



## wwPDB EM Validation Summary Report ⓘ

Aug 28, 2024 – 01:12 AM JST

PDB ID : 8WOE  
EMDB ID : EMD-37684  
Title : Cryo-EM structure of the intact flagellar motor-hook complex in the CW state  
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.  
Deposited on : 2023-10-07  
Resolution : 4.30 Å(reported)  
Based on initial models : ., ?

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev112  
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) : 2.38.2

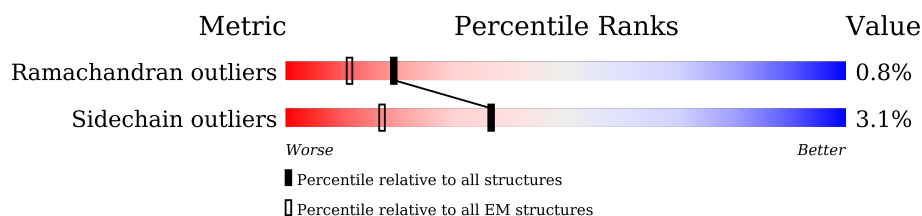
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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.



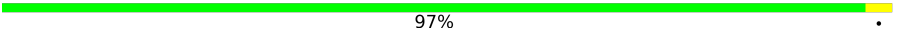
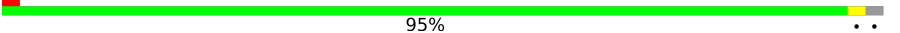

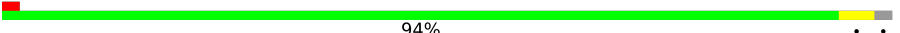

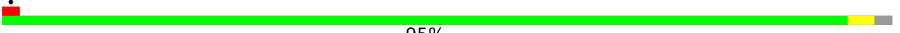









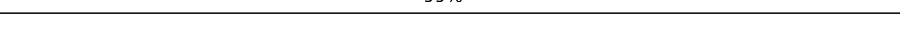









Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	0	260	
1	1	260	
1	2	260	
1	3	260	
1	4	260	
1	5	260	
1	6	260	
1	7	260	
1	8	260	



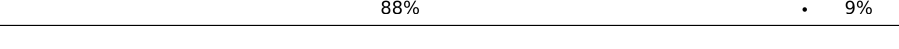
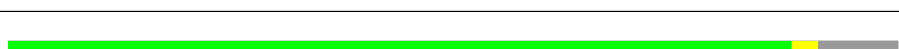



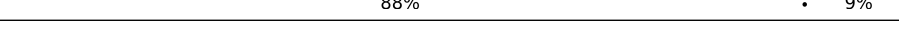



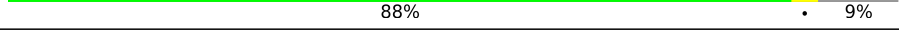

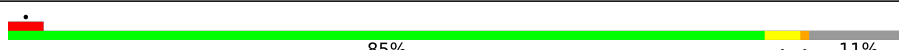
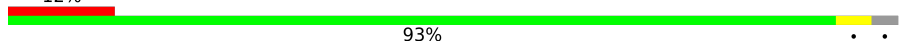

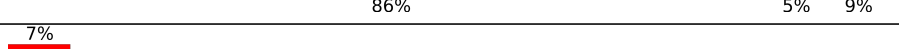







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Mol	Chain	Length	Quality of chain
1	9	260	 97%
1	AF	260	 95%
1	AG	260	 95%
1	AH	260	 94%
1	AI	260	 93% 5%
1	AJ	260	 95%
1	AK	260	 92% 7%
1	AL	260	 92% 5%
1	AM	260	 92% 5%
1	AN	260	 93% 5%
1	ZA	260	 98%
1	ZB	260	 96%
1	ZC	260	 98%
1	ZD	260	 98%
1	ZE	260	 99%
2	A	232	 88% 9%
2	B	232	 88% 9%
2	C	232	 88% 9%
2	D	232	 88% 9%
2	E	232	 88% 9%
2	F	232	 87% 9%
2	G	232	 88% 9%
2	H	232	 88% 9%
2	I	232	 88% 9%
2	J	232	 88% 9%

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Mol	Chain	Length	Quality of chain
2	K	232	
2	L	232	
2	M	232	
2	N	232	
2	O	232	
2	P	232	
2	Q	232	
2	R	232	
2	S	232	
2	T	232	
2	U	232	
2	V	232	
2	W	232	
2	X	232	
2	Y	232	
2	Z	232	
3	A0	138	
3	A6	138	
3	A7	138	
3	A8	138	
3	A9	138	
4	A1	104	
4	A2	104	
4	A3	104	
4	A4	104	






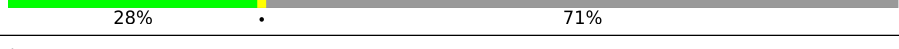

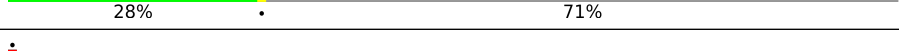
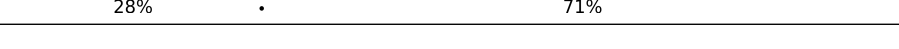
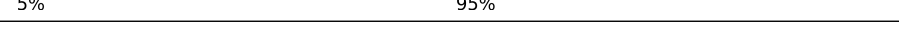
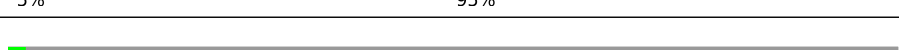
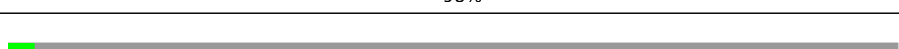

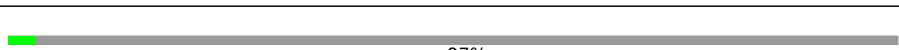
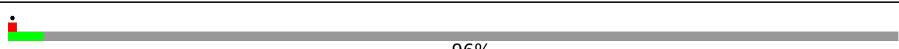


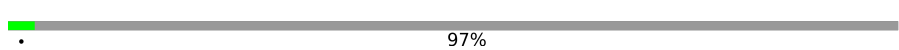
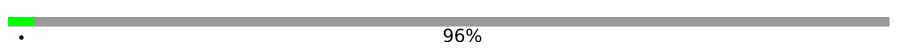
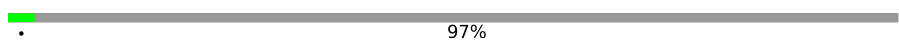
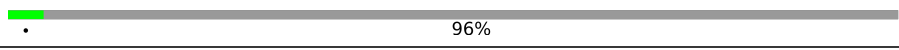




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Mol	Chain	Length	Quality of chain
4	A5	104	85% 12%
4	Az	104	52% 5% 43%
5	AA	251	13% 96%
5	AB	251	8% 98%
5	AC	251	5% 97%
5	AD	251	99%
5	AE	251	98%
6	AO	560	28% 71%
6	AP	560	28% 71%
6	AQ	560	28% 71%
6	AR	560	28% 71%
6	AS	560	28% 71%
6	AT	560	28% 71%
6	AU	560	28% 71%
6	AV	560	28% 71%
6	AW	560	28% 71%
6	AX	560	28% 71%
6	AY	560	28% 71%
6	AZ	560	28% 71%
6	Aa	560	28% 71%
6	Ac	560	28% 71%
6	Ad	560	28% 71%
6	Ae	560	28% 71%
6	Af	560	28% 71%
6	Ag	560	28% 71%





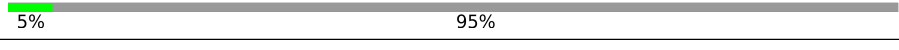
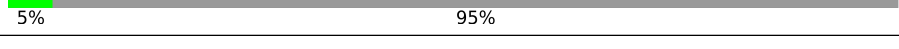
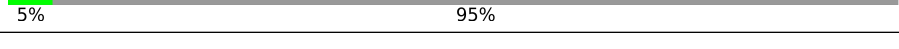
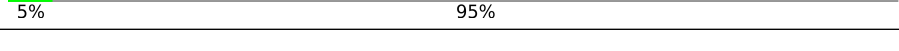
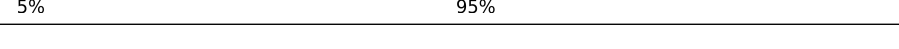
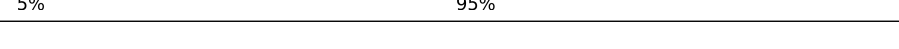
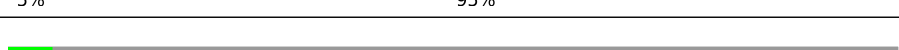
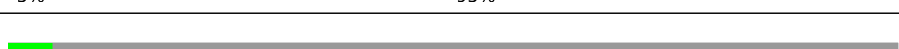

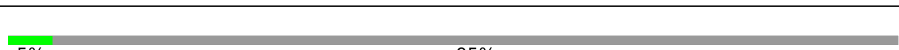
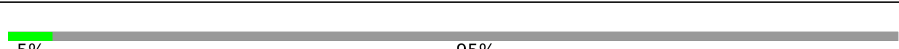


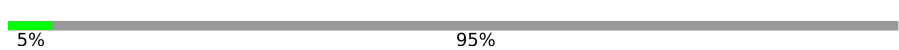
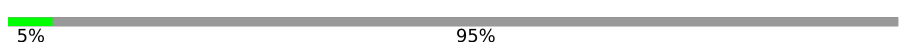
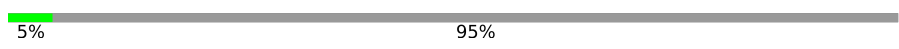
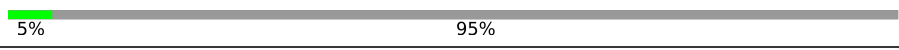
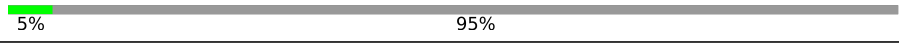
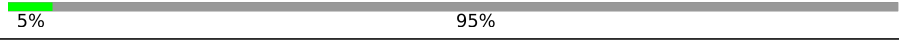
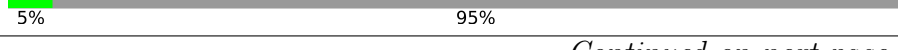

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Mol	Chain	Length	Quality of chain
6	Ah	560	 28%71%
6	Ai	560	 28%71%
6	Aj	560	 28%71%
6	Ak	560	 28%71%
6	Al	560	 28%71%
6	Am	560	 28%71%
6	An	560	 28%71%
6	Ao	560	 28%71%
6	Ap	560	 28%71%
6	B0	560	 5%95%
6	B3	560	 5%95%
6	BG	560	 98%
6	BH	560	 97%
6	BI	560	 96%
6	BJ	560	 97%
6	BK	560	 96%
6	BL	560	 97%
6	BM	560	 96%
6	BN	560	 97%
6	BO	560	 96%
6	BP	560	 97%
6	BQ	560	 96%
6	BR	560	 28%71%
6	BS	560	 28%71%
6	BT	560	 28%71%

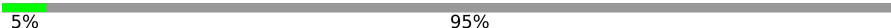
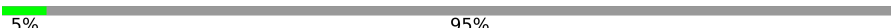
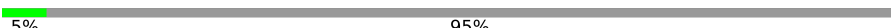










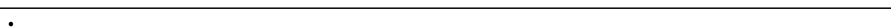











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Mol	Chain	Length	Quality of chain
6	BU	560	 28% 71%
6	BV	560	 28% 71%
6	BW	560	 28% 71%
6	BX	560	 28% 71%
6	Ba	560	 5% 95%
6	Bh	560	 5% 95%
6	Bo	560	 5% 95%
6	Bv	560	 5% 95%
6	CG	560	 5% 95%
6	CN	560	 5% 95%
6	CU	560	 5% 95%
6	Cb	560	 5% 95%
6	Ci	560	 5% 95%
6	Cp	560	 5% 95%
6	Cw	560	 5% 95%
6	DE	560	 5% 95%
6	DL	560	 5% 95%
6	EH	560	 5% 95%
6	EO	560	 5% 95%
6	EV	560	 5% 95%
6	Ea	560	 5% 95%
6	Eb	560	 5% 95%
6	Ec	560	 5% 95%
6	Ed	560	 5% 95%
6	Ee	560	 5% 95%

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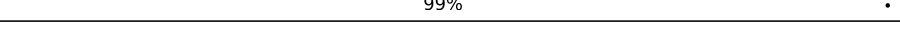
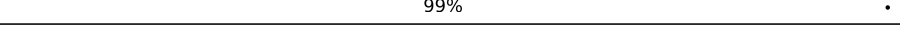
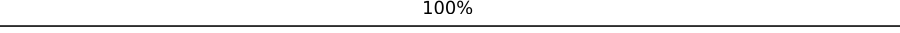
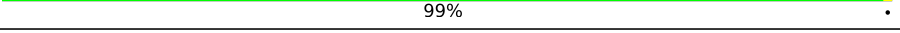



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Mol	Chain	Length	Quality of chain
6	Ef	560	 5% 95%
6	Eg	560	 5% 95%
6	Eh	560	 5% 95%
6	Ei	560	 5% 95%
6	Ej	560	 5% 95%
6	Ek	560	 5% 95%
6	El	560	 5% 95%
6	Em	560	 5% 95%
6	En	560	 5% 95%
6	Eo	560	 5% 95%
6	Ep	560	 5% 95%
6	UI	560	 25% 72%
6	UJ	560	 25% 72%
6	UK	560	 25% 72%
6	UL	560	 25% 72%
6	UM	560	 25% 72%
6	UN	560	 25% 72%
6	UO	560	 25% 72%
6	UP	560	 25% 72%
6	WA	560	 18% 80%
6	WB	560	 18% 80%
6	WC	560	 17% 81%
6	WD	560	 18% 80%
6	WE	560	 18% 80%
6	WF	560	 18% 80%

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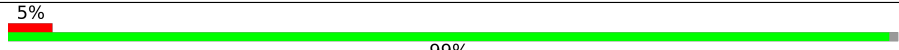
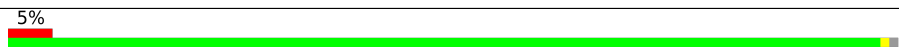
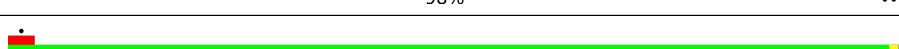
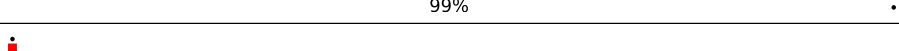
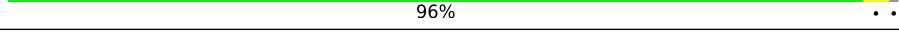
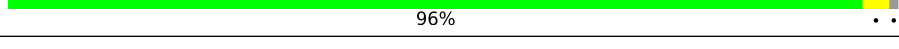
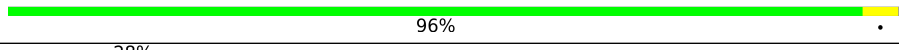
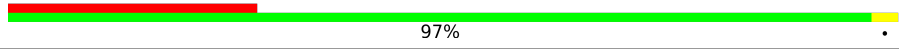
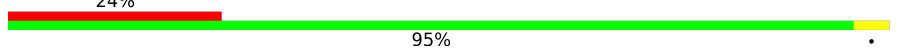
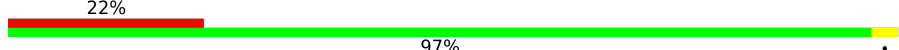
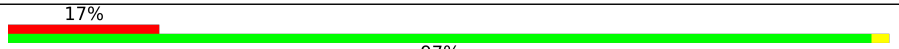

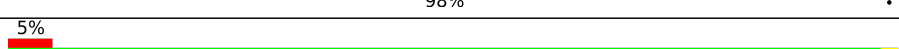
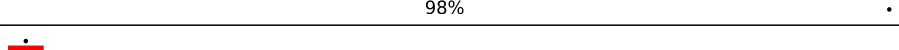
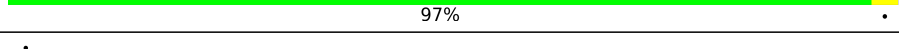
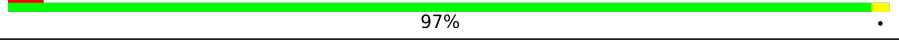
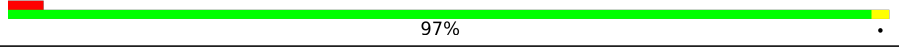
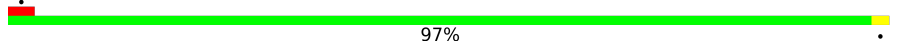
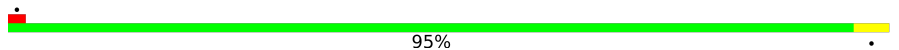
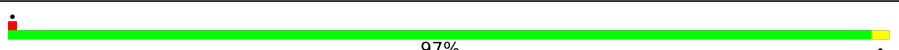

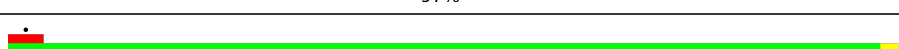
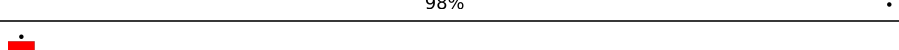


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Mol	Chain	Length	Quality of chain
6	WG	560	 18% . 80%
6	WH	560	 16% . 83%
6	WI	560	 15% . 83%
6	WJ	560	 16% . 82%
6	WK	560	 16% . 82%
6	WL	560	 14% . 85%
6	WM	560	 14% . 85%
6	WN	560	 14% . 85%
6	WO	560	 16% . 83%
6	WP	560	 16% . 82%
6	WQ	560	 18% . 80%
6	WR	560	 17% . 80%
6	WS	560	 18% . 80%
6	WT	560	 17% . 80%
6	WU	560	 19% . 80%
6	WV	560	 17% . 80%
6	WW	560	 18% .. 80%
7	Ab	89	 99% .
7	Aq	89	 99% .
7	Ar	89	 100%
7	As	89	 99% .
8	At	264	 91% . . .
9	Au	245	 81% . 16%
9	Av	245	 82% . 15%
9	Aw	245	 83% . 15%

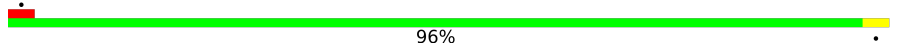
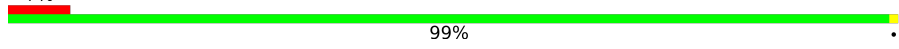
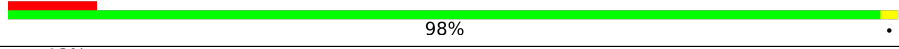
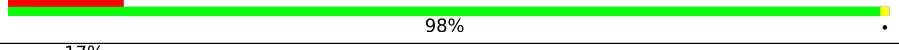
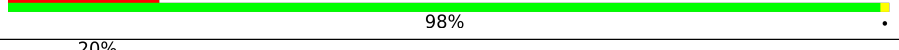
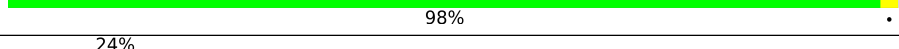
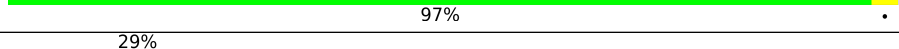
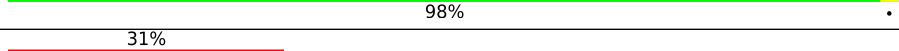
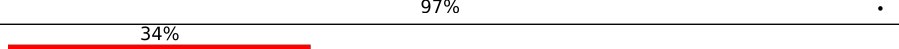
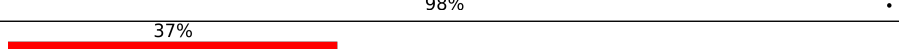
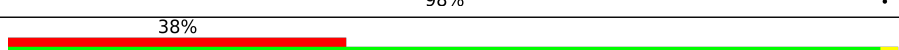
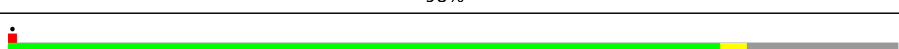
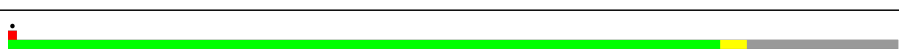

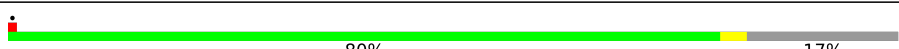





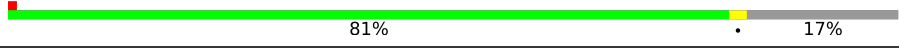
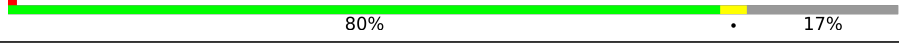



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Mol	Chain	Length	Quality of chain
9	Ax	245	
9	Ay	245	
10	BA	134	
10	BB	134	
10	BC	134	
10	BD	134	
10	BE	134	
10	BF	134	
11	ZF	403	
11	ZG	403	
11	ZH	403	
11	ZI	403	
11	ZJ	403	
11	ZK	403	
11	ZL	403	
11	ZM	403	
11	ZN	403	
11	ZO	403	
11	ZP	403	
11	ZQ	403	
11	ZR	403	
11	ZS	403	
11	ZT	403	
11	ZU	403	
11	ZV	403	







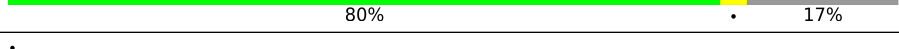
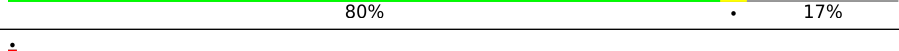
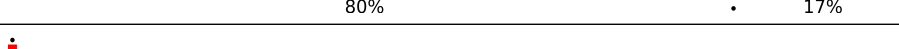
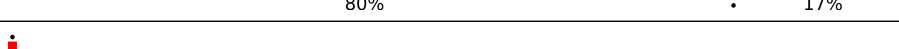
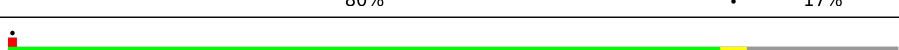

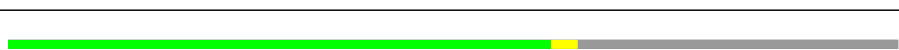

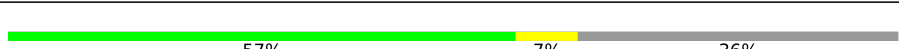





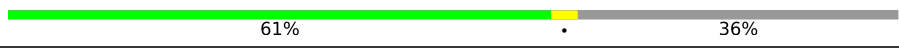
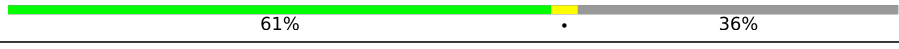



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Mol	Chain	Length	Quality of chain
11	ZW	403	
11	ZX	403	
11	ZY	403	
11	ZZ	403	
11	Za	403	
11	Zb	403	
11	Zc	403	
11	Zd	403	
11	Ze	403	
11	Zf	403	
11	Zg	403	
11	Zh	403	
12	a	365	
12	b	365	
12	c	365	
12	d	365	
12	e	365	
12	f	365	
12	g	365	
12	h	365	
12	i	365	
12	j	365	
12	k	365	
12	l	365	
12	m	365	











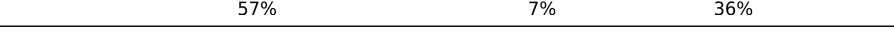
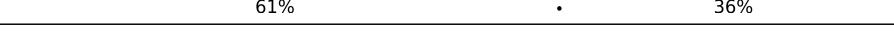
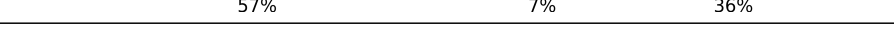


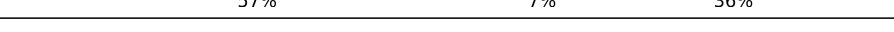









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Mol	Chain	Length	Quality of chain
12	n	365	
12	o	365	
12	p	365	
12	q	365	
12	r	365	
12	s	365	
12	t	365	
12	u	365	
12	v	365	
12	w	365	
12	x	365	
12	y	365	
12	z	365	
13	B1	137	
13	B2	137	
13	B7	137	
13	B8	137	
13	B9	137	
13	BY	137	
13	BZ	137	
13	Be	137	
13	Bf	137	
13	Bg	137	
13	Bl	137	
13	Bm	137	











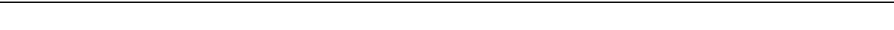

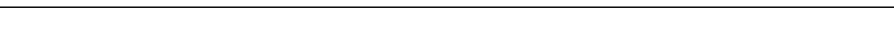
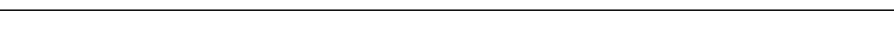











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Mol	Chain	Length	Quality of chain
13	Bn	137	
13	Bs	137	
13	Bt	137	
13	Bu	137	
13	Bz	137	
13	C1	137	
13	C2	137	
13	C3	137	
13	C4	137	
13	C5	137	
13	C8	137	
13	C9	137	
13	CD	137	
13	CE	137	
13	CF	137	
13	CK	137	
13	CL	137	
13	CM	137	
13	CR	137	
13	CS	137	
13	CT	137	
13	CY	137	
13	CZ	137	
13	Ca	137	
13	Cf	137	











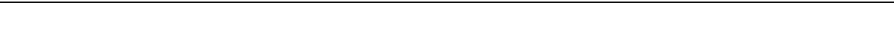

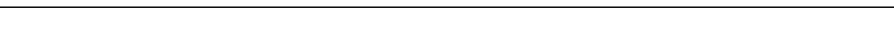
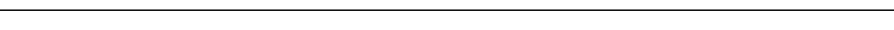











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Mol	Chain	Length	Quality of chain
13	Cg	137	
13	Ch	137	
13	Cm	137	
13	Cn	137	
13	Co	137	
13	Ct	137	
13	Cu	137	
13	Cv	137	
13	D1	137	
13	D5	137	
13	D6	137	
13	D7	137	
13	DD	137	
13	DI	137	
13	DJ	137	
13	DK	137	
13	DM	137	
13	DN	137	
13	DO	137	
13	DP	137	
13	DQ	137	
13	DR	137	
13	DS	137	
13	DT	137	
13	DU	137	












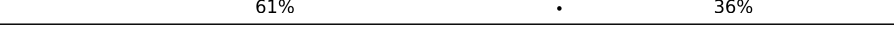







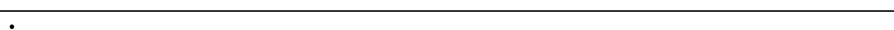

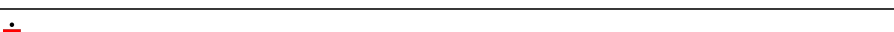
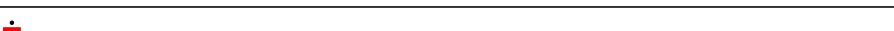


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Mol	Chain	Length	Quality of chain
13	DV	137	
13	DW	137	
13	Da	137	
13	Db	137	
13	Dc	137	
13	Dg	137	
13	Dh	137	
13	Di	137	
13	Dm	137	
13	Dn	137	
13	Do	137	
13	Ds	137	
13	Dt	137	
13	Du	137	
13	Dy	137	
13	Dz	137	
13	EA	137	
13	EB	137	
13	EE	137	
13	EF	137	
13	EG	137	
13	EL	137	
13	EM	137	
13	EN	137	
13	ES	137	

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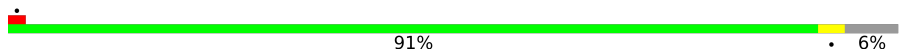
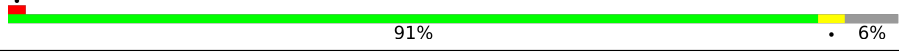
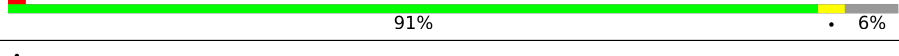
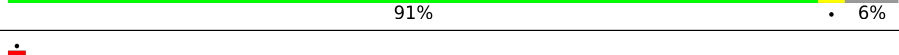
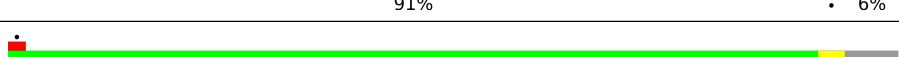
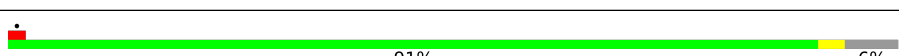
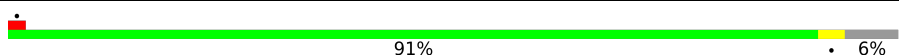
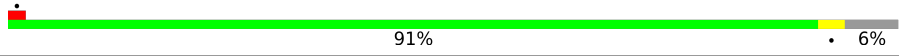
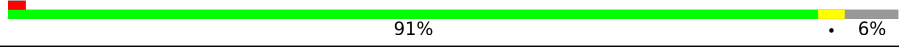
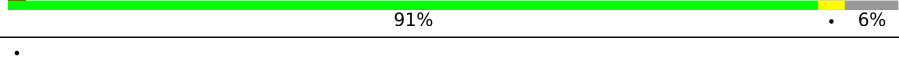
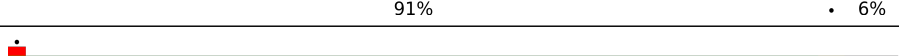
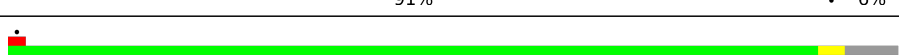
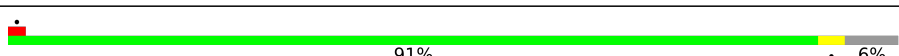
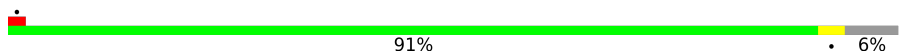
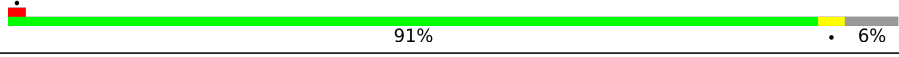
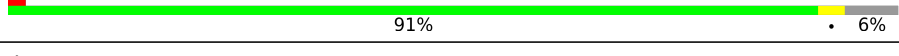
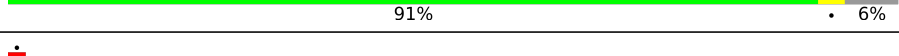
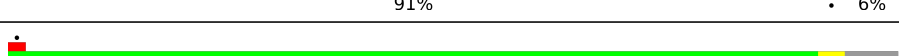
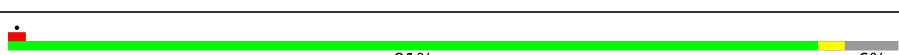
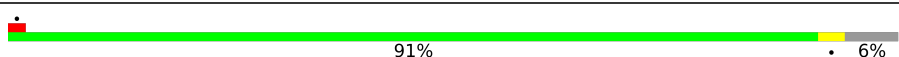
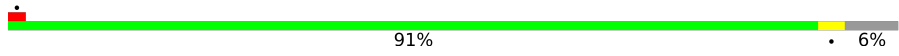
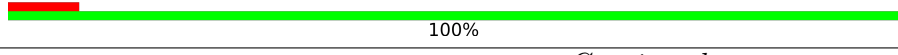


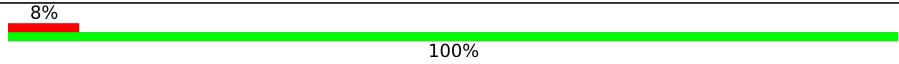
*Continued from previous page...*

Mol	Chain	Length	Quality of chain
13	ET	137	
13	EU	137	
13	EZ	137	
13	FC	137	
13	FD	137	
13	FE	137	
13	FF	137	
13	FG	137	
13	FH	137	
13	FI	137	
13	FJ	137	
13	FK	137	
13	FL	137	
13	FM	137	
13	FN	137	
14	B5	331	
14	Bc	331	
14	Bj	331	
14	Bq	331	
14	Bx	331	
14	C6	331	
14	CB	331	
14	CI	331	
14	CP	331	
14	CW	331	

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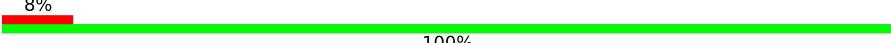
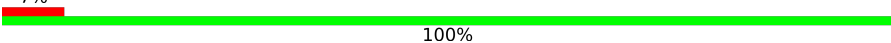
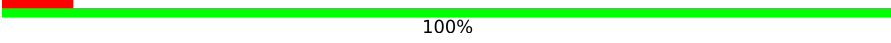
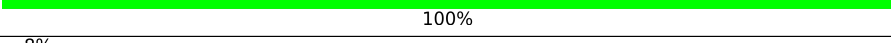
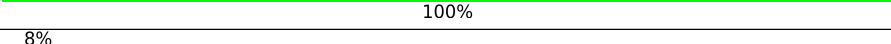
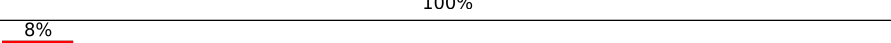
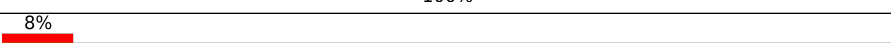

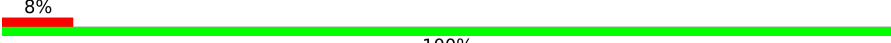
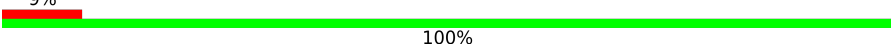
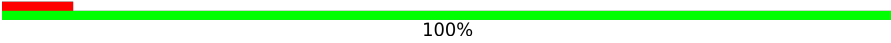
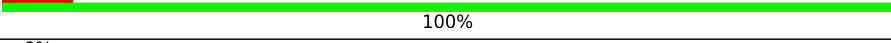
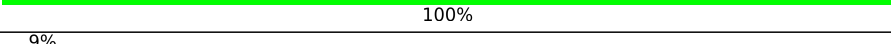
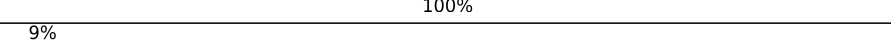
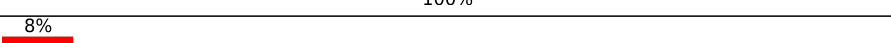


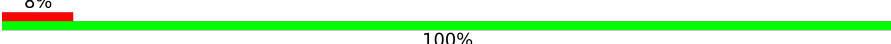
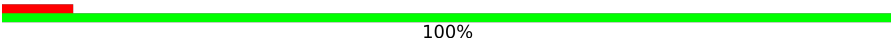
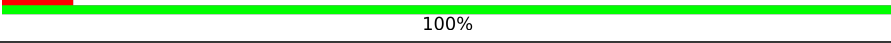
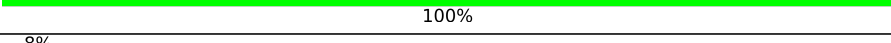
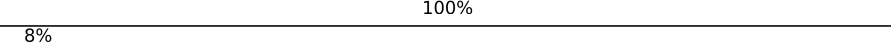
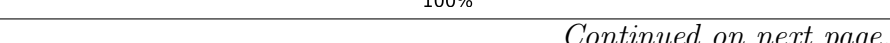




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Mol	Chain	Length	Quality of chain
14	Cd	331	
14	Ck	331	
14	Cr	331	
14	Cy	331	
14	D3	331	
14	D9	331	
14	DA	331	
14	DG	331	
14	DY	331	
14	De	331	
14	Dk	331	
14	Dq	331	
14	Dw	331	
14	E1	331	
14	E2	331	
14	E3	331	
14	E4	331	
14	EC	331	
14	EJ	331	
14	EQ	331	
14	EX	331	
14	Ex	331	
14	Ey	331	
14	Ez	331	
15	B6	129	

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Mol	Chain	Length	Quality of chain
15	Bd	129	8%  100%
15	Bk	129	7%  100%
15	Br	129	8%  100%
15	By	129	8%  100%
15	C7	129	8%  100%
15	CC	129	8%  100%
15	CJ	129	8%  100%
15	CQ	129	8%  100%
15	CX	129	9%  100%
15	Ce	129	8%  100%
15	Cl	129	9%  100%
15	Cs	129	8%  100%
15	Cz	129	8%  100%
15	D0	129	8%  100%
15	D4	129	9%  100%
15	DB	129	9%  100%
15	DH	129	8%  100%
15	DZ	129	8%  100%
15	Df	129	8%  100%
15	Dl	129	8%  100%
15	Dr	129	8%  100%
15	Dx	129	8%  100%
15	E0	129	9%  100%
15	E6	129	8%  100%
15	E7	129	8%  100%



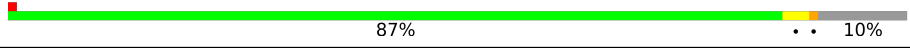



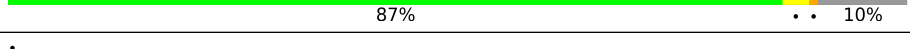
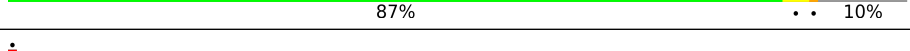
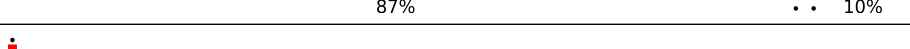
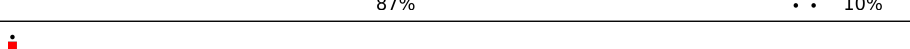
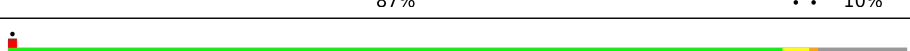



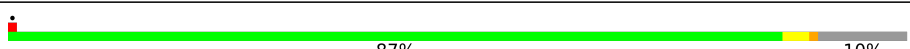


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Mol	Chain	Length	Quality of chain
15	E8	129	<div> <div>9%</div> <div>100%</div> </div>
15	E9	129	<div> <div>9%</div> <div>100%</div> </div>
15	ED	129	<div> <div>8%</div> <div>100%</div> </div>
15	EK	129	<div> <div>8%</div> <div>100%</div> </div>
15	ER	129	<div> <div>8%</div> <div>100%</div> </div>
15	EY	129	<div> <div>9%</div> <div>100%</div> </div>
15	FA	129	<div> <div>8%</div> <div>100%</div> </div>
15	FB	129	<div> <div>9%</div> <div>100%</div> </div>
16	B4	334	<div> <div>87%</div> <div>10%</div> </div>
16	Bb	334	<div> <div>87%</div> <div>10%</div> </div>
16	Bi	334	<div> <div>87%</div> <div>10%</div> </div>
16	Bp	334	<div> <div>87%</div> <div>10%</div> </div>
16	Bw	334	<div> <div>87%</div> <div>10%</div> </div>
16	C0	334	<div> <div>87%</div> <div>10%</div> </div>
16	CA	334	<div> <div>87%</div> <div>10%</div> </div>
16	CH	334	<div> <div>87%</div> <div>10%</div> </div>
16	CO	334	<div> <div>87%</div> <div>10%</div> </div>
16	CV	334	<div> <div>87%</div> <div>10%</div> </div>
16	Cc	334	<div> <div>87%</div> <div>10%</div> </div>
16	Cj	334	<div> <div>87%</div> <div>10%</div> </div>
16	Cq	334	<div> <div>87%</div> <div>10%</div> </div>
16	Cx	334	<div> <div>87%</div> <div>10%</div> </div>
16	D2	334	<div> <div>87%</div> <div>10%</div> </div>
16	D8	334	<div> <div>87%</div> <div>10%</div> </div>
16	DC	334	<div> <div>87%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
16	DF	334	
16	DX	334	
16	Dd	334	
16	Dj	334	
16	Dp	334	
16	Dv	334	
16	E5	334	
16	EI	334	
16	EP	334	
16	EW	334	
16	Eq	334	
16	Er	334	
16	Es	334	
16	Et	334	
16	Eu	334	
16	Ev	334	
16	Ew	334	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 614043 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 basal-body rod protein FlgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
1	1	252	Total	C	N	O	S	0	0
			1894	1172	331	385	6		
1	2	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	3	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	4	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	5	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	6	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	7	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	8	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	9	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	AF	254	Total	C	N	O	S	0	0
			1903	1175	334	389	5		
1	AG	255	Total	C	N	O	S	0	0
			1911	1181	335	390	5		
1	AH	256	Total	C	N	O	S	0	0
			1919	1186	336	391	6		
1	AI	254	Total	C	N	O	S	0	0
			1903	1175	334	389	5		
1	AJ	255	Total	C	N	O	S	0	0
			1911	1181	335	390	5		
1	AK	243	Total	C	N	O	S	0	0
			1823	1127	318	373	5		
1	AL	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AM	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
1	AN	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
1	ZA	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	ZB	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	ZC	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	ZD	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	ZE	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	B	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	C	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	D	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	E	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	F	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	G	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	H	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	I	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	J	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	K	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	L	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	N	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	O	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	P	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	Q	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	R	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	S	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	T	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	U	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	V	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	W	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	X	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	Y	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
2	Z	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		

- Molecule 3 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A0	123	Total	C	N	O	S	0	0
			950	588	172	185	5		
3	A6	134	Total	C	N	O	S	0	0
			1030	633	189	203	5		
3	A7	121	Total	C	N	O	S	0	0
			942	583	172	182	5		
3	A8	125	Total	C	N	O	S	0	0
			967	598	177	187	5		
3	A9	127	Total	C	N	O	S	0	0
			982	606	182	189	5		

- Molecule 4 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A1	91	Total	C	N	O	S	0	0
			672	415	121	129	7		
4	A2	93	Total	C	N	O	S	0	0
			686	424	123	132	7		
4	A3	93	Total	C	N	O	S	0	0
			686	424	123	132	7		
4	A4	93	Total	C	N	O	S	0	0
			686	424	123	132	7		
4	A5	92	Total	C	N	O	S	0	0
			679	420	122	130	7		
4	Az	59	Total	C	N	O	S	0	0
			429	265	74	83	7		

- Molecule 5 is a protein called Flagellar basal-body rod protein FlgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AA	248	Total	C	N	O	S	0	0
			1804	1106	324	367	7		
5	AB	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
5	AC	250	Total	C	N	O	S	0	0
			1820	1116	326	369	9		
5	AD	250	Total	C	N	O	S	0	0
			1820	1116	326	369	9		
5	AE	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		

- Molecule 6 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AO	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	AP	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	AQ	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	AR	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	AS	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	AT	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	AU	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	AV	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	AW	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	AX	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	AY	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	AZ	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Aa	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Ac	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Ad	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Ae	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Af	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Ag	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Ah	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Ai	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Aj	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Ak	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Al	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Am	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	An	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Ao	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	Ap	164	Total 1275	C 776	N 237	O 259	S 3	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
6	BG	13	Total 81	C 50	N 15	O 16	0	0	
6	BH	16	Total 103	C 64	N 19	O 20	0	0	
6	BI	20	Total 133	C 83	N 23	O 27	0	0	
6	BJ	16	Total 103	C 64	N 19	O 20	0	0	
6	BK	21	Total 140	C 88	N 24	O 28	0	0	
6	BL	16	Total 103	C 64	N 19	O 20	0	0	
6	BM	21	Total 140	C 88	N 24	O 28	0	0	
6	BN	16	Total 103	C 64	N 19	O 20	0	0	
6	BO	20	Total 133	C 83	N 23	O 27	0	0	
6	BP	16	Total 103	C 64	N 19	O 20	0	0	
6	BQ	21	Total 140	C 88	N 24	O 28	0	0	
6	BR	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	BS	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	BT	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	BU	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	BV	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	BW	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	BX	164	Total 1275	C 776	N 237	O 259	S 3	0	0
6	UI	155	Total 1172	C 733	N 211	O 226	S 2	0	0
6	UJ	155	Total 1172	C 733	N 211	O 226	S 2	0	0
6	UK	155	Total 1172	C 733	N 211	O 226	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	UL	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
6	UM	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
6	UN	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
6	UO	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
6	UP	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
6	WA	113	Total	C	N	O	S	0	0
			849	534	148	166	1		
6	WB	111	Total	C	N	O	S	0	0
			836	526	146	163	1		
6	WC	108	Total	C	N	O	S	0	0
			812	510	142	159	1		
6	WD	110	Total	C	N	O	S	0	0
			827	522	144	160	1		
6	WE	112	Total	C	N	O	S	0	0
			843	531	147	164	1		
6	WF	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
6	WG	112	Total	C	N	O	S	0	0
			843	531	147	164	1		
6	WH	95	Total	C	N	O	S	0	0
			703	439	126	137	1		
6	WI	95	Total	C	N	O	S	0	0
			703	439	126	137	1		
6	WJ	99	Total	C	N	O	S	0	0
			737	462	131	143	1		
6	WK	98	Total	C	N	O	S	0	0
			729	456	130	142	1		
6	WL	85	Total	C	N	O	S	0	0
			622	389	110	122	1		
6	WM	82	Total	C	N	O	S	0	0
			596	372	107	116	1		
6	WN	84	Total	C	N	O	S	0	0
			611	380	109	121	1		
6	WO	96	Total	C	N	O	S	0	0
			714	448	127	138	1		
6	WP	100	Total	C	N	O	S	0	0
			741	464	132	144	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	WQ	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
6	WR	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
6	WS	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
6	WT	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
6	WU	112	Total	C	N	O	S	0	0
			843	531	147	164	1		
6	WV	110	Total	C	N	O	S	0	0
			827	521	144	161	1		
6	WW	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
6	DE	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	DL	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	B0	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	B3	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	EH	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	EO	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	EV	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Ba	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Bh	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Bo	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Bv	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Ea	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	CG	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	CN	27	Total	C	N	O	S	0	0
			224	135	44	42	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	CU	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Cb	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Ci	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Cp	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Cw	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Eb	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Ec	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Ed	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Ee	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Ef	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Eg	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Eh	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Ei	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Ej	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Ek	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	El	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Em	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	En	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Eo	27	Total 224	C 135	N 44	O 42	S 3	0	0
6	Ep	27	Total 224	C 135	N 44	O 42	S 3	0	0

- Molecule 7 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ab	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
7	Aq	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
7	Ar	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
7	As	89	Total	C	N	O	S	0	0
			670	449	100	114	7		

- Molecule 8 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	At	253	Total	C	N	O	S	0	0
			1945	1305	307	318	15		

- Molecule 9 is a protein called Flagellar biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Au	207	Total	C	N	O	S	0	0
			1605	1072	249	272	12		
9	Av	209	Total	C	N	O	S	0	0
			1626	1086	252	276	12		
9	Aw	208	Total	C	N	O	S	0	0
			1614	1077	251	274	12		
9	Ax	208	Total	C	N	O	S	0	0
			1614	1077	251	274	12		
9	Ay	209	Total	C	N	O	S	0	0
			1623	1084	251	276	12		

- Molecule 10 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BA	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
10	BB	132	Total	C	N	O	S	0	0
			964	601	166	192	5		
10	BC	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
10	BD	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
10	BE	133	Total	C	N	O	S	0	0
			969	604	167	193	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	BF	133	Total	C	N	O	S	0	0
			969	604	167	193	5		

- Molecule 11 is a protein called Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	ZF	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZG	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZH	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZI	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZJ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZK	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZL	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZM	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZN	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZO	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZP	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZQ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZR	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZS	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZT	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZU	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZV	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZW	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	ZX	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZY	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	ZZ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	Za	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	Zb	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	Zc	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	Zd	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	Ze	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	Zf	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	Zg	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
11	Zh	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

- Molecule 12 is a protein called Flagellar P-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	b	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	c	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	d	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	e	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	f	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	g	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	h	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	j	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	k	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	l	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	m	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	n	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	o	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	p	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	q	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	r	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	s	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	t	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	u	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	v	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	w	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	x	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	y	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
12	z	303	Total 2228	C 1364	N 405	O 446	S 13	0	0

- Molecule 13 is a protein called Flagellar motor switch protein FliN.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C3	87	Total 675	C 427	N 118	O 126	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	C4	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	C5	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	C8	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	C9	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DD	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DI	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DJ	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DK	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DM	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DN	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DO	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DP	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DQ	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DR	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DS	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DT	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DU	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DV	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	DW	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Da	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Db	87	Total 675	C 427	N 118	O 126	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	Dc	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Dg	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Dh	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Di	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Dm	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Dn	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Do	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Ds	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Dt	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Du	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Dy	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Dz	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	D1	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	D5	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	D6	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	D7	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	EA	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	EB	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	B1	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	B2	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	B7	87	Total 675	C 427	N 118	O 126	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	B8	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	B9	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	EE	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	EF	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	EG	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	EL	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	EM	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	EN	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	ES	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	ET	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	EU	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	EZ	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	BY	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	BZ	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Be	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Bf	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Bg	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Bl	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Bm	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Bn	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Bs	87	Total 675	C 427	N 118	O 126	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	Bt	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Bu	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Bz	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	C1	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	C2	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CD	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CE	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CF	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CK	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CL	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CM	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CR	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CS	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CT	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CY	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	CZ	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Ca	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Cf	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Cg	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Ch	87	Total 675	C 427	N 118	O 126	S 4	0	0
13	Cm	87	Total 675	C 427	N 118	O 126	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	Cn	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Co	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Ct	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Cu	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Cv	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FC	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FD	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FE	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FF	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FG	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FH	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FI	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FJ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FK	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FL	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FM	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	FN	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

- Molecule 14 is a protein called Flagellar motor switch protein FliG.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C6	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	DA	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	DG	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	DY	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	De	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	Dk	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	Dq	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	Dw	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	D3	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	D9	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	B5	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	EC	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	EJ	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	EQ	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	EX	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	Bc	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	Bj	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	Bq	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	Bx	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	CB	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	CI	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	CP	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
14	CW	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	Cd	310	Total 2428	C 1515	N 430	O 474	S 9	0	0
14	Ck	310	Total 2428	C 1515	N 430	O 474	S 9	0	0
14	Cr	310	Total 2428	C 1515	N 430	O 474	S 9	0	0
14	Cy	310	Total 2428	C 1515	N 430	O 474	S 9	0	0
14	Ex	310	Total 2428	C 1515	N 430	O 474	S 9	0	0
14	Ey	310	Total 2428	C 1515	N 430	O 474	S 9	0	0
14	Ez	310	Total 2428	C 1515	N 430	O 474	S 9	0	0
14	E1	310	Total 2428	C 1515	N 430	O 474	S 9	0	0
14	E2	310	Total 2428	C 1515	N 430	O 474	S 9	0	0
14	E3	310	Total 2428	C 1515	N 430	O 474	S 9	0	0
14	E4	310	Total 2428	C 1515	N 430	O 474	S 9	0	0

- Molecule 15 is a protein called Chemotaxis protein CheY.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C7	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	DB	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	DH	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	DZ	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Df	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Dl	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Dr	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Dx	129	Total 991	C 634	N 165	O 185	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	D4	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	D0	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	B6	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	ED	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	EK	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	ER	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	EY	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Bd	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Bk	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Br	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	By	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	CC	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	CJ	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	CQ	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	CX	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Ce	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Cl	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Cs	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	Cz	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	E6	129	Total 991	C 634	N 165	O 185	S 7	0	0
15	E7	129	Total 991	C 634	N 165	O 185	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	E8	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
15	E9	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
15	E0	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
15	FA	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
15	FB	129	Total	C	N	O	S	0	0
			991	634	165	185	7		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C7	13	LYS	ASP	engineered mutation	UNP P0A2D5
C7	106	TRP	TYR	engineered mutation	UNP P0A2D5
DB	13	LYS	ASP	engineered mutation	UNP P0A2D5
DB	106	TRP	TYR	engineered mutation	UNP P0A2D5
DH	13	LYS	ASP	engineered mutation	UNP P0A2D5
DH	106	TRP	TYR	engineered mutation	UNP P0A2D5
DZ	13	LYS	ASP	engineered mutation	UNP P0A2D5
DZ	106	TRP	TYR	engineered mutation	UNP P0A2D5
Df	13	LYS	ASP	engineered mutation	UNP P0A2D5
Df	106	TRP	TYR	engineered mutation	UNP P0A2D5
Dl	13	LYS	ASP	engineered mutation	UNP P0A2D5
Dl	106	TRP	TYR	engineered mutation	UNP P0A2D5
Dr	13	LYS	ASP	engineered mutation	UNP P0A2D5
Dr	106	TRP	TYR	engineered mutation	UNP P0A2D5
Dx	13	LYS	ASP	engineered mutation	UNP P0A2D5
Dx	106	TRP	TYR	engineered mutation	UNP P0A2D5
D4	13	LYS	ASP	engineered mutation	UNP P0A2D5
D4	106	TRP	TYR	engineered mutation	UNP P0A2D5
D0	13	LYS	ASP	engineered mutation	UNP P0A2D5
D0	106	TRP	TYR	engineered mutation	UNP P0A2D5
B6	13	LYS	ASP	engineered mutation	UNP P0A2D5
B6	106	TRP	TYR	engineered mutation	UNP P0A2D5
ED	13	LYS	ASP	engineered mutation	UNP P0A2D5
ED	106	TRP	TYR	engineered mutation	UNP P0A2D5
EK	13	LYS	ASP	engineered mutation	UNP P0A2D5
EK	106	TRP	TYR	engineered mutation	UNP P0A2D5
ER	13	LYS	ASP	engineered mutation	UNP P0A2D5
ER	106	TRP	TYR	engineered mutation	UNP P0A2D5
EY	13	LYS	ASP	engineered mutation	UNP P0A2D5

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Chain	Residue	Modelled	Actual	Comment	Reference
EY	106	TRP	TYR	engineered mutation	UNP P0A2D5
Bd	13	LYS	ASP	engineered mutation	UNP P0A2D5
Bd	106	TRP	TYR	engineered mutation	UNP P0A2D5
Bk	13	LYS	ASP	engineered mutation	UNP P0A2D5
Bk	106	TRP	TYR	engineered mutation	UNP P0A2D5
Br	13	LYS	ASP	engineered mutation	UNP P0A2D5
Br	106	TRP	TYR	engineered mutation	UNP P0A2D5
By	13	LYS	ASP	engineered mutation	UNP P0A2D5
By	106	TRP	TYR	engineered mutation	UNP P0A2D5
CC	13	LYS	ASP	engineered mutation	UNP P0A2D5
CC	106	TRP	TYR	engineered mutation	UNP P0A2D5
CJ	13	LYS	ASP	engineered mutation	UNP P0A2D5
CJ	106	TRP	TYR	engineered mutation	UNP P0A2D5
CQ	13	LYS	ASP	engineered mutation	UNP P0A2D5
CQ	106	TRP	TYR	engineered mutation	UNP P0A2D5
CX	13	LYS	ASP	engineered mutation	UNP P0A2D5
CX	106	TRP	TYR	engineered mutation	UNP P0A2D5
Ce	13	LYS	ASP	engineered mutation	UNP P0A2D5
Ce	106	TRP	TYR	engineered mutation	UNP P0A2D5
Cl	13	LYS	ASP	engineered mutation	UNP P0A2D5
Cl	106	TRP	TYR	engineered mutation	UNP P0A2D5
Cs	13	LYS	ASP	engineered mutation	UNP P0A2D5
Cs	106	TRP	TYR	engineered mutation	UNP P0A2D5
Cz	13	LYS	ASP	engineered mutation	UNP P0A2D5
Cz	106	TRP	TYR	engineered mutation	UNP P0A2D5
E6	13	LYS	ASP	engineered mutation	UNP P0A2D5
E6	106	TRP	TYR	engineered mutation	UNP P0A2D5
E7	13	LYS	ASP	engineered mutation	UNP P0A2D5
E7	106	TRP	TYR	engineered mutation	UNP P0A2D5
E8	13	LYS	ASP	engineered mutation	UNP P0A2D5
E8	106	TRP	TYR	engineered mutation	UNP P0A2D5
E9	13	LYS	ASP	engineered mutation	UNP P0A2D5
E9	106	TRP	TYR	engineered mutation	UNP P0A2D5
E0	13	LYS	ASP	engineered mutation	UNP P0A2D5
E0	106	TRP	TYR	engineered mutation	UNP P0A2D5
FA	13	LYS	ASP	engineered mutation	UNP P0A2D5
FA	106	TRP	TYR	engineered mutation	UNP P0A2D5
FB	13	LYS	ASP	engineered mutation	UNP P0A2D5
FB	106	TRP	TYR	engineered mutation	UNP P0A2D5

- Molecule 16 is a protein called Flagellar motor switch protein FliM.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C0	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	DC	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	DF	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	DX	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	Dd	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	Dj	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	Dp	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	Dv	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	D2	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	D8	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	B4	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	EI	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	EP	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	EW	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	Bb	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	Bi	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	Bp	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	Bw	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	CA	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	CH	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	CO	301	Total 2431	C 1549	N 437	O 440	S 5	0	0
16	CV	301	Total 2431	C 1549	N 437	O 440	S 5	0	0

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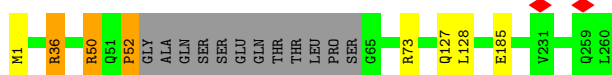
Mol	Chain	Residues	Atoms					AltConf	Trace
16	Cc	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	Cj	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	Cq	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	Cx	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	Eq	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	Er	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	Es	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	Et	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	Eu	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	Ev	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	Ew	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
16	E5	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		

### 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 basal-body rod protein FlgG

Chain 0:  92% .. 5%



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain 1:  93% ..



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain 2:  98% .



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain 3:  98% .



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain 4:  97% .



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain 5:  97%



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain 6:  97%



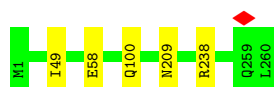
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain 7:  98%



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain 8:  98%



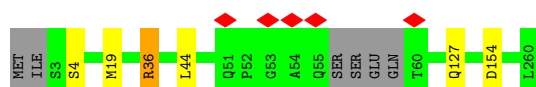
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain 9:  97%



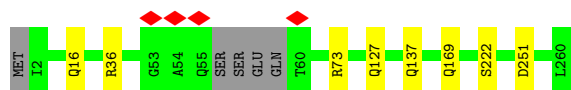
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain AF:  95%

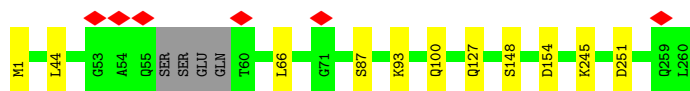


- Molecule 1: Flagellar basal-body rod protein FlgG

Chain AG:  95%



- Molecule 1: Flagellar basal-body rod protein FlgG



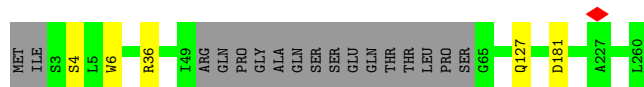
- Molecule 1: Flagellar basal-body rod protein FlgG



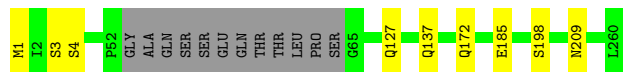
- Molecule 1: Flagellar basal-body rod protein FlgG



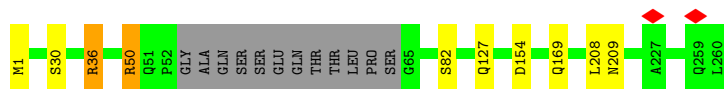
- Molecule 1: Flagellar basal-body rod protein FlgG



- Molecule 1: Flagellar basal-body rod protein FlgG



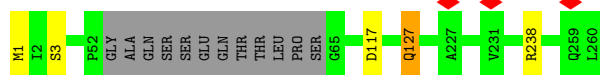
- Molecule 1: Flagellar basal-body rod protein FlgG



- Molecule 1: Flagellar basal-body rod protein FlgG



Chain AN:  93% • 5%



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain ZA:  98% •



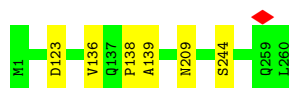
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain ZB:  96% •



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain ZC:  98% •



- Molecule 1: Flagellar basal-body rod protein FlgG

Chain ZD:  98% •




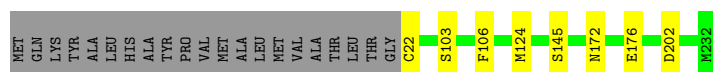
- Molecule 1: Flagellar basal-body rod protein FlgG

Chain ZE:  99% •



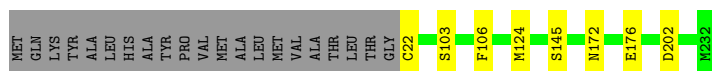
- Molecule 2: Flagellar L-ring protein

Chain A:  88% • 9%




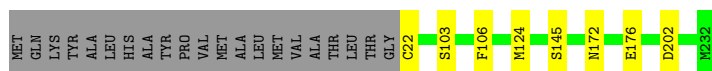
- Molecule 2: Flagellar L-ring protein

Chain B:  88% 9%




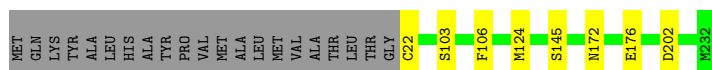
• Molecule 2: Flagellar L-ring protein

Chain C:  88% 9%




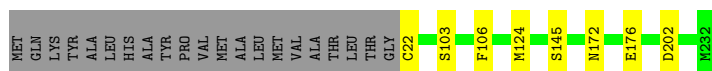
• Molecule 2: Flagellar L-ring protein

Chain D:  88% 9%




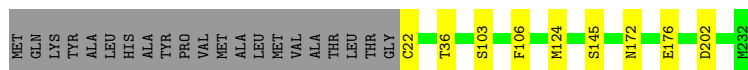
• Molecule 2: Flagellar L-ring protein

Chain E:  88% 9%




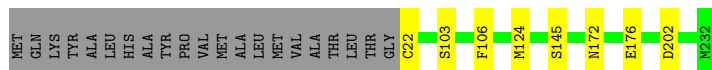
• Molecule 2: Flagellar L-ring protein

Chain F:  87% 9%



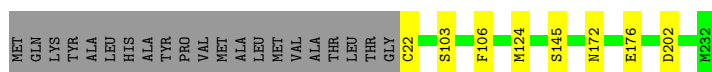
• Molecule 2: Flagellar L-ring protein

Chain G:  88% 9%




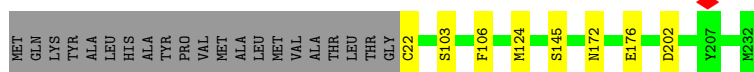
• Molecule 2: Flagellar L-ring protein

Chain H:  88% 9%



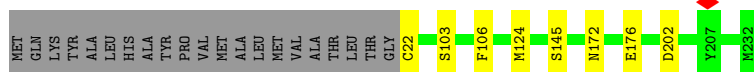
• Molecule 2: Flagellar L-ring protein

Chain I:  88% 9%



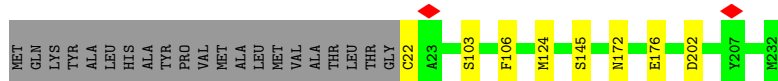
- Molecule 2: Flagellar L-ring protein

Chain J:  88% 9%




- Molecule 2: Flagellar L-ring protein

Chain K:  88% 9%



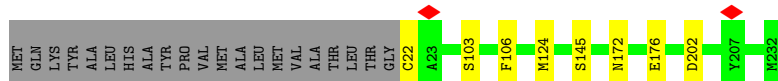
- Molecule 2: Flagellar L-ring protein

Chain L:  88% 9%



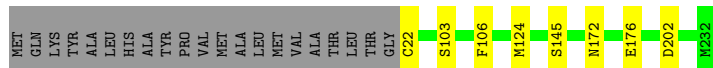
- Molecule 2: Flagellar L-ring protein

Chain M:  88% 9%



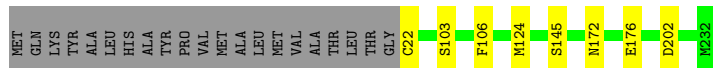
- Molecule 2: Flagellar L-ring protein

Chain N:  88% 9%


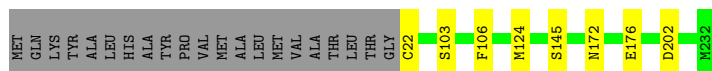


- Molecule 2: Flagellar L-ring protein

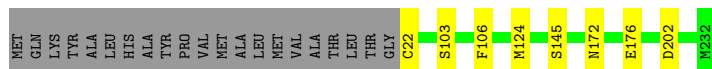
Chain O:  88% 9%



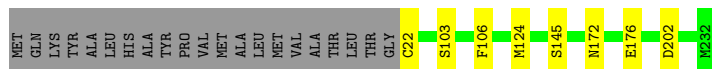
## • Molecule 2: Flagellar L-ring protein

Chain P:  88% 9%


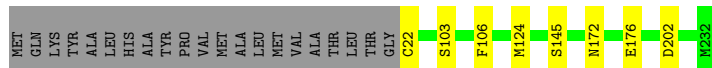
## • Molecule 2: Flagellar L-ring protein

Chain Q:  88% 9%


## • Molecule 2: Flagellar L-ring protein

Chain R:  88% 9%


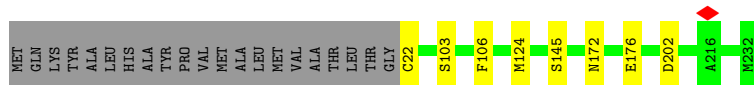
## • Molecule 2: Flagellar L-ring protein

Chain S:  88% 9%


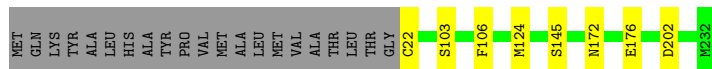
## • Molecule 2: Flagellar L-ring protein

Chain T:  88% 9%

## • Molecule 2: Flagellar L-ring protein

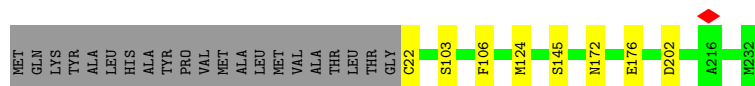
Chain U:  88% 9%

## • Molecule 2: Flagellar L-ring protein


Chain V:  88% 9%

- Molecule 2: Flagellar L-ring protein

Chain W:  88% 9%




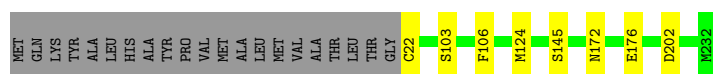
- Molecule 2: Flagellar L-ring protein

Chain X:  88% 9%




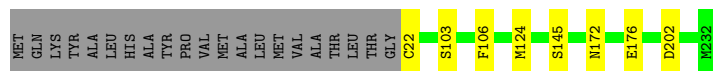
- Molecule 2: Flagellar L-ring protein

Chain Y:  88% 9%




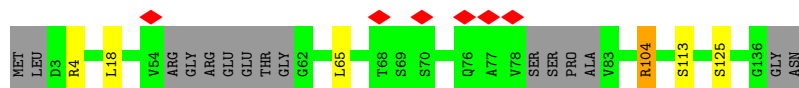
- Molecule 2: Flagellar L-ring protein

Chain Z:  88% 9%



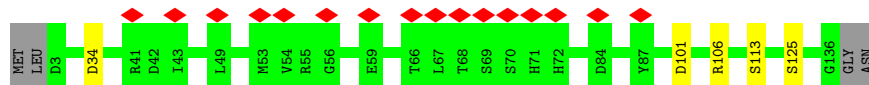
- Molecule 3: Flagellar basal body rod protein FlgB

Chain A0:  85% 11%




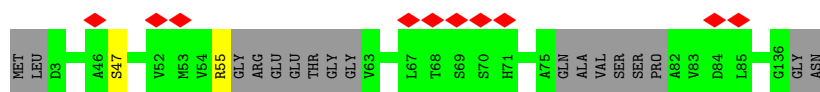
- Molecule 3: Flagellar basal body rod protein FlgB

Chain A6:  12% 93%

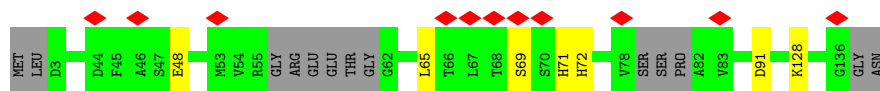
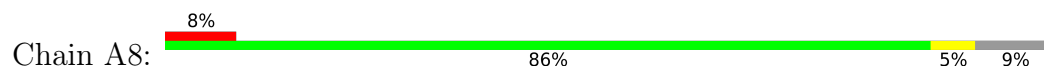


- Molecule 3: Flagellar basal body rod protein FlgB

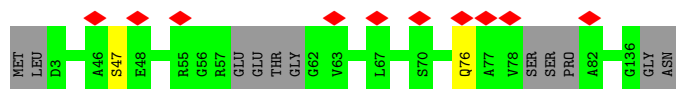
Chain A7:  7% 86% 12%



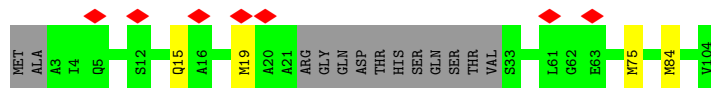
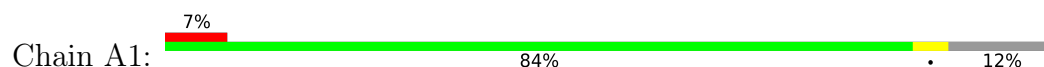
- Molecule 3: Flagellar basal body rod protein FlgB



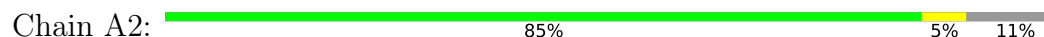
- Molecule 3: Flagellar basal body rod protein FlgB



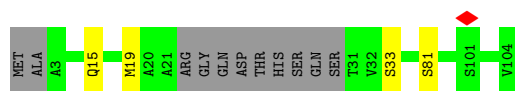
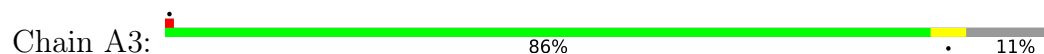
- Molecule 4: Flagellar hook-basal body complex protein FliE



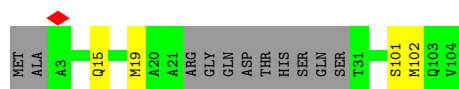
- Molecule 4: Flagellar hook-basal body complex protein FliE




- Molecule 4: Flagellar hook-basal body complex protein FliE

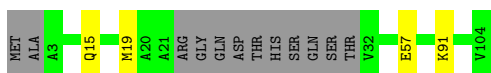


- Molecule 4: Flagellar hook-basal body complex protein FliE



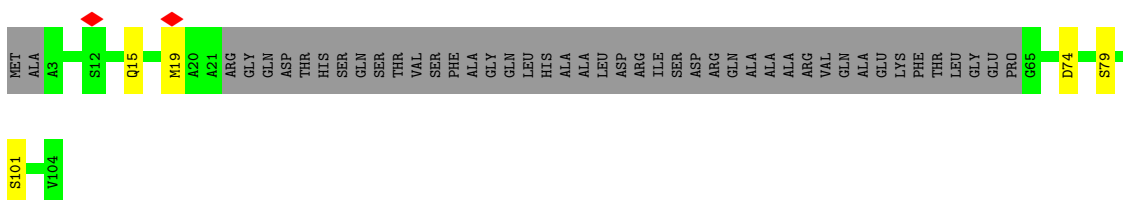
- Molecule 4: Flagellar hook-basal body complex protein FliE

Chain A5:  85% 12%



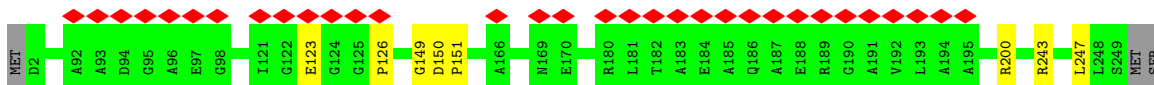
- Molecule 4: Flagellar hook-basal body complex protein FliE

Chain Az:  52% 5% 43%



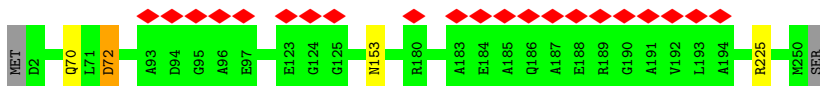
- Molecule 5: Flagellar basal-body rod protein FlgF

Chain AA:  13% 96%



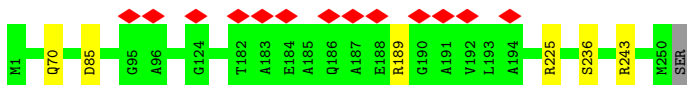
- Molecule 5: Flagellar basal-body rod protein FlgF

Chain AB:  8% 98%



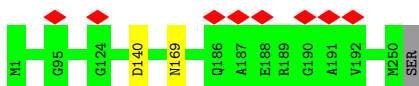
- Molecule 5: Flagellar basal-body rod protein FlgF

Chain AC:  5% 97%



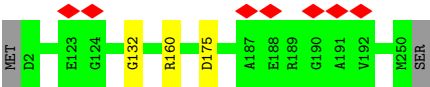
- Molecule 5: Flagellar basal-body rod protein FlgF

Chain AD:  99%



- Molecule 5: Flagellar basal-body rod protein FlgF

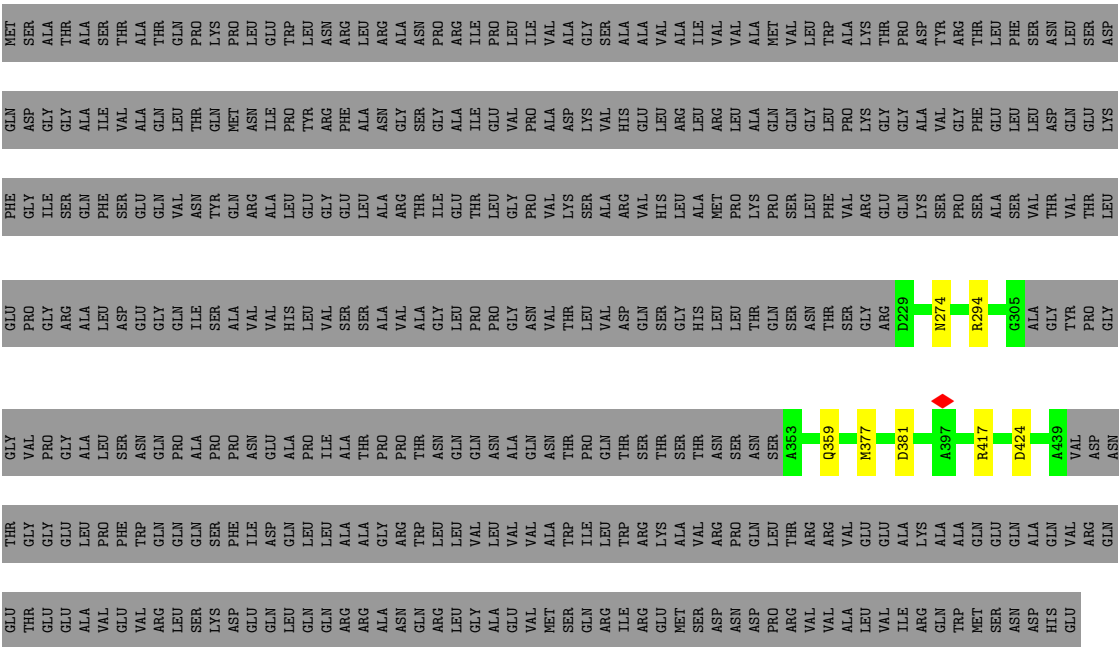
Chain AE:  98%



• Molecule 6: Flagellar M-ring protein



• Molecule 6: Flagellar M-ring protein



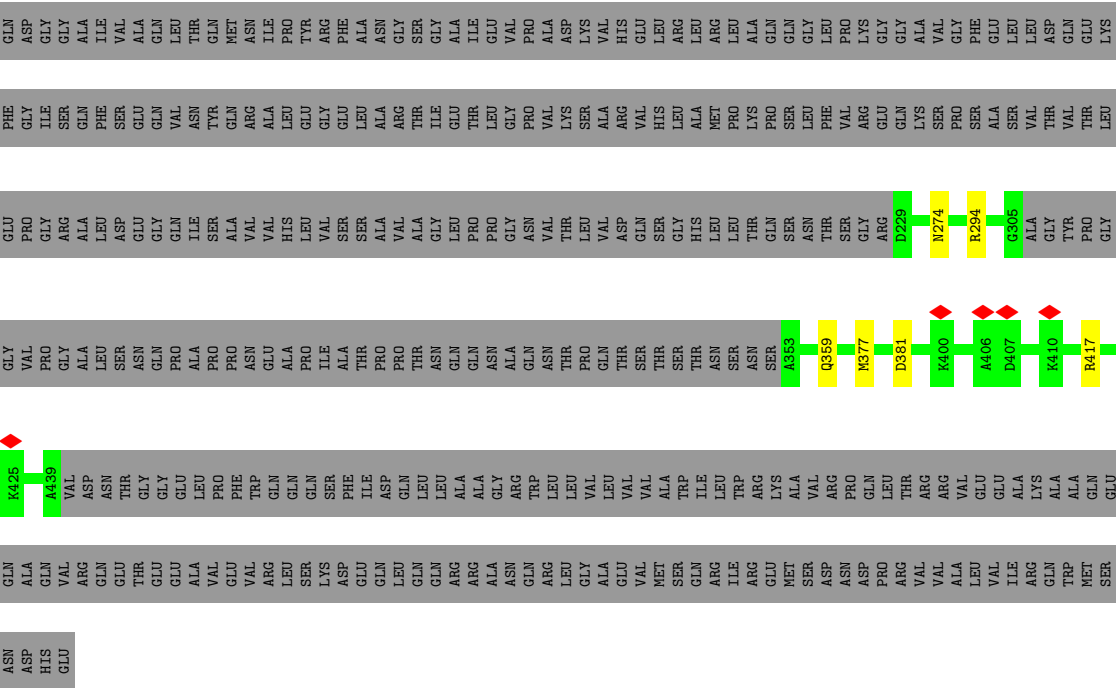
• Molecule 6: Flagellar M-ring protein



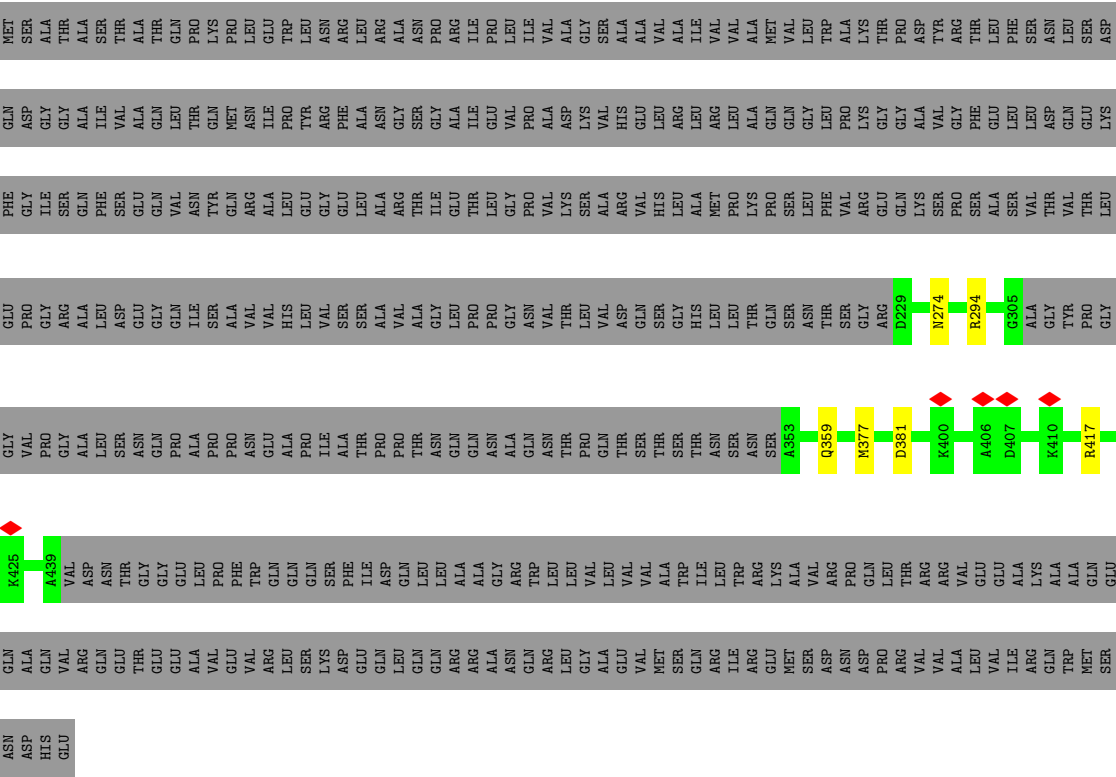
[illegible]

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GLU	GLY	GLU	ALA	ARG	GLN	ALA	THR
ALA	LEU	LEU	LEU	ASP	PHE	ILE	SER
VAL	PRO	PRO	SER	ASP	SER	VAL	THR
GLU	PHE	ASN	ASN	GLU	GLU	ALA	THR
VAL	THR	GLN	GLN	GLY	GLN	LEU	THR
ARG	GLN	GLN	PRO	ILE	ASN	THR	PRO
LEU	SER	SER	PRO	SER	TYR	GLN	LYS
LYS	LYS	SER	PRO	ALA	GLN	MET	PRO
ASP	GLU	ILE	ASN	VAL	ASN	LEU	LEU
GLN	ASP	ASP	ALA	HIS	LEU	TRP	TRP
LEU	GLN	GLN	ALA	VAL	GLY	TYR	LEU
GLN	LEU	LEU	ILE	VAL	GLY	ARG	ASN
GLN	LEU	LEU	ALA	SER	GLU	PHE	ARG
ARG	ALA	ALA	THR	SER	GLU	ALA	LEU
ARG	ALA	ALA	PRO	VAL	ALA	ASN	ARG
ALA	GLY	GLY	PRO	VAL	ARG	GLY	ALA
ASN	ARG	THR	THR	ALA	THR	SER	ASN
GLN	TRP	LEU	ASN	GLY	ILE	GLY	PRO
ARG	LEU	LEU	GLN	LEU	GLU	ALA	ARG
LEU	VAL	VAL	ASN	PRO	THR	ILE	PRO
GLU	VAL	VAL	GLN	ASN	GLY	VAL	LEU
VAL	VAL	VAL	ASN	VAL	VAL	ALA	ILE
MET	MET	ALA	THR	THR	LYS	ASP	VAL
SER	GLN	ILE	GLN	VAL	SER	GLY	ALA
THR	LEU	LEU	THR	ASP	ALA	HIS	SER
ARG	ARG	LEU	THR	THR	VAL	GLN	ALA
ILE	TRP	TRP	SER	SER	VAL	LEU	VAL
ARG	ARG	ARG	THR	SER	HIS	ARG	VAL
GLU	LYS	LYS	SER	GLY	LEU	ARG	VAL
MET	ALA	ALA	THR	HIS	ALA	ILE	VAL
SER	VAL	ASN	ASN	LEU	MET	ARG	VAL
ASP	ARG	ARG	SER	THR	PRO	LEU	VAL
ASN	PRO	PRO	ASN	THR	LYS	ALA	ALA
ASP	GLN	SER	SER	GLN	PRO	GLN	MET
PRO	LEU	GLN	ARG	SER	SER	GLN	VAL
ARG	THR	THR	THR	ASN	LEU	GLY	VAL
VAL	ARG	ARG	VAL	THR	PHE	LEU	TRP
VAL	VAL	VAL	ARG	SER	VAL	PRO	ALA
ALA	VAL	VAL	M377	GLY	ARG	LYS	LYS
LEU	GLU	GLU	D381	ARG	GLU	GLY	THR
VAL	ILE	ALA	D381	D329	GLN	GLY	PRO
ILE	ARG	ALA	D381	D329	ALA	ALA	ASP
ARG	GLN	LYS	A397	N274	SER	VAL	TYR
GLN	ALA	ALA	D398	N274	PRO	GLY	ARG
TRP	ALA	ALA	D398	R294	SER	PHE	THR
MET	GLN	GLN	R417	G305	ALA	GLU	LEU
SER	GLU	GLU	R417	G305	SER	LEU	PHE
ASN	GLN	GLN	D424	ALA	VAL	LEU	ASN
ASP	ALA	ALA	D424	GLY	THR	ASP	ASN
HIS	GLN	GLN	A439	TYR	VAL	GLN	ASN
GLU	VAL	ARG	VAL	PRO	THR	GLU	SER
				GLY	LEU	LYS	

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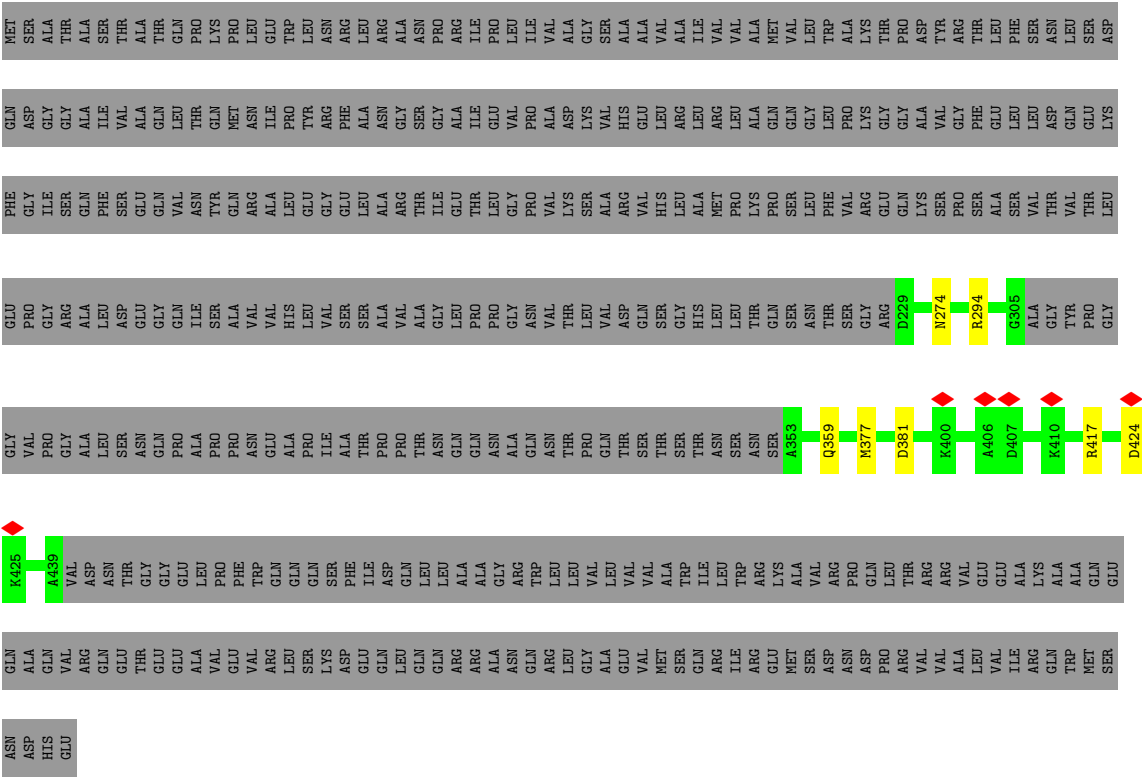


• Molecule 6: Flagellar M-ring protein

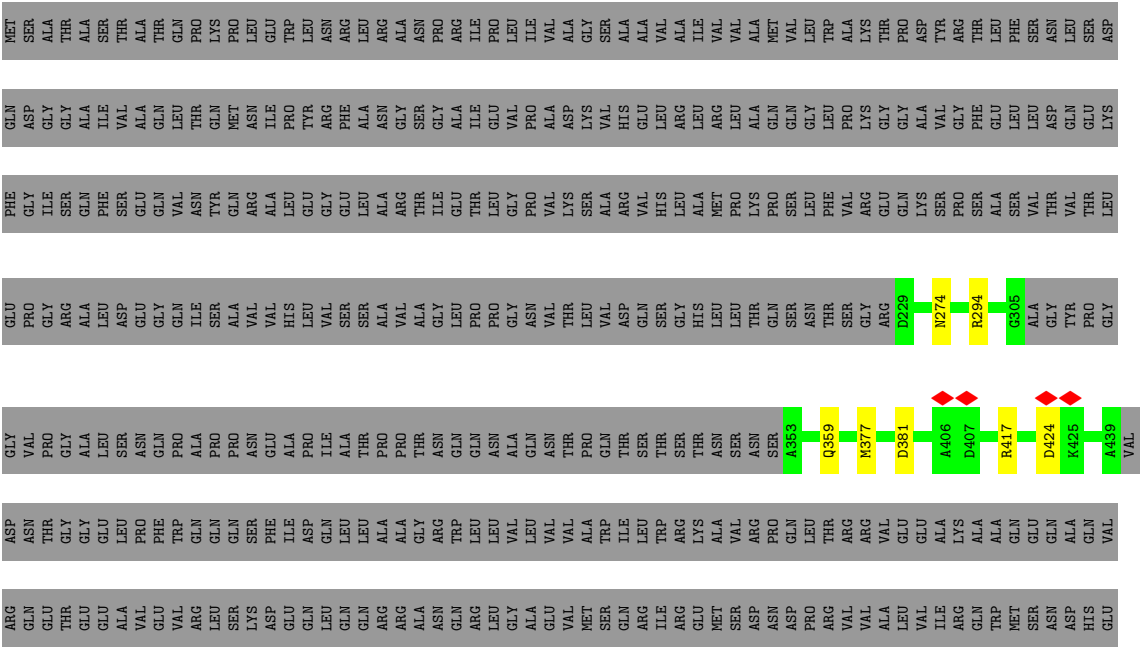


• Molecule 6: Flagellar M-ring protein





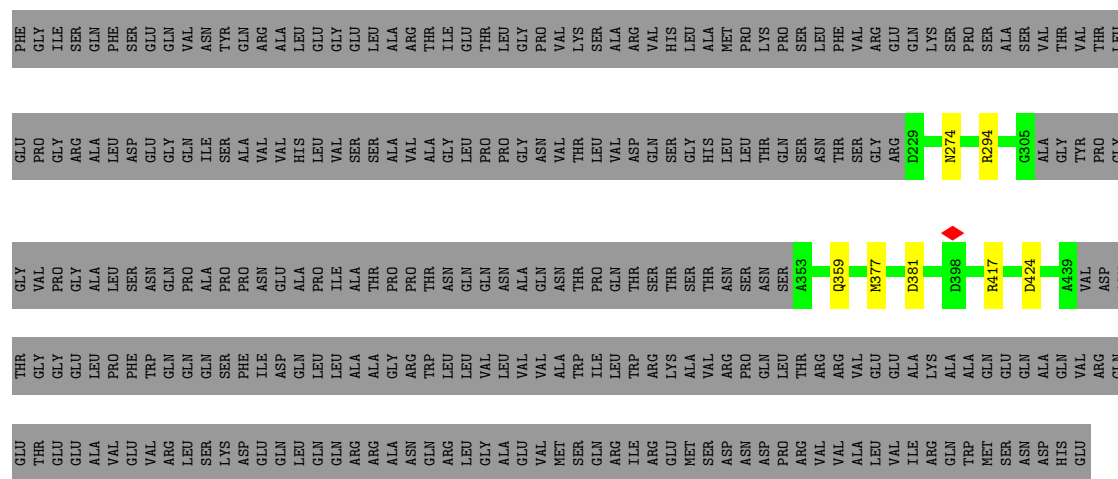
● Molecule 6: Flagellar M-ring protein



● Molecule 6: Flagellar M-ring protein







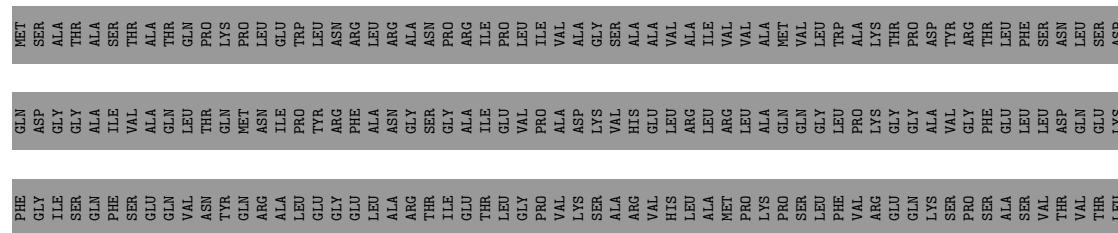
- Molecule 6: Flagellar M-ring protein

Chain AZ:  28% 71%

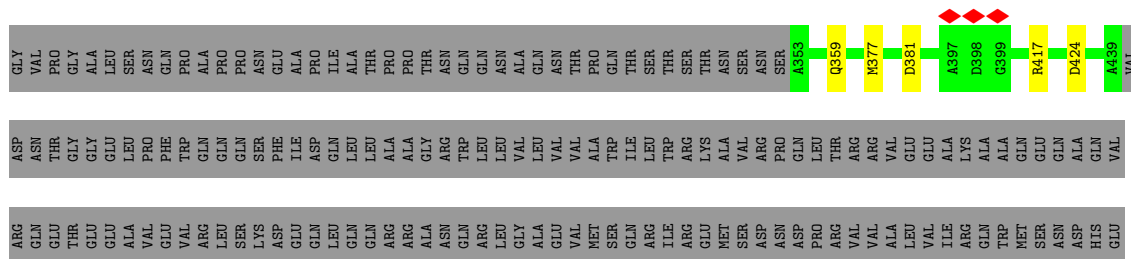


- Molecule 6: Flagellar M-ring protein

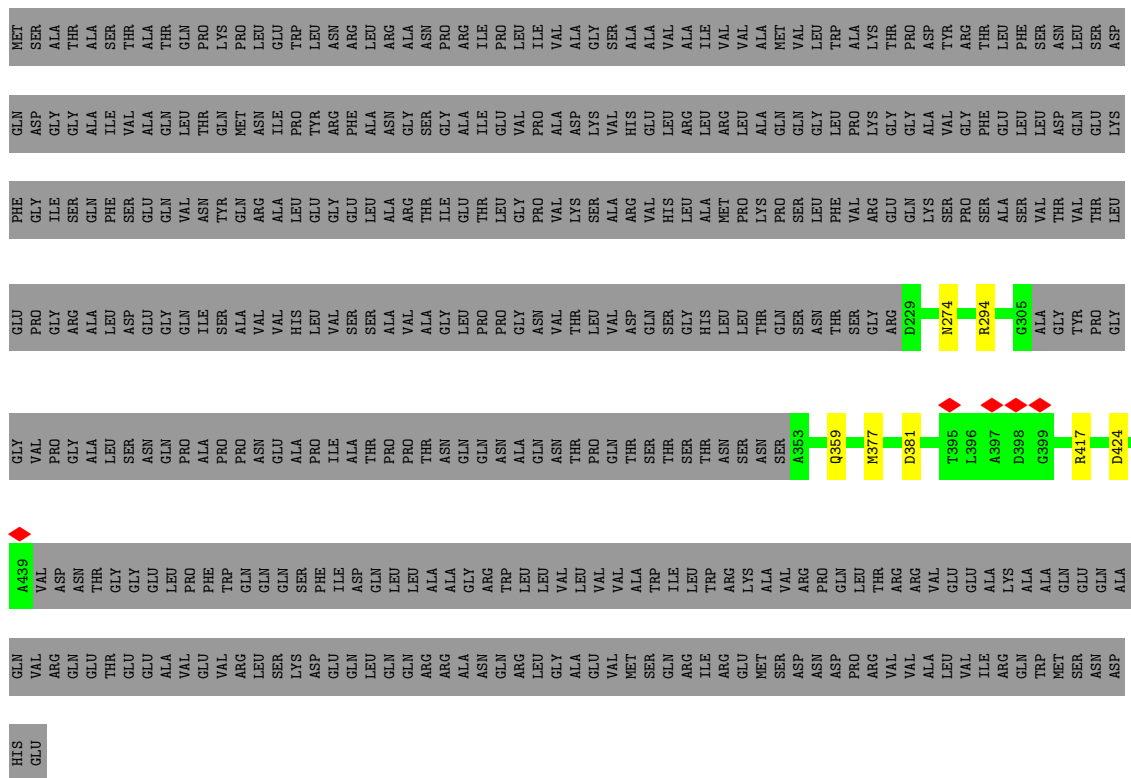
Chain Aa:  28% 71%



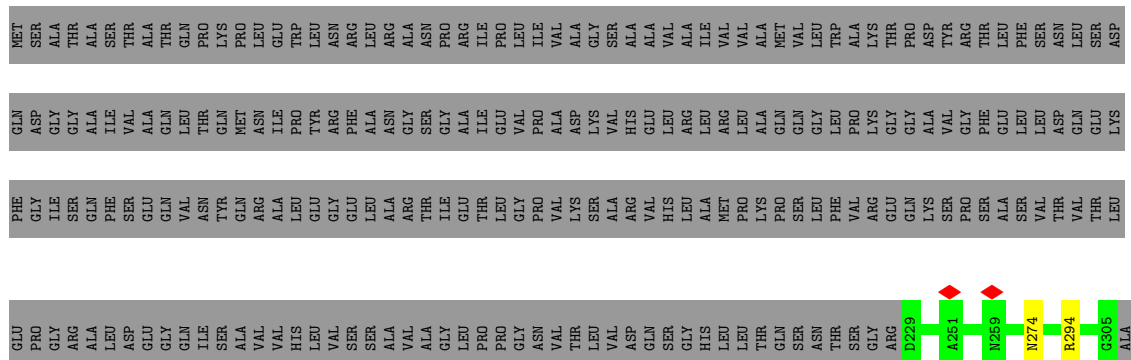


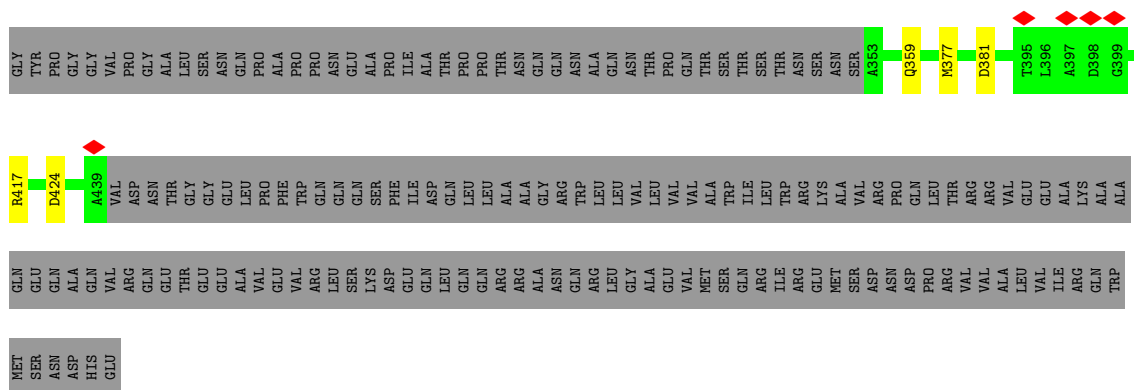


- Molecule 6: Flagellar M-ring protein

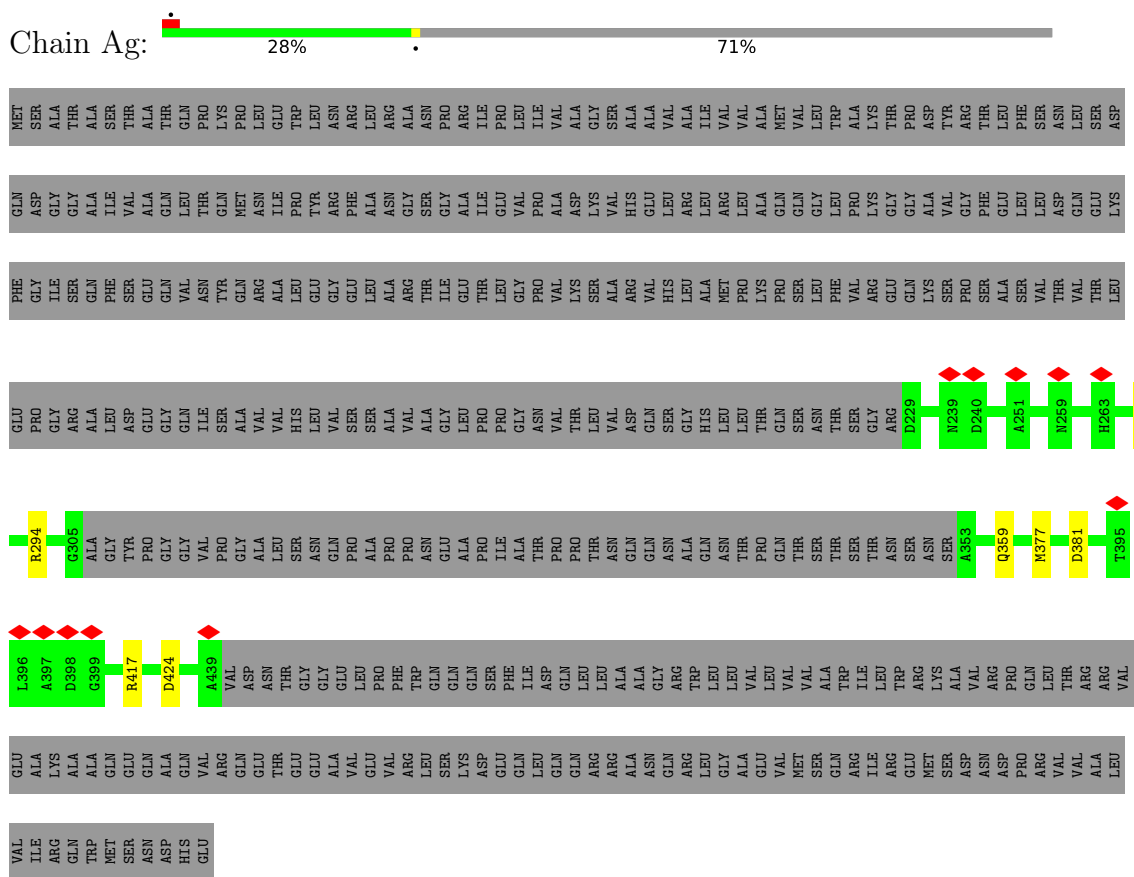


- Molecule 6: Flagellar M-ring protein

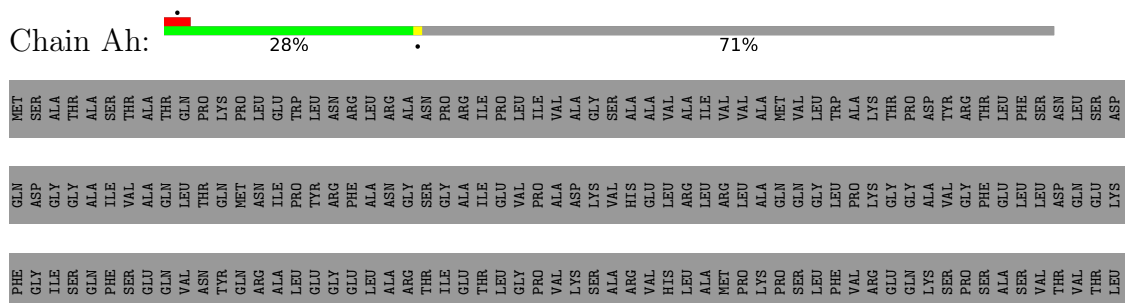




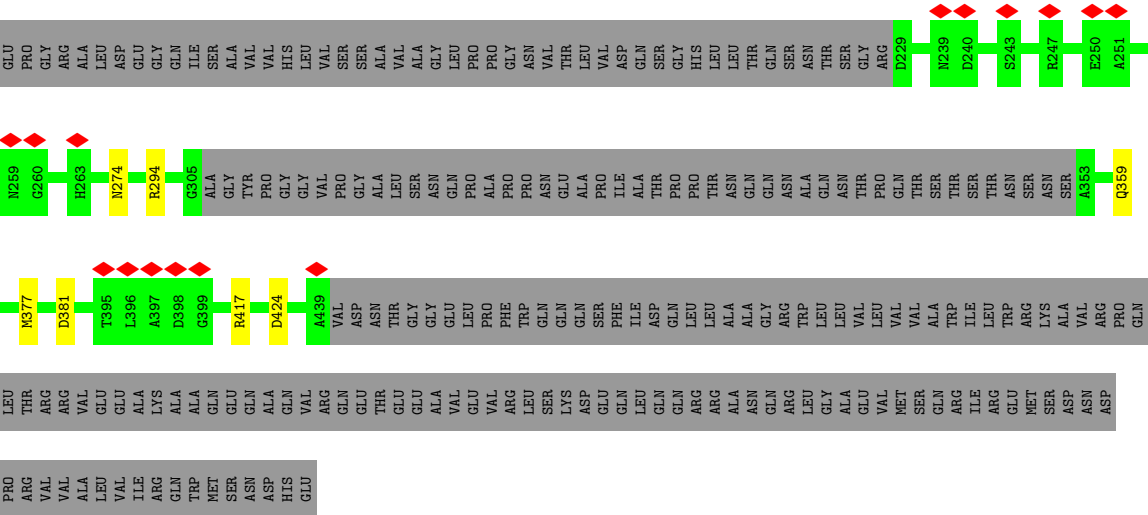
- Molecule 6: Flagellar M-ring protein



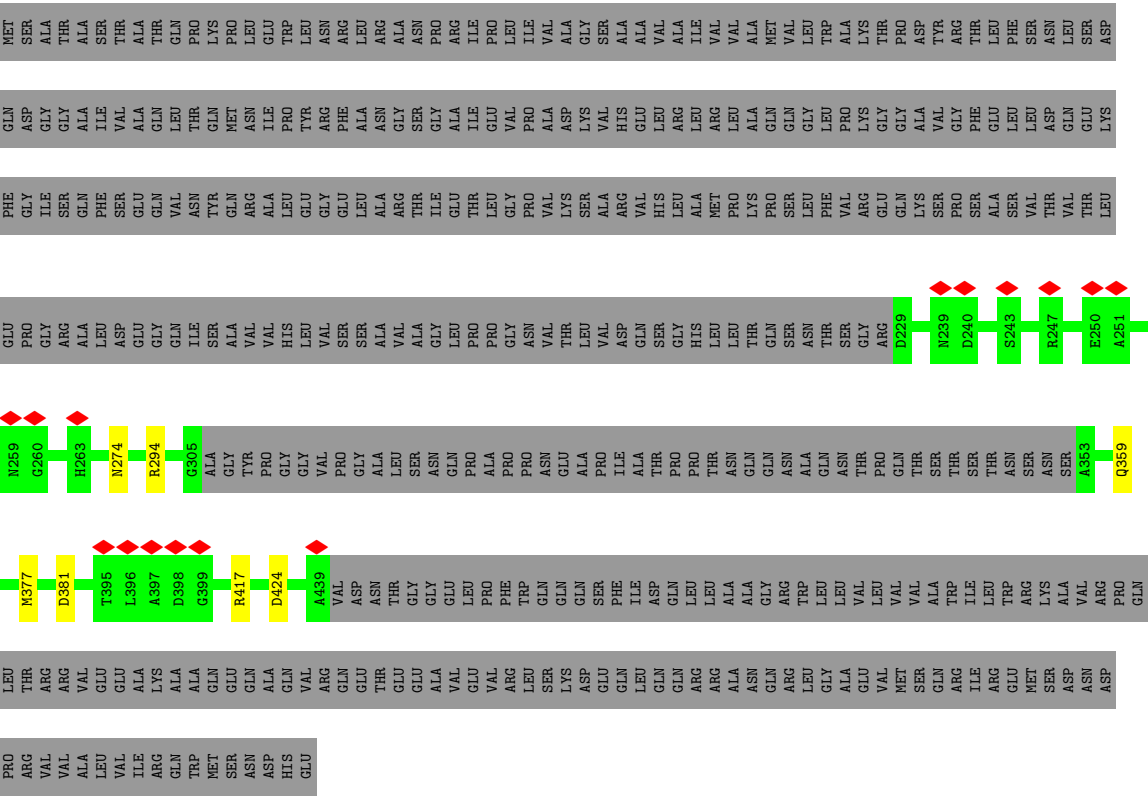
- Molecule 6: Flagellar M-ring protein



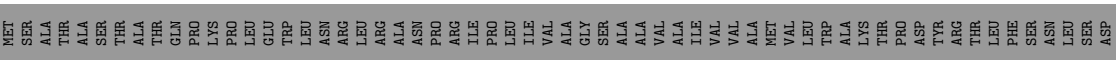


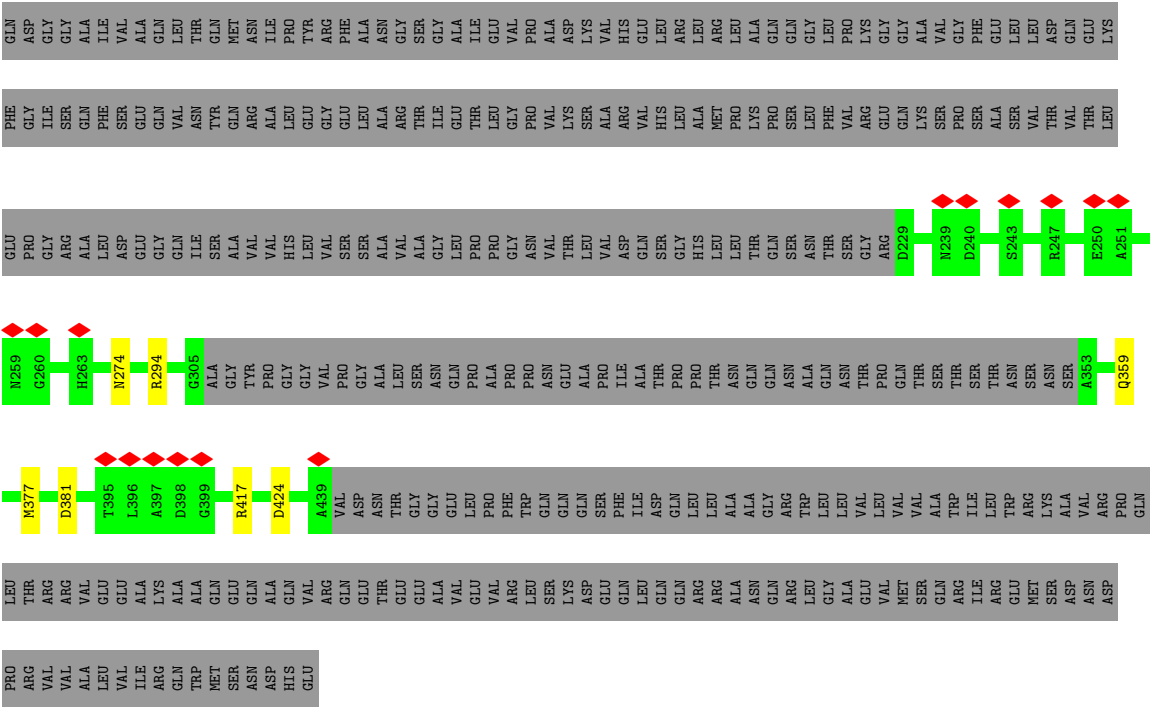


• Molecule 6: Flagellar M-ring protein

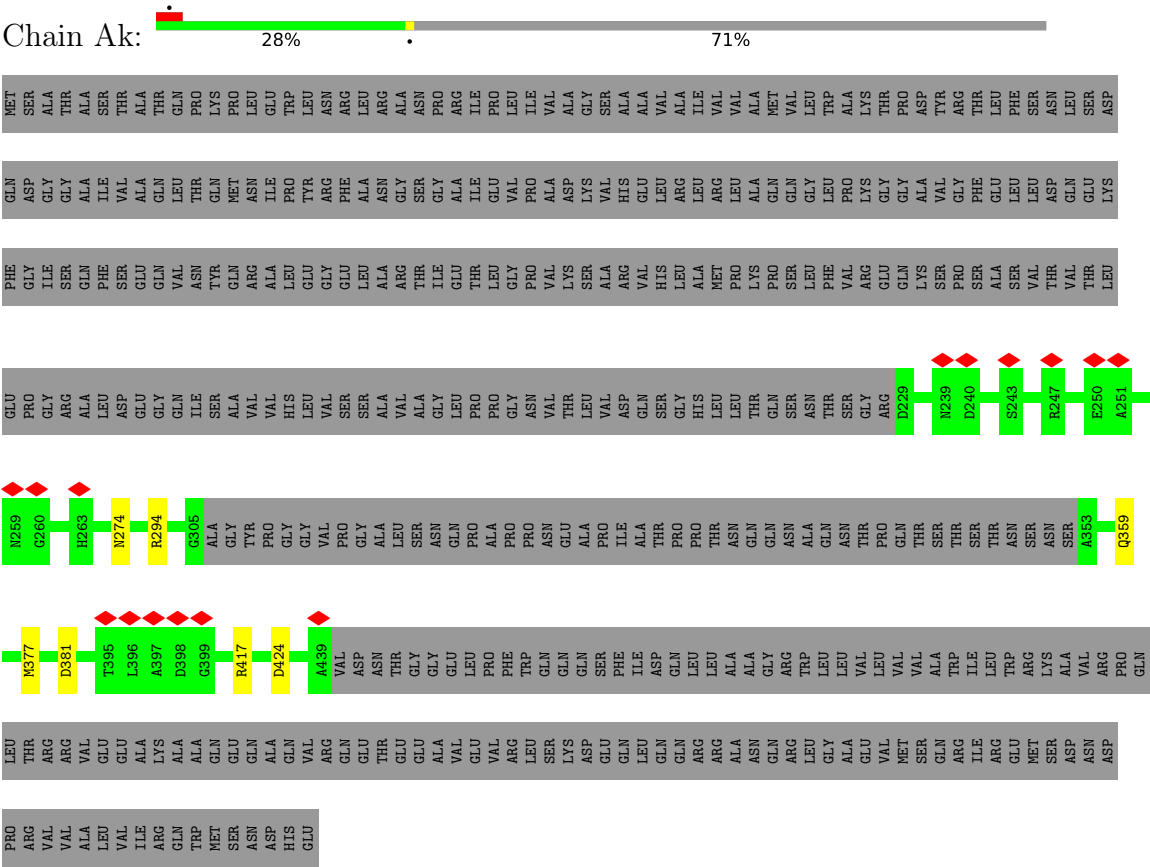


• Molecule 6: Flagellar M-ring protein

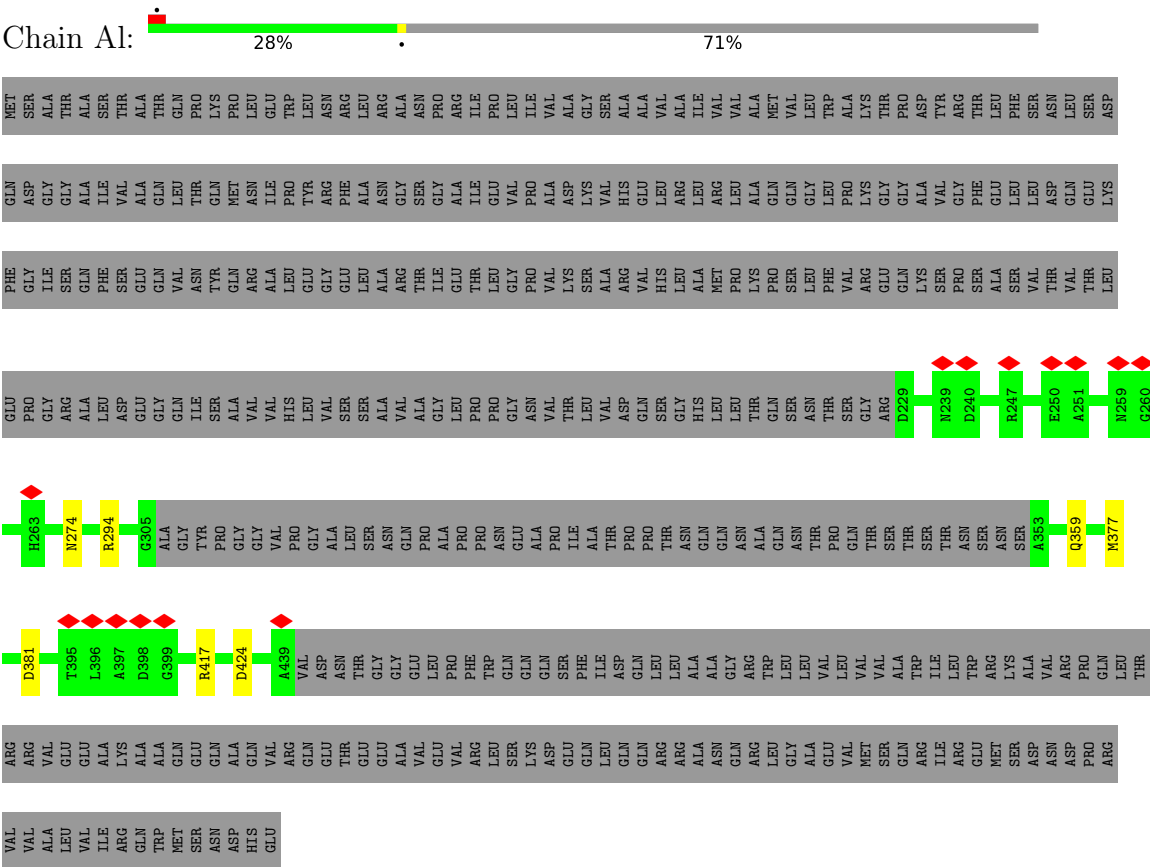




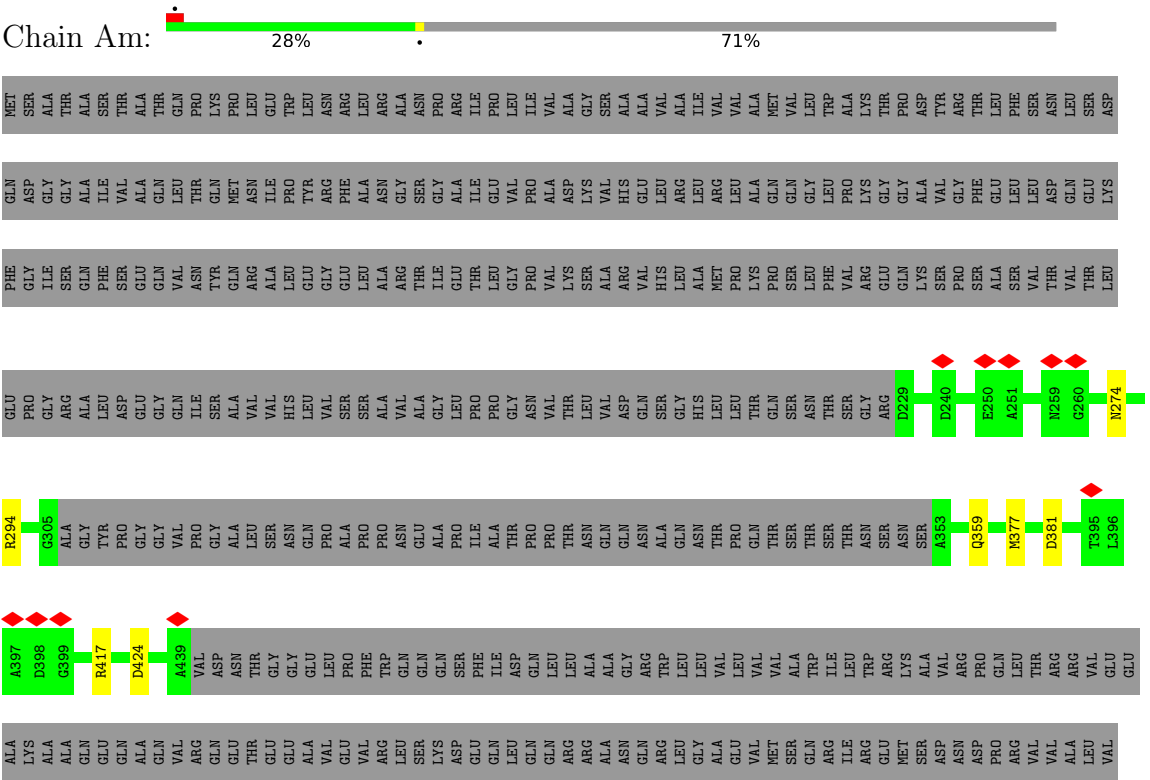
• Molecule 6: Flagellar M-ring protein



• Molecule 6: Flagellar M-ring protein



• Molecule 6: Flagellar M-ring protein





ASN	GLN
ASP	ALA
HIS	ARG
GLU	VAL

- Molecule 6: Flagellar M-ring protein



NET	SER	ALA	ALA	ALA	SER	THR	THR	ALA	GLN	PRO	LYS	PRO	LEU	GLU	TRP	LEU	ASN	ARG	ANG	LEU	ARG	ALA	ALA	ALA	ASN	PRO	ARG	ILE	ILE	ILE	VAL	VAL	ALA	GLY	SER	ALA	ALA	ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	NET	VAL	VAL	LEU	THR	THR	PRO	ASP	TYR	ARG	THR	LEU	PHE	SER	ASN	LEU	SER	SER	
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GLN	ASP	GLY	GLY	ALA	ILE	VAL	ALA	ALA	GLN	THR	GLN	MET	ASN	ILE	TYR	PRO	ARG	PHE	ALA	ALA	ASN	GLY	GLY	GLY	ILE	GLU	VAL	VAL	PRO	PRO	ALA	ASP	LYS	VAL	VAL	GLU	LEU	LEU	ARG	LEU	ALA	GLN	GLN	GLY	LEU	LEU	PRO	PRO	LYS	GLY	GLY	VAL	VAL	GLY	PHE	GLU	LEU	LEU	ASP	GLN	GLN	GLU	LYS
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PHE	GLY	ILE	GLN	SER	PHE	SER	GLU	GLN	VAL	ASN	TYR	GLN	ARG	ALA	LEU	GLY	GLY	GLU	LEU	ALA	ARG	THR	ILE	GLU	THR	LEU	GLY	PRO	VAL	LYS	SER	ALA	ARG	VAL	HIS	LEU	ALA	MET	PRO	LYS	PRO	SER	LEU	PHE	VAL	ARG	GLN	LYS	SER	PRO	SER	ALA	VAL	THR	VAL	THR	LEU
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- Molecule 6: Flagellar M-ring protein



MET	SER	ALA	ALA	THR	THR	SER	THR	ALA	ALA	GLN	PRO	PRO	LYS	PRO	LEU	GLU	TRP	LEU	ASN	ARG	ARG	ARG	ASN	PRO	ARG	ILE	PRO	PRO	LEU	LEU	ILE	VAL	ALA	GLY	SER	ALA	ALA	VAL	VAL	VAL	VAL	MET	VAL	LEU	TRP	ALA	ALA	LYS	THR	PRO	ASP	TYR	ARG	THR	LEU	PHE	SER	ASN	LEU	SER	ASN	ASP
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- Molecule 6: Flagellar M-ring protein

Chain BH:  97%

[illegible]

- Molecule 6: Flagellar M-ring protein

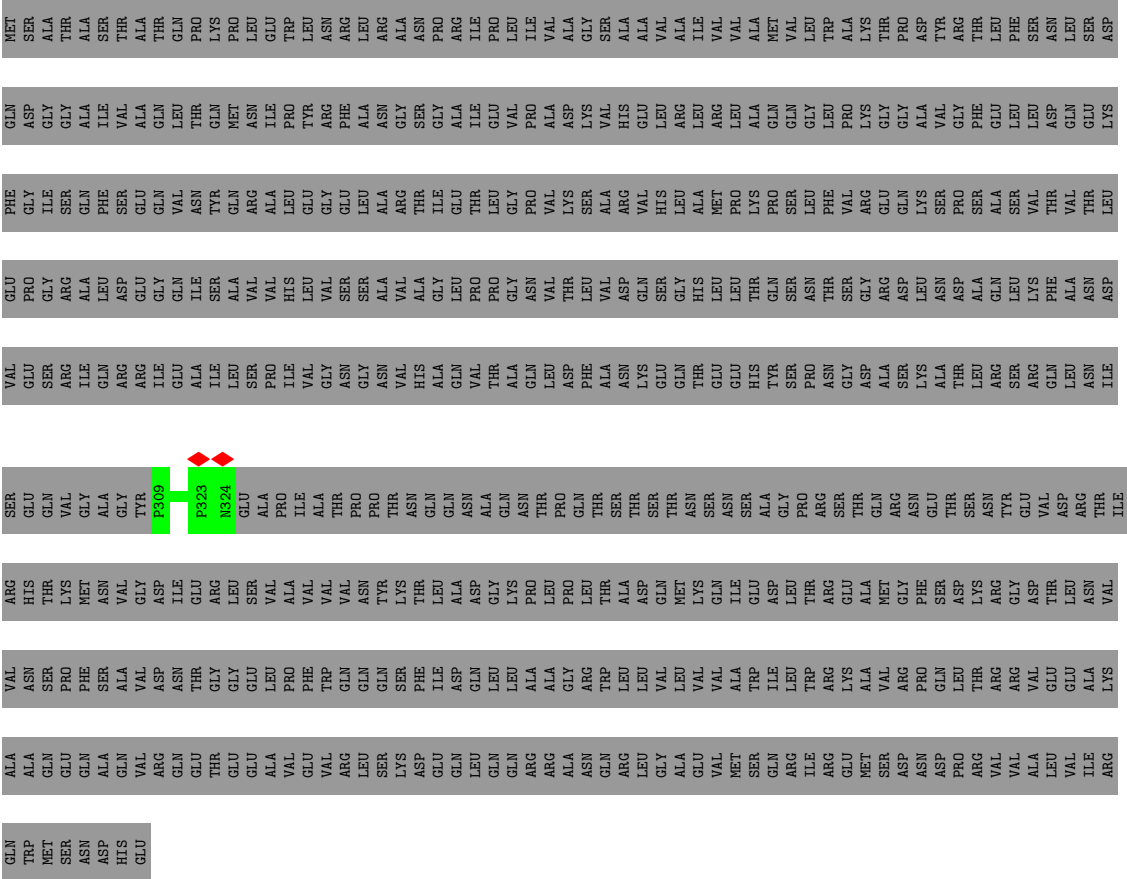
Chain BI:  96%

[illegible]



• Molecule 6: Flagellar M-ring protein

Chain BJ: . 97%



• Molecule 6: Flagellar M-ring protein

Chain BK: . 96%





[illegible]

- Molecule 6: Flagellar M-ring protein

Chain BM:  96%

MET	SER	ALA	ALA	THR	THR	SER	THR	ALA	ALA	GLN	PRO	LYS	PRO	LEU	LEU	GLU	TRP	LEU	ASN	ARG	ARG	LEU	ALA	ALA	ASN	PRO	ARG	ILE	PRO	PRO	LEU	LEU	ILE	VAL	ALA	GLY	SER	ALA	ALA	ALA	VAL	VAL	ALA	ILE	VAL	VAL	VAL	VAL	MET	VAL	VAL	LEU	LEU	TRP	TRP	ALA	LYS	THR	PRO	PRO	ASP	TYSR	ARG	THR	LEU	PHE	SER	ASN	LEU	LEU	SER	SER	ASN	SER	ASN	ARG
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PRO	PHE	SER	ALA	VAL	ASP	ASN	THR	GLY	GLY	GLU	LEU	PRO	PHE	TRP	GLN	GLN	SER	PHE	ILE	ASP	GLN	LEU	LEU	ALA	ALA	GLY	TRP	LEU	VAL	VAL	VAL	ALA	TRP	ILE	ARG	LYS	ARG	VAL	VAL	PRO	PRO	LEU	LEU	THR	ARG	ARG	VAL	VAL	GLU	GLU	ALA	LYS	ALA	ALA	GLN
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[illegible]

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- Molecule 6: Flagellar M-ring protein

Chain BN:  97%

[illegible]

GLN	ASP	GLY	GLY	ALA	ALA	VAL	ILE	GLN	THR	GLN	ASN	ILE	TYR	ARG	PHE	ALA	ASN	GLY	GLY	GLY	GLY	ALA	ILE	GLU	VAL	PRO	PRO	ALA	ASP	LYS	VAL	HIS	VAL	GLU	LEU	LEU	ARG	ARG	LEU	LEU	ALA	ALA	GLN	GLN	GLY	GLY	VAL	VAL	PHE	GLY	GLY	LEU	LEU	ASP	GLN	GLY	LYS
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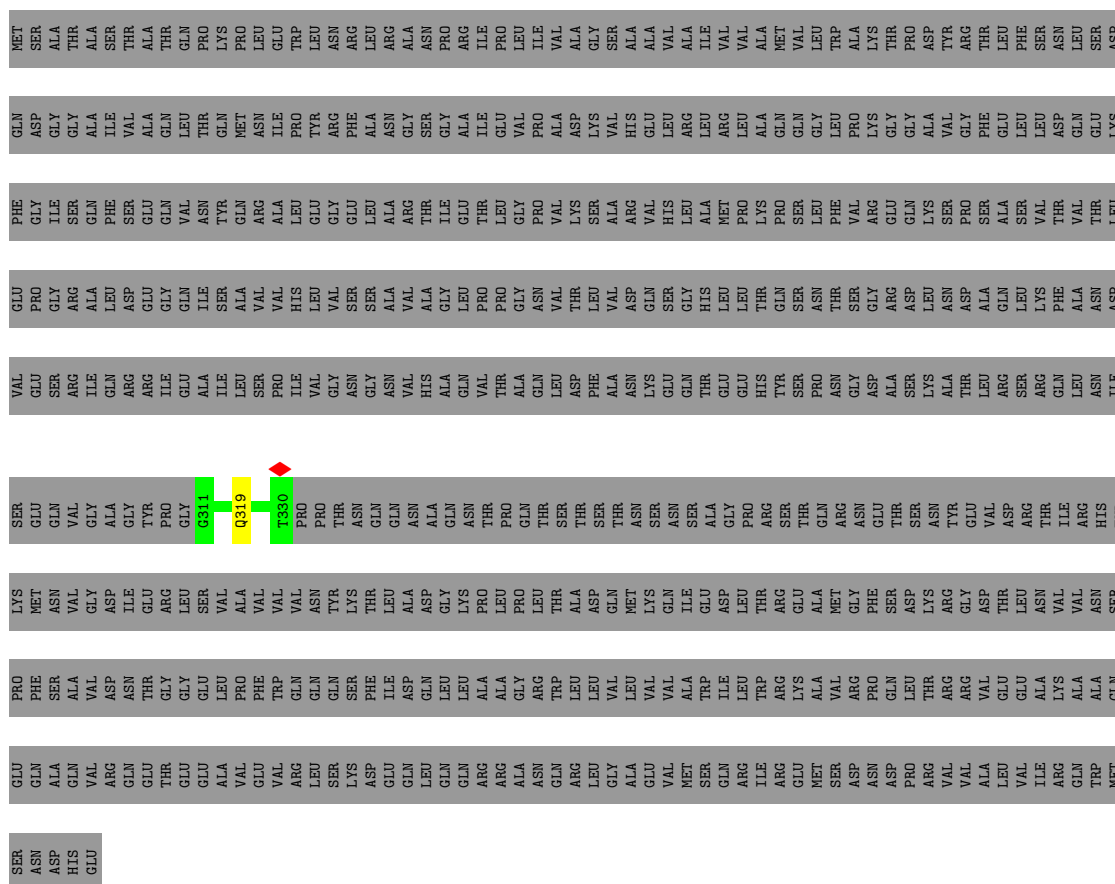
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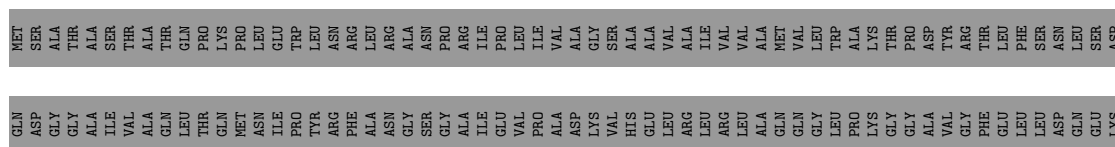
- Molecule 6: Flagellar M-ring protein

Chain BO:  96%



- Molecule 6: Flagellar M-ring protein

Chain BP:  97%



[illegible]

- Molecule 6: Flagellar M-ring protein

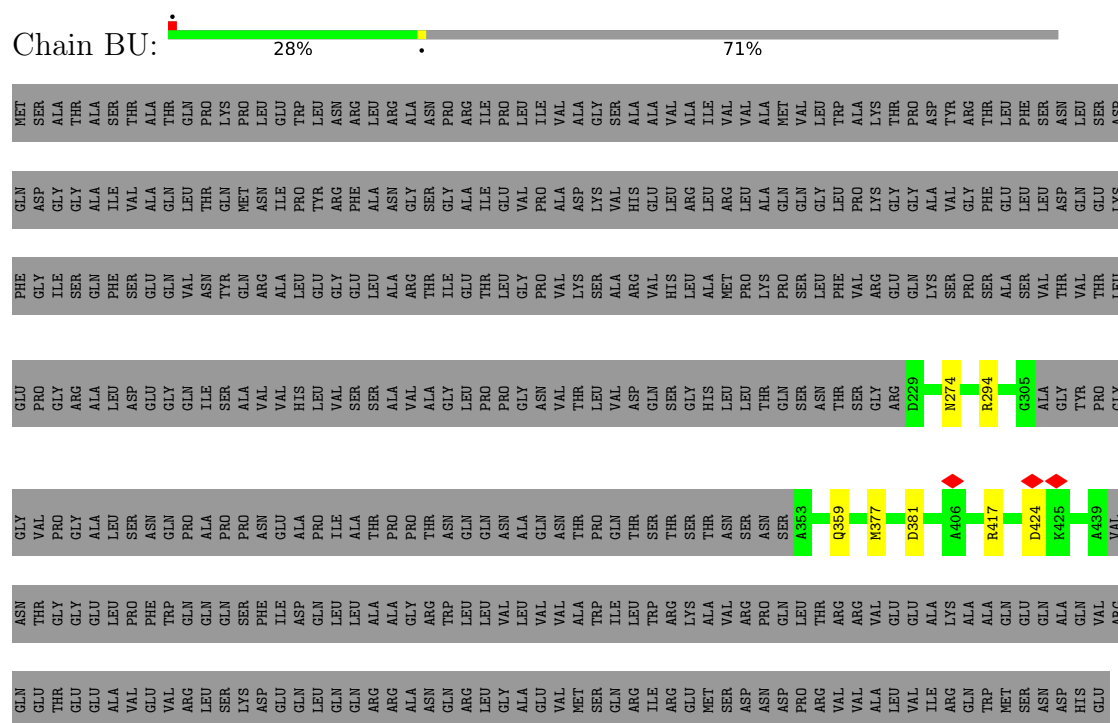
Chain BQ:  96%

ASN	GLN	PHE	MET	SER	VAL	GLU	PHE	GLN	MET
ASP	ALA	SER	ASN	GLU	GLU	GLU	GLU	GLY	GLY
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GLU	VAL	ARG	GLY	VAL	ILE	ARG	GLN	ALA	ALA
	GLN	ASN	ILE	ALA	ALA	GLN	PHE	ILE	SER
	GLU	THR	GLU	GLY	ARG	ASP	SER	VAL	THR
	THR	GLY	ARG	TYR	ARG	GLU	GLU	ALA	ALA
	GLU	GLY	LEU	PRO	ILE	GLY	GLN	GLN	THR
	GLU	GLU	SER	PRO	GLU	GLN	VAL	LEU	LEU
	VAL	VAL	VAL	G311	ALA	ILE	ASN	THR	THR
	ALA	PRO	ALA		ILE	SER	TYR	GLN	PRO
	GLU	PHE	VAL	R318	LEU	ALA	GLN	MET	PRO
	VAL	THR	VAL		SER	VAL	ALA	ILE	LEU
	ARG	GLN	VAL	P331	PRO	PRO	ALA	ALA	THR
	LEU	GLN	ASN	PRO	ILE	HIS	GLY	GLY	TRP
	LEU	GLN	ASN	THR	VAL	GLY	GLU	TYR	ASN
	LYS	SER	LYS	ASN	GLY	VAL	GLY	GLY	ASN
	ASP	PHE	THR	ASN	ASN	SER	GLU	ARG	ARG
	GLU	ILE	LEU	GLN	GLY	GLY	THR	GLY	LEU
	GLN	ASP	ALA	GLN	VAL	VAL	ALA	ALA	THR
	LEU	GLN	GLY	ALA	HIS	HIS	THR	GLY	THR
	GLN	LEU	LYS	GLN	ALA	GLN	ILE	GLY	ASN
	ARG	ALA	PRO	ASN	ALA	LEU	GLU	VAL	GLN
	ARG	ALA	LEU	THR	THR	ASP	THR	VAL	ARG
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	GLU	VAL	LYS	SER	ASN	LYS	VAL	GLY	GLY
	VAL	VAL	ILE	ASN	ASN	GLN	GLN	GLY	GLY
	MET	ALA	ILE	ASN	GLY	SER	HIS	LEU	VAL
	SER	THR	GLU	ALA	GLN	GLY	LEU	ARG	ALA
	GLN	ILE	ASP	GLY	GLU	HIS	THR	LEU	THR
	ARG	THR	THR	ARG	HIS	THR	GLY	GLY	THR
	ILE	TRP	THR	ARG	TYR	GLY	ARG	GLY	THR
	ARG	ARG	ARG	SER	ASN	ASP	GLY	PRO	GLY
	GLU	LYS	GLU	THR	TYR	ALA	GLU	LYS	GLY
	MET	VAL	ALA	GLN	GLN	SER	GLN	GLY	GLY
	ASP	VAL	MET	ARG	PRO	ASN	LEU	LEU	GLY
	ASN	ARG	GLY	ASN	ASN	ASN	THR	VAL	VAL
	ASP	PRO	PHE	GLU	GLY	ASP	ARG	GLY	VAL
	ASP	ASN	SER	THR	ASP	ALA	GLY	GLY	THR
	PRO	LEU	ASN	SER	SER	THR	GLU	GLY	THR
	ARG	THR	LYS	THR	ALA	THR	TYR	GLY	GLY
	VAL	ALA	ALA	GLN	SER	SER	SER	GLN	GLY
	MET	VAL	ALA	GLN	THR	ASP	THR	GLN	GLY
	GLY	VAL	GLN	THR	PHE	GLN	LEU	VAL	ASP
	GLU	ILE	ASP	GLY	GLY	GLN	HIS	ARG	GLY
	ARG	THR	THR	PRO	GLU	GLY	LEU	LEU	GLY
	ILE	TRP	THR	ARG	GLY	GLY	THR	LEU	GLY
	ARG	ARG	ARG	SER	HIS	HIS	THR	ALA	GLY
	GLU	LYS	GLU	THR	TYR	THR	GLN	GLY	GLY
	MET	VAL	ALA	GLN	PRO	LEU	ASP	GLY	GLY
	ASP	VAL	MET	ARG	ASN	SER	ASN	GLY	GLY
	ASN	ARG	MET	ASN	LYS	GLN	GLN	GLY	GLY
	ASP	THR	THR	THR	THR	GLY	GLY	GLY	GLY
	GLU	GLY	ASN	GLU	VAL	VAL	VAL	VAL	GLY
	MET	ILE	ILE	ALA	GLN	GLN	HIS	ALA	GLY
	GLN	THR	THR	GLY	THR	LEU	GLY	GLY	GLY
	ARG	VAL	GLY	GLY	ARG	GLY	GLY	GLY	GLY
	GLY	ARG	ASN	THR	SER	GLY	GLY	GLY	GLY
	THR	ALA	LEU	ARG	ALA	GLY	GLY	GLY	GLY
	ASN	GLU	THR	ASN	THR	GLY	GLY	GLY	GLY
	MET	GLY	GLN	GLU	GLY	GLY	GLY	GLY	GLY

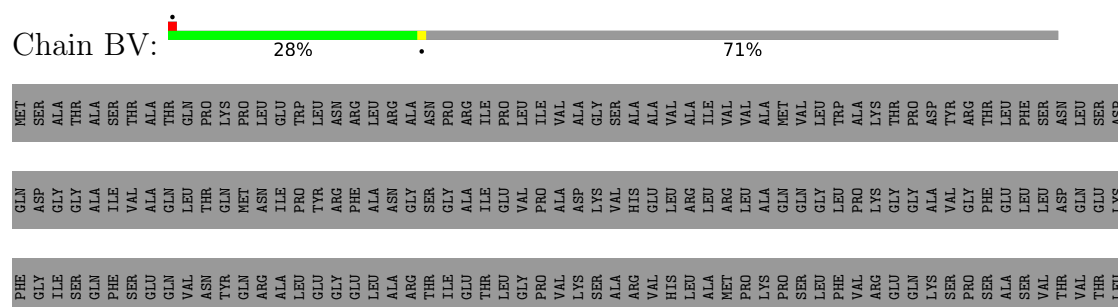


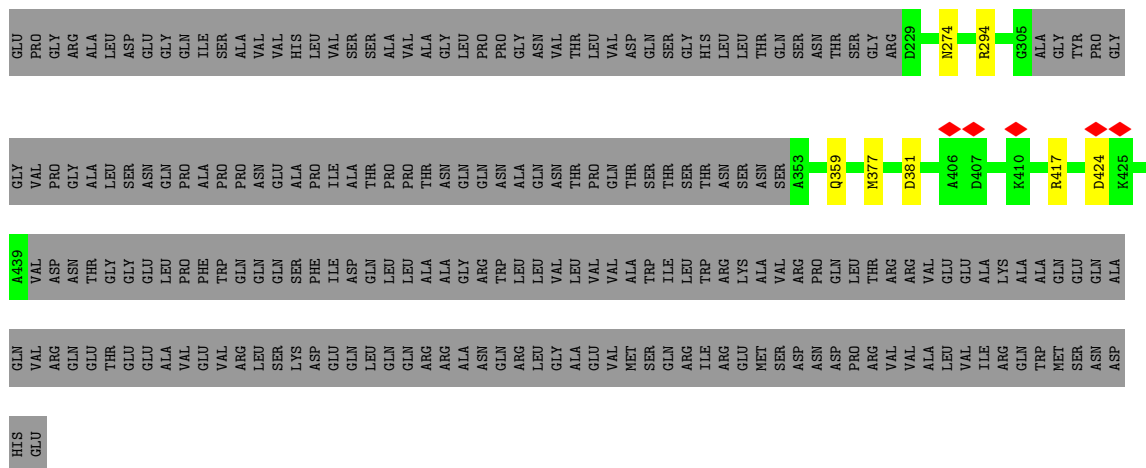


- Molecule 6: Flagellar M-ring protein

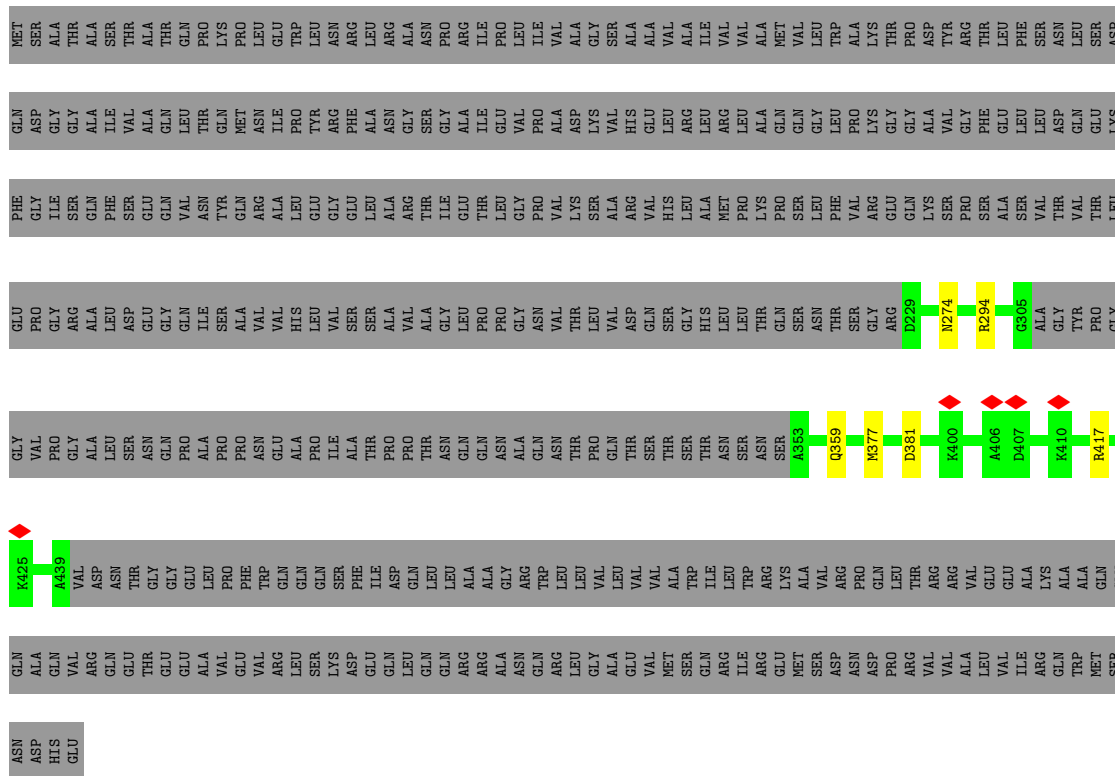


- Molecule 6: Flagellar M-ring protein

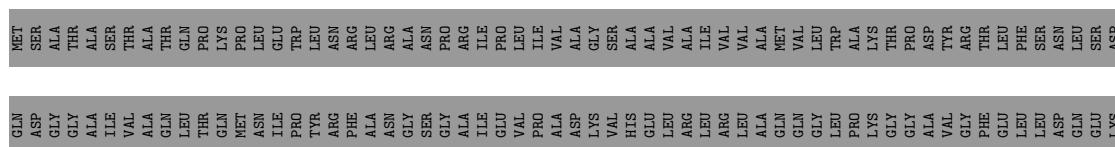




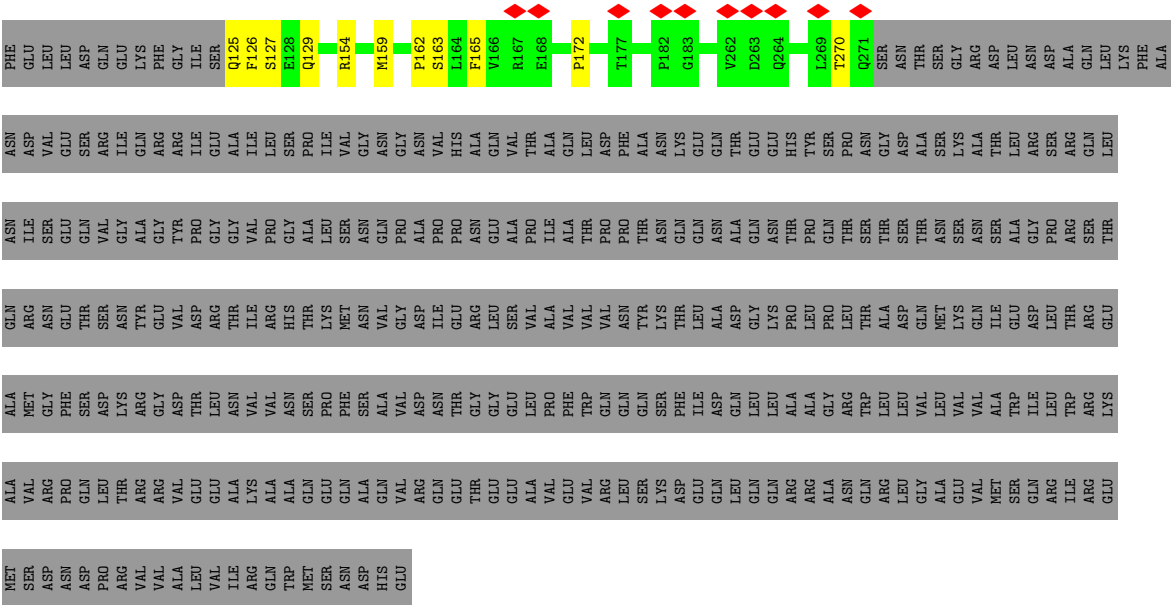
- Molecule 6: Flagellar M-ring protein



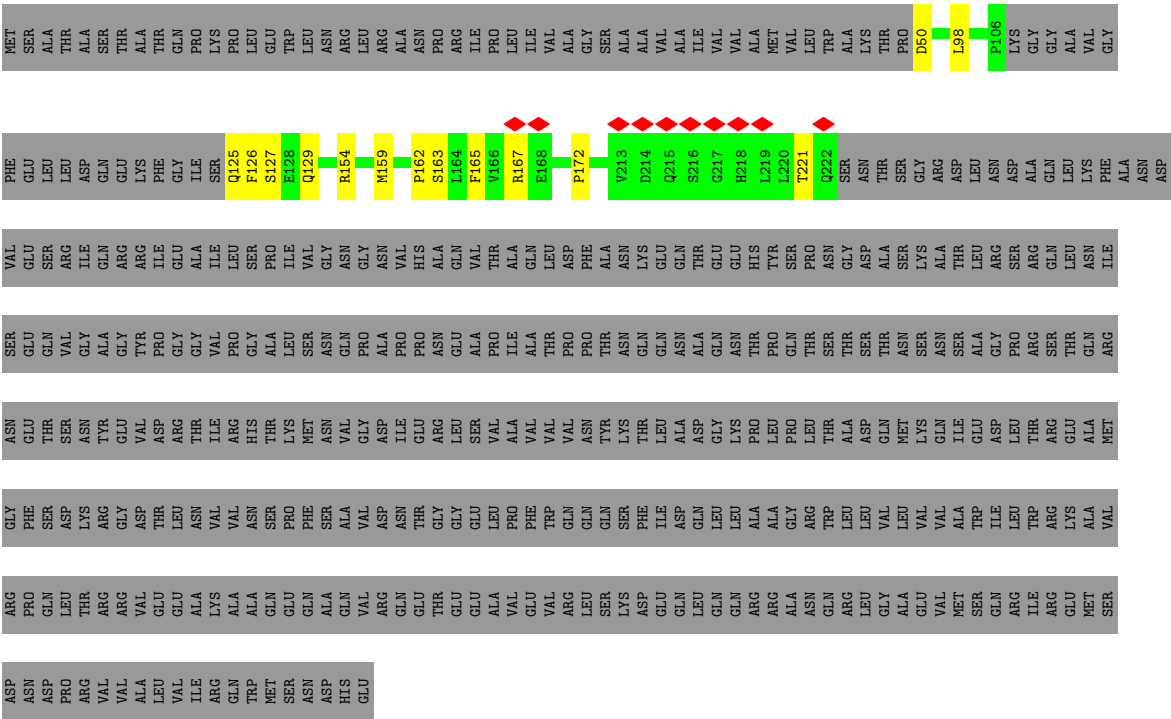
- Molecule 6: Flagellar M-ring protein



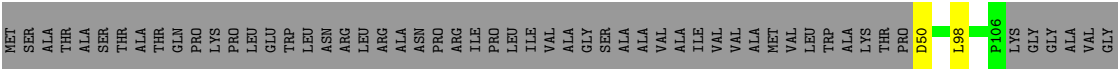




● Molecule 6: Flagellar M-ring protein

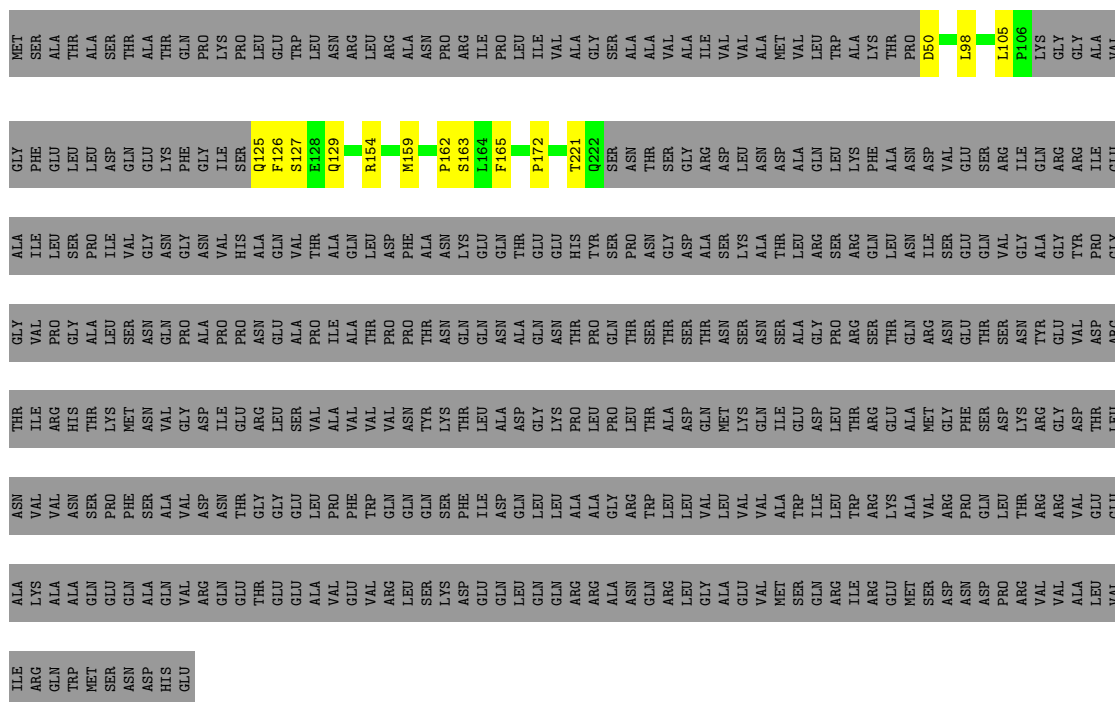


● Molecule 6: Flagellar M-ring protein

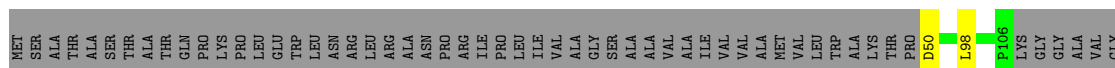


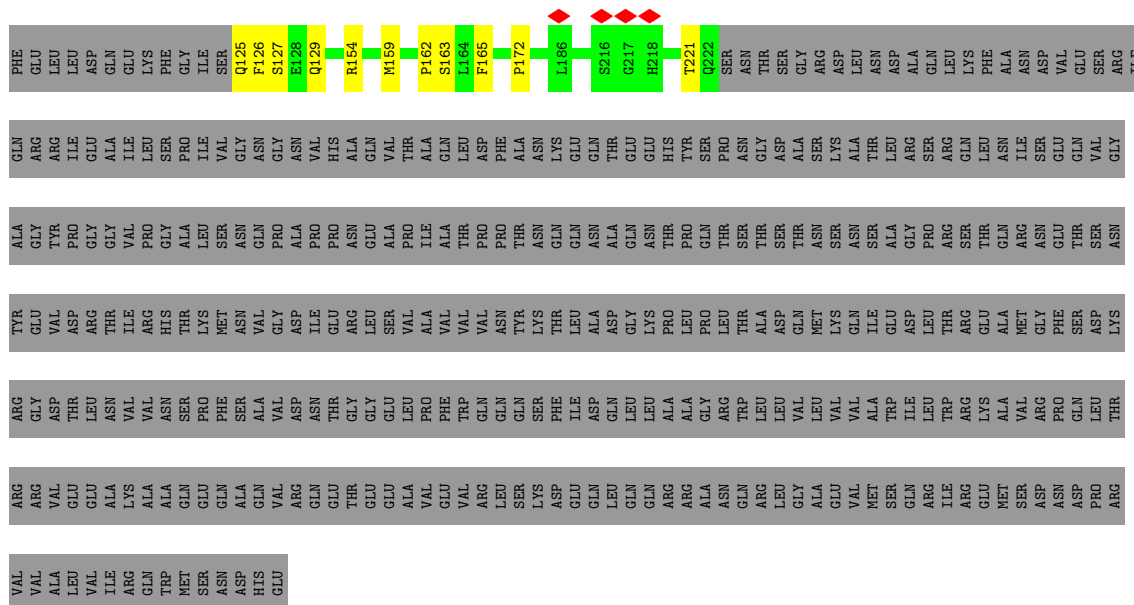


- Molecule 6: Flagellar M-ring protein

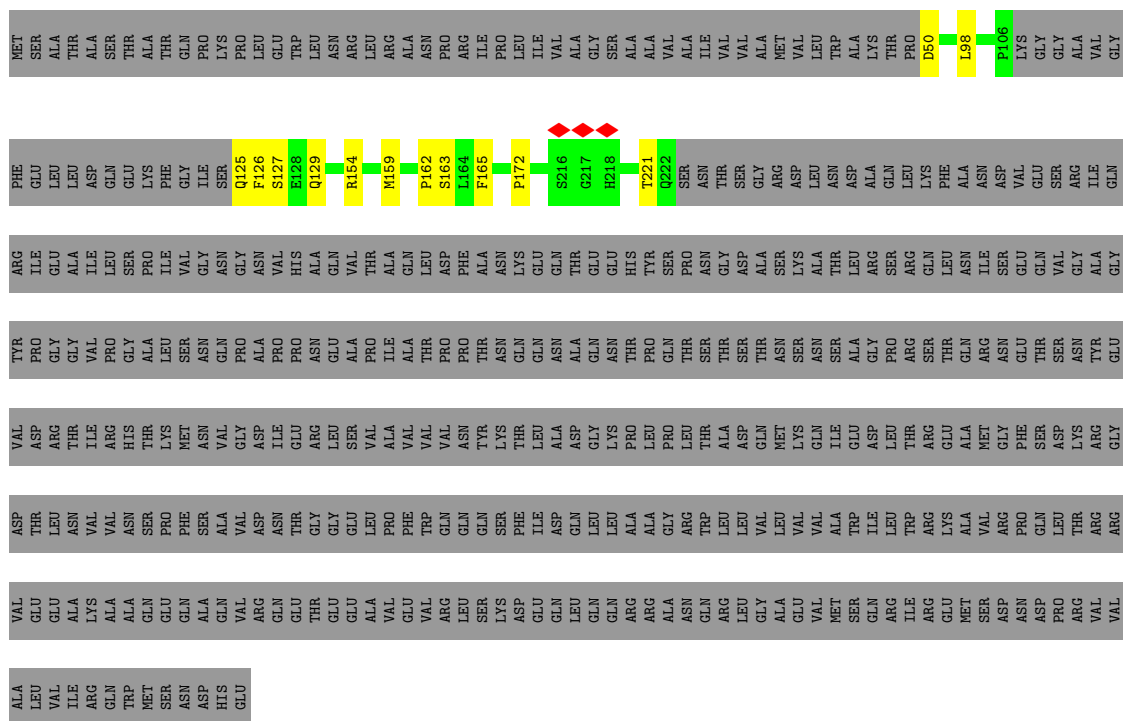


- Molecule 6: Flagellar M-ring protein

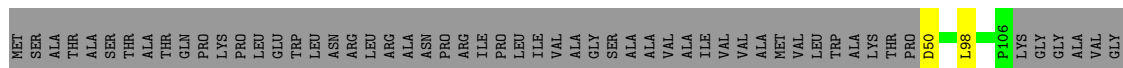


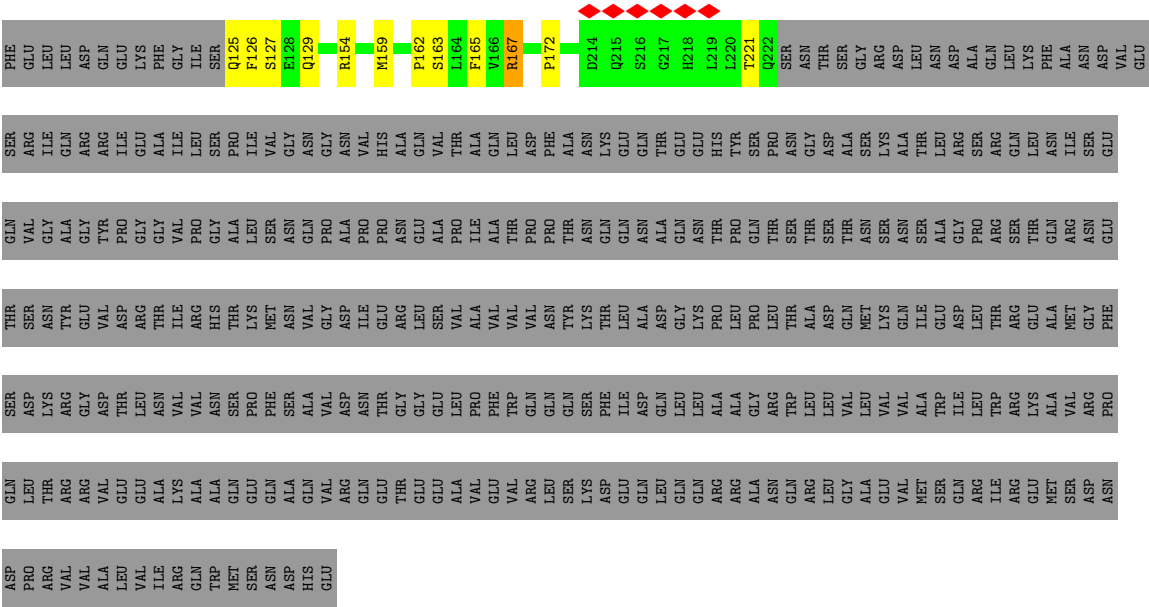


- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein

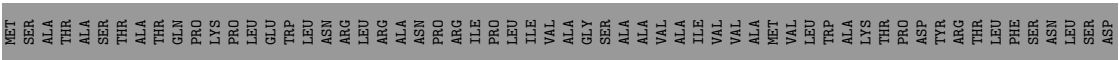




● Molecule 6: Flagellar M-ring protein

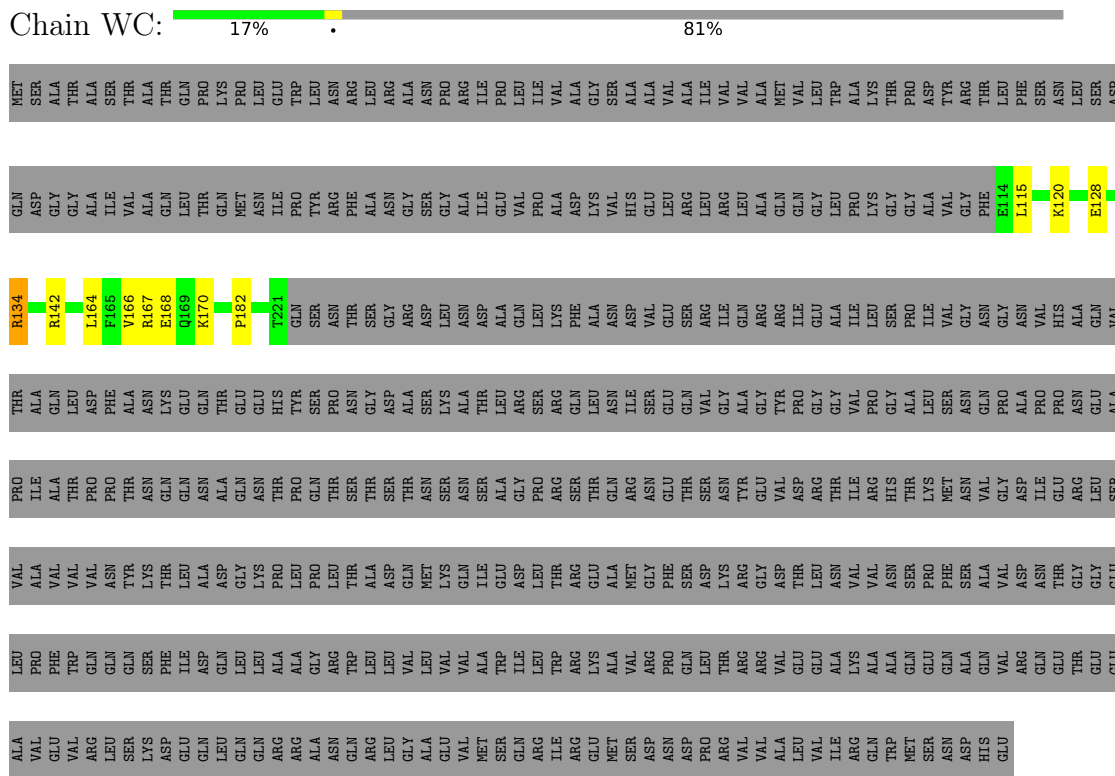


● Molecule 6: Flagellar M-ring protein

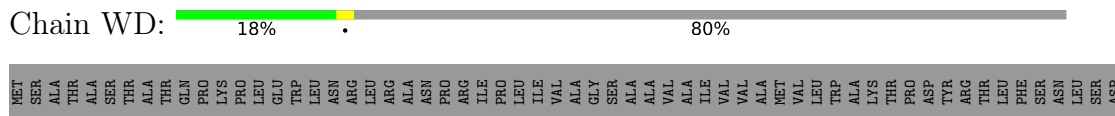


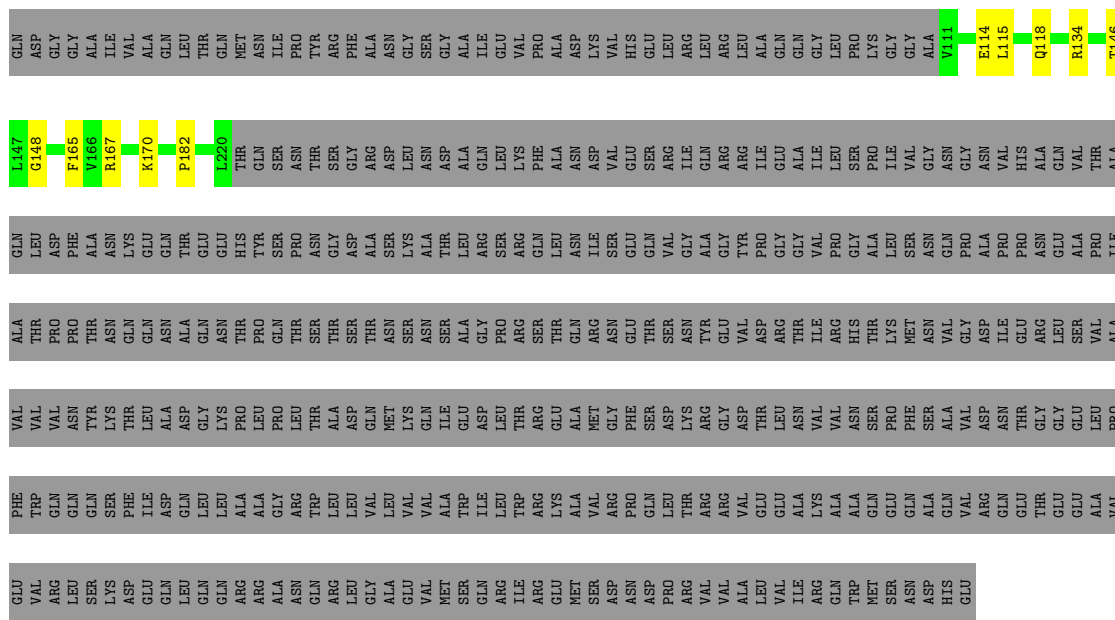


- Molecule 6: Flagellar M-ring protein

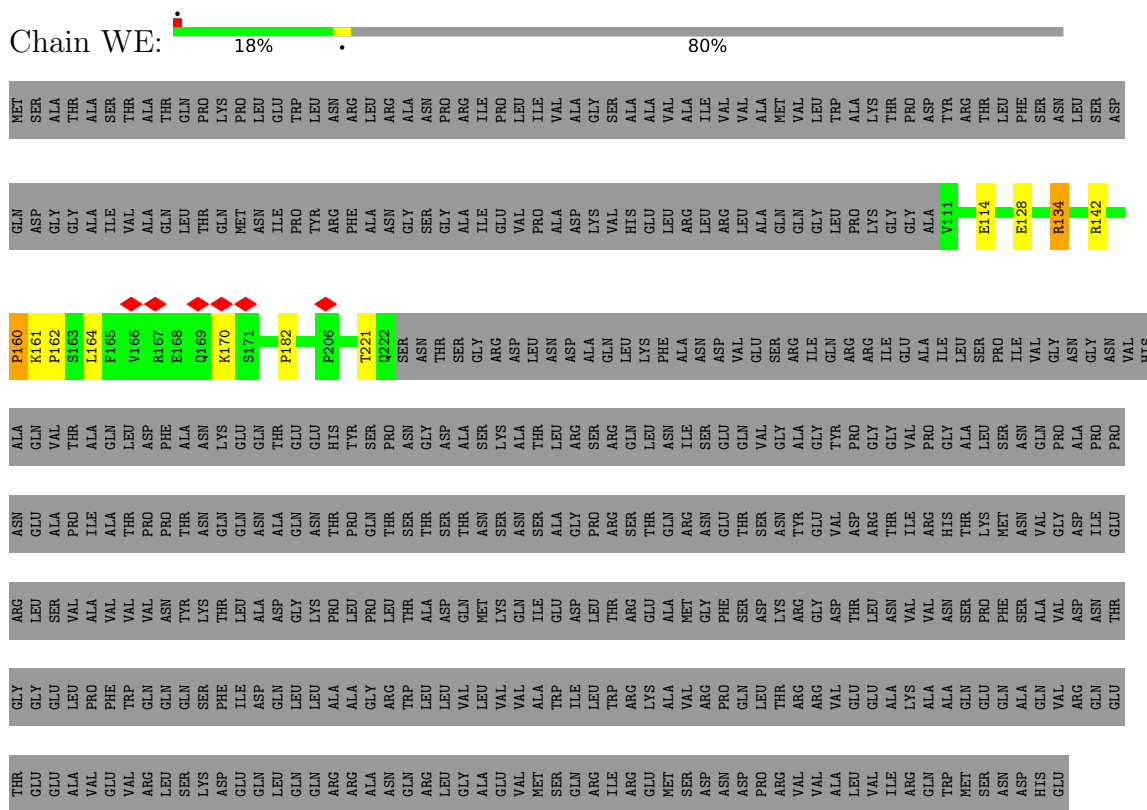


- Molecule 6: Flagellar M-ring protein

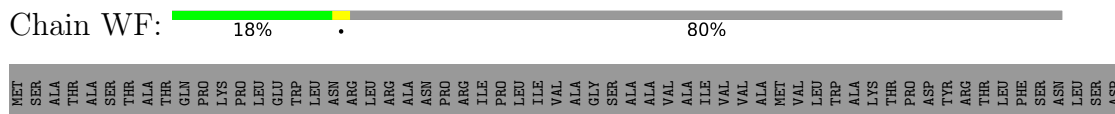


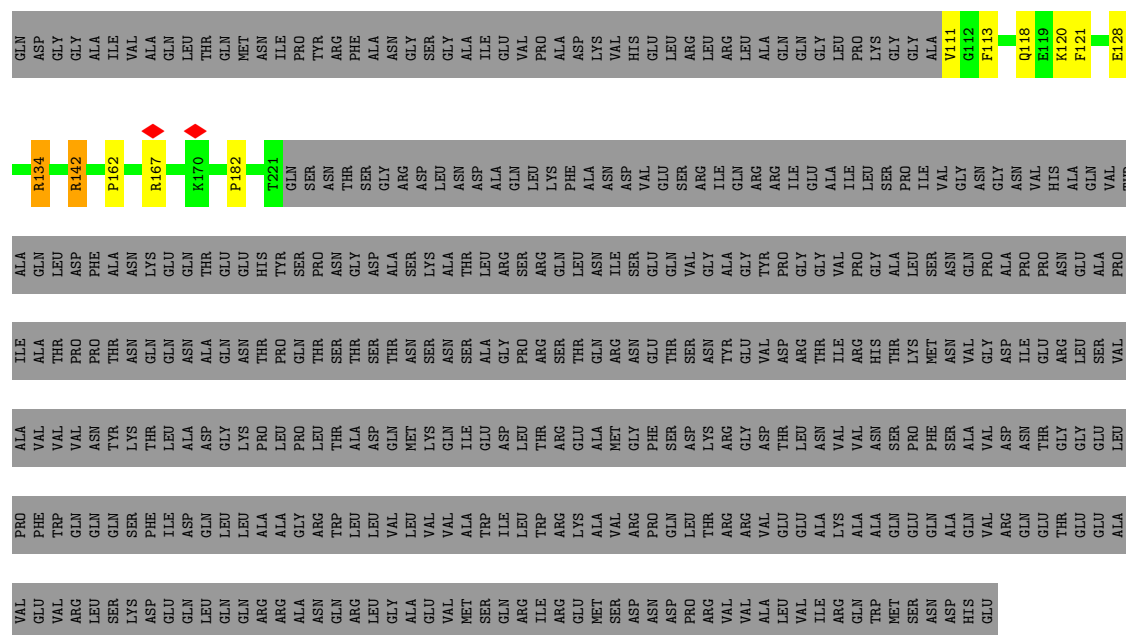


- Molecule 6: Flagellar M-ring protein

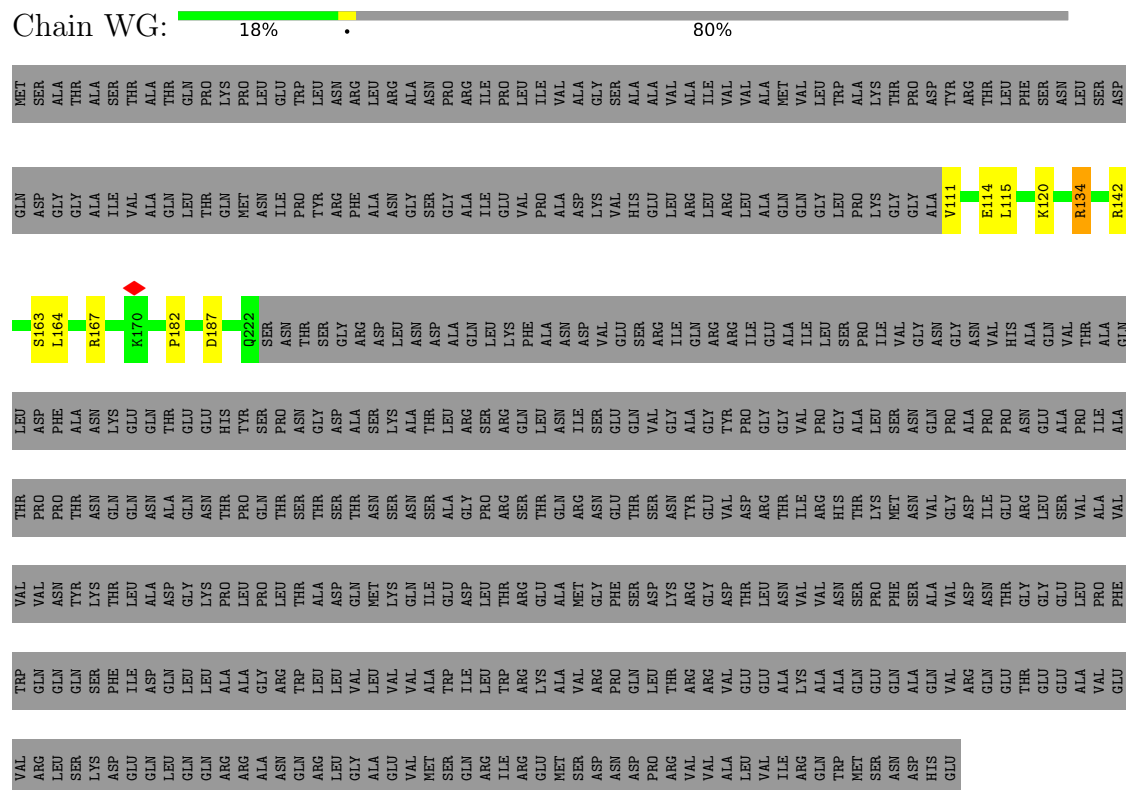


- Molecule 6: Flagellar M-ring protein

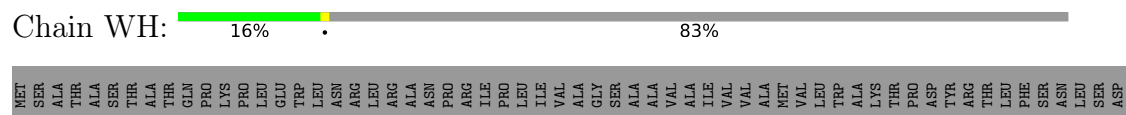


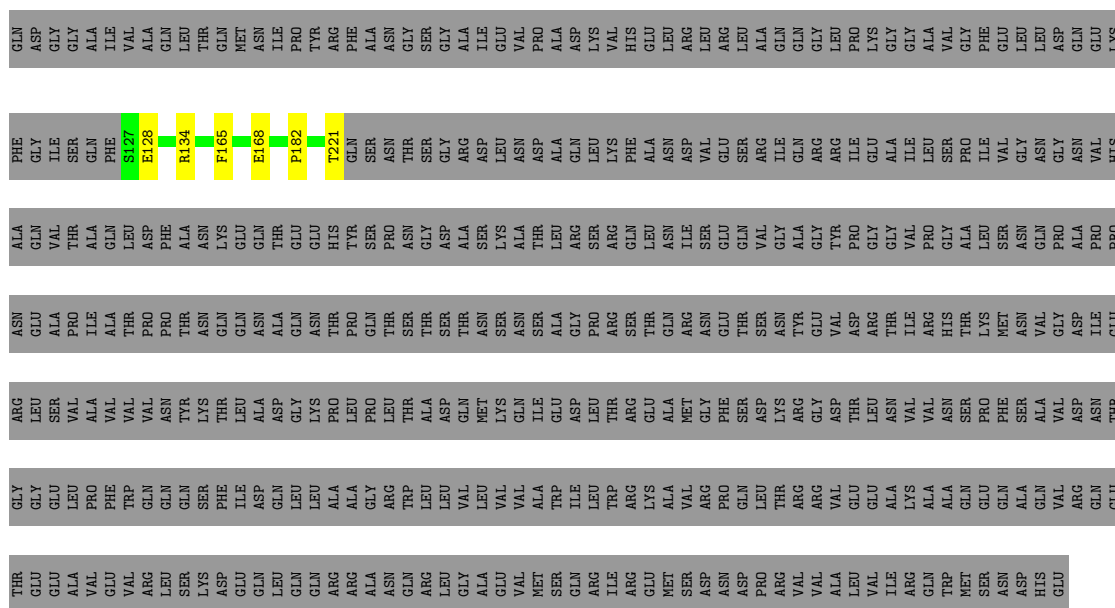


- Molecule 6: Flagellar M-ring protein

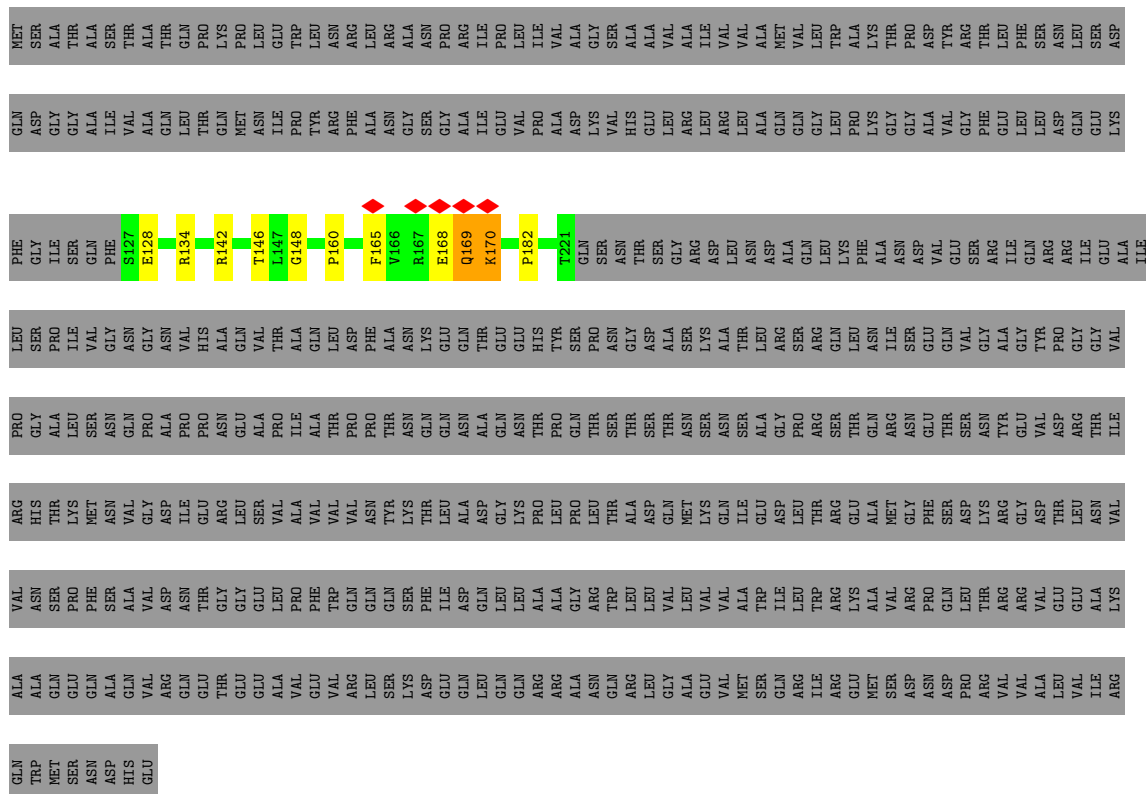


- Molecule 6: Flagellar M-ring protein

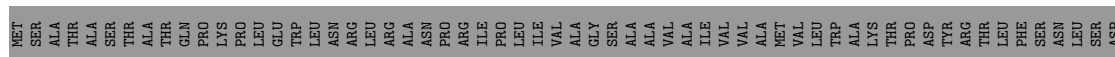




- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein



[illegible]

- Molecule 6: Flagellar M-ring protein

Chain WK:  16% . 82%

[illegible]

- Molecule 6: Flagellar M-ring protein

Chain WL:  14% . 85%

MET	SER	ALA	ALA	THR	THR	SER	THR	ALA	ALA	GLN	PRO	LYS	PRO	LEU	LEU	ASN	ARG	LEU	ALA	ARG	ALA	ASN	PRO	ARG	ILE	PRO	PRO	LEU	ILE	VAL	VAL	ALA	GLY	SER	ALA	ALA	VAL	ALA	VAL	ILE	VAL	VAL	VAL	MET	VAL	VAL	TRP	TRP	ALA	ALA	LYS	THR	PRO	ASP	TYR	ARG	THR	LEU	PHE	SER	ASN	LEU	SER	SEN
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[illegible]

- Molecule 6: Flagellar M-ring protein

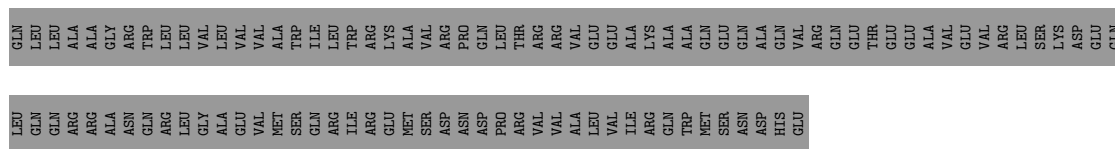
Chain WT:  17% 80%

[illegible]

- Molecule 6: Flagellar M-ring protein

Chain WU:  19% 80%

[illegible]



- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein



[illegible]

- Molecule 6: Flagellar M-ring protein

Chain DE: 

[illegible]

- Molecule 6: Flagellar M-ring protein

Chain DL:  5% 95%

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

ARG	PRO	GLN	GLN	LEU	THR	ARG	ARG	VAL	GLU	GLU	GLY	ALA	LYS	ALA	ALA	GLN	GLN	GLN	GLN	ALA	GLN	GLY	VAL	VAL	GLU	VAL	ARG	ARG	VAL	LEU	SER	LYS	ASP	GLU	GLN	GLN	LEU	GLN	GLN	GLN	ARG	ARG	ALA	ASN	GLN	GLN	ARG	LEU	GLY	ALA	GLU	VAL	M532	D568	HIS	TIT
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- Chain B0:  5% 95%

G O U N N U R R G G L L U U U A A S S A A N N U N U A A L L G G N N U R R U U U A A L L U U L L L L G G G U U R R S S P P U U N U N N N N G G G A A N N N N G U Y Y A A U L L L L L

- Chain B3: 

VAL	GLU	SER	ARG	ILE	GLN	ARG	ARG	ILE	GLU	ALA	ALA	LEU	SER	PRO	ILE	VAL	GLY	ASN	GLY	ASN	VAL	HIS	ALA	GLN	VAL	THR	ALA	GLN	GLN	LEU	ASP	PHE	ALA	ASN	LYS	GLU	GLN	THR	GLU	GLU	GLY	TYP	SER	PRO	ASN	ASP	ALA	SER	LYS	ALA	THR	ARG	SER	GLN	LEU	ASN	TYR
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ARG	GLY	ASN	SER	VAL	GLU
PRO	PHE	GLN	GLU	GLU	PRO
GLN	SER	THR	GLY	SER	GLY
LEU	ASP	SER	VAL	GLY	ARG
THR	LYS	ASN	GLY	ILE	ALA
ARG	ARG	TYR	ALA	GLN	LEU
ARG	GLY	GLU	GLY	ARG	ASP
VAL	ASP	VAL	TYR	GLU	GLU
GLU	THR	ASP	PRO	ILE	GLY
GLU	THR	ARG	GLY	GLN	GLN
ALA	ASN	THR	VAL	ALA	ILE
LYS	VAL	ILE	VAL	ILE	SER
ALA	VAL	ARG	PRO	LEU	ALA
ALA	ASN	HIS	GLY	SER	VAL
GLN	SER	THR	ALA	PRO	VAL
GLU	PRO	LYS	LEU	ILE	HIS
GLN	PHE	MET	SER	VAL	LEU
ALA	SER	ASN	ASN	GLY	VAL
GLN	ALA	VAL	GLN	ASN	SER
VAL	VAL	GLY	PRO	GLY	SER
ASP	ASP	ASP	ALA	ASN	ALA
GLN	ASN	ILE	PRO	VAL	VAL
GLU	THR	GLU	PRO	HIS	ALA
THR	GLY	ARG	ASN	ALA	GLY
GLU	GLY	LEU	GLU	GLN	LEU
GLU	GLU	SER	ALA	VAL	PRO
ALA	LEU	VAL	ALA	ALA	GLY
VAL	PHE	VAL	ALA	GLN	ASN
VAL	TRP	VAL	THR	LEU	VAL
ARG	GLN	VAL	PRO	ASP	THR
LEU	GLN	ASN	PRO	PHE	LEU
SER	GLN	ASN	THR	ALA	VAL
LYS	SER	LYS	ASN	ASN	ASN
ASP	PHE	THR	GLN	LYS	GLN
GLU	ILE	LEU	ASN	GLU	SER
GLN	GLN	ALA	GLN	GLY	GLY
GLN	GLN	ASP	ALA	THR	HIS
GLN	LEU	GLY	GLN	GLU	LEU
GLN	LEU	LYS	ASN	GLU	LEU
ARG	ALA	PRO	THR	HIS	THR
ARG	ALA	LEU	PRO	TYR	GLN
ALA	GLY	PRO	SER	SER	GLN
ASN	ARG	LEU	THR	PRO	ASN
GLN	TRP	GLN	SER	ASN	THR
ARG	LEU	ALA	THR	GLY	SER
LEU	LEU	ASP	SER	ASP	GLY
GLY	VAL	GLN	THR	ALA	ARG
ALA	LEU	MET	ASN	SER	ASP
GLU	VAL	LYS	SER	LYS	ASP
M532	VAL	GLN	ASN	ALA	ASN
I558	VAL	ILE	SER	ASP	ASN
	TRP	GLU	ALA	LEU	ALA
	ILE	ASP	GLY	ARG	ALA
HIS	TRP	LEU	PRO	SER	GLN
GLU	TRP	THR	ARG	GLY	GLN
	LYS	GLU	SER	LEU	ASN
	ARG	THR	THR	ALA	PHE
	VAL	MET	GLN	ASN	LYS
	VAL	THR	ARG	ILE	ASN

- Molecule 6: Flagellar M-ring protein

Chain Bh:  5% 95%

[illegible]

- Molecule 6: Flagellar M-ring protein

Chain Bo:  5% 95%

[illegible]

- Molecule 6: Flagellar M-ring protein

Chain Bv:  5% 95%

[illegible]

- Molecule 6: Flagellar M-ring protein

Chain Ea:  5% 95%

[illegible]

- Molecule 6: Flagellar M-ring protein

Chain CG: 

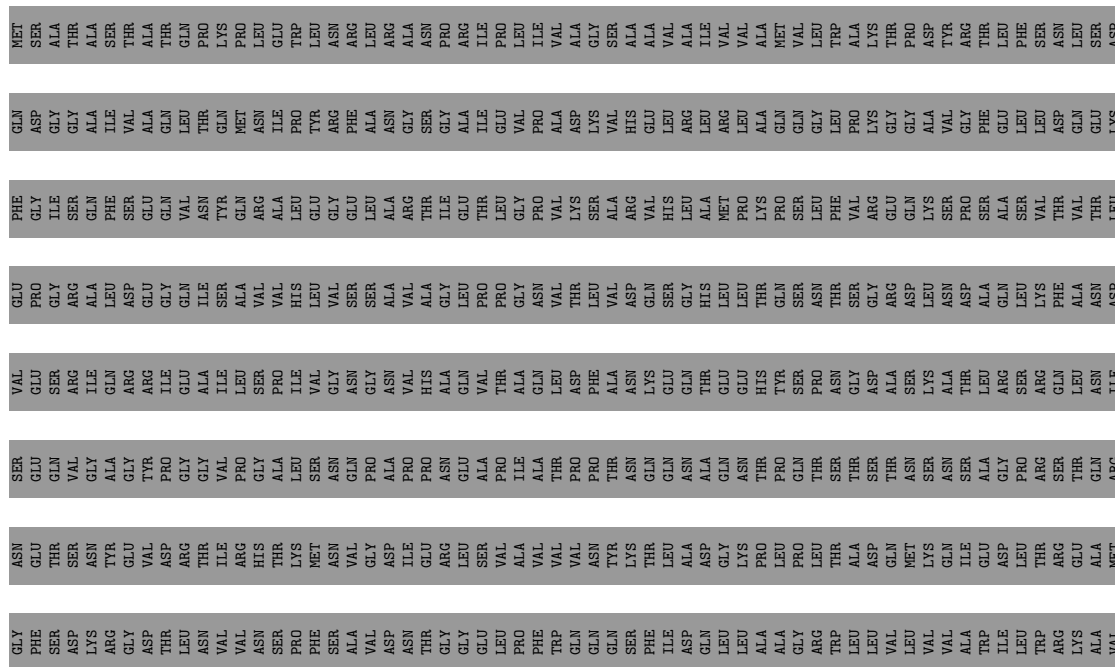
[illegible]

- Molecule 6: Flagellar M-ring protein

Chain CN:  5% 95%



- Molecule 6: Flagellar M-ring protein









	ARG	PRO	GLN	LEU	THR	ARG	ARG	VAL	GLU	GLY	GLN	ALA	LYS	ALA	ALA	GLN	GLU	GLN	GLN	ALA	GLN	VAL	ARG	ASP	LYS	GLY	GLN	GLN	GLN	GLN	ARG	ALA	ASN	GLN	ARG	LEU	SER	THR	GLY	GLU	ALA	VAL	VAL	GLY	GLU	VAL	M632	D568	HIS	TIT
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Chain Ed:  5% 95%

G O U N U N U R R G G L L U U U U A A S S A A N N U N U N A A L L G G N N U R R U U U A A L L U U L L L L G G U U U R R S S P P U U U N U N U N N N G G G G A A A N N N G U U Y Y A A U U L L L L

Chain Ee: 

[illegible]





ARG	GLY	ASN	SER	VAL	GLU	PRO
PRO	PHE	GLN	THR	GLU	GLY	GLY
GLN	SER	THR	GLN	VAL	SER	ARG
LEU	ASP	ASN	GLY	ILE	ALA	LEU
THR	ARG	THR	ALA	GLY	ARG	ASP
ARG	GLY	GLU	GLY	THR	GLU	GLY
VAL	ASP	VAL	VAL	TYR	ARG	GLY
GLU	THR	ASP	GLY	GLY	ILE	GLY
GLU	LEU	ARG	PRO	GLN	GLN	ILE
ALA	ASN	THR	VAL	GLY	ALA	SER
ALA	VAL	ILE	VAL	ILE	SER	ALA
ALA	VAL	ARG	PRO	LEU	ALA	ALA
ALA	ASN	HIS	GLY	SER	VAL	VAL
GLN	SER	THR	ALA	VAL	PRO	VAL
GLU	PRO	LYS	LEU	ILE	HIS	HIS
GLN	PHE	MET	SER	VAL	LEU	VAL
GLN	SER	ASN	ASN	GLY	VAL	SER
ALA	ALA	VAL	GLN	ASN	SER	SER
GLN	VAL	GLY	PRO	GLY	GLY	SER
ARG	ASP	ASP	ALA	ASN	VAL	VAL
GLN	ASN	ILE	PRO	VAL	VAL	ALA
GLU	THR	GLU	PRO	HIS	ALA	ALA
THR	GLY	ARG	GLU	ASN	GLY	GLY
GLU	GLY	LEU	GLU	GLN	LEU	LEU
GLU	GLU	SER	SER	ALA	PRO	PRO
ALA	LEU	VAL	ALA	ILE	LEU	THR
VAL	PHE	VAL	ALA	THR	LEU	VAL
VAL	TRP	VAL	THR	LEU	ASP	THR
ARG	GLN	VAL	PRO	PRO	ASP	THR
LEU	GLN	ASN	PRO	ALA	GLN	GLN
SER	GLN	ASN	PRO	PHE	LEU	THR
LYS	LYS	TYR	THR	ALA	GLY	GLN
ASP	PHE	THR	GLN	LYS	GLY	SER
GLU	ILE	LEU	ASN	GLN	GLN	HIS
GLN	GLN	ASP	ALA	GLN	GLU	LEU
ARG	ALA	PRO	THR	ASN	GLU	THR
ARG	ALA	LEU	PRO	TYR	THR	GLN
ALA	GLY	PRO	GLN	SER	SER	ASN
ASN	ARG	LEU	THR	PRO	THR	THR
GLN	TRP	ALA	ALA	GLY	GLY	GLY
ARG	LEU	ASP	SER	ASP	ALA	ARG
GLY	VAL	GLN	THR	THR	SER	GLY
ALA	LEU	MET	ASN	SER	ASP	GLY
GLU	VAL	LYS	SER	SER	ASP	ARG
GLU	VAL	GLN	LYS	LEU	ASP	ASP
VAL	VAL	ILE	ASN	ALA	LEU	ASN
M532	TRP	ALA	SER	THR	ASP	ASN
I558	ALA	GLU	GLY	ALA	LEU	ALA
	TRP	ILE	ASP	ALA	THR	ALA
HIS	GLU	THR	PRO	GLY	ARG	GLN
GLU	TRP	LEU	ALA	SER	THR	GLN
	LYS	ARG	SER	LEU	GLN	LYS
	ARG	GLU	SER	ALA	THR	PHE
	VAL	MET	ASN	THR	GLN	ALA
	VAL	THR	GLN	ILE	ASN	ASN

- Molecule 6: Flagellar M-ring protein

Chain Ej:  5% 95%

[illegible]

- Molecule 6: Flagellar M-ring protein

Chain Ek:  5%  95%

[illegible]

- Molecule 6: Flagellar M-ring protein

Chain El:  5% 95%

- Molecule 6: Flagellar M-ring protein

Chain Em:  5% 95%

MET	SER	ALA	ALA	ALA	SER	THR	ALA	ALA	GLN	PRO	PRO	LYS	LEU	GLY	TRP	LEU	ASN	ARG	LEU	ALA	ARG	ALA	ASN	PRO	ARG	ILE	PRO	PRO	LEU	ILE	VAL	ALA	GLY	SER	ALA	ALA	VAL	VAL	ALA	ALA	VAL	MET	VAL	LEU	LEU	TRP	ALA	ALA	LYS	THR	PRO	ASP	TYR	ARG	THR	LEU	PHE	SER	ASN	LEU	SER	SER	
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- Molecule 6: Flagellar M-ring protein

Chain En:  5% 95%

[illegible]

- Molecule 6: Flagellar M-ring protein

Chain Eo:  5% 95%





Chain Ab:  99%



- Molecule 7: Flagellar biosynthetic protein FliQ

Chain Aq:  99%



- Molecule 7: Flagellar biosynthetic protein FliQ

Chain Ar:  100%


There are no outlier residues recorded for this chain.

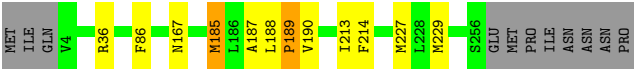
- Molecule 7: Flagellar biosynthetic protein FliQ

Chain As:  99%




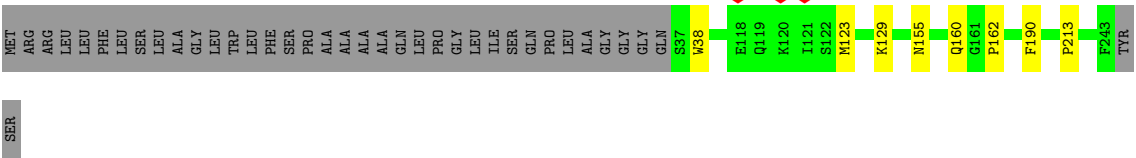
- Molecule 8: Flagellar biosynthetic protein FliR

Chain At:  91%




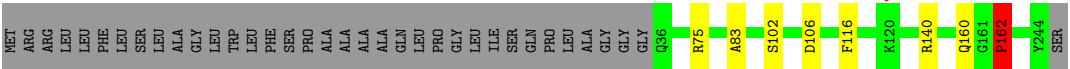
- Molecule 9: Flagellar biosynthetic protein FliP

Chain Au:  81%




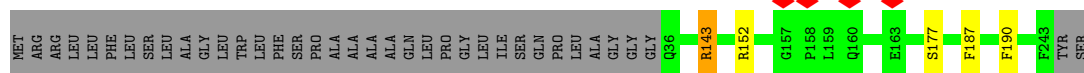
- Molecule 9: Flagellar biosynthetic protein FliP

Chain Av:  82%




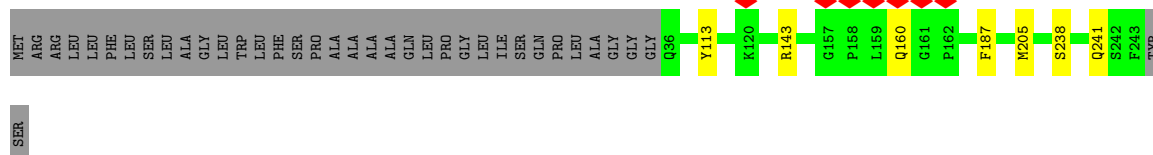
- Molecule 9: Flagellar biosynthetic protein FlpP

Chain Aw:  83% 15%




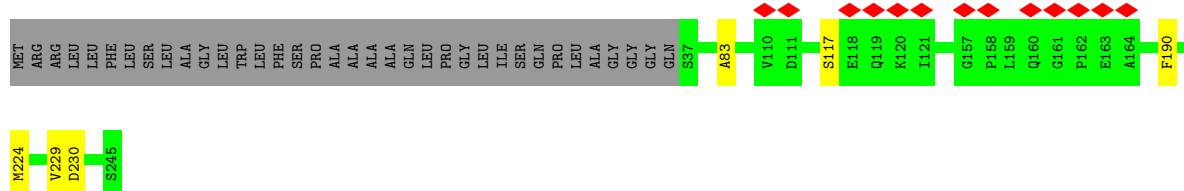
- Molecule 9: Flagellar biosynthetic protein FlpP

Chain Ax:  82% 15%



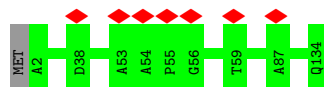
- Molecule 9: Flagellar biosynthetic protein FlpP

Chain Ay:  5% 83% 15%



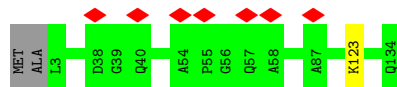
- Molecule 10: Flagellar basal-body rod protein FlgC

Chain BA:  5% 99%



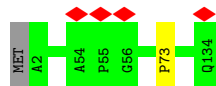
- Molecule 10: Flagellar basal-body rod protein FlgC

Chain BB:  5% 98%



- Molecule 10: Flagellar basal-body rod protein FlgC

Chain BC:  99%



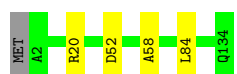
- Molecule 10: Flagellar basal-body rod protein FlgC

Chain BD:  96%



- Molecule 10: Flagellar basal-body rod protein FlgC

Chain BE:  96%



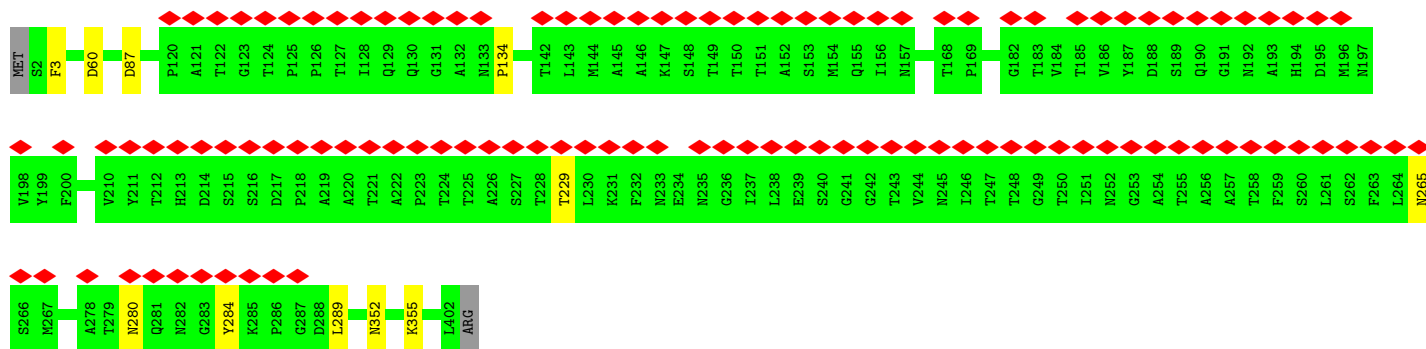
- Molecule 10: Flagellar basal-body rod protein FlgC

Chain BF:  96%



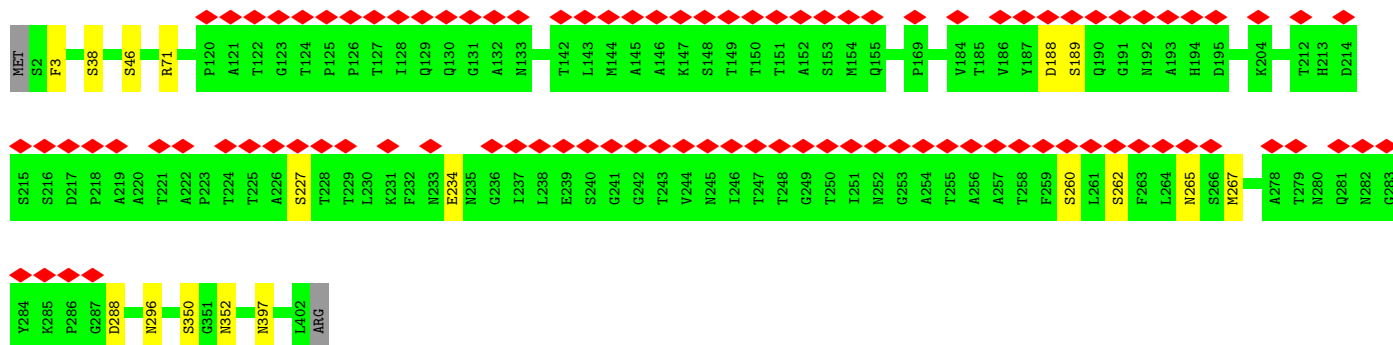
- Molecule 11: Flagellar hook protein FlgE

Chain ZF:  28% 97%

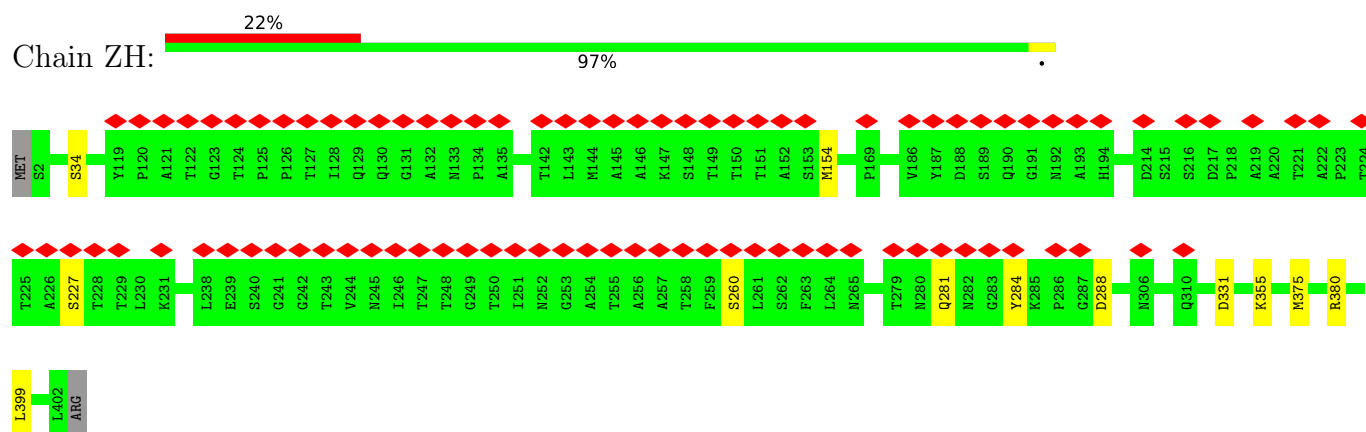


- Molecule 11: Flagellar hook protein FlgE

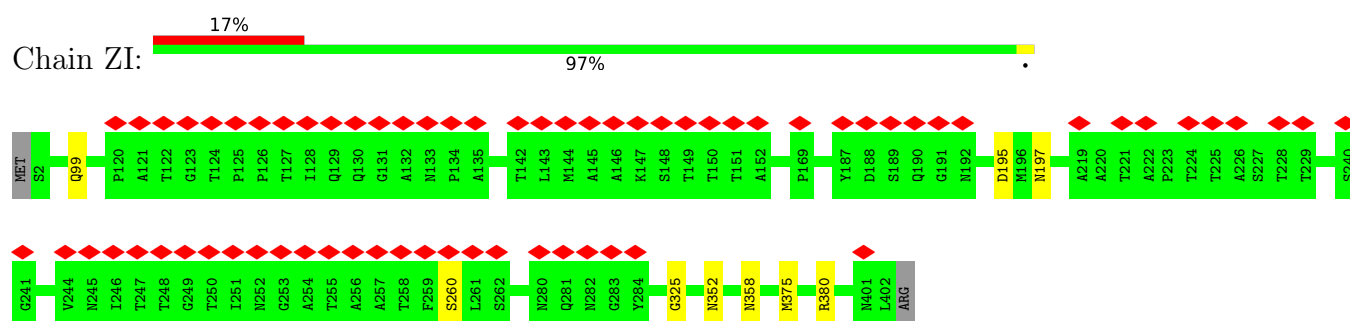
Chain ZG:  24% 95%



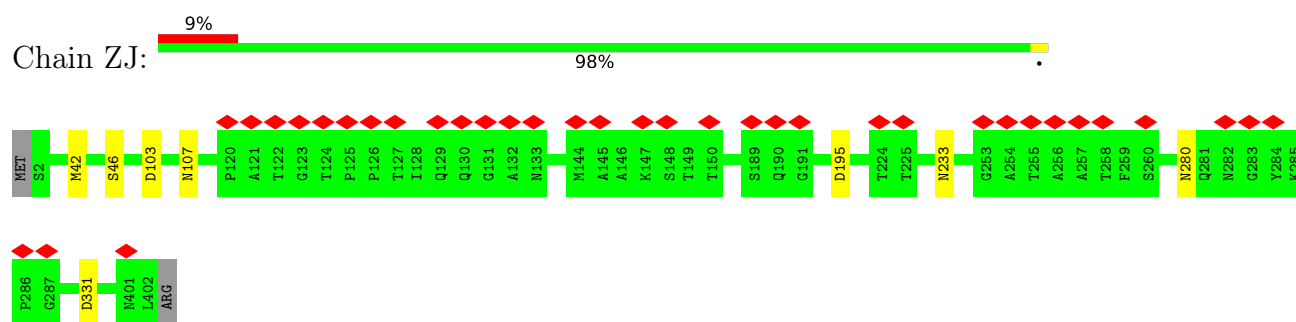
## ● Molecule 11: Flagellar hook protein FlgE



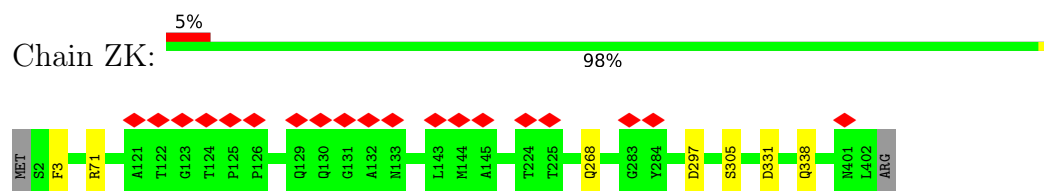
## ● Molecule 11: Flagellar hook protein FlgE



## ● Molecule 11: Flagellar hook protein FlgE

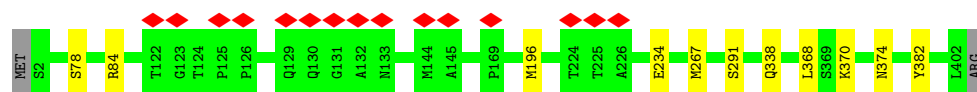


## ● Molecule 11: Flagellar hook protein FlgE



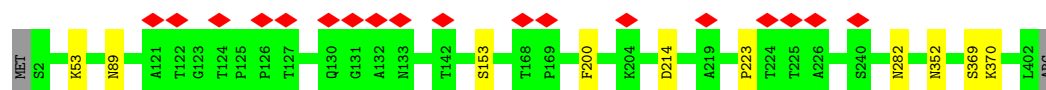
## ● Molecule 11: Flagellar hook protein FlgE





- Molecule 11: Flagellar hook protein FlgE

Chain ZM: 97%



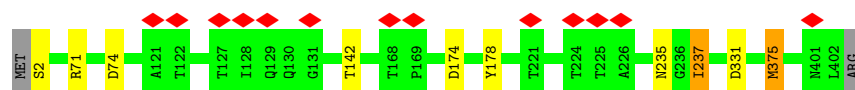
- Molecule 11: Flagellar hook protein FlgE

Chain ZN: 97%



- Molecule 11: Flagellar hook protein FlgE

Chain ZO: 97%



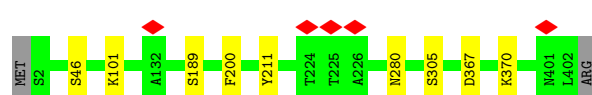
- Molecule 11: Flagellar hook protein FlgE

Chain ZP: 95%



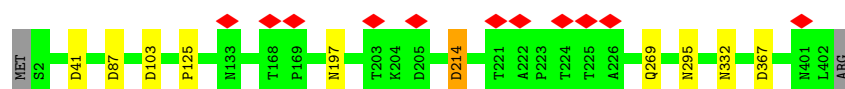
- Molecule 11: Flagellar hook protein FlgE

Chain ZQ: 97%



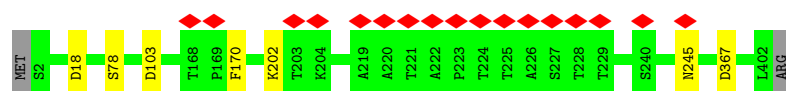
- Molecule 11: Flagellar hook protein FlgE

Chain ZR: 97%



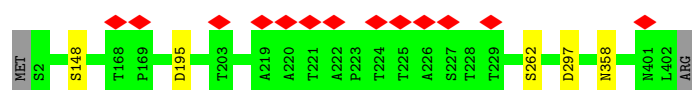
- Molecule 11: Flagellar hook protein FlgE

Chain ZS:  98%



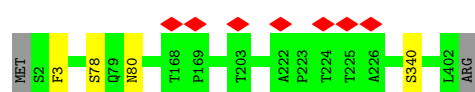
- Molecule 11: Flagellar hook protein FlgE

Chain ZT:  98%



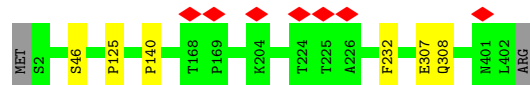
- Molecule 11: Flagellar hook protein FlgE

Chain ZU:  99%



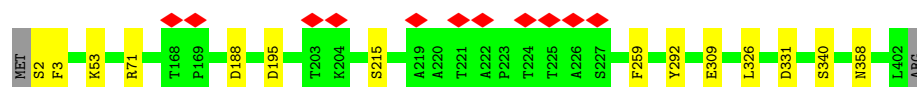
- Molecule 11: Flagellar hook protein FlgE

Chain ZV:  98%



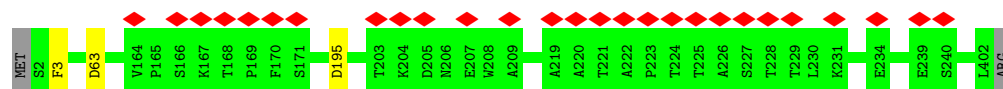
- Molecule 11: Flagellar hook protein FlgE

Chain ZW:  96%



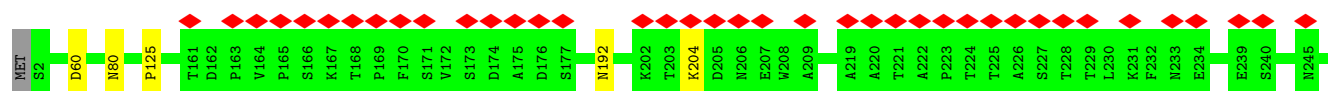
- Molecule 11: Flagellar hook protein FlgE

Chain ZX:  7% 99%



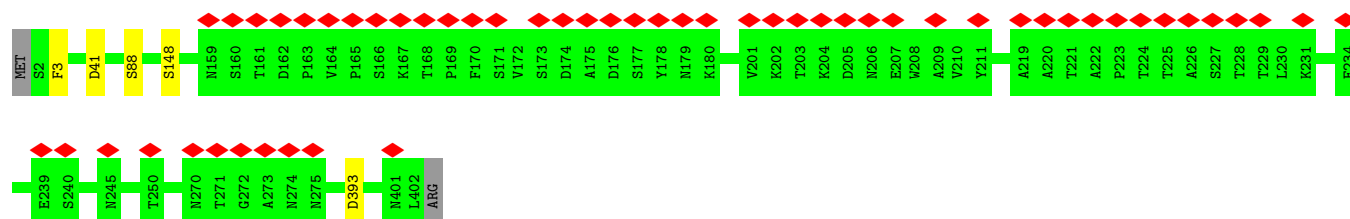
- Molecule 11: Flagellar hook protein FlgE

Chain ZY:  10% 98%

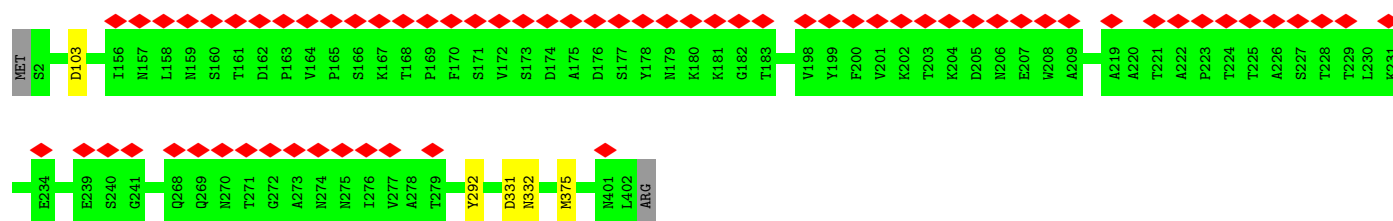




- Molecule 11: Flagellar hook protein FlgE



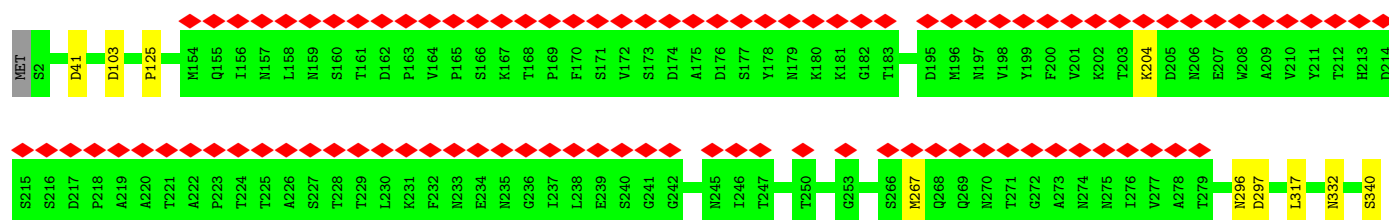
- Molecule 11: Flagellar hook protein FlgE



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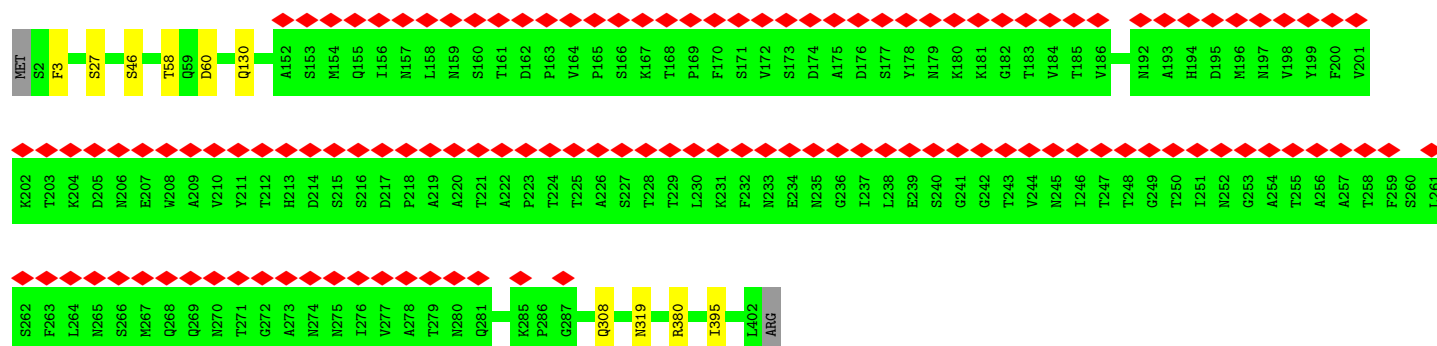




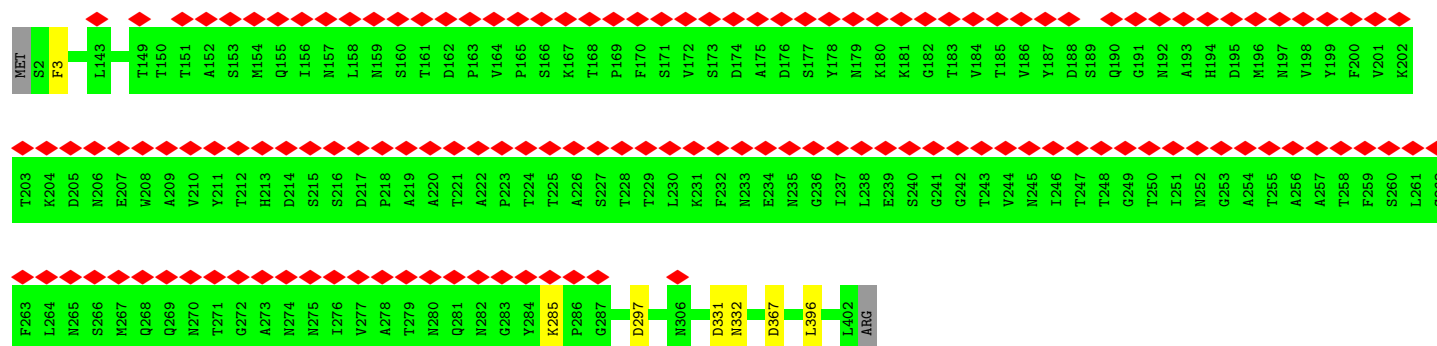
• Molecule 11: Flagellar hook protein FlgE



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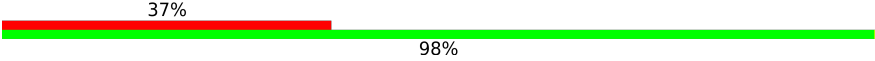


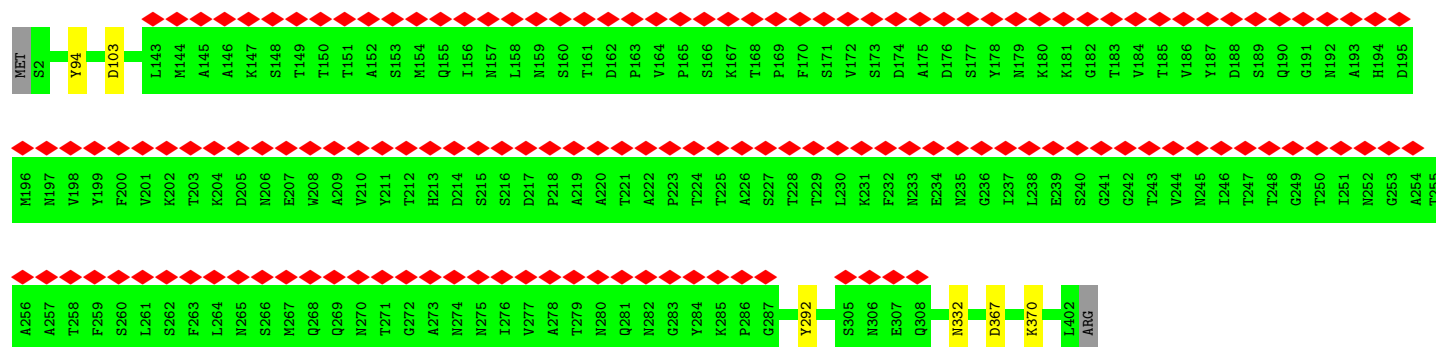
• Molecule 11: Flagellar hook protein FlgE



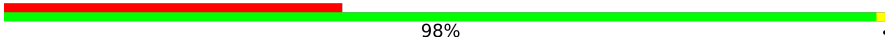
• Molecule 11: Flagellar hook protein FlgE

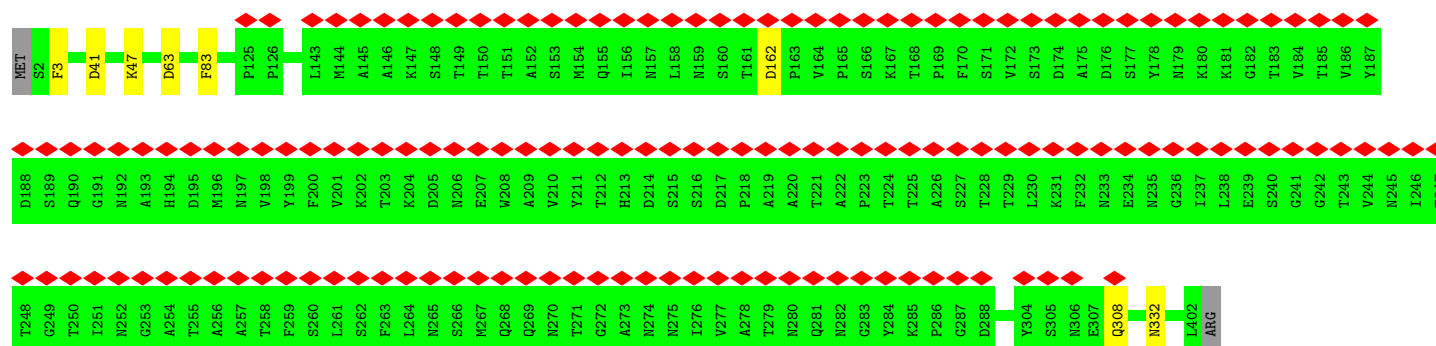


Chain Zg:  37% 98%




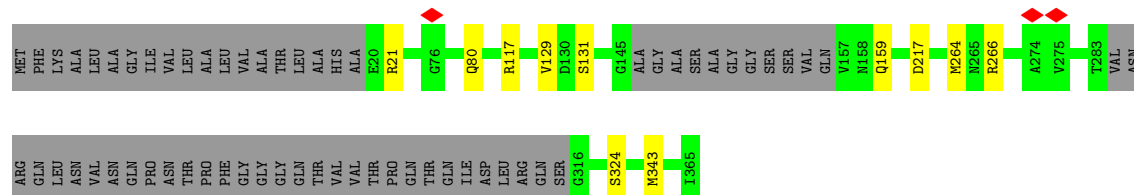
• Molecule 11: Flagellar hook protein FlgE

Chain Zh:  38% 98%




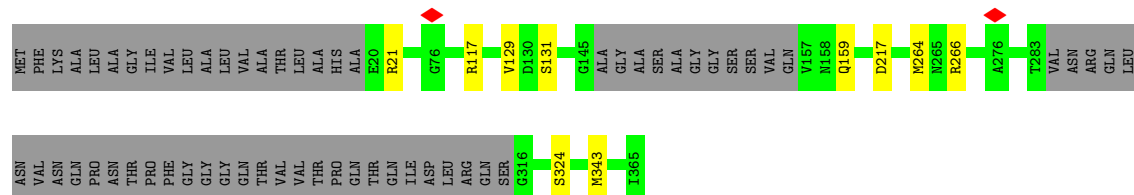
• Molecule 12: Flagellar P-ring protein

Chain a:  80% 17%




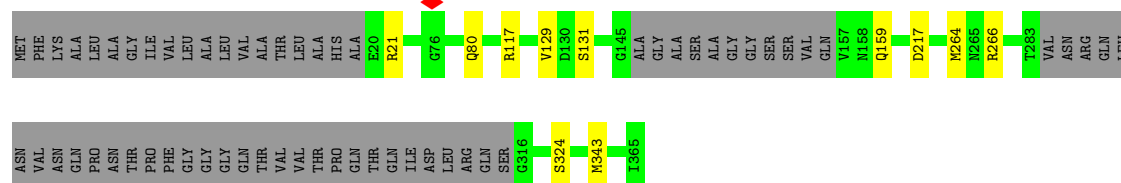
• Molecule 12: Flagellar P-ring protein

Chain b:  80% 17%




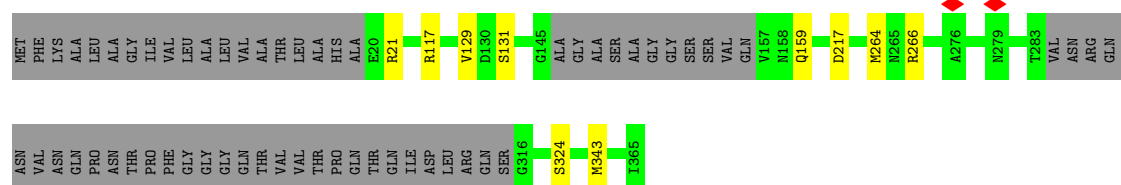
• Molecule 12: Flagellar P-ring protein

Chain c:  80% 17%




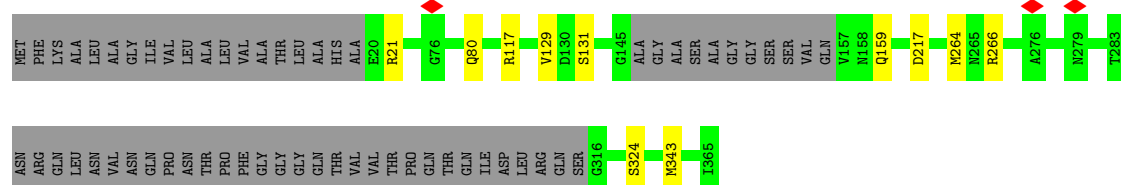
• Molecule 12: Flagellar P-ring protein

Chain d:  80% 17%




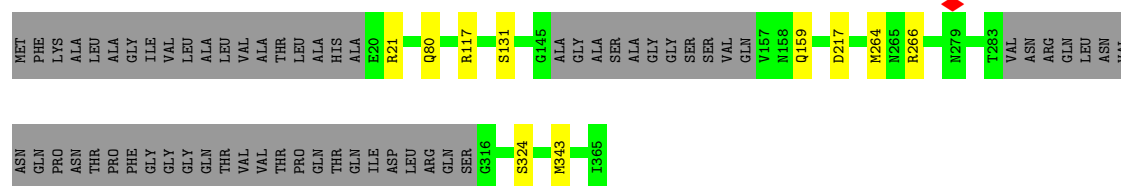
• Molecule 12: Flagellar P-ring protein

Chain e:  80% 17%




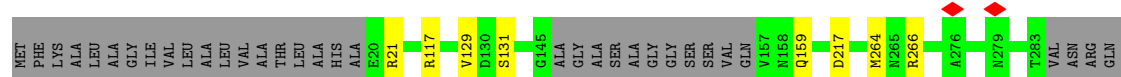
• Molecule 12: Flagellar P-ring protein

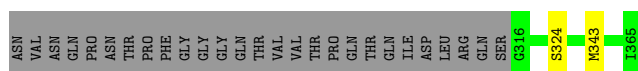
Chain f:  80% 17%



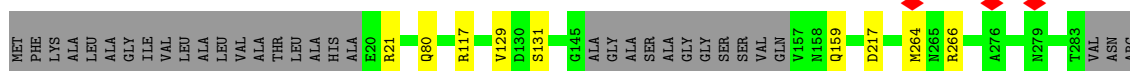
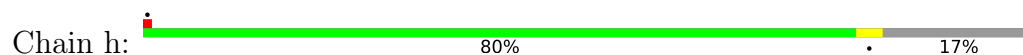
• Molecule 12: Flagellar P-ring protein

Chain g:  80% 17%

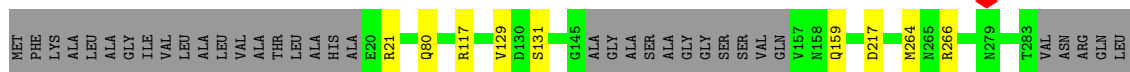
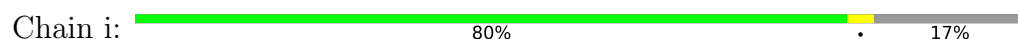




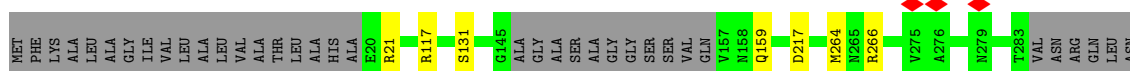
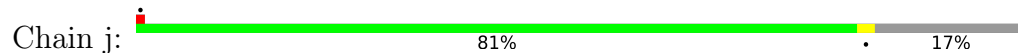
- Molecule 12: Flagellar P-ring protein



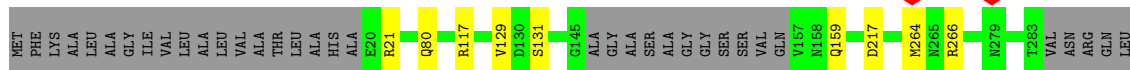
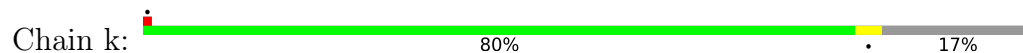
- Molecule 12: Flagellar P-ring protein



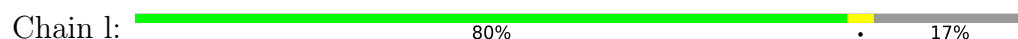
- Molecule 12: Flagellar P-ring protein

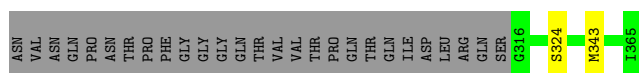
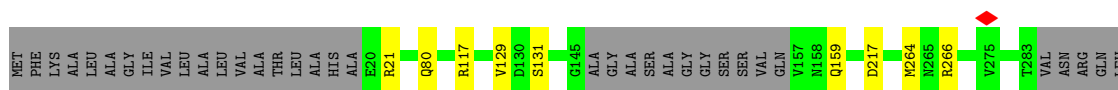


- Molecule 12: Flagellar P-ring protein

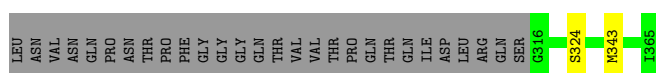
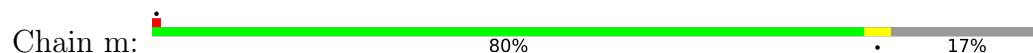


- Molecule 12: Flagellar P-ring protein

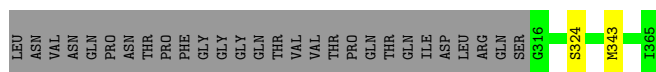
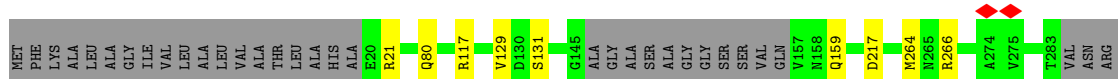
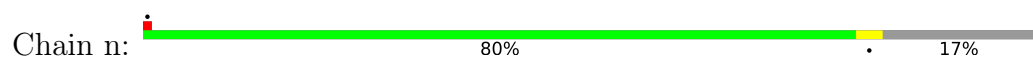




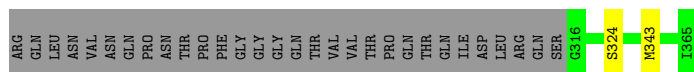
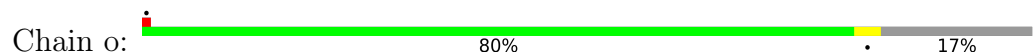
• Molecule 12: Flagellar P-ring protein



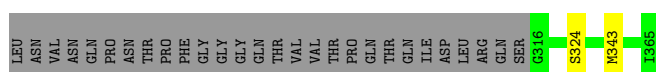
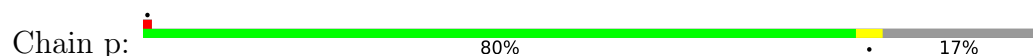
• Molecule 12: Flagellar P-ring protein




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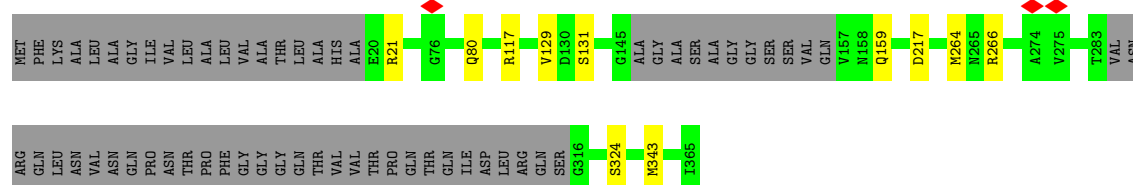


• Molecule 12: Flagellar P-ring protein




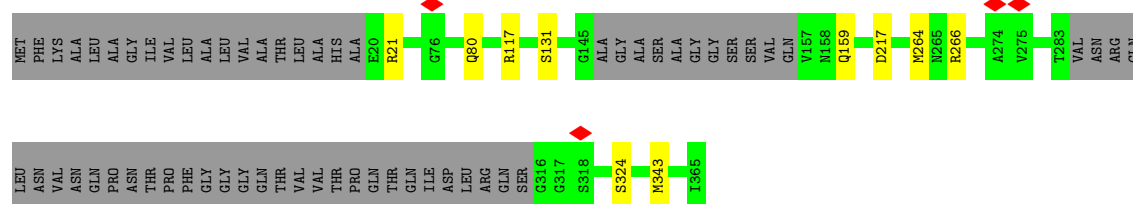
- Molecule 12: Flagellar P-ring protein

Chain q:  80% 17%




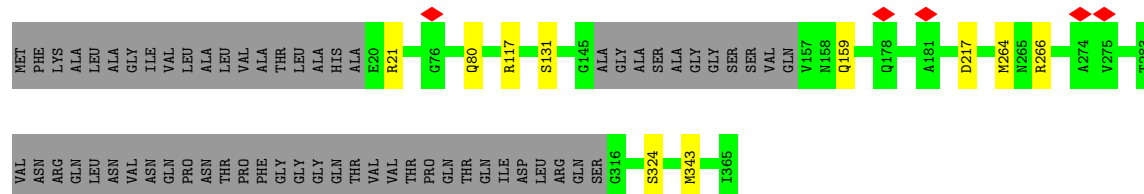
- Molecule 12: Flagellar P-ring protein

Chain r:  80% 17%




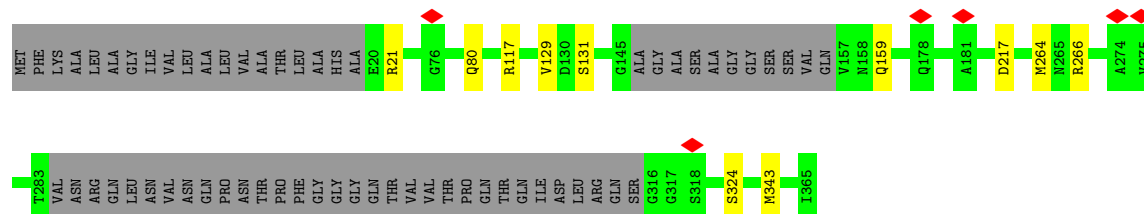
- Molecule 12: Flagellar P-ring protein

Chain s:  80% 17%




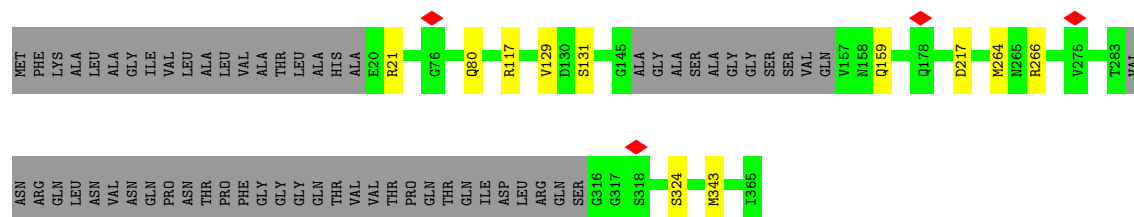
- Molecule 12: Flagellar P-ring protein

Chain t:  80% 17%

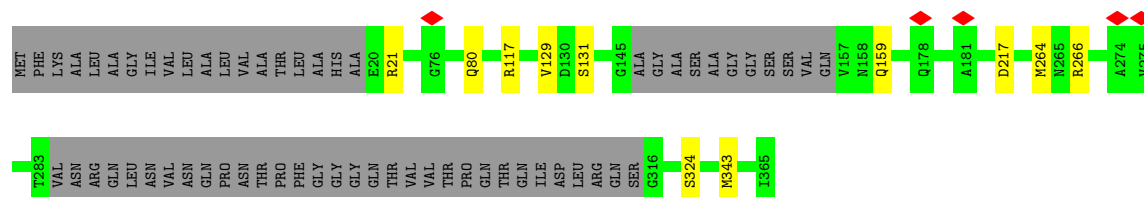
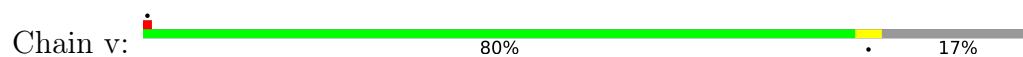


- Molecule 12: Flagellar P-ring protein

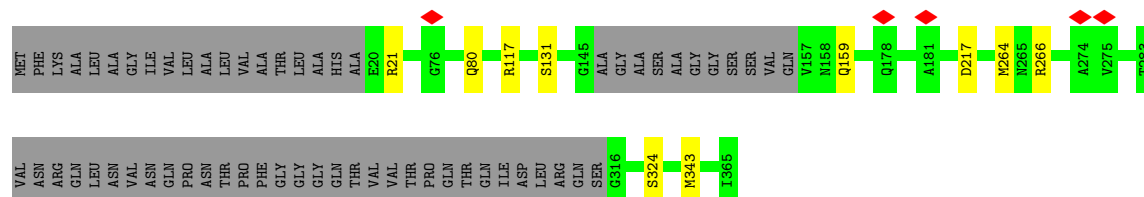
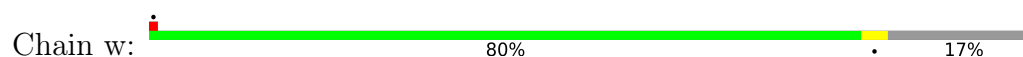
Chain u:  80% 17%



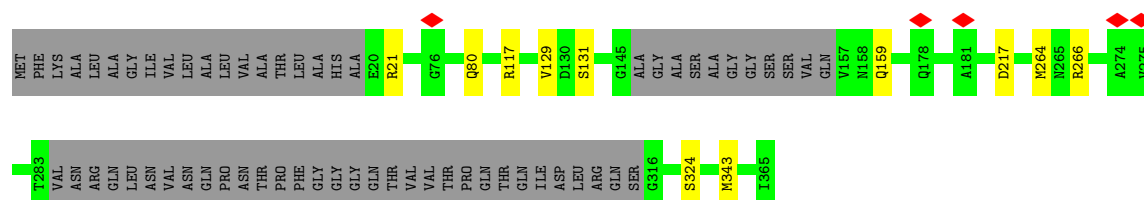
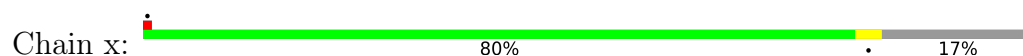
• Molecule 12: Flagellar P-ring protein



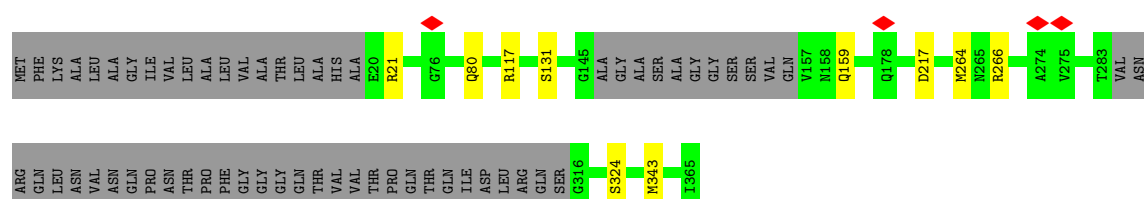
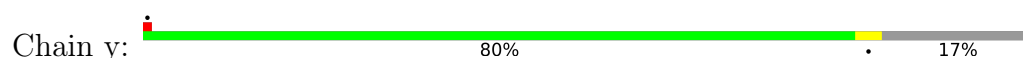
• Molecule 12: Flagellar P-ring protein



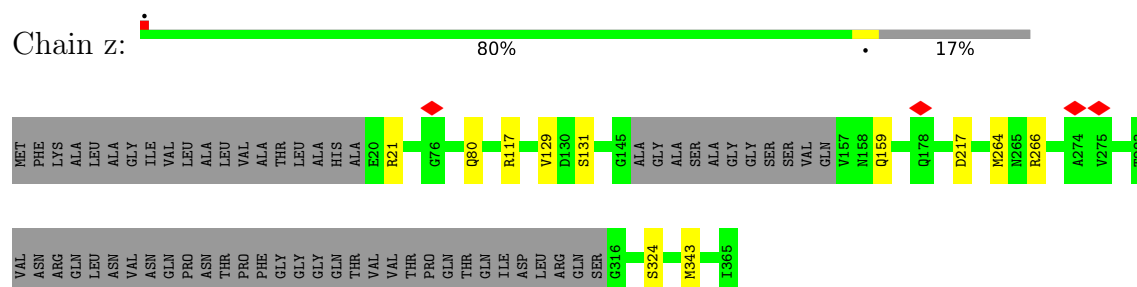
• Molecule 12: Flagellar P-ring protein



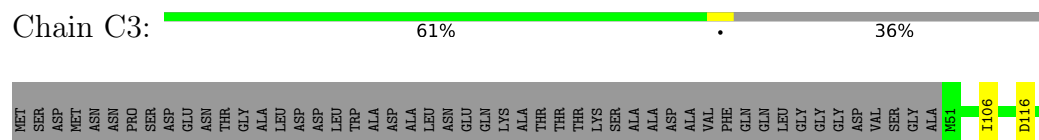
• Molecule 12: Flagellar P-ring protein



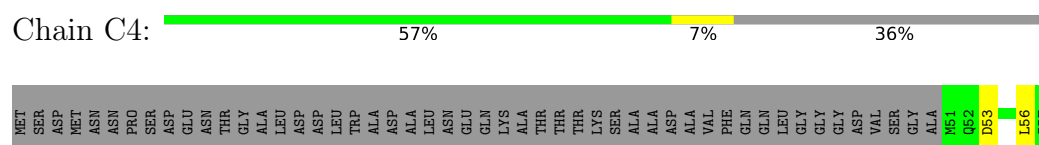
- Molecule 12: Flagellar P-ring protein



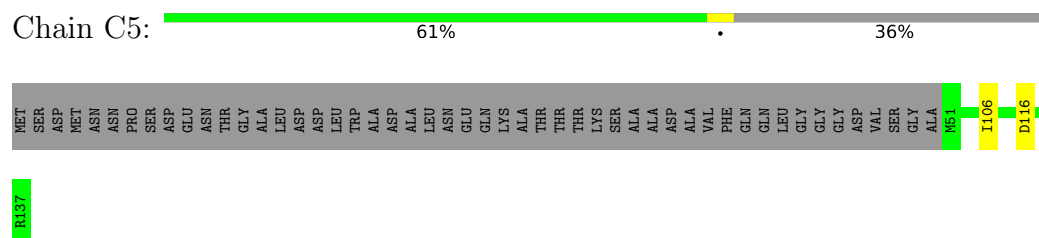
- Molecule 13: Flagellar motor switch protein FliN



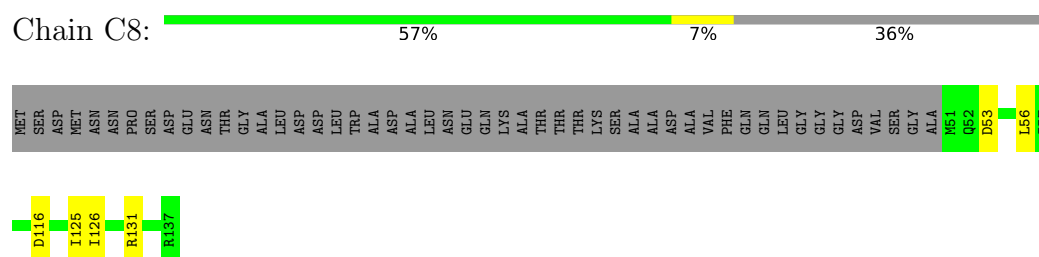
- Molecule 13: Flagellar motor switch protein FliN



- Molecule 13: Flagellar motor switch protein FliN

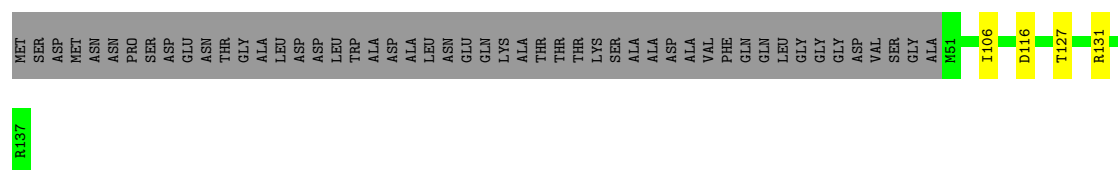


- Molecule 13: Flagellar motor switch protein FliN




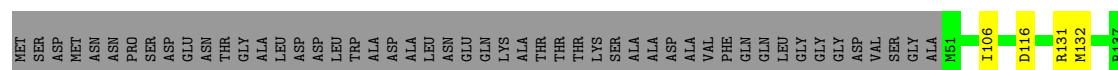
- Molecule 13: Flagellar motor switch protein FliN

Chain C9:  61% 36%



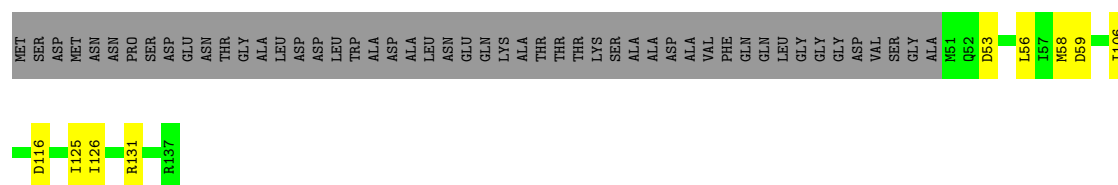
- Molecule 13: Flagellar motor switch protein FliN

Chain DD:  61% 36%



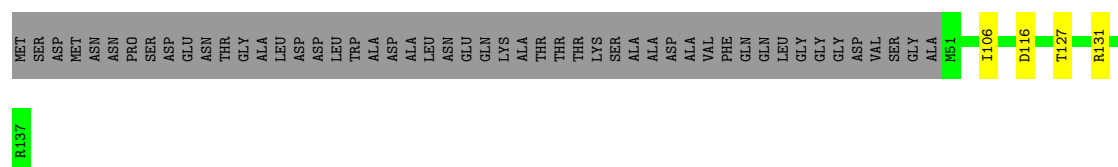
- Molecule 13: Flagellar motor switch protein FliN

Chain DI:  57% 7% 36%



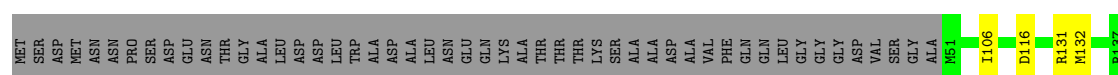
- Molecule 13: Flagellar motor switch protein FliN

Chain DJ:  61% 36%



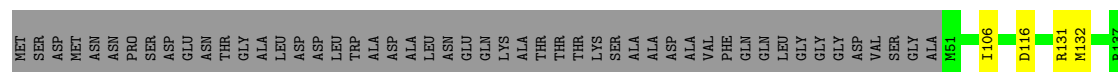
- Molecule 13: Flagellar motor switch protein FliN

Chain DK:  61% 36%



- Molecule 13: Flagellar motor switch protein FliN

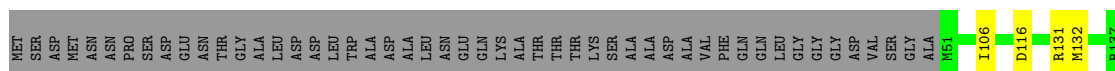
Chain DM:  61% 36%



- Molecule 13: Flagellar motor switch protein FliN

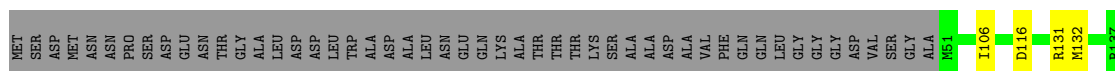


Chain DN:  61% 36%



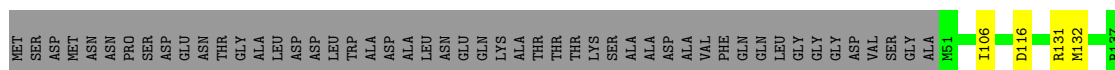
- Molecule 13: Flagellar motor switch protein FlhN

Chain DO:  61% 36%



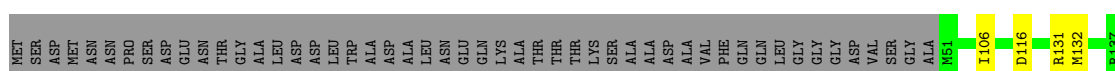
- Molecule 13: Flagellar motor switch protein FlhN

Chain DP:  61% 36%



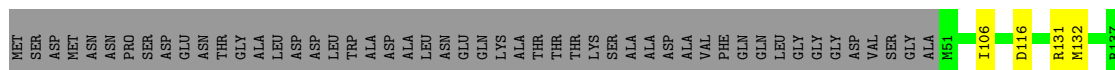
- Molecule 13: Flagellar motor switch protein FlhN

Chain DQ:  61% 36%



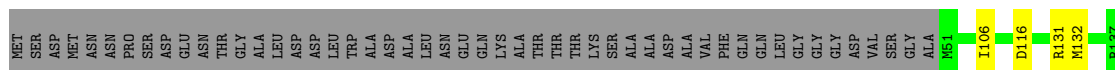
- Molecule 13: Flagellar motor switch protein FlhN

Chain DR:  61% 36%



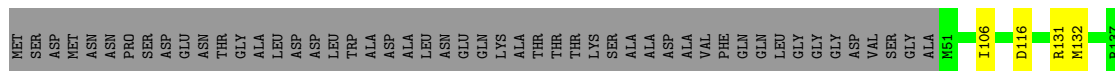
- Molecule 13: Flagellar motor switch protein FlhN

Chain DS:  61% 36%



- Molecule 13: Flagellar motor switch protein FlhN

Chain DT:  61% 36%



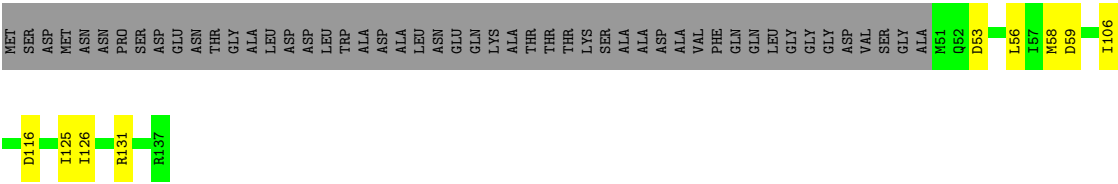
- Molecule 13: Flagellar motor switch protein FlhN

Chain DU: 

57%

7%

36%



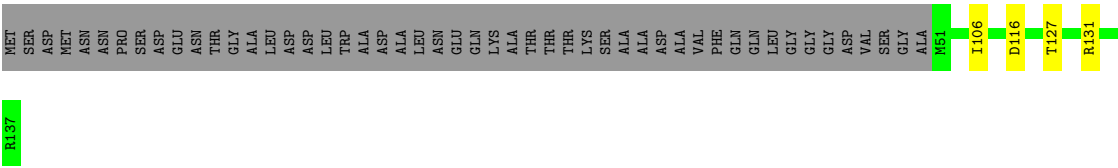
- Molecule 13: Flagellar motor switch protein FliN

Chain DV: 

61%

•

36%



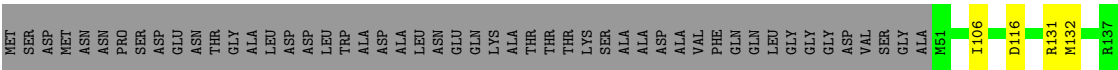
- Molecule 13: Flagellar motor switch protein FliN

Chain DW: 

61%

•

36%



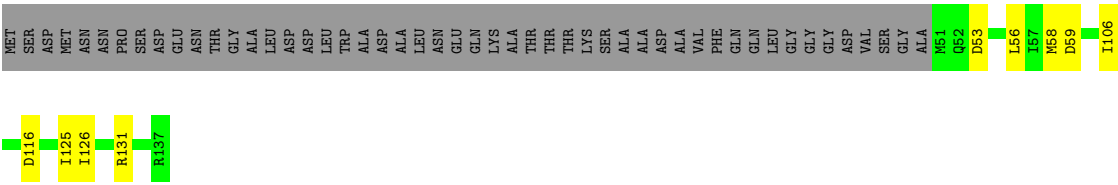
- Molecule 13: Flagellar motor switch protein FliN

Chain Da: 

57%

7%

36%



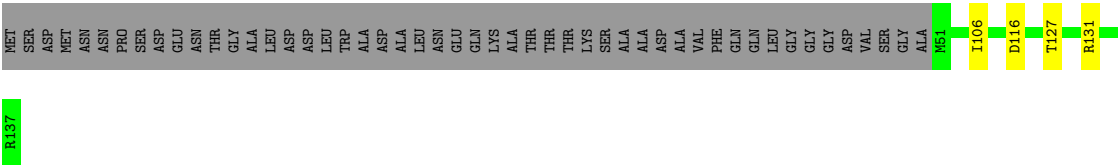
- Molecule 13: Flagellar motor switch protein FliN

Chain Db: 

61%

•

36%



- Molecule 13: Flagellar motor switch protein FliN

Chain Dc: 

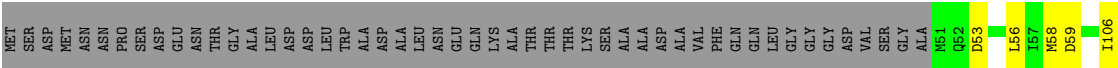
61%

•

36%



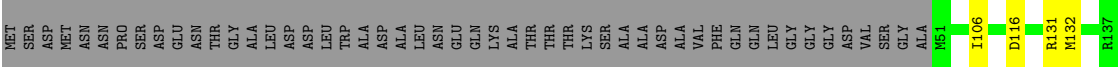
● Molecule 13: Flagellar motor switch protein FliN



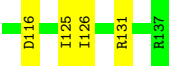
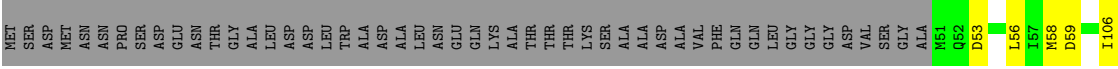
● Molecule 13: Flagellar motor switch protein FliN



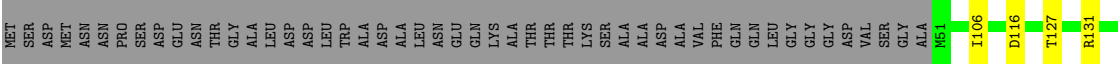
● Molecule 13: Flagellar motor switch protein FliN



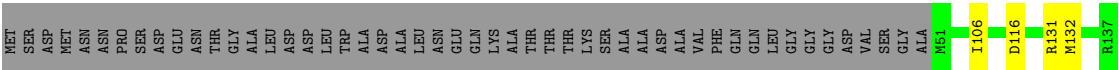
● Molecule 13: Flagellar motor switch protein FliN



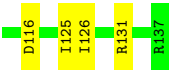
● Molecule 13: Flagellar motor switch protein FliN



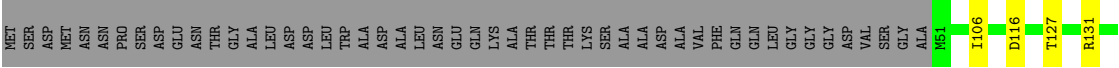
● Molecule 13: Flagellar motor switch protein FliN



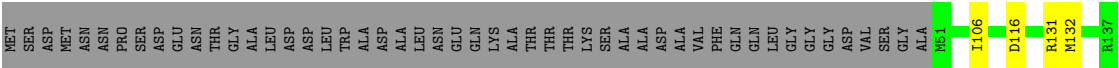
● Molecule 13: Flagellar motor switch protein FliN



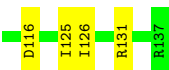
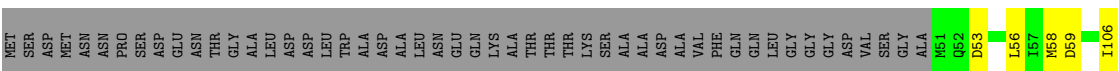
● Molecule 13: Flagellar motor switch protein FliN



● Molecule 13: Flagellar motor switch protein FliN

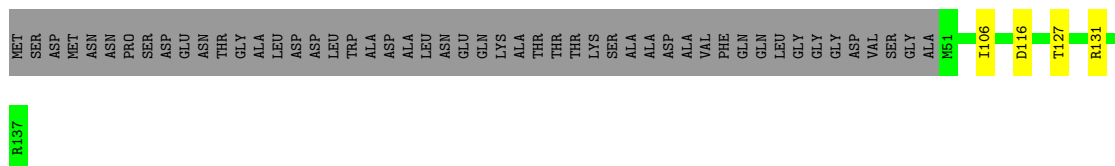


● Molecule 13: Flagellar motor switch protein FliN

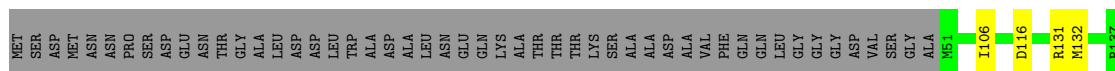


● Molecule 13: Flagellar motor switch protein FliN

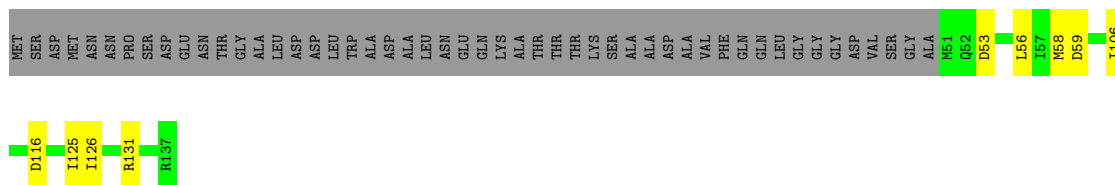




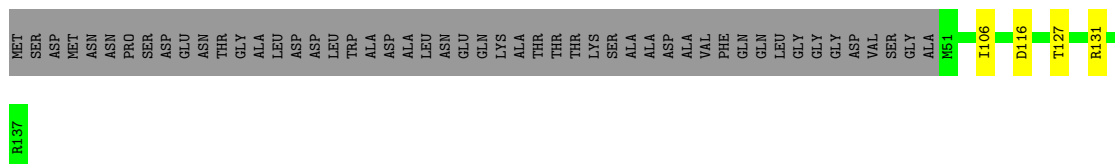
- Molecule 13: Flagellar motor switch protein FliN



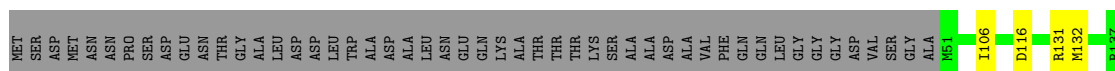
- Molecule 13: Flagellar motor switch protein FliN



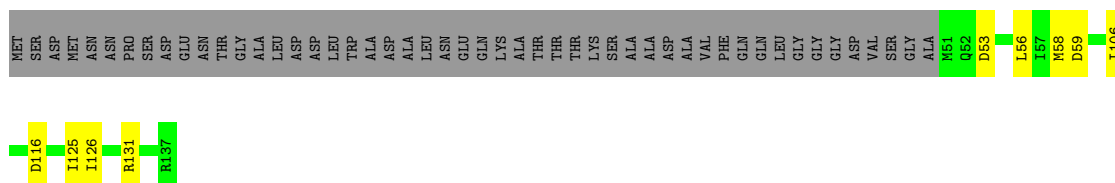
- Molecule 13: Flagellar motor switch protein FliN



- Molecule 13: Flagellar motor switch protein FliN

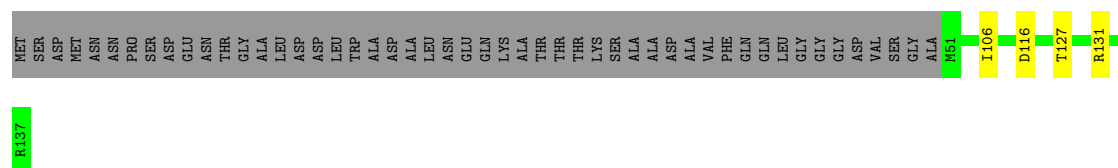


- Molecule 13: Flagellar motor switch protein FliN



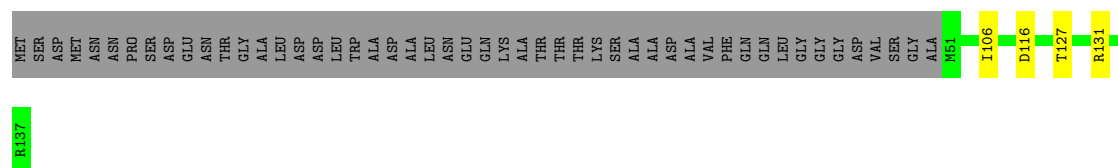
- Molecule 13: Flagellar motor switch protein FliN

Chain EB:  61% 36%



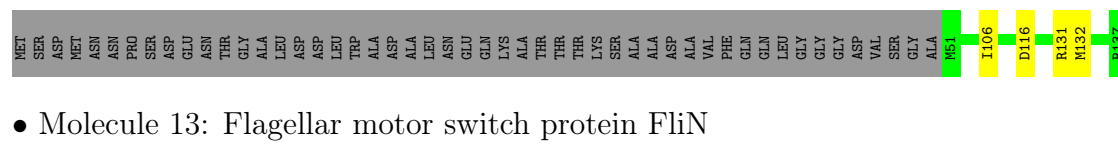
- Molecule 13: Flagellar motor switch protein FliN

Chain B1:  61% 36%



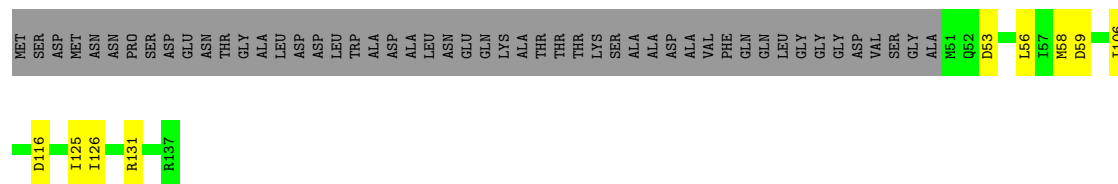
- Molecule 13: Flagellar motor switch protein FliN

Chain B2:  61% 36%



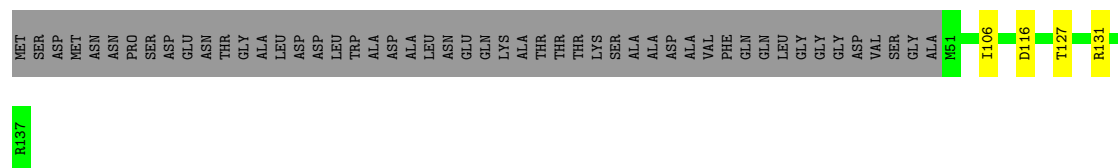
- Molecule 13: Flagellar motor switch protein FliN

Chain B7:  57% 7% 36%



- Molecule 13: Flagellar motor switch protein FliN

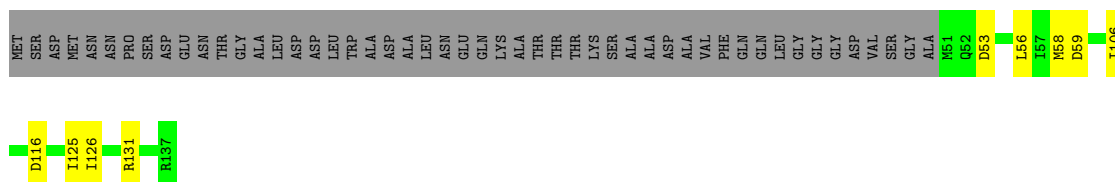
Chain B8:  61% 36%



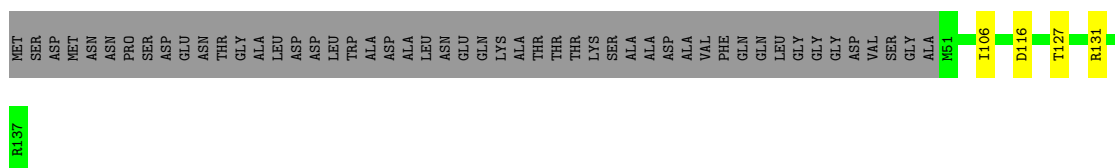
- Molecule 13: Flagellar motor switch protein FliN

Chain B9:  61% 36%

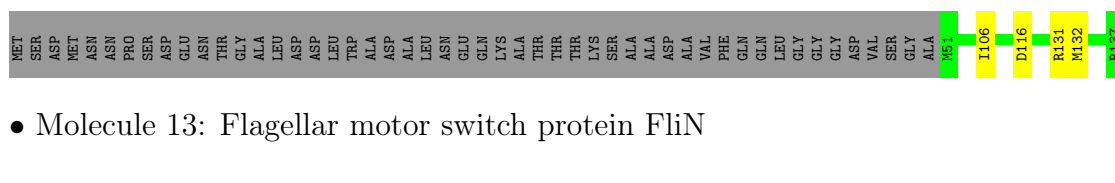
- Molecule 13: Flagellar motor switch protein FliN



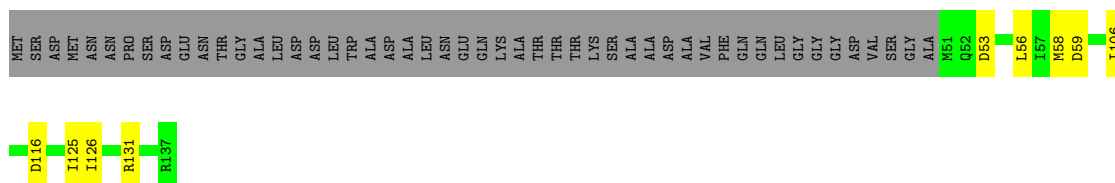
- Molecule 13: Flagellar motor switch protein FliN



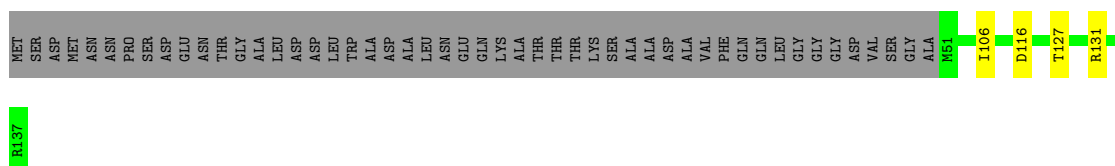
- Molecule 13: Flagellar motor switch protein FliN



- Molecule 13: Flagellar motor switch protein FliN

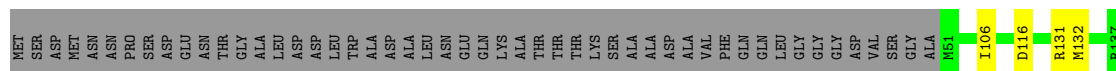


- Molecule 13: Flagellar motor switch protein FliN



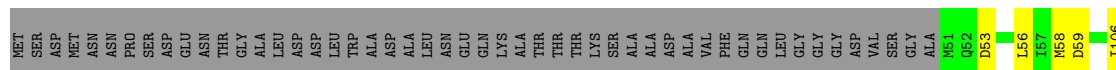
- Molecule 13: Flagellar motor switch protein FliN

Chain EN:  61% 36%



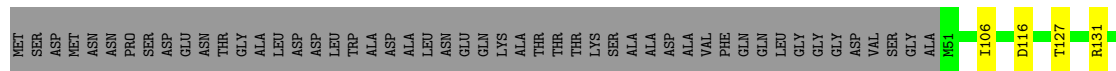
- Molecule 13: Flagellar motor switch protein FliN

Chain ES:  57% 7% 36%



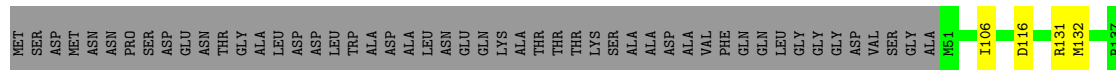
- Molecule 13: Flagellar motor switch protein FliN

Chain ET:  61% 36%



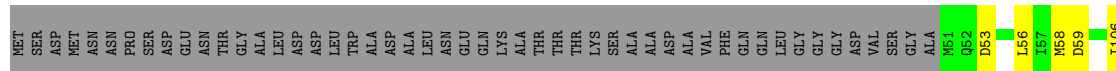
- Molecule 13: Flagellar motor switch protein FliN

Chain EU:  61% 36%



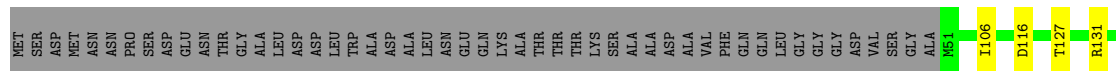
- Molecule 13: Flagellar motor switch protein FliN

Chain EZ:  57% 7% 36%



- Molecule 13: Flagellar motor switch protein FliN

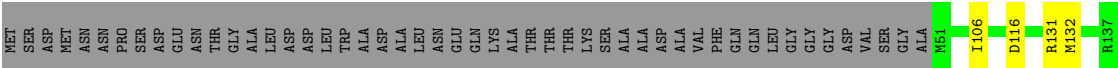
Chain BY:  61% 36%



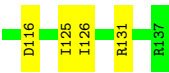
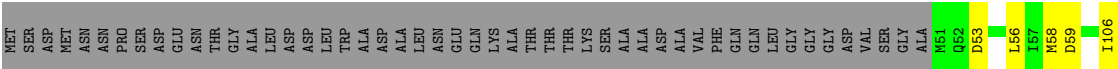


R137

- Molecule 13: Flagellar motor switch protein FliN



- Molecule 13: Flagellar motor switch protein FliN

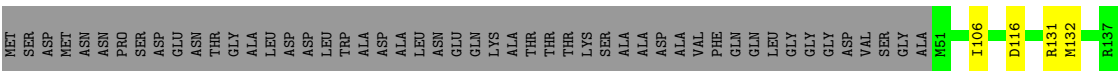


- Molecule 13: Flagellar motor switch protein FliN

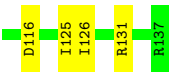


R137

- Molecule 13: Flagellar motor switch protein FliN



- Molecule 13: Flagellar motor switch protein FliN



- Molecule 13: Flagellar motor switch protein FliN

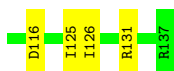




- Chain Bn:  61% 36%



- Chain Bs:  57% 7% 36%



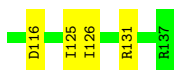
- Chain Bt:  61% 0% 36%



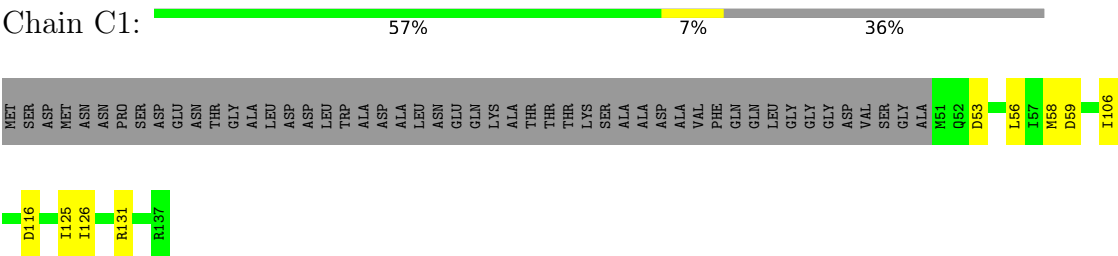
- Chain Bu:  61% 36%



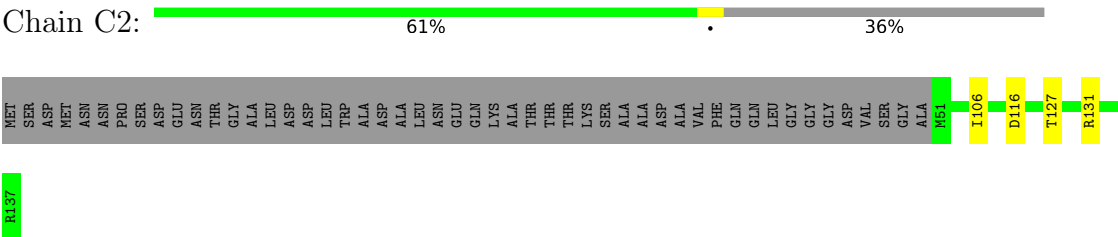
- Chain Bz:  57% 7% 36%



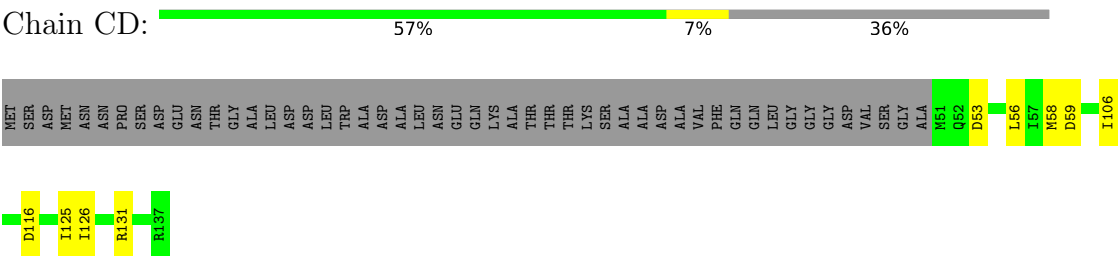
• Molecule 13: Flagellar motor switch protein FliN



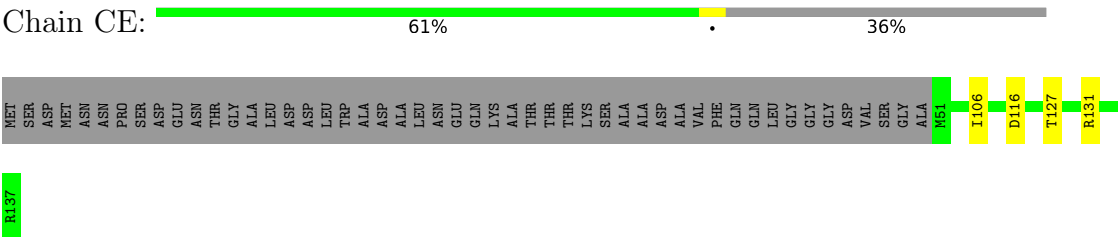
• Molecule 13: Flagellar motor switch protein FliN



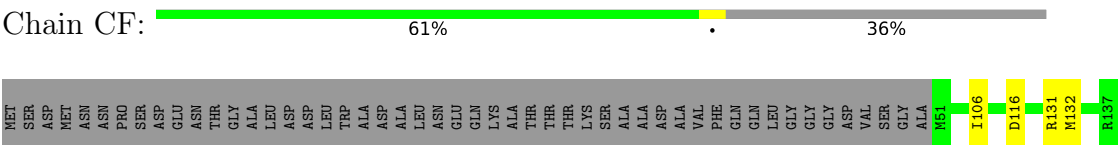
• Molecule 13: Flagellar motor switch protein FliN



• Molecule 13: Flagellar motor switch protein FliN

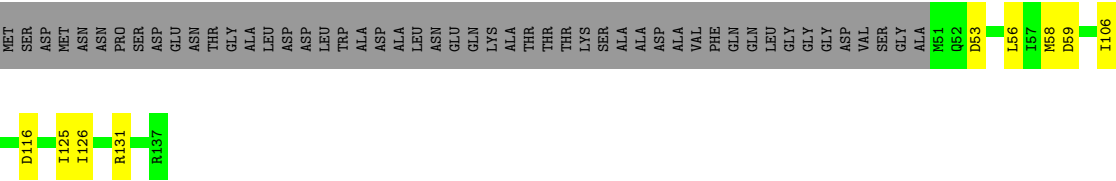


• Molecule 13: Flagellar motor switch protein FliN

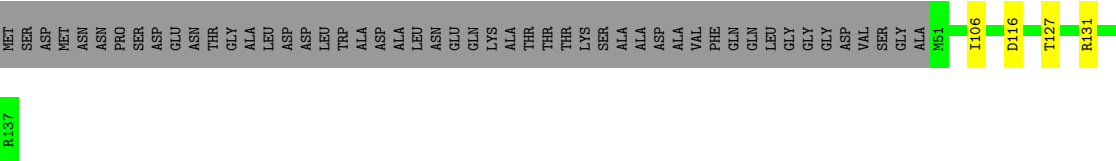


• Molecule 13: Flagellar motor switch protein FliN

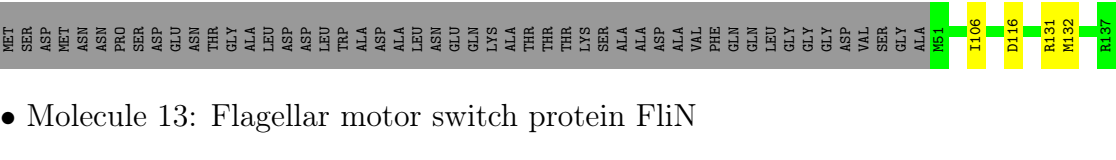




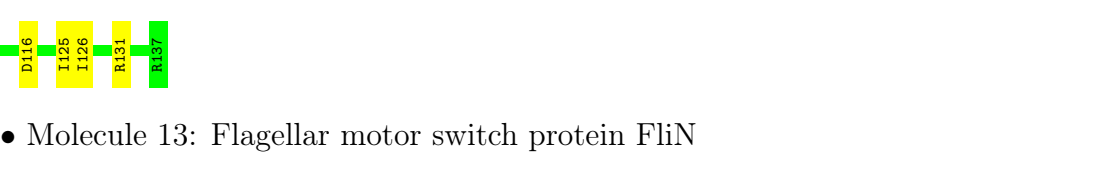
• Molecule 13: Flagellar motor switch protein FliN



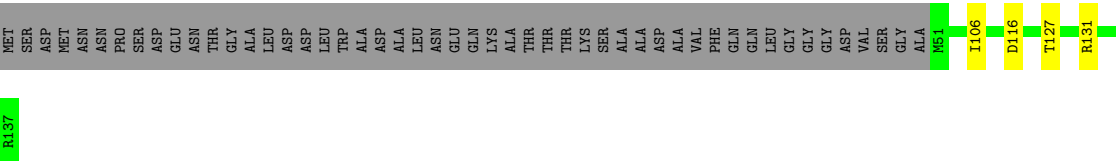
• Molecule 13: Flagellar motor switch protein FliN



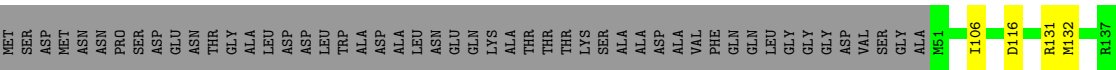
• Molecule 13: Flagellar motor switch protein FliN



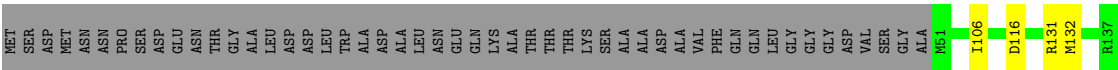
• Molecule 13: Flagellar motor switch protein FliN



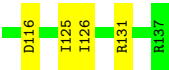
• Molecule 13: Flagellar motor switch protein FliN



- Chain Ch:  61% 0% 36%



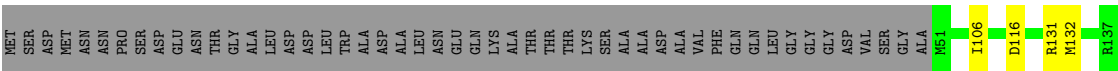
• Molecule 13: Flagellar motor switch protein FliN



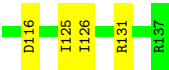
• Molecule 13: Flagellar motor switch protein FliN



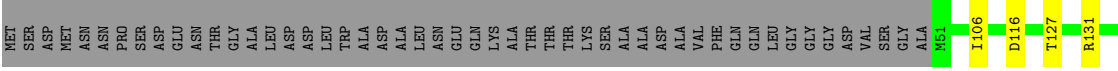
• Molecule 13: Flagellar motor switch protein FliN



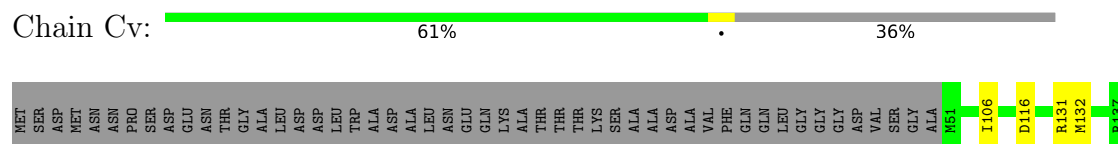
• Molecule 13: Flagellar motor switch protein FliN



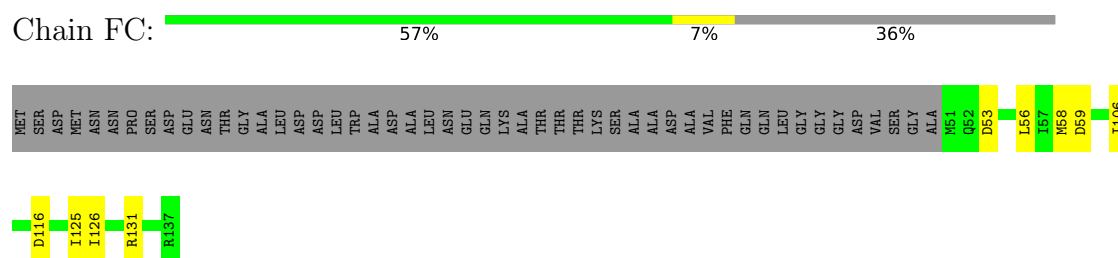
• Molecule 13: Flagellar motor switch protein FliN



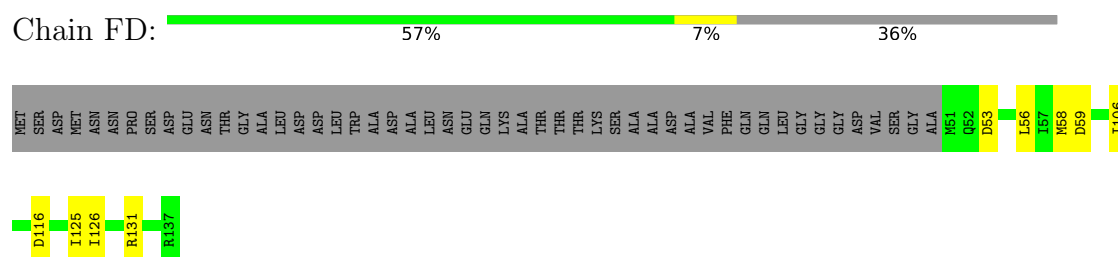
- Molecule 13: Flagellar motor switch protein FliN



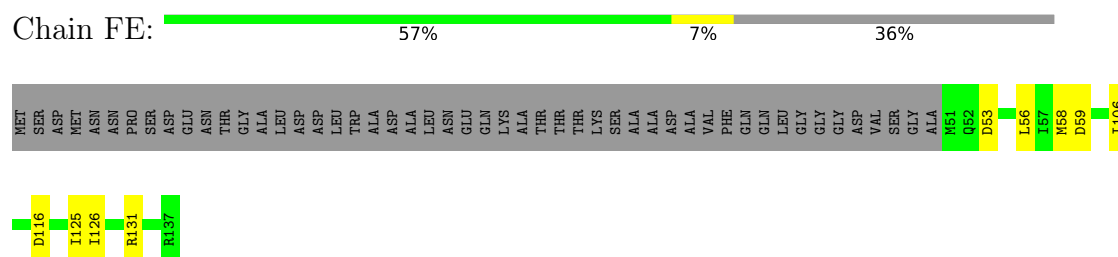
- Molecule 13: Flagellar motor switch protein FliN



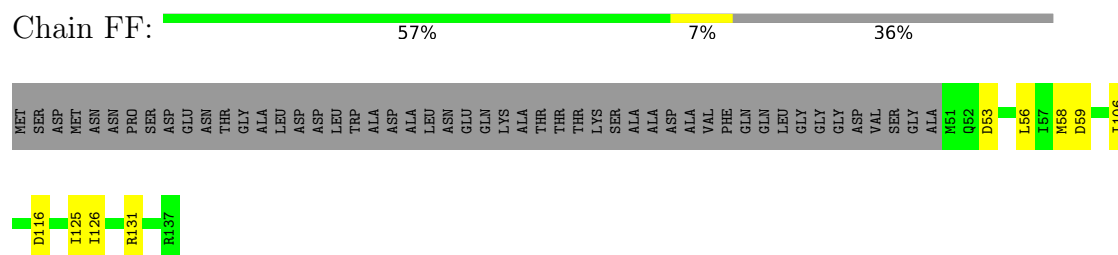
- Molecule 13: Flagellar motor switch protein FliN



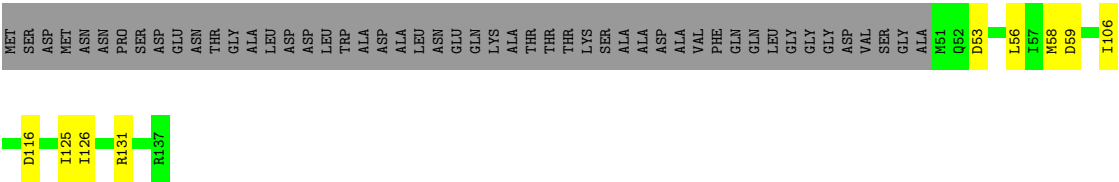
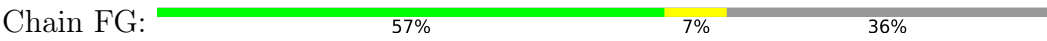
- Molecule 13: Flagellar motor switch protein FliN



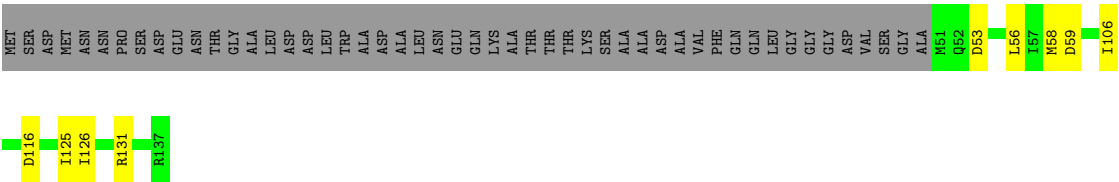
- Molecule 13: Flagellar motor switch protein FliN



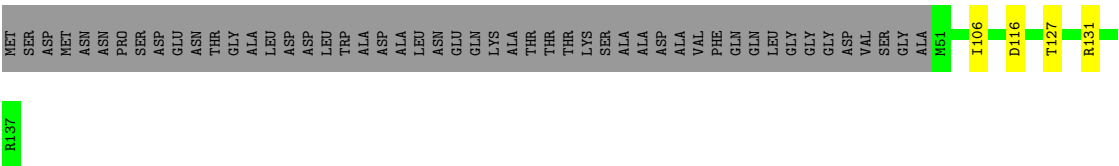
- Molecule 13: Flagellar motor switch protein FliN



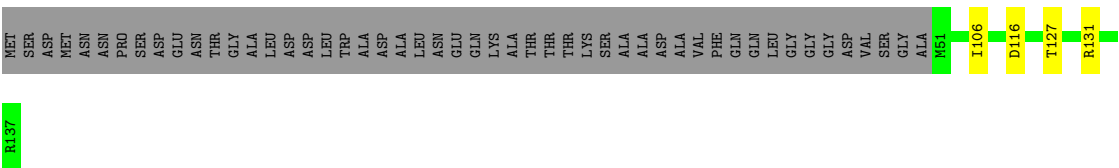
- Molecule 13: Flagellar motor switch protein FliN



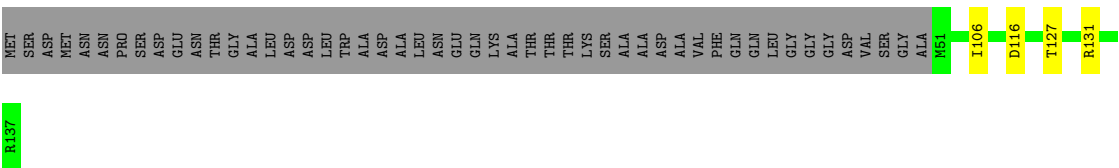
- Molecule 13: Flagellar motor switch protein FliN



- Molecule 13: Flagellar motor switch protein FliN



- Molecule 13: Flagellar motor switch protein FliN



- Molecule 13: Flagellar motor switch protein FliN





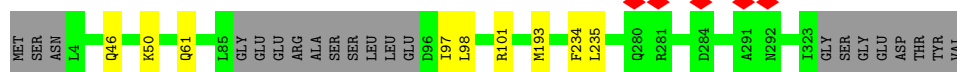
## ● Molecule 14: Flagellar motor switch protein Flig

Chain DY:  91% 6%

## ● Molecule 14: Flagellar motor switch protein Flig

Chain De:  91% 6%

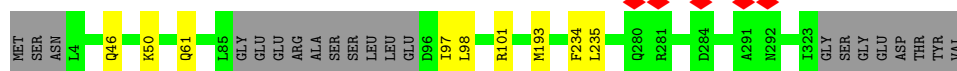
## ● Molecule 14: Flagellar motor switch protein Flig

Chain Dk:  91% 6%

## ● Molecule 14: Flagellar motor switch protein Flig

Chain Dq:  91% 6%

## ● Molecule 14: Flagellar motor switch protein Flig

Chain Dw:  91% 6%

## ● Molecule 14: Flagellar motor switch protein Flig

Chain D3:  91% 6%

## ● Molecule 14: Flagellar motor switch protein Flig

Chain D9:  91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain B5: 91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain EC: 91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain EJ: 91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain EQ: 91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain EX: 91% 6%




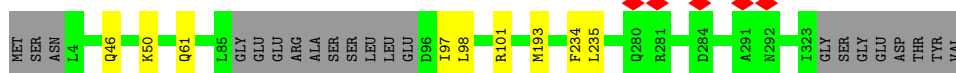
- Molecule 14: Flagellar motor switch protein Flig

Chain Bc: 91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain Bj:  91% 6%



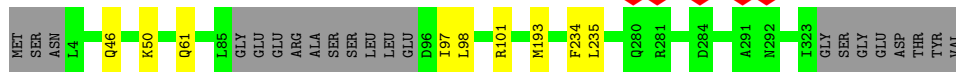
- Molecule 14: Flagellar motor switch protein FlgG

Chain Bq:  91% 6%



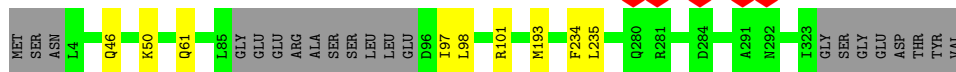
- Molecule 14: Flagellar motor switch protein FlgG

Chain Bx:  91% 6%




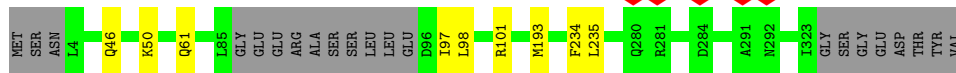
- Molecule 14: Flagellar motor switch protein FlgG

Chain CB:  91% 6%



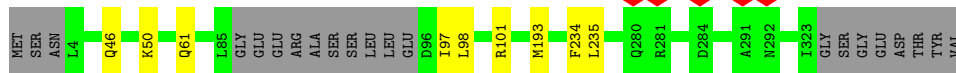
- Molecule 14: Flagellar motor switch protein FlgG

Chain CI:  91% 6%



- Molecule 14: Flagellar motor switch protein FlgG

Chain CP:  91% 6%



- Molecule 14: Flagellar motor switch protein FlgG

Chain CW:  91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain Cd: 91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain Ck: 91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain Cr: 91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain Cy: 91% 6%



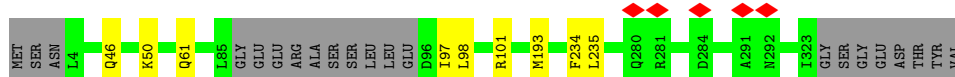
- Molecule 14: Flagellar motor switch protein Flig

Chain Ex: 91% 6%



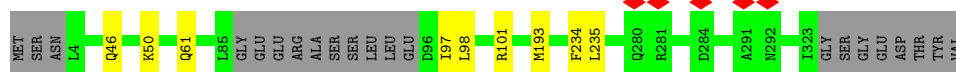
- Molecule 14: Flagellar motor switch protein Flig

Chain Ey: 91% 6%



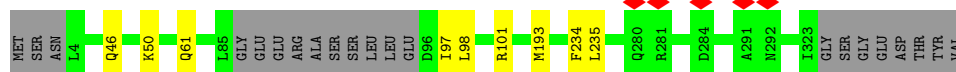
- Molecule 14: Flagellar motor switch protein Flig

Chain Ez:  91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain E1:  91% 6%



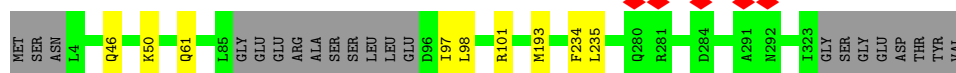
- Molecule 14: Flagellar motor switch protein Flig

Chain E2:  91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain E3:  91% 6%



- Molecule 14: Flagellar motor switch protein Flig

Chain E4:  91% 6%



- Molecule 15: Chemotaxis protein CheY

Chain C7:  8% 100%



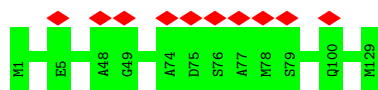
- Molecule 15: Chemotaxis protein CheY

Chain DB:  9% 100%



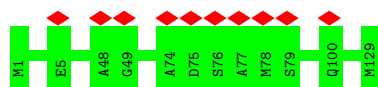
## • Molecule 15: Chemotaxis protein CheY

Chain DH:  100%



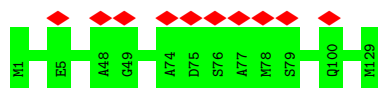
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Chain DZ:  100%



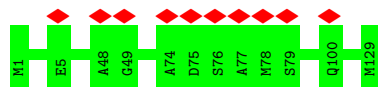
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Chain Df:  100%



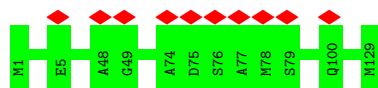
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Chain DI:  100%



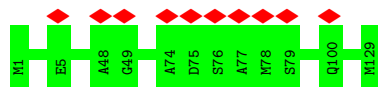
## • Molecule 15: Chemotaxis protein CheY

Chain Dr:  100%



## • Molecule 15: Chemotaxis protein CheY

Chain Dx:  100%

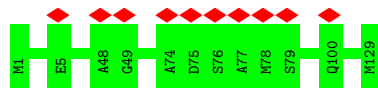


## • Molecule 15: Chemotaxis protein CheY

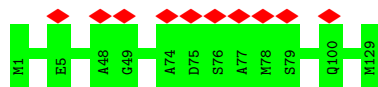
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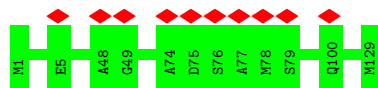
- Molecule 15: Chemotaxis protein CheY



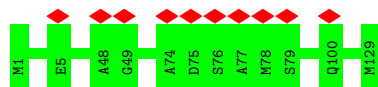
- Molecule 15: Chemotaxis protein CheY



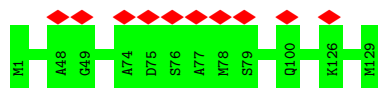
- Molecule 15: Chemotaxis protein CheY



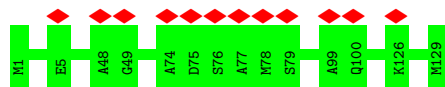
- Molecule 15: Chemotaxis protein CheY



- Molecule 15: Chemotaxis protein CheY

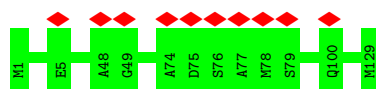


- Molecule 15: Chemotaxis protein CheY

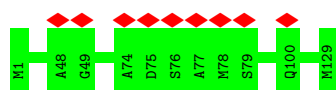


- Molecule 15: Chemotaxis protein CheY

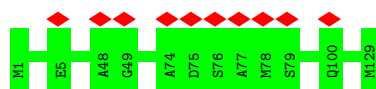




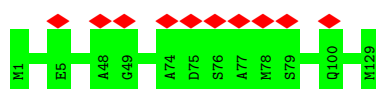
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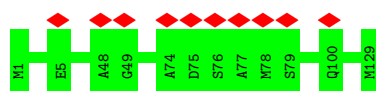
- Molecule 15: Chemotaxis protein CheY



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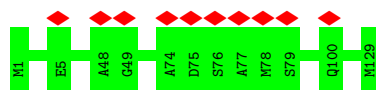


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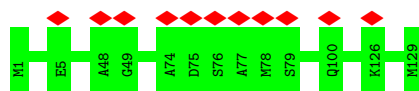


- Molecule 15: Chemotaxis protein CheY





- Molecule 15: Chemotaxis protein CheY



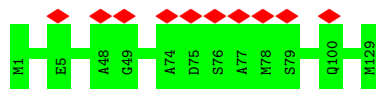
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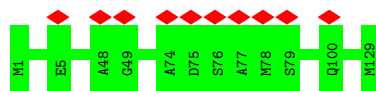
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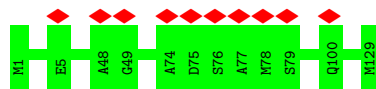
- Molecule 15: Chemotaxis protein CheY



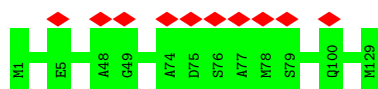
- Molecule 15: Chemotaxis protein CheY



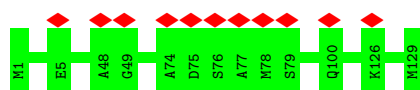
- Molecule 15: Chemotaxis protein CheY



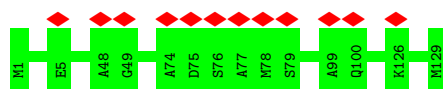
- Molecule 15: Chemotaxis protein CheY



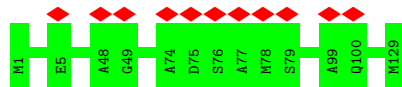
- Molecule 15: Chemotaxis protein CheY



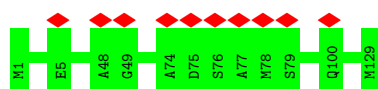
- Molecule 15: Chemotaxis protein CheY



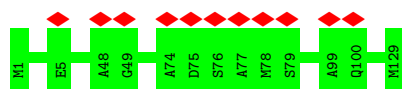
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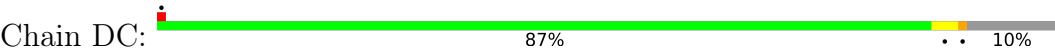


- Molecule 16: Flagellar motor switch protein FlhM



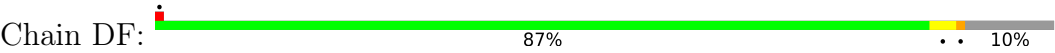
GLN  
PRO  
LYS

• Molecule 16: Flagellar motor switch protein FliM



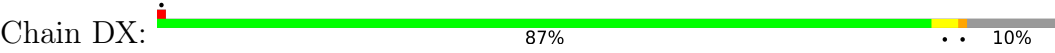
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PRO  
LYS

• Molecule 16: Flagellar motor switch protein FliM



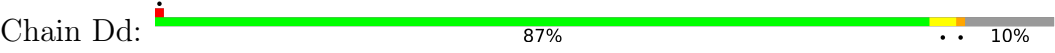
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• Molecule 16: Flagellar motor switch protein FliM



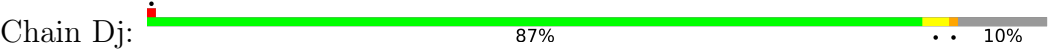
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• Molecule 16: Flagellar motor switch protein FliM



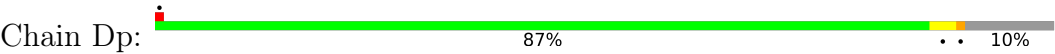
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• Molecule 16: Flagellar motor switch protein FliM



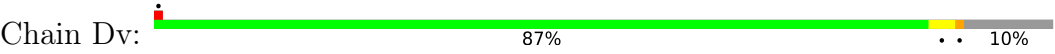
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• Molecule 16: Flagellar motor switch protein FlIM



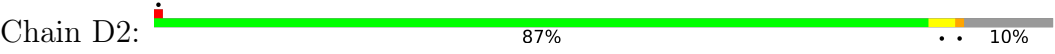
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• Molecule 16: Flagellar motor switch protein FlIM



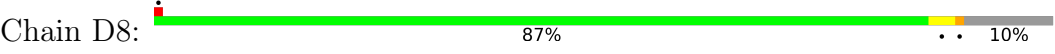
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• Molecule 16: Flagellar motor switch protein FlIM



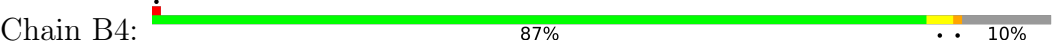
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• Molecule 16: Flagellar motor switch protein FlIM



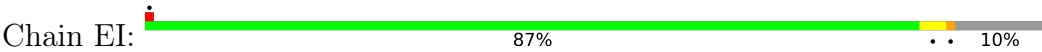
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• Molecule 16: Flagellar motor switch protein FlIM



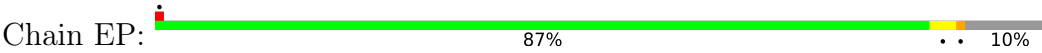
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• Molecule 16: Flagellar motor switch protein FliM



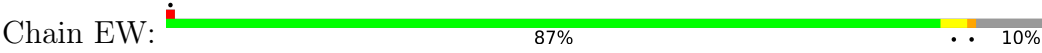
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LYS

• Molecule 16: Flagellar motor switch protein FliM



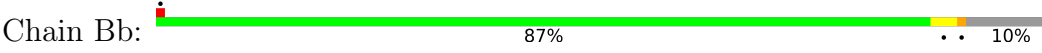
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LYS

• Molecule 16: Flagellar motor switch protein FliM



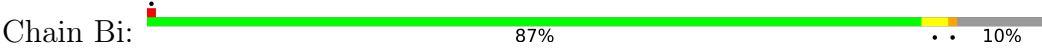
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PRO  
LYS

• Molecule 16: Flagellar motor switch protein FliM



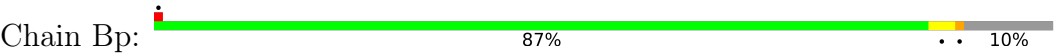
GLN  
PRO  
LYS

• Molecule 16: Flagellar motor switch protein FliM



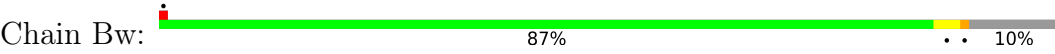
GLN  
PRO  
LYS

• Molecule 16: Flagellar motor switch protein FlIM



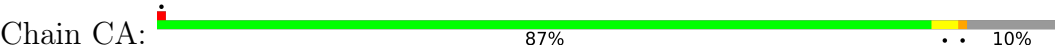
GLN  
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• Molecule 16: Flagellar motor switch protein FlIM



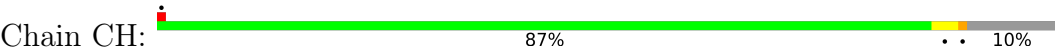
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• Molecule 16: Flagellar motor switch protein FlIM



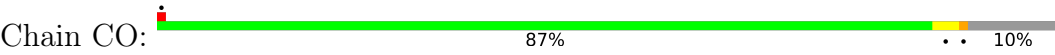
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• Molecule 16: Flagellar motor switch protein FlIM



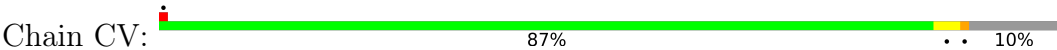
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LYS

• Molecule 16: Flagellar motor switch protein FlIM



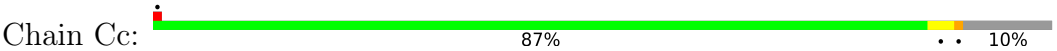
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• Molecule 16: Flagellar motor switch protein FliM



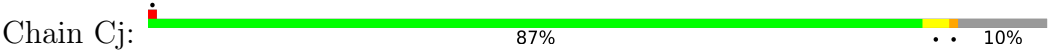
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• Molecule 16: Flagellar motor switch protein FliM



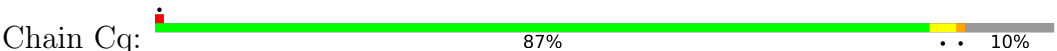
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• Molecule 16: Flagellar motor switch protein FliM



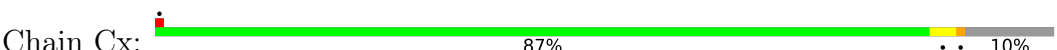
GLN  
PRO  
LYS

• Molecule 16: Flagellar motor switch protein FliM



GLN  
PRO  
LYS

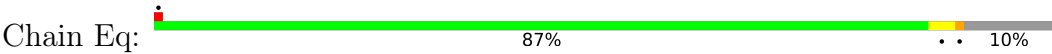
• Molecule 16: Flagellar motor switch protein FliM





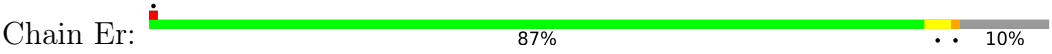
GLN  
PRO  
LYS

• Molecule 16: Flagellar motor switch protein FlIM



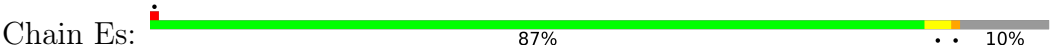
GLN  
PRO  
LYS

• Molecule 16: Flagellar motor switch protein FlIM



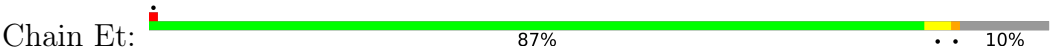
GLN  
PRO  
LYS

• Molecule 16: Flagellar motor switch protein FlIM



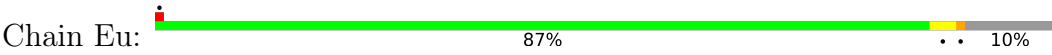
GLN  
PRO  
LYS

• Molecule 16: Flagellar motor switch protein FlIM



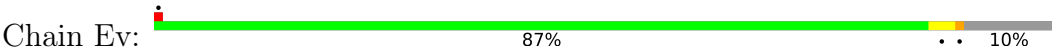
GLN  
PRO  
LYS

• Molecule 16: Flagellar motor switch protein FlIM



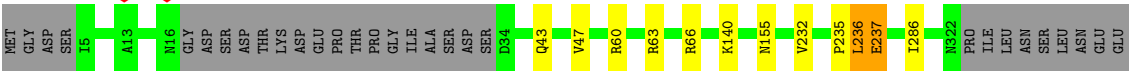
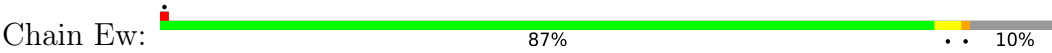
GLN  
PRO  
LYS

• Molecule 16: Flagellar motor switch protein FliM



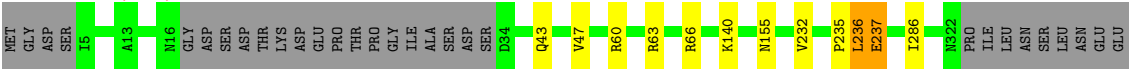
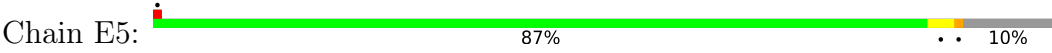
GLN  
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• Molecule 16: Flagellar motor switch protein FliM



GLN  
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• Molecule 16: Flagellar motor switch protein FliM



GLN  
PRO  
LYS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	26921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.415	Depositor
Minimum map value	-0.224	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	1008.00006, 1008.00006, 1008.00006	wwPDB
Map dimensions	840, 840, 840	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	0	0.30	0/1888	0.52	1/2564 (0.0%)
1	1	0.31	0/1917	0.50	0/2605
1	2	0.27	0/1973	0.48	0/2682
1	3	0.28	0/1973	0.50	0/2682
1	4	0.28	0/1973	0.50	0/2682
1	5	0.32	0/1973	0.52	0/2682
1	6	0.31	0/1973	0.52	0/2682
1	7	0.28	0/1973	0.51	0/2682
1	8	0.30	0/1973	0.52	0/2682
1	9	0.29	0/1973	0.54	1/2682 (0.0%)
1	AF	0.33	0/1926	0.53	0/2618
1	AG	0.36	0/1934	0.56	0/2629
1	AH	0.33	0/1942	0.55	0/2639
1	AI	0.33	0/1926	0.57	1/2618 (0.0%)
1	AJ	0.30	0/1934	0.51	0/2629
1	AK	0.32	0/1844	0.51	0/2505
1	AL	0.31	0/1888	0.51	0/2564
1	AM	0.30	0/1888	0.54	1/2564 (0.0%)
1	AN	0.30	0/1888	0.51	0/2564
1	ZA	0.29	0/1973	0.52	0/2682
1	ZB	0.29	0/1973	0.49	0/2682
1	ZC	0.28	0/1973	0.51	0/2682
1	ZD	0.28	0/1973	0.51	0/2682
1	ZE	0.28	0/1973	0.50	1/2682 (0.0%)
2	A	0.27	0/1613	0.51	0/2194
2	B	0.27	0/1613	0.51	0/2194
2	C	0.27	0/1613	0.51	0/2194
2	D	0.27	0/1613	0.51	0/2194
2	E	0.27	0/1613	0.51	0/2194
2	F	0.27	0/1613	0.51	0/2194
2	G	0.27	0/1613	0.51	0/2194
2	H	0.27	0/1613	0.51	0/2194
2	I	0.27	0/1613	0.51	0/2194
2	J	0.27	0/1613	0.51	0/2194

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	K	0.27	0/1613	0.51	0/2194
2	L	0.27	0/1613	0.51	0/2194
2	M	0.27	0/1613	0.51	0/2194
2	N	0.27	0/1613	0.51	0/2194
2	O	0.27	0/1613	0.51	0/2194
2	P	0.27	0/1613	0.51	0/2194
2	Q	0.27	0/1613	0.51	0/2194
2	R	0.27	0/1613	0.51	0/2194
2	S	0.27	0/1613	0.51	0/2194
2	T	0.27	0/1613	0.51	0/2194
2	U	0.27	0/1613	0.51	0/2194
2	V	0.27	0/1613	0.51	0/2194
2	W	0.27	0/1613	0.51	0/2194
2	X	0.27	0/1613	0.51	0/2194
2	Y	0.27	0/1613	0.51	0/2194
2	Z	0.27	0/1613	0.51	0/2194
3	A0	0.34	0/959	0.50	0/1293
3	A6	0.36	0/1042	0.55	0/1408
3	A7	0.33	0/951	0.50	0/1282
3	A8	0.35	0/976	0.57	0/1316
3	A9	0.34	0/991	0.54	0/1335
4	A1	0.36	0/675	0.49	0/905
4	A2	0.37	0/689	0.52	0/925
4	A3	0.36	0/689	0.51	0/925
4	A4	0.37	0/689	0.53	0/925
4	A5	0.37	0/682	0.51	0/915
4	Az	0.42	0/428	0.53	0/572
5	AA	0.33	0/1828	0.56	0/2492
5	AB	0.29	0/1836	0.54	1/2502 (0.0%)
5	AC	0.28	0/1844	0.54	0/2512
5	AD	0.27	0/1844	0.53	0/2512
5	AE	0.31	0/1836	0.55	0/2502
6	AO	0.27	0/1289	0.53	0/1741
6	AP	0.27	0/1289	0.53	0/1741
6	AQ	0.27	0/1289	0.53	0/1741
6	AR	0.27	0/1289	0.53	0/1741
6	AS	0.27	0/1289	0.53	0/1741
6	AT	0.27	0/1289	0.53	0/1741
6	AU	0.27	0/1289	0.53	0/1741
6	AV	0.27	0/1289	0.53	0/1741
6	AW	0.27	0/1289	0.53	0/1741
6	AX	0.27	0/1289	0.53	0/1741
6	AY	0.27	0/1289	0.53	0/1741

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	AZ	0.27	0/1289	0.53	0/1741
6	Aa	0.27	0/1289	0.53	0/1741
6	Ac	0.27	0/1289	0.53	0/1741
6	Ad	0.27	0/1289	0.53	0/1741
6	Ae	0.27	0/1289	0.53	0/1741
6	Af	0.27	0/1289	0.53	0/1741
6	Ag	0.27	0/1289	0.53	0/1741
6	Ah	0.27	0/1289	0.53	0/1741
6	Ai	0.27	0/1289	0.53	0/1741
6	Aj	0.27	0/1289	0.53	0/1741
6	Ak	0.27	0/1289	0.53	0/1741
6	Al	0.27	0/1289	0.53	0/1741
6	Am	0.27	0/1289	0.53	0/1741
6	An	0.27	0/1289	0.53	0/1741
6	Ao	0.27	0/1289	0.53	0/1741
6	Ap	0.26	0/1289	0.53	0/1741
6	B0	0.22	0/226	0.50	0/303
6	B3	0.22	0/226	0.48	0/303
6	BG	0.52	0/83	0.63	0/114
6	BH	0.27	0/107	0.38	0/148
6	BI	0.30	0/137	0.49	0/191
6	BJ	0.28	0/107	0.56	0/148
6	BK	1.36	1/145 (0.7%)	1.49	3/203 (1.5%)
6	BL	0.33	0/107	0.51	0/148
6	BM	0.26	0/145	0.44	0/203
6	BN	0.30	0/107	0.38	0/148
6	BO	0.30	0/137	0.57	0/191
6	BP	0.30	0/107	0.37	0/148
6	BQ	0.29	0/145	0.45	0/203
6	BR	0.27	0/1289	0.52	0/1741
6	BS	0.27	0/1289	0.53	0/1741
6	BT	0.27	0/1289	0.53	0/1741
6	BU	0.27	0/1289	0.53	0/1741
6	BV	0.27	0/1289	0.53	0/1741
6	BW	0.26	0/1289	0.53	0/1741
6	BX	0.27	0/1289	0.53	0/1741
6	Ba	0.22	0/226	0.49	0/303
6	Bh	0.22	0/226	0.49	0/303
6	Bo	0.22	0/226	0.49	0/303
6	Bv	0.22	0/226	0.49	0/303
6	CG	0.22	0/226	0.49	0/303
6	CN	0.22	0/226	0.49	0/303
6	CU	0.22	0/226	0.49	0/303

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	Cb	0.22	0/226	0.49	0/303
6	Ci	0.22	0/226	0.49	0/303
6	Cp	0.22	0/226	0.49	0/303
6	Cw	0.22	0/226	0.49	0/303
6	DE	0.22	0/226	0.49	0/303
6	DL	0.22	0/226	0.49	0/303
6	EH	0.22	0/226	0.49	0/303
6	EO	0.22	0/226	0.49	0/303
6	EV	0.22	0/226	0.49	0/303
6	Ea	0.22	0/226	0.49	0/303
6	Eb	0.22	0/226	0.48	0/303
6	Ec	0.22	0/226	0.49	0/303
6	Ed	0.22	0/226	0.49	0/303
6	Ee	0.23	0/226	0.49	0/303
6	Ef	0.22	0/226	0.48	0/303
6	Eg	0.22	0/226	0.49	0/303
6	Eh	0.22	0/226	0.49	0/303
6	Ei	0.22	0/226	0.49	0/303
6	Ej	0.22	0/226	0.50	0/303
6	Ek	0.22	0/226	0.49	0/303
6	El	0.22	0/226	0.49	0/303
6	Em	0.22	0/226	0.48	0/303
6	En	0.22	0/226	0.49	0/303
6	Eo	0.22	0/226	0.49	0/303
6	Ep	0.22	0/226	0.49	0/303
6	UI	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UJ	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UK	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UL	0.82	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UM	0.84	3/1191 (0.3%)	0.82	4/1618 (0.2%)
6	UN	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UO	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UP	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	WA	0.61	0/863	0.72	1/1172 (0.1%)
6	WB	0.59	0/850	0.69	0/1154
6	WC	0.59	0/825	0.68	0/1121
6	WD	0.61	0/841	0.68	0/1142
6	WE	0.60	0/857	0.71	0/1164
6	WF	0.60	0/848	0.69	0/1152
6	WG	0.60	0/857	0.68	0/1164
6	WH	0.60	0/714	0.69	0/973
6	WI	0.60	0/714	0.74	0/973
6	WJ	0.61	0/749	0.72	1/1020 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	WK	0.60	0/741	0.69	0/1009
6	WL	0.60	0/631	0.70	0/860
6	WM	0.59	0/604	0.70	0/824
6	WN	0.60	0/619	0.70	0/844
6	WO	0.60	0/726	0.72	1/989 (0.1%)
6	WP	0.60	0/753	0.69	0/1025
6	WQ	0.60	0/848	0.69	0/1152
6	WR	0.60	0/848	0.69	0/1152
6	WS	0.61	0/848	0.69	0/1152
6	WT	0.60	0/848	0.70	0/1152
6	WU	0.60	0/857	0.67	0/1164
6	WV	0.61	0/841	0.69	0/1142
6	WW	0.60	0/848	0.70	0/1152
7	Ab	0.29	0/681	0.47	0/930
7	Aq	0.26	0/681	0.49	0/930
7	Ar	0.28	0/681	0.48	0/930
7	As	0.29	0/681	0.49	0/930
8	At	0.38	1/1994 (0.1%)	0.55	1/2724 (0.0%)
9	Au	0.36	0/1643	0.62	2/2237 (0.1%)
9	Av	0.30	0/1665	0.49	1/2267 (0.0%)
9	Aw	0.29	0/1652	0.48	0/2249
9	Ax	0.28	0/1652	0.46	0/2249
9	Ay	0.31	0/1662	0.49	0/2263
10	BA	0.28	0/981	0.44	0/1334
10	BB	0.26	0/976	0.46	0/1327
10	BC	0.57	2/981 (0.2%)	0.95	3/1334 (0.2%)
10	BD	0.28	0/981	0.52	1/1334 (0.1%)
10	BE	0.26	0/981	0.47	0/1334
10	BF	0.28	0/981	0.47	0/1334
11	ZF	0.28	0/2991	0.49	0/4076
11	ZG	0.31	0/2991	0.50	0/4076
11	ZH	0.28	0/2991	0.50	0/4076
11	ZI	0.30	0/2991	0.51	0/4076
11	ZJ	0.31	0/2991	0.51	0/4076
11	ZK	0.26	0/2991	0.48	0/4076
11	ZL	0.28	0/2991	0.49	0/4076
11	ZM	0.29	0/2991	0.53	1/4076 (0.0%)
11	ZN	0.28	0/2991	0.51	0/4076
11	ZO	0.30	0/2991	0.50	0/4076
11	ZP	0.28	0/2991	0.50	1/4076 (0.0%)
11	ZQ	0.29	0/2991	0.51	0/4076
11	ZR	0.30	1/2991 (0.0%)	0.55	3/4076 (0.1%)
11	ZS	0.29	0/2991	0.52	1/4076 (0.0%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	ZT	0.26	0/2991	0.47	0/4076
11	ZU	0.28	0/2991	0.50	0/4076
11	ZV	0.50	4/2991 (0.1%)	0.67	6/4076 (0.1%)
11	ZW	0.26	0/2991	0.48	0/4076
11	ZX	0.28	0/2991	0.48	0/4076
11	ZY	0.30	1/2991 (0.0%)	0.54	2/4076 (0.0%)
11	ZZ	0.25	0/2991	0.46	0/4076
11	Za	0.28	0/2991	0.49	0/4076
11	Zb	0.29	0/2991	0.50	0/4076
11	Zc	0.29	0/2991	0.53	2/4076 (0.0%)
11	Zd	0.29	0/2991	0.50	0/4076
11	Ze	0.27	0/2991	0.48	0/4076
11	Zf	0.27	0/2991	0.48	0/4076
11	Zg	0.27	0/2991	0.49	0/4076
11	Zh	0.26	0/2991	0.48	0/4076
12	a	0.26	0/2243	0.51	0/3041
12	b	0.26	0/2243	0.51	0/3041
12	c	0.26	0/2243	0.51	0/3041
12	d	0.26	0/2243	0.51	0/3041
12	e	0.26	0/2243	0.51	0/3041
12	f	0.26	0/2243	0.51	0/3041
12	g	0.26	0/2243	0.51	0/3041
12	h	0.26	0/2243	0.51	0/3041
12	i	0.26	0/2243	0.51	0/3041
12	j	0.26	0/2243	0.51	0/3041
12	k	0.26	0/2243	0.51	0/3041
12	l	0.26	0/2243	0.51	0/3041
12	m	0.26	0/2243	0.51	0/3041
12	n	0.26	0/2243	0.51	0/3041
12	o	0.26	0/2243	0.51	0/3041
12	p	0.26	0/2243	0.51	0/3041
12	q	0.26	0/2243	0.51	0/3041
12	r	0.26	0/2243	0.51	0/3041
12	s	0.26	0/2243	0.51	0/3041
12	t	0.26	0/2243	0.51	0/3041
12	u	0.26	0/2243	0.51	0/3041
12	v	0.26	0/2243	0.51	0/3041
12	w	0.26	0/2243	0.51	0/3041
12	x	0.26	0/2243	0.51	0/3041
12	y	0.26	0/2243	0.51	0/3041
12	z	0.26	0/2243	0.51	0/3041
13	B1	0.31	0/679	0.54	0/917
13	B2	0.29	0/679	0.53	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
13	B7	0.39	0/679	0.57	0/917
13	B8	0.31	0/679	0.55	0/917
13	B9	0.29	0/679	0.53	0/917
13	BY	0.31	0/679	0.54	0/917
13	BZ	0.29	0/679	0.53	0/917
13	Be	0.39	0/679	0.57	0/917
13	Bf	0.31	0/679	0.54	0/917
13	Bg	0.29	0/679	0.53	0/917
13	Bl	0.39	0/679	0.57	0/917
13	Bm	0.31	0/679	0.54	0/917
13	Bn	0.29	0/679	0.53	0/917
13	Bs	0.39	0/679	0.57	0/917
13	Bt	0.31	0/679	0.54	0/917
13	Bu	0.30	0/679	0.53	0/917
13	Bz	0.39	0/679	0.57	0/917
13	C1	0.39	0/679	0.57	0/917
13	C2	0.31	0/679	0.54	0/917
13	C3	0.29	0/679	0.53	0/917
13	C4	0.39	0/679	0.57	0/917
13	C5	0.31	0/679	0.54	0/917
13	C8	0.39	0/679	0.57	0/917
13	C9	0.31	0/679	0.54	0/917
13	CD	0.39	0/679	0.57	0/917
13	CE	0.31	0/679	0.54	0/917
13	CF	0.29	0/679	0.53	0/917
13	CK	0.39	0/679	0.57	0/917
13	CL	0.31	0/679	0.54	0/917
13	CM	0.29	0/679	0.53	0/917
13	CR	0.39	0/679	0.57	0/917
13	CS	0.31	0/679	0.54	0/917
13	CT	0.29	0/679	0.53	0/917
13	CY	0.39	0/679	0.57	0/917
13	CZ	0.31	0/679	0.54	0/917
13	Ca	0.29	0/679	0.53	0/917
13	Cf	0.39	0/679	0.57	0/917
13	Cg	0.31	0/679	0.54	0/917
13	Ch	0.29	0/679	0.53	0/917
13	Cm	0.39	0/679	0.57	0/917
13	Cn	0.32	0/679	0.54	0/917
13	Co	0.30	0/679	0.53	0/917
13	Ct	0.39	0/679	0.57	0/917
13	Cu	0.31	0/679	0.55	0/917
13	Cv	0.29	0/679	0.53	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
13	D1	0.29	0/679	0.53	0/917
13	D5	0.39	0/679	0.57	0/917
13	D6	0.31	0/679	0.54	0/917
13	D7	0.29	0/679	0.53	0/917
13	DD	0.30	0/679	0.53	0/917
13	DI	0.39	0/679	0.57	0/917
13	DJ	0.31	0/679	0.54	0/917
13	DK	0.29	0/679	0.53	0/917
13	DM	0.29	0/679	0.53	0/917
13	DN	0.29	0/679	0.53	0/917
13	DO	0.29	0/679	0.53	0/917
13	DP	0.29	0/679	0.53	0/917
13	DQ	0.29	0/679	0.53	0/917
13	DR	0.29	0/679	0.53	0/917
13	DS	0.29	0/679	0.53	0/917
13	DT	0.29	0/679	0.53	0/917
13	DU	0.39	0/679	0.57	0/917
13	DV	0.31	0/679	0.54	0/917
13	DW	0.29	0/679	0.53	0/917
13	Da	0.39	0/679	0.57	0/917
13	Db	0.31	0/679	0.54	0/917
13	Dc	0.29	0/679	0.53	0/917
13	Dg	0.39	0/679	0.57	0/917
13	Dh	0.31	0/679	0.54	0/917
13	Di	0.29	0/679	0.53	0/917
13	Dm	0.39	0/679	0.57	0/917
13	Dn	0.31	0/679	0.54	0/917
13	Do	0.29	0/679	0.53	0/917
13	Ds	0.39	0/679	0.57	0/917
13	Dt	0.31	0/679	0.54	0/917
13	Du	0.29	0/679	0.53	0/917
13	Dy	0.39	0/679	0.57	0/917
13	Dz	0.31	0/679	0.54	0/917
13	EA	0.39	0/679	0.57	0/917
13	EB	0.31	0/679	0.54	0/917
13	EE	0.39	0/679	0.57	0/917
13	EF	0.31	0/679	0.54	0/917
13	EG	0.30	0/679	0.53	0/917
13	EL	0.39	0/679	0.57	0/917
13	EM	0.31	0/679	0.54	0/917
13	EN	0.29	0/679	0.53	0/917
13	ES	0.39	0/679	0.57	0/917
13	ET	0.31	0/679	0.54	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
13	EU	0.29	0/679	0.53	0/917
13	EZ	0.39	0/679	0.57	0/917
13	FC	0.39	0/679	0.57	0/917
13	FD	0.39	0/679	0.57	0/917
13	FE	0.39	0/679	0.57	0/917
13	FF	0.39	0/679	0.57	0/917
13	FG	0.39	0/679	0.57	0/917
13	FH	0.39	0/679	0.57	0/917
13	FI	0.31	0/679	0.54	0/917
13	FJ	0.31	0/679	0.54	0/917
13	FK	0.31	0/679	0.54	0/917
13	FL	0.31	0/679	0.54	0/917
13	FM	0.31	0/679	0.54	0/917
13	FN	0.31	0/679	0.54	0/917
14	B5	0.24	0/2447	0.46	0/3300
14	Bc	0.23	0/2447	0.46	0/3300
14	Bj	0.23	0/2447	0.46	0/3300
14	Bq	0.23	0/2447	0.46	0/3300
14	Bx	0.24	0/2447	0.46	0/3300
14	C6	0.23	0/2447	0.46	0/3300
14	CB	0.23	0/2447	0.46	0/3300
14	CI	0.23	0/2447	0.46	0/3300
14	CP	0.23	0/2447	0.46	0/3300
14	CW	0.23	0/2447	0.46	0/3300
14	Cd	0.23	0/2447	0.46	0/3300
14	Ck	0.23	0/2447	0.46	0/3300
14	Cr	0.23	0/2447	0.46	0/3300
14	Cy	0.23	0/2447	0.46	0/3300
14	D3	0.23	0/2447	0.46	0/3300
14	D9	0.23	0/2447	0.46	0/3300
14	DA	0.24	0/2447	0.46	0/3300
14	DG	0.23	0/2447	0.46	0/3300
14	DY	0.23	0/2447	0.46	0/3300
14	De	0.23	0/2447	0.46	0/3300
14	Dk	0.23	0/2447	0.46	0/3300
14	Dq	0.23	0/2447	0.46	0/3300
14	Dw	0.24	0/2447	0.46	0/3300
14	E1	0.23	0/2447	0.46	0/3300
14	E2	0.23	0/2447	0.46	0/3300
14	E3	0.23	0/2447	0.46	0/3300
14	E4	0.23	0/2447	0.46	0/3300
14	EC	0.23	0/2447	0.46	0/3300
14	EJ	0.23	0/2447	0.46	0/3300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
14	EQ	0.23	0/2447	0.46	0/3300
14	EX	0.23	0/2447	0.46	0/3300
14	Ex	0.23	0/2447	0.46	0/3300
14	Ey	0.23	0/2447	0.46	0/3300
14	Ez	0.23	0/2447	0.46	0/3300
15	B6	0.24	0/1004	0.41	0/1349
15	Bd	0.24	0/1004	0.41	0/1349
15	Bk	0.24	0/1004	0.40	0/1349
15	Br	0.24	0/1004	0.41	0/1349
15	By	0.24	0/1004	0.41	0/1349
15	C7	0.24	0/1004	0.41	0/1349
15	CC	0.24	0/1004	0.41	0/1349
15	CJ	0.24	0/1004	0.40	0/1349
15	CQ	0.24	0/1004	0.41	0/1349
15	CX	0.24	0/1004	0.41	0/1349
15	Ce	0.24	0/1004	0.41	0/1349
15	Cl	0.24	0/1004	0.41	0/1349
15	Cs	0.24	0/1004	0.41	0/1349
15	Cz	0.24	0/1004	0.41	0/1349
15	D0	0.24	0/1004	0.41	0/1349
15	D4	0.24	0/1004	0.41	0/1349
15	DB	0.24	0/1004	0.41	0/1349
15	DH	0.24	0/1004	0.40	0/1349
15	DZ	0.24	0/1004	0.41	0/1349
15	Df	0.24	0/1004	0.41	0/1349
15	Dl	0.24	0/1004	0.41	0/1349
15	Dr	0.24	0/1004	0.41	0/1349
15	Dx	0.24	0/1004	0.41	0/1349
15	E0	0.24	0/1004	0.41	0/1349
15	E6	0.24	0/1004	0.41	0/1349
15	E7	0.23	0/1004	0.41	0/1349
15	E8	0.24	0/1004	0.41	0/1349
15	E9	0.24	0/1004	0.41	0/1349
15	ED	0.24	0/1004	0.41	0/1349
15	EK	0.24	0/1004	0.41	0/1349
15	ER	0.24	0/1004	0.41	0/1349
15	EY	0.24	0/1004	0.40	0/1349
15	FA	0.24	0/1004	0.40	0/1349
15	FB	0.24	0/1004	0.41	0/1349
16	B4	0.27	0/2482	0.50	0/3375
16	Bb	0.28	0/2482	0.50	0/3375
16	Bi	0.28	0/2482	0.50	0/3375
16	Bp	0.28	0/2482	0.50	0/3375

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	Bw	0.27	0/2482	0.50	0/3375
16	C0	0.27	0/2482	0.50	0/3375
16	CA	0.27	0/2482	0.50	0/3375
16	CH	0.28	0/2482	0.50	0/3375
16	CO	0.28	0/2482	0.50	0/3375
16	CV	0.28	0/2482	0.50	0/3375
16	Cc	0.28	0/2482	0.50	0/3375
16	Cj	0.28	0/2482	0.50	0/3375
16	Cq	0.27	0/2482	0.50	0/3375
16	Cx	0.28	0/2482	0.50	0/3375
16	D2	0.27	0/2482	0.50	0/3375
16	D8	0.27	0/2482	0.50	0/3375
16	DC	0.28	0/2482	0.50	0/3375
16	DF	0.28	0/2482	0.50	0/3375
16	DX	0.28	0/2482	0.50	0/3375
16	Dd	0.28	0/2482	0.50	0/3375
16	Dj	0.28	0/2482	0.50	0/3375
16	Dp	0.28	0/2482	0.50	0/3375
16	Dv	0.28	0/2482	0.50	0/3375
16	E5	0.27	0/2482	0.50	0/3375
16	EI	0.28	0/2482	0.50	0/3375
16	EP	0.28	0/2482	0.50	0/3375
16	EW	0.28	0/2482	0.50	0/3375
16	Eq	0.27	0/2482	0.50	0/3375
16	Er	0.28	0/2482	0.50	0/3375
16	Es	0.28	0/2482	0.50	0/3375
16	Et	0.27	0/2482	0.50	0/3375
16	Eu	0.27	0/2482	0.50	0/3375
16	Ev	0.27	0/2482	0.50	0/3375
16	Ew	0.28	0/2482	0.50	0/3375
All	All	0.31	27/621926 (0.0%)	0.52	68/842993 (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	0	0	2
1	1	0	1
1	5	0	1
1	6	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	8	0	1
1	AF	0	1
1	AI	0	1
1	AM	0	2
1	AN	0	1
1	ZA	0	1
3	A0	0	1
3	A6	0	1
5	AA	0	2
5	AB	0	1
5	AC	0	1
5	AE	0	1
6	UI	0	2
6	UJ	0	2
6	UK	0	3
6	UL	0	3
6	UM	0	2
6	UN	0	2
6	UO	0	2
6	UP	0	3
6	WA	0	3
6	WB	0	4
6	WC	0	3
6	WD	0	1
6	WE	0	2
6	WF	0	3
6	WG	0	3
6	WI	0	1
6	WJ	0	3
6	WK	0	2
6	WL	0	2
6	WM	0	1
6	WN	0	1
6	WO	0	1
6	WP	0	3
6	WQ	0	2
6	WR	0	3
6	WS	0	1
6	WT	0	2
6	WU	0	2
6	WV	0	3
6	WW	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	Aw	0	1
10	BD	0	1
10	BF	0	1
11	ZG	0	1
11	ZI	0	1
11	ZK	0	1
11	ZO	0	1
11	ZW	0	1
11	Zb	0	1
11	Zd	0	1
11	Ze	0	1
12	a	0	1
12	b	0	1
12	c	0	1
12	d	0	1
12	e	0	1
12	f	0	1
12	g	0	1
12	h	0	1
12	i	0	1
12	j	0	1
12	k	0	1
12	l	0	1
12	m	0	1
12	n	0	1
12	o	0	1
12	p	0	1
12	q	0	1
12	r	0	1
12	s	0	1
12	t	0	1
12	u	0	1
12	v	0	1
12	w	0	1
12	x	0	1
12	y	0	1
12	z	0	1
13	B1	0	1
13	B2	0	1
13	B7	0	1
13	B8	0	1
13	B9	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	BY	0	1
13	BZ	0	1
13	Be	0	1
13	Bf	0	1
13	Bg	0	1
13	Bl	0	1
13	Bm	0	1
13	Bn	0	1
13	Bs	0	1
13	Bt	0	1
13	Bu	0	1
13	Bz	0	1
13	C1	0	1
13	C2	0	1
13	C3	0	1
13	C4	0	1
13	C5	0	1
13	C8	0	1
13	C9	0	1
13	CD	0	1
13	CE	0	1
13	CF	0	1
13	CK	0	1
13	CL	0	1
13	CM	0	1
13	CR	0	1
13	CS	0	1
13	CT	0	1
13	CY	0	1
13	CZ	0	1
13	Ca	0	1
13	Cf	0	1
13	Cg	0	1
13	Ch	0	1
13	Cm	0	1
13	Cn	0	1
13	Co	0	1
13	Ct	0	1
13	Cu	0	1
13	Cv	0	1
13	D1	0	1
13	D5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	D6	0	1
13	D7	0	1
13	DD	0	1
13	DI	0	1
13	DJ	0	1
13	DK	0	1
13	DM	0	1
13	DN	0	1
13	DO	0	1
13	DP	0	1
13	DQ	0	1
13	DR	0	1
13	DS	0	1
13	DT	0	1
13	DU	0	1
13	DV	0	1
13	DW	0	1
13	Da	0	1
13	Db	0	1
13	Dc	0	1
13	Dg	0	1
13	Dh	0	1
13	Di	0	1
13	Dm	0	1
13	Dn	0	1
13	Do	0	1
13	Ds	0	1
13	Dt	0	1
13	Du	0	1
13	Dy	0	1
13	Dz	0	1
13	EA	0	1
13	EB	0	1
13	EE	0	1
13	EF	0	1
13	EG	0	1
13	EL	0	1
13	EM	0	1
13	EN	0	1
13	ES	0	1
13	ET	0	1
13	EU	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	EZ	0	1
13	FC	0	1
13	FD	0	1
13	FE	0	1
13	FF	0	1
13	FG	0	1
13	FH	0	1
13	FI	0	1
13	FJ	0	1
13	FK	0	1
13	FL	0	1
13	FM	0	1
13	FN	0	1
16	B4	0	2
16	Bb	0	2
16	Bi	0	2
16	Bp	0	2
16	Bw	0	2
16	C0	0	2
16	CA	0	2
16	CH	0	2
16	CO	0	2
16	CV	0	2
16	Cc	0	2
16	Cj	0	2
16	Cq	0	2
16	Cx	0	2
16	D2	0	2
16	D8	0	2
16	DC	0	2
16	DF	0	2
16	DX	0	2
16	Dd	0	2
16	Dj	0	2
16	Dp	0	2
16	Dv	0	2
16	E5	0	2
16	EI	0	2
16	EP	0	2
16	EW	0	2
16	Eq	0	2
16	Er	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	Es	0	2
16	Et	0	2
16	Eu	0	2
16	Ev	0	2
16	Ew	0	2
All	All	0	293

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	ZV	140	PRO	CG-CD	-16.08	0.97	1.50
6	BK	331	PRO	CG-CD	-14.23	1.03	1.50
10	BC	73	PRO	CG-CD	-12.74	1.08	1.50
11	ZV	125	PRO	CG-CD	-10.17	1.17	1.50
6	UM	172	PRO	N-CD	-9.56	1.34	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BC	73	PRO	N-CD-CG	-18.84	74.94	103.20
10	BC	73	PRO	CB-CG-CD	18.81	179.84	106.50
11	ZV	140	PRO	N-CD-CG	-17.35	77.18	103.20
6	BK	331	PRO	N-CD-CG	-16.11	79.04	103.20
10	BC	73	PRO	CA-CB-CG	-14.02	77.37	104.00

There are no chirality outliers.

5 of 293 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	36	ARG	Sidechain
1	0	50	ARG	Sidechain
1	1	36	ARG	Sidechain
1	5	50	ARG	Sidechain
1	6	153	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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	0	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	67
1	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	67
1	2	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	53
1	3	258/260 (99%)	248 (96%)	8 (3%)	2 (1%)	16	53
1	4	258/260 (99%)	248 (96%)	7 (3%)	3 (1%)	11	43
1	5	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	53
1	6	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	53
1	7	258/260 (99%)	245 (95%)	10 (4%)	3 (1%)	11	43
1	8	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	53
1	9	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	53
1	AF	250/260 (96%)	238 (95%)	11 (4%)	1 (0%)	30	67
1	AG	251/260 (96%)	237 (94%)	13 (5%)	1 (0%)	30	67
1	AH	252/260 (97%)	241 (96%)	10 (4%)	1 (0%)	30	67
1	AI	250/260 (96%)	241 (96%)	7 (3%)	2 (1%)	16	53
1	AJ	251/260 (96%)	241 (96%)	9 (4%)	1 (0%)	30	67
1	AK	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	30	67
1	AL	244/260 (94%)	237 (97%)	4 (2%)	3 (1%)	11	43
1	AM	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	67
1	AN	244/260 (94%)	240 (98%)	3 (1%)	1 (0%)	30	67
1	ZA	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	43
1	ZB	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	43
1	ZC	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	43
1	ZD	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	53
1	ZE	258/260 (99%)	245 (95%)	12 (5%)	1 (0%)	30	67
2	A	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	C	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	D	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	E	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	63
2	F	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	63
2	G	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	H	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	63
2	I	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	J	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	K	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	L	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	M	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	N	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	63
2	O	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	P	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	Q	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	R	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	S	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	T	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	U	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	V	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	W	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	X	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	Y	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	63
2	Z	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
3	A0	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
3	A6	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
3	A7	115/138 (83%)	114 (99%)	1 (1%)	0	100	100
3	A8	119/138 (86%)	116 (98%)	3 (2%)	0	100	100
3	A9	121/138 (88%)	118 (98%)	3 (2%)	0	100	100
4	A1	87/104 (84%)	87 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A2	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
4	A3	89/104 (86%)	89 (100%)	0	0	100	100
4	A4	89/104 (86%)	89 (100%)	0	0	100	100
4	A5	88/104 (85%)	88 (100%)	0	0	100	100
4	Az	55/104 (53%)	53 (96%)	2 (4%)	0	100	100
5	AA	246/251 (98%)	232 (94%)	11 (4%)	3 (1%)	11	43
5	AB	247/251 (98%)	241 (98%)	6 (2%)	0	100	100
5	AC	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
5	AD	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
5	AE	247/251 (98%)	233 (94%)	13 (5%)	1 (0%)	30	67
6	AO	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AP	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AQ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AR	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AS	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AT	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AU	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AV	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AW	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AX	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AY	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AZ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Aa	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ac	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ad	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ae	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Af	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ag	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ah	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ai	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Aj	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Ak	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Al	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Am	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	An	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ao	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ap	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	B0	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	B3	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	BG	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
6	BH	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
6	BI	18/560 (3%)	18 (100%)	0	0	100	100
6	BJ	14/560 (2%)	14 (100%)	0	0	100	100
6	BK	19/560 (3%)	19 (100%)	0	0	100	100
6	BL	14/560 (2%)	13 (93%)	1 (7%)	0	100	100
6	BM	19/560 (3%)	19 (100%)	0	0	100	100
6	BN	14/560 (2%)	14 (100%)	0	0	100	100
6	BO	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
6	BP	14/560 (2%)	14 (100%)	0	0	100	100
6	BQ	19/560 (3%)	19 (100%)	0	0	100	100
6	BR	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BS	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BT	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BU	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BV	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BW	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BX	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ba	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Bh	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Bo	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Bv	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	CG	25/560 (4%)	24 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CN	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	CU	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Cb	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ci	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Cp	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Cw	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	DE	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	DL	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	EH	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	EO	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	EV	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ea	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Eb	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ec	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ed	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ee	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ef	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Eg	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Eh	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ei	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ej	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ek	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	El	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Em	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	En	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Eo	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ep	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	UI	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UJ	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UK	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UL	151/560 (27%)	142 (94%)	7 (5%)	2 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	UM	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UN	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UO	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UP	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	WA	111/560 (20%)	99 (89%)	9 (8%)	3 (3%)	4	26
6	WB	109/560 (20%)	94 (86%)	10 (9%)	5 (5%)	2	18
6	WC	106/560 (19%)	96 (91%)	9 (8%)	1 (1%)	14	50
6	WD	108/560 (19%)	99 (92%)	4 (4%)	5 (5%)	2	18
6	WE	110/560 (20%)	98 (89%)	8 (7%)	4 (4%)	3	21
6	WF	109/560 (20%)	98 (90%)	8 (7%)	3 (3%)	4	25
6	WG	110/560 (20%)	98 (89%)	10 (9%)	2 (2%)	7	34
6	WH	93/560 (17%)	86 (92%)	5 (5%)	2 (2%)	5	30
6	WI	93/560 (17%)	82 (88%)	5 (5%)	6 (6%)	1	13
6	WJ	97/560 (17%)	89 (92%)	7 (7%)	1 (1%)	13	48
6	WK	96/560 (17%)	84 (88%)	9 (9%)	3 (3%)	3	23
6	WL	81/560 (14%)	75 (93%)	4 (5%)	2 (2%)	4	27
6	WM	78/560 (14%)	72 (92%)	4 (5%)	2 (3%)	4	26
6	WN	80/560 (14%)	75 (94%)	2 (2%)	3 (4%)	2	20
6	WO	94/560 (17%)	85 (90%)	7 (7%)	2 (2%)	5	31
6	WP	98/560 (18%)	87 (89%)	6 (6%)	5 (5%)	1	16
6	WQ	109/560 (20%)	100 (92%)	5 (5%)	4 (4%)	2	21
6	WR	109/560 (20%)	94 (86%)	8 (7%)	7 (6%)	1	13
6	WS	109/560 (20%)	96 (88%)	7 (6%)	6 (6%)	1	15
6	WT	109/560 (20%)	97 (89%)	5 (5%)	7 (6%)	1	13
6	WU	110/560 (20%)	101 (92%)	8 (7%)	1 (1%)	14	50
6	WV	108/560 (19%)	97 (90%)	9 (8%)	2 (2%)	6	33
6	WW	109/560 (20%)	95 (87%)	9 (8%)	5 (5%)	2	18
7	Ab	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
7	Aq	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
7	Ar	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
7	As	87/89 (98%)	85 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	At	251/264 (95%)	232 (92%)	13 (5%)	6 (2%)	5	28
9	Au	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
9	Av	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13	48
9	Aw	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
9	Ax	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25	63
9	Ay	207/245 (84%)	201 (97%)	4 (2%)	2 (1%)	13	48
10	BA	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
10	BB	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
10	BC	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
10	BD	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
10	BE	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16	53
10	BF	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
11	ZF	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	ZG	399/403 (99%)	392 (98%)	6 (2%)	1 (0%)	37	72
11	ZH	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25	63
11	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
11	ZK	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
11	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	72
11	ZM	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	ZN	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	ZO	399/403 (99%)	381 (96%)	15 (4%)	3 (1%)	16	53
11	ZP	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	72
11	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
11	ZR	399/403 (99%)	390 (98%)	8 (2%)	1 (0%)	37	72
11	ZS	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
11	ZT	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
11	ZU	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
11	ZV	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
11	ZW	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
11	ZX	399/403 (99%)	388 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	ZY	399/403 (99%)	384 (96%)	15 (4%)	0	100	100
11	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
11	Za	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	Zb	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
11	Zc	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
11	Zd	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	Ze	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
11	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
11	Zg	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
11	Zh	399/403 (99%)	393 (98%)	6 (2%)	0	100	100
12	a	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	b	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	c	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	d	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	e	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	f	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	g	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	h	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	i	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	j	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	k	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	l	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	m	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	n	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	o	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	p	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	q	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	r	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	s	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	t	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	u	297/365 (81%)	293 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	v	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	w	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	x	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	y	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	z	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
13	B1	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	B2	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	B7	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	B8	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	B9	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	BY	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	BZ	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Be	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Bf	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Bg	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Bl	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Bm	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Bn	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Bs	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Bt	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Bu	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Bz	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	C1	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	C2	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	C3	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	C4	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	C5	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	C8	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	C9	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	CD	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	CE	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CF	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	CK	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	CL	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	CM	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	CR	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	CS	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	CT	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	CY	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	CZ	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Ca	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Cf	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Cg	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Ch	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Cm	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Cn	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Co	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Ct	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Cu	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Cv	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	D1	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	D5	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	D6	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	D7	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DD	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DI	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	DJ	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	DK	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DM	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DN	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DO	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DP	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	DQ	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DR	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DS	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DT	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DU	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	DV	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	DW	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Da	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Db	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Dc	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Dg	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Dh	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Di	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Dm	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Dn	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Do	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Ds	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Dt	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Du	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Dy	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Dz	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	EA	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	EB	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	EE	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	EF	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	EG	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	EL	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	EM	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	EN	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	ES	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	ET	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	EU	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	EZ	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	FC	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	FD	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	FE	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	FF	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	FG	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	FH	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	FI	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	FJ	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	FK	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	FL	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	FM	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	FN	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
14	B5	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Bc	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Bj	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Bq	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Bx	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	C6	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	CB	306/331 (92%)	296 (97%)	9 (3%)	1 (0%)	37	72
14	CI	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	CP	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	CW	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Cd	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Ck	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Cr	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Cy	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	D3	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	D9	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	DA	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	DG	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	DY	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	De	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Dk	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Dq	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Dw	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	E1	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	E2	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	E3	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	E4	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	EC	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	EJ	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	EQ	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	EX	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Ex	306/331 (92%)	296 (97%)	9 (3%)	1 (0%)	37	72
14	Ey	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Ez	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
15	B6	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Bd	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Bk	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Br	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	By	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	C7	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	CC	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	CJ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	CQ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	CX	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Ce	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Cl	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Cs	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Cz	127/129 (98%)	125 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	D0	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	D4	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	DB	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	DH	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	DZ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Df	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Dl	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Dr	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Dx	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	E0	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	E6	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	E7	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	E8	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	E9	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	ED	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	EK	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	ER	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	EY	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	FA	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	FB	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
16	B4	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Bb	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Bi	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Bp	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Bw	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	C0	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	CA	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	CH	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	CO	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	CV	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Cc	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Cj	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Cq	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Cx	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	D2	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	D8	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	DC	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	DF	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	DX	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Dd	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Dj	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Dp	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Dv	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	E5	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	EI	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	EP	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	EW	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Eq	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Er	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Es	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Et	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Eu	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Ev	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Ew	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
All	All	79048/141237 (56%)	76302 (96%)	2146 (3%)	600 (1%)	19	53

5 of 600 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	209	ASN
1	5	209	ASN
1	8	209	ASN
5	AA	123	GLU
8	At	188	LEU

### 5.3.2 Protein sidechains ⓘ

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	0	205/215 (95%)	198 (97%)	7 (3%)	32	54
1	1	209/215 (97%)	201 (96%)	8 (4%)	28	50
1	2	215/215 (100%)	212 (99%)	3 (1%)	62	76
1	3	215/215 (100%)	211 (98%)	4 (2%)	52	70
1	4	215/215 (100%)	211 (98%)	4 (2%)	52	70
1	5	215/215 (100%)	211 (98%)	4 (2%)	52	70
1	6	215/215 (100%)	210 (98%)	5 (2%)	45	65
1	7	215/215 (100%)	214 (100%)	1 (0%)	86	90
1	8	215/215 (100%)	213 (99%)	2 (1%)	75	83
1	9	215/215 (100%)	211 (98%)	4 (2%)	52	70
1	AF	209/215 (97%)	204 (98%)	5 (2%)	44	64
1	AG	210/215 (98%)	203 (97%)	7 (3%)	33	55
1	AH	211/215 (98%)	201 (95%)	10 (5%)	22	45
1	AI	209/215 (97%)	200 (96%)	9 (4%)	25	48
1	AJ	210/215 (98%)	202 (96%)	8 (4%)	28	50
1	AK	200/215 (93%)	196 (98%)	4 (2%)	50	69
1	AL	205/215 (95%)	199 (97%)	6 (3%)	37	58
1	AM	205/215 (95%)	197 (96%)	8 (4%)	27	50
1	AN	205/215 (95%)	201 (98%)	4 (2%)	50	69
1	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	83
1	ZB	215/215 (100%)	207 (96%)	8 (4%)	29	51
1	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	76
1	ZD	215/215 (100%)	212 (99%)	3 (1%)	62	76
1	ZE	215/215 (100%)	214 (100%)	1 (0%)	86	90
2	A	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	B	170/186 (91%)	163 (96%)	7 (4%)	26	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	D	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	E	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	F	170/186 (91%)	162 (95%)	8 (5%)	22	45
2	G	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	H	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	I	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	J	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	K	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	L	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	M	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	N	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	O	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	P	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	Q	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	R	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	S	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	T	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	U	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	V	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	W	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	X	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	Y	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	Z	170/186 (91%)	163 (96%)	7 (4%)	26	49
3	A0	102/113 (90%)	96 (94%)	6 (6%)	16	39
3	A6	110/113 (97%)	106 (96%)	4 (4%)	30	52
3	A7	101/113 (89%)	99 (98%)	2 (2%)	50	69
3	A8	103/113 (91%)	96 (93%)	7 (7%)	13	34
3	A9	104/113 (92%)	102 (98%)	2 (2%)	52	70
4	A1	68/79 (86%)	64 (94%)	4 (6%)	16	39
4	A2	70/79 (89%)	65 (93%)	5 (7%)	12	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A3	70/79 (89%)	66 (94%)	4 (6%)	17	40
4	A4	70/79 (89%)	66 (94%)	4 (6%)	17	40
4	A5	69/79 (87%)	65 (94%)	4 (6%)	17	39
4	Az	45/79 (57%)	40 (89%)	5 (11%)	5	19
5	AA	190/193 (98%)	187 (98%)	3 (2%)	58	74
5	AB	191/193 (99%)	188 (98%)	3 (2%)	58	74
5	AC	192/193 (100%)	187 (97%)	5 (3%)	41	61
5	AD	192/193 (100%)	190 (99%)	2 (1%)	73	82
5	AE	191/193 (99%)	190 (100%)	1 (0%)	86	90
6	AO	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AP	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AQ	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AR	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AS	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AT	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AU	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AV	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AW	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AX	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AY	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AZ	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Aa	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ac	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ad	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ae	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Af	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ag	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ah	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ai	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Aj	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ak	141/467 (30%)	134 (95%)	7 (5%)	20	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Al	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Am	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	An	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ao	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ap	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	B0	26/467 (6%)	26 (100%)	0	100	100
6	B3	26/467 (6%)	26 (100%)	0	100	100
6	BG	8/467 (2%)	8 (100%)	0	100	100
6	BH	11/467 (2%)	10 (91%)	1 (9%)	7	25
6	BI	14/467 (3%)	12 (86%)	2 (14%)	2	14
6	BJ	11/467 (2%)	11 (100%)	0	100	100
6	BK	15/467 (3%)	15 (100%)	0	100	100
6	BL	11/467 (2%)	11 (100%)	0	100	100
6	BM	15/467 (3%)	15 (100%)	0	100	100
6	BN	11/467 (2%)	11 (100%)	0	100	100
6	BO	14/467 (3%)	13 (93%)	1 (7%)	12	33
6	BP	11/467 (2%)	11 (100%)	0	100	100
6	BQ	15/467 (3%)	14 (93%)	1 (7%)	13	35
6	BR	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BS	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BT	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BU	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BV	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BW	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BX	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ba	26/467 (6%)	26 (100%)	0	100	100
6	Bh	26/467 (6%)	26 (100%)	0	100	100
6	Bo	26/467 (6%)	26 (100%)	0	100	100
6	Bv	26/467 (6%)	26 (100%)	0	100	100
6	CG	26/467 (6%)	26 (100%)	0	100	100
6	CN	26/467 (6%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	CU	26/467 (6%)	26 (100%)	0	100	100
6	Cb	26/467 (6%)	26 (100%)	0	100	100
6	Ci	26/467 (6%)	26 (100%)	0	100	100
6	Cp	26/467 (6%)	26 (100%)	0	100	100
6	Cw	26/467 (6%)	26 (100%)	0	100	100
6	DE	26/467 (6%)	26 (100%)	0	100	100
6	DL	26/467 (6%)	26 (100%)	0	100	100
6	EH	26/467 (6%)	26 (100%)	0	100	100
6	EO	26/467 (6%)	26 (100%)	0	100	100
6	EV	26/467 (6%)	26 (100%)	0	100	100
6	Ea	26/467 (6%)	26 (100%)	0	100	100
6	Eb	26/467 (6%)	26 (100%)	0	100	100
6	Ec	26/467 (6%)	26 (100%)	0	100	100
6	Ed	26/467 (6%)	26 (100%)	0	100	100
6	Ee	26/467 (6%)	26 (100%)	0	100	100
6	Ef	26/467 (6%)	26 (100%)	0	100	100
6	Eg	26/467 (6%)	26 (100%)	0	100	100
6	Eh	26/467 (6%)	26 (100%)	0	100	100
6	Ei	26/467 (6%)	26 (100%)	0	100	100
6	Ej	26/467 (6%)	26 (100%)	0	100	100
6	Ek	26/467 (6%)	26 (100%)	0	100	100
6	El	26/467 (6%)	26 (100%)	0	100	100
6	Em	26/467 (6%)	26 (100%)	0	100	100
6	En	26/467 (6%)	26 (100%)	0	100	100
6	Eo	26/467 (6%)	26 (100%)	0	100	100
6	Ep	26/467 (6%)	26 (100%)	0	100	100
6	UI	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UJ	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UK	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UL	128/467 (27%)	122 (95%)	6 (5%)	22	45
6	UM	128/467 (27%)	123 (96%)	5 (4%)	27	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	UN	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UO	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UP	128/467 (27%)	122 (95%)	6 (5%)	22	45
6	WA	95/467 (20%)	91 (96%)	4 (4%)	25	48
6	WB	93/467 (20%)	87 (94%)	6 (6%)	14	36
6	WC	91/467 (20%)	83 (91%)	8 (9%)	8	26
6	WD	92/467 (20%)	88 (96%)	4 (4%)	25	48
6	WE	94/467 (20%)	87 (93%)	7 (7%)	11	31
6	WF	93/467 (20%)	86 (92%)	7 (8%)	11	31
6	WG	94/467 (20%)	87 (93%)	7 (7%)	11	31
6	WH	79/467 (17%)	75 (95%)	4 (5%)	20	43
6	WI	79/467 (17%)	73 (92%)	6 (8%)	11	31
6	WJ	83/467 (18%)	79 (95%)	4 (5%)	21	44
6	WK	82/467 (18%)	77 (94%)	5 (6%)	15	38
6	WL	69/467 (15%)	66 (96%)	3 (4%)	25	48
6	WM	66/467 (14%)	65 (98%)	1 (2%)	60	75
6	WN	68/467 (15%)	66 (97%)	2 (3%)	37	58
6	WO	80/467 (17%)	76 (95%)	4 (5%)	20	43
6	WP	83/467 (18%)	77 (93%)	6 (7%)	12	32
6	WQ	93/467 (20%)	91 (98%)	2 (2%)	47	66
6	WR	93/467 (20%)	86 (92%)	7 (8%)	11	31
6	WS	93/467 (20%)	87 (94%)	6 (6%)	14	36
6	WT	93/467 (20%)	86 (92%)	7 (8%)	11	31
6	WU	94/467 (20%)	90 (96%)	4 (4%)	25	48
6	WV	92/467 (20%)	83 (90%)	9 (10%)	6	22
6	WW	93/467 (20%)	85 (91%)	8 (9%)	8	27
7	Ab	74/74 (100%)	73 (99%)	1 (1%)	62	76
7	Aq	74/74 (100%)	73 (99%)	1 (1%)	62	76
7	Ar	74/74 (100%)	74 (100%)	0	100	100
7	As	74/74 (100%)	73 (99%)	1 (1%)	62	76
8	At	210/221 (95%)	204 (97%)	6 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Au	177/204 (87%)	170 (96%)	7 (4%)	27	49
9	Av	179/204 (88%)	172 (96%)	7 (4%)	27	50
9	Aw	178/204 (87%)	173 (97%)	5 (3%)	38	59
9	Ax	178/204 (87%)	172 (97%)	6 (3%)	32	54
9	Ay	179/204 (88%)	175 (98%)	4 (2%)	47	66
10	BA	104/105 (99%)	104 (100%)	0	100	100
10	BB	104/105 (99%)	103 (99%)	1 (1%)	73	82
10	BC	104/105 (99%)	104 (100%)	0	100	100
10	BD	104/105 (99%)	102 (98%)	2 (2%)	52	70
10	BE	104/105 (99%)	101 (97%)	3 (3%)	37	58
10	BF	104/105 (99%)	100 (96%)	4 (4%)	28	50
11	ZF	321/323 (99%)	310 (97%)	11 (3%)	32	54
11	ZG	321/323 (99%)	306 (95%)	15 (5%)	22	45
11	ZH	321/323 (99%)	309 (96%)	12 (4%)	29	51
11	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	ZJ	321/323 (99%)	313 (98%)	8 (2%)	42	63
11	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	56
11	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	59
11	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	56
11	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	63
11	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	45
11	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	59
11	ZR	321/323 (99%)	313 (98%)	8 (2%)	42	63
11	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	ZT	321/323 (99%)	316 (98%)	5 (2%)	58	74
11	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	79
11	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	79
11	ZW	321/323 (99%)	308 (96%)	13 (4%)	27	49
11	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	83
11	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	74
11	Za	321/323 (99%)	316 (98%)	5 (2%)	58	74
11	Zb	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	54
11	Zd	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	Ze	321/323 (99%)	312 (97%)	9 (3%)	38	59
11	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	66
11	Zg	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	Zh	321/323 (99%)	313 (98%)	8 (2%)	42	63
12	a	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	b	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	c	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	d	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	e	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	f	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	g	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	h	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	i	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	j	248/294 (84%)	240 (97%)	8 (3%)	34	55
12	k	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	l	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	m	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	n	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	o	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	p	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	q	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	r	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	s	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	t	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	u	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	v	248/294 (84%)	238 (96%)	10 (4%)	27	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	w	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	x	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	y	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	z	248/294 (84%)	238 (96%)	10 (4%)	27	49
13	B1	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	B2	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	B7	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	B8	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	B9	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	BY	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	BZ	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Be	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Bf	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Bg	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Bl	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Bm	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Bn	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Bs	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Bt	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Bu	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Bz	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	C1	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	C2	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	C3	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	C4	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	C5	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	C8	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	C9	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	CD	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	CE	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	CF	76/113 (67%)	74 (97%)	2 (3%)	41	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	CK	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	CL	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	CM	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	CR	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	CS	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	CT	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	CY	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	CZ	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Ca	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Cf	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Cg	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Ch	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Cm	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Cn	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Co	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Ct	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Cu	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Cv	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	D1	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	D5	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	D6	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	D7	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DD	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DI	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	DJ	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	DK	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DM	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DN	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DO	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DP	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DQ	76/113 (67%)	74 (97%)	2 (3%)	41	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	DR	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DS	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DT	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DU	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	DV	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	DW	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Da	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Db	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Dc	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Dg	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Dh	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Di	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Dm	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Dn	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Do	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Ds	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Dt	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Du	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Dy	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Dz	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	EA	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	EB	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	EE	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	EF	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	EG	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	EL	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	EM	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	EN	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	ES	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	ET	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	EU	76/113 (67%)	74 (97%)	2 (3%)	41	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	EZ	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FC	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FD	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FE	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FF	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FG	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FH	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FI	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	FJ	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	FK	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	FL	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	FM	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	FN	76/113 (67%)	75 (99%)	1 (1%)	65	77
14	B5	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Bc	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Bj	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Bq	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Bx	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	C6	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	CB	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	CI	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	CP	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	CW	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Cd	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Ck	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Cr	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Cy	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	D3	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	D9	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	DA	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	DG	265/282 (94%)	257 (97%)	8 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	DY	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	De	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Dk	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Dq	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Dw	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	E1	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	E2	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	E3	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	E4	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	EC	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	EJ	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	EQ	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	EX	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Ex	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Ey	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Ez	265/282 (94%)	257 (97%)	8 (3%)	36	57
15	B6	104/104 (100%)	104 (100%)	0	100	100
15	Bd	104/104 (100%)	104 (100%)	0	100	100
15	Bk	104/104 (100%)	104 (100%)	0	100	100
15	Br	104/104 (100%)	104 (100%)	0	100	100
15	By	104/104 (100%)	104 (100%)	0	100	100
15	C7	104/104 (100%)	104 (100%)	0	100	100
15	CC	104/104 (100%)	104 (100%)	0	100	100
15	CJ	104/104 (100%)	104 (100%)	0	100	100
15	CQ	104/104 (100%)	104 (100%)	0	100	100
15	CX	104/104 (100%)	104 (100%)	0	100	100
15	Ce	104/104 (100%)	104 (100%)	0	100	100
15	Cl	104/104 (100%)	104 (100%)	0	100	100
15	Cs	104/104 (100%)	104 (100%)	0	100	100
15	Cz	104/104 (100%)	104 (100%)	0	100	100
15	D0	104/104 (100%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	D4	104/104 (100%)	104 (100%)	0	100	100
15	DB	104/104 (100%)	104 (100%)	0	100	100
15	DH	104/104 (100%)	104 (100%)	0	100	100
15	DZ	104/104 (100%)	104 (100%)	0	100	100
15	Df	104/104 (100%)	104 (100%)	0	100	100
15	Dl	104/104 (100%)	104 (100%)	0	100	100
15	Dr	104/104 (100%)	104 (100%)	0	100	100
15	Dx	104/104 (100%)	104 (100%)	0	100	100
15	E0	104/104 (100%)	104 (100%)	0	100	100
15	E6	104/104 (100%)	104 (100%)	0	100	100
15	E7	104/104 (100%)	104 (100%)	0	100	100
15	E8	104/104 (100%)	104 (100%)	0	100	100
15	E9	104/104 (100%)	104 (100%)	0	100	100
15	ED	104/104 (100%)	104 (100%)	0	100	100
15	EK	104/104 (100%)	104 (100%)	0	100	100
15	ER	104/104 (100%)	104 (100%)	0	100	100
15	EY	104/104 (100%)	104 (100%)	0	100	100
15	FA	104/104 (100%)	104 (100%)	0	100	100
15	FB	104/104 (100%)	104 (100%)	0	100	100
16	B4	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Bb	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Bi	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Bp	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Bw	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	C0	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	CA	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	CH	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	CO	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	CV	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Cc	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Cj	272/301 (90%)	264 (97%)	8 (3%)	37	58

*Continued on next page...*

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Cq	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Cx	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	D2	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	D8	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	DC	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	DF	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	DX	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Dd	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Dj	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Dp	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Dv	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	E5	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	EI	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	EP	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	EW	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Eq	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Er	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Es	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Et	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Eu	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Ev	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Ew	272/301 (90%)	264 (97%)	8 (3%)	37	58
All	All	67515/117432 (58%)	65434 (97%)	2081 (3%)	37	56

5 of 2081 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	Cc	237	GLU
14	Cr	235	LEU
16	Cc	155	ASN
13	FN	106	ILE
6	WW	168	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1341 such sidechains are listed below:

Mol	Chain	Res	Type
12	j	178	GLN
16	DC	245	ASN
12	l	178	GLN
12	j	161	ASN
12	s	54	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

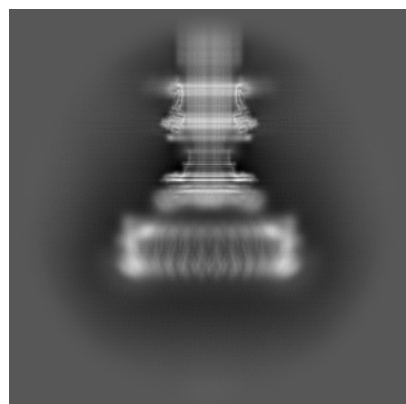
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37684. These allow visual inspection of the internal detail of the map and identification of artifacts.

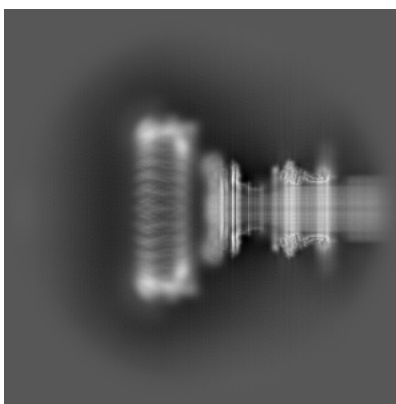
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

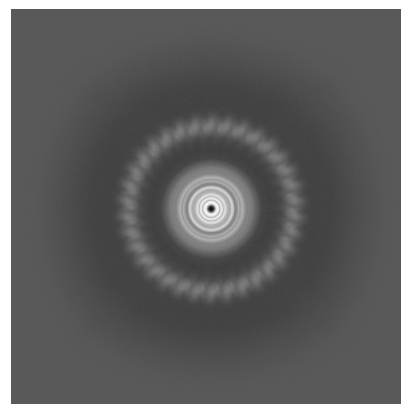
#### 6.1.1 Primary map



X

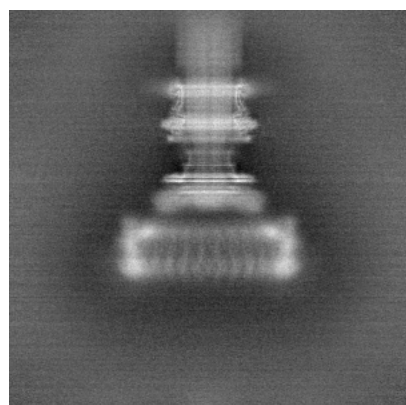


Y

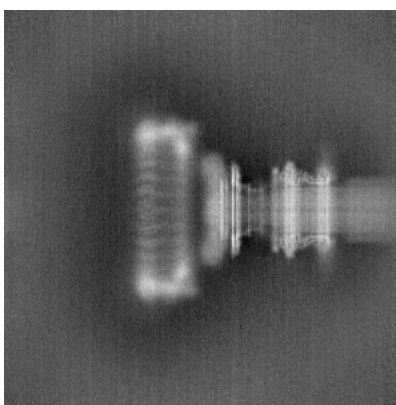


Z

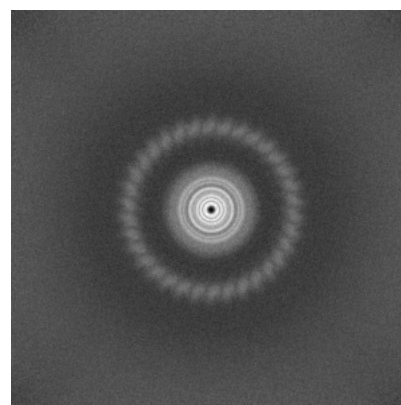
#### 6.1.2 Raw map



X



Y

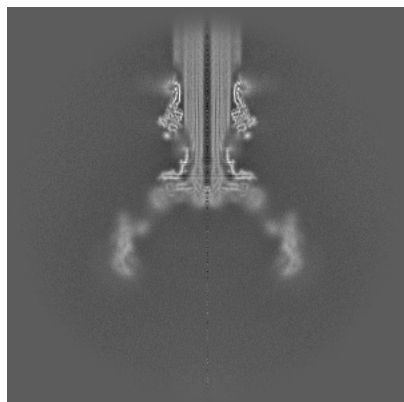


Z

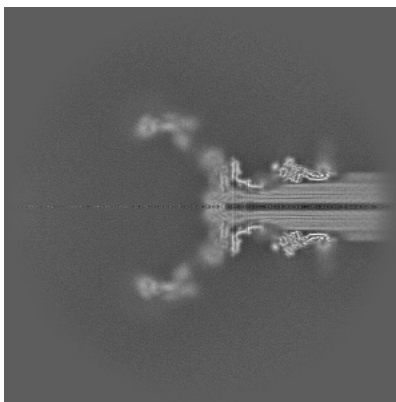
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

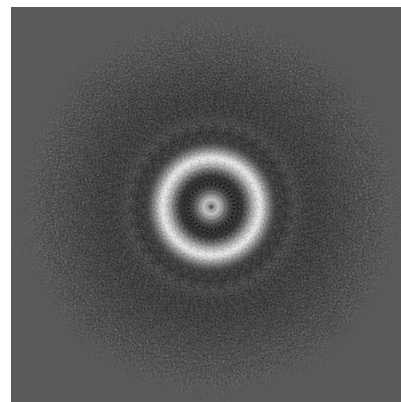
### 6.2.1 Primary map



X Index: 420



Y Index: 420

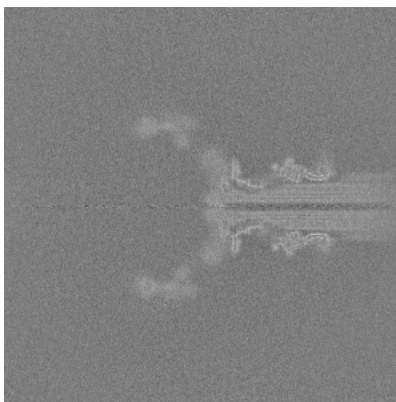


Z Index: 420

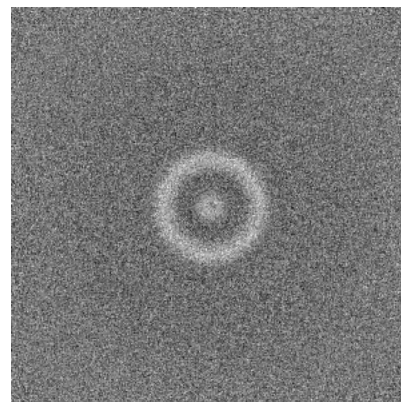
### 6.2.2 Raw map



X Index: 420



Y Index: 420

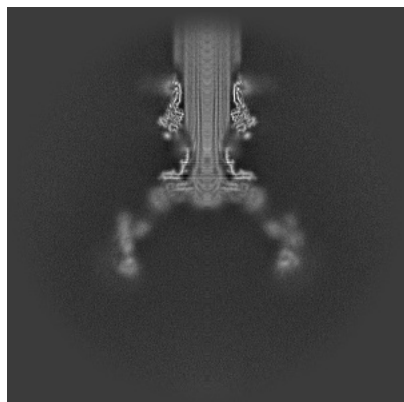


Z Index: 420

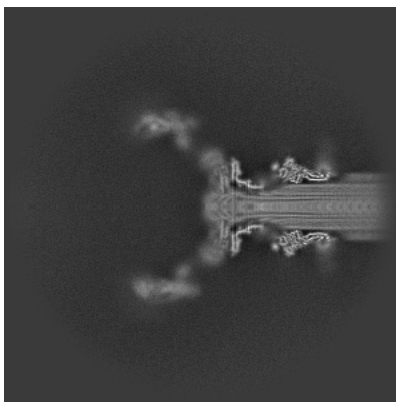
The images above show central slices of the map in three orthogonal directions.

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

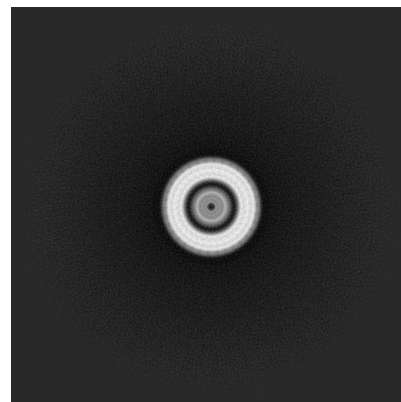
### 6.3.1 Primary map



X Index: 431



Y Index: 431

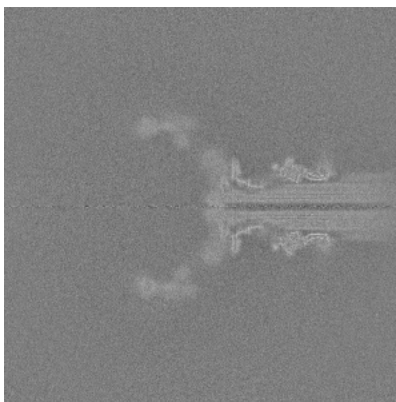


Z Index: 481

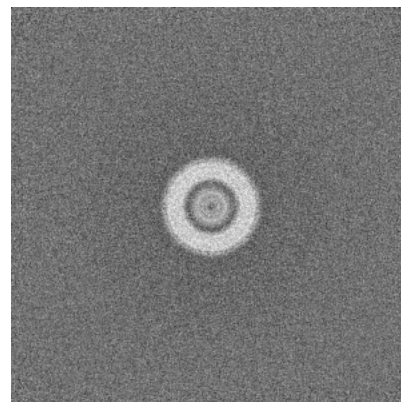
### 6.3.2 Raw map



X Index: 420



Y Index: 420



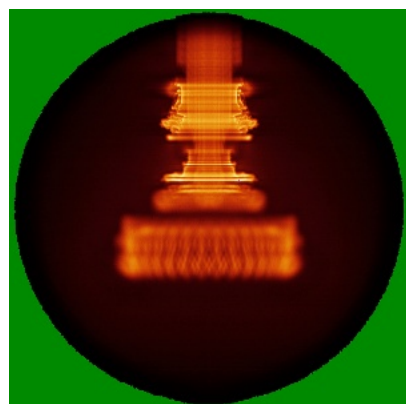
Z Index: 481

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

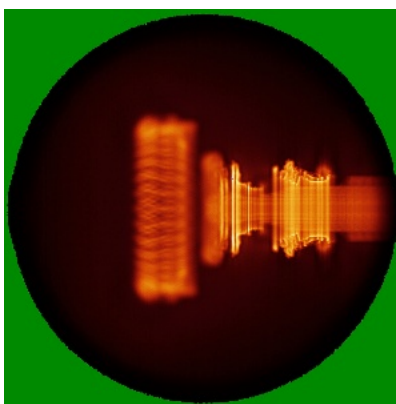


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

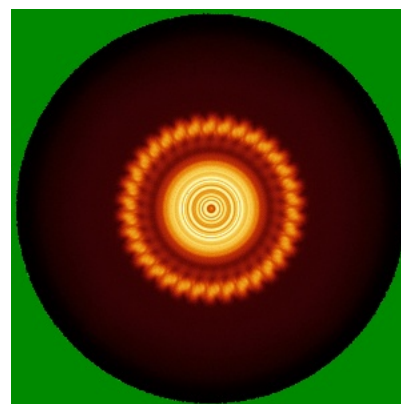
### 6.4.1 Primary map



X

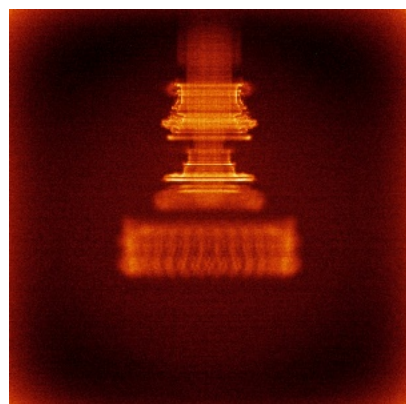


Y

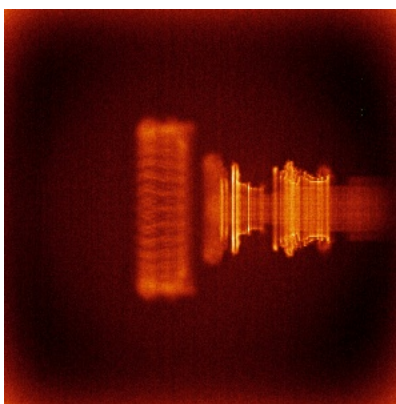


Z

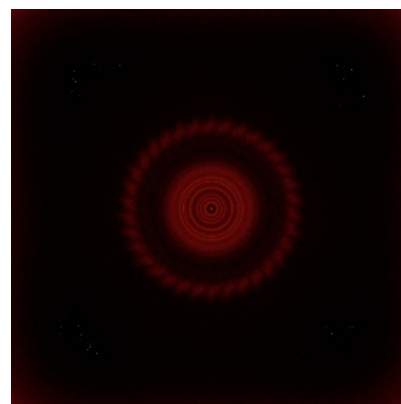
### 6.4.2 Raw map



X



Y



Z

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

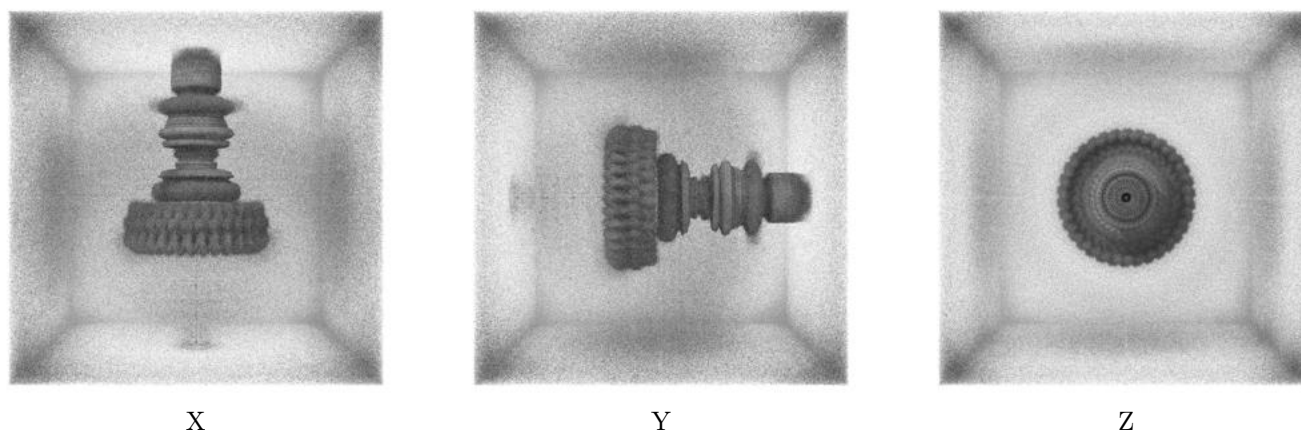
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

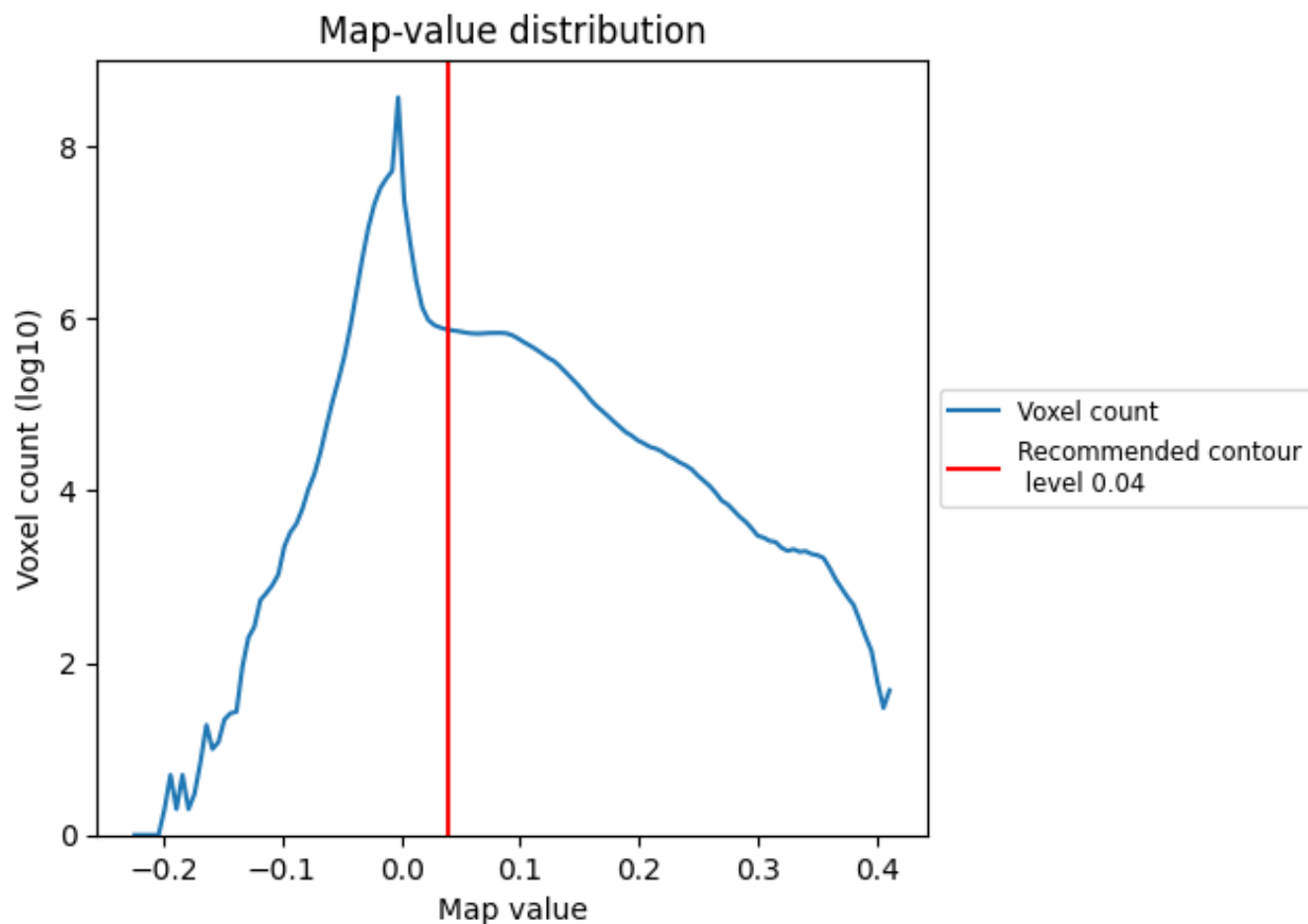
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

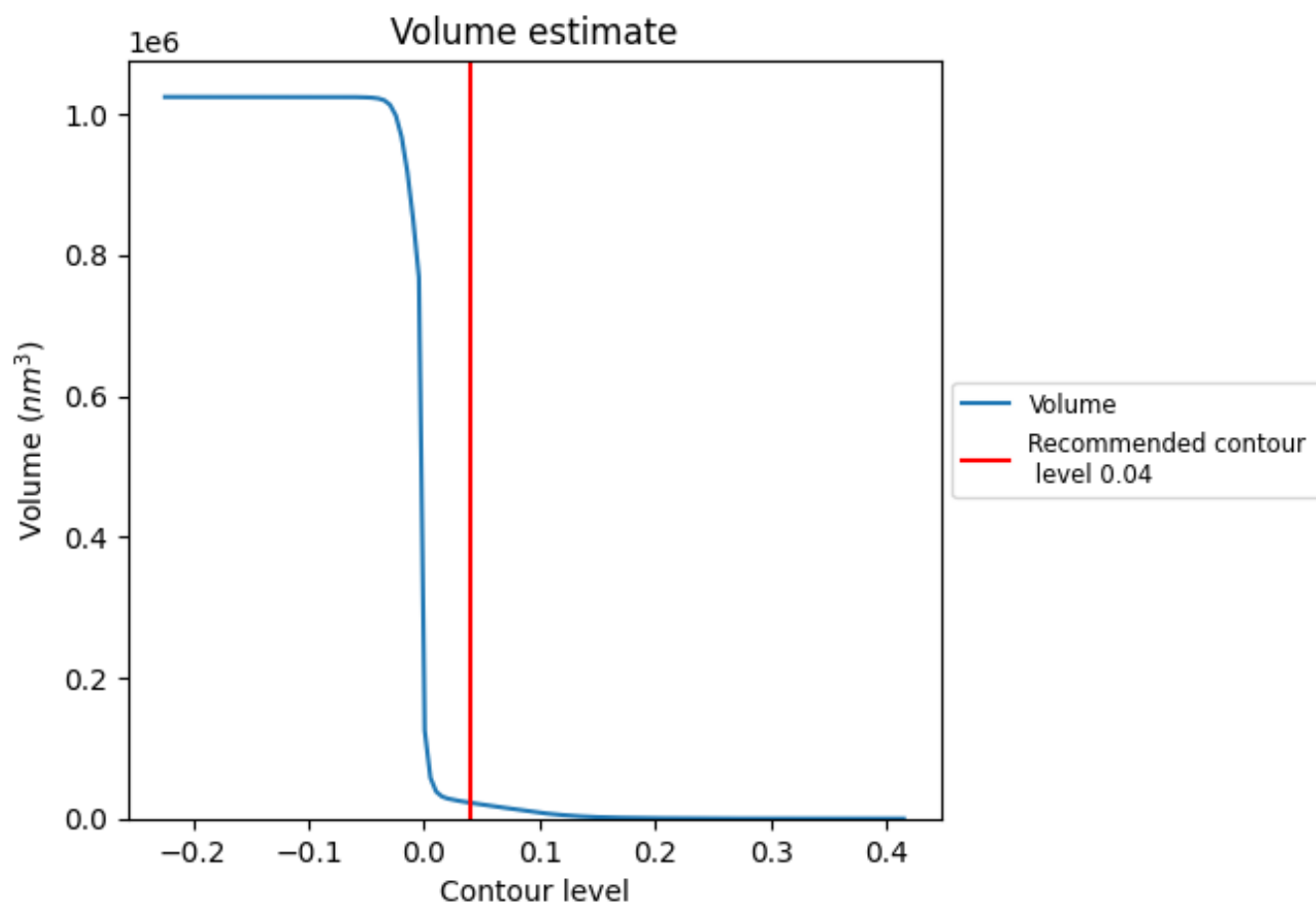
This section contains the results of statistical analysis of the map.

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



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

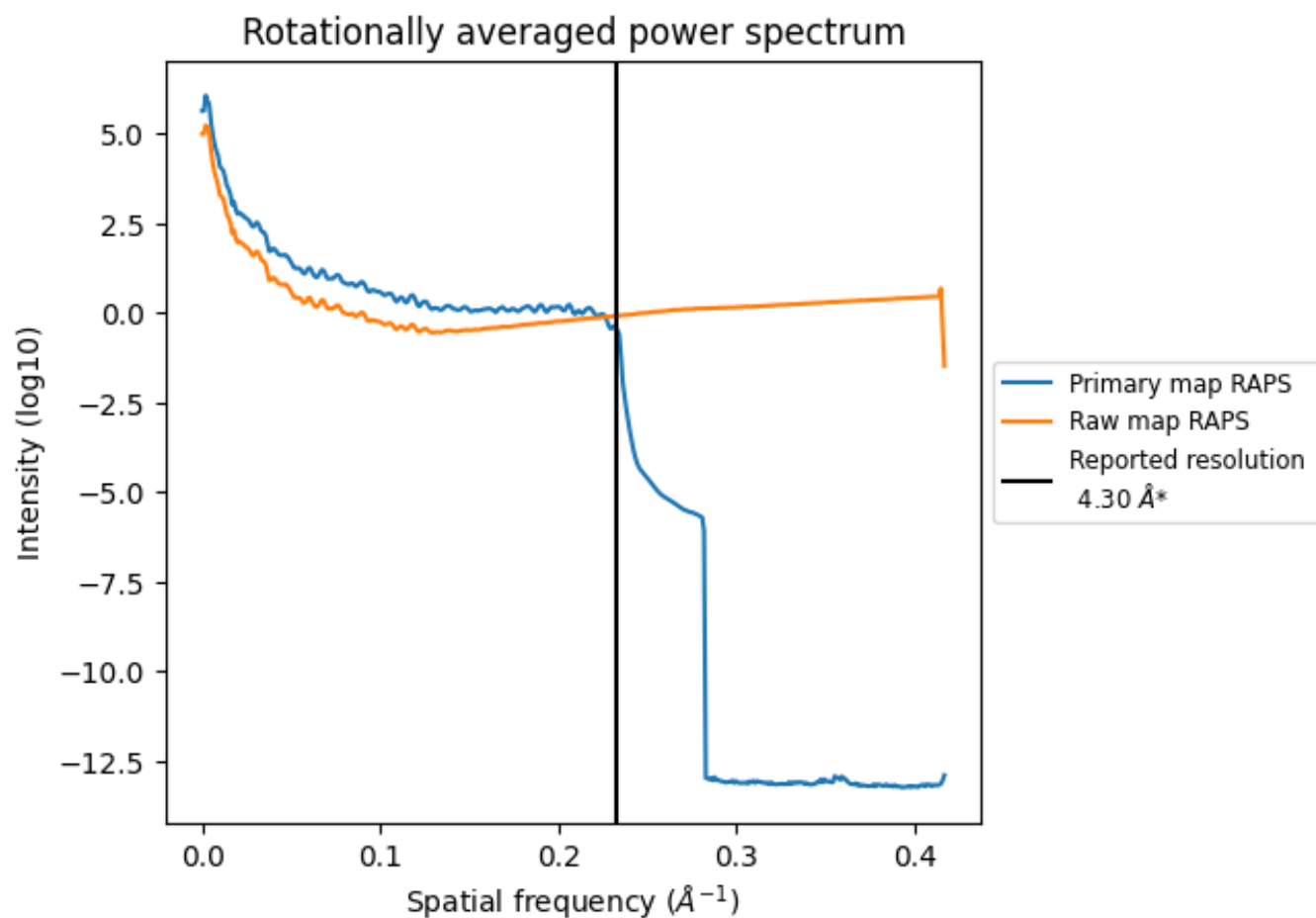
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 22548 nm<sup>3</sup>; this corresponds to an approximate mass of 20368 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 ⓘ

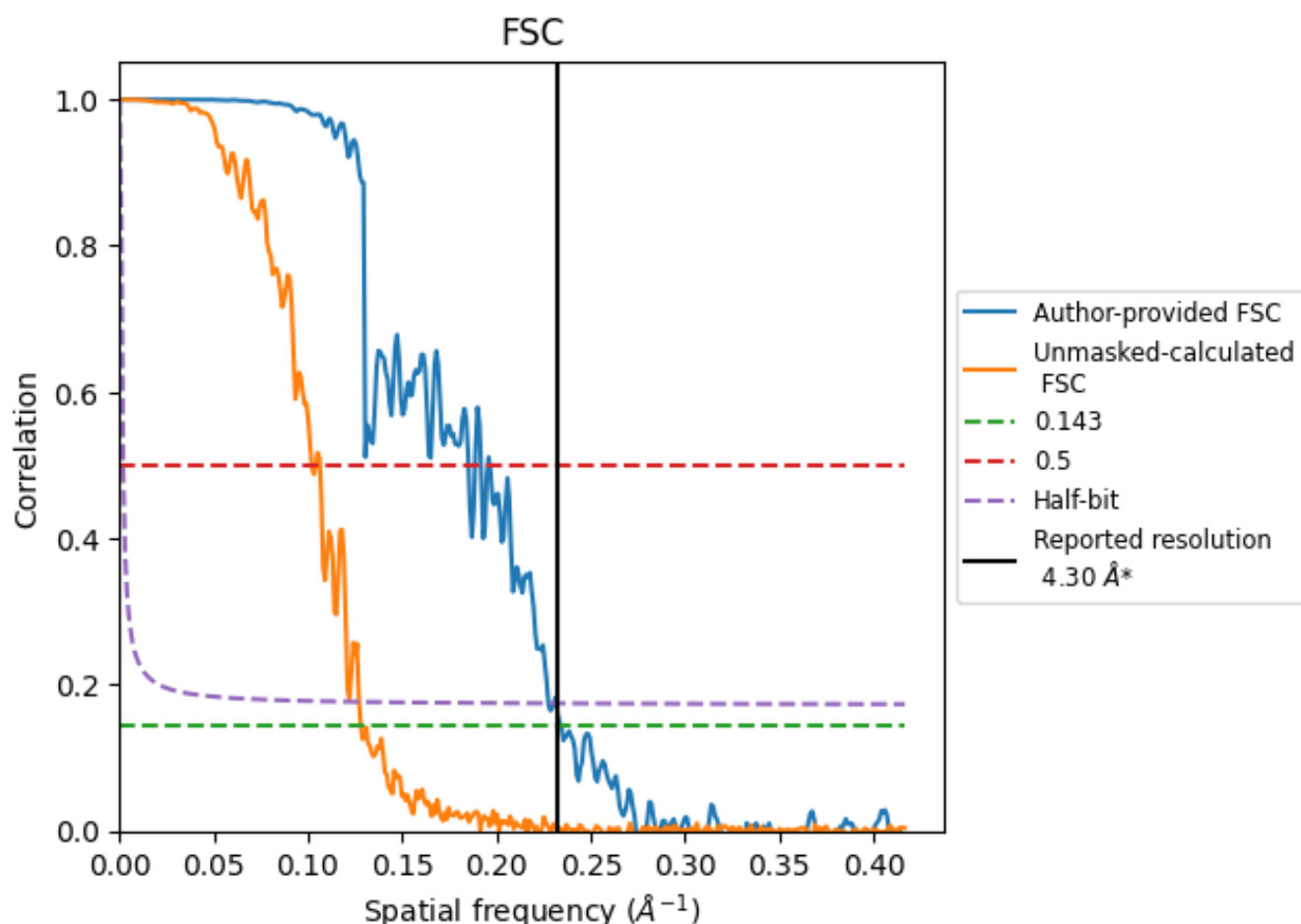


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.27	5.40	4.39
Unmasked-calculated*	7.81	9.80	7.86

\*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 7.81 differs from the reported value 4.3 by more than 10 %

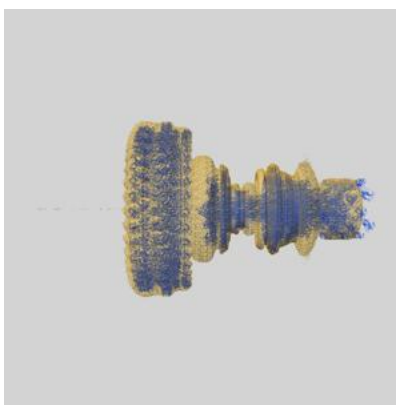
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37684 and PDB model 8WOE. Per-residue inclusion information can be found in section [3](#) on page [46](#).

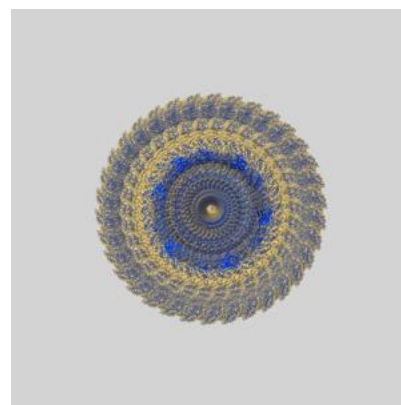
### 9.1 Map-model overlay [i](#)



X



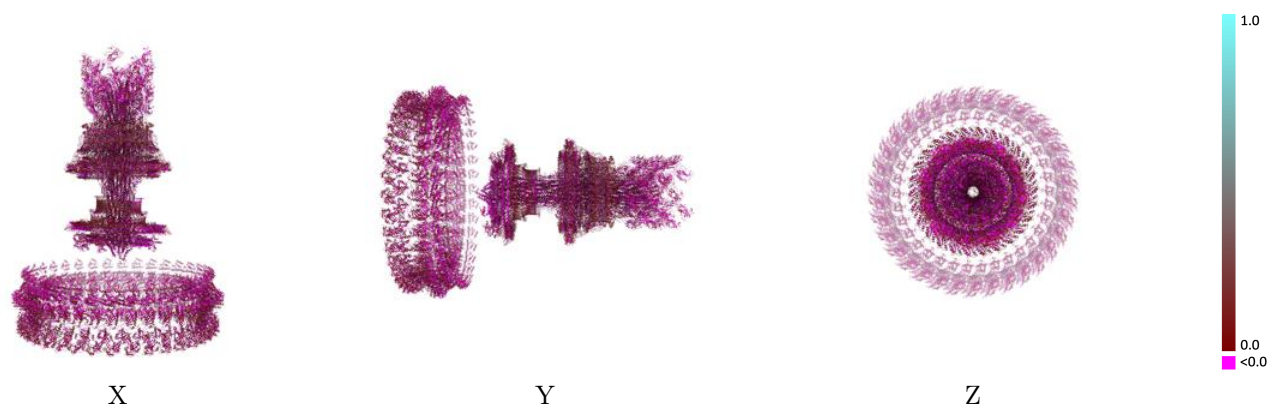
Y



Z

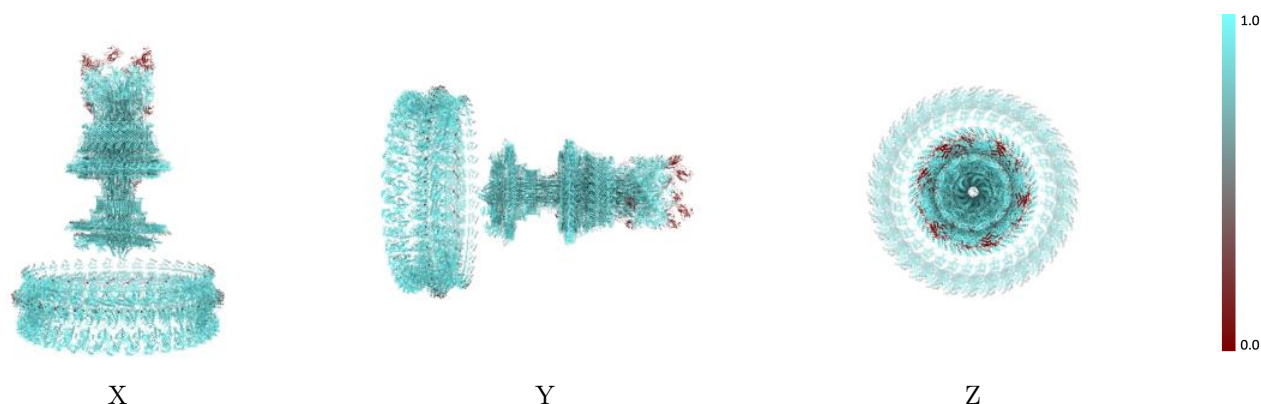
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



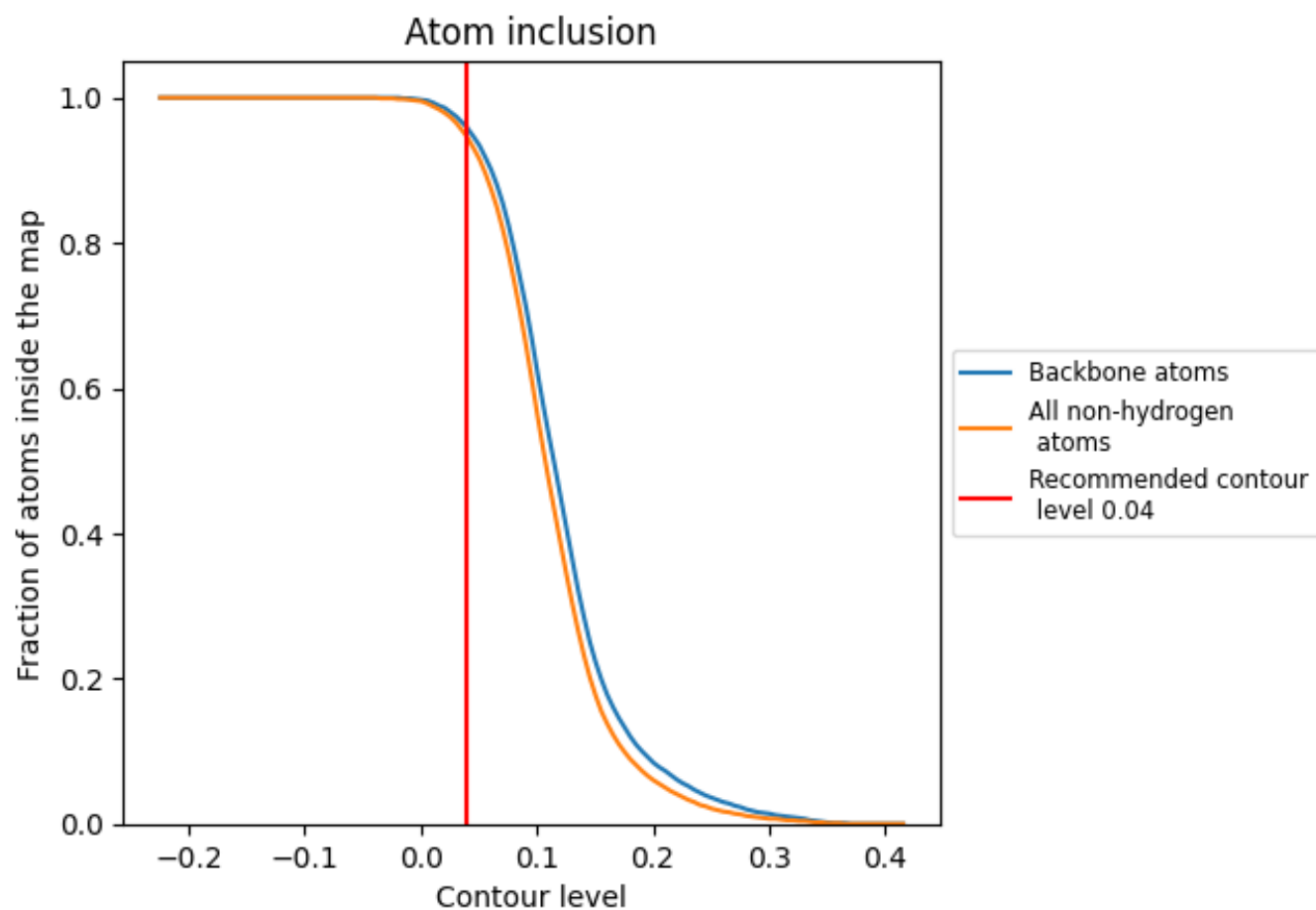
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.0660
0	 0.9630	 0.0640
1	 0.9600	 0.0700
2	 0.9620	 0.0710
3	 0.9620	 0.0670
4	 0.9560	 0.0560
5	 0.9560	 0.0480
6	 0.9570	 0.0700
7	 0.9660	 0.0710
8	 0.9720	 0.0770
9	 0.9740	 0.0690
A	 0.9370	 0.1470
A0	 0.9020	 0.0500
A1	 0.8930	 0.0440
A2	 0.9510	 0.0550
A3	 0.9540	 0.0720
A4	 0.9590	 0.1040
A5	 0.9510	 0.0930
A6	 0.8340	 0.0610
A7	 0.8770	 0.0350
A8	 0.8850	 0.0360
A9	 0.8790	 0.0380
AA	 0.8630	 0.0360
AB	 0.8980	 0.0310
AC	 0.9290	 0.0380
AD	 0.9510	 0.0550
AE	 0.9590	 0.0710
AF	 0.9670	 0.0760
AG	 0.9660	 0.0660
AH	 0.9710	 0.0590
AI	 0.9670	 0.0480
AJ	 0.9690	 0.0690
AK	 0.9730	 0.0660
AL	 0.9680	 0.0800
AM	 0.9690	 0.0620























































































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Chain	Atom inclusion	Q-score
AN	 0.9590	 0.0450
AO	 0.9620	 0.0790
AP	 0.9750	 0.1060
AQ	 0.9780	 0.1230
AR	 0.9740	 0.1190
AS	 0.9290	 0.0700
AT	 0.9320	 0.0710
AU	 0.9330	 0.0790
AV	 0.9450	 0.0910
AW	 0.9550	 0.1070
AX	 0.9680	 0.1250
AY	 0.9730	 0.1440
AZ	 0.9770	 0.1450
Aa	 0.9770	 0.1370
Ab	 0.9870	 0.0060
Ac	 0.9650	 0.0970
Ad	 0.9540	 0.0750
Ae	 0.9420	 0.0550
Af	 0.9220	 0.0390
Ag	 0.9110	 0.0280
Ah	 0.8980	 0.0200
Ai	 0.8930	 0.0130
Aj	 0.8920	 0.0120
Ak	 0.8960	 0.0120
Al	 0.9010	 0.0150
Am	 0.9110	 0.0190
An	 0.9210	 0.0240
Ao	 0.9380	 0.0320
Ap	 0.9470	 0.0510
Aq	 1.0000	 -0.0100
Ar	 1.0000	 0.0070
As	 0.9940	 0.0470
At	 0.9950	 0.0390
Au	 0.9690	 0.0360
Av	 0.9840	 0.0330
Aw	 0.9770	 0.0160
Ax	 0.9580	 0.0210
Ay	 0.9240	 0.0430
Az	 0.9110	 0.0700
B	 0.9360	 0.1430
B0	 0.9910	 0.0380
B1	 0.9940	 0.1100





















































































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Chain	Atom inclusion	Q-score
B2	 0.9920	 0.0680
B3	 0.9910	 0.0420
B4	 0.9880	 0.0820
B5	 0.9740	 0.0320
B6	 0.8860	 0.0460
B7	 0.9970	 0.0820
B8	 0.9940	 0.1080
B9	 0.9920	 0.0710
BA	 0.9450	 0.0370
BB	 0.9490	 0.0440
BC	 0.9530	 0.0250
BD	 0.9790	 0.0710
BE	 0.9890	 0.0930
BF	 0.9940	 0.0690
BG	 1.0000	 0.0830
BH	 0.8450	 0.0020
BI	 0.5710	 -0.0320
BJ	 0.8350	 -0.0060
BK	 0.6860	 -0.0090
BL	 0.8640	 -0.0320
BM	 0.8210	 0.0250
BN	 0.9710	 0.0730
BO	 0.9320	 0.1020
BP	 0.9610	 0.0190
BQ	 0.8570	 0.0660
BR	 0.9820	 0.1300
BS	 0.9740	 0.1260
BT	 0.9660	 0.1160
BU	 0.9480	 0.1040
BV	 0.9380	 0.0920
BW	 0.9330	 0.0800
BX	 0.9290	 0.0720
BY	 0.9940	 0.1110
BZ	 0.9920	 0.0700
Ba	 0.9910	 0.0390
Bb	 0.9870	 0.0820
Bc	 0.9730	 0.0320
Bd	 0.8770	 0.0430
Be	 0.9950	 0.0790
Bf	 0.9940	 0.1120
Bg	 0.9920	 0.0670
Bh	 0.9910	 0.0380





















































































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Chain	Atom inclusion	Q-score
Bi	 0.9870	 0.0820
Bj	 0.9730	 0.0320
Bk	 0.8760	 0.0440
Bl	 0.9950	 0.0790
Bm	 0.9940	 0.1080
Bn	 0.9920	 0.0690
Bo	 0.9910	 0.0370
Bp	 0.9870	 0.0830
Bq	 0.9720	 0.0310
Br	 0.8730	 0.0450
Bs	 0.9970	 0.0810
Bt	 0.9940	 0.1050
Bu	 0.9920	 0.0700
Bv	 0.9910	 0.0420
Bw	 0.9870	 0.0830
Bx	 0.9730	 0.0330
By	 0.8770	 0.0450
Bz	 0.9950	 0.0810
C	 0.9410	 0.1460
C0	 0.9880	 0.0800
C1	 0.9970	 0.0790
C2	 0.9940	 0.1060
C3	 0.9920	 0.0720
C4	 0.9970	 0.0790
C5	 0.9940	 0.1050
C6	 0.9720	 0.0320
C7	 0.8770	 0.0370
C8	 0.9950	 0.0780
C9	 0.9940	 0.1080
CA	 0.9880	 0.0820
CB	 0.9740	 0.0320
CC	 0.8820	 0.0450
CD	 0.9950	 0.0810
CE	 0.9940	 0.1100
CF	 0.9920	 0.0700
CG	 0.9910	 0.0360
CH	 0.9880	 0.0820
CI	 0.9720	 0.0300
CJ	 0.8800	 0.0420
CK	 0.9970	 0.0810
CL	 0.9940	 0.1100
CM	 0.9920	 0.0710





















































































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Chain	Atom inclusion	Q-score
CN	 0.9910	 0.0410
CO	 0.9880	 0.0820
CP	 0.9730	 0.0310
CQ	 0.8810	 0.0420
CR	 0.9970	 0.0790
CS	 0.9940	 0.1110
CT	 0.9920	 0.0730
CU	 0.9910	 0.0430
CV	 0.9870	 0.0810
CW	 0.9730	 0.0310
CX	 0.8730	 0.0430
CY	 0.9970	 0.0820
CZ	 0.9940	 0.1070
Ca	 0.9920	 0.0710
Cb	 0.9910	 0.0410
Cc	 0.9870	 0.0810
Cd	 0.9730	 0.0320
Ce	 0.8770	 0.0420
Cf	 0.9970	 0.0810
Cg	 0.9920	 0.1080
Ch	 0.9920	 0.0700
Ci	 0.9910	 0.0380
Cj	 0.9870	 0.0820
Ck	 0.9730	 0.0310
Cl	 0.8740	 0.0420
Cm	 0.9940	 0.0780
Cn	 0.9920	 0.1070
Co	 0.9920	 0.0710
Cp	 0.9910	 0.0360
Cq	 0.9870	 0.0820
Cr	 0.9730	 0.0330
Cs	 0.8780	 0.0400
Ct	 0.9950	 0.0790
Cu	 0.9940	 0.1080
Cv	 0.9920	 0.0720
Cw	 0.9910	 0.0420
Cx	 0.9870	 0.0810
Cy	 0.9740	 0.0320
Cz	 0.8770	 0.0410
D	 0.9350	 0.1440
D0	 0.8770	 0.0380
D1	 0.9920	 0.0690





















































































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Chain	Atom inclusion	Q-score
D2	 0.9870	 0.0810
D3	 0.9730	 0.0300
D4	 0.8730	 0.0380
D5	 0.9940	 0.0790
D6	 0.9940	 0.1060
D7	 0.9920	 0.0690
D8	 0.9870	 0.0820
D9	 0.9730	 0.0310
DA	 0.9740	 0.0300
DB	 0.8840	 0.0370
DC	 0.9880	 0.0810
DD	 0.9920	 0.0700
DE	 0.9910	 0.0410
DF	 0.9880	 0.0810
DG	 0.9740	 0.0310
DH	 0.8800	 0.0420
DI	 0.9950	 0.0800
DJ	 0.9940	 0.1070
DK	 0.9920	 0.0690
DL	 0.9910	 0.0360
DM	 0.9920	 0.0700
DN	 0.9920	 0.0720
DO	 0.9920	 0.0710
DP	 0.9920	 0.0720
DQ	 0.9920	 0.0690
DR	 0.9920	 0.0710
DS	 0.9920	 0.0710
DT	 0.9920	 0.0670
DU	 0.9970	 0.0800
DV	 0.9940	 0.1040
DW	 0.9920	 0.0710
DX	 0.9880	 0.0810
DY	 0.9730	 0.0300
DZ	 0.8800	 0.0410
Da	 0.9970	 0.0800
Db	 0.9940	 0.1060
Dc	 0.9920	 0.0700
Dd	 0.9880	 0.0810
De	 0.9720	 0.0290
Df	 0.8810	 0.0370
Dg	 0.9950	 0.0800
Dh	 0.9940	 0.1030





















































































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Chain	Atom inclusion	Q-score
Di	 0.9920	 0.0700
Dj	 0.9870	 0.0820
Dk	 0.9730	 0.0300
Dl	 0.8800	 0.0380
Dm	 0.9970	 0.0820
Dn	 0.9920	 0.1060
Do	 0.9920	 0.0720
Dp	 0.9870	 0.0800
Dq	 0.9720	 0.0290
Dr	 0.8760	 0.0390
Ds	 0.9970	 0.0830
Dt	 0.9940	 0.1050
Du	 0.9920	 0.0700
Dv	 0.9870	 0.0790
Dw	 0.9730	 0.0310
Dx	 0.8790	 0.0380
Dy	 0.9970	 0.0820
Dz	 0.9920	 0.1060
E	 0.9410	 0.1370
E0	 0.8750	 0.0390
E1	 0.9730	 0.0310
E2	 0.9730	 0.0310
E3	 0.9730	 0.0310
E4	 0.9720	 0.0300
E5	 0.9870	 0.0810
E6	 0.8810	 0.0390
E7	 0.8790	 0.0390
E8	 0.8780	 0.0380
E9	 0.8720	 0.0400
EA	 0.9950	 0.0810
EB	 0.9940	 0.1080
EC	 0.9720	 0.0330
ED	 0.8820	 0.0420
EE	 0.9970	 0.0800
EF	 0.9940	 0.1080
EG	 0.9920	 0.0680
EH	 0.9910	 0.0400
EI	 0.9880	 0.0810
EJ	 0.9720	 0.0320
EK	 0.8830	 0.0410
EL	 0.9970	 0.0820
EM	 0.9940	 0.1080

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

































































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Chain	Atom inclusion	Q-score
EN	 0.9920	 0.0710
EO	 0.9910	 0.0380
EP	 0.9880	 0.0820
EQ	 0.9730	 0.0300
ER	 0.8790	 0.0430
ES	 0.9970	 0.0810
ET	 0.9940	 0.1050
EU	 0.9920	 0.0700
EV	 0.9910	 0.0380
EW	 0.9870	 0.0810
EX	 0.9740	 0.0310
EY	 0.8730	 0.0440
EZ	 0.9970	 0.0820
Ea	 0.9910	 0.0400
Eb	 0.9910	 0.0390
Ec	 0.9910	 0.0370
Ed	 0.9910	 0.0410
Ee	 0.9910	 0.0430
Ef	 0.9910	 0.0420
Eg	 0.9910	 0.0400
Eh	 0.9910	 0.0410
Ei	 0.9910	 0.0430
Ej	 0.9910	 0.0430
Ek	 0.9910	 0.0420
El	 0.9910	 0.0420
Em	 0.9910	 0.0370
En	 0.9910	 0.0390
Eo	 0.9910	 0.0390
Ep	 0.9910	 0.0410
Eq	 0.9870	 0.0800
Er	 0.9870	 0.0810
Es	 0.9880	 0.0820
Et	 0.9870	 0.0820
Eu	 0.9870	 0.0810
Ev	 0.9870	 0.0820
Ew	 0.9870	 0.0820
Ex	 0.9720	 0.0310
Ey	 0.9730	 0.0310
Ez	 0.9730	 0.0290
F	 0.9400	 0.1370
FA	 0.8750	 0.0390
FB	 0.8720	 0.0370

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


































































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Chain	Atom inclusion	Q-score
FC	 0.9970	 0.0770
FD	 0.9970	 0.0810
FE	 0.9970	 0.0780
FF	 0.9970	 0.0780
FG	 0.9950	 0.0780
FH	 0.9950	 0.0760
FI	 0.9940	 0.1080
FJ	 0.9940	 0.1060
FK	 0.9940	 0.1040
FL	 0.9940	 0.1060
FM	 0.9940	 0.1060
FN	 0.9910	 0.1050
G	 0.9380	 0.1350
H	 0.9270	 0.1260
I	 0.9320	 0.1250
J	 0.9320	 0.1310
K	 0.9250	 0.1270
L	 0.9310	 0.1300
M	 0.9320	 0.1390
N	 0.9280	 0.1400
O	 0.9320	 0.1430
P	 0.9300	 0.1450
Q	 0.9270	 0.1460
R	 0.9320	 0.1450
S	 0.9280	 0.1430
T	 0.9260	 0.1340
U	 0.9260	 0.1350
UI	 0.9360	 0.0490
UJ	 0.8960	 0.0090
UK	 0.9260	 0.0530
UL	 0.9260	 0.0540
UM	 0.9890	 -0.0010
UN	 0.9710	 0.0110
UO	 0.9670	 0.0410
UP	 0.9440	 0.0470
V	 0.9310	 0.1360
W	 0.9290	 0.1290
WA	 0.9710	 0.0730
WB	 0.9830	 0.0770
WC	 0.9800	 0.0500
WD	 0.9770	 0.0590
WE	 0.9280	 0.0460















































































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Chain	Atom inclusion	Q-score
WF	 0.9610	 0.0770
WG	 0.9650	 0.0590
WH	 0.9710	 0.0900
WI	 0.9160	 0.0950
WJ	 0.9780	 0.0620
WK	 0.9900	 0.0270
WL	 0.9870	 -0.0210
WM	 0.9630	 -0.0210
WN	 0.9470	 -0.0240
WO	 0.9390	 -0.0120
WP	 0.9550	 -0.0220
WQ	 0.9670	 -0.0370
WR	 0.9790	 0.0110
WS	 0.9840	 -0.0140
WT	 0.9850	 0.0440
WU	 0.9930	 0.0540
WV	 0.9940	 0.0760
WW	 0.9990	 0.0740
X	 0.9310	 0.1380
Y	 0.9320	 0.1400
Z	 0.9380	 0.1440
ZA	 0.9800	 0.0510
ZB	 0.9730	 0.0500
ZC	 0.9800	 0.0600
ZD	 0.9840	 0.0610
ZE	 0.9850	 0.0580
ZF	 0.7050	 0.0240
ZG	 0.7380	 0.0300
ZH	 0.7700	 0.0230
ZI	 0.8220	 0.0400
ZJ	 0.9000	 0.0460
ZK	 0.9360	 0.0390
ZL	 0.9480	 0.0130
ZM	 0.9360	 0.0410
ZN	 0.9380	 0.0410
ZO	 0.9600	 0.0390
ZP	 0.9680	 0.0320
ZQ	 0.9760	 0.0280
ZR	 0.9660	 0.0280
ZS	 0.9540	 0.0280
ZT	 0.9630	 0.0360
ZU	 0.9720	 0.0270

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Chain	Atom inclusion	Q-score
ZV	 0.9710	 0.0330
ZW	 0.9530	 0.0160
ZX	 0.9180	 0.0250
ZY	 0.8790	 0.0320
ZZ	 0.8510	 0.0130
Za	 0.8220	 0.0190
Zb	 0.7790	 0.0210
Zc	 0.7410	 0.0330
Zd	 0.7020	 0.0120
Ze	 0.6730	 0.0270
Zf	 0.6350	 0.0300
Zg	 0.6210	 0.0330
Zh	 0.6050	 0.0180
a	 0.9660	 0.1240
b	 0.9680	 0.1300
c	 0.9660	 0.1280
d	 0.9640	 0.1270
e	 0.9650	 0.1130
f	 0.9640	 0.1140
g	 0.9650	 0.1160
h	 0.9610	 0.1030
i	 0.9630	 0.1090
j	 0.9620	 0.1150
k	 0.9620	 0.1130
l	 0.9670	 0.1210
m	 0.9640	 0.1210
n	 0.9620	 0.1290
o	 0.9640	 0.1300
p	 0.9620	 0.1220
q	 0.9660	 0.1240
r	 0.9610	 0.1200
s	 0.9580	 0.1080
t	 0.9570	 0.1070
u	 0.9580	 0.1040
v	 0.9550	 0.0950
w	 0.9550	 0.0960
x	 0.9630	 0.1090
y	 0.9590	 0.1170
z	 0.9620	 0.1170