wwPDB EM Validation Summary Report

Mar 31, 2025 – 08:25 PM JST

PDB ID	:	7CGO / pdb_00007cgo
EMDB ID	:	EMD-30359
Title	:	Cryo-EM structure of the flagellar motor-hook complex from Salmonella
Authors	:	Tan, J.X.; Chang, S.H.; Wang, X.F.; Xu, C.H.; Zhou, Y.; Zhang, X.; Zhu, Y.Q.
Deposited on	:	2020-07-01
Resolution	:	3.90 Å(reported)

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

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

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

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

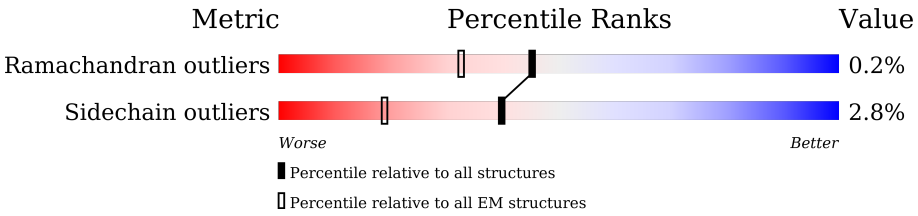
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	260	98%
1	B	260	99%
1	C	260	99%
1	D	260	100%
1	E	260	98%
1	F	260	100%
1	G	260	98%
1	H	260	99%
1	I	260	98%

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Mol	Chain	Length	Quality of chain
1	J	260	99%
1	K	260	98%
1	L	260	98%
1	M	260	99%
1	N	260	96%
1	O	260	97%
1	P	260	95% 5%
1	Q	260	93% 5%
1	R	260	94%
1	S	260	94% 5%
1	T	260	97%
1	U	260	99%
1	V	260	98%
1	W	260	98%
1	X	260	98%
2	a	251	97%
2	b	251	97%
2	c	251	97%
2	d	251	98%
2	e	251	98%
3	0	15	100%
3	1	15	100%
3	2	15	100%
3	3	15	100%
3	4	15	100%

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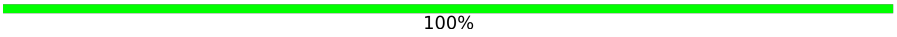
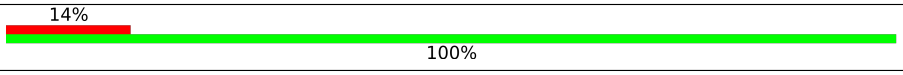
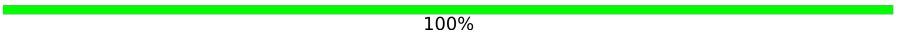
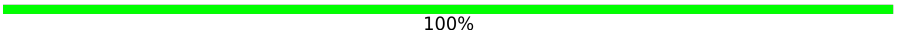
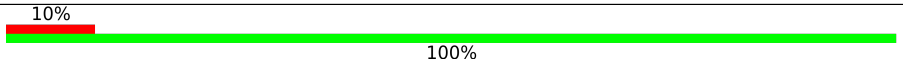
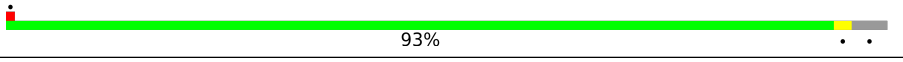
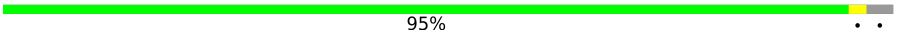
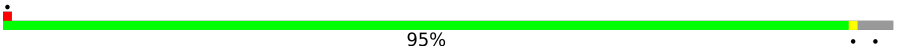
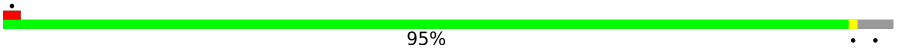
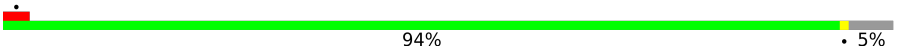
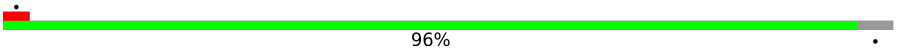
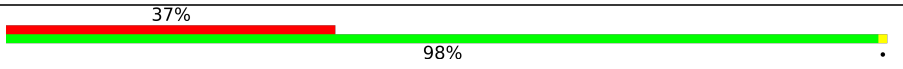
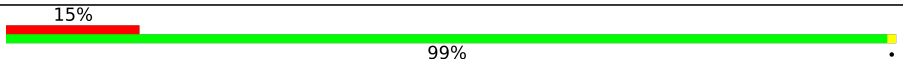
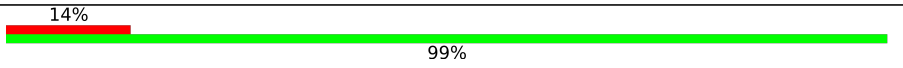
Mol	Chain	Length	Quality of chain
4	5	21	
4	6	21	
4	7	21	
4	8	21	
4	9	21	
5	f	134	
5	g	134	
5	h	134	
5	i	134	
5	j	134	
5	p	134	
6	k	138	
6	l	138	
6	m	138	
6	n	138	
6	o	138	
7	q	104	
7	r	104	
7	s	104	
7	t	104	
7	u	104	
7	v	104	
8	DA	403	
8	DB	403	
8	DC	403	

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Mol	Chain	Length	Quality of chain
8	DD	403	17% 99%
8	DE	403	17% 99%
8	DF	403	19% 99%
8	DG	403	19% 99%
8	DH	403	19% 98%
8	DI	403	24% 98%
8	DJ	403	28% 98%
8	DK	403	33% 99%
8	DL	403	44% 93% 5%
8	DM	403	40% 96%
8	DN	403	46% 96%
8	DO	403	47% 93% 6%
8	DP	403	56% 98%
8	DQ	403	56% 98%
8	DR	403	59% 100%
8	DS	403	63% 98%
8	DT	403	60% 99%
8	DU	403	68% 98%
8	DV	403	69% 99%
8	DW	403	69% 99%
8	DX	403	75% 99%
8	DY	403	75% 99%
8	DZ	403	77% 99%
8	EA	403	84% 100%
8	EB	403	81% 99%

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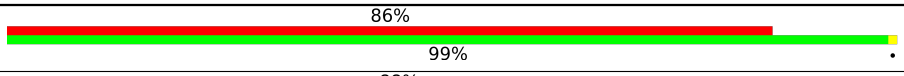
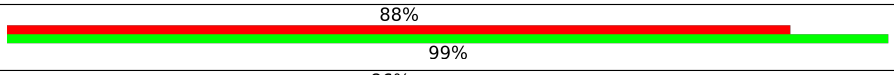
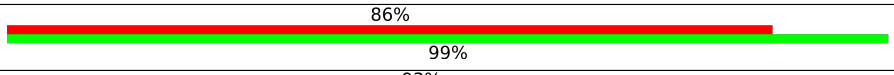
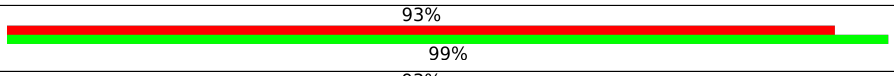
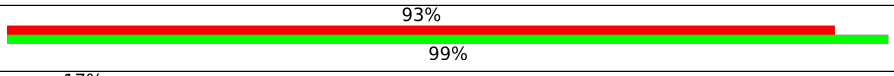
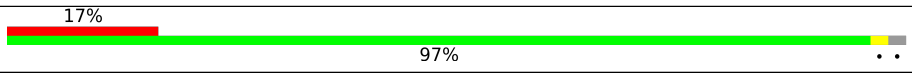
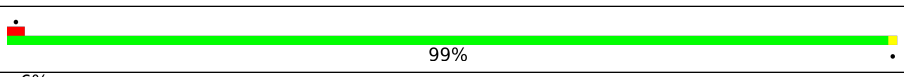
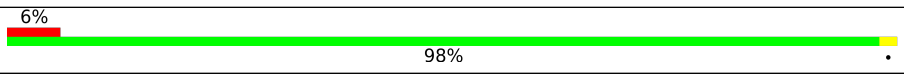
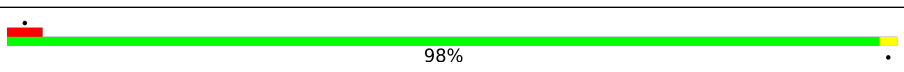
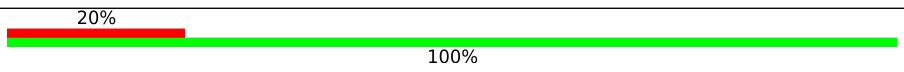
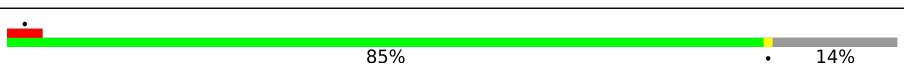
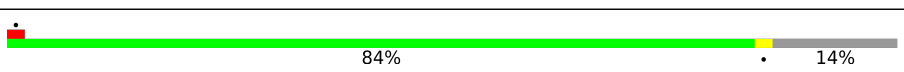
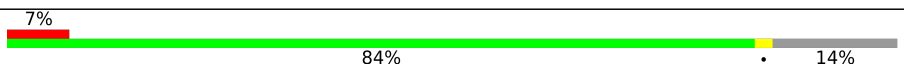
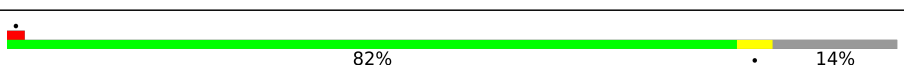
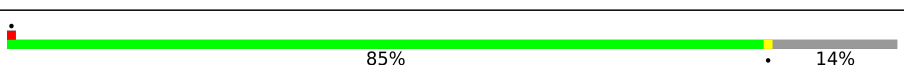
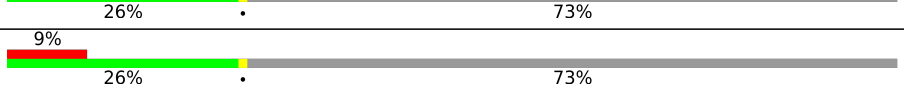
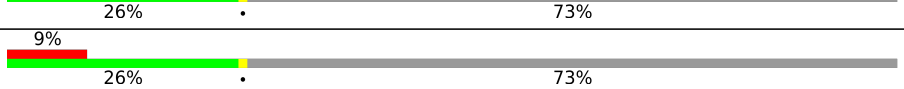
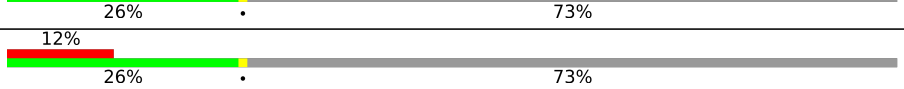
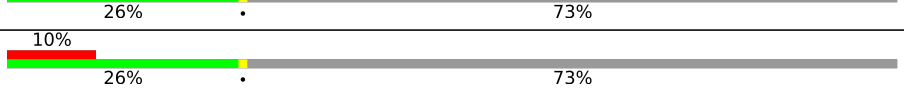
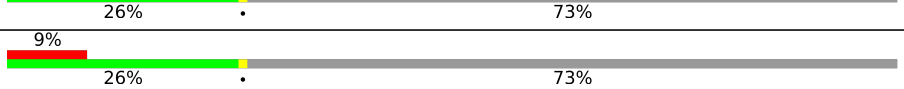
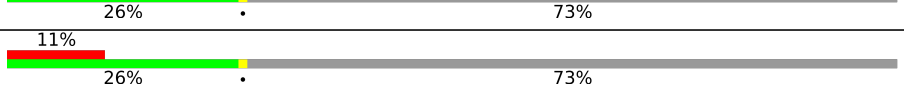
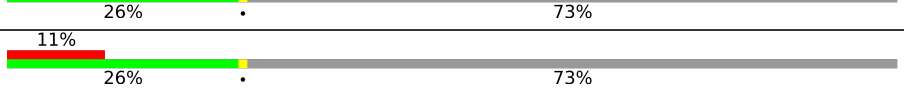
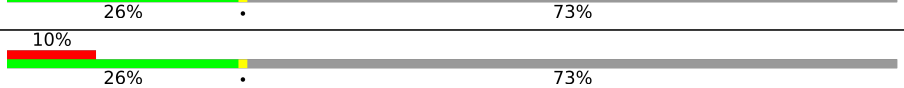
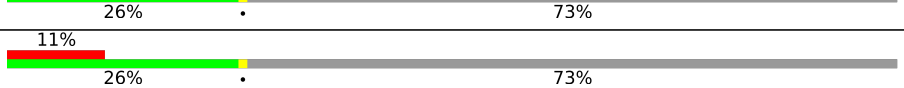
Mol	Chain	Length	Quality of chain
8	EC	403	
8	ED	403	
8	EE	403	
8	EF	403	
8	EG	403	
9	CE	264	
10	CA	89	
10	CB	89	
10	CC	89	
10	CD	89	
11	CF	245	
11	w	245	
11	x	245	
11	y	245	
11	z	245	
12	Ca	560	
12	Cb	560	
12	Cc	560	
12	Cd	560	
12	Ce	560	
12	Cf	560	
12	Cg	560	
12	Ch	560	
12	Ci	560	
12	Cj	560	

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Mol	Chain	Length	Quality of chain
12	Ck	560	12% 26% 73%
12	Cl	560	11% 26% 73%
12	Cm	560	12% 26% 73%
12	Cn	560	11% 26% 73%
12	Co	560	11% 26% 73%
12	Cp	560	11% 26% 73%
12	Cq	560	11% 26% 73%
12	Cr	560	12% 26% 73%
12	Cs	560	10% 26% 73%
12	Ct	560	10% 26% 73%
12	Cu	560	9% 26% 73%
12	Cv	560	10% 26% 73%
12	Cw	560	9% 26% 73%
12	Cx	560	9% 26% 73%
12	Cy	560	9% 26% 73%
12	Cz	560	8% 26% 73%
12	Da	560	19% 81%
12	Db	560	18% 81%
12	Dc	560	18% 81%
12	Dd	560	5% 19% 81%
12	De	560	17% 82%
12	Df	560	17% 83%
12	Dg	560	5% 15% 84%
12	Dh	560	6% 15% 84%
12	Di	560	7% 15% 84%

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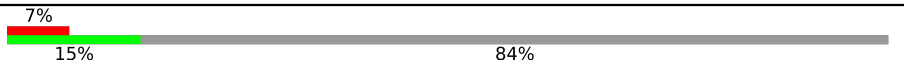
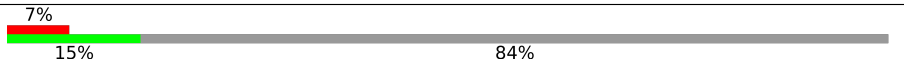
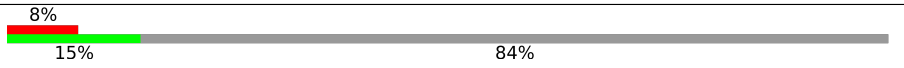
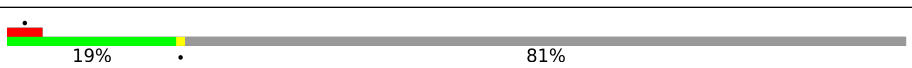
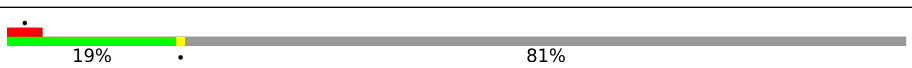
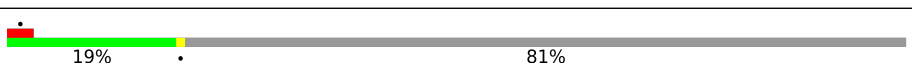
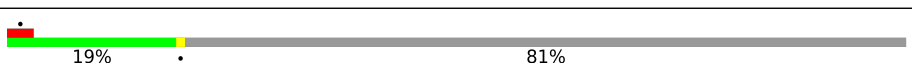
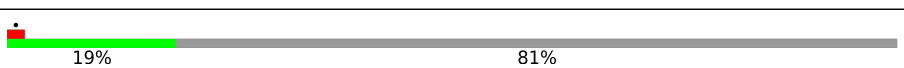
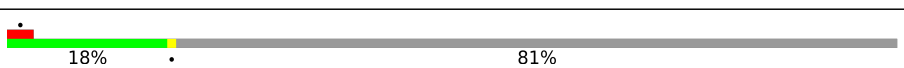
Mol	Chain	Length	Quality of chain
12	Dj	560	
12	Dk	560	
12	Dl	560	
12	Dm	560	
12	Dn	560	
12	Do	560	
12	Dp	560	
12	Dq	560	
12	Dr	560	
12	Ds	560	
12	Dt	560	
12	Du	560	
12	Dv	560	
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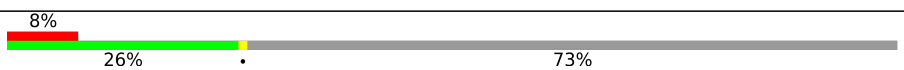
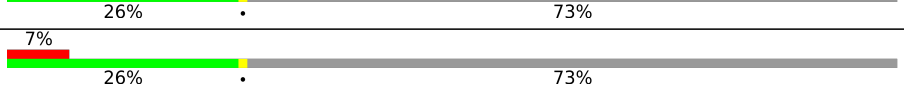
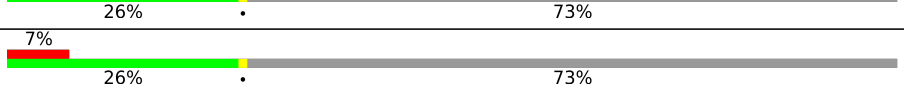
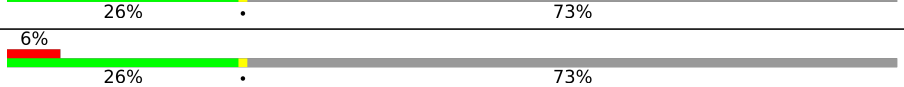
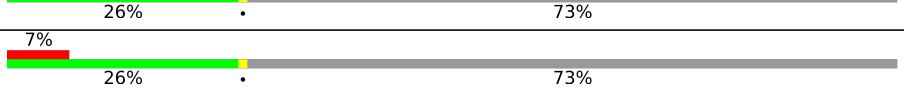
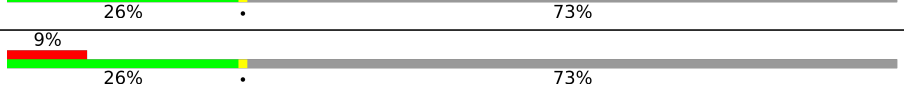
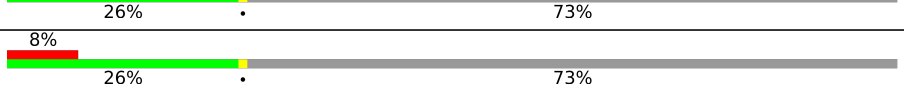
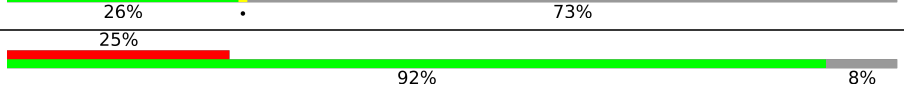
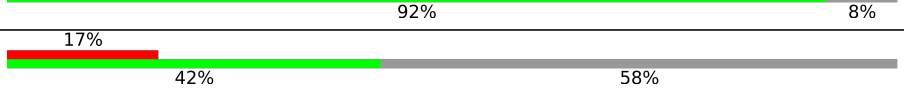
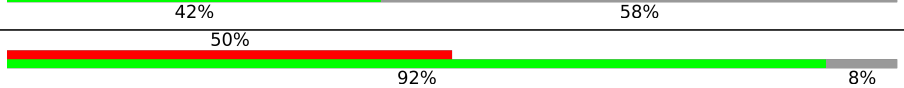
12	Ea	560	
12	Eb	560	
12	Ec	560	
12	Ed	560	
12	Ee	560	
12	Ef	560	
12	Eg	560	
12	Eh	560	
13	GA	12	
13	GB	12	
13	GC	12	

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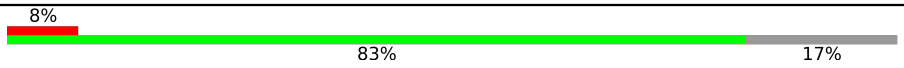
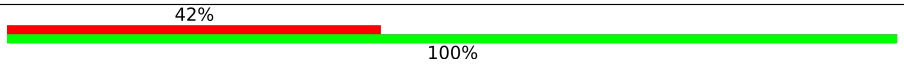
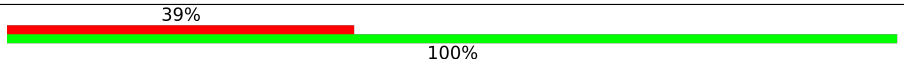
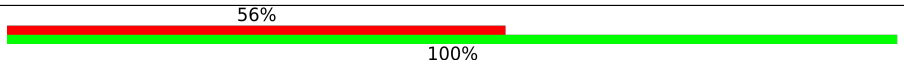
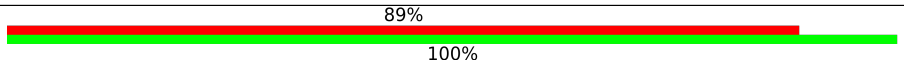
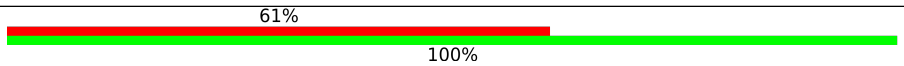
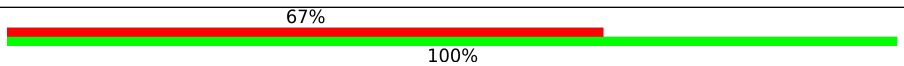
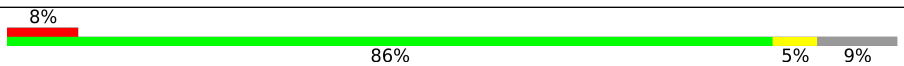
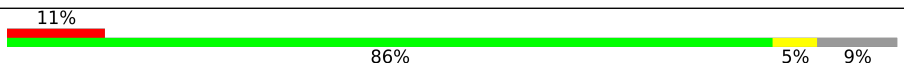
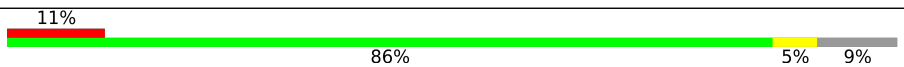
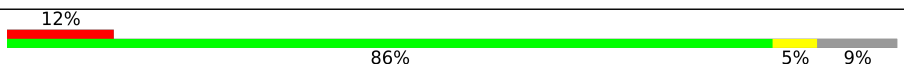
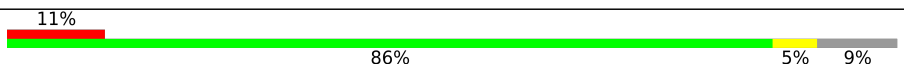
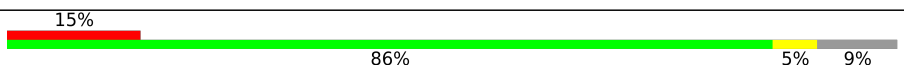
Mol	Chain	Length	Quality of chain
13	GD	12	
13	GE	12	
14	GF	18	
14	GG	18	
14	GH	18	
14	GI	18	
14	GJ	18	
14	GK	18	
15	AA	232	
15	AB	232	
15	AC	232	
15	AD	232	
15	AE	232	
15	AF	232	
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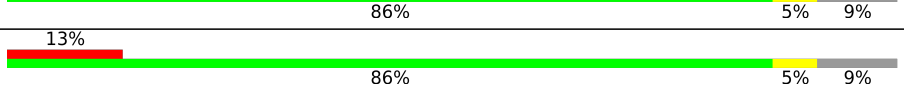
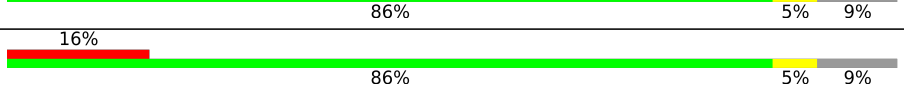
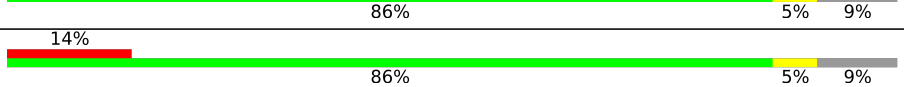
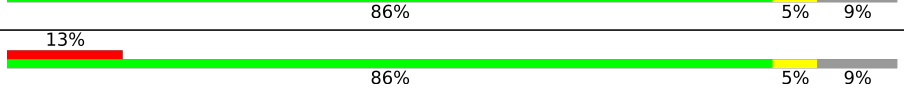
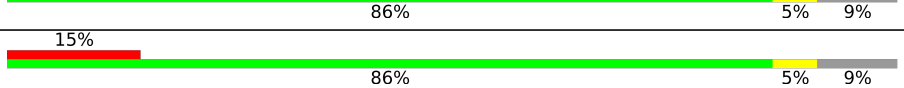
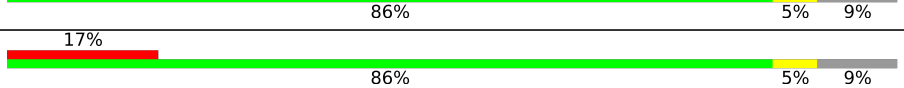
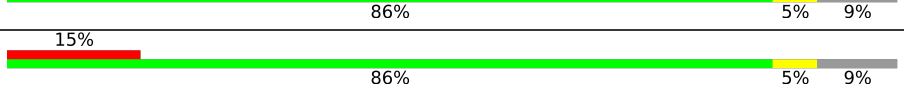
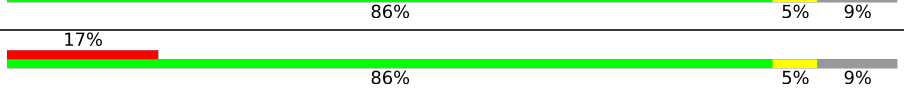
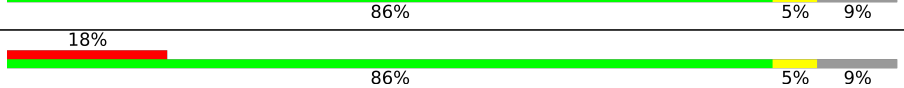
15	AH	232	
15	AI	232	
15	AJ	232	
15	AK	232	
15	AL	232	
15	AM	232	
15	AN	232	
15	AO	232	
15	AP	232	
15	AQ	232	

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Mol	Chain	Length	Quality of chain
15	AR	232	15% 86% 5% 9%
15	AS	232	15% 86% 5% 9%
15	AT	232	14% 86% 5% 9%
15	AU	232	16% 86% 5% 9%
15	AV	232	12% 86% 5% 9%
15	AW	232	11% 86% 5% 9%
15	AX	232	13% 86% 5% 9%
15	AY	232	13% 86% 5% 9%
15	AZ	232	11% 86% 5% 9%
16	BA	365	7% 79% 17%
16	BB	365	6% 80% 17%
16	BC	365	8% 79% 17%
16	BD	365	8% 80% 17%
16	BE	365	6% 79% 17%
16	BF	365	8% 80% 17%
16	BG	365	8% 79% 17%
16	BH	365	8% 79% 17%
16	BI	365	7% 80% 17%
16	BJ	365	9% 80% 17%
16	BK	365	10% 79% 17%
16	BL	365	10% 80% 17%
16	BM	365	10% 79% 17%
16	BN	365	10% 79% 17%
16	BO	365	10% 79% 17%
16	BP	365	11% 79% 17%

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Mol	Chain	Length	Quality of chain
16	BQ	365	11% 79% 17%
16	BR	365	9% 79% 17%
16	BS	365	10% 80% 17%
16	BT	365	12% 79% 17%
16	BU	365	10% 79% 17%
16	BV	365	9% 79% 17%
16	BW	365	8% 79% 17%
16	BX	365	8% 80% 17%
16	BY	365	7% 79% 17%
16	BZ	365	6% 80% 17%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 335722 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	A	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	B	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	C	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	D	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	E	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	F	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	G	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	H	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	I	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	J	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	K	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	L	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		
1	M	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		
1	N	251	Total	C	N	O	S	0	0
			1887	1167	330	384	6		
1	O	252	Total	C	N	O	S	0	0
			1894	1172	331	385	6		
1	P	248	Total	C	N	O	S	0	0
			1862	1151	327	379	5		
1	Q	247	Total	C	N	O	S	0	0
			1858	1149	326	378	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	250	Total	C	N	O	S	0	0
			1875	1159	329	382	5		
1	S	247	Total	C	N	O	S	0	0
			1858	1149	326	378	5		
1	T	253	Total	C	N	O	S	0	0
			1902	1176	333	388	5		
1	U	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		
1	V	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		
1	W	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		
1	X	259	Total	C	N	O	S	0	0
			1941	1197	340	399	5		

- Molecule 2 is a protein called Flagellar basal-body rod protein FlgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
2	b	248	Total	C	N	O	S	0	0
			1804	1106	324	367	7		
2	c	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
2	d	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
2	e	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		

- Molecule 3 is a protein called Flagellar MS ring L2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	0	15	Total	C	N	O	0	0
			75	45	15	15		
3	1	15	Total	C	N	O	0	0
			75	45	15	15		
3	2	15	Total	C	N	O	0	0
			75	45	15	15		
3	3	15	Total	C	N	O	0	0
			75	45	15	15		
3	4	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 4 is a protein called Flagellar MS ring L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	5	21	Total	C	N	O	0	0
			140	88	24	28		
4	6	21	Total	C	N	O	0	0
			140	88	24	28		
4	7	21	Total	C	N	O	0	0
			140	88	24	28		
4	9	21	Total	C	N	O	0	0
			140	88	24	28		
4	8	21	Total	C	N	O	0	0
			140	88	24	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	128	Total	C	N	O	S	0	0
			936	585	160	186	5		
5	g	130	Total	C	N	O	S	0	0
			949	592	163	189	5		
5	h	128	Total	C	N	O	S	0	0
			935	584	160	186	5		
5	j	127	Total	C	N	O	S	0	0
			931	582	159	185	5		
5	p	129	Total	C	N	O	S	0	0
			940	587	161	187	5		
5	i	129	Total	C	N	O	S	0	0
			944	589	162	188	5		

- Molecule 6 is a protein called Flagellar basal body rod protein FlgB.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	l	106	Total	C	N	O	S	0	0
			833	515	150	163	5		
6	m	106	Total	C	N	O	S	0	0
			833	515	150	163	5		
6	o	109	Total	C	N	O	S	0	0
			856	529	156	166	5		
6	k	108	Total	C	N	O	S	0	0
			852	527	155	165	5		
6	n	107	Total	C	N	O	S	0	0
			844	521	154	164	5		

- Molecule 7 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	q	71	Total	C	N	O	S	0	0
			536	330	98	102	6		
7	r	70	Total	C	N	O	S	0	0
			526	323	97	100	6		
7	s	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
7	t	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
7	u	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
7	v	38	Total	C	N	O	S	0	0
			289	178	50	55	6		

- Molecule 8 is a protein called Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	DA	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DB	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DC	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DD	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DE	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DF	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DG	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DH	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DI	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DJ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DK	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DL	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DM	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DN	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	DO	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DP	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DQ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DR	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DS	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DT	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DU	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DV	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DW	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DX	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DY	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	DZ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	EA	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	EB	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	EC	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	ED	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	EE	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	EF	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
8	EG	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CE	260	Total	C	N	O	S	0	0
			2002	1339	317	330	16		

- Molecule 10 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CA	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
10	CB	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
10	CC	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
10	CD	89	Total	C	N	O	S	0	0
			670	449	100	114	7		

- Molecule 11 is a protein called Flagellar biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	w	211	Total	C	N	O	S	0	0
			1636	1091	254	279	12		
11	x	211	Total	C	N	O	S	0	0
			1636	1091	254	279	12		
11	y	211	Total	C	N	O	S	0	0
			1636	1091	254	279	12		
11	z	211	Total	C	N	O	S	0	0
			1636	1091	254	279	12		
11	CF	211	Total	C	N	O	S	0	0
			1636	1091	254	279	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Da	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Db	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Dc	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Dd	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	De	99	Total	C	N	O	S	0	0
			696	432	125	138	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	Df	97	Total	C	N	O	S	0	0
			687	427	123	136	1		
12	Dg	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
12	Dh	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
12	Di	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
12	Dj	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
12	Dk	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
12	Dl	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
12	Dm	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
12	Dn	87	Total	C	N	O	S	0	0
			637	397	113	126	1		
12	Do	97	Total	C	N	O	S	0	0
			687	427	123	136	1		
12	Dp	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Dq	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Dr	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Ds	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Dt	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Du	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Dv	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Dw	109	Total	C	N	O	S	0	0
			746	462	135	148	1		
12	Ca	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cb	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cc	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	Cd	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Ce	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cf	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cg	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Ch	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Ci	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cj	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Ck	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cl	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cm	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cn	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Co	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cp	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cq	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cr	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cs	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Ct	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cu	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cv	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cw	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cx	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	Cy	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Cz	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Ea	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Eb	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Ec	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Ed	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Ee	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Ef	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Eg	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		
12	Eh	150	Total	C	N	O	S	0	0
			1185	722	221	239	3		

- Molecule 13 is a protein called FlgB-Dc loop.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	GA	11	Total	C	N	O	0	0
			55	33	11	11		
13	GC	11	Total	C	N	O	0	0
			55	33	11	11		
13	GE	12	Total	C	N	O	0	0
			60	36	12	12		
13	GD	10	Total	C	N	O	0	0
			50	30	10	10		
13	GB	5	Total	C	N	O	0	0
			25	15	5	5		

- Molecule 14 is a protein called FliE helix 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	GF	18	Total	C	N	O	0	0
			90	54	18	18		
14	GG	18	Total	C	N	O	0	0
			90	54	18	18		

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Mol	Chain	Residues	Atoms				AltConf	Trace
14	GH	18	Total 90	C 54	N 18	O 18	0	0
14	GI	15	Total 75	C 45	N 15	O 15	0	0
14	GJ	18	Total 90	C 54	N 18	O 18	0	0
14	GK	18	Total 90	C 54	N 18	O 18	0	0

- Molecule 15 is a protein called Flagellar L-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AA	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AB	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AC	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AD	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AE	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AF	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AG	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AH	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AI	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AJ	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AK	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AL	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AM	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AN	211	Total 1589	C 993	N 282	O 310	S 4	0	0
15	AO	211	Total 1589	C 993	N 282	O 310	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		
15	AQ	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		
15	AR	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		
15	AS	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		
15	AT	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		
15	AU	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		
15	AV	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		
15	AW	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		
15	AX	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		
15	AY	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		
15	AZ	211	Total	C	N	O	S	0	0
			1589	993	282	310	4		

- Molecule 16 is a protein called Flagellar P-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BA	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BB	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BC	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BD	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BE	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BF	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BG	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BH	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		

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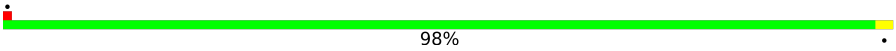
Mol	Chain	Residues	Atoms					AltConf	Trace
16	BI	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BJ	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BK	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BL	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BM	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BN	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BO	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BP	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BQ	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BR	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BS	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BT	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BU	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BV	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BW	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BX	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BY	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
16	BZ	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		

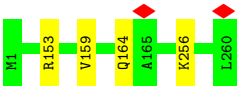
3 Residue-property plots (i)

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

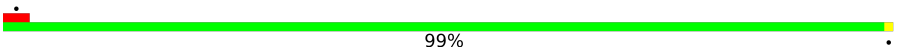
Chain A:

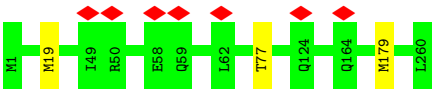




• Molecule 1: Flagellar basal-body rod protein FlgG

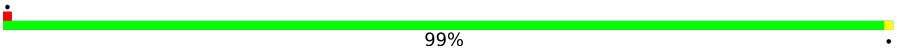
Chain B:

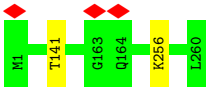




• Molecule 1: Flagellar basal-body rod protein FlgG

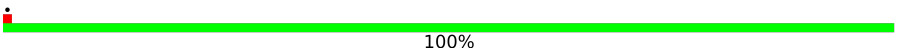
Chain C:

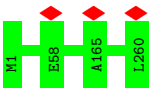




• Molecule 1: Flagellar basal-body rod protein FlgG

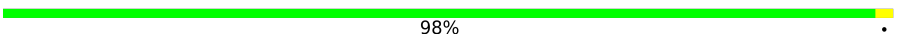
Chain D:





• Molecule 1: Flagellar basal-body rod protein FlgG

Chain E:

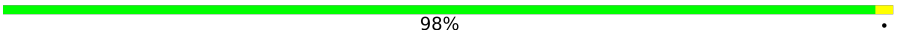


• Molecule 1: Flagellar basal-body rod protein FlgG

Chain F:

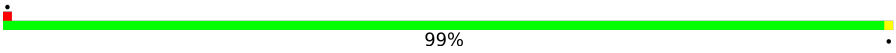
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain G:



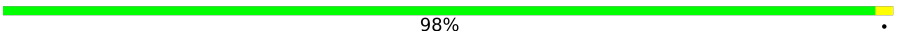
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain H:



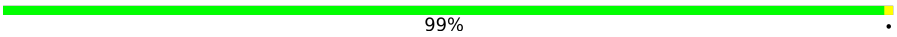
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain I:



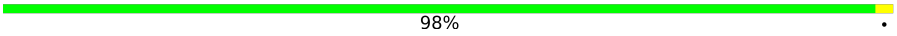
• Molecule 1: Flagellar basal-body rod protein FlgG

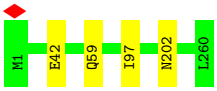
Chain J:



• Molecule 1: Flagellar basal-body rod protein FlgG

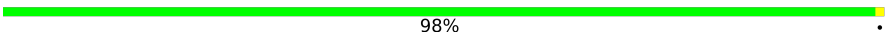
Chain K:





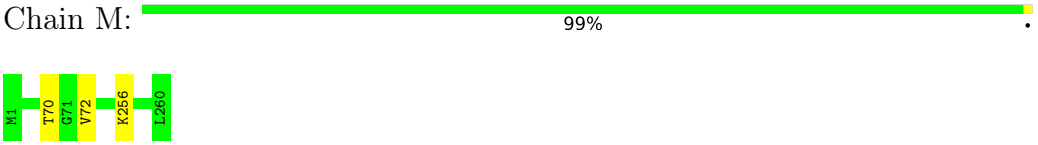
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain L:



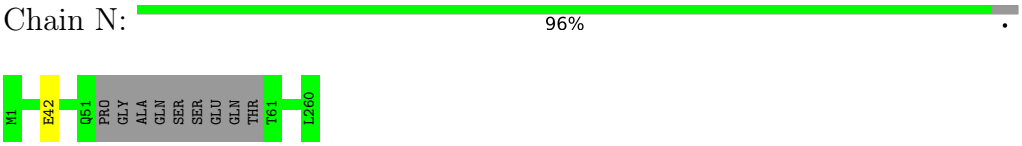
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain M:



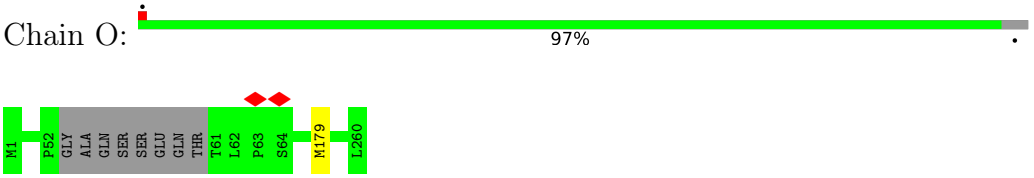
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain N:



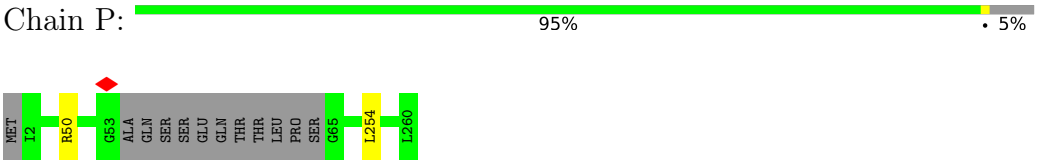
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain O:



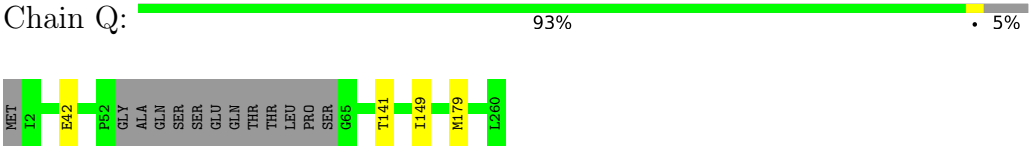
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain P:



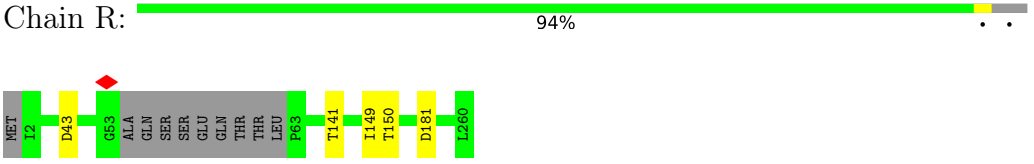
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain Q:



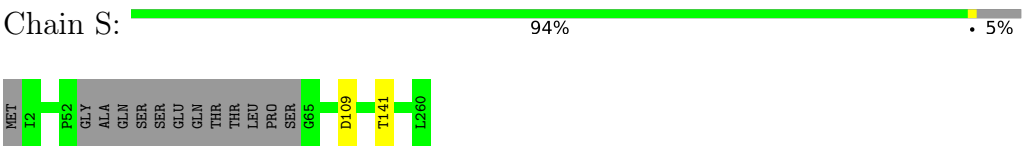
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain R:



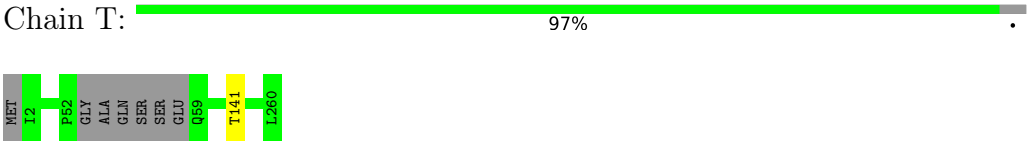
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain S:



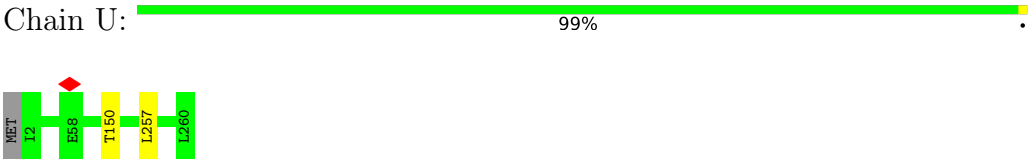
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain T:



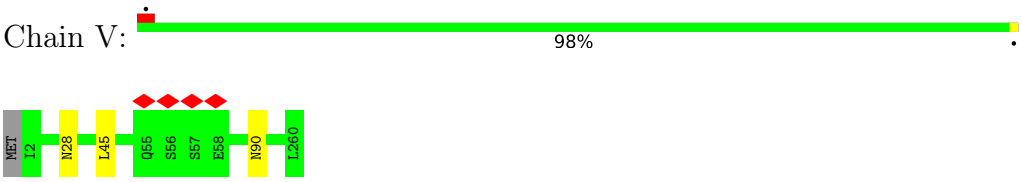
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain U:



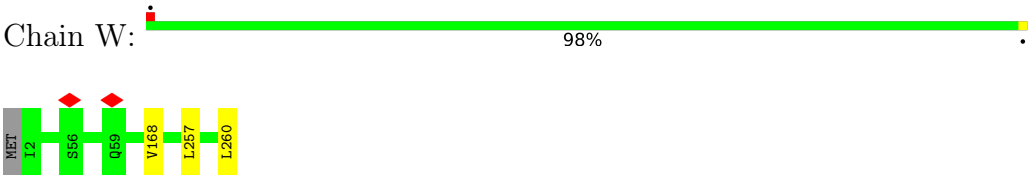
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain V:



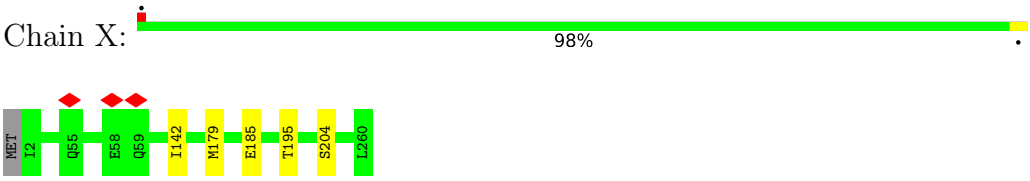
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain W:



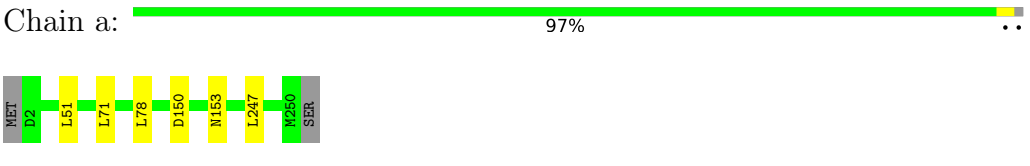
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain X:



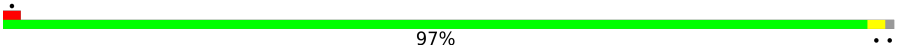
• Molecule 2: Flagellar basal-body rod protein FlgF

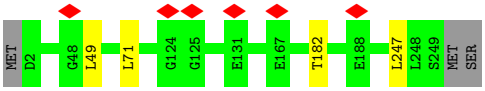
Chain a:



• Molecule 2: Flagellar basal-body rod protein FlgF

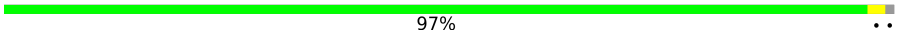
Chain b:

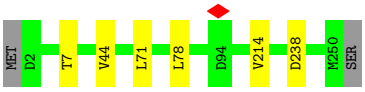




• Molecule 2: Flagellar basal-body rod protein FlgF

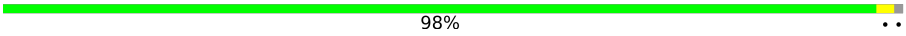
Chain c:

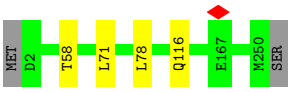




• Molecule 2: Flagellar basal-body rod protein FlgF

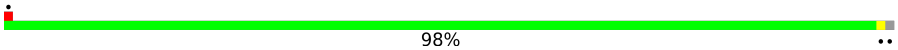
Chain d:

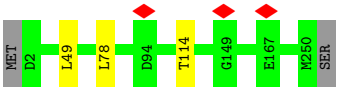




• Molecule 2: Flagellar basal-body rod protein FlgF

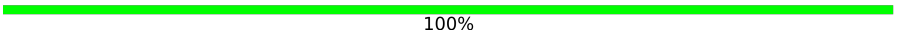
Chain e:





• Molecule 3: Flagellar MS ring L2

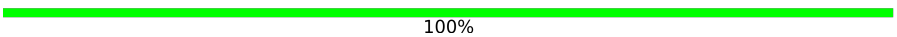
Chain 0:



There are no outlier residues recorded for this chain.

• Molecule 3: Flagellar MS ring L2

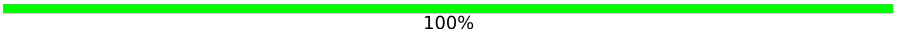
Chain 1:



There are no outlier residues recorded for this chain.

• Molecule 3: Flagellar MS ring L2

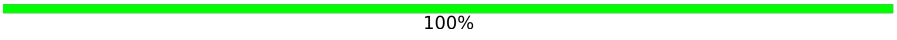
Chain 2:



There are no outlier residues recorded for this chain.

• Molecule 3: Flagellar MS ring L2

Chain 3:



There are no outlier residues recorded for this chain.

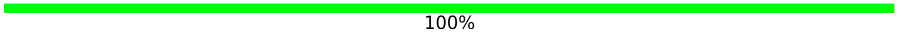
• Molecule 3: Flagellar MS ring L2

Chain 4:

There are no outlier residues recorded for this chain.

• Molecule 4: Flagellar MS ring L1

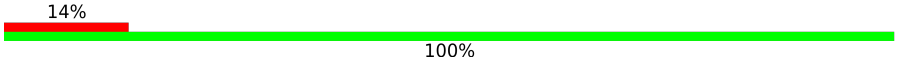
Chain 5:

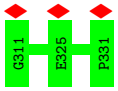


There are no outlier residues recorded for this chain.

• Molecule 4: Flagellar MS ring L1

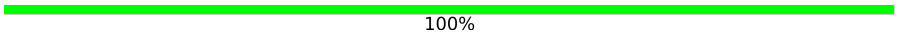
Chain 6:





• Molecule 4: Flagellar MS ring L1

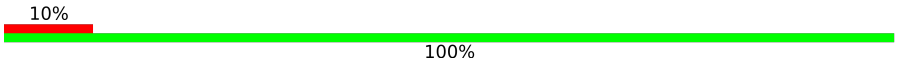
Chain 7:

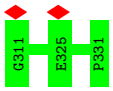


There are no outlier residues recorded for this chain.

• Molecule 4: Flagellar MS ring L1

Chain 9:





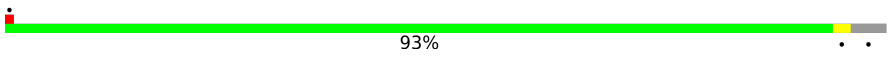
• Molecule 4: Flagellar MS ring L1

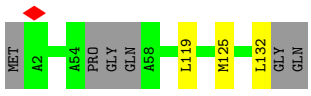
Chain 8:

There are no outlier residues recorded for this chain.

• Molecule 5: Flagellar basal-body rod protein FlgC

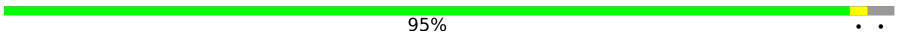
Chain f:

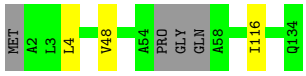




• Molecule 5: Flagellar basal-body rod protein FlgC

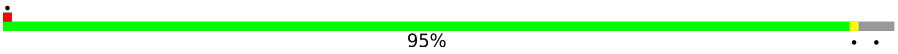
Chain g:

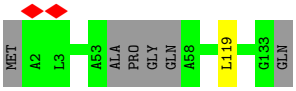




• Molecule 5: Flagellar basal-body rod protein FlgC

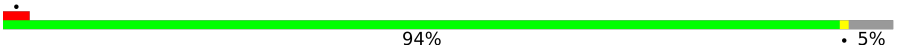
Chain h:

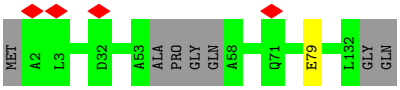




• Molecule 5: Flagellar basal-body rod protein FlgC

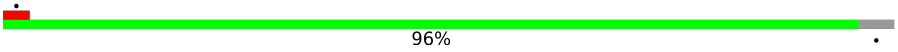
Chain j:

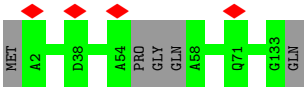




• Molecule 5: Flagellar basal-body rod protein FlgC

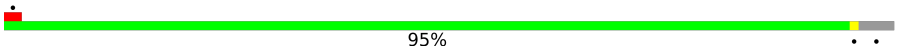
Chain p:

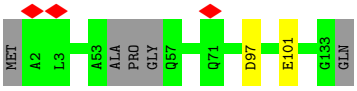




• Molecule 5: Flagellar basal-body rod protein FlgC

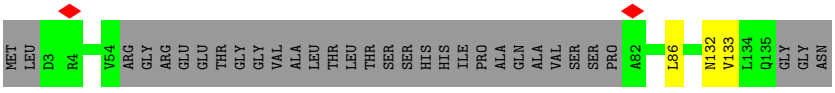
Chain i:





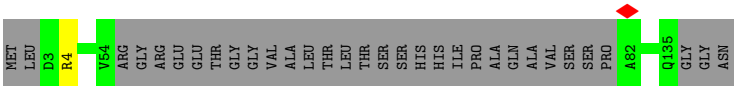
• Molecule 6: Flagellar basal body rod protein FlgB

Chain l:



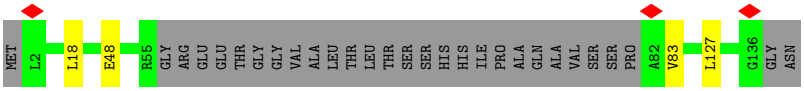
• Molecule 6: Flagellar basal body rod protein FlgB

Chain m:

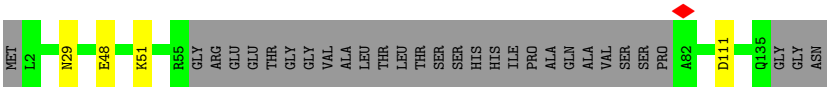


• Molecule 6: Flagellar basal body rod protein FlgB

Chain o:

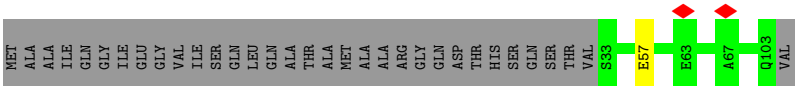


• Molecule 6: Flagellar basal body rod protein FlgB

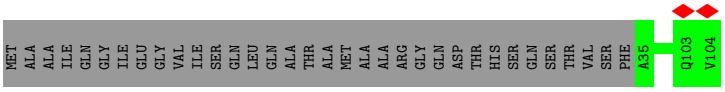


• Molecule 6: Flagellar basal body rod protein FlgB

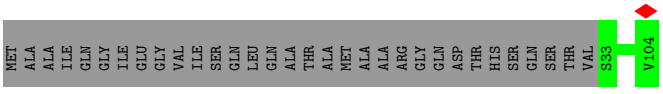
• Molecule 7: Flagellar hook-basal body complex protein FliE



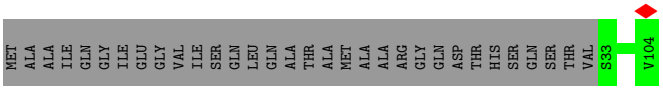
• Molecule 7: Flagellar hook-basal body complex protein FliE



• Molecule 7: Flagellar hook-basal body complex protein FliE



• Molecule 7: Flagellar hook-basal body complex protein FliE



• Molecule 7: Flagellar hook-basal body complex protein FliE

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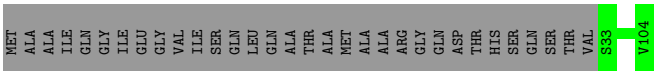

• Molecule 7: Flagellar hook-basal body complex protein FliE

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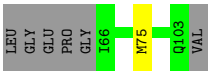

• Molecule 8: Flagellar hook protein FlgE

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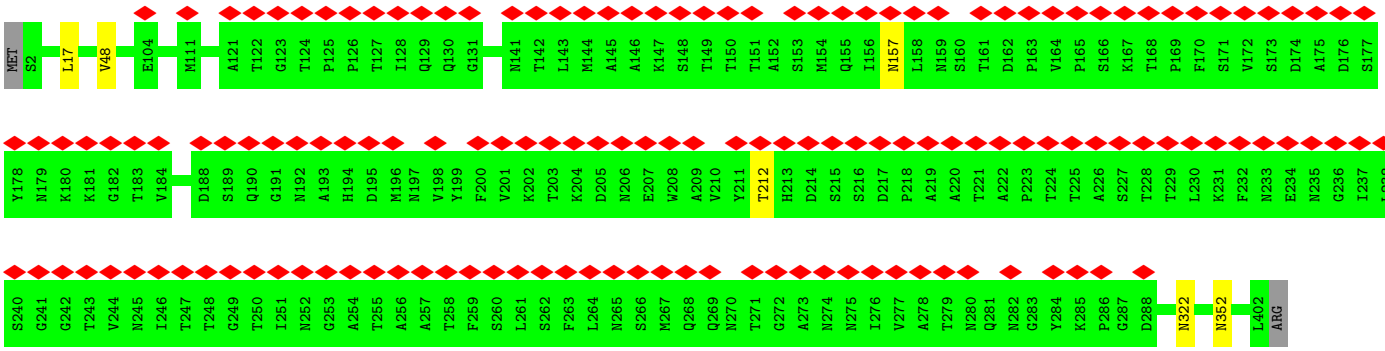

• Molecule 8: Flagellar hook protein FlgE

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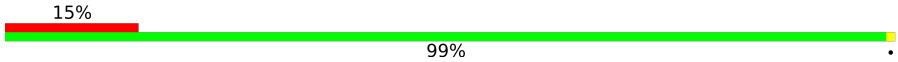

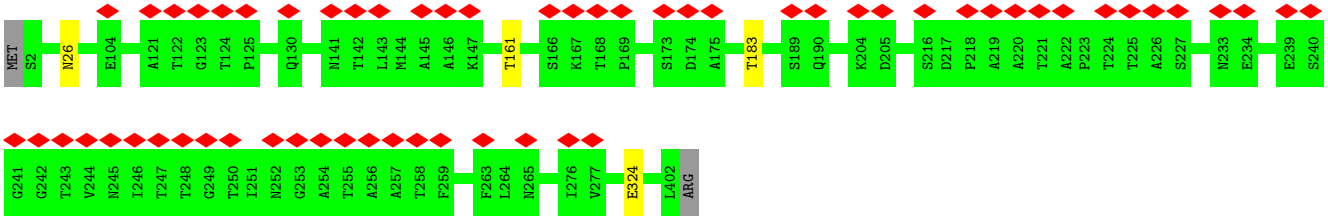

• Molecule 8: Flagellar hook protein FlgE

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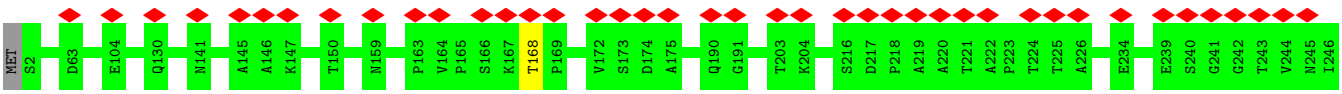

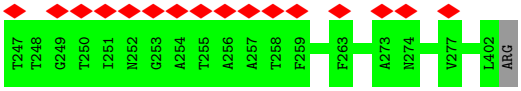

• Molecule 8: Flagellar hook protein FlgE

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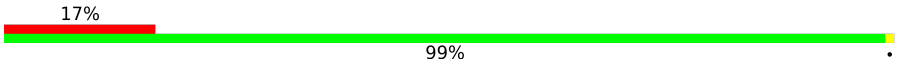

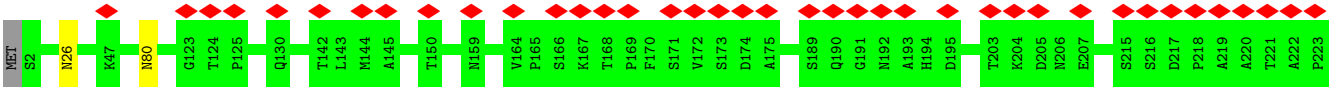

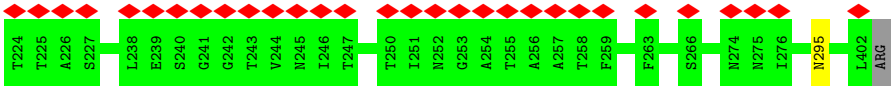

• Molecule 8: Flagellar hook protein FlgE

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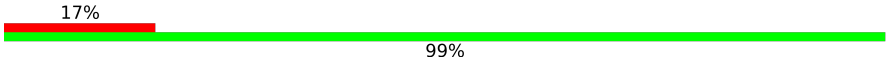

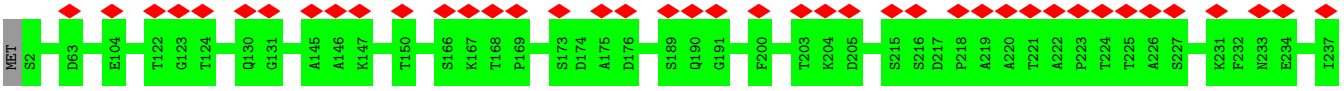

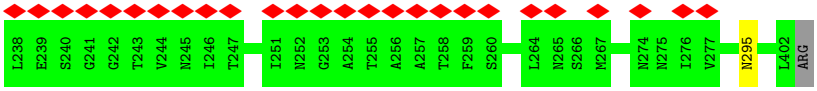

• Molecule 8: Flagellar hook protein FlgE

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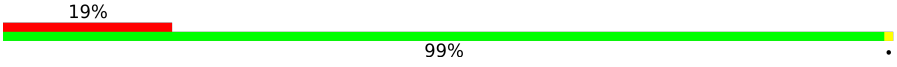

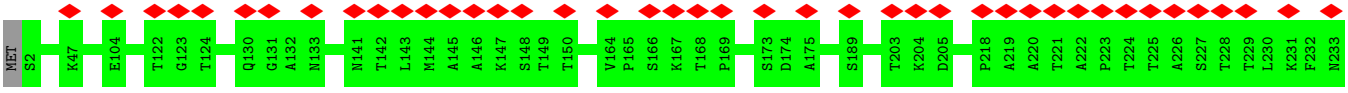

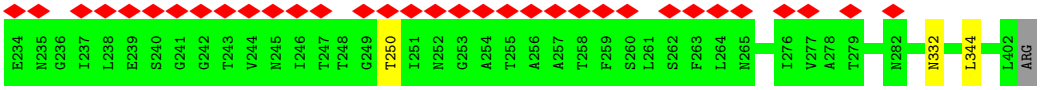

• Molecule 8: Flagellar hook protein FlgE

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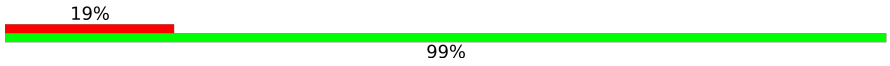

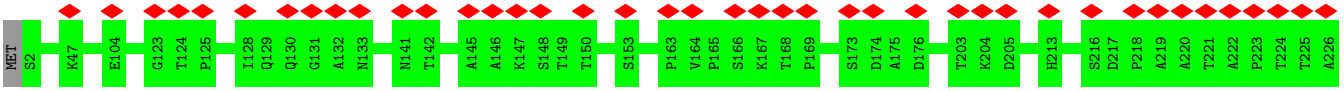

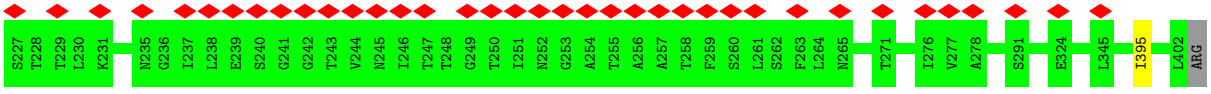

• Molecule 8: Flagellar hook protein FlgE

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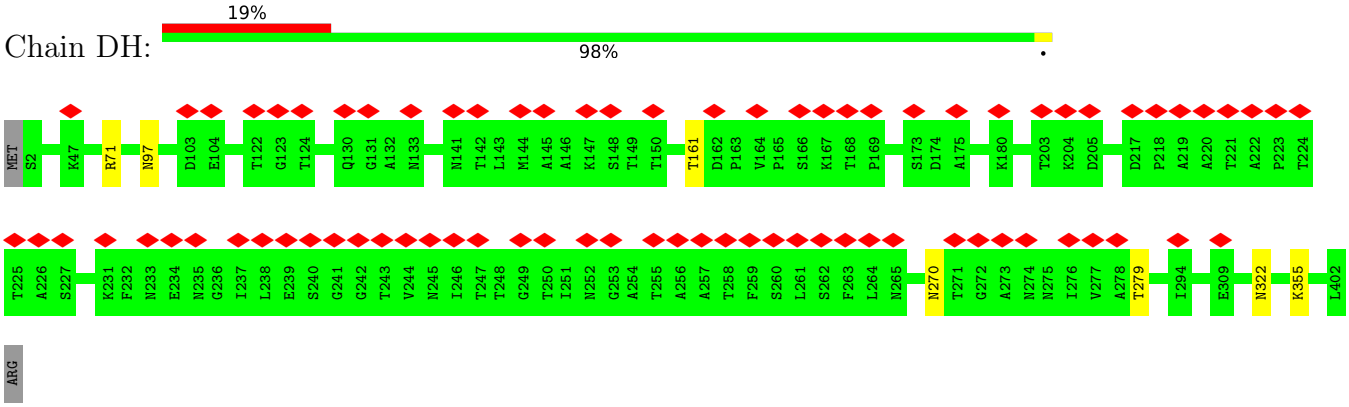

• Molecule 8: Flagellar hook protein FlgE

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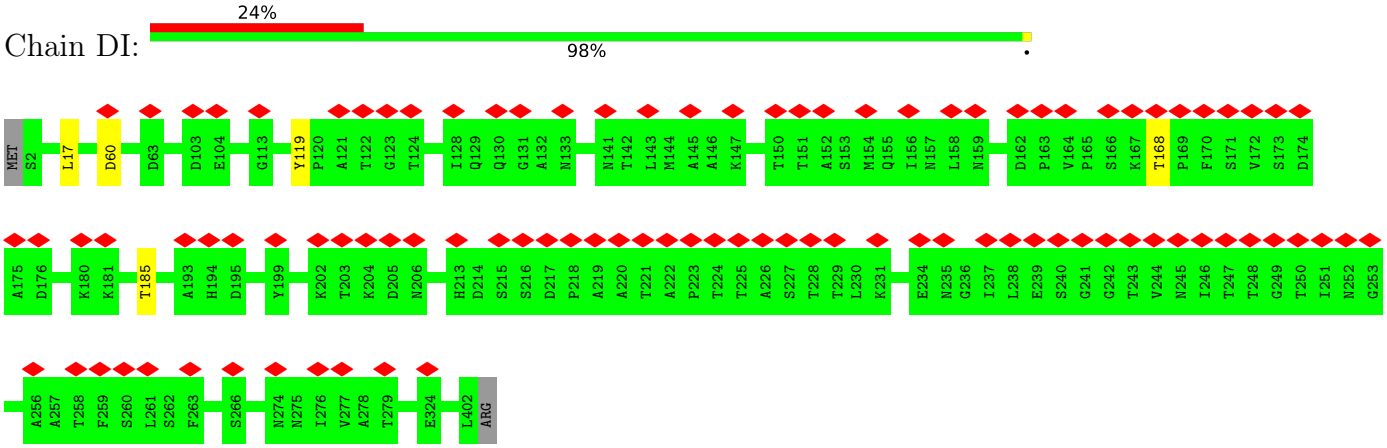

• Molecule 8: Flagellar hook protein FlgE

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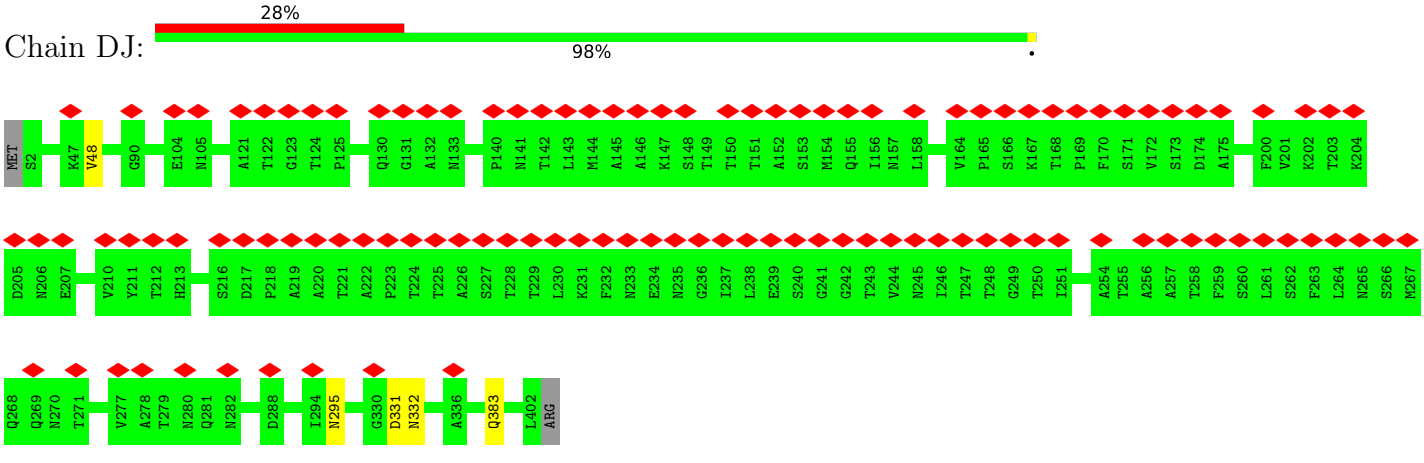

• Molecule 8: Flagellar hook protein FlgE

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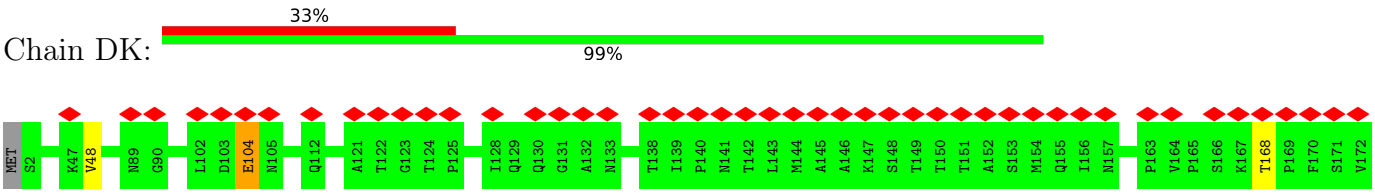
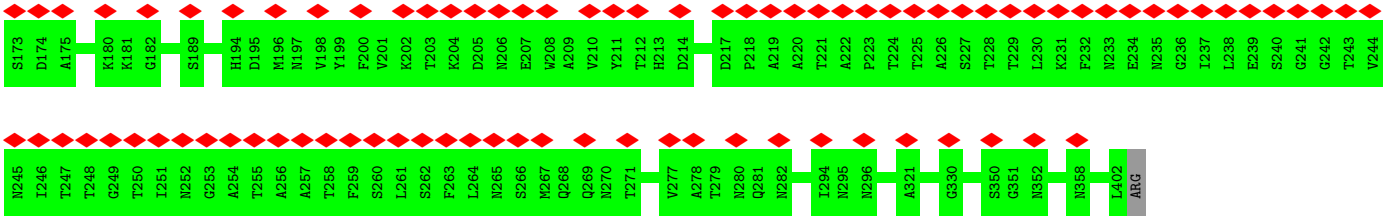
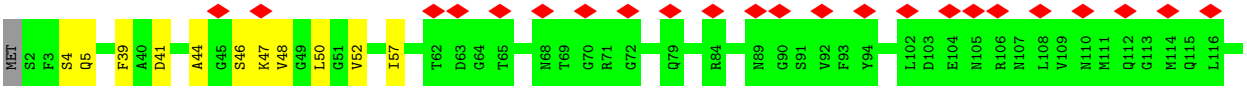
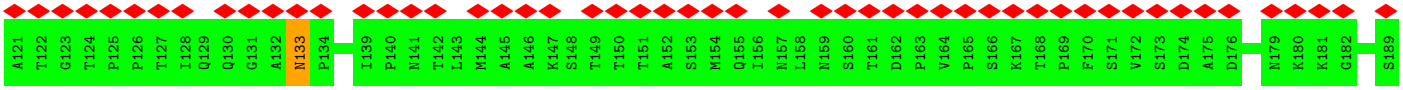
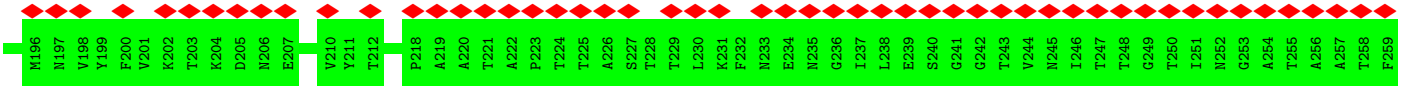


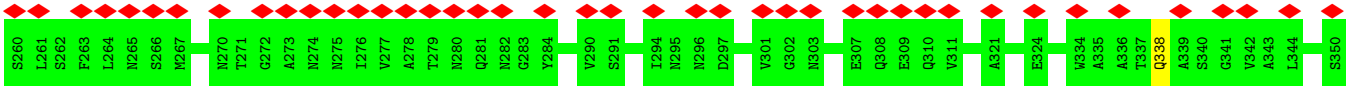


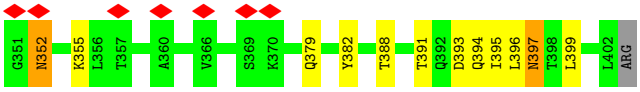
• Molecule 8: Flagellar hook protein FlgE



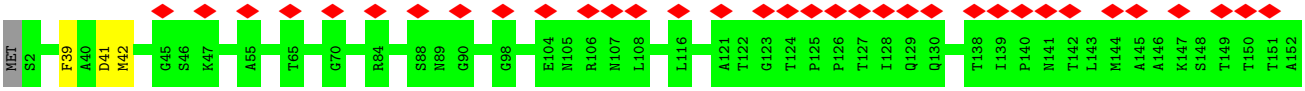


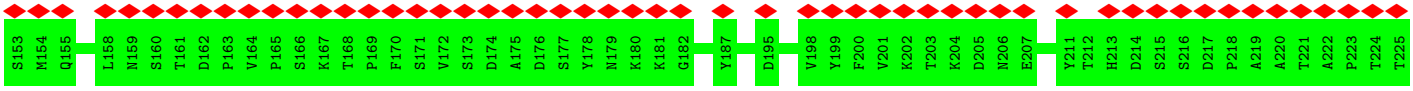


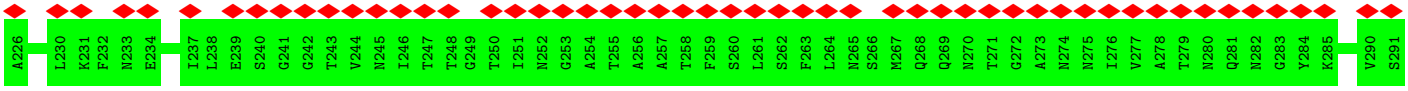


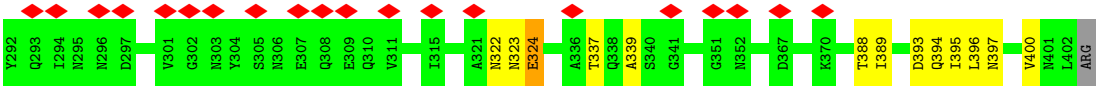


• Molecule 8: Flagellar hook protein FlgE







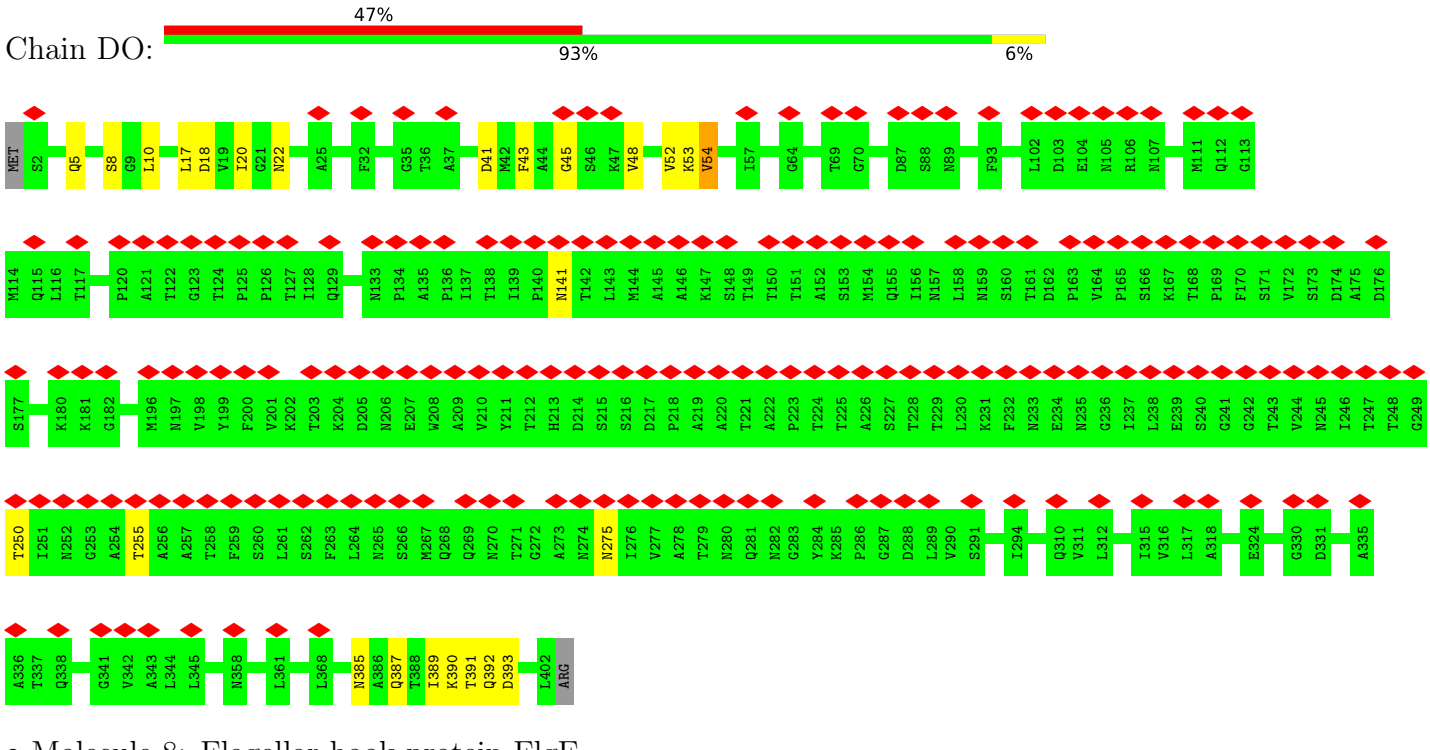


• Molecule 8: Flagellar hook protein FlgE

Chain DN:

• Molecule 8: Flagellar hook protein FlgE

Chain DO:



• Molecule 8: Flagellar hook protein FlgE

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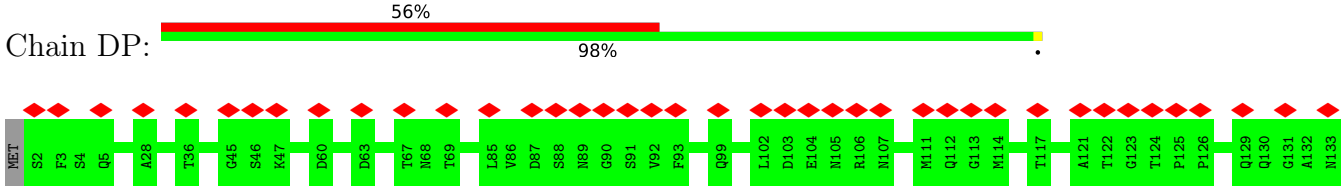

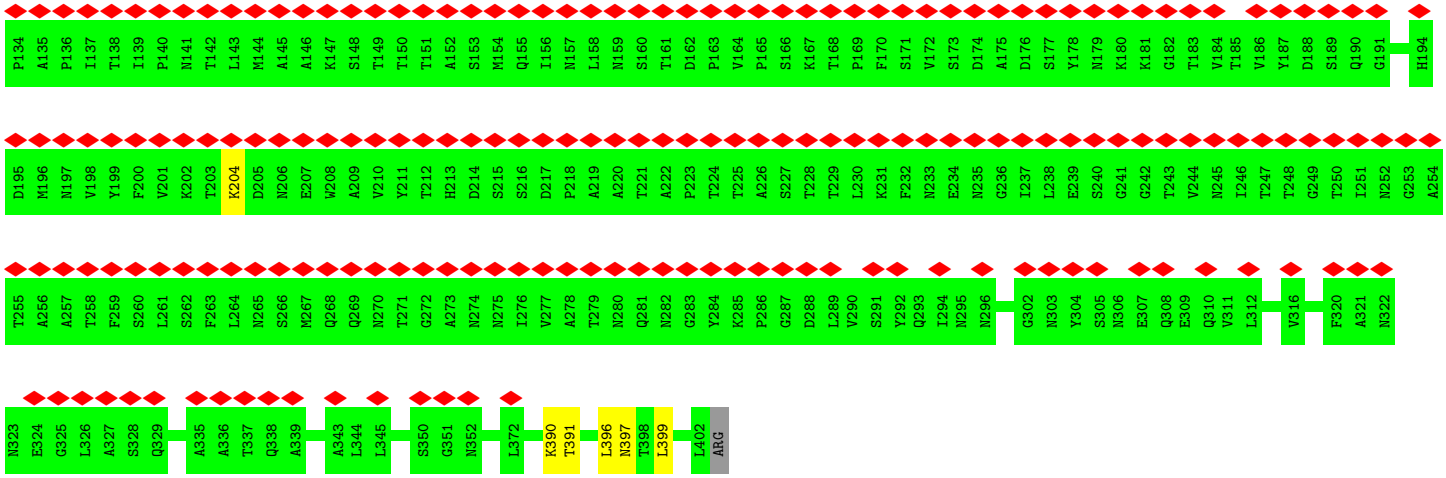

• Molecule 8: Flagellar hook protein FlgE

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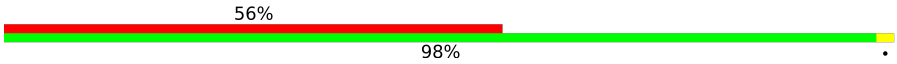

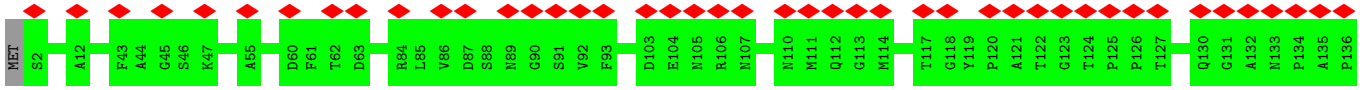

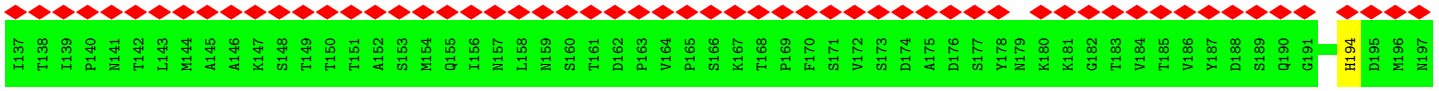

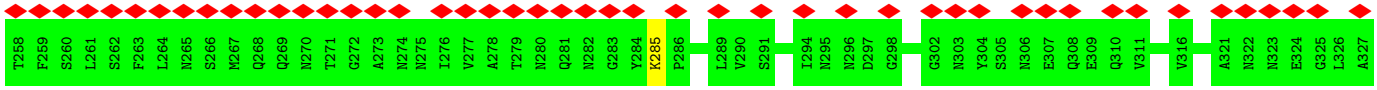

• Molecule 8: Flagellar hook protein FlgE

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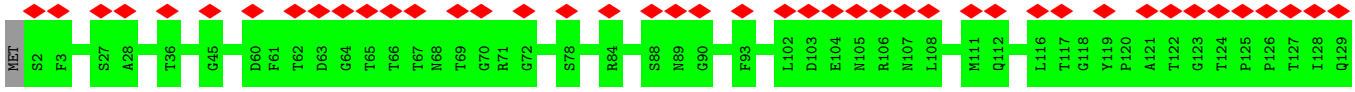
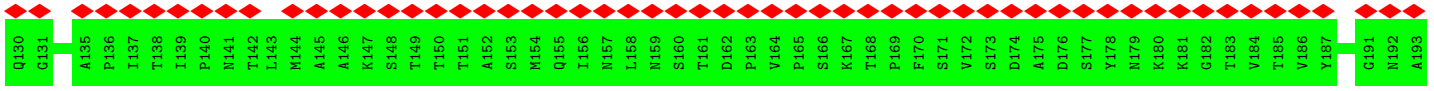
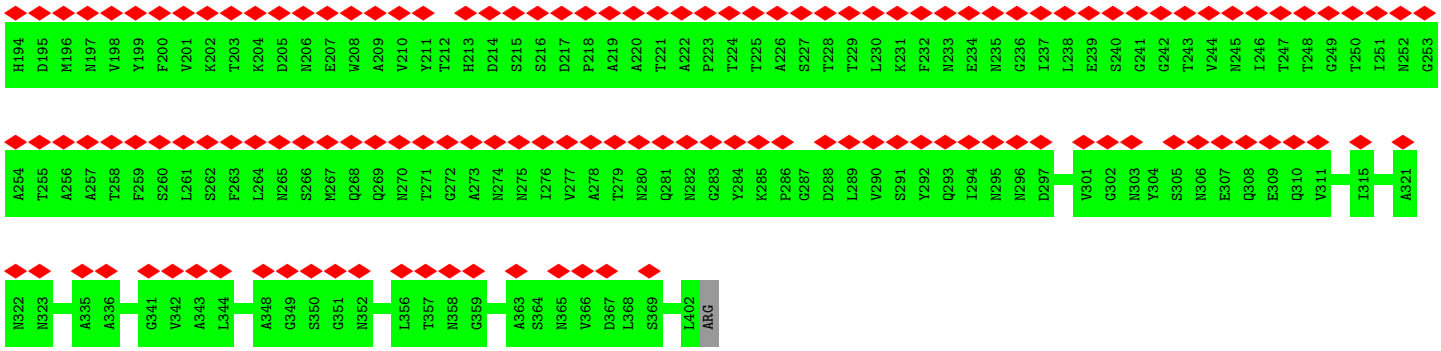
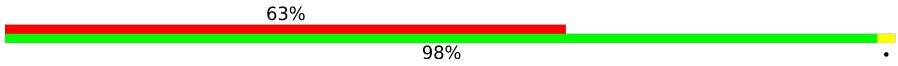


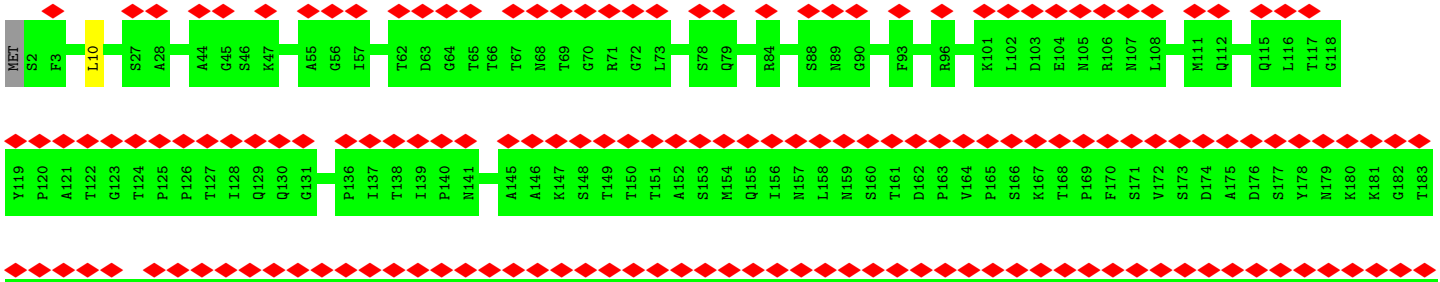


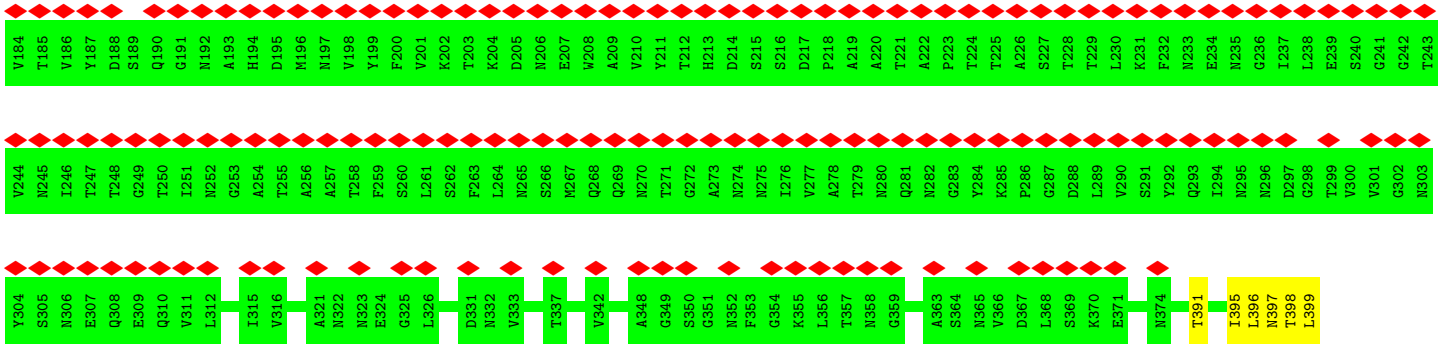


• Molecule 8: Flagellar hook protein FlgE

Chain DS:







• Molecule 8: Flagellar hook protein FlgE

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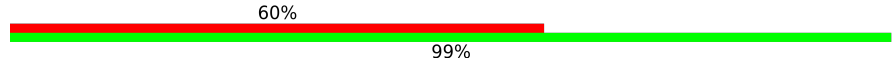
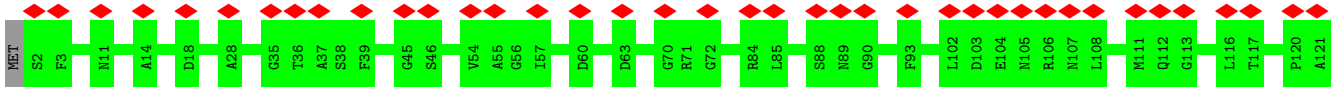
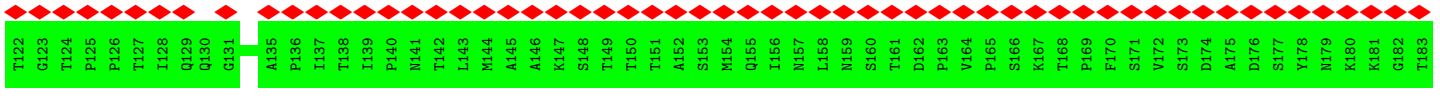
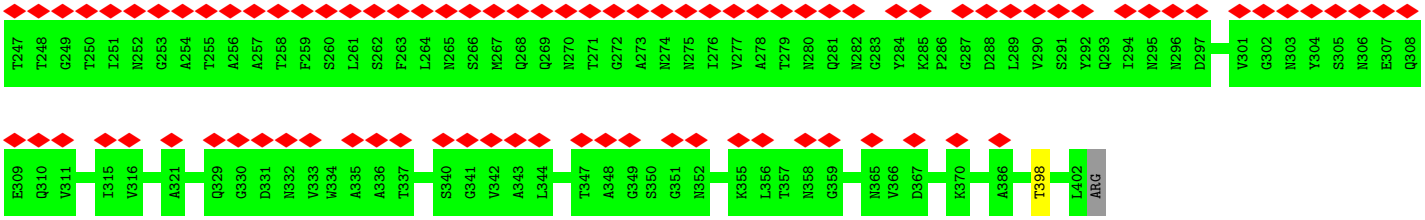


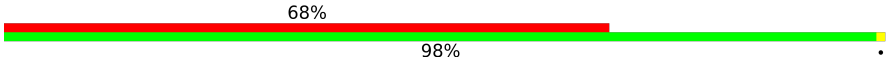


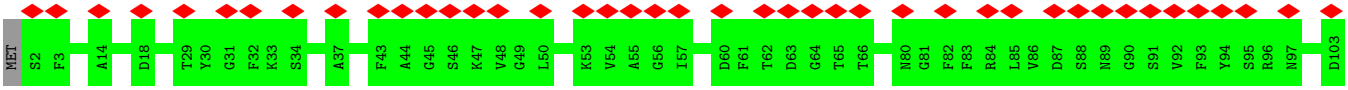


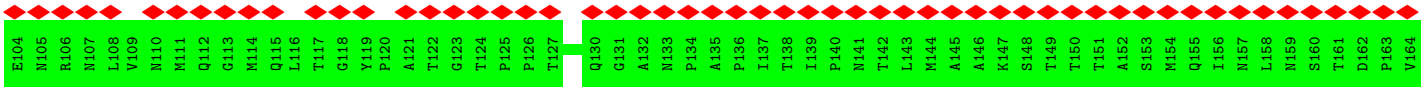


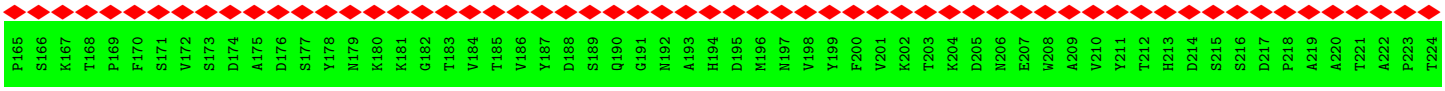
• Molecule 8: Flagellar hook protein FlgE

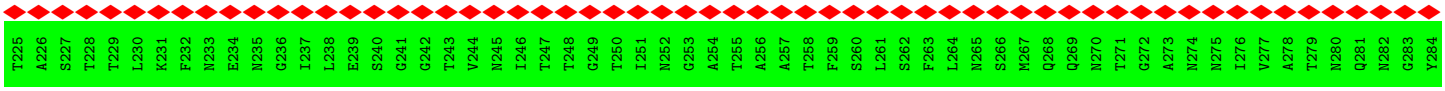
Chain DU:

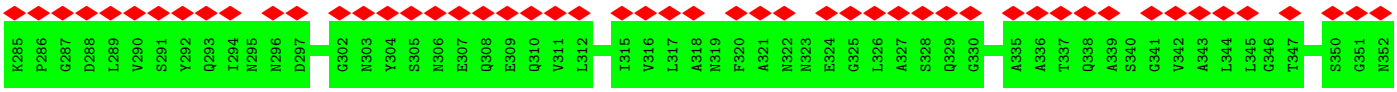


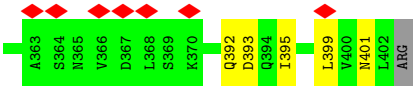






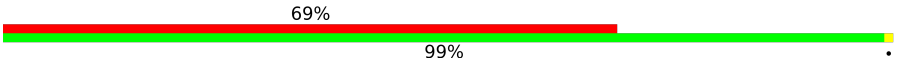


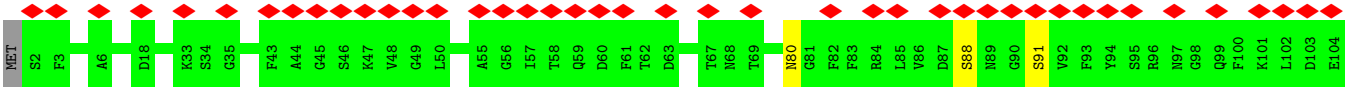


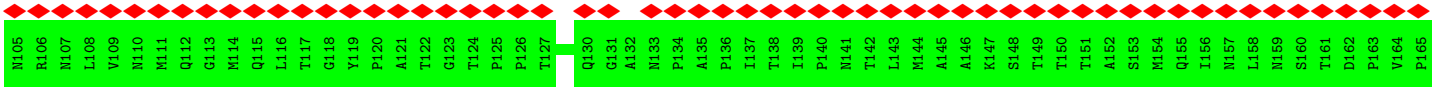


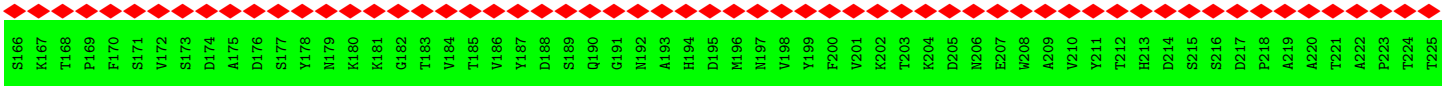
• Molecule 8: Flagellar hook protein FlgE

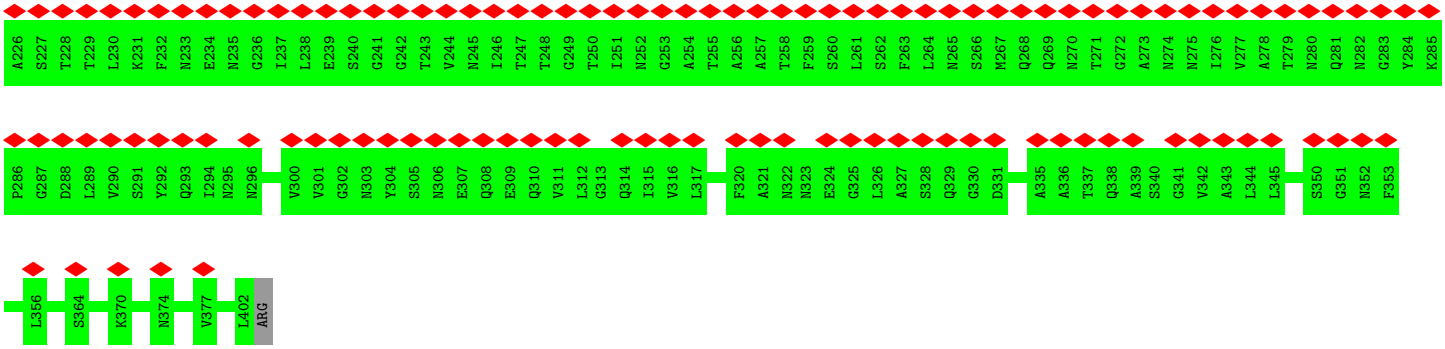
Chain DV:





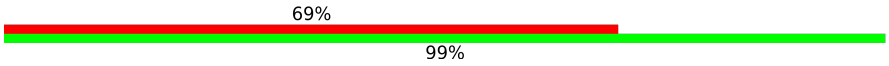


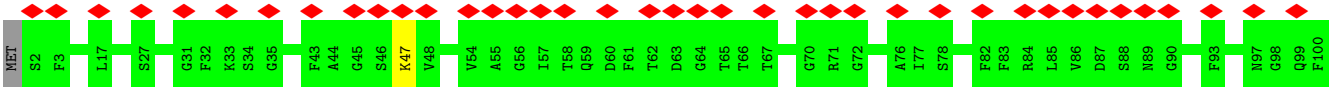




• Molecule 8: Flagellar hook protein FlgE

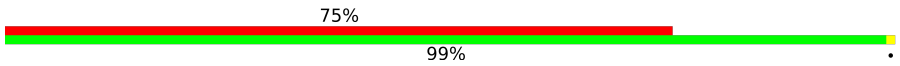
Chain DW:

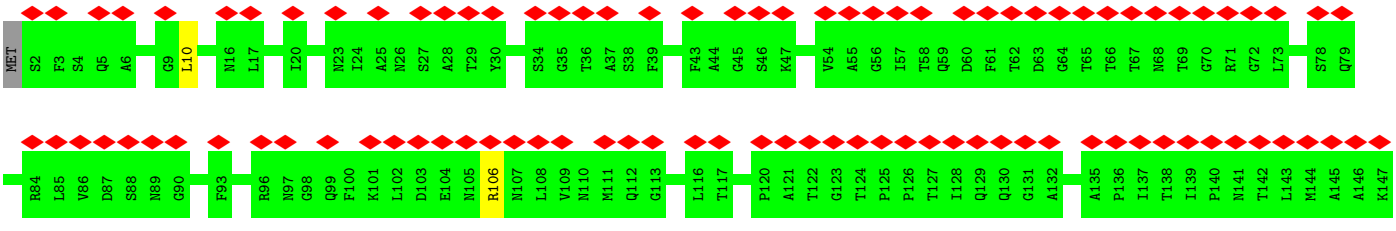


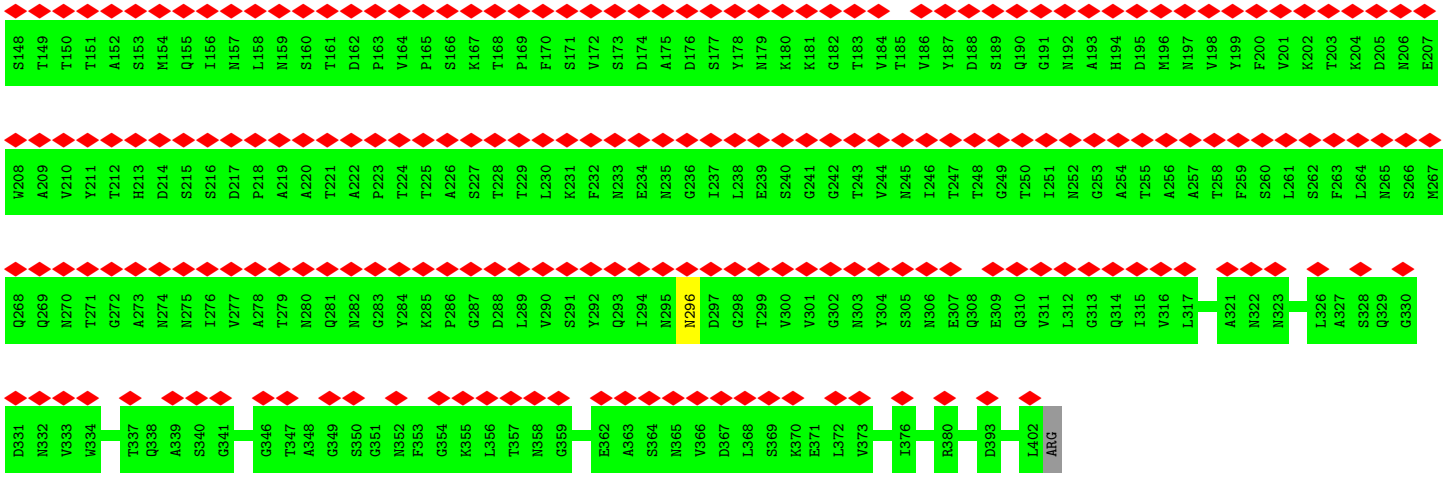


• Molecule 8: Flagellar hook protein FlgE

Chain DX:

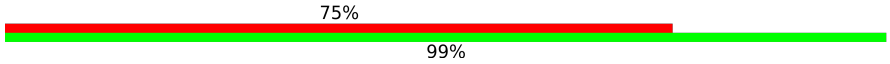


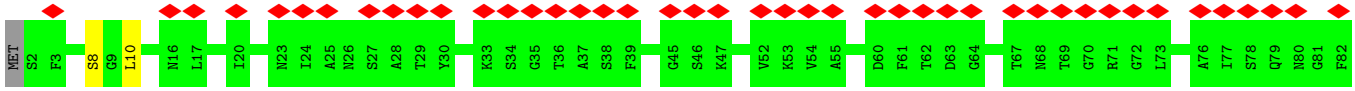




• Molecule 8: Flagellar hook protein FlgE

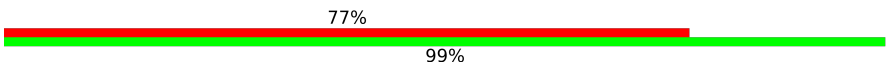
Chain DY:

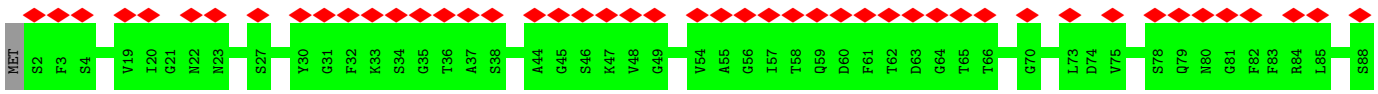


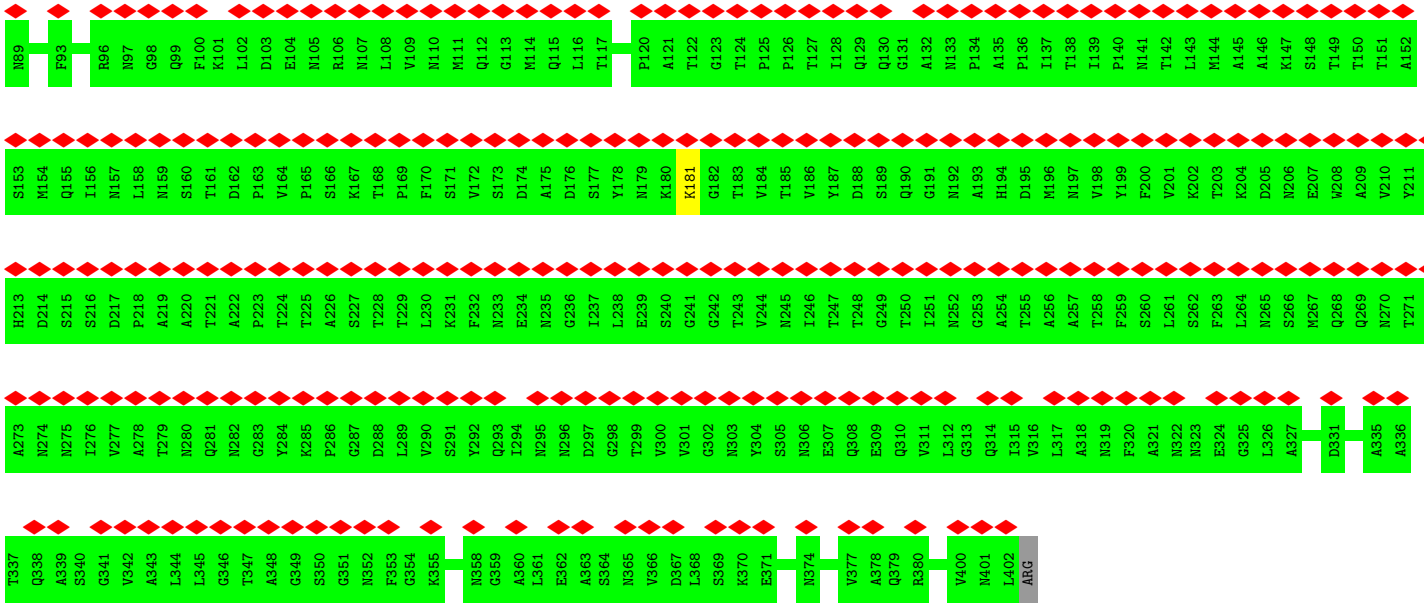


• Molecule 8: Flagellar hook protein FlgE

Chain DZ:

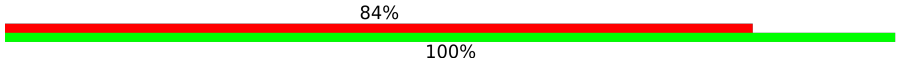


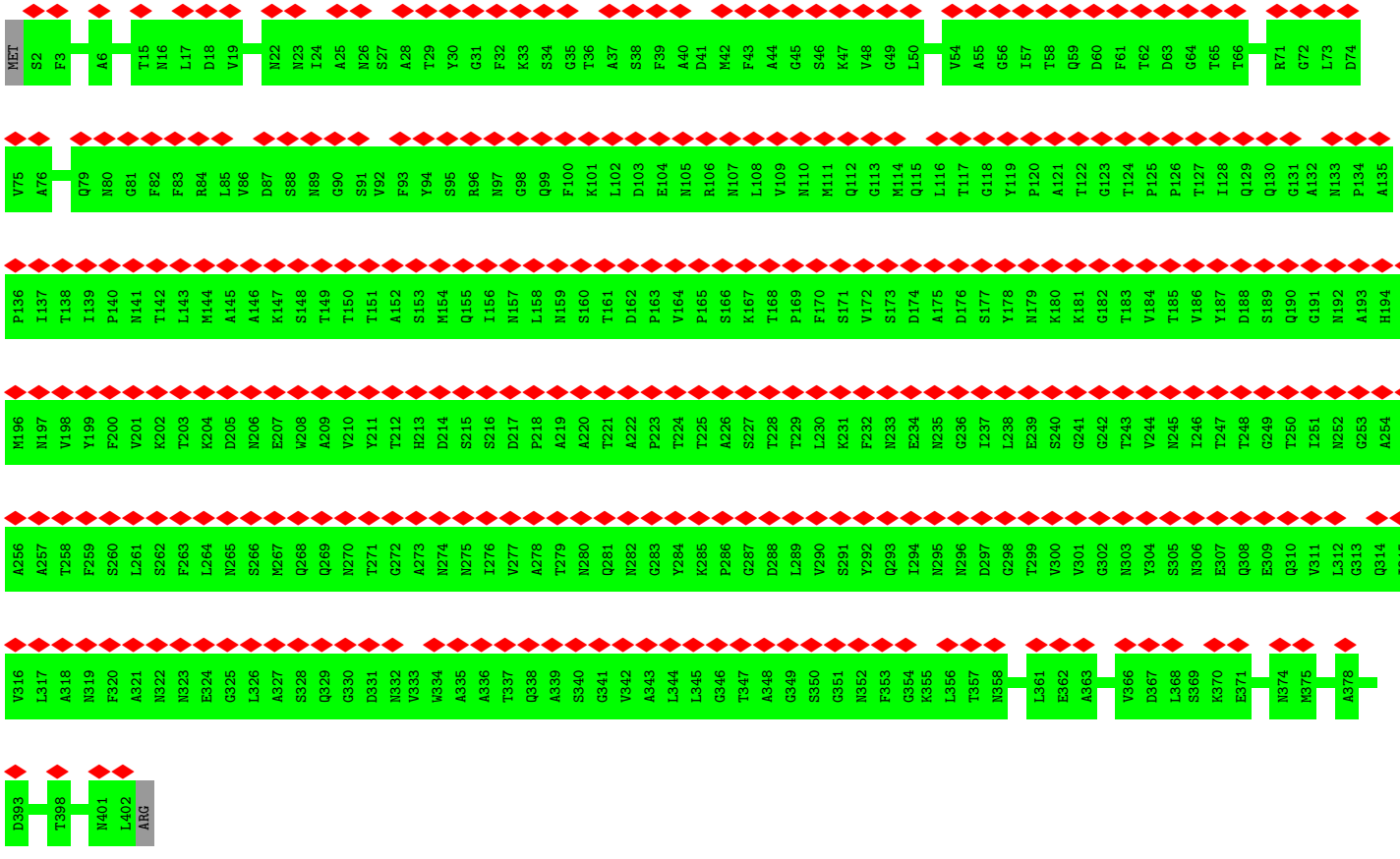




• Molecule 8: Flagellar hook protein FlgE

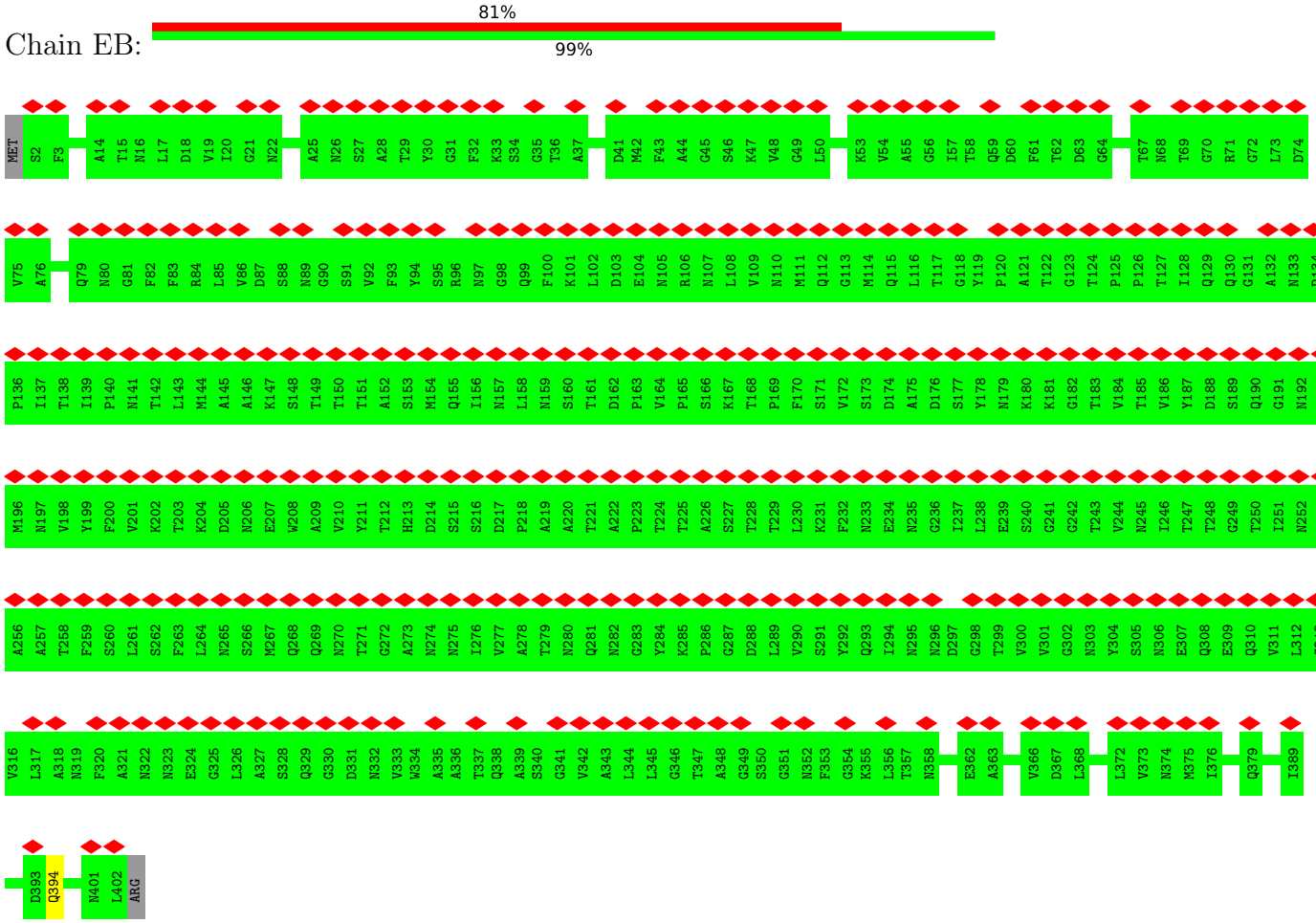
Chain EA:





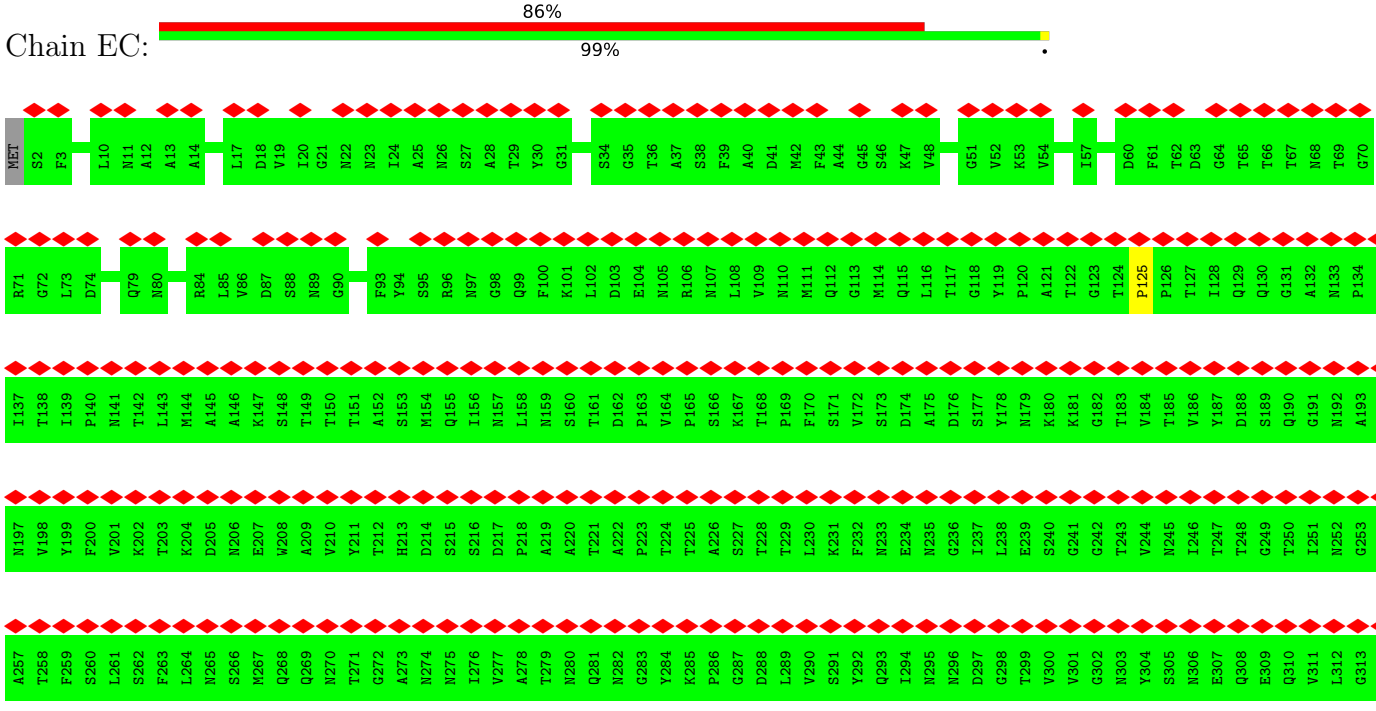
• Molecule 8: Flagellar hook protein FlgE

Chain EB:



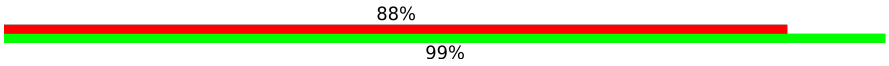
• Molecule 8: Flagellar hook protein FlgE

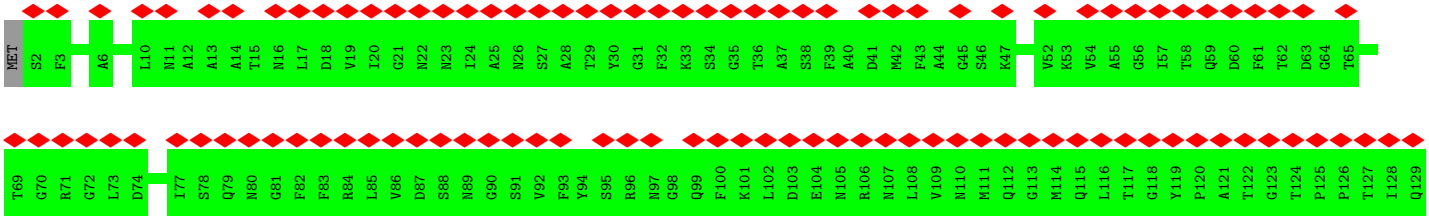
Chain EC:



• Molecule 8: Flagellar hook protein FlgE

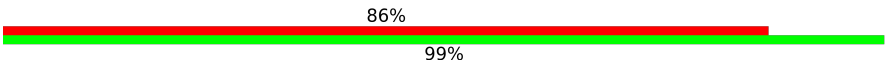
Chain ED:

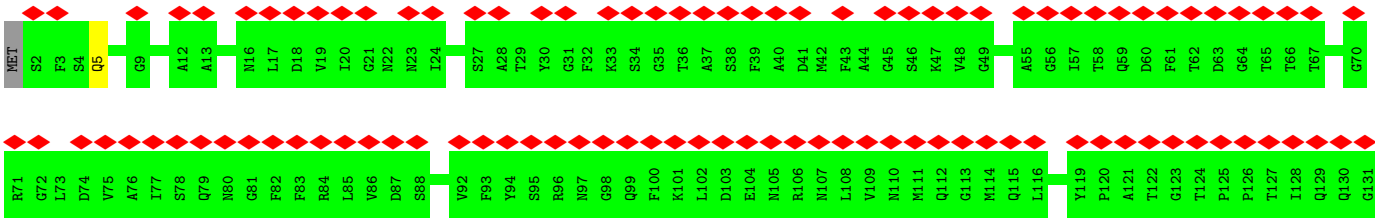


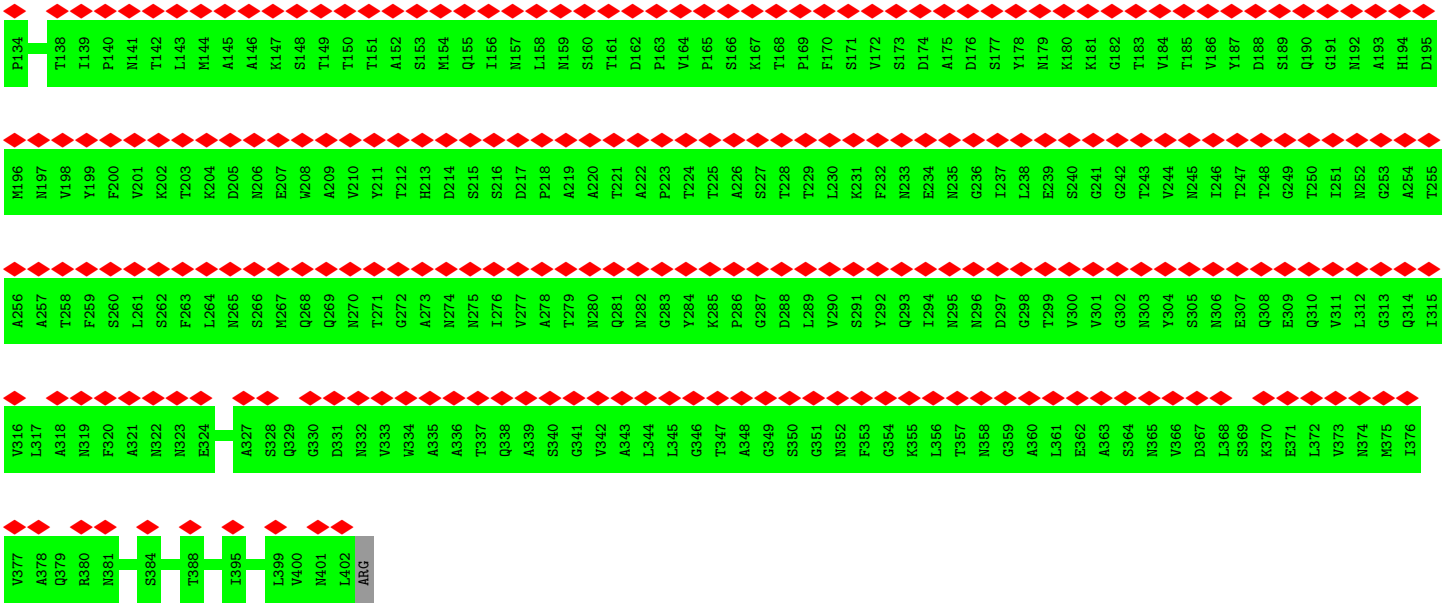


• Molecule 8: Flagellar hook protein FlgE

Chain EE:

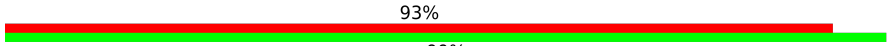


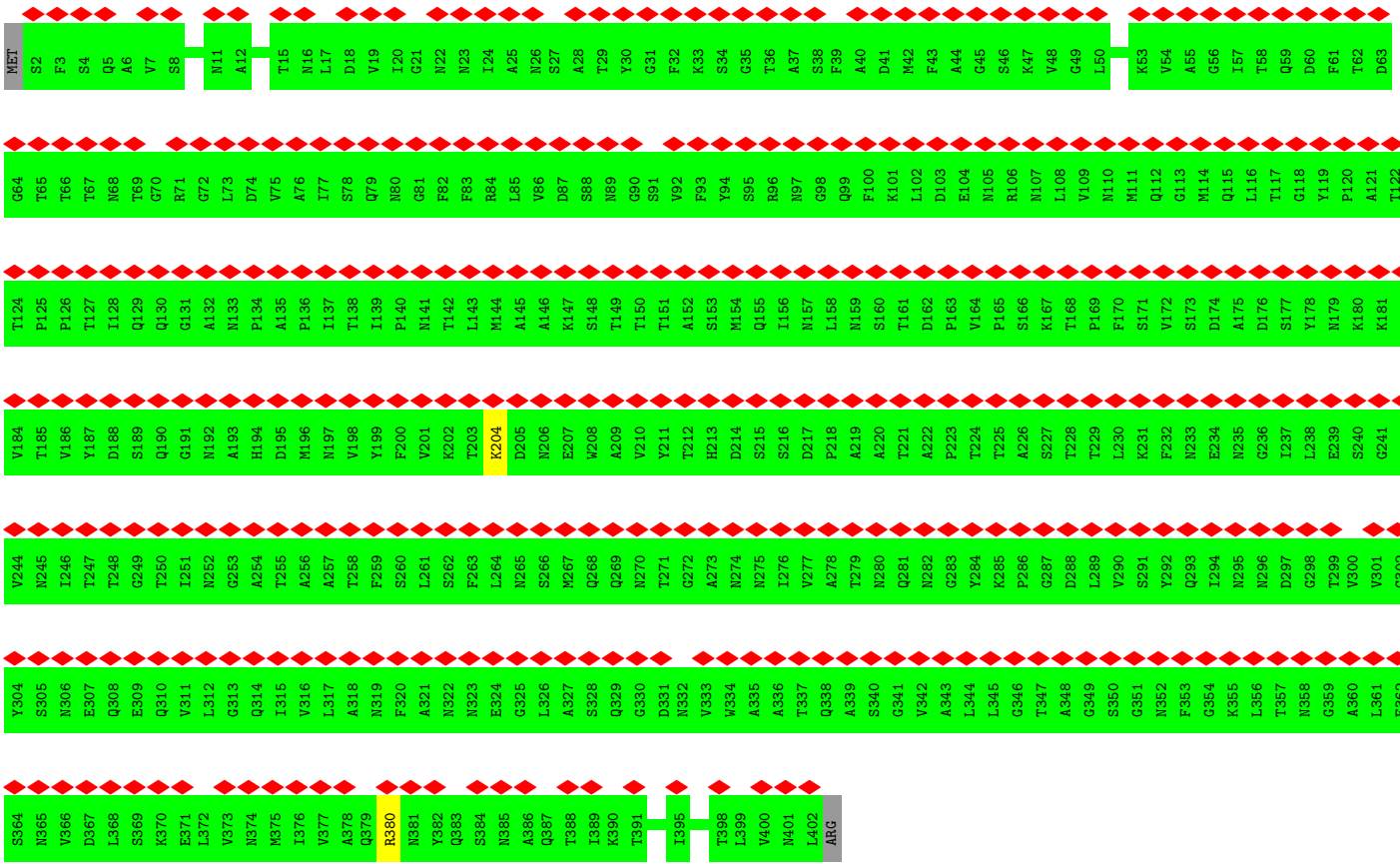




• Molecule 8: Flagellar hook protein FlgE

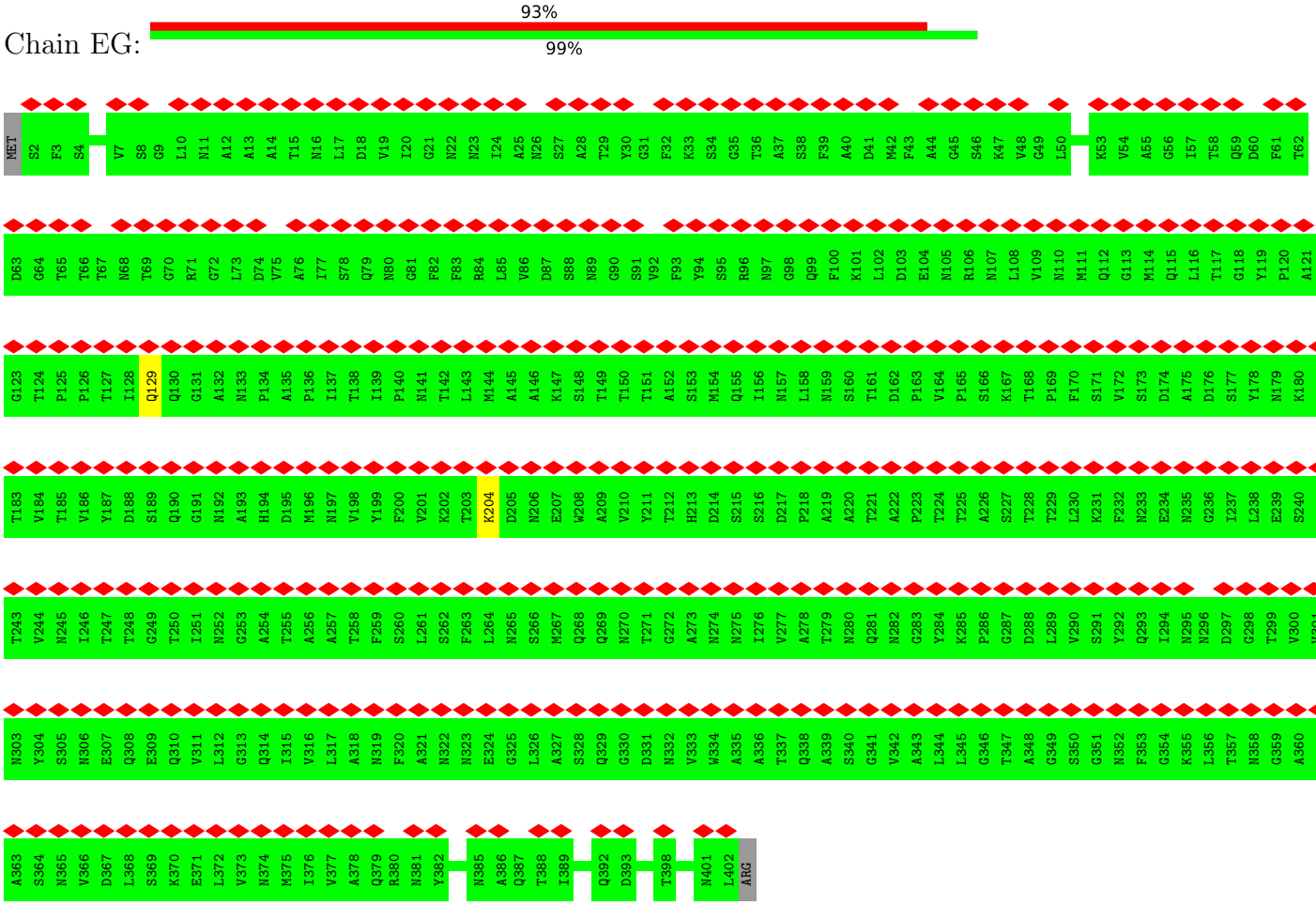
Chain EF:





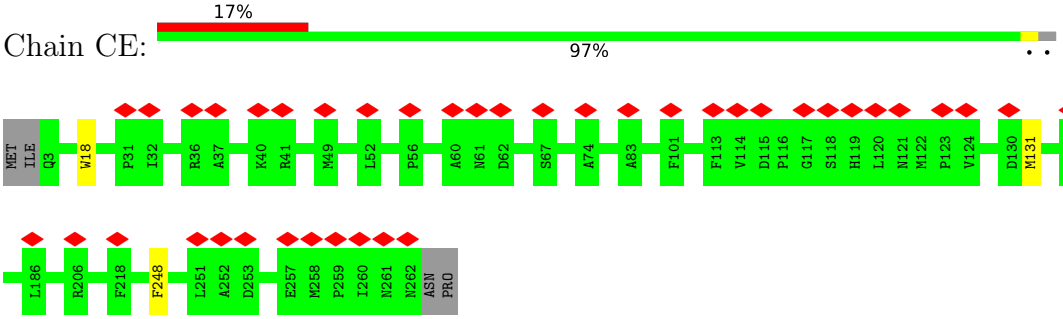
• Molecule 8: Flagellar hook protein FlgE

Chain EG:



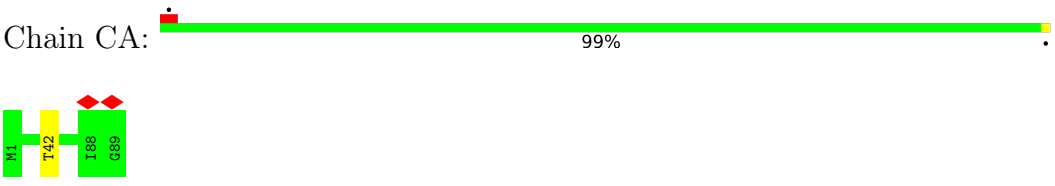
• Molecule 9: Flagellar biosynthetic protein FliR

Chain CE:



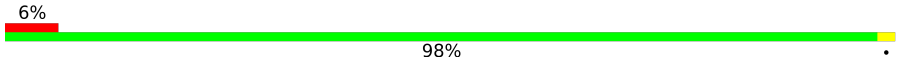
• Molecule 10: Flagellar biosynthetic protein FliQ

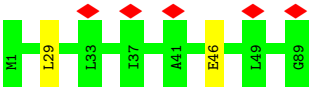
Chain CA:



• Molecule 10: Flagellar biosynthetic protein FliQ

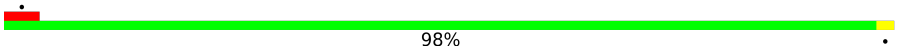
Chain CB:

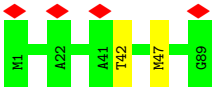




• Molecule 10: Flagellar biosynthetic protein FliQ

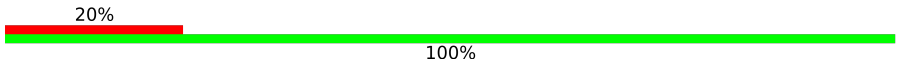
Chain CC:

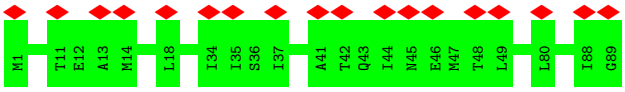




• Molecule 10: Flagellar biosynthetic protein FliQ

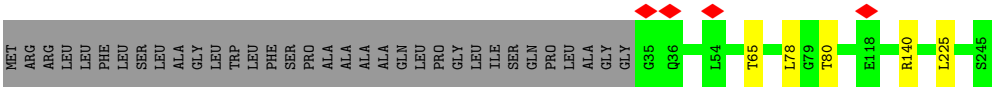
Chain CD:





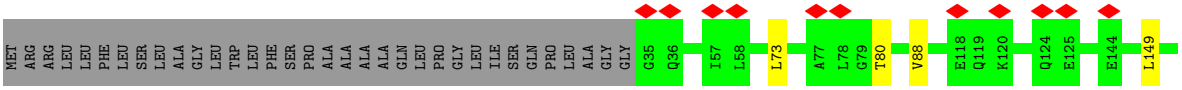
• Molecule 11: Flagellar biosynthetic protein FliP

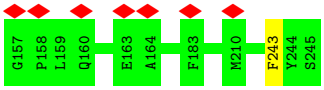
Chain w:



• Molecule 11: Flagellar biosynthetic protein FliP

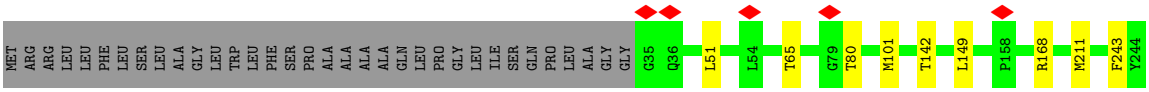
Chain x:





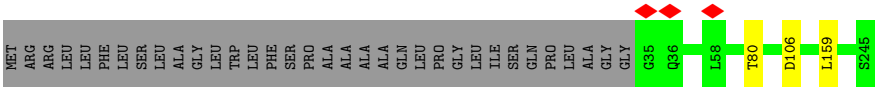
• Molecule 11: Flagellar biosynthetic protein FliP

Chain y:



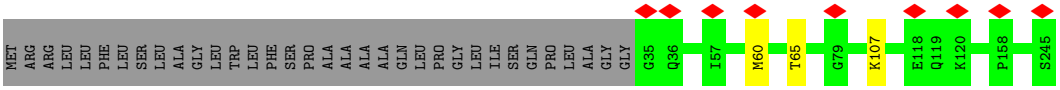
• Molecule 11: Flagellar biosynthetic protein FliP

Chain z:



• Molecule 11: Flagellar biosynthetic protein FliP

Chain CF:

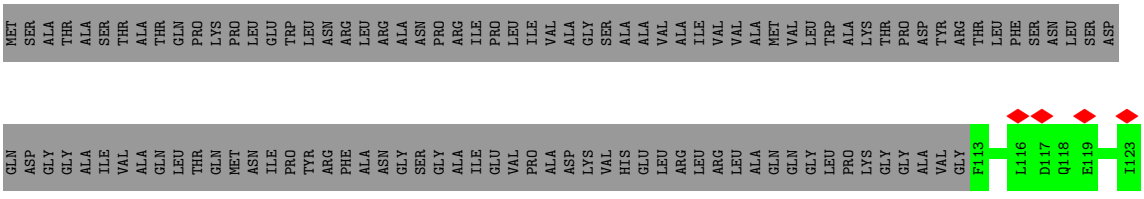


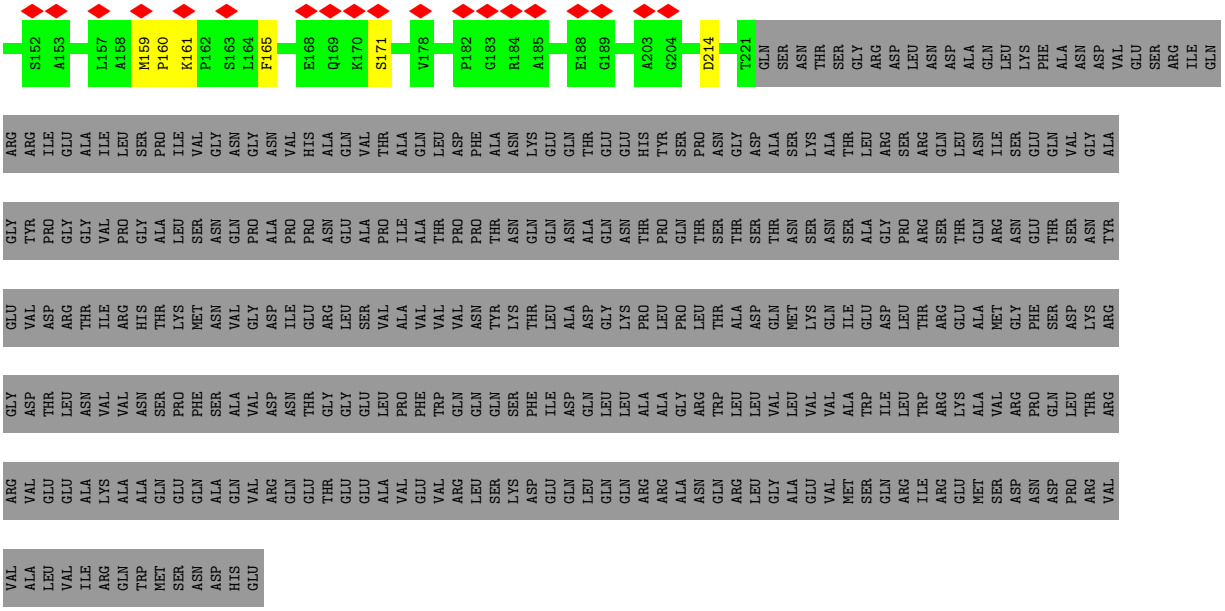
• Molecule 12: Flagellar M-ring protein

Chain Da:

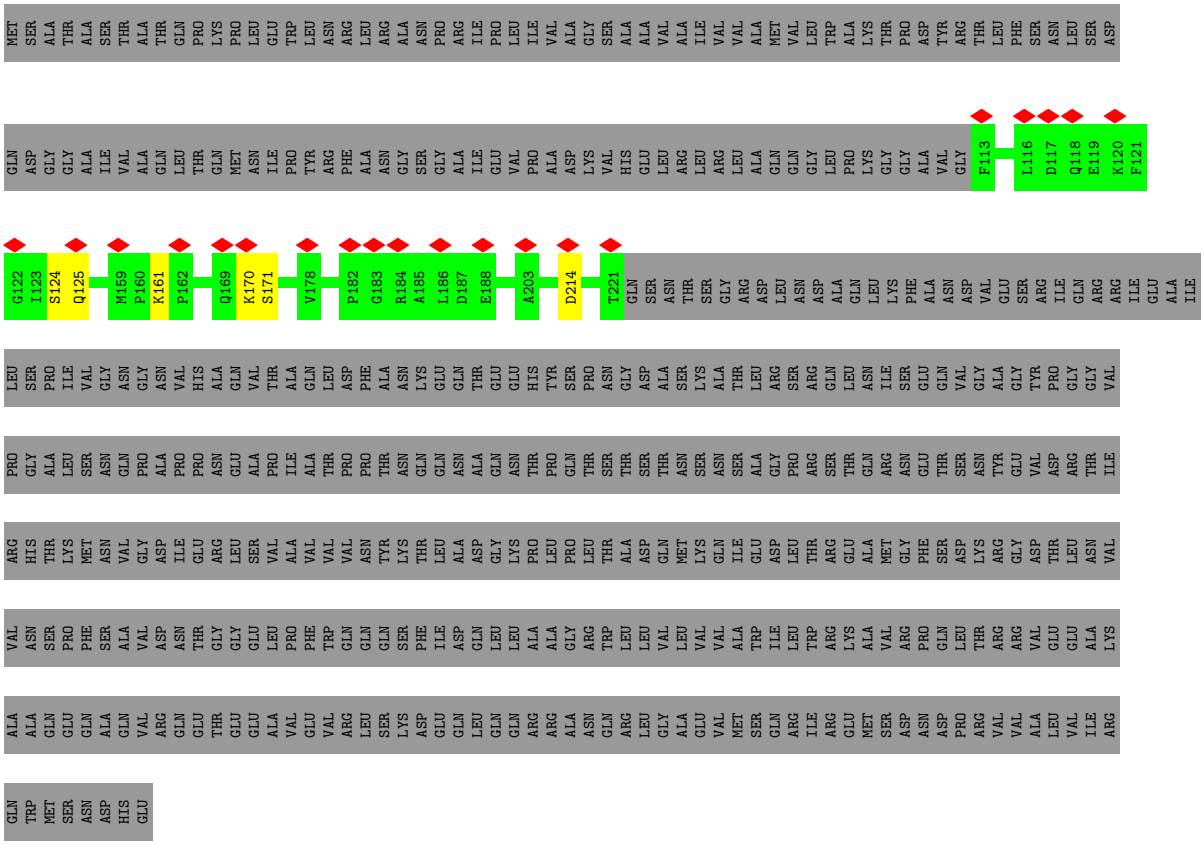
• Molecule 12: Flagellar M-ring protein

Chain Db:

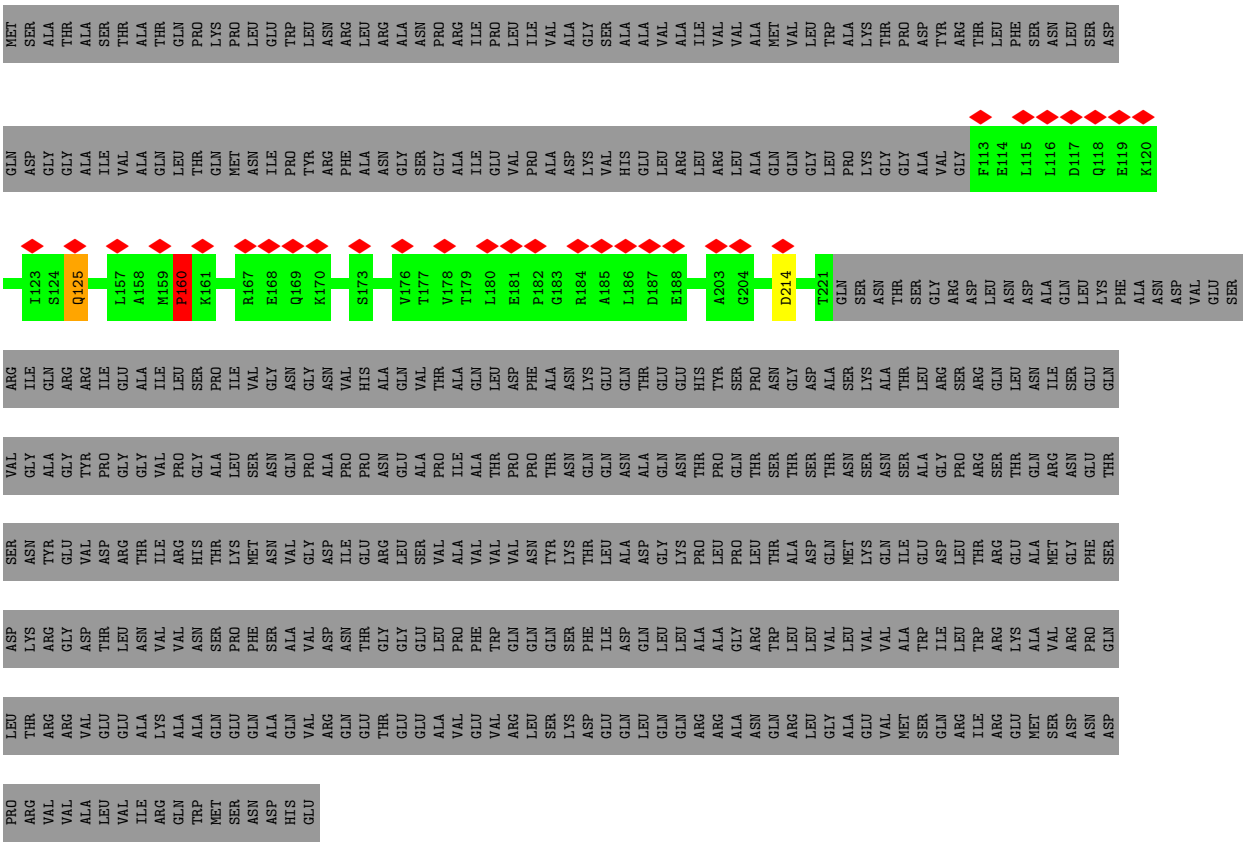




• Molecule 12: Flagellar M-ring protein



• Molecule 12: Flagellar M-ring protein



• Molecule 12: Flagellar M-ring protein

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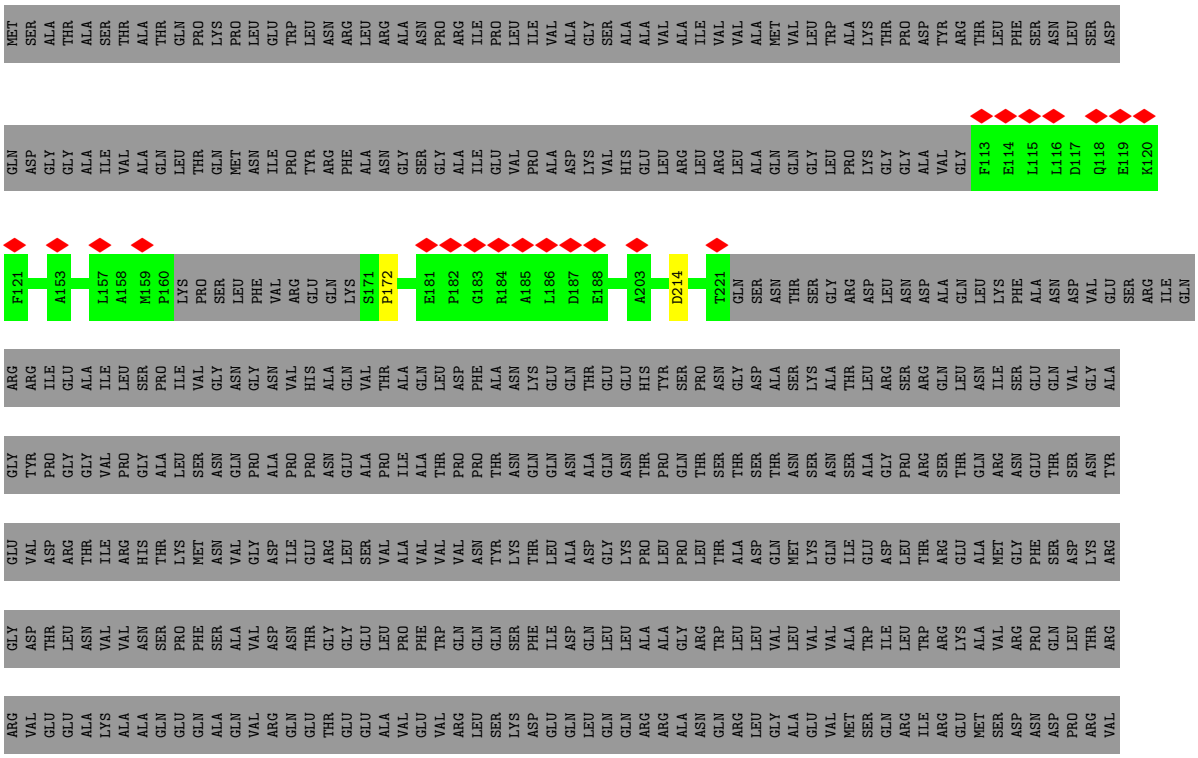

• Molecule 12: Flagellar M-ring protein

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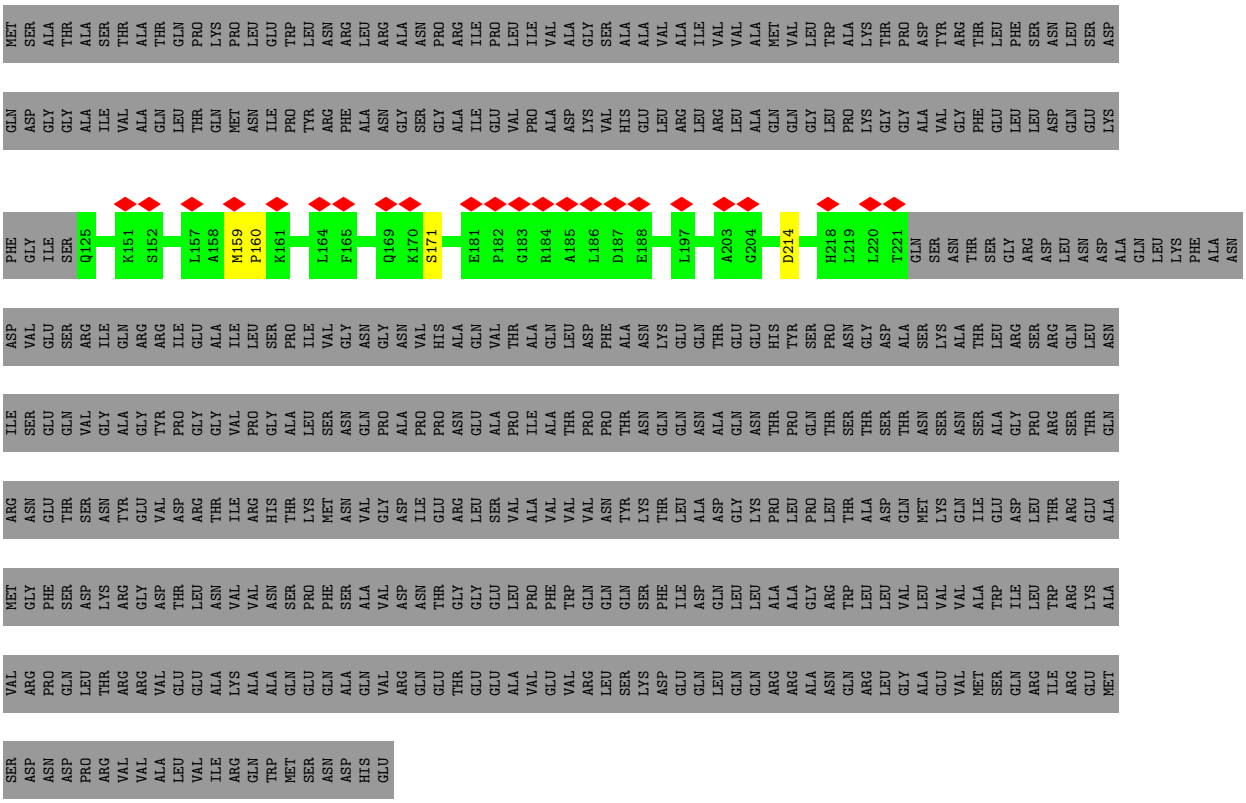

• Molecule 12: Flagellar M-ring protein

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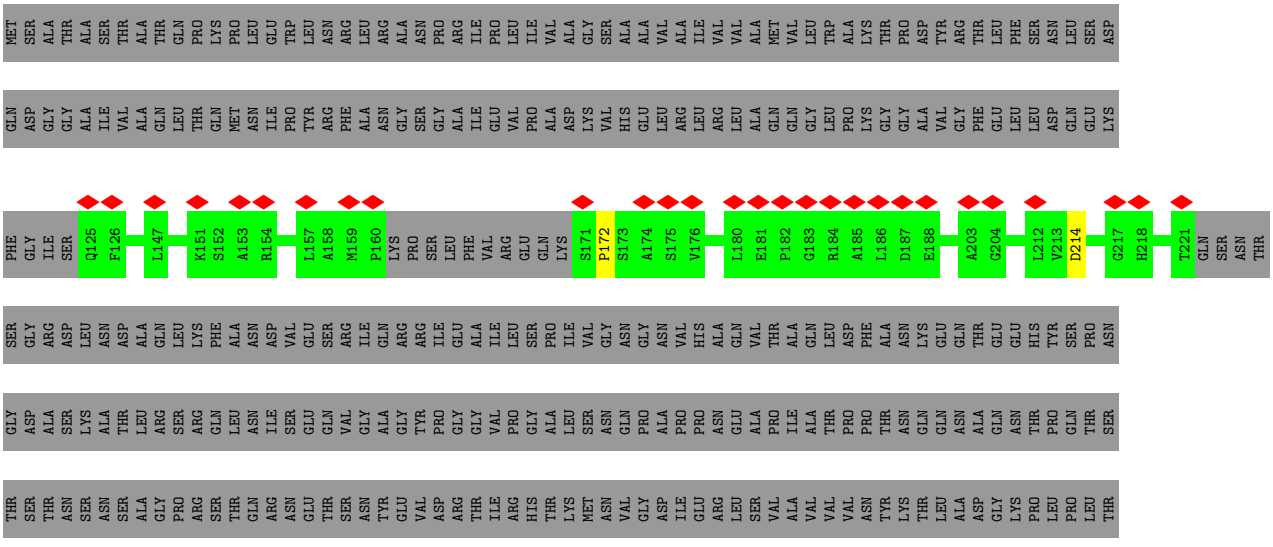

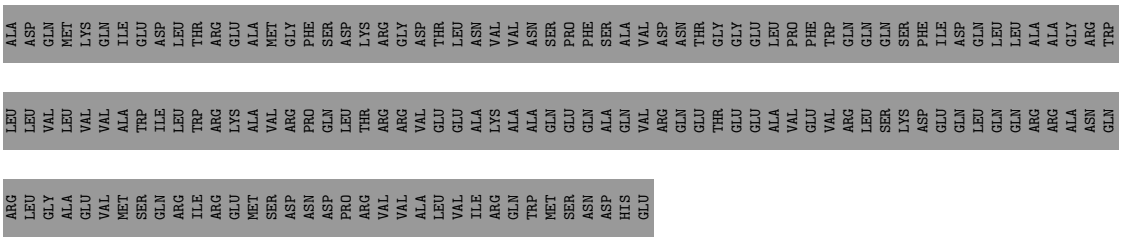

• Molecule 12: Flagellar M-ring protein

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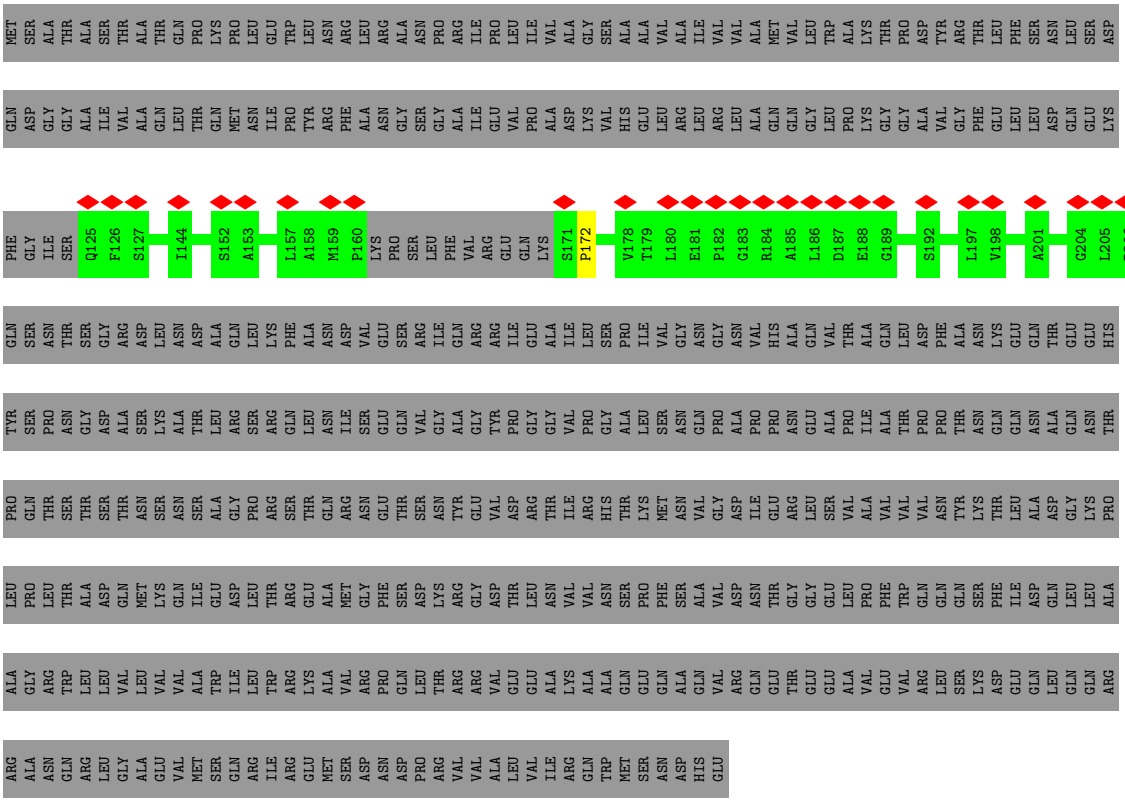

• Molecule 12: Flagellar M-ring protein

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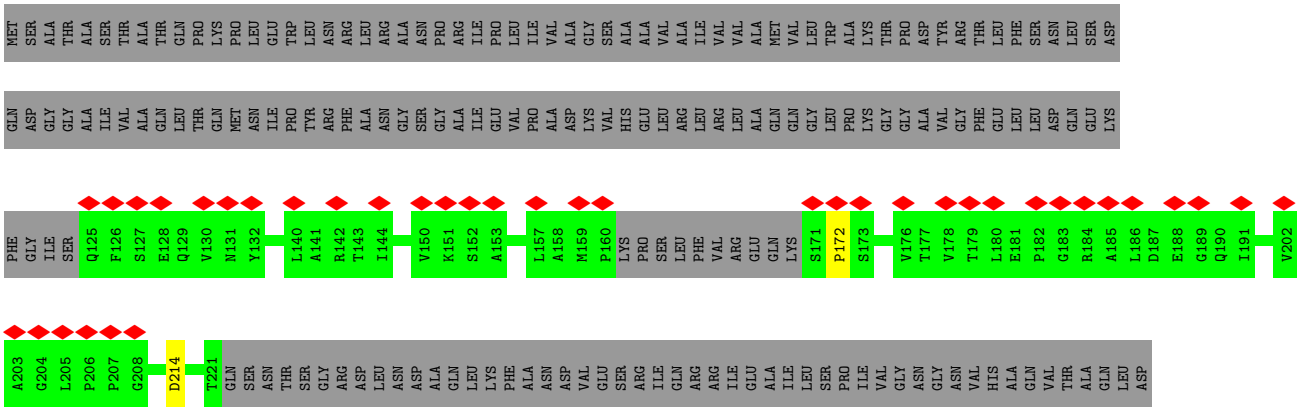

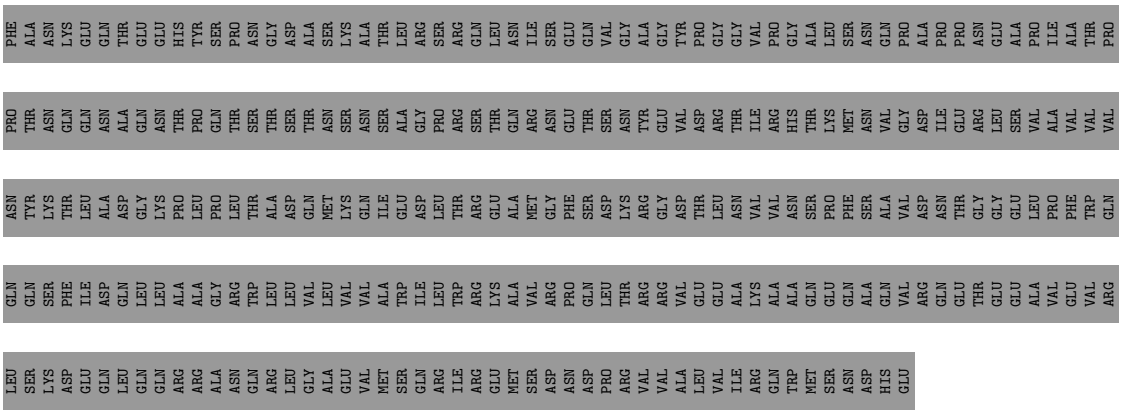

• Molecule 12: Flagellar M-ring protein

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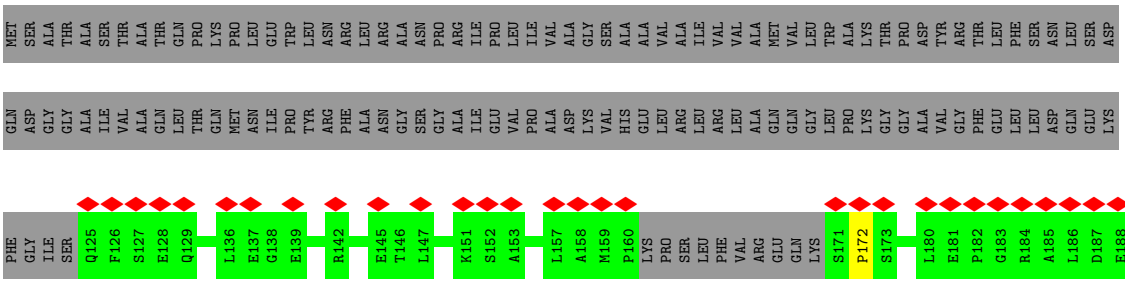

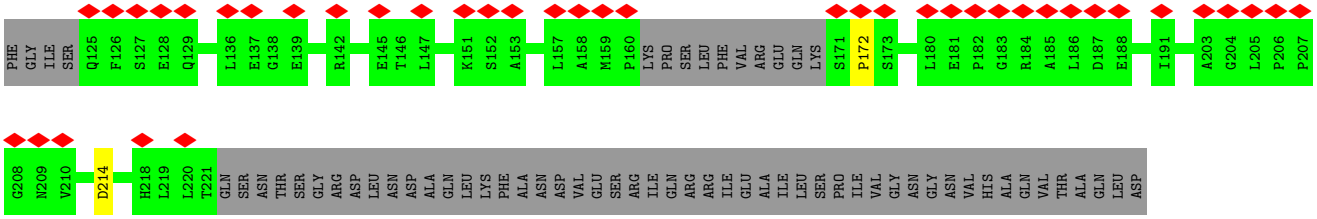

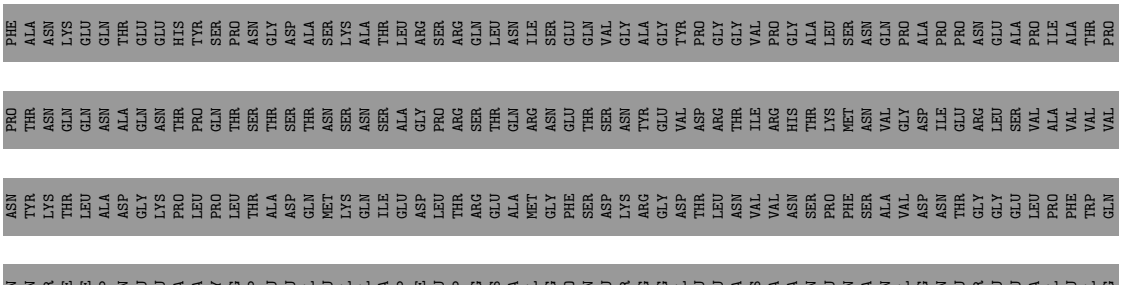

• Molecule 12: Flagellar M-ring protein

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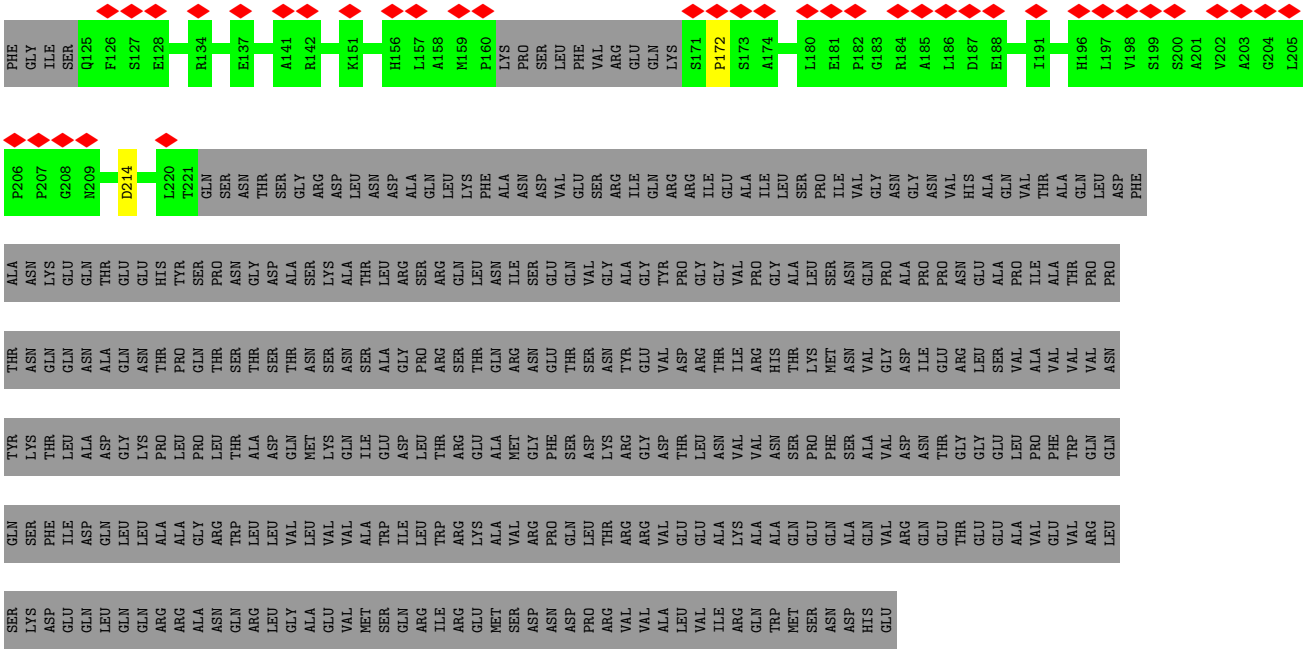

• Molecule 12: Flagellar M-ring protein

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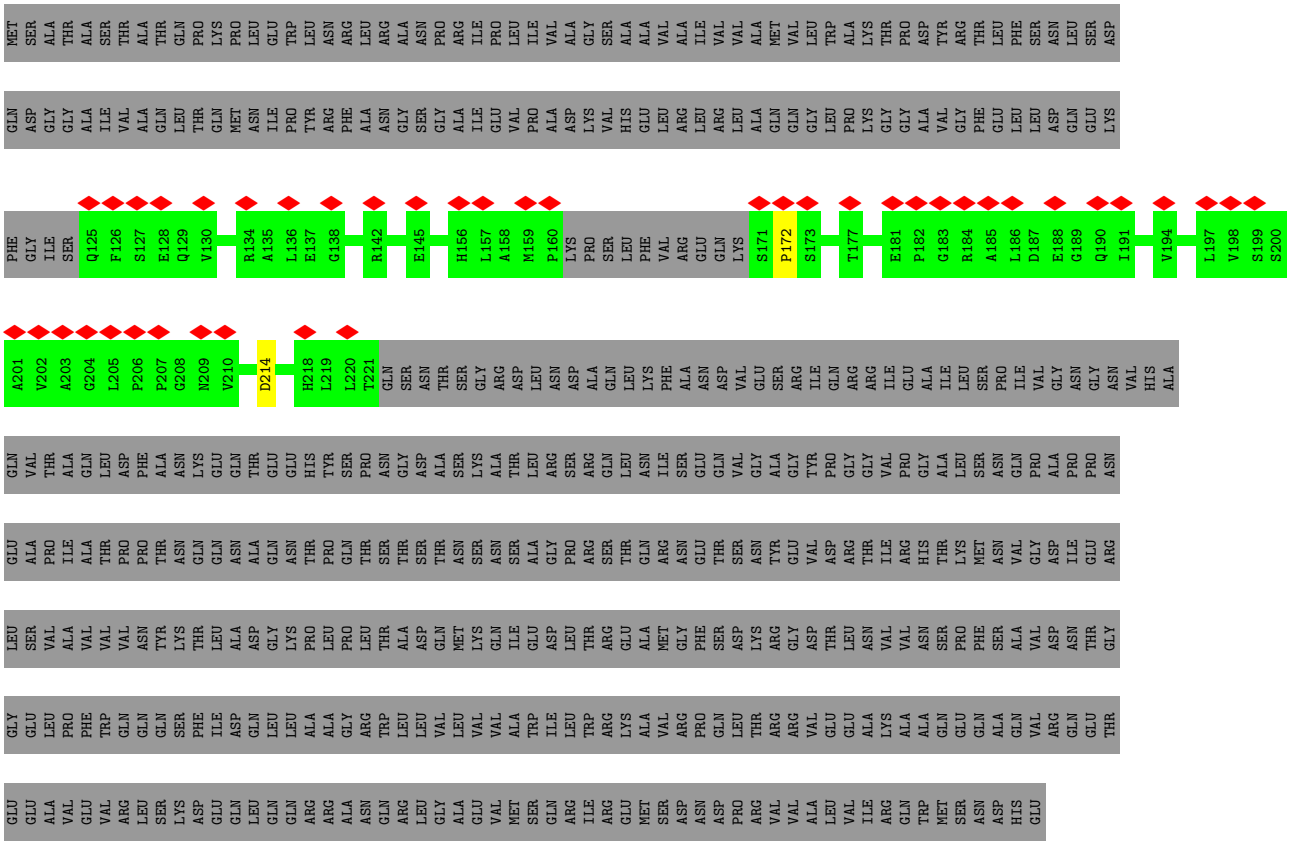

• Molecule 12: Flagellar M-ring protein

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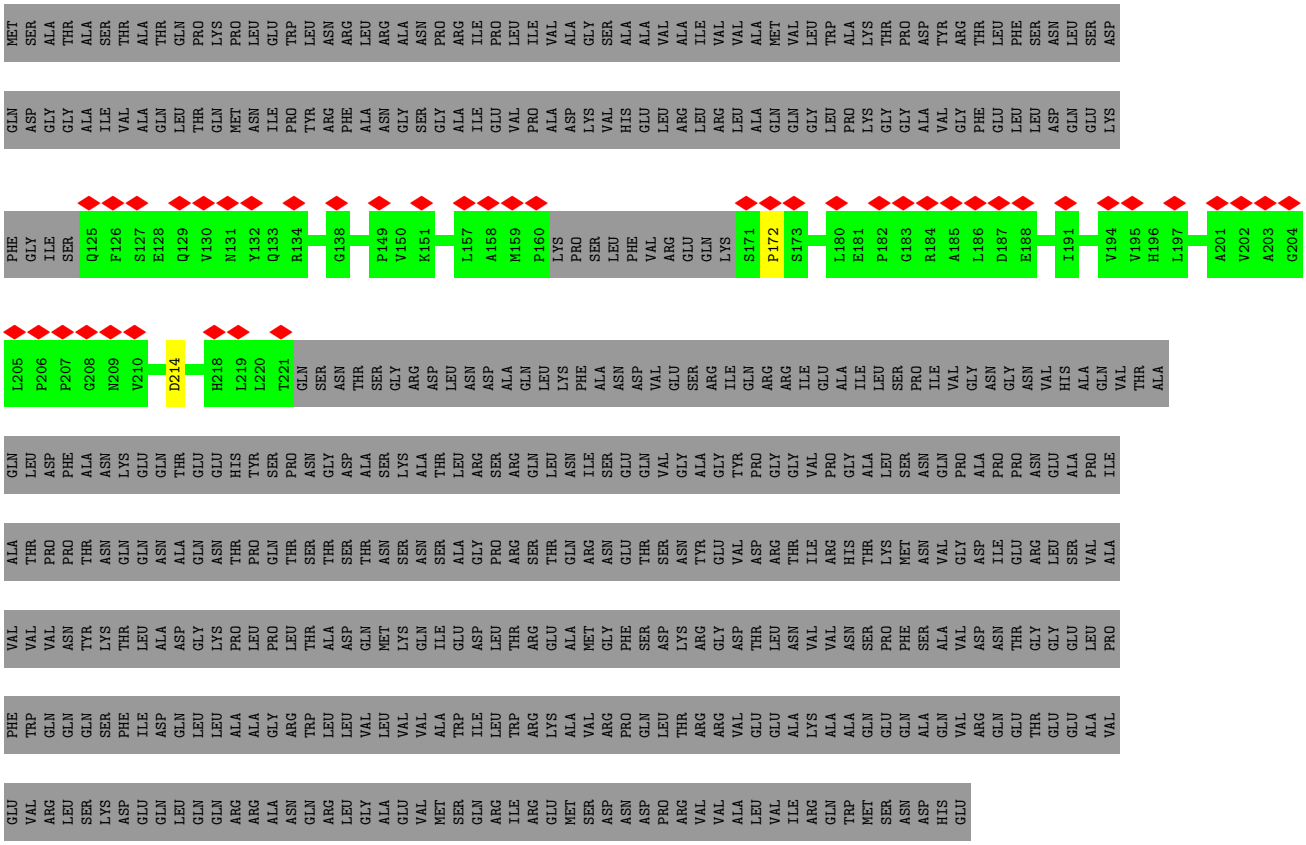

• Molecule 12: Flagellar M-ring protein

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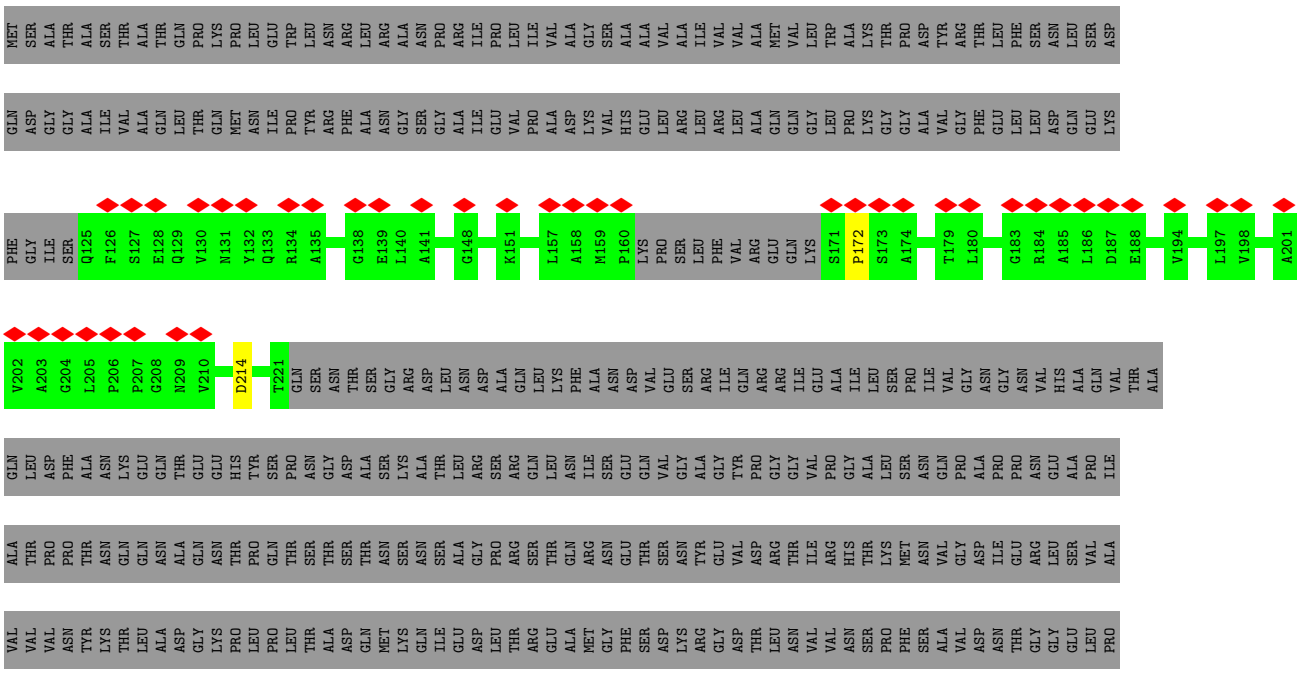

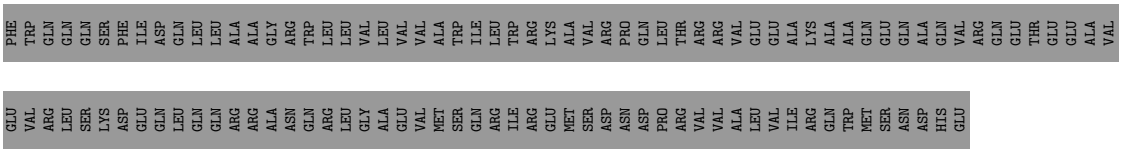

• Molecule 12: Flagellar M-ring protein

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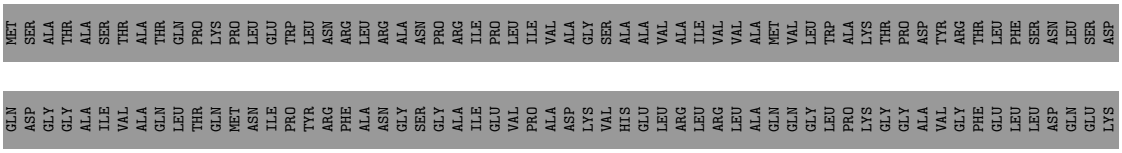

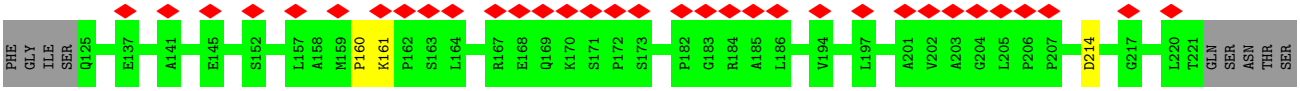

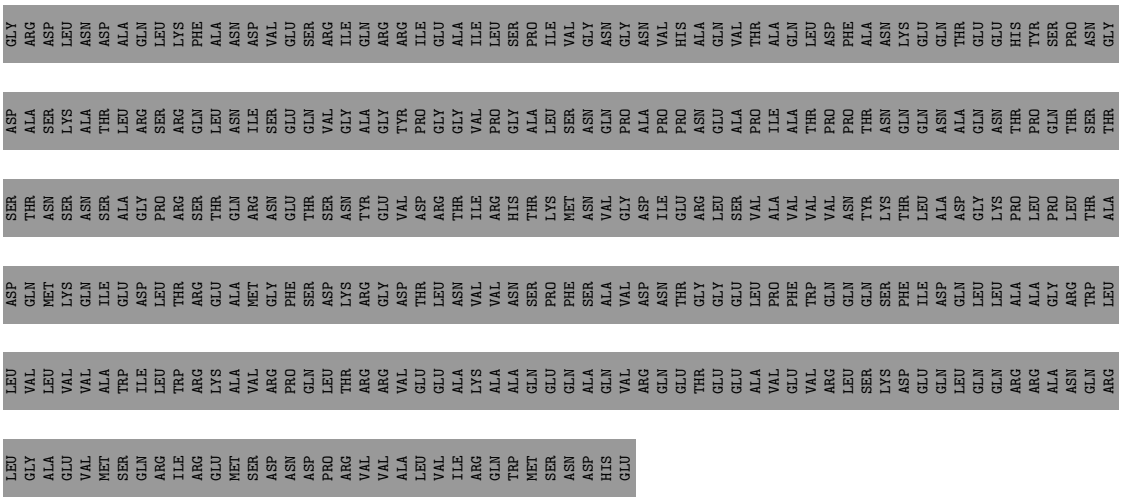

• Molecule 12: Flagellar M-ring protein

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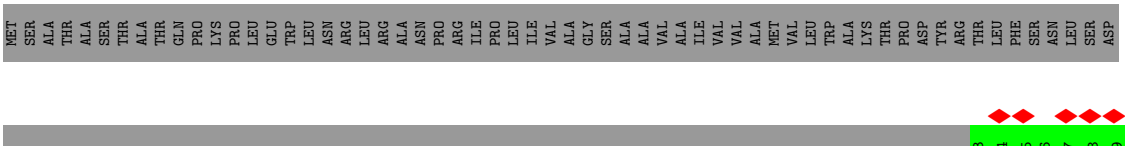

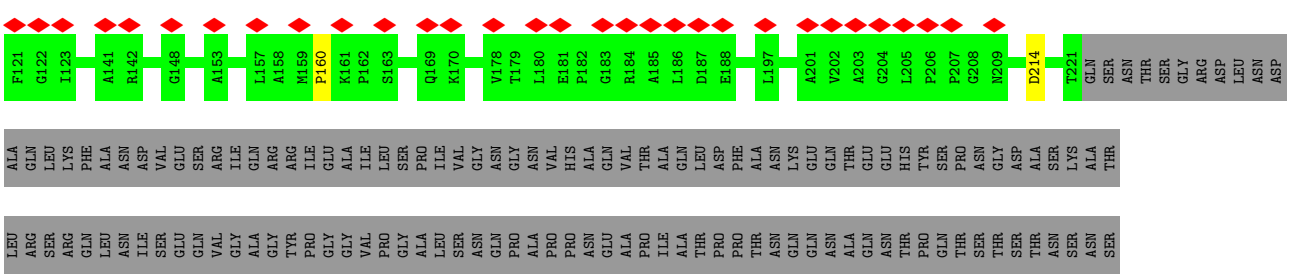

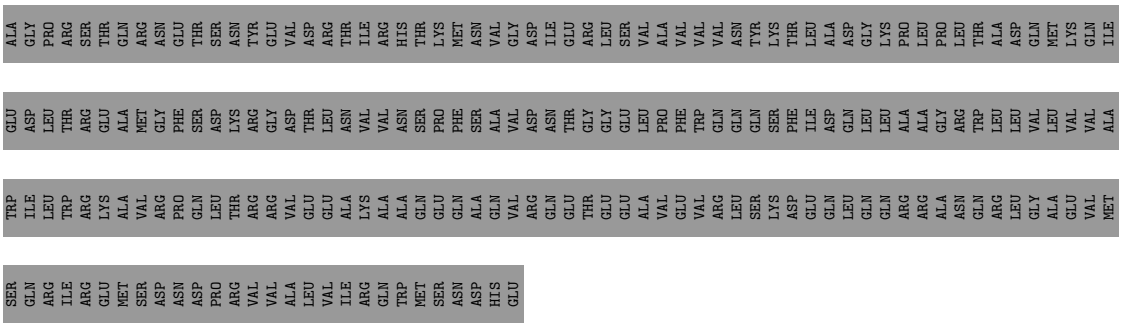

• Molecule 12: Flagellar M-ring protein

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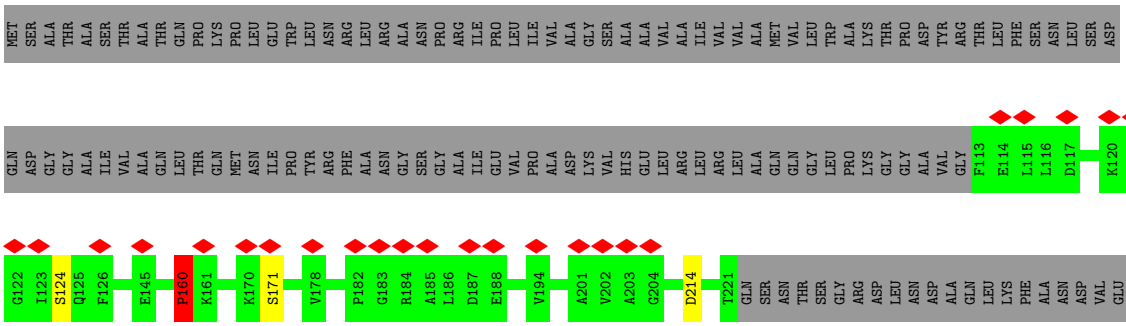

• Molecule 12: Flagellar M-ring protein

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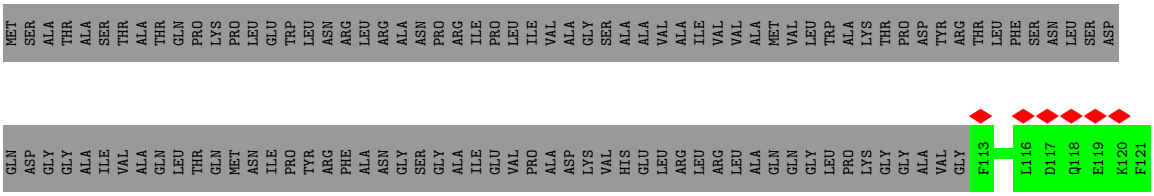

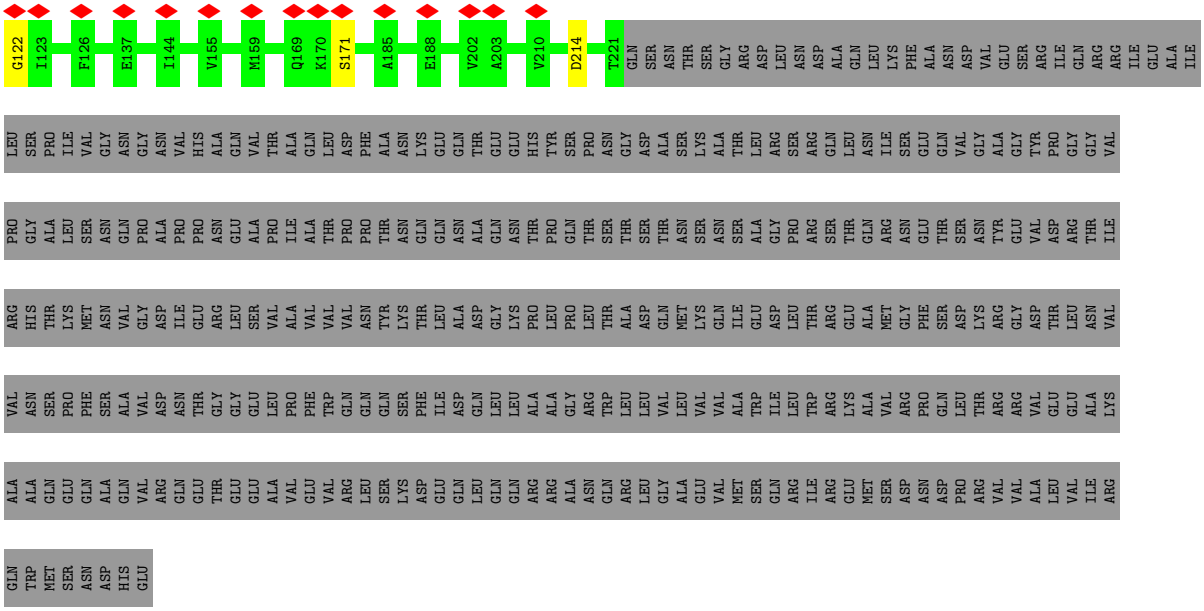

• Molecule 12: Flagellar M-ring protein

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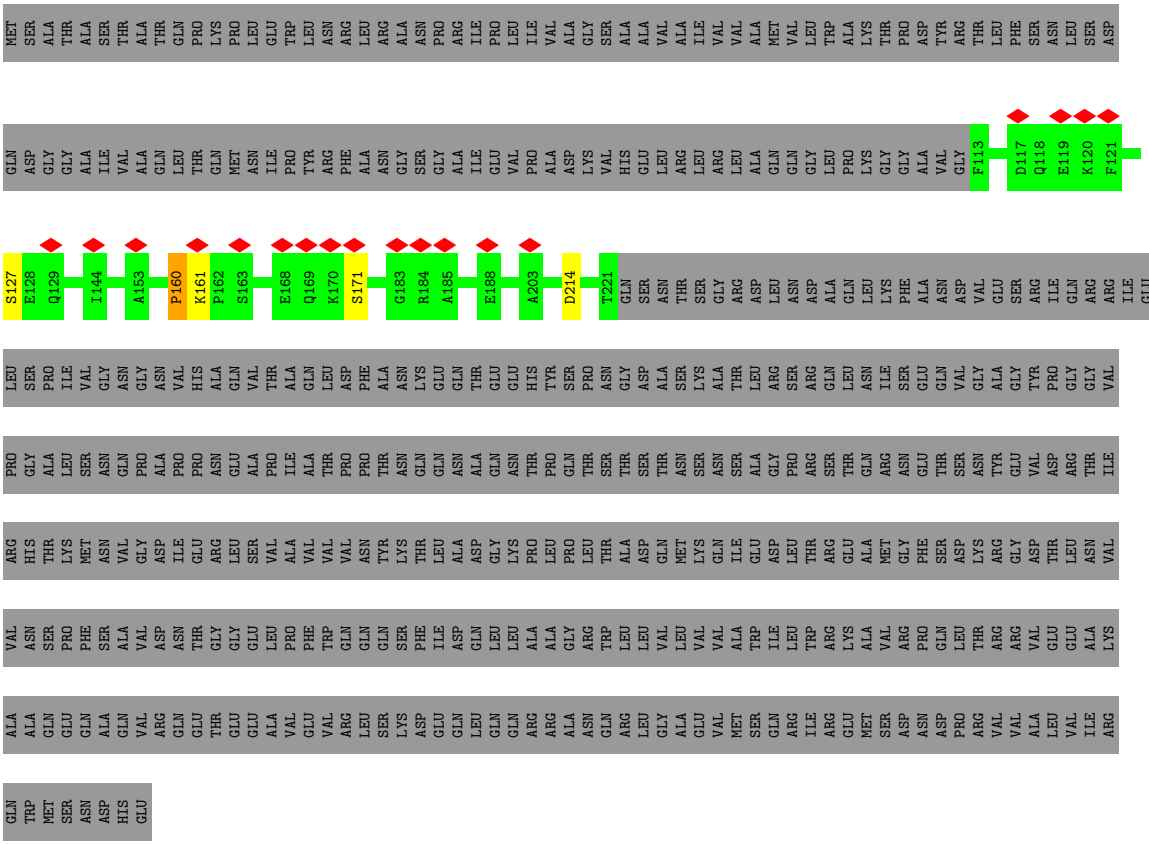

• Molecule 12: Flagellar M-ring protein

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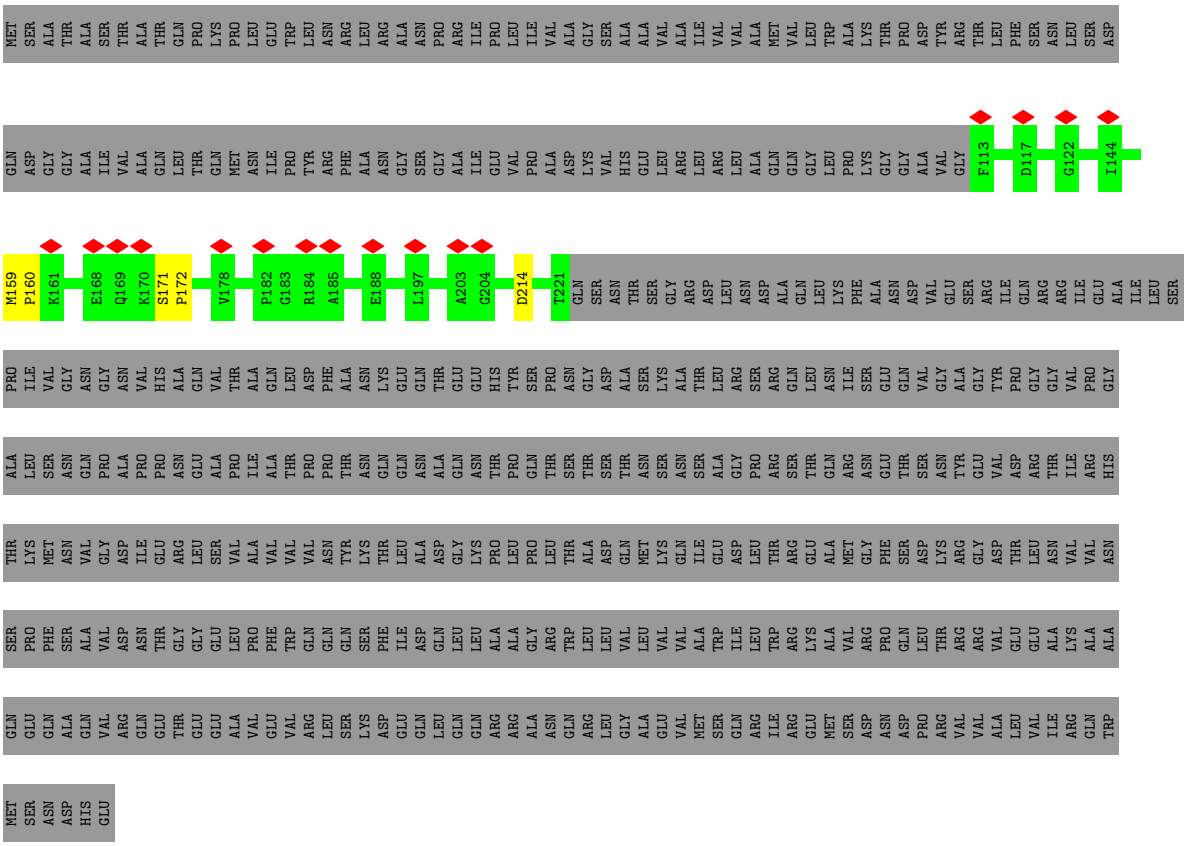

• Molecule 12: Flagellar M-ring protein

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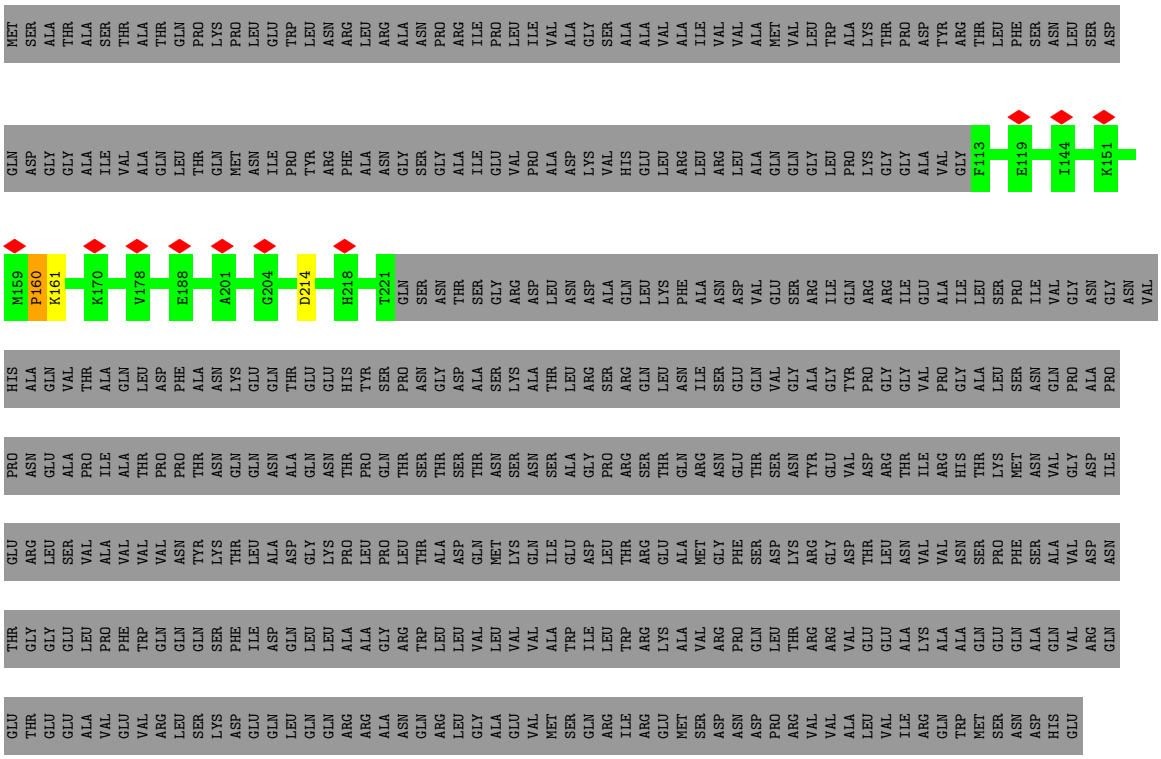

• Molecule 12: Flagellar M-ring protein

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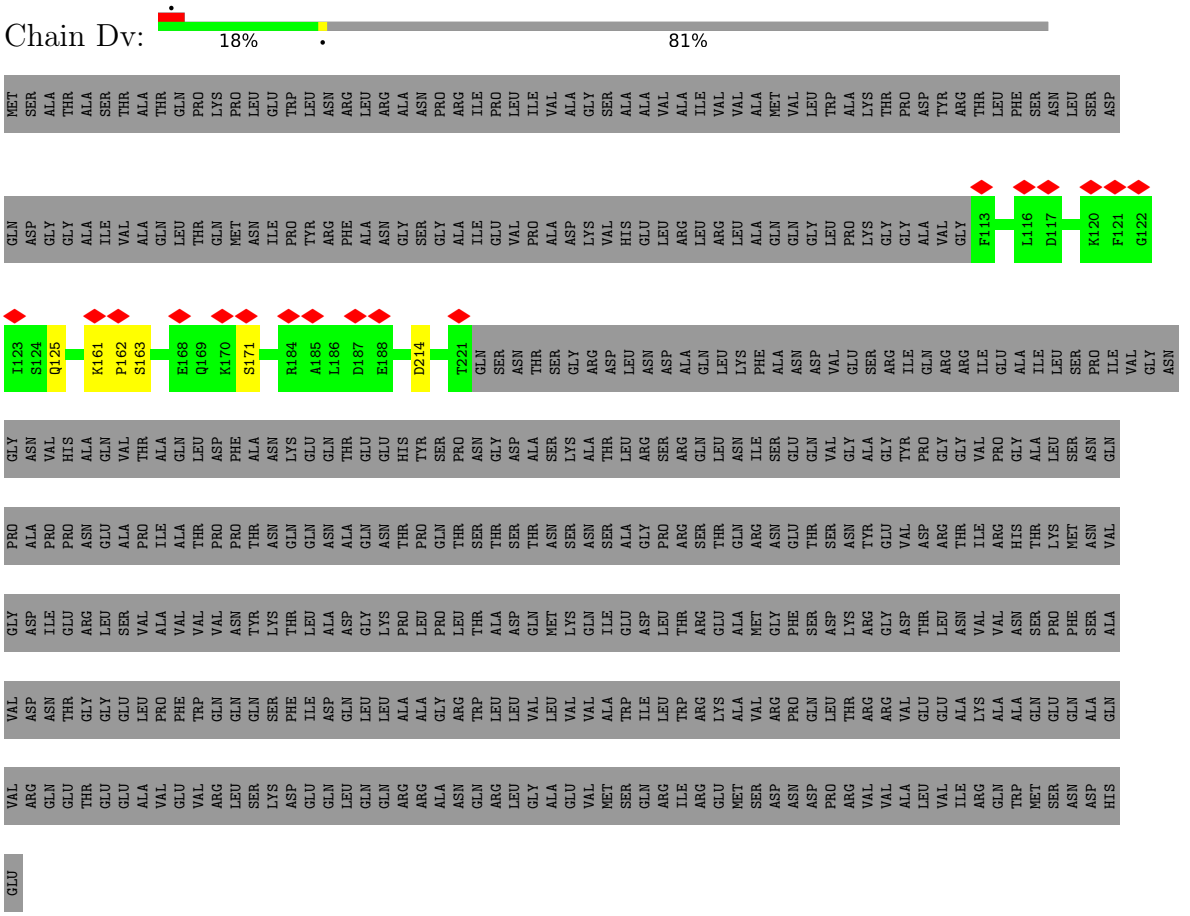

• Molecule 12: Flagellar M-ring protein

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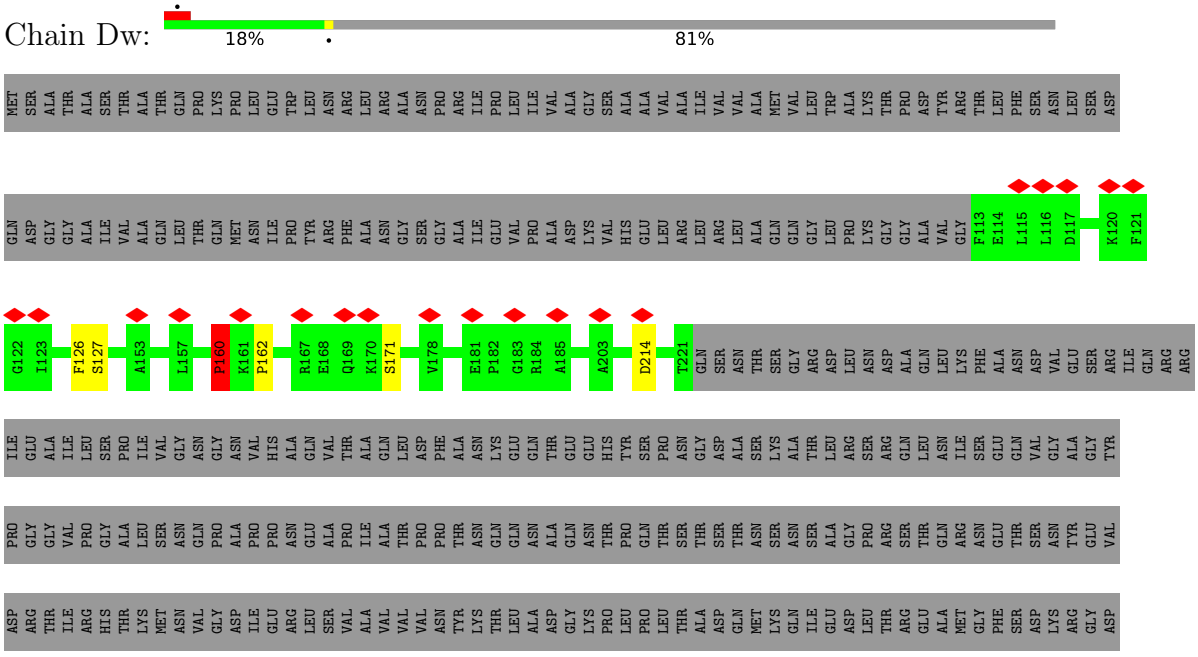

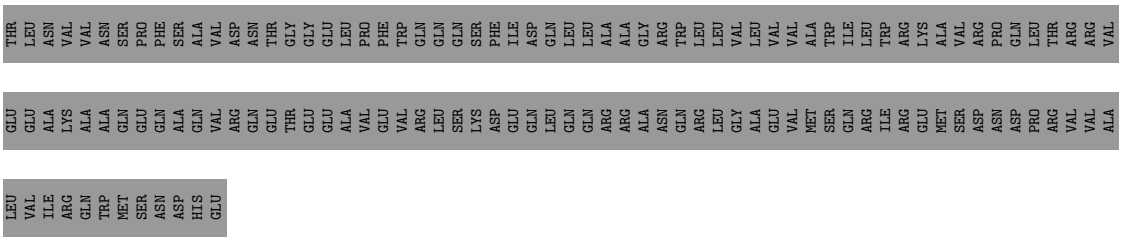

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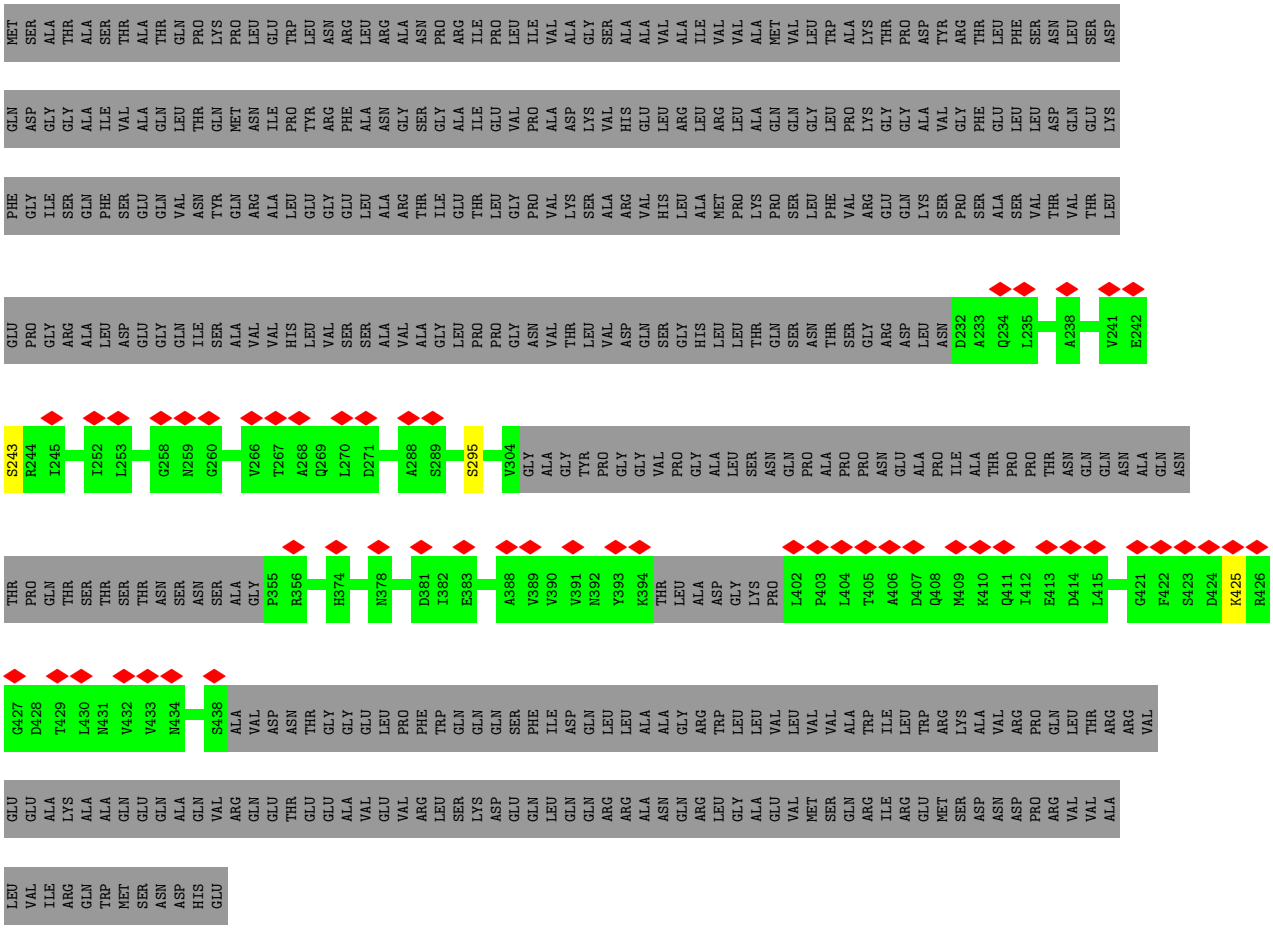
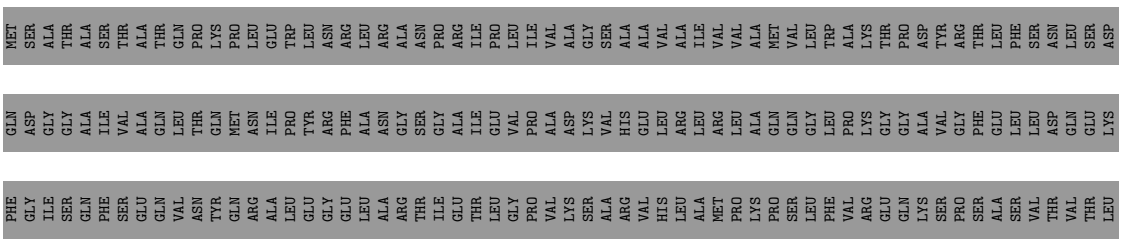
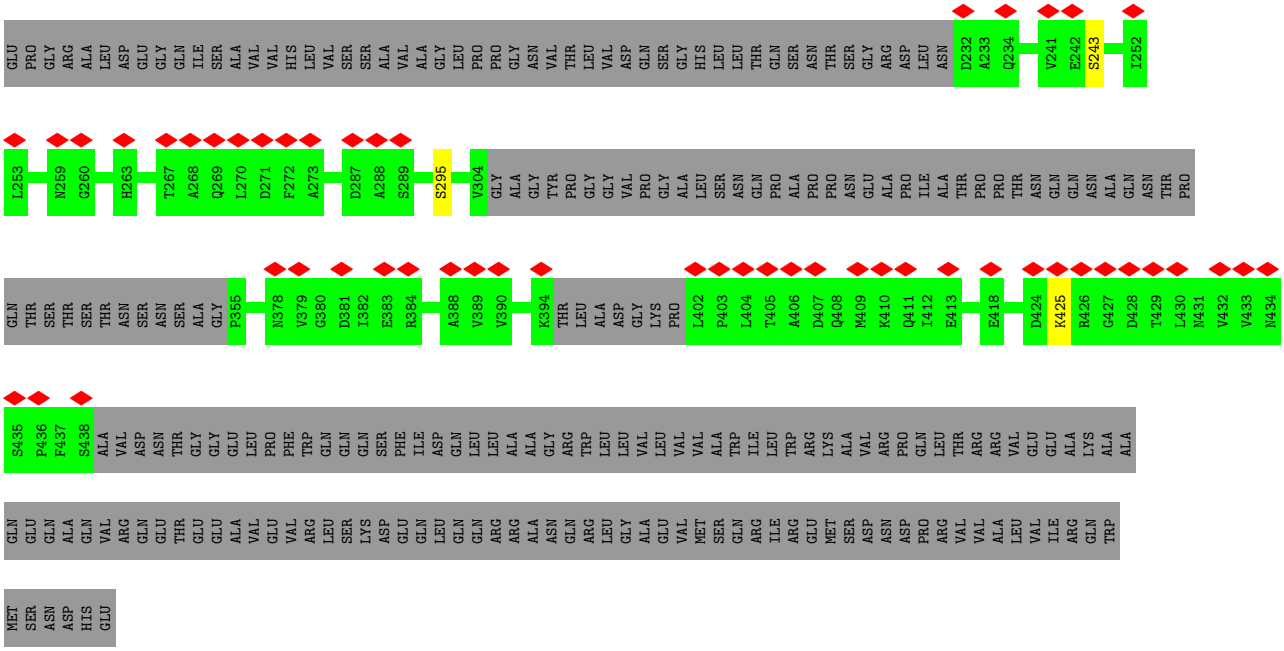
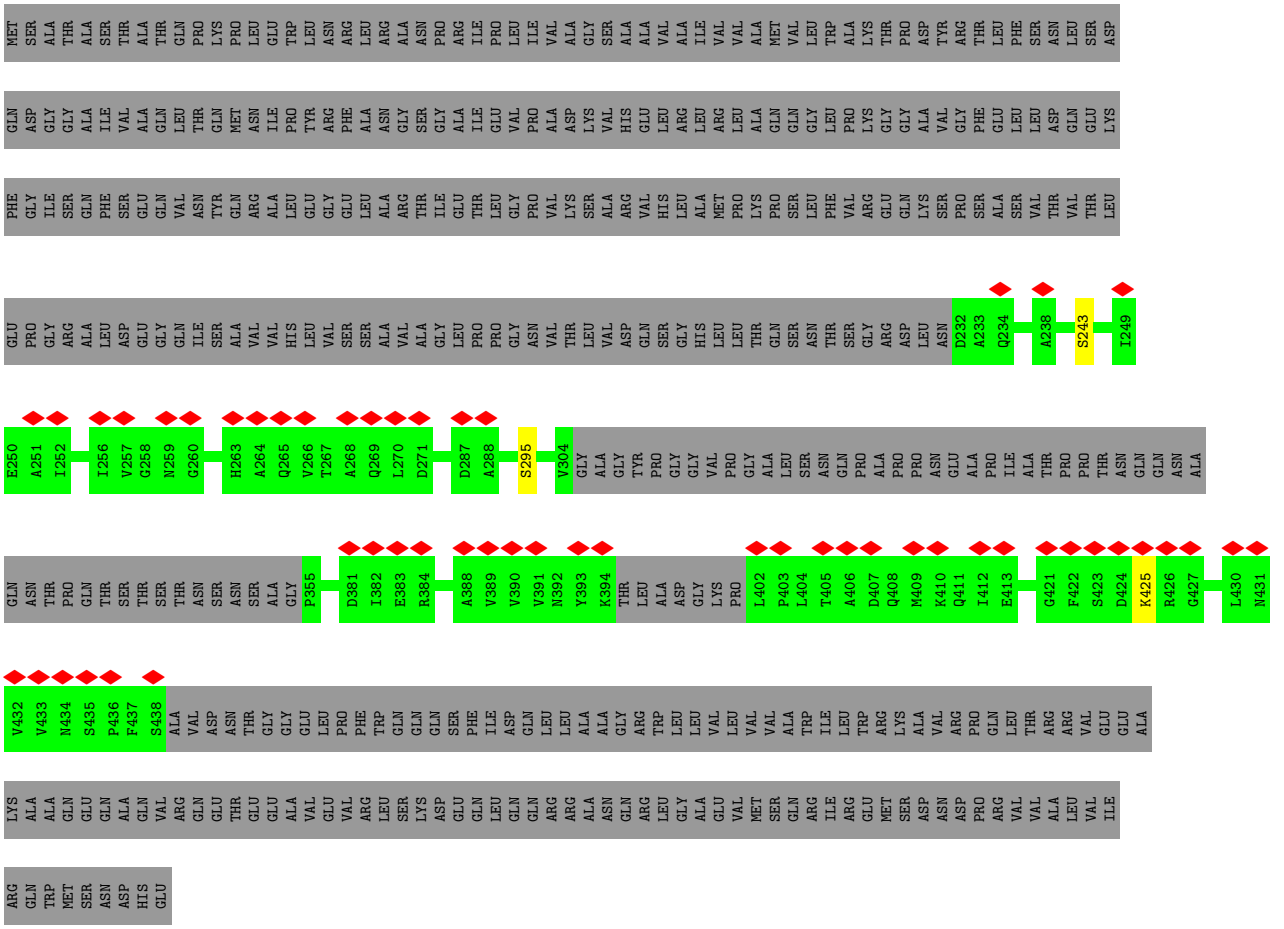


• Molecule 12: Flagellar M-ring protein





• Molecule 12: Flagellar M-ring protein



• Molecule 12: Flagellar M-ring protein

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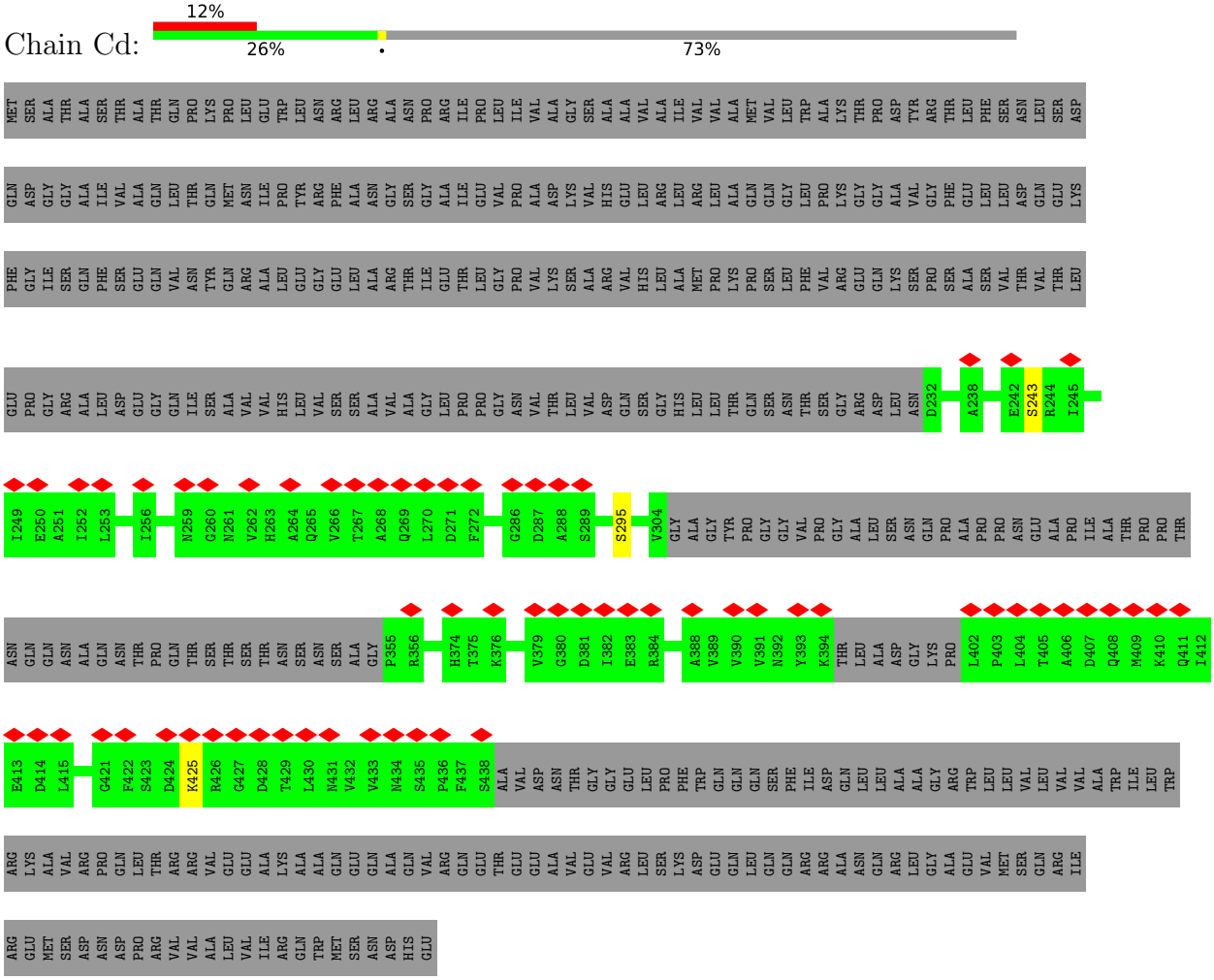

• Molecule 12: Flagellar M-ring protein

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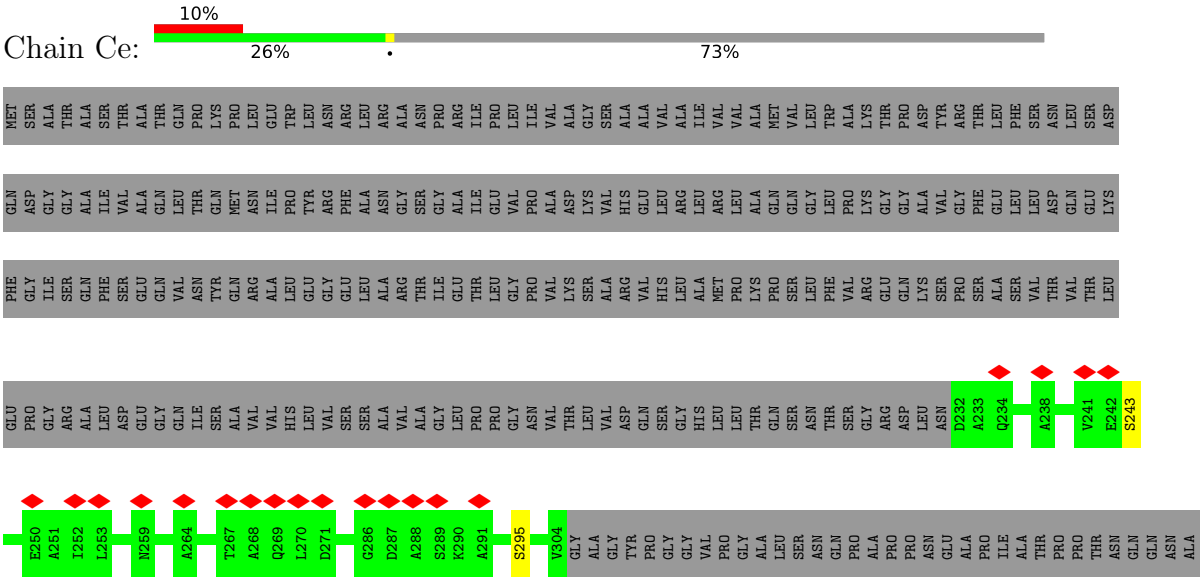

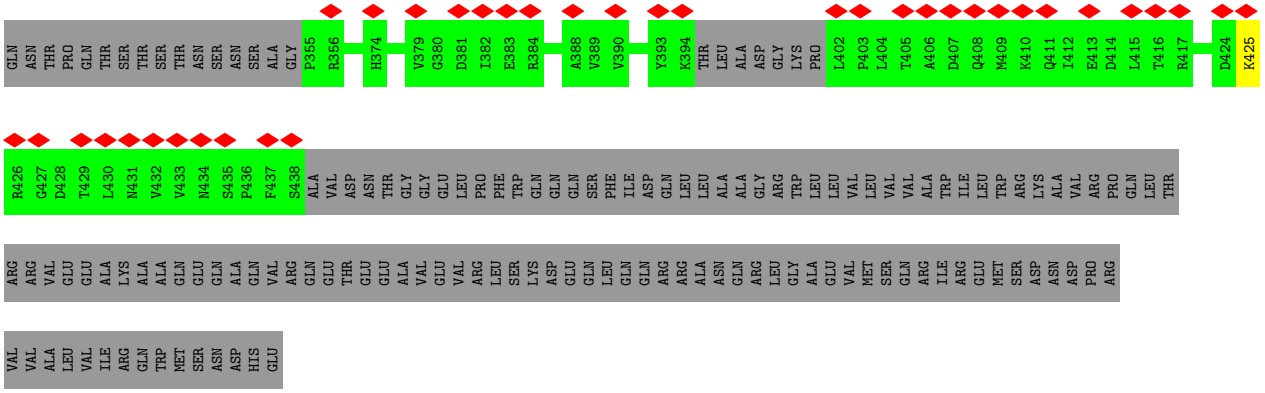

• Molecule 12: Flagellar M-ring protein

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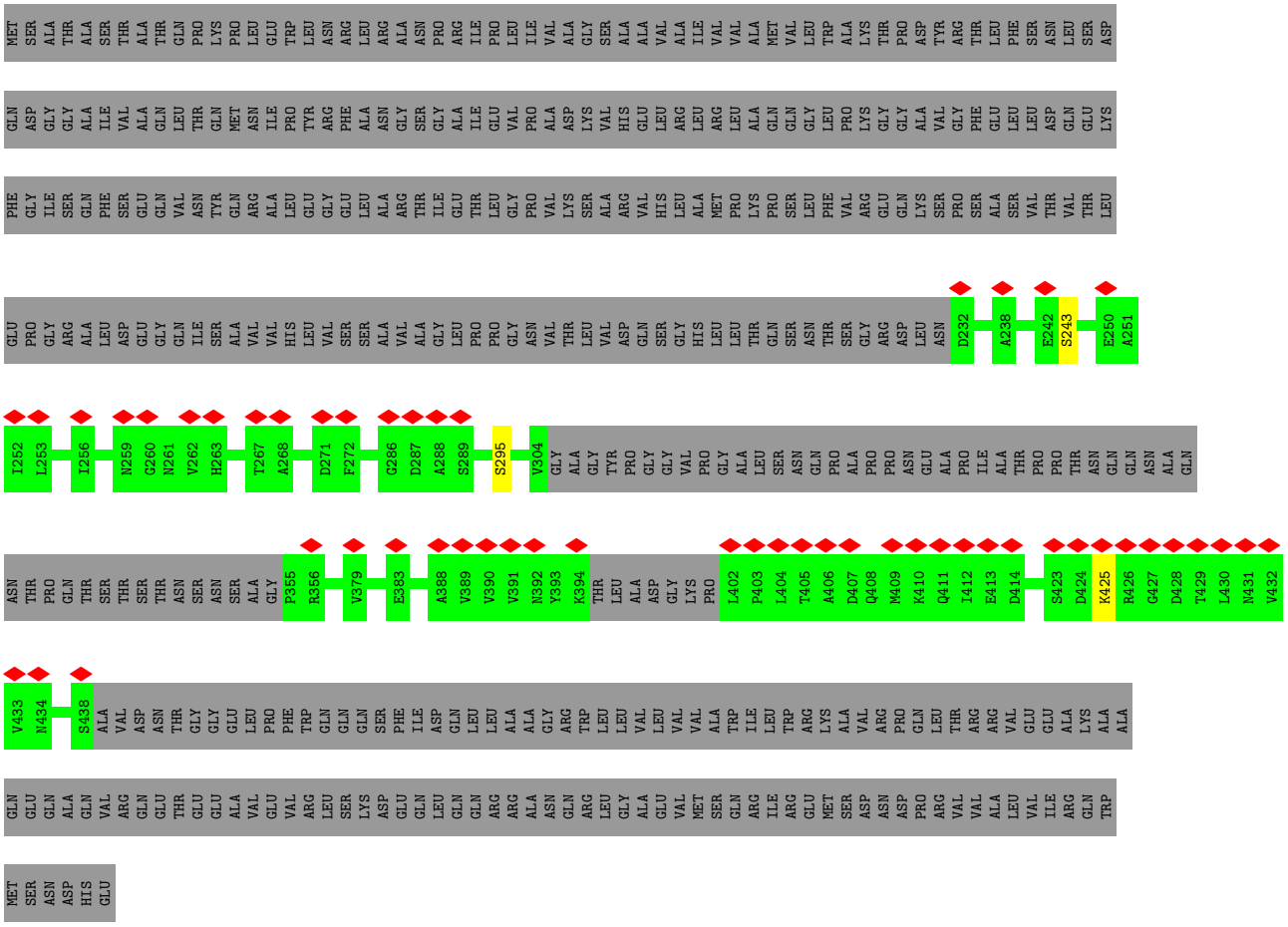

• Molecule 12: Flagellar M-ring protein

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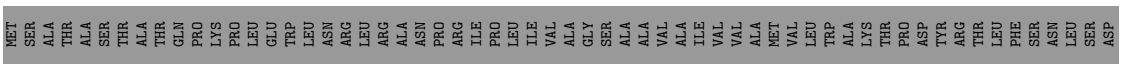

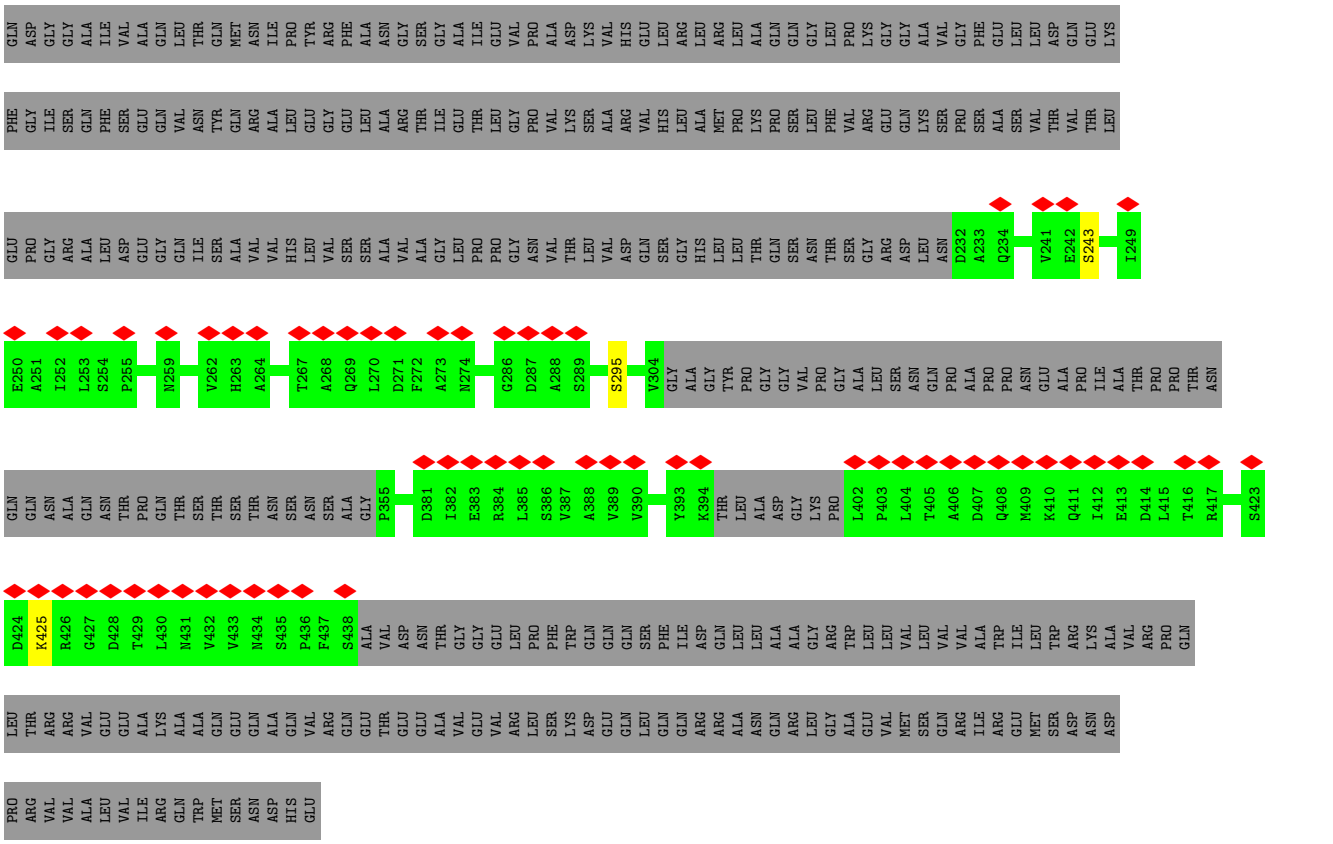

• Molecule 12: Flagellar M-ring protein

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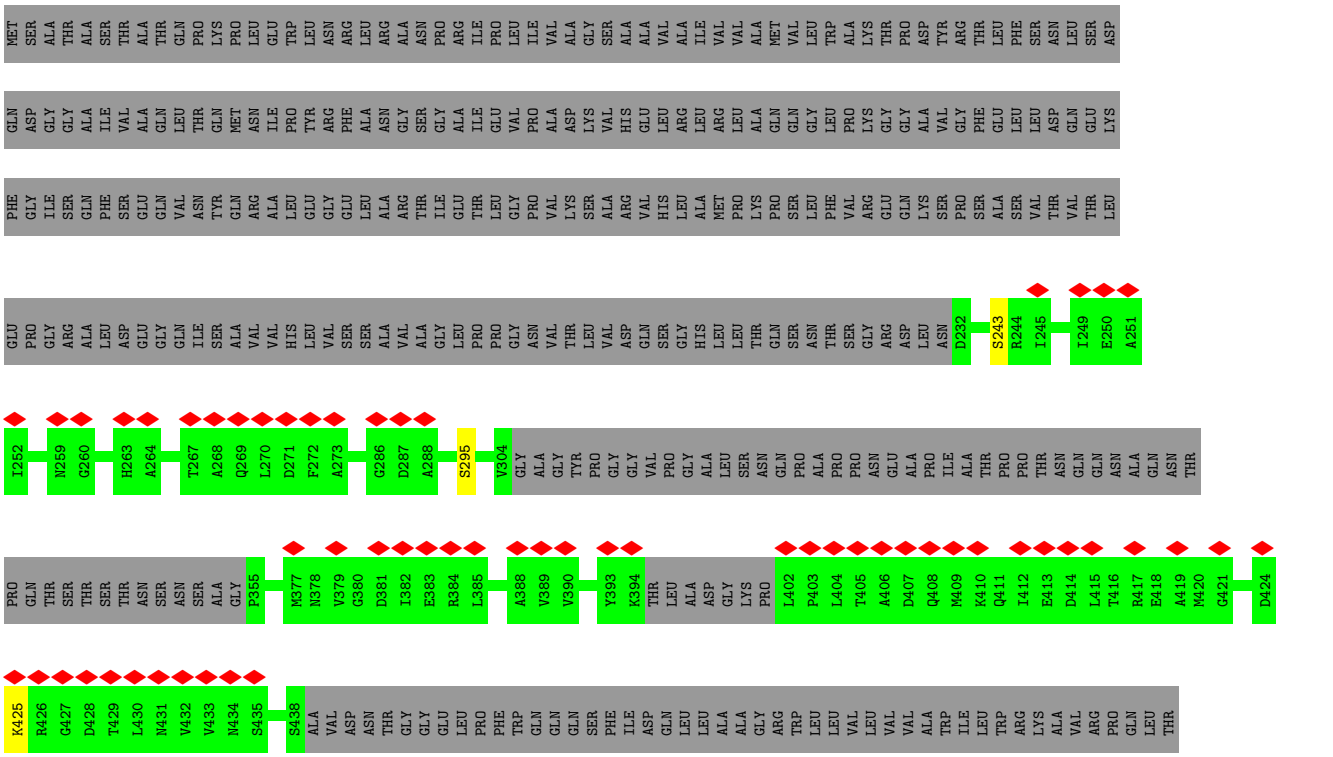
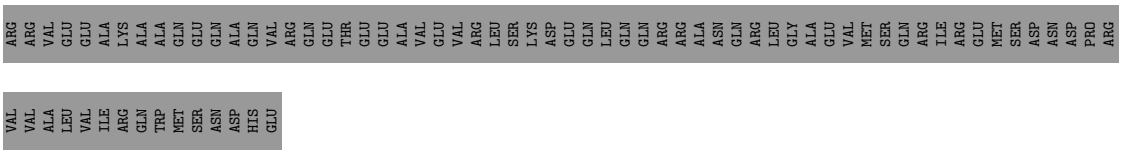
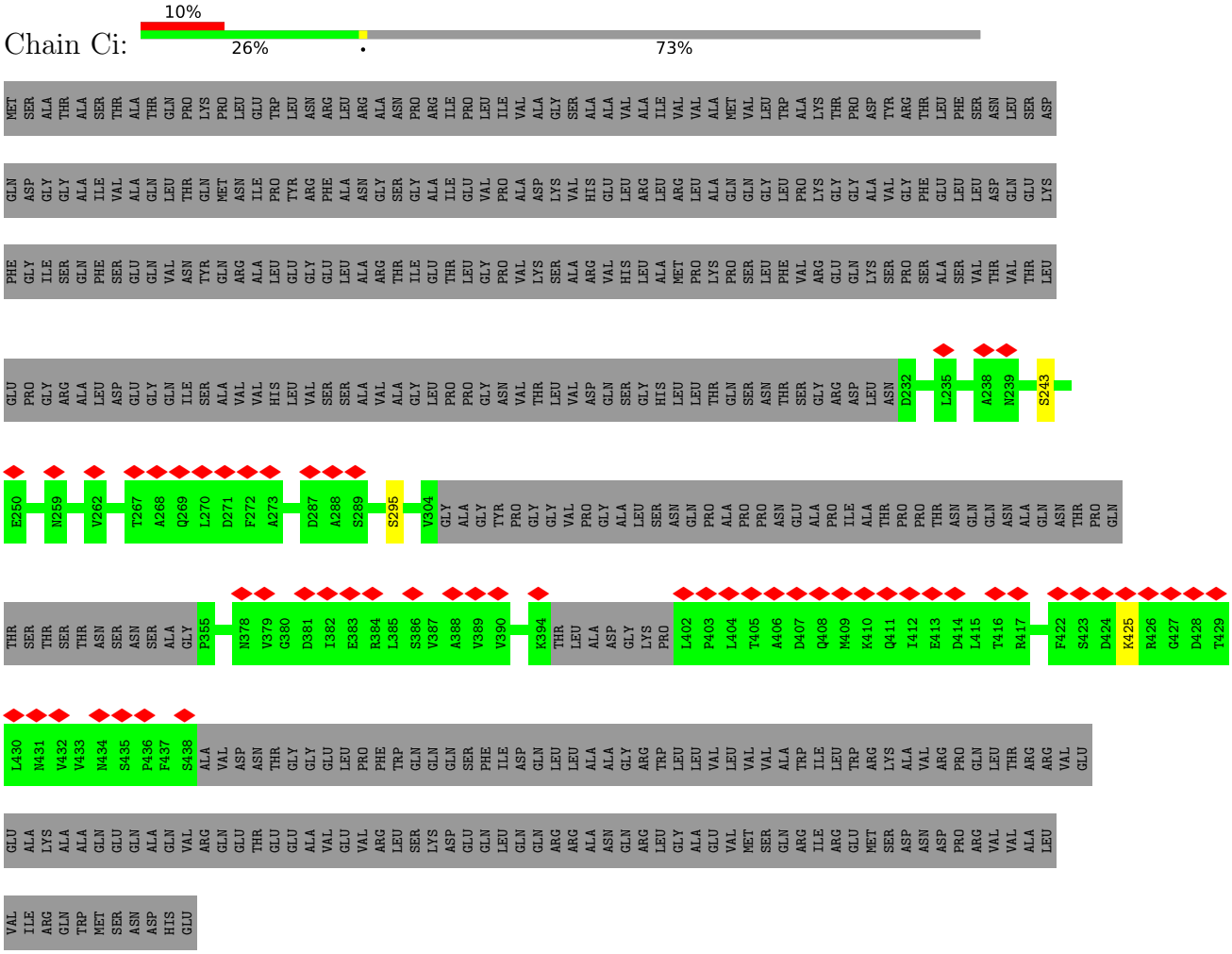
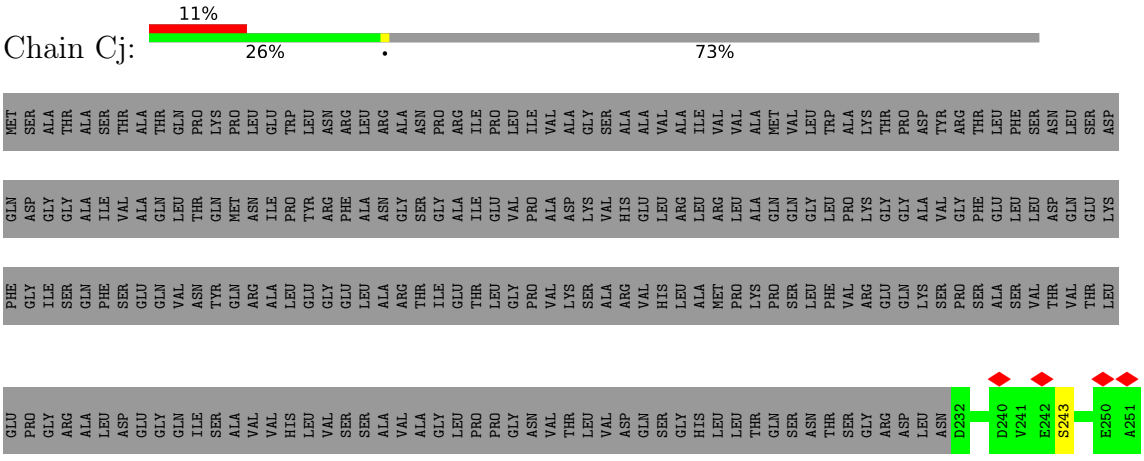


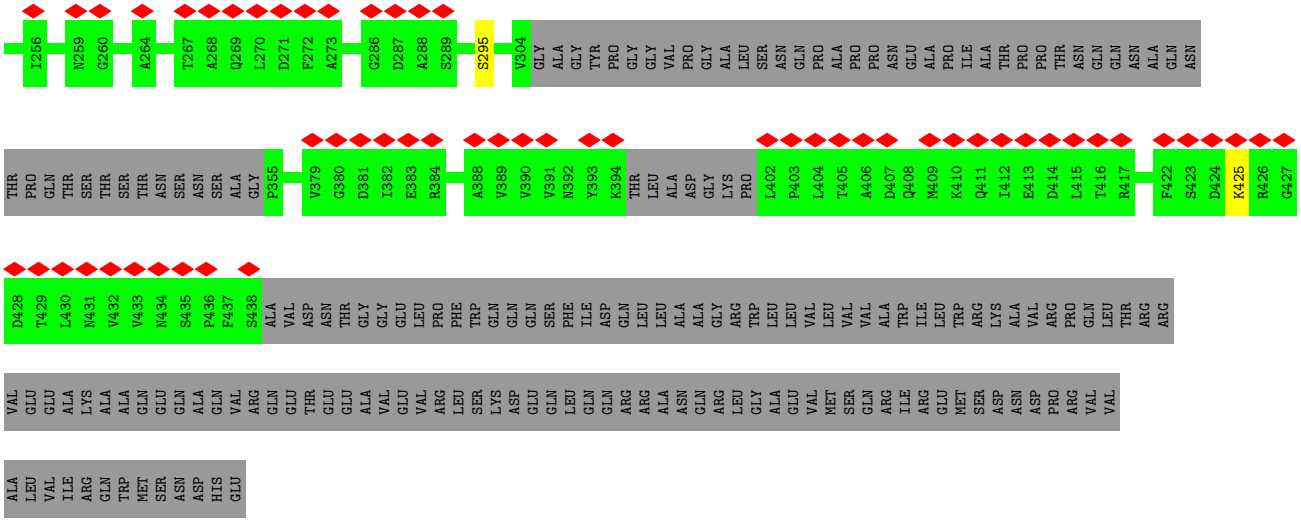


• Molecule 12: Flagellar M-ring protein



• Molecule 12: Flagellar M-ring protein





• Molecule 12: Flagellar M-ring protein

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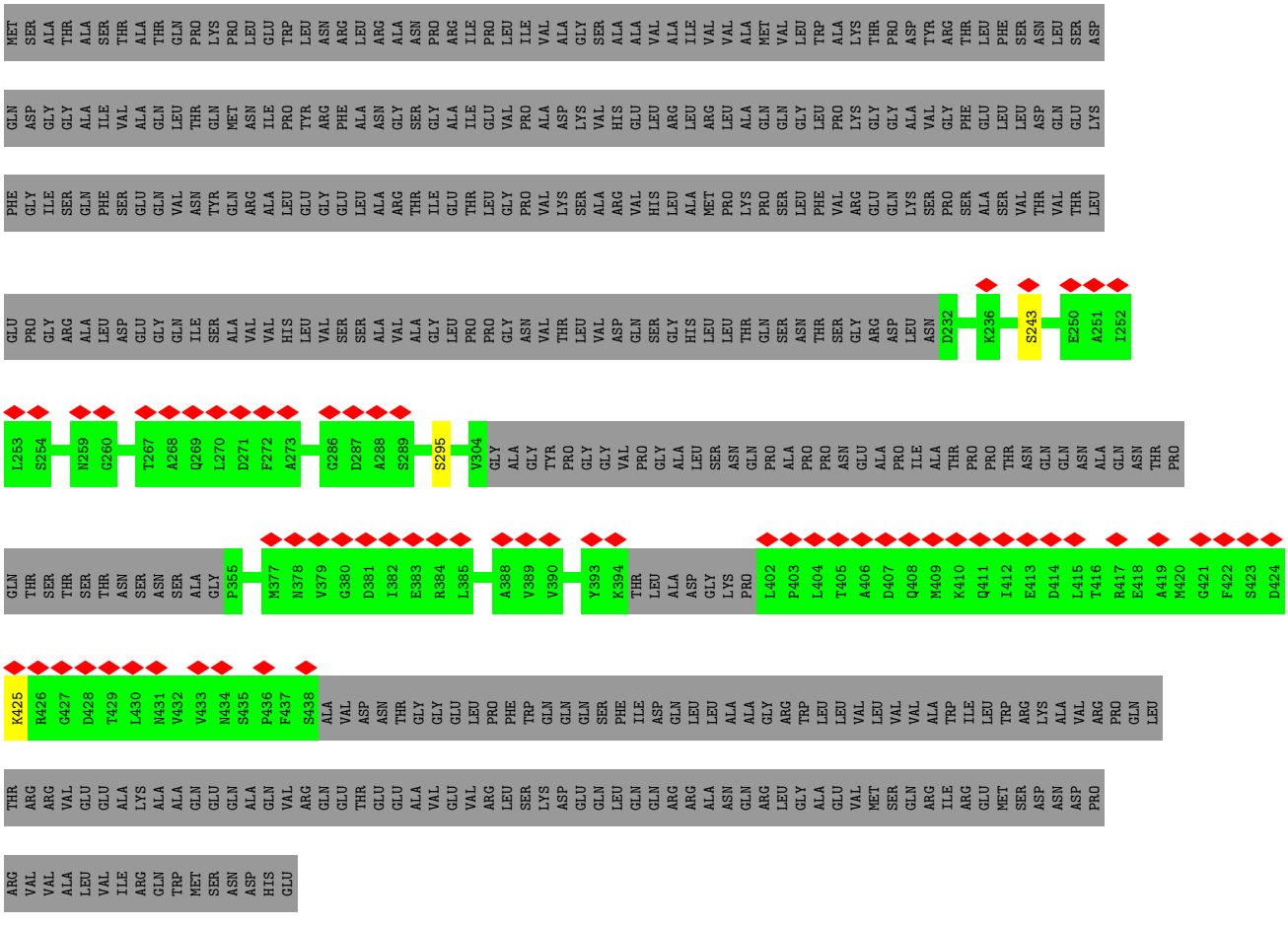

• Molecule 12: Flagellar M-ring protein

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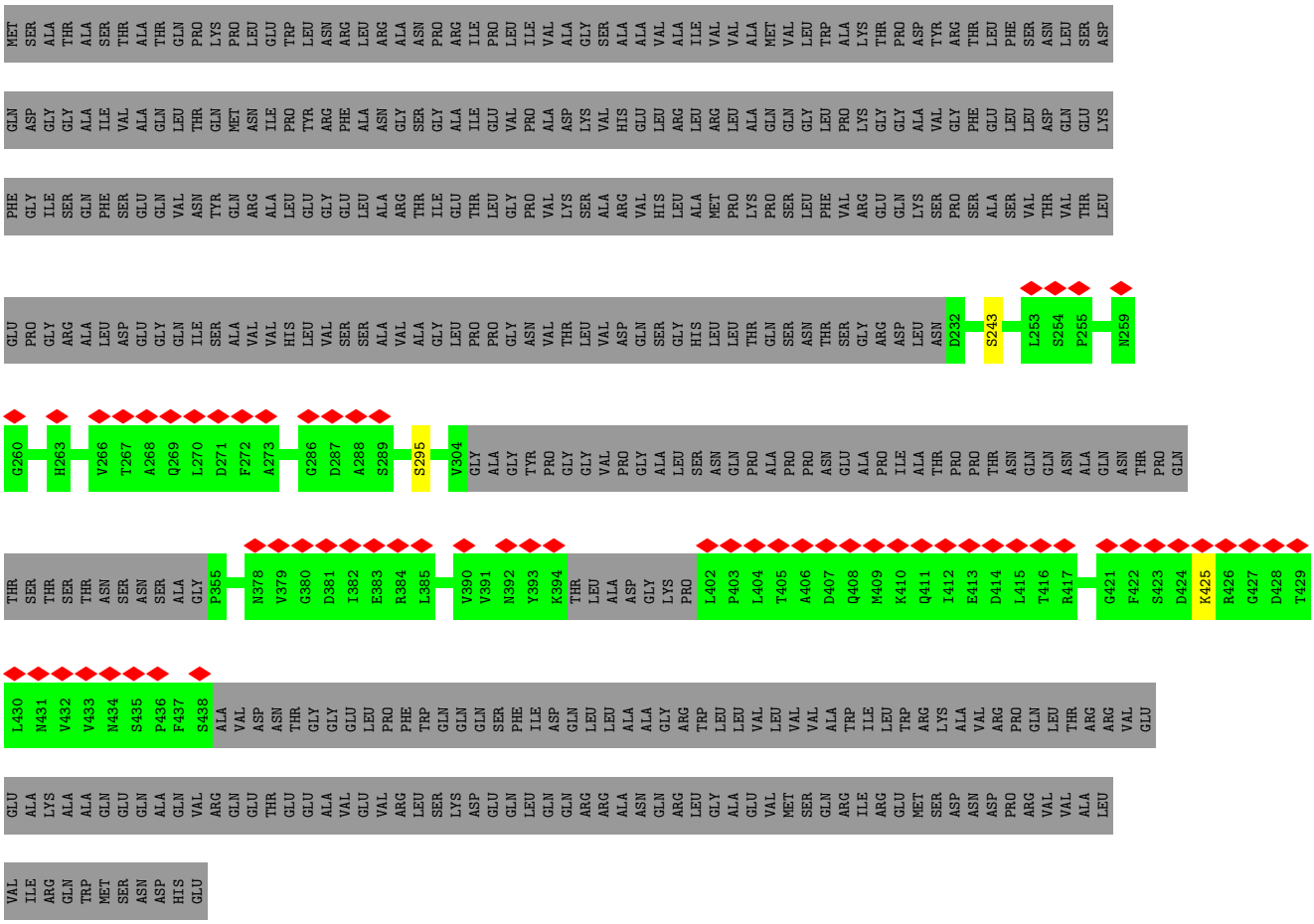

• Molecule 12: Flagellar M-ring protein

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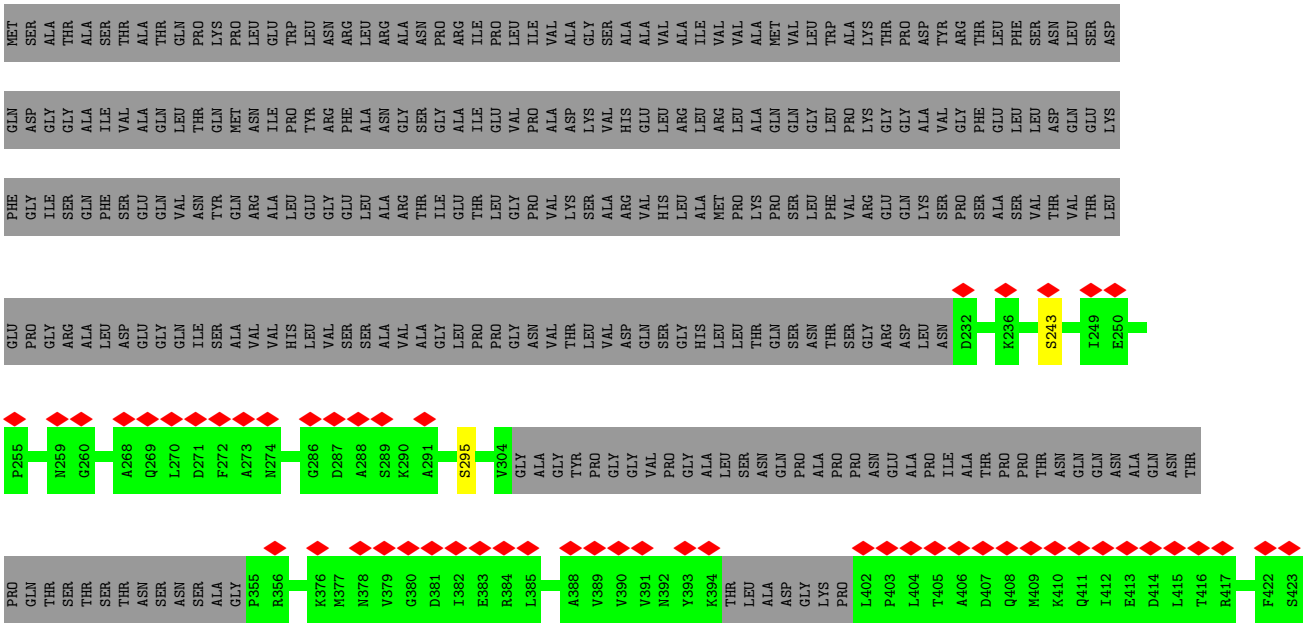

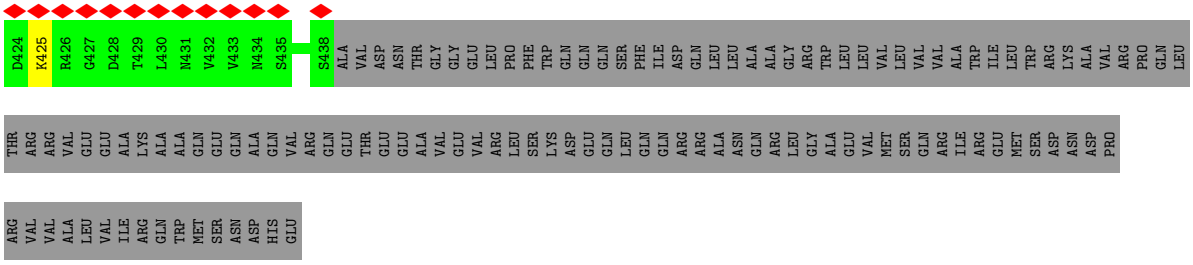

• Molecule 12: Flagellar M-ring protein

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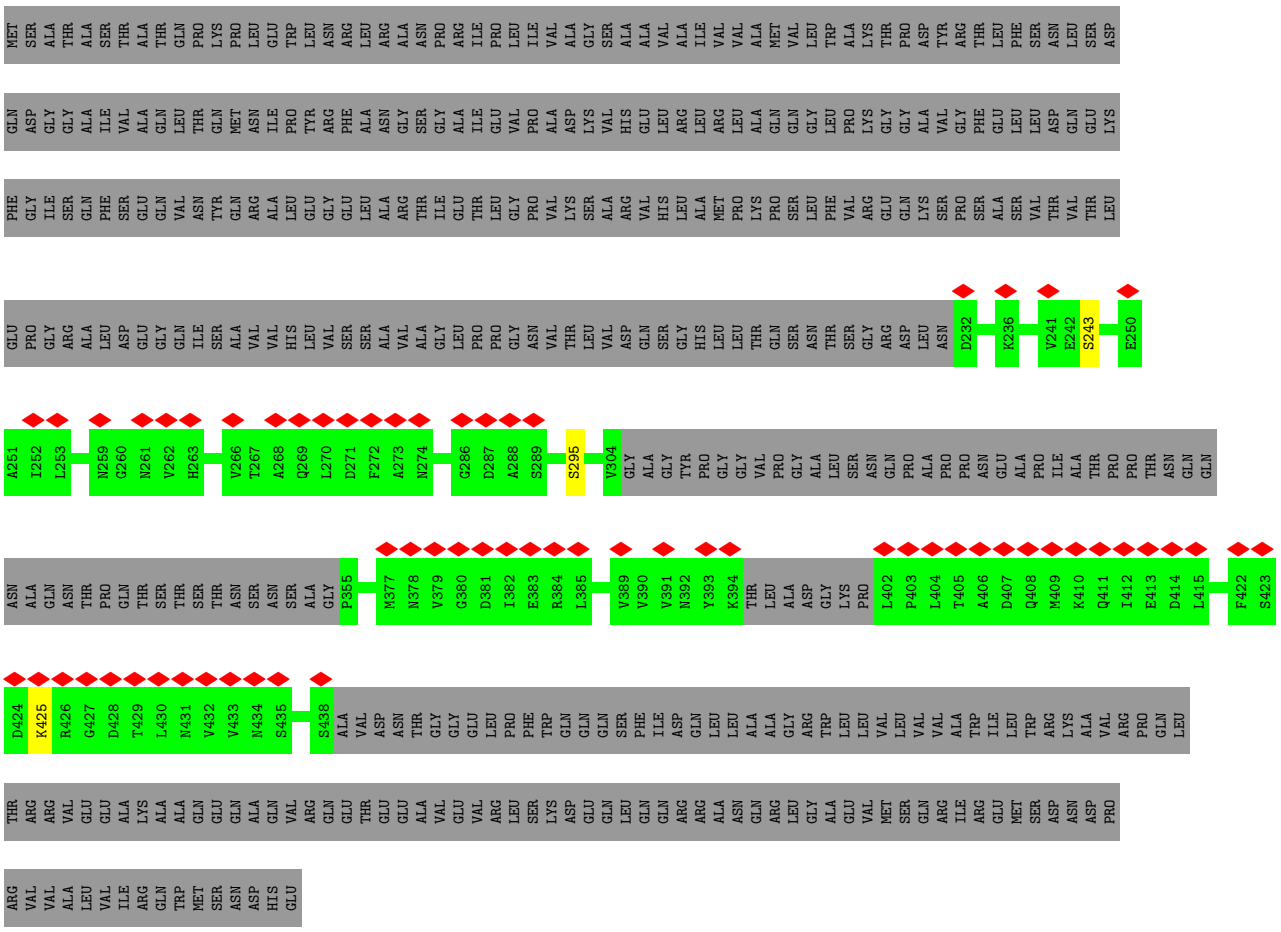

• Molecule 12: Flagellar M-ring protein

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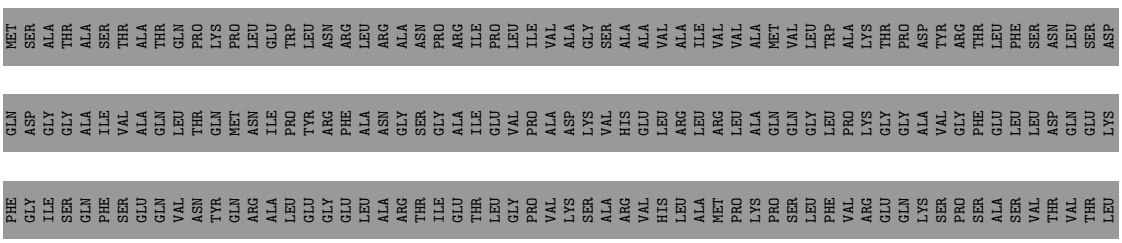
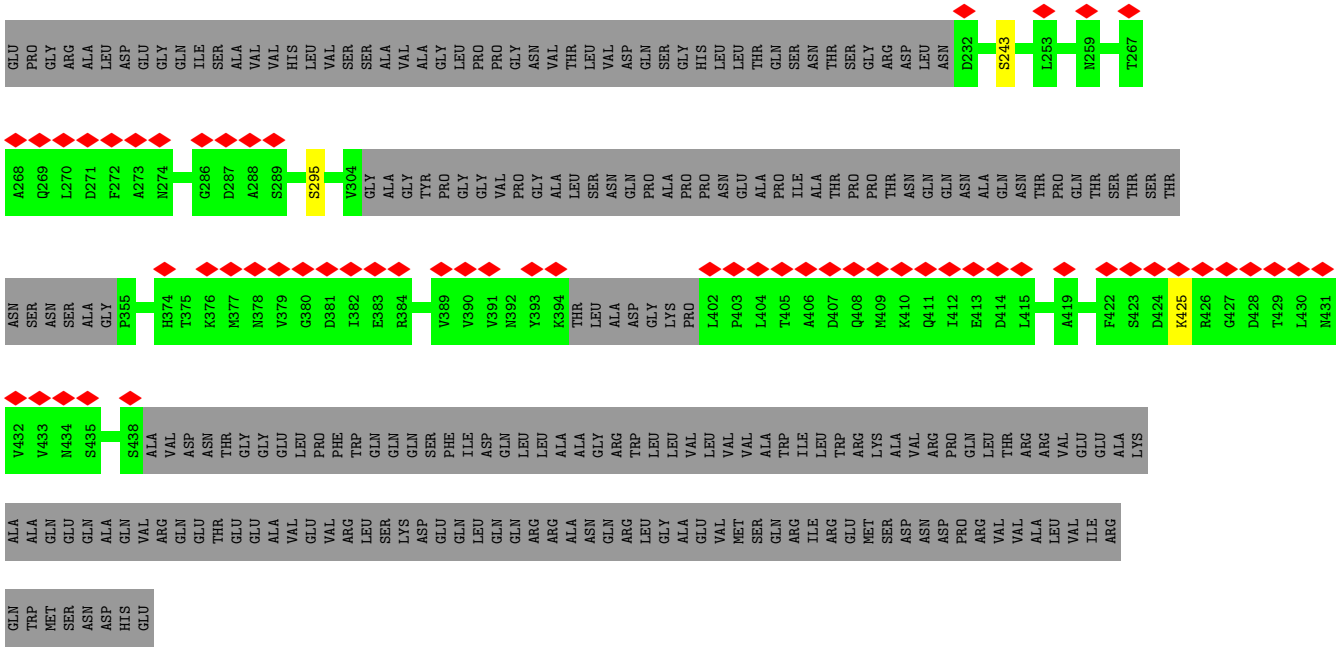
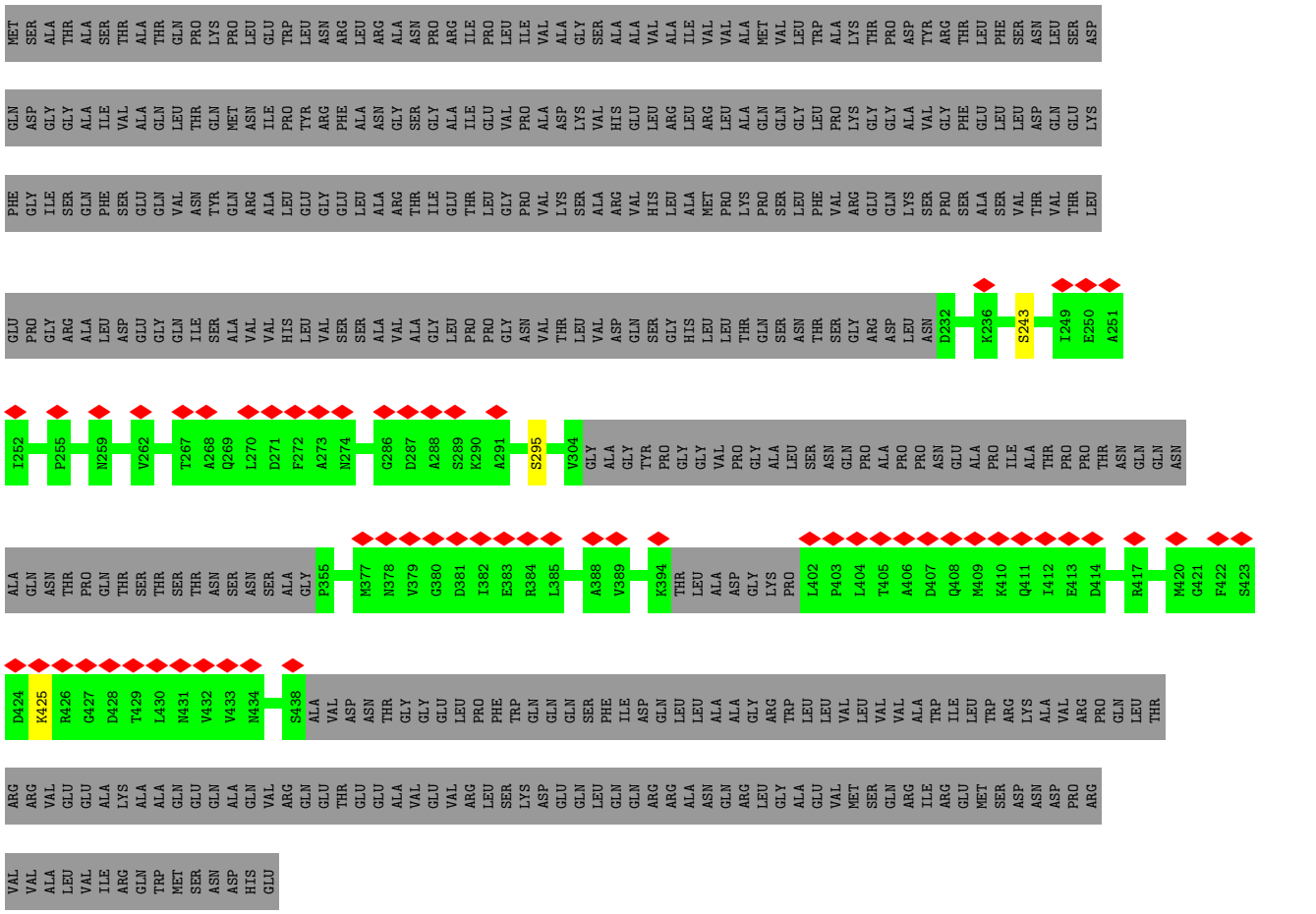




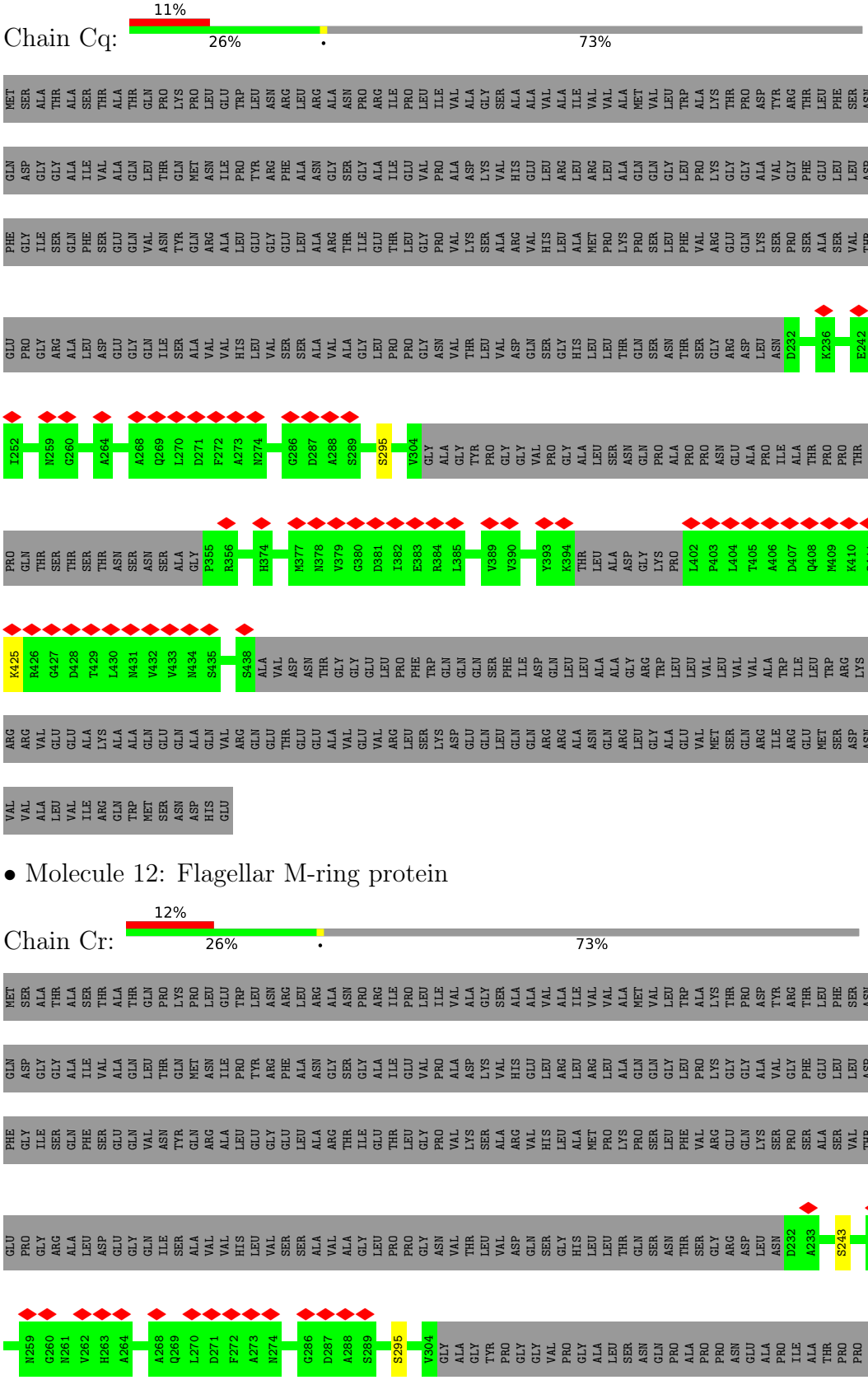
• Molecule 12: Flagellar M-ring protein

Chain Cp:



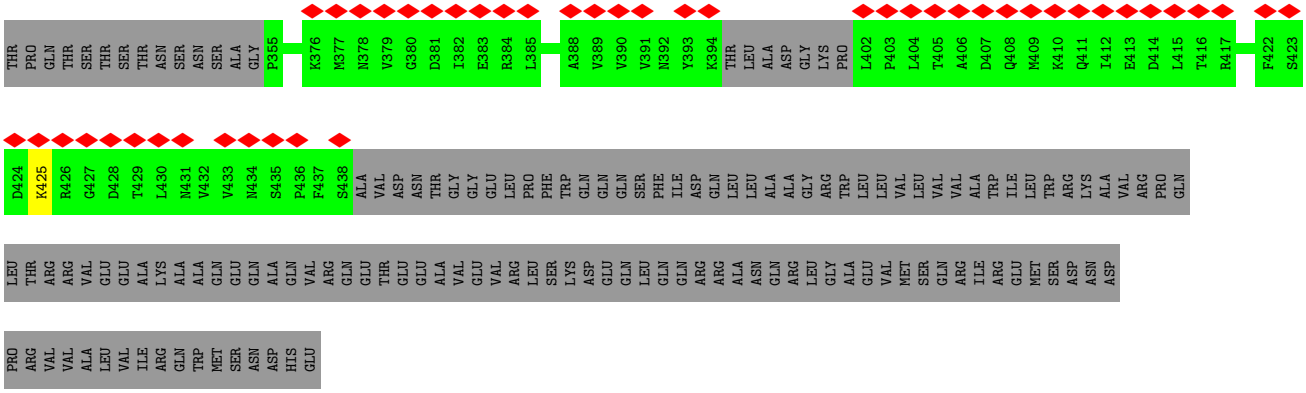
• Molecule 12: Flagellar M-ring protein

Chain Cq:



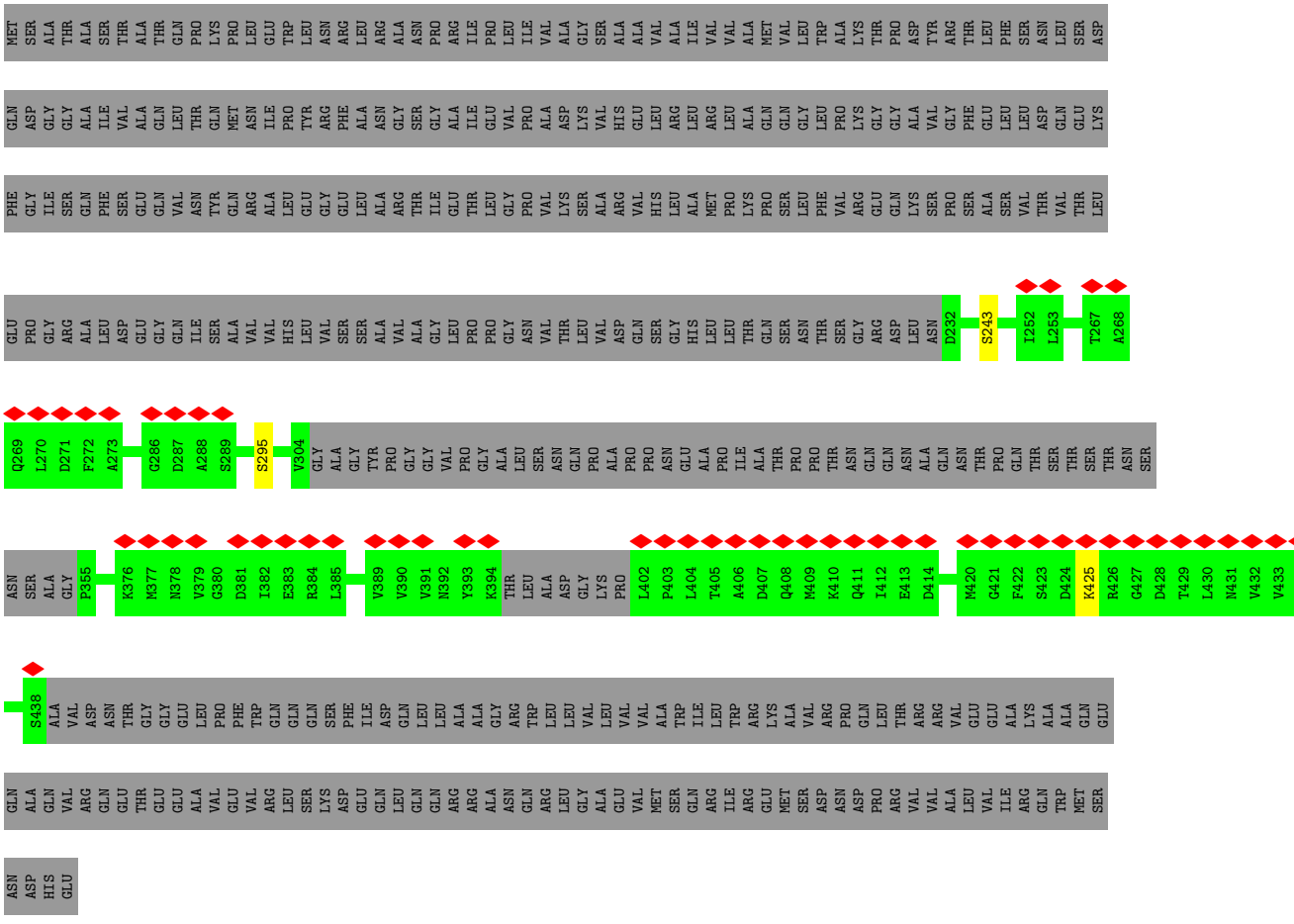
• Molecule 12: Flagellar M-ring protein

Chain Cr:



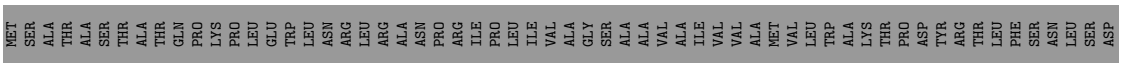
• Molecule 12: Flagellar M-ring protein

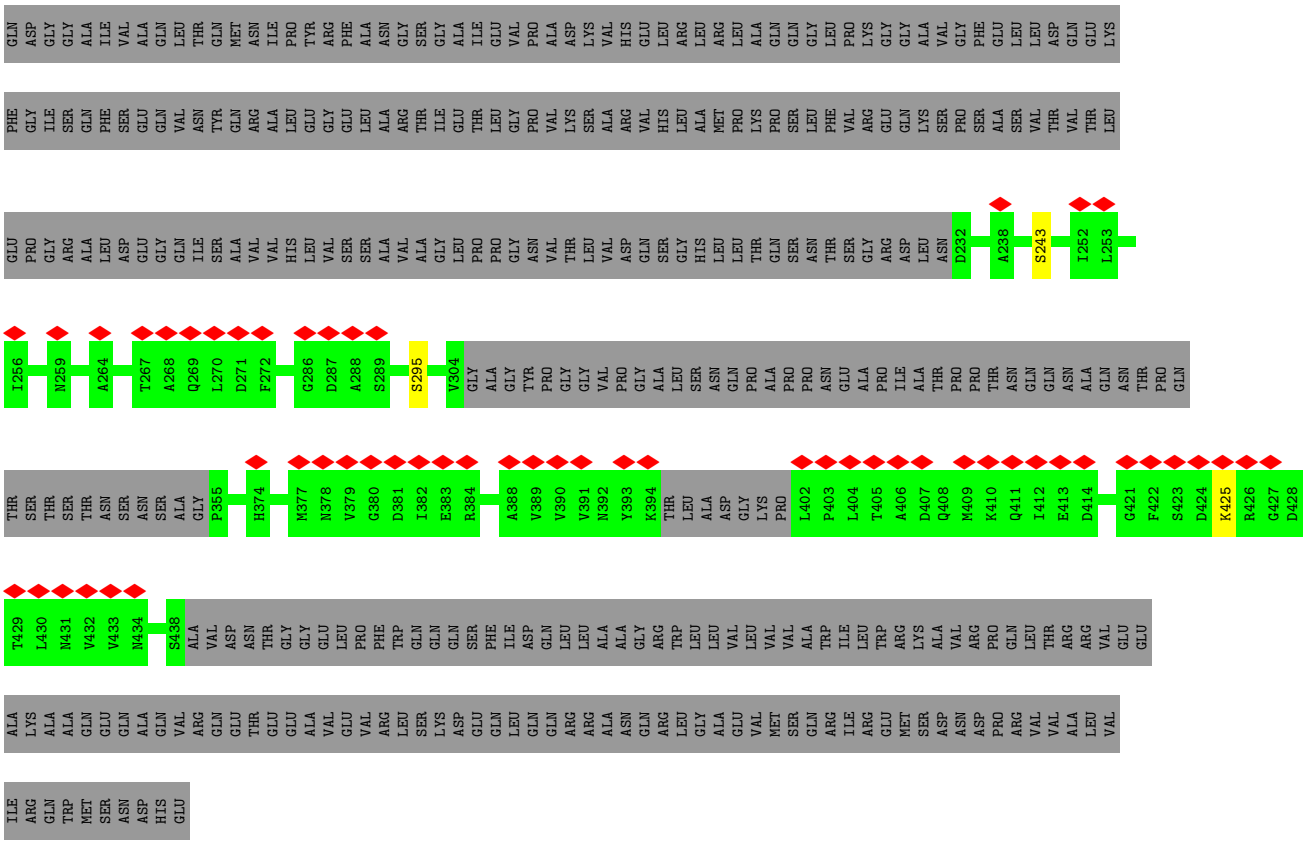
Chain Cs:



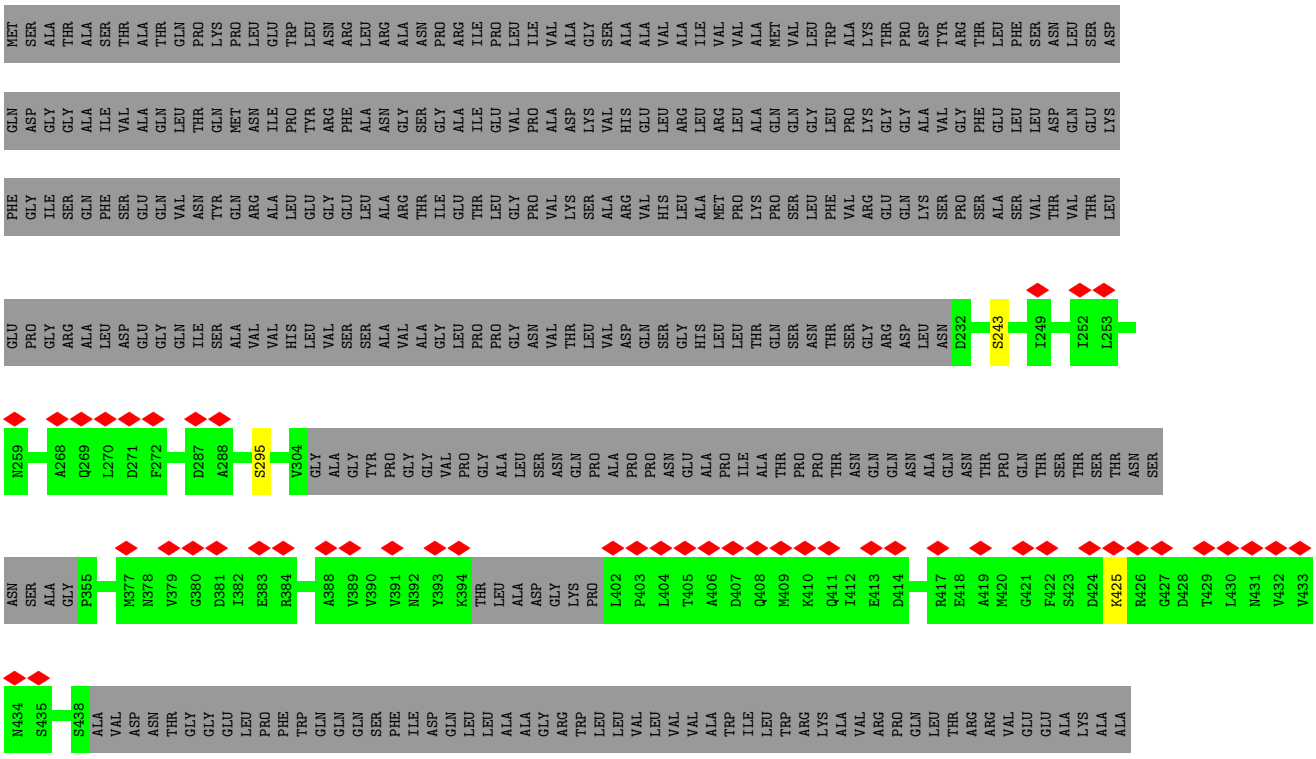
• Molecule 12: Flagellar M-ring protein

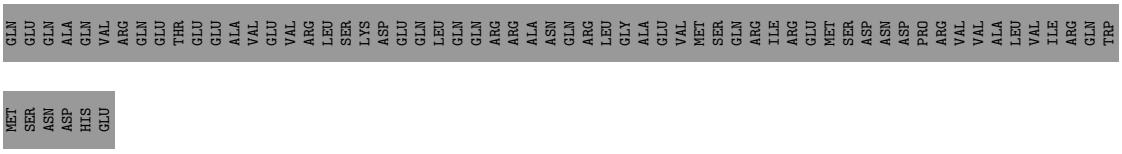
Chain Ct:



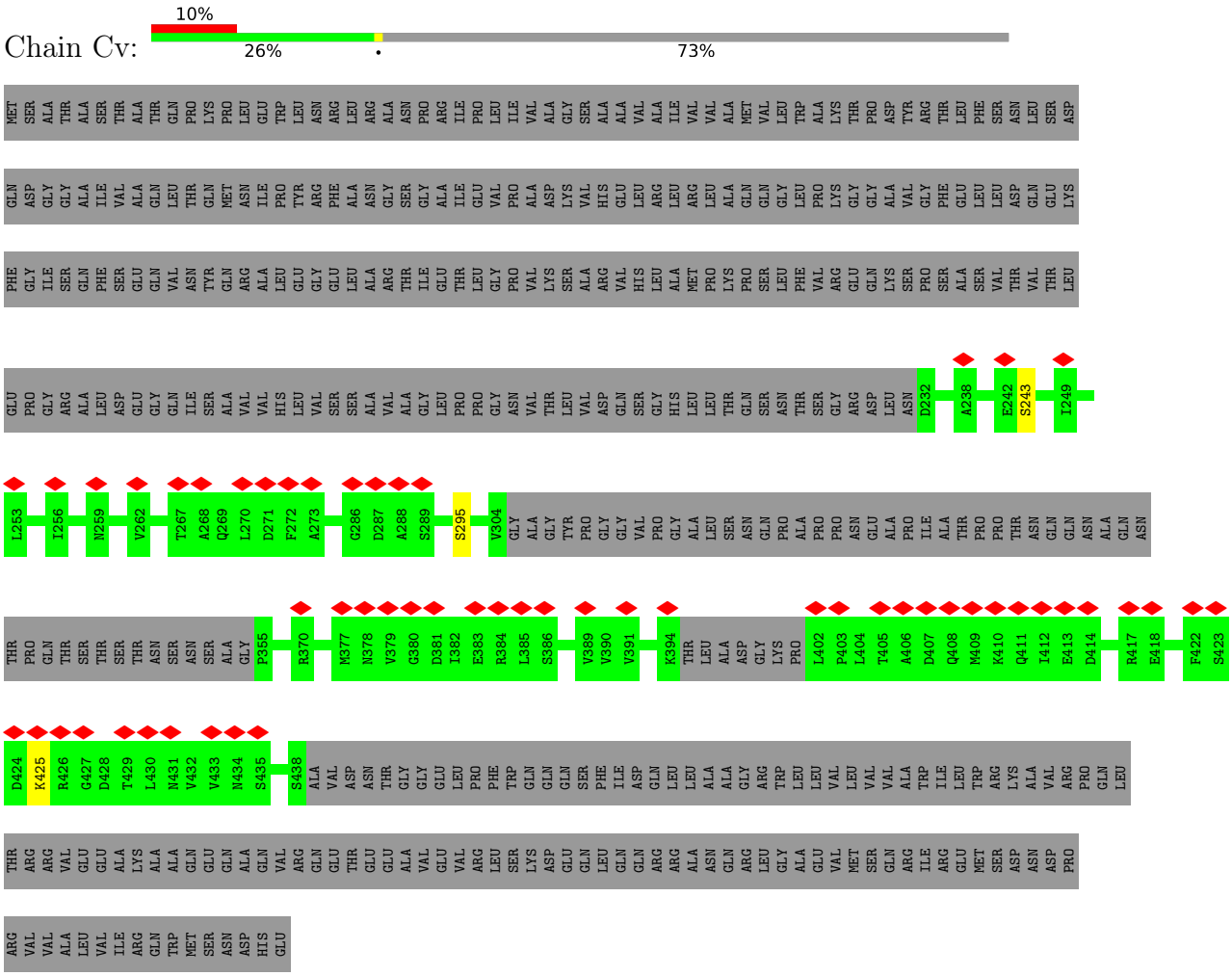


• Molecule 12: Flagellar M-ring protein

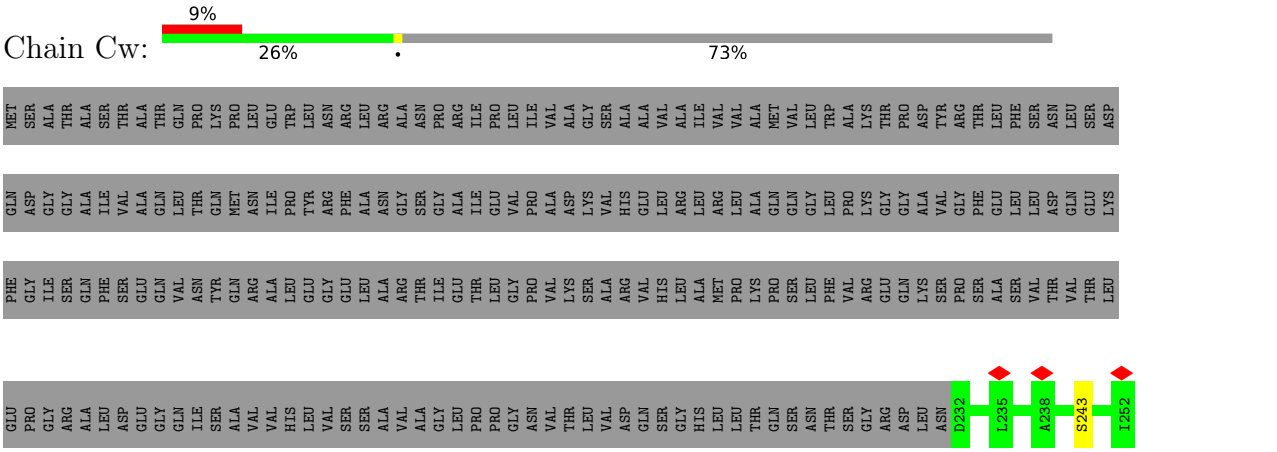


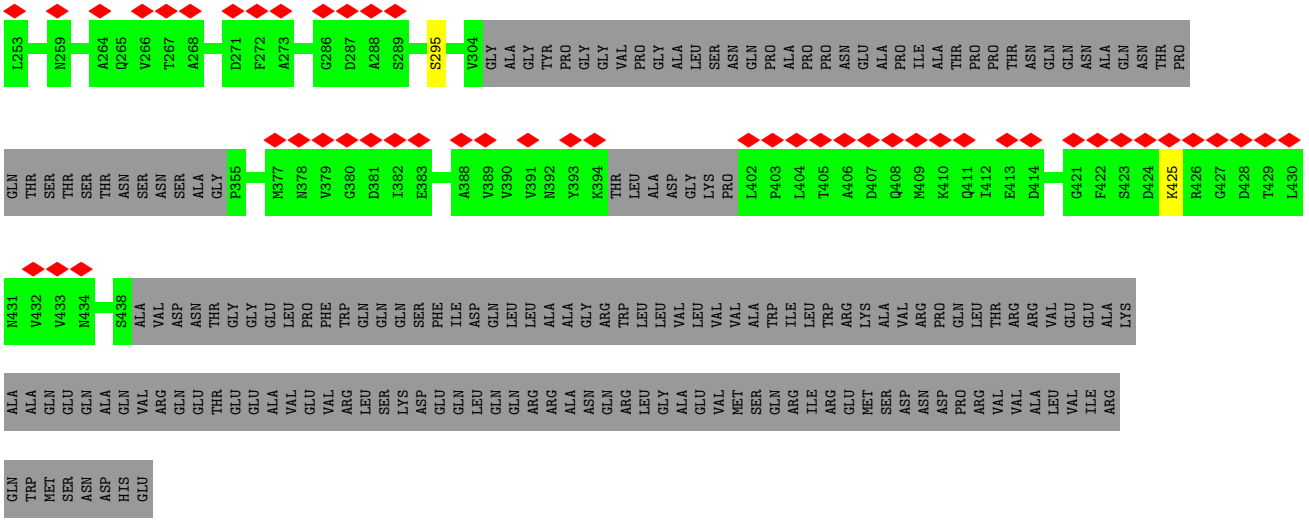


• Molecule 12: Flagellar M-ring protein



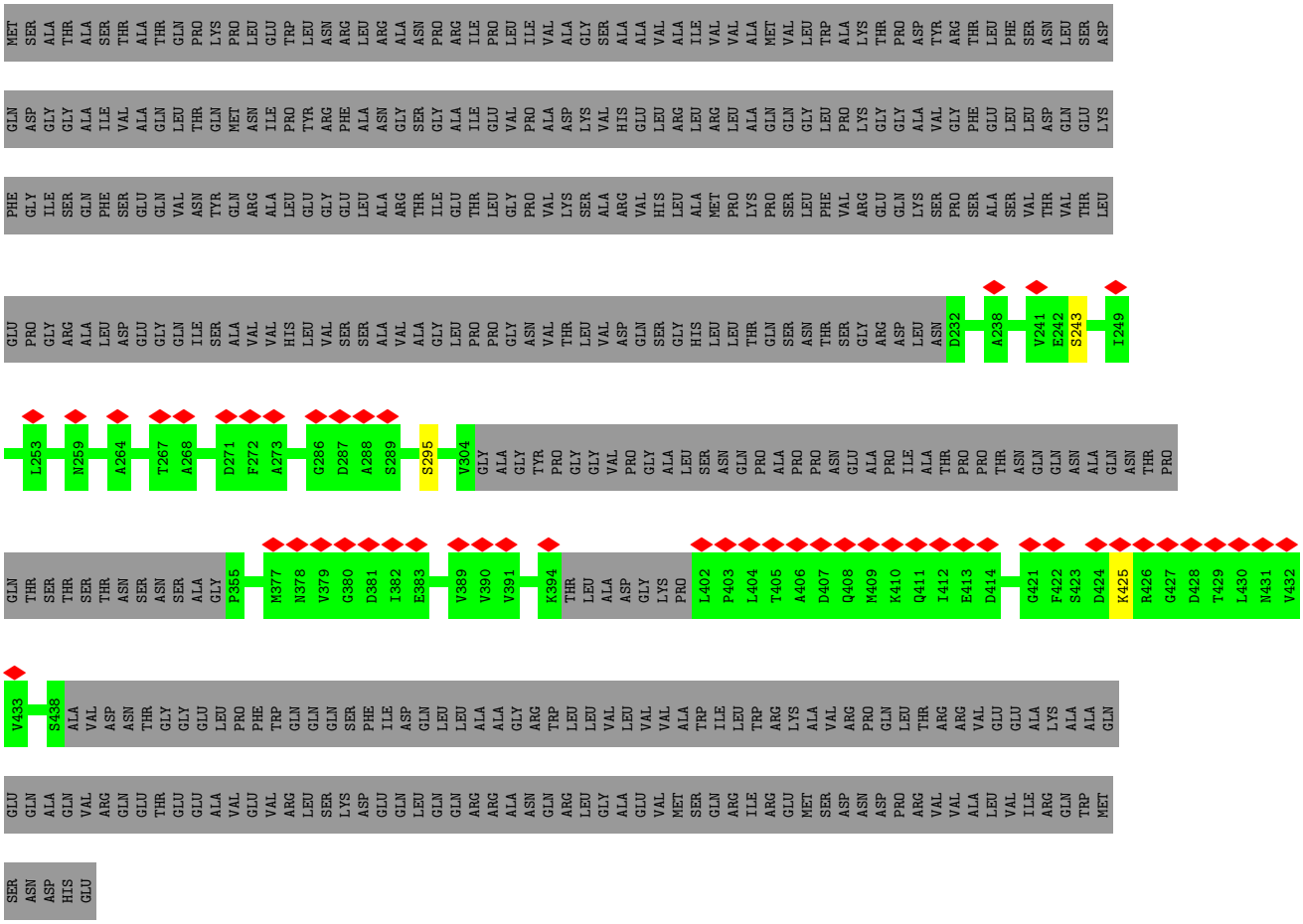
• Molecule 12: Flagellar M-ring protein





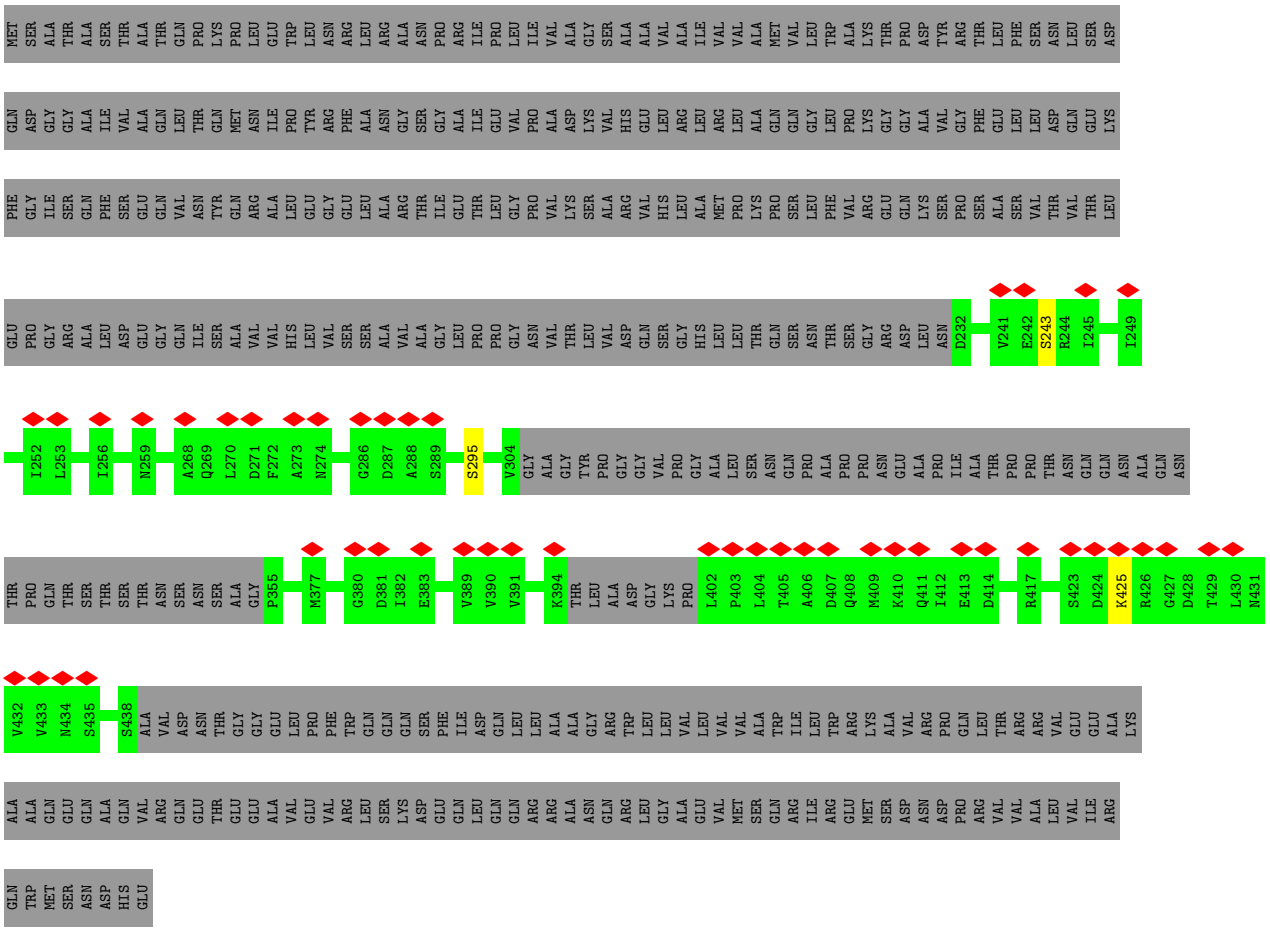
• Molecule 12: Flagellar M-ring protein

Chain Cx:



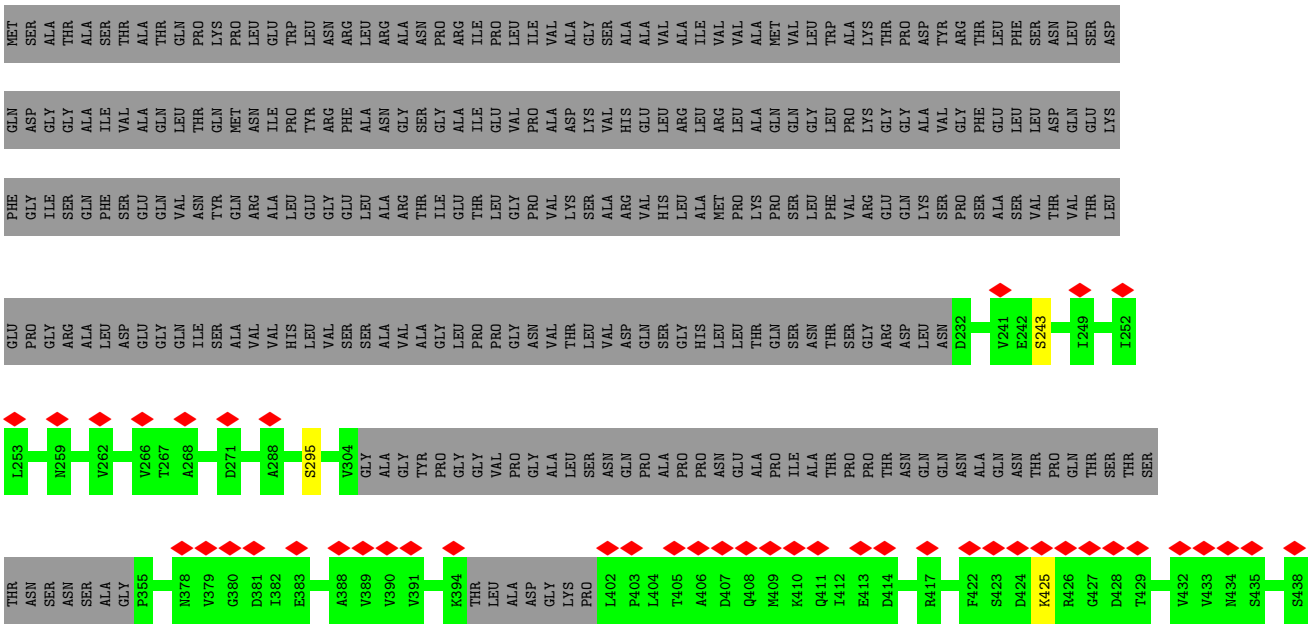
• Molecule 12: Flagellar M-ring protein

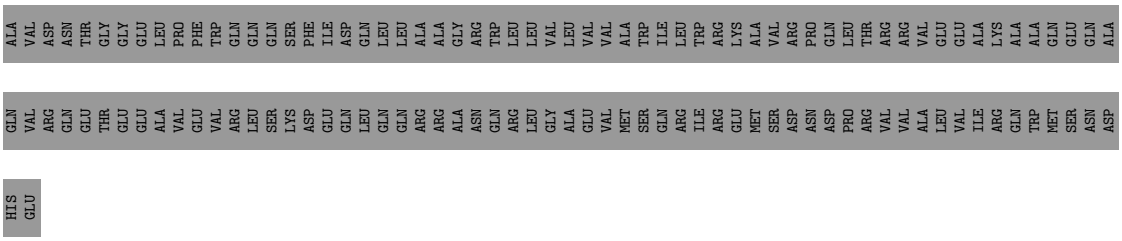
Chain Cy:



• Molecule 12: Flagellar M-ring protein

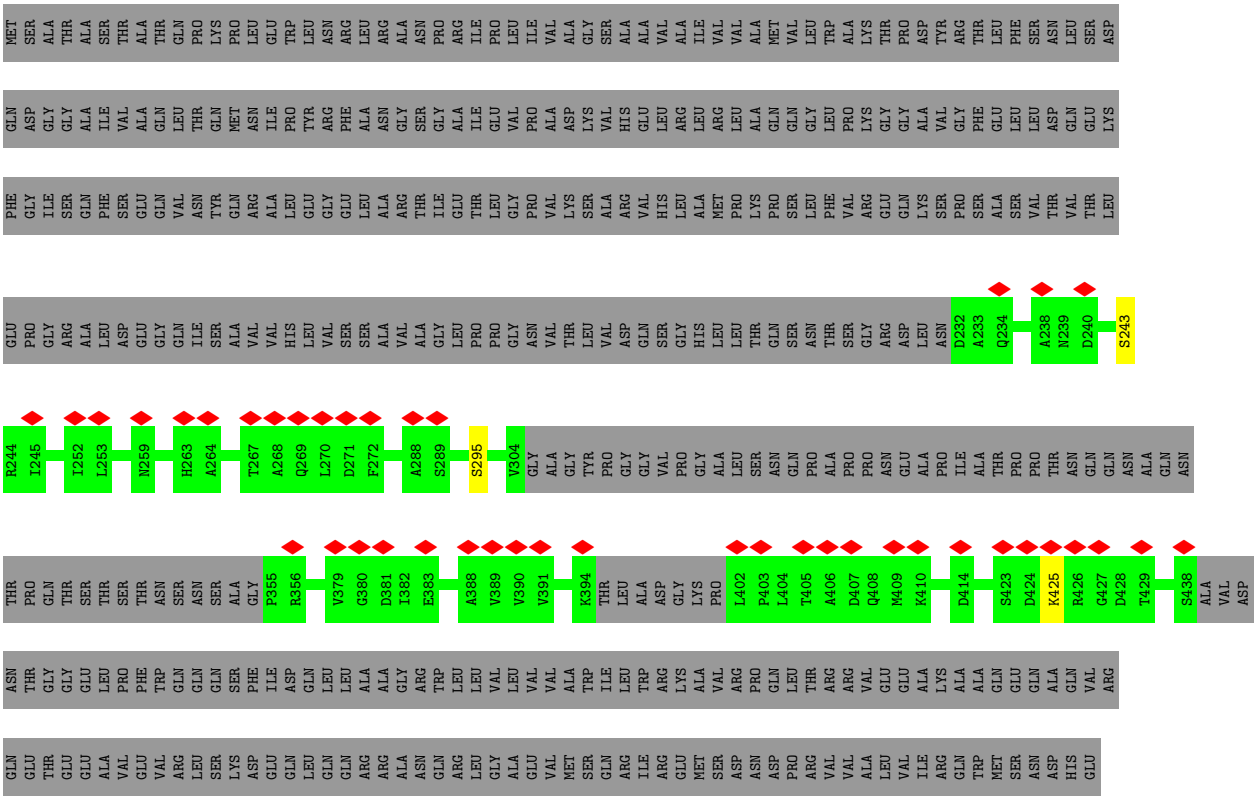
Chain Cz:





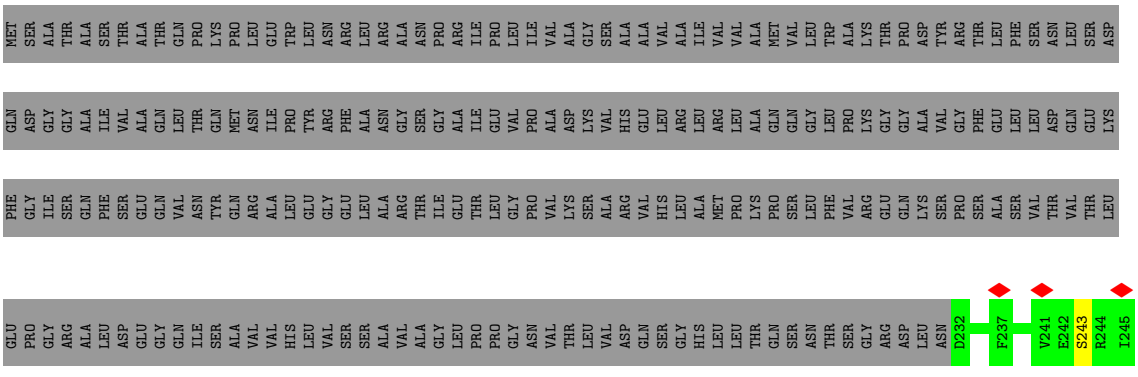
• Molecule 12: Flagellar M-ring protein

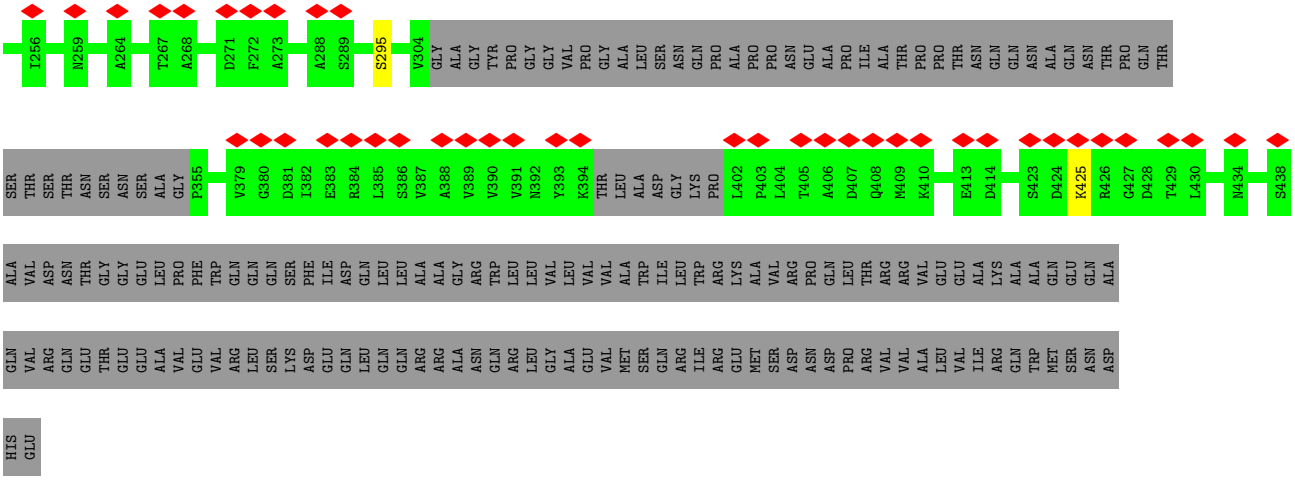
Chain Ea:



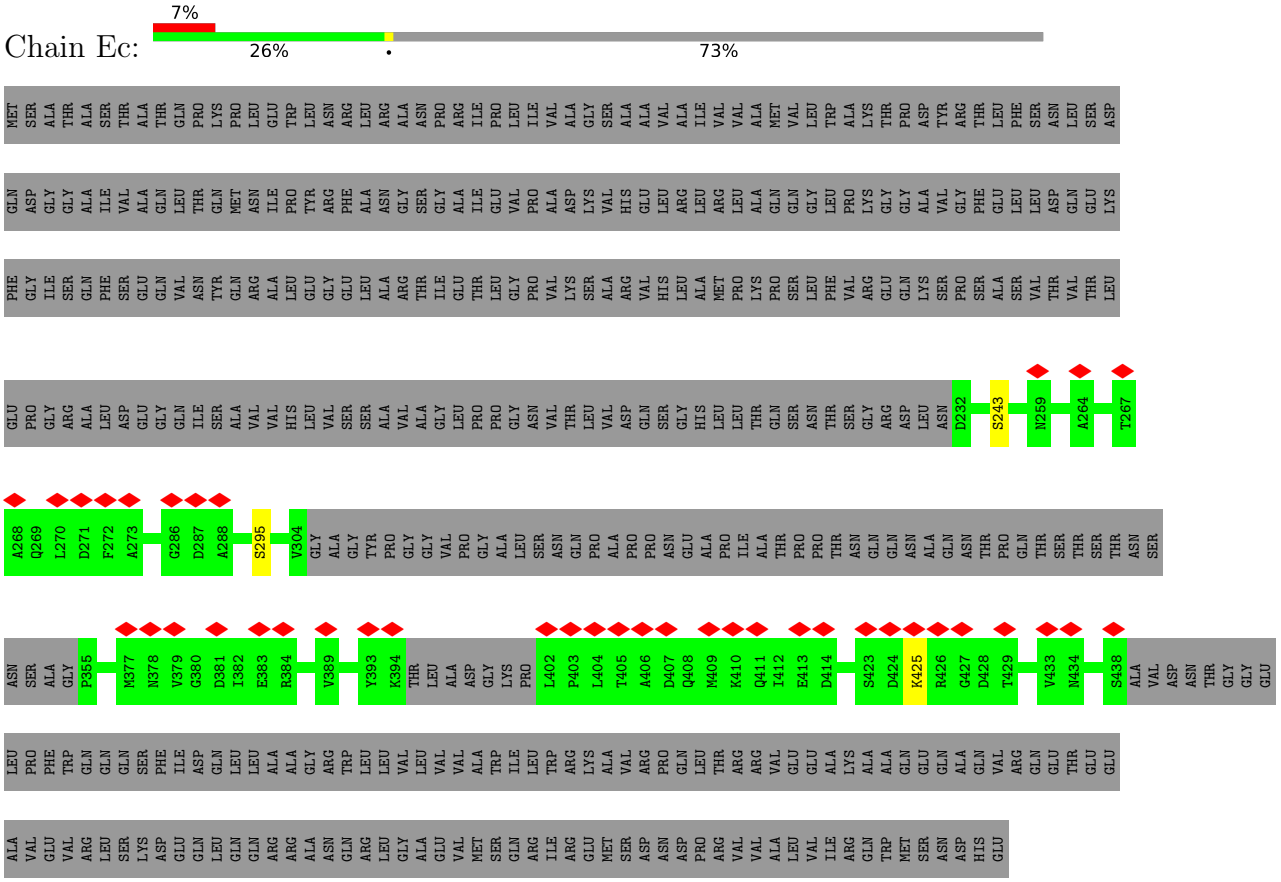
• Molecule 12: Flagellar M-ring protein

Chain Eb:

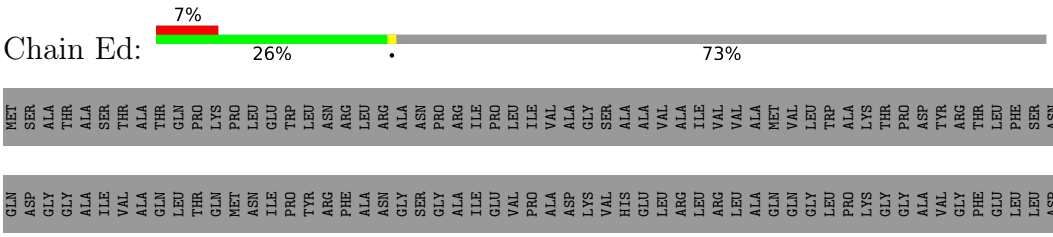


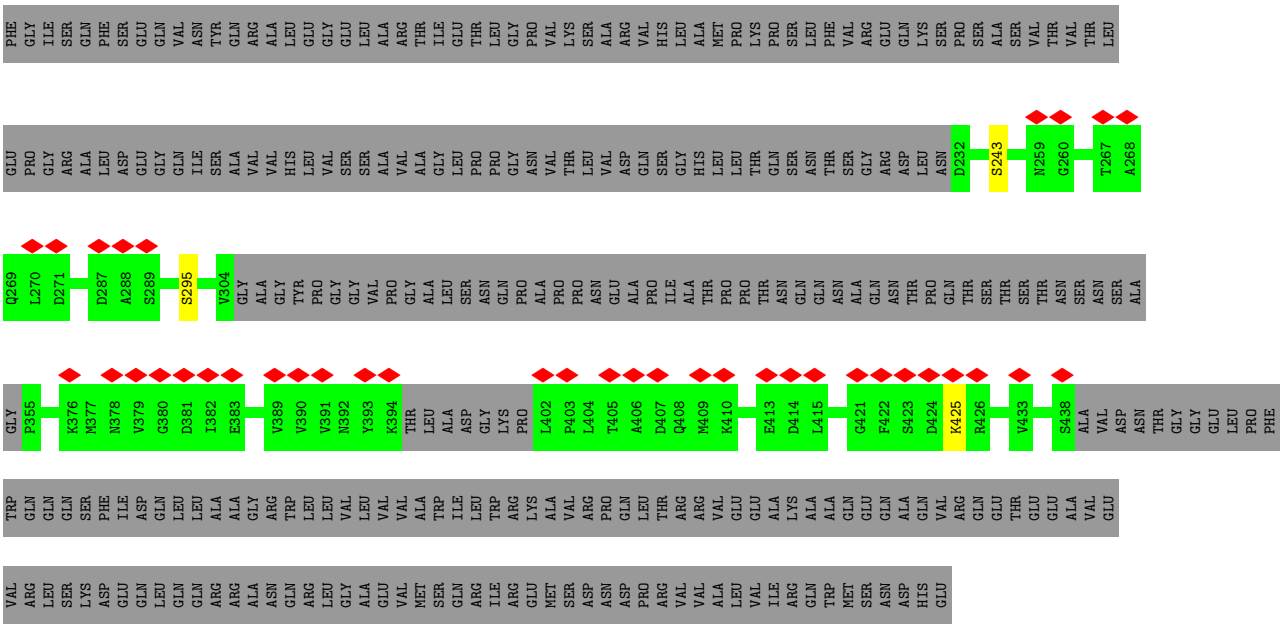


• Molecule 12: Flagellar M-ring protein



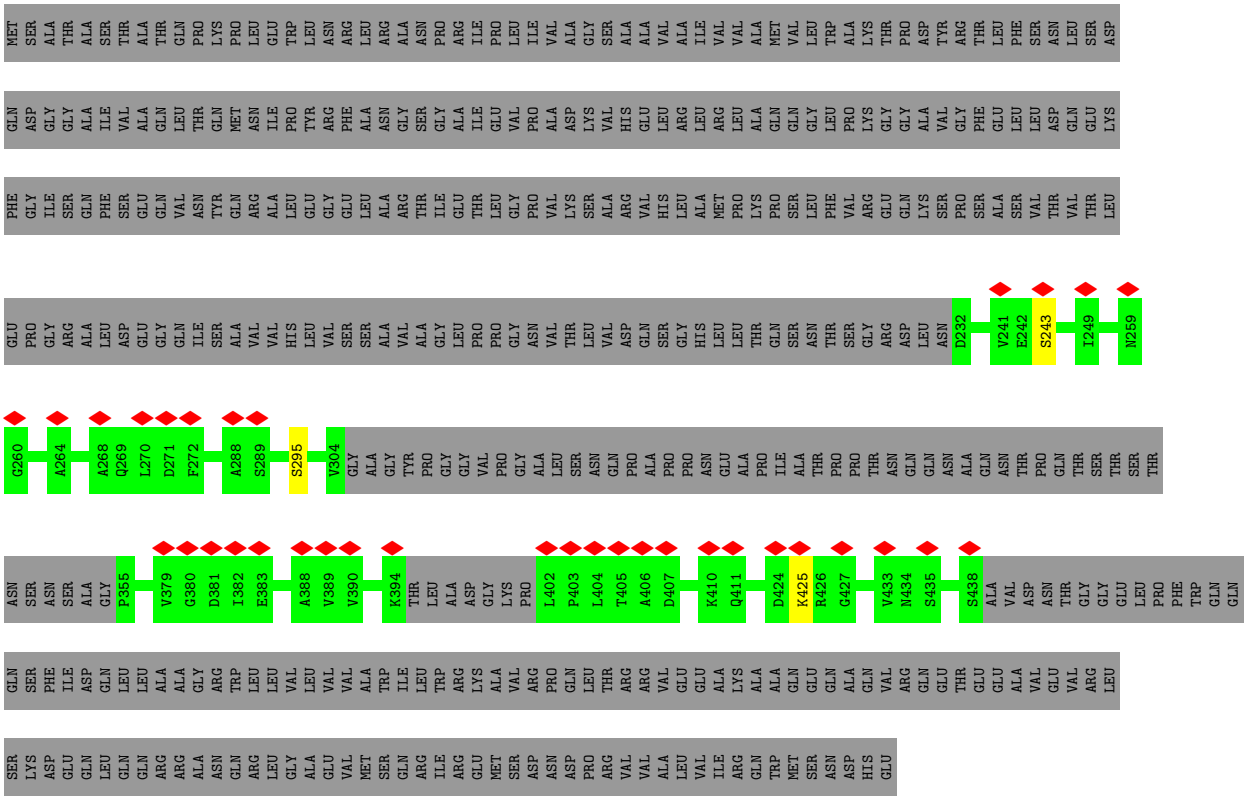
• Molecule 12: Flagellar M-ring protein





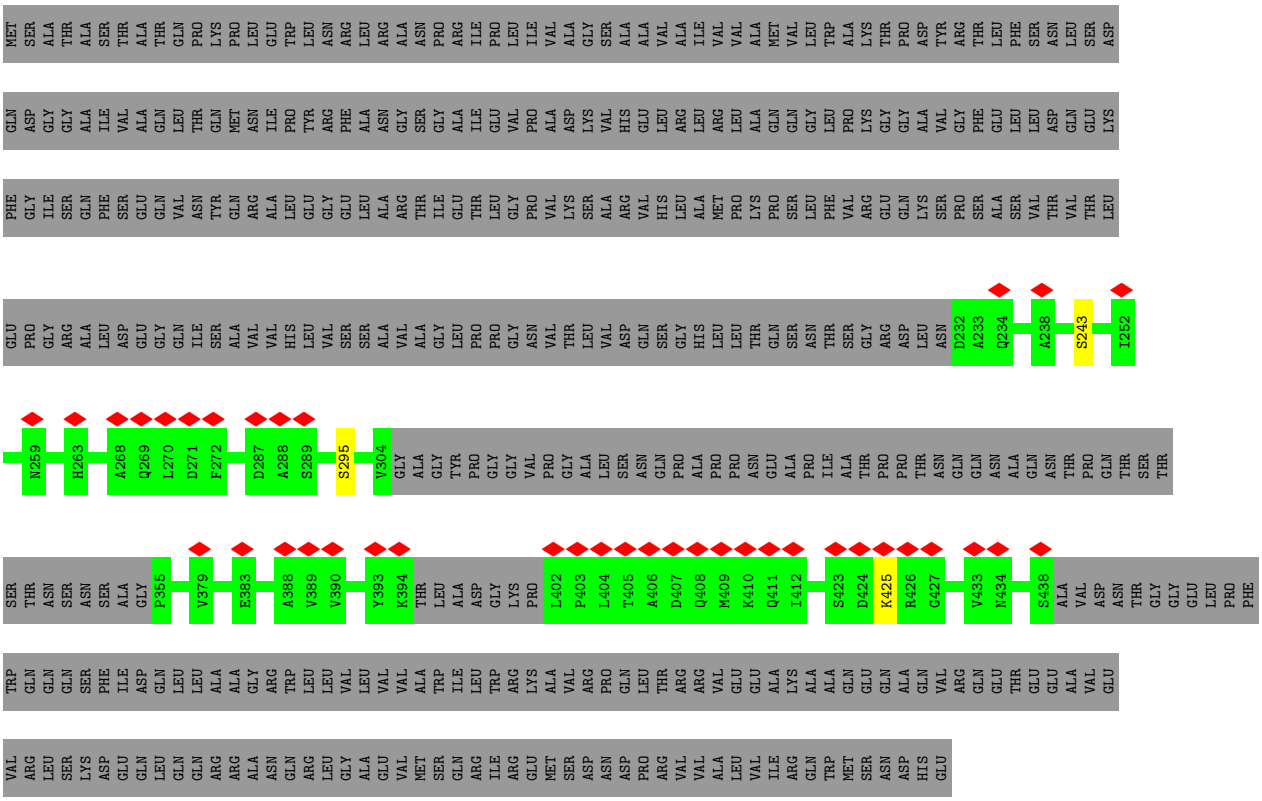
• Molecule 12: Flagellar M-ring protein

Chain Ee:



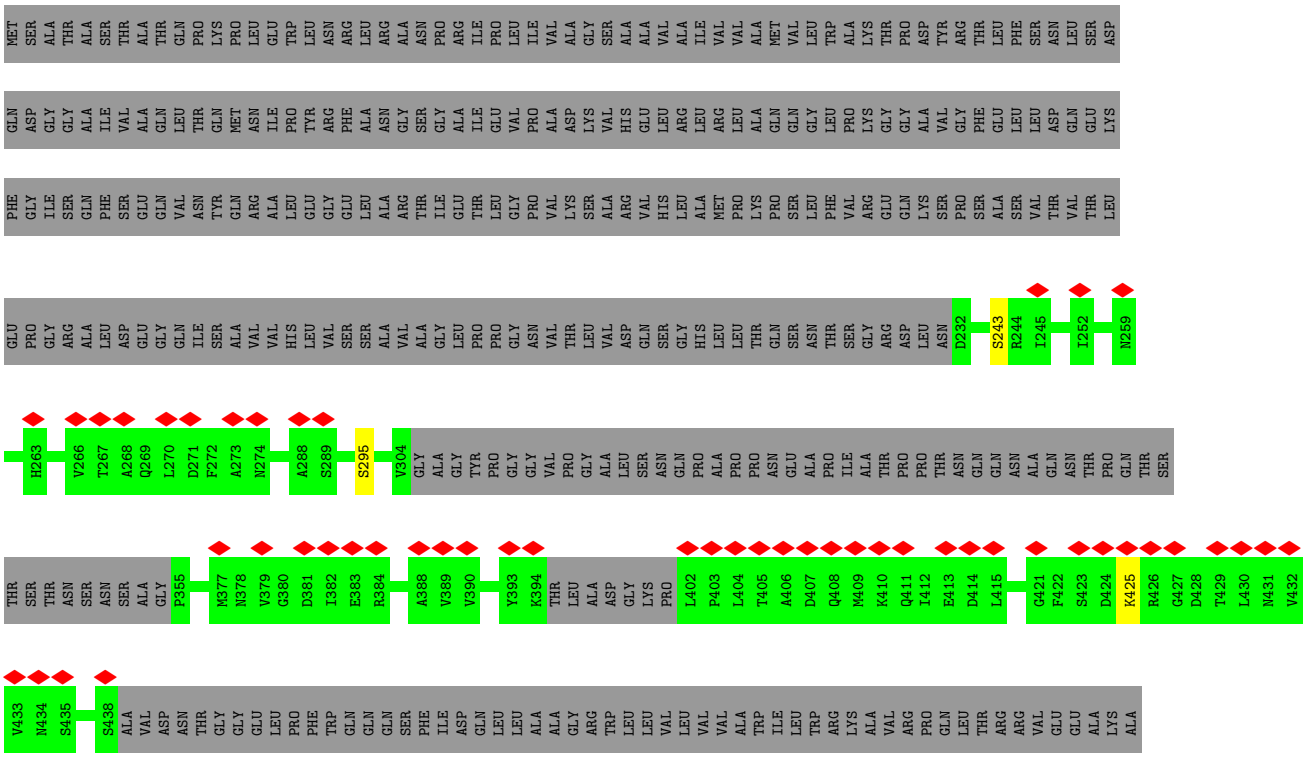
• Molecule 12: Flagellar M-ring protein

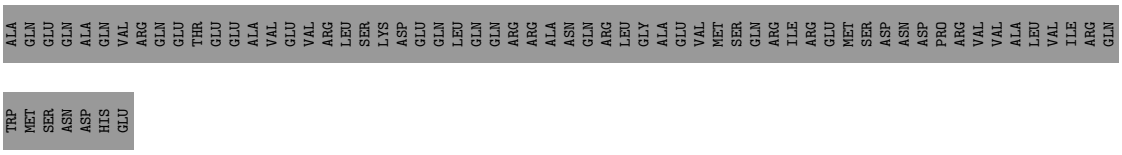
Chain Ef:



• Molecule 12: Flagellar M-ring protein

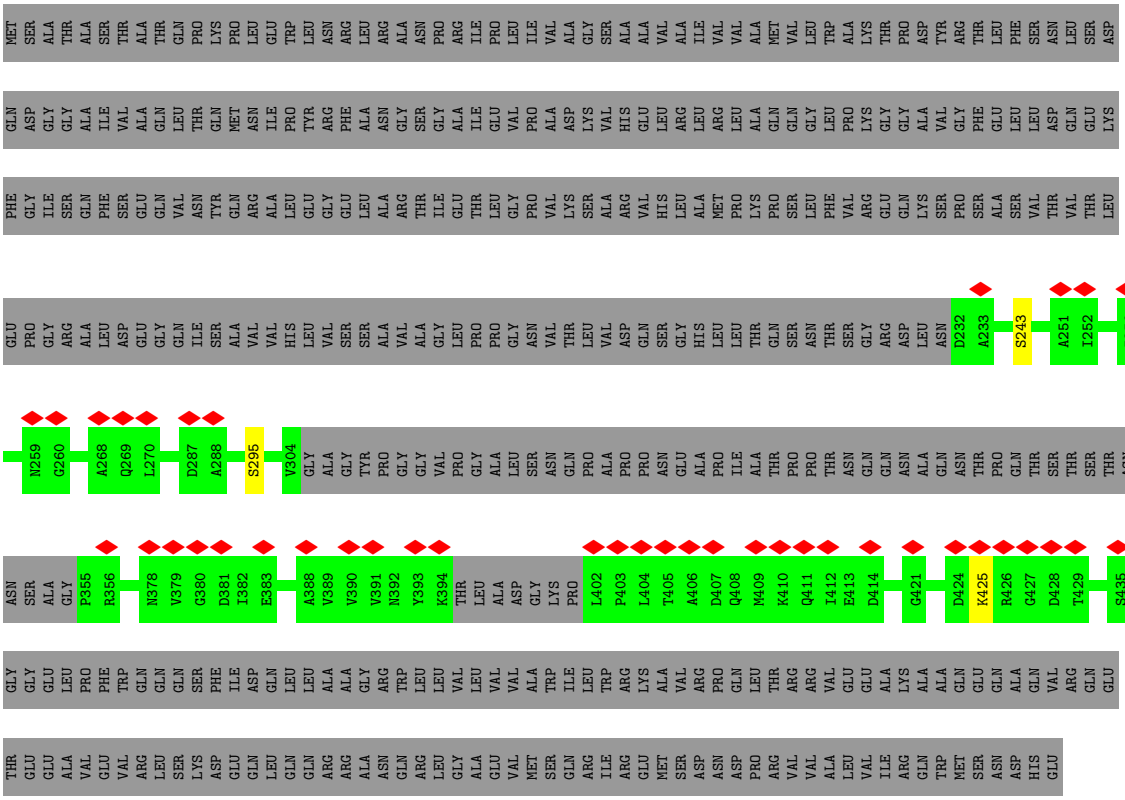
Chain Eg:





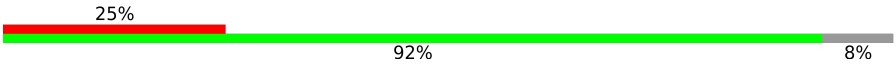
• Molecule 12: Flagellar M-ring protein

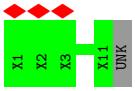
Chain Eh:



• Molecule 13: FlgB-Dc loop

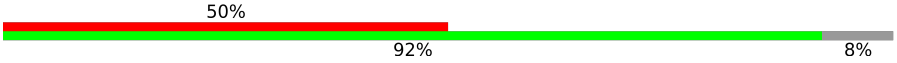
Chain GA:

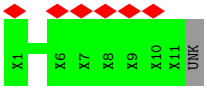




• Molecule 13: FlgB-Dc loop

Chain GC:





• Molecule 13: FlgB-Dc loop

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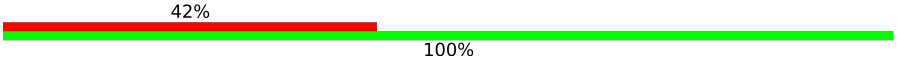
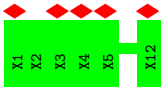
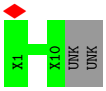




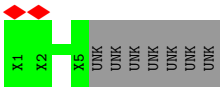
• Molecule 13: FlgB-Dc loop

Chain GD:



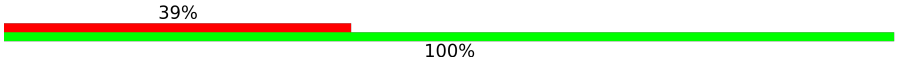
• Molecule 13: FlgB-Dc loop

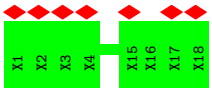
Chain GB:



• Molecule 14: FliE helix 1

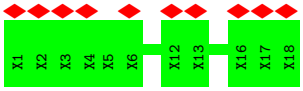
Chain GF:





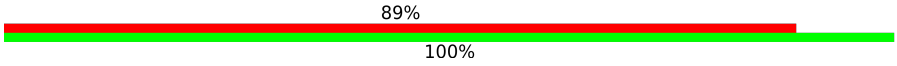
• Molecule 14: FliE helix 1

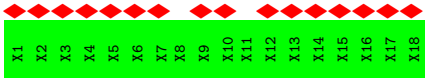
Chain GG:



• Molecule 14: FliE helix 1

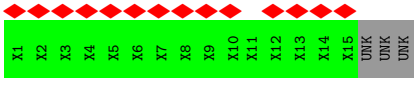
Chain GH:





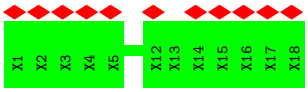
• Molecule 14: FliE helix 1

Chain GI:



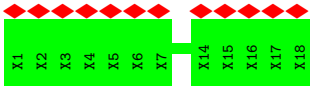
• Molecule 14: FliE helix 1

Chain GJ:



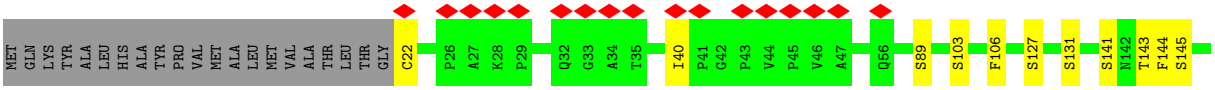
• Molecule 14: FliE helix 1

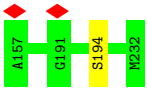
Chain GK:



• Molecule 15: Flagellar L-ring protein

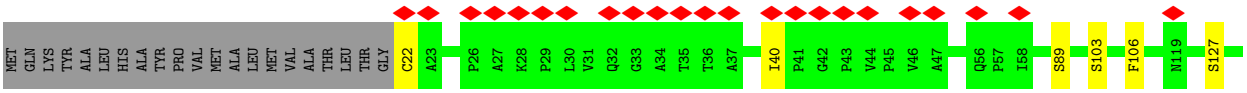
Chain AA:

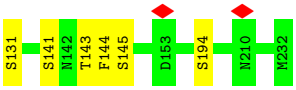




• Molecule 15: Flagellar L-ring protein

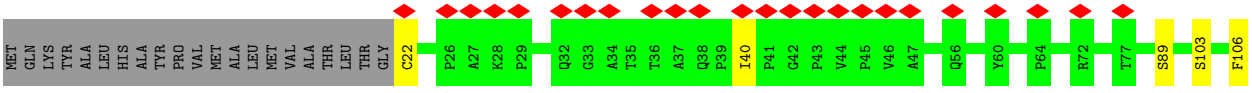
Chain AB:

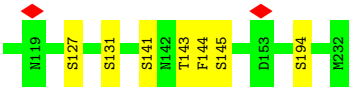




• Molecule 15: Flagellar L-ring protein

Chain AC:

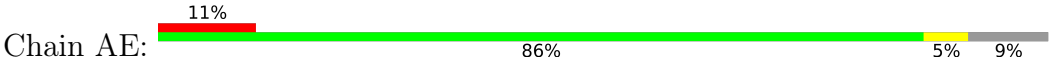


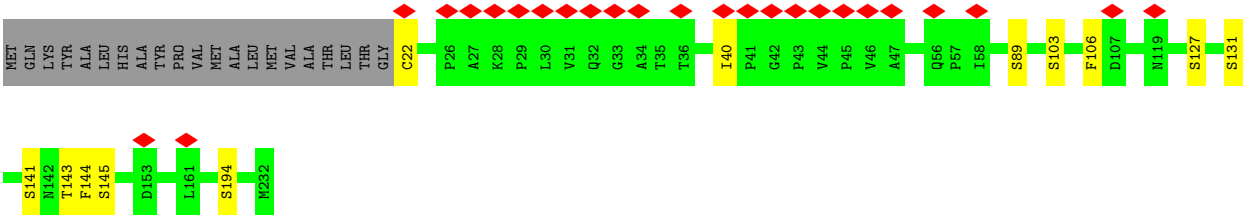


• Molecule 15: Flagellar L-ring protein

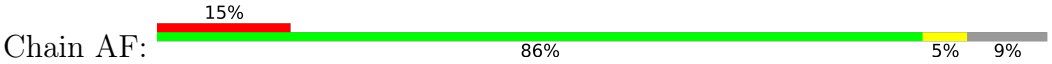
Chain AD:

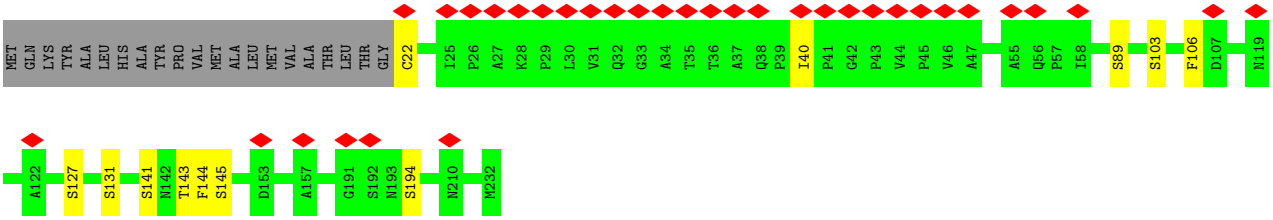
• Molecule 15: Flagellar L-ring protein



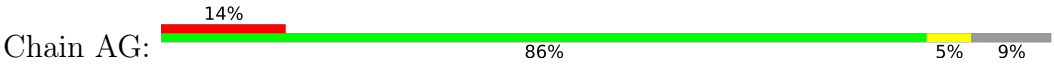


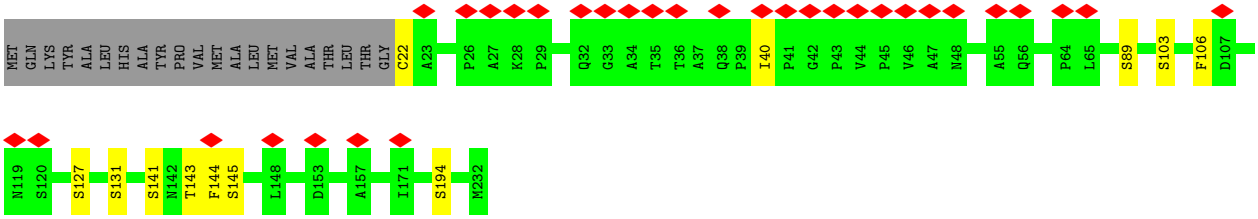
• Molecule 15: Flagellar L-ring protein



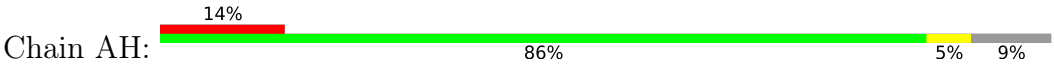


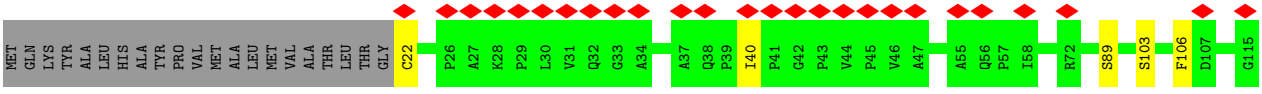
• Molecule 15: Flagellar L-ring protein

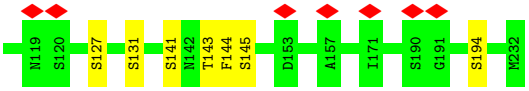




• Molecule 15: Flagellar L-ring protein







• Molecule 15: Flagellar L-ring protein

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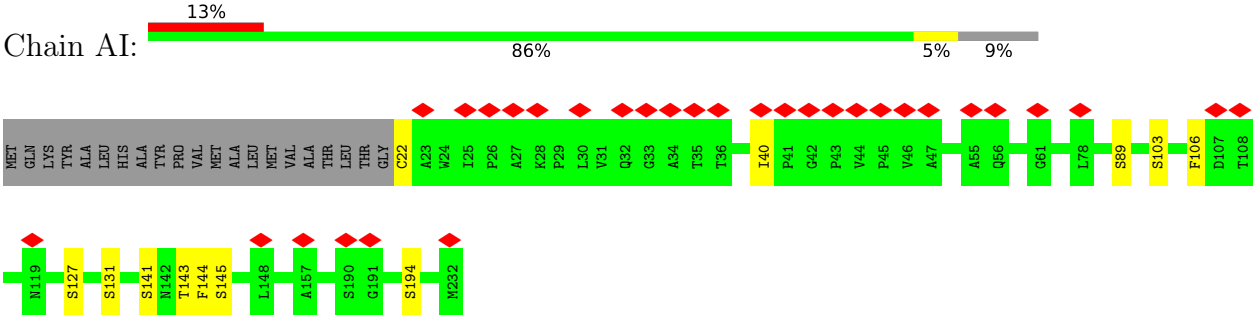
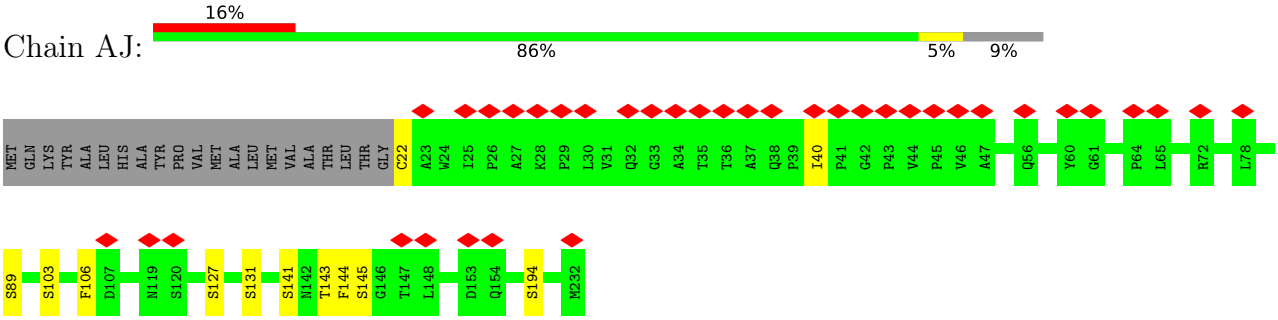


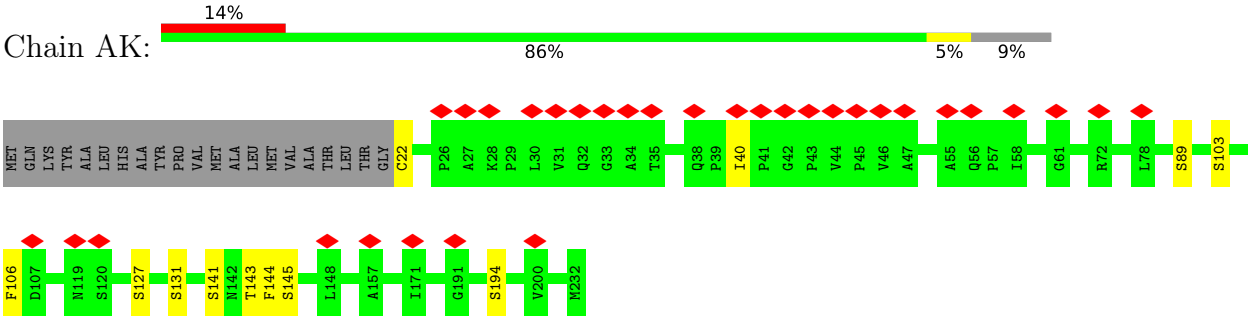
• Molecule 15: Flagellar L-ring protein

Chain AJ:



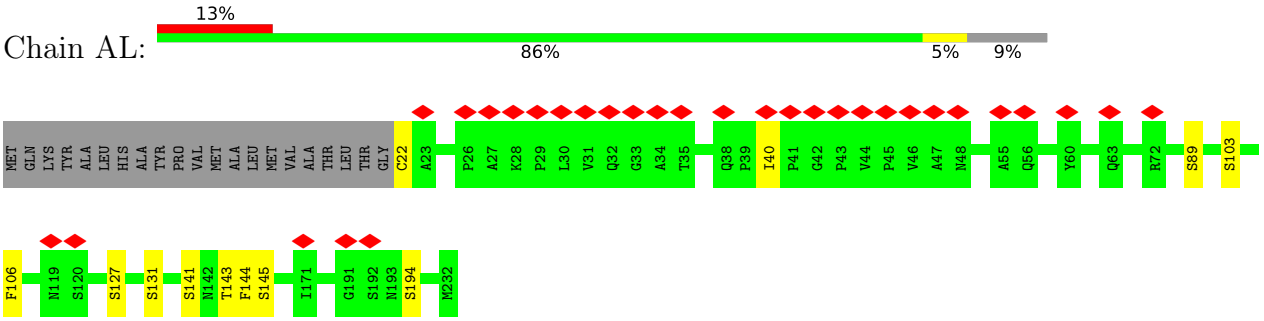
• Molecule 15: Flagellar L-ring protein

Chain AK:



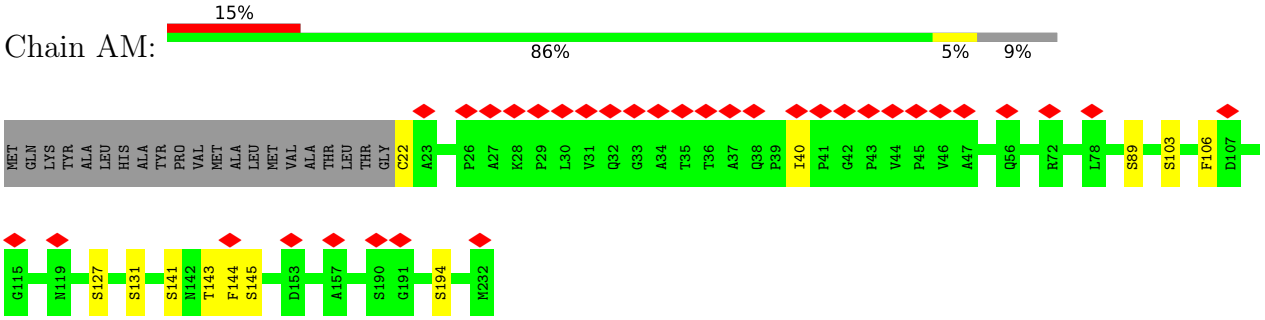
• Molecule 15: Flagellar L-ring protein

Chain AL:



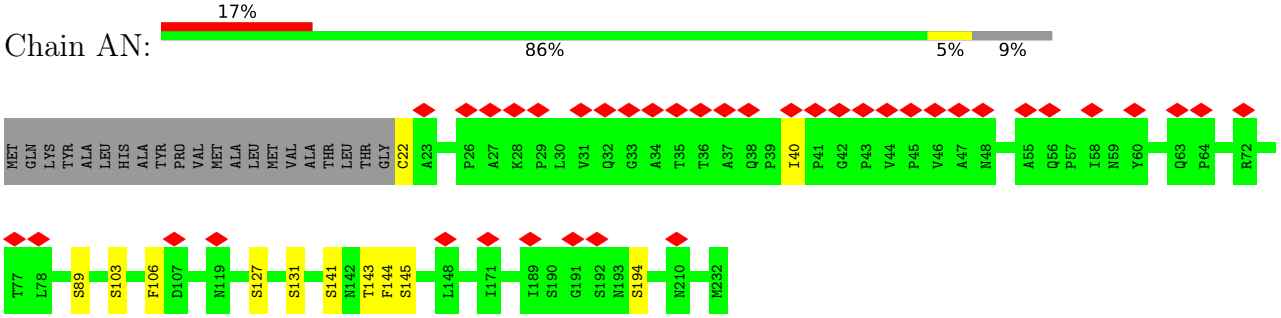
• Molecule 15: Flagellar L-ring protein

Chain AM:



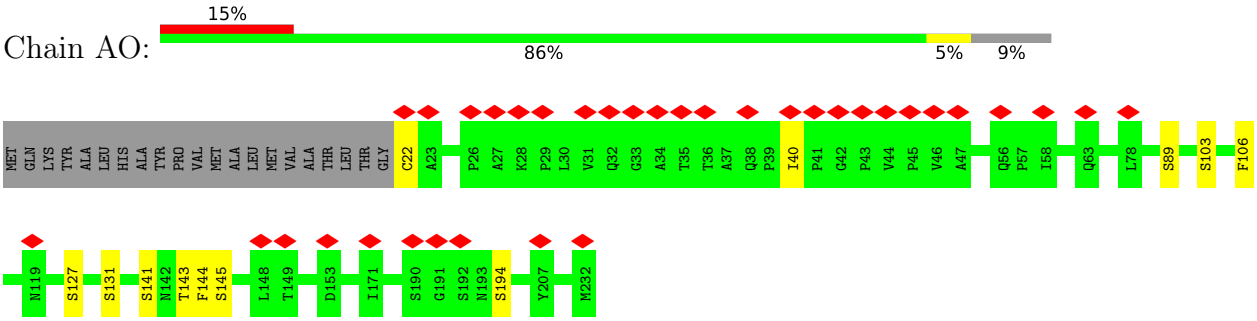
• Molecule 15: Flagellar L-ring protein

Chain AN:



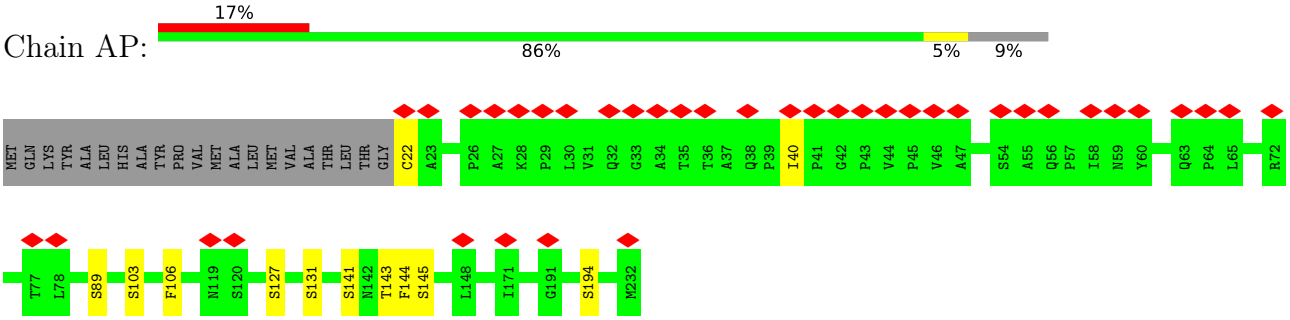
• Molecule 15: Flagellar L-ring protein

Chain AO:



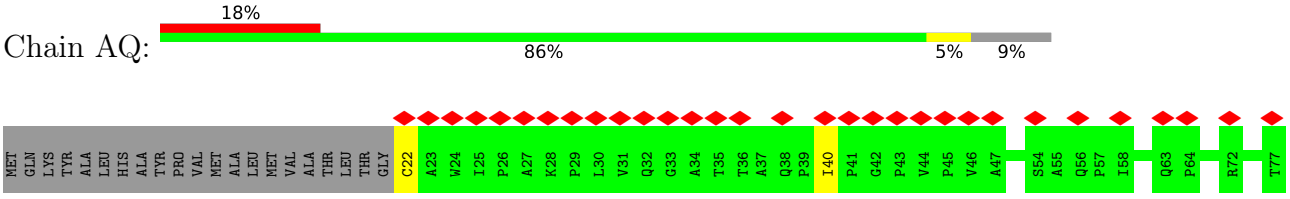
• Molecule 15: Flagellar L-ring protein

Chain AP:



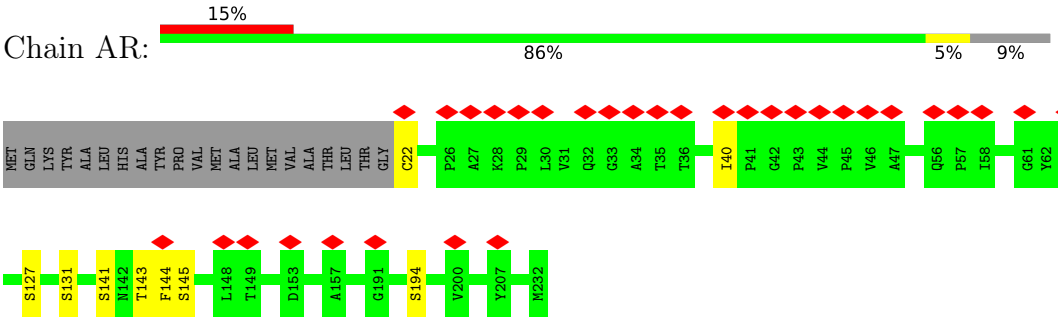
• Molecule 15: Flagellar L-ring protein

Chain AQ:



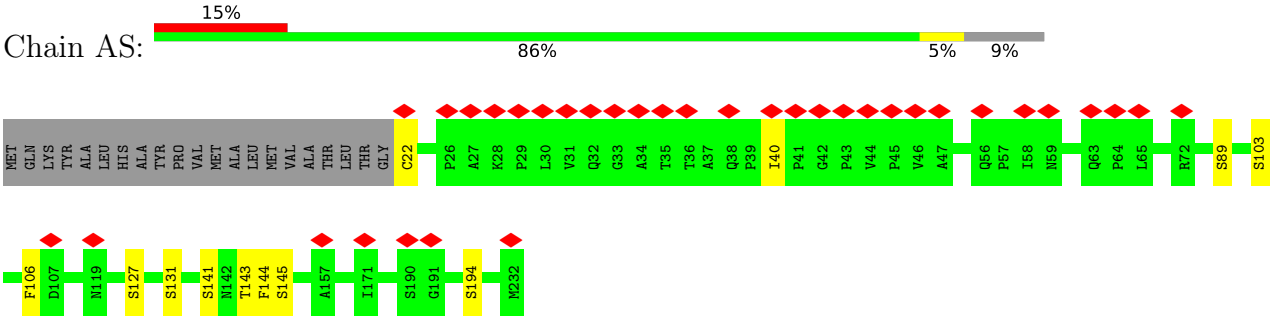
• Molecule 15: Flagellar L-ring protein

Chain AR:



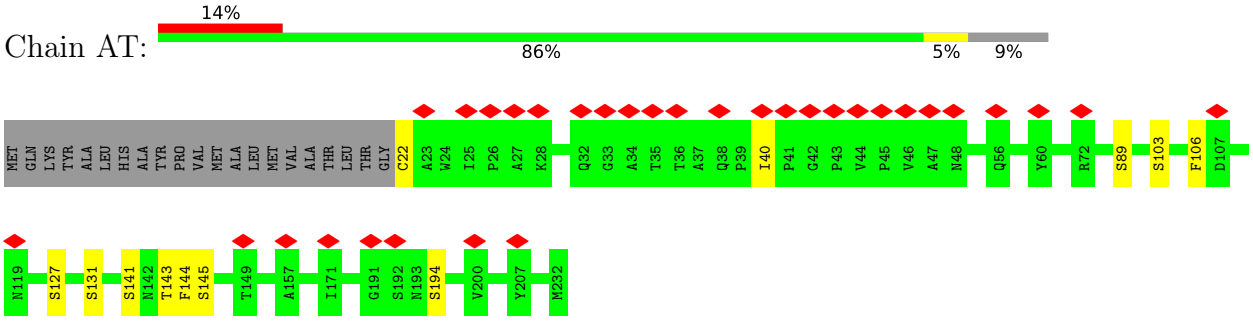
• Molecule 15: Flagellar L-ring protein

Chain AS:



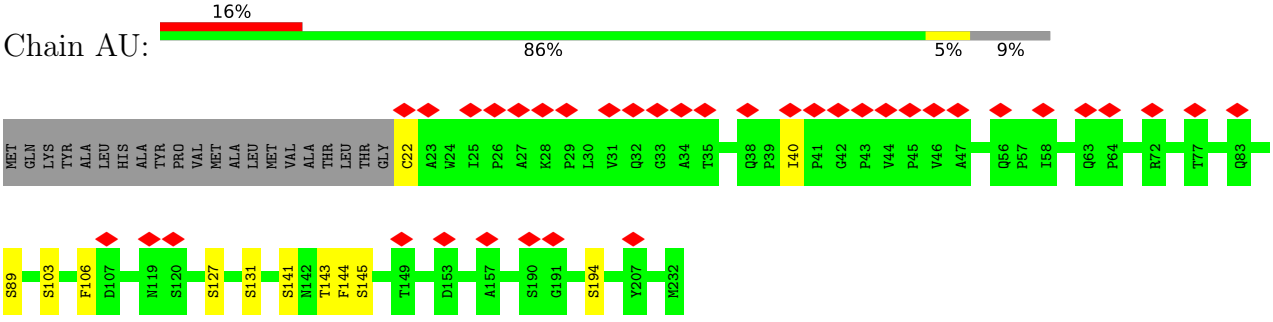
• Molecule 15: Flagellar L-ring protein

Chain AT:



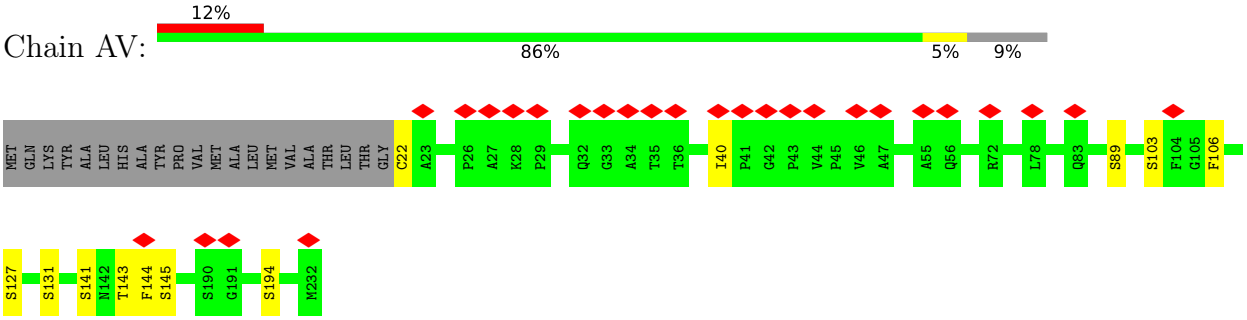
• Molecule 15: Flagellar L-ring protein

Chain AU:



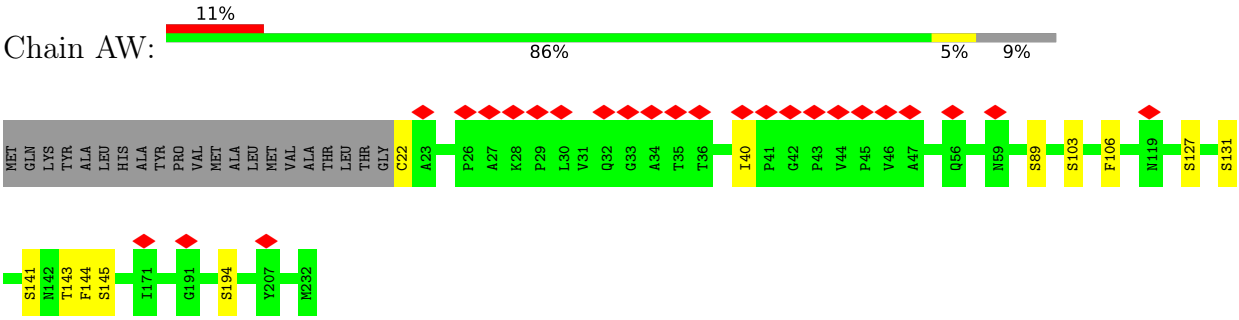
• Molecule 15: Flagellar L-ring protein

Chain AV:



• Molecule 15: Flagellar L-ring protein

Chain AW:



• Molecule 15: Flagellar L-ring protein

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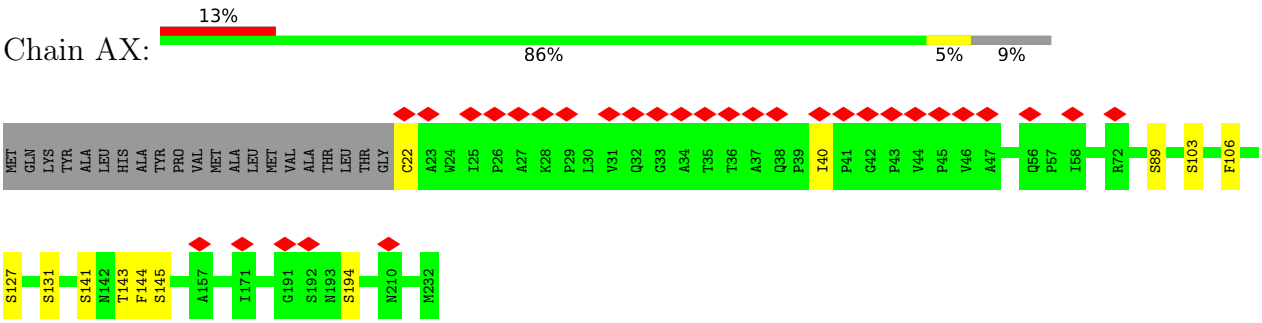

• Molecule 15: Flagellar L-ring protein

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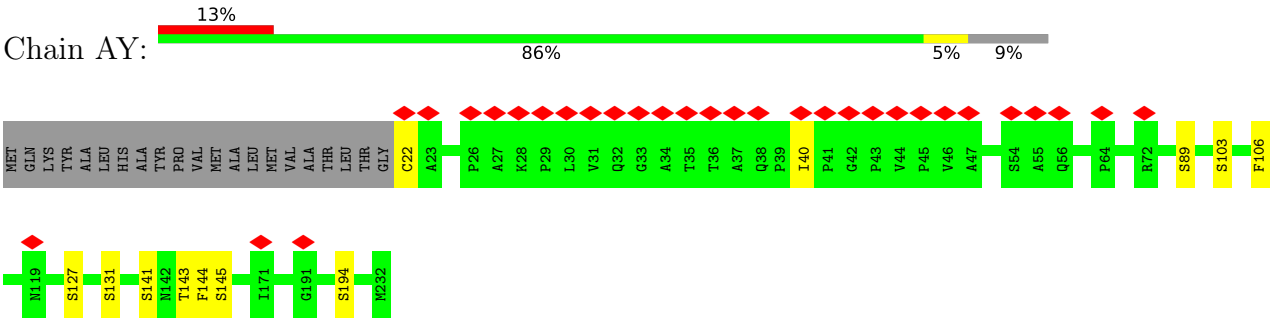

• Molecule 15: Flagellar L-ring protein

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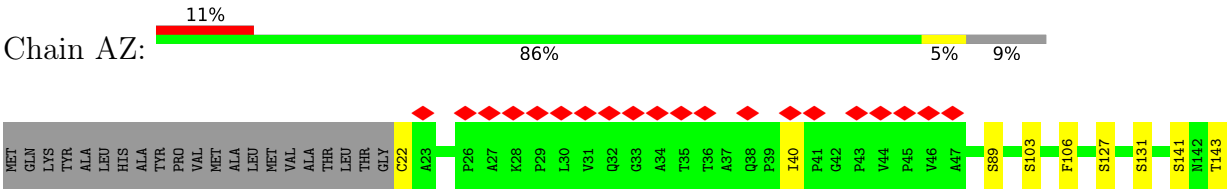
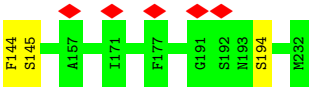
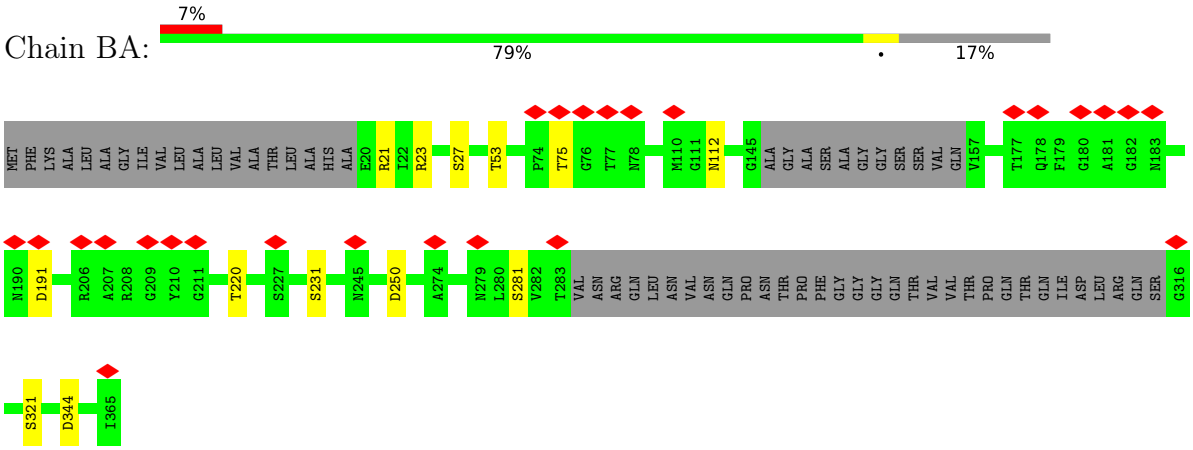




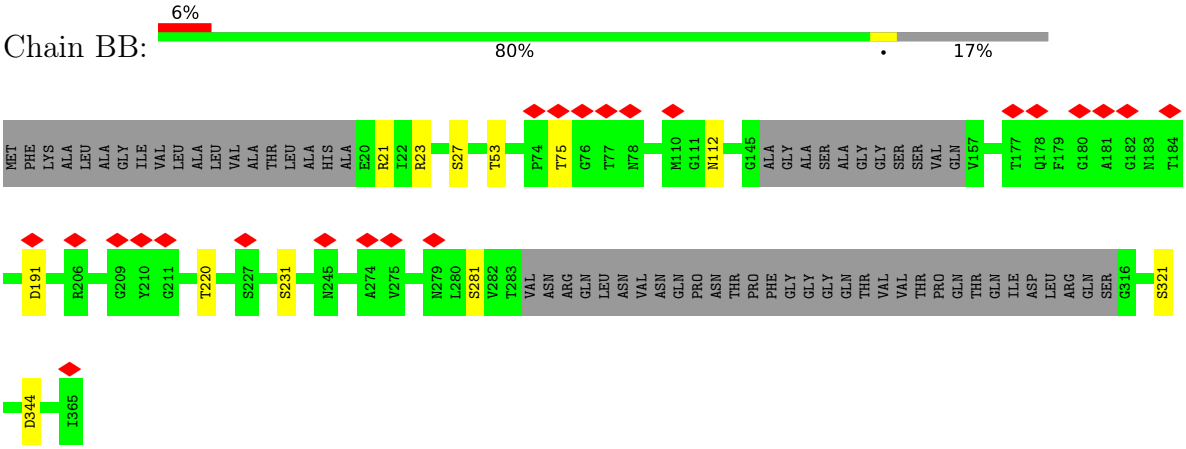
• Molecule 16: Flagellar P-ring protein

Chain BA:



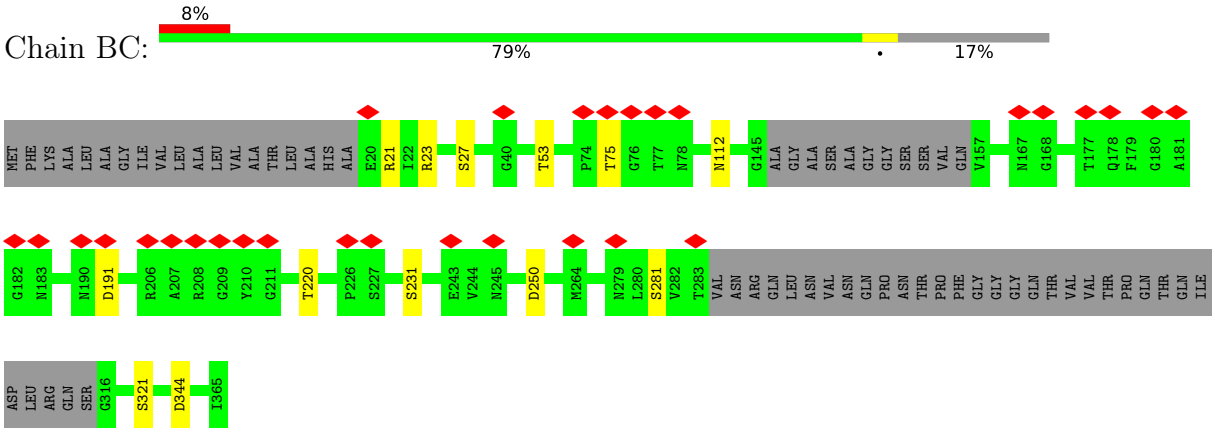
• Molecule 16: Flagellar P-ring protein

Chain BB:



• Molecule 16: Flagellar P-ring protein

Chain BC:



• Molecule 16: Flagellar P-ring protein

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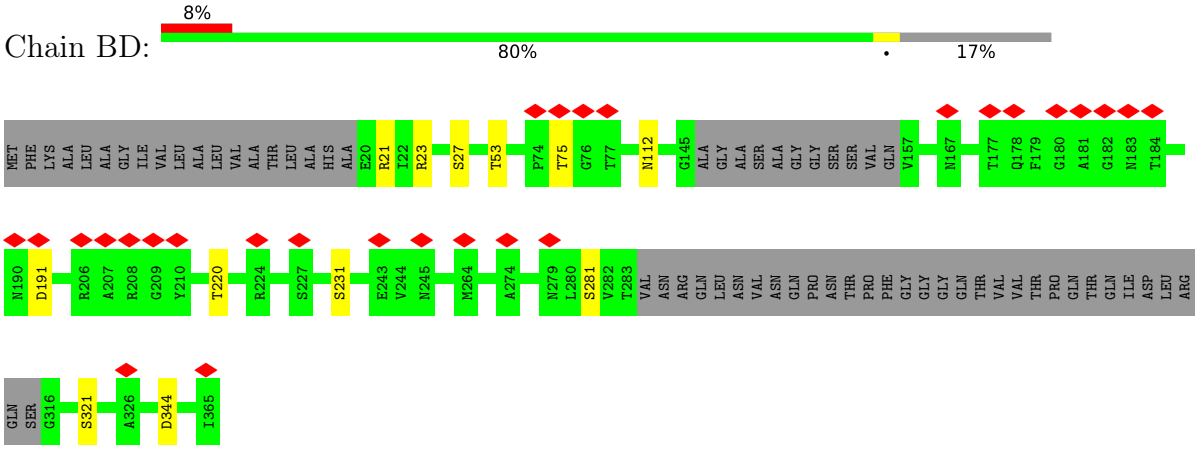

• Molecule 16: Flagellar P-ring protein

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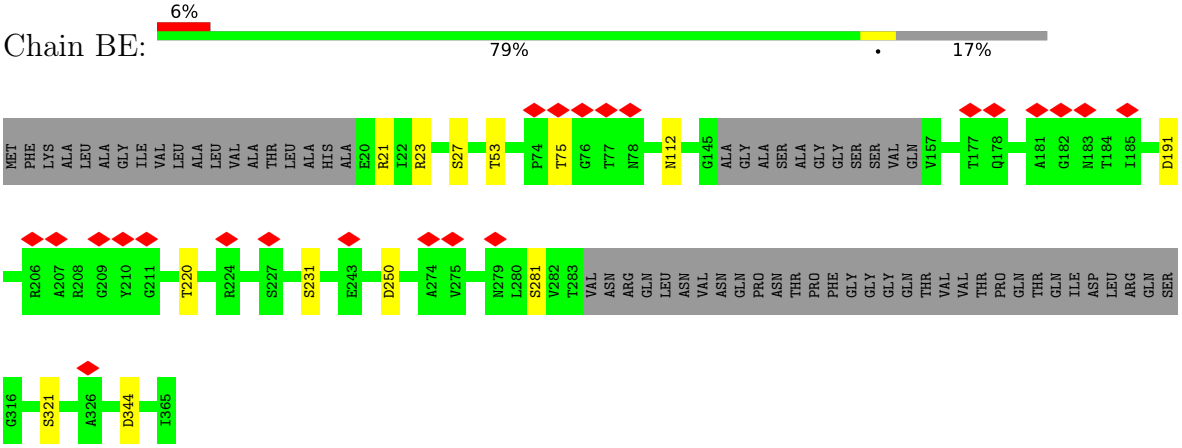
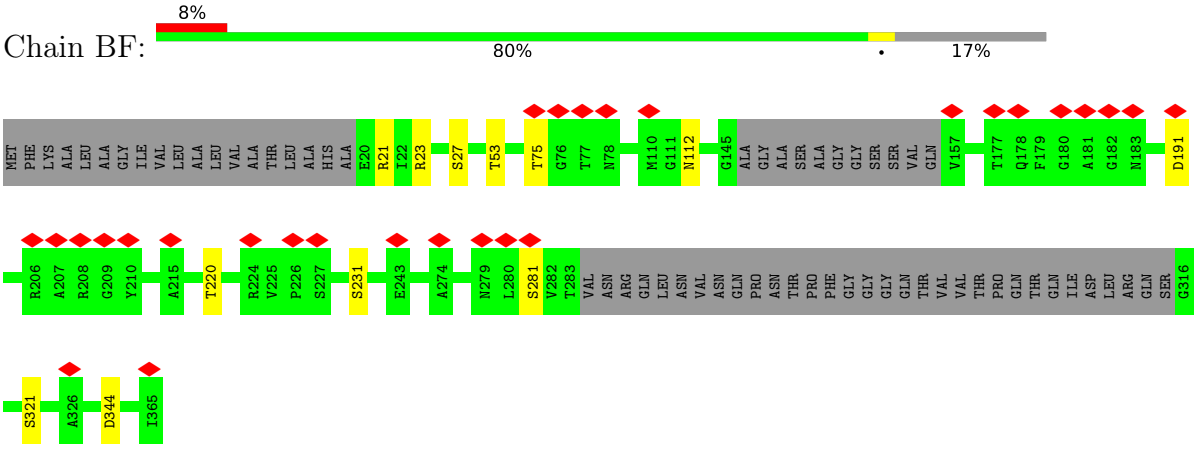


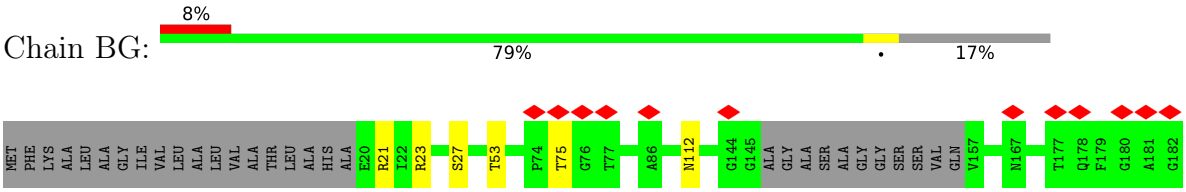
• Molecule 16: Flagellar P-ring protein

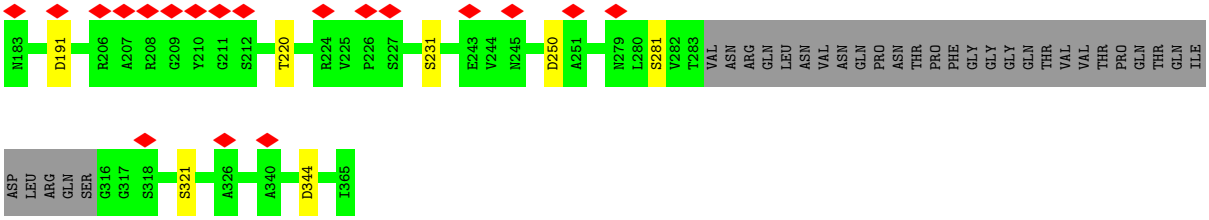
Chain BF:



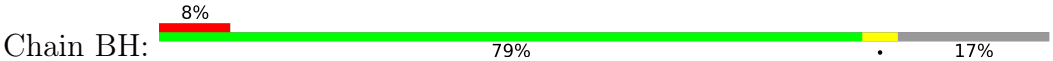
• Molecule 16: Flagellar P-ring protein

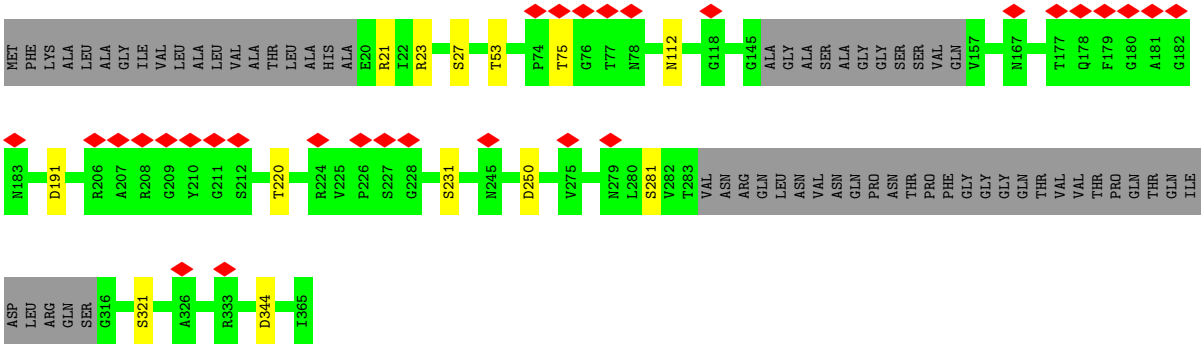
Chain BG:



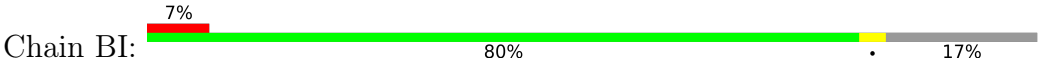


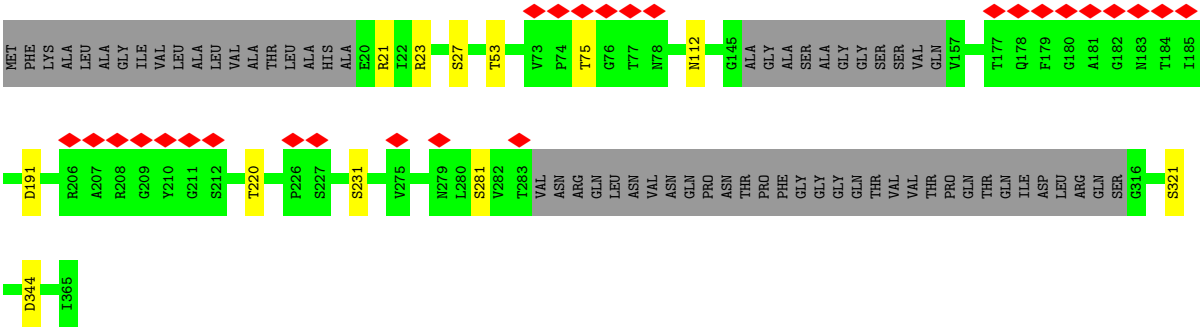
• Molecule 16: Flagellar P-ring protein



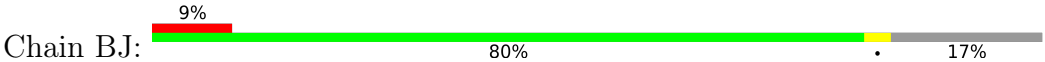


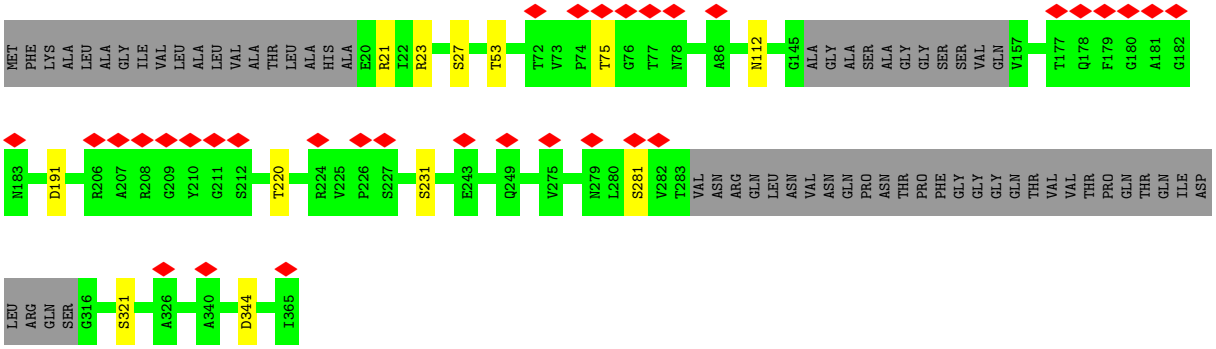
• Molecule 16: Flagellar P-ring protein





• Molecule 16: Flagellar P-ring protein





• Molecule 16: Flagellar P-ring protein

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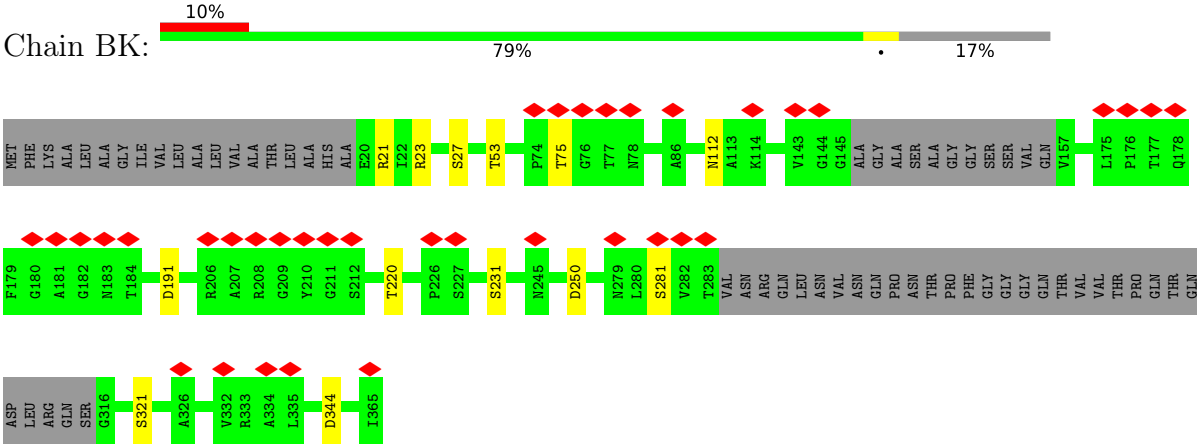
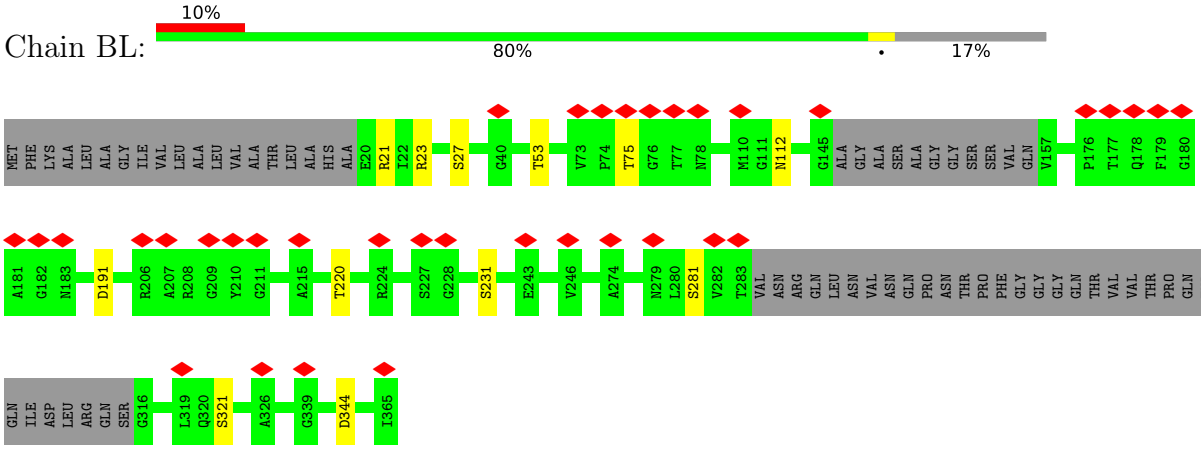


• Molecule 16: Flagellar P-ring protein

Chain BL:



• Molecule 16: Flagellar P-ring protein

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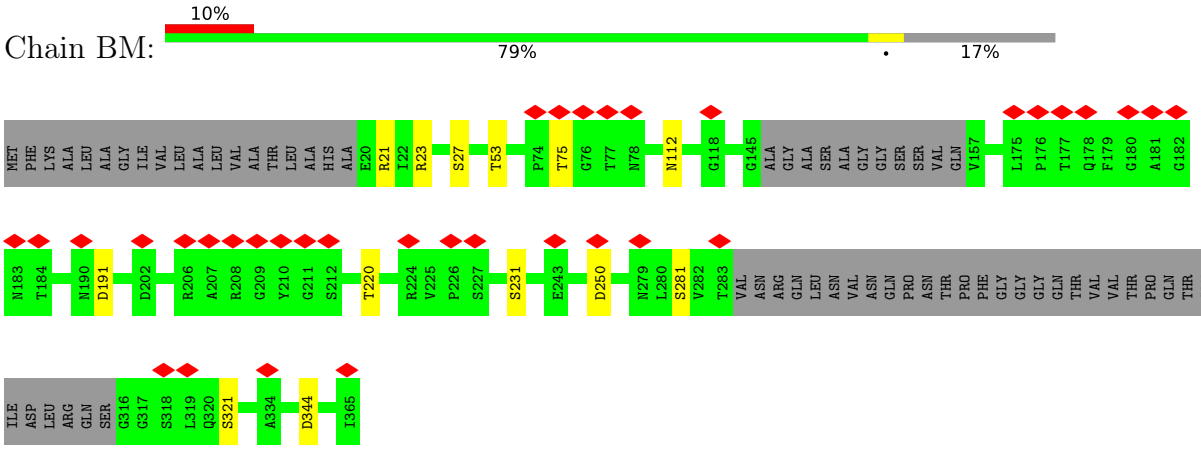
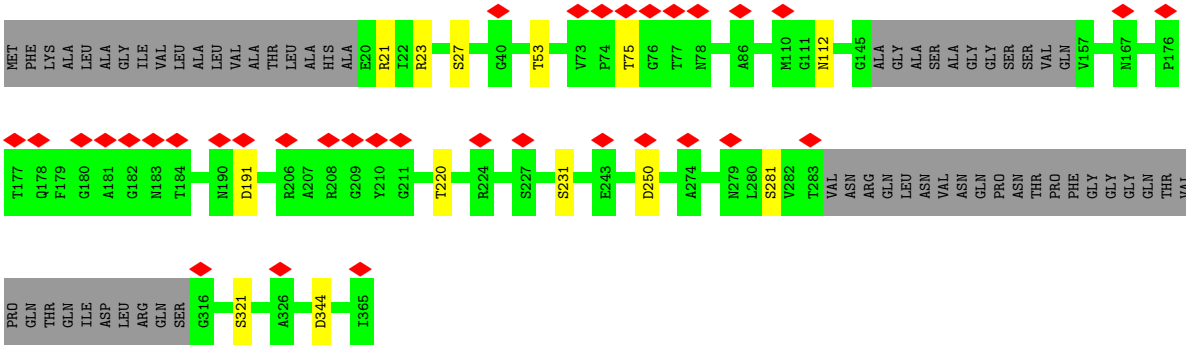
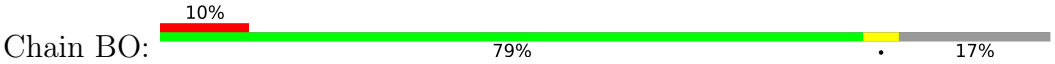


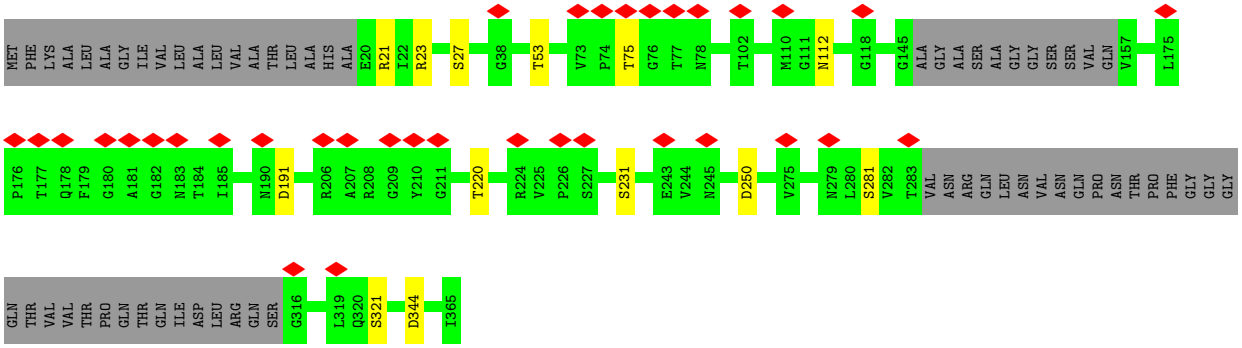
• Molecule 16: Flagellar P-ring protein

Chain BN:

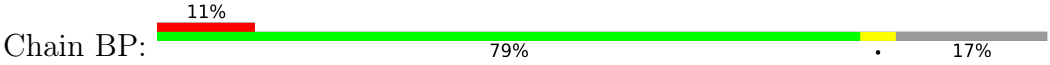


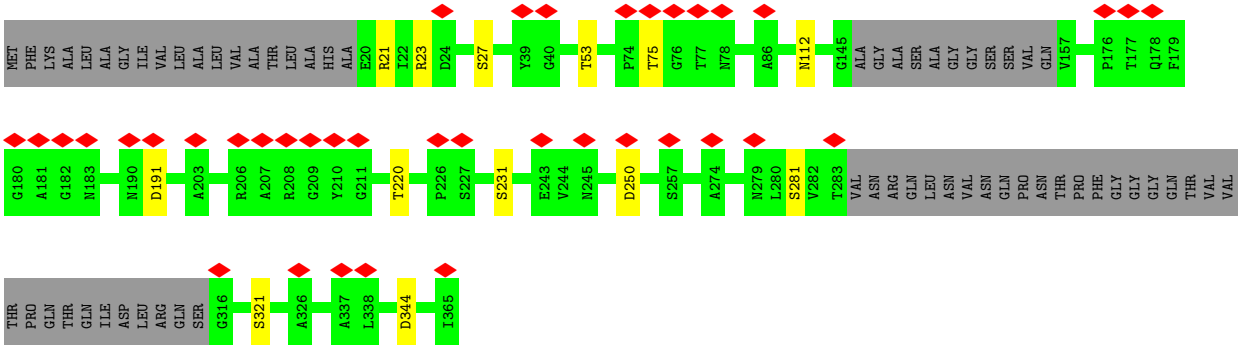
• Molecule 16: Flagellar P-ring protein



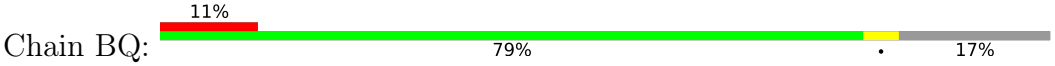


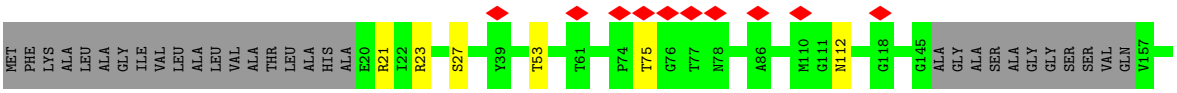
• Molecule 16: Flagellar P-ring protein

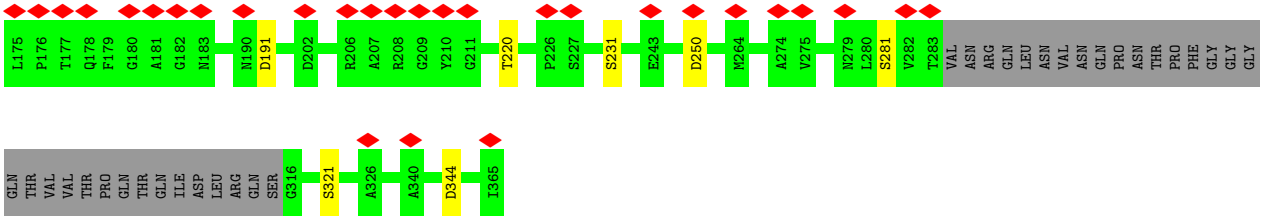




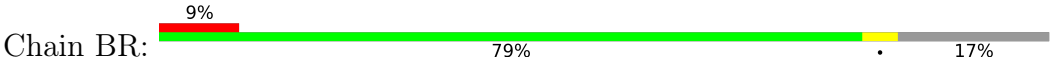
• Molecule 16: Flagellar P-ring protein

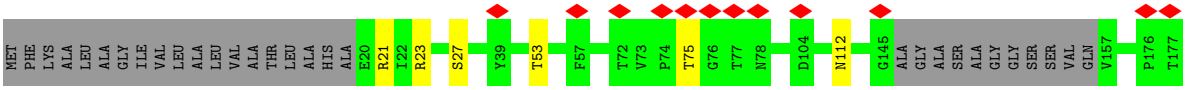


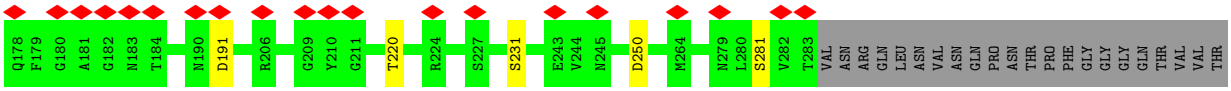


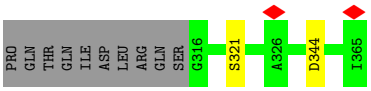


• Molecule 16: Flagellar P-ring protein

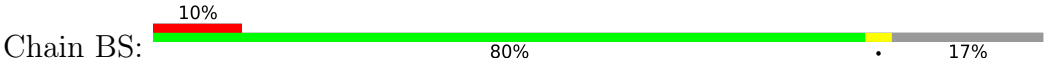


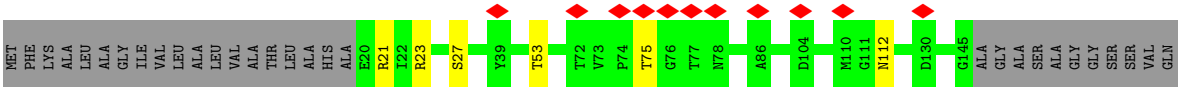


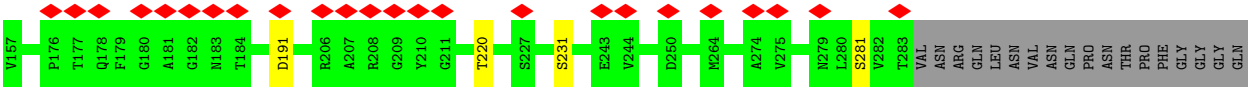


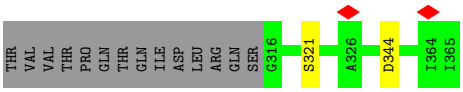


• Molecule 16: Flagellar P-ring protein

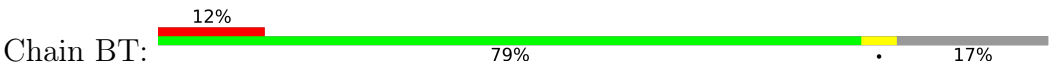


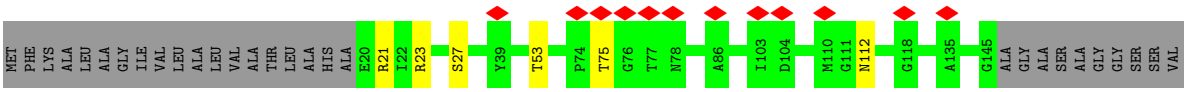


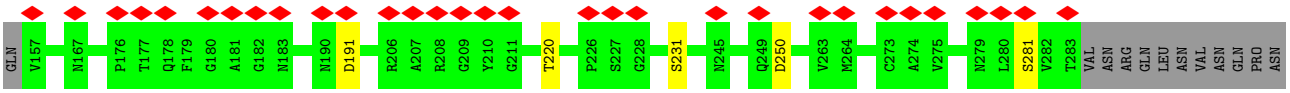


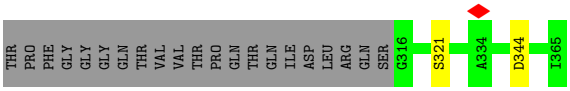


• Molecule 16: Flagellar P-ring protein



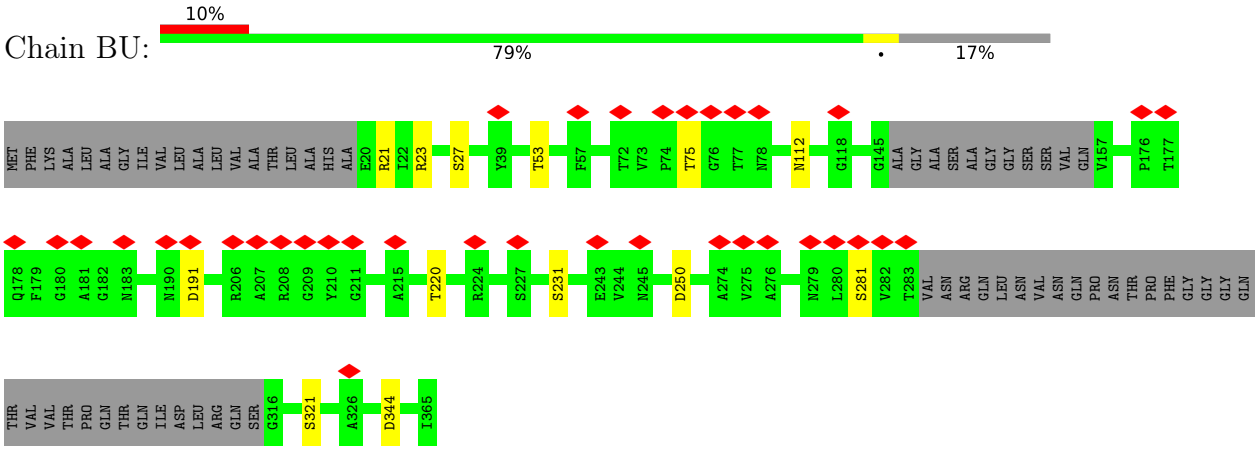






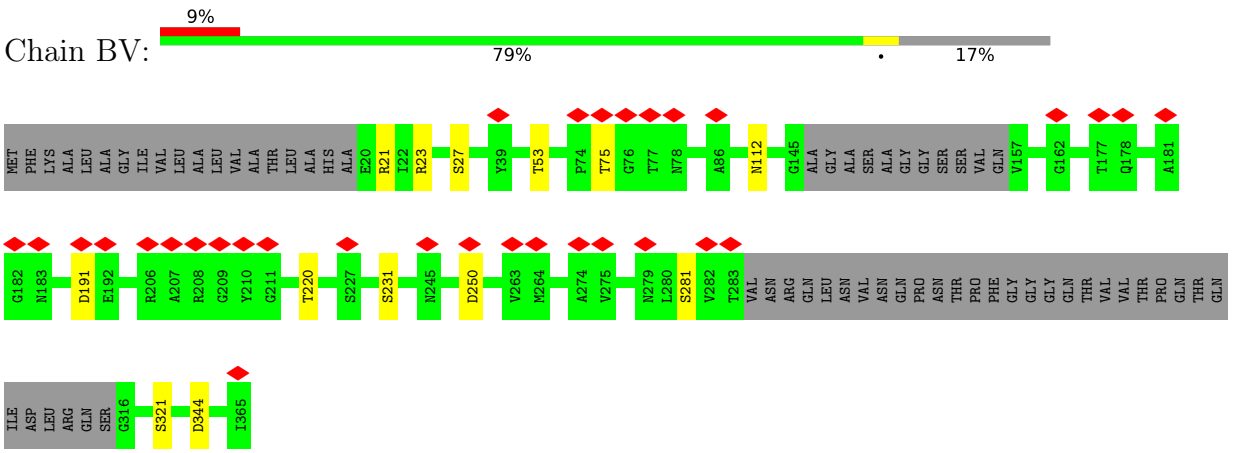
• Molecule 16: Flagellar P-ring protein

Chain BU:



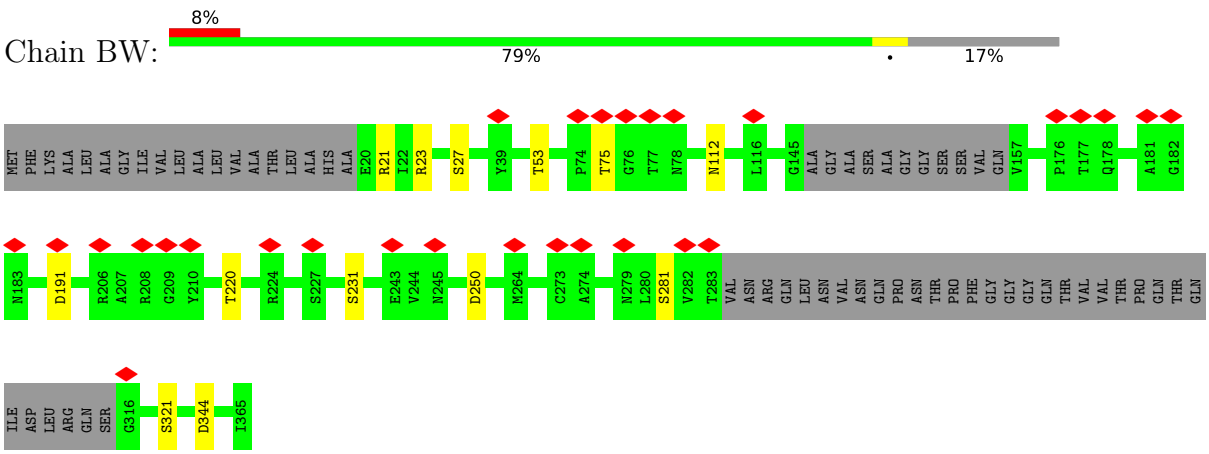
• Molecule 16: Flagellar P-ring protein

Chain BV:



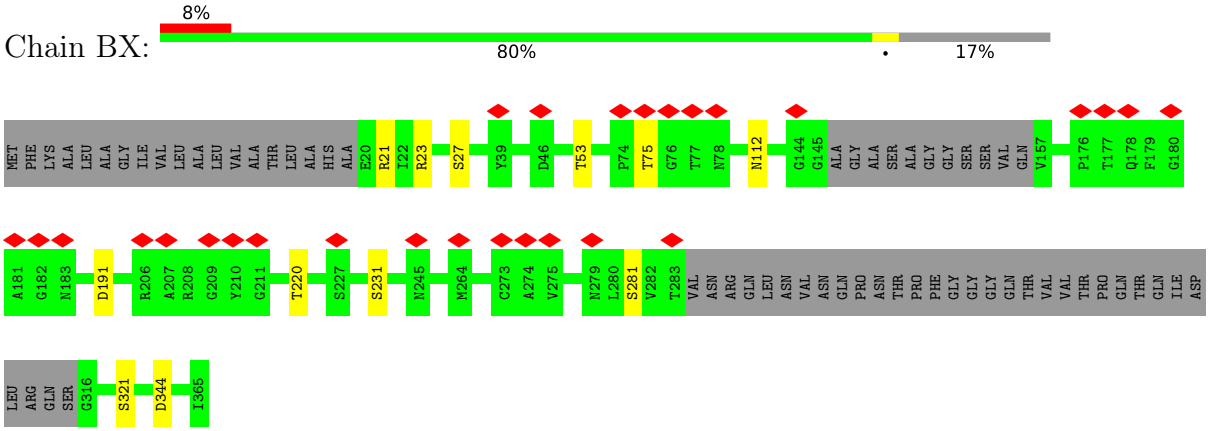
• Molecule 16: Flagellar P-ring protein

Chain BW:



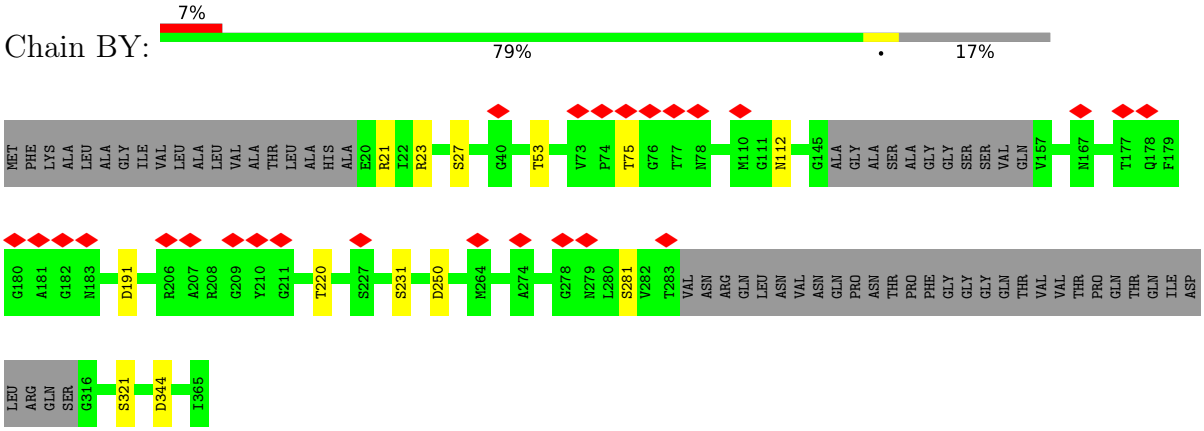
• Molecule 16: Flagellar P-ring protein

Chain BX:



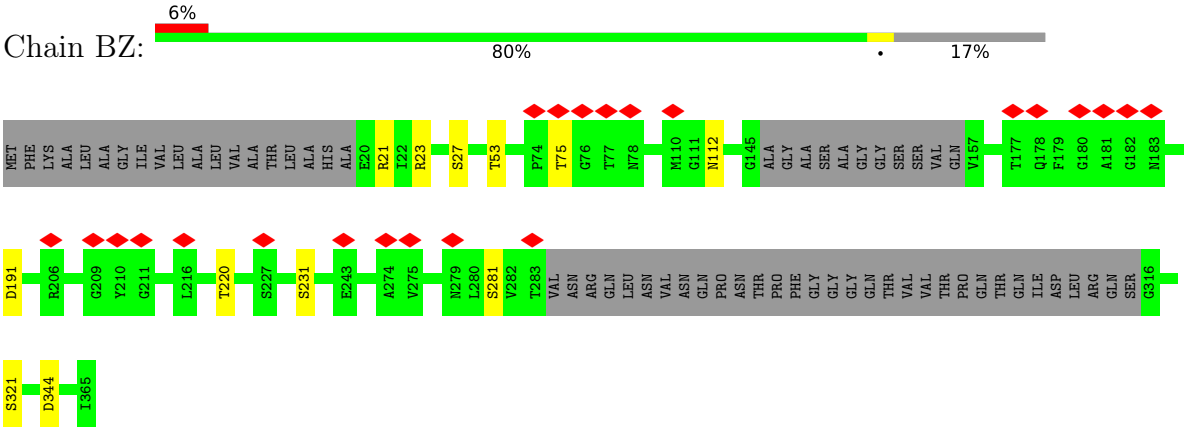
• Molecule 16: Flagellar P-ring protein

Chain BY:



• Molecule 16: Flagellar P-ring protein

Chain BZ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52714	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 ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.383	Depositor
Minimum map value	-0.418	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	669.184, 669.184, 669.184	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: P1L

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	A	0.27	0/1973	0.48	0/2682
1	B	0.27	0/1973	0.48	0/2682
1	C	0.27	0/1973	0.48	0/2682
1	D	0.28	0/1973	0.48	0/2682
1	E	0.27	0/1973	0.49	0/2682
1	F	0.28	0/1973	0.48	0/2682
1	G	0.28	0/1973	0.49	0/2682
1	H	0.27	0/1973	0.48	0/2682
1	I	0.28	0/1973	0.49	0/2682
1	J	0.28	0/1973	0.48	0/2682
1	K	0.28	0/1973	0.50	0/2682
1	L	0.28	0/1965	0.47	0/2672
1	M	0.28	0/1973	0.48	0/2682
1	N	0.28	0/1909	0.47	0/2593
1	O	0.28	0/1917	0.48	0/2605
1	P	0.28	0/1884	0.48	0/2559
1	Q	0.28	0/1880	0.48	0/2554
1	R	0.28	0/1898	0.48	0/2578
1	S	0.29	0/1880	0.50	0/2554
1	T	0.28	0/1925	0.47	0/2617
1	U	0.28	0/1965	0.48	0/2672
1	V	0.28	0/1965	0.47	0/2672
1	W	0.29	0/1965	0.49	0/2672
1	X	0.27	0/1965	0.49	1/2672 (0.0%)
2	a	0.27	0/1836	0.50	0/2502
2	b	0.26	0/1828	0.49	0/2492
2	c	0.27	0/1836	0.49	0/2502
2	d	0.27	0/1836	0.50	0/2502
2	e	0.26	0/1836	0.50	0/2502
4	5	0.28	0/145	0.42	0/203
4	6	0.26	0/145	0.43	0/203
4	7	0.40	0/145	0.55	0/203

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	8	0.27	0/145	0.41	0/203
4	9	0.26	0/145	0.44	0/203
5	f	0.27	0/946	0.44	0/1285
5	g	0.27	0/959	0.45	0/1302
5	h	0.28	0/945	0.45	0/1283
5	i	0.28	0/954	0.46	0/1295
5	j	0.28	0/941	0.46	0/1278
5	p	0.27	0/950	0.43	0/1290
6	k	0.26	0/859	0.48	0/1156
6	l	0.26	0/840	0.48	0/1131
6	m	0.26	0/840	0.47	0/1131
6	n	0.26	0/851	0.49	0/1145
6	o	0.25	0/863	0.50	0/1161
7	q	0.26	0/540	0.44	0/723
7	r	0.26	0/529	0.46	0/709
7	s	0.26	0/547	0.44	0/733
7	t	0.25	0/547	0.44	0/733
7	u	0.25	0/547	0.46	0/733
7	v	0.24	0/289	0.39	0/385
8	DA	0.26	0/2991	0.45	0/4076
8	DB	0.26	0/2991	0.45	0/4076
8	DC	0.26	0/2991	0.45	0/4076
8	DD	0.26	0/2991	0.45	0/4076
8	DE	0.26	0/2991	0.45	0/4076
8	DF	0.25	0/2991	0.45	0/4076
8	DG	0.25	0/2991	0.45	0/4076
8	DH	0.26	0/2991	0.45	0/4076
8	DI	0.26	0/2991	0.46	0/4076
8	DJ	0.28	0/2991	0.48	1/4076 (0.0%)
8	DK	0.26	0/2991	0.47	1/4076 (0.0%)
8	DL	0.45	1/2991 (0.0%)	0.67	3/4076 (0.1%)
8	DM	0.34	0/2991	0.60	1/4076 (0.0%)
8	DN	0.41	1/2991 (0.0%)	0.65	1/4076 (0.0%)
8	DO	0.39	0/2991	0.65	0/4076
8	DP	0.29	0/2991	0.55	1/4076 (0.0%)
8	DQ	0.33	1/2991 (0.0%)	0.55	0/4076
8	DR	0.26	0/2991	0.51	0/4076
8	DS	0.28	0/2991	0.53	1/4076 (0.0%)
8	DT	0.27	0/2991	0.49	0/4076
8	DU	0.28	0/2991	0.54	1/4076 (0.0%)
8	DV	0.27	0/2991	0.52	0/4076
8	DW	0.26	0/2991	0.51	1/4076 (0.0%)
8	DX	0.26	0/2991	0.49	1/4076 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
8	DY	0.27	0/2991	0.51	1/4076 (0.0%)
8	DZ	0.27	0/2991	0.50	0/4076
8	EA	0.26	0/2991	0.50	0/4076
8	EB	0.26	0/2991	0.50	0/4076
8	EC	0.27	0/2991	0.51	1/4076 (0.0%)
8	ED	0.26	0/2991	0.49	0/4076
8	EE	0.26	0/2991	0.49	0/4076
8	EF	0.26	0/2991	0.49	0/4076
8	EG	0.26	0/2991	0.50	0/4076
9	CE	0.25	0/2052	0.44	0/2803
10	CA	0.24	0/681	0.45	1/930 (0.1%)
10	CB	0.25	0/681	0.44	0/930
10	CC	0.24	0/681	0.46	1/930 (0.1%)
10	CD	0.24	0/681	0.46	0/930
11	CF	0.25	0/1675	0.44	0/2280
11	w	0.27	0/1675	0.44	0/2280
11	x	0.26	0/1675	0.44	0/2280
11	y	0.26	0/1675	0.46	0/2280
11	z	0.26	0/1675	0.44	0/2280
12	Ca	0.31	0/1197	0.45	0/1613
12	Cb	0.31	0/1197	0.45	0/1613
12	Cc	0.31	0/1197	0.45	0/1613
12	Cd	0.31	0/1197	0.45	0/1613
12	Ce	0.31	0/1197	0.45	0/1613
12	Cf	0.32	0/1197	0.45	0/1613
12	Cg	0.31	0/1197	0.45	0/1613
12	Ch	0.32	0/1197	0.45	0/1613
12	Ci	0.31	0/1197	0.45	0/1613
12	Cj	0.31	0/1197	0.45	0/1613
12	Ck	0.31	0/1197	0.45	0/1613
12	Cl	0.32	0/1197	0.45	0/1613
12	Cm	0.31	0/1197	0.45	0/1613
12	Cn	0.31	0/1197	0.45	0/1613
12	Co	0.31	0/1197	0.45	0/1613
12	Cp	0.31	0/1197	0.45	0/1613
12	Cq	0.31	0/1197	0.45	0/1613
12	Cr	0.32	0/1197	0.45	0/1613
12	Cs	0.31	0/1197	0.45	0/1613
12	Ct	0.32	0/1197	0.45	0/1613
12	Cu	0.31	0/1197	0.45	0/1613
12	Cv	0.31	0/1197	0.45	0/1613
12	Cw	0.31	0/1197	0.45	0/1613
12	Cx	0.31	0/1197	0.45	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
12	Cy	0.31	0/1197	0.45	0/1613
12	Cz	0.31	0/1197	0.45	0/1613
12	Da	0.45	0/756	0.59	0/1036
12	Db	0.76	3/756 (0.4%)	0.67	1/1036 (0.1%)
12	Dc	0.46	0/756	0.56	0/1036
12	Dd	0.45	0/756	0.66	1/1036 (0.1%)
12	De	0.40	0/705	0.53	0/963
12	Df	0.76	3/697 (0.4%)	0.68	1/954 (0.1%)
12	Dg	0.37	0/646	0.52	0/881
12	Dh	0.37	0/646	0.52	0/881
12	Di	0.37	0/646	0.52	0/881
12	Dj	0.37	0/646	0.52	0/881
12	Dk	0.37	0/646	0.52	0/881
12	Dl	0.37	0/646	0.52	0/881
12	Dm	0.37	0/646	0.52	0/881
12	Dn	0.37	0/646	0.52	0/881
12	Do	0.38	0/697	0.53	0/954
12	Dp	0.44	0/756	0.58	0/1036
12	Dq	0.46	0/756	0.73	3/1036 (0.3%)
12	Dr	0.55	1/756 (0.1%)	0.59	0/1036
12	Ds	0.55	1/756 (0.1%)	0.66	2/1036 (0.2%)
12	Dt	0.45	0/756	0.59	0/1036
12	Du	0.45	0/756	0.62	1/1036 (0.1%)
12	Dv	0.44	0/756	0.58	0/1036
12	Dw	0.45	0/756	0.66	1/1036 (0.1%)
12	Ea	0.31	0/1197	0.45	0/1613
12	Eb	0.31	0/1197	0.45	0/1613
12	Ec	0.32	0/1197	0.45	0/1613
12	Ed	0.31	0/1197	0.45	0/1613
12	Ee	0.31	0/1197	0.45	0/1613
12	Ef	0.31	0/1197	0.45	0/1613
12	Eg	0.31	0/1197	0.45	0/1613
12	Eh	0.31	0/1197	0.45	0/1613
15	AA	0.36	0/1607	0.48	0/2186
15	AB	0.36	0/1607	0.47	0/2186
15	AC	0.36	0/1607	0.47	0/2186
15	AD	0.36	0/1607	0.47	0/2186
15	AE	0.36	0/1607	0.47	0/2186
15	AF	0.36	0/1607	0.47	0/2186
15	AG	0.36	0/1607	0.47	0/2186
15	AH	0.36	0/1607	0.47	0/2186
15	AI	0.36	0/1607	0.47	0/2186
15	AJ	0.36	0/1607	0.47	0/2186

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
15	AK	0.36	0/1607	0.47	0/2186
15	AL	0.36	0/1607	0.47	0/2186
15	AM	0.36	0/1607	0.47	0/2186
15	AN	0.36	0/1607	0.47	0/2186
15	AO	0.36	0/1607	0.47	0/2186
15	AP	0.36	0/1607	0.47	0/2186
15	AQ	0.36	0/1607	0.47	0/2186
15	AR	0.36	0/1607	0.47	0/2186
15	AS	0.36	0/1607	0.47	0/2186
15	AT	0.36	0/1607	0.47	0/2186
15	AU	0.36	0/1607	0.47	0/2186
15	AV	0.36	0/1607	0.47	0/2186
15	AW	0.36	0/1607	0.47	0/2186
15	AX	0.36	0/1607	0.48	0/2186
15	AY	0.36	0/1607	0.47	0/2186
15	AZ	0.36	0/1607	0.47	0/2186
16	BA	0.33	0/2243	0.47	0/3041
16	BB	0.33	0/2243	0.47	0/3041
16	BC	0.33	0/2243	0.47	0/3041
16	BD	0.33	0/2243	0.47	0/3041
16	BE	0.33	0/2243	0.47	0/3041
16	BF	0.33	0/2243	0.47	0/3041
16	BG	0.33	0/2243	0.47	0/3041
16	BH	0.33	0/2243	0.47	0/3041
16	BI	0.33	0/2243	0.47	0/3041
16	BJ	0.33	0/2243	0.47	0/3041
16	BK	0.33	0/2243	0.47	0/3041
16	BL	0.33	0/2243	0.47	0/3041
16	BM	0.33	0/2243	0.47	0/3041
16	BN	0.33	0/2243	0.47	0/3041
16	BO	0.33	0/2243	0.47	0/3041
16	BP	0.33	0/2243	0.47	0/3041
16	BQ	0.33	0/2243	0.47	0/3041
16	BR	0.33	0/2243	0.47	0/3041
16	BS	0.33	0/2243	0.47	0/3041
16	BT	0.33	0/2243	0.47	0/3041
16	BU	0.33	0/2243	0.47	0/3041
16	BV	0.33	0/2243	0.47	0/3041
16	BW	0.33	0/2243	0.47	0/3041
16	BX	0.33	0/2243	0.47	0/3041
16	BY	0.33	0/2243	0.47	0/3041
16	BZ	0.33	0/2243	0.47	0/3041
All	All	0.31	11/338629 (0.0%)	0.49	27/460118 (0.0%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Db	160	PRO	N-CA	13.20	1.69	1.47
12	Df	160	PRO	N-CA	13.19	1.69	1.47
12	Df	171	SER	C-N	8.88	1.51	1.34
8	DL	133	ASN	C-N	8.75	1.50	1.34
8	DQ	285	LYS	C-N	8.73	1.50	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	Df	160	PRO	CA-N-CD	-10.68	96.54	111.50
12	Dq	160	PRO	N-CA-CB	-10.52	90.67	103.30
12	Db	160	PRO	CA-N-CD	-10.51	96.78	111.50
12	Dd	160	PRO	N-CA-CB	-9.96	91.34	103.30
12	Dw	160	PRO	N-CA-CB	-8.37	93.25	103.30

There are no chirality outliers.

There are no planarity outliers.

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	A	258/260 (99%)	249 (96%)	9 (4%)	0	100	100
1	B	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	C	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	D	258/260 (99%)	248 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
1	F	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	G	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	H	258/260 (99%)	245 (95%)	13 (5%)	0	100	100
1	I	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	J	258/260 (99%)	251 (97%)	7 (3%)	0	100	100
1	K	258/260 (99%)	248 (96%)	10 (4%)	0	100	100
1	L	257/260 (99%)	250 (97%)	7 (3%)	0	100	100
1	M	258/260 (99%)	247 (96%)	11 (4%)	0	100	100
1	N	247/260 (95%)	240 (97%)	7 (3%)	0	100	100
1	O	248/260 (95%)	240 (97%)	8 (3%)	0	100	100
1	P	244/260 (94%)	236 (97%)	8 (3%)	0	100	100
1	Q	243/260 (94%)	237 (98%)	6 (2%)	0	100	100
1	R	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
1	S	243/260 (94%)	235 (97%)	8 (3%)	0	100	100
1	T	249/260 (96%)	241 (97%)	8 (3%)	0	100	100
1	U	257/260 (99%)	243 (95%)	14 (5%)	0	100	100
1	V	257/260 (99%)	249 (97%)	8 (3%)	0	100	100
1	W	257/260 (99%)	242 (94%)	15 (6%)	0	100	100
1	X	257/260 (99%)	244 (95%)	13 (5%)	0	100	100
2	a	247/251 (98%)	235 (95%)	12 (5%)	0	100	100
2	b	246/251 (98%)	236 (96%)	10 (4%)	0	100	100
2	c	247/251 (98%)	237 (96%)	10 (4%)	0	100	100
2	d	247/251 (98%)	232 (94%)	15 (6%)	0	100	100
2	e	247/251 (98%)	231 (94%)	16 (6%)	0	100	100
4	5	19/21 (90%)	19 (100%)	0	0	100	100
4	6	19/21 (90%)	19 (100%)	0	0	100	100
4	7	19/21 (90%)	19 (100%)	0	0	100	100
4	8	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
4	9	19/21 (90%)	19 (100%)	0	0	100	100
5	f	124/134 (92%)	121 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	g	126/134 (94%)	121 (96%)	5 (4%)	0	100	100
5	h	124/134 (92%)	120 (97%)	4 (3%)	0	100	100
5	i	125/134 (93%)	121 (97%)	4 (3%)	0	100	100
5	j	123/134 (92%)	119 (97%)	4 (3%)	0	100	100
5	p	125/134 (93%)	120 (96%)	5 (4%)	0	100	100
6	k	104/138 (75%)	99 (95%)	5 (5%)	0	100	100
6	l	102/138 (74%)	101 (99%)	1 (1%)	0	100	100
6	m	102/138 (74%)	99 (97%)	3 (3%)	0	100	100
6	n	103/138 (75%)	99 (96%)	4 (4%)	0	100	100
6	o	105/138 (76%)	103 (98%)	2 (2%)	0	100	100
7	q	69/104 (66%)	68 (99%)	1 (1%)	0	100	100
7	r	68/104 (65%)	64 (94%)	4 (6%)	0	100	100
7	s	70/104 (67%)	70 (100%)	0	0	100	100
7	t	70/104 (67%)	69 (99%)	1 (1%)	0	100	100
7	u	70/104 (67%)	70 (100%)	0	0	100	100
7	v	36/104 (35%)	36 (100%)	0	0	100	100
8	DA	399/403 (99%)	377 (94%)	22 (6%)	0	100	100
8	DB	399/403 (99%)	377 (94%)	22 (6%)	0	100	100
8	DC	399/403 (99%)	375 (94%)	24 (6%)	0	100	100
8	DD	399/403 (99%)	378 (95%)	21 (5%)	0	100	100
8	DE	399/403 (99%)	380 (95%)	19 (5%)	0	100	100
8	DF	399/403 (99%)	376 (94%)	23 (6%)	0	100	100
8	DG	399/403 (99%)	382 (96%)	17 (4%)	0	100	100
8	DH	399/403 (99%)	378 (95%)	19 (5%)	2 (0%)	25	60
8	DI	399/403 (99%)	381 (96%)	18 (4%)	0	100	100
8	DJ	399/403 (99%)	375 (94%)	23 (6%)	1 (0%)	37	70
8	DK	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
8	DL	399/403 (99%)	369 (92%)	27 (7%)	3 (1%)	16	51
8	DM	399/403 (99%)	383 (96%)	14 (4%)	2 (0%)	25	60
8	DN	399/403 (99%)	366 (92%)	31 (8%)	2 (0%)	25	60
8	DO	399/403 (99%)	373 (94%)	23 (6%)	3 (1%)	16	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	DP	399/403 (99%)	375 (94%)	24 (6%)	0	100	100
8	DQ	399/403 (99%)	379 (95%)	20 (5%)	0	100	100
8	DR	399/403 (99%)	382 (96%)	17 (4%)	0	100	100
8	DS	399/403 (99%)	381 (96%)	18 (4%)	0	100	100
8	DT	399/403 (99%)	377 (94%)	22 (6%)	0	100	100
8	DU	399/403 (99%)	381 (96%)	18 (4%)	0	100	100
8	DV	399/403 (99%)	374 (94%)	23 (6%)	2 (0%)	25	60
8	DW	399/403 (99%)	381 (96%)	18 (4%)	0	100	100
8	DX	399/403 (99%)	380 (95%)	19 (5%)	0	100	100
8	DY	399/403 (99%)	378 (95%)	21 (5%)	0	100	100
8	DZ	399/403 (99%)	377 (94%)	22 (6%)	0	100	100
8	EA	399/403 (99%)	378 (95%)	21 (5%)	0	100	100
8	EB	399/403 (99%)	373 (94%)	26 (6%)	0	100	100
8	EC	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
8	ED	399/403 (99%)	380 (95%)	19 (5%)	0	100	100
8	EE	399/403 (99%)	379 (95%)	20 (5%)	0	100	100
8	EF	399/403 (99%)	379 (95%)	20 (5%)	0	100	100
8	EG	399/403 (99%)	376 (94%)	23 (6%)	0	100	100
9	CE	258/264 (98%)	239 (93%)	18 (7%)	1 (0%)	30	65
10	CA	87/89 (98%)	77 (88%)	10 (12%)	0	100	100
10	CB	87/89 (98%)	78 (90%)	9 (10%)	0	100	100
10	CC	87/89 (98%)	77 (88%)	10 (12%)	0	100	100
10	CD	87/89 (98%)	77 (88%)	10 (12%)	0	100	100
11	CF	209/245 (85%)	203 (97%)	6 (3%)	0	100	100
11	w	209/245 (85%)	203 (97%)	6 (3%)	0	100	100
11	x	209/245 (85%)	197 (94%)	12 (6%)	0	100	100
11	y	209/245 (85%)	201 (96%)	8 (4%)	0	100	100
11	z	209/245 (85%)	204 (98%)	5 (2%)	0	100	100
12	Ca	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cb	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cc	144/560 (26%)	136 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Cd	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Ce	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cf	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cg	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Ch	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Ci	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cj	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Ck	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cl	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cm	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cn	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Co	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cp	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cq	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cr	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cs	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Ct	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cu	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cv	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cw	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cx	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cy	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Cz	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Da	107/560 (19%)	94 (88%)	10 (9%)	3 (3%)	4	28
12	Db	107/560 (19%)	95 (89%)	10 (9%)	2 (2%)	6	34
12	Dc	107/560 (19%)	93 (87%)	10 (9%)	4 (4%)	2	23
12	Dd	107/560 (19%)	93 (87%)	12 (11%)	2 (2%)	6	34
12	De	95/560 (17%)	86 (90%)	8 (8%)	1 (1%)	12	45
12	Df	95/560 (17%)	83 (87%)	12 (13%)	0	100	100
12	Dg	83/560 (15%)	75 (90%)	7 (8%)	1 (1%)	11	43
12	Dh	83/560 (15%)	75 (90%)	7 (8%)	1 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Di	83/560 (15%)	75 (90%)	7 (8%)	1 (1%)	11	43
12	Dj	83/560 (15%)	75 (90%)	7 (8%)	1 (1%)	11	43
12	Dk	83/560 (15%)	75 (90%)	7 (8%)	1 (1%)	11	43
12	Dl	83/560 (15%)	76 (92%)	6 (7%)	1 (1%)	11	43
12	Dm	83/560 (15%)	75 (90%)	7 (8%)	1 (1%)	11	43
12	Dn	83/560 (15%)	75 (90%)	7 (8%)	1 (1%)	11	43
12	Do	95/560 (17%)	86 (90%)	7 (7%)	2 (2%)	5	33
12	Dp	107/560 (19%)	94 (88%)	12 (11%)	1 (1%)	14	48
12	Dq	107/560 (19%)	96 (90%)	8 (8%)	3 (3%)	4	28
12	Dr	107/560 (19%)	96 (90%)	10 (9%)	1 (1%)	14	48
12	Ds	107/560 (19%)	93 (87%)	11 (10%)	3 (3%)	4	28
12	Dt	107/560 (19%)	93 (87%)	11 (10%)	3 (3%)	4	28
12	Du	107/560 (19%)	94 (88%)	11 (10%)	2 (2%)	6	34
12	Dv	107/560 (19%)	96 (90%)	8 (8%)	3 (3%)	4	28
12	Dw	107/560 (19%)	90 (84%)	13 (12%)	4 (4%)	2	23
12	Ea	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Eb	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Ec	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Ed	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Ee	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Ef	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Eg	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
12	Eh	144/560 (26%)	136 (94%)	8 (6%)	0	100	100
15	AA	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AB	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AC	209/232 (90%)	198 (95%)	11 (5%)	0	100	100
15	AD	209/232 (90%)	198 (95%)	11 (5%)	0	100	100
15	AE	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AF	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AG	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AH	209/232 (90%)	198 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	AI	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AJ	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AK	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AL	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AM	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AN	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AO	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AP	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AQ	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AR	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AS	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AT	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AU	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AV	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AW	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AX	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
15	AY	209/232 (90%)	198 (95%)	11 (5%)	0	100	100
15	AZ	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
16	BA	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37	70
16	BB	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37	70
16	BC	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37	70
16	BD	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37	70
16	BE	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37	70
16	BF	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37	70
16	BG	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37	70
16	BH	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37	70
16	BI	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37	70
16	BJ	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37	70
16	BK	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37	70
16	BL	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37	70
16	BM	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	BN	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37 70
16	BO	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37 70
16	BP	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37 70
16	BQ	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37 70
16	BR	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37 70
16	BS	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	37 70
16	BT	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37 70
16	BU	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37 70
16	BV	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37 70
16	BW	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37 70
16	BX	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37 70
16	BY	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37 70
16	BZ	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	37 70
All	All	44179/72304 (61%)	42089 (95%)	2006 (4%)	84 (0%)	45 75

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	DJ	332	ASN
12	Dc	124	SER
12	Dc	125	GLN
12	Dd	160	PRO
12	Dq	124	SER

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	A	215/215 (100%)	211 (98%)	4 (2%)	52 70
1	B	215/215 (100%)	212 (99%)	3 (1%)	62 75
1	C	215/215 (100%)	213 (99%)	2 (1%)	75 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	215/215 (100%)	215 (100%)	0	100	100
1	E	215/215 (100%)	210 (98%)	5 (2%)	45	64
1	F	215/215 (100%)	214 (100%)	1 (0%)	86	90
1	G	215/215 (100%)	209 (97%)	6 (3%)	38	59
1	H	215/215 (100%)	213 (99%)	2 (1%)	75	83
1	I	215/215 (100%)	211 (98%)	4 (2%)	52	70
1	J	215/215 (100%)	213 (99%)	2 (1%)	75	83
1	K	215/215 (100%)	211 (98%)	4 (2%)	52	70
1	L	214/215 (100%)	211 (99%)	3 (1%)	62	75
1	M	215/215 (100%)	212 (99%)	3 (1%)	62	75
1	N	208/215 (97%)	207 (100%)	1 (0%)	86	90
1	O	209/215 (97%)	208 (100%)	1 (0%)	86	90
1	P	204/215 (95%)	202 (99%)	2 (1%)	73	81
1	Q	204/215 (95%)	200 (98%)	4 (2%)	50	68
1	R	206/215 (96%)	201 (98%)	5 (2%)	44	63
1	S	204/215 (95%)	202 (99%)	2 (1%)	73	81
1	T	210/215 (98%)	209 (100%)	1 (0%)	86	90
1	U	214/215 (100%)	212 (99%)	2 (1%)	75	83
1	V	214/215 (100%)	211 (99%)	3 (1%)	62	75
1	W	214/215 (100%)	211 (99%)	3 (1%)	62	75
1	X	214/215 (100%)	210 (98%)	4 (2%)	52	70
2	a	191/193 (99%)	185 (97%)	6 (3%)	35	56
2	b	190/193 (98%)	186 (98%)	4 (2%)	48	67
2	c	191/193 (99%)	185 (97%)	6 (3%)	35	56
2	d	191/193 (99%)	187 (98%)	4 (2%)	48	67
2	e	191/193 (99%)	188 (98%)	3 (2%)	58	73
4	5	15/15 (100%)	15 (100%)	0	100	100
4	6	15/15 (100%)	15 (100%)	0	100	100
4	7	15/15 (100%)	15 (100%)	0	100	100
4	8	15/15 (100%)	15 (100%)	0	100	100
4	9	15/15 (100%)	15 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	f	101/105 (96%)	98 (97%)	3 (3%)	36	58
5	g	102/105 (97%)	99 (97%)	3 (3%)	37	59
5	h	101/105 (96%)	100 (99%)	1 (1%)	73	81
5	i	102/105 (97%)	100 (98%)	2 (2%)	50	68
5	j	101/105 (96%)	100 (99%)	1 (1%)	73	81
5	p	101/105 (96%)	101 (100%)	0	100	100
6	k	91/113 (80%)	87 (96%)	4 (4%)	24	48
6	l	89/113 (79%)	86 (97%)	3 (3%)	32	55
6	m	89/113 (79%)	88 (99%)	1 (1%)	70	79
6	n	90/113 (80%)	87 (97%)	3 (3%)	33	56
6	o	91/113 (80%)	87 (96%)	4 (4%)	24	48
7	q	55/79 (70%)	54 (98%)	1 (2%)	54	71
7	r	54/79 (68%)	54 (100%)	0	100	100
7	s	56/79 (71%)	56 (100%)	0	100	100
7	t	56/79 (71%)	56 (100%)	0	100	100
7	u	56/79 (71%)	56 (100%)	0	100	100
7	v	32/79 (40%)	31 (97%)	1 (3%)	35	56
8	DA	321/323 (99%)	315 (98%)	6 (2%)	52	70
8	DB	321/323 (99%)	317 (99%)	4 (1%)	67	78
8	DC	321/323 (99%)	320 (100%)	1 (0%)	91	92
8	DD	321/323 (99%)	318 (99%)	3 (1%)	75	83
8	DE	321/323 (99%)	320 (100%)	1 (0%)	91	92
8	DF	321/323 (99%)	318 (99%)	3 (1%)	75	83
8	DG	321/323 (99%)	320 (100%)	1 (0%)	91	92
8	DH	321/323 (99%)	316 (98%)	5 (2%)	58	73
8	DI	321/323 (99%)	316 (98%)	5 (2%)	58	73
8	DJ	321/323 (99%)	318 (99%)	3 (1%)	75	83
8	DK	321/323 (99%)	318 (99%)	3 (1%)	75	83
8	DL	321/323 (99%)	300 (94%)	21 (6%)	14	39
8	DM	321/323 (99%)	307 (96%)	14 (4%)	24	48
8	DN	321/323 (99%)	308 (96%)	13 (4%)	27	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	DO	321/323 (99%)	298 (93%)	23 (7%)	12 36
8	DP	321/323 (99%)	316 (98%)	5 (2%)	58 73
8	DQ	321/323 (99%)	315 (98%)	6 (2%)	52 70
8	DR	321/323 (99%)	321 (100%)	0	100 100
8	DS	321/323 (99%)	314 (98%)	7 (2%)	47 65
8	DT	321/323 (99%)	320 (100%)	1 (0%)	91 92
8	DU	321/323 (99%)	317 (99%)	4 (1%)	67 78
8	DV	321/323 (99%)	320 (100%)	1 (0%)	91 92
8	DW	321/323 (99%)	320 (100%)	1 (0%)	91 92
8	DX	321/323 (99%)	319 (99%)	2 (1%)	84 88
8	DY	321/323 (99%)	320 (100%)	1 (0%)	91 92
8	DZ	321/323 (99%)	320 (100%)	1 (0%)	91 92
8	EA	321/323 (99%)	321 (100%)	0	100 100
8	EB	321/323 (99%)	320 (100%)	1 (0%)	91 92
8	EC	321/323 (99%)	319 (99%)	2 (1%)	84 88
8	ED	321/323 (99%)	320 (100%)	1 (0%)	91 92
8	EE	321/323 (99%)	320 (100%)	1 (0%)	91 92
8	EF	321/323 (99%)	319 (99%)	2 (1%)	84 88
8	EG	321/323 (99%)	319 (99%)	2 (1%)	84 88
9	CE	217/221 (98%)	214 (99%)	3 (1%)	62 75
10	CA	74/74 (100%)	74 (100%)	0	100 100
10	CB	74/74 (100%)	72 (97%)	2 (3%)	40 60
10	CC	74/74 (100%)	73 (99%)	1 (1%)	62 75
10	CD	74/74 (100%)	74 (100%)	0	100 100
11	CF	180/204 (88%)	177 (98%)	3 (2%)	56 72
11	w	180/204 (88%)	175 (97%)	5 (3%)	38 59
11	x	180/204 (88%)	175 (97%)	5 (3%)	38 59
11	y	180/204 (88%)	171 (95%)	9 (5%)	20 45
11	z	180/204 (88%)	177 (98%)	3 (2%)	56 72
12	Ca	133/467 (28%)	130 (98%)	3 (2%)	45 64
12	Cb	133/467 (28%)	130 (98%)	3 (2%)	45 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Cc	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cd	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Ce	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cf	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cg	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Ch	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Ci	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cj	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Ck	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cl	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cm	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cn	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Co	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cp	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cq	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cr	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cs	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Ct	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cu	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cv	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cw	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cx	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cy	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Cz	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Da	71/467 (15%)	69 (97%)	2 (3%)	38	59
12	Db	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dc	71/467 (15%)	69 (97%)	2 (3%)	38	59
12	Dd	71/467 (15%)	68 (96%)	3 (4%)	25	49
12	De	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Df	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dg	71/467 (15%)	70 (99%)	1 (1%)	62	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Dh	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Di	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dj	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dk	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dl	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dm	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dn	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Do	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dp	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dq	71/467 (15%)	69 (97%)	2 (3%)	38	59
12	Dr	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Ds	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dt	71/467 (15%)	69 (97%)	2 (3%)	38	59
12	Du	71/467 (15%)	70 (99%)	1 (1%)	62	75
12	Dv	71/467 (15%)	68 (96%)	3 (4%)	25	49
12	Dw	71/467 (15%)	68 (96%)	3 (4%)	25	49
12	Ea	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Eb	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Ec	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Ed	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Ee	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Ef	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Eg	133/467 (28%)	130 (98%)	3 (2%)	45	64
12	Eh	133/467 (28%)	130 (98%)	3 (2%)	45	64
15	AA	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AB	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AC	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AD	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AE	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AF	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AG	169/185 (91%)	158 (94%)	11 (6%)	14	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AH	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AI	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AJ	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AK	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AL	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AM	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AN	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AO	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AP	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AQ	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AR	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AS	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AT	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AU	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AV	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AW	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AX	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AY	169/185 (91%)	158 (94%)	11 (6%)	14	39
15	AZ	169/185 (91%)	158 (94%)	11 (6%)	14	39
16	BA	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BB	248/294 (84%)	237 (96%)	11 (4%)	24	48
16	BC	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BD	248/294 (84%)	237 (96%)	11 (4%)	24	48
16	BE	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BF	248/294 (84%)	237 (96%)	11 (4%)	24	48
16	BG	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BH	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BI	248/294 (84%)	237 (96%)	11 (4%)	24	48
16	BJ	248/294 (84%)	237 (96%)	11 (4%)	24	48
16	BK	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BL	248/294 (84%)	237 (96%)	11 (4%)	24	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	BM	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BN	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BO	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BP	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BQ	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BR	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BS	248/294 (84%)	237 (96%)	11 (4%)	24	48
16	BT	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BU	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BV	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BW	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BX	248/294 (84%)	237 (96%)	11 (4%)	24	48
16	BY	248/294 (84%)	236 (95%)	12 (5%)	21	46
16	BZ	248/294 (84%)	237 (96%)	11 (4%)	24	48
All	All	36494/59138 (62%)	35478 (97%)	1016 (3%)	40	59

5 of 1016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	AN	103	SER
16	BY	27	SER
15	AX	103	SER
16	BX	75	THR
8	DN	143	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 518 such sidechains are listed below:

Mol	Chain	Res	Type
8	DO	274	ASN
8	DQ	129	GLN
8	DO	252	ASN
15	AS	119	ASN
15	AR	133	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

26 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	P1L	AT	22	15	13,14,23	0.85	0	10,15,25	1.93	3 (30%)
15	P1L	AV	22	15	13,14,23	0.85	0	10,15,25	1.92	3 (30%)
15	P1L	AU	22	15	13,14,23	0.84	0	10,15,25	1.97	3 (30%)
15	P1L	AA	22	15	13,14,23	0.87	0	10,15,25	1.95	3 (30%)
15	P1L	AP	22	15	13,14,23	0.86	0	10,15,25	1.94	3 (30%)
15	P1L	AY	22	15	13,14,23	0.84	0	10,15,25	1.94	3 (30%)
15	P1L	AF	22	15	13,14,23	0.87	0	10,15,25	1.93	3 (30%)
15	P1L	AW	22	15	13,14,23	0.87	0	10,15,25	1.95	3 (30%)
15	P1L	AJ	22	15	13,14,23	0.84	0	10,15,25	1.95	3 (30%)
15	P1L	AS	22	15	13,14,23	0.86	0	10,15,25	1.96	3 (30%)
15	P1L	AR	22	15	13,14,23	0.86	0	10,15,25	1.92	3 (30%)
15	P1L	AC	22	15	13,14,23	0.84	0	10,15,25	1.95	3 (30%)
15	P1L	AK	22	15	13,14,23	0.86	0	10,15,25	1.92	3 (30%)
15	P1L	AN	22	15	13,14,23	0.88	0	10,15,25	1.95	3 (30%)
15	P1L	AX	22	15	13,14,23	0.84	0	10,15,25	1.97	3 (30%)
15	P1L	AQ	22	15	13,14,23	0.83	0	10,15,25	1.93	3 (30%)
15	P1L	AD	22	15	13,14,23	0.84	0	10,15,25	1.93	3 (30%)
15	P1L	AL	22	15	13,14,23	0.87	0	10,15,25	1.93	3 (30%)
15	P1L	AI	22	15	13,14,23	0.87	0	10,15,25	1.93	3 (30%)
15	P1L	AG	22	15	13,14,23	0.86	0	10,15,25	1.93	3 (30%)
15	P1L	AZ	22	15	13,14,23	0.86	0	10,15,25	1.94	3 (30%)
15	P1L	AH	22	15	13,14,23	0.86	0	10,15,25	1.95	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	P1L	AO	22	15	13,14,23	0.86	0	10,15,25	1.90	3 (30%)
15	P1L	AE	22	15	13,14,23	0.85	0	10,15,25	1.94	3 (30%)
15	P1L	AB	22	15	13,14,23	0.86	0	10,15,25	1.96	3 (30%)
15	P1L	AM	22	15	13,14,23	0.84	0	10,15,25	1.94	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	P1L	AT	22	15	-	7/12/14/24	-
15	P1L	AV	22	15	-	7/12/14/24	-
15	P1L	AU	22	15	-	7/12/14/24	-
15	P1L	AA	22	15	-	7/12/14/24	-
15	P1L	AP	22	15	-	7/12/14/24	-
15	P1L	AY	22	15	-	7/12/14/24	-
15	P1L	AF	22	15	-	7/12/14/24	-
15	P1L	AW	22	15	-	7/12/14/24	-
15	P1L	AJ	22	15	-	7/12/14/24	-
15	P1L	AS	22	15	-	7/12/14/24	-
15	P1L	AR	22	15	-	7/12/14/24	-
15	P1L	AC	22	15	-	7/12/14/24	-
15	P1L	AK	22	15	-	7/12/14/24	-
15	P1L	AN	22	15	-	7/12/14/24	-
15	P1L	AX	22	15	-	7/12/14/24	-
15	P1L	AQ	22	15	-	7/12/14/24	-
15	P1L	AD	22	15	-	7/12/14/24	-
15	P1L	AL	22	15	-	7/12/14/24	-
15	P1L	AI	22	15	-	7/12/14/24	-
15	P1L	AG	22	15	-	7/12/14/24	-
15	P1L	AZ	22	15	-	7/12/14/24	-
15	P1L	AH	22	15	-	7/12/14/24	-
15	P1L	AO	22	15	-	7/12/14/24	-
15	P1L	AE	22	15	-	7/12/14/24	-
15	P1L	AB	22	15	-	7/12/14/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	P1L	AM	22	15	-	7/12/14/24	-

There are no bond length outliers.

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	AU	22	P1L	C8-C7-SG	-4.29	108.46	113.46
15	AX	22	P1L	C8-C7-SG	-4.25	108.50	113.46
15	AJ	22	P1L	C8-C7-SG	-4.23	108.53	113.46
15	AC	22	P1L	C8-C7-SG	-4.23	108.54	113.46
15	AB	22	P1L	C8-C7-SG	-4.20	108.56	113.46

There are no chirality outliers.

5 of 182 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	AA	22	P1L	CA-CB-SG-C7
15	AA	22	P1L	O7-C7-SG-CB
15	AA	22	P1L	C8-C7-SG-CB
15	AB	22	P1L	CA-CB-SG-C7
15	AB	22	P1L	O7-C7-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

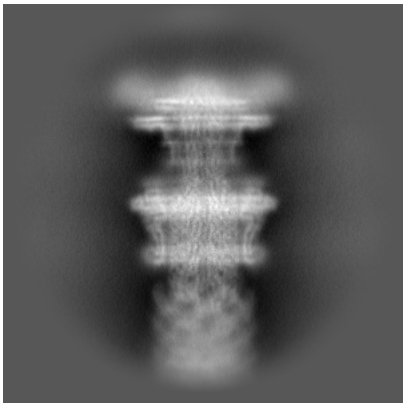
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30359. These allow visual inspection of the internal detail of the map and identification of artifacts.

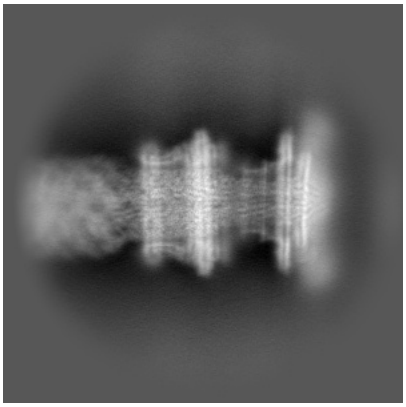
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

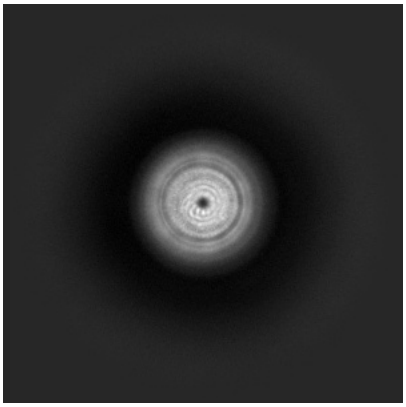
6.1.1 Primary map



X



Y

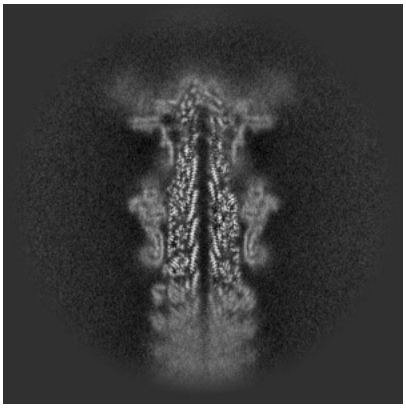


Z

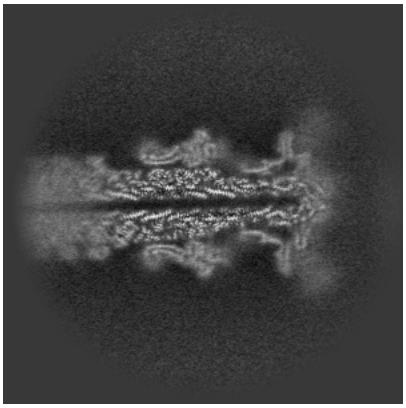
The images above show the map projected in three orthogonal directions.

6.2 Central slices

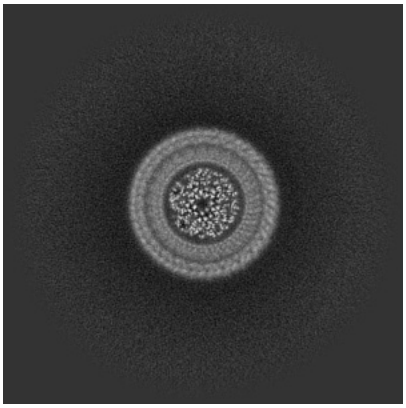
6.2.1 Primary map



X Index: 256



Y Index: 256

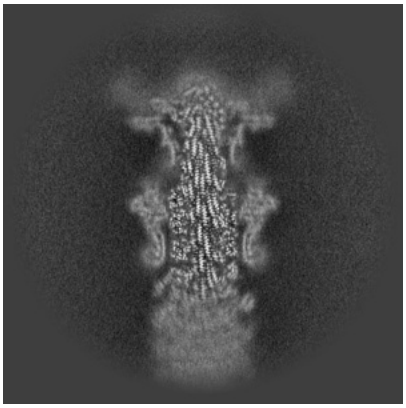


Z Index: 256

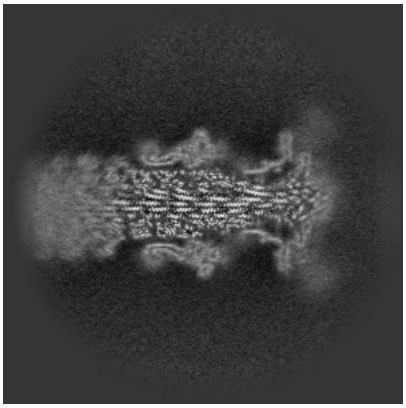
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

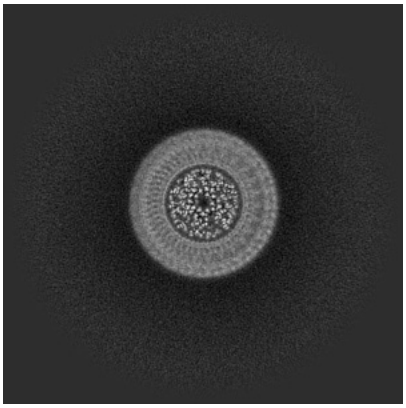
6.3.1 Primary map



X Index: 269



Y Index: 244

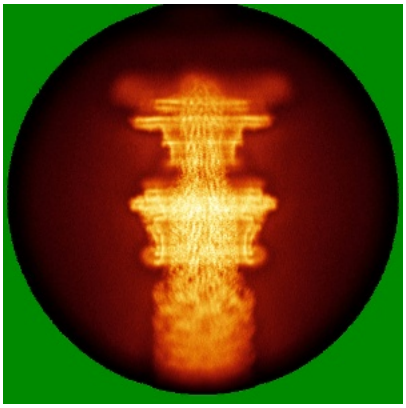


Z Index: 251

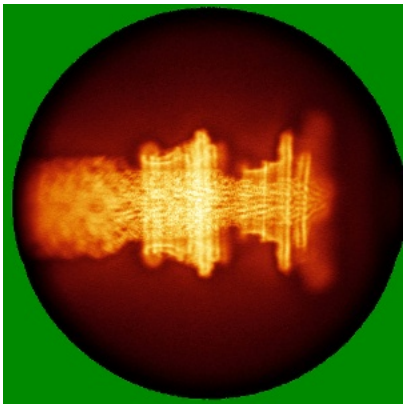
The images above show the largest variance slices of the map in three orthogonal directions.

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

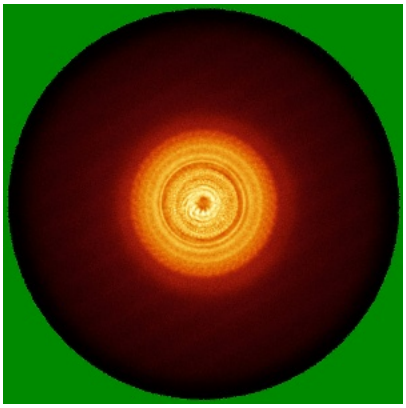
6.4.1 Primary map



X



Y



Z

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 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

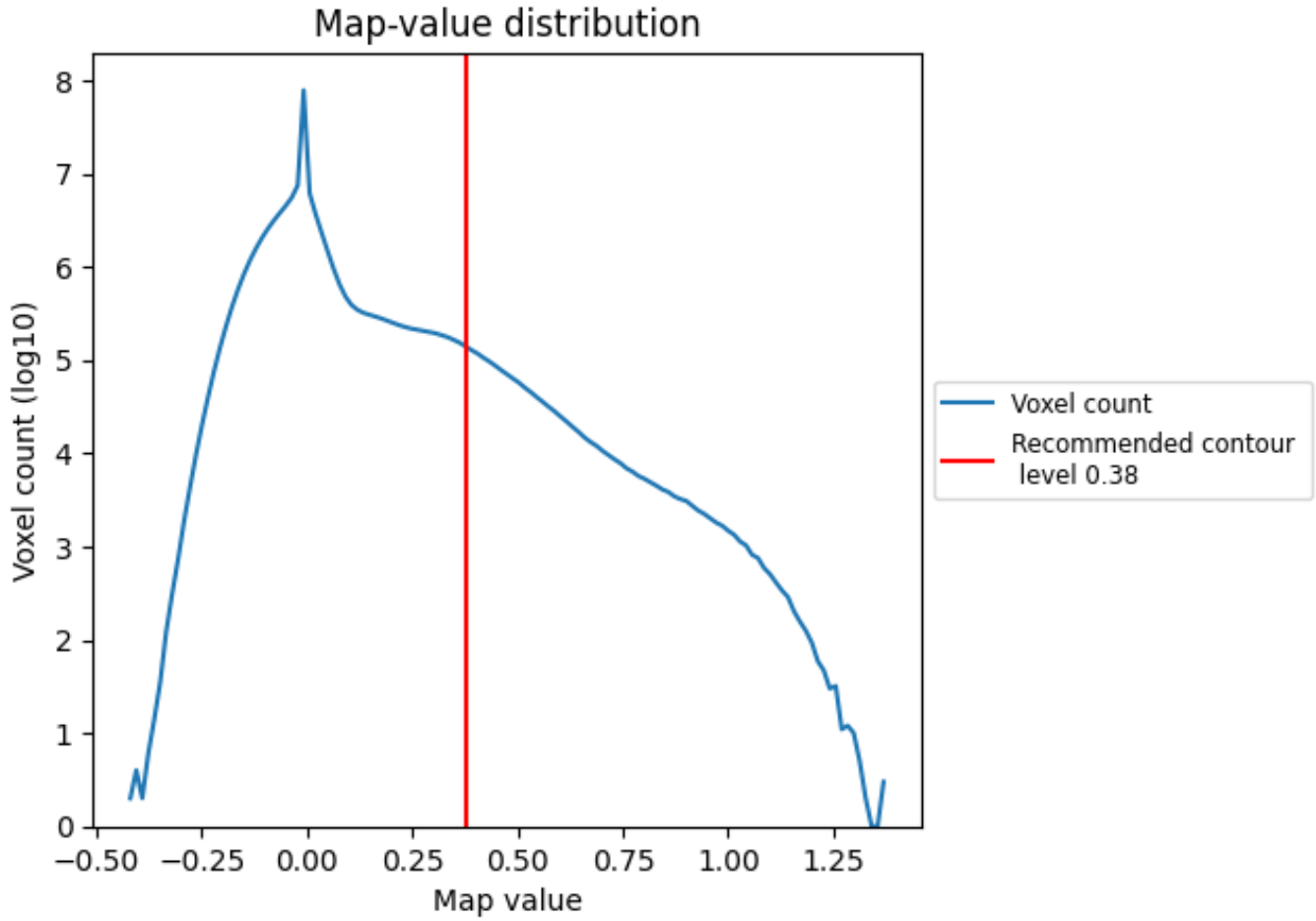
6.6 Mask visualisation (i)

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

7 Map analysis

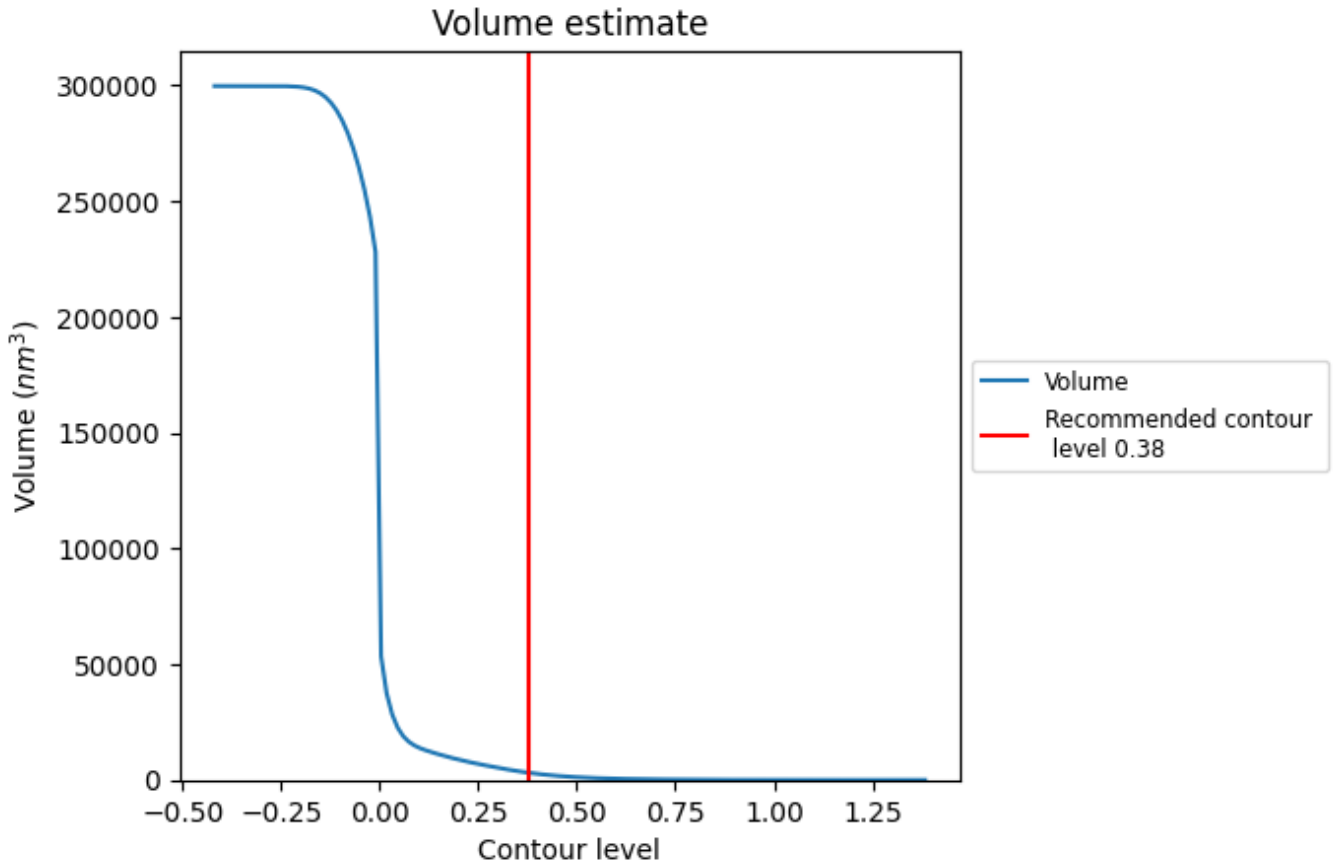
This section contains the results of statistical analysis of the map.

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.

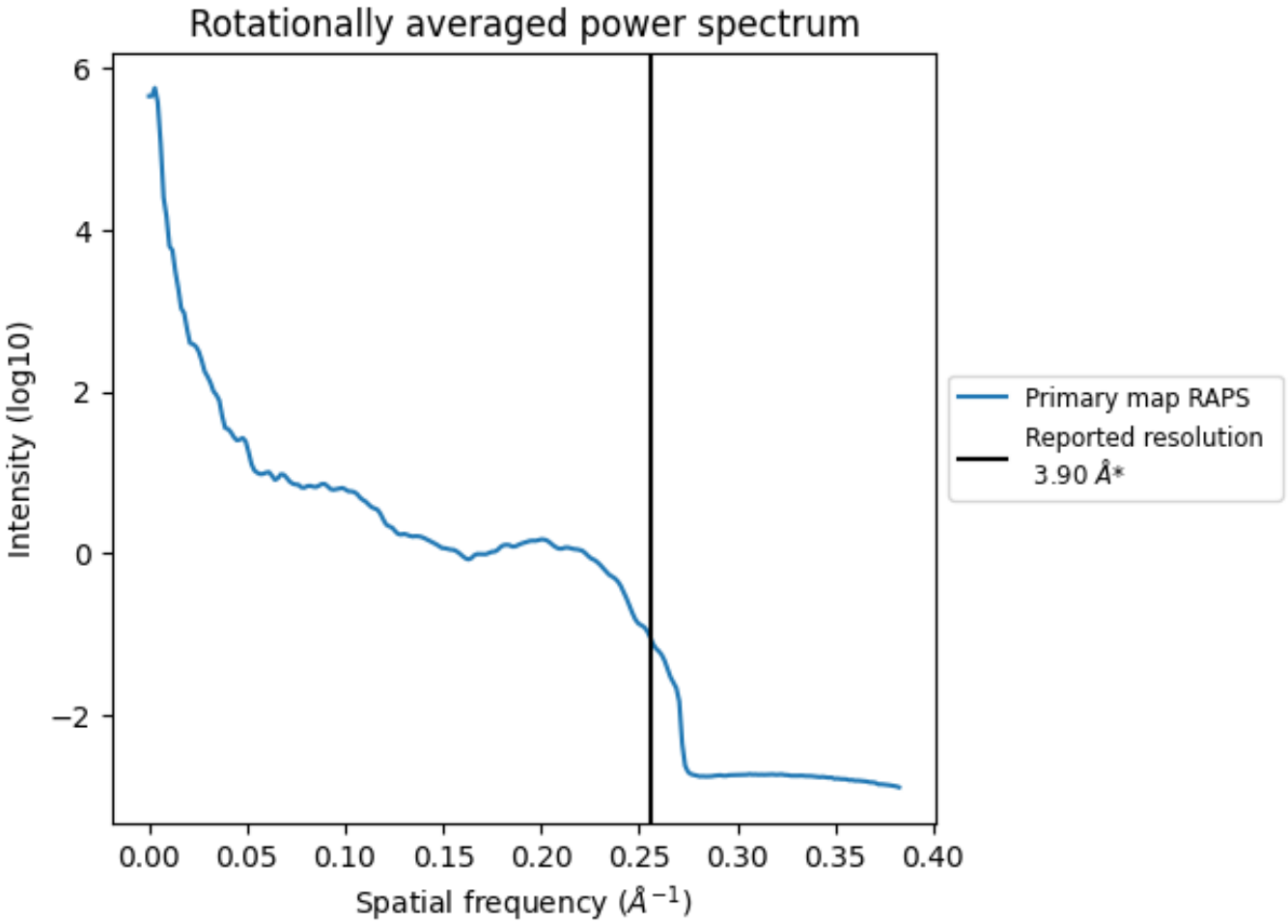
7.2 Volume estimate (i)



The volume at the recommended contour level is 3068 nm^3; this corresponds to an approximate mass of 2771 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 0.256 Å^{-1}

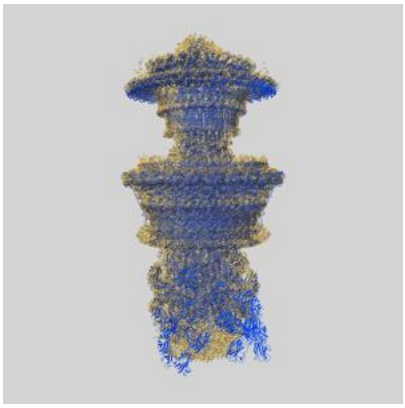
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

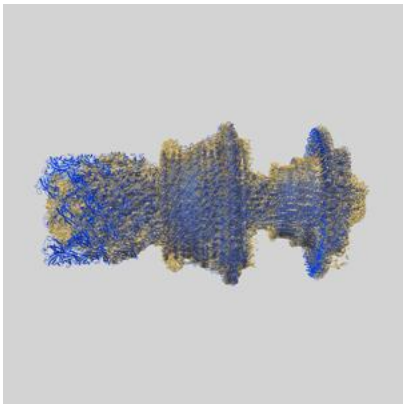
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30359 and PDB model 7CGO. Per-residue inclusion information can be found in section 3 on page 24.

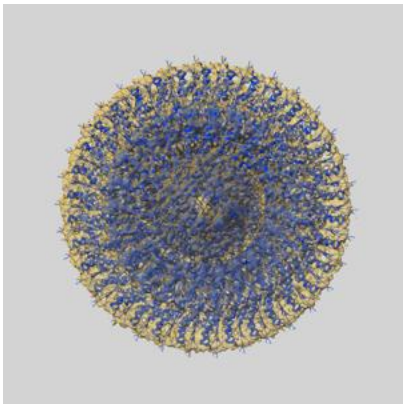
9.1 Map-model overlay



X



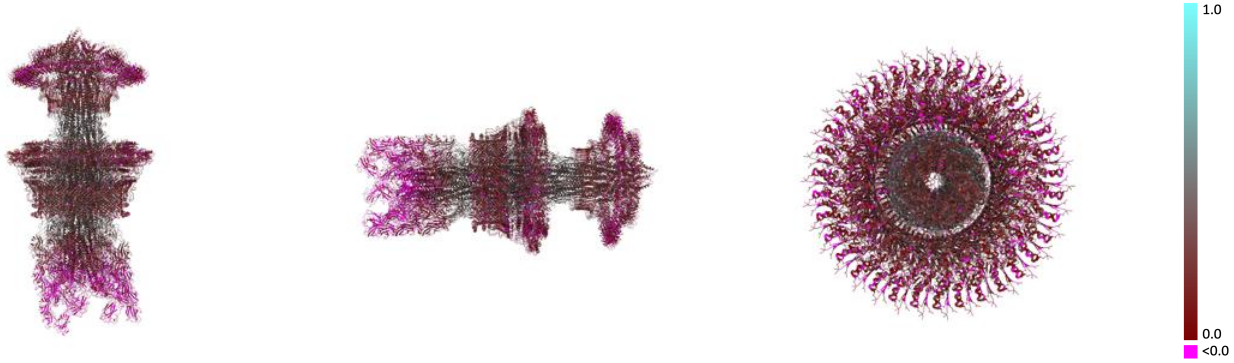
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

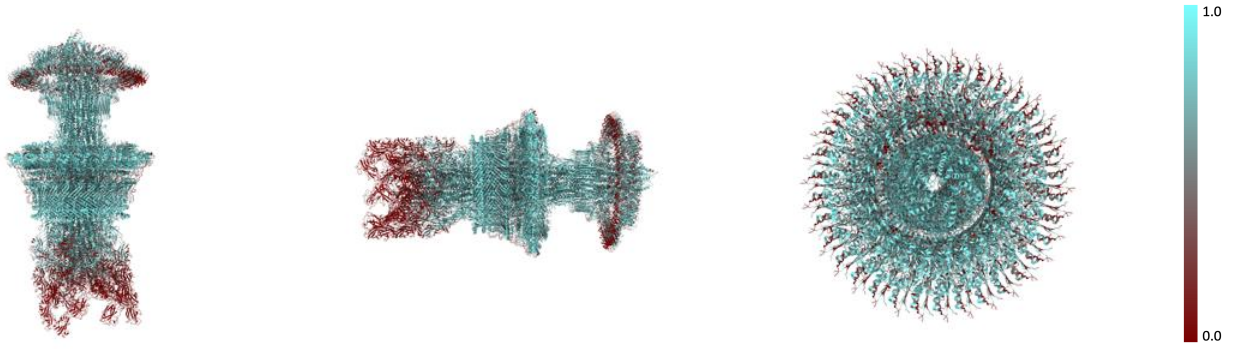
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

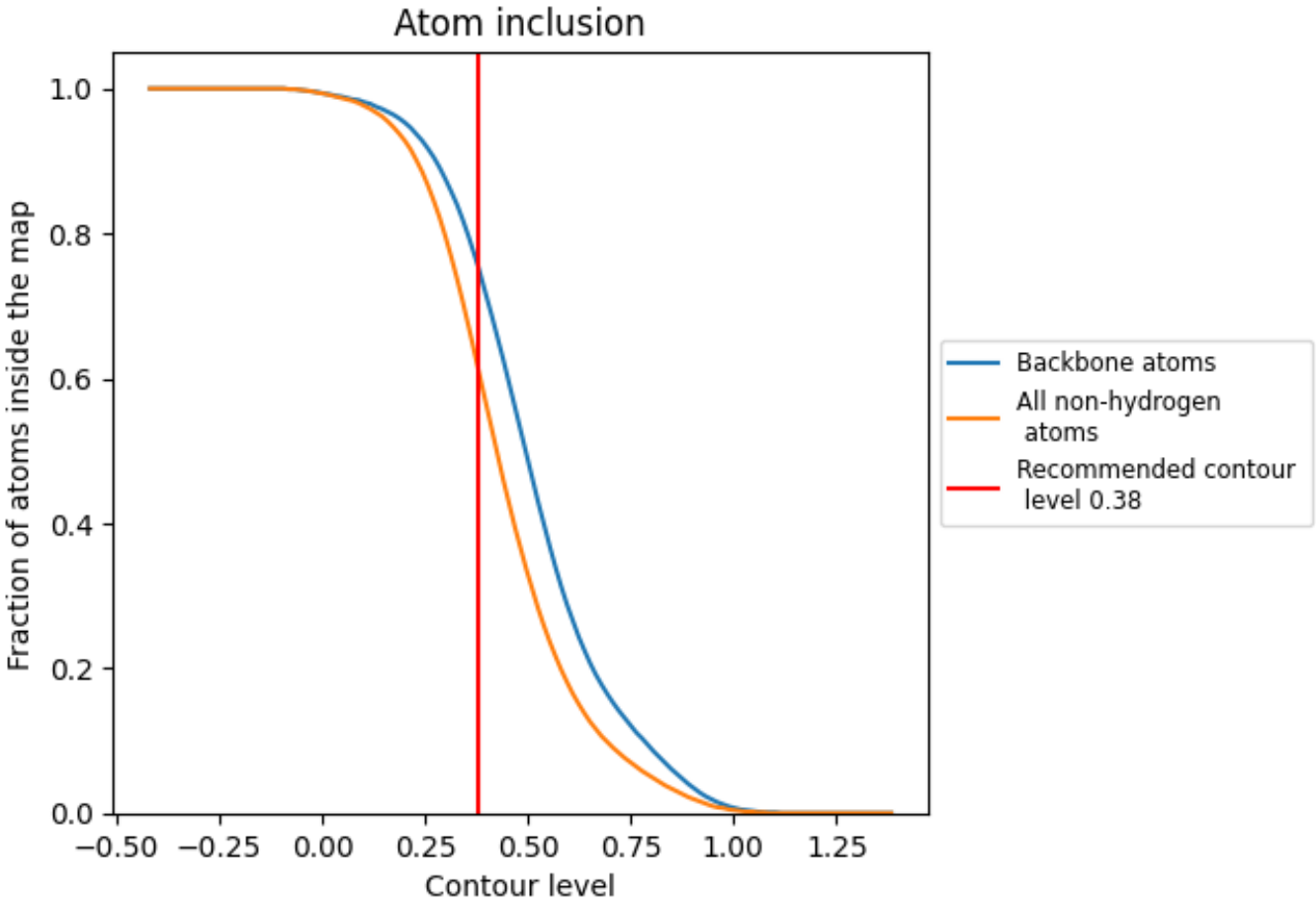
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.38).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 61% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6110	0.2210
0	0.8930	0.4500
1	0.9070	0.4270
2	0.9470	0.4930
3	0.8800	0.4400
4	0.9070	0.4600
5	0.8500	0.4640
6	0.6710	0.4240
7	0.8430	0.4520
8	0.8360	0.4430
9	0.7790	0.4420
A	0.8060	0.4250
AA	0.7250	0.2400
AB	0.7370	0.2460
AC	0.7250	0.2380
AD	0.7050	0.2210
AE	0.7160	0.2310
AF	0.7060	0.2190
AG	0.6930	0.2240
AH	0.6950	0.2120
AI	0.6800	0.1990
AJ	0.6700	0.1870
AK	0.6920	0.1890
AL	0.6770	0.1720
AM	0.6600	0.1770
AN	0.6500	0.1490
AO	0.6650	0.1540
AP	0.6580	0.1350
AQ	0.6620	0.1360
AR	0.6750	0.1550
AS	0.6750	0.1610
AT	0.6690	0.1560
AU	0.6770	0.1750
AV	0.7060	0.2050
AW	0.7130	0.2040

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Chain	Atom inclusion	Q-score
AX	0.7150	0.2290
AY	0.7160	0.2250
AZ	0.7220	0.2230
B	0.7740	0.4090
BA	0.7860	0.2310
BB	0.7710	0.2260
BC	0.7680	0.2300
BD	0.7700	0.2210
BE	0.7750	0.2290
BF	0.7640	0.2150
BG	0.7690	0.2040
BH	0.7640	0.1980
BI	0.7720	0.1930
BJ	0.7580	0.1830
BK	0.7580	0.1780
BL	0.7350	0.1660
BM	0.7320	0.1510
BN	0.7410	0.1320
BO	0.7290	0.1340
BP	0.7180	0.1220
BQ	0.7080	0.1270
BR	0.7270	0.1310
BS	0.7380	0.1460
BT	0.7320	0.1390
BU	0.7440	0.1520
BV	0.7600	0.1690
BW	0.7740	0.1900
BX	0.7690	0.2040
BY	0.7830	0.2250
BZ	0.7850	0.2240
C	0.8110	0.4230
CA	0.7230	0.2260
CB	0.7290	0.2420
CC	0.6840	0.2410
CD	0.6140	0.2210
CE	0.6420	0.2360
CF	0.7260	0.2860
Ca	0.5340	0.1090
Cb	0.5340	0.1260
Cc	0.5090	0.1180
Cd	0.4790	0.1030
Ce	0.5060	0.1160

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Chain	Atom inclusion	Q-score
Cf	0.5020	0.1070
Cg	0.4830	0.0970
Ch	0.4930	0.1200
Ci	0.4830	0.1190
Cj	0.4800	0.1320
Ck	0.4660	0.1320
Cl	0.4920	0.1390
Cm	0.4740	0.1490
Cn	0.4560	0.1390
Co	0.4720	0.1570
Cp	0.4670	0.1430
Cq	0.4660	0.1300
Cr	0.4710	0.1280
Cs	0.5010	0.1350
Ct	0.5300	0.1630
Cu	0.5200	0.1290
Cv	0.5220	0.1370
Cw	0.5250	0.1430
Cx	0.5220	0.1370
Cy	0.5470	0.1620
Cz	0.5420	0.1400
D	0.8060	0.4220
DA	0.5190	0.3360
DB	0.6960	0.3470
DC	0.6990	0.3310
DD	0.6760	0.3100
DE	0.6800	0.3230
DF	0.6560	0.3150
DG	0.6630	0.3140
DH	0.6610	0.3080
DI	0.6180	0.2800
DJ	0.5790	0.2670
DK	0.5320	0.2560
DL	0.4750	0.1410
DM	0.4900	0.1570
DN	0.4540	0.1470
DO	0.4430	0.1660
DP	0.3490	0.0950
DQ	0.3590	0.1350
DR	0.3420	0.0940
DS	0.3010	0.0620
DT	0.3400	0.1240

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Chain	Atom inclusion	Q-score
DU	0.2570	0.0660
DV	0.2390	0.0520
DW	0.2520	0.0960
DX	0.2110	0.0180
DY	0.2050	0.0410
DZ	0.1940	0.0600
Da	0.7030	0.2190
Db	0.6490	0.1990
Dc	0.6540	0.1900
Dd	0.6380	0.1770
De	0.6100	0.1800
Df	0.6060	0.1740
Dg	0.5560	0.1100
Dh	0.5060	0.1350
Di	0.4540	0.1110
Dj	0.4310	0.1280
Dk	0.4510	0.1440
Dl	0.4140	0.1010
Dm	0.4240	0.1170
Dn	0.4590	0.1250
Do	0.5000	0.1580
Dp	0.5780	0.1810
Dq	0.6360	0.1880
Dr	0.6280	0.1980
Ds	0.6320	0.2160
Dt	0.6590	0.2010
Du	0.7020	0.2200
Dv	0.6770	0.2320
Dw	0.6570	0.2050
E	0.8200	0.4270
EA	0.1370	0.0090
EB	0.1620	0.0480
EC	0.1270	0.0050
ED	0.1040	-0.0140
EE	0.1200	0.0400
EF	0.0810	0.0100
EG	0.0760	0.0240
Ea	0.5680	0.1500
Eb	0.5590	0.1460
Ec	0.5710	0.1320
Ed	0.5820	0.1580
Ee	0.5950	0.1340

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Chain	Atom inclusion	Q-score
Ef	0.5800	0.1450
Eg	0.5330	0.1300
Eh	0.5560	0.1230
F	0.8110	0.4240
G	0.8110	0.4290
GA	0.6360	0.2900
GB	0.6400	0.2500
GC	0.4730	0.2790
GD	0.7200	0.3160
GE	0.6670	0.2860
GF	0.5330	0.2750
GG	0.4330	0.3040
GH	0.2220	0.2370
GI	0.1330	0.1770
GJ	0.4000	0.2520
GK	0.3330	0.2420
H	0.8130	0.4320
I	0.8190	0.4330
J	0.8120	0.4360
K	0.8040	0.4360
L	0.8070	0.4340
M	0.8140	0.4340
N	0.7950	0.4370
O	0.8110	0.4320
P	0.8100	0.4310
Q	0.8120	0.4300
R	0.8060	0.4290
S	0.8120	0.4270
T	0.8140	0.4330
U	0.8240	0.4380
V	0.8180	0.4300
W	0.8200	0.4360
X	0.8070	0.4230
a	0.8490	0.4350
b	0.8160	0.4130
c	0.8470	0.4370
d	0.8320	0.4260
e	0.8100	0.4220
f	0.8210	0.4150
g	0.8060	0.3760
h	0.8240	0.4170
i	0.8280	0.4180

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Chain	Atom inclusion	Q-score
j	0.8070	0.4120
k	0.8160	0.3950
l	0.7790	0.3840
m	0.8260	0.4000
n	0.8150	0.3870
o	0.7960	0.3830
p	0.8000	0.3950
q	0.7720	0.3570
r	0.7580	0.3120
s	0.7530	0.3550
t	0.7810	0.3660
u	0.7550	0.3500
v	0.6850	0.3130
w	0.7330	0.3110
x	0.6670	0.2840
y	0.7330	0.3080
z	0.7340	0.3040