



# wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 04:50 PM JST

PDB ID : 8WL2  
EMDB ID : EMD-37611  
Title : Cryo-EM structure of the membrane-anchored part of the flagellar motor-hook complex in the CW state.  
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.  
Deposited on : 2023-09-29  
Resolution : 3.40 Å (reported)  
Based on initial models : ?, .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

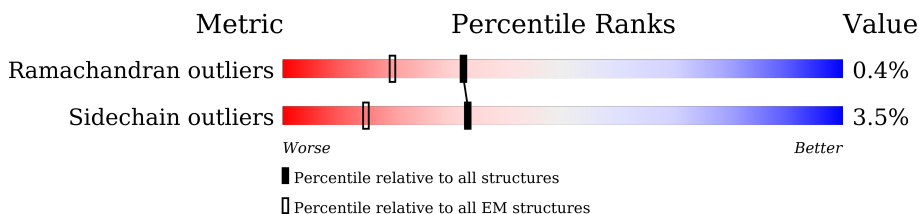
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	232	
1	B	232	
1	C	232	
1	D	232	
1	E	232	
1	F	232	
1	G	232	
1	H	232	
1	I	232	

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Mol	Chain	Length	Quality of chain
1	J	232	45% 88% 9%
1	K	232	41% 88% 9%
1	L	232	44% 88% 9%
1	M	232	47% 88% 9%
1	N	232	44% 88% 9%
1	O	232	50% 88% 9%
1	P	232	41% 88% 9%
1	Q	232	46% 88% 9%
1	R	232	42% 88% 9%
1	S	232	47% 88% 9%
1	T	232	49% 88% 9%
1	U	232	47% 88% 9%
1	V	232	47% 88% 9%
1	W	232	50% 88% 9%
1	X	232	46% 88% 9%
1	Y	232	48% 88% 9%
1	Z	232	47% 88% 9%
2	a	365	56% 80% 17%
2	b	365	55% 80% 17%
2	c	365	54% 80% 17%
2	d	365	55% 80% 17%
2	e	365	55% 80% 17%
2	f	365	55% 80% 17%
2	g	365	52% 80% 17%
2	h	365	57% 80% 17%

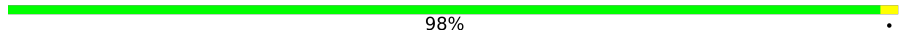
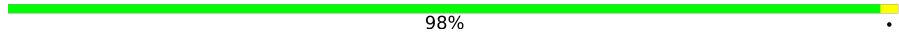
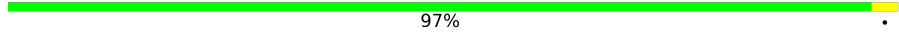
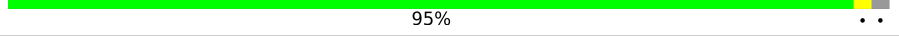
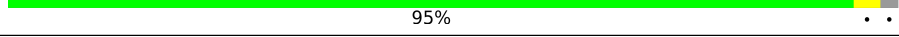
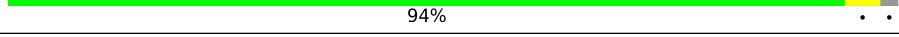
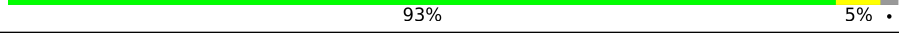
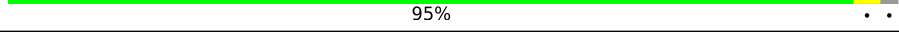
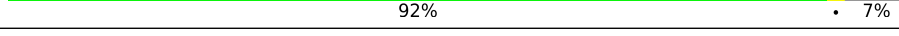
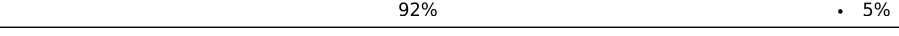
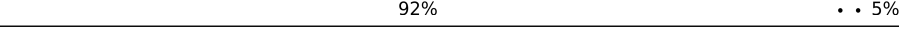
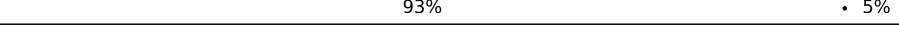
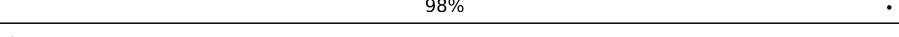
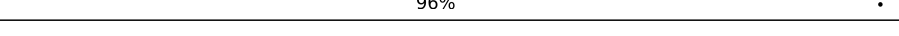
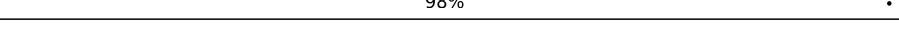
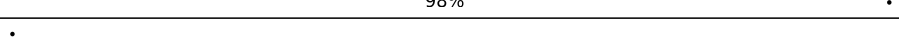
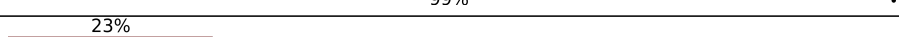
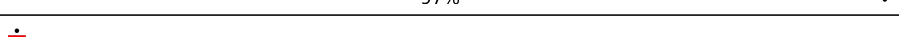
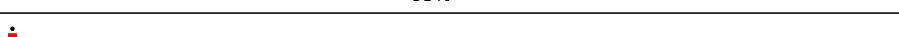






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Mol	Chain	Length	Quality of chain
2	i	365	57% 80% 17%
2	j	365	53% 81% 17%
2	k	365	58% 80% 17%
2	l	365	57% 80% 17%
2	m	365	54% 80% 17%
2	n	365	55% 80% 17%
2	o	365	55% 80% 17%
2	p	365	53% 80% 17%
2	q	365	57% 80% 17%
2	r	365	51% 80% 17%
2	s	365	54% 80% 17%
2	t	365	55% 80% 17%
2	u	365	62% 80% 17%
2	v	365	59% 80% 17%
2	w	365	57% 80% 17%
2	x	365	59% 80% 17%
2	y	365	60% 80% 17%
2	z	365	58% 80% 17%
3	0	260	93% 5%
3	1	260	93%
3	2	260	98%
3	3	260	98%
3	4	260	97%
3	5	260	97%
3	6	260	97%

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Mol	Chain	Length	Quality of chain
3	7	260	 98%
3	8	260	 98%
3	9	260	 97%
3	AF	260	 95%
3	AG	260	 95%
3	AH	260	 94%
3	AI	260	 93% 5%
3	AJ	260	 95%
3	AK	260	 92% 7%
3	AL	260	 92% 5%
3	AM	260	 92% 5%
3	AN	260	 93% 5%
3	ZA	260	 98%
3	ZB	260	 96%
3	ZC	260	 98%
3	ZD	260	 98%
3	ZE	260	 99%
4	ZF	403	 23% 97%
4	ZG	403	 95%
4	ZH	403	 97%
4	ZI	403	 97%
4	ZJ	403	 98%
4	ZK	403	 98%
4	ZL	403	 97%
4	ZM	403	 97%

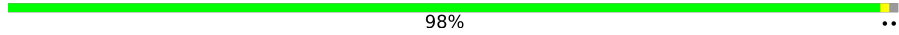






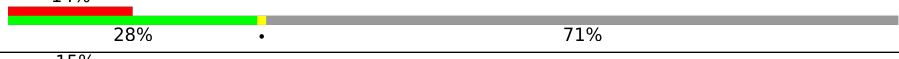









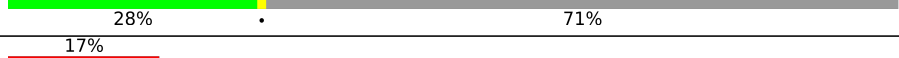





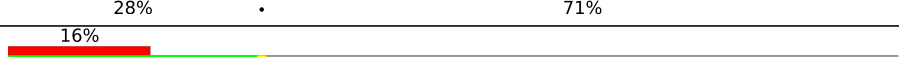

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Mol	Chain	Length	Quality of chain
4	ZN	403	97%
4	ZO	403	97%
4	ZP	403	95%
4	ZQ	403	97%
4	ZR	403	97%
4	ZS	403	98%
4	ZT	403	6% 98%
4	ZU	403	9% 99%
4	ZV	403	11% 98%
4	ZW	403	16% 96%
4	ZX	403	18% 99%
4	ZY	403	26% 98%
4	ZZ	403	29% 98%
4	Za	403	34% 98%
4	Zb	403	34% 98%
4	Zc	403	38% 97%
4	Zd	403	42% 98%
4	Ze	403	45% 97%
4	Zf	403	47% 98%
4	Zg	403	51% 98%
4	Zh	403	53% 98%
5	AA	251	96%
5	AB	251	98%
5	AC	251	97%
5	AD	251	99%



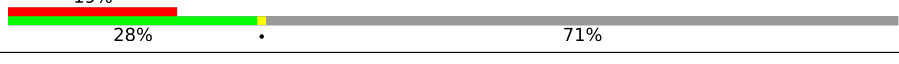
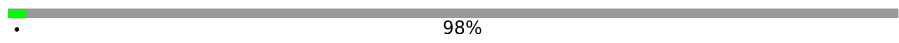


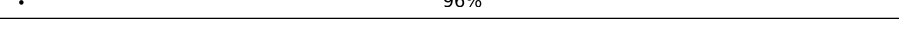
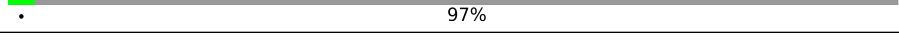
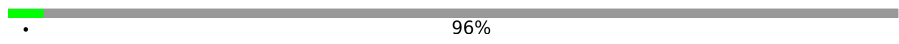


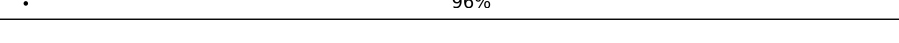
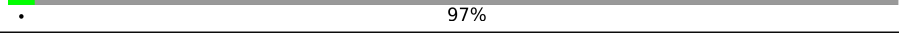
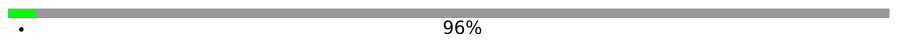
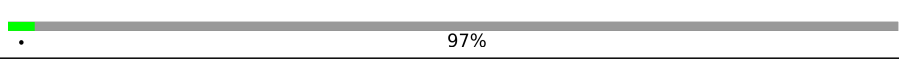
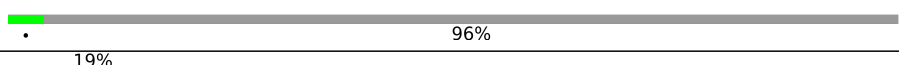




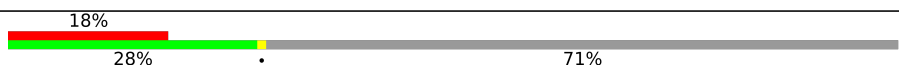




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Mol	Chain	Length	Quality of chain
5	AE	251	 98%
6	AO	560	 18% 28% 71%
6	AP	560	 18% 28% 71%
6	AQ	560	 19% 28% 71%
6	AR	560	 14% 28% 71%
6	AS	560	 17% 28% 71%
6	AT	560	 15% 28% 71%
6	AU	560	 14% 28% 71%
6	AV	560	 15% 28% 71%
6	AW	560	 15% 28% 71%
6	AX	560	 13% 28% 71%
6	AY	560	 14% 28% 71%
6	AZ	560	 14% 28% 71%
6	Aa	560	 14% 28% 71%
6	Ac	560	 17% 28% 71%
6	Ad	560	 15% 28% 71%
6	Ae	560	 16% 28% 71%
6	Af	560	 17% 28% 71%
6	Ag	560	 17% 28% 71%
6	Ah	560	 18% 28% 71%
6	Ai	560	 20% 28% 71%
6	Aj	560	 18% 28% 71%
6	Ak	560	 19% 28% 71%
6	Al	560	 18% 28% 71%
6	Am	560	 16% 28% 71%

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Mol	Chain	Length	Quality of chain
6	An	560	 15% 28% 71%
6	Ao	560	 15% 28% 71%
6	Ap	560	 19% 28% 71%
6	BG	560	 98%
6	BH	560	 97%
6	BI	560	 96%
6	BJ	560	 97%
6	BK	560	 96%
6	BL	560	 97%
6	BM	560	 96%
6	BN	560	 97%
6	BO	560	 96%
6	BP	560	 97%
6	BQ	560	 96%
6	BR	560	 19% 28% 71%
6	BS	560	 18% 28% 71%
6	BT	560	 20% 28% 71%
6	BU	560	 20% 28% 71%
6	BV	560	 19% 28% 71%
6	BW	560	 18% 28% 71%
6	BX	560	 18% 28% 71%
6	UI	560	 27% 25% 72%
6	UJ	560	 27% 25% 72%
6	UK	560	 28% 25% 72%
6	UL	560	 27% 25% 72%

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Mol	Chain	Length	Quality of chain
6	UM	560	27% 25% 72%
6	UN	560	27% 25% 72%
6	UO	560	27% 25% 72%
6	UP	560	27% 25% 72%
6	WA	560	6% 18% 80%
6	WB	560	7% 18% 80%
6	WC	560	7% 17% 81%
6	WD	560	9% 18% 80%
6	WE	560	9% 18% 80%
6	WF	560	11% 18% 80%
6	WG	560	13% 18% 80%
6	WH	560	11% 16% 83%
6	WI	560	13% 15% 83%
6	WJ	560	14% 16% 82%
6	WK	560	14% 16% 82%
6	WL	560	13% 14% 85%
6	WM	560	12% 14% 85%
6	WN	560	12% 14% 85%
6	WO	560	10% 16% 83%
6	WP	560	9% 16% 82%
6	WQ	560	9% 18% 80%
6	WR	560	10% 17% 80%
6	WS	560	7% 18% 80%
6	WT	560	6% 17% 80%
6	WU	560	8% 19% 80%

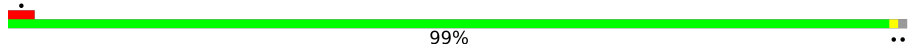
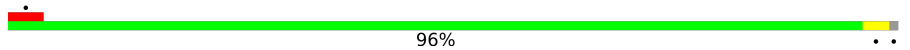
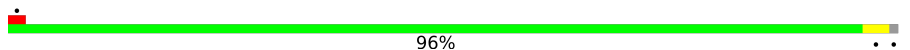

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Mol	Chain	Length	Quality of chain
6	WV	560	8% 17% 80%
6	WW	560	8% 18% 80%
7	Ab	89	13% 99%
7	Aq	89	99%
7	Ar	89	100%
7	As	89	7% 99%
8	At	264	10% 91%
9	Au	245	81% 16%
9	Av	245	82% 15%
9	Aw	245	83% 15%
9	Ax	245	82% 15%
9	Ay	245	83% 15%
10	A1	104	12% 84% 12%
10	A2	104	10% 85% 11% 5%
10	A3	104	11% 86% 11%
10	A4	104	18% 86% 11%
10	A5	104	20% 85% 12%
10	Az	104	16% 52% 43% 5%
11	A0	138	9% 85% 11%
11	A6	138	7% 93%
11	A7	138	7% 86% 12%
11	A8	138	7% 86% 9% 5%
11	A9	138	9% 91% 8%
12	BA	134	99%
12	BB	134	98%

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Mol	Chain	Length	Quality of chain
12	BC	134	 99%
12	BD	134	 96%
12	BE	134	 96%
12	BF	134	 96%

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 338677 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 L-ring protein.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
3	1	252	Total	C	N	O	S	0	0
			1894	1172	331	385	6		
3	2	260	Total	C	N	O	S	0	0
			1949	1202	341	400	6		

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

- Molecule 4 is a protein called Flagellar hook protein FlgE.

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AP	164	1275	776	237	259	3	0	0
6	AQ	164	1275	776	237	259	3	0	0
6	UI	155	1172	733	211	226	2	0	0
6	UJ	155	1172	733	211	226	2	0	0
6	UK	155	1172	733	211	226	2	0	0
6	UL	155	1172	733	211	226	2	0	0
6	UM	155	1172	733	211	226	2	0	0
6	UN	155	1172	733	211	226	2	0	0
6	UO	155	1172	733	211	226	2	0	0
6	UP	155	1172	733	211	226	2	0	0
6	WA	113	849	534	148	166	1	0	0
6	WB	111	836	526	146	163	1	0	0
6	WC	108	812	510	142	159	1	0	0
6	WD	110	827	522	144	160	1	0	0
6	WE	112	843	531	147	164	1	0	0
6	WF	111	834	526	145	162	1	0	0
6	WG	112	843	531	147	164	1	0	0
6	WH	95	703	439	126	137	1	0	0
6	WI	95	703	439	126	137	1	0	0
6	WJ	99	737	462	131	143	1	0	0
6	WK	98	729	456	130	142	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	WL	85	Total 622	C 389	N 110	O 122	S 1	0	0
6	WM	82	Total 596	C 372	N 107	O 116	S 1	0	0
6	WN	84	Total 611	C 380	N 109	O 121	S 1	0	0
6	WO	96	Total 714	C 448	N 127	O 138	S 1	0	0
6	WP	100	Total 741	C 464	N 132	O 144	S 1	0	0
6	WQ	111	Total 834	C 526	N 145	O 162	S 1	0	0
6	WR	111	Total 834	C 526	N 145	O 162	S 1	0	0
6	WS	111	Total 834	C 526	N 145	O 162	S 1	0	0
6	WT	111	Total 834	C 526	N 145	O 162	S 1	0	0
6	WU	112	Total 843	C 531	N 147	O 164	S 1	0	0
6	WV	110	Total 827	C 521	N 144	O 161	S 1	0	0
6	WW	111	Total 834	C 526	N 145	O 162	S 1	0	0
6	BG	13	Total 81	C 50	N 15	O 16		0	0
6	BH	16	Total 103	C 64	N 19	O 20		0	0
6	BI	20	Total 133	C 83	N 23	O 27		0	0
6	BJ	16	Total 103	C 64	N 19	O 20		0	0
6	BK	21	Total 140	C 88	N 24	O 28		0	0
6	BL	16	Total 103	C 64	N 19	O 20		0	0
6	BM	21	Total 140	C 88	N 24	O 28		0	0
6	BN	16	Total 103	C 64	N 19	O 20		0	0
6	BO	20	Total 133	C 83	N 23	O 27		0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	BP	16	Total	C	N	O			
			103	64	19	20	0	0	
6	BQ	21	Total	C	N	O			
			140	88	24	28	0	0	
6	BR	164	Total	C	N	O	S		
			1275	776	237	259	3	0	
6	BS	164	Total	C	N	O	S		
			1275	776	237	259	3	0	
6	BT	164	Total	C	N	O	S		
			1275	776	237	259	3	0	
6	BU	164	Total	C	N	O	S		
			1275	776	237	259	3	0	
6	BV	164	Total	C	N	O	S		
			1275	776	237	259	3	0	
6	BW	164	Total	C	N	O	S		
			1275	776	237	259	3	0	
6	BX	164	Total	C	N	O	S		
			1275	776	237	259	3	0	

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Au	207	Total	C	N	O	S		
			1605	1072	249	272	12	0	

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

- Molecule 10 is a protein called Flagellar hook-basal body complex protein FliE.

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

- Molecule 11 is a protein called Flagellar basal body rod protein FlgB.

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

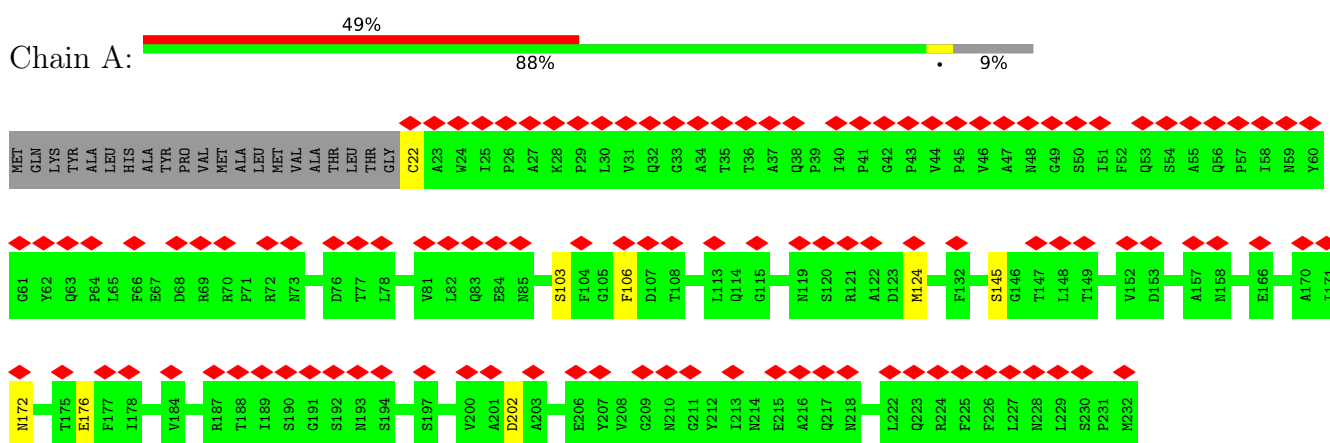
- Molecule 12 is a protein called Flagellar basal-body rod protein FlgC.

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

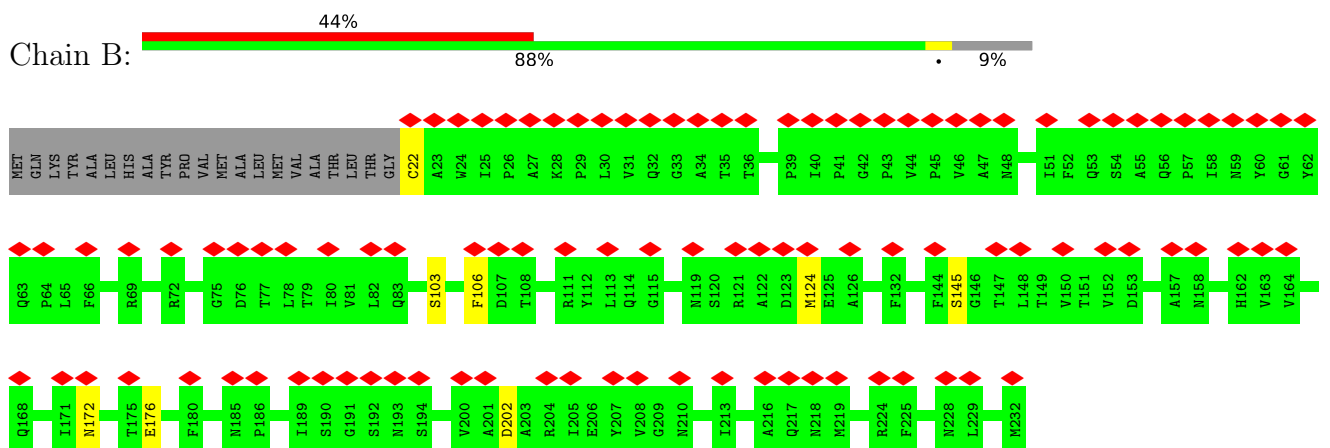
### 3 Residue-property plots [i](#)

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

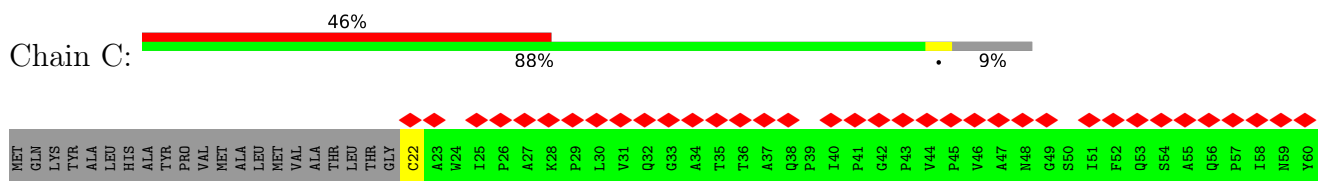
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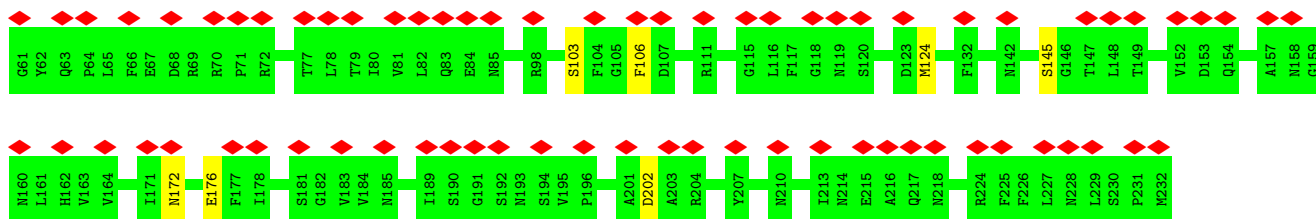
- Molecule 1: Flagellar L-ring protein



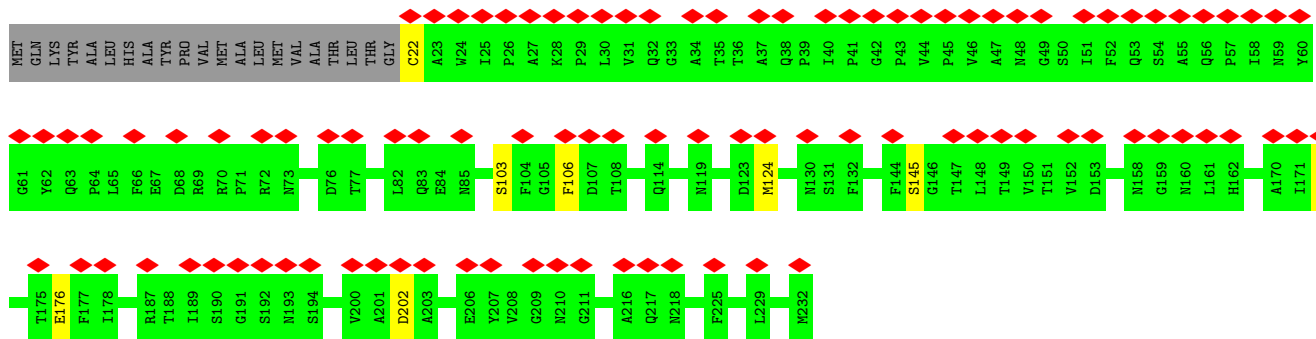
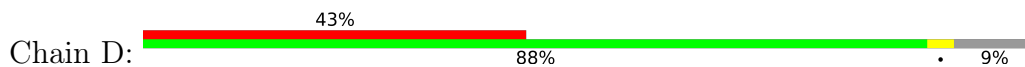
- Molecule 1: Flagellar L-ring protein



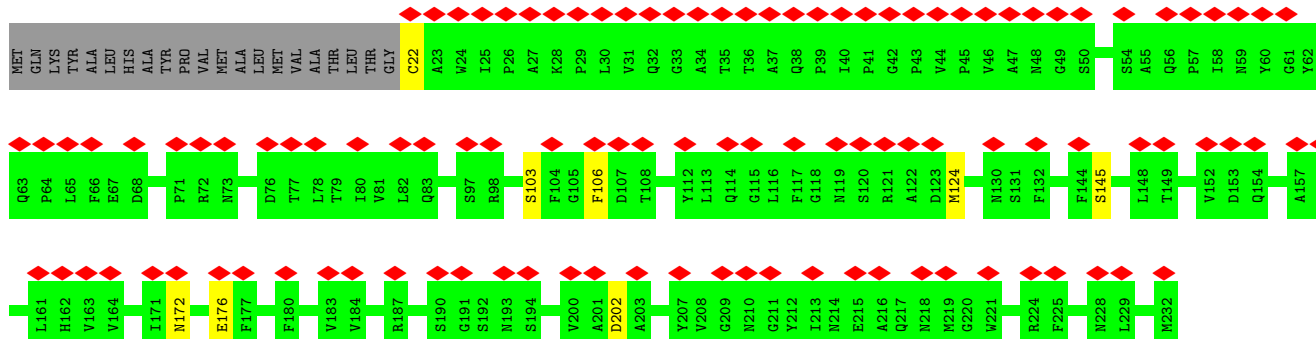
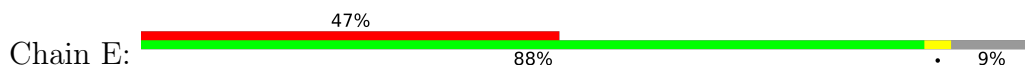




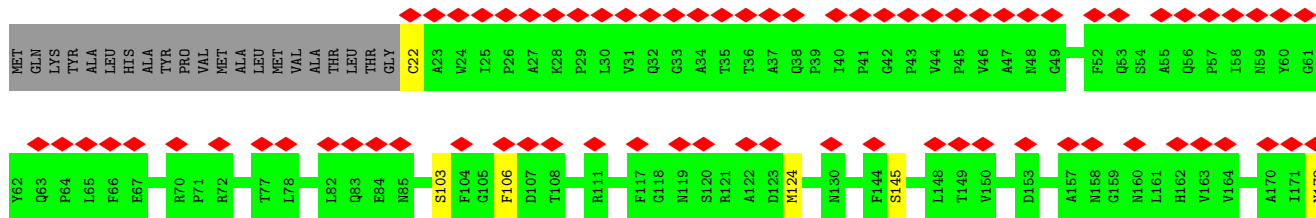
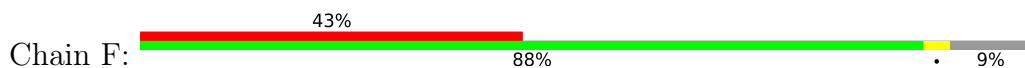
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

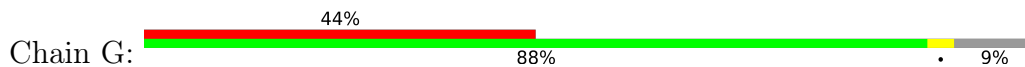


• Molecule 1: Flagellar L-ring protein

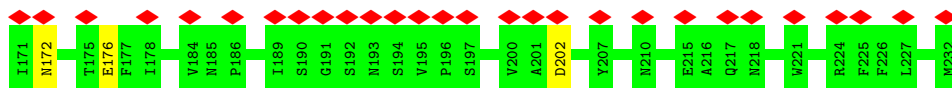
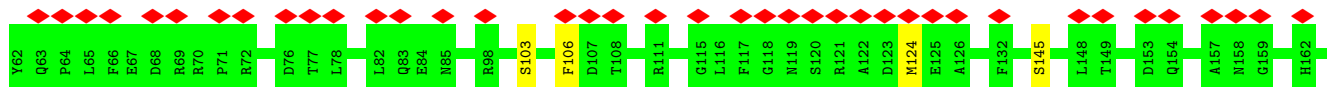
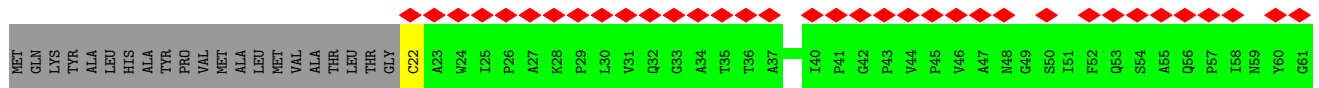




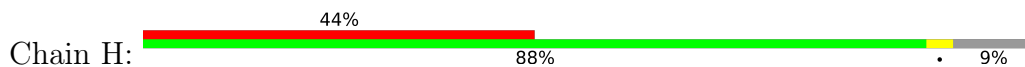
• Molecule 1: Flagellar L-ring protein



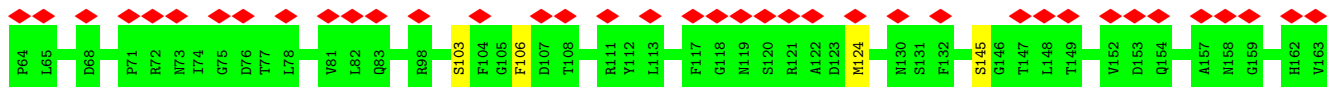
Chain G:



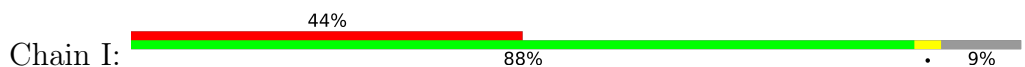
• Molecule 1: Flagellar L-ring protein



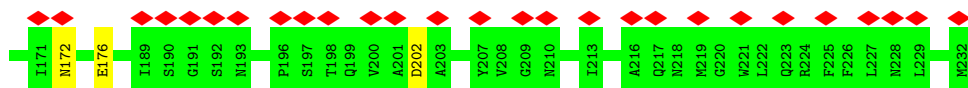
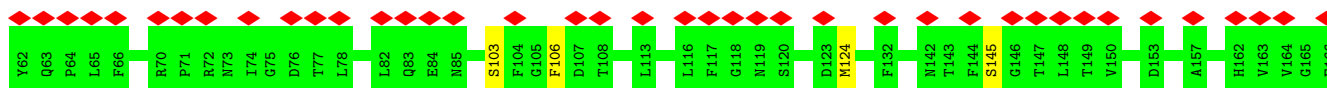
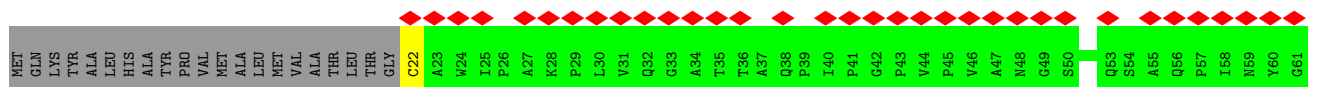
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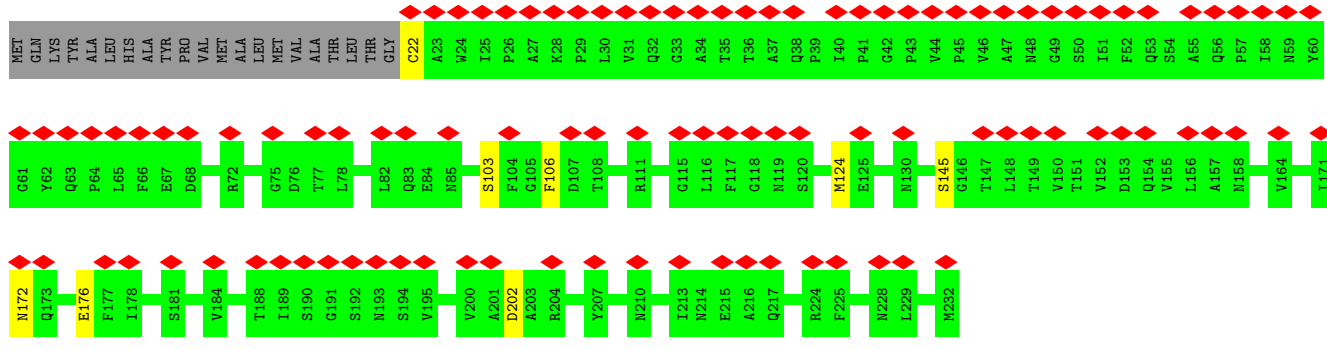
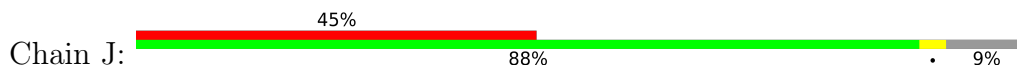
• Molecule 1: Flagellar L-ring protein



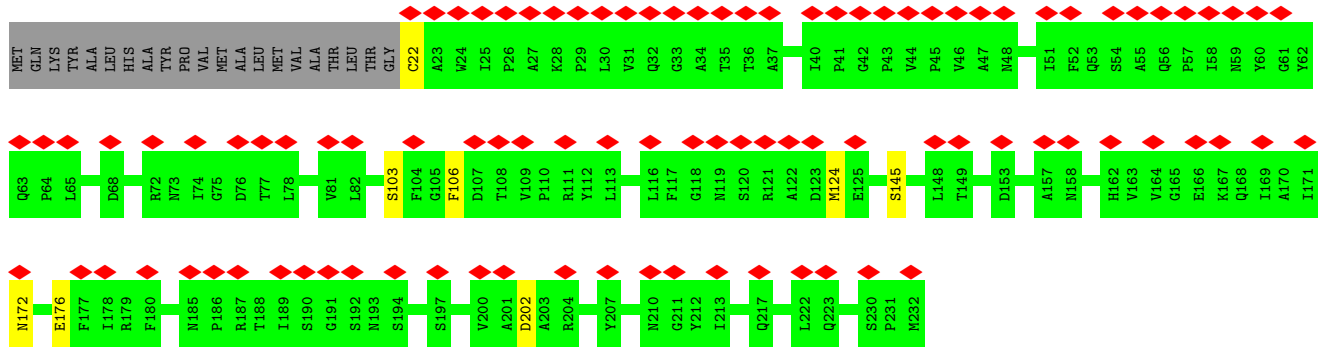
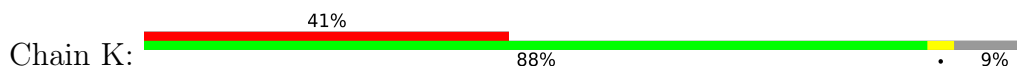
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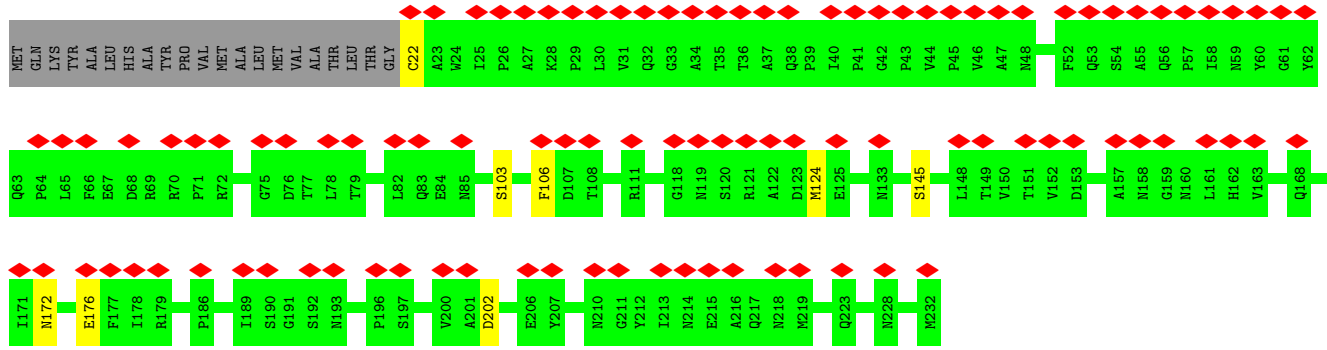
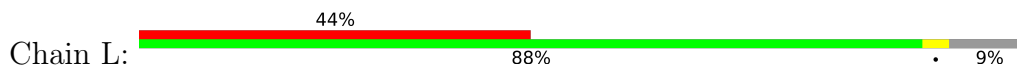
• Molecule 1: Flagellar L-ring protein



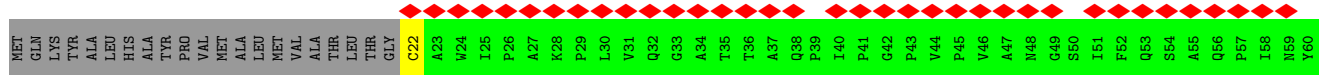
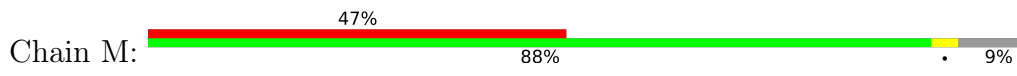
• Molecule 1: Flagellar L-ring protein

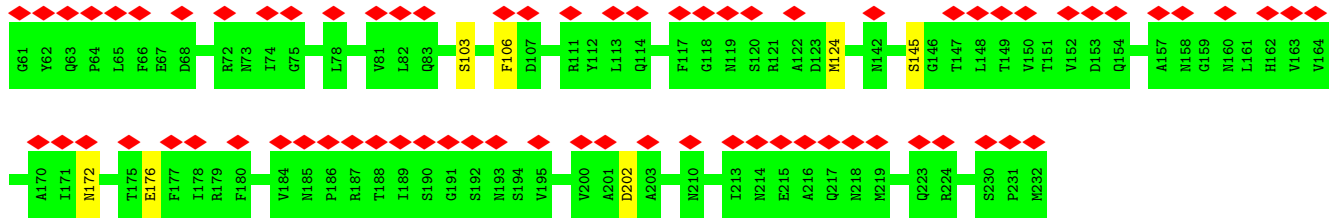


• Molecule 1: Flagellar L-ring protein

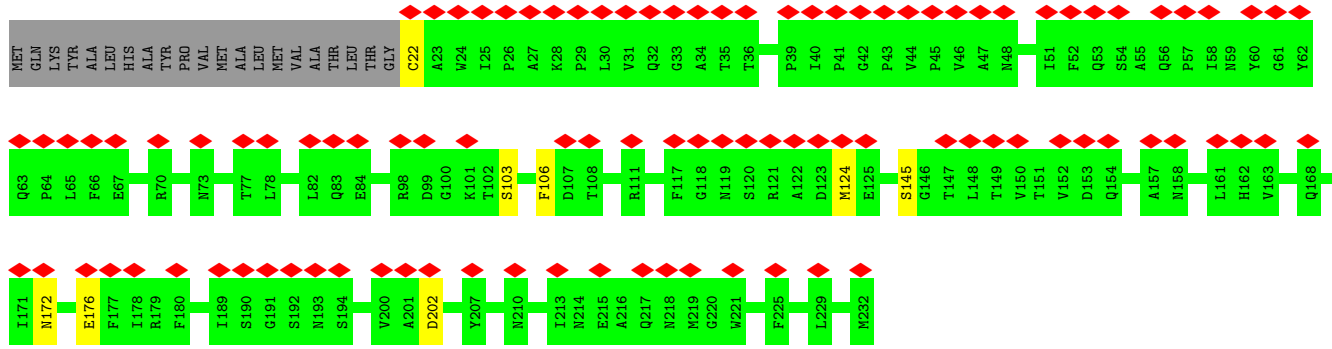
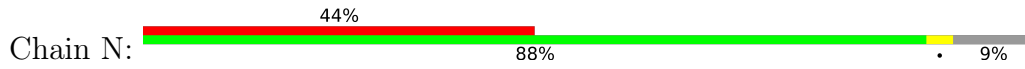


• Molecule 1: Flagellar L-ring protein

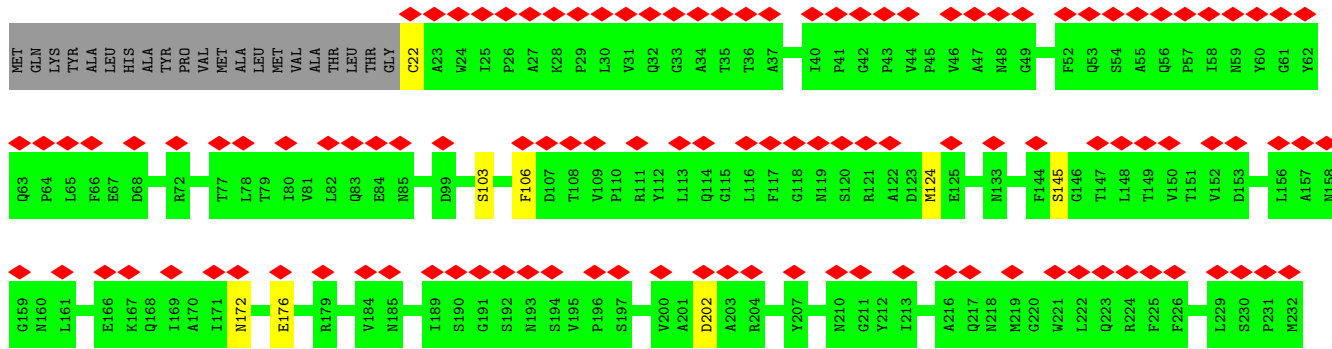
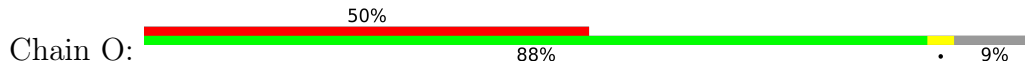




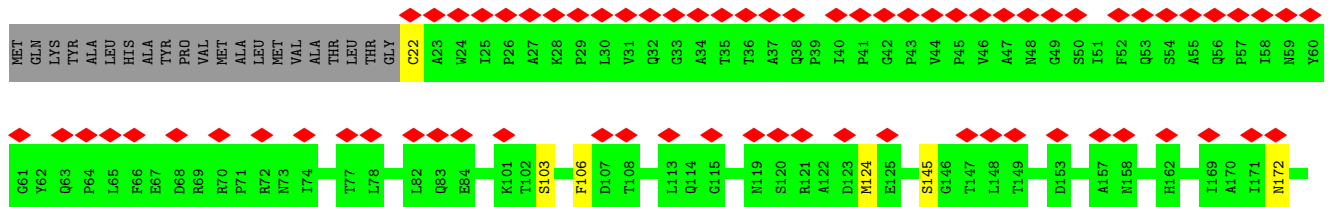
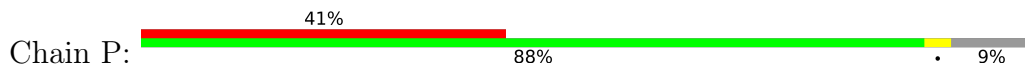
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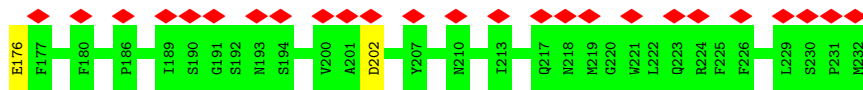


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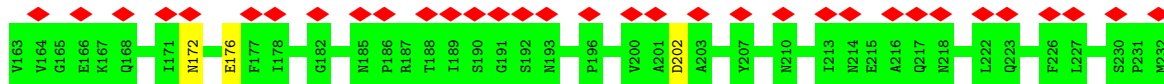
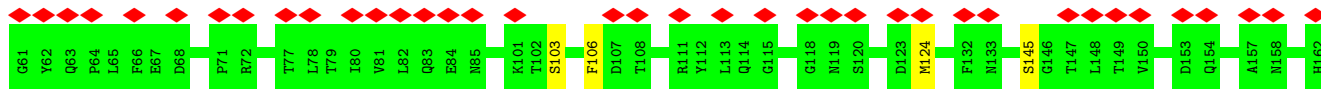
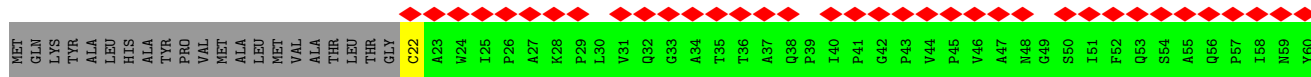
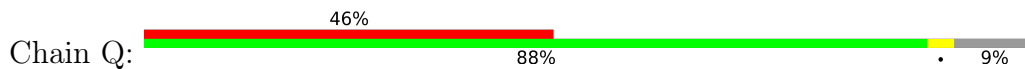


• Molecule 1: Flagellar L-ring protein

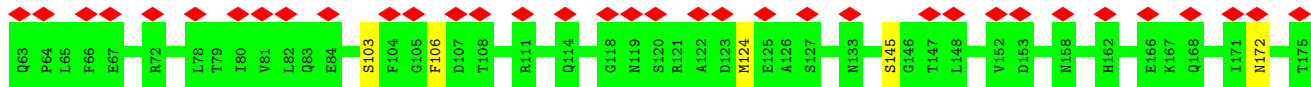
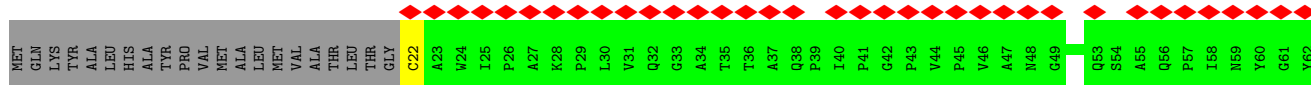
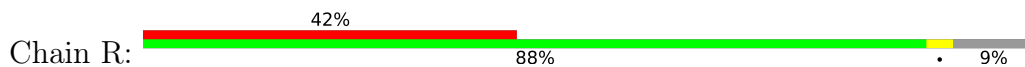




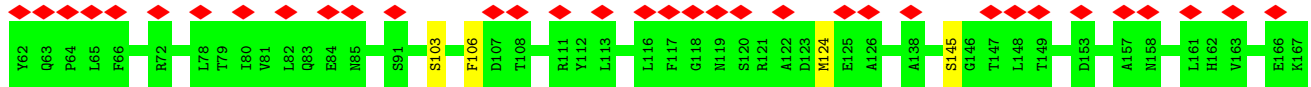
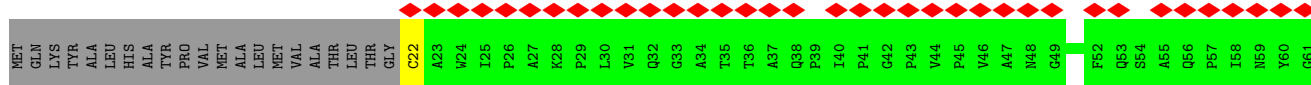
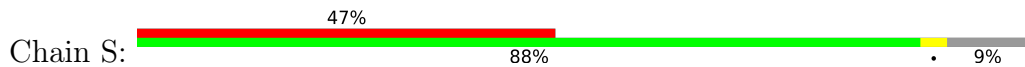
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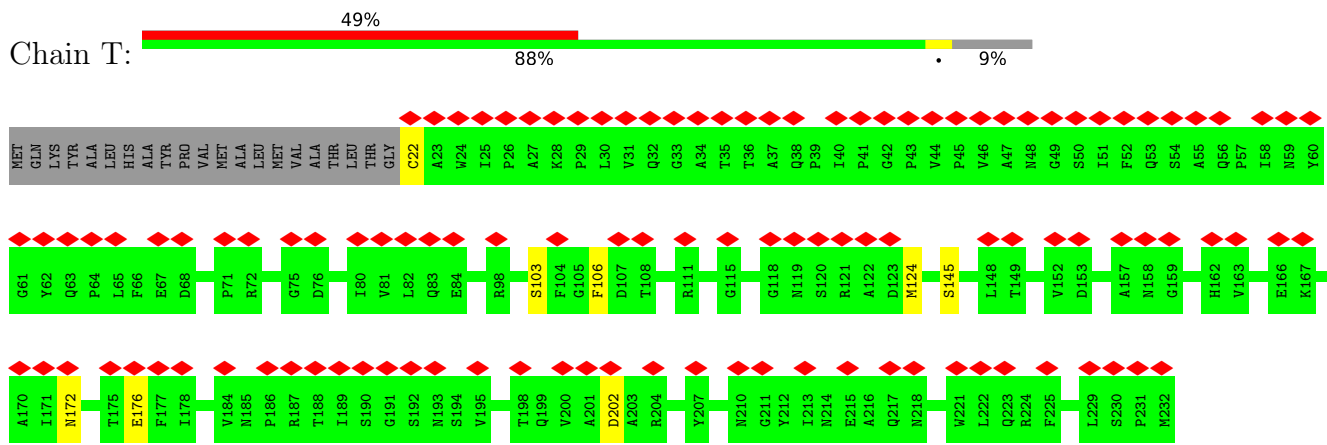
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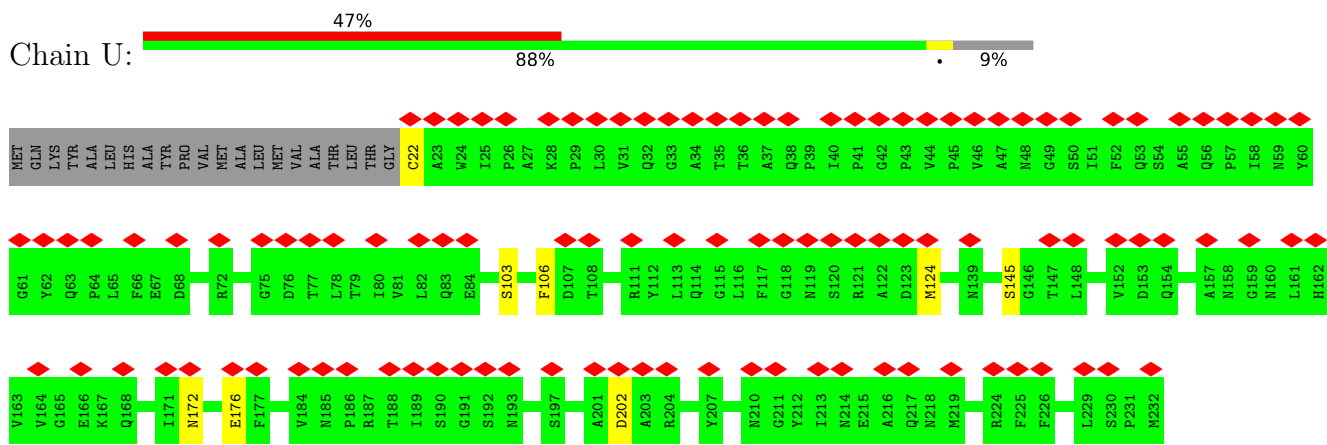
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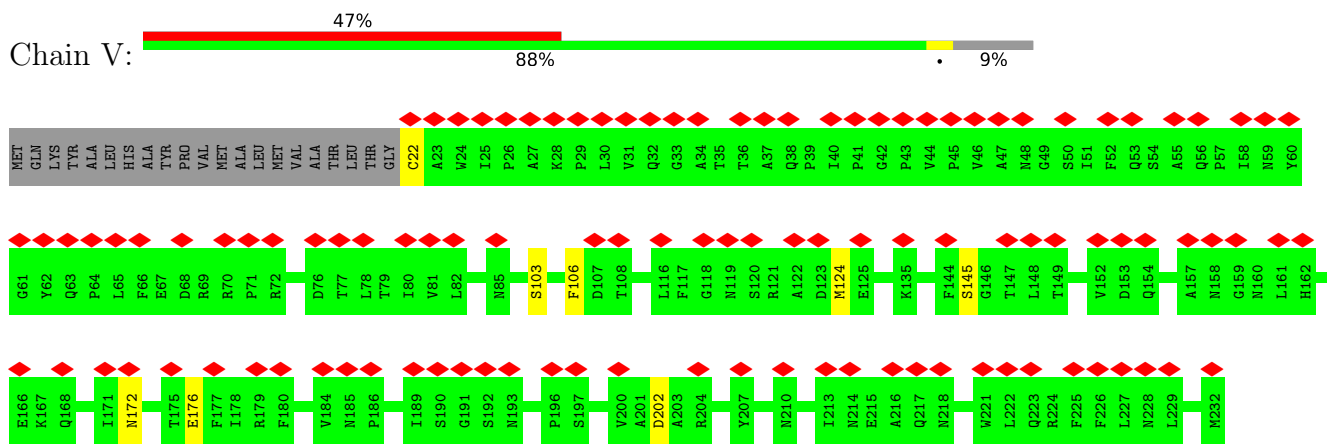
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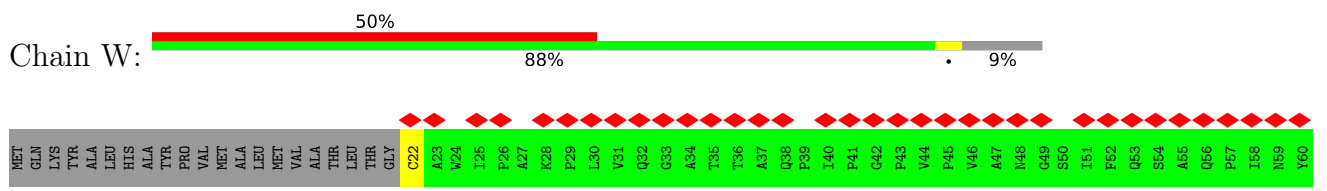
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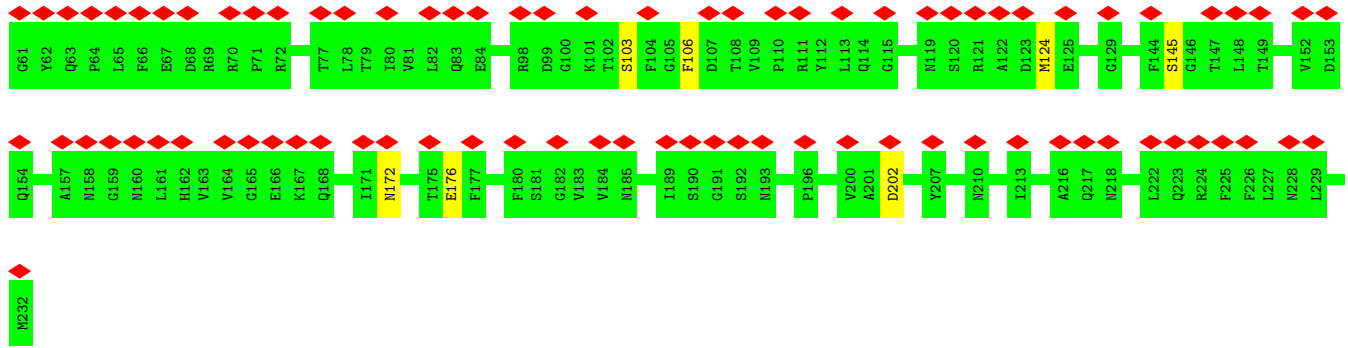


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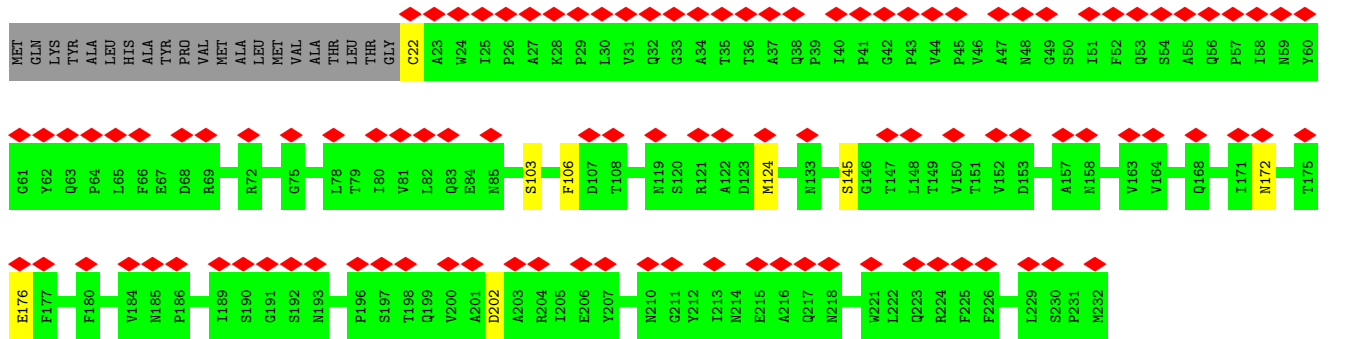
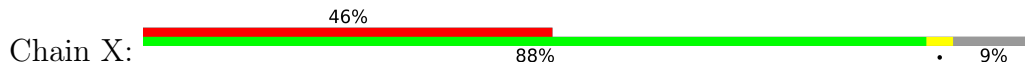


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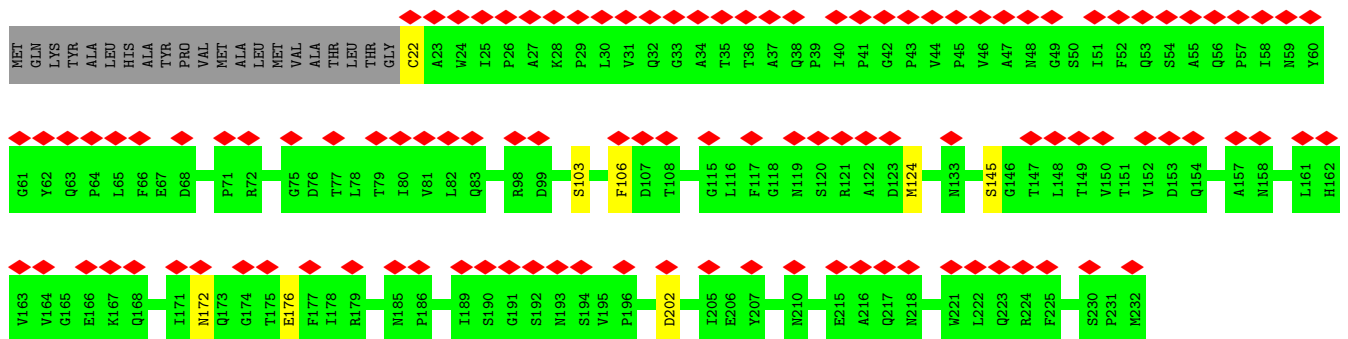
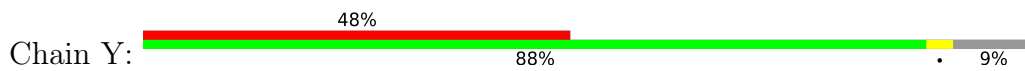




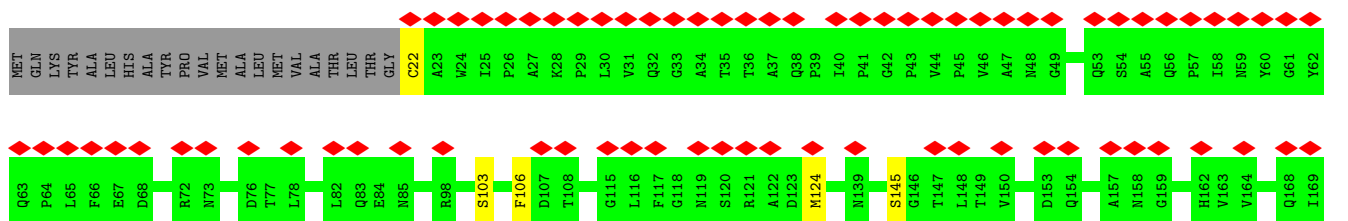
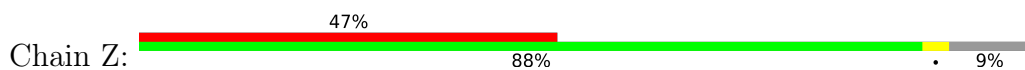
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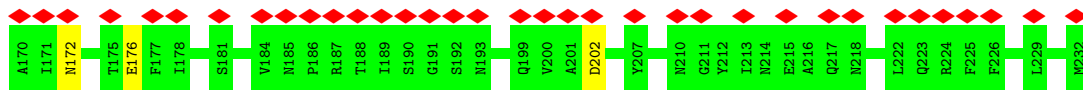


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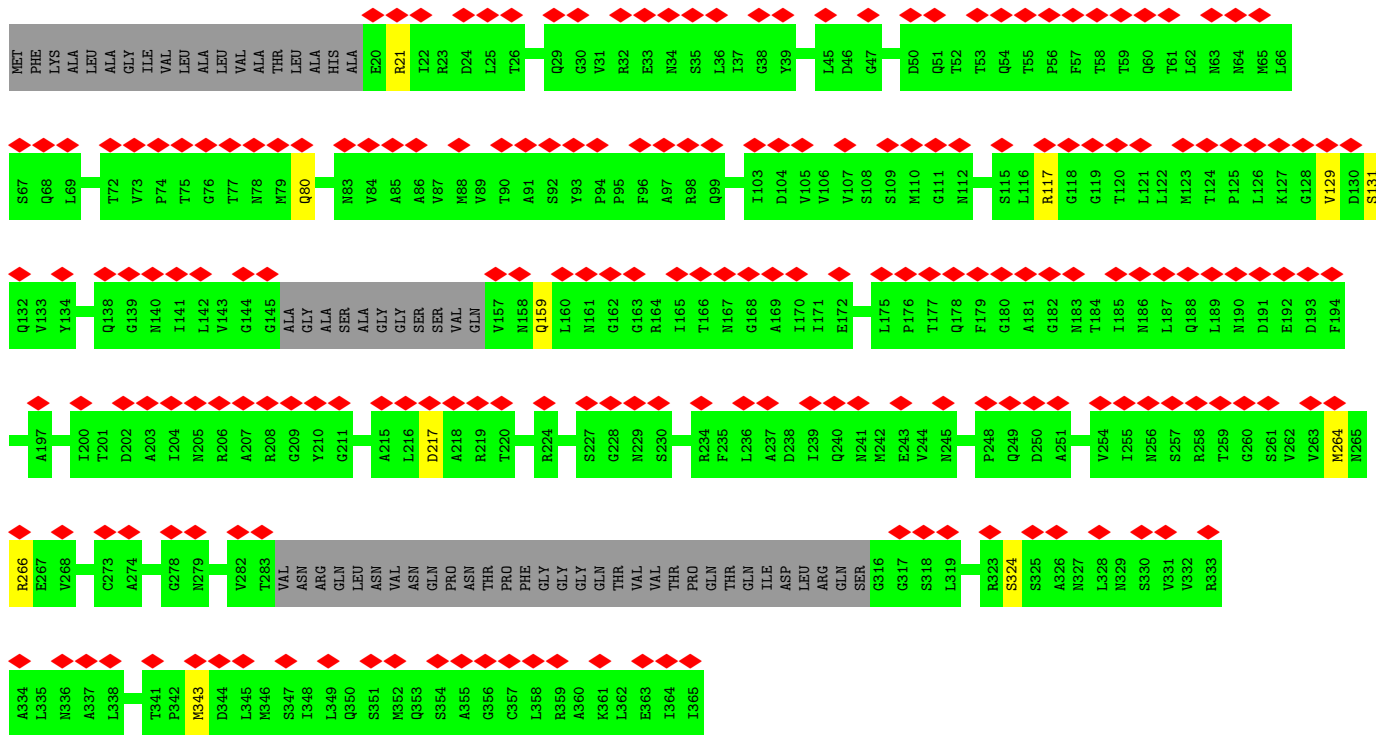
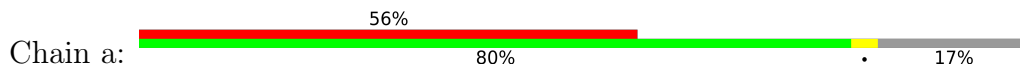


• Molecule 1: Flagellar L-ring protein

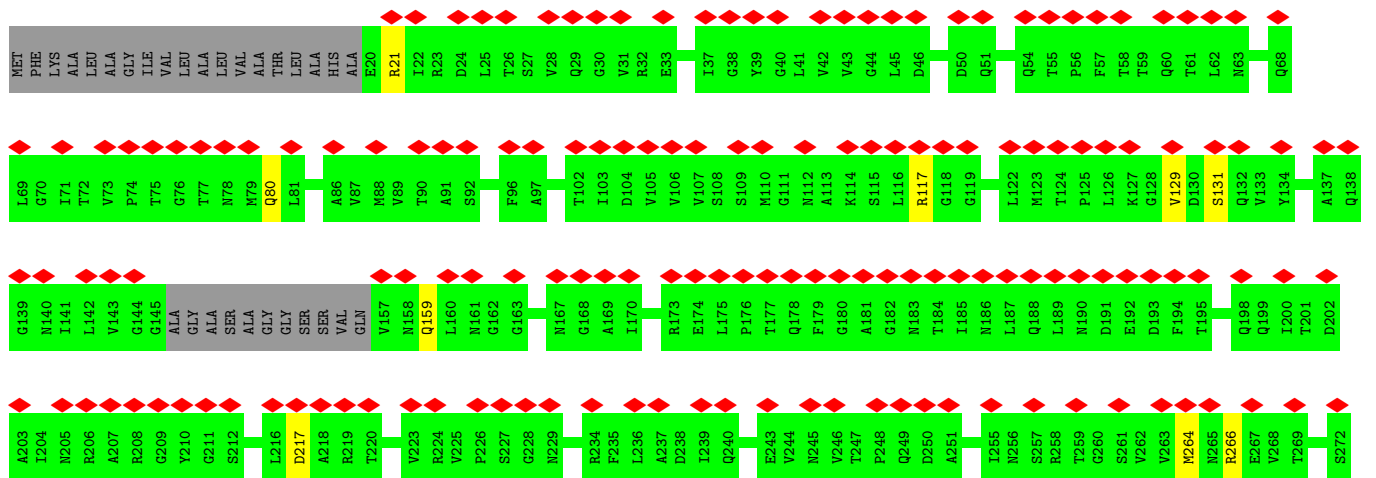
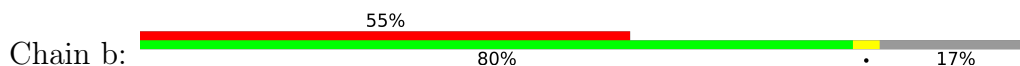




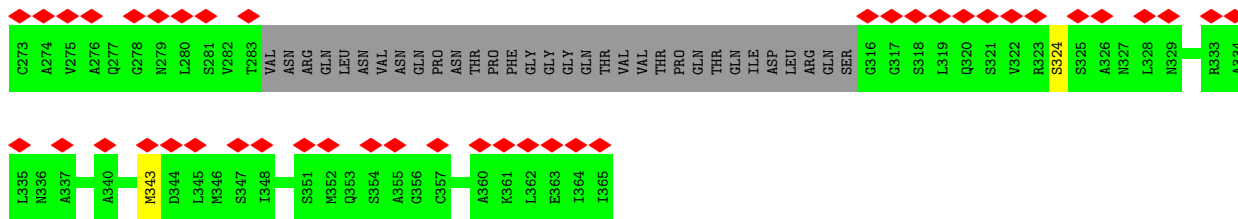
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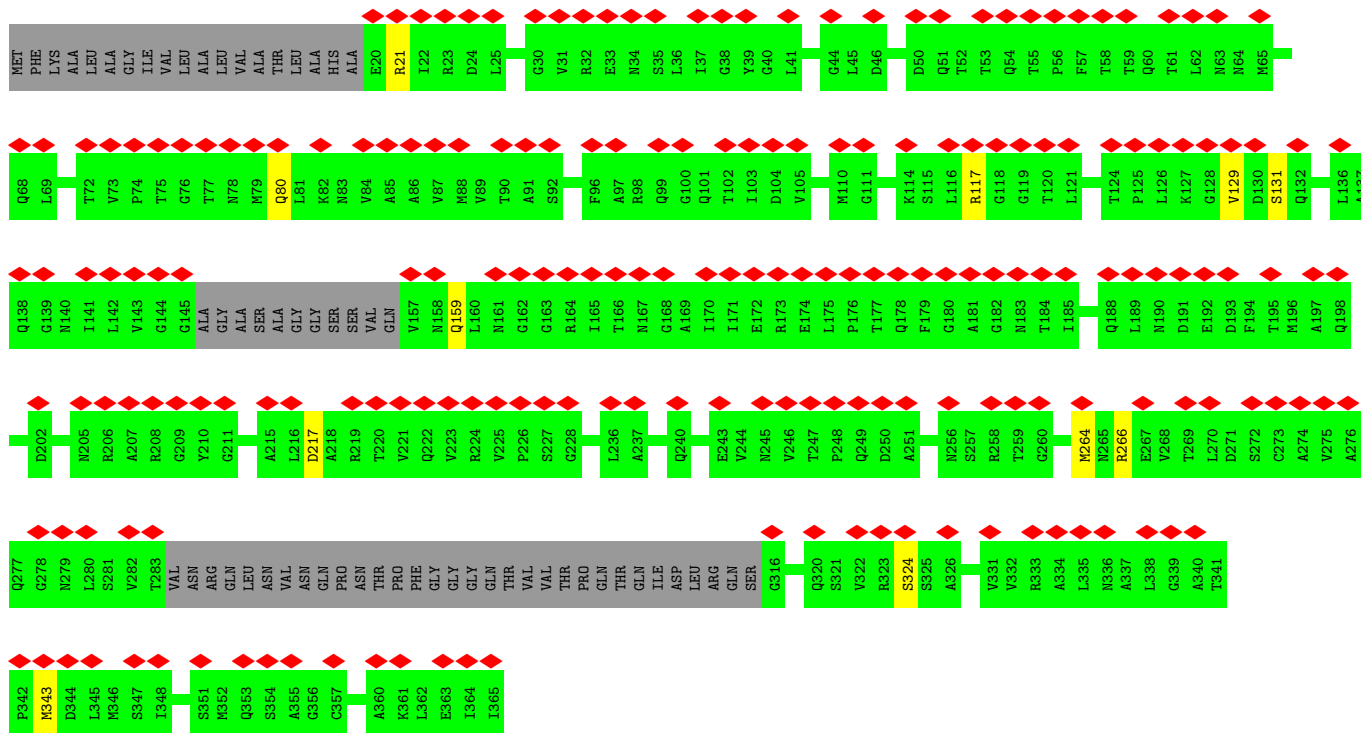
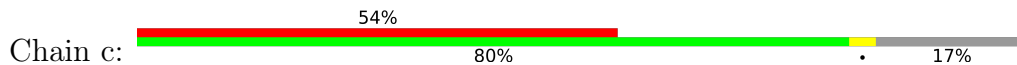
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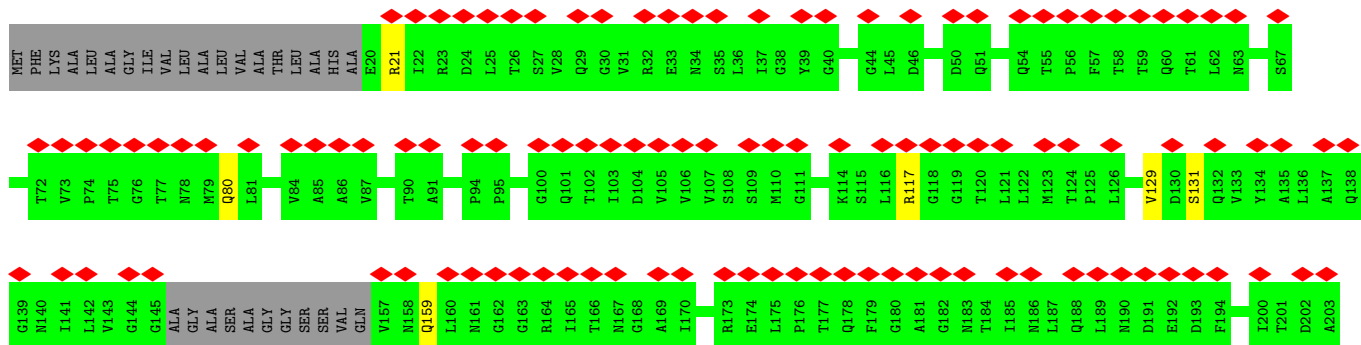
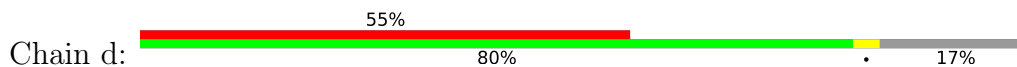


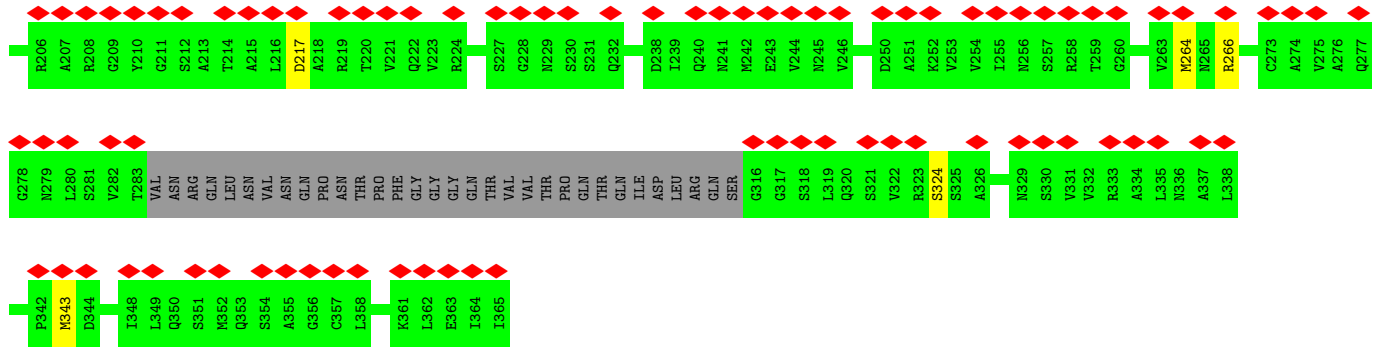


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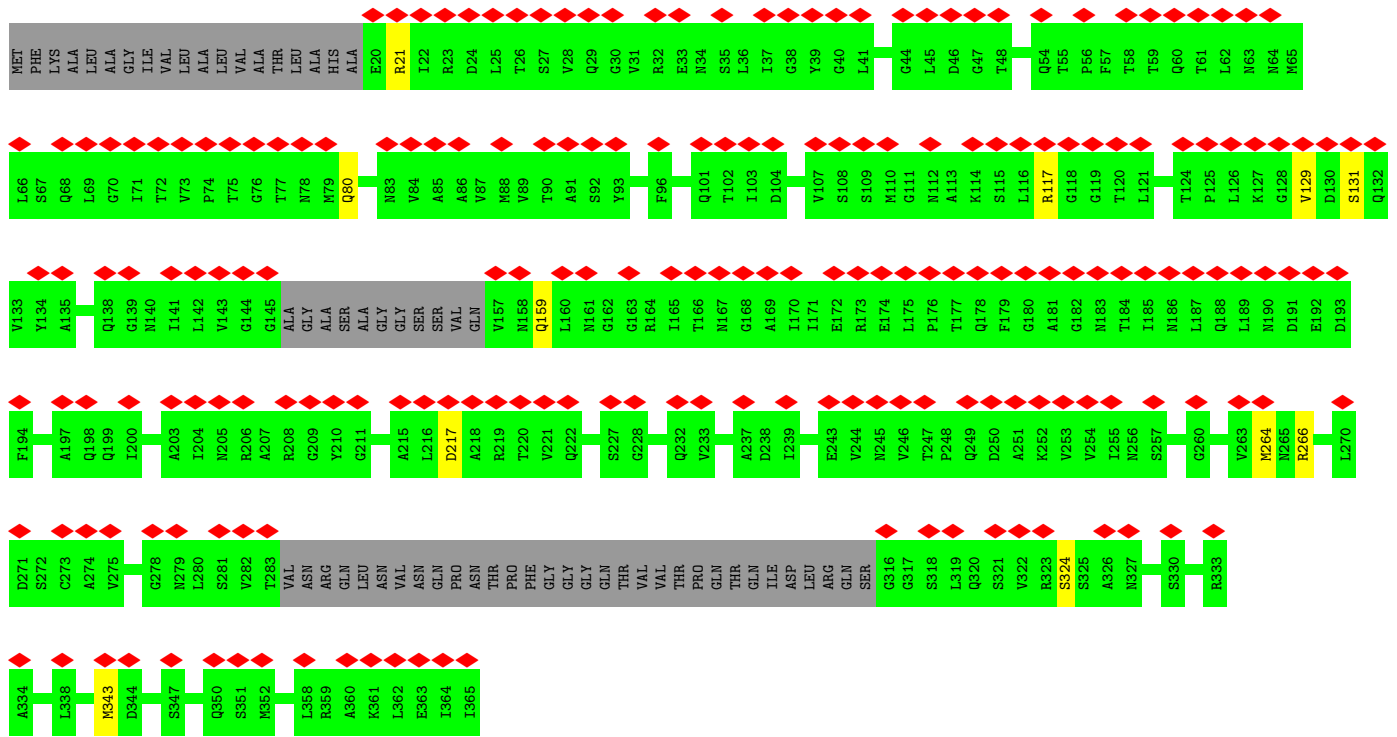
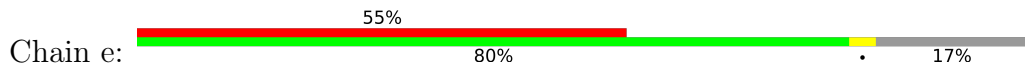


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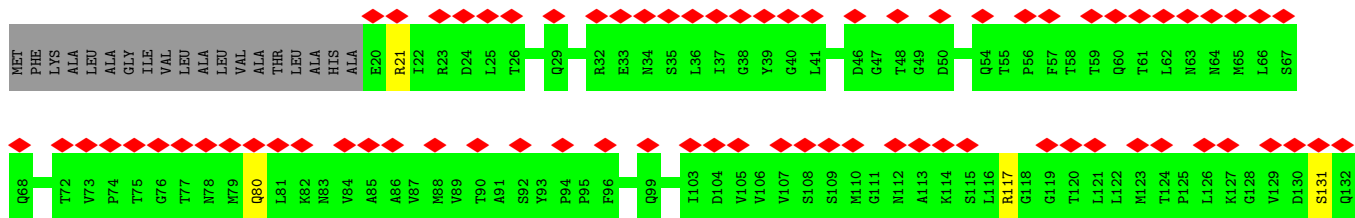
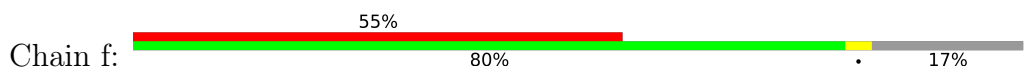


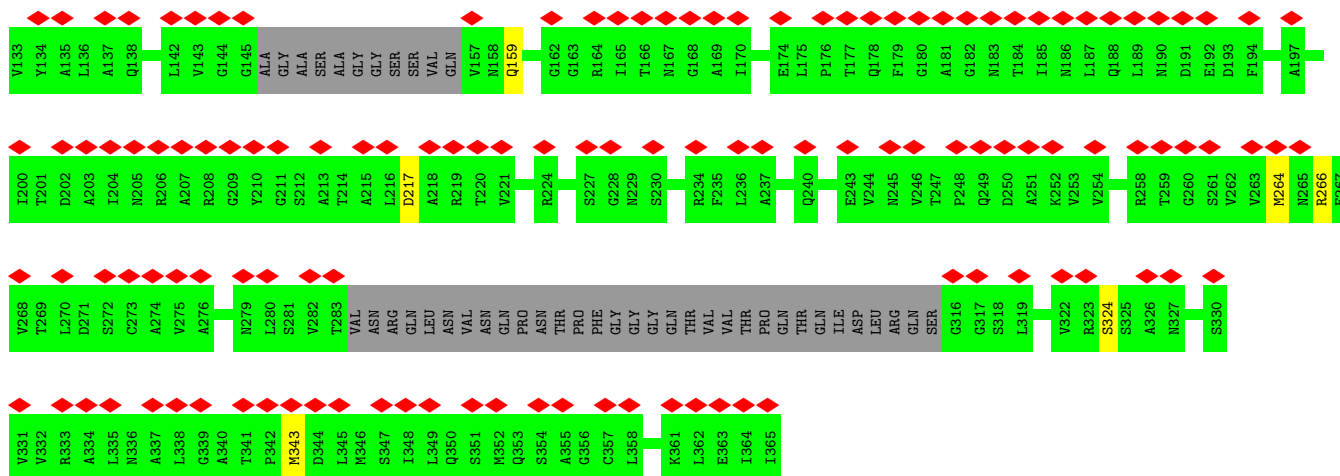


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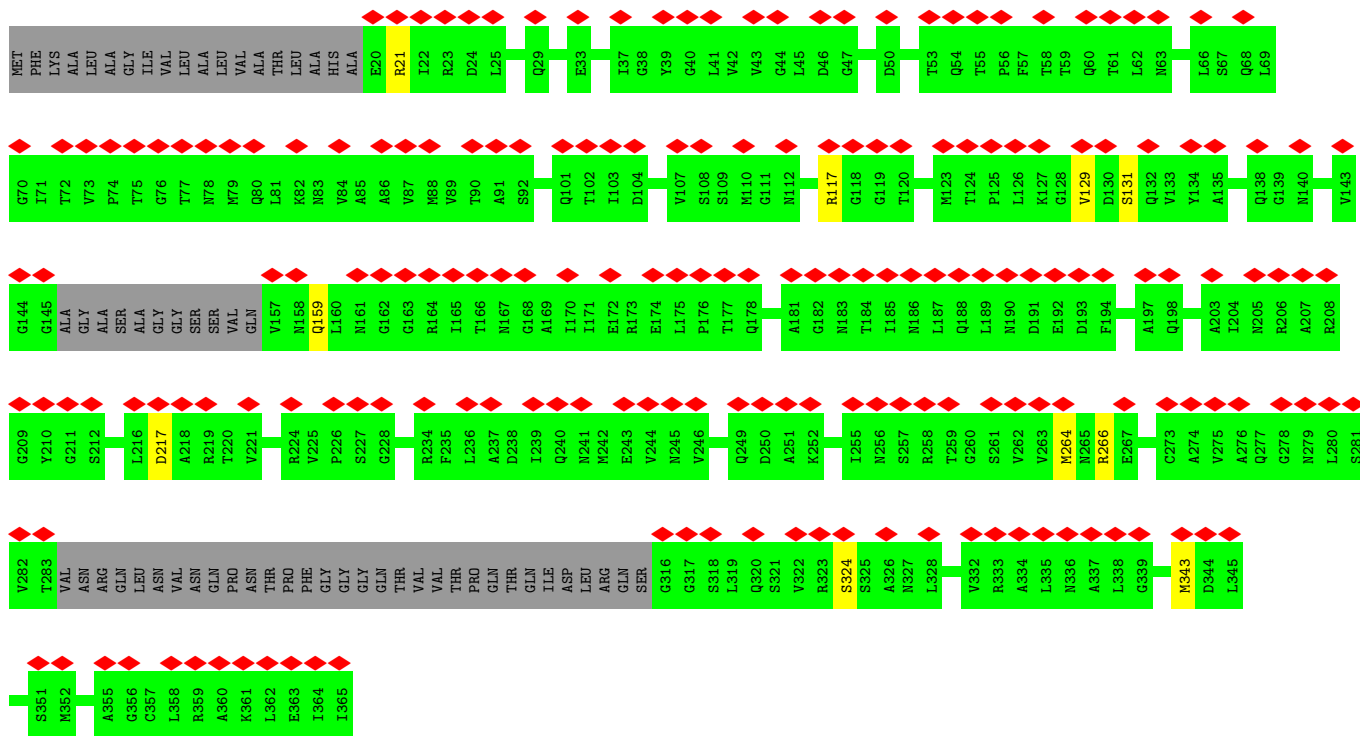
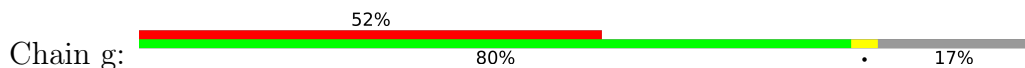


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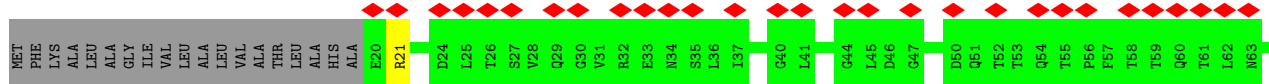
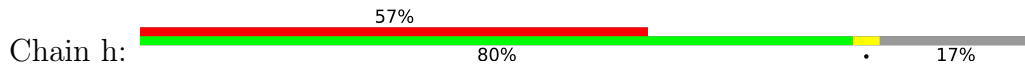


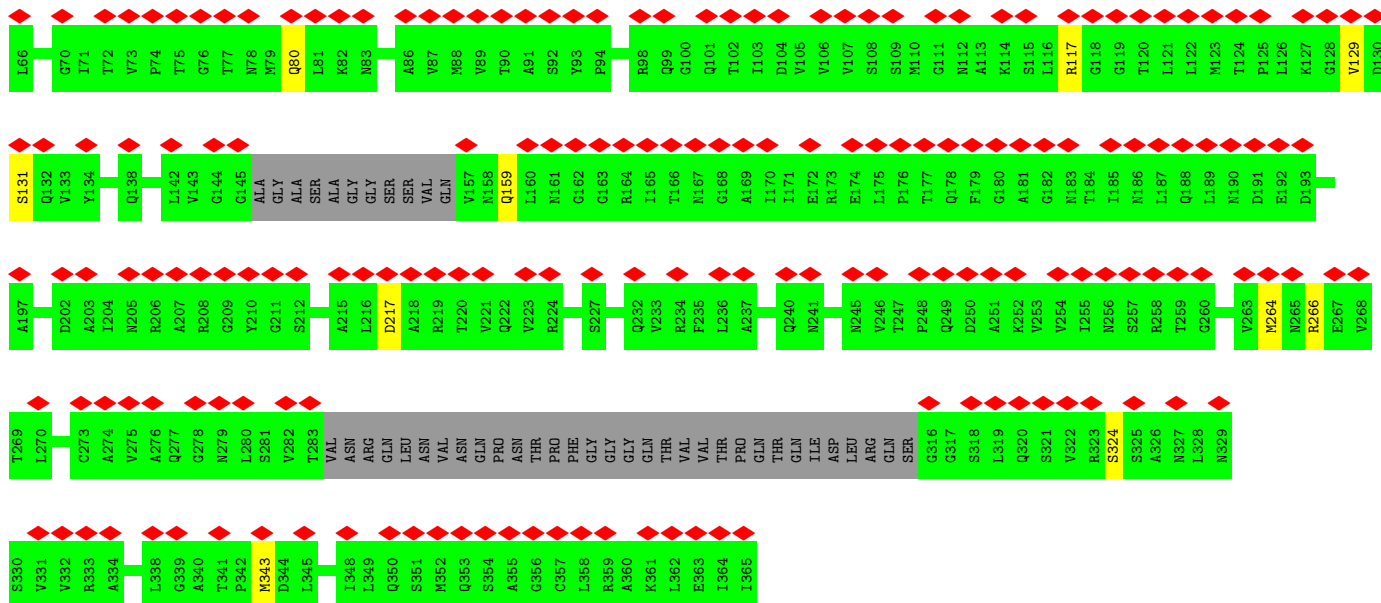


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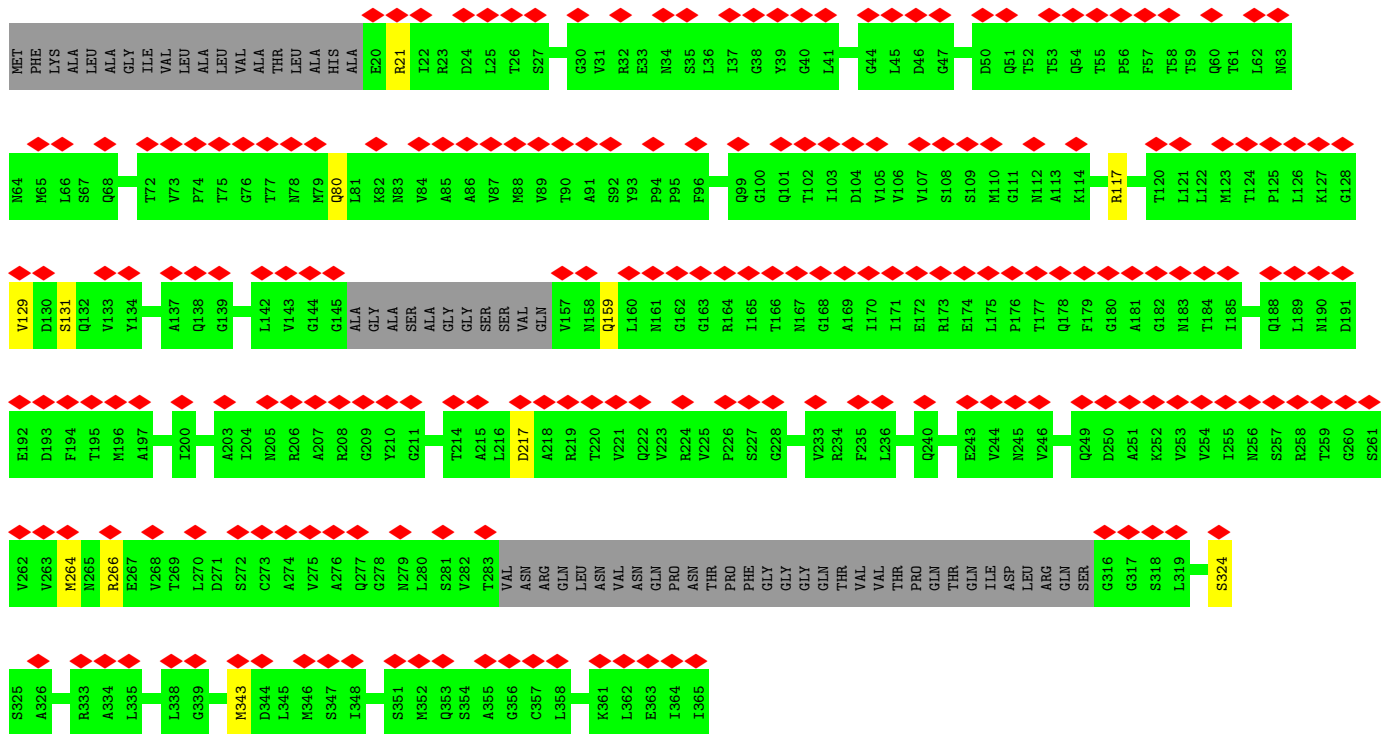
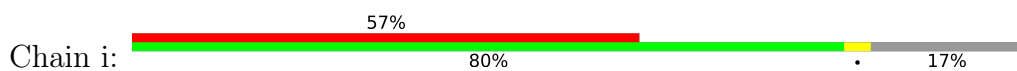


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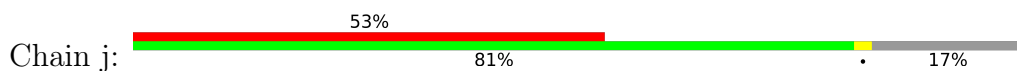


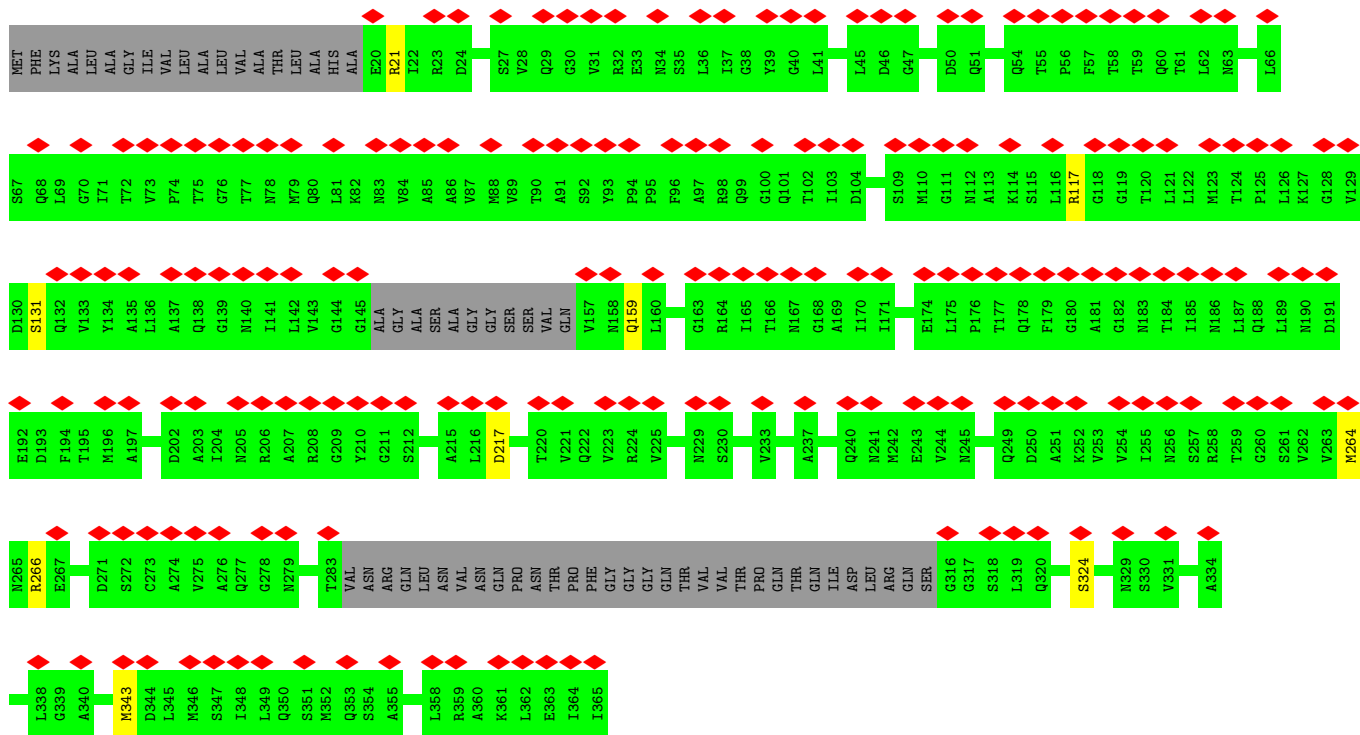


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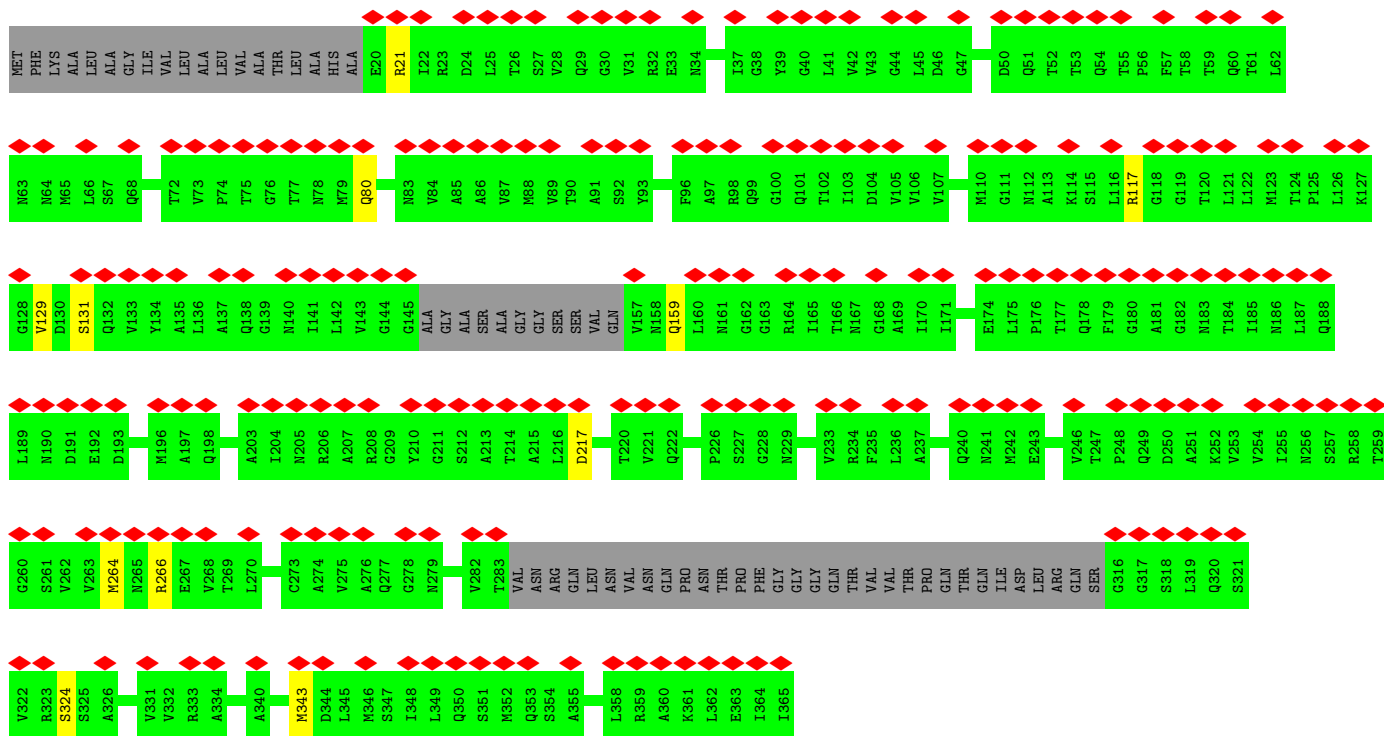
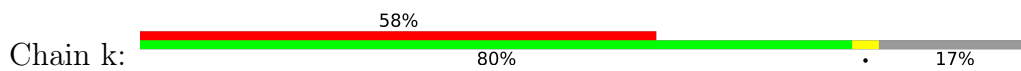


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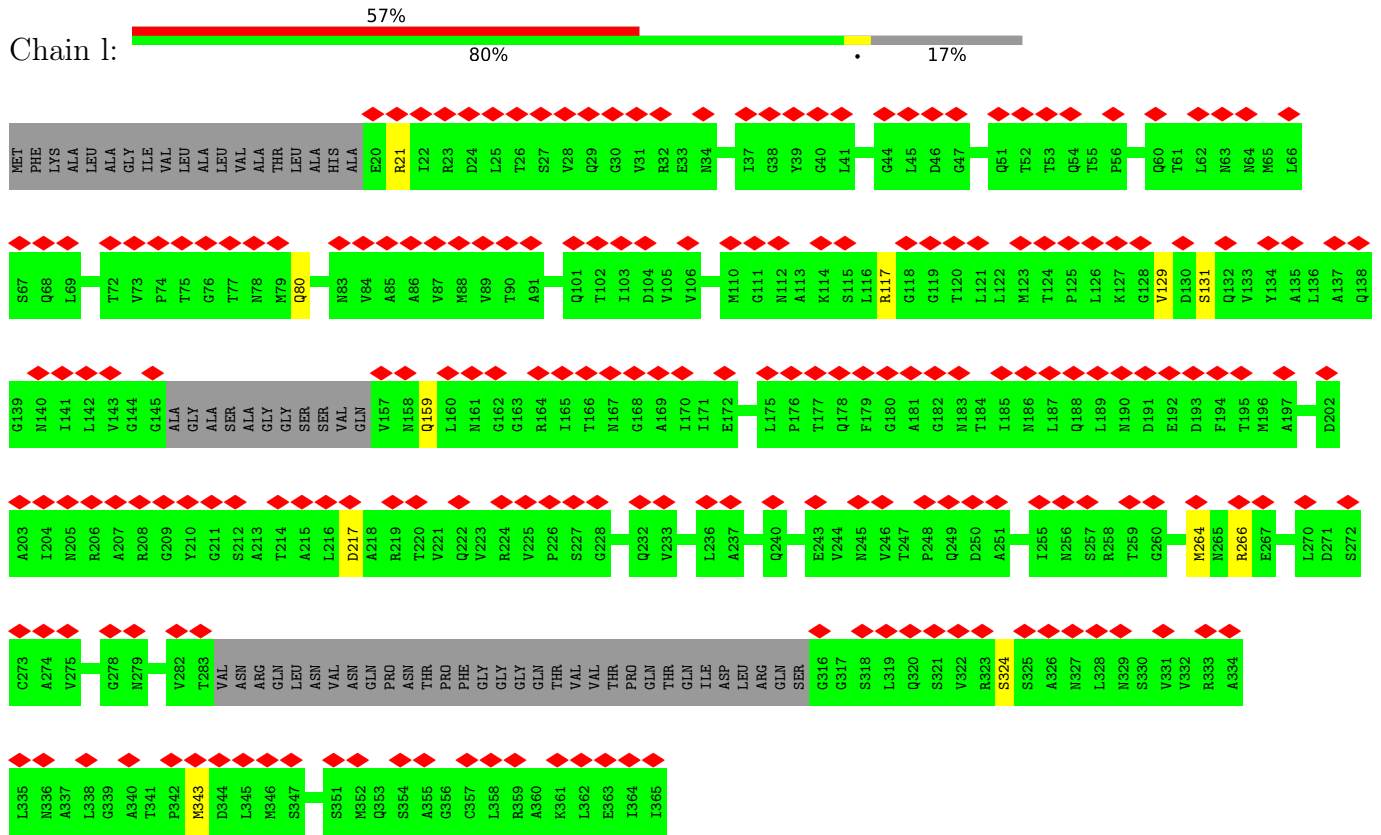




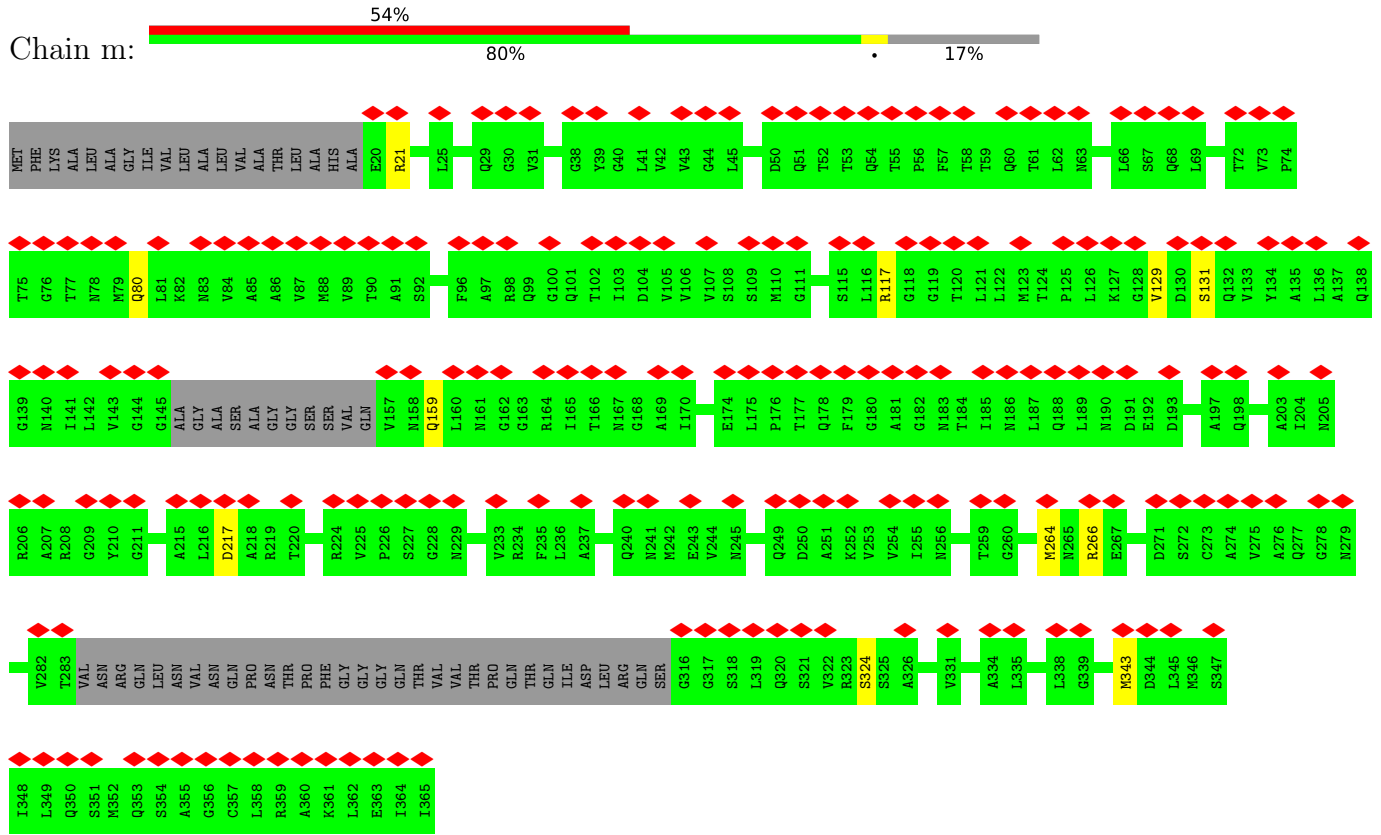
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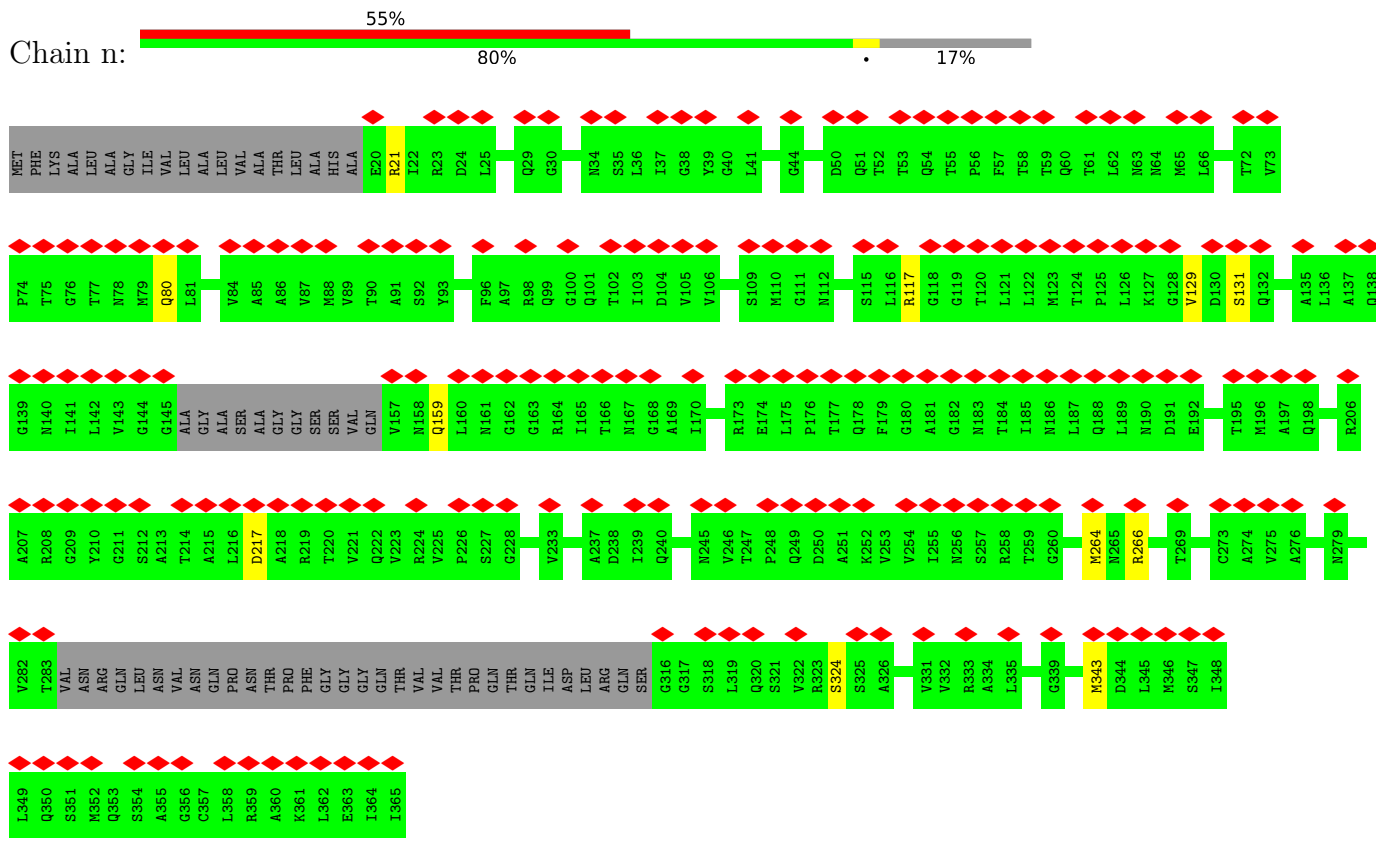
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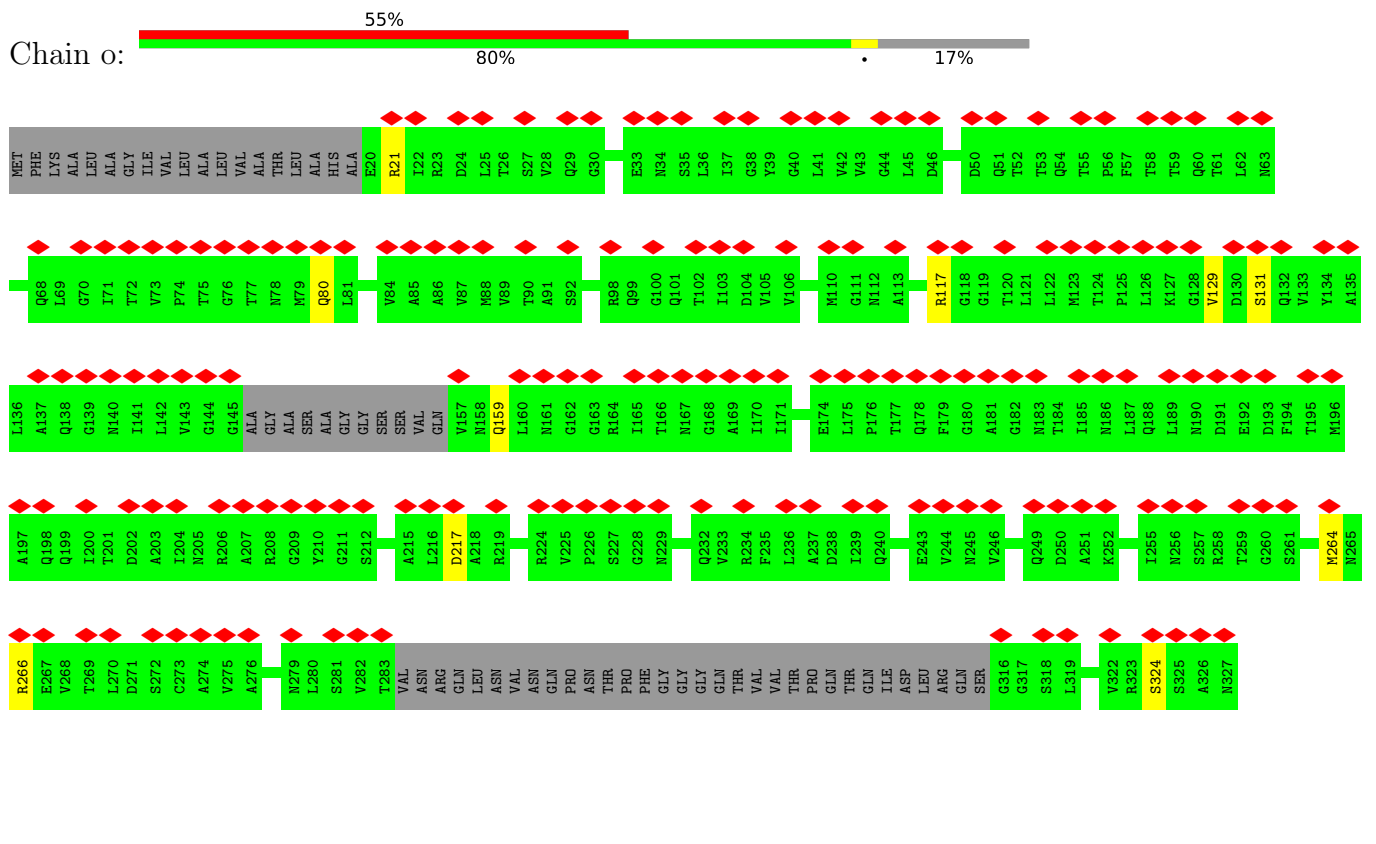
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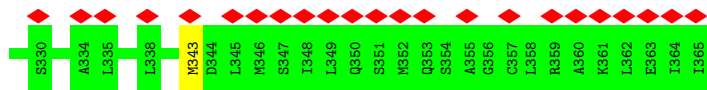


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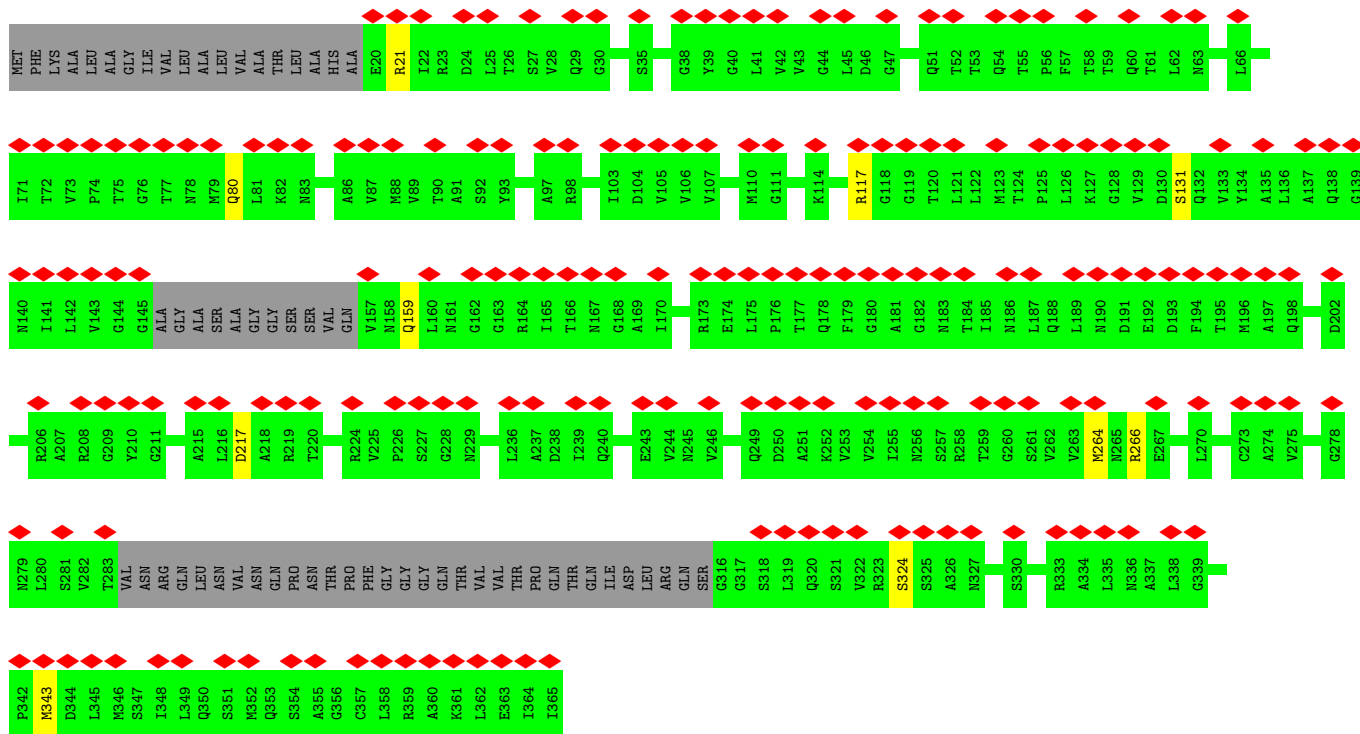
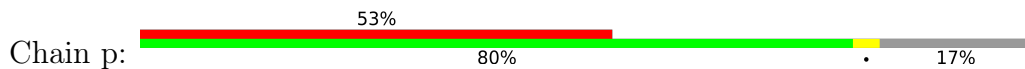


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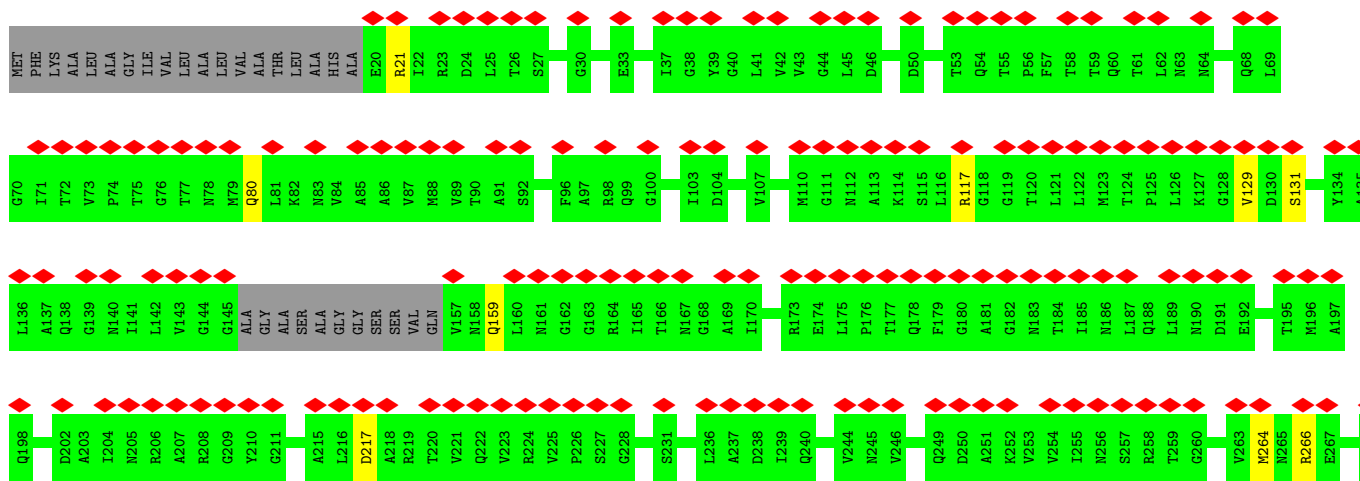
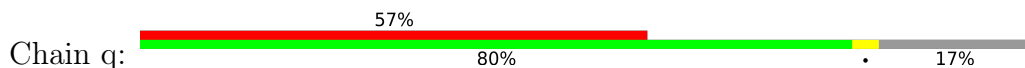




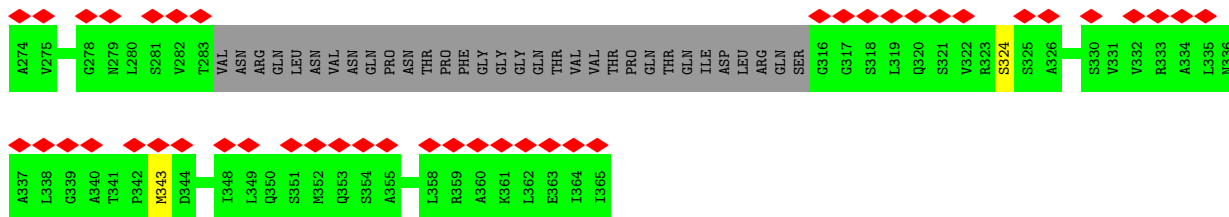
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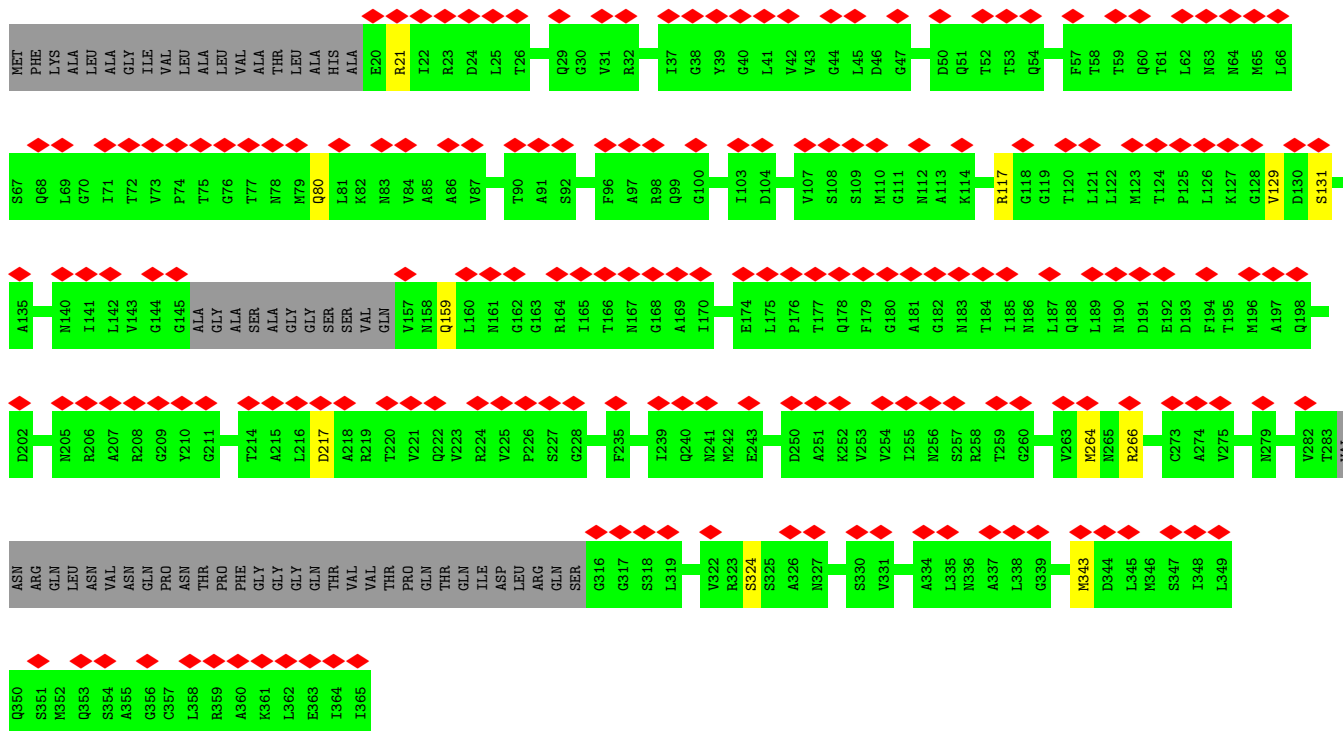
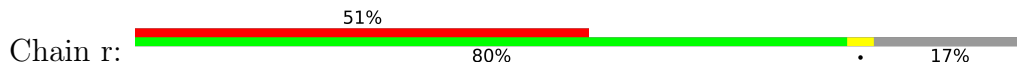
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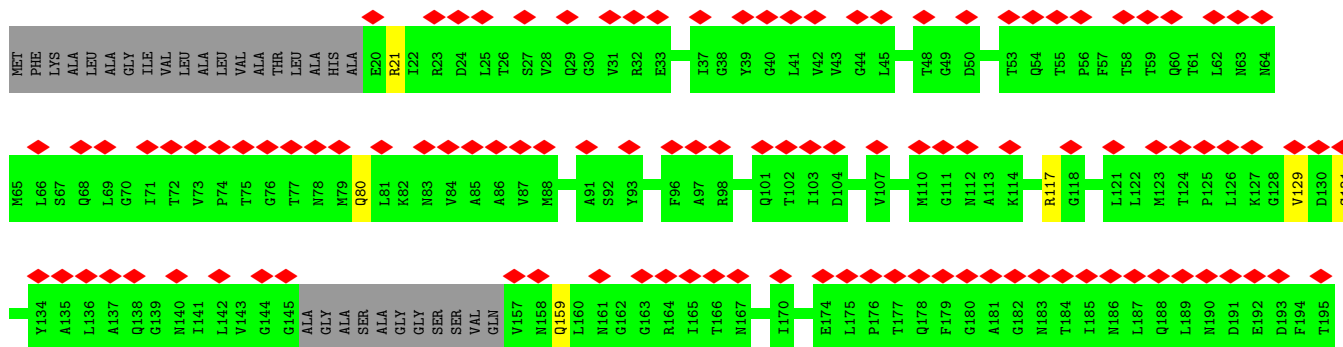
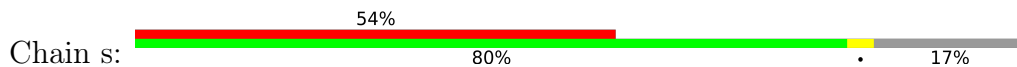


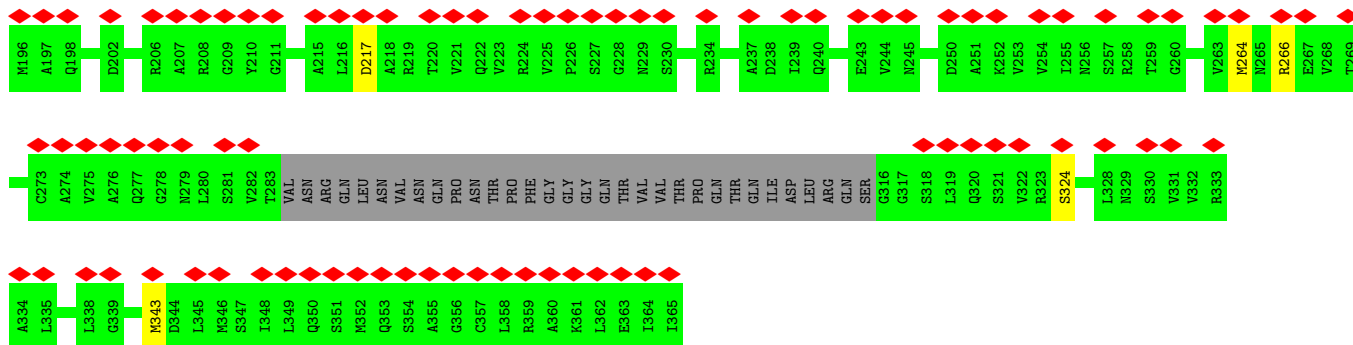


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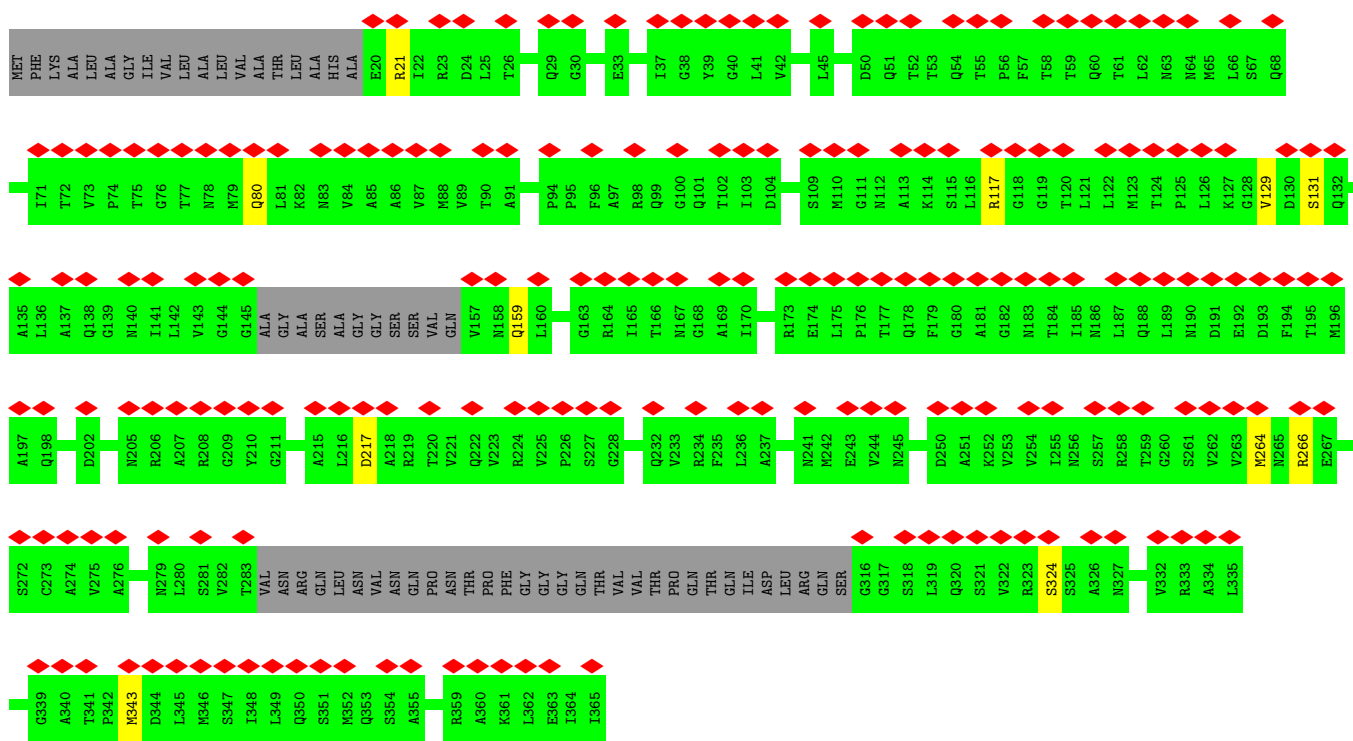
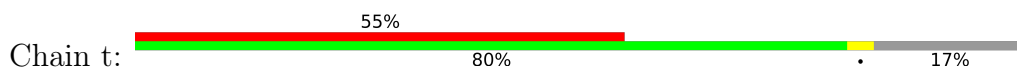


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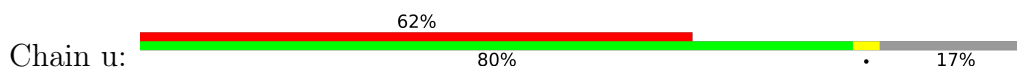


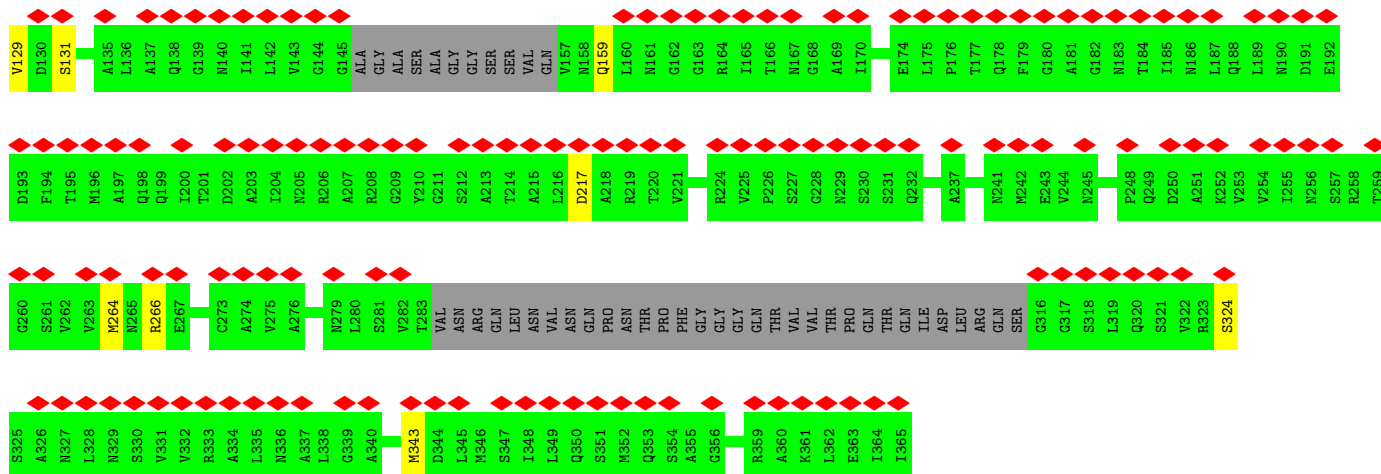


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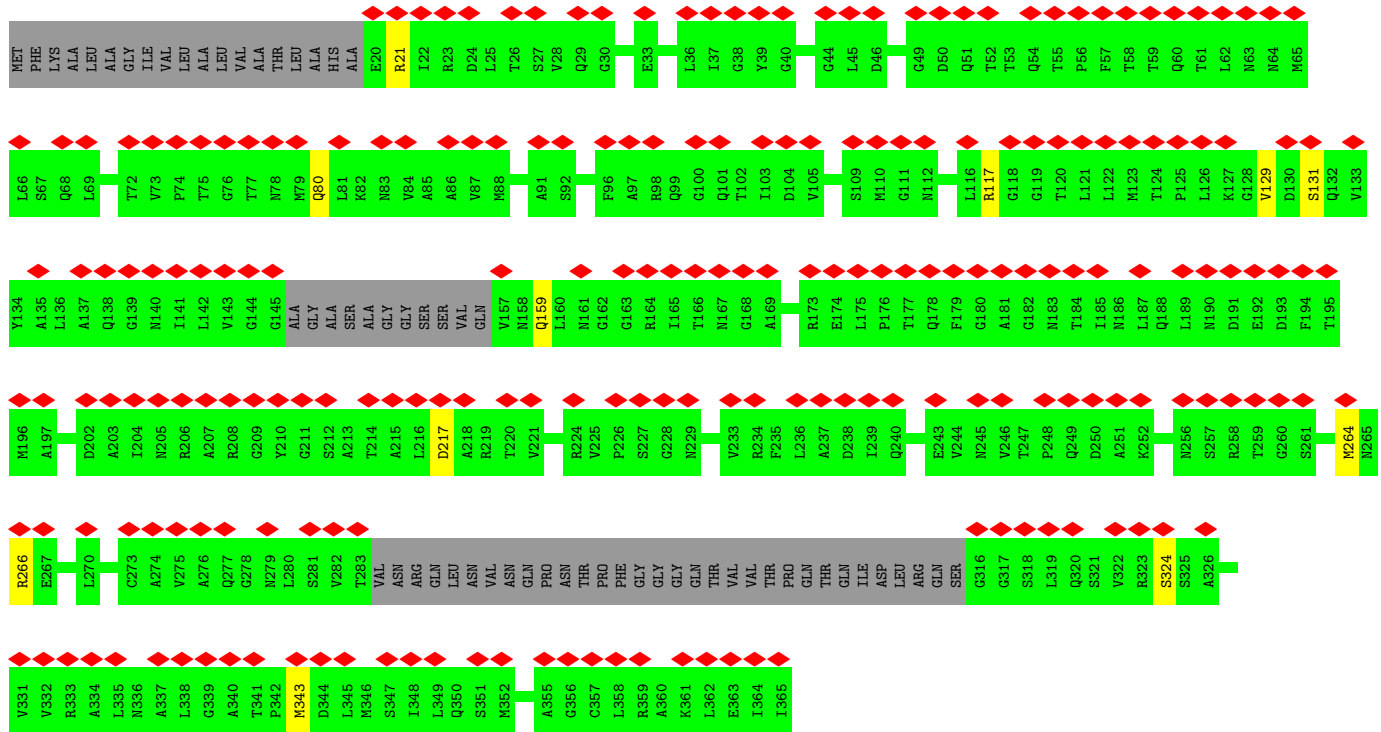
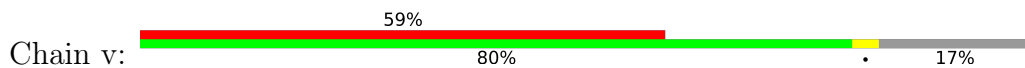


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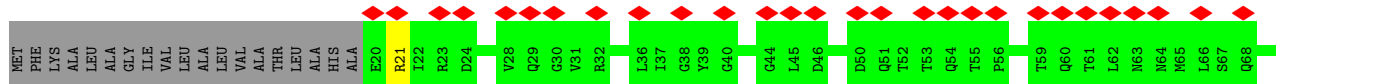
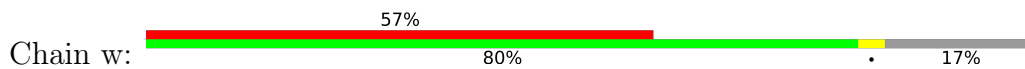


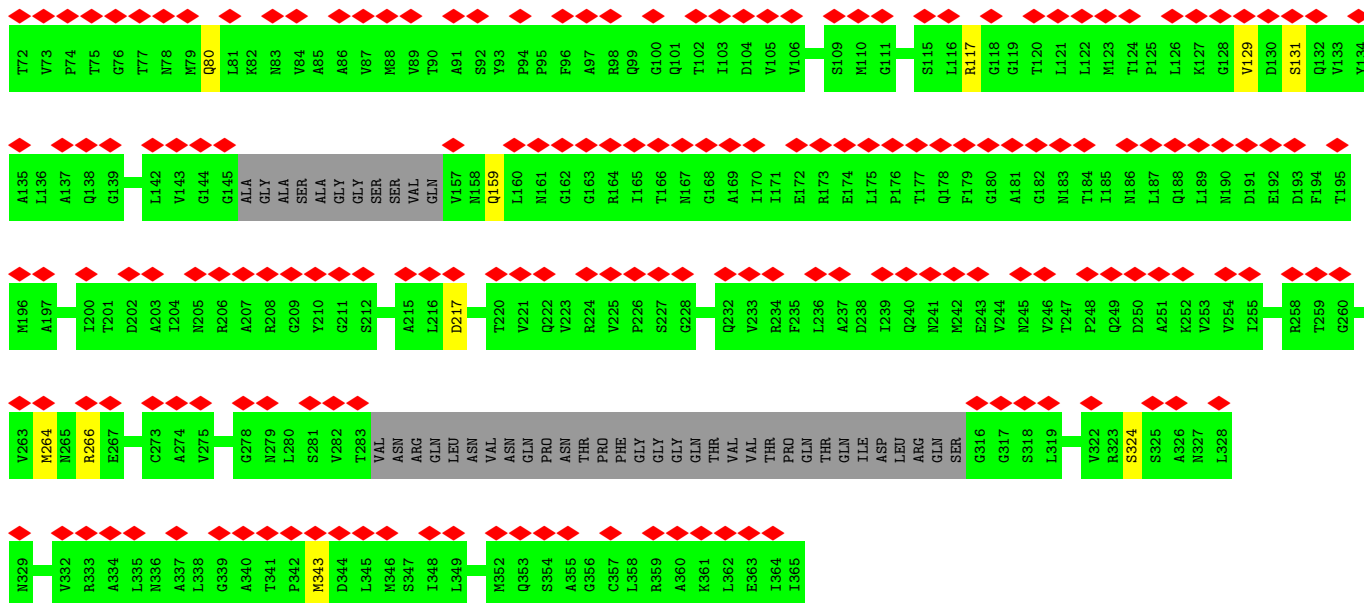


• Molecule 2: Flagellar P-ring protein

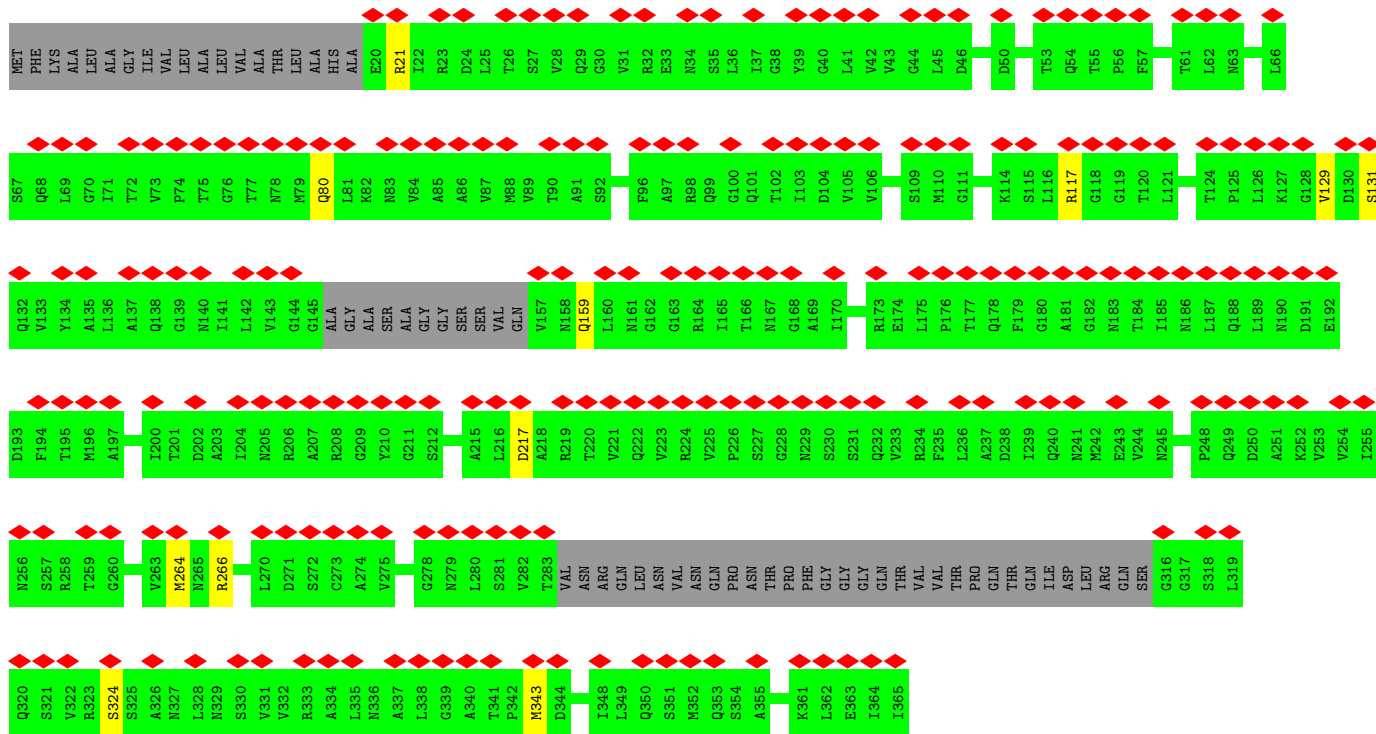
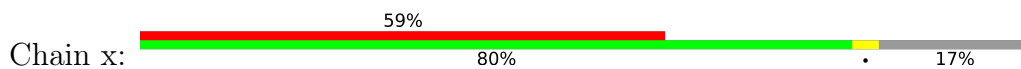


• Molecule 2: Flagellar P-ring protein

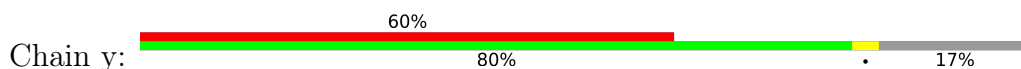


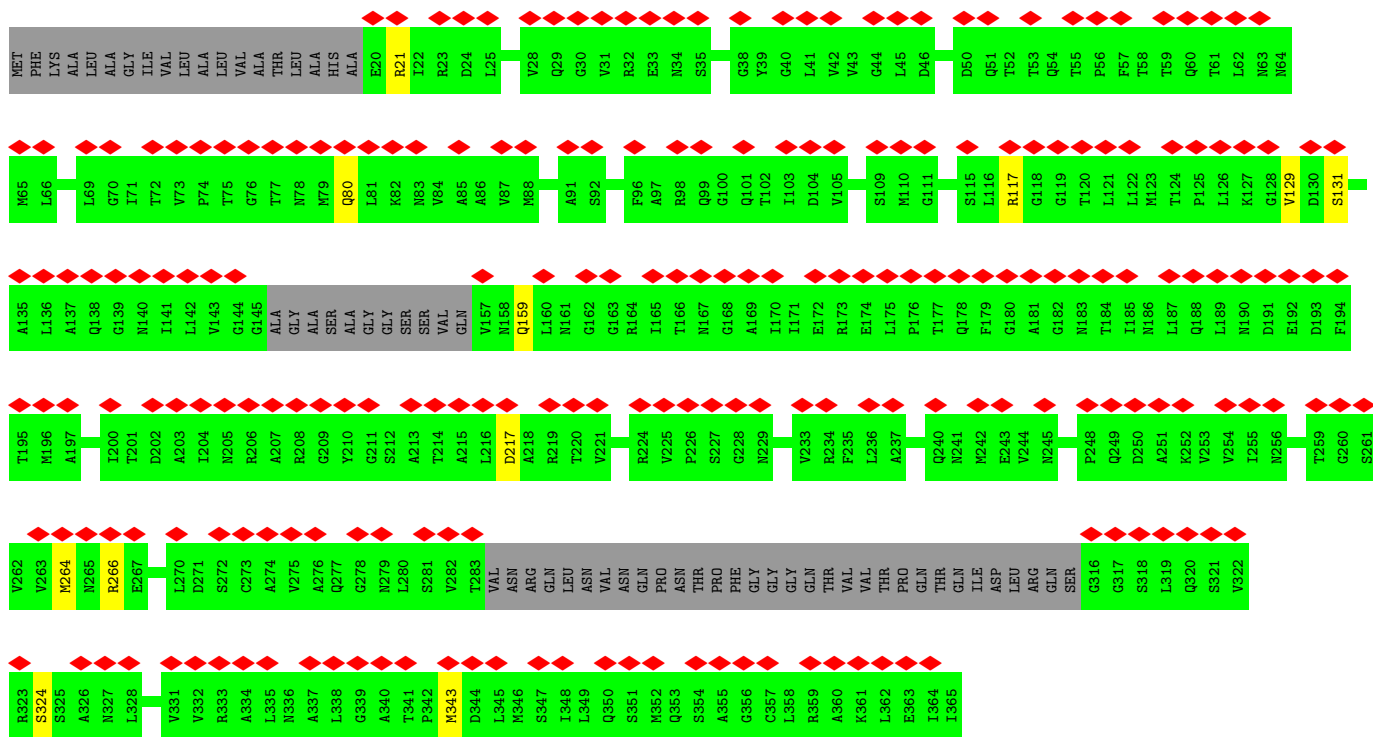


• Molecule 2: Flagellar P-ring protein

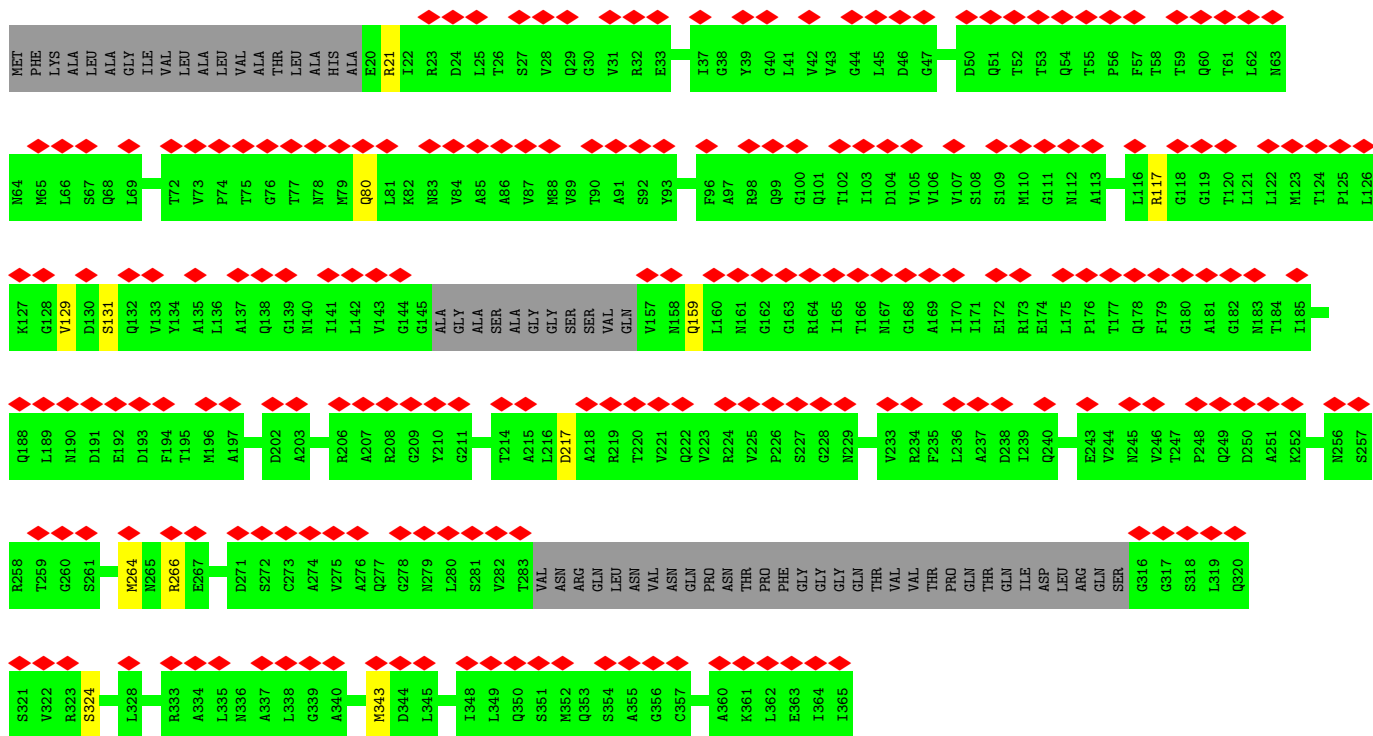
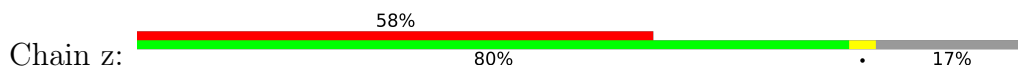


• Molecule 2: Flagellar P-ring protein



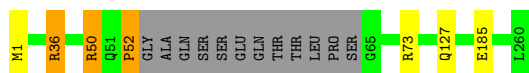


• Molecule 2: Flagellar P-ring protein



• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 0:  93% .. 5%



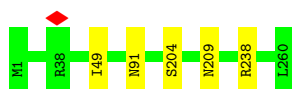
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 1:  93% ..



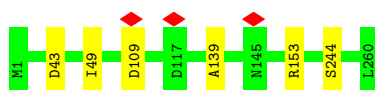
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 2:  98% .



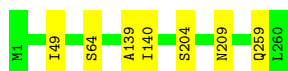
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 3:  98% .



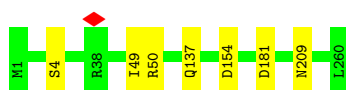
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 4:  97% .



• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 5:  97% .



• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 6:  97% .



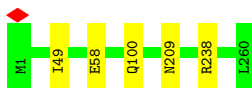
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 7:  98%



• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 8:  98%



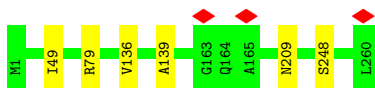
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 9:  97%



• Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZA:  98%



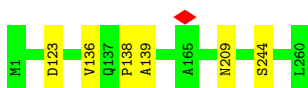
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZB:  96%



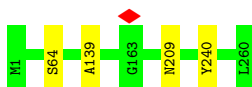
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZC:  98%



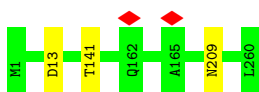
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZD:  98%



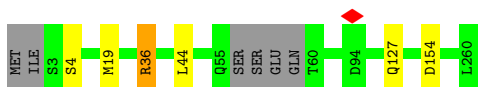
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZE:  99%



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AF:  95%



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AG:  95%



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AH:  94%



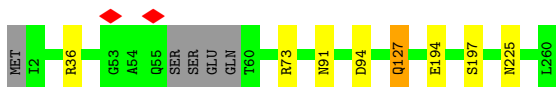
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AI:  93% 5%



- Molecule 3: Flagellar basal-body rod protein FlgG

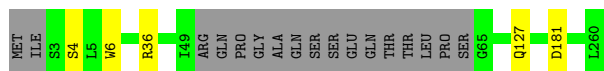
Chain AJ:  95%



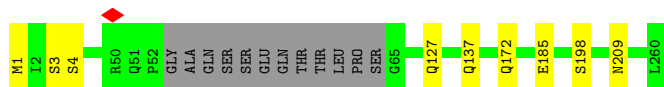
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AK:  92% 7%

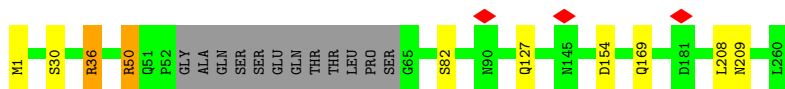




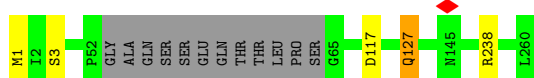
• Molecule 3: Flagellar basal-body rod protein FlgG



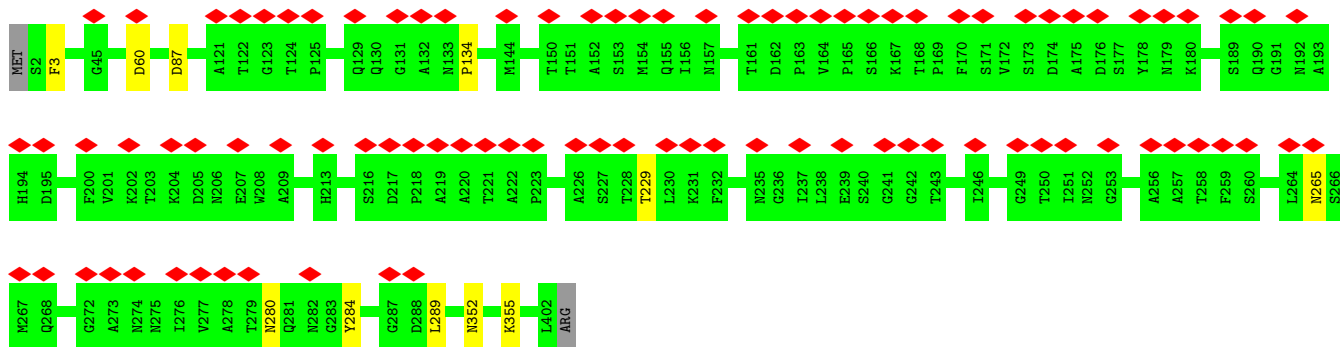
• Molecule 3: Flagellar basal-body rod protein FlgG



• Molecule 3: Flagellar basal-body rod protein FlgG



• Molecule 4: Flagellar hook protein FlgE

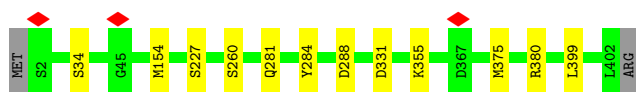


• Molecule 4: Flagellar hook protein FlgE



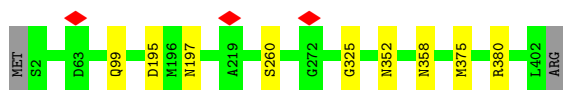
• Molecule 4: Flagellar hook protein FlgE

Chain ZH:  97%



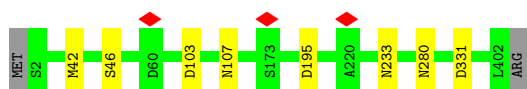
• Molecule 4: Flagellar hook protein FlgE

Chain ZI:  97%



• Molecule 4: Flagellar hook protein FlgE

Chain ZJ:  98%



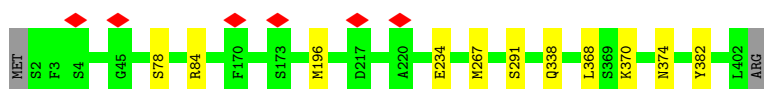
• Molecule 4: Flagellar hook protein FlgE

Chain ZK:  98%



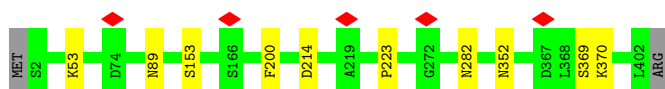
• Molecule 4: Flagellar hook protein FlgE

Chain ZL:  97%



• Molecule 4: Flagellar hook protein FlgE

Chain ZM:  97%



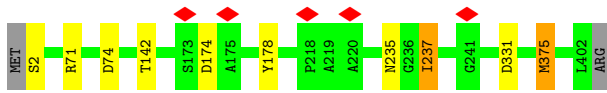
• Molecule 4: Flagellar hook protein FlgE

Chain ZN:  97%



- Molecule 4: Flagellar hook protein FlgE

Chain ZO:  97%



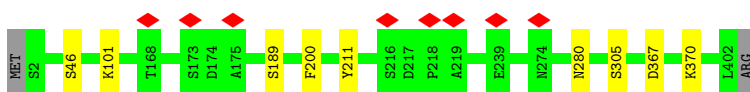
- Molecule 4: Flagellar hook protein FlgE

Chain ZP:  95%



- Molecule 4: Flagellar hook protein FlgE

Chain ZQ:  97%



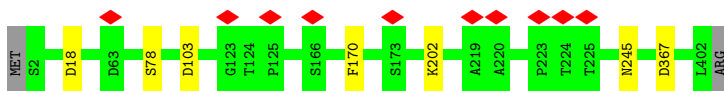
- Molecule 4: Flagellar hook protein FlgE

Chain ZR:  97%



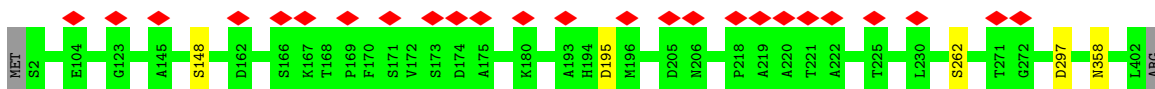
- Molecule 4: Flagellar hook protein FlgE

Chain ZS:  98%



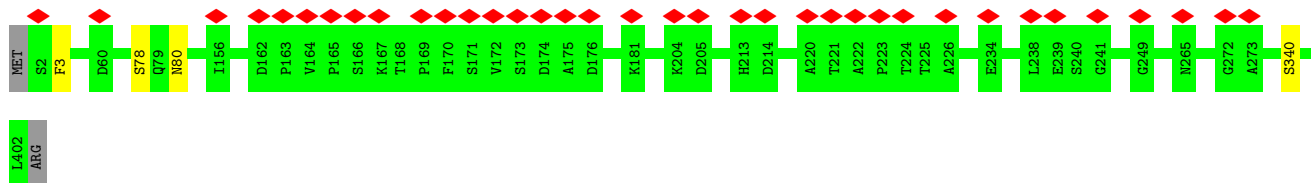
- Molecule 4: Flagellar hook protein FlgE

Chain ZT:  98%

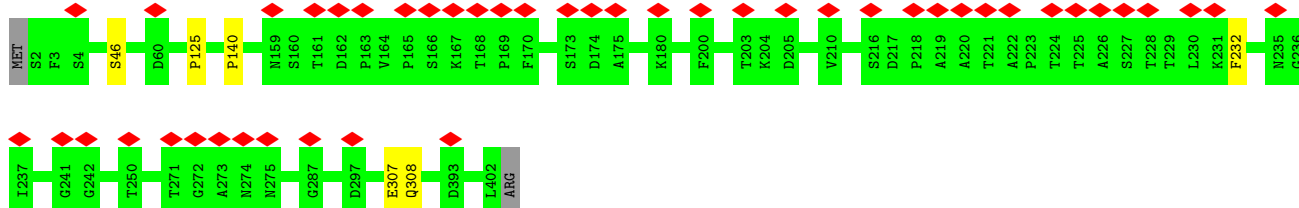


- Molecule 4: Flagellar hook protein FlgE

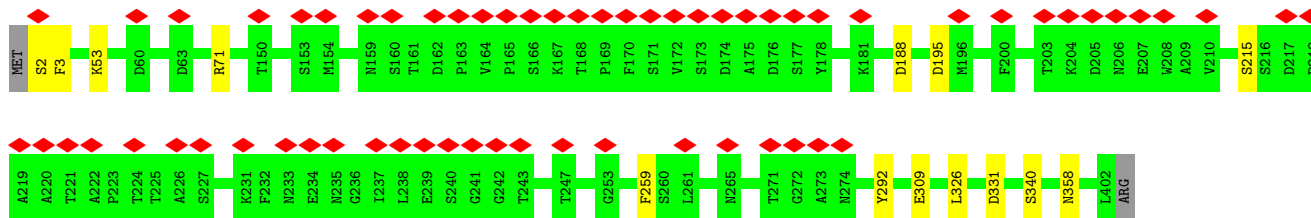
Chain ZU:  99%



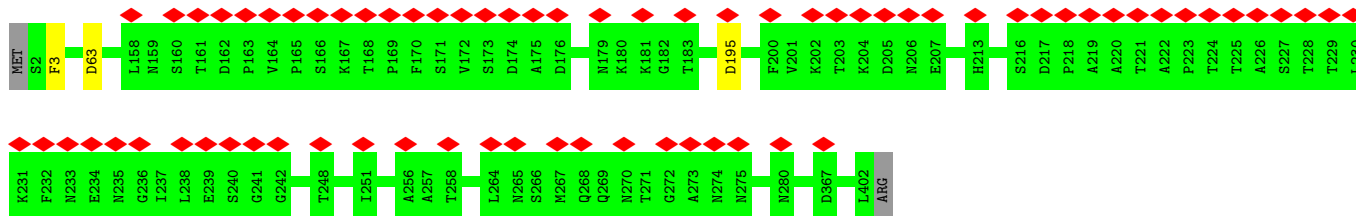
• Molecule 4: Flagellar hook protein FlgE



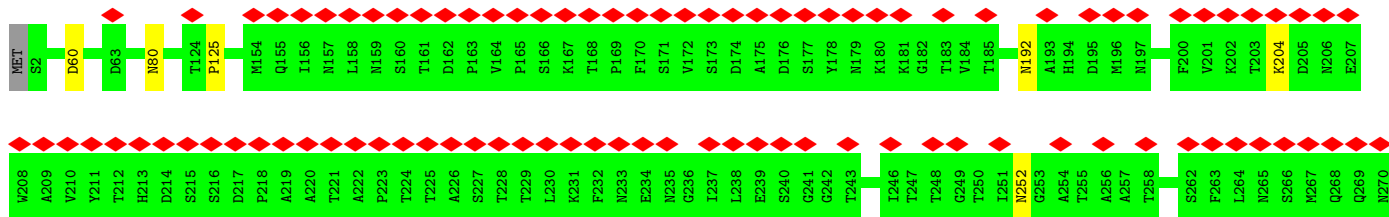
• Molecule 4: Flagellar hook protein FlgE

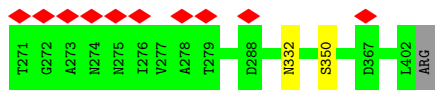


• Molecule 4: Flagellar hook protein FlgE

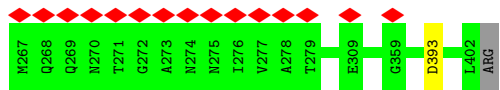
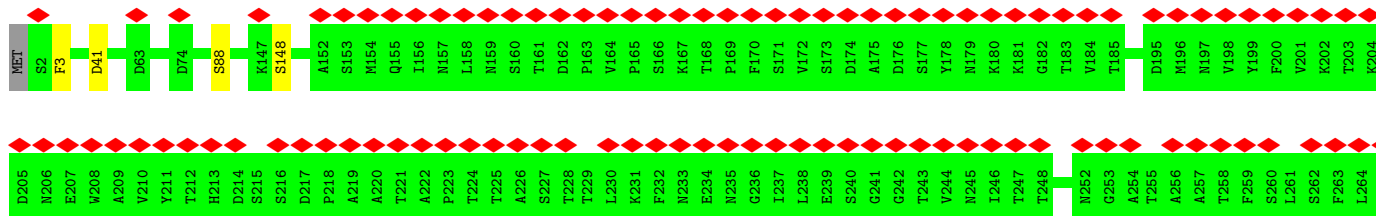


• Molecule 4: Flagellar hook protein FlgE

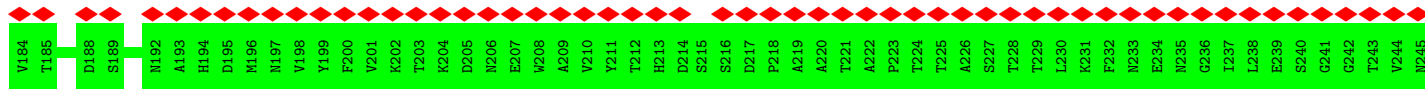
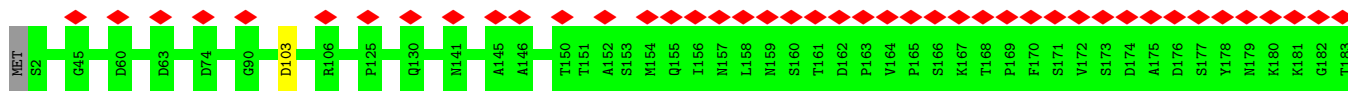




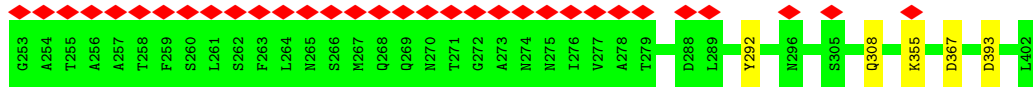
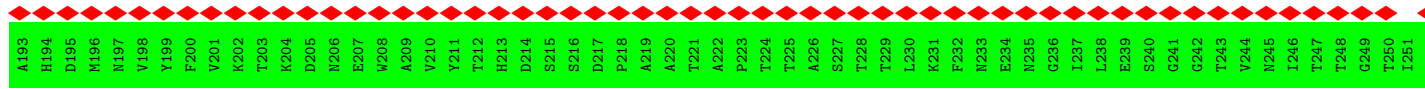
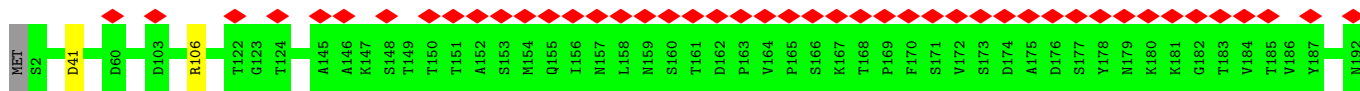
• Molecule 4: Flagellar hook protein FlgE



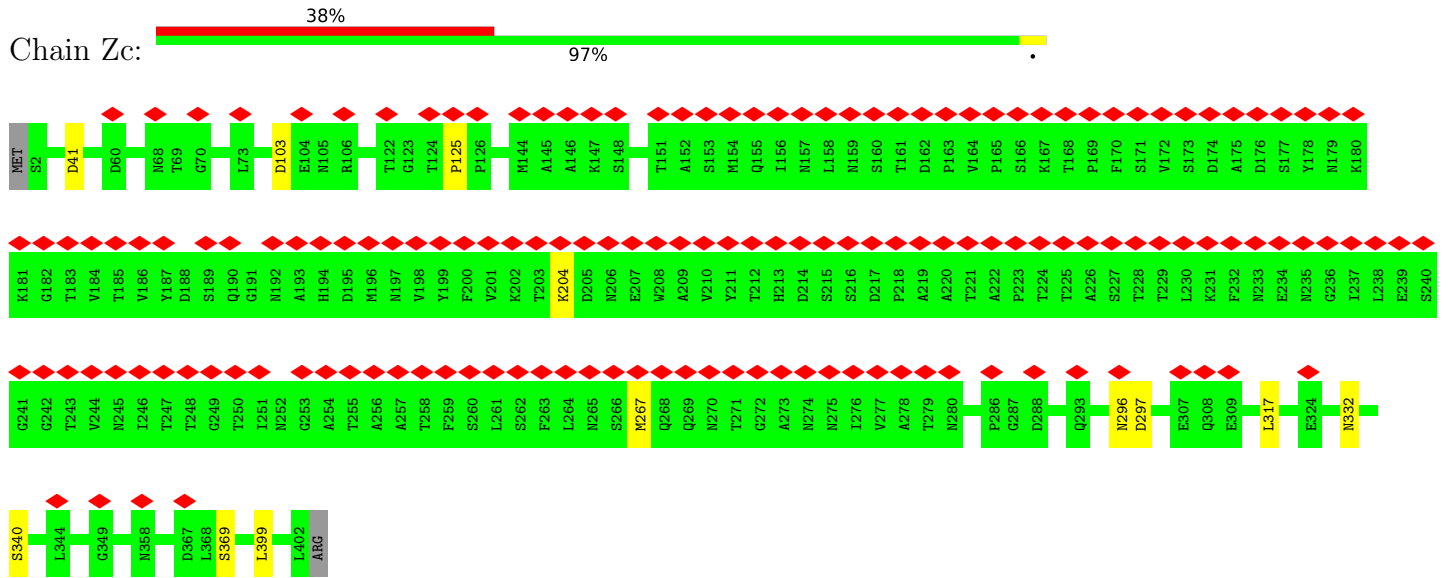
• Molecule 4: Flagellar hook protein FlgE



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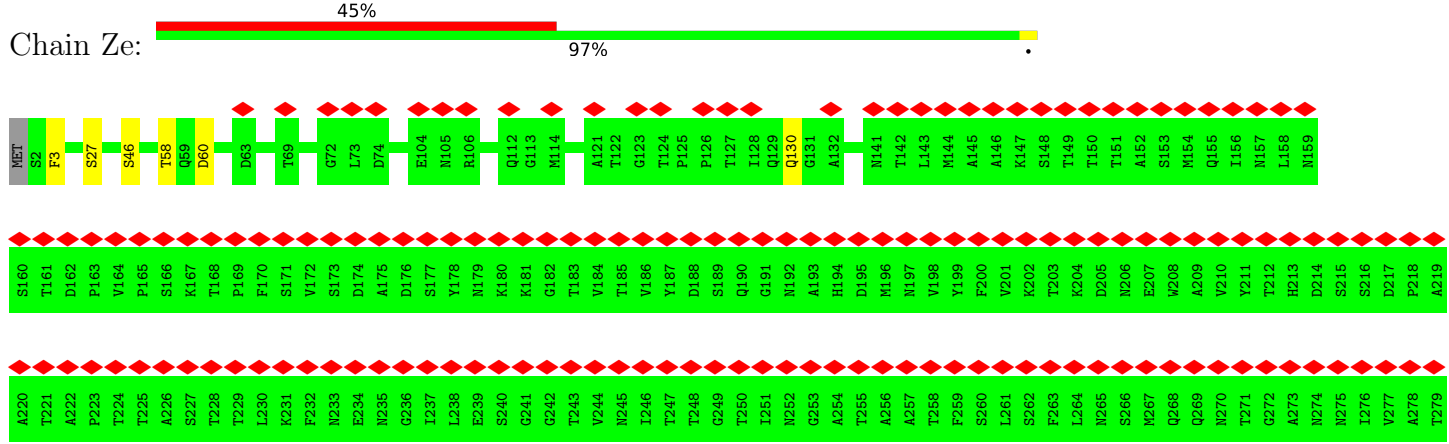
• Molecule 4: Flagellar hook protein FlgE

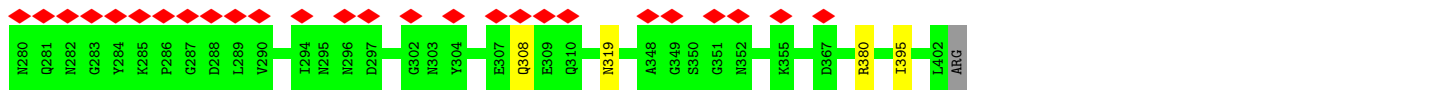


• Molecule 4: Flagellar hook protein FlgE

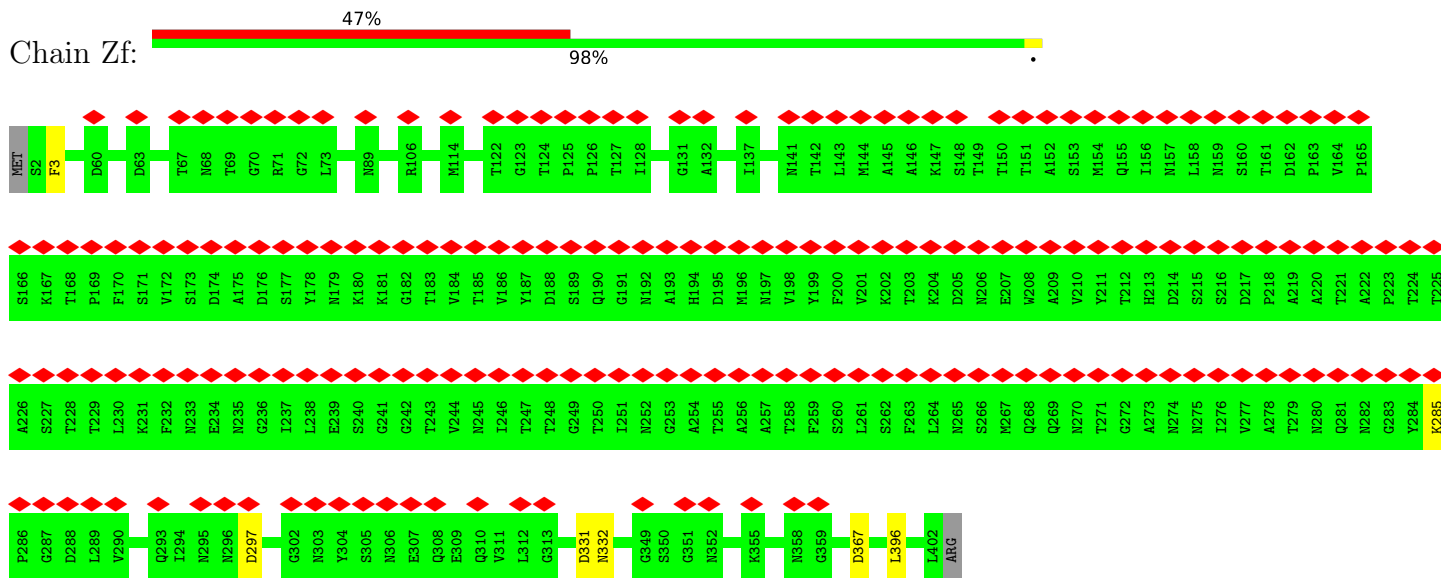


• Molecule 4: Flagellar hook protein FlgE

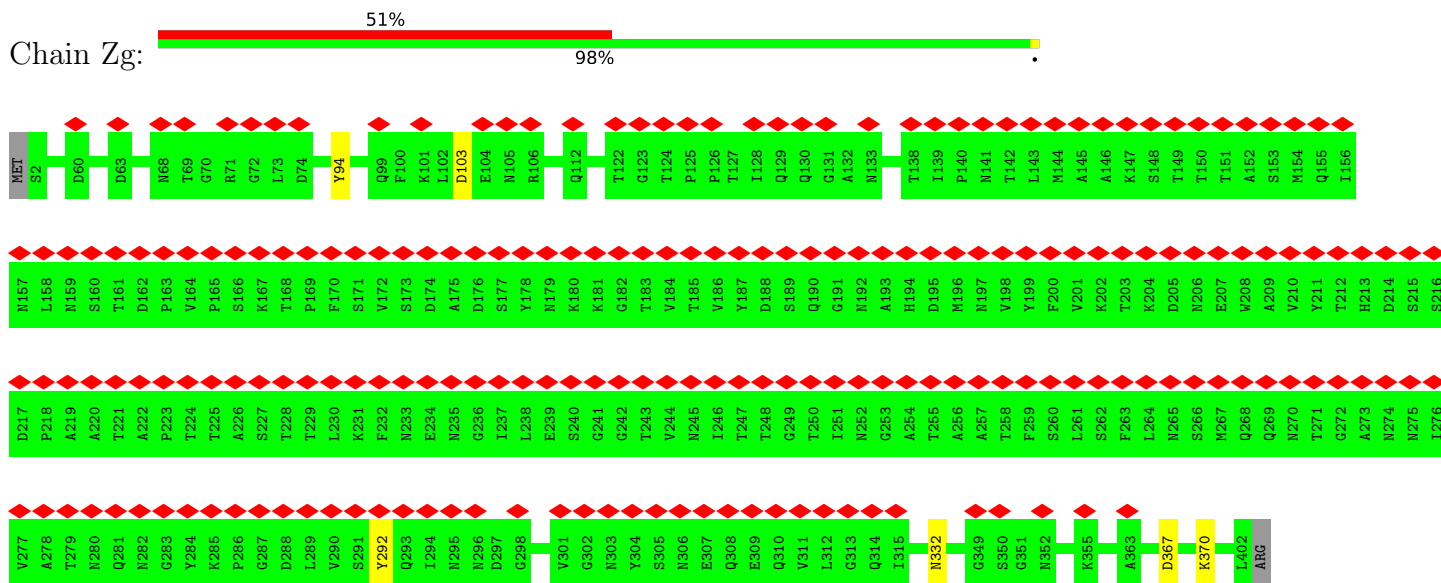




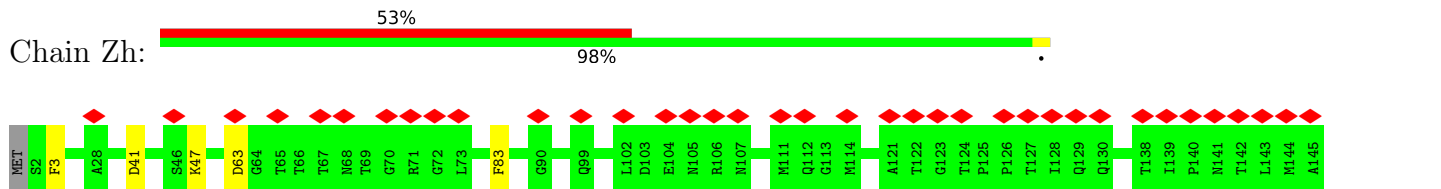
• Molecule 4: Flagellar hook protein FlgE

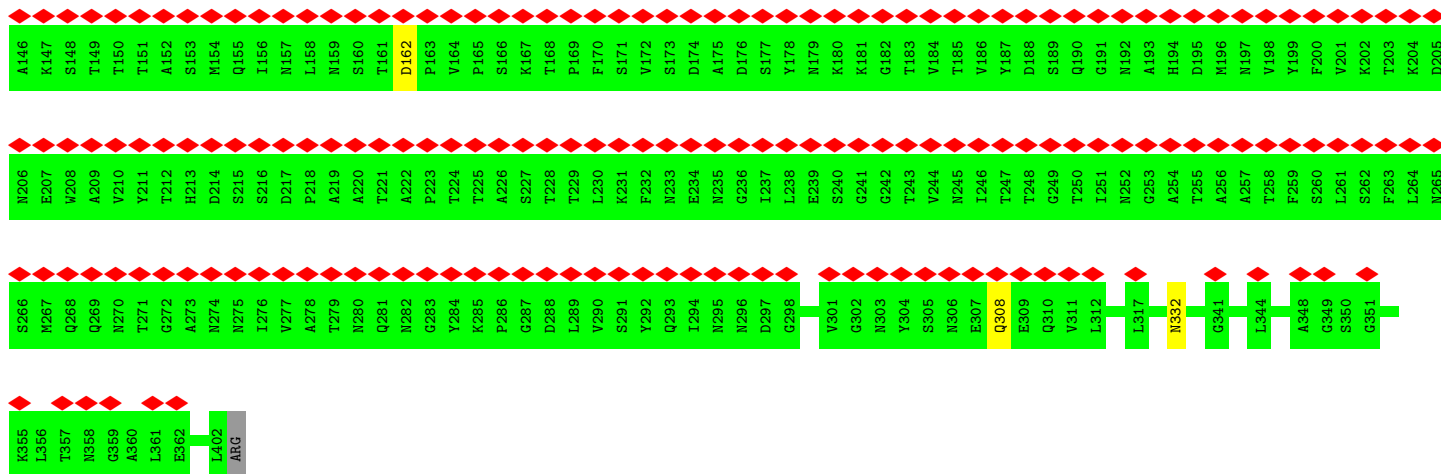


• Molecule 4: Flagellar hook protein FlgE



• Molecule 4: Flagellar hook protein FlgE

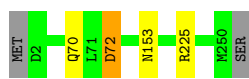




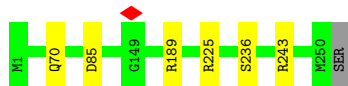
• Molecule 5: Flagellar basal-body rod protein FlgF



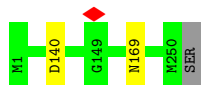
• Molecule 5: Flagellar basal-body rod protein FlgF



• Molecule 5: Flagellar basal-body rod protein FlgF



• Molecule 5: Flagellar basal-body rod protein FlgF



• Molecule 5: Flagellar basal-body rod protein FlgF

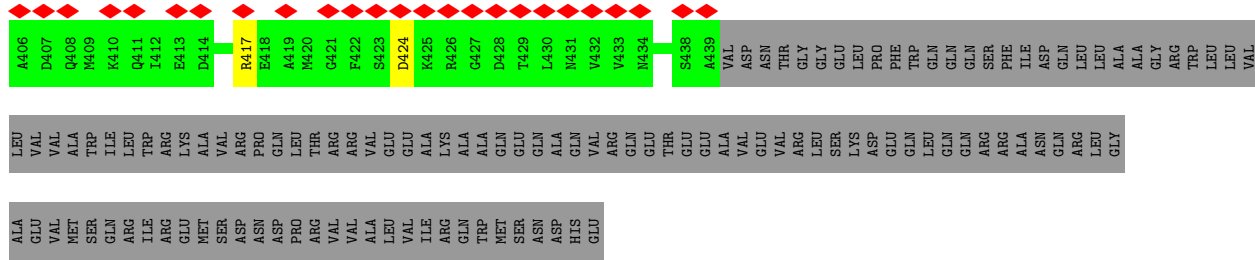




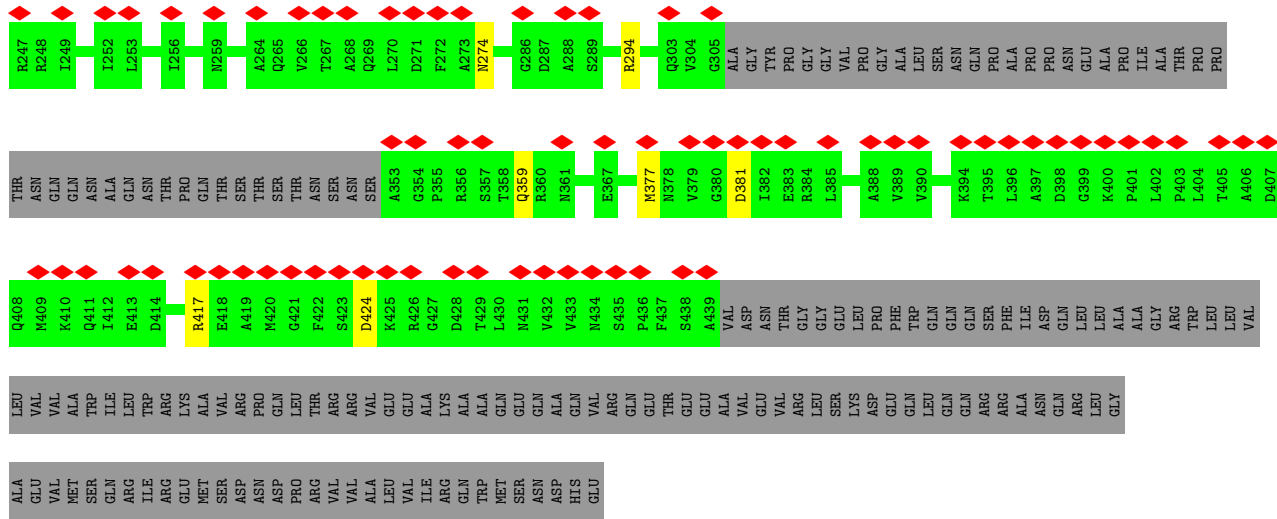
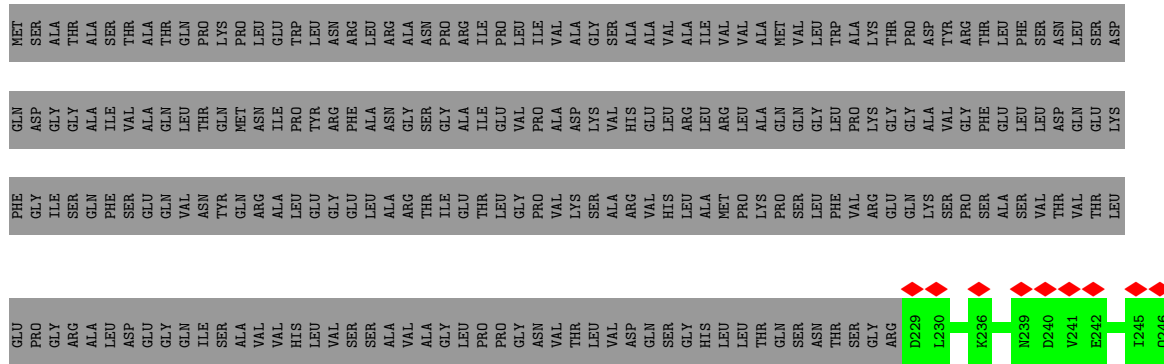




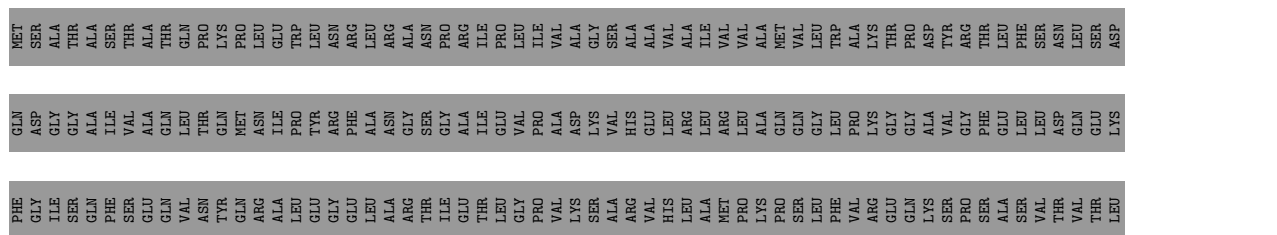




● Molecule 6: Flagellar M-ring protein



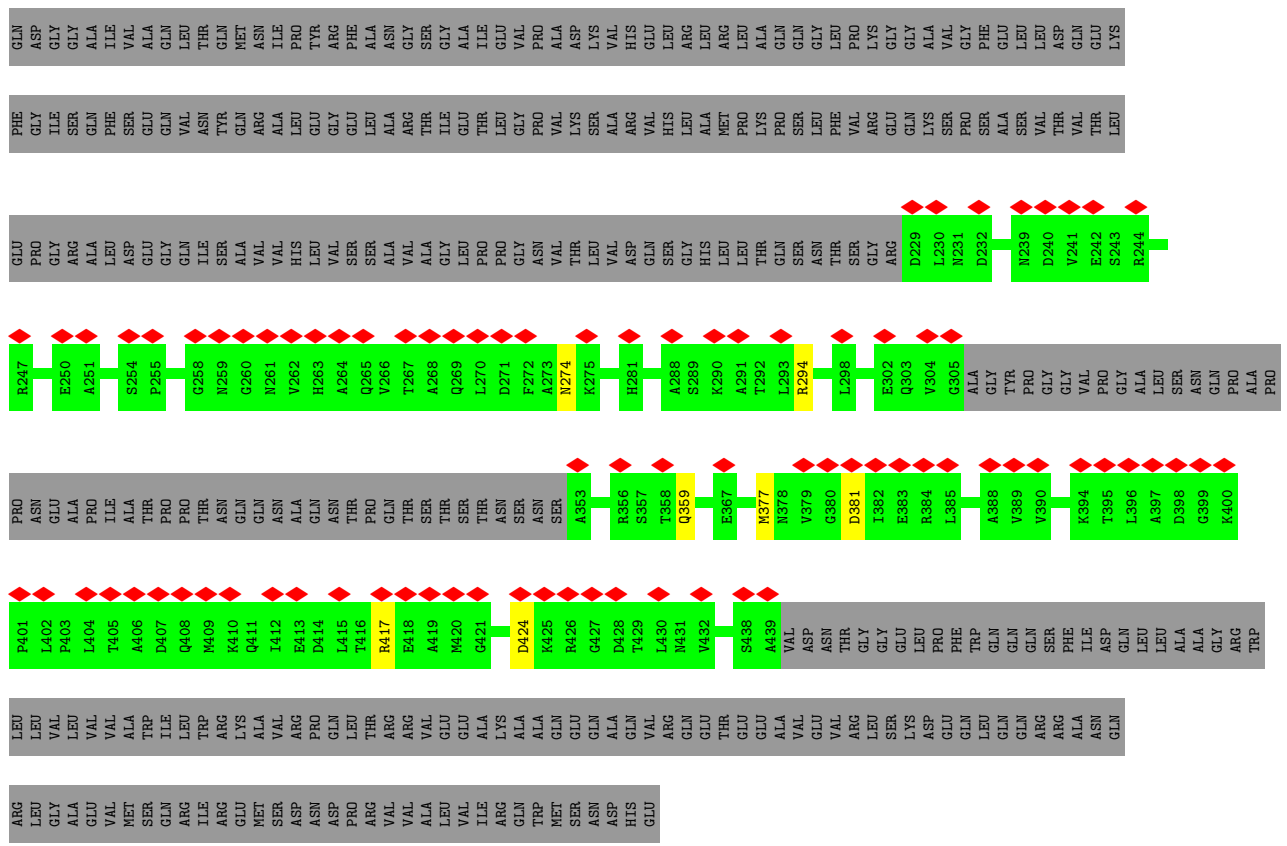
● Molecule 6: Flagellar M-ring protein



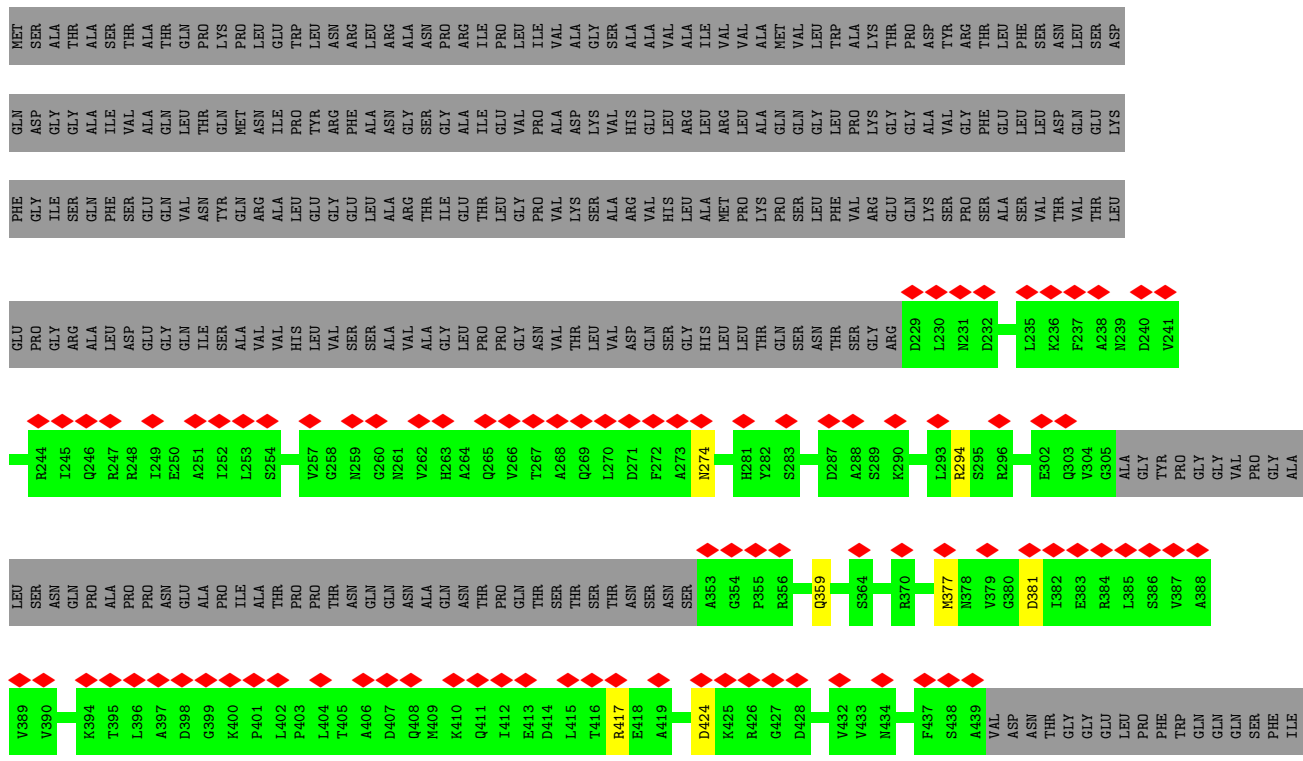








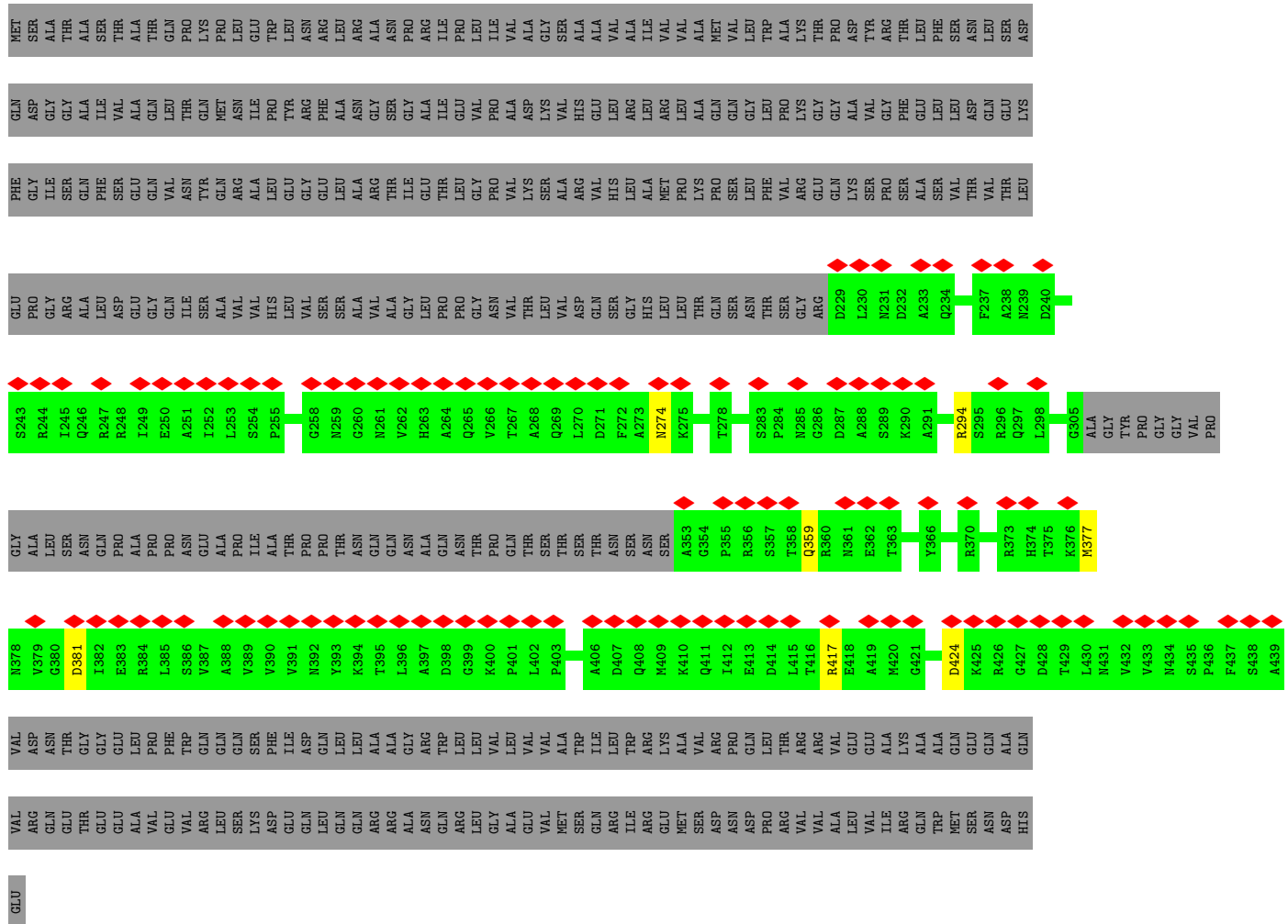
● Molecule 6: Flagellar M-ring protein



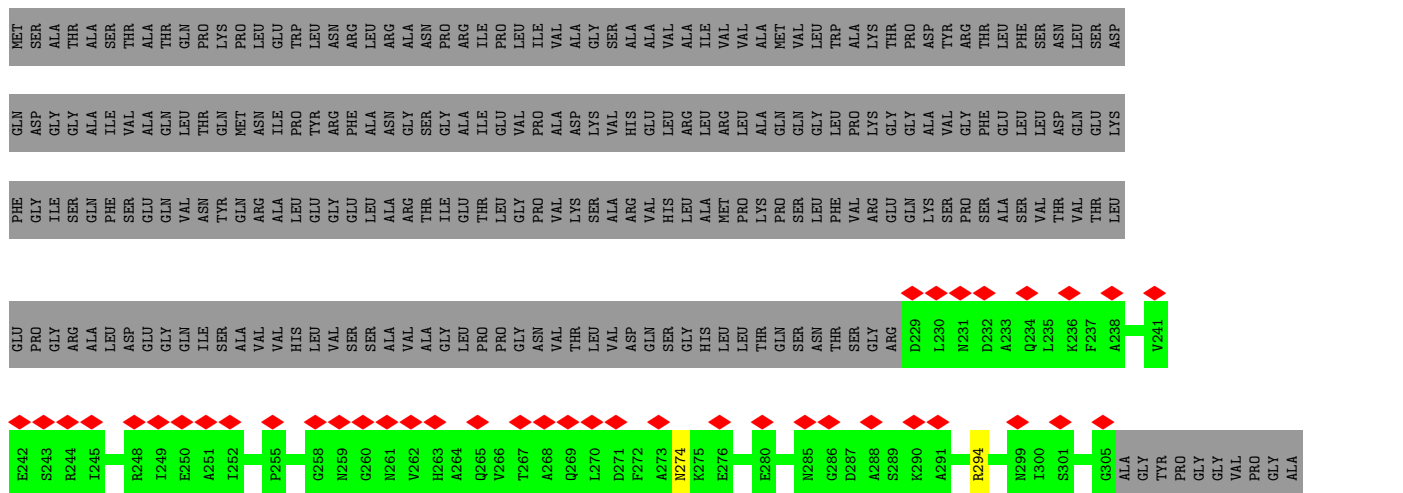


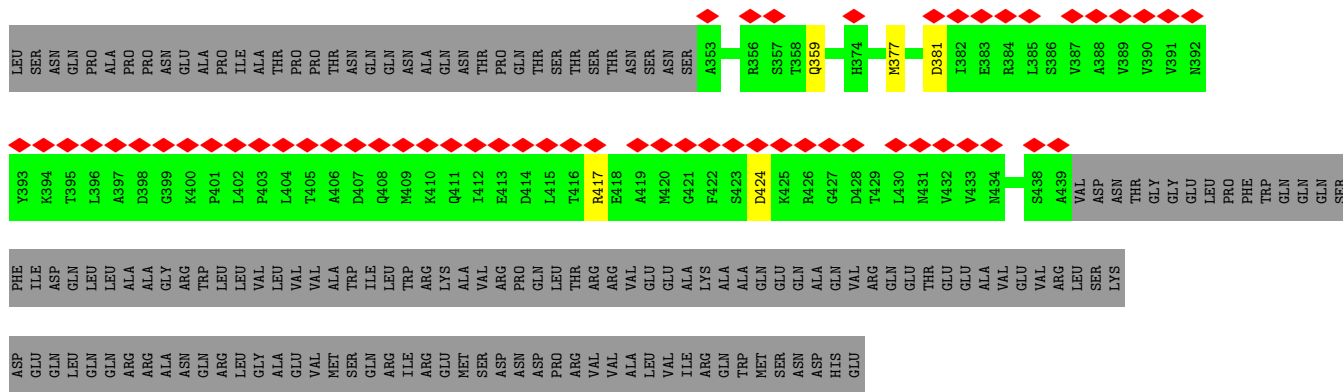




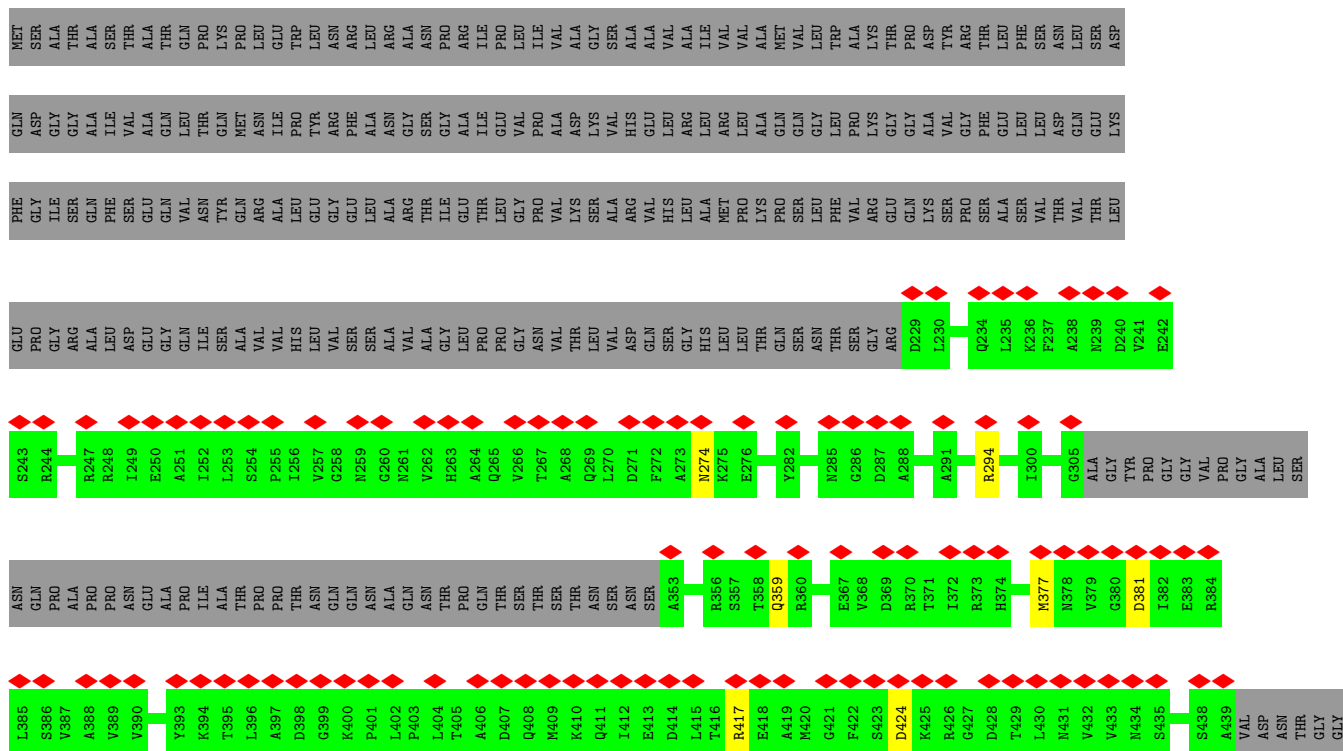


● Molecule 6: Flagellar M-ring protein

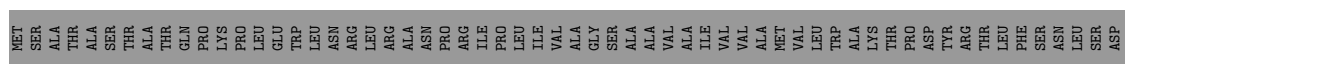


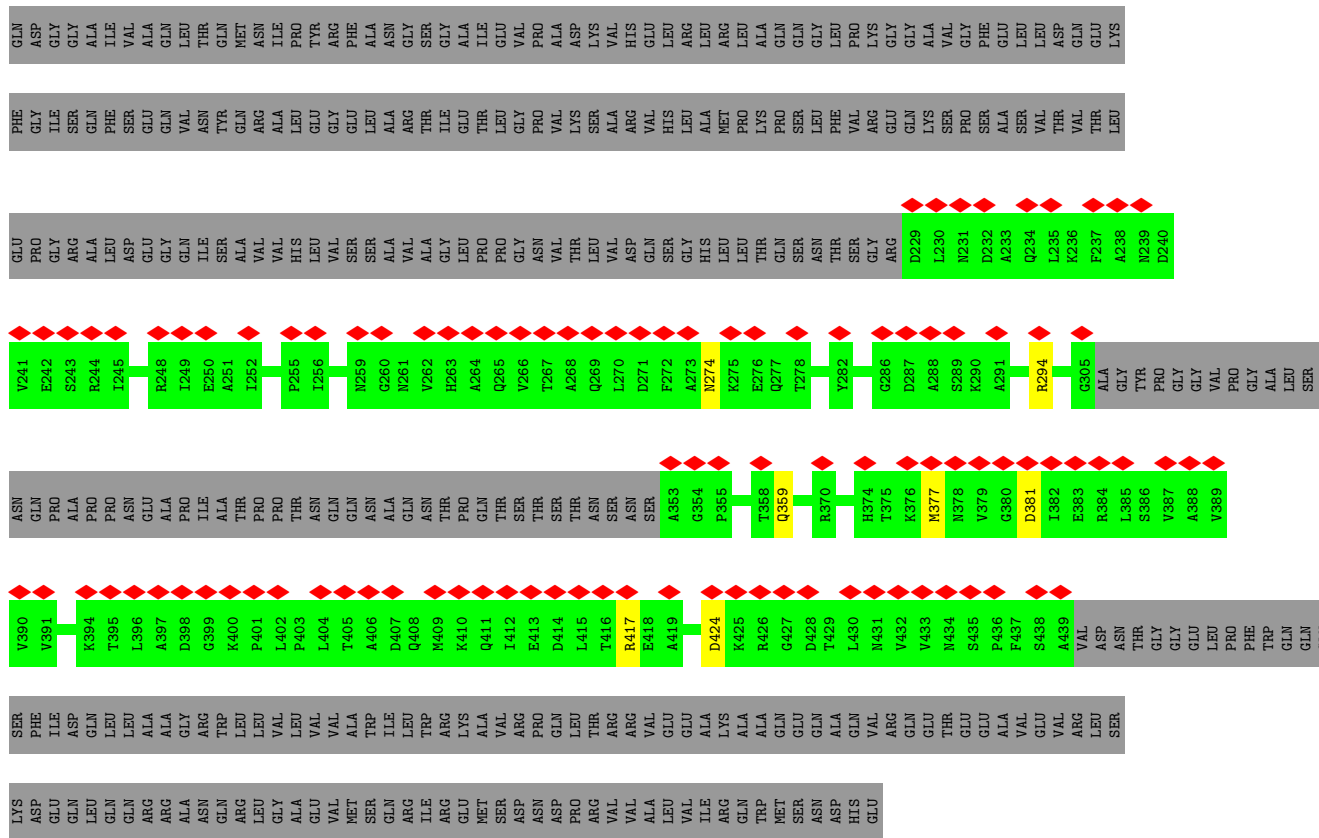


• Molecule 6: Flagellar M-ring protein

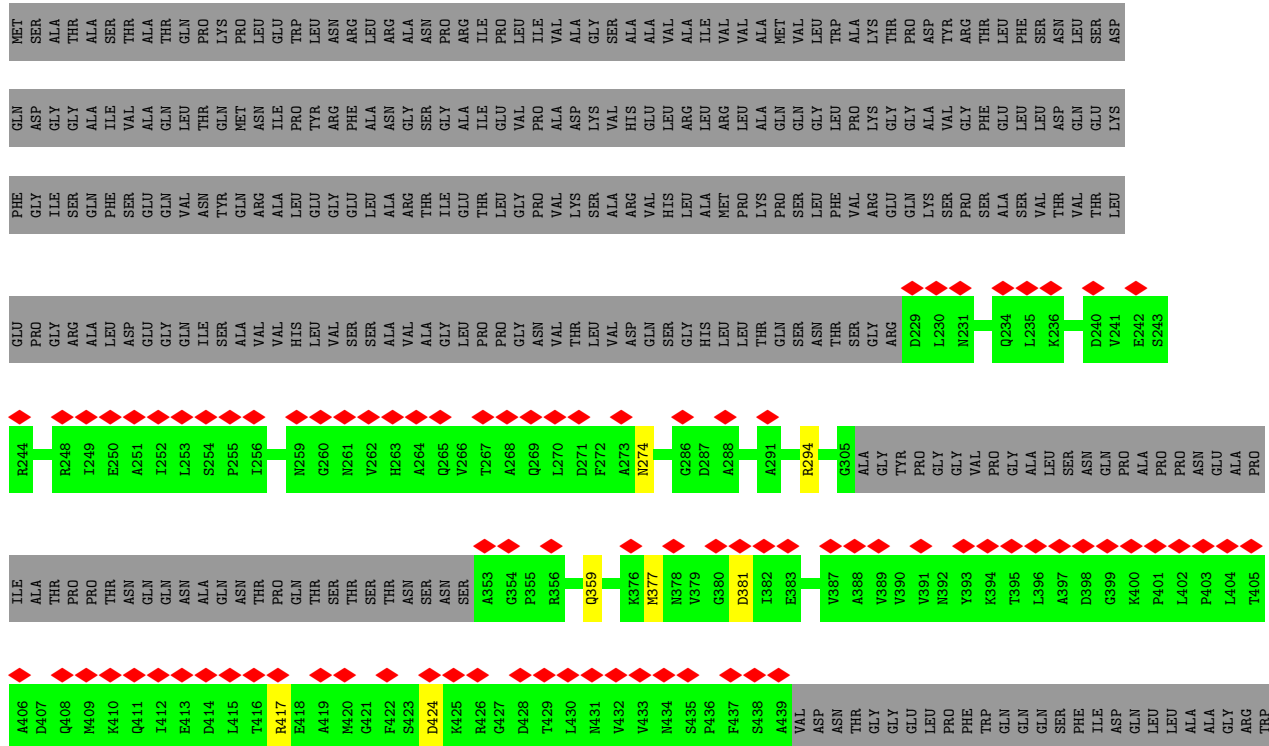


• Molecule 6: Flagellar M-ring protein

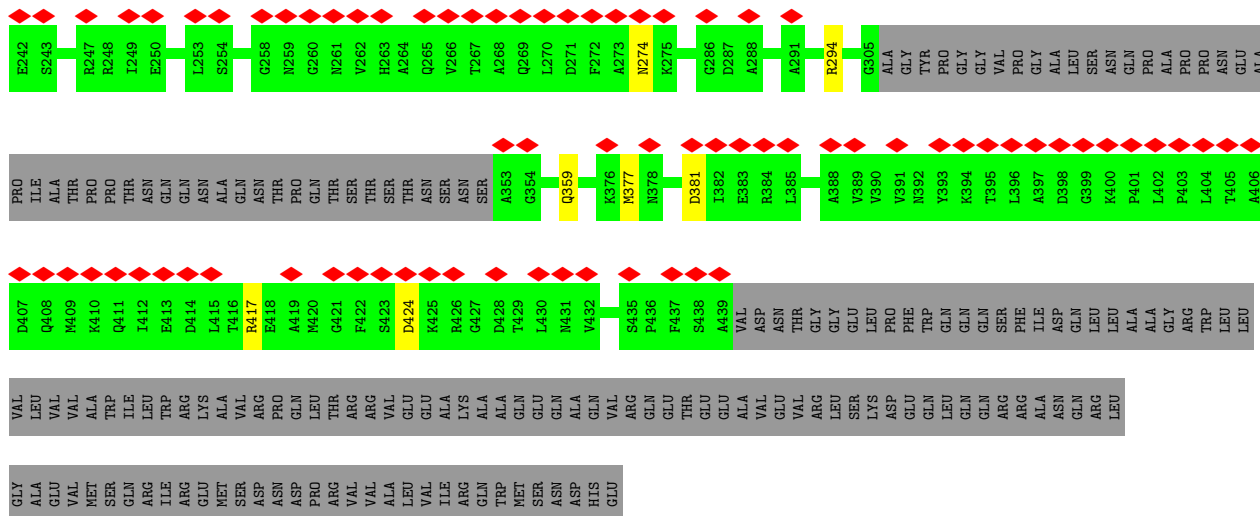




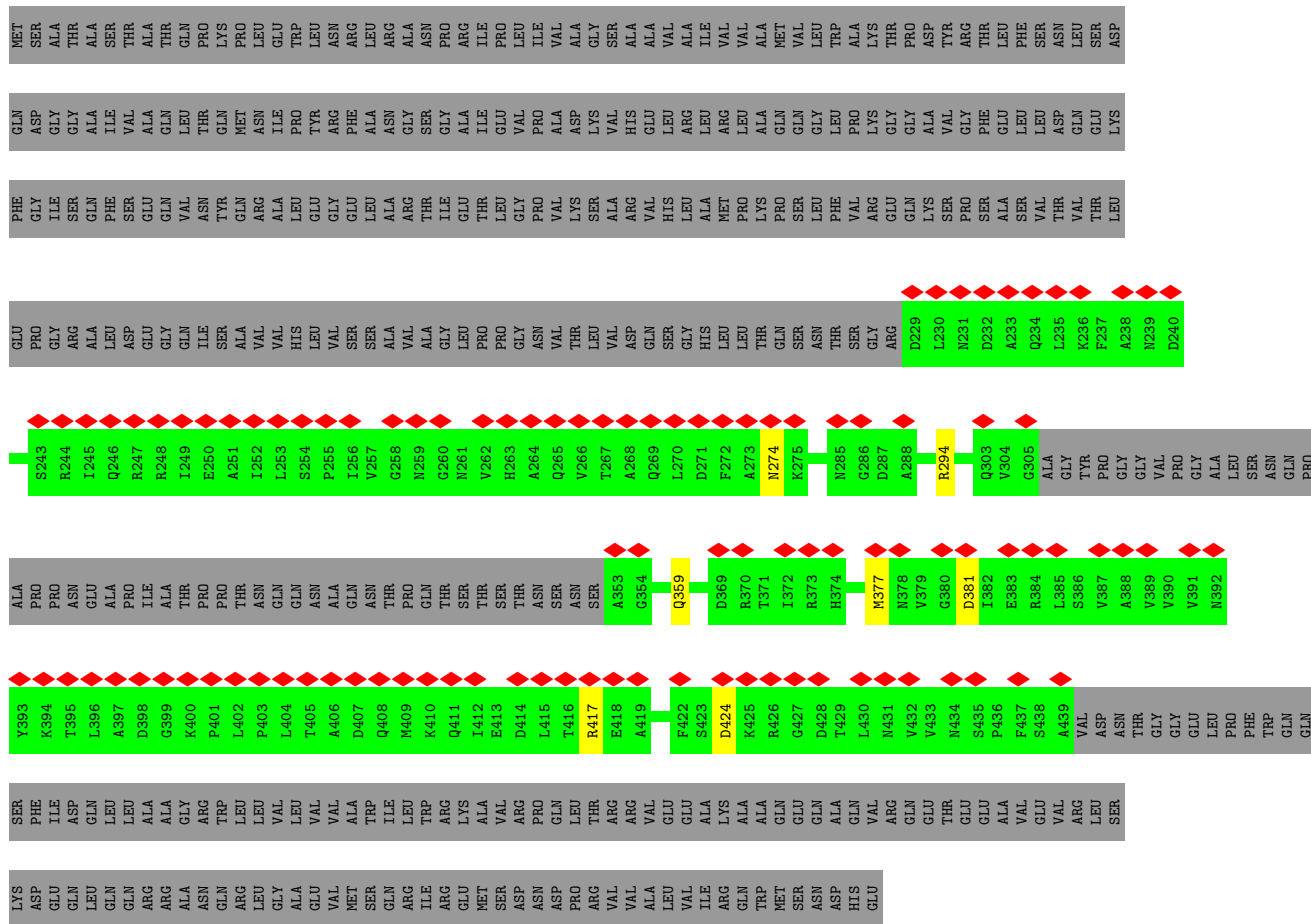
● Molecule 6: Flagellar M-ring protein





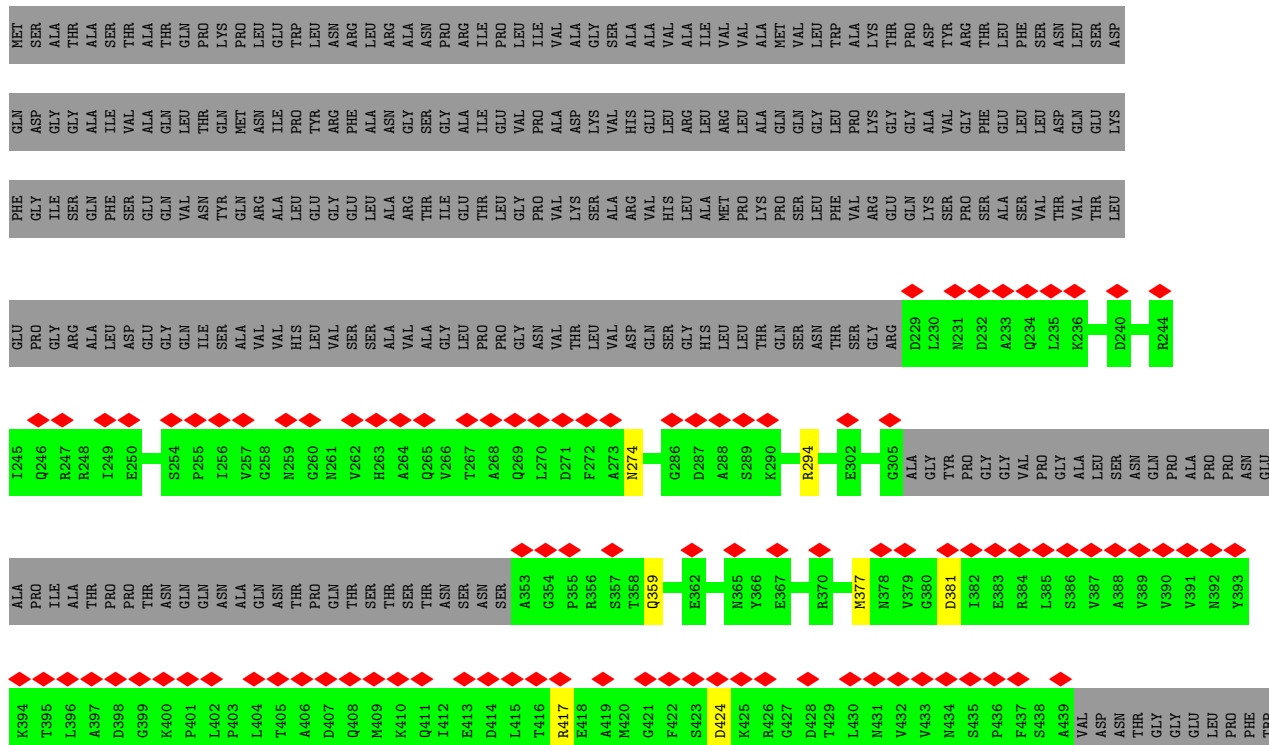


### • Molecule 6: Flagellar M-ring protein

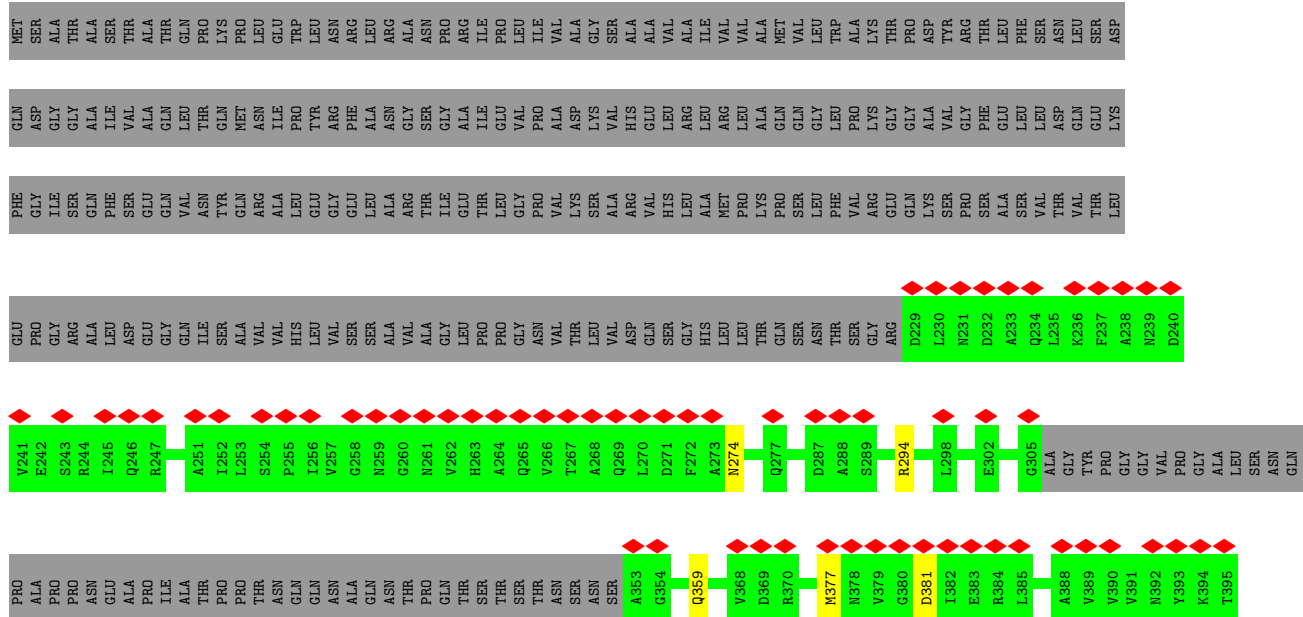


### • Molecule 6: Flagellar M-ring protein





Molecule 6: Flagellar M-ring protein











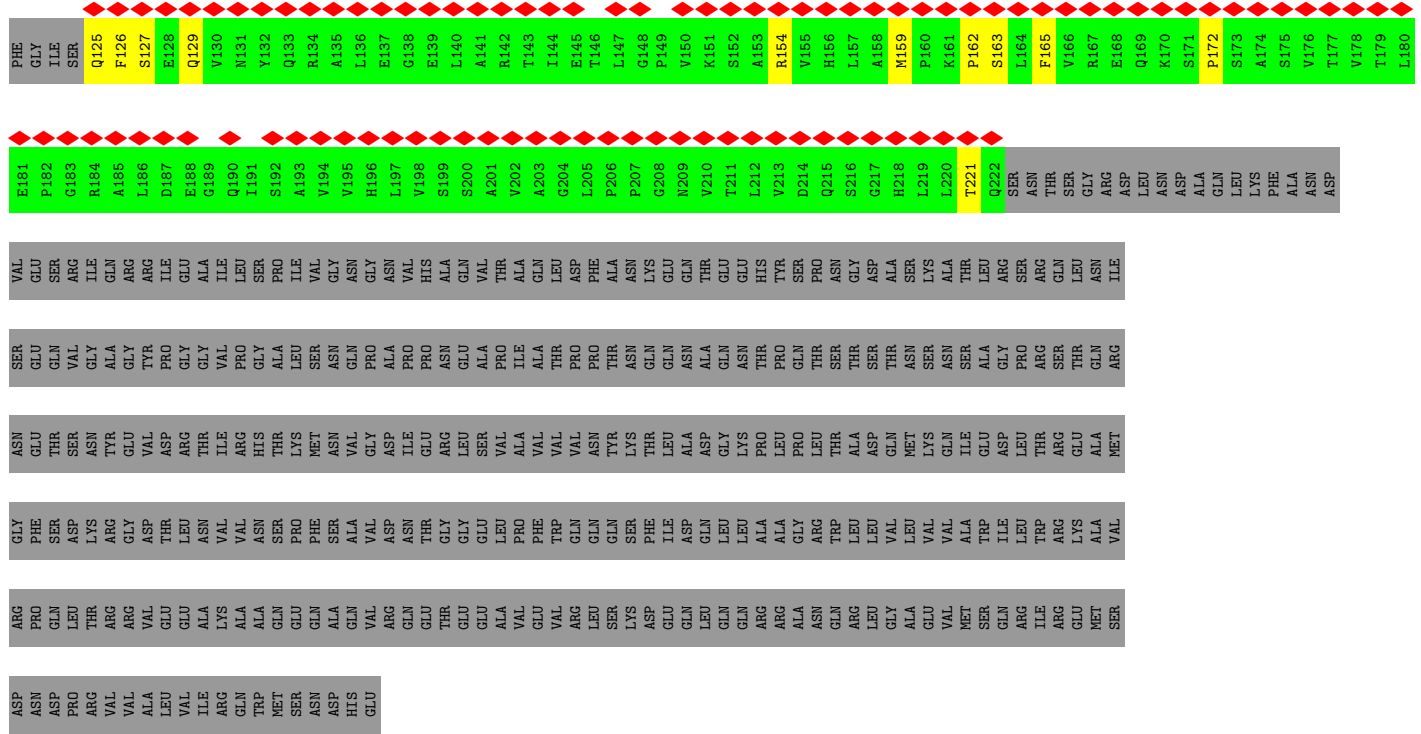
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ARG	E181	P182	G183	R184	A185	L186	D187	E188	G189	Q190	I191	S192	A193	V194	V195	H196	L197	V198	S199	S200	A201	V202	A203	G204	L205	P206	P207	G208	N209	V210	T211	L212	L213	D214	Q215	S216	G217	H218	L219	L220	T221	Q222	ASN	THR	SER	GLY	ARG	ASP	LEU	ASN	ASP	ALA	GLN	LEU	PHE	ALA	ASN	ASP
VAL	GLU	SER	ARG	ILE	GLN	GLY	ALA	VAL	ILE	PRO	GLY	VAL	ASP	ASN	GLY	ASN	ALA	THR	ALA	ILE	ALA	GLN	THR	ASP	PHE	THR	ALA	GLN	THR	GLN	THR	PRO	ASN	TRP	GLY	LEU	ASP	VAL	ALA	LEU	ARG	THR	ASP	GLY	ARG	GLN	SER	THR	THR	GLN	ALA	ALA	ILE					
SER	GLU	GLN	SER	VAL	ARG	ILE	GLN	ALA	VAL	PRO	GLY	VAL	ASP	ASN	GLY	ASN	ALA	THR	ALA	ILE	ALA	GLN	THR	ASP	PHE	THR	ALA	GLN	THR	PRO	ASN	TRP	GLY	LEU	ASP	VAL	ALA	LEU	ARG	THR	ASP	GLY	ARG	GLN	SER	THR	THR	GLN	ALA	ALA	ILE							
ASN	GLU	THR	SER	ASN	TYR	GLU	VAL	ASP	THR	ASN	GLY	VAL	ASP	ASN	VAL	GLY	ASN	THR	ALA	ILE	ALA	GLN	THR	ASP	PHE	THR	ALA	GLN	THR	PRO	ASN	TRP	GLY	LEU	ASP	VAL	ALA	LEU	ARG	THR	ASP	GLY	ARG	GLN	SER	THR	THR	GLN	ALA	ALA	MET							
GLY	PHE	SER	ASP	LYS	ARG	GLY	ASP	THR	LEU	ASN	VAL	VAL	ASN	SER	THR	GLN	THR	ALA	PRO	ALA	PHE	THR	GLN	GLY	SER	THR	ALA	ALA	GLY	LEU	VAL	ALA	ARG	ALA	GLY	VAL	VAL	VAL	ALA	THR	TRP	ILE	ILE	TRP	ARG	GLY	THR	ALA	ALA	VAL	VAL	SER						
ARG	PRO	GLN	LEU	THR	ARG	VAL	GLU	GLY	ALA	ASN	GLY	VAL	ASP	ASN	GLN	VAL	ARG	ALA	PRO	ALA	VAL	GLU	GLY	GLN	SER	THR	ALA	GLN	THR	PRO	ASN	TRP	GLY	LEU	ASP	VAL	ALA	LEU	ARG	ALA	GLN	THR	TRP	ILE	ARG	GLY	THR	THR	ALA	ALA	MET	SER						
ASP	ASN	ASP	PRO	ARG	VAL	VAL	LEU	VAL	VAL	GLN	TRP	MET	SER	ASN	ASP	HIS	GLU																																									

• Molecule 6: Flagellar M-ring protein

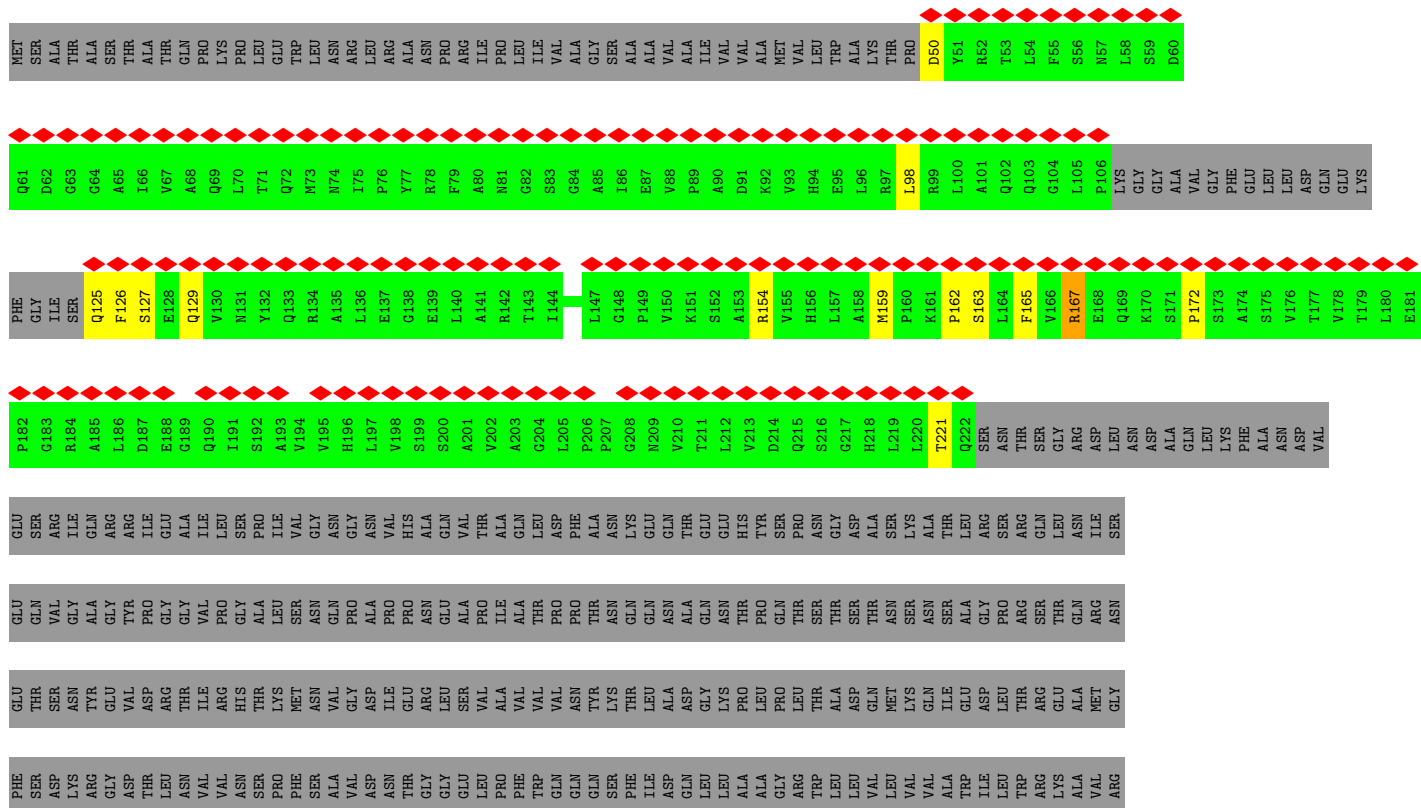


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Q61	D62	G63	G64	A65	I66	V67	A68	Q69	L70	T71	Q72	M73	N74	I75	P76	Y77	R78	F79	A80	N81	G82	S83	G84	A85	I86	E87	V88	P89	A90	D91	K92	V93	H94	E95	L96	R97	L98	R99	L100	A101	Q102	Q103	G104	F105	L106	L107	L108	L109	P110	L111	G112	L113	L114	L115	L116	L117	L118	L119	L120	L121	L122	L123	L124	L125	L126	L127	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180
VAL	GLU	SER	ARG	ILE	GLN	GLY	ALA	VAL	ILE	PRO	GLY	VAL	ASP	ASN	GLY	ASN	ALA	THR	ALA	ILE	ALA	GLN	THR	ASP	PHE	THR	ALA	GLN	THR	PRO	ASN	TRP	GLY	LEU	ASP	VAL	ALA	LEU	ARG	THR	ASP	GLY	ARG	GLN	SER	THR	THR	GLN	ALA	ALA	ILE																																																																				
SER	GLU	GLN	SER	VAL	ARG	ILE	GLN	ALA	VAL	PRO	GLY	VAL	ASP	ASN	GLY	ASN	ALA	THR	ALA	ILE	ALA	GLN	THR	ASP	PHE	THR	ALA	GLN	THR	PRO	ASN	TRP	GLY	LEU	ASP	VAL	ALA	LEU	ARG	THR	ASP	GLY	ARG	GLN	SER	THR	THR	GLN	ALA	ALA	ILE																																																																				
ASN	GLU	THR	SER	ASN	TYR	GLU	VAL	ASP	THR	ASN	GLY	VAL	ASP	ASN	VAL	GLY	ASN	THR	ALA	ILE	ALA	GLN	THR	ASP	PHE	THR	ALA	GLN	THR	PRO	ASN	TRP	GLY	LEU	ASP	VAL	ALA	LEU	ARG	THR	ASP	GLY	ARG	GLN	SER	THR	THR	GLN	ALA	ALA	ILE																																																																				
GLY	PHE	SER	ASP	LYS	ARG	GLY	ASP	THR	LEU	ASN	VAL	VAL	ASN	SER	THR	GLN	VAL	ARG	ALA	PRO	ALA	PHE	THR	GLN	GLY	SER	THR	ALA	GLN	THR	PRO	ASN	TRP	GLY	LEU	ASP	VAL	ALA	LEU	ARG	THR	ASP	GLY	ARG	GLN	SER	THR	THR	GLN	ALA	ALA	ILE																																																																			





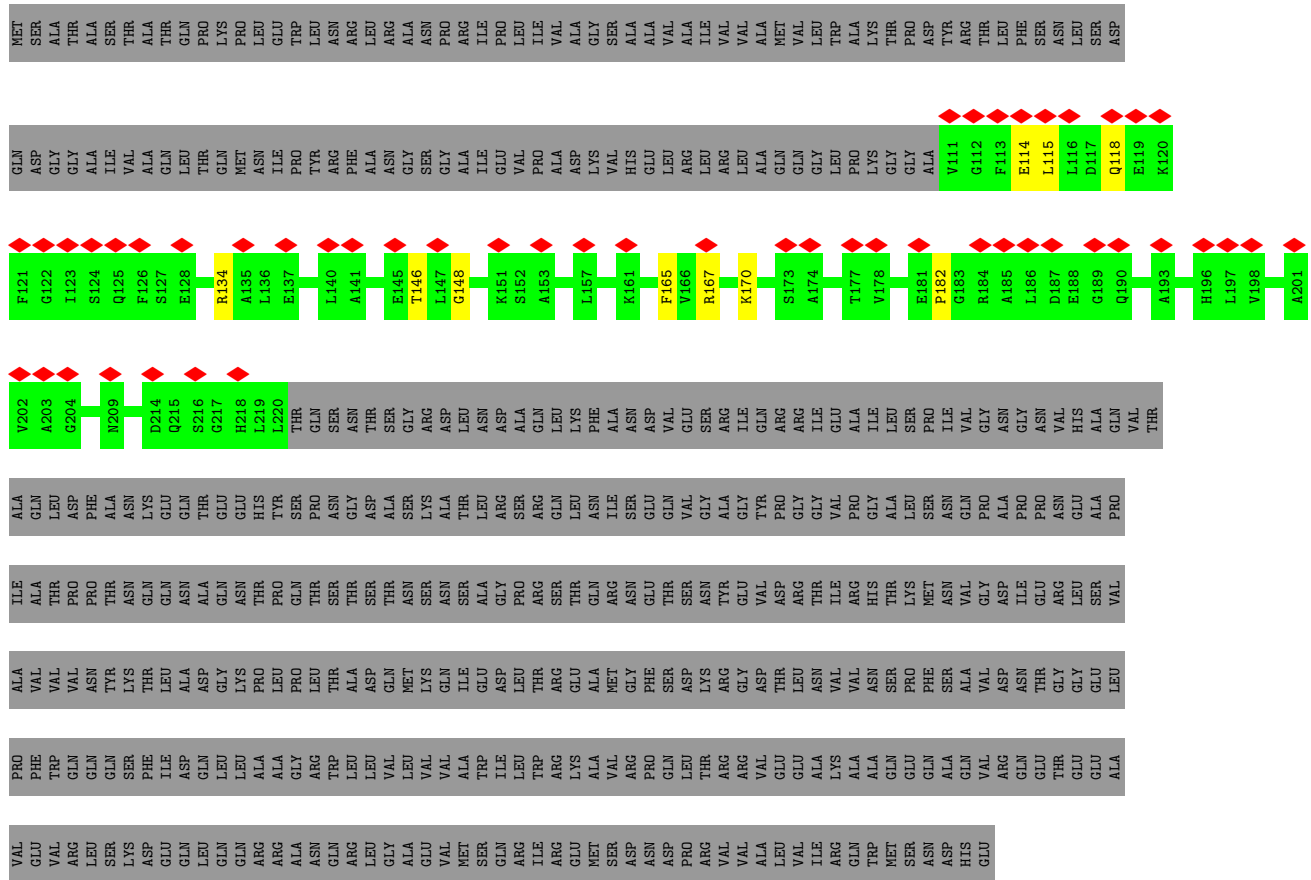
● Molecule 6: Flagellar M-ring protein



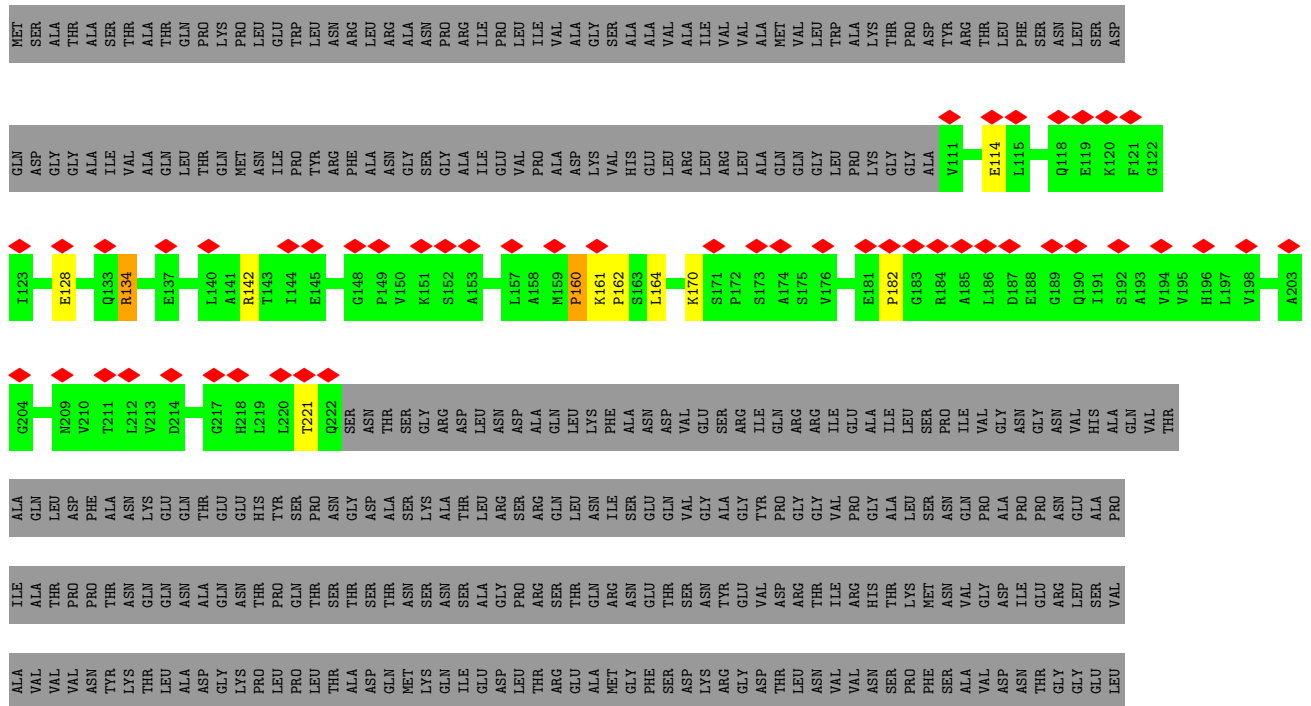




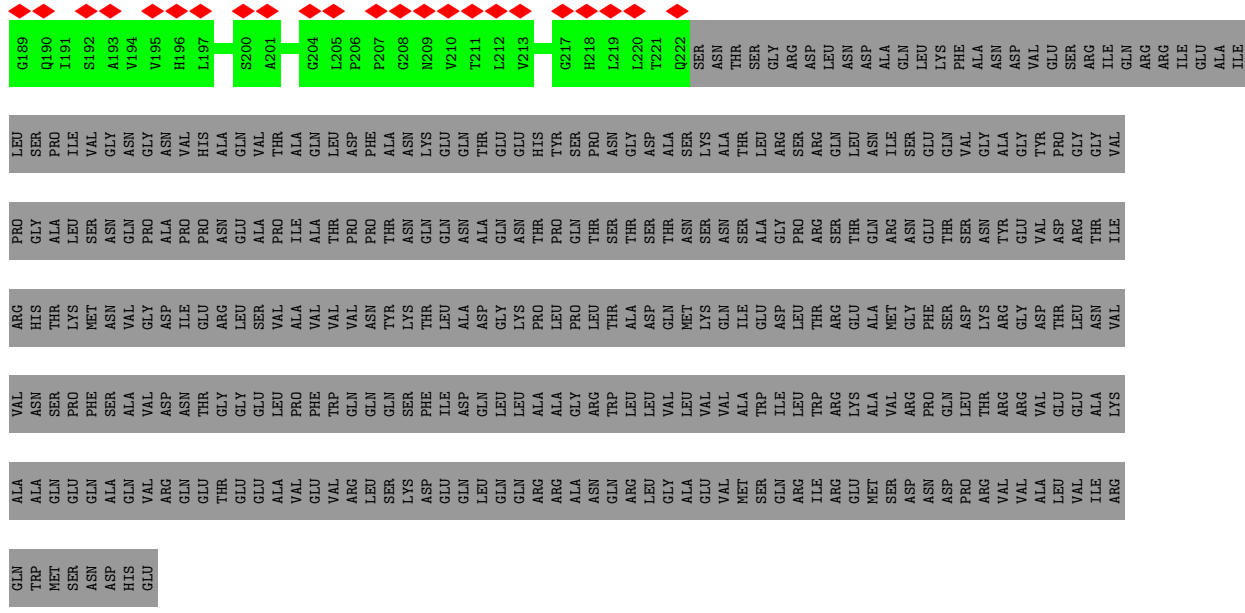




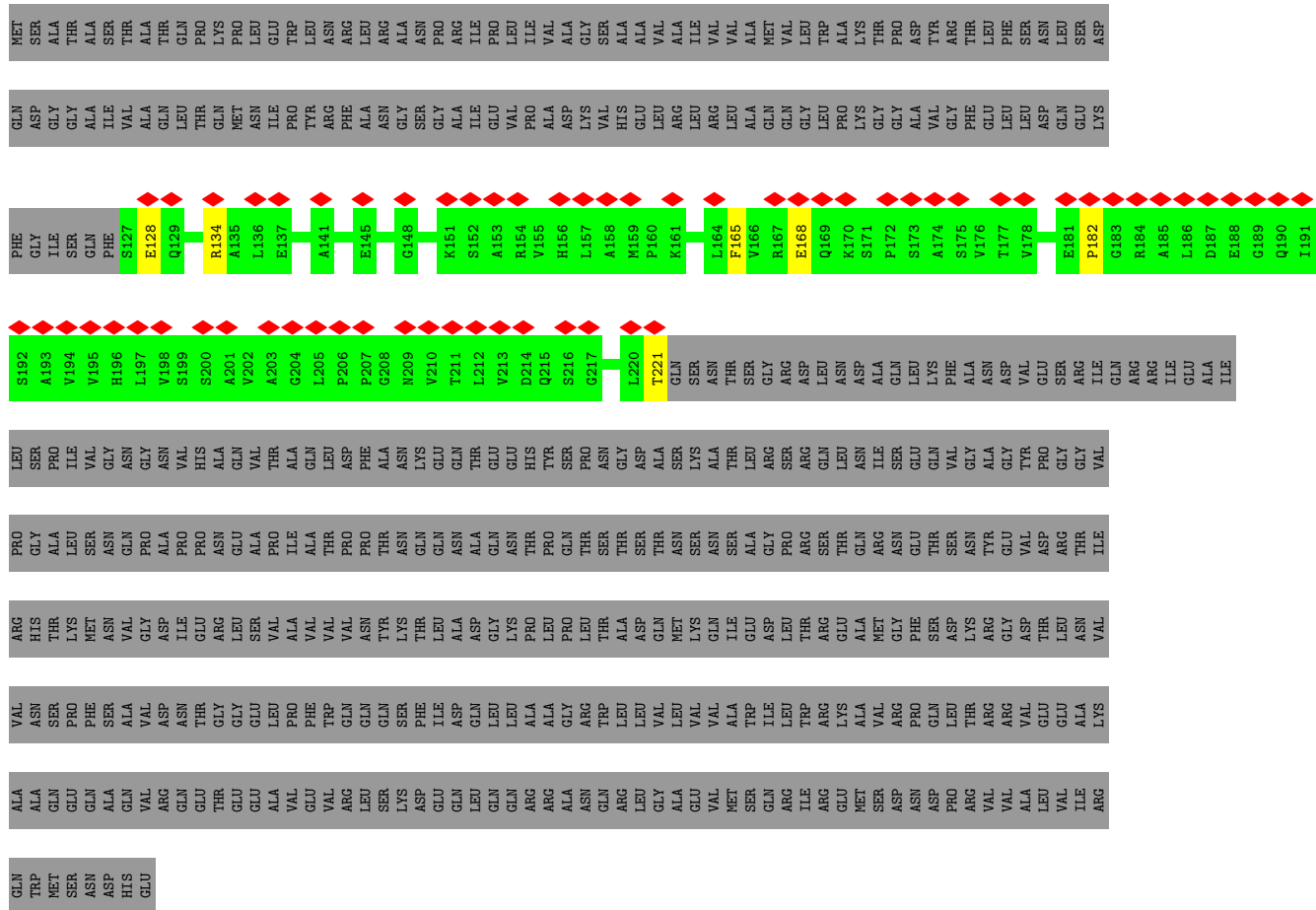
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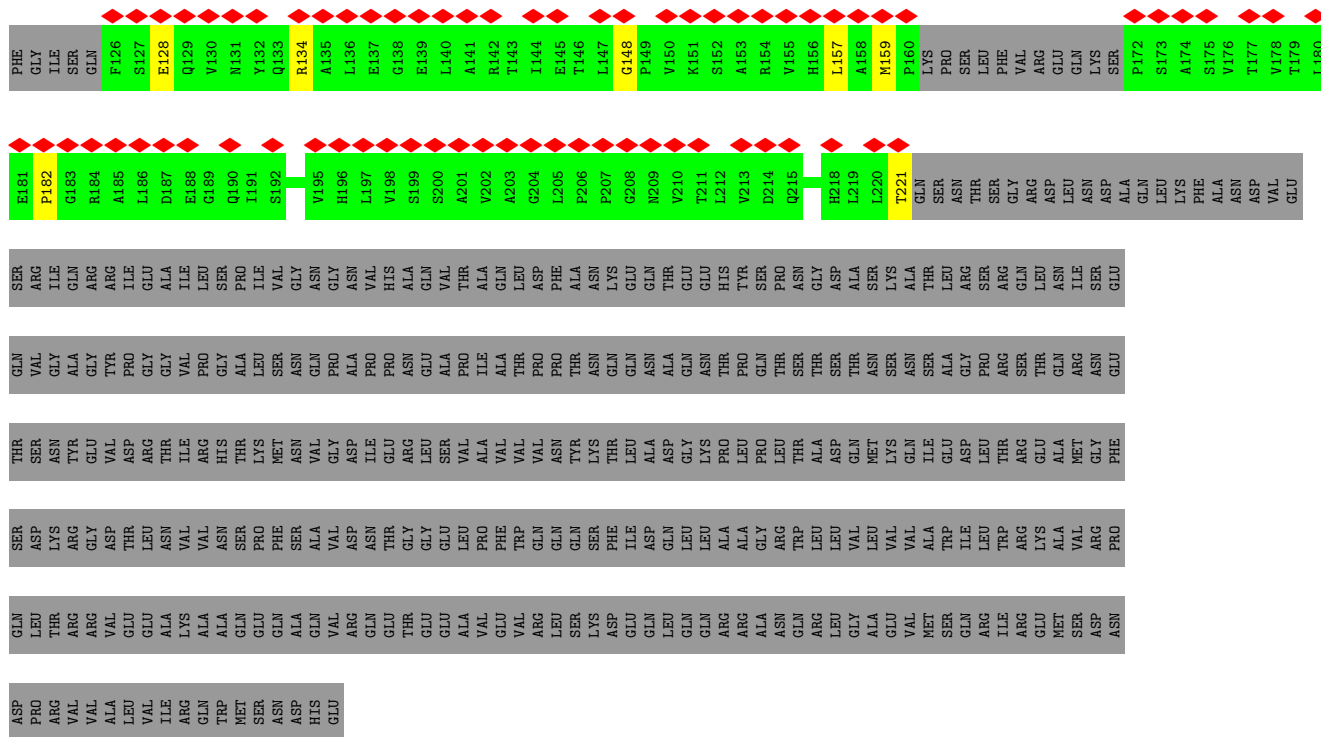
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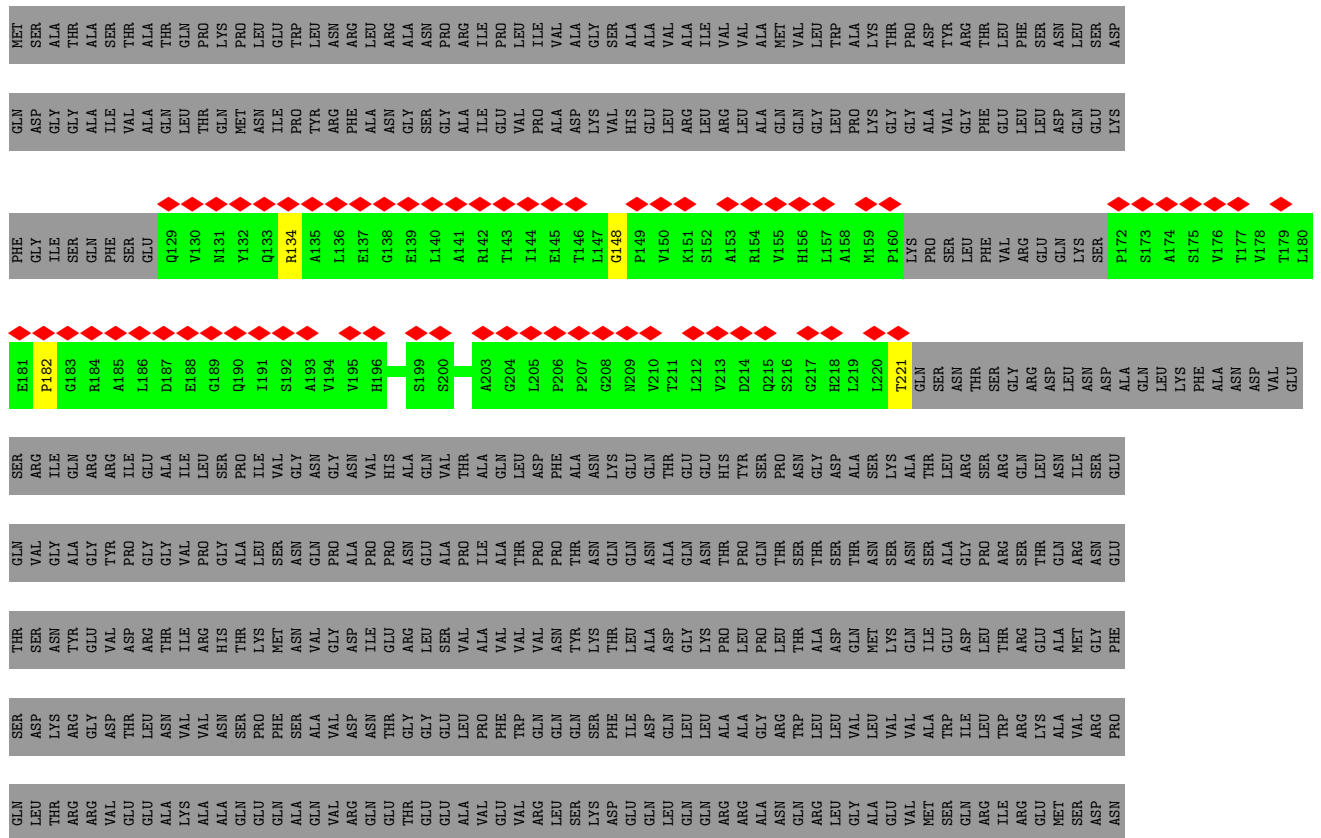
● Molecule 6: Flagellar M-ring protein







● Molecule 6: Flagellar M-ring protein



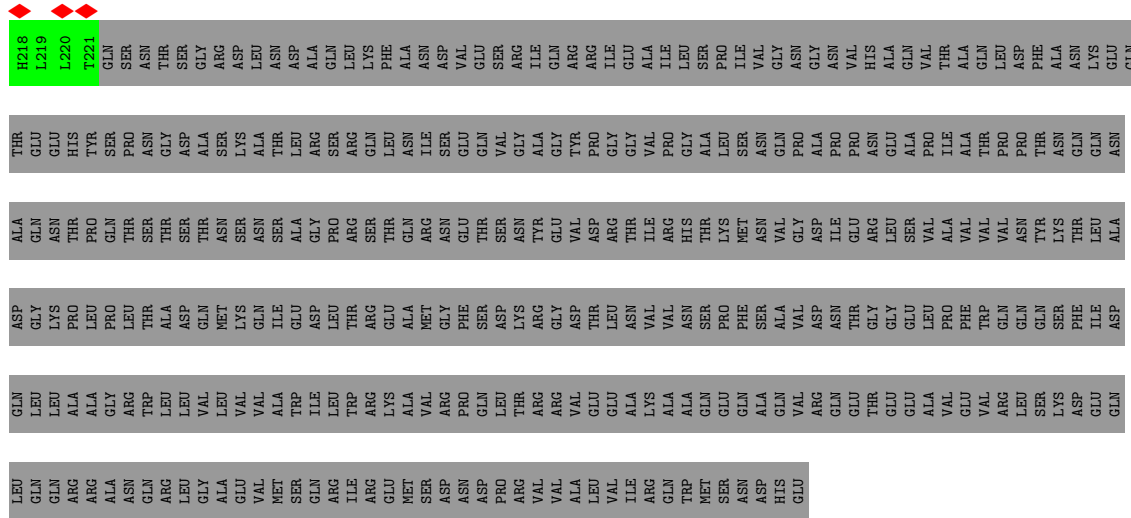




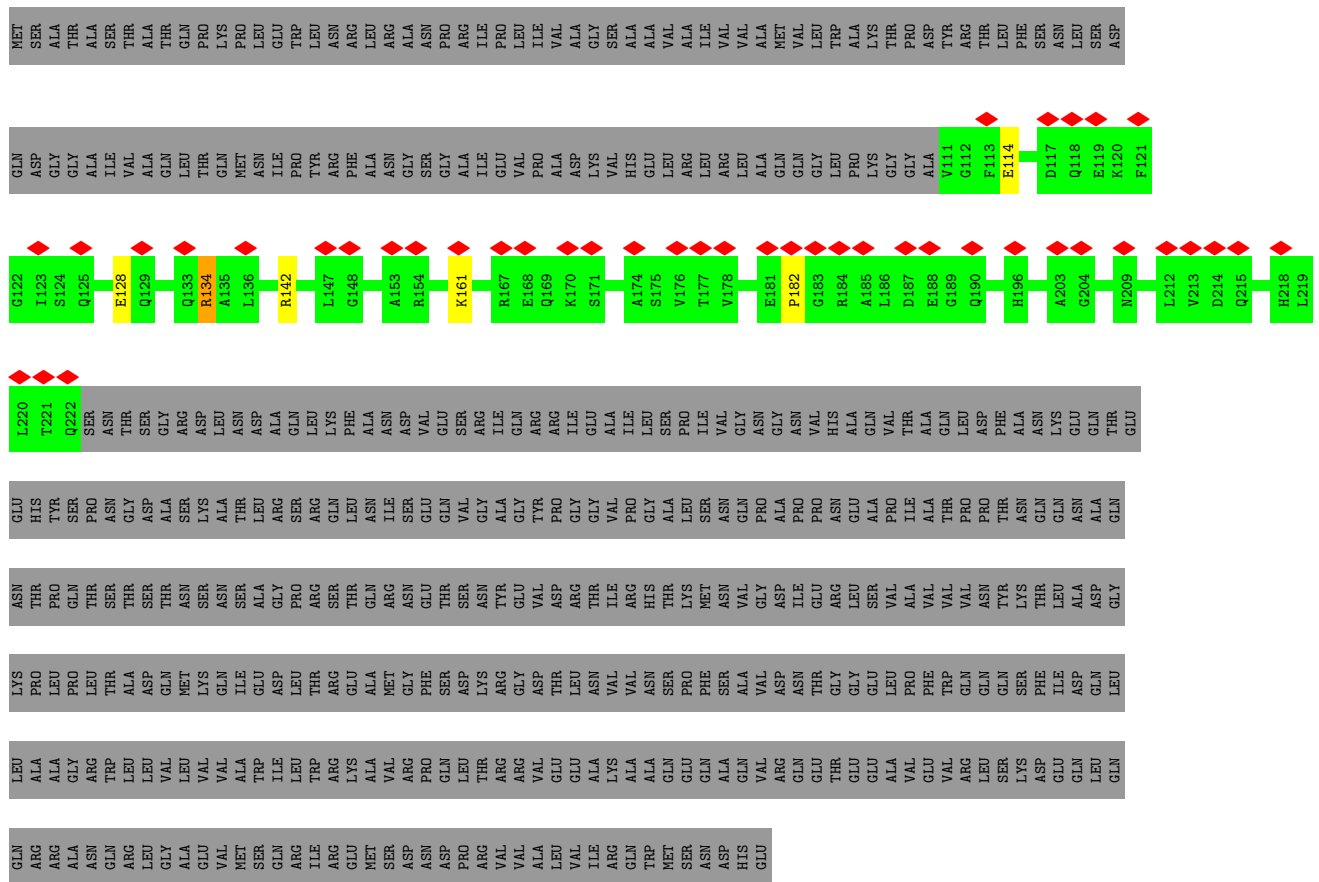








• Molecule 6: Flagellar M-ring protein



• Molecule 6: Flagellar M-ring protein













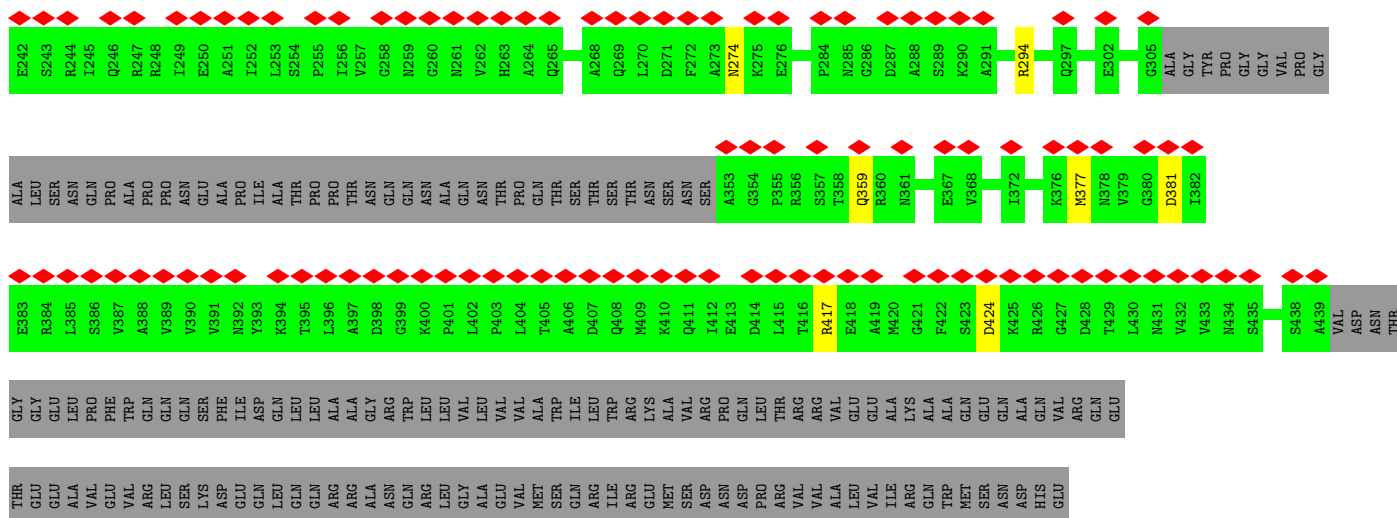




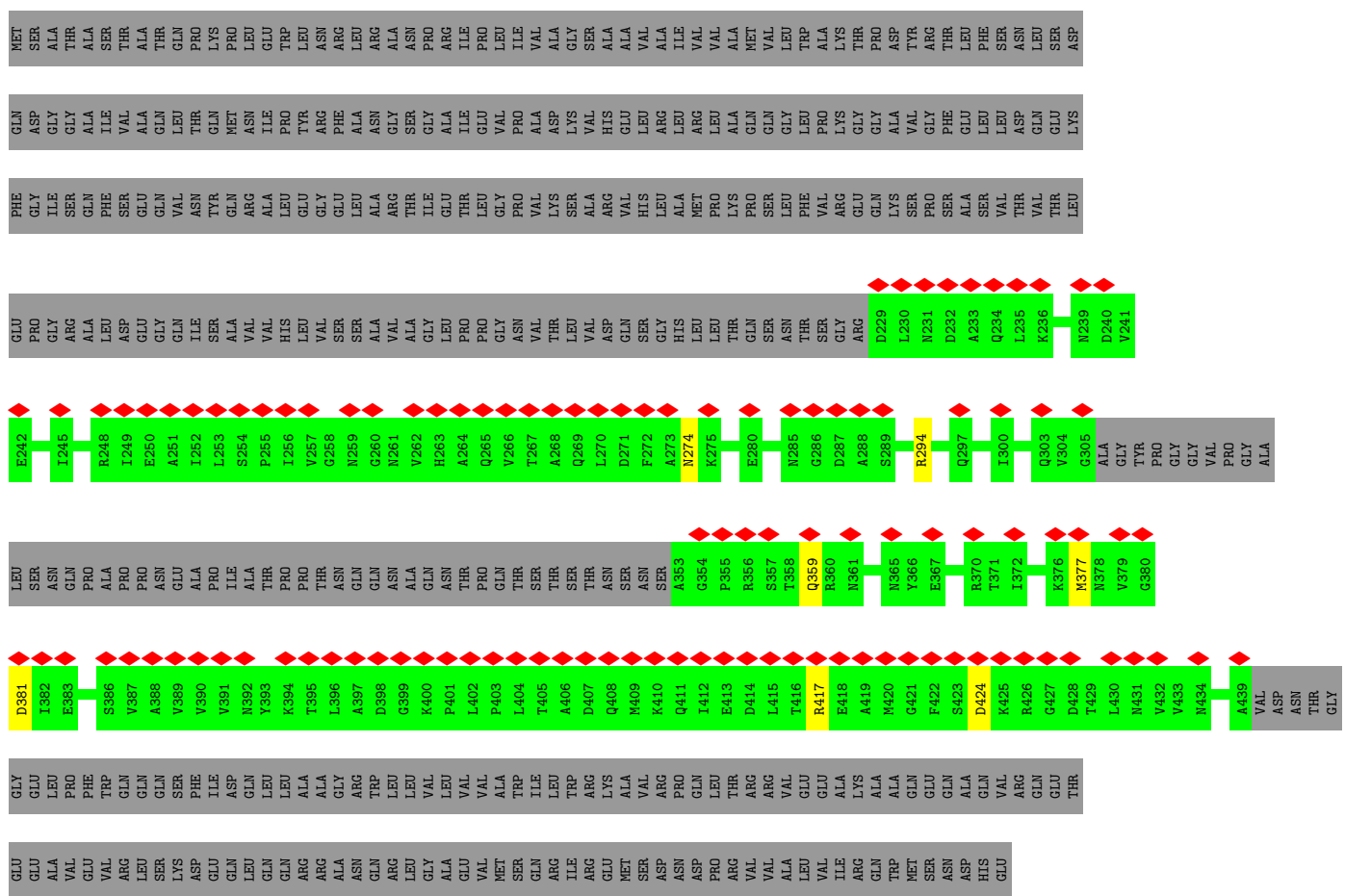






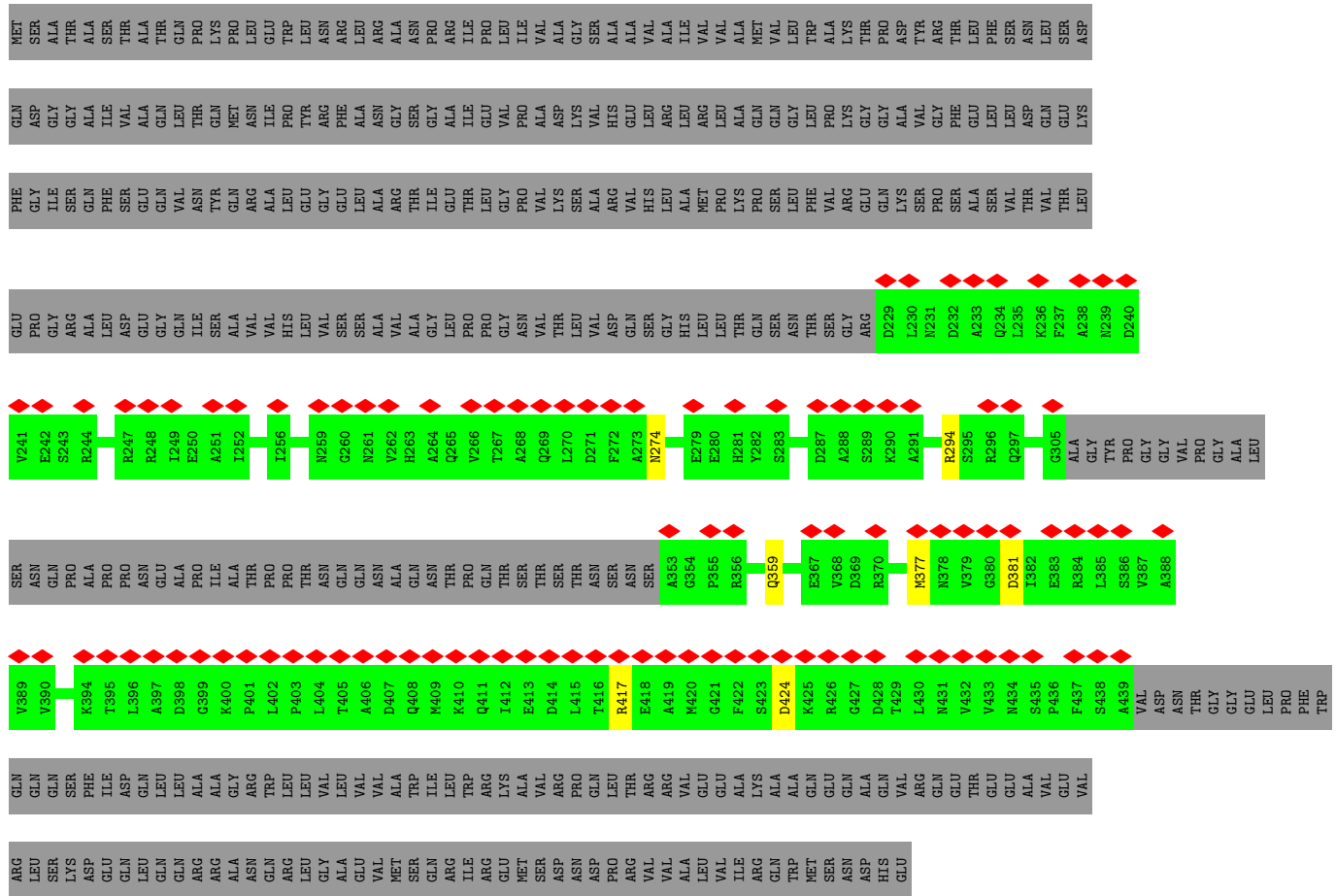


• Molecule 6: Flagellar M-ring protein

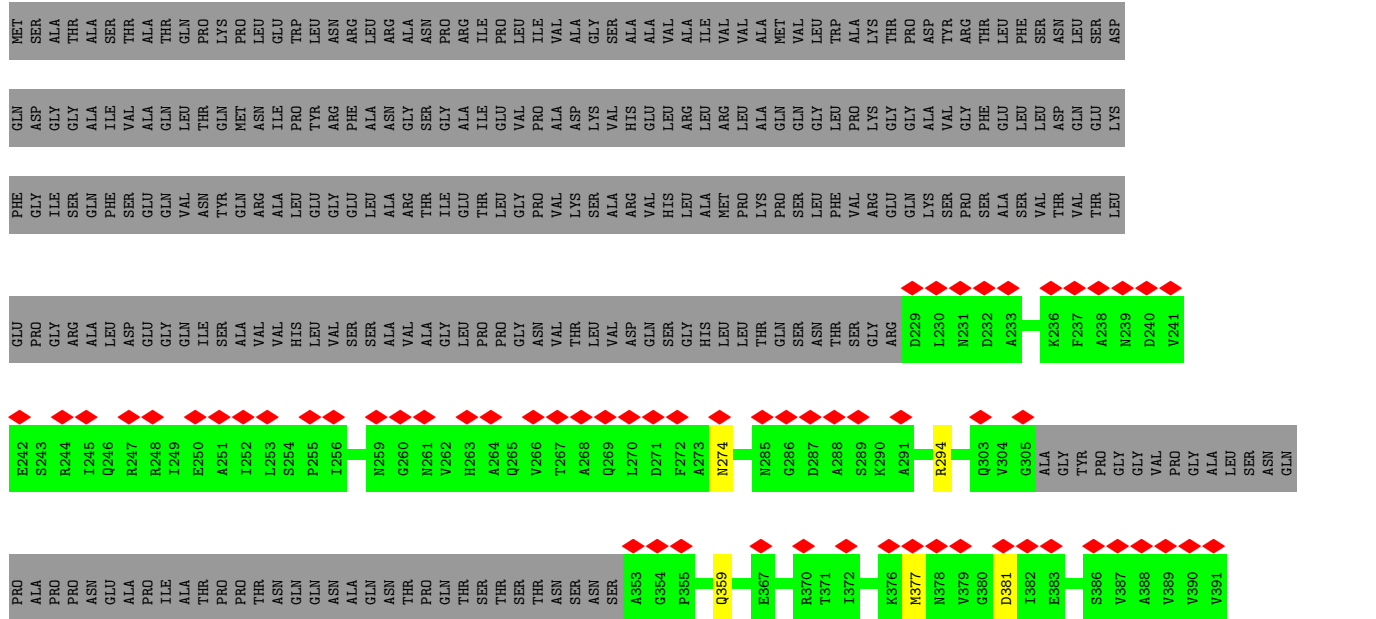


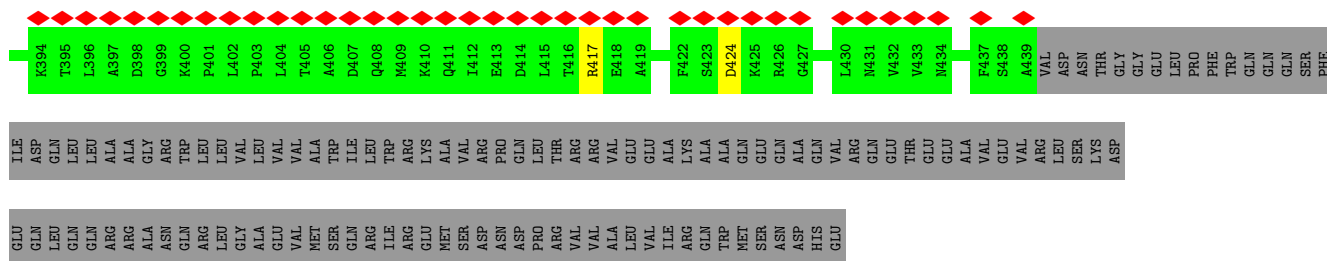
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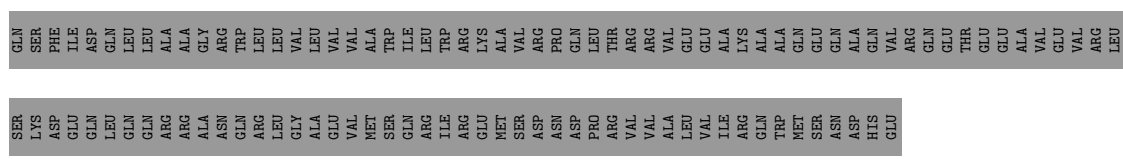
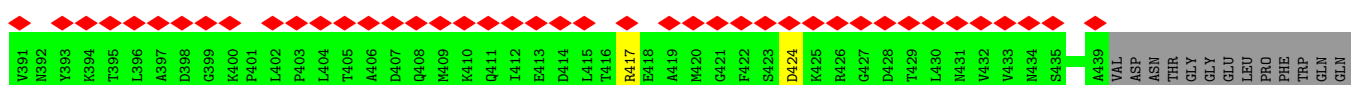
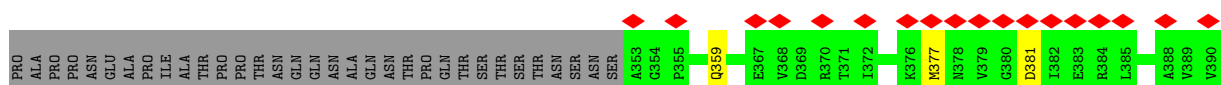
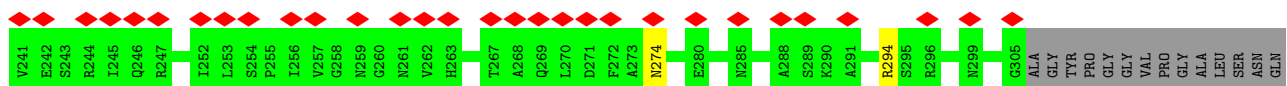
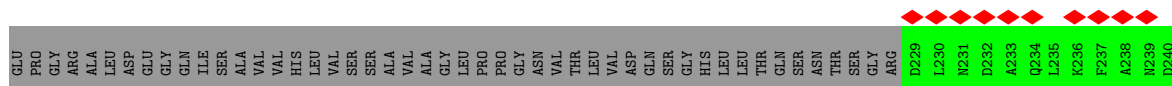
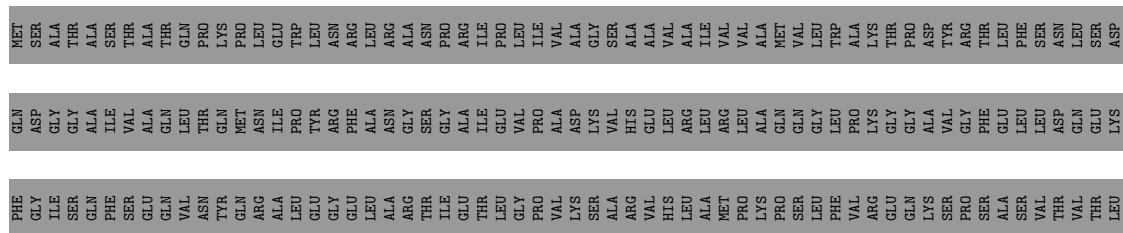


### • Molecule 6: Flagellar M-ring protein

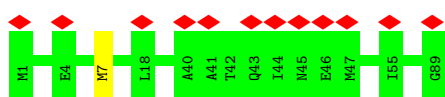




• Molecule 6: Flagellar M-ring protein

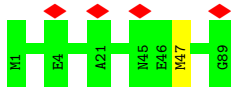


• Molecule 7: Flagellar biosynthetic protein FliQ

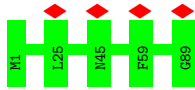


• Molecule 7: Flagellar biosynthetic protein FliQ

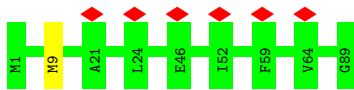




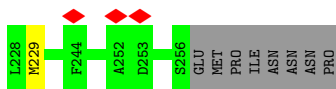
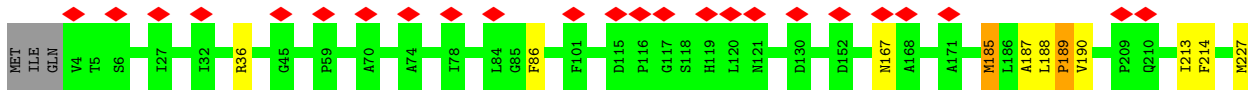
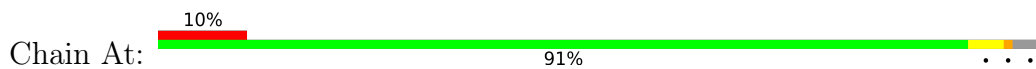
- Molecule 7: Flagellar biosynthetic protein FliQ



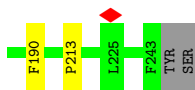
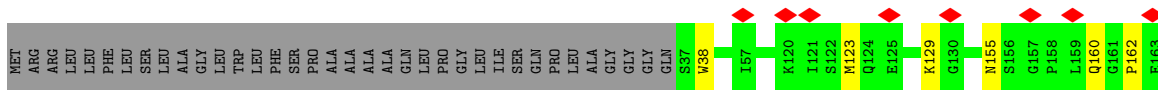
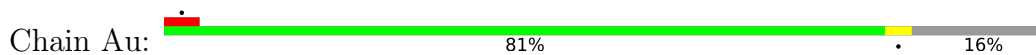
- Molecule 7: Flagellar biosynthetic protein FliQ



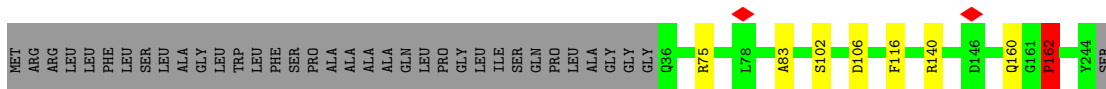
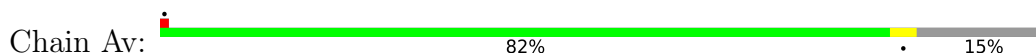
- Molecule 8: Flagellar biosynthetic protein FliR



- Molecule 9: Flagellar biosynthetic protein FliP

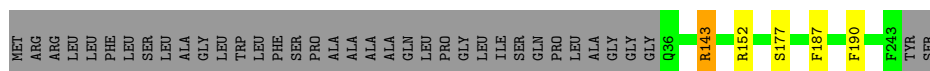
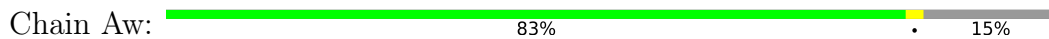


- Molecule 9: Flagellar biosynthetic protein FliP

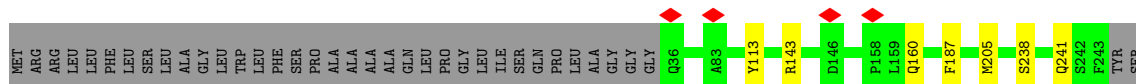
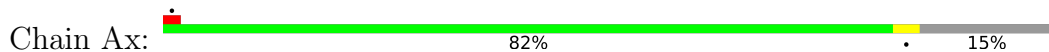


- Molecule 9: Flagellar biosynthetic protein FliP

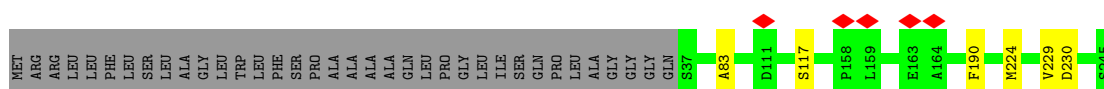
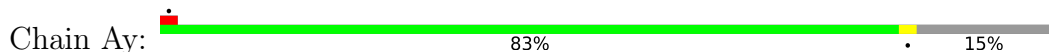




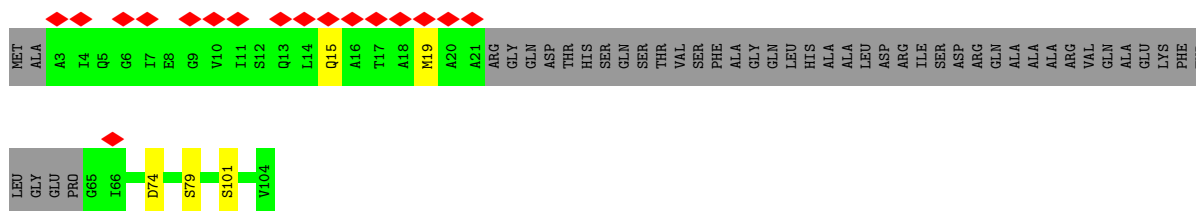
• Molecule 9: Flagellar biosynthetic protein FliP



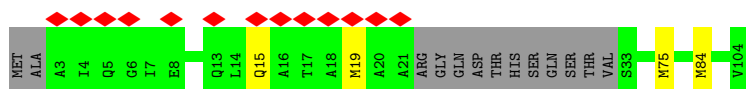
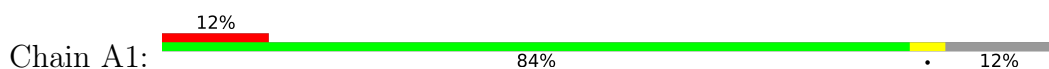
• Molecule 9: Flagellar biosynthetic protein FliP



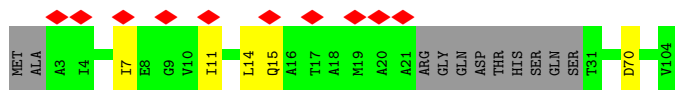
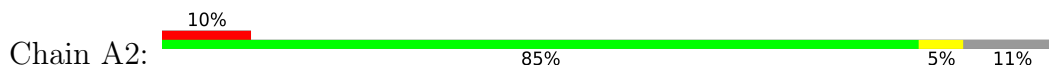
• Molecule 10: Flagellar hook-basal body complex protein FliE



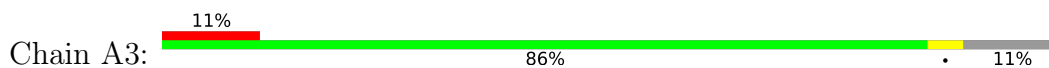
• Molecule 10: Flagellar hook-basal body complex protein FliE

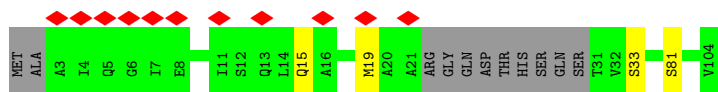


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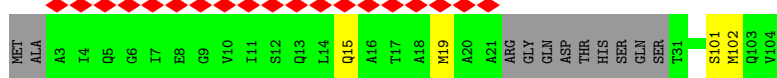
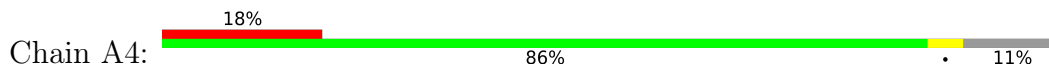


• Molecule 10: Flagellar hook-basal body complex protein FliE

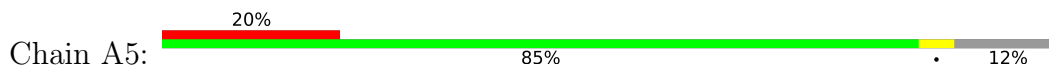




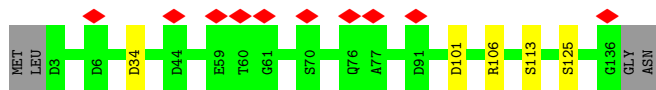
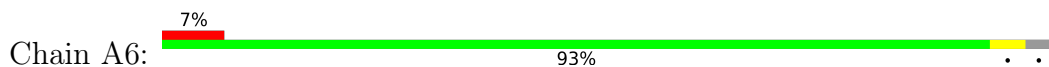
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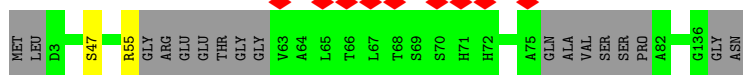
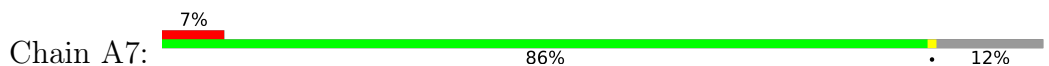
• Molecule 10: Flagellar hook-basal body complex protein FliE



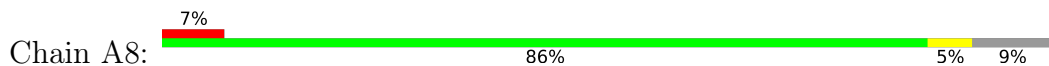
• Molecule 11: Flagellar basal body rod protein FlgB



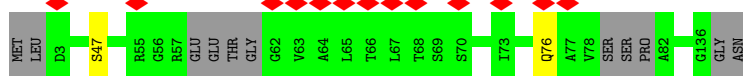
• Molecule 11: Flagellar basal body rod protein FlgB



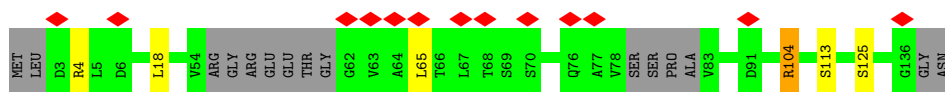
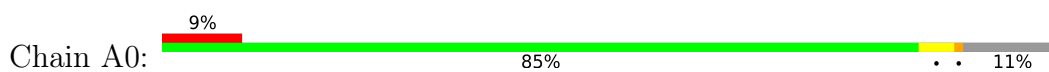
• Molecule 11: Flagellar basal body rod protein FlgB



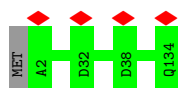
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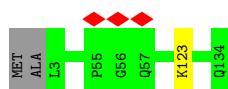
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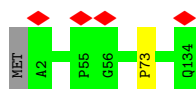
- Molecule 12: Flagellar basal-body rod protein FlgC



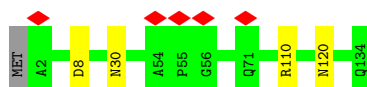
- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.118	Depositor
Minimum map value	-0.684	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.18	Depositor
Map size ( $\text{\AA}$ )	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.2, 1.2, 1.2	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/1613	0.51	0/2194
1	B	0.27	0/1613	0.51	0/2194
1	C	0.27	0/1613	0.51	0/2194
1	D	0.27	0/1613	0.51	0/2194
1	E	0.27	0/1613	0.51	0/2194
1	F	0.27	0/1613	0.51	0/2194
1	G	0.27	0/1613	0.51	0/2194
1	H	0.27	0/1613	0.51	0/2194
1	I	0.27	0/1613	0.51	0/2194
1	J	0.27	0/1613	0.51	0/2194
1	K	0.27	0/1613	0.51	0/2194
1	L	0.27	0/1613	0.51	0/2194
1	M	0.27	0/1613	0.51	0/2194
1	N	0.27	0/1613	0.51	0/2194
1	O	0.27	0/1613	0.51	0/2194
1	P	0.27	0/1613	0.51	0/2194
1	Q	0.27	0/1613	0.51	0/2194
1	R	0.27	0/1613	0.51	0/2194
1	S	0.27	0/1613	0.51	0/2194
1	T	0.27	0/1613	0.51	0/2194
1	U	0.27	0/1613	0.51	0/2194
1	V	0.27	0/1613	0.51	0/2194
1	W	0.27	0/1613	0.51	0/2194
1	X	0.27	0/1613	0.51	0/2194
1	Y	0.27	0/1613	0.51	0/2194
1	Z	0.27	0/1613	0.51	0/2194
2	a	0.26	0/2243	0.51	0/3041
2	b	0.26	0/2243	0.51	0/3041
2	c	0.26	0/2243	0.51	0/3041
2	d	0.26	0/2243	0.51	0/3041
2	e	0.26	0/2243	0.51	0/3041
2	f	0.26	0/2243	0.51	0/3041
2	g	0.26	0/2243	0.51	0/3041
2	h	0.26	0/2243	0.51	0/3041

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	i	0.26	0/2243	0.51	0/3041
2	j	0.26	0/2243	0.51	0/3041
2	k	0.26	0/2243	0.51	0/3041
2	l	0.26	0/2243	0.51	0/3041
2	m	0.26	0/2243	0.51	0/3041
2	n	0.26	0/2243	0.51	0/3041
2	o	0.26	0/2243	0.51	0/3041
2	p	0.26	0/2243	0.51	0/3041
2	q	0.25	0/2243	0.51	0/3041
2	r	0.26	0/2243	0.51	0/3041
2	s	0.26	0/2243	0.51	0/3041
2	t	0.26	0/2243	0.51	0/3041
2	u	0.26	0/2243	0.51	0/3041
2	v	0.26	0/2243	0.51	0/3041
2	w	0.26	0/2243	0.51	0/3041
2	x	0.26	0/2243	0.51	0/3041
2	y	0.26	0/2243	0.51	0/3041
2	z	0.26	0/2243	0.51	0/3041
3	0	0.30	0/1888	0.52	1/2564 (0.0%)
3	1	0.31	0/1917	0.50	0/2605
3	2	0.27	0/1973	0.48	0/2682
3	3	0.28	0/1973	0.50	0/2682
3	4	0.28	0/1973	0.50	0/2682
3	5	0.32	0/1973	0.52	0/2682
3	6	0.30	0/1973	0.52	0/2682
3	7	0.28	0/1973	0.51	0/2682
3	8	0.30	0/1973	0.52	0/2682
3	9	0.29	0/1973	0.54	1/2682 (0.0%)
3	AF	0.33	0/1926	0.53	0/2618
3	AG	0.36	0/1934	0.56	0/2629
3	AH	0.33	0/1942	0.55	0/2639
3	AI	0.32	0/1926	0.57	1/2618 (0.0%)
3	AJ	0.30	0/1934	0.51	0/2629
3	AK	0.32	0/1844	0.51	0/2505
3	AL	0.31	0/1888	0.51	0/2564
3	AM	0.30	0/1888	0.54	1/2564 (0.0%)
3	AN	0.30	0/1888	0.51	0/2564
3	ZA	0.29	0/1973	0.52	0/2682
3	ZB	0.29	0/1973	0.49	0/2682
3	ZC	0.28	0/1973	0.51	0/2682
3	ZD	0.28	0/1973	0.51	0/2682
3	ZE	0.28	0/1973	0.50	1/2682 (0.0%)
4	ZF	0.28	0/2991	0.49	0/4076

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	ZG	0.31	0/2991	0.50	0/4076
4	ZH	0.28	0/2991	0.50	0/4076
4	ZI	0.30	0/2991	0.51	0/4076
4	ZJ	0.31	0/2991	0.51	0/4076
4	ZK	0.26	0/2991	0.48	0/4076
4	ZL	0.28	0/2991	0.49	0/4076
4	ZM	0.29	0/2991	0.53	1/4076 (0.0%)
4	ZN	0.28	0/2991	0.51	0/4076
4	ZO	0.30	0/2991	0.50	0/4076
4	ZP	0.28	0/2991	0.50	1/4076 (0.0%)
4	ZQ	0.29	0/2991	0.51	0/4076
4	ZR	0.30	1/2991 (0.0%)	0.55	3/4076 (0.1%)
4	ZS	0.29	0/2991	0.52	1/4076 (0.0%)
4	ZT	0.26	0/2991	0.47	0/4076
4	ZU	0.28	0/2991	0.50	0/4076
4	ZV	0.50	4/2991 (0.1%)	0.67	6/4076 (0.1%)
4	ZW	0.25	0/2991	0.48	0/4076
4	ZX	0.28	0/2991	0.48	0/4076
4	ZY	0.30	1/2991 (0.0%)	0.54	2/4076 (0.0%)
4	ZZ	0.25	0/2991	0.46	0/4076
4	Za	0.27	0/2991	0.49	0/4076
4	Zb	0.29	0/2991	0.50	0/4076
4	Zc	0.29	0/2991	0.53	2/4076 (0.0%)
4	Zd	0.29	0/2991	0.50	0/4076
4	Ze	0.27	0/2991	0.48	0/4076
4	Zf	0.27	0/2991	0.48	0/4076
4	Zg	0.27	0/2991	0.49	0/4076
4	Zh	0.26	0/2991	0.48	0/4076
5	AA	0.33	0/1828	0.56	0/2492
5	AB	0.29	0/1836	0.54	1/2502 (0.0%)
5	AC	0.28	0/1844	0.54	0/2512
5	AD	0.27	0/1844	0.53	0/2512
5	AE	0.31	0/1836	0.55	0/2502
6	AO	0.27	0/1289	0.53	0/1741
6	AP	0.27	0/1289	0.53	0/1741
6	AQ	0.27	0/1289	0.53	0/1741
6	AR	0.26	0/1289	0.53	0/1741
6	AS	0.27	0/1289	0.53	0/1741
6	AT	0.27	0/1289	0.53	0/1741
6	AU	0.27	0/1289	0.53	0/1741
6	AV	0.27	0/1289	0.53	0/1741
6	AW	0.27	0/1289	0.53	0/1741
6	AX	0.27	0/1289	0.53	0/1741

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	AY	0.27	0/1289	0.53	0/1741
6	AZ	0.27	0/1289	0.53	0/1741
6	Aa	0.27	0/1289	0.53	0/1741
6	Ac	0.27	0/1289	0.53	0/1741
6	Ad	0.27	0/1289	0.53	0/1741
6	Ae	0.27	0/1289	0.53	0/1741
6	Af	0.27	0/1289	0.53	0/1741
6	Ag	0.27	0/1289	0.53	0/1741
6	Ah	0.26	0/1289	0.53	0/1741
6	Ai	0.27	0/1289	0.53	0/1741
6	Aj	0.27	0/1289	0.53	0/1741
6	Ak	0.26	0/1289	0.53	0/1741
6	Al	0.27	0/1289	0.53	0/1741
6	Am	0.27	0/1289	0.53	0/1741
6	An	0.27	0/1289	0.53	0/1741
6	Ao	0.27	0/1289	0.53	0/1741
6	Ap	0.26	0/1289	0.53	0/1741
6	BG	0.52	0/83	0.63	0/114
6	BH	0.27	0/107	0.38	0/148
6	BI	0.30	0/137	0.49	0/191
6	BJ	0.28	0/107	0.56	0/148
6	BK	1.36	1/145 (0.7%)	1.49	3/203 (1.5%)
6	BL	0.33	0/107	0.51	0/148
6	BM	0.26	0/145	0.44	0/203
6	BN	0.30	0/107	0.38	0/148
6	BO	0.30	0/137	0.57	0/191
6	BP	0.30	0/107	0.37	0/148
6	BQ	0.29	0/145	0.45	0/203
6	BR	0.27	0/1289	0.52	0/1741
6	BS	0.27	0/1289	0.53	0/1741
6	BT	0.27	0/1289	0.53	0/1741
6	BU	0.27	0/1289	0.53	0/1741
6	BV	0.27	0/1289	0.53	0/1741
6	BW	0.26	0/1289	0.52	0/1741
6	BX	0.27	0/1289	0.53	0/1741
6	UI	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UJ	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UK	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UL	0.82	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UM	0.84	3/1191 (0.3%)	0.82	4/1618 (0.2%)
6	UN	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UO	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UP	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
6	WA	0.61	0/863	0.72	1/1172 (0.1%)
6	WB	0.59	0/850	0.69	0/1154
6	WC	0.59	0/825	0.68	0/1121
6	WD	0.61	0/841	0.68	0/1142
6	WE	0.60	0/857	0.71	0/1164
6	WF	0.60	0/848	0.69	0/1152
6	WG	0.60	0/857	0.68	0/1164
6	WH	0.60	0/714	0.69	0/973
6	WI	0.60	0/714	0.74	0/973
6	WJ	0.61	0/749	0.72	1/1020 (0.1%)
6	WK	0.60	0/741	0.69	0/1009
6	WL	0.60	0/631	0.70	0/860
6	WM	0.59	0/604	0.70	0/824
6	WN	0.60	0/619	0.70	0/844
6	WO	0.60	0/726	0.72	1/989 (0.1%)
6	WP	0.60	0/753	0.69	0/1025
6	WQ	0.60	0/848	0.69	0/1152
6	WR	0.60	0/848	0.69	0/1152
6	WS	0.60	0/848	0.69	0/1152
6	WT	0.60	0/848	0.70	0/1152
6	WU	0.60	0/857	0.67	0/1164
6	WV	0.61	0/841	0.69	0/1142
6	WW	0.60	0/848	0.70	0/1152
7	Ab	0.29	0/681	0.47	0/930
7	Aq	0.26	0/681	0.49	0/930
7	Ar	0.28	0/681	0.48	0/930
7	As	0.29	0/681	0.49	0/930
8	At	0.38	1/1994 (0.1%)	0.56	1/2724 (0.0%)
9	Au	0.36	0/1643	0.62	2/2237 (0.1%)
9	Av	0.29	0/1665	0.49	1/2267 (0.0%)
9	Aw	0.29	0/1652	0.48	0/2249
9	Ax	0.28	0/1652	0.46	0/2249
9	Ay	0.31	0/1662	0.49	0/2263
10	A1	0.36	0/675	0.49	0/905
10	A2	0.37	0/689	0.52	0/925
10	A3	0.36	0/689	0.50	0/925
10	A4	0.37	0/689	0.53	0/925
10	A5	0.37	0/682	0.51	0/915
10	Az	0.42	0/428	0.53	0/572
11	A0	0.34	0/959	0.50	0/1293
11	A6	0.36	0/1042	0.55	0/1408
11	A7	0.33	0/951	0.49	0/1282
11	A8	0.35	0/976	0.57	0/1316

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	A9	0.34	0/991	0.54	0/1335
12	BA	0.28	0/981	0.44	0/1334
12	BB	0.26	0/976	0.46	0/1327
12	BC	0.57	2/981 (0.2%)	0.95	3/1334 (0.2%)
12	BD	0.28	0/981	0.52	1/1334 (0.1%)
12	BE	0.26	0/981	0.47	0/1334
12	BF	0.28	0/981	0.47	0/1334
All	All	0.34	27/343262 (0.0%)	0.54	68/466341 (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
2	a	0	1
2	b	0	1
2	c	0	1
2	d	0	1
2	e	0	1
2	f	0	1
2	g	0	1
2	h	0	1
2	i	0	1
2	j	0	1
2	k	0	1
2	l	0	1
2	m	0	1
2	n	0	1
2	o	0	1
2	p	0	1
2	q	0	1
2	r	0	1
2	s	0	1
2	t	0	1
2	u	0	1
2	v	0	1
2	w	0	1
2	x	0	1
2	y	0	1
2	z	0	1
3	0	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	1	0	1
3	5	0	1
3	6	0	1
3	8	0	1
3	AF	0	1
3	AI	0	1
3	AM	0	2
3	AN	0	1
3	ZA	0	1
4	ZG	0	1
4	ZI	0	1
4	ZK	0	1
4	ZO	0	1
4	ZW	0	1
4	Zb	0	1
4	Zd	0	1
4	Ze	0	1
5	AA	0	2
5	AB	0	1
5	AC	0	1
5	AE	0	1
6	UI	0	2
6	UJ	0	2
6	UK	0	3
6	UL	0	3
6	UM	0	2
6	UN	0	2
6	UO	0	2
6	UP	0	3
6	WA	0	3
6	WB	0	4
6	WC	0	3
6	WD	0	1
6	WE	0	2
6	WF	0	3
6	WG	0	3
6	WI	0	1
6	WJ	0	3
6	WK	0	2
6	WL	0	2
6	WM	0	1
6	WN	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	WO	0	1
6	WP	0	3
6	WQ	0	2
6	WR	0	3
6	WS	0	1
6	WT	0	2
6	WU	0	2
6	WV	0	3
6	WW	0	2
9	Aw	0	1
11	A0	0	1
11	A6	0	1
12	BD	0	1
12	BF	0	1
All	All	0	123

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	ZV	140	PRO	CG-CD	-16.09	0.97	1.50
6	BK	331	PRO	CG-CD	-14.22	1.03	1.50
12	BC	73	PRO	CG-CD	-12.75	1.08	1.50
4	ZV	125	PRO	CG-CD	-10.16	1.17	1.50
6	UM	172	PRO	N-CD	-9.55	1.34	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BC	73	PRO	N-CD-CG	-18.82	74.97	103.20
12	BC	73	PRO	CB-CG-CD	18.82	179.88	106.50
4	ZV	140	PRO	N-CD-CG	-17.33	77.21	103.20
6	BK	331	PRO	N-CD-CG	-16.14	78.99	103.20
12	BC	73	PRO	CA-CB-CG	-14.02	77.37	104.00

There are no chirality outliers.

5 of 123 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	a	117	ARG	Sidechain
2	b	117	ARG	Sidechain
2	c	117	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	d	117	ARG	Sidechain
2	e	117	ARG	Sidechain

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	B	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	C	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	D	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	E	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	F	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	54
1	G	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	H	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	I	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	J	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	K	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	L	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	M	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	N	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	O	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	P	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	Q	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	S	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	T	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	U	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	V	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	W	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	X	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	Y	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
1	Z	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
2	a	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	b	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	c	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	d	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	e	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	f	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	g	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	h	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	i	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	j	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	k	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	l	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	m	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	n	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	o	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	p	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	q	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	r	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	s	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	t	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	u	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	v	297/365 (81%)	293 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	w	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	x	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	y	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	z	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
3	0	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	60
3	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	60
3	2	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	44
3	3	258/260 (99%)	248 (96%)	8 (3%)	2 (1%)	16	44
3	4	258/260 (99%)	248 (96%)	7 (3%)	3 (1%)	11	35
3	5	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	44
3	6	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	44
3	7	258/260 (99%)	245 (95%)	10 (4%)	3 (1%)	11	35
3	8	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	44
3	9	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	44
3	AF	250/260 (96%)	237 (95%)	12 (5%)	1 (0%)	30	60
3	AG	251/260 (96%)	237 (94%)	13 (5%)	1 (0%)	30	60
3	AH	252/260 (97%)	241 (96%)	10 (4%)	1 (0%)	30	60
3	AI	250/260 (96%)	242 (97%)	6 (2%)	2 (1%)	16	44
3	AJ	251/260 (96%)	241 (96%)	9 (4%)	1 (0%)	30	60
3	AK	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	30	60
3	AL	244/260 (94%)	237 (97%)	4 (2%)	3 (1%)	11	35
3	AM	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	60
3	AN	244/260 (94%)	240 (98%)	3 (1%)	1 (0%)	30	60
3	ZA	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	11	35
3	ZB	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	35
3	ZC	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	35
3	ZD	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	44
3	ZE	258/260 (99%)	245 (95%)	12 (5%)	1 (0%)	30	60
4	ZF	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	ZG	399/403 (99%)	392 (98%)	6 (2%)	1 (0%)	37	66
4	ZH	399/403 (99%)	388 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25	54
4	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
4	ZK	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
4	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	66
4	ZM	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	ZN	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	ZO	399/403 (99%)	381 (96%)	15 (4%)	3 (1%)	16	44
4	ZP	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	66
4	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
4	ZR	399/403 (99%)	390 (98%)	8 (2%)	1 (0%)	37	66
4	ZS	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
4	ZT	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
4	ZU	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
4	ZV	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
4	ZW	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
4	ZX	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	ZY	399/403 (99%)	384 (96%)	15 (4%)	0	100	100
4	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
4	Za	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	Zb	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
4	Zc	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
4	Zd	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	Ze	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
4	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
4	Zg	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
4	Zh	399/403 (99%)	393 (98%)	6 (2%)	0	100	100
5	AA	246/251 (98%)	232 (94%)	11 (4%)	3 (1%)	11	35
5	AB	247/251 (98%)	241 (98%)	6 (2%)	0	100	100
5	AC	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
5	AD	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
5	AE	247/251 (98%)	233 (94%)	13 (5%)	1 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AO	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AP	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AQ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AR	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AS	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AT	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AU	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AV	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AW	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AX	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AY	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AZ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Aa	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ac	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ad	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ae	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Af	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ag	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ah	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ai	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Aj	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ak	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Al	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Am	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	An	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ao	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ap	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BG	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
6	BH	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
6	BI	18/560 (3%)	18 (100%)	0	0	100	100
6	BJ	14/560 (2%)	14 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BK	19/560 (3%)	19 (100%)	0	0	100	100
6	BL	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
6	BM	19/560 (3%)	19 (100%)	0	0	100	100
6	BN	14/560 (2%)	14 (100%)	0	0	100	100
6	BO	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
6	BP	14/560 (2%)	14 (100%)	0	0	100	100
6	BQ	19/560 (3%)	19 (100%)	0	0	100	100
6	BR	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BS	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BT	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BU	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BV	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BW	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BX	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	UI	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UJ	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UK	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UL	151/560 (27%)	142 (94%)	7 (5%)	2 (1%)	10	33
6	UM	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UN	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UO	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UP	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	WA	111/560 (20%)	99 (89%)	9 (8%)	3 (3%)	4	21
6	WB	109/560 (20%)	94 (86%)	10 (9%)	5 (5%)	2	12
6	WC	106/560 (19%)	96 (91%)	9 (8%)	1 (1%)	14	41
6	WD	108/560 (19%)	99 (92%)	4 (4%)	5 (5%)	2	12
6	WE	110/560 (20%)	98 (89%)	8 (7%)	4 (4%)	3	16
6	WF	109/560 (20%)	98 (90%)	8 (7%)	3 (3%)	4	20
6	WG	110/560 (20%)	98 (89%)	10 (9%)	2 (2%)	7	27
6	WH	93/560 (17%)	86 (92%)	5 (5%)	2 (2%)	5	24
6	WI	93/560 (17%)	82 (88%)	5 (5%)	6 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	WJ	97/560 (17%)	89 (92%)	7 (7%)	1 (1%)	13	39
6	WK	96/560 (17%)	84 (88%)	9 (9%)	3 (3%)	3	18
6	WL	81/560 (14%)	75 (93%)	4 (5%)	2 (2%)	4	22
6	WM	78/560 (14%)	72 (92%)	4 (5%)	2 (3%)	4	22
6	WN	80/560 (14%)	75 (94%)	2 (2%)	3 (4%)	2	15
6	WO	94/560 (17%)	85 (90%)	7 (7%)	2 (2%)	5	24
6	WP	98/560 (18%)	87 (89%)	6 (6%)	5 (5%)	1	11
6	WQ	109/560 (20%)	100 (92%)	5 (5%)	4 (4%)	2	16
6	WR	109/560 (20%)	94 (86%)	8 (7%)	7 (6%)	1	7
6	WS	109/560 (20%)	96 (88%)	7 (6%)	6 (6%)	1	10
6	WT	109/560 (20%)	97 (89%)	5 (5%)	7 (6%)	1	7
6	WU	110/560 (20%)	101 (92%)	8 (7%)	1 (1%)	14	41
6	WV	108/560 (19%)	97 (90%)	9 (8%)	2 (2%)	6	26
6	WW	109/560 (20%)	95 (87%)	9 (8%)	5 (5%)	2	12
7	Ab	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
7	Aq	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
7	Ar	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
7	As	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
8	At	251/264 (95%)	231 (92%)	14 (6%)	6 (2%)	5	23
9	Au	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
9	Av	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13	39
9	Aw	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
9	Ax	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25	54
9	Ay	207/245 (84%)	201 (97%)	4 (2%)	2 (1%)	13	39
10	A1	87/104 (84%)	87 (100%)	0	0	100	100
10	A2	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
10	A3	89/104 (86%)	89 (100%)	0	0	100	100
10	A4	89/104 (86%)	89 (100%)	0	0	100	100
10	A5	88/104 (85%)	88 (100%)	0	0	100	100
10	Az	55/104 (53%)	53 (96%)	2 (4%)	0	100	100
11	A0	117/138 (85%)	115 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	A6	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
11	A7	115/138 (83%)	114 (99%)	1 (1%)	0	100	100
11	A8	119/138 (86%)	116 (98%)	3 (2%)	0	100	100
11	A9	121/138 (88%)	118 (98%)	3 (2%)	0	100	100
12	BA	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
12	BB	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
12	BC	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
12	BD	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
12	BE	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16	44
12	BF	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
All	All	44708/81227 (55%)	43390 (97%)	1126 (2%)	192 (0%)	32	60

5 of 192 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	209	ASN
3	5	209	ASN
3	8	209	ASN
3	ZA	209	ASN
3	ZB	164	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	B	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	C	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	D	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	E	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	F	170/186 (91%)	163 (96%)	7 (4%)	26	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	H	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	I	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	J	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	K	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	L	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	M	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	N	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	O	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	P	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	Q	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	R	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	S	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	T	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	U	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	V	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	W	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	X	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	Y	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	Z	170/186 (91%)	163 (96%)	7 (4%)	26	51
2	a	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	b	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	c	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	d	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	e	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	f	248/294 (84%)	239 (96%)	9 (4%)	30	56
2	g	248/294 (84%)	239 (96%)	9 (4%)	30	56
2	h	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	i	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	j	248/294 (84%)	240 (97%)	8 (3%)	34	59
2	k	248/294 (84%)	238 (96%)	10 (4%)	27	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	l	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	m	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	n	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	o	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	p	248/294 (84%)	239 (96%)	9 (4%)	30	56
2	q	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	r	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	s	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	t	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	u	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	v	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	w	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	x	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	y	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	z	248/294 (84%)	238 (96%)	10 (4%)	27	52
3	0	205/215 (95%)	199 (97%)	6 (3%)	37	61
3	1	209/215 (97%)	201 (96%)	8 (4%)	28	54
3	2	215/215 (100%)	212 (99%)	3 (1%)	62	77
3	3	215/215 (100%)	211 (98%)	4 (2%)	52	71
3	4	215/215 (100%)	211 (98%)	4 (2%)	52	71
3	5	215/215 (100%)	211 (98%)	4 (2%)	52	71
3	6	215/215 (100%)	210 (98%)	5 (2%)	45	67
3	7	215/215 (100%)	214 (100%)	1 (0%)	86	91
3	8	215/215 (100%)	213 (99%)	2 (1%)	75	86
3	9	215/215 (100%)	211 (98%)	4 (2%)	52	71
3	AF	209/215 (97%)	204 (98%)	5 (2%)	44	66
3	AG	210/215 (98%)	203 (97%)	7 (3%)	33	58
3	AH	211/215 (98%)	201 (95%)	10 (5%)	22	49
3	AI	209/215 (97%)	200 (96%)	9 (4%)	25	50
3	AJ	210/215 (98%)	202 (96%)	8 (4%)	28	54
3	AK	200/215 (93%)	196 (98%)	4 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AL	205/215 (95%)	199 (97%)	6 (3%)	37	61
3	AM	205/215 (95%)	197 (96%)	8 (4%)	27	53
3	AN	205/215 (95%)	201 (98%)	4 (2%)	50	70
3	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	86
3	ZB	215/215 (100%)	207 (96%)	8 (4%)	29	54
3	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	77
3	ZD	215/215 (100%)	213 (99%)	2 (1%)	75	86
3	ZE	215/215 (100%)	214 (100%)	1 (0%)	86	91
4	ZF	321/323 (99%)	310 (97%)	11 (3%)	32	57
4	ZG	321/323 (99%)	306 (95%)	15 (5%)	22	49
4	ZH	321/323 (99%)	309 (96%)	12 (4%)	29	54
4	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	ZJ	321/323 (99%)	313 (98%)	8 (2%)	42	65
4	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	60
4	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	62
4	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	60
4	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	65
4	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	49
4	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	62
4	ZR	321/323 (99%)	313 (98%)	8 (2%)	42	65
4	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	ZT	321/323 (99%)	316 (98%)	5 (2%)	58	75
4	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	80
4	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	80
4	ZW	321/323 (99%)	308 (96%)	13 (4%)	27	52
4	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	86
4	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	68
4	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	75
4	Za	321/323 (99%)	316 (98%)	5 (2%)	58	75
4	Zb	321/323 (99%)	315 (98%)	6 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	57
4	Zd	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	Ze	321/323 (99%)	312 (97%)	9 (3%)	38	62
4	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	68
4	Zg	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	Zh	321/323 (99%)	313 (98%)	8 (2%)	42	65
5	AA	190/193 (98%)	187 (98%)	3 (2%)	58	75
5	AB	191/193 (99%)	188 (98%)	3 (2%)	58	75
5	AC	192/193 (100%)	187 (97%)	5 (3%)	41	64
5	AD	192/193 (100%)	190 (99%)	2 (1%)	73	83
5	AE	191/193 (99%)	190 (100%)	1 (0%)	86	91
6	AO	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AP	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AQ	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AR	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AS	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AT	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AU	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AV	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AW	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AX	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AY	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AZ	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Aa	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ac	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ad	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ae	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Af	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ag	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ah	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ai	141/467 (30%)	134 (95%)	7 (5%)	20	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Aj	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ak	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Al	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Am	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	An	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ao	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ap	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	BG	8/467 (2%)	8 (100%)	0	100	100
6	BH	11/467 (2%)	10 (91%)	1 (9%)	7	26
6	BI	14/467 (3%)	12 (86%)	2 (14%)	2	10
6	BJ	11/467 (2%)	11 (100%)	0	100	100
6	BK	15/467 (3%)	15 (100%)	0	100	100
6	BL	11/467 (2%)	11 (100%)	0	100	100
6	BM	15/467 (3%)	15 (100%)	0	100	100
6	BN	11/467 (2%)	11 (100%)	0	100	100
6	BO	14/467 (3%)	13 (93%)	1 (7%)	12	37
6	BP	11/467 (2%)	11 (100%)	0	100	100
6	BQ	15/467 (3%)	14 (93%)	1 (7%)	13	38
6	BR	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	BS	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	BT	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	BU	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	BV	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	BW	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	BX	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	UI	128/467 (27%)	123 (96%)	5 (4%)	27	53
6	UJ	128/467 (27%)	123 (96%)	5 (4%)	27	53
6	UK	128/467 (27%)	123 (96%)	5 (4%)	27	53
6	UL	128/467 (27%)	122 (95%)	6 (5%)	22	49
6	UM	128/467 (27%)	123 (96%)	5 (4%)	27	53
6	UN	128/467 (27%)	123 (96%)	5 (4%)	27	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	UO	128/467 (27%)	123 (96%)	5 (4%)	27	53
6	UP	128/467 (27%)	122 (95%)	6 (5%)	22	49
6	WA	95/467 (20%)	91 (96%)	4 (4%)	25	51
6	WB	93/467 (20%)	87 (94%)	6 (6%)	14	39
6	WC	91/467 (20%)	83 (91%)	8 (9%)	8	28
6	WD	92/467 (20%)	88 (96%)	4 (4%)	25	50
6	WE	94/467 (20%)	87 (93%)	7 (7%)	11	35
6	WF	93/467 (20%)	86 (92%)	7 (8%)	11	35
6	WG	94/467 (20%)	87 (93%)	7 (7%)	11	35
6	WH	79/467 (17%)	75 (95%)	4 (5%)	20	46
6	WI	79/467 (17%)	73 (92%)	6 (8%)	11	34
6	WJ	83/467 (18%)	79 (95%)	4 (5%)	21	48
6	WK	82/467 (18%)	77 (94%)	5 (6%)	15	40
6	WL	69/467 (15%)	66 (96%)	3 (4%)	25	50
6	WM	66/467 (14%)	65 (98%)	1 (2%)	60	76
6	WN	68/467 (15%)	66 (97%)	2 (3%)	37	61
6	WO	80/467 (17%)	76 (95%)	4 (5%)	20	46
6	WP	83/467 (18%)	77 (93%)	6 (7%)	12	37
6	WQ	93/467 (20%)	91 (98%)	2 (2%)	47	68
6	WR	93/467 (20%)	86 (92%)	7 (8%)	11	35
6	WS	93/467 (20%)	87 (94%)	6 (6%)	14	39
6	WT	93/467 (20%)	86 (92%)	7 (8%)	11	35
6	WU	94/467 (20%)	90 (96%)	4 (4%)	25	50
6	WV	92/467 (20%)	83 (90%)	9 (10%)	6	23
6	WW	93/467 (20%)	85 (91%)	8 (9%)	8	29
7	Ab	74/74 (100%)	73 (99%)	1 (1%)	62	77
7	Aq	74/74 (100%)	73 (99%)	1 (1%)	62	77
7	Ar	74/74 (100%)	74 (100%)	0	100	100
7	As	74/74 (100%)	73 (99%)	1 (1%)	62	77
8	At	210/221 (95%)	204 (97%)	6 (3%)	37	61
9	Au	177/204 (87%)	170 (96%)	7 (4%)	27	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Av	179/204 (88%)	172 (96%)	7 (4%)	27	53
9	Aw	178/204 (87%)	173 (97%)	5 (3%)	38	62
9	Ax	178/204 (87%)	172 (97%)	6 (3%)	32	57
9	Ay	179/204 (88%)	175 (98%)	4 (2%)	47	68
10	A1	68/79 (86%)	64 (94%)	4 (6%)	16	41
10	A2	70/79 (89%)	65 (93%)	5 (7%)	12	37
10	A3	70/79 (89%)	66 (94%)	4 (6%)	17	43
10	A4	70/79 (89%)	66 (94%)	4 (6%)	17	43
10	A5	69/79 (87%)	65 (94%)	4 (6%)	17	42
10	Az	45/79 (57%)	40 (89%)	5 (11%)	5	18
11	A0	102/113 (90%)	96 (94%)	6 (6%)	16	41
11	A6	110/113 (97%)	106 (96%)	4 (4%)	30	56
11	A7	101/113 (89%)	99 (98%)	2 (2%)	50	70
11	A8	103/113 (91%)	96 (93%)	7 (7%)	13	38
11	A9	104/113 (92%)	102 (98%)	2 (2%)	52	71
12	BA	104/105 (99%)	104 (100%)	0	100	100
12	BB	104/105 (99%)	103 (99%)	1 (1%)	73	83
12	BC	104/105 (99%)	104 (100%)	0	100	100
12	BD	104/105 (99%)	102 (98%)	2 (2%)	52	71
12	BE	104/105 (99%)	101 (97%)	3 (3%)	37	61
12	BF	104/105 (99%)	100 (96%)	4 (4%)	28	54
All	All	37085/66670 (56%)	35783 (96%)	1302 (4%)	33	56

5 of 1302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	Aj	417	ARG
6	WE	170	LYS
6	An	381	ASP
6	Aj	381	ASP
10	A2	15	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1144 such sidechains are listed below:

Mol	Chain	Res	Type
3	AG	223	ASN
3	AK	127	GLN
3	AG	145	ASN
6	AO	303	GLN
2	1	198	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

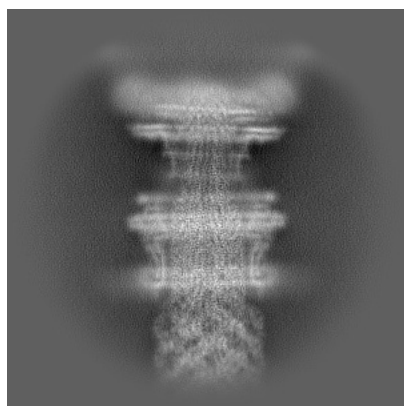
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37611. These allow visual inspection of the internal detail of the map and identification of artifacts.

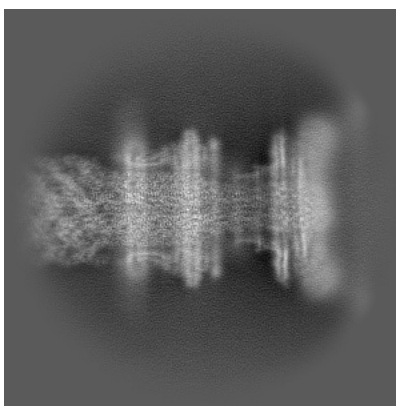
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

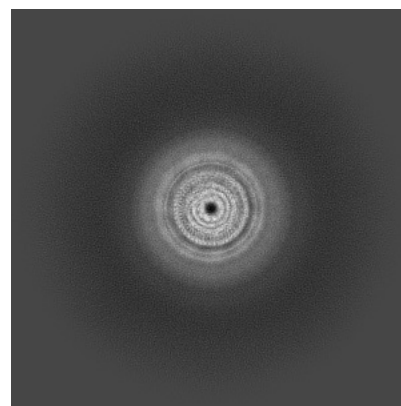
#### 6.1.1 Primary map



X

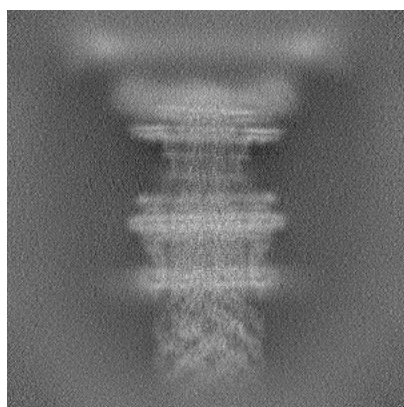


Y

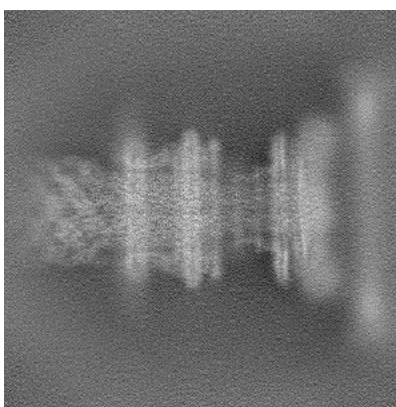


Z

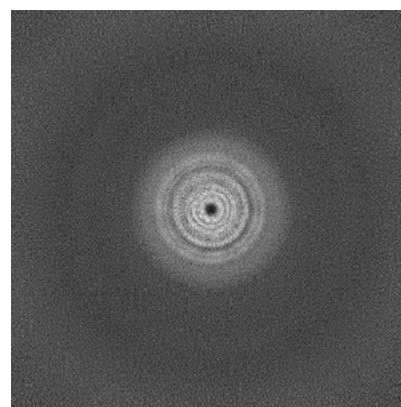
#### 6.1.2 Raw map



X



Y

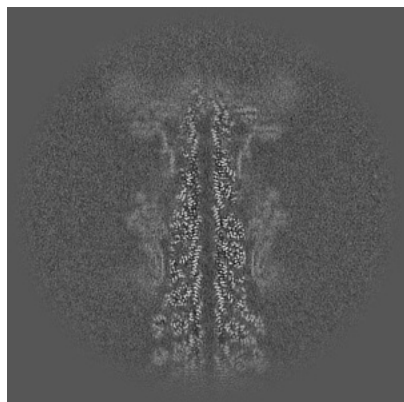


Z

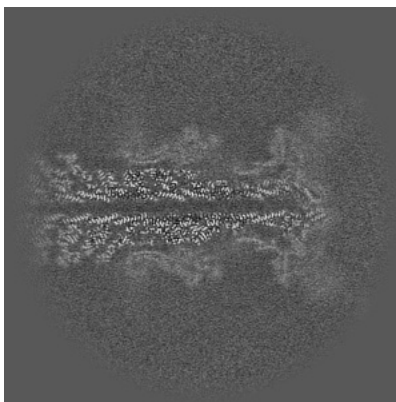
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

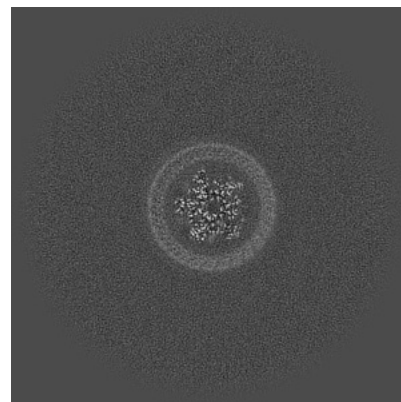
### 6.2.1 Primary map



X Index: 256

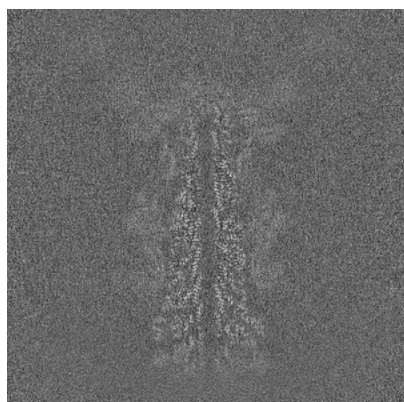


Y Index: 256

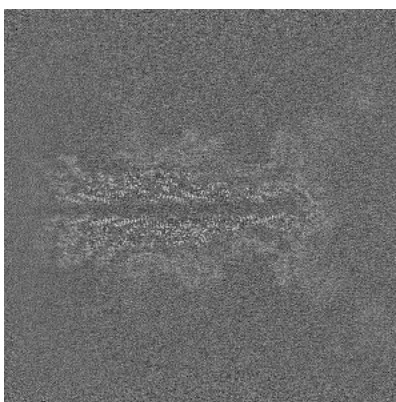


Z Index: 256

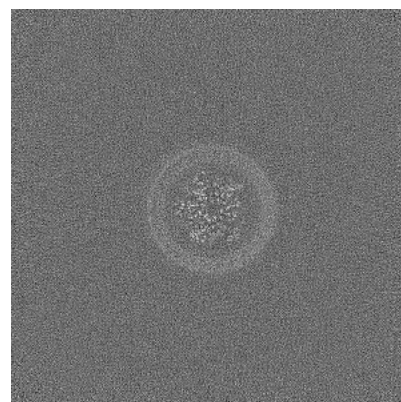
### 6.2.2 Raw map



X Index: 256



Y Index: 256

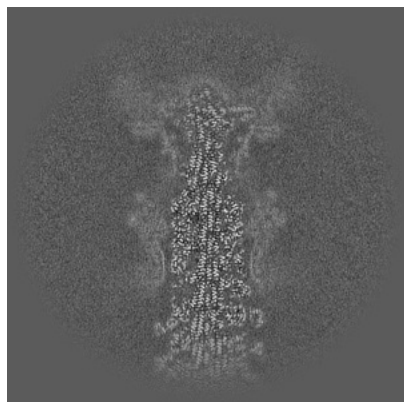


Z Index: 256

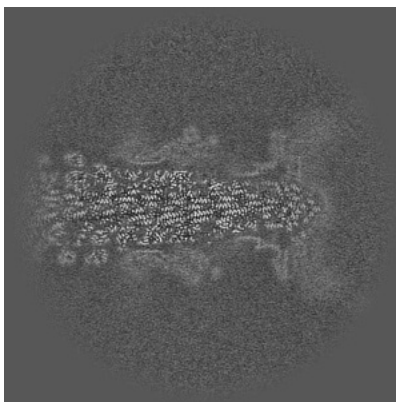
The images above show central slices of the map in three orthogonal directions.

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

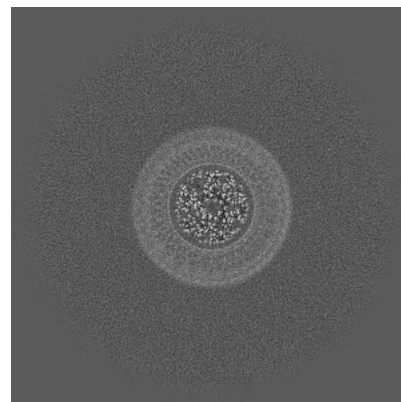
### 6.3.1 Primary map



X Index: 242

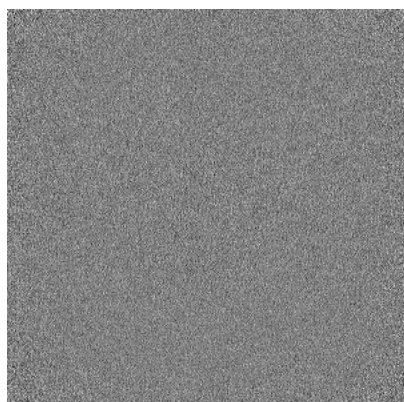


Y Index: 268

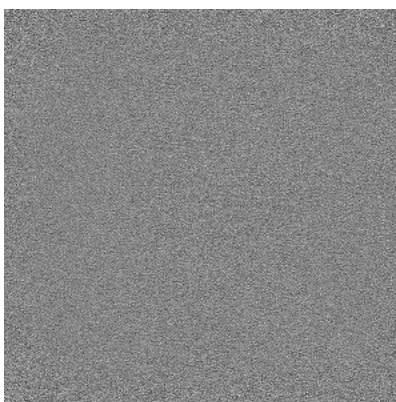


Z Index: 234

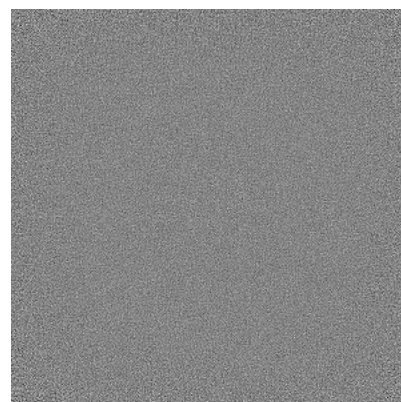
### 6.3.2 Raw map



X Index: 0



Y Index: 0

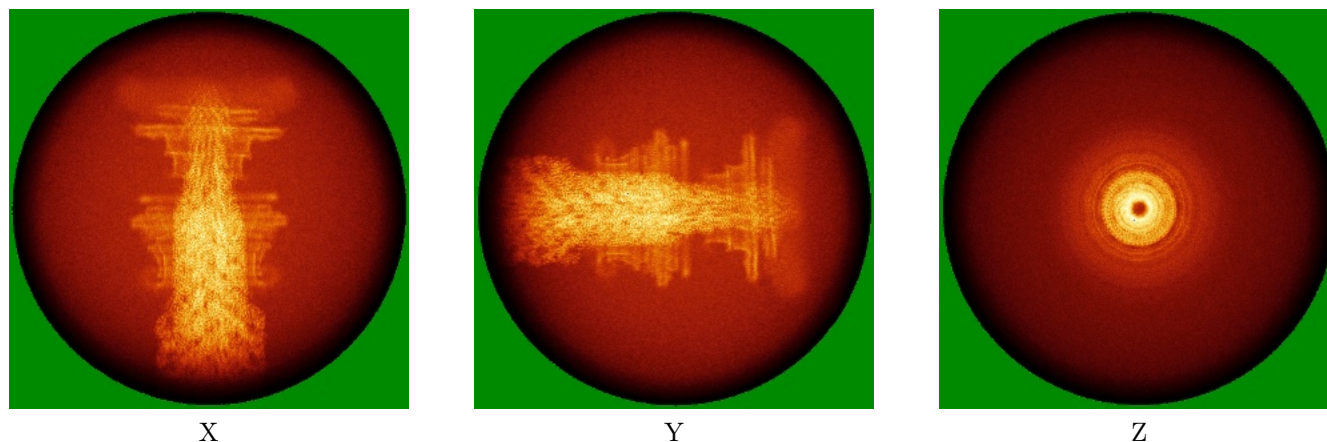


Z Index: 0

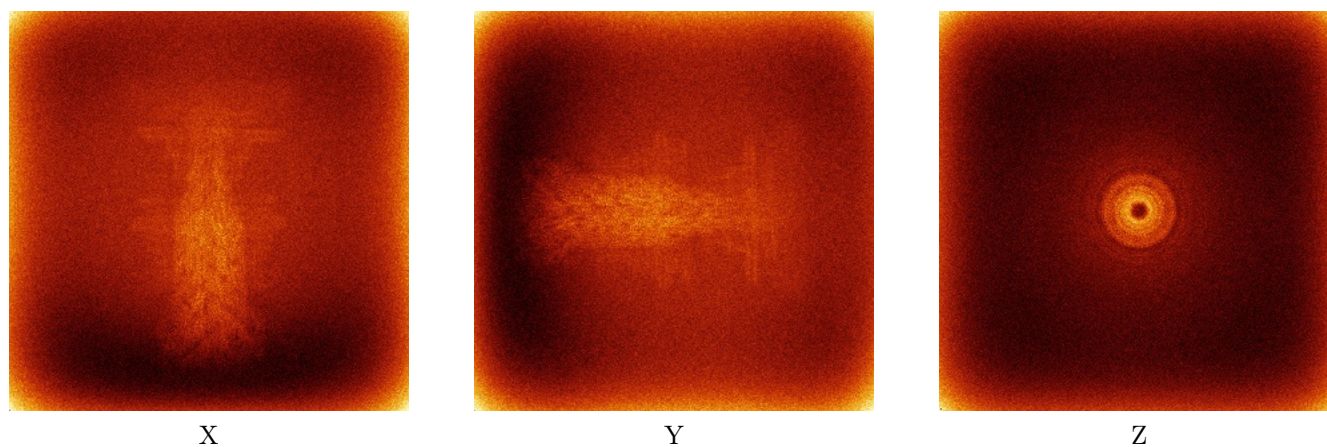
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map

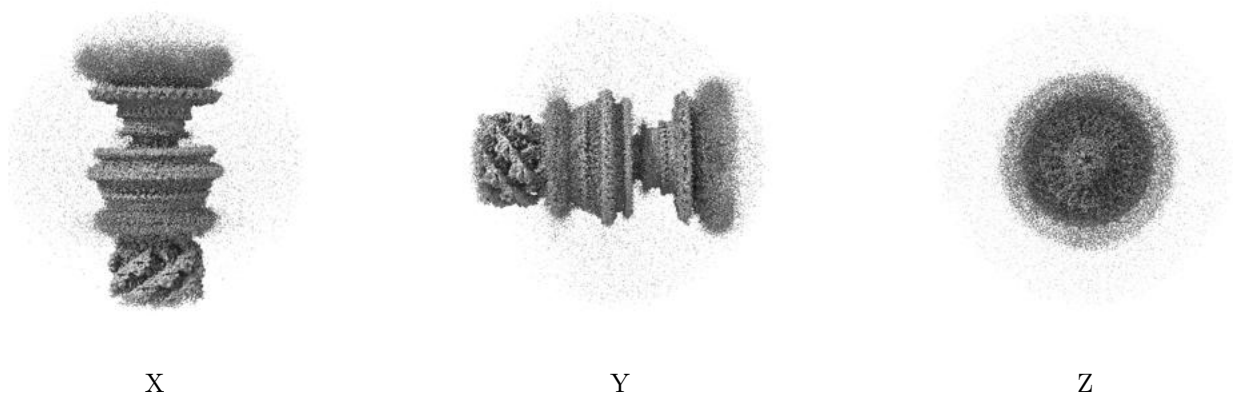


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



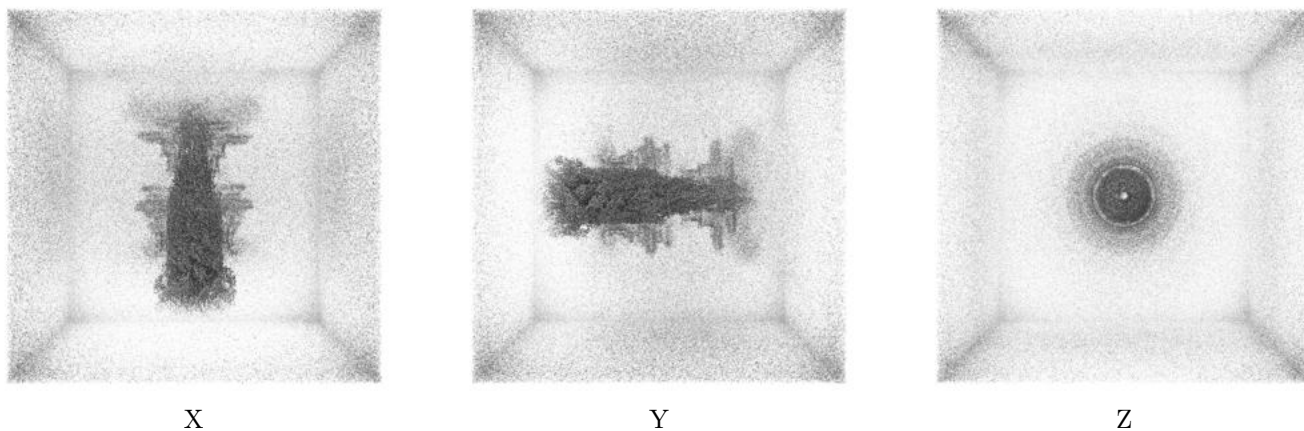
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

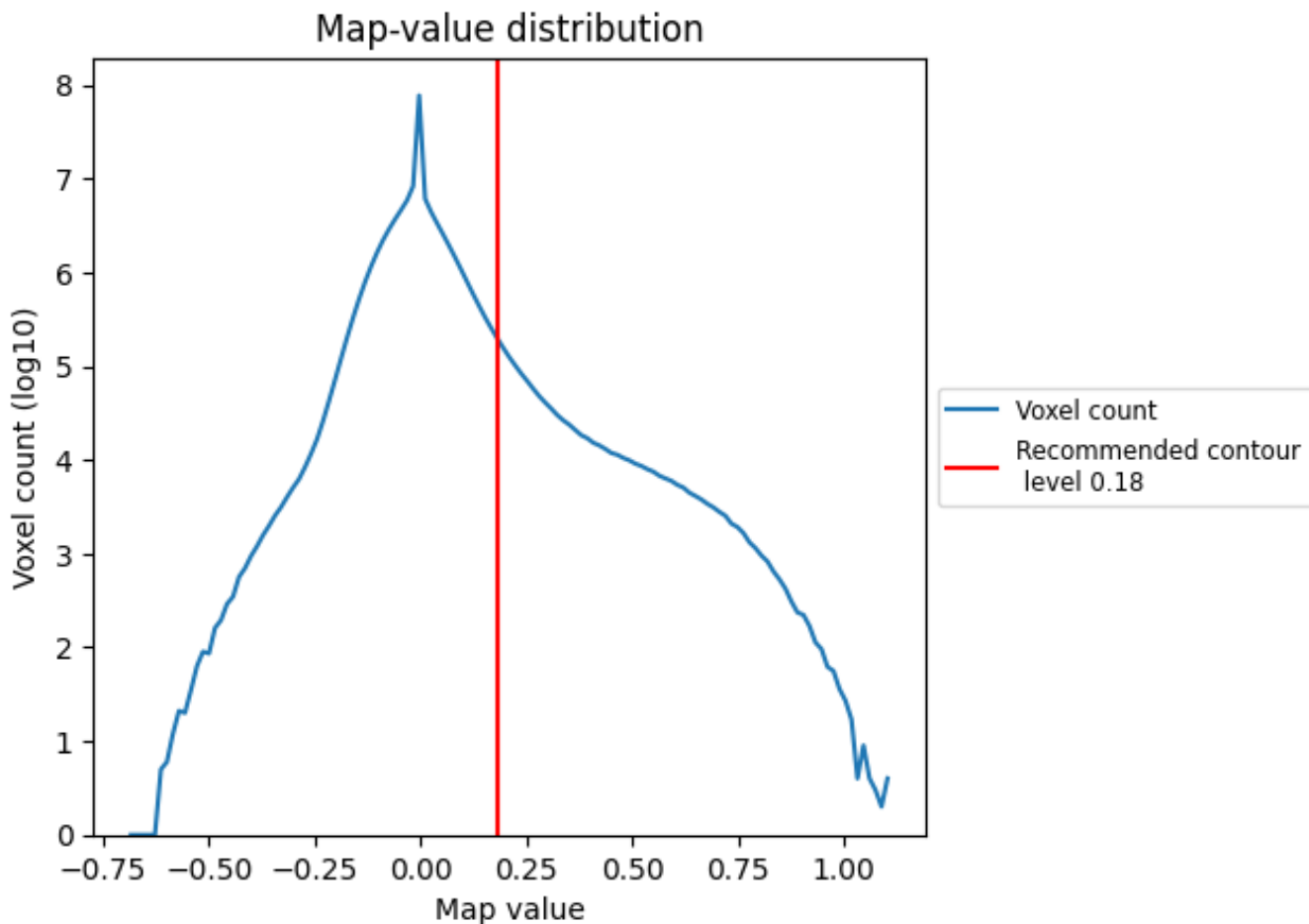
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

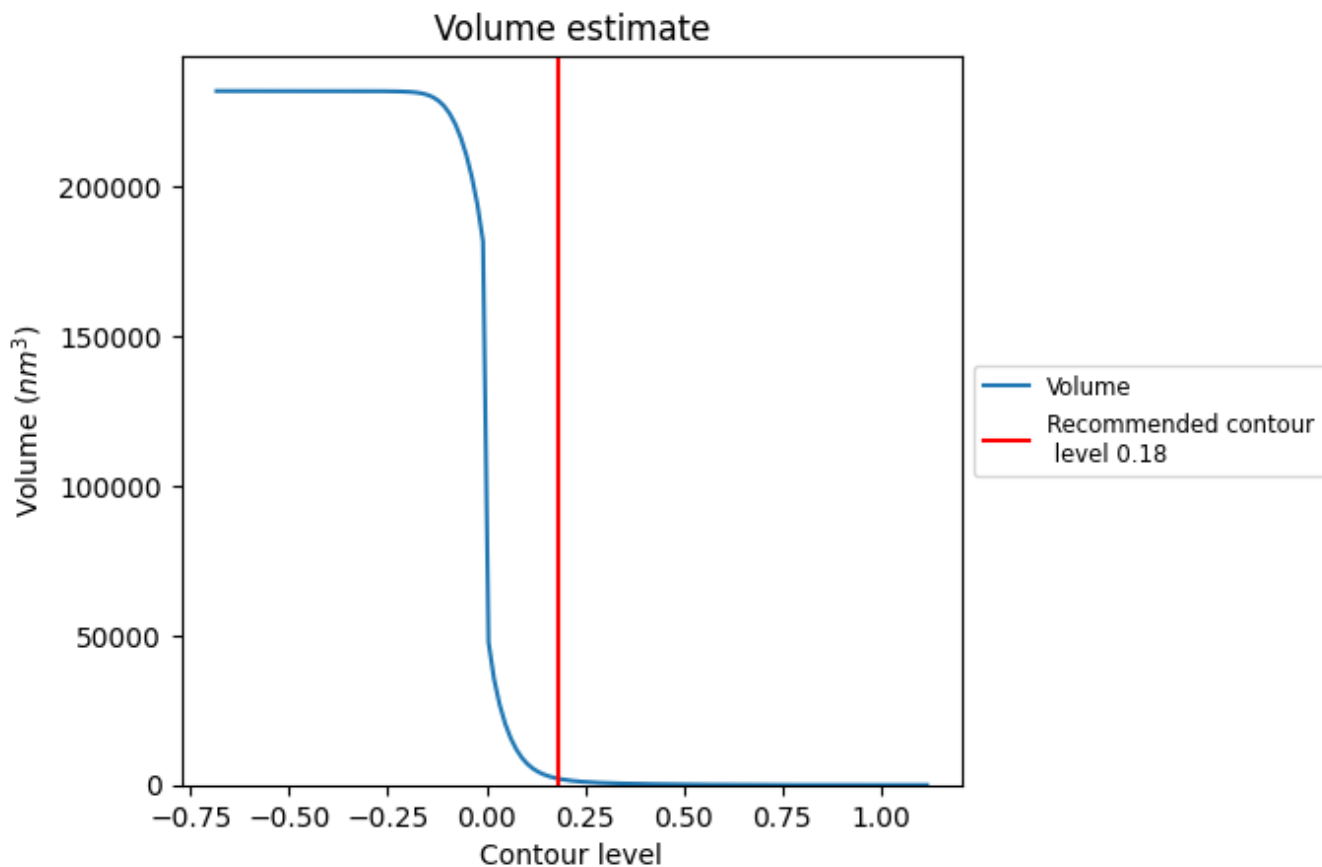
This section contains the results of statistical analysis of the map.

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



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

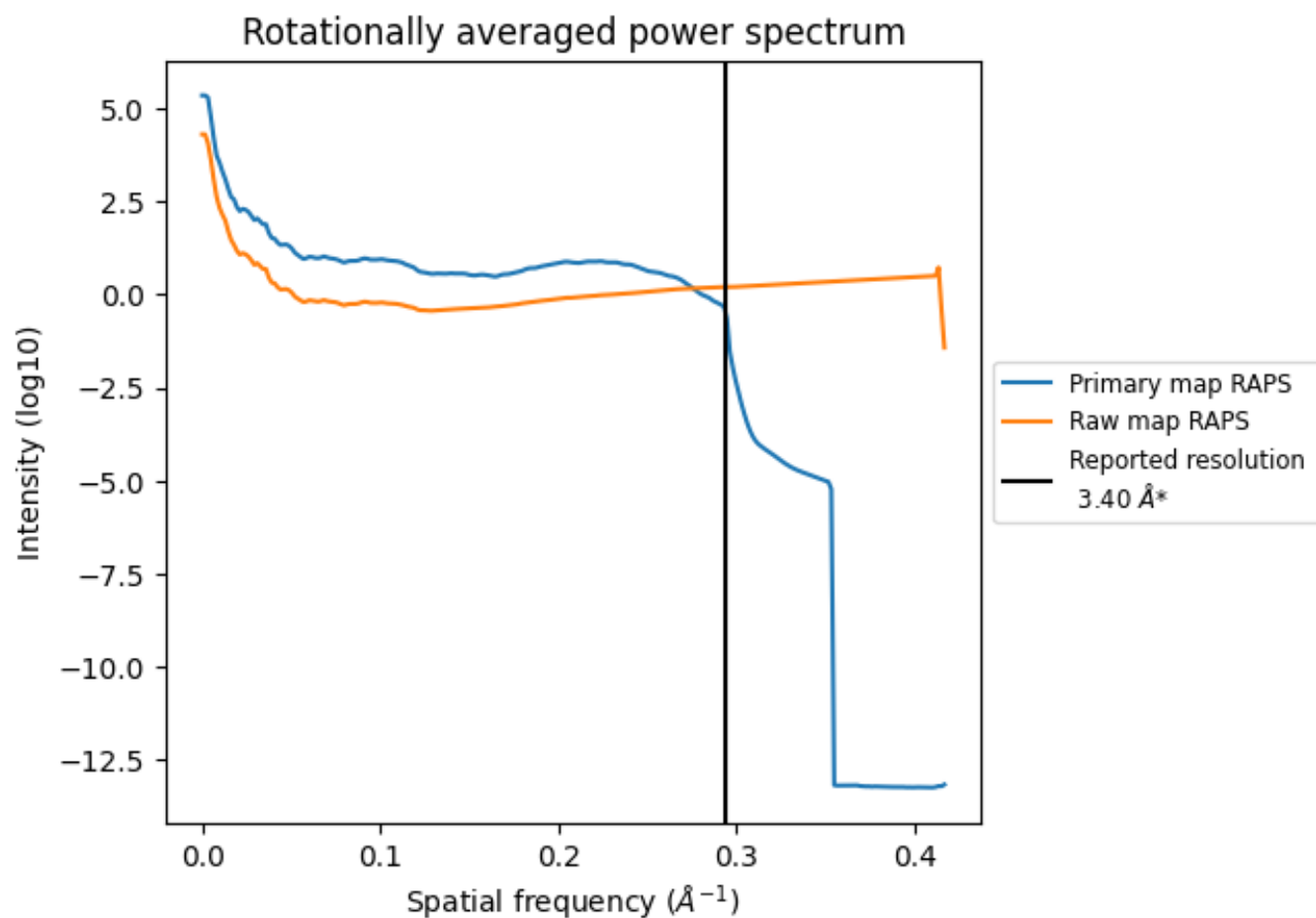
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2188 nm<sup>3</sup>; this corresponds to an approximate mass of 1977 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

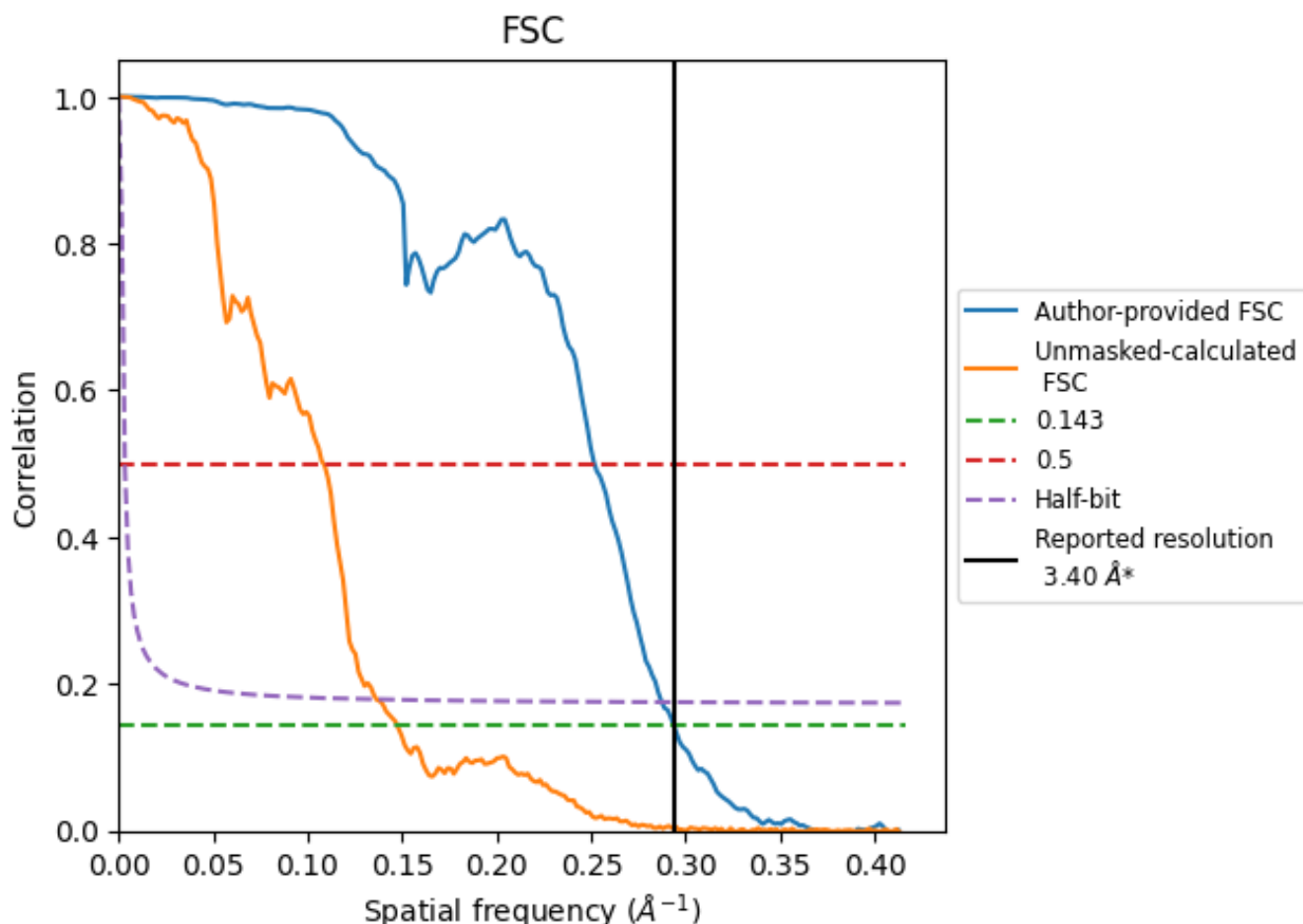


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

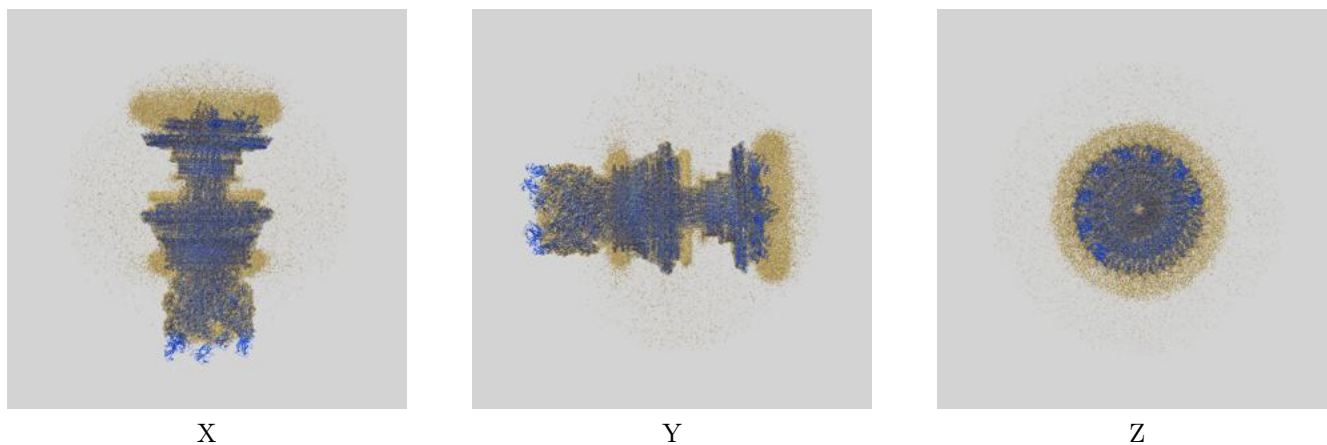
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.97	3.48
Unmasked-calculated*	6.78	9.23	7.33

\*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 6.78 differs from the reported value 3.4 by more than 10 %

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

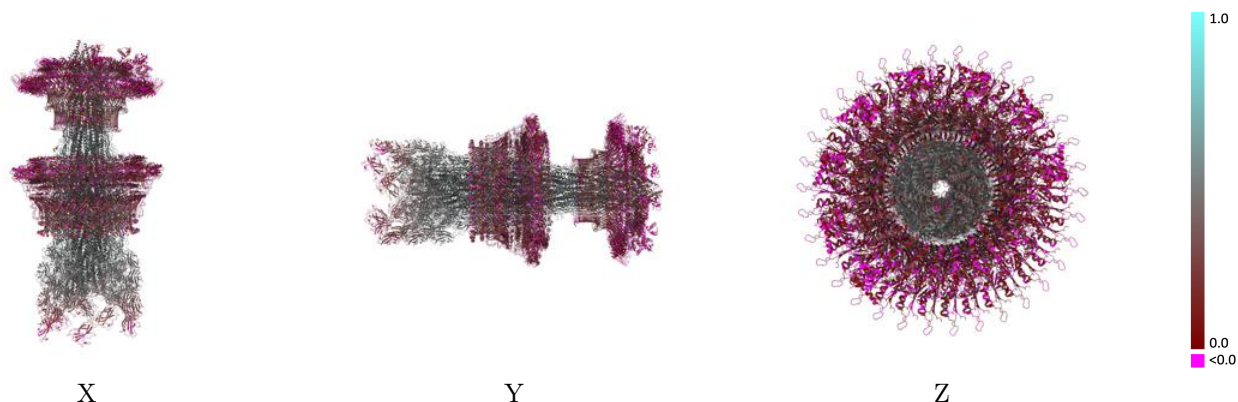
This section contains information regarding the fit between EMDB map EMD-37611 and PDB model 8WL2. Per-residue inclusion information can be found in section 3 on page 24.

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



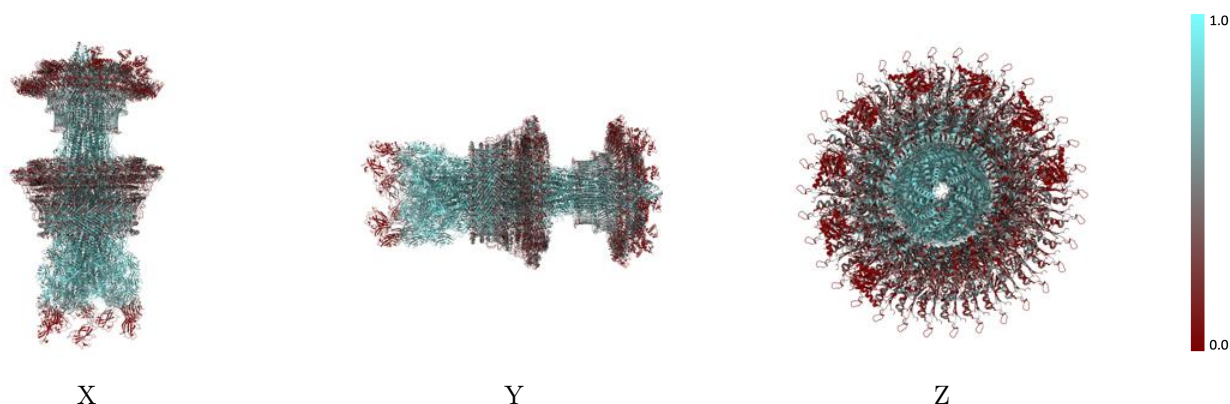
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

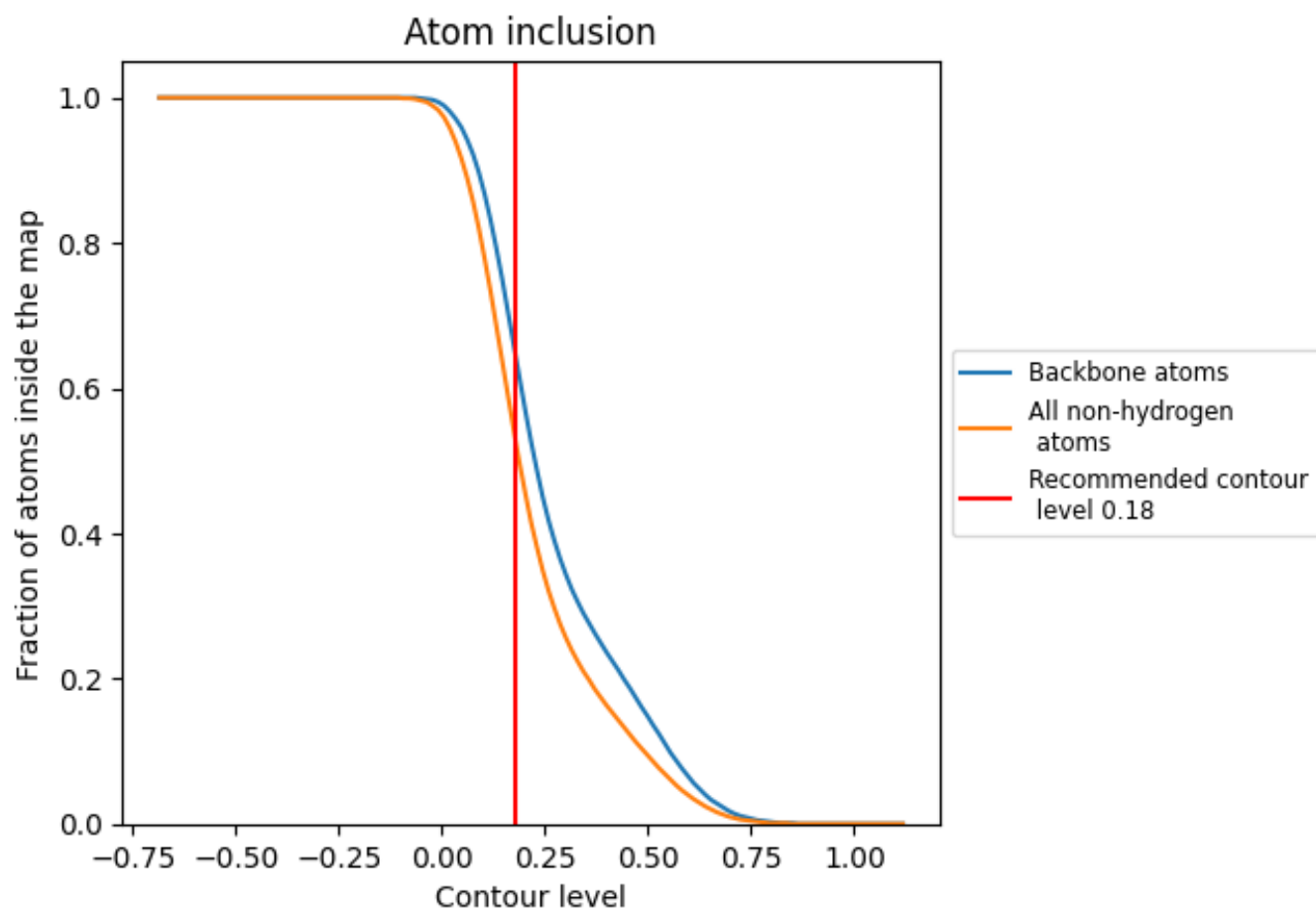
## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5240	 0.3100
0	 0.8020	 0.5090
1	 0.7900	 0.5090
2	 0.7950	 0.5130
3	 0.7850	 0.5070
4	 0.7900	 0.5030
5	 0.7960	 0.5030
6	 0.8020	 0.5080
7	 0.7970	 0.5020
8	 0.7960	 0.5040
9	 0.8000	 0.5090
A	 0.3850	 0.2080
A0	 0.7190	 0.4510
A1	 0.6820	 0.4090
A2	 0.7020	 0.4120
A3	 0.7000	 0.4350
A4	 0.6560	 0.3930
A5	 0.6150	 0.3870
A6	 0.7010	 0.4630
A7	 0.7480	 0.4640
A8	 0.7500	 0.4690
A9	 0.7310	 0.4640
AA	 0.7600	 0.5010
AB	 0.8190	 0.5150
AC	 0.8150	 0.5130
AD	 0.8120	 0.5120
AE	 0.7910	 0.4970
AF	 0.7780	 0.5070
AG	 0.8070	 0.5130
AH	 0.8030	 0.5070
AI	 0.8010	 0.5170
AJ	 0.7940	 0.5080
AK	 0.7960	 0.5130
AL	 0.8000	 0.5060
AM	 0.7940	 0.5090























































































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Chain	Atom inclusion	Q-score
AN	 0.8010	 0.5120
AO	 0.3380	 0.1640
AP	 0.3490	 0.1710
AQ	 0.3360	 0.1640
AR	 0.4180	 0.1610
AS	 0.3560	 0.1480
AT	 0.3970	 0.1610
AU	 0.4010	 0.1700
AV	 0.4010	 0.1490
AW	 0.4060	 0.1660
AX	 0.4240	 0.1740
AY	 0.4270	 0.1780
AZ	 0.4290	 0.1660
Aa	 0.4270	 0.1780
Ab	 0.6140	 0.3500
Ac	 0.3860	 0.1240
Ad	 0.3920	 0.1320
Ae	 0.3650	 0.1210
Af	 0.3730	 0.1160
Ag	 0.3340	 0.0990
Ah	 0.3330	 0.0830
Ai	 0.3180	 0.0890
Aj	 0.3380	 0.1030
Ak	 0.3440	 0.1450
Al	 0.3450	 0.1410
Am	 0.3770	 0.1600
An	 0.3770	 0.1760
Ao	 0.3710	 0.1760
Ap	 0.3450	 0.1640
Aq	 0.7130	 0.3970
Ar	 0.7130	 0.3910
As	 0.6690	 0.3770
At	 0.6300	 0.3800
Au	 0.7040	 0.4150
Av	 0.7440	 0.4450
Aw	 0.7660	 0.4570
Ax	 0.7460	 0.4570
Ay	 0.7020	 0.4330
Az	 0.5680	 0.3510
B	 0.3860	 0.2100
BA	 0.7550	 0.4860
BB	 0.7870	 0.5020

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Chain	Atom inclusion	Q-score
BC	 0.7890	 0.5030
BD	 0.7900	 0.4940
BE	 0.7900	 0.4970
BF	 0.7590	 0.4810
BG	 0.6170	 0.4660
BH	 0.7180	 0.4850
BI	 0.7370	 0.4830
BJ	 0.8160	 0.5020
BK	 0.7790	 0.4960
BL	 0.7570	 0.5110
BM	 0.8500	 0.5000
BN	 0.7280	 0.4740
BO	 0.8200	 0.4880
BP	 0.7090	 0.4900
BQ	 0.7790	 0.4970
BR	 0.3280	 0.1360
BS	 0.3230	 0.1370
BT	 0.3040	 0.1250
BU	 0.3200	 0.1330
BV	 0.3420	 0.1530
BW	 0.3410	 0.1290
BX	 0.3550	 0.1470
C	 0.3820	 0.2010
D	 0.4050	 0.2210
E	 0.3900	 0.1980
F	 0.4010	 0.2100
G	 0.3990	 0.2110
H	 0.4010	 0.1950
I	 0.3930	 0.1990
J	 0.3770	 0.1840
K	 0.4020	 0.2130
L	 0.3930	 0.1900
M	 0.3930	 0.1980
N	 0.3970	 0.1950
O	 0.3710	 0.1920
P	 0.4060	 0.2080
Q	 0.3950	 0.2020
R	 0.4030	 0.2000
S	 0.3840	 0.1850
T	 0.3800	 0.1880
U	 0.3720	 0.2040
UI	 0.0730	 0.0730





















































































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Chain	Atom inclusion	Q-score
UJ	0.0820	0.0660
UK	0.0470	0.0870
UL	0.0550	0.0410
UM	0.0440	0.0280
UN	0.0700	0.0480
UO	0.0660	0.0660
UP	0.0720	0.0510
V	0.3900	0.2060
W	0.3700	0.2020
WA	0.5050	0.2590
WB	0.4920	0.2350
WC	0.4740	0.2500
WD	0.4420	0.2190
WE	0.4360	0.2360
WF	0.3890	0.2250
WG	0.3190	0.1870
WH	0.2930	0.1630
WI	0.2800	0.1510
WJ	0.2700	0.1580
WK	0.2070	0.1260
WL	0.1940	0.0880
WM	0.2250	0.1040
WN	0.2470	0.1100
WO	0.3410	0.1590
WP	0.4010	0.1750
WQ	0.4120	0.2190
WR	0.4230	0.2080
WS	0.4750	0.2340
WT	0.4910	0.2460
WU	0.4830	0.2110
WV	0.4840	0.2430
WW	0.4710	0.2400
X	0.3790	0.2040
Y	0.3830	0.2120
Z	0.3850	0.2080
ZA	0.7820	0.4990
ZB	0.8050	0.5050
ZC	0.8020	0.5020
ZD	0.7950	0.4990
ZE	0.7860	0.4940
ZF	0.6200	0.4500
ZG	0.7670	0.4800

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Chain	Atom inclusion	Q-score
ZH	 0.8040	 0.4840
ZI	 0.8010	 0.4820
ZJ	 0.8020	 0.4780
ZK	 0.7950	 0.4740
ZL	 0.7990	 0.4730
ZM	 0.7980	 0.4730
ZN	 0.7960	 0.4690
ZO	 0.7900	 0.4690
ZP	 0.7840	 0.4620
ZQ	 0.7650	 0.4540
ZR	 0.7520	 0.4520
ZS	 0.7520	 0.4530
ZT	 0.7300	 0.4370
ZU	 0.7080	 0.4320
ZV	 0.6860	 0.4250
ZW	 0.6600	 0.4250
ZX	 0.6380	 0.4160
ZY	 0.5890	 0.4060
ZZ	 0.5560	 0.3950
Za	 0.5220	 0.3800
Zb	 0.5020	 0.3870
Zc	 0.4820	 0.3740
Zd	 0.4430	 0.3490
Ze	 0.4150	 0.3440
Zf	 0.3900	 0.3300
Zg	 0.3620	 0.3120
Zh	 0.3480	 0.3080
a	 0.3210	 0.1760
b	 0.3200	 0.1710
c	 0.3090	 0.1790
d	 0.3240	 0.1660
e	 0.3130	 0.1690
f	 0.3160	 0.1750
g	 0.3270	 0.1590
h	 0.3060	 0.1600
i	 0.3170	 0.1580
j	 0.3240	 0.1730
k	 0.3040	 0.1510
l	 0.3020	 0.1620
m	 0.3210	 0.1550
n	 0.3140	 0.1640
o	 0.3250	 0.1600

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Chain	Atom inclusion	Q-score
p	■ 0.3230	■ 0.1910
q	■ 0.3040	■ 0.1610
r	■ 0.3300	■ 0.1840
s	■ 0.3010	■ 0.1560
t	■ 0.3010	■ 0.1710
u	■ 0.2760	■ 0.1590
v	■ 0.3060	■ 0.1650
w	■ 0.2970	■ 0.1650
x	■ 0.2910	■ 0.1570
y	■ 0.2720	■ 0.1480
z	■ 0.3090	■ 0.1790