wwPDB EM Validation Summary Report

Mar 18, 2025 – 10:37 PM JST

PDB ID	:	8WKQ
EMDB ID	:	EMD-37605
Title	:	Cryo-EM structure of the MS ring (C1) with export apparatus and proximal rod within the flagellar motor-hook complex in the CW state.
Authors	:	Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on	:	2023-09-28
Resolution	:	3.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

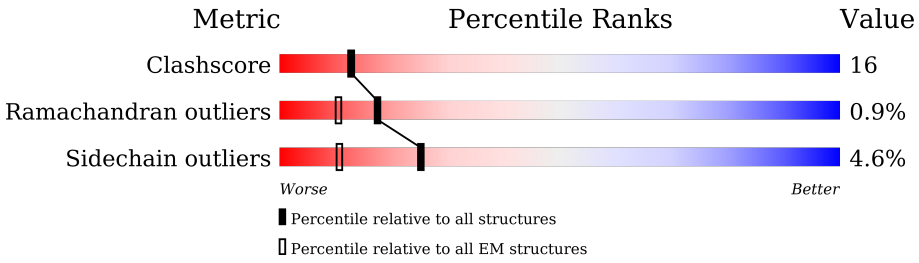
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	0	560	23% 6% 71%
1	1	560	22% 7% 71%
1	2	560	22% 6% 71%
1	3	560	23% 6% 71%
1	4	560	23% 6% 71%
1	5	560	23% 6% 71%
1	6	560	22% 7% 71%
1	7	560	22% 7% 71%

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Mol	Chain	Length	Quality of chain
1	8	560	23% 6% 71%
1	9	560	23% 6% 71%
1	AA	560	23% 6% 71%
1	AB	560	22% 6% 71%
1	AC	560	23% 6% 71%
1	AD	560	22% 7% 71%
1	AE	560	23% 6% 71%
1	AF	560	23% 6% 71%
1	AG	560	23% 6% 71%
1	AH	560	22% 6% 71%
1	AI	560	23% 6% 71%
1	AJ	560	23% 6% 71%
1	AK	560	23% 6% 71%
1	AL	560	23% 6% 71%
1	AM	560	23% 6% 71%
1	AN	560	23% 6% 71%
1	AO	560	22% 7% 71%
1	AP	560	22% 6% 71%
1	AQ	560	23% 6% 71%
1	UI	560	8% 18% 8% 72%
1	UJ	560	10% 17% 9% 72%
1	UK	560	14% 18% 8% 72%
1	UL	560	16% 17% 9% 72%
1	UM	560	20% 17% 9% 72%
1	UN	560	16% 17% 9% 72%

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Mol	Chain	Length	Quality of chain
1	UO	560	12% 18% 8% 72%
1	UP	560	10% 18% 8% 72%
1	WA	560	11% 8% 80%
1	WB	560	11% 7% 80%
1	WC	560	10% 8% 81%
1	WD	560	10% 8% 80%
1	WE	560	12% 7% 80%
1	WF	560	11% 8% 80%
1	WG	560	10% 9% 80%
1	WH	560	10% 6% 83%
1	WI	560	8% 8% 83%
1	WJ	560	10% 7% 82%
1	WK	560	9% 8% 82%
1	WL	560	8% 6% 85%
1	WM	560	9% 6% 85%
1	WN	560	9% 6% 85%
1	WO	560	10% 7% 83%
1	WP	560	9% 7% 82%
1	WQ	560	10% 9% 80%
1	WR	560	10% 8% 80%
1	WS	560	9% 9% 80%
1	WT	560	10% 8% 80%
1	WU	560	11% 8% 80%
1	WV	560	10% 8% 80%
1	WW	560	9% 9% 80%

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Mol	Chain	Length	Quality of chain
1	b	560	98%
1	c	560	97%
1	d	560	96%
1	e	560	97%
1	f	560	96%
1	g	560	97%
1	h	560	96%
1	i	560	97%
1	j	560	96%
1	k	560	97%
1	l	560	96%
1	t	560	28% 71%
1	u	560	28% 71%
1	v	560	28% 71%
1	w	560	28% 71%
1	x	560	28% 71%
1	y	560	28% 71%
1	z	560	28% 71%
2	A	89	74% 26%
2	B	89	66% 34%
2	C	89	69% 31%
2	D	89	67% 33%
3	E	264	65% 28%
4	F	245	53% 30% 16%
4	G	245	61% 23% 15%

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Mol	Chain	Length	Quality of chain
4	H	245	64% 19% 15%
4	I	245	62% 20% 15%
4	J	245	58% 26% 15%
5	K	104	37% 18% 43%
5	L	104	71% 14% 12%
5	M	104	71% 13% 5% 11%
5	N	104	69% 19% 11%
5	O	104	68% 20% 11%
5	P	104	68% 18% 12%
6	Q	138	70% 26%
6	R	138	67% 20% 12%
6	S	138	5% 63% 25% 9%
6	T	138	8% 72% 20% 8%
6	U	138	15% 67% 20% 11%
7	V	134	40% 84% 16%
7	W	134	49% 81% 16%
7	X	134	55% 84% 16%
7	Y	134	63% 83% 16%
7	Z	134	67% 77% 22%
7	a	134	75% 96%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 99073 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	UI	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
1	UJ	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
1	UK	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
1	UL	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
1	UM	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
1	UN	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
1	UO	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
1	UP	155	Total	C	N	O	S	0	0
			1172	733	211	226	2		
1	WA	113	Total	C	N	O	S	0	0
			849	534	148	166	1		
1	WB	111	Total	C	N	O	S	0	0
			836	526	146	163	1		
1	WC	108	Total	C	N	O	S	0	0
			812	510	142	159	1		
1	WD	110	Total	C	N	O	S	0	0
			827	522	144	160	1		
1	WE	112	Total	C	N	O	S	0	0
			843	531	147	164	1		
1	WF	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
1	WG	112	Total	C	N	O	S	0	0
			843	531	147	164	1		
1	WH	95	Total	C	N	O	S	0	0
			703	439	126	137	1		
1	WI	95	Total	C	N	O	S	0	0
			703	439	126	137	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	WJ	99	Total	C	N	O	S	0	0
			737	462	131	143	1		
1	WK	98	Total	C	N	O	S	0	0
			729	456	130	142	1		
1	WL	85	Total	C	N	O	S	0	0
			622	389	110	122	1		
1	WM	82	Total	C	N	O	S	0	0
			596	372	107	116	1		
1	WN	84	Total	C	N	O	S	0	0
			611	380	109	121	1		
1	WO	96	Total	C	N	O	S	0	0
			714	448	127	138	1		
1	WP	100	Total	C	N	O	S	0	0
			741	464	132	144	1		
1	WQ	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
1	WR	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
1	WS	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
1	WT	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
1	WU	112	Total	C	N	O	S	0	0
			843	531	147	164	1		
1	WV	110	Total	C	N	O	S	0	0
			827	521	144	161	1		
1	WW	111	Total	C	N	O	S	0	0
			834	526	145	162	1		
1	b	13	Total	C	N	O		0	0
			81	50	15	16			
1	c	16	Total	C	N	O		0	0
			103	64	19	20			
1	d	20	Total	C	N	O		0	0
			133	83	23	27			
1	e	16	Total	C	N	O		0	0
			103	64	19	20			
1	f	21	Total	C	N	O		0	0
			140	88	24	28			
1	g	16	Total	C	N	O		0	0
			103	64	19	20			
1	h	21	Total	C	N	O		0	0
			140	88	24	28			

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	16	Total	C	N	O		0	0
			103	64	19	20			
1	j	20	Total	C	N	O		0	0
			133	83	23	27			
1	k	16	Total	C	N	O		0	0
			103	64	19	20			
1	l	21	Total	C	N	O		0	0
			140	88	24	28			
1	t	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	u	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	v	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	w	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	x	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	y	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	z	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	1	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	2	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	3	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	4	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	5	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	6	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	7	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	8	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	9	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	0	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AB	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AC	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AD	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AE	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AF	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AG	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AH	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AI	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AJ	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AK	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AL	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AM	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AN	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AO	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AP	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		
1	AQ	164	Total	C	N	O	S	0	0
			1275	776	237	259	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
2	B	89	Total	C	N	O	S	0	0
			670	449	100	114	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	89	Total	C	N	O	S	0	0
			670	449	100	114	7		
2	D	89	Total	C	N	O	S	0	0
			670	449	100	114	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	207	Total	C	N	O	S	0	0
			1605	1072	249	272	12		
4	G	209	Total	C	N	O	S	0	0
			1626	1086	252	276	12		
4	H	208	Total	C	N	O	S	0	0
			1614	1077	251	274	12		
4	I	208	Total	C	N	O	S	0	0
			1614	1077	251	274	12		
4	J	209	Total	C	N	O	S	0	0
			1623	1084	251	276	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	59	Total	C	N	O	S	0	0
			429	265	74	83	7		
5	L	91	Total	C	N	O	S	0	0
			672	415	121	129	7		
5	M	93	Total	C	N	O	S	0	0
			686	424	123	132	7		
5	N	93	Total	C	N	O	S	0	0
			686	424	123	132	7		
5	O	93	Total	C	N	O	S	0	0
			686	424	123	132	7		
5	P	92	Total	C	N	O	S	0	0
			679	420	122	130	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	134	Total	C	N	O	S	0	0
			1030	633	189	203	5		
6	R	121	Total	C	N	O	S	0	0
			942	583	172	182	5		
6	S	125	Total	C	N	O	S	0	0
			967	598	177	187	5		
6	T	127	Total	C	N	O	S	0	0
			982	606	182	189	5		
6	U	123	Total	C	N	O	S	0	0
			950	588	172	185	5		

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

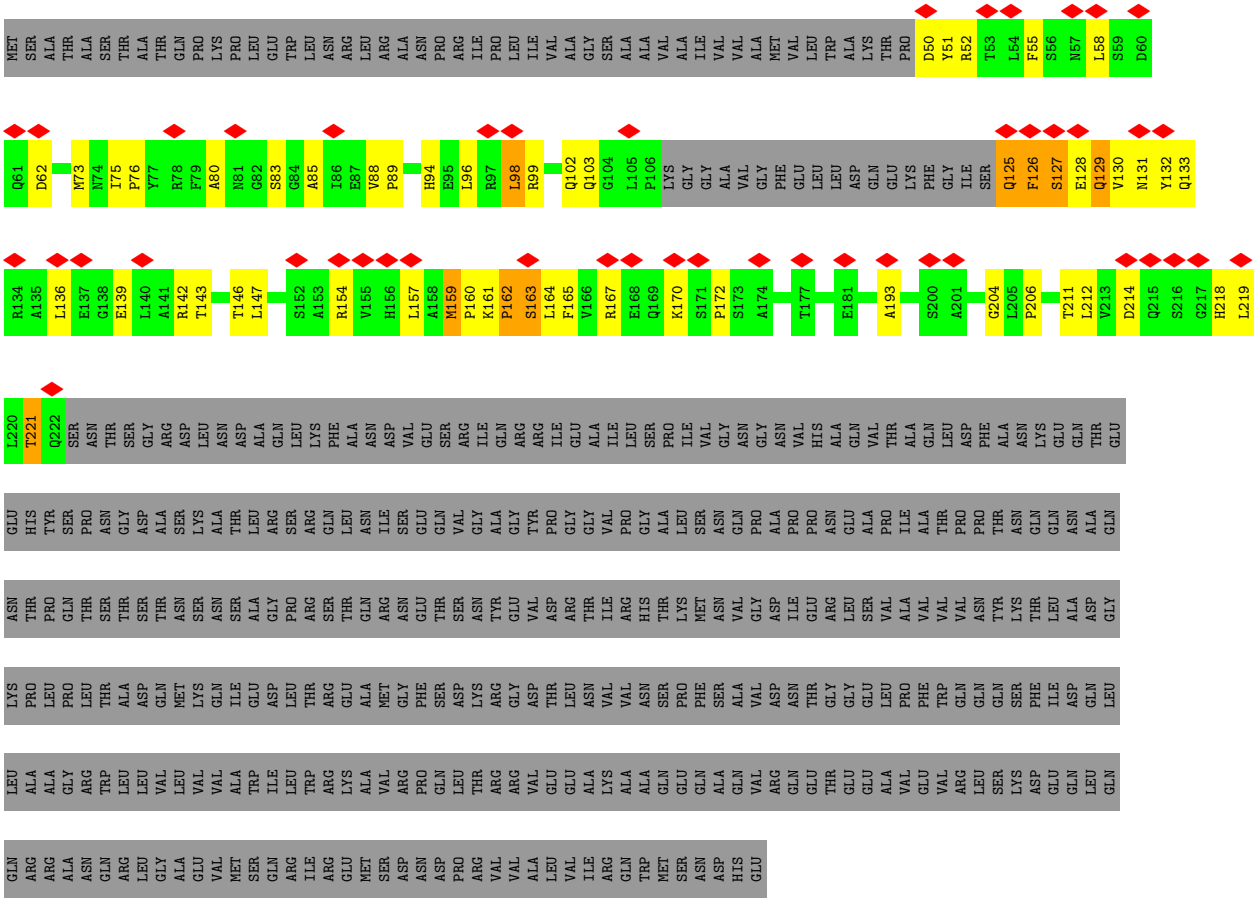
Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	W	132	Total	C	N	O	S	0	0
			964	601	166	192	5		
7	X	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	Y	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	Z	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
7	a	133	Total	C	N	O	S	0	0
			969	604	167	193	5		

3 Residue-property plots (i)

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

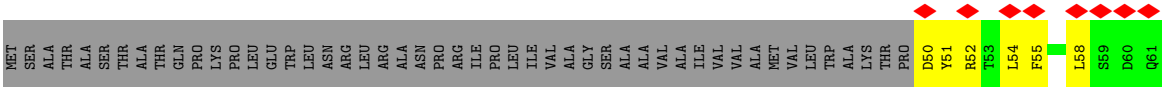
• Molecule 1: Flagellar M-ring protein

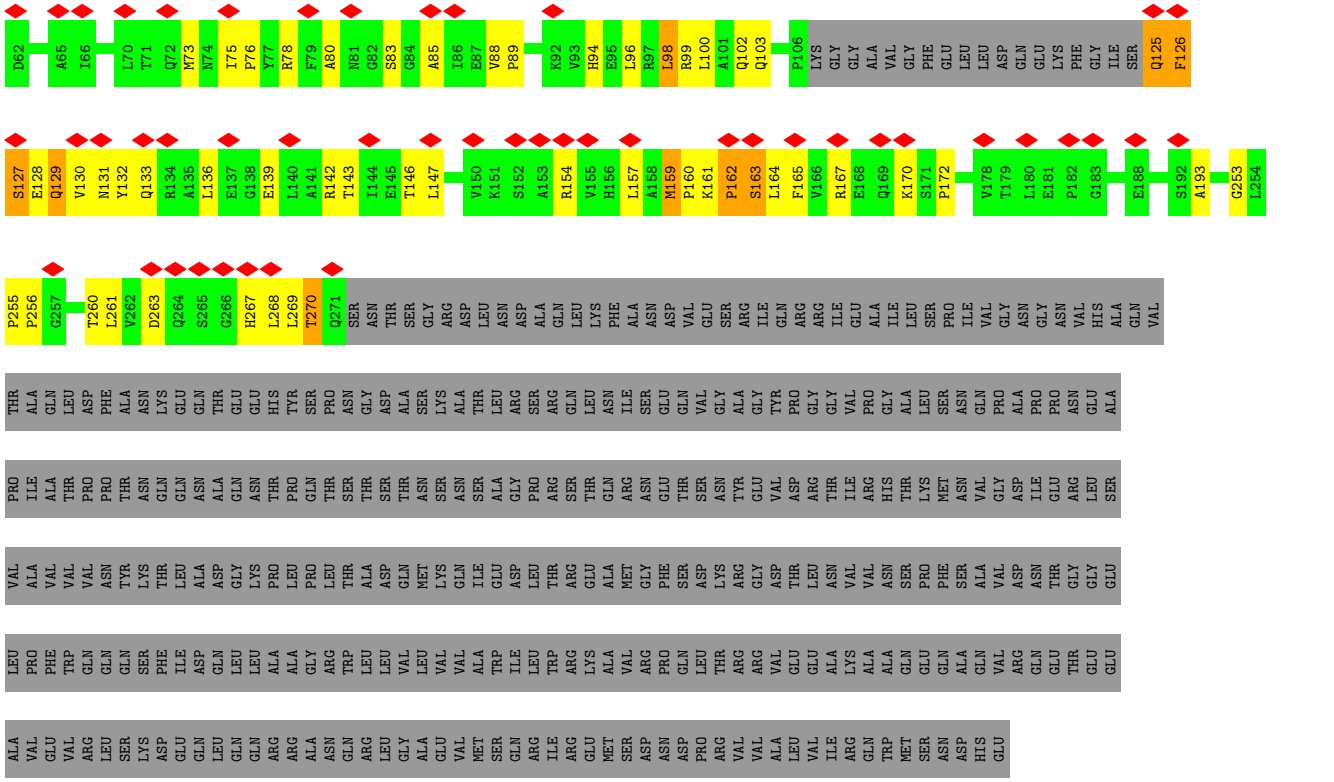
Chain UI:



• Molecule 1: Flagellar M-ring protein

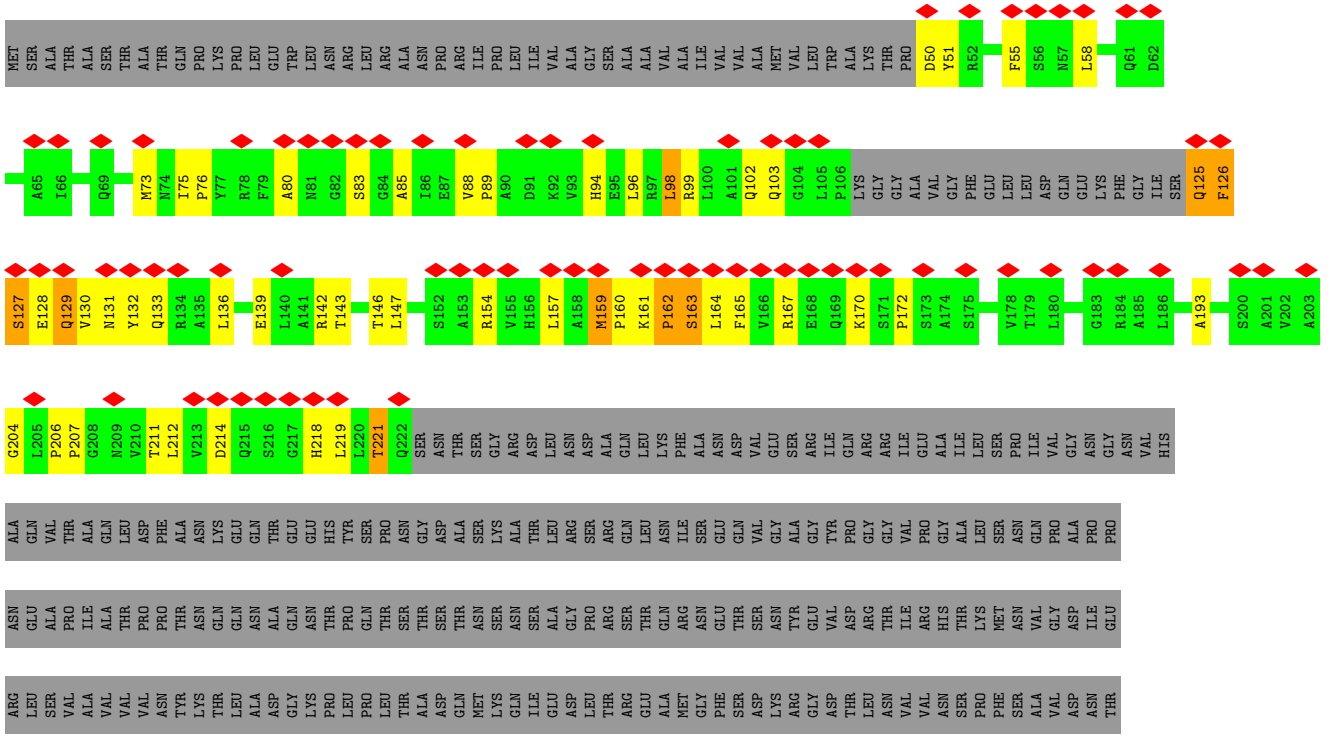
Chain UJ:

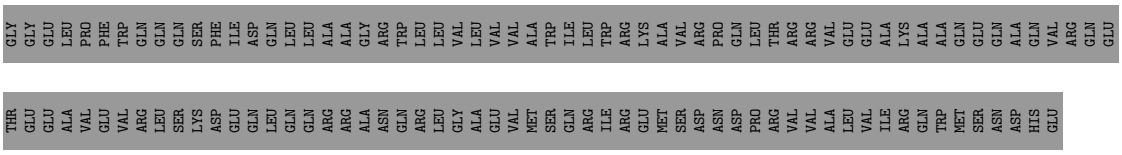




• Molecule 1: Flagellar M-ring protein

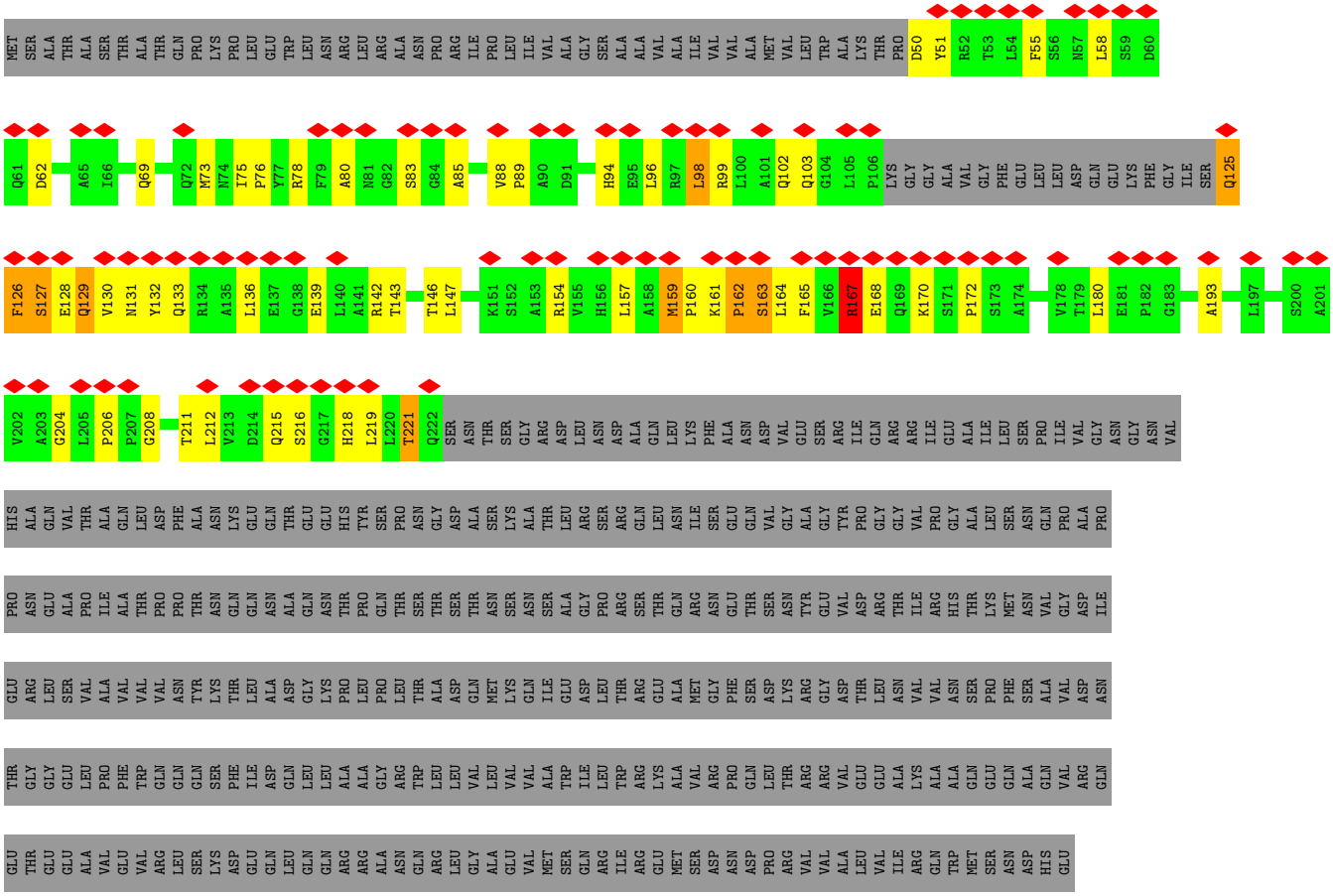
Chain UK:





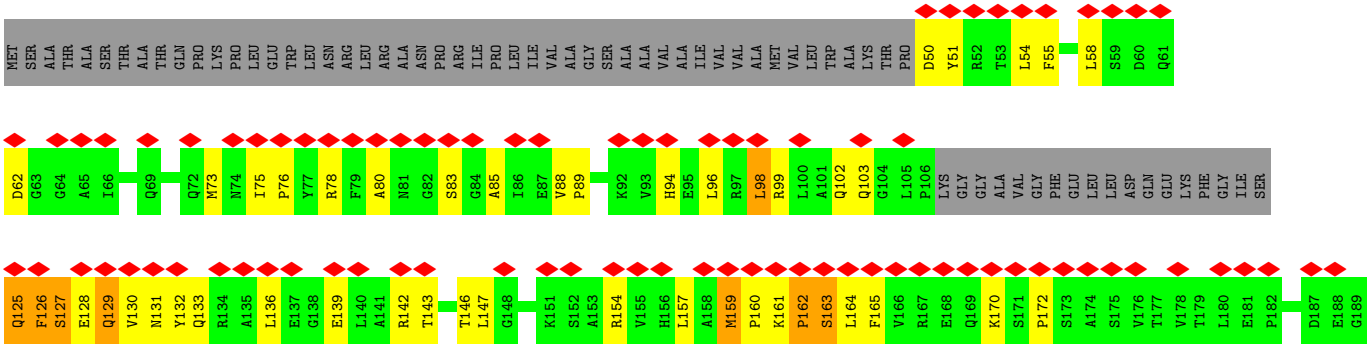
• Molecule 1: Flagellar M-ring protein

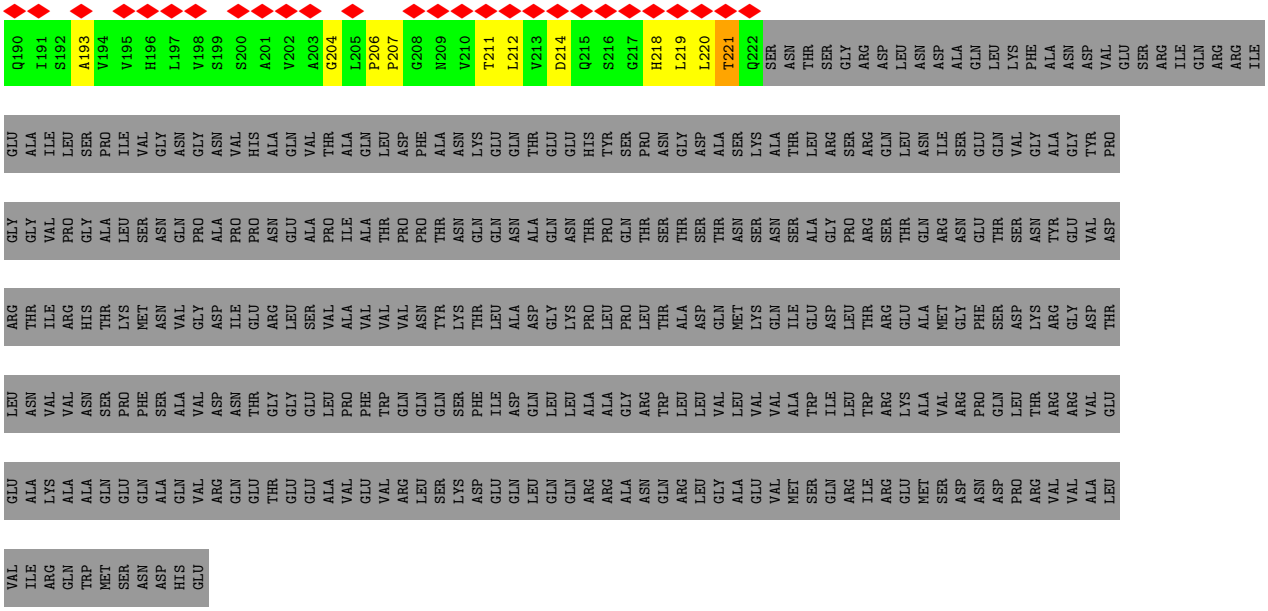
Chain UL:



• Molecule 1: Flagellar M-ring protein

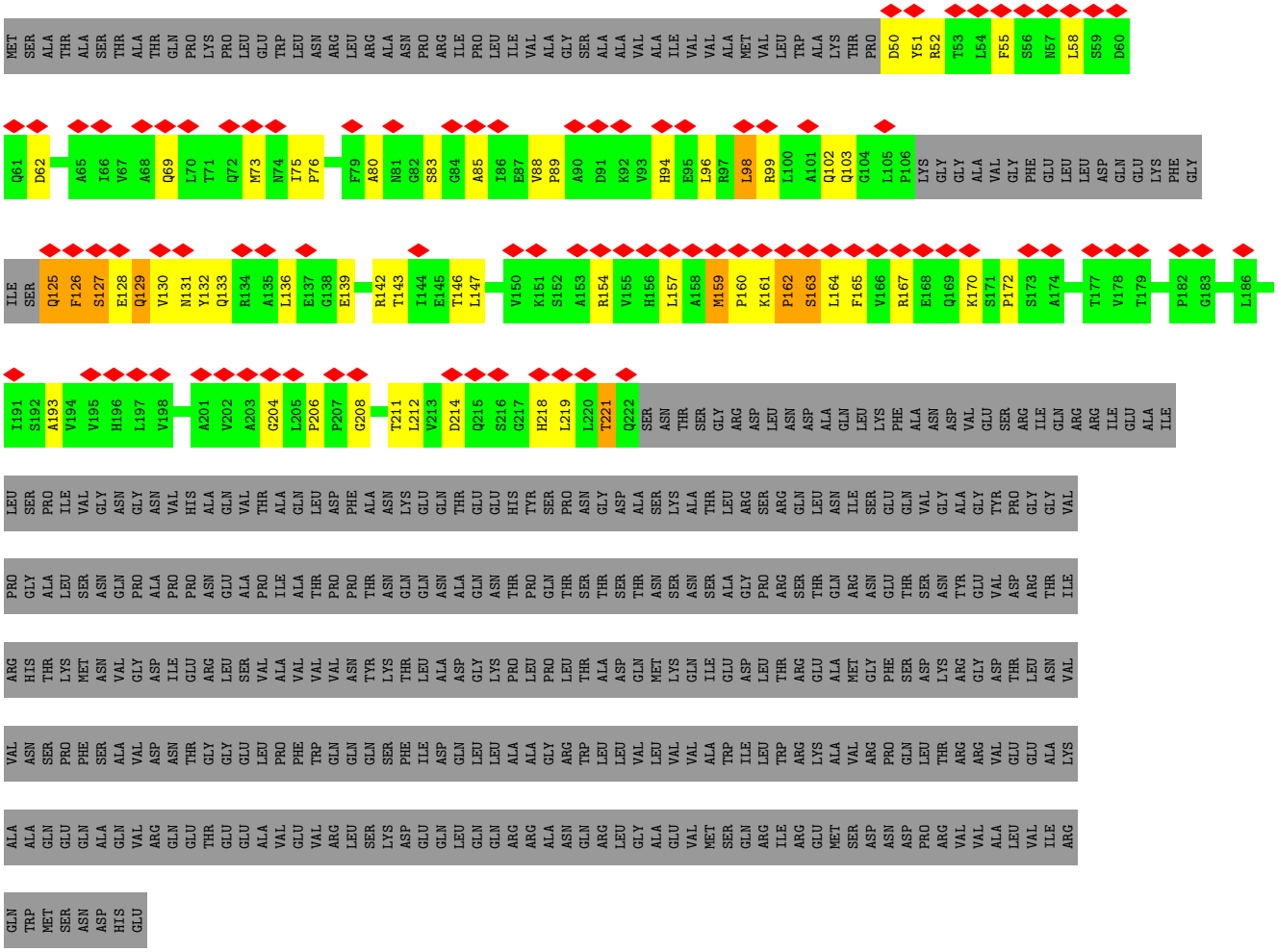
Chain UM:





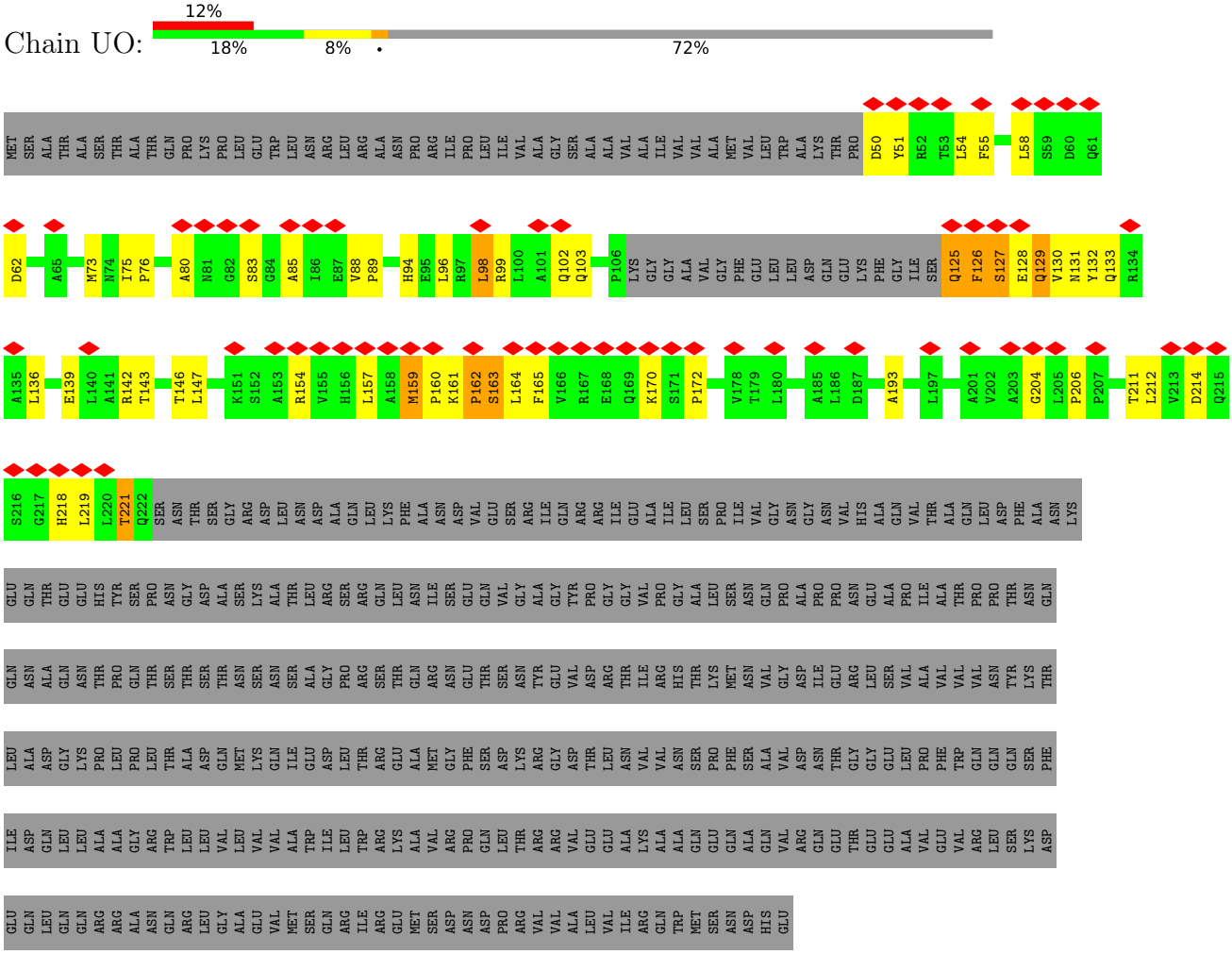
• Molecule 1: Flagellar M-ring protein

Chain UN:



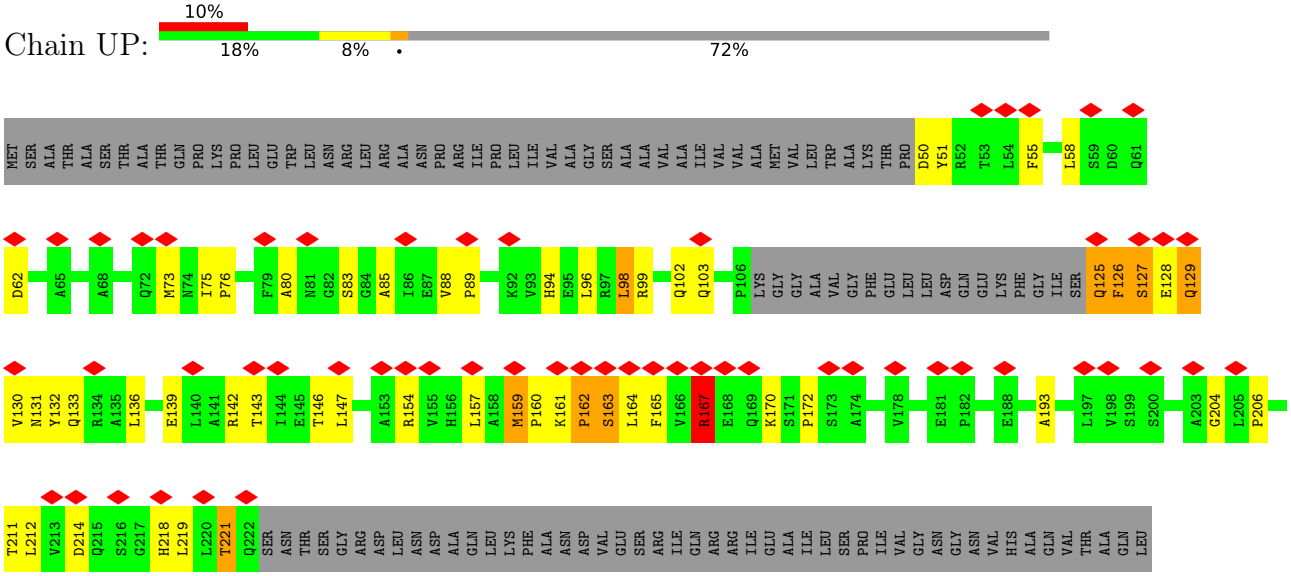
• Molecule 1: Flagellar M-ring protein

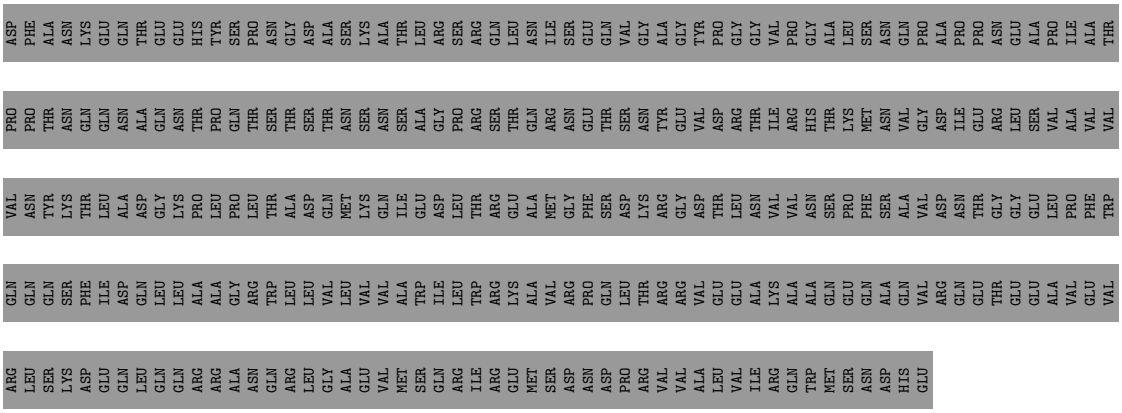
Chain UO:



• Molecule 1: Flagellar M-ring protein

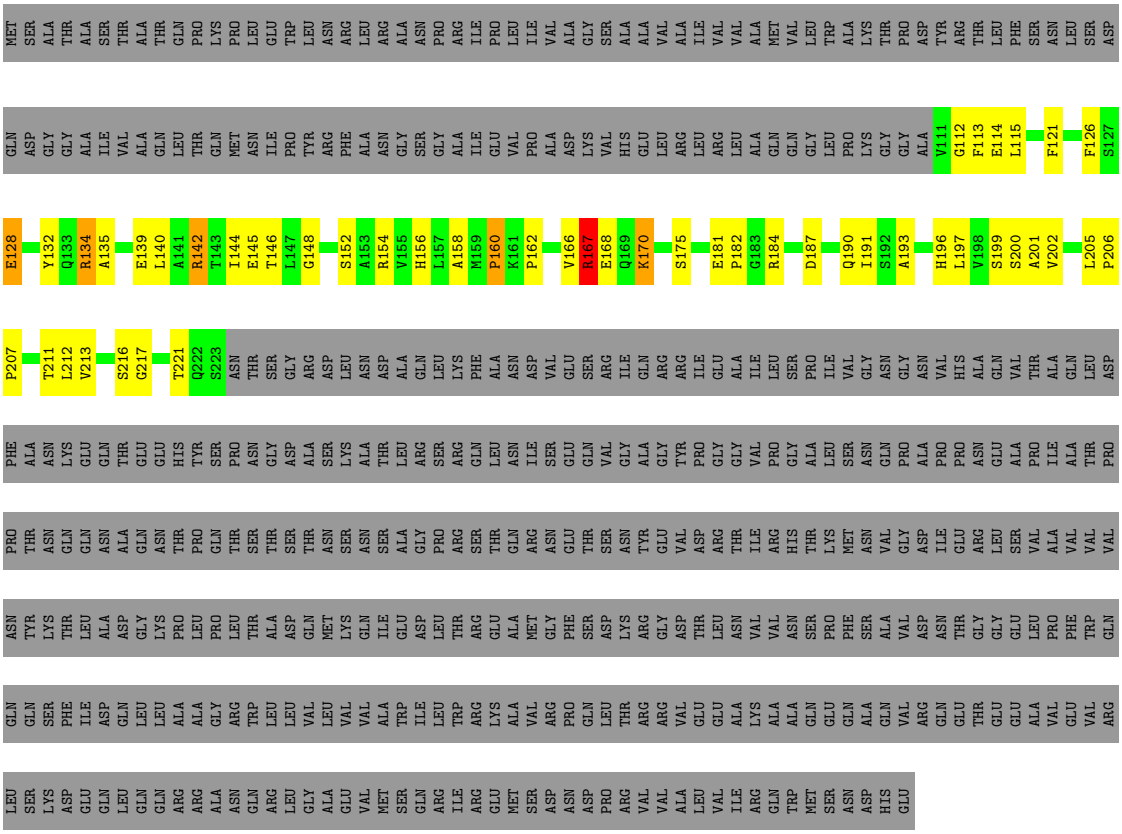
Chain UP:





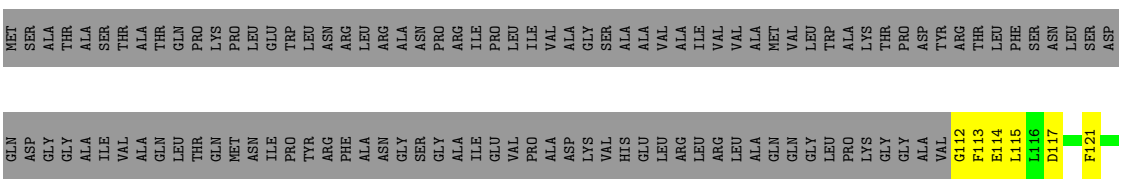
• Molecule 1: Flagellar M-ring protein

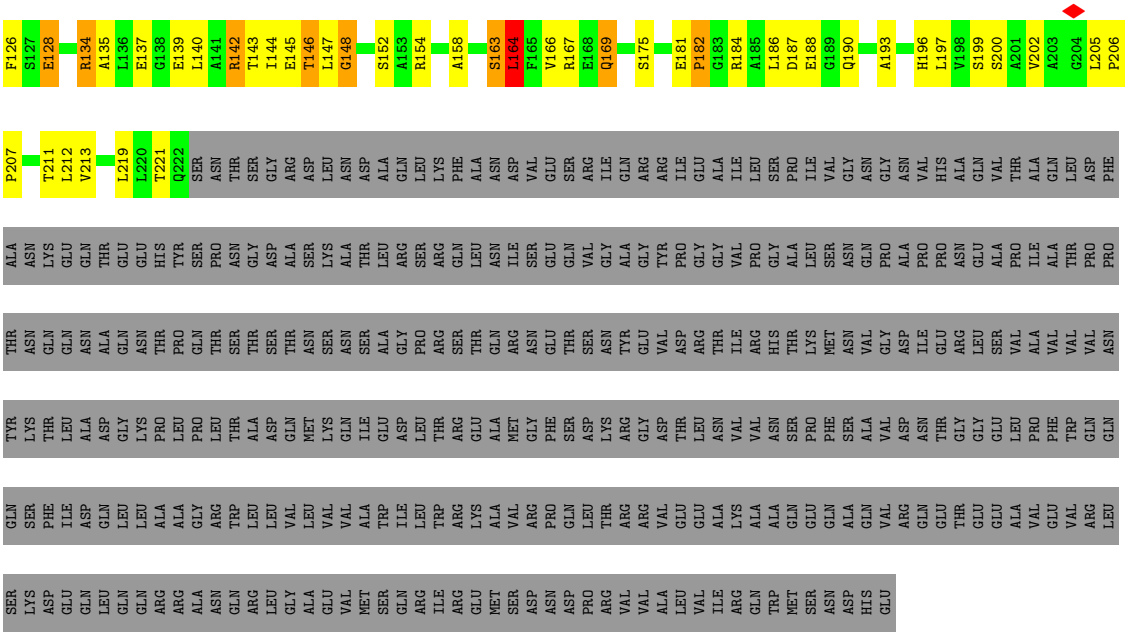
Chain WA:



• Molecule 1: Flagellar M-ring protein

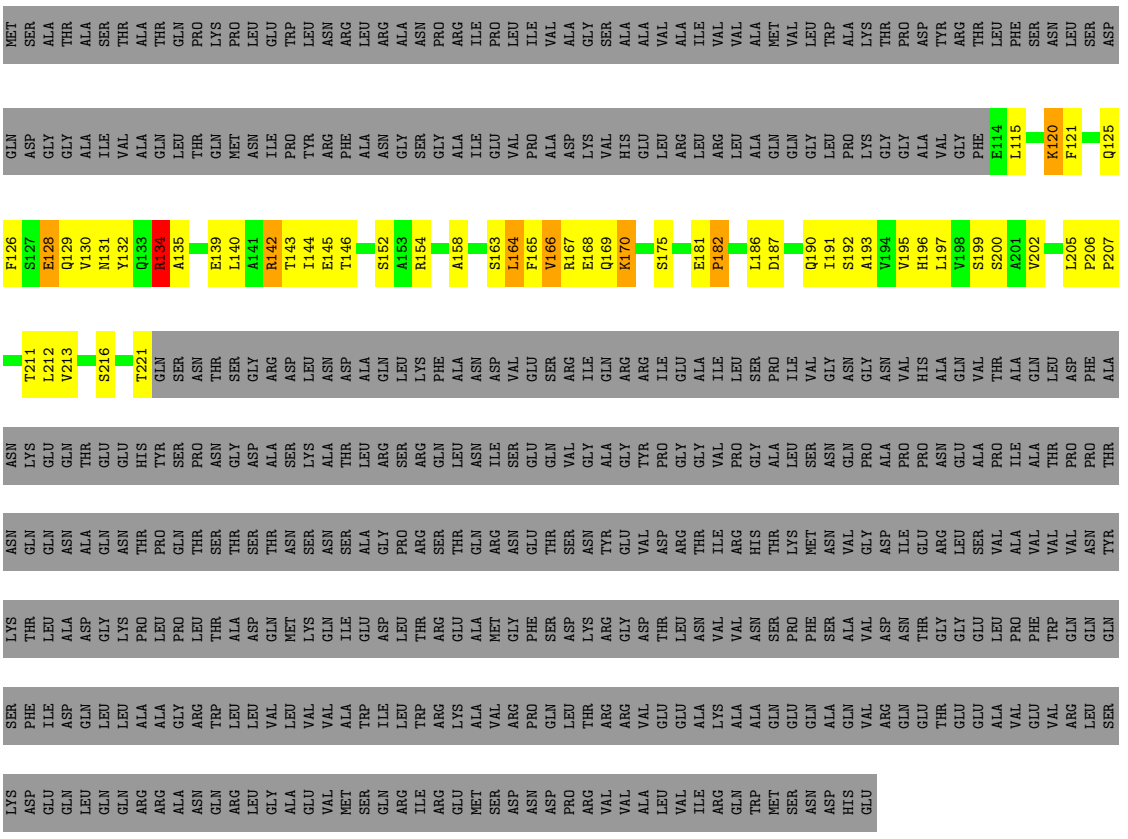
Chain WB:





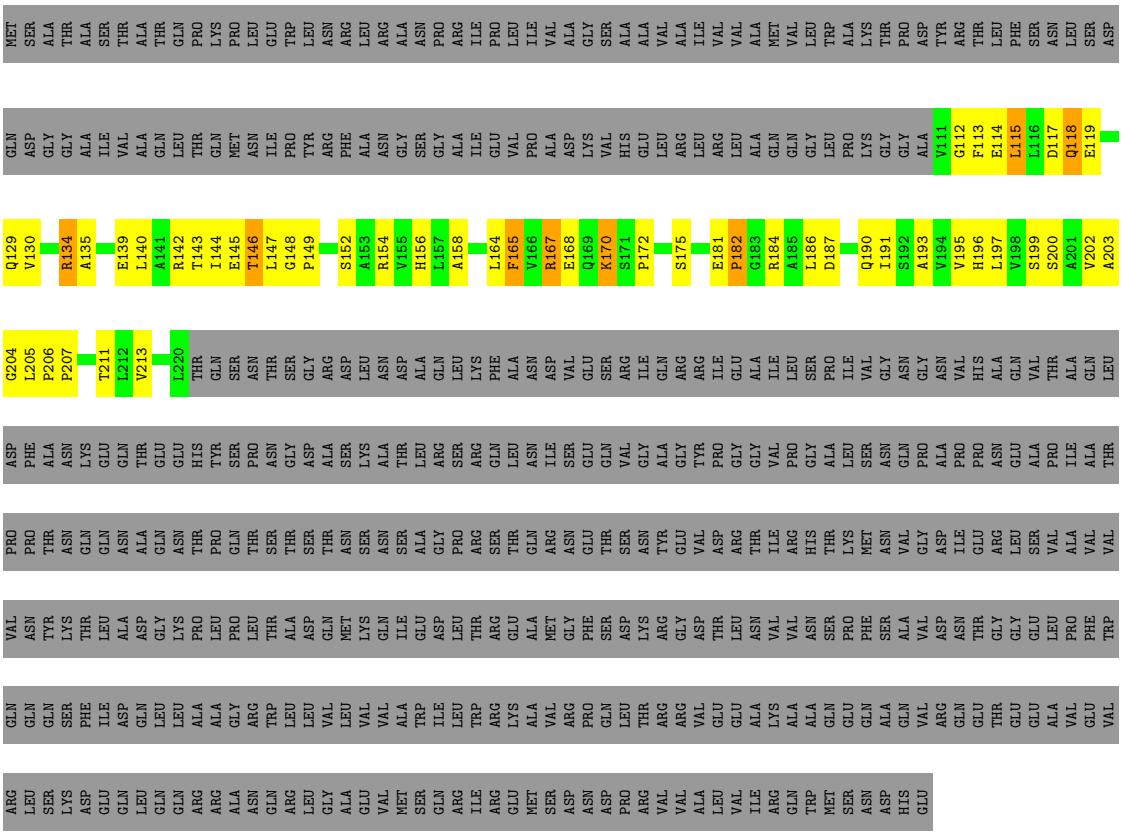
• Molecule 1: Flagellar M-ring protein

Chain WC:



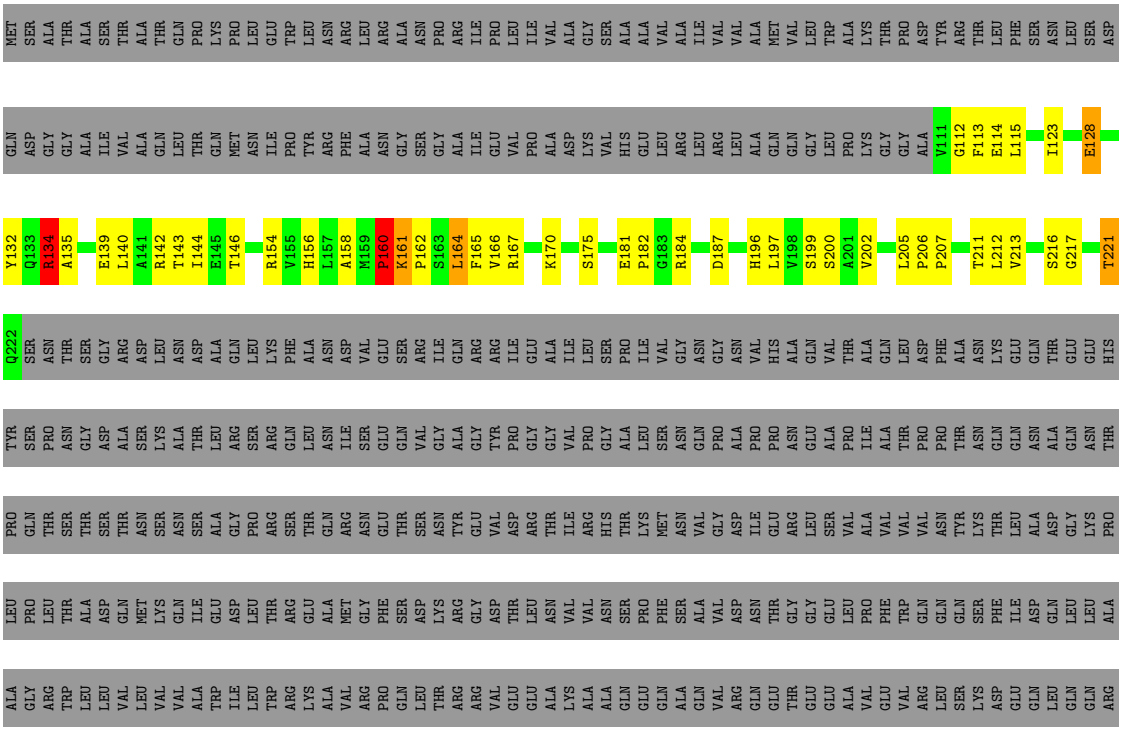
• Molecule 1: Flagellar M-ring protein

Chain WD:



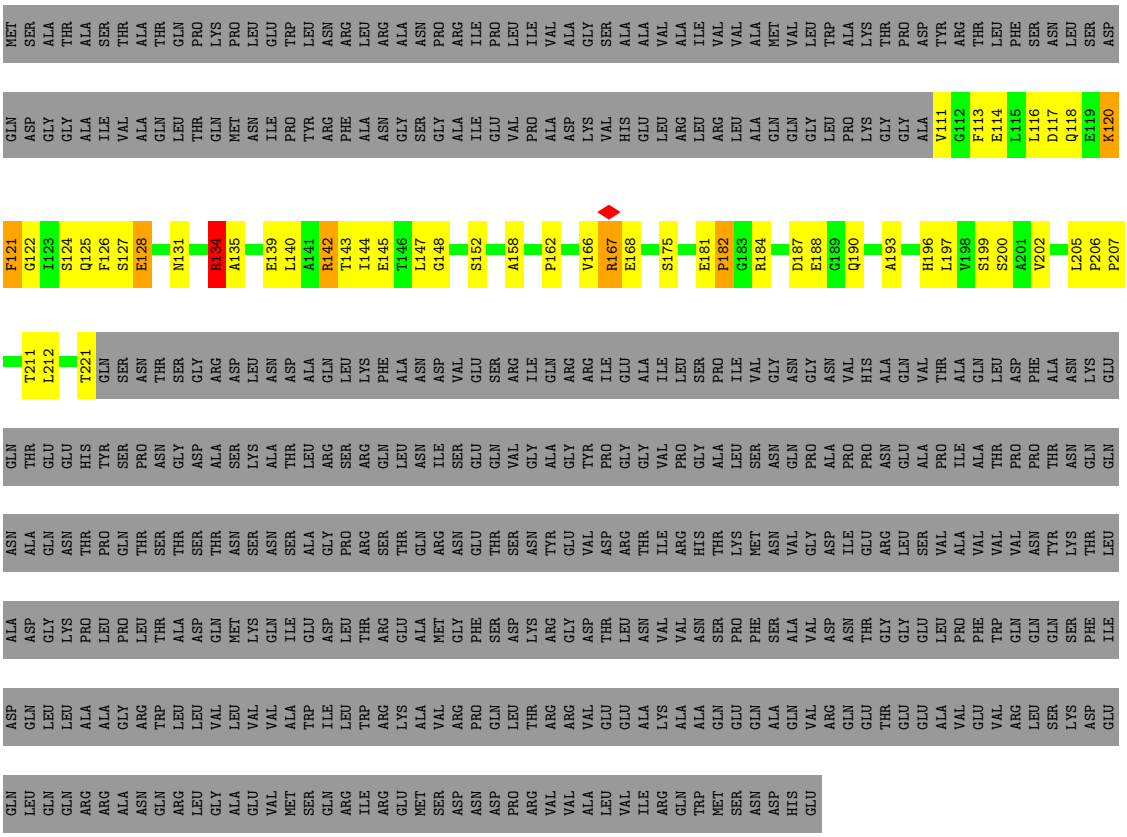
• Molecule 1: Flagellar M-ring protein

Chain WE:



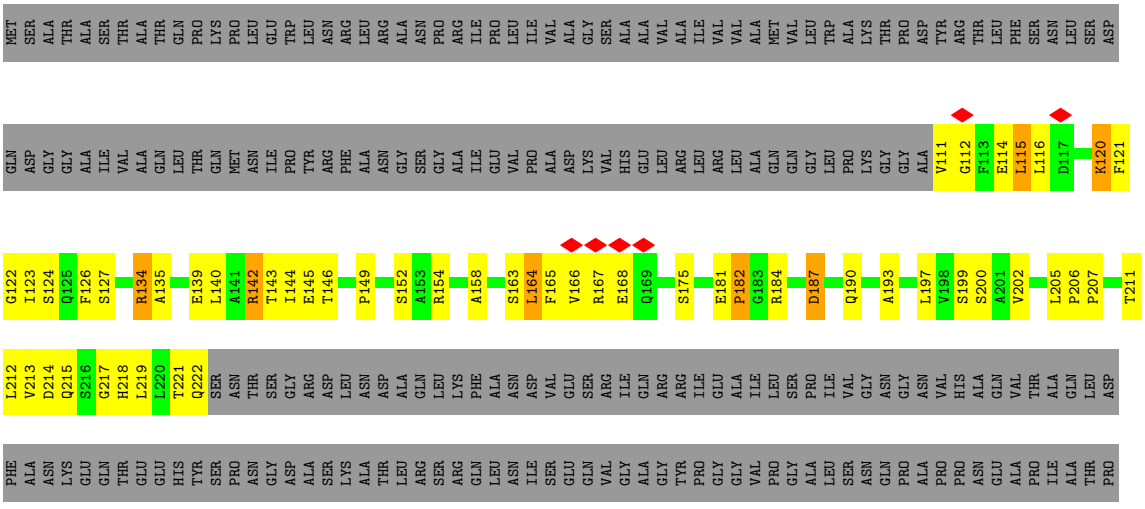
• Molecule 1: Flagellar M-ring protein

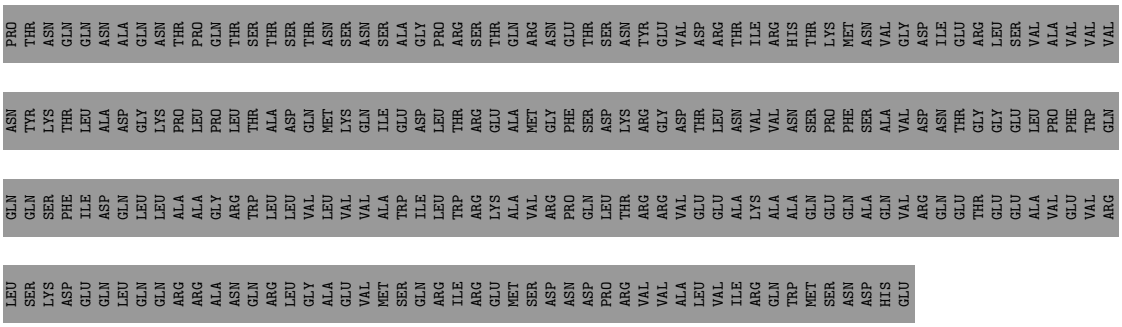
Chain WF:



• Molecule 1: Flagellar M-ring protein

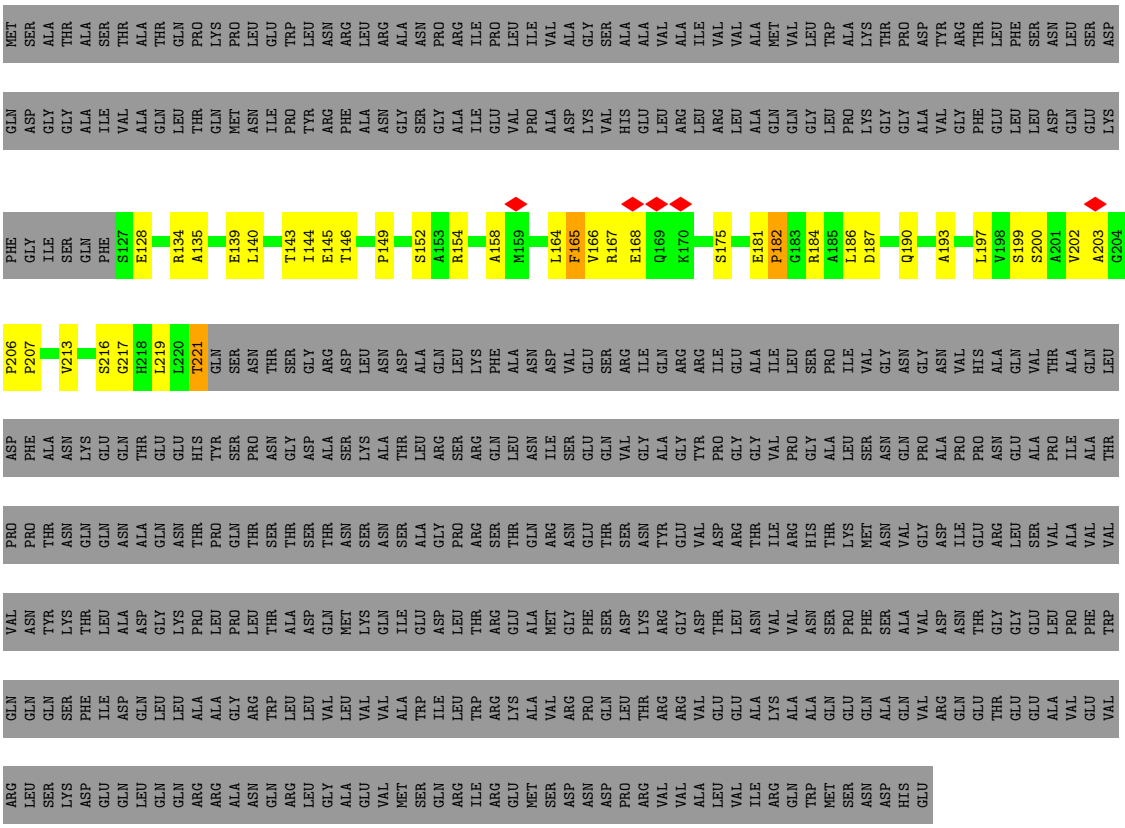
Chain WG:





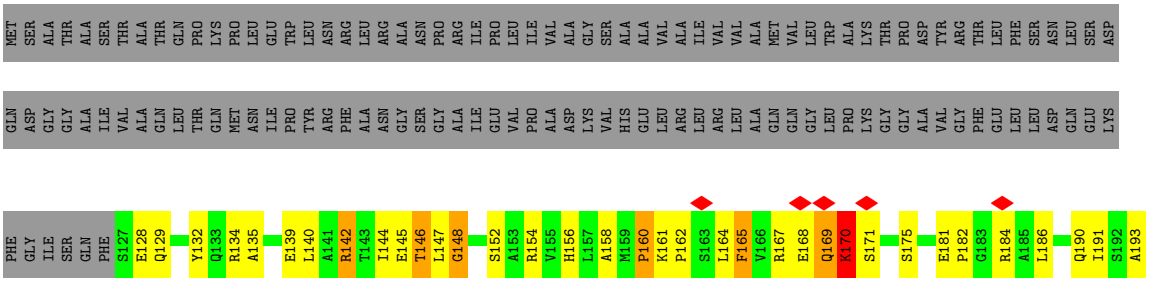
• Molecule 1: Flagellar M-ring protein

Chain WH:



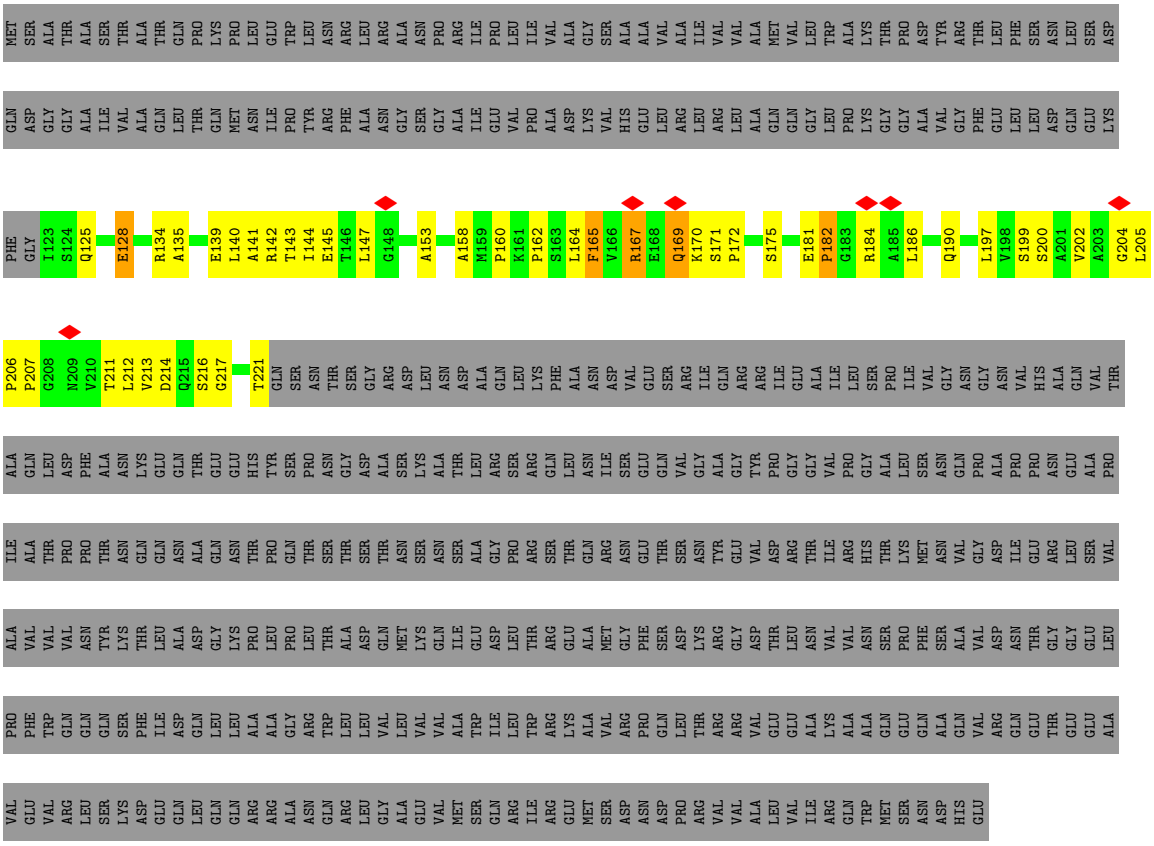
• Molecule 1: Flagellar M-ring protein

Chain WI:



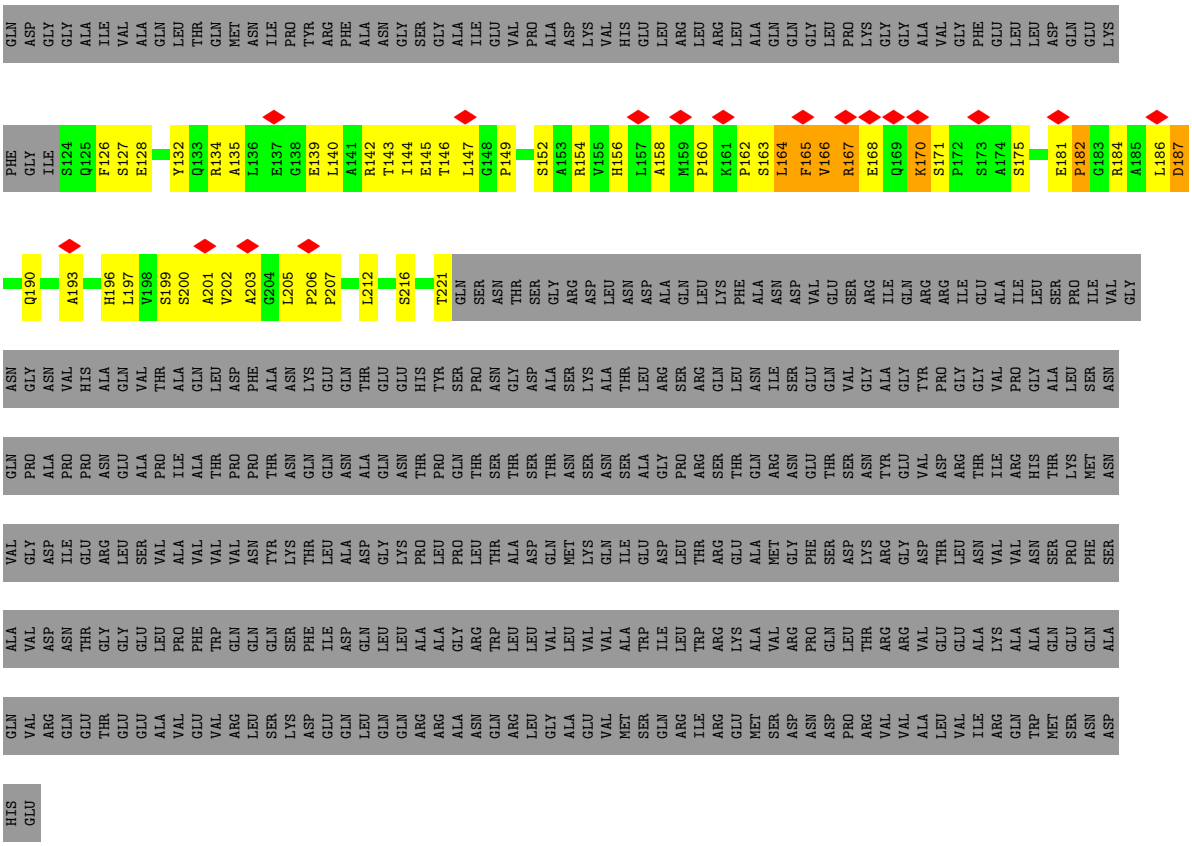
• Molecule 1: Flagellar M-ring protein

Chain WJ:



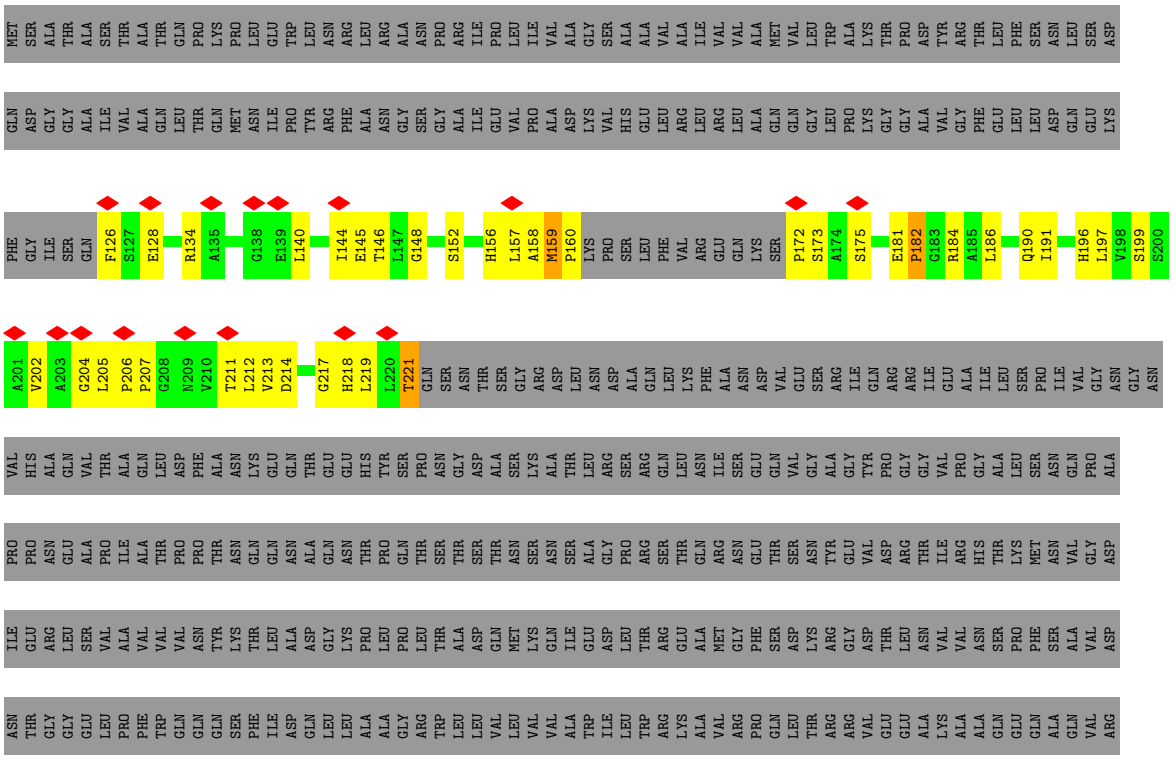
• Molecule 1: Flagellar M-ring protein

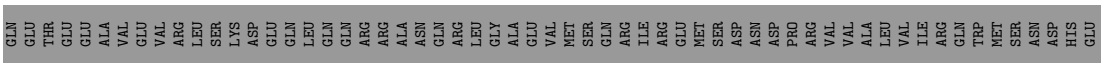
Chain WK:



• Molecule 1: Flagellar M-ring protein

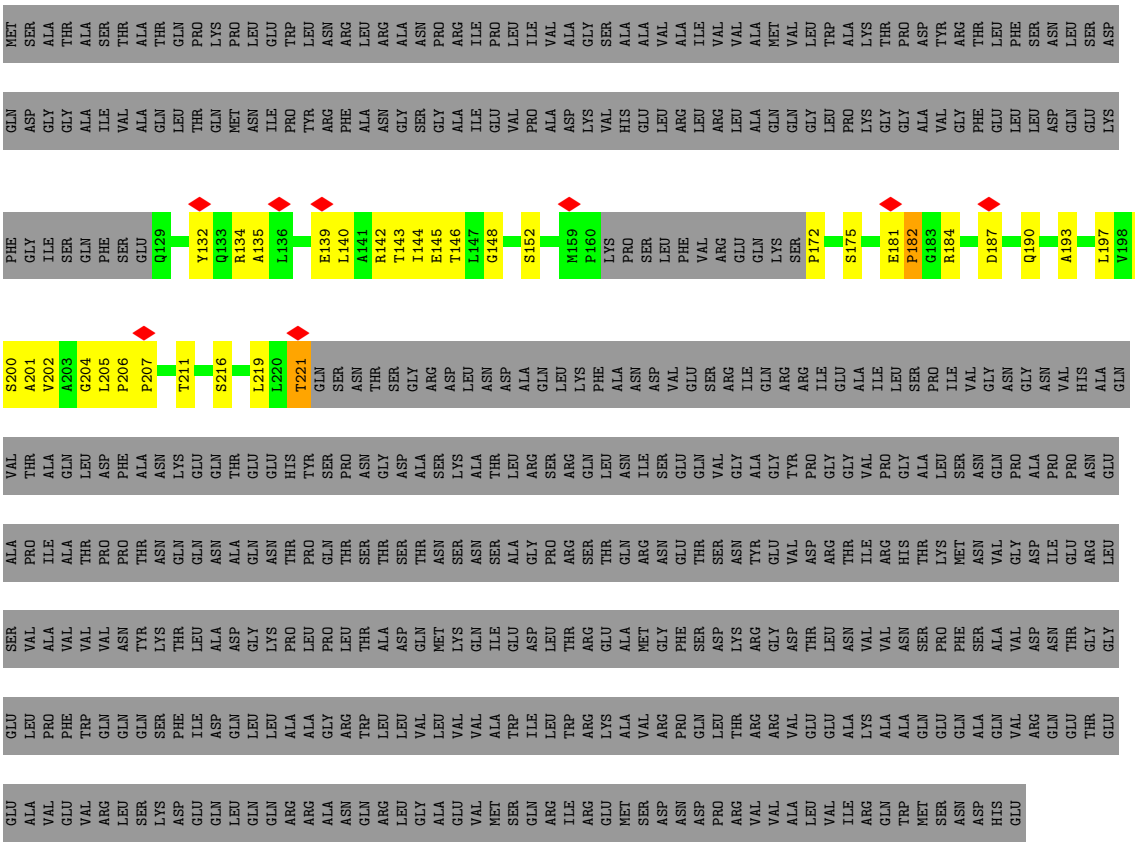
Chain WL:





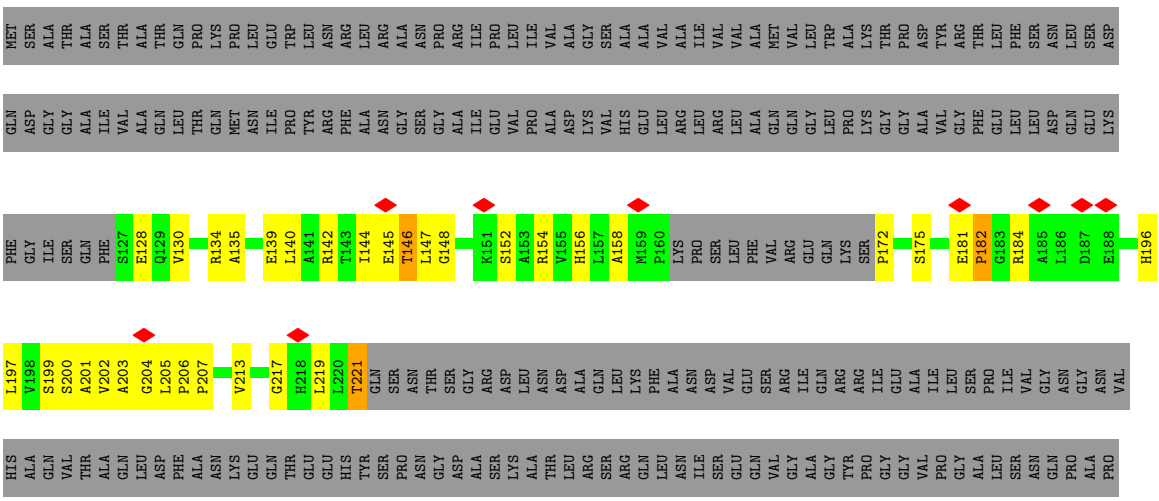
• Molecule 1: Flagellar M-ring protein

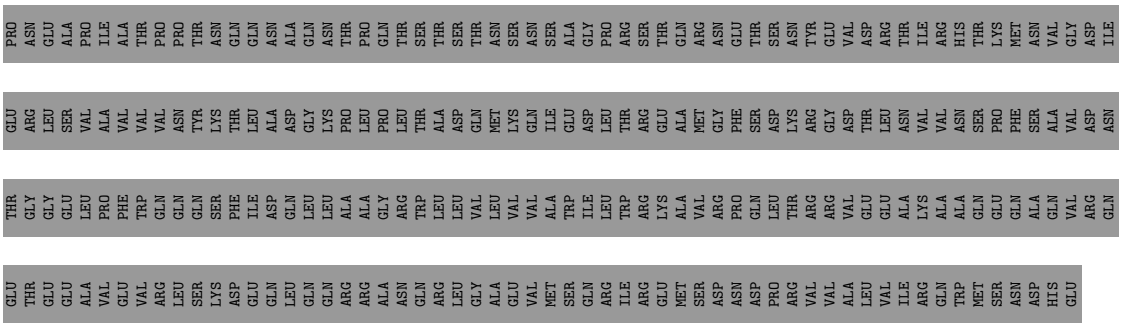
Chain WM:



• Molecule 1: Flagellar M-ring protein

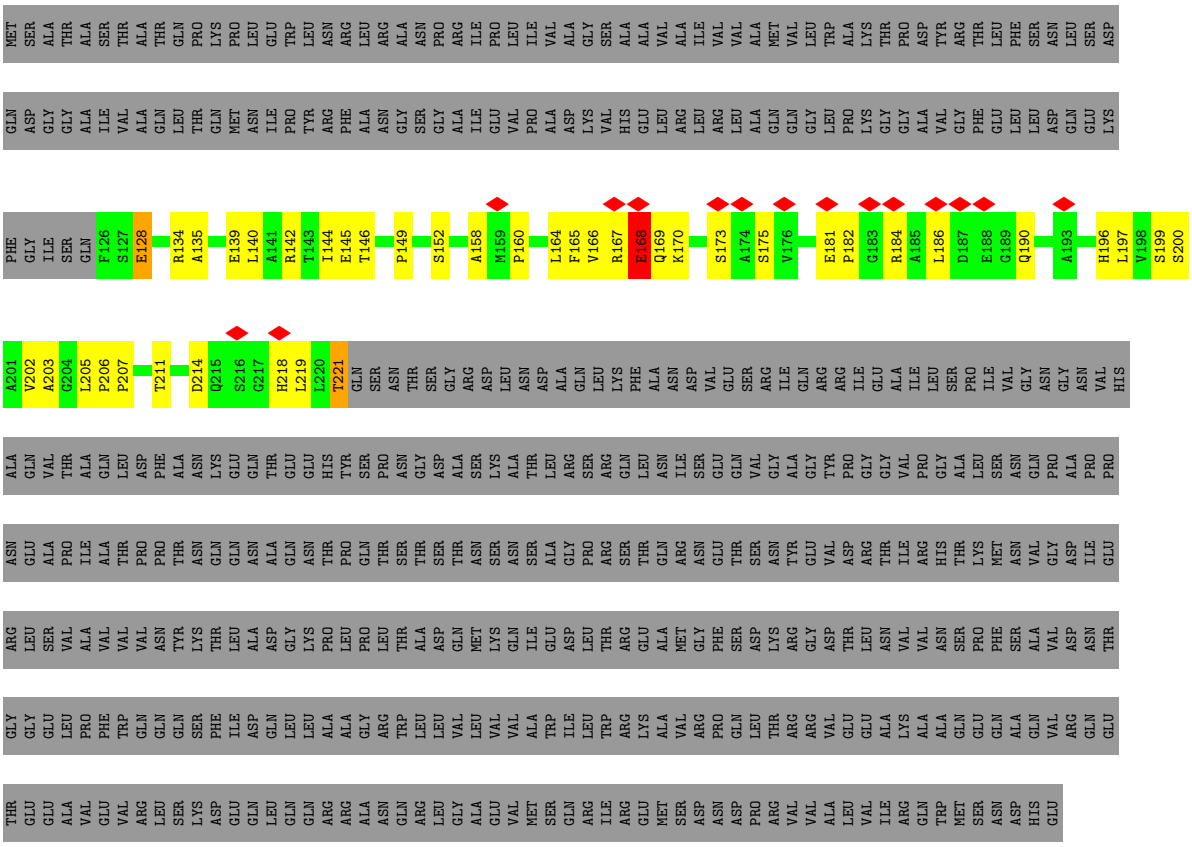
Chain WN:





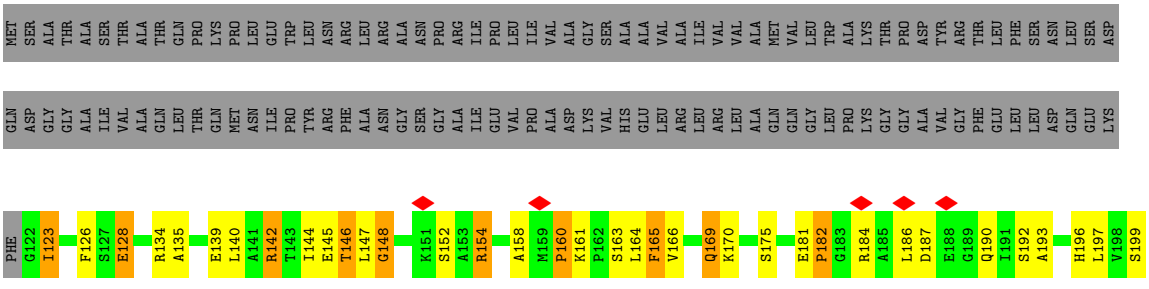
• Molecule 1: Flagellar M-ring protein

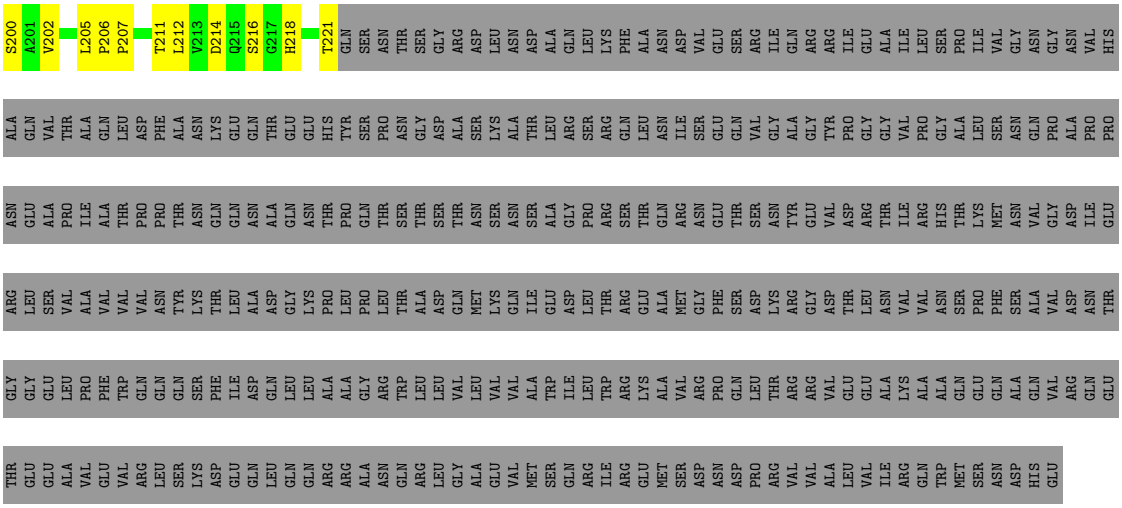
Chain WO:



• Molecule 1: Flagellar M-ring protein

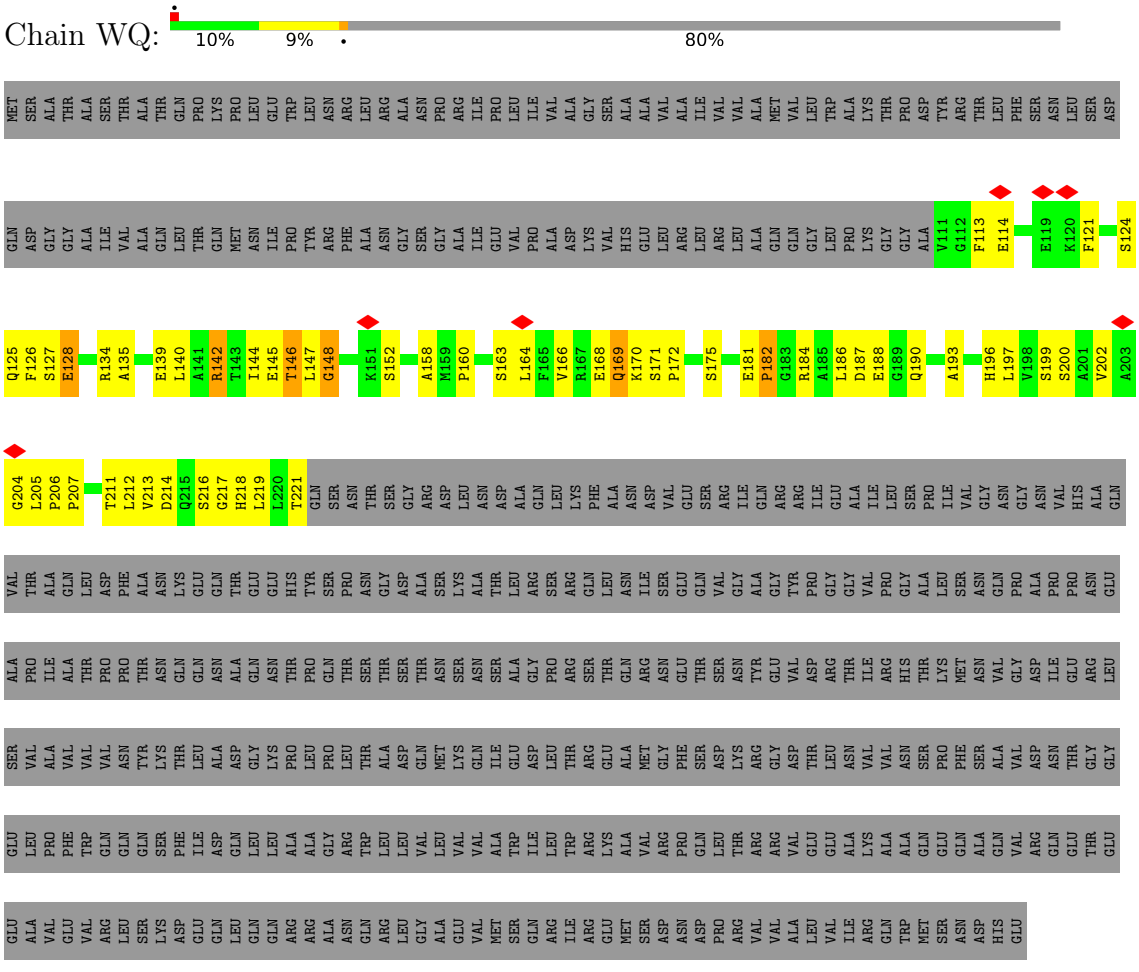
Chain WP:





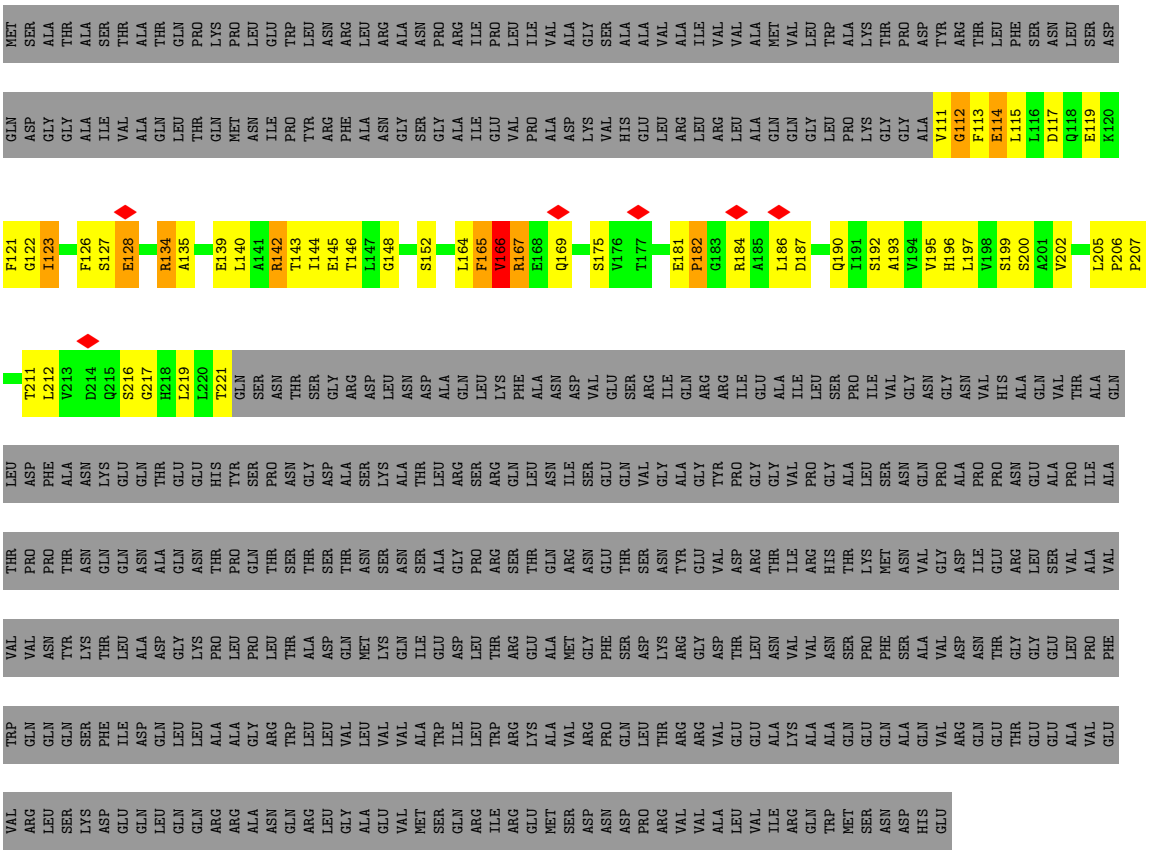
• Molecule 1: Flagellar M-ring protein

Chain WQ:



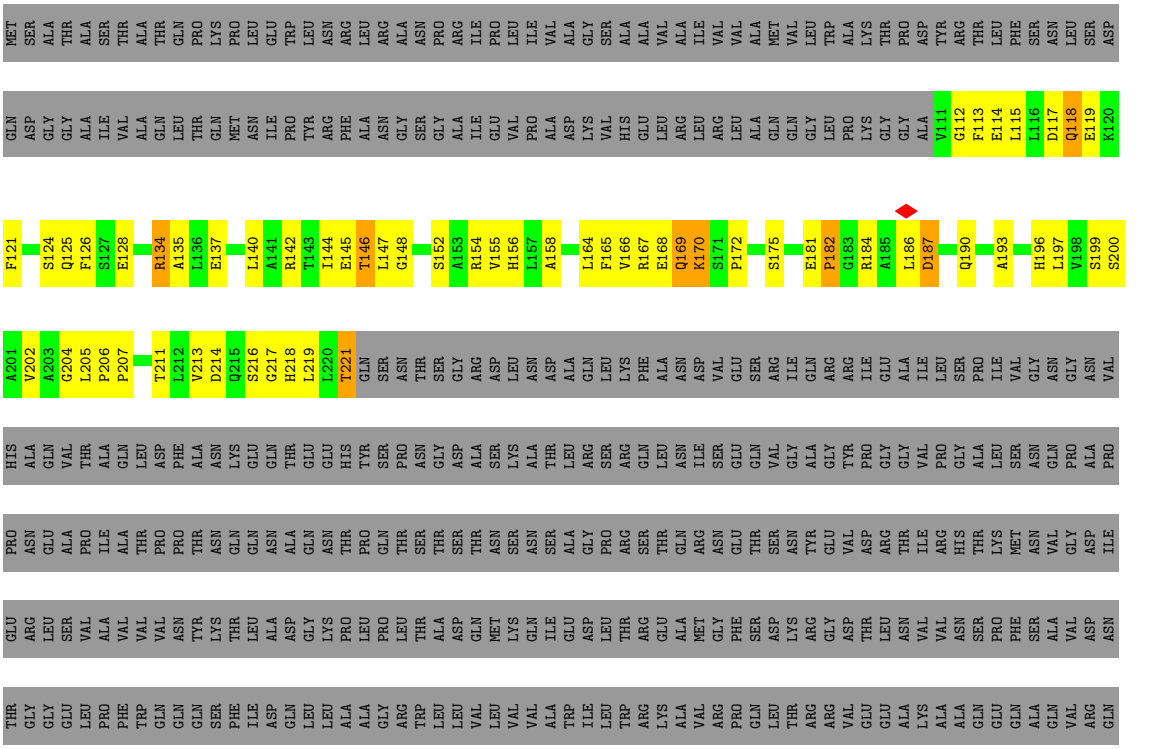
• Molecule 1: Flagellar M-ring protein

Chain WR:



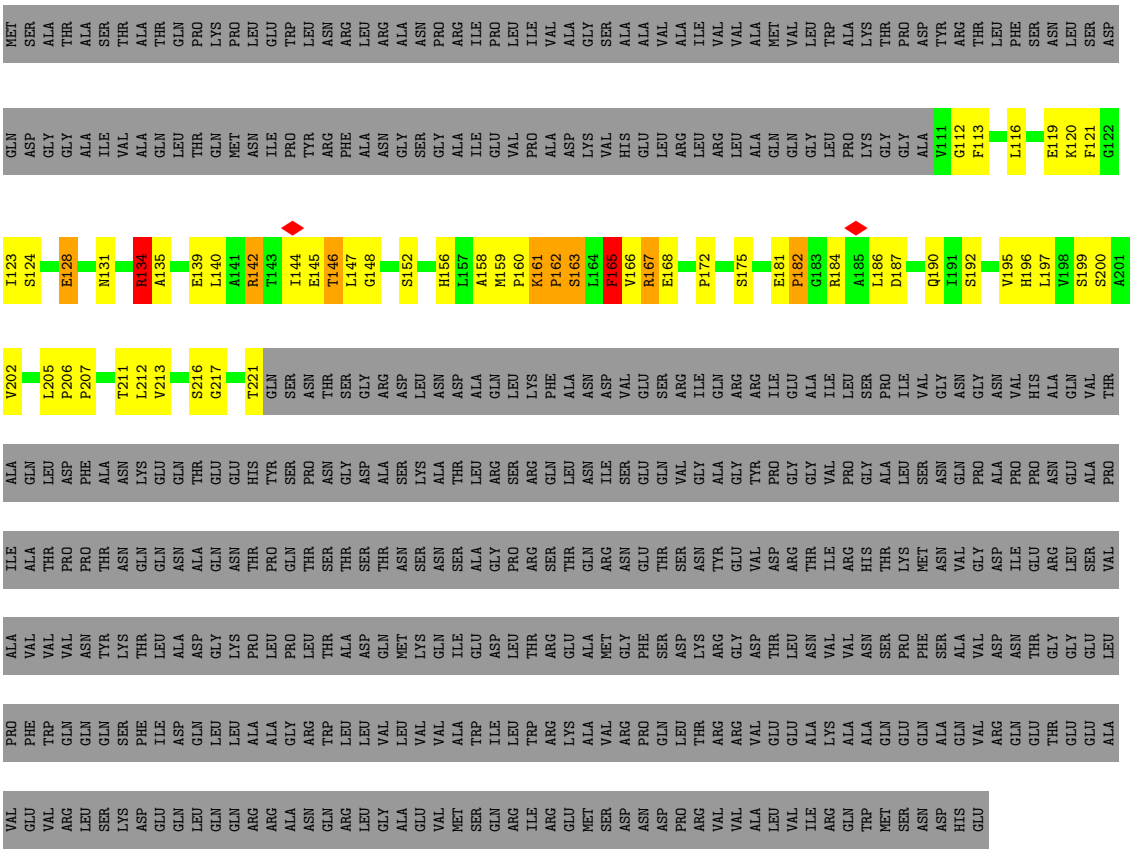
• Molecule 1: Flagellar M-ring protein

Chain WS: 9% 9% 80%



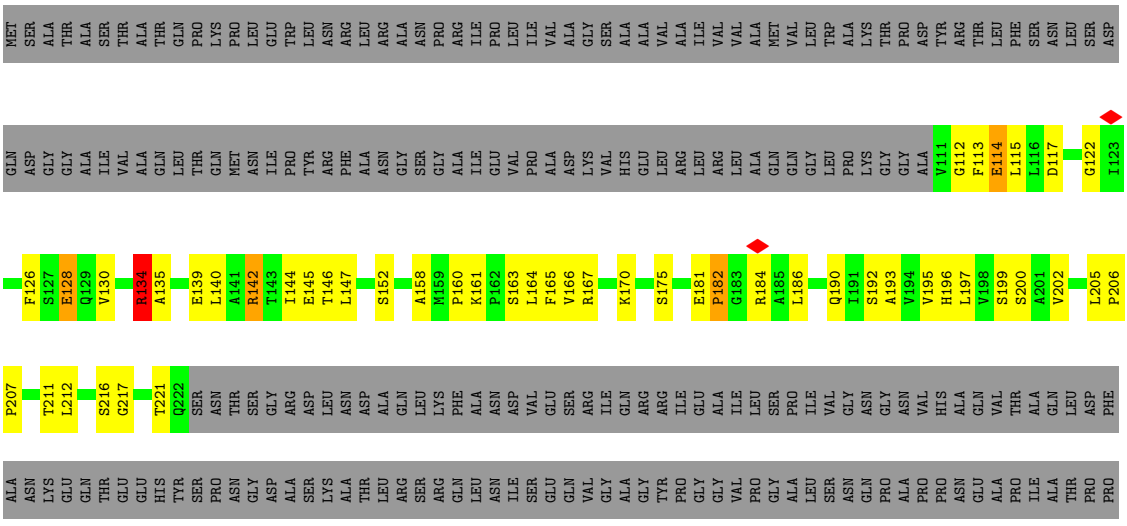
• Molecule 1: Flagellar M-ring protein

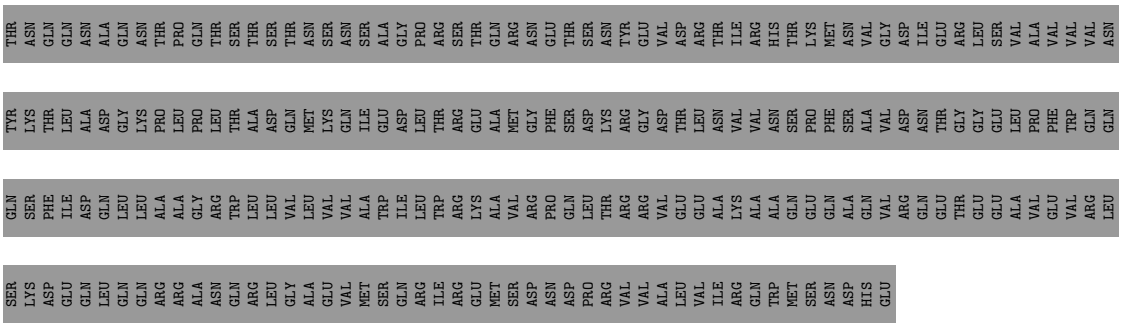
Chain WT:



• Molecule 1: Flagellar M-ring protein

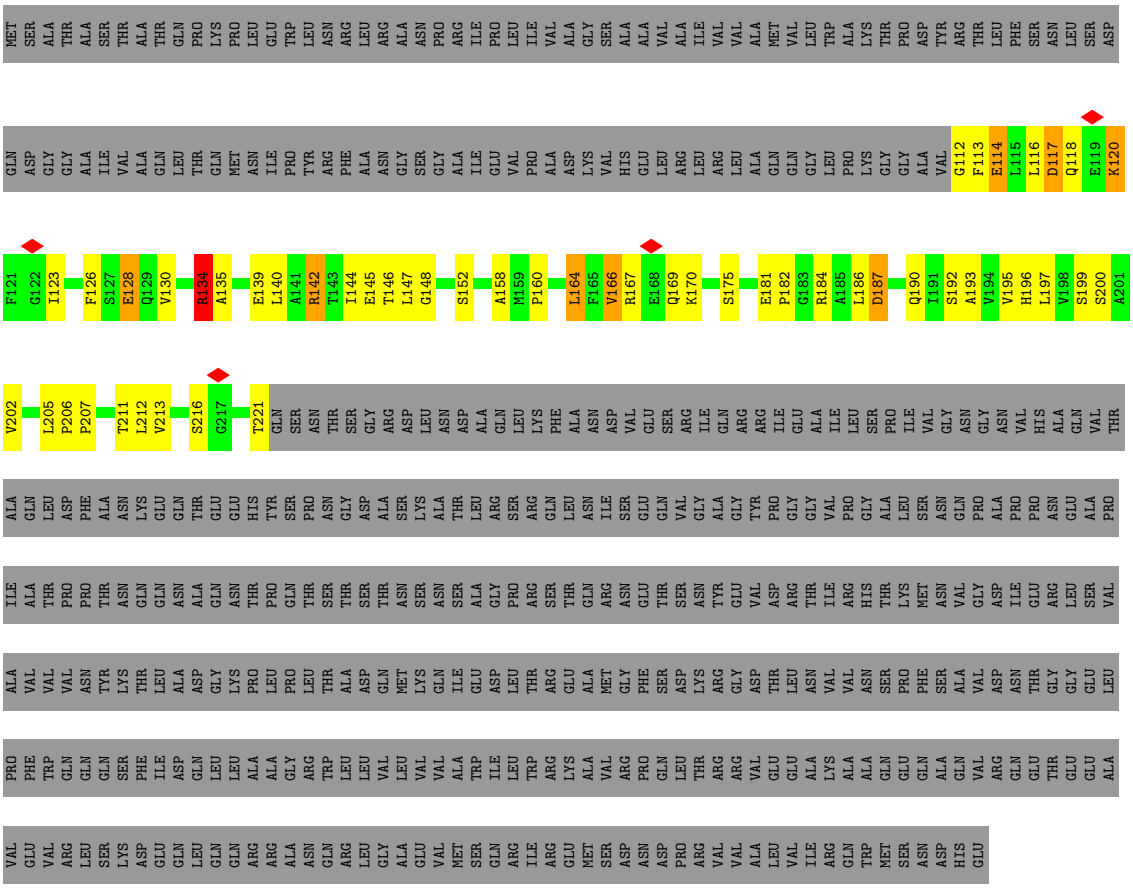
Chain WU:





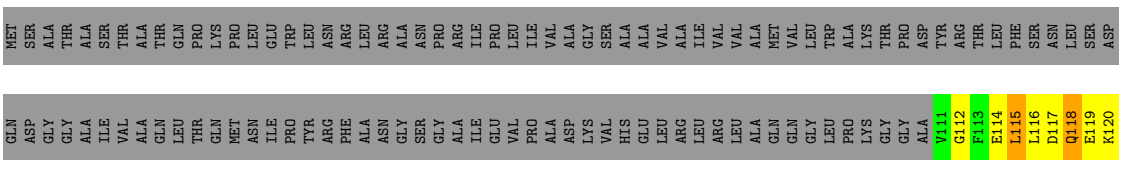
• Molecule 1: Flagellar M-ring protein

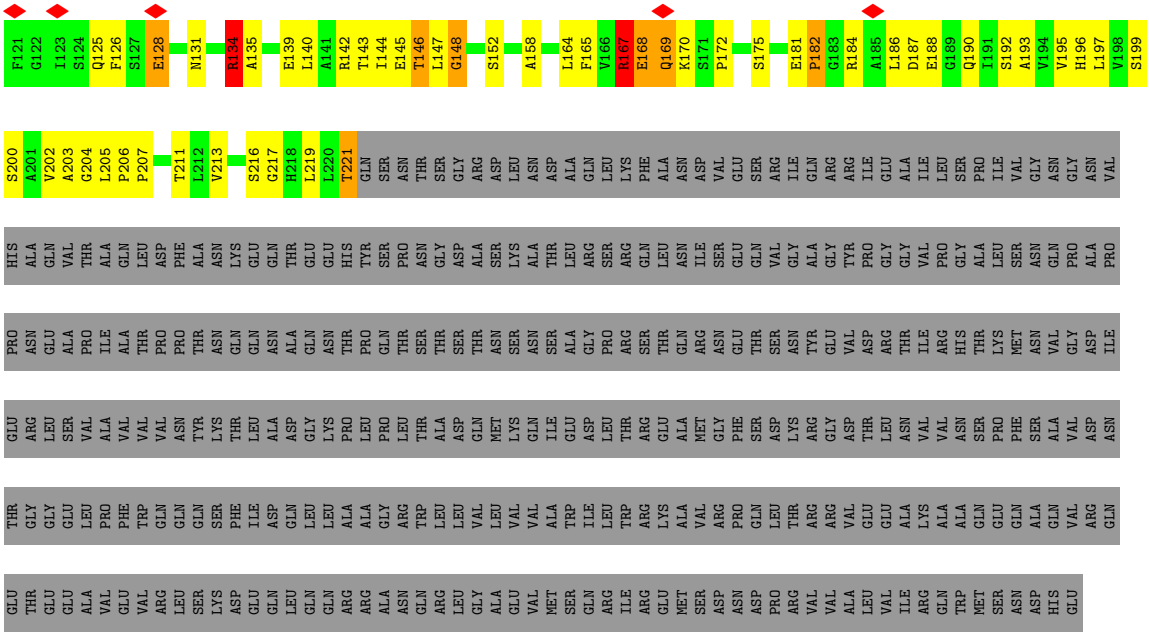
Chain WV:



• Molecule 1: Flagellar M-ring protein

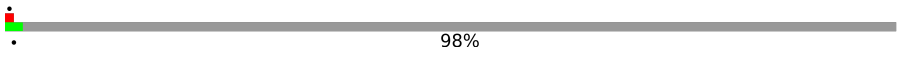
Chain WW:

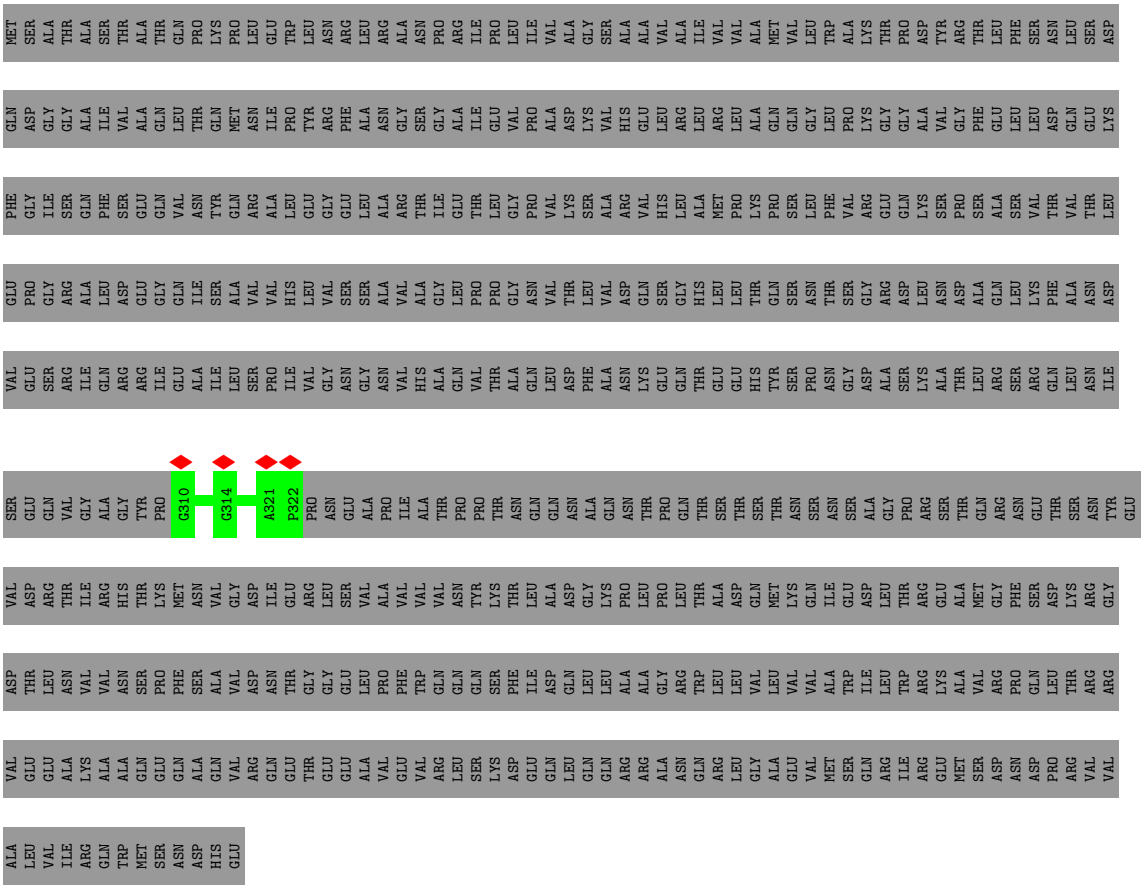




• Molecule 1: Flagellar M-ring protein

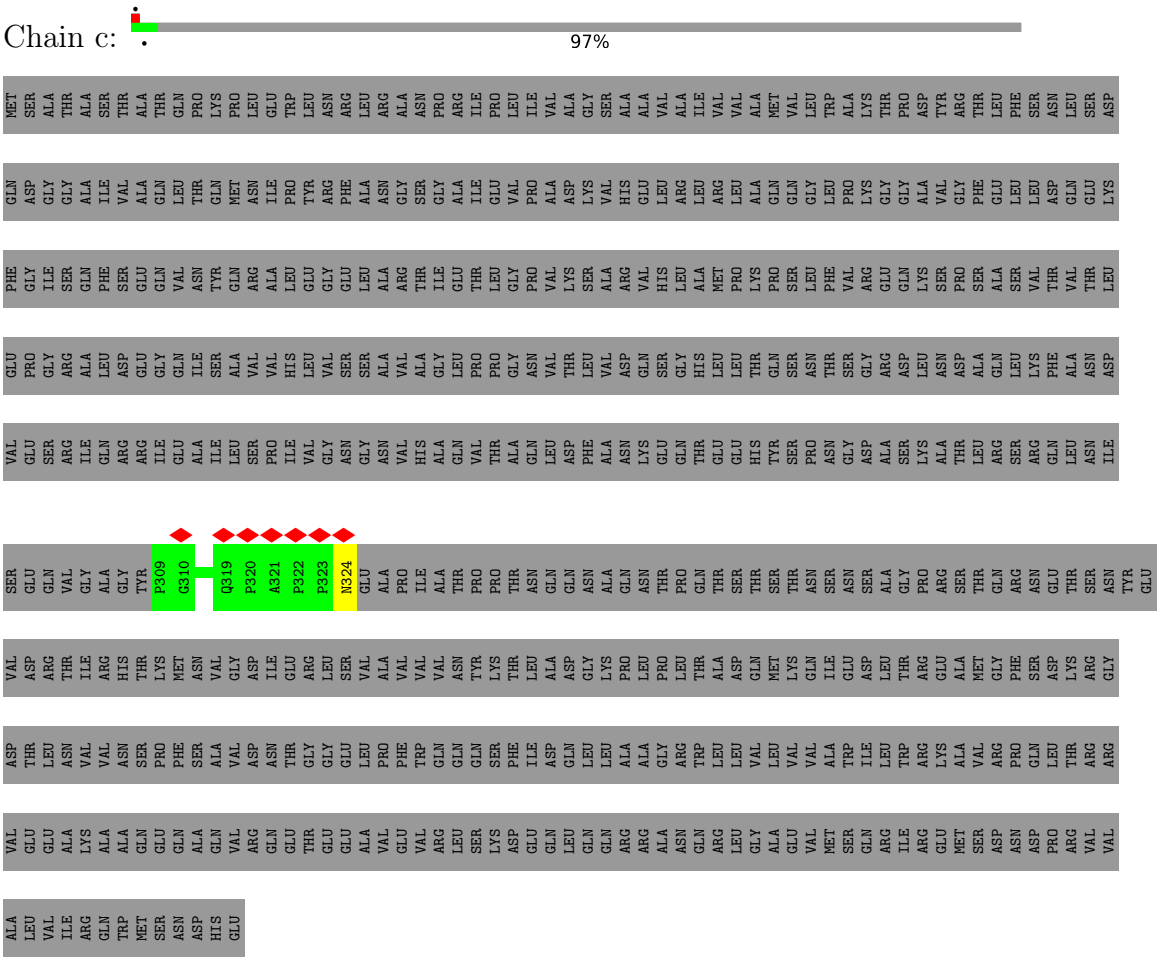
Chain b:





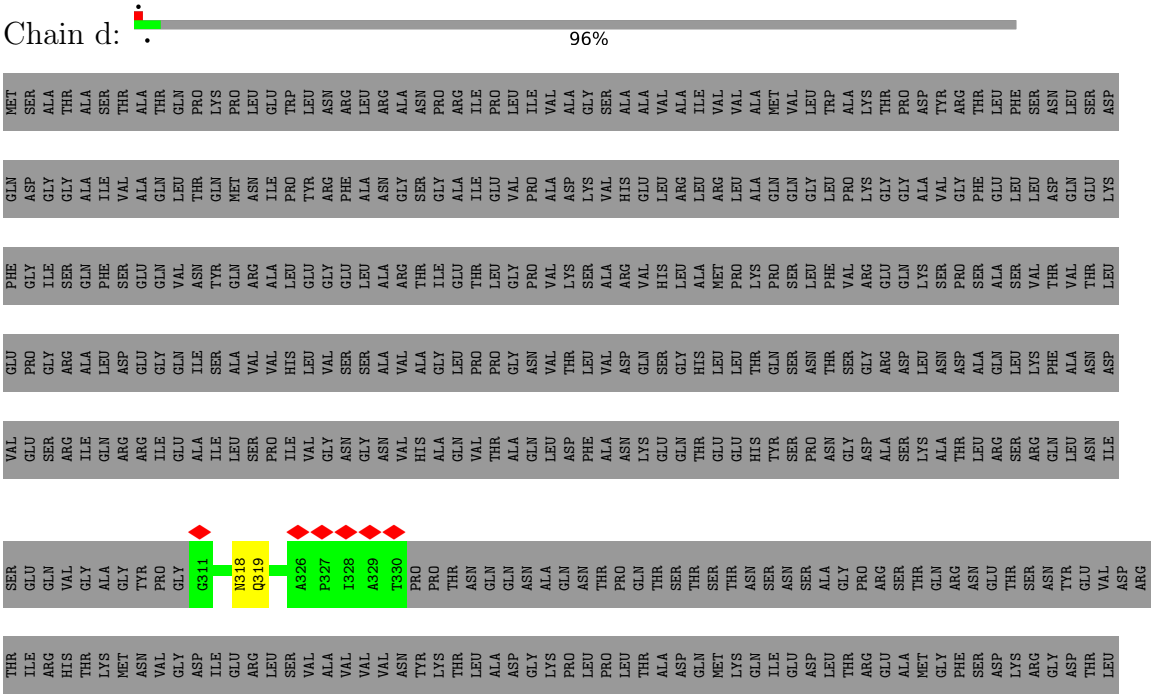
• Molecule 1: Flagellar M-ring protein

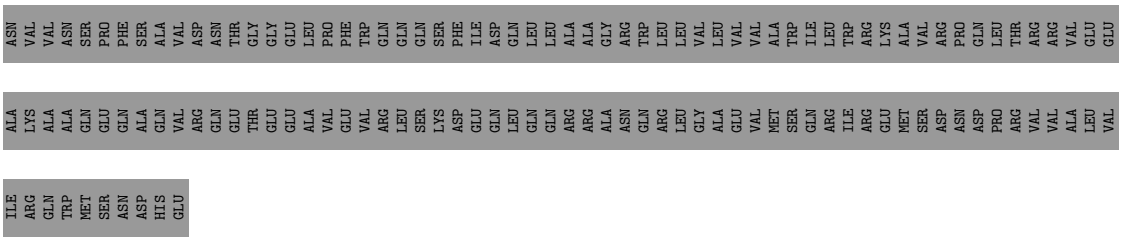
Chain c:



• Molecule 1: Flagellar M-ring protein

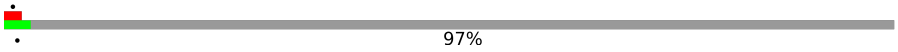
Chain d:

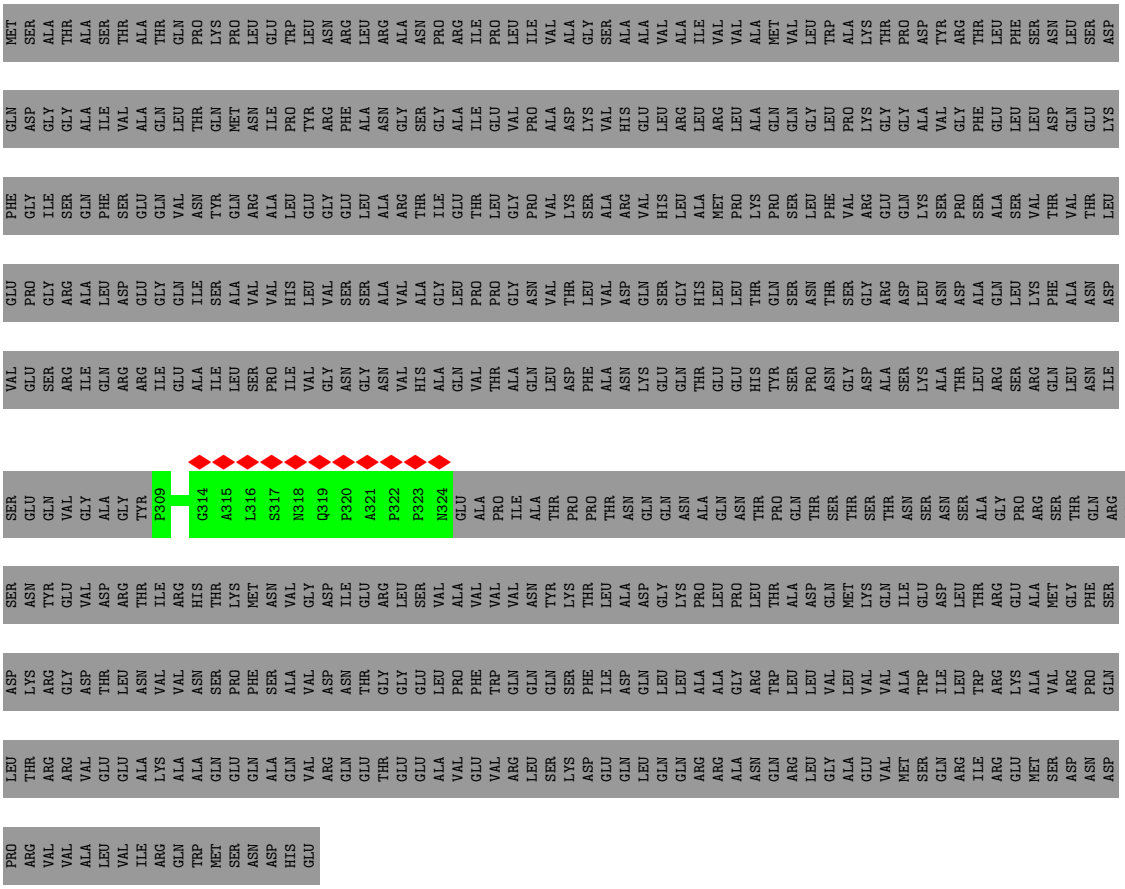




• Molecule 1: Flagellar M-ring protein

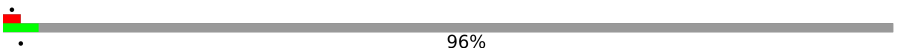
Chain e:

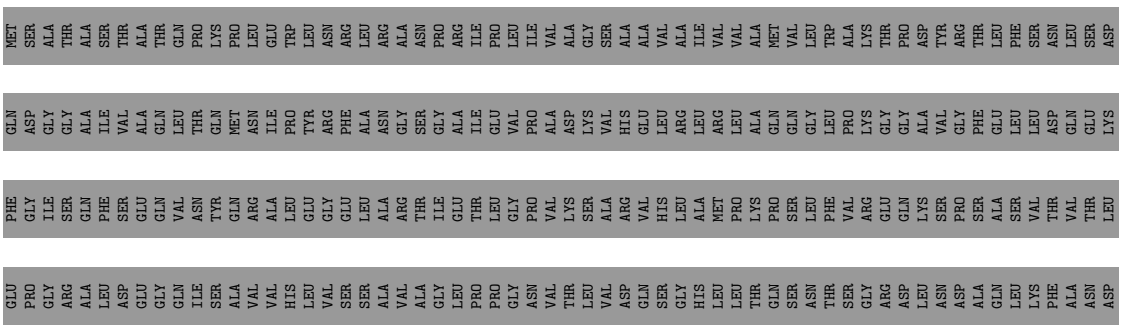




• Molecule 1: Flagellar M-ring protein

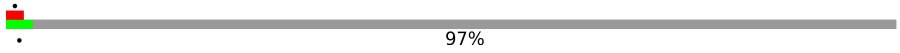
Chain f:

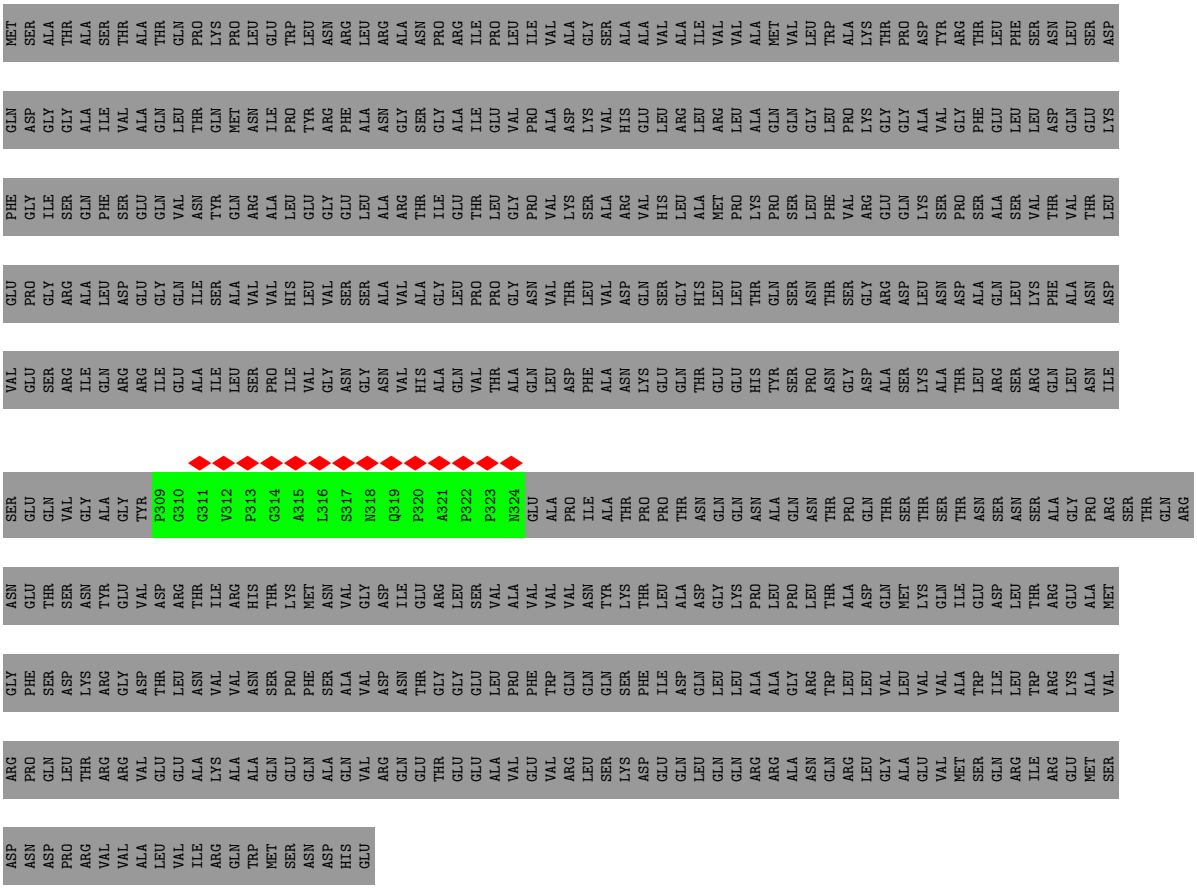




• Molecule 1: Flagellar M-ring protein

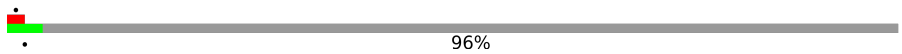
Chain g:

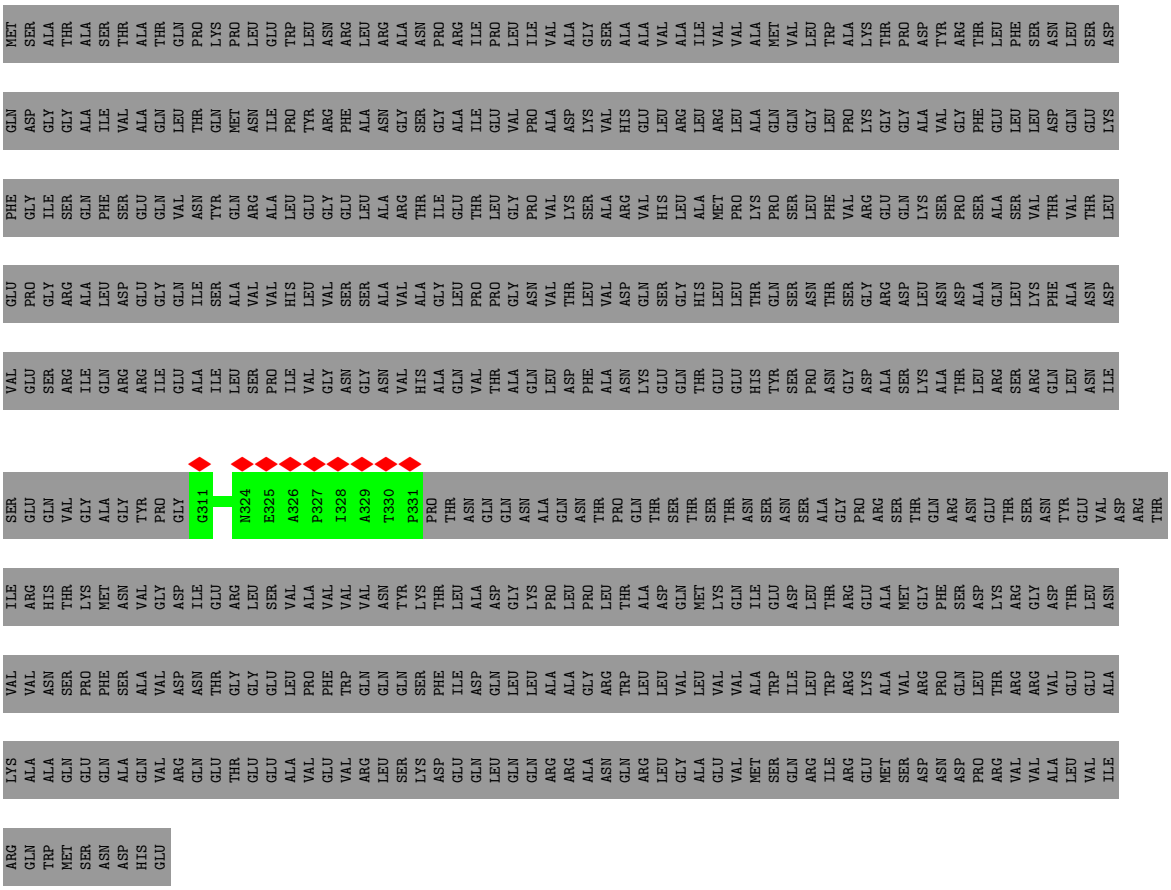




• Molecule 1: Flagellar M-ring protein

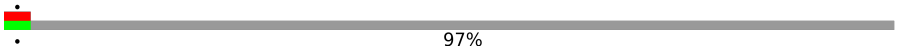
Chain h:

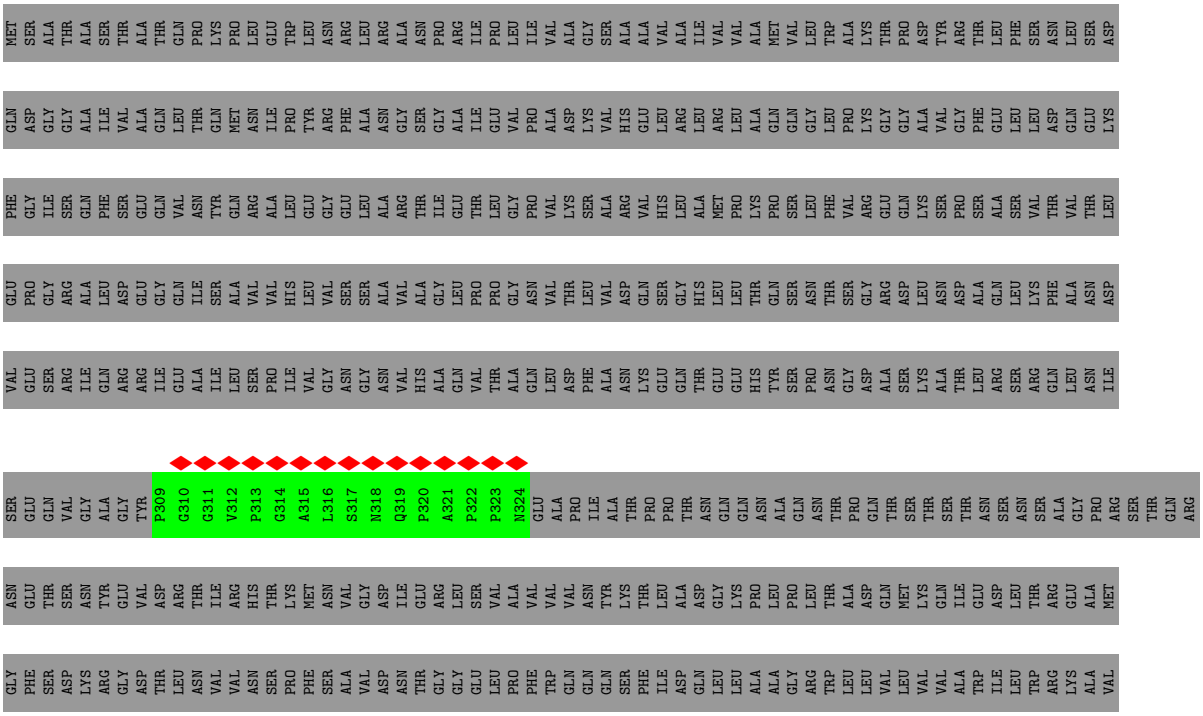


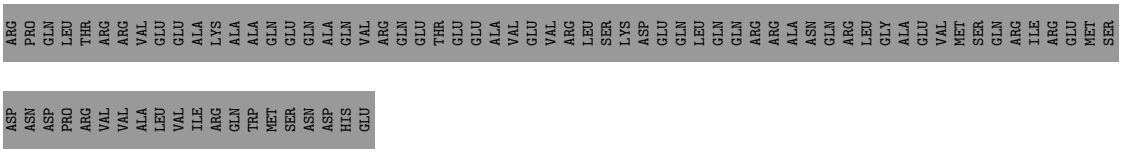


• Molecule 1: Flagellar M-ring protein

Chain i:

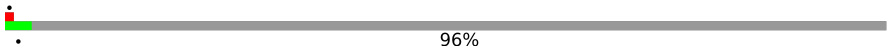


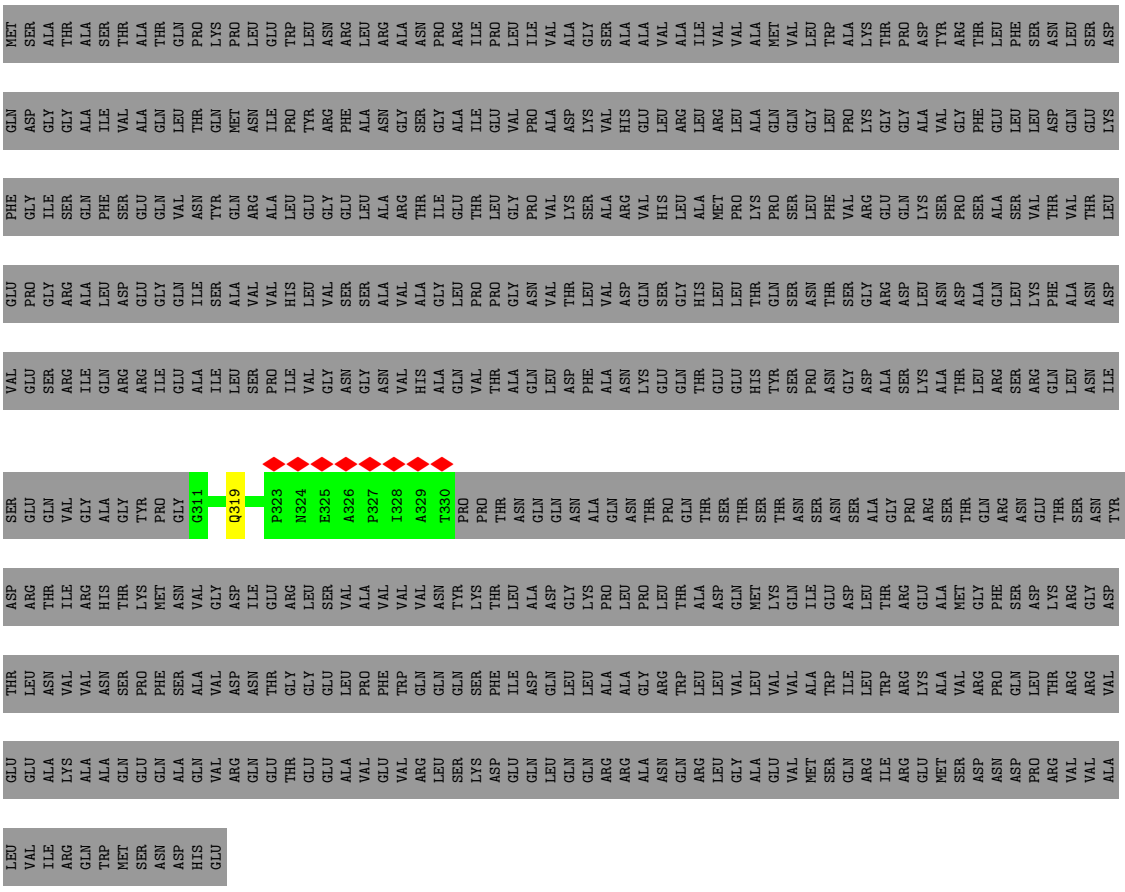




• Molecule 1: Flagellar M-ring protein

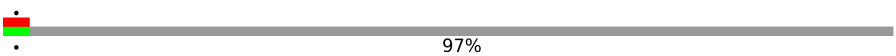
Chain j:

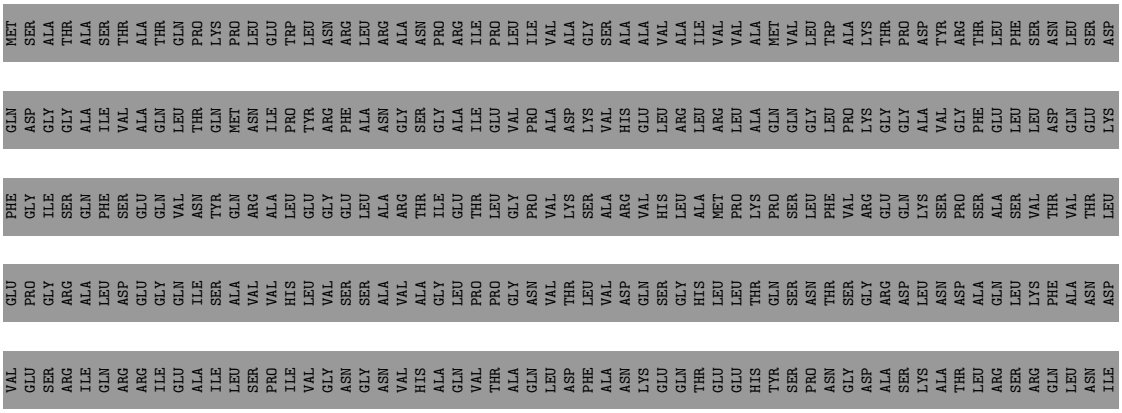


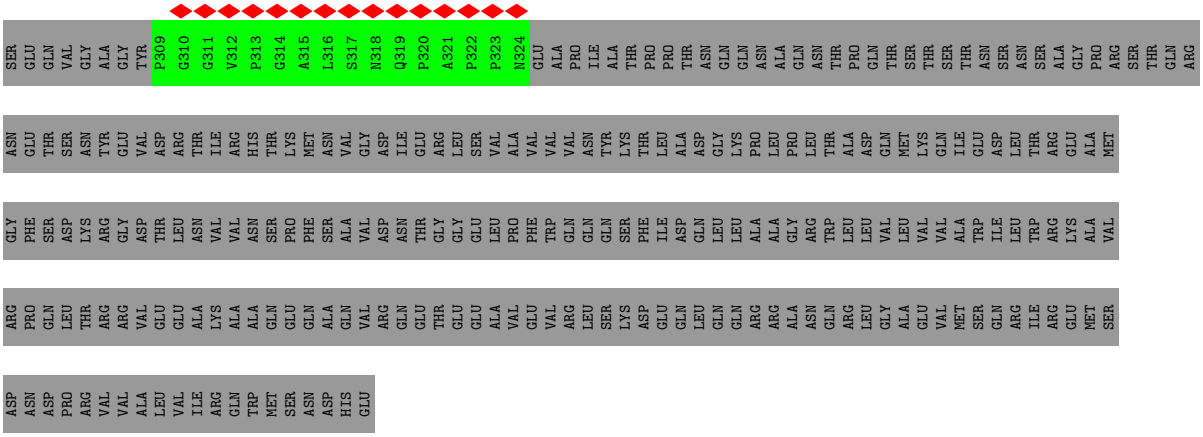


• Molecule 1: Flagellar M-ring protein

Chain k:

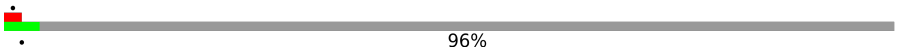


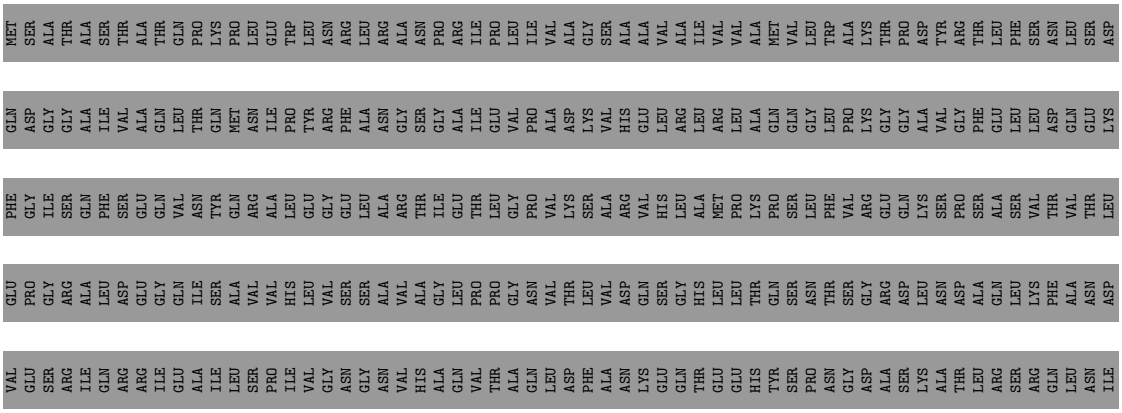


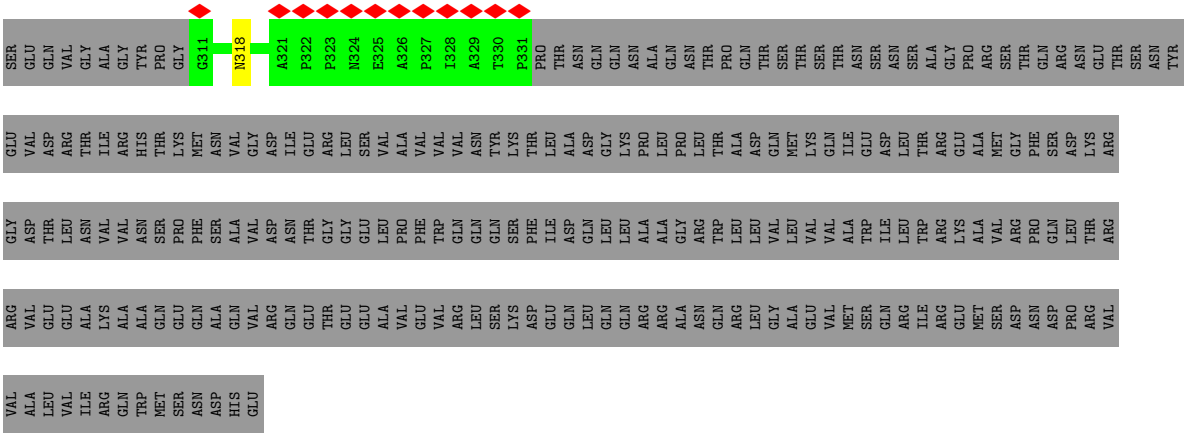


• Molecule 1: Flagellar M-ring protein

Chain l:

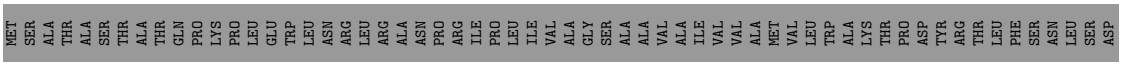






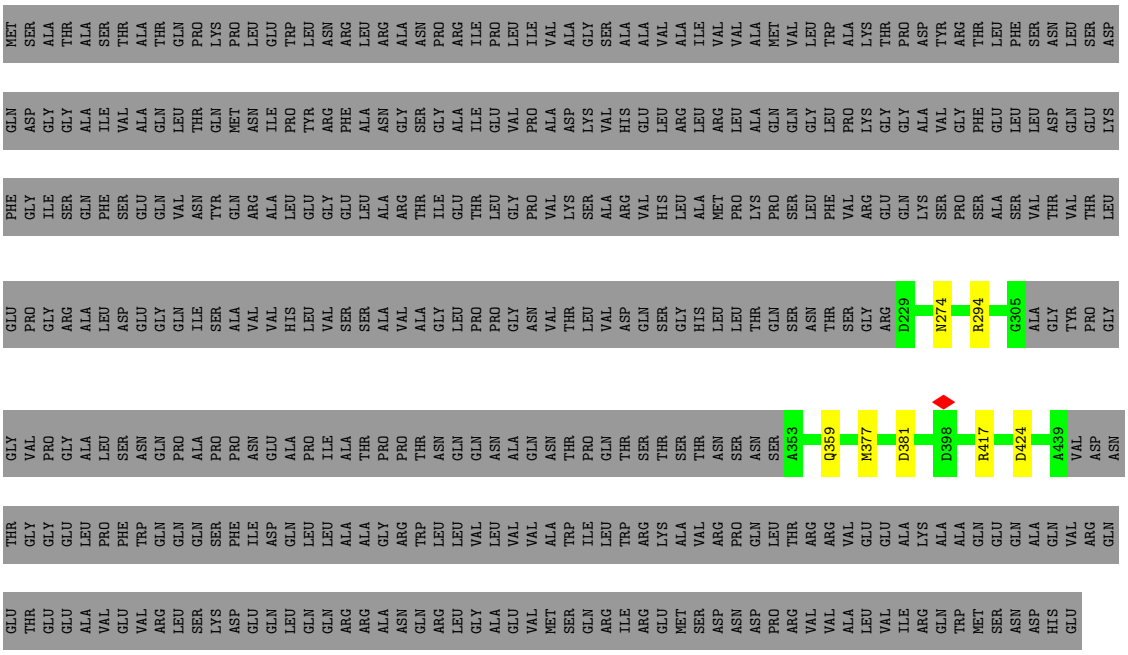
• Molecule 1: Flagellar M-ring protein

Chain t:



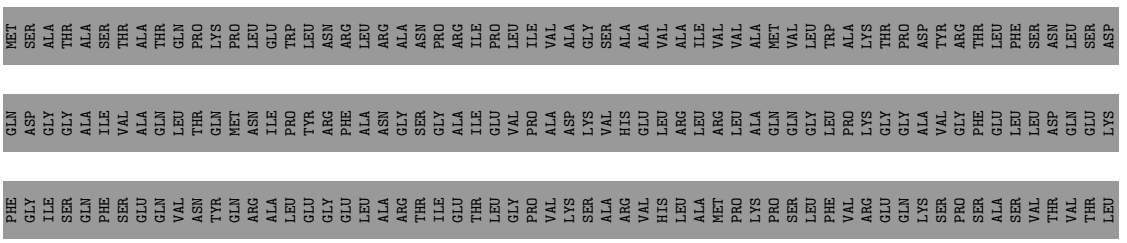
• Molecule 1: Flagellar M-ring protein

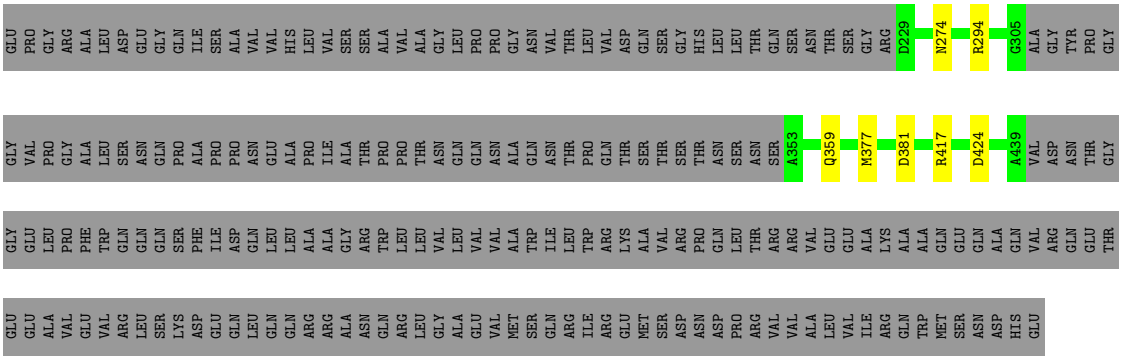
Chain u:



• Molecule 1: Flagellar M-ring protein

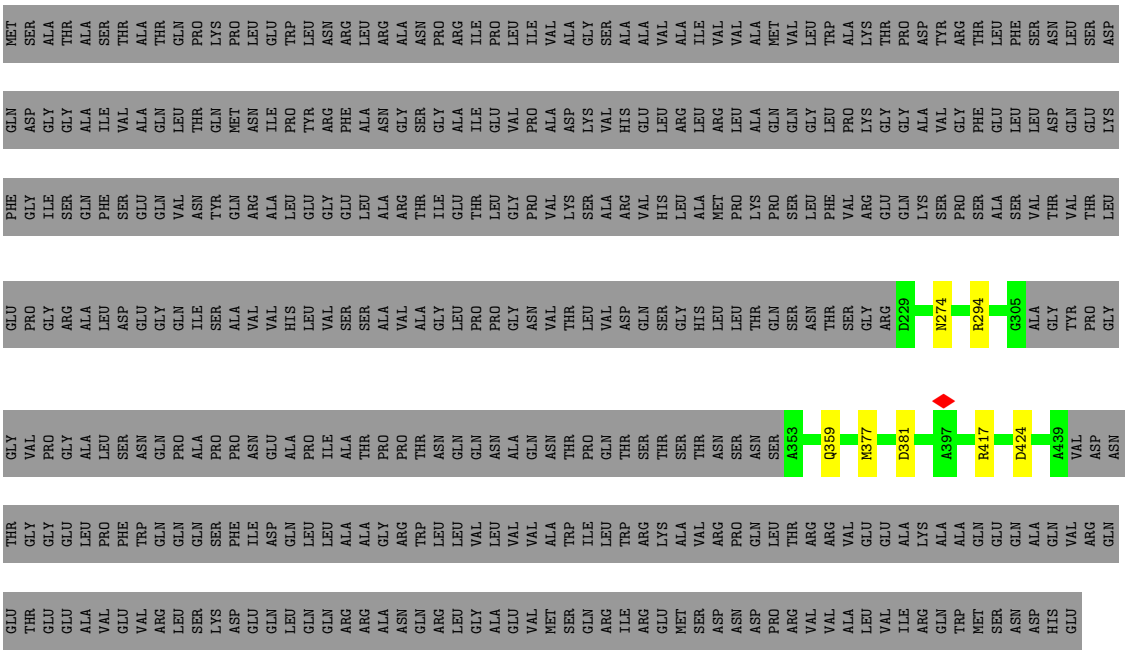
Chain v:





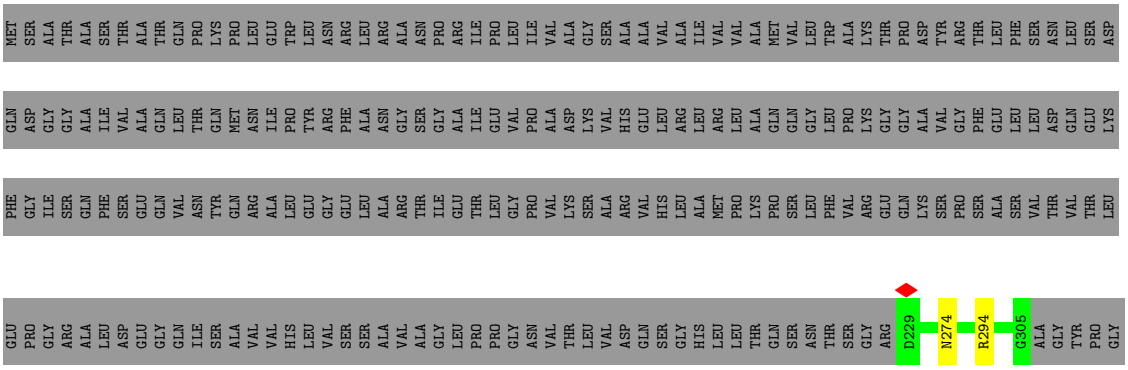
• Molecule 1: Flagellar M-ring protein

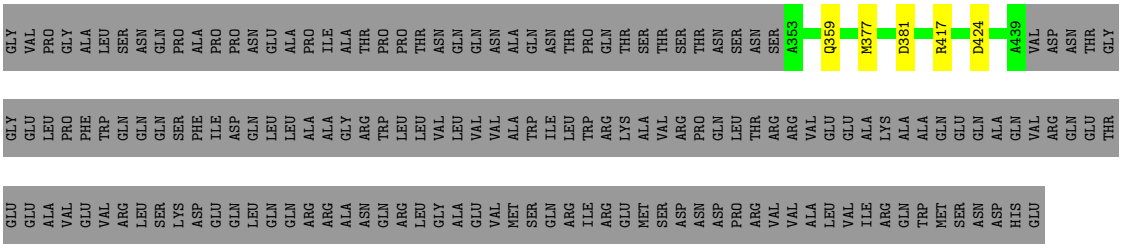
Chain w:



• Molecule 1: Flagellar M-ring protein

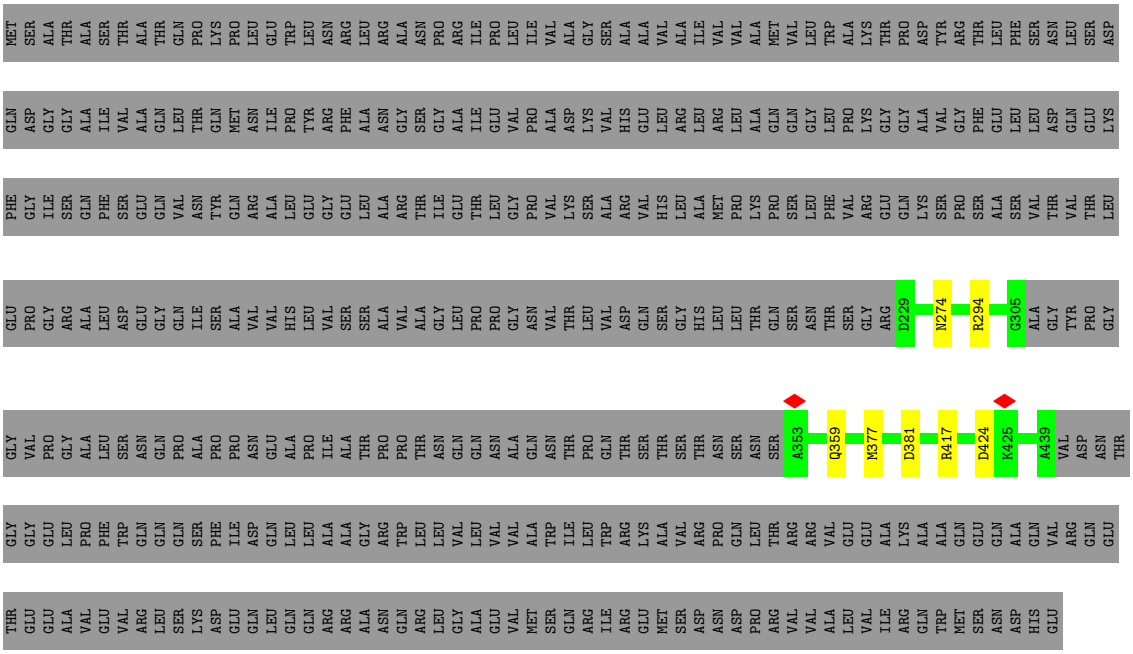
Chain x:





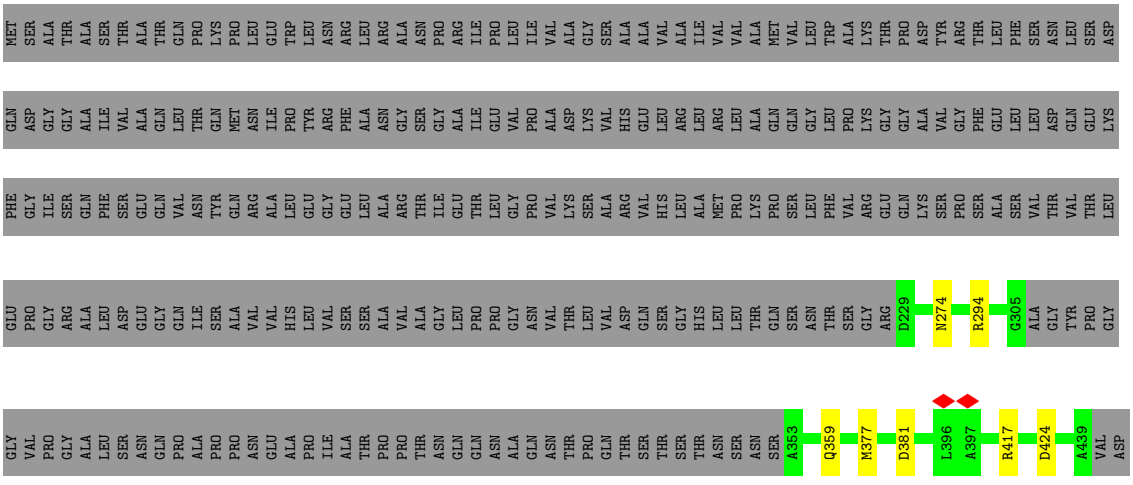
• Molecule 1: Flagellar M-ring protein

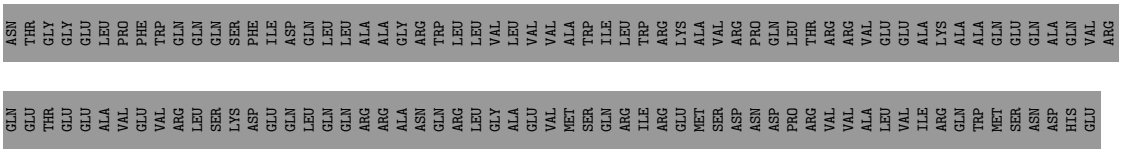
Chain y:



• Molecule 1: Flagellar M-ring protein

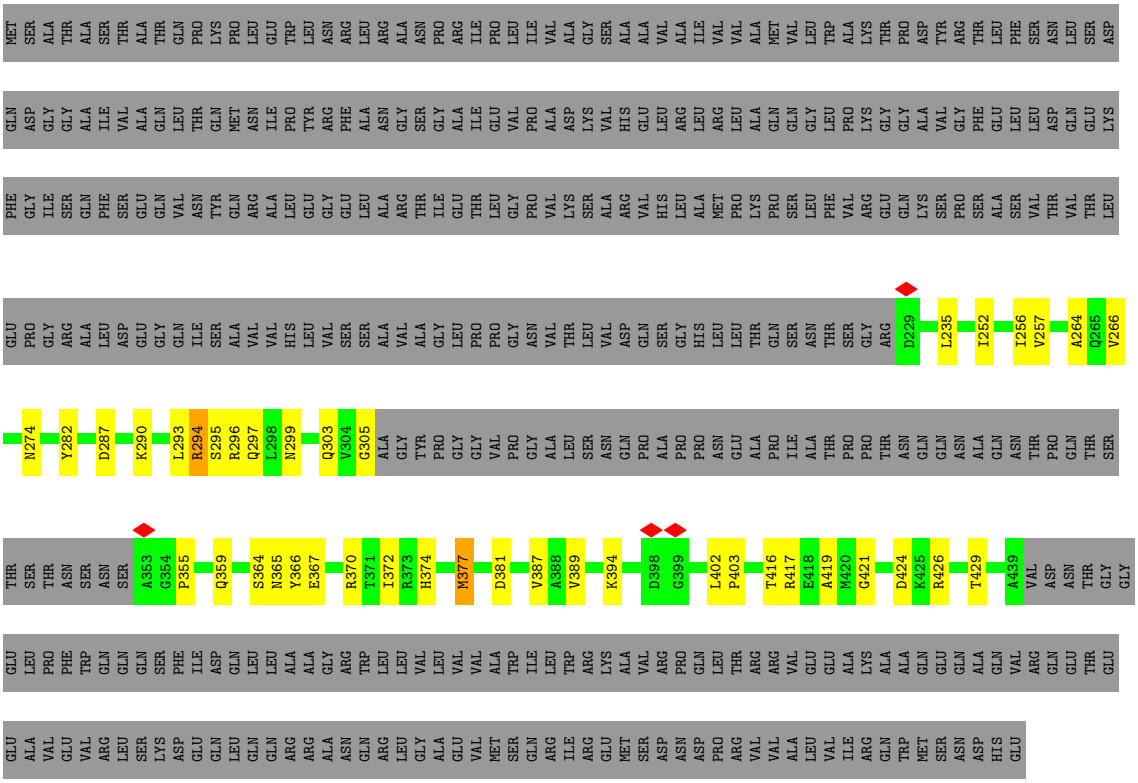
Chain z:





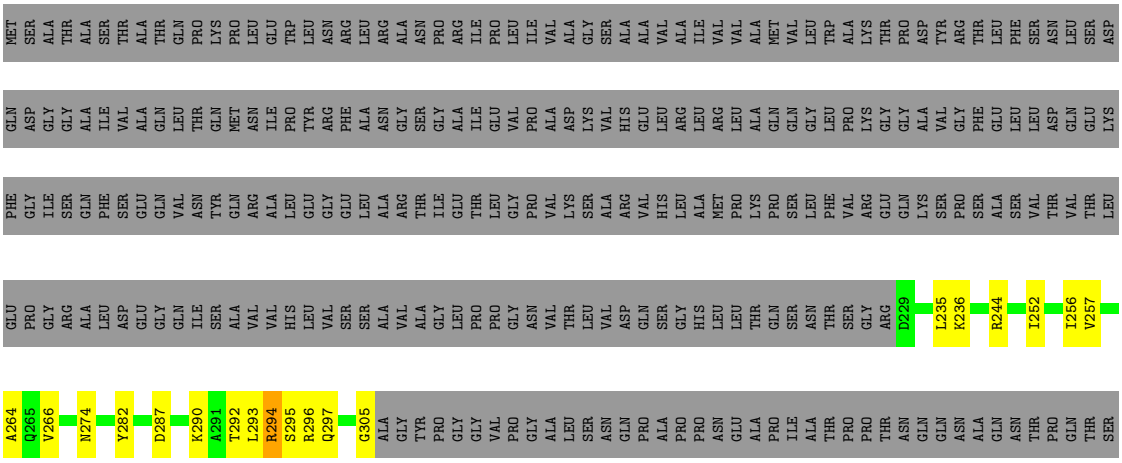
• Molecule 1: Flagellar M-ring protein

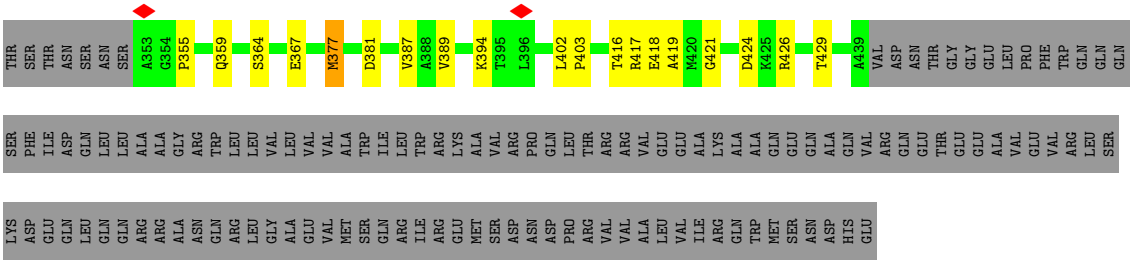
Chain 1:



• Molecule 1: Flagellar M-ring protein

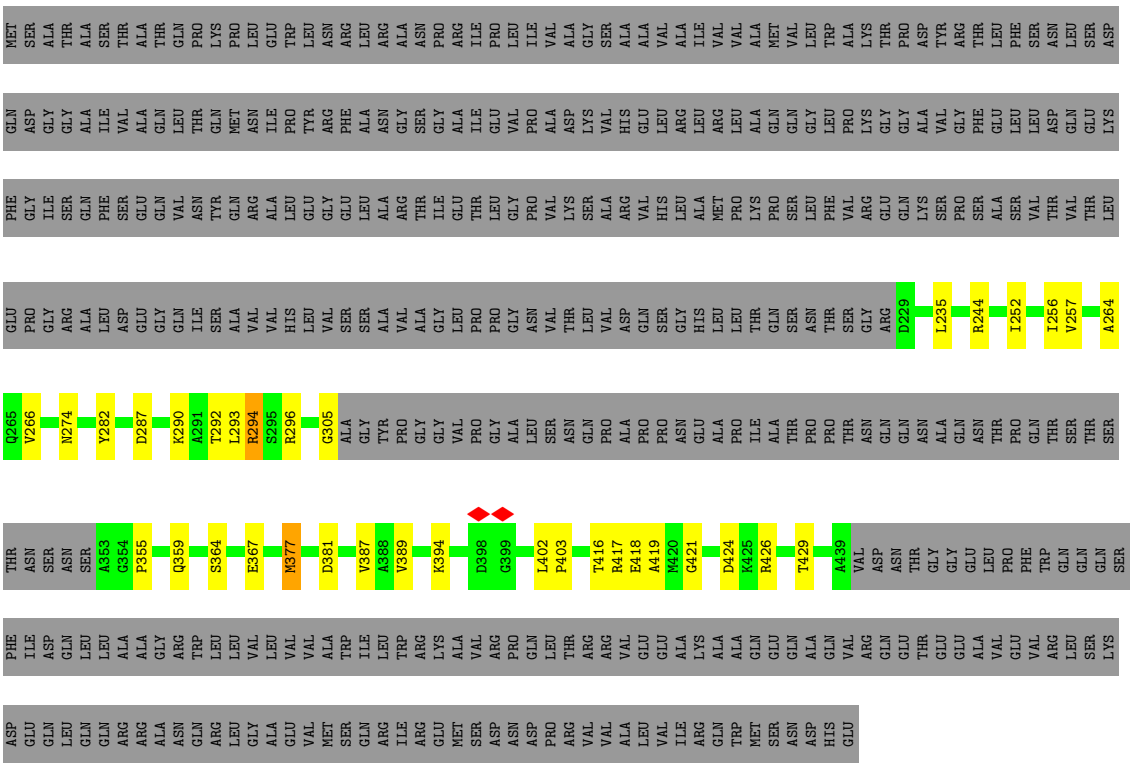
Chain 2:





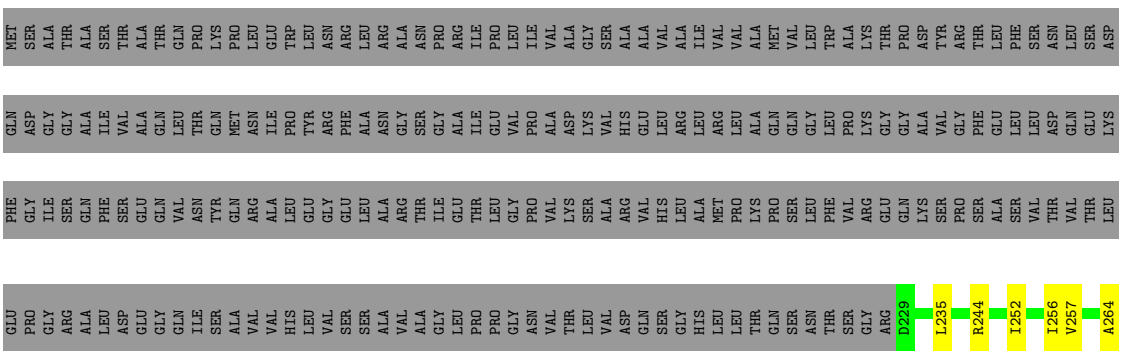
• Molecule 1: Flagellar M-ring protein

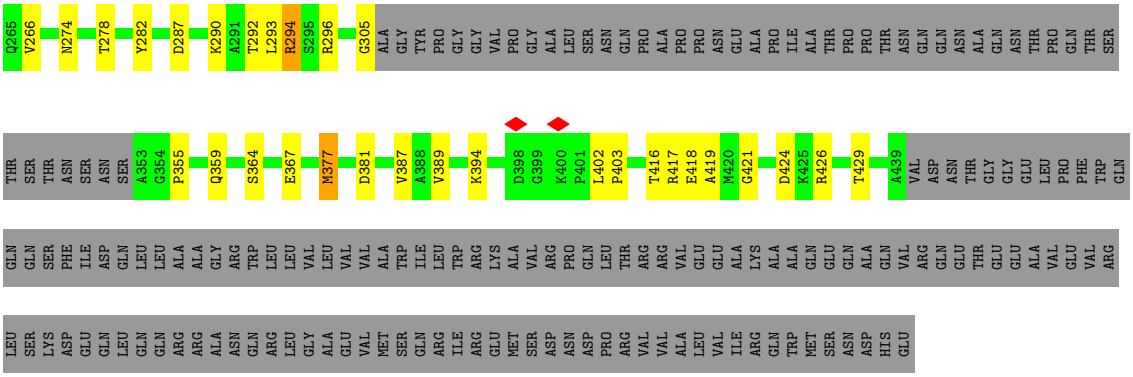
Chain 3:



• Molecule 1: Flagellar M-ring protein

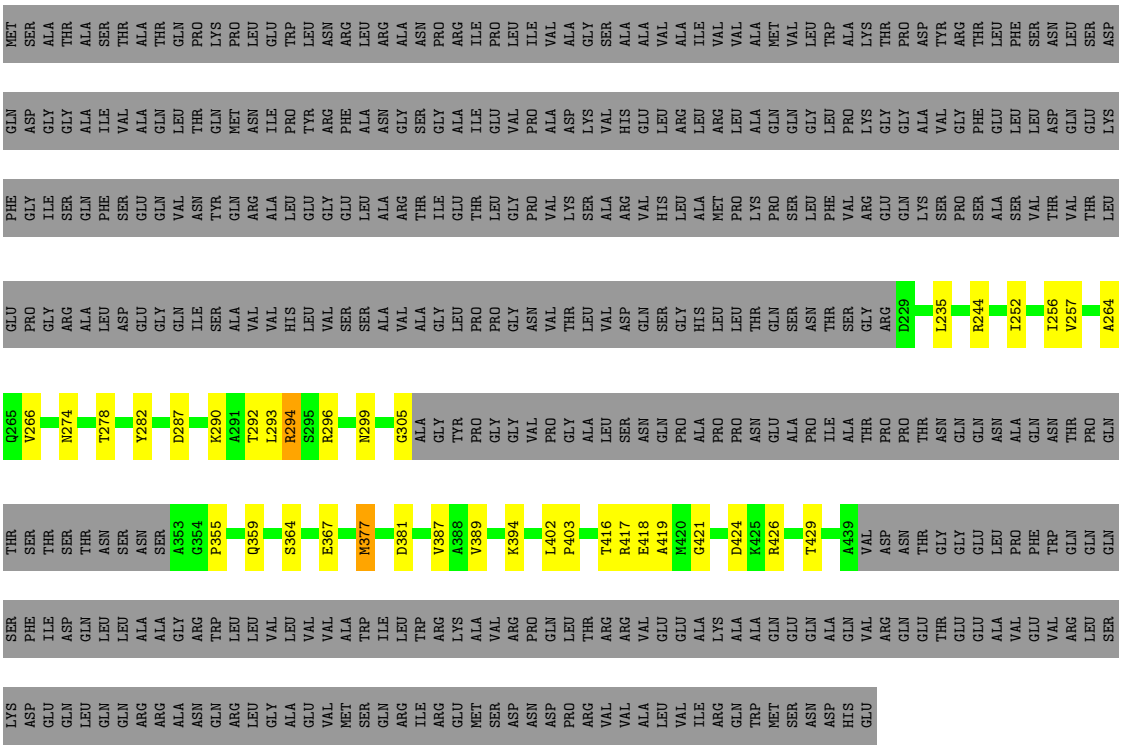
Chain 4:





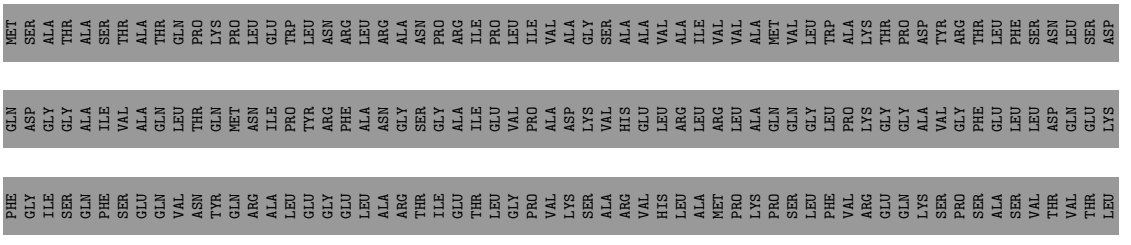
• Molecule 1: Flagellar M-ring protein

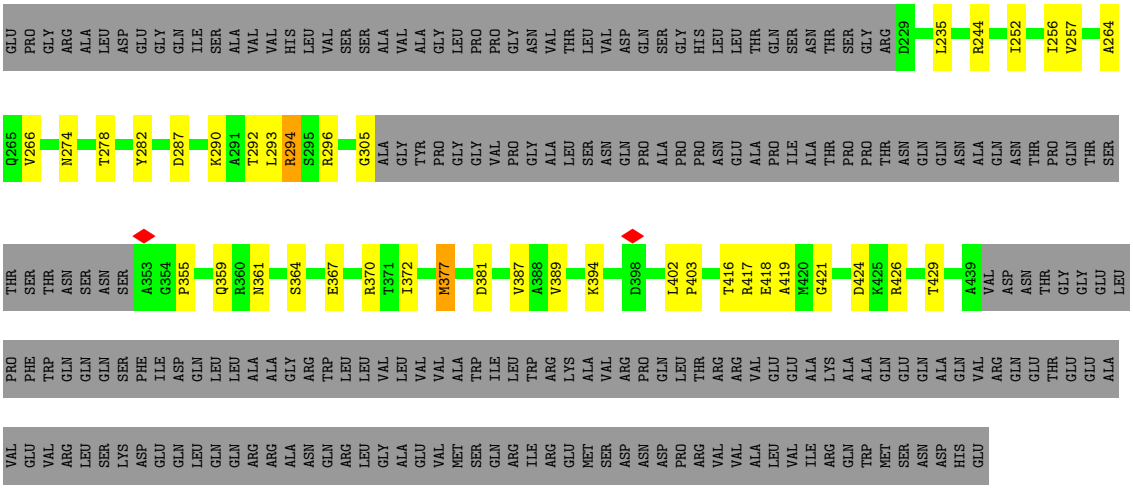
Chain 5:



• Molecule 1: Flagellar M-ring protein

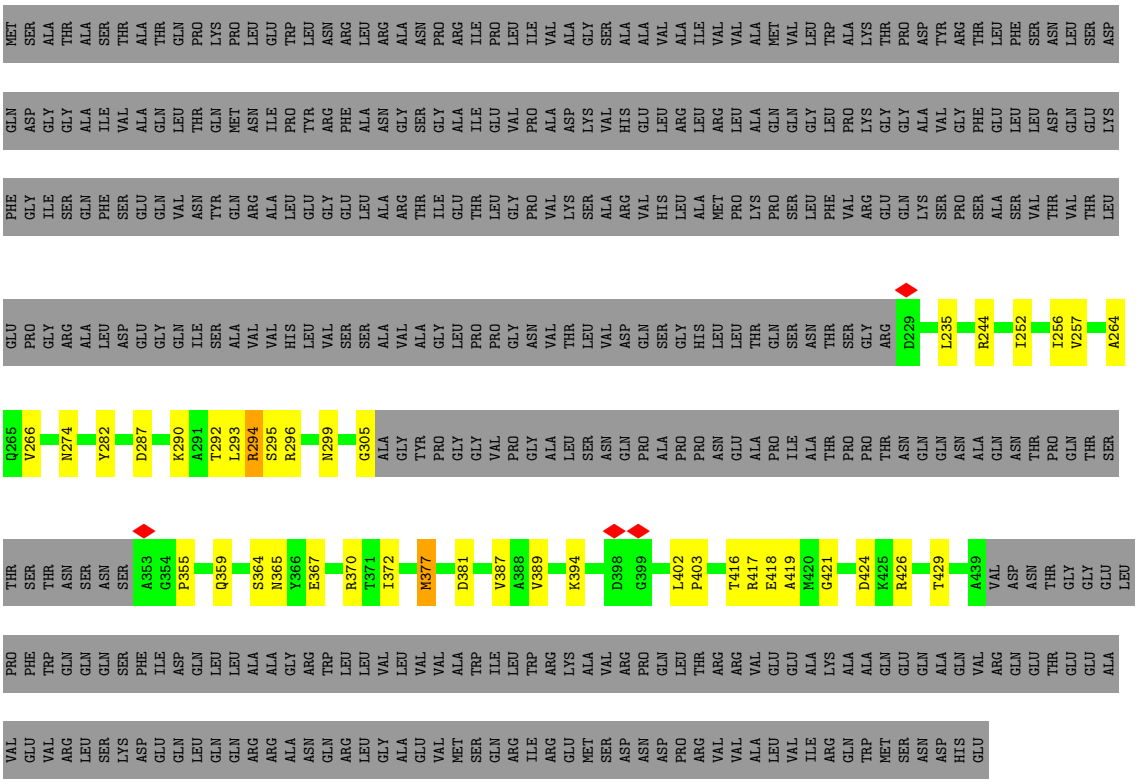
Chain 6:





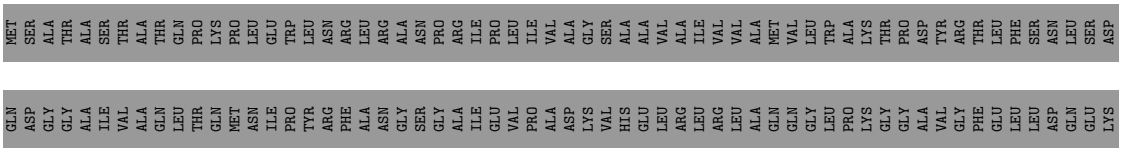
• Molecule 1: Flagellar M-ring protein

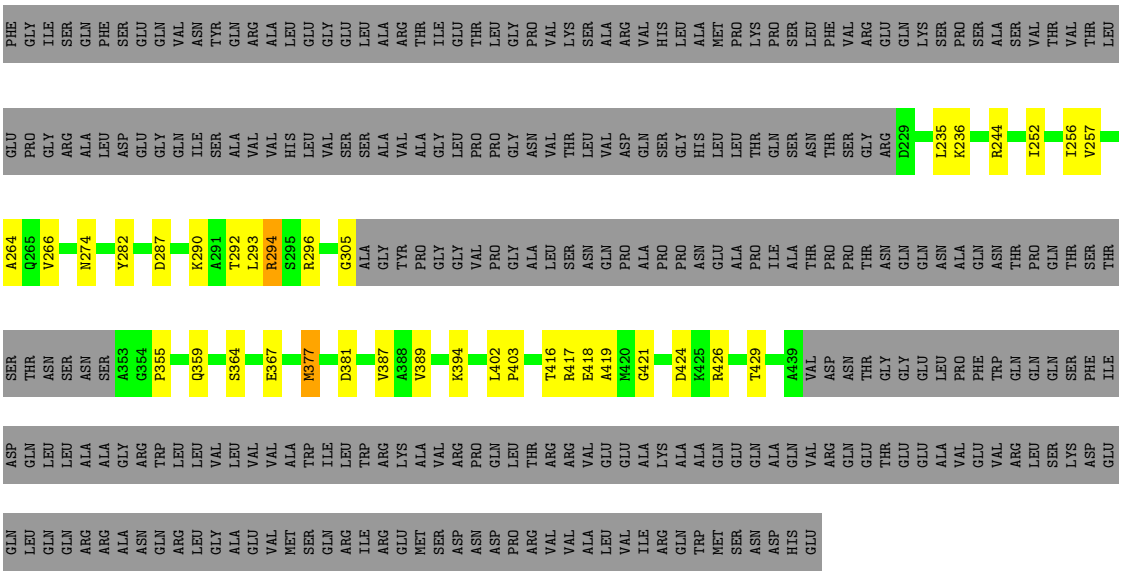
Chain 7:



• Molecule 1: Flagellar M-ring protein

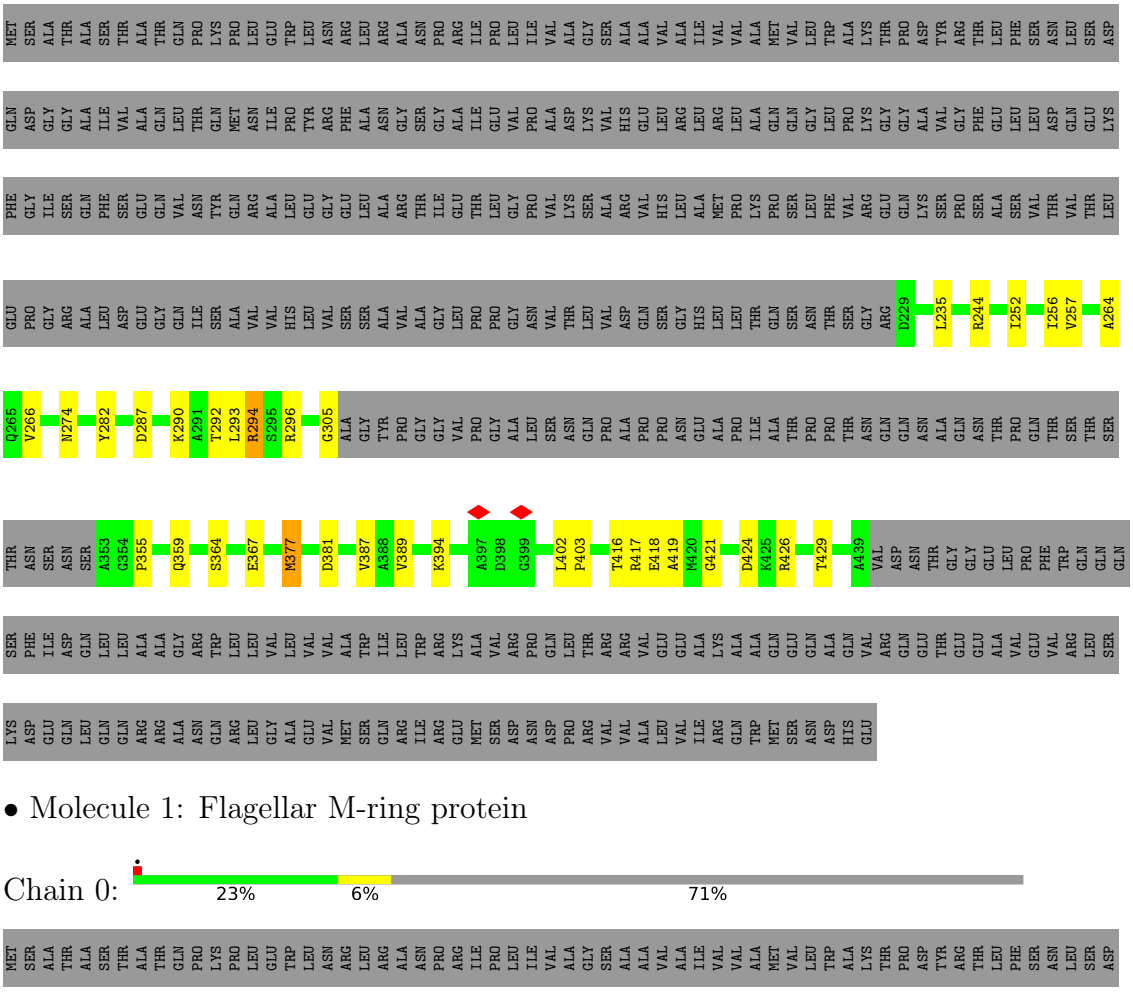
Chain 8:





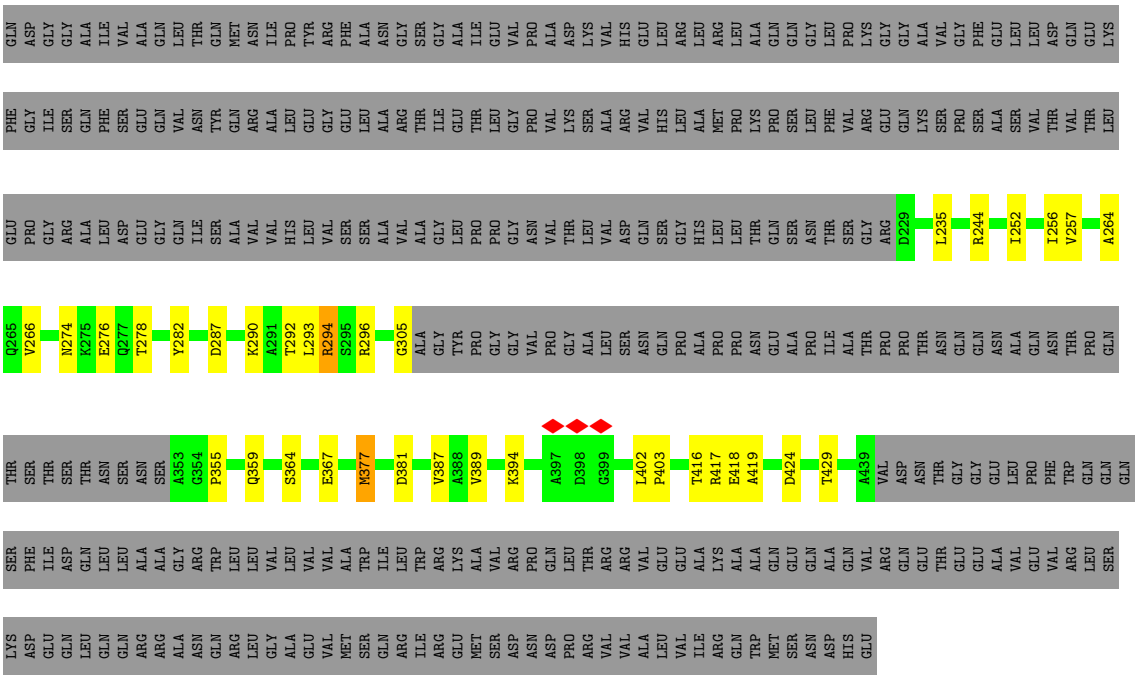
• Molecule 1: Flagellar M-ring protein

Chain 9:



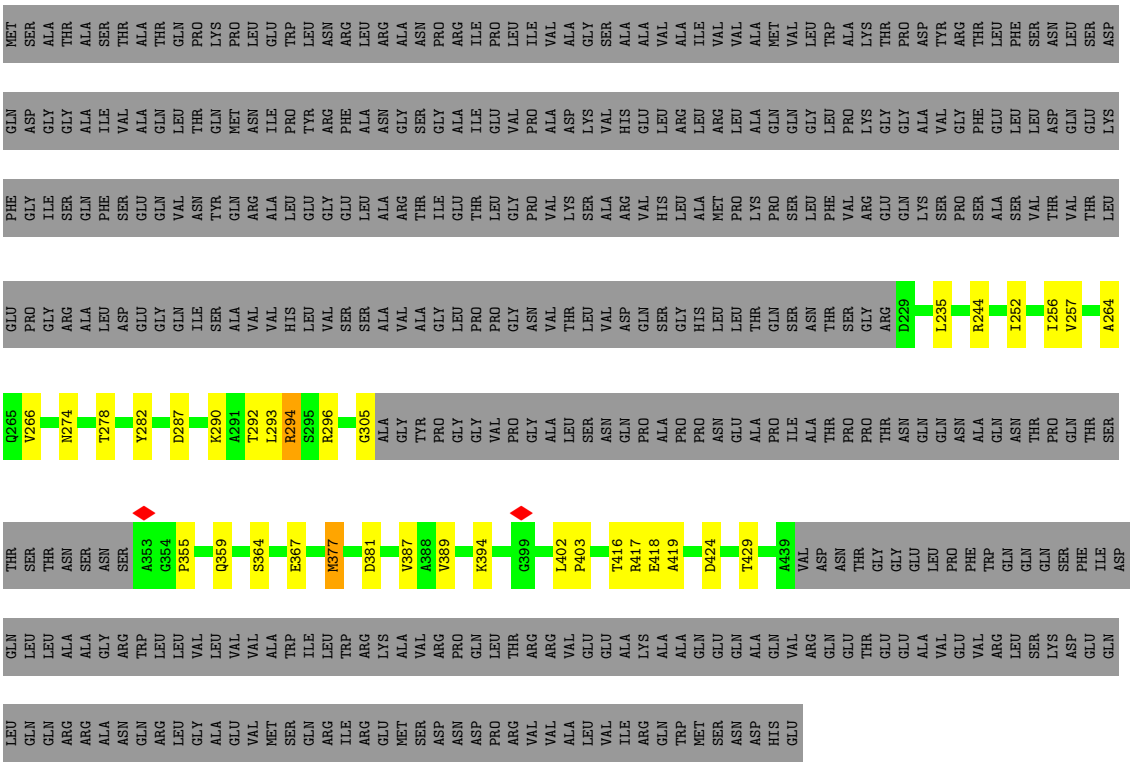
• Molecule 1: Flagellar M-ring protein

Chain 0:



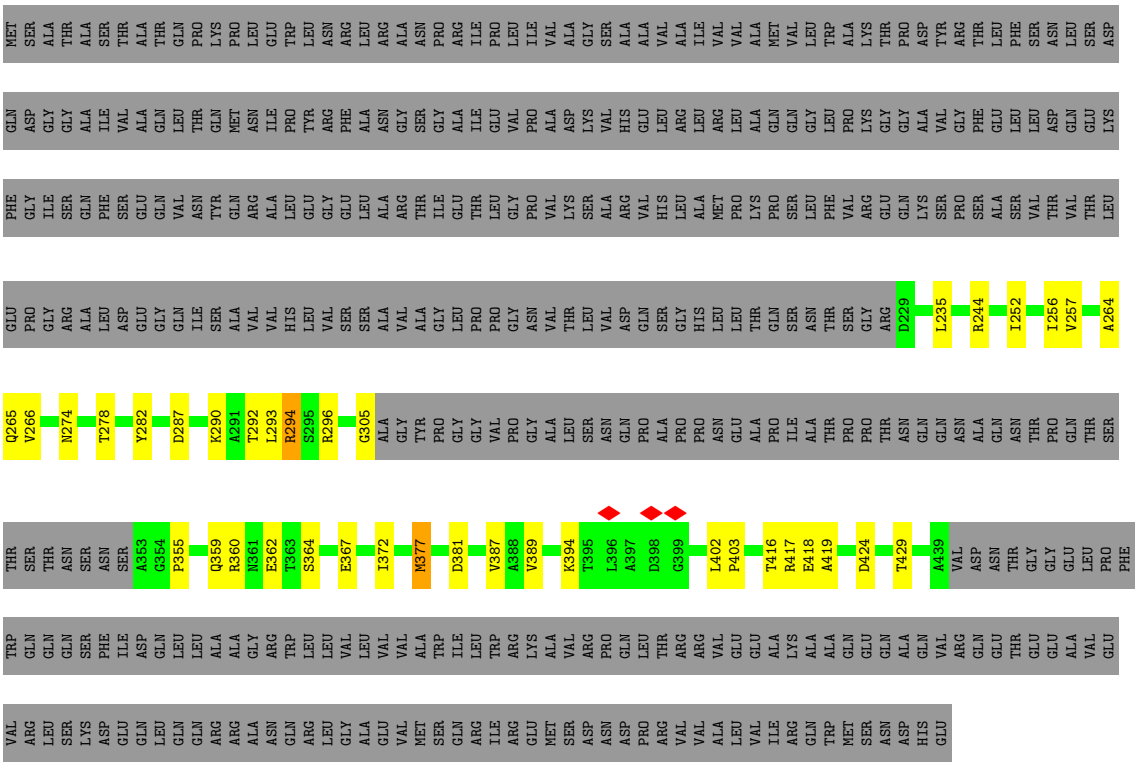
• Molecule 1: Flagellar M-ring protein

Chain AA:



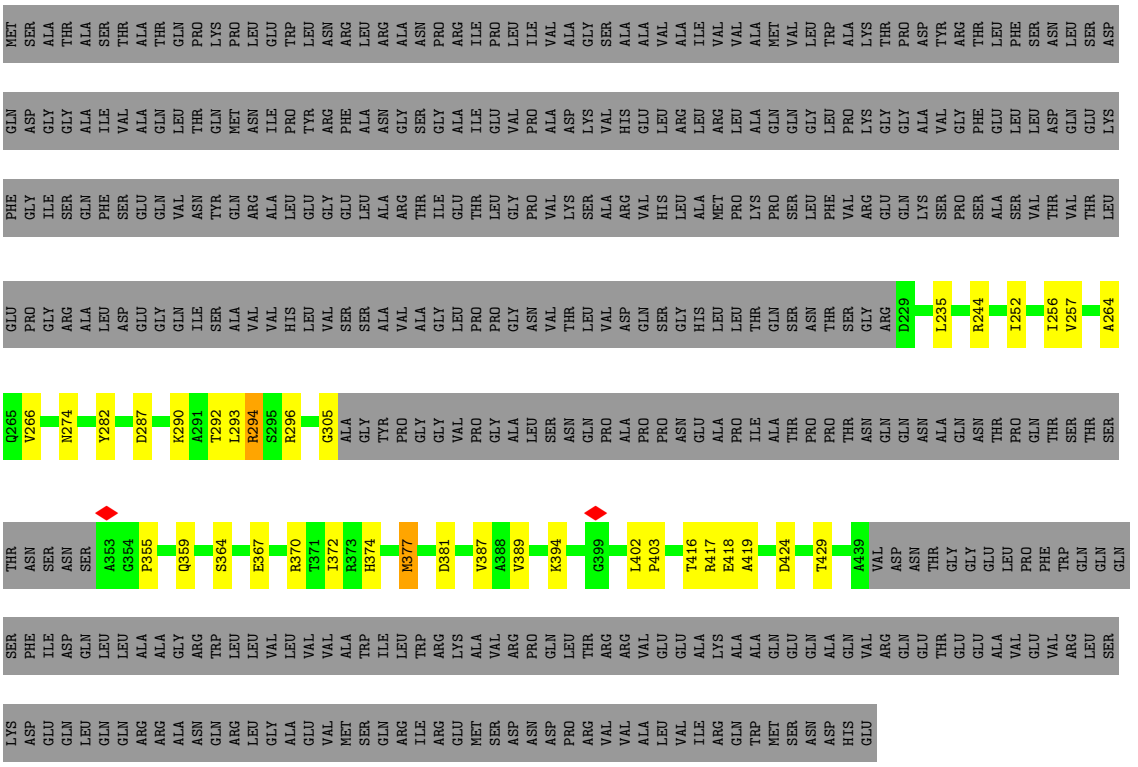
• Molecule 1: Flagellar M-ring protein

Chain AB:



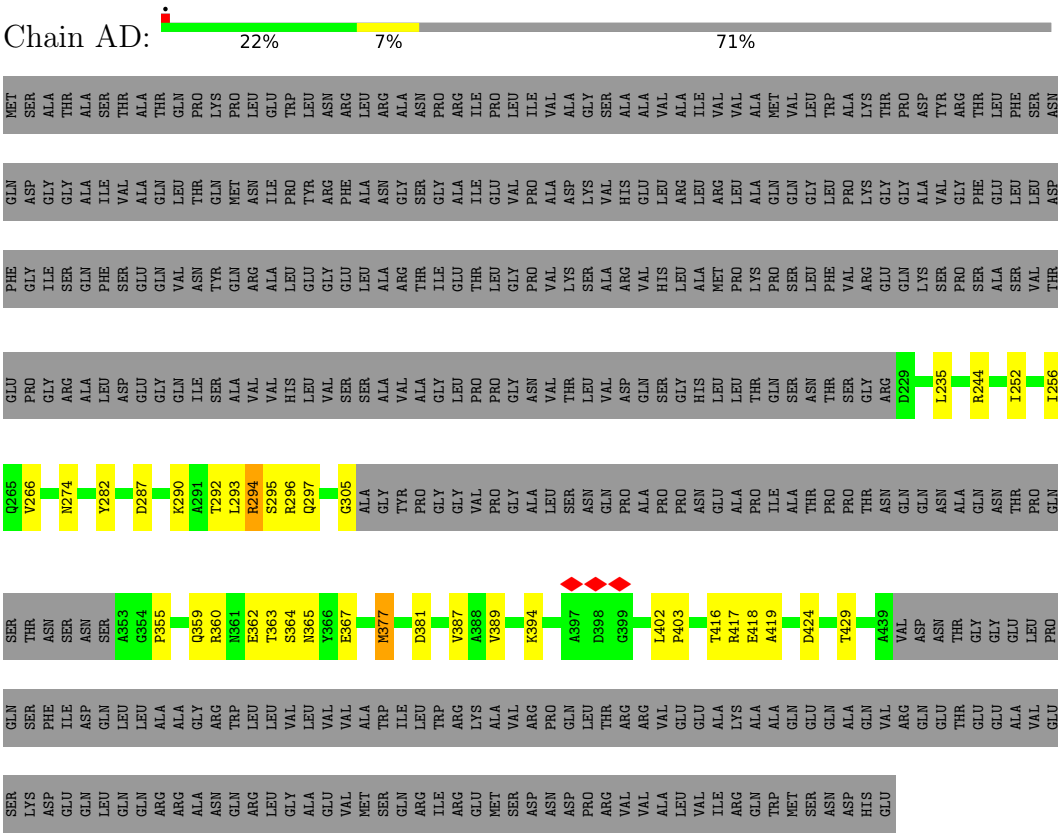
• Molecule 1: Flagellar M-ring protein

Chain AC:



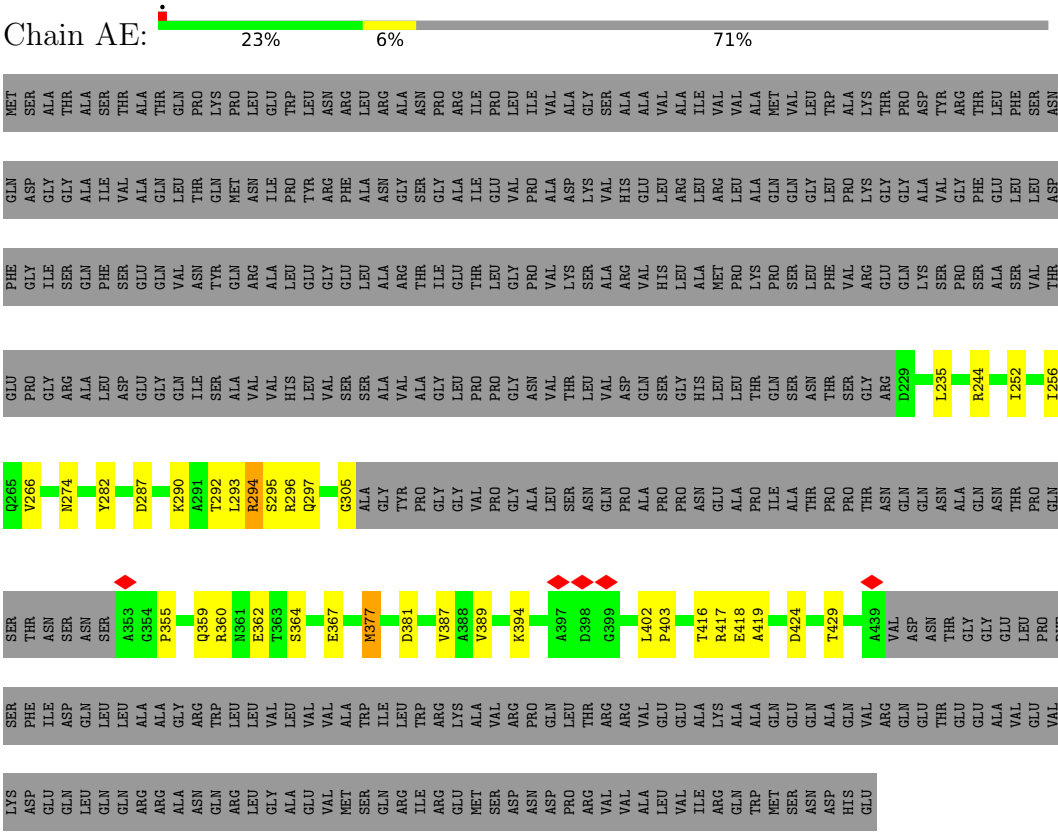
• Molecule 1: Flagellar M-ring protein

Chain AD:



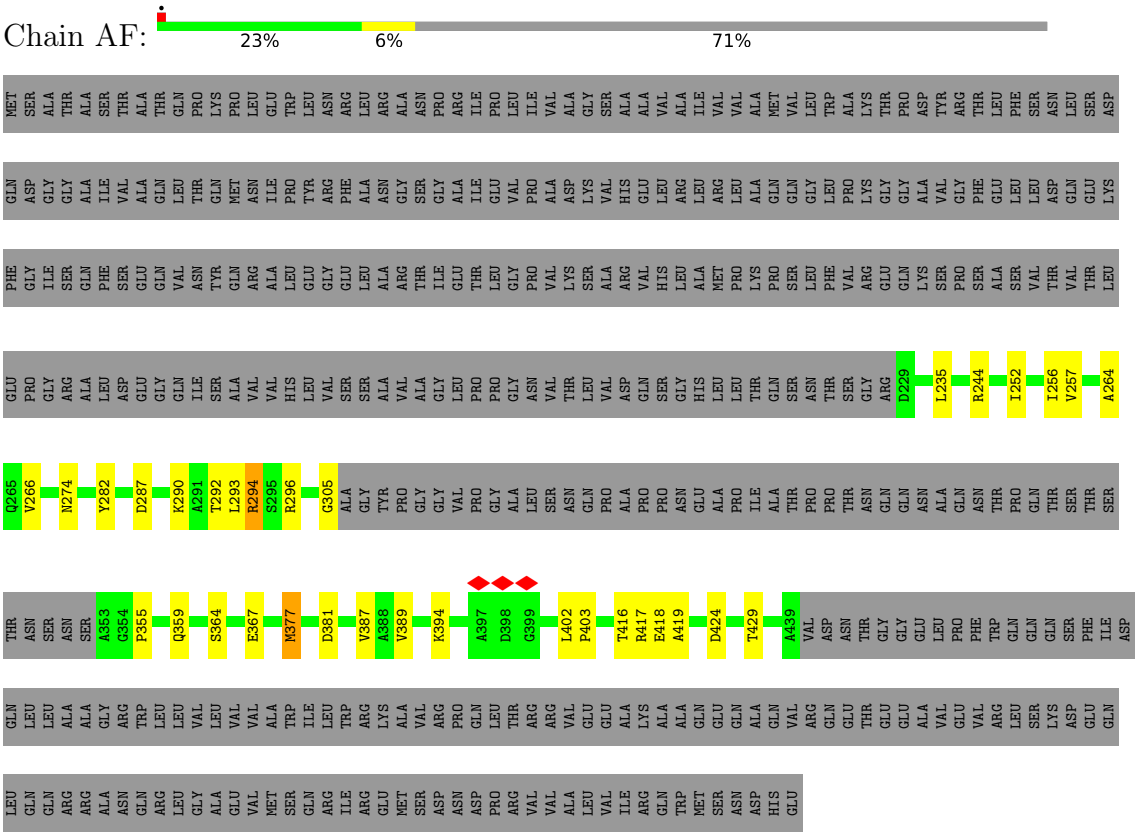
• Molecule 1: Flagellar M-ring protein

Chain AE:



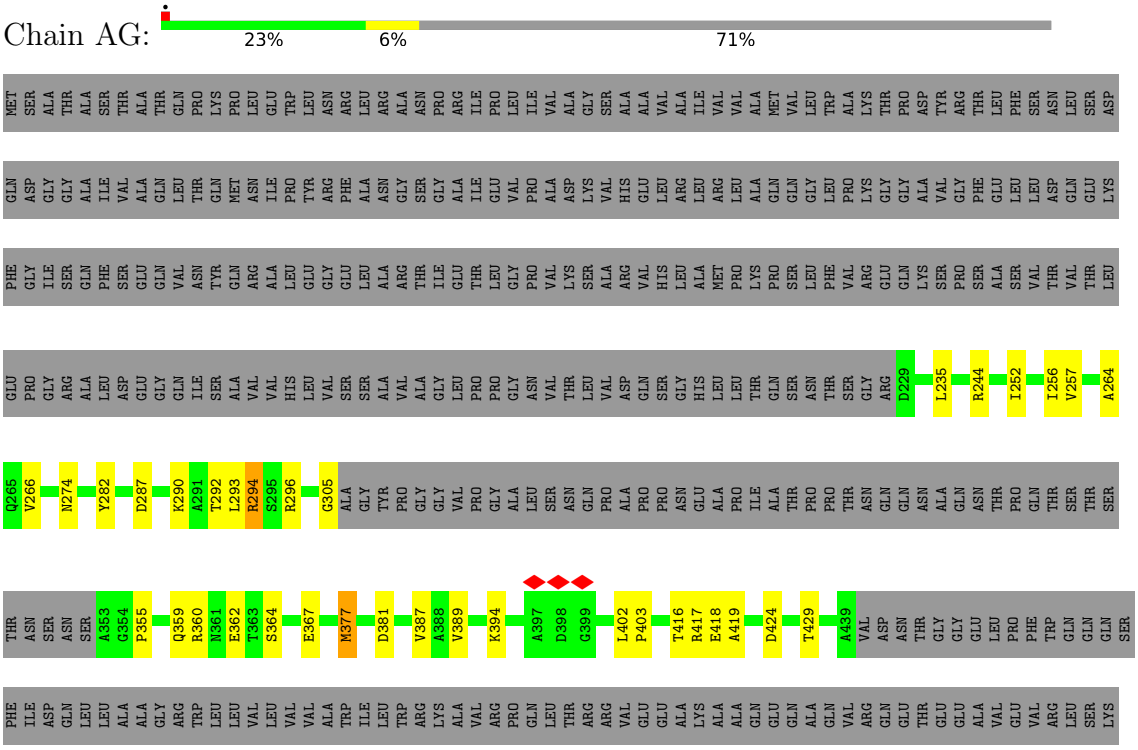
• Molecule 1: Flagellar M-ring protein

Chain AF:



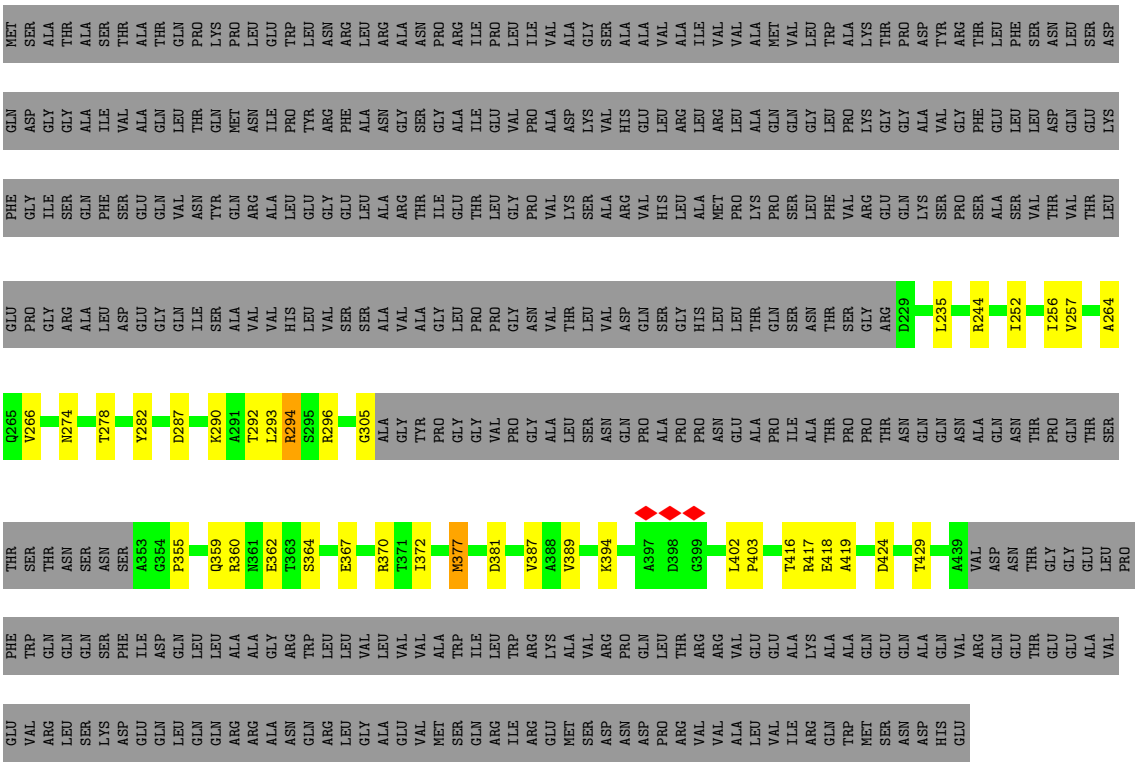
• Molecule 1: Flagellar M-ring protein

Chain AG:



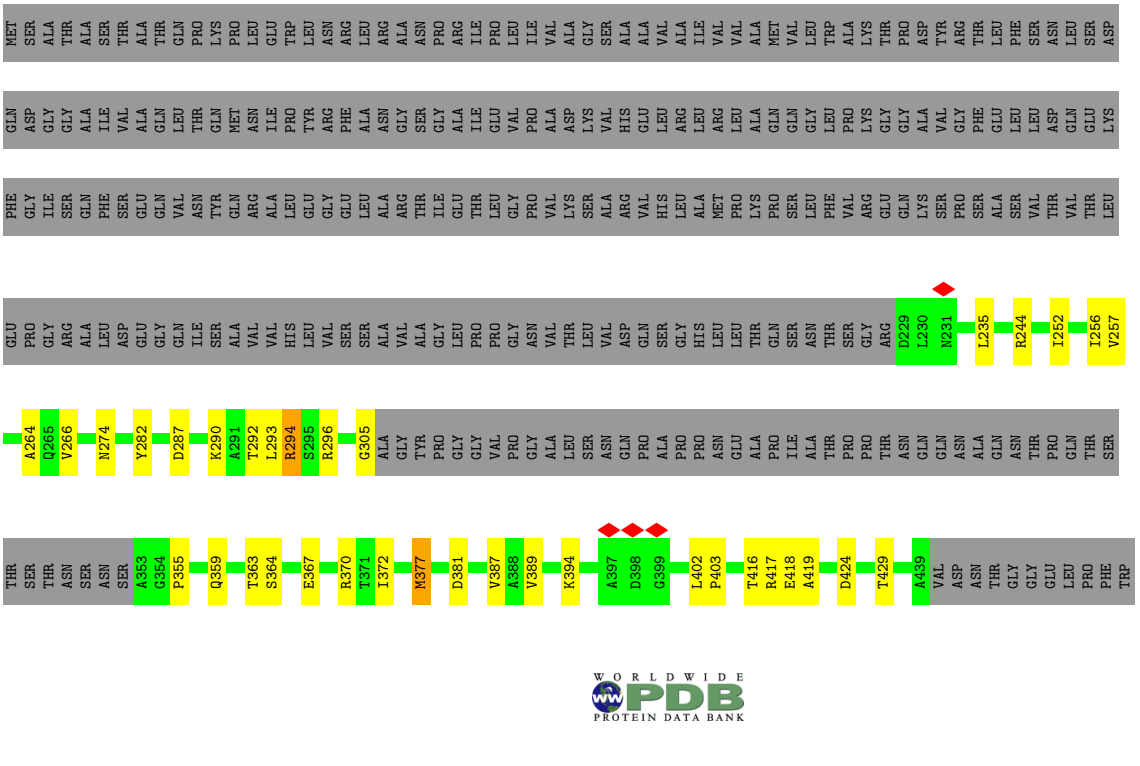
• Molecule 1: Flagellar M-ring protein

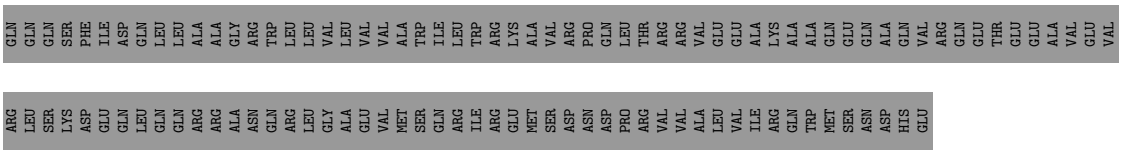
Chain AH:



• Molecule 1: Flagellar M-ring protein

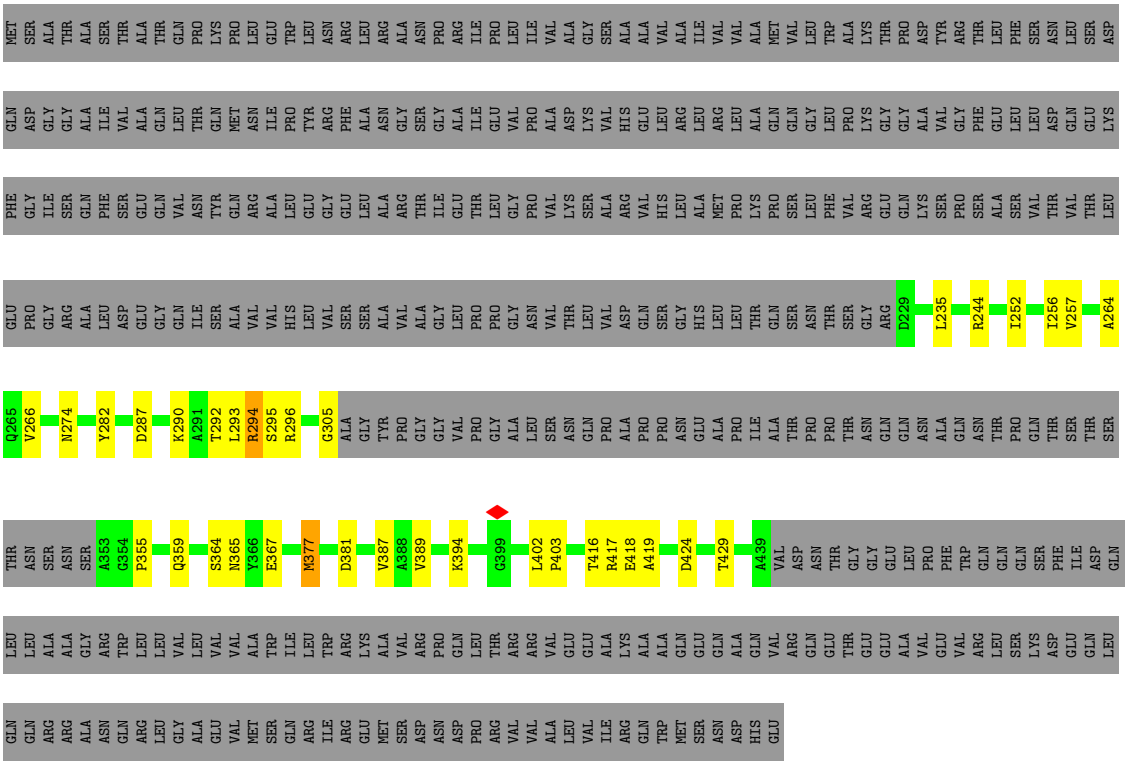
Chain AI:





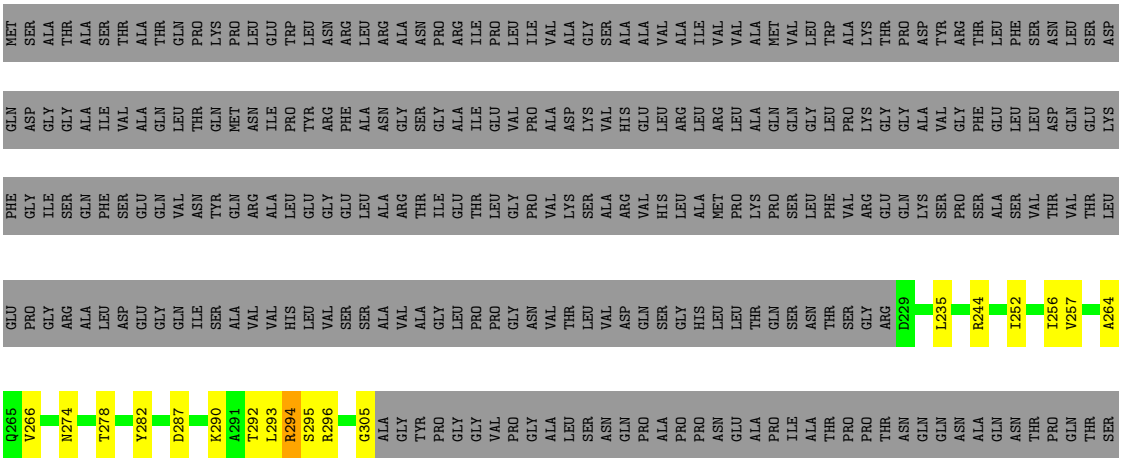
• Molecule 1: Flagellar M-ring protein

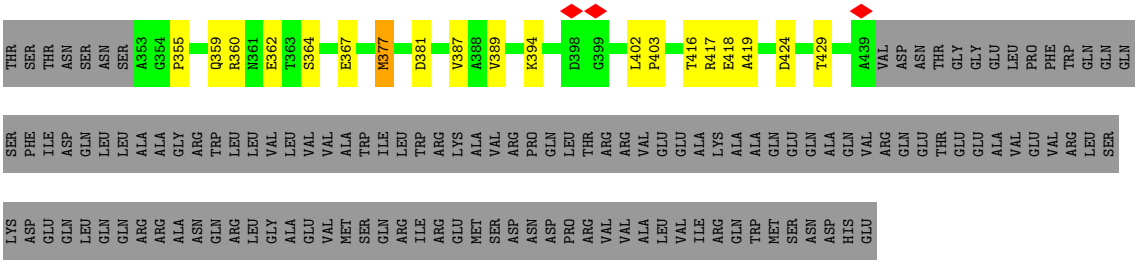
Chain AJ: 23% 6% 71%



• Molecule 1: Flagellar M-ring protein

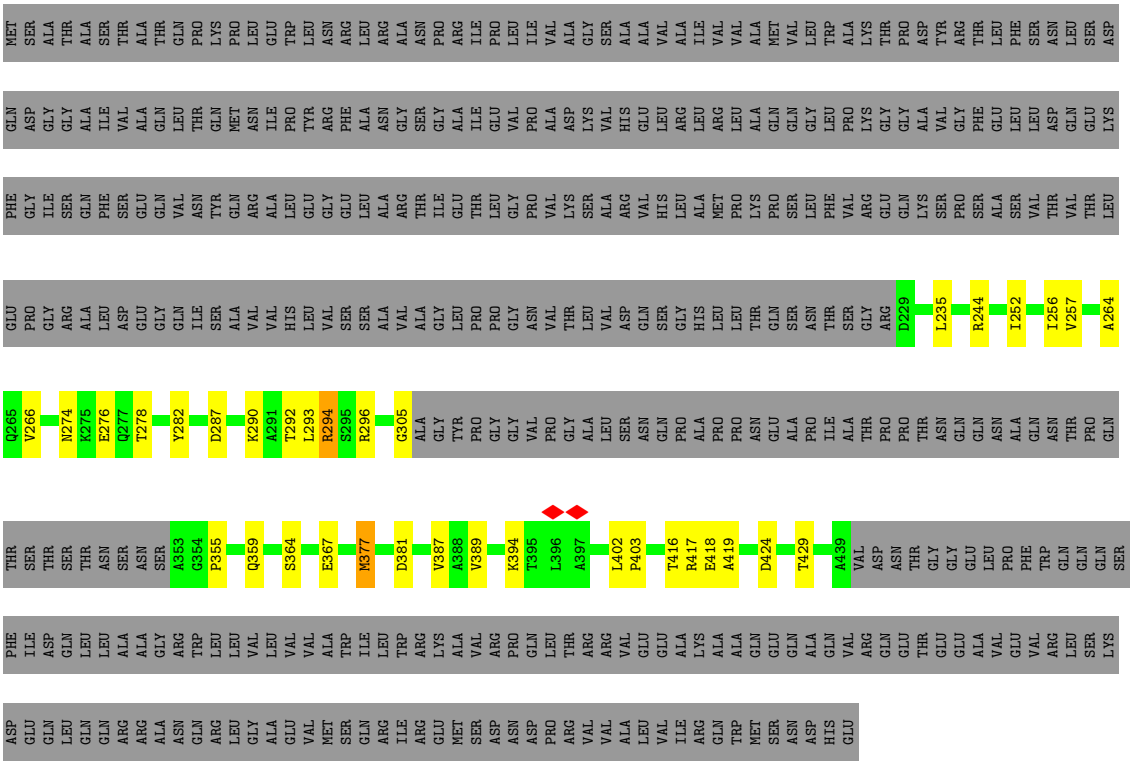
Chain AK: 23% 6% 71%





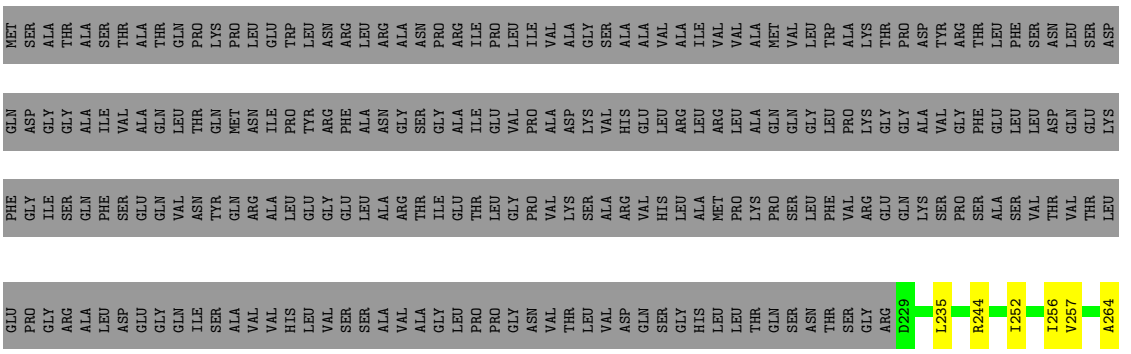
• Molecule 1: Flagellar M-ring protein

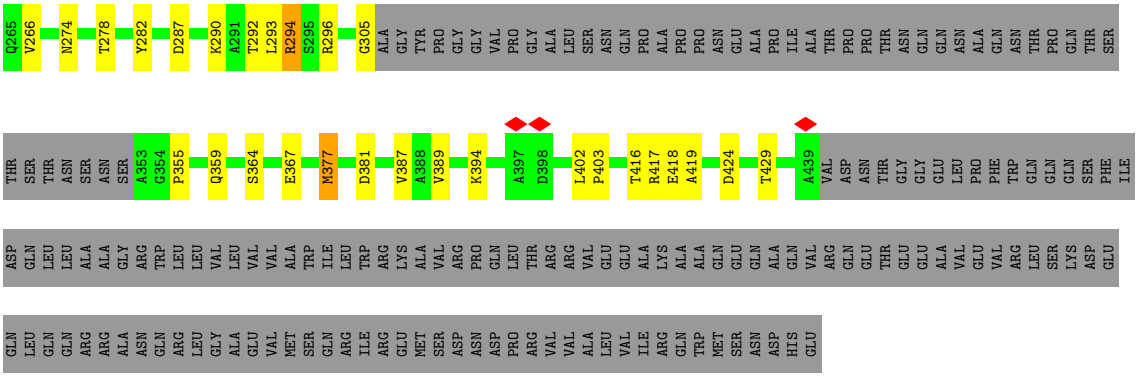
Chain AL:



• Molecule 1: Flagellar M-ring protein

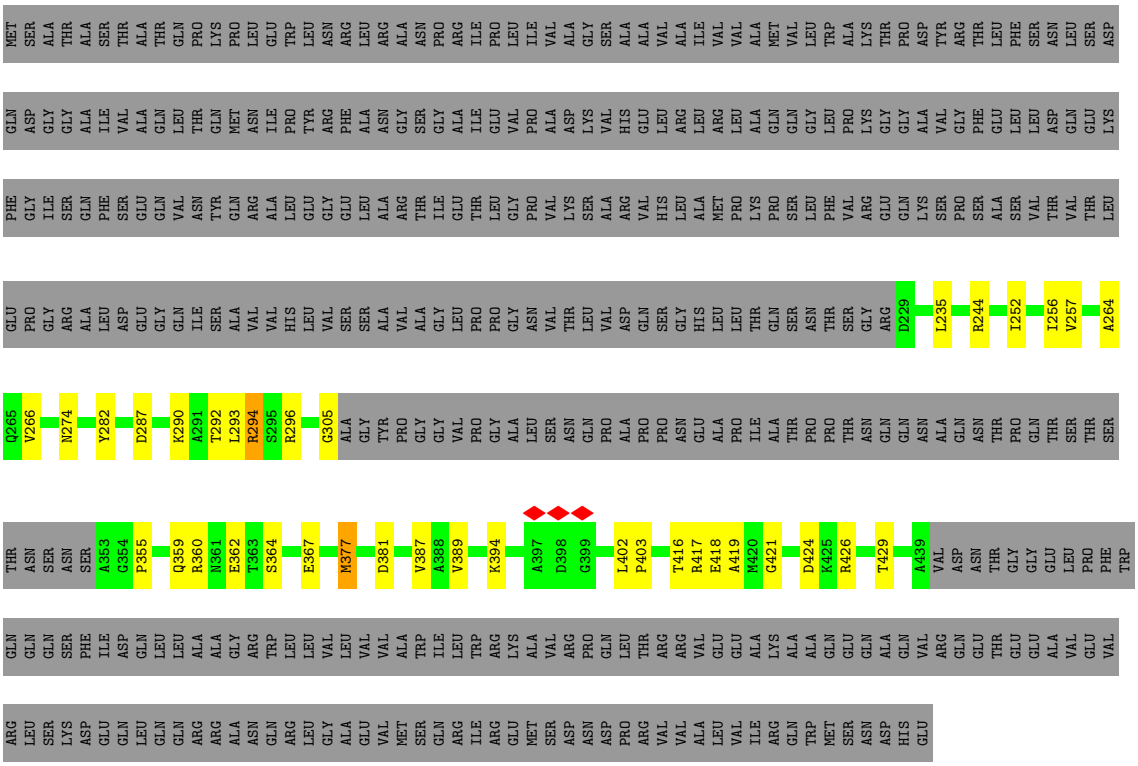
Chain AM:





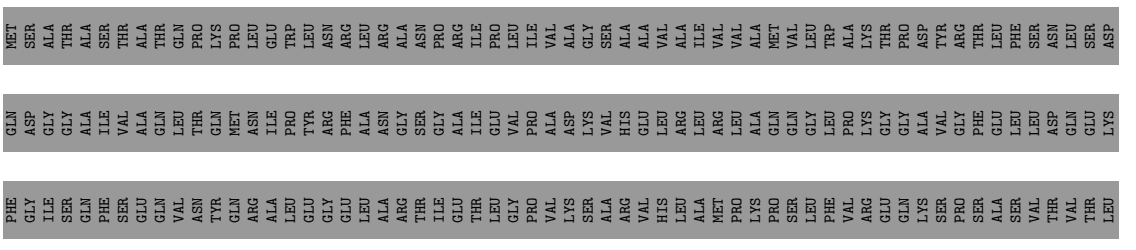
• Molecule 1: Flagellar M-ring protein

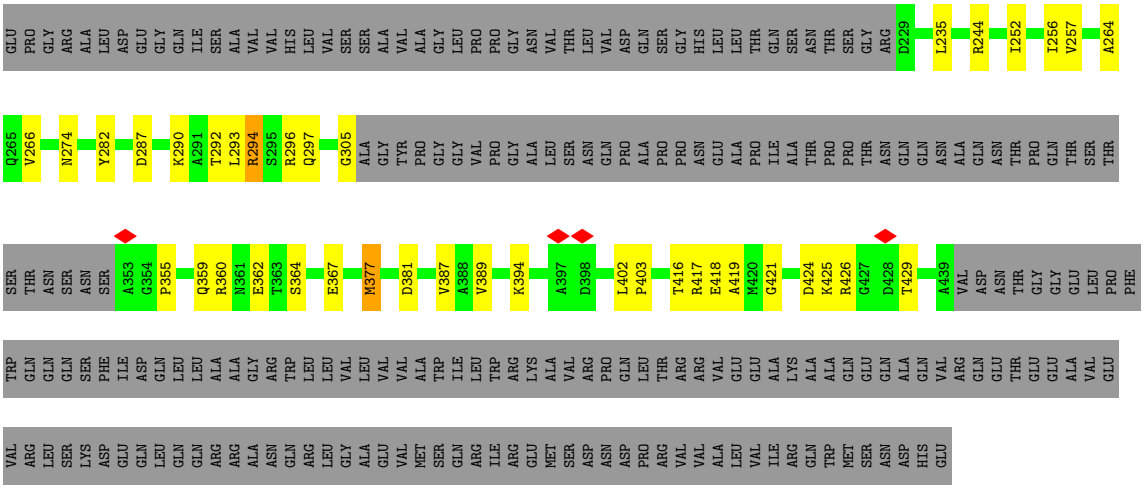
Chain AN:



• Molecule 1: Flagellar M-ring protein

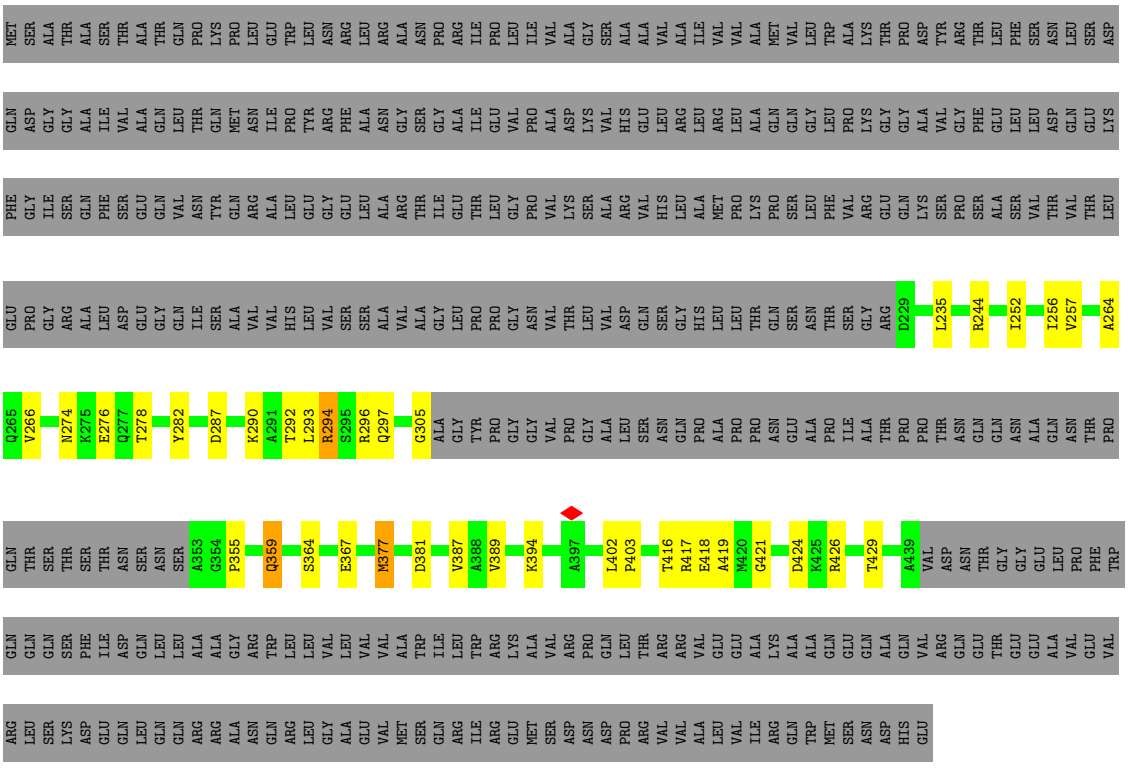
Chain AO:





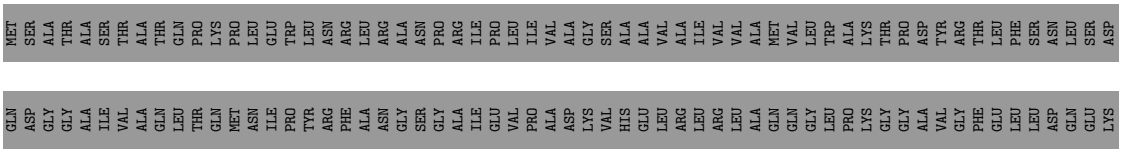
• Molecule 1: Flagellar M-ring protein

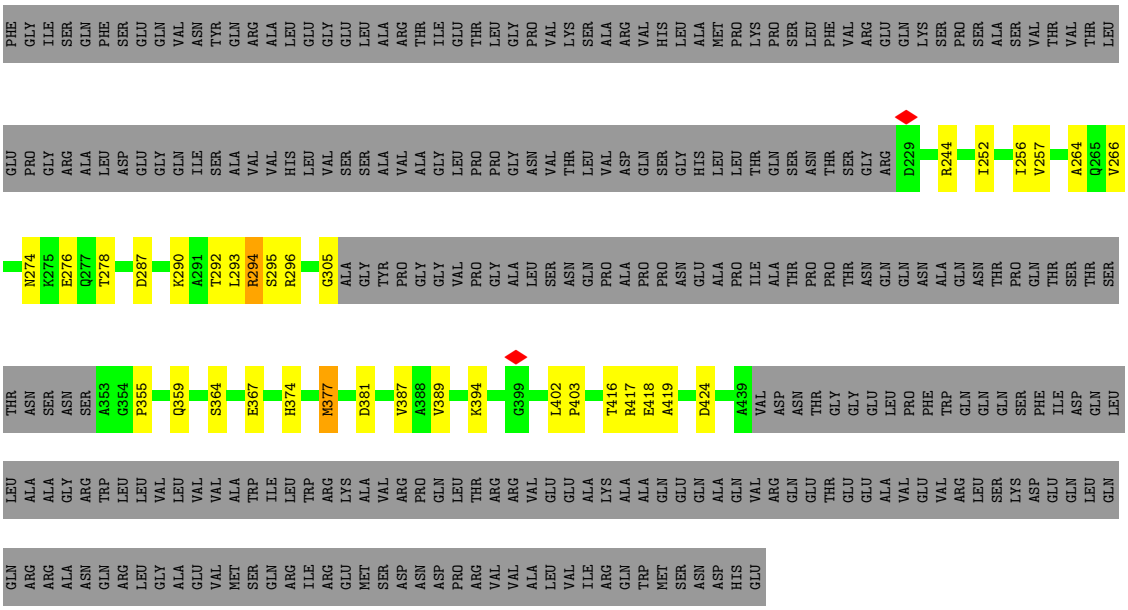
Chain AP:



• Molecule 1: Flagellar M-ring protein

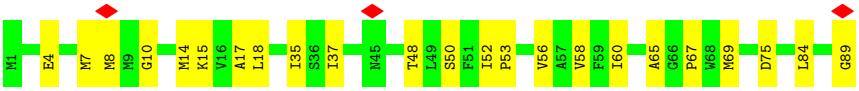
Chain AQ:





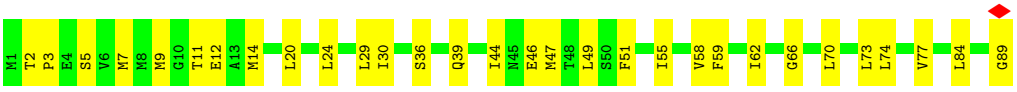
• Molecule 2: Flagellar biosynthetic protein FliQ

Chain A:



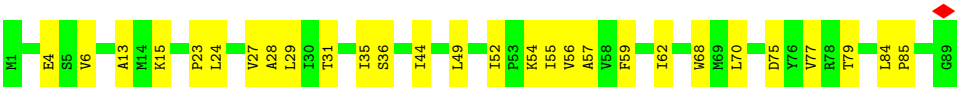
• Molecule 2: Flagellar biosynthetic protein FliQ

Chain B:



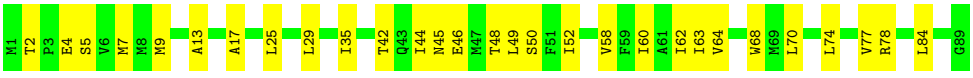
• Molecule 2: Flagellar biosynthetic protein FliQ

Chain C:



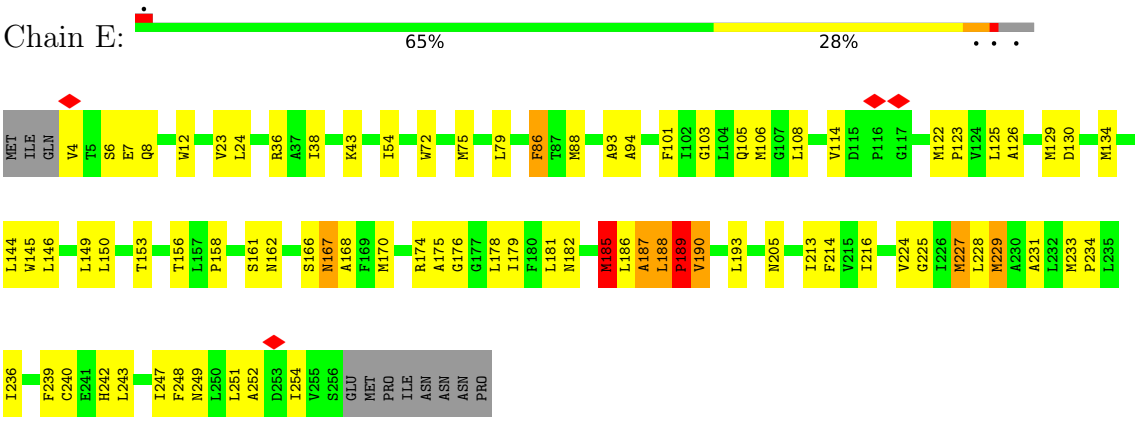
• Molecule 2: Flagellar biosynthetic protein FliQ

Chain D:



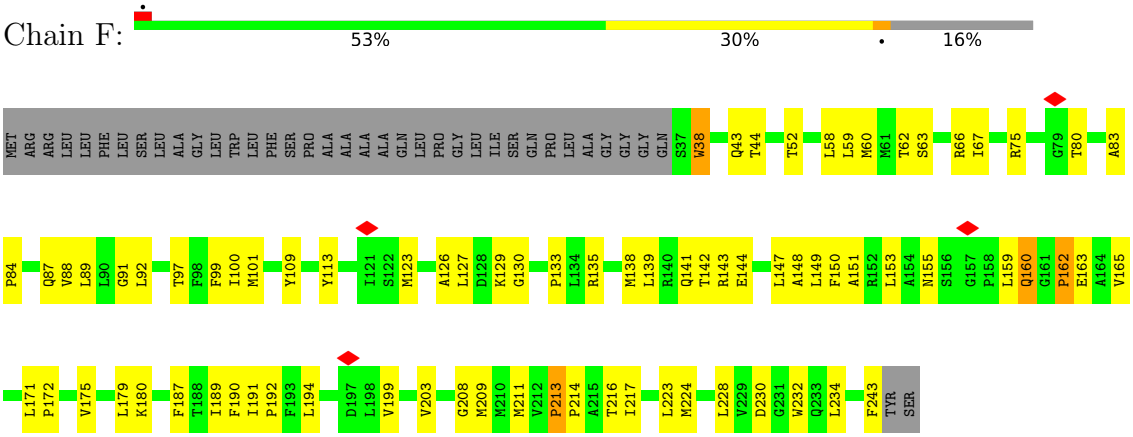
• Molecule 3: Flagellar biosynthetic protein FliR

Chain E:



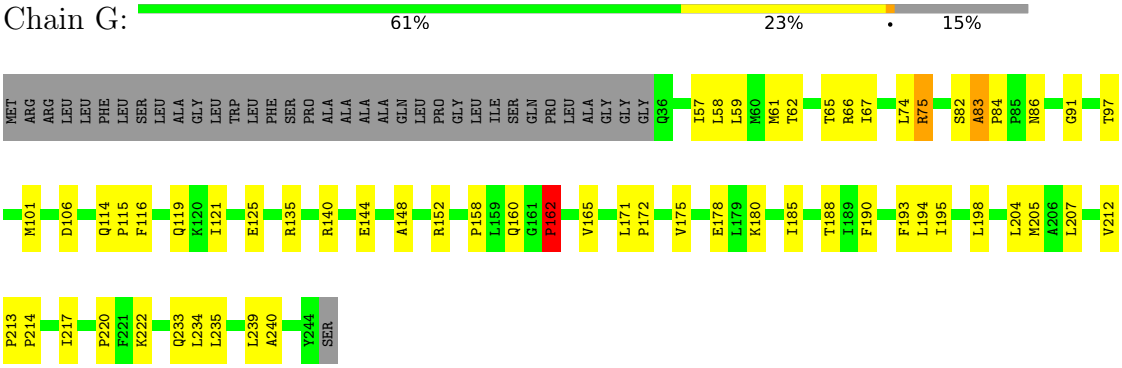
• Molecule 4: Flagellar biosynthetic protein FliP

Chain F:



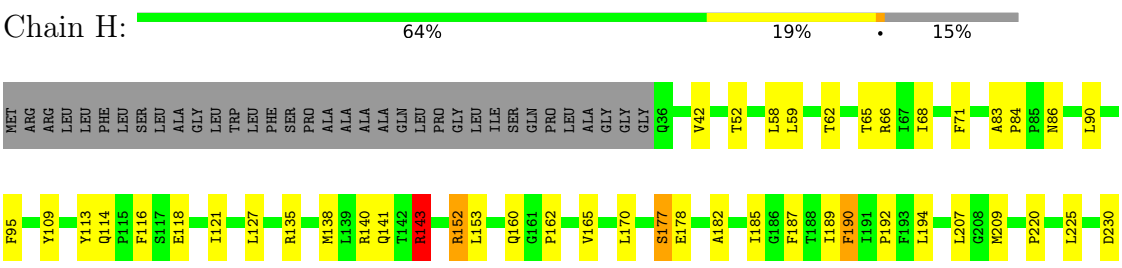
• Molecule 4: Flagellar biosynthetic protein FliP

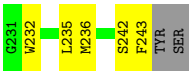
Chain G:



• Molecule 4: Flagellar biosynthetic protein FliP

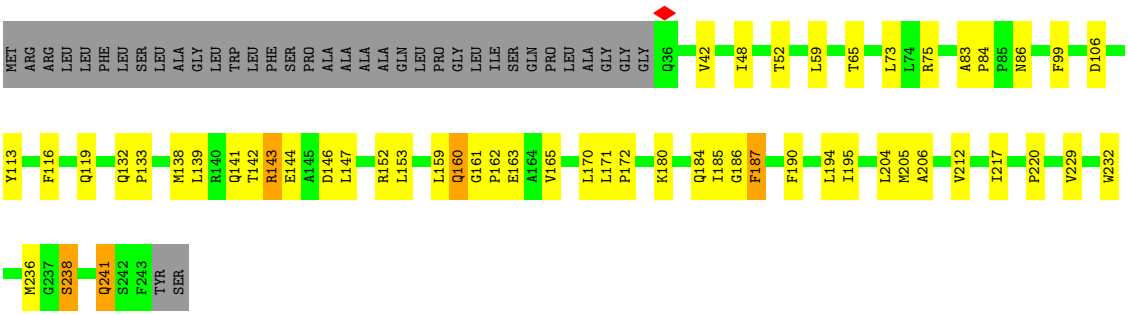
Chain H:





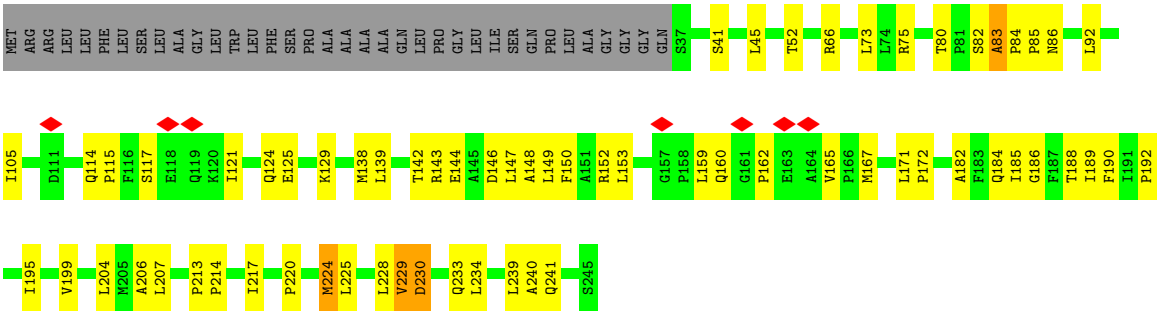
• Molecule 4: Flagellar biosynthetic protein FliP

Chain I:



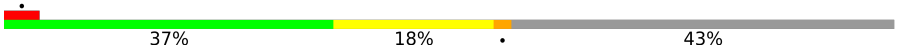
• Molecule 4: Flagellar biosynthetic protein FliP

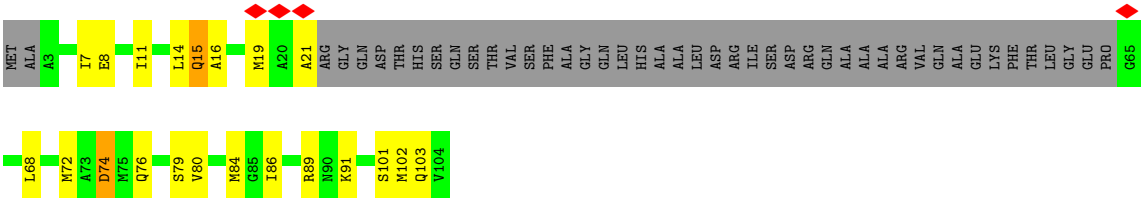
Chain J:



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

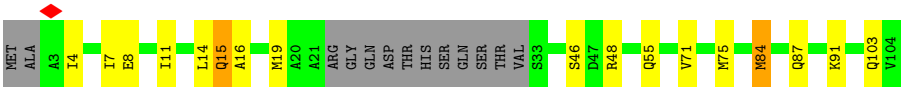
Chain K:





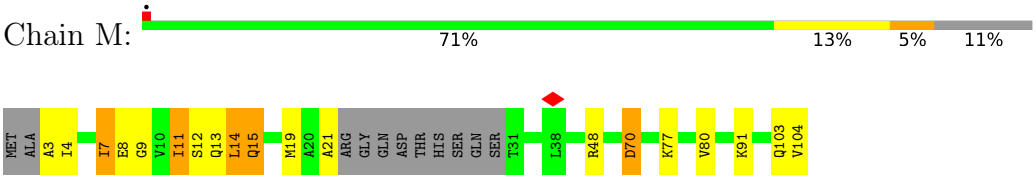
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain L:



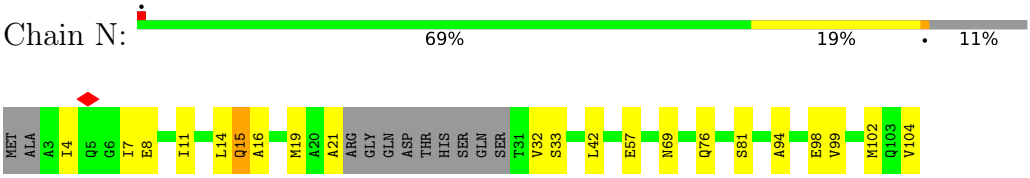
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain M:



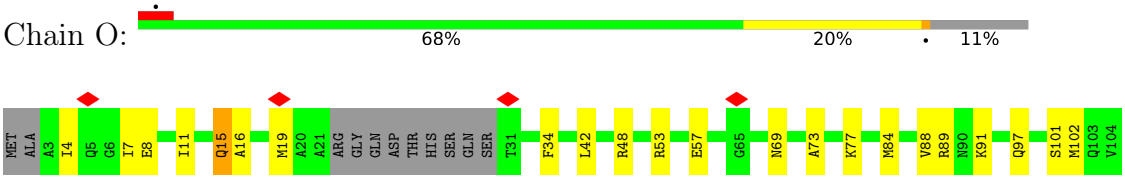
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain N:



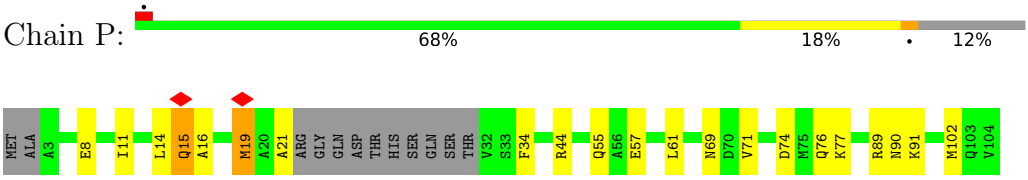
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain O:



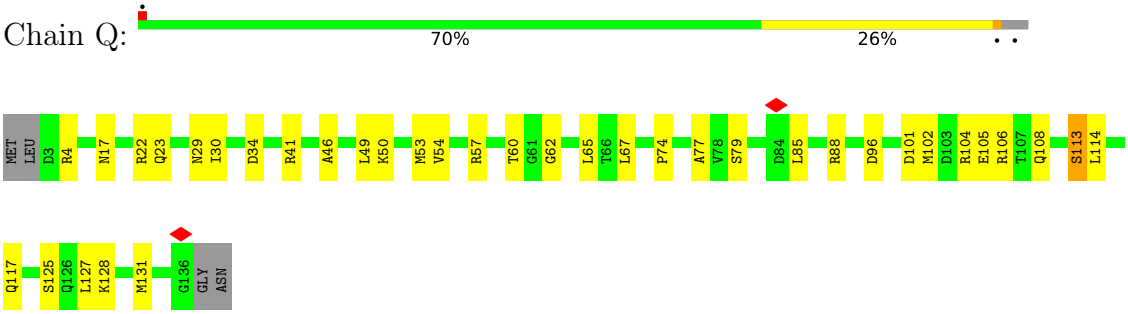
• Molecule 5: Flagellar hook-basal body complex protein FliE

Chain P:



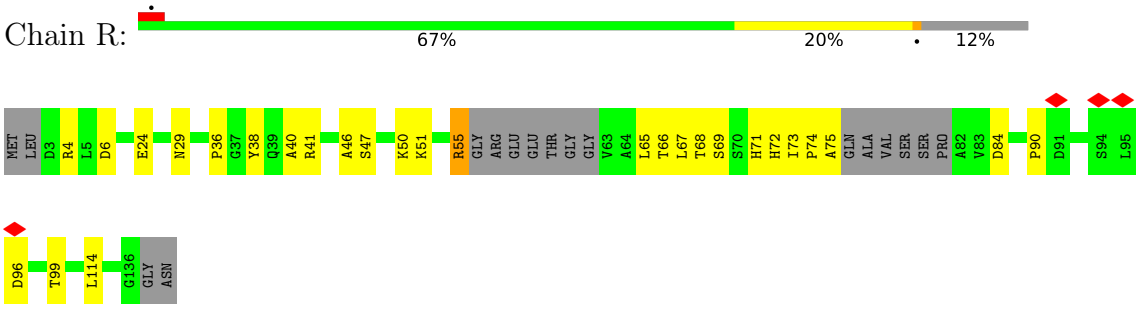
• Molecule 6: Flagellar basal body rod protein FlgB

Chain Q:



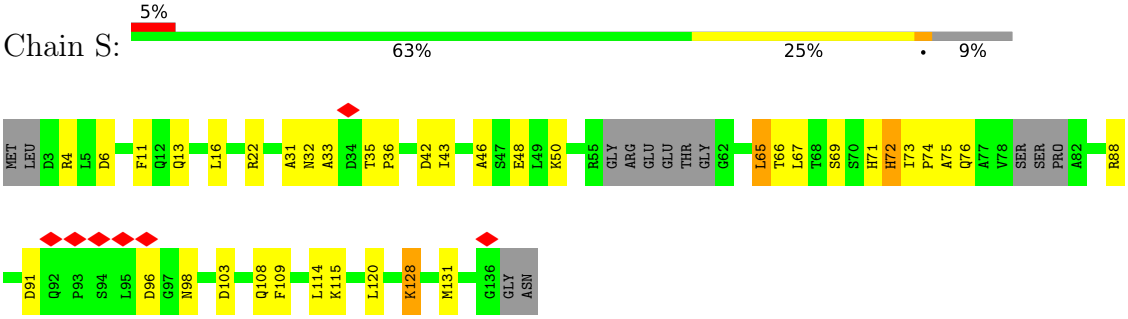
• Molecule 6: Flagellar basal body rod protein FlgB

Chain R:



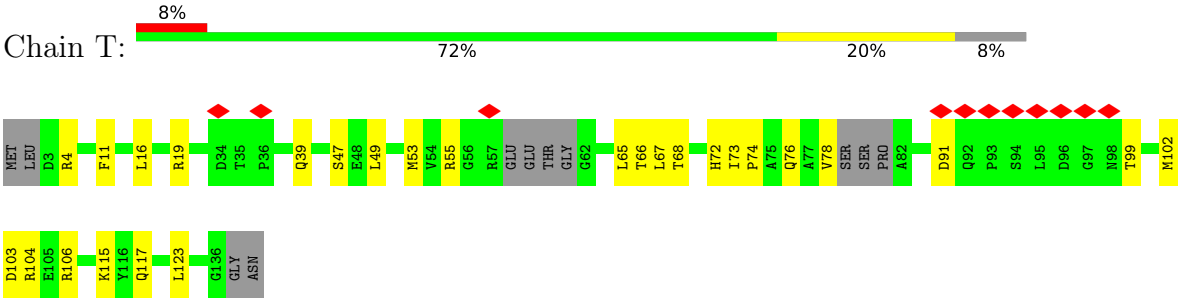
• Molecule 6: Flagellar basal body rod protein FlgB

Chain S:



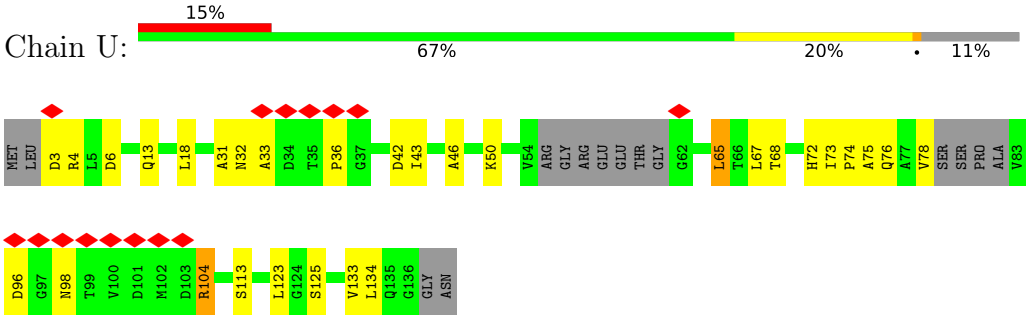
• Molecule 6: Flagellar basal body rod protein FlgB

Chain T:



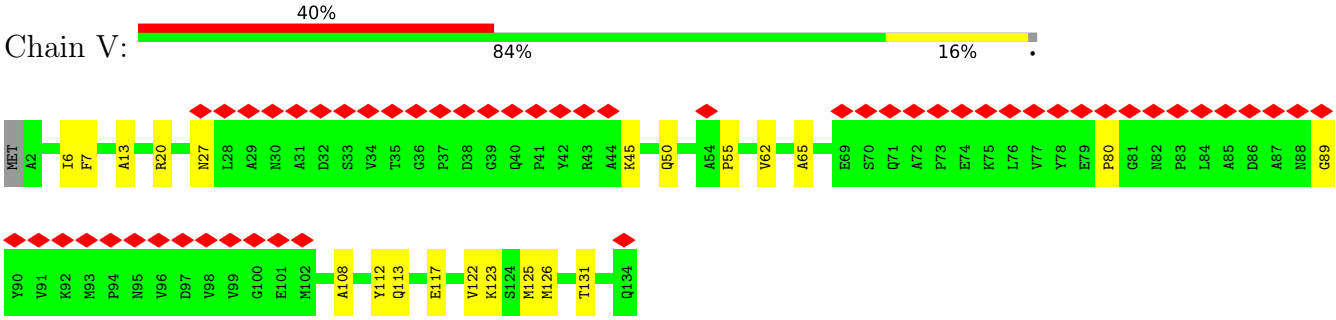
• Molecule 6: Flagellar basal body rod protein FlgB

Chain U:



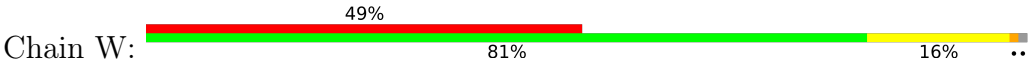
• Molecule 7: Flagellar basal-body rod protein FlgC

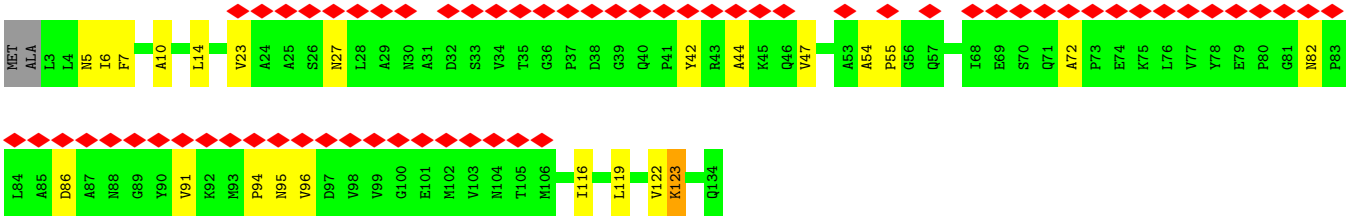
Chain V:



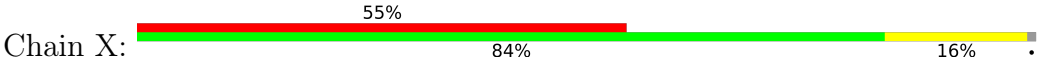
• Molecule 7: Flagellar basal-body rod protein FlgC

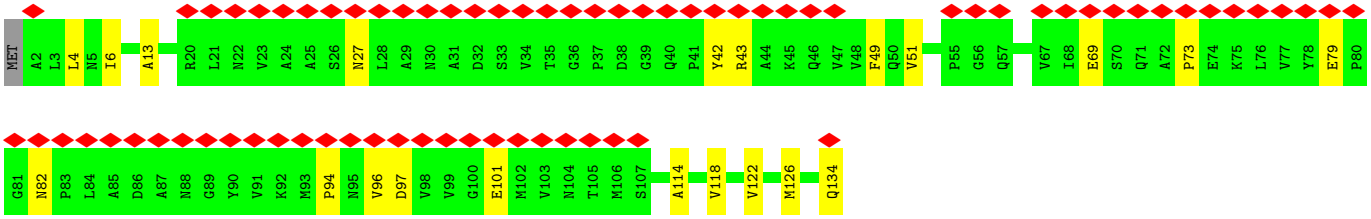
Chain W:



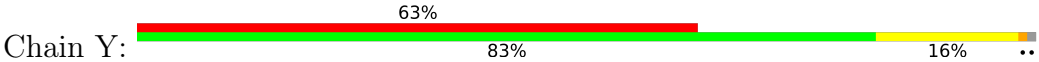


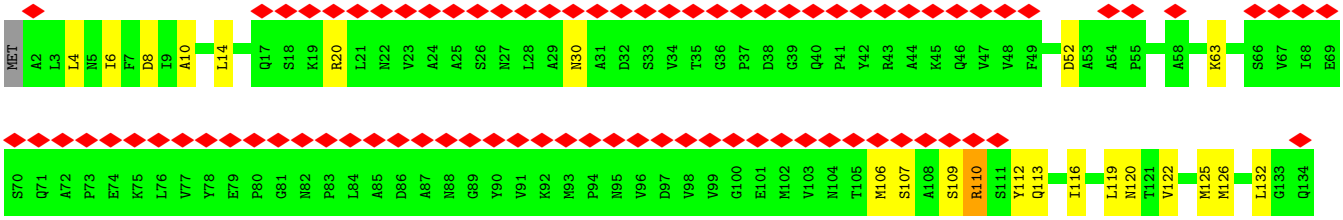
• Molecule 7: Flagellar basal-body rod protein FlgC



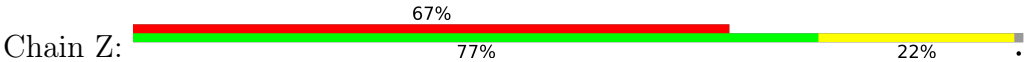


• Molecule 7: Flagellar basal-body rod protein FlgC

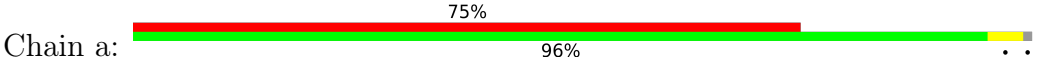


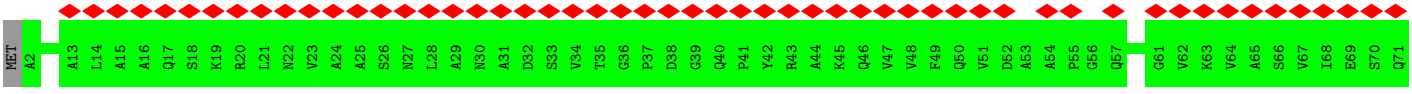


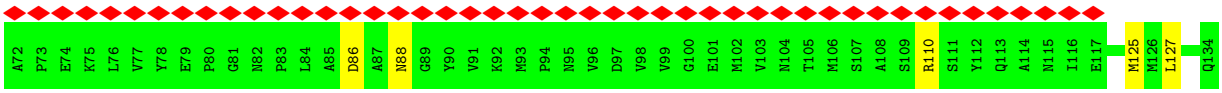
• Molecule 7: Flagellar basal-body rod protein FlgC



• Molecule 7: Flagellar basal-body rod protein FlgC






A72
P73
E74
K75
L76
V77
Y78
E79
P80
G81
N82
P83
L84
A85
D86
A87
N88
G89
Y90
V91
K92
M93
P94
N95
V96
D97
V98
V99
G100
E101
M102
V103
N104
T105
M106
S107
A108
S109
R110
S111
Y112
Q113
A114
N115
I116
E117
M125
M126
L127
Q134

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24190	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.867	Depositor
Minimum map value	-0.441	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	614.4, 614.4, 614.4	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.26	0/1289	0.53	0/1741
1	1	0.26	0/1289	0.53	0/1741
1	2	0.27	0/1289	0.53	0/1741
1	3	0.27	0/1289	0.53	0/1741
1	4	0.27	0/1289	0.53	0/1741
1	5	0.27	0/1289	0.53	0/1741
1	6	0.27	0/1289	0.53	0/1741
1	7	0.27	0/1289	0.53	0/1741
1	8	0.27	0/1289	0.53	0/1741
1	9	0.26	0/1289	0.53	0/1741
1	AA	0.27	0/1289	0.53	0/1741
1	AB	0.27	0/1289	0.53	0/1741
1	AC	0.27	0/1289	0.53	0/1741
1	AD	0.27	0/1289	0.53	0/1741
1	AE	0.27	0/1289	0.53	0/1741
1	AF	0.26	0/1289	0.53	0/1741
1	AG	0.27	0/1289	0.53	0/1741
1	AH	0.27	0/1289	0.53	0/1741
1	AI	0.26	0/1289	0.53	0/1741
1	AJ	0.27	0/1289	0.53	0/1741
1	AK	0.26	0/1289	0.53	0/1741
1	AL	0.27	0/1289	0.53	0/1741
1	AM	0.27	0/1289	0.53	0/1741
1	AN	0.26	0/1289	0.53	0/1741
1	AO	0.27	0/1289	0.53	0/1741
1	AP	0.27	0/1289	0.53	0/1741
1	AQ	0.26	0/1289	0.53	0/1741
1	UI	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UJ	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UK	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UL	0.82	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UM	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UN	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	UO	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	UP	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
1	WA	0.60	0/863	0.72	1/1172 (0.1%)
1	WB	0.59	0/850	0.69	0/1154
1	WC	0.59	0/825	0.68	0/1121
1	WD	0.61	0/841	0.68	0/1142
1	WE	0.60	0/857	0.71	0/1164
1	WF	0.60	0/848	0.69	0/1152
1	WG	0.60	0/857	0.68	0/1164
1	WH	0.60	0/714	0.69	0/973
1	WI	0.59	0/714	0.74	0/973
1	WJ	0.61	0/749	0.72	1/1020 (0.1%)
1	WK	0.60	0/741	0.69	0/1009
1	WL	0.60	0/631	0.70	0/860
1	WM	0.59	0/604	0.70	0/824
1	WN	0.60	0/619	0.70	0/844
1	WO	0.60	0/726	0.72	1/989 (0.1%)
1	WP	0.60	0/753	0.69	0/1025
1	WQ	0.60	0/848	0.69	0/1152
1	WR	0.60	0/848	0.69	0/1152
1	WS	0.60	0/848	0.69	0/1152
1	WT	0.60	0/848	0.70	0/1152
1	WU	0.60	0/857	0.67	0/1164
1	WV	0.61	0/841	0.69	0/1142
1	WW	0.60	0/848	0.70	0/1152
1	b	0.52	0/83	0.63	0/114
1	c	0.26	0/107	0.38	0/148
1	d	0.31	0/137	0.49	0/191
1	e	0.28	0/107	0.56	0/148
1	f	1.36	1/145 (0.7%)	1.49	3/203 (1.5%)
1	g	0.33	0/107	0.51	0/148
1	h	0.26	0/145	0.44	0/203
1	i	0.30	0/107	0.38	0/148
1	j	0.30	0/137	0.57	0/191
1	k	0.30	0/107	0.37	0/148
1	l	0.29	0/145	0.45	0/203
1	t	0.26	0/1289	0.53	0/1741
1	u	0.26	0/1289	0.53	0/1741
1	v	0.27	0/1289	0.53	0/1741
1	w	0.27	0/1289	0.53	0/1741
1	x	0.27	0/1289	0.53	0/1741
1	y	0.26	0/1289	0.53	0/1741
1	z	0.27	0/1289	0.53	0/1741
2	A	0.29	0/681	0.47	0/930

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	B	0.26	0/681	0.49	0/930
2	C	0.28	0/681	0.48	0/930
2	D	0.29	0/681	0.49	0/930
3	E	0.38	1/1994 (0.1%)	0.56	1/2724 (0.0%)
4	F	0.36	0/1643	0.62	2/2237 (0.1%)
4	G	0.29	0/1665	0.49	1/2267 (0.0%)
4	H	0.29	0/1652	0.48	0/2249
4	I	0.28	0/1652	0.46	0/2249
4	J	0.30	0/1662	0.49	0/2263
5	K	0.42	0/428	0.53	0/572
5	L	0.36	0/675	0.49	0/905
5	M	0.36	0/689	0.52	0/925
5	N	0.36	0/689	0.50	0/925
5	O	0.37	0/689	0.53	0/925
5	P	0.37	0/682	0.51	0/915
6	Q	0.36	0/1042	0.55	0/1408
6	R	0.33	0/951	0.50	0/1282
6	S	0.35	0/976	0.56	0/1316
6	T	0.34	0/991	0.54	0/1335
6	U	0.34	0/959	0.50	0/1293
7	V	0.28	0/981	0.44	0/1334
7	W	0.26	0/976	0.46	0/1327
7	X	0.57	2/981 (0.2%)	0.95	3/1334 (0.2%)
7	Y	0.28	0/981	0.52	1/1334 (0.1%)
7	Z	0.26	0/981	0.47	0/1334
7	a	0.28	0/981	0.47	0/1334
All	All	0.44	20/100455 (0.0%)	0.60	46/136142 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	UI	0	2
1	UJ	0	2
1	UK	0	3
1	UL	0	3
1	UM	0	2
1	UN	0	2
1	UO	0	2
1	UP	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	WA	0	3
1	WB	0	4
1	WC	0	3
1	WD	0	1
1	WE	0	2
1	WF	0	3
1	WG	0	3
1	WI	0	1
1	WJ	0	3
1	WK	0	2
1	WL	0	2
1	WM	0	1
1	WN	0	1
1	WO	0	1
1	WP	0	3
1	WQ	0	2
1	WR	0	3
1	WS	0	1
1	WT	0	2
1	WU	0	2
1	WV	0	3
1	WW	0	2
4	H	0	1
6	Q	0	1
6	U	0	1
7	Y	0	1
7	a	0	1
All	All	0	72

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	331	PRO	CG-CD	-14.23	1.03	1.50
7	X	73	PRO	CG-CD	-12.74	1.08	1.50
1	UL	172	PRO	N-CD	-9.53	1.34	1.47
1	UM	172	PRO	N-CD	-9.52	1.34	1.47
1	UP	172	PRO	N-CD	-9.50	1.34	1.47

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	73	PRO	CB-CG-CD	18.81	179.86	106.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	73	PRO	N-CD-CG	-18.80	75.00	103.20
1	f	331	PRO	N-CD-CG	-16.10	79.05	103.20
7	X	73	PRO	CA-CB-CG	-14.00	77.40	104.00
4	F	162	PRO	CA-N-CD	-12.05	94.62	111.50

There are no chirality outliers.

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	UI	221	THR	Mainchain
1	UI	50	ASP	Mainchain
1	UJ	270	THR	Mainchain
1	UJ	50	ASP	Mainchain
1	UK	50	ASP	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1275	0	1254	30	0
1	1	1275	0	1254	50	0
1	2	1275	0	1254	36	0
1	3	1275	0	1254	27	0
1	4	1275	0	1254	33	0
1	5	1275	0	1254	35	0
1	6	1275	0	1254	46	0
1	7	1275	0	1254	50	0
1	8	1275	0	1254	30	0
1	9	1275	0	1254	28	0
1	AA	1275	0	1254	26	0
1	AB	1275	0	1254	40	0
1	AC	1275	0	1254	43	0
1	AD	1275	0	1254	43	0
1	AE	1275	0	1254	42	0
1	AF	1275	0	1254	25	0
1	AG	1275	0	1254	25	0
1	AH	1275	0	1254	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AI	1275	0	1254	44	0
1	AJ	1275	0	1254	38	0
1	AK	1275	0	1254	37	0
1	AL	1275	0	1254	34	0
1	AM	1275	0	1254	31	0
1	AN	1275	0	1254	27	0
1	AO	1275	0	1254	30	0
1	AP	1275	0	1254	35	0
1	AQ	1275	0	1254	24	0
1	UI	1172	0	1181	62	0
1	UJ	1172	0	1181	78	0
1	UK	1172	0	1181	71	0
1	UL	1172	0	1181	68	0
1	UM	1172	0	1181	67	0
1	UN	1172	0	1181	69	0
1	UO	1172	0	1181	62	0
1	UP	1172	0	1181	65	0
1	WA	849	0	860	79	0
1	WB	836	0	846	79	0
1	WC	812	0	826	68	0
1	WD	827	0	840	93	0
1	WE	843	0	855	88	0
1	WF	834	0	847	62	0
1	WG	843	0	855	71	0
1	WH	703	0	722	67	0
1	WI	703	0	722	74	0
1	WJ	737	0	755	90	0
1	WK	729	0	744	85	0
1	WL	622	0	632	59	0
1	WM	596	0	612	48	0
1	WN	611	0	623	56	0
1	WO	714	0	731	51	0
1	WP	741	0	758	71	0
1	WQ	834	0	847	72	0
1	WR	834	0	847	62	0
1	WS	834	0	847	78	0
1	WT	834	0	847	75	0
1	WU	843	0	855	68	0
1	WV	827	0	838	65	0
1	WW	834	0	847	86	0
1	b	81	0	78	0	0
1	c	103	0	99	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	133	0	129	0	0
1	e	103	0	99	0	0
1	f	140	0	136	0	0
1	g	103	0	99	0	0
1	h	140	0	136	0	0
1	i	103	0	99	0	0
1	j	133	0	129	0	0
1	k	103	0	99	0	0
1	l	140	0	136	0	0
1	t	1275	0	1254	0	0
1	u	1275	0	1254	0	0
1	v	1275	0	1254	0	0
1	w	1275	0	1254	0	0
1	x	1275	0	1254	0	0
1	y	1275	0	1254	0	0
1	z	1275	0	1254	0	0
2	A	670	0	739	34	0
2	B	670	0	739	35	0
2	C	670	0	739	31	0
2	D	670	0	739	32	0
3	E	1945	0	2063	113	0
4	F	1605	0	1701	78	0
4	G	1626	0	1718	58	0
4	H	1614	0	1709	52	0
4	I	1614	0	1709	71	0
4	J	1623	0	1715	83	0
5	K	429	0	445	37	0
5	L	672	0	684	49	0
5	M	686	0	700	52	0
5	N	686	0	700	43	0
5	O	686	0	700	22	0
5	P	679	0	693	28	0
6	Q	1030	0	1025	23	0
6	R	942	0	943	35	0
6	S	967	0	968	59	0
6	T	982	0	984	43	0
6	U	950	0	946	51	0
7	V	969	0	981	17	0
7	W	964	0	976	15	0
7	X	969	0	981	14	0
7	Y	969	0	981	15	0
7	Z	969	0	981	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	a	969	0	981	0	0
All	All	99073	0	99719	3015	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 3015 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WD:168:GLU:CD	1:WD:170:LYS:HE3	1.40	1.38
1:WC:121:PHE:HZ	2:C:15:LYS:NZ	1.21	1.35
1:UP:103:GLN:HG2	1:WW:182:PRO:CB	1.58	1.33
1:UP:103:GLN:CG	1:WW:182:PRO:HB3	1.56	1.32
5:L:11:ILE:HG22	1:AH:372:ILE:CD1	1.58	1.32

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	1	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	2	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	3	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	4	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	5	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	6	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	7	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	9	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AA	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AB	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AC	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AD	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AE	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AF	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AG	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AH	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AI	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AJ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AK	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AL	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AM	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AN	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AO	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AP	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	AQ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	UI	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UJ	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UK	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UL	151/560 (27%)	142 (94%)	7 (5%)	2 (1%)	10	39
1	UM	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UN	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UO	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	UP	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	39
1	WA	111/560 (20%)	99 (89%)	9 (8%)	3 (3%)	4	27
1	WB	109/560 (20%)	94 (86%)	10 (9%)	5 (5%)	2	19
1	WC	106/560 (19%)	96 (91%)	9 (8%)	1 (1%)	14	45
1	WD	108/560 (19%)	99 (92%)	4 (4%)	5 (5%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	WE	110/560 (20%)	98 (89%)	8 (7%)	4 (4%)	3	23
1	WF	109/560 (20%)	98 (90%)	8 (7%)	3 (3%)	4	27
1	WG	110/560 (20%)	98 (89%)	10 (9%)	2 (2%)	7	34
1	WH	93/560 (17%)	86 (92%)	5 (5%)	2 (2%)	5	30
1	WI	93/560 (17%)	82 (88%)	5 (5%)	6 (6%)	1	14
1	WJ	97/560 (17%)	89 (92%)	7 (7%)	1 (1%)	13	44
1	WK	96/560 (17%)	84 (88%)	9 (9%)	3 (3%)	3	25
1	WL	81/560 (14%)	75 (93%)	4 (5%)	2 (2%)	4	28
1	WM	78/560 (14%)	72 (92%)	4 (5%)	2 (3%)	4	28
1	WN	80/560 (14%)	75 (94%)	2 (2%)	3 (4%)	2	21
1	WO	94/560 (17%)	85 (90%)	7 (7%)	2 (2%)	5	32
1	WP	98/560 (18%)	87 (89%)	6 (6%)	5 (5%)	1	17
1	WQ	109/560 (20%)	100 (92%)	5 (5%)	4 (4%)	2	22
1	WR	109/560 (20%)	94 (86%)	8 (7%)	7 (6%)	1	14
1	WS	109/560 (20%)	96 (88%)	7 (6%)	6 (6%)	1	16
1	WT	109/560 (20%)	97 (89%)	5 (5%)	7 (6%)	1	14
1	WU	110/560 (20%)	101 (92%)	8 (7%)	1 (1%)	14	45
1	WV	108/560 (19%)	97 (90%)	9 (8%)	2 (2%)	6	33
1	WW	109/560 (20%)	95 (87%)	9 (8%)	5 (5%)	2	19
1	b	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
1	c	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
1	d	18/560 (3%)	18 (100%)	0	0	100	100
1	e	14/560 (2%)	14 (100%)	0	0	100	100
1	f	19/560 (3%)	19 (100%)	0	0	100	100
1	g	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
1	h	19/560 (3%)	19 (100%)	0	0	100	100
1	i	14/560 (2%)	14 (100%)	0	0	100	100
1	j	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
1	k	14/560 (2%)	14 (100%)	0	0	100	100
1	l	19/560 (3%)	19 (100%)	0	0	100	100
1	t	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	v	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	w	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	x	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	y	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
1	z	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
2	A	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
2	B	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
2	C	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
2	D	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
3	E	251/264 (95%)	231 (92%)	14 (6%)	6 (2%)	5	29
4	F	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
4	G	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13	44
4	H	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
4	I	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25	58
4	J	207/245 (84%)	201 (97%)	4 (2%)	2 (1%)	13	44
5	K	55/104 (53%)	53 (96%)	2 (4%)	0	100	100
5	L	87/104 (84%)	87 (100%)	0	0	100	100
5	M	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
5	N	89/104 (86%)	89 (100%)	0	0	100	100
5	O	89/104 (86%)	89 (100%)	0	0	100	100
5	P	88/104 (85%)	88 (100%)	0	0	100	100
6	Q	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
6	R	115/138 (83%)	114 (99%)	1 (1%)	0	100	100
6	S	119/138 (86%)	116 (98%)	3 (2%)	0	100	100
6	T	121/138 (88%)	118 (98%)	3 (2%)	0	100	100
6	U	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
7	V	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
7	W	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
7	X	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
7	Y	131/134 (98%)	127 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	Z	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16 49
7	a	131/134 (98%)	125 (95%)	6 (5%)	0	100 100
All	All	12674/46523 (27%)	12203 (96%)	362 (3%)	109 (1%)	17 45

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	WO	168	GLU
1	WR	123	ILE
1	WR	165	PHE
1	WR	166	VAL
1	WS	187	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	1	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	2	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	3	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	4	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	5	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	6	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	7	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	8	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	9	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	AA	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	AB	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	AC	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	AD	141/467 (30%)	134 (95%)	7 (5%)	20 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AE	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AF	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AG	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AH	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AI	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AJ	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AK	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AL	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AM	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AN	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AO	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AP	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	AQ	141/467 (30%)	134 (95%)	7 (5%)	20	45
1	UI	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UJ	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UK	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UL	128/467 (27%)	122 (95%)	6 (5%)	22	46
1	UM	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UN	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UO	128/467 (27%)	123 (96%)	5 (4%)	27	51
1	UP	128/467 (27%)	122 (95%)	6 (5%)	22	46
1	WA	95/467 (20%)	91 (96%)	4 (4%)	25	49
1	WB	93/467 (20%)	87 (94%)	6 (6%)	14	39
1	WC	91/467 (20%)	83 (91%)	8 (9%)	8	30
1	WD	92/467 (20%)	88 (96%)	4 (4%)	25	49
1	WE	94/467 (20%)	87 (93%)	7 (7%)	11	35
1	WF	93/467 (20%)	86 (92%)	7 (8%)	11	35
1	WG	94/467 (20%)	87 (93%)	7 (7%)	11	35
1	WH	79/467 (17%)	75 (95%)	4 (5%)	20	45
1	WI	79/467 (17%)	73 (92%)	6 (8%)	11	34
1	WJ	83/467 (18%)	79 (95%)	4 (5%)	21	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	WK	82/467 (18%)	77 (94%)	5 (6%)	15 41
1	WL	69/467 (15%)	66 (96%)	3 (4%)	25 49
1	WM	66/467 (14%)	65 (98%)	1 (2%)	60 74
1	WN	68/467 (15%)	66 (97%)	2 (3%)	37 58
1	WO	80/467 (17%)	76 (95%)	4 (5%)	20 45
1	WP	83/467 (18%)	77 (93%)	6 (7%)	12 36
1	WQ	93/467 (20%)	91 (98%)	2 (2%)	47 64
1	WR	93/467 (20%)	86 (92%)	7 (8%)	11 35
1	WS	93/467 (20%)	87 (94%)	6 (6%)	14 39
1	WT	93/467 (20%)	86 (92%)	7 (8%)	11 35
1	WU	94/467 (20%)	90 (96%)	4 (4%)	25 49
1	WV	92/467 (20%)	83 (90%)	9 (10%)	6 25
1	WW	93/467 (20%)	85 (91%)	8 (9%)	8 31
1	b	8/467 (2%)	8 (100%)	0	100 100
1	c	11/467 (2%)	10 (91%)	1 (9%)	7 28
1	d	14/467 (3%)	12 (86%)	2 (14%)	2 16
1	e	11/467 (2%)	11 (100%)	0	100 100
1	f	15/467 (3%)	15 (100%)	0	100 100
1	g	11/467 (2%)	11 (100%)	0	100 100
1	h	15/467 (3%)	15 (100%)	0	100 100
1	i	11/467 (2%)	11 (100%)	0	100 100
1	j	14/467 (3%)	13 (93%)	1 (7%)	12 36
1	k	11/467 (2%)	11 (100%)	0	100 100
1	l	15/467 (3%)	14 (93%)	1 (7%)	13 38
1	t	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	u	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	v	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	w	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	x	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	y	141/467 (30%)	134 (95%)	7 (5%)	20 45
1	z	141/467 (30%)	134 (95%)	7 (5%)	20 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	74/74 (100%)	73 (99%)	1 (1%)	62	75
2	B	74/74 (100%)	73 (99%)	1 (1%)	62	75
2	C	74/74 (100%)	74 (100%)	0	100	100
2	D	74/74 (100%)	73 (99%)	1 (1%)	62	75
3	E	210/221 (95%)	204 (97%)	6 (3%)	37	58
4	F	177/204 (87%)	170 (96%)	7 (4%)	27	50
4	G	179/204 (88%)	173 (97%)	6 (3%)	32	55
4	H	178/204 (87%)	173 (97%)	5 (3%)	38	59
4	I	178/204 (87%)	172 (97%)	6 (3%)	32	55
4	J	179/204 (88%)	175 (98%)	4 (2%)	47	64
5	K	45/79 (57%)	40 (89%)	5 (11%)	5	21
5	L	68/79 (86%)	64 (94%)	4 (6%)	16	41
5	M	70/79 (89%)	65 (93%)	5 (7%)	12	36
5	N	70/79 (89%)	66 (94%)	4 (6%)	17	43
5	O	70/79 (89%)	66 (94%)	4 (6%)	17	43
5	P	69/79 (87%)	65 (94%)	4 (6%)	17	42
6	Q	110/113 (97%)	106 (96%)	4 (4%)	30	54
6	R	101/113 (89%)	99 (98%)	2 (2%)	50	68
6	S	103/113 (91%)	96 (93%)	7 (7%)	13	38
6	T	104/113 (92%)	102 (98%)	2 (2%)	52	69
6	U	102/113 (90%)	96 (94%)	6 (6%)	16	41
7	V	104/105 (99%)	104 (100%)	0	100	100
7	W	104/105 (99%)	103 (99%)	1 (1%)	73	80
7	X	104/105 (99%)	104 (100%)	0	100	100
7	Y	104/105 (99%)	102 (98%)	2 (2%)	52	69
7	Z	104/105 (99%)	101 (97%)	3 (3%)	37	58
7	a	104/105 (99%)	100 (96%)	4 (4%)	28	52
All	All	10879/38698 (28%)	10379 (95%)	500 (5%)	25	47

5 of 500 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	R	55	ARG

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Mol	Chain	Res	Type
1	AI	424	ASP
1	w	377	MET
1	AI	294	ARG
1	AN	294	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
1	0	374	HIS
1	AK	303	GLN
1	AB	374	HIS
1	AF	374	HIS
1	AM	374	HIS

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.

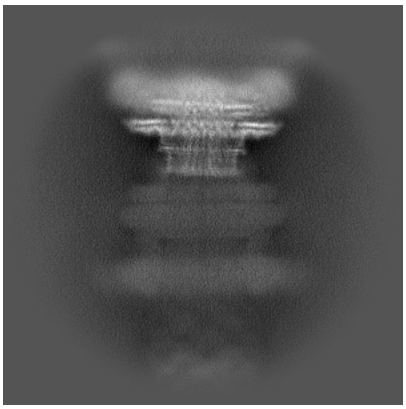
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37605. These allow visual inspection of the internal detail of the map and identification of artifacts.

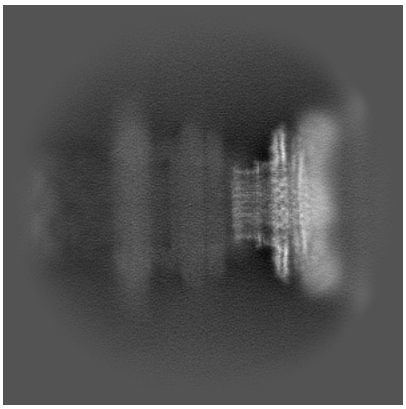
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

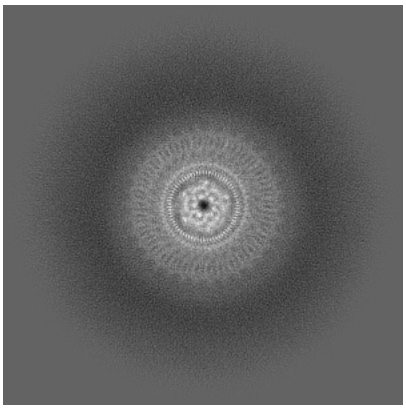
6.1.1 Primary map



X

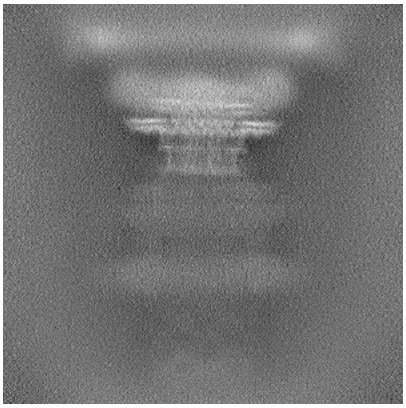


Y

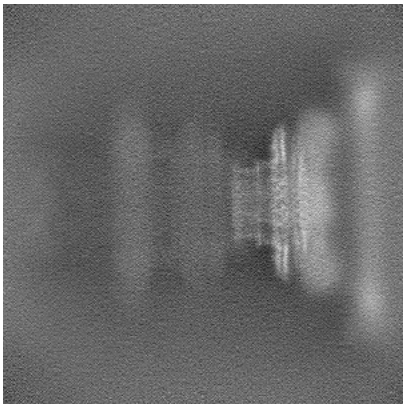


Z

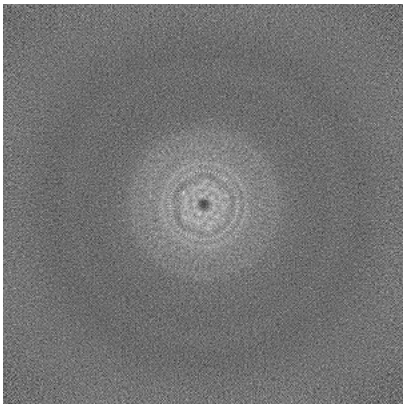
6.1.2 Raw map



X



Y

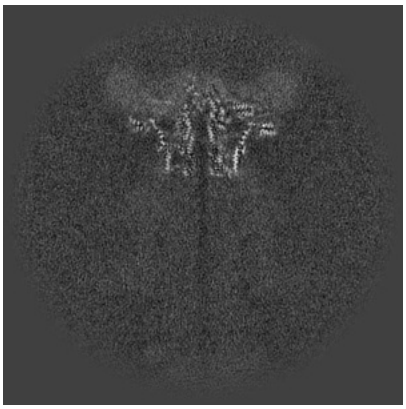


Z

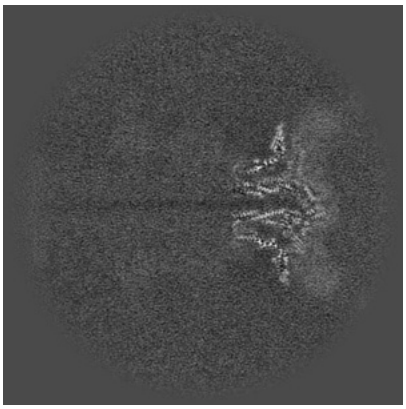
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

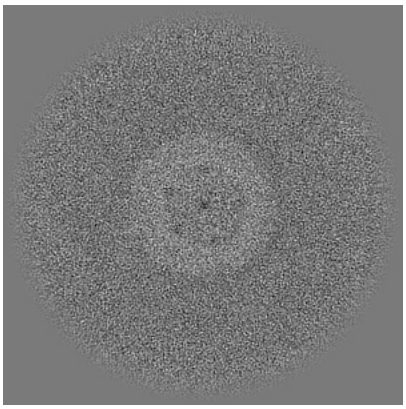
6.2.1 Primary map



X Index: 256

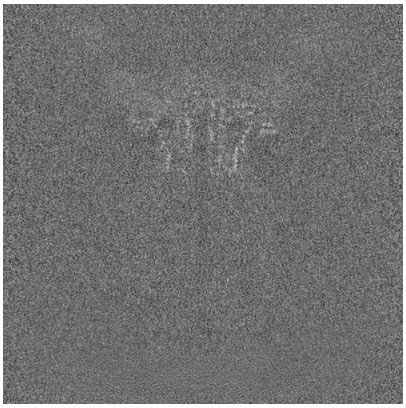


Y Index: 256

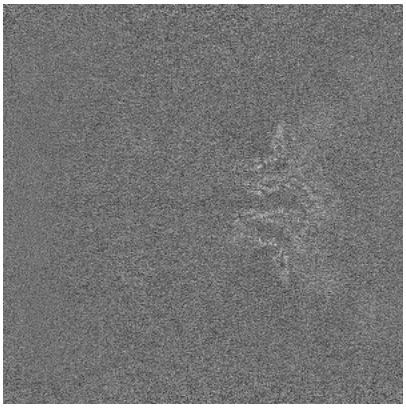


Z Index: 256

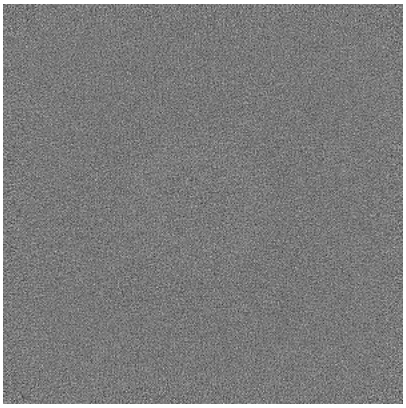
6.2.2 Raw map



X Index: 256



Y Index: 256

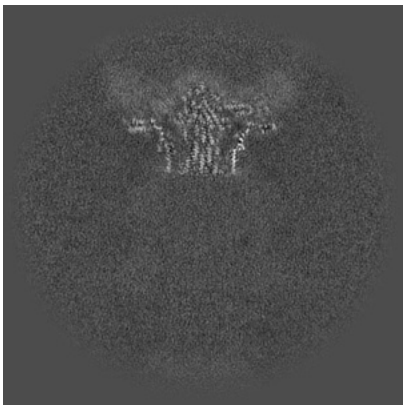


Z Index: 256

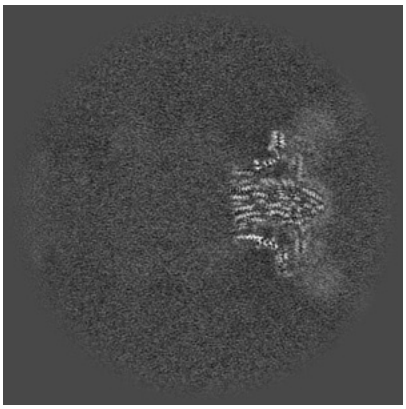
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

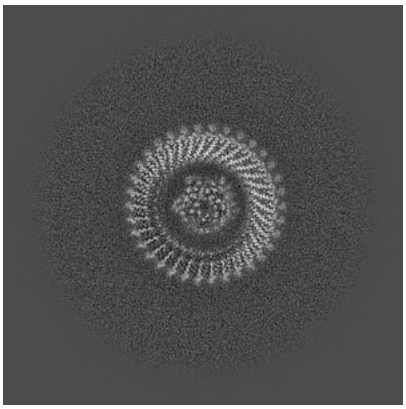
6.3.1 Primary map



X Index: 244

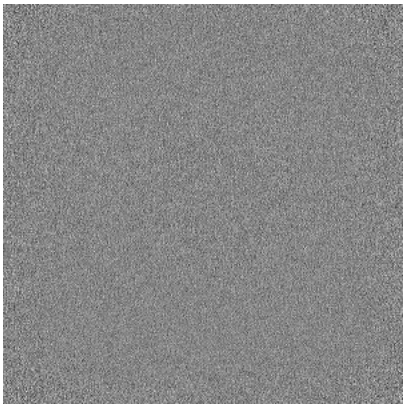


Y Index: 265

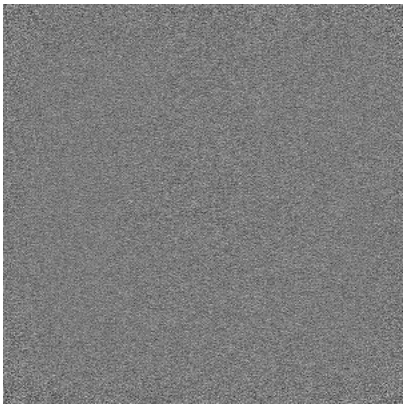


Z Index: 358

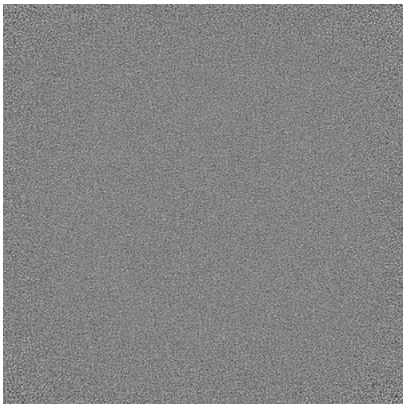
6.3.2 Raw map



X Index: 0



Y Index: 0

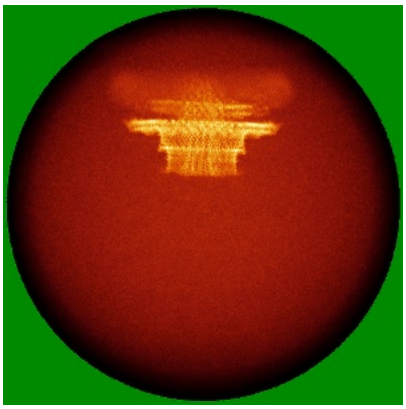


Z Index: 0

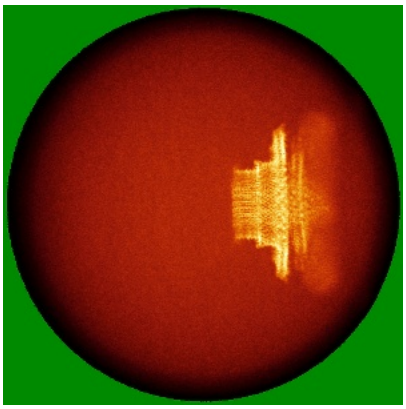
The images above show the largest variance slices of the map in three orthogonal directions.

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

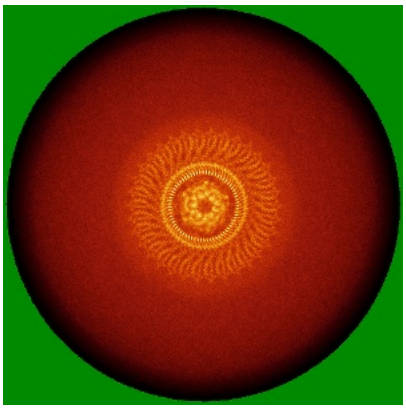
6.4.1 Primary map



X

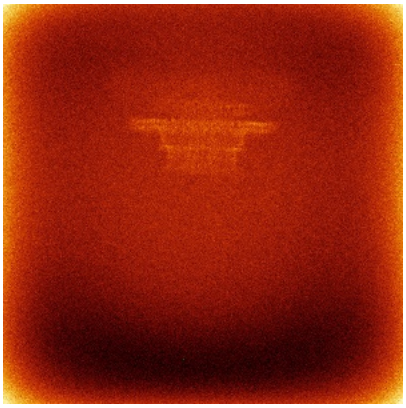


Y

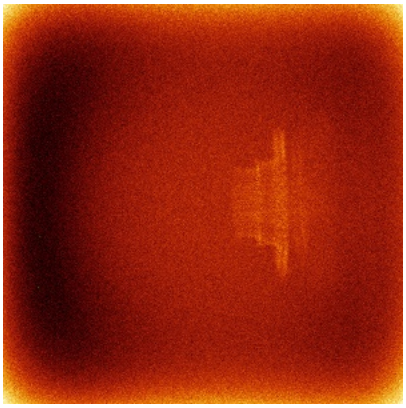


Z

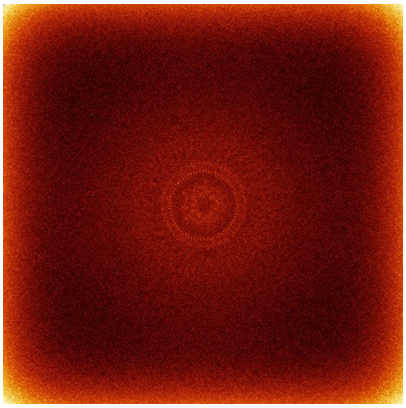
6.4.2 Raw map



X



Y

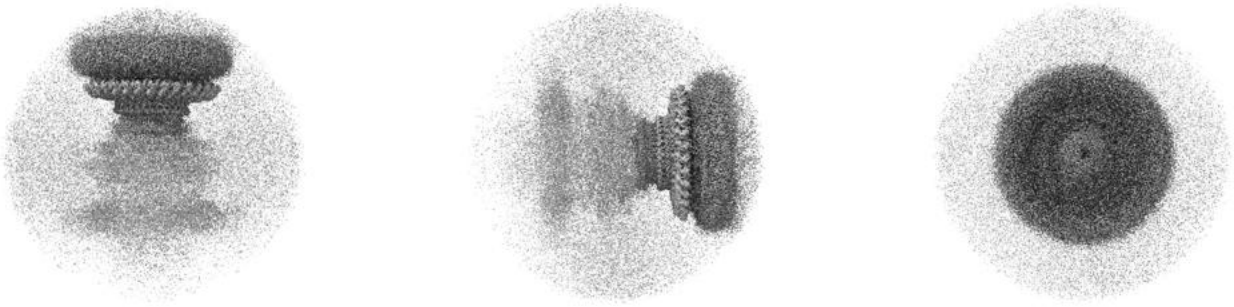


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

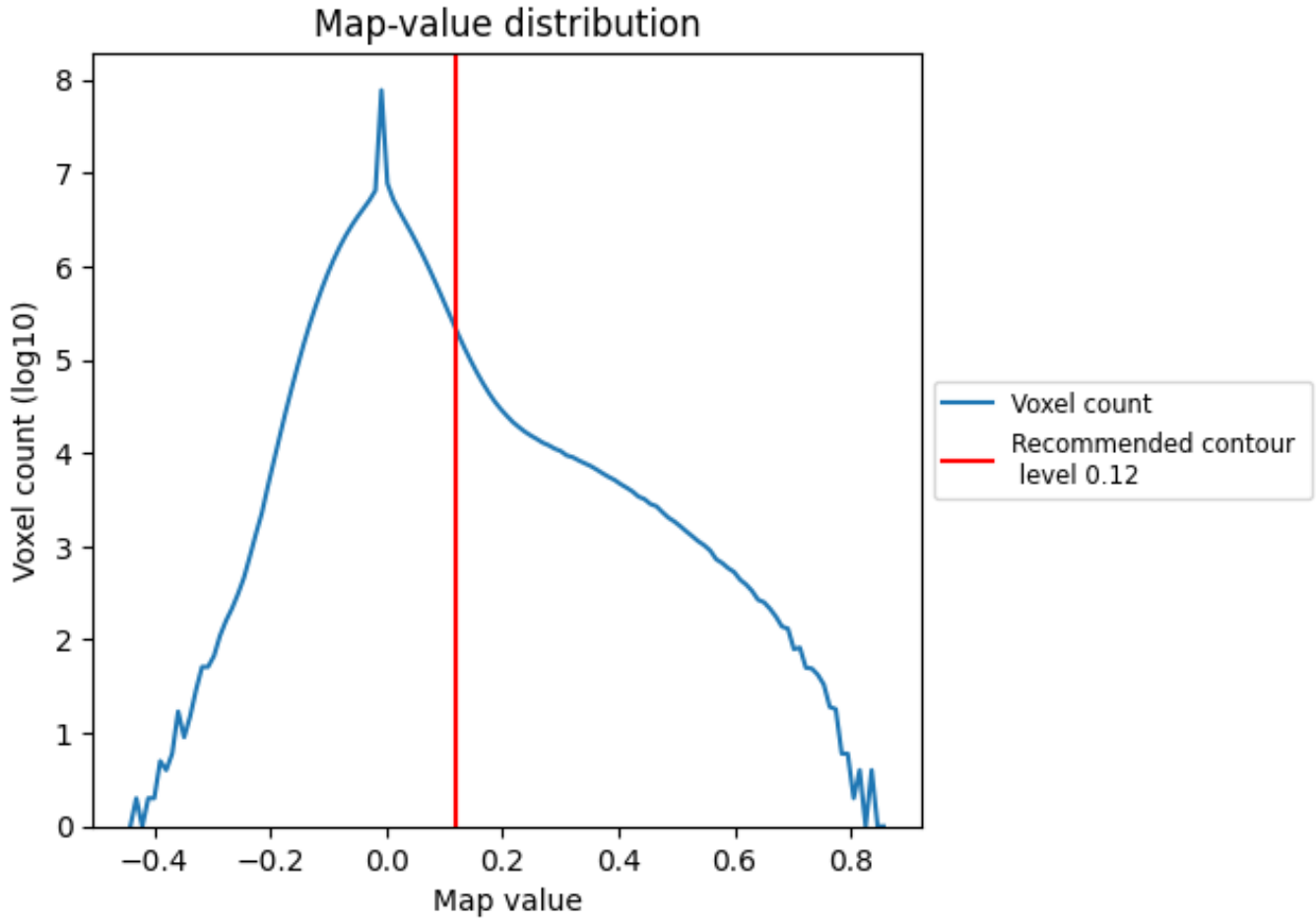
6.6 Mask visualisation (i)

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

7 Map analysis

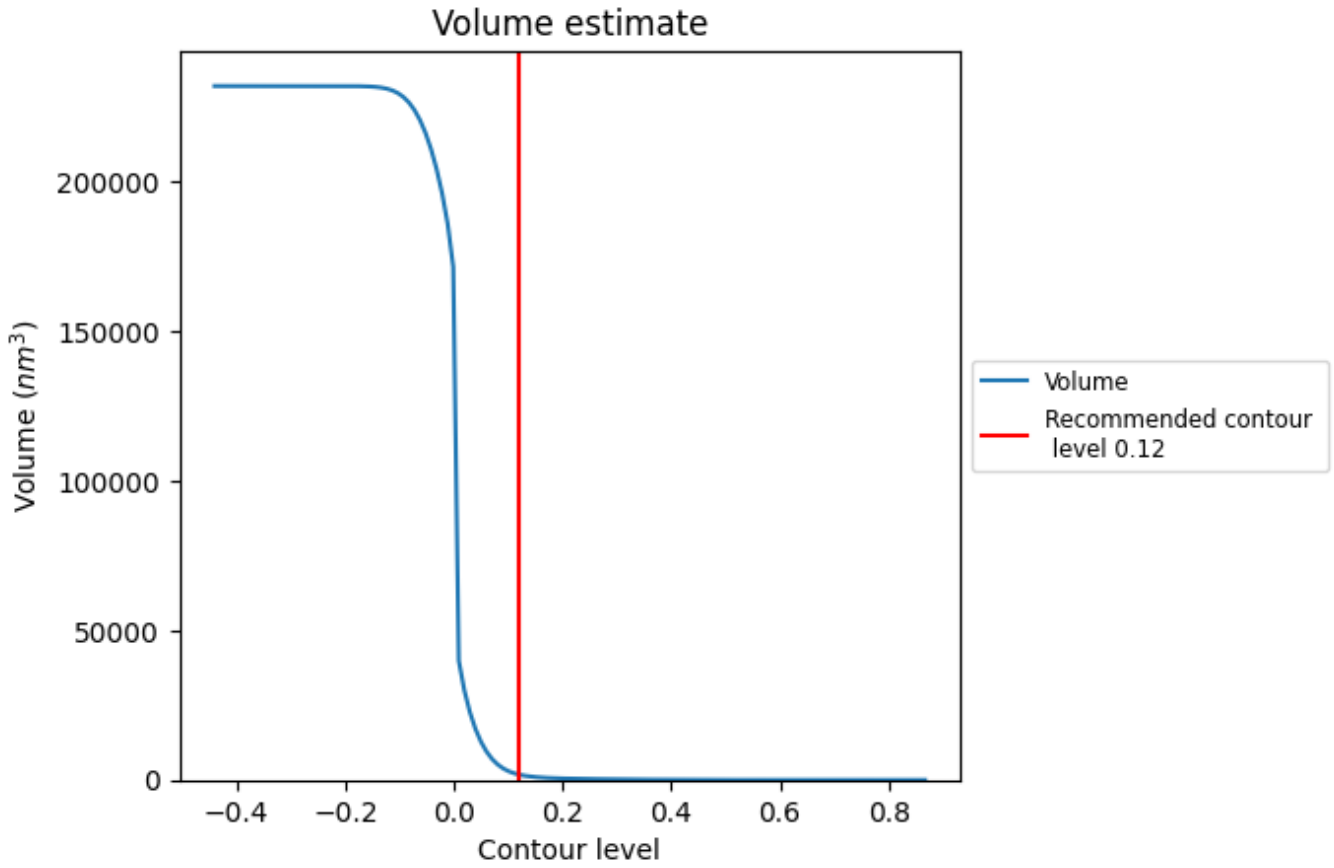
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

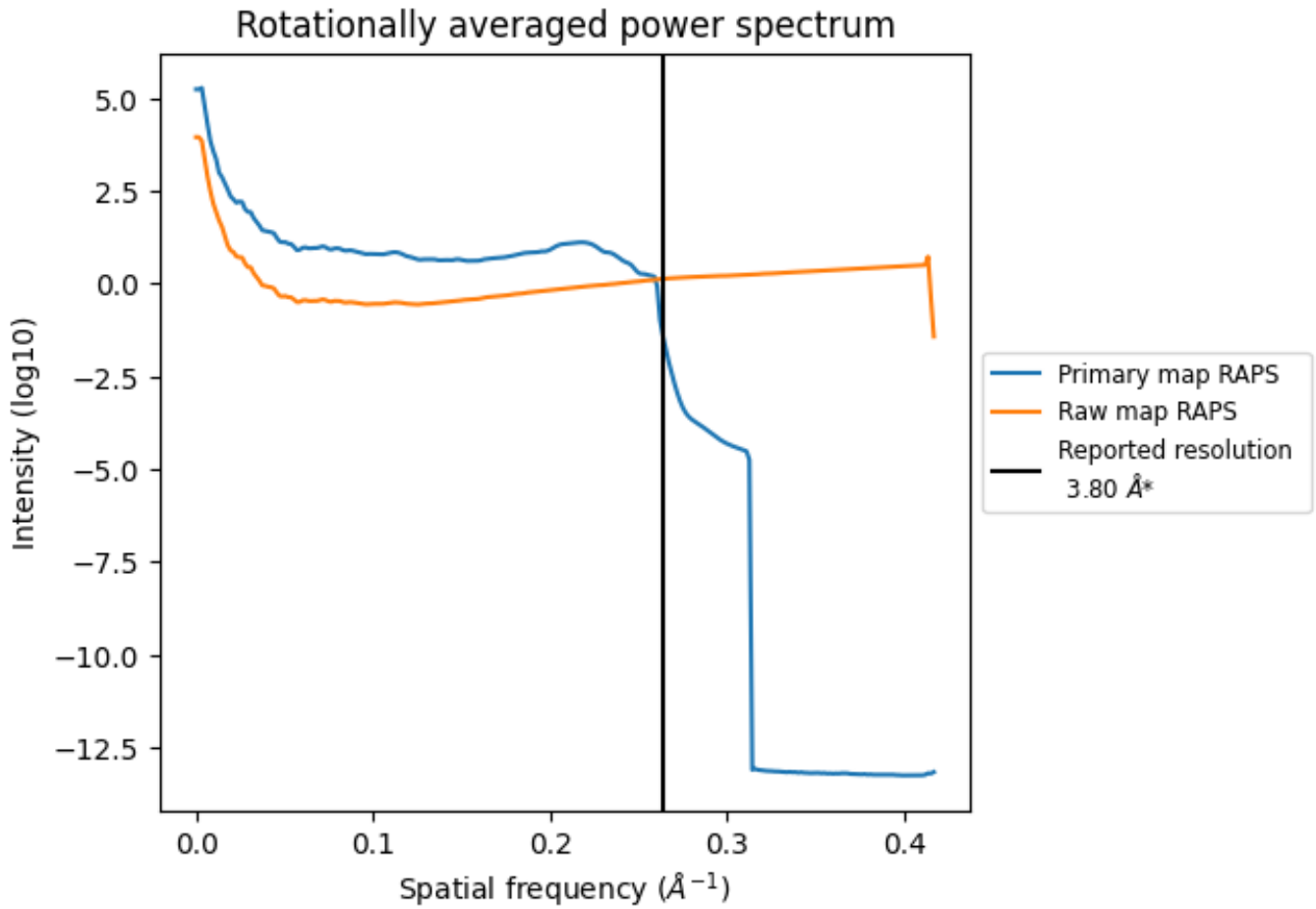
7.2 Volume estimate (i)



The volume at the recommended contour level is 1782 nm^3; this corresponds to an approximate mass of 1610 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)

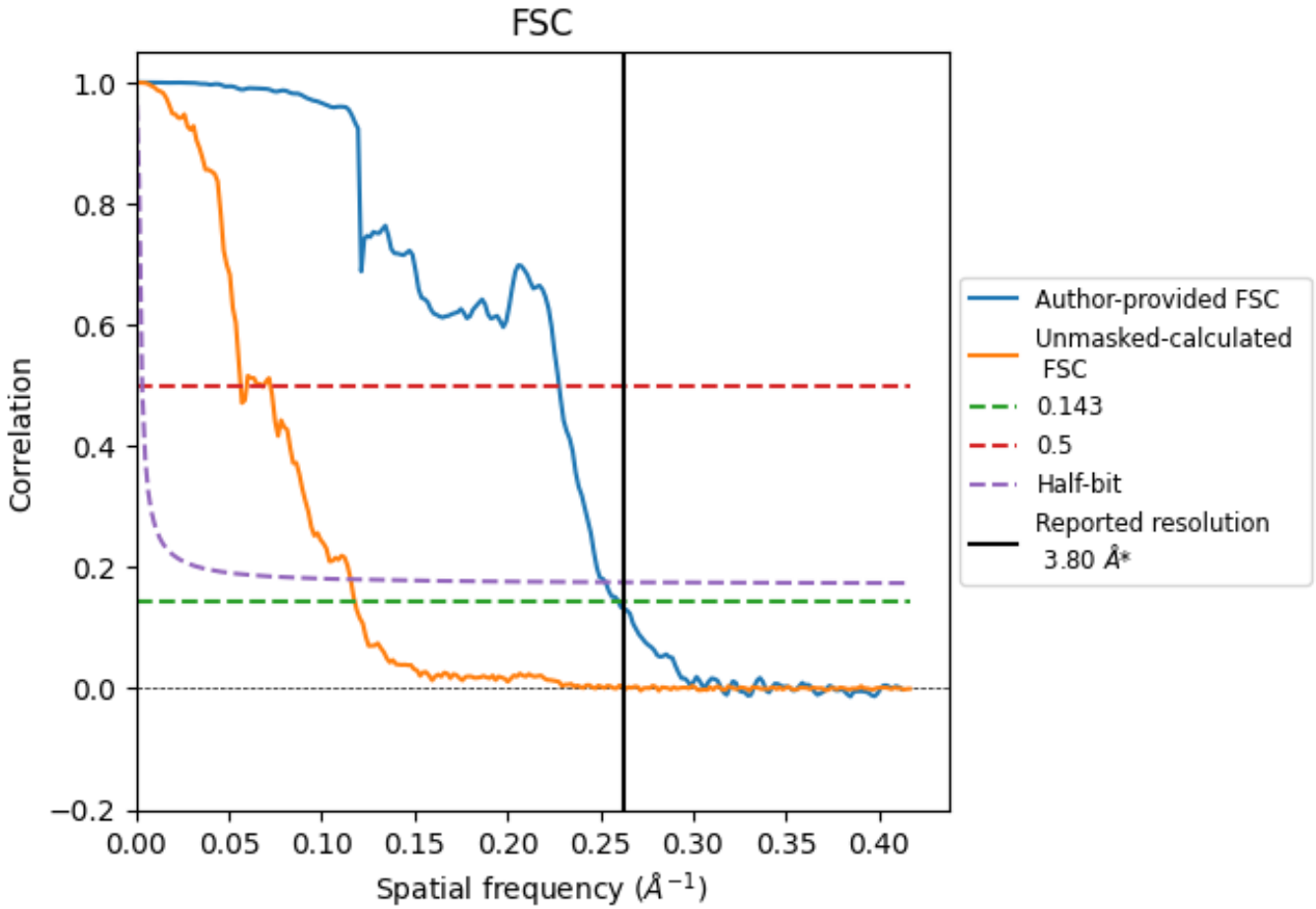


*Reported resolution corresponds to spatial frequency of 0.263 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

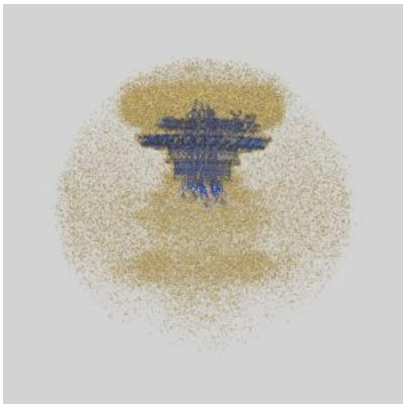
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.85	4.39	3.96
Unmasked-calculated*	8.49	17.76	8.65

*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 8.49 differs from the reported value 3.8 by more than 10 %

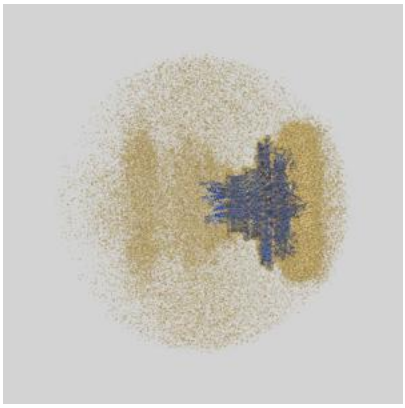
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37605 and PDB model 8WKQ. Per-residue inclusion information can be found in section 3 on page 13.

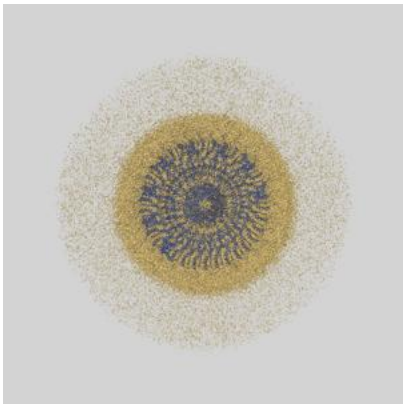
9.1 Map-model overlay



X



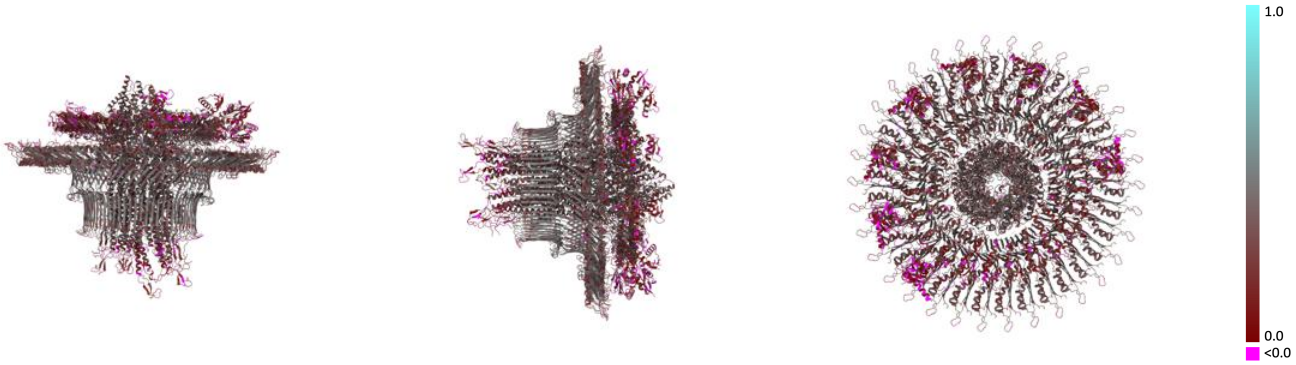
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

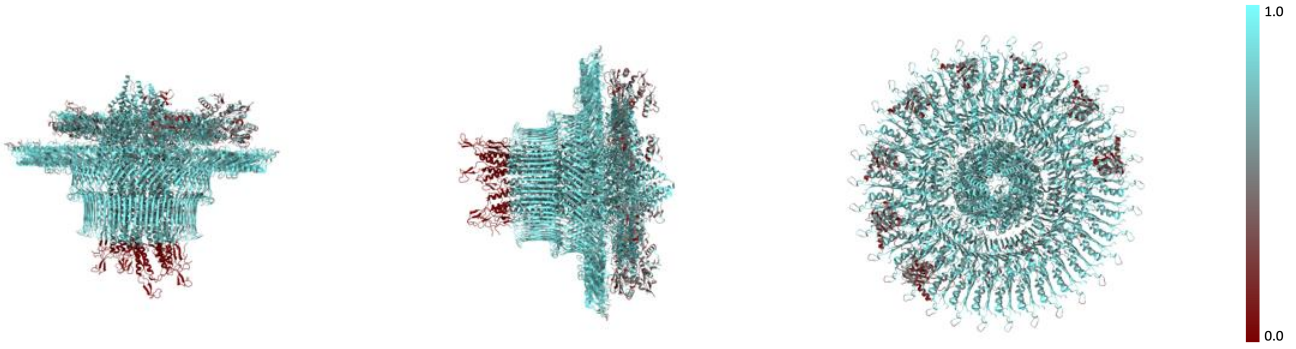
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

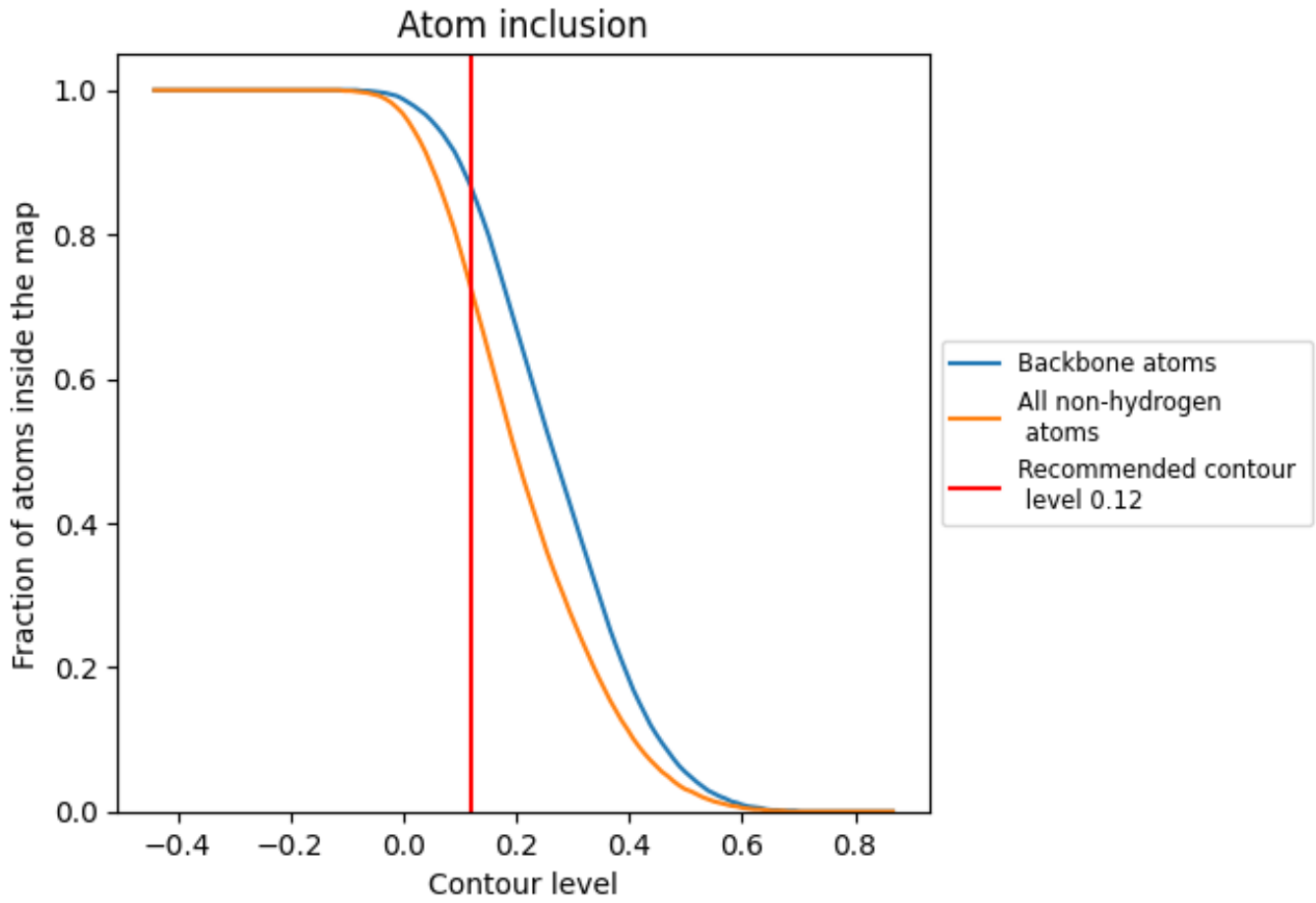
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 72% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.3190
0	0.8170	0.3700
1	0.8140	0.3590
2	0.8250	0.3680
3	0.8290	0.3720
4	0.8250	0.3740
5	0.8190	0.3730
6	0.8280	0.3770
7	0.8200	0.3750
8	0.8340	0.3860
9	0.8330	0.3850
A	0.7670	0.3160
AA	0.8140	0.3660
AB	0.8210	0.3660
AC	0.8210	0.3690
AD	0.8240	0.3640
AE	0.8180	0.3720
AF	0.8290	0.3590
AG	0.8120	0.3470
AH	0.8200	0.3540
AI	0.8010	0.3490
AJ	0.8220	0.3610
AK	0.8270	0.3650
AL	0.8140	0.3620
AM	0.8110	0.3650
AN	0.8040	0.3640
AO	0.8250	0.3750
AP	0.8220	0.3740
AQ	0.8160	0.3700
B	0.8150	0.3480
C	0.8200	0.3510
D	0.8090	0.3460
E	0.7840	0.3500
F	0.7940	0.3610
G	0.8120	0.3750

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Chain	Atom inclusion	Q-score
H	0.7990	0.3690
I	0.7870	0.3680
J	0.7640	0.3640
K	0.7300	0.3590
L	0.7890	0.3540
M	0.7750	0.3500
N	0.7680	0.3580
O	0.7610	0.3430
P	0.7660	0.3520
Q	0.7750	0.3790
R	0.7740	0.3690
S	0.7420	0.3670
T	0.7260	0.3610
U	0.6610	0.3390
UI	0.5160	0.2040
UJ	0.4890	0.1640
UK	0.4160	0.1540
UL	0.3670	0.1180
UM	0.2850	0.0510
UN	0.3590	0.0800
UO	0.4200	0.1310
UP	0.4760	0.1390
V	0.5020	0.3110
W	0.4120	0.2850
WA	0.7920	0.3380
WB	0.7910	0.3290
WC	0.8040	0.3460
WD	0.7890	0.3400
WE	0.7680	0.3210
WF	0.7780	0.3230
WG	0.7460	0.2860
WH	0.7690	0.2810
WI	0.7200	0.2360
WJ	0.6920	0.2170
WK	0.6500	0.1970
WL	0.6770	0.1880
WM	0.7090	0.2250
WN	0.6880	0.1660
WO	0.6630	0.1650
WP	0.7480	0.2330
WQ	0.7300	0.2510
WR	0.7300	0.2820

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Chain	Atom inclusion	Q-score
WS	0.7870	0.2910
WT	0.7950	0.3240
WU	0.7600	0.2930
WV	0.7590	0.2860
WW	0.7790	0.3220
X	0.3500	0.2540
Y	0.2900	0.2230
Z	0.2590	0.2420
a	0.2050	0.2240
b	0.6670	0.3370
c	0.5050	0.3570
d	0.5640	0.3320
e	0.2430	0.2510
f	0.4930	0.2610
g	0.0870	0.1150
h	0.4360	0.2610
i	0.0680	0.1250
j	0.4510	0.2720
k	0.0780	0.1940
l	0.3360	0.2730
t	0.8270	0.3780
u	0.8270	0.3630
v	0.8240	0.3710
w	0.8280	0.3750
x	0.8300	0.3680
y	0.8260	0.3730
z	0.8250	0.3740