Full wwPDB EM Validation Report ⓘ

Mar 18, 2025 – 11:19 PM JST

PDB ID	:	8YJT
EMDB ID	:	EMD-39349
Title	:	Cryo-EM structure of the flagellar C ring in the CCW state
Authors	:	Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on	:	2024-03-02
Resolution	:	5.90 Å(reported)
Based on initial models	:	., ?

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

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

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

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

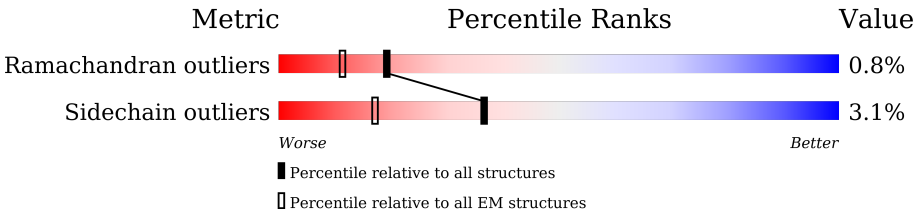
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance

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

The reported resolution of this entry is 5.90 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	3	331	7% 93% · 5%
1	9	331	7% 93% · 5%
1	A1	331	7% 93% · 5%
1	A7	331	6% 93% · 5%
1	AE	331	7% 93% · 5%
1	AK	331	6% 93% · 5%
1	AQ	331	7% 93% · 5%
1	AW	331	7% 93% · 5%
1	Ac	331	7% 93% · 5%

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Mol	Chain	Length	Quality of chain
1	Ai	331	6% 93% 5%
1	Ao	331	8% 93% 5%
1	Au	331	7% 93% 5%
1	B5	331	7% 93% 5%
1	BC	331	7% 93% 5%
1	BI	331	8% 93% 5%
1	BO	331	7% 93% 5%
1	BU	331	7% 93% 5%
1	Ba	331	7% 93% 5%
1	Bg	331	7% 93% 5%
1	Bm	331	7% 93% 5%
1	Bs	331	7% 93% 5%
1	By	331	6% 93% 5%
1	CA	331	7% 93% 5%
1	CG	331	7% 93% 5%
1	CM	331	6% 93% 5%
1	CS	331	8% 93% 5%
1	CY	331	7% 93% 5%
1	Ce	331	7% 93% 5%
1	Ck	331	6% 93% 5%
1	Cq	331	7% 93% 5%
1	Cw	331	8% 93% 5%
1	k	331	7% 93% 5%
1	q	331	7% 93% 5%
1	w	331	7% 93% 5%

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Mol	Chain	Length	Quality of chain
2	0	560	5% 95%
2	4	560	5% 95%
2	A2	560	5% 95%
2	A8	560	5% 95%
2	AF	560	5% 95%
2	AL	560	5% 95%
2	AR	560	5% 95%
2	AX	560	5% 95%
2	Ad	560	5% 95%
2	Aj	560	5% 95%
2	Ap	560	5% 95%
2	Av	560	5% 95%
2	B6	560	5% 95%
2	BD	560	5% 95%
2	BJ	560	5% 95%
2	BP	560	5% 95%
2	BV	560	5% 95%
2	Bb	560	5% 95%
2	Bh	560	5% 95%
2	Bn	560	5% 95%
2	Bt	560	5% 95%
2	Bz	560	5% 95%
2	CB	560	5% 95%
2	CH	560	5% 95%
2	CN	560	5% 95%

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Mol	Chain	Length	Quality of chain
2	CT	560	5% 95%
2	CZ	560	5% 95%
2	Cf	560	5% 95%
2	Cl	560	5% 95%
2	Cr	560	5% 95%
2	Cx	560	5% 95%
2	l	560	5% 95%
2	r	560	5% 95%
2	x	560	5% 95%
3	5	334	82% 13%
3	A3	334	82% 13%
3	A9	334	82% 13%
3	AA	334	82% 13%
3	AG	334	82% 13%
3	AM	334	82% 13%
3	AS	334	82% 13%
3	AY	334	82% 13%
3	Ae	334	82% 13%
3	Ak	334	82% 13%
3	Aq	334	82% 13%
3	Aw	334	82% 13%
3	B1	334	82% 13%
3	B7	334	82% 13%
3	BE	334	82% 13%
3	BK	334	82% 13%

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Mol	Chain	Length	Quality of chain
3	BQ	334	82% · 13%
3	BW	334	82% · 13%
3	Bc	334	82% · 13%
3	Bi	334	82% · 13%
3	Bo	334	82% · 13%
3	Bu	334	82% · 13%
3	CC	334	82% · 13%
3	CI	334	82% · 13%
3	CO	334	82% · 13%
3	CU	334	82% · 13%
3	Ca	334	82% · 13%
3	Cg	334	82% · 13%
3	Cm	334	82% · 13%
3	Cs	334	82% · 13%
3	Cy	334	82% · 13%
3	m	334	82% · 13%
3	s	334	82% · 13%
3	y	334	82% · 13%
4	1	137	61% · 36%
4	2	137	61% · 36%
4	6	137	61% · 36%
4	7	137	61% · 36%
4	8	137	61% · 36%
4	A0	137	61% · 36%
4	A4	137	61% · 36%

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Mol	Chain	Length	Quality of chain
4	A5	137	61% 36%
4	A6	137	61% 36%
4	AB	137	61% 36%
4	AC	137	61% 36%
4	AD	137	61% 36%
4	AH	137	61% 36%
4	AI	137	61% 36%
4	AJ	137	61% 36%
4	AN	137	61% 36%
4	AO	137	61% 36%
4	AP	137	61% 36%
4	AT	137	61% 36%
4	AU	137	61% 36%
4	AV	137	61% 36%
4	AZ	137	61% 36%
4	Aa	137	61% 36%
4	Ab	137	61% 36%
4	Af	137	61% 36%
4	Ag	137	61% 36%
4	Ah	137	61% 36%
4	Al	137	61% 36%
4	Am	137	61% 36%
4	An	137	61% 36%
4	Ar	137	61% 36%
4	As	137	61% 36%

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Mol	Chain	Length	Quality of chain
4	At	137	61% 36%
4	Ax	137	61% 36%
4	Ay	137	61% 36%
4	Az	137	61% 36%
4	B0	137	61% 36%
4	B2	137	61% 36%
4	B3	137	61% 36%
4	B4	137	61% 36%
4	B8	137	61% 36%
4	B9	137	61% 36%
4	BA	137	61% 36%
4	BB	137	61% 36%
4	BF	137	61% 36%
4	BG	137	61% 36%
4	BH	137	61% 36%
4	BL	137	61% 36%
4	BM	137	61% 36%
4	BN	137	61% 36%
4	BR	137	61% 36%
4	BS	137	61% 36%
4	BT	137	61% 36%
4	BX	137	61% 36%
4	BY	137	61% 36%
4	BZ	137	61% 36%
4	Bd	137	61% 36%

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Mol	Chain	Length	Quality of chain
4	Be	137	61% 36%
4	Bf	137	61% 36%
4	Bj	137	61% 36%
4	Bk	137	61% 36%
4	Bl	137	61% 36%
4	Bp	137	61% 36%
4	Bq	137	61% 36%
4	Br	137	61% 36%
4	Bv	137	61% 36%
4	Bw	137	61% 36%
4	Bx	137	61% 36%
4	C1	137	61% 36%
4	C2	137	61% 36%
4	CD	137	61% 36%
4	CE	137	61% 36%
4	CF	137	61% 36%
4	CJ	137	61% 36%
4	CK	137	61% 36%
4	CL	137	61% 36%
4	CP	137	61% 36%
4	CQ	137	61% 36%
4	CR	137	61% 36%
4	CV	137	61% 36%
4	CW	137	61% 36%
4	CX	137	61% 36%

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Mol	Chain	Length	Quality of chain
4	Cb	137	61% 36%
4	Cc	137	61% 36%
4	Cd	137	61% 36%
4	Ch	137	61% 36%
4	Ci	137	61% 36%
4	Cj	137	61% 36%
4	Cn	137	61% 36%
4	Co	137	61% 36%
4	Cp	137	61% 36%
4	Ct	137	61% 36%
4	Cu	137	61% 36%
4	Cv	137	61% 36%
4	Cz	137	61% 36%
4	n	137	61% 36%
4	o	137	61% 36%
4	p	137	61% 36%
4	t	137	61% 36%
4	u	137	61% 36%
4	v	137	61% 36%
4	z	137	61% 36%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 239768 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 motor switch protein FliG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	k	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	q	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	w	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	3	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	9	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	AE	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	AK	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	AQ	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	AW	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Ac	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Ai	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Ao	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Au	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	A1	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	A7	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	BC	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	BI	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BO	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	BU	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Ba	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Bg	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Bm	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Bs	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	By	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	B5	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	CA	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	CG	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	CM	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	CS	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	CY	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Ce	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Ck	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Cq	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
1	Cw	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		

- Molecule 2 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	l	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	r	27	Total	C	N	O	S	0	0
			224	135	44	42	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	x	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	4	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	0	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	AF	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	AL	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	AR	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	AX	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Ad	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Aj	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Ap	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Av	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	A2	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	A8	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	BD	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	BJ	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	BP	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	BV	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Bb	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Bh	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Bn	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Bt	27	Total	C	N	O	S	0	0
			224	135	44	42	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bz	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	B6	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	CB	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	CH	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	CN	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	CT	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	CZ	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Cf	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Cl	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Cr	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Cx	27	Total	C	N	O	S	0	0
			224	135	44	42	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	m	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	s	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	y	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	5	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	AA	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	AG	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	AM	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	AS	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	AY	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Ae	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Ak	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Aq	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Aw	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	A3	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	A9	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	BE	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	BK	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	BQ	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	BW	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Bc	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Bi	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Bo	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Bu	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	B1	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	B7	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	CC	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	CI	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	CO	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	CU	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ca	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Cg	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Cm	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Cs	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
3	Cy	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	o	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	p	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	t	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	u	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	v	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	z	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	1	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	2	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	6	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	7	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	8	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AB	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AC	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AH	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AI	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AJ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AN	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AO	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AP	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AT	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AU	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AV	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	AZ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Aa	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Ab	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Af	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Ag	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Ah	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Al	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Am	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	An	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Ar	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	As	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	At	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Ax	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Ay	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Az	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	A4	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	A5	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	A6	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	A0	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BA	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BB	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BF	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BG	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BH	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BL	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BM	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BN	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BR	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BS	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BT	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BX	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	BY	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	BZ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Bd	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Be	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Bf	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Bj	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Bk	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Bl	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Bp	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Bq	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Br	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Bv	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Bw	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Bx	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	B2	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	B3	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	B4	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	B8	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	B9	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	B0	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CD	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CE	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	CF	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CJ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CK	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CL	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CP	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CQ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CR	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CV	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CW	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	CX	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Cb	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Cc	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Cd	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Ch	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Ci	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Cj	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Cn	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Co	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Cp	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Ct	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Cu	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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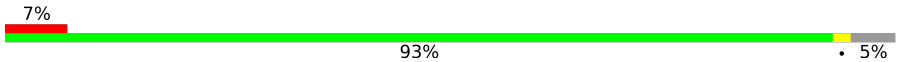
Mol	Chain	Residues	Atoms					AltConf	Trace
4	Cv	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	Cz	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	C1	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
4	C2	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

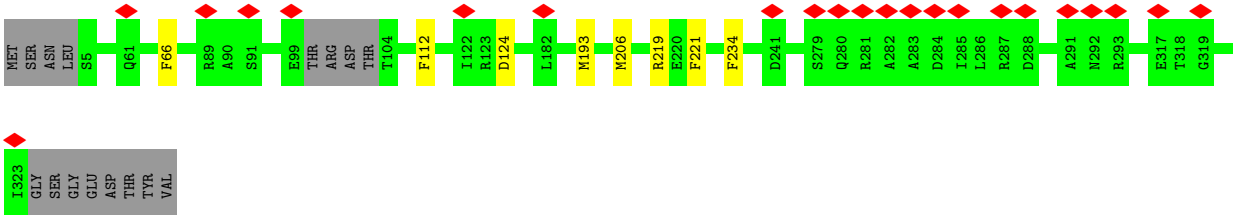
3 Residue-property plots (i)

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

• Molecule 1: Flagellar motor switch protein FliG

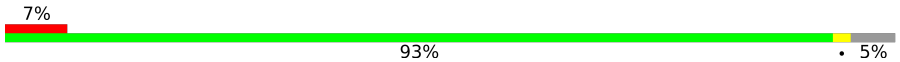
Chain k:

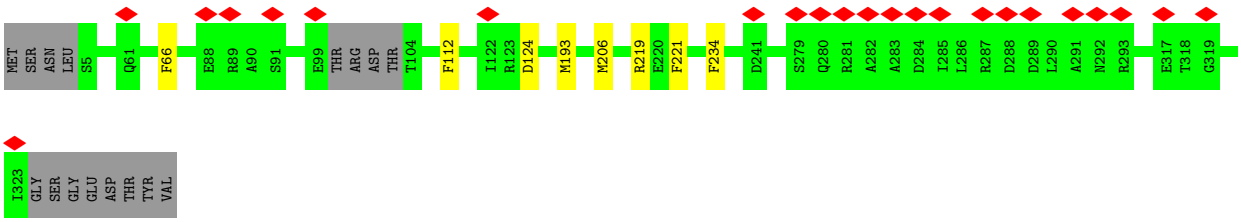




• Molecule 1: Flagellar motor switch protein FliG

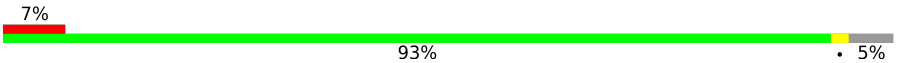
Chain q:

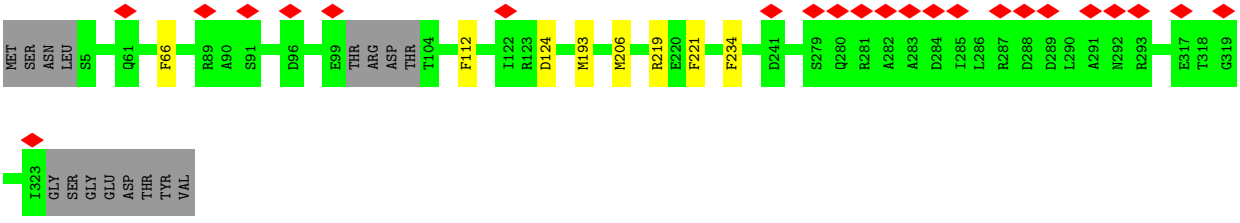




• Molecule 1: Flagellar motor switch protein FliG

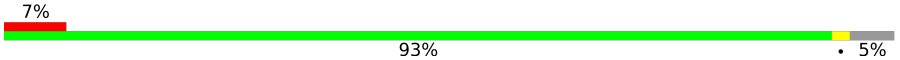
Chain w:

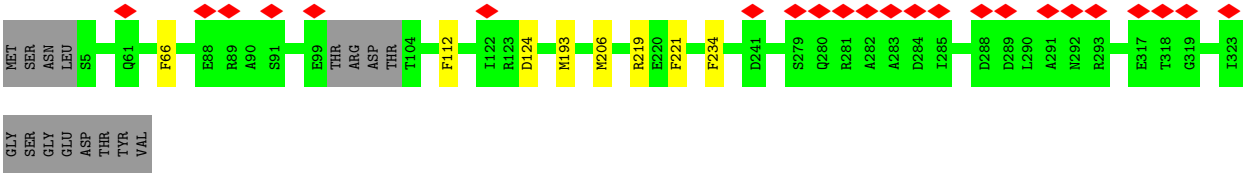




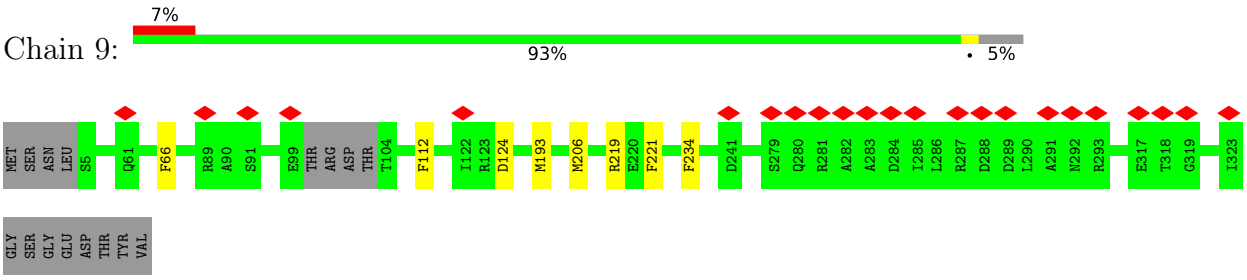
• Molecule 1: Flagellar motor switch protein FliG

Chain 3:

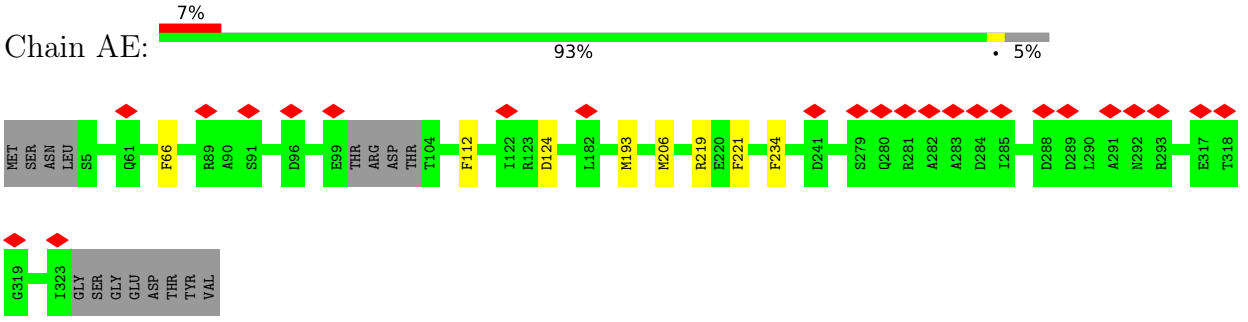




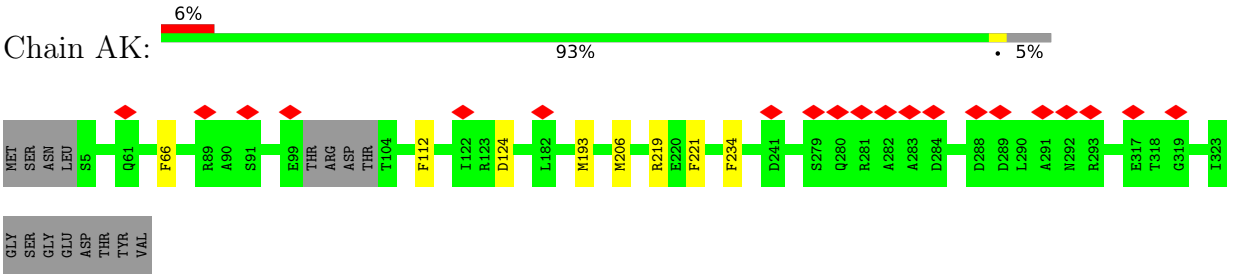
• Molecule 1: Flagellar motor switch protein FliG



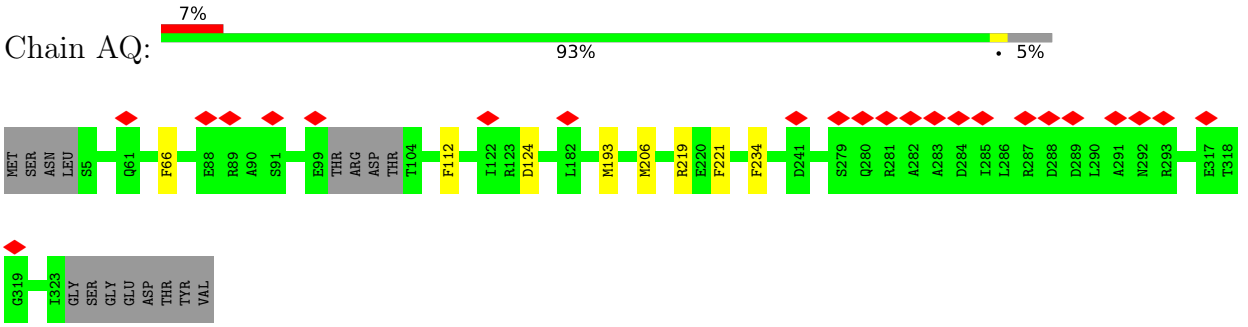
• Molecule 1: Flagellar motor switch protein FliG



• Molecule 1: Flagellar motor switch protein FliG

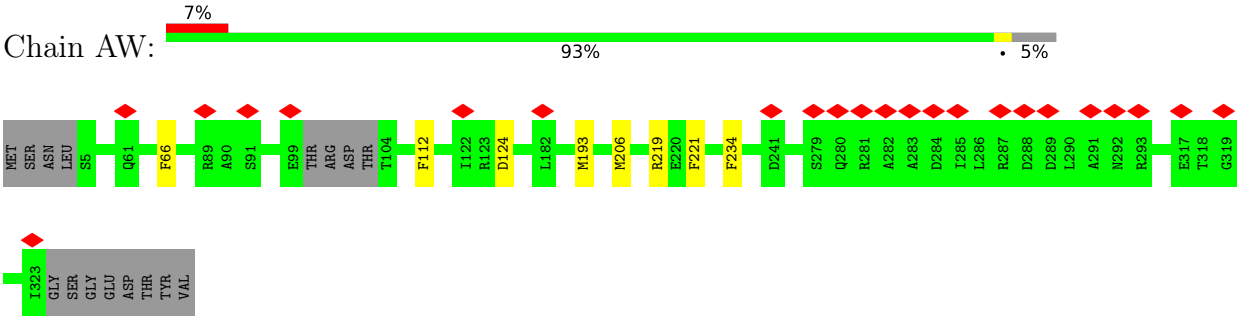


• Molecule 1: Flagellar motor switch protein FliG



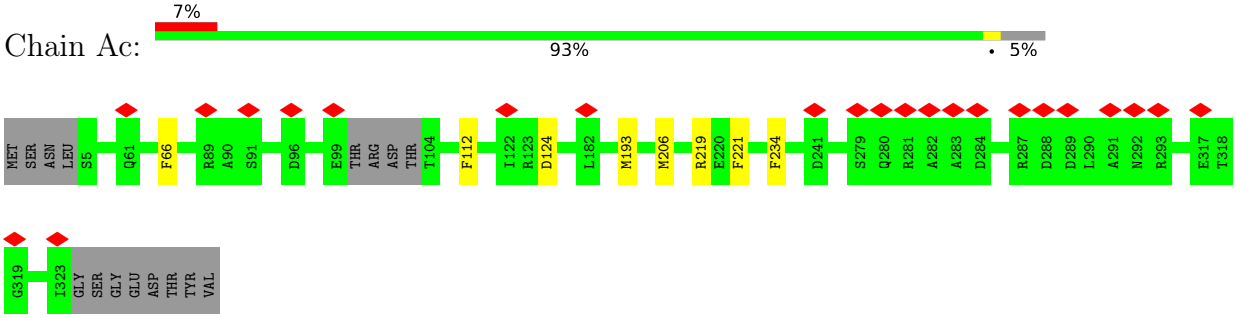
• Molecule 1: Flagellar motor switch protein FliG

Chain AW:



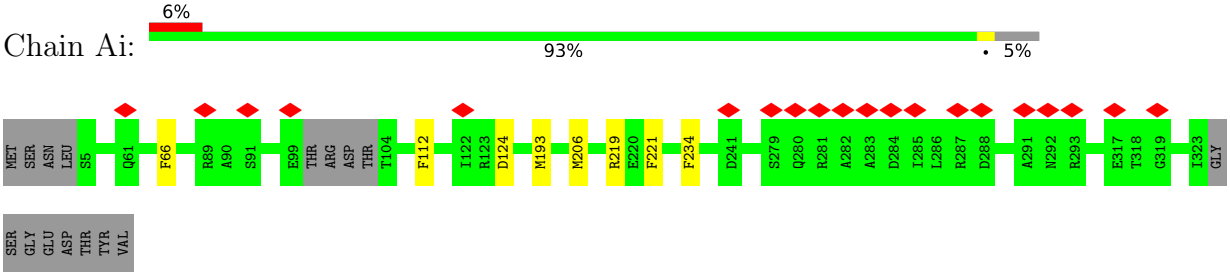
• Molecule 1: Flagellar motor switch protein FliG

Chain Ac:



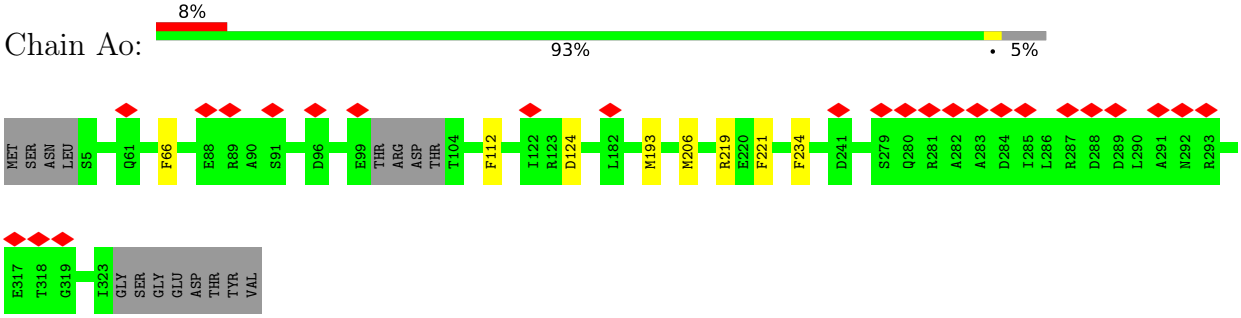
• Molecule 1: Flagellar motor switch protein FliG

Chain Ai:



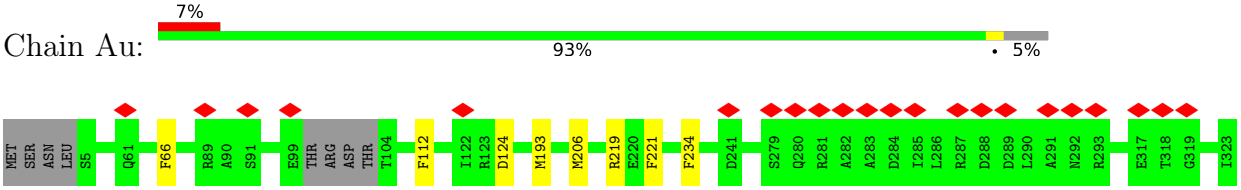
• Molecule 1: Flagellar motor switch protein FliG

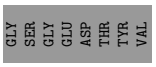
Chain Ao:



• Molecule 1: Flagellar motor switch protein FliG

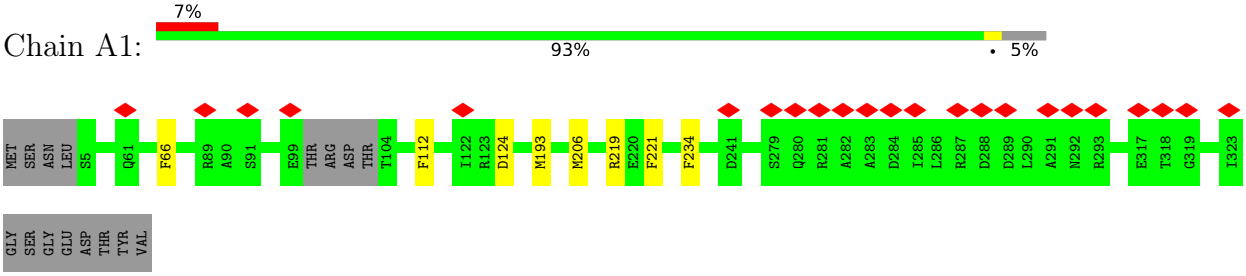
Chain Au:





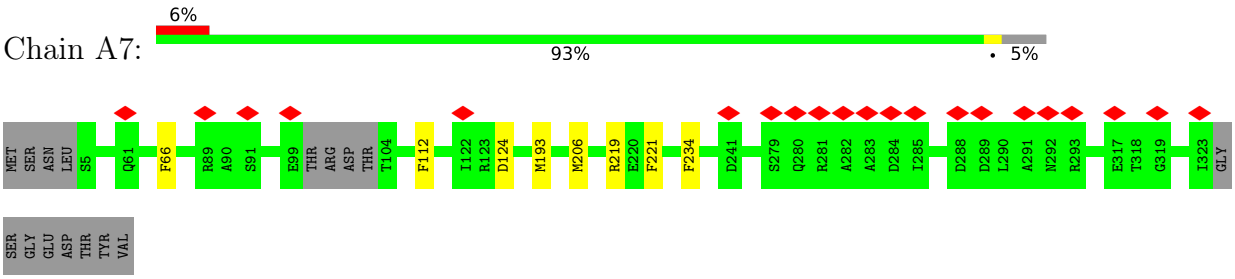
• Molecule 1: Flagellar motor switch protein FliG

Chain A1:



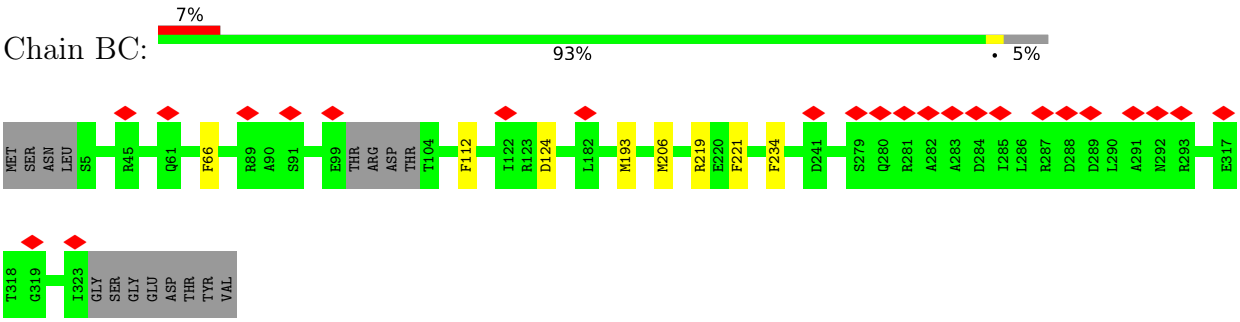
• Molecule 1: Flagellar motor switch protein FliG

Chain A7:



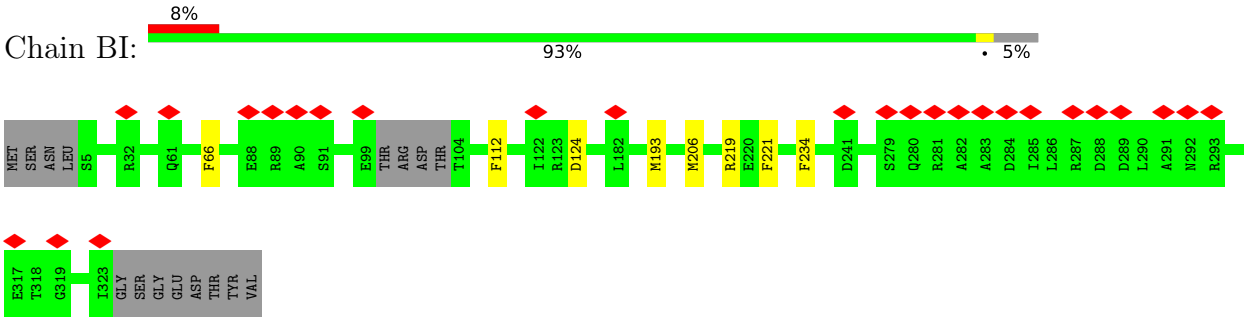
• Molecule 1: Flagellar motor switch protein FliG

Chain BC:



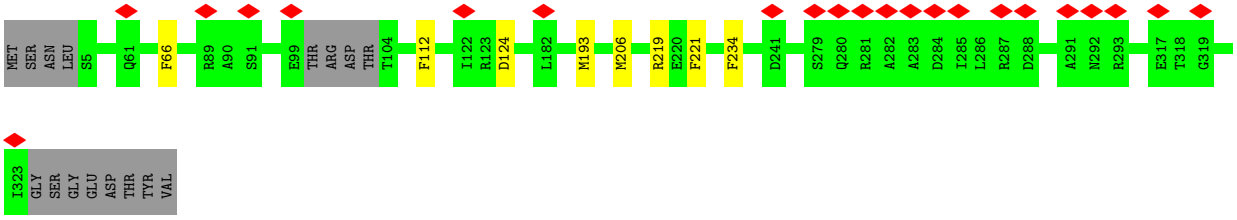
• Molecule 1: Flagellar motor switch protein FliG

Chain BI:

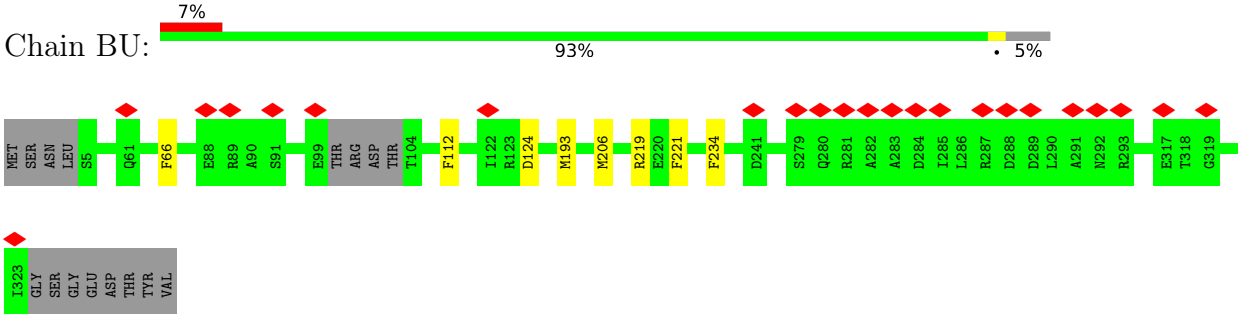


• Molecule 1: Flagellar motor switch protein FliG

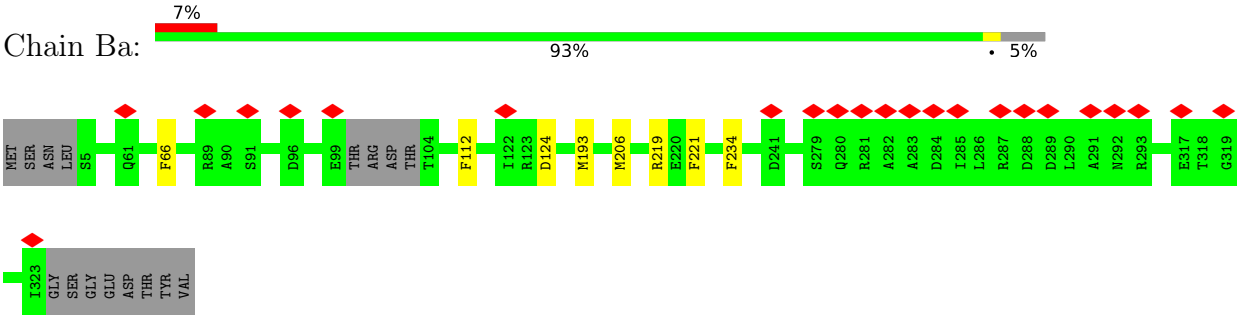
Chain BO:



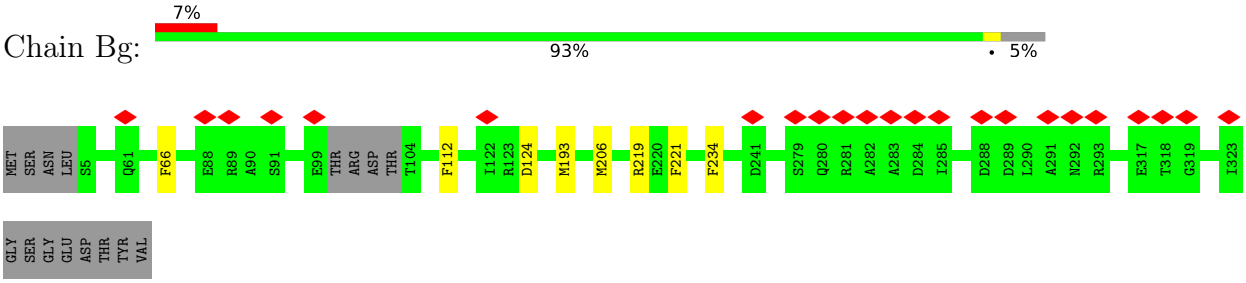
• Molecule 1: Flagellar motor switch protein FliG



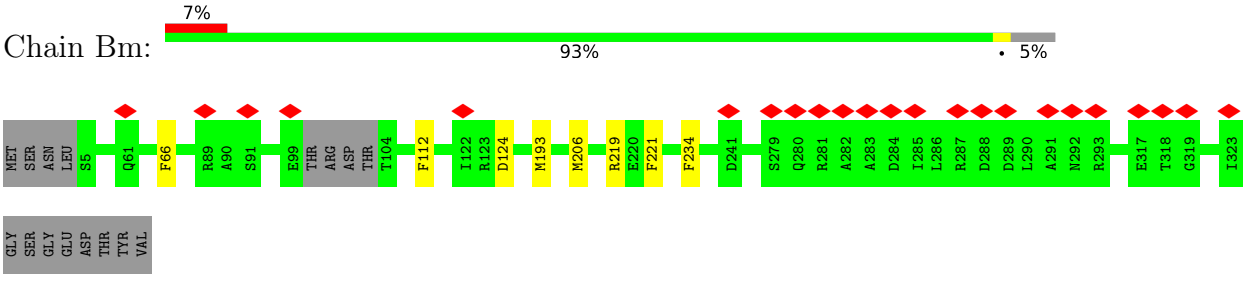
• Molecule 1: Flagellar motor switch protein FliG



• Molecule 1: Flagellar motor switch protein FliG

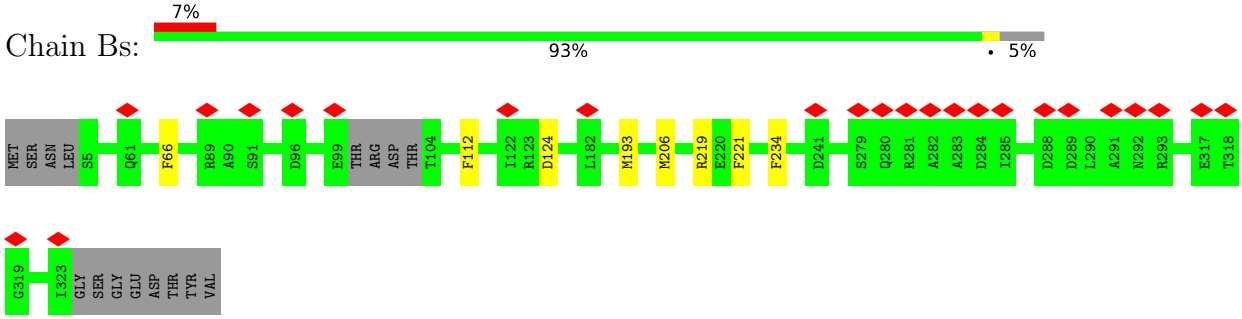


• Molecule 1: Flagellar motor switch protein FliG



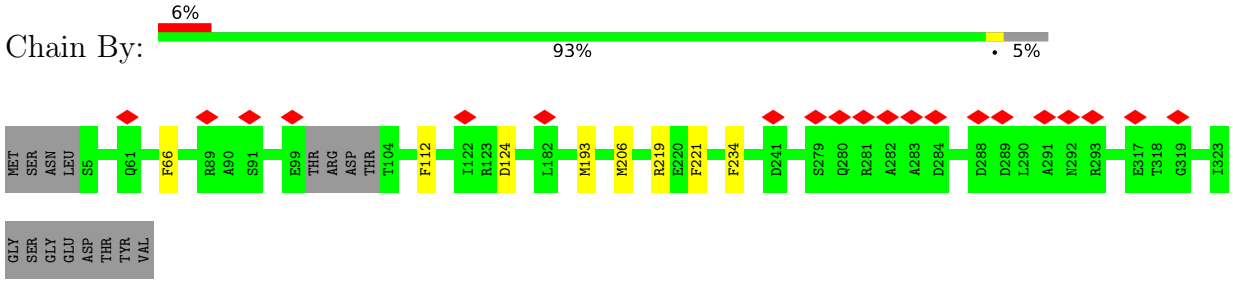
• Molecule 1: Flagellar motor switch protein FliG

Chain Bs:



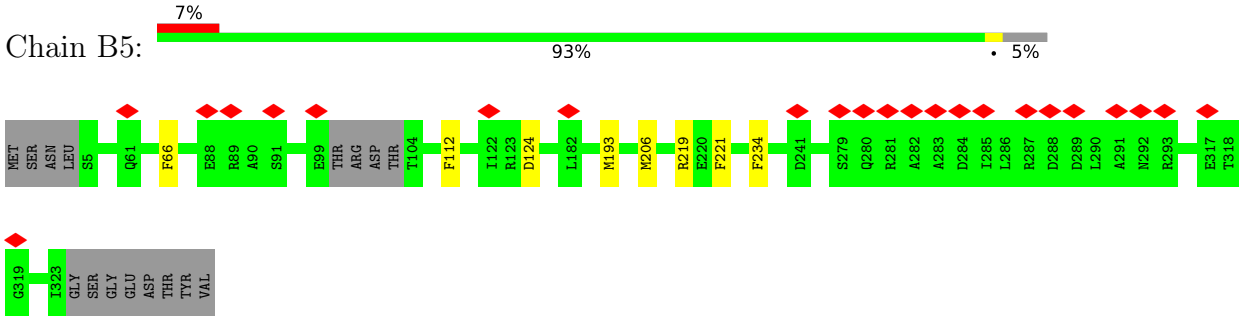
• Molecule 1: Flagellar motor switch protein FliG

Chain By:



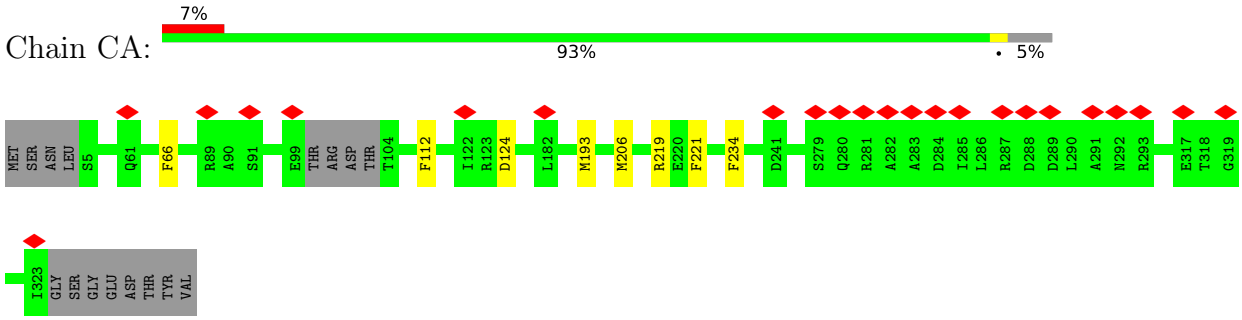
• Molecule 1: Flagellar motor switch protein FliG

Chain B5:



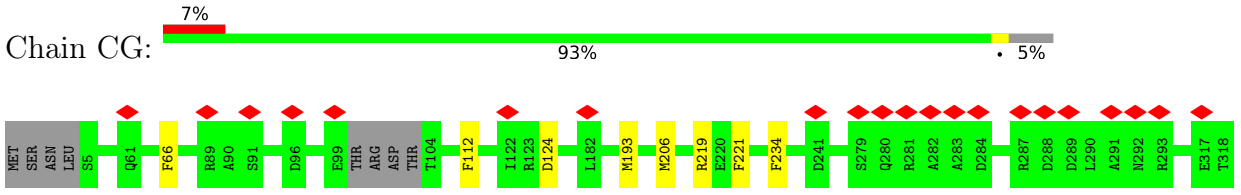
• Molecule 1: Flagellar motor switch protein FliG

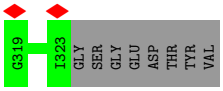
Chain CA:



• Molecule 1: Flagellar motor switch protein FliG

Chain CG:





• Molecule 1: Flagellar motor switch protein FliG

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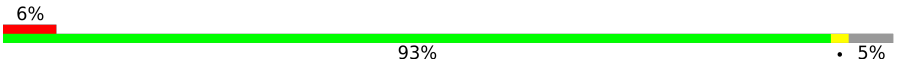
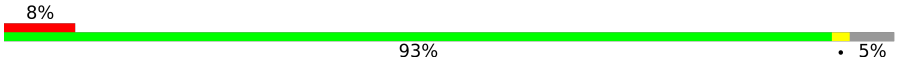
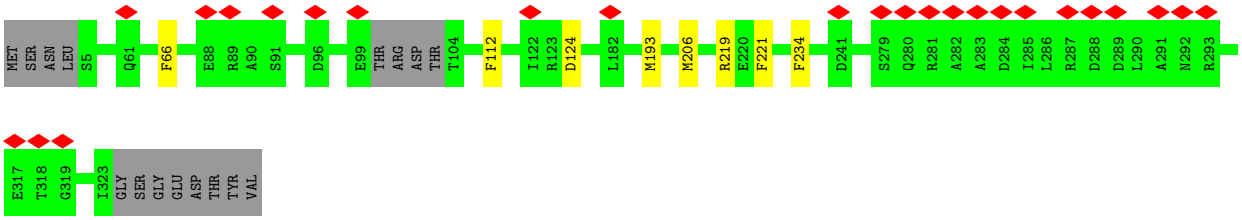


• Molecule 1: Flagellar motor switch protein FliG

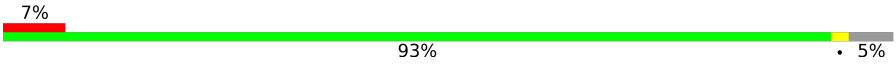
Chain CS:

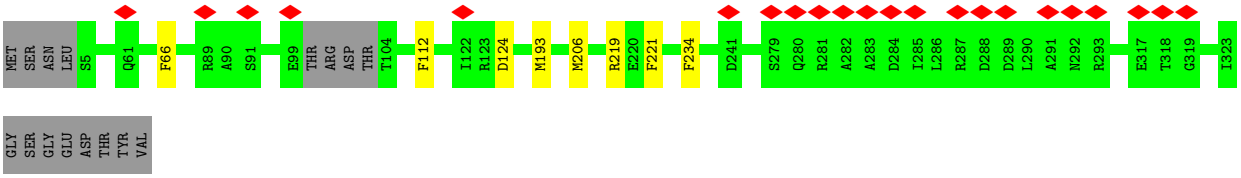




• Molecule 1: Flagellar motor switch protein FliG

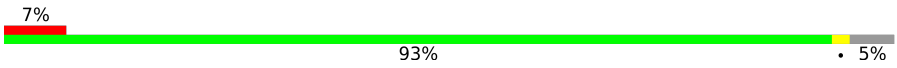
Chain CY:





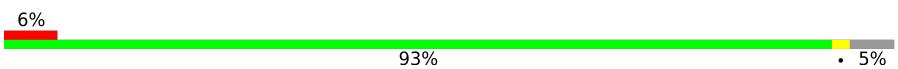
• Molecule 1: Flagellar motor switch protein FliG

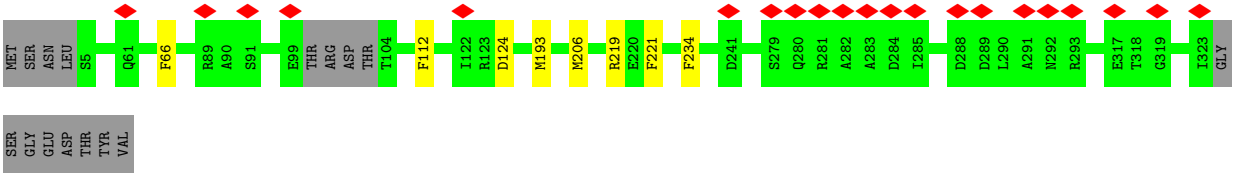
Chain Ce:



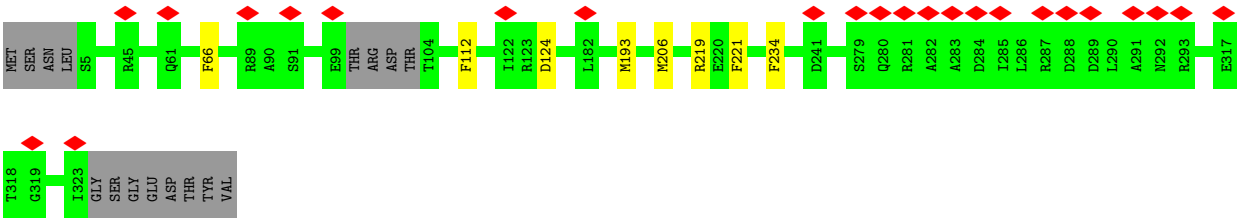
• Molecule 1: Flagellar motor switch protein FliG

Chain Ck:

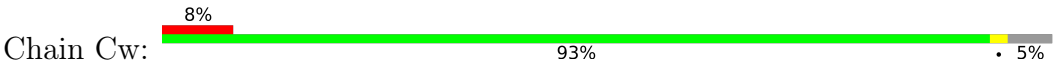


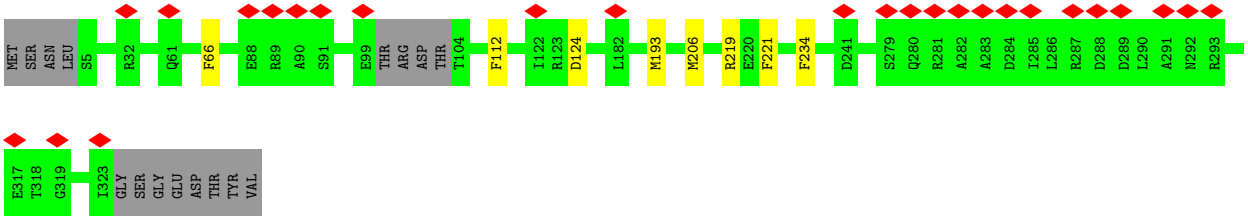


• Molecule 1: Flagellar motor switch protein FliG

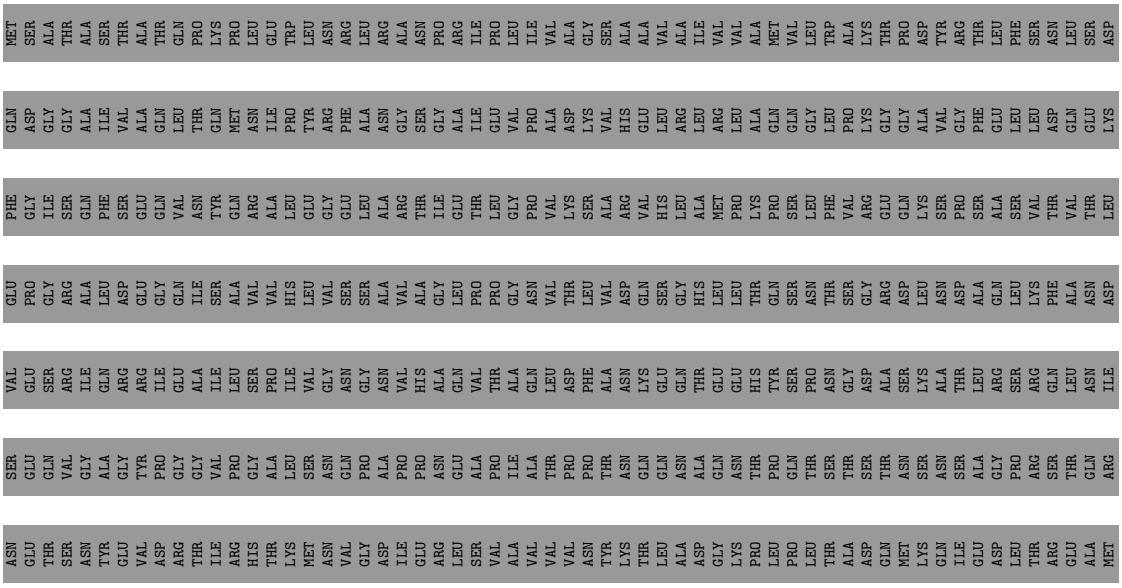


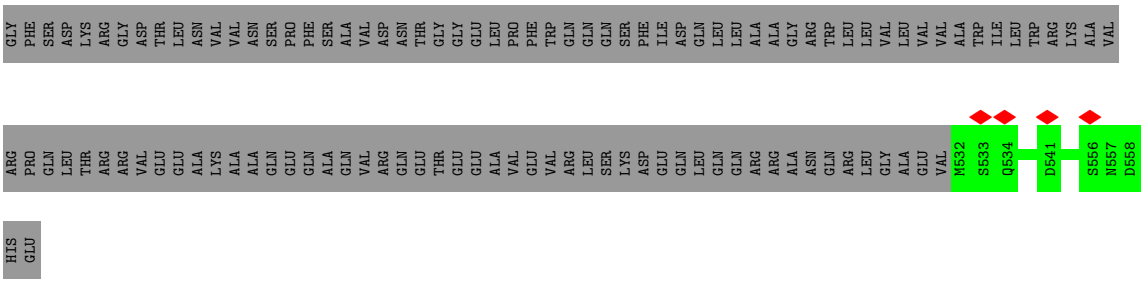
• Molecule 1: Flagellar motor switch protein FliG





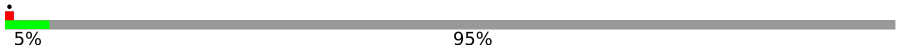
• Molecule 2: Flagellar M-ring protein

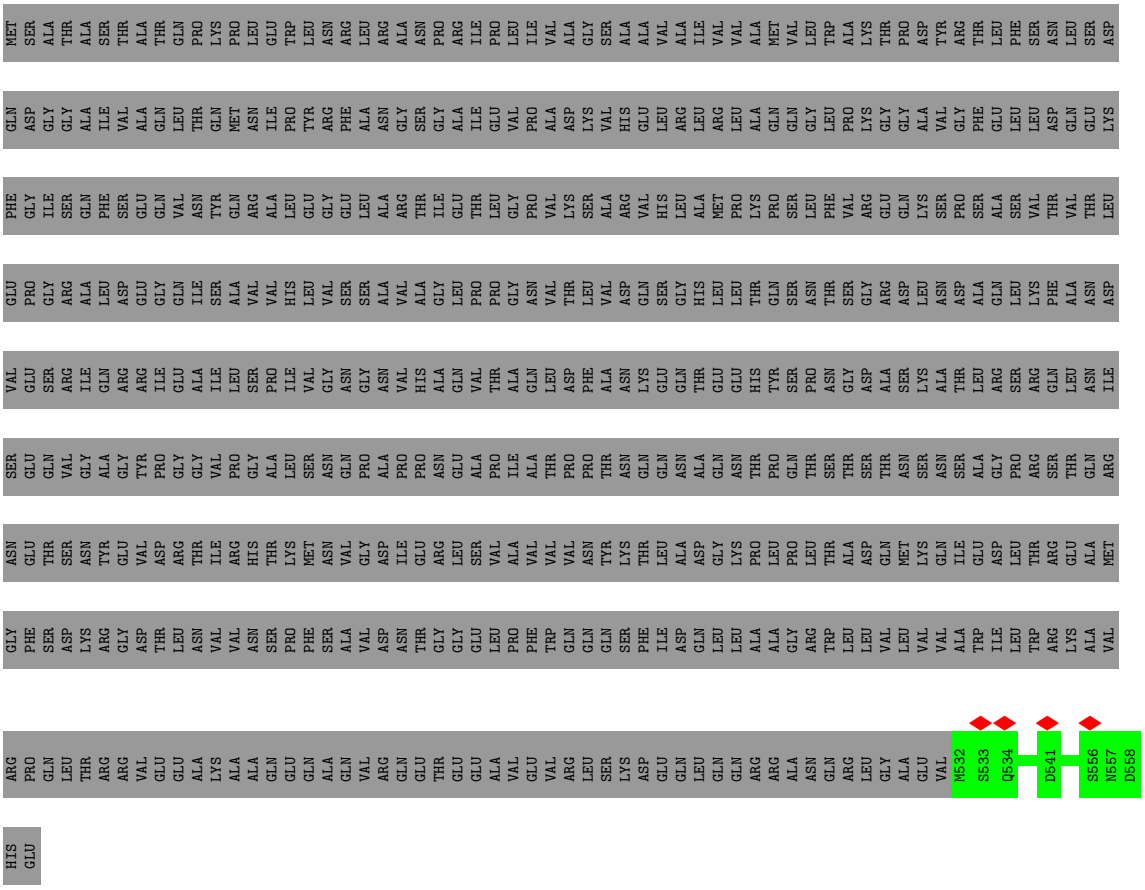




• Molecule 2: Flagellar M-ring protein

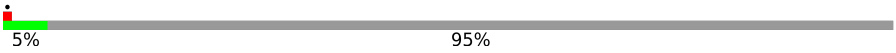
Chain r:

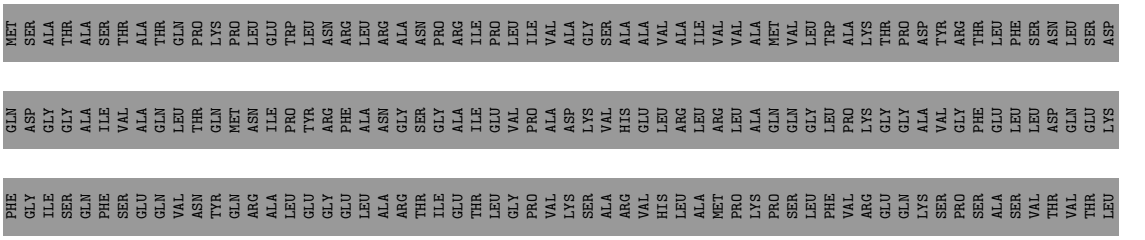


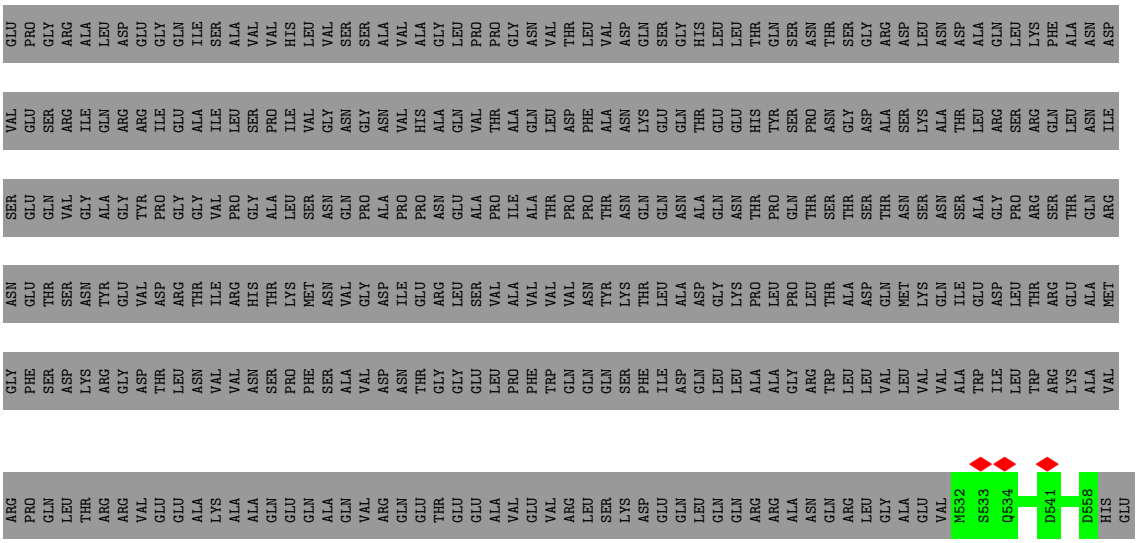


• Molecule 2: Flagellar M-ring protein

Chain x:

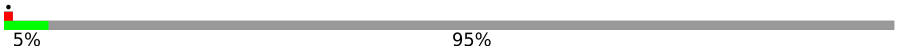


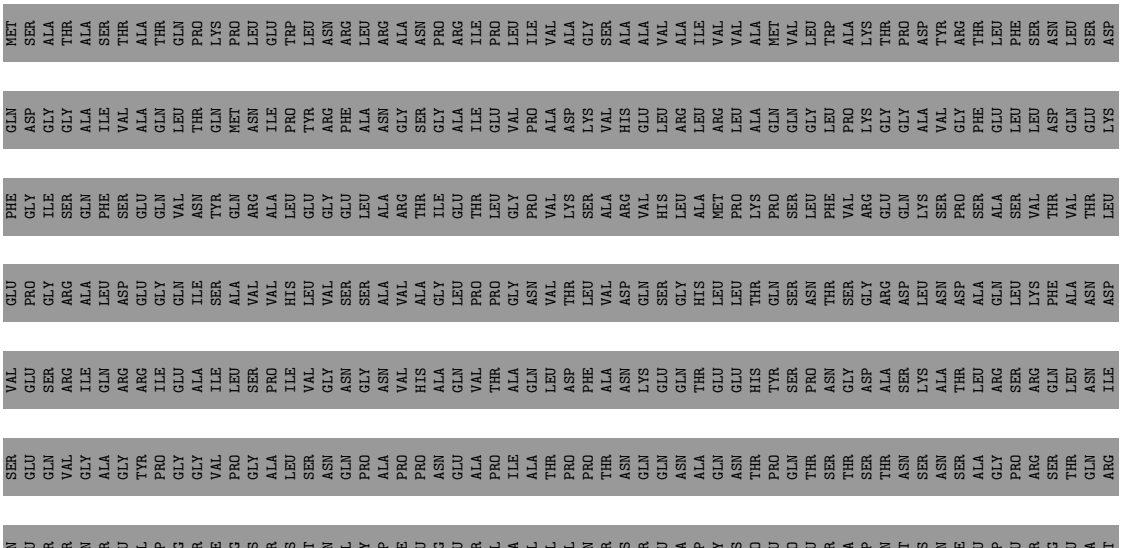




• Molecule 2: Flagellar M-ring protein

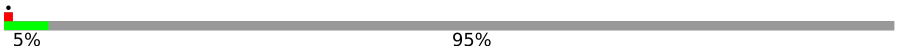
Chain 4:

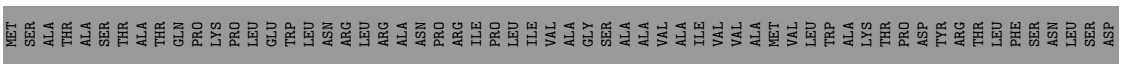


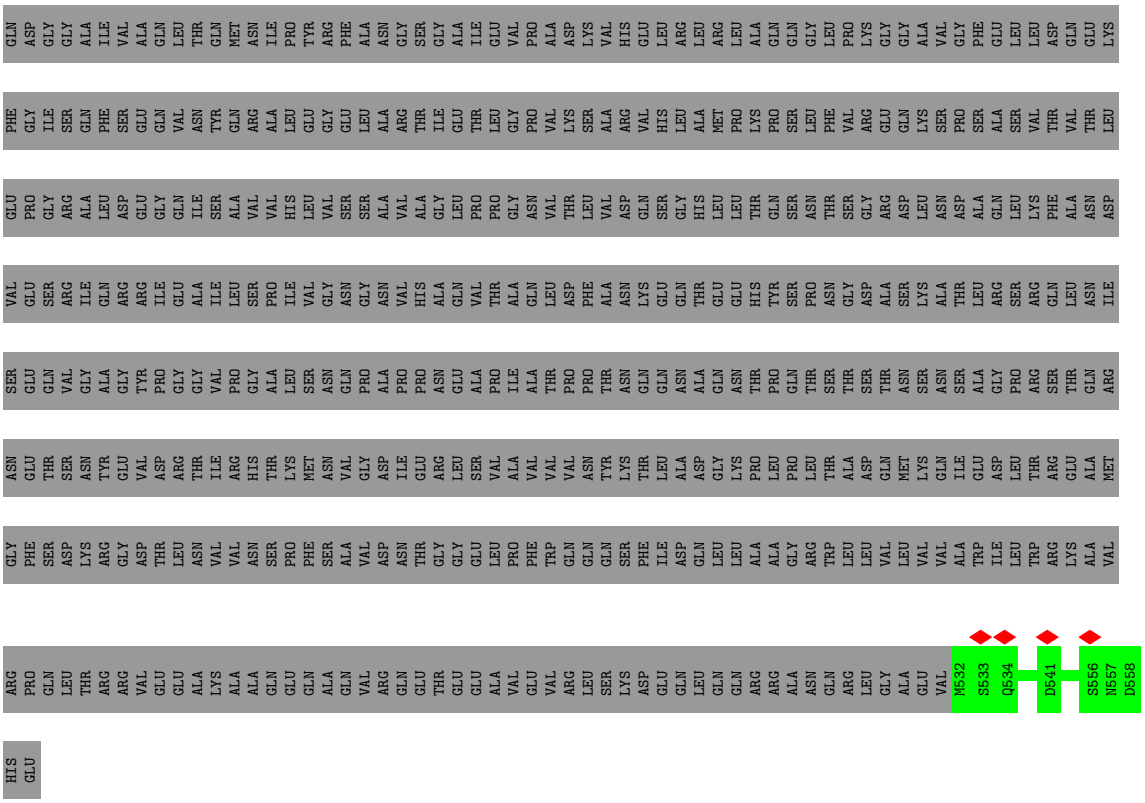


• Molecule 2: Flagellar M-ring protein

Chain 0:

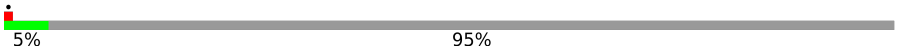


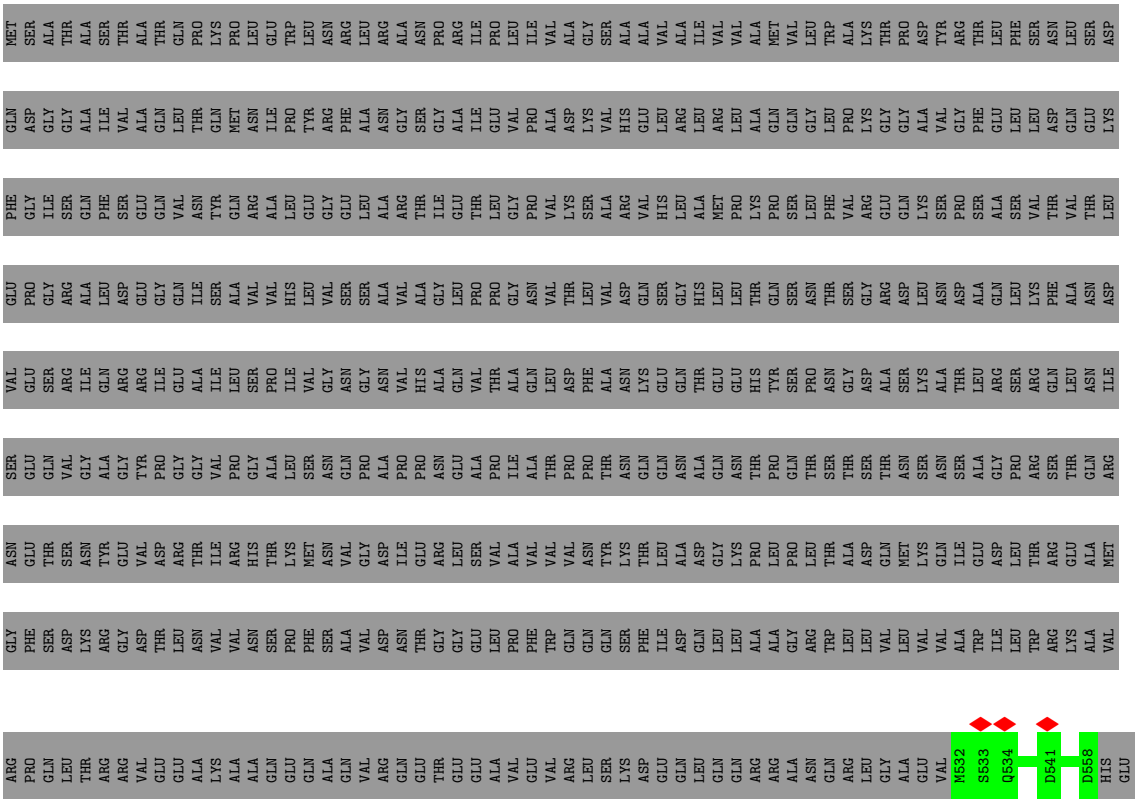




• Molecule 2: Flagellar M-ring protein

Chain AF:





• Molecule 2: Flagellar M-ring protein

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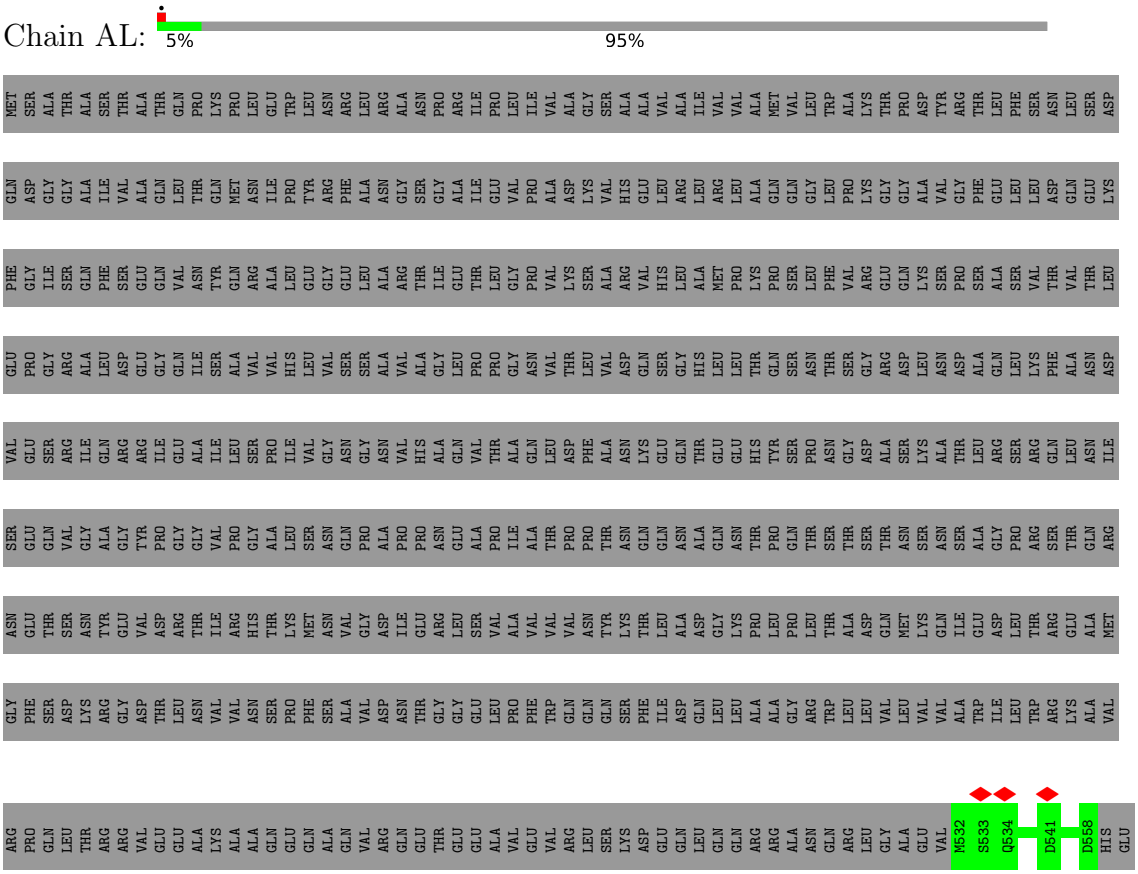

• Molecule 2: Flagellar M-ring protein

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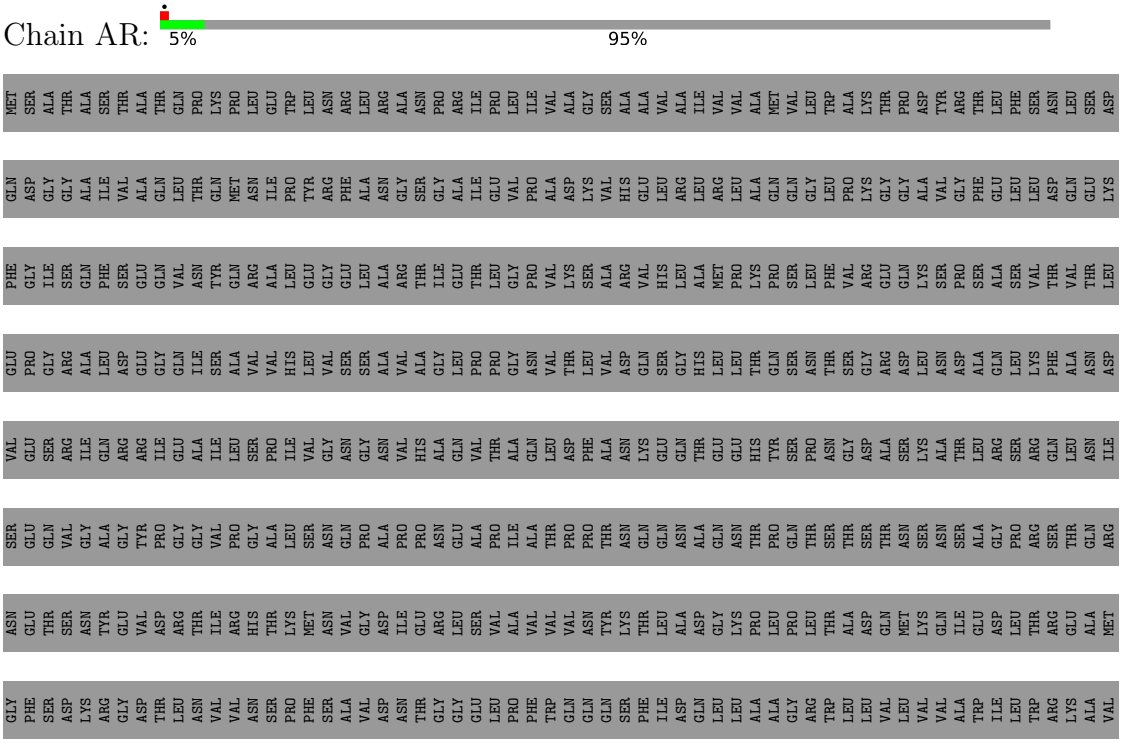
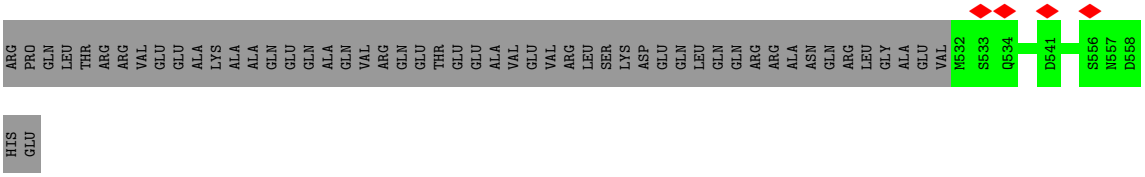
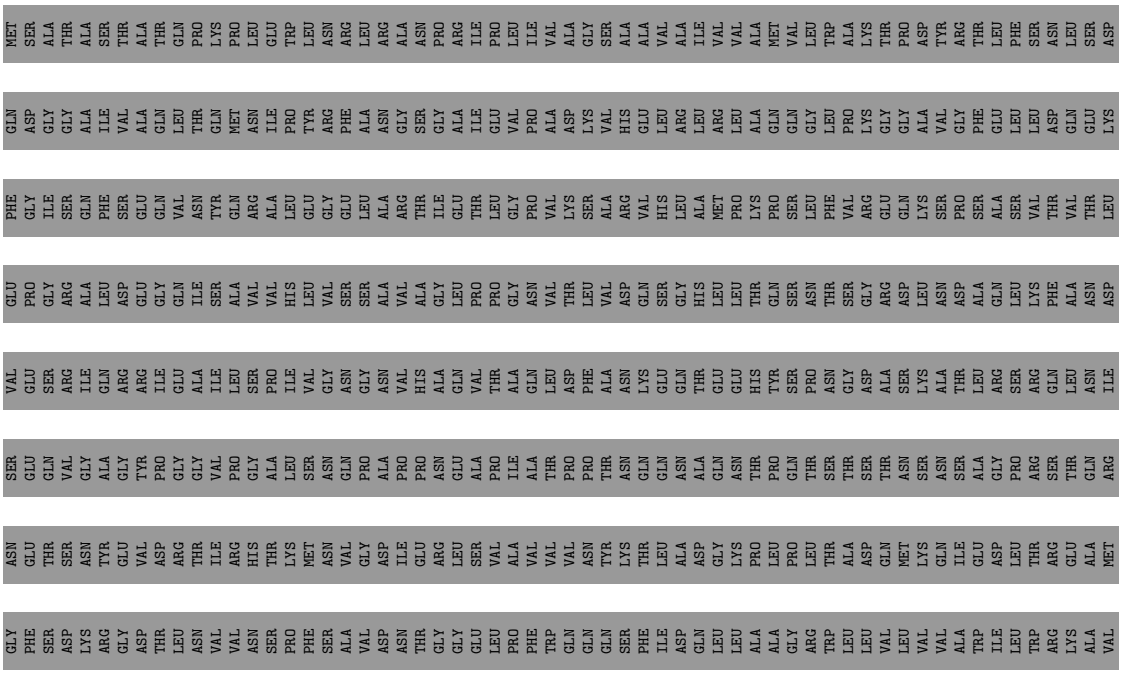




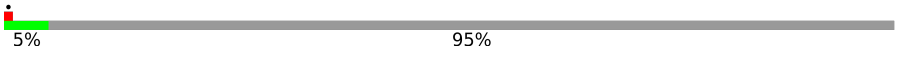
• Molecule 2: Flagellar M-ring protein

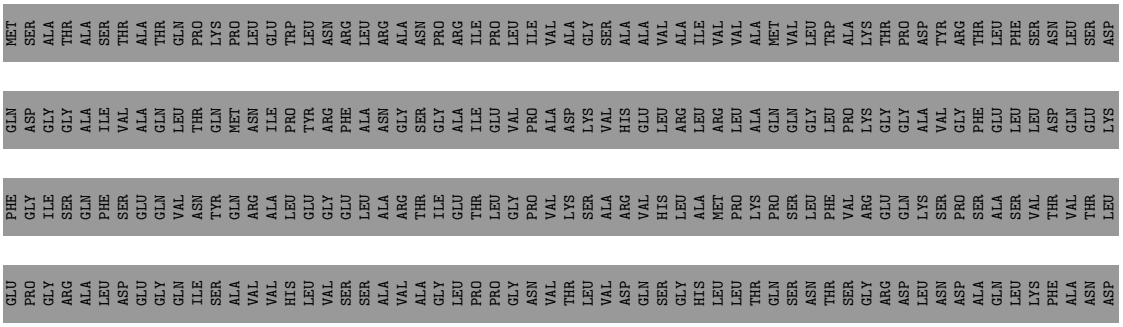
Chain AX:



• Molecule 2: Flagellar M-ring protein

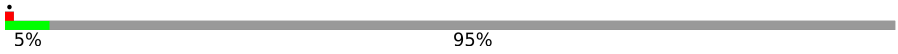
Chain Ad:

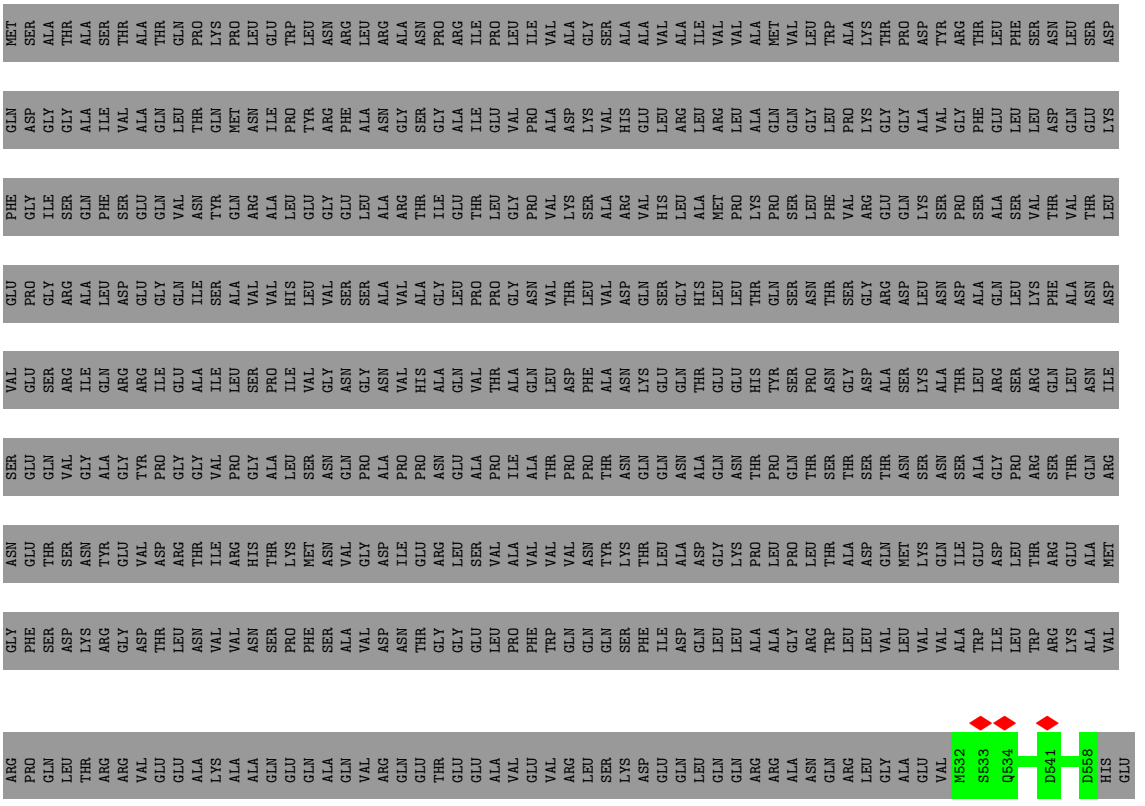




• Molecule 2: Flagellar M-ring protein

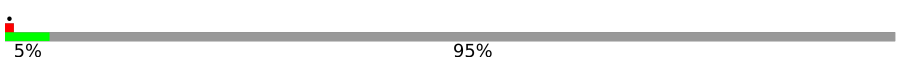
Chain Aj:

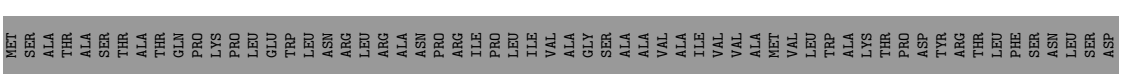


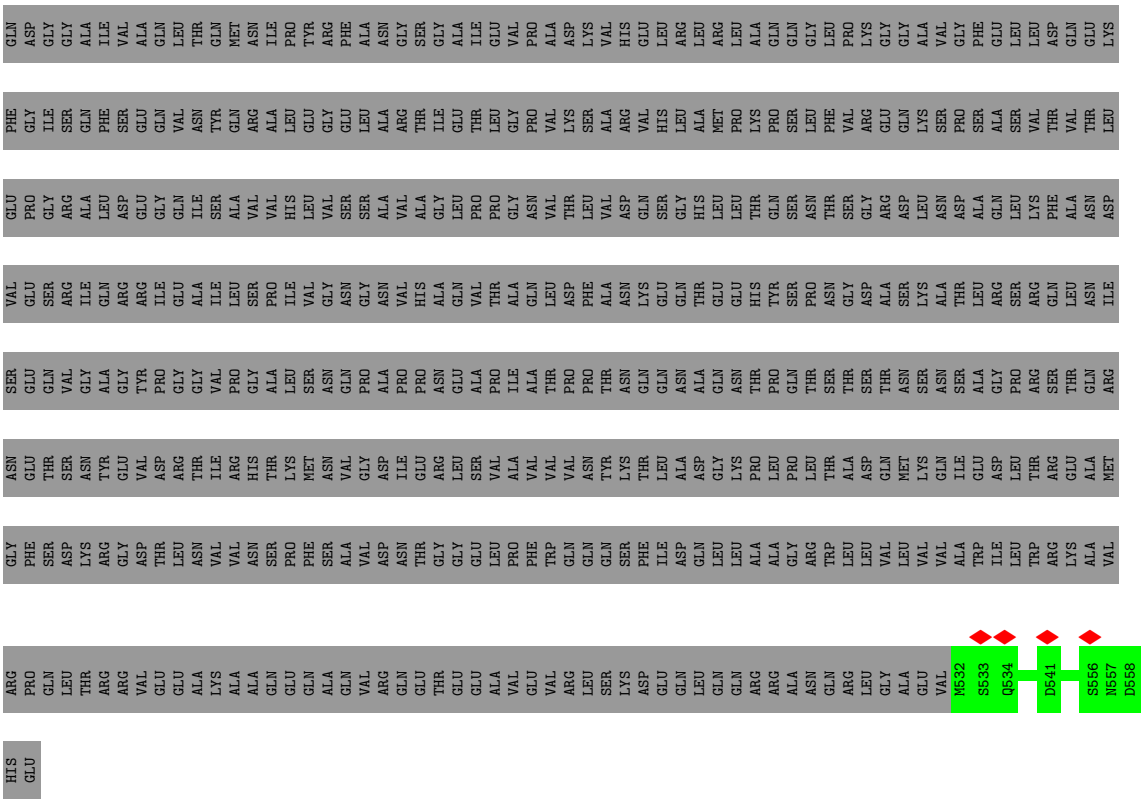


• Molecule 2: Flagellar M-ring protein

Chain Ap:

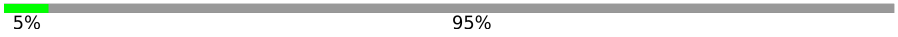


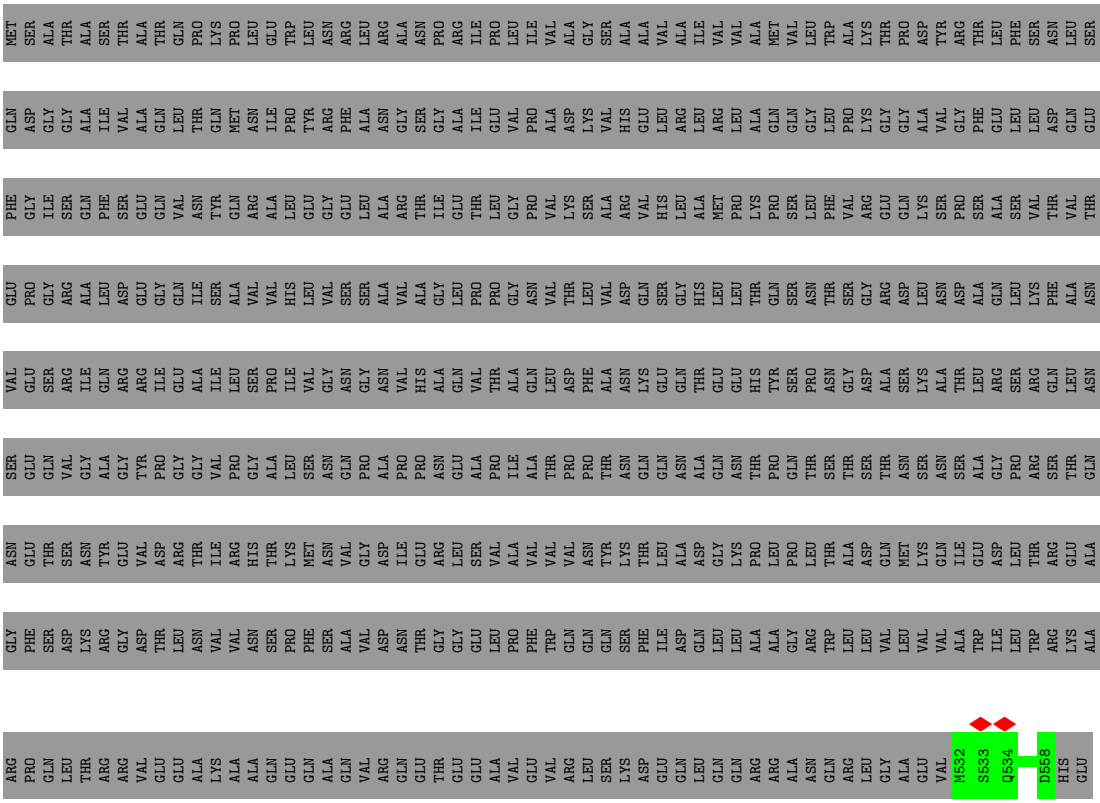




• Molecule 2: Flagellar M-ring protein

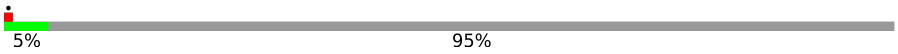
Chain Av:

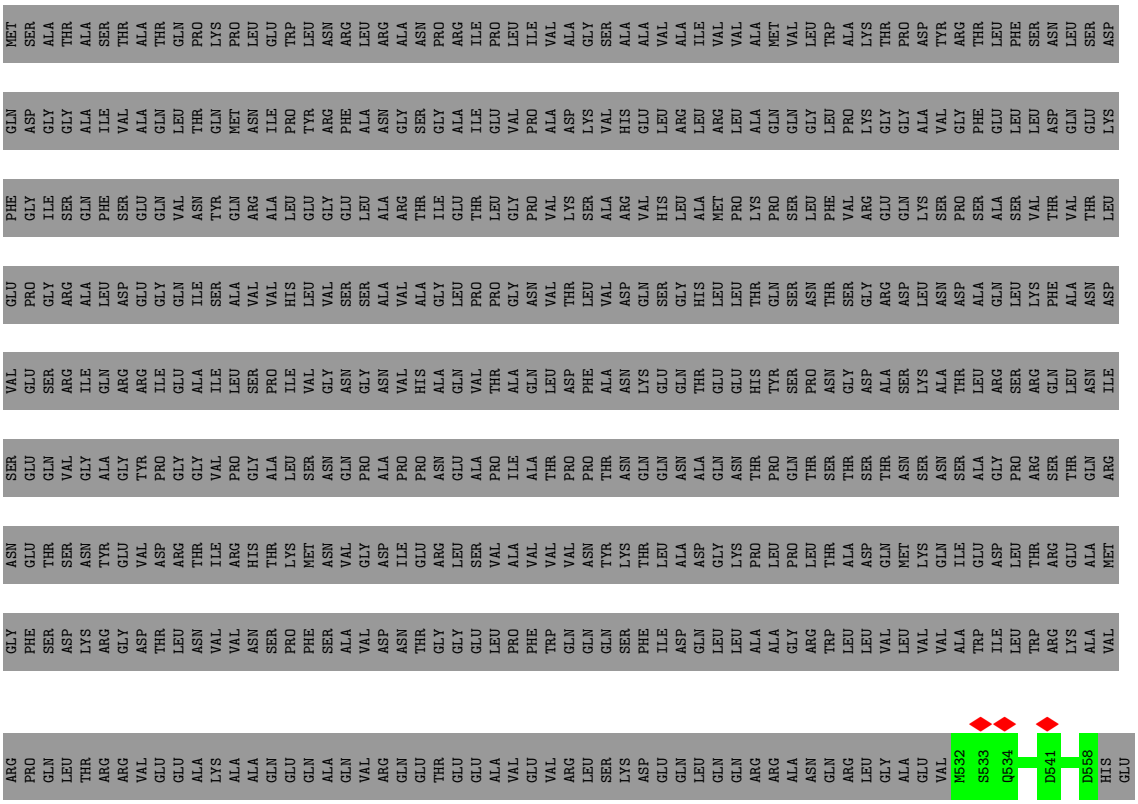




• Molecule 2: Flagellar M-ring protein

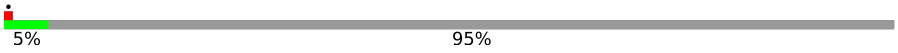
Chain A2:

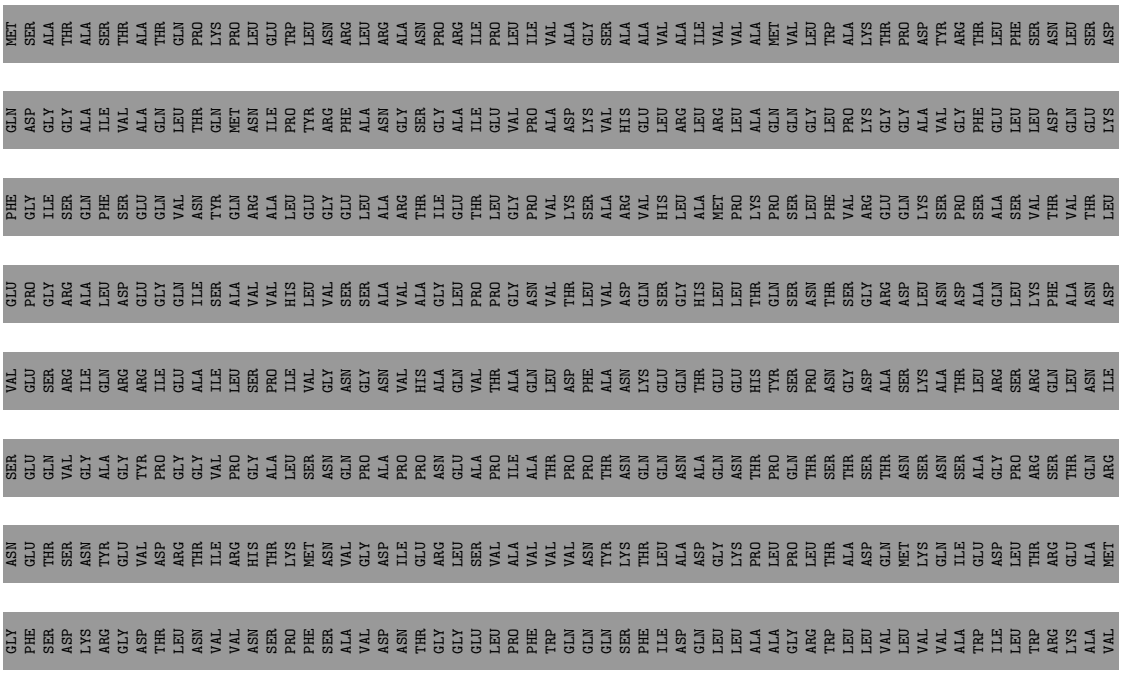


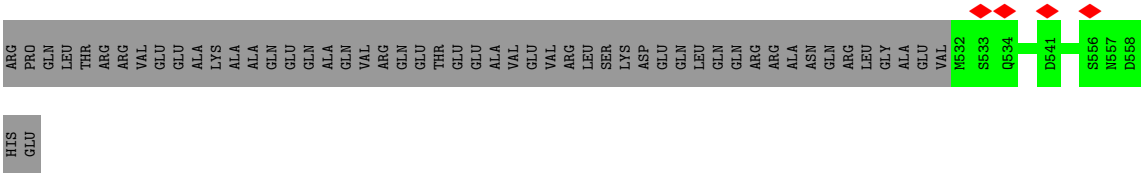


• Molecule 2: Flagellar M-ring protein

Chain A8:

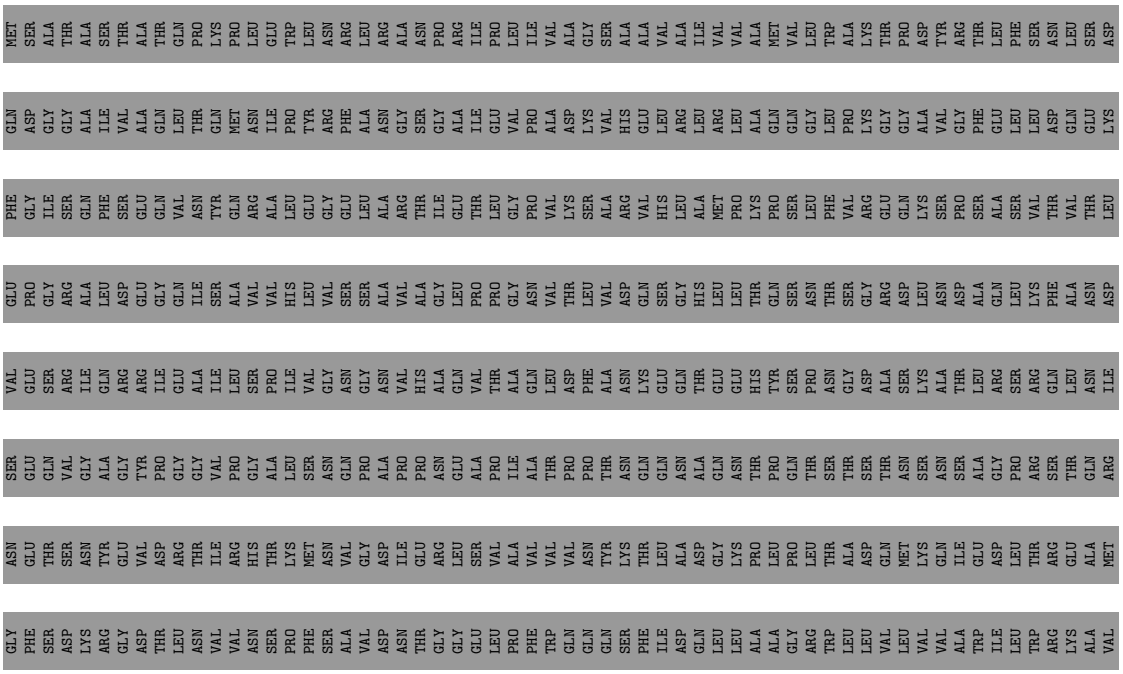






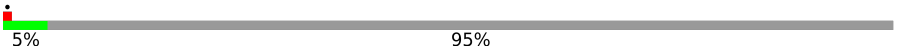
• Molecule 2: Flagellar M-ring protein

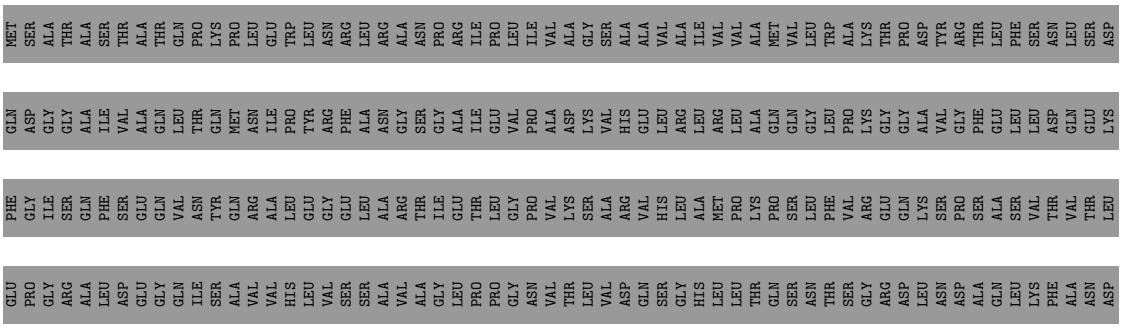
Chain BD:

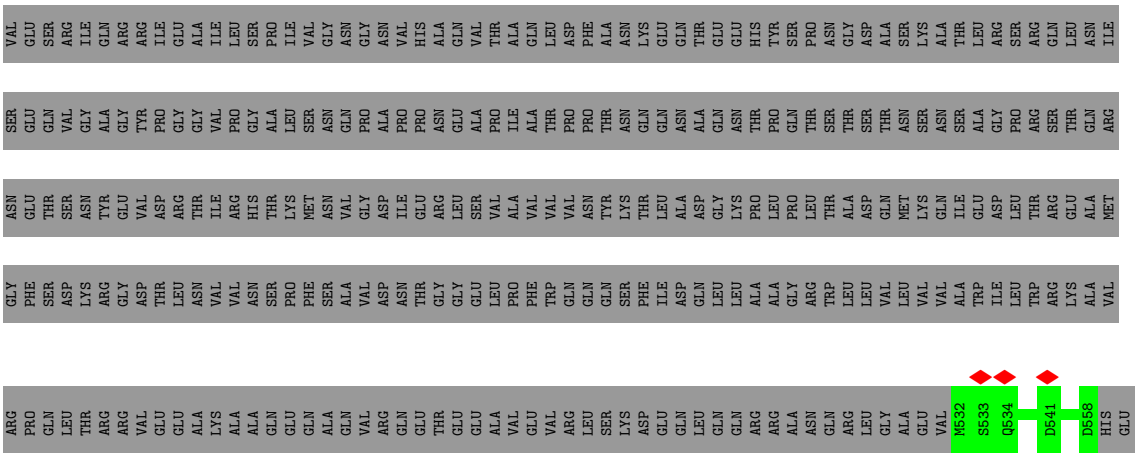


• Molecule 2: Flagellar M-ring protein

Chain BJ:

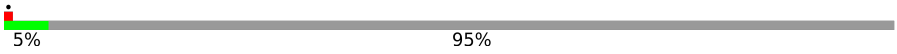


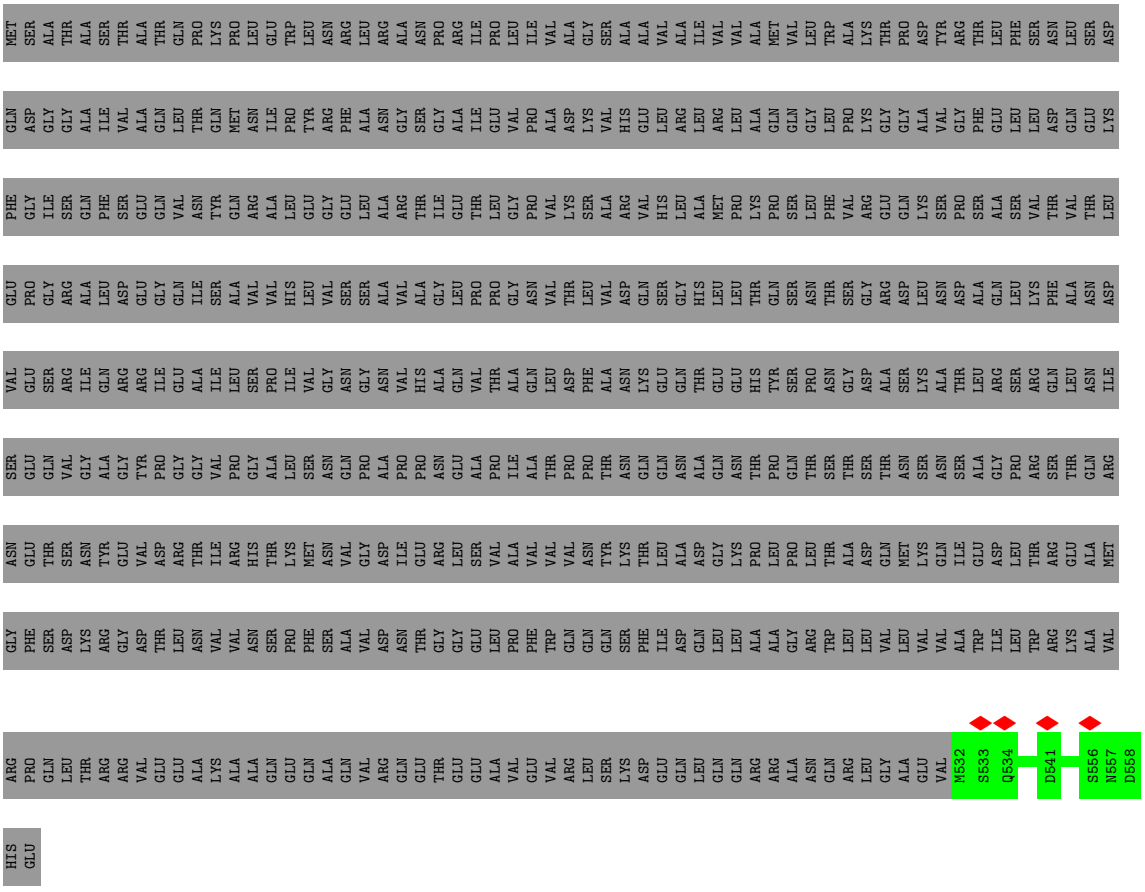




• Molecule 2: Flagellar M-ring protein

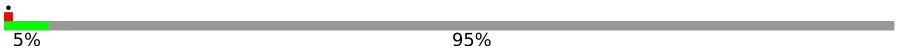
Chain BP:

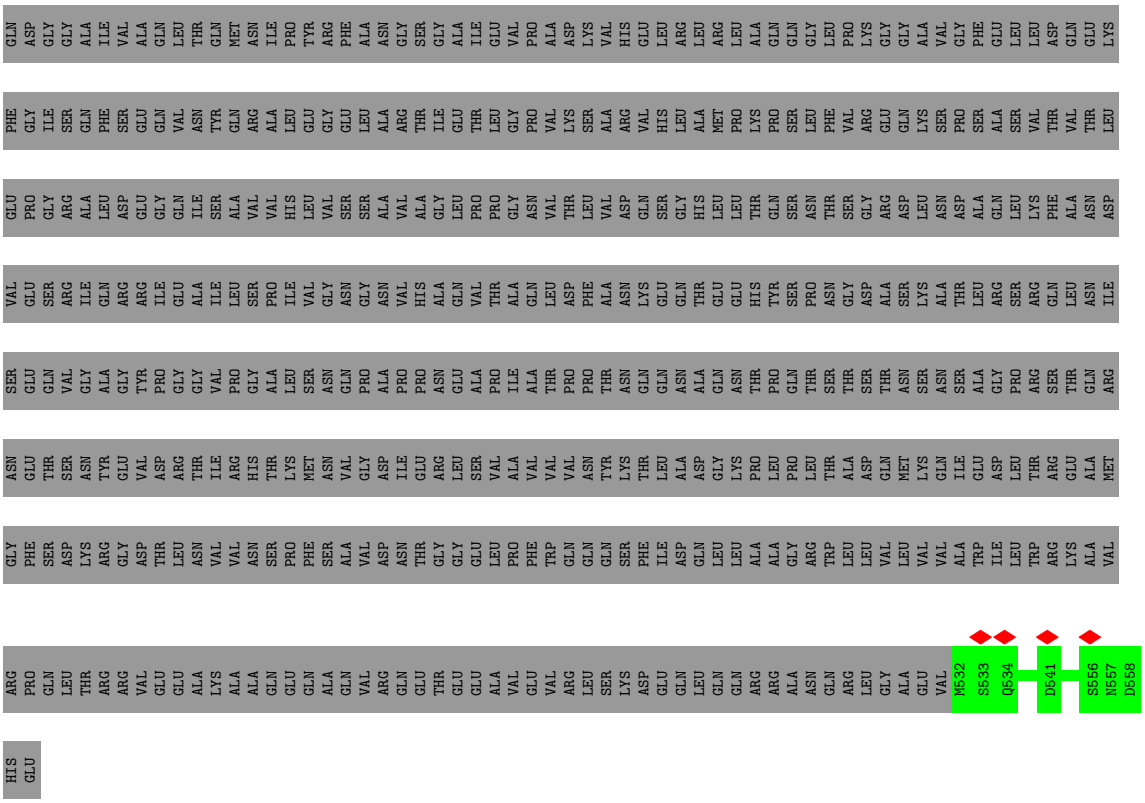




• Molecule 2: Flagellar M-ring protein

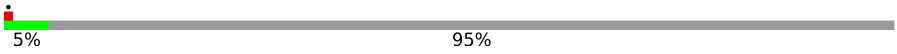
Chain BV:

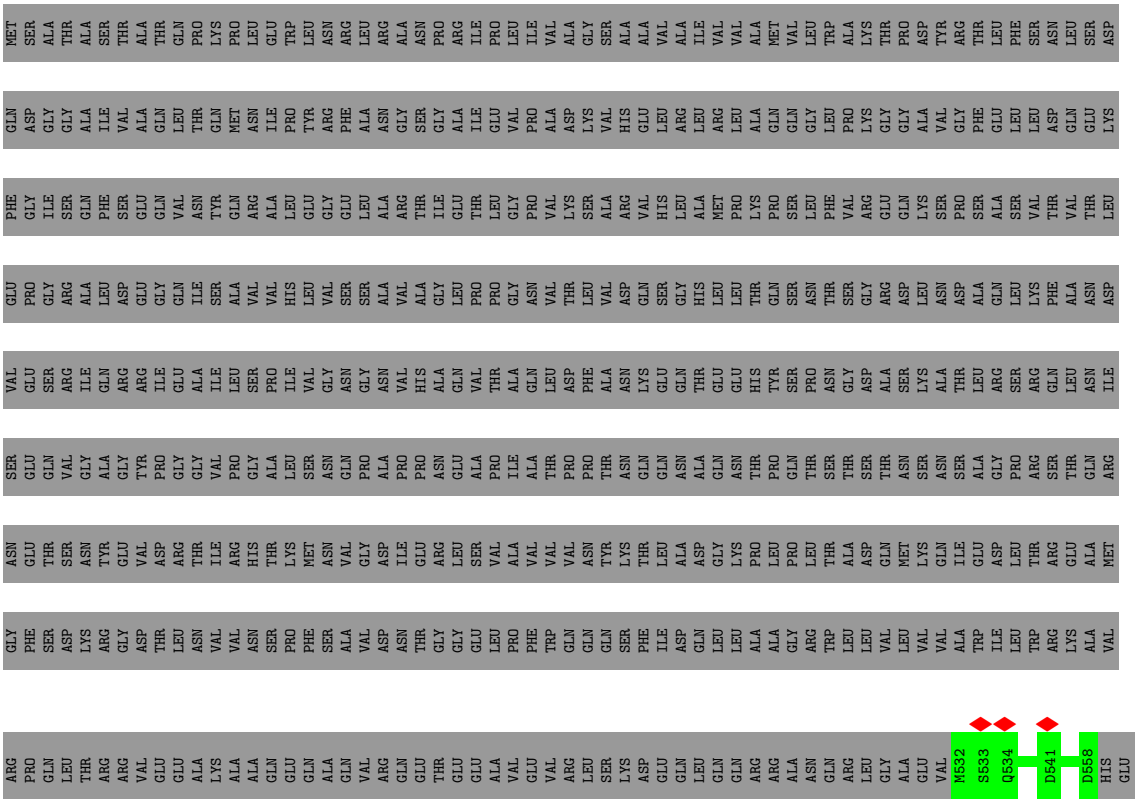




• Molecule 2: Flagellar M-ring protein

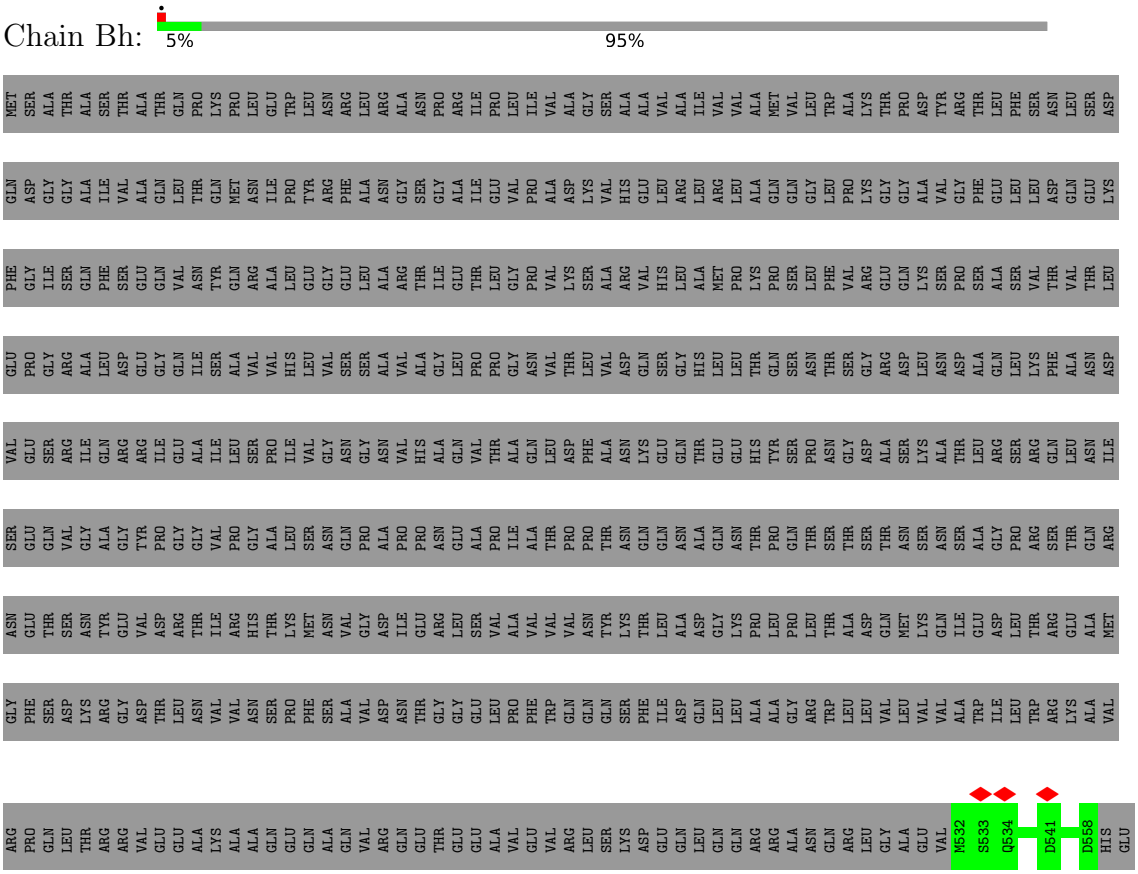
Chain Bb:





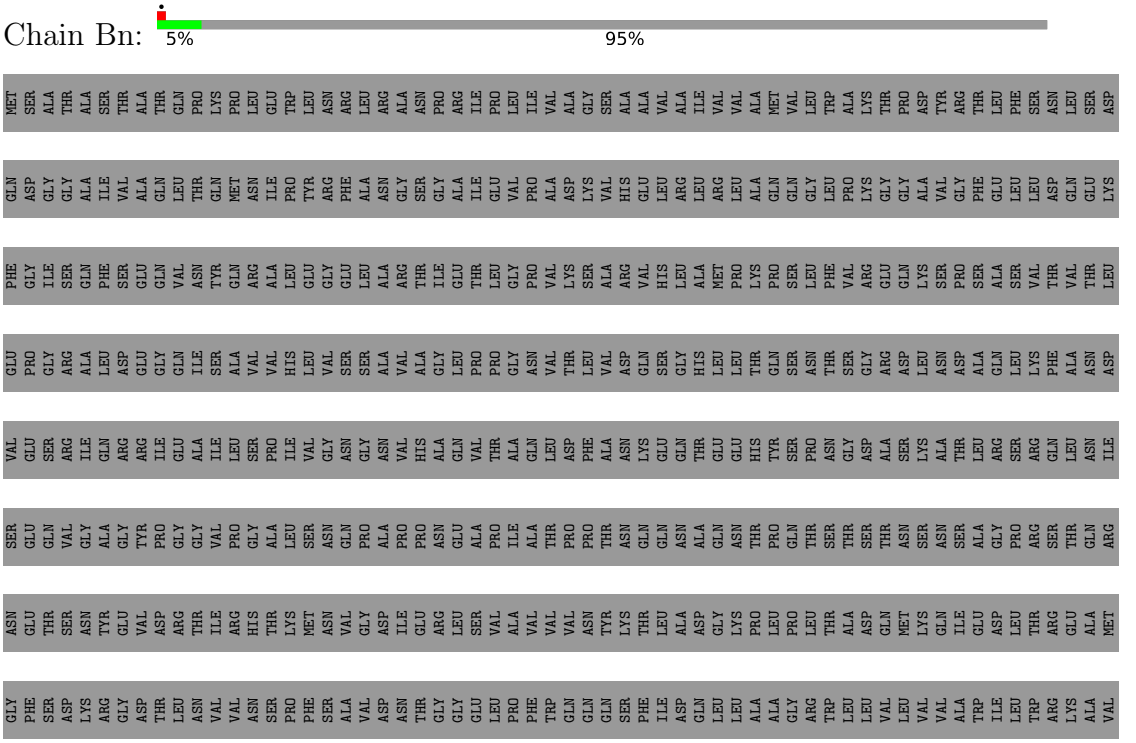
• Molecule 2: Flagellar M-ring protein

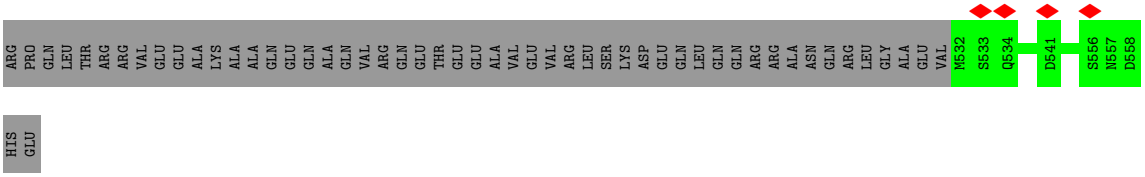
Chain Bh:



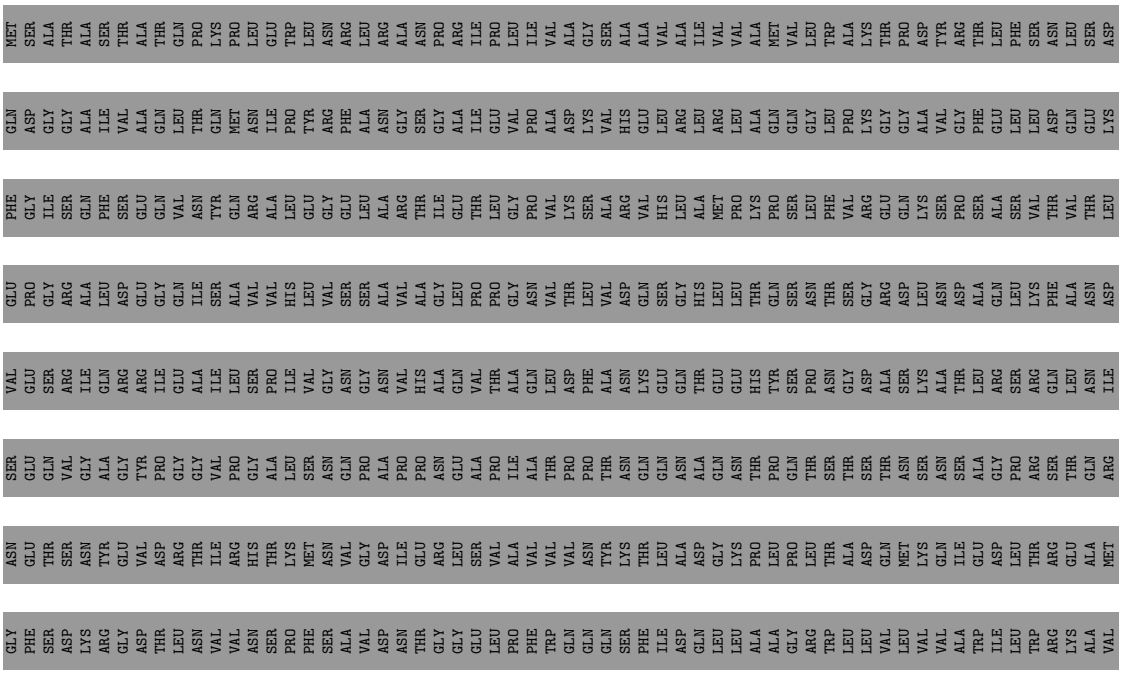
• Molecule 2: Flagellar M-ring protein

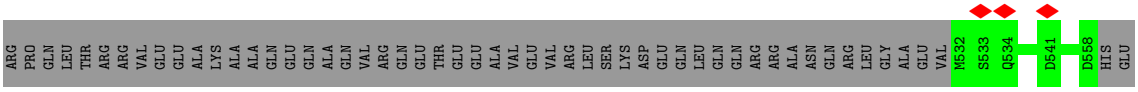
Chain Bn:



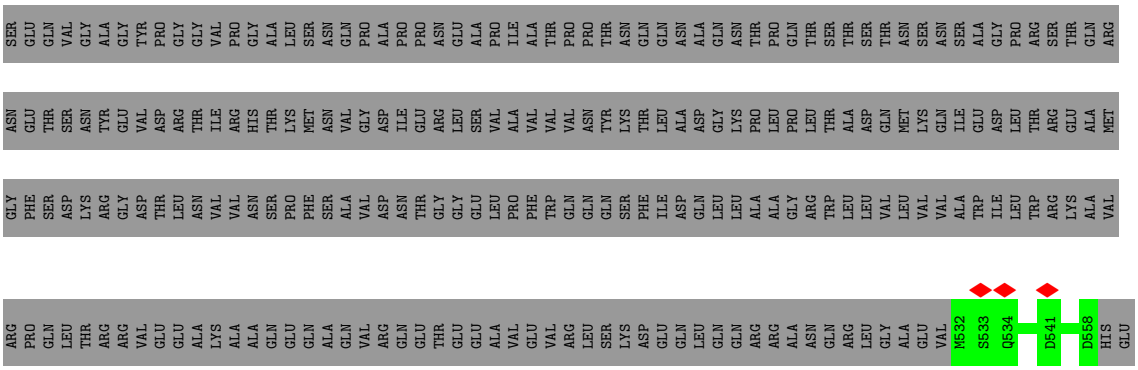


• Molecule 2: Flagellar M-ring protein



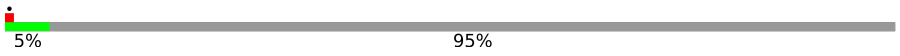


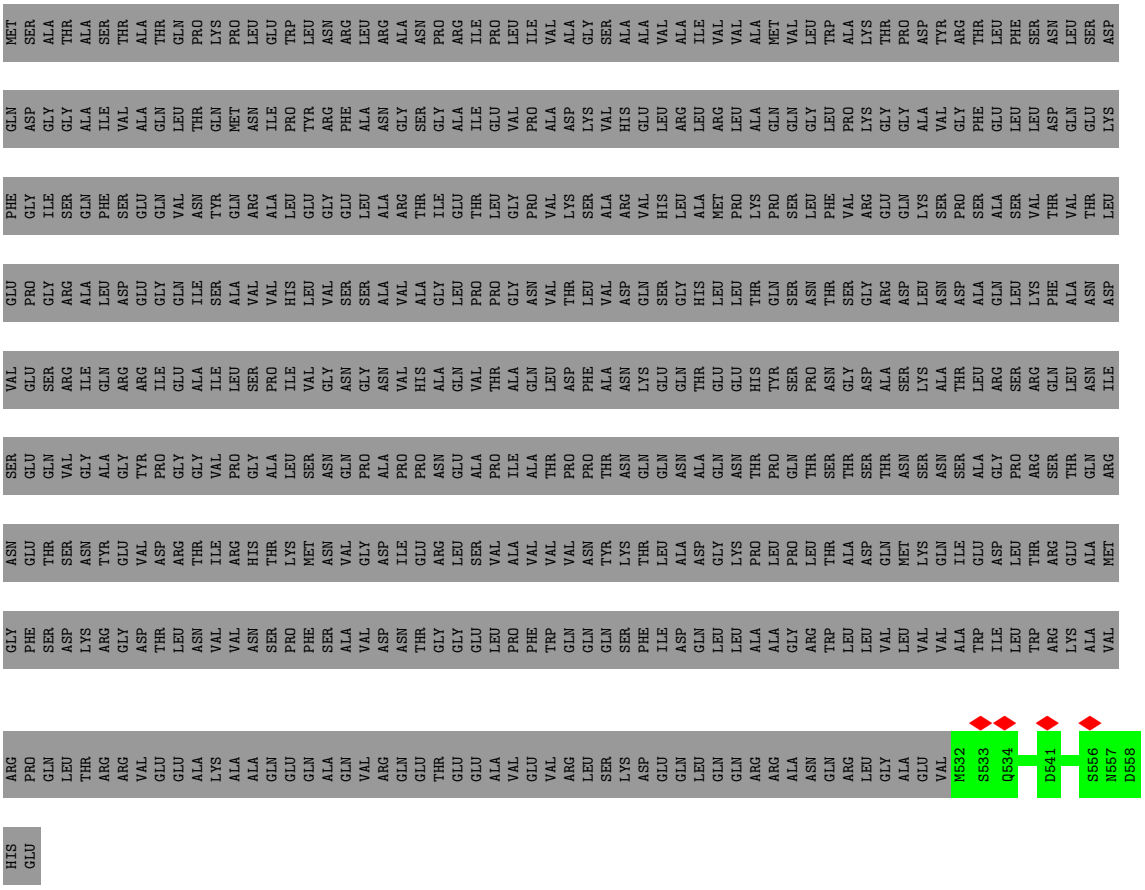
• Molecule 2: Flagellar M-ring protein



• Molecule 2: Flagellar M-ring protein

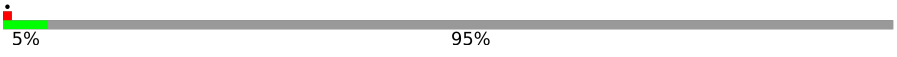
Chain B6:

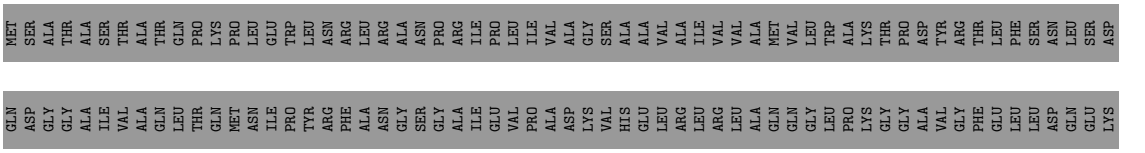




• Molecule 2: Flagellar M-ring protein

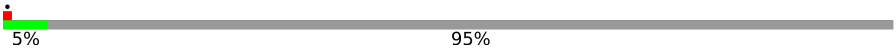
Chain CB:

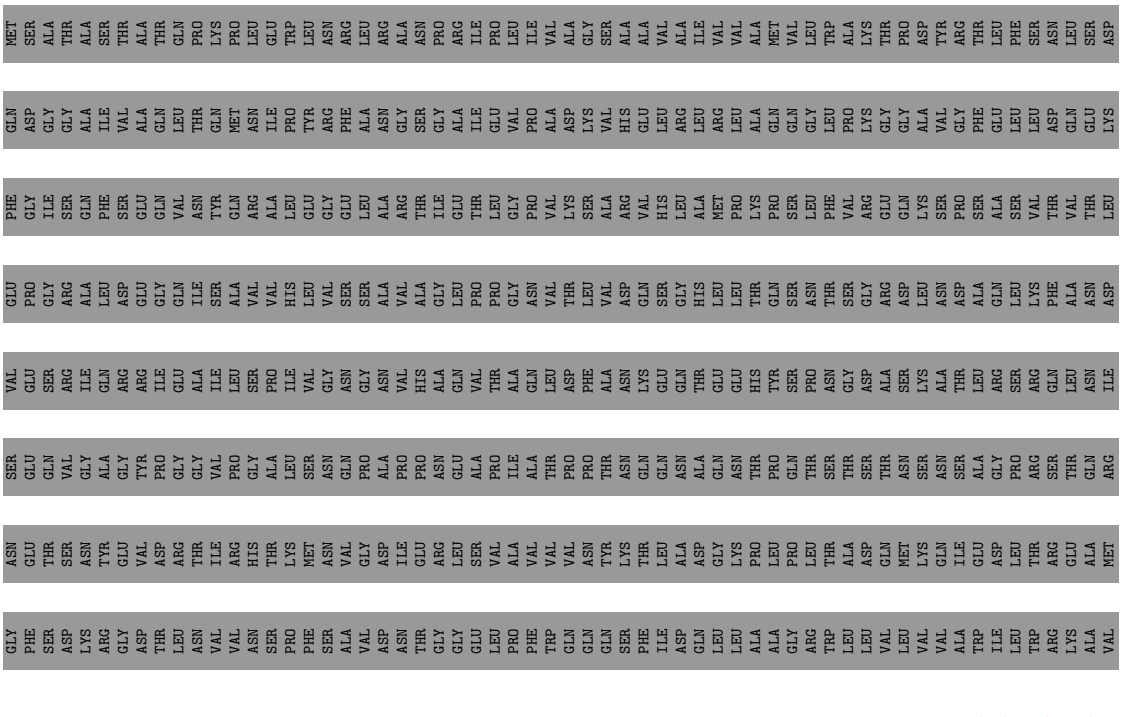




- Molecule 2: Flagellar M-ring protein

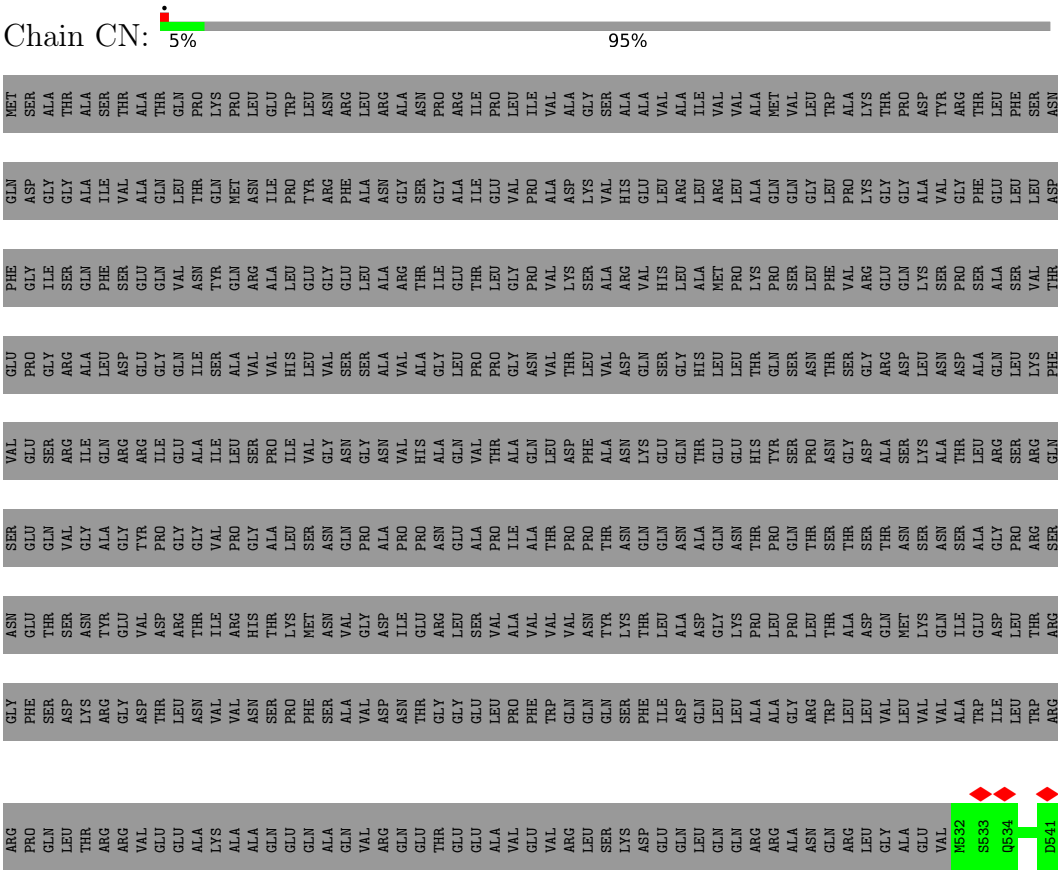
Chain CH:





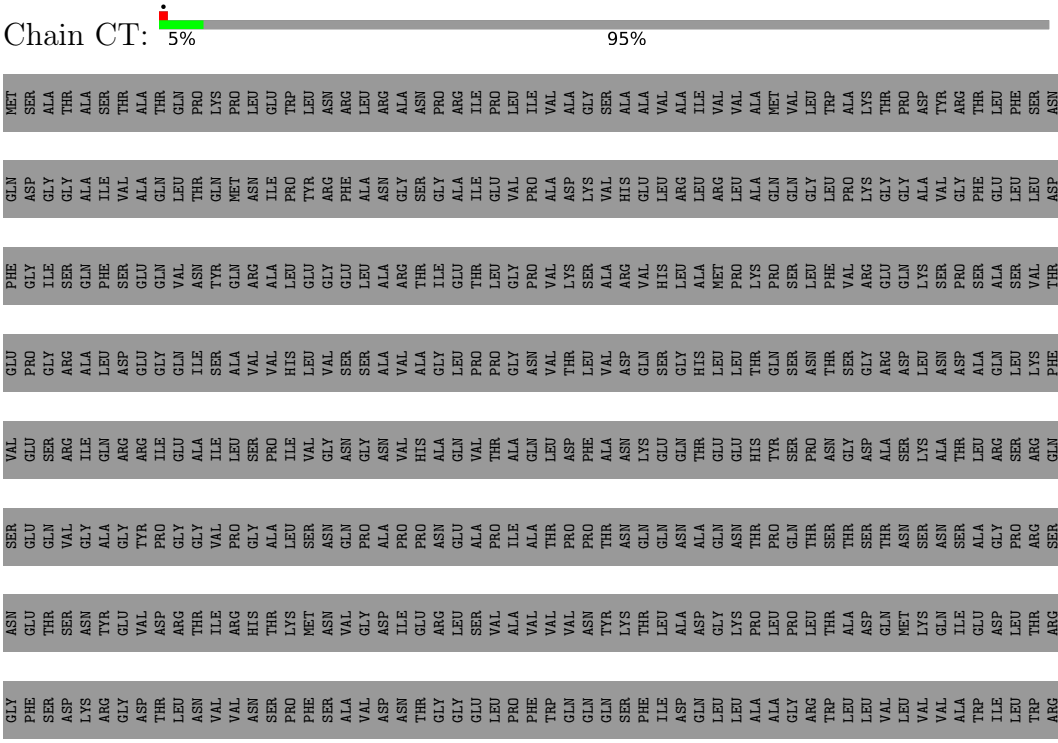
• Molecule 2: Flagellar M-ring protein

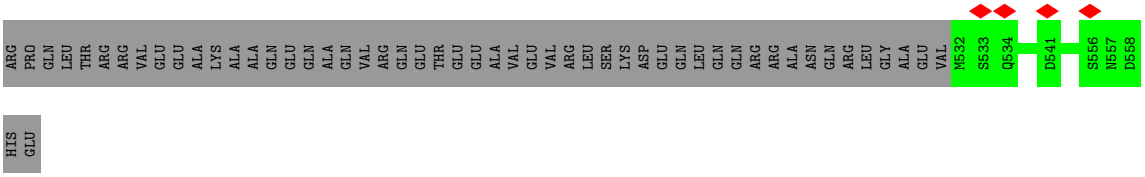
Chain CN:



• Molecule 2: Flagellar M-ring protein

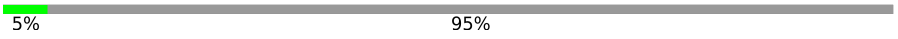
Chain CT:

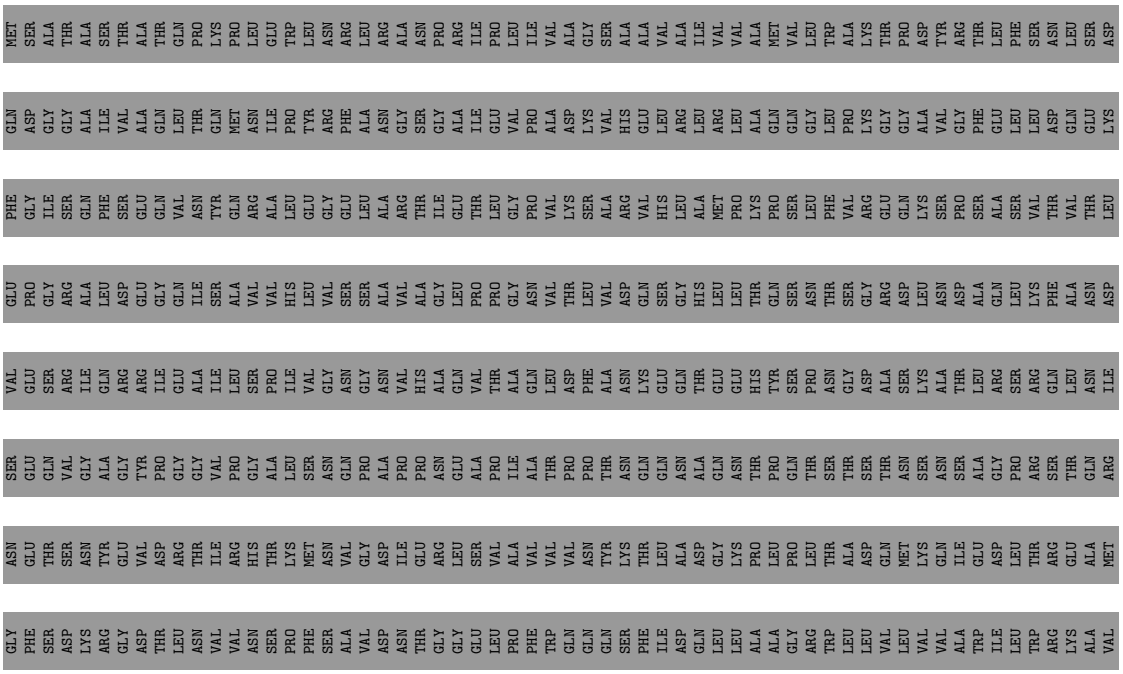


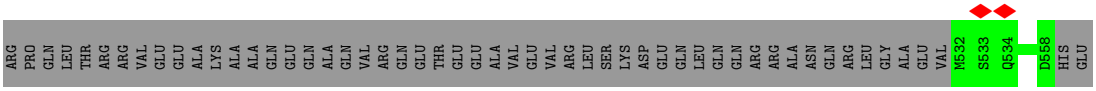


• Molecule 2: Flagellar M-ring protein

Chain CZ:

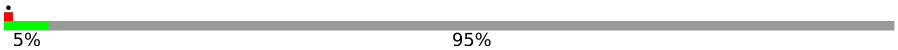


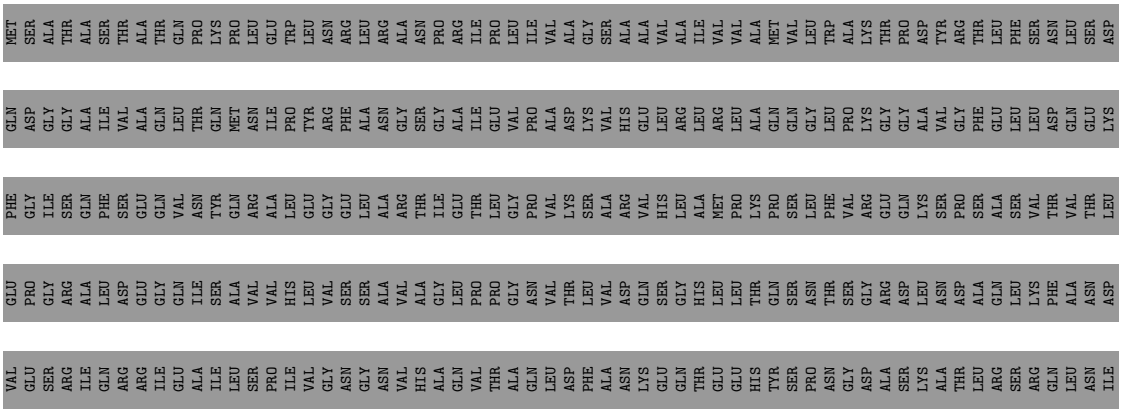


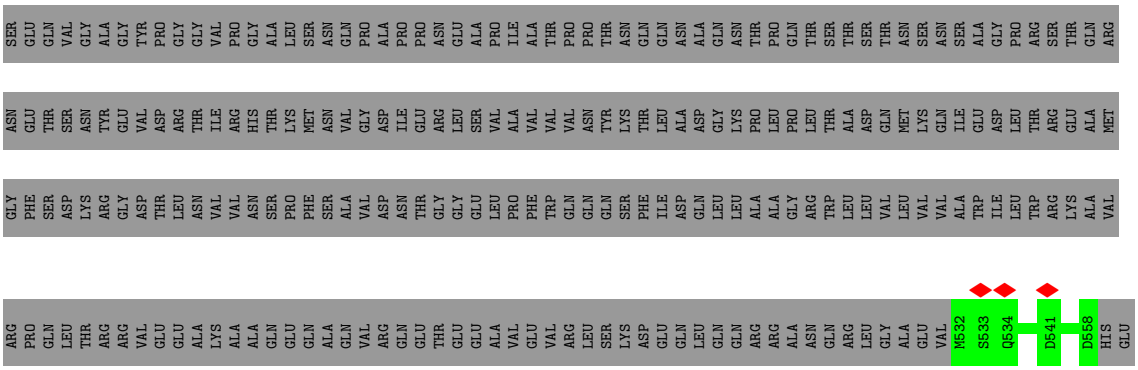


• Molecule 2: Flagellar M-ring protein

Chain Cf:

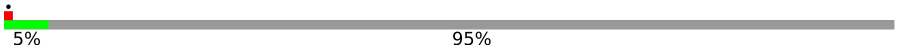


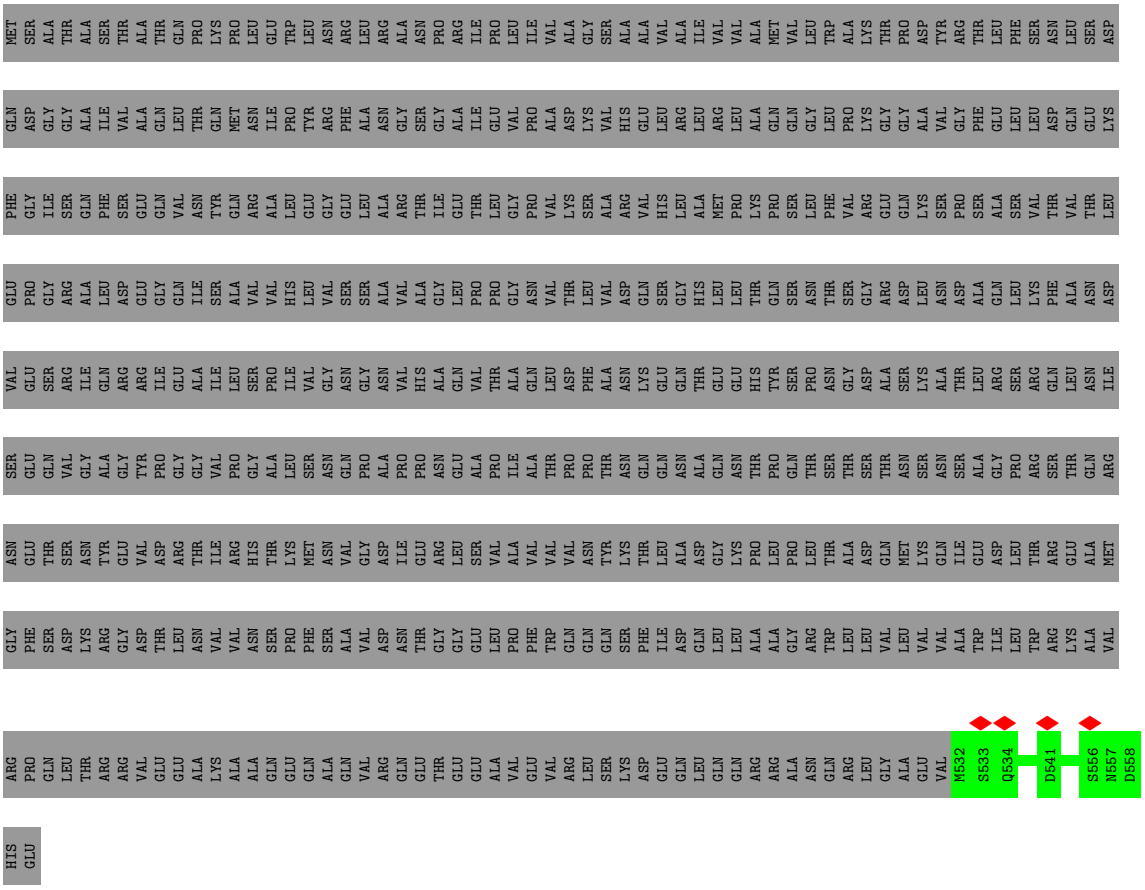




• Molecule 2: Flagellar M-ring protein

Chain Cl:





• Molecule 2: Flagellar M-ring protein

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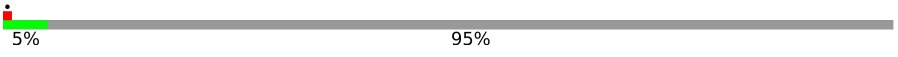
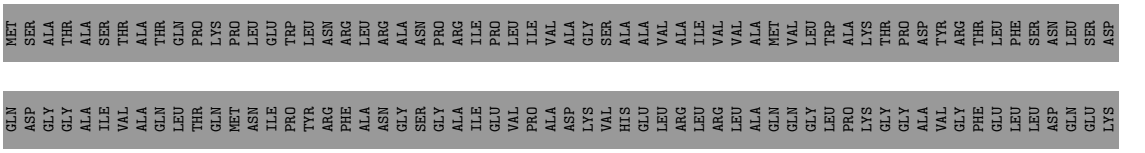
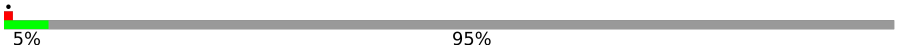
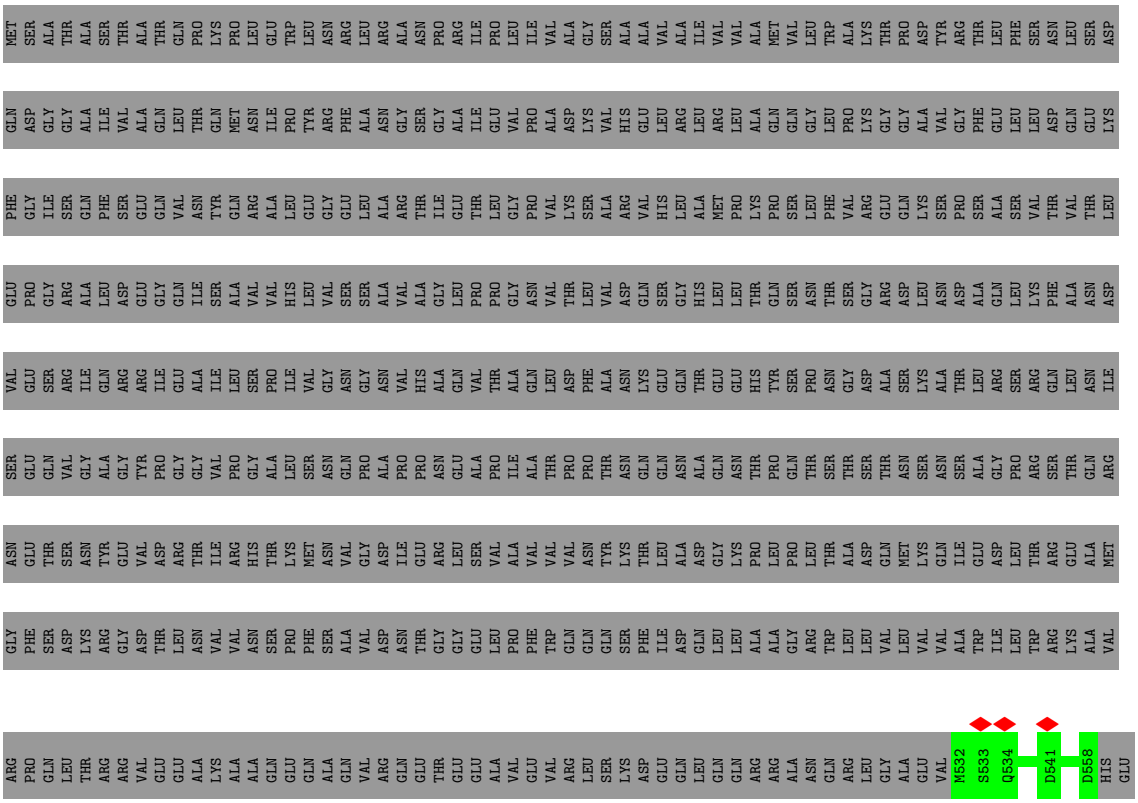




• Molecule 2: Flagellar M-ring protein

Chain Cx:





• Molecule 3: Flagellar motor switch protein FliM

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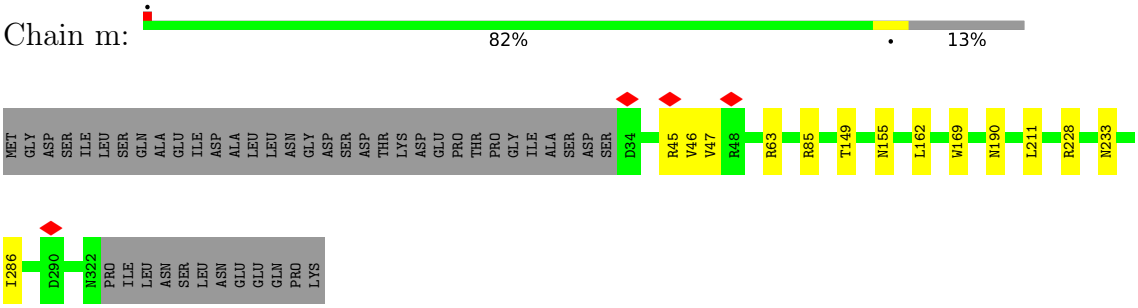

• Molecule 3: Flagellar motor switch protein FliM

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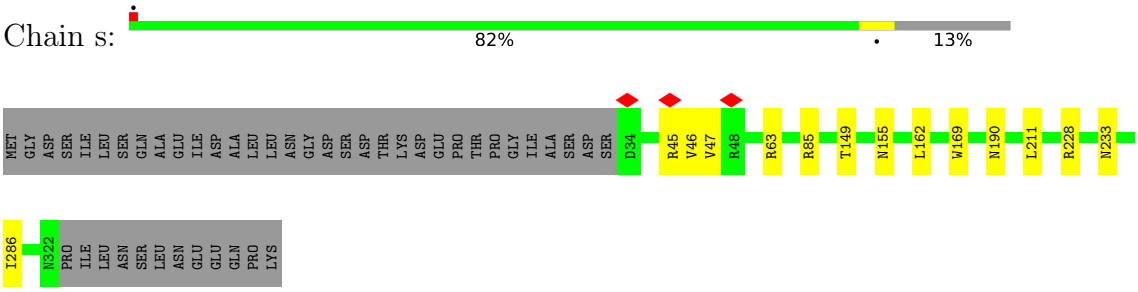

• Molecule 3: Flagellar motor switch protein FliM

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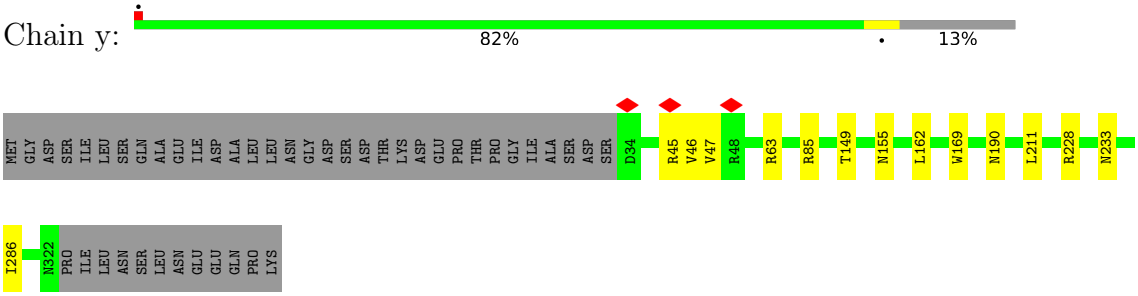
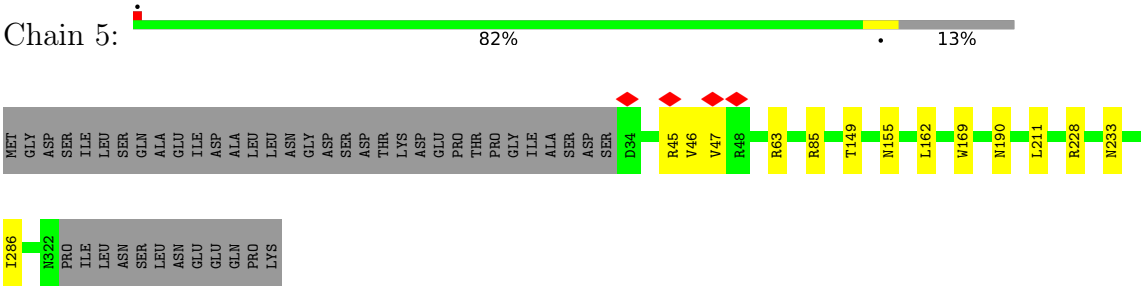


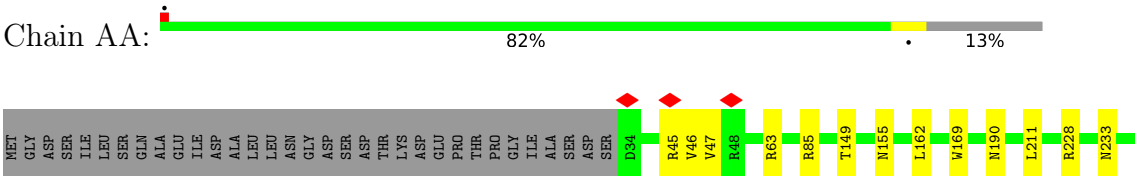
• Molecule 3: Flagellar motor switch protein FliM

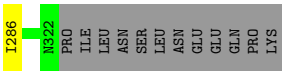
Chain 5:



• Molecule 3: Flagellar motor switch protein FliM

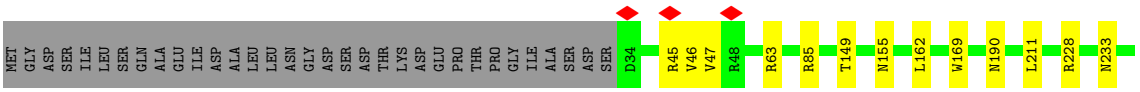
Chain AA:

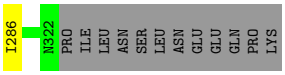




• Molecule 3: Flagellar motor switch protein FliM

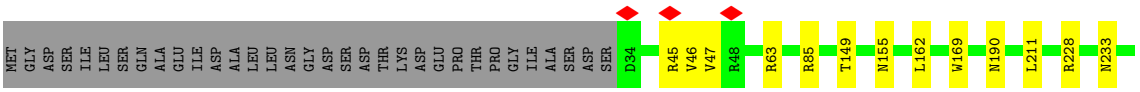
Chain AG:

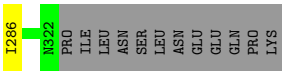




• Molecule 3: Flagellar motor switch protein FliM

Chain AM:





• Molecule 3: Flagellar motor switch protein FliM

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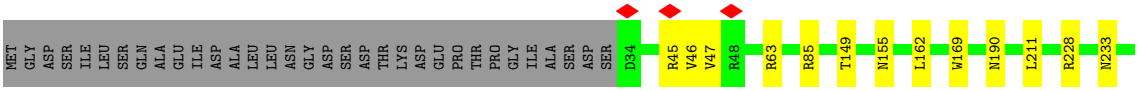
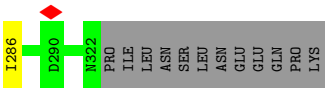
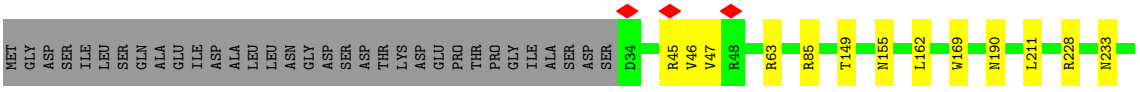
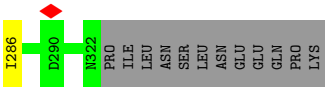




• Molecule 3: Flagellar motor switch protein FliM

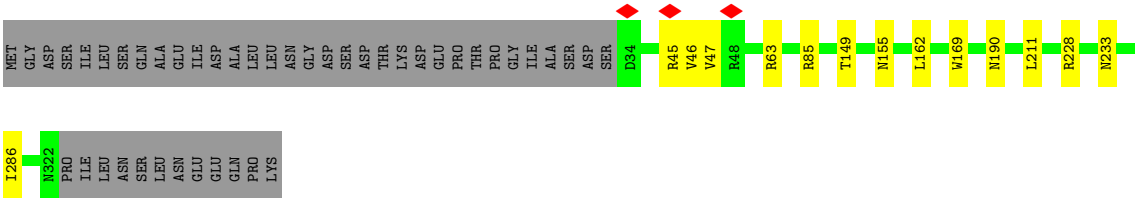
Chain AY:





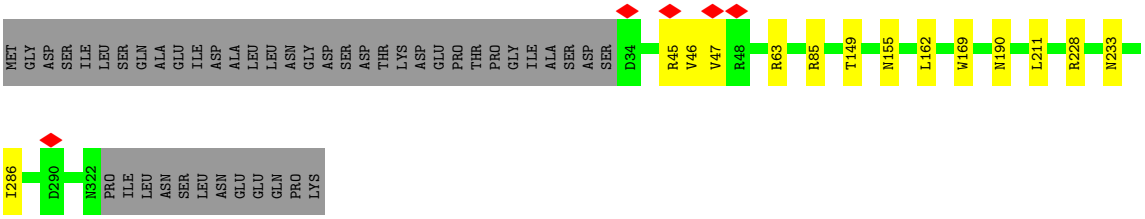
• Molecule 3: Flagellar motor switch protein FliM

Chain Ae:



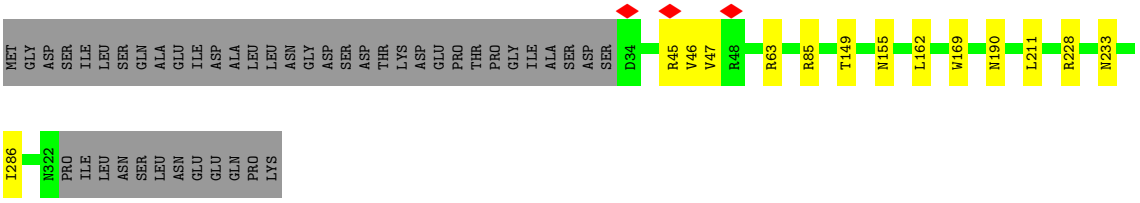
• Molecule 3: Flagellar motor switch protein FliM

Chain Ak:



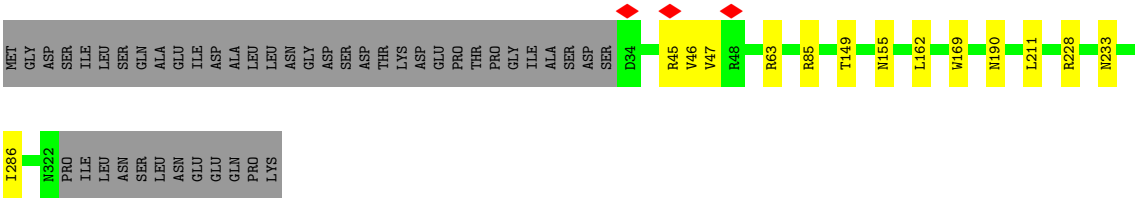
• Molecule 3: Flagellar motor switch protein FliM

Chain Aq:



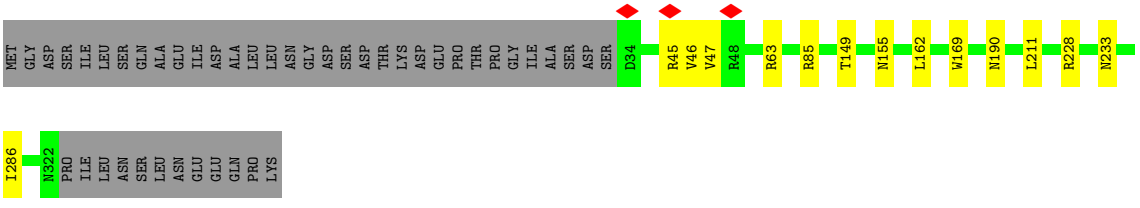
• Molecule 3: Flagellar motor switch protein FliM

Chain Aw:



• Molecule 3: Flagellar motor switch protein FliM

Chain A3:



• Molecule 3: Flagellar motor switch protein FliM

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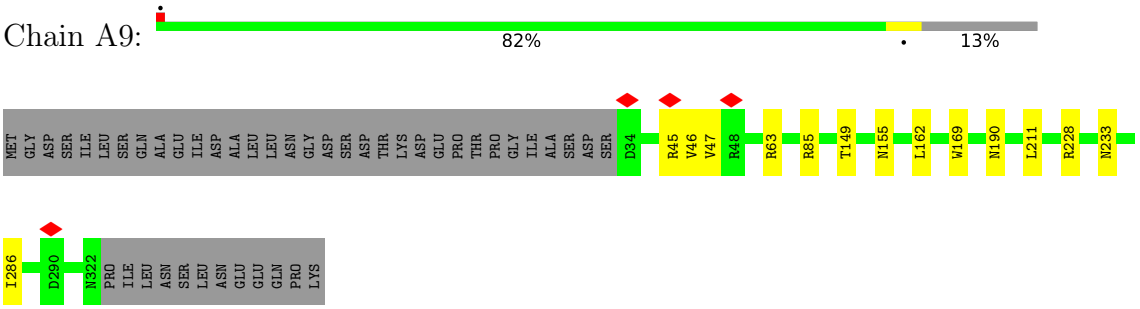
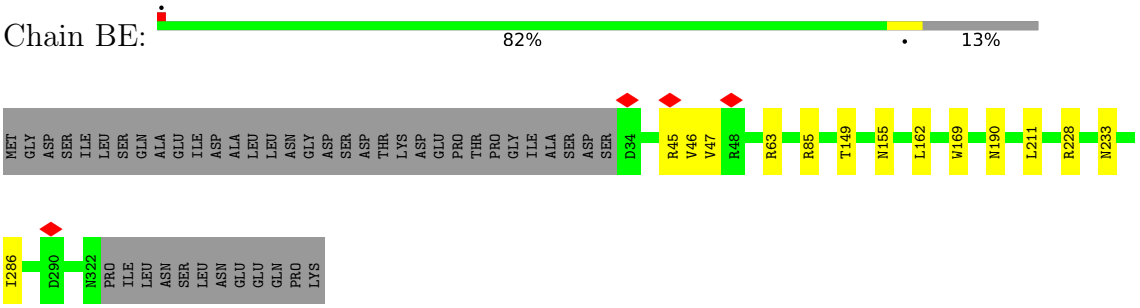


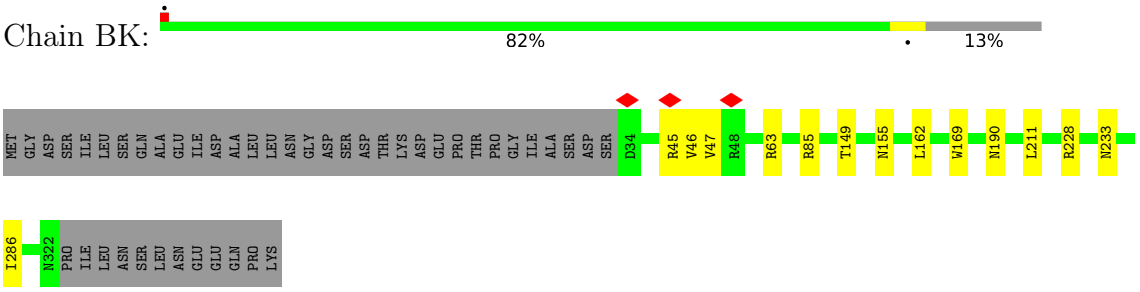
• Molecule 3: Flagellar motor switch protein FliM

Chain BE:



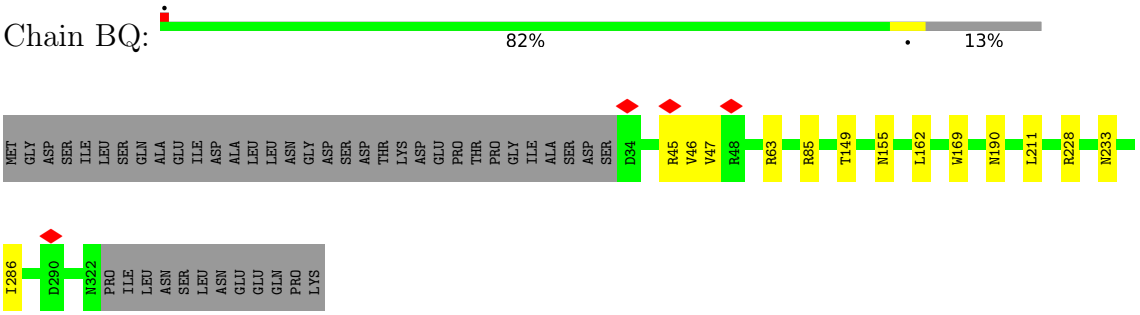
• Molecule 3: Flagellar motor switch protein FliM

Chain BK:



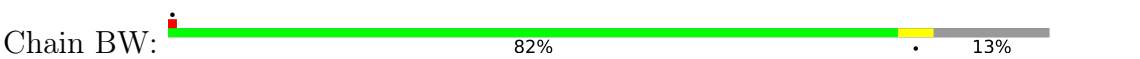
• Molecule 3: Flagellar motor switch protein FliM

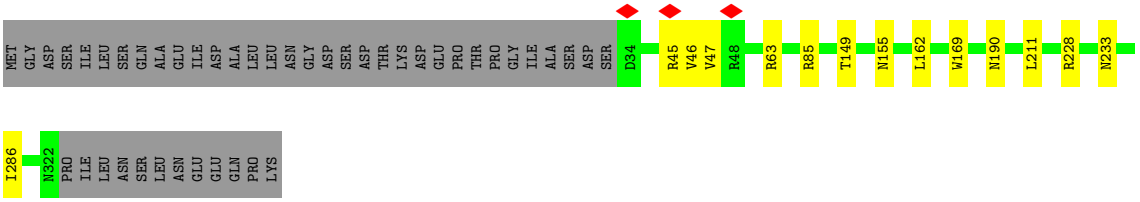
Chain BQ:



• Molecule 3: Flagellar motor switch protein FliM

Chain BW:





• Molecule 3: Flagellar motor switch protein FliM

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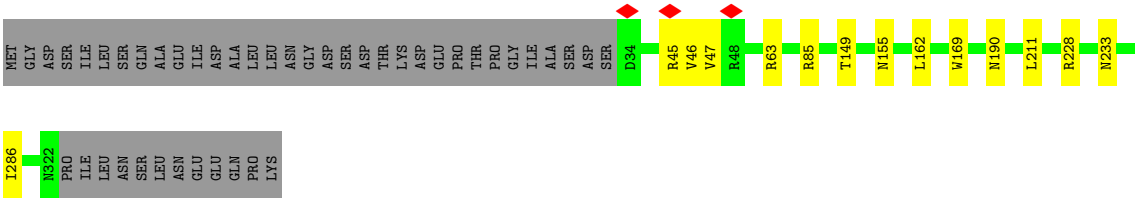

• Molecule 3: Flagellar motor switch protein FliM

Chain Bi:

• Molecule 3: Flagellar motor switch protein FliM

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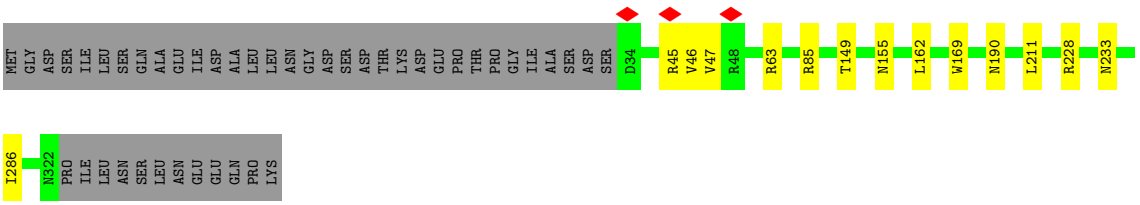

• Molecule 3: Flagellar motor switch protein FliM

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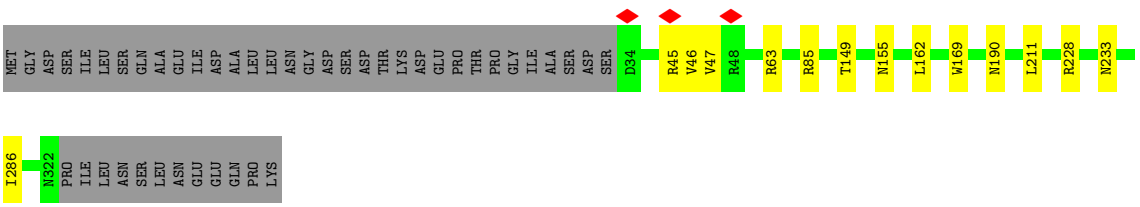

• Molecule 3: Flagellar motor switch protein FliM

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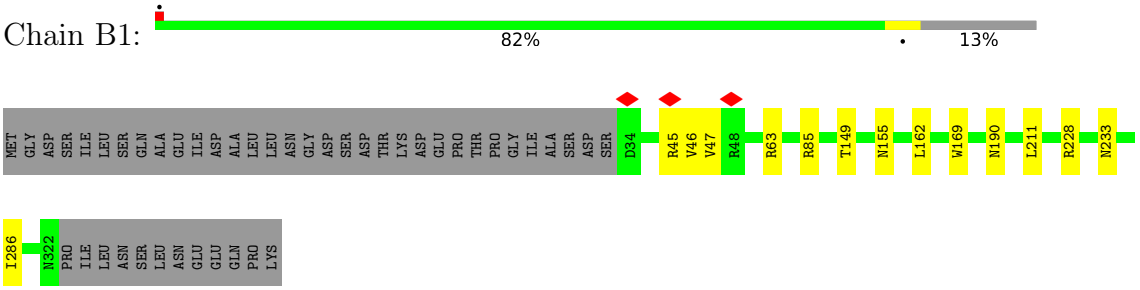

• Molecule 3: Flagellar motor switch protein FliM

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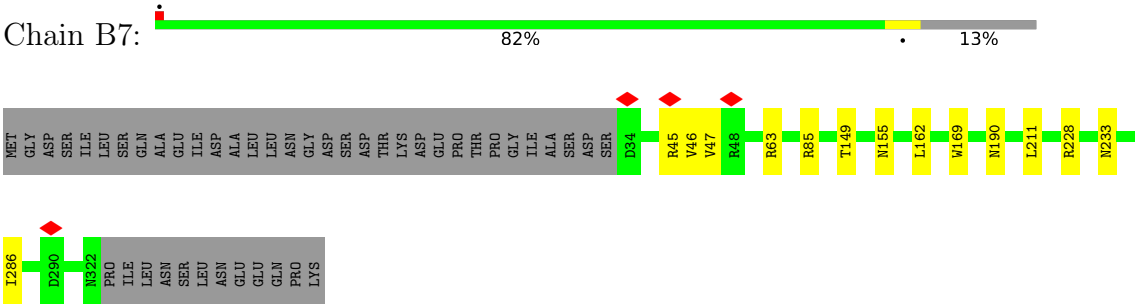

• Molecule 3: Flagellar motor switch protein FliM

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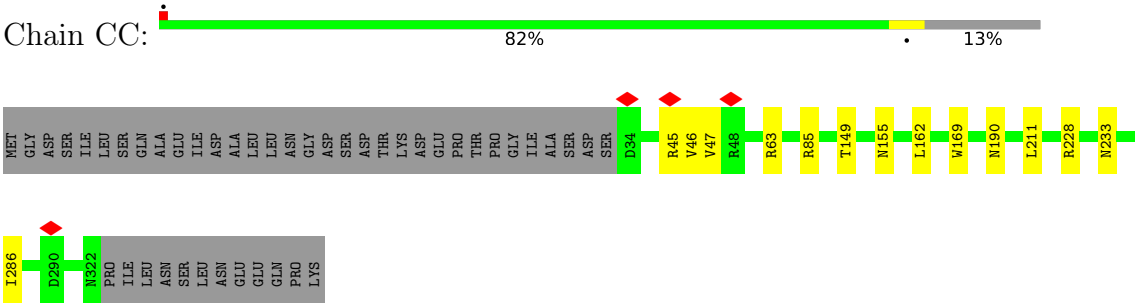

• Molecule 3: Flagellar motor switch protein FliM

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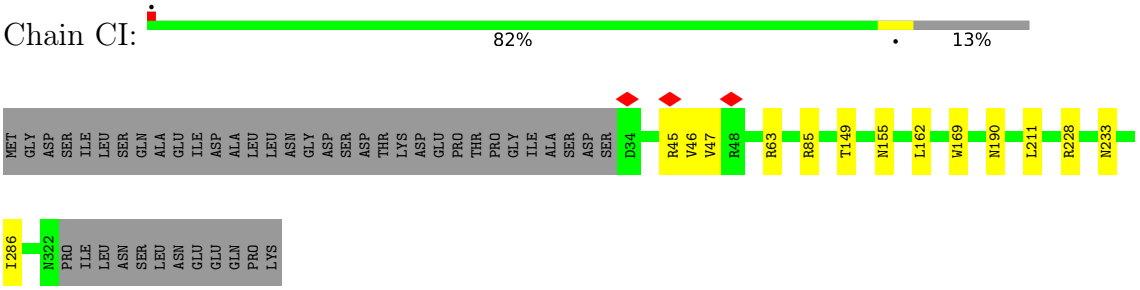

• Molecule 3: Flagellar motor switch protein FliM

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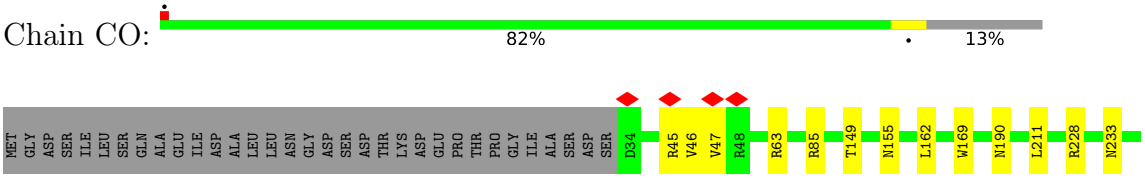

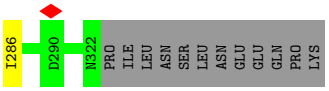

• Molecule 3: Flagellar motor switch protein FliM

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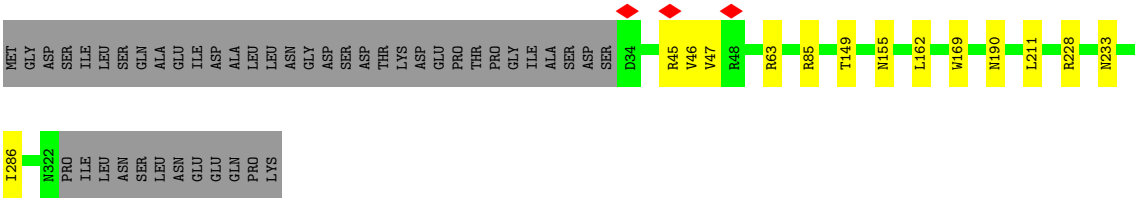

• Molecule 3: Flagellar motor switch protein FliM

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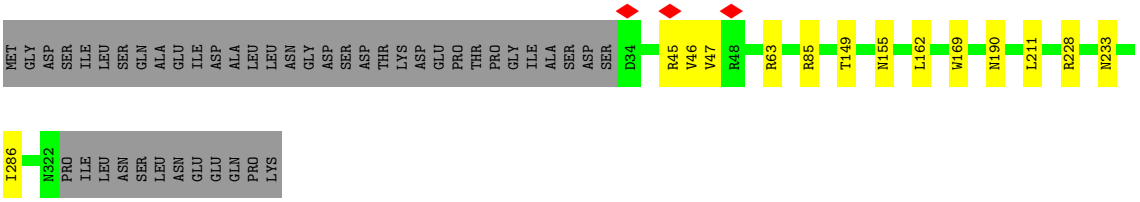

• Molecule 3: Flagellar motor switch protein FliM

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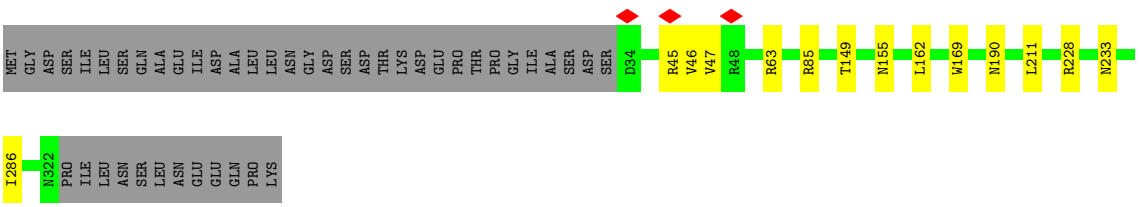

• Molecule 3: Flagellar motor switch protein FliM

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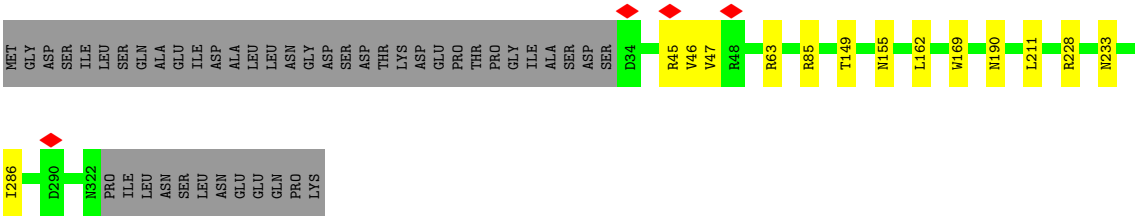

• Molecule 3: Flagellar motor switch protein FliM

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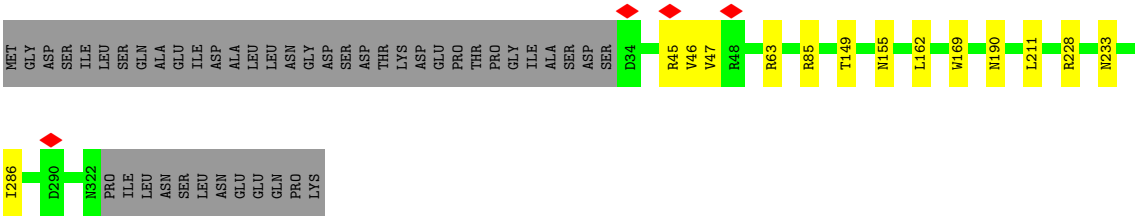
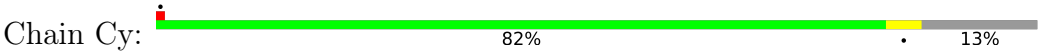
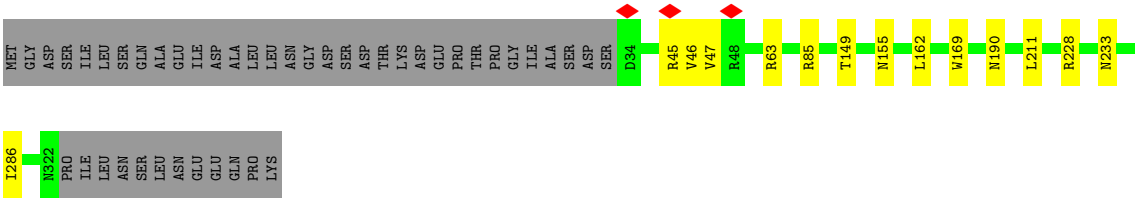
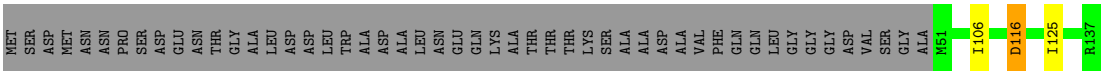


• Molecule 3: Flagellar motor switch protein FliM

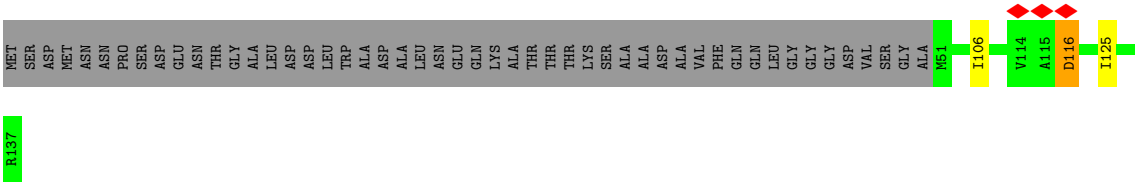




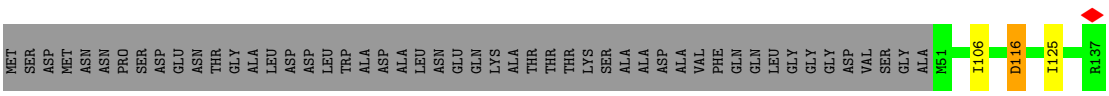
• Molecule 4: Flagellar motor switch protein FliN



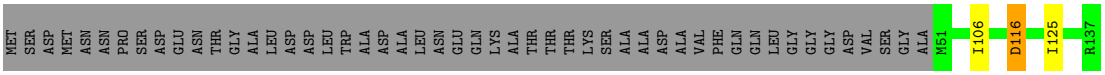
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

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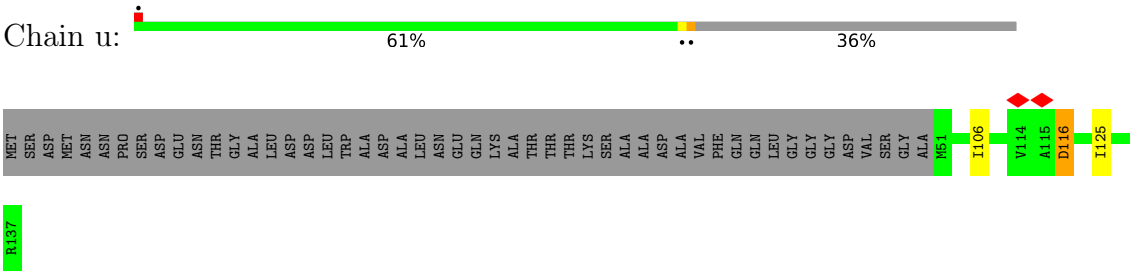

• Molecule 4: Flagellar motor switch protein FliN

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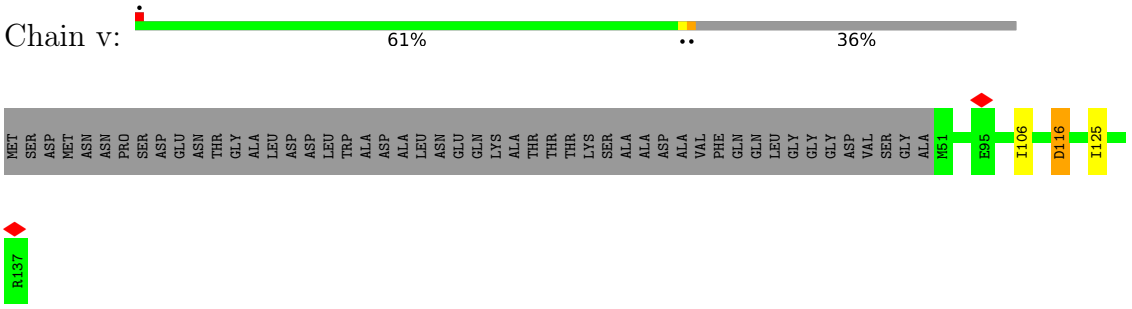

• Molecule 4: Flagellar motor switch protein FliN

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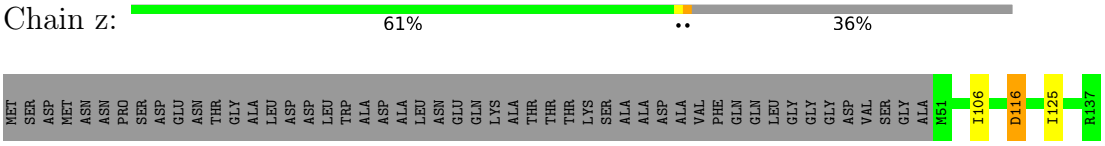

• Molecule 4: Flagellar motor switch protein FliN

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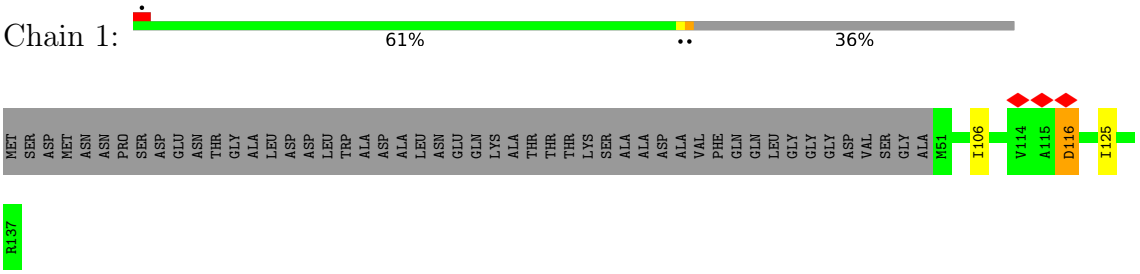

• Molecule 4: Flagellar motor switch protein FliN

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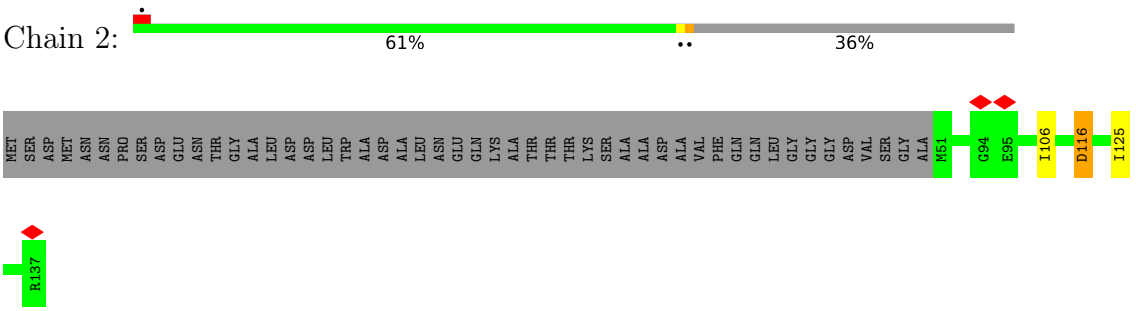

• Molecule 4: Flagellar motor switch protein FliN

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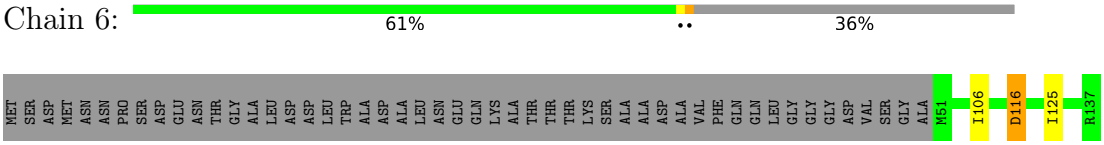

• Molecule 4: Flagellar motor switch protein FliN

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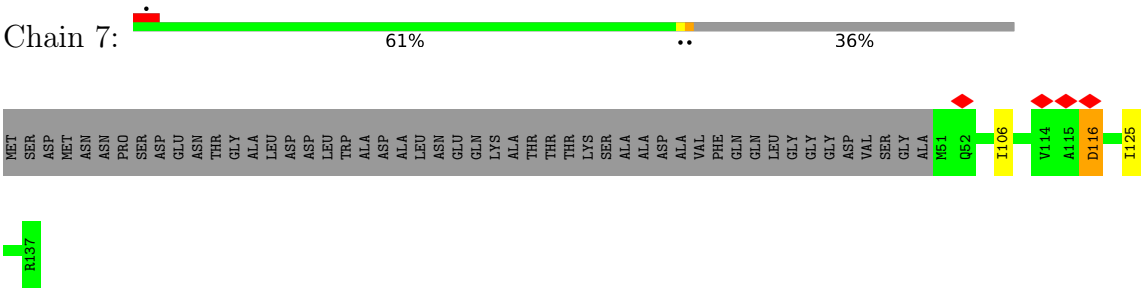

• Molecule 4: Flagellar motor switch protein FliN

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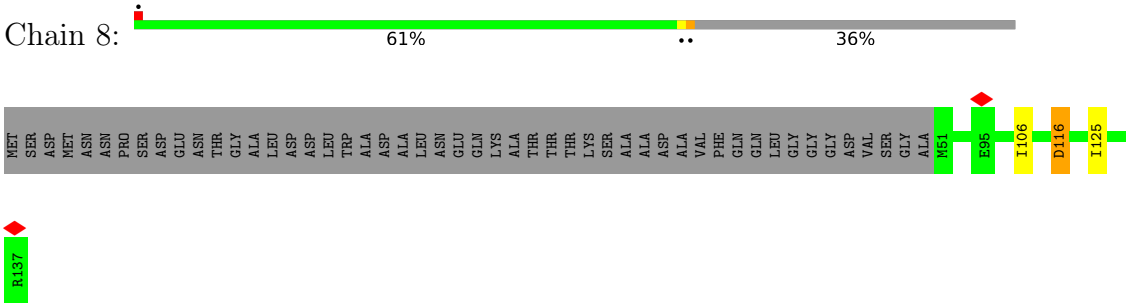

• Molecule 4: Flagellar motor switch protein FliN

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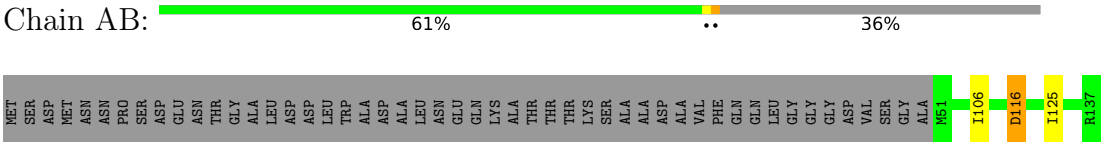

• Molecule 4: Flagellar motor switch protein FliN

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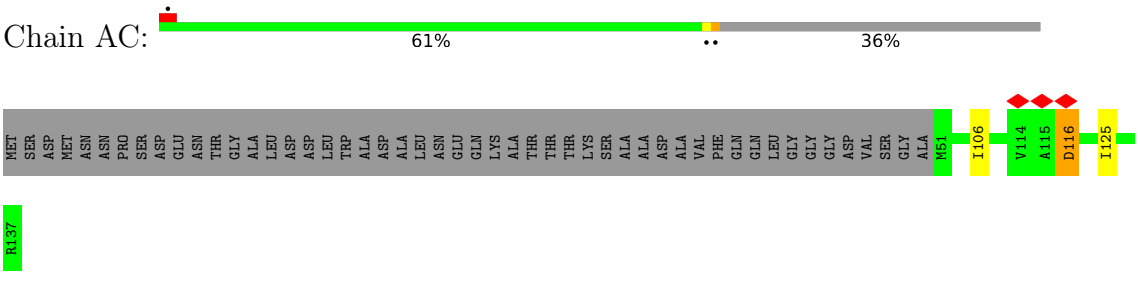

• Molecule 4: Flagellar motor switch protein FliN

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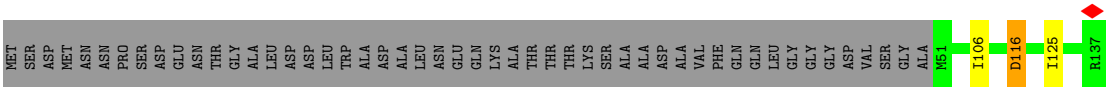
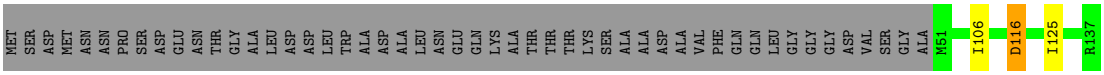
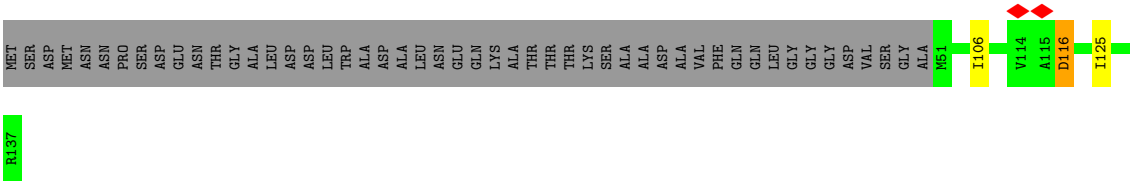


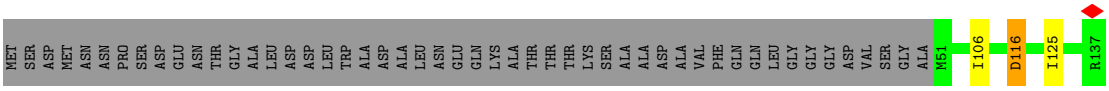
• Molecule 4: Flagellar motor switch protein FliN



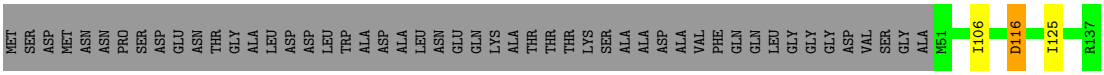
• Molecule 4: Flagellar motor switch protein FliN



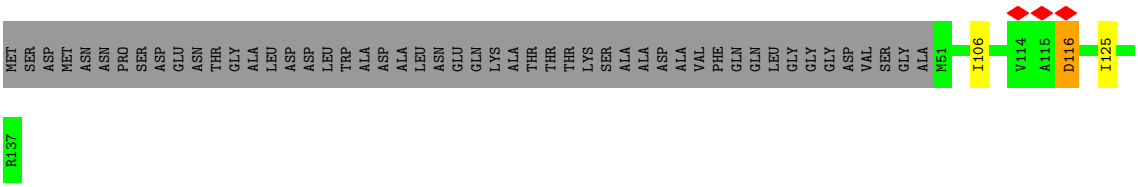
• Molecule 4: Flagellar motor switch protein FliN



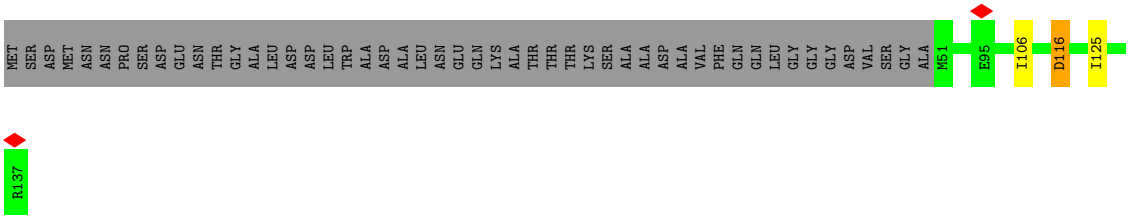
• Molecule 4: Flagellar motor switch protein FliN



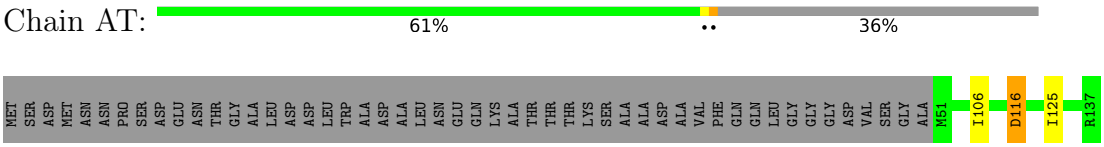
• Molecule 4: Flagellar motor switch protein FliN



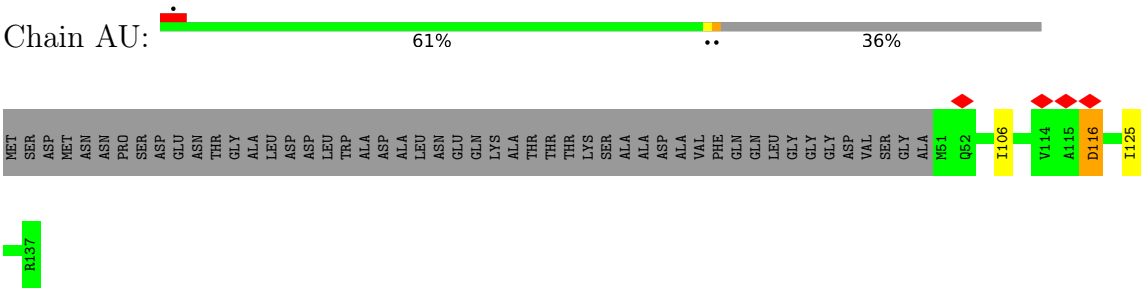
• Molecule 4: Flagellar motor switch protein FliN



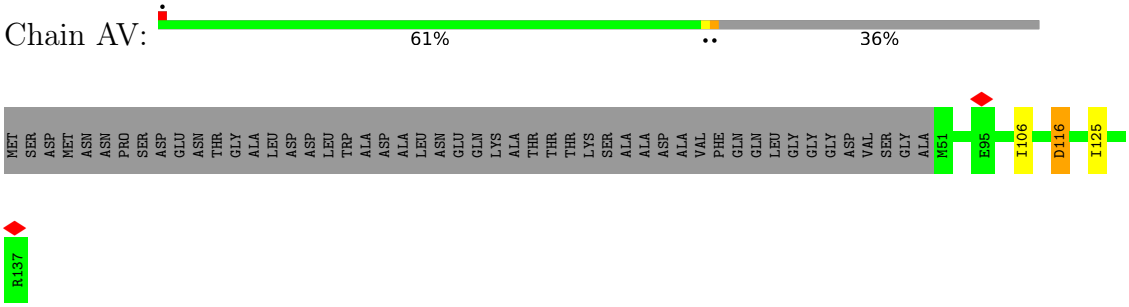
• Molecule 4: Flagellar motor switch protein FliN



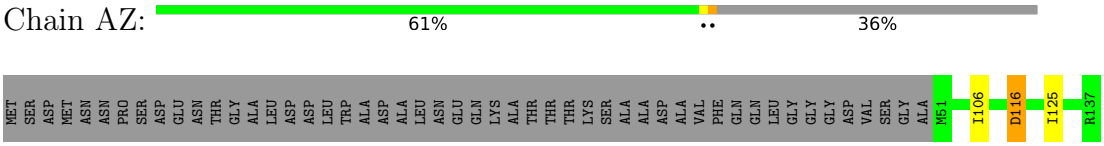
• Molecule 4: Flagellar motor switch protein FliN



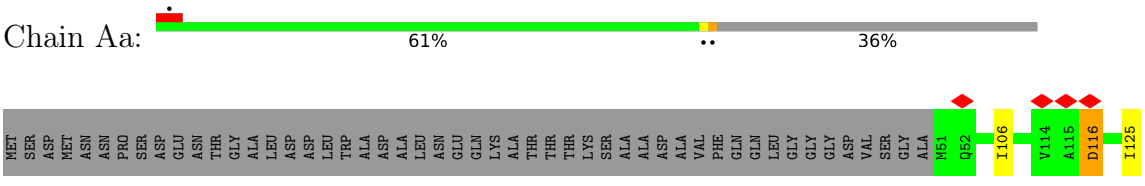
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

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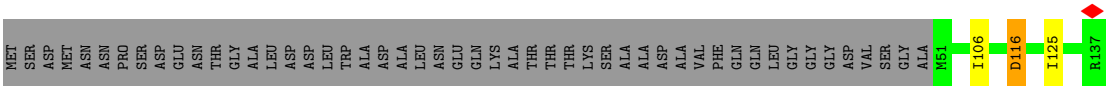

• Molecule 4: Flagellar motor switch protein FliN

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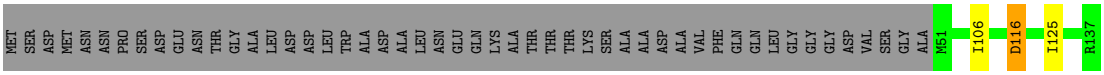

• Molecule 4: Flagellar motor switch protein FliN

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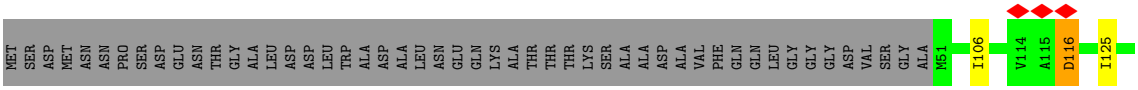

• Molecule 4: Flagellar motor switch protein FliN

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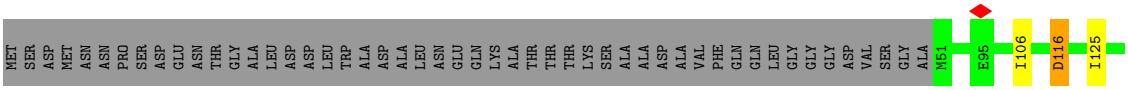

• Molecule 4: Flagellar motor switch protein FliN

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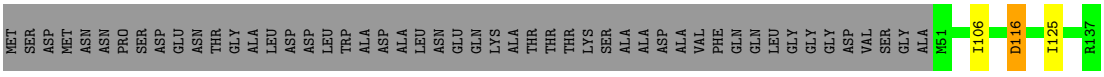

• Molecule 4: Flagellar motor switch protein FliN

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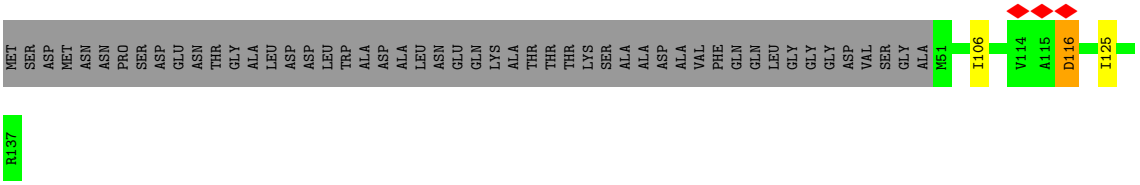
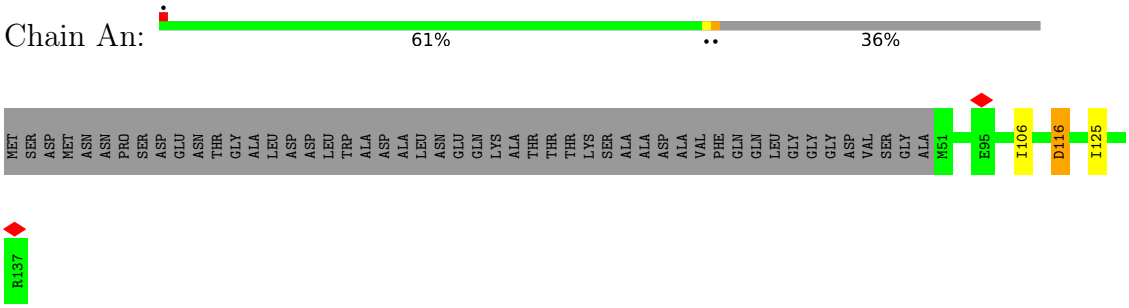
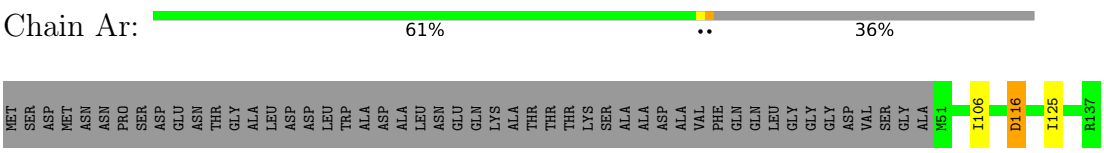


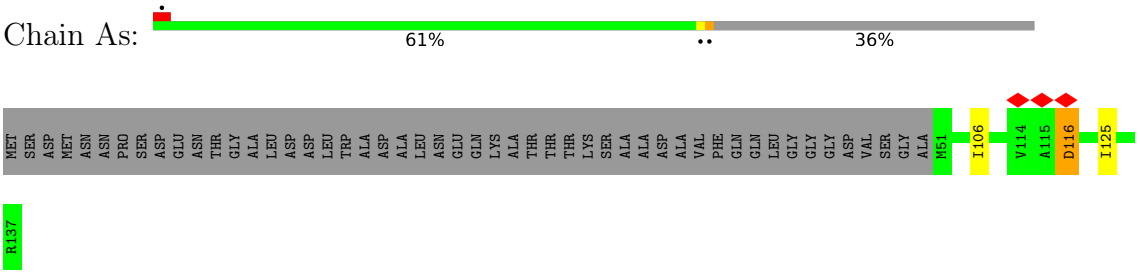
• Molecule 4: Flagellar motor switch protein FliN



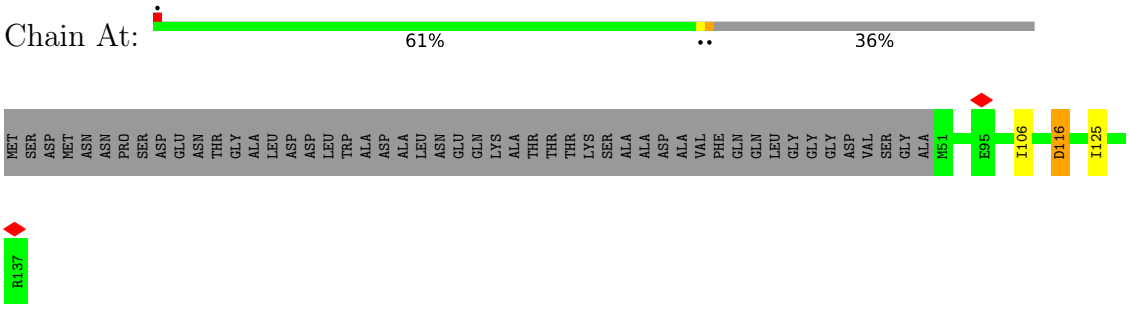
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



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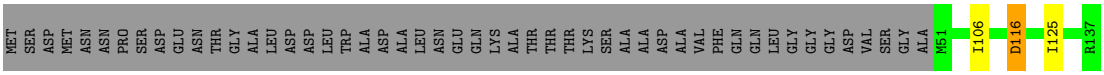
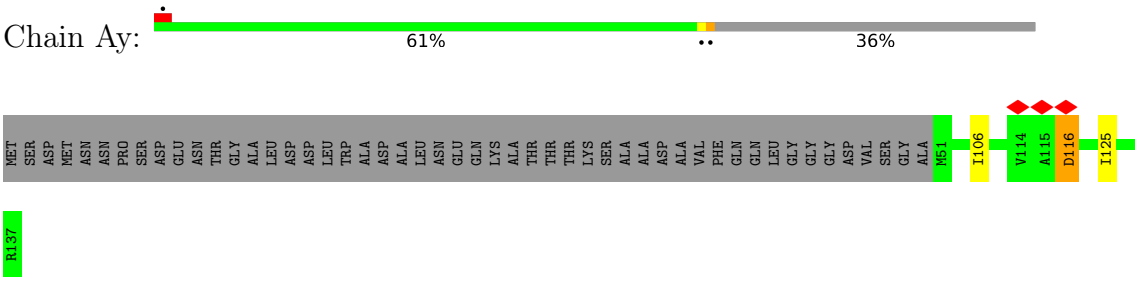
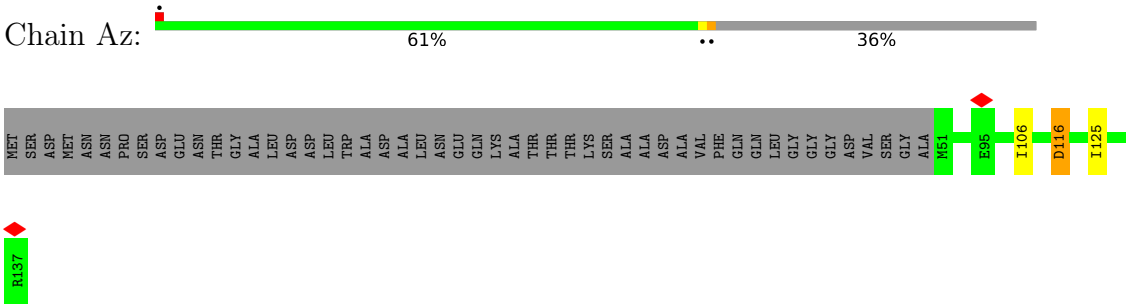


• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

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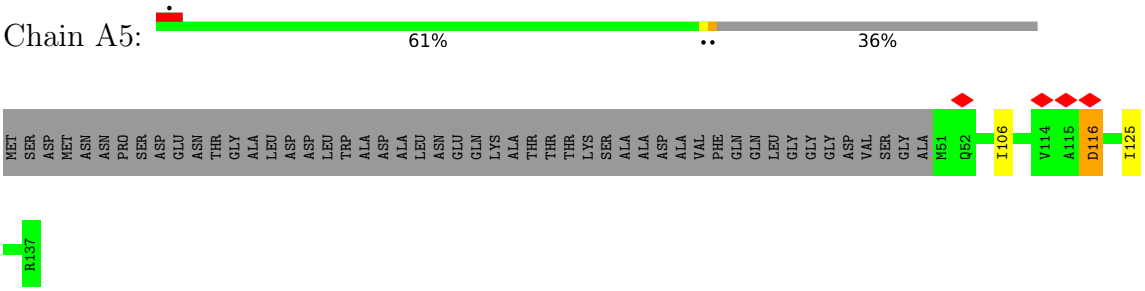
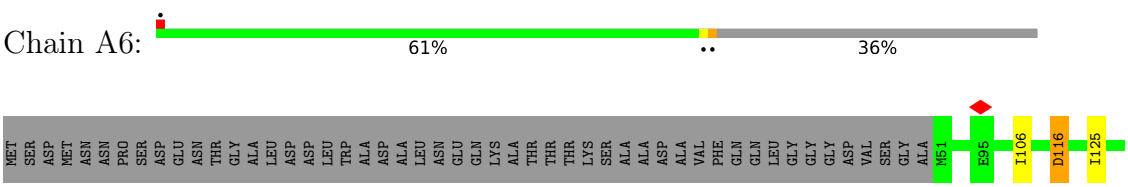


• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

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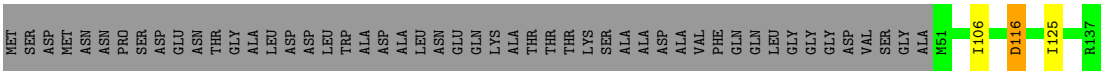

• Molecule 4: Flagellar motor switch protein FliN

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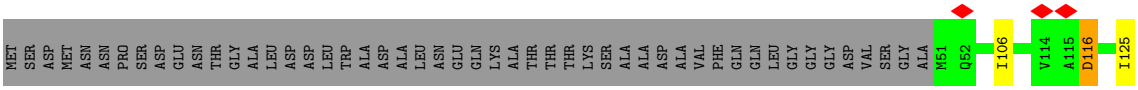

• Molecule 4: Flagellar motor switch protein FliN

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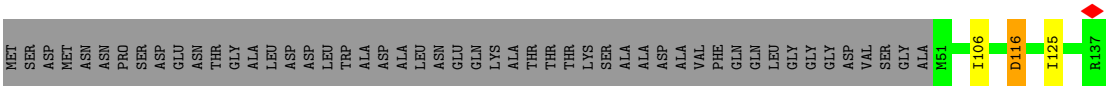

• Molecule 4: Flagellar motor switch protein FliN

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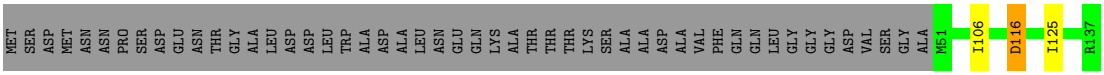

• Molecule 4: Flagellar motor switch protein FliN

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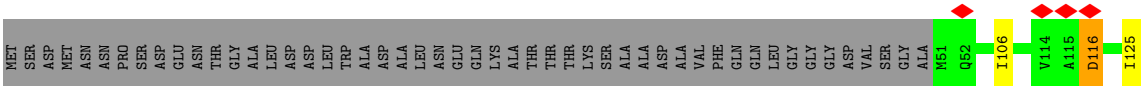

• Molecule 4: Flagellar motor switch protein FliN

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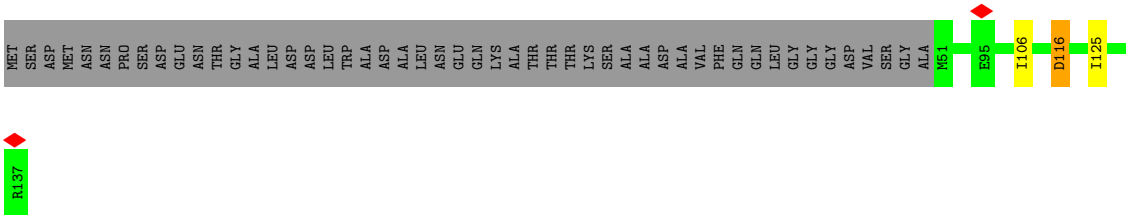

• Molecule 4: Flagellar motor switch protein FliN

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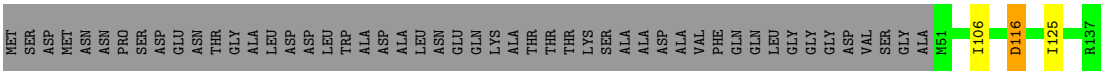

• Molecule 4: Flagellar motor switch protein FliN

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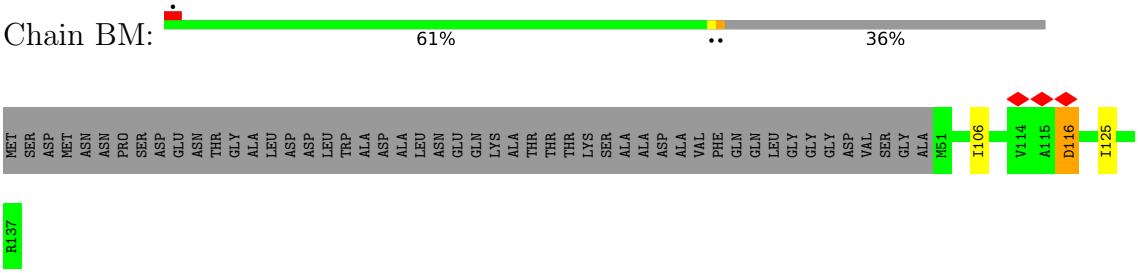

• Molecule 4: Flagellar motor switch protein FliN

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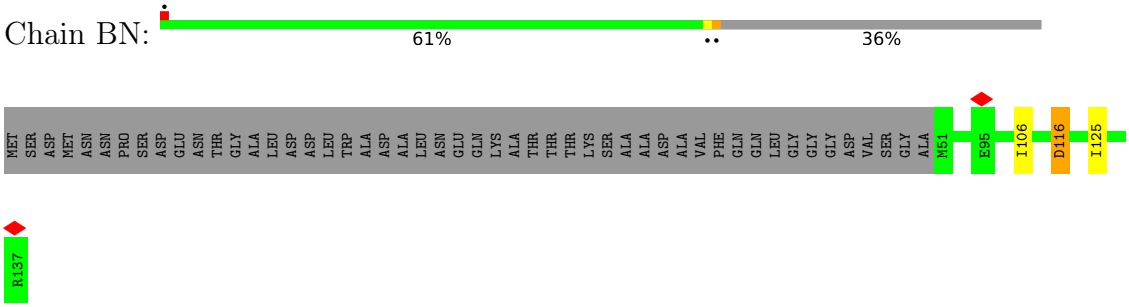

• Molecule 4: Flagellar motor switch protein FliN

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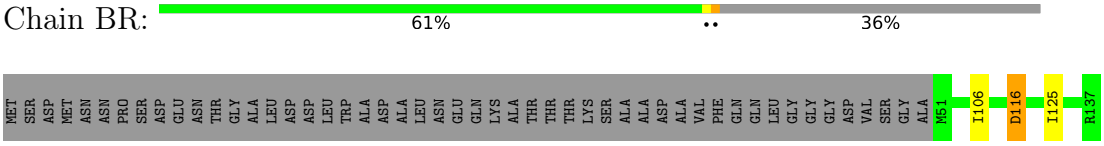

• Molecule 4: Flagellar motor switch protein FliN

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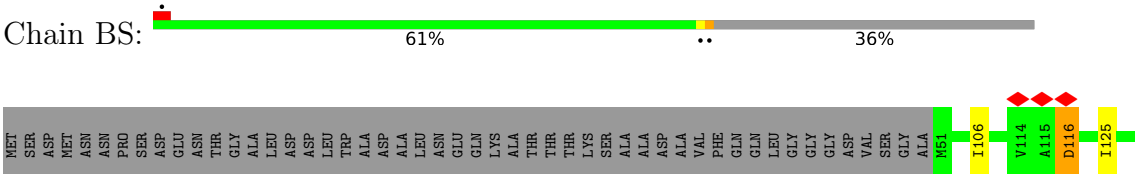

• Molecule 4: Flagellar motor switch protein FliN

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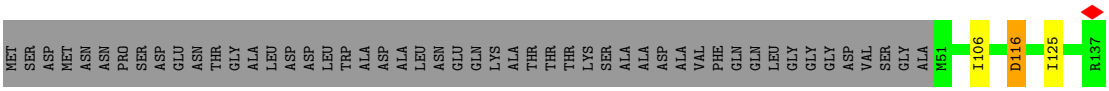

• Molecule 4: Flagellar motor switch protein FliN

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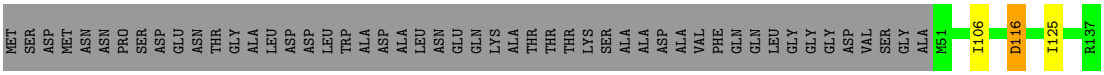

• Molecule 4: Flagellar motor switch protein FliN

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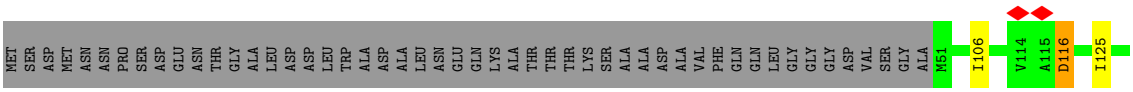

• Molecule 4: Flagellar motor switch protein FliN

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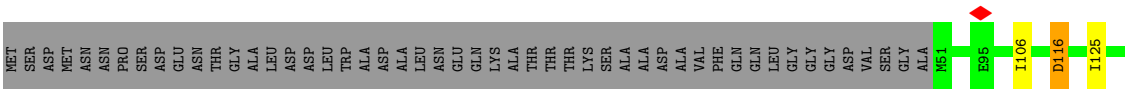

• Molecule 4: Flagellar motor switch protein FliN

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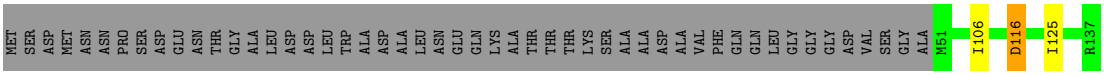

• Molecule 4: Flagellar motor switch protein FliN

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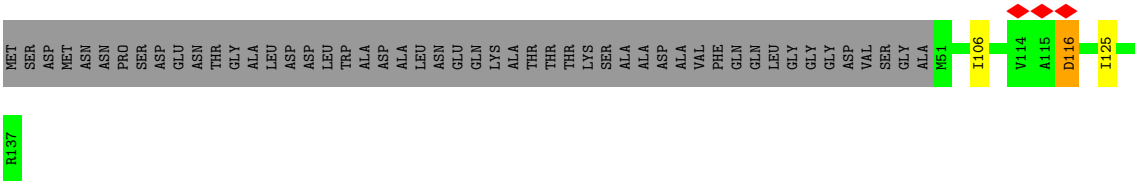
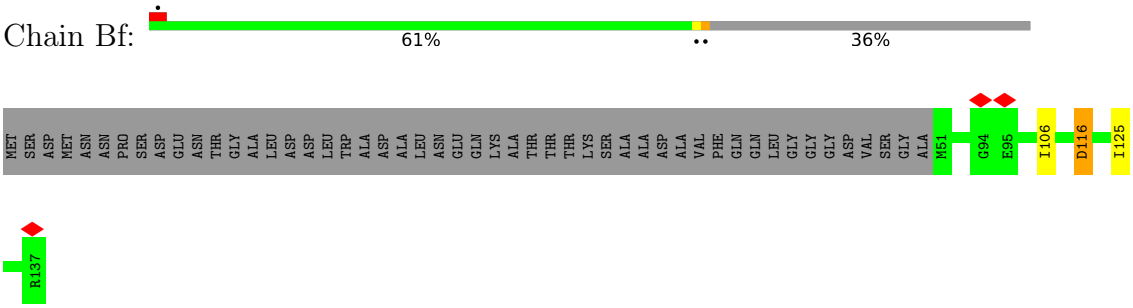
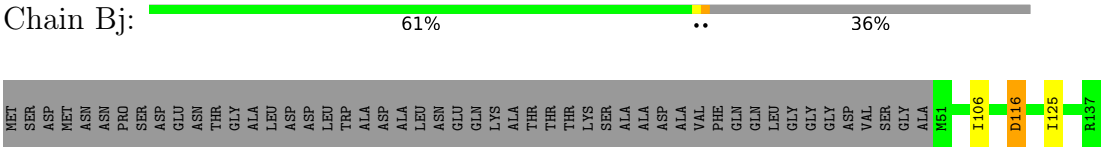


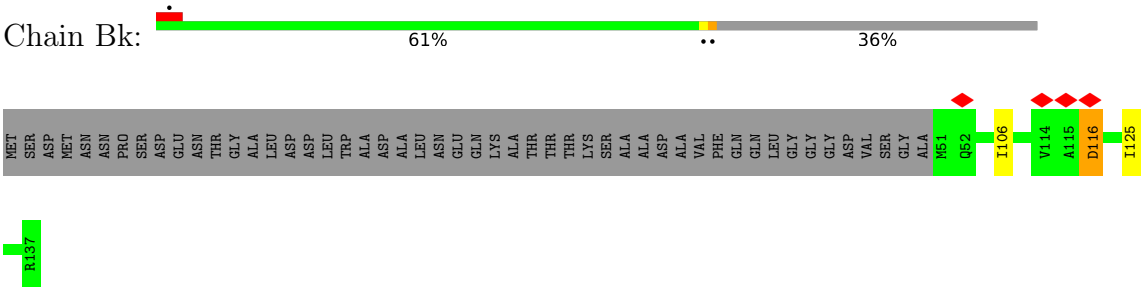
• Molecule 4: Flagellar motor switch protein FliN



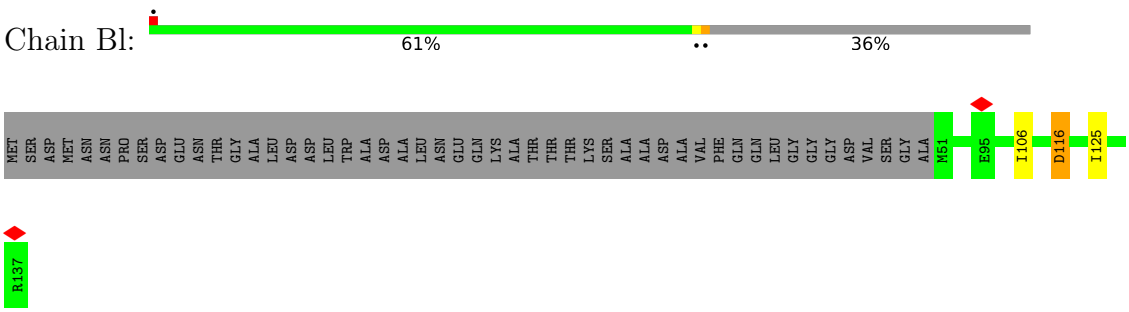
• Molecule 4: Flagellar motor switch protein FliN



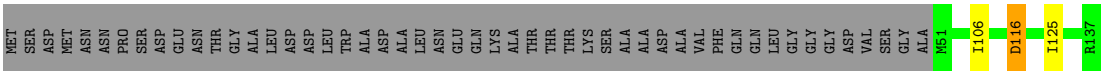
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

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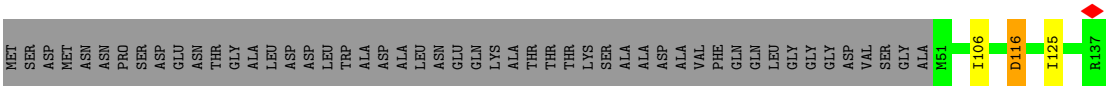
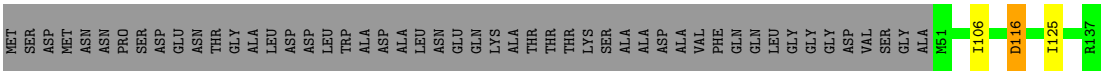
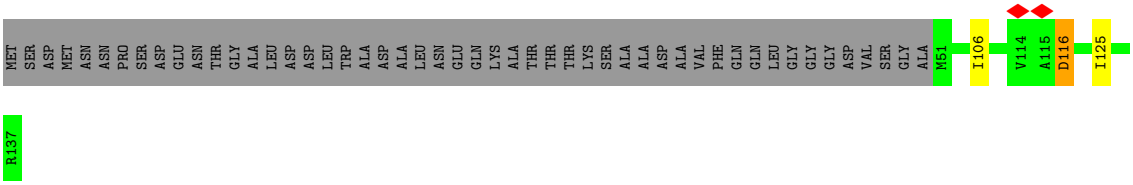


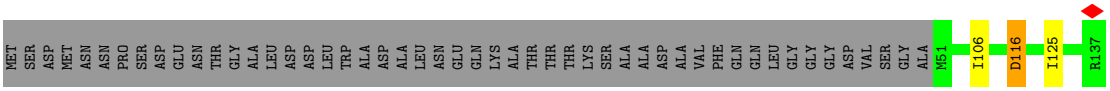
• Molecule 4: Flagellar motor switch protein FliN



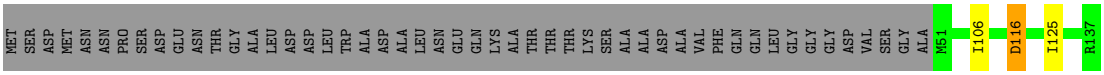
• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

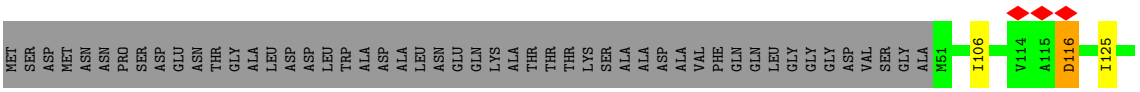


• Molecule 4: Flagellar motor switch protein FliN



• Molecule 4: Flagellar motor switch protein FliN

Chain B3:



• Molecule 4: Flagellar motor switch protein FliN

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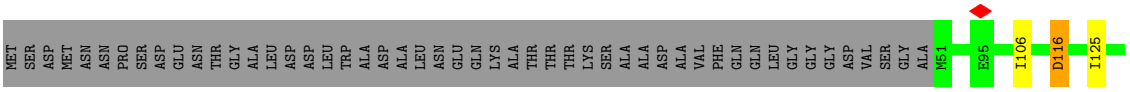

• Molecule 4: Flagellar motor switch protein FliN

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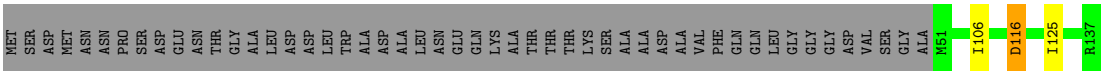

• Molecule 4: Flagellar motor switch protein FliN

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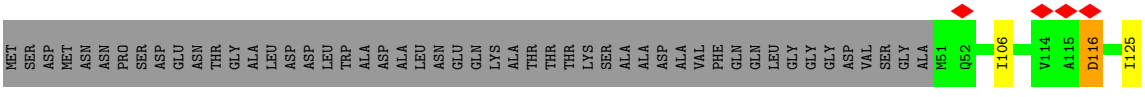

• Molecule 4: Flagellar motor switch protein FliN

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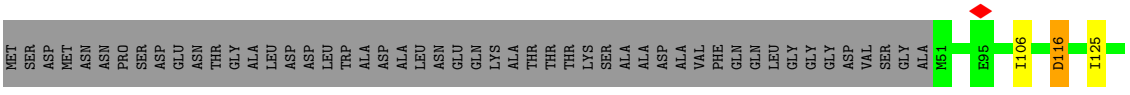

• Molecule 4: Flagellar motor switch protein FliN

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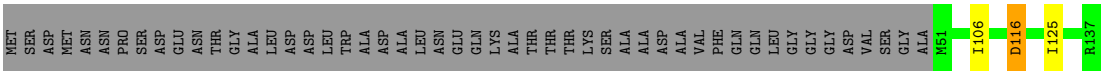

• Molecule 4: Flagellar motor switch protein FliN

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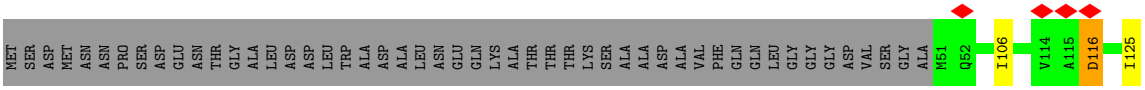

• Molecule 4: Flagellar motor switch protein FliN

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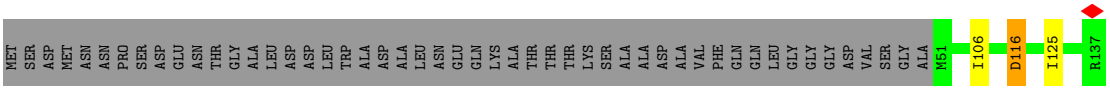

• Molecule 4: Flagellar motor switch protein FliN

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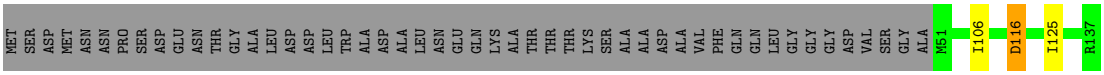
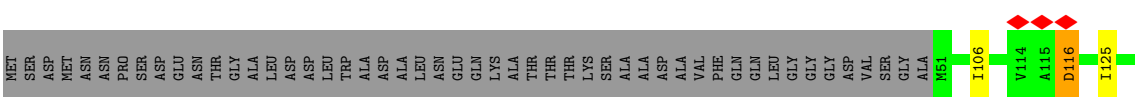


• Molecule 4: Flagellar motor switch protein FliN

Chain CK:



• Molecule 4: Flagellar motor switch protein FliN

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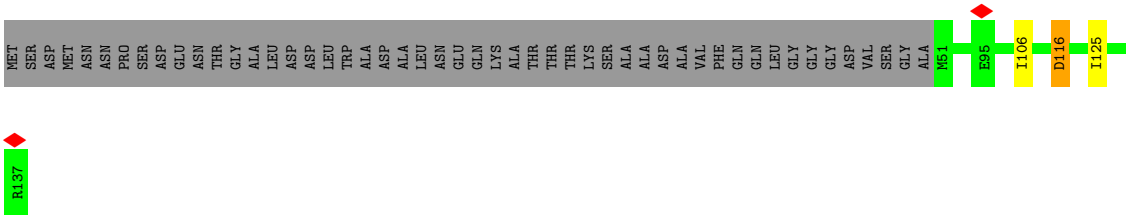
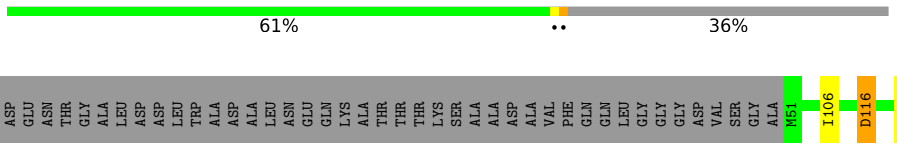


• Molecule 4: Flagellar motor switch protein FliN

Chain CP:



• Molecule 4: Flagellar motor switch protein FliN

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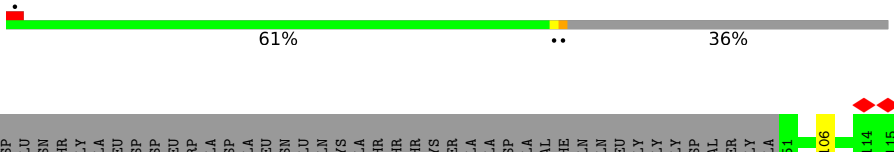

• Molecule 4: Flagellar motor switch protein FliN

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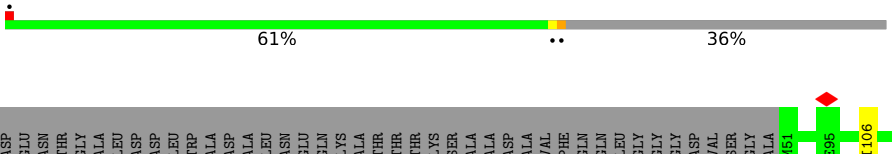

• Molecule 4: Flagellar motor switch protein FliN

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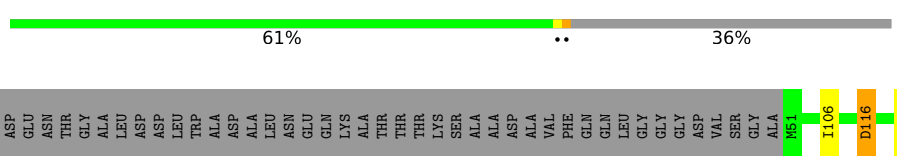

• Molecule 4: Flagellar motor switch protein FliN

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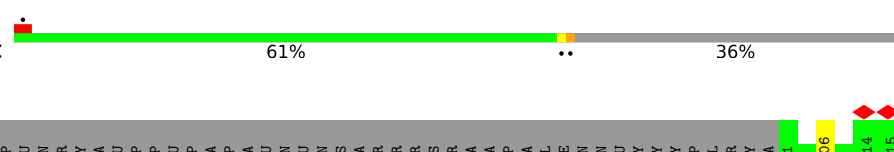
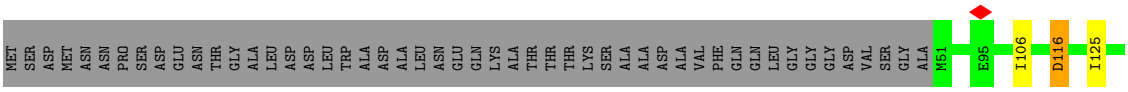


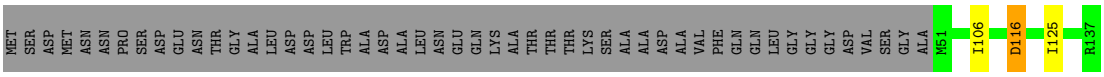
• Molecule 4: Flagellar motor switch protein FliN

Chain CX:



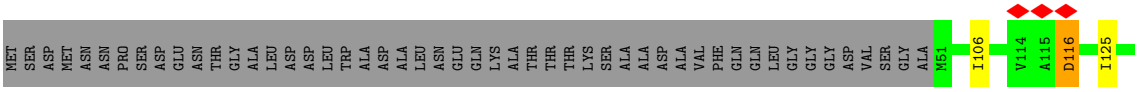
• Molecule 4: Flagellar motor switch protein FliN

Chain Cb:



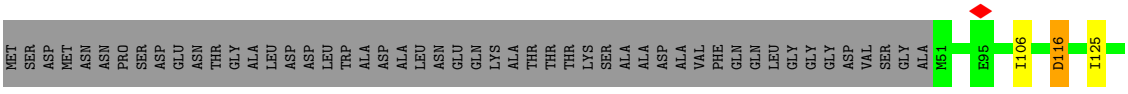
• Molecule 4: Flagellar motor switch protein FliN

Chain Cc:



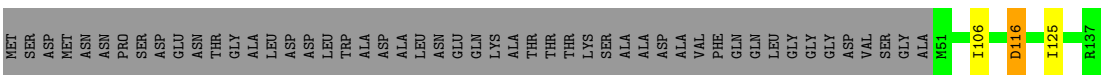
• Molecule 4: Flagellar motor switch protein FliN

Chain Cd:



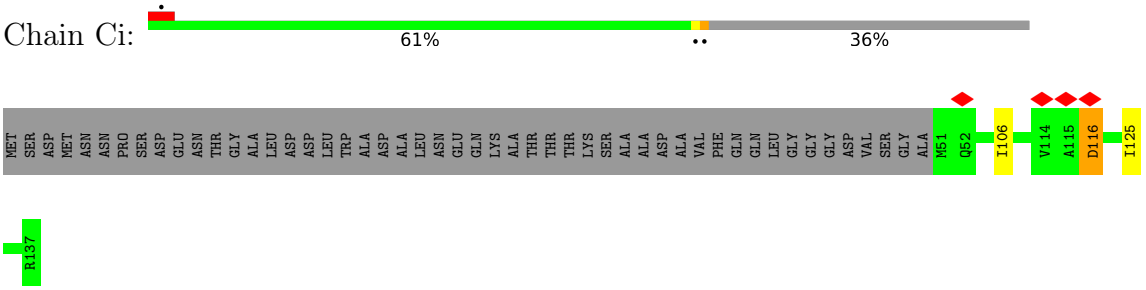
• Molecule 4: Flagellar motor switch protein FliN

Chain Ch:



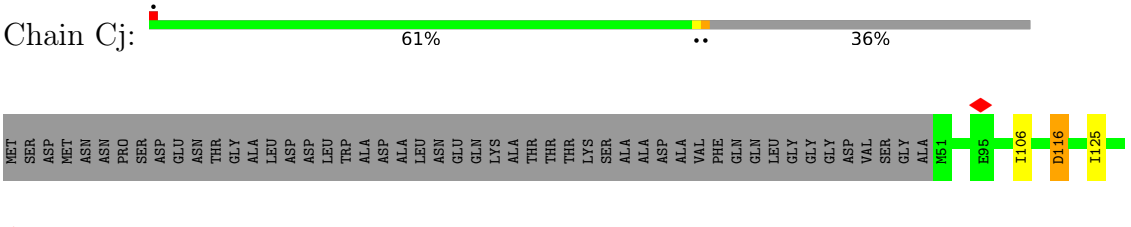
• Molecule 4: Flagellar motor switch protein FliN

Chain Ci:



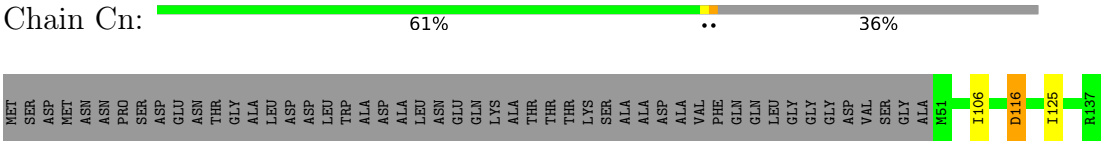
• Molecule 4: Flagellar motor switch protein FliN

Chain Cj:



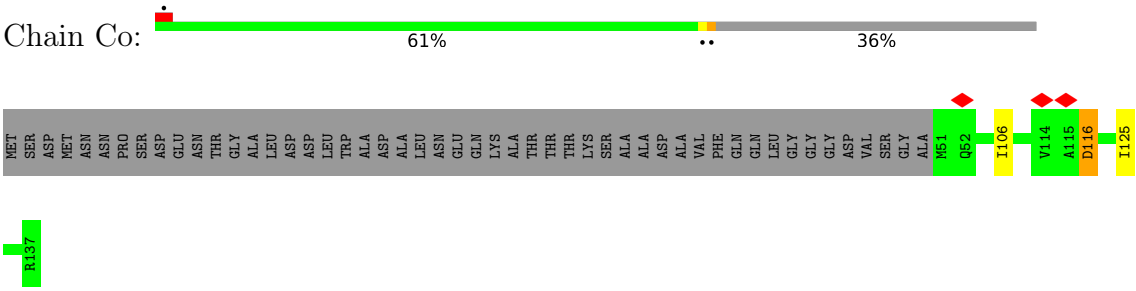
• Molecule 4: Flagellar motor switch protein FliN

Chain Cn:



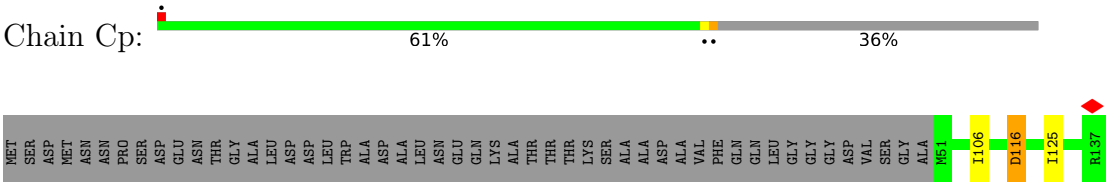
• Molecule 4: Flagellar motor switch protein FliN

Chain Co:



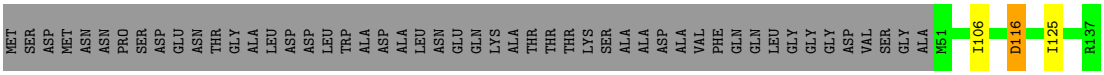
• Molecule 4: Flagellar motor switch protein FliN

Chain Cp:



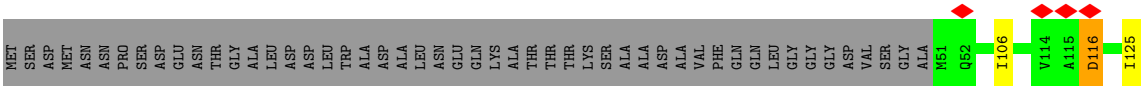
• Molecule 4: Flagellar motor switch protein FliN

Chain Ct:



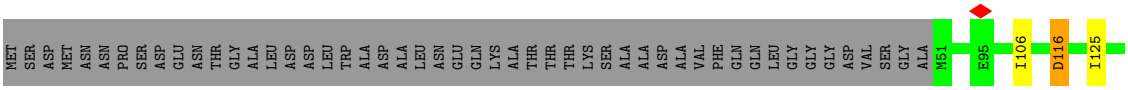
• Molecule 4: Flagellar motor switch protein FliN

Chain Cu:



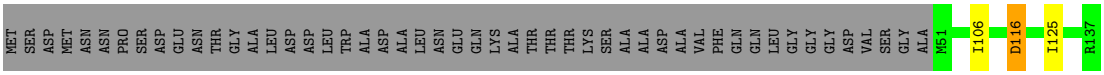
• Molecule 4: Flagellar motor switch protein FliN

Chain Cv:



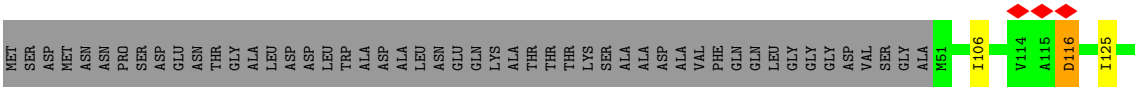
• Molecule 4: Flagellar motor switch protein FliN

Chain Cz:



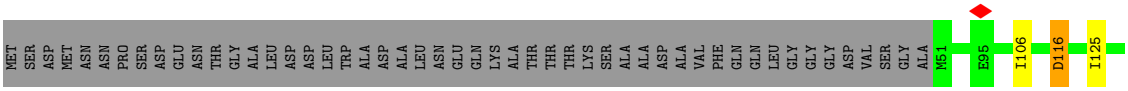
• Molecule 4: Flagellar motor switch protein FliN

Chain C1:



• Molecule 4: Flagellar motor switch protein FliN

Chain C2:



R137

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	19627	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.498	Depositor
Minimum map value	-0.276	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	660.0, 660.0, 660.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	3	0.27	0/2481	0.48	1/3344 (0.0%)
1	9	0.27	0/2481	0.48	1/3344 (0.0%)
1	A1	0.27	0/2481	0.48	1/3344 (0.0%)
1	A7	0.28	0/2481	0.48	1/3344 (0.0%)
1	AE	0.27	0/2481	0.48	1/3344 (0.0%)
1	AK	0.27	0/2481	0.48	1/3344 (0.0%)
1	AQ	0.27	0/2481	0.48	1/3344 (0.0%)
1	AW	0.27	0/2481	0.48	1/3344 (0.0%)
1	Ac	0.28	0/2481	0.48	1/3344 (0.0%)
1	Ai	0.28	0/2481	0.48	1/3344 (0.0%)
1	Ao	0.28	0/2481	0.48	1/3344 (0.0%)
1	Au	0.28	0/2481	0.48	1/3344 (0.0%)
1	B5	0.27	0/2481	0.48	1/3344 (0.0%)
1	BC	0.28	0/2481	0.48	1/3344 (0.0%)
1	BI	0.28	0/2481	0.48	1/3344 (0.0%)
1	BO	0.27	0/2481	0.48	1/3344 (0.0%)
1	BU	0.28	0/2481	0.48	1/3344 (0.0%)
1	Ba	0.27	0/2481	0.48	1/3344 (0.0%)
1	Bg	0.27	0/2481	0.48	1/3344 (0.0%)
1	Bm	0.27	0/2481	0.48	1/3344 (0.0%)
1	Bs	0.27	0/2481	0.48	1/3344 (0.0%)
1	By	0.27	0/2481	0.48	1/3344 (0.0%)
1	CA	0.28	0/2481	0.48	1/3344 (0.0%)
1	CG	0.28	0/2481	0.48	1/3344 (0.0%)
1	CM	0.28	0/2481	0.48	1/3344 (0.0%)
1	CS	0.28	0/2481	0.48	1/3344 (0.0%)
1	CY	0.28	0/2481	0.48	1/3344 (0.0%)
1	Ce	0.27	0/2481	0.48	1/3344 (0.0%)
1	Ck	0.28	0/2481	0.48	1/3344 (0.0%)
1	Cq	0.28	0/2481	0.48	1/3344 (0.0%)
1	Cw	0.28	0/2481	0.48	1/3344 (0.0%)
1	k	0.27	0/2481	0.48	1/3344 (0.0%)
1	q	0.27	0/2481	0.48	1/3344 (0.0%)
1	w	0.27	0/2481	0.48	1/3344 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	0	0.22	0/226	0.49	0/303
2	4	0.22	0/226	0.48	0/303
2	A2	0.22	0/226	0.49	0/303
2	A8	0.22	0/226	0.49	0/303
2	AF	0.22	0/226	0.49	0/303
2	AL	0.22	0/226	0.48	0/303
2	AR	0.22	0/226	0.49	0/303
2	AX	0.22	0/226	0.48	0/303
2	Ad	0.22	0/226	0.49	0/303
2	Aj	0.22	0/226	0.49	0/303
2	Ap	0.22	0/226	0.48	0/303
2	Av	0.22	0/226	0.49	0/303
2	B6	0.22	0/226	0.49	0/303
2	BD	0.22	0/226	0.49	0/303
2	BJ	0.22	0/226	0.48	0/303
2	BP	0.22	0/226	0.49	0/303
2	BV	0.22	0/226	0.48	0/303
2	Bb	0.22	0/226	0.48	0/303
2	Bh	0.22	0/226	0.48	0/303
2	Bn	0.22	0/226	0.50	0/303
2	Bt	0.22	0/226	0.49	0/303
2	Bz	0.22	0/226	0.48	0/303
2	CB	0.22	0/226	0.49	0/303
2	CH	0.22	0/226	0.49	0/303
2	CN	0.22	0/226	0.49	0/303
2	CT	0.22	0/226	0.49	0/303
2	CZ	0.22	0/226	0.49	0/303
2	Cf	0.22	0/226	0.49	0/303
2	Cl	0.22	0/226	0.48	0/303
2	Cr	0.22	0/226	0.48	0/303
2	Cx	0.22	0/226	0.49	0/303
2	l	0.22	0/226	0.49	0/303
2	r	0.22	0/226	0.48	0/303
2	x	0.22	0/226	0.48	0/303
3	5	0.25	0/2393	0.50	0/3255
3	A3	0.25	0/2393	0.50	0/3255
3	A9	0.25	0/2393	0.50	0/3255
3	AA	0.25	0/2393	0.50	0/3255
3	AG	0.25	0/2393	0.50	0/3255
3	AM	0.25	0/2393	0.50	0/3255
3	AS	0.25	0/2393	0.50	0/3255
3	AY	0.25	0/2393	0.50	0/3255
3	Ae	0.25	0/2393	0.50	0/3255

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	Ak	0.25	0/2393	0.50	0/3255
3	Aq	0.25	0/2393	0.50	0/3255
3	Aw	0.25	0/2393	0.50	0/3255
3	B1	0.25	0/2393	0.50	0/3255
3	B7	0.25	0/2393	0.50	0/3255
3	BE	0.25	0/2393	0.50	0/3255
3	BK	0.25	0/2393	0.50	0/3255
3	BQ	0.25	0/2393	0.50	0/3255
3	BW	0.25	0/2393	0.50	0/3255
3	Bc	0.25	0/2393	0.50	0/3255
3	Bi	0.25	0/2393	0.50	0/3255
3	Bo	0.25	0/2393	0.50	0/3255
3	Bu	0.25	0/2393	0.50	0/3255
3	CC	0.25	0/2393	0.50	0/3255
3	CI	0.25	0/2393	0.50	0/3255
3	CO	0.25	0/2393	0.50	0/3255
3	CU	0.25	0/2393	0.50	0/3255
3	Ca	0.25	0/2393	0.50	0/3255
3	Cg	0.25	0/2393	0.50	0/3255
3	Cm	0.25	0/2393	0.50	0/3255
3	Cs	0.25	0/2393	0.50	0/3255
3	Cy	0.25	0/2393	0.50	0/3255
3	m	0.25	0/2393	0.50	0/3255
3	s	0.25	0/2393	0.50	0/3255
3	y	0.25	0/2393	0.50	0/3255
4	1	0.23	0/679	0.52	0/917
4	2	0.23	0/679	0.53	0/917
4	6	0.23	0/679	0.53	0/917
4	7	0.23	0/679	0.53	0/917
4	8	0.23	0/679	0.53	0/917
4	A0	0.23	0/679	0.53	0/917
4	A4	0.23	0/679	0.53	0/917
4	A5	0.23	0/679	0.52	0/917
4	A6	0.23	0/679	0.53	0/917
4	AB	0.23	0/679	0.53	0/917
4	AC	0.23	0/679	0.53	0/917
4	AD	0.23	0/679	0.53	0/917
4	AH	0.23	0/679	0.53	0/917
4	AI	0.23	0/679	0.52	0/917
4	AJ	0.23	0/679	0.53	0/917
4	AN	0.23	0/679	0.53	0/917
4	AO	0.23	0/679	0.53	0/917
4	AP	0.23	0/679	0.53	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	AT	0.23	0/679	0.53	0/917
4	AU	0.23	0/679	0.52	0/917
4	AV	0.23	0/679	0.53	0/917
4	AZ	0.23	0/679	0.53	0/917
4	Aa	0.23	0/679	0.52	0/917
4	Ab	0.23	0/679	0.53	0/917
4	Af	0.23	0/679	0.53	0/917
4	Ag	0.23	0/679	0.52	0/917
4	Ah	0.23	0/679	0.53	0/917
4	Al	0.23	0/679	0.53	0/917
4	Am	0.23	0/679	0.53	0/917
4	An	0.23	0/679	0.53	0/917
4	Ar	0.23	0/679	0.53	0/917
4	As	0.23	0/679	0.52	0/917
4	At	0.23	0/679	0.53	0/917
4	Ax	0.23	0/679	0.52	0/917
4	Ay	0.23	0/679	0.53	0/917
4	Az	0.23	0/679	0.53	0/917
4	B0	0.23	0/679	0.53	0/917
4	B2	0.23	0/679	0.53	0/917
4	B3	0.23	0/679	0.53	0/917
4	B4	0.23	0/679	0.53	0/917
4	B8	0.23	0/679	0.53	0/917
4	B9	0.23	0/679	0.52	0/917
4	BA	0.23	0/679	0.52	0/917
4	BB	0.23	0/679	0.53	0/917
4	BF	0.23	0/679	0.52	0/917
4	BG	0.23	0/679	0.52	0/917
4	BH	0.23	0/679	0.53	0/917
4	BL	0.23	0/679	0.52	0/917
4	BM	0.23	0/679	0.52	0/917
4	BN	0.23	0/679	0.53	0/917
4	BR	0.23	0/679	0.53	0/917
4	BS	0.23	0/679	0.53	0/917
4	BT	0.23	0/679	0.53	0/917
4	BX	0.23	0/679	0.53	0/917
4	BY	0.23	0/679	0.52	0/917
4	BZ	0.23	0/679	0.53	0/917
4	Bd	0.23	0/679	0.53	0/917
4	Be	0.23	0/679	0.52	0/917
4	Bf	0.23	0/679	0.53	0/917
4	Bj	0.23	0/679	0.53	0/917
4	Bk	0.23	0/679	0.52	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	Bl	0.23	0/679	0.53	0/917
4	Bp	0.23	0/679	0.53	0/917
4	Bq	0.23	0/679	0.53	0/917
4	Br	0.23	0/679	0.53	0/917
4	Bv	0.23	0/679	0.53	0/917
4	Bw	0.23	0/679	0.52	0/917
4	Bx	0.23	0/679	0.53	0/917
4	C1	0.23	0/679	0.52	0/917
4	C2	0.23	0/679	0.53	0/917
4	CD	0.23	0/679	0.53	0/917
4	CE	0.23	0/679	0.52	0/917
4	CF	0.23	0/679	0.53	0/917
4	CJ	0.23	0/679	0.53	0/917
4	CK	0.23	0/679	0.52	0/917
4	CL	0.23	0/679	0.53	0/917
4	CP	0.23	0/679	0.53	0/917
4	CQ	0.23	0/679	0.53	0/917
4	CR	0.23	0/679	0.53	0/917
4	CV	0.23	0/679	0.53	0/917
4	CW	0.23	0/679	0.52	0/917
4	CX	0.23	0/679	0.53	0/917
4	Cb	0.23	0/679	0.53	0/917
4	Cc	0.23	0/679	0.52	0/917
4	Cd	0.23	0/679	0.53	0/917
4	Ch	0.23	0/679	0.53	0/917
4	Ci	0.23	0/679	0.52	0/917
4	Cj	0.23	0/679	0.53	0/917
4	Cn	0.23	0/679	0.53	0/917
4	Co	0.23	0/679	0.53	0/917
4	Cp	0.23	0/679	0.53	0/917
4	Ct	0.23	0/679	0.52	0/917
4	Cu	0.23	0/679	0.52	0/917
4	Cv	0.23	0/679	0.53	0/917
4	Cz	0.23	0/679	0.52	0/917
4	n	0.23	0/679	0.53	0/917
4	o	0.23	0/679	0.53	0/917
4	p	0.23	0/679	0.53	0/917
4	t	0.23	0/679	0.53	0/917
4	u	0.23	0/679	0.52	0/917
4	v	0.23	0/679	0.53	0/917
4	z	0.23	0/679	0.53	0/917
All	All	0.25	0/242658	0.50	34/328202 (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
1	3	0	2
1	9	0	2
1	A1	0	2
1	A7	0	2
1	AE	0	2
1	AK	0	2
1	AQ	0	2
1	AW	0	2
1	Ac	0	2
1	Ai	0	2
1	Ao	0	2
1	Au	0	2
1	B5	0	2
1	BC	0	2
1	BI	0	2
1	BO	0	2
1	BU	0	2
1	Ba	0	2
1	Bg	0	2
1	Bm	0	2
1	Bs	0	2
1	By	0	2
1	CA	0	2
1	CG	0	2
1	CM	0	2
1	CS	0	2
1	CY	0	2
1	Ce	0	2
1	Ck	0	2
1	Cq	0	2
1	Cw	0	2
1	k	0	2
1	q	0	2
1	w	0	2
All	All	0	68

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ac	66	PHE	C-N-CA	5.15	134.58	121.70
1	CG	66	PHE	C-N-CA	5.15	134.58	121.70
1	AK	66	PHE	C-N-CA	5.15	134.57	121.70
1	By	66	PHE	C-N-CA	5.15	134.57	121.70
1	q	66	PHE	C-N-CA	5.14	134.56	121.70
1	BU	66	PHE	C-N-CA	5.14	134.56	121.70
1	3	66	PHE	C-N-CA	5.14	134.55	121.70
1	AQ	66	PHE	C-N-CA	5.14	134.54	121.70
1	Bg	66	PHE	C-N-CA	5.14	134.55	121.70
1	CY	66	PHE	C-N-CA	5.14	134.54	121.70
1	Ce	66	PHE	C-N-CA	5.14	134.54	121.70
1	Cw	66	PHE	C-N-CA	5.13	134.54	121.70
1	AW	66	PHE	C-N-CA	5.13	134.53	121.70
1	A7	66	PHE	C-N-CA	5.13	134.53	121.70
1	CA	66	PHE	C-N-CA	5.13	134.52	121.70
1	A1	66	PHE	C-N-CA	5.13	134.52	121.70
1	B5	66	PHE	C-N-CA	5.13	134.52	121.70
1	k	66	PHE	C-N-CA	5.12	134.50	121.70
1	w	66	PHE	C-N-CA	5.12	134.50	121.70
1	Ba	66	PHE	C-N-CA	5.12	134.50	121.70
1	Au	66	PHE	C-N-CA	5.12	134.50	121.70
1	BI	66	PHE	C-N-CA	5.12	134.50	121.70
1	AE	66	PHE	C-N-CA	5.12	134.49	121.70
1	Ao	66	PHE	C-N-CA	5.12	134.49	121.70
1	CS	66	PHE	C-N-CA	5.12	134.49	121.70
1	9	66	PHE	C-N-CA	5.11	134.47	121.70
1	Ai	66	PHE	C-N-CA	5.11	134.47	121.70
1	BO	66	PHE	C-N-CA	5.11	134.47	121.70
1	Bm	66	PHE	C-N-CA	5.11	134.47	121.70
1	Bs	66	PHE	C-N-CA	5.11	134.47	121.70
1	CM	66	PHE	C-N-CA	5.11	134.47	121.70
1	BC	66	PHE	C-N-CA	5.11	134.46	121.70
1	Ck	66	PHE	C-N-CA	5.11	134.46	121.70
1	Cq	66	PHE	C-N-CA	5.11	134.46	121.70

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	206	MET	Mainchain
1	3	219	ARG	Sidechain
1	9	206	MET	Mainchain
1	9	219	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A1	206	MET	Mainchain
1	A1	219	ARG	Sidechain
1	A7	206	MET	Mainchain
1	A7	219	ARG	Sidechain
1	AE	206	MET	Mainchain
1	AE	219	ARG	Sidechain
1	AK	206	MET	Mainchain
1	AK	219	ARG	Sidechain
1	AQ	206	MET	Mainchain
1	AQ	219	ARG	Sidechain
1	AW	206	MET	Mainchain
1	AW	219	ARG	Sidechain
1	Ac	206	MET	Mainchain
1	Ac	219	ARG	Sidechain
1	Ai	206	MET	Mainchain
1	Ai	219	ARG	Sidechain
1	Ao	206	MET	Mainchain
1	Ao	219	ARG	Sidechain
1	Au	206	MET	Mainchain
1	Au	219	ARG	Sidechain
1	B5	206	MET	Mainchain
1	B5	219	ARG	Sidechain
1	BC	206	MET	Mainchain
1	BC	219	ARG	Sidechain
1	BI	206	MET	Mainchain
1	BI	219	ARG	Sidechain
1	BO	206	MET	Mainchain
1	BO	219	ARG	Sidechain
1	BU	206	MET	Mainchain
1	BU	219	ARG	Sidechain
1	Ba	206	MET	Mainchain
1	Ba	219	ARG	Sidechain
1	Bg	206	MET	Mainchain
1	Bg	219	ARG	Sidechain
1	Bm	206	MET	Mainchain
1	Bm	219	ARG	Sidechain
1	Bs	206	MET	Mainchain
1	Bs	219	ARG	Sidechain
1	By	206	MET	Mainchain
1	By	219	ARG	Sidechain
1	CA	206	MET	Mainchain
1	CA	219	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	CG	206	MET	Mainchain
1	CG	219	ARG	Sidechain
1	CM	206	MET	Mainchain
1	CM	219	ARG	Sidechain
1	CS	206	MET	Mainchain
1	CS	219	ARG	Sidechain
1	CY	206	MET	Mainchain
1	CY	219	ARG	Sidechain
1	Ce	206	MET	Mainchain
1	Ce	219	ARG	Sidechain
1	Ck	206	MET	Mainchain
1	Ck	219	ARG	Sidechain
1	Cq	206	MET	Mainchain
1	Cq	219	ARG	Sidechain
1	Cw	206	MET	Mainchain
1	Cw	219	ARG	Sidechain
1	k	206	MET	Mainchain
1	k	219	ARG	Sidechain
1	q	206	MET	Mainchain
1	q	219	ARG	Sidechain
1	w	206	MET	Mainchain
1	w	219	ARG	Sidechain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	3	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22 61
1	9	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	A7	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	AE	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	AK	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	AQ	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	AW	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Ac	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Ai	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Ao	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Au	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	B5	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	BC	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	BI	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	BO	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	BU	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Ba	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Bg	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Bm	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Bs	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	By	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	CA	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	CG	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	CM	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	CS	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	CY	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Ce	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Ck	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Cq	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	Cw	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	k	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
1	q	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	61
2	0	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	4	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	A2	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	A8	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	AF	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	AL	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	AR	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	AX	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Ad	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Aj	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Ap	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Av	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	B6	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	BD	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	BJ	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	BP	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	BV	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Bb	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Bh	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Bn	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Bt	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Bz	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	CB	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	CH	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	CN	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	CT	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	CZ	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Cf	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Cl	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Cr	25/560 (4%)	24 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Cx	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	l	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	r	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	x	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
3	5	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	A3	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	A9	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	AA	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	AG	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	AM	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	AS	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	AY	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Ae	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Ak	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Aq	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Aw	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	B1	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	B7	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	BE	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	BK	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	BQ	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	BW	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Bc	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Bi	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Bo	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Bu	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	CC	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	CI	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	CO	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	CU	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Ca	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Cg	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Cm	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Cs	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	Cy	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	m	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	s	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
3	y	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
4	1	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	2	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	6	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	7	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	8	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	A0	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	A4	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	A5	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	A6	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AB	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AC	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AD	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AH	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AI	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AJ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AN	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AO	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AP	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AT	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AU	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AV	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	AZ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Aa	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Ab	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Af	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Ag	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Ah	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Al	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Am	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	An	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Ar	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	As	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	At	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Ax	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Ay	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Az	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	B0	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	B2	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	B3	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	B4	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	B8	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	B9	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BA	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BB	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BF	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BG	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BH	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BL	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BM	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BN	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BR	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BS	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BT	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BX	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	BY	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	BZ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Bd	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Be	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Bf	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Bj	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Bk	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Bl	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Bp	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Bq	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Br	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Bv	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Bw	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Bx	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	C1	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	C2	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CD	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CE	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CF	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CJ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CK	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CL	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CP	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CQ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CR	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CV	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CW	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	CX	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Cb	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Cc	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Cd	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Ch	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Ci	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Cj	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Cn	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Co	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Cp	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Ct	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Cu	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Cv	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	Cz	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	n	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	o	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	p	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	t	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	u	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	v	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
4	z	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
All	All	29852/55624 (54%)	28526 (96%)	1088 (4%)	238 (1%)	19	55

All (238) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	n	116	ASP
4	o	116	ASP
4	p	116	ASP
4	t	116	ASP
4	u	116	ASP
4	v	116	ASP
4	z	116	ASP
4	1	116	ASP
4	2	116	ASP
4	6	116	ASP
4	7	116	ASP
4	8	116	ASP
4	AB	116	ASP
4	AC	116	ASP
4	AD	116	ASP

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Mol	Chain	Res	Type
4	AH	116	ASP
4	AI	116	ASP
4	AJ	116	ASP
4	AN	116	ASP
4	AO	116	ASP
4	AP	116	ASP
4	AT	116	ASP
4	AU	116	ASP
4	AV	116	ASP
4	AZ	116	ASP
4	Aa	116	ASP
4	Ab	116	ASP
4	Af	116	ASP
4	Ag	116	ASP
4	Ah	116	ASP
4	Al	116	ASP
4	Am	116	ASP
4	An	116	ASP
4	Ar	116	ASP
4	As	116	ASP
4	At	116	ASP
4	Ax	116	ASP
4	Ay	116	ASP
4	Az	116	ASP
4	A4	116	ASP
4	A5	116	ASP
4	A6	116	ASP
4	A0	116	ASP
4	BA	116	ASP
4	BB	116	ASP
4	BF	116	ASP
4	BG	116	ASP
4	BH	116	ASP
4	BL	116	ASP
4	BM	116	ASP
4	BN	116	ASP
4	BR	116	ASP
4	BS	116	ASP
4	BT	116	ASP
4	BX	116	ASP
4	BY	116	ASP
4	BZ	116	ASP

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Mol	Chain	Res	Type
4	Bd	116	ASP
4	Be	116	ASP
4	Bf	116	ASP
4	Bj	116	ASP
4	Bk	116	ASP
4	Bl	116	ASP
4	Bp	116	ASP
4	Bq	116	ASP
4	Br	116	ASP
4	Bv	116	ASP
4	Bw	116	ASP
4	Bx	116	ASP
4	B2	116	ASP
4	B3	116	ASP
4	B4	116	ASP
4	B8	116	ASP
4	B9	116	ASP
4	B0	116	ASP
4	CD	116	ASP
4	CE	116	ASP
4	CF	116	ASP
4	CJ	116	ASP
4	CK	116	ASP
4	CL	116	ASP
4	CP	116	ASP
4	CQ	116	ASP
4	CR	116	ASP
4	CV	116	ASP
4	CW	116	ASP
4	CX	116	ASP
4	Cb	116	ASP
4	Cc	116	ASP
4	Cd	116	ASP
4	Ch	116	ASP
4	Ci	116	ASP
4	Cj	116	ASP
4	Cn	116	ASP
4	Co	116	ASP
4	Cp	116	ASP
4	Ct	116	ASP
4	Cu	116	ASP
4	Cv	116	ASP

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Mol	Chain	Res	Type
4	Cz	116	ASP
4	C1	116	ASP
4	C2	116	ASP
1	k	221	PHE
3	m	47	VAL
1	q	221	PHE
3	s	47	VAL
1	w	221	PHE
3	y	47	VAL
1	3	221	PHE
3	5	47	VAL
1	9	221	PHE
3	AA	47	VAL
1	AE	221	PHE
3	AG	47	VAL
1	AK	221	PHE
3	AM	47	VAL
1	AQ	221	PHE
3	AS	47	VAL
1	AW	221	PHE
3	AY	47	VAL
1	Ac	221	PHE
3	Ae	47	VAL
1	Ai	221	PHE
3	Ak	47	VAL
1	Ao	221	PHE
3	Aq	47	VAL
1	Au	221	PHE
3	Aw	47	VAL
1	A1	221	PHE
3	A3	47	VAL
1	A7	221	PHE
3	A9	47	VAL
1	BC	221	PHE
3	BE	47	VAL
1	BI	221	PHE
3	BK	47	VAL
1	BO	221	PHE
3	BQ	47	VAL
1	BU	221	PHE
3	BW	47	VAL
1	Ba	221	PHE

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Mol	Chain	Res	Type
3	Bc	47	VAL
1	Bg	221	PHE
3	Bi	47	VAL
1	Bm	221	PHE
3	Bo	47	VAL
1	Bs	221	PHE
3	Bu	47	VAL
1	By	221	PHE
3	B1	47	VAL
1	B5	221	PHE
3	B7	47	VAL
1	CA	221	PHE
3	CC	47	VAL
1	CG	221	PHE
3	CI	47	VAL
1	CM	221	PHE
3	CO	47	VAL
1	CS	221	PHE
3	CU	47	VAL
1	CY	221	PHE
3	Ca	47	VAL
1	Ce	221	PHE
3	Cg	47	VAL
1	Ck	221	PHE
3	Cm	47	VAL
1	Cq	221	PHE
3	Cs	47	VAL
1	Cw	221	PHE
3	Cy	47	VAL
1	k	234	PHE
1	q	234	PHE
3	s	190	ASN
1	w	234	PHE
1	3	234	PHE
3	5	190	ASN
1	9	234	PHE
3	AA	190	ASN
1	AE	234	PHE
3	AG	190	ASN
1	AK	234	PHE
1	AQ	234	PHE
1	AW	234	PHE

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Mol	Chain	Res	Type
1	Ac	234	PHE
1	Ai	234	PHE
3	Ak	190	ASN
1	Ao	234	PHE
1	Au	234	PHE
1	A1	234	PHE
3	A3	190	ASN
1	A7	234	PHE
1	BC	234	PHE
3	BE	190	ASN
1	BI	234	PHE
1	BO	234	PHE
1	BU	234	PHE
3	BW	190	ASN
1	Ba	234	PHE
1	Bg	234	PHE
3	Bi	190	ASN
1	Bm	234	PHE
3	Bo	190	ASN
1	Bs	234	PHE
3	Bu	190	ASN
1	By	234	PHE
1	B5	234	PHE
1	CA	234	PHE
1	CG	234	PHE
1	CM	234	PHE
3	CO	190	ASN
1	CS	234	PHE
1	CY	234	PHE
1	Ce	234	PHE
1	Ck	234	PHE
1	Cq	234	PHE
3	Cs	190	ASN
1	Cw	234	PHE
3	m	190	ASN
3	y	190	ASN
3	AM	190	ASN
3	AS	190	ASN
3	AY	190	ASN
3	Ae	190	ASN
3	Aq	190	ASN
3	Aw	190	ASN

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Mol	Chain	Res	Type
3	A9	190	ASN
3	BK	190	ASN
3	BQ	190	ASN
3	Bc	190	ASN
3	B1	190	ASN
3	B7	190	ASN
3	CC	190	ASN
3	CI	190	ASN
3	CU	190	ASN
3	Ca	190	ASN
3	Cg	190	ASN
3	Cm	190	ASN
3	Cy	190	ASN

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	3	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	9	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	A1	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	A7	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	AE	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	AK	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	AQ	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	AW	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Ac	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Ai	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Ao	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Au	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	B5	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	BC	268/282 (95%)	265 (99%)	3 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BI	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	BO	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	BU	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Ba	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Bg	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Bm	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Bs	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	By	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	CA	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	CG	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	CM	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	CS	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	CY	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Ce	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Ck	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Cq	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	Cw	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	k	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	q	268/282 (95%)	265 (99%)	3 (1%)	70	80
1	w	268/282 (95%)	265 (99%)	3 (1%)	70	80
2	0	26/467 (6%)	26 (100%)	0	100	100
2	4	26/467 (6%)	26 (100%)	0	100	100
2	A2	26/467 (6%)	26 (100%)	0	100	100
2	A8	26/467 (6%)	26 (100%)	0	100	100
2	AF	26/467 (6%)	26 (100%)	0	100	100
2	AL	26/467 (6%)	26 (100%)	0	100	100
2	AR	26/467 (6%)	26 (100%)	0	100	100
2	AX	26/467 (6%)	26 (100%)	0	100	100
2	Ad	26/467 (6%)	26 (100%)	0	100	100
2	Aj	26/467 (6%)	26 (100%)	0	100	100
2	Ap	26/467 (6%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Av	26/467 (6%)	26 (100%)	0	100	100
2	B6	26/467 (6%)	26 (100%)	0	100	100
2	BD	26/467 (6%)	26 (100%)	0	100	100
2	BJ	26/467 (6%)	26 (100%)	0	100	100
2	BP	26/467 (6%)	26 (100%)	0	100	100
2	BV	26/467 (6%)	26 (100%)	0	100	100
2	Bb	26/467 (6%)	26 (100%)	0	100	100
2	Bh	26/467 (6%)	26 (100%)	0	100	100
2	Bn	26/467 (6%)	26 (100%)	0	100	100
2	Bt	26/467 (6%)	26 (100%)	0	100	100
2	Bz	26/467 (6%)	26 (100%)	0	100	100
2	CB	26/467 (6%)	26 (100%)	0	100	100
2	CH	26/467 (6%)	26 (100%)	0	100	100
2	CN	26/467 (6%)	26 (100%)	0	100	100
2	CT	26/467 (6%)	26 (100%)	0	100	100
2	CZ	26/467 (6%)	26 (100%)	0	100	100
2	Cf	26/467 (6%)	26 (100%)	0	100	100
2	Cl	26/467 (6%)	26 (100%)	0	100	100
2	Cr	26/467 (6%)	26 (100%)	0	100	100
2	Cx	26/467 (6%)	26 (100%)	0	100	100
2	l	26/467 (6%)	26 (100%)	0	100	100
2	r	26/467 (6%)	26 (100%)	0	100	100
2	x	26/467 (6%)	26 (100%)	0	100	100
3	5	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	A3	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	A9	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	AA	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	AG	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	AM	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	AS	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	AY	262/301 (87%)	250 (95%)	12 (5%)	23	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Ae	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Ak	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Aq	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Aw	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	B1	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	B7	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	BE	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	BK	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	BQ	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	BW	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Bc	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Bi	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Bo	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Bu	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	CC	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	CI	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	CO	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	CU	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Ca	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Cg	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Cm	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Cs	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	Cy	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	m	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	s	262/301 (87%)	250 (95%)	12 (5%)	23	44
3	y	262/301 (87%)	250 (95%)	12 (5%)	23	44
4	1	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	2	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	6	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	7	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	8	76/113 (67%)	73 (96%)	3 (4%)	27	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A0	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	A4	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	A5	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	A6	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AB	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AC	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AD	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AH	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AI	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AJ	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AN	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AO	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AP	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AT	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AU	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AV	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	AZ	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Aa	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Ab	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Af	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Ag	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Ah	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Al	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Am	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	An	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Ar	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	As	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	At	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Ax	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Ay	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Az	76/113 (67%)	73 (96%)	3 (4%)	27	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B0	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	B2	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	B3	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	B4	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	B8	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	B9	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BA	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BB	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BF	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BG	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BH	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BL	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BM	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BN	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BR	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BS	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BT	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BX	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BY	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	BZ	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Bd	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Be	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Bf	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Bj	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Bk	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Bl	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Bp	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Bq	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Br	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Bv	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Bw	76/113 (67%)	73 (96%)	3 (4%)	27	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Bx	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	C1	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	C2	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CD	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CE	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CF	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CJ	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CK	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CL	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CP	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CQ	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CR	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CV	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CW	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	CX	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Cb	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Cc	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Cd	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Ch	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Ci	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Cj	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Cn	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Co	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Cp	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Ct	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Cu	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Cv	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	Cz	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	n	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	o	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	p	76/113 (67%)	73 (96%)	3 (4%)	27	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	t	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	u	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	v	76/113 (67%)	73 (96%)	3 (4%)	27	48
4	z	76/113 (67%)	73 (96%)	3 (4%)	27	48
All	All	26656/47226 (56%)	25840 (97%)	816 (3%)	37	54

All (816) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	k	112	PHE
1	k	124	ASP
1	k	193	MET
3	m	45	ARG
3	m	46	VAL
3	m	63	ARG
3	m	85	ARG
3	m	149	THR
3	m	155	ASN
3	m	162	LEU
3	m	169	TRP
3	m	211	LEU
3	m	228	ARG
3	m	233	ASN
3	m	286	ILE
4	n	106	ILE
4	n	116	ASP
4	n	125	ILE
4	o	106	ILE
4	o	116	ASP
4	o	125	ILE
4	p	106	ILE
4	p	116	ASP
4	p	125	ILE
1	q	112	PHE
1	q	124	ASP
1	q	193	MET
3	s	45	ARG
3	s	46	VAL
3	s	63	ARG
3	s	85	ARG
3	s	149	THR

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Mol	Chain	Res	Type
3	s	155	ASN
3	s	162	LEU
3	s	169	TRP
3	s	211	LEU
3	s	228	ARG
3	s	233	ASN
3	s	286	ILE
4	t	106	ILE
4	t	116	ASP
4	t	125	ILE
4	u	106	ILE
4	u	116	ASP
4	u	125	ILE
4	v	106	ILE
4	v	116	ASP
4	v	125	ILE
1	w	112	PHE
1	w	124	ASP
1	w	193	MET
3	y	45	ARG
3	y	46	VAL
3	y	63	ARG
3	y	85	ARG
3	y	149	THR
3	y	155	ASN
3	y	162	LEU
3	y	169	TRP
3	y	211	LEU
3	y	228	ARG
3	y	233	ASN
3	y	286	ILE
4	z	106	ILE
4	z	116	ASP
4	z	125	ILE
4	1	106	ILE
4	1	116	ASP
4	1	125	ILE
4	2	106	ILE
4	2	116	ASP
4	2	125	ILE
1	3	112	PHE
1	3	124	ASP

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Mol	Chain	Res	Type
1	3	193	MET
3	5	45	ARG
3	5	46	VAL
3	5	63	ARG
3	5	85	ARG
3	5	149	THR
3	5	155	ASN
3	5	162	LEU
3	5	169	TRP
3	5	211	LEU
3	5	228	ARG
3	5	233	ASN
3	5	286	ILE
4	6	106	ILE
4	6	116	ASP
4	6	125	ILE
4	7	106	ILE
4	7	116	ASP
4	7	125	ILE
4	8	106	ILE
4	8	116	ASP
4	8	125	ILE
1	9	112	PHE
1	9	124	ASP
1	9	193	MET
3	AA	45	ARG
3	AA	46	VAL
3	AA	63	ARG
3	AA	85	ARG
3	AA	149	THR
3	AA	155	ASN
3	AA	162	LEU
3	AA	169	TRP
3	AA	211	LEU
3	AA	228	ARG
3	AA	233	ASN
3	AA	286	ILE
4	AB	106	ILE
4	AB	116	ASP
4	AB	125	ILE
4	AC	106	ILE
4	AC	116	ASP

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Mol	Chain	Res	Type
4	AC	125	ILE
4	AD	106	ILE
4	AD	116	ASP
4	AD	125	ILE
1	AE	112	PHE
1	AE	124	ASP
1	AE	193	MET
3	AG	45	ARG
3	AG	46	VAL
3	AG	63	ARG
3	AG	85	ARG
3	AG	149	THR
3	AG	155	ASN
3	AG	162	LEU
3	AG	169	TRP
3	AG	211	LEU
3	AG	228	ARG
3	AG	233	ASN
3	AG	286	ILE
4	AH	106	ILE
4	AH	116	ASP
4	AH	125	ILE
4	AI	106	ILE
4	AI	116	ASP
4	AI	125	ILE
4	AJ	106	ILE
4	AJ	116	ASP
4	AJ	125	ILE
1	AK	112	PHE
1	AK	124	ASP
1	AK	193	MET
3	AM	45	ARG
3	AM	46	VAL
3	AM	63	ARG
3	AM	85	ARG
3	AM	149	THR
3	AM	155	ASN
3	AM	162	LEU
3	AM	169	TRP
3	AM	211	LEU
3	AM	228	ARG
3	AM	233	ASN

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Mol	Chain	Res	Type
3	AM	286	ILE
4	AN	106	ILE
4	AN	116	ASP
4	AN	125	ILE
4	AO	106	ILE
4	AO	116	ASP
4	AO	125	ILE
4	AP	106	ILE
4	AP	116	ASP
4	AP	125	ILE
1	AQ	112	PHE
1	AQ	124	ASP
1	AQ	193	MET
3	AS	45	ARG
3	AS	46	VAL
3	AS	63	ARG
3	AS	85	ARG
3	AS	149	THR
3	AS	155	ASN
3	AS	162	LEU
3	AS	169	TRP
3	AS	211	LEU
3	AS	228	ARG
3	AS	233	ASN
3	AS	286	ILE
4	AT	106	ILE
4	AT	116	ASP
4	AT	125	ILE
4	AU	106	ILE
4	AU	116	ASP
4	AU	125	ILE
4	AV	106	ILE
4	AV	116	ASP
4	AV	125	ILE
1	AW	112	PHE
1	AW	124	ASP
1	AW	193	MET
3	AY	45	ARG
3	AY	46	VAL
3	AY	63	ARG
3	AY	85	ARG
3	AY	149	THR

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Mol	Chain	Res	Type
3	AY	155	ASN
3	AY	162	LEU
3	AY	169	TRP
3	AY	211	LEU
3	AY	228	ARG
3	AY	233	ASN
3	AY	286	ILE
4	AZ	106	ILE
4	AZ	116	ASP
4	AZ	125	ILE
4	Aa	106	ILE
4	Aa	116	ASP
4	Aa	125	ILE
4	Ab	106	ILE
4	Ab	116	ASP
4	Ab	125	ILE
1	Ac	112	PHE
1	Ac	124	ASP
1	Ac	193	MET
3	Ae	45	ARG
3	Ae	46	VAL
3	Ae	63	ARG
3	Ae	85	ARG
3	Ae	149	THR
3	Ae	155	ASN
3	Ae	162	LEU
3	Ae	169	TRP
3	Ae	211	LEU
3	Ae	228	ARG
3	Ae	233	ASN
3	Ae	286	ILE
4	Af	106	ILE
4	Af	116	ASP
4	Af	125	ILE
4	Ag	106	ILE
4	Ag	116	ASP
4	Ag	125	ILE
4	Ah	106	ILE
4	Ah	116	ASP
4	Ah	125	ILE
1	Ai	112	PHE
1	Ai	124	ASP

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Mol	Chain	Res	Type
1	Ai	193	MET
3	Ak	45	ARG
3	Ak	46	VAL
3	Ak	63	ARG
3	Ak	85	ARG
3	Ak	149	THR
3	Ak	155	ASN
3	Ak	162	LEU
3	Ak	169	TRP
3	Ak	211	LEU
3	Ak	228	ARG
3	Ak	233	ASN
3	Ak	286	ILE
4	Al	106	ILE
4	Al	116	ASP
4	Al	125	ILE
4	Am	106	ILE
4	Am	116	ASP
4	Am	125	ILE
4	An	106	ILE
4	An	116	ASP
4	An	125	ILE
1	Ao	112	PHE
1	Ao	124	ASP
1	Ao	193	MET
3	Aq	45	ARG
3	Aq	46	VAL
3	Aq	63	ARG
3	Aq	85	ARG
3	Aq	149	THR
3	Aq	155	ASN
3	Aq	162	LEU
3	Aq	169	TRP
3	Aq	211	LEU
3	Aq	228	ARG
3	Aq	233	ASN
3	Aq	286	ILE
4	Ar	106	ILE
4	Ar	116	ASP
4	Ar	125	ILE
4	As	106	ILE
4	As	116	ASP

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Mol	Chain	Res	Type
4	As	125	ILE
4	At	106	ILE
4	At	116	ASP
4	At	125	ILE
1	Au	112	PHE
1	Au	124	ASP
1	Au	193	MET
3	Aw	45	ARG
3	Aw	46	VAL
3	Aw	63	ARG
3	Aw	85	ARG
3	Aw	149	THR
3	Aw	155	ASN
3	Aw	162	LEU
3	Aw	169	TRP
3	Aw	211	LEU
3	Aw	228	ARG
3	Aw	233	ASN
3	Aw	286	ILE
4	Ax	106	ILE
4	Ax	116	ASP
4	Ax	125	ILE
4	Ay	106	ILE
4	Ay	116	ASP
4	Ay	125	ILE
4	Az	106	ILE
4	Az	116	ASP
4	Az	125	ILE
1	A1	112	PHE
1	A1	124	ASP
1	A1	193	MET
3	A3	45	ARG
3	A3	46	VAL
3	A3	63	ARG
3	A3	85	ARG
3	A3	149	THR
3	A3	155	ASN
3	A3	162	LEU
3	A3	169	TRP
3	A3	211	LEU
3	A3	228	ARG
3	A3	233	ASN

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Mol	Chain	Res	Type
3	A3	286	ILE
4	A4	106	ILE
4	A4	116	ASP
4	A4	125	ILE
4	A5	106	ILE
4	A5	116	ASP
4	A5	125	ILE
4	A6	106	ILE
4	A6	116	ASP
4	A6	125	ILE
1	A7	112	PHE
1	A7	124	ASP
1	A7	193	MET
3	A9	45	ARG
3	A9	46	VAL
3	A9	63	ARG
3	A9	85	ARG
3	A9	149	THR
3	A9	155	ASN
3	A9	162	LEU
3	A9	169	TRP
3	A9	211	LEU
3	A9	228	ARG
3	A9	233	ASN
3	A9	286	ILE
4	A0	106	ILE
4	A0	116	ASP
4	A0	125	ILE
4	BA	106	ILE
4	BA	116	ASP
4	BA	125	ILE
4	BB	106	ILE
4	BB	116	ASP
4	BB	125	ILE
1	BC	112	PHE
1	BC	124	ASP
1	BC	193	MET
3	BE	45	ARG
3	BE	46	VAL
3	BE	63	ARG
3	BE	85	ARG
3	BE	149	THR

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Mol	Chain	Res	Type
3	BE	155	ASN
3	BE	162	LEU
3	BE	169	TRP
3	BE	211	LEU
3	BE	228	ARG
3	BE	233	ASN
3	BE	286	ILE
4	BF	106	ILE
4	BF	116	ASP
4	BF	125	ILE
4	BG	106	ILE
4	BG	116	ASP
4	BG	125	ILE
4	BH	106	ILE
4	BH	116	ASP
4	BH	125	ILE
1	BI	112	PHE
1	BI	124	ASP
1	BI	193	MET
3	BK	45	ARG
3	BK	46	VAL
3	BK	63	ARG
3	BK	85	ARG
3	BK	149	THR
3	BK	155	ASN
3	BK	162	LEU
3	BK	169	TRP
3	BK	211	LEU
3	BK	228	ARG
3	BK	233	ASN
3	BK	286	ILE
4	BL	106	ILE
4	BL	116	ASP
4	BL	125	ILE
4	BM	106	ILE
4	BM	116	ASP
4	BM	125	ILE
4	BN	106	ILE
4	BN	116	ASP
4	BN	125	ILE
1	BO	112	PHE
1	BO	124	ASP

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Mol	Chain	Res	Type
1	BO	193	MET
3	BQ	45	ARG
3	BQ	46	VAL
3	BQ	63	ARG
3	BQ	85	ARG
3	BQ	149	THR
3	BQ	155	ASN
3	BQ	162	LEU
3	BQ	169	TRP
3	BQ	211	LEU
3	BQ	228	ARG
3	BQ	233	ASN
3	BQ	286	ILE
4	BR	106	ILE
4	BR	116	ASP
4	BR	125	ILE
4	BS	106	ILE
4	BS	116	ASP
4	BS	125	ILE
4	BT	106	ILE
4	BT	116	ASP
4	BT	125	ILE
1	BU	112	PHE
1	BU	124	ASP
1	BU	193	MET
3	BW	45	ARG
3	BW	46	VAL
3	BW	63	ARG
3	BW	85	ARG
3	BW	149	THR
3	BW	155	ASN
3	BW	162	LEU
3	BW	169	TRP
3	BW	211	LEU
3	BW	228	ARG
3	BW	233	ASN
3	BW	286	ILE
4	BX	106	ILE
4	BX	116	ASP
4	BX	125	ILE
4	BY	106	ILE
4	BY	116	ASP

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Mol	Chain	Res	Type
4	BY	125	ILE
4	BZ	106	ILE
4	BZ	116	ASP
4	BZ	125	ILE
1	Ba	112	PHE
1	Ba	124	ASP
1	Ba	193	MET
3	Bc	45	ARG
3	Bc	46	VAL
3	Bc	63	ARG
3	Bc	85	ARG
3	Bc	149	THR
3	Bc	155	ASN
3	Bc	162	LEU
3	Bc	169	TRP
3	Bc	211	LEU
3	Bc	228	ARG
3	Bc	233	ASN
3	Bc	286	ILE
4	Bd	106	ILE
4	Bd	116	ASP
4	Bd	125	ILE
4	Be	106	ILE
4	Be	116	ASP
4	Be	125	ILE
4	Bf	106	ILE
4	Bf	116	ASP
4	Bf	125	ILE
1	Bg	112	PHE
1	Bg	124	ASP
1	Bg	193	MET
3	Bi	45	ARG
3	Bi	46	VAL
3	Bi	63	ARG
3	Bi	85	ARG
3	Bi	149	THR
3	Bi	155	ASN
3	Bi	162	LEU
3	Bi	169	TRP
3	Bi	211	LEU
3	Bi	228	ARG
3	Bi	233	ASN

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Mol	Chain	Res	Type
3	Bi	286	ILE
4	Bj	106	ILE
4	Bj	116	ASP
4	Bj	125	ILE
4	Bk	106	ILE
4	Bk	116	ASP
4	Bk	125	ILE
4	Bl	106	ILE
4	Bl	116	ASP
4	Bl	125	ILE
1	Bm	112	PHE
1	Bm	124	ASP
1	Bm	193	MET
3	Bo	45	ARG
3	Bo	46	VAL
3	Bo	63	ARG
3	Bo	85	ARG
3	Bo	149	THR
3	Bo	155	ASN
3	Bo	162	LEU
3	Bo	169	TRP
3	Bo	211	LEU
3	Bo	228	ARG
3	Bo	233	ASN
3	Bo	286	ILE
4	Bp	106	ILE
4	Bp	116	ASP
4	Bp	125	ILE
4	Bq	106	ILE
4	Bq	116	ASP
4	Bq	125	ILE
4	Br	106	ILE
4	Br	116	ASP
4	Br	125	ILE
1	Bs	112	PHE
1	Bs	124	ASP
1	Bs	193	MET
3	Bu	45	ARG
3	Bu	46	VAL
3	Bu	63	ARG
3	Bu	85	ARG
3	Bu	149	THR

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Mol	Chain	Res	Type
3	Bu	155	ASN
3	Bu	162	LEU
3	Bu	169	TRP
3	Bu	211	LEU
3	Bu	228	ARG
3	Bu	233	ASN
3	Bu	286	ILE
4	Bv	106	ILE
4	Bv	116	ASP
4	Bv	125	ILE
4	Bw	106	ILE
4	Bw	116	ASP
4	Bw	125	ILE
4	Bx	106	ILE
4	Bx	116	ASP
4	Bx	125	ILE
1	By	112	PHE
1	By	124	ASP
1	By	193	MET
3	B1	45	ARG
3	B1	46	VAL
3	B1	63	ARG
3	B1	85	ARG
3	B1	149	THR
3	B1	155	ASN
3	B1	162	LEU
3	B1	169	TRP
3	B1	211	LEU
3	B1	228	ARG
3	B1	233	ASN
3	B1	286	ILE
4	B2	106	ILE
4	B2	116	ASP
4	B2	125	ILE
4	B3	106	ILE
4	B3	116	ASP
4	B3	125	ILE
4	B4	106	ILE
4	B4	116	ASP
4	B4	125	ILE
1	B5	112	PHE
1	B5	124	ASP

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Mol	Chain	Res	Type
1	B5	193	MET
3	B7	45	ARG
3	B7	46	VAL
3	B7	63	ARG
3	B7	85	ARG
3	B7	149	THR
3	B7	155	ASN
3	B7	162	LEU
3	B7	169	TRP
3	B7	211	LEU
3	B7	228	ARG
3	B7	233	ASN
3	B7	286	ILE
4	B8	106	ILE
4	B8	116	ASP
4	B8	125	ILE
4	B9	106	ILE
4	B9	116	ASP
4	B9	125	ILE
4	B0	106	ILE
4	B0	116	ASP
4	B0	125	ILE
1	CA	112	PHE
1	CA	124	ASP
1	CA	193	MET
3	CC	45	ARG
3	CC	46	VAL
3	CC	63	ARG
3	CC	85	ARG
3	CC	149	THR
3	CC	155	ASN
3	CC	162	LEU
3	CC	169	TRP
3	CC	211	LEU
3	CC	228	ARG
3	CC	233	ASN
3	CC	286	ILE
4	CD	106	ILE
4	CD	116	ASP
4	CD	125	ILE
4	CE	106	ILE
4	CE	116	ASP

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Mol	Chain	Res	Type
4	CE	125	ILE
4	CF	106	ILE
4	CF	116	ASP
4	CF	125	ILE
1	CG	112	PHE
1	CG	124	ASP
1	CG	193	MET
3	CI	45	ARG
3	CI	46	VAL
3	CI	63	ARG
3	CI	85	ARG
3	CI	149	THR
3	CI	155	ASN
3	CI	162	LEU
3	CI	169	TRP
3	CI	211	LEU
3	CI	228	ARG
3	CI	233	ASN
3	CI	286	ILE
4	CJ	106	ILE
4	CJ	116	ASP
4	CJ	125	ILE
4	CK	106	ILE
4	CK	116	ASP
4	CK	125	ILE
4	CL	106	ILE
4	CL	116	ASP
4	CL	125	ILE
1	CM	112	PHE
1	CM	124	ASP
1	CM	193	MET
3	CO	45	ARG
3	CO	46	VAL
3	CO	63	ARG
3	CO	85	ARG
3	CO	149	THR
3	CO	155	ASN
3	CO	162	LEU
3	CO	169	TRP
3	CO	211	LEU
3	CO	228	ARG
3	CO	233	ASN

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Mol	Chain	Res	Type
3	CO	286	ILE
4	CP	106	ILE
4	CP	116	ASP
4	CP	125	ILE
4	CQ	106	ILE
4	CQ	116	ASP
4	CQ	125	ILE
4	CR	106	ILE
4	CR	116	ASP
4	CR	125	ILE
1	CS	112	PHE
1	CS	124	ASP
1	CS	193	MET
3	CU	45	ARG
3	CU	46	VAL
3	CU	63	ARG
3	CU	85	ARG
3	CU	149	THR
3	CU	155	ASN
3	CU	162	LEU
3	CU	169	TRP
3	CU	211	LEU
3	CU	228	ARG
3	CU	233	ASN
3	CU	286	ILE
4	CV	106	ILE
4	CV	116	ASP
4	CV	125	ILE
4	CW	106	ILE
4	CW	116	ASP
4	CW	125	ILE
4	CX	106	ILE
4	CX	116	ASP
4	CX	125	ILE
1	CY	112	PHE
1	CY	124	ASP
1	CY	193	MET
3	Ca	45	ARG
3	Ca	46	VAL
3	Ca	63	ARG
3	Ca	85	ARG
3	Ca	149	THR

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Mol	Chain	Res	Type
3	Ca	155	ASN
3	Ca	162	LEU
3	Ca	169	TRP
3	Ca	211	LEU
3	Ca	228	ARG
3	Ca	233	ASN
3	Ca	286	ILE
4	Cb	106	ILE
4	Cb	116	ASP
4	Cb	125	ILE
4	Cc	106	ILE
4	Cc	116	ASP
4	Cc	125	ILE
4	Cd	106	ILE
4	Cd	116	ASP
4	Cd	125	ILE
1	Ce	112	PHE
1	Ce	124	ASP
1	Ce	193	MET
3	Cg	45	ARG
3	Cg	46	VAL
3	Cg	63	ARG
3	Cg	85	ARG
3	Cg	149	THR
3	Cg	155	ASN
3	Cg	162	LEU
3	Cg	169	TRP
3	Cg	211	LEU
3	Cg	228	ARG
3	Cg	233	ASN
3	Cg	286	ILE
4	Ch	106	ILE
4	Ch	116	ASP
4	Ch	125	ILE
4	Ci	106	ILE
4	Ci	116	ASP
4	Ci	125	ILE
4	Cj	106	ILE
4	Cj	116	ASP
4	Cj	125	ILE
1	Ck	112	PHE
1	Ck	124	ASP

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Mol	Chain	Res	Type
1	Ck	193	MET
3	Cm	45	ARG
3	Cm	46	VAL
3	Cm	63	ARG
3	Cm	85	ARG
3	Cm	149	THR
3	Cm	155	ASN
3	Cm	162	LEU
3	Cm	169	TRP
3	Cm	211	LEU
3	Cm	228	ARG
3	Cm	233	ASN
3	Cm	286	ILE
4	Cn	106	ILE
4	Cn	116	ASP
4	Cn	125	ILE
4	Co	106	ILE
4	Co	116	ASP
4	Co	125	ILE
4	Cp	106	ILE
4	Cp	116	ASP
4	Cp	125	ILE
1	Cq	112	PHE
1	Cq	124	ASP
1	Cq	193	MET
3	Cs	45	ARG
3	Cs	46	VAL
3	Cs	63	ARG
3	Cs	85	ARG
3	Cs	149	THR
3	Cs	155	ASN
3	Cs	162	LEU
3	Cs	169	TRP
3	Cs	211	LEU
3	Cs	228	ARG
3	Cs	233	ASN
3	Cs	286	ILE
4	Ct	106	ILE
4	Ct	116	ASP
4	Ct	125	ILE
4	Cu	106	ILE
4	Cu	116	ASP

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Mol	Chain	Res	Type
4	Cu	125	ILE
4	Cv	106	ILE
4	Cv	116	ASP
4	Cv	125	ILE
1	Cw	112	PHE
1	Cw	124	ASP
1	Cw	193	MET
3	Cy	45	ARG
3	Cy	46	VAL
3	Cy	63	ARG
3	Cy	85	ARG
3	Cy	149	THR
3	Cy	155	ASN
3	Cy	162	LEU
3	Cy	169	TRP
3	Cy	211	LEU
3	Cy	228	ARG
3	Cy	233	ASN
3	Cy	286	ILE
4	Cz	106	ILE
4	Cz	116	ASP
4	Cz	125	ILE
4	C1	106	ILE
4	C1	116	ASP
4	C1	125	ILE
4	C2	106	ILE
4	C2	116	ASP
4	C2	125	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (320) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	35	GLN
1	k	46	GLN
1	k	49	ASN
1	k	180	ASN
1	k	186	GLN
3	m	148	HIS
3	m	245	ASN
4	o	102	ASN
4	p	83	GLN
1	q	35	GLN

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Mol	Chain	Res	Type
1	q	46	GLN
1	q	49	ASN
1	q	180	ASN
1	q	186	GLN
3	s	148	HIS
3	s	245	ASN
4	u	102	ASN
4	v	83	GLN
1	w	35	GLN
1	w	46	GLN
1	w	49	ASN
1	w	180	ASN
1	w	186	GLN
3	y	87	GLN
3	y	148	HIS
3	y	245	ASN
4	1	102	ASN
4	2	83	GLN
1	3	35	GLN
1	3	46	GLN
1	3	49	ASN
1	3	180	ASN
1	3	186	GLN
3	5	87	GLN
3	5	148	HIS
3	5	245	ASN
4	7	102	ASN
4	8	83	GLN
1	9	35	GLN
1	9	46	GLN
1	9	49	ASN
1	9	180	ASN
1	9	186	GLN
3	AA	148	HIS
3	AA	245	ASN
4	AC	102	ASN
4	AD	83	GLN
1	AE	35	GLN
1	AE	46	GLN
1	AE	49	ASN
1	AE	180	ASN
1	AE	186	GLN

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Mol	Chain	Res	Type
3	AG	87	GLN
3	AG	148	HIS
3	AG	245	ASN
4	AI	102	ASN
4	AJ	83	GLN
1	AK	35	GLN
1	AK	46	GLN
1	AK	49	ASN
1	AK	180	ASN
1	AK	186	GLN
3	AM	87	GLN
3	AM	148	HIS
3	AM	245	ASN
4	AO	102	ASN
4	AP	83	GLN
1	AQ	35	GLN
1	AQ	46	GLN
1	AQ	49	ASN
1	AQ	180	ASN
1	AQ	186	GLN
3	AS	87	GLN
3	AS	148	HIS
3	AS	245	ASN
4	AU	102	ASN
4	AV	83	GLN
1	AW	35	GLN
1	AW	46	GLN
1	AW	49	ASN
1	AW	180	ASN
1	AW	186	GLN
3	AY	87	GLN
3	AY	148	HIS
3	AY	245	ASN
4	Aa	102	ASN
4	Ab	83	GLN
1	Ac	35	GLN
1	Ac	46	GLN
1	Ac	49	ASN
1	Ac	180	ASN
1	Ac	186	GLN
3	Ae	87	GLN
3	Ae	148	HIS

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Mol	Chain	Res	Type
3	Ae	245	ASN
4	Ag	102	ASN
4	Ah	83	GLN
1	Ai	35	GLN
1	Ai	46	GLN
1	Ai	49	ASN
1	Ai	180	ASN
1	Ai	186	GLN
3	Ak	87	GLN
3	Ak	148	HIS
3	Ak	245	ASN
4	Am	102	ASN
4	An	83	GLN
1	Ao	35	GLN
1	Ao	46	GLN
1	Ao	49	ASN
1	Ao	180	ASN
1	Ao	186	GLN
3	Aq	148	HIS
3	Aq	245	ASN
4	As	102	ASN
4	At	83	GLN
1	Au	35	GLN
1	Au	46	GLN
1	Au	49	ASN
1	Au	180	ASN
1	Au	186	GLN
3	Aw	148	HIS
3	Aw	245	ASN
4	Ay	102	ASN
4	Az	83	GLN
1	A1	35	GLN
1	A1	46	GLN
1	A1	49	ASN
1	A1	180	ASN
1	A1	186	GLN
3	A3	87	GLN
3	A3	148	HIS
3	A3	190	ASN
3	A3	245	ASN
4	A5	102	ASN
4	A6	83	GLN

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Mol	Chain	Res	Type
1	A7	35	GLN
1	A7	46	GLN
1	A7	49	ASN
1	A7	180	ASN
1	A7	186	GLN
3	A9	148	HIS
3	A9	245	ASN
4	BA	102	ASN
4	BB	83	GLN
1	BC	35	GLN
1	BC	46	GLN
1	BC	49	ASN
1	BC	180	ASN
1	BC	186	GLN
3	BE	87	GLN
3	BE	148	HIS
3	BE	245	ASN
4	BG	102	ASN
4	BH	83	GLN
1	BI	35	GLN
1	BI	46	GLN
1	BI	49	ASN
1	BI	180	ASN
1	BI	186	GLN
3	BK	148	HIS
3	BK	245	ASN
4	BM	102	ASN
4	BN	83	GLN
1	BO	35	GLN
1	BO	46	GLN
1	BO	49	ASN
1	BO	180	ASN
1	BO	186	GLN
3	BQ	148	HIS
3	BQ	190	ASN
3	BQ	245	ASN
4	BS	102	ASN
4	BT	83	GLN
1	BU	35	GLN
1	BU	46	GLN
1	BU	49	ASN
1	BU	180	ASN

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Mol	Chain	Res	Type
1	BU	186	GLN
3	BW	148	HIS
3	BW	245	ASN
4	BY	102	ASN
4	BZ	83	GLN
1	Ba	35	GLN
1	Ba	46	GLN
1	Ba	49	ASN
1	Ba	180	ASN
1	Ba	186	GLN
3	Bc	148	HIS
3	Bc	245	ASN
4	Be	102	ASN
4	Bf	83	GLN
1	Bg	35	GLN
1	Bg	46	GLN
1	Bg	49	ASN
1	Bg	180	ASN
1	Bg	186	GLN
3	Bi	87	GLN
3	Bi	148	HIS
3	Bi	190	ASN
3	Bi	245	ASN
4	Bk	102	ASN
4	Bl	83	GLN
1	Bm	35	GLN
1	Bm	46	GLN
1	Bm	49	ASN
1	Bm	180	ASN
1	Bm	186	GLN
3	Bo	148	HIS
3	Bo	245	ASN
4	Bq	102	ASN
4	Br	83	GLN
1	Bs	35	GLN
1	Bs	46	GLN
1	Bs	49	ASN
1	Bs	180	ASN
1	Bs	186	GLN
3	Bu	148	HIS
3	Bu	245	ASN
4	Bw	102	ASN

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Mol	Chain	Res	Type
4	Bx	83	GLN
1	By	35	GLN
1	By	46	GLN
1	By	49	ASN
1	By	180	ASN
1	By	186	GLN
3	B1	148	HIS
3	B1	245	ASN
4	B3	102	ASN
4	B4	83	GLN
1	B5	35	GLN
1	B5	46	GLN
1	B5	49	ASN
1	B5	180	ASN
1	B5	186	GLN
3	B7	148	HIS
3	B7	245	ASN
4	B9	102	ASN
4	B0	83	GLN
1	CA	35	GLN
1	CA	46	GLN
1	CA	49	ASN
1	CA	180	ASN
1	CA	186	GLN
3	CC	148	HIS
3	CC	245	ASN
4	CE	102	ASN
4	CF	83	GLN
1	CG	35	GLN
1	CG	46	GLN
1	CG	49	ASN
1	CG	180	ASN
1	CG	186	GLN
3	CI	148	HIS
3	CI	245	ASN
4	CK	102	ASN
4	CL	83	GLN
1	CM	35	GLN
1	CM	46	GLN
1	CM	49	ASN
1	CM	180	ASN
1	CM	186	GLN

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Mol	Chain	Res	Type
3	CO	148	HIS
3	CO	245	ASN
4	CQ	102	ASN
4	CR	83	GLN
1	CS	35	GLN
1	CS	46	GLN
1	CS	49	ASN
1	CS	180	ASN
1	CS	186	GLN
3	CU	148	HIS
3	CU	245	ASN
4	CW	102	ASN
4	CX	83	GLN
1	CY	35	GLN
1	CY	46	GLN
1	CY	49	ASN
1	CY	180	ASN
1	CY	186	GLN
3	Ca	148	HIS
3	Ca	245	ASN
4	Cc	102	ASN
4	Cd	83	GLN
1	Ce	35	GLN
1	Ce	46	GLN
1	Ce	49	ASN
1	Ce	180	ASN
1	Ce	186	GLN
3	Cg	148	HIS
3	Cg	245	ASN
4	Ci	102	ASN
4	Cj	83	GLN
1	Ck	35	GLN
1	Ck	46	GLN
1	Ck	49	ASN
1	Ck	180	ASN
1	Ck	186	GLN
3	Cm	148	HIS
3	Cm	245	ASN
4	Co	102	ASN
4	Cp	83	GLN
1	Cq	35	GLN
1	Cq	46	GLN

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Mol	Chain	Res	Type
1	Cq	49	ASN
1	Cq	180	ASN
1	Cq	186	GLN
3	Cs	148	HIS
3	Cs	245	ASN
4	Cu	102	ASN
4	Cv	83	GLN
1	Cw	35	GLN
1	Cw	46	GLN
1	Cw	49	ASN
1	Cw	180	ASN
1	Cw	186	GLN
3	Cy	148	HIS
3	Cy	245	ASN
4	C1	102	ASN
4	C2	83	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

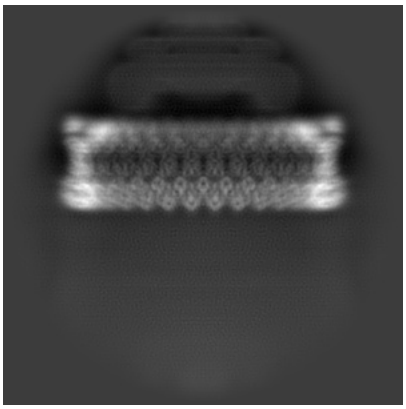
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39349. These allow visual inspection of the internal detail of the map and identification of artifacts.

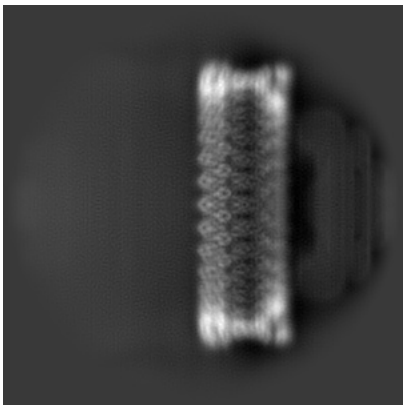
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

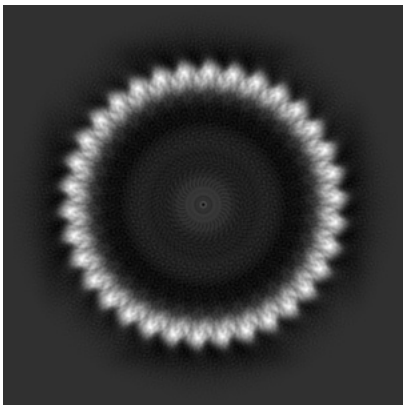
6.1.1 Primary map



X

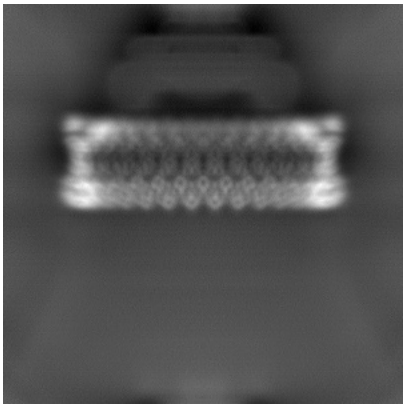


Y

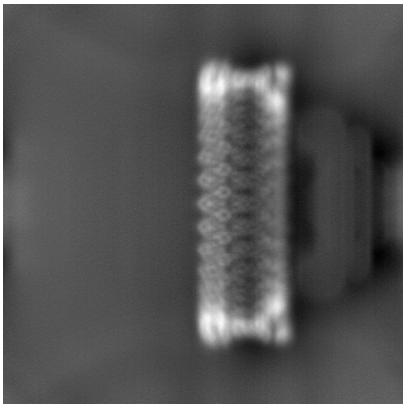


Z

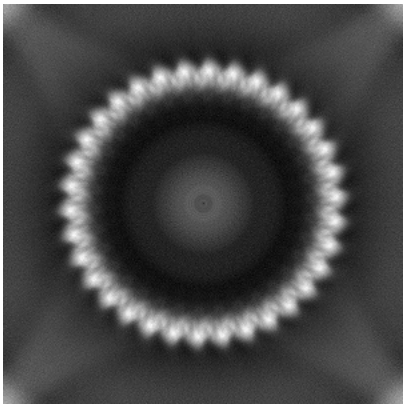
6.1.2 Raw map



X



Y

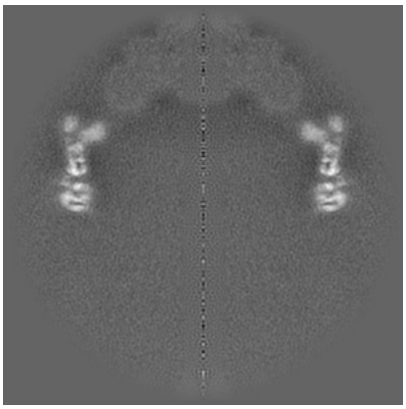


Z

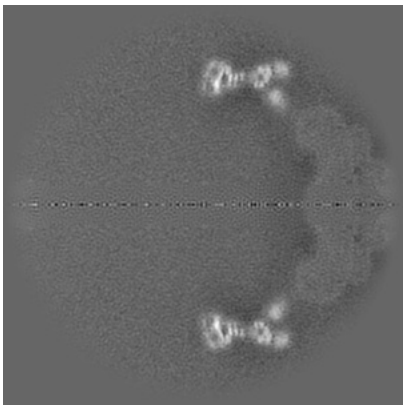
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

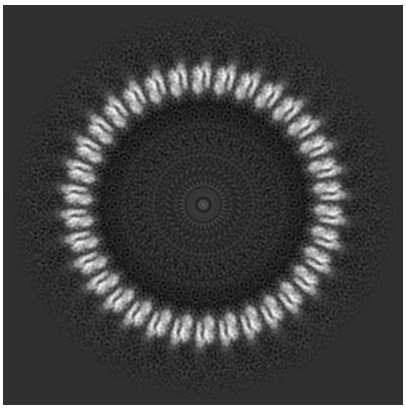
6.2.1 Primary map



X Index: 300

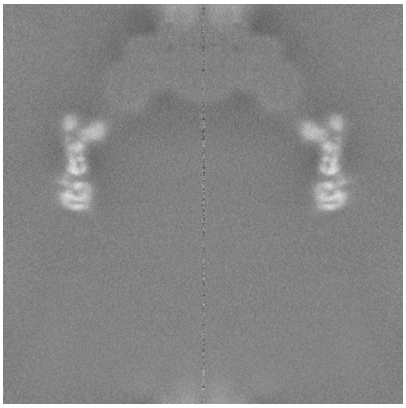


Y Index: 300

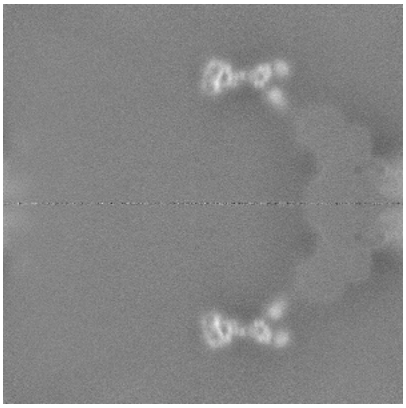


Z Index: 300

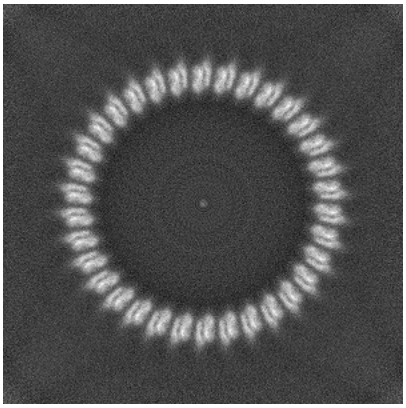
6.2.2 Raw map



X Index: 300



Y Index: 300

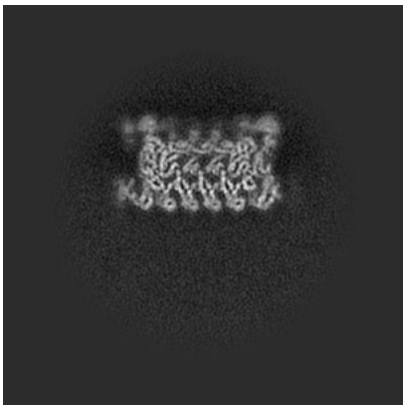


Z Index: 300

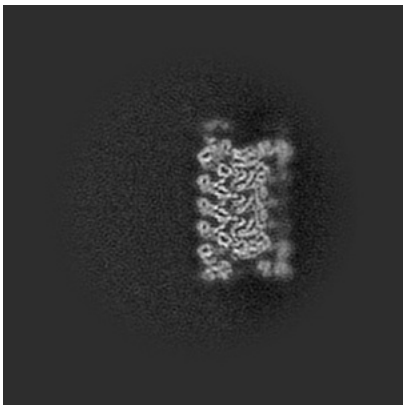
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

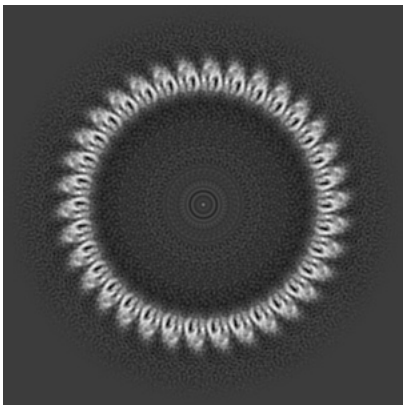
6.3.1 Primary map



X Index: 120

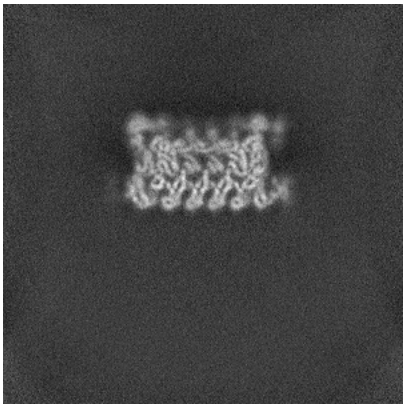


Y Index: 483

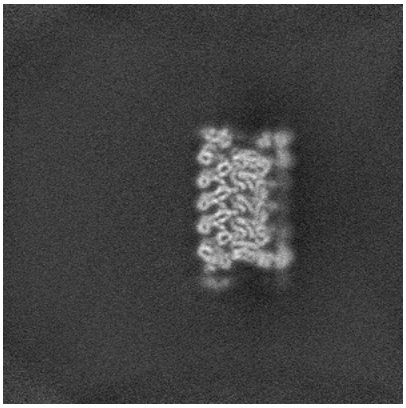


Z Index: 328

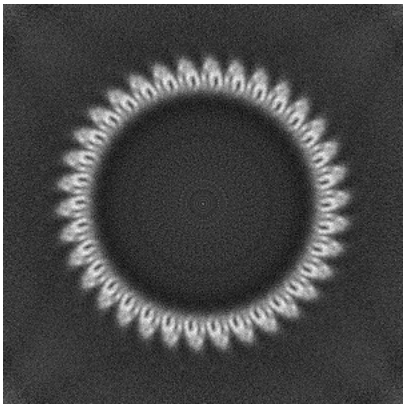
6.3.2 Raw map



X Index: 480



Y Index: 117

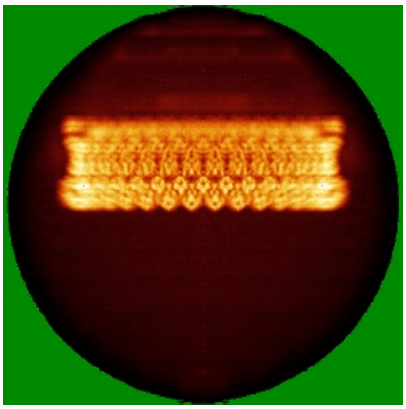


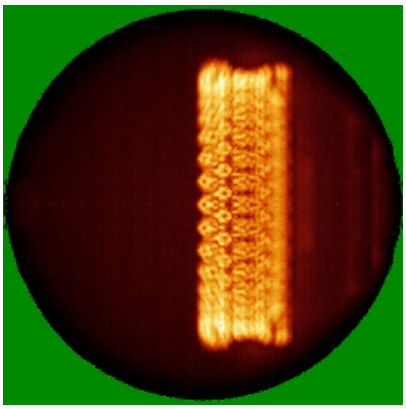
Z Index: 327

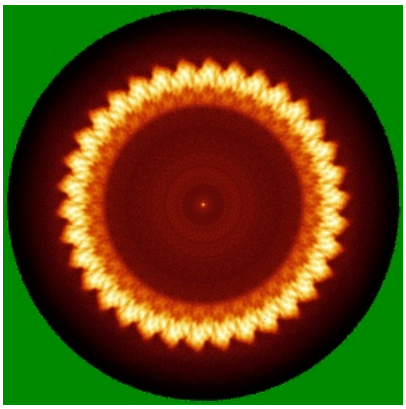
The images above show the largest variance slices of the map in three orthogonal directions.

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

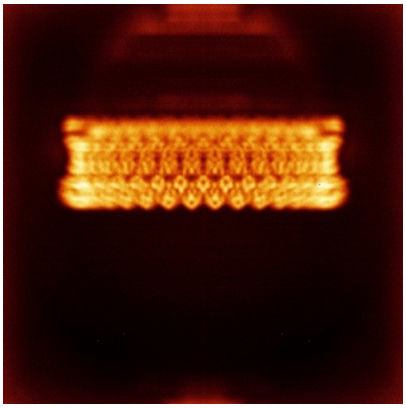
6.4.1 Primary map

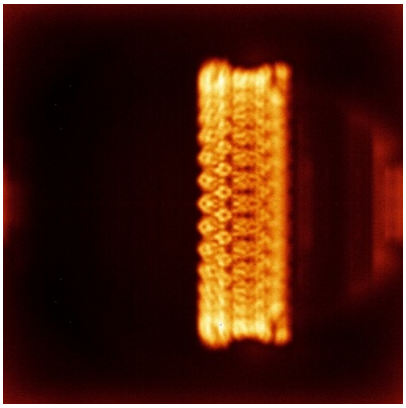

X

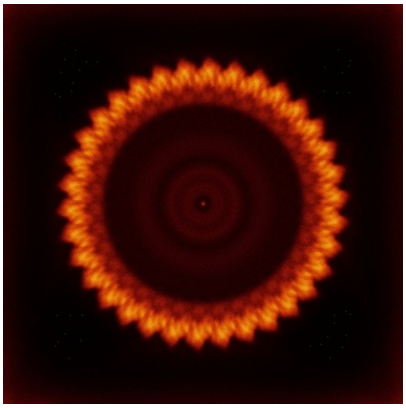

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

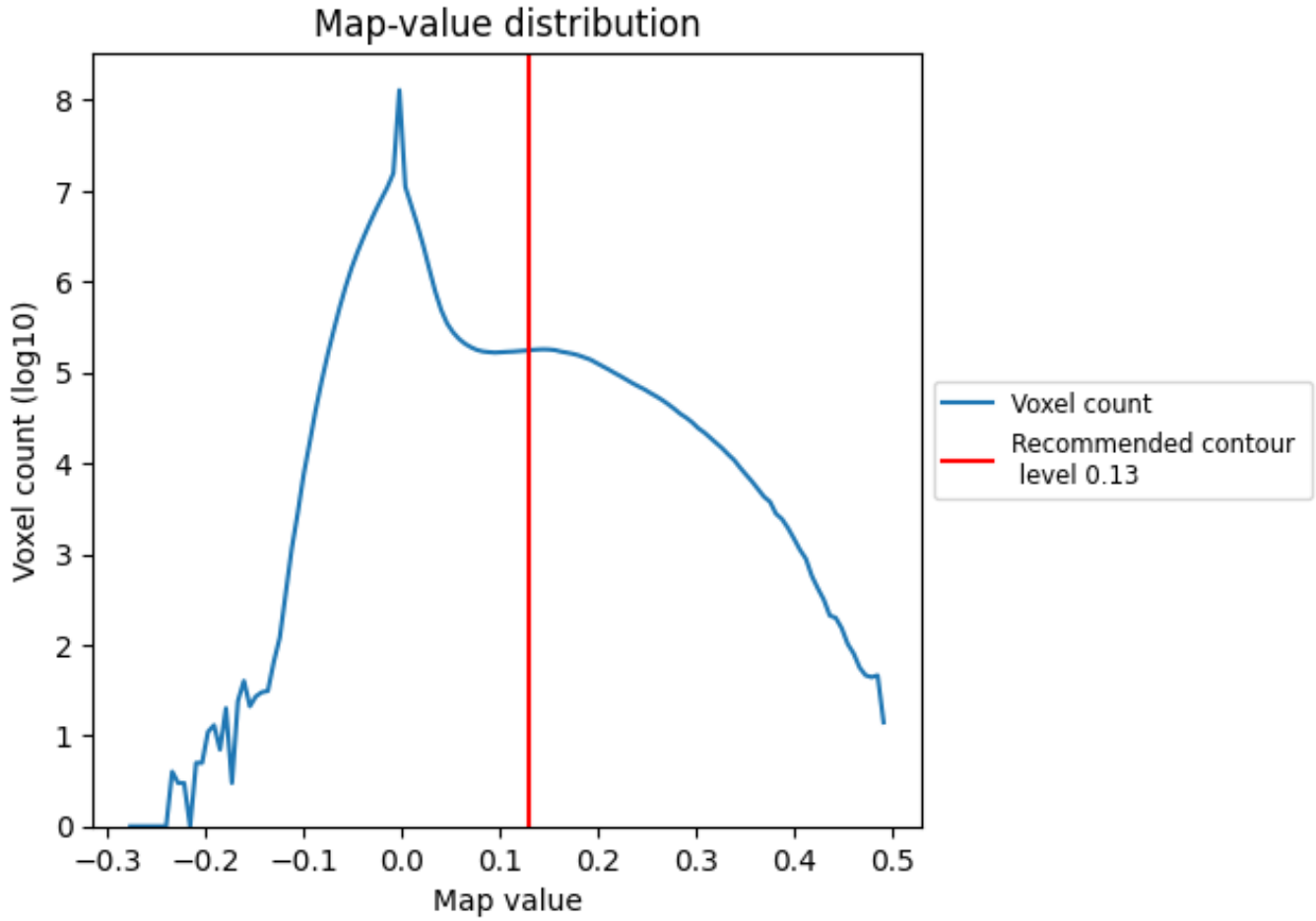
6.6 Mask visualisation (i)

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

7 Map analysis

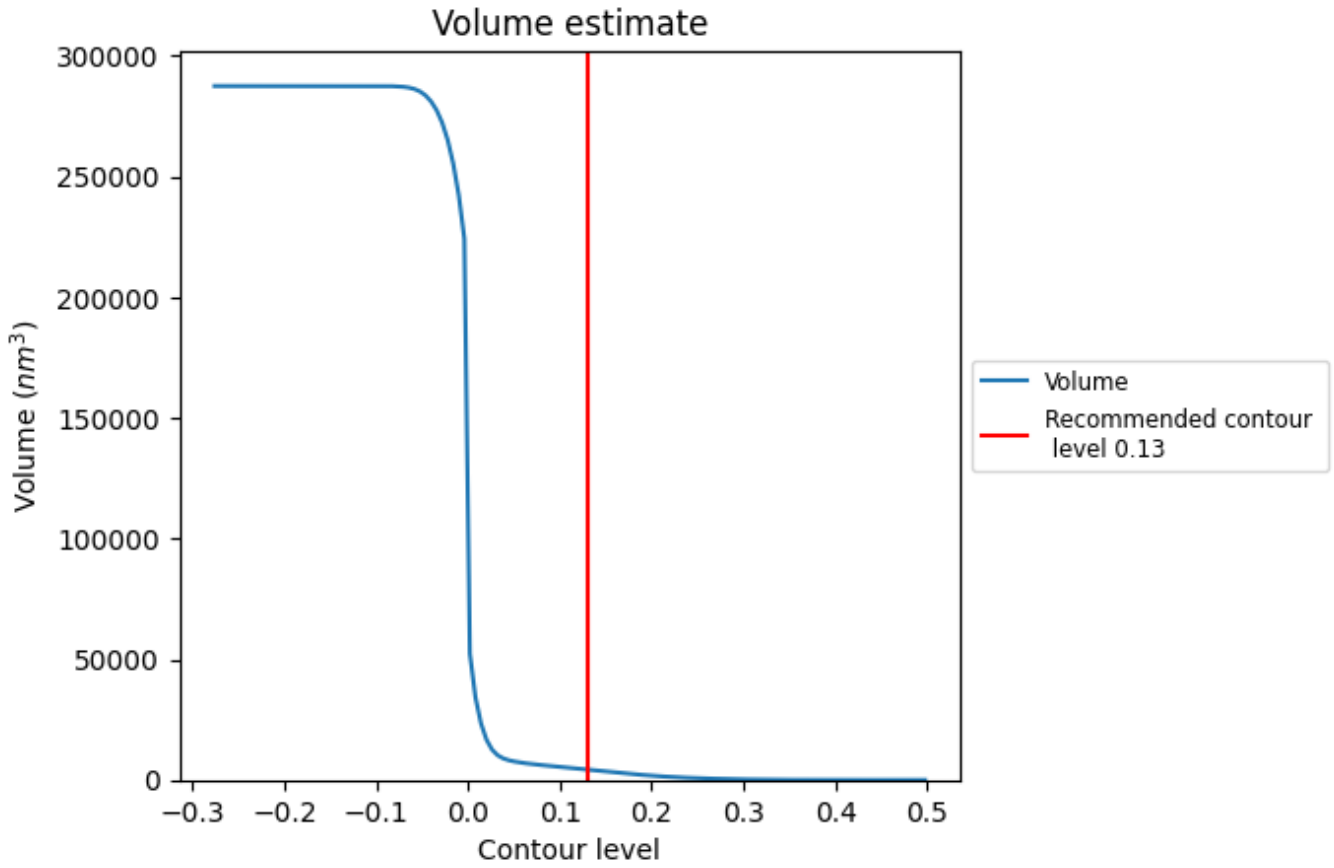
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

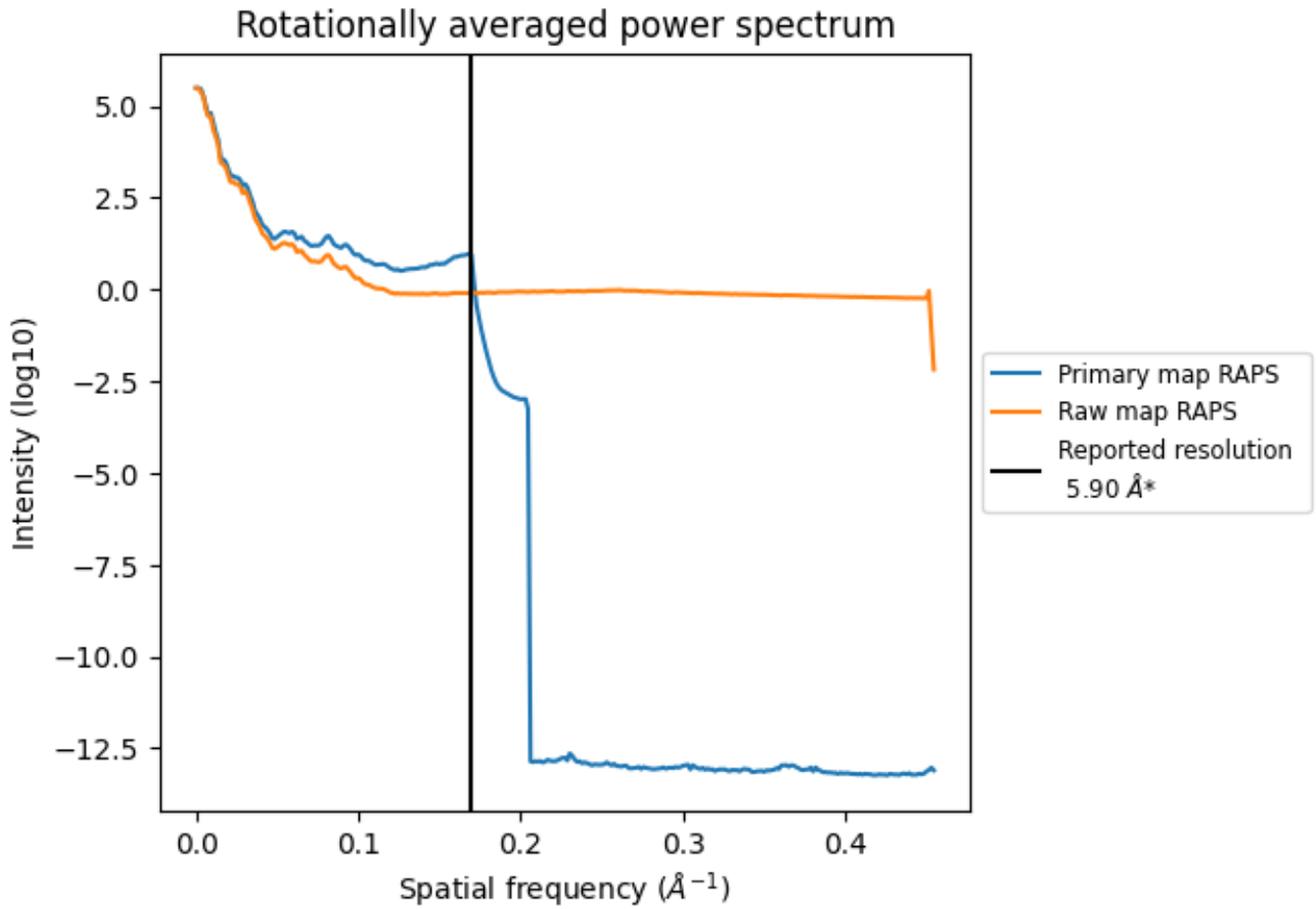
7.2 Volume estimate



The volume at the recommended contour level is 4303 nm^3; this corresponds to an approximate mass of 3887 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)

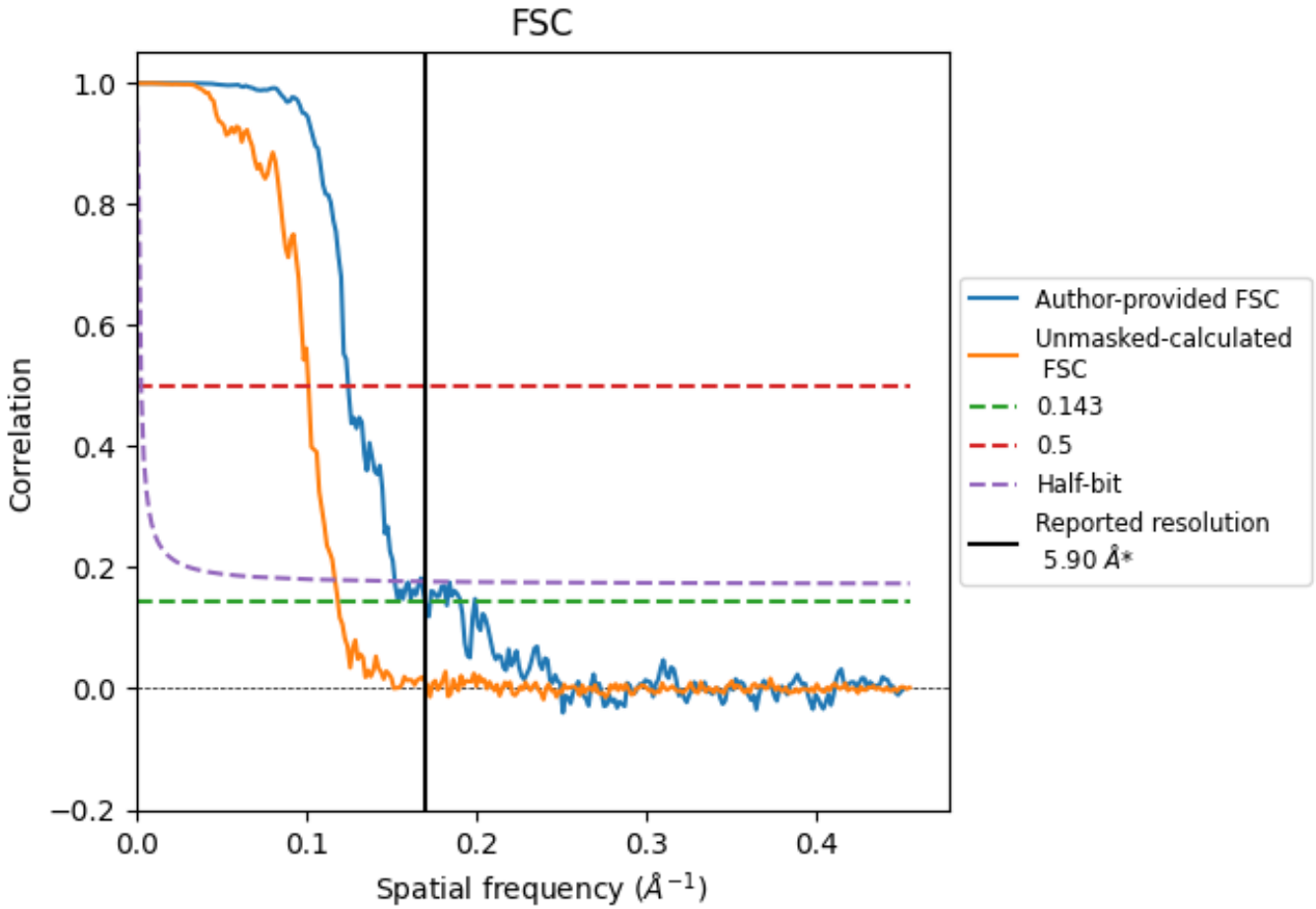


*Reported resolution corresponds to spatial frequency of 0.169 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.169 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	5.89	8.03	6.58
Unmasked-calculated*	8.43	9.87	8.56

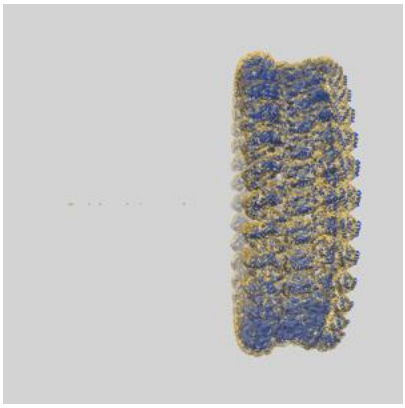
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.43 differs from the reported value 5.9 by more than 10 %

9 Map-model fit

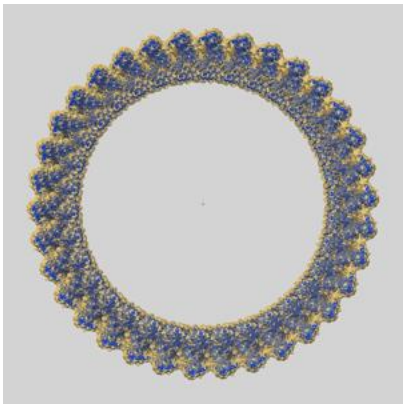
This section contains information regarding the fit between EMDB map EMD-39349 and PDB model 8YJT. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay

X



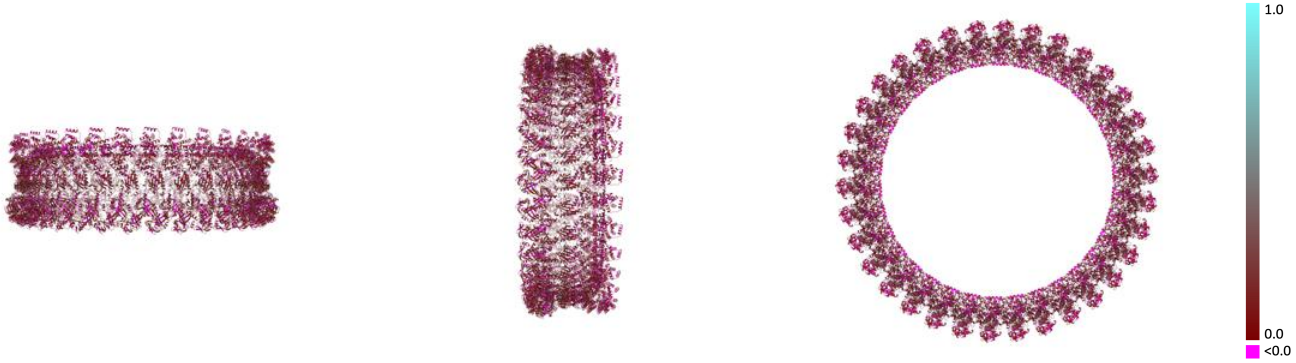
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

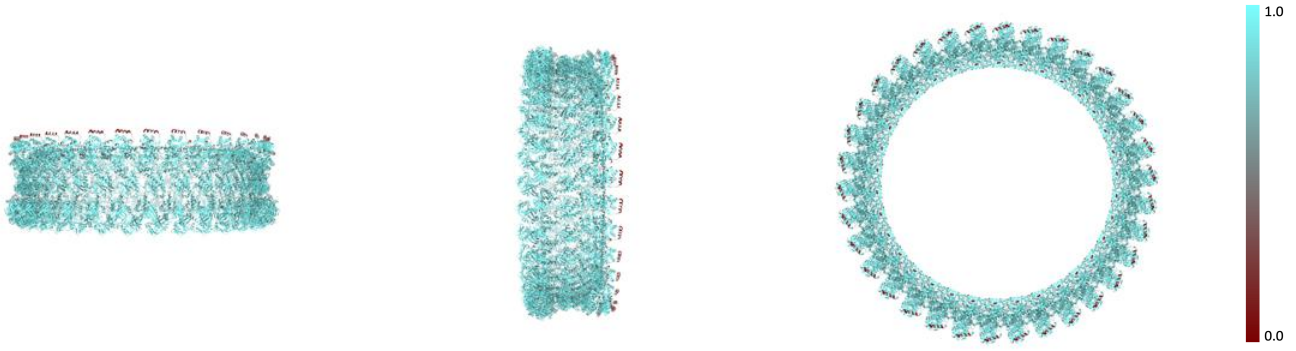
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

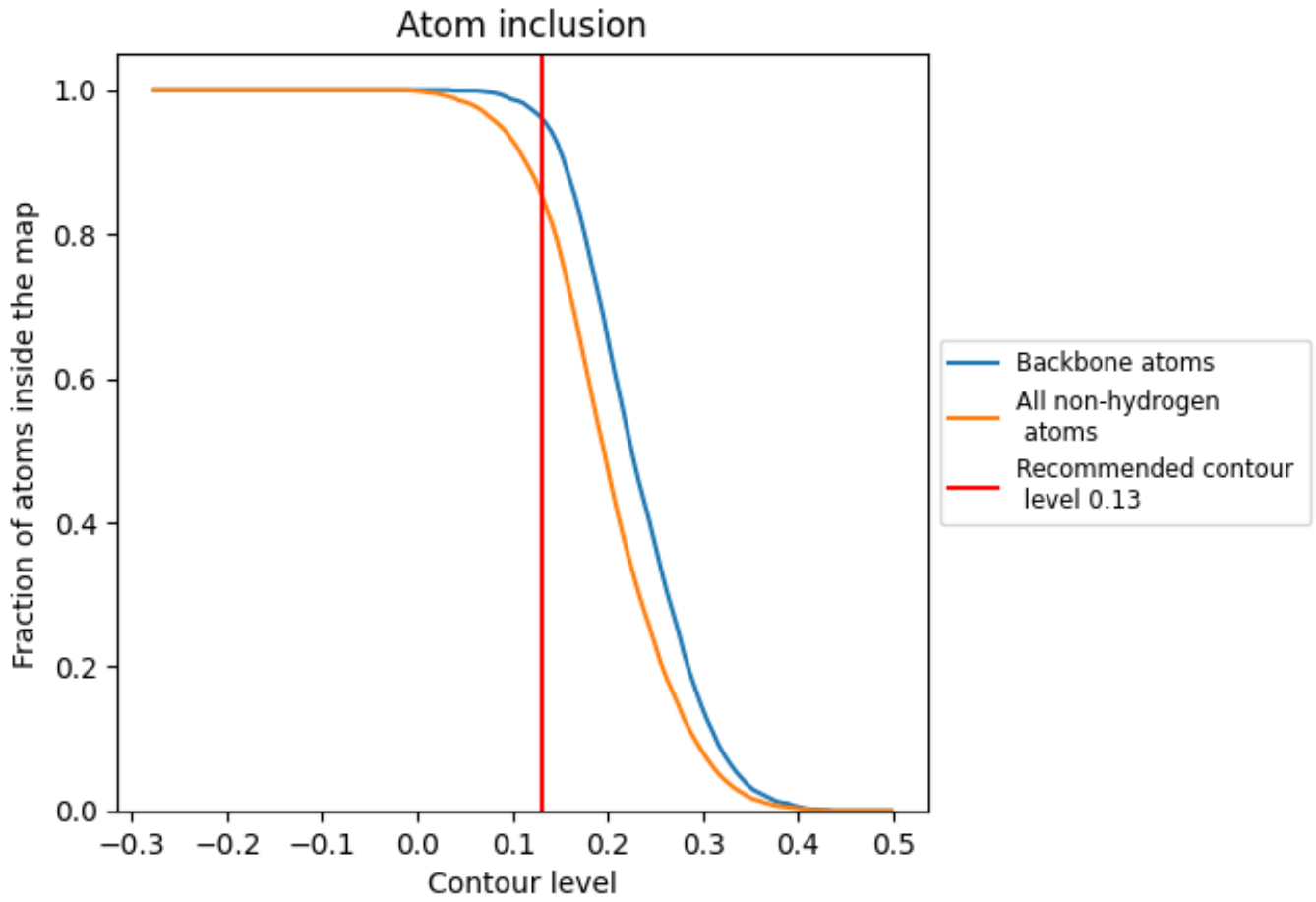
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8560	0.1470
0	0.7670	0.1200
1	0.8620	0.1690
2	0.8680	0.1500
3	0.8380	0.1240
4	0.7810	0.1120
5	0.8650	0.1660
6	0.8860	0.1530
7	0.8570	0.1660
8	0.8690	0.1530
9	0.8390	0.1260
A0	0.8840	0.1500
A1	0.8380	0.1260
A2	0.7770	0.1110
A3	0.8700	0.1660
A4	0.8830	0.1520
A5	0.8620	0.1690
A6	0.8770	0.1500
A7	0.8400	0.1240
A8	0.7810	0.1160
A9	0.8680	0.1650
AA	0.8700	0.1650
AB	0.8840	0.1530
AC	0.8650	0.1650
AD	0.8750	0.1530
AE	0.8400	0.1270
AF	0.7810	0.1160
AG	0.8690	0.1650
AH	0.8830	0.1520
AI	0.8580	0.1670
AJ	0.8780	0.1510
AK	0.8420	0.1250
AL	0.7770	0.1130
AM	0.8660	0.1650
AN	0.8800	0.1530

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Chain	Atom inclusion	Q-score
AO	0.8600	0.1660
AP	0.8770	0.1510
AQ	0.8390	0.1270
AR	0.7770	0.1160
AS	0.8660	0.1660
AT	0.8800	0.1520
AU	0.8580	0.1670
AV	0.8750	0.1500
AW	0.8360	0.1250
AX	0.7770	0.1130
AY	0.8650	0.1630
AZ	0.8830	0.1520
Aa	0.8580	0.1660
Ab	0.8830	0.1520
Ac	0.8410	0.1250
Ad	0.7720	0.1160
Ae	0.8700	0.1650
Af	0.8860	0.1510
Ag	0.8600	0.1650
Ah	0.8720	0.1530
Ai	0.8420	0.1260
Aj	0.7770	0.1200
Ak	0.8690	0.1650
Al	0.8840	0.1500
Am	0.8580	0.1660
An	0.8680	0.1520
Ao	0.8410	0.1240
Ap	0.7860	0.1150
Aq	0.8680	0.1650
Ar	0.8860	0.1520
As	0.8570	0.1660
At	0.8710	0.1510
Au	0.8390	0.1250
Av	0.7860	0.1120
Aw	0.8670	0.1660
Ax	0.8800	0.1530
Ay	0.8600	0.1690
Az	0.8750	0.1520
B0	0.8750	0.1540
B1	0.8660	0.1670
B2	0.8800	0.1540
B3	0.8600	0.1690

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Chain	Atom inclusion	Q-score
B4	0.8770	0.1560
B5	0.8390	0.1260
B6	0.7770	0.1140
B7	0.8660	0.1670
B8	0.8800	0.1520
B9	0.8580	0.1700
BA	0.8570	0.1690
BB	0.8740	0.1530
BC	0.8400	0.1230
BD	0.7670	0.1170
BE	0.8660	0.1660
BF	0.8800	0.1520
BG	0.8570	0.1700
BH	0.8750	0.1550
BI	0.8330	0.1250
BJ	0.7860	0.1160
BK	0.8660	0.1670
BL	0.8770	0.1500
BM	0.8620	0.1690
BN	0.8780	0.1560
BO	0.8400	0.1240
BP	0.7670	0.1140
BQ	0.8690	0.1660
BR	0.8870	0.1530
BS	0.8580	0.1710
BT	0.8770	0.1570
BU	0.8410	0.1230
BV	0.7770	0.1100
BW	0.8690	0.1660
BX	0.8840	0.1500
BY	0.8580	0.1690
BZ	0.8680	0.1570
Ba	0.8430	0.1240
Bb	0.7770	0.1080
Bc	0.8660	0.1650
Bd	0.8800	0.1540
Be	0.8620	0.1740
Bf	0.8680	0.1550
Bg	0.8380	0.1240
Bh	0.7810	0.1100
Bi	0.8650	0.1660
Bj	0.8860	0.1520

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Chain	Atom inclusion	Q-score
Bk	0.8570	0.1700
Bl	0.8690	0.1580
Bm	0.8390	0.1250
Bn	0.7670	0.1210
Bo	0.8700	0.1660
Bp	0.8840	0.1520
Bq	0.8650	0.1690
Br	0.8750	0.1570
Bs	0.8400	0.1260
Bt	0.7810	0.1150
Bu	0.8690	0.1660
Bv	0.8830	0.1520
Bw	0.8580	0.1700
Bx	0.8780	0.1580
By	0.8420	0.1240
Bz	0.7770	0.1130
C1	0.8620	0.1660
C2	0.8780	0.1520
CA	0.8360	0.1240
CB	0.7770	0.1130
CC	0.8650	0.1640
CD	0.8830	0.1530
CE	0.8580	0.1680
CF	0.8830	0.1560
CG	0.8410	0.1240
CH	0.7720	0.1130
CI	0.8700	0.1650
CJ	0.8860	0.1500
CK	0.8600	0.1690
CL	0.8720	0.1560
CM	0.8420	0.1250
CN	0.7770	0.1160
CO	0.8690	0.1650
CP	0.8840	0.1520
CQ	0.8580	0.1670
CR	0.8680	0.1550
CS	0.8410	0.1240
CT	0.7860	0.1110
CU	0.8680	0.1640
CV	0.8860	0.1530
CW	0.8570	0.1670
CX	0.8710	0.1540

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Chain	Atom inclusion	Q-score
CY	0.8390	0.1240
CZ	0.7860	0.1110
Ca	0.8670	0.1650
Cb	0.8800	0.1540
Cc	0.8600	0.1690
Cd	0.8750	0.1560
Ce	0.8380	0.1260
Cf	0.7770	0.1120
Cg	0.8700	0.1660
Ch	0.8830	0.1520
Ci	0.8620	0.1670
Cj	0.8770	0.1530
Ck	0.8400	0.1250
Cl	0.7810	0.1140
Cm	0.8680	0.1650
Cn	0.8840	0.1510
Co	0.8570	0.1670
Cp	0.8740	0.1560
Cq	0.8400	0.1230
Cr	0.7670	0.1190
Cs	0.8660	0.1640
Ct	0.8800	0.1500
Cu	0.8570	0.1670
Cv	0.8750	0.1540
Cw	0.8330	0.1270
Cx	0.7860	0.1120
Cy	0.8660	0.1650
Cz	0.8770	0.1510
k	0.8400	0.1260
l	0.7670	0.1130
m	0.8690	0.1640
n	0.8870	0.1510
o	0.8580	0.1670
p	0.8770	0.1530
q	0.8410	0.1240
r	0.7770	0.1100
s	0.8690	0.1660
t	0.8840	0.1480
u	0.8580	0.1660
v	0.8680	0.1530
w	0.8430	0.1260
x	0.7770	0.1100

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Chain	Atom inclusion	Q-score
y	0.8660	0.1660
z	0.8800	0.1530