Full wwPDB EM Validation Report ⓘ

Mar 19, 2025 – 02:02 AM JST

PDB ID	:	8WO5
EMDB ID	:	EMD-37679
Title	:	Cryo-EM structure of the intact flagellar motor-hook complex in the CCW state
Authors	:	Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on	:	2023-10-06
Resolution	:	7.40 Å(reported)
Based on initial models	:	., ?

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

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

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

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

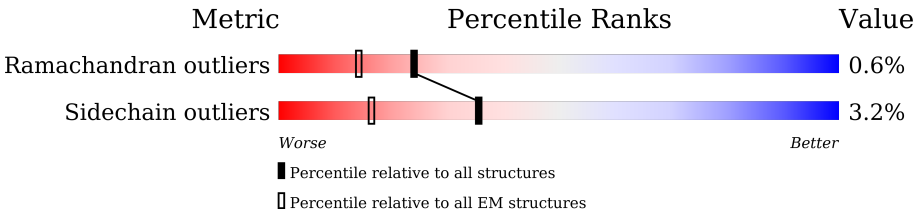
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	0	260	21% 92% • • 5%
1	1	260	13% 93% • •
1	2	260	16% 98% •
1	3	260	19% 98% •
1	4	260	26% 97% •
1	5	260	27% 97% •
1	6	260	26% 97% •
1	7	260	21% 98% •
1	8	260	24% 96% •

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Mol	Chain	Length	Quality of chain
1	9	260	27% 98%
1	AF	260	15% 95%
1	AG	260	14% 94%
1	AH	260	18% 93% 5%
1	AI	260	21% 92% 6%
1	AJ	260	22% 92% 5%
1	AK	260	16% 91% 7%
1	AL	260	15% 90% 5% 5%
1	AM	260	19% 92% 5%
1	AN	260	23% 92% 5%
1	ZA	260	29% 98%
1	ZB	260	27% 97%
1	ZC	260	19% 98%
1	ZD	260	17% 97%
1	ZE	260	19% 97%
2	A	232	16% 88% 9%
2	B	232	18% 88% 9%
2	C	232	16% 88% 9%
2	D	232	16% 88% 9%
2	E	232	16% 88% 9%
2	F	232	16% 88% 9%
2	G	232	16% 88% 9%
2	H	232	16% 88% 9%
2	I	232	19% 88% 9%
2	J	232	20% 88% 9%

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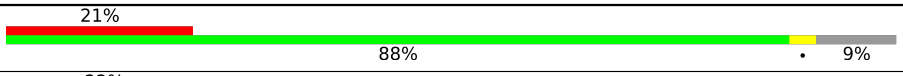
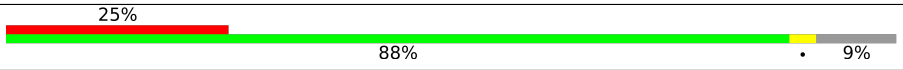
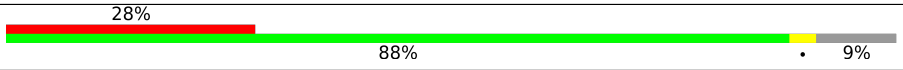
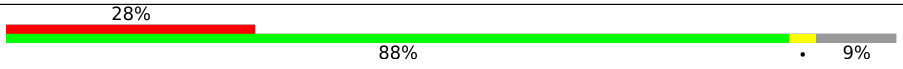
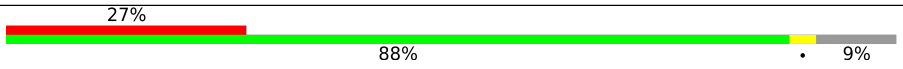
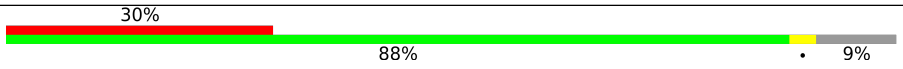
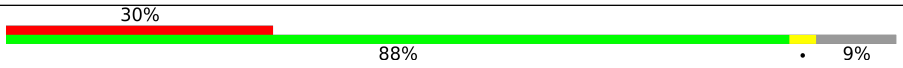
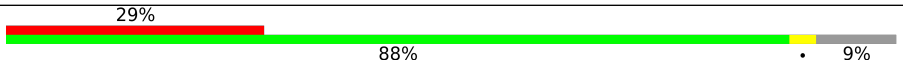
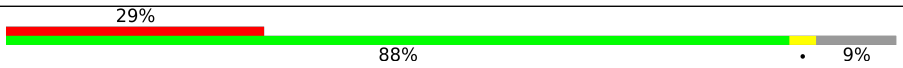
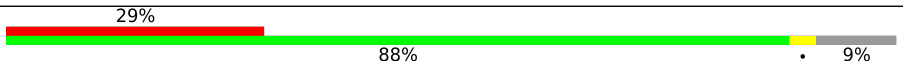
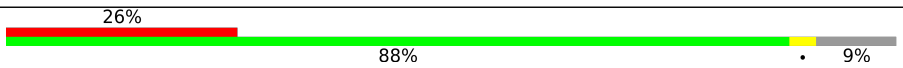
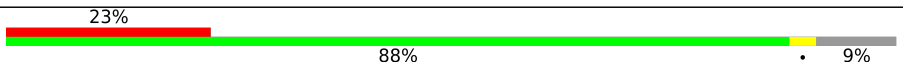
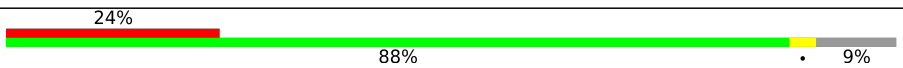
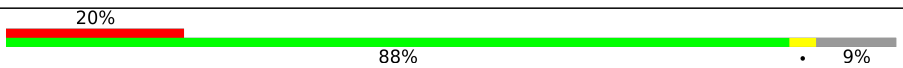
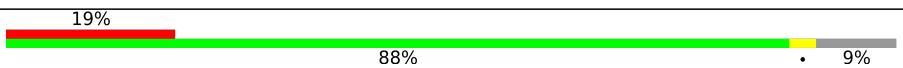
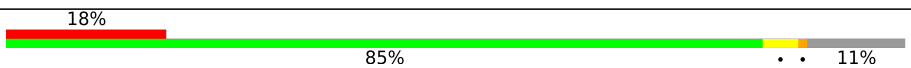
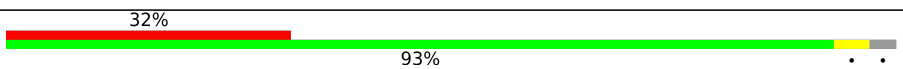
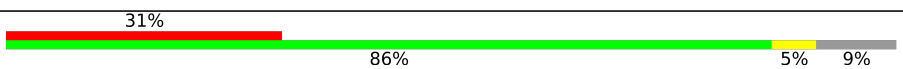
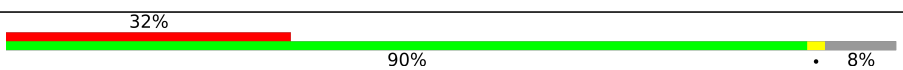
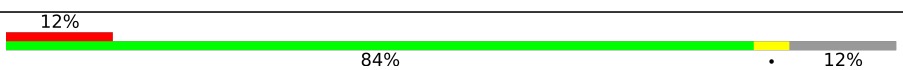
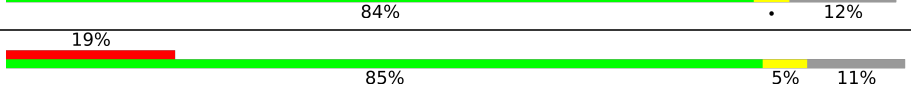
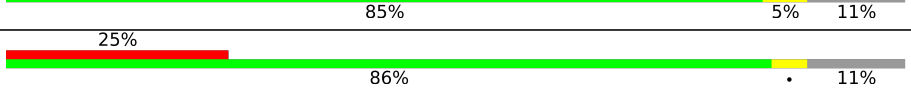
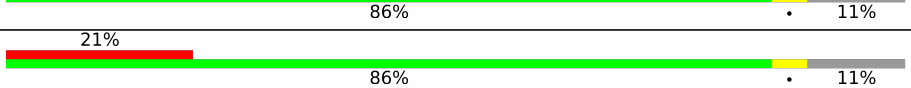
Mol	Chain	Length	Quality of chain
2	K	232	
2	L	232	
2	M	232	
2	N	232	
2	O	232	
2	P	232	
2	Q	232	
2	R	232	
2	S	232	
2	T	232	
2	U	232	
2	V	232	
2	W	232	
2	X	232	
2	Y	232	
2	Z	232	
3	A0	138	
3	A6	138	
3	A7	138	
3	A8	138	
3	A9	138	
4	A1	104	
4	A2	104	
4	A3	104	
4	A4	104	

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Mol	Chain	Length	Quality of chain
4	A5	104	13% 84% 5% 12%
4	Az	104	51% 6% 43%
5	AA	251	29% 97%
5	AB	251	24% 96%
5	AC	251	25% 98%
5	AD	251	23% 96%
5	AE	251	24% 98%
6	AO	560	28% 71%
6	AP	560	28% 71%
6	AQ	560	28% 71%
6	AR	560	28% 71%
6	AS	560	5% 28% 71%
6	AT	560	5% 28% 71%
6	AU	560	5% 28% 71%
6	AV	560	5% 28% 71%
6	AW	560	5% 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	B6	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%
6	BU	560	28% 71%

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Mol	Chain	Length	Quality of chain
6	BV	560	28% 71%
6	BW	560	28% 71%
6	BX	560	5% 28% 71%
6	Bb	560	5% 95%
6	Bh	560	5% 95%
6	Bn	560	5% 95%
6	Bt	560	5% 95%
6	Bz	560	5% 95%
6	C3	560	5% 95%
6	C7	560	5% 95%
6	CB	560	5% 95%
6	CH	560	5% 95%
6	CN	560	5% 95%
6	CT	560	5% 95%
6	CZ	560	5% 95%
6	Cf	560	5% 95%
6	Cl	560	5% 95%
6	Cr	560	5% 95%
6	Cx	560	5% 95%
6	D2	560	5% 95%
6	D8	560	5% 95%
6	DE	560	5% 95%
6	DK	560	5% 95%
6	DR	560	5% 95%
6	DX	560	5% 95%

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Mol	Chain	Length	Quality of chain
6	Dd	560	5% 95%
6	Dj	560	5% 95%
6	Dp	560	5% 95%
6	Dv	560	5% 95%
6	EF	560	5% 95%
6	EL	560	5% 95%
6	ER	560	5% 95%
6	EX	560	5% 95%
6	Eb	560	5% 95%
6	Eh	560	5% 95%
6	En	560	5% 95%
6	UI	560	8% 25% 72%
6	UJ	560	9% 25% 72%
6	UK	560	8% 25% 72%
6	UL	560	8% 25% 72%
6	UM	560	25% 72%
6	UN	560	25% 72%
6	UO	560	25% 72%
6	UP	560	7% 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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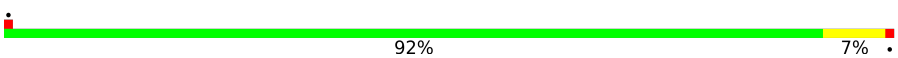
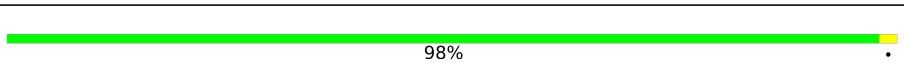
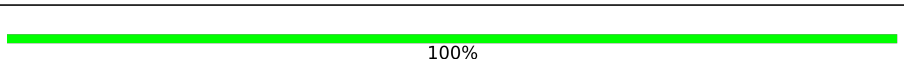
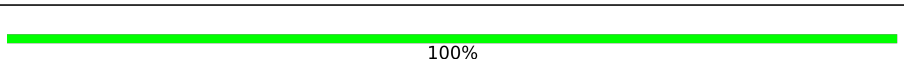
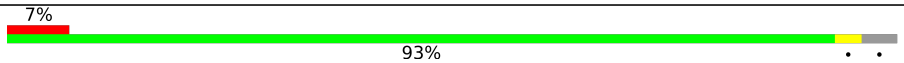
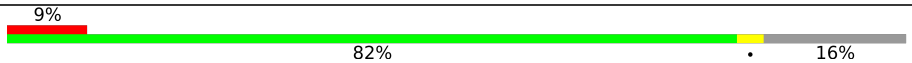
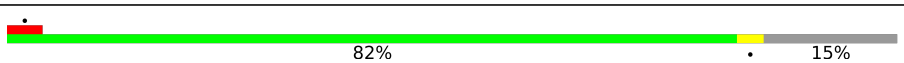
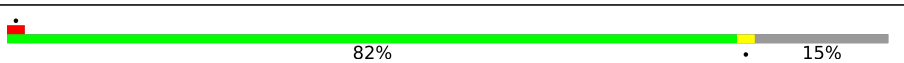
Mol	Chain	Length	Quality of chain
6	WG	560	
6	WH	560	
6	WI	560	
6	WJ	560	
6	WK	560	
6	WL	560	
6	WM	560	
6	WN	560	
6	WO	560	
6	WP	560	
6	WQ	560	
6	WR	560	
6	WS	560	
6	WT	560	
6	WU	560	
6	WV	560	
6	WW	560	
7	Ab	89	
7	Aq	89	
7	Ar	89	
7	As	89	
8	At	264	
9	Au	245	
9	Av	245	
9	Aw	245	

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Mol	Chain	Length	Quality of chain
9	Ax	245	9% 82% 15%
9	Ay	245	16% 80% 15%
10	BA	134	19% 99%
10	BB	134	16% 96%
10	BC	134	12% 98%
10	BD	134	18% 93% 6%
10	BE	134	14% 94%
10	BF	134	9% 94% 5%
11	ZF	403	48% 97%
11	ZG	403	45% 95%
11	ZH	403	41% 96%
11	ZI	403	38% 97%
11	ZJ	403	31% 97%
11	ZK	403	26% 98%
11	ZL	403	23% 97%
11	ZM	403	19% 97%
11	ZN	403	13% 97%
11	ZO	403	11% 97%
11	ZP	403	11% 95%
11	ZQ	403	11% 97%
11	ZR	403	10% 98%
11	ZS	403	9% 98%
11	ZT	403	6% 97%
11	ZU	403	6% 98%
11	ZV	403	6% 98%

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Mol	Chain	Length	Quality of chain
11	ZW	403	7% 96%
11	ZX	403	7% 99%
11	ZY	403	9% 98%
11	ZZ	403	11% 98%
11	Za	403	15% 98%
11	Zb	403	18% 98%
11	Zc	403	22% 97%
11	Zd	403	24% 98%
11	Ze	403	28% 97%
11	Zf	403	32% 98%
11	Zg	403	35% 98%
11	Zh	403	37% 98%
12	a	365	7% 82% 17%
12	b	365	5% 82% 17%
12	c	365	6% 82% 17%
12	d	365	7% 82% 17%
12	e	365	8% 82% 17%
12	f	365	8% 82% 17%
12	g	365	9% 82% 17%
12	h	365	13% 82% 17%
12	i	365	13% 82% 17%
12	j	365	14% 82% 17%
12	k	365	16% 82% 17%
12	l	365	16% 82% 17%
12	m	365	16% 82% 17%

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Mol	Chain	Length	Quality of chain
12	n	365	18% 82% 17%
12	o	365	17% 82% 17%
12	p	365	16% 82% 17%
12	q	365	15% 82% 17%
12	r	365	13% 82% 17%
12	s	365	13% 82% 17%
12	t	365	13% 82% 17%
12	u	365	10% 82% 17%
12	v	365	12% 82% 17%
12	w	365	10% 82% 17%
12	x	365	8% 82% 17%
12	y	365	7% 82% 17%
12	z	365	7% 82% 17%
13	B0	137	61% 36%
13	B2	137	61% 36%
13	B3	137	61% 36%
13	B4	137	61% 36%
13	B8	137	61% 36%
13	B9	137	61% 36%
13	BY	137	61% 36%
13	BZ	137	61% 36%
13	Bd	137	61% 36%
13	Be	137	61% 36%
13	Bf	137	61% 36%
13	Bj	137	61% 36%

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Mol	Chain	Length	Quality of chain
13	Bk	137	61% 36%
13	Bl	137	61% 36%
13	Bp	137	61% 36%
13	Bq	137	61% 36%
13	Br	137	61% 36%
13	Bv	137	61% 36%
13	Bw	137	61% 36%
13	Bx	137	61% 36%
13	C0	137	61% 36%
13	C1	137	61% 36%
13	C2	137	61% 36%
13	C4	137	61% 36%
13	C5	137	61% 36%
13	C9	137	61% 36%
13	CD	137	61% 36%
13	CE	137	61% 36%
13	CF	137	61% 36%
13	CJ	137	61% 36%
13	CK	137	61% 36%
13	CL	137	61% 36%
13	CP	137	61% 36%
13	CQ	137	61% 36%
13	CR	137	61% 36%
13	CV	137	61% 36%
13	CW	137	61% 36%

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Mol	Chain	Length	Quality of chain
13	CX	137	61% 36%
13	Cb	137	61% 36%
13	Cc	137	61% 36%
13	Cd	137	61% 36%
13	Ch	137	61% 36%
13	Ci	137	61% 36%
13	Cj	137	61% 36%
13	Cn	137	61% 36%
13	Co	137	61% 36%
13	Cp	137	61% 36%
13	Ct	137	61% 36%
13	Cu	137	61% 36%
13	Cv	137	61% 36%
13	Cz	137	61% 36%
13	D0	137	61% 36%
13	D4	137	61% 36%
13	D5	137	61% 36%
13	D6	137	61% 36%
13	DA	137	61% 36%
13	DC	137	61% 36%
13	DG	137	61% 36%
13	DH	137	61% 36%
13	DI	137	61% 36%
13	DN	137	61% 36%
13	DO	137	61% 36%

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Mol	Chain	Length	Quality of chain
13	DP	137	61% 36%
13	DT	137	61% 36%
13	DU	137	61% 36%
13	DV	137	61% 36%
13	DZ	137	61% 36%
13	Da	137	61% 36%
13	Db	137	61% 36%
13	Df	137	61% 36%
13	Dg	137	61% 36%
13	Dh	137	61% 36%
13	Dl	137	61% 36%
13	Dm	137	61% 36%
13	Dn	137	61% 36%
13	Dr	137	61% 36%
13	Ds	137	61% 36%
13	Dt	137	61% 36%
13	Dx	137	61% 36%
13	Dy	137	61% 36%
13	Dz	137	61% 36%
13	EA	137	61% 36%
13	EB	137	61% 36%
13	EC	137	61% 36%
13	ED	137	61% 36%
13	EH	137	61% 36%
13	EI	137	61% 36%

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Mol	Chain	Length	Quality of chain
13	EJ	137	61% 36%
13	EN	137	61% 36%
13	EO	137	61% 36%
13	EP	137	61% 36%
13	ET	137	61% 36%
13	EU	137	61% 36%
13	EV	137	61% 36%
13	EZ	137	61% 36%
13	Ed	137	61% 36%
13	Ee	137	61% 36%
13	Ef	137	61% 36%
13	Ej	137	61% 36%
13	Ek	137	61% 36%
13	El	137	61% 36%
13	Ep	137	61% 36%
14	B5	331	93% 5%
14	Ba	331	93% 5%
14	Bg	331	93% 5%
14	Bm	331	93% 5%
14	Bs	331	93% 5%
14	By	331	93% 5%
14	C6	331	93% 5%
14	CA	331	93% 5%
14	CG	331	93% 5%
14	CM	331	93% 5%

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Mol	Chain	Length	Quality of chain
14	CS	331	93% • 5%
14	CY	331	93% • 5%
14	Ce	331	93% • 5%
14	Ck	331	93% • 5%
14	Cq	331	93% • 5%
14	Cw	331	93% • 5%
14	D1	331	93% • 5%
14	D7	331	93% • 5%
14	DB	331	93% • 5%
14	DD	331	93% • 5%
14	DJ	331	93% • 5%
14	DQ	331	93% • 5%
14	DW	331	93% • 5%
14	Dc	331	93% • 5%
14	Di	331	93% • 5%
14	Do	331	93% • 5%
14	Du	331	93% • 5%
14	EE	331	93% • 5%
14	EK	331	93% • 5%
14	EQ	331	93% • 5%
14	EW	331	93% • 5%
14	Ea	331	93% • 5%
14	Eg	331	93% • 5%
14	Em	331	93% • 5%
15	B1	334	82% • 13%

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Mol	Chain	Length	Quality of chain
15	B7	334	82% · 13%
15	Bc	334	82% · 13%
15	Bi	334	82% · 13%
15	Bo	334	82% · 13%
15	Bu	334	82% · 13%
15	C8	334	82% · 13%
15	CC	334	82% · 13%
15	CI	334	82% · 13%
15	CO	334	82% · 13%
15	CU	334	82% · 13%
15	Ca	334	82% · 13%
15	Cg	334	82% · 13%
15	Cm	334	82% · 13%
15	Cs	334	82% · 13%
15	Cy	334	82% · 13%
15	D3	334	82% · 13%
15	D9	334	82% · 13%
15	DF	334	82% · 13%
15	DL	334	82% · 13%
15	DM	334	82% · 13%
15	DS	334	82% · 13%
15	DY	334	82% · 13%
15	De	334	82% · 13%
15	Dk	334	82% · 13%
15	Dq	334	82% · 13%

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Mol	Chain	Length	Quality of chain
15	Dw	334	82% · 13%
15	EG	334	82% · 13%
15	EM	334	82% · 13%
15	ES	334	82% · 13%
15	EY	334	82% · 13%
15	Ec	334	82% · 13%
15	Ei	334	82% · 13%
15	Eo	334	82% · 13%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 578432 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	C	N	O	S	0	0
			1275	776	237	259	3		
6	AV	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	AW	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	AX	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	AY	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	AZ	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Aa	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Ac	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Ad	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Ae	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Af	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Ag	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Ah	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Ai	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Aj	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Ak	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Al	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	Am	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
6	An	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
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		

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Mol	Chain	Residues	Atoms	AltConf	Trace
6	BG	13	Total C N O 81 50 15 16	0	0
6	BH	16	Total C N O 103 64 19 20	0	0
6	BI	20	Total C N O 133 83 23 27	0	0
6	BJ	16	Total C N O 103 64 19 20	0	0
6	BK	21	Total C N O 140 88 24 28	0	0
6	BL	16	Total C N O 103 64 19 20	0	0
6	BM	21	Total C N O 140 88 24 28	0	0
6	BN	16	Total C N O 103 64 19 20	0	0
6	BO	20	Total C N O 133 83 23 27	0	0
6	BP	16	Total C N O 103 64 19 20	0	0
6	BQ	21	Total C N O 140 88 24 28	0	0
6	BR	164	Total C N O S 1275 776 237 259 3	0	0
6	BS	164	Total C N O S 1275 776 237 259 3	0	0
6	BT	164	Total C N O S 1275 776 237 259 3	0	0
6	BU	164	Total C N O S 1275 776 237 259 3	0	0
6	BV	164	Total C N O S 1275 776 237 259 3	0	0
6	BW	164	Total C N O S 1275 776 237 259 3	0	0
6	BX	164	Total C N O S 1275 776 237 259 3	0	0
6	UI	155	Total C N O S 1172 733 211 226 2	0	0
6	UJ	155	Total C N O S 1172 733 211 226 2	0	0
6	UK	155	Total C N O S 1172 733 211 226 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	C3	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	C7	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	DE	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	DK	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	DR	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	DX	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Dd	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Dj	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Dp	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Dv	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	D2	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	D8	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	B6	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	EF	27	Total	C	N	O	S	0	0
			224	135	44	42	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	EL	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	ER	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	EX	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Bb	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	Bn	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Bt	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Bz	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	CB	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	CH	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		
6	CT	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	CZ	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Cf	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Cl	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Cr	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Cx	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
6	Eb	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	En	27	Total	C	N	O	S	0	0
			224	135	44	42	3		

- 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	131	Total	C	N	O	S	0	0
			956	595	165	191	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	C	N	O	S	0	0
			2228	1364	405	446	13		
12	j	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	k	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	l	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	m	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	n	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	o	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	p	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	q	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	r	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	s	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	t	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	u	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	v	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	w	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	x	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	y	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
12	z	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C4	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	C5	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	C9	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	C0	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DA	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DC	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DG	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DH	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DI	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DN	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DO	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DP	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DT	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DU	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DV	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	DZ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Da	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Db	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Df	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Dg	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Dh	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Dl	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	Dm	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Dn	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Dr	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Ds	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Dt	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Dx	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Dy	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Dz	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	D4	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	D5	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	D6	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	D0	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EA	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EB	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	B0	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	B2	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	B3	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	B4	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	B8	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	B9	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EC	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	ED	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EH	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EI	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EJ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EN	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EO	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EP	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	ET	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EU	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EV	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	EZ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	BY	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	BZ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Bd	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Be	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Bf	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Bj	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Bk	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Bl	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Bp	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Bq	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	Br	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Bv	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Bw	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Bx	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	C1	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	C2	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	CD	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	CE	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	CF	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	CJ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	CK	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	CL	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	CP	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	CQ	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	CR	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	CW	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	CX	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Cb	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Cc	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Cd	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	Ch	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Ci	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Cj	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
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	Cp	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	Cz	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Ed	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Ee	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Ef	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Ej	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Ek	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	El	87	Total	C	N	O	S	0	0
			675	427	118	126	4		
13	Ep	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	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	DB	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	DD	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	DJ	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	DQ	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	DW	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Dc	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Di	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Do	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Du	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	D1	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	D7	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	B5	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	EE	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	EK	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	EQ	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	EW	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Ba	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Bg	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Bm	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Bs	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	By	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	CA	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	CG	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	CM	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	CS	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	CY	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Ce	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Ck	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Cq	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Cw	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Ea	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Eg	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		
14	Em	315	Total	C	N	O	S	0	0
			2462	1535	435	483	9		

- Molecule 15 is a protein called Flagellar motor switch protein FliM.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C8	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	DF	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	DL	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	DM	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	DS	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	DY	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	De	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Dk	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	Dq	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Dw	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	D3	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	D9	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	B1	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	B7	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	EG	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	EM	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	ES	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	EY	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Bc	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Bi	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Bo	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Bu	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	CC	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	CI	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	CO	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	CU	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Ca	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Cg	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Cm	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		

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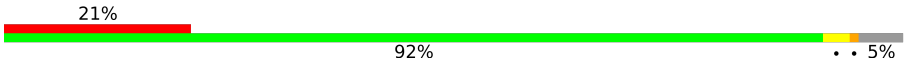
Mol	Chain	Residues	Atoms					AltConf	Trace
15	Cs	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Cy	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Ec	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Ei	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		
15	Eo	289	Total	C	N	O	S	0	0
			2341	1492	423	421	5		

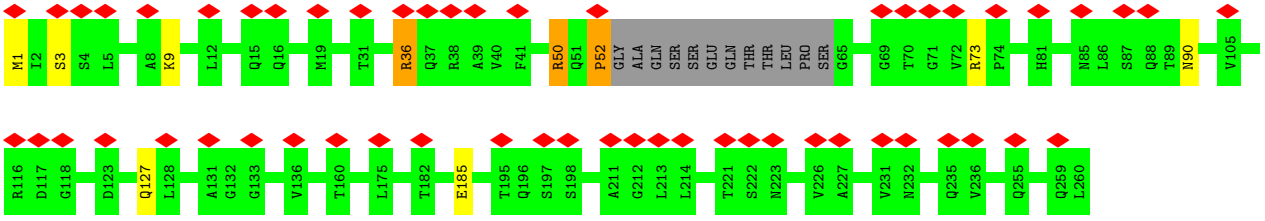
3 Residue-property plots (i)

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

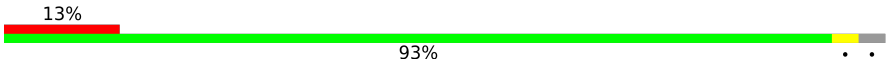
Chain 0:

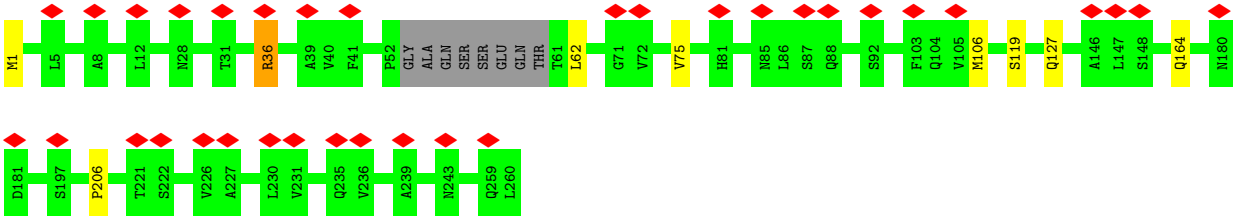




• Molecule 1: Flagellar basal-body rod protein FlgG

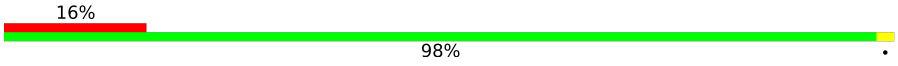
Chain 1:

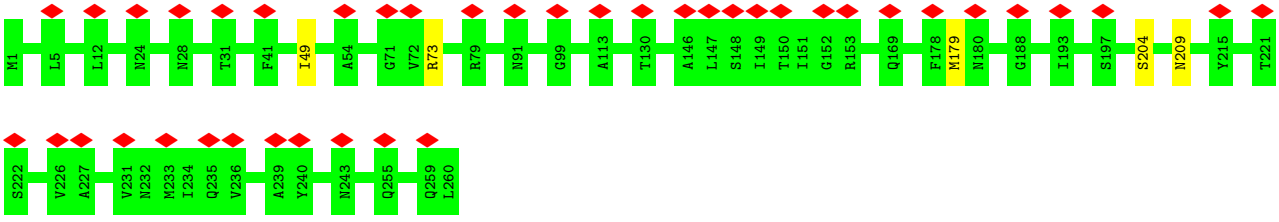




• Molecule 1: Flagellar basal-body rod protein FlgG

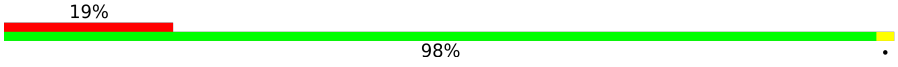
Chain 2:

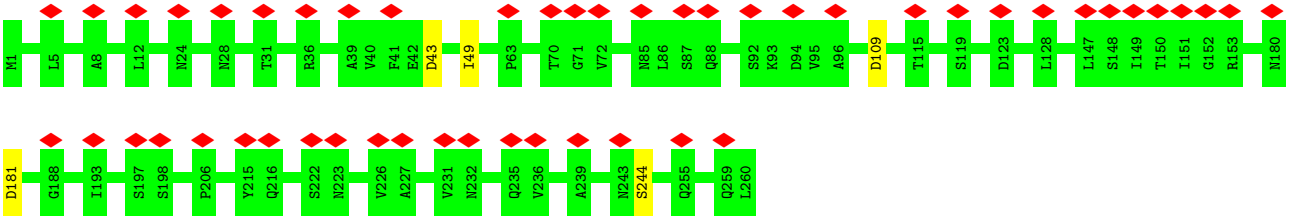




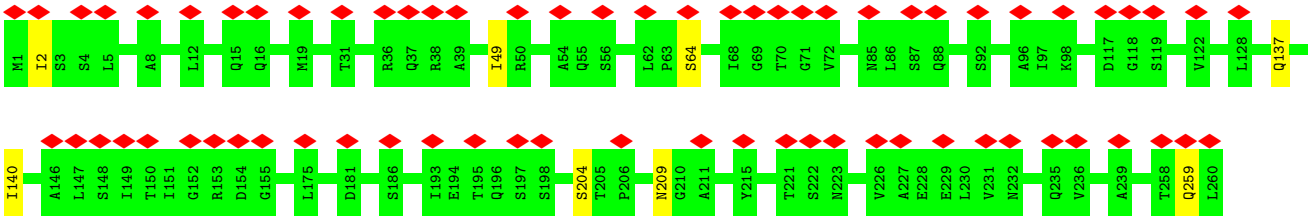
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain 3:

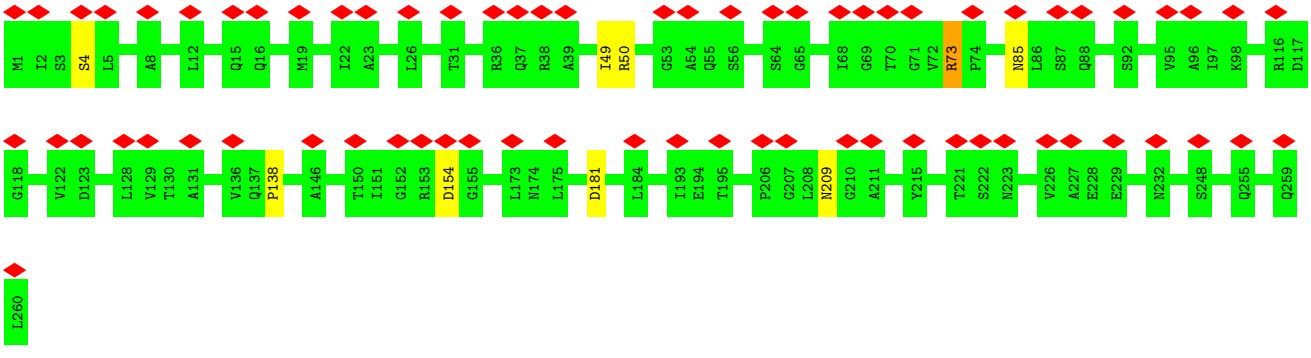




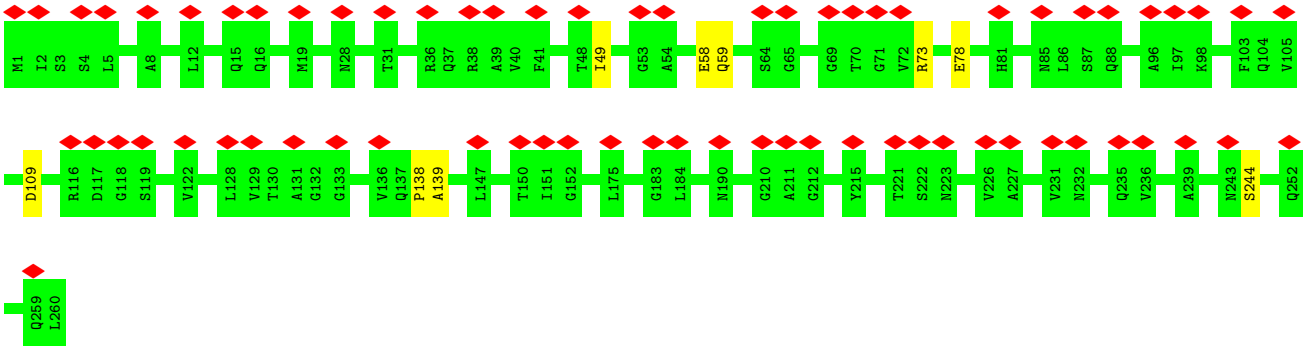
• Molecule 1: Flagellar basal-body rod protein FlgG



• Molecule 1: Flagellar basal-body rod protein FlgG

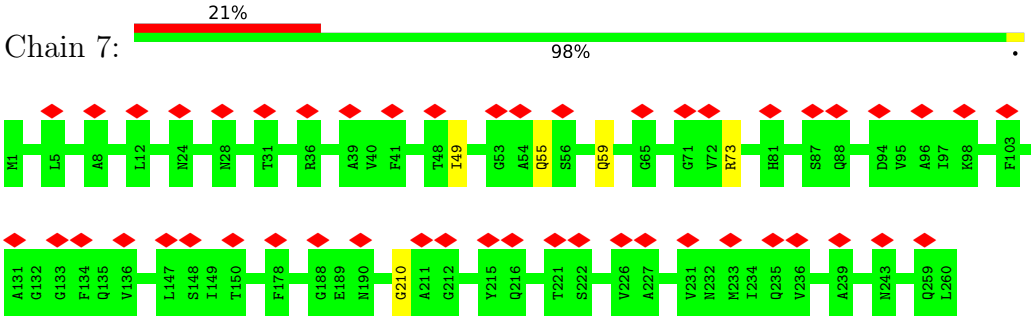


• Molecule 1: Flagellar basal-body rod protein FlgG



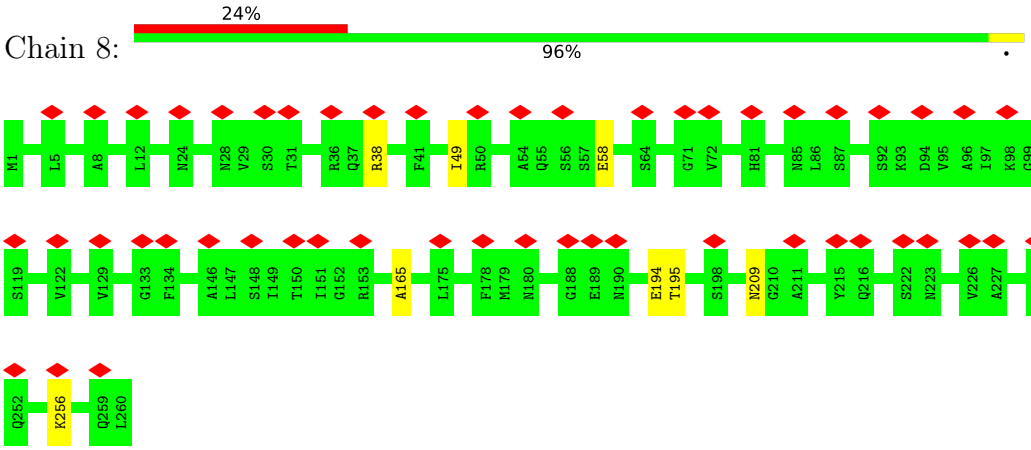
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain 7:



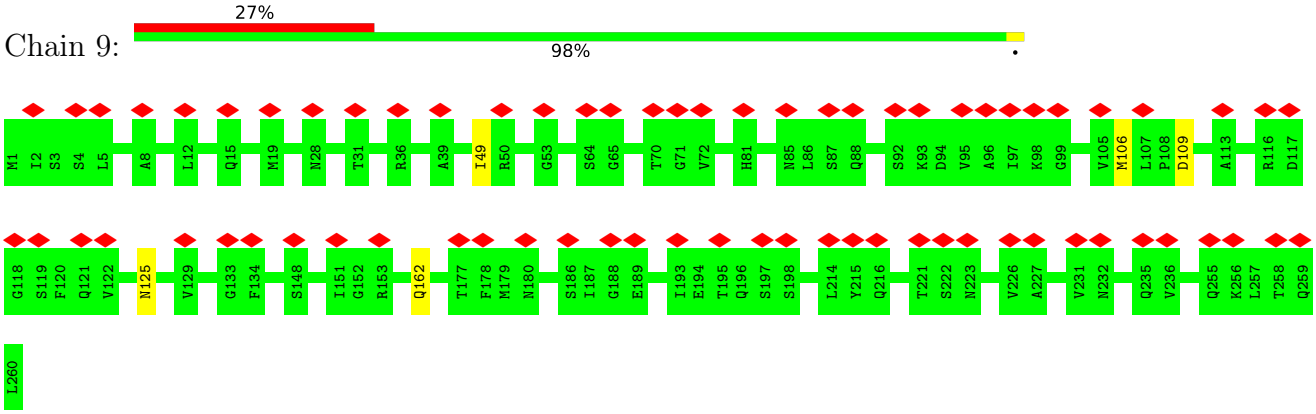
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain 8:



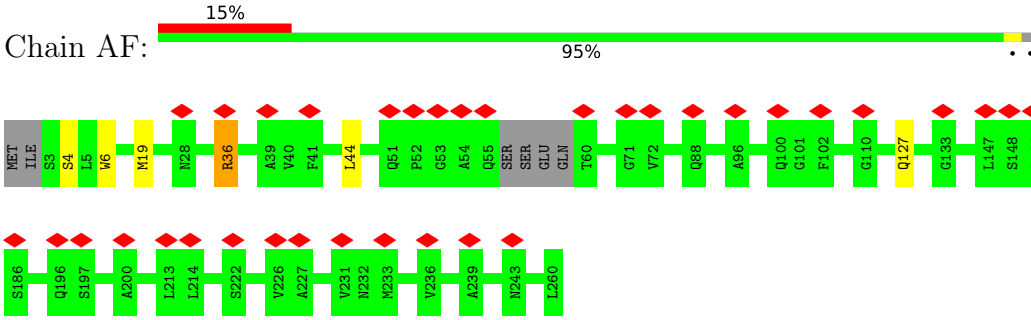
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain 9:



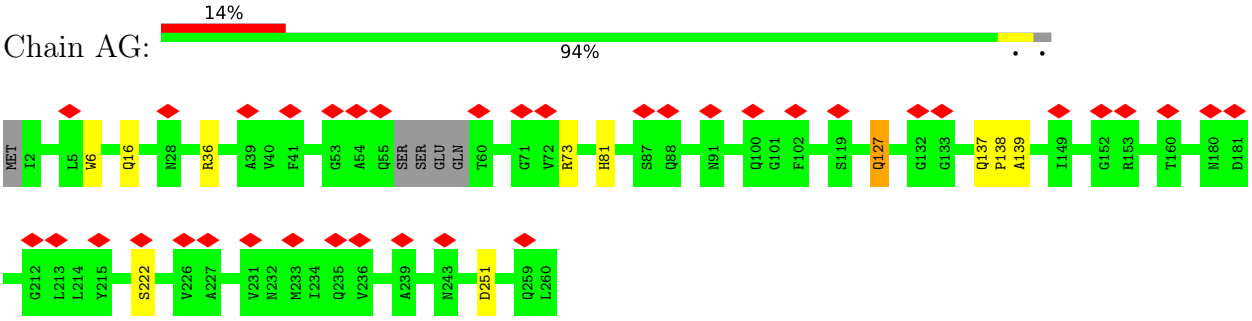
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain AF:



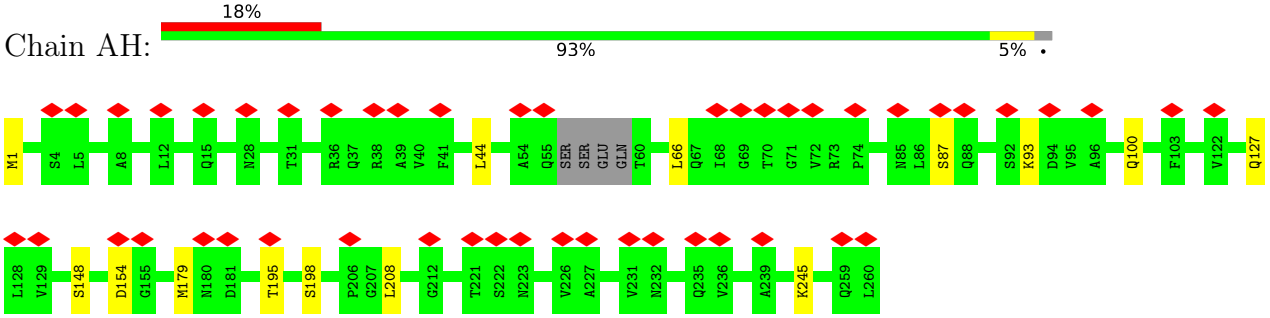
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain AG:



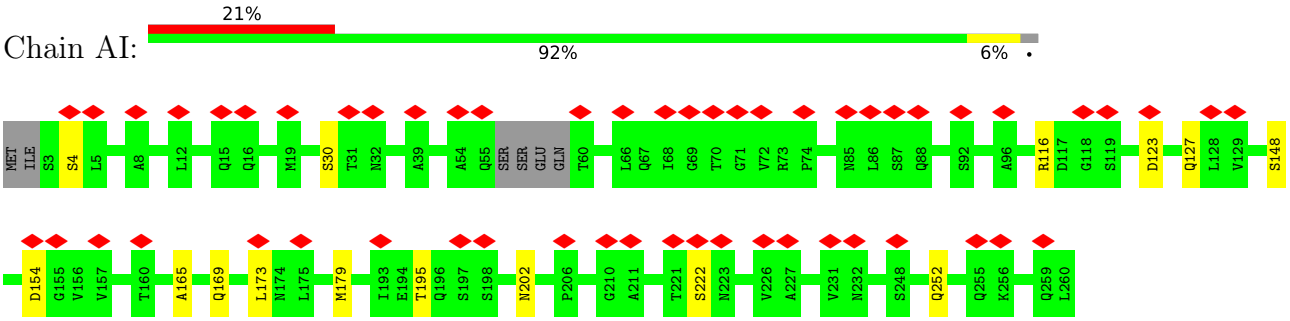
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain AH:



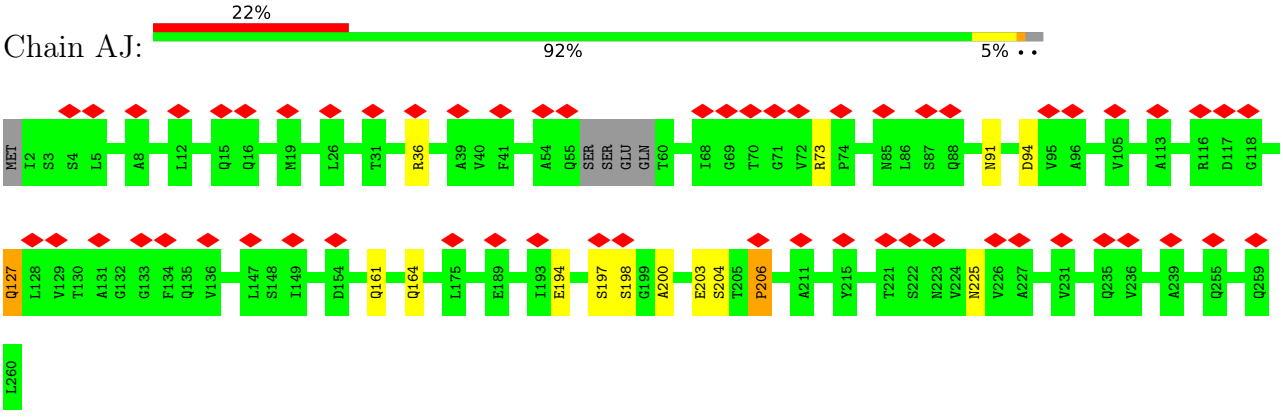
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain AI:



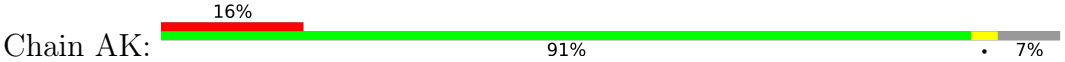
• Molecule 1: Flagellar basal-body rod protein FlgG

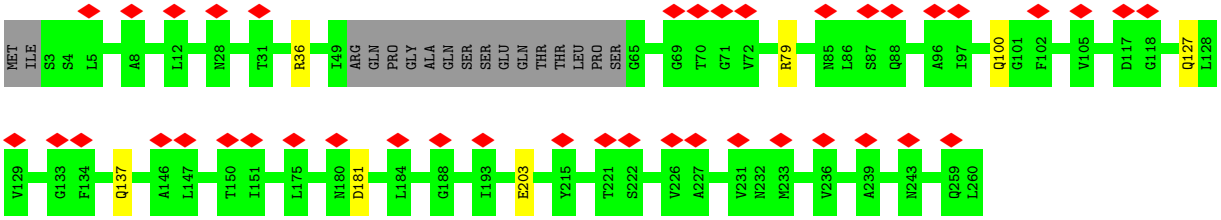
Chain AJ:



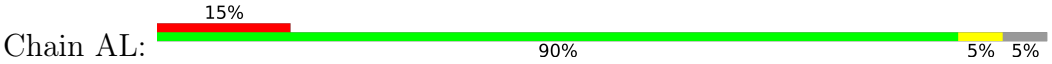
• Molecule 1: Flagellar basal-body rod protein FlgG

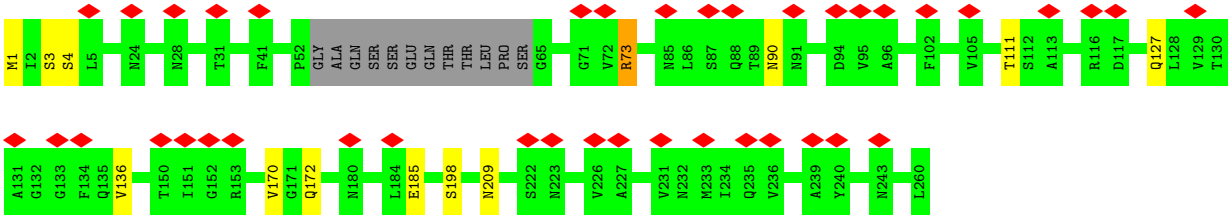
Chain AK:



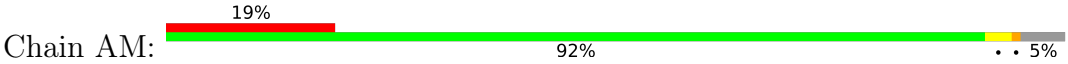


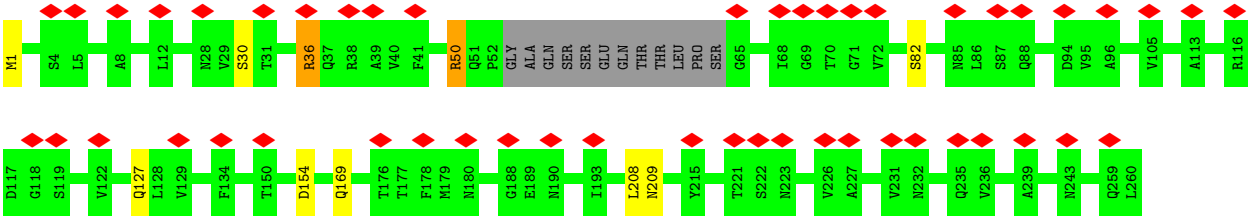
• Molecule 1: Flagellar basal-body rod protein FlgG



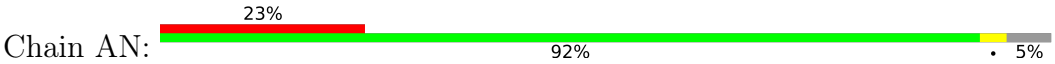


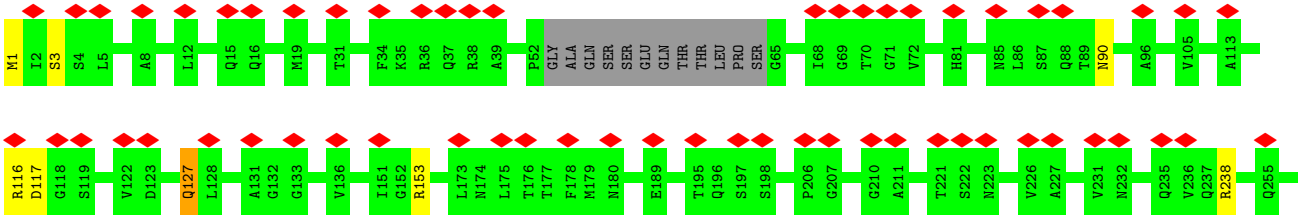
• Molecule 1: Flagellar basal-body rod protein FlgG



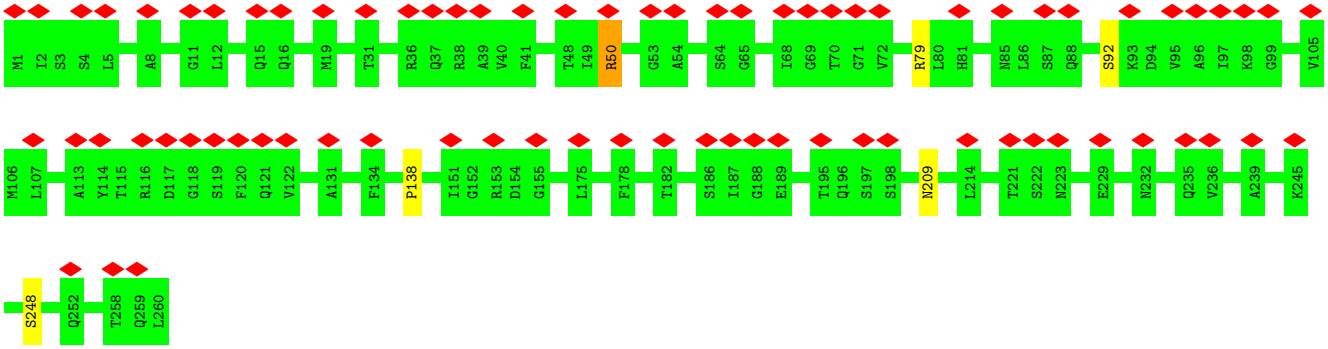


• Molecule 1: Flagellar basal-body rod protein FlgG

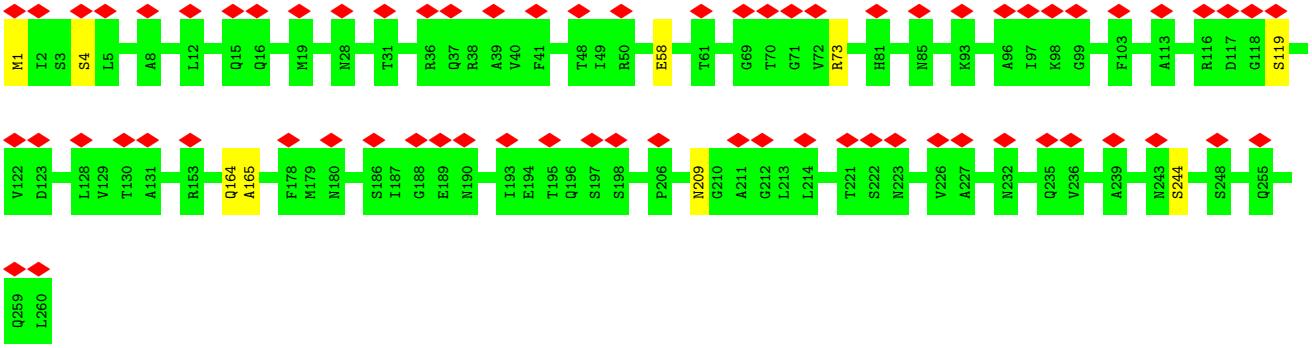




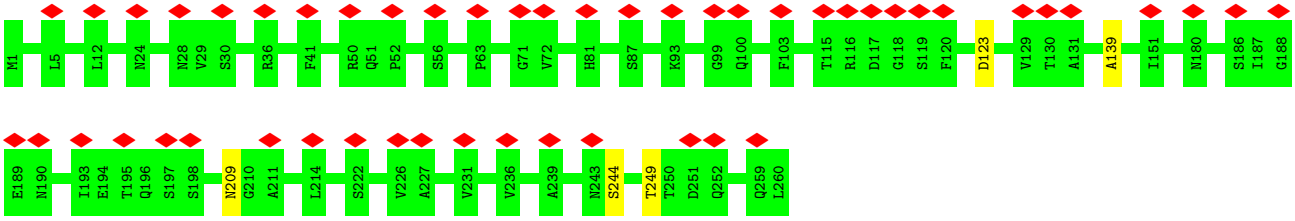
• Molecule 1: Flagellar basal-body rod protein FlgG



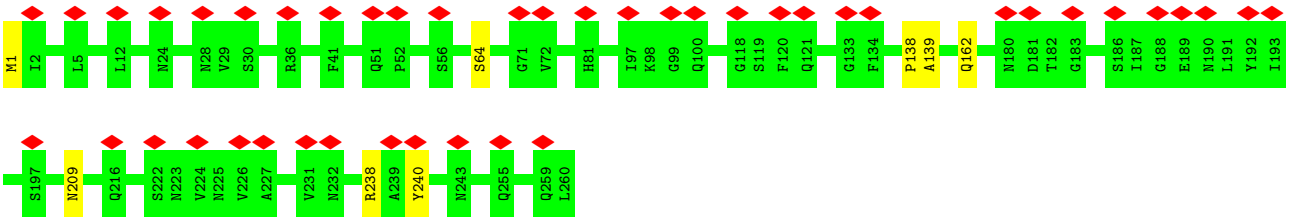
• Molecule 1: Flagellar basal-body rod protein FlgG



• Molecule 1: Flagellar basal-body rod protein FlgG

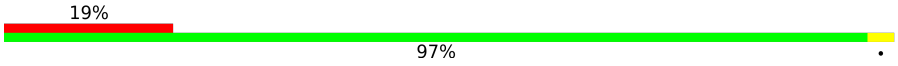


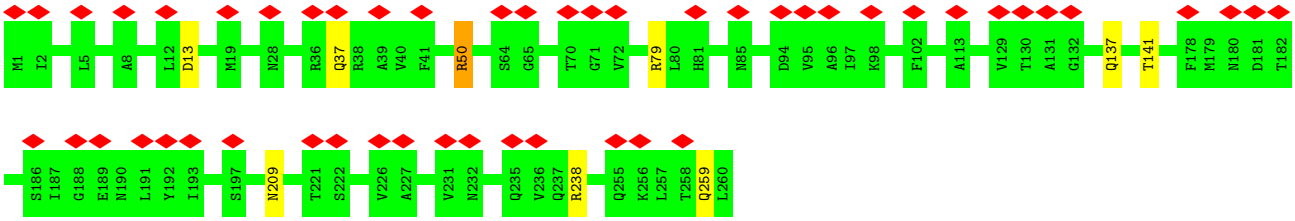
• Molecule 1: Flagellar basal-body rod protein FlgG



• Molecule 1: Flagellar basal-body rod protein FlgG

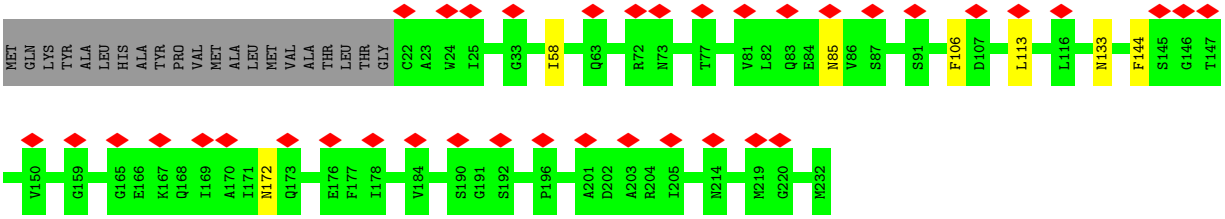
Chain ZE:





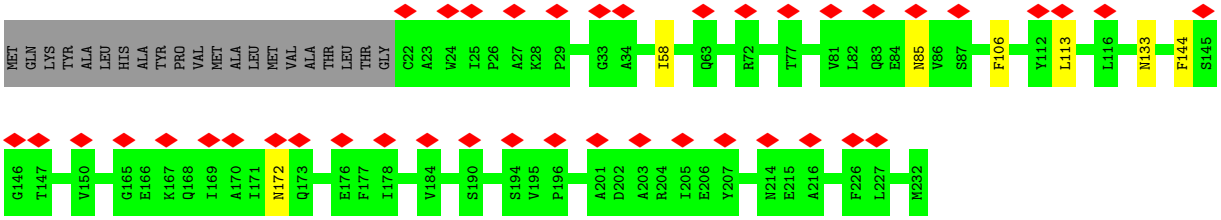
• Molecule 2: Flagellar L-ring protein

Chain A:



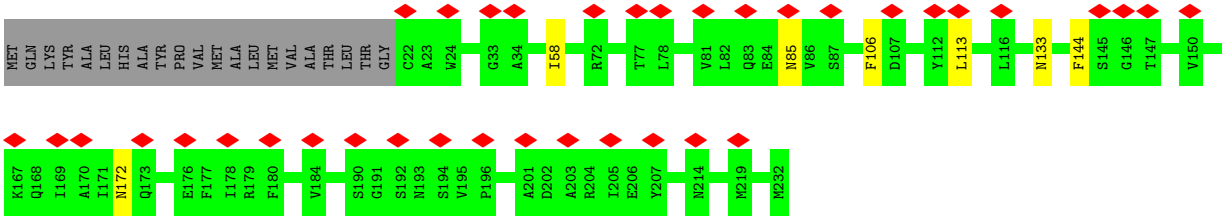
• Molecule 2: Flagellar L-ring protein

Chain B:



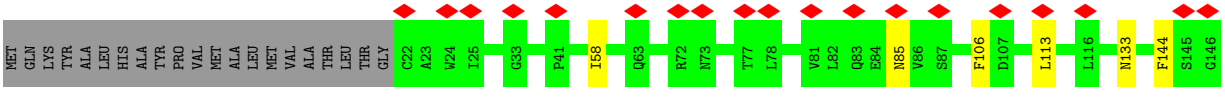
• Molecule 2: Flagellar L-ring protein

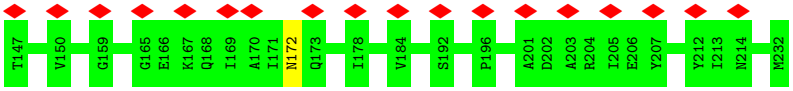
Chain C:



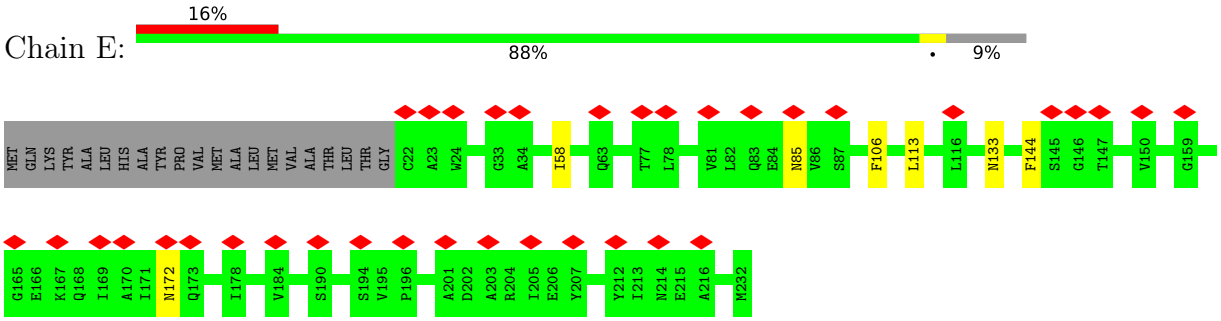
• Molecule 2: Flagellar L-ring protein

Chain D:

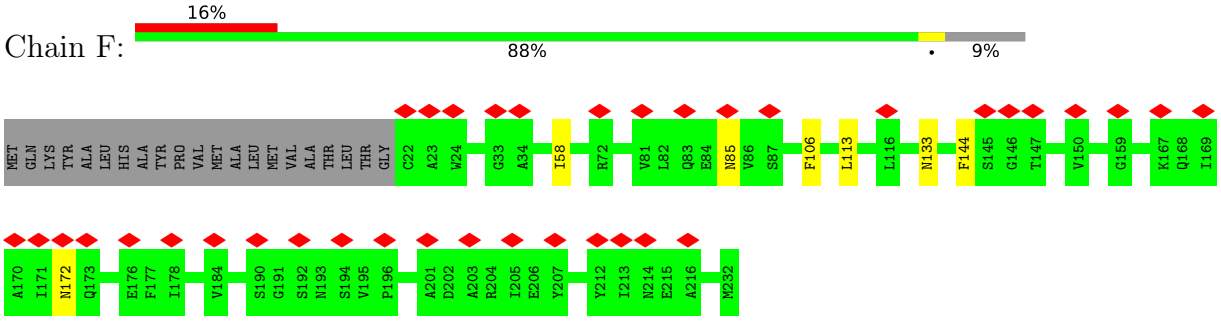




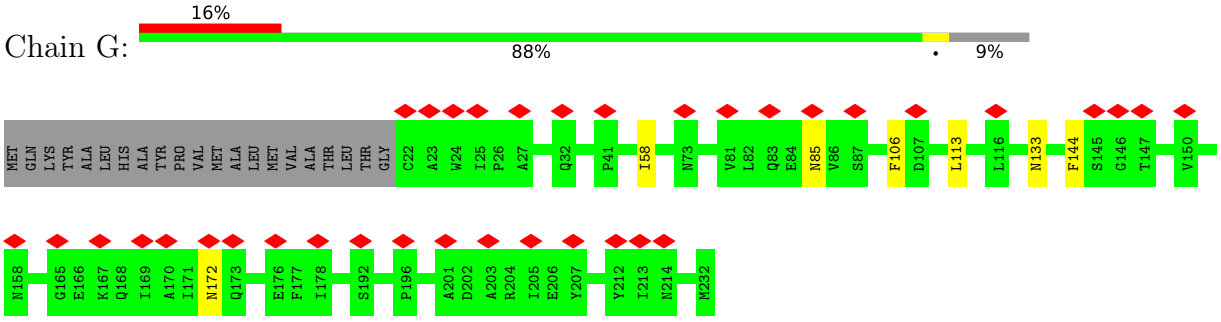
• Molecule 2: Flagellar L-ring protein



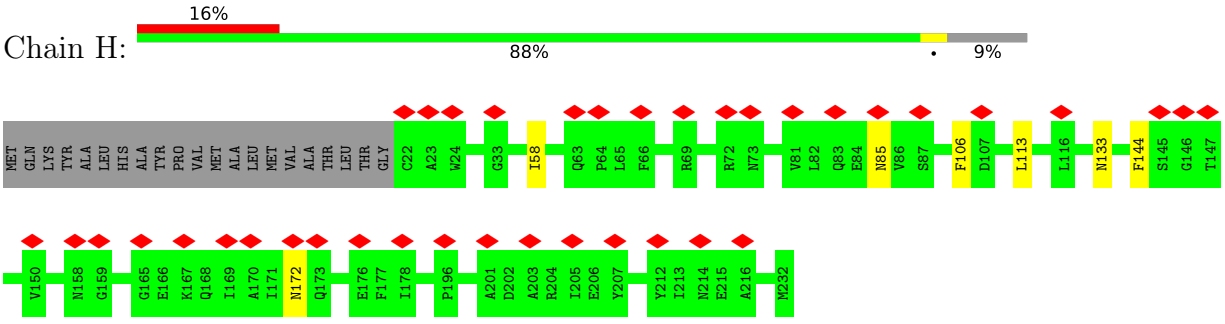
• Molecule 2: Flagellar L-ring protein



• Molecule 2: Flagellar L-ring protein

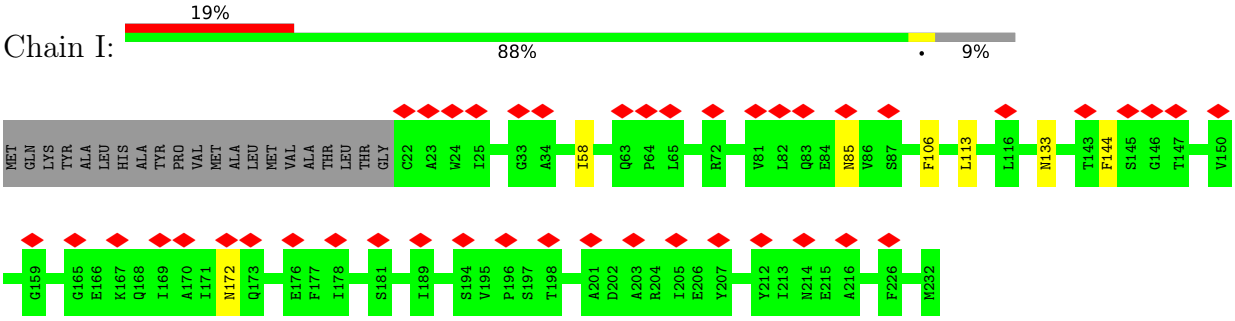


• Molecule 2: Flagellar L-ring protein



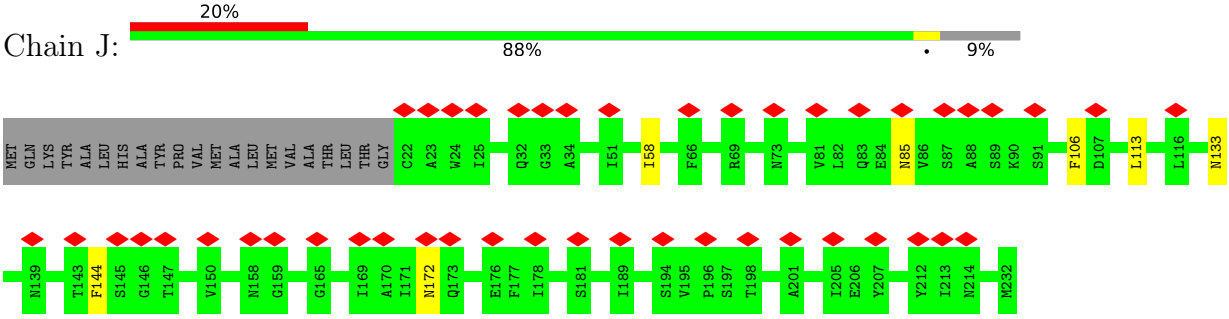
• Molecule 2: Flagellar L-ring protein

Chain I:



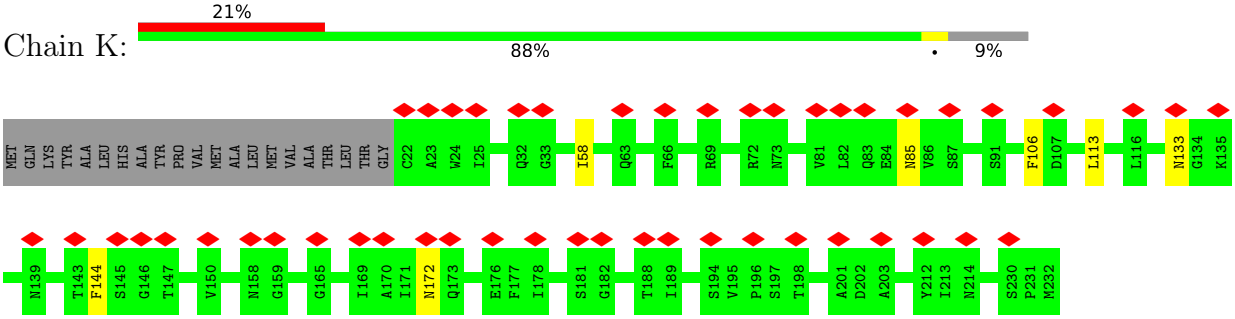
• Molecule 2: Flagellar L-ring protein

Chain J:



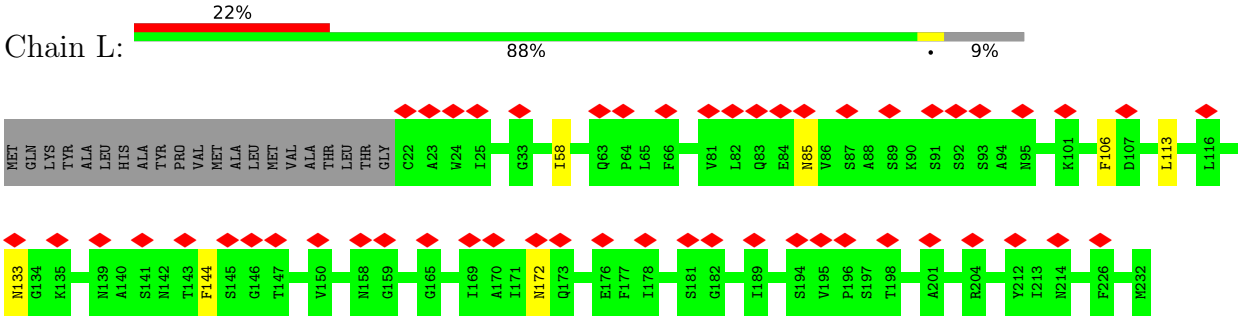
• Molecule 2: Flagellar L-ring protein

Chain K:



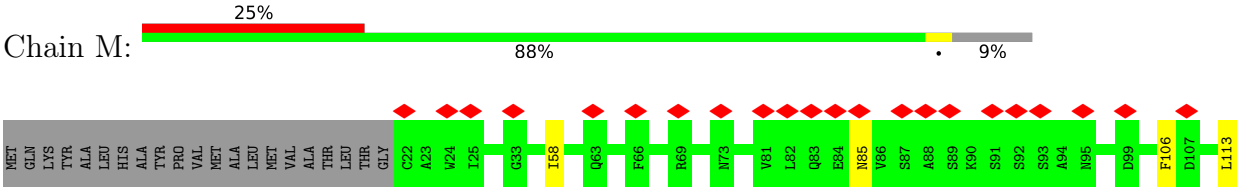
• Molecule 2: Flagellar L-ring protein

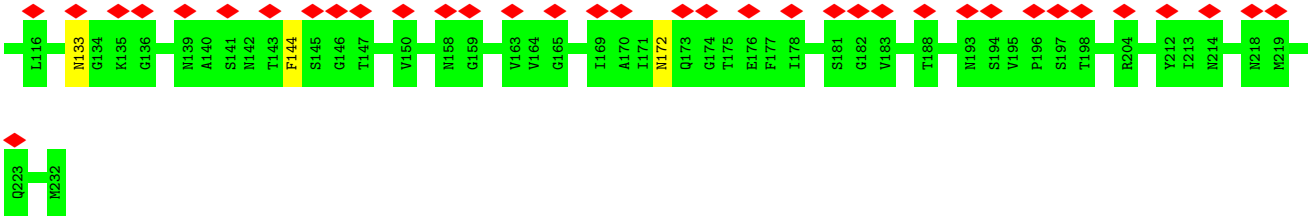
Chain L:



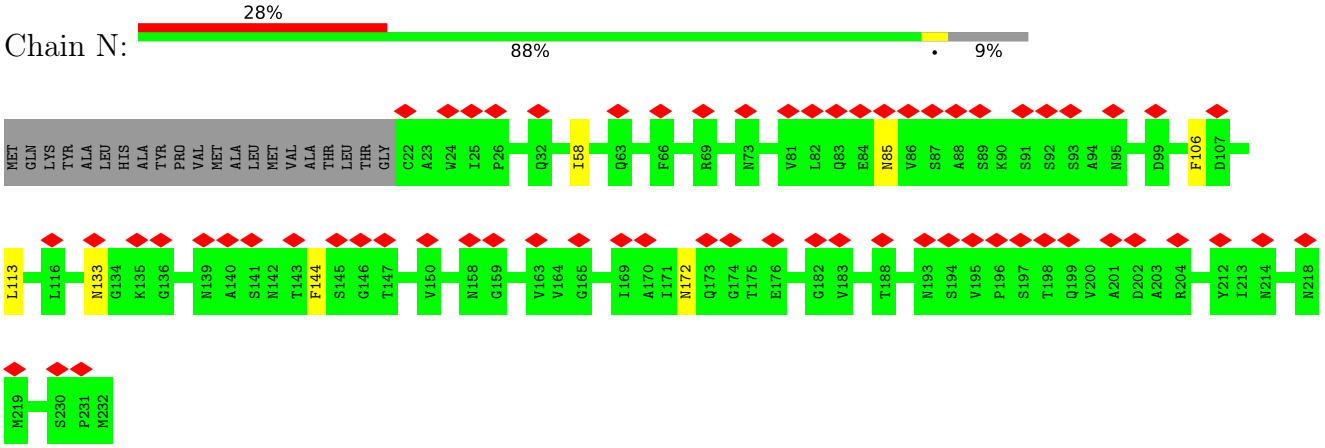
• Molecule 2: Flagellar L-ring protein

Chain M:

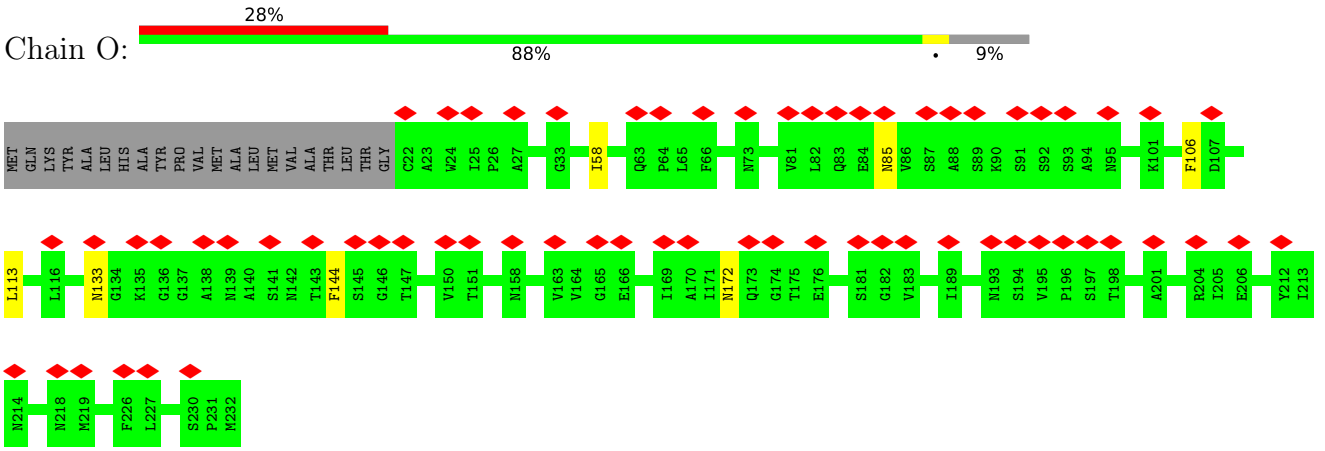




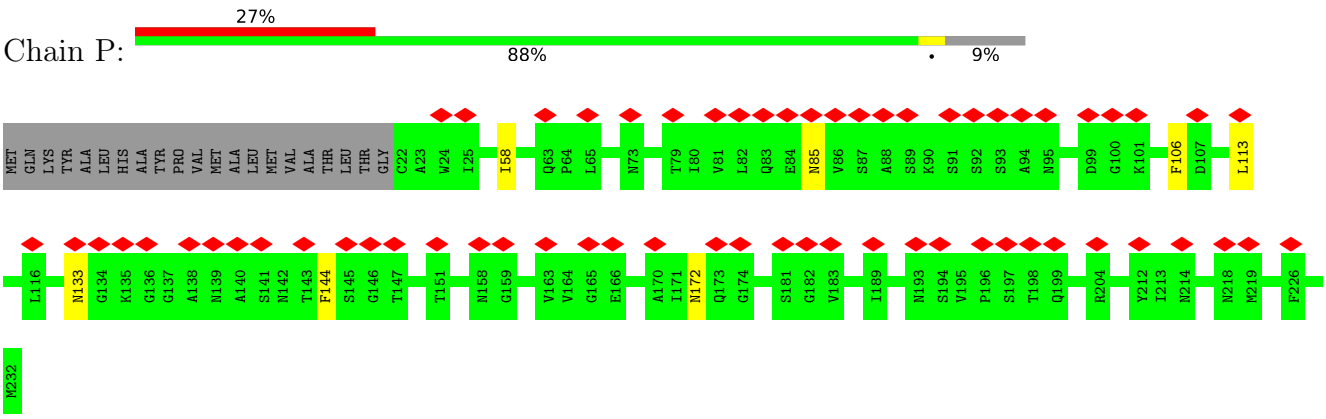
• Molecule 2: Flagellar L-ring protein



• Molecule 2: Flagellar L-ring protein

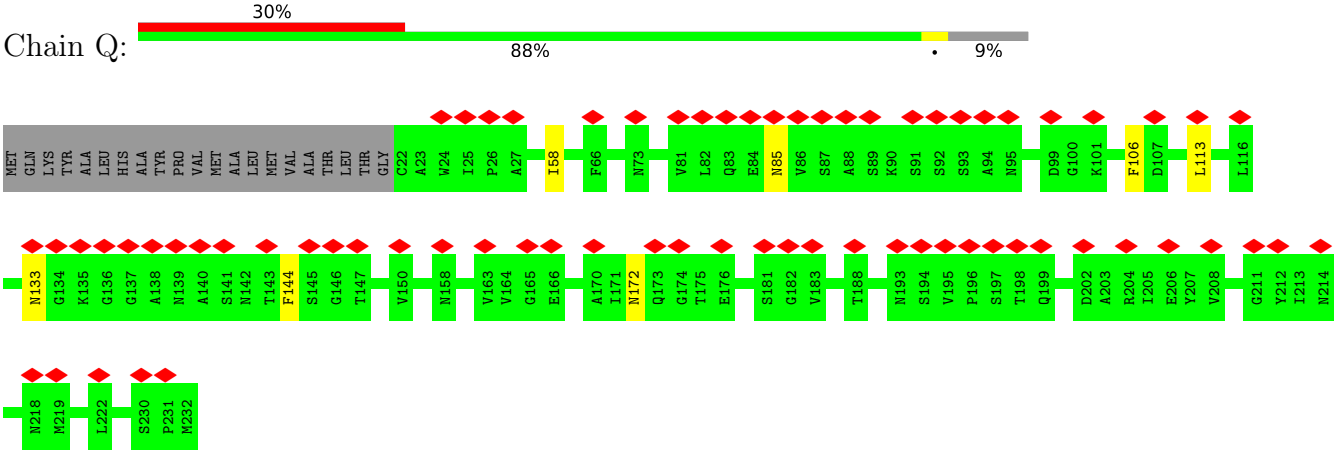


• Molecule 2: Flagellar L-ring protein



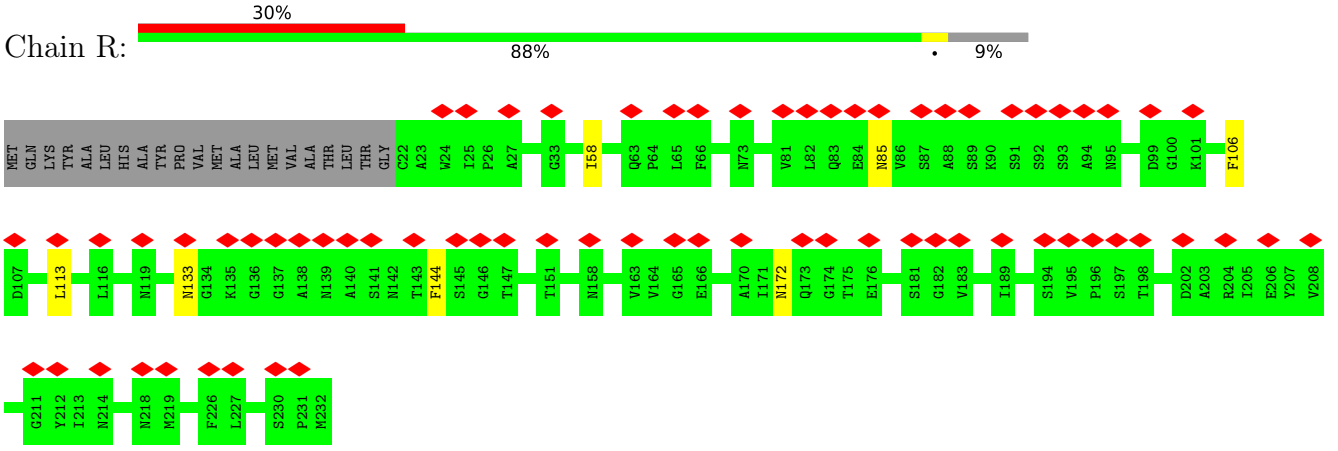
• Molecule 2: Flagellar L-ring protein

Chain Q:



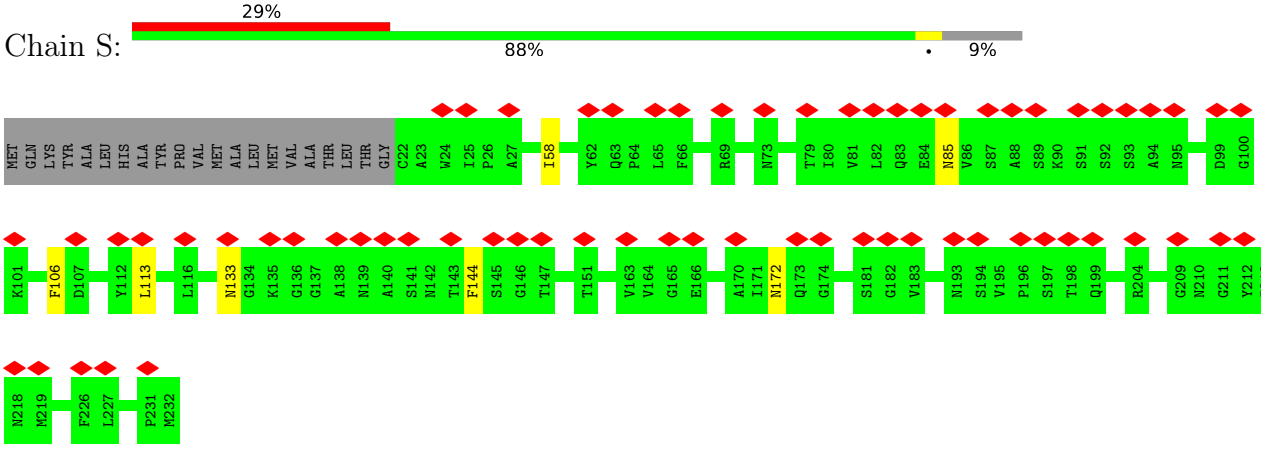
• Molecule 2: Flagellar L-ring protein

Chain R:



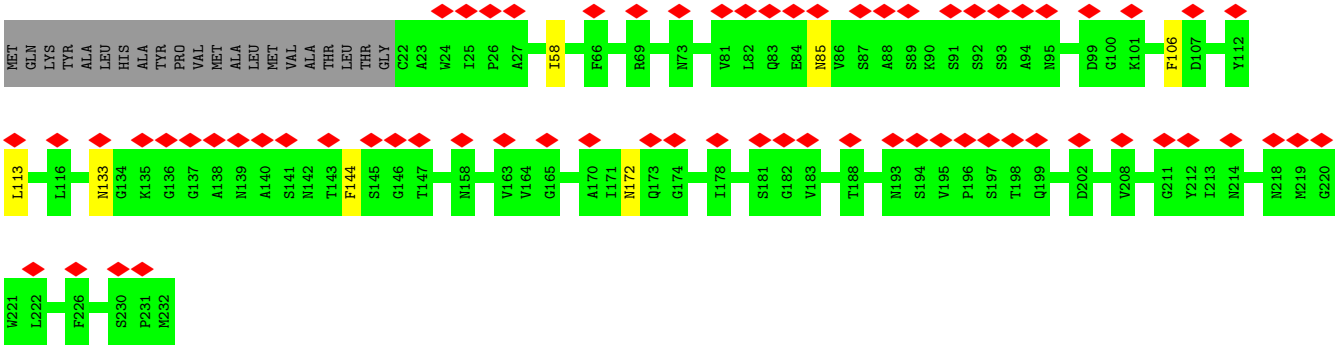
• Molecule 2: Flagellar L-ring protein

Chain S:



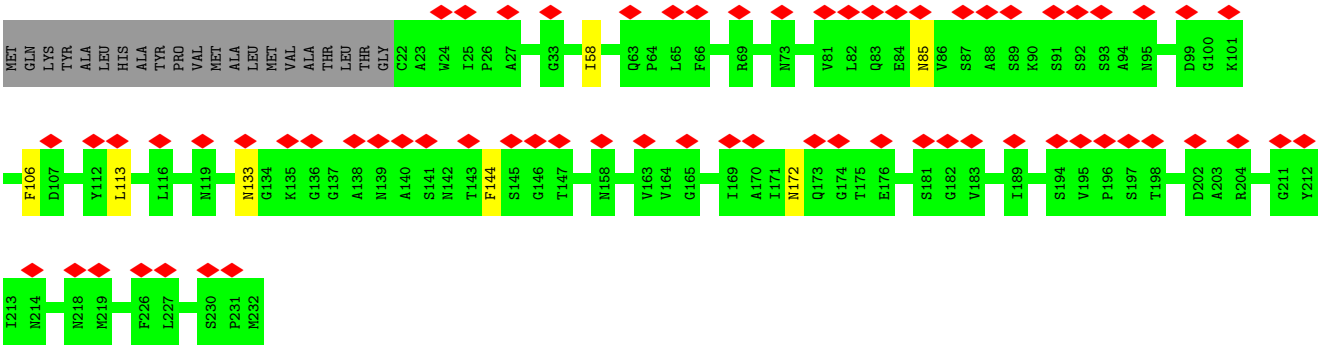
• Molecule 2: Flagellar L-ring protein

Chain T:



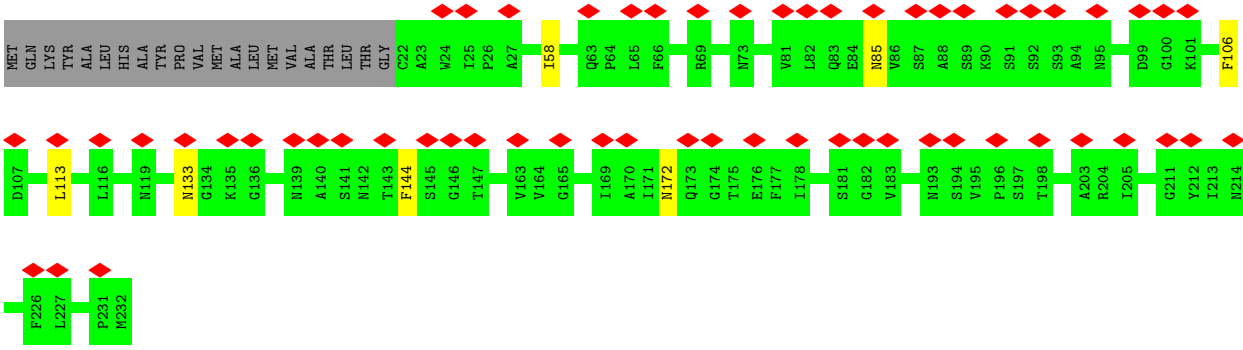
• Molecule 2: Flagellar L-ring protein

Chain U:



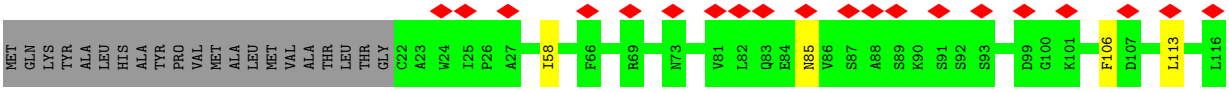
• Molecule 2: Flagellar L-ring protein

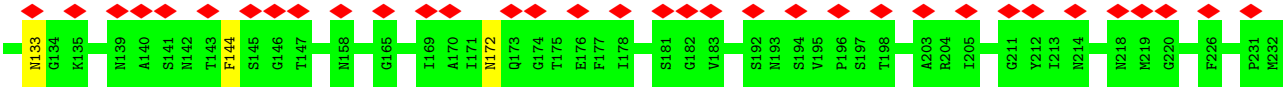
Chain V:



• Molecule 2: Flagellar L-ring protein

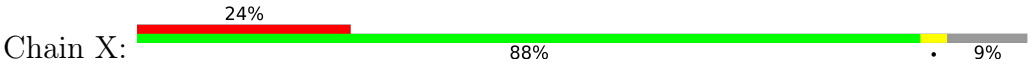
Chain W:

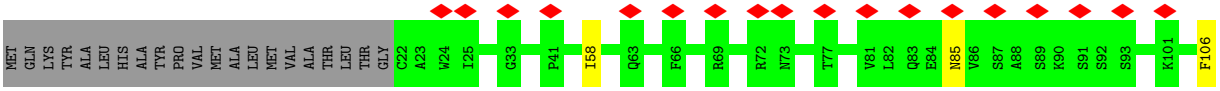


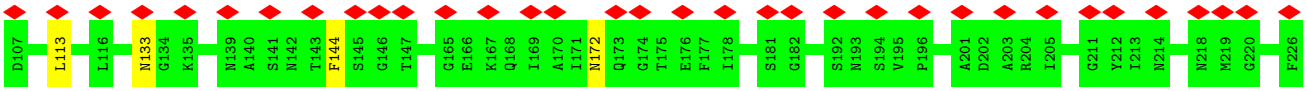


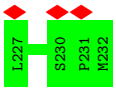
• Molecule 2: Flagellar L-ring protein

Chain X:



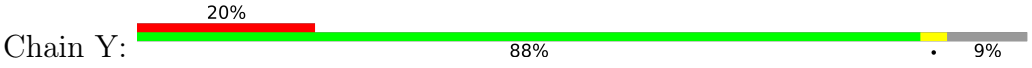


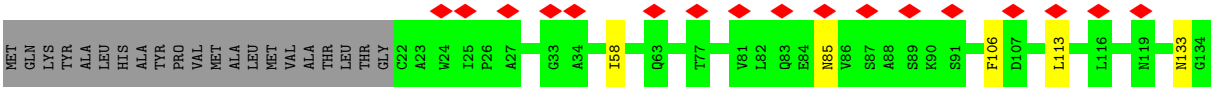


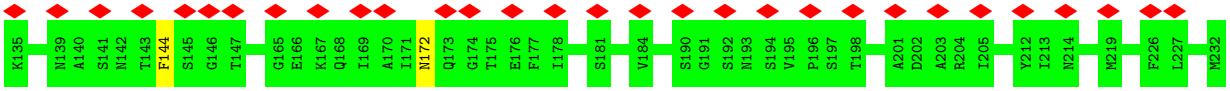


• Molecule 2: Flagellar L-ring protein

Chain Y:

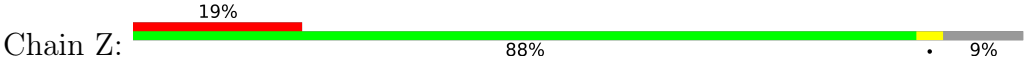


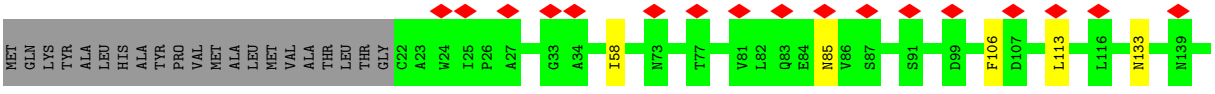


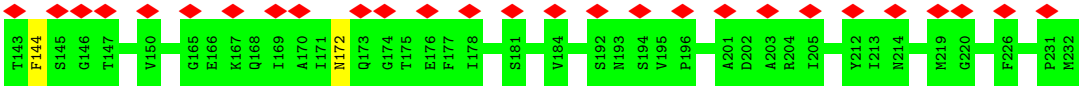


• Molecule 2: Flagellar L-ring protein

Chain Z:

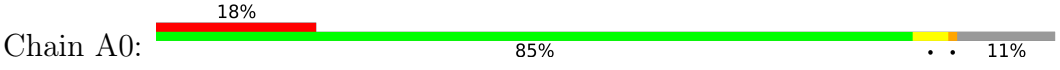


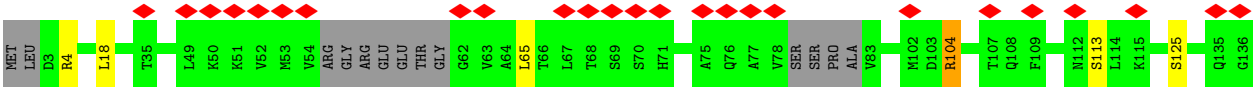




• Molecule 3: Flagellar basal body rod protein FlgB

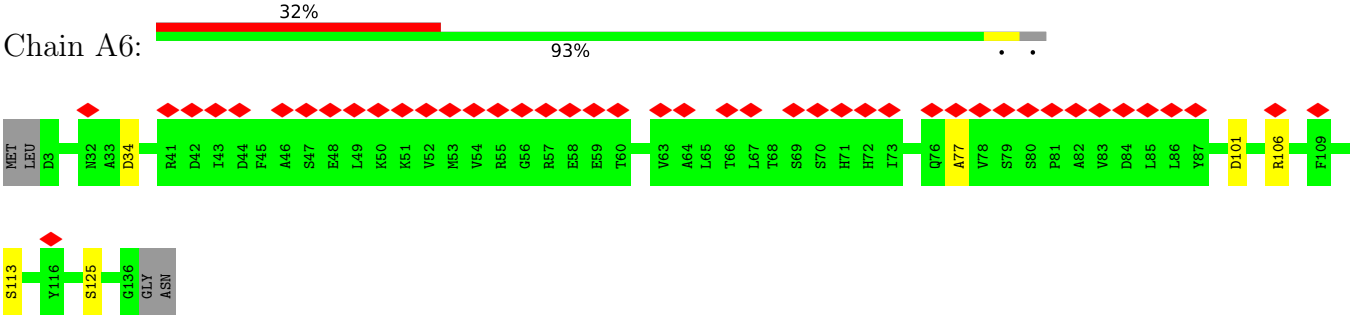
Chain A0:





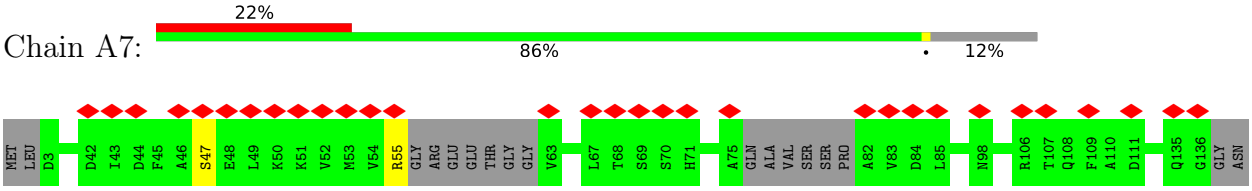
• Molecule 3: Flagellar basal body rod protein FlgB

Chain A6:



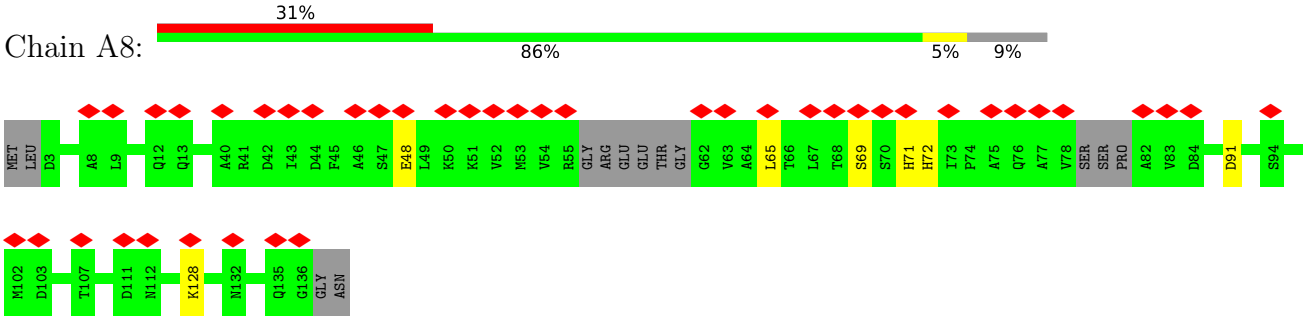
• Molecule 3: Flagellar basal body rod protein FlgB

Chain A7:



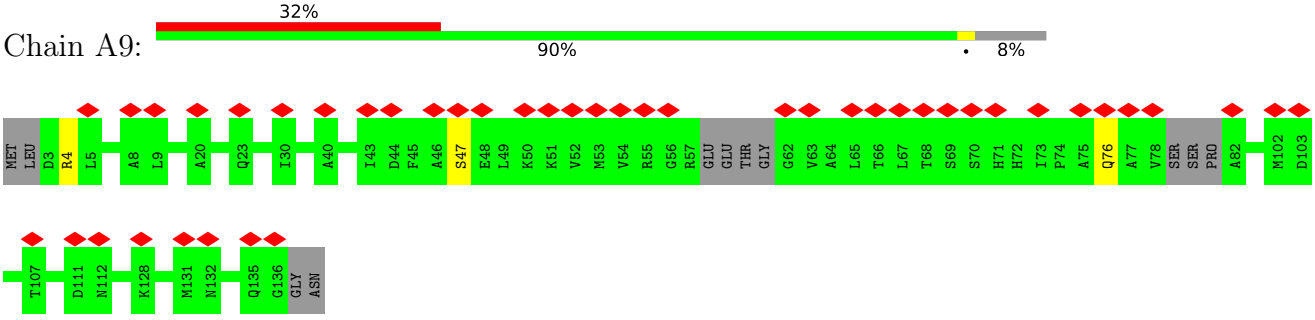
• Molecule 3: Flagellar basal body rod protein FlgB

Chain A8:



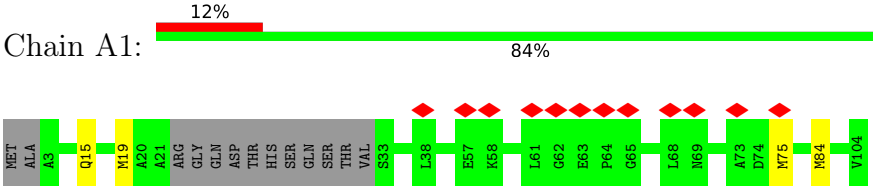
• Molecule 3: Flagellar basal body rod protein FlgB

Chain A9:



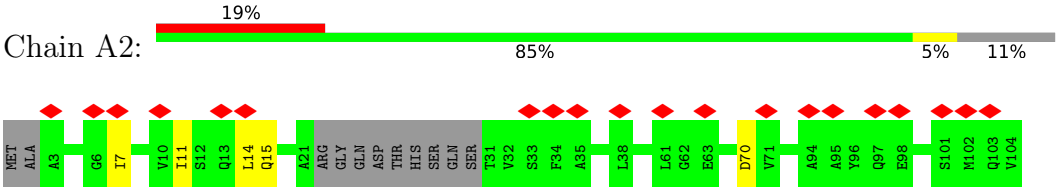
• Molecule 4: Flagellar hook-basal body complex protein FliE

Chain A1:



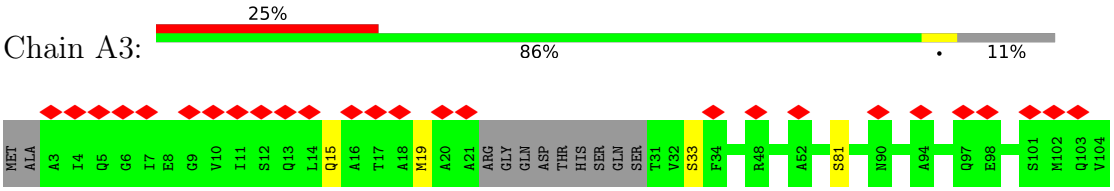
• Molecule 4: Flagellar hook-basal body complex protein FliE

Chain A2:



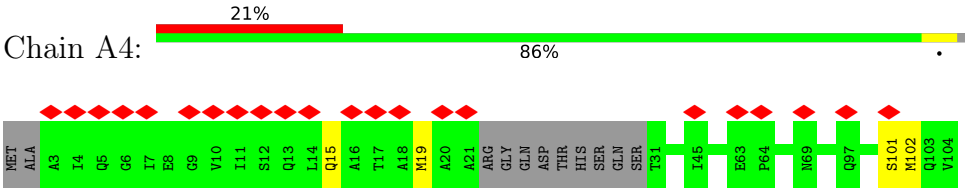
• Molecule 4: Flagellar hook-basal body complex protein FliE

Chain A3:



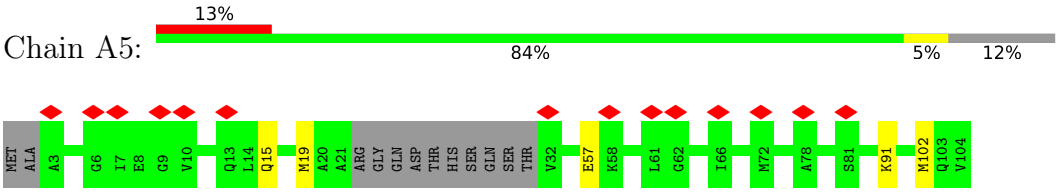
• Molecule 4: Flagellar hook-basal body complex protein FliE

Chain A4:



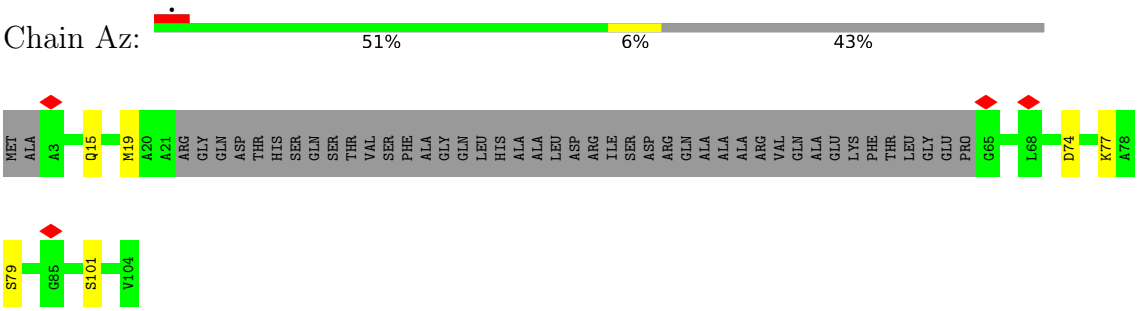
• Molecule 4: Flagellar hook-basal body complex protein FliE

Chain A5:



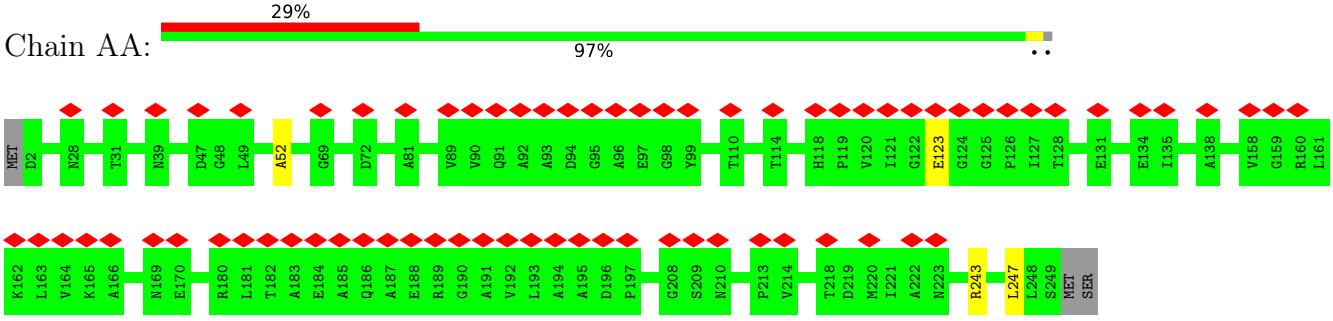
• Molecule 4: Flagellar hook-basal body complex protein FliE

Chain Az:



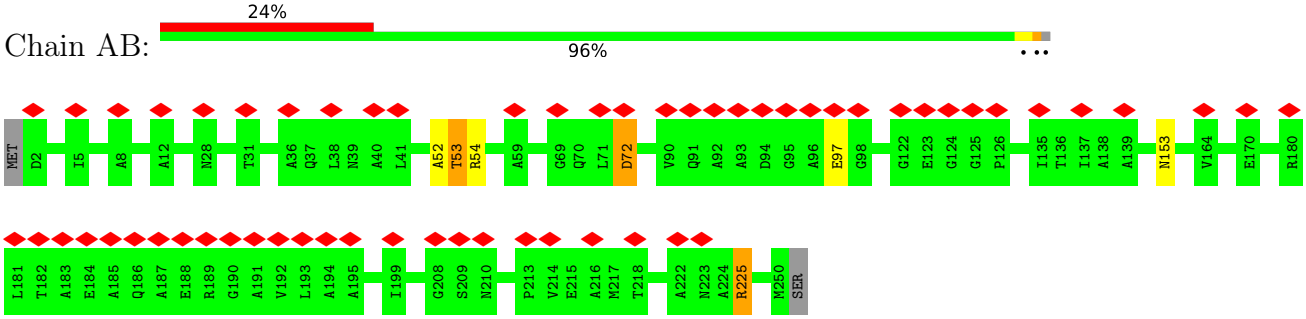
• Molecule 5: Flagellar basal-body rod protein FlgF

Chain AA:



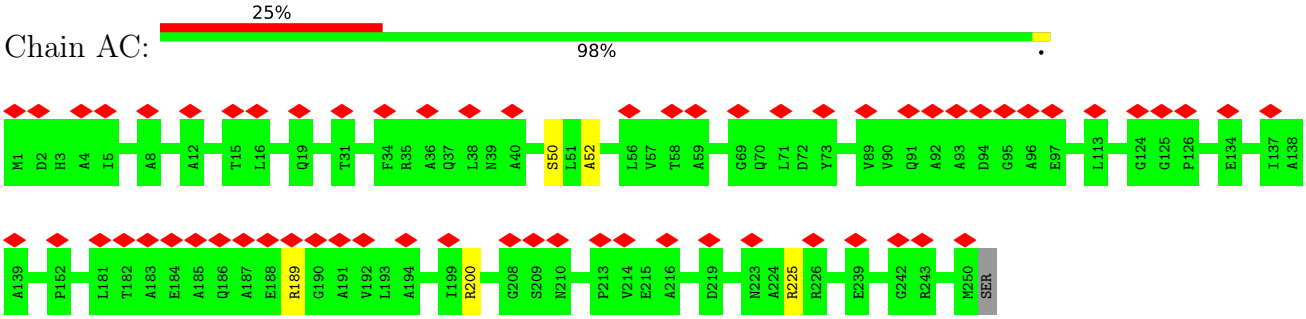
• Molecule 5: Flagellar basal-body rod protein FlgF

Chain AB:



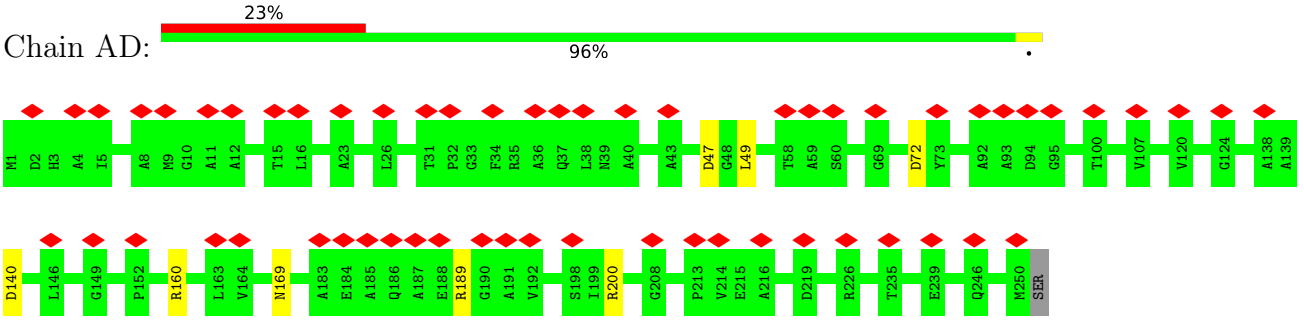
• Molecule 5: Flagellar basal-body rod protein FlgF

Chain AC:



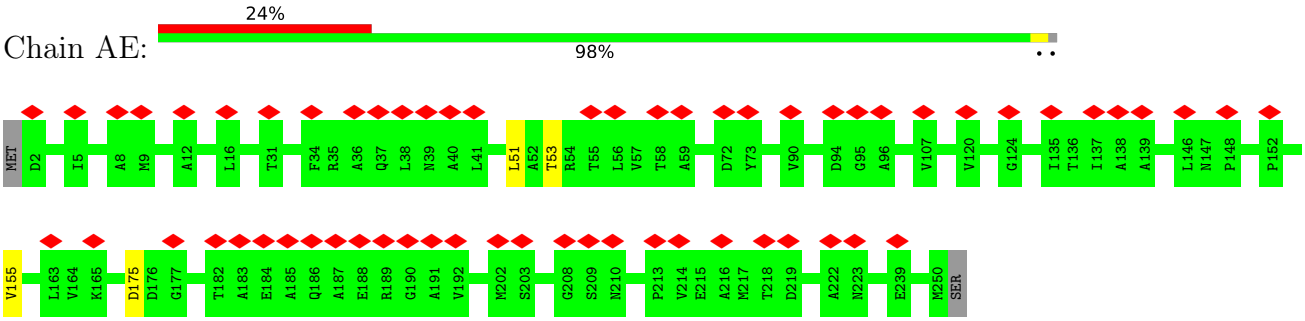
• Molecule 5: Flagellar basal-body rod protein FlgF

Chain AD:



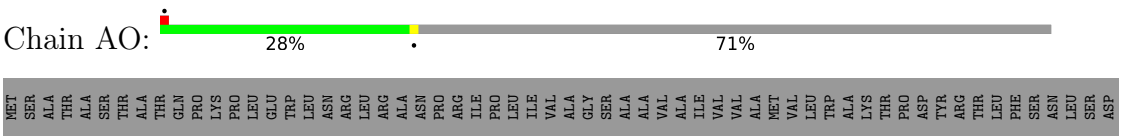
• Molecule 5: Flagellar basal-body rod protein FlgF

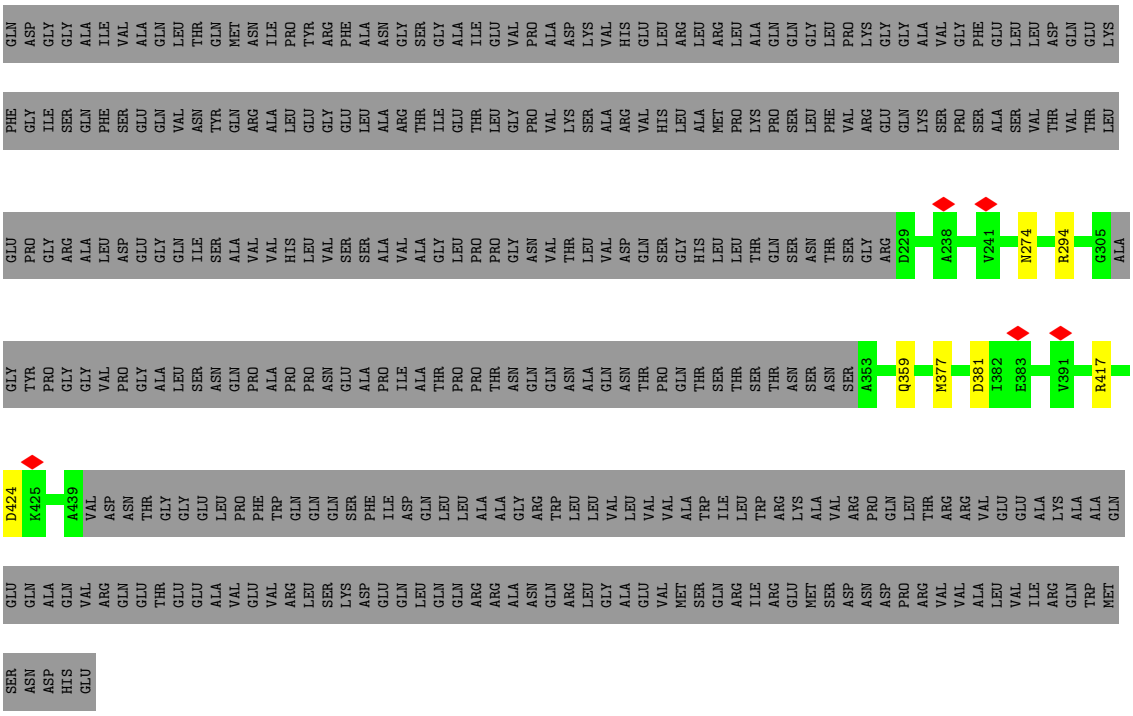
Chain AE:



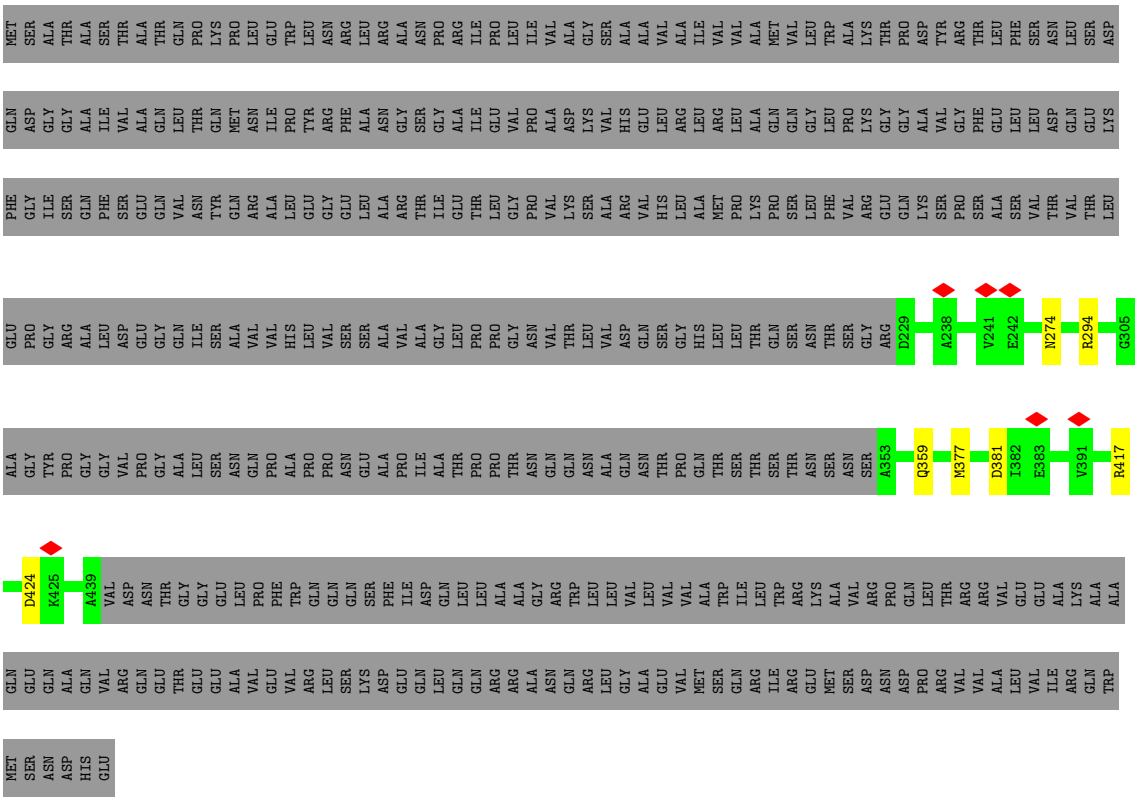
• Molecule 6: Flagellar M-ring protein

Chain AO:



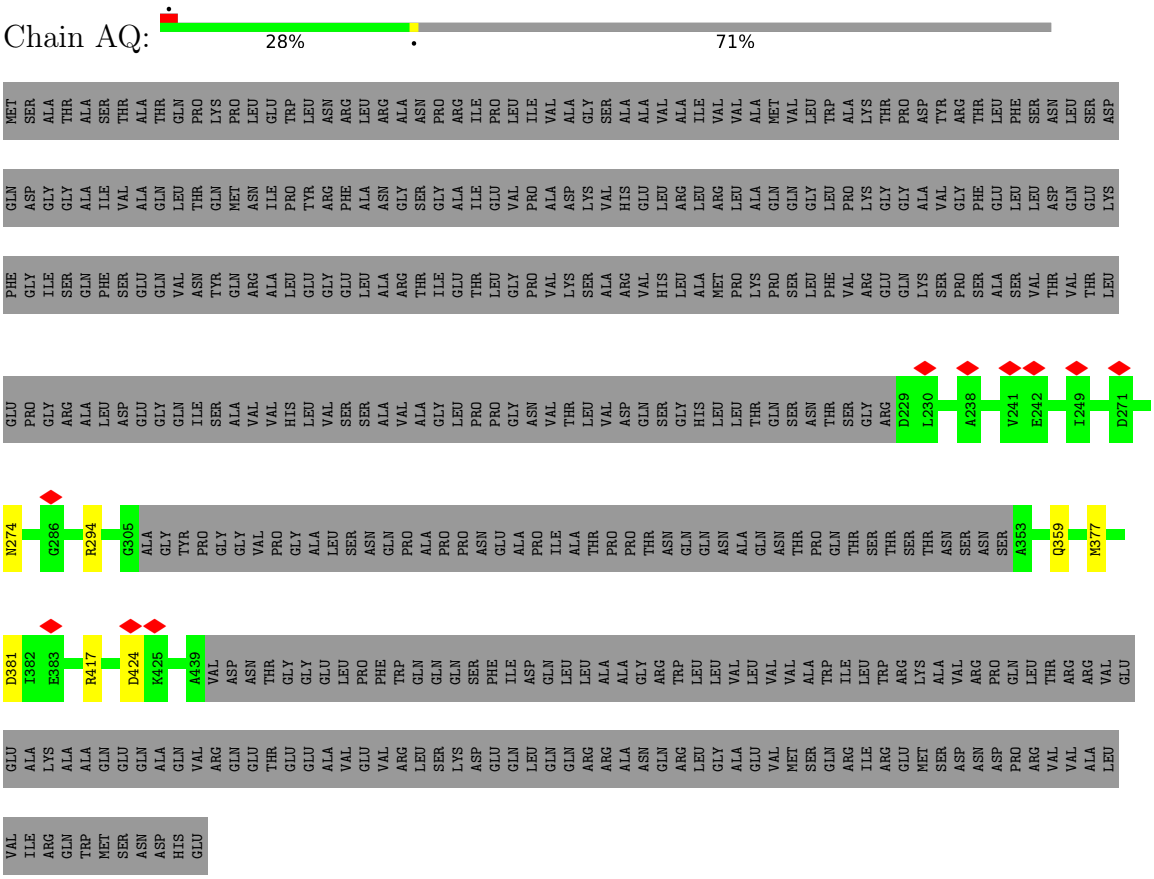


• Molecule 6: Flagellar M-ring protein



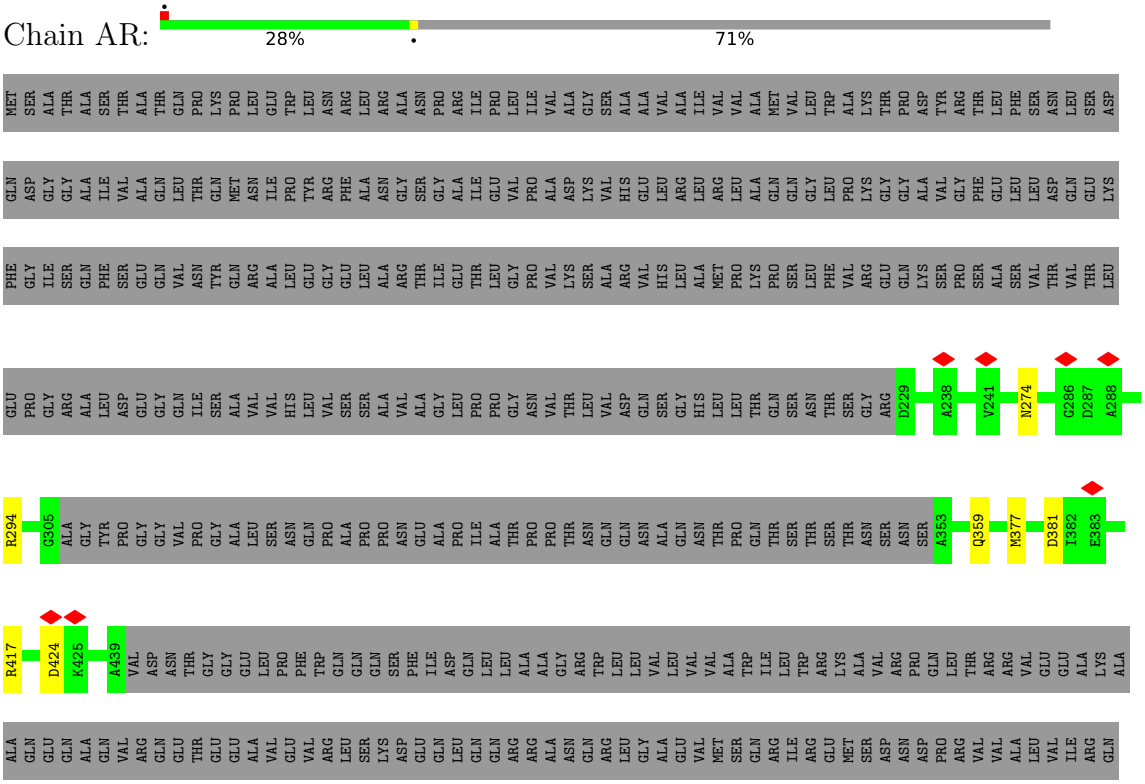
• Molecule 6: Flagellar M-ring protein

Chain AQ:



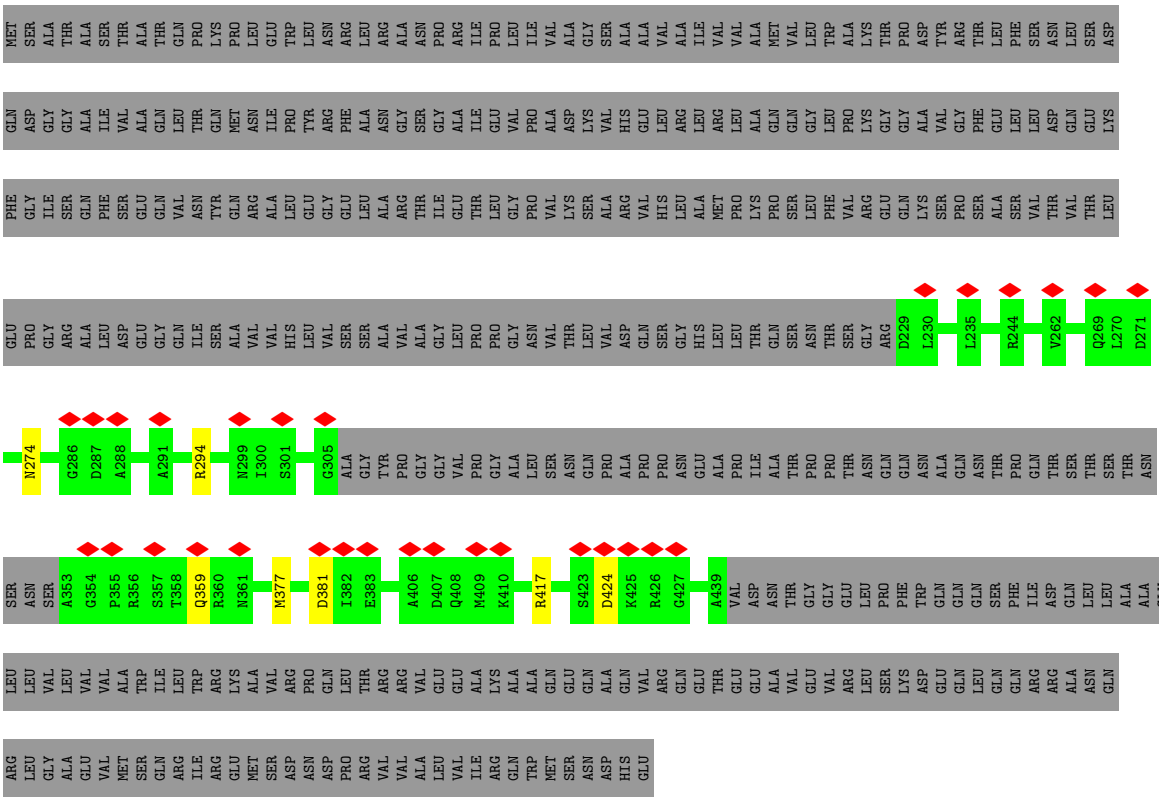
• Molecule 6: Flagellar M-ring protein

Chain AR:



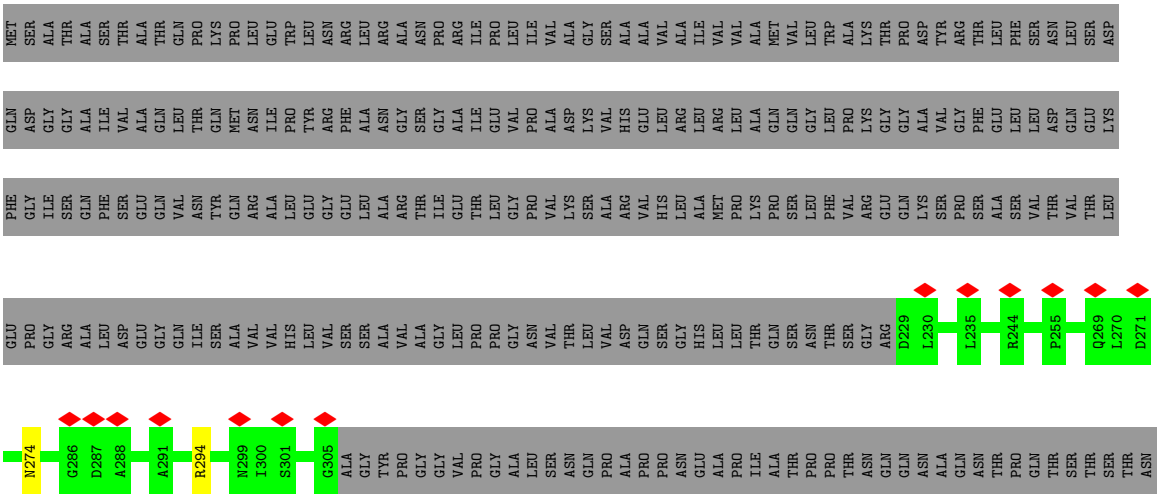
• Molecule 6: Flagellar M-ring protein

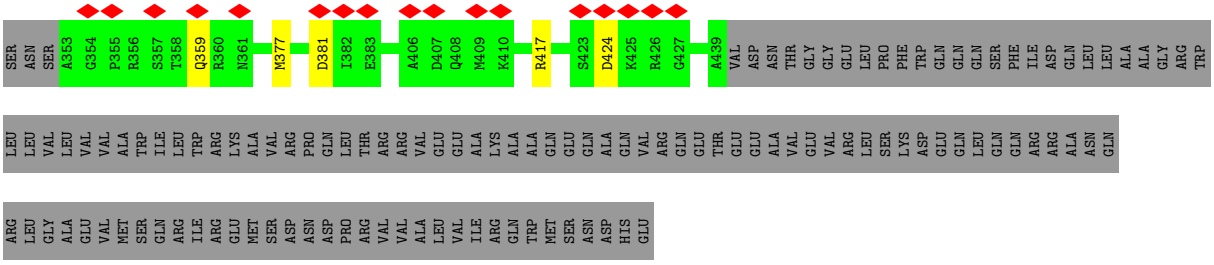
Chain AS:



• Molecule 6: Flagellar M-ring protein

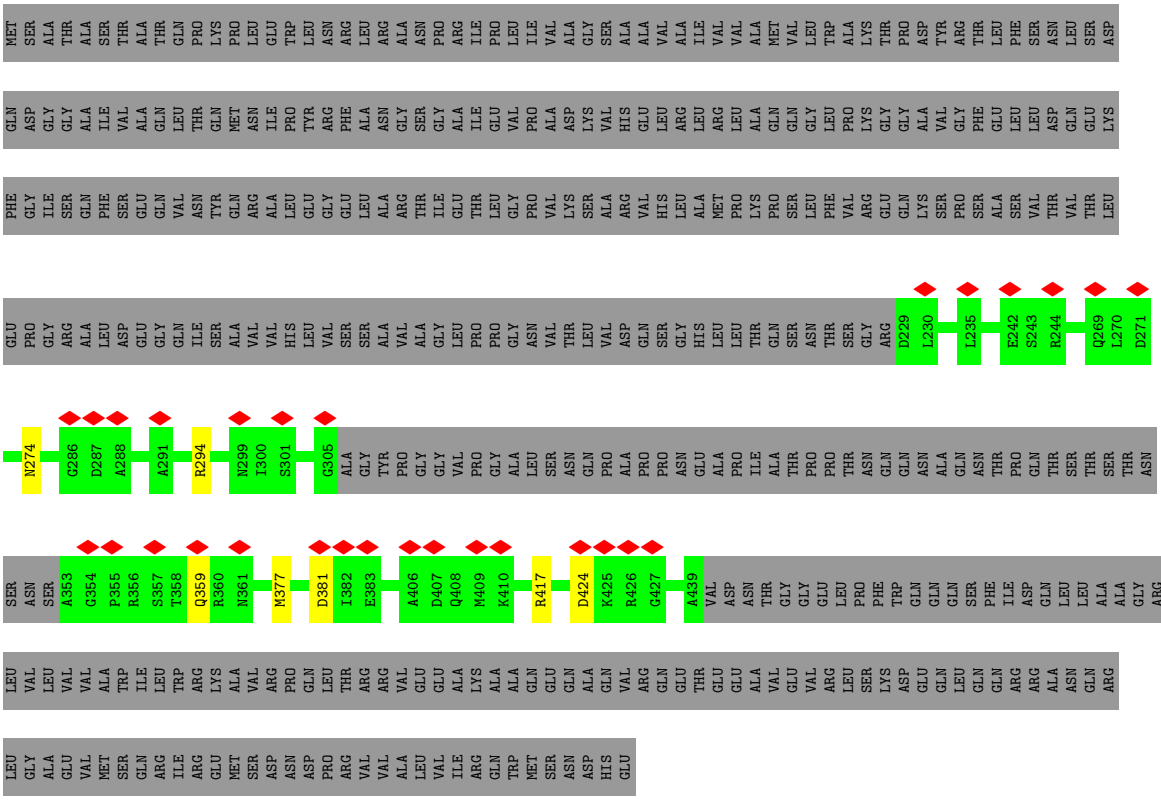
Chain AT:





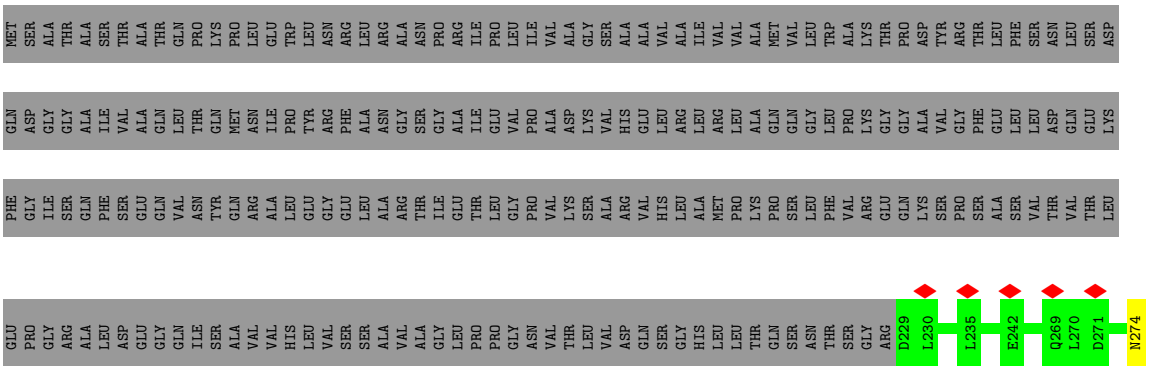
• Molecule 6: Flagellar M-ring protein

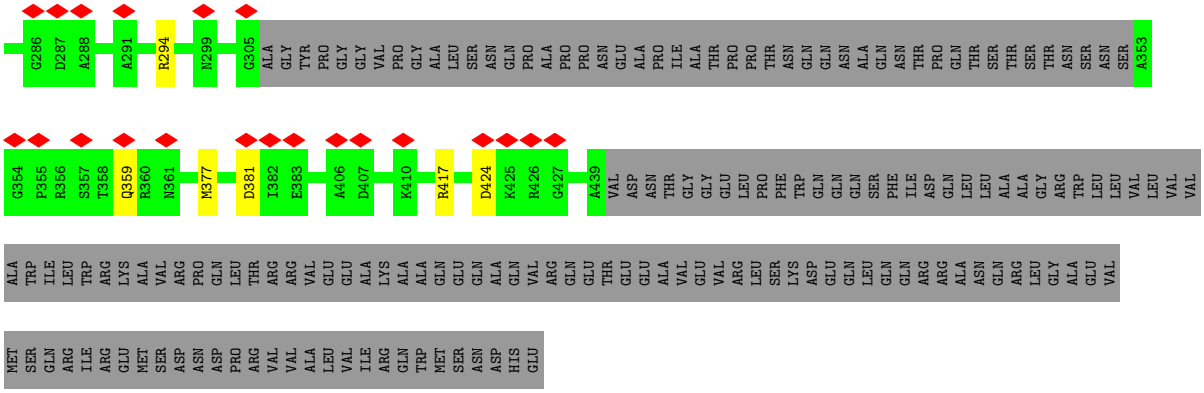
Chain AU:



• Molecule 6: Flagellar M-ring protein

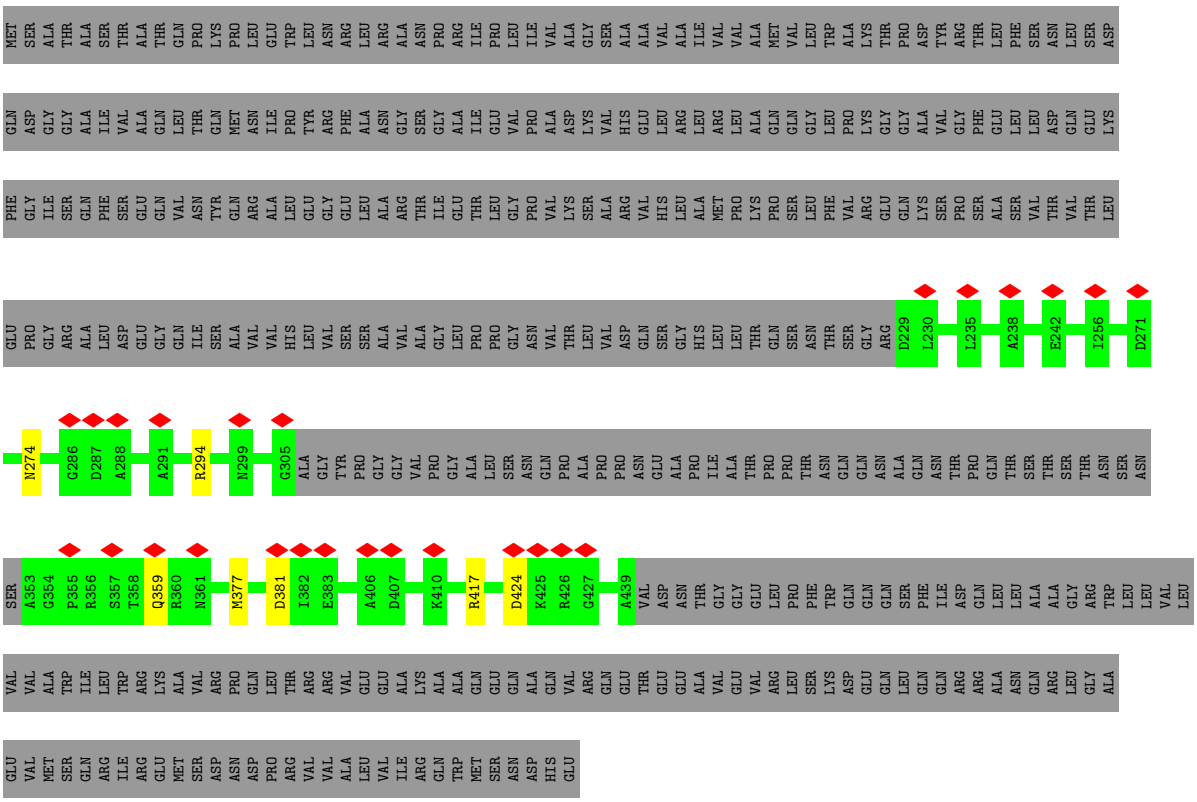
Chain AV:





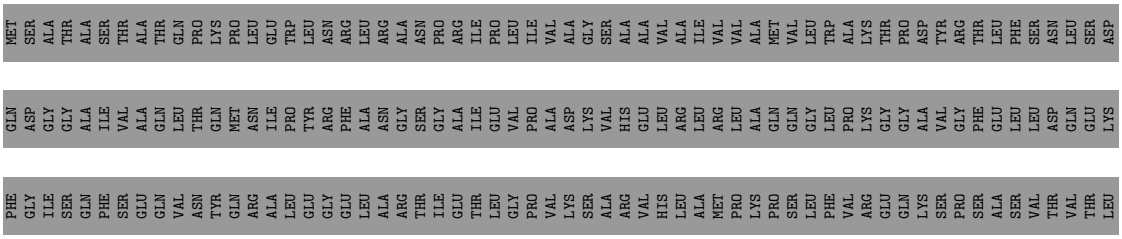
• Molecule 6: Flagellar M-ring protein

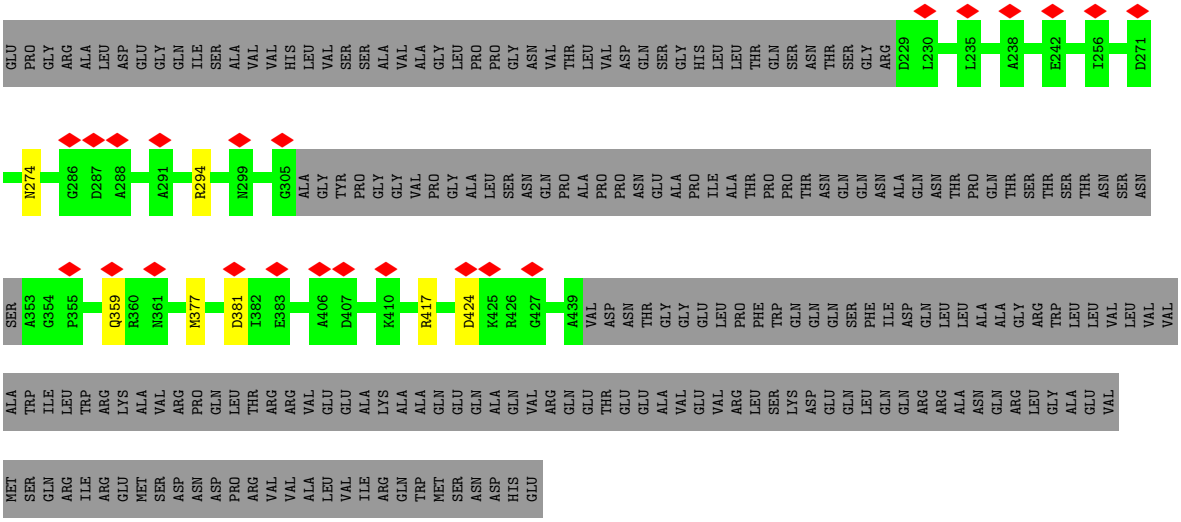
Chain AW:



• Molecule 6: Flagellar M-ring protein

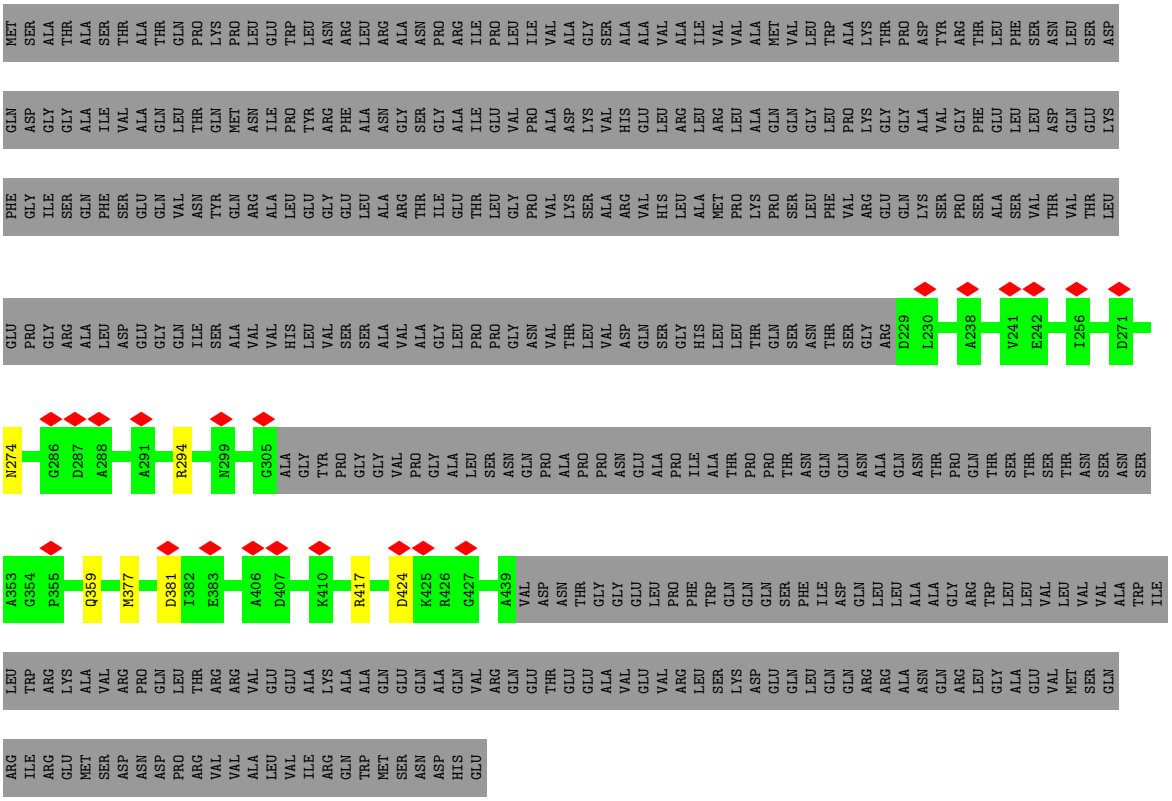
Chain AX:





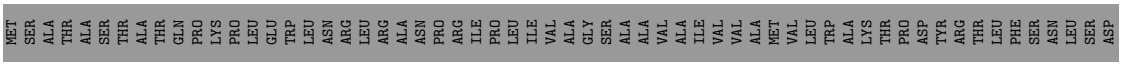
• Molecule 6: Flagellar M-ring protein

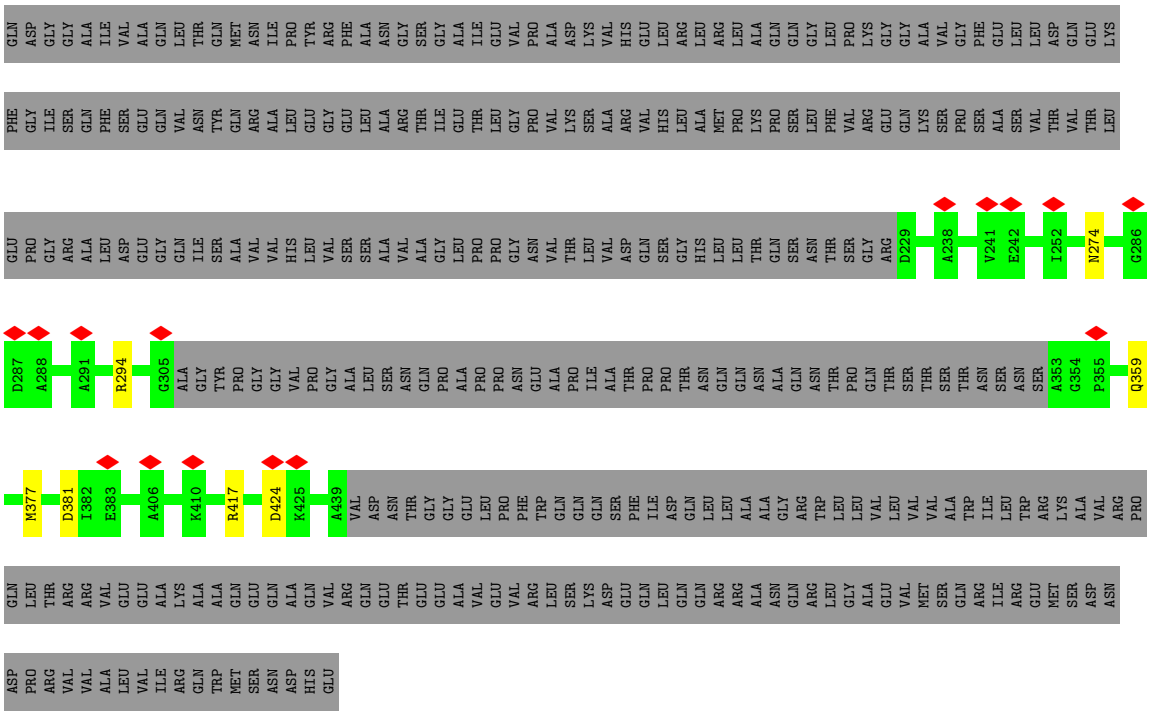
Chain AY:



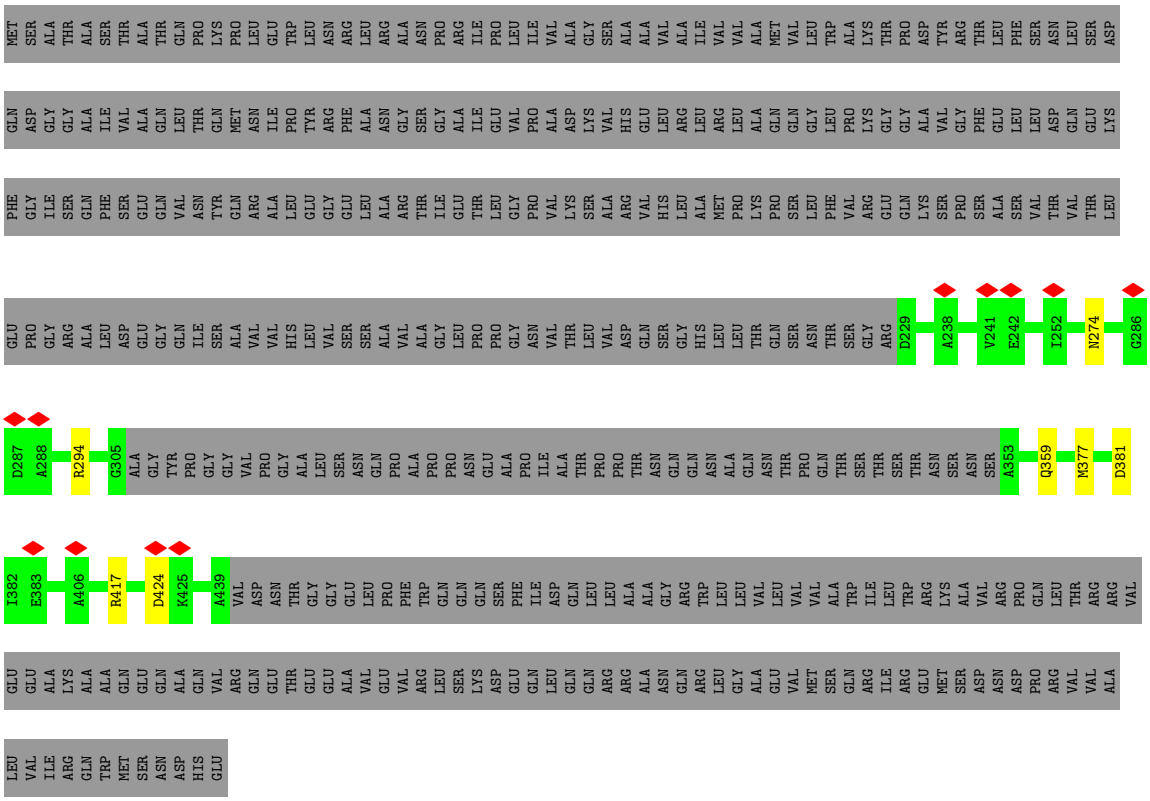
• Molecule 6: Flagellar M-ring protein

Chain AZ:



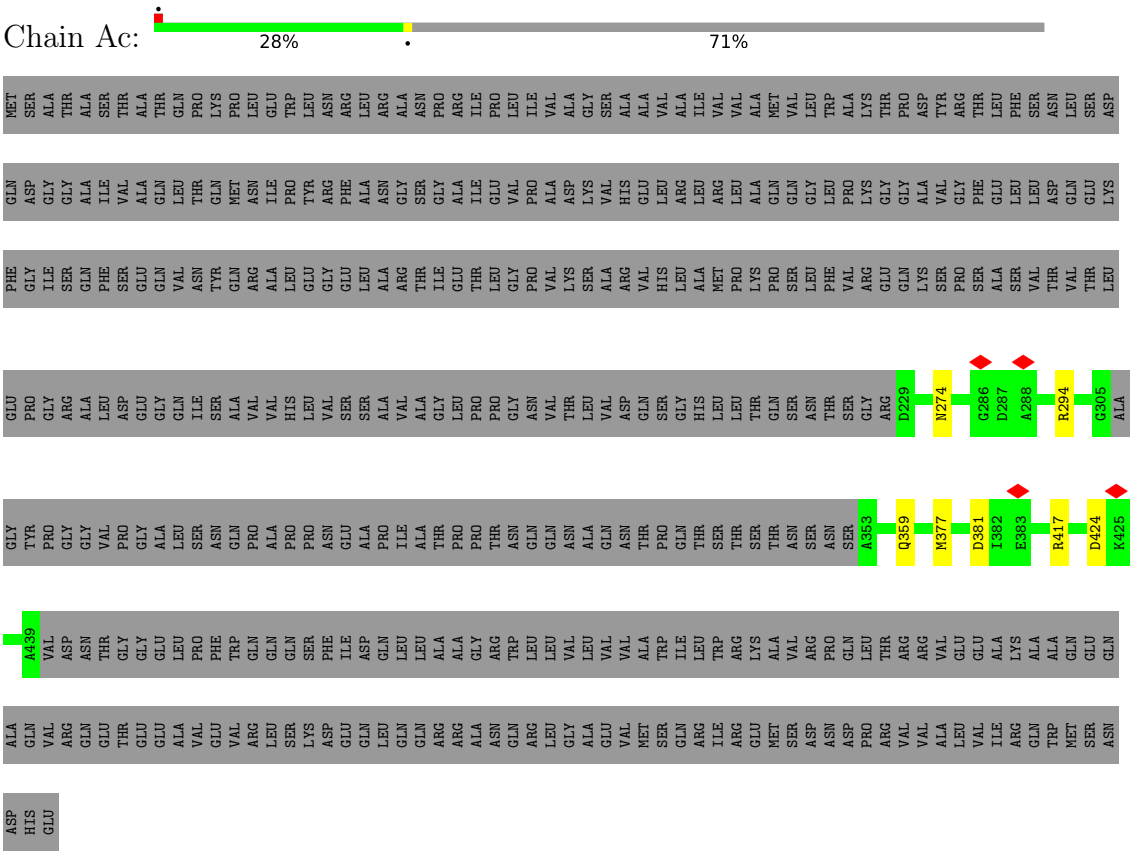


• Molecule 6: Flagellar M-ring protein



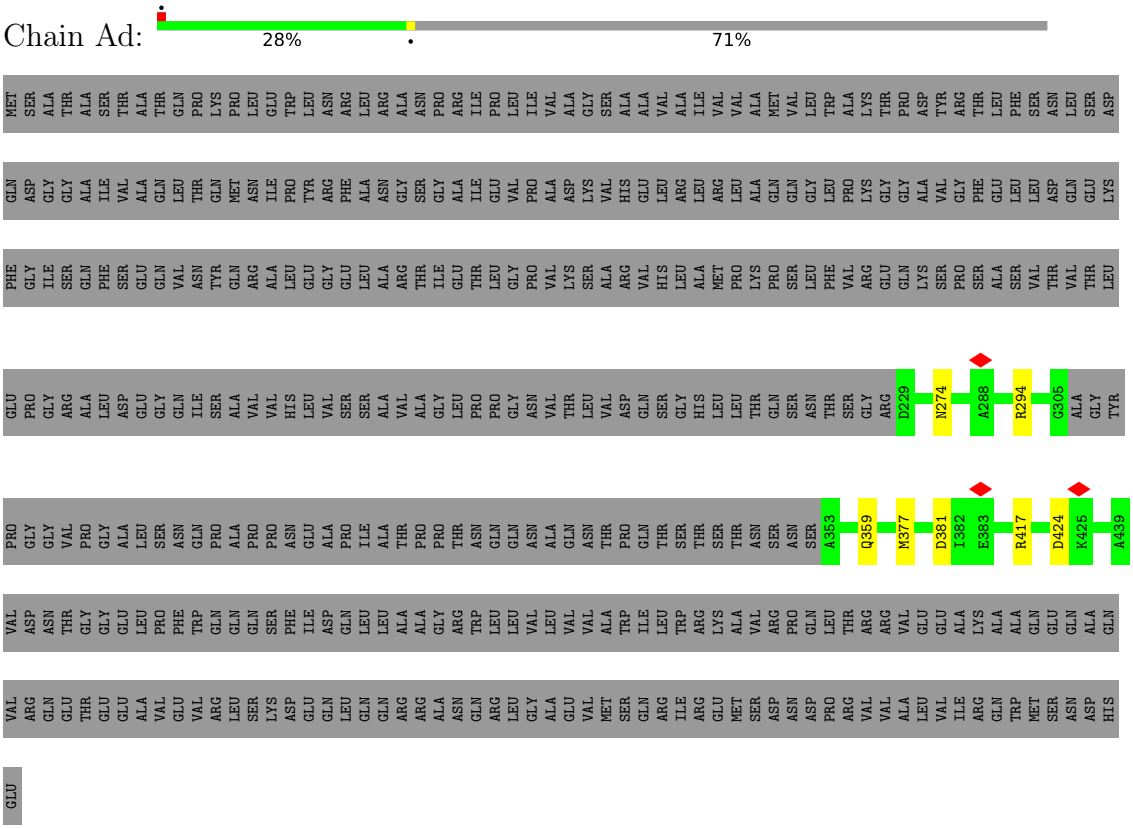
• Molecule 6: Flagellar M-ring protein

Chain Ac:



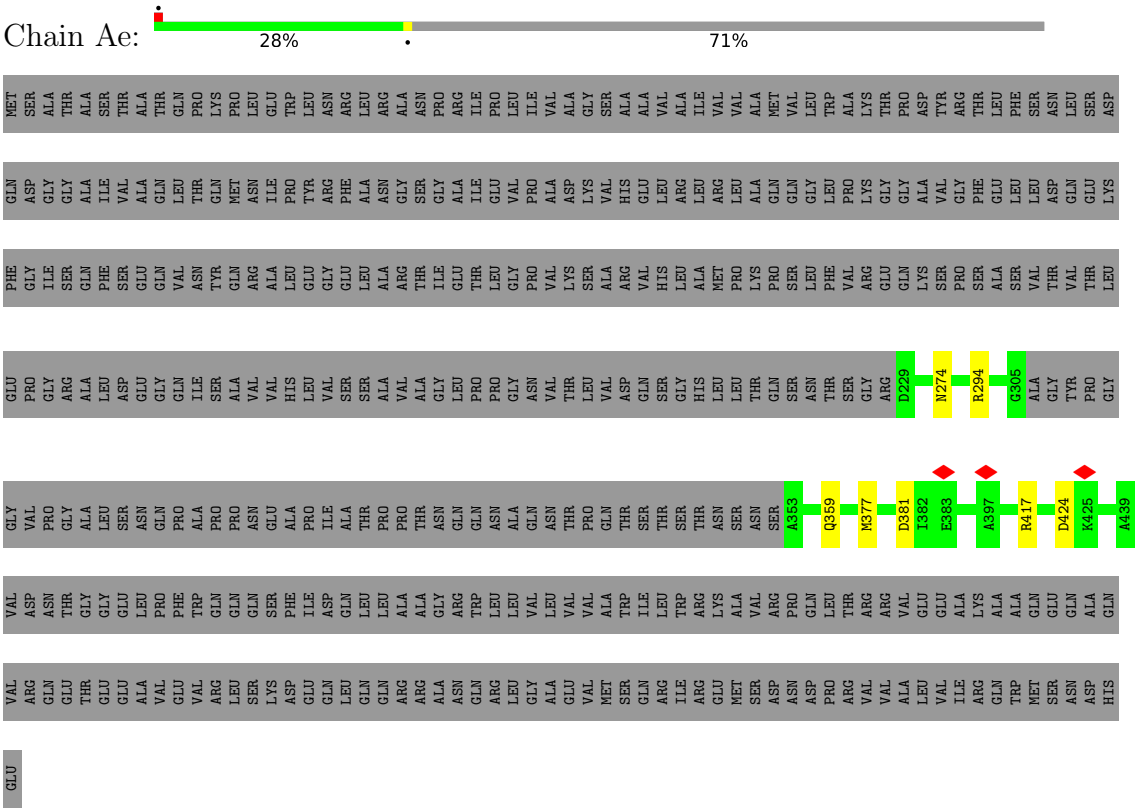
• Molecule 6: Flagellar M-ring protein

Chain Ad:



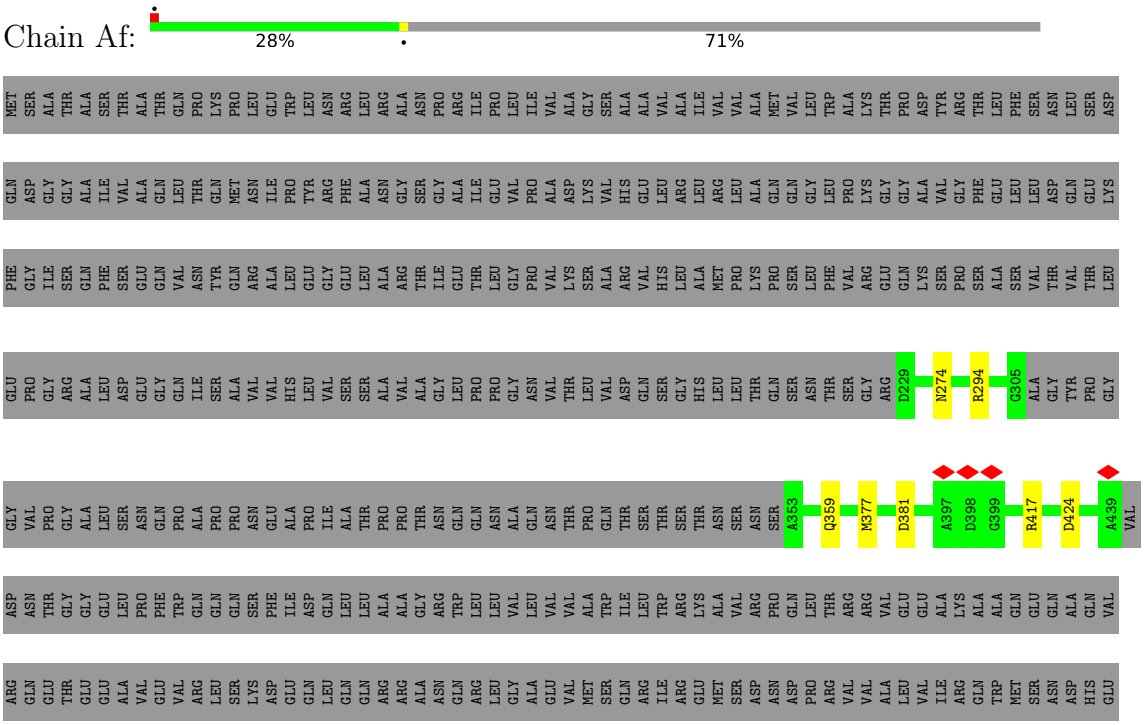
• Molecule 6: Flagellar M-ring protein

Chain Ae:



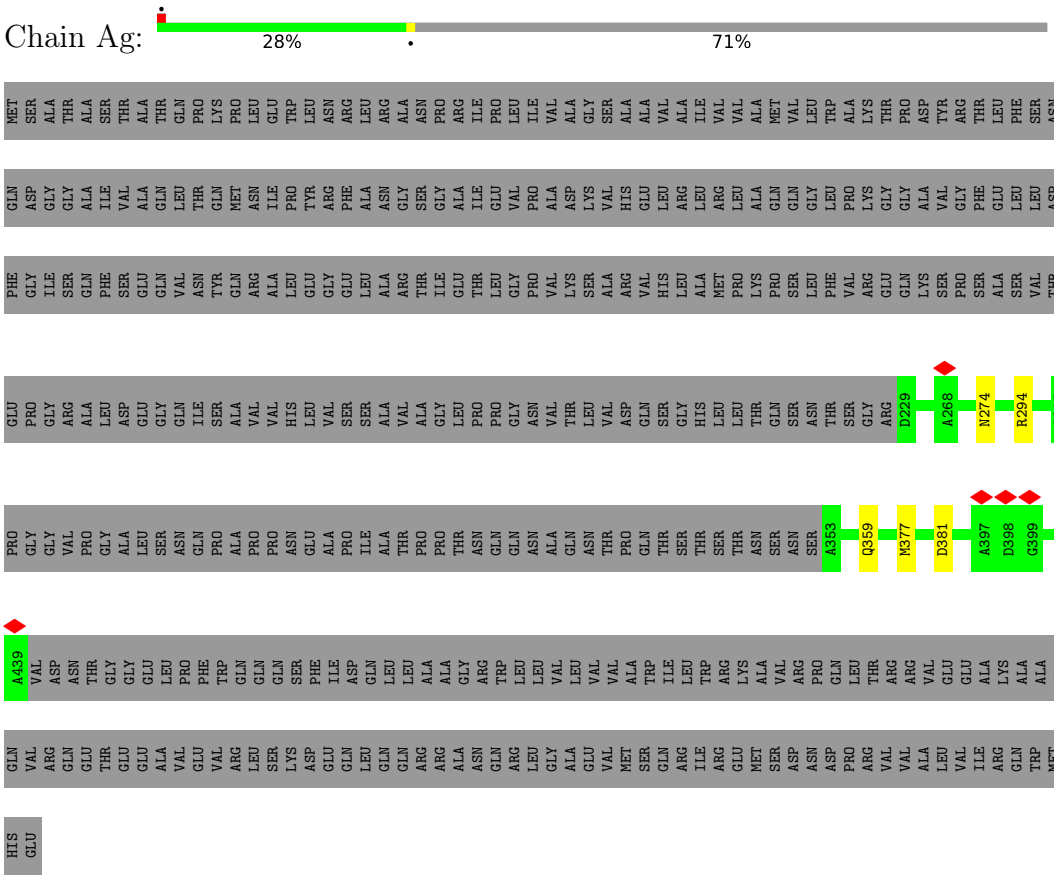
• Molecule 6: Flagellar M-ring protein

Chain Af:



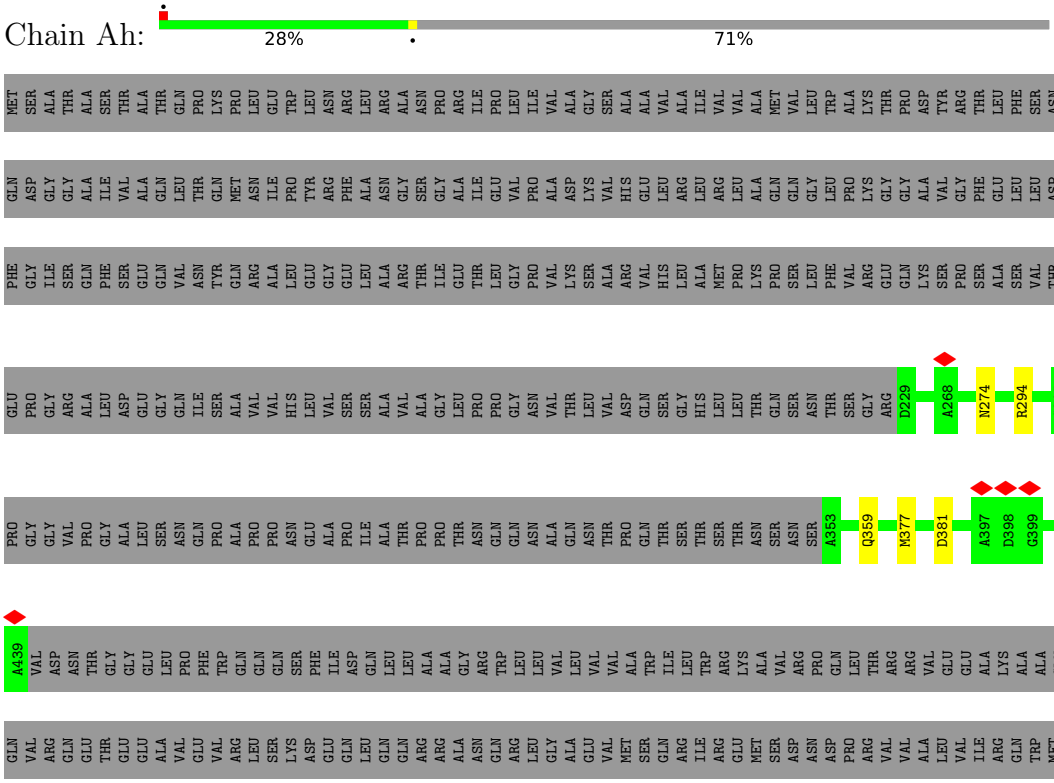
• Molecule 6: Flagellar M-ring protein

Chain Ag:



• Molecule 6: Flagellar M-ring protein

Chain Ah:



• Molecule 6: Flagellar M-ring protein

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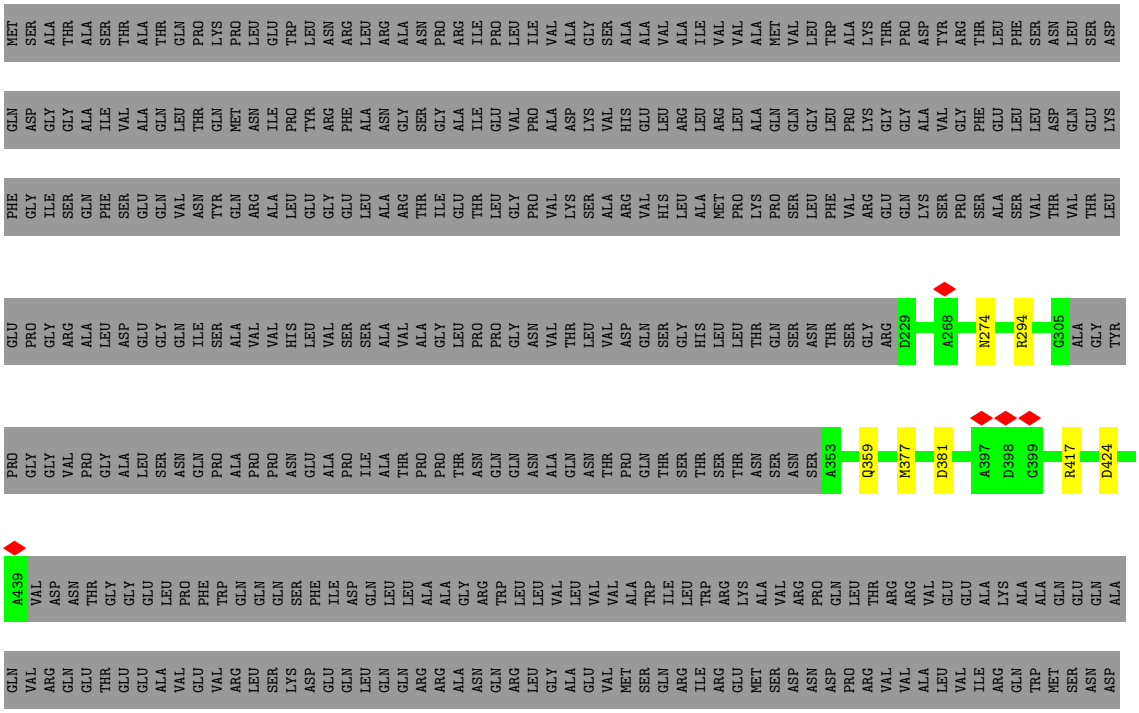
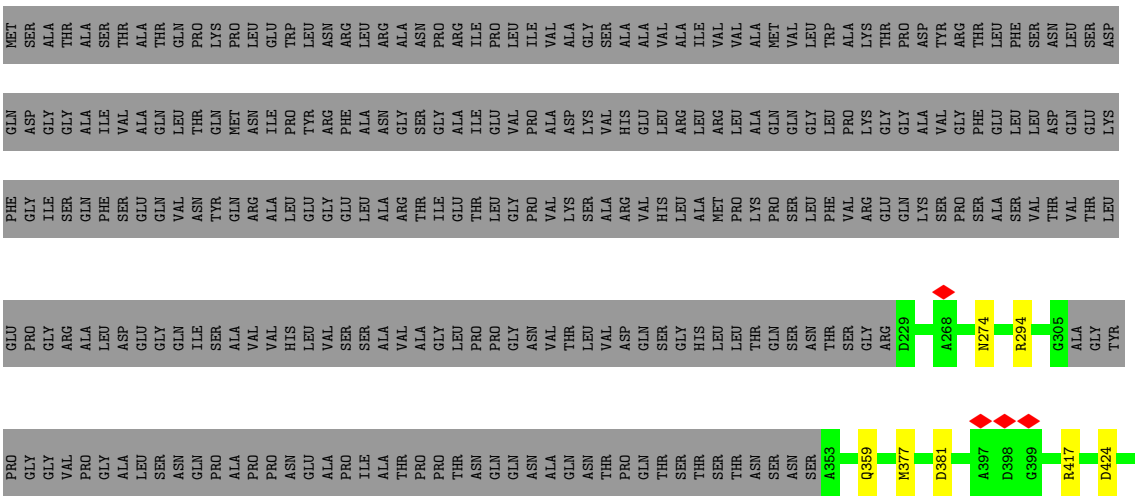
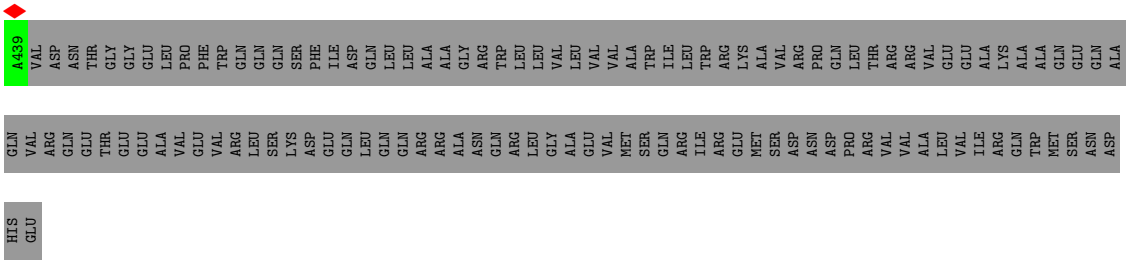


• Molecule 6: Flagellar M-ring protein

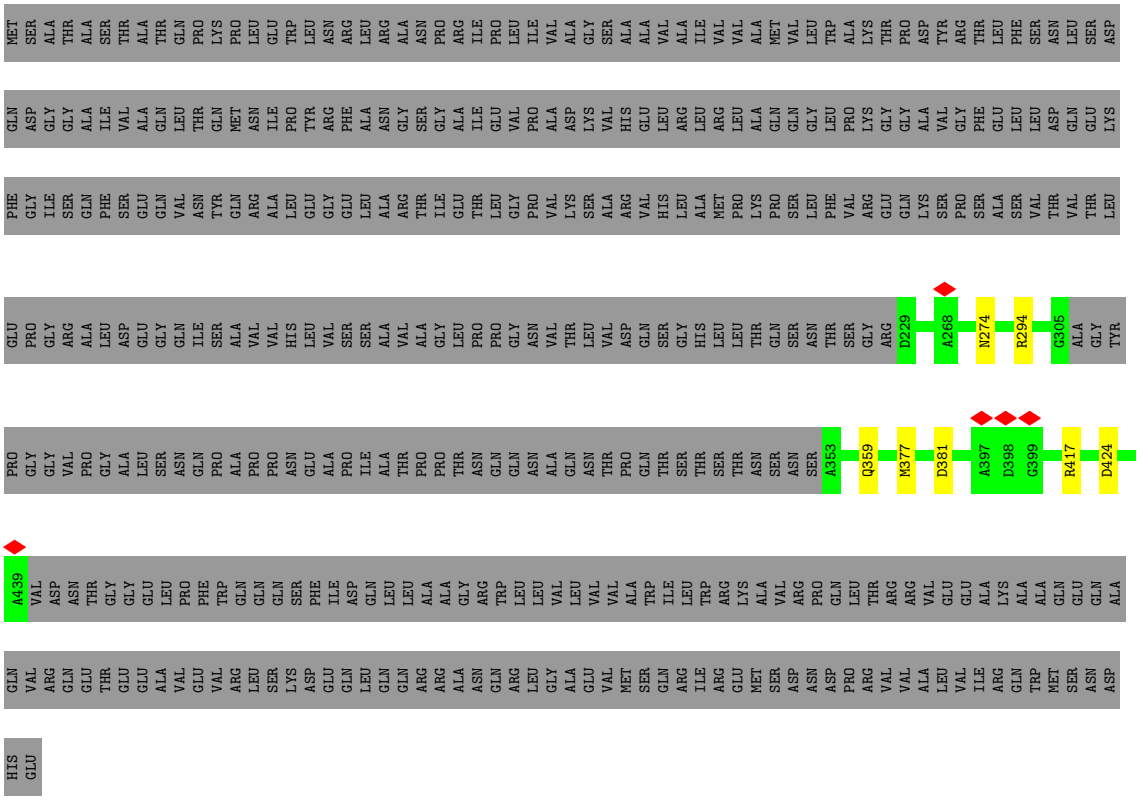
Chain Aj:





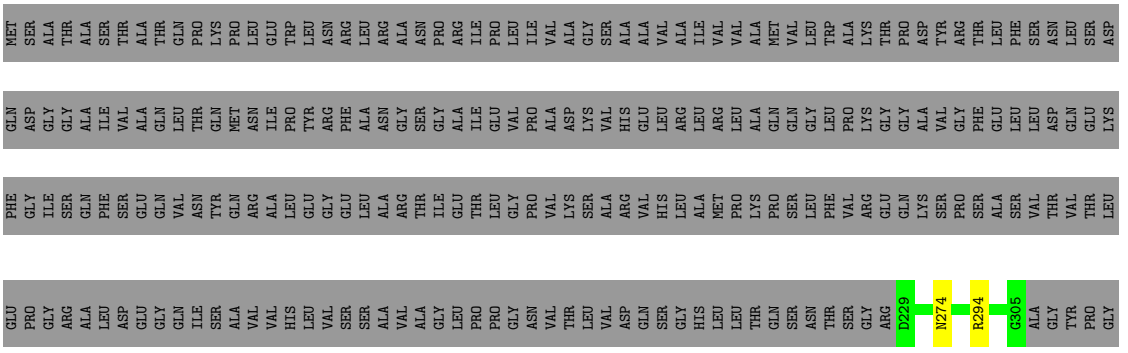
• Molecule 6: Flagellar M-ring protein

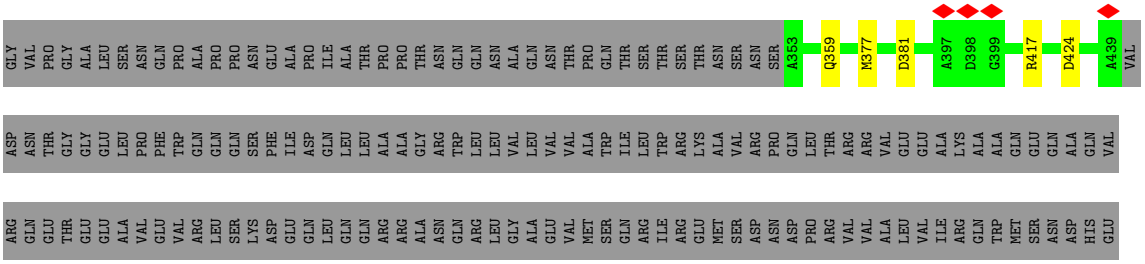
Chain Ak:



• Molecule 6: Flagellar M-ring protein

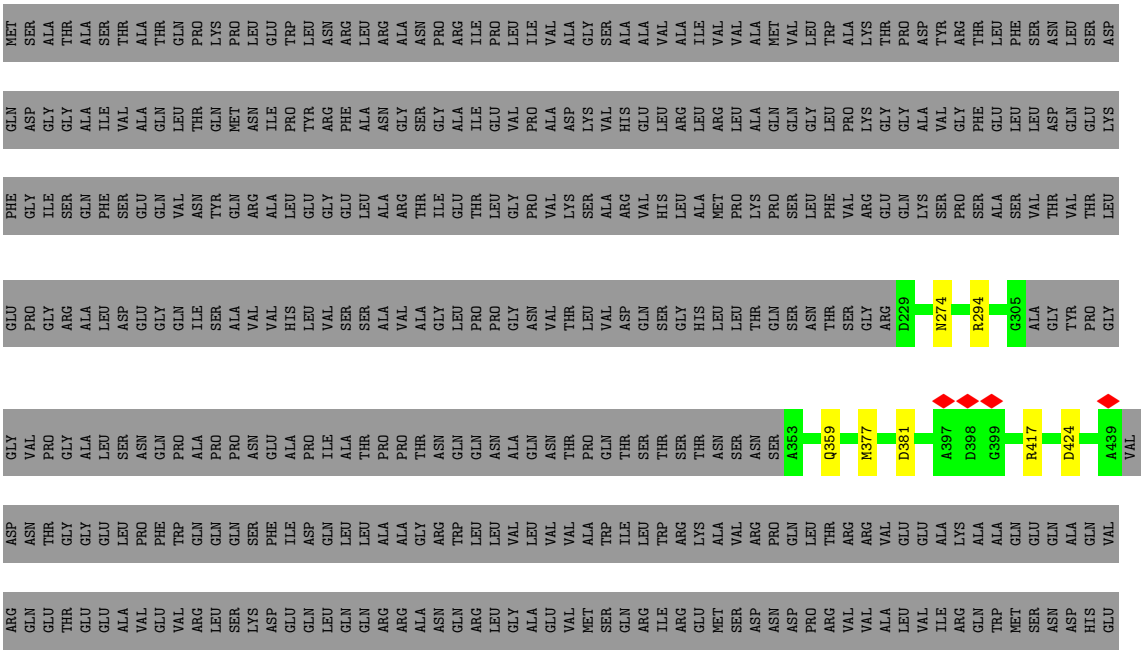
Chain Al:





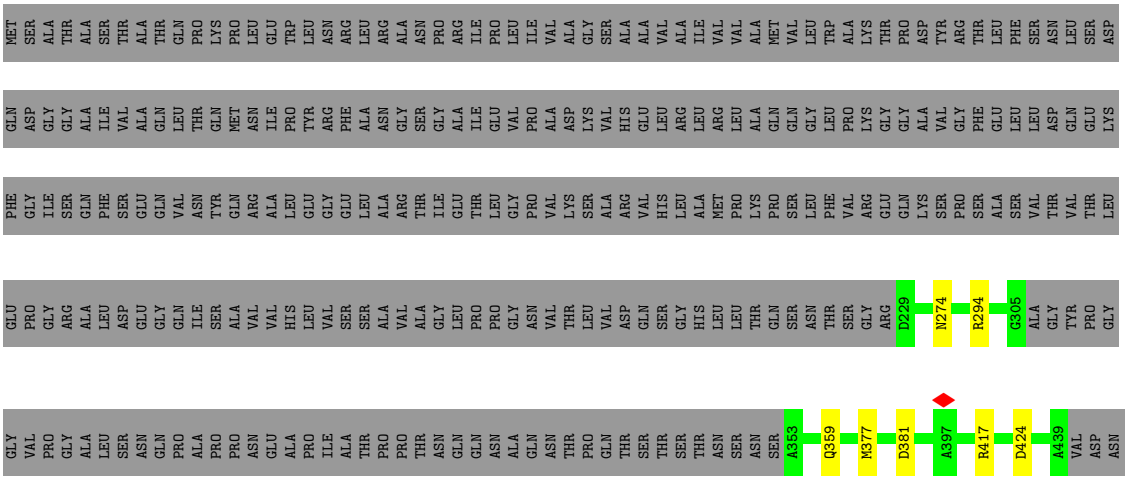
• Molecule 6: Flagellar M-ring protein

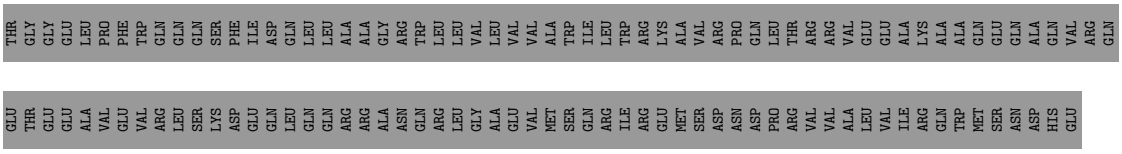
Chain Am:



• Molecule 6: Flagellar M-ring protein

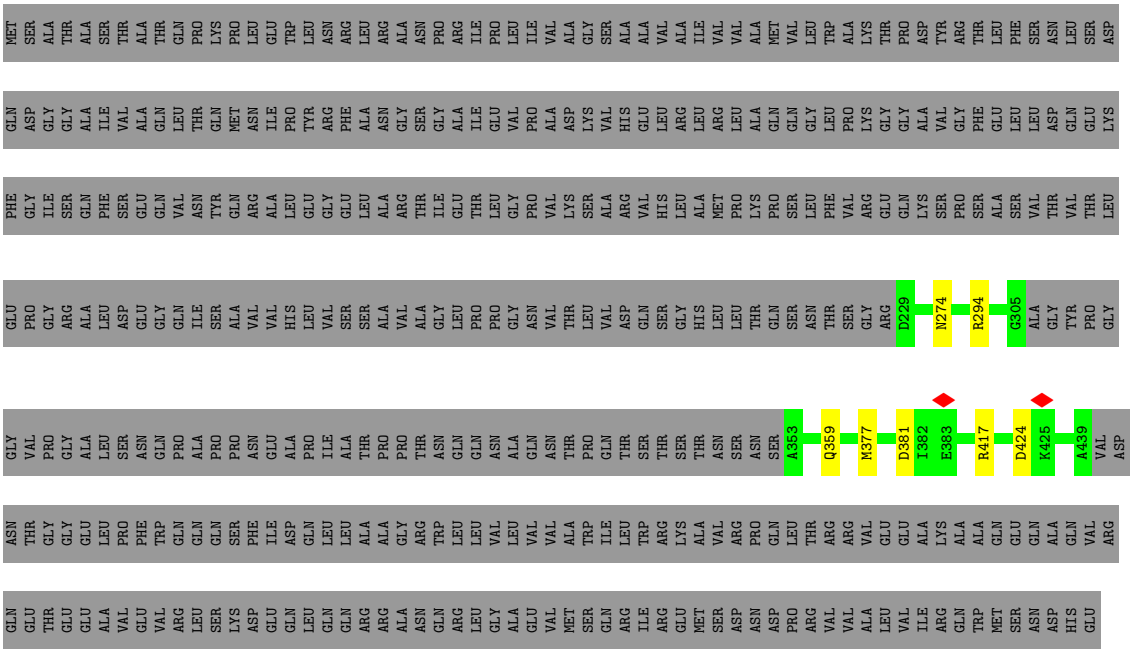
Chain An:





• Molecule 6: Flagellar M-ring protein

Chain Ao:



• Molecule 6: Flagellar M-ring protein

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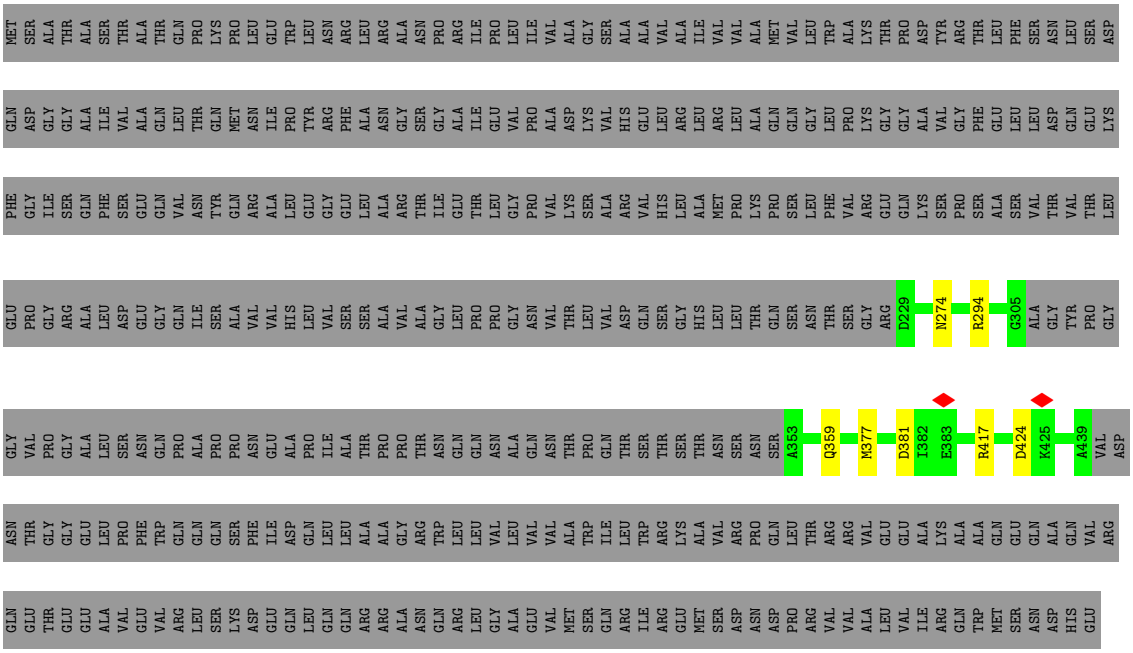
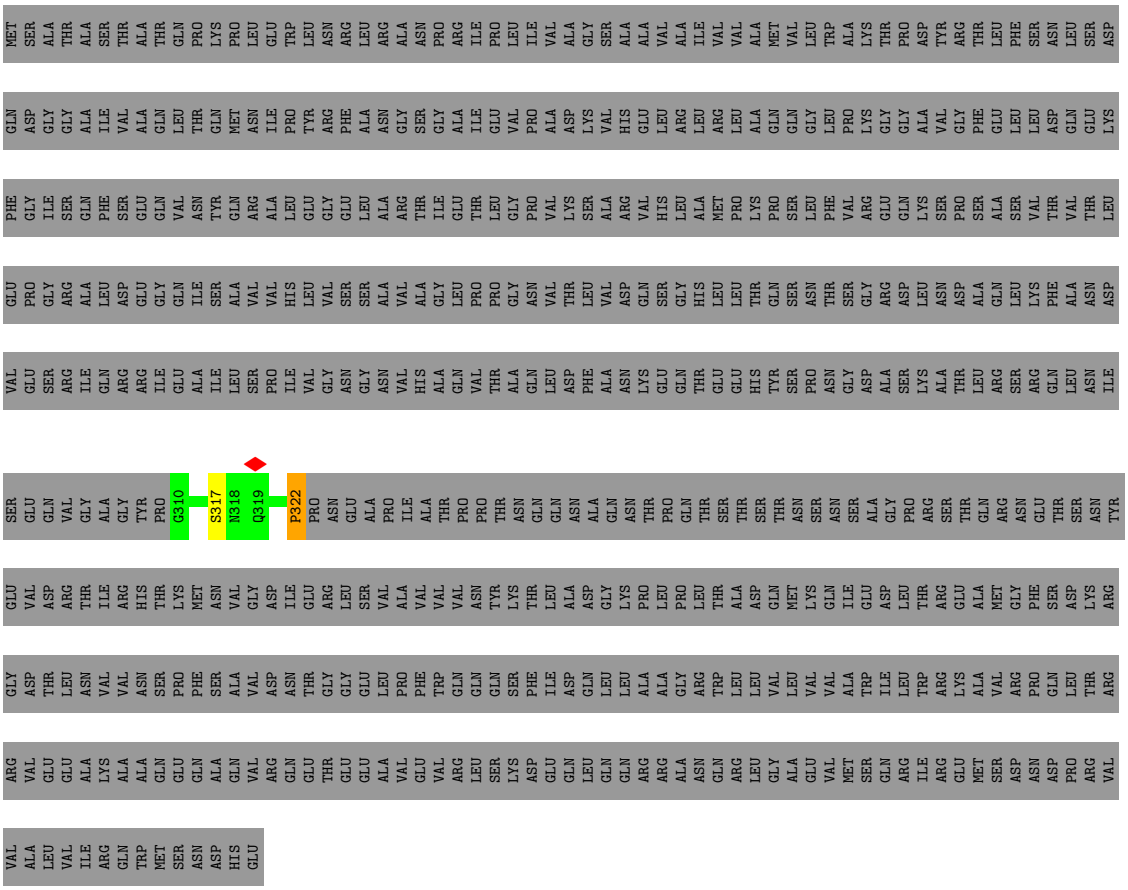


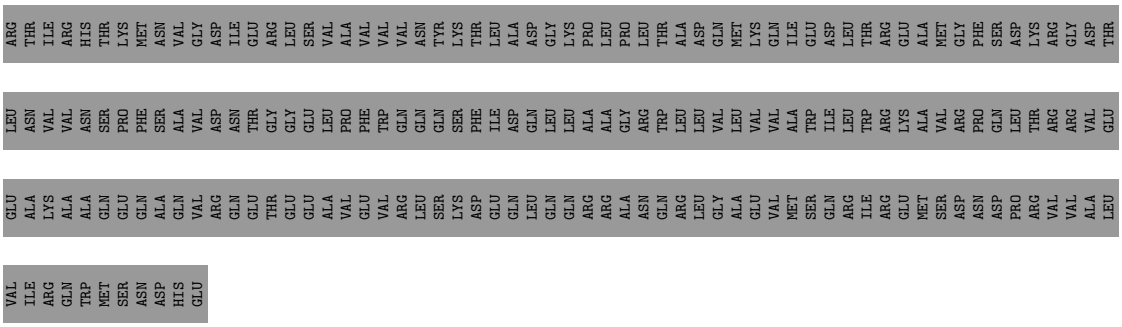
• Molecule 6: Flagellar M-ring protein

Chain BG:



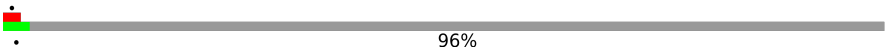
• Molecule 6: Flagellar M-ring protein

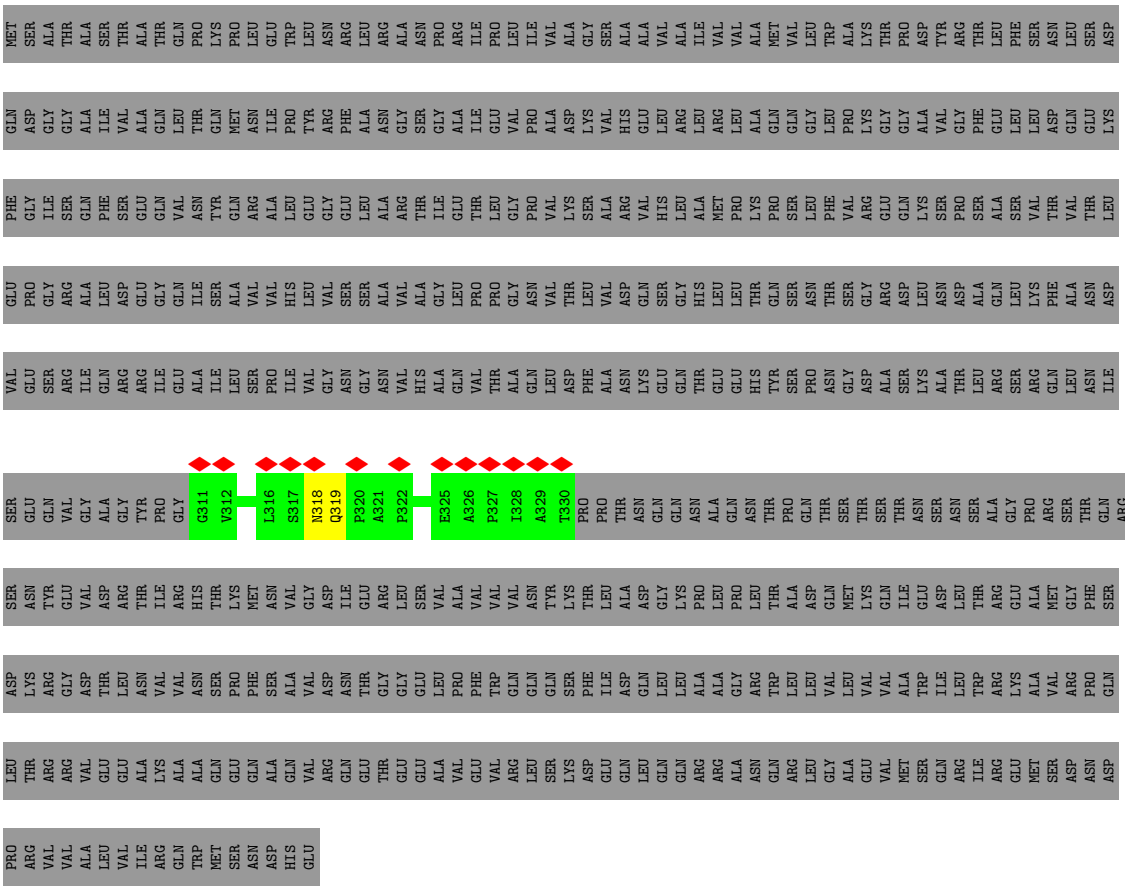
Chain BH:



• Molecule 6: Flagellar M-ring protein

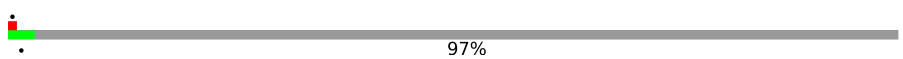
Chain BI:

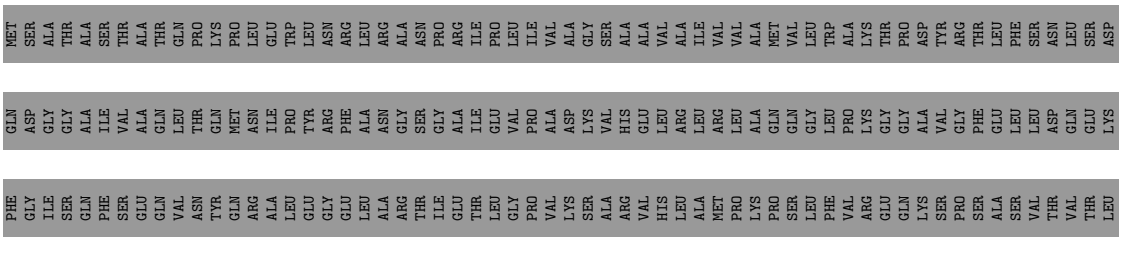


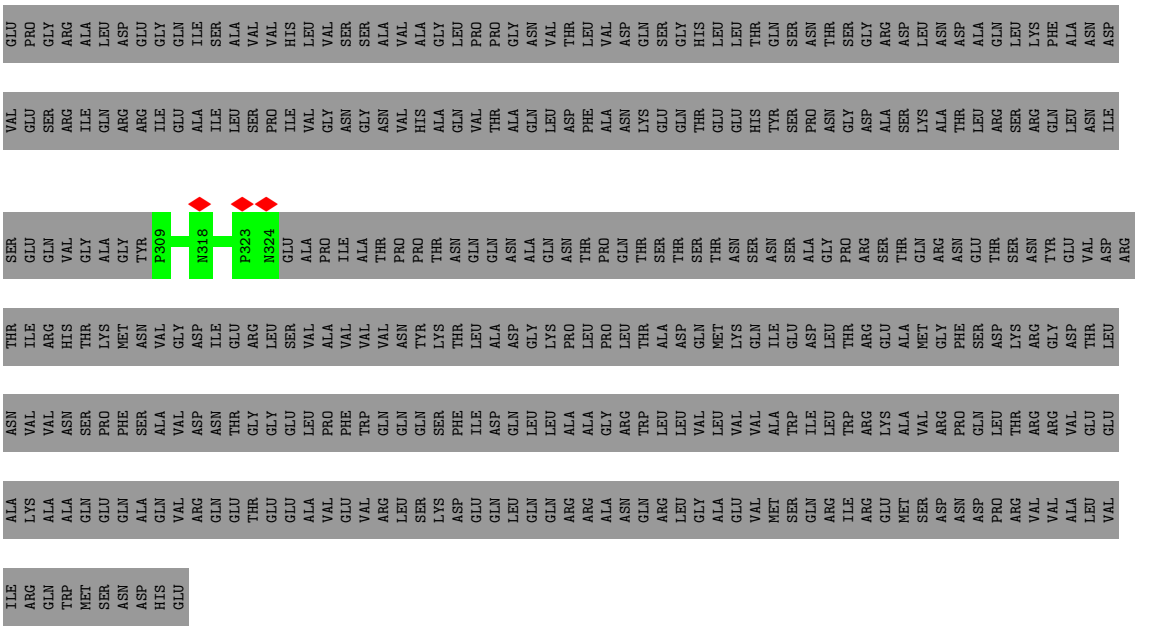


• Molecule 6: Flagellar M-ring protein

Chain BJ:

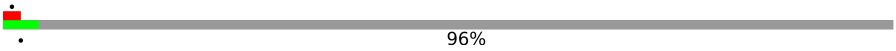


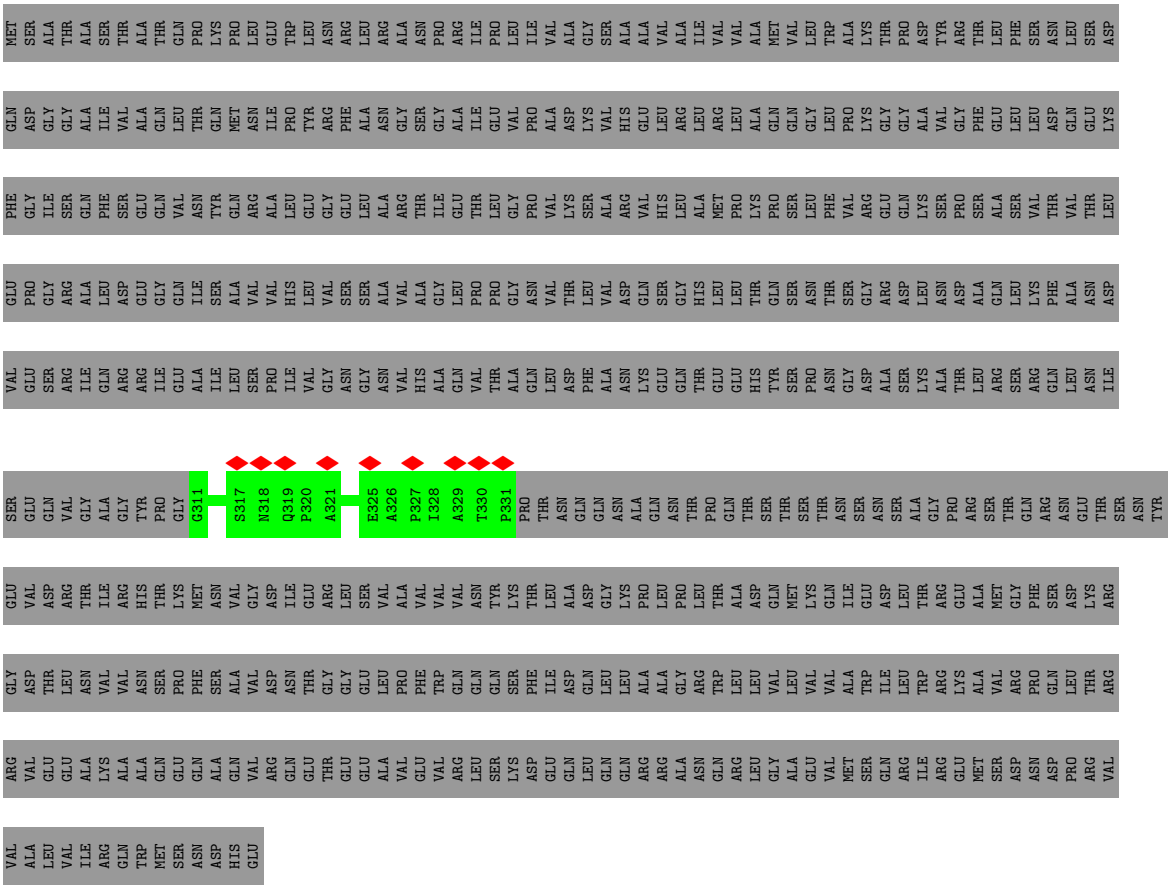




• Molecule 6: Flagellar M-ring protein

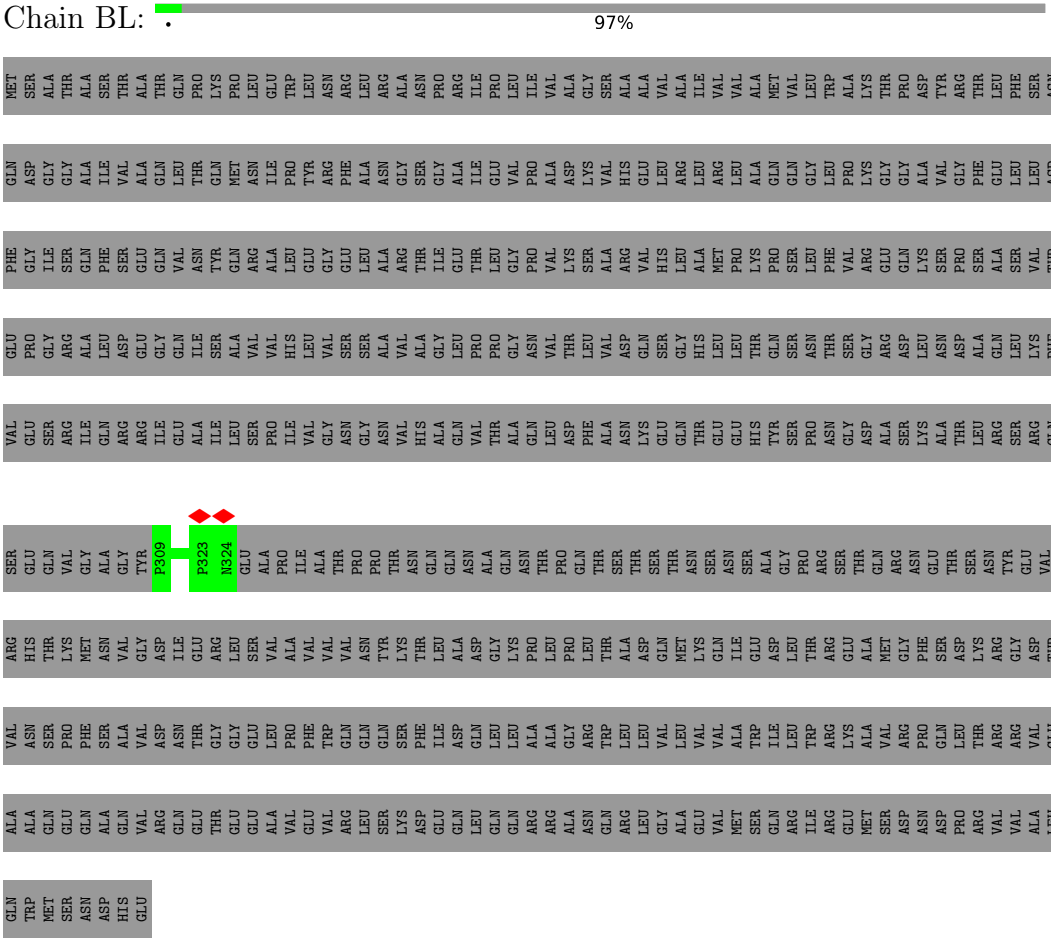
Chain BK:





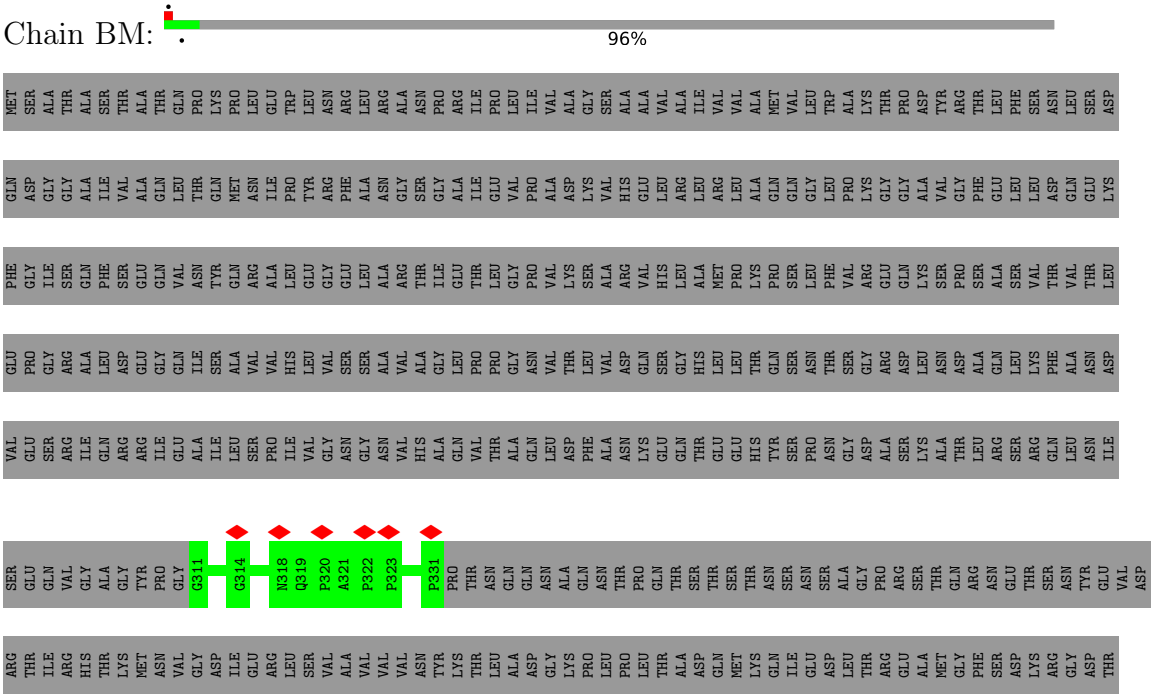
• Molecule 6: Flagellar M-ring protein

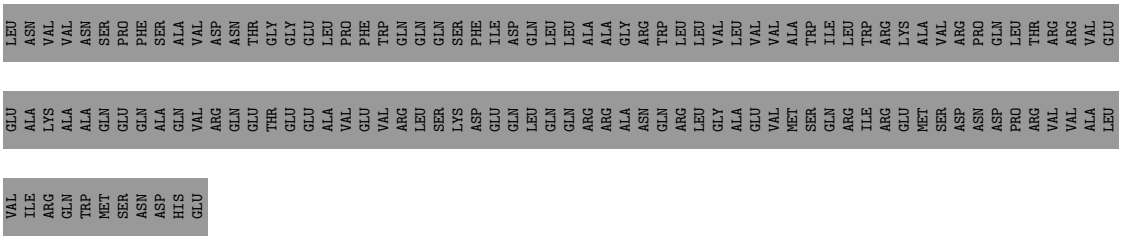
Chain BL:



• Molecule 6: Flagellar M-ring protein

Chain BM:



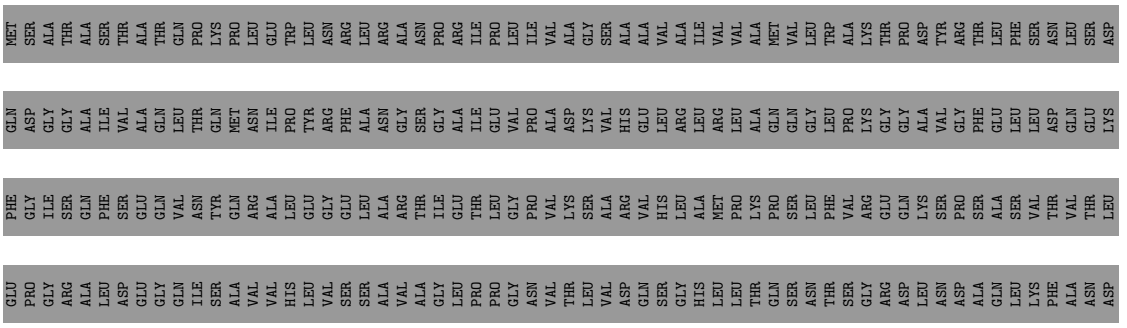


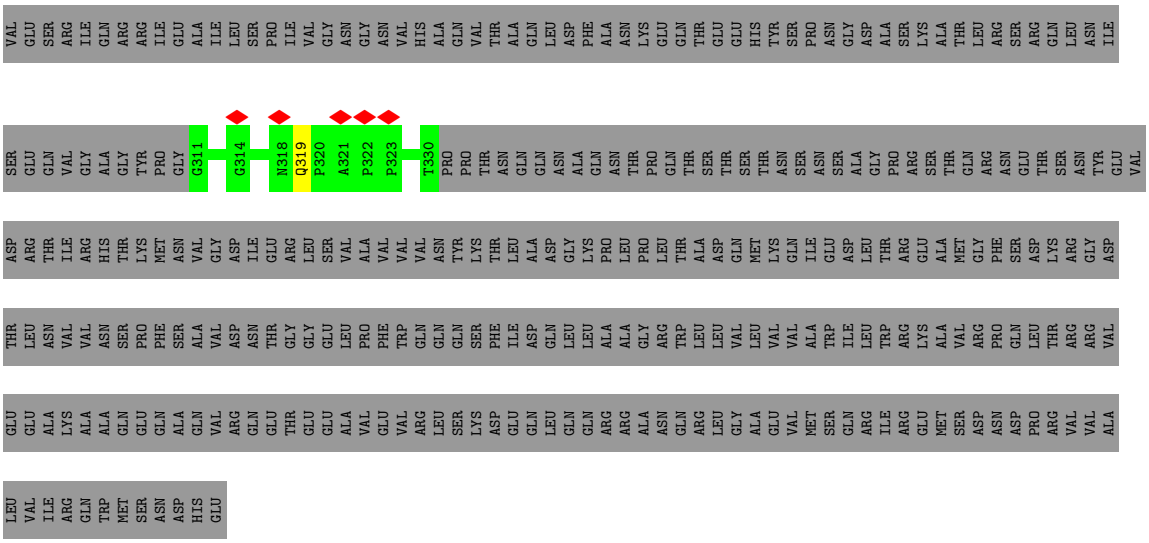
• Molecule 6: Flagellar M-ring protein

Chain BN: 97%

• Molecule 6: Flagellar M-ring protein

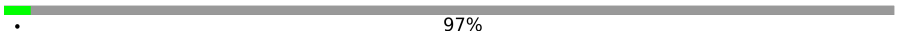
Chain BO: 96%

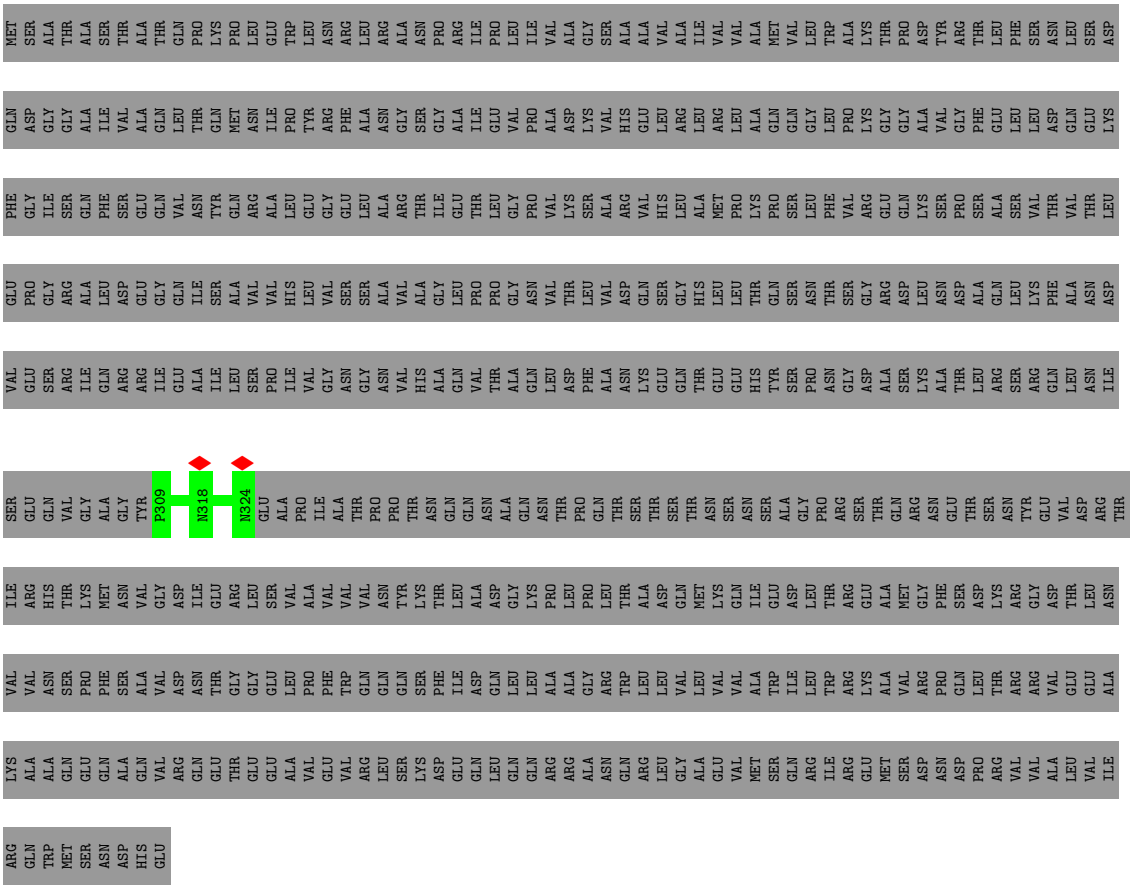




• Molecule 6: Flagellar M-ring protein

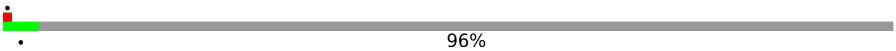
Chain BP:

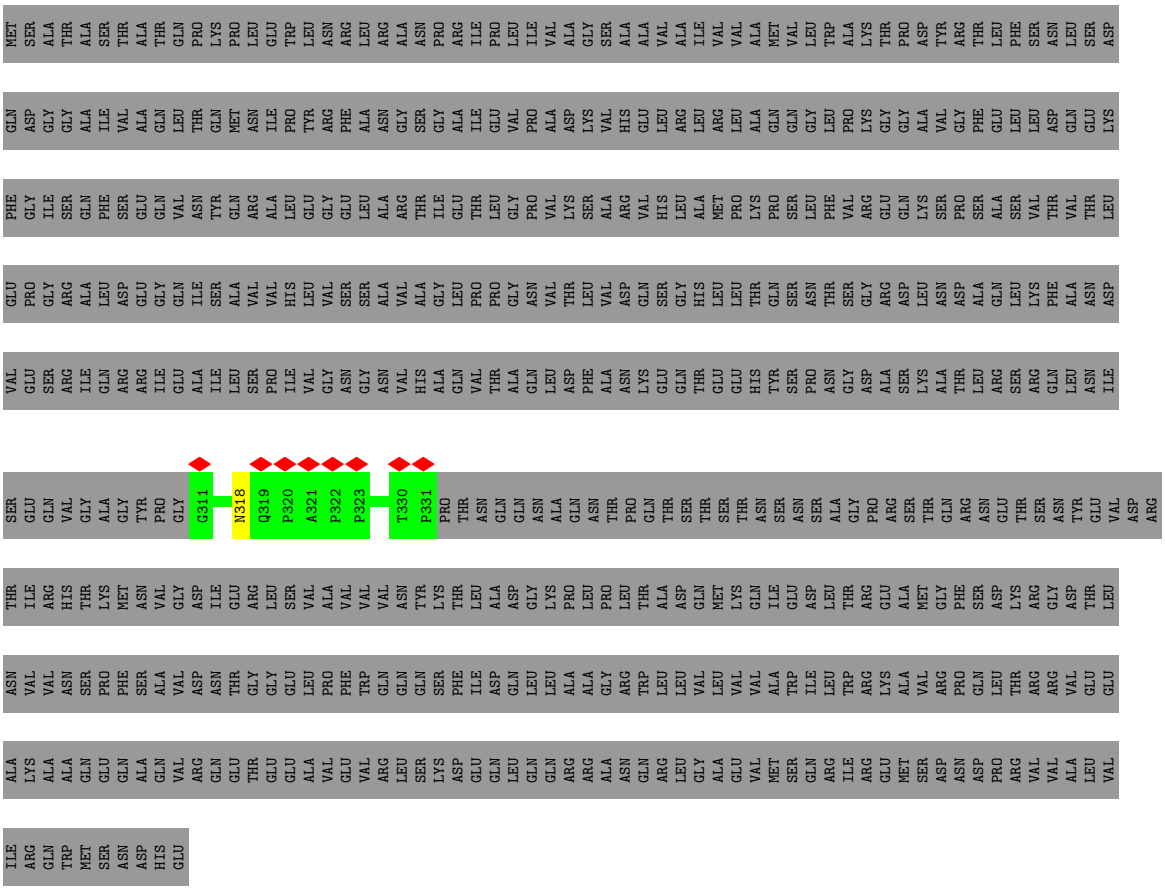




• Molecule 6: Flagellar M-ring protein

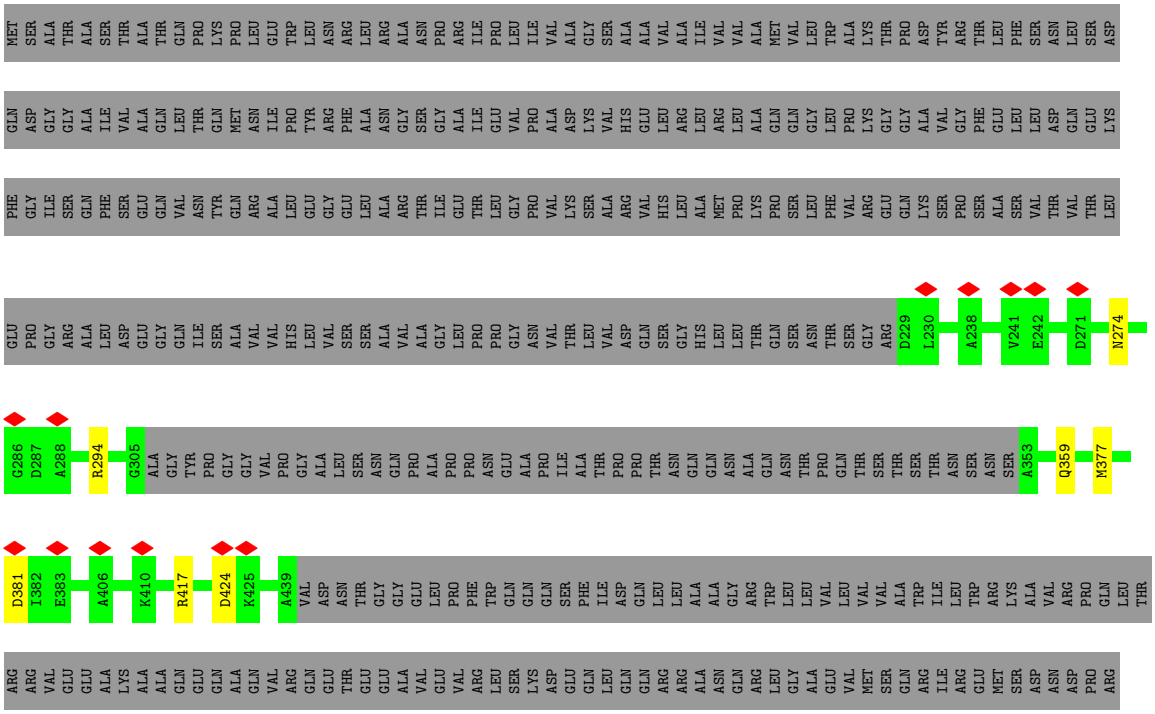
Chain BQ:





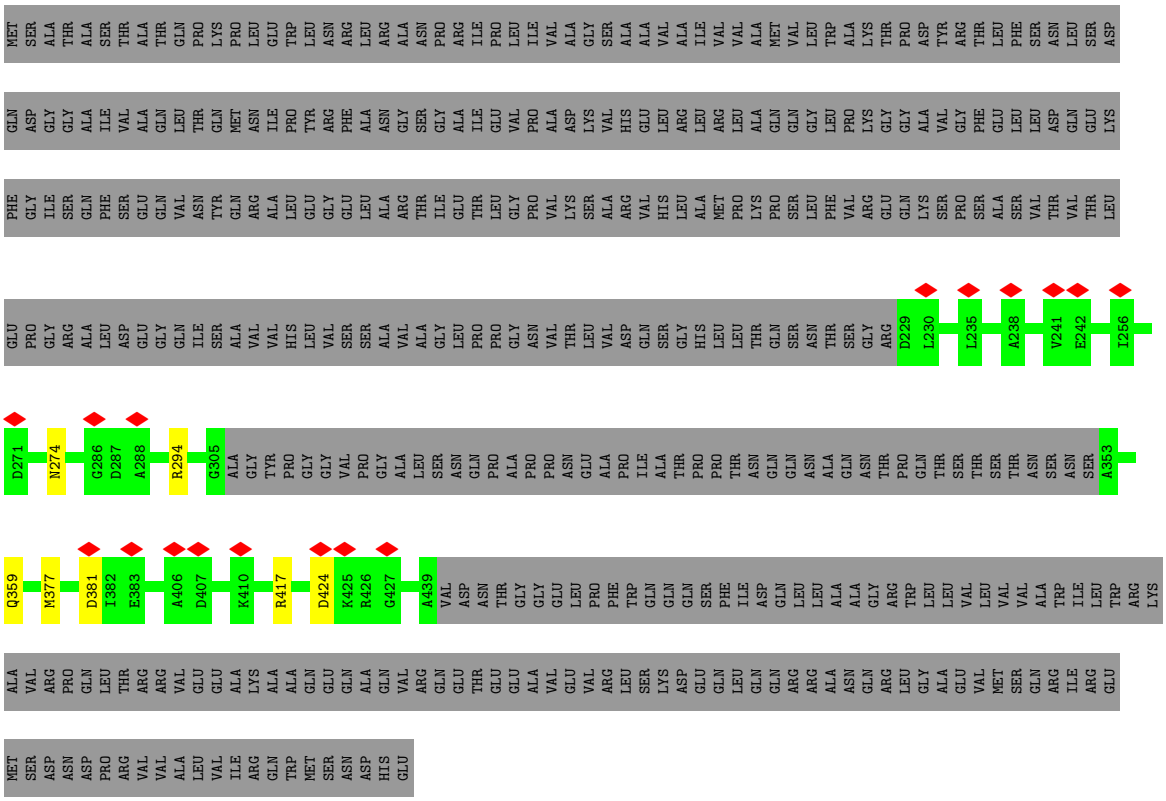
• Molecule 6: Flagellar M-ring protein

Chain BR:



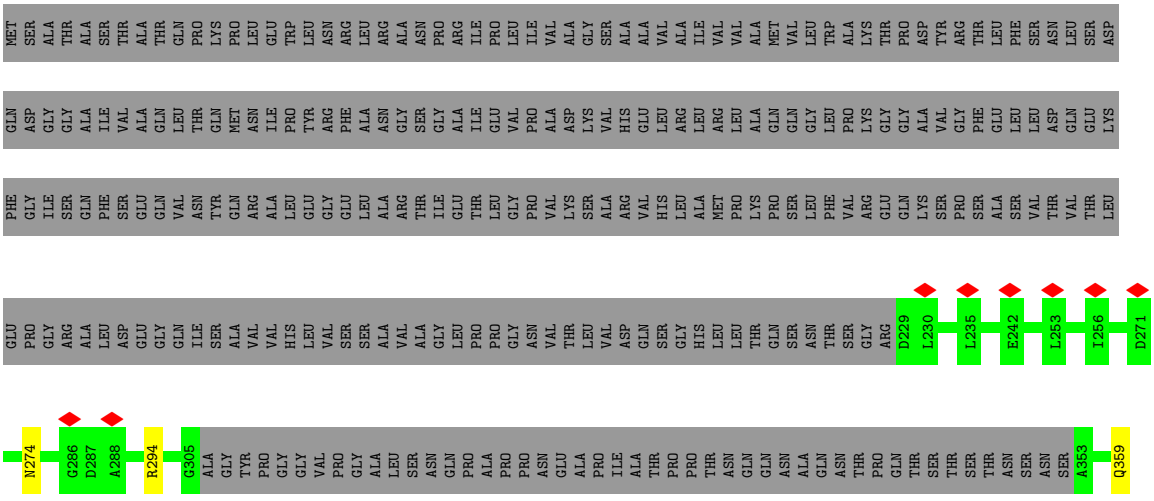
• Molecule 6: Flagellar M-ring protein

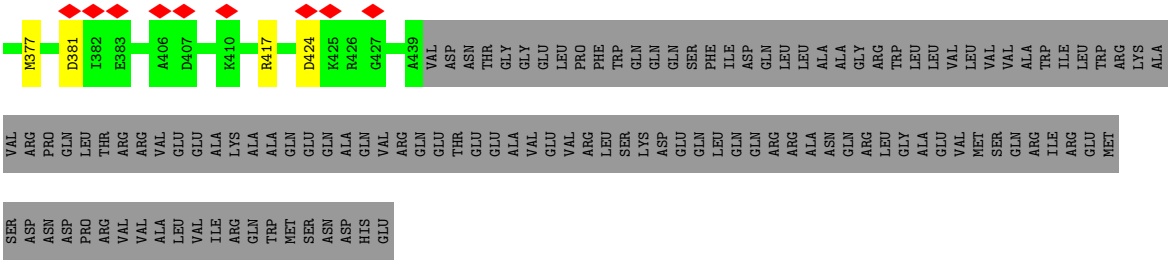
Chain BS:



• Molecule 6: Flagellar M-ring protein

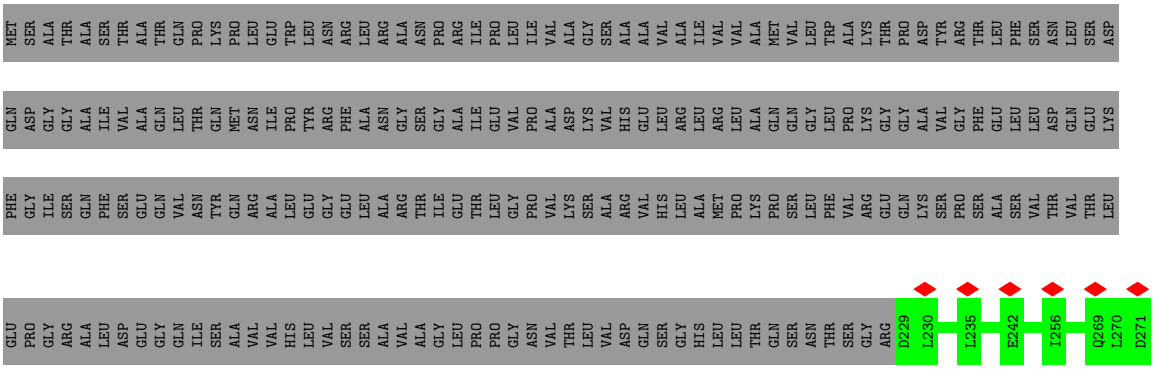
Chain BT:

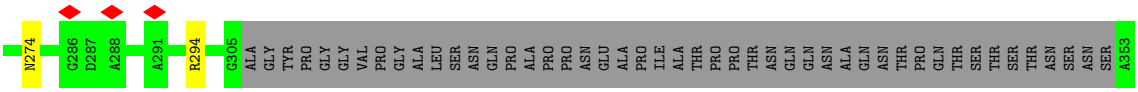


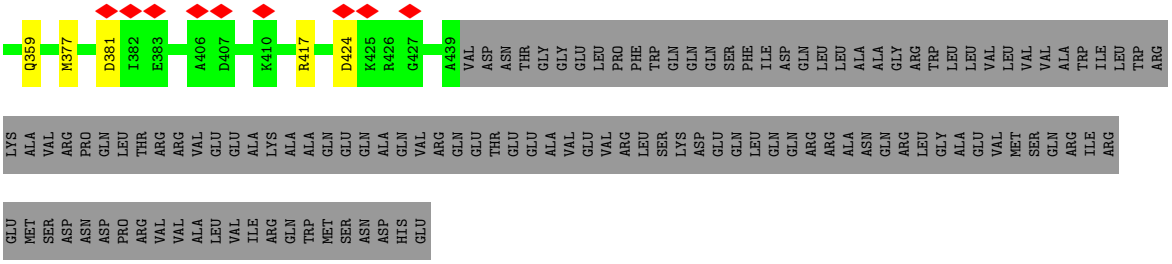


• Molecule 6: Flagellar M-ring protein

Chain BU:

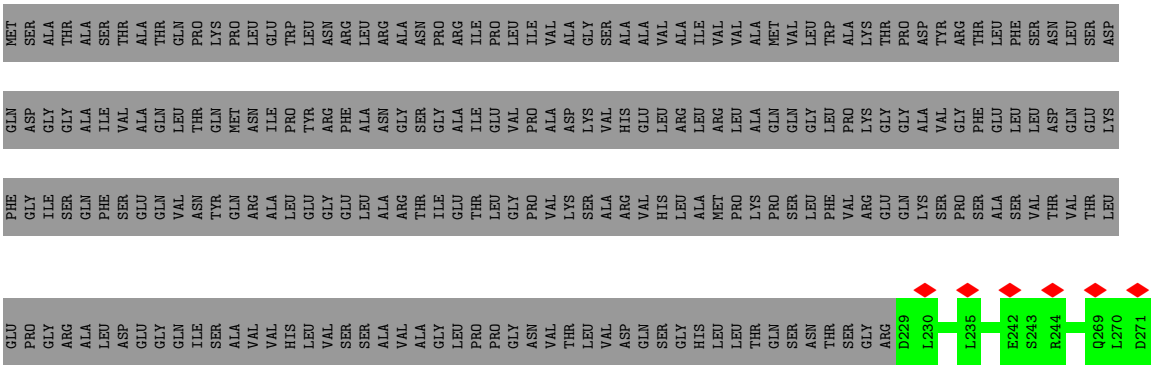


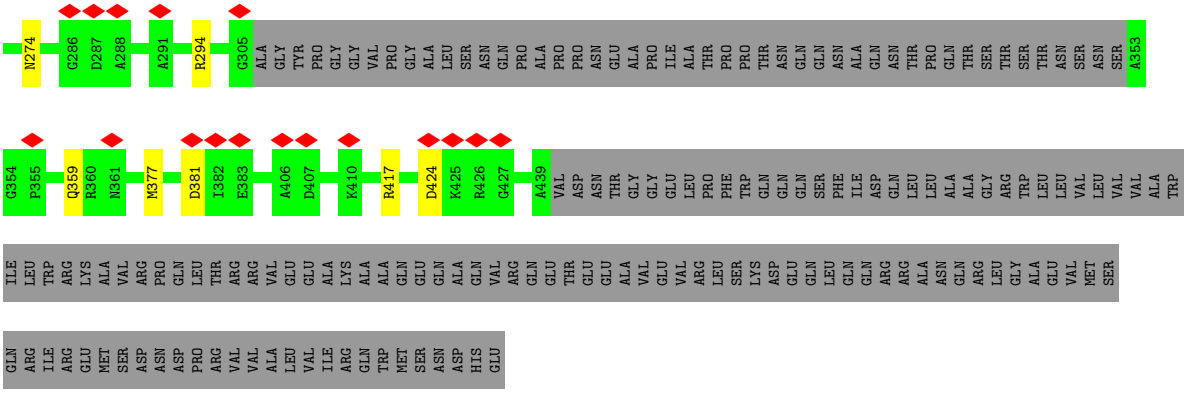




• Molecule 6: Flagellar M-ring protein

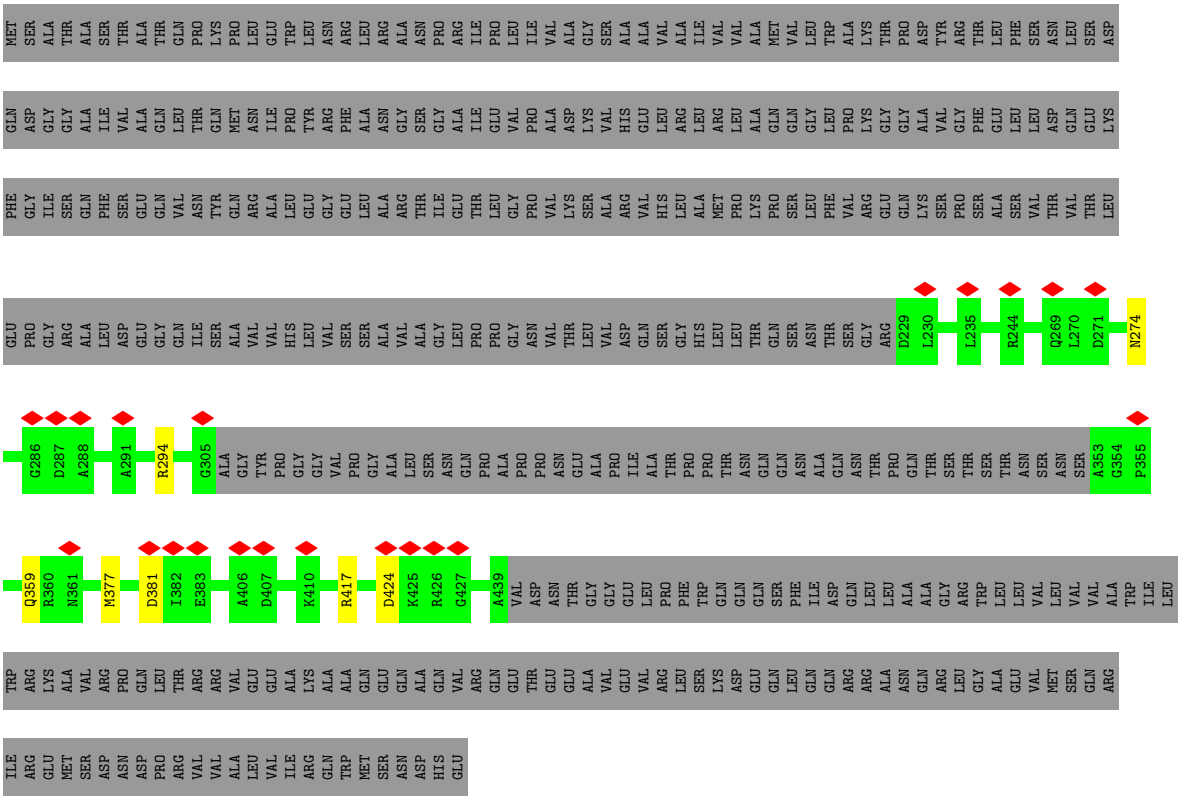
Chain BV:





• Molecule 6: Flagellar M-ring protein

Chain BW:



• Molecule 6: Flagellar M-ring protein

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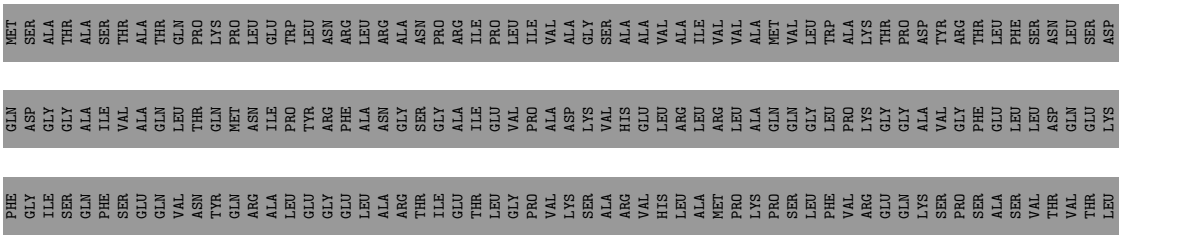

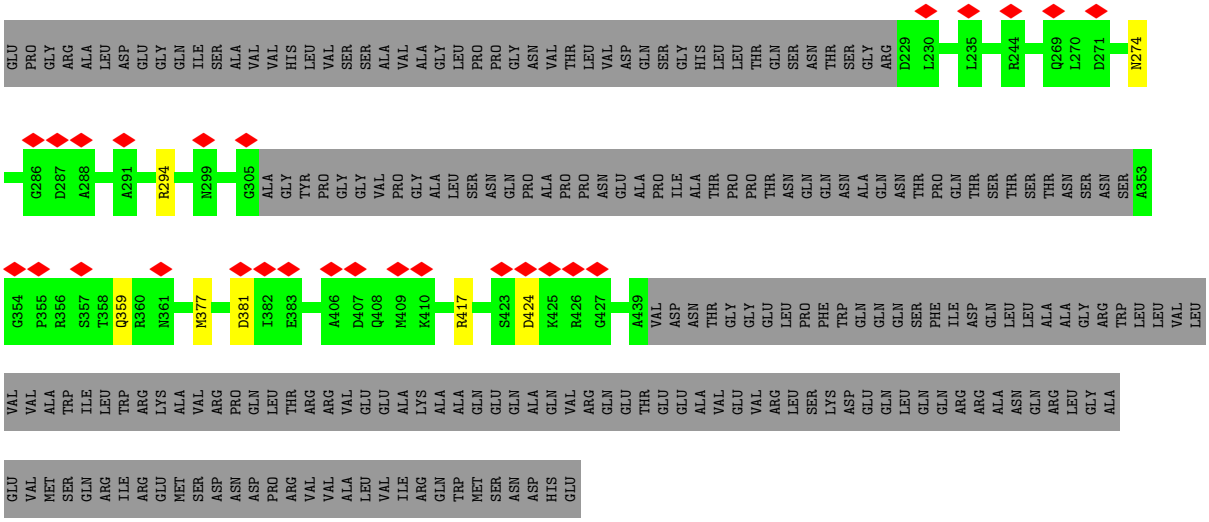

• Molecule 6: Flagellar M-ring protein

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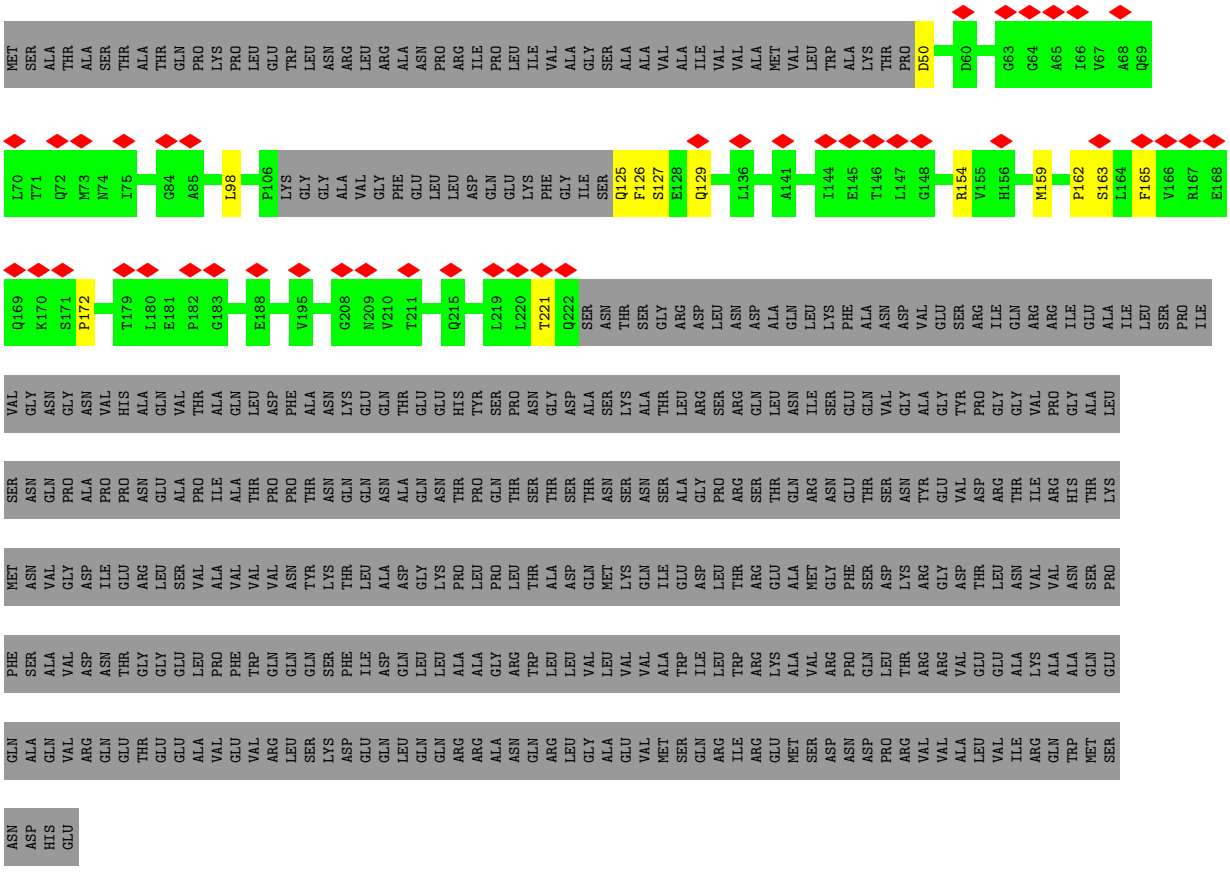
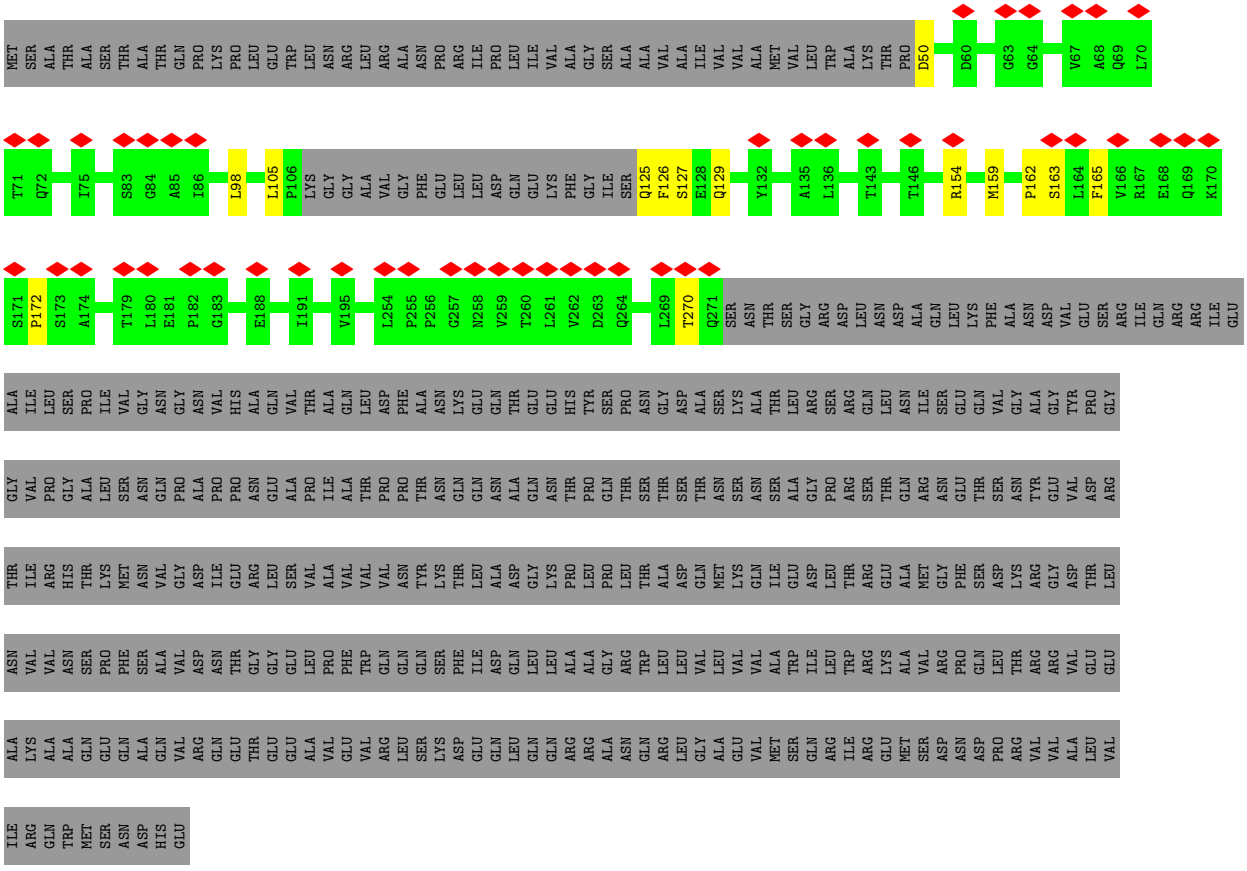


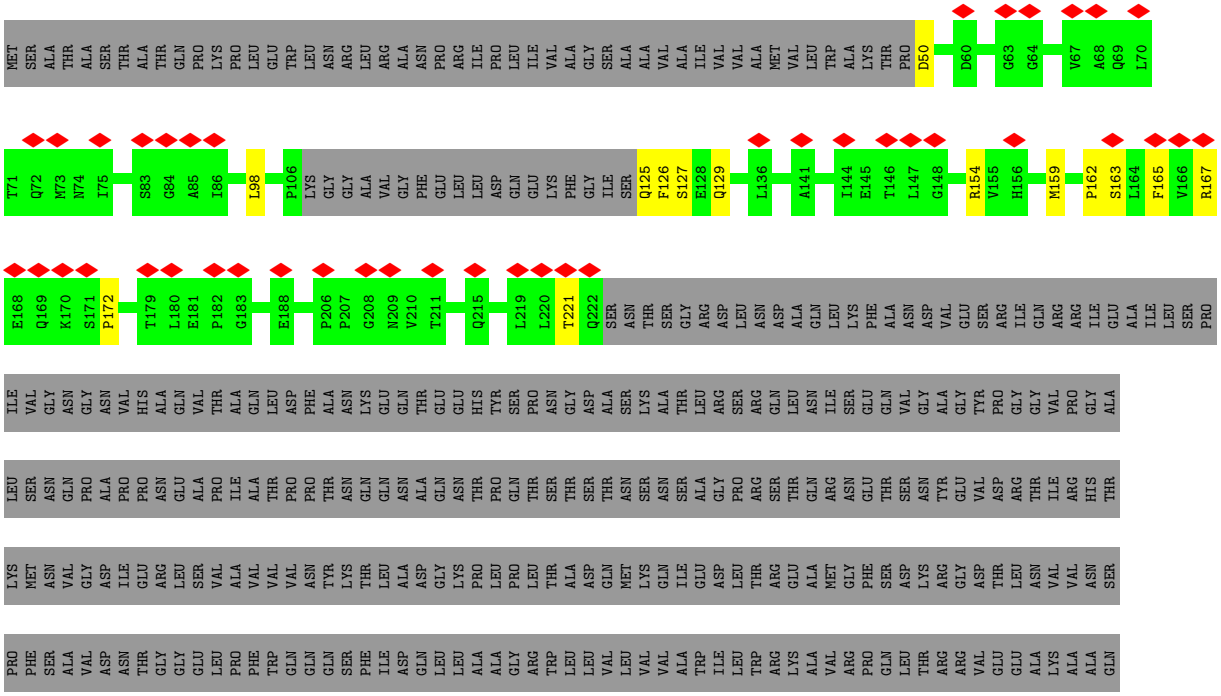
• Molecule 6: Flagellar M-ring protein

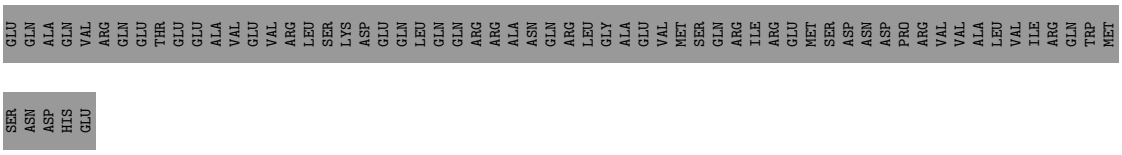
Chain UJ:



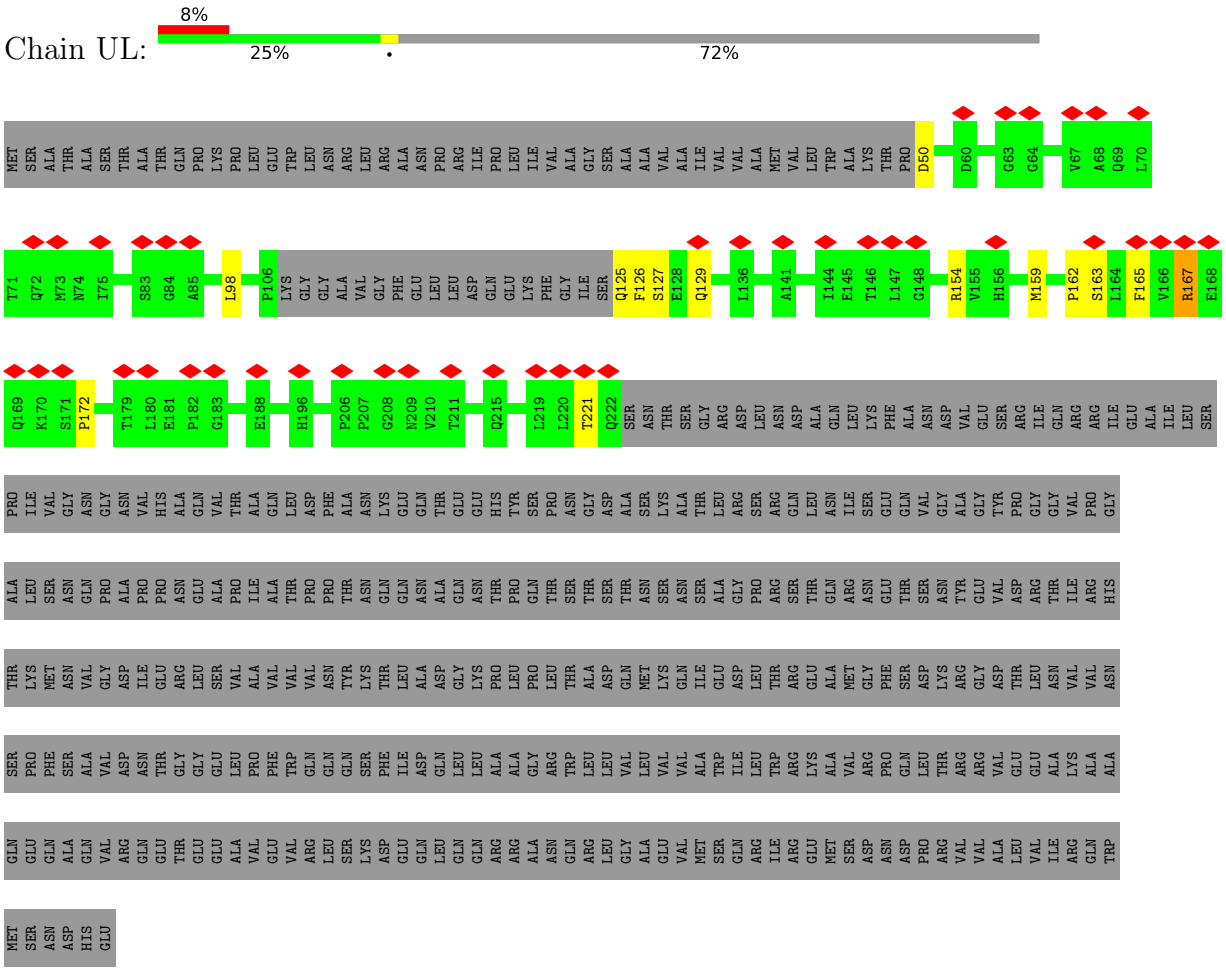
• Molecule 6: Flagellar M-ring protein

Chain UK:

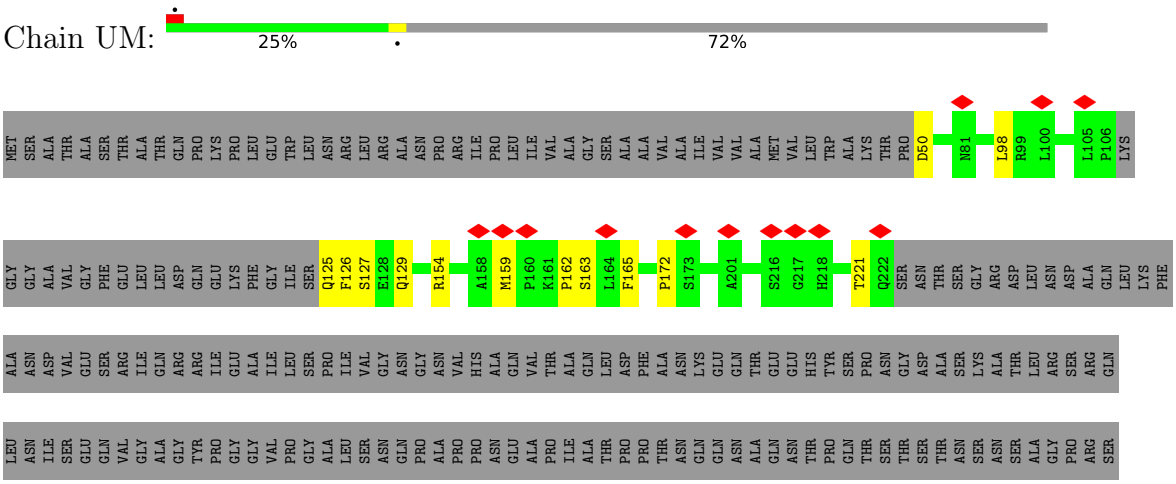


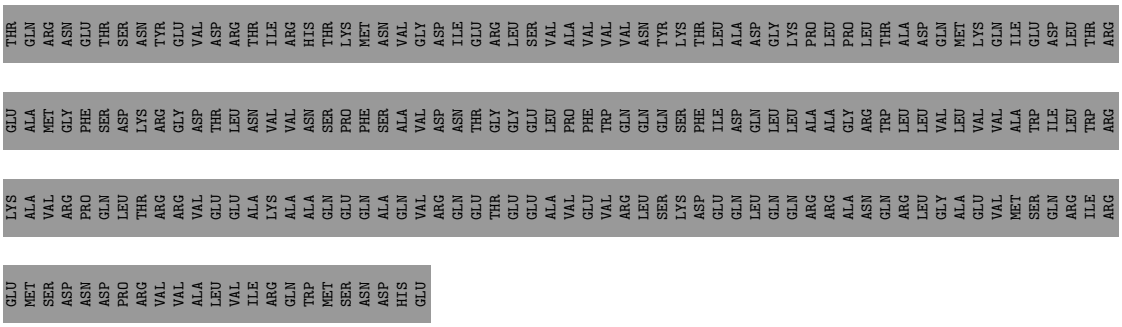


• Molecule 6: Flagellar M-ring protein



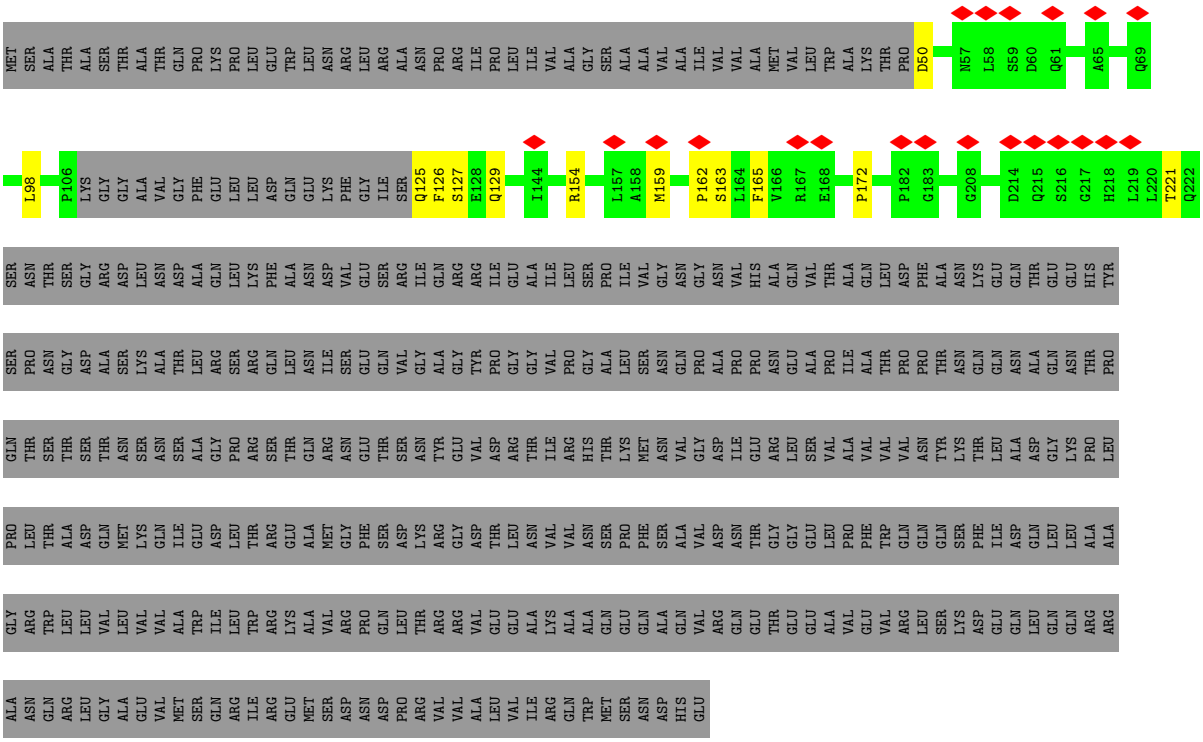
• Molecule 6: Flagellar M-ring protein





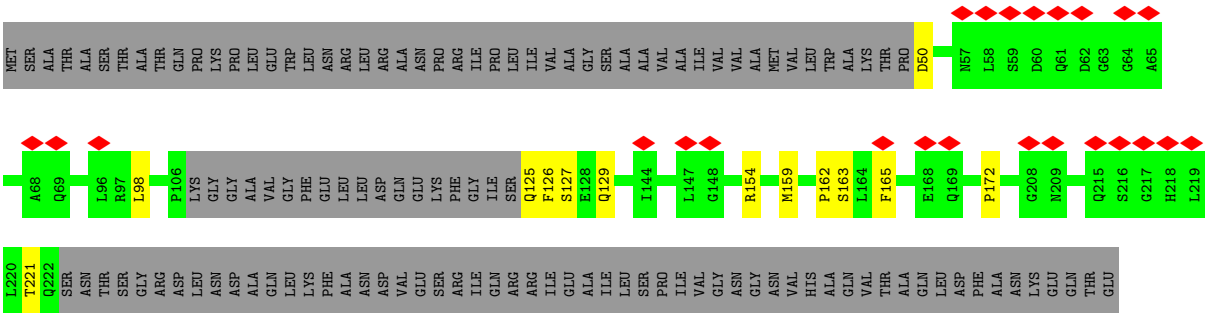
• Molecule 6: Flagellar M-ring protein

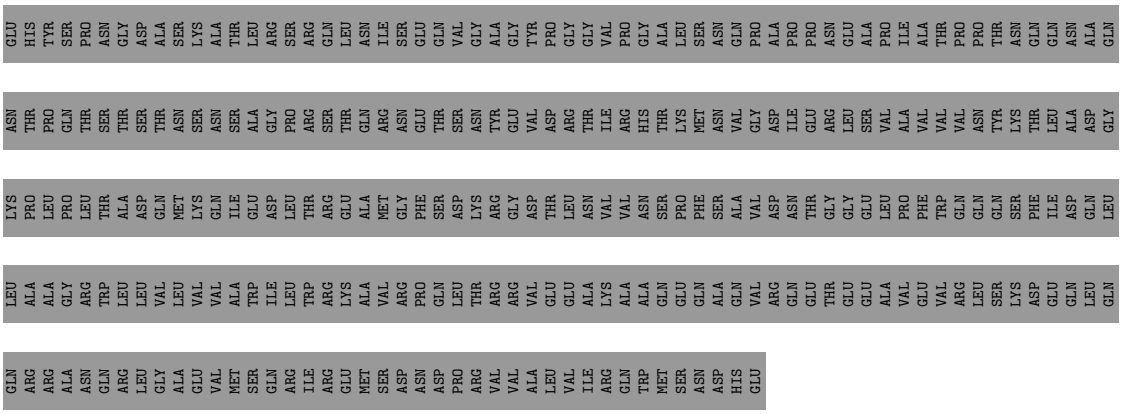
Chain UN:



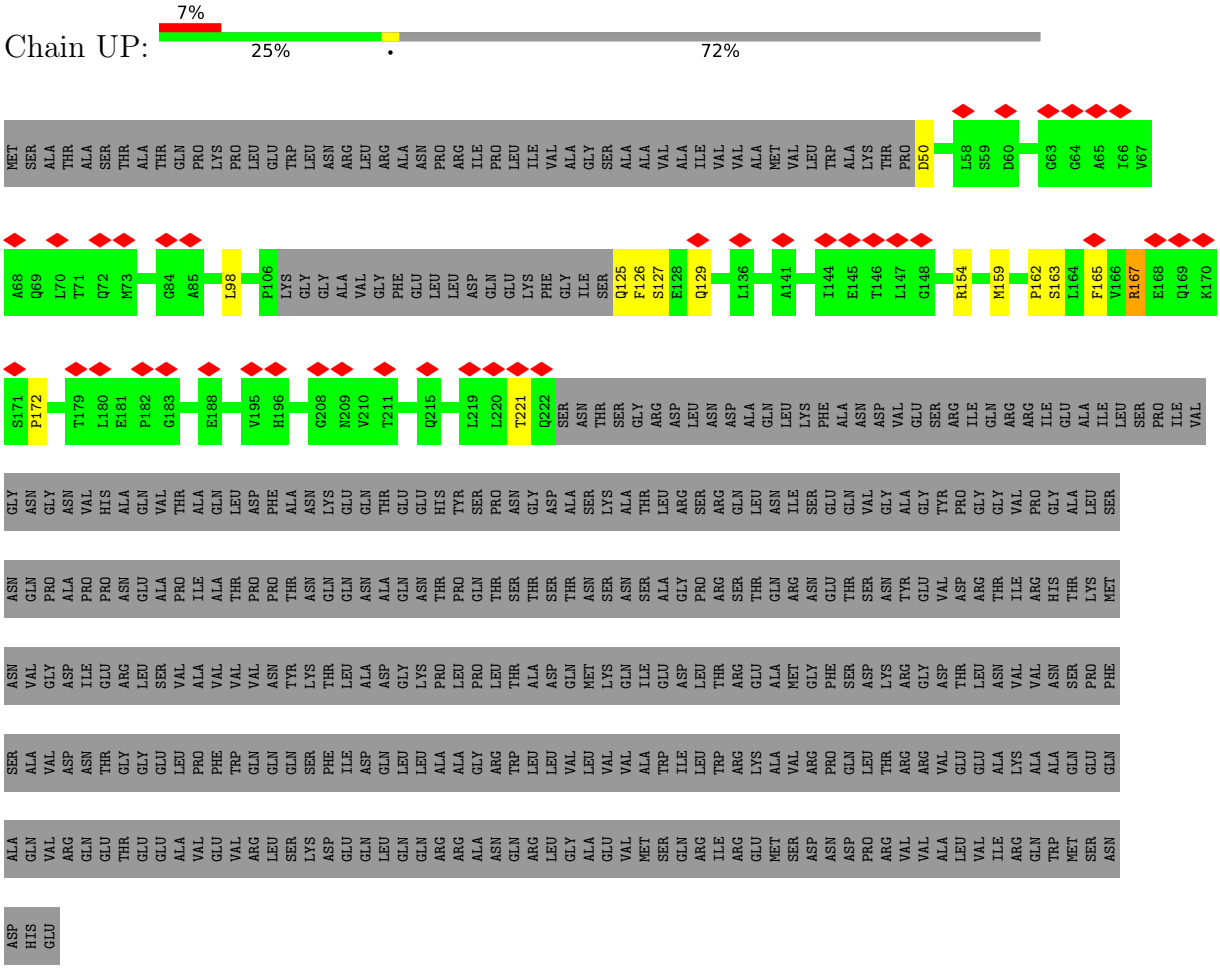
• Molecule 6: Flagellar M-ring protein

Chain UO:

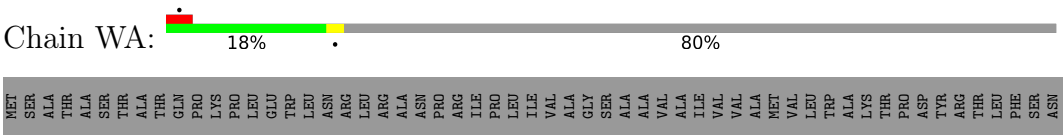


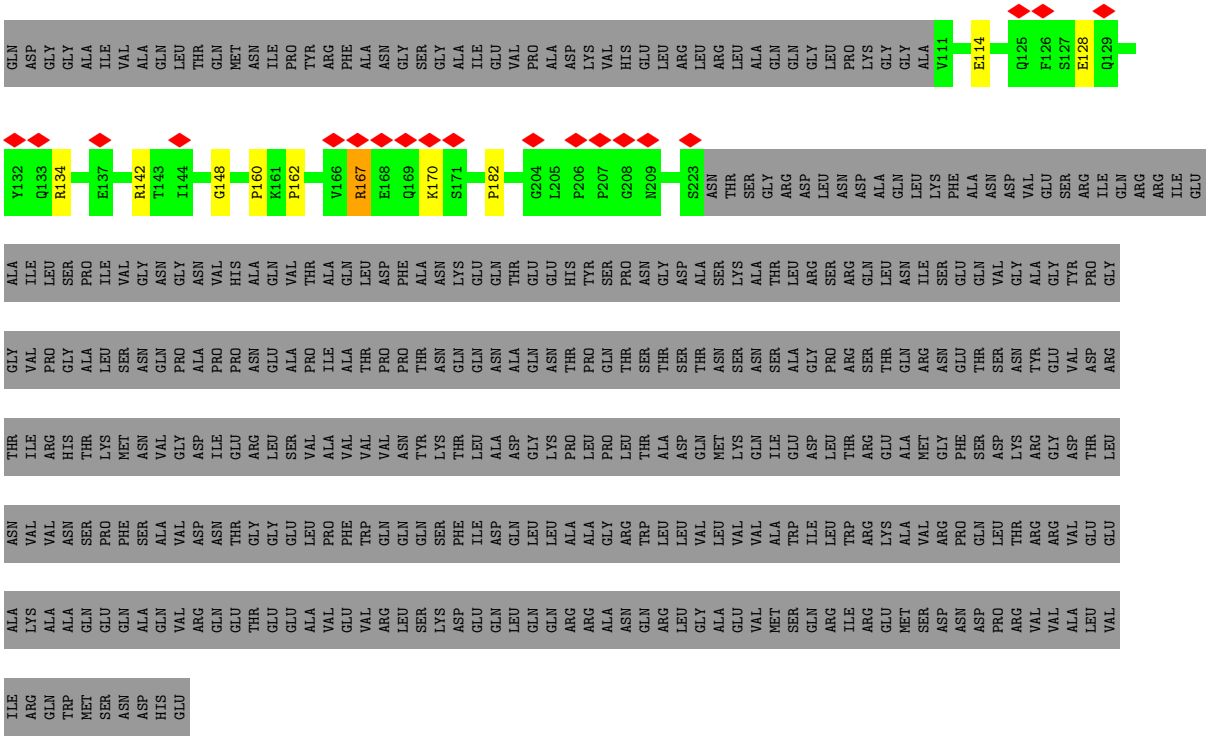


• Molecule 6: Flagellar M-ring protein



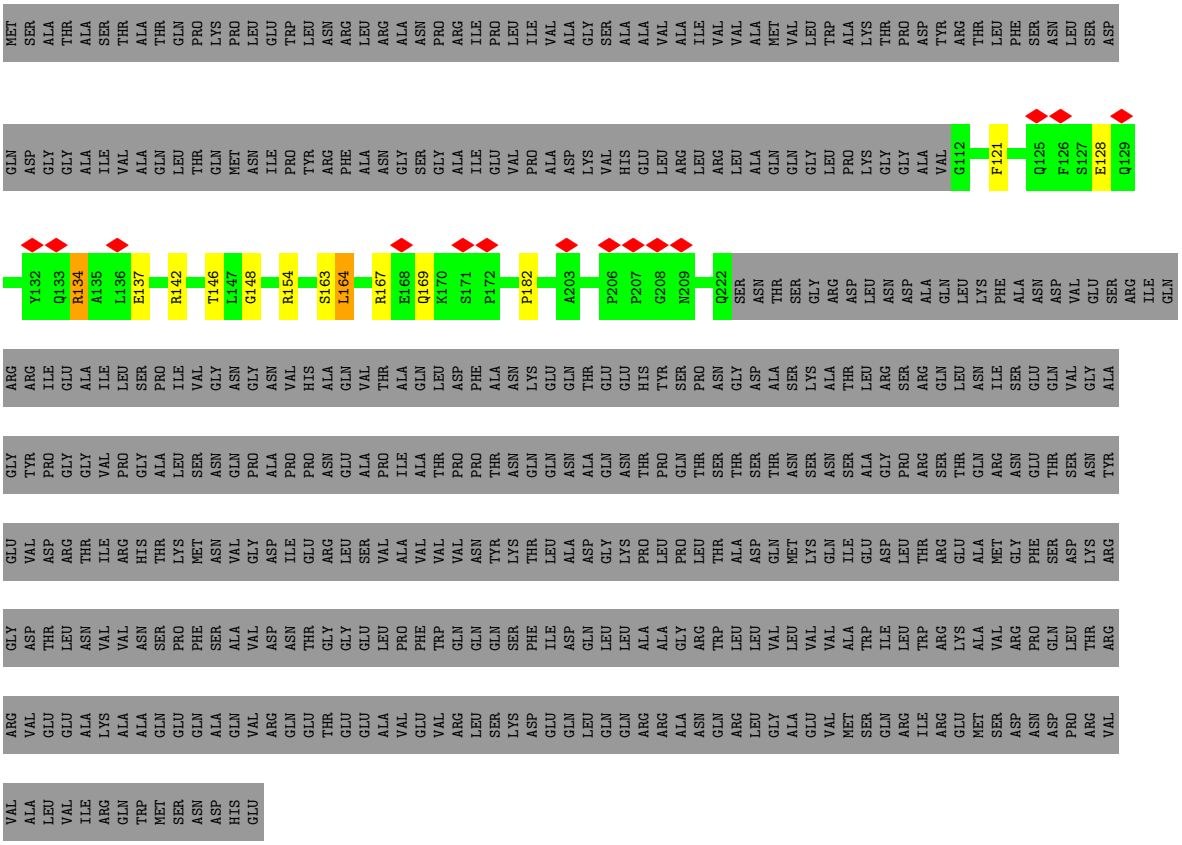
• Molecule 6: Flagellar M-ring protein





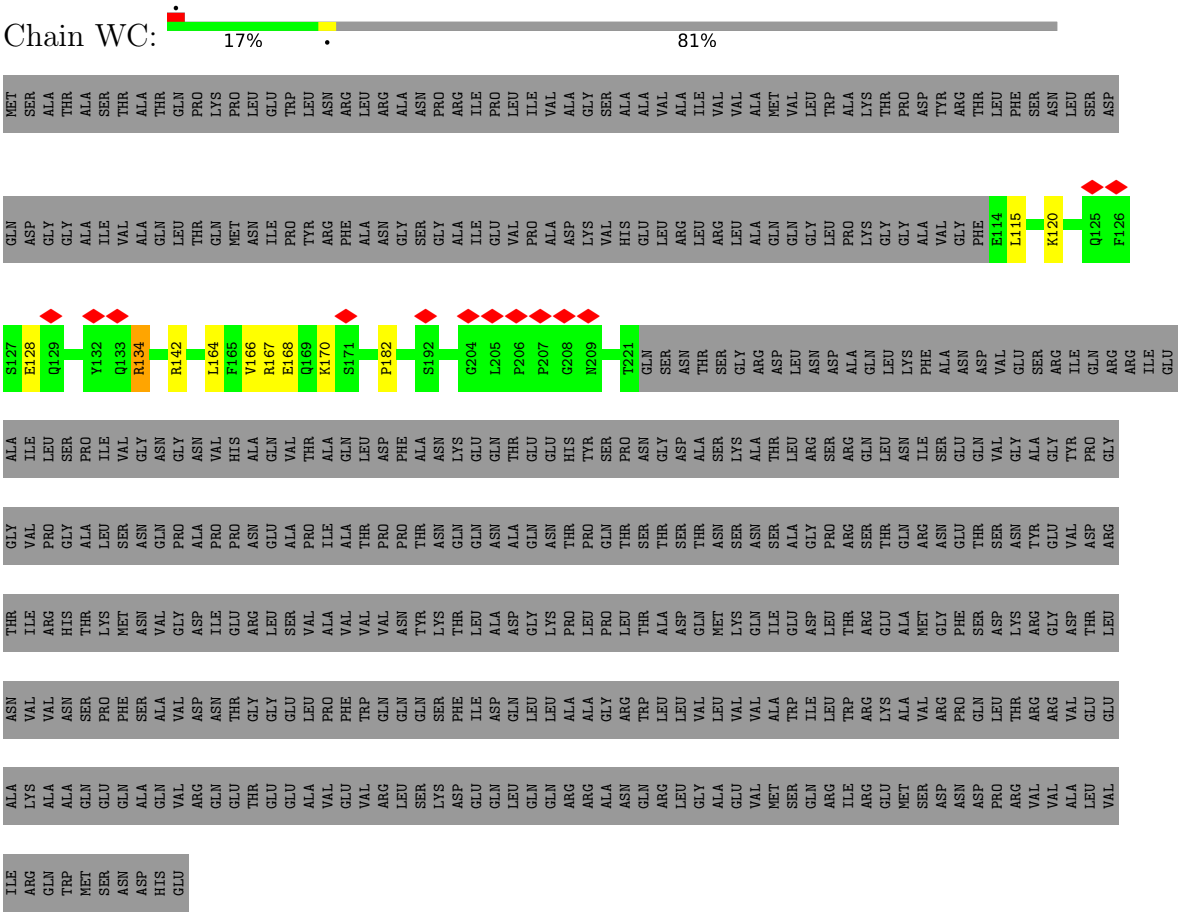
• Molecule 6: Flagellar M-ring protein

Chain WB:



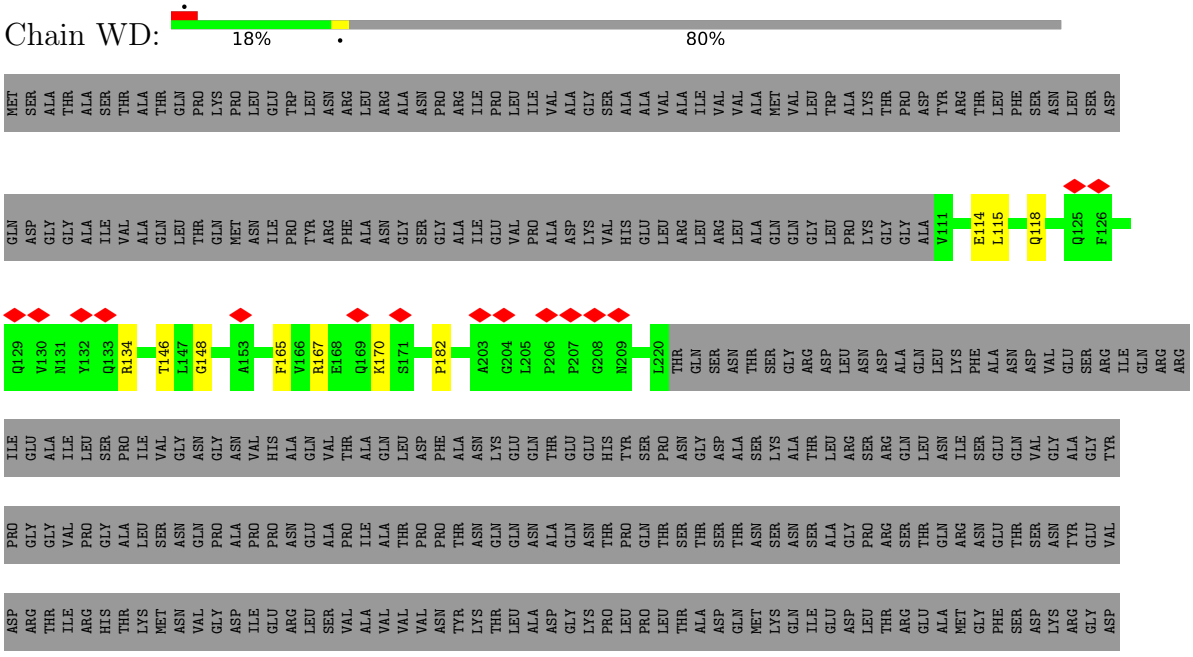
• Molecule 6: Flagellar M-ring protein

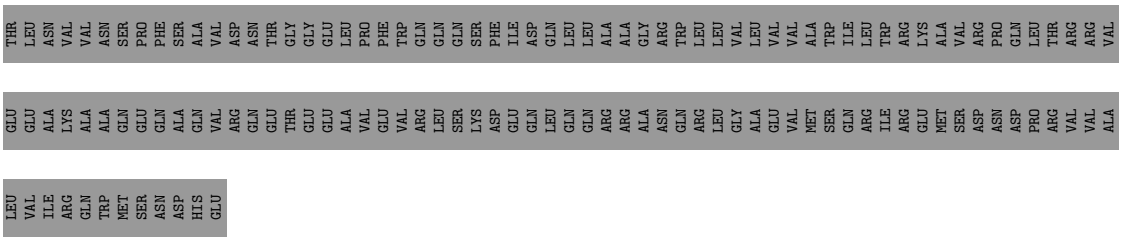
Chain WC:



• Molecule 6: Flagellar M-ring protein

Chain WD:





• Molecule 6: Flagellar M-ring protein

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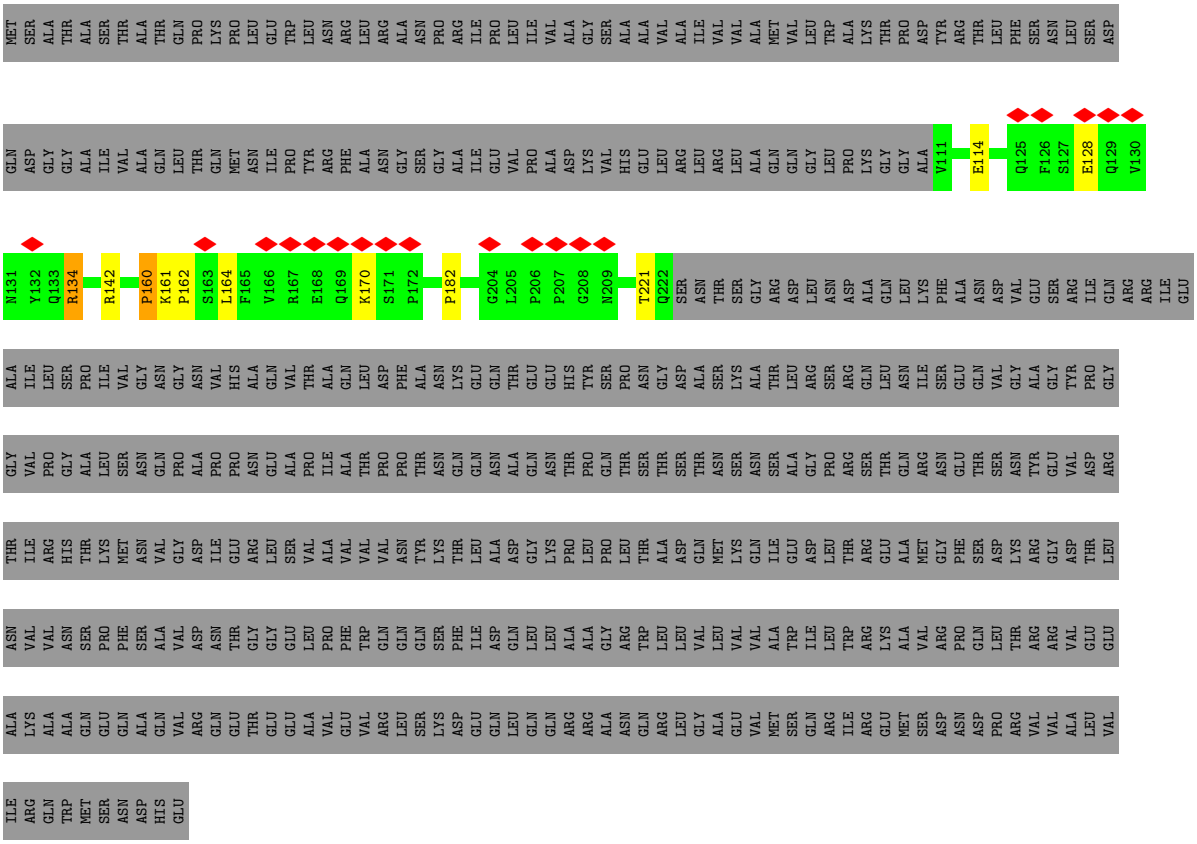

• Molecule 6: Flagellar M-ring protein

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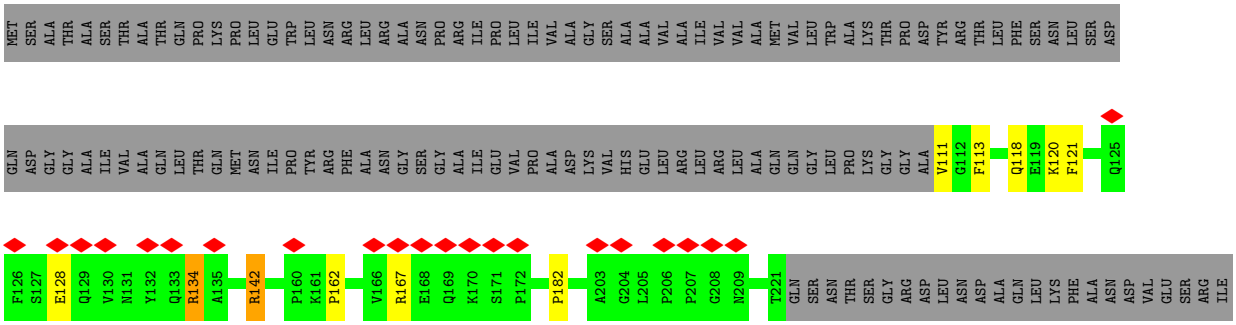

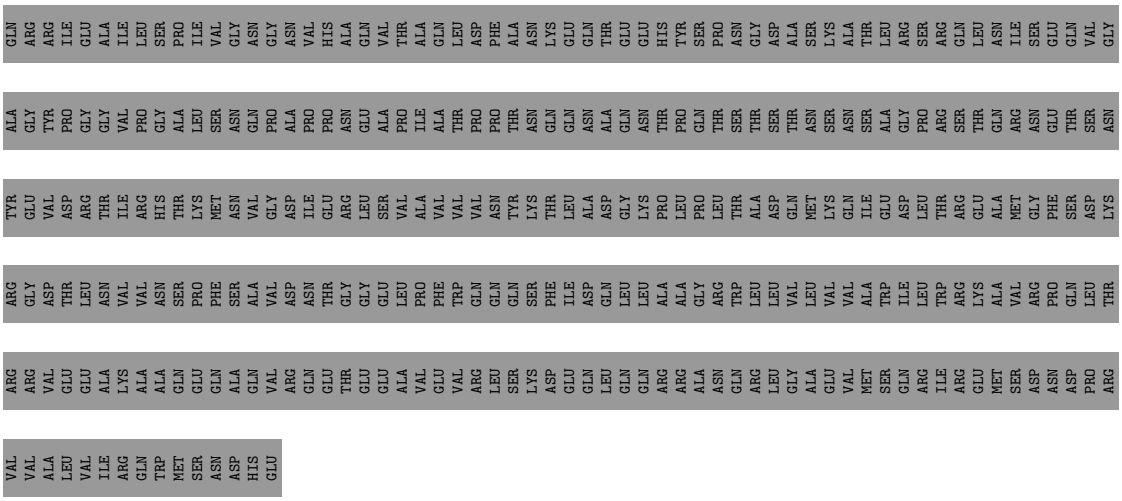

• Molecule 6: Flagellar M-ring protein

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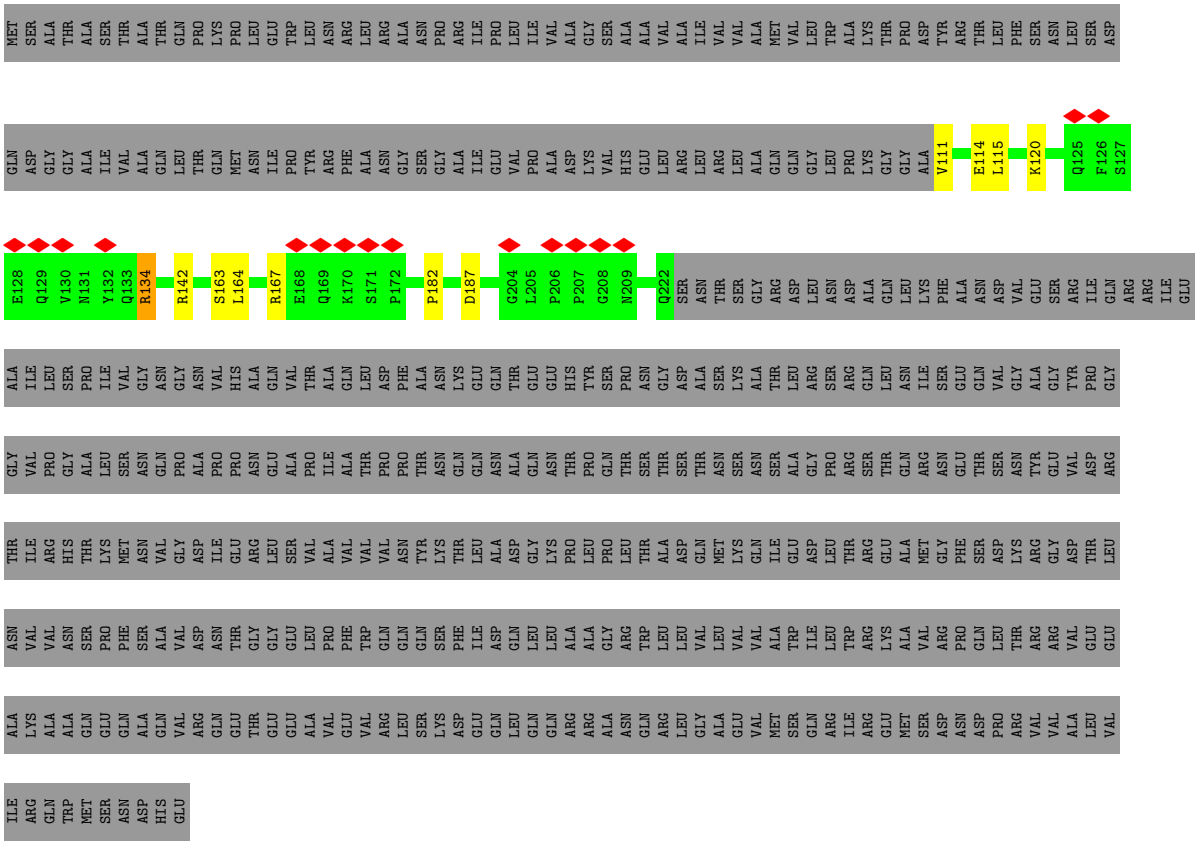

• Molecule 6: Flagellar M-ring protein

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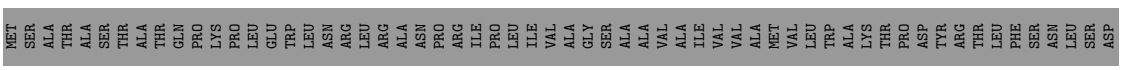

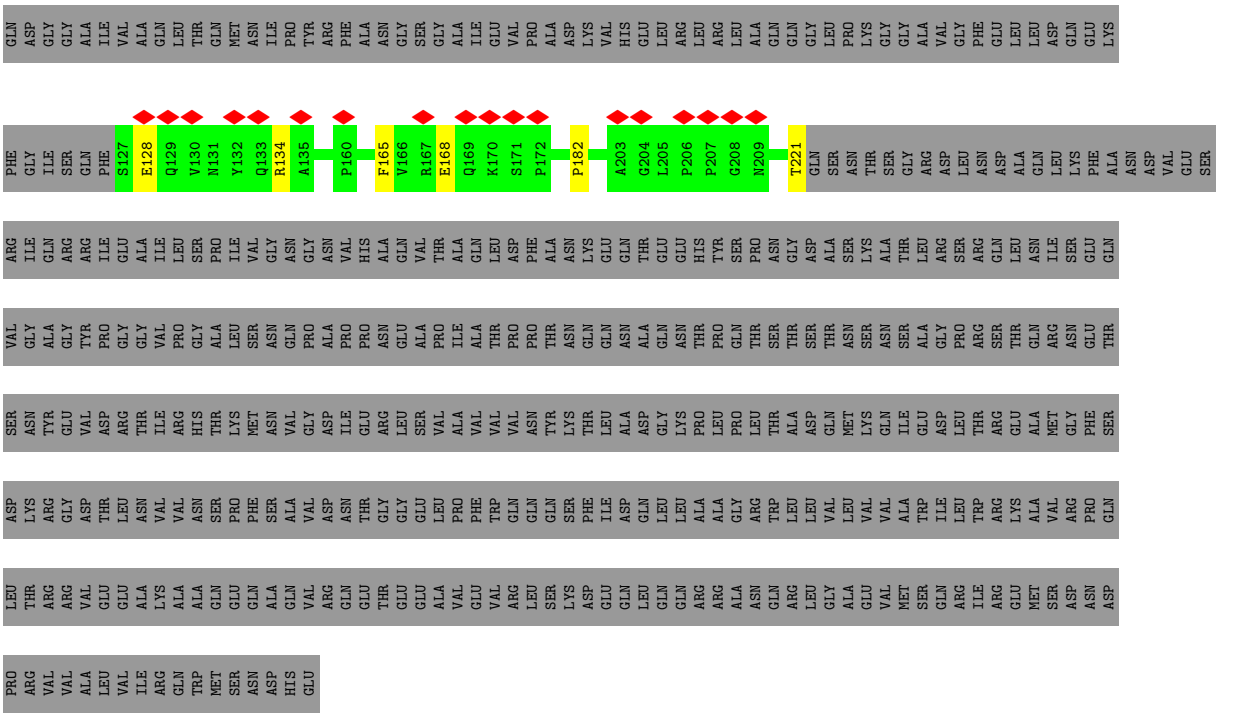

• Molecule 6: Flagellar M-ring protein

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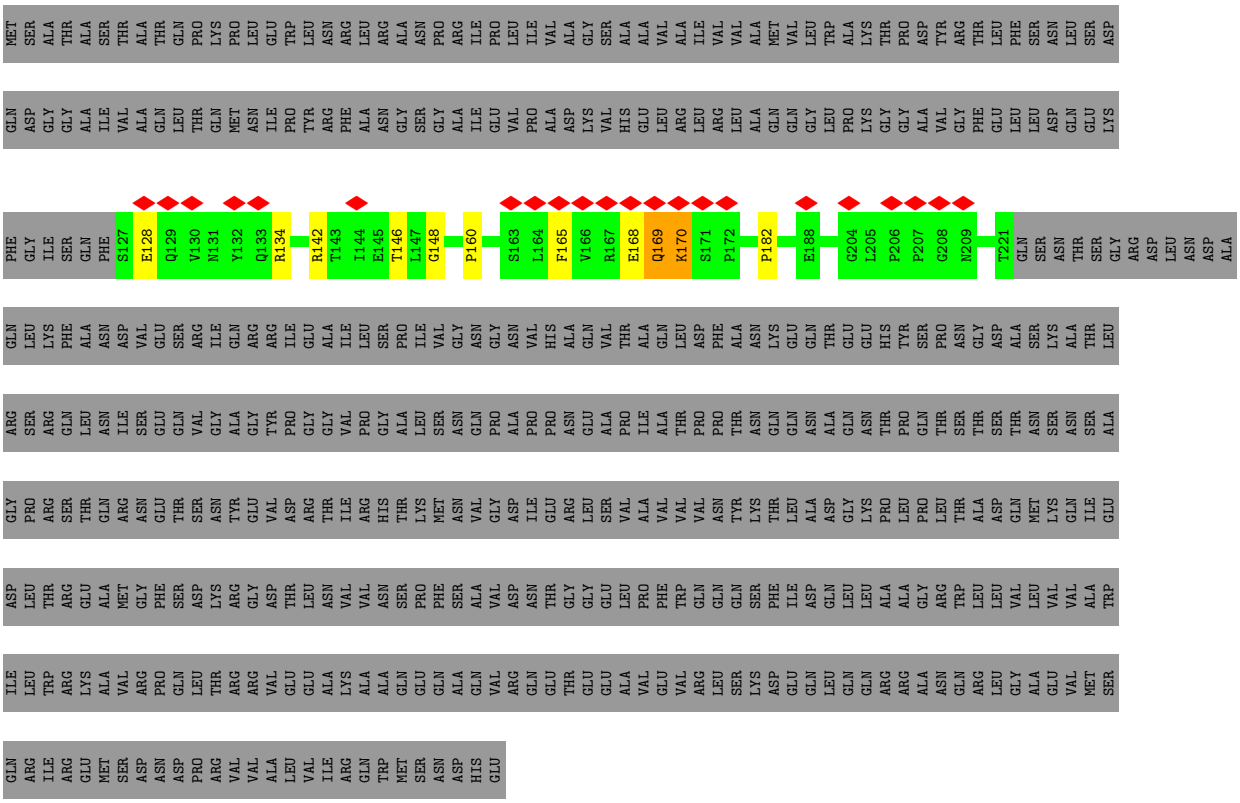

• Molecule 6: Flagellar M-ring protein

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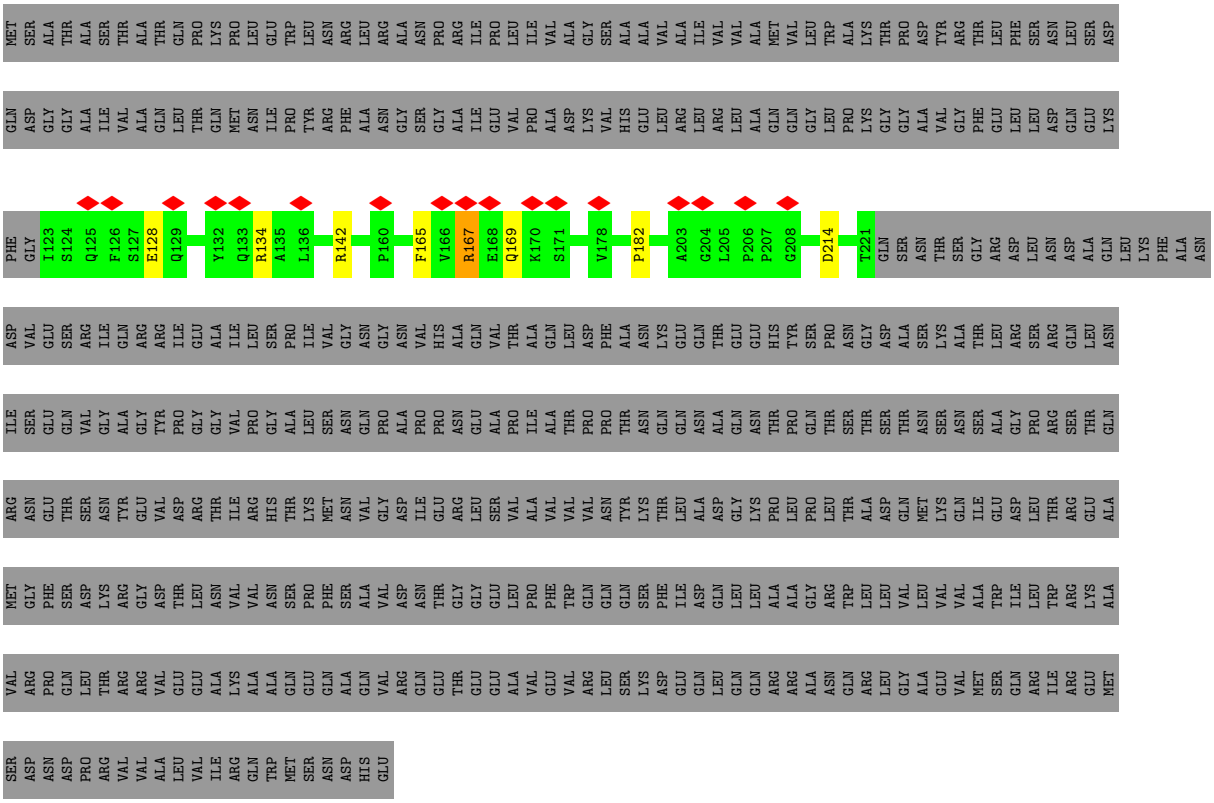

• Molecule 6: Flagellar M-ring protein

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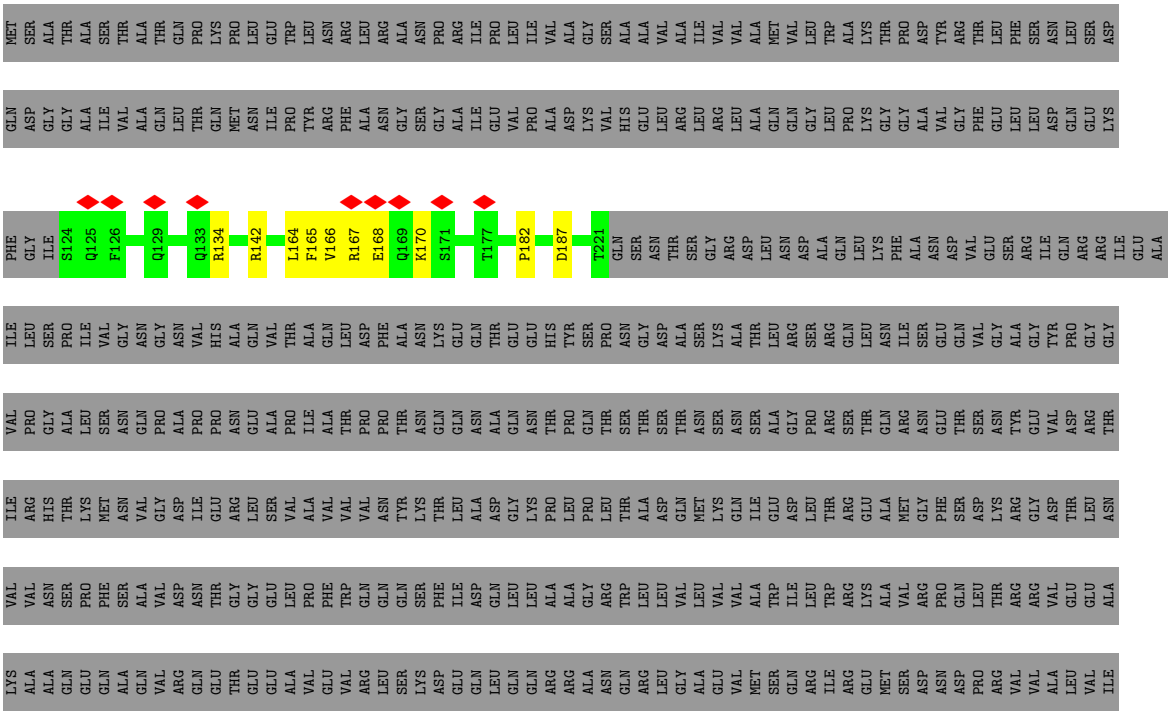

• Molecule 6: Flagellar M-ring protein

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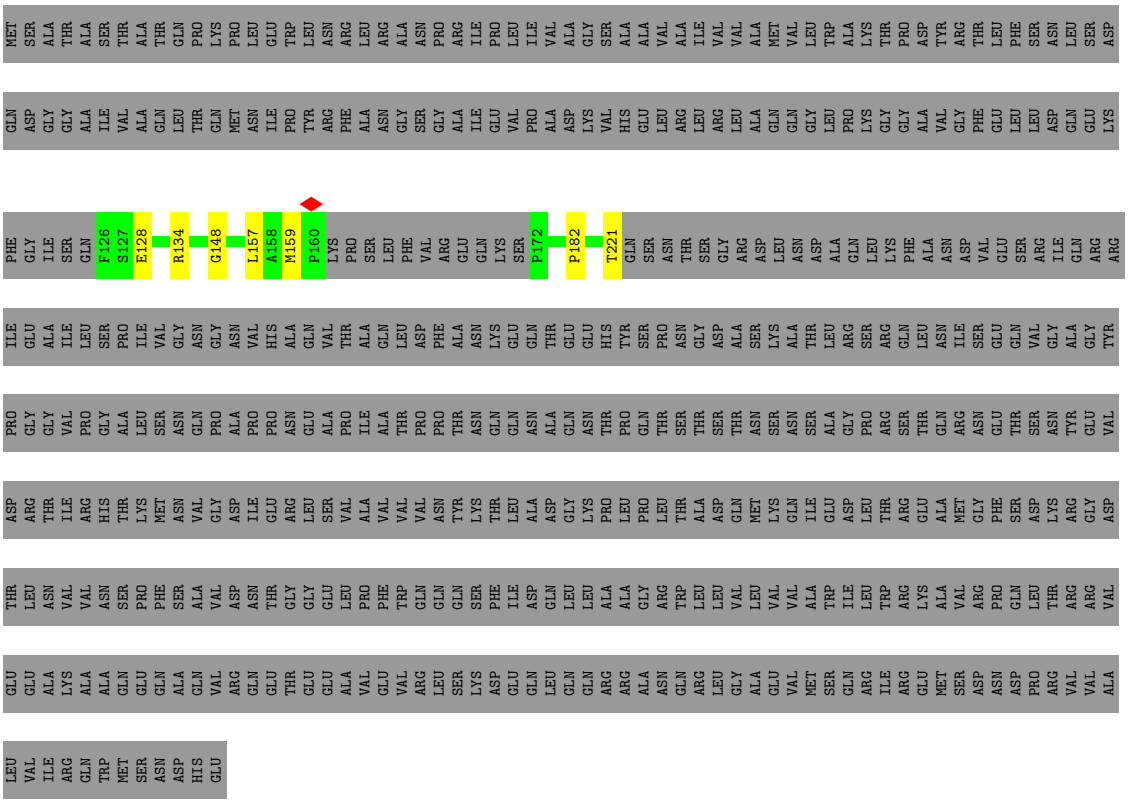

• Molecule 6: Flagellar M-ring protein

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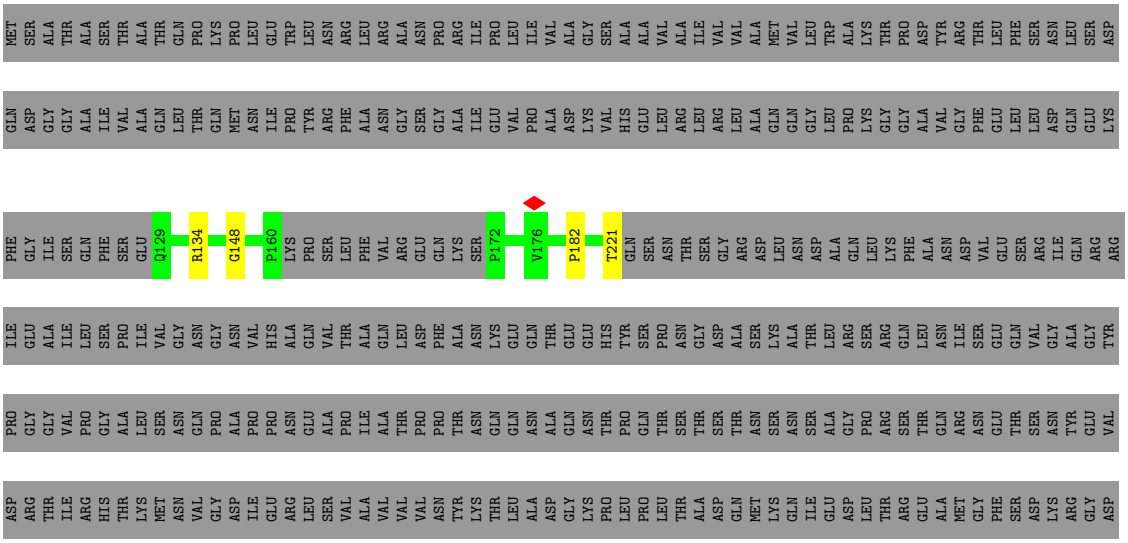

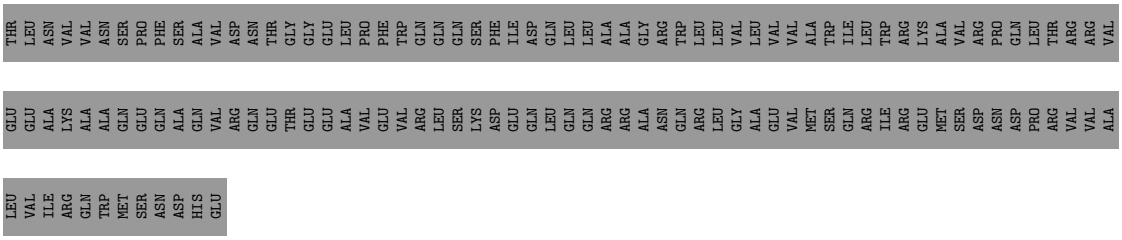

• Molecule 6: Flagellar M-ring protein

Chain WN:

• Molecule 6: Flagellar M-ring protein

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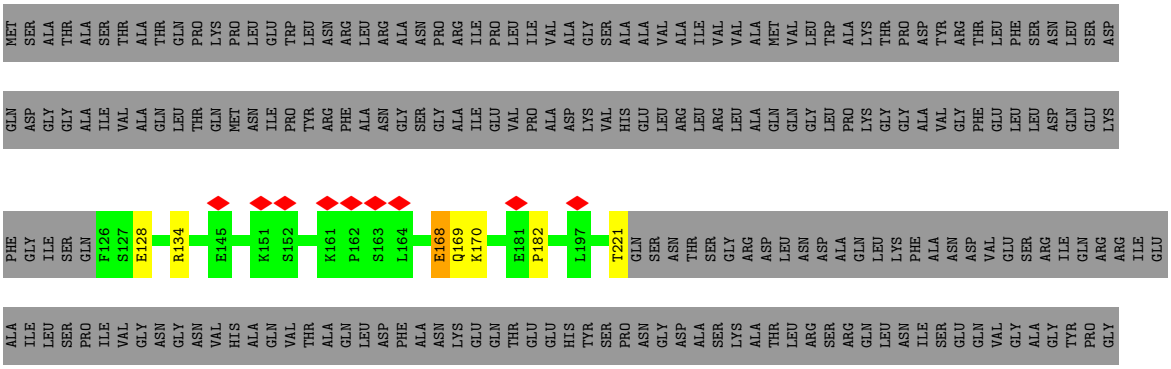

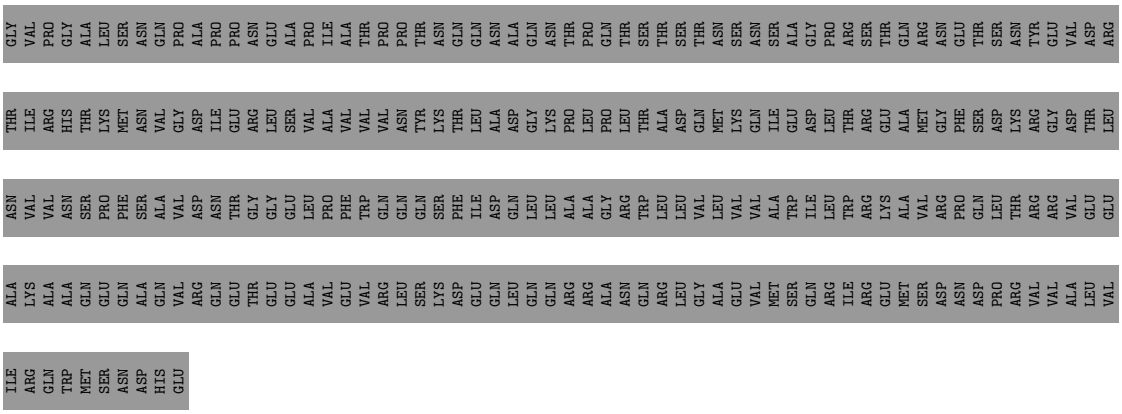

• Molecule 6: Flagellar M-ring protein

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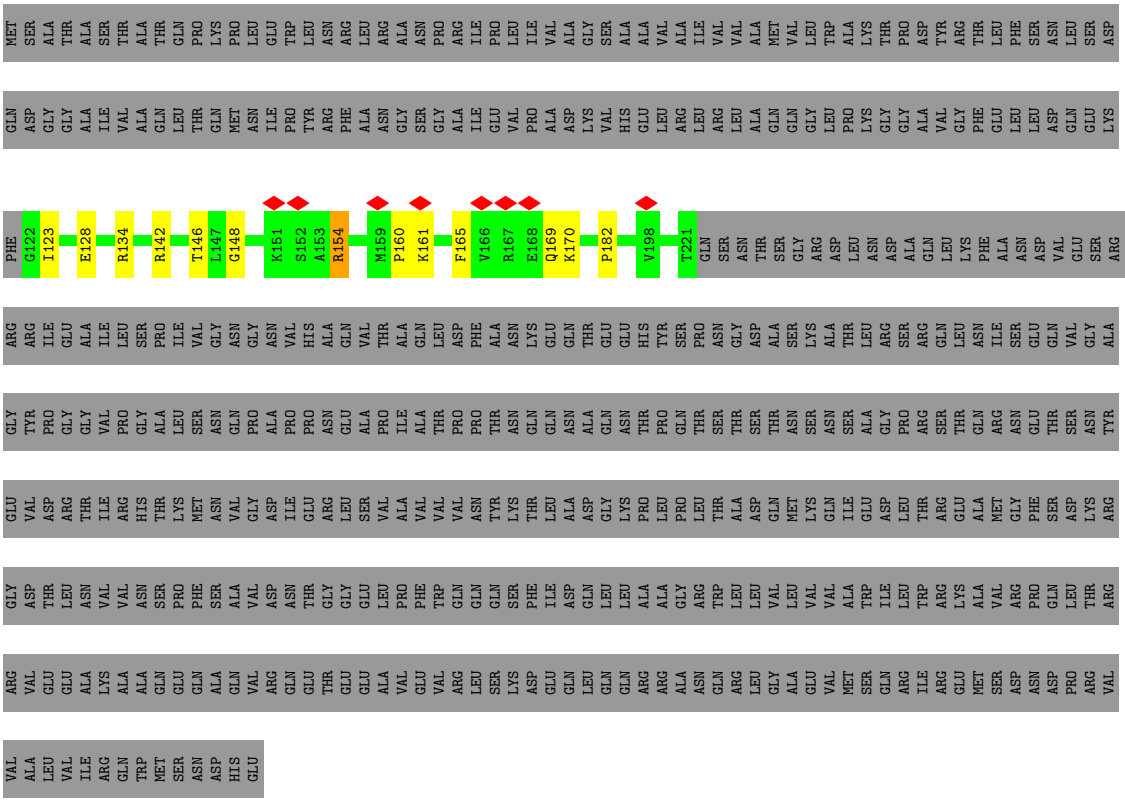

• Molecule 6: Flagellar M-ring protein

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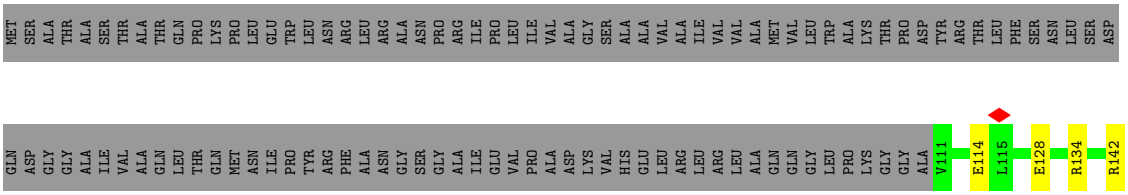

• Molecule 6: Flagellar M-ring protein

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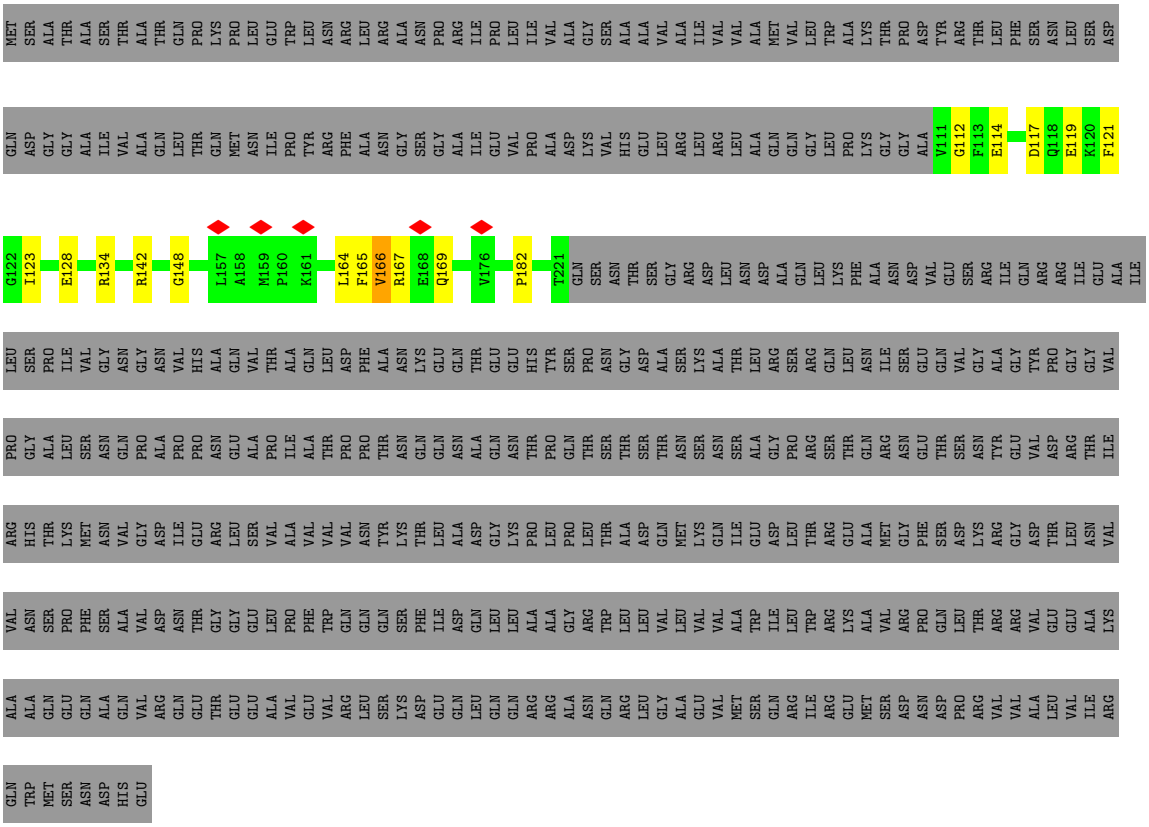
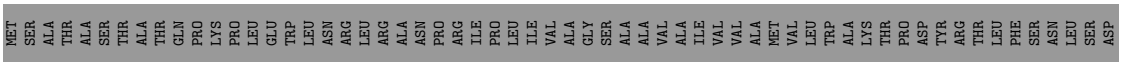
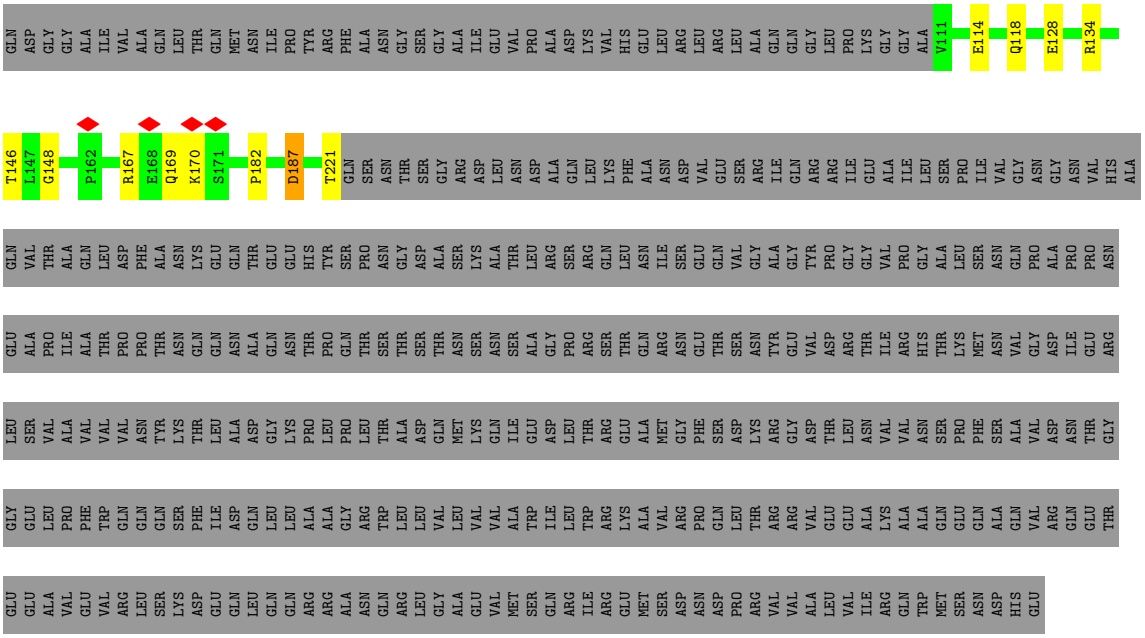


• Molecule 6: Flagellar M-ring protein

Chain WS:





• Molecule 6: Flagellar M-ring protein

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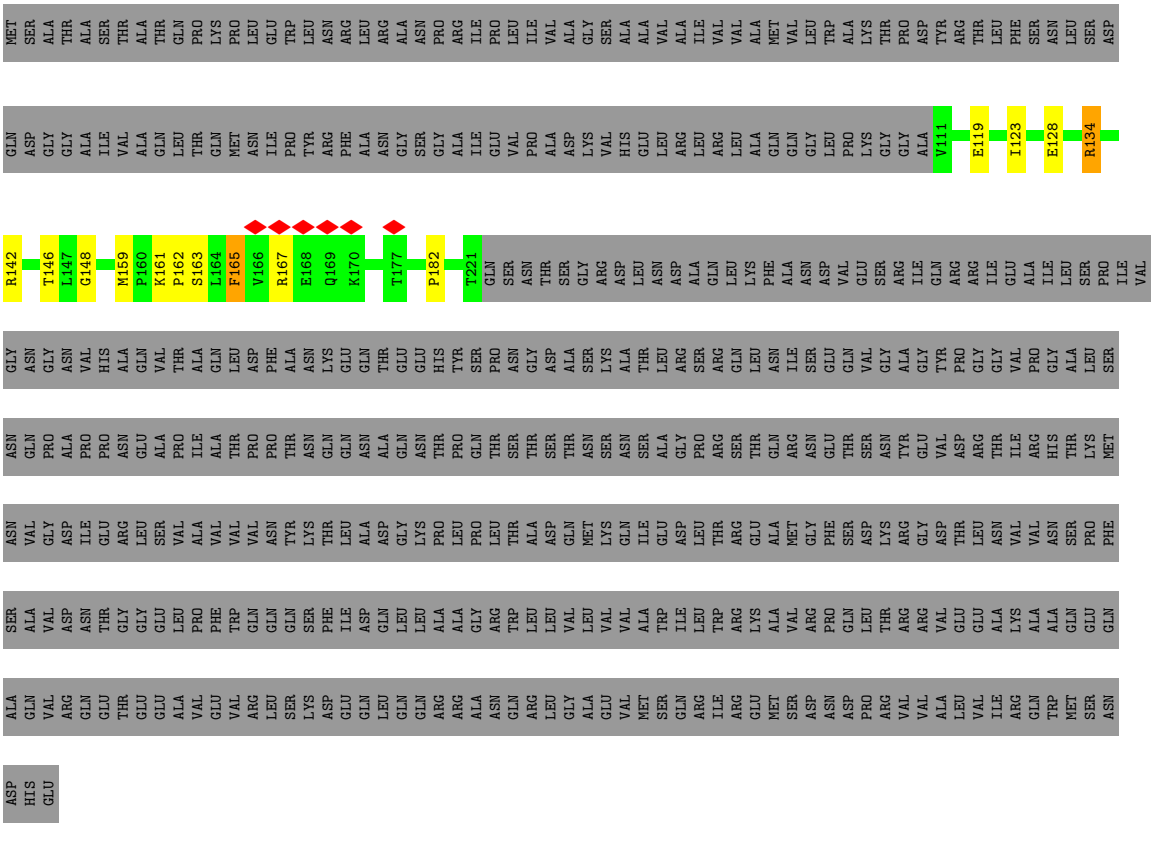

• Molecule 6: Flagellar M-ring protein

Chain WU:

- Molecule 6: Flagellar M-ring protein

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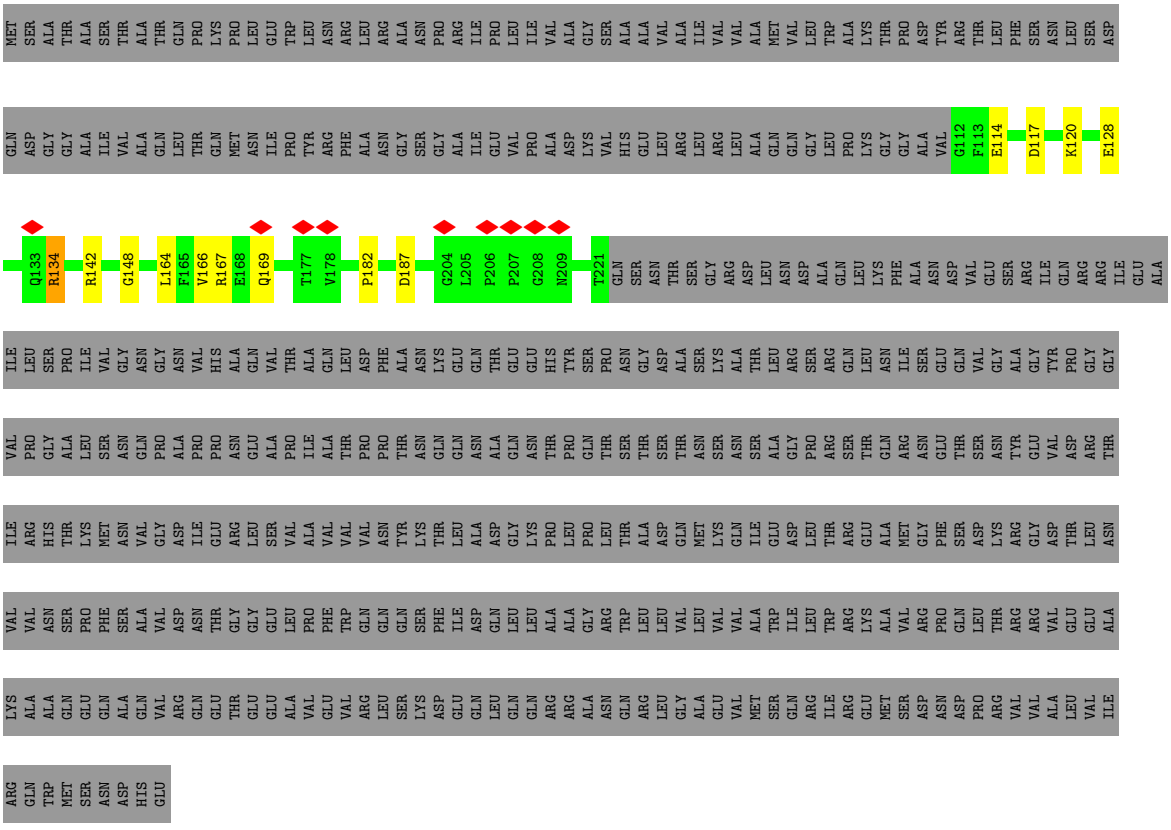

• Molecule 6: Flagellar M-ring protein

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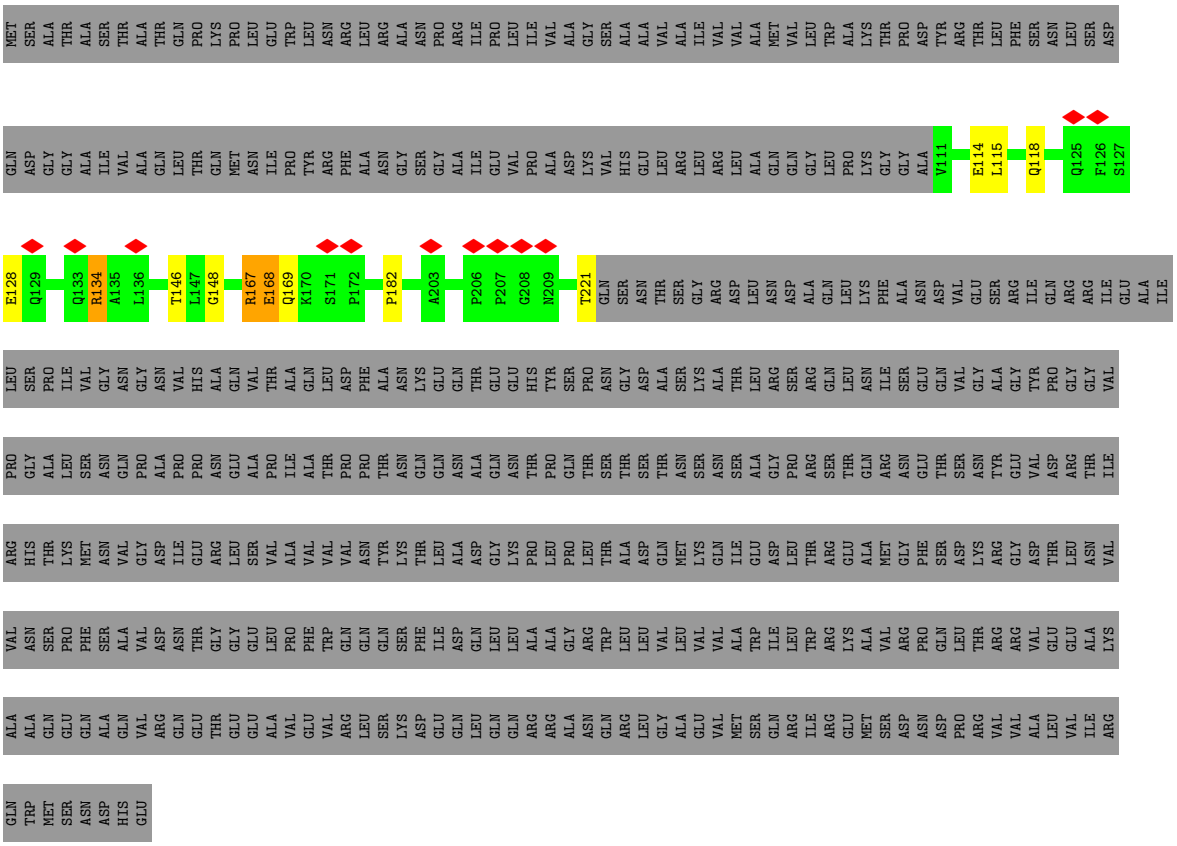
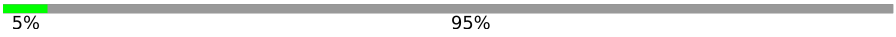
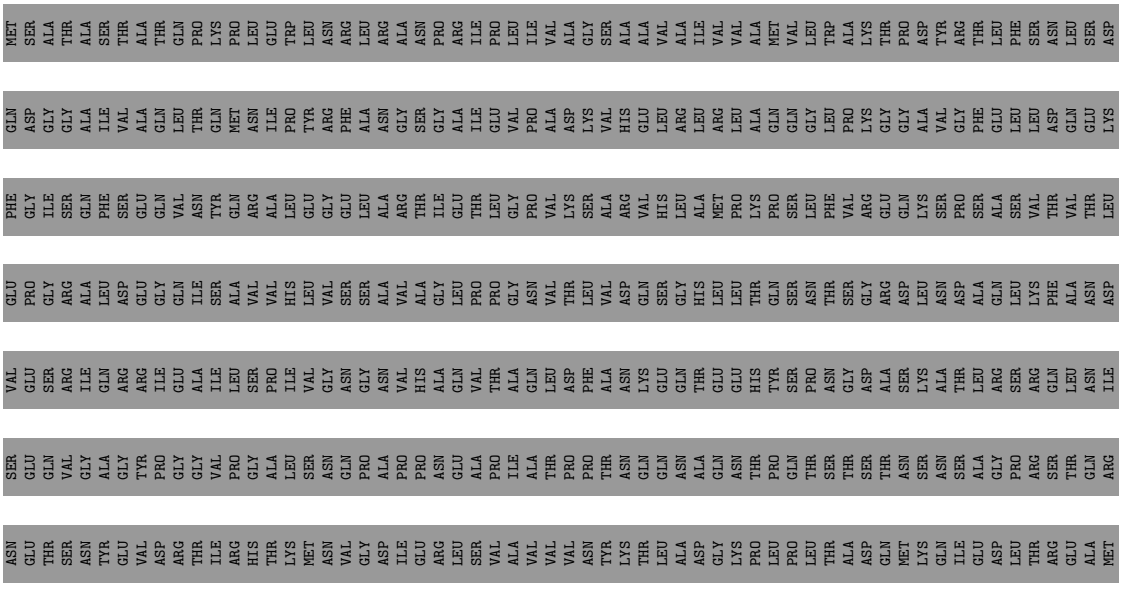
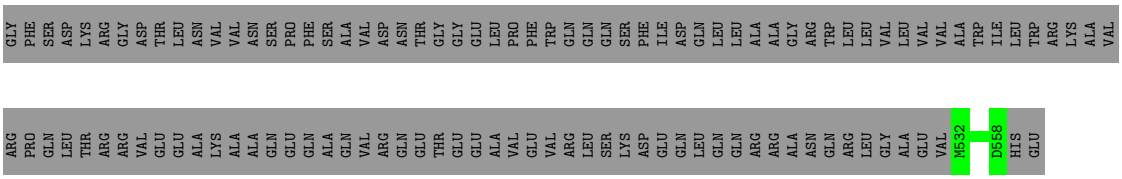


• Molecule 6: Flagellar M-ring protein

Chain C3:

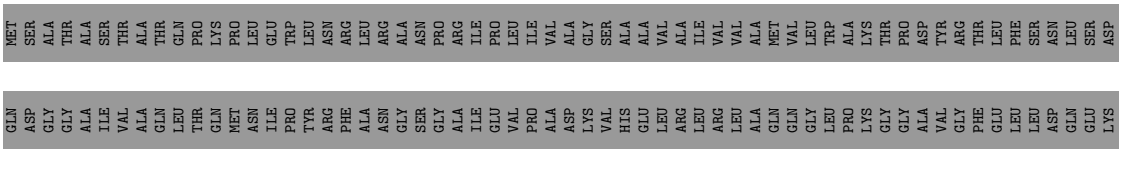






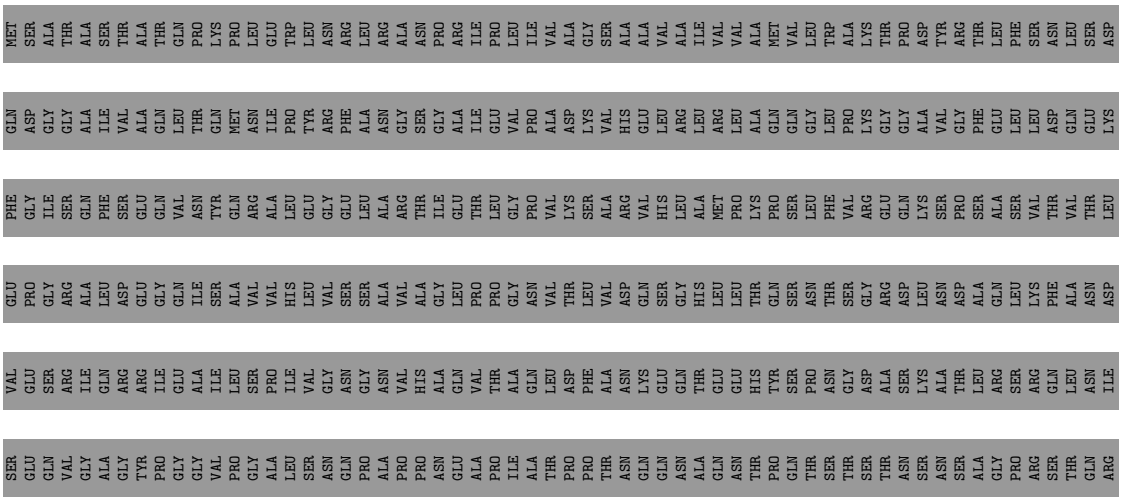
• Molecule 6: Flagellar M-ring protein

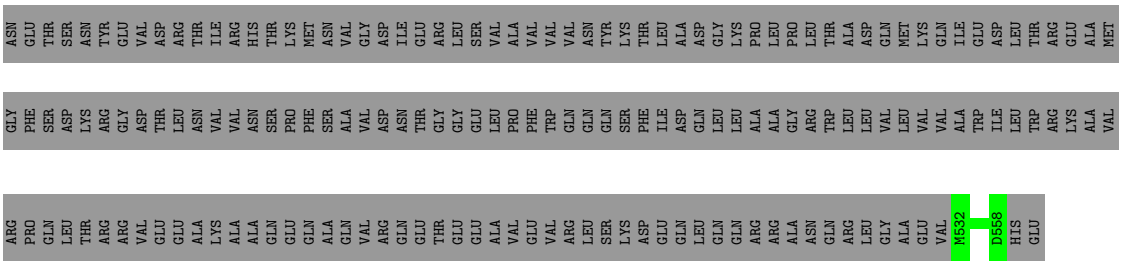
Chain C7: 5% 95%



• Molecule 6: Flagellar M-ring protein

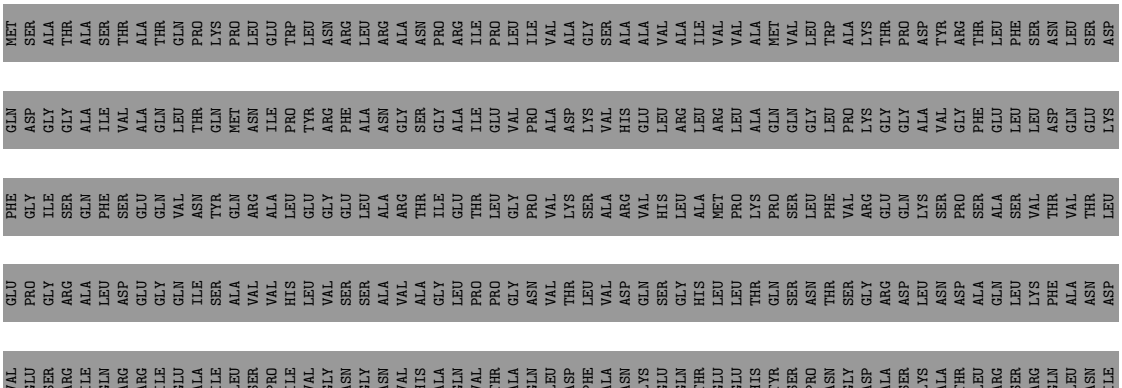
Chain DE: 5% 95%





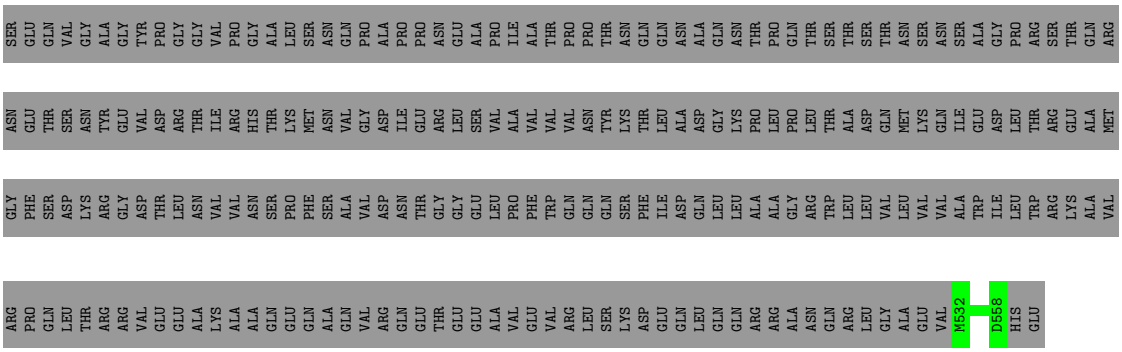
• Molecule 6: Flagellar M-ring protein

Chain DK: 5% 95%



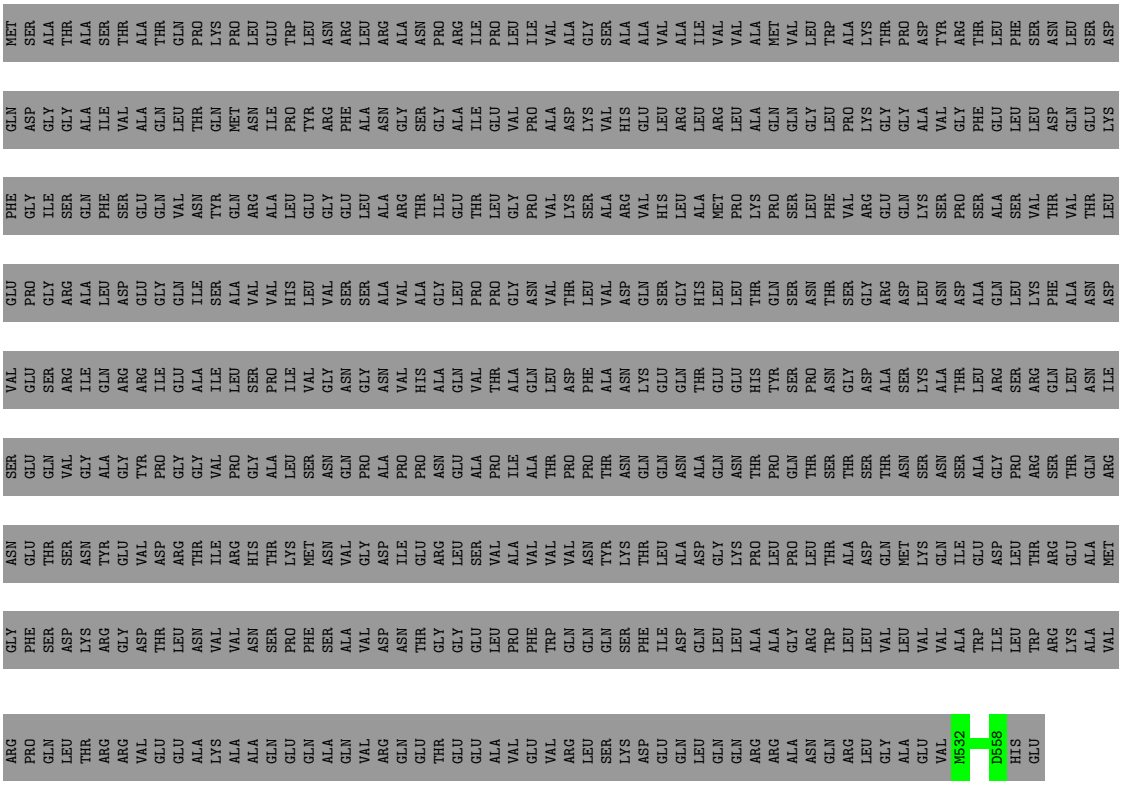
• Molecule 6: Flagellar M-ring protein

Chain DR: 5% 95%



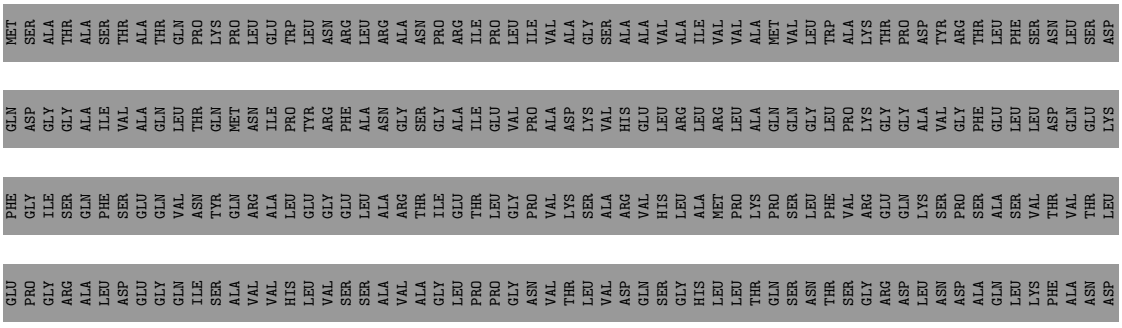
• Molecule 6: Flagellar M-ring protein

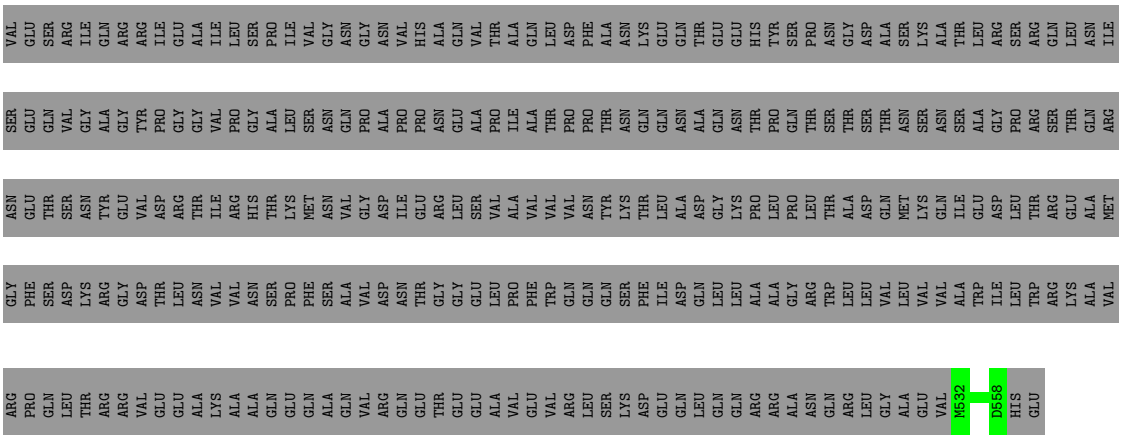
Chain DX: 5% 95%



• Molecule 6: Flagellar M-ring protein

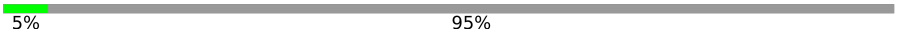
Chain Dd: 5% 95%

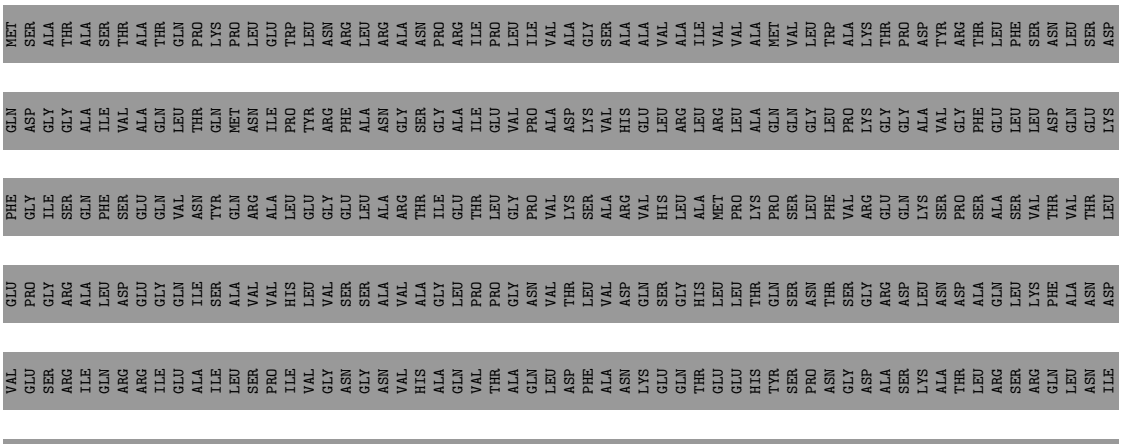




• Molecule 6: Flagellar M-ring protein

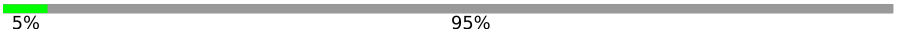
Chain Dj:

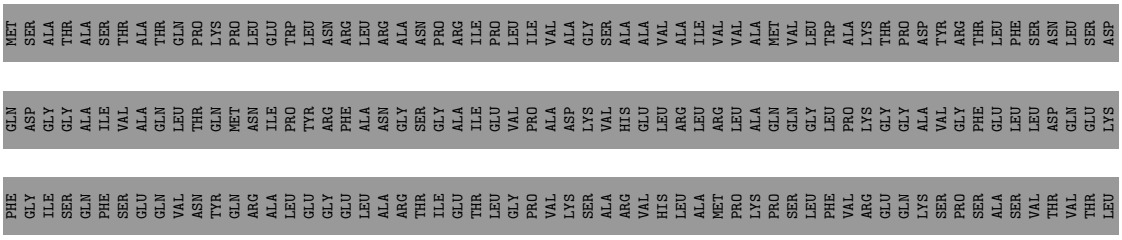


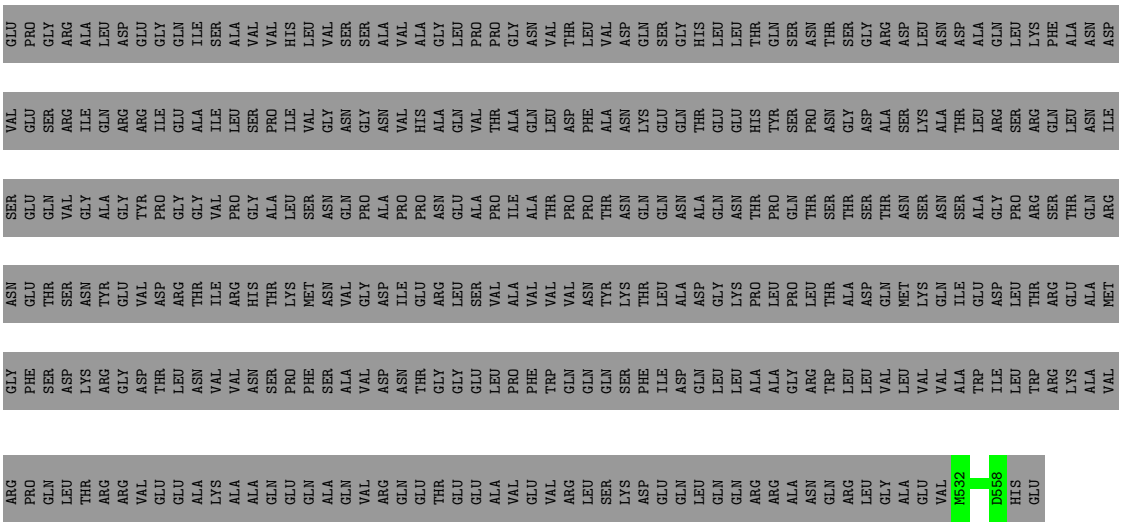


• Molecule 6: Flagellar M-ring protein

Chain Dp:

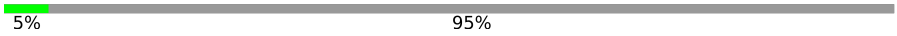


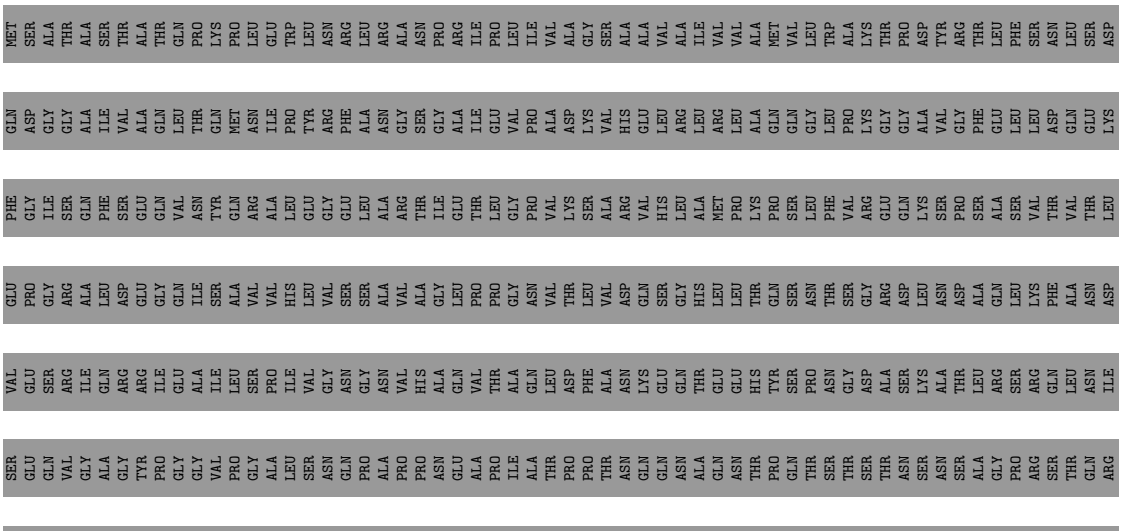




• Molecule 6: Flagellar M-ring protein

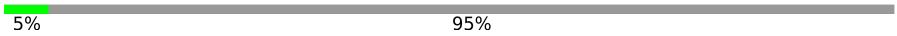
Chain Dv:

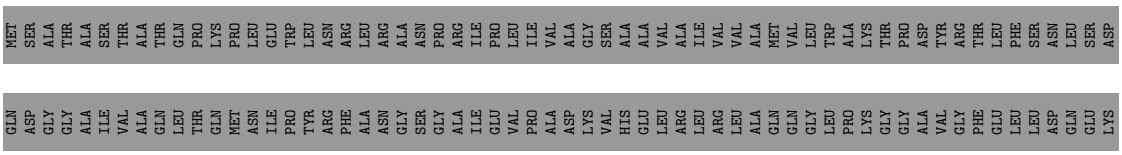




• Molecule 6: Flagellar M-ring protein

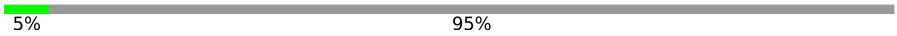
Chain D2:

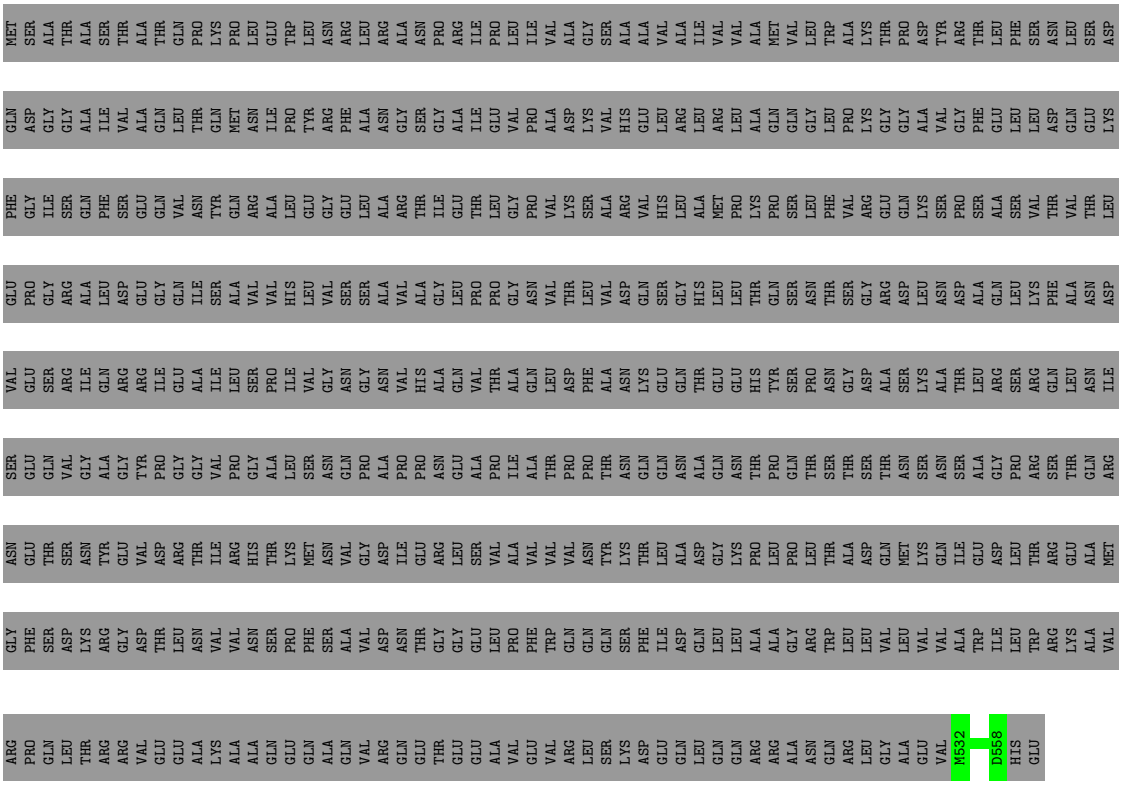




• Molecule 6: Flagellar M-ring protein

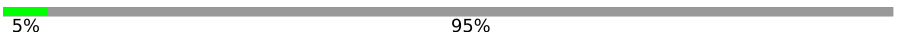
Chain D8:

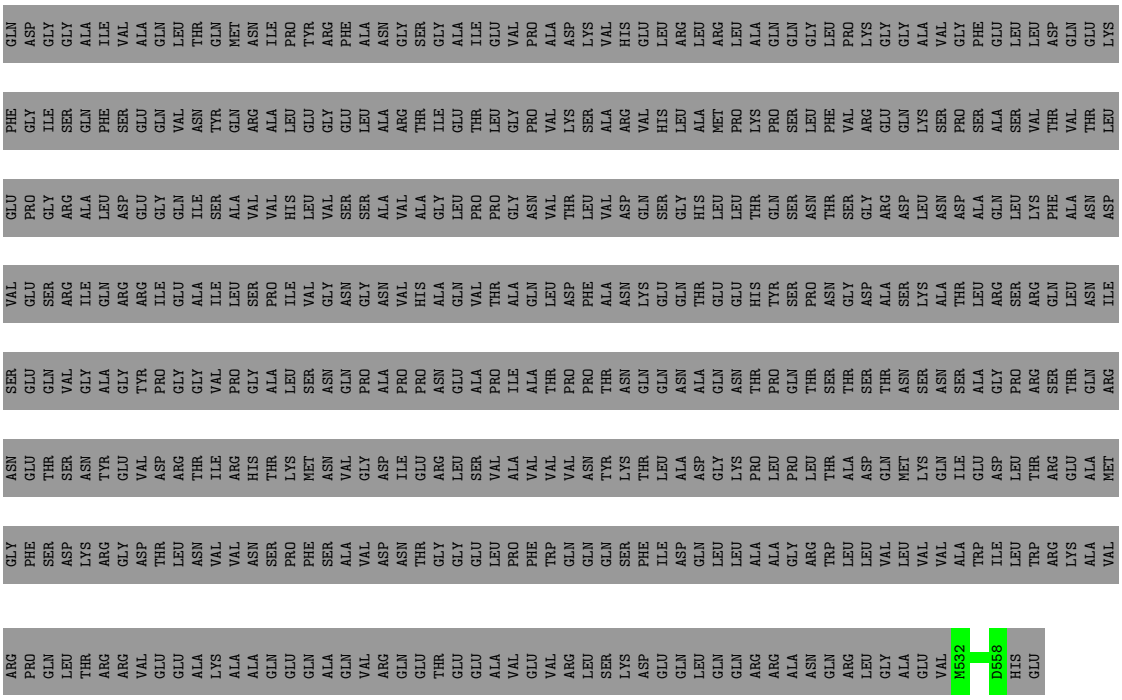




• Molecule 6: Flagellar M-ring protein

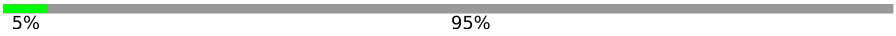
Chain B6:

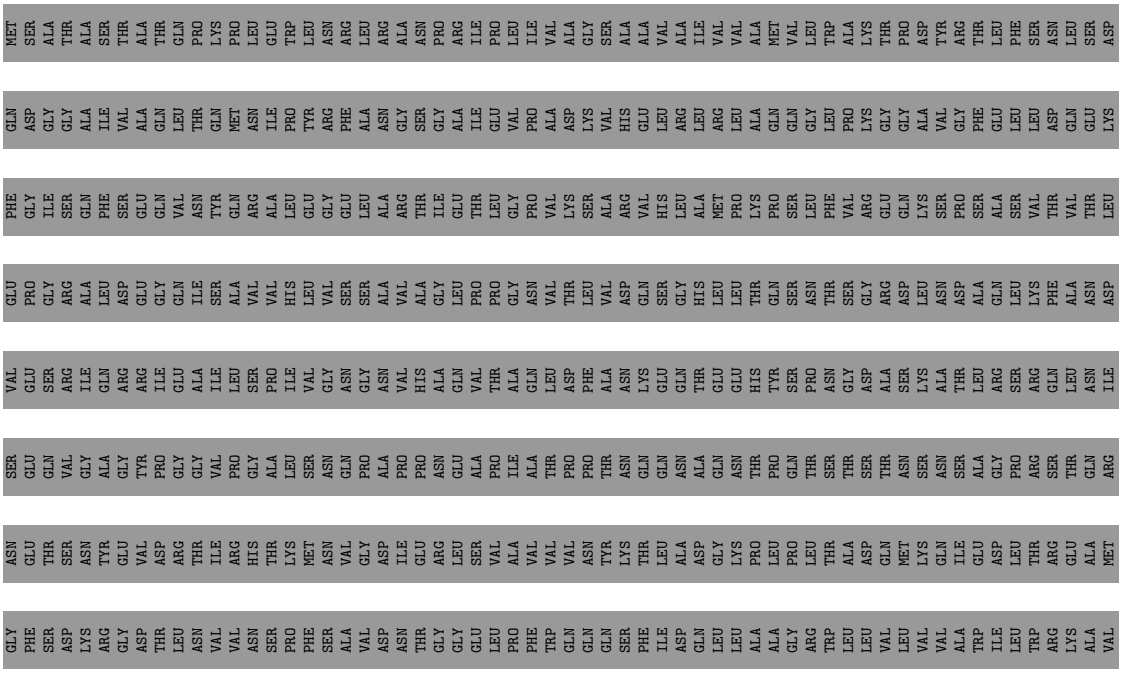




• Molecule 6: Flagellar M-ring protein

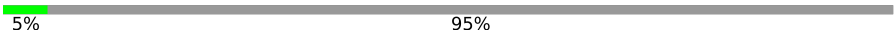
Chain EF:

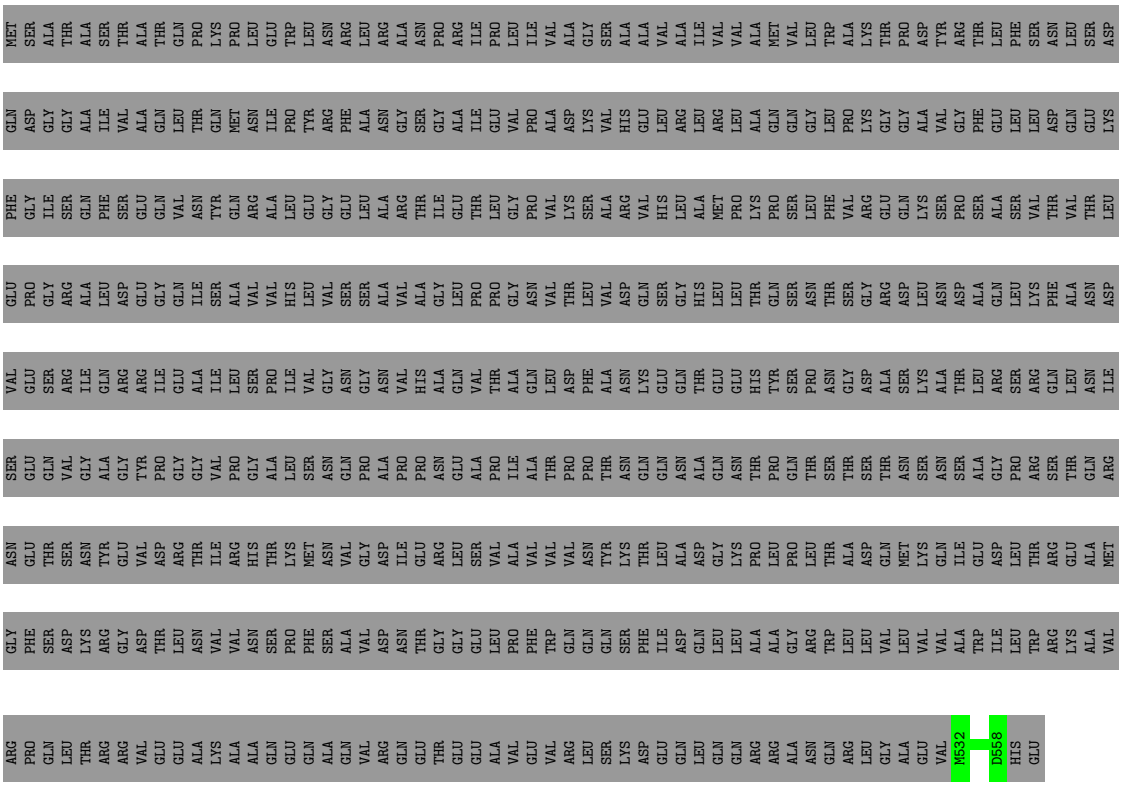




• Molecule 6: Flagellar M-ring protein

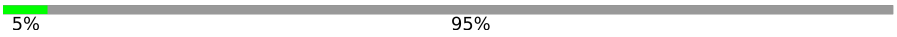
Chain EL:

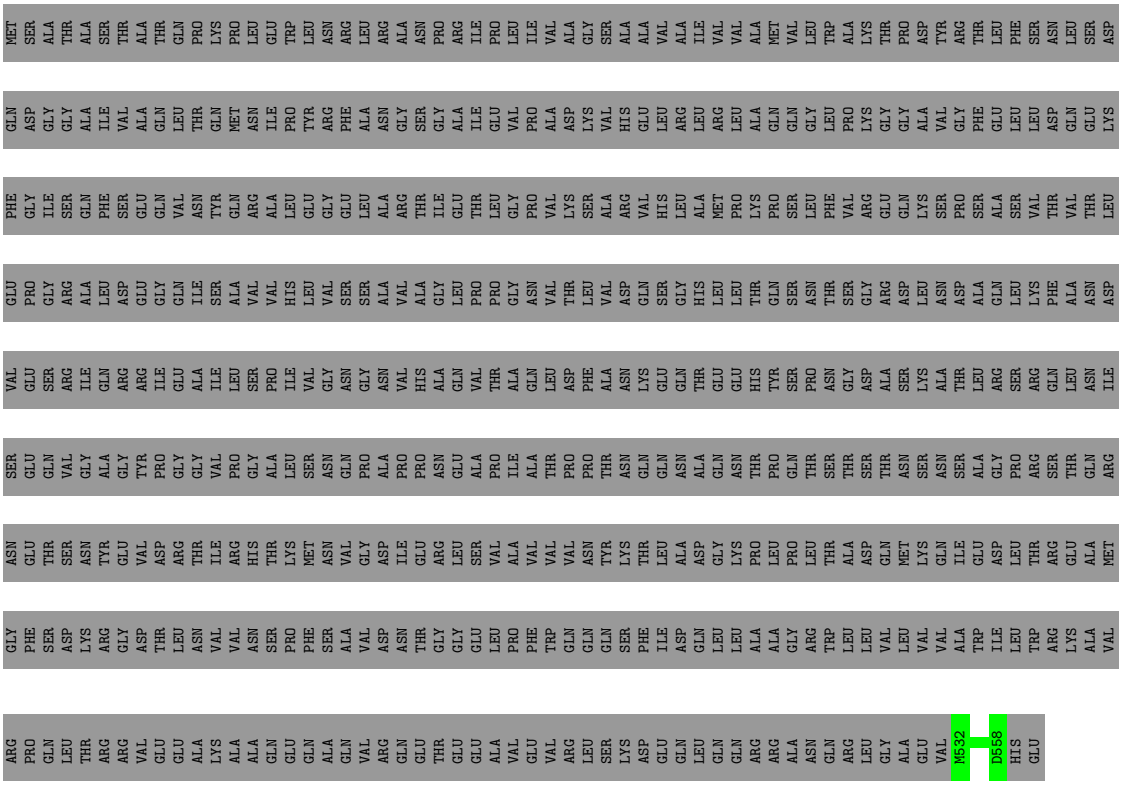




• Molecule 6: Flagellar M-ring protein

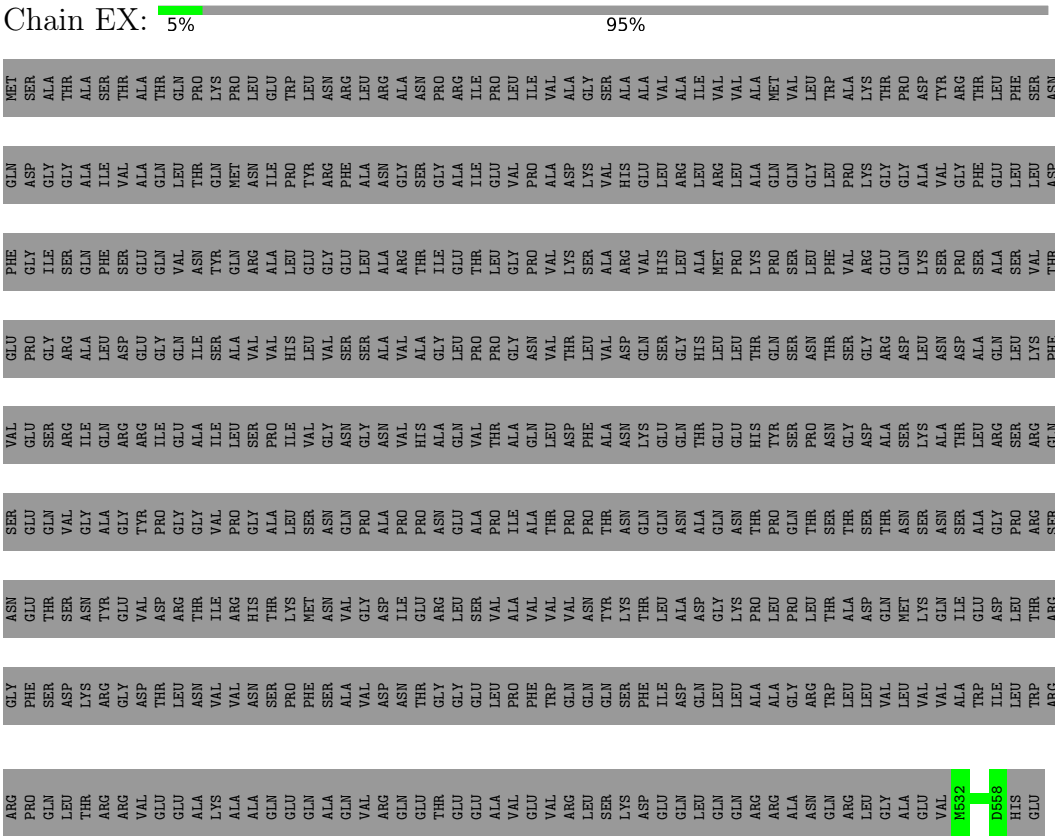
Chain ER:





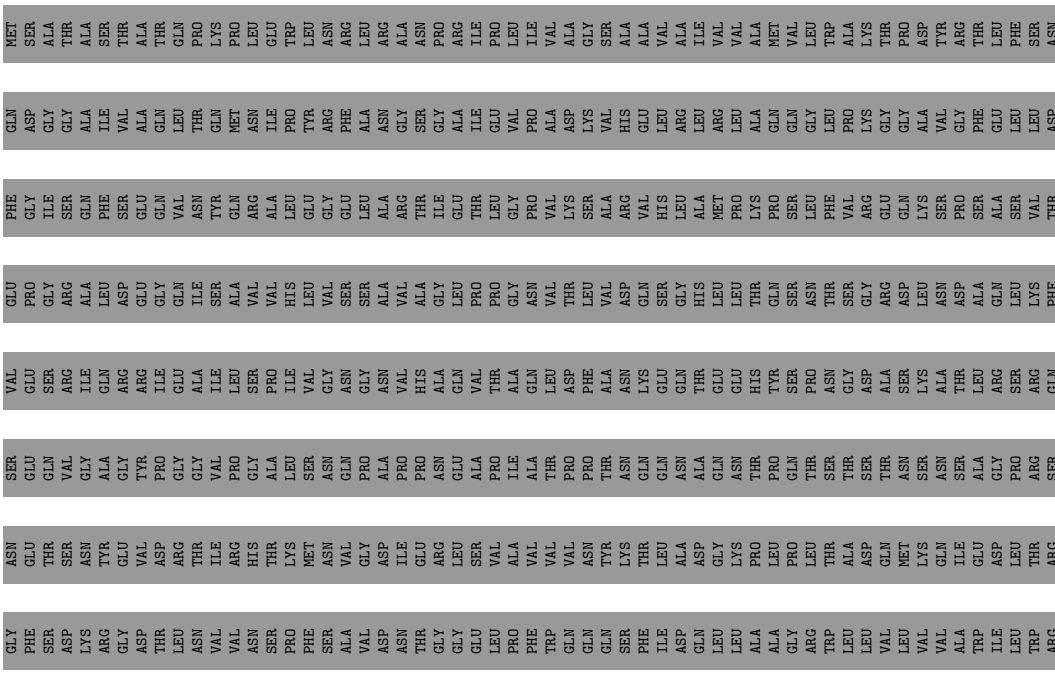
• Molecule 6: Flagellar M-ring protein

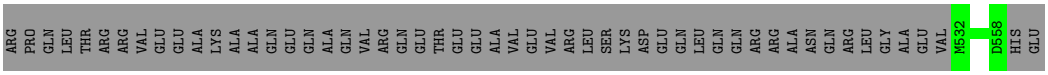
Chain EX:



• Molecule 6: Flagellar M-ring protein

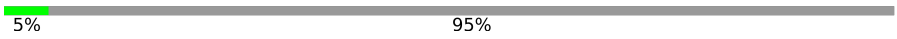
Chain Bb:

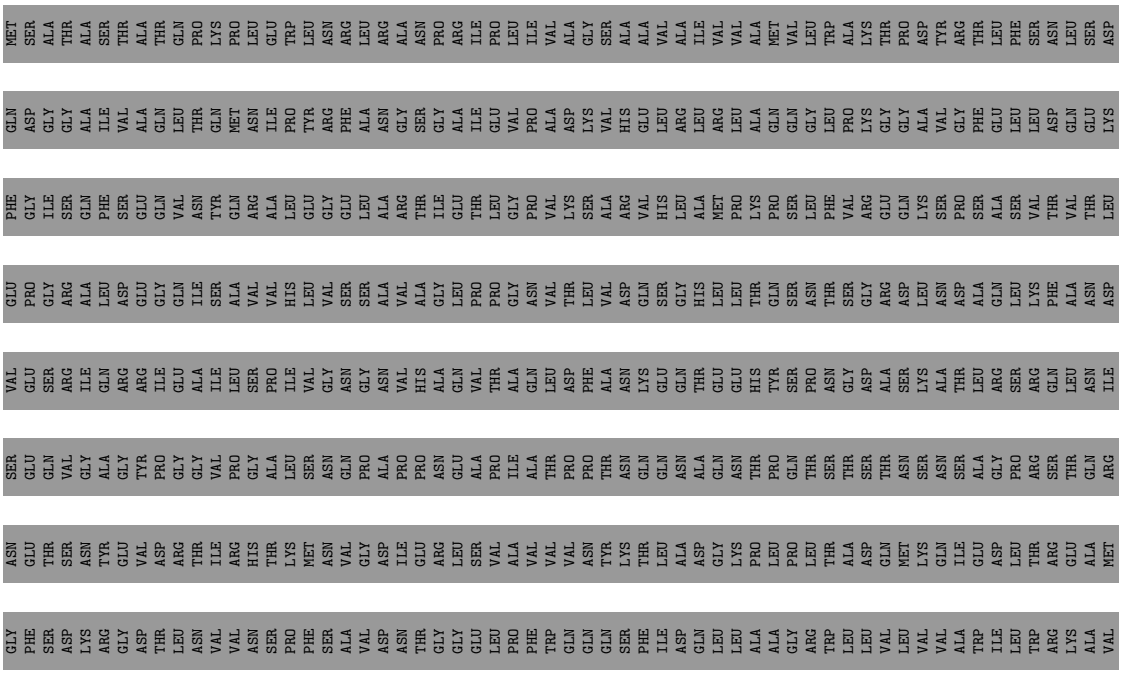




• Molecule 6: Flagellar M-ring protein

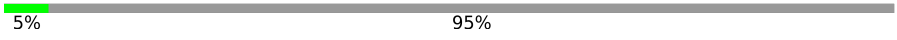
Chain Bh:

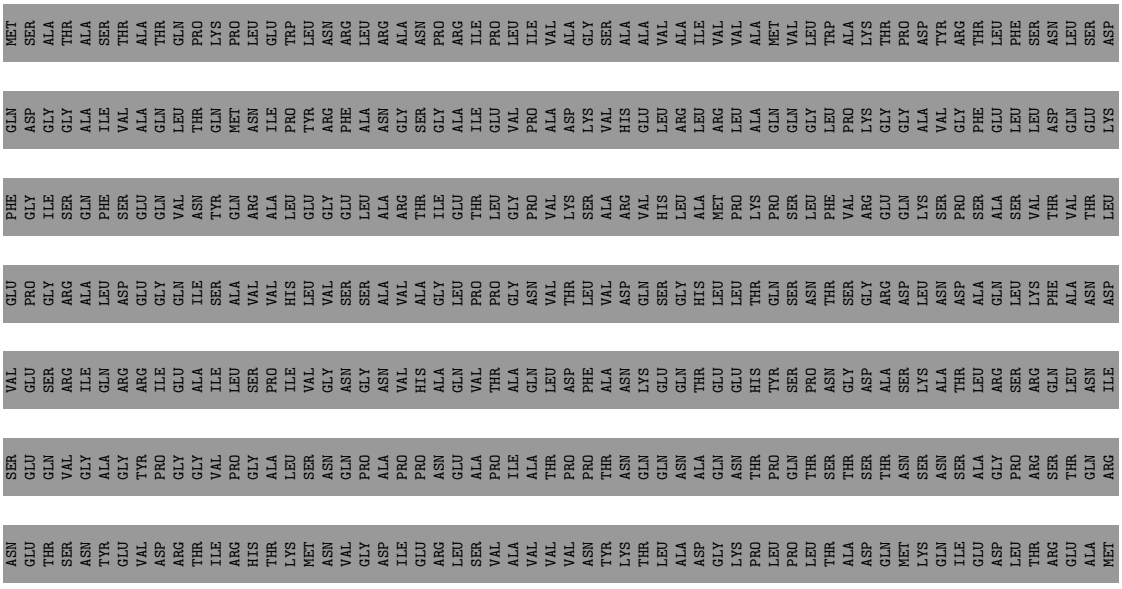


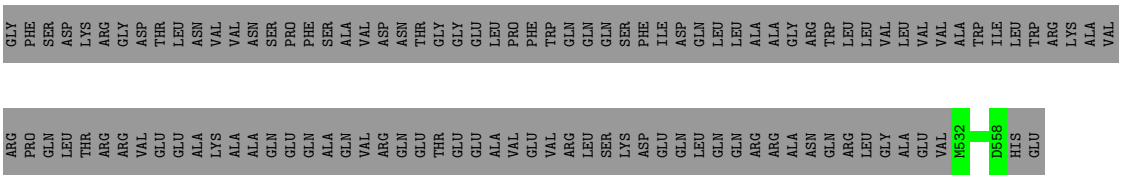


• Molecule 6: Flagellar M-ring protein

Chain Bn:

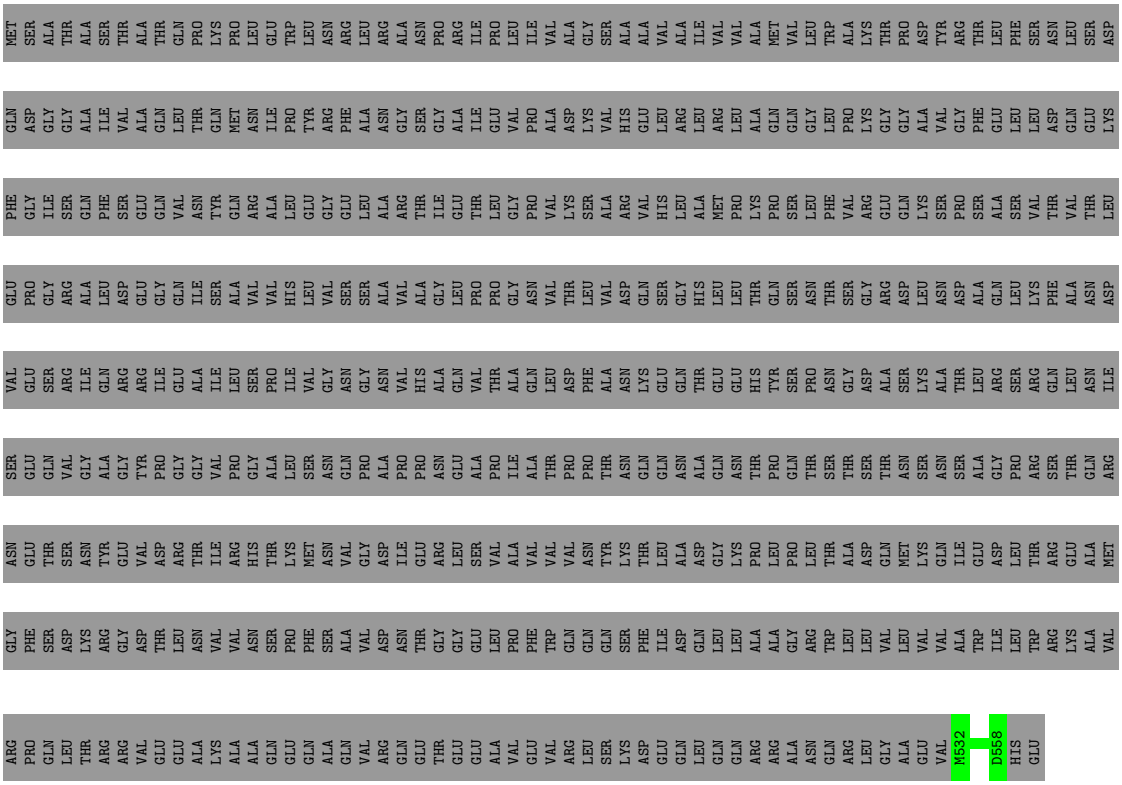






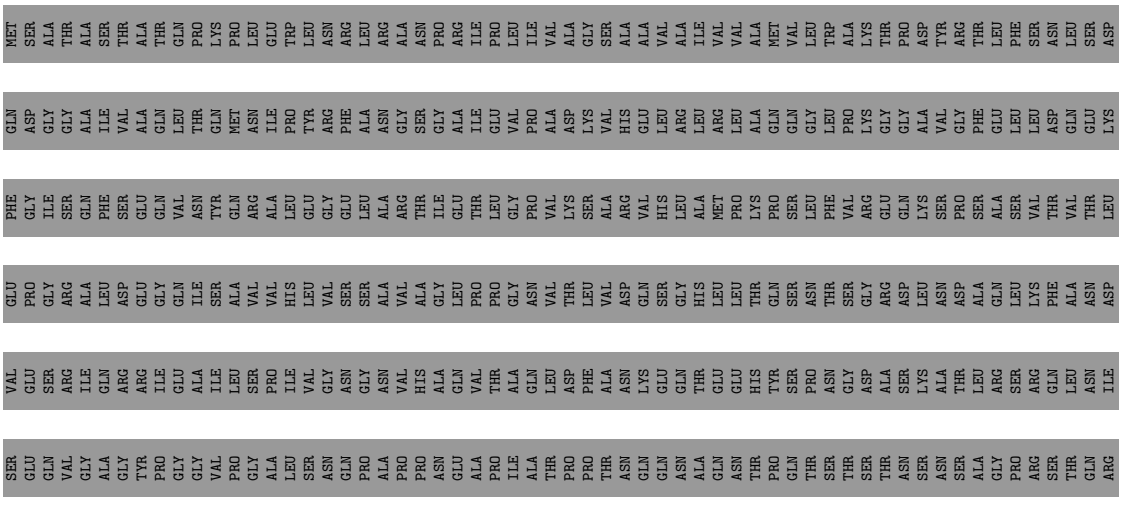
• Molecule 6: Flagellar M-ring protein

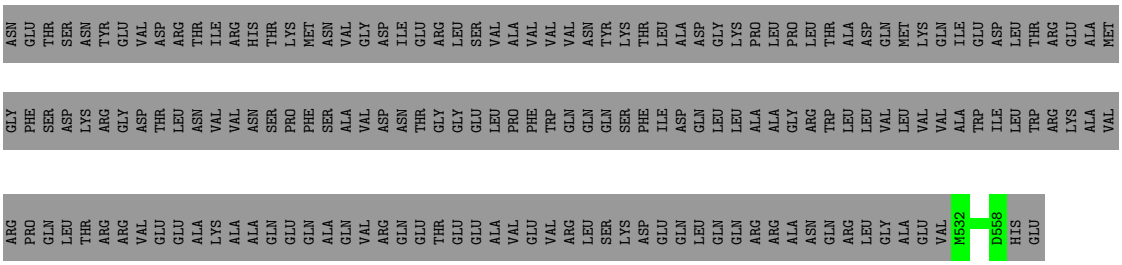
Chain Bt: 5% 95%



• Molecule 6: Flagellar M-ring protein

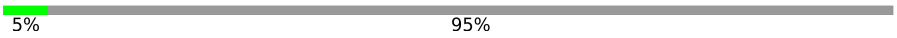
Chain Bz: 5% 95%

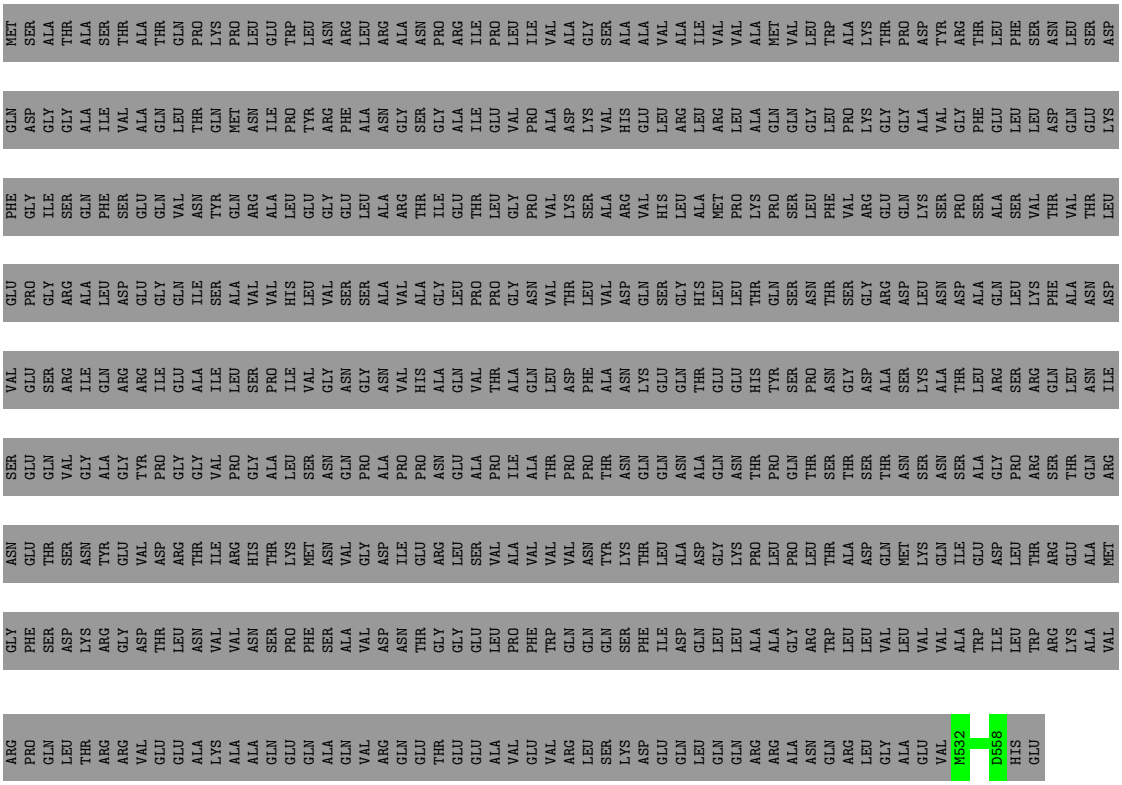




• Molecule 6: Flagellar M-ring protein

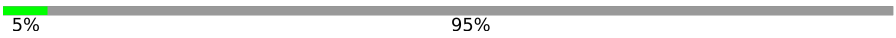
Chain CB:

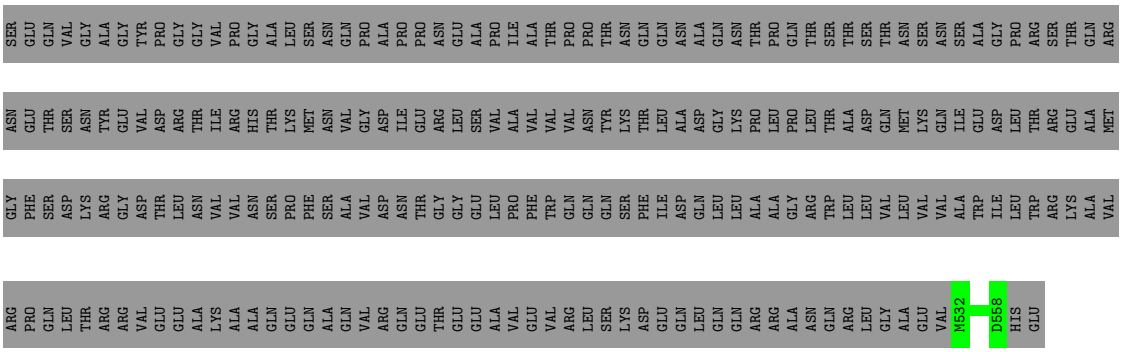




• Molecule 6: Flagellar M-ring protein

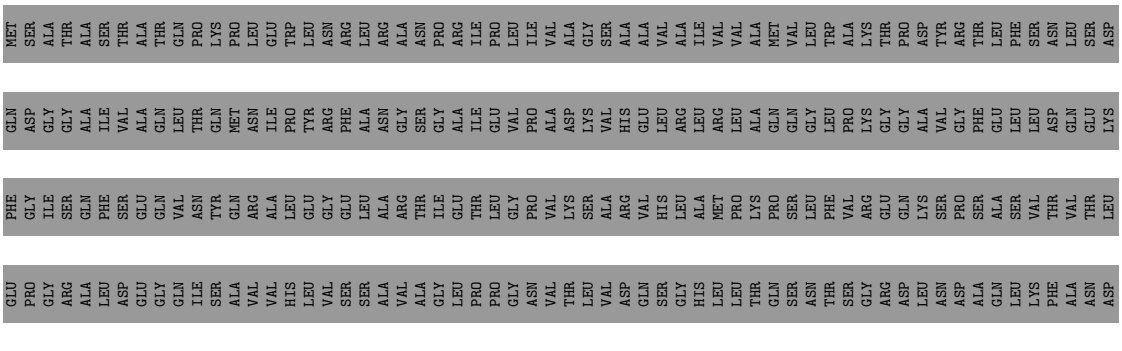
Chain CH:





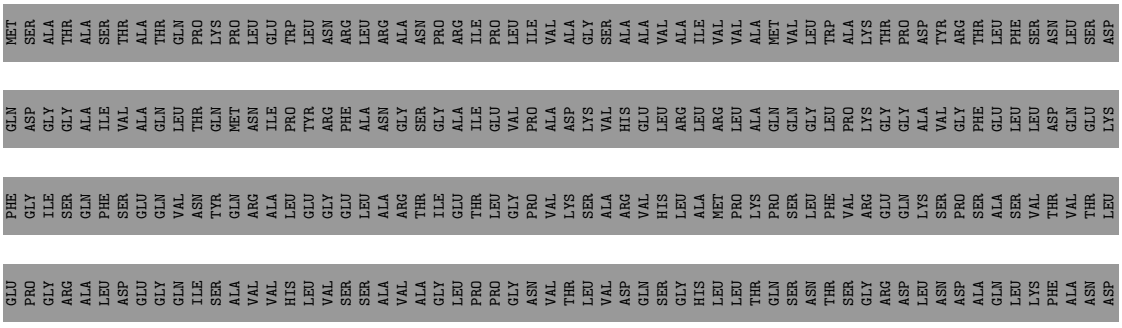
• Molecule 6: Flagellar M-ring protein

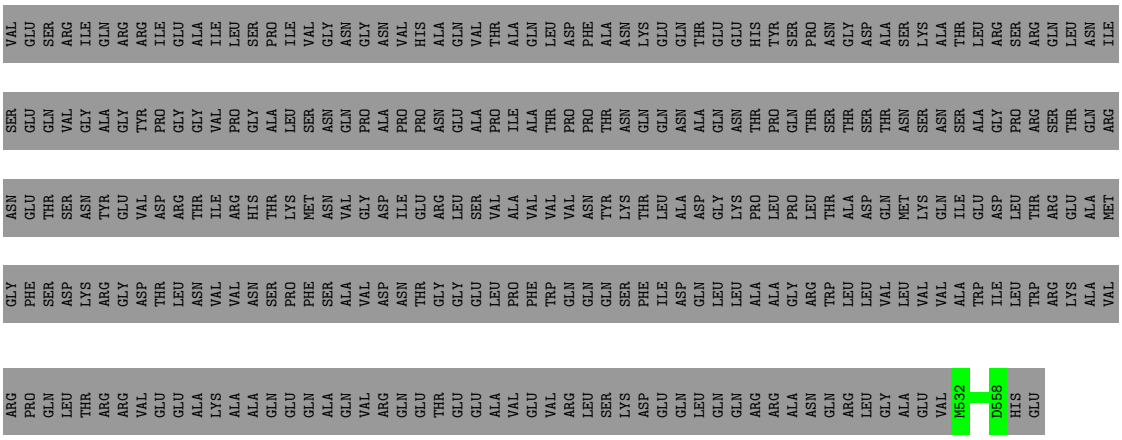
Chain CN: 5% 95%



• Molecule 6: Flagellar M-ring protein

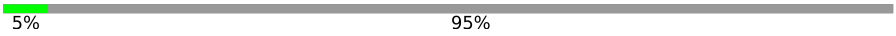
Chain CT: 5% 95%





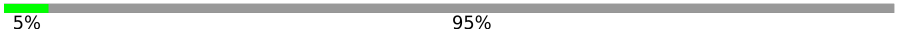
• Molecule 6: Flagellar M-ring protein

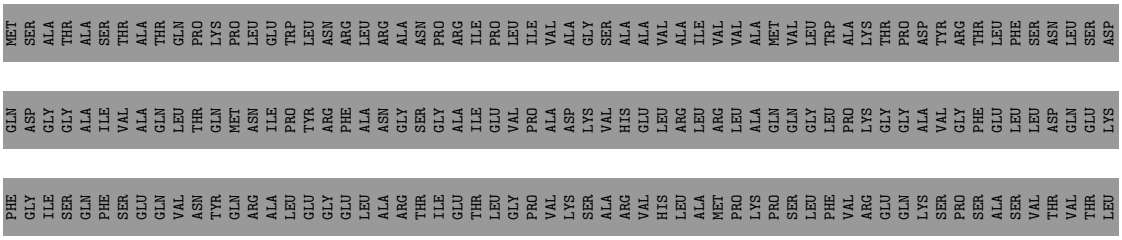
Chain CZ:

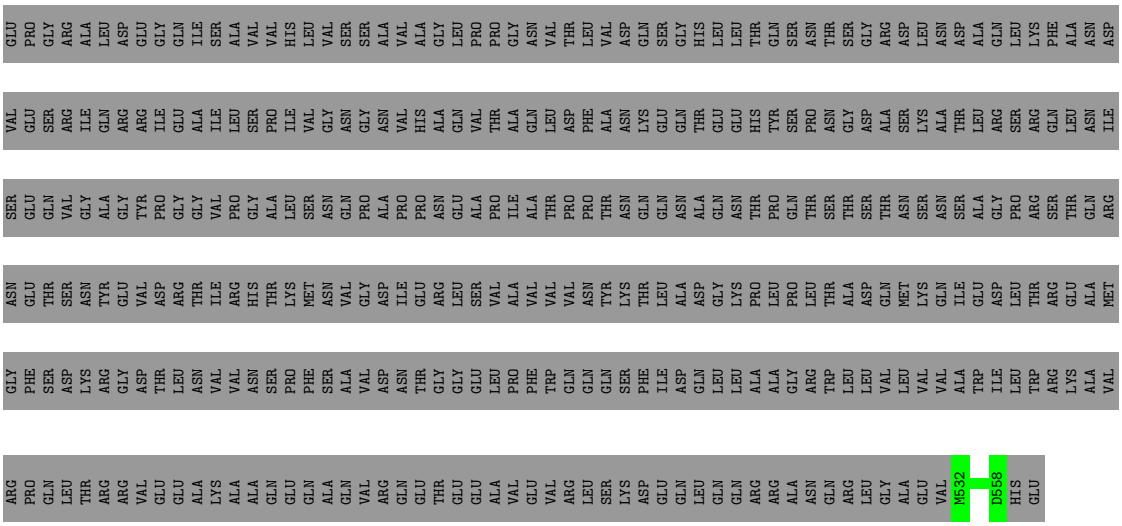


• Molecule 6: Flagellar M-ring protein

Chain Cf:

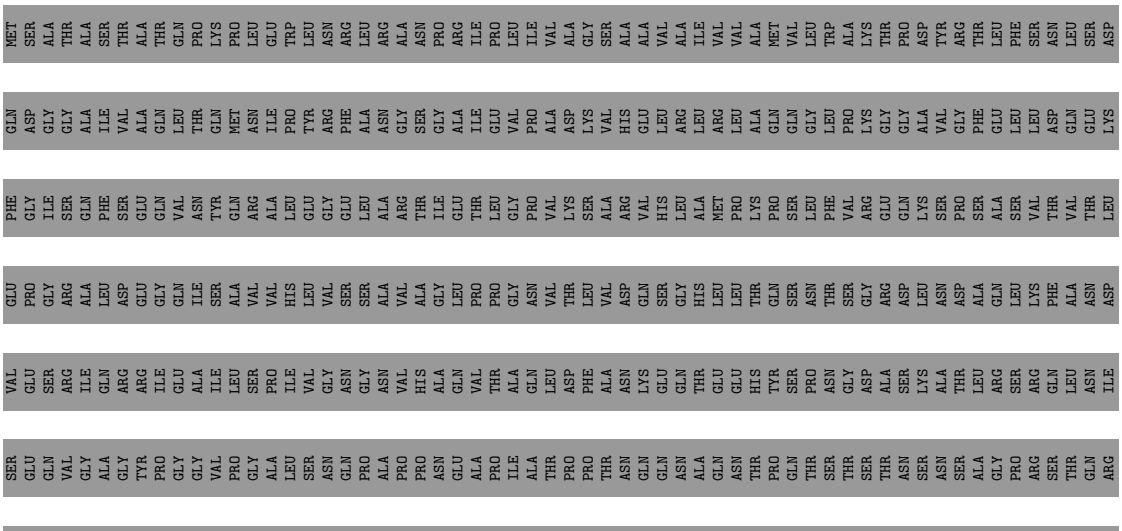






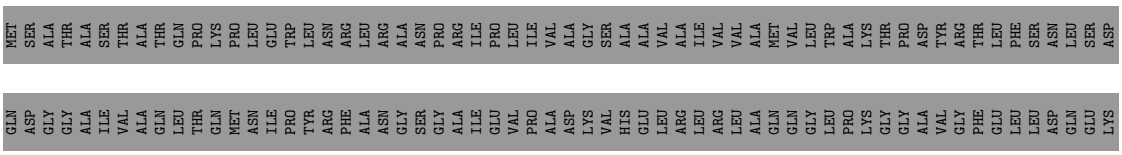
• Molecule 6: Flagellar M-ring protein

Chain Cl: 5% 95%



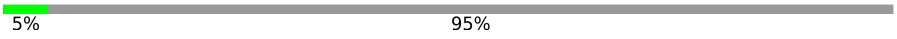
• Molecule 6: Flagellar M-ring protein

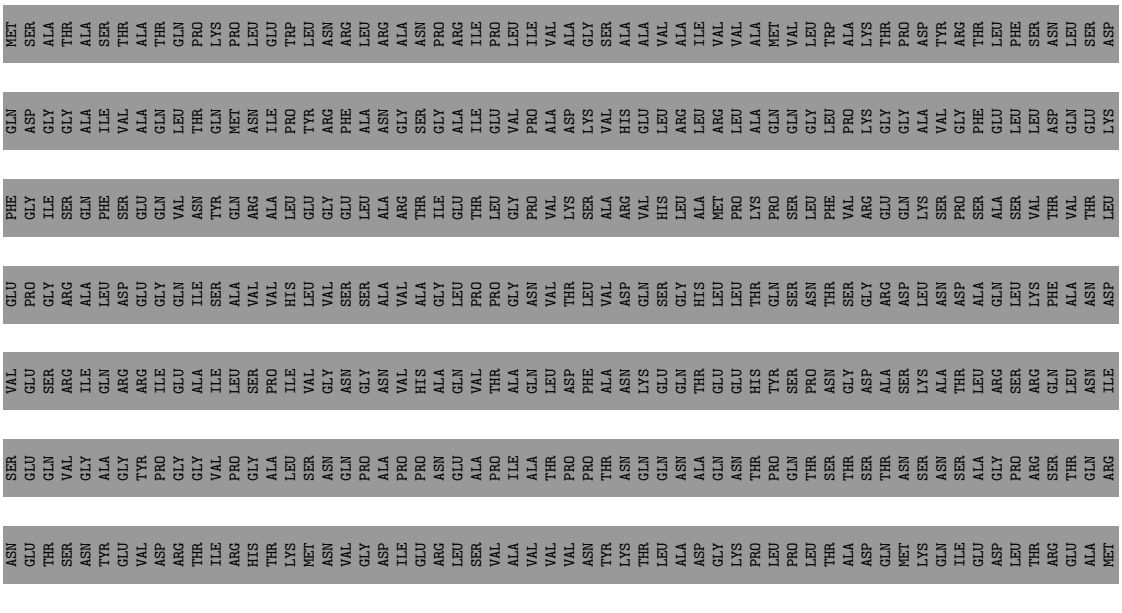
Chain Cr: 5% 95%



• Molecule 6: Flagellar M-ring protein

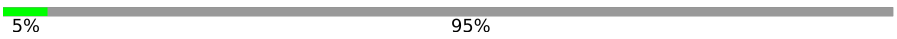
Chain Cx:

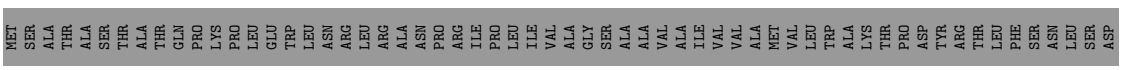


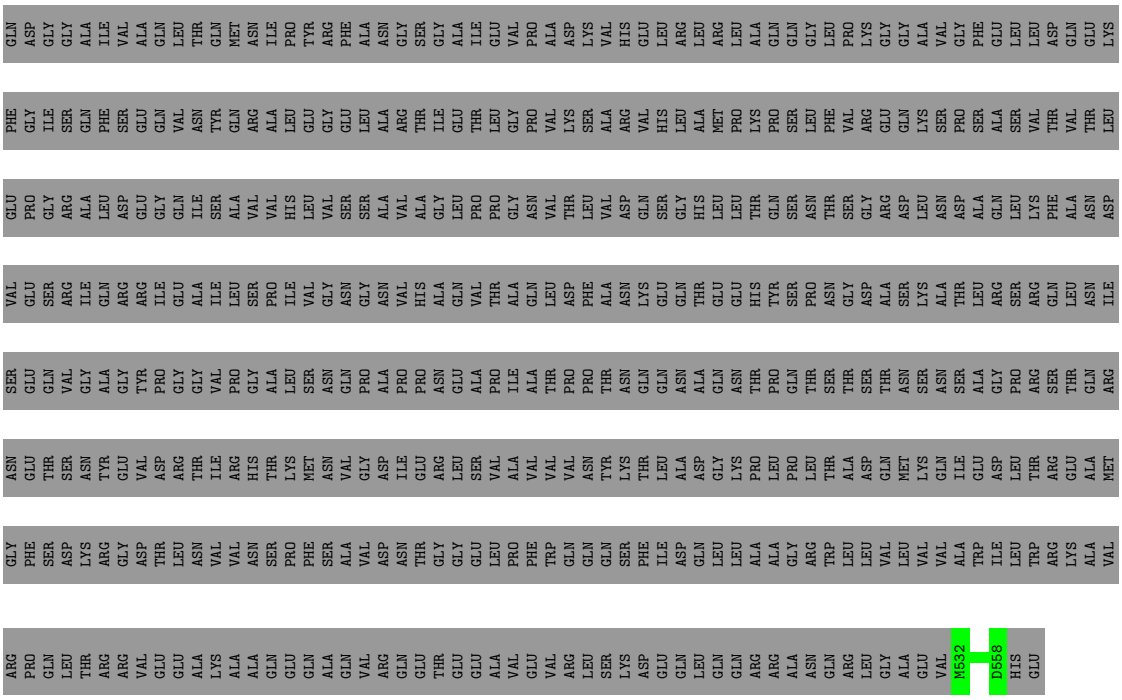


• Molecule 6: Flagellar M-ring protein

Chain Eb:







• Molecule 6: Flagellar M-ring protein

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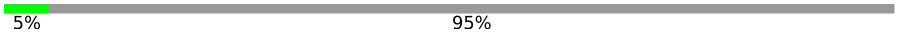

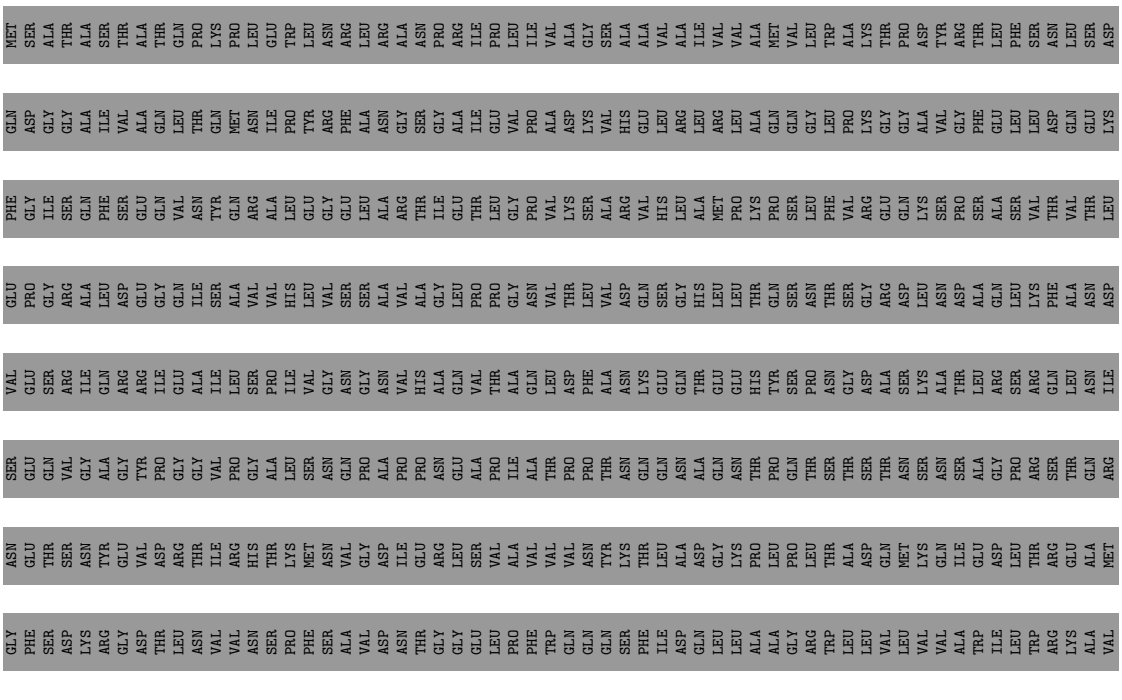

• Molecule 6: Flagellar M-ring protein

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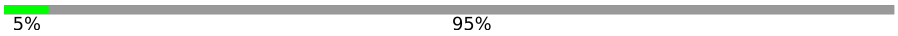

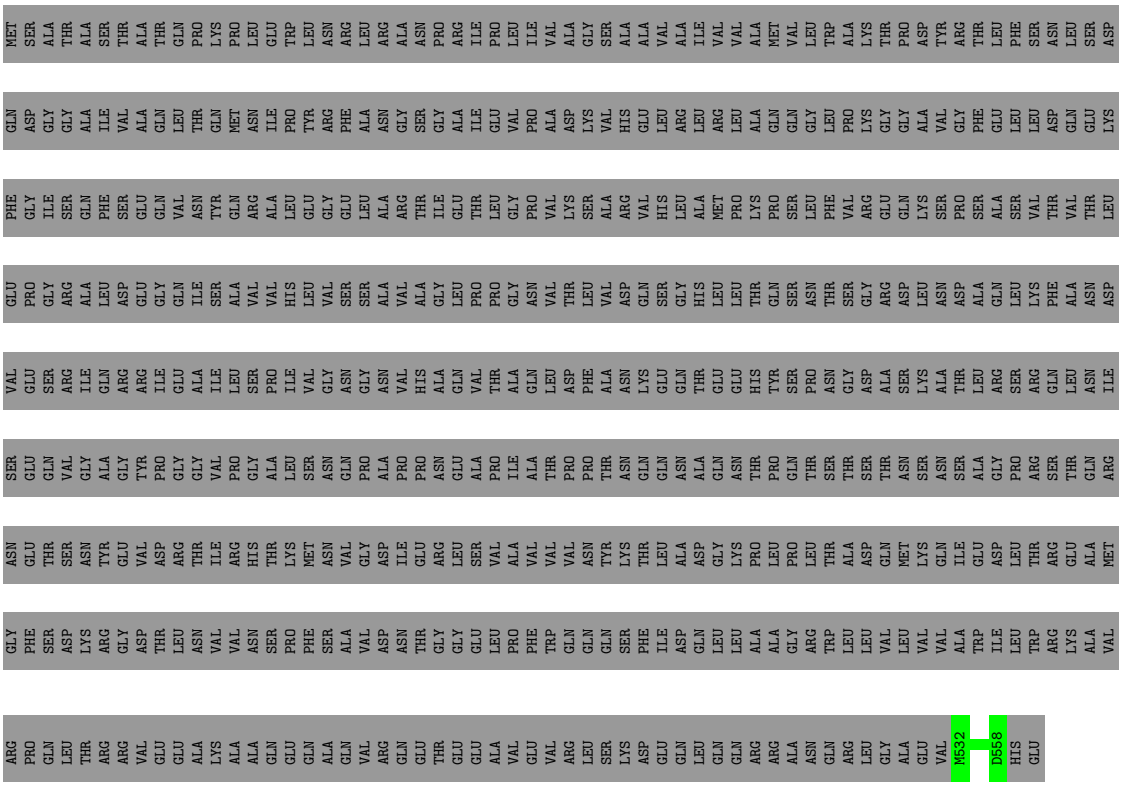

• Molecule 7: Flagellar biosynthetic protein FliQ

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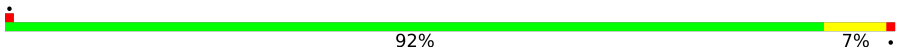

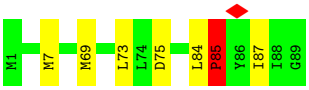

• Molecule 7: Flagellar biosynthetic protein FliQ

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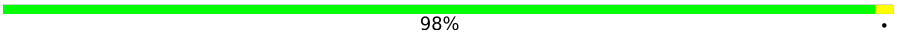

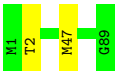

• Molecule 7: Flagellar biosynthetic protein FliQ

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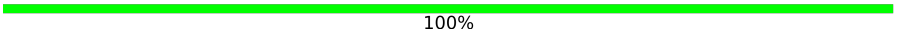
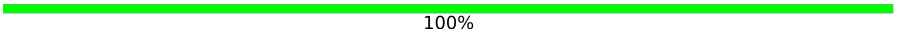


There are no outlier residues recorded for this chain.

• Molecule 7: Flagellar biosynthetic protein FliQ

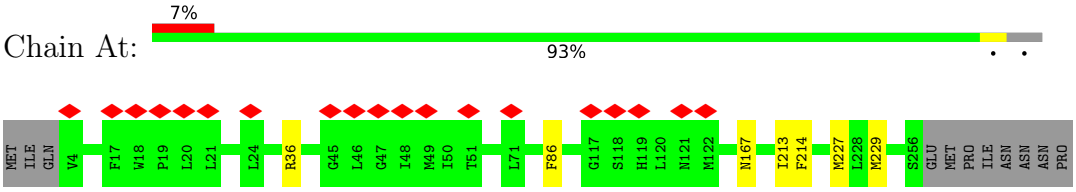
Chain As:



There are no outlier residues recorded for this chain.

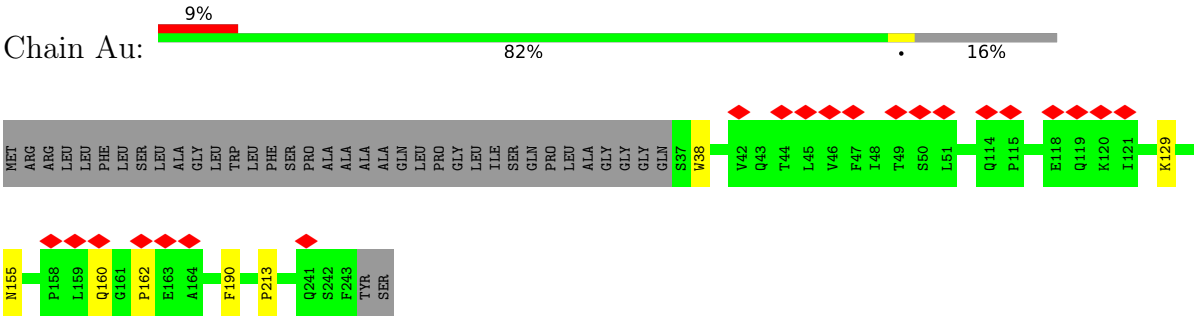
• Molecule 8: Flagellar biosynthetic protein FliR

Chain At:



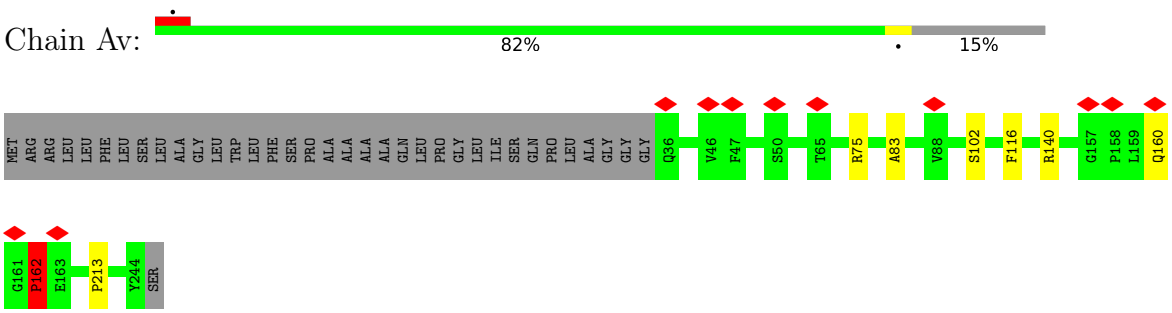
• Molecule 9: Flagellar biosynthetic protein FliP

Chain Au:



• Molecule 9: Flagellar biosynthetic protein FliP

Chain Av:



• Molecule 9: Flagellar biosynthetic protein FliP

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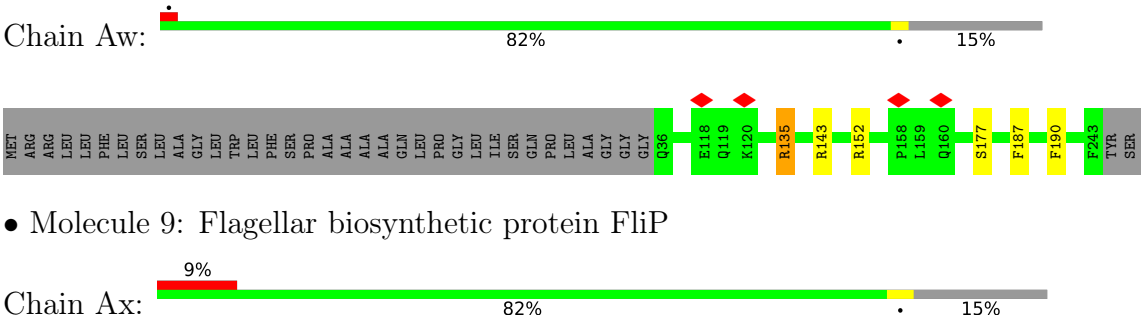

• Molecule 9: Flagellar biosynthetic protein FliP

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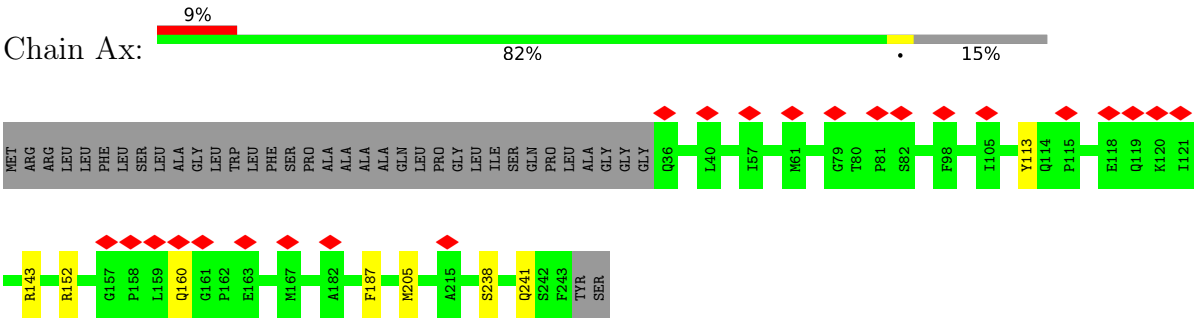

• Molecule 9: Flagellar biosynthetic protein FliP

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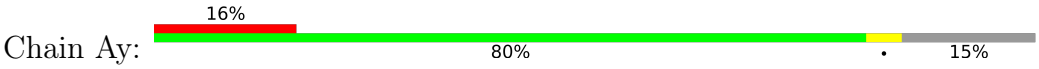
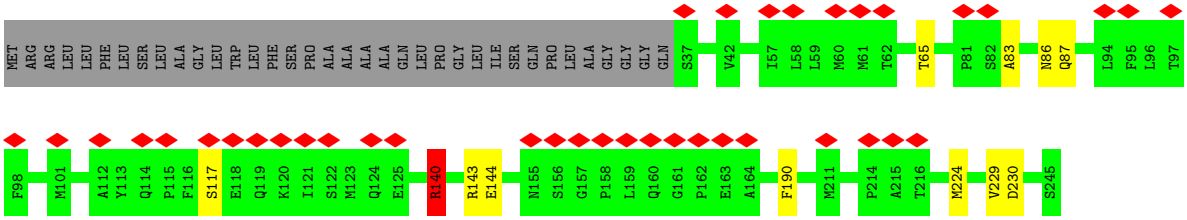
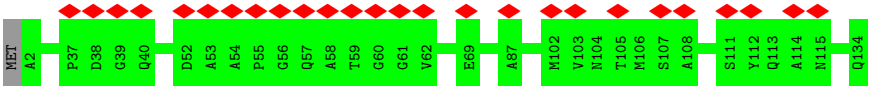
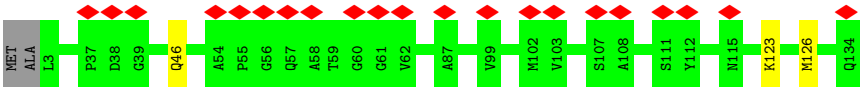




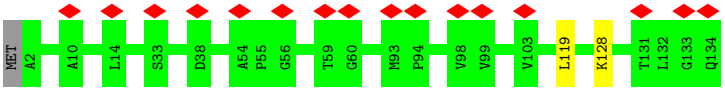
• Molecule 10: Flagellar basal-body rod protein FlgC



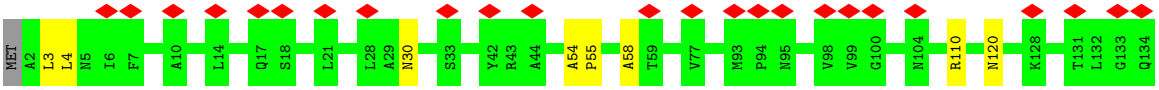
• Molecule 10: Flagellar basal-body rod protein FlgC



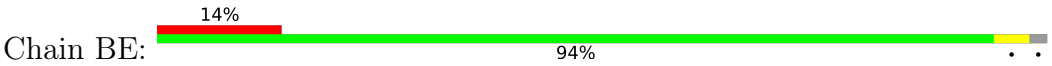
• Molecule 10: Flagellar basal-body rod protein FlgC

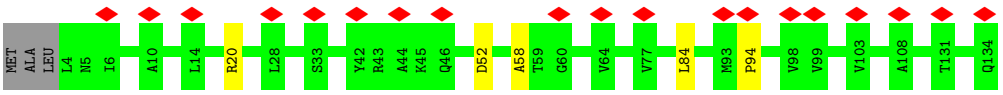


• Molecule 10: Flagellar basal-body rod protein FlgC

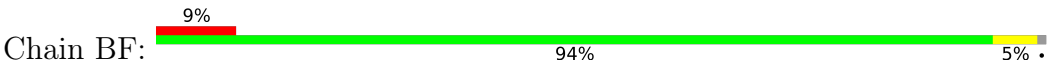


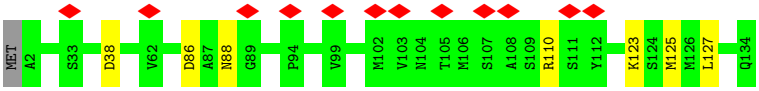
• Molecule 10: Flagellar basal-body rod protein FlgC





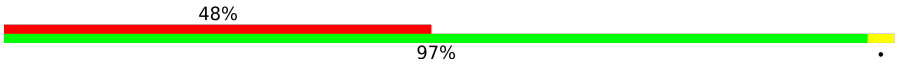
• Molecule 10: Flagellar basal-body rod protein FlgC

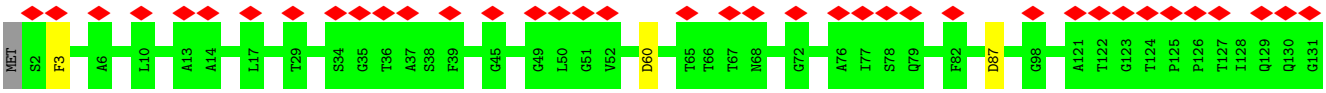


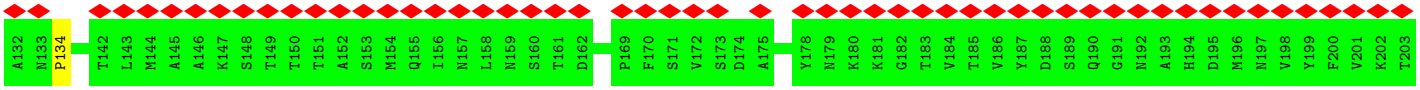


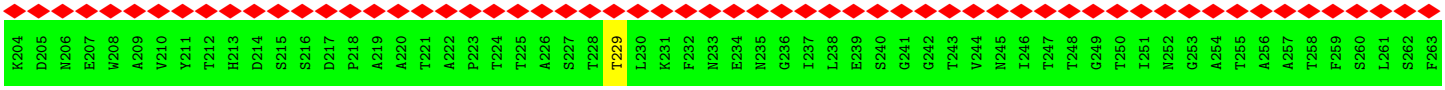
• Molecule 11: Flagellar hook protein FlgE

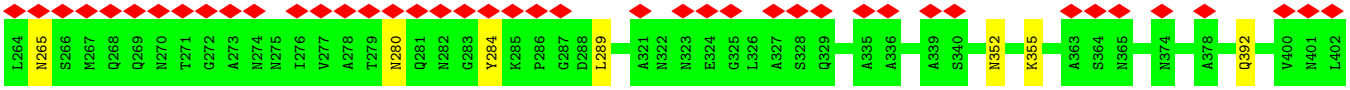
Chain ZF:





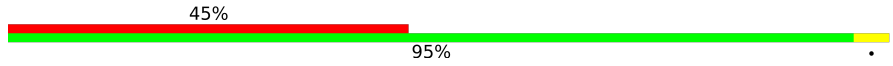


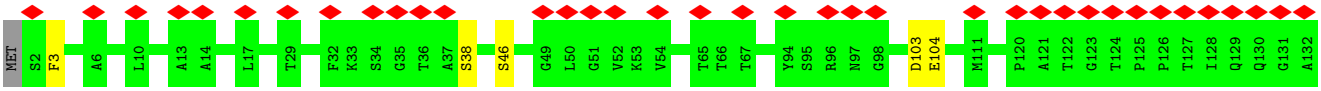


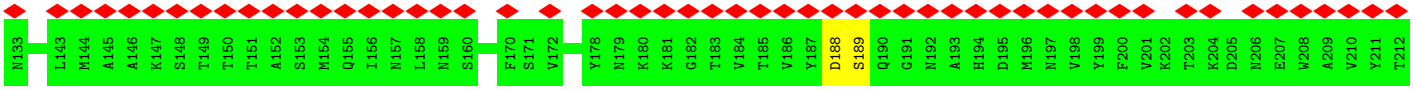


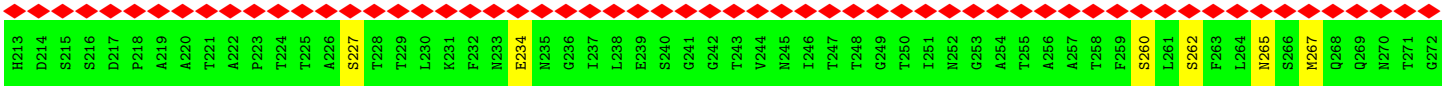
• Molecule 11: Flagellar hook protein FlgE

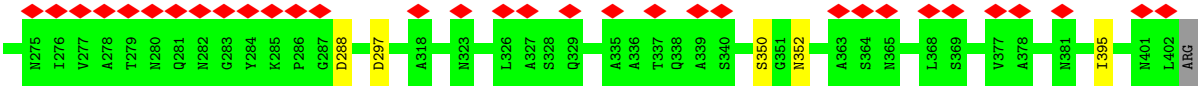
Chain ZG:





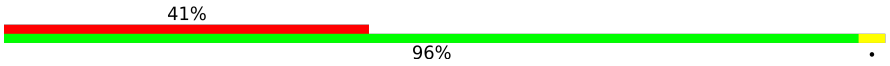


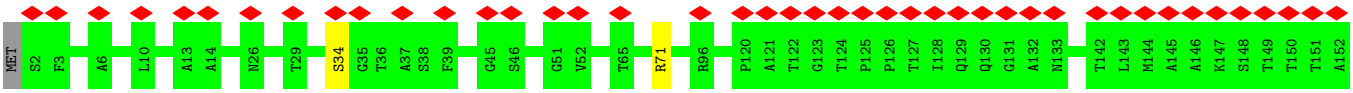


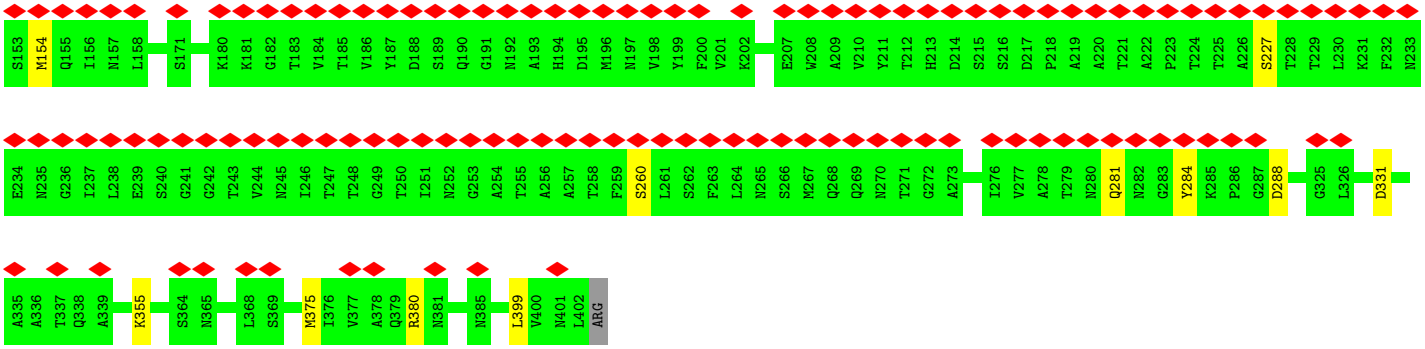


• Molecule 11: Flagellar hook protein FlgE

Chain ZH:

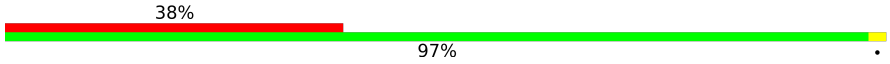


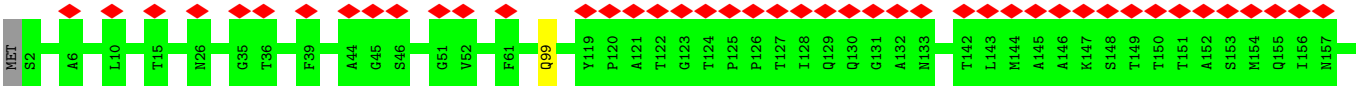


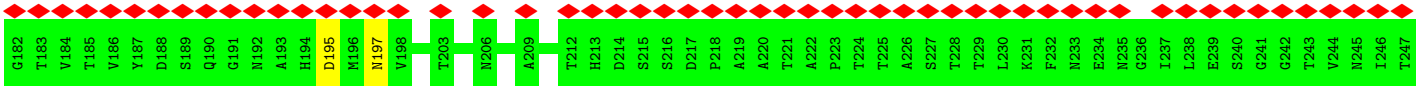


• Molecule 11: Flagellar hook protein FlgE

Chain ZI:

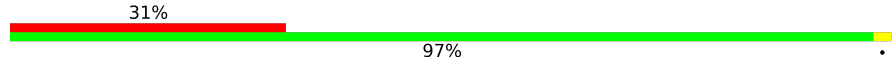


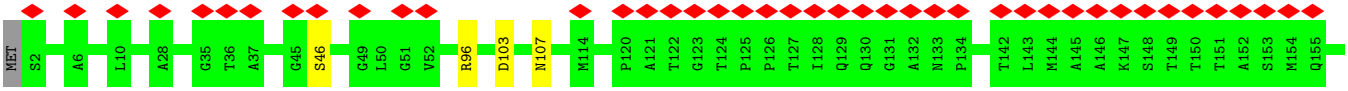


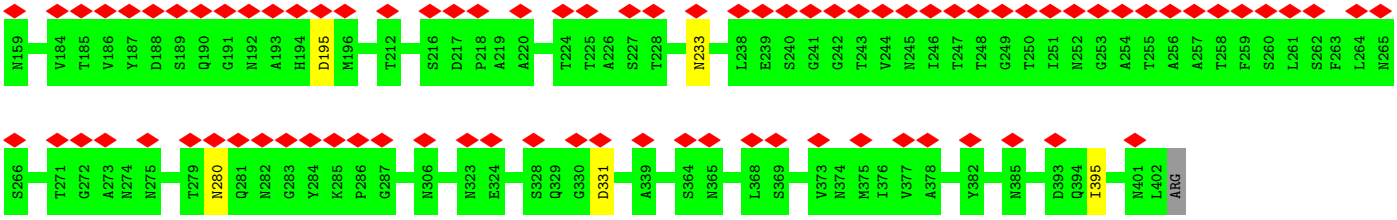


• Molecule 11: Flagellar hook protein FlgE

Chain ZJ:

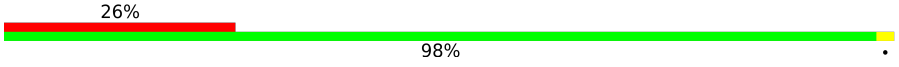


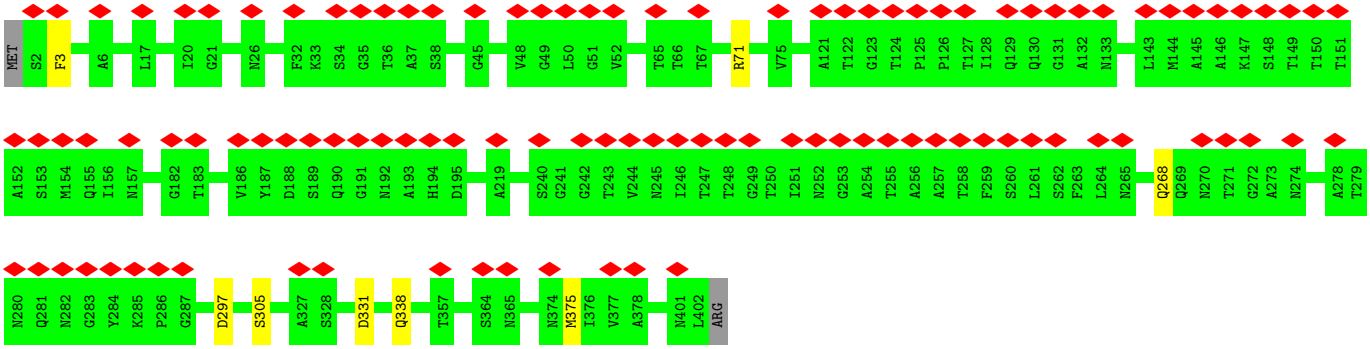




• Molecule 11: Flagellar hook protein FlgE

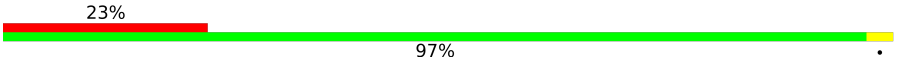
Chain ZK:

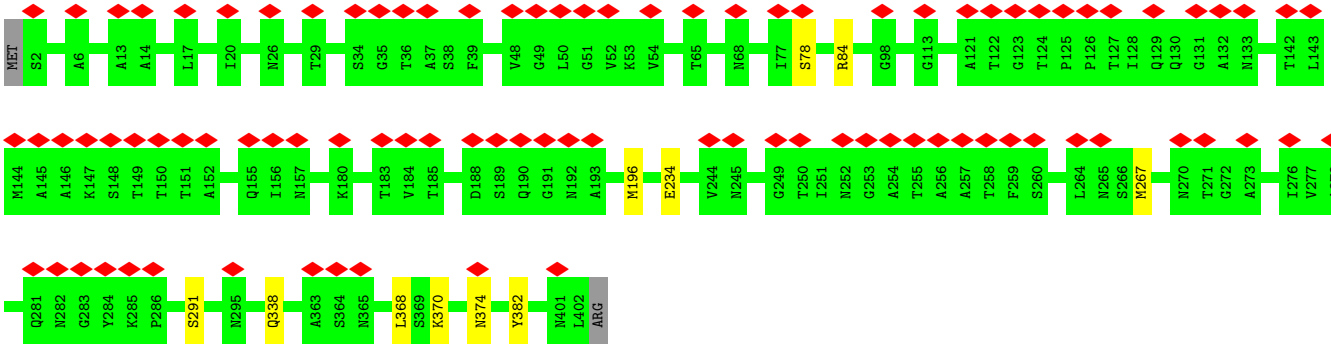




• Molecule 11: Flagellar hook protein FlgE

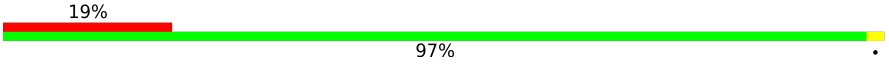
Chain ZL:

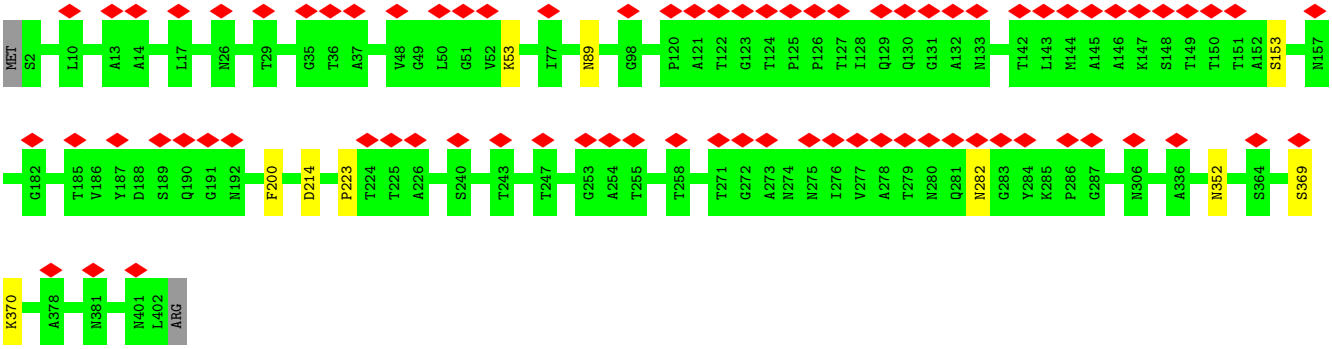




• Molecule 11: Flagellar hook protein FlgE

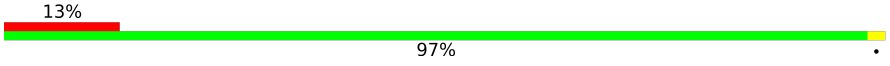
Chain ZM:

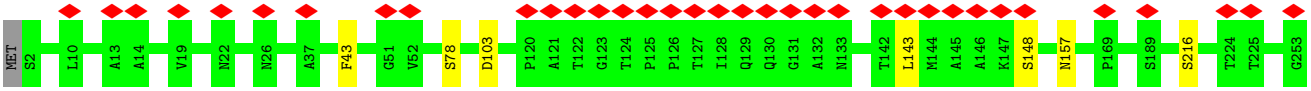


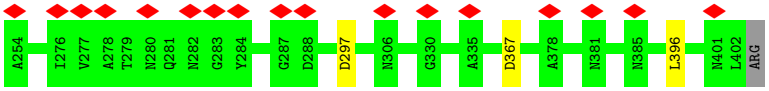


• Molecule 11: Flagellar hook protein FlgE

Chain ZN:

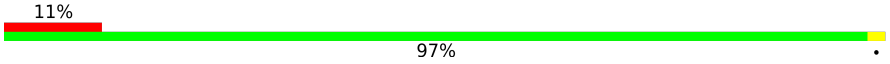


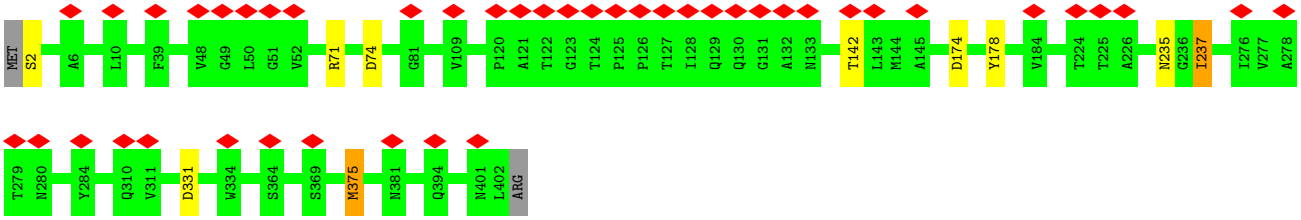




• Molecule 11: Flagellar hook protein FlgE

Chain ZO:





• Molecule 11: Flagellar hook protein FlgE

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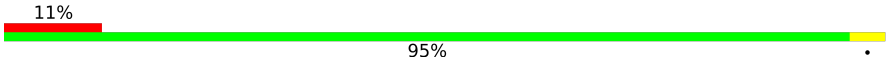
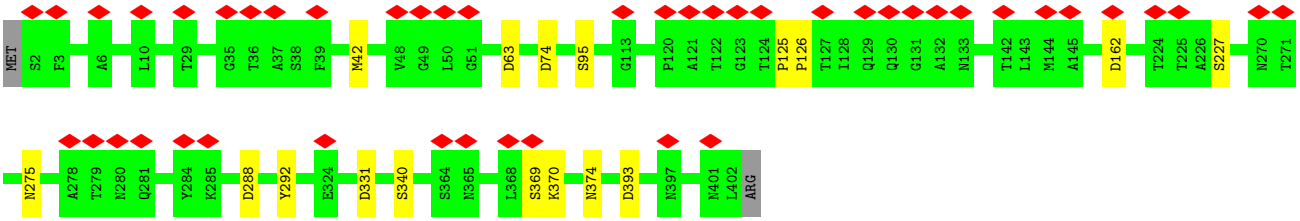
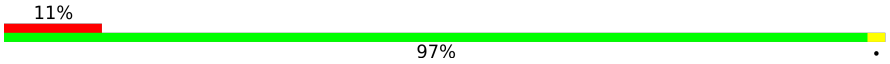
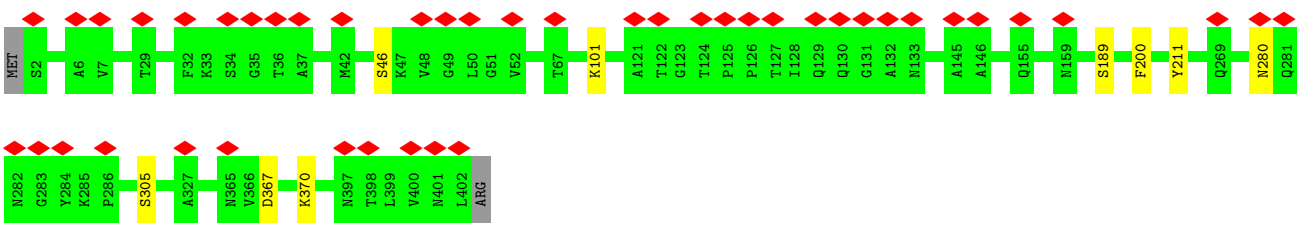




• Molecule 11: Flagellar hook protein FlgE

Chain ZQ:





• Molecule 11: Flagellar hook protein FlgE

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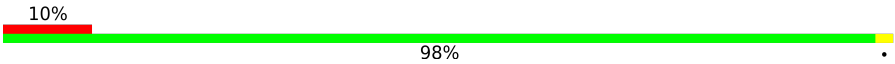
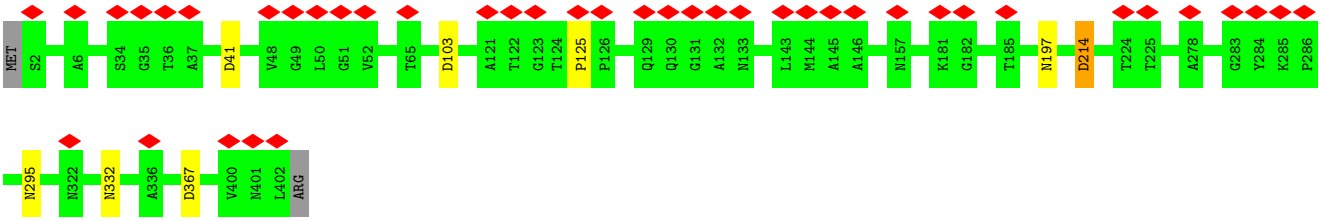
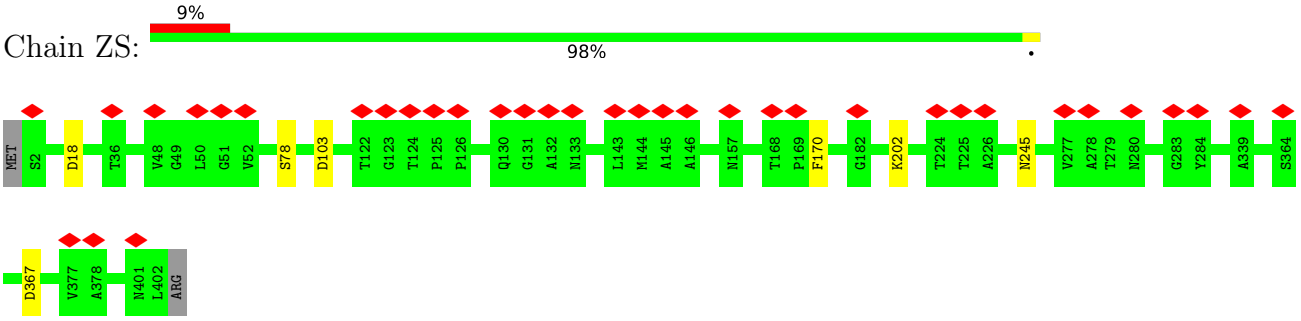




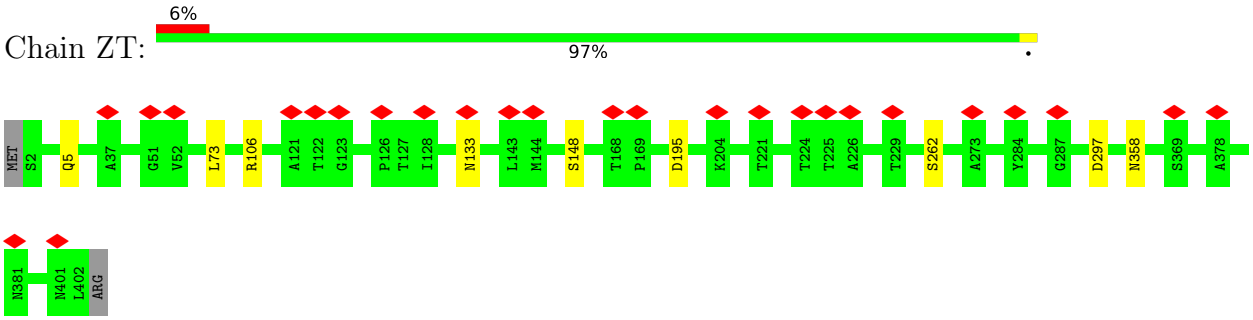
• Molecule 11: Flagellar hook protein FlgE

Chain ZS:



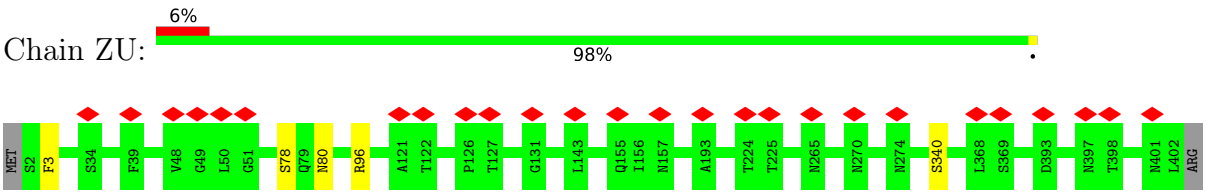
• Molecule 11: Flagellar hook protein FlgE

Chain ZT:



• Molecule 11: Flagellar hook protein FlgE

Chain ZU:



• Molecule 11: Flagellar hook protein FlgE

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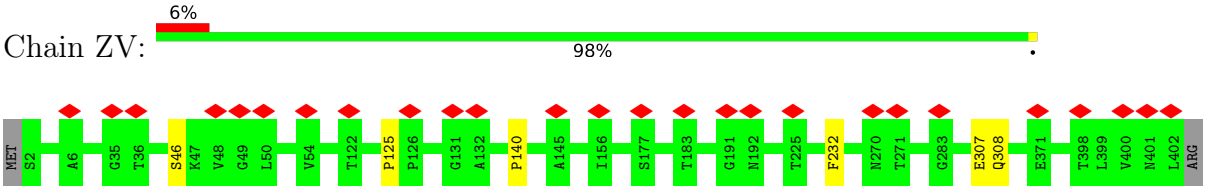
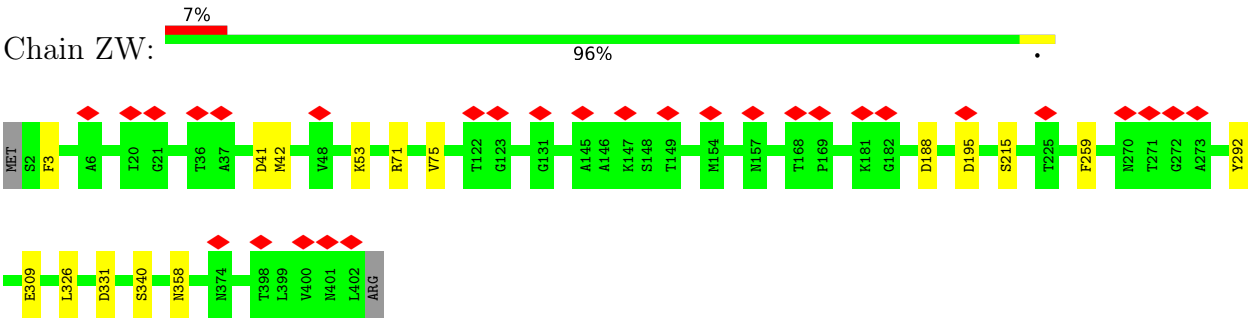


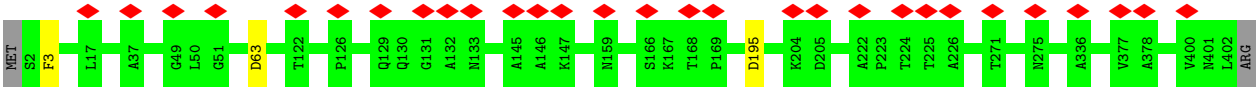
• Molecule 11: Flagellar hook protein FlgE

Chain ZW:



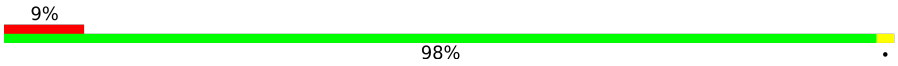
• Molecule 11: Flagellar hook protein FlgE

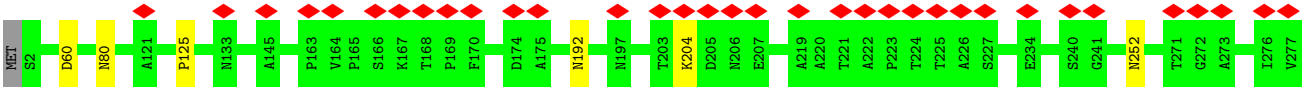
Chain ZX:

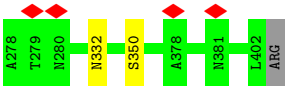


• Molecule 11: Flagellar hook protein FlgE

Chain ZY:

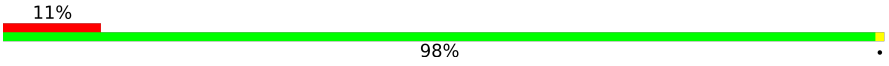


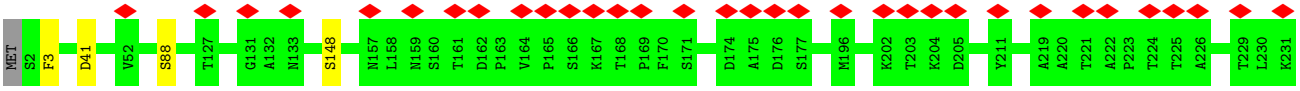


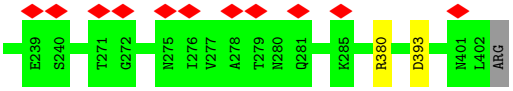


• Molecule 11: Flagellar hook protein FlgE

Chain ZZ:

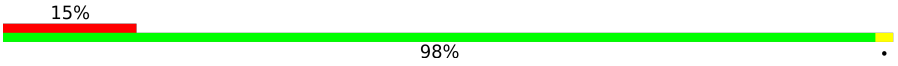


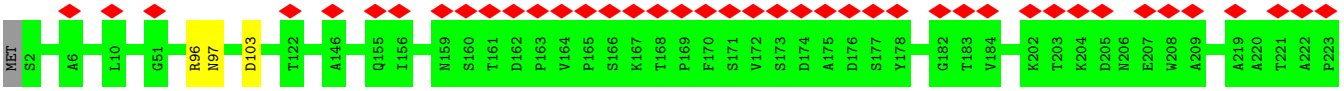


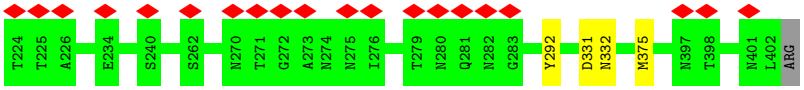


• Molecule 11: Flagellar hook protein FlgE

Chain Za:







• Molecule 11: Flagellar hook protein FlgE

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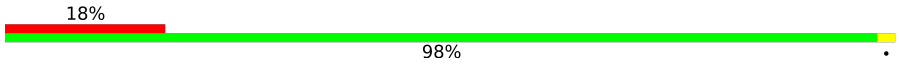

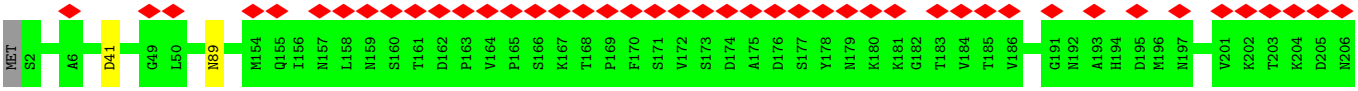

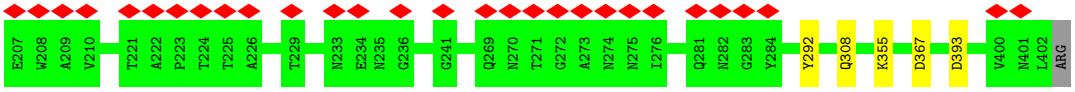

• Molecule 11: Flagellar hook protein FlgE

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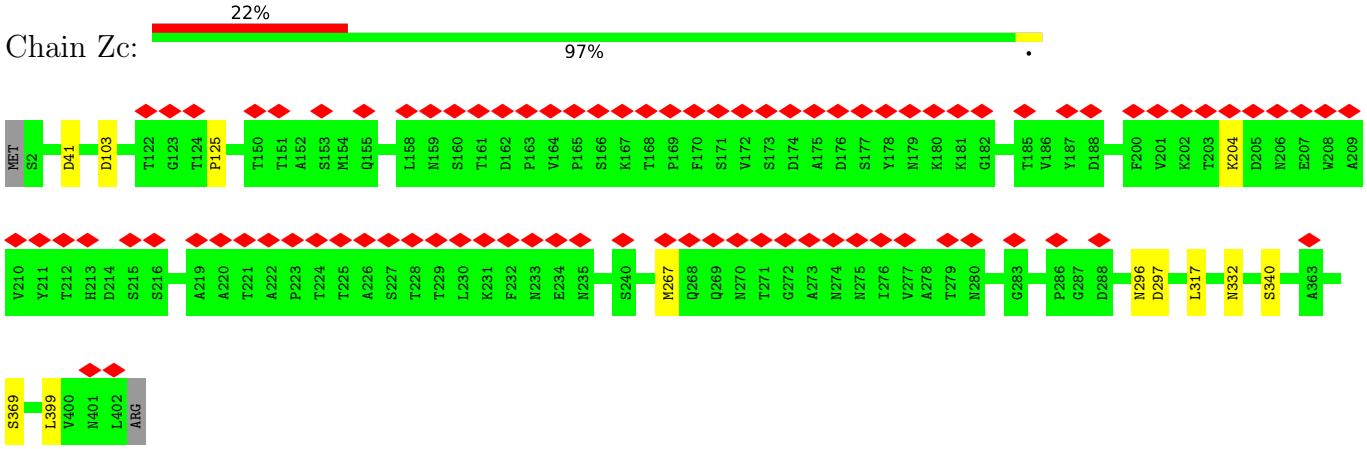
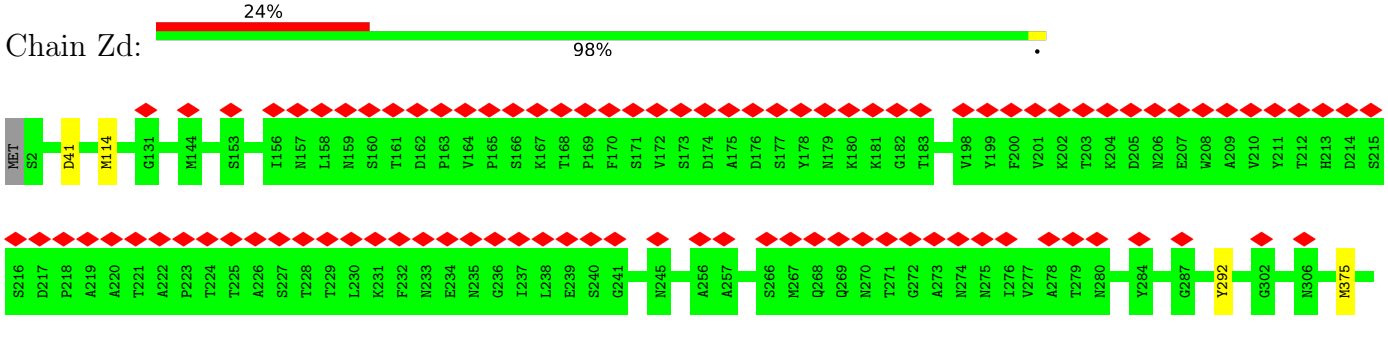


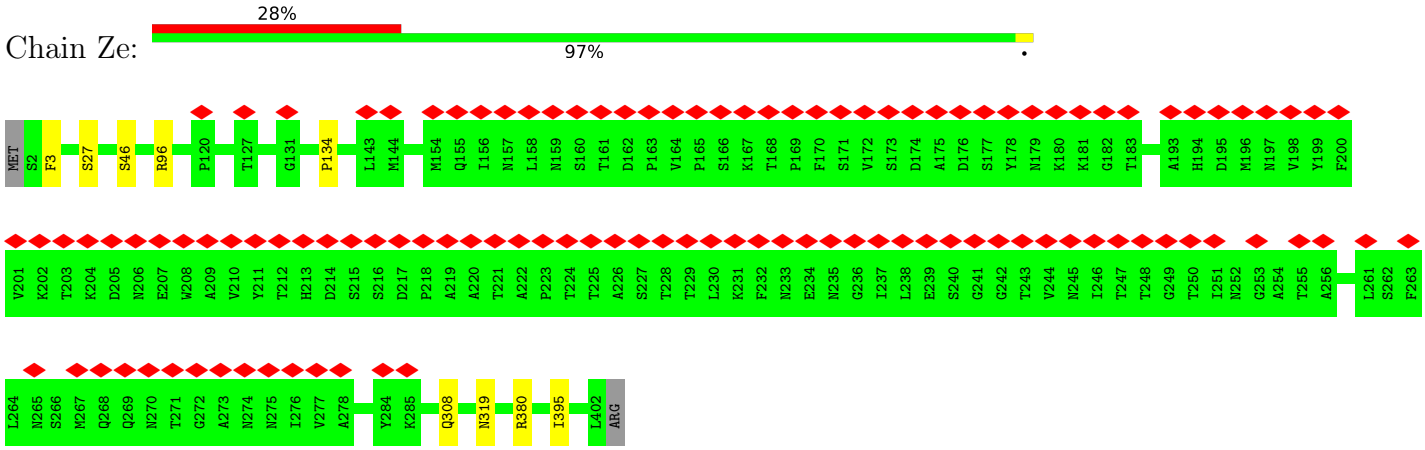
• Molecule 11: Flagellar hook protein FlgE

Chain Zd:



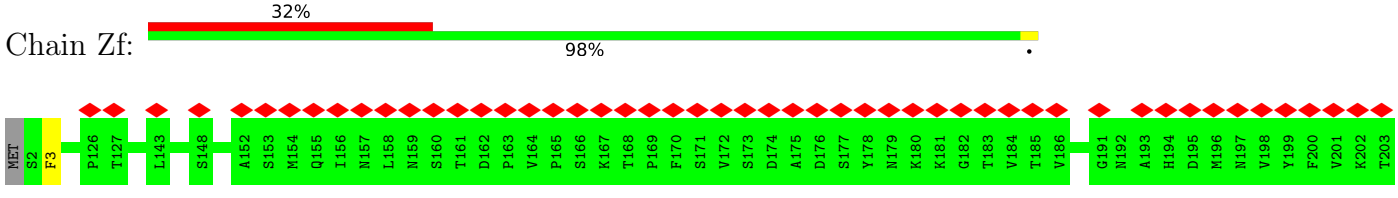
• Molecule 11: Flagellar hook protein FlgE

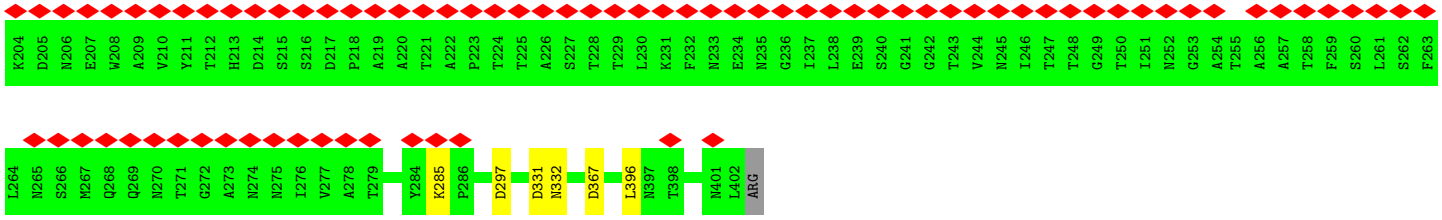
Chain Ze:



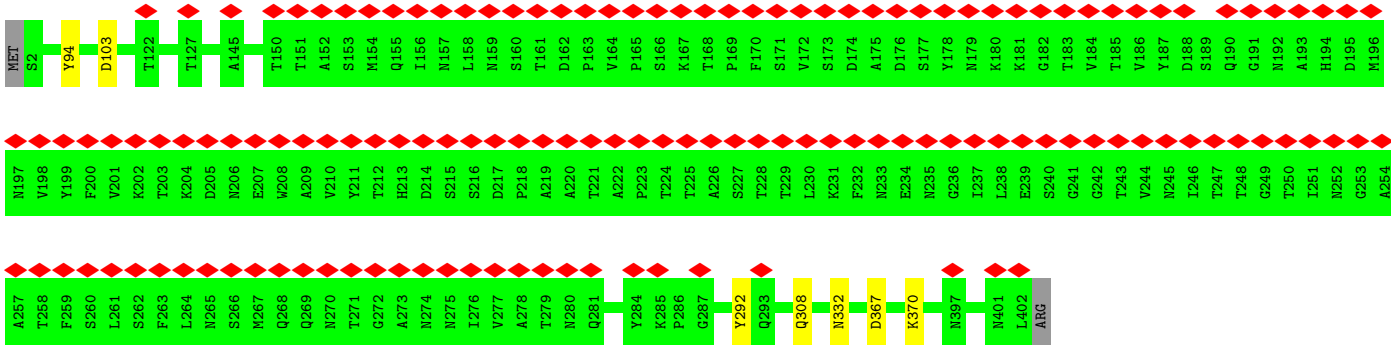
• Molecule 11: Flagellar hook protein FlgE

Chain Zf:

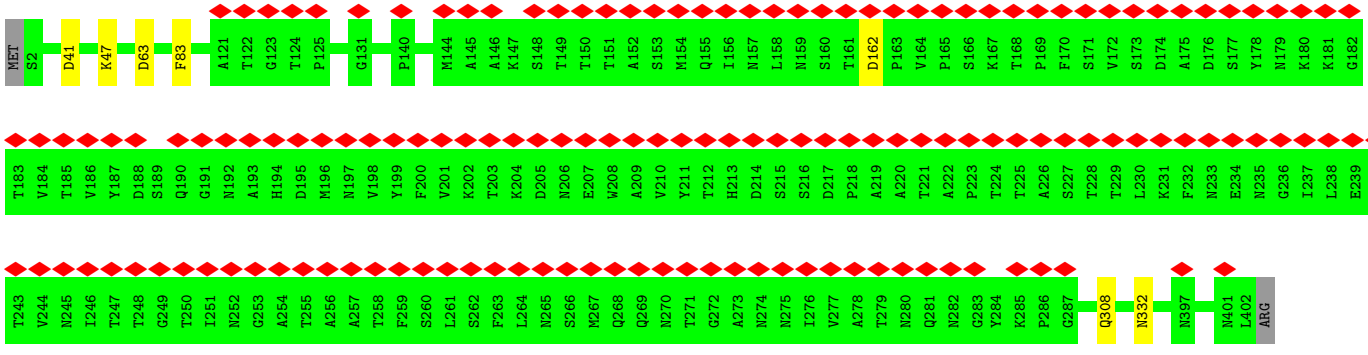




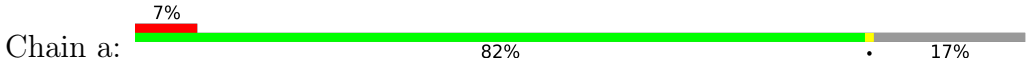
• Molecule 11: Flagellar hook protein FlgE

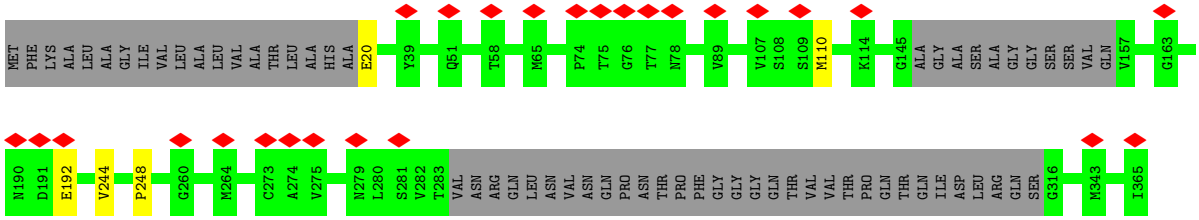


• Molecule 11: Flagellar hook protein FlgE



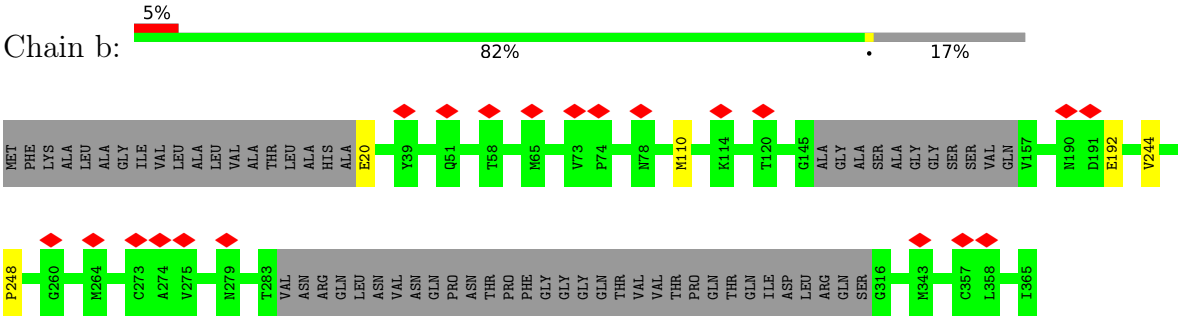
• Molecule 12: Flagellar P-ring protein





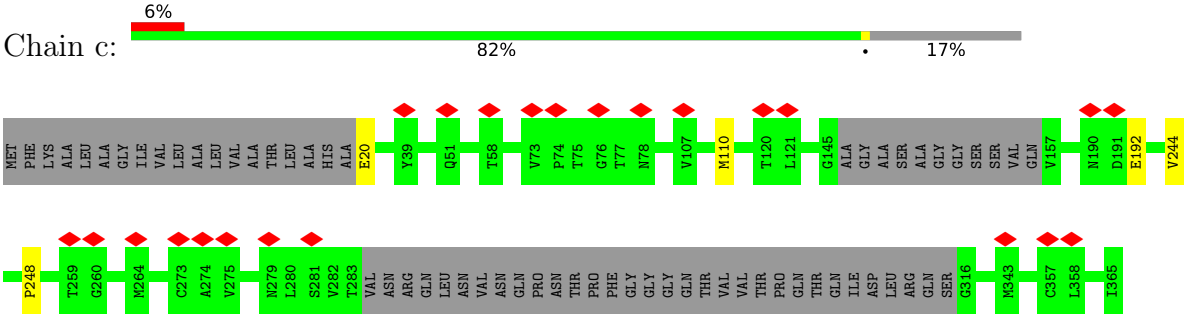
• Molecule 12: Flagellar P-ring protein

Chain b:



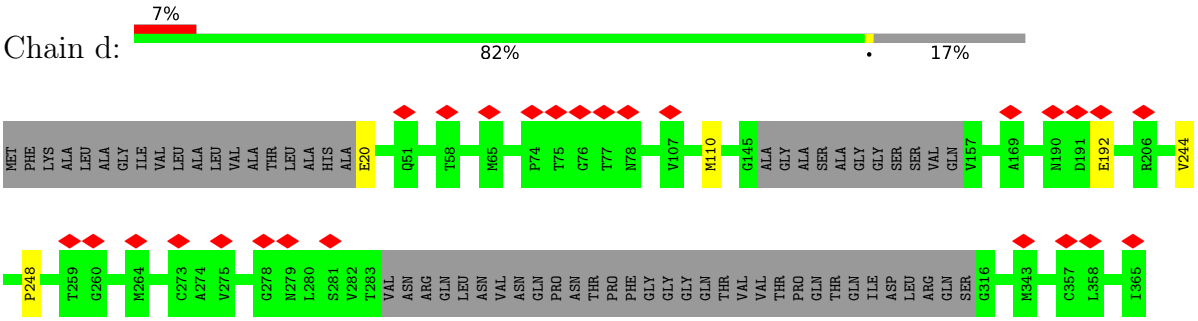
• Molecule 12: Flagellar P-ring protein

Chain c:



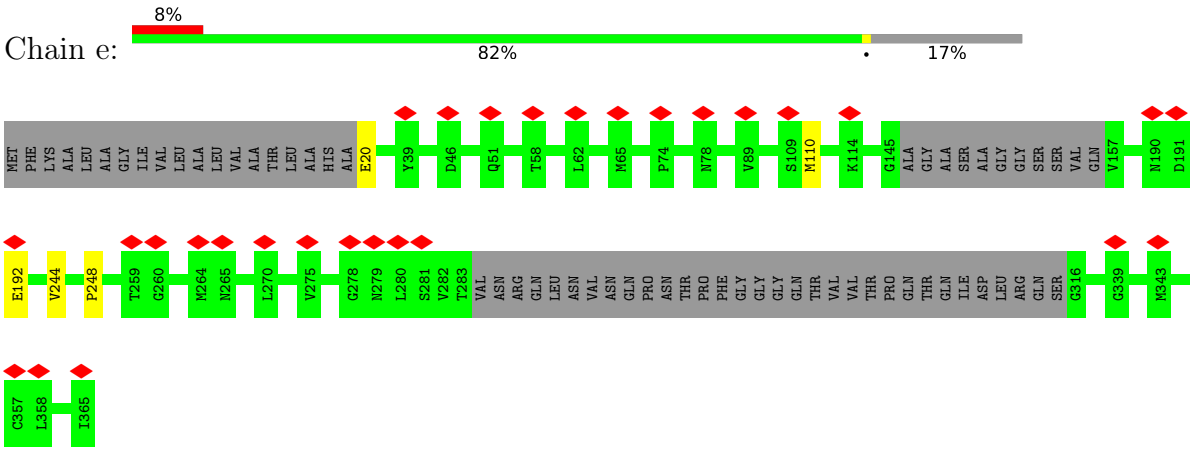
• Molecule 12: Flagellar P-ring protein

Chain d:



• Molecule 12: Flagellar P-ring protein

Chain e:



• Molecule 12: Flagellar P-ring protein

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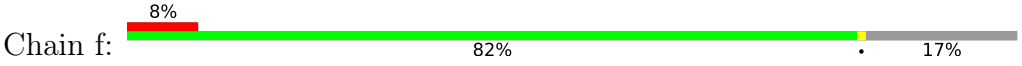
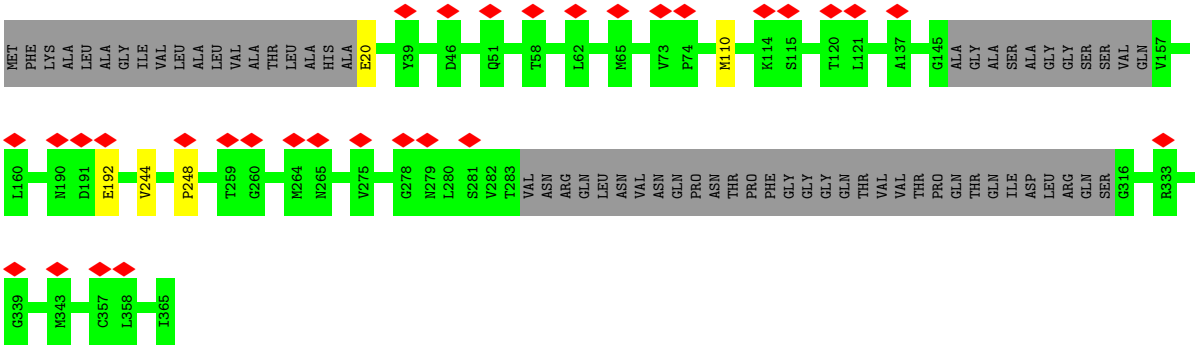
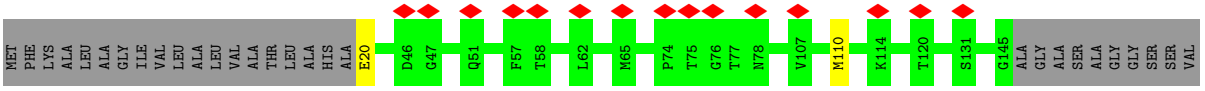
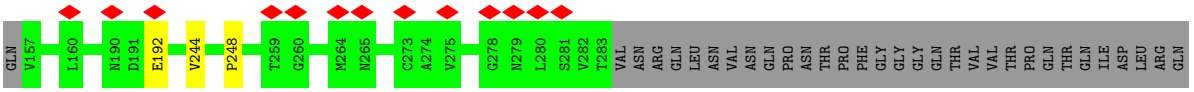


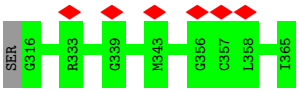


• Molecule 12: Flagellar P-ring protein

Chain g:

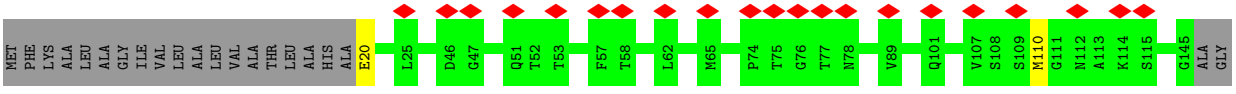


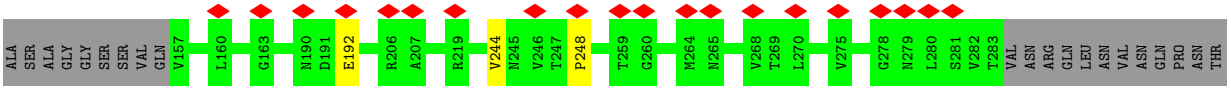


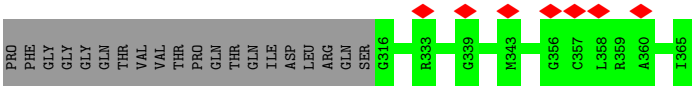


• Molecule 12: Flagellar P-ring protein

Chain h:

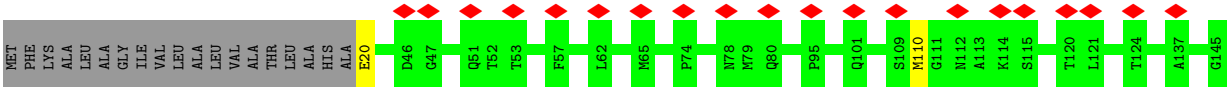


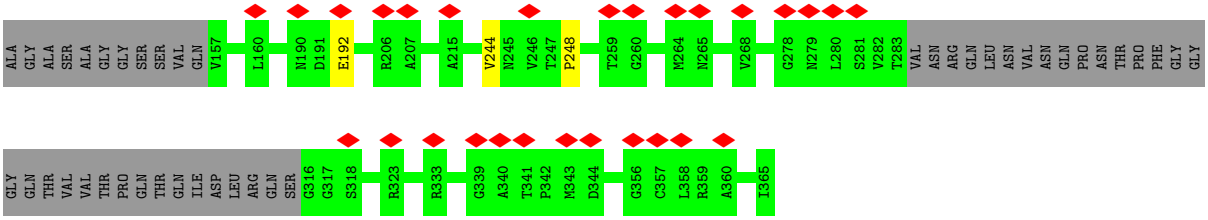




• Molecule 12: Flagellar P-ring protein

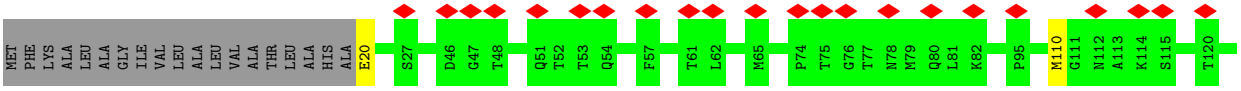
Chain i:

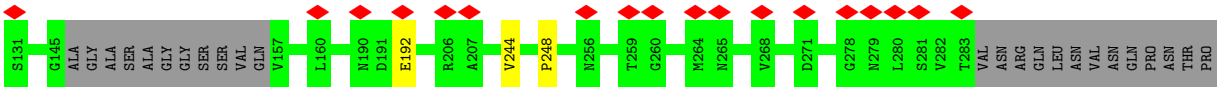


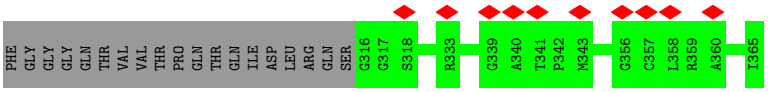


• Molecule 12: Flagellar P-ring protein

Chain j:

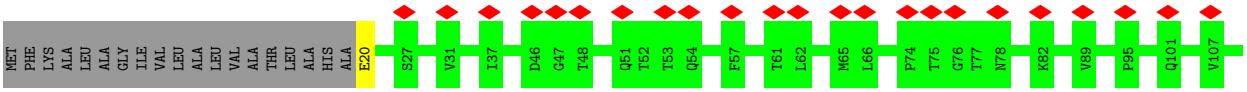


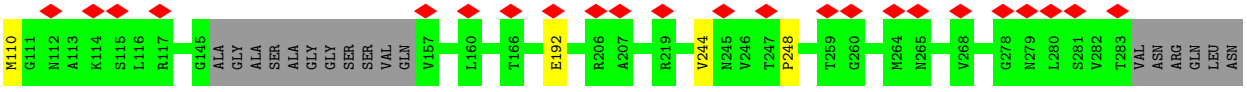


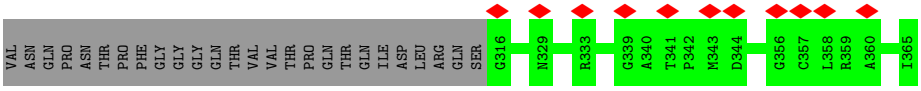


• Molecule 12: Flagellar P-ring protein

Chain k:

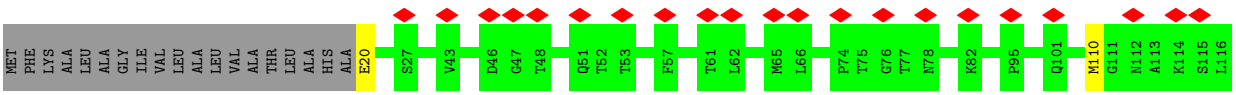


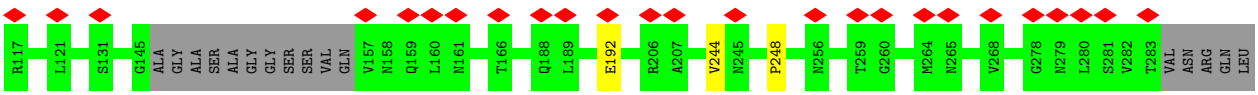


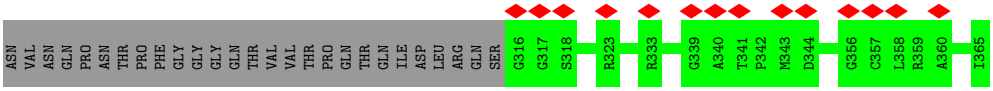


• Molecule 12: Flagellar P-ring protein

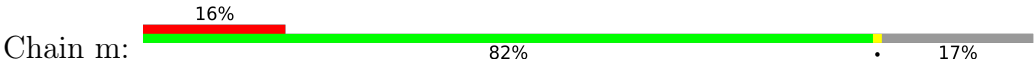
Chain l:

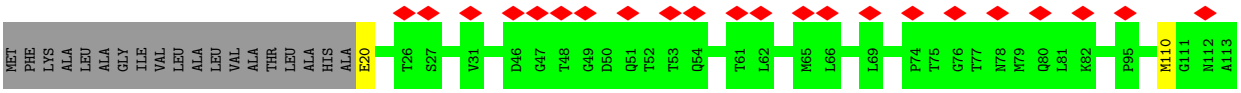


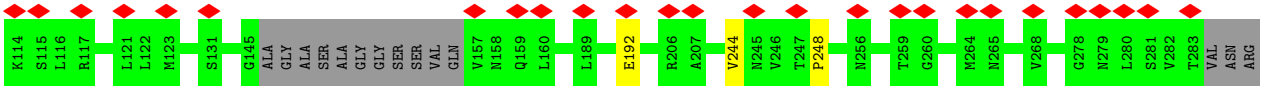


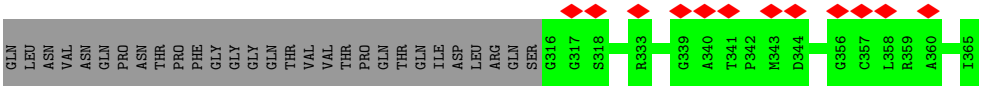


• Molecule 12: Flagellar P-ring protein

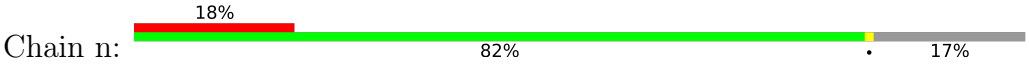


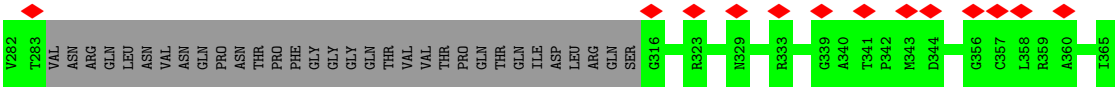




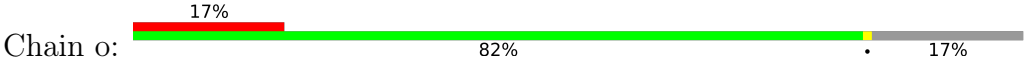


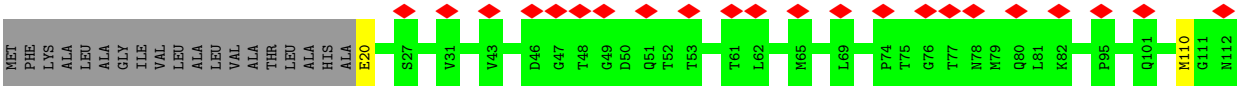
• Molecule 12: Flagellar P-ring protein

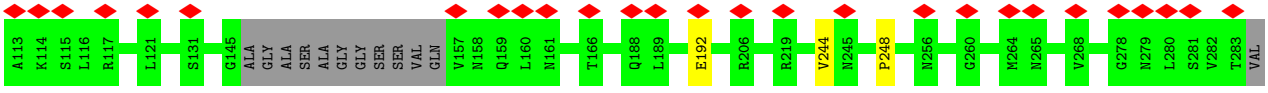




• Molecule 12: Flagellar P-ring protein

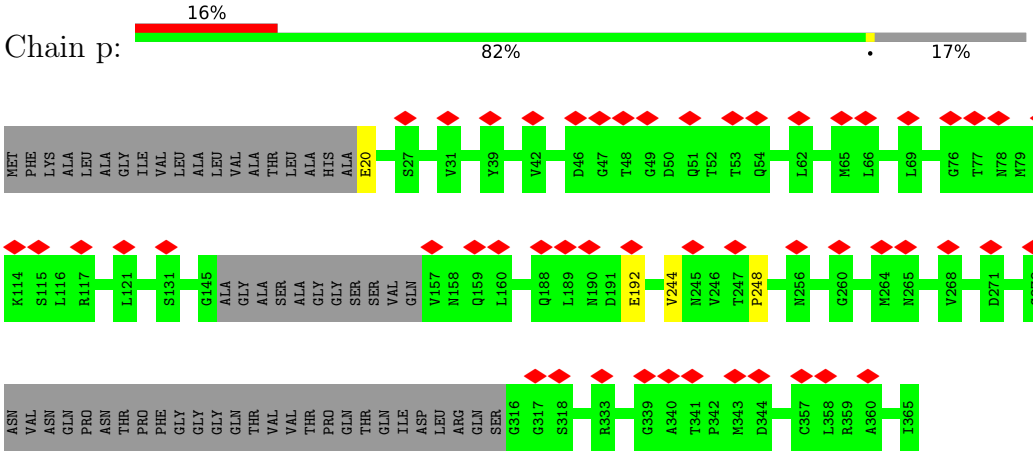






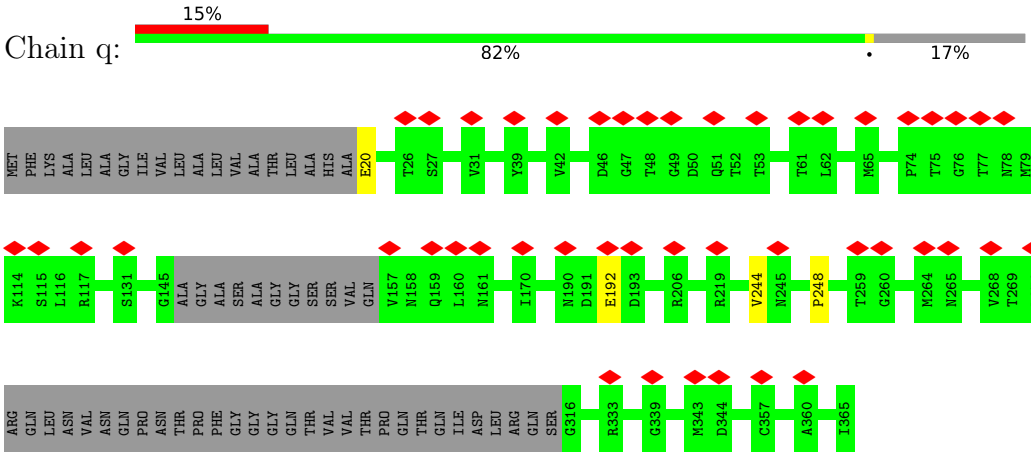
• Molecule 12: Flagellar P-ring protein

Chain p:



• Molecule 12: Flagellar P-ring protein

Chain q:



• Molecule 12: Flagellar P-ring protein

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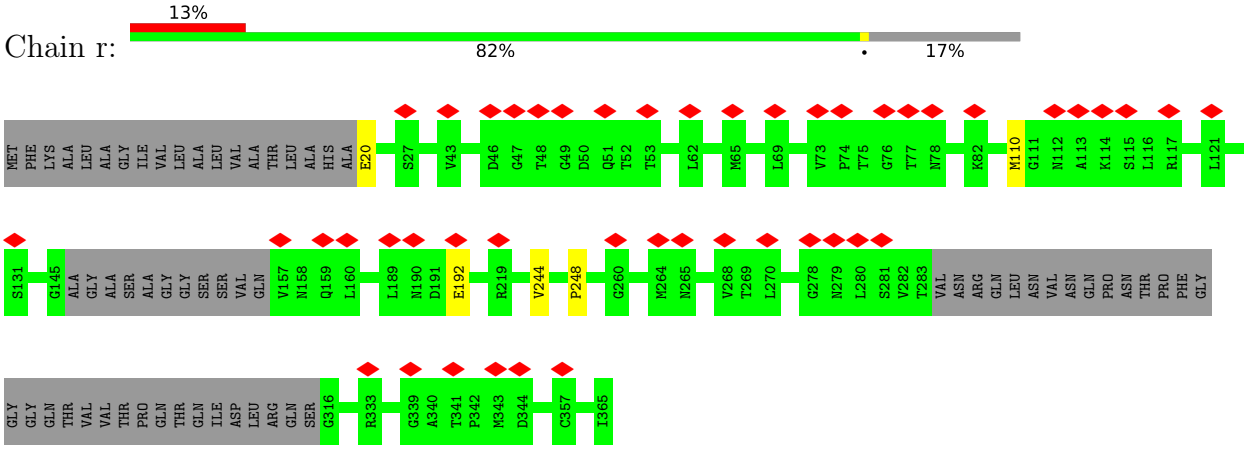

• Molecule 12: Flagellar P-ring protein

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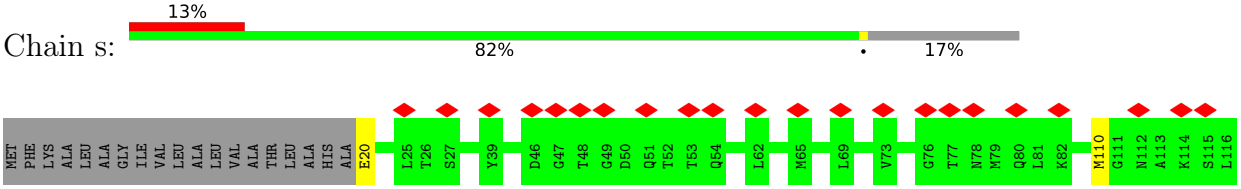
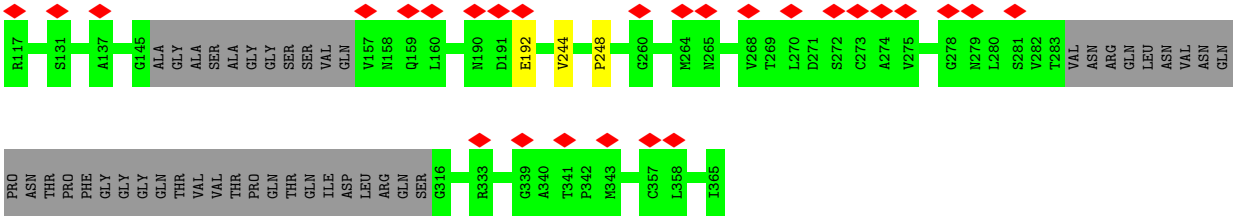
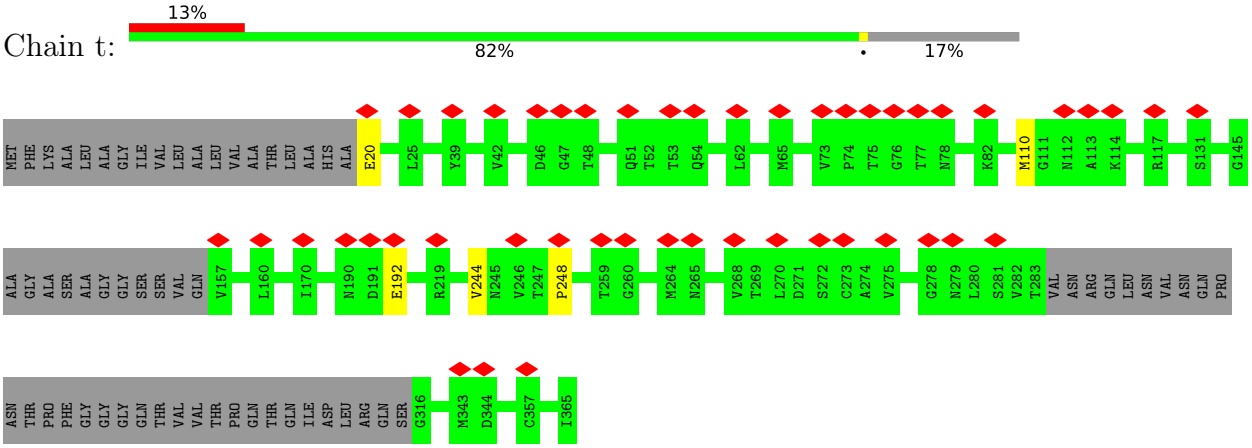
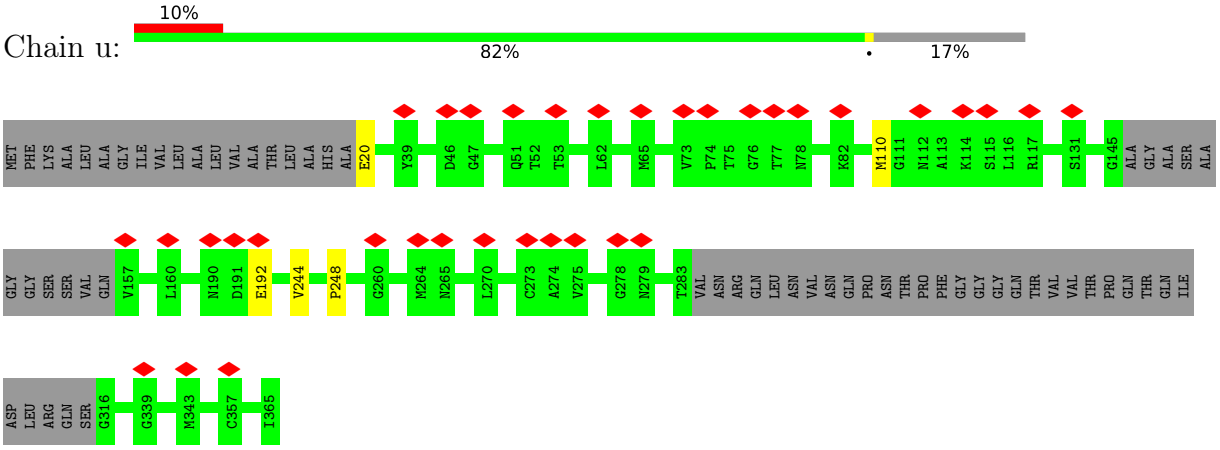




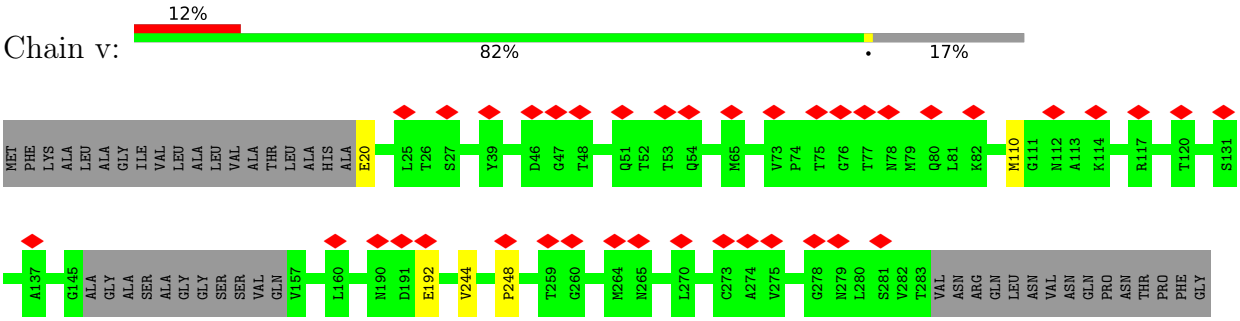
• Molecule 12: Flagellar P-ring protein

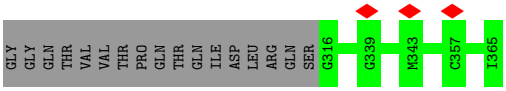


• Molecule 12: Flagellar P-ring protein



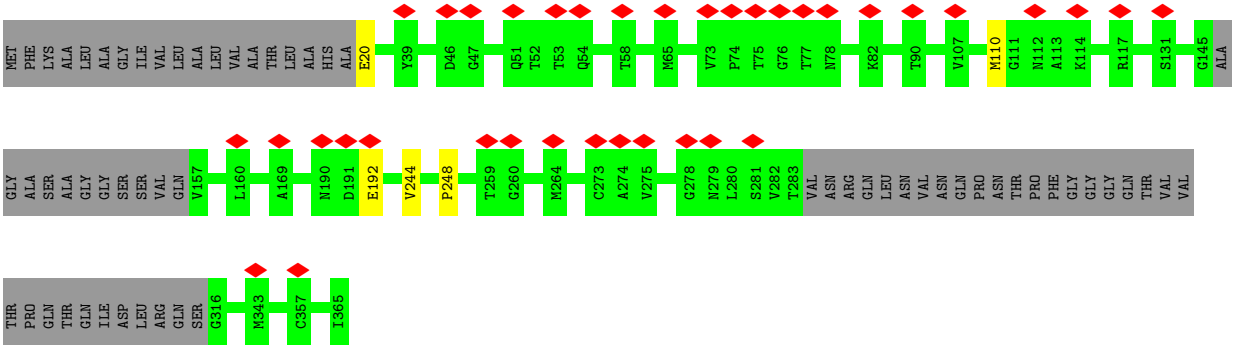
• Molecule 12: Flagellar P-ring protein





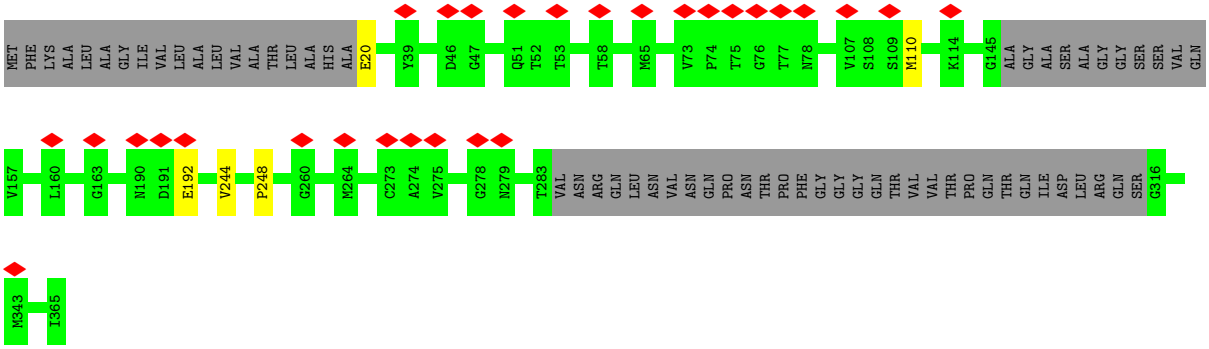
• Molecule 12: Flagellar P-ring protein

Chain w:



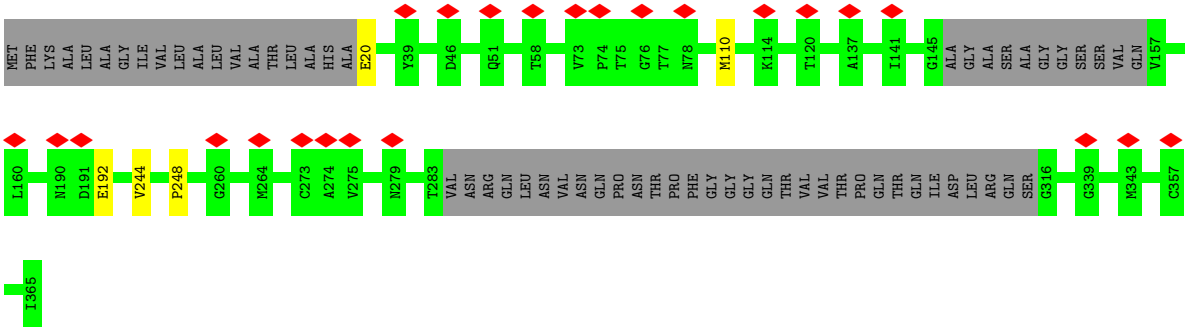
• Molecule 12: Flagellar P-ring protein

Chain x:



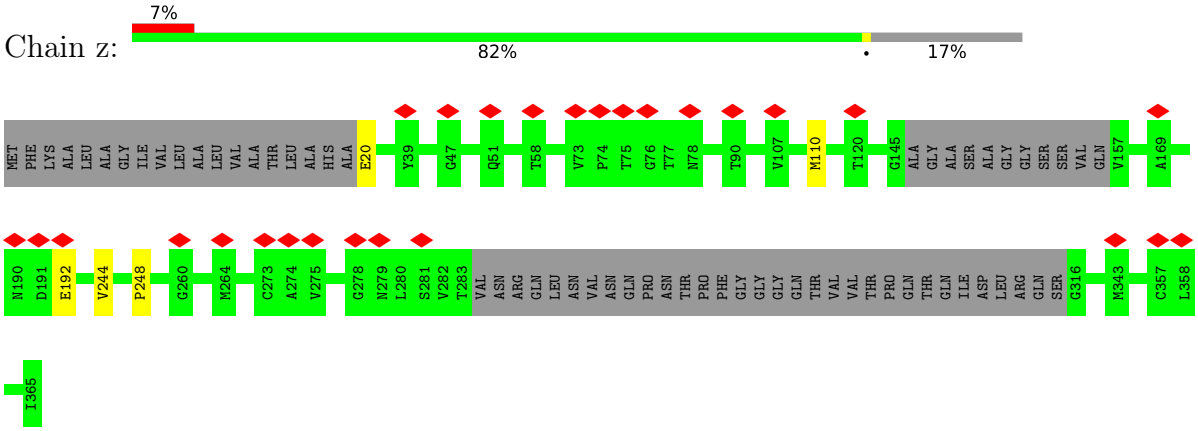
• Molecule 12: Flagellar P-ring protein

Chain y:



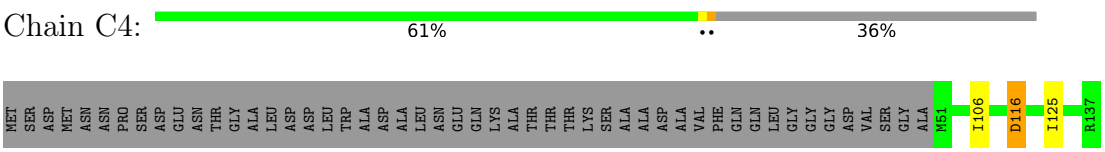
• Molecule 12: Flagellar P-ring protein

Chain z:



• Molecule 13: Flagellar motor switch protein FliN

Chain C4:



• Molecule 13: Flagellar motor switch protein FliN

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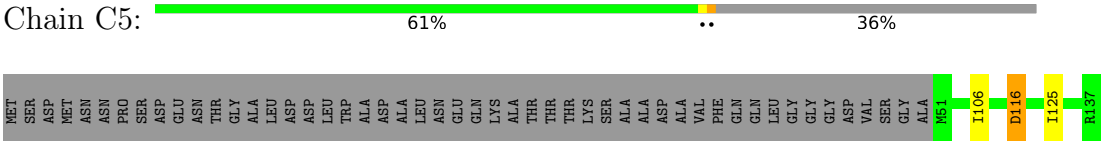

• Molecule 13: Flagellar motor switch protein FliN

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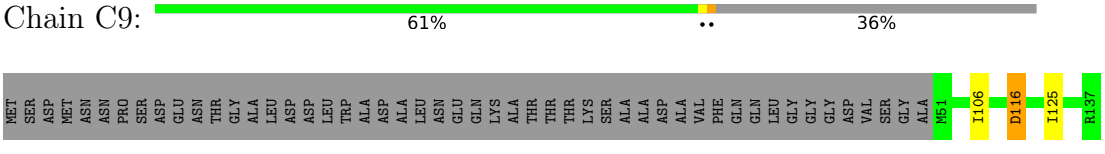
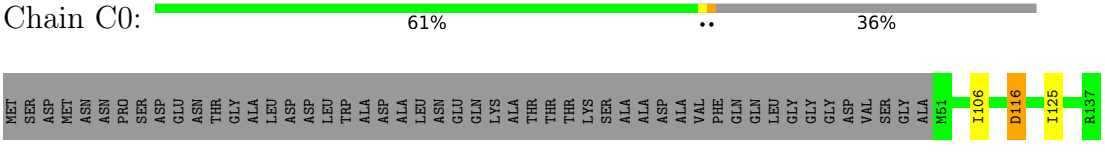


• Molecule 13: Flagellar motor switch protein FliN

Chain C0:



• Molecule 13: Flagellar motor switch protein FliN

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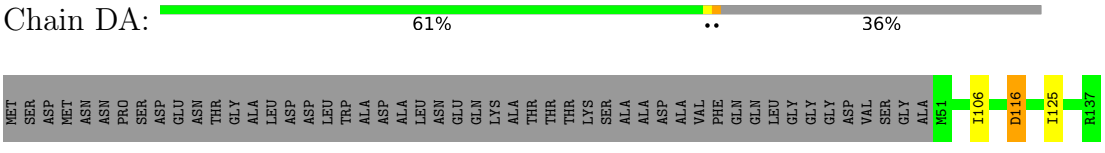

• Molecule 13: Flagellar motor switch protein FliN

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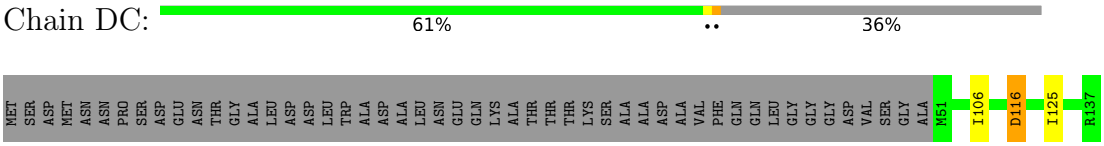
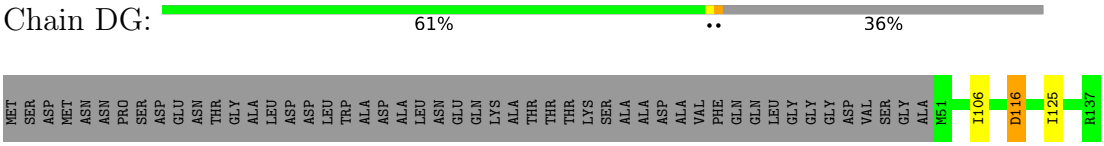


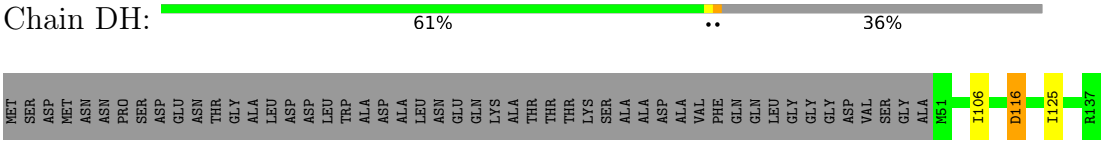
• Molecule 13: Flagellar motor switch protein FliN

Chain DG:



• Molecule 13: Flagellar motor switch protein FliN

Chain DH:



• Molecule 13: Flagellar motor switch protein FliN

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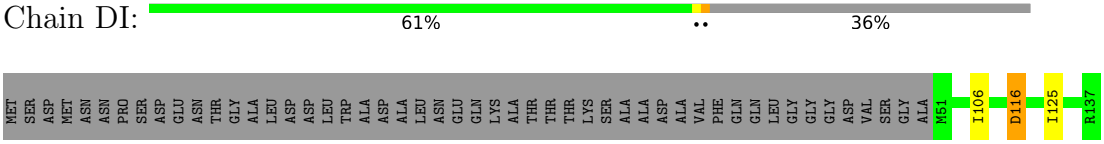

• Molecule 13: Flagellar motor switch protein FliN

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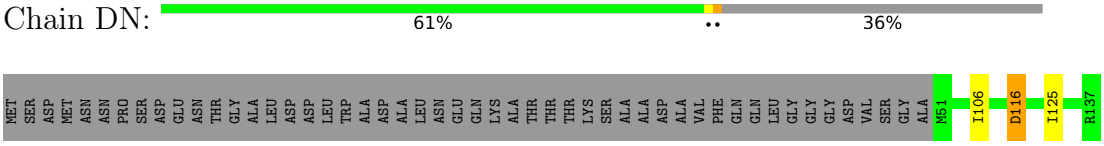

• Molecule 13: Flagellar motor switch protein FliN

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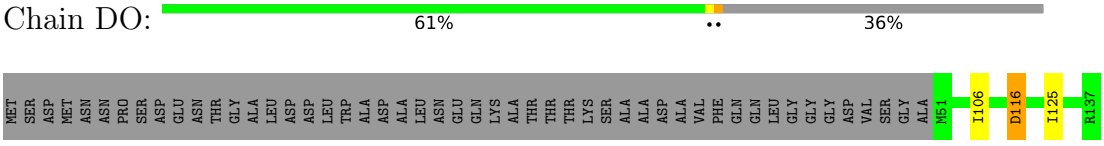

• Molecule 13: Flagellar motor switch protein FliN

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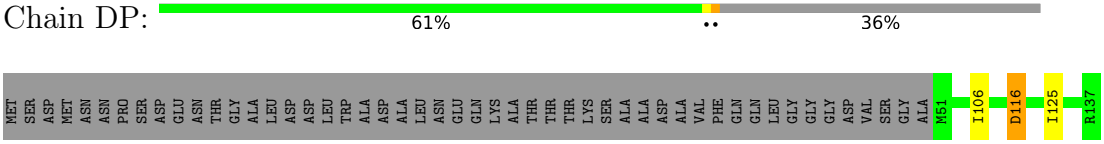
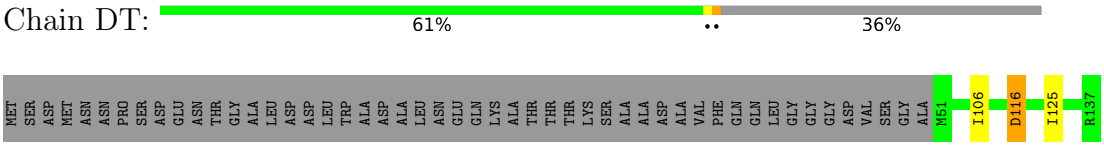


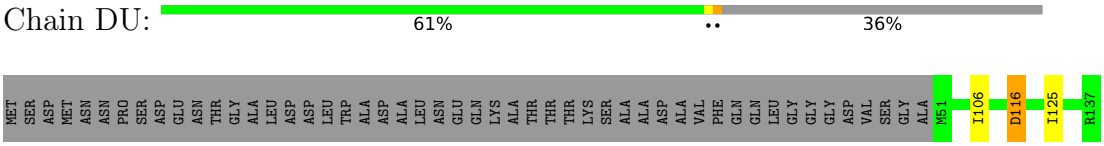
• Molecule 13: Flagellar motor switch protein FliN

Chain DT:



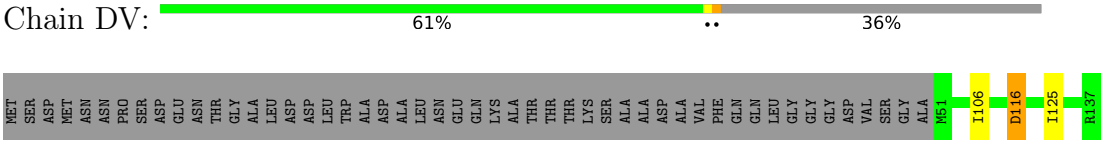
• Molecule 13: Flagellar motor switch protein FliN

Chain DU:



• Molecule 13: Flagellar motor switch protein FliN

Chain DV:



• Molecule 13: Flagellar motor switch protein FliN

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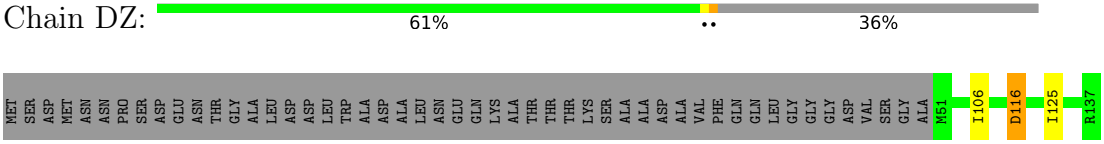
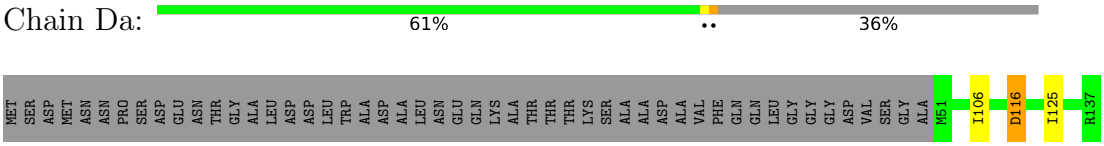


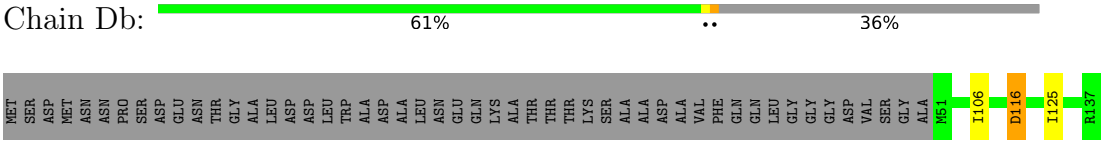
• Molecule 13: Flagellar motor switch protein FliN

Chain Da:



• Molecule 13: Flagellar motor switch protein FliN

Chain Db:



• Molecule 13: Flagellar motor switch protein FliN

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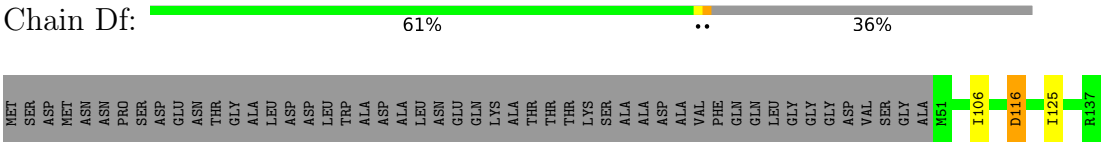

• Molecule 13: Flagellar motor switch protein FliN

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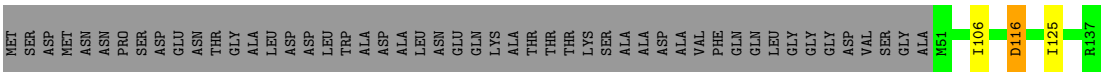

• Molecule 13: Flagellar motor switch protein FliN

Chain Dh:

• Molecule 13: Flagellar motor switch protein FliN

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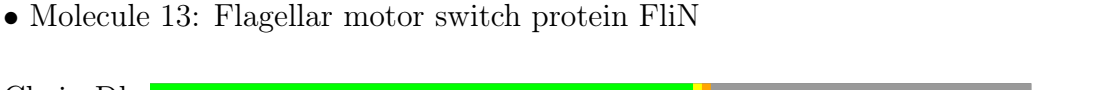

• Molecule 13: Flagellar motor switch protein FliN

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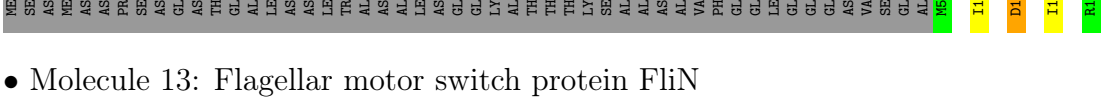
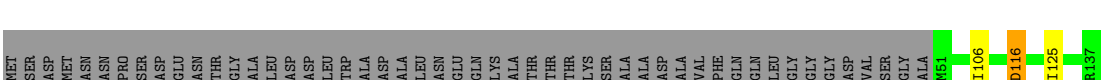


• Molecule 13: Flagellar motor switch protein FliN

Chain Dn:

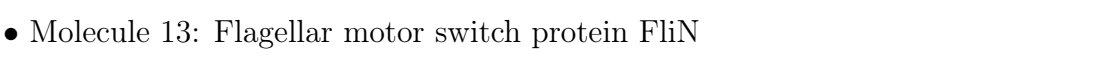


• Molecule 13: Flagellar motor switch protein FliN

Chain Dr:

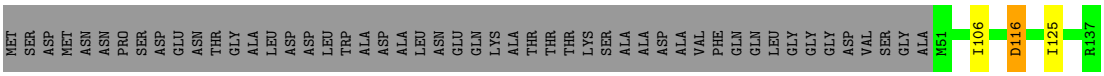
• Molecule 13: Flagellar motor switch protein FliN

Chain Ds:



• Molecule 13: Flagellar motor switch protein FliN

Chain Dt:



• Molecule 13: Flagellar motor switch protein FliN

Chain Dx:

• Molecule 13: Flagellar motor switch protein FliN

Chain Dy:

• Molecule 13: Flagellar motor switch protein FliN

Chain Dz:

• Molecule 13: Flagellar motor switch protein FliN

Chain D4:

• Molecule 13: Flagellar motor switch protein FliN

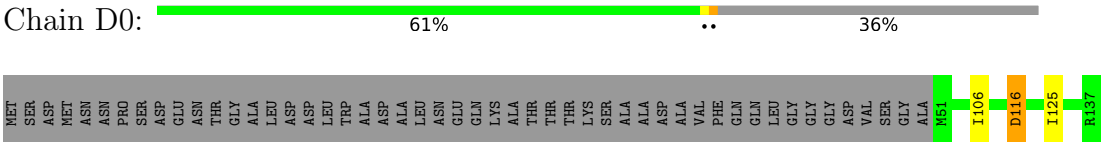
Chain D5:

• Molecule 13: Flagellar motor switch protein FliN

Chain D6:

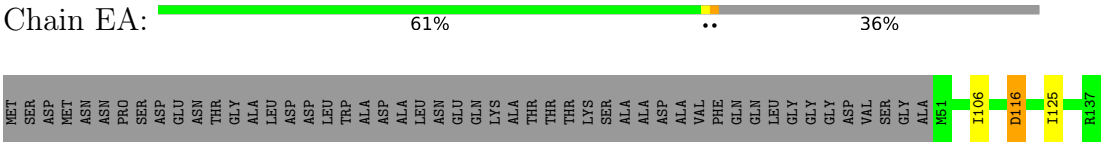
• Molecule 13: Flagellar motor switch protein FliN

Chain D0:



• Molecule 13: Flagellar motor switch protein FliN

Chain EA:



• Molecule 13: Flagellar motor switch protein FliN

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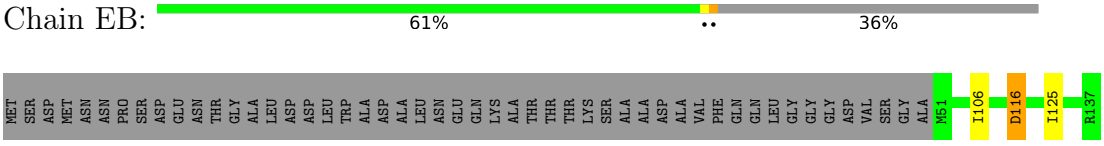
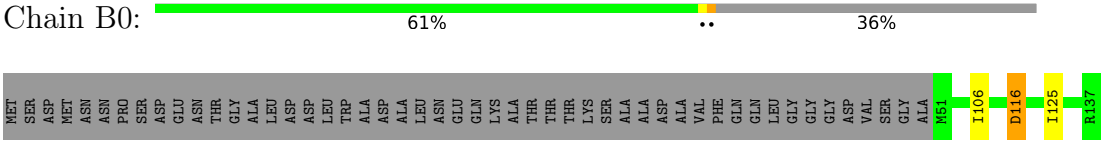


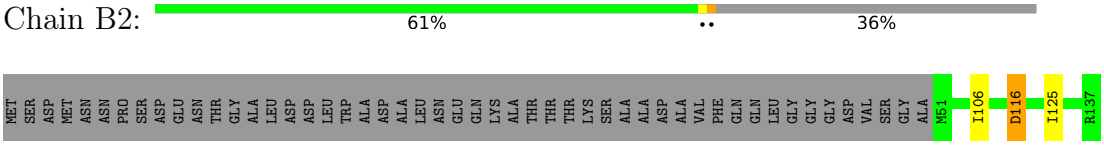
• Molecule 13: Flagellar motor switch protein FliN

Chain B0:



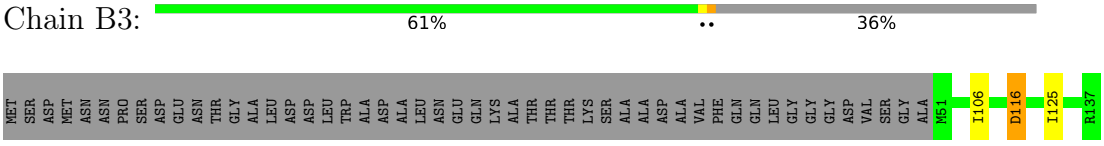
• Molecule 13: Flagellar motor switch protein FliN

Chain B2:



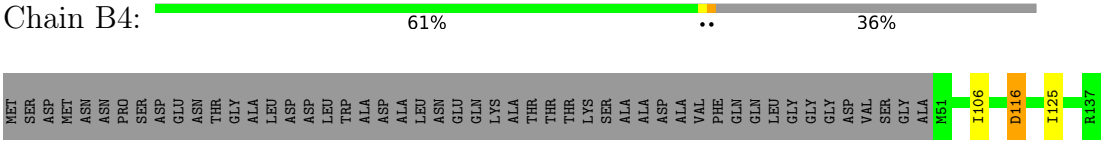
• Molecule 13: Flagellar motor switch protein FliN

Chain B3:



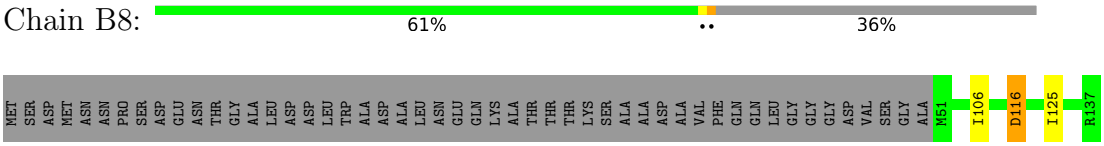
• Molecule 13: Flagellar motor switch protein FliN

Chain B4:



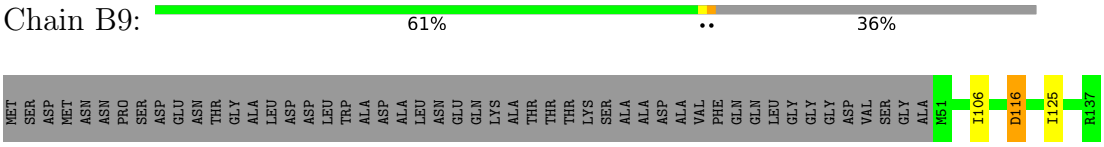
• Molecule 13: Flagellar motor switch protein FliN

Chain B8:



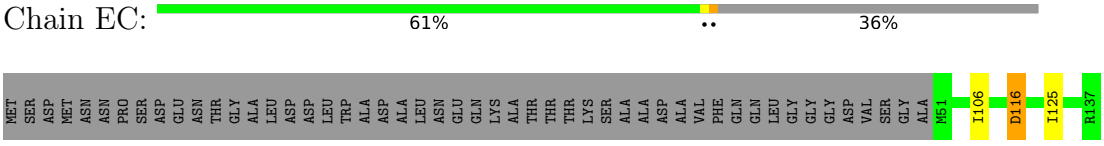
• Molecule 13: Flagellar motor switch protein FliN

Chain B9:



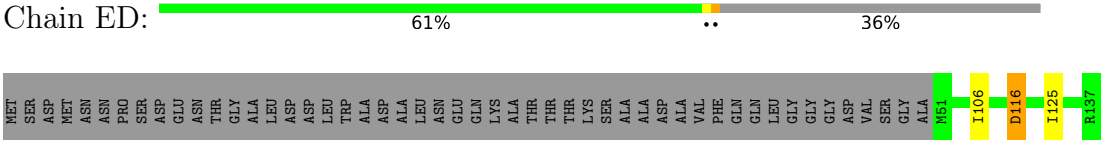
• Molecule 13: Flagellar motor switch protein FliN

Chain EC:



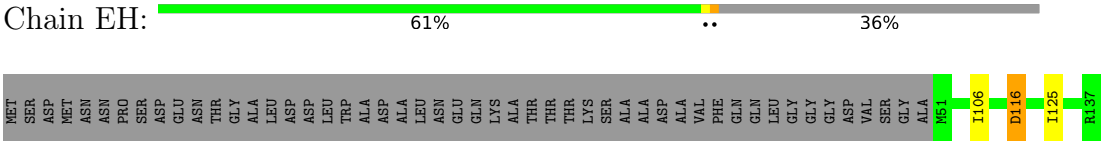
• Molecule 13: Flagellar motor switch protein FliN

Chain ED:



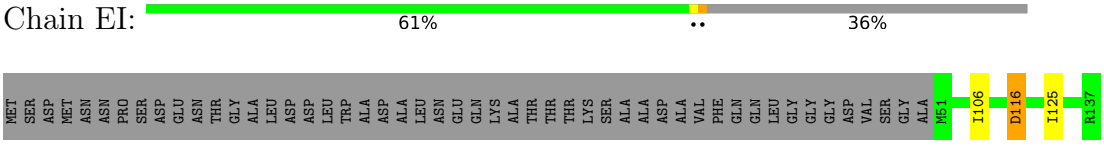
• Molecule 13: Flagellar motor switch protein FliN

Chain EH:



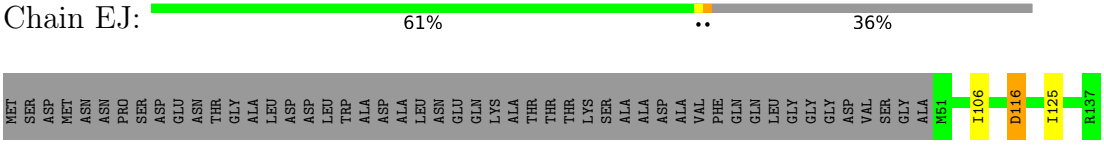
• Molecule 13: Flagellar motor switch protein FliN

Chain EI:



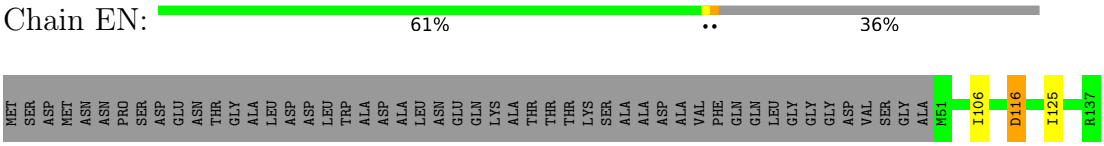
• Molecule 13: Flagellar motor switch protein FliN

Chain EJ:



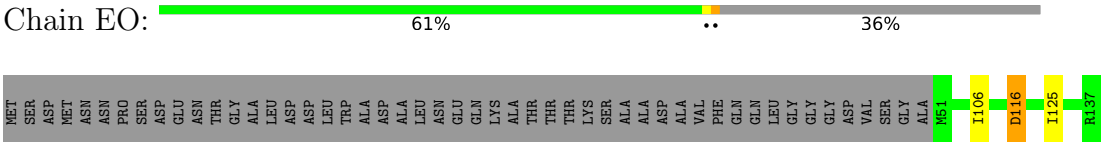
• Molecule 13: Flagellar motor switch protein FliN

Chain EN:



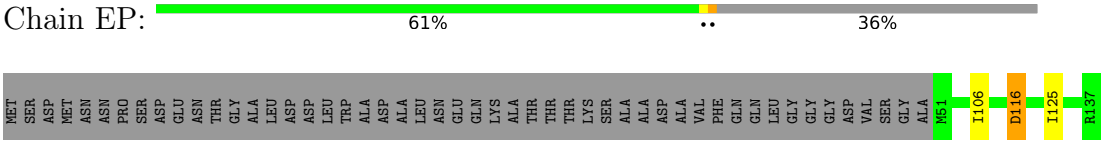
• Molecule 13: Flagellar motor switch protein FliN

Chain EO:



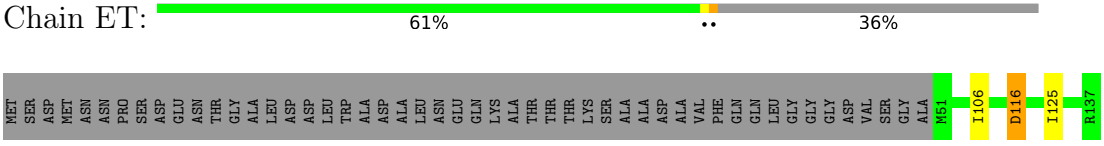
• Molecule 13: Flagellar motor switch protein FliN

Chain EP:



• Molecule 13: Flagellar motor switch protein FliN

Chain ET:



• Molecule 13: Flagellar motor switch protein FliN

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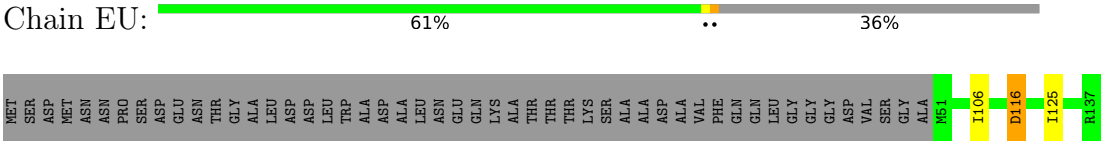
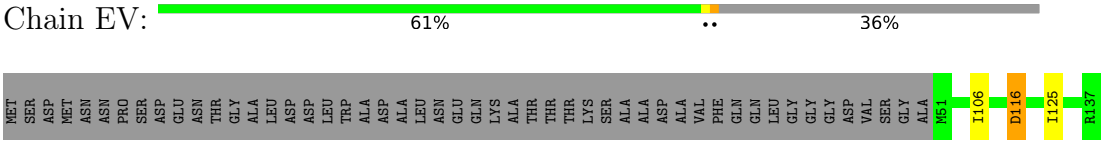


• Molecule 13: Flagellar motor switch protein FliN

Chain EV:



• Molecule 13: Flagellar motor switch protein FliN

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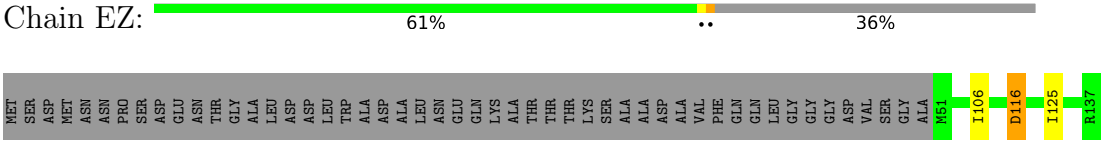
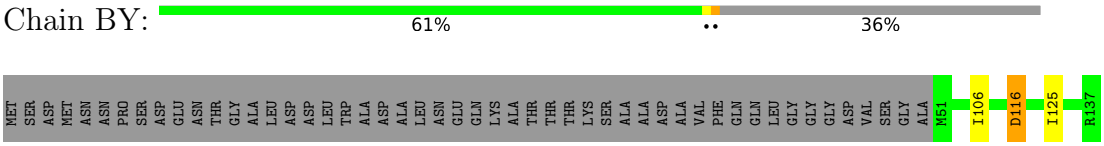


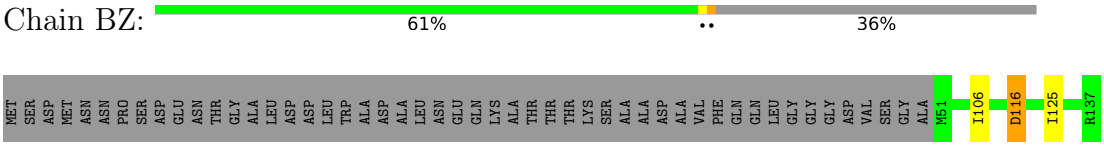
• Molecule 13: Flagellar motor switch protein FliN

Chain BY:



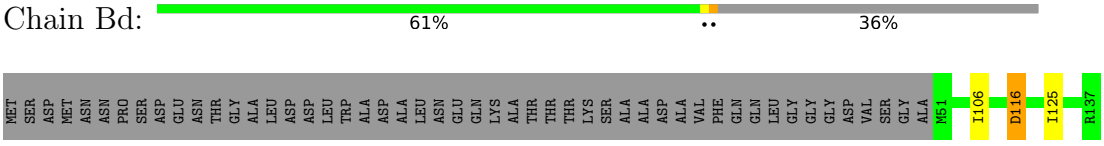
• Molecule 13: Flagellar motor switch protein FliN

Chain BZ:



• Molecule 13: Flagellar motor switch protein FliN

Chain Bd:



• Molecule 13: Flagellar motor switch protein FliN

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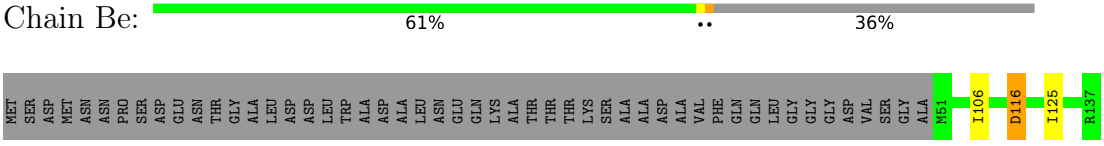
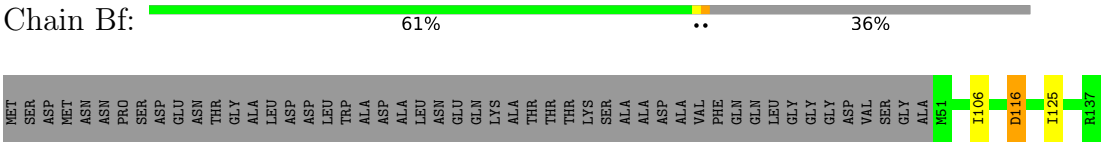


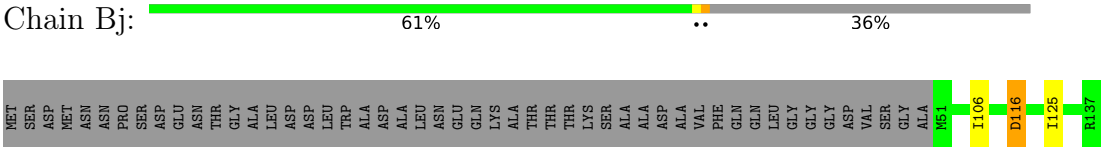
• Molecule 13: Flagellar motor switch protein FliN

Chain Bf:



• Molecule 13: Flagellar motor switch protein FliN

Chain Bj:



• Molecule 13: Flagellar motor switch protein FliN

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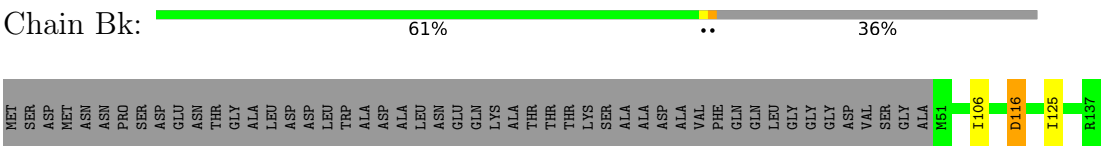

• Molecule 13: Flagellar motor switch protein FliN

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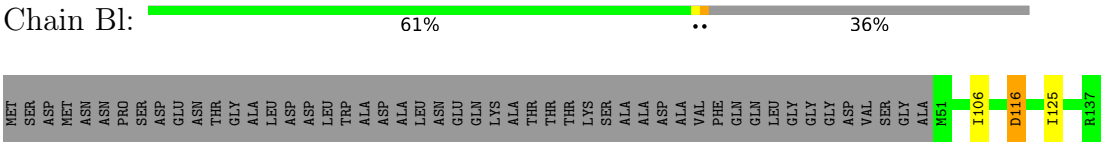

• Molecule 13: Flagellar motor switch protein FliN

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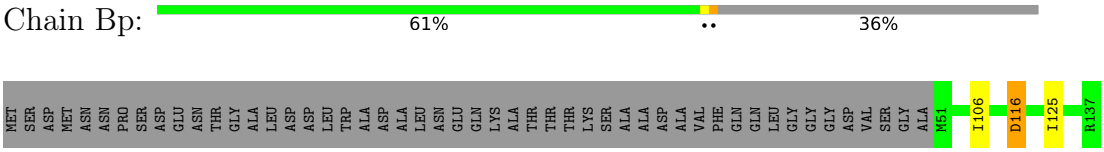
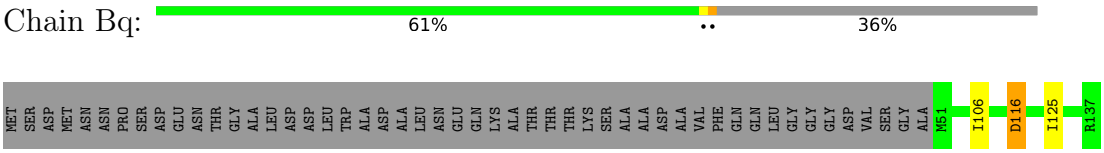


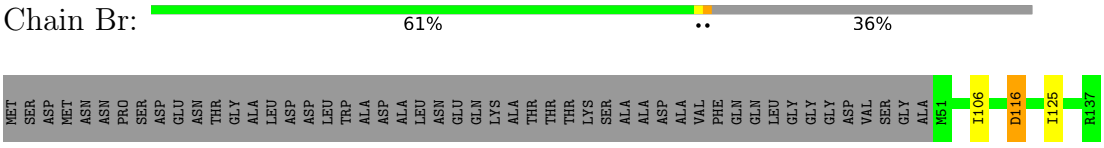
• Molecule 13: Flagellar motor switch protein FliN

Chain Bq:



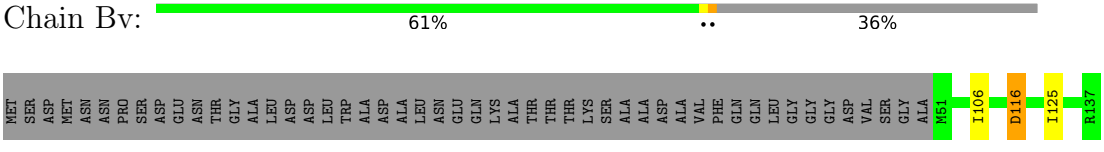
• Molecule 13: Flagellar motor switch protein FliN

Chain Br:



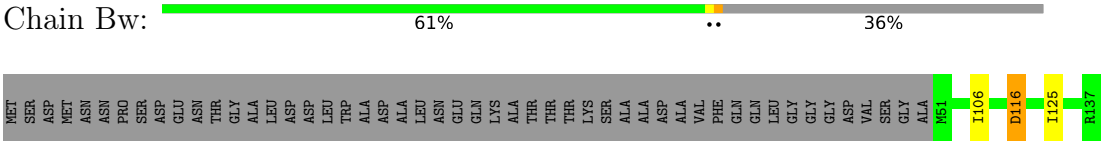
• Molecule 13: Flagellar motor switch protein FliN

Chain Bv:



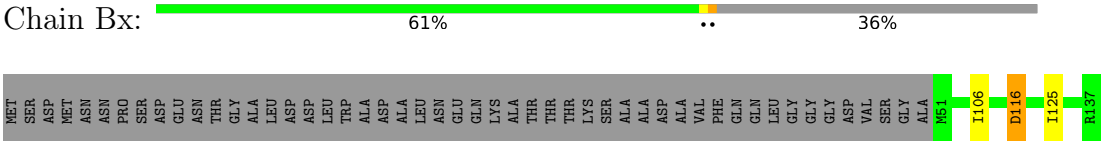
• Molecule 13: Flagellar motor switch protein FliN

Chain Bw:



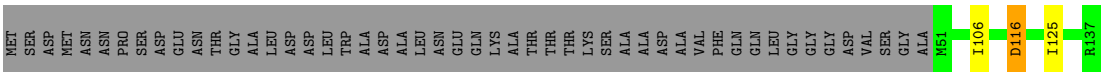
• Molecule 13: Flagellar motor switch protein FliN

Chain Bx:



• Molecule 13: Flagellar motor switch protein FliN

Chain C1:

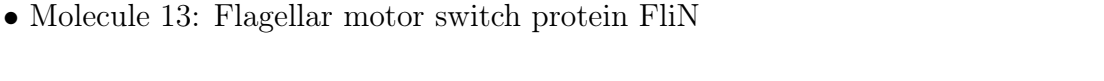


• Molecule 13: Flagellar motor switch protein FliN

Chain C2:

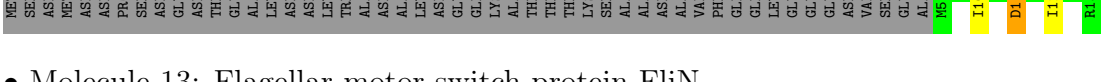
• Molecule 13: Flagellar motor switch protein FliN

Chain CD:



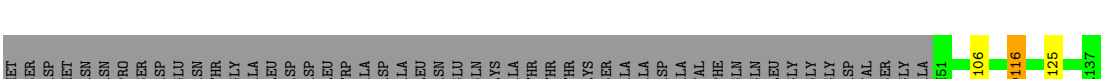
• Molecule 13: Flagellar motor switch protein FliN

Chain CE:



• Molecule 13: Flagellar motor switch protein FliN

Chain CF:

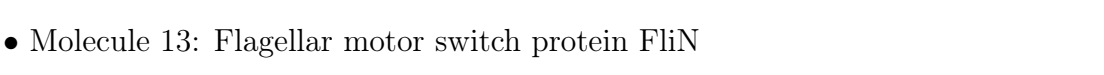


• Molecule 13: Flagellar motor switch protein FliN

Chain CJ:

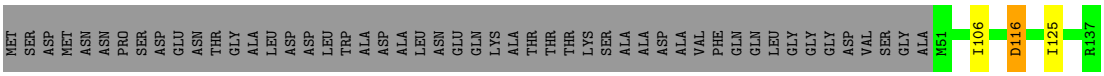
• Molecule 13: Flagellar motor switch protein FliN

Chain CK:



• Molecule 13: Flagellar motor switch protein FliN

Chain CL:



• Molecule 13: Flagellar motor switch protein FliN

Chain CP:

• Molecule 13: Flagellar motor switch protein FliN

Chain CQ:

• Molecule 13: Flagellar motor switch protein FliN

Chain CR:

• Molecule 13: Flagellar motor switch protein FliN

Chain CV:

• Molecule 13: Flagellar motor switch protein FliN

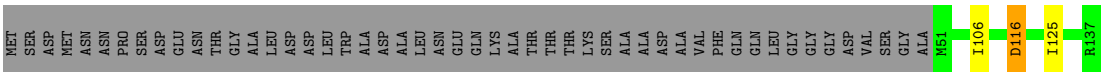
Chain CW:

• Molecule 13: Flagellar motor switch protein FliN

Chain CX:

• Molecule 13: Flagellar motor switch protein FliN

Chain Cb:



• Molecule 13: Flagellar motor switch protein FliN

Chain Cc:

• Molecule 13: Flagellar motor switch protein FliN

Chain Cd:

• Molecule 13: Flagellar motor switch protein FliN

Chain Ch:

• Molecule 13: Flagellar motor switch protein FliN

Chain Ci:

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Chain Cj:

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Chain Cn:

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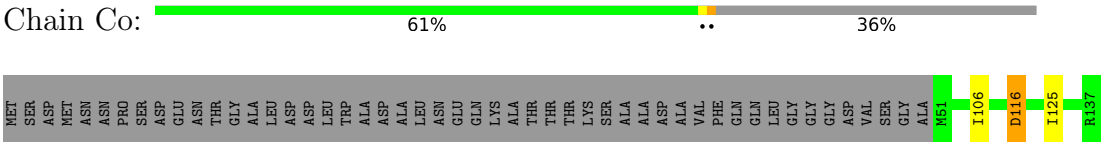
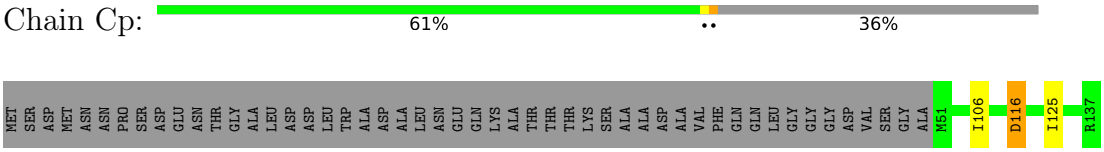
Chain Co:



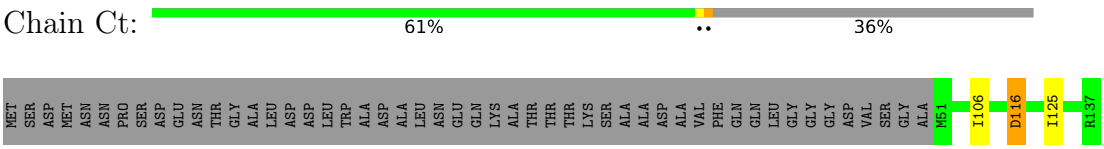
• Molecule 13: Flagellar motor switch protein FliN

Chain Cp:



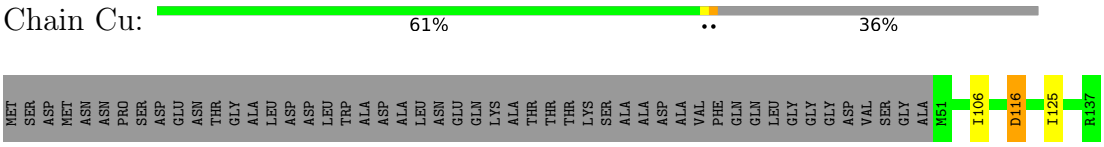
• Molecule 13: Flagellar motor switch protein FliN

Chain Ct:



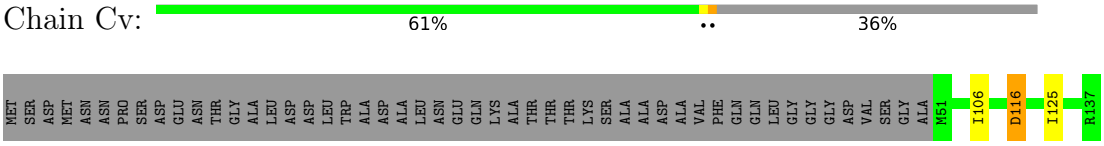
• Molecule 13: Flagellar motor switch protein FliN

Chain Cu:



• Molecule 13: Flagellar motor switch protein FliN

Chain Cv:



• Molecule 13: Flagellar motor switch protein FliN

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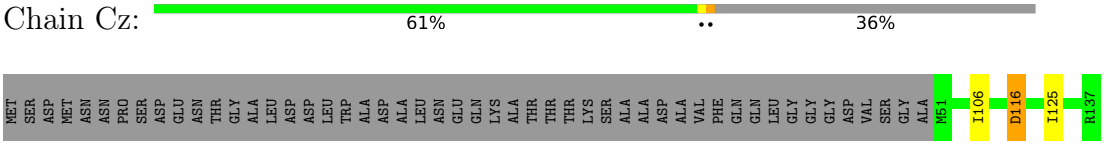

• Molecule 13: Flagellar motor switch protein FliN

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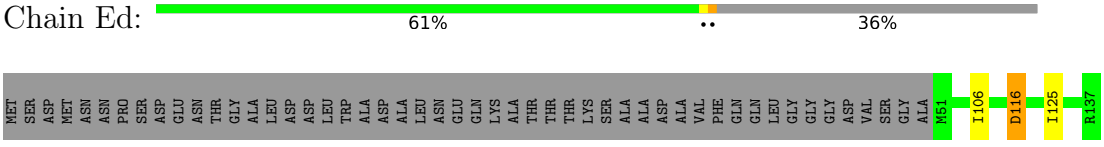
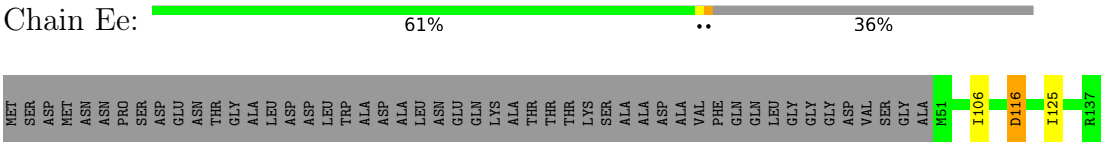


• Molecule 13: Flagellar motor switch protein FliN

Chain Ee:



• Molecule 13: Flagellar motor switch protein FliN

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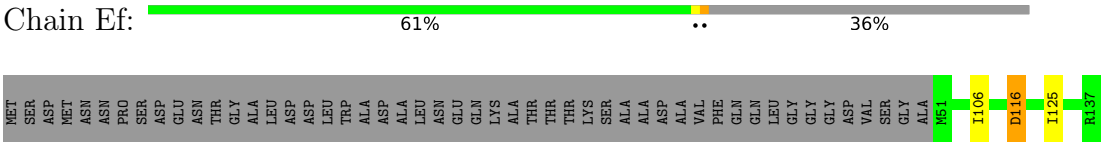

• Molecule 13: Flagellar motor switch protein FliN

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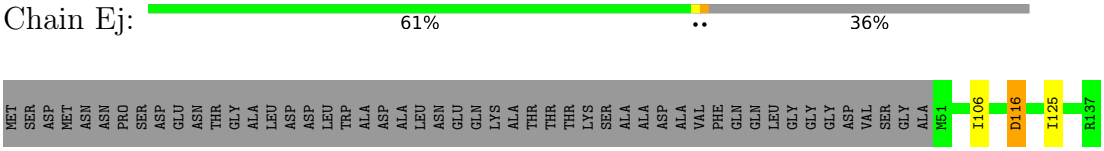

• Molecule 13: Flagellar motor switch protein FliN

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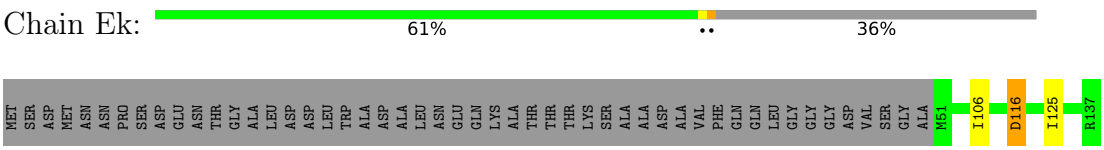

• Molecule 13: Flagellar motor switch protein FliN

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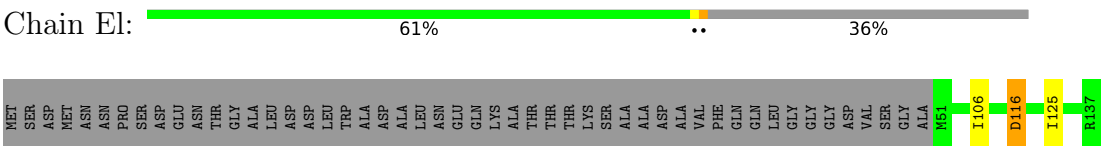

• Molecule 13: Flagellar motor switch protein FliN

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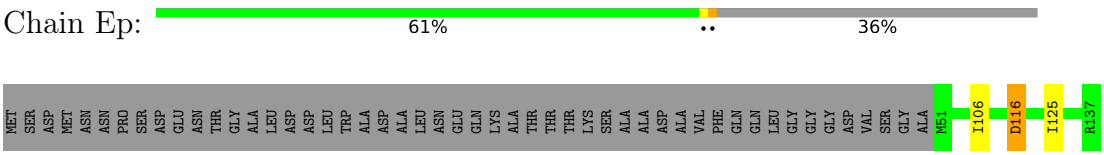
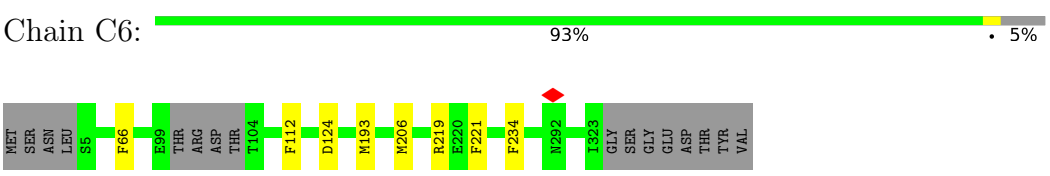


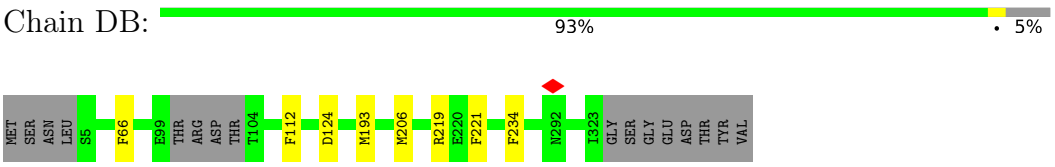
• Molecule 14: Flagellar motor switch protein FliG

Chain C6:



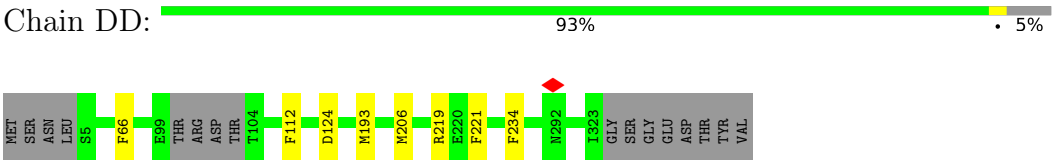
• Molecule 14: Flagellar motor switch protein FliG

Chain DB:



• Molecule 14: Flagellar motor switch protein FliG

Chain DD:



• Molecule 14: Flagellar motor switch protein FliG

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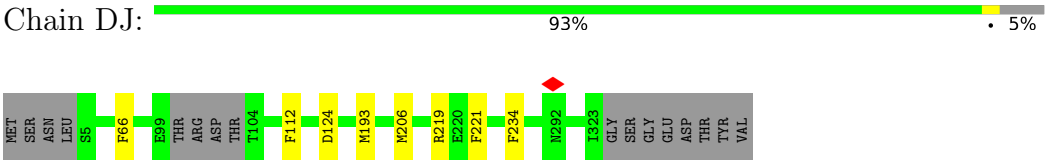
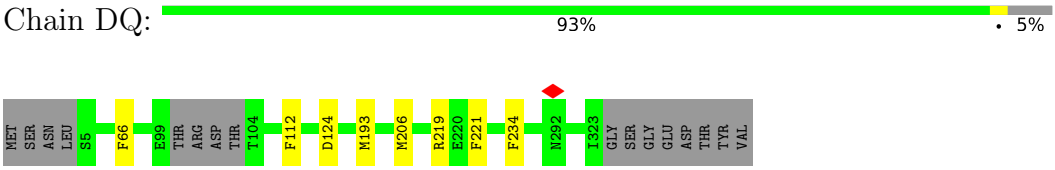


• Molecule 14: Flagellar motor switch protein FliG

Chain DQ:



• Molecule 14: Flagellar motor switch protein FliG

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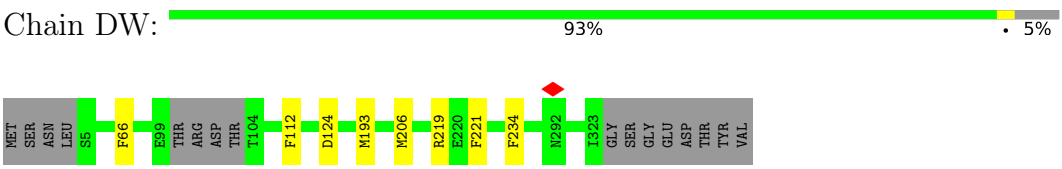

• Molecule 14: Flagellar motor switch protein FliG

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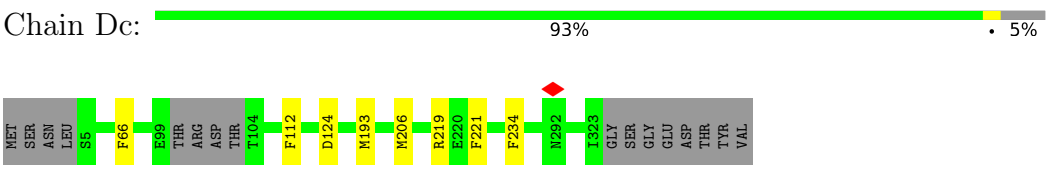

• Molecule 14: Flagellar motor switch protein FliG

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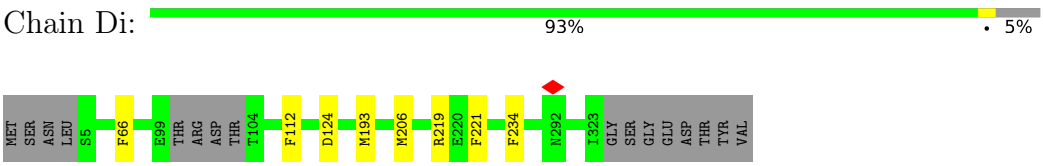
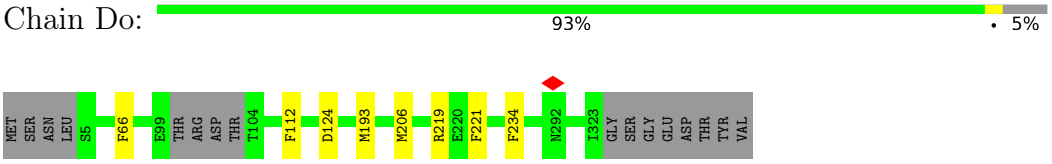


• Molecule 14: Flagellar motor switch protein FliG

Chain Do:



• Molecule 14: Flagellar motor switch protein FliG

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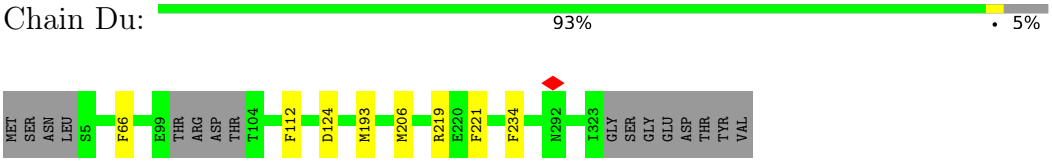
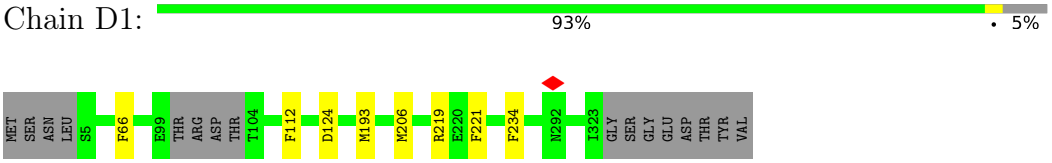


• Molecule 14: Flagellar motor switch protein FliG

Chain D1:



• Molecule 14: Flagellar motor switch protein FliG

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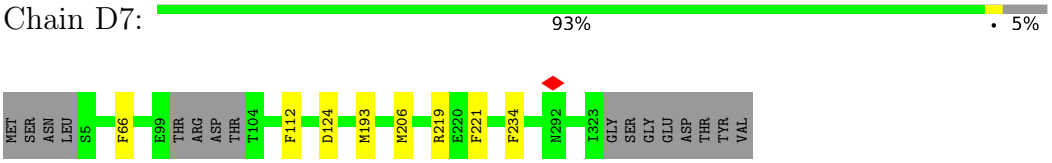
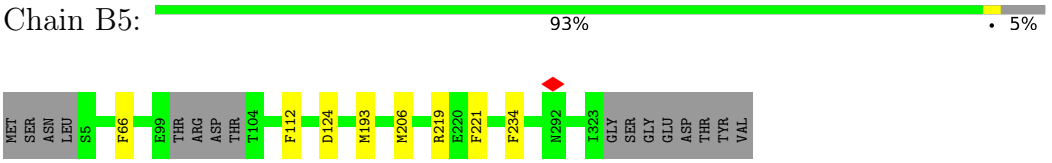


• Molecule 14: Flagellar motor switch protein FliG

Chain B5:



• Molecule 14: Flagellar motor switch protein FliG

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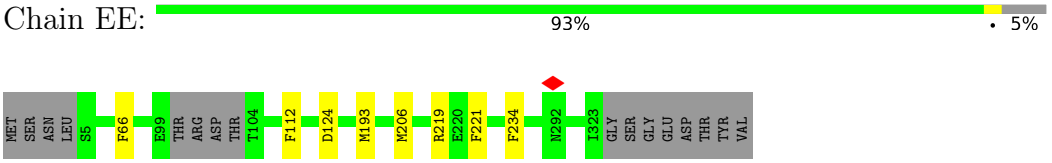
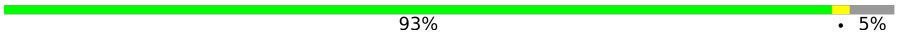


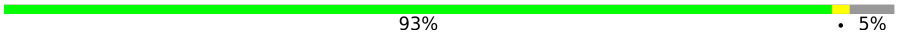
• Molecule 14: Flagellar motor switch protein FliG

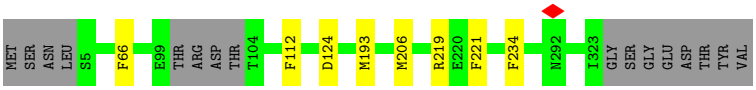
Chain EK:



• Molecule 14: Flagellar motor switch protein FliG

Chain EQ:





• Molecule 14: Flagellar motor switch protein FliG

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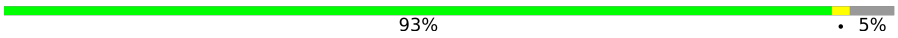

• Molecule 14: Flagellar motor switch protein FliG

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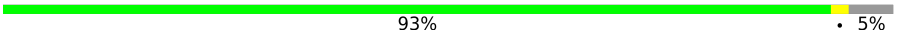

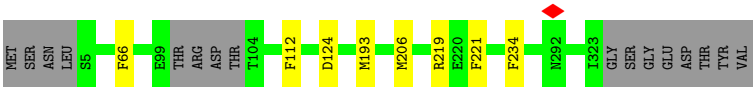

• Molecule 14: Flagellar motor switch protein FliG

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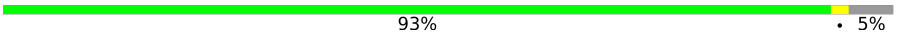
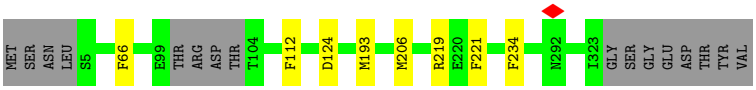
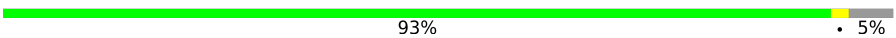
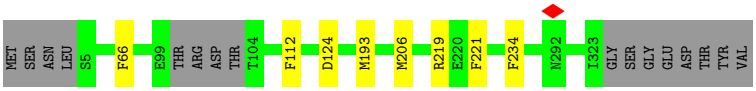




• Molecule 14: Flagellar motor switch protein FliG

Chain Bm:





• Molecule 14: Flagellar motor switch protein FliG

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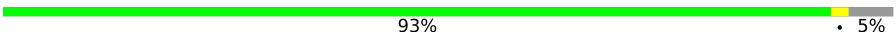
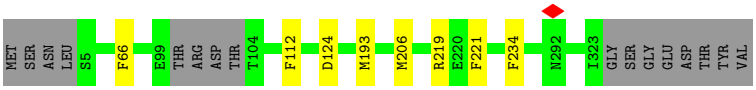
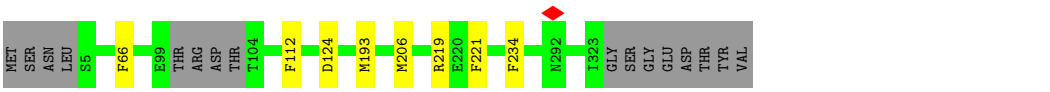




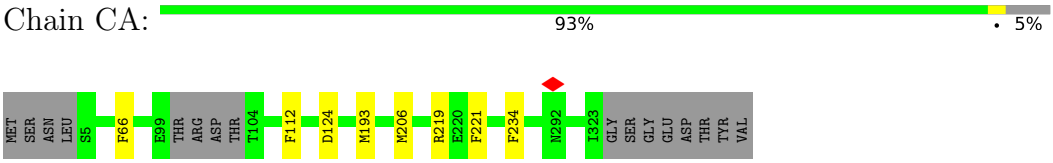
• Molecule 14: Flagellar motor switch protein FliG

Chain By:



• Molecule 14: Flagellar motor switch protein FliG

Chain CA:



• Molecule 14: Flagellar motor switch protein FliG

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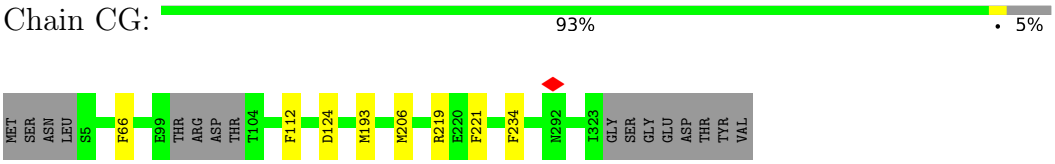

• Molecule 14: Flagellar motor switch protein FliG

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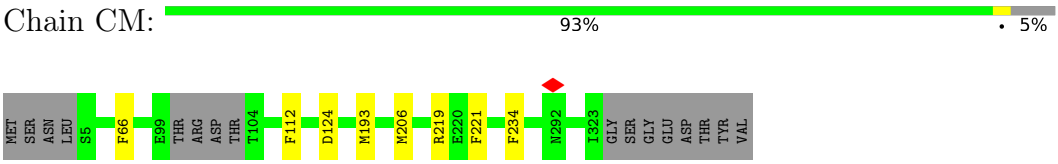

• Molecule 14: Flagellar motor switch protein FliG

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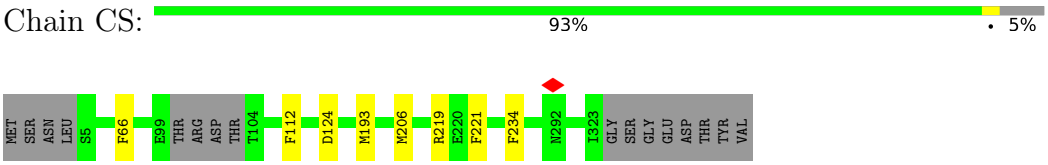

• Molecule 14: Flagellar motor switch protein FliG

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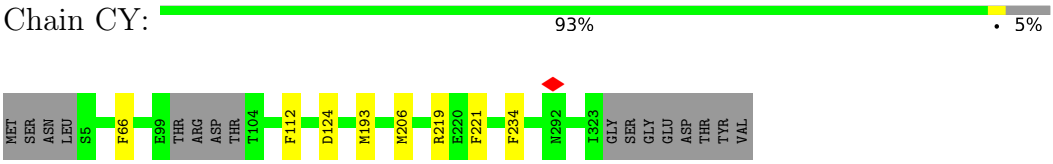

• Molecule 14: Flagellar motor switch protein FliG

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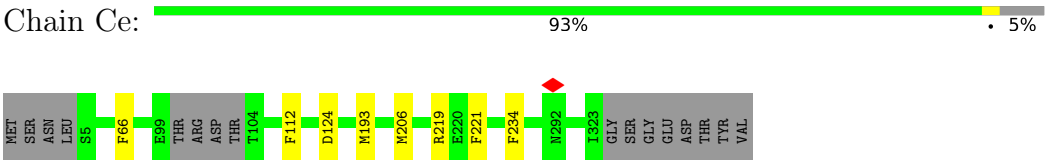

• Molecule 14: Flagellar motor switch protein FliG

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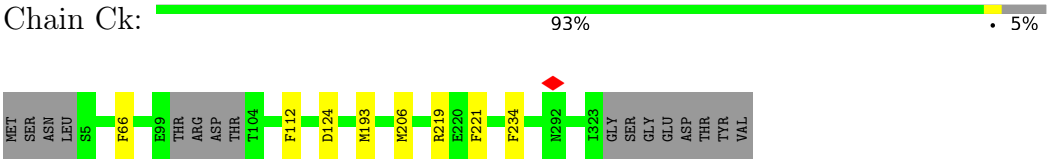

• Molecule 14: Flagellar motor switch protein FliG

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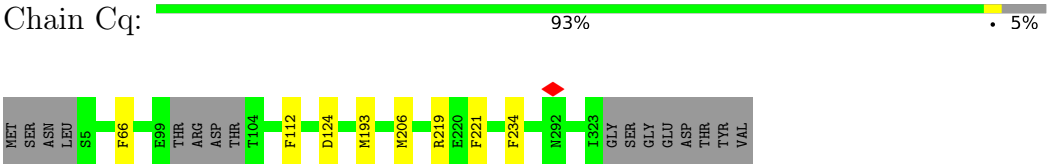
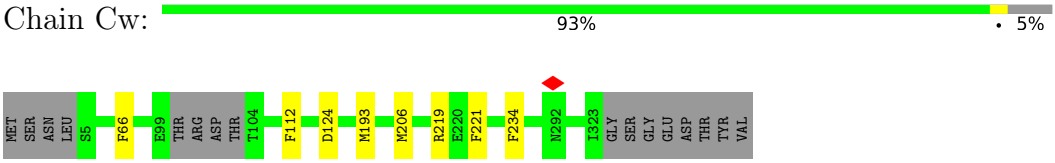


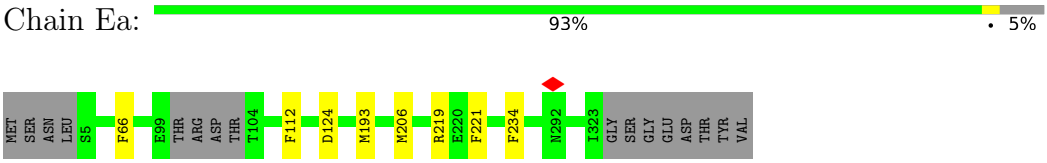
• Molecule 14: Flagellar motor switch protein FliG

Chain Cw:



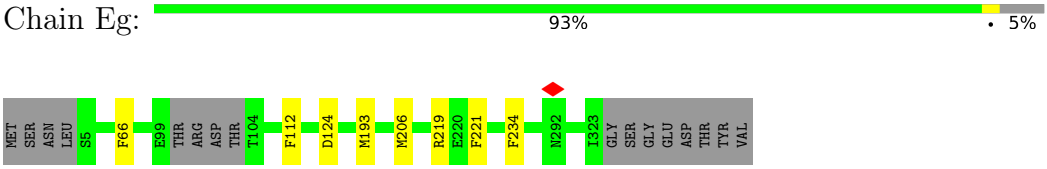
• Molecule 14: Flagellar motor switch protein FliG

Chain Ea:



• Molecule 14: Flagellar motor switch protein FliG

Chain Eg:



• Molecule 14: Flagellar motor switch protein FliG

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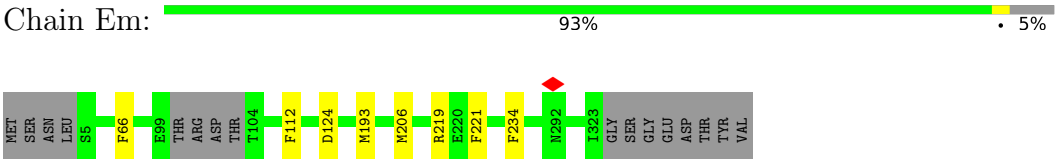
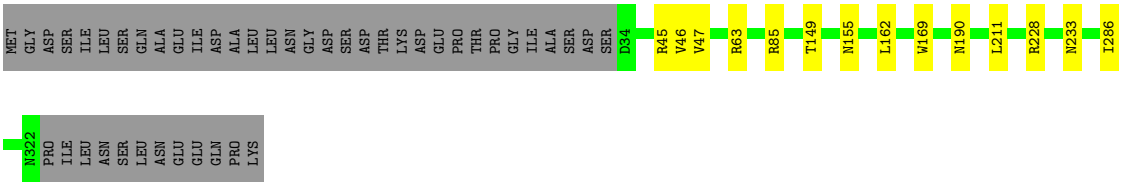


• Molecule 15: Flagellar motor switch protein FliM

Chain C8:



• Molecule 15: Flagellar motor switch protein FliM

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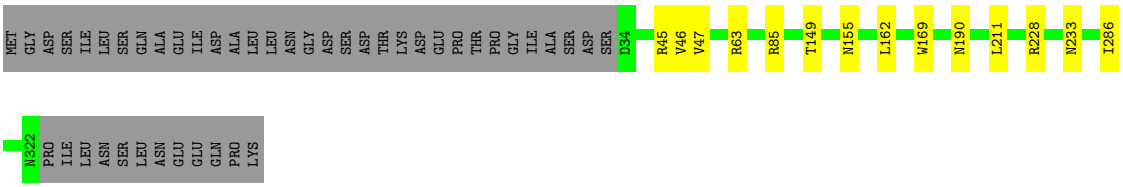
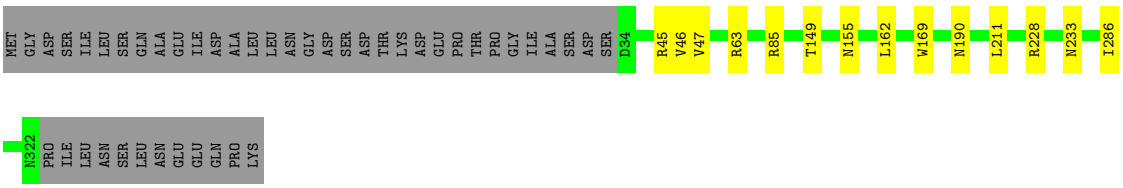


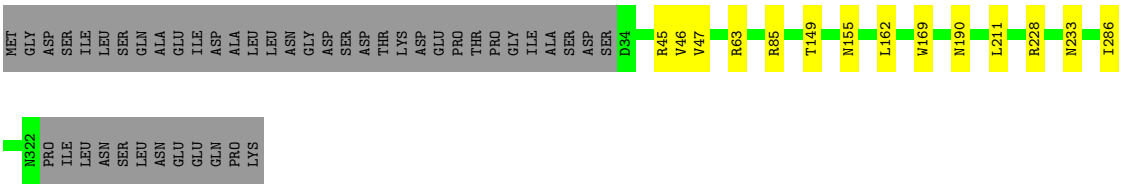
• Molecule 15: Flagellar motor switch protein FliM

Chain DL:



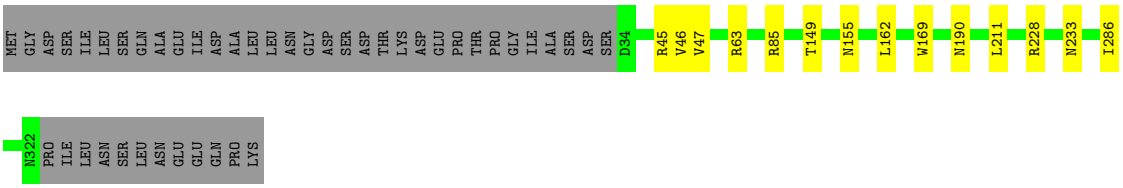
• Molecule 15: Flagellar motor switch protein FliM

Chain DM:



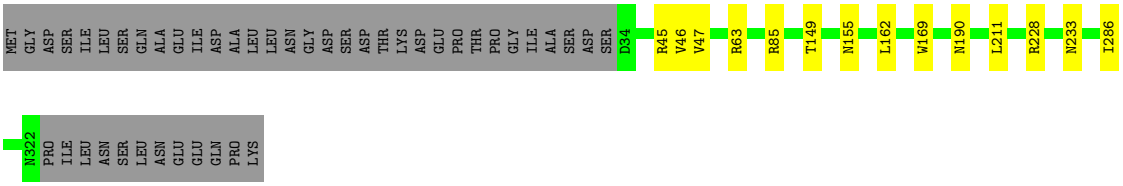
• Molecule 15: Flagellar motor switch protein FliM

Chain DS:



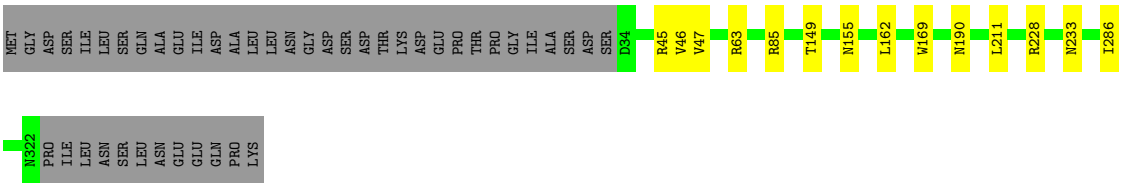
• Molecule 15: Flagellar motor switch protein FliM

Chain DY:



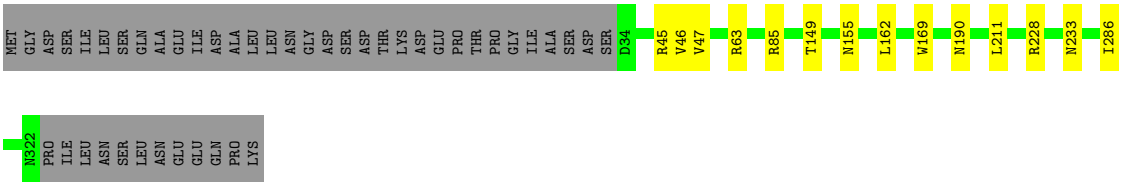
• Molecule 15: Flagellar motor switch protein FliM

Chain De:



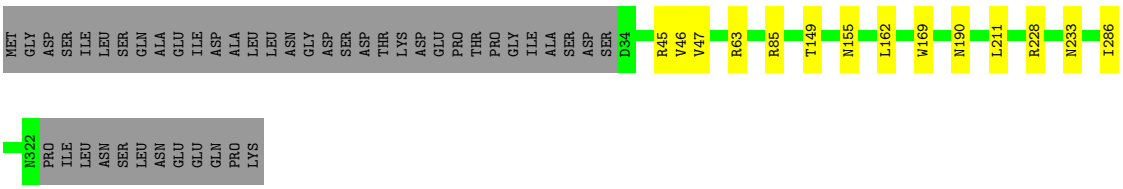
• Molecule 15: Flagellar motor switch protein FliM

Chain Dk:



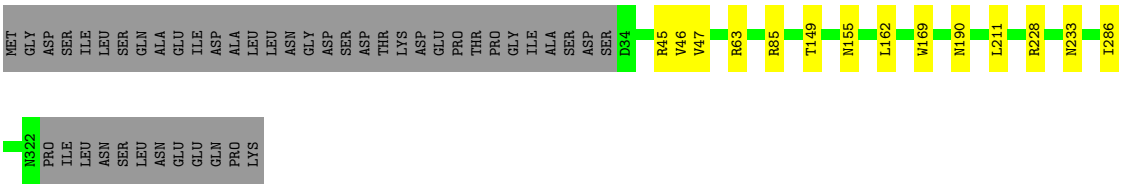
• Molecule 15: Flagellar motor switch protein FliM

Chain Dq:



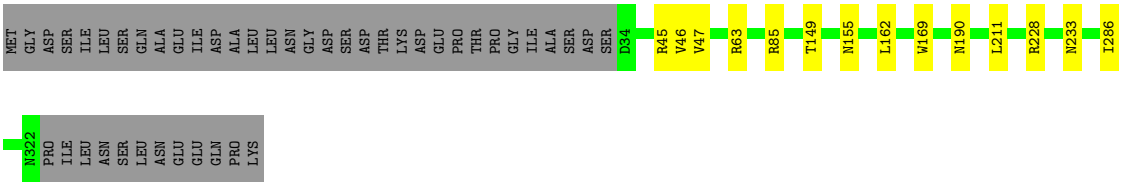
• Molecule 15: Flagellar motor switch protein FliM

Chain Dw:



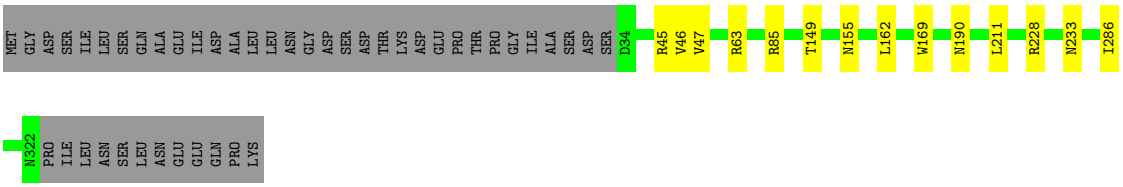
• Molecule 15: Flagellar motor switch protein FliM

Chain D3:



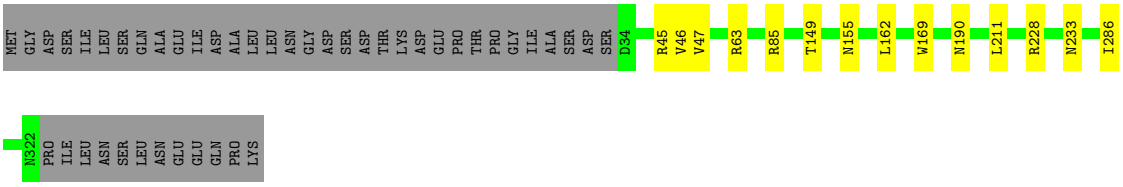
• Molecule 15: Flagellar motor switch protein FliM

Chain D9:



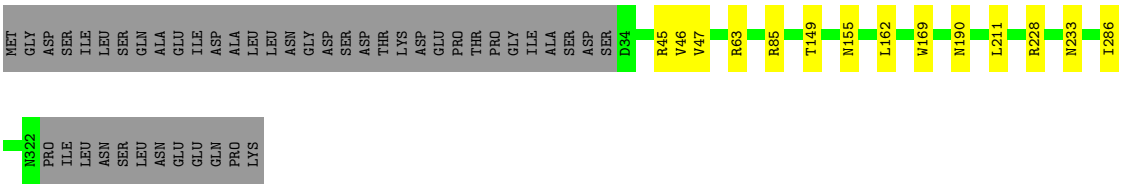
• Molecule 15: Flagellar motor switch protein FliM

Chain B1:



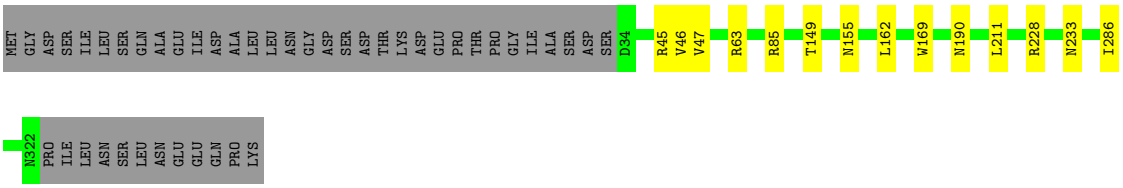
• Molecule 15: Flagellar motor switch protein FliM

Chain B7:



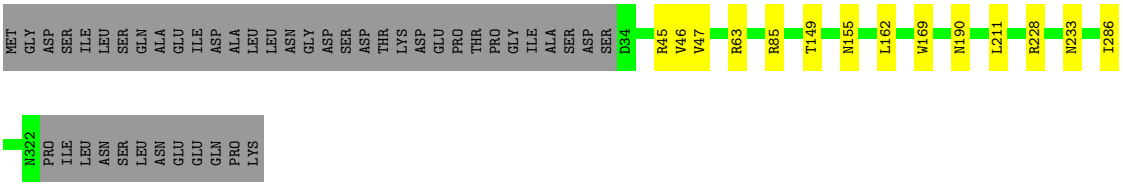
• Molecule 15: Flagellar motor switch protein FliM

Chain EG:



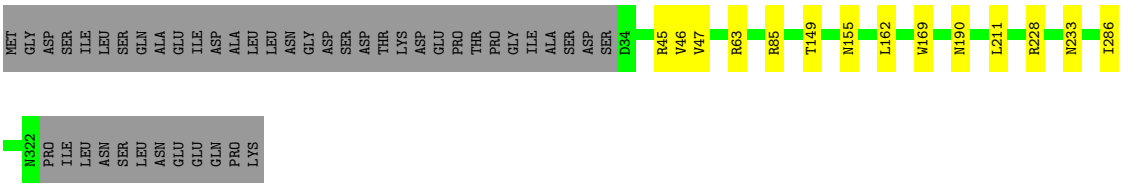
• Molecule 15: Flagellar motor switch protein FliM

Chain EM:



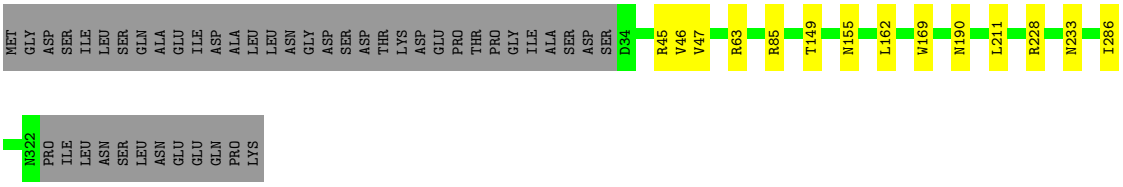
• Molecule 15: Flagellar motor switch protein FliM

Chain ES:



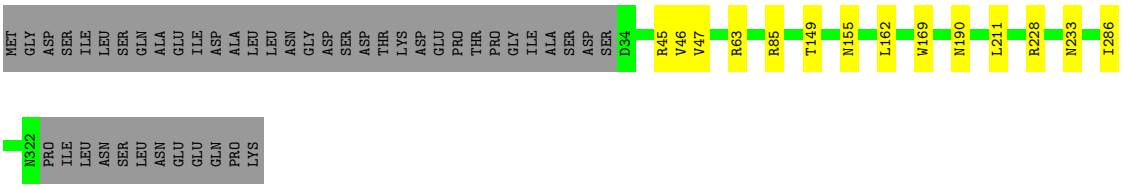
• Molecule 15: Flagellar motor switch protein FliM

Chain EY:



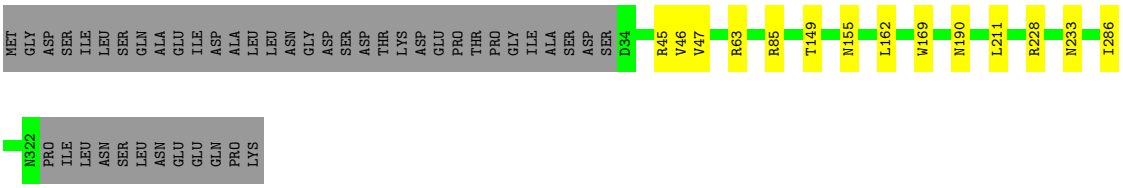
• Molecule 15: Flagellar motor switch protein FliM

Chain Bc:



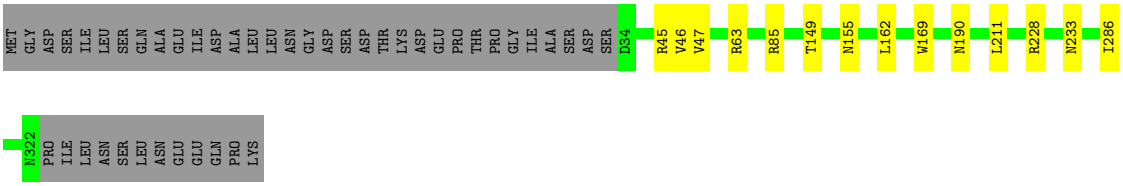
• Molecule 15: Flagellar motor switch protein FliM

Chain Bi:



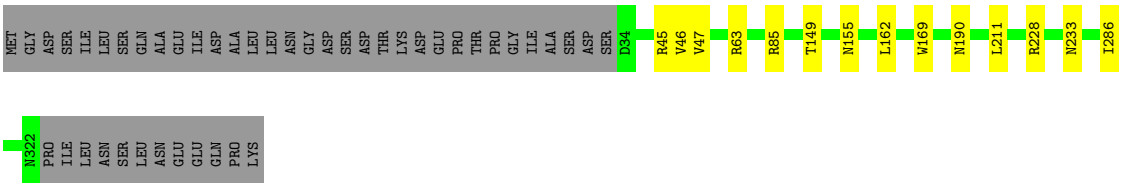
• Molecule 15: Flagellar motor switch protein FliM

Chain Bo:



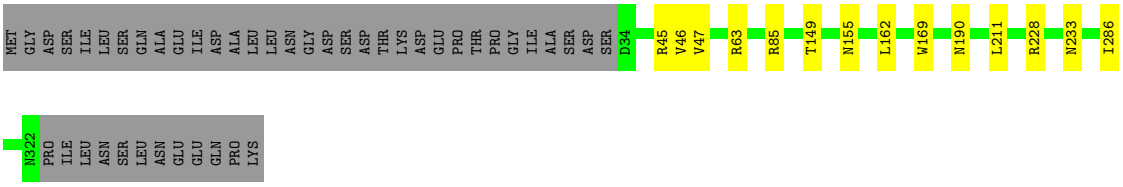
• Molecule 15: Flagellar motor switch protein FliM

Chain Bu:



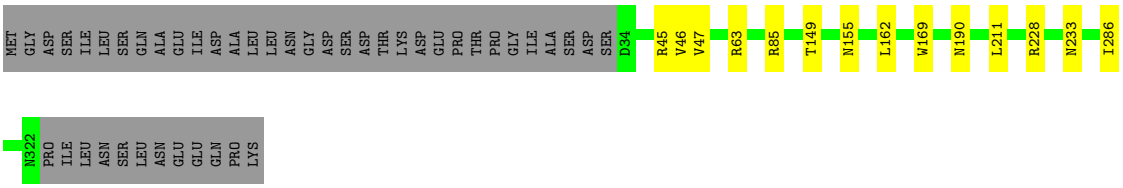
• Molecule 15: Flagellar motor switch protein FliM

Chain CC:



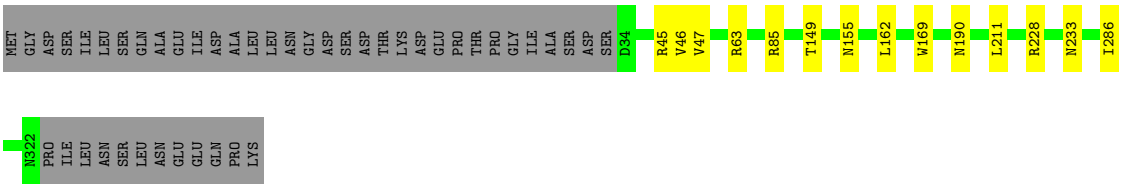
• Molecule 15: Flagellar motor switch protein FliM

Chain CI:



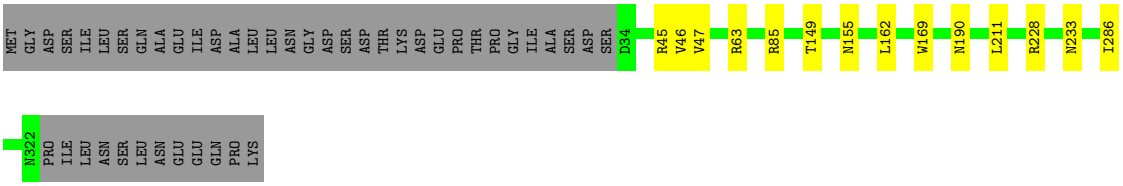
• Molecule 15: Flagellar motor switch protein FliM

Chain CO:



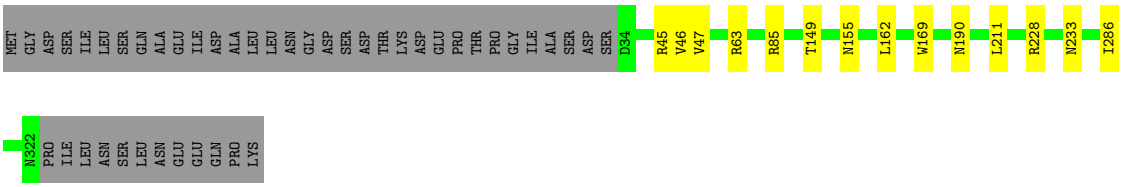
• Molecule 15: Flagellar motor switch protein FliM

Chain CU:



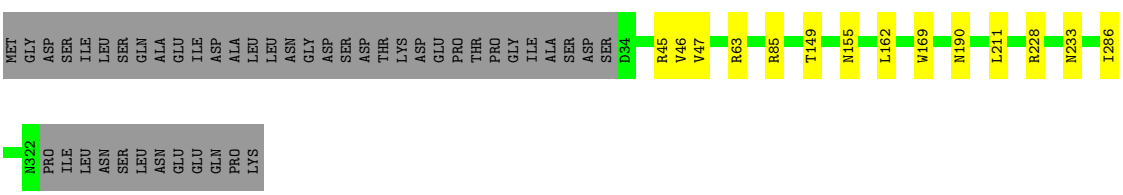
• Molecule 15: Flagellar motor switch protein FliM

Chain Ca:



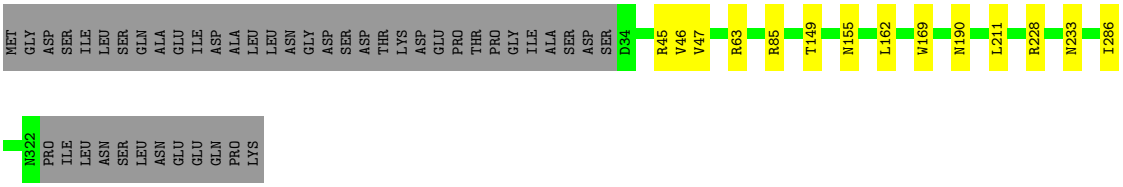
• Molecule 15: Flagellar motor switch protein FliM

Chain Cg:



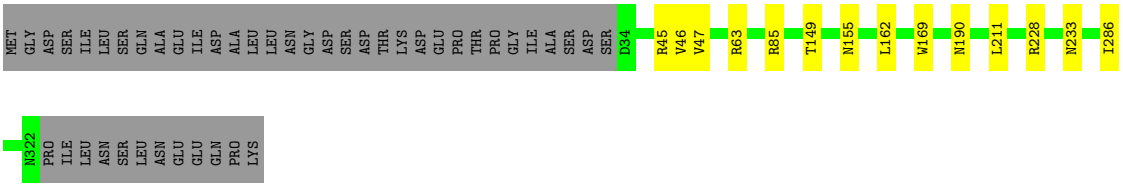
• Molecule 15: Flagellar motor switch protein FliM

Chain Cm:



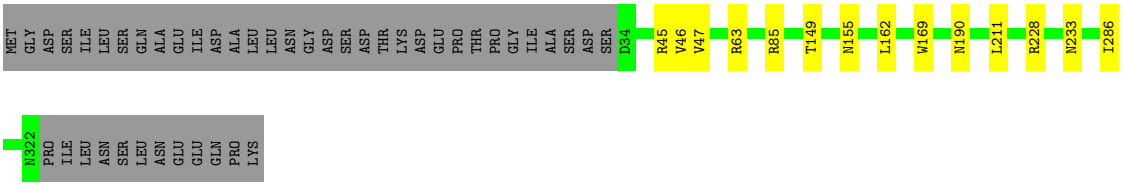
• Molecule 15: Flagellar motor switch protein FliM

Chain Cs:



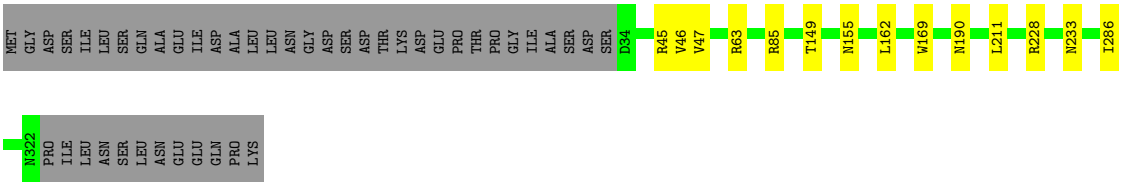
• Molecule 15: Flagellar motor switch protein FliM

Chain Cy:



• Molecule 15: Flagellar motor switch protein FliM

Chain Ec:

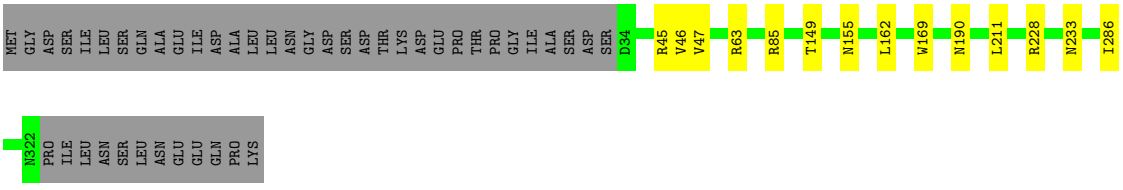


• Molecule 15: Flagellar motor switch protein FliM

Chain Ei:

• Molecule 15: Flagellar motor switch protein FliM

Chain Eo:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	10318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	41	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.608	Depositor
Minimum map value	-0.537	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	880.0, 880.0, 880.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.33	0/1888	0.54	1/2564 (0.0%)
1	1	0.31	0/1917	0.51	0/2605
1	2	0.29	0/1973	0.50	0/2682
1	3	0.28	0/1973	0.52	0/2682
1	4	0.28	0/1973	0.51	0/2682
1	5	0.33	0/1973	0.52	0/2682
1	6	0.32	0/1973	0.54	0/2682
1	7	0.32	0/1973	0.53	0/2682
1	8	0.33	0/1973	0.56	0/2682
1	9	0.30	0/1973	0.53	1/2682 (0.0%)
1	AF	0.34	0/1926	0.53	0/2618
1	AG	0.38	0/1934	0.59	0/2629
1	AH	0.39	0/1942	0.56	0/2639
1	AI	0.35	0/1926	0.58	1/2618 (0.0%)
1	AJ	0.34	0/1934	0.54	0/2629
1	AK	0.34	0/1844	0.51	0/2505
1	AL	0.33	0/1888	0.52	0/2564
1	AM	0.33	0/1888	0.56	1/2564 (0.0%)
1	AN	0.31	0/1888	0.52	0/2564
1	ZA	0.31	0/1973	0.53	0/2682
1	ZB	0.29	0/1973	0.49	0/2682
1	ZC	0.34	0/1973	0.54	0/2682
1	ZD	0.31	0/1973	0.52	0/2682
1	ZE	0.30	0/1973	0.51	1/2682 (0.0%)
2	A	0.30	0/1613	0.51	0/2194
2	B	0.30	0/1613	0.51	0/2194
2	C	0.30	0/1613	0.51	0/2194
2	D	0.30	0/1613	0.51	0/2194
2	E	0.30	0/1613	0.51	0/2194
2	F	0.30	0/1613	0.51	0/2194
2	G	0.30	0/1613	0.51	0/2194
2	H	0.30	0/1613	0.51	0/2194
2	I	0.30	0/1613	0.51	0/2194
2	J	0.30	0/1613	0.51	0/2194

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	K	0.30	0/1613	0.51	0/2194
2	L	0.30	0/1613	0.51	0/2194
2	M	0.30	0/1613	0.51	0/2194
2	N	0.30	0/1613	0.51	0/2194
2	O	0.30	0/1613	0.51	0/2194
2	P	0.30	0/1613	0.51	0/2194
2	Q	0.30	0/1613	0.51	0/2194
2	R	0.30	0/1613	0.51	0/2194
2	S	0.30	0/1613	0.51	0/2194
2	T	0.29	0/1613	0.51	0/2194
2	U	0.30	0/1613	0.51	0/2194
2	V	0.30	0/1613	0.51	0/2194
2	W	0.29	0/1613	0.51	0/2194
2	X	0.30	0/1613	0.51	0/2194
2	Y	0.30	0/1613	0.51	0/2194
2	Z	0.30	0/1613	0.51	0/2194
3	A0	0.34	0/959	0.50	0/1293
3	A6	0.37	0/1042	0.56	0/1408
3	A7	0.33	0/951	0.50	0/1282
3	A8	0.35	0/976	0.56	0/1316
3	A9	0.35	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	0.50	0/925
4	A4	0.37	0/689	0.53	0/925
4	A5	0.40	0/682	0.52	0/915
4	Az	0.43	0/428	0.57	0/572
5	AA	0.33	0/1828	0.56	0/2492
5	AB	0.33	0/1836	0.56	2/2502 (0.1%)
5	AC	0.37	0/1844	0.57	0/2512
5	AD	0.33	0/1844	0.57	0/2512
5	AE	0.33	0/1836	0.58	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	0.27	0/1289	0.53	0/1741
6	B6	0.22	0/226	0.48	0/303
6	BG	0.46	0/83	0.87	1/114 (0.9%)
6	BH	0.26	0/107	0.38	0/148
6	BI	0.31	0/137	0.49	0/191
6	BJ	0.28	0/107	0.57	0/148
6	BK	0.40	0/145	0.55	0/203
6	BL	0.33	0/107	0.51	0/148
6	BM	0.26	0/145	0.43	0/203
6	BN	0.30	0/107	0.38	0/148
6	BO	0.33	0/137	0.70	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	0.53	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	0.27	0/1289	0.52	0/1741
6	BX	0.27	0/1289	0.53	0/1741
6	Bb	0.22	0/226	0.48	0/303
6	Bh	0.22	0/226	0.48	0/303
6	Bn	0.22	0/226	0.49	0/303
6	Bt	0.22	0/226	0.50	0/303
6	Bz	0.22	0/226	0.48	0/303
6	C3	0.22	0/226	0.49	0/303
6	C7	0.22	0/226	0.49	0/303
6	CB	0.22	0/226	0.49	0/303

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	CH	0.22	0/226	0.48	0/303
6	CN	0.22	0/226	0.49	0/303
6	CT	0.21	0/226	0.48	0/303
6	CZ	0.22	0/226	0.49	0/303
6	Cf	0.22	0/226	0.49	0/303
6	Cl	0.22	0/226	0.49	0/303
6	Cr	0.22	0/226	0.49	0/303
6	Cx	0.22	0/226	0.49	0/303
6	D2	0.22	0/226	0.49	0/303
6	D8	0.22	0/226	0.48	0/303
6	DE	0.22	0/226	0.49	0/303
6	DK	0.22	0/226	0.48	0/303
6	DR	0.22	0/226	0.49	0/303
6	DX	0.22	0/226	0.49	0/303
6	Dd	0.22	0/226	0.48	0/303
6	Dj	0.22	0/226	0.48	0/303
6	Dp	0.22	0/226	0.48	0/303
6	Dv	0.22	0/226	0.49	0/303
6	EF	0.21	0/226	0.49	0/303
6	EL	0.22	0/226	0.49	0/303
6	ER	0.22	0/226	0.49	0/303
6	EX	0.22	0/226	0.49	0/303
6	Eb	0.22	0/226	0.49	0/303
6	Eh	0.22	0/226	0.48	0/303
6	En	0.22	0/226	0.48	0/303
6	UI	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UJ	0.84	3/1191 (0.3%)	0.82	4/1618 (0.2%)
6	UK	0.83	2/1191 (0.2%)	0.83	4/1618 (0.2%)
6	UL	0.82	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UM	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UN	0.84	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	0.60	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	0.59	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	0.71	0/1152
6	WU	0.60	0/857	0.67	0/1164
6	WV	0.62	0/841	0.69	0/1142
6	WW	0.60	0/848	0.70	0/1152
7	Ab	0.45	0/681	0.67	1/930 (0.1%)
7	Aq	0.33	0/681	0.53	0/930
7	Ar	0.28	0/681	0.50	0/930
7	As	0.27	0/681	0.48	0/930
8	At	0.31	0/1994	0.52	0/2724
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	0.50	0/2249
9	Ax	0.29	0/1652	0.47	0/2249
9	Ay	0.33	0/1662	0.52	0/2263
10	BA	0.30	0/981	0.47	0/1334
10	BB	0.29	0/976	0.50	0/1327
10	BC	0.34	0/981	0.50	0/1334
10	BD	0.33	0/981	0.62	0/1334
10	BE	0.29	0/968	0.48	0/1316
10	BF	0.36	0/981	0.52	0/1334
11	ZF	0.28	0/2991	0.49	0/4076
11	ZG	0.34	0/2991	0.52	1/4076 (0.0%)
11	ZH	0.29	0/2991	0.50	0/4076
11	ZI	0.30	0/2991	0.51	0/4076
11	ZJ	0.31	0/2991	0.49	0/4076
11	ZK	0.30	0/2991	0.50	0/4076
11	ZL	0.29	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	0.29	0/2991	0.48	0/4076
11	ZU	0.29	0/2991	0.50	0/4076
11	ZV	0.50	4/2991 (0.1%)	0.67	6/4076 (0.1%)
11	ZW	0.27	0/2991	0.49	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	0.26	0/2991	0.46	0/4076
11	Za	0.28	0/2991	0.49	0/4076
11	Zb	0.30	0/2991	0.49	0/4076
11	Zc	0.29	0/2991	0.52	2/4076 (0.0%)
11	Zd	0.30	0/2991	0.51	0/4076
11	Ze	0.28	0/2991	0.48	0/4076
11	Zf	0.27	0/2991	0.48	0/4076
11	Zg	0.28	0/2991	0.50	0/4076
11	Zh	0.28	0/2991	0.48	0/4076
12	a	0.31	0/2243	0.55	0/3041
12	b	0.31	0/2243	0.55	0/3041
12	c	0.31	0/2243	0.55	0/3041
12	d	0.31	0/2243	0.55	0/3041
12	e	0.31	0/2243	0.55	0/3041
12	f	0.31	0/2243	0.55	0/3041
12	g	0.30	0/2243	0.55	0/3041
12	h	0.31	0/2243	0.55	0/3041
12	i	0.31	0/2243	0.55	0/3041
12	j	0.31	0/2243	0.55	0/3041
12	k	0.31	0/2243	0.55	0/3041
12	l	0.30	0/2243	0.55	0/3041
12	m	0.30	0/2243	0.55	0/3041
12	n	0.31	0/2243	0.55	0/3041
12	o	0.30	0/2243	0.55	0/3041
12	p	0.31	0/2243	0.55	0/3041
12	q	0.31	0/2243	0.54	0/3041
12	r	0.31	0/2243	0.55	0/3041
12	s	0.30	0/2243	0.55	0/3041
12	t	0.31	0/2243	0.55	0/3041
12	u	0.31	0/2243	0.55	0/3041
12	v	0.31	0/2243	0.55	0/3041
12	w	0.31	0/2243	0.55	0/3041
12	x	0.31	0/2243	0.55	0/3041
12	y	0.31	0/2243	0.55	0/3041
12	z	0.31	0/2243	0.55	0/3041
13	B0	0.23	0/679	0.53	0/917
13	B2	0.23	0/679	0.52	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
13	B3	0.23	0/679	0.52	0/917
13	B4	0.23	0/679	0.53	0/917
13	B8	0.23	0/679	0.53	0/917
13	B9	0.23	0/679	0.53	0/917
13	BY	0.23	0/679	0.53	0/917
13	BZ	0.23	0/679	0.53	0/917
13	Bd	0.23	0/679	0.53	0/917
13	Be	0.23	0/679	0.52	0/917
13	Bf	0.23	0/679	0.53	0/917
13	Bj	0.23	0/679	0.53	0/917
13	Bk	0.23	0/679	0.53	0/917
13	Bl	0.23	0/679	0.53	0/917
13	Bp	0.23	0/679	0.53	0/917
13	Bq	0.23	0/679	0.52	0/917
13	Br	0.23	0/679	0.53	0/917
13	Bv	0.23	0/679	0.53	0/917
13	Bw	0.23	0/679	0.52	0/917
13	Bx	0.23	0/679	0.53	0/917
13	C0	0.23	0/679	0.52	0/917
13	C1	0.23	0/679	0.52	0/917
13	C2	0.23	0/679	0.53	0/917
13	C4	0.23	0/679	0.52	0/917
13	C5	0.23	0/679	0.53	0/917
13	C9	0.23	0/679	0.53	0/917
13	CD	0.23	0/679	0.53	0/917
13	CE	0.23	0/679	0.52	0/917
13	CF	0.23	0/679	0.53	0/917
13	CJ	0.23	0/679	0.52	0/917
13	CK	0.23	0/679	0.52	0/917
13	CL	0.23	0/679	0.53	0/917
13	CP	0.23	0/679	0.53	0/917
13	CQ	0.23	0/679	0.53	0/917
13	CR	0.23	0/679	0.53	0/917
13	CV	0.23	0/679	0.53	0/917
13	CW	0.23	0/679	0.52	0/917
13	CX	0.23	0/679	0.53	0/917
13	Cb	0.23	0/679	0.53	0/917
13	Cc	0.23	0/679	0.52	0/917
13	Cd	0.23	0/679	0.53	0/917
13	Ch	0.23	0/679	0.53	0/917
13	Ci	0.23	0/679	0.53	0/917
13	Cj	0.23	0/679	0.53	0/917
13	Cn	0.23	0/679	0.53	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
13	Co	0.23	0/679	0.52	0/917
13	Cp	0.23	0/679	0.53	0/917
13	Ct	0.23	0/679	0.53	0/917
13	Cu	0.23	0/679	0.53	0/917
13	Cv	0.23	0/679	0.53	0/917
13	Cz	0.23	0/679	0.52	0/917
13	D0	0.23	0/679	0.53	0/917
13	D4	0.23	0/679	0.53	0/917
13	D5	0.23	0/679	0.52	0/917
13	D6	0.23	0/679	0.53	0/917
13	DA	0.23	0/679	0.53	0/917
13	DC	0.23	0/679	0.53	0/917
13	DG	0.23	0/679	0.53	0/917
13	DH	0.23	0/679	0.53	0/917
13	DI	0.23	0/679	0.53	0/917
13	DN	0.23	0/679	0.53	0/917
13	DO	0.23	0/679	0.52	0/917
13	DP	0.23	0/679	0.53	0/917
13	DT	0.23	0/679	0.53	0/917
13	DU	0.23	0/679	0.52	0/917
13	DV	0.23	0/679	0.53	0/917
13	DZ	0.23	0/679	0.52	0/917
13	Da	0.23	0/679	0.52	0/917
13	Db	0.23	0/679	0.53	0/917
13	Df	0.23	0/679	0.53	0/917
13	Dg	0.23	0/679	0.53	0/917
13	Dh	0.23	0/679	0.53	0/917
13	Dl	0.23	0/679	0.53	0/917
13	Dm	0.23	0/679	0.53	0/917
13	Dn	0.23	0/679	0.53	0/917
13	Dr	0.23	0/679	0.52	0/917
13	Ds	0.23	0/679	0.52	0/917
13	Dt	0.23	0/679	0.53	0/917
13	Dx	0.23	0/679	0.53	0/917
13	Dy	0.23	0/679	0.53	0/917
13	Dz	0.23	0/679	0.53	0/917
13	EA	0.23	0/679	0.53	0/917
13	EB	0.23	0/679	0.53	0/917
13	EC	0.23	0/679	0.52	0/917
13	ED	0.23	0/679	0.53	0/917
13	EH	0.23	0/679	0.53	0/917
13	EI	0.23	0/679	0.52	0/917
13	EJ	0.23	0/679	0.53	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
13	EN	0.23	0/679	0.52	0/917
13	EO	0.23	0/679	0.52	0/917
13	EP	0.23	0/679	0.53	0/917
13	ET	0.23	0/679	0.53	0/917
13	EU	0.23	0/679	0.53	0/917
13	EV	0.23	0/679	0.53	0/917
13	EZ	0.23	0/679	0.53	0/917
13	Ed	0.23	0/679	0.53	0/917
13	Ee	0.23	0/679	0.52	0/917
13	Ef	0.23	0/679	0.53	0/917
13	Ej	0.23	0/679	0.53	0/917
13	Ek	0.23	0/679	0.52	0/917
13	El	0.23	0/679	0.53	0/917
13	Ep	0.23	0/679	0.53	0/917
14	B5	0.27	0/2481	0.48	1/3344 (0.0%)
14	Ba	0.27	0/2481	0.48	1/3344 (0.0%)
14	Bg	0.27	0/2481	0.48	1/3344 (0.0%)
14	Bm	0.28	0/2481	0.48	1/3344 (0.0%)
14	Bs	0.27	0/2481	0.48	1/3344 (0.0%)
14	By	0.27	0/2481	0.48	1/3344 (0.0%)
14	C6	0.27	0/2481	0.48	1/3344 (0.0%)
14	CA	0.28	0/2481	0.48	1/3344 (0.0%)
14	CG	0.28	0/2481	0.48	1/3344 (0.0%)
14	CM	0.28	0/2481	0.48	1/3344 (0.0%)
14	CS	0.28	0/2481	0.48	1/3344 (0.0%)
14	CY	0.28	0/2481	0.48	1/3344 (0.0%)
14	Ce	0.28	0/2481	0.48	1/3344 (0.0%)
14	Ck	0.28	0/2481	0.48	1/3344 (0.0%)
14	Cq	0.28	0/2481	0.48	1/3344 (0.0%)
14	Cw	0.28	0/2481	0.48	1/3344 (0.0%)
14	D1	0.28	0/2481	0.48	1/3344 (0.0%)
14	D7	0.28	0/2481	0.48	1/3344 (0.0%)
14	DB	0.28	0/2481	0.48	1/3344 (0.0%)
14	DD	0.28	0/2481	0.48	1/3344 (0.0%)
14	DJ	0.28	0/2481	0.48	1/3344 (0.0%)
14	DQ	0.27	0/2481	0.48	1/3344 (0.0%)
14	DW	0.28	0/2481	0.48	1/3344 (0.0%)
14	Dc	0.28	0/2481	0.48	1/3344 (0.0%)
14	Di	0.28	0/2481	0.48	1/3344 (0.0%)
14	Do	0.28	0/2481	0.48	1/3344 (0.0%)
14	Du	0.28	0/2481	0.48	1/3344 (0.0%)
14	EE	0.28	0/2481	0.48	1/3344 (0.0%)
14	EK	0.28	0/2481	0.48	1/3344 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	EQ	0.27	0/2481	0.48	1/3344 (0.0%)
14	EW	0.27	0/2481	0.48	1/3344 (0.0%)
14	Ea	0.27	0/2481	0.48	1/3344 (0.0%)
14	Eg	0.28	0/2481	0.48	1/3344 (0.0%)
14	Em	0.27	0/2481	0.48	1/3344 (0.0%)
15	B1	0.25	0/2393	0.50	0/3255
15	B7	0.25	0/2393	0.50	0/3255
15	Bc	0.25	0/2393	0.50	0/3255
15	Bi	0.25	0/2393	0.50	0/3255
15	Bo	0.25	0/2393	0.50	0/3255
15	Bu	0.25	0/2393	0.50	0/3255
15	C8	0.25	0/2393	0.50	0/3255
15	CC	0.25	0/2393	0.50	0/3255
15	CI	0.25	0/2393	0.50	0/3255
15	CO	0.25	0/2393	0.50	0/3255
15	CU	0.25	0/2393	0.50	0/3255
15	Ca	0.25	0/2393	0.50	0/3255
15	Cg	0.25	0/2393	0.50	0/3255
15	Cm	0.25	0/2393	0.50	0/3255
15	Cs	0.25	0/2393	0.50	0/3255
15	Cy	0.25	0/2393	0.50	0/3255
15	D3	0.25	0/2393	0.50	0/3255
15	D9	0.25	0/2393	0.50	0/3255
15	DF	0.25	0/2393	0.50	0/3255
15	DL	0.25	0/2393	0.50	0/3255
15	DM	0.25	0/2393	0.50	0/3255
15	DS	0.25	0/2393	0.50	0/3255
15	DY	0.25	0/2393	0.50	0/3255
15	De	0.25	0/2393	0.50	0/3255
15	Dk	0.25	0/2393	0.50	0/3255
15	Dq	0.25	0/2393	0.50	0/3255
15	Dw	0.25	0/2393	0.50	0/3255
15	EG	0.25	0/2393	0.50	0/3255
15	EM	0.25	0/2393	0.50	0/3255
15	ES	0.25	0/2393	0.50	0/3255
15	EY	0.25	0/2393	0.50	0/3255
15	Ec	0.25	0/2393	0.50	0/3255
15	Ei	0.25	0/2393	0.50	0/3255
15	Eo	0.25	0/2393	0.50	0/3255
All	All	0.31	23/585907 (0.0%)	0.53	98/794525 (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	2
1	7	0	1
1	8	0	2
1	AF	0	1
1	AI	0	1
1	AK	0	1
1	AL	0	1
1	AM	0	2
1	AN	0	3
1	ZA	0	2
1	ZD	0	1
1	ZE	0	3
3	A0	0	1
3	A6	0	1
3	A7	0	1
3	A9	0	1
5	AA	0	1
5	AB	0	2
5	AD	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

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Mol	Chain	#Chirality outliers	#Planarity outliers
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
9	Aw	0	2
9	Ay	0	2
10	BD	0	1
10	BF	0	1
11	ZI	0	1
11	ZK	0	1
11	ZO	0	1
11	ZT	0	1
11	ZU	0	1
11	ZW	0	1
11	ZZ	0	1
11	Zd	0	1
11	Ze	0	1
14	B5	0	2
14	Ba	0	2
14	Bg	0	2
14	Bm	0	2
14	Bs	0	2
14	By	0	2
14	C6	0	2
14	CA	0	2
14	CG	0	2
14	CM	0	2
14	CS	0	2
14	CY	0	2
14	Ce	0	2
14	Ck	0	2
14	Cq	0	2
14	Cw	0	2
14	D1	0	2
14	D7	0	2
14	DB	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	DD	0	2
14	DJ	0	2
14	DQ	0	2
14	DW	0	2
14	Dc	0	2
14	Di	0	2
14	Do	0	2
14	Du	0	2
14	EE	0	2
14	EK	0	2
14	EQ	0	2
14	EW	0	2
14	Ea	0	2
14	Eg	0	2
14	Em	0	2
All	All	0	181

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	ZV	140	PRO	CG-CD	-16.11	0.97	1.50
11	ZV	125	PRO	CG-CD	-10.15	1.17	1.50
6	UL	172	PRO	N-CD	-9.55	1.34	1.47
6	UI	172	PRO	N-CD	-9.53	1.34	1.47
6	UM	172	PRO	N-CD	-9.52	1.34	1.47
6	UN	172	PRO	N-CD	-9.52	1.34	1.47
6	UO	172	PRO	N-CD	-9.47	1.34	1.47
6	UK	172	PRO	N-CD	-9.42	1.34	1.47
6	UJ	172	PRO	N-CD	-9.40	1.34	1.47
6	UP	172	PRO	N-CD	-9.39	1.34	1.47
11	ZV	140	PRO	N-CD	8.32	1.59	1.47
6	UJ	125	GLN	C-N	7.70	1.51	1.34
6	UK	125	GLN	C-N	7.65	1.51	1.34
6	UO	125	GLN	C-N	7.60	1.51	1.34
6	UI	125	GLN	C-N	7.59	1.51	1.34
6	UP	125	GLN	C-N	7.59	1.51	1.34
6	UN	125	GLN	C-N	7.58	1.51	1.34
6	UL	125	GLN	C-N	7.57	1.51	1.34
6	UM	125	GLN	C-N	7.53	1.51	1.34
11	ZV	125	PRO	N-CD	6.65	1.57	1.47
11	ZY	125	PRO	CG-CD	-5.47	1.32	1.50
11	ZR	125	PRO	CG-CD	-5.11	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	UJ	105	LEU	C-N	-5.01	1.24	1.34

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	ZV	140	PRO	N-CD-CG	-17.34	77.20	103.20
11	ZR	125	PRO	CA-N-CD	-13.98	91.92	111.50
11	ZY	125	PRO	CA-N-CD	-13.29	92.89	111.50
11	ZV	125	PRO	CA-N-CD	-13.25	92.96	111.50
9	Au	162	PRO	CA-N-CD	-11.97	94.74	111.50
11	Zc	125	PRO	CA-N-CD	-11.28	95.71	111.50
11	ZV	125	PRO	N-CD-CG	-11.25	86.32	103.20
11	ZV	140	PRO	CA-N-CD	-10.20	97.22	111.50
11	ZV	140	PRO	CA-CB-CG	-9.29	86.35	104.00
6	UO	126	PHE	O-C-N	8.83	136.82	122.70
6	UL	126	PHE	O-C-N	8.82	136.82	122.70
6	UN	126	PHE	O-C-N	8.80	136.78	122.70
6	UJ	126	PHE	O-C-N	8.80	136.78	122.70
6	UI	126	PHE	O-C-N	8.79	136.76	122.70
6	UK	126	PHE	O-C-N	8.79	136.76	122.70
6	UP	126	PHE	O-C-N	8.78	136.74	122.70
6	UM	126	PHE	O-C-N	8.76	136.72	122.70
11	ZM	223	PRO	CA-N-CD	-8.39	99.76	111.50
11	ZR	125	PRO	N-CD-CG	-7.59	91.82	103.20
11	ZY	125	PRO	N-CD-CG	-7.43	92.05	103.20
6	UL	126	PHE	CA-C-N	-6.79	102.26	117.20
6	UO	126	PHE	CA-C-N	-6.78	102.28	117.20
6	UK	126	PHE	CA-C-N	-6.77	102.30	117.20
6	UJ	126	PHE	CA-C-N	-6.76	102.33	117.20
6	UP	126	PHE	CA-C-N	-6.74	102.37	117.20
6	UI	126	PHE	CA-C-N	-6.74	102.38	117.20
6	UM	126	PHE	CA-C-N	-6.73	102.38	117.20
6	UN	126	PHE	CA-C-N	-6.71	102.44	117.20
9	Au	162	PRO	N-CD-CG	-6.59	93.31	103.20
6	UK	129	GLN	O-C-N	6.42	132.97	122.70
6	UP	129	GLN	O-C-N	6.39	132.93	122.70
6	UO	129	GLN	O-C-N	6.35	132.87	122.70
6	UL	129	GLN	O-C-N	6.31	132.79	122.70
6	UM	129	GLN	O-C-N	6.30	132.79	122.70
6	WA	162	PRO	N-CA-C	6.30	128.47	112.10
6	UJ	129	GLN	O-C-N	6.29	132.77	122.70
6	UN	129	GLN	O-C-N	6.29	132.77	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	UI	129	GLN	O-C-N	6.27	132.73	122.70
1	AI	154	ASP	CB-CG-OD2	6.22	123.90	118.30
11	ZG	297	ASP	CB-CG-OD2	6.17	123.86	118.30
11	ZR	214	ASP	CB-CG-OD1	6.02	123.72	118.30
7	Ab	85	PRO	CA-N-CD	-5.86	103.29	111.50
11	Zc	125	PRO	N-CD-CG	-5.85	94.43	103.20
1	AM	154	ASP	CB-CG-OD1	5.76	123.48	118.30
6	UL	126	PHE	C-N-CA	-5.76	107.30	121.70
6	UO	126	PHE	C-N-CA	-5.74	107.35	121.70
1	0	52	PRO	N-CA-CB	-5.74	96.29	102.60
6	UM	126	PHE	C-N-CA	-5.74	107.35	121.70
6	UJ	126	PHE	C-N-CA	-5.74	107.36	121.70
6	UP	126	PHE	C-N-CA	-5.74	107.36	121.70
6	UK	126	PHE	C-N-CA	-5.74	107.36	121.70
6	UN	126	PHE	C-N-CA	-5.72	107.40	121.70
11	ZS	18	ASP	CB-CG-OD1	5.72	123.44	118.30
6	UI	126	PHE	C-N-CA	-5.70	107.45	121.70
11	ZV	125	PRO	CA-CB-CG	-5.68	93.22	104.00
5	AB	53	THR	CB-CA-C	-5.62	96.41	111.60
11	ZP	125	PRO	CA-N-CD	-5.57	103.70	111.50
1	ZE	13	ASP	CB-CG-OD1	5.51	123.26	118.30
9	Av	162	PRO	N-CA-CB	-5.29	96.78	102.60
5	AB	72	ASP	CB-CG-OD1	5.24	123.02	118.30
6	BG	322	PRO	N-CA-CB	-5.21	96.86	102.60
6	WJ	214	ASP	CB-CA-C	-5.20	100.00	110.40
1	9	109	ASP	CB-CG-OD2	5.20	122.98	118.30
14	Cw	66	PHE	C-N-CA	5.16	134.60	121.70
14	CG	66	PHE	C-N-CA	5.16	134.59	121.70
14	DJ	66	PHE	C-N-CA	5.15	134.58	121.70
14	DW	66	PHE	C-N-CA	5.15	134.57	121.70
14	Em	66	PHE	C-N-CA	5.15	134.57	121.70
14	Do	66	PHE	C-N-CA	5.14	134.56	121.70
14	CA	66	PHE	C-N-CA	5.14	134.56	121.70
14	By	66	PHE	C-N-CA	5.14	134.55	121.70
14	EQ	66	PHE	C-N-CA	5.14	134.54	121.70
14	Bg	66	PHE	C-N-CA	5.14	134.54	121.70
14	EK	66	PHE	C-N-CA	5.13	134.53	121.70
14	Eg	66	PHE	C-N-CA	5.13	134.53	121.70
14	Ce	66	PHE	C-N-CA	5.13	134.53	121.70
14	DQ	66	PHE	C-N-CA	5.13	134.52	121.70
14	Di	66	PHE	C-N-CA	5.13	134.52	121.70
14	D7	66	PHE	C-N-CA	5.13	134.52	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	Ck	66	PHE	C-N-CA	5.13	134.52	121.70
14	Ea	66	PHE	C-N-CA	5.12	134.51	121.70
14	DD	66	PHE	C-N-CA	5.12	134.51	121.70
14	Bs	66	PHE	C-N-CA	5.12	134.51	121.70
14	Ba	66	PHE	C-N-CA	5.12	134.50	121.70
14	C6	66	PHE	C-N-CA	5.12	134.50	121.70
14	DB	66	PHE	C-N-CA	5.12	134.50	121.70
14	EW	66	PHE	C-N-CA	5.12	134.50	121.70
14	Dc	66	PHE	C-N-CA	5.12	134.49	121.70
14	B5	66	PHE	C-N-CA	5.12	134.49	121.70
14	EE	66	PHE	C-N-CA	5.12	134.50	121.70
14	Bm	66	PHE	C-N-CA	5.12	134.49	121.70
14	Cq	66	PHE	C-N-CA	5.12	134.50	121.70
14	CY	66	PHE	C-N-CA	5.11	134.48	121.70
14	D1	66	PHE	C-N-CA	5.10	134.46	121.70
14	CS	66	PHE	C-N-CA	5.10	134.46	121.70
14	Du	66	PHE	C-N-CA	5.10	134.45	121.70
14	CM	66	PHE	C-N-CA	5.10	134.45	121.70
6	WO	168	GLU	CB-CA-C	-5.05	100.29	110.40

There are no chirality outliers.

All (181) 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	5	73	ARG	Sidechain
1	7	73	ARG	Sidechain
1	8	238	ARG	Sidechain
1	8	38	ARG	Sidechain
3	A0	104	ARG	Sidechain
3	A6	106	ARG	Sidechain
3	A7	55	ARG	Sidechain
3	A9	4	ARG	Sidechain
5	AA	243	ARG	Sidechain
5	AB	225	ARG	Sidechain
5	AB	54	ARG	Sidechain
5	AD	200	ARG	Sidechain
1	AF	36	ARG	Sidechain
1	AI	116	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	AK	79	ARG	Sidechain
1	AL	73	ARG	Sidechain
1	AM	36	ARG	Sidechain
1	AM	50	ARG	Sidechain
1	AN	116	ARG	Sidechain
1	AN	153	ARG	Sidechain
1	AN	238	ARG	Sidechain
9	Aw	135	ARG	Sidechain
9	Aw	143	ARG	Sidechain
9	Ay	140	ARG	Sidechain
9	Ay	143	ARG	Sidechain
14	B5	206	MET	Mainchain
14	B5	219	ARG	Sidechain
10	BD	110	ARG	Sidechain
10	BF	110	ARG	Sidechain
14	Ba	206	MET	Mainchain
14	Ba	219	ARG	Sidechain
14	Bg	206	MET	Mainchain
14	Bg	219	ARG	Sidechain
14	Bm	206	MET	Mainchain
14	Bm	219	ARG	Sidechain
14	Bs	206	MET	Mainchain
14	Bs	219	ARG	Sidechain
14	By	206	MET	Mainchain
14	By	219	ARG	Sidechain
14	C6	206	MET	Mainchain
14	C6	219	ARG	Sidechain
14	CA	206	MET	Mainchain
14	CA	219	ARG	Sidechain
14	CG	206	MET	Mainchain
14	CG	219	ARG	Sidechain
14	CM	206	MET	Mainchain
14	CM	219	ARG	Sidechain
14	CS	206	MET	Mainchain
14	CS	219	ARG	Sidechain
14	CY	206	MET	Mainchain
14	CY	219	ARG	Sidechain
14	Ce	206	MET	Mainchain
14	Ce	219	ARG	Sidechain
14	Ck	206	MET	Mainchain
14	Ck	219	ARG	Sidechain
14	Cq	206	MET	Mainchain

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Mol	Chain	Res	Type	Group
14	Cq	219	ARG	Sidechain
14	Cw	206	MET	Mainchain
14	Cw	219	ARG	Sidechain
14	D1	206	MET	Mainchain
14	D1	219	ARG	Sidechain
14	D7	206	MET	Mainchain
14	D7	219	ARG	Sidechain
14	DB	206	MET	Mainchain
14	DB	219	ARG	Sidechain
14	DD	206	MET	Mainchain
14	DD	219	ARG	Sidechain
14	DJ	206	MET	Mainchain
14	DJ	219	ARG	Sidechain
14	DQ	206	MET	Mainchain
14	DQ	219	ARG	Sidechain
14	DW	206	MET	Mainchain
14	DW	219	ARG	Sidechain
14	Dc	206	MET	Mainchain
14	Dc	219	ARG	Sidechain
14	Di	206	MET	Mainchain
14	Di	219	ARG	Sidechain
14	Do	206	MET	Mainchain
14	Do	219	ARG	Sidechain
14	Du	206	MET	Mainchain
14	Du	219	ARG	Sidechain
14	EE	206	MET	Mainchain
14	EE	219	ARG	Sidechain
14	EK	206	MET	Mainchain
14	EK	219	ARG	Sidechain
14	EQ	206	MET	Mainchain
14	EQ	219	ARG	Sidechain
14	EW	206	MET	Mainchain
14	EW	219	ARG	Sidechain
14	Ea	206	MET	Mainchain
14	Ea	219	ARG	Sidechain
14	Eg	206	MET	Mainchain
14	Eg	219	ARG	Sidechain
14	Em	206	MET	Mainchain
14	Em	219	ARG	Sidechain
6	UI	221	THR	Mainchain
6	UI	50	ASP	Mainchain
6	UJ	270	THR	Mainchain

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Mol	Chain	Res	Type	Group
6	UJ	50	ASP	Mainchain
6	UK	167	ARG	Sidechain
6	UK	221	THR	Mainchain
6	UK	50	ASP	Mainchain
6	UL	167	ARG	Sidechain
6	UL	221	THR	Mainchain
6	UL	50	ASP	Mainchain
6	UM	221	THR	Mainchain
6	UM	50	ASP	Mainchain
6	UN	221	THR	Mainchain
6	UN	50	ASP	Mainchain
6	UO	221	THR	Mainchain
6	UO	50	ASP	Mainchain
6	UP	167	ARG	Sidechain
6	UP	221	THR	Mainchain
6	UP	50	ASP	Mainchain
6	WA	134	ARG	Sidechain
6	WA	142	ARG	Sidechain
6	WA	167	ARG	Sidechain
6	WB	134	ARG	Sidechain
6	WB	142	ARG	Sidechain
6	WB	154	ARG	Sidechain
6	WB	167	ARG	Sidechain
6	WC	134	ARG	Sidechain
6	WC	142	ARG	Sidechain
6	WC	167	ARG	Sidechain
6	WD	134	ARG	Sidechain
6	WE	134	ARG	Sidechain
6	WE	142	ARG	Sidechain
6	WF	134	ARG	Sidechain
6	WF	142	ARG	Sidechain
6	WF	167	ARG	Sidechain
6	WG	134	ARG	Sidechain
6	WG	142	ARG	Sidechain
6	WG	167	ARG	Sidechain
6	WI	142	ARG	Sidechain
6	WJ	134	ARG	Sidechain
6	WJ	142	ARG	Sidechain
6	WJ	167	ARG	Sidechain
6	WK	134	ARG	Sidechain
6	WK	142	ARG	Sidechain
6	WL	134	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	WL	157	LEU	Mainchain
6	WM	134	ARG	Sidechain
6	WN	134	ARG	Sidechain
6	WO	134	ARG	Sidechain
6	WP	134	ARG	Sidechain
6	WP	142	ARG	Sidechain
6	WP	154	ARG	Sidechain
6	WQ	134	ARG	Sidechain
6	WQ	142	ARG	Sidechain
6	WR	134	ARG	Sidechain
6	WR	142	ARG	Sidechain
6	WR	167	ARG	Sidechain
6	WS	167	ARG	Sidechain
6	WT	134	ARG	Sidechain
6	WT	142	ARG	Sidechain
6	WU	134	ARG	Sidechain
6	WU	142	ARG	Sidechain
6	WV	134	ARG	Sidechain
6	WV	142	ARG	Sidechain
6	WV	167	ARG	Sidechain
6	WW	134	ARG	Sidechain
6	WW	167	ARG	Sidechain
1	ZA	50	ARG	Sidechain
1	ZA	79	ARG	Sidechain
1	ZD	238	ARG	Sidechain
1	ZE	238	ARG	Sidechain
1	ZE	50	ARG	Sidechain
1	ZE	79	ARG	Sidechain
11	ZI	380	ARG	Sidechain
11	ZK	71	ARG	Sidechain
11	ZO	71	ARG	Sidechain
11	ZT	106	ARG	Sidechain
11	ZU	96	ARG	Sidechain
11	ZW	71	ARG	Sidechain
11	ZZ	380	ARG	Sidechain
11	Zd	380	ARG	Sidechain
11	Ze	380	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	244/260 (94%)	236 (97%)	5 (2%)	3 (1%)	11	44
1	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	68
1	2	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	55
1	3	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	55
1	4	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	55
1	5	258/260 (99%)	240 (93%)	15 (6%)	3 (1%)	11	44
1	6	258/260 (99%)	244 (95%)	10 (4%)	4 (2%)	8	38
1	7	258/260 (99%)	244 (95%)	11 (4%)	3 (1%)	11	44
1	8	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	44
1	9	258/260 (99%)	244 (95%)	13 (5%)	1 (0%)	30	68
1	AF	250/260 (96%)	238 (95%)	11 (4%)	1 (0%)	30	68
1	AG	251/260 (96%)	234 (93%)	14 (6%)	3 (1%)	11	44
1	AH	252/260 (97%)	234 (93%)	16 (6%)	2 (1%)	16	55
1	AI	250/260 (96%)	239 (96%)	9 (4%)	2 (1%)	16	55
1	AJ	251/260 (96%)	235 (94%)	10 (4%)	6 (2%)	5	27
1	AK	239/260 (92%)	231 (97%)	7 (3%)	1 (0%)	30	68
1	AL	244/260 (94%)	229 (94%)	10 (4%)	5 (2%)	6	32
1	AM	244/260 (94%)	234 (96%)	9 (4%)	1 (0%)	30	68
1	AN	244/260 (94%)	239 (98%)	4 (2%)	1 (0%)	30	68
1	ZA	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	44
1	ZB	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	11	44
1	ZC	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	55
1	ZD	258/260 (99%)	237 (92%)	18 (7%)	3 (1%)	11	44
1	ZE	258/260 (99%)	243 (94%)	14 (5%)	1 (0%)	30	68
2	A	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	C	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	D	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	E	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	F	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	G	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	H	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	I	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	J	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	K	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	L	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	M	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	N	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	O	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	P	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	Q	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	R	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	S	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	T	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	U	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	V	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	W	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	X	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	Y	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
2	Z	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	64
3	A0	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
3	A6	132/138 (96%)	127 (96%)	4 (3%)	1 (1%)	16	55
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%)	119 (98%)	2 (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%)	52 (94%)	3 (6%)	0	100	100
5	AA	246/251 (98%)	238 (97%)	7 (3%)	1 (0%)	30	68
5	AB	247/251 (98%)	241 (98%)	5 (2%)	1 (0%)	30	68
5	AC	248/251 (99%)	233 (94%)	13 (5%)	2 (1%)	16	55
5	AD	248/251 (99%)	235 (95%)	13 (5%)	0	100	100
5	AE	247/251 (98%)	236 (96%)	9 (4%)	2 (1%)	16	55
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	B6	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	BG	11/560 (2%)	9 (82%)	2 (18%)	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%)	17 (90%)	2 (10%)	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%)	18 (100%)	0	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	Bb	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Bh	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Bn	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Bt	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Bz	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	C3	25/560 (4%)	24 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C7	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	CB	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	CH	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	CN	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	CT	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	CZ	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Cf	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Cl	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Cr	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Cx	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	D2	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	D8	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	DE	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	DK	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	DR	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	DX	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Dd	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Dj	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Dp	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Dv	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	EF	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	EL	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	ER	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	EX	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Eb	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Eh	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	En	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	UI	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	43
6	UJ	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	43
6	UK	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	43
6	UL	151/560 (27%)	142 (94%)	7 (5%)	2 (1%)	10	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	UM	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	43
6	UN	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	43
6	UO	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	43
6	UP	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	43
6	WA	111/560 (20%)	99 (89%)	9 (8%)	3 (3%)	4	25
6	WB	109/560 (20%)	94 (86%)	10 (9%)	5 (5%)	2	17
6	WC	106/560 (19%)	96 (91%)	9 (8%)	1 (1%)	14	52
6	WD	108/560 (19%)	99 (92%)	4 (4%)	5 (5%)	2	17
6	WE	110/560 (20%)	98 (89%)	8 (7%)	4 (4%)	3	20
6	WF	109/560 (20%)	98 (90%)	8 (7%)	3 (3%)	4	24
6	WG	110/560 (20%)	98 (89%)	10 (9%)	2 (2%)	7	35
6	WH	93/560 (17%)	86 (92%)	5 (5%)	2 (2%)	5	29
6	WI	93/560 (17%)	82 (88%)	5 (5%)	6 (6%)	1	12
6	WJ	97/560 (17%)	89 (92%)	7 (7%)	1 (1%)	13	49
6	WK	96/560 (17%)	84 (88%)	9 (9%)	3 (3%)	3	22
6	WL	81/560 (14%)	75 (93%)	4 (5%)	2 (2%)	4	26
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	19
6	WO	94/560 (17%)	85 (90%)	7 (7%)	2 (2%)	5	30
6	WP	98/560 (18%)	87 (89%)	6 (6%)	5 (5%)	1	15
6	WQ	109/560 (20%)	100 (92%)	5 (5%)	4 (4%)	2	20
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	52
6	WV	108/560 (19%)	97 (90%)	9 (8%)	2 (2%)	6	32
6	WW	109/560 (20%)	95 (87%)	9 (8%)	5 (5%)	2	17
7	Ab	87/89 (98%)	81 (93%)	4 (5%)	2 (2%)	5	28
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%)	233 (93%)	16 (6%)	2 (1%)	16 55
9	Au	205/245 (84%)	197 (96%)	8 (4%)	0	100 100
9	Av	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13 49
9	Aw	206/245 (84%)	201 (98%)	5 (2%)	0	100 100
9	Ax	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25 64
9	Ay	207/245 (84%)	192 (93%)	10 (5%)	5 (2%)	5 27
10	BA	131/134 (98%)	122 (93%)	9 (7%)	0	100 100
10	BB	130/134 (97%)	123 (95%)	7 (5%)	0	100 100
10	BC	131/134 (98%)	124 (95%)	7 (5%)	0	100 100
10	BD	131/134 (98%)	121 (92%)	7 (5%)	3 (2%)	5 28
10	BE	129/134 (96%)	123 (95%)	5 (4%)	1 (1%)	16 55
10	BF	131/134 (98%)	124 (95%)	7 (5%)	0	100 100
11	ZF	399/403 (99%)	387 (97%)	12 (3%)	0	100 100
11	ZG	399/403 (99%)	388 (97%)	10 (2%)	1 (0%)	37 73
11	ZH	399/403 (99%)	385 (96%)	14 (4%)	0	100 100
11	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25 64
11	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100 100
11	ZK	399/403 (99%)	387 (97%)	11 (3%)	1 (0%)	37 73
11	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37 73
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 55
11	ZP	399/403 (99%)	386 (97%)	12 (3%)	1 (0%)	37 73
11	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100 100
11	ZR	399/403 (99%)	391 (98%)	8 (2%)	0	100 100
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%)	380 (95%)	18 (4%)	1 (0%)	37 73
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%)	385 (96%)	14 (4%)	0	100	100
11	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
11	Za	399/403 (99%)	386 (97%)	12 (3%)	1 (0%)	37	73
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%)	384 (96%)	15 (4%)	0	100	100
11	Ze	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	73
11	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
11	Zg	399/403 (99%)	383 (96%)	16 (4%)	0	100	100
11	Zh	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
12	a	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	b	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	c	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	d	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	e	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	f	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	g	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	h	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	i	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	j	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	k	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	l	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	m	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	n	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	o	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	p	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	q	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	r	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	s	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	t	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	u	297/365 (81%)	288 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	v	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	w	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
12	x	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	y	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
12	z	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
13	B0	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	B2	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	B3	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	B4	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	B8	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	B9	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	BY	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	BZ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Bd	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Be	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Bf	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Bj	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Bk	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Bl	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Bp	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Bq	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Br	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Bv	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Bw	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Bx	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	C0	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	C1	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	C2	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	C4	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	C5	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	C9	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CD	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CE	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CF	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CJ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CK	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CL	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CP	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CQ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CR	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CV	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CW	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	CX	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Cb	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Cc	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Cd	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Ch	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Ci	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Cj	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Cn	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Co	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Cp	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Ct	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Cu	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Cv	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Cz	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	D0	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	D4	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	D5	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	D6	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DA	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DC	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	DG	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DH	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DI	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DN	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DO	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DP	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DT	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DU	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DV	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	DZ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Da	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Db	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Df	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Dg	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Dh	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Dl	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Dm	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Dn	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Dr	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Ds	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Dt	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Dx	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Dy	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Dz	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EA	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EB	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EC	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	ED	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EH	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EI	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EJ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	EN	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EO	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EP	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	ET	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EU	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EV	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	EZ	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Ed	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Ee	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Ef	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Ej	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Ek	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	El	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
13	Ep	85/137 (62%)	79 (93%)	5 (6%)	1 (1%)	11	44
14	B5	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Ba	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Bg	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Bm	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Bs	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	By	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	C6	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	CA	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	CG	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	CM	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	CS	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	CY	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Ce	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Ck	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Cq	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Cw	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	D1	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	D7	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	DB	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	DD	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	DJ	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	DQ	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	DW	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Dc	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Di	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Do	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Du	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	EE	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	EK	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	EQ	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	EW	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Ea	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Eg	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
14	Em	311/331 (94%)	302 (97%)	7 (2%)	2 (1%)	22	60
15	B1	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	B7	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Bc	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Bi	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Bo	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Bu	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	C8	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	CC	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	CI	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	CO	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	CU	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Ca	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Cg	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Cm	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	Cs	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Cy	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	D3	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	D9	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	DF	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	DL	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	DM	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	DS	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	DY	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	De	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Dk	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Dq	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Dw	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	EG	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	EM	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	ES	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	EY	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Ec	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Ei	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
15	Eo	287/334 (86%)	276 (96%)	9 (3%)	2 (1%)	19	57
All	All	74558/136851 (54%)	71664 (96%)	2440 (3%)	454 (1%)	24	60

All (454) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	209	ASN
1	4	140	ILE
1	5	209	ASN
1	6	139	ALA
1	8	209	ASN
5	AE	155	VAL
1	AL	90	ASN
7	Ab	84	LEU
9	Ay	83	ALA
9	Ay	87	GLN

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Mol	Chain	Res	Type
6	WO	168	GLU
6	WR	123	ILE
6	WR	165	PHE
6	WR	166	VAL
6	WS	187	ASP
1	ZA	92	SER
1	ZA	209	ASN
1	ZB	164	GLN
11	ZG	46	SER
13	C4	116	ASP
13	C5	116	ASP
13	C9	116	ASP
13	C0	116	ASP
13	DA	116	ASP
13	DC	116	ASP
13	DG	116	ASP
13	DH	116	ASP
13	DI	116	ASP
13	DN	116	ASP
13	DO	116	ASP
13	DP	116	ASP
13	DT	116	ASP
13	DU	116	ASP
13	DV	116	ASP
13	DZ	116	ASP
13	Da	116	ASP
13	Db	116	ASP
13	Df	116	ASP
13	Dg	116	ASP
13	Dh	116	ASP
13	Dl	116	ASP
13	Dm	116	ASP
13	Dn	116	ASP
13	Dr	116	ASP
13	Ds	116	ASP
13	Dt	116	ASP
13	Dx	116	ASP
13	Dy	116	ASP
13	Dz	116	ASP
13	D4	116	ASP
13	D5	116	ASP
13	D6	116	ASP

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Mol	Chain	Res	Type
13	D0	116	ASP
13	EA	116	ASP
13	EB	116	ASP
13	B0	116	ASP
13	B2	116	ASP
13	B3	116	ASP
13	B4	116	ASP
13	B8	116	ASP
13	B9	116	ASP
13	EC	116	ASP
13	ED	116	ASP
13	EH	116	ASP
13	EI	116	ASP
13	EJ	116	ASP
13	EN	116	ASP
13	EO	116	ASP
13	EP	116	ASP
13	ET	116	ASP
13	EU	116	ASP
13	EV	116	ASP
13	EZ	116	ASP
13	BY	116	ASP
13	BZ	116	ASP
13	Bd	116	ASP
13	Be	116	ASP
13	Bf	116	ASP
13	Bj	116	ASP
13	Bk	116	ASP
13	Bl	116	ASP
13	Bp	116	ASP
13	Bq	116	ASP
13	Br	116	ASP
13	Bv	116	ASP
13	Bw	116	ASP
13	Bx	116	ASP
13	C1	116	ASP
13	C2	116	ASP
13	CD	116	ASP
13	CE	116	ASP
13	CF	116	ASP
13	CJ	116	ASP
13	CK	116	ASP

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Mol	Chain	Res	Type
13	CL	116	ASP
13	CP	116	ASP
13	CQ	116	ASP
13	CR	116	ASP
13	CV	116	ASP
13	CW	116	ASP
13	CX	116	ASP
13	Cb	116	ASP
13	Cc	116	ASP
13	Cd	116	ASP
13	Ch	116	ASP
13	Ci	116	ASP
13	Cj	116	ASP
13	Cn	116	ASP
13	Co	116	ASP
13	Cp	116	ASP
13	Ct	116	ASP
13	Cu	116	ASP
13	Cv	116	ASP
13	Cz	116	ASP
13	Ed	116	ASP
13	Ee	116	ASP
13	Ef	116	ASP
13	Ej	116	ASP
13	Ek	116	ASP
13	El	116	ASP
13	Ep	116	ASP
1	0	90	ASN
1	8	165	ALA
5	AC	50	SER
5	AE	53	THR
1	AI	127	GLN
1	AI	165	ALA
1	AJ	204	SER
1	AL	4	SER
1	AN	127	GLN
8	At	167	ASN
8	At	213	ILE
9	Av	83	ALA
9	Ax	160	GLN
9	Ay	86	ASN
10	BD	54	ALA

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Mol	Chain	Res	Type
6	WB	148	GLY
6	WB	163	SER
6	WD	146	THR
6	WD	148	GLY
6	WF	118	GLN
6	WI	146	THR
6	WI	160	PRO
6	WI	170	LYS
6	WK	166	VAL
6	WM	148	GLY
6	WN	146	THR
6	WN	148	GLY
6	WP	146	THR
6	WQ	146	THR
6	WQ	148	GLY
6	WQ	169	GLN
6	WS	146	THR
6	WT	146	THR
6	WT	162	PRO
6	WW	146	THR
6	WW	148	GLY
1	ZB	165	ALA
1	ZB	209	ASN
1	ZC	209	ASN
1	ZD	209	ASN
1	ZE	209	ASN
11	ZI	375	MET
11	ZO	237	ILE
14	C6	221	PHE
15	C8	47	VAL
14	DB	221	PHE
14	DD	221	PHE
15	DF	47	VAL
14	DJ	221	PHE
15	DL	47	VAL
15	DM	47	VAL
14	DQ	221	PHE
15	DS	47	VAL
14	DW	221	PHE
15	DY	47	VAL
14	Dc	221	PHE
15	De	47	VAL

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Mol	Chain	Res	Type
14	Di	221	PHE
15	Dk	47	VAL
14	Do	221	PHE
15	Dq	47	VAL
14	Du	221	PHE
15	Dw	47	VAL
14	D1	221	PHE
15	D3	47	VAL
14	D7	221	PHE
15	D9	47	VAL
15	B1	47	VAL
14	B5	221	PHE
15	B7	47	VAL
14	EE	221	PHE
15	EG	47	VAL
14	EK	221	PHE
15	EM	47	VAL
14	EQ	221	PHE
15	ES	47	VAL
14	EW	221	PHE
15	EY	47	VAL
14	Ba	221	PHE
15	Bc	47	VAL
14	Bg	221	PHE
15	Bi	47	VAL
14	Bm	221	PHE
15	Bo	47	VAL
14	Bs	221	PHE
15	Bu	47	VAL
14	By	221	PHE
14	CA	221	PHE
15	CC	47	VAL
14	CG	221	PHE
15	CI	47	VAL
14	CM	221	PHE
15	CO	47	VAL
14	CS	221	PHE
15	CU	47	VAL
14	CY	221	PHE
15	Ca	47	VAL
14	Ce	221	PHE
15	Cg	47	VAL

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Mol	Chain	Res	Type
14	Ck	221	PHE
15	Cm	47	VAL
14	Cq	221	PHE
15	Cs	47	VAL
14	Cw	221	PHE
15	Cy	47	VAL
14	Ea	221	PHE
15	Ec	47	VAL
14	Eg	221	PHE
15	Ei	47	VAL
14	Em	221	PHE
15	Eo	47	VAL
1	0	3	SER
1	0	127	GLN
1	2	49	ILE
1	3	49	ILE
1	3	181	ASP
1	4	49	ILE
1	5	49	ILE
1	6	138	PRO
1	7	55	GLN
3	A6	77	ALA
1	AF	127	GLN
1	AH	198	SER
1	AJ	164	GLN
1	AJ	206	PRO
1	AL	3	SER
1	AL	127	GLN
1	AM	127	GLN
9	Ay	140	ARG
10	BD	58	ALA
6	UI	162	PRO
6	UJ	162	PRO
6	UK	162	PRO
6	UL	162	PRO
6	UM	162	PRO
6	UN	162	PRO
6	UO	162	PRO
6	UP	162	PRO
6	WB	146	THR
6	WB	164	LEU
6	WD	118	GLN

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Mol	Chain	Res	Type
6	WE	160	PRO
6	WE	162	PRO
6	WI	148	GLY
6	WP	148	GLY
6	WS	118	GLN
6	WS	169	GLN
6	WT	165	PHE
6	WW	118	GLN
6	WW	168	GLU
11	ZK	375	MET
11	ZL	374	ASN
1	6	49	ILE
1	6	58	GLU
1	7	49	ILE
1	8	49	ILE
1	9	49	ILE
2	A	172	ASN
1	AG	81	HIS
1	AG	127	GLN
1	AJ	203	GLU
1	AK	127	GLN
2	B	172	ASN
10	BD	55	PRO
2	C	172	ASN
2	D	172	ASN
2	E	172	ASN
2	F	172	ASN
2	G	172	ASN
2	H	172	ASN
2	I	172	ASN
2	J	172	ASN
2	K	172	ASN
2	L	172	ASN
2	M	172	ASN
2	N	172	ASN
2	O	172	ASN
2	P	172	ASN
2	Q	172	ASN
2	R	172	ASN
2	S	172	ASN
2	T	172	ASN
2	U	172	ASN

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Mol	Chain	Res	Type
6	UI	163	SER
6	UJ	163	SER
6	UK	163	SER
6	UL	163	SER
6	UM	163	SER
6	UN	163	SER
6	UO	163	SER
6	UP	163	SER
2	V	172	ASN
2	W	172	ASN
6	WA	182	PRO
6	WB	182	PRO
6	WD	165	PHE
6	WD	182	PRO
6	WE	182	PRO
6	WF	182	PRO
6	WG	182	PRO
6	WH	165	PHE
6	WH	182	PRO
6	WI	169	GLN
6	WI	182	PRO
6	WJ	182	PRO
6	WK	182	PRO
6	WL	182	PRO
6	WM	182	PRO
6	WN	182	PRO
6	WO	182	PRO
6	WP	182	PRO
6	WQ	182	PRO
6	WR	112	GLY
6	WR	182	PRO
6	WS	182	PRO
6	WT	182	PRO
6	WU	182	PRO
6	WV	148	GLY
6	WV	182	PRO
6	WW	182	PRO
2	X	172	ASN
2	Y	172	ASN
2	Z	172	ASN
1	ZA	138	PRO
11	ZO	142	THR

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Mol	Chain	Res	Type
11	ZP	374	ASN
1	1	127	GLN
1	7	210	GLY
5	AC	52	ALA
1	AG	139	ALA
1	AH	127	GLN
1	AJ	127	GLN
7	Ab	85	PRO
9	Av	162	PRO
6	WK	168	GLU
6	WR	121	PHE
6	WT	163	SER
1	ZC	139	ALA
1	ZD	139	ALA
14	C6	234	PHE
14	DB	234	PHE
14	DD	234	PHE
15	DF	190	ASN
14	DJ	234	PHE
15	DL	190	ASN
15	DM	190	ASN
14	DQ	234	PHE
15	DS	190	ASN
14	DW	234	PHE
14	Dc	234	PHE
14	Di	234	PHE
14	Do	234	PHE
14	Du	234	PHE
14	D1	234	PHE
14	D7	234	PHE
15	B1	190	ASN
14	B5	234	PHE
15	B7	190	ASN
14	EE	234	PHE
15	EG	190	ASN
14	EK	234	PHE
14	EQ	234	PHE
14	EW	234	PHE
14	Ba	234	PHE
14	Bg	234	PHE
15	Bi	190	ASN
14	Bm	234	PHE

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Mol	Chain	Res	Type
14	Bs	234	PHE
14	By	234	PHE
14	CA	234	PHE
14	CG	234	PHE
14	CM	234	PHE
14	CS	234	PHE
14	CY	234	PHE
14	Ce	234	PHE
15	Cg	190	ASN
14	Ck	234	PHE
15	Cm	190	ASN
14	Cq	234	PHE
15	Cs	190	ASN
14	Cw	234	PHE
15	Cy	190	ASN
14	Ea	234	PHE
15	Ec	190	ASN
14	Eg	234	PHE
15	Ei	190	ASN
14	Em	234	PHE
5	AA	52	ALA
5	AB	52	ALA
1	AJ	200	ALA
10	BE	58	ALA
6	WC	182	PRO
6	WE	221	THR
6	WF	162	PRO
6	WG	163	SER
11	ZO	375	MET
11	Za	97	ASN
11	Ze	134	PRO
15	C8	190	ASN
15	DY	190	ASN
15	De	190	ASN
15	Dk	190	ASN
15	Dq	190	ASN
15	Dw	190	ASN
15	D3	190	ASN
15	D9	190	ASN
15	EM	190	ASN
15	ES	190	ASN
15	EY	190	ASN

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Mol	Chain	Res	Type
15	Bc	190	ASN
15	Bo	190	ASN
15	Bu	190	ASN
15	CC	190	ASN
15	CI	190	ASN
15	CO	190	ASN
15	CU	190	ASN
15	Ca	190	ASN
15	Eo	190	ASN
6	WA	160	PRO
6	WL	148	GLY
6	WS	148	GLY
6	WT	148	GLY
11	ZI	325	GLY
11	ZW	75	VAL
6	WA	148	GLY
6	WP	123	ILE
6	WR	148	GLY
1	5	138	PRO
1	AL	136	VAL
9	Ay	229	VAL
6	WP	160	PRO
6	WT	161	LYS
1	ZD	138	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	205/215 (95%)	198 (97%)	7 (3%)	32 51
1	1	209/215 (97%)	201 (96%)	8 (4%)	28 49
1	2	215/215 (100%)	212 (99%)	3 (1%)	62 75
1	3	215/215 (100%)	212 (99%)	3 (1%)	62 75
1	4	215/215 (100%)	209 (97%)	6 (3%)	38 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	215/215 (100%)	210 (98%)	5 (2%)	45	64
1	6	215/215 (100%)	210 (98%)	5 (2%)	45	64
1	7	215/215 (100%)	214 (100%)	1 (0%)	86	89
1	8	215/215 (100%)	210 (98%)	5 (2%)	45	64
1	9	215/215 (100%)	212 (99%)	3 (1%)	62	75
1	AF	209/215 (97%)	203 (97%)	6 (3%)	37	56
1	AG	210/215 (98%)	201 (96%)	9 (4%)	25	46
1	AH	211/215 (98%)	199 (94%)	12 (6%)	17	38
1	AI	209/215 (97%)	198 (95%)	11 (5%)	19	40
1	AJ	210/215 (98%)	199 (95%)	11 (5%)	19	40
1	AK	200/215 (93%)	195 (98%)	5 (2%)	42	61
1	AL	205/215 (95%)	197 (96%)	8 (4%)	27	48
1	AM	205/215 (95%)	197 (96%)	8 (4%)	27	48
1	AN	205/215 (95%)	200 (98%)	5 (2%)	44	62
1	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	83
1	ZB	215/215 (100%)	209 (97%)	6 (3%)	38	57
1	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	75
1	ZD	215/215 (100%)	211 (98%)	4 (2%)	52	69
1	ZE	215/215 (100%)	210 (98%)	5 (2%)	45	64
2	A	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	B	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	C	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	D	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	E	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	F	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	G	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	H	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	I	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	J	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	K	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	L	170/186 (91%)	164 (96%)	6 (4%)	31	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	N	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	O	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	P	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	Q	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	R	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	S	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	T	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	U	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	V	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	W	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	X	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	Y	170/186 (91%)	164 (96%)	6 (4%)	31	51
2	Z	170/186 (91%)	164 (96%)	6 (4%)	31	51
3	A0	102/113 (90%)	96 (94%)	6 (6%)	16	37
3	A6	110/113 (97%)	106 (96%)	4 (4%)	30	50
3	A7	101/113 (89%)	100 (99%)	1 (1%)	73	82
3	A8	103/113 (91%)	96 (93%)	7 (7%)	13	34
3	A9	104/113 (92%)	102 (98%)	2 (2%)	52	69
4	A1	68/79 (86%)	64 (94%)	4 (6%)	16	37
4	A2	70/79 (89%)	65 (93%)	5 (7%)	12	32
4	A3	70/79 (89%)	66 (94%)	4 (6%)	17	38
4	A4	70/79 (89%)	66 (94%)	4 (6%)	17	38
4	A5	69/79 (87%)	64 (93%)	5 (7%)	12	32
4	Az	45/79 (57%)	39 (87%)	6 (13%)	3	13
5	AA	190/193 (98%)	188 (99%)	2 (1%)	70	80
5	AB	191/193 (99%)	186 (97%)	5 (3%)	41	59
5	AC	192/193 (100%)	189 (98%)	3 (2%)	58	73
5	AD	192/193 (100%)	185 (96%)	7 (4%)	30	50
5	AE	191/193 (99%)	189 (99%)	2 (1%)	73	82
6	AO	141/467 (30%)	134 (95%)	7 (5%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	AP	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	AQ	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	AR	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	AS	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	AT	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	AU	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	AV	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	AW	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	AX	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	AY	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	AZ	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Aa	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Ac	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Ad	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Ae	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Af	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Ag	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Ah	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Ai	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Aj	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Ak	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Al	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Am	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	An	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Ao	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	Ap	141/467 (30%)	134 (95%)	7 (5%)	20 41
6	B6	26/467 (6%)	26 (100%)	0	100 100
6	BG	8/467 (2%)	6 (75%)	2 (25%)	0 3
6	BH	11/467 (2%)	10 (91%)	1 (9%)	7 24
6	BI	14/467 (3%)	12 (86%)	2 (14%)	2 12
6	BJ	11/467 (2%)	11 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	32
6	BP	11/467 (2%)	11 (100%)	0	100	100
6	BQ	15/467 (3%)	14 (93%)	1 (7%)	13	34
6	BR	141/467 (30%)	134 (95%)	7 (5%)	20	41
6	BS	141/467 (30%)	134 (95%)	7 (5%)	20	41
6	BT	141/467 (30%)	134 (95%)	7 (5%)	20	41
6	BU	141/467 (30%)	134 (95%)	7 (5%)	20	41
6	BV	141/467 (30%)	134 (95%)	7 (5%)	20	41
6	BW	141/467 (30%)	134 (95%)	7 (5%)	20	41
6	BX	141/467 (30%)	134 (95%)	7 (5%)	20	41
6	Bb	26/467 (6%)	26 (100%)	0	100	100
6	Bh	26/467 (6%)	26 (100%)	0	100	100
6	Bn	26/467 (6%)	26 (100%)	0	100	100
6	Bt	26/467 (6%)	26 (100%)	0	100	100
6	Bz	26/467 (6%)	26 (100%)	0	100	100
6	C3	26/467 (6%)	26 (100%)	0	100	100
6	C7	26/467 (6%)	26 (100%)	0	100	100
6	CB	26/467 (6%)	26 (100%)	0	100	100
6	CH	26/467 (6%)	26 (100%)	0	100	100
6	CN	26/467 (6%)	26 (100%)	0	100	100
6	CT	26/467 (6%)	26 (100%)	0	100	100
6	CZ	26/467 (6%)	26 (100%)	0	100	100
6	Cf	26/467 (6%)	26 (100%)	0	100	100
6	Cl	26/467 (6%)	26 (100%)	0	100	100
6	Cr	26/467 (6%)	26 (100%)	0	100	100
6	Cx	26/467 (6%)	26 (100%)	0	100	100
6	D2	26/467 (6%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	D8	26/467 (6%)	26 (100%)	0	100	100
6	DE	26/467 (6%)	26 (100%)	0	100	100
6	DK	26/467 (6%)	26 (100%)	0	100	100
6	DR	26/467 (6%)	26 (100%)	0	100	100
6	DX	26/467 (6%)	26 (100%)	0	100	100
6	Dd	26/467 (6%)	26 (100%)	0	100	100
6	Dj	26/467 (6%)	26 (100%)	0	100	100
6	Dp	26/467 (6%)	26 (100%)	0	100	100
6	Dv	26/467 (6%)	26 (100%)	0	100	100
6	EF	26/467 (6%)	26 (100%)	0	100	100
6	EL	26/467 (6%)	26 (100%)	0	100	100
6	ER	26/467 (6%)	26 (100%)	0	100	100
6	EX	26/467 (6%)	26 (100%)	0	100	100
6	Eb	26/467 (6%)	26 (100%)	0	100	100
6	Eh	26/467 (6%)	26 (100%)	0	100	100
6	En	26/467 (6%)	26 (100%)	0	100	100
6	UI	128/467 (27%)	123 (96%)	5 (4%)	27	48
6	UJ	128/467 (27%)	123 (96%)	5 (4%)	27	48
6	UK	128/467 (27%)	123 (96%)	5 (4%)	27	48
6	UL	128/467 (27%)	122 (95%)	6 (5%)	22	44
6	UM	128/467 (27%)	123 (96%)	5 (4%)	27	48
6	UN	128/467 (27%)	123 (96%)	5 (4%)	27	48
6	UO	128/467 (27%)	123 (96%)	5 (4%)	27	48
6	UP	128/467 (27%)	122 (95%)	6 (5%)	22	44
6	WA	95/467 (20%)	91 (96%)	4 (4%)	25	46
6	WB	93/467 (20%)	87 (94%)	6 (6%)	14	35
6	WC	91/467 (20%)	83 (91%)	8 (9%)	8	25
6	WD	92/467 (20%)	88 (96%)	4 (4%)	25	46
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	WH	79/467 (17%)	75 (95%)	4 (5%)	20 41
6	WI	79/467 (17%)	73 (92%)	6 (8%)	11 30
6	WJ	83/467 (18%)	79 (95%)	4 (5%)	21 43
6	WK	82/467 (18%)	77 (94%)	5 (6%)	15 37
6	WL	69/467 (15%)	66 (96%)	3 (4%)	25 46
6	WM	66/467 (14%)	65 (98%)	1 (2%)	60 75
6	WN	68/467 (15%)	66 (97%)	2 (3%)	37 56
6	WO	80/467 (17%)	76 (95%)	4 (5%)	20 41
6	WP	83/467 (18%)	77 (93%)	6 (7%)	12 32
6	WQ	93/467 (20%)	91 (98%)	2 (2%)	47 65
6	WR	93/467 (20%)	86 (92%)	7 (8%)	11 31
6	WS	93/467 (20%)	87 (94%)	6 (6%)	14 35
6	WT	93/467 (20%)	86 (92%)	7 (8%)	11 31
6	WU	94/467 (20%)	90 (96%)	4 (4%)	25 46
6	WV	92/467 (20%)	83 (90%)	9 (10%)	6 21
6	WW	93/467 (20%)	85 (91%)	8 (9%)	8 26
7	Ab	74/74 (100%)	68 (92%)	6 (8%)	9 28
7	Aq	74/74 (100%)	72 (97%)	2 (3%)	40 58
7	Ar	74/74 (100%)	74 (100%)	0	100 100
7	As	74/74 (100%)	74 (100%)	0	100 100
8	At	210/221 (95%)	205 (98%)	5 (2%)	44 62
9	Au	177/204 (87%)	171 (97%)	6 (3%)	32 51
9	Av	179/204 (88%)	172 (96%)	7 (4%)	27 48
9	Aw	178/204 (87%)	173 (97%)	5 (3%)	38 57
9	Ax	178/204 (87%)	171 (96%)	7 (4%)	27 48
9	Ay	179/204 (88%)	172 (96%)	7 (4%)	27 48
10	BA	104/105 (99%)	104 (100%)	0	100 100
10	BB	104/105 (99%)	101 (97%)	3 (3%)	37 56
10	BC	104/105 (99%)	102 (98%)	2 (2%)	52 69
10	BD	104/105 (99%)	100 (96%)	4 (4%)	28 49
10	BE	103/105 (98%)	99 (96%)	4 (4%)	27 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	BF	104/105 (99%)	98 (94%)	6 (6%)	17	38
11	ZF	321/323 (99%)	309 (96%)	12 (4%)	29	49
11	ZG	321/323 (99%)	305 (95%)	16 (5%)	20	41
11	ZH	321/323 (99%)	308 (96%)	13 (4%)	27	47
11	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	69
11	ZJ	321/323 (99%)	312 (97%)	9 (3%)	38	57
11	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	69
11	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	54
11	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	57
11	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	54
11	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	61
11	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	44
11	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	57
11	ZR	321/323 (99%)	314 (98%)	7 (2%)	47	65
11	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	69
11	ZT	321/323 (99%)	313 (98%)	8 (2%)	42	61
11	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	78
11	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	78
11	ZW	321/323 (99%)	307 (96%)	14 (4%)	24	45
11	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	83
11	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	65
11	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	73
11	Za	321/323 (99%)	315 (98%)	6 (2%)	52	69
11	Zb	321/323 (99%)	314 (98%)	7 (2%)	47	65
11	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	51
11	Zd	321/323 (99%)	315 (98%)	6 (2%)	52	69
11	Ze	321/323 (99%)	314 (98%)	7 (2%)	47	65
11	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	65
11	Zg	321/323 (99%)	314 (98%)	7 (2%)	47	65
11	Zh	321/323 (99%)	314 (98%)	7 (2%)	47	65
12	a	248/294 (84%)	243 (98%)	5 (2%)	50	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	b	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	c	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	d	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	e	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	f	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	g	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	h	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	i	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	j	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	k	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	l	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	m	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	n	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	o	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	p	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	q	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	r	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	s	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	t	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	u	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	v	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	w	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	x	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	y	248/294 (84%)	243 (98%)	5 (2%)	50	68
12	z	248/294 (84%)	243 (98%)	5 (2%)	50	68
13	B0	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	B2	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	B3	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	B4	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	B8	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	B9	76/113 (67%)	73 (96%)	3 (4%)	27	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	BY	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	BZ	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Bd	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Be	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Bf	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Bj	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Bk	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Bl	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Bp	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Bq	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Br	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Bv	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Bw	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Bx	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	C0	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	C1	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	C2	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	C4	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	C5	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	C9	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CD	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CE	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CF	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CJ	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CK	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CL	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CP	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CQ	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CR	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CV	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	CW	76/113 (67%)	73 (96%)	3 (4%)	27	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	CX	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Cb	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Cc	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Cd	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Ch	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Ci	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Cj	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Cn	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Co	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Cp	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Ct	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Cu	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Cv	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Cz	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	D0	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	D4	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	D5	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	D6	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DA	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DC	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DG	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DH	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DI	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DN	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DO	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DP	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DT	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DU	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DV	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	DZ	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Da	76/113 (67%)	73 (96%)	3 (4%)	27	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	Db	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Df	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Dg	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Dh	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Dl	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Dm	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Dn	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Dr	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Ds	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Dt	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Dx	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Dy	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Dz	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EA	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EB	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EC	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	ED	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EH	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EI	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EJ	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EN	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EO	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EP	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	ET	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EU	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EV	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	EZ	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Ed	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Ee	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Ef	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Ej	76/113 (67%)	73 (96%)	3 (4%)	27	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	Ek	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	El	76/113 (67%)	73 (96%)	3 (4%)	27	48
13	Ep	76/113 (67%)	73 (96%)	3 (4%)	27	48
14	B5	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Ba	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Bg	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Bm	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Bs	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	By	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	C6	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	CA	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	CG	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	CM	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	CS	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	CY	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Ce	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Ck	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Cq	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Cw	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	D1	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	D7	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	DB	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	DD	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	DJ	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	DQ	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	DW	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Dc	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Di	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Do	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Du	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	EE	268/282 (95%)	265 (99%)	3 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	EK	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	EQ	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	EW	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Ea	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Eg	268/282 (95%)	265 (99%)	3 (1%)	70	80
14	Em	268/282 (95%)	265 (99%)	3 (1%)	70	80
15	B1	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	B7	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Bc	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Bi	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Bo	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Bu	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	C8	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	CC	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	CI	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	CO	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	CU	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Ca	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Cg	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Cm	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Cs	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Cy	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	D3	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	D9	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	DF	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	DL	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	DM	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	DS	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	DY	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	De	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Dk	262/301 (87%)	250 (95%)	12 (5%)	23	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	Dq	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Dw	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	EG	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	EM	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	ES	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	EY	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Ec	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Ei	262/301 (87%)	250 (95%)	12 (5%)	23	44
15	Eo	262/301 (87%)	250 (95%)	12 (5%)	23	44
All	All	63740/113896 (56%)	61719 (97%)	2021 (3%)	36	53

All (2021) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	1	MET
1	0	9	LYS
1	0	36	ARG
1	0	50	ARG
1	0	52	PRO
1	0	73	ARG
1	0	185	GLU
1	1	1	MET
1	1	36	ARG
1	1	62	LEU
1	1	75	VAL
1	1	106	MET
1	1	119	SER
1	1	164	GLN
1	1	206	PRO
1	2	73	ARG
1	2	179	MET
1	2	204	SER
1	3	43	ASP
1	3	109	ASP
1	3	244	SER
1	4	2	ILE
1	4	64	SER
1	4	137	GLN
1	4	204	SER

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Mol	Chain	Res	Type
1	4	209	ASN
1	4	259	GLN
1	5	4	SER
1	5	73	ARG
1	5	85	ASN
1	5	154	ASP
1	5	181	ASP
1	6	59	GLN
1	6	73	ARG
1	6	78	GLU
1	6	109	ASP
1	6	244	SER
1	7	59	GLN
1	8	58	GLU
1	8	100	GLN
1	8	194	GLU
1	8	195	THR
1	8	256	LYS
1	9	106	MET
1	9	125	ASN
1	9	162	GLN
2	A	58	ILE
2	A	85	ASN
2	A	106	PHE
2	A	113	LEU
2	A	133	ASN
2	A	144	PHE
3	A0	4	ARG
3	A0	18	LEU
3	A0	65	LEU
3	A0	104	ARG
3	A0	113	SER
3	A0	125	SER
4	A1	15	GLN
4	A1	19	MET
4	A1	75	MET
4	A1	84	MET
4	A2	7	ILE
4	A2	11	ILE
4	A2	14	LEU
4	A2	15	GLN
4	A2	70	ASP

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Mol	Chain	Res	Type
4	A3	15	GLN
4	A3	19	MET
4	A3	33	SER
4	A3	81	SER
4	A4	15	GLN
4	A4	19	MET
4	A4	101	SER
4	A4	102	MET
4	A5	15	GLN
4	A5	19	MET
4	A5	57	GLU
4	A5	91	LYS
4	A5	102	MET
3	A6	34	ASP
3	A6	101	ASP
3	A6	113	SER
3	A6	125	SER
3	A7	47	SER
3	A8	48	GLU
3	A8	65	LEU
3	A8	69	SER
3	A8	71	HIS
3	A8	72	HIS
3	A8	91	ASP
3	A8	128	LYS
3	A9	47	SER
3	A9	76	GLN
5	AA	123	GLU
5	AA	247	LEU
5	AB	53	THR
5	AB	72	ASP
5	AB	97	GLU
5	AB	153	ASN
5	AB	225	ARG
5	AC	189	ARG
5	AC	200	ARG
5	AC	225	ARG
5	AD	47	ASP
5	AD	49	LEU
5	AD	72	ASP
5	AD	140	ASP
5	AD	160	ARG

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Mol	Chain	Res	Type
5	AD	169	ASN
5	AD	189	ARG
5	AE	51	LEU
5	AE	175	ASP
1	AF	4	SER
1	AF	6	TRP
1	AF	19	MET
1	AF	36	ARG
1	AF	44	LEU
1	AF	154	ASP
1	AG	6	TRP
1	AG	16	GLN
1	AG	36	ARG
1	AG	73	ARG
1	AG	127	GLN
1	AG	137	GLN
1	AG	138	PRO
1	AG	222	SER
1	AG	251	ASP
1	AH	1	MET
1	AH	44	LEU
1	AH	66	LEU
1	AH	87	SER
1	AH	93	LYS
1	AH	100	GLN
1	AH	148	SER
1	AH	154	ASP
1	AH	179	MET
1	AH	195	THR
1	AH	208	LEU
1	AH	245	LYS
1	AI	4	SER
1	AI	30	SER
1	AI	123	ASP
1	AI	148	SER
1	AI	169	GLN
1	AI	173	LEU
1	AI	179	MET
1	AI	195	THR
1	AI	202	ASN
1	AI	222	SER
1	AI	252	GLN

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Mol	Chain	Res	Type
1	AJ	36	ARG
1	AJ	73	ARG
1	AJ	91	ASN
1	AJ	94	ASP
1	AJ	127	GLN
1	AJ	161	GLN
1	AJ	194	GLU
1	AJ	197	SER
1	AJ	198	SER
1	AJ	206	PRO
1	AJ	225	ASN
1	AK	36	ARG
1	AK	100	GLN
1	AK	137	GLN
1	AK	181	ASP
1	AK	203	GLU
1	AL	1	MET
1	AL	73	ARG
1	AL	111	THR
1	AL	170	VAL
1	AL	172	GLN
1	AL	185	GLU
1	AL	198	SER
1	AL	209	ASN
1	AM	1	MET
1	AM	30	SER
1	AM	36	ARG
1	AM	50	ARG
1	AM	82	SER
1	AM	169	GLN
1	AM	208	LEU
1	AM	209	ASN
1	AN	1	MET
1	AN	3	SER
1	AN	90	ASN
1	AN	117	ASP
1	AN	127	GLN
6	AO	274	ASN
6	AO	294	ARG
6	AO	359	GLN
6	AO	377	MET
6	AO	381	ASP

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Mol	Chain	Res	Type
6	AO	417	ARG
6	AO	424	ASP
6	AP	274	ASN
6	AP	294	ARG
6	AP	359	GLN
6	AP	377	MET
6	AP	381	ASP
6	AP	417	ARG
6	AP	424	ASP
6	AQ	274	ASN
6	AQ	294	ARG
6	AQ	359	GLN
6	AQ	377	MET
6	AQ	381	ASP
6	AQ	417	ARG
6	AQ	424	ASP
6	AR	274	ASN
6	AR	294	ARG
6	AR	359	GLN
6	AR	377	MET
6	AR	381	ASP
6	AR	417	ARG
6	AR	424	ASP
6	AS	274	ASN
6	AS	294	ARG
6	AS	359	GLN
6	AS	377	MET
6	AS	381	ASP
6	AS	417	ARG
6	AS	424	ASP
6	AT	274	ASN
6	AT	294	ARG
6	AT	359	GLN
6	AT	377	MET
6	AT	381	ASP
6	AT	417	ARG
6	AT	424	ASP
6	AU	274	ASN
6	AU	294	ARG
6	AU	359	GLN
6	AU	377	MET
6	AU	381	ASP

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Mol	Chain	Res	Type
6	AU	417	ARG
6	AU	424	ASP
6	AV	274	ASN
6	AV	294	ARG
6	AV	359	GLN
6	AV	377	MET
6	AV	381	ASP
6	AV	417	ARG
6	AV	424	ASP
6	AW	274	ASN
6	AW	294	ARG
6	AW	359	GLN
6	AW	377	MET
6	AW	381	ASP
6	AW	417	ARG
6	AW	424	ASP
6	AX	274	ASN
6	AX	294	ARG
6	AX	359	GLN
6	AX	377	MET
6	AX	381	ASP
6	AX	417	ARG
6	AX	424	ASP
6	AY	274	ASN
6	AY	294	ARG
6	AY	359	GLN
6	AY	377	MET
6	AY	381	ASP
6	AY	417	ARG
6	AY	424	ASP
6	AZ	274	ASN
6	AZ	294	ARG
6	AZ	359	GLN
6	AZ	377	MET
6	AZ	381	ASP
6	AZ	417	ARG
6	AZ	424	ASP
6	Aa	274	ASN
6	Aa	294	ARG
6	Aa	359	GLN
6	Aa	377	MET
6	Aa	381	ASP

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Mol	Chain	Res	Type
6	Aa	417	ARG
6	Aa	424	ASP
7	Ab	7	MET
7	Ab	69	MET
7	Ab	73	LEU
7	Ab	75	ASP
7	Ab	85	PRO
7	Ab	87	ILE
6	Ac	274	ASN
6	Ac	294	ARG
6	Ac	359	GLN
6	Ac	377	MET
6	Ac	381	ASP
6	Ac	417	ARG
6	Ac	424	ASP
6	Ad	274	ASN
6	Ad	294	ARG
6	Ad	359	GLN
6	Ad	377	MET
6	Ad	381	ASP
6	Ad	417	ARG
6	Ad	424	ASP
6	Ae	274	ASN
6	Ae	294	ARG
6	Ae	359	GLN
6	Ae	377	MET
6	Ae	381	ASP
6	Ae	417	ARG
6	Ae	424	ASP
6	Af	274	ASN
6	Af	294	ARG
6	Af	359	GLN
6	Af	377	MET
6	Af	381	ASP
6	Af	417	ARG
6	Af	424	ASP
6	Ag	274	ASN
6	Ag	294	ARG
6	Ag	359	GLN
6	Ag	377	MET
6	Ag	381	ASP
6	Ag	417	ARG

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Mol	Chain	Res	Type
6	Ag	424	ASP
6	Ah	274	ASN
6	Ah	294	ARG
6	Ah	359	GLN
6	Ah	377	MET
6	Ah	381	ASP
6	Ah	417	ARG
6	Ah	424	ASP
6	Ai	274	ASN
6	Ai	294	ARG
6	Ai	359	GLN
6	Ai	377	MET
6	Ai	381	ASP
6	Ai	417	ARG
6	Ai	424	ASP
6	Aj	274	ASN
6	Aj	294	ARG
6	Aj	359	GLN
6	Aj	377	MET
6	Aj	381	ASP
6	Aj	417	ARG
6	Aj	424	ASP
6	Ak	274	ASN
6	Ak	294	ARG
6	Ak	359	GLN
6	Ak	377	MET
6	Ak	381	ASP
6	Ak	417	ARG
6	Ak	424	ASP
6	Al	274	ASN
6	Al	294	ARG
6	Al	359	GLN
6	Al	377	MET
6	Al	381	ASP
6	Al	417	ARG
6	Al	424	ASP
6	Am	274	ASN
6	Am	294	ARG
6	Am	359	GLN
6	Am	377	MET
6	Am	381	ASP
6	Am	417	ARG

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Mol	Chain	Res	Type
6	Am	424	ASP
6	An	274	ASN
6	An	294	ARG
6	An	359	GLN
6	An	377	MET
6	An	381	ASP
6	An	417	ARG
6	An	424	ASP
6	Ao	274	ASN
6	Ao	294	ARG
6	Ao	359	GLN
6	Ao	377	MET
6	Ao	381	ASP
6	Ao	417	ARG
6	Ao	424	ASP
6	Ap	274	ASN
6	Ap	294	ARG
6	Ap	359	GLN
6	Ap	377	MET
6	Ap	381	ASP
6	Ap	417	ARG
6	Ap	424	ASP
7	Aq	2	THR
7	Aq	47	MET
8	At	36	ARG
8	At	86	PHE
8	At	214	PHE
8	At	227	MET
8	At	229	MET
9	Au	38	TRP
9	Au	129	LYS
9	Au	155	ASN
9	Au	160	GLN
9	Au	190	PHE
9	Au	213	PRO
9	Av	75	ARG
9	Av	102	SER
9	Av	116	PHE
9	Av	140	ARG
9	Av	160	GLN
9	Av	162	PRO
9	Av	213	PRO

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Mol	Chain	Res	Type
9	Aw	135	ARG
9	Aw	152	ARG
9	Aw	177	SER
9	Aw	187	PHE
9	Aw	190	PHE
9	Ax	113	TYR
9	Ax	143	ARG
9	Ax	152	ARG
9	Ax	187	PHE
9	Ax	205	MET
9	Ax	238	SER
9	Ax	241	GLN
9	Ay	65	THR
9	Ay	117	SER
9	Ay	140	ARG
9	Ay	144	GLU
9	Ay	190	PHE
9	Ay	224	MET
9	Ay	230	ASP
4	Az	15	GLN
4	Az	19	MET
4	Az	74	ASP
4	Az	77	LYS
4	Az	79	SER
4	Az	101	SER
2	B	58	ILE
2	B	85	ASN
2	B	106	PHE
2	B	113	LEU
2	B	133	ASN
2	B	144	PHE
10	BB	46	GLN
10	BB	123	LYS
10	BB	126	MET
10	BC	119	LEU
10	BC	128	LYS
10	BD	3	LEU
10	BD	4	LEU
10	BD	30	ASN
10	BD	120	ASN
10	BE	20	ARG
10	BE	52	ASP

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Mol	Chain	Res	Type
10	BE	84	LEU
10	BE	94	PRO
10	BF	38	ASP
10	BF	86	ASP
10	BF	88	ASN
10	BF	123	LYS
10	BF	125	MET
10	BF	127	LEU
6	BG	317	SER
6	BG	322	PRO
6	BH	324	ASN
6	BI	318	ASN
6	BI	319	GLN
6	BO	319	GLN
6	BQ	318	ASN
6	BR	274	ASN
6	BR	294	ARG
6	BR	359	GLN
6	BR	377	MET
6	BR	381	ASP
6	BR	417	ARG
6	BR	424	ASP
6	BS	274	ASN
6	BS	294	ARG
6	BS	359	GLN
6	BS	377	MET
6	BS	381	ASP
6	BS	417	ARG
6	BS	424	ASP
6	BT	274	ASN
6	BT	294	ARG
6	BT	359	GLN
6	BT	377	MET
6	BT	381	ASP
6	BT	417	ARG
6	BT	424	ASP
6	BU	274	ASN
6	BU	294	ARG
6	BU	359	GLN
6	BU	377	MET
6	BU	381	ASP
6	BU	417	ARG

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Mol	Chain	Res	Type
6	BU	424	ASP
6	BV	274	ASN
6	BV	294	ARG
6	BV	359	GLN
6	BV	377	MET
6	BV	381	ASP
6	BV	417	ARG
6	BV	424	ASP
6	BW	274	ASN
6	BW	294	ARG
6	BW	359	GLN
6	BW	377	MET
6	BW	381	ASP
6	BW	417	ARG
6	BW	424	ASP
6	BX	274	ASN
6	BX	294	ARG
6	BX	359	GLN
6	BX	377	MET
6	BX	381	ASP
6	BX	417	ARG
6	BX	424	ASP
2	C	58	ILE
2	C	85	ASN
2	C	106	PHE
2	C	113	LEU
2	C	133	ASN
2	C	144	PHE
2	D	58	ILE
2	D	85	ASN
2	D	106	PHE
2	D	113	LEU
2	D	133	ASN
2	D	144	PHE
2	E	58	ILE
2	E	85	ASN
2	E	106	PHE
2	E	113	LEU
2	E	133	ASN
2	E	144	PHE
2	F	58	ILE
2	F	85	ASN

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Mol	Chain	Res	Type
2	F	106	PHE
2	F	113	LEU
2	F	133	ASN
2	F	144	PHE
2	G	58	ILE
2	G	85	ASN
2	G	106	PHE
2	G	113	LEU
2	G	133	ASN
2	G	144	PHE
2	H	58	ILE
2	H	85	ASN
2	H	106	PHE
2	H	113	LEU
2	H	133	ASN
2	H	144	PHE
2	I	58	ILE
2	I	85	ASN
2	I	106	PHE
2	I	113	LEU
2	I	133	ASN
2	I	144	PHE
2	J	58	ILE
2	J	85	ASN
2	J	106	PHE
2	J	113	LEU
2	J	133	ASN
2	J	144	PHE
2	K	58	ILE
2	K	85	ASN
2	K	106	PHE
2	K	113	LEU
2	K	133	ASN
2	K	144	PHE
2	L	58	ILE
2	L	85	ASN
2	L	106	PHE
2	L	113	LEU
2	L	133	ASN
2	L	144	PHE
2	M	58	ILE
2	M	85	ASN

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Mol	Chain	Res	Type
2	M	106	PHE
2	M	113	LEU
2	M	133	ASN
2	M	144	PHE
2	N	58	ILE
2	N	85	ASN
2	N	106	PHE
2	N	113	LEU
2	N	133	ASN
2	N	144	PHE
2	O	58	ILE
2	O	85	ASN
2	O	106	PHE
2	O	113	LEU
2	O	133	ASN
2	O	144	PHE
2	P	58	ILE
2	P	85	ASN
2	P	106	PHE
2	P	113	LEU
2	P	133	ASN
2	P	144	PHE
2	Q	58	ILE
2	Q	85	ASN
2	Q	106	PHE
2	Q	113	LEU
2	Q	133	ASN
2	Q	144	PHE
2	R	58	ILE
2	R	85	ASN
2	R	106	PHE
2	R	113	LEU
2	R	133	ASN
2	R	144	PHE
2	S	58	ILE
2	S	85	ASN
2	S	106	PHE
2	S	113	LEU
2	S	133	ASN
2	S	144	PHE
2	T	58	ILE
2	T	85	ASN

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Mol	Chain	Res	Type
2	T	106	PHE
2	T	113	LEU
2	T	133	ASN
2	T	144	PHE
2	U	58	ILE
2	U	85	ASN
2	U	106	PHE
2	U	113	LEU
2	U	133	ASN
2	U	144	PHE
6	UI	98	LEU
6	UI	127	SER
6	UI	154	ARG
6	UI	159	MET
6	UI	165	PHE
6	UJ	98	LEU
6	UJ	127	SER
6	UJ	154	ARG
6	UJ	159	MET
6	UJ	165	PHE
6	UK	98	LEU
6	UK	127	SER
6	UK	154	ARG
6	UK	159	MET
6	UK	165	PHE
6	UL	98	LEU
6	UL	127	SER
6	UL	154	ARG
6	UL	159	MET
6	UL	165	PHE
6	UL	167	ARG
6	UM	98	LEU
6	UM	127	SER
6	UM	154	ARG
6	UM	159	MET
6	UM	165	PHE
6	UN	98	LEU
6	UN	127	SER
6	UN	154	ARG
6	UN	159	MET
6	UN	165	PHE
6	UO	98	LEU

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Mol	Chain	Res	Type
6	UO	127	SER
6	UO	154	ARG
6	UO	159	MET
6	UO	165	PHE
6	UP	98	LEU
6	UP	127	SER
6	UP	154	ARG
6	UP	159	MET
6	UP	165	PHE
6	UP	167	ARG
2	V	58	ILE
2	V	85	ASN
2	V	106	PHE
2	V	113	LEU
2	V	133	ASN
2	V	144	PHE
2	W	58	ILE
2	W	85	ASN
2	W	106	PHE
2	W	113	LEU
2	W	133	ASN
2	W	144	PHE
6	WA	114	GLU
6	WA	128	GLU
6	WA	167	ARG
6	WA	170	LYS
6	WB	121	PHE
6	WB	128	GLU
6	WB	134	ARG
6	WB	137	GLU
6	WB	164	LEU
6	WB	169	GLN
6	WC	115	LEU
6	WC	120	LYS
6	WC	128	GLU
6	WC	134	ARG
6	WC	164	LEU
6	WC	166	VAL
6	WC	168	GLU
6	WC	170	LYS
6	WD	114	GLU
6	WD	115	LEU

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Mol	Chain	Res	Type
6	WD	167	ARG
6	WD	170	LYS
6	WE	114	GLU
6	WE	128	GLU
6	WE	134	ARG
6	WE	160	PRO
6	WE	161	LYS
6	WE	164	LEU
6	WE	170	LYS
6	WF	111	VAL
6	WF	113	PHE
6	WF	120	LYS
6	WF	121	PHE
6	WF	128	GLU
6	WF	134	ARG
6	WF	142	ARG
6	WG	111	VAL
6	WG	114	GLU
6	WG	115	LEU
6	WG	120	LYS
6	WG	134	ARG
6	WG	164	LEU
6	WG	187	ASP
6	WH	128	GLU
6	WH	134	ARG
6	WH	168	GLU
6	WH	221	THR
6	WI	128	GLU
6	WI	134	ARG
6	WI	165	PHE
6	WI	168	GLU
6	WI	169	GLN
6	WI	170	LYS
6	WJ	128	GLU
6	WJ	165	PHE
6	WJ	167	ARG
6	WJ	169	GLN
6	WK	164	LEU
6	WK	165	PHE
6	WK	167	ARG
6	WK	170	LYS
6	WK	187	ASP

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Mol	Chain	Res	Type
6	WL	128	GLU
6	WL	159	MET
6	WL	221	THR
6	WM	221	THR
6	WN	128	GLU
6	WN	221	THR
6	WO	128	GLU
6	WO	169	GLN
6	WO	170	LYS
6	WO	221	THR
6	WP	128	GLU
6	WP	154	ARG
6	WP	161	LYS
6	WP	165	PHE
6	WP	169	GLN
6	WP	170	LYS
6	WQ	114	GLU
6	WQ	128	GLU
6	WR	114	GLU
6	WR	117	ASP
6	WR	119	GLU
6	WR	128	GLU
6	WR	164	LEU
6	WR	166	VAL
6	WR	169	GLN
6	WS	114	GLU
6	WS	128	GLU
6	WS	134	ARG
6	WS	170	LYS
6	WS	187	ASP
6	WS	221	THR
6	WT	119	GLU
6	WT	123	ILE
6	WT	128	GLU
6	WT	134	ARG
6	WT	159	MET
6	WT	165	PHE
6	WT	167	ARG
6	WU	114	GLU
6	WU	128	GLU
6	WU	134	ARG
6	WU	161	LYS

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Mol	Chain	Res	Type
6	WV	114	GLU
6	WV	117	ASP
6	WV	120	LYS
6	WV	128	GLU
6	WV	134	ARG
6	WV	164	LEU
6	WV	166	VAL
6	WV	169	GLN
6	WV	187	ASP
6	WW	114	GLU
6	WW	115	LEU
6	WW	128	GLU
6	WW	134	ARG
6	WW	167	ARG
6	WW	168	GLU
6	WW	169	GLN
6	WW	221	THR
2	X	58	ILE
2	X	85	ASN
2	X	106	PHE
2	X	113	LEU
2	X	133	ASN
2	X	144	PHE
2	Y	58	ILE
2	Y	85	ASN
2	Y	106	PHE
2	Y	113	LEU
2	Y	133	ASN
2	Y	144	PHE
2	Z	58	ILE
2	Z	85	ASN
2	Z	106	PHE
2	Z	113	LEU
2	Z	133	ASN
2	Z	144	PHE
1	ZA	50	ARG
1	ZA	248	SER
1	ZB	1	MET
1	ZB	4	SER
1	ZB	58	GLU
1	ZB	73	ARG
1	ZB	119	SER

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Mol	Chain	Res	Type
1	ZB	244	SER
1	ZC	123	ASP
1	ZC	244	SER
1	ZC	249	THR
1	ZD	1	MET
1	ZD	64	SER
1	ZD	162	GLN
1	ZD	240	TYR
1	ZE	37	GLN
1	ZE	50	ARG
1	ZE	137	GLN
1	ZE	141	THR
1	ZE	259	GLN
11	ZF	3	PHE
11	ZF	60	ASP
11	ZF	87	ASP
11	ZF	134	PRO
11	ZF	229	THR
11	ZF	265	ASN
11	ZF	280	ASN
11	ZF	284	TYR
11	ZF	289	LEU
11	ZF	352	ASN
11	ZF	355	LYS
11	ZF	392	GLN
11	ZG	3	PHE
11	ZG	38	SER
11	ZG	103	ASP
11	ZG	104	GLU
11	ZG	188	ASP
11	ZG	189	SER
11	ZG	227	SER
11	ZG	234	GLU
11	ZG	260	SER
11	ZG	262	SER
11	ZG	265	ASN
11	ZG	267	MET
11	ZG	288	ASP
11	ZG	350	SER
11	ZG	352	ASN
11	ZG	395	ILE
11	ZH	34	SER

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Mol	Chain	Res	Type
11	ZH	71	ARG
11	ZH	154	MET
11	ZH	227	SER
11	ZH	260	SER
11	ZH	281	GLN
11	ZH	284	TYR
11	ZH	288	ASP
11	ZH	331	ASP
11	ZH	355	LYS
11	ZH	375	MET
11	ZH	380	ARG
11	ZH	399	LEU
11	ZI	99	GLN
11	ZI	195	ASP
11	ZI	197	ASN
11	ZI	260	SER
11	ZI	352	ASN
11	ZI	358	ASN
11	ZJ	46	SER
11	ZJ	96	ARG
11	ZJ	103	ASP
11	ZJ	107	ASN
11	ZJ	195	ASP
11	ZJ	233	ASN
11	ZJ	280	ASN
11	ZJ	331	ASP
11	ZJ	395	ILE
11	ZK	3	PHE
11	ZK	268	GLN
11	ZK	297	ASP
11	ZK	305	SER
11	ZK	331	ASP
11	ZK	338	GLN
11	ZL	78	SER
11	ZL	84	ARG
11	ZL	196	MET
11	ZL	234	GLU
11	ZL	267	MET
11	ZL	291	SER
11	ZL	338	GLN
11	ZL	368	LEU
11	ZL	370	LYS

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Mol	Chain	Res	Type
11	ZL	382	TYR
11	ZM	53	LYS
11	ZM	89	ASN
11	ZM	153	SER
11	ZM	200	PHE
11	ZM	214	ASP
11	ZM	282	ASN
11	ZM	352	ASN
11	ZM	369	SER
11	ZM	370	LYS
11	ZN	43	PHE
11	ZN	78	SER
11	ZN	103	ASP
11	ZN	143	LEU
11	ZN	148	SER
11	ZN	157	ASN
11	ZN	216	SER
11	ZN	297	ASP
11	ZN	367	ASP
11	ZN	396	LEU
11	ZO	2	SER
11	ZO	74	ASP
11	ZO	174	ASP
11	ZO	178	TYR
11	ZO	235	ASN
11	ZO	237	ILE
11	ZO	331	ASP
11	ZO	375	MET
11	ZP	42	MET
11	ZP	63	ASP
11	ZP	74	ASP
11	ZP	95	SER
11	ZP	126	PRO
11	ZP	162	ASP
11	ZP	227	SER
11	ZP	275	ASN
11	ZP	288	ASP
11	ZP	292	TYR
11	ZP	331	ASP
11	ZP	340	SER
11	ZP	369	SER
11	ZP	370	LYS

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Mol	Chain	Res	Type
11	ZP	393	ASP
11	ZQ	46	SER
11	ZQ	101	LYS
11	ZQ	189	SER
11	ZQ	200	PHE
11	ZQ	211	TYR
11	ZQ	280	ASN
11	ZQ	305	SER
11	ZQ	367	ASP
11	ZQ	370	LYS
11	ZR	41	ASP
11	ZR	103	ASP
11	ZR	197	ASN
11	ZR	214	ASP
11	ZR	295	ASN
11	ZR	332	ASN
11	ZR	367	ASP
11	ZS	78	SER
11	ZS	103	ASP
11	ZS	170	PHE
11	ZS	202	LYS
11	ZS	245	ASN
11	ZS	367	ASP
11	ZT	5	GLN
11	ZT	73	LEU
11	ZT	133	ASN
11	ZT	148	SER
11	ZT	195	ASP
11	ZT	262	SER
11	ZT	297	ASP
11	ZT	358	ASN
11	ZU	3	PHE
11	ZU	78	SER
11	ZU	80	ASN
11	ZU	340	SER
11	ZV	46	SER
11	ZV	232	PHE
11	ZV	307	GLU
11	ZV	308	GLN
11	ZW	3	PHE
11	ZW	41	ASP
11	ZW	42	MET

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Mol	Chain	Res	Type
11	ZW	53	LYS
11	ZW	188	ASP
11	ZW	195	ASP
11	ZW	215	SER
11	ZW	259	PHE
11	ZW	292	TYR
11	ZW	309	GLU
11	ZW	326	LEU
11	ZW	331	ASP
11	ZW	340	SER
11	ZW	358	ASN
11	ZX	3	PHE
11	ZX	63	ASP
11	ZX	195	ASP
11	ZY	60	ASP
11	ZY	80	ASN
11	ZY	192	ASN
11	ZY	204	LYS
11	ZY	252	ASN
11	ZY	332	ASN
11	ZY	350	SER
11	ZZ	3	PHE
11	ZZ	41	ASP
11	ZZ	88	SER
11	ZZ	148	SER
11	ZZ	393	ASP
11	Za	96	ARG
11	Za	103	ASP
11	Za	292	TYR
11	Za	331	ASP
11	Za	332	ASN
11	Za	375	MET
11	Zb	41	ASP
11	Zb	89	ASN
11	Zb	292	TYR
11	Zb	308	GLN
11	Zb	355	LYS
11	Zb	367	ASP
11	Zb	393	ASP
11	Zc	41	ASP
11	Zc	103	ASP
11	Zc	204	LYS

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Mol	Chain	Res	Type
11	Zc	267	MET
11	Zc	296	ASN
11	Zc	297	ASP
11	Zc	317	LEU
11	Zc	332	ASN
11	Zc	340	SER
11	Zc	369	SER
11	Zc	399	LEU
11	Zd	41	ASP
11	Zd	114	MET
11	Zd	292	TYR
11	Zd	375	MET
11	Zd	393	ASP
11	Zd	397	ASN
11	Ze	3	PHE
11	Ze	27	SER
11	Ze	46	SER
11	Ze	96	ARG
11	Ze	308	GLN
11	Ze	319	ASN
11	Ze	395	ILE
11	Zf	3	PHE
11	Zf	285	LYS
11	Zf	297	ASP
11	Zf	331	ASP
11	Zf	332	ASN
11	Zf	367	ASP
11	Zf	396	LEU
11	Zg	94	TYR
11	Zg	103	ASP
11	Zg	292	TYR
11	Zg	308	GLN
11	Zg	332	ASN
11	Zg	367	ASP
11	Zg	370	LYS
11	Zh	41	ASP
11	Zh	47	LYS
11	Zh	63	ASP
11	Zh	83	PHE
11	Zh	162	ASP
11	Zh	308	GLN
11	Zh	332	ASN

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Mol	Chain	Res	Type
12	a	20	GLU
12	a	110	MET
12	a	192	GLU
12	a	244	VAL
12	a	248	PRO
12	b	20	GLU
12	b	110	MET
12	b	192	GLU
12	b	244	VAL
12	b	248	PRO
12	c	20	GLU
12	c	110	MET
12	c	192	GLU
12	c	244	VAL
12	c	248	PRO
12	d	20	GLU
12	d	110	MET
12	d	192	GLU
12	d	244	VAL
12	d	248	PRO
12	e	20	GLU
12	e	110	MET
12	e	192	GLU
12	e	244	VAL
12	e	248	PRO
12	f	20	GLU
12	f	110	MET
12	f	192	GLU
12	f	244	VAL
12	f	248	PRO
12	g	20	GLU
12	g	110	MET
12	g	192	GLU
12	g	244	VAL
12	g	248	PRO
12	h	20	GLU
12	h	110	MET
12	h	192	GLU
12	h	244	VAL
12	h	248	PRO
12	i	20	GLU
12	i	110	MET

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Mol	Chain	Res	Type
12	i	192	GLU
12	i	244	VAL
12	i	248	PRO
12	j	20	GLU
12	j	110	MET
12	j	192	GLU
12	j	244	VAL
12	j	248	PRO
12	k	20	GLU
12	k	110	MET
12	k	192	GLU
12	k	244	VAL
12	k	248	PRO
12	l	20	GLU
12	l	110	MET
12	l	192	GLU
12	l	244	VAL
12	l	248	PRO
12	m	20	GLU
12	m	110	MET
12	m	192	GLU
12	m	244	VAL
12	m	248	PRO
12	n	20	GLU
12	n	110	MET
12	n	192	GLU
12	n	244	VAL
12	n	248	PRO
12	o	20	GLU
12	o	110	MET
12	o	192	GLU
12	o	244	VAL
12	o	248	PRO
12	p	20	GLU
12	p	110	MET
12	p	192	GLU
12	p	244	VAL
12	p	248	PRO
12	q	20	GLU
12	q	110	MET
12	q	192	GLU
12	q	244	VAL

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Mol	Chain	Res	Type
12	q	248	PRO
12	r	20	GLU
12	r	110	MET
12	r	192	GLU
12	r	244	VAL
12	r	248	PRO
12	s	20	GLU
12	s	110	MET
12	s	192	GLU
12	s	244	VAL
12	s	248	PRO
12	t	20	GLU
12	t	110	MET
12	t	192	GLU
12	t	244	VAL
12	t	248	PRO
12	u	20	GLU
12	u	110	MET
12	u	192	GLU
12	u	244	VAL
12	u	248	PRO
12	v	20	GLU
12	v	110	MET
12	v	192	GLU
12	v	244	VAL
12	v	248	PRO
12	w	20	GLU
12	w	110	MET
12	w	192	GLU
12	w	244	VAL
12	w	248	PRO
12	x	20	GLU
12	x	110	MET
12	x	192	GLU
12	x	244	VAL
12	x	248	PRO
12	y	20	GLU
12	y	110	MET
12	y	192	GLU
12	y	244	VAL
12	y	248	PRO
12	z	20	GLU

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Mol	Chain	Res	Type
12	z	110	MET
12	z	192	GLU
12	z	244	VAL
12	z	248	PRO
13	C4	106	ILE
13	C4	116	ASP
13	C4	125	ILE
13	C5	106	ILE
13	C5	116	ASP
13	C5	125	ILE
14	C6	112	PHE
14	C6	124	ASP
14	C6	193	MET
15	C8	45	ARG
15	C8	46	VAL
15	C8	63	ARG
15	C8	85	ARG
15	C8	149	THR
15	C8	155	ASN
15	C8	162	LEU
15	C8	169	TRP
15	C8	211	LEU
15	C8	228	ARG
15	C8	233	ASN
15	C8	286	ILE
13	C9	106	ILE
13	C9	116	ASP
13	C9	125	ILE
13	C0	106	ILE
13	C0	116	ASP
13	C0	125	ILE
13	DA	106	ILE
13	DA	116	ASP
13	DA	125	ILE
14	DB	112	PHE
14	DB	124	ASP
14	DB	193	MET
13	DC	106	ILE
13	DC	116	ASP
13	DC	125	ILE
14	DD	112	PHE
14	DD	124	ASP

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Mol	Chain	Res	Type
14	DD	193	MET
15	DF	45	ARG
15	DF	46	VAL
15	DF	63	ARG
15	DF	85	ARG
15	DF	149	THR
15	DF	155	ASN
15	DF	162	LEU
15	DF	169	TRP
15	DF	211	LEU
15	DF	228	ARG
15	DF	233	ASN
15	DF	286	ILE
13	DG	106	ILE
13	DG	116	ASP
13	DG	125	ILE
13	DH	106	ILE
13	DH	116	ASP
13	DH	125	ILE
13	DI	106	ILE
13	DI	116	ASP
13	DI	125	ILE
14	DJ	112	PHE
14	DJ	124	ASP
14	DJ	193	MET
15	DL	45	ARG
15	DL	46	VAL
15	DL	63	ARG
15	DL	85	ARG
15	DL	149	THR
15	DL	155	ASN
15	DL	162	LEU
15	DL	169	TRP
15	DL	211	LEU
15	DL	228	ARG
15	DL	233	ASN
15	DL	286	ILE
15	DM	45	ARG
15	DM	46	VAL
15	DM	63	ARG
15	DM	85	ARG
15	DM	149	THR

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Mol	Chain	Res	Type
15	DM	155	ASN
15	DM	162	LEU
15	DM	169	TRP
15	DM	211	LEU
15	DM	228	ARG
15	DM	233	ASN
15	DM	286	ILE
13	DN	106	ILE
13	DN	116	ASP
13	DN	125	ILE
13	DO	106	ILE
13	DO	116	ASP
13	DO	125	ILE
13	DP	106	ILE
13	DP	116	ASP
13	DP	125	ILE
14	DQ	112	PHE
14	DQ	124	ASP
14	DQ	193	MET
15	DS	45	ARG
15	DS	46	VAL
15	DS	63	ARG
15	DS	85	ARG
15	DS	149	THR
15	DS	155	ASN
15	DS	162	LEU
15	DS	169	TRP
15	DS	211	LEU
15	DS	228	ARG
15	DS	233	ASN
15	DS	286	ILE
13	DT	106	ILE
13	DT	116	ASP
13	DT	125	ILE
13	DU	106	ILE
13	DU	116	ASP
13	DU	125	ILE
13	DV	106	ILE
13	DV	116	ASP
13	DV	125	ILE
14	DW	112	PHE
14	DW	124	ASP

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Mol	Chain	Res	Type
14	DW	193	MET
15	DY	45	ARG
15	DY	46	VAL
15	DY	63	ARG
15	DY	85	ARG
15	DY	149	THR
15	DY	155	ASN
15	DY	162	LEU
15	DY	169	TRP
15	DY	211	LEU
15	DY	228	ARG
15	DY	233	ASN
15	DY	286	ILE
13	DZ	106	ILE
13	DZ	116	ASP
13	DZ	125	ILE
13	Da	106	ILE
13	Da	116	ASP
13	Da	125	ILE
13	Db	106	ILE
13	Db	116	ASP
13	Db	125	ILE
14	Dc	112	PHE
14	Dc	124	ASP
14	Dc	193	MET
15	De	45	ARG
15	De	46	VAL
15	De	63	ARG
15	De	85	ARG
15	De	149	THR
15	De	155	ASN
15	De	162	LEU
15	De	169	TRP
15	De	211	LEU
15	De	228	ARG
15	De	233	ASN
15	De	286	ILE
13	Df	106	ILE
13	Df	116	ASP
13	Df	125	ILE
13	Dg	106	ILE
13	Dg	116	ASP

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Mol	Chain	Res	Type
13	Dg	125	ILE
13	Dh	106	ILE
13	Dh	116	ASP
13	Dh	125	ILE
14	Di	112	PHE
14	Di	124	ASP
14	Di	193	MET
15	Dk	45	ARG
15	Dk	46	VAL
15	Dk	63	ARG
15	Dk	85	ARG
15	Dk	149	THR
15	Dk	155	ASN
15	Dk	162	LEU
15	Dk	169	TRP
15	Dk	211	LEU
15	Dk	228	ARG
15	Dk	233	ASN
15	Dk	286	ILE
13	Dl	106	ILE
13	Dl	116	ASP
13	Dl	125	ILE
13	Dm	106	ILE
13	Dm	116	ASP
13	Dm	125	ILE
13	Dn	106	ILE
13	Dn	116	ASP
13	Dn	125	ILE
14	Do	112	PHE
14	Do	124	ASP
14	Do	193	MET
15	Dq	45	ARG
15	Dq	46	VAL
15	Dq	63	ARG
15	Dq	85	ARG
15	Dq	149	THR
15	Dq	155	ASN
15	Dq	162	LEU
15	Dq	169	TRP
15	Dq	211	LEU
15	Dq	228	ARG
15	Dq	233	ASN

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Mol	Chain	Res	Type
15	Dq	286	ILE
13	Dr	106	ILE
13	Dr	116	ASP
13	Dr	125	ILE
13	Ds	106	ILE
13	Ds	116	ASP
13	Ds	125	ILE
13	Dt	106	ILE
13	Dt	116	ASP
13	Dt	125	ILE
14	Du	112	PHE
14	Du	124	ASP
14	Du	193	MET
15	Dw	45	ARG
15	Dw	46	VAL
15	Dw	63	ARG
15	Dw	85	ARG
15	Dw	149	THR
15	Dw	155	ASN
15	Dw	162	LEU
15	Dw	169	TRP
15	Dw	211	LEU
15	Dw	228	ARG
15	Dw	233	ASN
15	Dw	286	ILE
13	Dx	106	ILE
13	Dx	116	ASP
13	Dx	125	ILE
13	Dy	106	ILE
13	Dy	116	ASP
13	Dy	125	ILE
13	Dz	106	ILE
13	Dz	116	ASP
13	Dz	125	ILE
14	D1	112	PHE
14	D1	124	ASP
14	D1	193	MET
15	D3	45	ARG
15	D3	46	VAL
15	D3	63	ARG
15	D3	85	ARG
15	D3	149	THR

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Mol	Chain	Res	Type
15	D3	155	ASN
15	D3	162	LEU
15	D3	169	TRP
15	D3	211	LEU
15	D3	228	ARG
15	D3	233	ASN
15	D3	286	ILE
13	D4	106	ILE
13	D4	116	ASP
13	D4	125	ILE
13	D5	106	ILE
13	D5	116	ASP
13	D5	125	ILE
13	D6	106	ILE
13	D6	116	ASP
13	D6	125	ILE
14	D7	112	PHE
14	D7	124	ASP
14	D7	193	MET
15	D9	45	ARG
15	D9	46	VAL
15	D9	63	ARG
15	D9	85	ARG
15	D9	149	THR
15	D9	155	ASN
15	D9	162	LEU
15	D9	169	TRP
15	D9	211	LEU
15	D9	228	ARG
15	D9	233	ASN
15	D9	286	ILE
13	D0	106	ILE
13	D0	116	ASP
13	D0	125	ILE
13	EA	106	ILE
13	EA	116	ASP
13	EA	125	ILE
13	EB	106	ILE
13	EB	116	ASP
13	EB	125	ILE
13	B0	106	ILE
13	B0	116	ASP

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Mol	Chain	Res	Type
13	B0	125	ILE
15	B1	45	ARG
15	B1	46	VAL
15	B1	63	ARG
15	B1	85	ARG
15	B1	149	THR
15	B1	155	ASN
15	B1	162	LEU
15	B1	169	TRP
15	B1	211	LEU
15	B1	228	ARG
15	B1	233	ASN
15	B1	286	ILE
13	B2	106	ILE
13	B2	116	ASP
13	B2	125	ILE
13	B3	106	ILE
13	B3	116	ASP
13	B3	125	ILE
13	B4	106	ILE
13	B4	116	ASP
13	B4	125	ILE
14	B5	112	PHE
14	B5	124	ASP
14	B5	193	MET
15	B7	45	ARG
15	B7	46	VAL
15	B7	63	ARG
15	B7	85	ARG
15	B7	149	THR
15	B7	155	ASN
15	B7	162	LEU
15	B7	169	TRP
15	B7	211	LEU
15	B7	228	ARG
15	B7	233	ASN
15	B7	286	ILE
13	B8	106	ILE
13	B8	116	ASP
13	B8	125	ILE
13	B9	106	ILE
13	B9	116	ASP

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Mol	Chain	Res	Type
13	B9	125	ILE
13	EC	106	ILE
13	EC	116	ASP
13	EC	125	ILE
13	ED	106	ILE
13	ED	116	ASP
13	ED	125	ILE
14	EE	112	PHE
14	EE	124	ASP
14	EE	193	MET
15	EG	45	ARG
15	EG	46	VAL
15	EG	63	ARG
15	EG	85	ARG
15	EG	149	THR
15	EG	155	ASN
15	EG	162	LEU
15	EG	169	TRP
15	EG	211	LEU
15	EG	228	ARG
15	EG	233	ASN
15	EG	286	ILE
13	EH	106	ILE
13	EH	116	ASP
13	EH	125	ILE
13	EI	106	ILE
13	EI	116	ASP
13	EI	125	ILE
13	EJ	106	ILE
13	EJ	116	ASP
13	EJ	125	ILE
14	EK	112	PHE
14	EK	124	ASP
14	EK	193	MET
15	EM	45	ARG
15	EM	46	VAL
15	EM	63	ARG
15	EM	85	ARG
15	EM	149	THR
15	EM	155	ASN
15	EM	162	LEU
15	EM	169	TRP

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Mol	Chain	Res	Type
15	EM	211	LEU
15	EM	228	ARG
15	EM	233	ASN
15	EM	286	ILE
13	EN	106	ILE
13	EN	116	ASP
13	EN	125	ILE
13	EO	106	ILE
13	EO	116	ASP
13	EO	125	ILE
13	EP	106	ILE
13	EP	116	ASP
13	EP	125	ILE
14	EQ	112	PHE
14	EQ	124	ASP
14	EQ	193	MET
15	ES	45	ARG
15	ES	46	VAL
15	ES	63	ARG
15	ES	85	ARG
15	ES	149	THR
15	ES	155	ASN
15	ES	162	LEU
15	ES	169	TRP
15	ES	211	LEU
15	ES	228	ARG
15	ES	233	ASN
15	ES	286	ILE
13	ET	106	ILE
13	ET	116	ASP
13	ET	125	ILE
13	EU	106	ILE
13	EU	116	ASP
13	EU	125	ILE
13	EV	106	ILE
13	EV	116	ASP
13	EV	125	ILE
14	EW	112	PHE
14	EW	124	ASP
14	EW	193	MET
15	EY	45	ARG
15	EY	46	VAL

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Mol	Chain	Res	Type
15	EY	63	ARG
15	EY	85	ARG
15	EY	149	THR
15	EY	155	ASN
15	EY	162	LEU
15	EY	169	TRP
15	EY	211	LEU
15	EY	228	ARG
15	EY	233	ASN
15	EY	286	ILE
13	EZ	106	ILE
13	EZ	116	ASP
13	EZ	125	ILE
13	BY	106	ILE
13	BY	116	ASP
13	BY	125	ILE
13	BZ	106	ILE
13	BZ	116	ASP
13	BZ	125	ILE
14	Ba	112	PHE
14	Ba	124	ASP
14	Ba	193	MET
15	Bc	45	ARG
15	Bc	46	VAL
15	Bc	63	ARG
15	Bc	85	ARG
15	Bc	149	THR
15	Bc	155	ASN
15	Bc	162	LEU
15	Bc	169	TRP
15	Bc	211	LEU
15	Bc	228	ARG
15	Bc	233	ASN
15	Bc	286	ILE
13	Bd	106	ILE
13	Bd	116	ASP
13	Bd	125	ILE
13	Be	106	ILE
13	Be	116	ASP
13	Be	125	ILE
13	Bf	106	ILE
13	Bf	116	ASP

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Mol	Chain	Res	Type
13	Bf	125	ILE
14	Bg	112	PHE
14	Bg	124	ASP
14	Bg	193	MET
15	Bi	45	ARG
15	Bi	46	VAL
15	Bi	63	ARG
15	Bi	85	ARG
15	Bi	149	THR
15	Bi	155	ASN
15	Bi	162	LEU
15	Bi	169	TRP
15	Bi	211	LEU
15	Bi	228	ARG
15	Bi	233	ASN
15	Bi	286	ILE
13	Bj	106	ILE
13	Bj	116	ASP
13	Bj	125	ILE
13	Bk	106	ILE
13	Bk	116	ASP
13	Bk	125	ILE
13	Bl	106	ILE
13	Bl	116	ASP
13	Bl	125	ILE
14	Bm	112	PHE
14	Bm	124	ASP
14	Bm	193	MET
15	Bo	45	ARG
15	Bo	46	VAL
15	Bo	63	ARG
15	Bo	85	ARG
15	Bo	149	THR
15	Bo	155	ASN
15	Bo	162	LEU
15	Bo	169	TRP
15	Bo	211	LEU
15	Bo	228	ARG
15	Bo	233	ASN
15	Bo	286	ILE
13	Bp	106	ILE
13	Bp	116	ASP

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Mol	Chain	Res	Type
13	Bp	125	ILE
13	Bq	106	ILE
13	Bq	116	ASP
13	Bq	125	ILE
13	Br	106	ILE
13	Br	116	ASP
13	Br	125	ILE
14	Bs	112	PHE
14	Bs	124	ASP
14	Bs	193	MET
15	Bu	45	ARG
15	Bu	46	VAL
15	Bu	63	ARG
15	Bu	85	ARG
15	Bu	149	THR
15	Bu	155	ASN
15	Bu	162	LEU
15	Bu	169	TRP
15	Bu	211	LEU
15	Bu	228	ARG
15	Bu	233	ASN
15	Bu	286	ILE
13	Bv	106	ILE
13	Bv	116	ASP
13	Bv	125	ILE
13	Bw	106	ILE
13	Bw	116	ASP
13	Bw	125	ILE
13	Bx	106	ILE
13	Bx	116	ASP
13	Bx	125	ILE
14	By	112	PHE
14	By	124	ASP
14	By	193	MET
13	C1	106	ILE
13	C1	116	ASP
13	C1	125	ILE
13	C2	106	ILE
13	C2	116	ASP
13	C2	125	ILE
14	CA	112	PHE
14	CA	124	ASP

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Mol	Chain	Res	Type
14	CA	193	MET
15	CC	45	ARG
15	CC	46	VAL
15	CC	63	ARG
15	CC	85	ARG
15	CC	149	THR
15	CC	155	ASN
15	CC	162	LEU
15	CC	169	TRP
15	CC	211	LEU
15	CC	228	ARG
15	CC	233	ASN
15	CC	286	ILE
13	CD	106	ILE
13	CD	116	ASP
13	CD	125	ILE
13	CE	106	ILE
13	CE	116	ASP
13	CE	125	ILE
13	CF	106	ILE
13	CF	116	ASP
13	CF	125	ILE
14	CG	112	PHE
14	CG	124	ASP
14	CG	193	MET
15	CI	45	ARG
15	CI	46	VAL
15	CI	63	ARG
15	CI	85	ARG
15	CI	149	THR
15	CI	155	ASN
15	CI	162	LEU
15	CI	169	TRP
15	CI	211	LEU
15	CI	228	ARG
15	CI	233	ASN
15	CI	286	ILE
13	CJ	106	ILE
13	CJ	116	ASP
13	CJ	125	ILE
13	CK	106	ILE
13	CK	116	ASP

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Mol	Chain	Res	Type
13	CK	125	ILE
13	CL	106	ILE
13	CL	116	ASP
13	CL	125	ILE
14	CM	112	PHE
14	CM	124	ASP
14	CM	193	MET
15	CO	45	ARG
15	CO	46	VAL
15	CO	63	ARG
15	CO	85	ARG
15	CO	149	THR
15	CO	155	ASN
15	CO	162	LEU
15	CO	169	TRP
15	CO	211	LEU
15	CO	228	ARG
15	CO	233	ASN
15	CO	286	ILE
13	CP	106	ILE
13	CP	116	ASP
13	CP	125	ILE
13	CQ	106	ILE
13	CQ	116	ASP
13	CQ	125	ILE
13	CR	106	ILE
13	CR	116	ASP
13	CR	125	ILE
14	CS	112	PHE
14	CS	124	ASP
14	CS	193	MET
15	CU	45	ARG
15	CU	46	VAL
15	CU	63	ARG
15	CU	85	ARG
15	CU	149	THR
15	CU	155	ASN
15	CU	162	LEU
15	CU	169	TRP
15	CU	211	LEU
15	CU	228	ARG
15	CU	233	ASN

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Mol	Chain	Res	Type
15	CU	286	ILE
13	CV	106	ILE
13	CV	116	ASP
13	CV	125	ILE
13	CW	106	ILE
13	CW	116	ASP
13	CW	125	ILE
13	CX	106	ILE
13	CX	116	ASP
13	CX	125	ILE
14	CY	112	PHE
14	CY	124	ASP
14	CY	193	MET
15	Ca	45	ARG
15	Ca	46	VAL
15	Ca	63	ARG
15	Ca	85	ARG
15	Ca	149	THR
15	Ca	155	ASN
15	Ca	162	LEU
15	Ca	169	TRP
15	Ca	211	LEU
15	Ca	228	ARG
15	Ca	233	ASN
15	Ca	286	ILE
13	Cb	106	ILE
13	Cb	116	ASP
13	Cb	125	ILE
13	Cc	106	ILE
13	Cc	116	ASP
13	Cc	125	ILE
13	Cd	106	ILE
13	Cd	116	ASP
13	Cd	125	ILE
14	Ce	112	PHE
14	Ce	124	ASP
14	Ce	193	MET
15	Cg	45	ARG
15	Cg	46	VAL
15	Cg	63	ARG
15	Cg	85	ARG
15	Cg	149	THR

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Mol	Chain	Res	Type
15	Cg	155	ASN
15	Cg	162	LEU
15	Cg	169	TRP
15	Cg	211	LEU
15	Cg	228	ARG
15	Cg	233	ASN
15	Cg	286	ILE
13	Ch	106	ILE
13	Ch	116	ASP
13	Ch	125	ILE
13	Ci	106	ILE
13	Ci	116	ASP
13	Ci	125	ILE
13	Cj	106	ILE
13	Cj	116	ASP
13	Cj	125	ILE
14	Ck	112	PHE
14	Ck	124	ASP
14	Ck	193	MET
15	Cm	45	ARG
15	Cm	46	VAL
15	Cm	63	ARG
15	Cm	85	ARG
15	Cm	149	THR
15	Cm	155	ASN
15	Cm	162	LEU
15	Cm	169	TRP
15	Cm	211	LEU
15	Cm	228	ARG
15	Cm	233	ASN
15	Cm	286	ILE
13	Cn	106	ILE
13	Cn	116	ASP
13	Cn	125	ILE
13	Co	106	ILE
13	Co	116	ASP
13	Co	125	ILE
13	Cp	106	ILE
13	Cp	116	ASP
13	Cp	125	ILE
14	Cq	112	PHE
14	Cq	124	ASP

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Mol	Chain	Res	Type
14	Cq	193	MET
15	Cs	45	ARG
15	Cs	46	VAL
15	Cs	63	ARG
15	Cs	85	ARG
15	Cs	149	THR
15	Cs	155	ASN
15	Cs	162	LEU
15	Cs	169	TRP
15	Cs	211	LEU
15	Cs	228	ARG
15	Cs	233	ASN
15	Cs	286	ILE
13	Ct	106	ILE
13	Ct	116	ASP
13	Ct	125	ILE
13	Cu	106	ILE
13	Cu	116	ASP
13	Cu	125	ILE
13	Cv	106	ILE
13	Cv	116	ASP
13	Cv	125	ILE
14	Cw	112	PHE
14	Cw	124	ASP
14	Cw	193	MET
15	Cy	45	ARG
15	Cy	46	VAL
15	Cy	63	ARG
15	Cy	85	ARG
15	Cy	149	THR
15	Cy	155	ASN
15	Cy	162	LEU
15	Cy	169	TRP
15	Cy	211	LEU
15	Cy	228	ARG
15	Cy	233	ASN
15	Cy	286	ILE
13	Cz	106	ILE
13	Cz	116	ASP
13	Cz	125	ILE
14	Ea	112	PHE
14	Ea	124	ASP

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Mol	Chain	Res	Type
14	Ea	193	MET
15	Ec	45	ARG
15	Ec	46	VAL
15	Ec	63	ARG
15	Ec	85	ARG
15	Ec	149	THR
15	Ec	155	ASN
15	Ec	162	LEU
15	Ec	169	TRP
15	Ec	211	LEU
15	Ec	228	ARG
15	Ec	233	ASN
15	Ec	286	ILE
13	Ed	106	ILE
13	Ed	116	ASP
13	Ed	125	ILE
13	Ee	106	ILE
13	Ee	116	ASP
13	Ee	125	ILE
13	Ef	106	ILE
13	Ef	116	ASP
13	Ef	125	ILE
14	Eg	112	PHE
14	Eg	124	ASP
14	Eg	193	MET
15	Ei	45	ARG
15	Ei	46	VAL
15	Ei	63	ARG
15	Ei	85	ARG
15	Ei	149	THR
15	Ei	155	ASN
15	Ei	162	LEU
15	Ei	169	TRP
15	Ei	211	LEU
15	Ei	228	ARG
15	Ei	233	ASN
15	Ei	286	ILE
13	Ej	106	ILE
13	Ej	116	ASP
13	Ej	125	ILE
13	Ek	106	ILE
13	Ek	116	ASP

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Mol	Chain	Res	Type
13	Ek	125	ILE
13	El	106	ILE
13	El	116	ASP
13	El	125	ILE
14	Em	112	PHE
14	Em	124	ASP
14	Em	193	MET
15	Eo	45	ARG
15	Eo	46	VAL
15	Eo	63	ARG
15	Eo	85	ARG
15	Eo	149	THR
15	Eo	155	ASN
15	Eo	162	LEU
15	Eo	169	TRP
15	Eo	211	LEU
15	Eo	228	ARG
15	Eo	233	ASN
15	Eo	286	ILE
13	Ep	106	ILE
13	Ep	116	ASP
13	Ep	125	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1300) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	16	GLN
1	0	47	GLN
1	0	100	GLN
1	0	135	GLN
1	0	196	GLN
1	0	235	GLN
1	0	255	GLN
1	1	47	GLN
1	1	67	GLN
1	1	83	GLN
1	1	85	ASN
1	1	91	ASN
1	1	121	GLN
1	1	223	ASN
1	1	252	GLN
1	2	51	GLN

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Mol	Chain	Res	Type
1	2	145	ASN
1	2	164	GLN
1	2	232	ASN
1	2	235	GLN
1	2	255	GLN
1	3	67	GLN
1	3	121	GLN
1	3	161	GLN
1	3	255	GLN
1	4	32	ASN
1	4	37	GLN
1	4	47	GLN
1	4	51	GLN
1	4	125	ASN
1	4	127	GLN
1	4	137	GLN
1	4	174	ASN
1	4	216	GLN
1	4	235	GLN
1	4	243	ASN
1	4	259	GLN
1	5	55	GLN
1	5	85	ASN
1	5	100	GLN
1	5	121	GLN
1	5	237	GLN
1	6	59	GLN
1	6	121	GLN
1	6	127	GLN
1	6	135	GLN
1	6	137	GLN
1	6	209	ASN
1	6	235	GLN
1	6	237	GLN
1	7	24	ASN
1	7	55	GLN
1	7	85	ASN
1	7	164	GLN
1	7	235	GLN
1	8	24	ASN
1	8	28	ASN
1	8	83	GLN

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Mol	Chain	Res	Type
1	8	91	ASN
1	9	37	GLN
1	9	55	GLN
1	9	85	ASN
1	9	91	ASN
1	9	127	GLN
1	9	259	GLN
2	A	130	ASN
2	A	142	ASN
2	A	160	ASN
2	A	173	GLN
2	A	214	ASN
2	A	217	GLN
2	A	223	GLN
3	A0	72	HIS
3	A0	76	GLN
3	A0	112	ASN
4	A1	15	GLN
4	A1	87	GLN
4	A1	90	ASN
4	A2	103	GLN
4	A3	87	GLN
4	A4	55	GLN
3	A6	17	ASN
3	A7	23	GLN
3	A7	29	ASN
3	A7	92	GLN
3	A7	117	GLN
3	A8	32	ASN
3	A8	76	GLN
3	A8	92	GLN
3	A9	17	ASN
3	A9	21	GLN
3	A9	32	ASN
3	A9	72	HIS
3	A9	76	GLN
3	A9	117	GLN
5	AA	102	ASN
5	AB	18	GLN
5	AB	70	GLN
5	AB	106	GLN
5	AB	116	GLN

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Mol	Chain	Res	Type
5	AB	172	GLN
5	AB	210	ASN
5	AB	223	ASN
5	AB	240	ASN
5	AC	14	GLN
5	AC	18	GLN
5	AC	28	ASN
5	AC	70	GLN
5	AC	104	ASN
5	AC	106	GLN
5	AC	186	GLN
5	AD	17	ASN
5	AD	28	ASN
5	AD	104	ASN
5	AD	106	GLN
5	AD	210	ASN
5	AD	240	ASN
5	AE	18	GLN
5	AE	104	ASN
5	AE	106	GLN
5	AE	112	GLN
5	AE	116	GLN
5	AE	118	HIS
5	AE	153	ASN
5	AE	240	ASN
1	AF	47	GLN
1	AF	121	GLN
1	AF	135	GLN
1	AF	169	GLN
1	AF	172	GLN
1	AF	180	ASN
1	AF	223	ASN
1	AG	16	GLN
1	AG	28	ASN
1	AG	88	GLN
1	AG	145	ASN
1	AG	180	ASN
1	AG	259	GLN
1	AH	85	ASN
1	AH	104	GLN
1	AH	127	GLN
1	AH	137	GLN

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Mol	Chain	Res	Type
1	AH	172	GLN
1	AH	174	ASN
1	AH	196	GLN
1	AH	259	GLN
1	AI	16	GLN
1	AI	32	ASN
1	AI	47	GLN
1	AI	67	GLN
1	AI	162	GLN
1	AI	209	ASN
1	AI	235	GLN
1	AJ	47	GLN
1	AJ	67	GLN
1	AJ	90	ASN
1	AJ	125	ASN
1	AJ	127	GLN
1	AJ	137	GLN
1	AJ	169	GLN
1	AJ	172	GLN
1	AJ	174	ASN
1	AJ	232	ASN
1	AJ	235	GLN
1	AJ	252	GLN
1	AK	28	ASN
1	AK	47	GLN
1	AK	104	GLN
1	AK	121	GLN
1	AK	135	GLN
1	AK	145	ASN
1	AK	174	ASN
1	AK	196	GLN
1	AK	202	ASN
1	AK	223	ASN
1	AK	235	GLN
1	AL	32	ASN
1	AL	47	GLN
1	AL	83	GLN
1	AL	127	GLN
1	AL	145	ASN
1	AL	209	ASN
1	AM	25	ASN
1	AM	37	GLN

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Mol	Chain	Res	Type
1	AM	51	GLN
1	AM	125	ASN
1	AM	127	GLN
1	AM	137	GLN
1	AM	209	ASN
1	AM	223	ASN
1	AM	252	GLN
1	AN	67	GLN
1	AN	125	ASN
6	AO	297	GLN
6	AO	303	GLN
6	AO	374	HIS
6	AO	434	ASN
6	AP	297	GLN
6	AP	299	ASN
6	AP	303	GLN
6	AP	359	GLN
6	AP	374	HIS
6	AP	434	ASN
6	AQ	303	GLN
6	AQ	374	HIS
6	AQ	434	ASN
6	AR	303	GLN
6	AR	374	HIS
6	AS	297	GLN
6	AS	299	ASN
6	AS	303	GLN
6	AS	374	HIS
6	AT	303	GLN
6	AT	374	HIS
6	AU	303	GLN
6	AU	374	HIS
6	AV	303	GLN
6	AV	374	HIS
6	AW	299	ASN
6	AW	303	GLN
6	AW	374	HIS
6	AX	303	GLN
6	AX	374	HIS
6	AY	299	ASN
6	AY	303	GLN
6	AY	374	HIS

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Mol	Chain	Res	Type
6	AZ	303	GLN
6	AZ	374	HIS
6	Aa	303	GLN
6	Aa	374	HIS
6	Ac	303	GLN
6	Ad	265	GLN
6	Ad	303	GLN
6	Ad	374	HIS
6	Ae	303	GLN
6	Ae	374	HIS
6	Af	297	GLN
6	Af	303	GLN
6	Af	365	ASN
6	Af	374	HIS
6	Ag	297	GLN
6	Ag	303	GLN
6	Ag	374	HIS
6	Ah	303	GLN
6	Ah	374	HIS
6	Ai	303	GLN
6	Ai	374	HIS
6	Aj	303	GLN
6	Aj	374	HIS
6	Ak	303	GLN
6	Ak	374	HIS
6	Al	303	GLN
6	Al	374	HIS
6	Am	303	GLN
6	Am	374	HIS
6	An	303	GLN
6	An	374	HIS
6	An	434	ASN
6	Ao	374	HIS
6	Ao	434	ASN
6	Ap	374	HIS
6	Ap	434	ASN
7	As	39	GLN
8	At	162	ASN
8	At	182	ASN
8	At	205	ASN
9	Au	119	GLN
9	Au	141	GLN

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Mol	Chain	Res	Type
9	Aw	36	GLN
9	Aw	160	GLN
9	Aw	233	GLN
9	Ax	160	GLN
9	Ax	184	GLN
9	Ax	233	GLN
9	Ay	114	GLN
9	Ay	155	ASN
9	Ay	241	GLN
4	Az	69	ASN
4	Az	83	GLN
4	Az	103	GLN
2	B	130	ASN
2	B	142	ASN
2	B	160	ASN
2	B	173	GLN
2	B	214	ASN
2	B	217	GLN
2	B	223	GLN
10	BA	30	ASN
10	BB	5	ASN
10	BB	22	ASN
10	BC	22	ASN
10	BC	50	GLN
10	BC	57	GLN
10	BC	134	GLN
10	BD	22	ASN
10	BE	17	GLN
10	BE	30	ASN
10	BF	57	GLN
10	BF	115	ASN
6	BG	318	ASN
6	BG	319	GLN
6	BI	319	GLN
6	BJ	324	ASN
6	BO	318	ASN
6	BQ	319	GLN
6	BQ	324	ASN
6	BR	303	GLN
6	BR	374	HIS
6	BR	434	ASN
6	BS	303	GLN

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Mol	Chain	Res	Type
6	BS	374	HIS
6	BT	303	GLN
6	BT	374	HIS
6	BU	303	GLN
6	BU	374	HIS
6	BV	303	GLN
6	BV	374	HIS
6	BW	303	GLN
6	BW	374	HIS
6	BX	297	GLN
6	BX	303	GLN
6	BX	374	HIS
2	C	130	ASN
2	C	142	ASN
2	C	160	ASN
2	C	173	GLN
2	C	214	ASN
2	C	217	GLN
2	C	223	GLN
2	D	130	ASN
2	D	142	ASN
2	D	160	ASN
2	D	173	GLN
2	D	214	ASN
2	D	217	GLN
2	D	223	GLN
2	E	130	ASN
2	E	142	ASN
2	E	160	ASN
2	E	173	GLN
2	E	214	ASN
2	E	217	GLN
2	E	223	GLN
2	F	130	ASN
2	F	142	ASN
2	F	160	ASN
2	F	173	GLN
2	F	214	ASN
2	F	217	GLN
2	F	223	GLN
2	G	130	ASN
2	G	142	ASN

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Mol	Chain	Res	Type
2	G	160	ASN
2	G	173	GLN
2	G	214	ASN
2	G	217	GLN
2	G	223	GLN
2	H	130	ASN
2	H	142	ASN
2	H	160	ASN
2	H	173	GLN
2	H	214	ASN
2	H	217	GLN
2	I	130	ASN
2	I	142	ASN
2	I	160	ASN
2	I	173	GLN
2	I	214	ASN
2	I	217	GLN
2	I	223	GLN
2	J	130	ASN
2	J	142	ASN
2	J	160	ASN
2	J	173	GLN
2	J	214	ASN
2	J	217	GLN
2	J	223	GLN
2	K	130	ASN
2	K	142	ASN
2	K	160	ASN
2	K	173	GLN
2	K	214	ASN
2	K	217	GLN
2	K	223	GLN
2	L	130	ASN
2	L	142	ASN
2	L	160	ASN
2	L	173	GLN
2	L	214	ASN
2	L	217	GLN
2	L	223	GLN
2	M	130	ASN
2	M	142	ASN
2	M	160	ASN

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Mol	Chain	Res	Type
2	M	173	GLN
2	M	214	ASN
2	M	217	GLN
2	M	223	GLN
2	N	130	ASN
2	N	142	ASN
2	N	160	ASN
2	N	173	GLN
2	N	214	ASN
2	N	217	GLN
2	N	223	GLN
2	O	130	ASN
2	O	142	ASN
2	O	160	ASN
2	O	173	GLN
2	O	214	ASN
2	O	217	GLN
2	O	223	GLN
2	P	130	ASN
2	P	142	ASN
2	P	160	ASN
2	P	173	GLN
2	P	214	ASN
2	P	217	GLN
2	P	223	GLN
2	Q	130	ASN
2	Q	142	ASN
2	Q	160	ASN
2	Q	173	GLN
2	Q	214	ASN
2	Q	217	GLN
2	Q	223	GLN
2	R	130	ASN
2	R	142	ASN
2	R	160	ASN
2	R	173	GLN
2	R	214	ASN
2	R	217	GLN
2	R	223	GLN
2	S	130	ASN
2	S	142	ASN
2	S	160	ASN

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Mol	Chain	Res	Type
2	S	173	GLN
2	S	214	ASN
2	S	217	GLN
2	S	223	GLN
2	T	130	ASN
2	T	142	ASN
2	T	160	ASN
2	T	173	GLN
2	T	214	ASN
2	T	217	GLN
2	T	223	GLN
2	U	130	ASN
2	U	142	ASN
2	U	160	ASN
2	U	173	GLN
2	U	214	ASN
2	U	217	GLN
2	U	223	GLN
6	UI	196	HIS
6	UJ	245	HIS
6	UK	196	HIS
6	UL	69	GLN
6	UL	196	HIS
6	UM	196	HIS
6	UN	69	GLN
6	UN	196	HIS
6	UO	196	HIS
6	UP	196	HIS
2	V	130	ASN
2	V	142	ASN
2	V	160	ASN
2	V	173	GLN
2	V	214	ASN
2	V	217	GLN
2	V	223	GLN
2	W	130	ASN
2	W	142	ASN
2	W	160	ASN
2	W	173	GLN
2	W	214	ASN
2	W	217	GLN
2	W	223	GLN

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Mol	Chain	Res	Type
6	WB	169	GLN
6	WE	156	HIS
6	WE	209	ASN
6	WF	118	GLN
6	WH	156	HIS
6	WI	129	GLN
6	WI	156	HIS
6	WJ	169	GLN
6	WJ	209	ASN
6	WO	209	ASN
6	WP	209	ASN
6	WV	169	GLN
6	WW	169	GLN
2	X	130	ASN
2	X	142	ASN
2	X	160	ASN
2	X	173	GLN
2	X	214	ASN
2	X	217	GLN
2	X	223	GLN
2	Y	130	ASN
2	Y	142	ASN
2	Y	160	ASN
2	Y	173	GLN
2	Y	214	ASN
2	Y	217	GLN
2	Y	223	GLN
2	Z	130	ASN
2	Z	142	ASN
2	Z	160	ASN
2	Z	173	GLN
2	Z	214	ASN
2	Z	217	GLN
2	Z	223	GLN
1	ZA	37	GLN
1	ZA	137	GLN
1	ZA	235	GLN
1	ZB	24	ASN
1	ZB	25	ASN
1	ZB	28	ASN
1	ZB	37	GLN
1	ZB	135	GLN

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Mol	Chain	Res	Type
1	ZB	137	GLN
1	ZB	237	GLN
1	ZC	16	GLN
1	ZC	37	GLN
1	ZC	88	GLN
1	ZC	100	GLN
1	ZC	137	GLN
1	ZD	24	ASN
1	ZD	67	GLN
1	ZD	88	GLN
1	ZD	91	ASN
1	ZD	135	GLN
1	ZD	235	GLN
1	ZD	237	GLN
1	ZE	24	ASN
1	ZE	37	GLN
1	ZE	67	GLN
1	ZE	121	GLN
1	ZE	235	GLN
1	ZE	252	GLN
11	ZF	5	GLN
11	ZF	16	ASN
11	ZF	107	ASN
11	ZF	155	GLN
11	ZF	157	ASN
11	ZF	197	ASN
11	ZF	358	ASN
11	ZF	392	GLN
11	ZF	401	ASN
11	ZG	107	ASN
11	ZG	112	GLN
11	ZG	130	GLN
11	ZG	133	ASN
11	ZG	332	ASN
11	ZG	387	GLN
11	ZG	394	GLN
11	ZH	5	GLN
11	ZH	155	GLN
11	ZH	157	ASN
11	ZH	206	ASN
11	ZH	270	ASN
11	ZH	296	ASN

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Mol	Chain	Res	Type
11	ZH	352	ASN
11	ZH	365	ASN
11	ZH	379	GLN
11	ZI	79	GLN
11	ZI	89	ASN
11	ZI	197	ASN
11	ZI	269	GLN
11	ZI	310	GLN
11	ZI	385	ASN
11	ZI	392	GLN
11	ZI	394	GLN
11	ZI	401	ASN
11	ZJ	89	ASN
11	ZJ	107	ASN
11	ZJ	133	ASN
11	ZJ	159	ASN
11	ZJ	197	ASN
11	ZJ	265	ASN
11	ZJ	274	ASN
11	ZJ	282	ASN
11	ZJ	379	GLN
11	ZJ	392	GLN
11	ZK	89	ASN
11	ZK	107	ASN
11	ZK	197	ASN
11	ZK	252	ASN
11	ZK	270	ASN
11	ZK	303	ASN
11	ZK	319	ASN
11	ZK	392	GLN
11	ZK	401	ASN
11	ZL	5	GLN
11	ZL	79	GLN
11	ZL	89	ASN
11	ZL	179	ASN
11	ZL	190	GLN
11	ZL	197	ASN
11	ZL	269	GLN
11	ZL	282	ASN
11	ZL	310	GLN
11	ZL	338	GLN
11	ZL	394	GLN

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Mol	Chain	Res	Type
11	ZL	401	ASN
11	ZM	5	GLN
11	ZM	59	GLN
11	ZM	89	ASN
11	ZM	197	ASN
11	ZM	213	HIS
11	ZM	235	ASN
11	ZM	252	ASN
11	ZM	381	ASN
11	ZN	79	GLN
11	ZN	107	ASN
11	ZN	112	GLN
11	ZN	129	GLN
11	ZN	133	ASN
11	ZN	190	GLN
11	ZN	197	ASN
11	ZN	319	ASN
11	ZN	332	ASN
11	ZN	379	GLN
11	ZN	385	ASN
11	ZN	401	ASN
11	ZO	5	GLN
11	ZO	89	ASN
11	ZO	141	ASN
11	ZO	235	ASN
11	ZO	268	GLN
11	ZO	332	ASN
11	ZP	5	GLN
11	ZP	11	ASN
11	ZP	107	ASN
11	ZP	129	GLN
11	ZP	194	HIS
11	ZP	269	GLN
11	ZP	270	ASN
11	ZP	314	GLN
11	ZP	322	ASN
11	ZP	338	GLN
11	ZP	379	GLN
11	ZP	381	ASN
11	ZP	385	ASN
11	ZQ	5	GLN
11	ZQ	89	ASN

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Mol	Chain	Res	Type
11	ZQ	97	ASN
11	ZQ	133	ASN
11	ZQ	141	ASN
11	ZQ	155	GLN
11	ZQ	157	ASN
11	ZQ	197	ASN
11	ZQ	233	ASN
11	ZQ	338	GLN
11	ZQ	387	GLN
11	ZR	5	GLN
11	ZR	89	ASN
11	ZR	107	ASN
11	ZR	268	GLN
11	ZR	269	GLN
11	ZR	293	GLN
11	ZR	295	ASN
11	ZR	401	ASN
11	ZS	133	ASN
11	ZS	192	ASN
11	ZS	197	ASN
11	ZS	387	GLN
11	ZS	394	GLN
11	ZT	99	GLN
11	ZT	129	GLN
11	ZT	190	GLN
11	ZT	197	ASN
11	ZT	213	HIS
11	ZT	235	ASN
11	ZT	275	ASN
11	ZT	293	GLN
11	ZT	314	GLN
11	ZT	352	ASN
11	ZT	392	GLN
11	ZU	97	ASN
11	ZU	107	ASN
11	ZU	133	ASN
11	ZU	159	ASN
11	ZU	190	GLN
11	ZU	268	GLN
11	ZU	269	GLN
11	ZU	293	GLN
11	ZU	379	GLN

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Mol	Chain	Res	Type
11	ZV	5	GLN
11	ZV	107	ASN
11	ZV	133	ASN
11	ZV	197	ASN
11	ZV	269	GLN
11	ZV	280	ASN
11	ZV	303	ASN
11	ZV	314	GLN
11	ZV	381	ASN
11	ZV	387	GLN
11	ZV	394	GLN
11	ZV	397	ASN
11	ZV	401	ASN
11	ZW	5	GLN
11	ZW	26	ASN
11	ZW	107	ASN
11	ZW	129	GLN
11	ZW	133	ASN
11	ZW	155	GLN
11	ZW	197	ASN
11	ZW	252	ASN
11	ZW	310	GLN
11	ZW	314	GLN
11	ZW	332	ASN
11	ZX	11	ASN
11	ZX	80	ASN
11	ZX	133	ASN
11	ZX	159	ASN
11	ZX	314	GLN
11	ZX	352	ASN
11	ZX	387	GLN
11	ZY	5	GLN
11	ZY	115	GLN
11	ZY	159	ASN
11	ZY	197	ASN
11	ZY	268	GLN
11	ZY	392	GLN
11	ZZ	5	GLN
11	ZZ	26	ASN
11	ZZ	99	GLN
11	ZZ	107	ASN
11	ZZ	133	ASN

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Mol	Chain	Res	Type
11	ZZ	194	HIS
11	ZZ	197	ASN
11	ZZ	314	GLN
11	ZZ	332	ASN
11	ZZ	401	ASN
11	Za	115	GLN
11	Za	129	GLN
11	Za	133	ASN
11	Za	157	ASN
11	Za	190	GLN
11	Za	197	ASN
11	Za	332	ASN
11	Zb	5	GLN
11	Zb	79	GLN
11	Zb	107	ASN
11	Zb	129	GLN
11	Zb	130	GLN
11	Zb	190	GLN
11	Zb	197	ASN
11	Zb	293	GLN
11	Zb	308	GLN
11	Zb	322	ASN
11	Zb	332	ASN
11	Zb	358	ASN
11	Zb	381	ASN
11	Zb	387	GLN
11	Zc	5	GLN
11	Zc	107	ASN
11	Zc	129	GLN
11	Zc	133	ASN
11	Zc	159	ASN
11	Zc	197	ASN
11	Zc	379	GLN
11	Zc	387	GLN
11	Zc	397	ASN
11	Zd	5	GLN
11	Zd	105	ASN
11	Zd	129	GLN
11	Zd	130	GLN
11	Zd	293	GLN
11	Zd	295	ASN
11	Zd	322	ASN

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Mol	Chain	Res	Type
11	Zd	397	ASN
11	Ze	99	GLN
11	Ze	107	ASN
11	Ze	133	ASN
11	Ze	197	ASN
11	Ze	394	GLN
11	Zf	105	ASN
11	Zf	133	ASN
11	Zf	197	ASN
11	Zf	252	ASN
11	Zf	314	GLN
11	Zf	397	ASN
11	Zg	5	GLN
11	Zg	107	ASN
11	Zg	129	GLN
11	Zg	133	ASN
11	Zg	197	ASN
11	Zg	310	GLN
11	Zh	5	GLN
11	Zh	115	GLN
11	Zh	129	GLN
11	Zh	197	ASN
11	Zh	379	GLN
11	Zh	392	GLN
12	a	63	ASN
12	a	80	GLN
12	a	140	ASN
12	a	159	GLN
12	a	178	GLN
12	a	188	GLN
12	a	350	GLN
12	b	54	GLN
12	b	63	ASN
12	b	140	ASN
12	b	159	GLN
12	b	178	GLN
12	b	188	GLN
12	b	350	GLN
12	c	54	GLN
12	c	63	ASN
12	c	80	GLN
12	c	140	ASN

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Mol	Chain	Res	Type
12	c	159	GLN
12	c	178	GLN
12	c	188	GLN
12	c	350	GLN
12	d	63	ASN
12	d	80	GLN
12	d	140	ASN
12	d	159	GLN
12	d	178	GLN
12	d	188	GLN
12	d	350	GLN
12	e	63	ASN
12	e	80	GLN
12	e	140	ASN
12	e	159	GLN
12	e	178	GLN
12	e	188	GLN
12	e	350	GLN
12	f	63	ASN
12	f	80	GLN
12	f	140	ASN
12	f	159	GLN
12	f	178	GLN
12	f	188	GLN
12	f	350	GLN
12	g	54	GLN
12	g	63	ASN
12	g	80	GLN
12	g	140	ASN
12	g	159	GLN
12	g	178	GLN
12	g	188	GLN
12	g	350	GLN
12	h	54	GLN
12	h	63	ASN
12	h	80	GLN
12	h	140	ASN
12	h	159	GLN
12	h	178	GLN
12	h	188	GLN
12	h	350	GLN
12	i	54	GLN

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Mol	Chain	Res	Type
12	i	63	ASN
12	i	80	GLN
12	i	140	ASN
12	i	159	GLN
12	i	178	GLN
12	i	188	GLN
12	i	350	GLN
12	j	63	ASN
12	j	80	GLN
12	j	140	ASN
12	j	159	GLN
12	j	178	GLN
12	j	188	GLN
12	j	350	GLN
12	k	54	GLN
12	k	63	ASN
12	k	140	ASN
12	k	159	GLN
12	k	178	GLN
12	k	188	GLN
12	k	350	GLN
12	l	63	ASN
12	l	140	ASN
12	l	159	GLN
12	l	178	GLN
12	l	188	GLN
12	l	350	GLN
12	m	63	ASN
12	m	140	ASN
12	m	159	GLN
12	m	178	GLN
12	m	188	GLN
12	m	350	GLN
12	n	54	GLN
12	n	63	ASN
12	n	140	ASN
12	n	159	GLN
12	n	178	GLN
12	n	188	GLN
12	n	350	GLN
12	o	54	GLN
12	o	63	ASN

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Mol	Chain	Res	Type
12	o	80	GLN
12	o	140	ASN
12	o	159	GLN
12	o	178	GLN
12	o	188	GLN
12	o	350	GLN
12	p	54	GLN
12	p	63	ASN
12	p	140	ASN
12	p	159	GLN
12	p	178	GLN
12	p	188	GLN
12	p	350	GLN
12	q	63	ASN
12	q	140	ASN
12	q	159	GLN
12	q	178	GLN
12	q	188	GLN
12	q	350	GLN
12	r	63	ASN
12	r	140	ASN
12	r	159	GLN
12	r	178	GLN
12	r	188	GLN
12	r	350	GLN
12	s	63	ASN
12	s	80	GLN
12	s	140	ASN
12	s	159	GLN
12	s	178	GLN
12	s	188	GLN
12	s	350	GLN
12	t	54	GLN
12	t	63	ASN
12	t	80	GLN
12	t	140	ASN
12	t	159	GLN
12	t	178	GLN
12	t	188	GLN
12	t	350	GLN
12	u	54	GLN
12	u	63	ASN

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Mol	Chain	Res	Type
12	u	140	ASN
12	u	159	GLN
12	u	178	GLN
12	u	188	GLN
12	u	350	GLN
12	v	63	ASN
12	v	140	ASN
12	v	159	GLN
12	v	178	GLN
12	v	188	GLN
12	v	350	GLN
12	w	63	ASN
12	w	80	GLN
12	w	140	ASN
12	w	159	GLN
12	w	178	GLN
12	w	188	GLN
12	w	350	GLN
12	x	51	GLN
12	x	63	ASN
12	x	80	GLN
12	x	140	ASN
12	x	159	GLN
12	x	178	GLN
12	x	188	GLN
12	x	350	GLN
12	y	54	GLN
12	y	63	ASN
12	y	80	GLN
12	y	140	ASN
12	y	159	GLN
12	y	178	GLN
12	y	188	GLN
12	y	350	GLN
12	z	54	GLN
12	z	63	ASN
12	z	80	GLN
12	z	140	ASN
12	z	159	GLN
12	z	178	GLN
12	z	188	GLN
12	z	350	GLN

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Mol	Chain	Res	Type
13	C4	102	ASN
13	C5	83	GLN
14	C6	35	GLN
14	C6	46	GLN
14	C6	49	ASN
14	C6	180	ASN
14	C6	186	GLN
15	C8	148	HIS
15	C8	245	ASN
13	C0	102	ASN
13	DA	83	GLN
14	DB	35	GLN
14	DB	46	GLN
14	DB	49	ASN
14	DB	180	ASN
14	DB	186	GLN
14	DD	35	GLN
14	DD	46	GLN
14	DD	49	ASN
14	DD	180	ASN
14	DD	186	GLN
15	DF	148	HIS
15	DF	245	ASN
13	DH	102	ASN
13	DI	83	GLN
14	DJ	35	GLN
14	DJ	46	GLN
14	DJ	49	ASN
14	DJ	180	ASN
14	DJ	186	GLN
15	DL	148	HIS
15	DL	245	ASN
15	DM	148	HIS
15	DM	245	ASN
13	DO	102	ASN
13	DP	83	GLN
14	DQ	35	GLN
14	DQ	46	GLN
14	DQ	49	ASN
14	DQ	180	ASN
14	DQ	186	GLN
15	DS	87	GLN

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Mol	Chain	Res	Type
15	DS	148	HIS
15	DS	245	ASN
13	DU	102	ASN
13	DV	83	GLN
14	DW	35	GLN
14	DW	46	GLN
14	DW	49	ASN
14	DW	180	ASN
14	DW	186	GLN
15	DY	87	GLN
15	DY	148	HIS
15	DY	245	ASN
13	Da	102	ASN
13	Db	83	GLN
14	Dc	35	GLN
14	Dc	46	GLN
14	Dc	49	ASN
14	Dc	180	ASN
14	Dc	186	GLN
15	De	87	GLN
15	De	148	HIS
15	De	245	ASN
13	Dg	102	ASN
13	Dh	83	GLN
14	Di	35	GLN
14	Di	46	GLN
14	Di	49	ASN
14	Di	180	ASN
14	Di	186	GLN
15	Dk	87	GLN
15	Dk	148	HIS
15	Dk	190	ASN
15	Dk	245	ASN
13	Dm	102	ASN
13	Dn	83	GLN
14	Do	35	GLN
14	Do	46	GLN
14	Do	49	ASN
14	Do	180	ASN
14	Do	186	GLN
15	Dq	87	GLN
15	Dq	148	HIS

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Mol	Chain	Res	Type
15	Dq	245	ASN
13	Ds	102	ASN
13	Dt	83	GLN
14	Du	35	GLN
14	Du	46	GLN
14	Du	49	ASN
14	Du	180	ASN
14	Du	186	GLN
15	Dw	87	GLN
15	Dw	148	HIS
15	Dw	245	ASN
13	Dy	102	ASN
13	Dz	83	GLN
14	D1	35	GLN
14	D1	46	GLN
14	D1	49	ASN
14	D1	180	ASN
14	D1	186	GLN
15	D3	148	HIS
15	D3	245	ASN
13	D5	102	ASN
13	D6	83	GLN
14	D7	35	GLN
14	D7	46	GLN
14	D7	49	ASN
14	D7	180	ASN
14	D7	186	GLN
15	D9	87	GLN
15	D9	148	HIS
15	D9	190	ASN
15	D9	245	ASN
13	EA	102	ASN
13	EB	83	GLN
13	B0	83	GLN
15	B1	148	HIS
15	B1	190	ASN
15	B1	245	ASN
13	B3	102	ASN
13	B4	83	GLN
14	B5	35	GLN
14	B5	46	GLN
14	B5	49	ASN

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Mol	Chain	Res	Type
14	B5	180	ASN
14	B5	186	GLN
15	B7	148	HIS
15	B7	245	ASN
13	B9	102	ASN
13	EC	102	ASN
13	ED	83	GLN
14	EE	35	GLN
14	EE	46	GLN
14	EE	49	ASN
14	EE	180	ASN
14	EE	186	GLN
15	EG	148	HIS
15	EG	190	ASN
15	EG	245	ASN
13	EI	102	ASN
13	EJ	83	GLN
14	EK	35	GLN
14	EK	46	GLN
14	EK	49	ASN
14	EK	180	ASN
14	EK	186	GLN
15	EM	148	HIS
15	EM	245	ASN
13	EO	102	ASN
13	EP	83	GLN
14	EQ	35	GLN
14	EQ	46	GLN
14	EQ	49	ASN
14	EQ	180	ASN
14	EQ	186	GLN
15	ES	148	HIS
15	ES	245	ASN
13	EU	102	ASN
13	EV	83	GLN
14	EW	35	GLN
14	EW	46	GLN
14	EW	49	ASN
14	EW	180	ASN
14	EW	186	GLN
15	EY	148	HIS
15	EY	245	ASN

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Mol	Chain	Res	Type
13	BY	102	ASN
13	BZ	83	GLN
14	Ba	35	GLN
14	Ba	46	GLN
14	Ba	49	ASN
14	Ba	180	ASN
14	Ba	186	GLN
15	Bc	148	HIS
15	Bc	245	ASN
13	Be	102	ASN
13	Bf	83	GLN
14	Bg	35	GLN
14	Bg	46	GLN
14	Bg	49	ASN
14	Bg	180	ASN
14	Bg	186	GLN
15	Bi	148	HIS
15	Bi	245	ASN
13	Bk	102	ASN
13	Bl	83	GLN
14	Bm	35	GLN
14	Bm	46	GLN
14	Bm	49	ASN
14	Bm	180	ASN
14	Bm	186	GLN
15	Bo	148	HIS
15	Bo	245	ASN
13	Bq	102	ASN
13	Br	83	GLN
14	Bs	35	GLN
14	Bs	46	GLN
14	Bs	49	ASN
14	Bs	180	ASN
14	Bs	186	GLN
15	Bu	148	HIS
15	Bu	245	ASN
13	Bw	102	ASN
13	Bx	83	GLN
14	By	35	GLN
14	By	46	GLN
14	By	49	ASN
14	By	180	ASN

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Mol	Chain	Res	Type
14	By	186	GLN
13	C1	102	ASN
13	C2	83	GLN
14	CA	35	GLN
14	CA	46	GLN
14	CA	49	ASN
14	CA	180	ASN
14	CA	186	GLN
15	CC	148	HIS
15	CC	245	ASN
13	CE	102	ASN
13	CF	83	GLN
14	CG	35	GLN
14	CG	46	GLN
14	CG	49	ASN
14	CG	180	ASN
14	CG	186	GLN
15	CI	148	HIS
15	CI	245	ASN
13	CK	102	ASN
13	CL	83	GLN
14	CM	35	GLN
14	CM	46	GLN
14	CM	49	ASN
14	CM	180	ASN
14	CM	186	GLN
15	CO	148	HIS
15	CO	245	ASN
13	CQ	102	ASN
13	CR	83	GLN
14	CS	35	GLN
14	CS	46	GLN
14	CS	49	ASN
14	CS	180	ASN
14	CS	186	GLN
15	CU	148	HIS
15	CU	245	ASN
13	CW	102	ASN
13	CX	83	GLN
14	CY	35	GLN
14	CY	46	GLN
14	CY	49	ASN

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Mol	Chain	Res	Type
14	CY	180	ASN
14	CY	186	GLN
15	Ca	87	GLN
15	Ca	148	HIS
15	Ca	245	ASN
13	Cc	102	ASN
13	Cd	83	GLN
14	Ce	35	GLN
14	Ce	46	GLN
14	Ce	49	ASN
14	Ce	180	ASN
14	Ce	186	GLN
15	Cg	148	HIS
15	Cg	245	ASN
13	Ci	102	ASN
13	Cj	83	GLN
14	Ck	35	GLN
14	Ck	46	GLN
14	Ck	49	ASN
14	Ck	180	ASN
14	Ck	186	GLN
15	Cm	148	HIS
15	Cm	245	ASN
13	Co	102	ASN
13	Cp	83	GLN
14	Cq	35	GLN
14	Cq	46	GLN
14	Cq	49	ASN
14	Cq	180	ASN
14	Cq	186	GLN
15	Cs	148	HIS
15	Cs	245	ASN
13	Cu	102	ASN
13	Cv	83	GLN
14	Cw	35	GLN
14	Cw	46	GLN
14	Cw	49	ASN
14	Cw	180	ASN
14	Cw	186	GLN
15	Cy	148	HIS
15	Cy	245	ASN
14	Ea	35	GLN

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Mol	Chain	Res	Type
14	Ea	46	GLN
14	Ea	49	ASN
14	Ea	180	ASN
14	Ea	186	GLN
15	Ec	148	HIS
15	Ec	245	ASN
13	Ee	102	ASN
13	Ef	83	GLN
14	Eg	35	GLN
14	Eg	46	GLN
14	Eg	49	ASN
14	Eg	180	ASN
14	Eg	186	GLN
15	Ei	148	HIS
15	Ei	245	ASN
13	Ek	102	ASN
13	El	83	GLN
14	Em	35	GLN
14	Em	46	GLN
14	Em	49	ASN
14	Em	180	ASN
14	Em	186	GLN
15	Eo	148	HIS
15	Eo	245	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

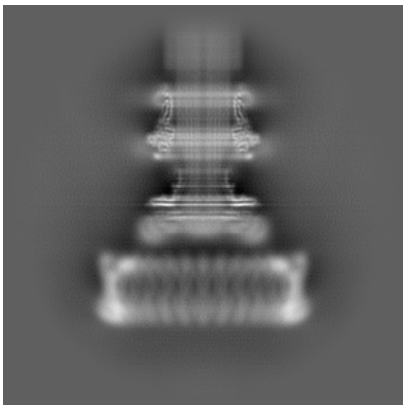
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37679. These allow visual inspection of the internal detail of the map and identification of artifacts.

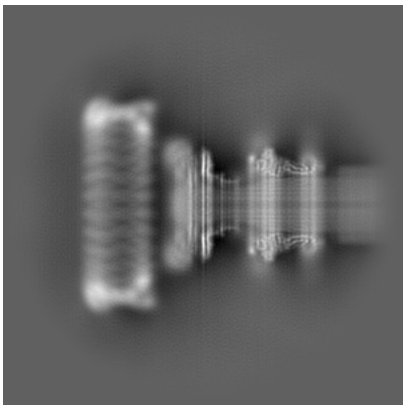
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

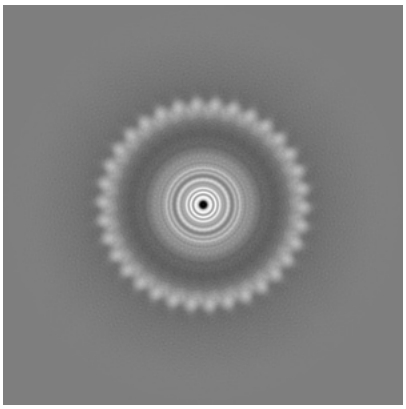
6.1.1 Primary map



X

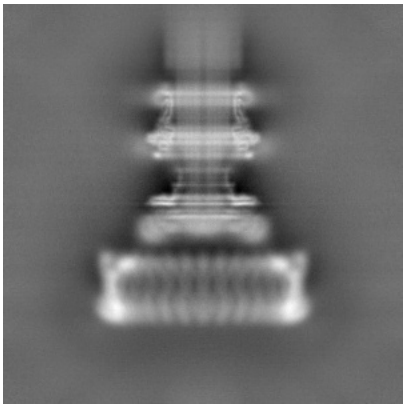


Y

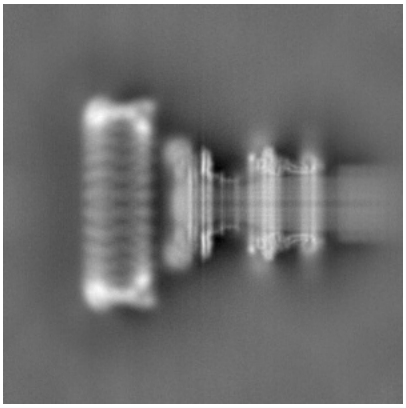


Z

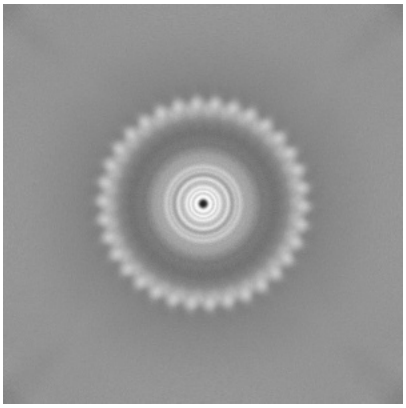
6.1.2 Raw map



X



Y

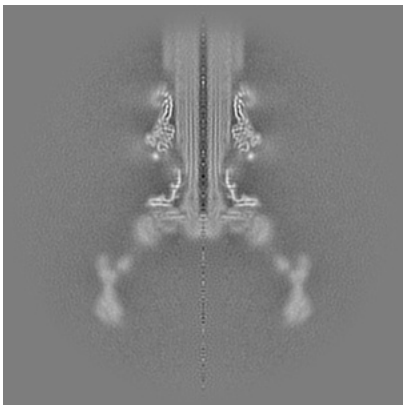


Z

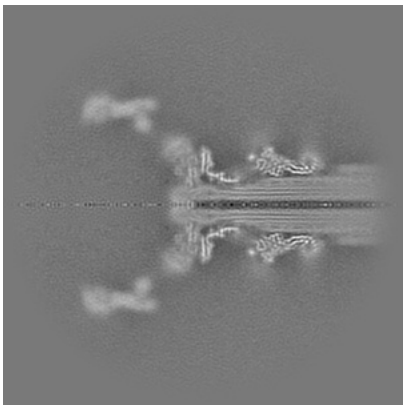
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

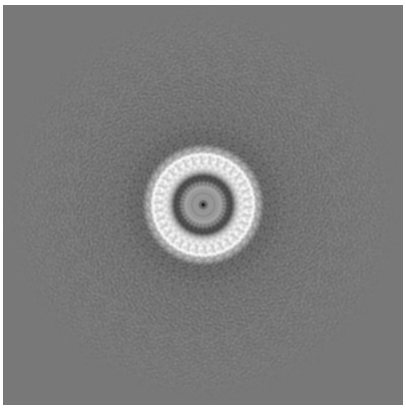
6.2.1 Primary map



X Index: 400

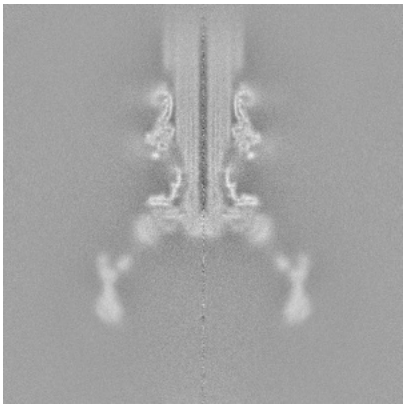


Y Index: 400

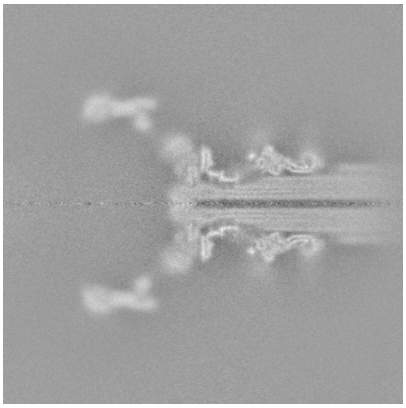


Z Index: 400

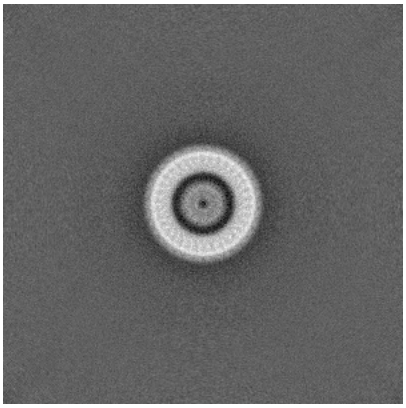
6.2.2 Raw map



X Index: 400



Y Index: 400

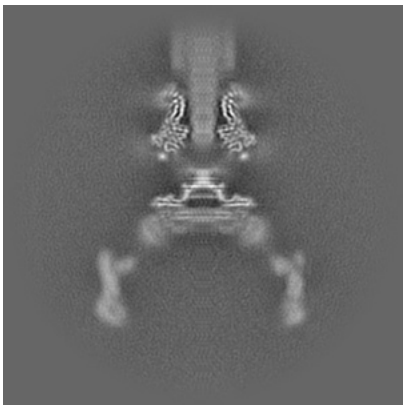


Z Index: 400

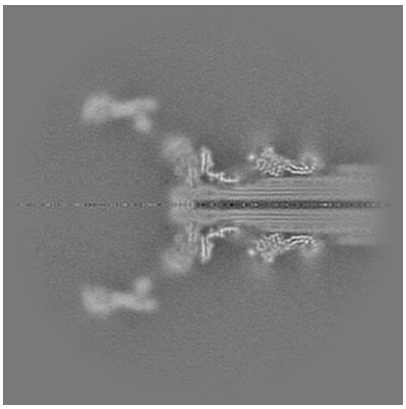
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

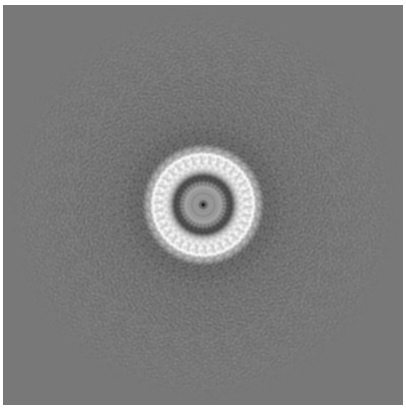
6.3.1 Primary map



X Index: 449

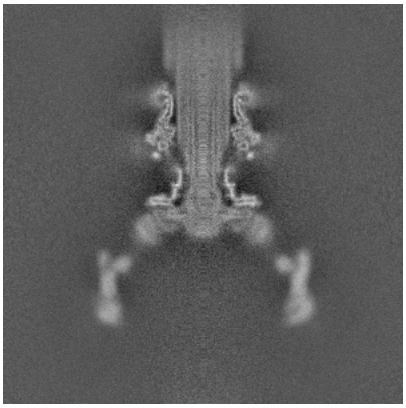


Y Index: 400

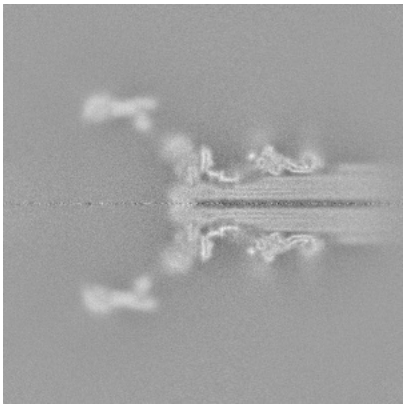


Z Index: 400

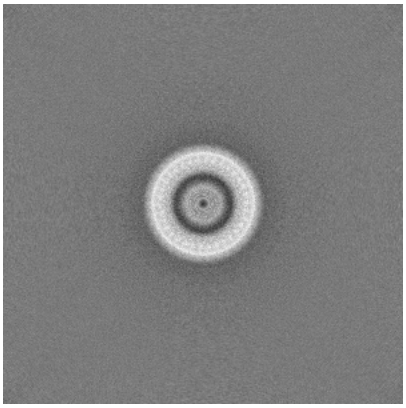
6.3.2 Raw map



X Index: 386



Y Index: 400

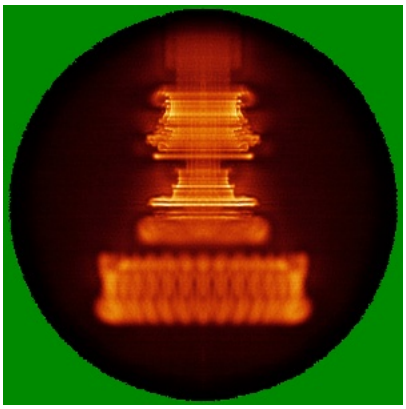


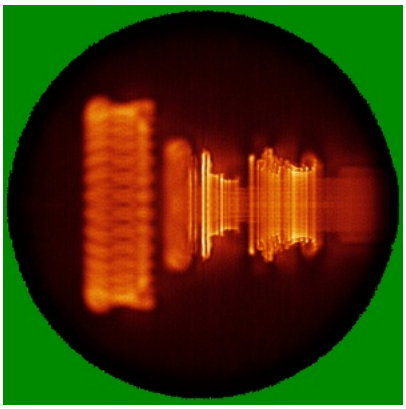
Z Index: 401

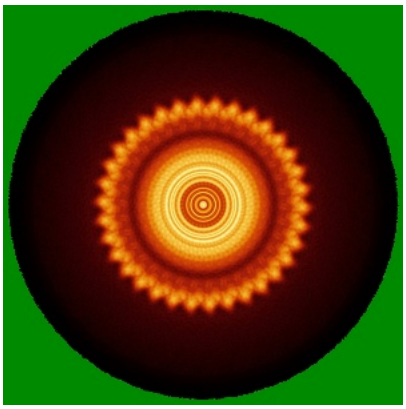
The images above show the largest variance slices of the map in three orthogonal directions.

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

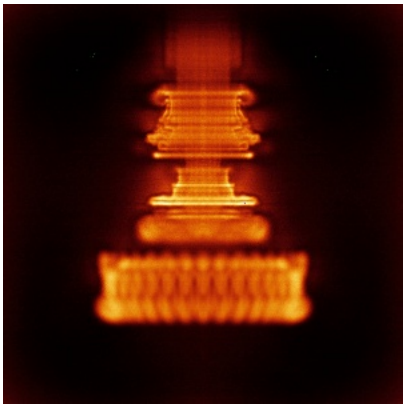
6.4.1 Primary map

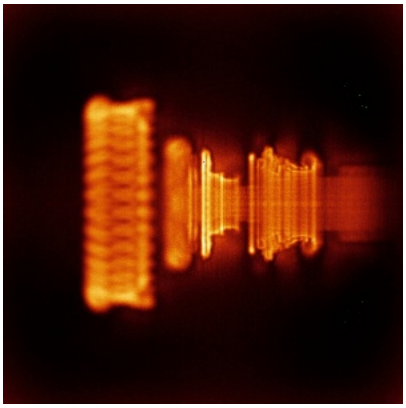

X

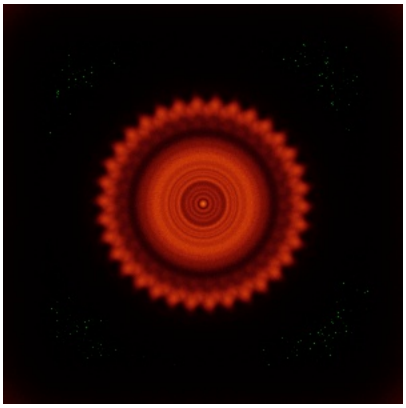

Y


Z

6.4.2 Raw map


X


Y

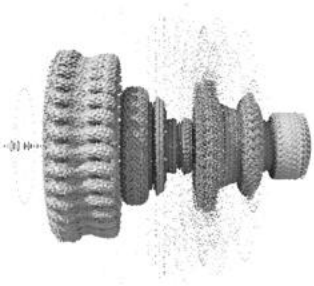

Z

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

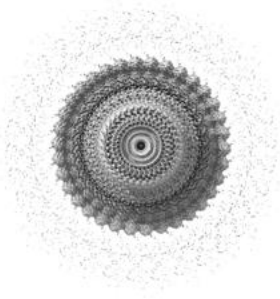
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X



Y



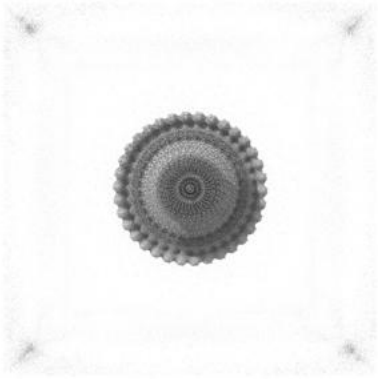
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X

Y



Z

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

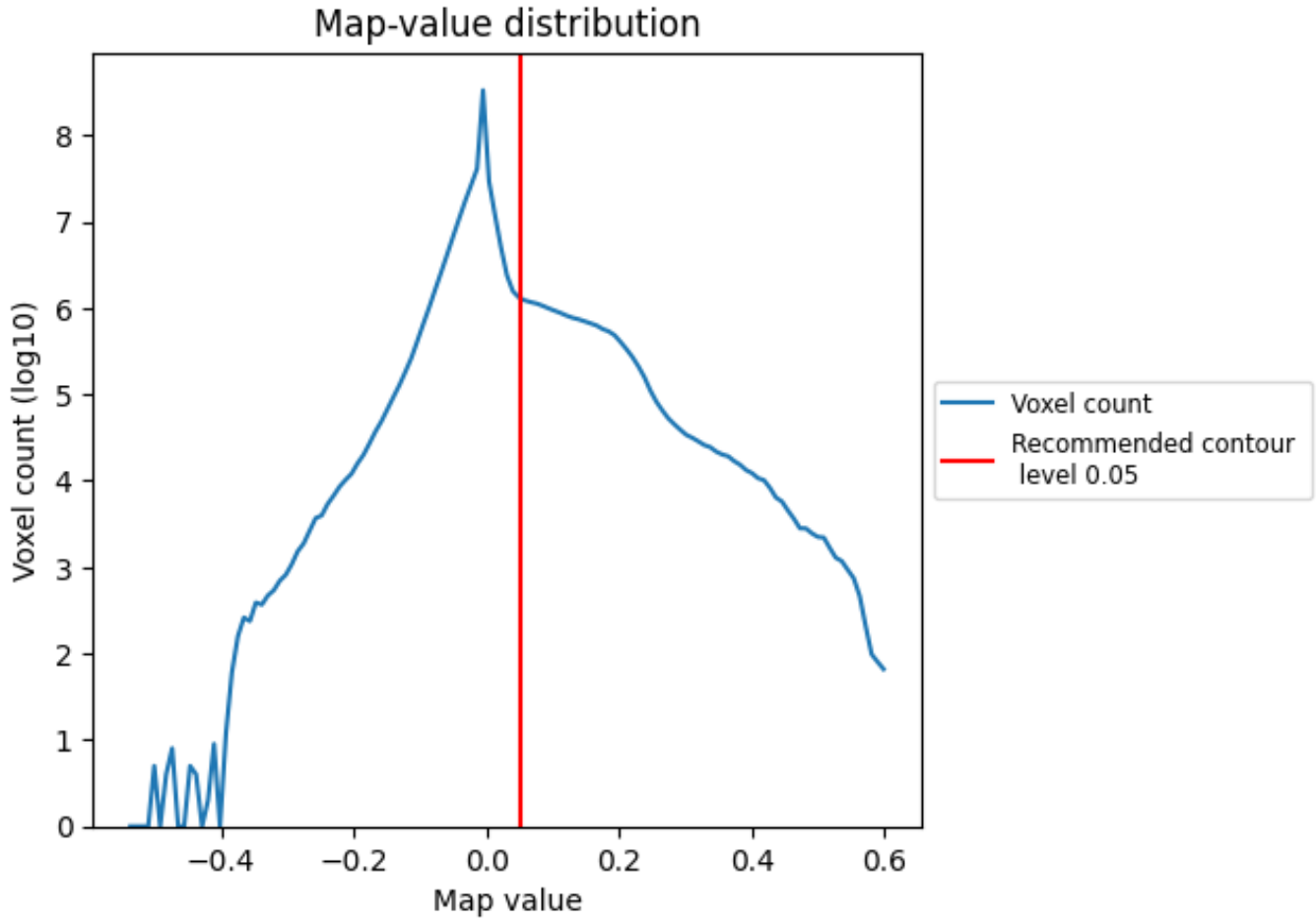
6.6 Mask visualisation (i)

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

7 Map analysis

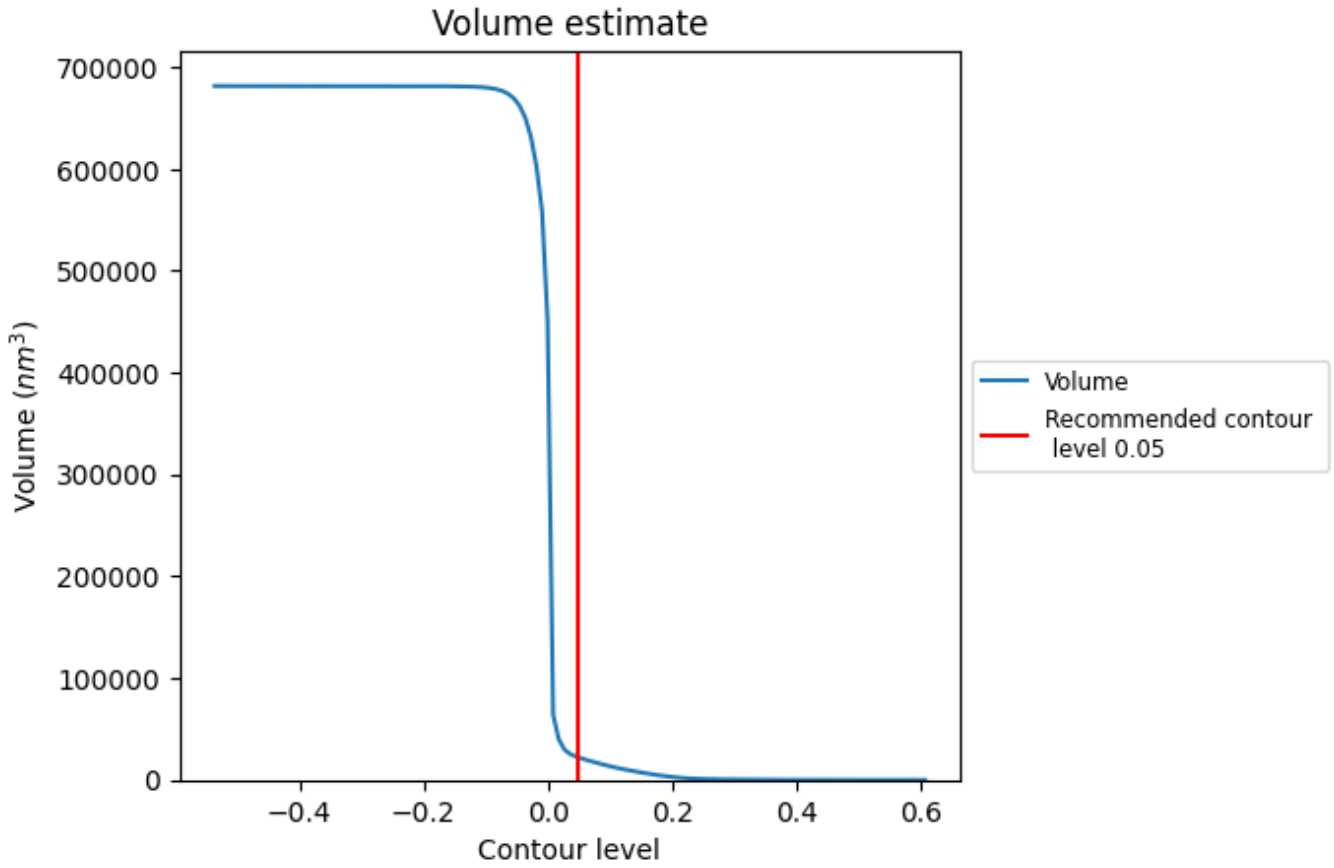
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

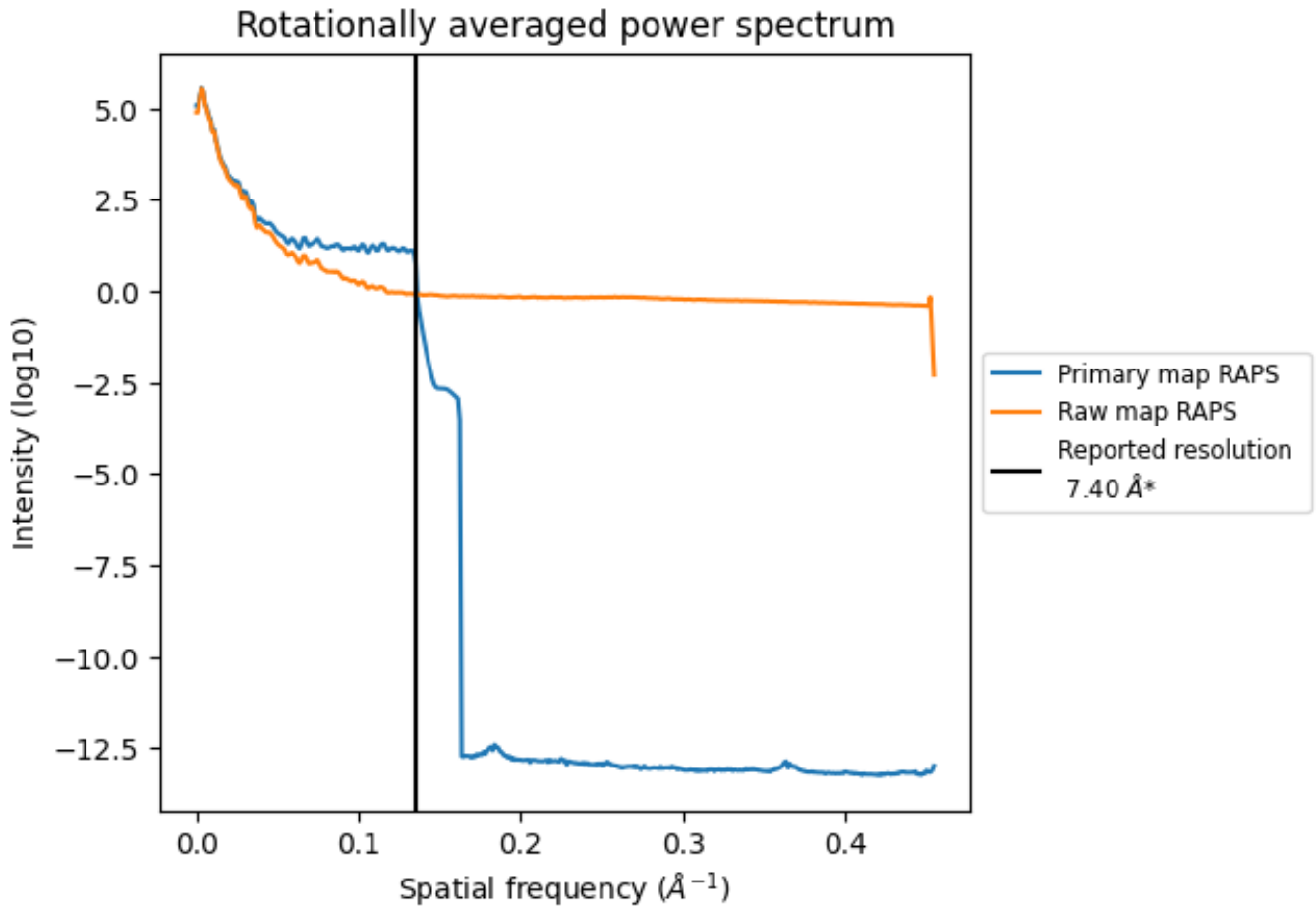
7.2 Volume estimate



The volume at the recommended contour level is 22073 nm^3; this corresponds to an approximate mass of 19939 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

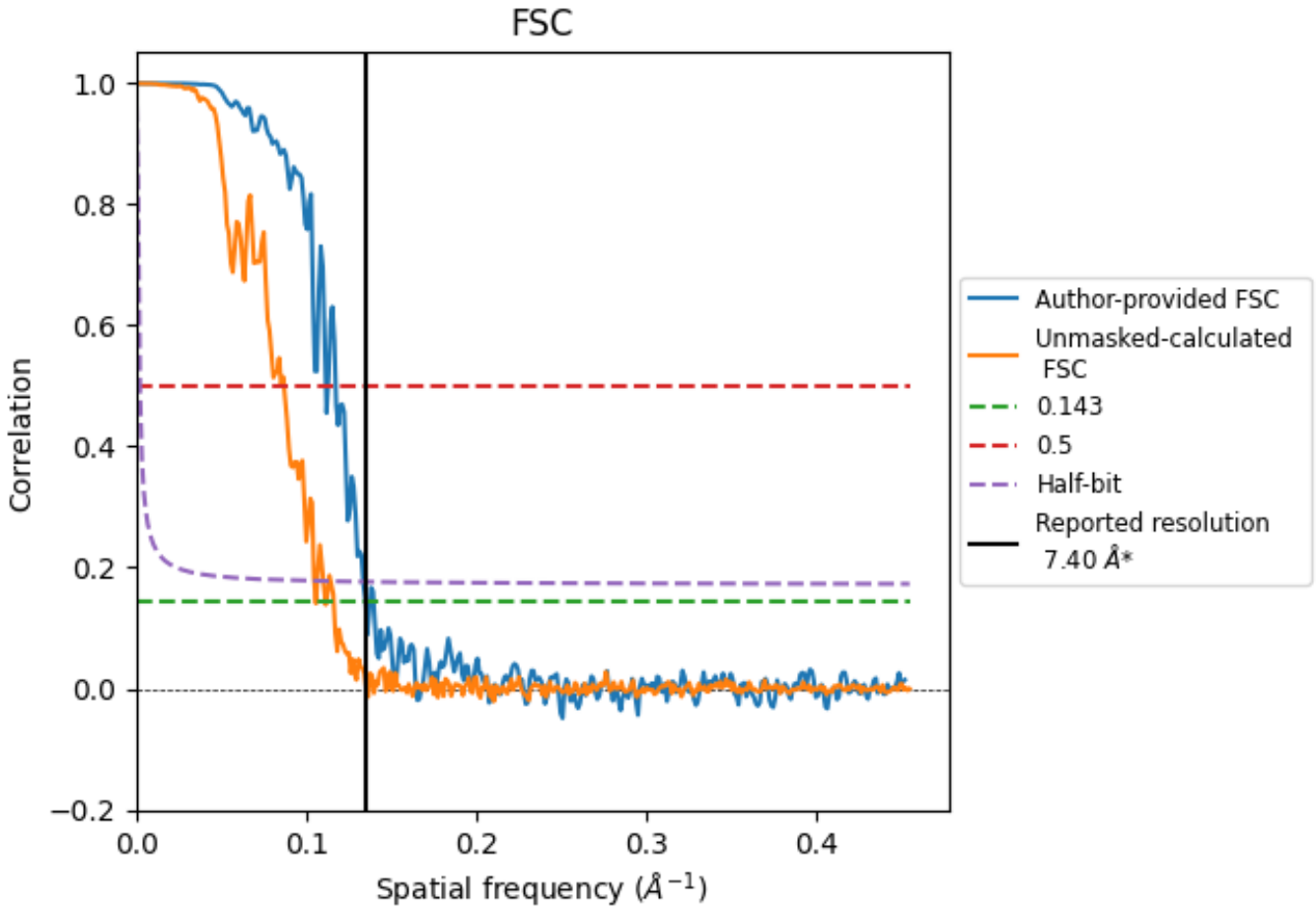


*Reported resolution corresponds to spatial frequency of 0.135 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.135 Å^{-1}

8.2 Resolution estimates (i)

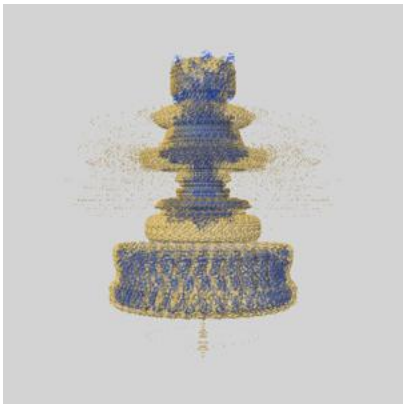
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.40	-	-
Author-provided FSC curve	7.42	8.97	7.50
Unmasked-calculated*	9.47	11.52	9.55

*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 9.47 differs from the reported value 7.4 by more than 10 %

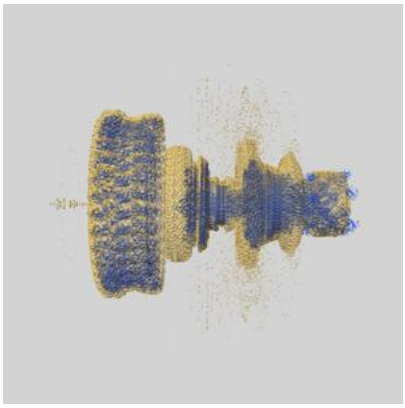
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37679 and PDB model 8WO5. Per-residue inclusion information can be found in section 3 on page 42.

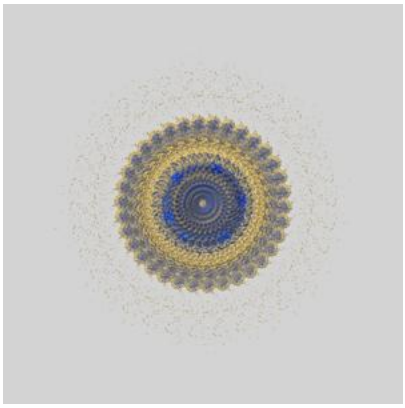
9.1 Map-model overlay



X



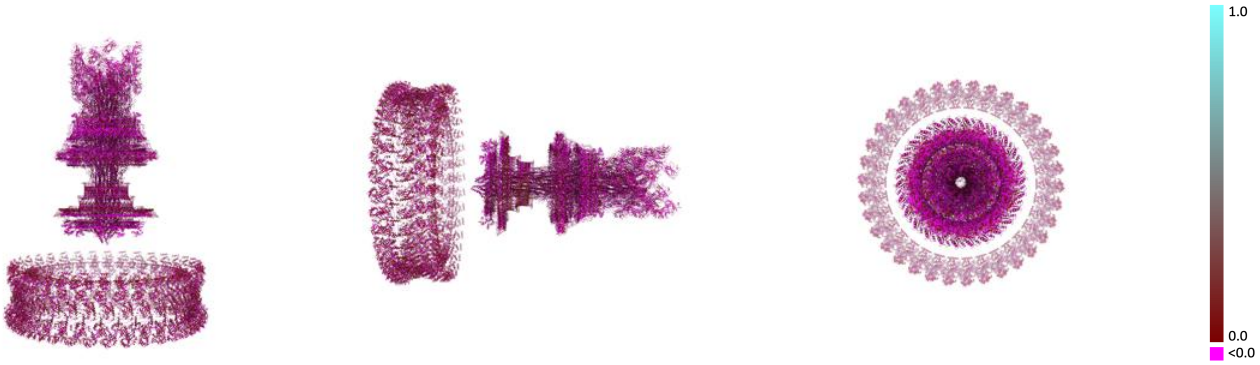
Y



Z

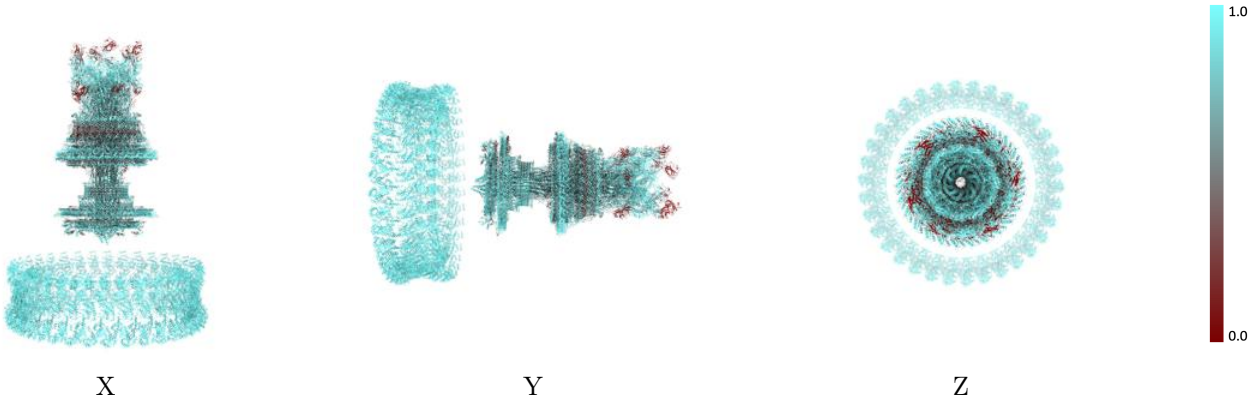
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



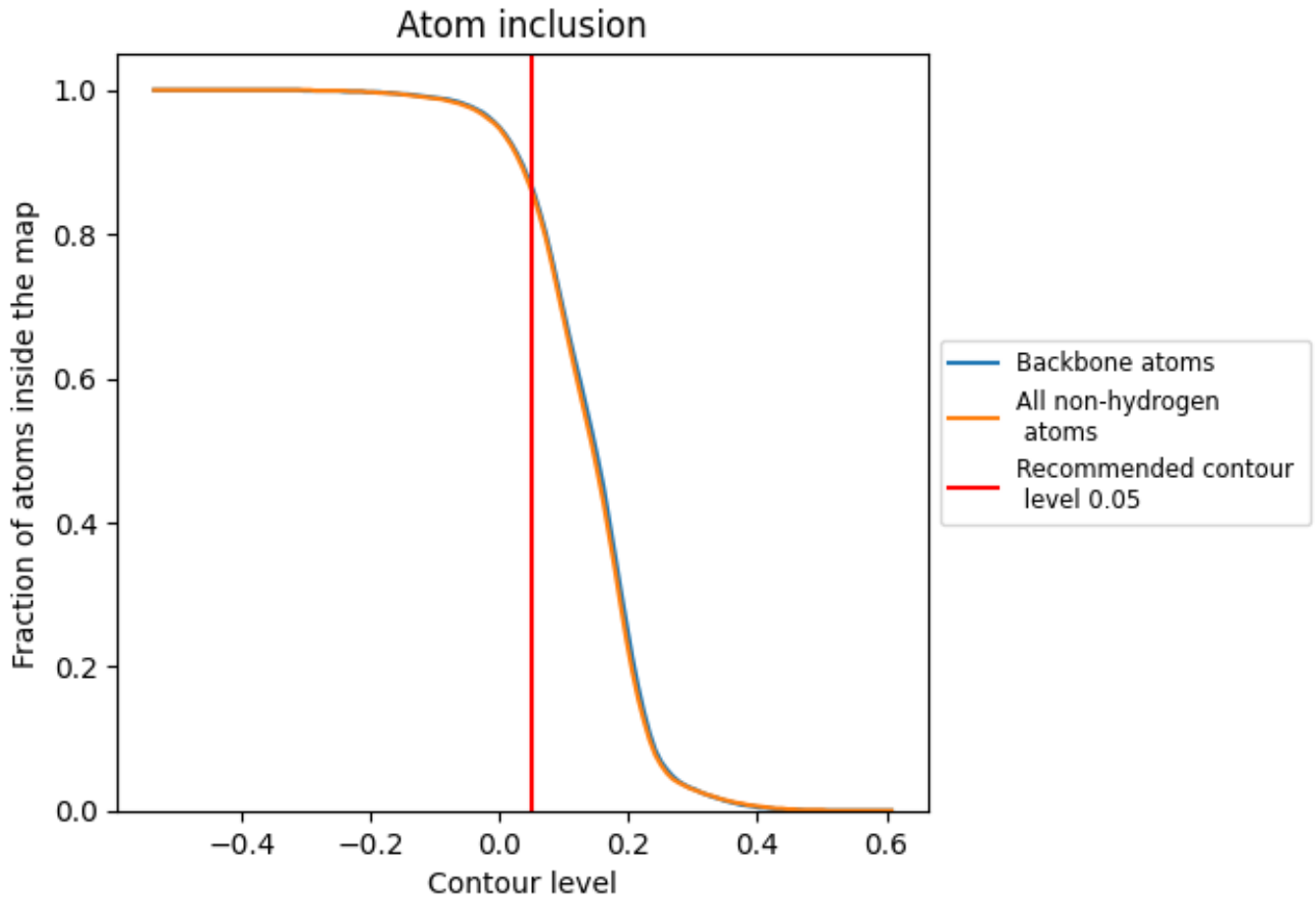
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.0430
0	0.7170	0.0180
1	0.7610	0.0370
2	0.7570	0.0390
3	0.7340	0.0320
4	0.6870	0.0250
5	0.6840	0.0200
6	0.6950	0.0420
7	0.6990	0.0360
8	0.6780	0.0300
9	0.6590	0.0250
A	0.6940	-0.0090
A0	0.7210	0.0380
A1	0.7980	0.0570
A2	0.7710	0.0690
A3	0.6850	0.0450
A4	0.7360	0.0850
A5	0.8160	0.1000
A6	0.6100	0.0700
A7	0.6630	0.0510
A8	0.6310	-0.0010
A9	0.6230	-0.0040
AA	0.6360	0.0280
AB	0.6800	0.0340
AC	0.6880	0.0180
AD	0.6980	0.0070
AE	0.7110	0.0250
AF	0.7700	0.0470
AG	0.7710	0.0510
AH	0.7380	0.0360
AI	0.7140	0.0160
AJ	0.7220	0.0220
AK	0.7460	0.0310
AL	0.7460	0.0370
AM	0.7320	0.0380

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Chain	Atom inclusion	Q-score
AN	0.6910	0.0160
AO	0.9130	0.1010
AP	0.9000	0.0900
AQ	0.8750	0.0730
AR	0.8820	0.0730
AS	0.7540	0.0040
AT	0.7510	0.0050
AU	0.7550	0.0070
AV	0.7670	0.0130
AW	0.7880	0.0190
AX	0.8100	0.0250
AY	0.8210	0.0330
AZ	0.8450	0.0450
Aa	0.8640	0.0590
Ab	0.9820	0.0000
Ac	0.9070	0.0860
Ad	0.9250	0.0970
Ae	0.9230	0.1020
Af	0.9260	0.1070
Ag	0.9250	0.1040
Ah	0.9240	0.0980
Ai	0.9210	0.0940
Aj	0.9210	0.0940
Ak	0.9220	0.0950
Al	0.9280	0.0990
Am	0.9260	0.1010
An	0.9290	0.1040
Ao	0.9300	0.1060
Ap	0.9300	0.1050
Aq	0.9970	0.0450
Ar	0.9900	0.0010
As	0.9770	0.0290
At	0.9080	0.0220
Au	0.8760	0.0190
Av	0.9260	0.0300
Aw	0.9460	0.0380
Ax	0.8700	0.0260
Ay	0.7880	0.0060
Az	0.8400	0.0610
B	0.6860	-0.0020
B0	0.9970	0.0690
B1	0.9970	0.0760

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Chain	Atom inclusion	Q-score
B2	1.0000	0.0730
B3	0.9950	0.0790
B4	0.9950	0.0660
B5	0.9940	0.0800
B6	0.9770	0.0860
B7	0.9970	0.0750
B8	1.0000	0.0730
B9	0.9950	0.0790
BA	0.7660	0.0390
BB	0.7840	0.0580
BC	0.8180	0.0580
BD	0.7760	0.0470
BE	0.8030	0.0510
BF	0.8230	0.0510
BG	0.7780	0.0630
BH	0.6600	0.0360
BI	0.2780	-0.0440
BJ	0.6800	-0.0350
BK	0.4710	-0.0230
BL	0.7380	-0.0610
BM	0.6000	-0.0520
BN	0.7670	-0.0470
BO	0.7820	-0.0020
BP	0.7670	-0.0250
BQ	0.6430	-0.0010
BR	0.8570	0.0530
BS	0.8300	0.0390
BT	0.8150	0.0280
BU	0.8000	0.0190
BV	0.7860	0.0110
BW	0.7760	0.0090
BX	0.7630	0.0070
BY	0.9950	0.0800
BZ	0.9940	0.0660
Ba	0.9940	0.0800
Bb	0.9770	0.0880
Bc	0.9970	0.0740
Bd	0.9970	0.0740
Be	0.9950	0.0800
Bf	0.9940	0.0650
Bg	0.9930	0.0780
Bh	0.9770	0.0870

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Chain	Atom inclusion	Q-score
Bi	0.9970	0.0750
Bj	0.9950	0.0730
Bk	0.9950	0.0800
Bl	0.9920	0.0630
Bm	0.9930	0.0780
Bn	0.9770	0.0880
Bo	0.9970	0.0760
Bp	0.9970	0.0730
Bq	0.9970	0.0820
Br	0.9970	0.0640
Bs	0.9930	0.0790
Bt	0.9770	0.0860
Bu	0.9970	0.0760
Bv	0.9970	0.0740
Bw	0.9950	0.0770
Bx	0.9940	0.0650
By	0.9930	0.0800
Bz	0.9770	0.0860
C	0.7190	0.0070
C0	0.9950	0.0740
C1	0.9950	0.0720
C2	0.9970	0.0580
C3	0.9770	0.0890
C4	0.9950	0.0750
C5	0.9940	0.0580
C6	0.9930	0.0790
C7	0.9770	0.0870
C8	0.9970	0.0740
C9	0.9950	0.0720
CA	0.9940	0.0810
CB	0.9770	0.0880
CC	0.9970	0.0730
CD	0.9970	0.0700
CE	0.9950	0.0790
CF	0.9950	0.0660
CG	0.9930	0.0800
CH	0.9770	0.0890
CI	0.9970	0.0740
CJ	0.9970	0.0700
CK	0.9950	0.0780
CL	0.9920	0.0660
CM	0.9930	0.0800

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Chain	Atom inclusion	Q-score
CN	0.9770	0.0900
CO	0.9970	0.0740
CP	0.9970	0.0720
CQ	0.9950	0.0770
CR	0.9940	0.0630
CS	0.9930	0.0800
CT	0.9770	0.0870
CU	0.9970	0.0740
CV	0.9970	0.0710
CW	0.9950	0.0750
CX	0.9920	0.0640
CY	0.9930	0.0800
CZ	0.9770	0.0910
Ca	0.9970	0.0740
Cb	0.9990	0.0740
Cc	0.9950	0.0750
Cd	0.9940	0.0650
Ce	0.9930	0.0800
Cf	0.9770	0.0860
Cg	0.9980	0.0740
Ch	0.9970	0.0710
Ci	0.9950	0.0750
Cj	0.9970	0.0630
Ck	0.9930	0.0810
Cl	0.9770	0.0880
Cm	0.9980	0.0750
Cn	0.9990	0.0720
Co	0.9950	0.0740
Cp	0.9950	0.0610
Cq	0.9930	0.0810
Cr	0.9770	0.0880
Cs	0.9980	0.0740
Ct	1.0000	0.0710
Cu	0.9950	0.0750
Cv	0.9970	0.0600
Cw	0.9930	0.0790
Cx	0.9770	0.0870
Cy	0.9970	0.0730
Cz	0.9970	0.0710
D	0.7040	0.0010
D0	0.9990	0.0740
D1	0.9930	0.0810

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Chain	Atom inclusion	Q-score
D2	0.9770	0.0840
D3	0.9970	0.0740
D4	0.9970	0.0720
D5	0.9950	0.0750
D6	0.9920	0.0580
D7	0.9930	0.0800
D8	0.9770	0.0910
D9	0.9970	0.0750
DA	0.9920	0.0560
DB	0.9930	0.0800
DC	0.9990	0.0740
DD	0.9930	0.0790
DE	0.9770	0.0850
DF	0.9980	0.0740
DG	0.9970	0.0730
DH	0.9950	0.0760
DI	0.9970	0.0610
DJ	0.9930	0.0790
DK	0.9770	0.0810
DL	0.9980	0.0740
DM	0.9970	0.0750
DN	0.9970	0.0730
DO	0.9970	0.0750
DP	0.9970	0.0560
DQ	0.9930	0.0800
DR	0.9770	0.0850
DS	0.9970	0.0750
DT	0.9970	0.0740
DU	0.9950	0.0730
DV	0.9940	0.0570
DW	0.9930	0.0800
DX	0.9770	0.0870
DY	0.9970	0.0740
DZ	1.0000	0.0710
Da	0.9950	0.0740
Db	0.9950	0.0570
Dc	0.9940	0.0790
Dd	0.9770	0.0830
De	0.9970	0.0740
Df	1.0000	0.0730
Dg	0.9950	0.0760
Dh	0.9970	0.0580

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Chain	Atom inclusion	Q-score
Di	0.9940	0.0800
Dj	0.9770	0.0850
Dk	0.9970	0.0740
Dl	0.9970	0.0730
Dm	0.9950	0.0760
Dn	0.9950	0.0550
Do	0.9930	0.0790
Dp	0.9770	0.0860
Dq	0.9970	0.0730
Dr	0.9990	0.0750
Ds	0.9950	0.0750
Dt	0.9920	0.0570
Du	0.9930	0.0790
Dv	0.9770	0.0830
Dw	0.9970	0.0740
Dx	0.9970	0.0750
Dy	0.9950	0.0770
Dz	0.9940	0.0570
E	0.6970	-0.0030
EA	0.9950	0.0750
EB	0.9940	0.0590
EC	0.9950	0.0780
ED	0.9950	0.0610
EE	0.9930	0.0790
EF	0.9770	0.0850
EG	0.9980	0.0740
EH	1.0000	0.0730
EI	0.9950	0.0810
EJ	0.9970	0.0610
EK	0.9930	0.0790
EL	0.9770	0.0850
EM	0.9970	0.0740
EN	0.9970	0.0750
EO	0.9950	0.0800
EP	0.9970	0.0620
EQ	0.9930	0.0790
ER	0.9770	0.0850
ES	0.9980	0.0740
ET	1.0000	0.0740
EU	0.9950	0.0800
EV	0.9950	0.0640
EW	0.9930	0.0800

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Chain	Atom inclusion	Q-score
EX	0.9770	0.0860
EY	0.9970	0.0740
EZ	0.9970	0.0740
Ea	0.9930	0.0800
Eb	0.9770	0.0880
Ec	0.9980	0.0730
Ed	1.0000	0.0720
Ee	0.9950	0.0740
Ef	0.9950	0.0590
Eg	0.9930	0.0790
Eh	0.9770	0.0850
Ei	0.9970	0.0730
Ej	0.9970	0.0720
Ek	0.9950	0.0720
El	0.9940	0.0610
Em	0.9940	0.0800
En	0.9770	0.0860
Eo	0.9970	0.0750
Ep	0.9970	0.0720
F	0.7120	0.0030
G	0.6990	-0.0030
H	0.6910	-0.0120
I	0.6700	-0.0170
J	0.6700	-0.0170
K	0.6630	-0.0300
L	0.6410	-0.0370
M	0.6260	-0.0320
N	0.6150	-0.0390
O	0.5980	-0.0470
P	0.6190	-0.0380
Q	0.6000	-0.0400
R	0.5940	-0.0480
S	0.6030	-0.0420
T	0.6100	-0.0420
U	0.6080	-0.0500
UI	0.6650	-0.0450
UJ	0.6400	-0.0520
UK	0.6640	-0.0480
UL	0.6590	-0.0440
UM	0.8510	0.0160
UN	0.8150	0.0450
UO	0.7780	0.0210

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Chain	Atom inclusion	Q-score
UP	0.6750	-0.0370
V	0.6260	-0.0390
W	0.6440	-0.0310
WA	0.7880	-0.0090
WB	0.8100	-0.0250
WC	0.8050	-0.0070
WD	0.7790	-0.0300
WE	0.7440	-0.0310
WF	0.7410	-0.0450
WG	0.7740	-0.0190
WH	0.7500	-0.0220
WI	0.7240	-0.0050
WJ	0.7820	0.0170
WK	0.8440	0.0470
WL	0.9360	0.0870
WM	0.9280	0.0500
WN	0.9090	0.0130
WO	0.8520	-0.0100
WP	0.8600	0.0070
WQ	0.8980	0.0350
WR	0.9190	0.0650
WS	0.9270	0.0850
WT	0.9020	0.0880
WU	0.8910	0.0510
WV	0.8540	0.0140
WW	0.8570	0.0130
X	0.6480	-0.0350
Y	0.6630	-0.0200
Z	0.6780	-0.0100
ZA	0.6510	0.0230
ZB	0.6780	0.0340
ZC	0.7270	0.0340
ZD	0.7520	0.0390
ZE	0.7340	0.0240
ZF	0.4700	0.0050
ZG	0.5140	0.0190
ZH	0.5380	0.0170
ZI	0.5800	0.0250
ZJ	0.6450	0.0240
ZK	0.6950	0.0050
ZL	0.7360	0.0140
ZM	0.7700	0.0180

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Chain	Atom inclusion	Q-score
ZN	0.8160	0.0320
ZO	0.8390	0.0320
ZP	0.8440	0.0150
ZQ	0.8500	0.0060
ZR	0.8690	0.0250
ZS	0.8750	0.0160
ZT	0.8940	0.0220
ZU	0.9000	0.0250
ZV	0.8910	0.0120
ZW	0.8970	0.0100
ZX	0.8850	0.0100
ZY	0.8750	0.0210
ZZ	0.8520	0.0160
Za	0.8210	0.0070
Zb	0.7820	-0.0030
Zc	0.7430	0.0000
Zd	0.7170	0.0130
Ze	0.6840	0.0140
Zf	0.6510	0.0160
Zg	0.6240	0.0090
Zh	0.6060	0.0060
a	0.8530	0.0460
b	0.8590	0.0460
c	0.8510	0.0480
d	0.8450	0.0410
e	0.8330	0.0410
f	0.8250	0.0330
g	0.8040	0.0190
h	0.7890	0.0180
i	0.7860	0.0090
j	0.7530	-0.0010
k	0.7490	0.0010
l	0.7530	-0.0040
m	0.7340	-0.0080
n	0.7310	-0.0050
o	0.7360	-0.0050
p	0.7370	-0.0080
q	0.7510	-0.0060
r	0.7670	0.0000
s	0.7800	0.0010
t	0.7750	0.0050
u	0.8050	0.0180

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Chain	Atom inclusion	Q-score
v	0.8130	0.0200
w	0.8170	0.0250
x	0.8350	0.0350
y	0.8500	0.0370
z	0.8540	0.0410