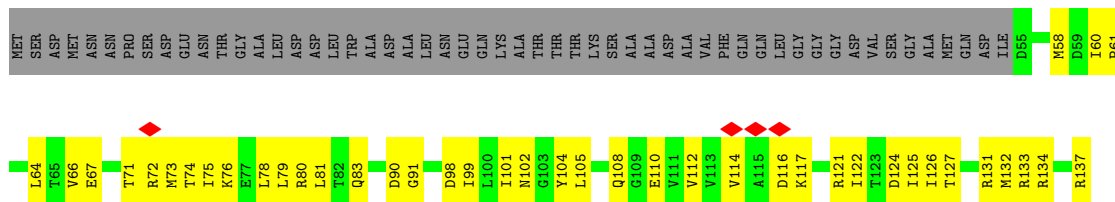
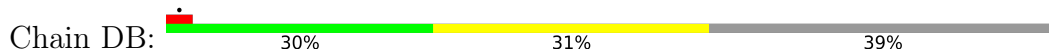


• Molecule 4: Flagellar motor switch protein FliN

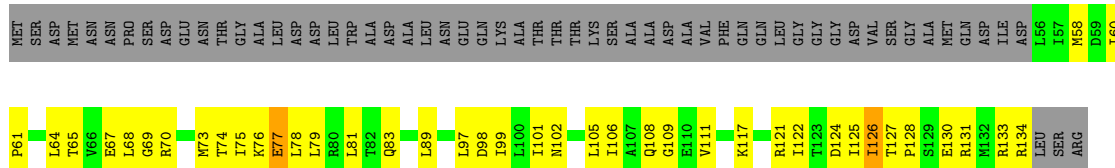
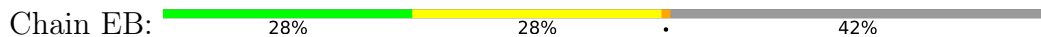


• Molecule 4: Flagellar motor switch protein FliN

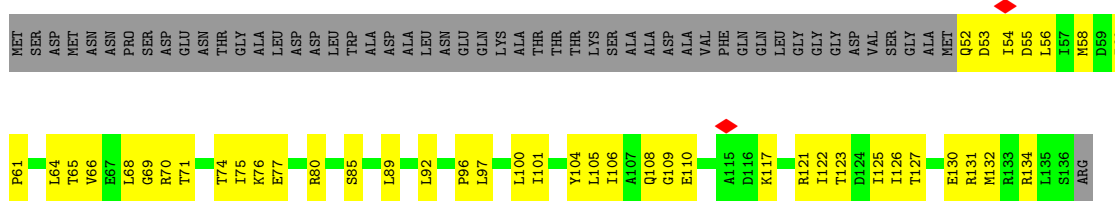




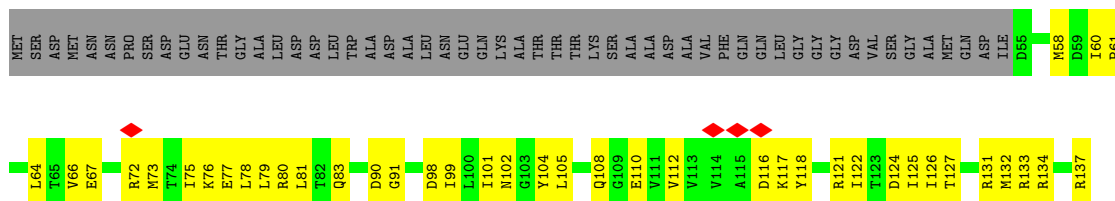
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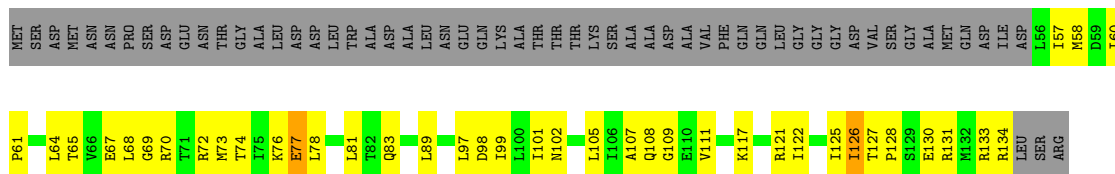
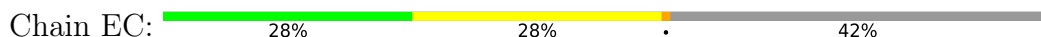
- Molecule 4: Flagellar motor switch protein FliN



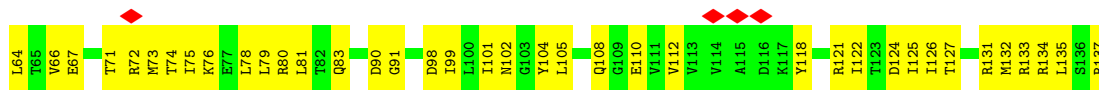
- Molecule 4: Flagellar motor switch protein FliN



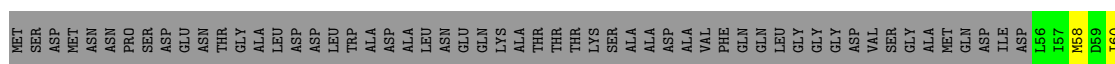
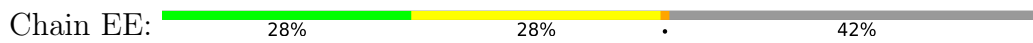
- Molecule 4: Flagellar motor switch protein FliN



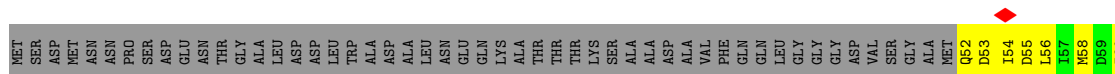
- Molecule 4: Flagellar motor switch protein FliN



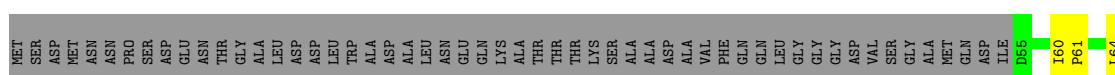
• Molecule 4: Flagellar motor switch protein FliN



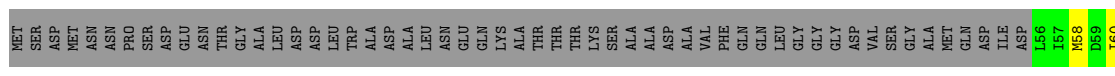
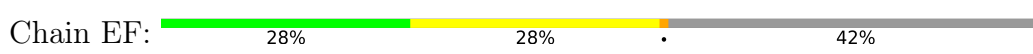
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

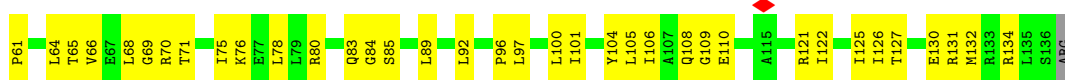
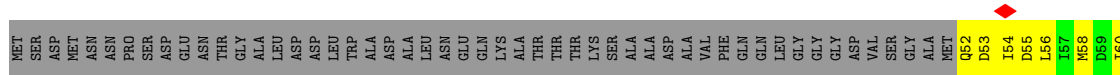


• Molecule 4: Flagellar motor switch protein FliN

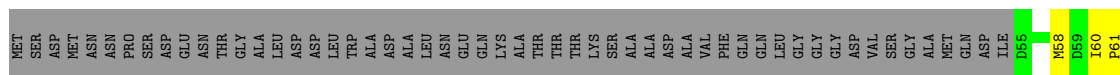


• Molecule 4: Flagellar motor switch protein FliN

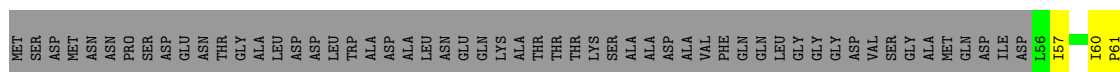
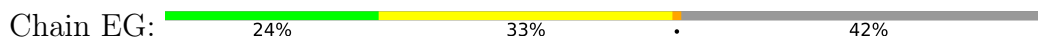




• Molecule 4: Flagellar motor switch protein FliN

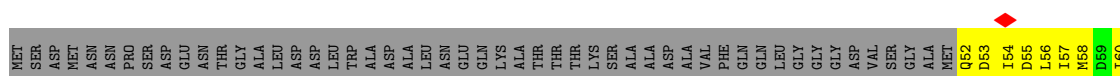


• Molecule 4: Flagellar motor switch protein FliN



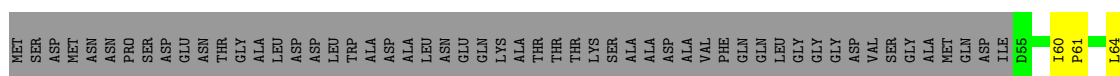
ARG

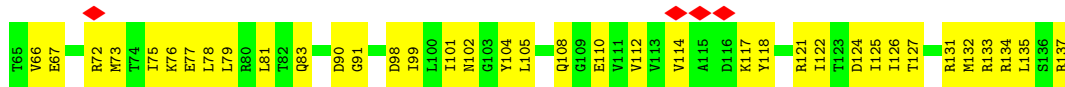
• Molecule 4: Flagellar motor switch protein FliN



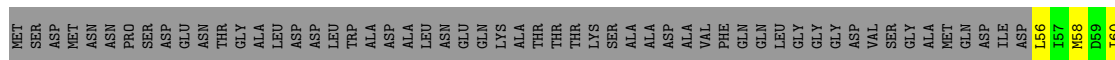
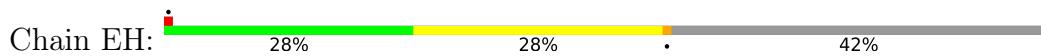
S136 ARG

• Molecule 4: Flagellar motor switch protein FliN

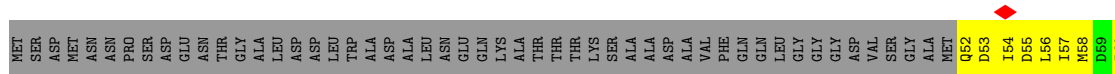




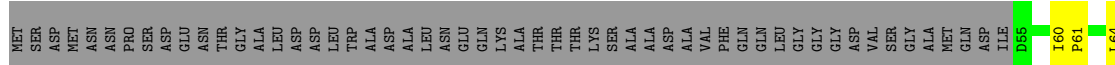
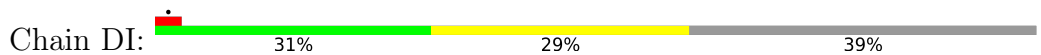
• Molecule 4: Flagellar motor switch protein FliN



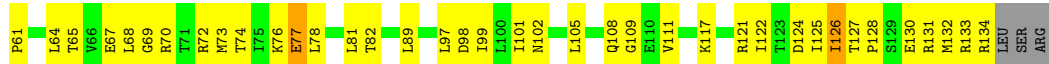
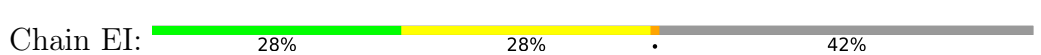
• Molecule 4: Flagellar motor switch protein FliN



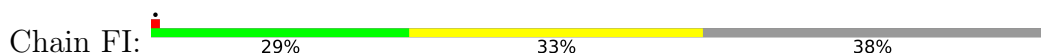
• Molecule 4: Flagellar motor switch protein FliN

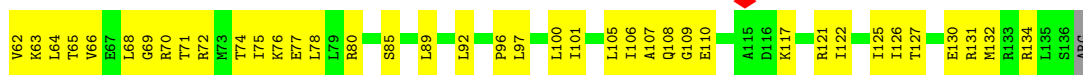
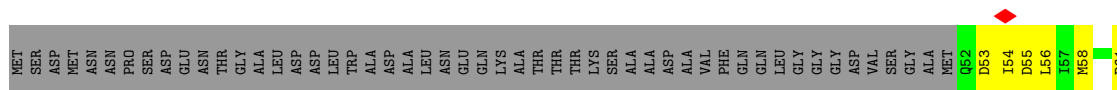


• Molecule 4: Flagellar motor switch protein FliN

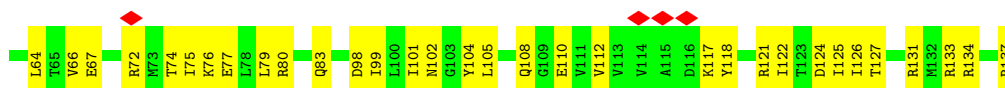
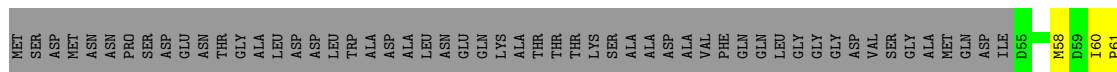


• Molecule 4: Flagellar motor switch protein FliN

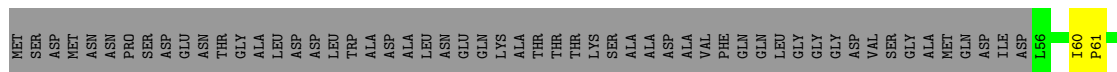
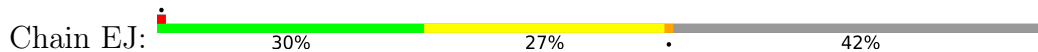




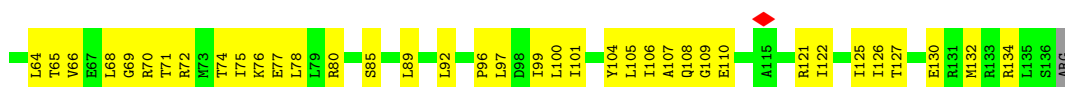
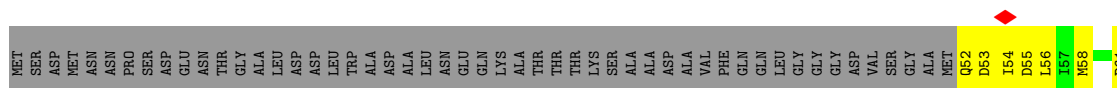
• Molecule 4: Flagellar motor switch protein FliN



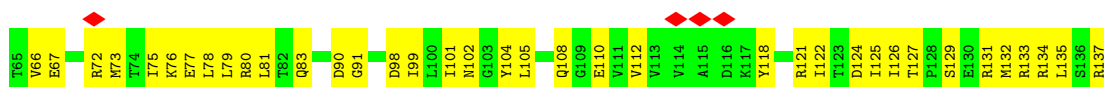
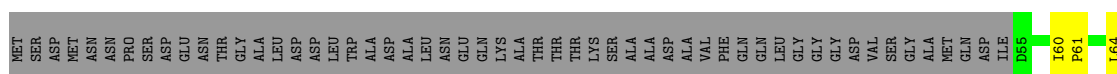
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

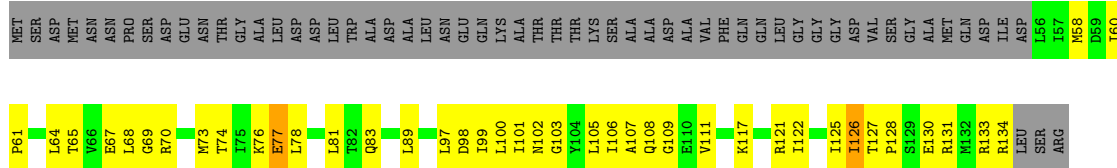


• Molecule 4: Flagellar motor switch protein FliN



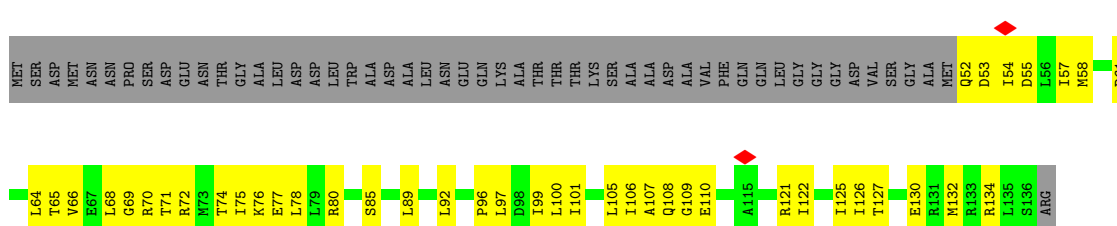
• Molecule 4: Flagellar motor switch protein FliN

Chain EK: 28% 28% 42%



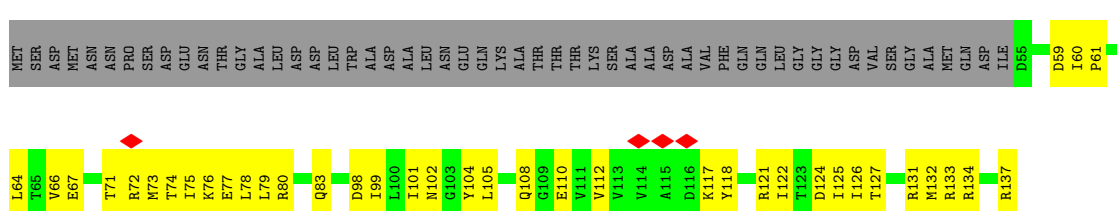
• Molecule 4: Flagellar motor switch protein FliN

Chain FK: 31% 31% 38%



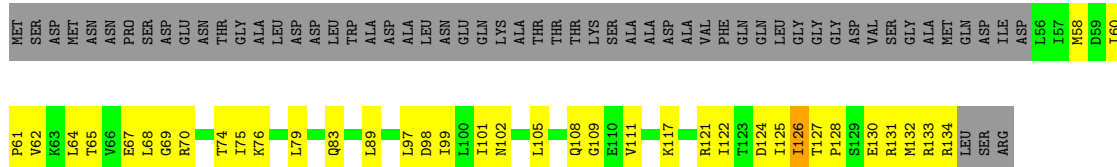
• Molecule 4: Flagellar motor switch protein FliN

Chain DL: 32% 28% 39%



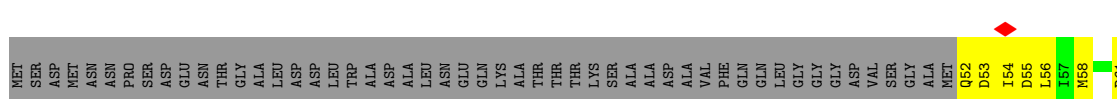
• Molecule 4: Flagellar motor switch protein FliN

Chain EL: 30% 27% 42%

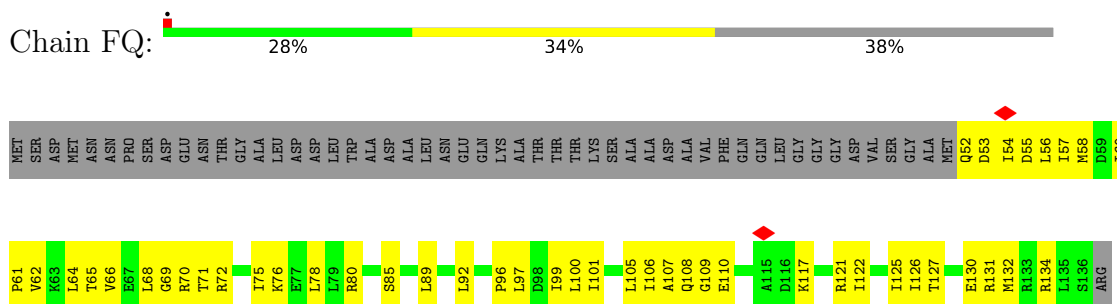


• Molecule 4: Flagellar motor switch protein FliN

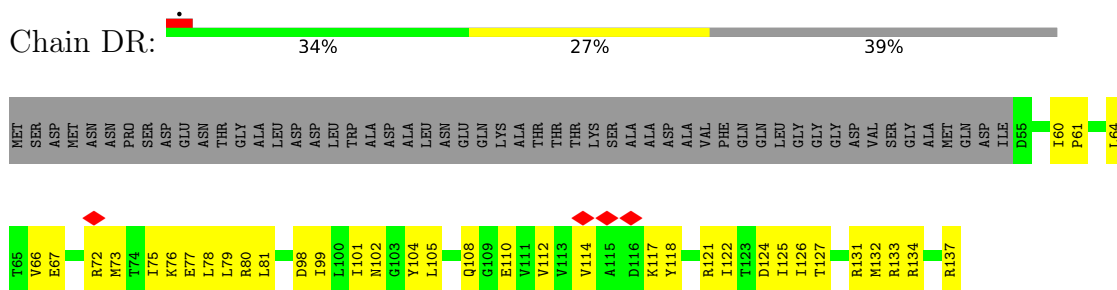
Chain FL: 31% 31% 38%



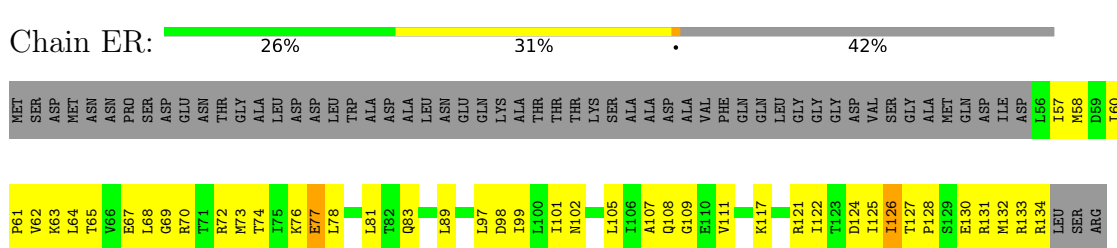
• Molecule 4: Flagellar motor switch protein FliN



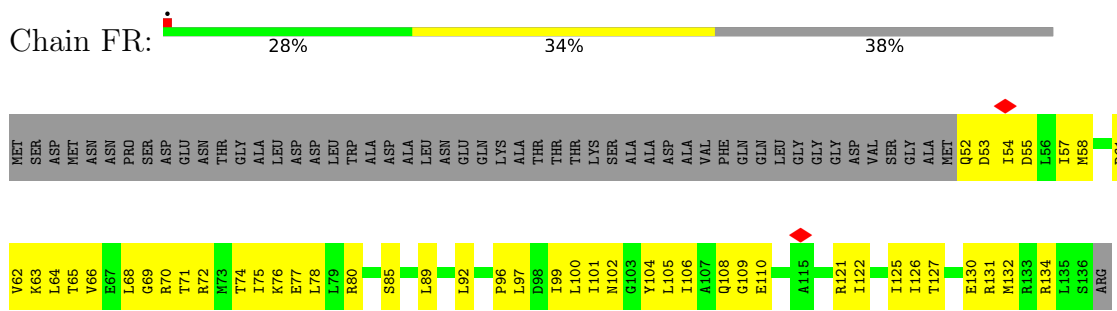
• Molecule 4: Flagellar motor switch protein FliN



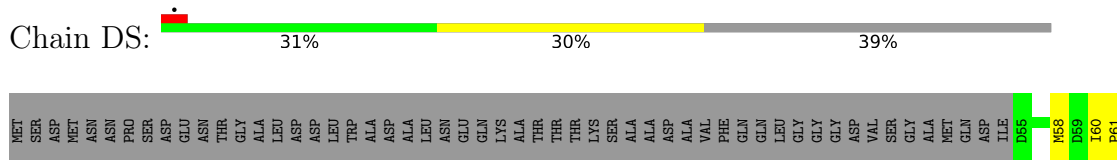
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

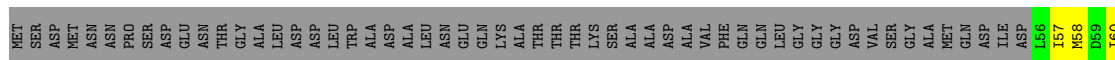
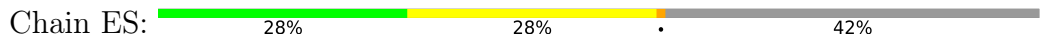


• Molecule 4: Flagellar motor switch protein FliN

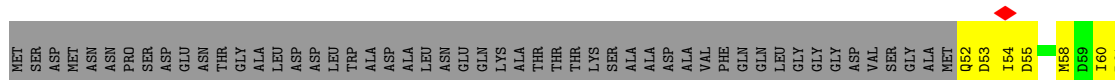




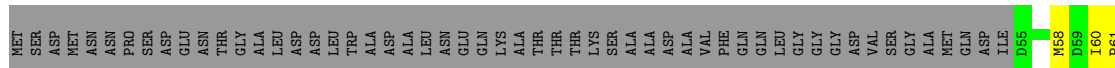
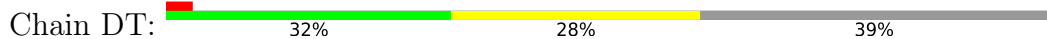
- Molecule 4: Flagellar motor switch protein FliN



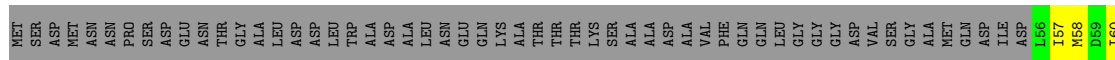
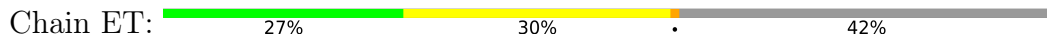
- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN

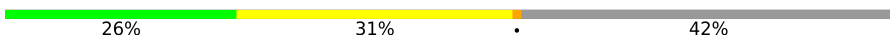


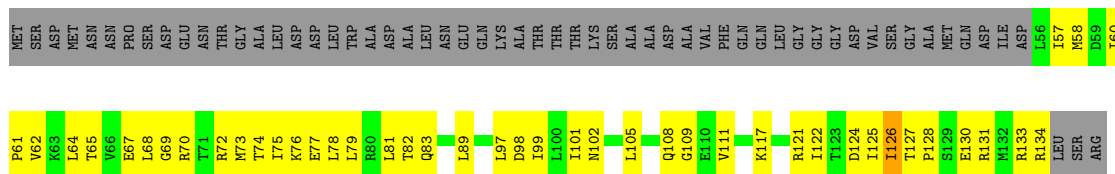
- Molecule 4: Flagellar motor switch protein FliN



- Molecule 4: Flagellar motor switch protein FliN

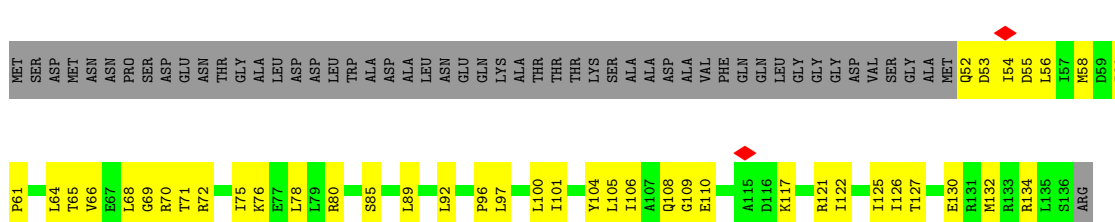


Chain EV: 



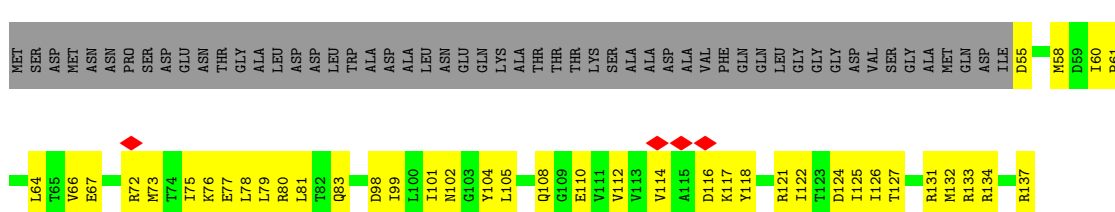
• Molecule 4: Flagellar motor switch protein FliN

Chain FV: 



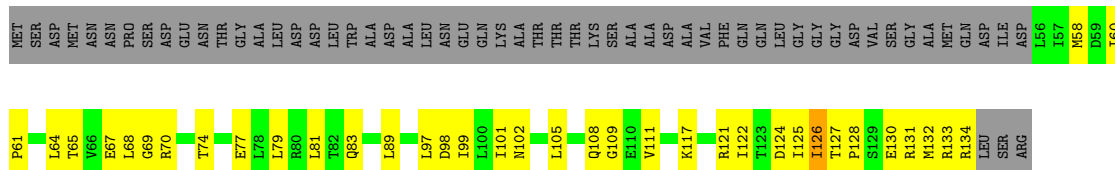
• Molecule 4: Flagellar motor switch protein FliN

Chain DW: 



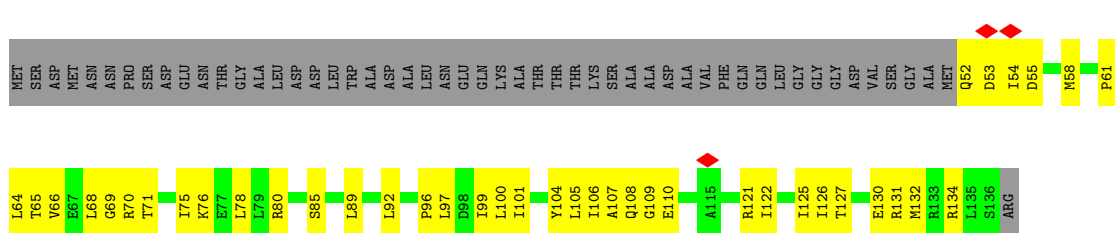
• Molecule 4: Flagellar motor switch protein FliN

Chain EW: 



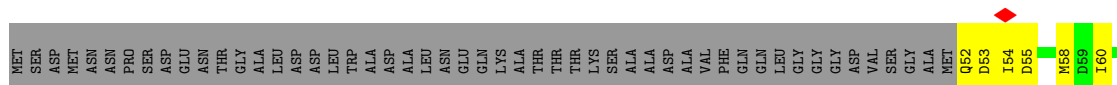
• Molecule 4: Flagellar motor switch protein FliN

Chain FW: 





- Molecule 4: Flagellar motor switch protein FliN



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.15	0/370	0.37	0/494
1	A2	0.13	0/370	0.36	0/494
1	A3	0.15	0/370	0.38	0/494
1	A4	0.13	0/370	0.36	0/494
1	A5	0.13	0/370	0.36	0/494
1	A6	0.15	0/370	0.39	0/494
1	A7	0.13	0/370	0.36	0/494
1	A8	0.13	0/370	0.36	0/494
1	A9	0.15	0/370	0.39	0/494
1	AA	0.14	0/370	0.38	0/494
1	AB	0.13	0/370	0.37	0/494
1	AC	0.14	0/370	0.37	0/494
1	AD	0.13	0/370	0.38	0/494
1	AE	0.14	0/370	0.37	0/494
1	AF	0.12	0/370	0.35	0/494
1	AG	0.12	0/370	0.34	0/494
1	AH	0.15	0/370	0.40	0/494
1	AI	0.13	0/370	0.35	0/494
1	AJ	0.13	0/370	0.35	0/494
1	AK	0.14	0/370	0.37	0/494
1	AL	0.14	0/370	0.36	0/494
1	AM	0.14	0/370	0.36	0/494
1	AN	0.15	0/370	0.38	0/494
1	AO	0.14	0/370	0.37	0/494
1	AP	0.13	0/370	0.38	0/494
1	AQ	0.13	0/370	0.36	0/494
1	AR	0.14	0/370	0.38	0/494
1	AS	0.13	0/370	0.35	0/494
1	AT	0.13	0/370	0.34	0/494
1	AU	0.13	0/370	0.38	0/494
1	AV	0.15	0/370	0.38	0/494
1	AW	0.13	0/370	0.37	0/494
1	AX	0.13	0/370	0.35	0/494
1	AY	0.14	0/370	0.38	0/494

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	B1	0.15	0/2586	0.37	0/3485
2	B2	0.14	0/2586	0.37	0/3485
2	B3	0.14	0/2586	0.37	0/3485
2	B4	0.15	0/2586	0.39	0/3485
2	B5	0.14	0/2586	0.38	0/3485
2	B6	0.14	0/2586	0.37	0/3485
2	B7	0.14	0/2586	0.37	0/3485
2	B8	0.14	0/2586	0.36	0/3485
2	B9	0.15	0/2586	0.37	1/3485 (0.0%)
2	BA	0.14	0/2586	0.36	0/3485
2	BB	0.14	0/2586	0.37	0/3485
2	BC	0.14	0/2586	0.37	0/3485
2	BD	0.14	0/2586	0.37	0/3485
2	BE	0.14	0/2586	0.36	0/3485
2	BF	0.14	0/2586	0.37	0/3485
2	BG	0.14	0/2586	0.37	0/3485
2	BH	0.14	0/2586	0.37	0/3485
2	BI	0.14	0/2586	0.37	0/3485
2	BJ	0.14	0/2586	0.37	0/3485
2	BK	0.13	0/2586	0.36	0/3485
2	BL	0.14	0/2586	0.36	0/3485
2	BM	0.14	0/2586	0.37	0/3485
2	BN	0.15	0/2586	0.39	0/3485
2	BO	0.14	0/2586	0.37	0/3485
2	BP	0.14	0/2586	0.37	0/3485
2	BQ	0.14	0/2586	0.39	0/3485
2	BR	0.14	0/2586	0.38	1/3485 (0.0%)
2	BS	0.15	0/2586	0.37	0/3485
2	BT	0.14	0/2586	0.37	0/3485
2	BU	0.15	0/2586	0.39	0/3485
2	BV	0.15	0/2586	0.39	0/3485
2	BW	0.15	0/2586	0.39	1/3485 (0.0%)
2	BX	0.15	0/2586	0.38	0/3485
2	BY	0.14	0/2586	0.39	0/3485
3	C1	0.15	0/2377	0.38	0/3233
3	C2	0.14	0/2377	0.39	0/3233
3	C3	0.15	0/2377	0.41	0/3233
3	C4	0.14	0/2377	0.40	0/3233
3	C5	0.15	0/2377	0.39	0/3233
3	C6	0.15	0/2377	0.38	0/3233
3	C7	0.15	0/2377	0.39	0/3233
3	C8	0.16	0/2377	0.41	0/3233
3	C9	0.16	0/2377	0.41	0/3233

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	CA	0.17	0/2377	0.43	0/3233
3	CB	0.16	0/2377	0.40	0/3233
3	CC	0.16	0/2377	0.42	0/3233
3	CD	0.16	0/2377	0.40	0/3233
3	CE	0.15	0/2377	0.39	0/3233
3	CF	0.15	0/2377	0.38	0/3233
3	CG	0.15	0/2377	0.38	0/3233
3	CH	0.14	0/2377	0.38	0/3233
3	CI	0.15	0/2377	0.39	0/3233
3	CJ	0.15	0/2377	0.41	0/3233
3	CK	0.15	0/2377	0.40	0/3233
3	CL	0.15	0/2377	0.40	0/3233
3	CM	0.15	0/2377	0.40	0/3233
3	CN	0.15	0/2377	0.40	0/3233
3	CO	0.14	0/2377	0.38	0/3233
3	CP	0.15	0/2377	0.38	0/3233
3	CQ	0.15	0/2377	0.41	0/3233
3	CR	0.15	0/2377	0.38	0/3233
3	CS	0.14	0/2377	0.38	0/3233
3	CT	0.16	0/2377	0.42	0/3233
3	CU	0.15	0/2377	0.40	0/3233
3	CV	0.15	0/2377	0.39	0/3233
3	CW	0.14	0/2377	0.38	0/3233
3	CX	0.14	0/2377	0.39	0/3233
3	CY	0.14	0/2377	0.38	0/3233
4	D1	0.16	0/647	0.47	0/873
4	D2	0.15	0/647	0.45	0/873
4	D3	0.17	0/647	0.48	0/873
4	D4	0.18	0/647	0.53	0/873
4	D5	0.17	0/647	0.48	0/873
4	D6	0.17	0/647	0.48	0/873
4	D7	0.21	0/647	0.51	0/873
4	D8	0.18	0/647	0.47	0/873
4	D9	0.16	0/647	0.46	0/873
4	DA	0.18	0/647	0.50	0/873
4	DB	0.17	0/647	0.50	0/873
4	DC	0.16	0/647	0.47	0/873
4	DD	0.15	0/647	0.46	0/873
4	DE	0.18	0/647	0.52	0/873
4	DF	0.17	0/647	0.49	0/873
4	DG	0.15	0/647	0.45	0/873
4	DH	0.17	0/647	0.48	0/873
4	DI	0.15	0/647	0.43	0/873

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	DJ	0.16	0/647	0.45	0/873
4	DK	0.17	0/647	0.47	0/873
4	DL	0.18	0/647	0.53	0/873
4	DM	0.18	0/647	0.50	0/873
4	DN	0.17	0/647	0.49	0/873
4	DO	0.17	0/647	0.47	0/873
4	DP	0.17	0/647	0.48	0/873
4	DQ	0.16	0/647	0.46	0/873
4	DR	0.17	0/647	0.49	0/873
4	DS	0.17	0/647	0.51	0/873
4	DT	0.17	0/647	0.49	0/873
4	DU	0.15	0/647	0.45	0/873
4	DV	0.16	0/647	0.45	0/873
4	DW	0.16	0/647	0.49	0/873
4	DX	0.15	0/647	0.46	0/873
4	DY	0.17	0/647	0.50	0/873
4	E1	0.18	0/613	0.52	0/829
4	E2	0.17	0/613	0.52	0/829
4	E3	0.19	0/613	0.53	0/829
4	E4	0.16	0/613	0.47	0/829
4	E5	0.18	0/613	0.50	0/829
4	E6	0.19	0/613	0.53	0/829
4	E7	0.19	0/613	0.53	0/829
4	E8	0.16	0/613	0.47	0/829
4	E9	0.18	0/613	0.51	0/829
4	EA	0.20	0/613	0.51	0/829
4	EB	0.19	0/613	0.54	0/829
4	EC	0.20	0/613	0.52	0/829
4	ED	0.18	0/613	0.54	0/829
4	EE	0.18	0/613	0.52	0/829
4	EF	0.19	0/613	0.53	0/829
4	EG	0.18	0/613	0.52	0/829
4	EH	0.20	0/613	0.54	0/829
4	EI	0.18	0/613	0.51	0/829
4	EJ	0.19	0/613	0.52	0/829
4	EK	0.19	0/613	0.54	0/829
4	EL	0.15	0/613	0.46	0/829
4	EM	0.16	0/613	0.46	0/829
4	EN	0.18	0/613	0.53	0/829
4	EO	0.16	0/613	0.48	0/829
4	EP	0.16	0/613	0.48	0/829
4	EQ	0.21	0/613	0.52	0/829
4	ER	0.19	0/613	0.52	0/829

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	ES	0.19	0/613	0.52	0/829
4	ET	0.17	0/613	0.52	0/829
4	EU	0.20	0/613	0.55	0/829
4	EV	0.26	0/613	0.56	0/829
4	EW	0.15	0/613	0.46	0/829
4	EX	0.18	0/613	0.52	0/829
4	EY	0.17	0/613	0.48	0/829
4	F1	0.16	0/660	0.50	0/893
4	F2	0.16	0/660	0.46	0/893
4	F3	0.16	0/660	0.47	0/893
4	F4	0.15	0/660	0.46	0/893
4	F5	0.15	0/660	0.46	0/893
4	F6	0.15	0/660	0.48	0/893
4	F7	0.17	0/660	0.48	0/893
4	F8	0.17	0/660	0.50	0/893
4	F9	0.17	0/660	0.51	0/893
4	FA	0.16	0/660	0.48	0/893
4	FB	0.17	0/660	0.51	0/893
4	FC	0.15	0/660	0.47	0/893
4	FD	0.17	0/660	0.52	0/893
4	FE	0.17	0/660	0.49	0/893
4	FF	0.16	0/660	0.49	0/893
4	FG	0.17	0/660	0.50	0/893
4	FH	0.16	0/660	0.52	0/893
4	FI	0.16	0/660	0.47	0/893
4	FJ	0.17	0/660	0.48	0/893
4	FK	0.16	0/660	0.46	0/893
4	FL	0.16	0/660	0.48	0/893
4	FM	0.17	0/660	0.49	0/893
4	FN	0.16	0/660	0.49	0/893
4	FO	0.16	0/660	0.48	0/893
4	FP	0.17	0/660	0.50	0/893
4	FQ	0.16	0/660	0.48	0/893
4	FR	0.17	0/660	0.50	0/893
4	FS	0.16	0/660	0.49	0/893
4	FT	0.16	0/660	0.48	0/893
4	FU	0.19	0/660	0.50	0/893
4	FV	0.17	0/660	0.48	0/893
4	FW	0.15	0/660	0.49	0/893
4	FX	0.16	0/660	0.48	0/893
4	FY	0.16	0/660	0.50	0/893
All	All	0.15	0/246602	0.41	3/333438 (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.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BR	193	MET	CA-CB-CG	5.78	125.66	114.10
2	BW	193	MET	CA-CB-CG	5.73	125.56	114.10
2	B9	235	LEU	CB-CA-C	-5.01	109.83	115.79

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E1	77	GLU	Peptide
4	E3	77	GLU	Peptide
4	E5	77	GLU	Peptide

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Mol	Chain	Res	Type	Group
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	29	0
1	A2	367	0	361	29	0
1	A3	367	0	361	29	0
1	A4	367	0	361	29	0
1	A5	367	0	361	26	0
1	A6	367	0	361	26	0
1	A7	367	0	361	26	0
1	A8	367	0	361	26	0
1	A9	367	0	361	29	0
1	AA	367	0	361	27	0
1	AB	367	0	361	26	0
1	AC	367	0	361	26	0
1	AD	367	0	361	27	0
1	AE	367	0	361	29	0
1	AF	367	0	361	24	0
1	AG	367	0	361	23	0
1	AH	367	0	361	33	0
1	AI	367	0	361	26	0
1	AJ	367	0	361	22	0
1	AK	367	0	361	26	0
1	AL	367	0	361	25	0
1	AM	367	0	361	24	0
1	AN	367	0	361	28	0
1	AO	367	0	361	30	0
1	AP	367	0	361	28	0
1	AQ	367	0	361	26	0
1	AR	367	0	361	26	0
1	AS	367	0	361	26	0
1	AT	367	0	361	22	0
1	AU	367	0	361	28	0
1	AV	367	0	361	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AW	367	0	361	27	0
1	AX	367	0	361	25	0
1	AY	367	0	361	28	0
2	B1	2566	0	2615	137	0
2	B2	2566	0	2615	135	0
2	B3	2566	0	2615	130	0
2	B4	2566	0	2615	142	0
2	B5	2566	0	2615	128	0
2	B6	2566	0	2615	130	0
2	B7	2566	0	2615	133	0
2	B8	2566	0	2615	132	0
2	B9	2566	0	2615	128	0
2	BA	2566	0	2615	134	0
2	BB	2566	0	2615	128	0
2	BC	2566	0	2615	127	0
2	BD	2566	0	2615	131	0
2	BE	2566	0	2615	134	0
2	BF	2566	0	2615	133	0
2	BG	2566	0	2615	133	0
2	BH	2566	0	2615	127	0
2	BI	2566	0	2615	138	0
2	BJ	2566	0	2615	134	0
2	BK	2566	0	2615	129	0
2	BL	2566	0	2615	129	0
2	BM	2566	0	2615	134	0
2	BN	2566	0	2615	129	0
2	BO	2566	0	2615	127	0
2	BP	2566	0	2615	126	0
2	BQ	2566	0	2615	131	0
2	BR	2566	0	2615	129	0
2	BS	2566	0	2615	130	0
2	BT	2566	0	2615	128	0
2	BU	2566	0	2615	129	0
2	BV	2566	0	2615	133	0
2	BW	2566	0	2615	134	0
2	BX	2566	0	2615	134	0
2	BY	2566	0	2615	136	0
3	C1	2325	0	2354	99	0
3	C2	2325	0	2354	95	0
3	C3	2325	0	2354	91	0
3	C4	2325	0	2354	96	0
3	C5	2325	0	2354	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C6	2325	0	2354	90	0
3	C7	2325	0	2354	97	0
3	C8	2325	0	2354	97	0
3	C9	2325	0	2354	97	0
3	CA	2325	0	2354	99	0
3	CB	2325	0	2354	97	0
3	CC	2325	0	2354	96	0
3	CD	2325	0	2354	95	0
3	CE	2325	0	2354	94	0
3	CF	2325	0	2354	97	0
3	CG	2325	0	2354	102	0
3	CH	2325	0	2354	89	0
3	CI	2325	0	2354	102	0
3	CJ	2325	0	2354	89	0
3	CK	2325	0	2354	90	0
3	CL	2325	0	2354	93	0
3	CM	2325	0	2354	86	0
3	CN	2325	0	2354	92	0
3	CO	2325	0	2354	99	0
3	CP	2325	0	2354	96	0
3	CQ	2325	0	2354	92	0
3	CR	2325	0	2354	88	0
3	CS	2325	0	2354	96	0
3	CT	2325	0	2354	94	0
3	CU	2325	0	2354	92	0
3	CV	2325	0	2354	92	0
3	CW	2325	0	2354	92	0
3	CX	2325	0	2354	96	0
3	CY	2325	0	2354	86	0
4	D1	643	0	694	37	0
4	D2	643	0	694	38	0
4	D3	643	0	694	37	0
4	D4	643	0	694	40	0
4	D5	643	0	694	33	0
4	D6	643	0	694	42	0
4	D7	643	0	694	34	0
4	D8	643	0	694	36	0
4	D9	643	0	694	42	0
4	DA	643	0	694	43	0
4	DB	643	0	694	40	0
4	DC	643	0	694	42	0
4	DD	643	0	694	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	DE	643	0	694	39	0
4	DF	643	0	694	42	0
4	DG	643	0	694	43	0
4	DH	643	0	694	39	0
4	DI	643	0	694	37	0
4	DJ	643	0	694	38	0
4	DK	643	0	694	40	0
4	DL	643	0	694	37	0
4	DM	643	0	694	35	0
4	DN	643	0	694	42	0
4	DO	643	0	694	38	0
4	DP	643	0	694	36	0
4	DQ	643	0	694	38	0
4	DR	643	0	694	36	0
4	DS	643	0	694	40	0
4	DT	643	0	694	40	0
4	DU	643	0	694	30	0
4	DV	643	0	694	34	0
4	DW	643	0	694	41	0
4	DX	643	0	694	38	0
4	DY	643	0	694	44	0
4	E1	609	0	661	41	0
4	E2	609	0	661	43	0
4	E3	609	0	661	43	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	41	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	44	0
4	EE	609	0	661	44	0
4	EF	609	0	661	40	0
4	EG	609	0	661	50	0
4	EH	609	0	661	46	0
4	EI	609	0	661	43	0
4	EJ	609	0	661	42	0
4	EK	609	0	661	42	0
4	EL	609	0	661	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	EM	609	0	661	42	0
4	EN	609	0	661	38	0
4	EO	609	0	661	40	0
4	EP	609	0	661	38	0
4	EQ	609	0	661	43	0
4	ER	609	0	661	51	0
4	ES	609	0	661	40	0
4	ET	609	0	661	45	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	40	0
4	EY	609	0	661	43	0
4	F1	656	0	704	47	0
4	F2	656	0	704	45	0
4	F3	656	0	704	44	0
4	F4	656	0	704	42	0
4	F5	656	0	704	49	0
4	F6	656	0	704	46	0
4	F7	656	0	704	56	0
4	F8	656	0	704	56	0
4	F9	656	0	704	55	0
4	FA	656	0	704	50	0
4	FB	656	0	704	53	0
4	FC	656	0	704	53	0
4	FD	656	0	704	48	0
4	FE	656	0	704	53	0
4	FF	656	0	704	42	0
4	FG	656	0	704	55	0
4	FH	656	0	704	49	0
4	FI	656	0	704	47	0
4	FJ	656	0	704	48	0
4	FK	656	0	704	44	0
4	FL	656	0	704	45	0
4	FM	656	0	704	47	0
4	FN	656	0	704	43	0
4	FO	656	0	704	48	0
4	FP	656	0	704	46	0
4	FQ	656	0	704	50	0
4	FR	656	0	704	53	0
4	FS	656	0	704	44	0
4	FT	656	0	704	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	FU	656	0	704	44	0
4	FV	656	0	704	47	0
4	FW	656	0	704	39	0
4	FX	656	0	704	46	0
4	FY	656	0	704	47	0
All	All	243644	0	251226	10170	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 21.

The worst 5 of 10170 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BT:158:MET:HE1	2:BU:218:VAL:HB	1.35	1.08
2:BX:158:MET:HE1	2:BY:218:VAL:HB	1.34	1.07
2:BC:158:MET:HE1	2:BD:218:VAL:HB	1.38	1.05
2:BG:158:MET:HE1	2:BH:218:VAL:HB	1.39	1.05
2:B5:135:VAL:HG21	2:B6:193:MET:HE2	1.41	1.00

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
1	A5	42/560 (8%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36	71
2	B2	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	36	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B3	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	36	71
2	B4	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	36	71
2	B5	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	36	71
2	B6	326/328 (99%)	312 (96%)	13 (4%)	1 (0%)	36	71
2	B7	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	36	71
2	B8	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	36	71
2	B9	326/328 (99%)	313 (96%)	12 (4%)	1 (0%)	36	71
2	BA	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	36	71
2	BB	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	36	71
2	BC	326/328 (99%)	313 (96%)	12 (4%)	1 (0%)	36	71
2	BD	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	36	71
2	BE	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	36	71
2	BF	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	36	71
2	BG	326/328 (99%)	313 (96%)	12 (4%)	1 (0%)	36	71
2	BH	326/328 (99%)	316 (97%)	10 (3%)	0	100	100
2	BI	326/328 (99%)	316 (97%)	9 (3%)	1 (0%)	36	71
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%)	36	71
2	BM	326/328 (99%)	316 (97%)	9 (3%)	1 (0%)	36	71
2	BN	326/328 (99%)	313 (96%)	12 (4%)	1 (0%)	36	71
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%)	36	71
2	BR	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	36	71
2	BS	326/328 (99%)	315 (97%)	10 (3%)	1 (0%)	36	71
2	BT	326/328 (99%)	312 (96%)	13 (4%)	1 (0%)	36	71
2	BU	326/328 (99%)	316 (97%)	9 (3%)	1 (0%)	36	71
2	BV	326/328 (99%)	314 (96%)	11 (3%)	1 (0%)	36	71
2	BW	326/328 (99%)	314 (96%)	12 (4%)	0	100	100
2	BX	326/328 (99%)	311 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
3	CU	285/334 (85%)	274 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
4	DR	81/137 (59%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	9	40
4	E2	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	E3	77/137 (56%)	70 (91%)	6 (8%)	1 (1%)	9	40
4	E4	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	E5	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	9	40
4	E6	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	E7	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	9	40
4	E8	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	E9	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	EA	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	9	40
4	EB	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	EC	77/137 (56%)	69 (90%)	7 (9%)	1 (1%)	9	40
4	ED	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	9	40
4	EE	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	EF	77/137 (56%)	70 (91%)	6 (8%)	1 (1%)	9	40
4	EG	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	9	40
4	EH	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	EI	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	EJ	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	EK	77/137 (56%)	70 (91%)	6 (8%)	1 (1%)	9	40
4	EL	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	EM	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	9	40
4	EN	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	EO	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	EP	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	9	40
4	EQ	77/137 (56%)	69 (90%)	7 (9%)	1 (1%)	9	40
4	ER	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	ES	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	9	40
4	ET	77/137 (56%)	70 (91%)	6 (8%)	1 (1%)	9	40
4	EU	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	EV	77/137 (56%)	70 (91%)	6 (8%)	1 (1%)	9	40
4	EW	77/137 (56%)	72 (94%)	4 (5%)	1 (1%)	9	40
4	EX	77/137 (56%)	71 (92%)	5 (6%)	1 (1%)	9	40
4	EY	77/137 (56%)	73 (95%)	3 (4%)	1 (1%)	9	40
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
4	FL	83/137 (61%)	77 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	44	77

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
1	A3	40/467 (9%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
1	AY	40/467 (9%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B1	281/281 (100%)	281 (100%)	0	100	100
2	B2	281/281 (100%)	281 (100%)	0	100	100
2	B3	281/281 (100%)	281 (100%)	0	100	100
2	B4	281/281 (100%)	281 (100%)	0	100	100
2	B5	281/281 (100%)	281 (100%)	0	100	100
2	B6	281/281 (100%)	281 (100%)	0	100	100
2	B7	281/281 (100%)	281 (100%)	0	100	100
2	B8	281/281 (100%)	281 (100%)	0	100	100
2	B9	281/281 (100%)	281 (100%)	0	100	100
2	BA	281/281 (100%)	281 (100%)	0	100	100
2	BB	281/281 (100%)	281 (100%)	0	100	100
2	BC	281/281 (100%)	281 (100%)	0	100	100
2	BD	281/281 (100%)	281 (100%)	0	100	100
2	BE	281/281 (100%)	281 (100%)	0	100	100
2	BF	281/281 (100%)	281 (100%)	0	100	100
2	BG	281/281 (100%)	281 (100%)	0	100	100
2	BH	281/281 (100%)	281 (100%)	0	100	100
2	BI	281/281 (100%)	281 (100%)	0	100	100
2	BJ	281/281 (100%)	281 (100%)	0	100	100
2	BK	281/281 (100%)	281 (100%)	0	100	100
2	BL	281/281 (100%)	281 (100%)	0	100	100
2	BM	281/281 (100%)	281 (100%)	0	100	100
2	BN	281/281 (100%)	281 (100%)	0	100	100
2	BO	281/281 (100%)	281 (100%)	0	100	100
2	BP	281/281 (100%)	281 (100%)	0	100	100
2	BQ	281/281 (100%)	281 (100%)	0	100	100
2	BR	281/281 (100%)	281 (100%)	0	100	100
2	BS	281/281 (100%)	281 (100%)	0	100	100
2	BT	281/281 (100%)	281 (100%)	0	100	100
2	BU	281/281 (100%)	281 (100%)	0	100	100
2	BV	281/281 (100%)	281 (100%)	0	100	100

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CT	260/301 (86%)	260 (100%)	0	100	100
3	CU	260/301 (86%)	260 (100%)	0	100	100
3	CV	260/301 (86%)	260 (100%)	0	100	100
3	CW	260/301 (86%)	260 (100%)	0	100	100
3	CX	260/301 (86%)	260 (100%)	0	100	100
3	CY	260/301 (86%)	260 (100%)	0	100	100
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
4	DP	72/113 (64%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
4	EM	68/113 (60%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
4	FJ	74/113 (66%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	27030 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 583 such sidechains are listed below:

Mol	Chain	Res	Type
2	BS	46	GLN
3	CY	43	GLN
4	FS	52	GLN
2	BS	28	HIS
2	BV	238	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

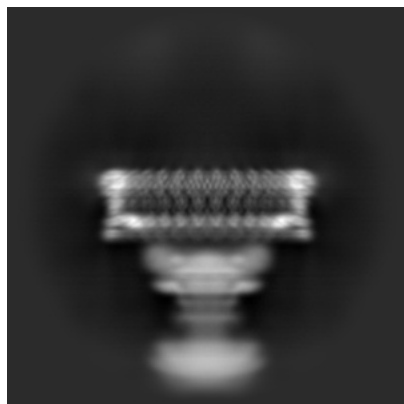
6 Map visualisation [i](#)

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

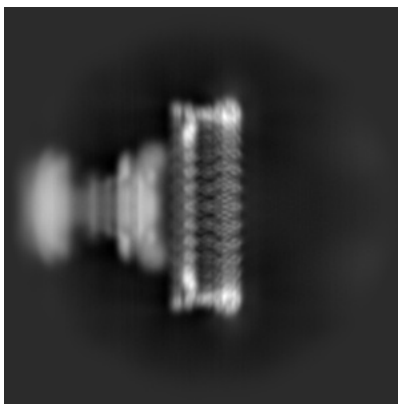
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

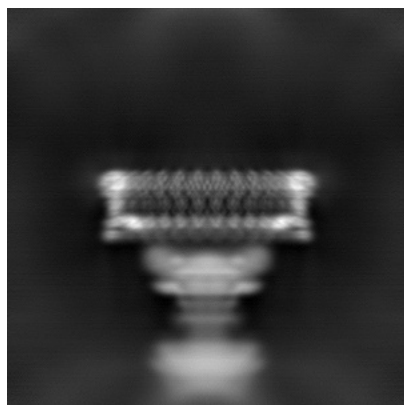


Y

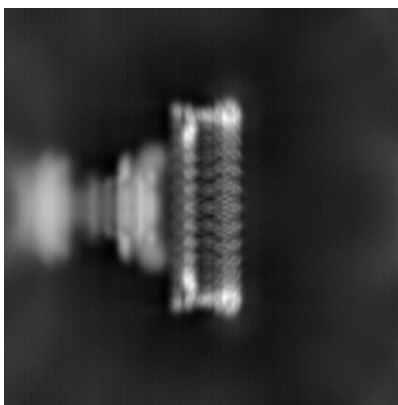


Z

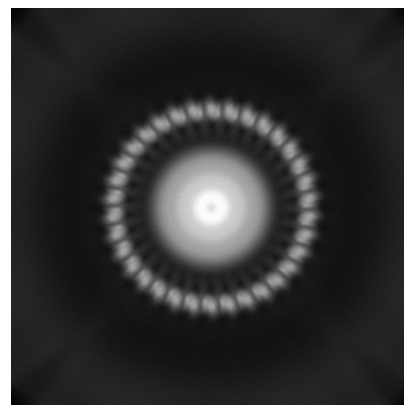
6.1.2 Raw map



X



Y

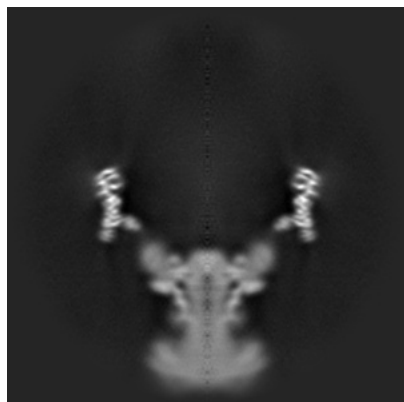


Z

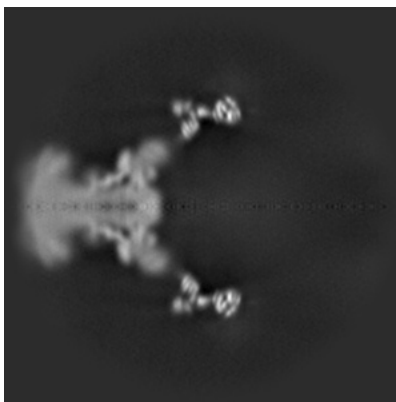
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

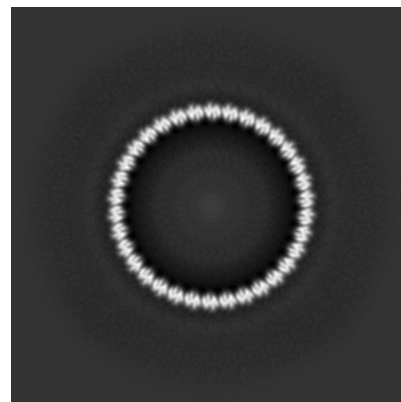
6.2.1 Primary map



X Index: 256

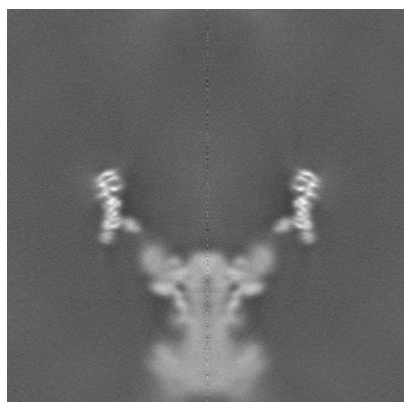


Y Index: 256

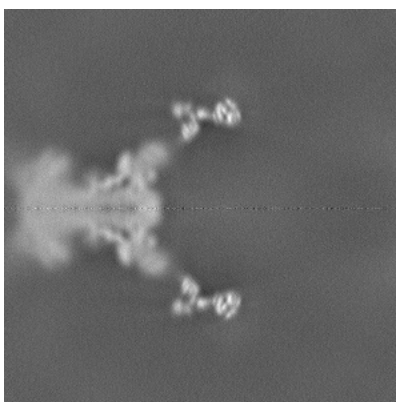


Z Index: 256

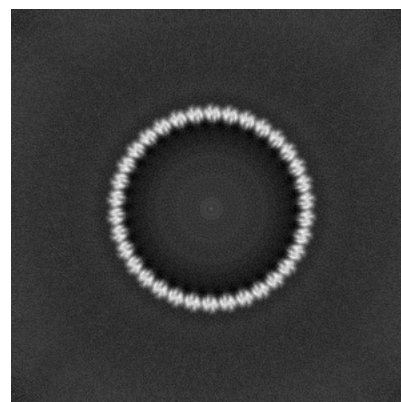
6.2.2 Raw map



X Index: 256



Y Index: 256

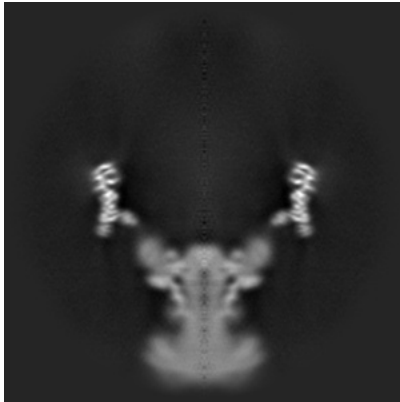


Z Index: 256

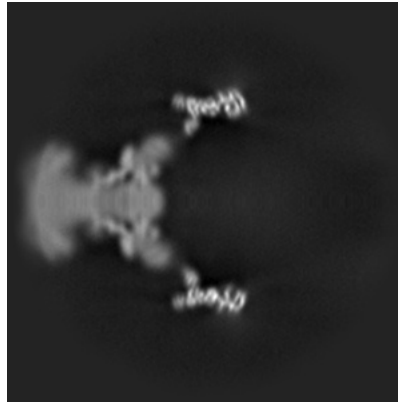
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

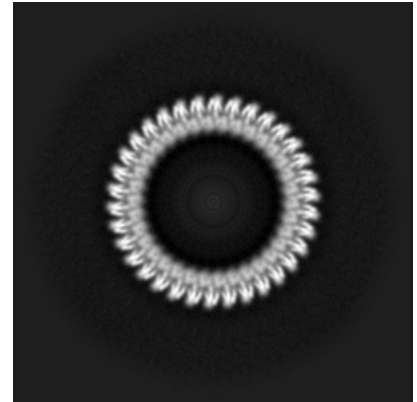
6.3.1 Primary map



X Index: 256

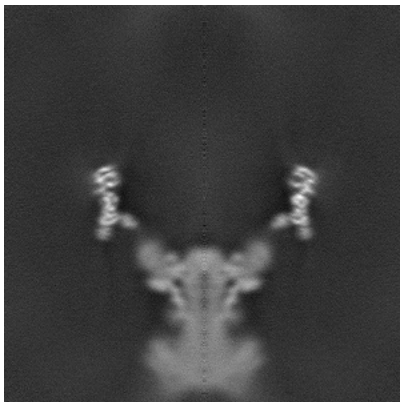


Y Index: 244

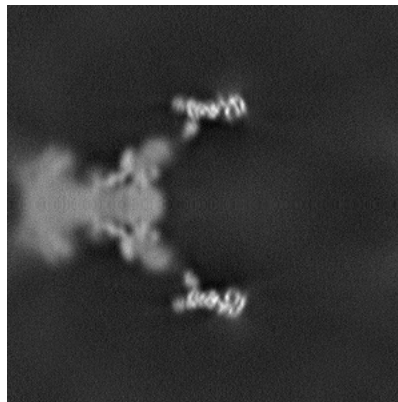


Z Index: 239

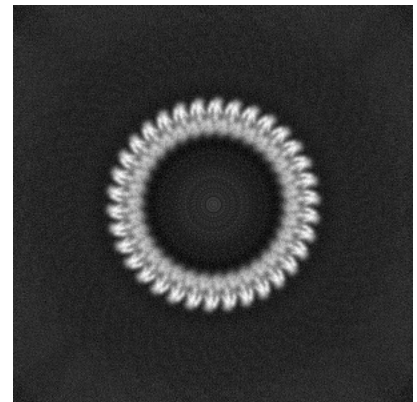
6.3.2 Raw map



X Index: 255



Y Index: 267

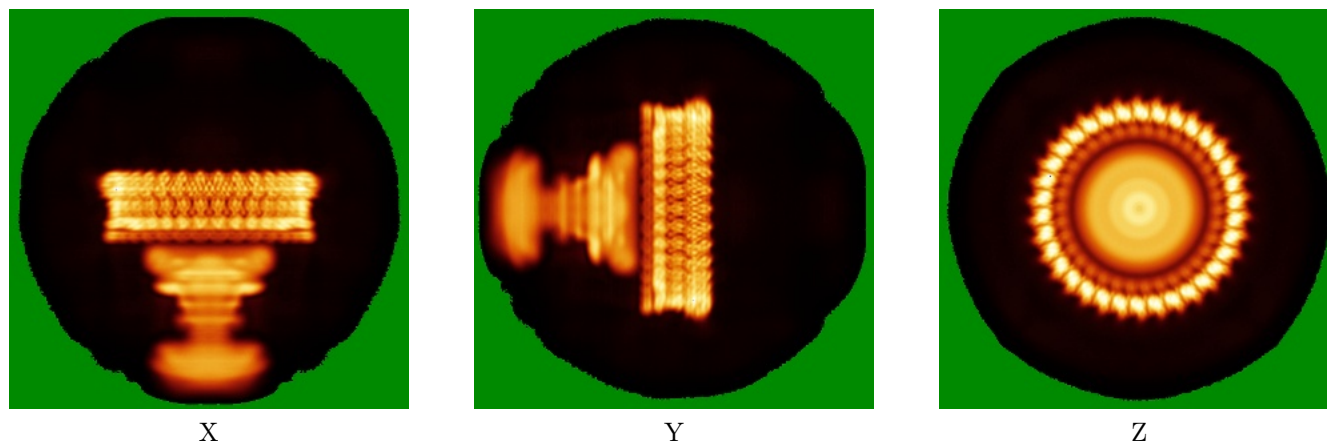


Z Index: 239

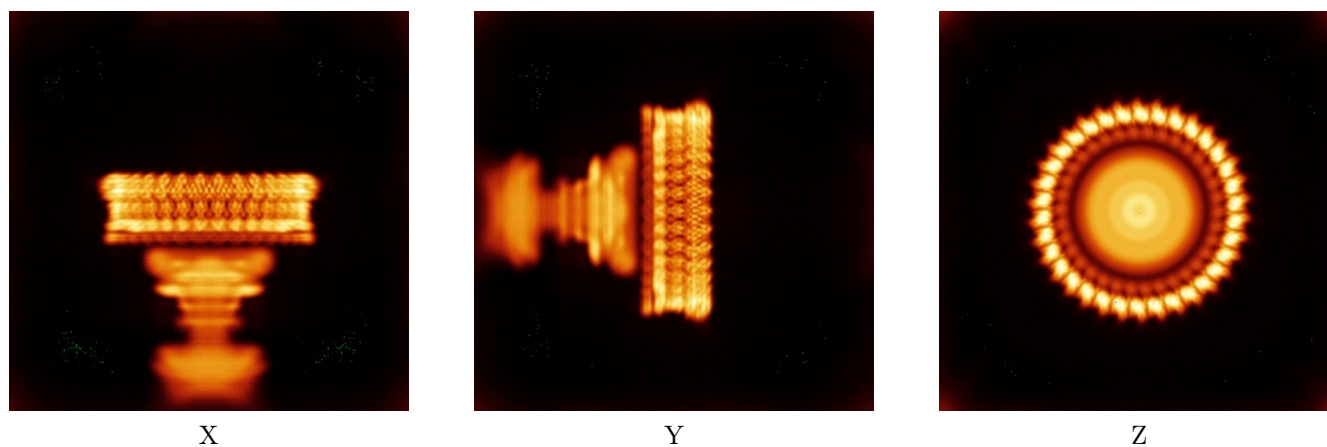
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

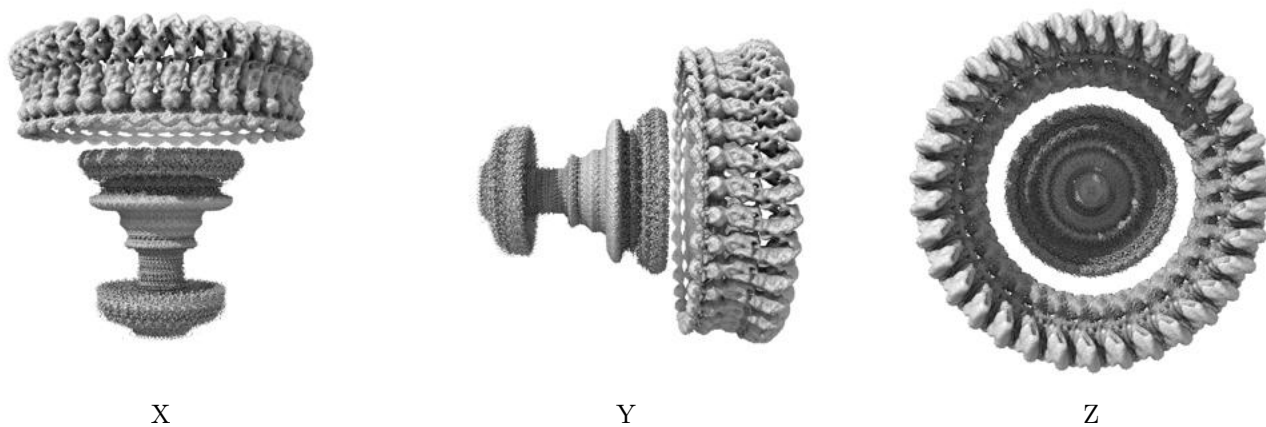
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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



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

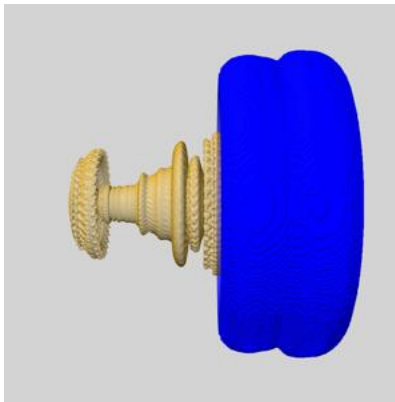
A mask typically either:

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

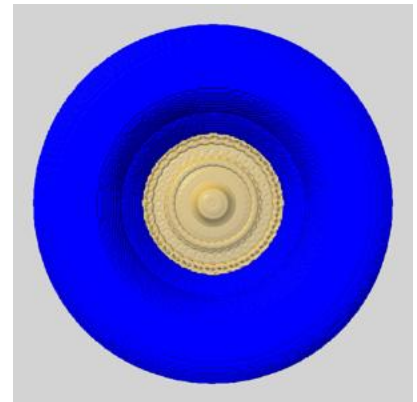
6.6.1 emd_42451_msk_1.map [i](#)



X



Y

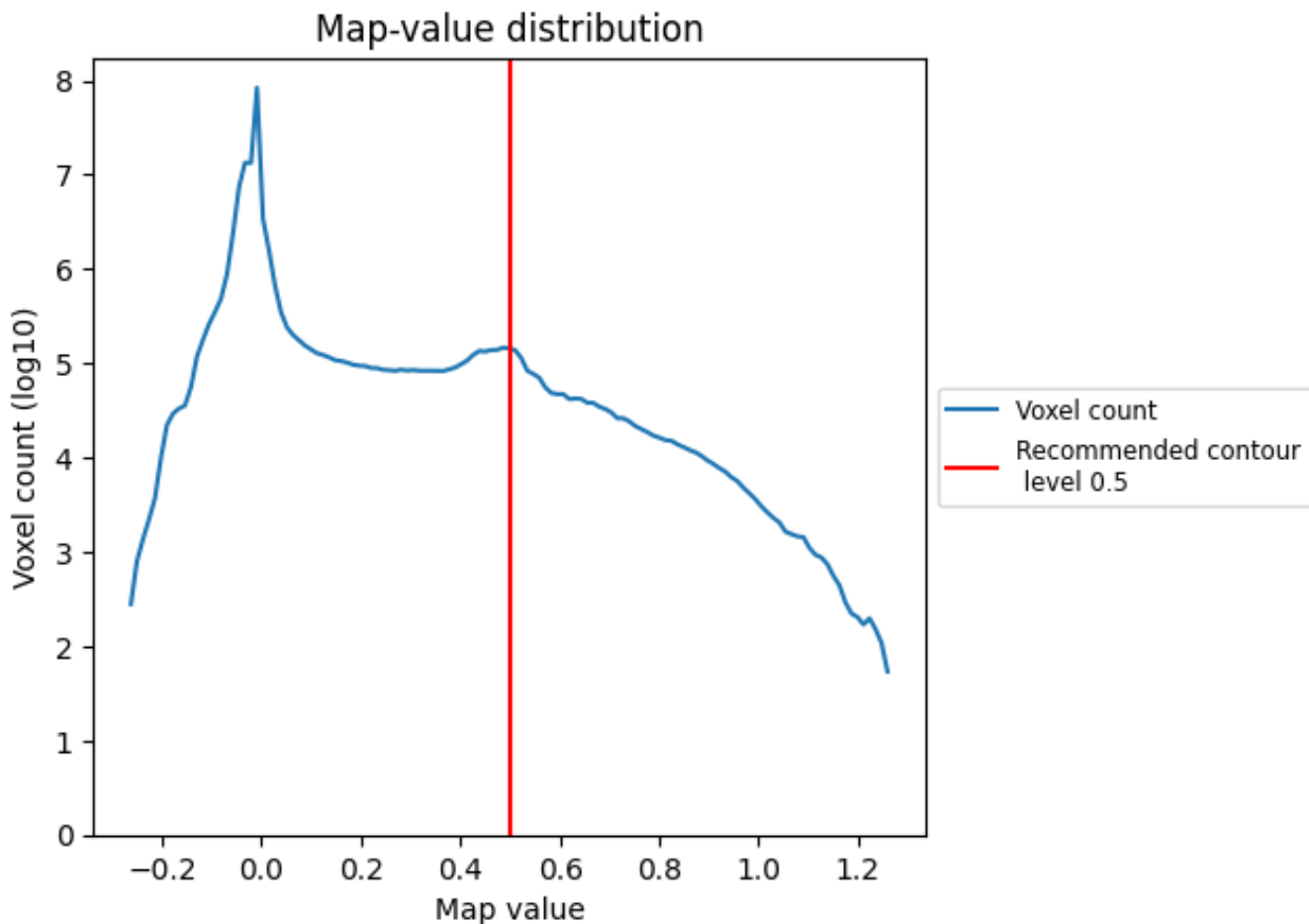


Z

7 Map analysis [i](#)

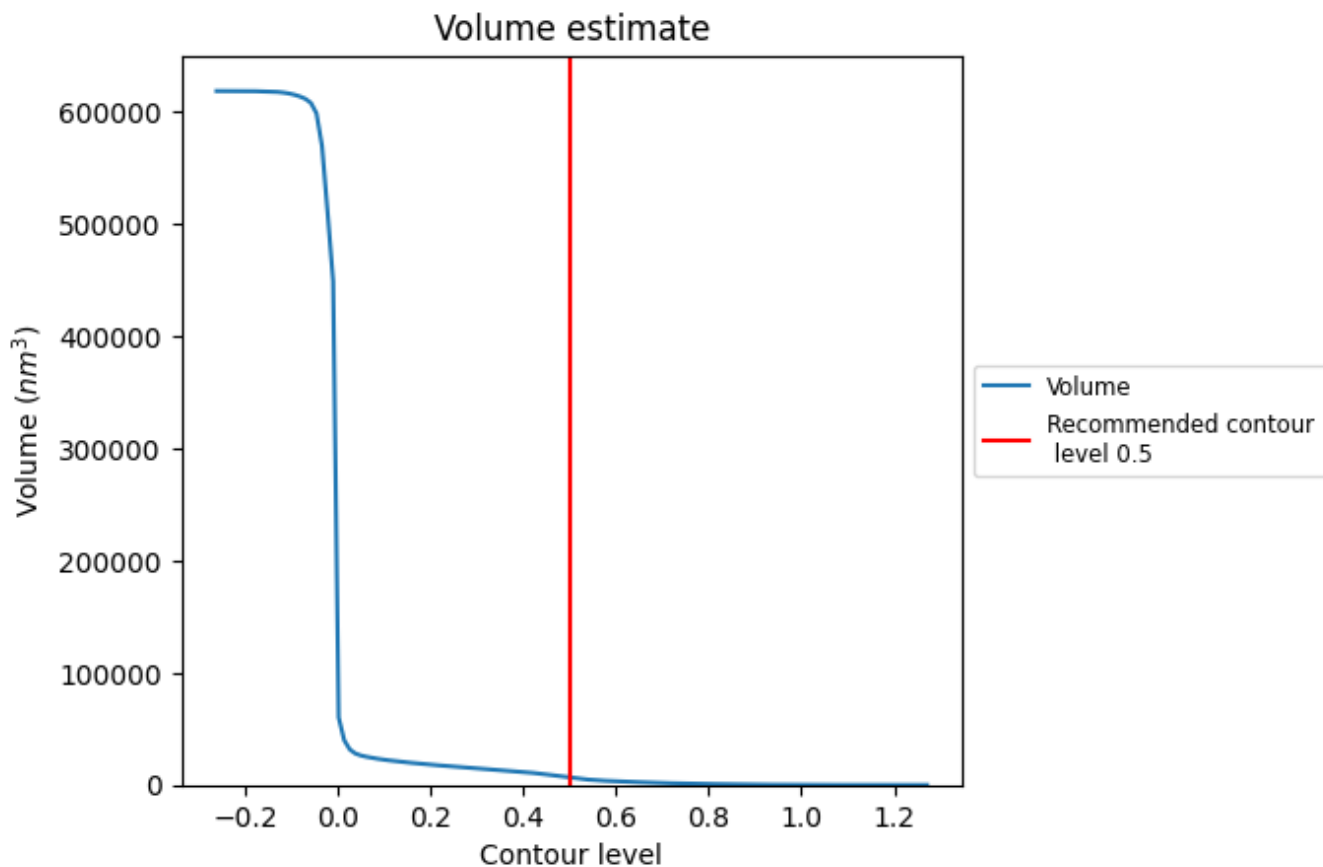
This section contains the results of statistical analysis of the map.

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.

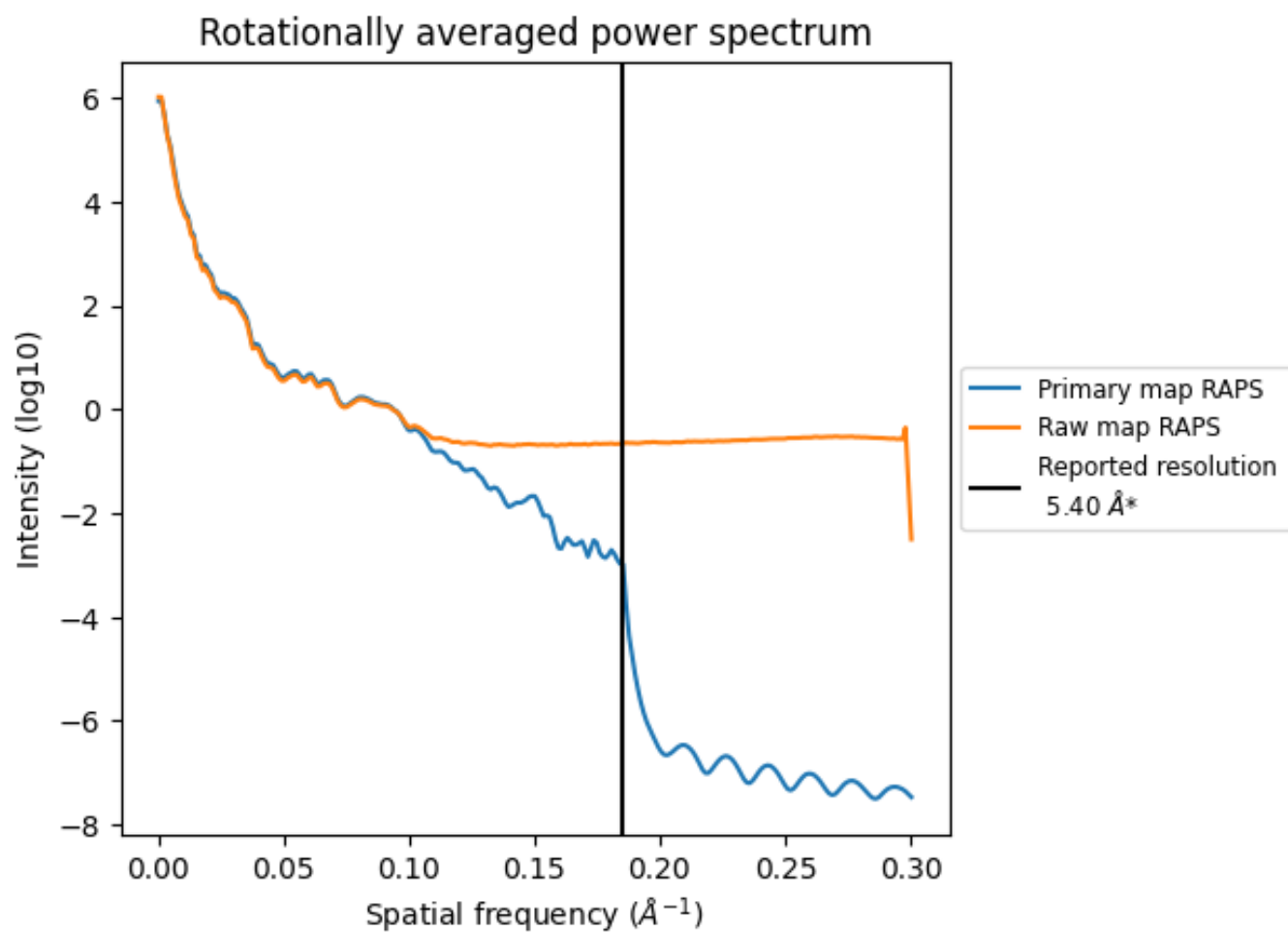
7.2 Volume estimate [\(i\)](#)



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

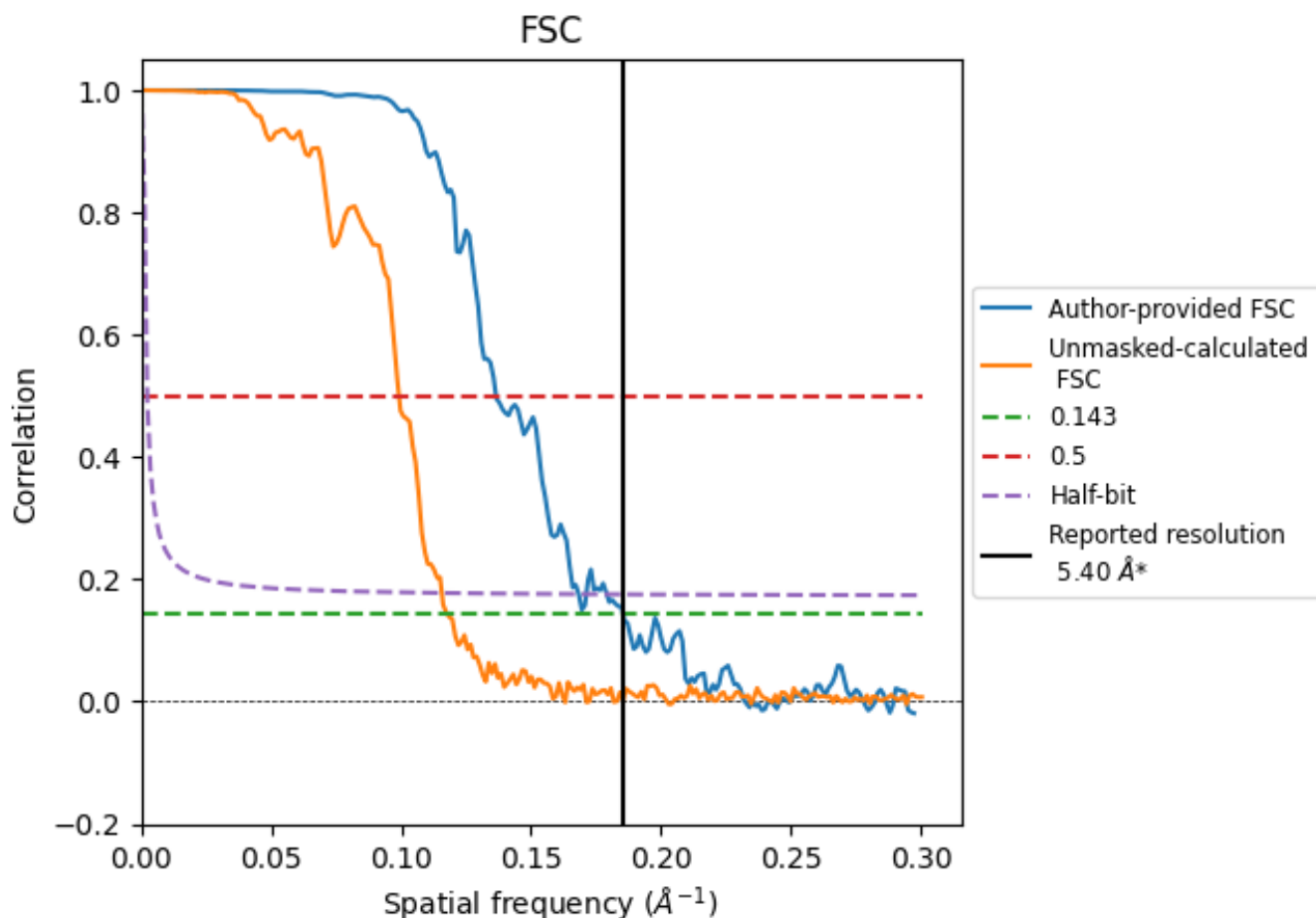


*Reported resolution corresponds to spatial frequency of 0.185 Å⁻¹

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](#)

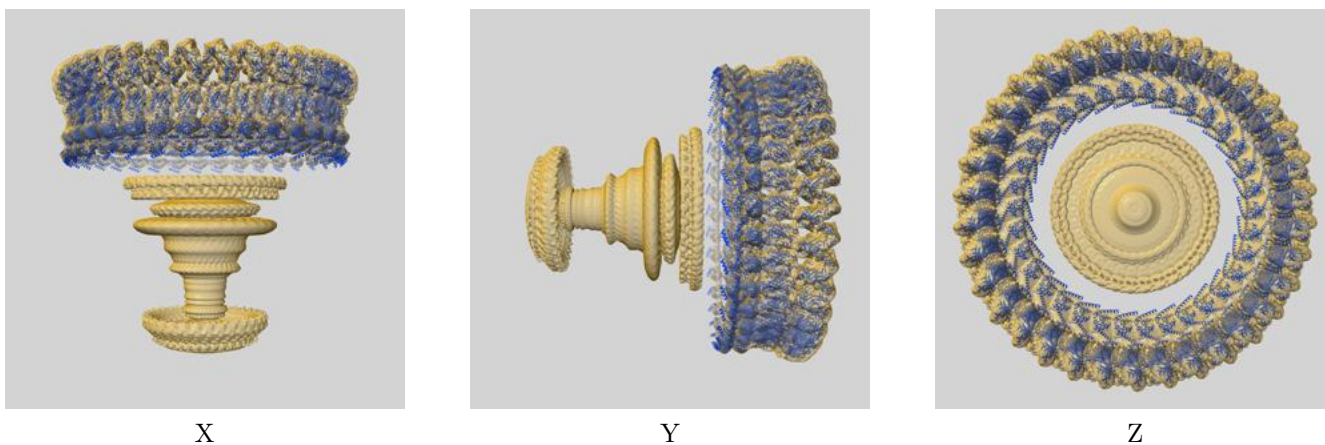
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.40	-	-
Author-provided FSC curve	5.39	7.32	5.94
Unmasked-calculated*	8.49	10.08	8.64

*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](#)

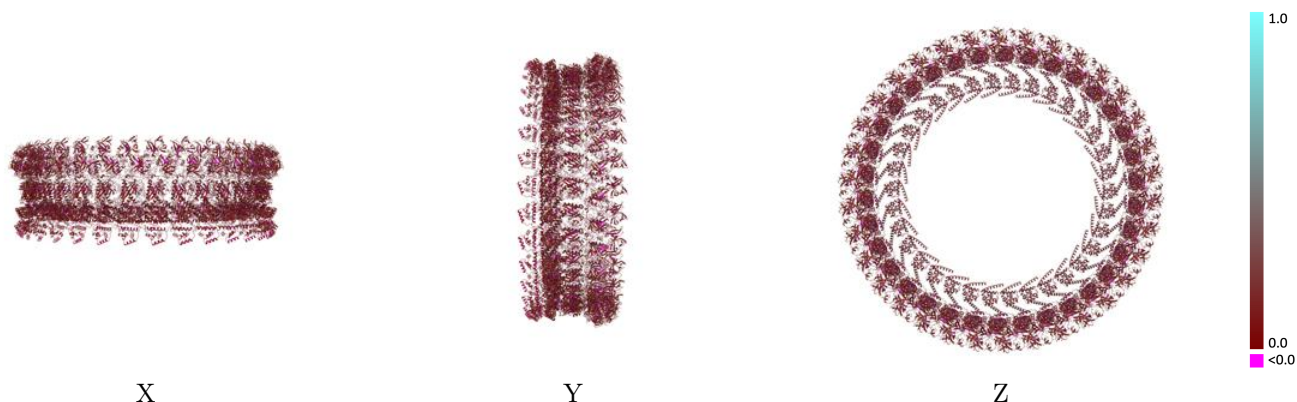
This section contains information regarding the fit between EMDB map EMD-42451 and PDB model 8UPL. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



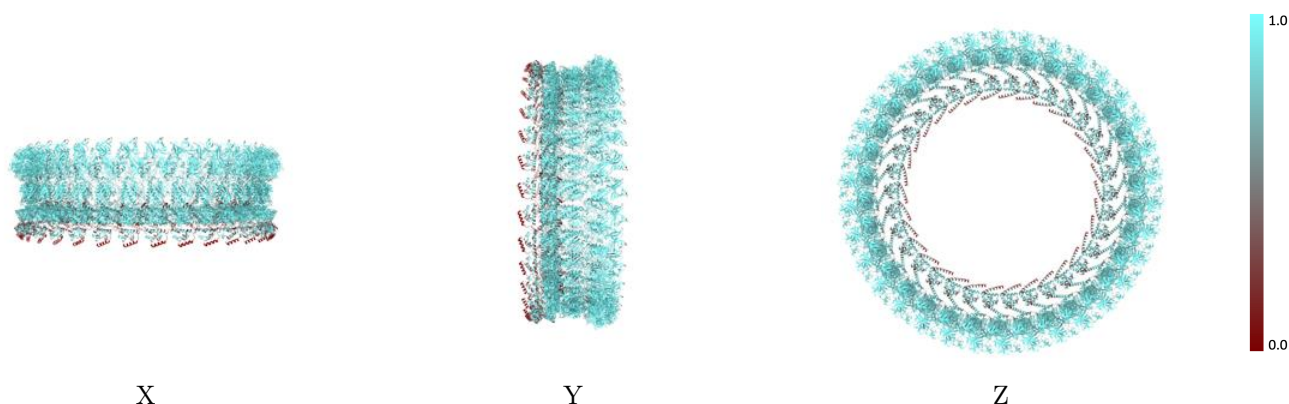
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



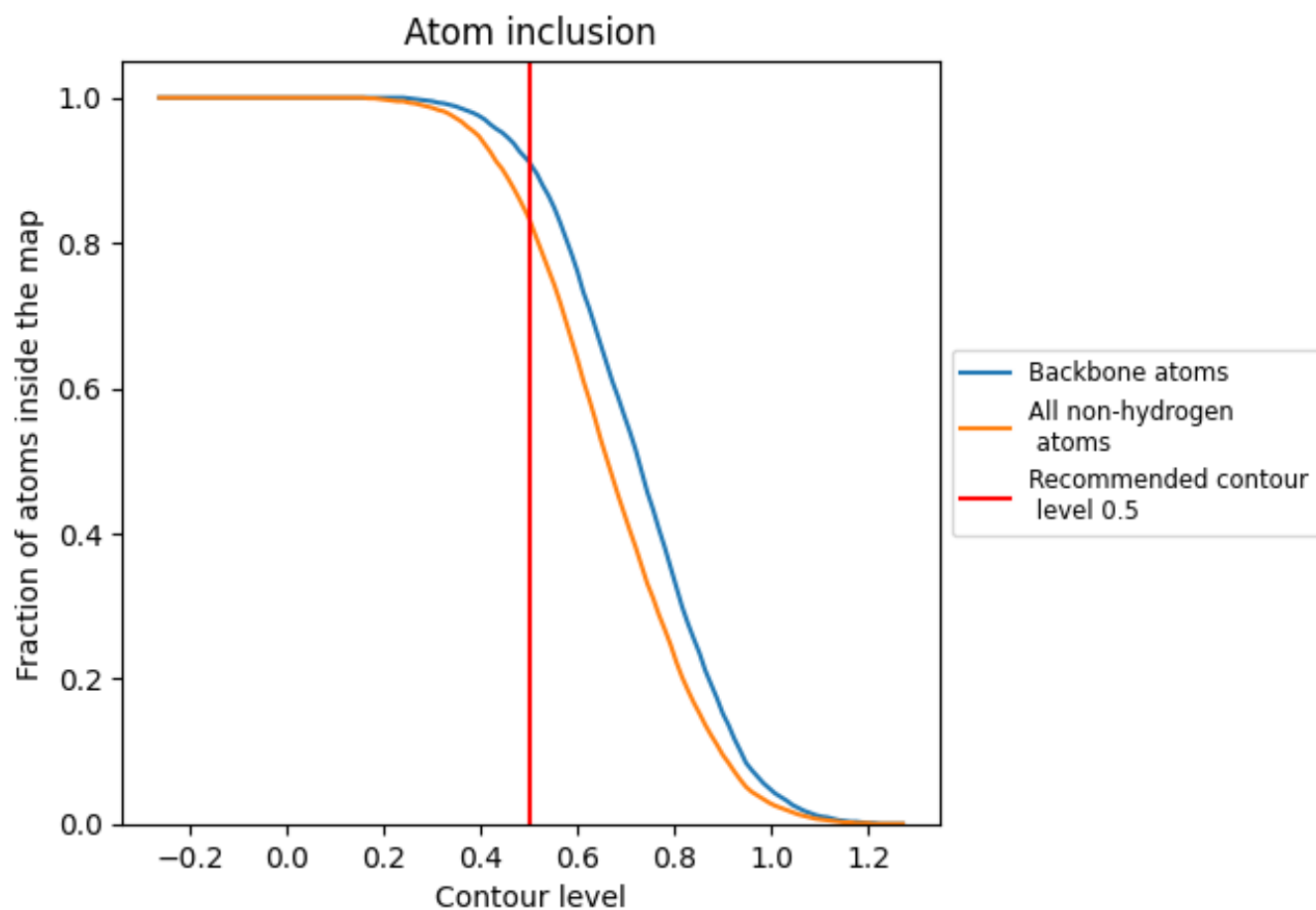
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































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





















































































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