Full wwPDB EM Validation Report ⓘ

Jul 7, 2021 – 03:33 pm BST

PDB ID	:	7NVG
EMDB ID	:	EMD-12603
Title	:	Salmonella flagellar basal body refined in C1 map
Authors	:	Johnson, S.; Furlong, E.; Lea, S.M.
Deposited on	:	2021-03-15
Resolution	:	3.70 Å(reported)

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

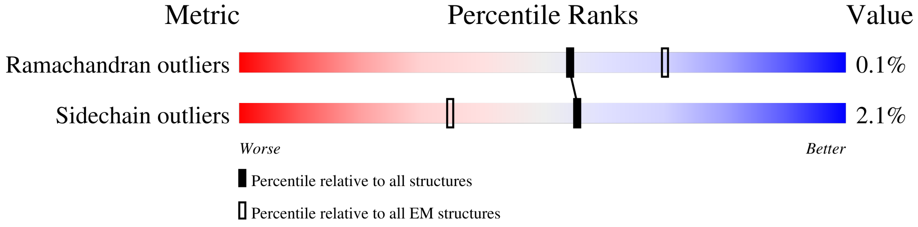
EMDB validation analysis	:	0.0.0.dev84
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

1 Overall quality at a glance (i)

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

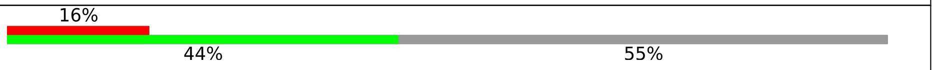
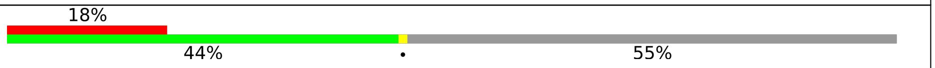
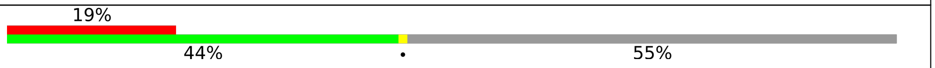
The reported resolution of this entry is 3.70 Å.

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	154571	4023
Sidechain outliers	154315	3826

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	A1	560	
1	B1	560	
1	C1	560	
1	D1	560	
1	E1	560	
1	F1	560	
1	G1	560	
1	H1	560	
1	I1	560	

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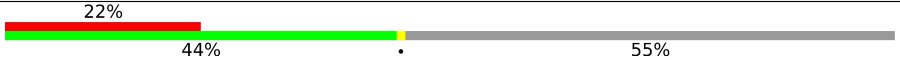
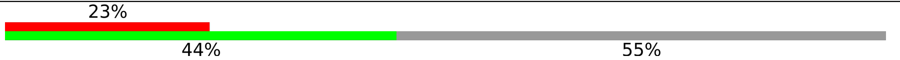
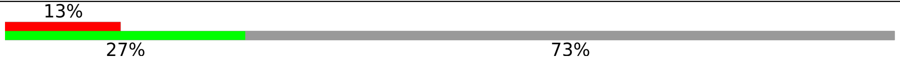
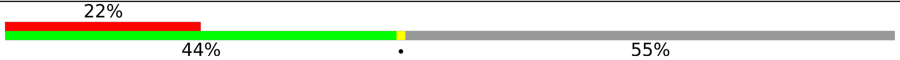
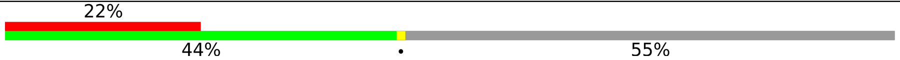
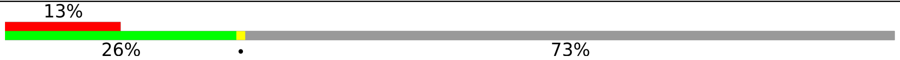
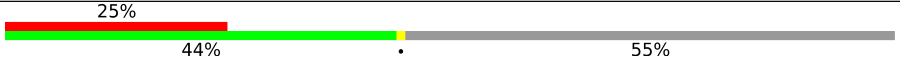
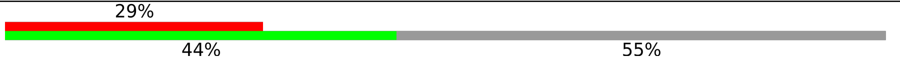
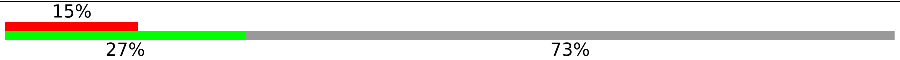
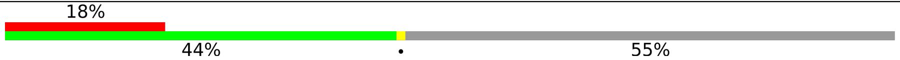
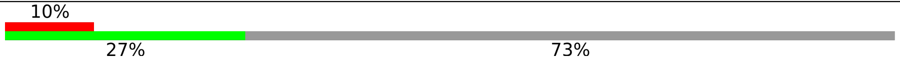
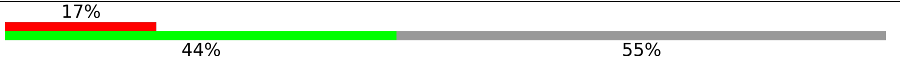
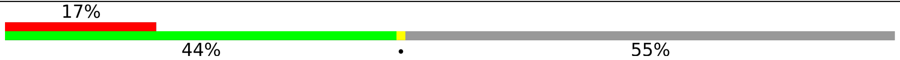
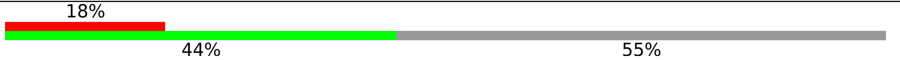
Mol	Chain	Length	Quality of chain
1	J1	560	 13% 26% • 73%
1	K1	560	 22% 44% • 55%
1	L1	560	 23% 44% 55%
1	M1	560	 13% 27% 73%
1	N1	560	 22% 44% • 55%
1	O1	560	 22% 44% • 55%
1	P1	560	 13% 26% • 73%
1	Q1	560	 25% 44% • 55%
1	R1	560	 29% 44% 55%
1	S1	560	 15% 27% 73%
1	T1	560	 31% 44% 55%
1	U1	560	 33% 44% 55%
1	V1	560	 16% 27% 73%
1	W1	560	 30% 44% • 55%
1	X1	560	 28% 44% • 55%
1	Y1	560	 25% 44% 55%
1	Z1	560	 14% 27% 73%
1	a1	560	 21% 44% • 55%
1	b1	560	 12% 27% 73%
1	c1	560	 20% 44% • 55%
1	d1	560	 18% 44% • 55%
1	e1	560	 10% 27% 73%
1	f1	560	 17% 44% 55%
1	g1	560	 17% 44% • 55%
1	h1	560	 18% 44% 55%

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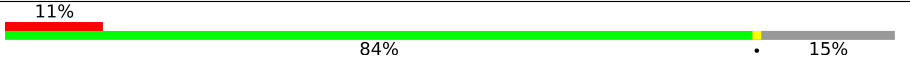
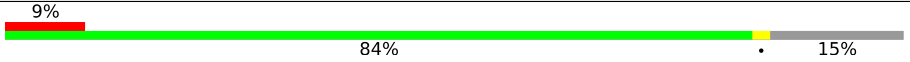
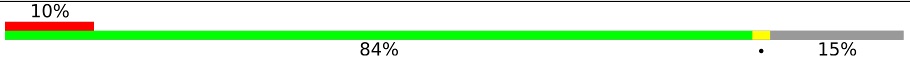
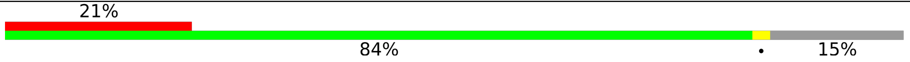
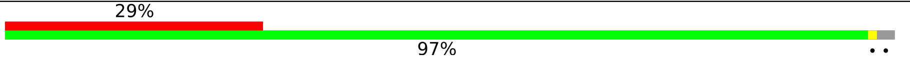
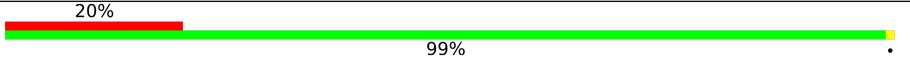
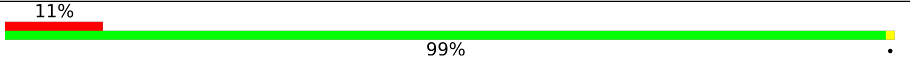
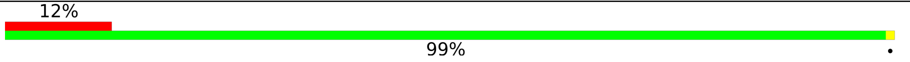
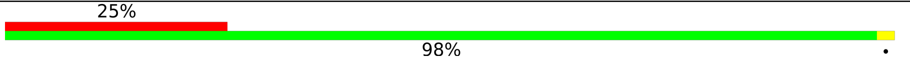
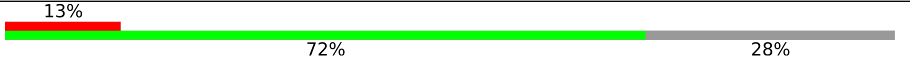
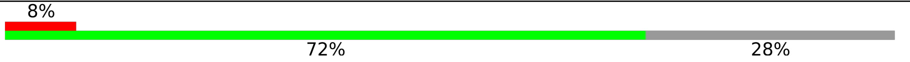
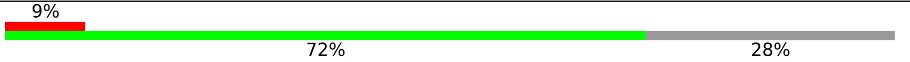
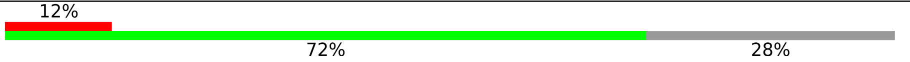
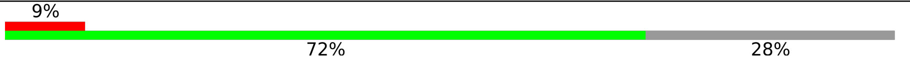
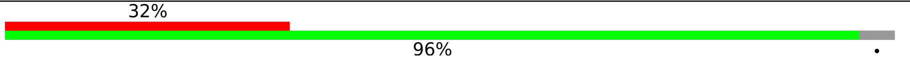
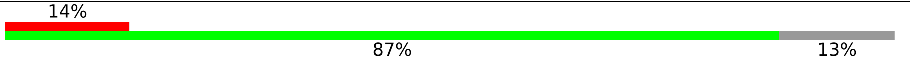
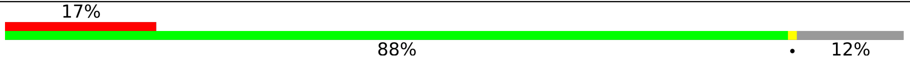
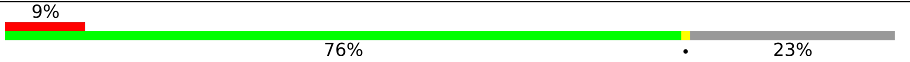
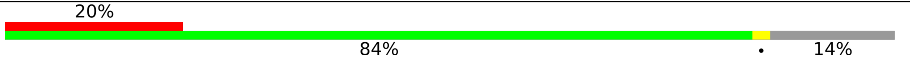
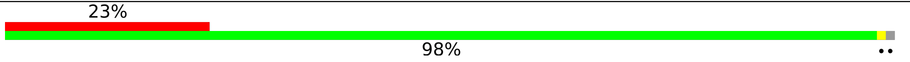
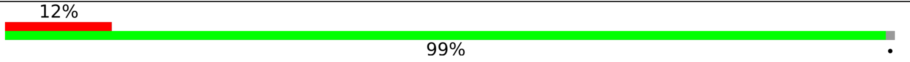
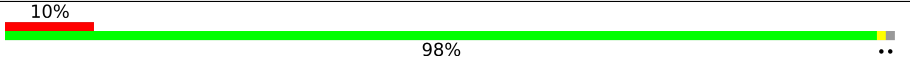
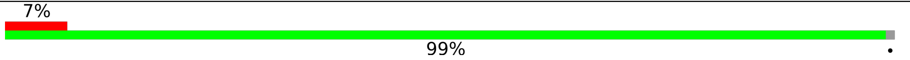
Mol	Chain	Length	Quality of chain
2	A2	245	
2	B2	245	
2	C2	245	
2	D2	245	
2	E2	245	
3	F2	264	
4	G2	89	
4	H2	89	
4	I2	89	
4	J2	89	
5	K2	104	
5	L2	104	
5	M2	104	
5	N2	104	
5	O2	104	
5	P2	104	
6	Q2	138	
6	R2	138	
6	S2	138	
6	T2	138	
6	U2	138	
7	V2	134	
7	W2	134	
7	X2	134	
7	Y2	134	

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Mol	Chain	Length	Quality of chain
7	Z2	134	10% 98% ••
7	a2	134	14% 99% •
8	b2	251	14% 98% •
8	c2	251	6% 98% ••
8	d2	251	• 99% •
8	e2	251	7% 98% ••
8	f2	251	7% 98% ••
9	12	260	19% 100%
9	22	260	19% 100%
9	32	260	23% 100%
9	42	260	72% 99% •
9	g2	260	7% 100%
9	h2	260	7% 100%
9	i2	260	5% 100%
9	j2	260	6% 100%
9	k2	260	6% 100%
9	l2	260	5% 96% •
9	m2	260	• 96% •
9	n2	260	5% 95% •
9	o2	260	5% 96% •
9	p2	260	5% 96% •
9	q2	260	• 96% •
9	r2	260	• 100%
9	s2	260	7% 100%
9	t2	260	6% 99% •

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Mol	Chain	Length	Quality of chain
9	u2	260	7% 100%
9	v2	260	6% 100%
9	w2	260	5% 100%
9	x2	260	9% 100%
9	y2	260	19% 100%
9	z2	260	27% 99% •
10	A3	232	85% 88% • 9%
10	B3	232	85% 88% • 9%
10	C3	232	85% 88% • 9%
10	D3	232	86% 88% • 9%
10	E3	232	85% 88% • 9%
10	F3	232	84% 88% • 9%
10	G3	232	86% 88% • 9%
10	H3	232	86% 88% • 9%
10	I3	232	87% 88% • 9%
10	J3	232	85% 88% • 9%
10	K3	232	85% 88% • 9%
10	L3	232	85% 88% • 9%
10	M3	232	86% 88% • 9%
10	N3	232	85% 88% • 9%
10	O3	232	86% 88% • 9%
10	P3	232	87% 88% • 9%
10	Q3	232	88% 88% • 9%
10	R3	232	86% 88% • 9%
10	S3	232	88% 88% • 9%

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Mol	Chain	Length	Quality of chain
10	T3	232	87% 88% • 9%
10	U3	232	87% 88% • 9%
10	V3	232	87% 88% • 9%
10	W3	232	86% 88% • 9%
10	X3	232	88% 88% • 9%
10	Y3	232	87% 88% • 9%
10	Z3	232	84% 88% • 9%
11	a3	365	83% 80% • 16%
11	b3	365	83% 80% • 16%
11	c3	365	84% 80% • 16%
11	d3	365	83% 80% • 16%
11	e3	365	83% 80% • 16%
11	f3	365	84% 80% • 16%
11	g3	365	83% 80% • 16%
11	h3	365	84% 80% • 16%
11	i3	365	83% 80% • 16%
11	j3	365	84% 80% • 16%
11	k3	365	84% 80% • 16%
11	l3	365	84% 80% • 16%
11	m3	365	84% 80% • 16%
11	n3	365	83% 80% • 16%
11	o3	365	84% 80% • 16%
11	p3	365	84% 80% • 16%
11	q3	365	84% 80% • 16%
11	r3	365	84% 80% • 16%

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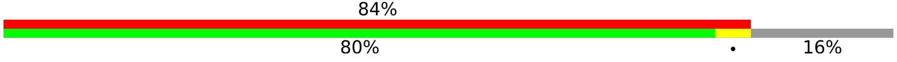
Mol	Chain	Length	Quality of chain
11	s3	365	
11	t3	365	
11	u3	365	
11	v3	365	
11	w3	365	
11	x3	365	
11	y3	365	
11	z3	365	
12	A4	232	
12	B4	232	
12	C4	232	
12	D4	232	
12	E4	232	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 246311 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A1	151	Total C N O S 1193 726 223 241 3	0	0
1	B1	250	Total C N O S 1931 1187 355 385 4	0	0
1	C1	250	Total C N O S 1931 1187 355 385 4	0	0
1	D1	151	Total C N O S 1193 726 223 241 3	0	0
1	E1	250	Total C N O S 1931 1187 355 385 4	0	0
1	F1	151	Total C N O S 1193 726 223 241 3	0	0
1	G1	250	Total C N O S 1931 1187 355 385 4	0	0
1	H1	250	Total C N O S 1931 1187 355 385 4	0	0
1	I1	250	Total C N O S 1931 1187 355 385 4	0	0
1	J1	151	Total C N O S 1193 726 223 241 3	0	0
1	K1	250	Total C N O S 1931 1187 355 385 4	0	0
1	L1	250	Total C N O S 1931 1187 355 385 4	0	0
1	M1	151	Total C N O S 1193 726 223 241 3	0	0
1	N1	250	Total C N O S 1931 1187 355 385 4	0	0
1	O1	250	Total C N O S 1931 1187 355 385 4	0	0
1	P1	151	Total C N O S 1193 726 223 241 3	0	0
1	Q1	250	Total C N O S 1931 1187 355 385 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	S1	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	T1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	U1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	V1	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	W1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	X1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	Y1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	Z1	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	a1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	b1	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	c1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	d1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	e1	151	Total 1193	C 726	N 223	O 241	S 3	0	0
1	f1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	g1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0
1	h1	250	Total 1931	C 1187	N 355	O 385	S 4	0	0

- Molecule 2 is a protein called Flagellar biosynthetic protein FliP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	209	Total 1623	C 1084	N 251	O 276	S 12	0	0
2	B2	209	Total 1623	C 1084	N 251	O 276	S 12	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
2	C2	209	Total C N O S 1623 1084 251 276 12	0	0
2	D2	209	Total C N O S 1623 1084 251 276 12	0	0
2	E2	209	Total C N O S 1623 1084 251 276 12	0	0

- Molecule 3 is a protein called Flagellar biosynthetic protein FliR.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	F2	258	Total C N O S 1986 1329 314 327 16	0	0

- Molecule 4 is a protein called Flagellar biosynthetic protein FliQ.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	G2	89	Total C N O S 670 449 100 114 7	0	0
4	H2	89	Total C N O S 670 449 100 114 7	0	0
4	I2	89	Total C N O S 670 449 100 114 7	0	0
4	J2	89	Total C N O S 670 449 100 114 7	0	0

- Molecule 5 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	K2	39	Total C N O S 296 183 51 56 6	0	0
5	L2	75	Total C N O S 563 347 102 108 6	0	0
5	M2	75	Total C N O S 563 347 102 108 6	0	0
5	N2	75	Total C N O S 563 347 102 108 6	0	0
5	O2	75	Total C N O S 563 347 102 108 6	0	0
5	P2	75	Total C N O S 563 347 102 108 6	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
6	Q2	133	Total C N O S 1023 630 188 200 5	0	0
6	R2	120	Total C N O S 932 578 169 180 5	0	0
6	S2	122	Total C N O S 942 583 173 181 5	0	0
6	T2	106	Total C N O S 835 516 153 161 5	0	0
6	U2	119	Total C N O S 925 573 168 179 5	0	0

- Molecule 7 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	V2	133	Total C N O S 969 604 167 193 5	0	0
7	W2	132	Total C N O S 964 601 166 192 5	0	0
7	X2	132	Total C N O S 964 601 166 192 5	0	0
7	Y2	132	Total C N O S 964 601 166 192 5	0	0
7	Z2	132	Total C N O S 964 601 166 192 5	0	0
7	a2	132	Total C N O S 964 601 166 192 5	0	0

- Molecule 8 is a protein called Flagellar basal body protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	b2	249	Total C N O S 1812 1111 325 368 8	0	0
8	c2	249	Total C N O S 1812 1111 325 368 8	0	0
8	d2	249	Total C N O S 1812 1111 325 368 8	0	0
8	e2	249	Total C N O S 1812 1111 325 368 8	0	0
8	f2	249	Total C N O S 1812 1111 325 368 8	0	0

- Molecule 9 is a protein called Flagellar basal-body rod protein FlgG.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	g2	260	Total C N O S 1949 1202 341 400 6	0	0
9	h2	260	Total C N O S 1949 1202 341 400 6	0	0
9	i2	260	Total C N O S 1949 1202 341 400 6	0	0
9	j2	260	Total C N O S 1949 1202 341 400 6	0	0
9	k2	260	Total C N O S 1949 1202 341 400 6	0	0
9	l2	249	Total C N O S 1871 1157 328 381 5	0	0
9	m2	249	Total C N O S 1871 1157 328 381 5	0	0
9	n2	249	Total C N O S 1871 1157 328 381 5	0	0
9	o2	249	Total C N O S 1871 1157 328 381 5	0	0
9	p2	249	Total C N O S 1871 1157 328 381 5	0	0
9	q2	251	Total C N O S 1885 1166 330 384 5	0	0
9	r2	260	Total C N O S 1949 1202 341 400 6	0	0
9	s2	260	Total C N O S 1949 1202 341 400 6	0	0
9	t2	260	Total C N O S 1949 1202 341 400 6	0	0
9	u2	260	Total C N O S 1949 1202 341 400 6	0	0
9	v2	260	Total C N O S 1949 1202 341 400 6	0	0
9	w2	260	Total C N O S 1949 1202 341 400 6	0	0
9	x2	260	Total C N O S 1949 1202 341 400 6	0	0
9	y2	260	Total C N O S 1949 1202 341 400 6	0	0
9	z2	260	Total C N O S 1949 1202 341 400 6	0	0
9	12	260	Total C N O S 1949 1202 341 400 6	0	0
9	22	260	Total C N O S 1949 1202 341 400 6	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
9	32	260	Total C N O S 1948 1202 340 400 6	0	0
9	42	260	Total C N O S 1949 1202 341 400 6	0	0

- Molecule 10 is a protein called Flagellar L-ring protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	A3	211	Total C N O S 1581 985 282 310 4	0	0
10	B3	211	Total C N O S 1581 985 282 310 4	0	0
10	C3	211	Total C N O S 1581 985 282 310 4	0	0
10	D3	211	Total C N O S 1581 985 282 310 4	0	0
10	E3	211	Total C N O S 1581 985 282 310 4	0	0
10	F3	211	Total C N O S 1581 985 282 310 4	0	0
10	G3	211	Total C N O S 1581 985 282 310 4	0	0
10	H3	211	Total C N O S 1581 985 282 310 4	0	0
10	I3	211	Total C N O S 1581 985 282 310 4	0	0
10	J3	211	Total C N O S 1581 985 282 310 4	0	0
10	K3	211	Total C N O S 1581 985 282 310 4	0	0
10	L3	211	Total C N O S 1581 985 282 310 4	0	0
10	M3	211	Total C N O S 1581 985 282 310 4	0	0
10	N3	211	Total C N O S 1581 985 282 310 4	0	0
10	O3	211	Total C N O S 1581 985 282 310 4	0	0
10	P3	211	Total C N O S 1581 985 282 310 4	0	0
10	Q3	211	Total C N O S 1581 985 282 310 4	0	0

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Mol	Chain	Residues	Atoms	AltConf	Trace
10	R3	211	Total C N O S 1581 985 282 310 4	0	0
10	S3	211	Total C N O S 1581 985 282 310 4	0	0
10	T3	211	Total C N O S 1581 985 282 310 4	0	0
10	U3	211	Total C N O S 1581 985 282 310 4	0	0
10	V3	211	Total C N O S 1581 985 282 310 4	0	0
10	W3	211	Total C N O S 1580 984 282 310 4	0	0
10	X3	211	Total C N O S 1581 985 282 310 4	0	0
10	Y3	211	Total C N O S 1581 985 282 310 4	0	0
10	Z3	211	Total C N O S 1581 985 282 310 4	0	0

- Molecule 11 is a protein called Flagellar P-ring protein.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	a3	306	Total C N O S 2252 1379 409 451 13	0	0
11	b3	306	Total C N O S 2252 1379 409 451 13	0	0
11	c3	306	Total C N O S 2252 1379 409 451 13	0	0
11	d3	306	Total C N O S 2252 1379 409 451 13	0	0
11	e3	306	Total C N O S 2252 1379 409 451 13	0	0
11	f3	306	Total C N O S 2252 1379 409 451 13	0	0
11	g3	306	Total C N O S 2252 1379 409 451 13	0	0
11	h3	306	Total C N O S 2251 1379 408 451 13	0	0
11	i3	306	Total C N O S 2252 1379 409 451 13	0	0
11	j3	306	Total C N O S 2252 1379 409 451 13	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	k3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	l3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	m3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	n3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	o3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	p3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	q3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	r3	306	Total 2251	C 1378	N 409	O 451	S 13	0	0
11	s3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	t3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	u3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	v3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	w3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	x3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	y3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0
11	z3	306	Total 2252	C 1379	N 409	O 451	S 13	0	0

- Molecule 12 is a protein called Basal-body rod modification protein FlgD.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A4	201	Total 1475	C 914	N 253	O 307	S 1	0	0
12	B4	204	Total 1493	C 924	N 256	O 312	S 1	0	0
12	C4	199	Total 1458	C 903	N 250	O 304	S 1	0	0

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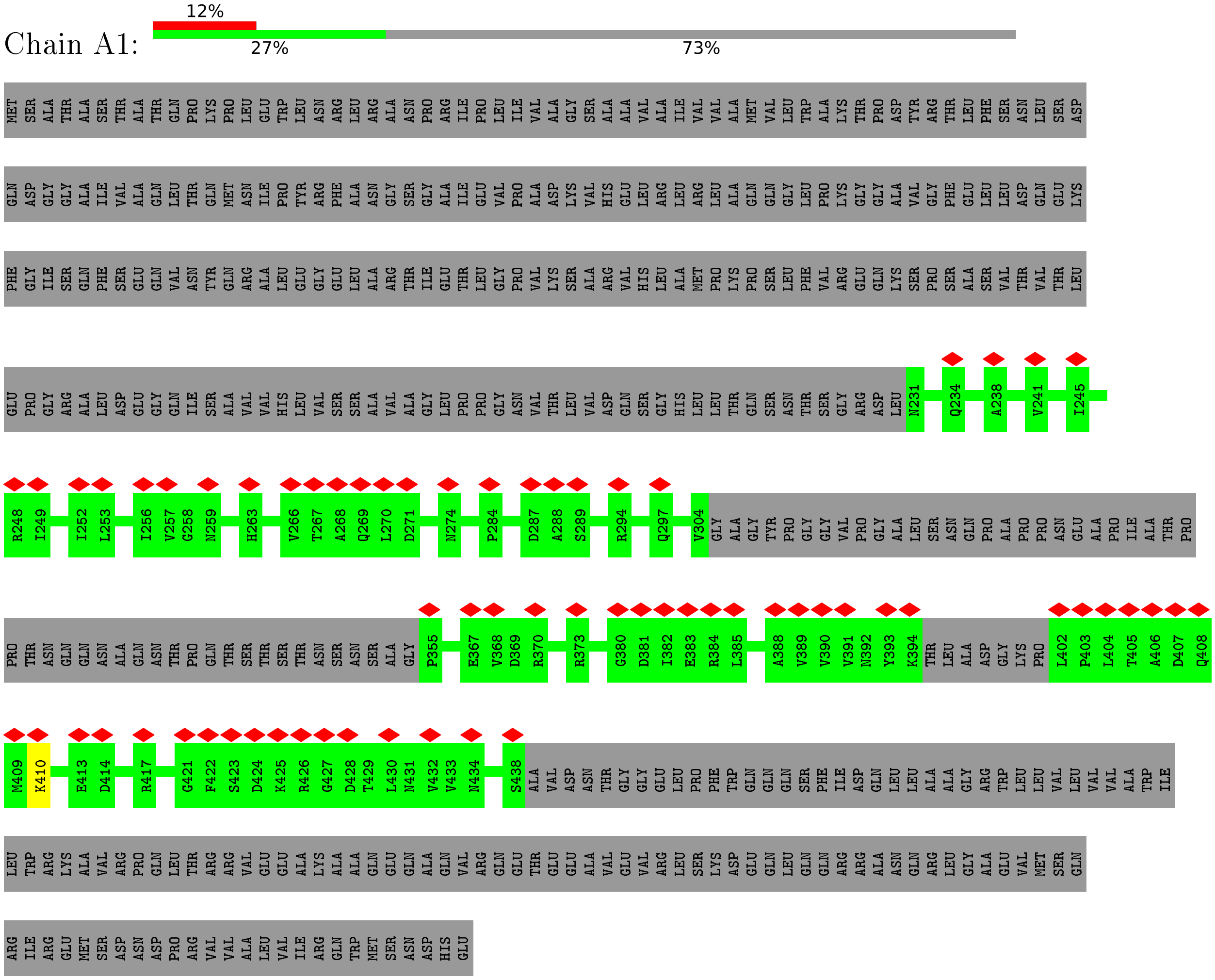
Mol	Chain	Residues	Atoms	AltConf	Trace
12	D4	202	Total C N O S 1482 917 254 310 1	0	0
12	E4	204	Total C N O S 1493 924 256 312 1	0	0

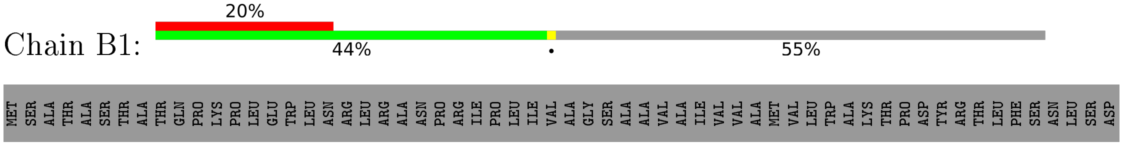
3 Residue-property plots ⓘ

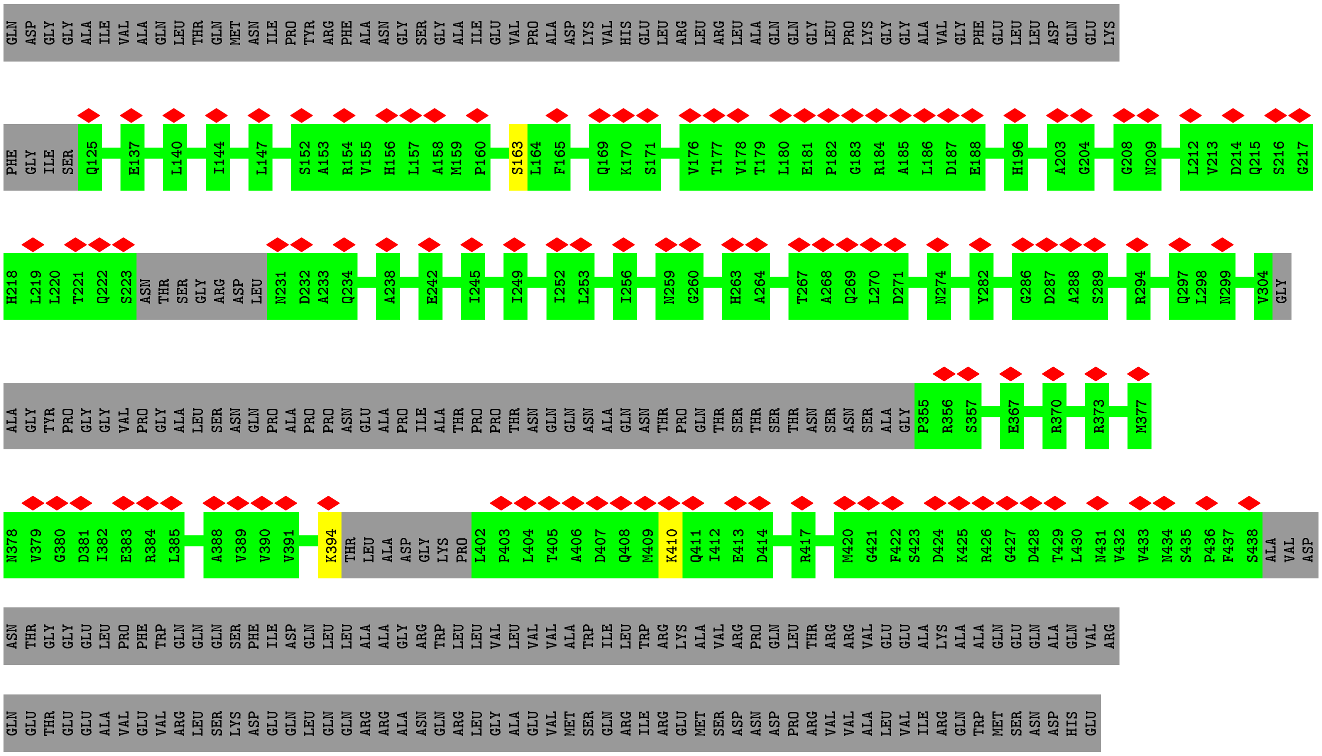
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 M-ring protein



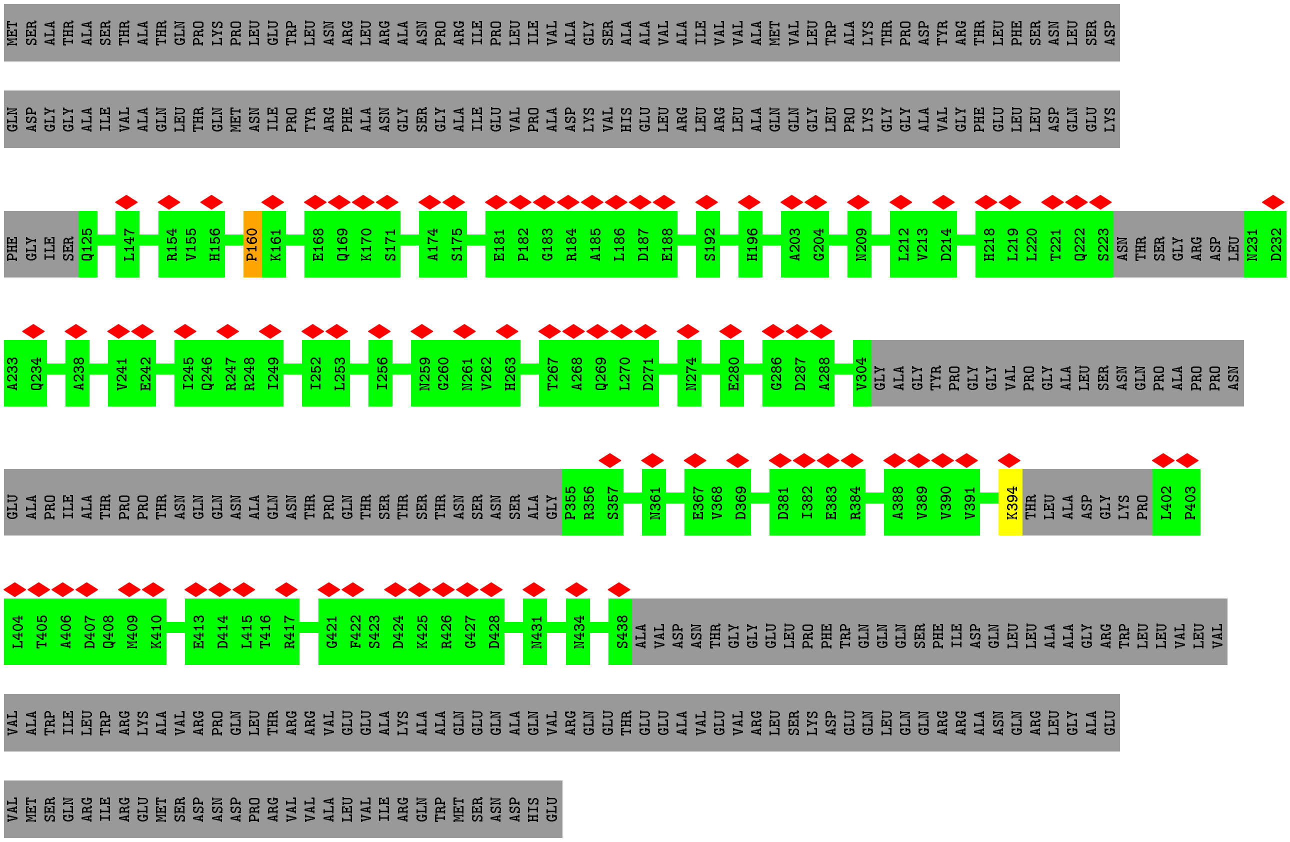
- Molecule 1: Flagellar M-ring protein



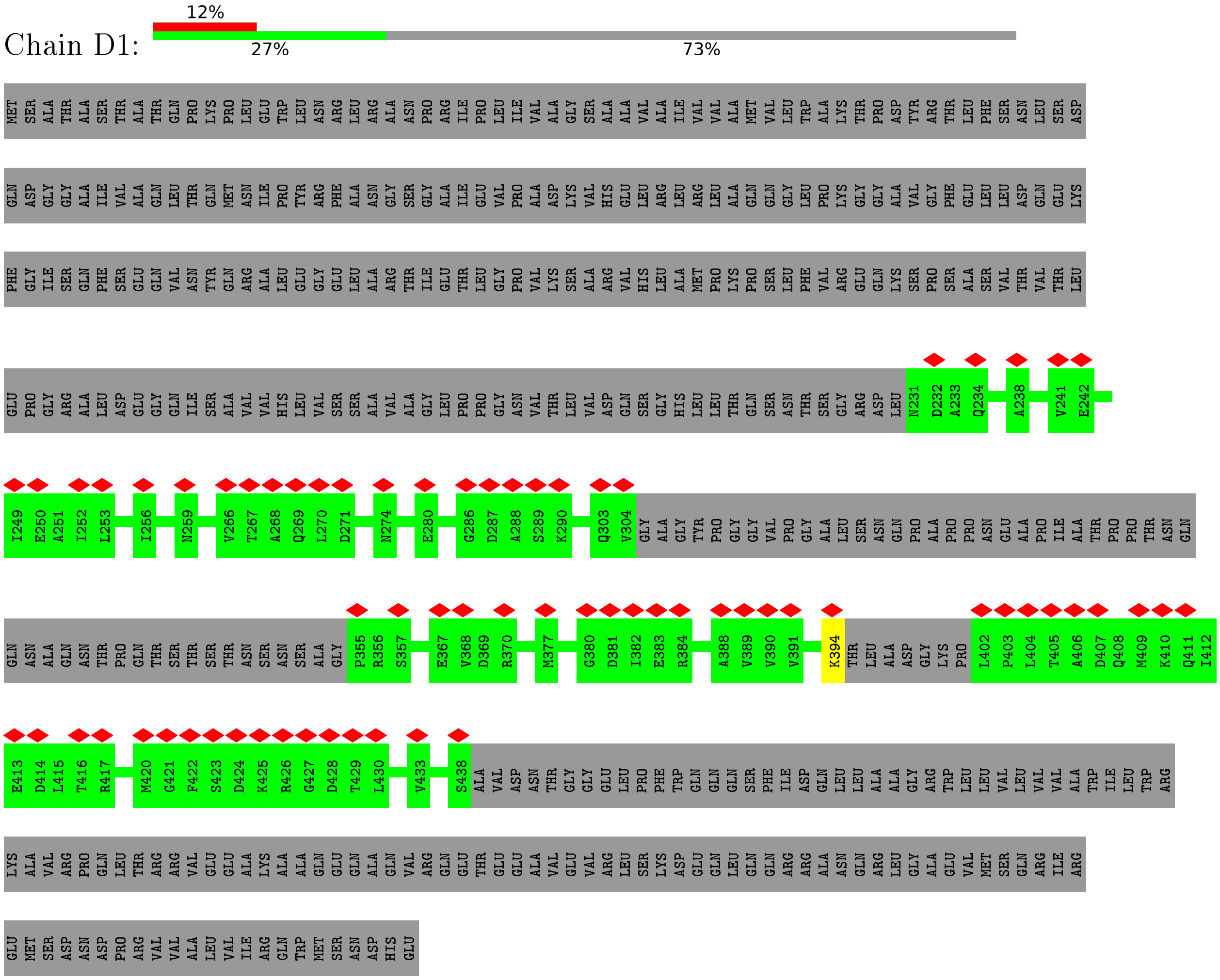


- Molecule 1: Flagellar M-ring protein

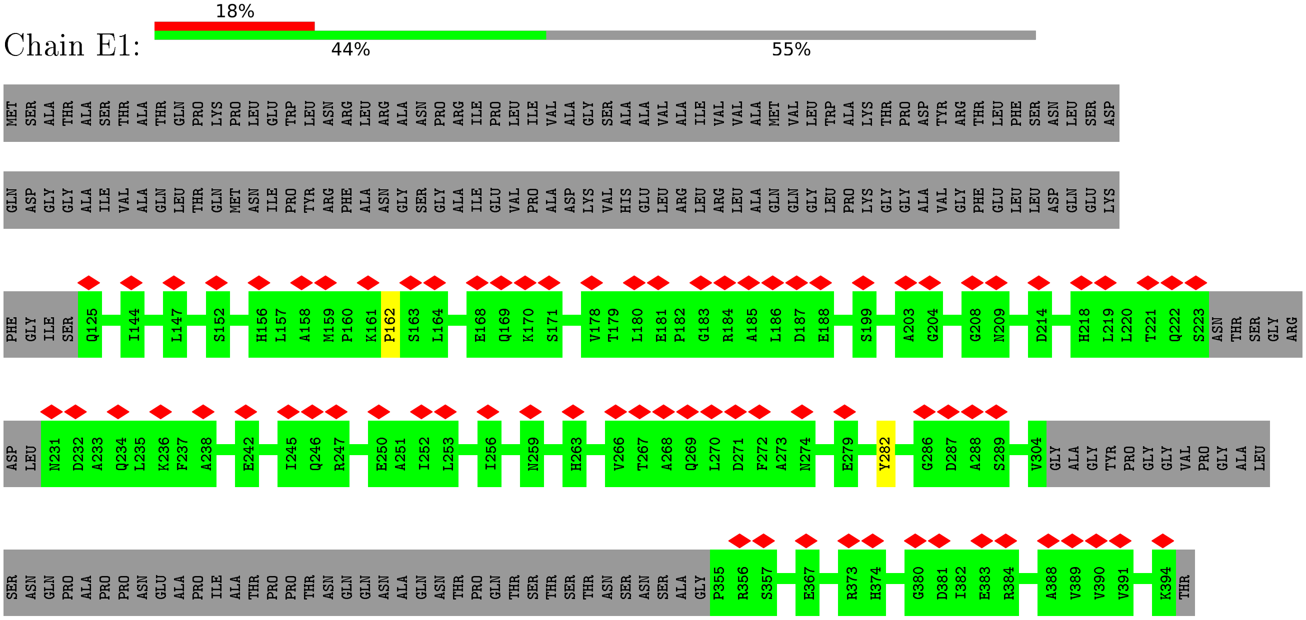
Chain C1:

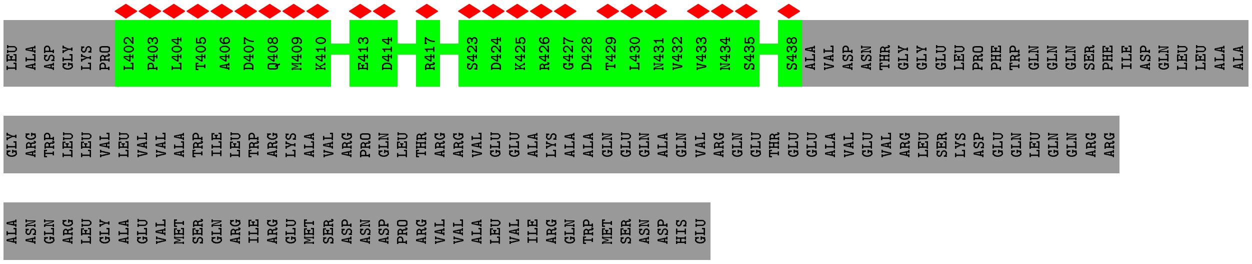


- Molecule 1: Flagellar M-ring protein

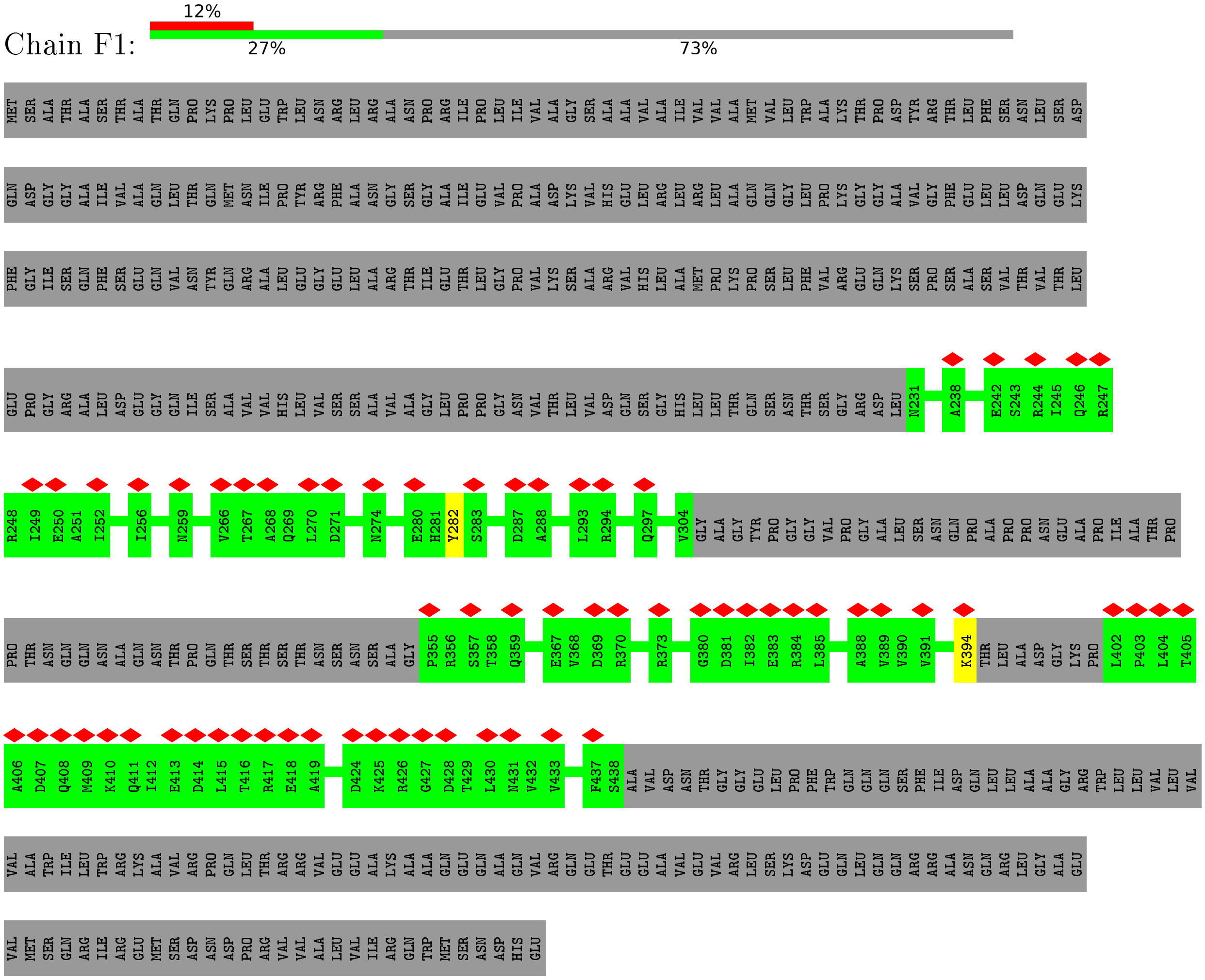


- Molecule 1: Flagellar M-ring protein

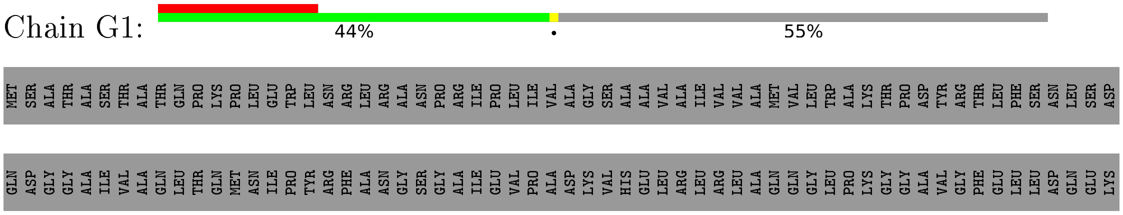


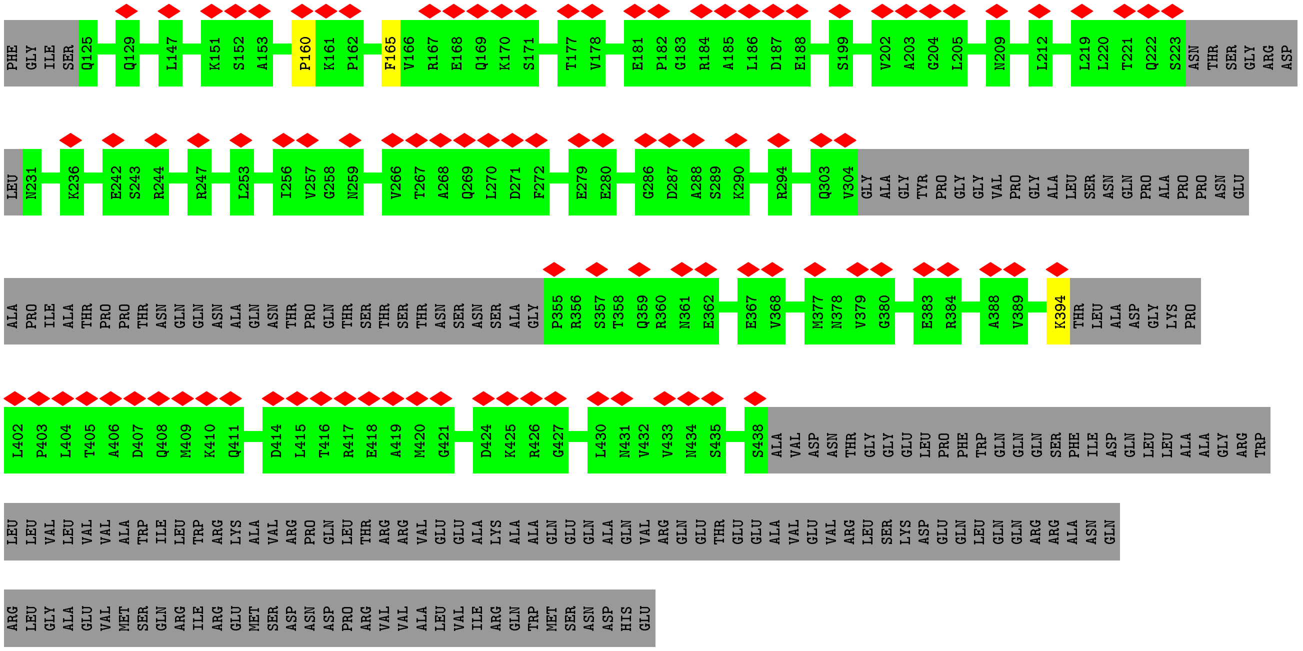


• Molecule 1: Flagellar M-ring protein



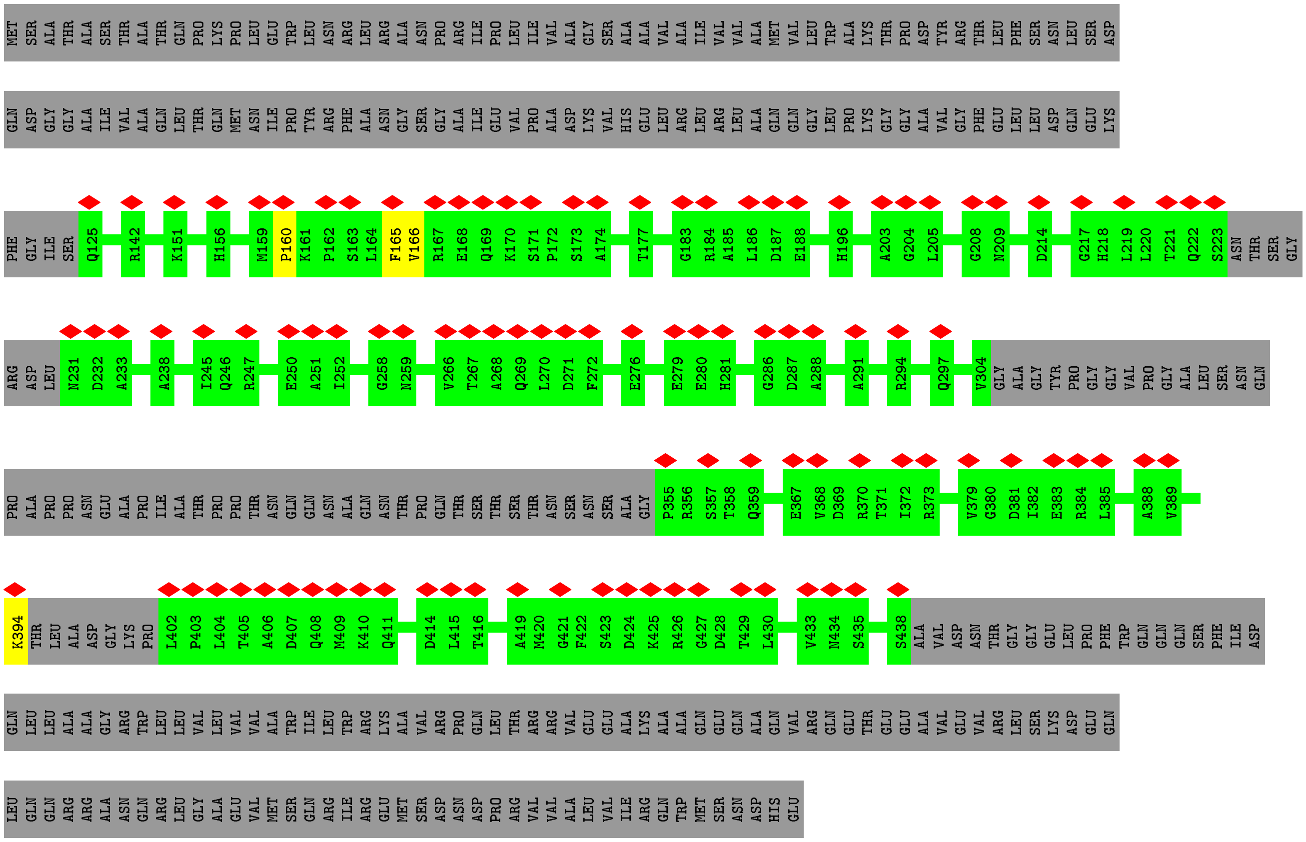
• Molecule 1: Flagellar M-ring protein



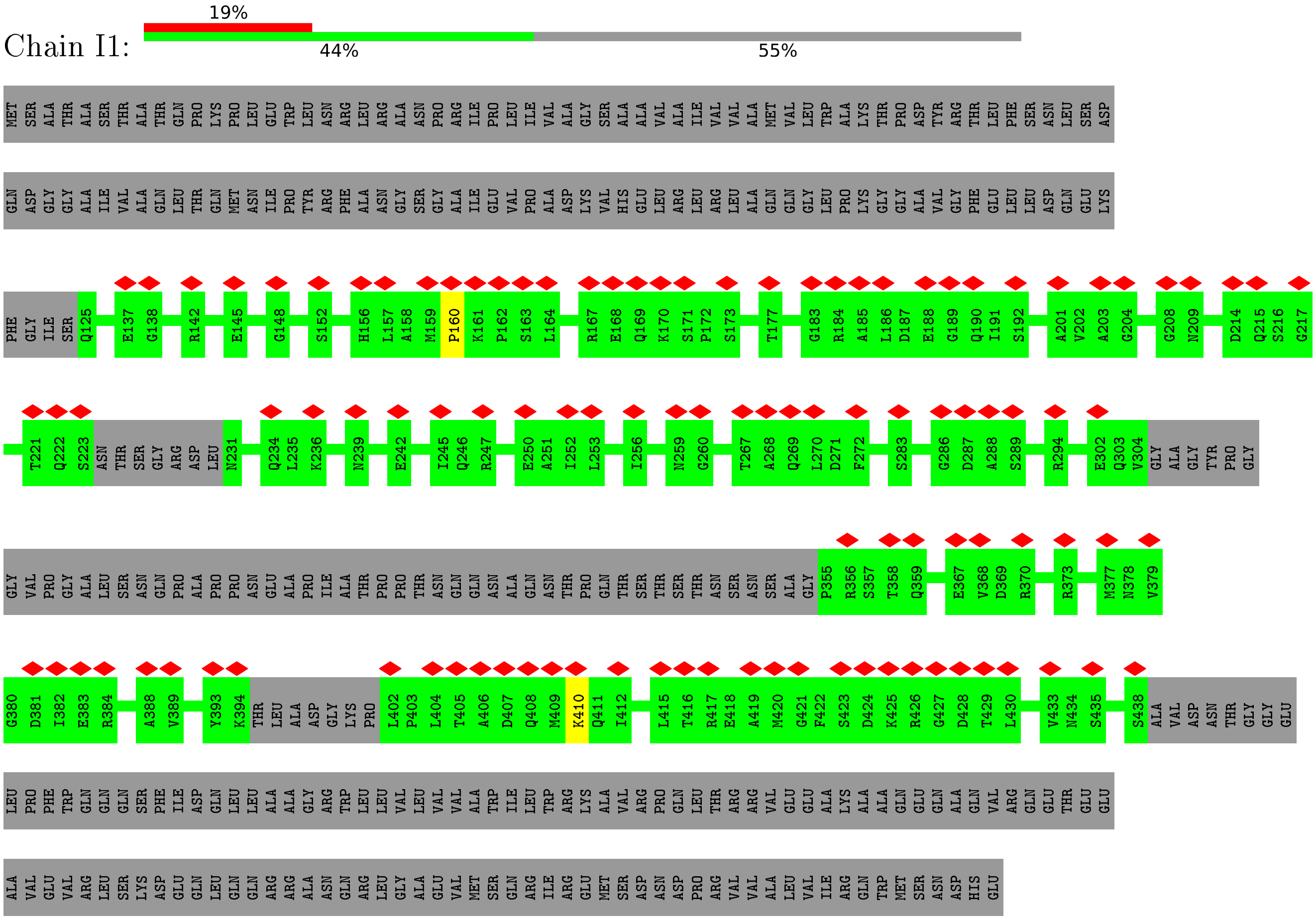


- Molecule 1: Flagellar M-ring protein

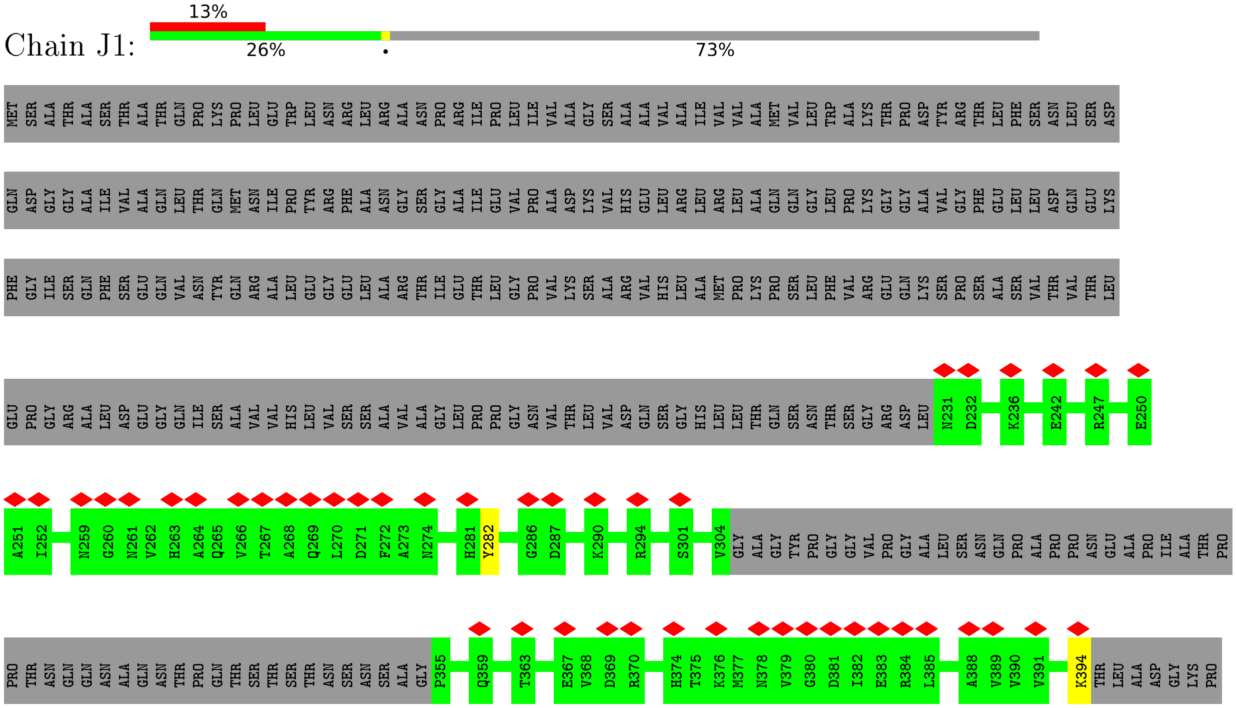
Chain H1:

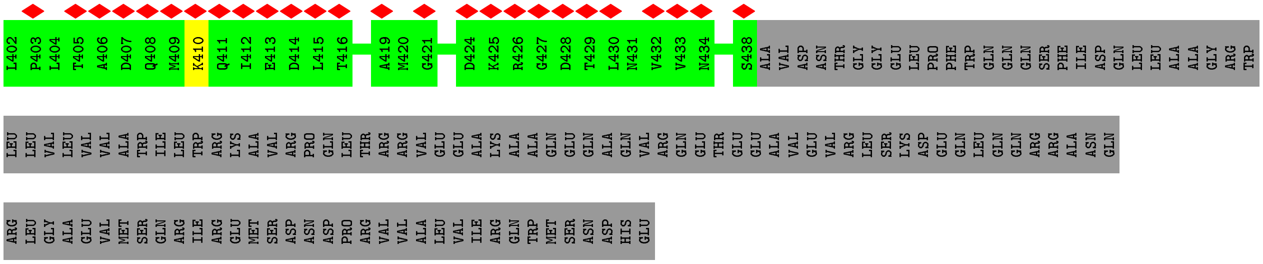


- Molecule 1: Flagellar M-ring protein

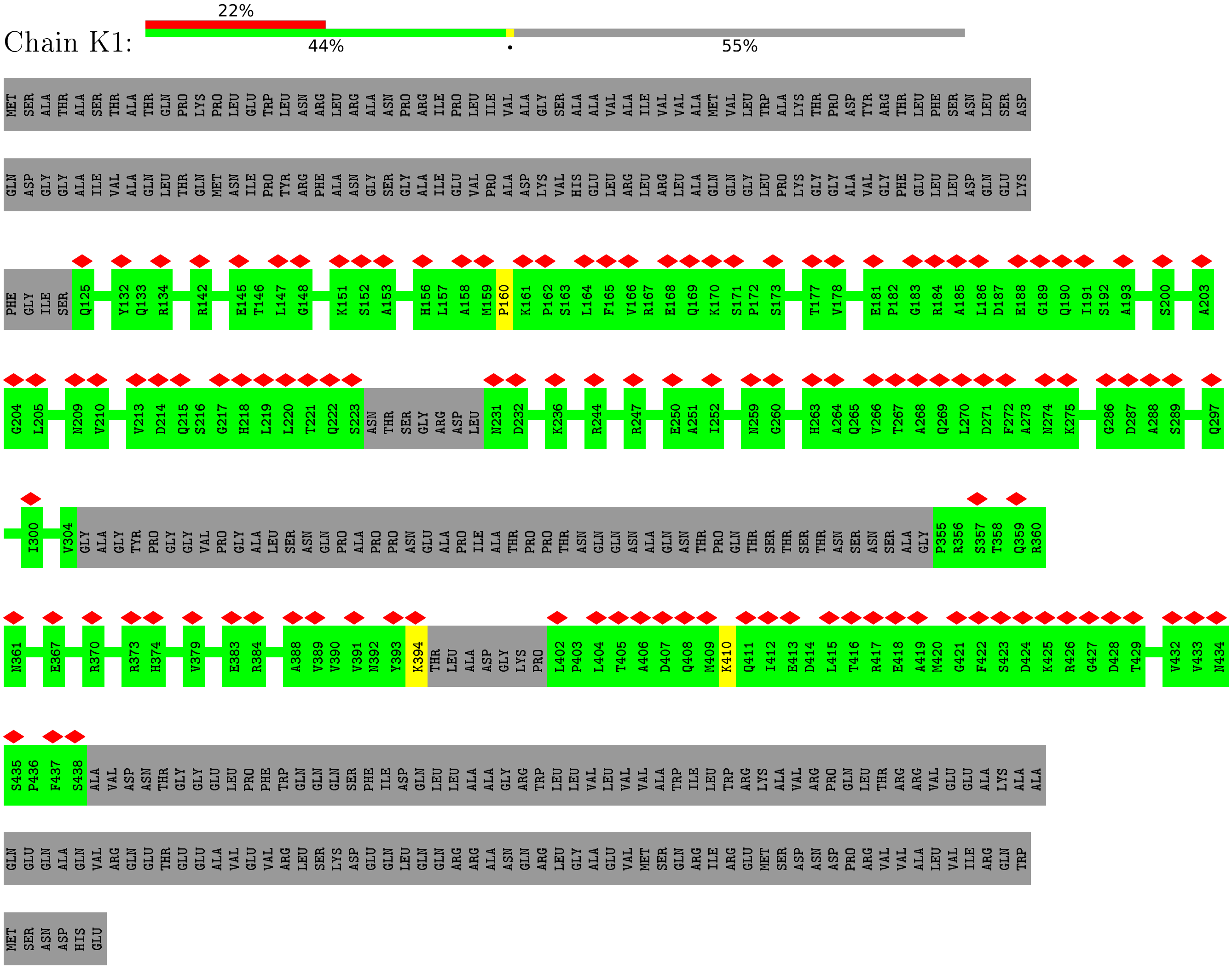


- Molecule 1: Flagellar M-ring protein

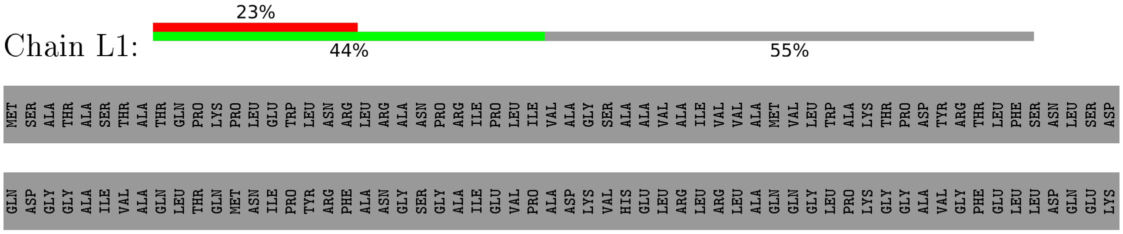


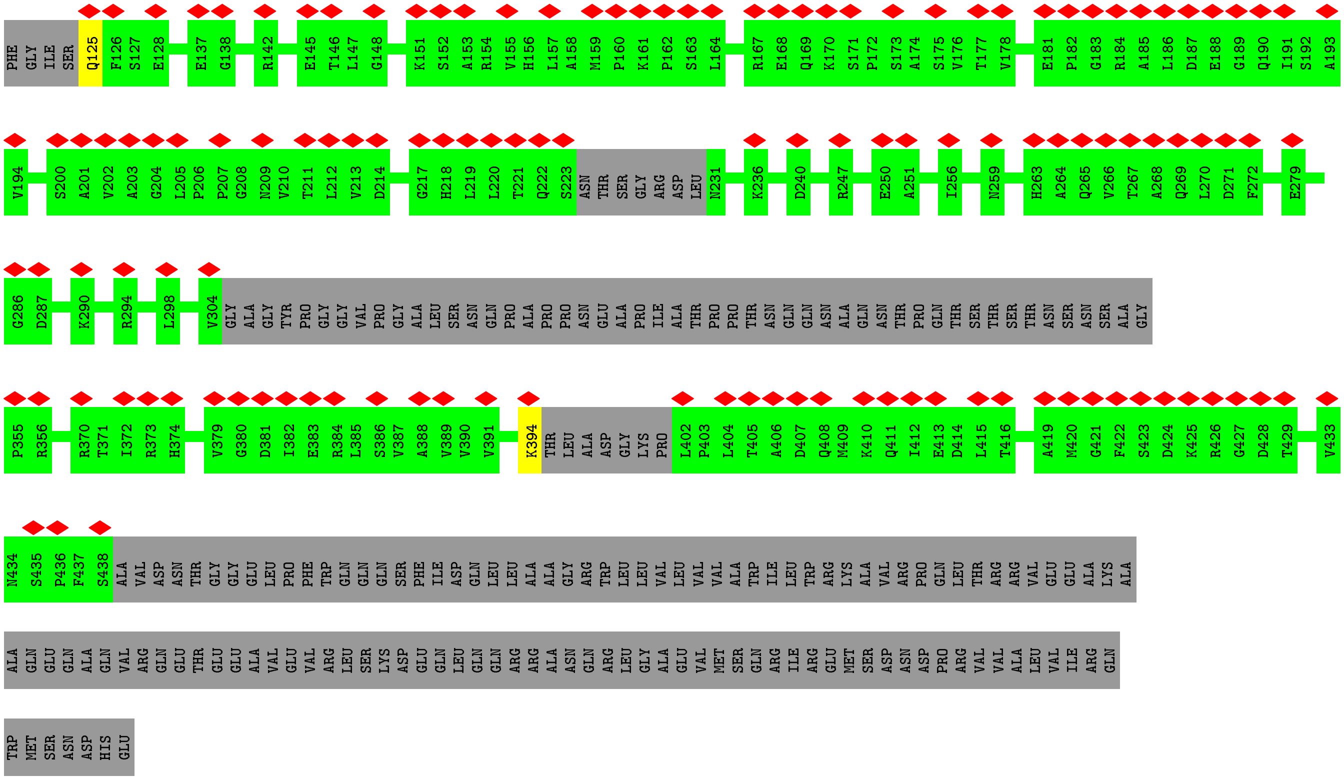


- Molecule 1: Flagellar M-ring protein



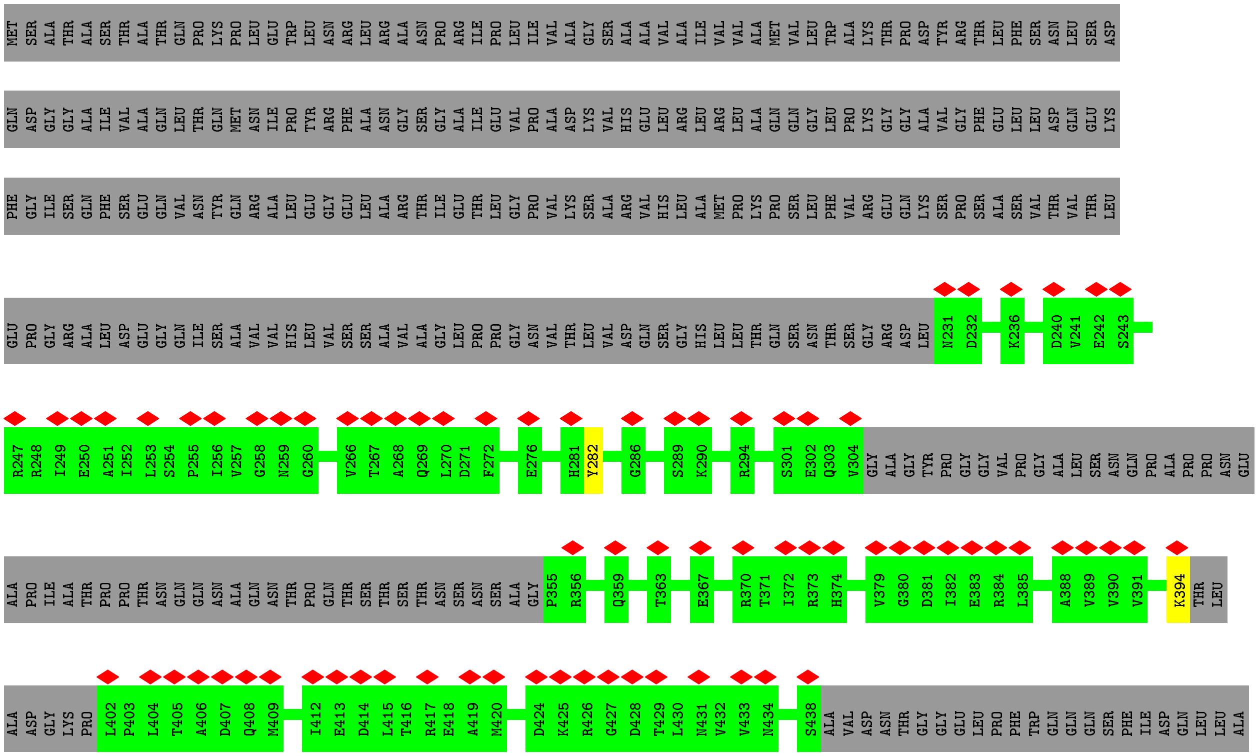
- Molecule 1: Flagellar M-ring protein

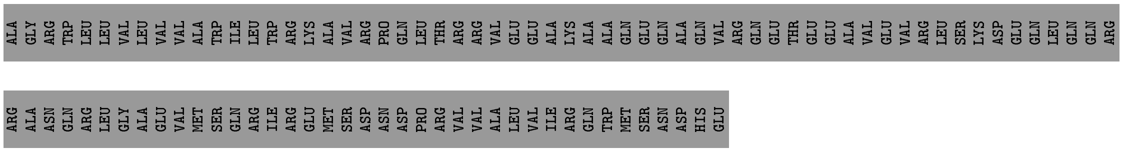




- Molecule 1: Flagellar M-ring protein

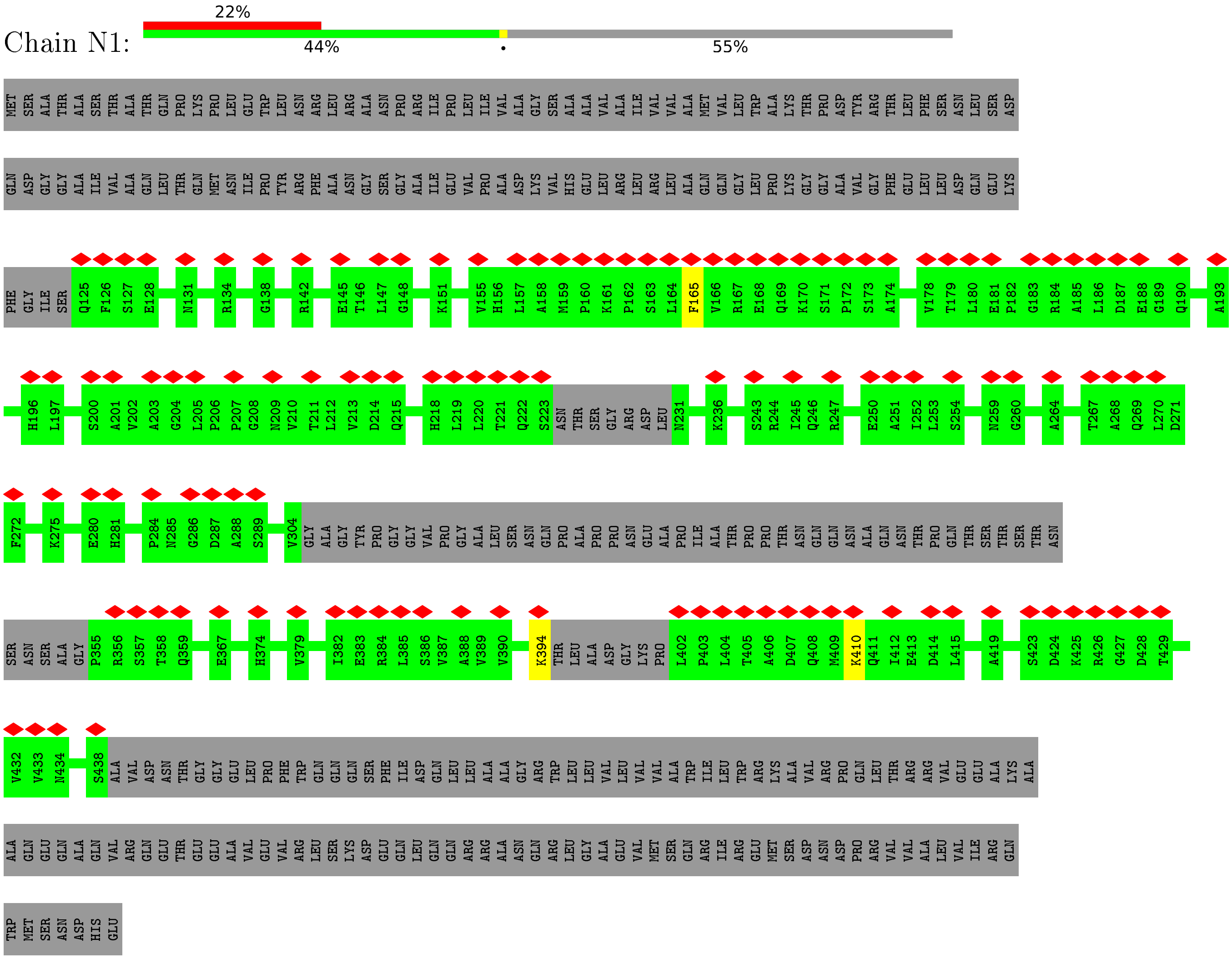
Chain M1:





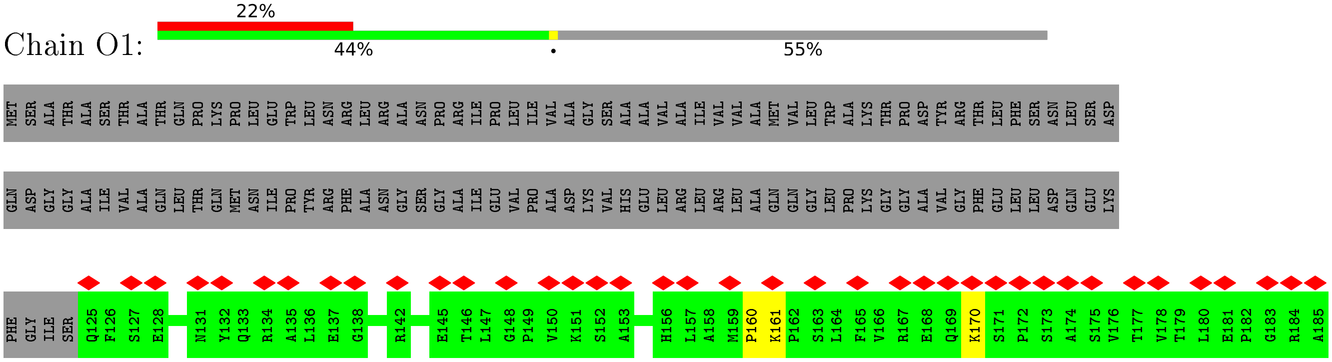
- Molecule 1: Flagellar M-ring protein

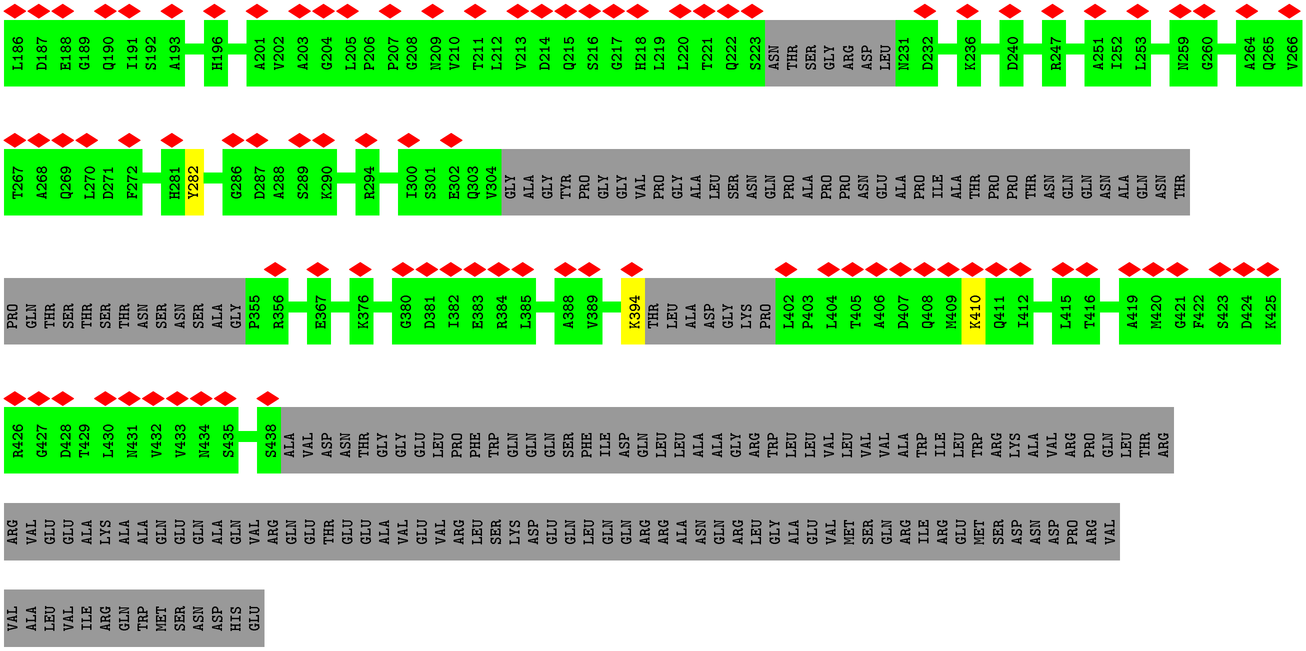
Chain N1:



- Molecule 1: Flagellar M-ring protein

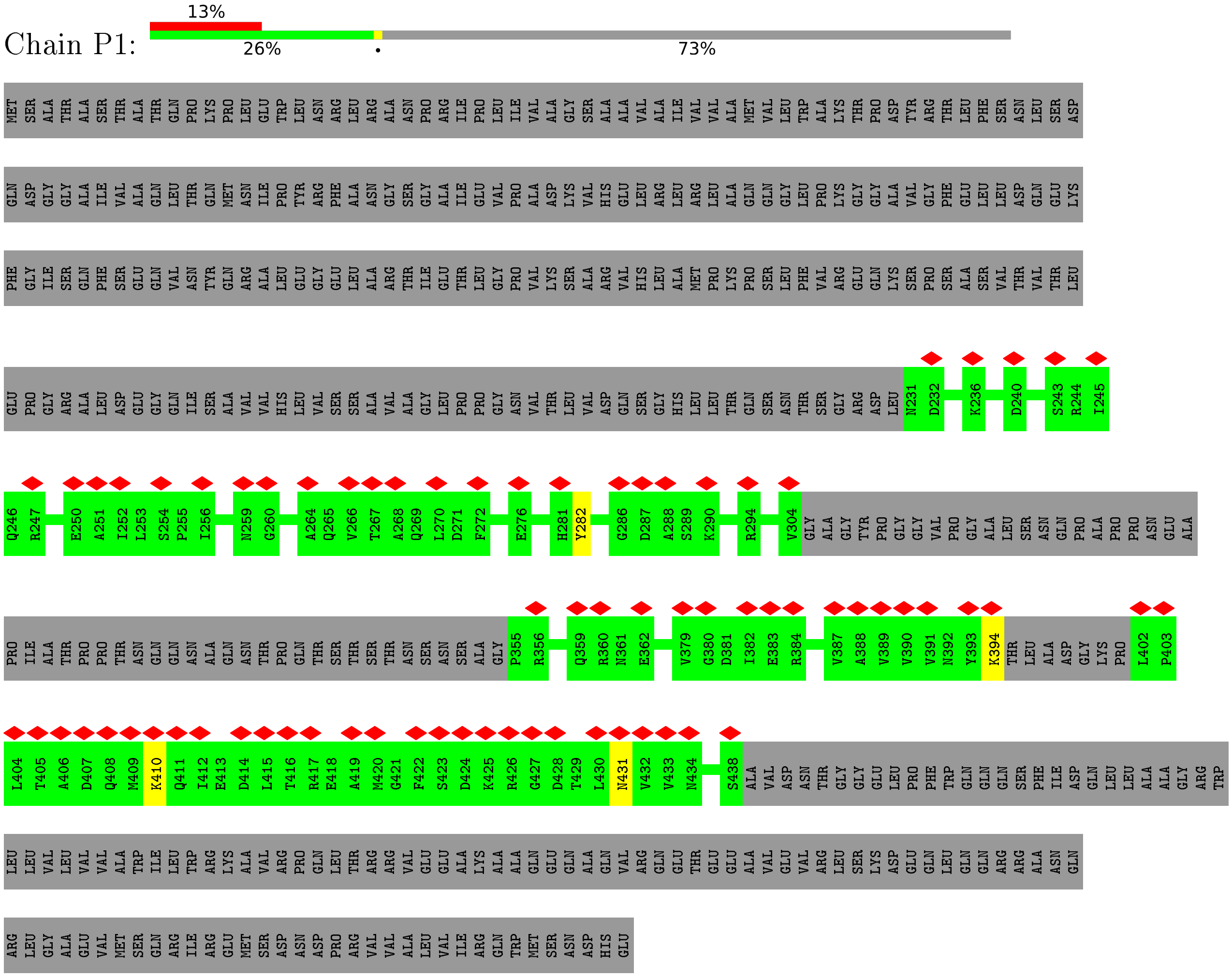
Chain O1:





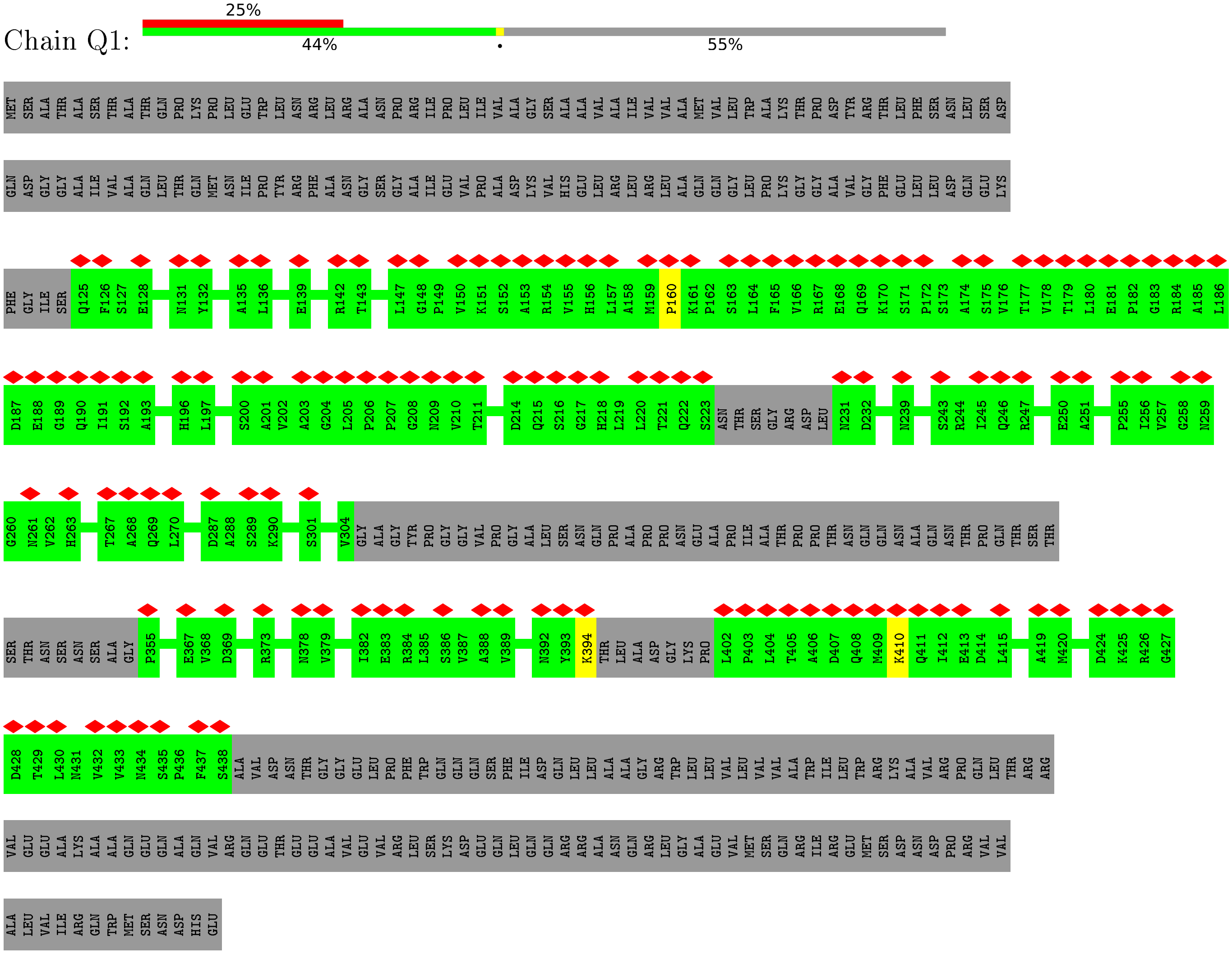
- Molecule 1: Flagellar M-ring protein

Chain P1:



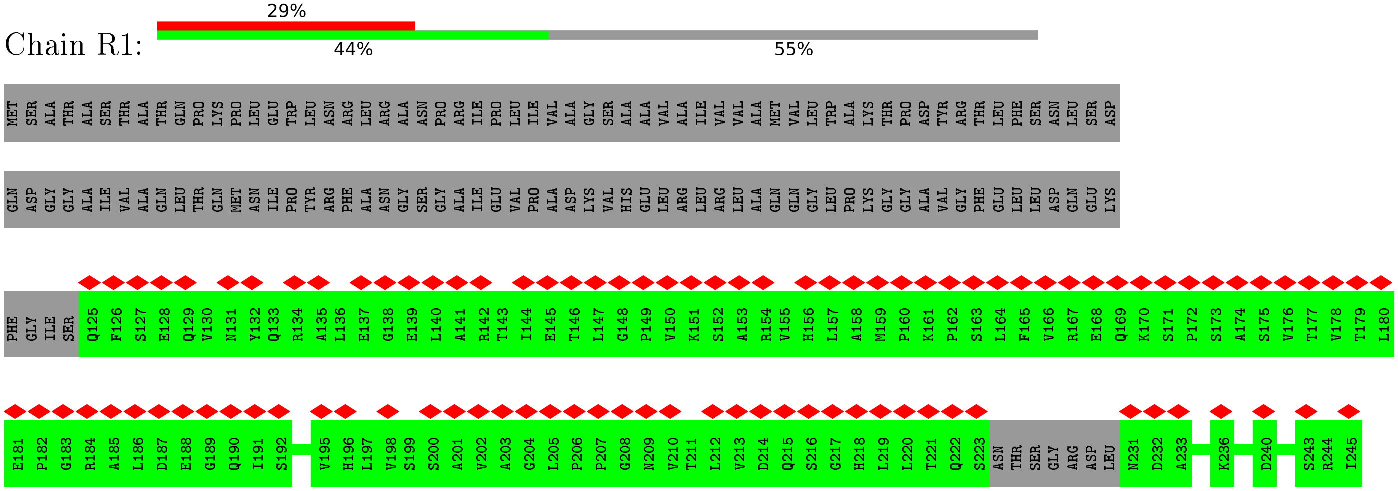
- Molecule 1: Flagellar M-ring protein

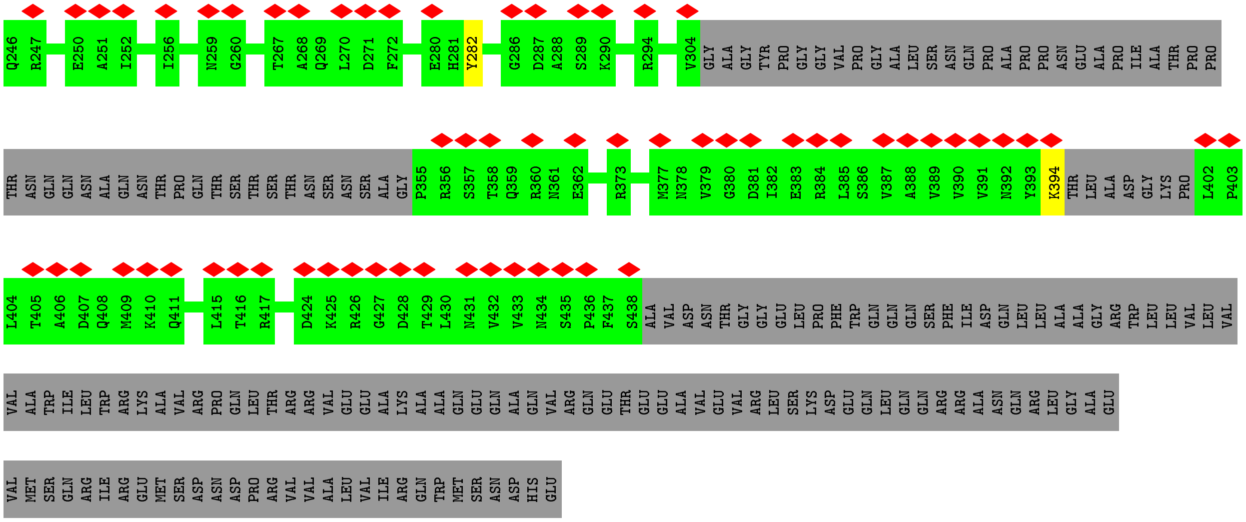
Chain Q1:



- Molecule 1: Flagellar M-ring protein

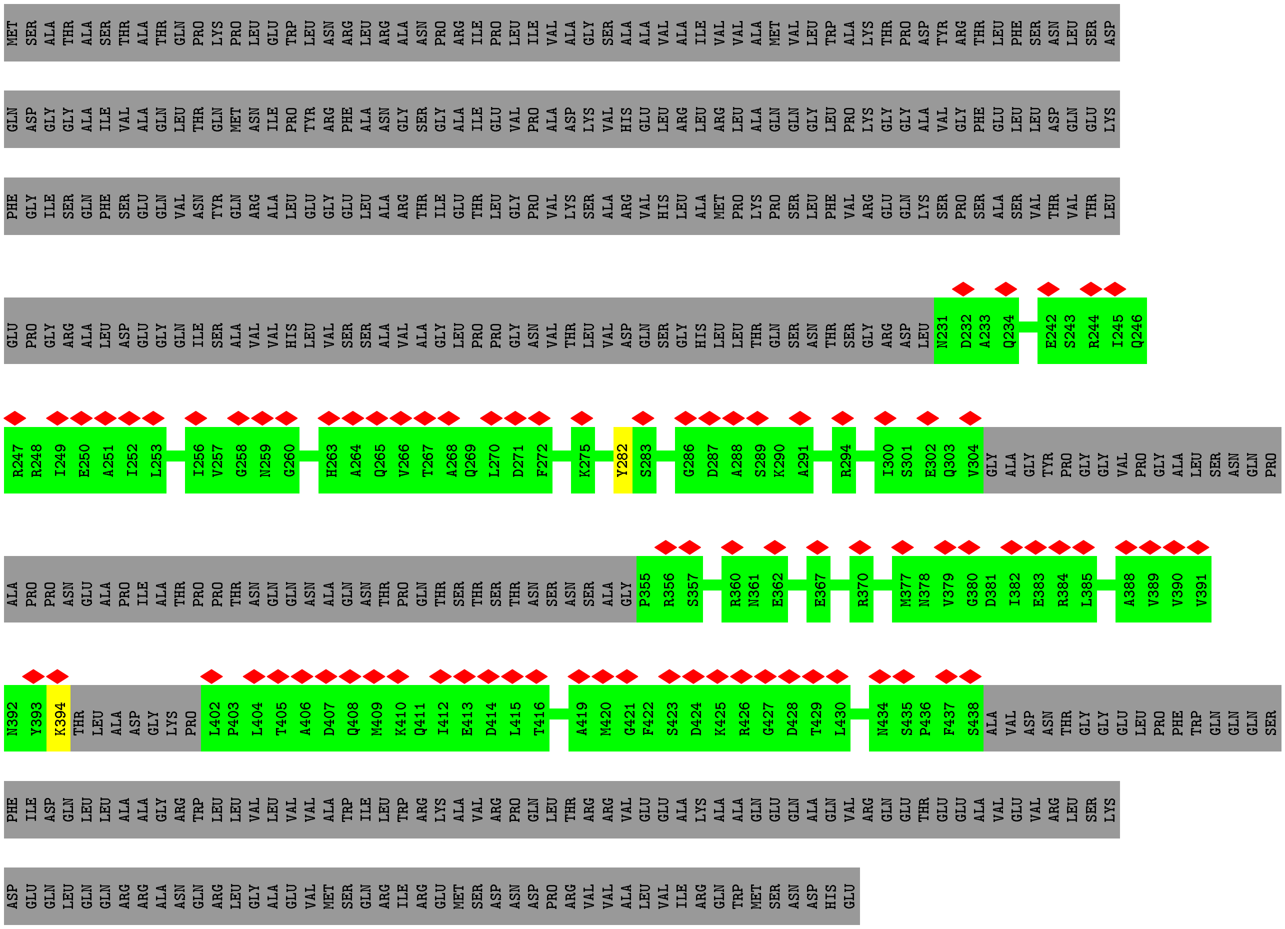
Chain R1:





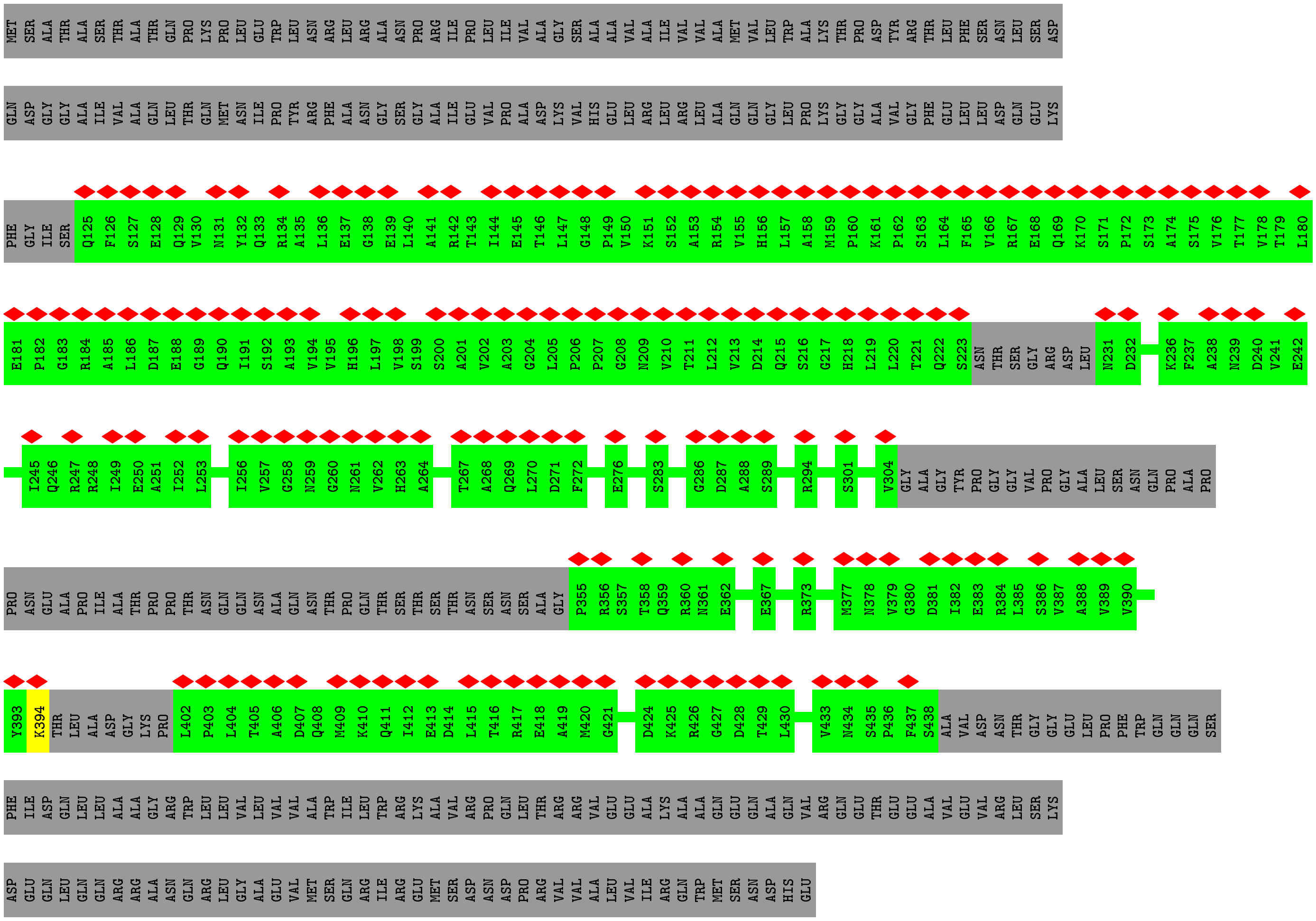
- Molecule 1: Flagellar M-ring protein

Chain S1:



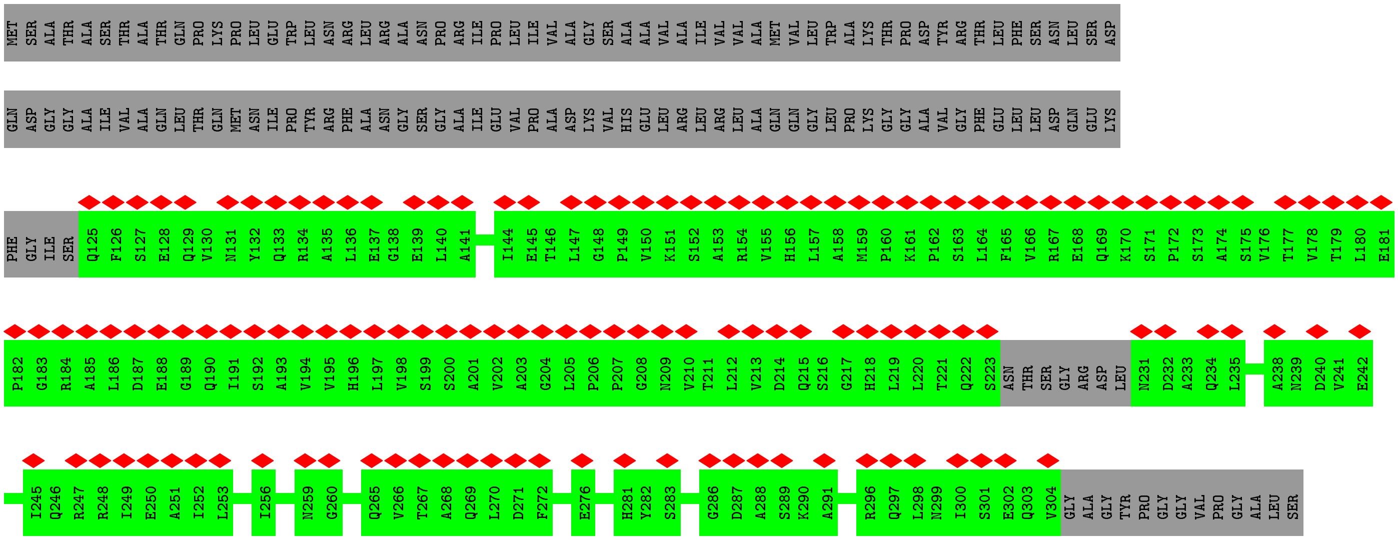
- Molecule 1: Flagellar M-ring protein

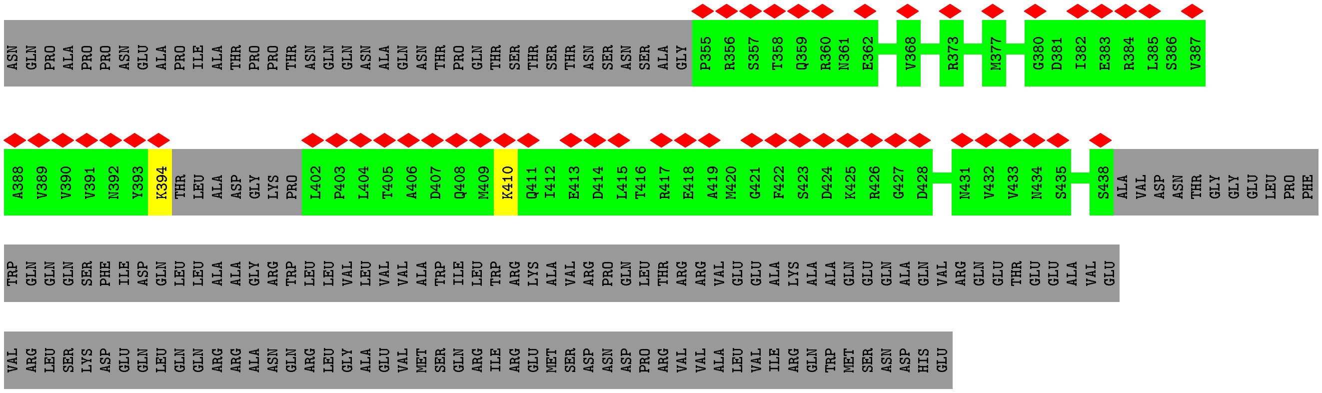
Chain T1:



- Molecule 1: Flagellar M-ring protein

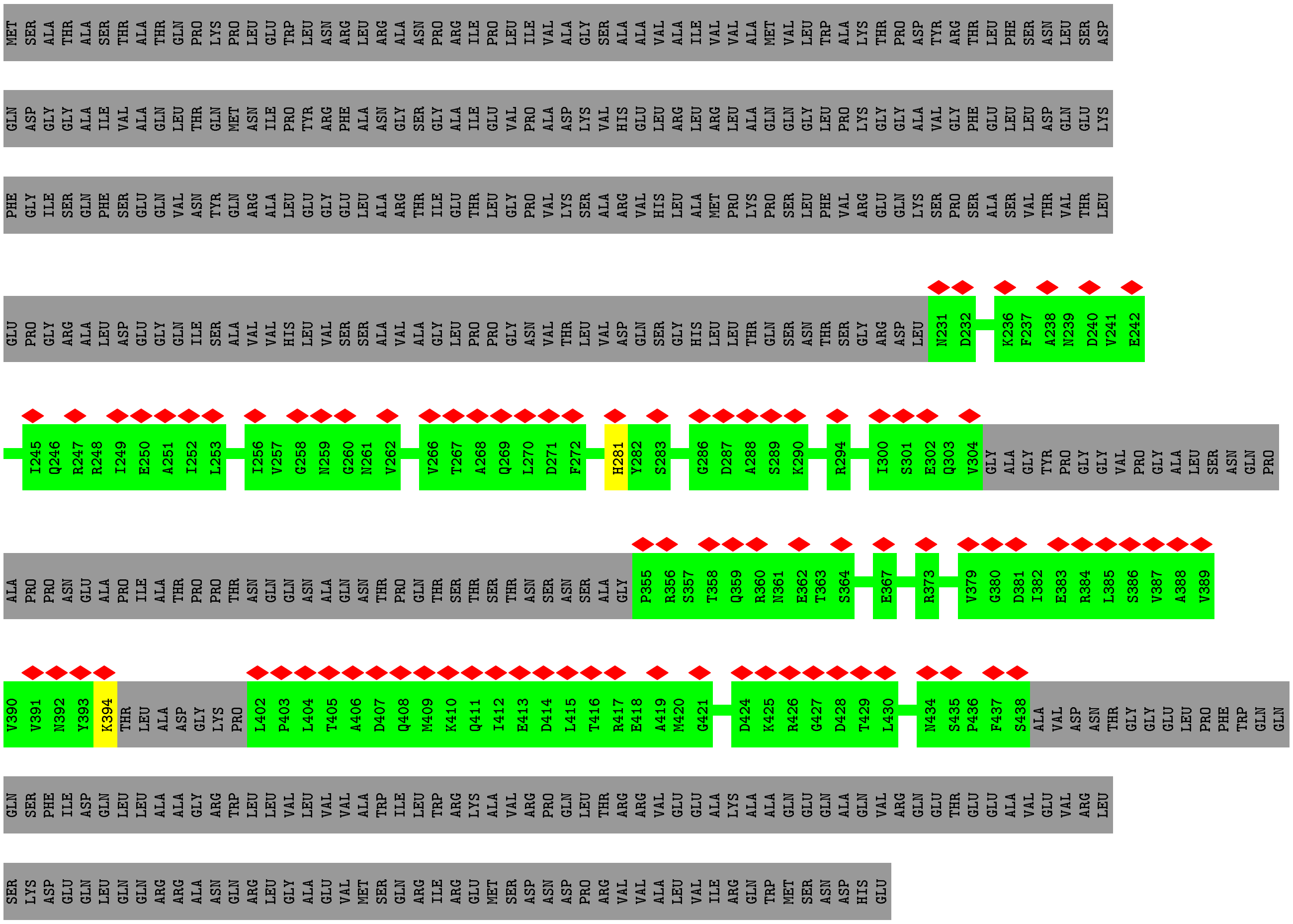
Chain U1:





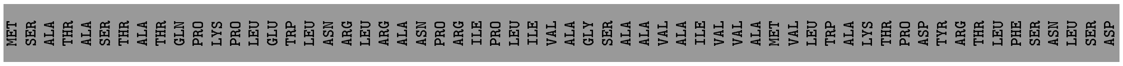
- Molecule 1: Flagellar M-ring protein

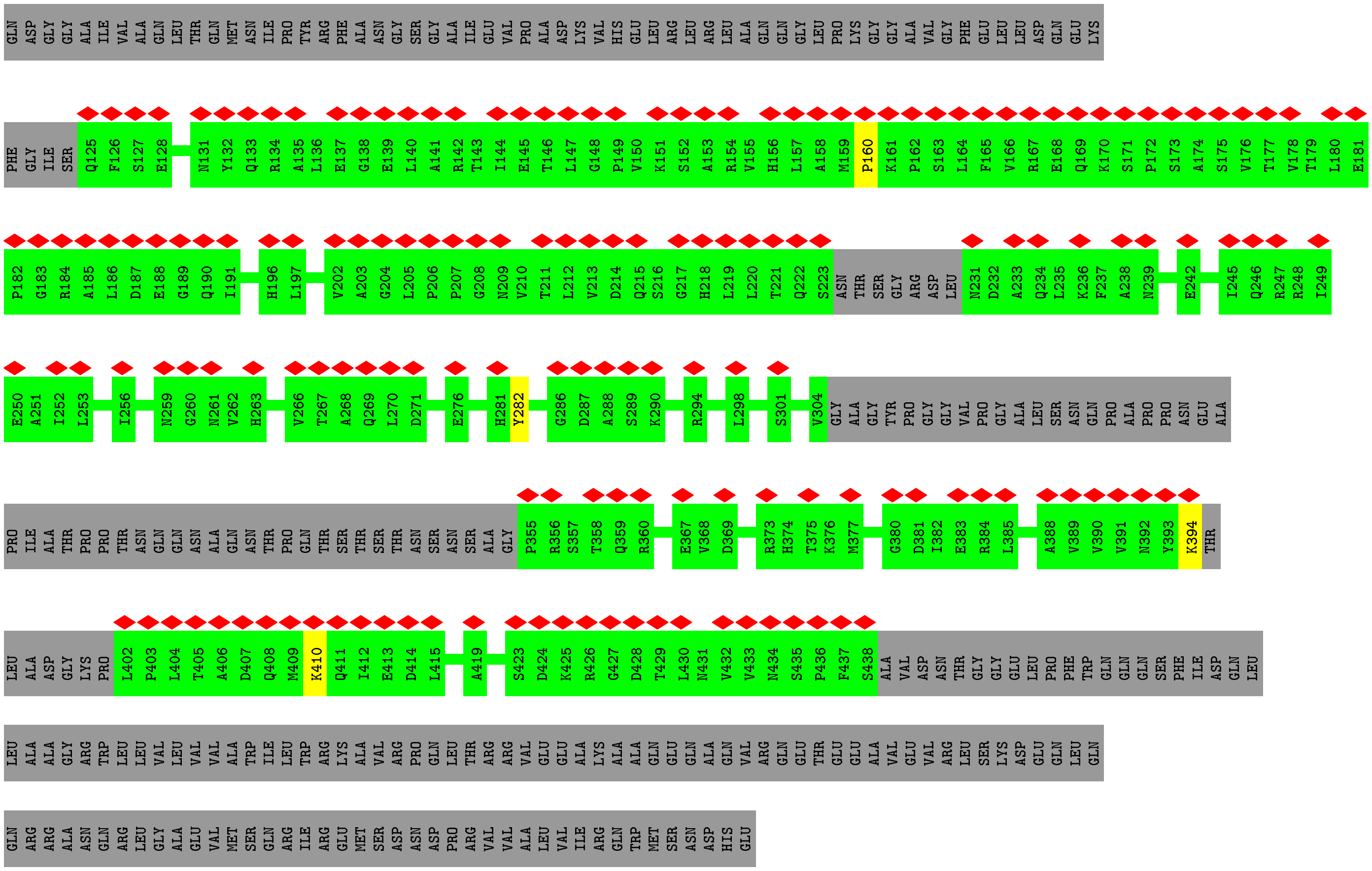
Chain V1:



- Molecule 1: Flagellar M-ring protein

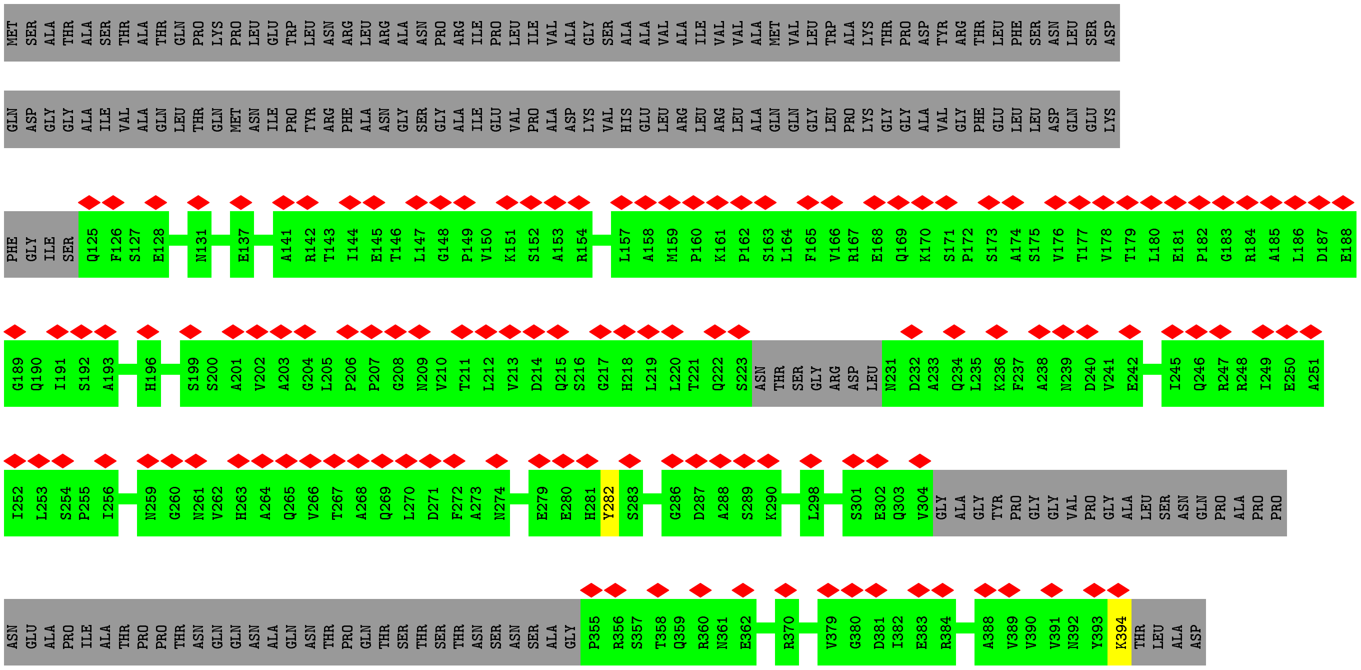
Chain W1:

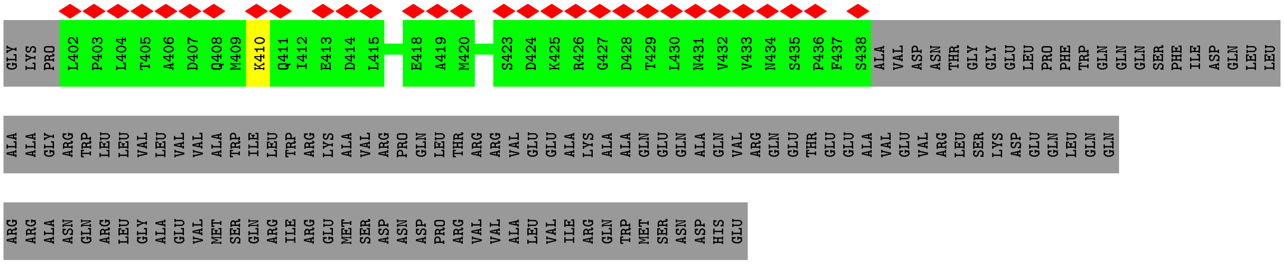




- Molecule 1: Flagellar M-ring protein

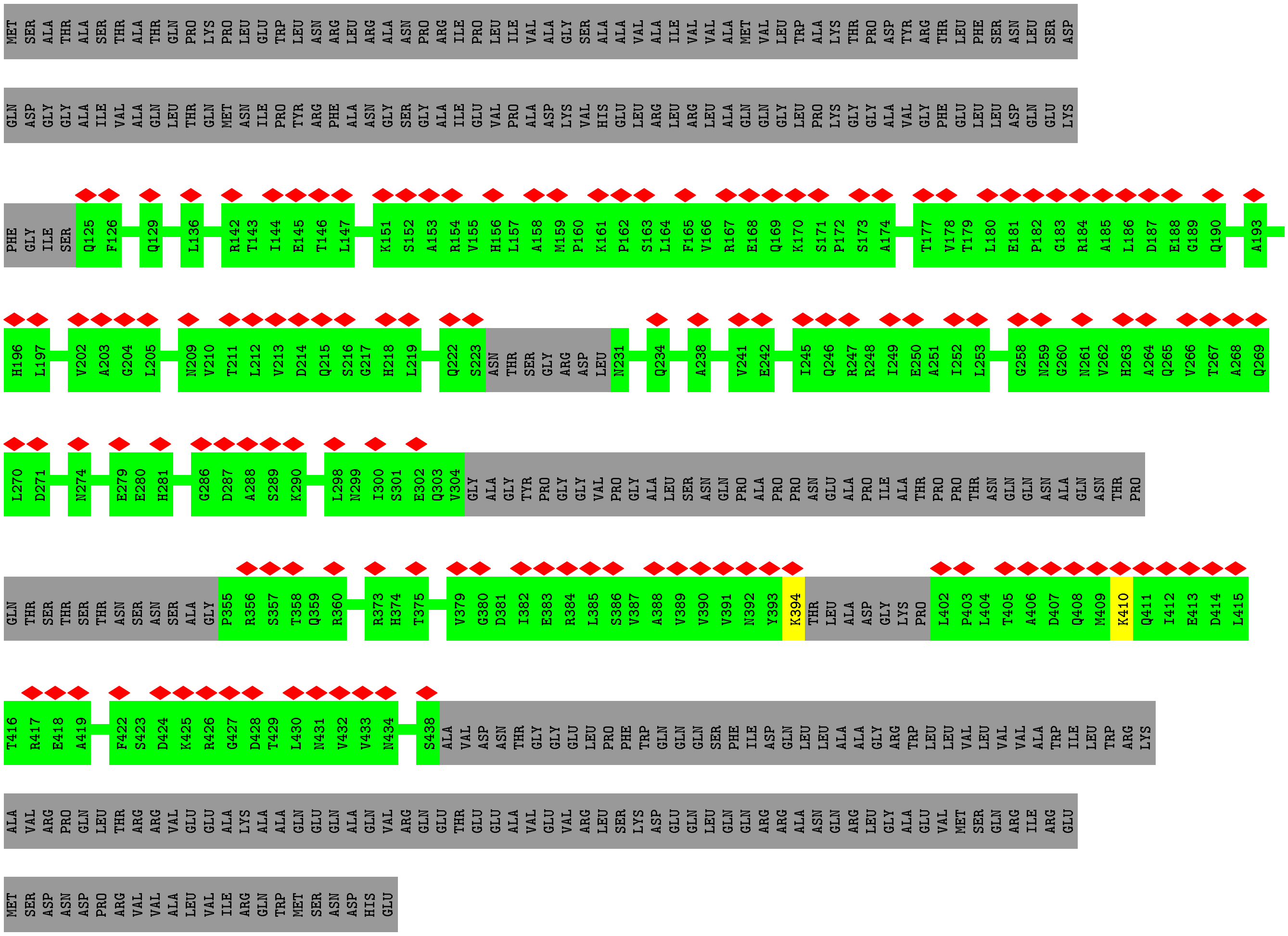
Chain X1:





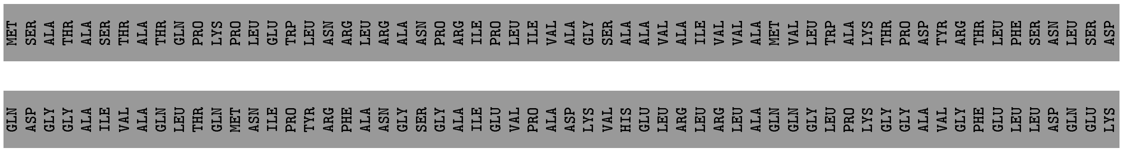
- Molecule 1: Flagellar M-ring protein

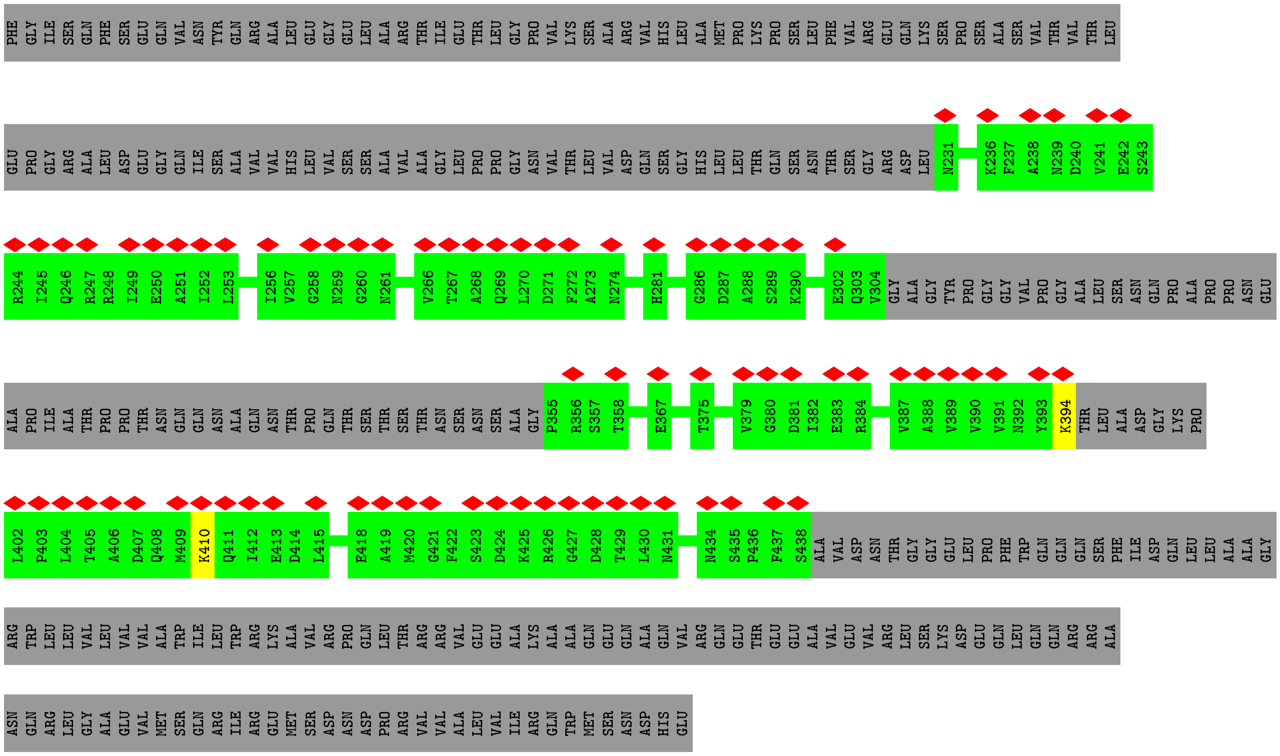
Chain Y1:



- Molecule 1: Flagellar M-ring protein

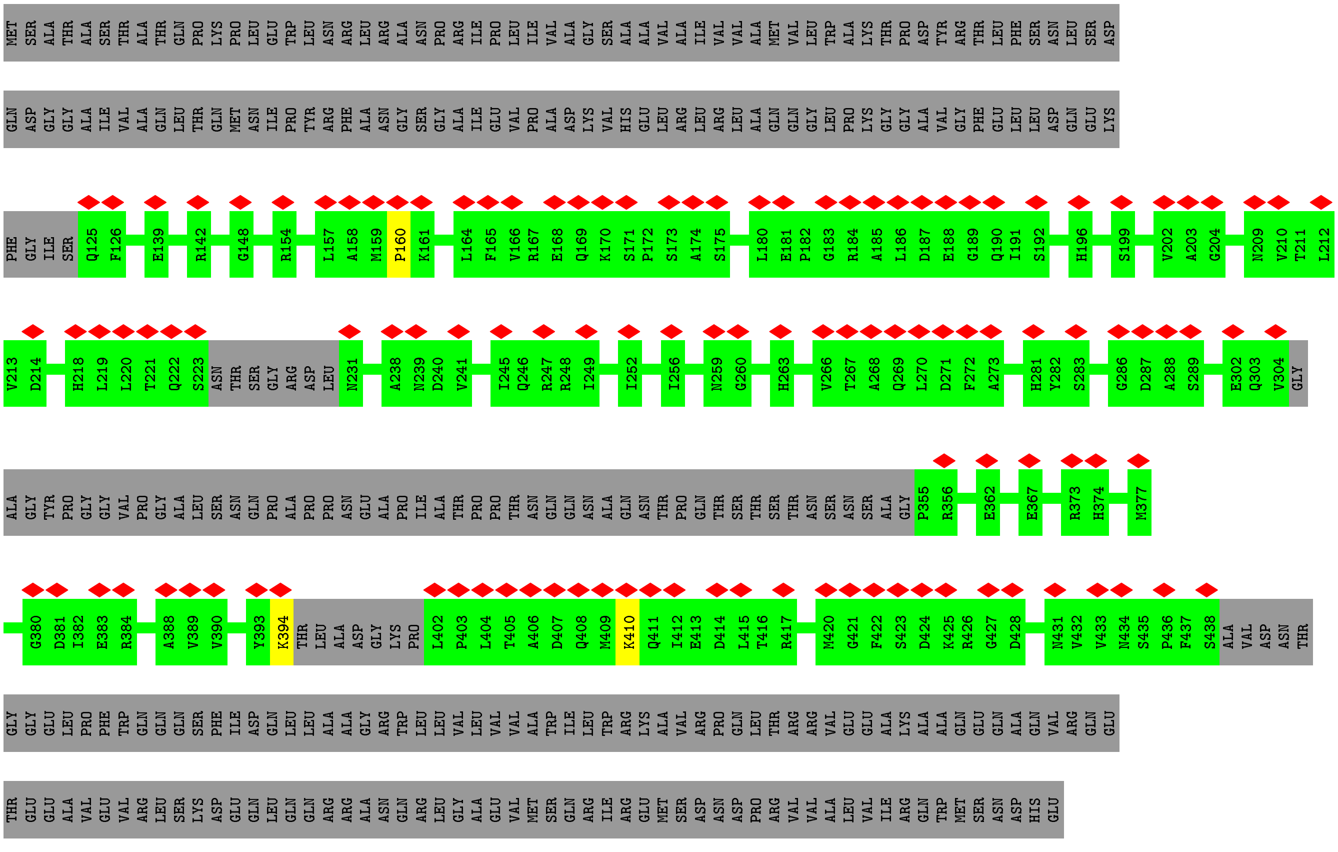
Chain Z1:





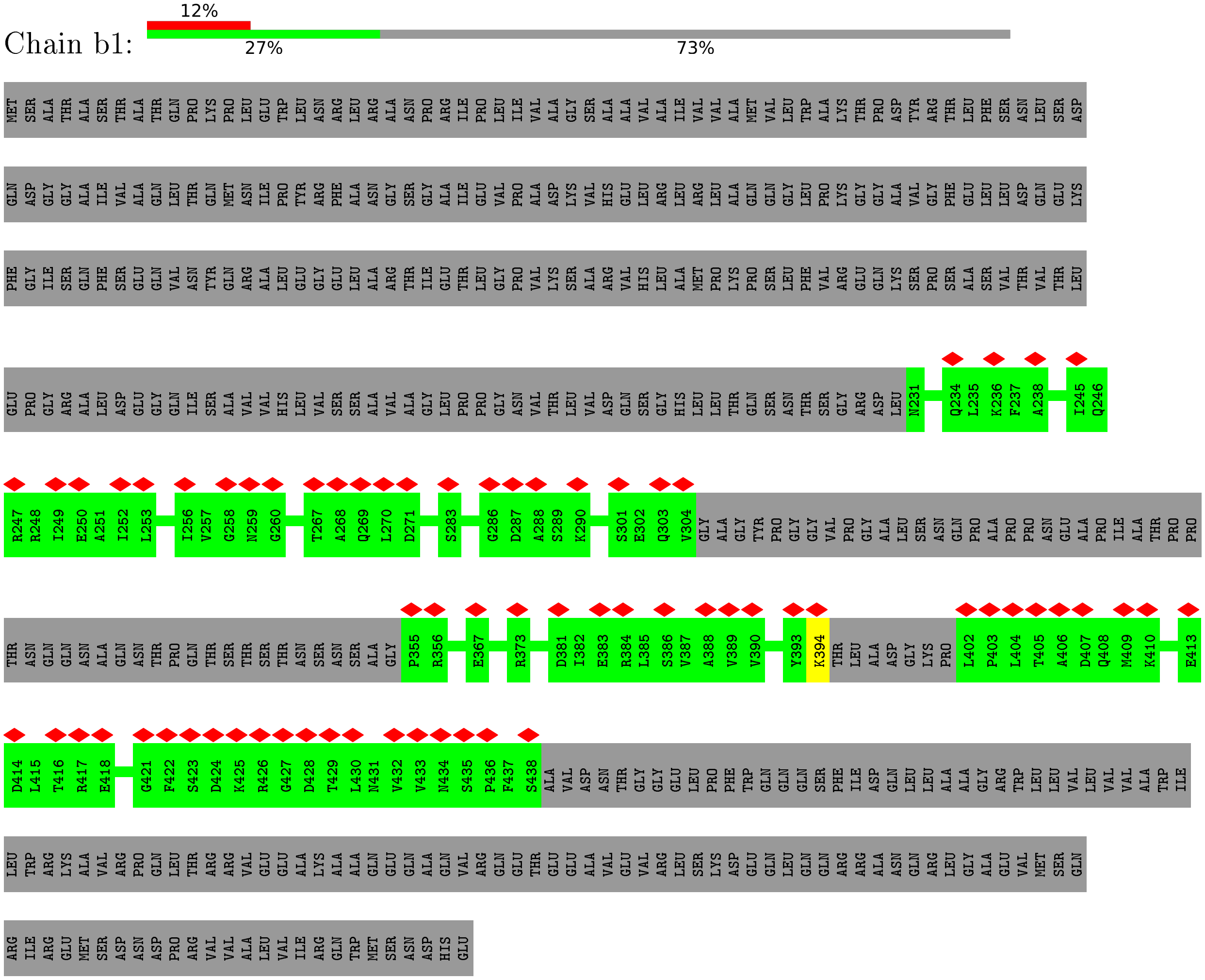
- Molecule 1: Flagellar M-ring protein

Chain a1:



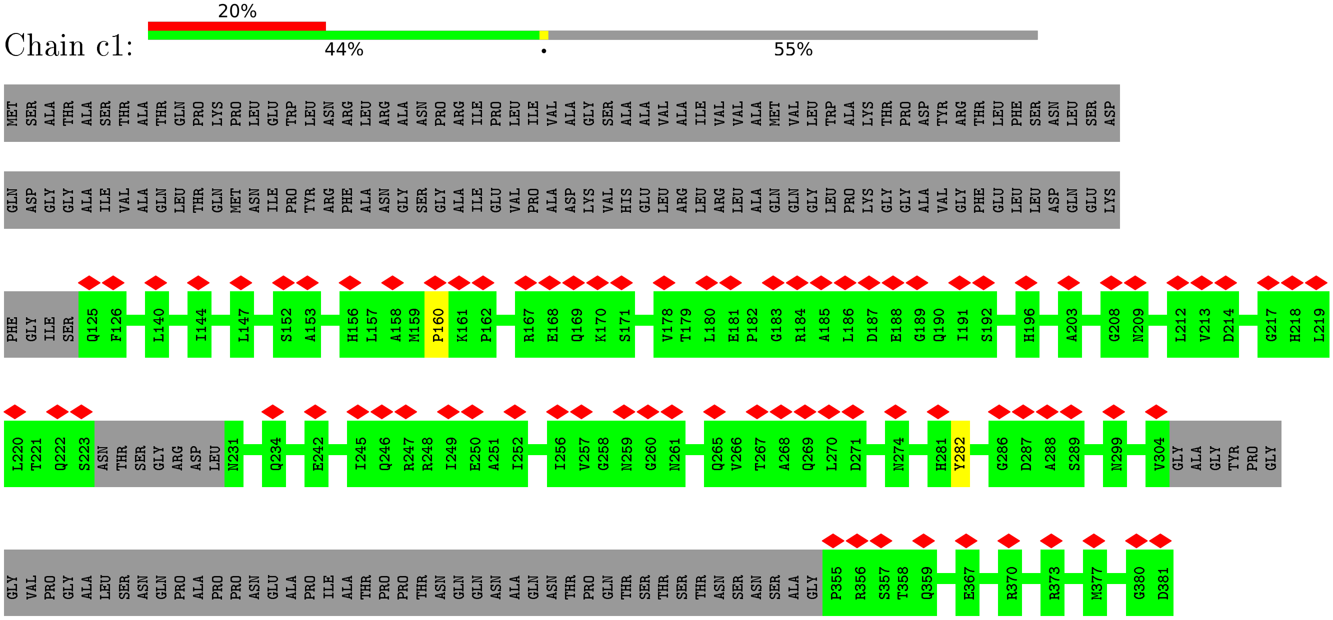
- Molecule 1: Flagellar M-ring protein

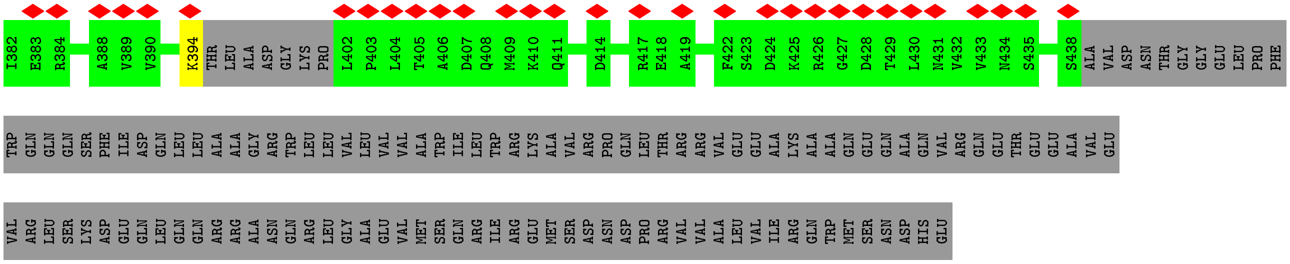
Chain b1:



- Molecule 1: Flagellar M-ring protein

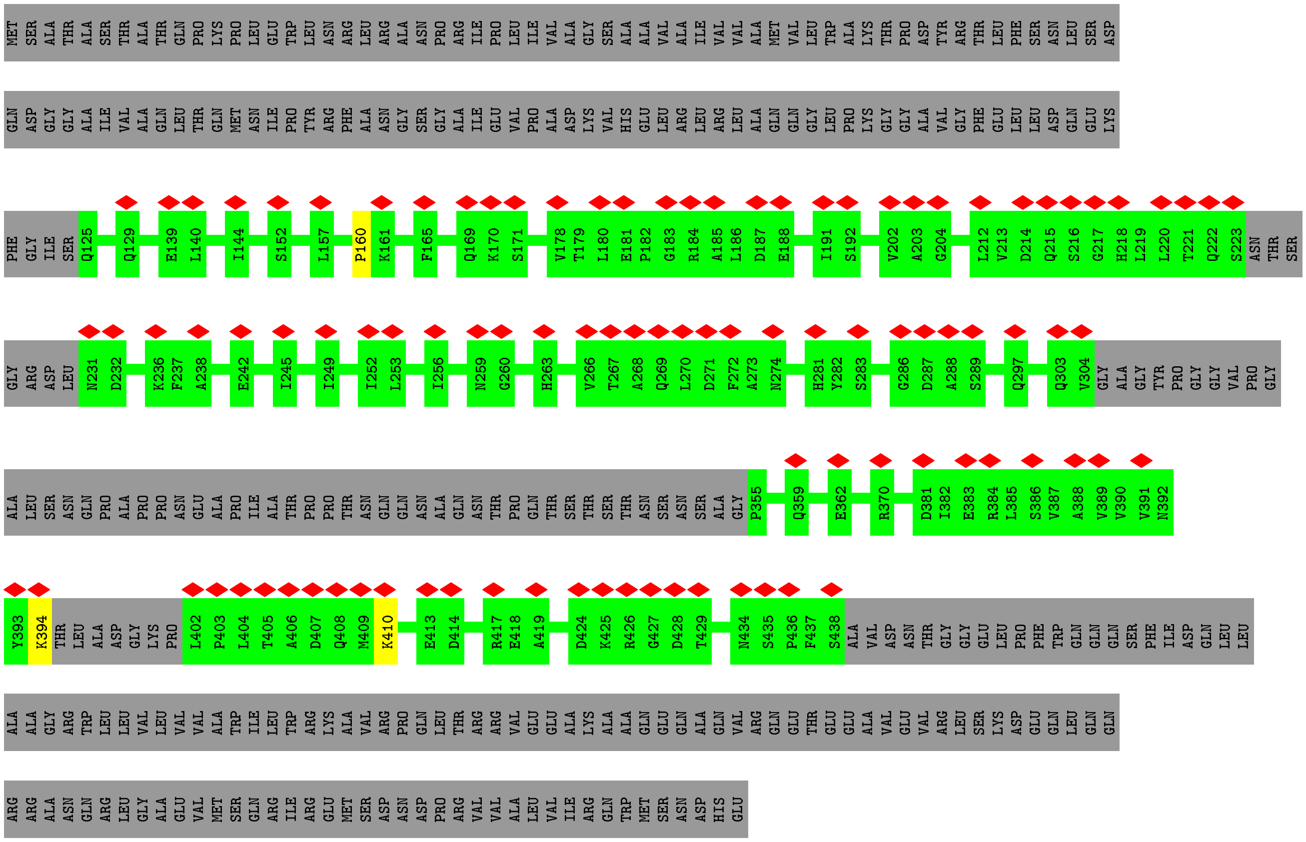
Chain c1:





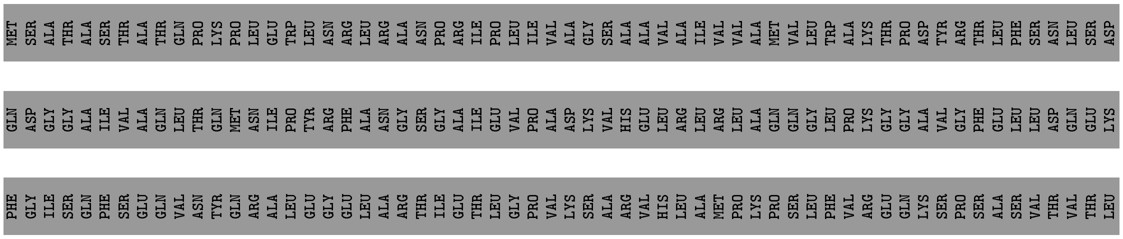
- Molecule 1: Flagellar M-ring protein

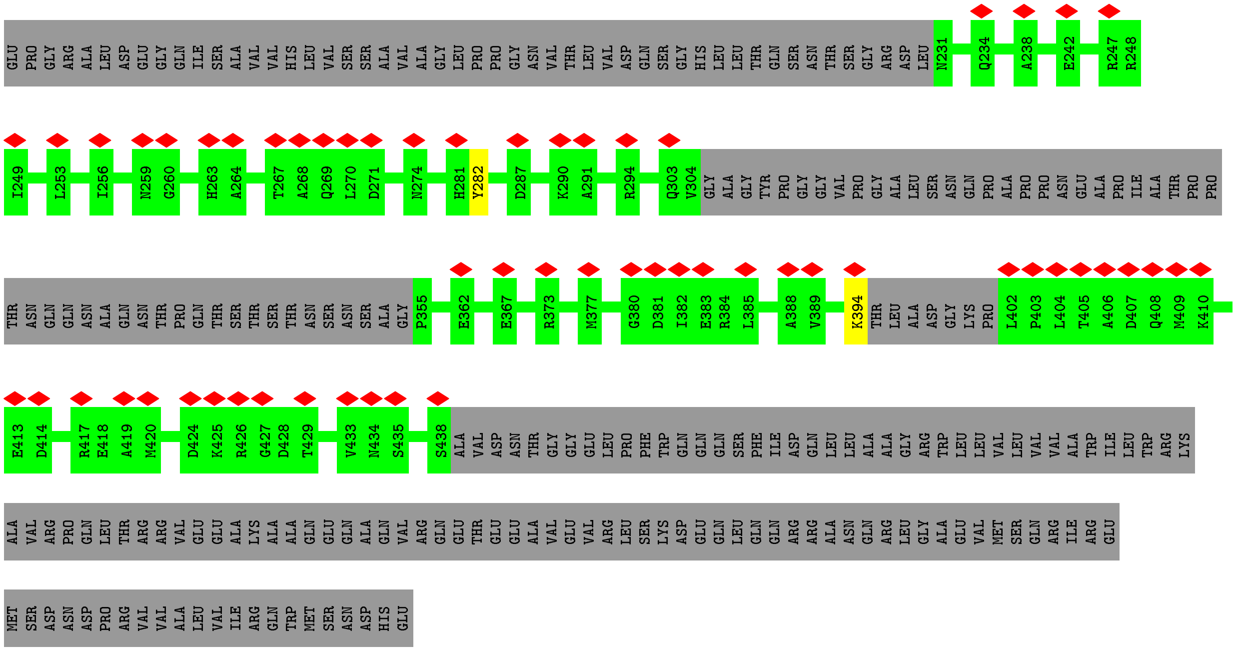
Chain d1:



- Molecule 1: Flagellar M-ring protein

Chain e1:



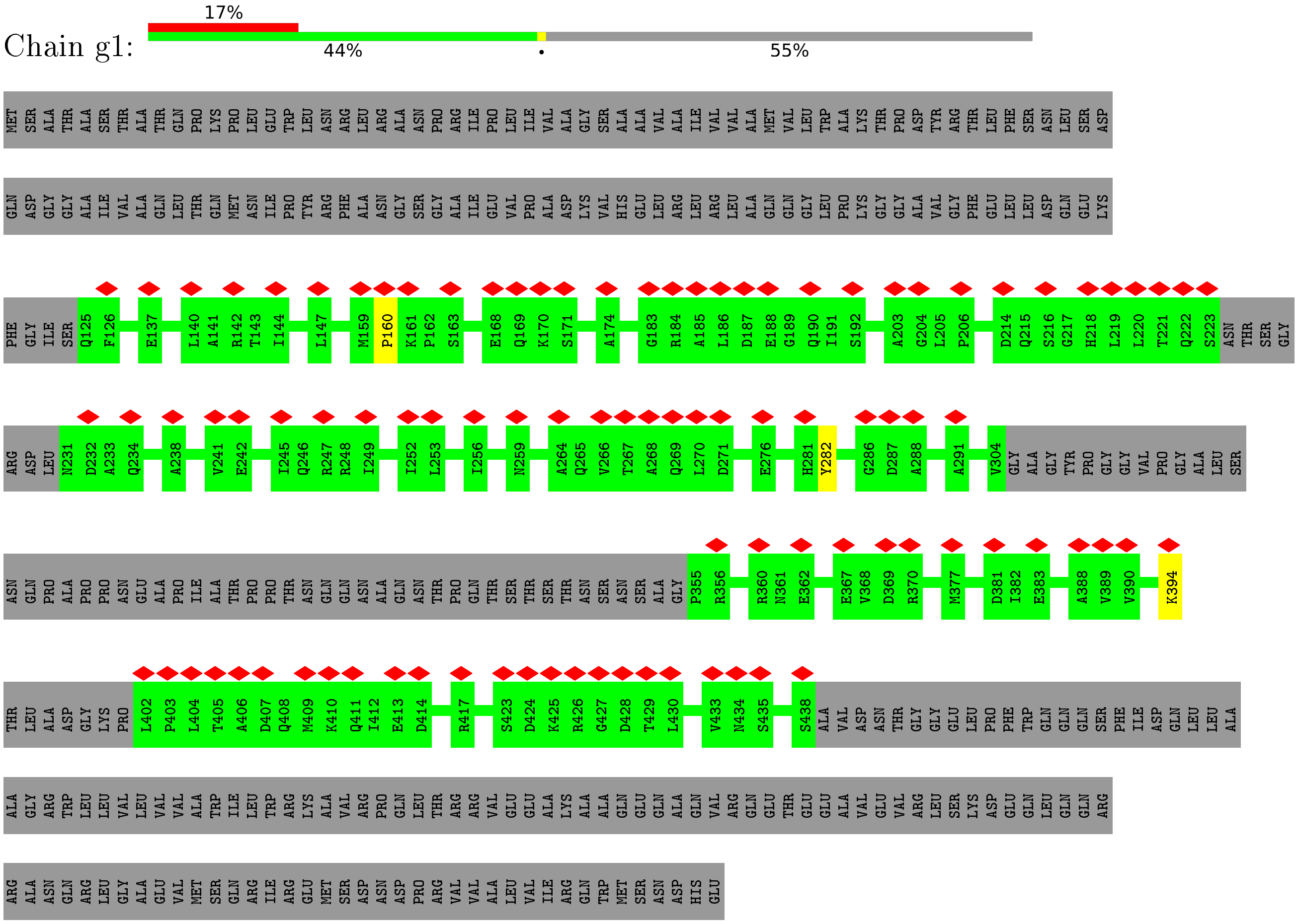


- Molecule 1: Flagellar M-ring protein

Chain f1:

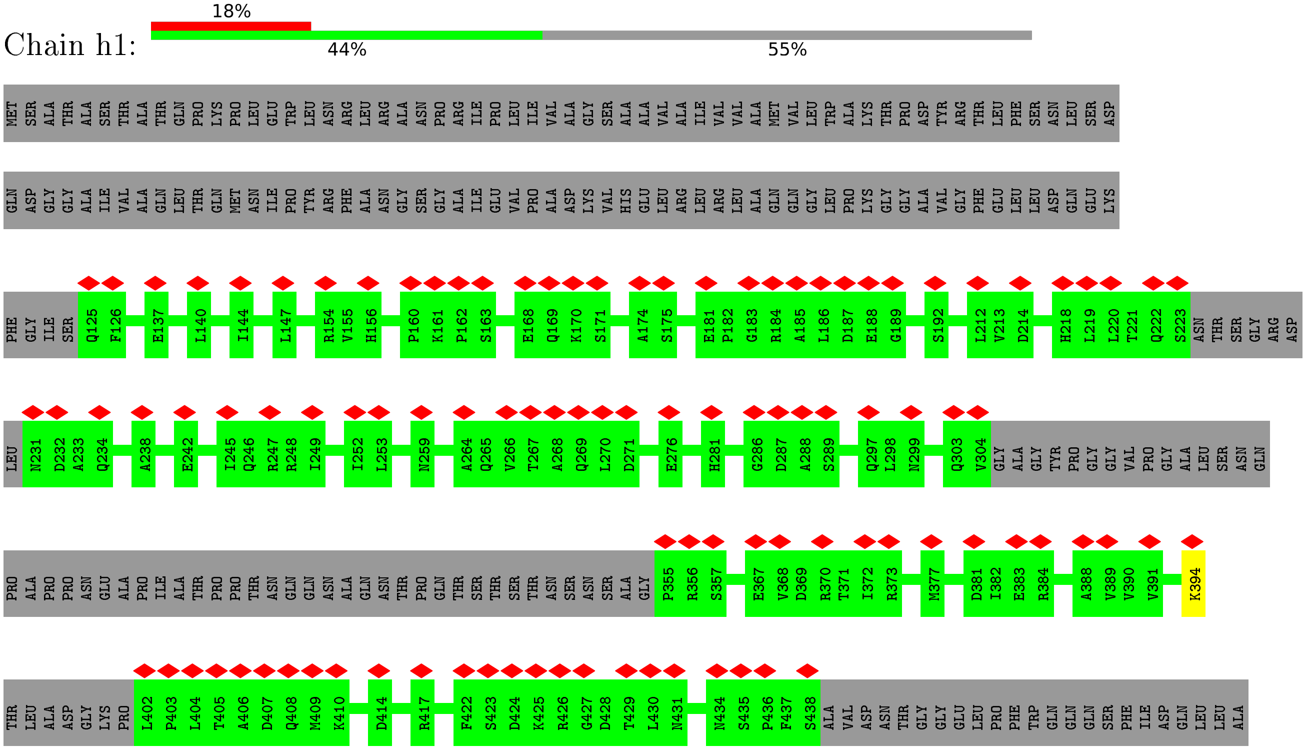
- Molecule 1: Flagellar M-ring protein

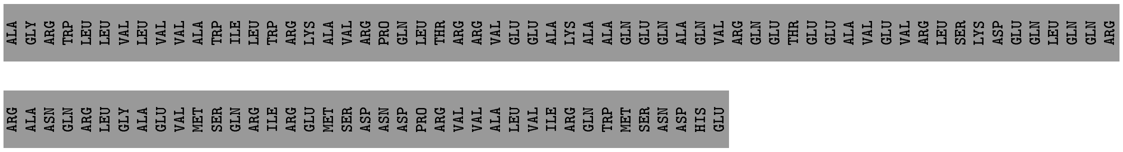
Chain g1:



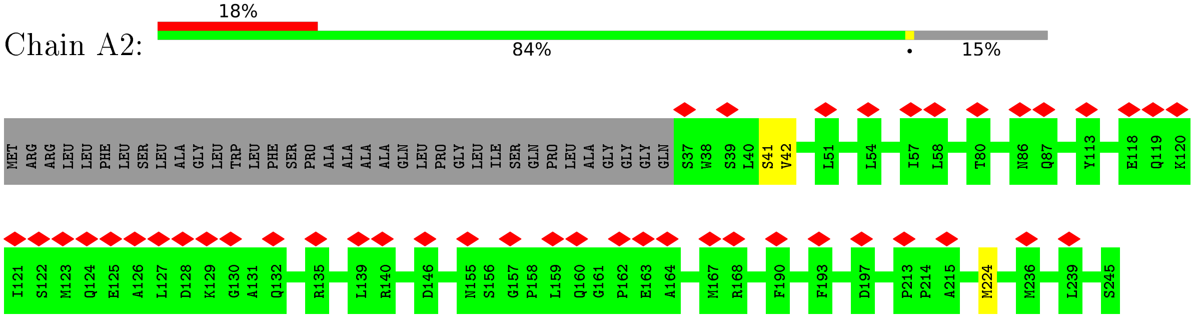
- Molecule 1: Flagellar M-ring protein

Chain h1:

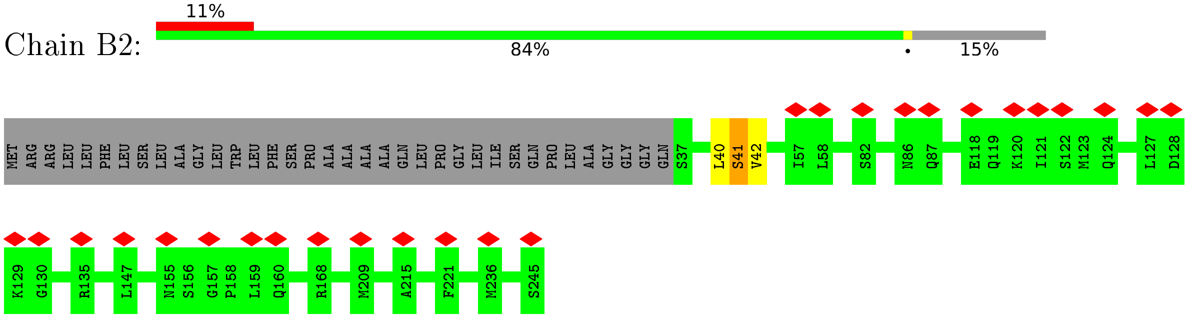




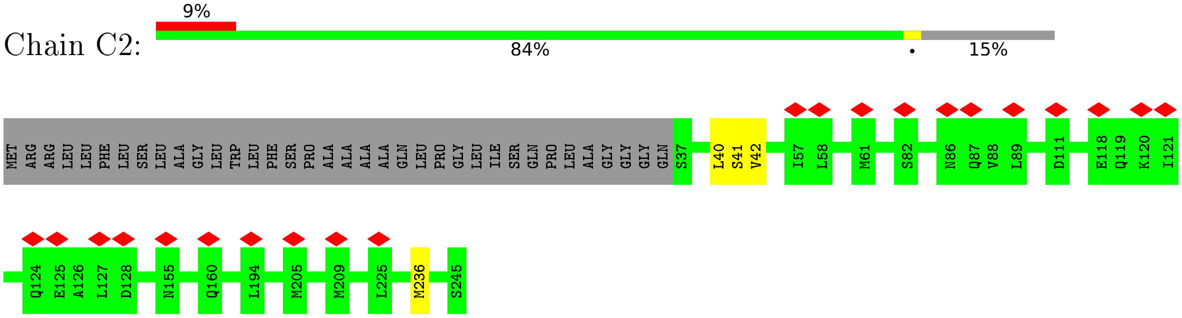
- Molecule 2: Flagellar biosynthetic protein FliP



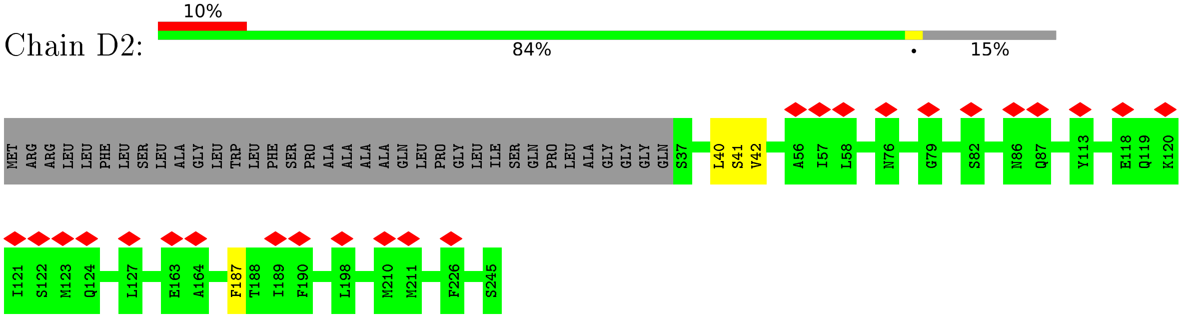
- Molecule 2: Flagellar biosynthetic protein FliP



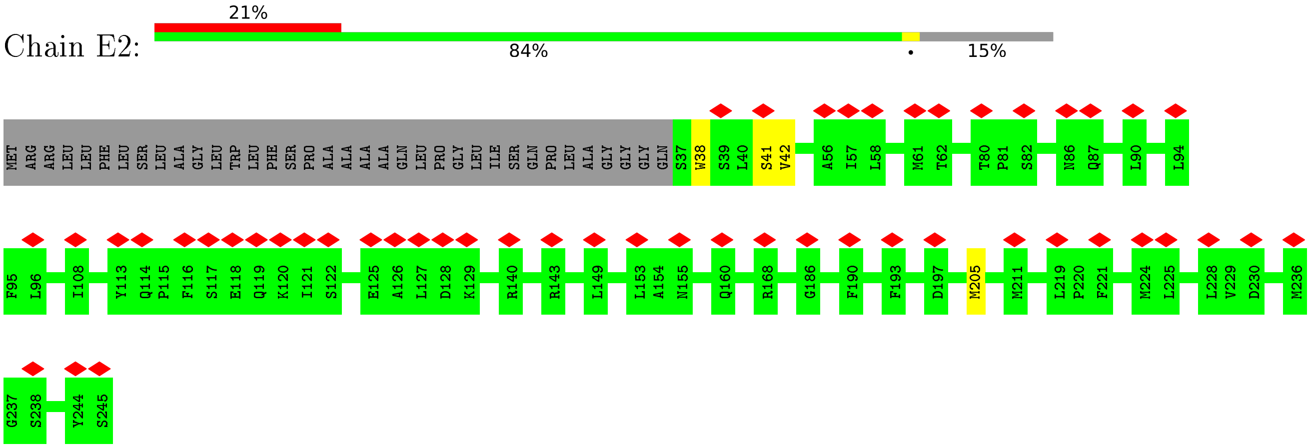
- Molecule 2: Flagellar biosynthetic protein FliP



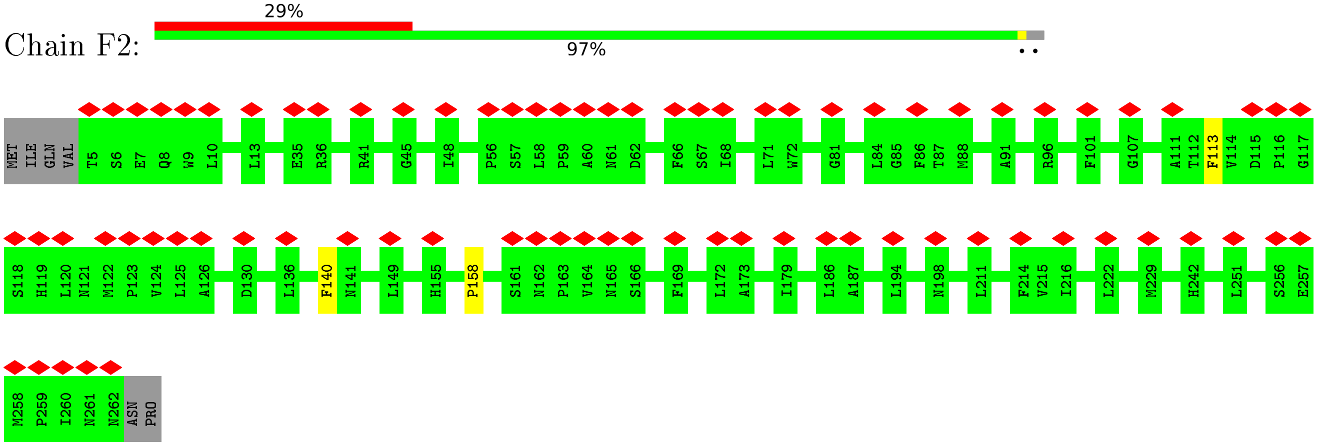
- Molecule 2: Flagellar biosynthetic protein FliP



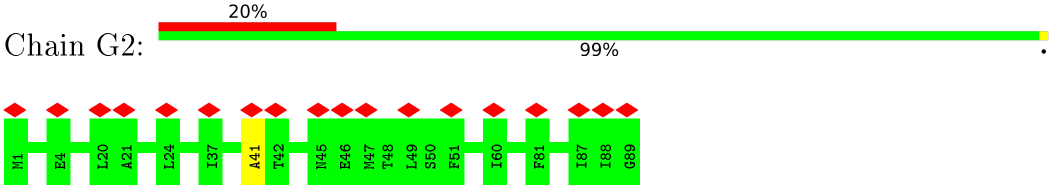
- Molecule 2: Flagellar biosynthetic protein FliP



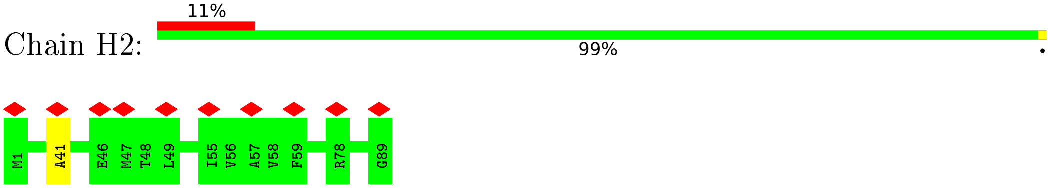
- Molecule 3: Flagellar biosynthetic protein FliR



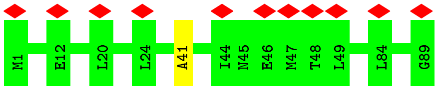
- Molecule 4: Flagellar biosynthetic protein FliQ



- Molecule 4: Flagellar biosynthetic protein FliQ

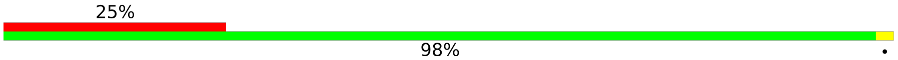


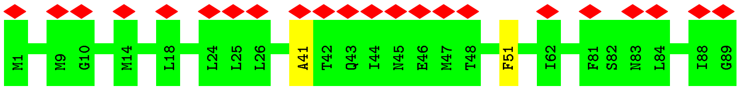
- Molecule 4: Flagellar biosynthetic protein FliQ



- Molecule 4: Flagellar biosynthetic protein FliQ

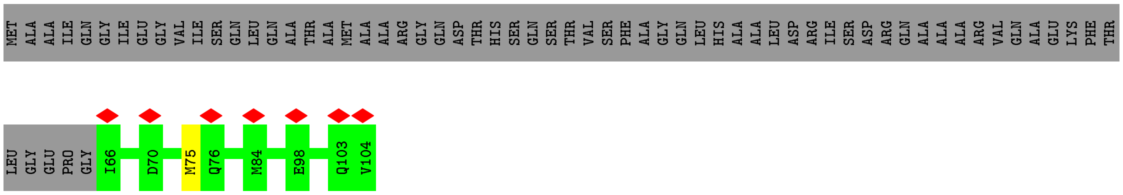
Chain J2:





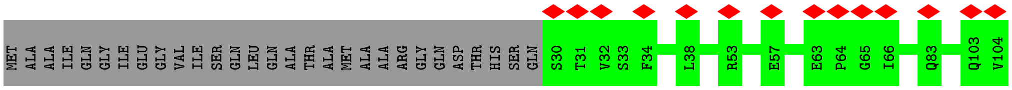
- Molecule 5: Flagellar hook-basal body complex protein FliE

Chain K2:



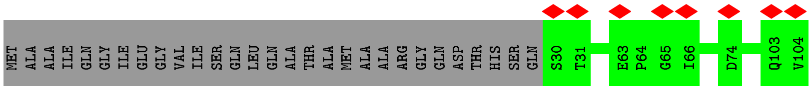
- Molecule 5: Flagellar hook-basal body complex protein FliE

Chain L2:



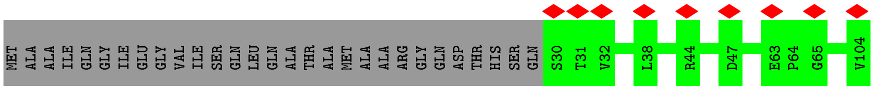
- Molecule 5: Flagellar hook-basal body complex protein FliE

Chain M2:



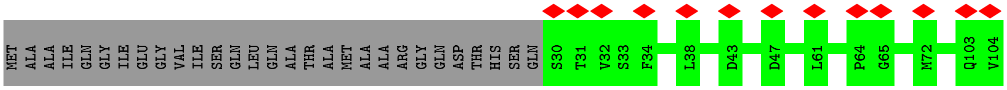
- Molecule 5: Flagellar hook-basal body complex protein FliE

Chain N2:



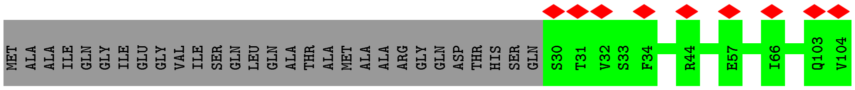
- Molecule 5: Flagellar hook-basal body complex protein FliE

Chain O2:



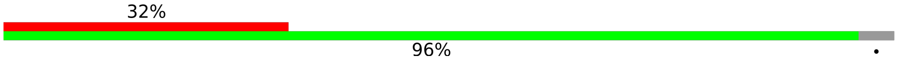
- Molecule 5: Flagellar hook-basal body complex protein FliE

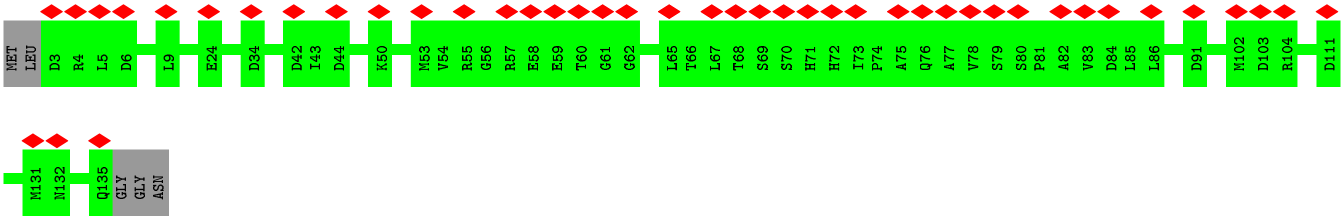
Chain P2:



- Molecule 6: Flagellar basal body rod protein FlgB

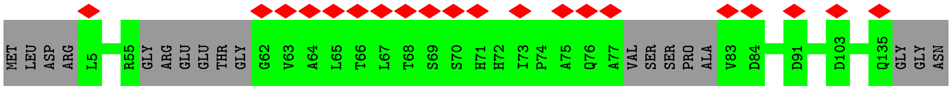
Chain Q2:





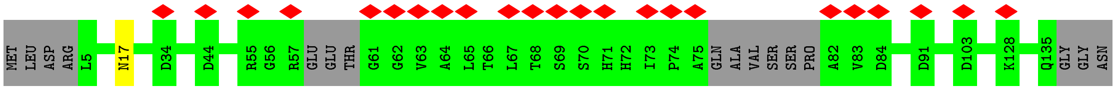
- Molecule 6: Flagellar basal body rod protein FlgB

Chain R2:



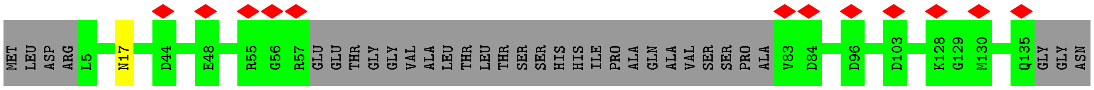
- Molecule 6: Flagellar basal body rod protein FlgB

Chain S2:



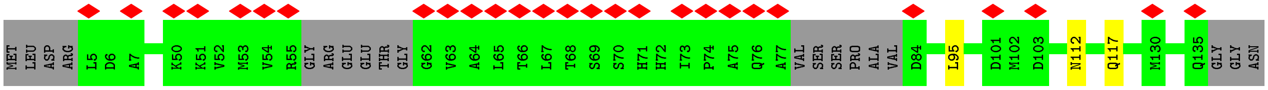
- Molecule 6: Flagellar basal body rod protein FlgB

Chain T2:



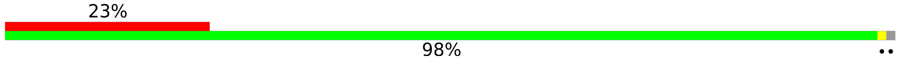
- Molecule 6: Flagellar basal body rod protein FlgB

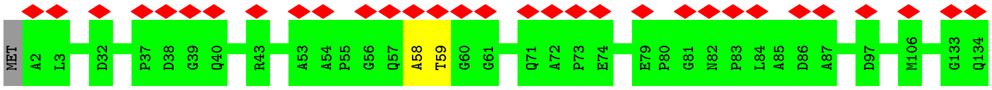
Chain U2:



- Molecule 7: Flagellar basal-body rod protein FlgC

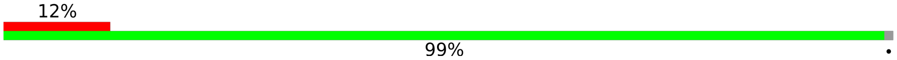
Chain V2:

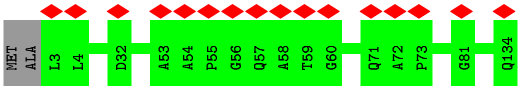




- Molecule 7: Flagellar basal-body rod protein FlgC

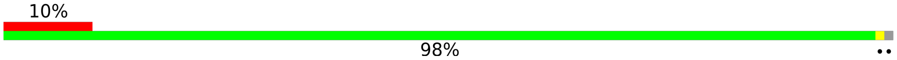
Chain W2:

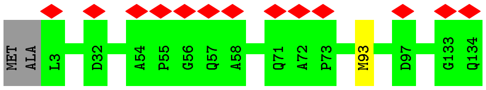




- Molecule 7: Flagellar basal-body rod protein FlgC

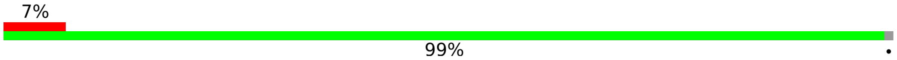
Chain X2:

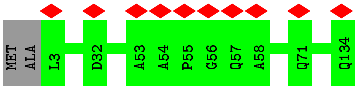




- Molecule 7: Flagellar basal-body rod protein FlgC

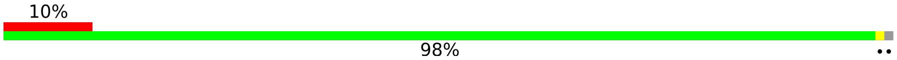
Chain Y2:

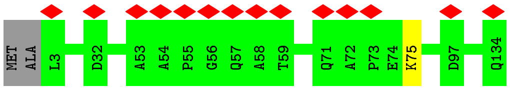




- Molecule 7: Flagellar basal-body rod protein FlgC

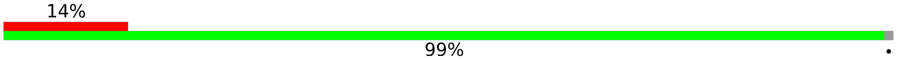
Chain Z2:

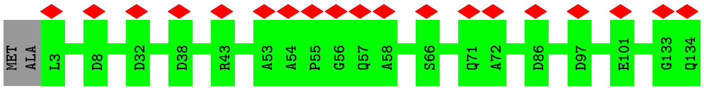




- Molecule 7: Flagellar basal-body rod protein FlgC

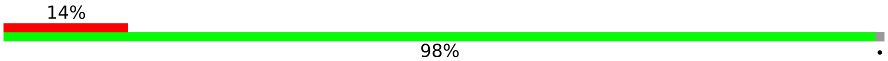
Chain a2:

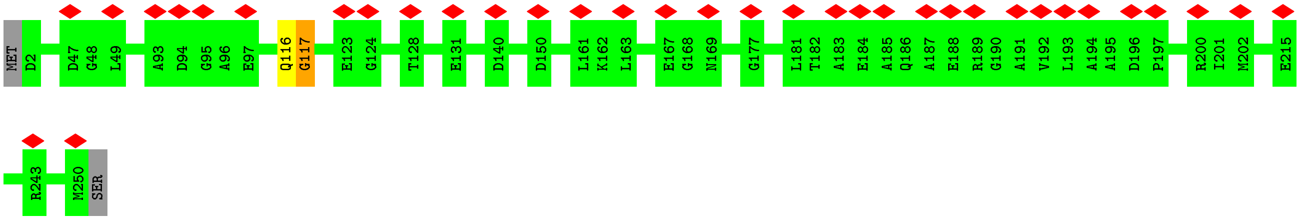




- Molecule 8: Flagellar basal body protein

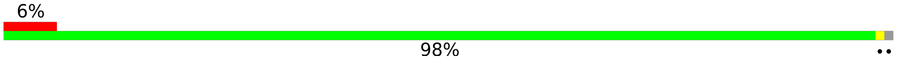
Chain b2:

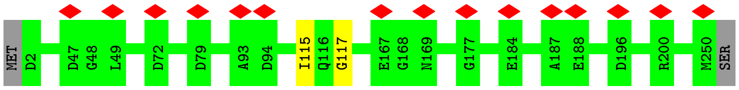




- Molecule 8: Flagellar basal body protein

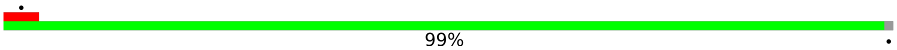
Chain c2:

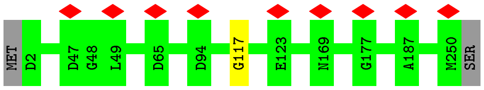




- Molecule 8: Flagellar basal body protein

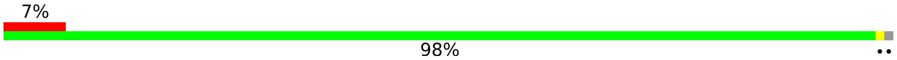
Chain d2:

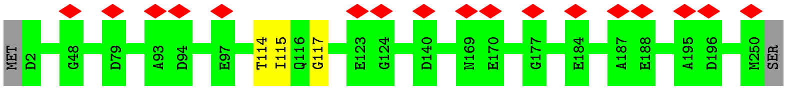




- Molecule 8: Flagellar basal body protein

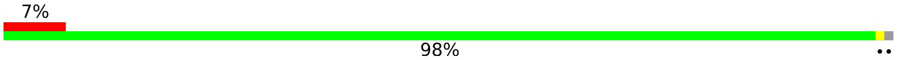
Chain e2:

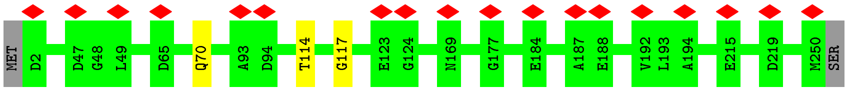




- Molecule 8: Flagellar basal body protein

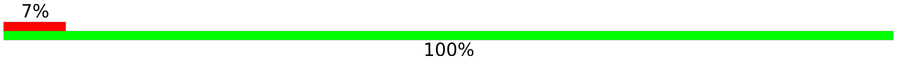
Chain f2:

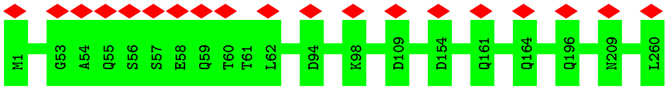




- Molecule 9: Flagellar basal-body rod protein FlgG

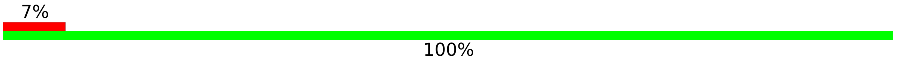
Chain g2:

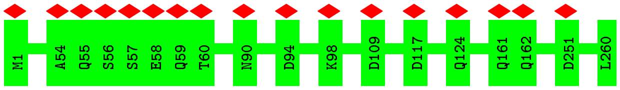




- Molecule 9: Flagellar basal-body rod protein FlgG

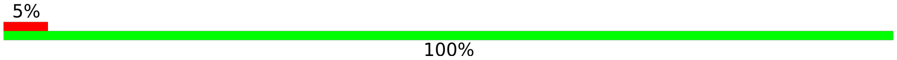
Chain h2:

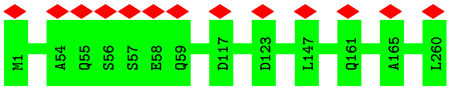




- Molecule 9: Flagellar basal-body rod protein FlgG

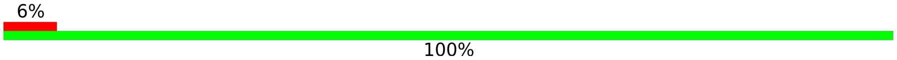
Chain i2:

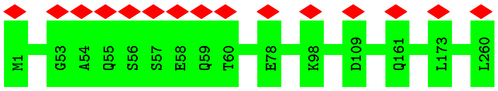




- Molecule 9: Flagellar basal-body rod protein FlgG

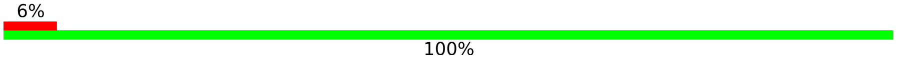
Chain j2:

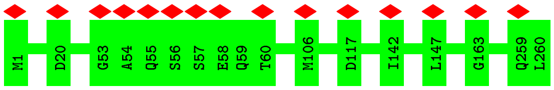




- Molecule 9: Flagellar basal-body rod protein FlgG

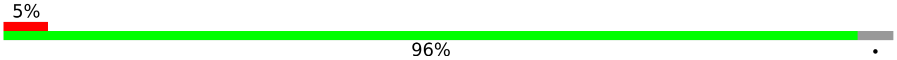
Chain k2:

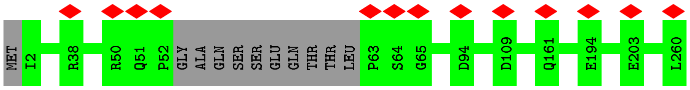




- Molecule 9: Flagellar basal-body rod protein FlgG

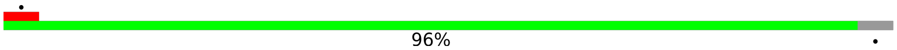
Chain l2:

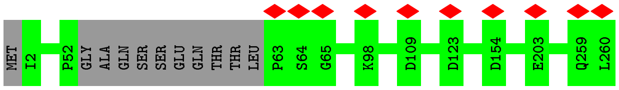




- Molecule 9: Flagellar basal-body rod protein FlgG

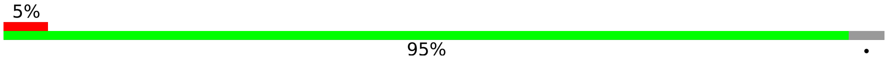
Chain m2:

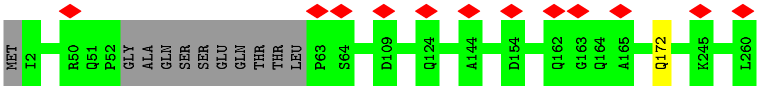




- Molecule 9: Flagellar basal-body rod protein FlgG

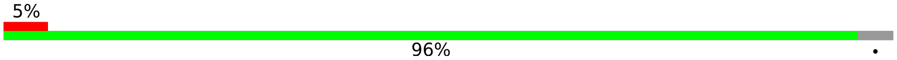
Chain n2:

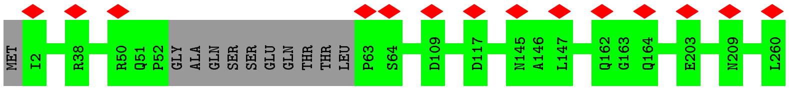




- Molecule 9: Flagellar basal-body rod protein FlgG

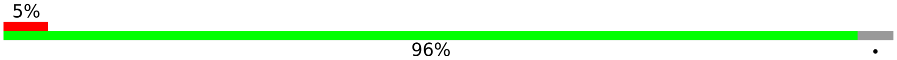
Chain o2:

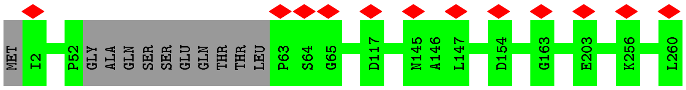




- Molecule 9: Flagellar basal-body rod protein FlgG

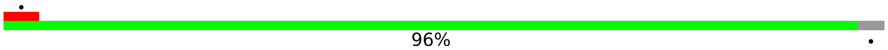
Chain p2:

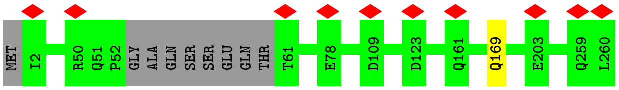




- Molecule 9: Flagellar basal-body rod protein FlgG

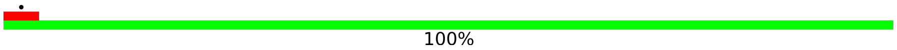
Chain q2:

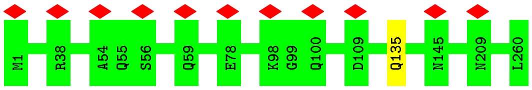




- Molecule 9: Flagellar basal-body rod protein FlgG

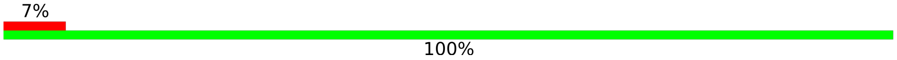
Chain r2:

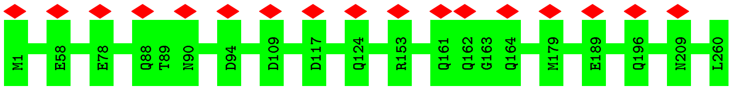




- Molecule 9: Flagellar basal-body rod protein FlgG

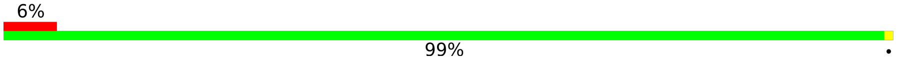
Chain s2:

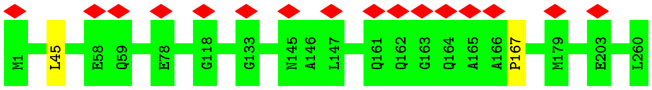




- Molecule 9: Flagellar basal-body rod protein FlgG

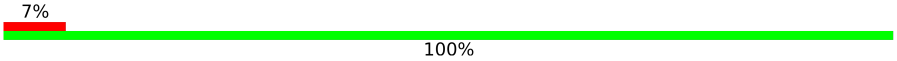
Chain t2:

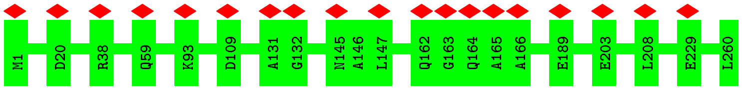




- Molecule 9: Flagellar basal-body rod protein FlgG

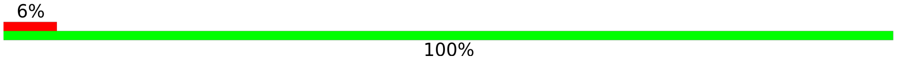
Chain u2:

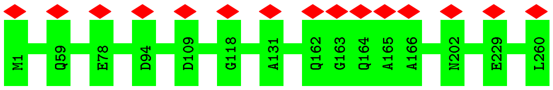




- Molecule 9: Flagellar basal-body rod protein FlgG

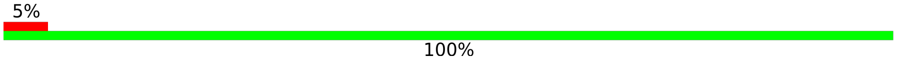
Chain v2:

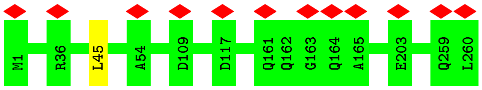




- Molecule 9: Flagellar basal-body rod protein FlgG

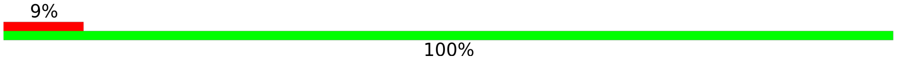
Chain w2:

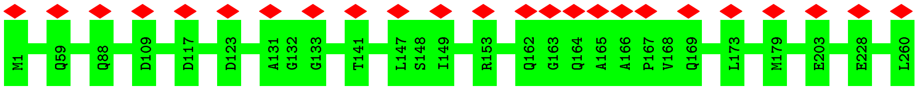




- Molecule 9: Flagellar basal-body rod protein FlgG

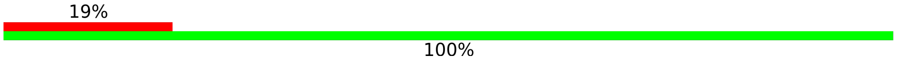
Chain x2:

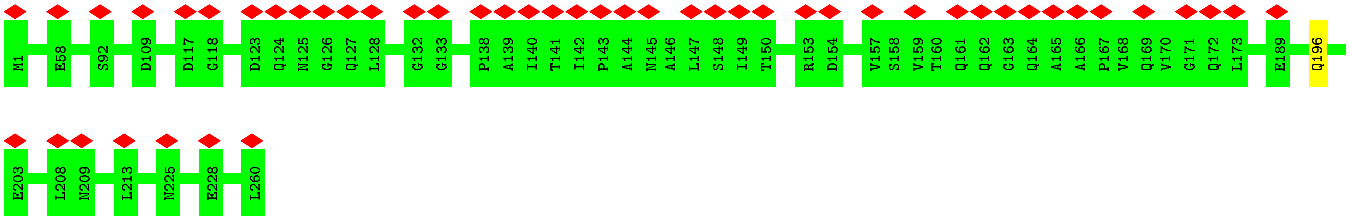




- Molecule 9: Flagellar basal-body rod protein FlgG

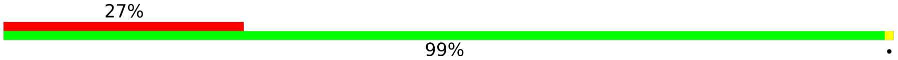
Chain y2:

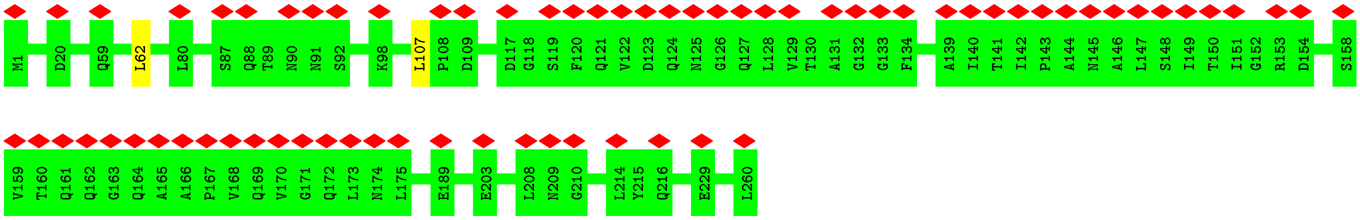




- Molecule 9: Flagellar basal-body rod protein FlgG

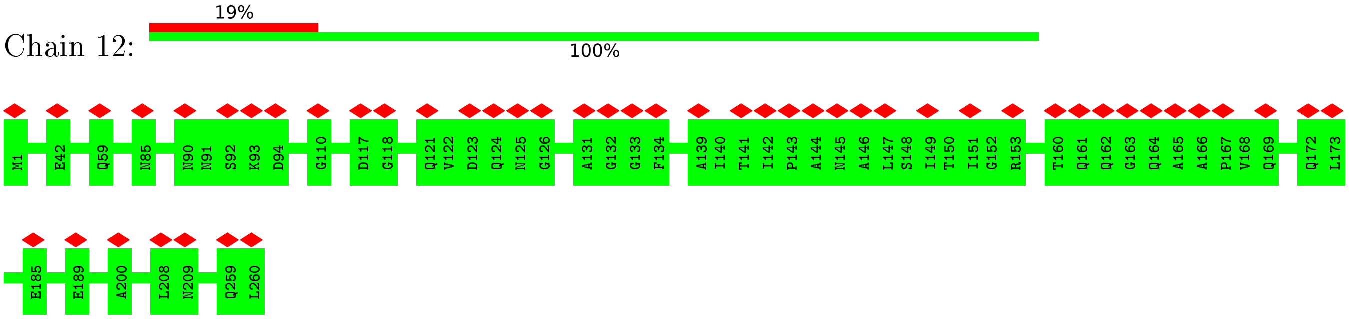
Chain z2:





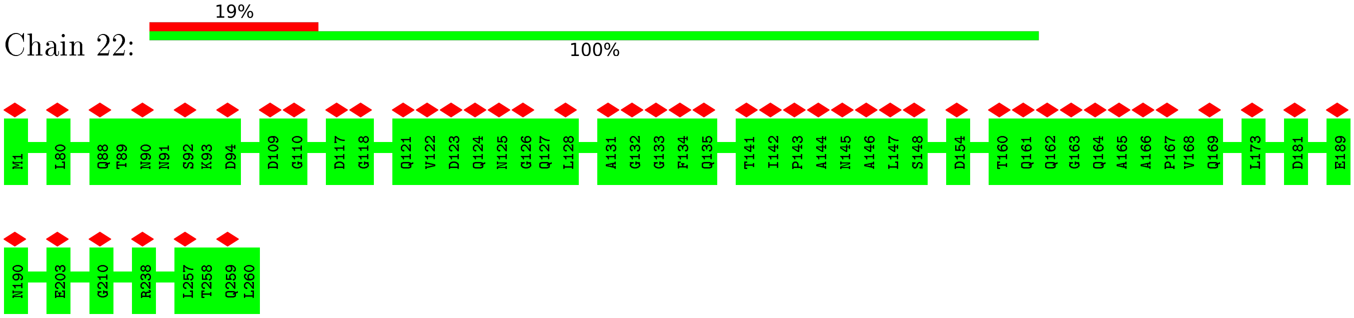
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain 12:



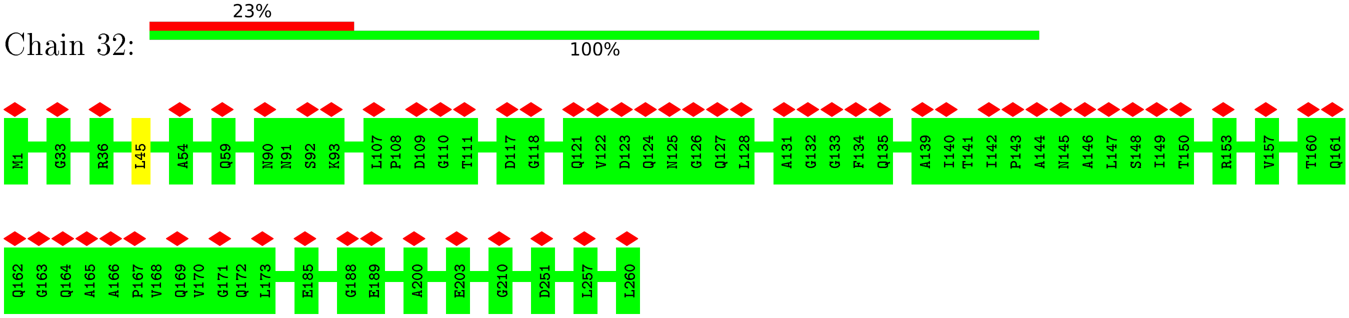
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain 22:



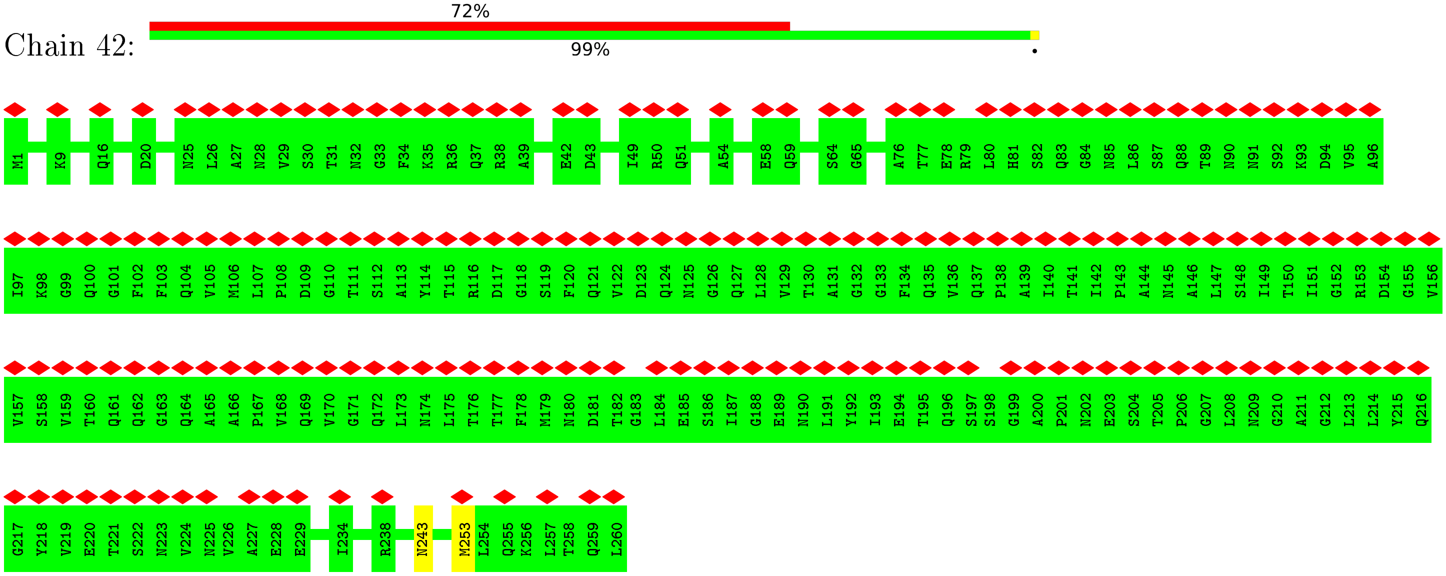
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain 32:



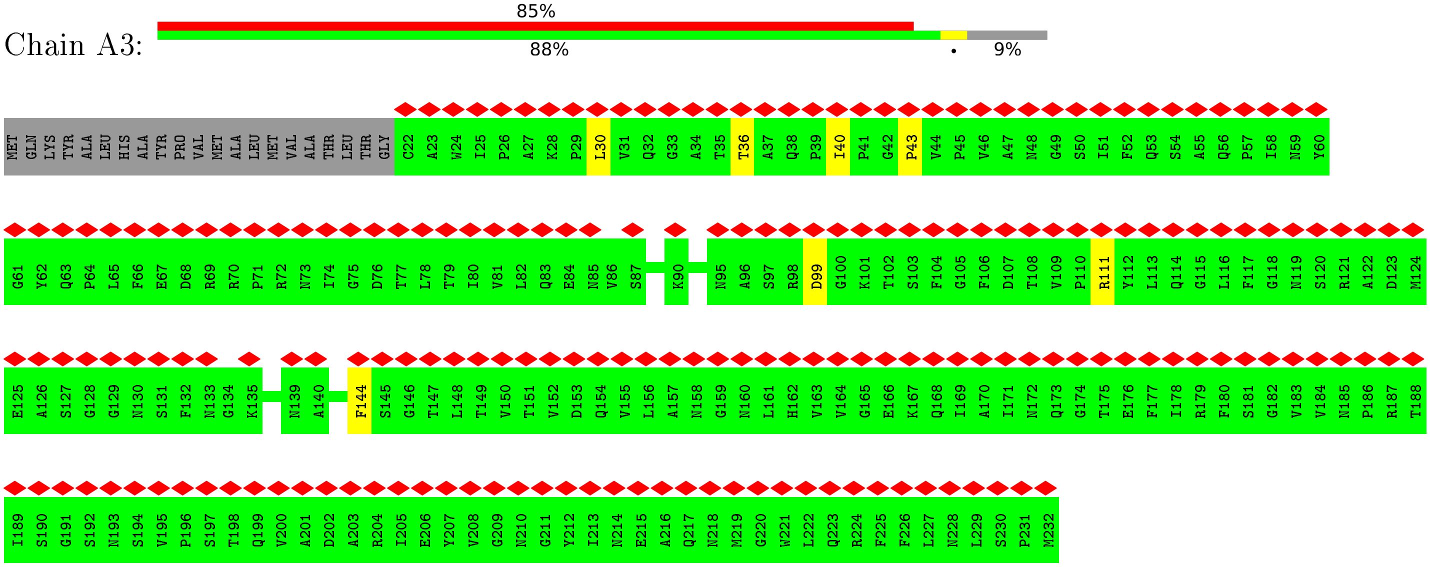
- Molecule 9: Flagellar basal-body rod protein FlgG

Chain 42:



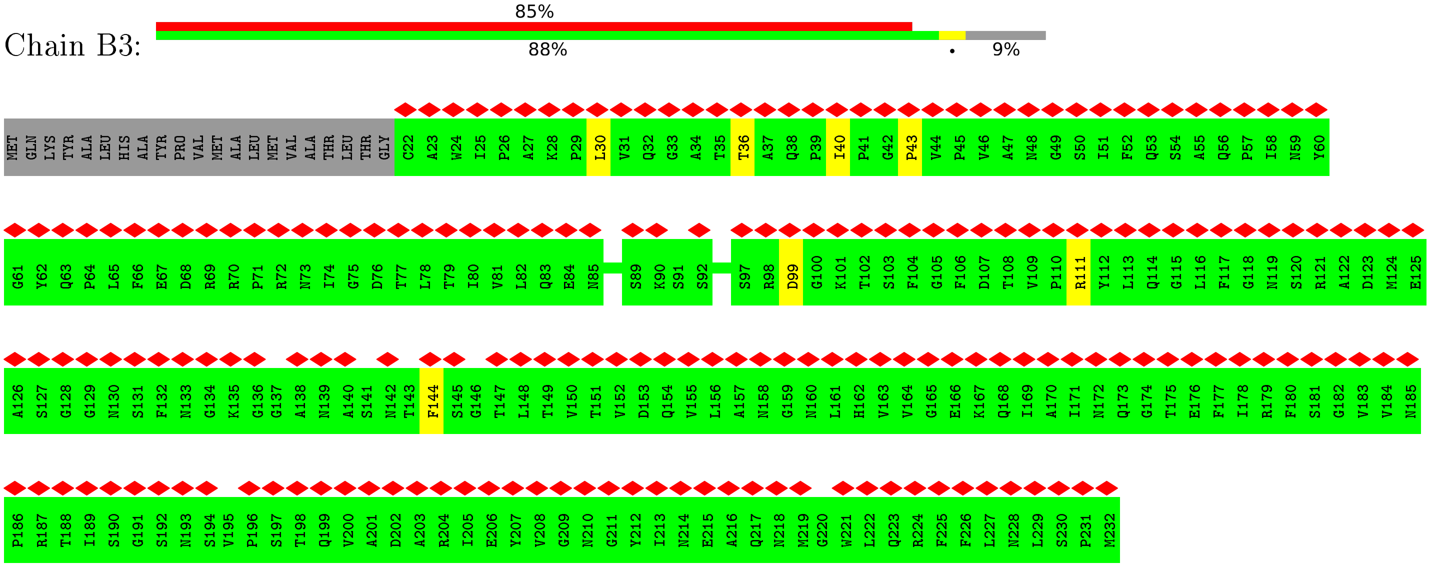
- Molecule 10: Flagellar L-ring protein

Chain A3:



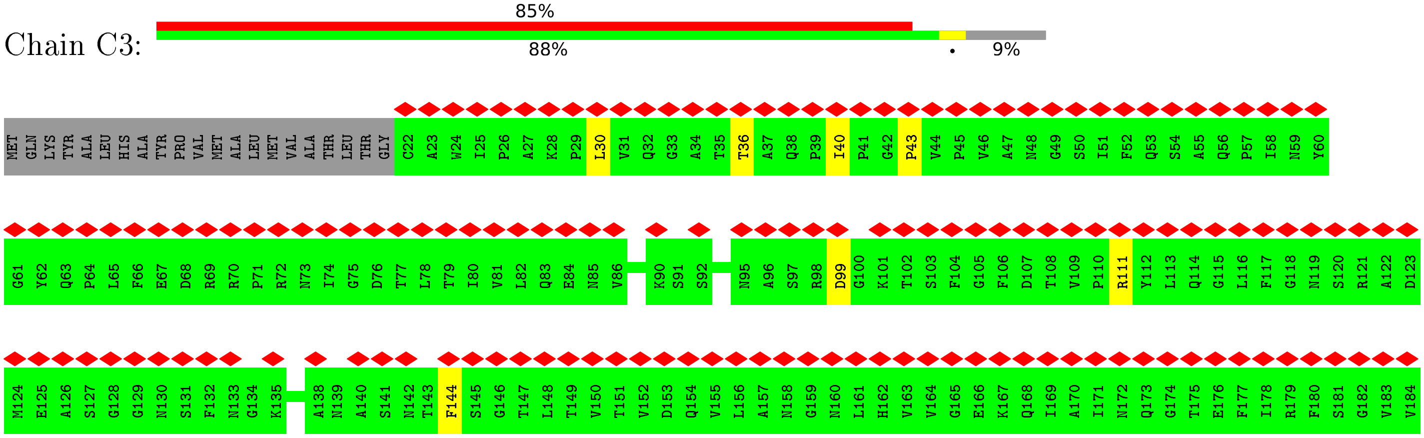
- Molecule 10: Flagellar L-ring protein

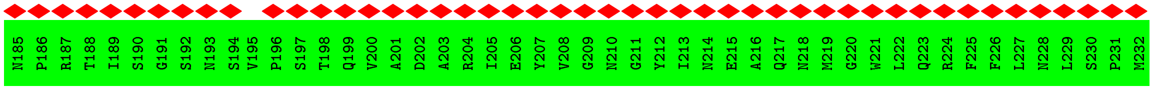
Chain B3:



- Molecule 10: Flagellar L-ring protein

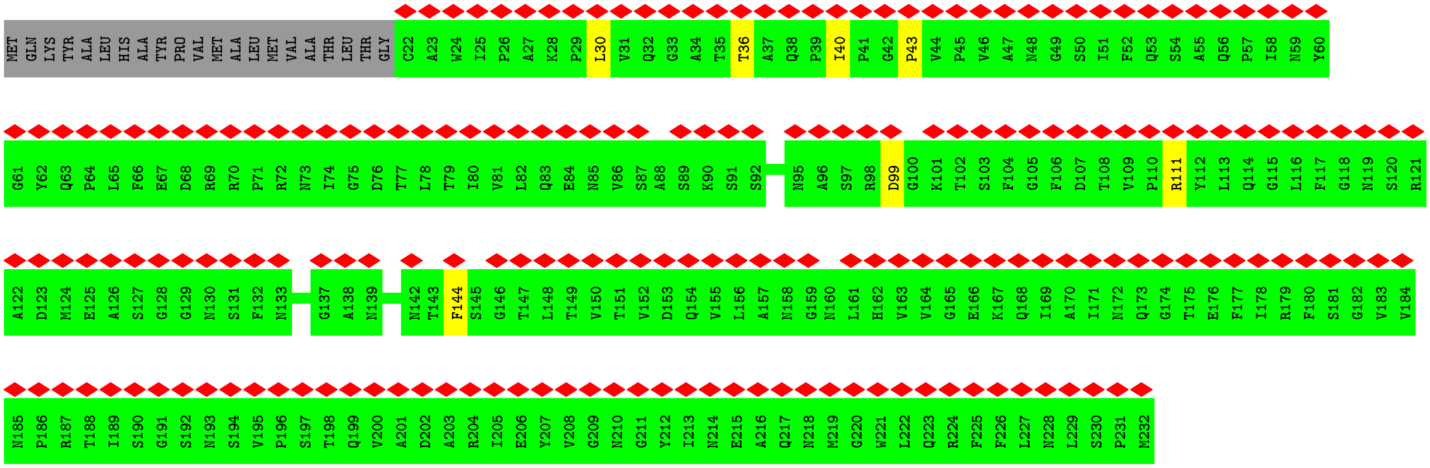
Chain C3:





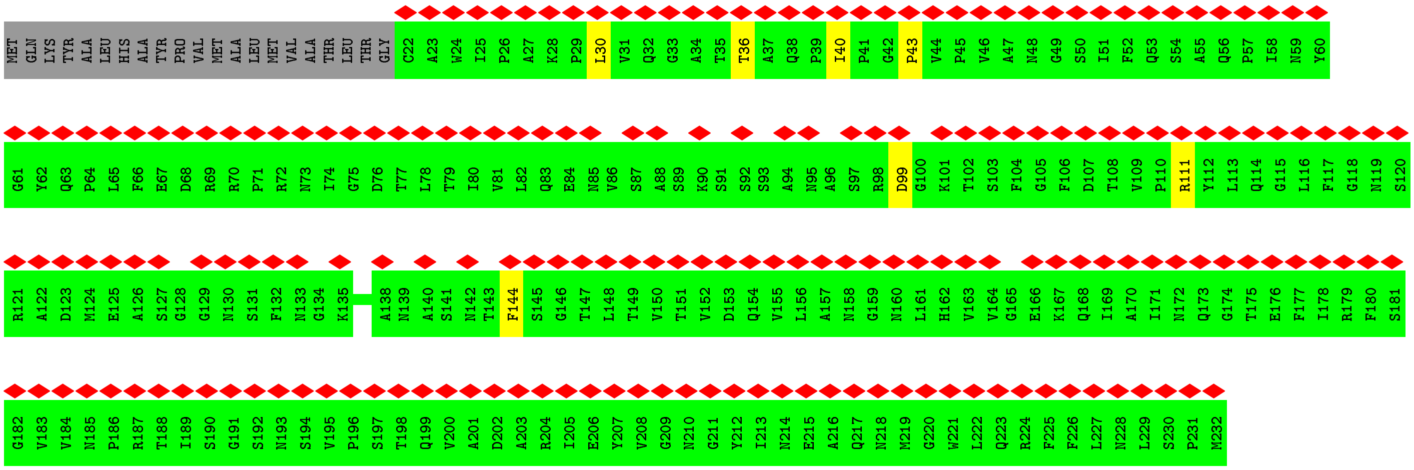
- Molecule 10: Flagellar L-ring protein

Chain D3:



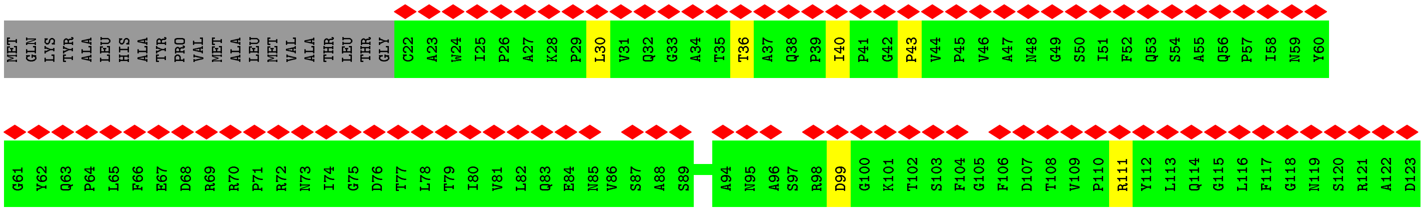
- Molecule 10: Flagellar L-ring protein

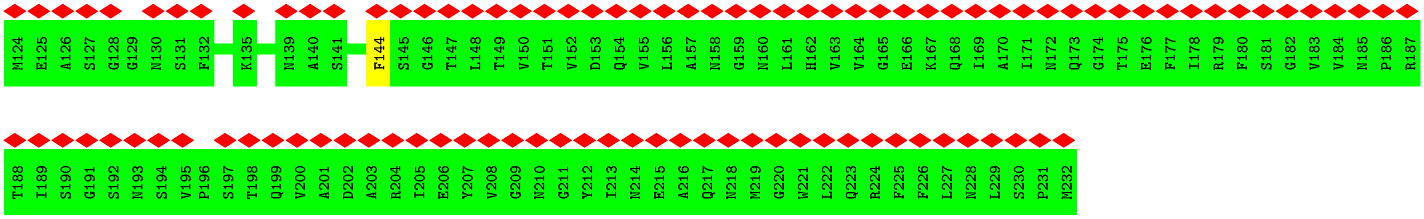
Chain E3:



- Molecule 10: Flagellar L-ring protein

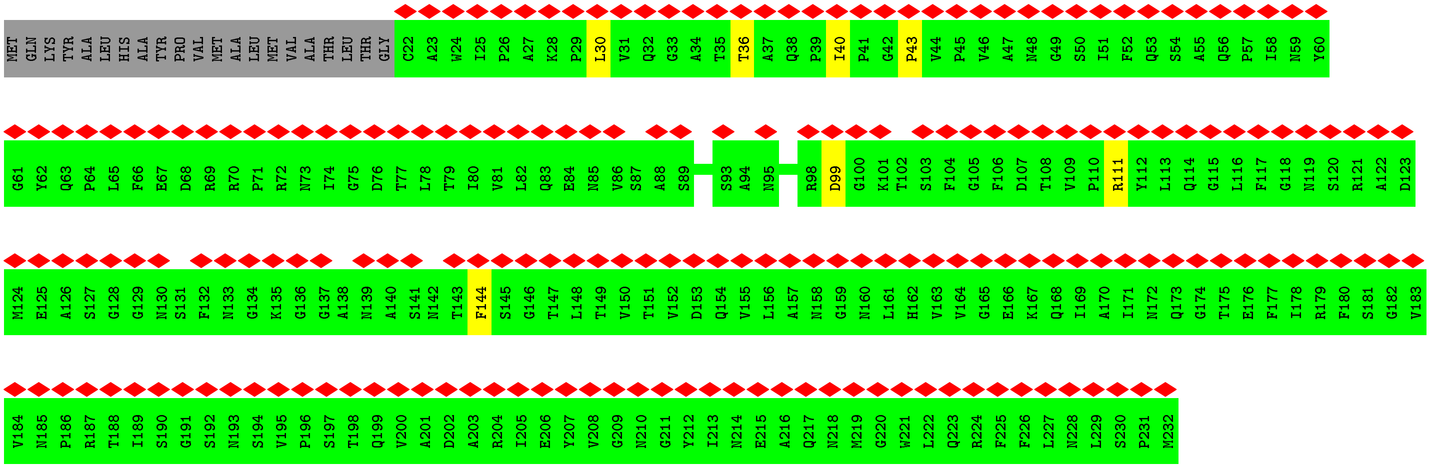
Chain F3:





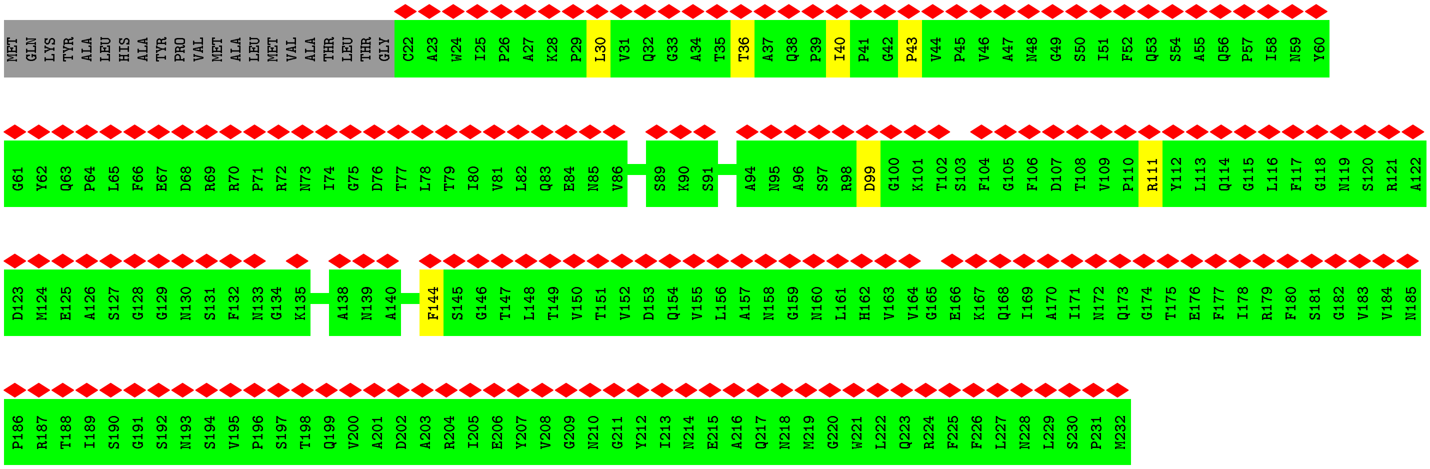
- Molecule 10: Flagellar L-ring protein

Chain G3:



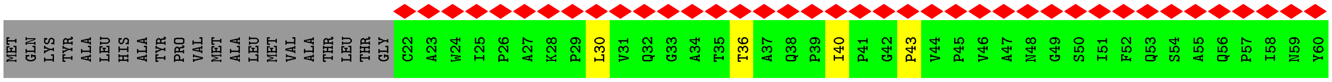
- Molecule 10: Flagellar L-ring protein

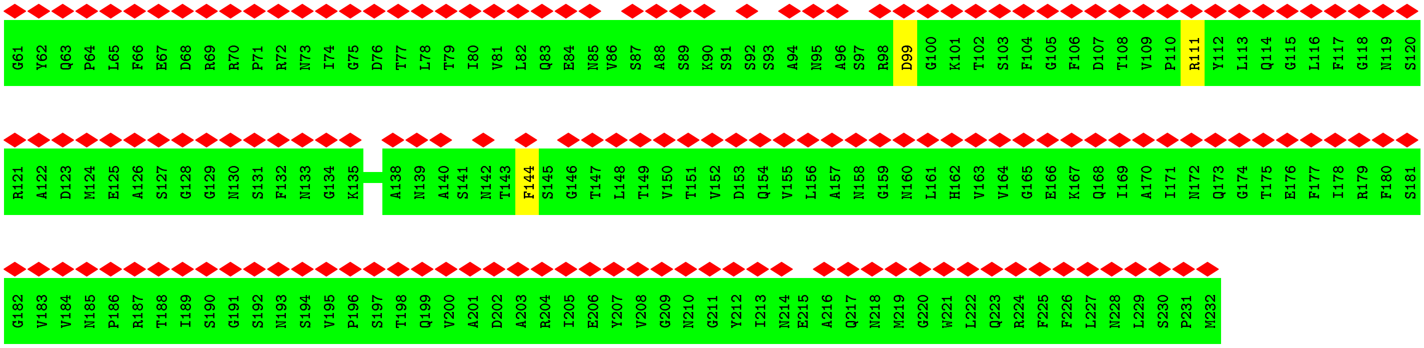
Chain H3:



- Molecule 10: Flagellar L-ring protein

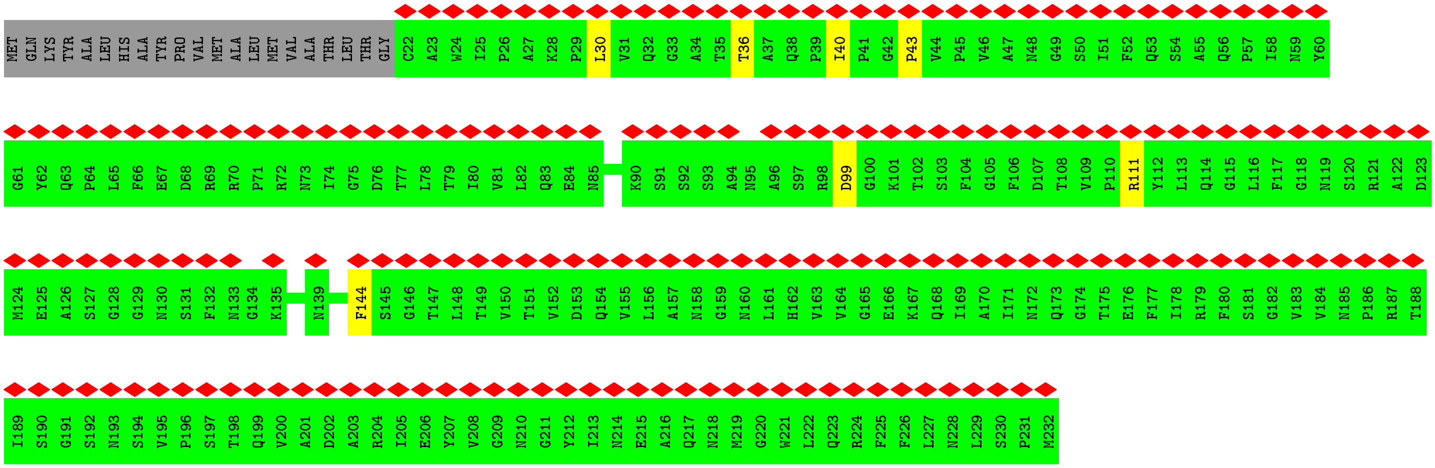
Chain I3:





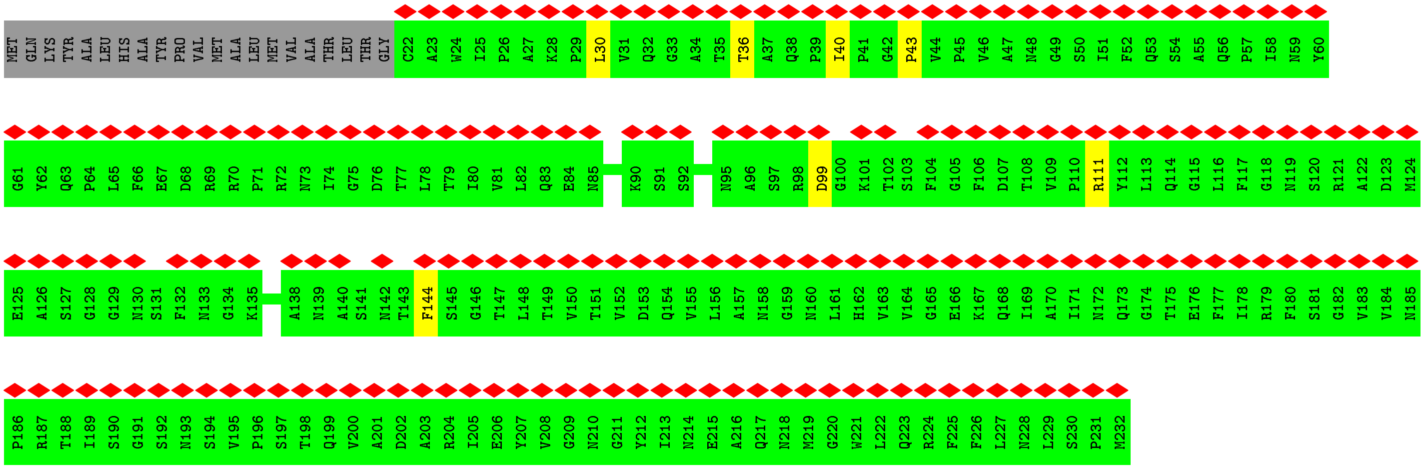
- Molecule 10: Flagellar L-ring protein

Chain J3:



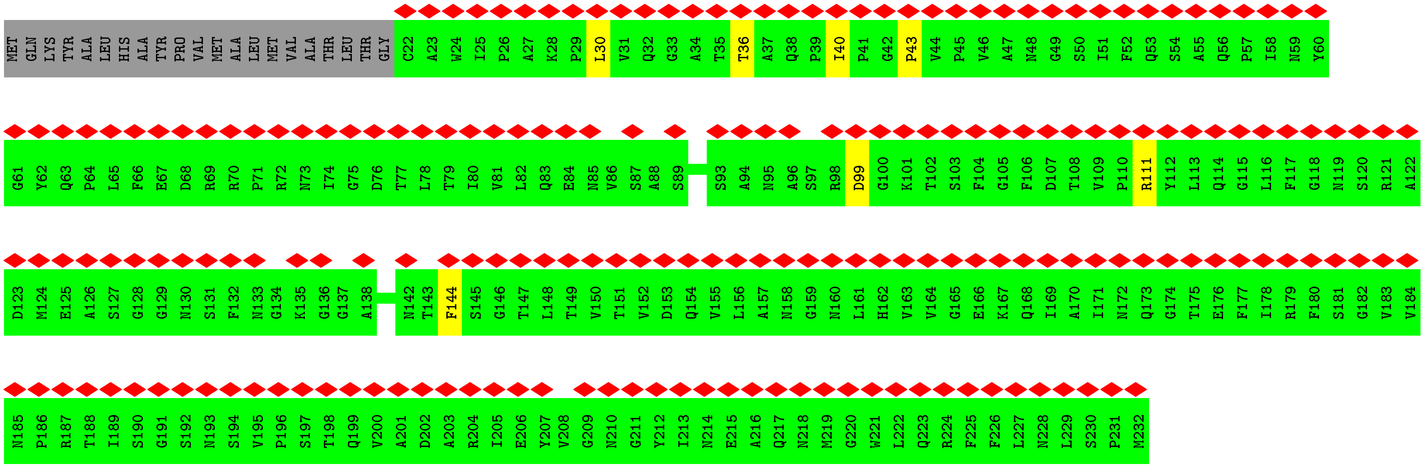
- Molecule 10: Flagellar L-ring protein

Chain K3:



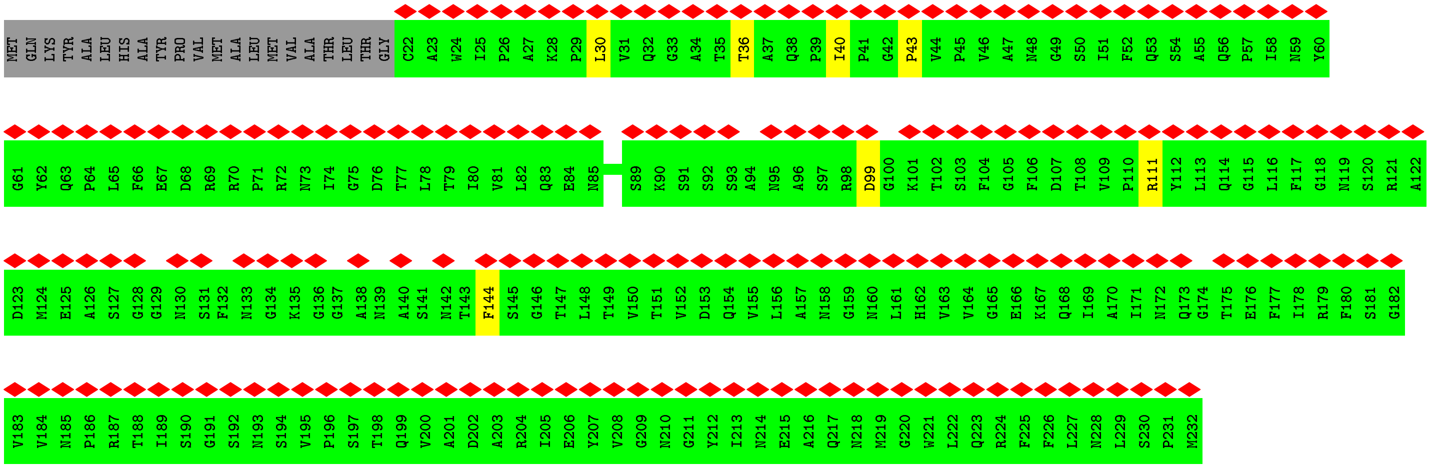
- Molecule 10: Flagellar L-ring protein

Chain L3:



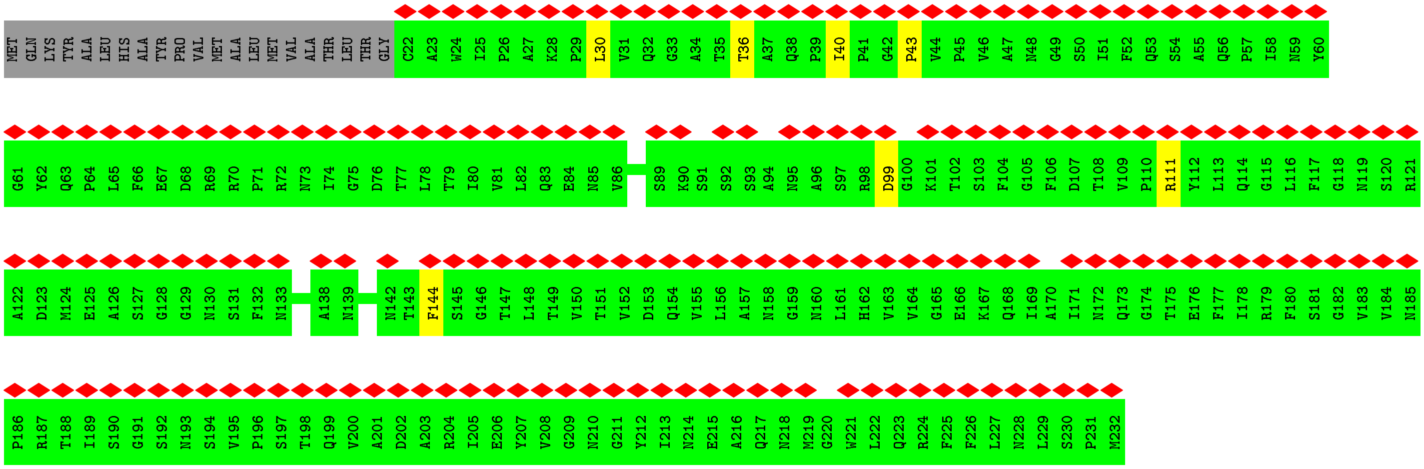
- Molecule 10: Flagellar L-ring protein

Chain M3:

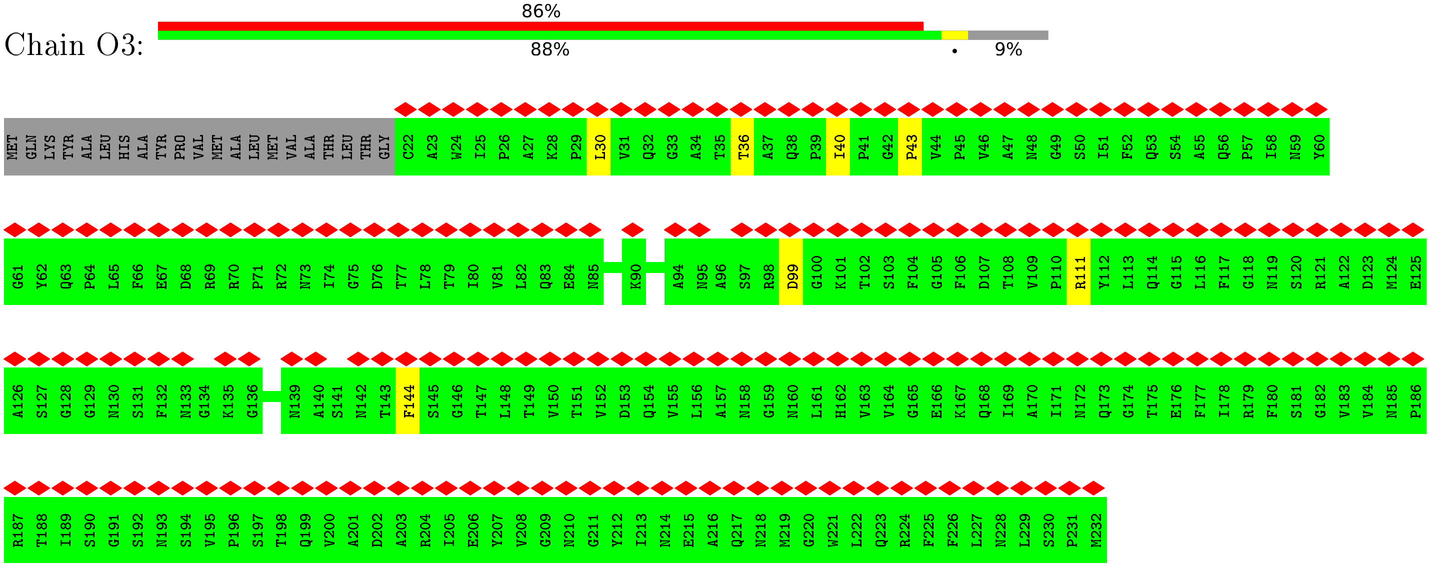


- Molecule 10: Flagellar L-ring protein

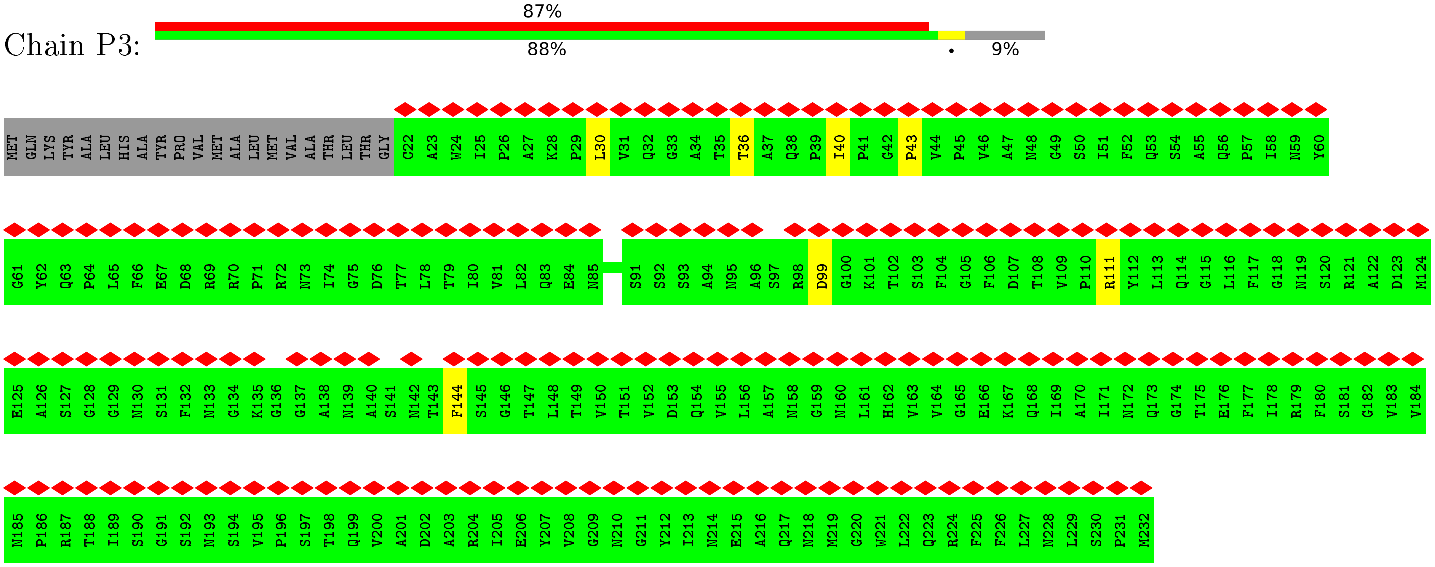
Chain N3:



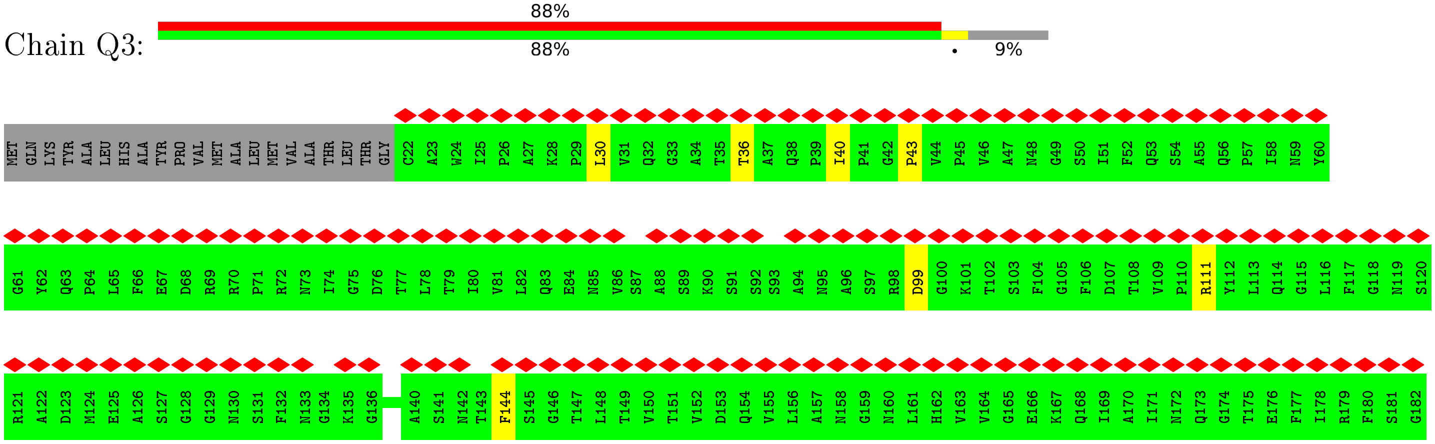
- Molecule 10: Flagellar L-ring protein

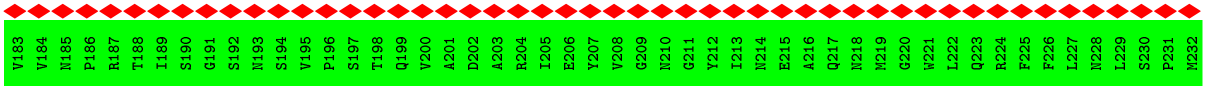


- Molecule 10: Flagellar L-ring protein



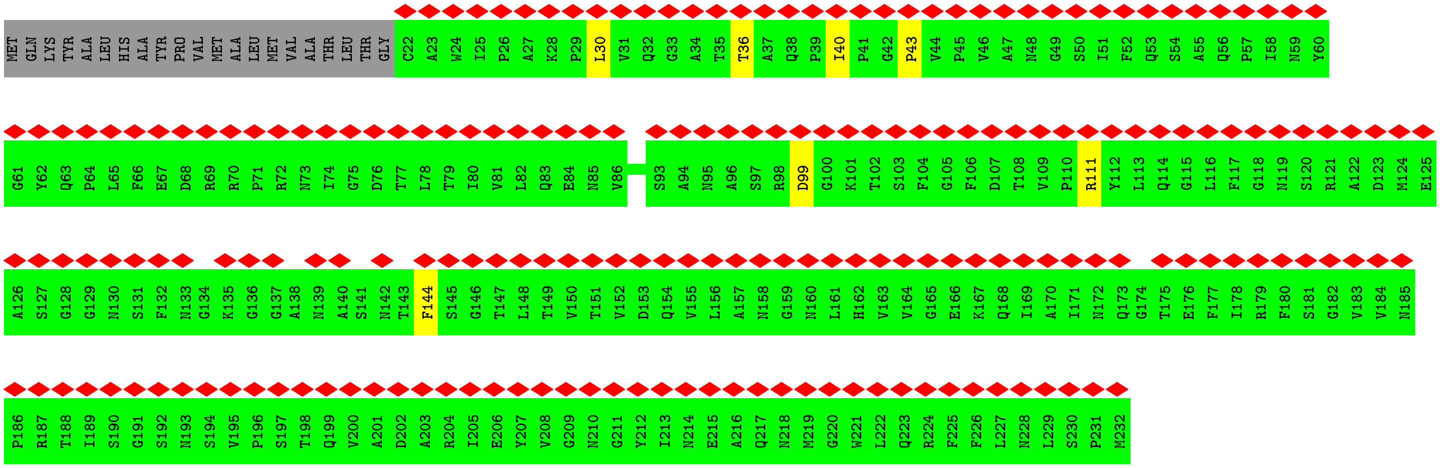
- Molecule 10: Flagellar L-ring protein





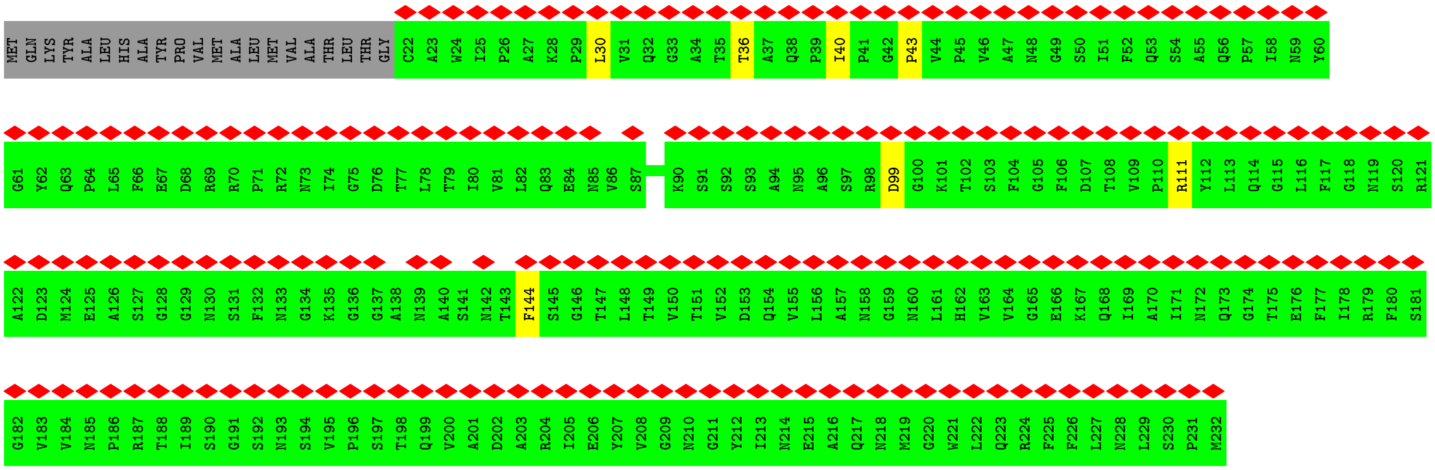
- Molecule 10: Flagellar L-ring protein

Chain R3:



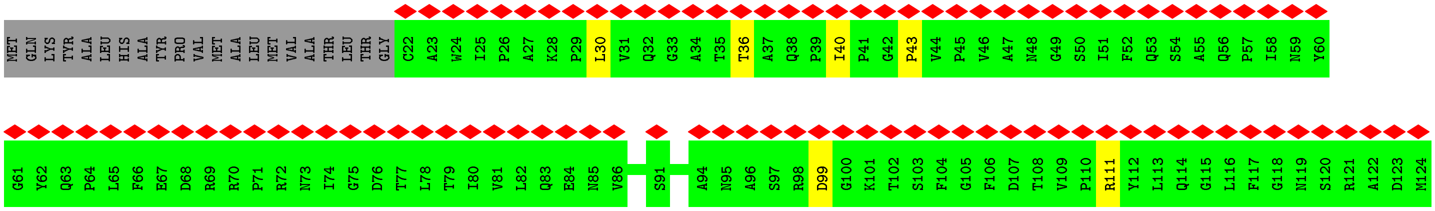
- Molecule 10: Flagellar L-ring protein

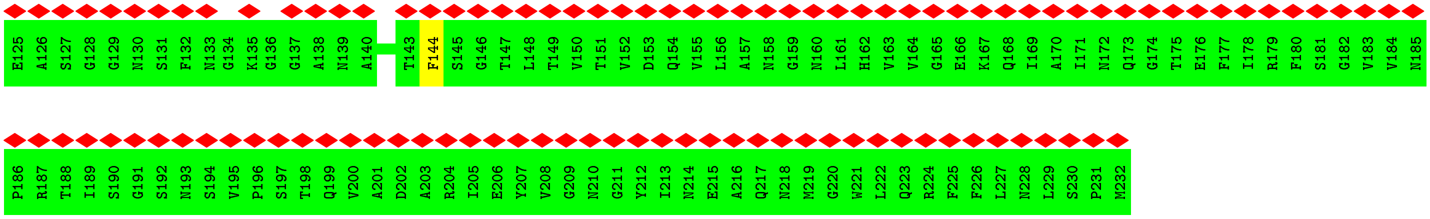
Chain S3:



- Molecule 10: Flagellar L-ring protein

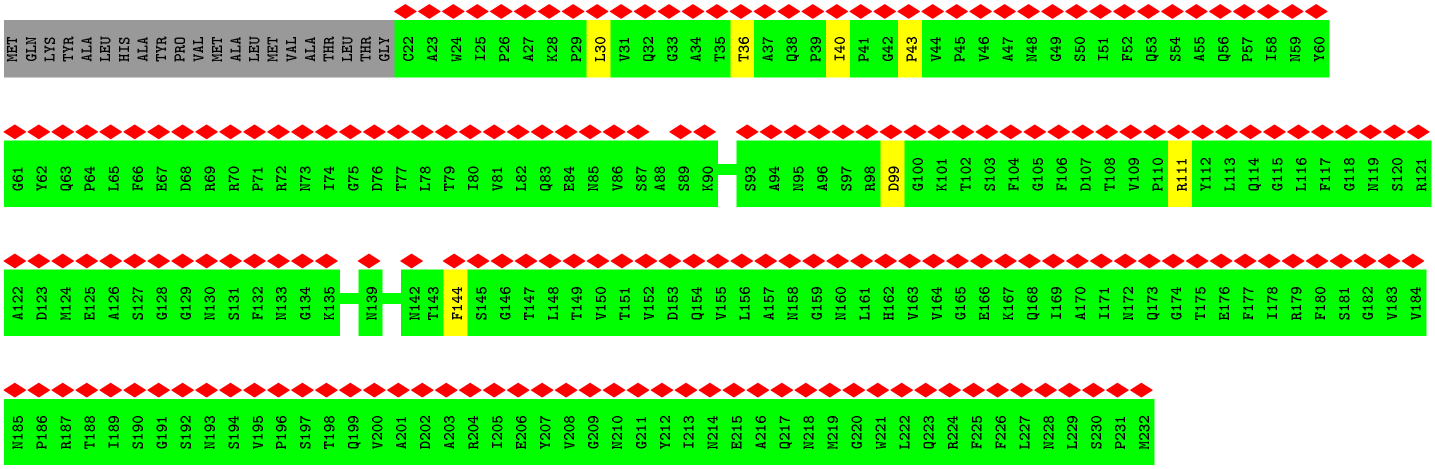
Chain T3:





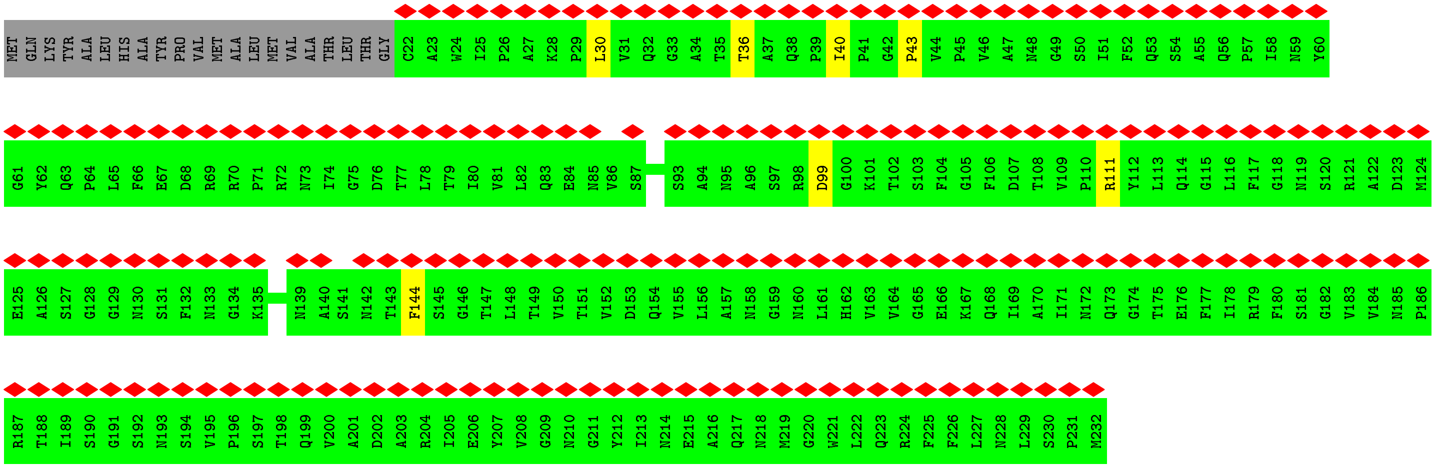
- Molecule 10: Flagellar L-ring protein

Chain U3:



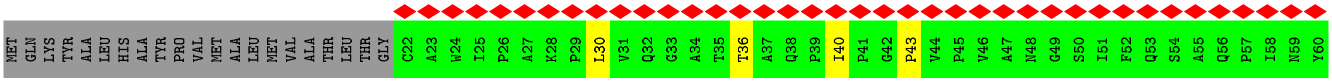
- Molecule 10: Flagellar L-ring protein

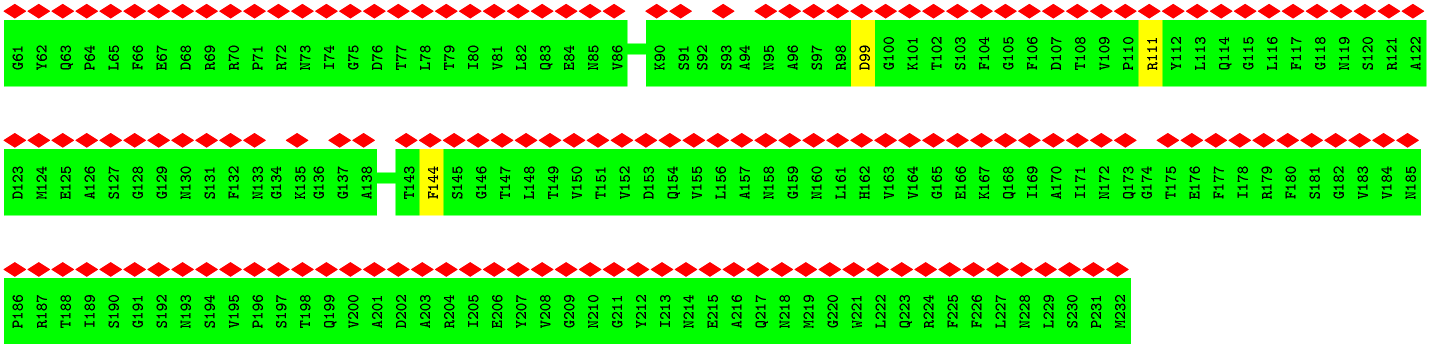
Chain V3:



- Molecule 10: Flagellar L-ring protein

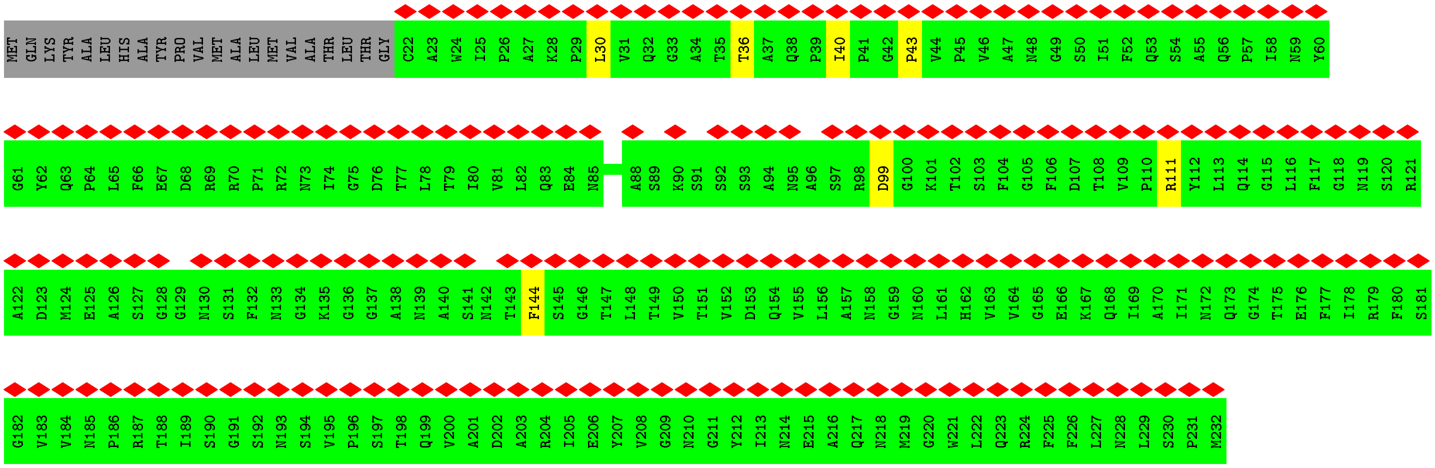
Chain W3:





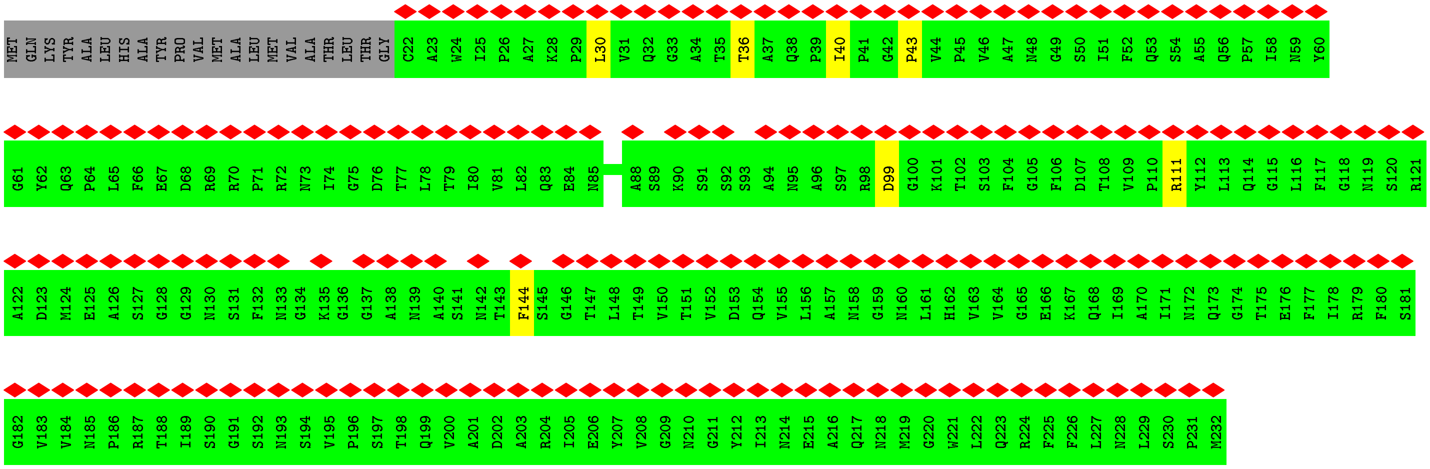
- Molecule 10: Flagellar L-ring protein

Chain X3:



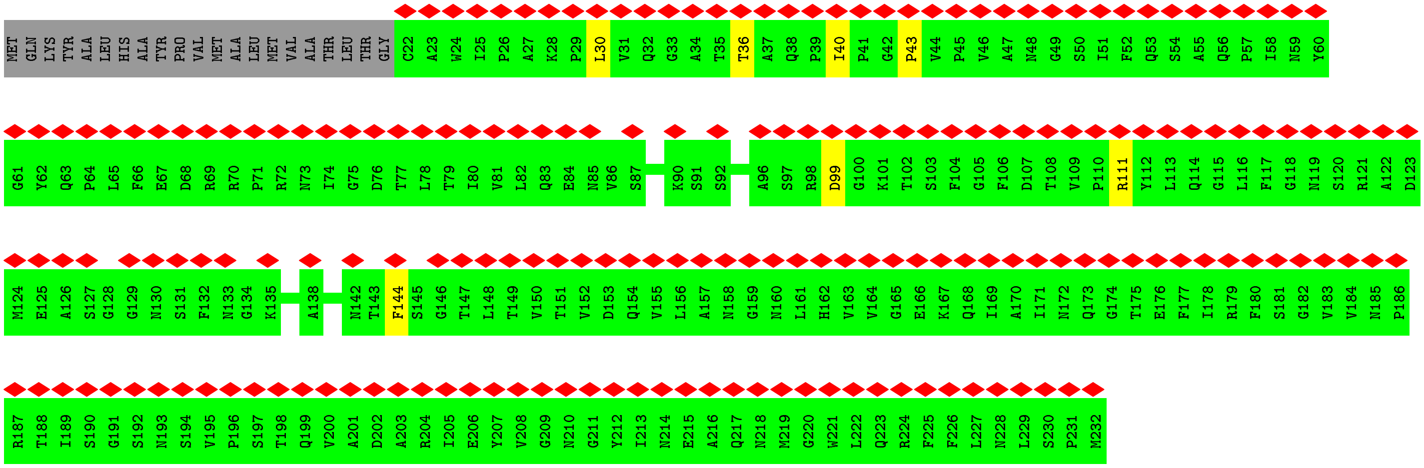
- Molecule 10: Flagellar L-ring protein

Chain Y3:



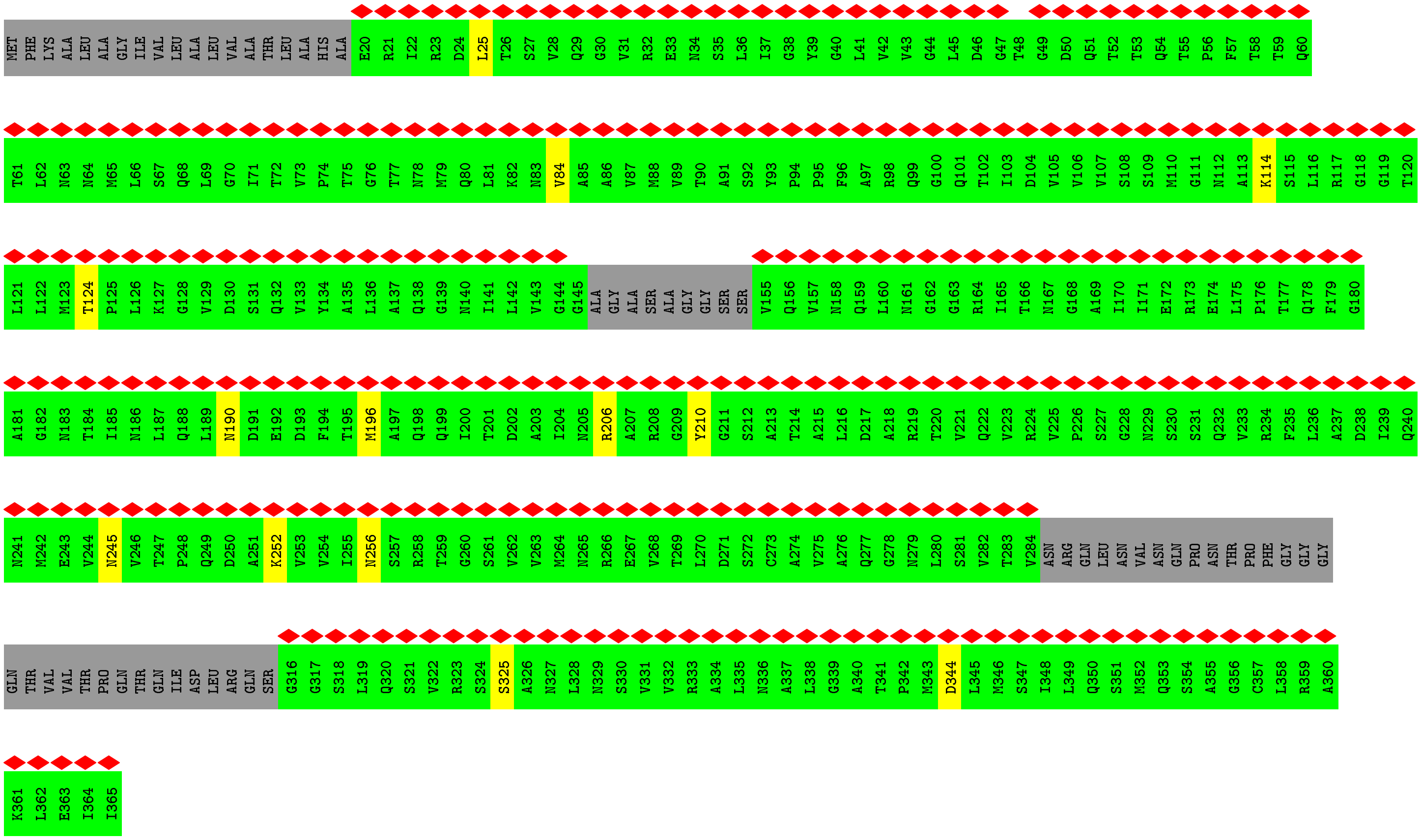
- Molecule 10: Flagellar L-ring protein

Chain Z3:



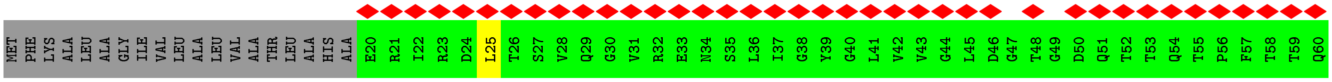
- Molecule 11: Flagellar P-ring protein

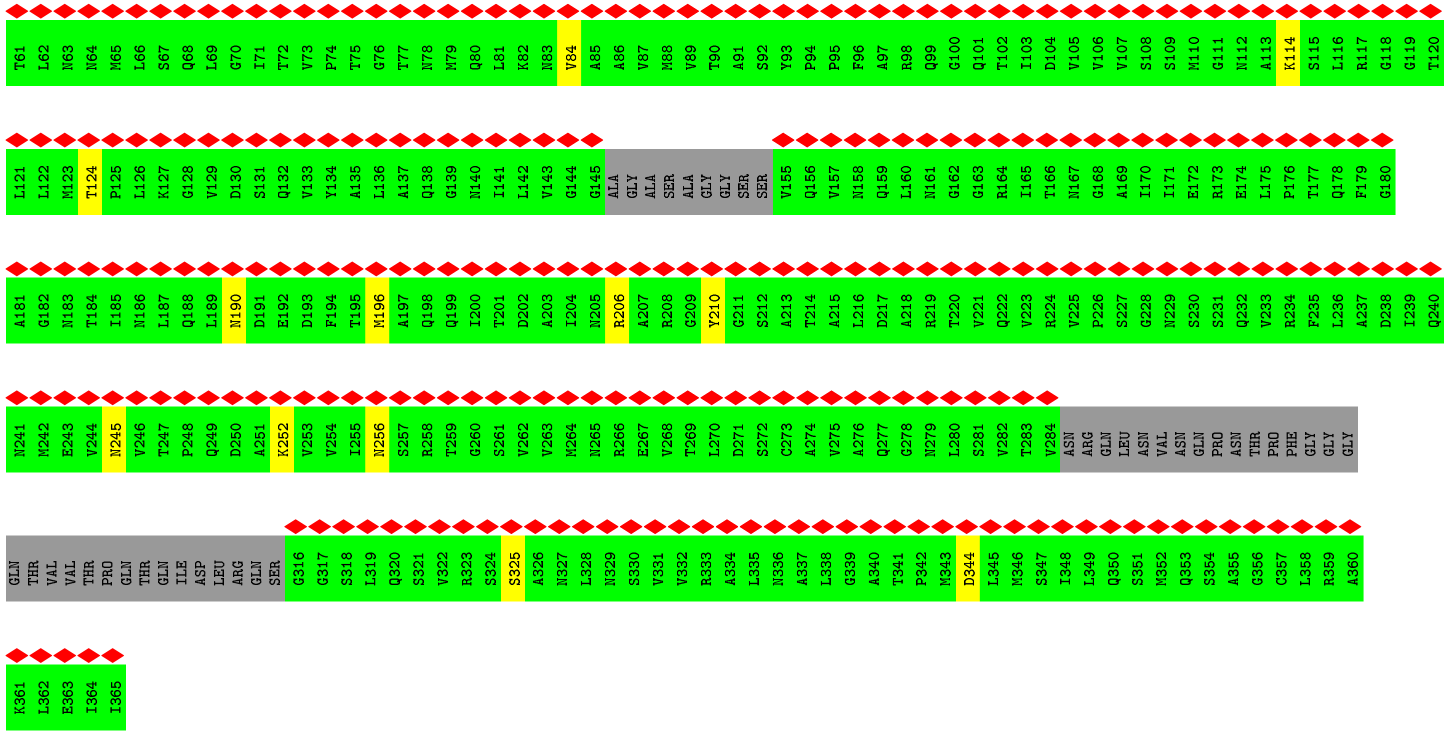
Chain a3:



- Molecule 11: Flagellar P-ring protein

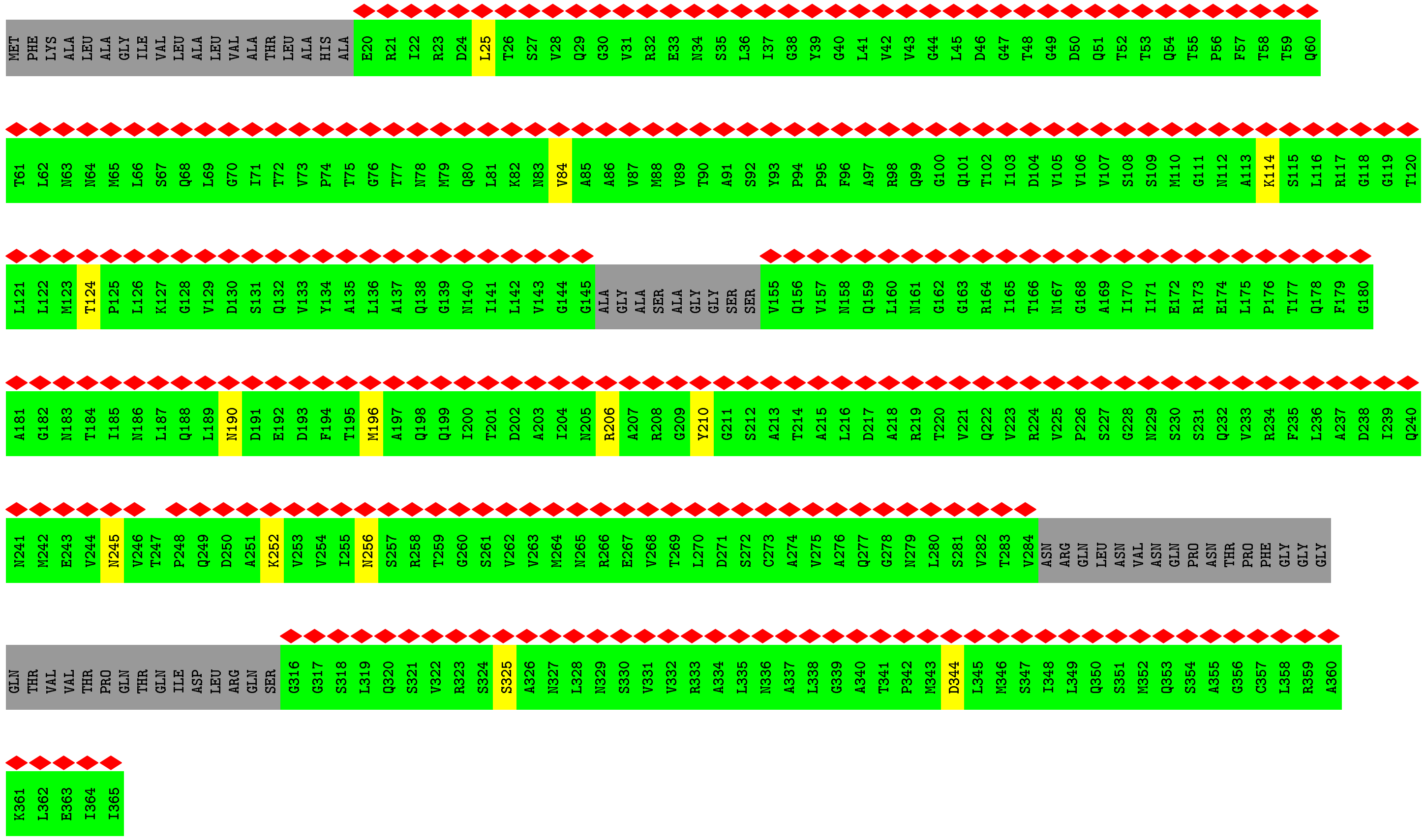
Chain b3:



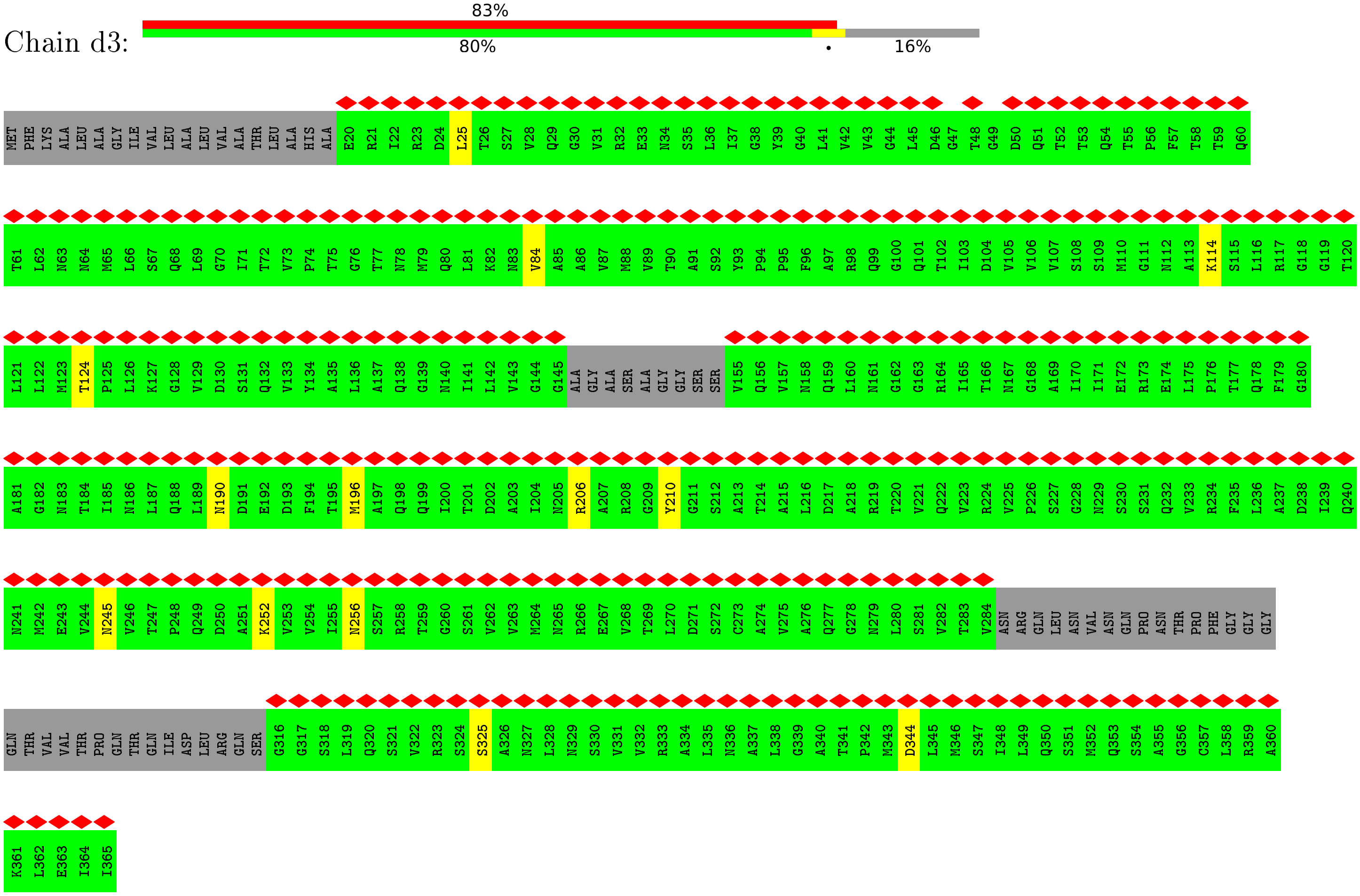


• Molecule 11: Flagellar P-ring protein

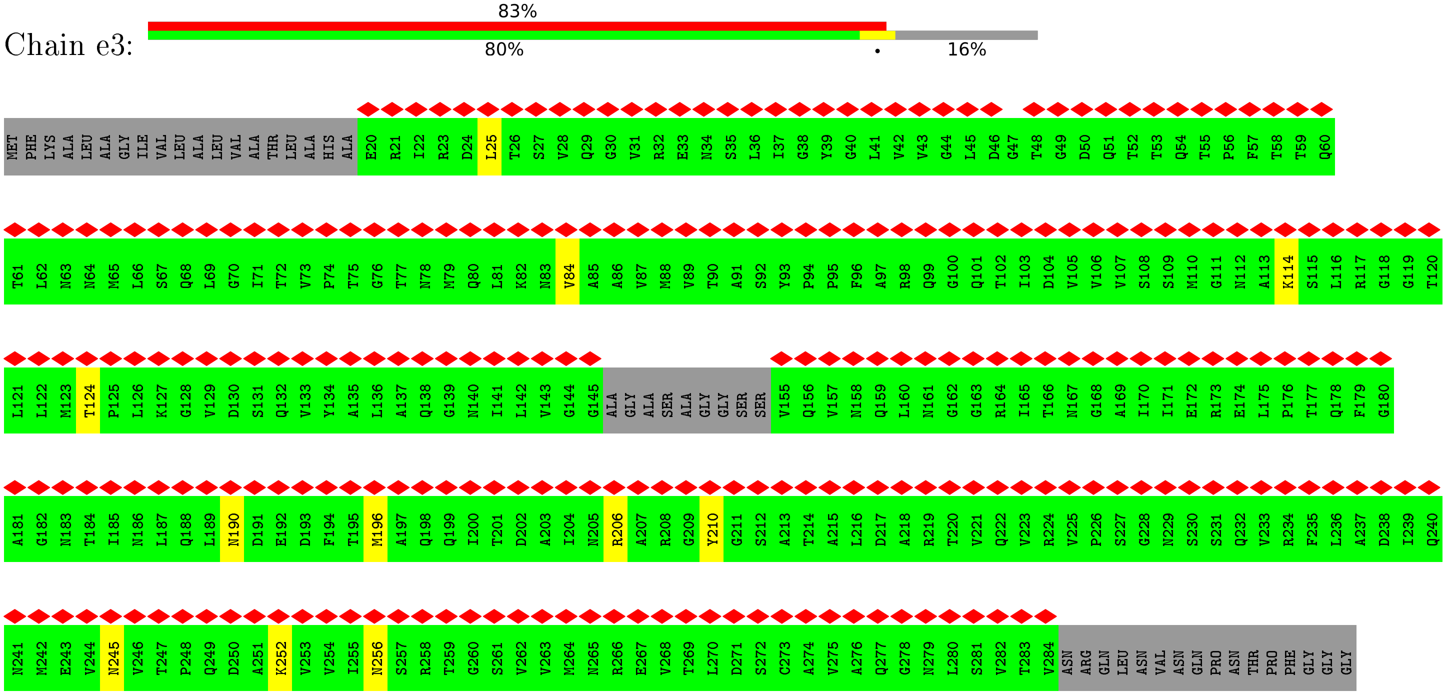
Chain c3:

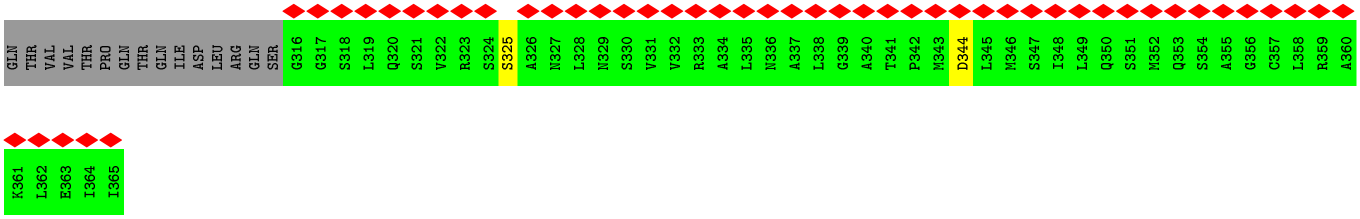


- Molecule 11: Flagellar P-ring protein



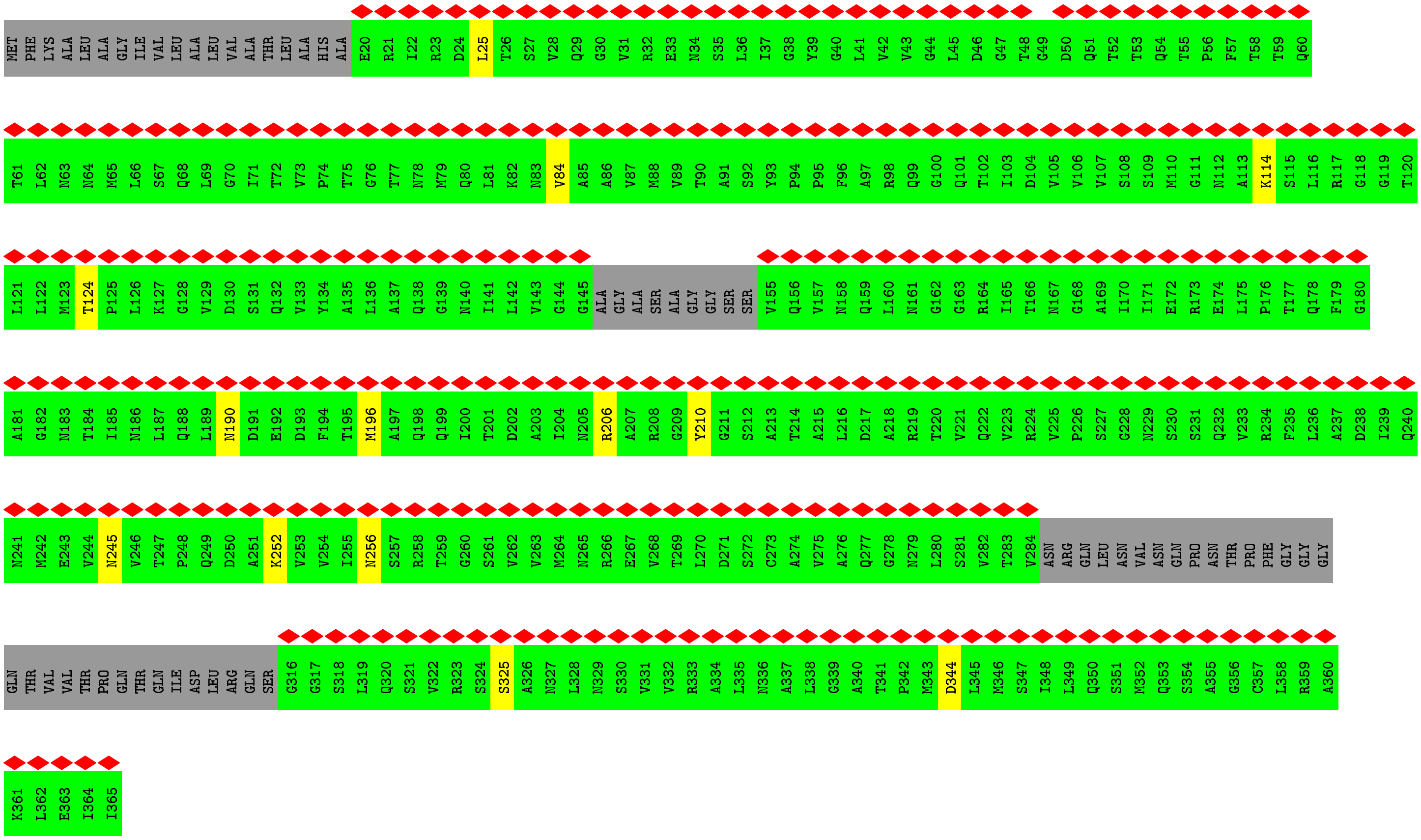
- Molecule 11: Flagellar P-ring protein





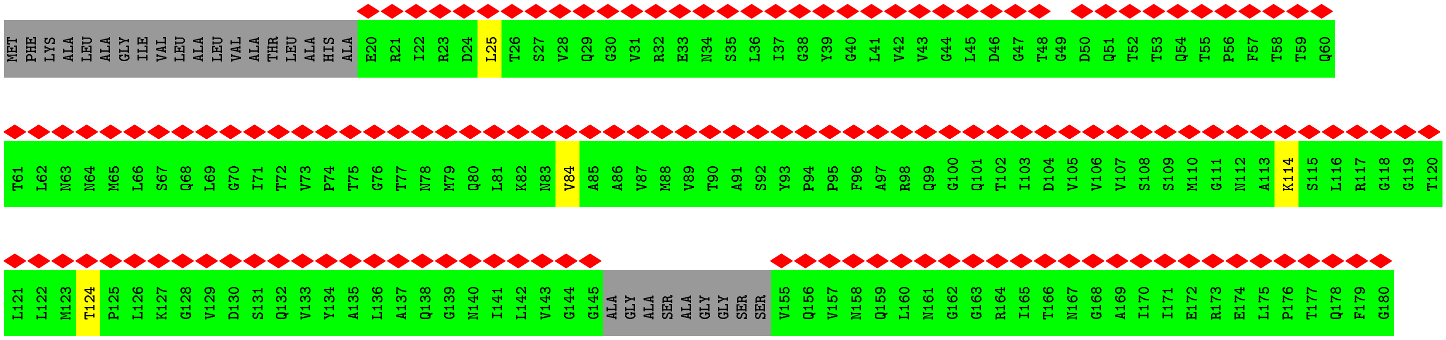
- Molecule 11: Flagellar P-ring protein

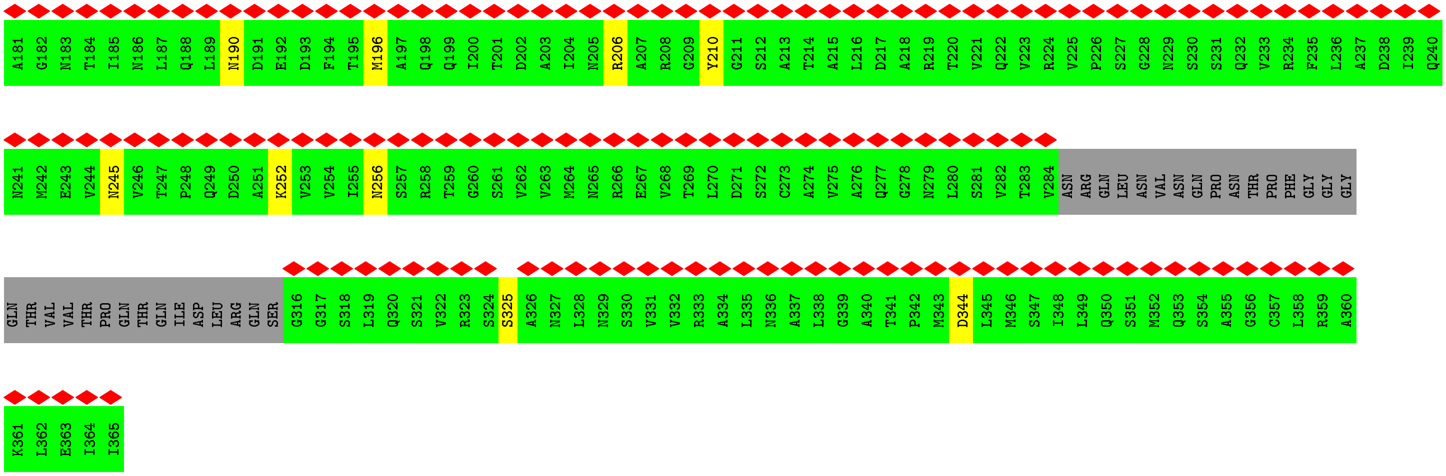
Chain f3:



- Molecule 11: Flagellar P-ring protein

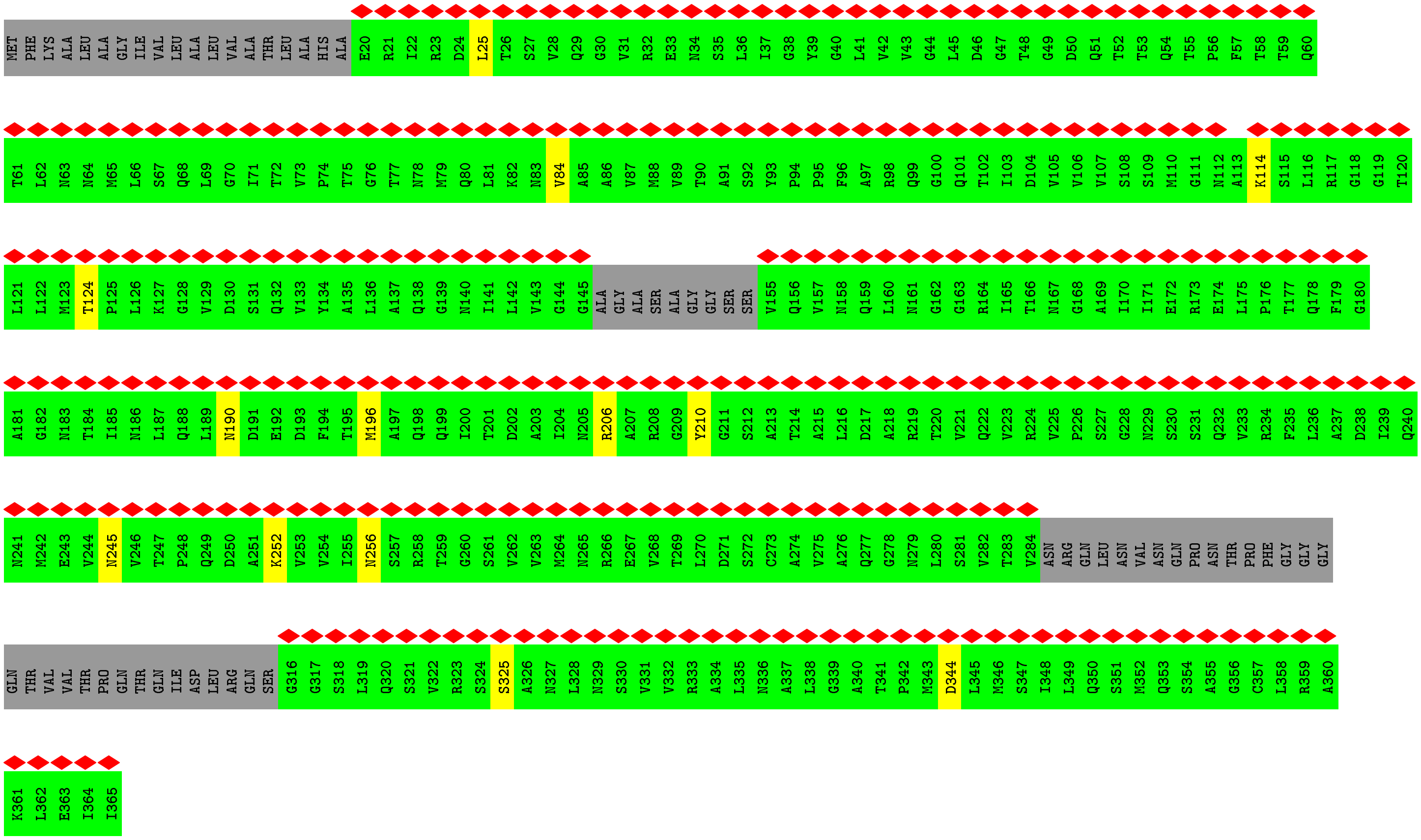
Chain g3:





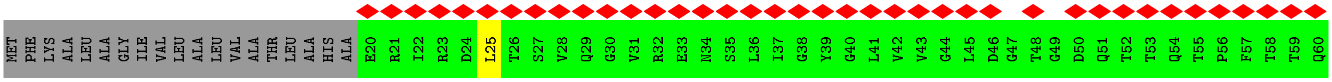
- Molecule 11: Flagellar P-ring protein

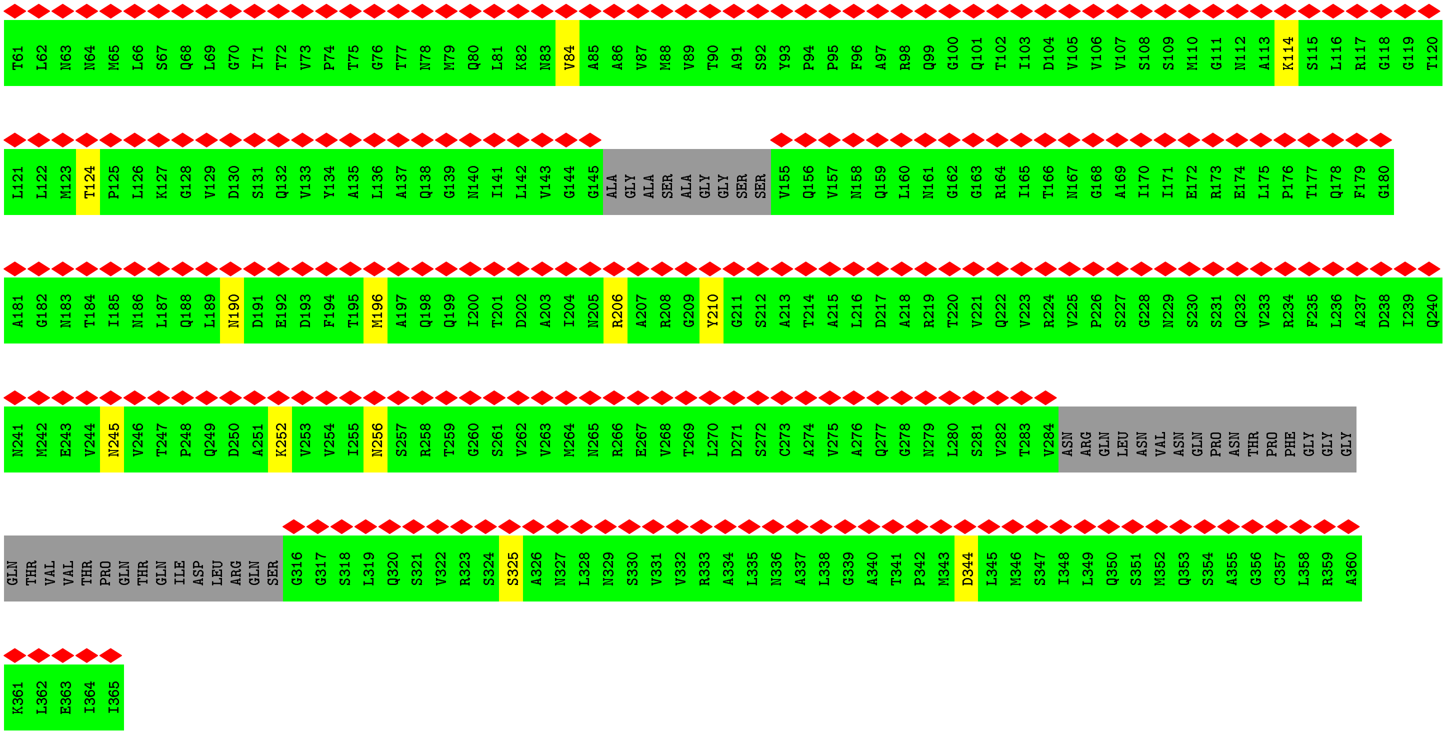
Chain h3:



- Molecule 11: Flagellar P-ring protein

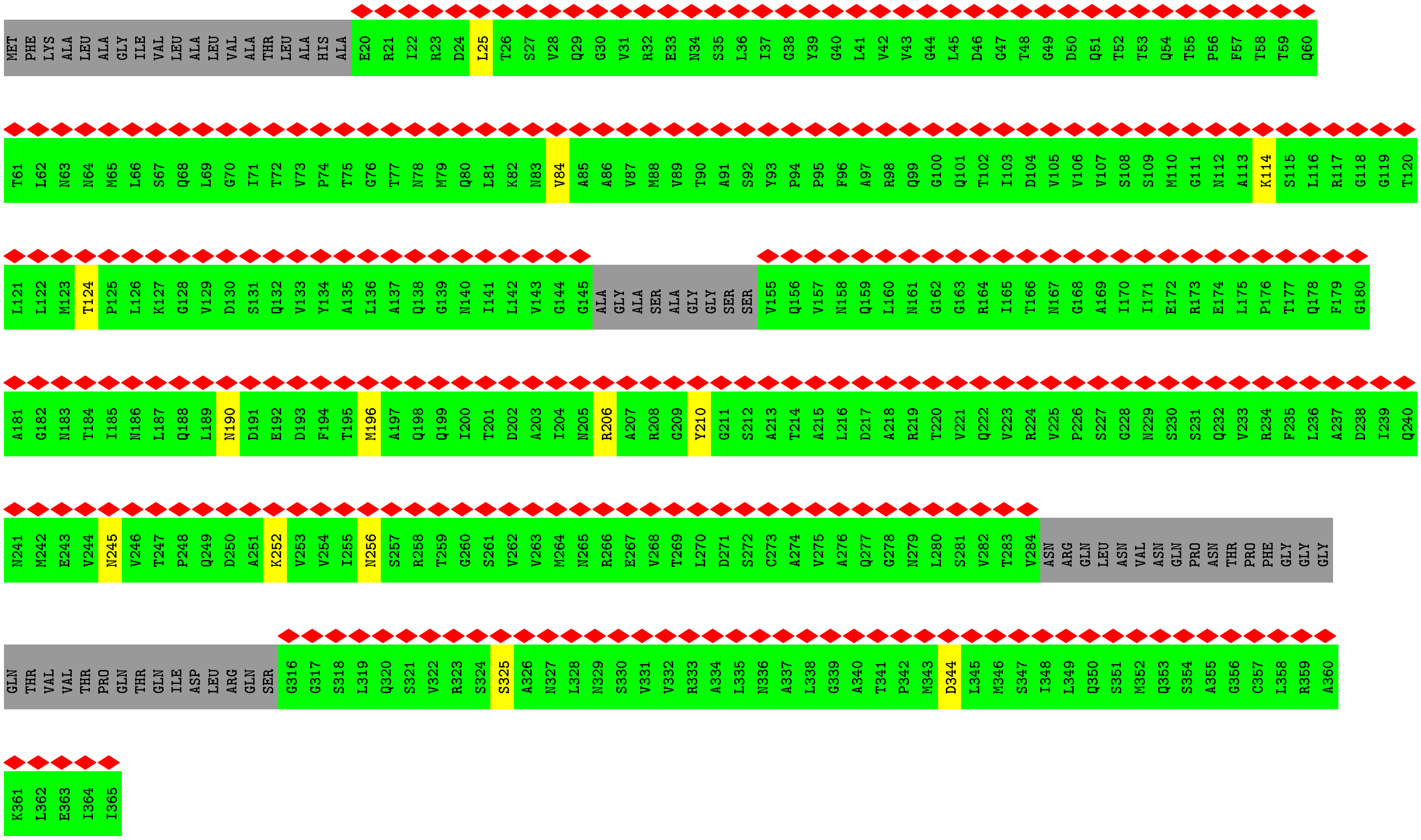
Chain i3:





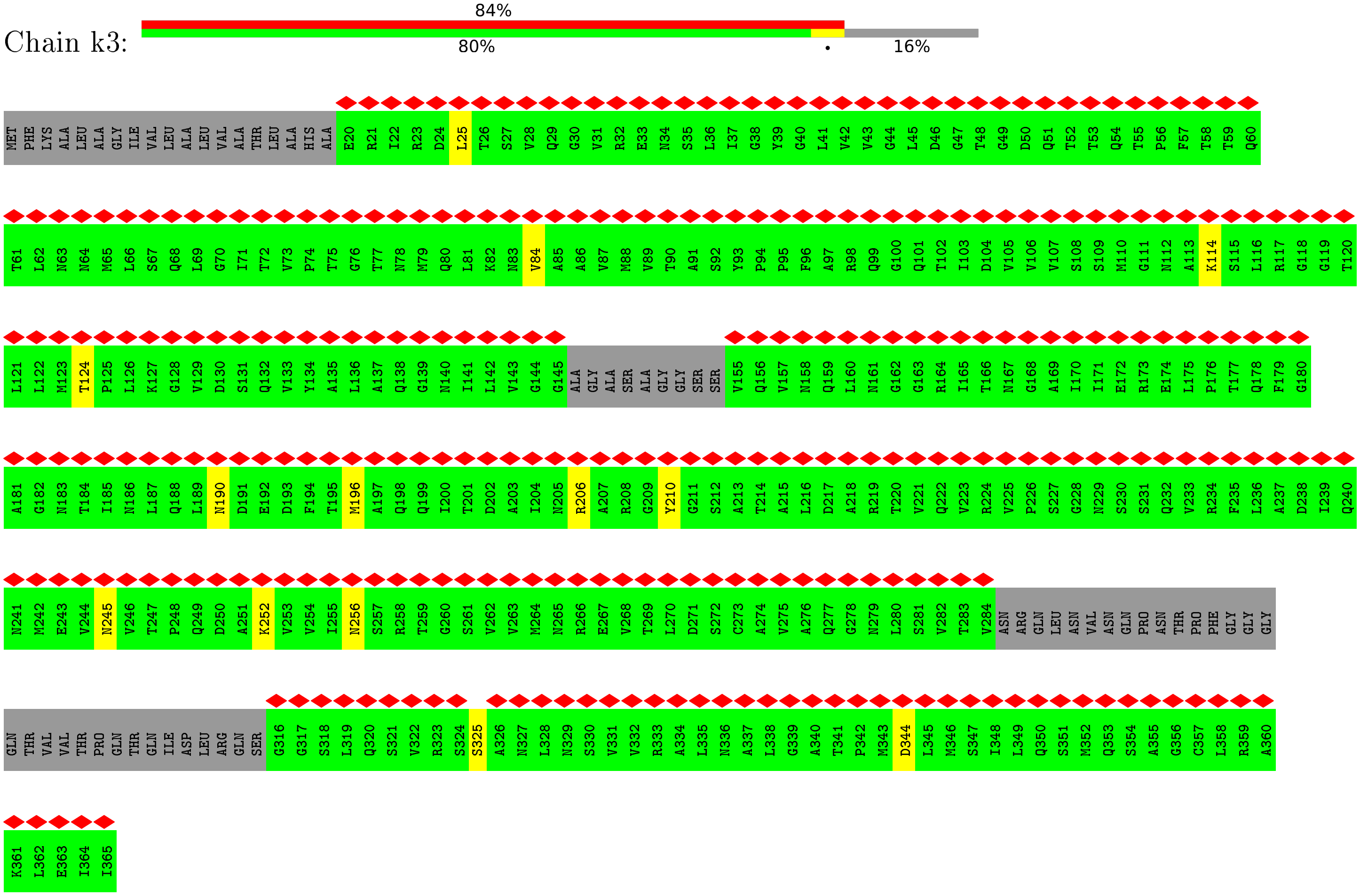
- Molecule 11: Flagellar P-ring protein

Chain j3:



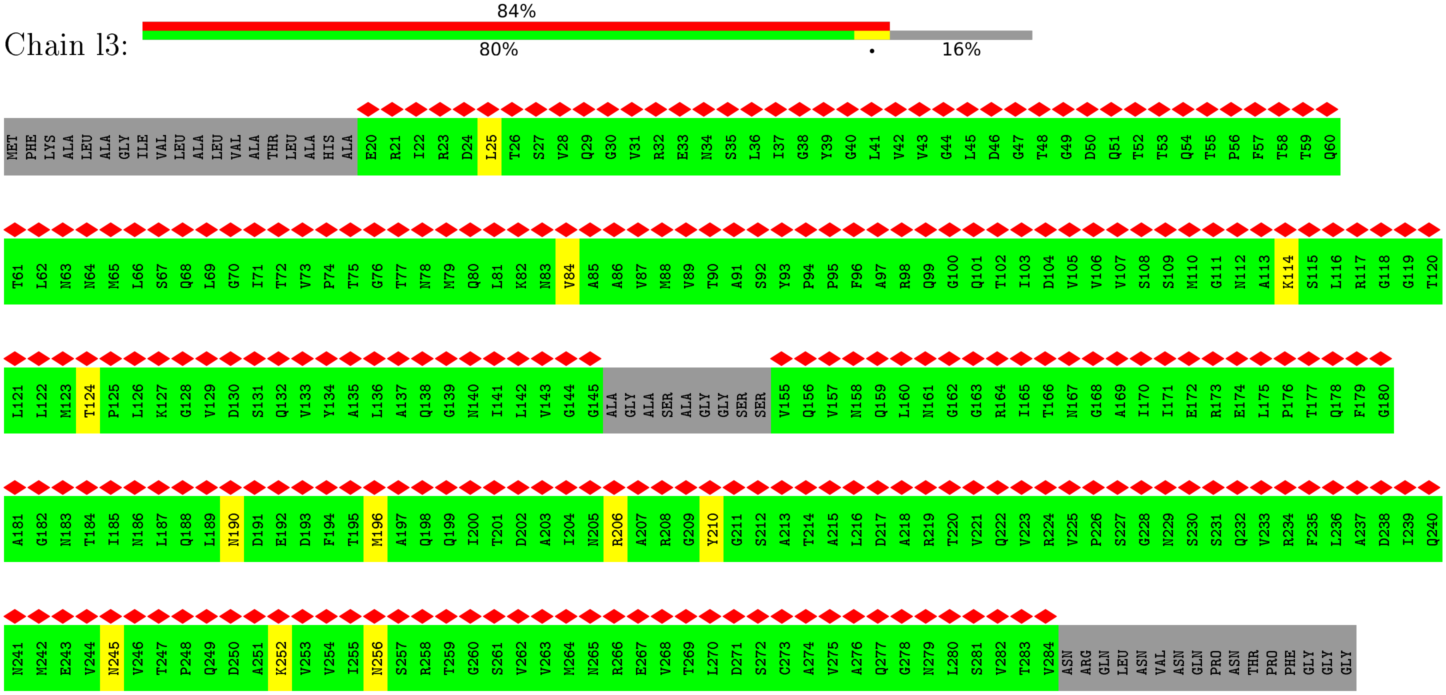
- Molecule 11: Flagellar P-ring protein

Chain k3:

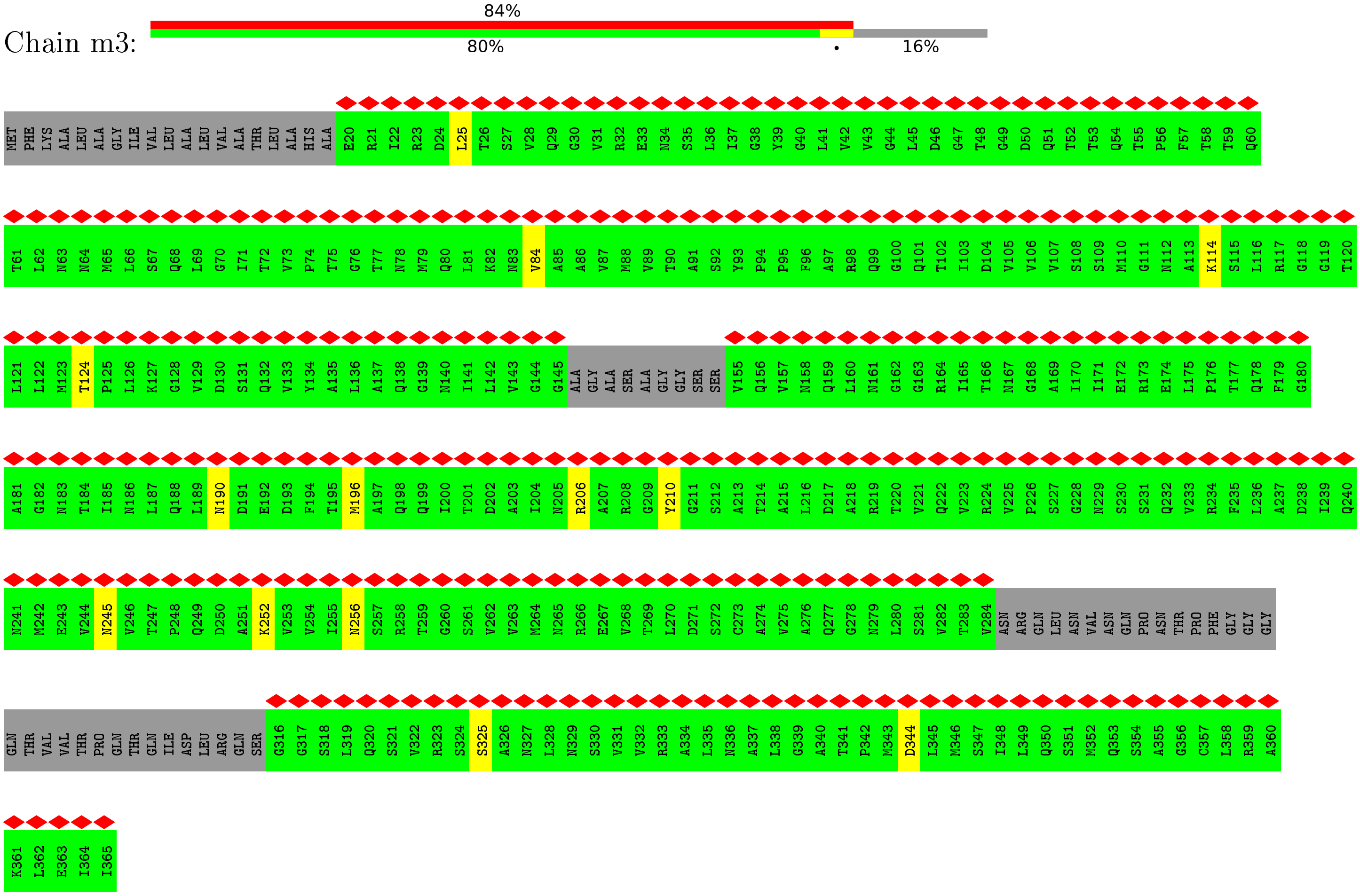


- Molecule 11: Flagellar P-ring protein

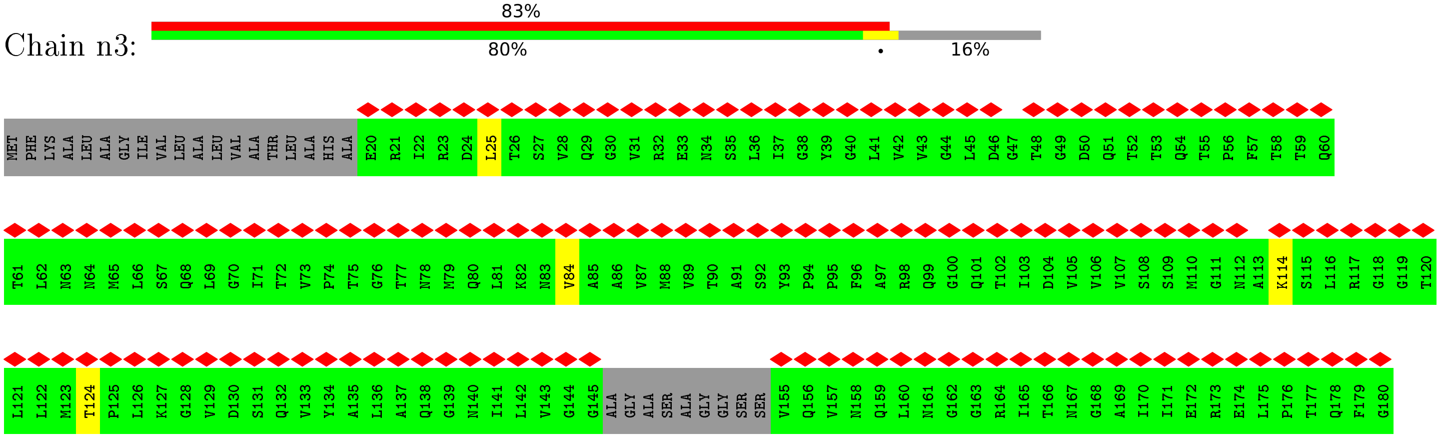
Chain l3:

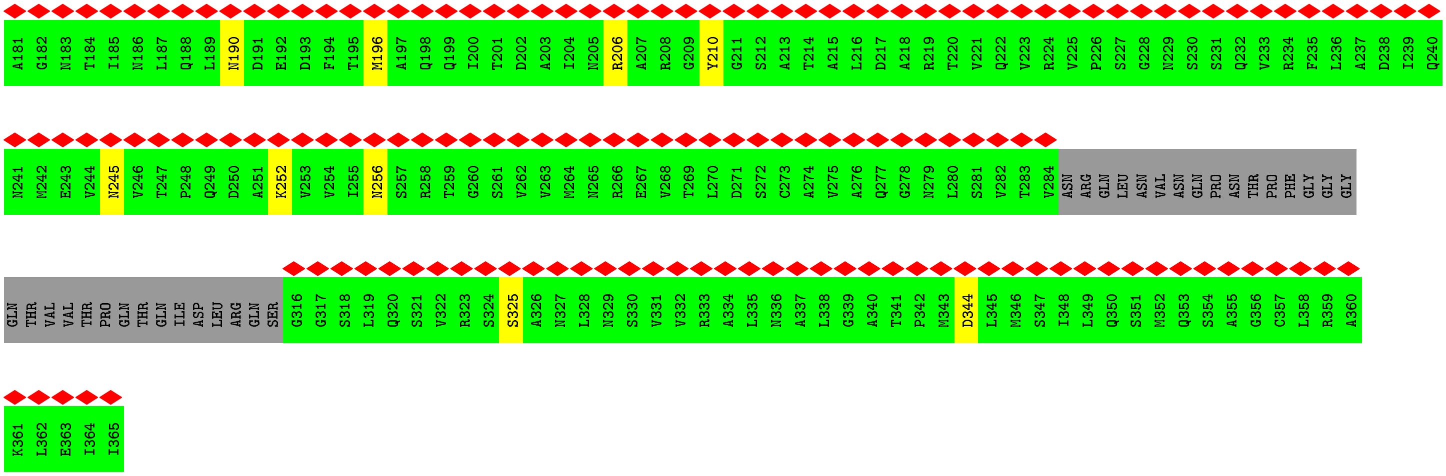


- Molecule 11: Flagellar P-ring protein



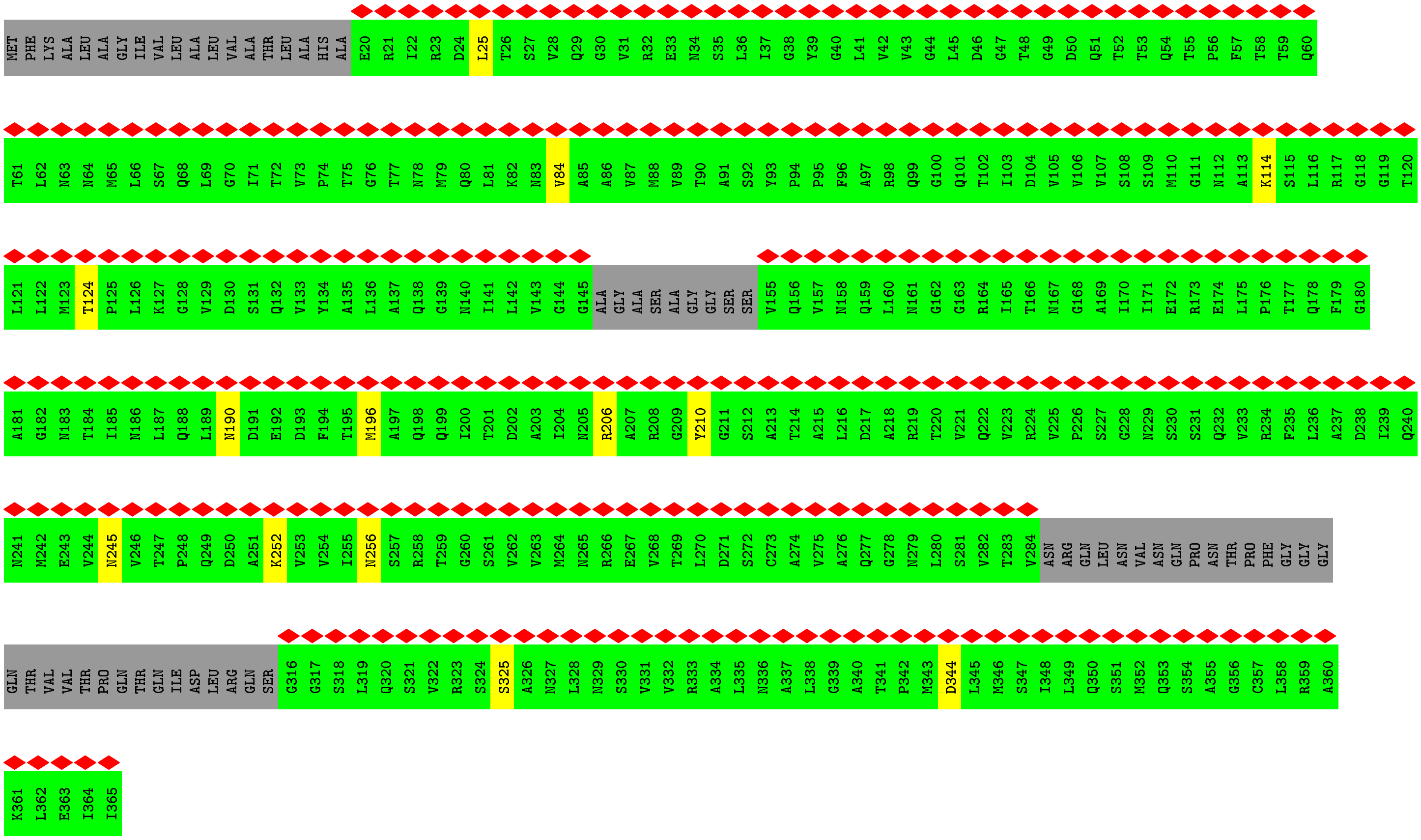
- Molecule 11: Flagellar P-ring protein





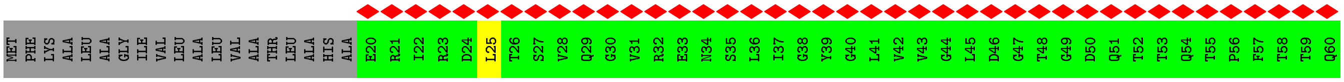
- Molecule 11: Flagellar P-ring protein

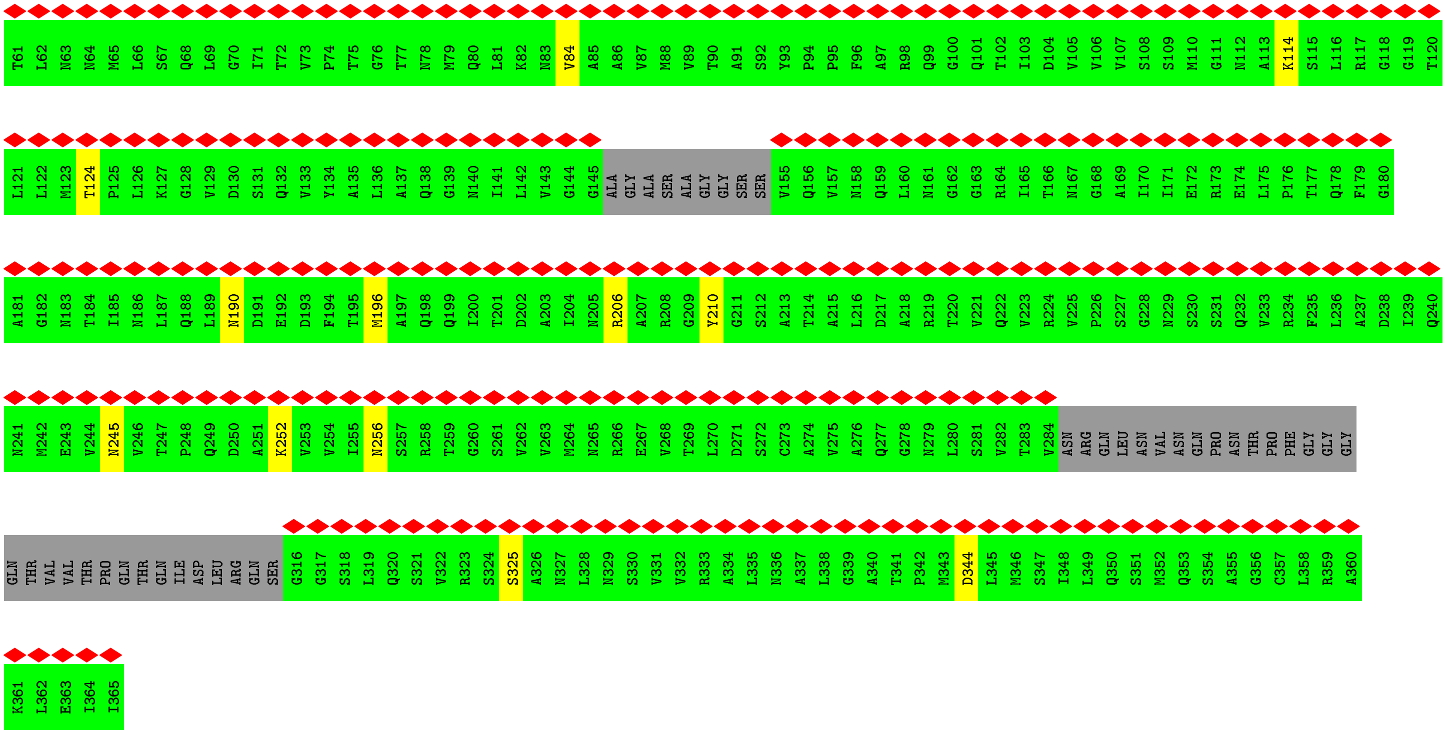
Chain o3:



- Molecule 11: Flagellar P-ring protein

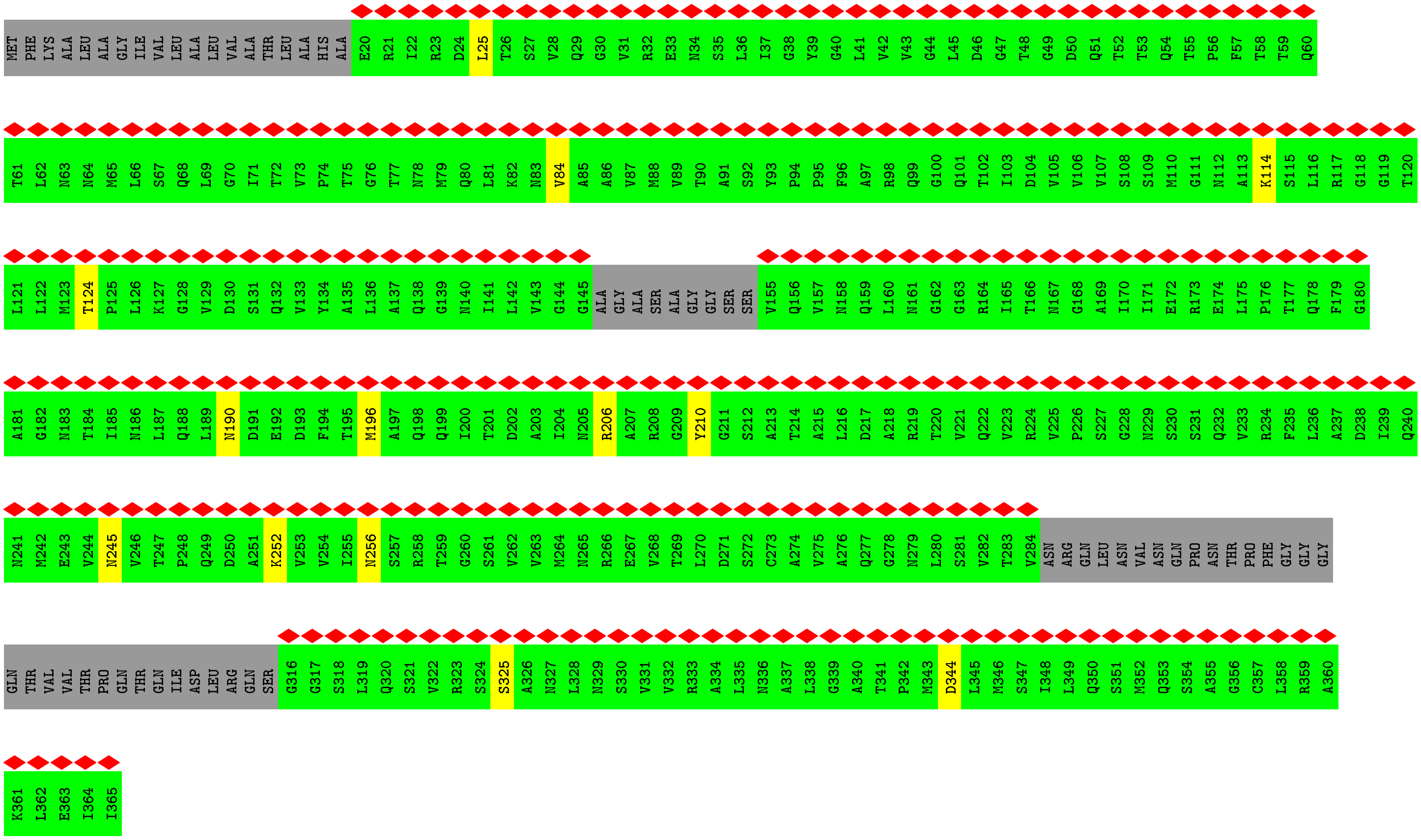
Chain p3:





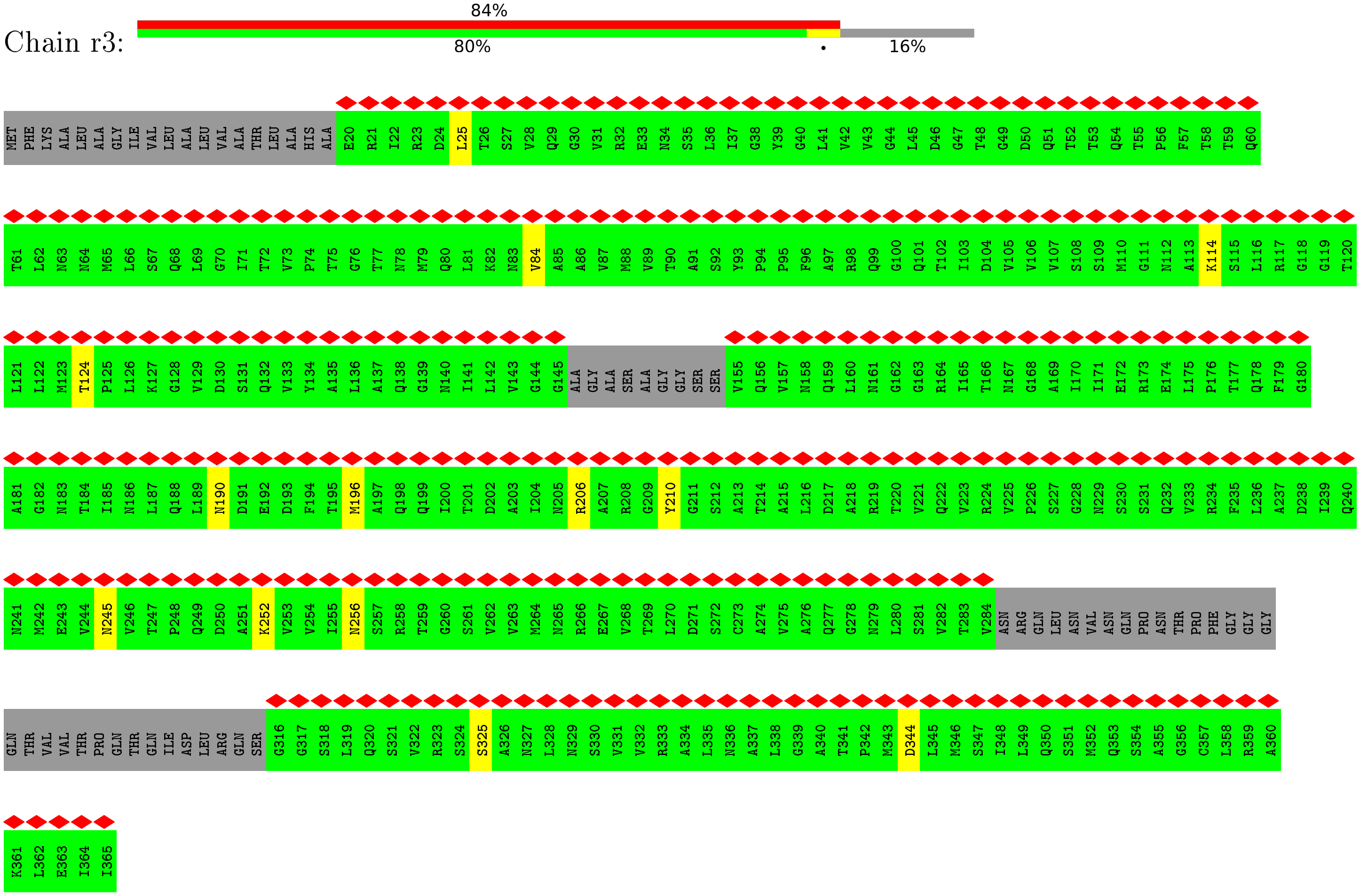
- Molecule 11: Flagellar P-ring protein

Chain q3:



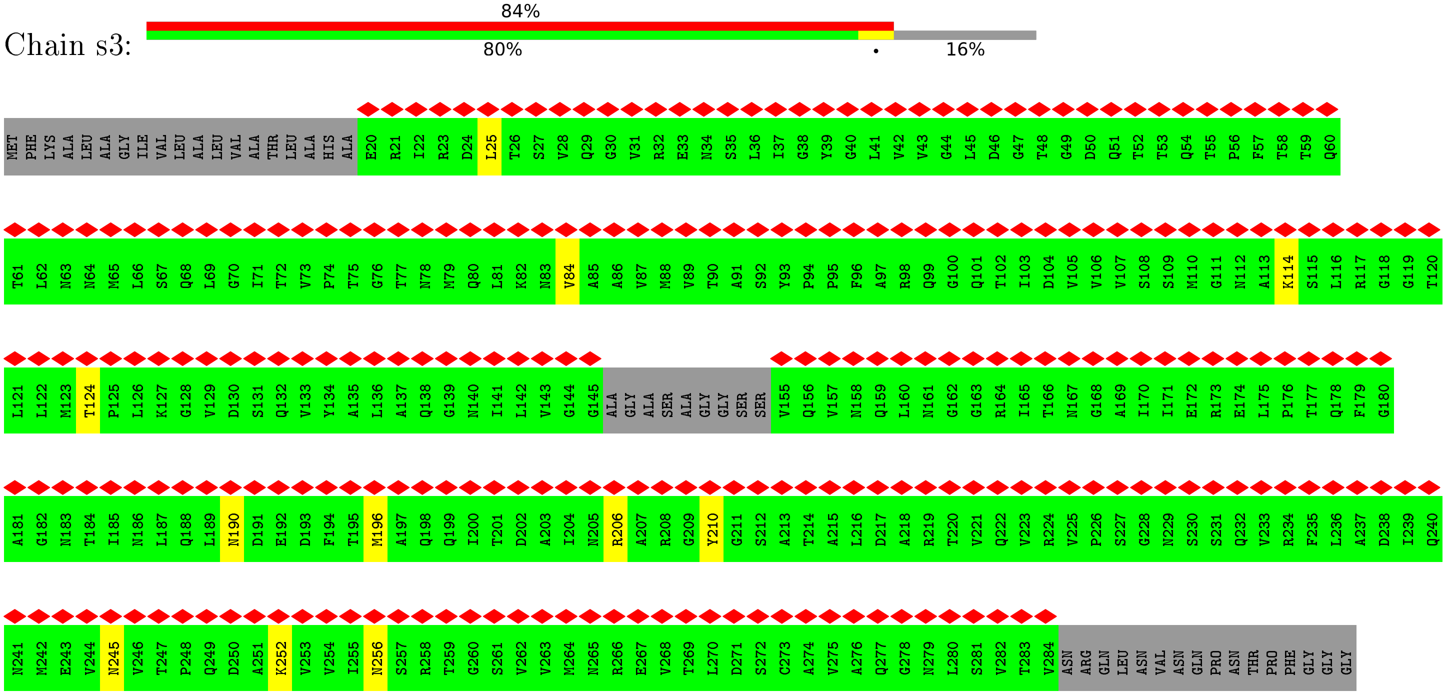
- Molecule 11: Flagellar P-ring protein

Chain r3:



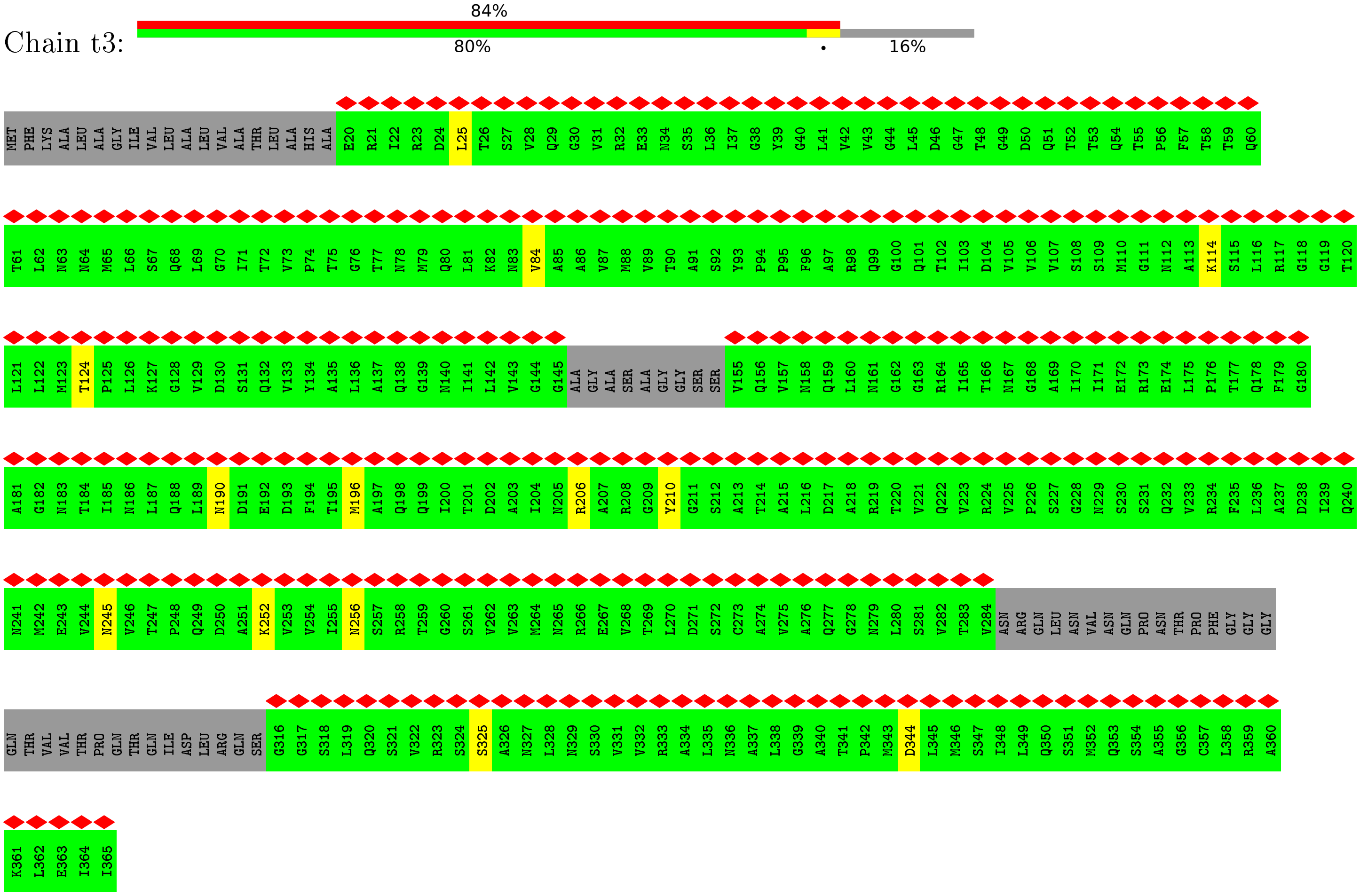
- Molecule 11: Flagellar P-ring protein

Chain s3:



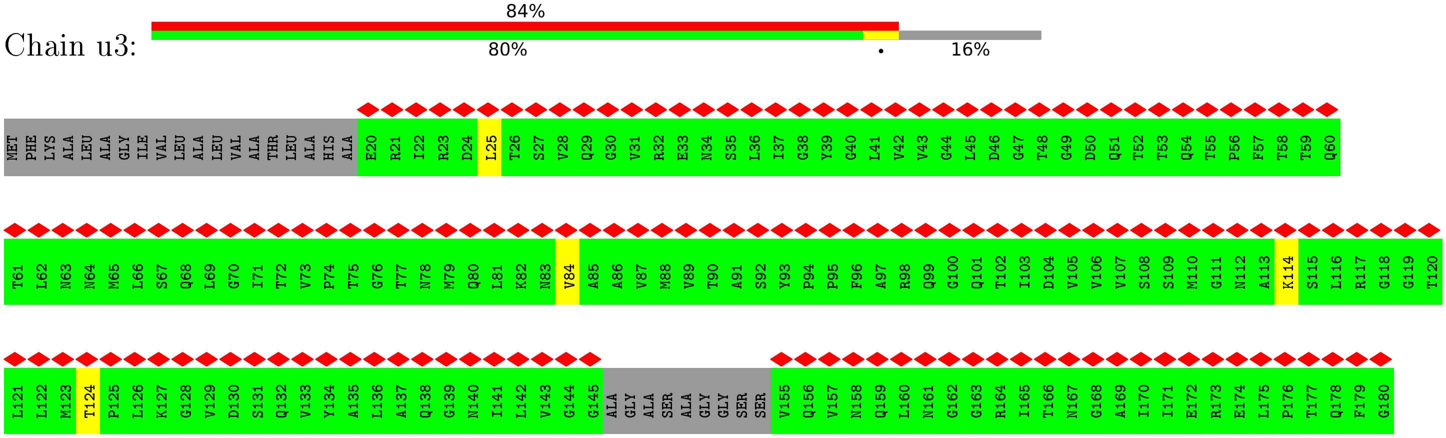
- Molecule 11: Flagellar P-ring protein

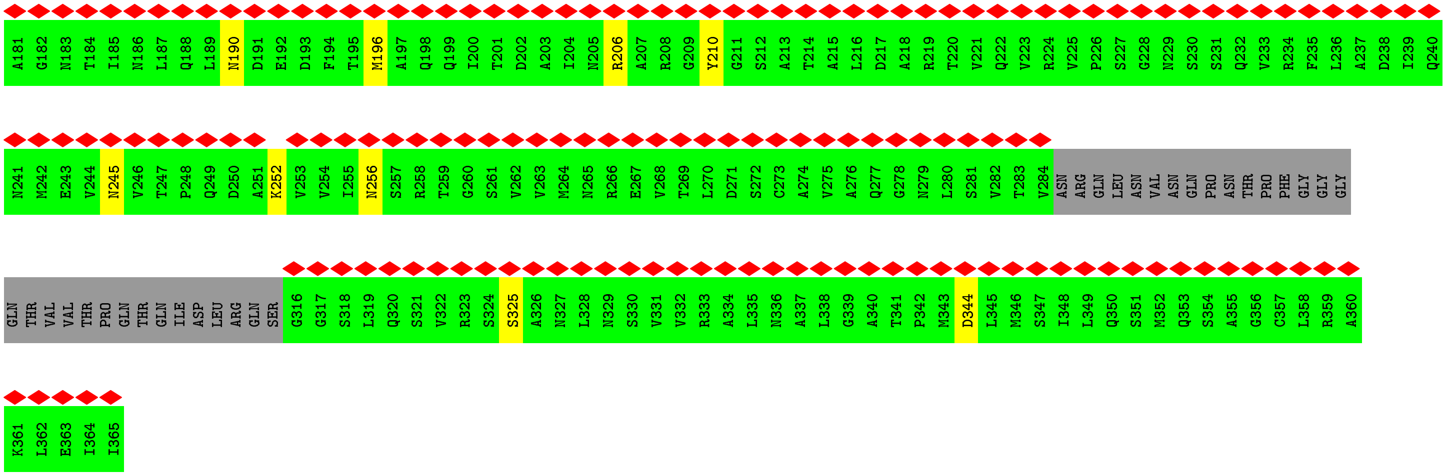
Chain t3:



- Molecule 11: Flagellar P-ring protein

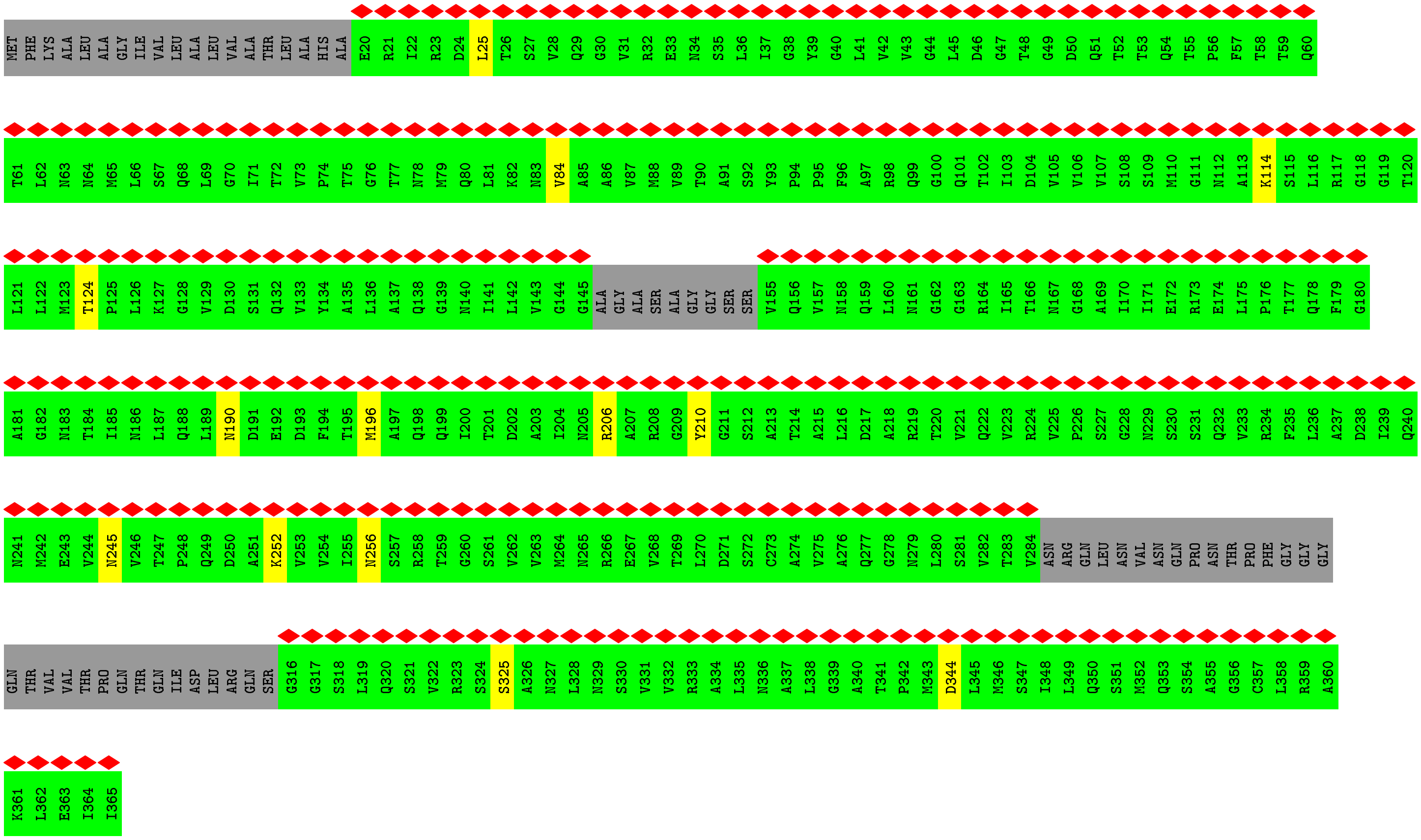
Chain u3:





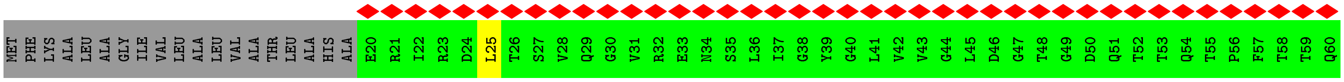
- Molecule 11: Flagellar P-ring protein

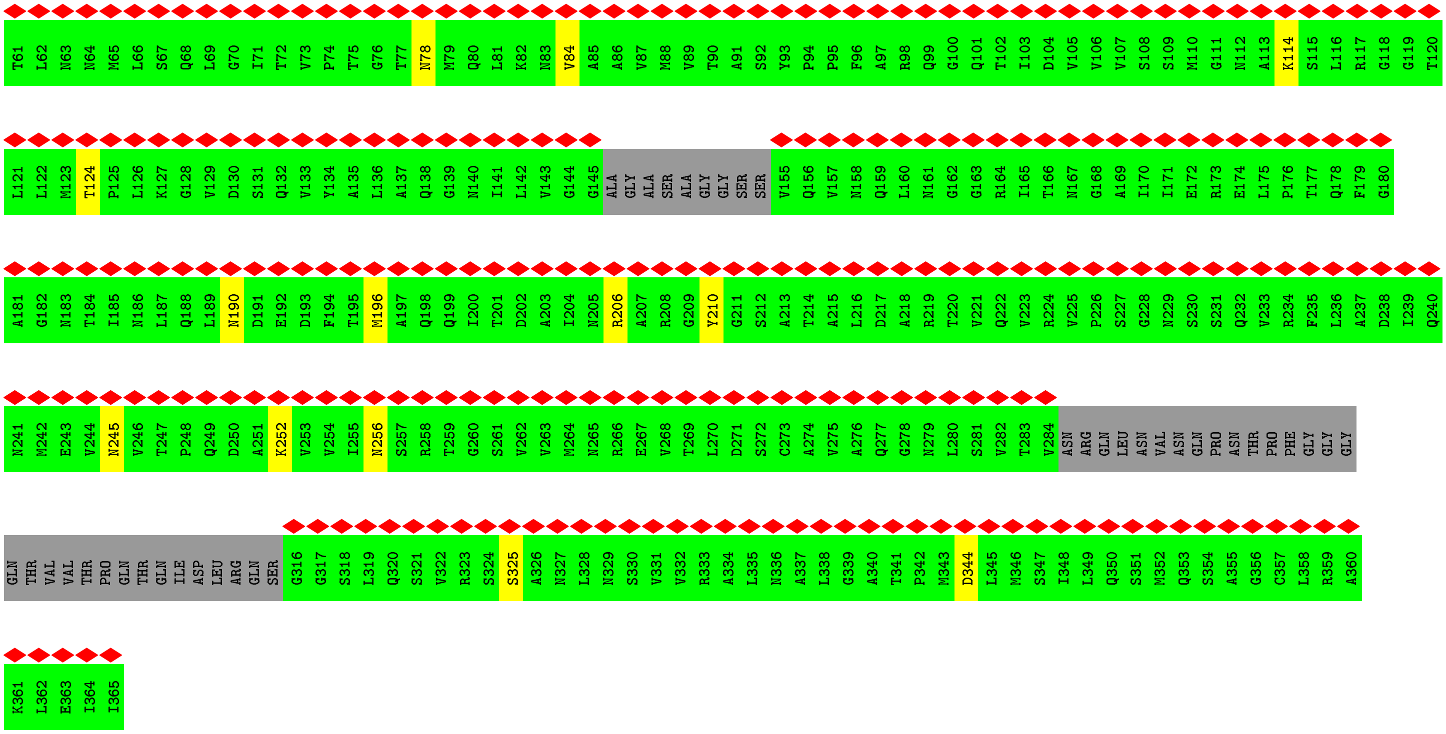
Chain v3:



- Molecule 11: Flagellar P-ring protein

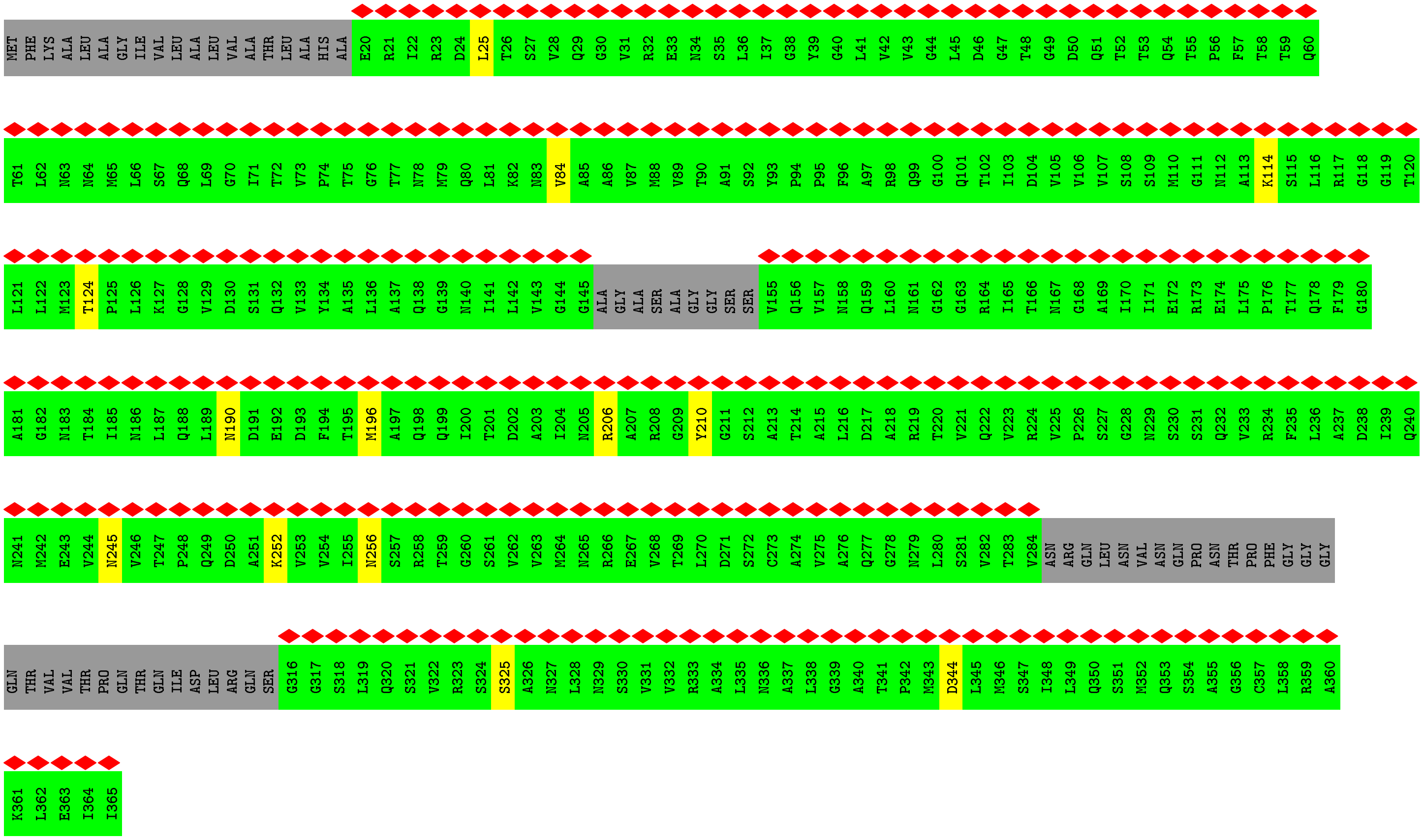
Chain w3:





- Molecule 11: Flagellar P-ring protein

Chain x3:

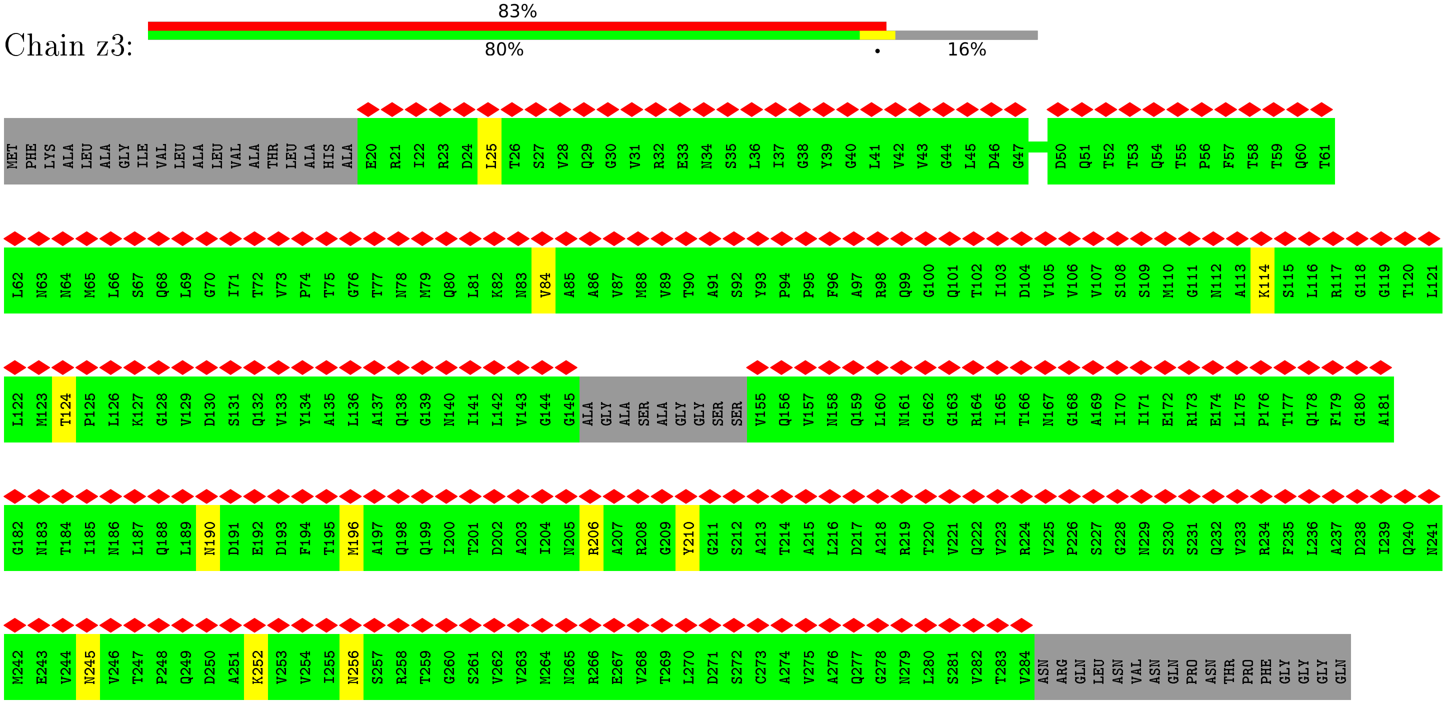


- Molecule 11: Flagellar P-ring protein

Chain y3:

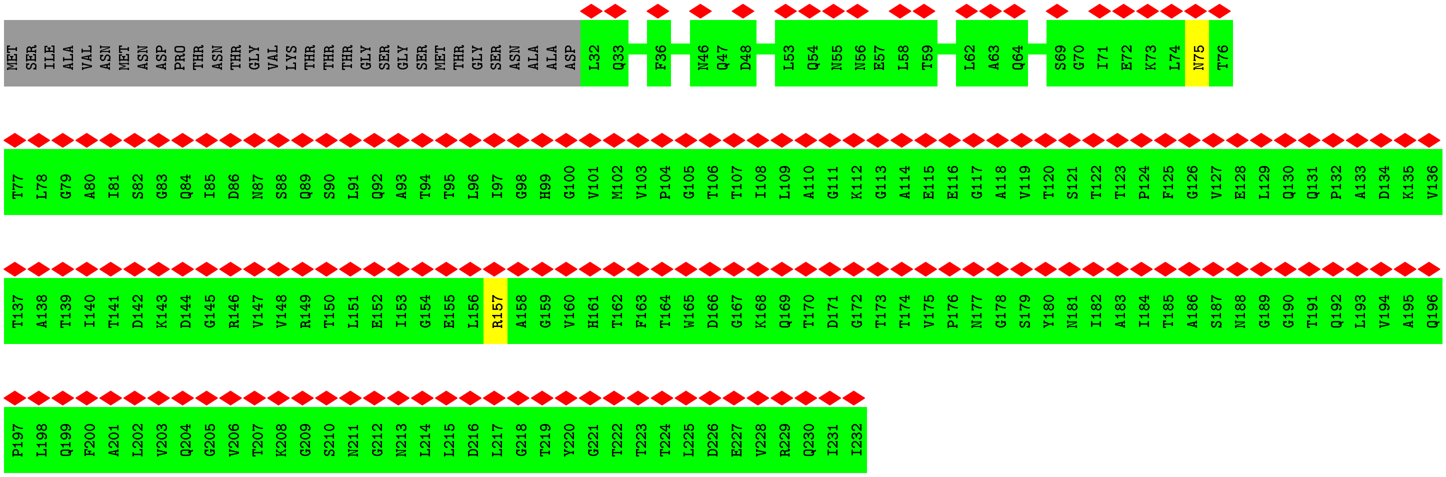
- Molecule 11: Flagellar P-ring protein

Chain z3:



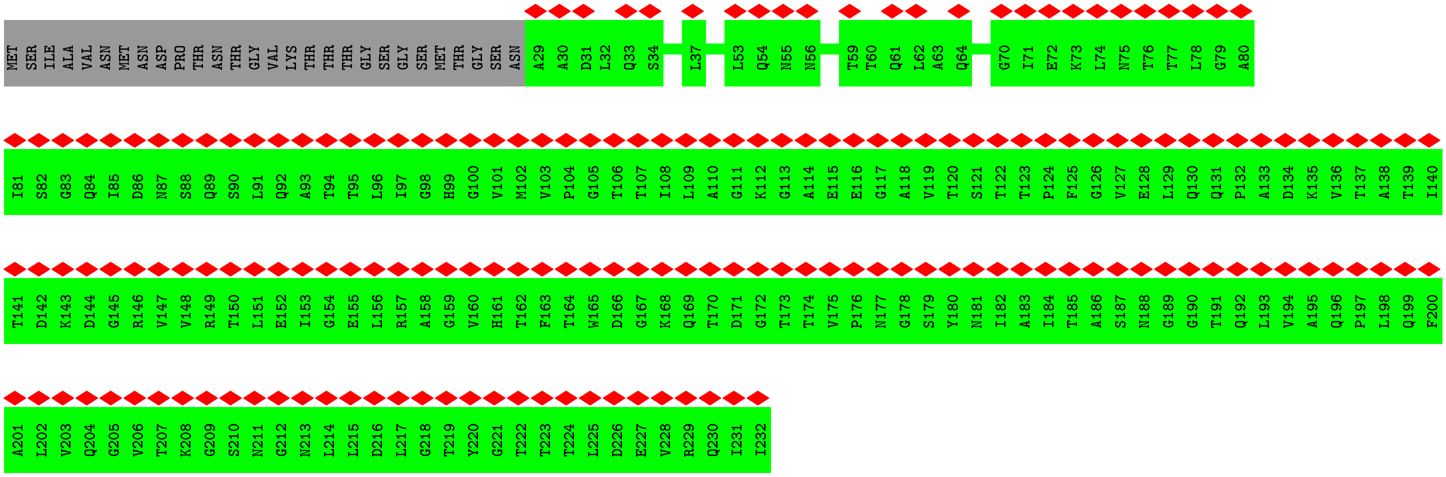
- Molecule 12: Basal-body rod modification protein FlgD

Chain A4:



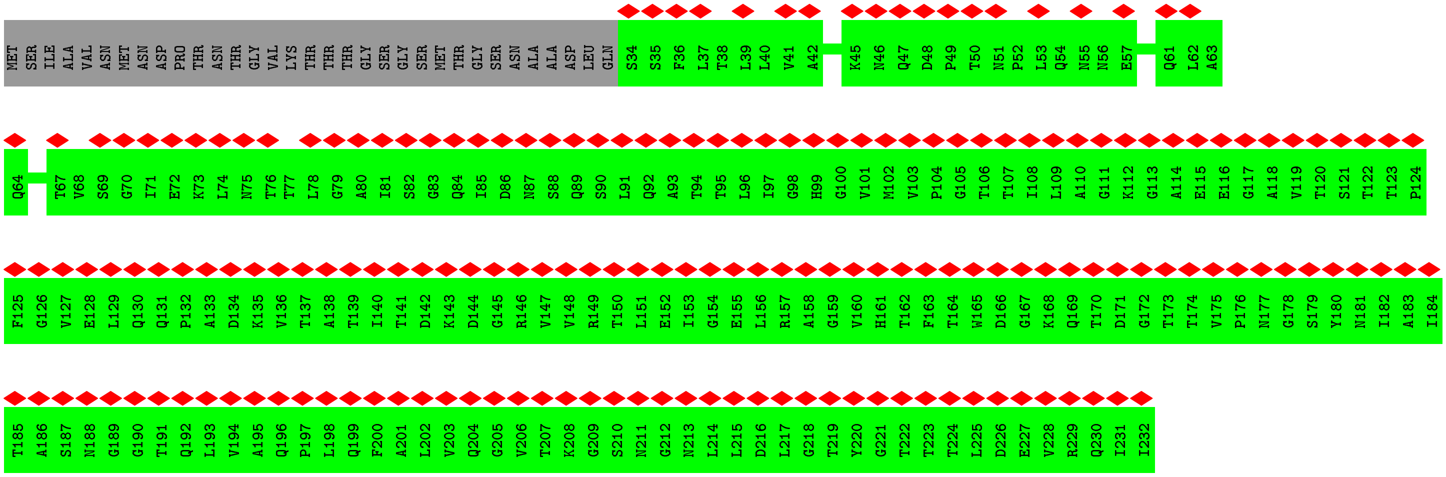
- Molecule 12: Basal-body rod modification protein FlgD

Chain B4:



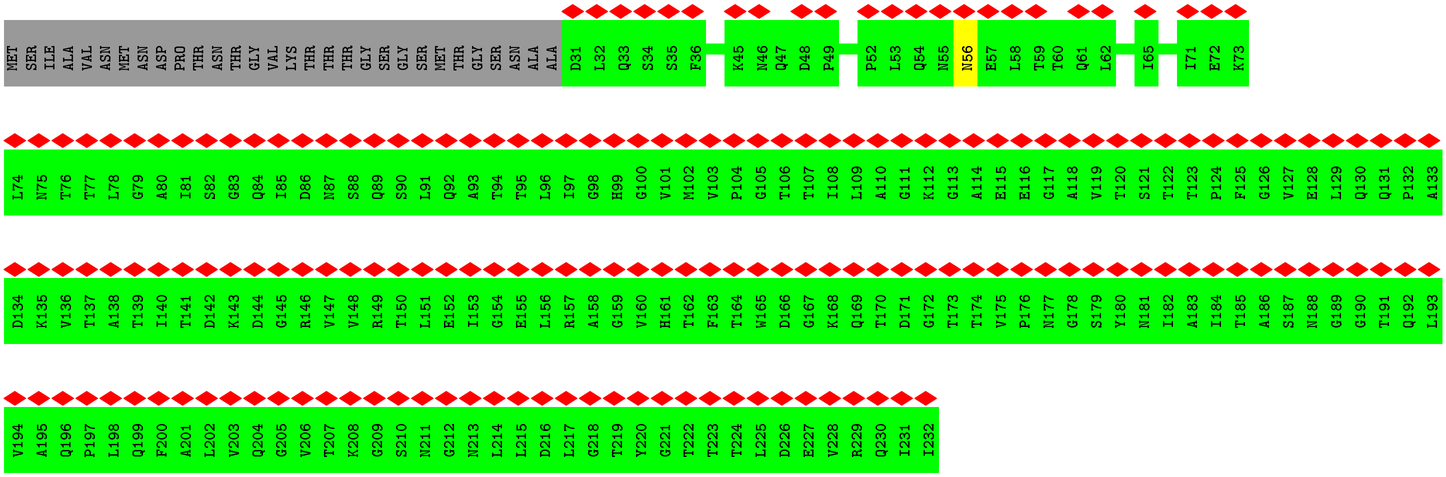
- Molecule 12: Basal-body rod modification protein FlgD

Chain C4:



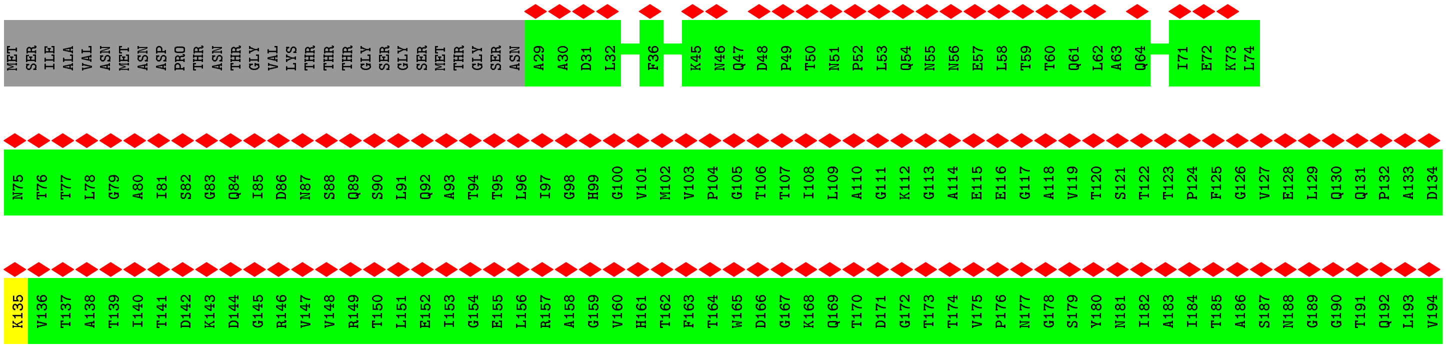
- Molecule 12: Basal-body rod modification protein FlgD

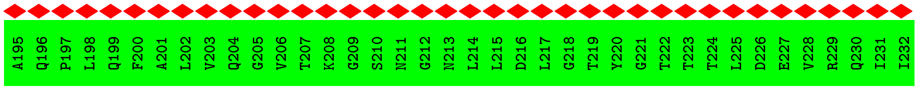
Chain D4:



- Molecule 12: Basal-body rod modification protein FlgD

Chain E4:




A195
Q196
P197
L198
Q199
F200
A201
L202
V203
Q204
G205
V206
T207
K208
G209
S210
N211
G212
N213
L214
L215
D216
L217
G218
T219
Y220
G221
T222
T223
T224
L225
D226
E227
V228
R229
Q230
I231
I232

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60497	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.010	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0075	Depositor
Map size (Å)	638.976, 638.976, 638.976	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A1	0.39	0/1205	0.52	0/1624
1	B1	0.38	0/1955	0.55	0/2645
1	C1	0.39	0/1955	0.54	1/2645 (0.0%)
1	D1	0.40	0/1205	0.53	0/1624
1	E1	0.38	0/1955	0.55	1/2645 (0.0%)
1	F1	0.39	0/1205	0.57	1/1624 (0.1%)
1	G1	0.37	0/1955	0.54	0/2645
1	H1	0.38	0/1955	0.56	0/2645
1	I1	0.37	0/1955	0.53	0/2645
1	J1	0.42	0/1205	0.53	1/1624 (0.1%)
1	K1	0.36	0/1955	0.52	0/2645
1	L1	0.36	0/1955	0.54	0/2645
1	M1	0.40	0/1205	0.55	1/1624 (0.1%)
1	N1	0.36	0/1955	0.55	0/2645
1	O1	0.35	0/1955	0.53	1/2645 (0.0%)
1	P1	0.37	0/1205	0.52	1/1624 (0.1%)
1	Q1	0.35	0/1955	0.52	0/2645
1	R1	0.35	0/1955	0.51	1/2645 (0.0%)
1	S1	0.38	0/1205	0.50	1/1624 (0.1%)
1	T1	0.35	0/1955	0.52	0/2645
1	U1	0.36	0/1955	0.56	0/2645
1	V1	0.38	0/1205	0.52	0/1624
1	W1	0.35	0/1955	0.52	1/2645 (0.0%)
1	X1	0.35	0/1955	0.52	1/2645 (0.0%)
1	Y1	0.34	0/1955	0.53	0/2645
1	Z1	0.41	0/1205	0.54	0/1624
1	a1	0.36	0/1955	0.53	0/2645
1	b1	0.39	0/1205	0.51	0/1624
1	c1	0.37	0/1955	0.53	1/2645 (0.0%)
1	d1	0.37	0/1955	0.54	0/2645
1	e1	0.39	0/1205	0.52	1/1624 (0.1%)
1	f1	0.37	0/1955	0.53	0/2645
1	g1	0.37	0/1955	0.54	1/2645 (0.0%)
1	h1	0.37	0/1955	0.51	0/2645

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	A2	0.39	0/1662	0.62	1/2263 (0.0%)
2	B2	0.41	0/1662	0.61	0/2263
2	C2	0.40	0/1662	0.61	0/2263
2	D2	0.43	1/1662 (0.1%)	0.58	0/2263
2	E2	0.61	1/1662 (0.1%)	0.71	1/2263 (0.0%)
3	F2	0.35	0/2035	0.58	0/2777
4	G2	0.34	0/681	0.61	0/930
4	H2	0.34	0/681	0.55	0/930
4	I2	0.37	0/681	0.53	0/930
4	J2	2.82	6/681 (0.9%)	0.65	0/930
5	K2	0.35	0/296	0.60	1/395 (0.3%)
5	L2	0.33	0/567	0.44	0/761
5	M2	0.36	0/567	0.45	0/761
5	N2	0.36	0/567	0.46	0/761
5	O2	0.34	0/567	0.47	0/761
5	P2	0.36	0/567	0.47	0/761
6	Q2	0.39	0/1035	0.52	0/1399
6	R2	0.37	0/941	0.53	0/1269
6	S2	0.40	0/951	0.51	0/1281
6	T2	0.40	0/842	0.53	0/1132
6	U2	0.37	0/934	0.50	0/1259
7	V2	0.44	0/981	0.65	0/1334
7	W2	0.44	0/976	0.57	0/1327
7	X2	0.48	0/976	0.56	0/1327
7	Y2	0.46	0/976	0.56	0/1327
7	Z2	0.46	0/976	0.55	0/1327
7	a2	0.42	0/976	0.57	0/1327
8	b2	0.39	0/1836	0.59	0/2502
8	c2	0.42	0/1836	0.59	0/2502
8	d2	0.44	0/1836	0.58	0/2502
8	e2	0.43	0/1836	0.56	0/2502
8	f2	0.40	0/1836	0.56	0/2502
9	12	0.38	0/1973	0.55	0/2682
9	22	0.37	0/1973	0.54	0/2682
9	32	0.36	0/1971	0.55	1/2677 (0.0%)
9	42	0.31	0/1973	0.56	1/2682 (0.0%)
9	g2	0.41	0/1973	0.52	0/2682
9	h2	0.43	0/1973	0.51	0/2682
9	i2	0.43	0/1973	0.53	0/2682
9	j2	0.44	0/1973	0.52	0/2682
9	k2	0.43	0/1973	0.54	0/2682
9	l2	0.43	0/1894	0.51	0/2573
9	m2	0.46	0/1894	0.54	0/2573

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	n2	0.43	0/1894	0.51	0/2573
9	o2	0.44	0/1894	0.53	0/2573
9	p2	0.44	0/1894	0.52	0/2573
9	q2	0.43	0/1907	0.52	0/2590
9	r2	0.42	0/1973	0.56	0/2682
9	s2	0.43	0/1973	0.56	0/2682
9	t2	0.42	0/1973	0.58	2/2682 (0.1%)
9	u2	0.42	0/1973	0.56	0/2682
9	v2	0.43	0/1973	0.54	0/2682
9	w2	0.42	0/1973	0.57	1/2682 (0.0%)
9	x2	0.39	0/1973	0.54	0/2682
9	y2	0.36	0/1973	0.53	0/2682
9	z2	0.35	0/1973	0.54	2/2682 (0.1%)
10	A3	0.26	0/1614	0.52	1/2194 (0.0%)
10	B3	0.27	0/1614	0.52	1/2194 (0.0%)
10	C3	0.26	0/1614	0.52	1/2194 (0.0%)
10	D3	0.26	0/1614	0.52	1/2194 (0.0%)
10	E3	0.26	0/1614	0.52	1/2194 (0.0%)
10	F3	0.26	0/1614	0.52	1/2194 (0.0%)
10	G3	0.26	0/1614	0.52	1/2194 (0.0%)
10	H3	0.26	0/1614	0.52	1/2194 (0.0%)
10	I3	0.26	0/1614	0.52	1/2194 (0.0%)
10	J3	0.26	0/1614	0.52	1/2194 (0.0%)
10	K3	0.26	0/1614	0.52	1/2194 (0.0%)
10	L3	0.26	0/1614	0.52	1/2194 (0.0%)
10	M3	0.26	0/1614	0.52	1/2194 (0.0%)
10	N3	0.26	0/1614	0.52	1/2194 (0.0%)
10	O3	0.26	0/1614	0.52	1/2194 (0.0%)
10	P3	0.26	0/1614	0.52	1/2194 (0.0%)
10	Q3	0.26	0/1614	0.52	1/2194 (0.0%)
10	R3	0.26	0/1614	0.52	1/2194 (0.0%)
10	S3	0.27	0/1614	0.52	1/2194 (0.0%)
10	T3	0.26	0/1614	0.52	1/2194 (0.0%)
10	U3	0.26	0/1614	0.52	1/2194 (0.0%)
10	V3	0.26	0/1614	0.52	1/2194 (0.0%)
10	W3	0.26	0/1611	0.52	1/2188 (0.0%)
10	X3	0.26	0/1614	0.52	1/2194 (0.0%)
10	Y3	0.26	0/1614	0.52	1/2194 (0.0%)
10	Z3	0.26	0/1614	0.52	1/2194 (0.0%)
11	a3	0.24	0/2267	0.50	0/3073
11	b3	0.24	0/2267	0.50	0/3073
11	c3	0.24	0/2267	0.50	0/3073
11	d3	0.24	0/2267	0.50	0/3073

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	e3	0.24	0/2267	0.50	0/3073
11	f3	0.24	0/2267	0.50	0/3073
11	g3	0.24	0/2267	0.50	0/3073
11	h3	0.24	0/2266	0.50	0/3071
11	i3	0.24	0/2267	0.50	0/3073
11	j3	0.24	0/2267	0.50	0/3073
11	k3	0.24	0/2267	0.50	0/3073
11	l3	0.24	0/2267	0.50	0/3073
11	m3	0.24	0/2267	0.50	0/3073
11	n3	0.24	0/2267	0.50	0/3073
11	o3	0.24	0/2267	0.50	0/3073
11	p3	0.24	0/2267	0.50	0/3073
11	q3	0.24	0/2267	0.50	0/3073
11	r3	0.24	0/2264	0.50	0/3066
11	s3	0.24	0/2267	0.50	0/3073
11	t3	0.24	0/2267	0.50	0/3073
11	u3	0.24	0/2267	0.50	0/3073
11	v3	0.24	0/2267	0.50	0/3073
11	w3	0.24	0/2267	0.50	0/3073
11	x3	0.24	0/2267	0.50	0/3073
11	y3	0.24	0/2267	0.50	0/3073
11	z3	0.24	0/2267	0.50	0/3073
12	A4	0.25	0/1491	0.47	0/2033
12	B4	0.25	0/1509	0.48	0/2058
12	C4	0.25	0/1474	0.48	0/2010
12	D4	0.25	0/1496	0.49	0/2040
12	E4	0.25	0/1509	0.48	0/2058
All	All	0.37	8/249431 (0.0%)	0.53	50/338382 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B1	0	1
1	E1	0	1
1	G1	0	1
1	H1	0	1
1	L1	0	1
1	N1	0	1
2	B2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	C2	0	2
2	D2	0	2
2	E2	0	1
3	F2	0	2
4	G2	0	1
4	H2	0	1
4	I2	0	1
4	J2	0	1
6	U2	0	1
8	b2	0	2
8	c2	0	2
8	d2	0	1
8	e2	0	3
8	f2	0	3
All	All	0	31

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J2	51	PHE	CE2-CZ	34.87	2.03	1.37
4	J2	51	PHE	CE1-CZ	33.72	2.01	1.37
4	J2	51	PHE	CD1-CE1	32.60	2.04	1.39
4	J2	51	PHE	CD2-CE2	31.33	2.02	1.39
4	J2	51	PHE	CG-CD1	21.84	1.71	1.38
4	J2	51	PHE	CG-CD2	21.32	1.70	1.38
2	E2	205	MET	SD-CE	19.73	2.88	1.77
2	D2	187	PHE	CB-CG	-5.18	1.42	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E2	205	MET	CG-SD-CE	20.16	132.46	100.20
9	t2	167	PRO	CA-N-CD	-8.46	99.66	111.50
1	E1	282	TYR	C-N-CA	-6.66	105.04	121.70
1	g1	282	TYR	C-N-CA	-6.65	105.07	121.70
10	Z3	43	PRO	CA-N-CD	-6.36	102.59	111.50
10	N3	43	PRO	CA-N-CD	-6.36	102.59	111.50
1	M1	282	TYR	C-N-CA	-6.36	105.80	121.70
10	M3	43	PRO	CA-N-CD	-6.36	102.60	111.50
10	A3	43	PRO	CA-N-CD	-6.35	102.61	111.50
10	J3	43	PRO	CA-N-CD	-6.34	102.62	111.50
10	Y3	43	PRO	CA-N-CD	-6.34	102.62	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	W3	43	PRO	CA-N-CD	-6.34	102.63	111.50
10	V3	43	PRO	CA-N-CD	-6.34	102.63	111.50
10	B3	43	PRO	CA-N-CD	-6.33	102.63	111.50
10	Q3	43	PRO	CA-N-CD	-6.33	102.63	111.50
10	D3	43	PRO	CA-N-CD	-6.33	102.64	111.50
10	H3	43	PRO	CA-N-CD	-6.33	102.64	111.50
10	I3	43	PRO	CA-N-CD	-6.32	102.65	111.50
10	R3	43	PRO	CA-N-CD	-6.32	102.65	111.50
10	F3	43	PRO	CA-N-CD	-6.32	102.65	111.50
10	S3	43	PRO	CA-N-CD	-6.32	102.66	111.50
10	G3	43	PRO	CA-N-CD	-6.31	102.67	111.50
10	T3	43	PRO	CA-N-CD	-6.31	102.67	111.50
10	C3	43	PRO	CA-N-CD	-6.30	102.67	111.50
10	L3	43	PRO	CA-N-CD	-6.30	102.69	111.50
10	K3	43	PRO	CA-N-CD	-6.29	102.69	111.50
10	U3	43	PRO	CA-N-CD	-6.29	102.69	111.50
10	O3	43	PRO	CA-N-CD	-6.29	102.69	111.50
10	P3	43	PRO	CA-N-CD	-6.29	102.70	111.50
10	X3	43	PRO	CA-N-CD	-6.29	102.70	111.50
10	E3	43	PRO	CA-N-CD	-6.28	102.70	111.50
2	A2	224	MET	CB-CG-SD	-6.22	93.75	112.40
9	t2	45	LEU	CB-CG-CD2	-6.03	100.74	111.00
1	R1	282	TYR	C-N-CA	-5.98	106.75	121.70
1	F1	282	TYR	C-N-CA	-5.90	106.94	121.70
1	X1	282	TYR	C-N-CA	-5.89	106.97	121.70
9	32	45	LEU	CA-CB-CG	5.80	128.63	115.30
1	O1	282	TYR	C-N-CA	-5.76	107.30	121.70
1	e1	282	TYR	C-N-CA	-5.75	107.34	121.70
9	42	253	MET	CG-SD-CE	-5.73	91.03	100.20
5	K2	75	MET	CA-CB-CG	5.60	122.82	113.30
1	S1	282	TYR	C-N-CA	-5.39	108.21	121.70
1	J1	282	TYR	C-N-CA	-5.34	108.35	121.70
1	W1	282	TYR	C-N-CA	-5.32	108.41	121.70
9	w2	45	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	c1	282	TYR	C-N-CA	-5.13	108.88	121.70
9	z2	107	LEU	CA-CB-CG	5.12	127.07	115.30
9	z2	62	LEU	CA-CB-CG	5.06	126.94	115.30
1	P1	282	TYR	C-N-CA	-5.04	109.10	121.70
1	C1	160	PRO	C-N-CA	5.03	134.28	121.70

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B1	163	SER	Peptide
2	B2	40	LEU	Peptide
2	B2	41	SER	Peptide
2	C2	40	LEU	Peptide
2	C2	41	SER	Peptide
2	D2	40	LEU	Peptide
2	D2	41	SER	Peptide
1	E1	162	PRO	Peptide
2	E2	38	TRP	Peptide
3	F2	113	PHE	Peptide
3	F2	140	PHE	Peptide
1	G1	165	PHE	Peptide
4	G2	41	ALA	Peptide
1	H1	165	PHE	Peptide
4	H2	41	ALA	Peptide
4	I2	41	ALA	Peptide
4	J2	41	ALA	Peptide
1	L1	125	GLN	Peptide
1	N1	165	PHE	Peptide
6	U2	95	LEU	Peptide
8	b2	116	GLN	Peptide
8	b2	117	GLY	Peptide
8	c2	115	ILE	Peptide
8	c2	117	GLY	Peptide
8	d2	117	GLY	Peptide
8	e2	114	THR	Peptide
8	e2	115	ILE	Peptide
8	e2	117	GLY	Peptide
8	f2	114	THR	Peptide
8	f2	117	GLY	Peptide
8	f2	70	GLN	Peptide

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	A1	145/560 (26%)	143 (99%)	2 (1%)	0	100	100
1	B1	242/560 (43%)	227 (94%)	15 (6%)	0	100	100
1	C1	242/560 (43%)	230 (95%)	11 (4%)	1 (0%)	34	69
1	D1	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	E1	242/560 (43%)	226 (93%)	16 (7%)	0	100	100
1	F1	145/560 (26%)	141 (97%)	4 (3%)	0	100	100
1	G1	242/560 (43%)	225 (93%)	16 (7%)	1 (0%)	34	69
1	H1	242/560 (43%)	221 (91%)	19 (8%)	2 (1%)	19	56
1	I1	242/560 (43%)	229 (95%)	12 (5%)	1 (0%)	34	69
1	J1	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	K1	242/560 (43%)	230 (95%)	11 (4%)	1 (0%)	34	69
1	L1	242/560 (43%)	224 (93%)	18 (7%)	0	100	100
1	M1	145/560 (26%)	141 (97%)	4 (3%)	0	100	100
1	N1	242/560 (43%)	223 (92%)	19 (8%)	0	100	100
1	O1	242/560 (43%)	231 (96%)	10 (4%)	1 (0%)	34	69
1	P1	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	Q1	242/560 (43%)	224 (93%)	17 (7%)	1 (0%)	34	69
1	R1	242/560 (43%)	229 (95%)	13 (5%)	0	100	100
1	S1	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	T1	242/560 (43%)	230 (95%)	12 (5%)	0	100	100
1	U1	242/560 (43%)	231 (96%)	11 (4%)	0	100	100
1	V1	145/560 (26%)	141 (97%)	4 (3%)	0	100	100
1	W1	242/560 (43%)	227 (94%)	14 (6%)	1 (0%)	34	69
1	X1	242/560 (43%)	225 (93%)	17 (7%)	0	100	100
1	Y1	242/560 (43%)	228 (94%)	14 (6%)	0	100	100
1	Z1	145/560 (26%)	142 (98%)	3 (2%)	0	100	100
1	a1	242/560 (43%)	227 (94%)	14 (6%)	1 (0%)	34	69
1	b1	145/560 (26%)	140 (97%)	5 (3%)	0	100	100
1	c1	242/560 (43%)	225 (93%)	16 (7%)	1 (0%)	34	69
1	d1	242/560 (43%)	225 (93%)	16 (7%)	1 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e1	145/560 (26%)	144 (99%)	1 (1%)	0	100	100
1	f1	242/560 (43%)	229 (95%)	12 (5%)	1 (0%)	34	69
1	g1	242/560 (43%)	226 (93%)	15 (6%)	1 (0%)	34	69
1	h1	242/560 (43%)	232 (96%)	10 (4%)	0	100	100
2	A2	207/245 (84%)	182 (88%)	23 (11%)	2 (1%)	15	51
2	B2	207/245 (84%)	183 (88%)	22 (11%)	2 (1%)	15	51
2	C2	207/245 (84%)	177 (86%)	29 (14%)	1 (0%)	29	66
2	D2	207/245 (84%)	181 (87%)	25 (12%)	1 (0%)	29	66
2	E2	207/245 (84%)	183 (88%)	22 (11%)	2 (1%)	15	51
3	F2	254/264 (96%)	223 (88%)	30 (12%)	1 (0%)	34	69
4	G2	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
4	H2	87/89 (98%)	77 (88%)	10 (12%)	0	100	100
4	I2	87/89 (98%)	78 (90%)	9 (10%)	0	100	100
4	J2	87/89 (98%)	77 (88%)	10 (12%)	0	100	100
5	K2	37/104 (36%)	37 (100%)	0	0	100	100
5	L2	73/104 (70%)	68 (93%)	5 (7%)	0	100	100
5	M2	73/104 (70%)	68 (93%)	5 (7%)	0	100	100
5	N2	73/104 (70%)	69 (94%)	4 (6%)	0	100	100
5	O2	73/104 (70%)	69 (94%)	4 (6%)	0	100	100
5	P2	73/104 (70%)	68 (93%)	5 (7%)	0	100	100
6	Q2	131/138 (95%)	115 (88%)	16 (12%)	0	100	100
6	R2	114/138 (83%)	98 (86%)	16 (14%)	0	100	100
6	S2	116/138 (84%)	104 (90%)	12 (10%)	0	100	100
6	T2	102/138 (74%)	95 (93%)	7 (7%)	0	100	100
6	U2	113/138 (82%)	102 (90%)	11 (10%)	0	100	100
7	V2	131/134 (98%)	112 (86%)	18 (14%)	1 (1%)	19	56
7	W2	130/134 (97%)	108 (83%)	22 (17%)	0	100	100
7	X2	130/134 (97%)	107 (82%)	22 (17%)	1 (1%)	19	56
7	Y2	130/134 (97%)	109 (84%)	21 (16%)	0	100	100
7	Z2	130/134 (97%)	113 (87%)	17 (13%)	0	100	100
7	a2	130/134 (97%)	109 (84%)	21 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	b2	247/251 (98%)	217 (88%)	29 (12%)	1 (0%)	34	69
8	c2	247/251 (98%)	212 (86%)	35 (14%)	0	100	100
8	d2	247/251 (98%)	215 (87%)	32 (13%)	0	100	100
8	e2	247/251 (98%)	212 (86%)	35 (14%)	0	100	100
8	f2	247/251 (98%)	210 (85%)	37 (15%)	0	100	100
9	12	258/260 (99%)	231 (90%)	27 (10%)	0	100	100
9	22	258/260 (99%)	231 (90%)	27 (10%)	0	100	100
9	32	256/260 (98%)	230 (90%)	26 (10%)	0	100	100
9	42	258/260 (99%)	239 (93%)	19 (7%)	0	100	100
9	g2	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
9	h2	258/260 (99%)	239 (93%)	19 (7%)	0	100	100
9	i2	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
9	j2	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
9	k2	258/260 (99%)	242 (94%)	16 (6%)	0	100	100
9	l2	245/260 (94%)	229 (94%)	16 (6%)	0	100	100
9	m2	245/260 (94%)	230 (94%)	15 (6%)	0	100	100
9	n2	245/260 (94%)	232 (95%)	13 (5%)	0	100	100
9	o2	245/260 (94%)	230 (94%)	15 (6%)	0	100	100
9	p2	245/260 (94%)	232 (95%)	13 (5%)	0	100	100
9	q2	247/260 (95%)	233 (94%)	14 (6%)	0	100	100
9	r2	258/260 (99%)	233 (90%)	25 (10%)	0	100	100
9	s2	258/260 (99%)	230 (89%)	28 (11%)	0	100	100
9	t2	258/260 (99%)	236 (92%)	22 (8%)	0	100	100
9	u2	258/260 (99%)	234 (91%)	24 (9%)	0	100	100
9	v2	258/260 (99%)	233 (90%)	25 (10%)	0	100	100
9	w2	258/260 (99%)	232 (90%)	26 (10%)	0	100	100
9	x2	258/260 (99%)	236 (92%)	22 (8%)	0	100	100
9	y2	258/260 (99%)	238 (92%)	20 (8%)	0	100	100
9	z2	258/260 (99%)	240 (93%)	18 (7%)	0	100	100
10	A3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	B3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	C3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	D3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	E3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	F3	209/232 (90%)	192 (92%)	17 (8%)	0	100	100
10	G3	209/232 (90%)	192 (92%)	17 (8%)	0	100	100
10	H3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	I3	209/232 (90%)	192 (92%)	17 (8%)	0	100	100
10	J3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	K3	209/232 (90%)	192 (92%)	17 (8%)	0	100	100
10	L3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	M3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	N3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	O3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	P3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	Q3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	R3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	S3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	T3	209/232 (90%)	192 (92%)	17 (8%)	0	100	100
10	U3	209/232 (90%)	192 (92%)	17 (8%)	0	100	100
10	V3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	W3	208/232 (90%)	192 (92%)	16 (8%)	0	100	100
10	X3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	Y3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
10	Z3	209/232 (90%)	193 (92%)	16 (8%)	0	100	100
11	a3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	b3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	c3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	d3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	e3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	f3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	g3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	h3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	i3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	j3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	k3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	l3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	m3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	n3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	o3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	p3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	q3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	r3	299/365 (82%)	288 (96%)	11 (4%)	0	100	100
11	s3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	t3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	u3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	v3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	w3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	x3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	y3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
11	z3	300/365 (82%)	288 (96%)	12 (4%)	0	100	100
12	A4	199/232 (86%)	194 (98%)	5 (2%)	0	100	100
12	B4	202/232 (87%)	200 (99%)	2 (1%)	0	100	100
12	C4	197/232 (85%)	185 (94%)	12 (6%)	0	100	100
12	D4	200/232 (86%)	194 (97%)	6 (3%)	0	100	100
12	E4	202/232 (87%)	197 (98%)	5 (2%)	0	100	100
All	All	32138/47180 (68%)	29936 (93%)	2176 (7%)	26 (0%)	54	83

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B2	42	VAL
2	C2	42	VAL
2	D2	42	VAL
2	A2	42	VAL
2	E2	42	VAL

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Mol	Chain	Res	Type
1	H1	160	PRO
1	O1	160	PRO
1	g1	160	PRO
2	E2	41	SER
1	K1	160	PRO
1	a1	160	PRO
2	A2	41	SER
2	B2	41	SER
7	V2	58	ALA
1	C1	160	PRO
1	H1	166	VAL
1	Q1	160	PRO
1	f1	160	PRO
3	F2	158	PRO
8	b2	117	GLY
1	G1	160	PRO
1	I1	160	PRO
1	W1	160	PRO
1	d1	160	PRO
1	c1	160	PRO
7	X2	93	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	B1	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	C1	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	D1	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	E1	217/467 (46%)	217 (100%)	0	100	100
1	F1	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	G1	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	H1	217/467 (46%)	216 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I1	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	J1	134/467 (29%)	132 (98%)	2 (2%)	65	81
1	K1	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	L1	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	M1	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	N1	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	O1	217/467 (46%)	213 (98%)	4 (2%)	59	77
1	P1	134/467 (29%)	131 (98%)	3 (2%)	52	72
1	Q1	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	R1	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	S1	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	T1	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	U1	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	V1	134/467 (29%)	132 (98%)	2 (2%)	65	81
1	W1	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	X1	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	Y1	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	Z1	134/467 (29%)	132 (98%)	2 (2%)	65	81
1	a1	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	b1	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	c1	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	d1	217/467 (46%)	215 (99%)	2 (1%)	78	88
1	e1	134/467 (29%)	133 (99%)	1 (1%)	84	91
1	f1	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	g1	217/467 (46%)	216 (100%)	1 (0%)	88	94
1	h1	217/467 (46%)	216 (100%)	1 (0%)	88	94
2	A2	179/204 (88%)	179 (100%)	0	100	100
2	B2	179/204 (88%)	179 (100%)	0	100	100
2	C2	179/204 (88%)	178 (99%)	1 (1%)	86	93
2	D2	179/204 (88%)	179 (100%)	0	100	100
2	E2	179/204 (88%)	179 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F2	215/221 (97%)	215 (100%)	0	100	100
4	G2	74/74 (100%)	74 (100%)	0	100	100
4	H2	74/74 (100%)	74 (100%)	0	100	100
4	I2	74/74 (100%)	74 (100%)	0	100	100
4	J2	74/74 (100%)	74 (100%)	0	100	100
5	K2	33/79 (42%)	33 (100%)	0	100	100
5	L2	59/79 (75%)	59 (100%)	0	100	100
5	M2	59/79 (75%)	59 (100%)	0	100	100
5	N2	59/79 (75%)	59 (100%)	0	100	100
5	O2	59/79 (75%)	59 (100%)	0	100	100
5	P2	59/79 (75%)	59 (100%)	0	100	100
6	Q2	109/113 (96%)	109 (100%)	0	100	100
6	R2	100/113 (88%)	100 (100%)	0	100	100
6	S2	100/113 (88%)	99 (99%)	1 (1%)	76	86
6	T2	89/113 (79%)	88 (99%)	1 (1%)	73	85
6	U2	99/113 (88%)	97 (98%)	2 (2%)	55	74
7	V2	104/105 (99%)	103 (99%)	1 (1%)	76	86
7	W2	104/105 (99%)	104 (100%)	0	100	100
7	X2	104/105 (99%)	104 (100%)	0	100	100
7	Y2	104/105 (99%)	104 (100%)	0	100	100
7	Z2	104/105 (99%)	103 (99%)	1 (1%)	76	86
7	a2	104/105 (99%)	104 (100%)	0	100	100
8	b2	191/193 (99%)	191 (100%)	0	100	100
8	c2	191/193 (99%)	191 (100%)	0	100	100
8	d2	191/193 (99%)	191 (100%)	0	100	100
8	e2	191/193 (99%)	191 (100%)	0	100	100
8	f2	191/193 (99%)	191 (100%)	0	100	100
9	12	215/215 (100%)	215 (100%)	0	100	100
9	22	215/215 (100%)	215 (100%)	0	100	100
9	32	214/215 (100%)	214 (100%)	0	100	100
9	42	215/215 (100%)	214 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	g2	215/215 (100%)	215 (100%)	0	100	100
9	h2	215/215 (100%)	215 (100%)	0	100	100
9	i2	215/215 (100%)	215 (100%)	0	100	100
9	j2	215/215 (100%)	215 (100%)	0	100	100
9	k2	215/215 (100%)	215 (100%)	0	100	100
9	l2	206/215 (96%)	206 (100%)	0	100	100
9	m2	206/215 (96%)	206 (100%)	0	100	100
9	n2	206/215 (96%)	205 (100%)	1 (0%)	88	94
9	o2	206/215 (96%)	206 (100%)	0	100	100
9	p2	206/215 (96%)	206 (100%)	0	100	100
9	q2	207/215 (96%)	206 (100%)	1 (0%)	88	94
9	r2	215/215 (100%)	214 (100%)	1 (0%)	88	94
9	s2	215/215 (100%)	215 (100%)	0	100	100
9	t2	215/215 (100%)	215 (100%)	0	100	100
9	u2	215/215 (100%)	215 (100%)	0	100	100
9	v2	215/215 (100%)	215 (100%)	0	100	100
9	w2	215/215 (100%)	215 (100%)	0	100	100
9	x2	215/215 (100%)	215 (100%)	0	100	100
9	y2	215/215 (100%)	214 (100%)	1 (0%)	88	94
9	z2	215/215 (100%)	215 (100%)	0	100	100
10	A3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	B3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	C3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	D3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	E3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	F3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	G3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	H3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	I3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	J3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	K3	170/186 (91%)	164 (96%)	6 (4%)	36	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	M3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	N3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	O3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	P3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	Q3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	R3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	S3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	T3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	U3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	V3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	W3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	X3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	Y3	170/186 (91%)	164 (96%)	6 (4%)	36	63
10	Z3	170/186 (91%)	164 (96%)	6 (4%)	36	63
11	a3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	b3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	c3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	d3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	e3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	f3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	g3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	h3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	i3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	j3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	k3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	l3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	m3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	n3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	o3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	p3	251/294 (85%)	238 (95%)	13 (5%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	q3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	r3	250/294 (85%)	237 (95%)	13 (5%)	23	55
11	s3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	t3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	u3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	v3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	w3	251/294 (85%)	237 (94%)	14 (6%)	21	53
11	x3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	y3	251/294 (85%)	238 (95%)	13 (5%)	23	55
11	z3	251/294 (85%)	238 (95%)	13 (5%)	23	55
12	A4	164/188 (87%)	162 (99%)	2 (1%)	71	84
12	B4	165/188 (88%)	165 (100%)	0	100	100
12	C4	162/188 (86%)	162 (100%)	0	100	100
12	D4	164/188 (87%)	163 (99%)	1 (1%)	86	93
12	E4	165/188 (88%)	164 (99%)	1 (1%)	86	93
All	All	27146/38629 (70%)	26584 (98%)	562 (2%)	56	74

All (562) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	410	LYS
1	B1	394	LYS
1	B1	410	LYS
1	C1	394	LYS
1	D1	394	LYS
1	F1	394	LYS
1	G1	394	LYS
1	H1	394	LYS
1	I1	410	LYS
1	J1	394	LYS
1	J1	410	LYS
1	K1	394	LYS
1	K1	410	LYS
1	L1	394	LYS
1	M1	394	LYS
1	N1	394	LYS
1	N1	410	LYS

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Mol	Chain	Res	Type
1	O1	161	LYS
1	O1	170	LYS
1	O1	394	LYS
1	O1	410	LYS
1	P1	394	LYS
1	P1	410	LYS
1	P1	431	ASN
1	Q1	394	LYS
1	Q1	410	LYS
1	R1	394	LYS
1	S1	394	LYS
1	T1	394	LYS
1	U1	394	LYS
1	U1	410	LYS
1	V1	281	HIS
1	V1	394	LYS
1	W1	394	LYS
1	W1	410	LYS
1	X1	394	LYS
1	X1	410	LYS
1	Y1	394	LYS
1	Y1	410	LYS
1	Z1	394	LYS
1	Z1	410	LYS
1	a1	394	LYS
1	a1	410	LYS
1	b1	394	LYS
1	c1	394	LYS
1	d1	394	LYS
1	d1	410	LYS
1	e1	394	LYS
1	f1	394	LYS
1	g1	394	LYS
1	h1	394	LYS
2	C2	236	MET
6	S2	17	ASN
6	T2	17	ASN
6	U2	112	ASN
6	U2	117	GLN
7	V2	59	THR
7	Z2	75	LYS
9	n2	172	GLN

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Mol	Chain	Res	Type
9	q2	169	GLN
9	r2	135	GLN
9	y2	196	GLN
9	42	243	ASN
10	A3	30	LEU
10	A3	36	THR
10	A3	40	ILE
10	A3	99	ASP
10	A3	111	ARG
10	A3	144	PHE
10	B3	30	LEU
10	B3	36	THR
10	B3	40	ILE
10	B3	99	ASP
10	B3	111	ARG
10	B3	144	PHE
10	C3	30	LEU
10	C3	36	THR
10	C3	40	ILE
10	C3	99	ASP
10	C3	111	ARG
10	C3	144	PHE
10	D3	30	LEU
10	D3	36	THR
10	D3	40	ILE
10	D3	99	ASP
10	D3	111	ARG
10	D3	144	PHE
10	E3	30	LEU
10	E3	36	THR
10	E3	40	ILE
10	E3	99	ASP
10	E3	111	ARG
10	E3	144	PHE
10	F3	30	LEU
10	F3	36	THR
10	F3	40	ILE
10	F3	99	ASP
10	F3	111	ARG
10	F3	144	PHE
10	G3	30	LEU
10	G3	36	THR

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Mol	Chain	Res	Type
10	G3	40	ILE
10	G3	99	ASP
10	G3	111	ARG
10	G3	144	PHE
10	H3	30	LEU
10	H3	36	THR
10	H3	40	ILE
10	H3	99	ASP
10	H3	111	ARG
10	H3	144	PHE
10	I3	30	LEU
10	I3	36	THR
10	I3	40	ILE
10	I3	99	ASP
10	I3	111	ARG
10	I3	144	PHE
10	J3	30	LEU
10	J3	36	THR
10	J3	40	ILE
10	J3	99	ASP
10	J3	111	ARG
10	J3	144	PHE
10	K3	30	LEU
10	K3	36	THR
10	K3	40	ILE
10	K3	99	ASP
10	K3	111	ARG
10	K3	144	PHE
10	L3	30	LEU
10	L3	36	THR
10	L3	40	ILE
10	L3	99	ASP
10	L3	111	ARG
10	L3	144	PHE
10	M3	30	LEU
10	M3	36	THR
10	M3	40	ILE
10	M3	99	ASP
10	M3	111	ARG
10	M3	144	PHE
10	N3	30	LEU
10	N3	36	THR

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Mol	Chain	Res	Type
10	N3	40	ILE
10	N3	99	ASP
10	N3	111	ARG
10	N3	144	PHE
10	O3	30	LEU
10	O3	36	THR
10	O3	40	ILE
10	O3	99	ASP
10	O3	111	ARG
10	O3	144	PHE
10	P3	30	LEU
10	P3	36	THR
10	P3	40	ILE
10	P3	99	ASP
10	P3	111	ARG
10	P3	144	PHE
10	Q3	30	LEU
10	Q3	36	THR
10	Q3	40	ILE
10	Q3	99	ASP
10	Q3	111	ARG
10	Q3	144	PHE
10	R3	30	LEU
10	R3	36	THR
10	R3	40	ILE
10	R3	99	ASP
10	R3	111	ARG
10	R3	144	PHE
10	S3	30	LEU
10	S3	36	THR
10	S3	40	ILE
10	S3	99	ASP
10	S3	111	ARG
10	S3	144	PHE
10	T3	30	LEU
10	T3	36	THR
10	T3	40	ILE
10	T3	99	ASP
10	T3	111	ARG
10	T3	144	PHE
10	U3	30	LEU
10	U3	36	THR

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Mol	Chain	Res	Type
10	U3	40	ILE
10	U3	99	ASP
10	U3	111	ARG
10	U3	144	PHE
10	V3	30	LEU
10	V3	36	THR
10	V3	40	ILE
10	V3	99	ASP
10	V3	111	ARG
10	V3	144	PHE
10	W3	30	LEU
10	W3	36	THR
10	W3	40	ILE
10	W3	99	ASP
10	W3	111	ARG
10	W3	144	PHE
10	X3	30	LEU
10	X3	36	THR
10	X3	40	ILE
10	X3	99	ASP
10	X3	111	ARG
10	X3	144	PHE
10	Y3	30	LEU
10	Y3	36	THR
10	Y3	40	ILE
10	Y3	99	ASP
10	Y3	111	ARG
10	Y3	144	PHE
10	Z3	30	LEU
10	Z3	36	THR
10	Z3	40	ILE
10	Z3	99	ASP
10	Z3	111	ARG
10	Z3	144	PHE
11	a3	25	LEU
11	a3	84	VAL
11	a3	114	LYS
11	a3	124	THR
11	a3	190	ASN
11	a3	196	MET
11	a3	206	ARG
11	a3	210	TYR

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Mol	Chain	Res	Type
11	a3	245	ASN
11	a3	252	LYS
11	a3	256	ASN
11	a3	325	SER
11	a3	344	ASP
11	b3	25	LEU
11	b3	84	VAL
11	b3	114	LYS
11	b3	124	THR
11	b3	190	ASN
11	b3	196	MET
11	b3	206	ARG
11	b3	210	TYR
11	b3	245	ASN
11	b3	252	LYS
11	b3	256	ASN
11	b3	325	SER
11	b3	344	ASP
11	c3	25	LEU
11	c3	84	VAL
11	c3	114	LYS
11	c3	124	THR
11	c3	190	ASN
11	c3	196	MET
11	c3	206	ARG
11	c3	210	TYR
11	c3	245	ASN
11	c3	252	LYS
11	c3	256	ASN
11	c3	325	SER
11	c3	344	ASP
11	d3	25	LEU
11	d3	84	VAL
11	d3	114	LYS
11	d3	124	THR
11	d3	190	ASN
11	d3	196	MET
11	d3	206	ARG
11	d3	210	TYR
11	d3	245	ASN
11	d3	252	LYS
11	d3	256	ASN

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Mol	Chain	Res	Type
11	d3	325	SER
11	d3	344	ASP
11	e3	25	LEU
11	e3	84	VAL
11	e3	114	LYS
11	e3	124	THR
11	e3	190	ASN
11	e3	196	MET
11	e3	206	ARG
11	e3	210	TYR
11	e3	245	ASN
11	e3	252	LYS
11	e3	256	ASN
11	e3	325	SER
11	e3	344	ASP
11	f3	25	LEU
11	f3	84	VAL
11	f3	114	LYS
11	f3	124	THR
11	f3	190	ASN
11	f3	196	MET
11	f3	206	ARG
11	f3	210	TYR
11	f3	245	ASN
11	f3	252	LYS
11	f3	256	ASN
11	f3	325	SER
11	f3	344	ASP
11	g3	25	LEU
11	g3	84	VAL
11	g3	114	LYS
11	g3	124	THR
11	g3	190	ASN
11	g3	196	MET
11	g3	206	ARG
11	g3	210	TYR
11	g3	245	ASN
11	g3	252	LYS
11	g3	256	ASN
11	g3	325	SER
11	g3	344	ASP
11	h3	25	LEU

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Mol	Chain	Res	Type
11	h3	84	VAL
11	h3	114	LYS
11	h3	124	THR
11	h3	190	ASN
11	h3	196	MET
11	h3	206	ARG
11	h3	210	TYR
11	h3	245	ASN
11	h3	252	LYS
11	h3	256	ASN
11	h3	325	SER
11	h3	344	ASP
11	i3	25	LEU
11	i3	84	VAL
11	i3	114	LYS
11	i3	124	THR
11	i3	190	ASN
11	i3	196	MET
11	i3	206	ARG
11	i3	210	TYR
11	i3	245	ASN
11	i3	252	LYS
11	i3	256	ASN
11	i3	325	SER
11	i3	344	ASP
11	j3	25	LEU
11	j3	84	VAL
11	j3	114	LYS
11	j3	124	THR
11	j3	190	ASN
11	j3	196	MET
11	j3	206	ARG
11	j3	210	TYR
11	j3	245	ASN
11	j3	252	LYS
11	j3	256	ASN
11	j3	325	SER
11	j3	344	ASP
11	k3	25	LEU
11	k3	84	VAL
11	k3	114	LYS
11	k3	124	THR

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Mol	Chain	Res	Type
11	k3	190	ASN
11	k3	196	MET
11	k3	206	ARG
11	k3	210	TYR
11	k3	245	ASN
11	k3	252	LYS
11	k3	256	ASN
11	k3	325	SER
11	k3	344	ASP
11	l3	25	LEU
11	l3	84	VAL
11	l3	114	LYS
11	l3	124	THR
11	l3	190	ASN
11	l3	196	MET
11	l3	206	ARG
11	l3	210	TYR
11	l3	245	ASN
11	l3	252	LYS
11	l3	256	ASN
11	l3	325	SER
11	l3	344	ASP
11	m3	25	LEU
11	m3	84	VAL
11	m3	114	LYS
11	m3	124	THR
11	m3	190	ASN
11	m3	196	MET
11	m3	206	ARG
11	m3	210	TYR
11	m3	245	ASN
11	m3	252	LYS
11	m3	256	ASN
11	m3	325	SER
11	m3	344	ASP
11	n3	25	LEU
11	n3	84	VAL
11	n3	114	LYS
11	n3	124	THR
11	n3	190	ASN
11	n3	196	MET
11	n3	206	ARG

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Mol	Chain	Res	Type
11	n3	210	TYR
11	n3	245	ASN
11	n3	252	LYS
11	n3	256	ASN
11	n3	325	SER
11	n3	344	ASP
11	o3	25	LEU
11	o3	84	VAL
11	o3	114	LYS
11	o3	124	THR
11	o3	190	ASN
11	o3	196	MET
11	o3	206	ARG
11	o3	210	TYR
11	o3	245	ASN
11	o3	252	LYS
11	o3	256	ASN
11	o3	325	SER
11	o3	344	ASP
11	p3	25	LEU
11	p3	84	VAL
11	p3	114	LYS
11	p3	124	THR
11	p3	190	ASN
11	p3	196	MET
11	p3	206	ARG
11	p3	210	TYR
11	p3	245	ASN
11	p3	252	LYS
11	p3	256	ASN
11	p3	325	SER
11	p3	344	ASP
11	q3	25	LEU
11	q3	84	VAL
11	q3	114	LYS
11	q3	124	THR
11	q3	190	ASN
11	q3	196	MET
11	q3	206	ARG
11	q3	210	TYR
11	q3	245	ASN
11	q3	252	LYS

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Mol	Chain	Res	Type
11	q3	256	ASN
11	q3	325	SER
11	q3	344	ASP
11	r3	25	LEU
11	r3	84	VAL
11	r3	114	LYS
11	r3	124	THR
11	r3	190	ASN
11	r3	196	MET
11	r3	206	ARG
11	r3	210	TYR
11	r3	245	ASN
11	r3	252	LYS
11	r3	256	ASN
11	r3	325	SER
11	r3	344	ASP
11	s3	25	LEU
11	s3	84	VAL
11	s3	114	LYS
11	s3	124	THR
11	s3	190	ASN
11	s3	196	MET
11	s3	206	ARG
11	s3	210	TYR
11	s3	245	ASN
11	s3	252	LYS
11	s3	256	ASN
11	s3	325	SER
11	s3	344	ASP
11	t3	25	LEU
11	t3	84	VAL
11	t3	114	LYS
11	t3	124	THR
11	t3	190	ASN
11	t3	196	MET
11	t3	206	ARG
11	t3	210	TYR
11	t3	245	ASN
11	t3	252	LYS
11	t3	256	ASN
11	t3	325	SER
11	t3	344	ASP

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Mol	Chain	Res	Type
11	u3	25	LEU
11	u3	84	VAL
11	u3	114	LYS
11	u3	124	THR
11	u3	190	ASN
11	u3	196	MET
11	u3	206	ARG
11	u3	210	TYR
11	u3	245	ASN
11	u3	252	LYS
11	u3	256	ASN
11	u3	325	SER
11	u3	344	ASP
11	v3	25	LEU
11	v3	84	VAL
11	v3	114	LYS
11	v3	124	THR
11	v3	190	ASN
11	v3	196	MET
11	v3	206	ARG
11	v3	210	TYR
11	v3	245	ASN
11	v3	252	LYS
11	v3	256	ASN
11	v3	325	SER
11	v3	344	ASP
11	w3	25	LEU
11	w3	78	ASN
11	w3	84	VAL
11	w3	114	LYS
11	w3	124	THR
11	w3	190	ASN
11	w3	196	MET
11	w3	206	ARG
11	w3	210	TYR
11	w3	245	ASN
11	w3	252	LYS
11	w3	256	ASN
11	w3	325	SER
11	w3	344	ASP
11	x3	25	LEU
11	x3	84	VAL

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Mol	Chain	Res	Type
11	x3	114	LYS
11	x3	124	THR
11	x3	190	ASN
11	x3	196	MET
11	x3	206	ARG
11	x3	210	TYR
11	x3	245	ASN
11	x3	252	LYS
11	x3	256	ASN
11	x3	325	SER
11	x3	344	ASP
11	y3	25	LEU
11	y3	84	VAL
11	y3	114	LYS
11	y3	124	THR
11	y3	190	ASN
11	y3	196	MET
11	y3	206	ARG
11	y3	210	TYR
11	y3	245	ASN
11	y3	252	LYS
11	y3	256	ASN
11	y3	325	SER
11	y3	344	ASP
11	z3	25	LEU
11	z3	84	VAL
11	z3	114	LYS
11	z3	124	THR
11	z3	190	ASN
11	z3	196	MET
11	z3	206	ARG
11	z3	210	TYR
11	z3	245	ASN
11	z3	252	LYS
11	z3	256	ASN
11	z3	325	SER
11	z3	344	ASP
12	A4	75	ASN
12	A4	157	ARG
12	D4	56	ASN
12	E4	135	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (200) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	434	ASN
1	B1	156	HIS
1	B1	434	ASN
1	C1	246	GLN
1	D1	434	ASN
1	E1	169	GLN
1	E1	297	GLN
1	E1	365	ASN
1	E1	434	ASN
1	G1	156	HIS
1	G1	169	GLN
1	H1	434	ASN
1	I1	169	GLN
1	J1	434	ASN
1	K1	133	GLN
1	K1	261	ASN
1	M1	277	GLN
1	M1	431	ASN
1	M1	434	ASN
1	N1	297	GLN
1	O1	361	ASN
1	P1	299	ASN
1	P1	359	GLN
1	P1	434	ASN
1	S1	411	GLN
1	S1	434	ASN
1	T1	156	HIS
1	W1	156	HIS
1	W1	431	ASN
1	W1	434	ASN
1	X1	434	ASN
1	Y1	359	GLN
1	Z1	297	GLN
1	Z1	299	ASN
1	Z1	434	ASN
1	a1	434	ASN
1	b1	265	GLN
1	d1	133	GLN
1	d1	218	HIS
1	e1	277	GLN
1	e1	434	ASN
1	f1	434	ASN

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Mol	Chain	Res	Type
2	A2	119	GLN
2	C2	119	GLN
3	F2	105	GLN
3	F2	141	ASN
6	Q2	13	GLN
6	Q2	92	GLN
6	Q2	112	ASN
6	S2	92	GLN
6	T2	92	GLN
7	V2	134	GLN
7	W2	22	ASN
7	X2	22	ASN
8	b2	37	GLN
8	c2	230	GLN
8	e2	83	GLN
8	e2	106	GLN
9	g2	67	GLN
9	h2	24	ASN
9	h2	47	GLN
9	h2	67	GLN
9	i2	121	GLN
9	j2	169	GLN
9	k2	135	GLN
9	m2	67	GLN
9	m2	135	GLN
9	m2	164	GLN
9	n2	169	GLN
9	n2	209	ASN
9	o2	67	GLN
9	o2	127	GLN
9	o2	161	GLN
9	o2	164	GLN
9	o2	169	GLN
9	o2	235	GLN
9	p2	85	ASN
9	p2	88	GLN
9	p2	145	ASN
9	p2	172	GLN
9	r2	180	ASN
9	s2	127	GLN
9	t2	67	GLN
9	t2	127	GLN

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Mol	Chain	Res	Type
9	t2	137	GLN
9	u2	55	GLN
9	u2	202	ASN
9	v2	88	GLN
9	w2	83	GLN
9	y2	16	GLN
9	y2	91	ASN
9	z2	164	GLN
9	z2	237	GLN
9	12	237	GLN
9	22	237	GLN
9	32	255	GLN
9	42	47	GLN
9	42	55	GLN
11	a3	99	GLN
11	a3	161	ASN
11	a3	350	GLN
11	b3	78	ASN
11	b3	99	GLN
11	b3	161	ASN
11	b3	350	GLN
11	c3	51	GLN
11	c3	54	GLN
11	c3	80	GLN
11	c3	99	GLN
11	c3	161	ASN
11	c3	350	GLN
11	d3	99	GLN
11	d3	161	ASN
11	d3	350	GLN
11	e3	99	GLN
11	e3	161	ASN
11	e3	350	GLN
11	f3	99	GLN
11	f3	161	ASN
11	f3	350	GLN
11	g3	99	GLN
11	g3	161	ASN
11	g3	350	GLN
11	h3	99	GLN
11	h3	161	ASN
11	h3	350	GLN

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Mol	Chain	Res	Type
11	i3	99	GLN
11	i3	161	ASN
11	i3	350	GLN
11	j3	99	GLN
11	j3	161	ASN
11	j3	350	GLN
11	k3	78	ASN
11	k3	99	GLN
11	k3	161	ASN
11	k3	350	GLN
11	l3	54	GLN
11	l3	78	ASN
11	l3	99	GLN
11	l3	161	ASN
11	l3	350	GLN
11	m3	54	GLN
11	m3	99	GLN
11	m3	161	ASN
11	m3	350	GLN
11	n3	99	GLN
11	n3	161	ASN
11	n3	350	GLN
11	o3	80	GLN
11	o3	99	GLN
11	o3	161	ASN
11	o3	350	GLN
11	p3	78	ASN
11	p3	99	GLN
11	p3	161	ASN
11	p3	350	GLN
11	q3	54	GLN
11	q3	99	GLN
11	q3	161	ASN
11	q3	350	GLN
11	r3	78	ASN
11	r3	99	GLN
11	r3	161	ASN
11	r3	350	GLN
11	s3	78	ASN
11	s3	80	GLN
11	s3	99	GLN
11	s3	161	ASN

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Mol	Chain	Res	Type
11	s3	350	GLN
11	t3	99	GLN
11	t3	161	ASN
11	t3	350	GLN
11	u3	80	GLN
11	u3	99	GLN
11	u3	161	ASN
11	u3	350	GLN
11	v3	78	ASN
11	v3	99	GLN
11	v3	161	ASN
11	v3	350	GLN
11	w3	99	GLN
11	w3	161	ASN
11	w3	350	GLN
11	x3	78	ASN
11	x3	99	GLN
11	x3	161	ASN
11	x3	350	GLN
11	y3	99	GLN
11	y3	161	ASN
11	y3	350	GLN
11	z3	80	GLN
11	z3	99	GLN
11	z3	161	ASN
11	z3	350	GLN
12	A4	55	ASN
12	A4	230	GLN
12	B4	46	ASN
12	B4	55	ASN
12	C4	84	GLN
12	E4	54	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	F2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F2	115:ASP	C	116:PRO	N	5.09

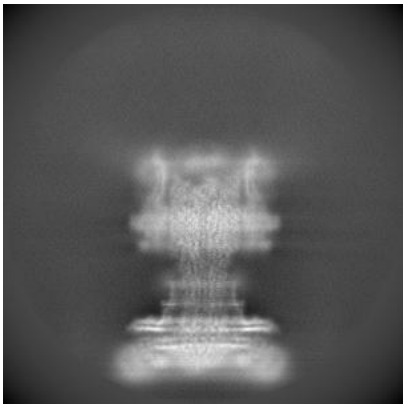
6 Map visualisation

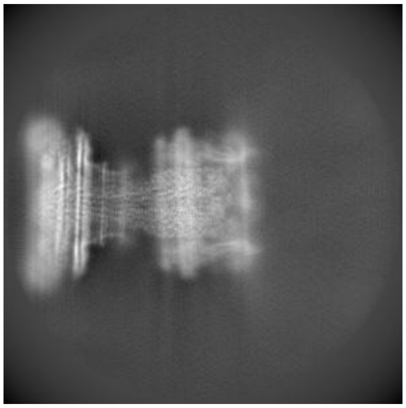
This section contains visualisations of the EMDB entry EMD-12603. These allow visual inspection of the internal detail of the map and identification of artifacts.

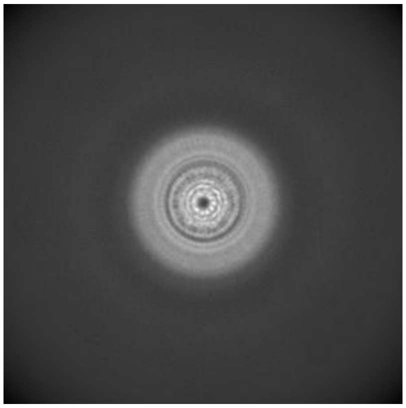
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

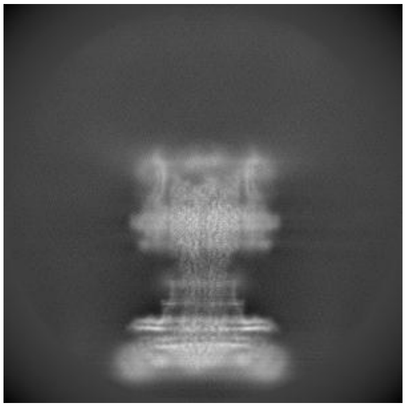
6.1.1 Primary map

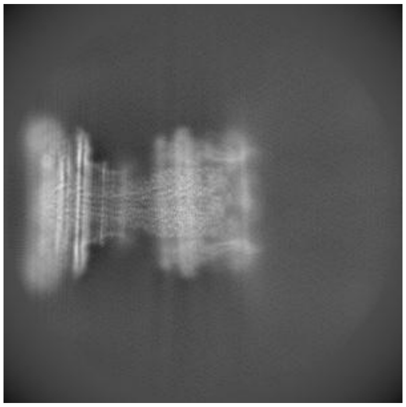

X

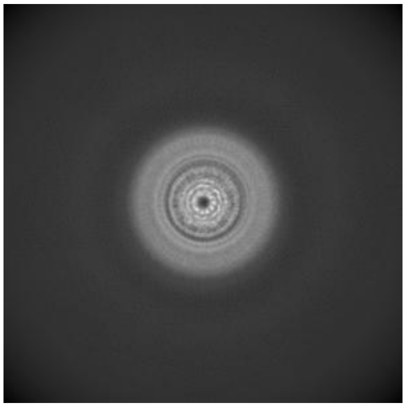

Y


Z

6.1.2 Raw map


X


Y


Z

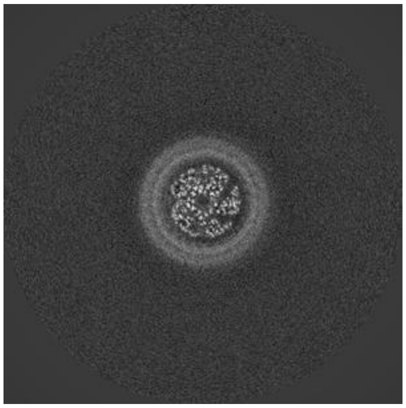
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

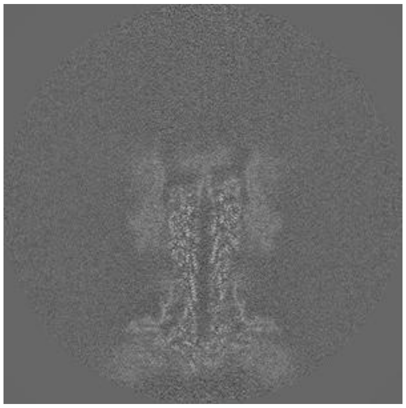
6.2.1 Primary map

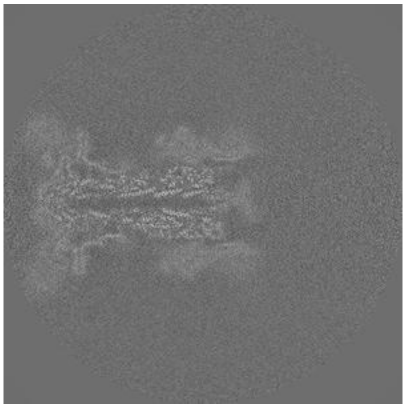

X Index: 384

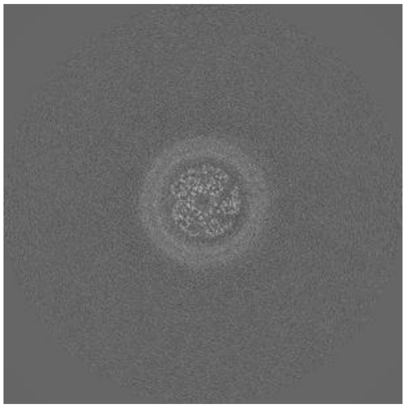

Y Index: 384


Z Index: 384

6.2.2 Raw map


X Index: 384


Y Index: 384

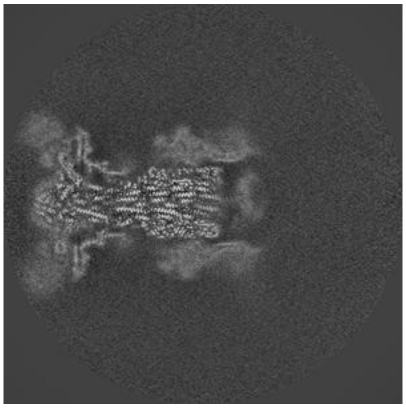

Z Index: 384

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

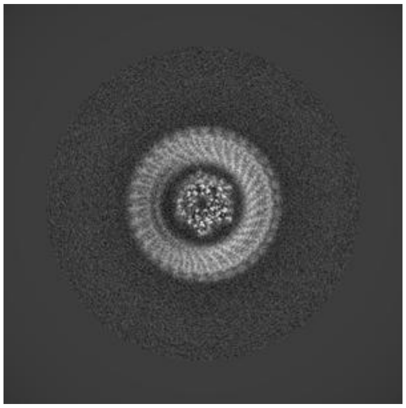
6.3 Largest variance slices

6.3.1 Primary map

X Index: 402

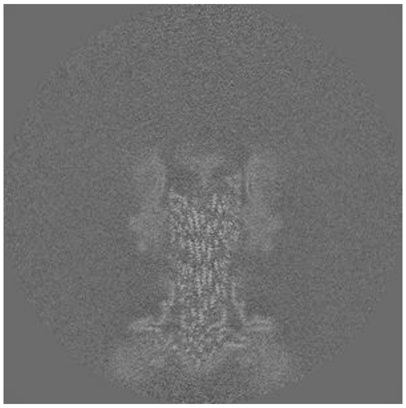


Y Index: 371

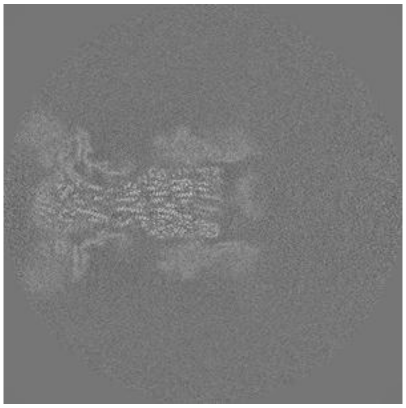


Z Index: 144

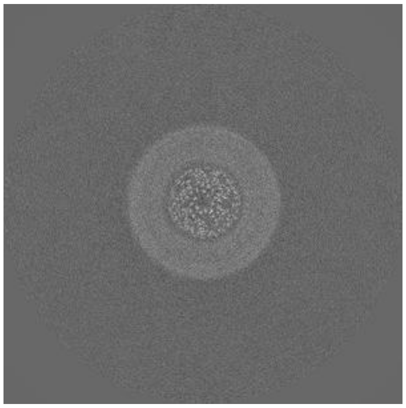
6.3.2 Raw map



X Index: 402



Y Index: 371

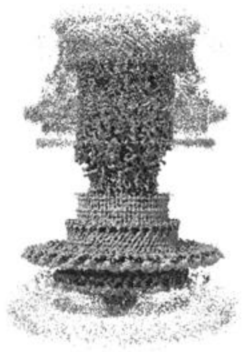


Z Index: 350

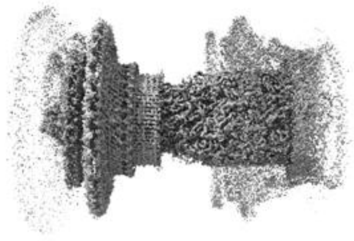
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

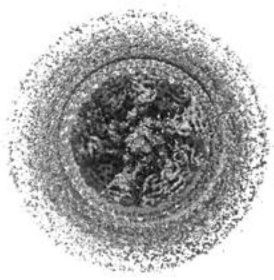
6.4.1 Primary map



X



Y

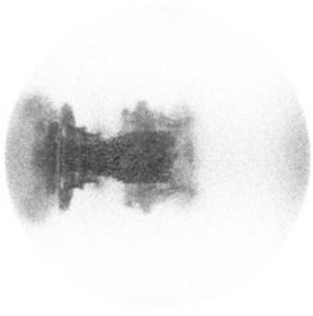


Z

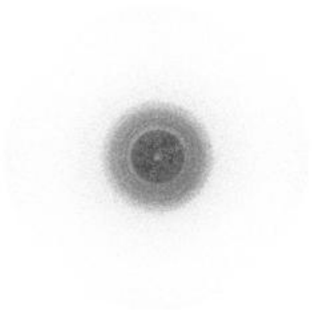
The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X



Y



Z

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

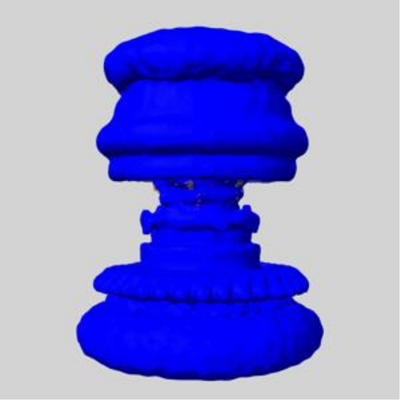
6.5 Mask visualisation ⓘ

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

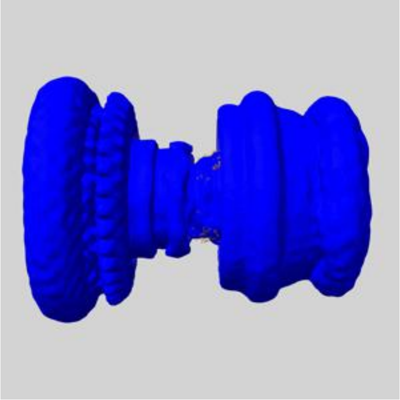
A mask typically either:

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

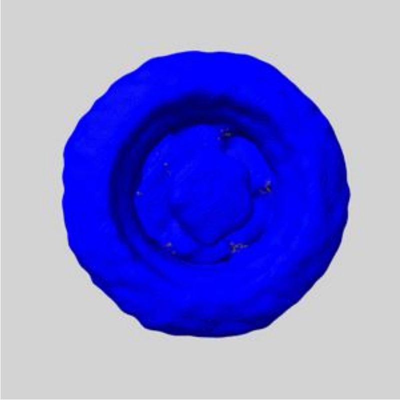
6.5.1 emd_12603_msk_1.map ⓘ



X



Y

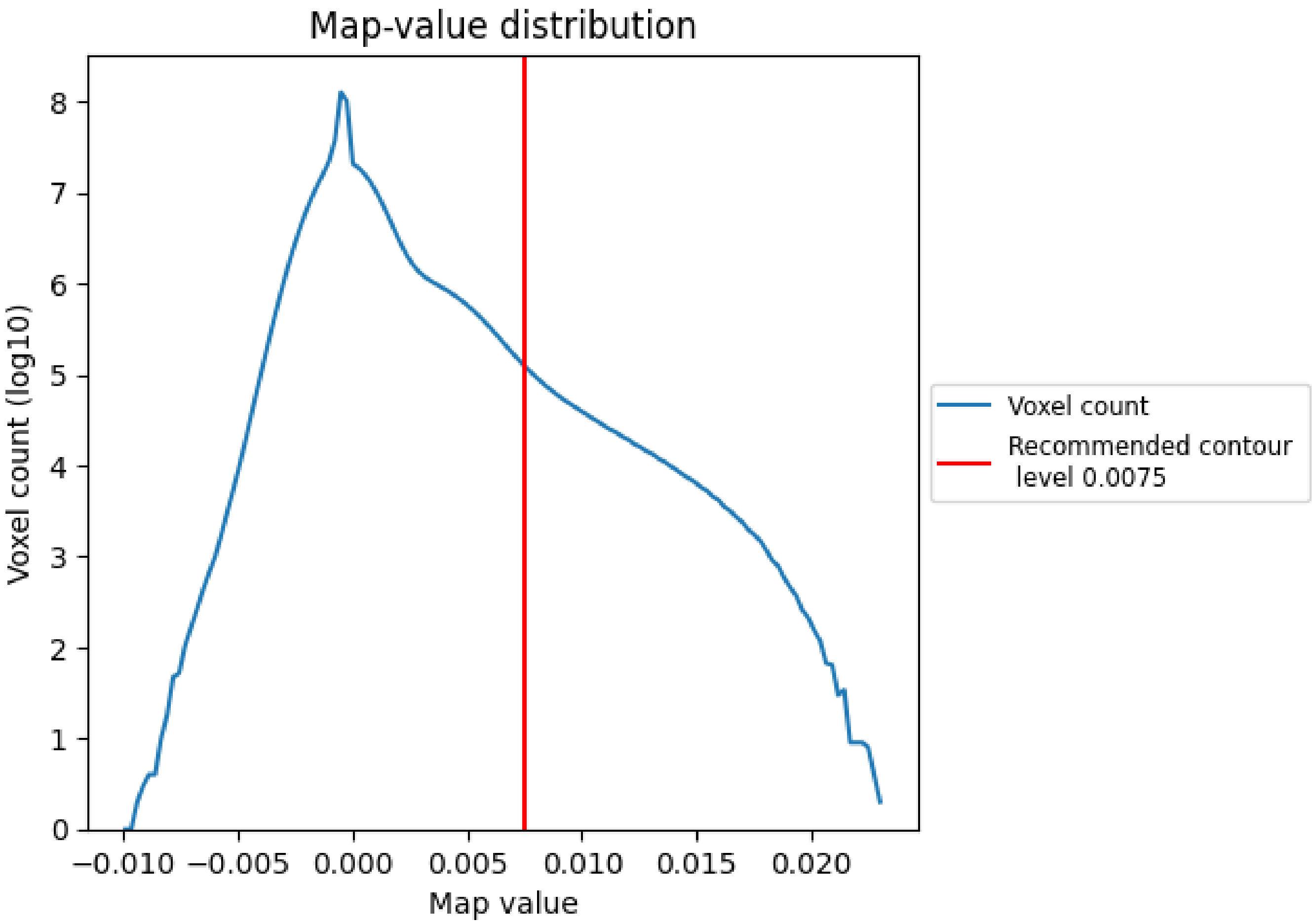


Z

7 Map analysis ⓘ

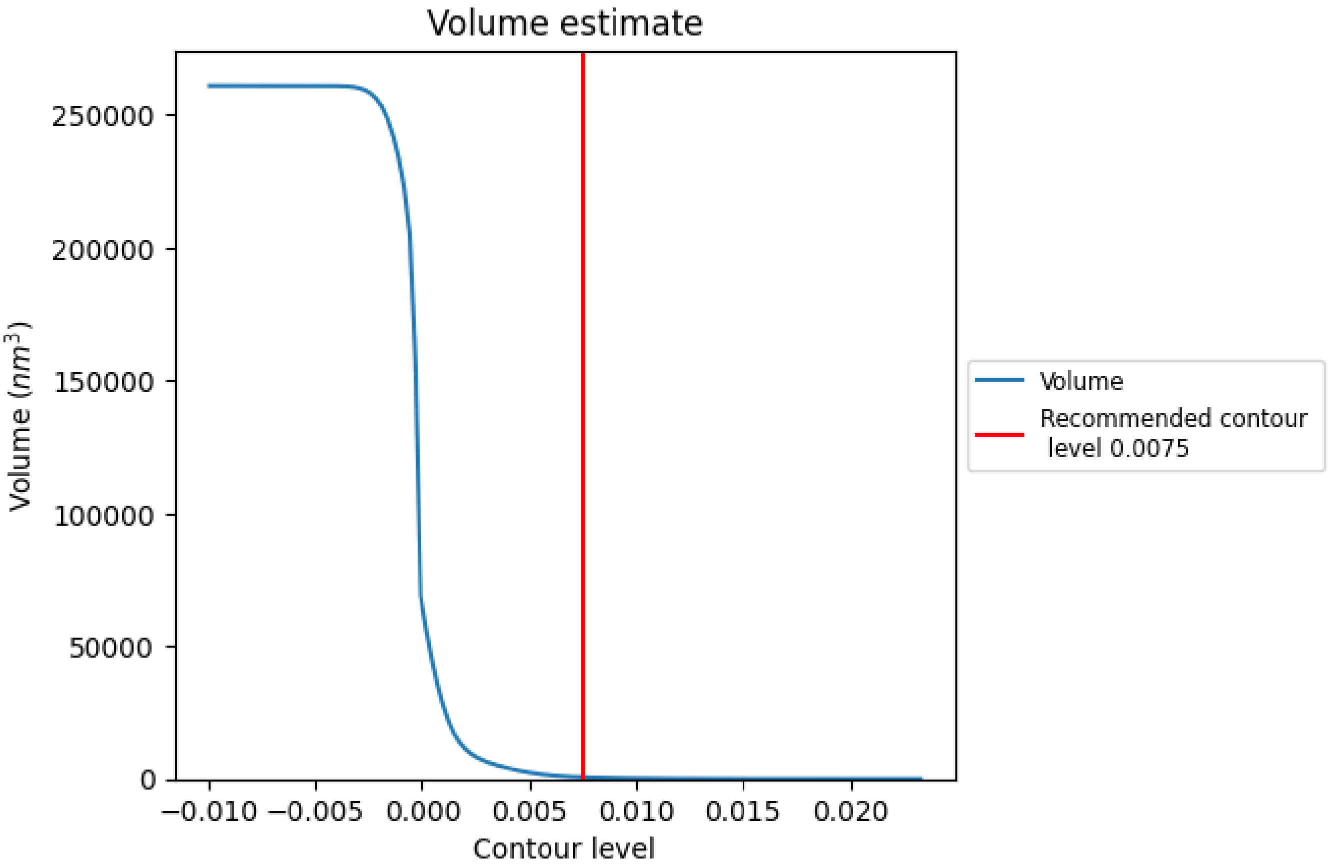
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

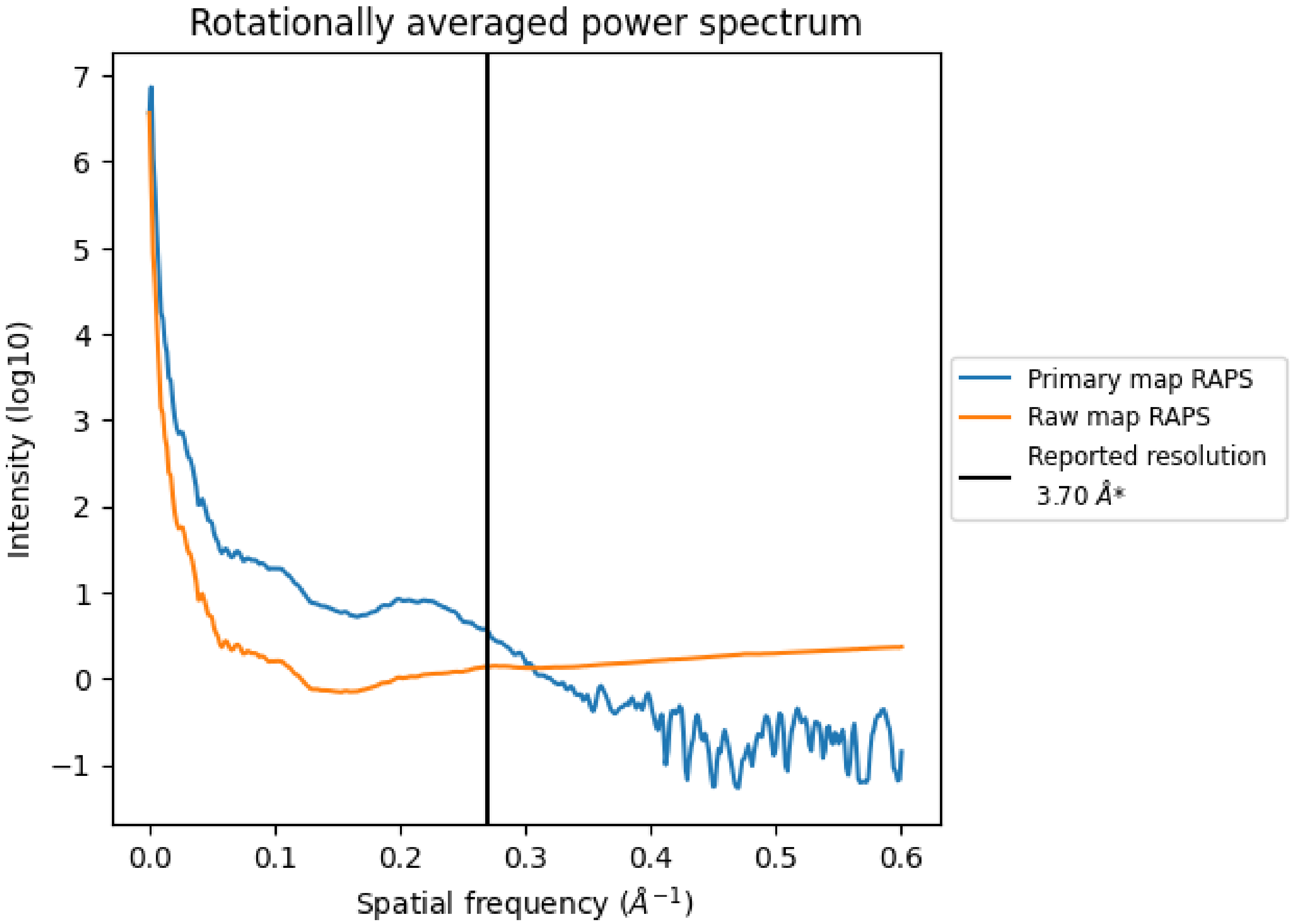
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 648 nm^3; this corresponds to an approximate mass of 586 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

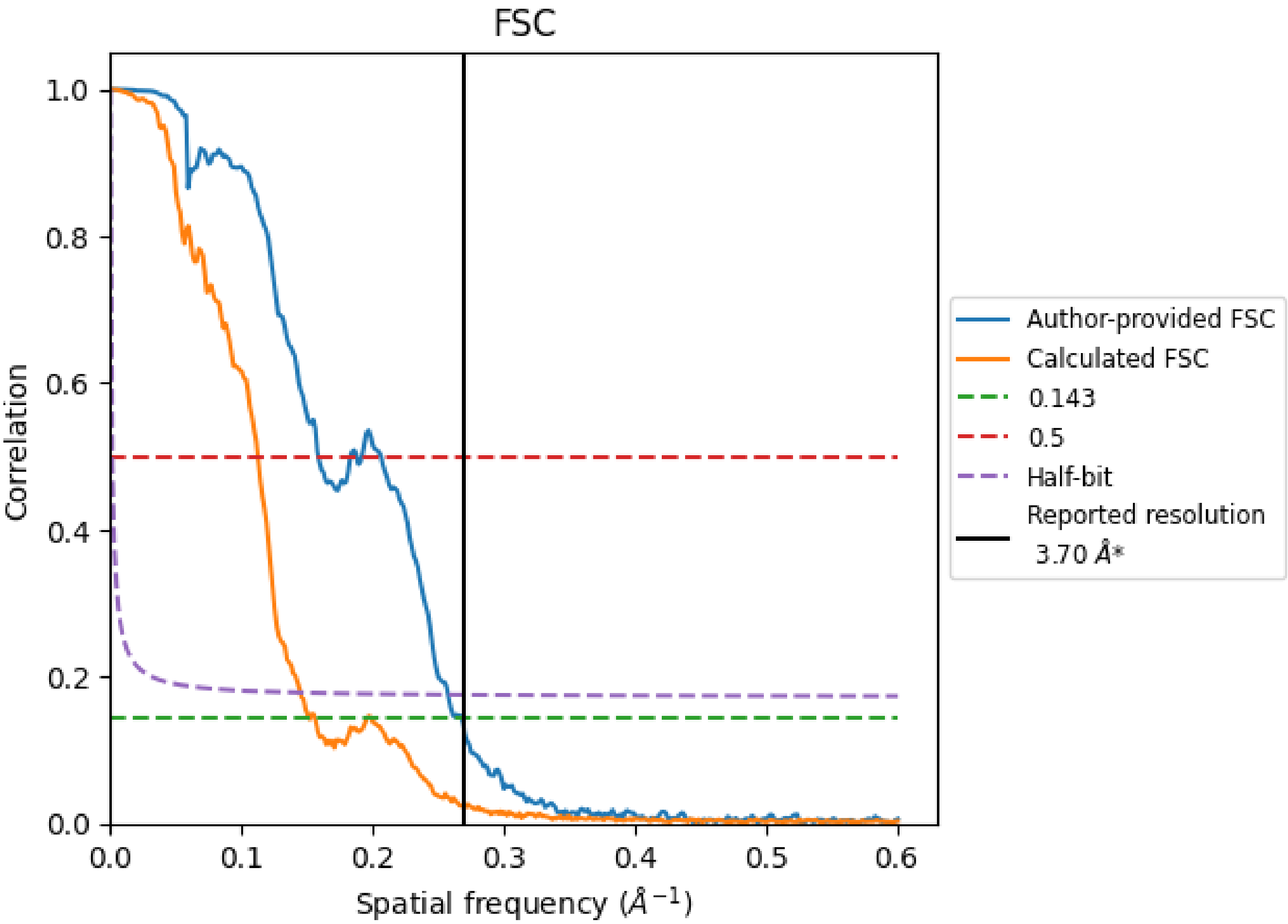


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates ⓘ

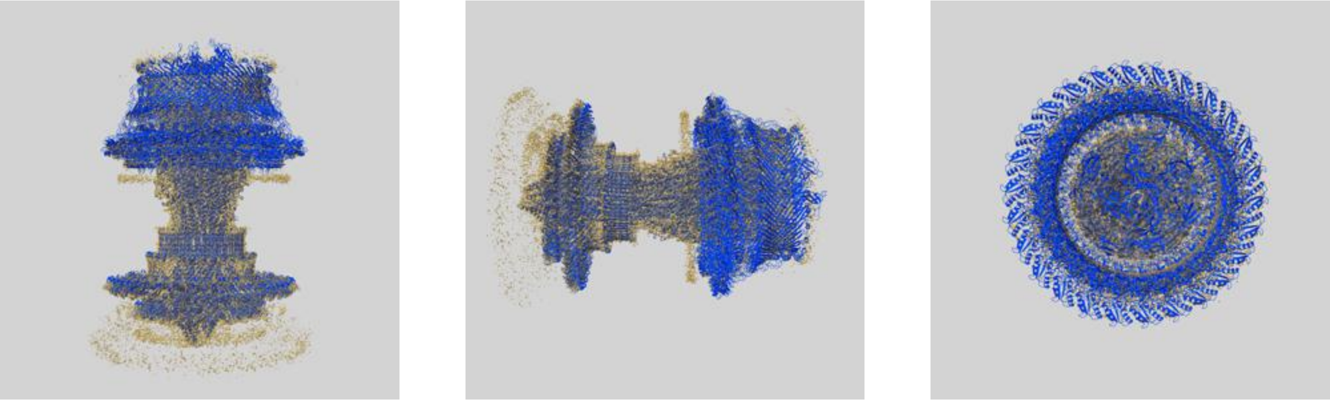
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	6.30	3.88
Calculated*	6.58	8.88	6.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.58 differs from the reported value 3.7 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-12603 and PDB model 7NVG. Per-residue inclusion information can be found in section 3 on page 18.

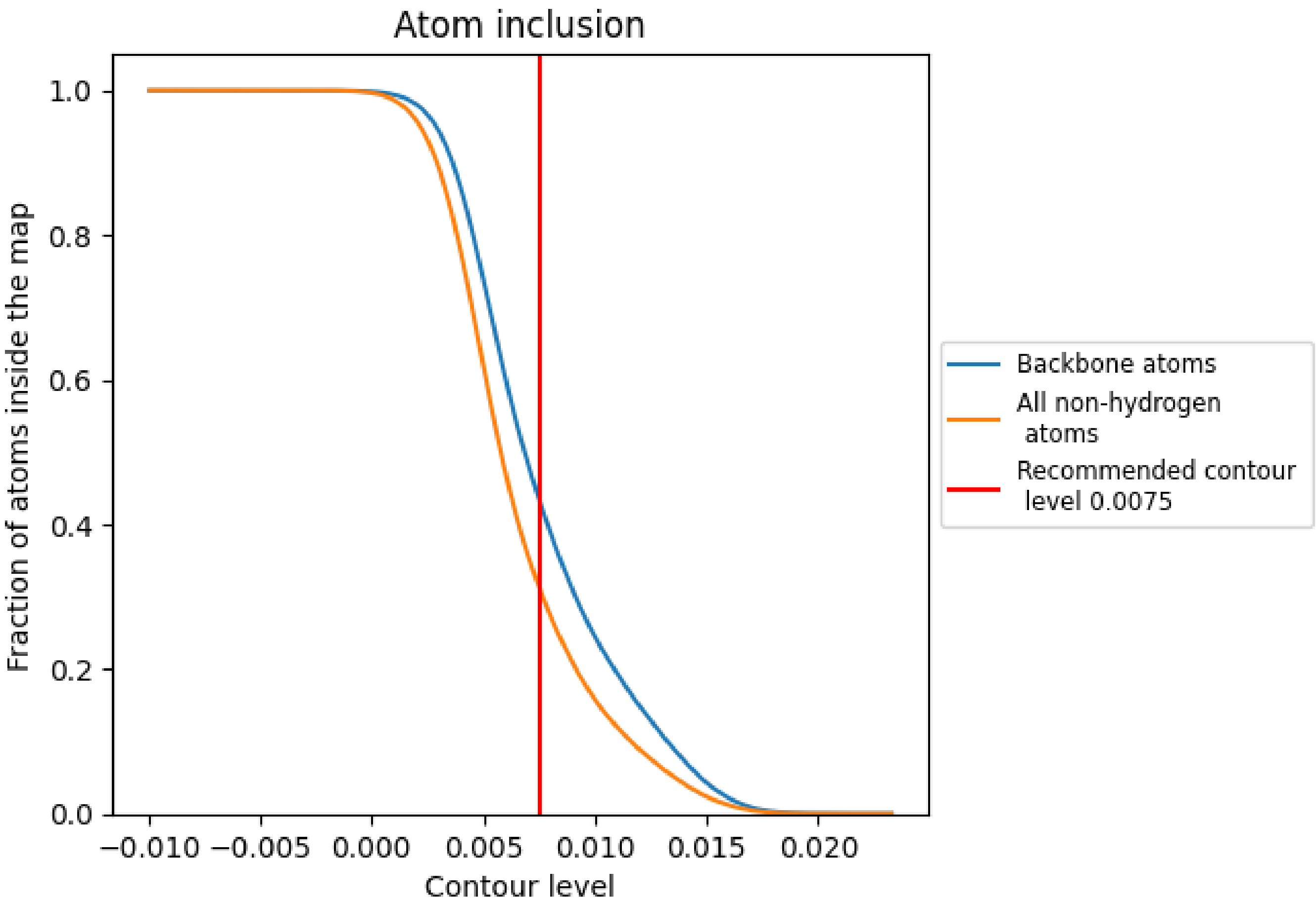
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075 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 Atom inclusion ⓘ



At the recommended contour level, 43% of all backbone atoms, 31% of all non-hydrogen atoms, are inside the map.