



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 04:50 PM JST

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

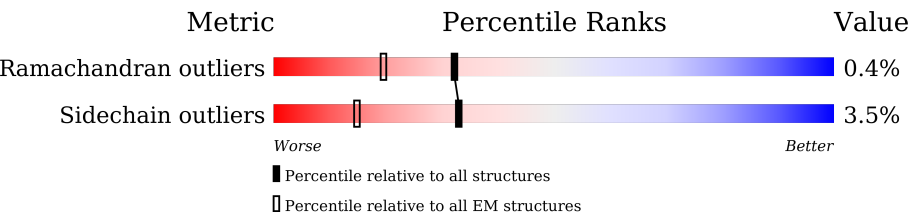
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 Å.

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



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

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

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

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

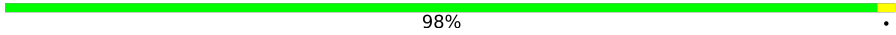
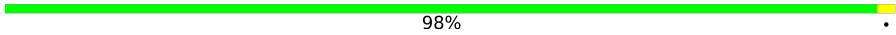
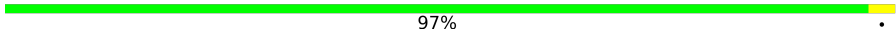
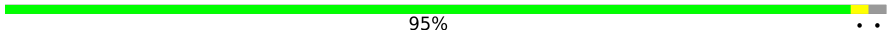
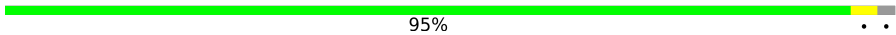
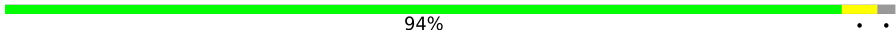
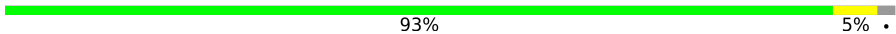
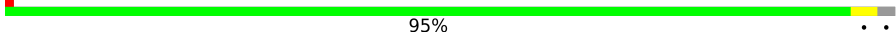




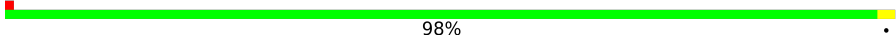
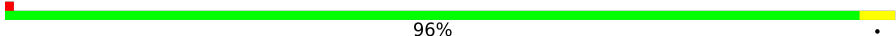
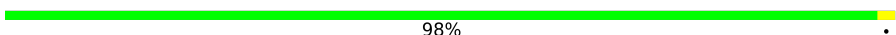
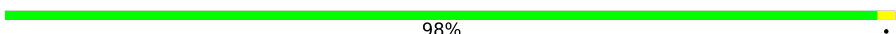
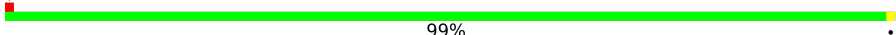
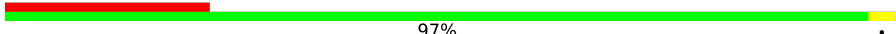
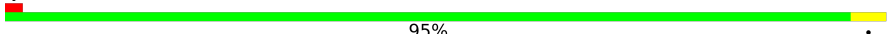
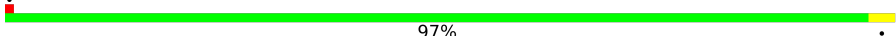
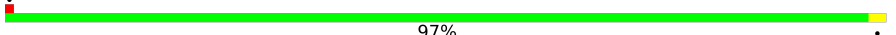
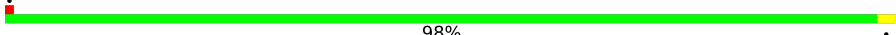
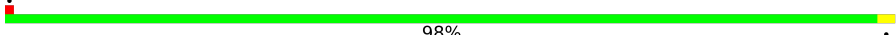
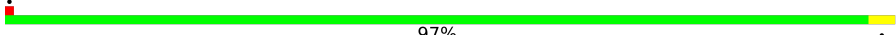
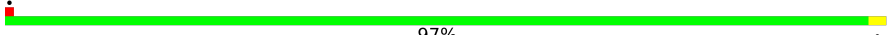
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Mol	Chain	Length	Quality of chain
2	i	365	<div> <div>57%</div> <div>80%</div> <div>17%</div> </div>
2	j	365	<div> <div>53%</div> <div>81%</div> <div>17%</div> </div>
2	k	365	<div> <div>58%</div> <div>80%</div> <div>17%</div> </div>
2	l	365	<div> <div>57%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

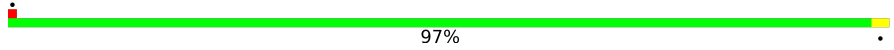
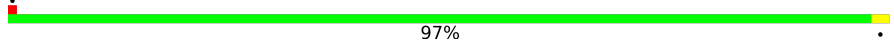
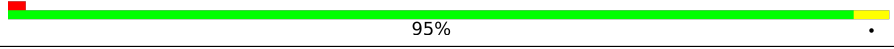
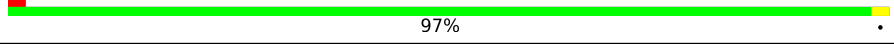
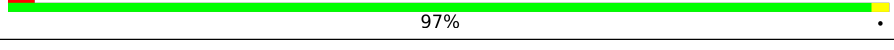
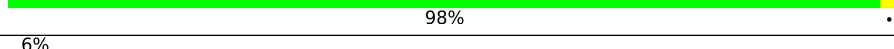
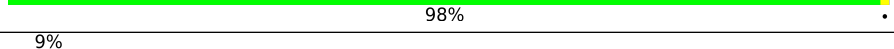
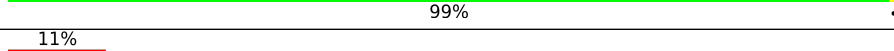
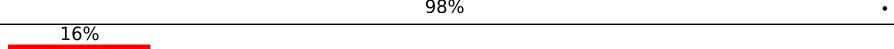
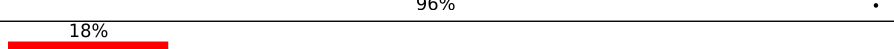
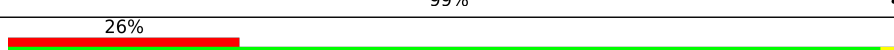
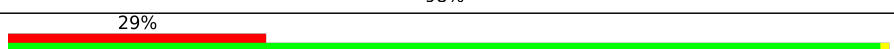
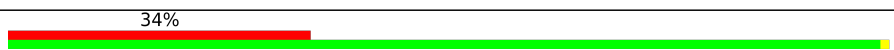
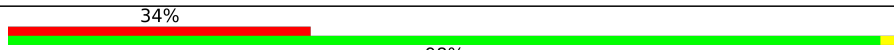
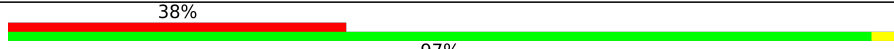
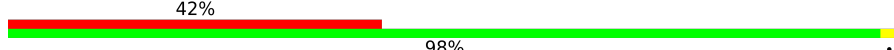

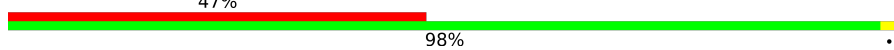
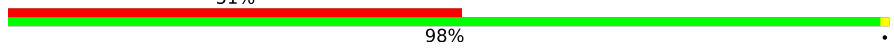
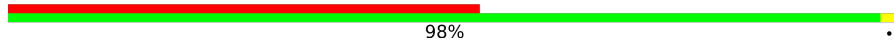
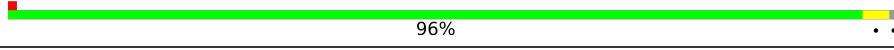
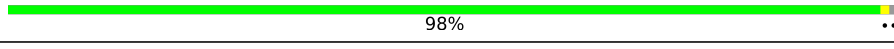
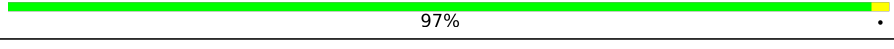
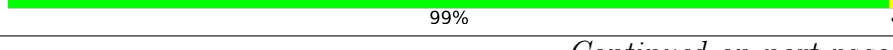

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Mol	Chain	Length	Quality of chain
3	7	260	 98%
3	8	260	 98%
3	9	260	 97%
3	AF	260	 95%
3	AG	260	 95%
3	AH	260	 94%
3	AI	260	 93%
3	AJ	260	 95%
3	AK	260	 92%
3	AL	260	 92%
3	AM	260	 92%
3	AN	260	 93%
3	ZA	260	 98%
3	ZB	260	 96%
3	ZC	260	 98%
3	ZD	260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

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Mol	Chain	Length	Quality of chain
4	ZN	403	 97%
4	ZO	403	 97%
4	ZP	403	 95%
4	ZQ	403	 97%
4	ZR	403	 97%
4	ZS	403	 98%
4	ZT	403	 98%
4	ZU	403	 99%
4	ZV	403	 98%
4	ZW	403	 96%
4	ZX	403	 99%
4	ZY	403	 98%
4	ZZ	403	 98%
4	Za	403	 98%
4	Zb	403	 98%
4	Zc	403	 97%
4	Zd	403	 98%
4	Ze	403	 97%
4	Zf	403	 98%
4	Zg	403	 98%
4	Zh	403	 98%
5	AA	251	 96%
5	AB	251	 98%
5	AC	251	 97%
5	AD	251	 99%

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

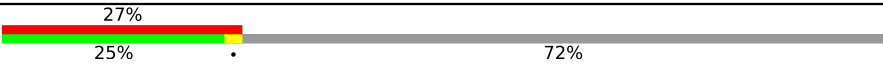


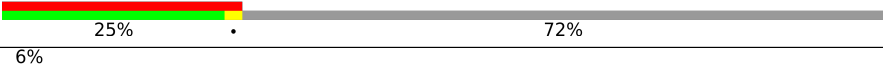



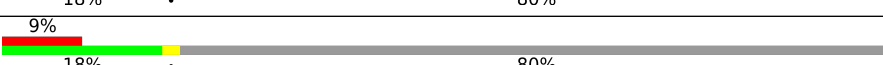
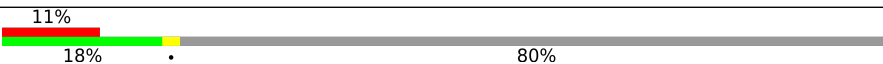

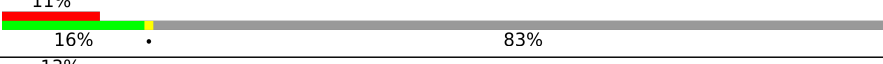




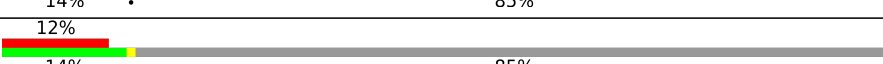









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Mol	Chain	Length	Quality of chain
6	An	560	
6	Ao	560	
6	Ap	560	
6	BG	560	
6	BH	560	
6	BI	560	
6	BJ	560	
6	BK	560	
6	BL	560	
6	BM	560	
6	BN	560	
6	BO	560	
6	BP	560	
6	BQ	560	
6	BR	560	
6	BS	560	
6	BT	560	
6	BU	560	
6	BV	560	
6	BW	560	
6	BX	560	
6	UI	560	
6	UJ	560	
6	UK	560	
6	UL	560	

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Mol	Chain	Length	Quality of chain	
6	UM	560		
6	UN	560		
6	UO	560		
6	UP	560		
6	WA	560		
6	WB	560		
6	WC	560		
6	WD	560		
6	WE	560		
6	WF	560		
6	WG	560		
6	WH	560		
6	WI	560		
6	WJ	560		
6	WK	560		
6	WL	560		
6	WM	560		
6	WN	560		
6	WO	560		
6	WP	560		
6	WQ	560		
6	WR	560		
6	WS	560		
6	WT	560		
6	WU	560		

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Mol	Chain	Length	Quality of chain
6	WV	560	
6	WW	560	
7	Ab	89	
7	Aq	89	
7	Ar	89	
7	As	89	
8	At	264	
9	Au	245	
9	Av	245	
9	Aw	245	
9	Ax	245	
9	Ay	245	
10	A1	104	
10	A2	104	
10	A3	104	
10	A4	104	
10	A5	104	
10	Az	104	
11	A0	138	
11	A6	138	
11	A7	138	
11	A8	138	
11	A9	138	
12	BA	134	
12	BB	134	

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Mol	Chain	Length	Quality of chain
12	BC	134	<div><div></div><div>99%</div><div></div></div>
12	BD	134	<div><div></div><div>96%</div><div></div></div>
12	BE	134	<div><div></div><div>96%</div><div></div></div>
12	BF	134	<div><div></div><div>96%</div><div></div></div>

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 338677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

3 Residue-property plots

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

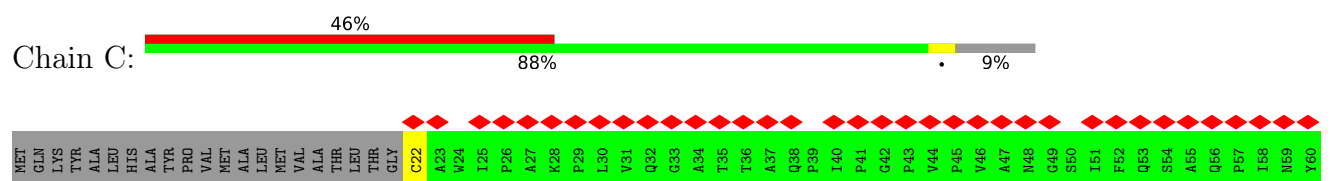
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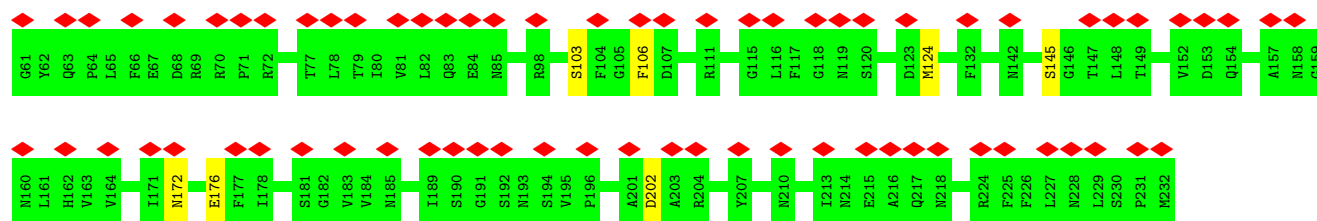


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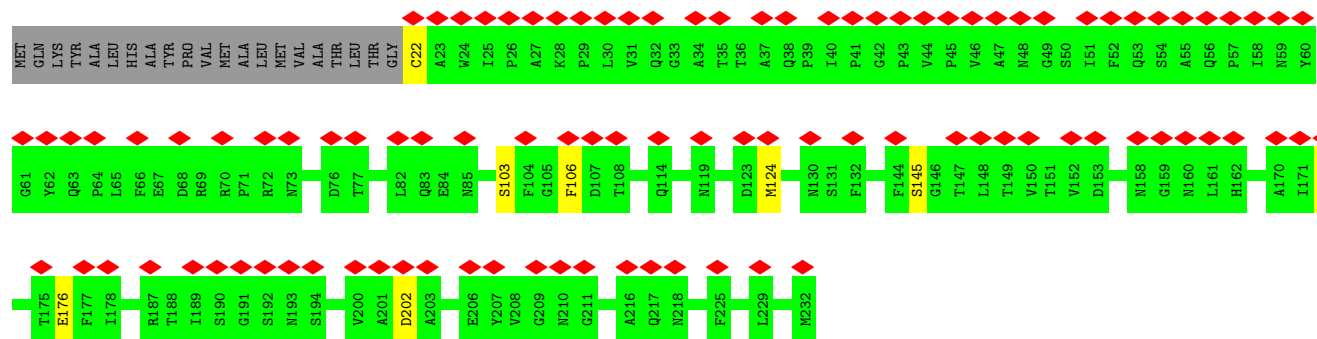
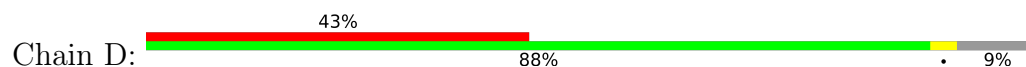


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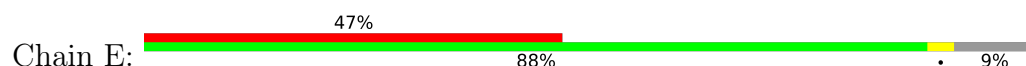




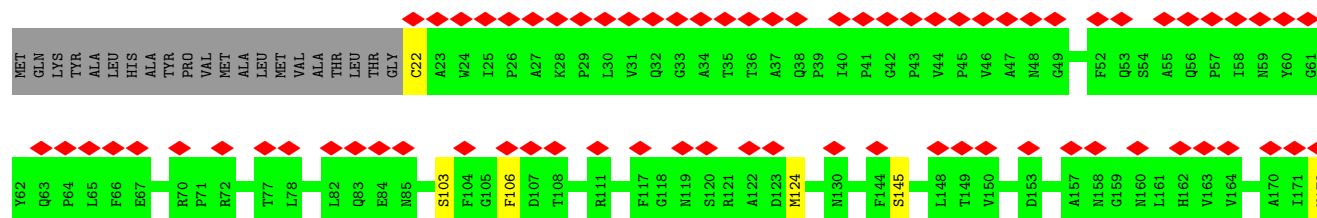
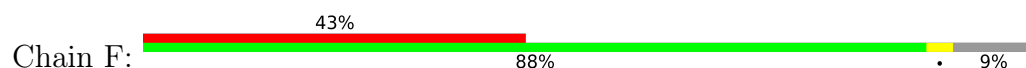
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

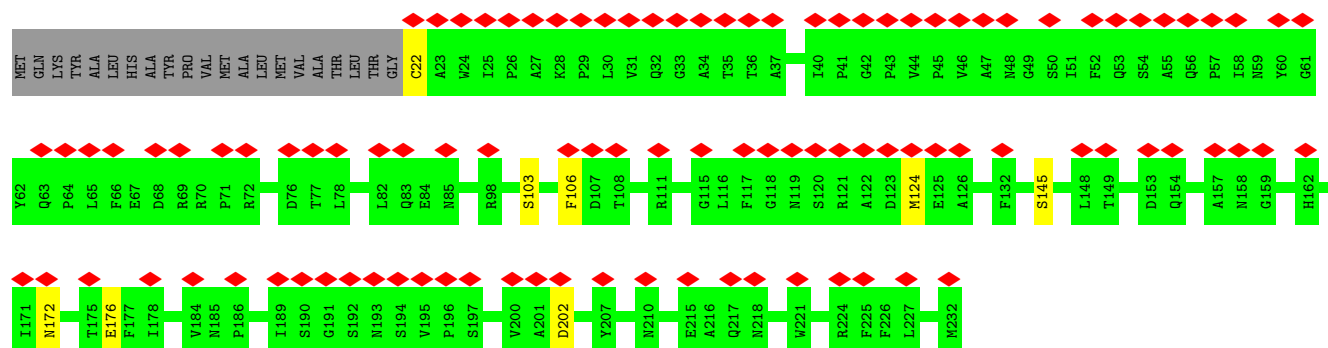
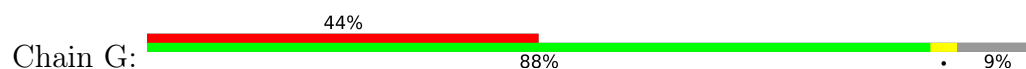


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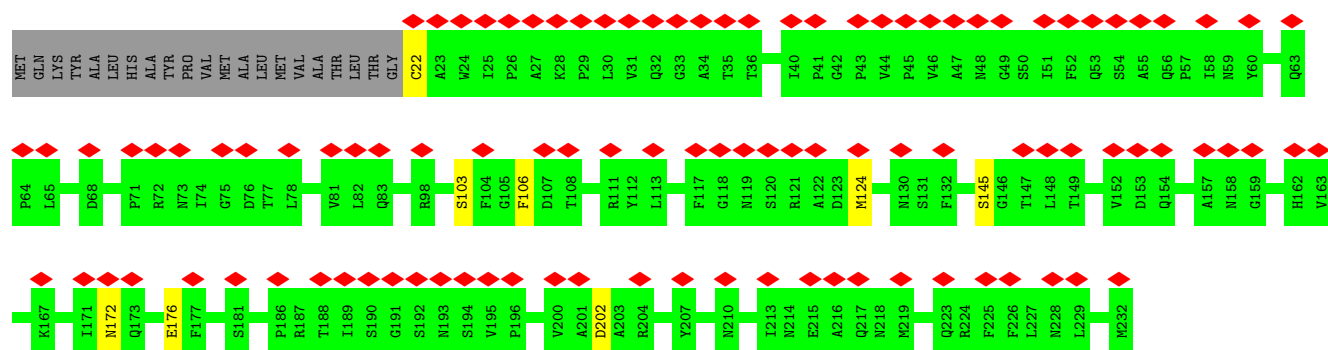
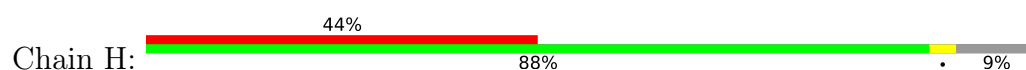




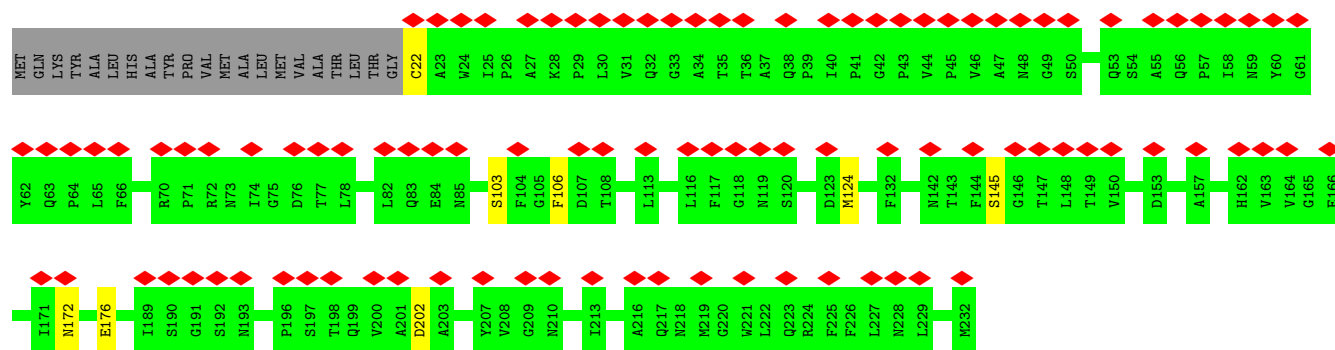
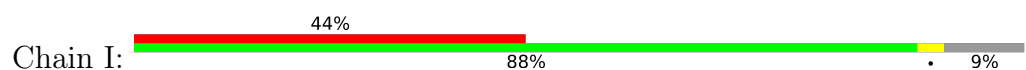
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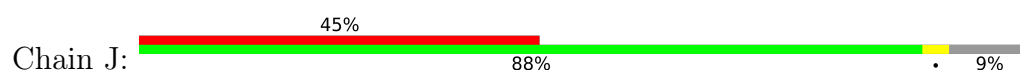
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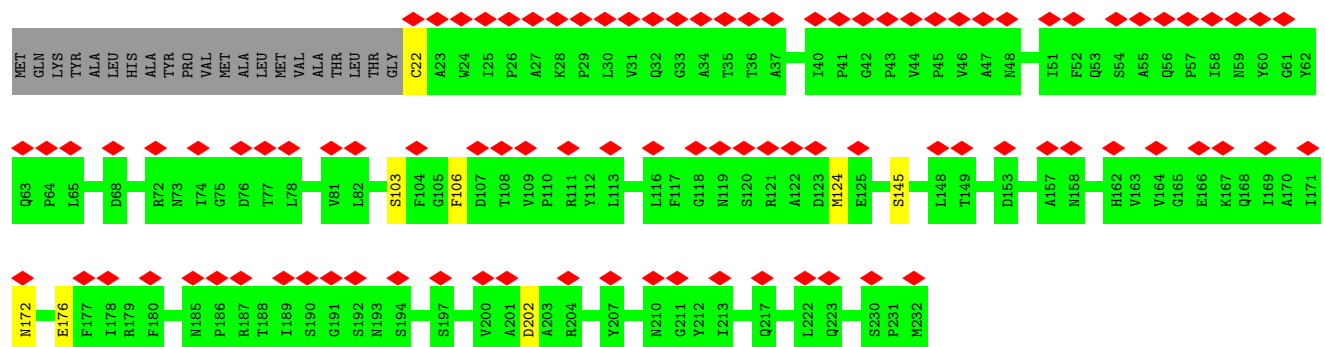
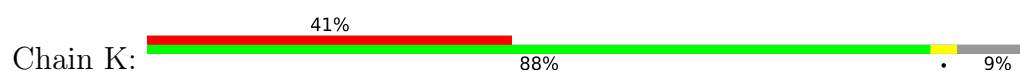
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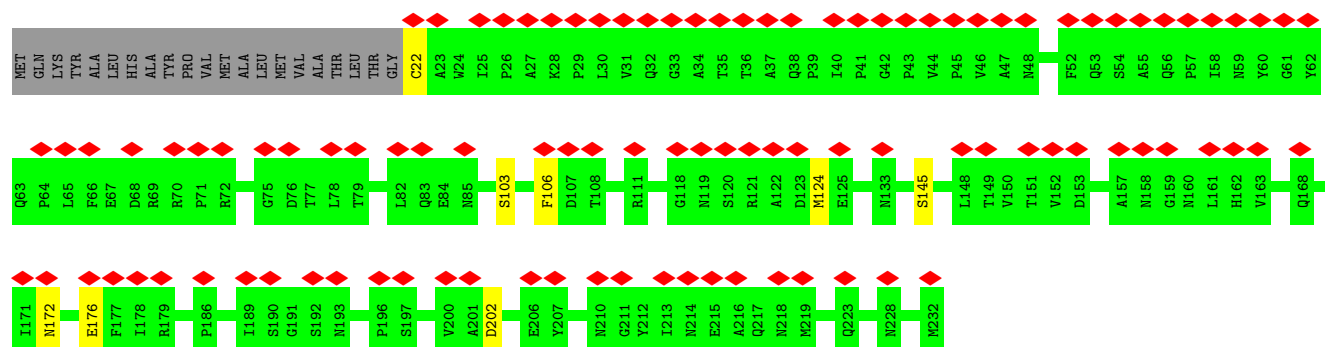
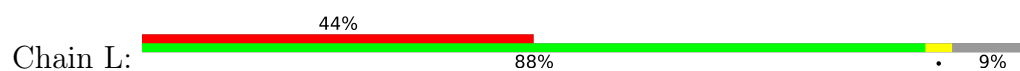
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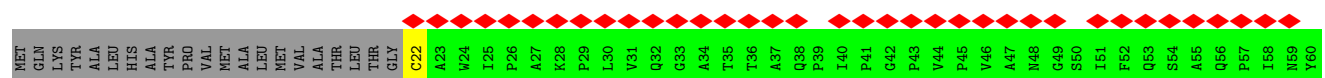
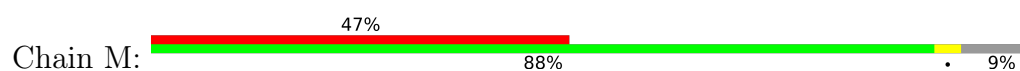
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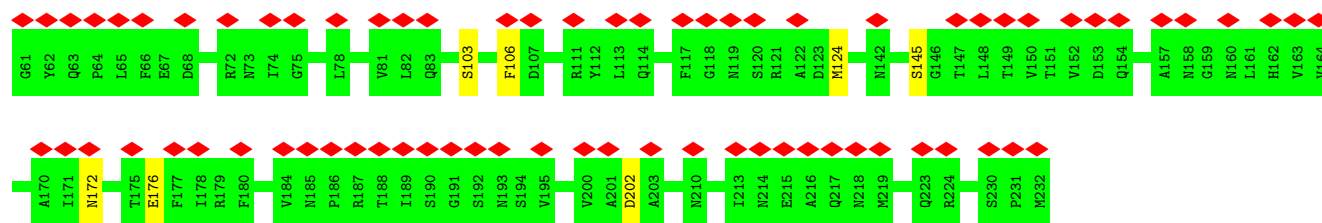


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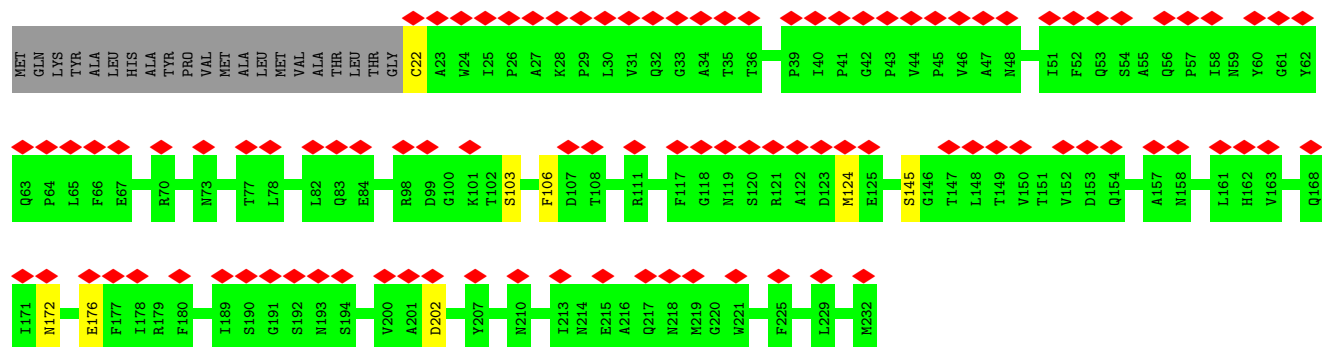
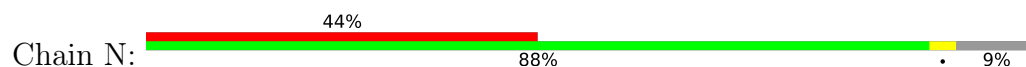


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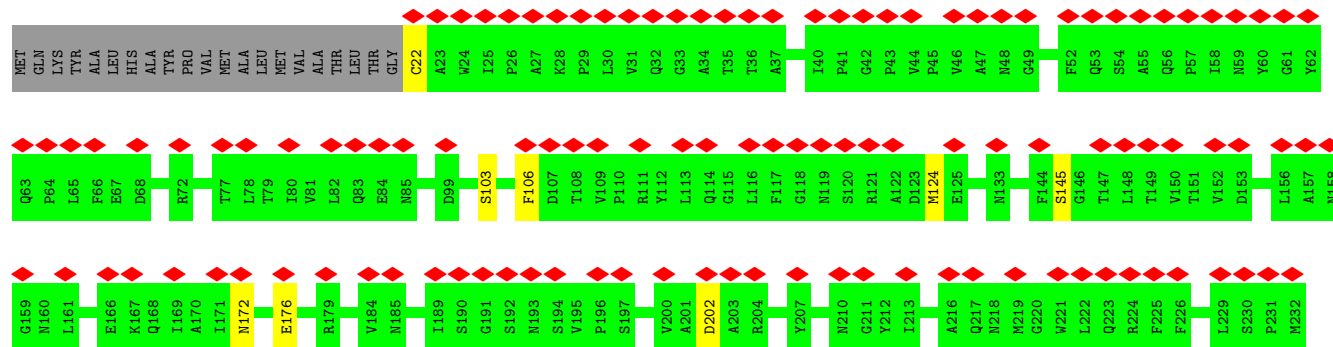
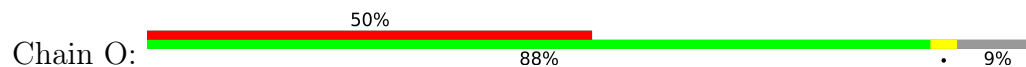




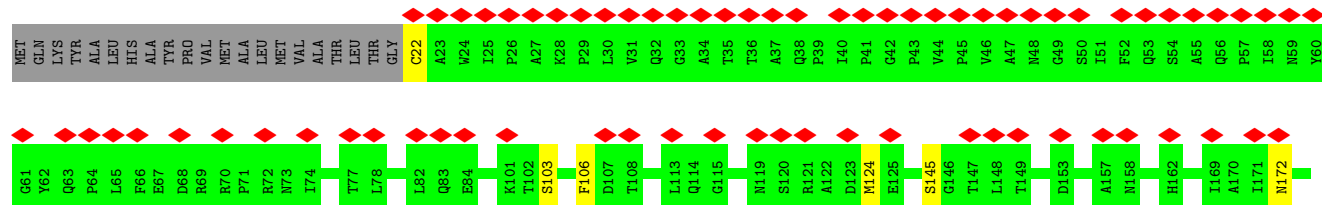
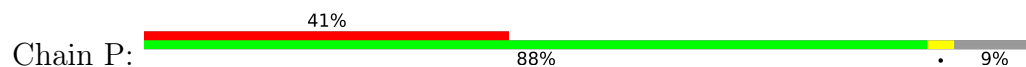
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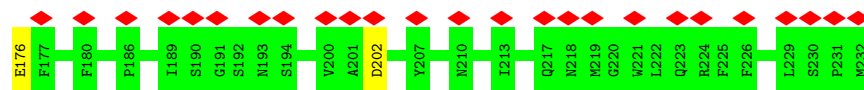


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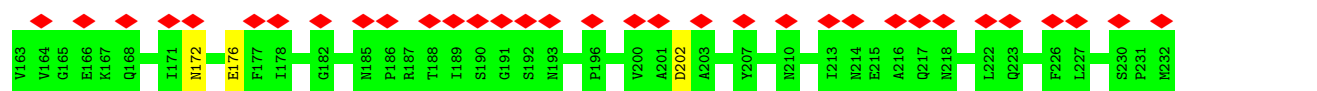
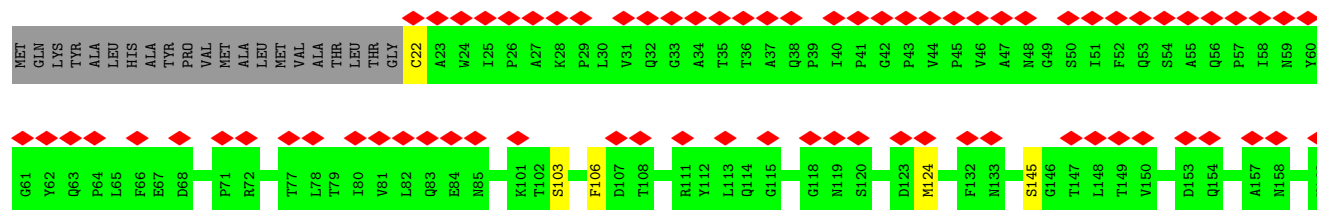
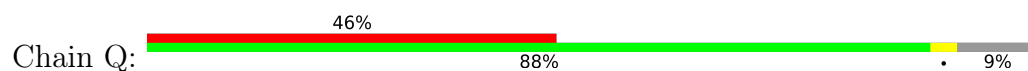


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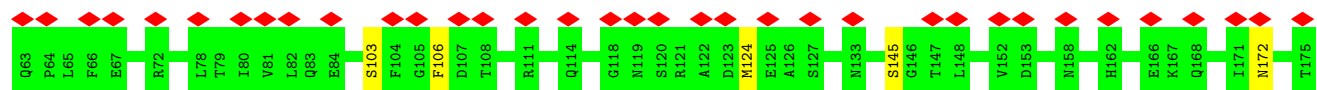
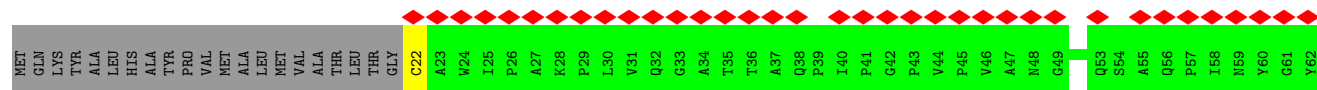
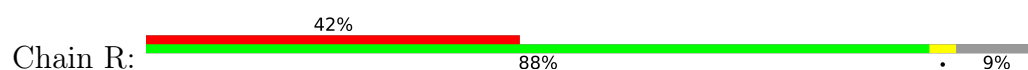




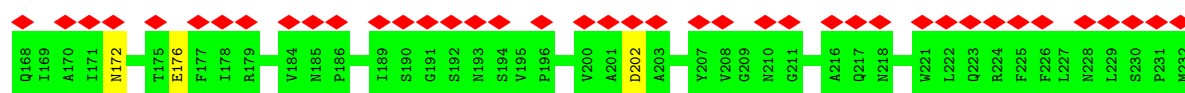
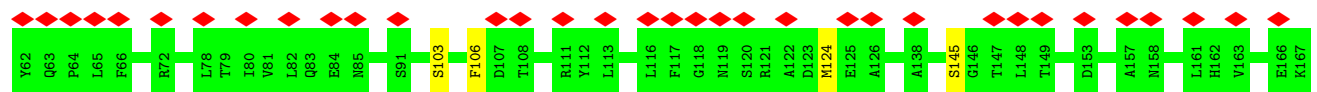
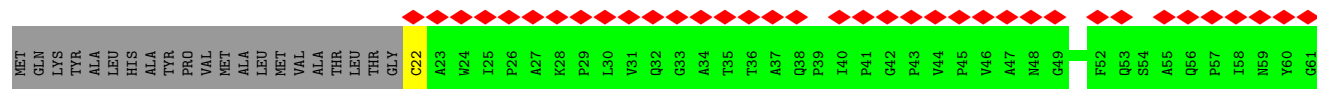
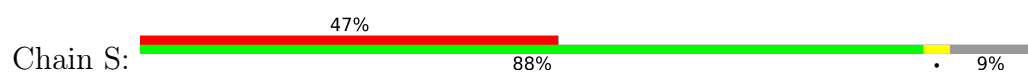
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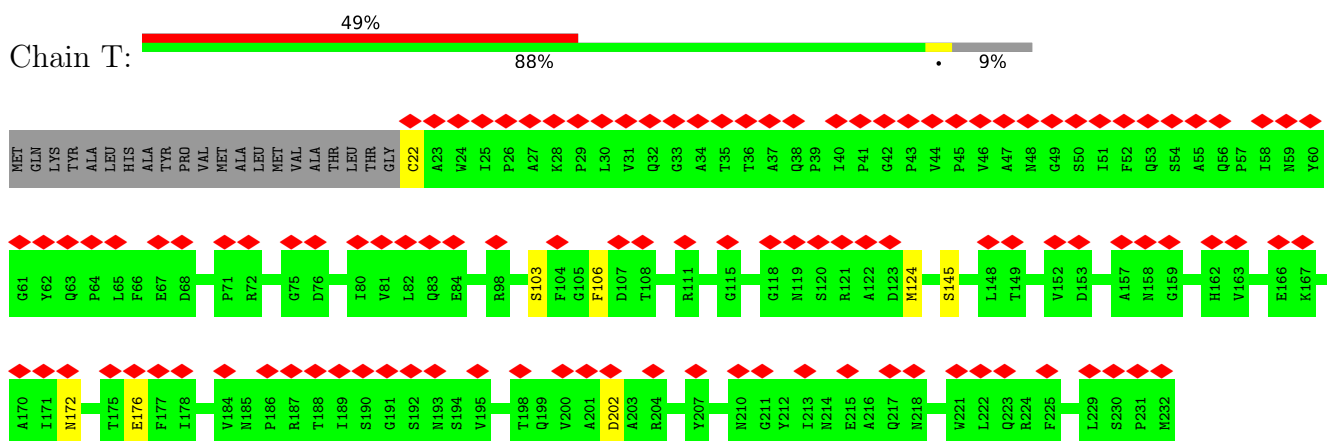
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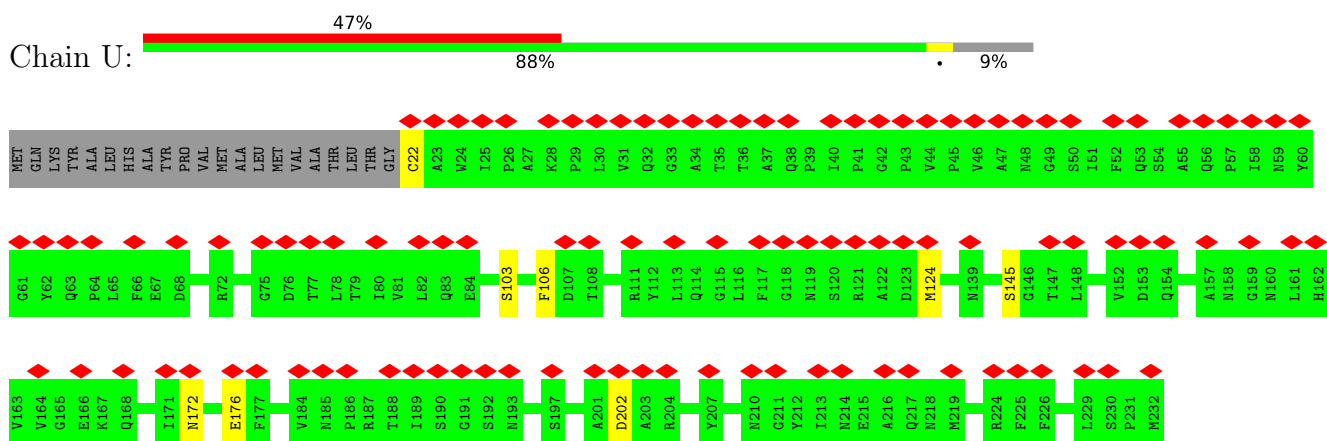
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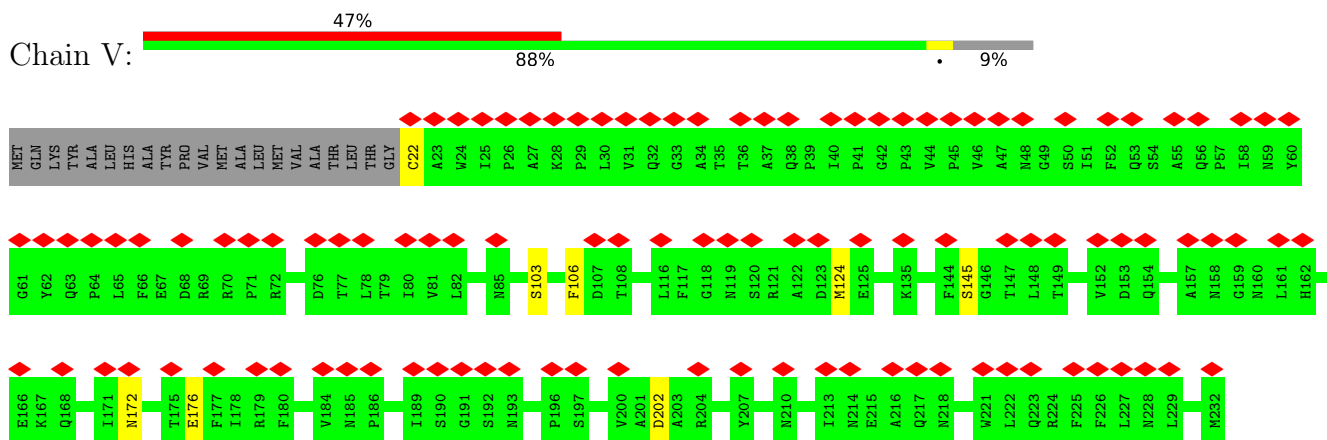
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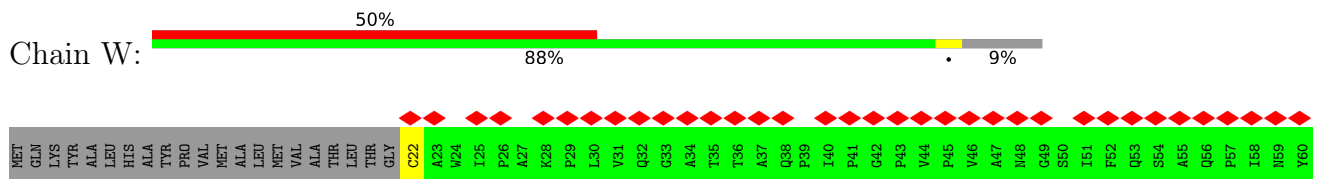
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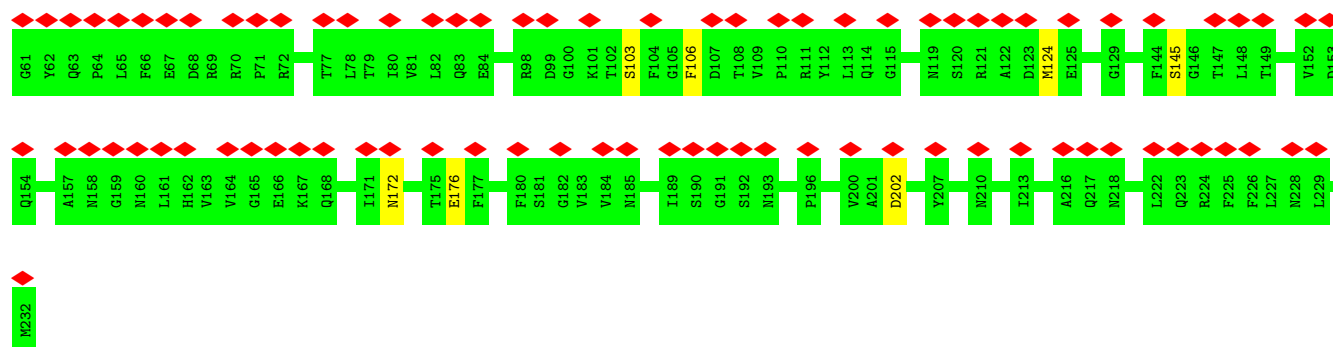


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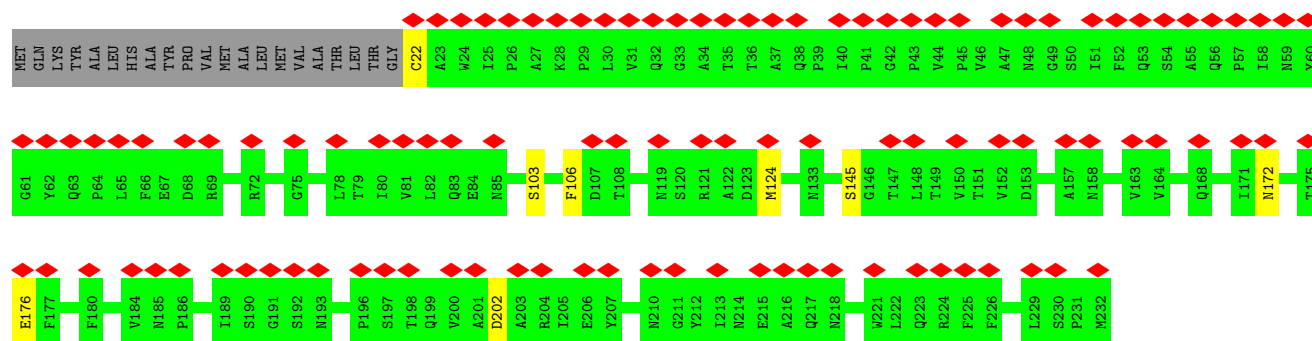
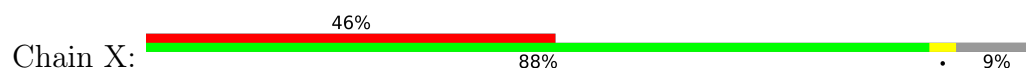


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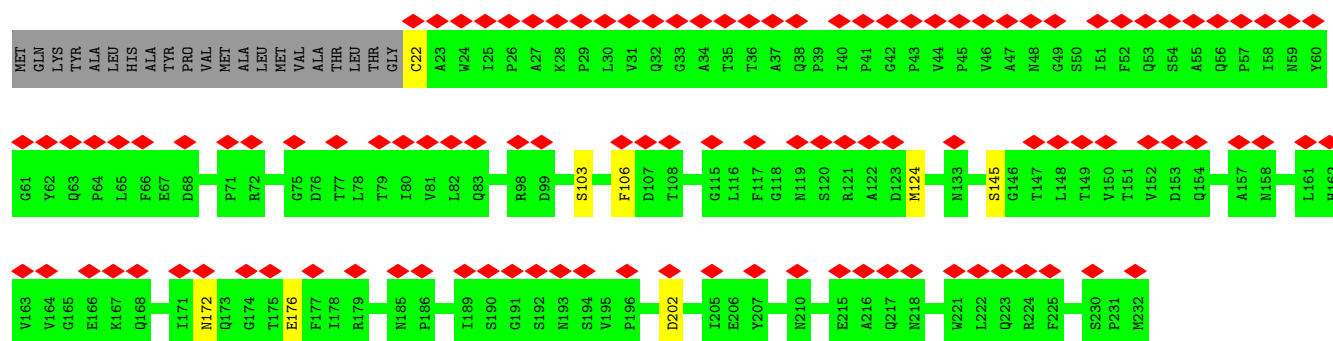
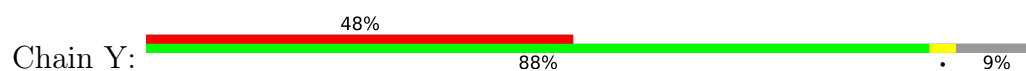




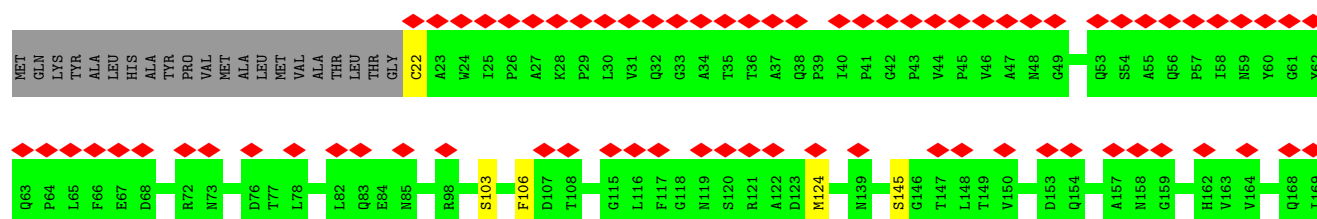
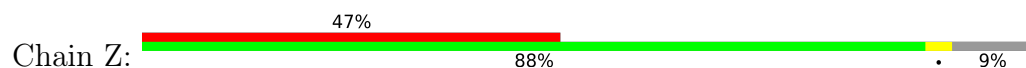
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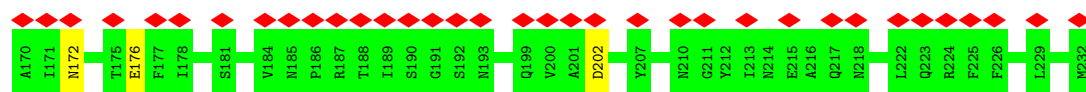


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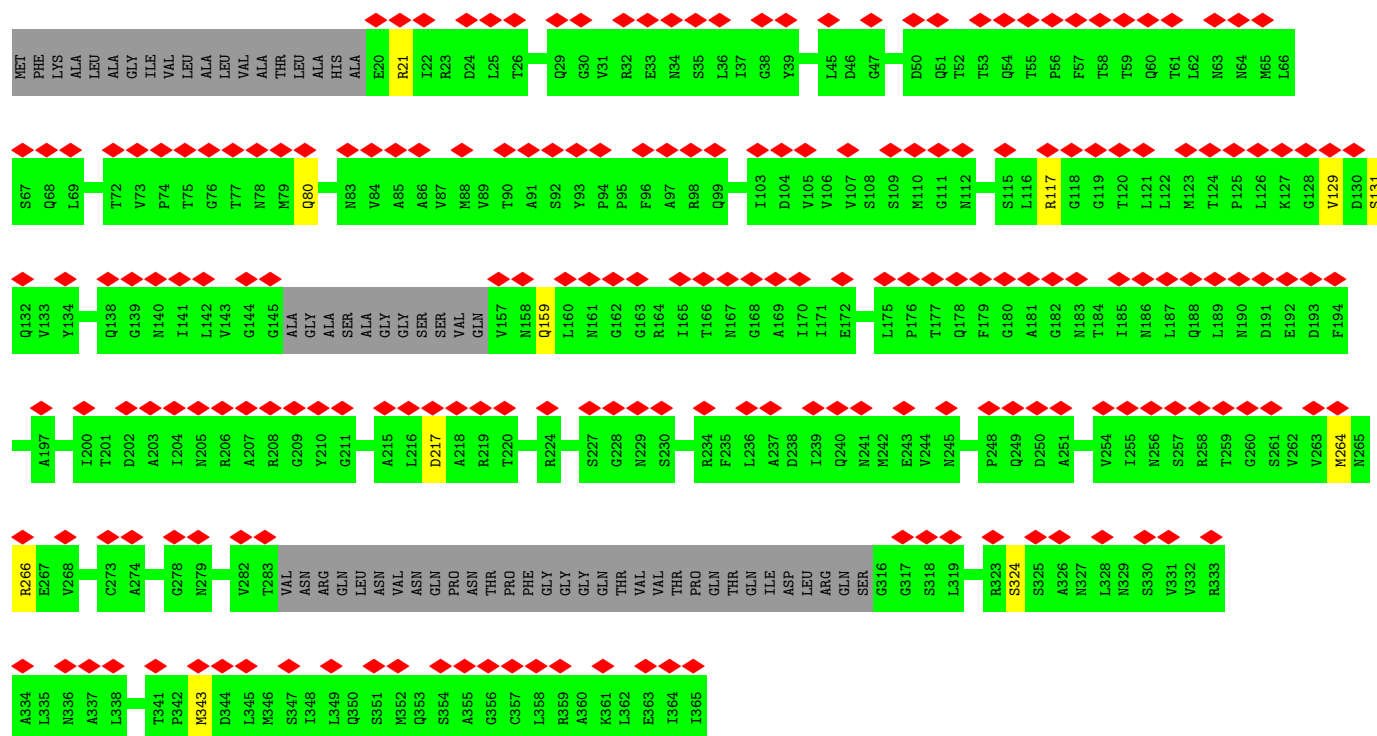
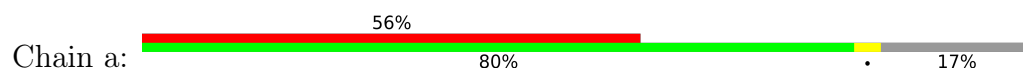


• Molecule 1: Flagellar L-ring protein

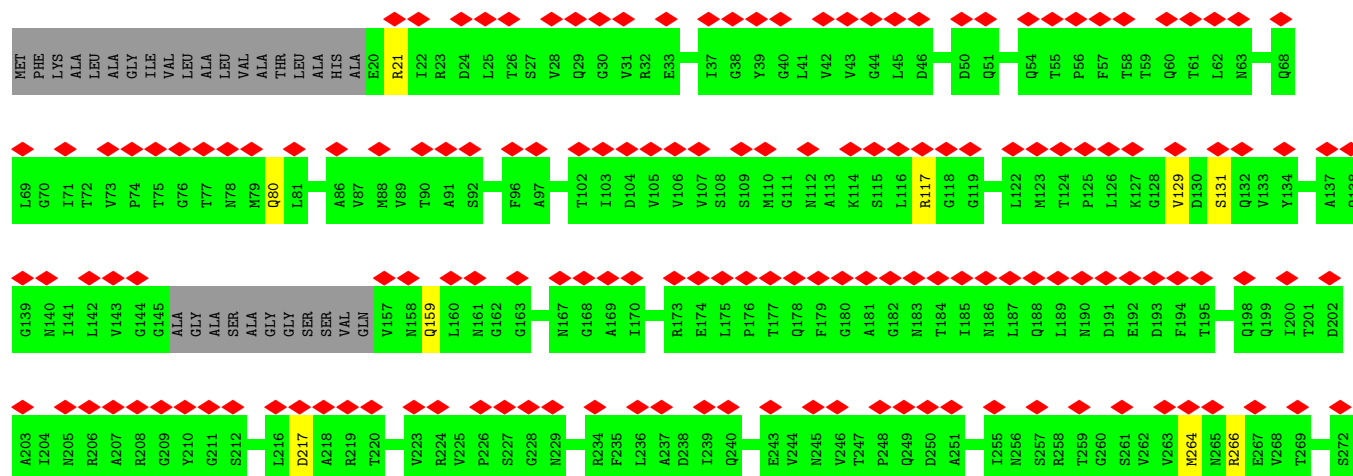
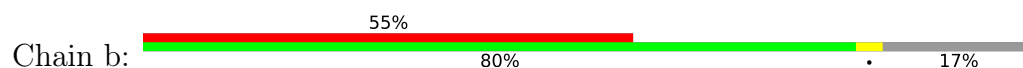


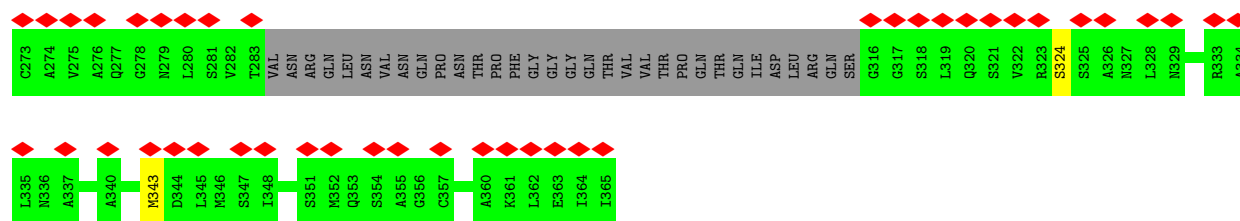


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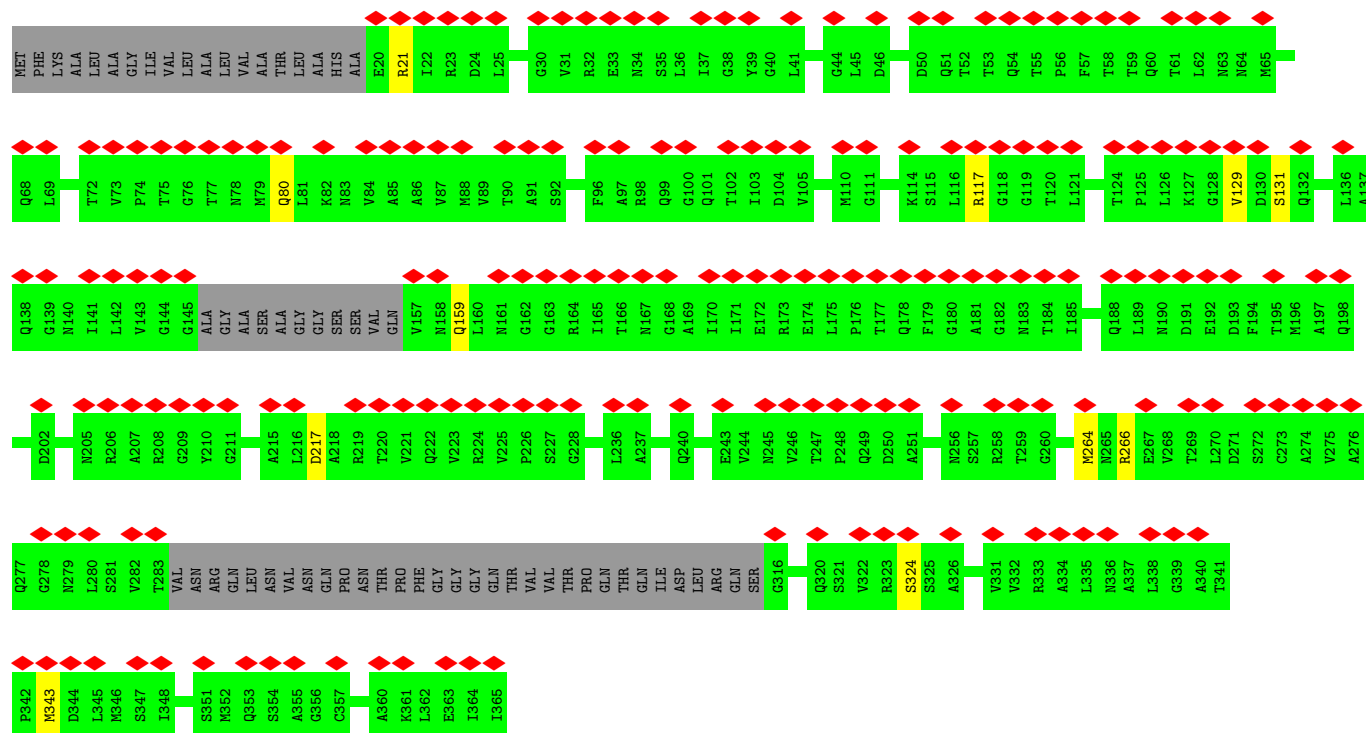
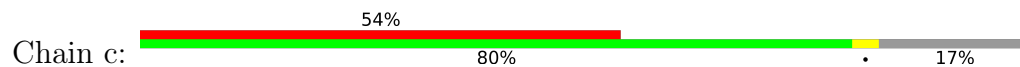


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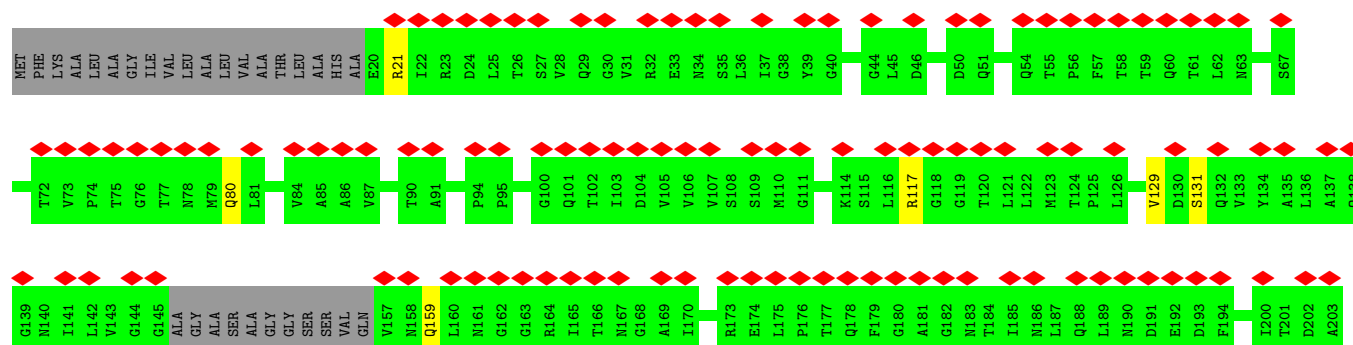
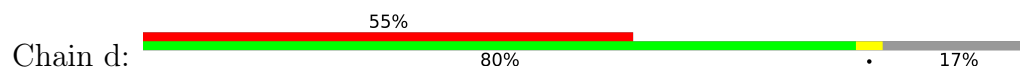




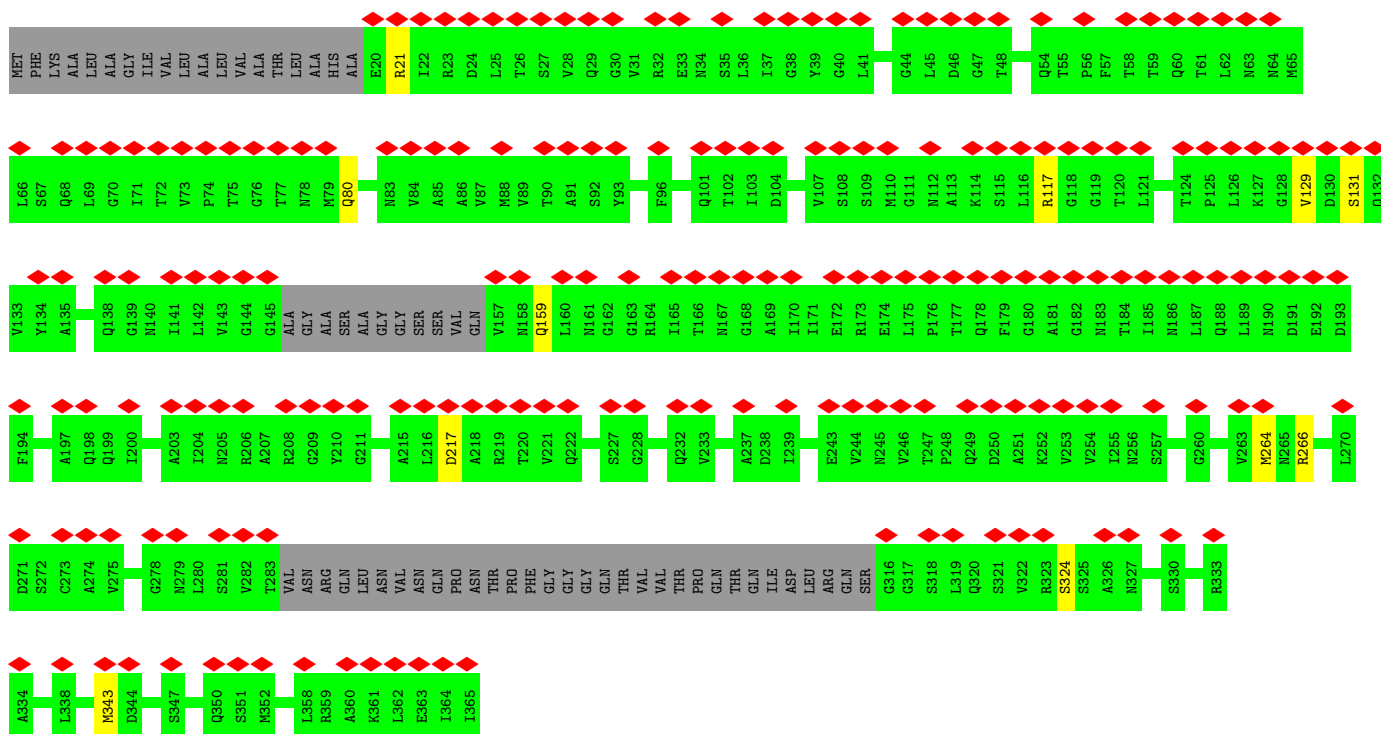
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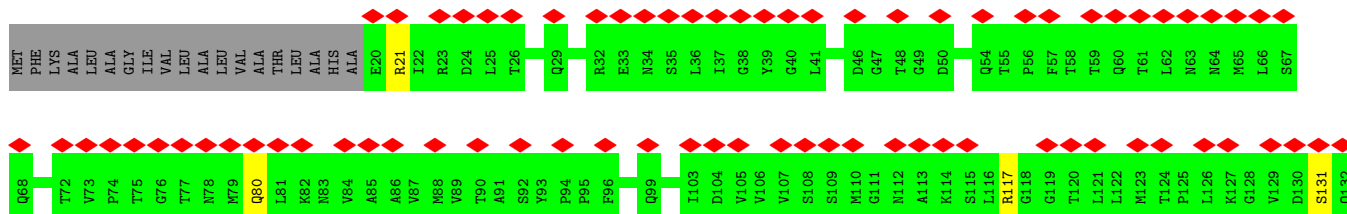
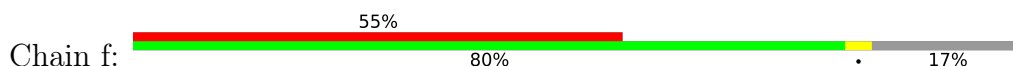
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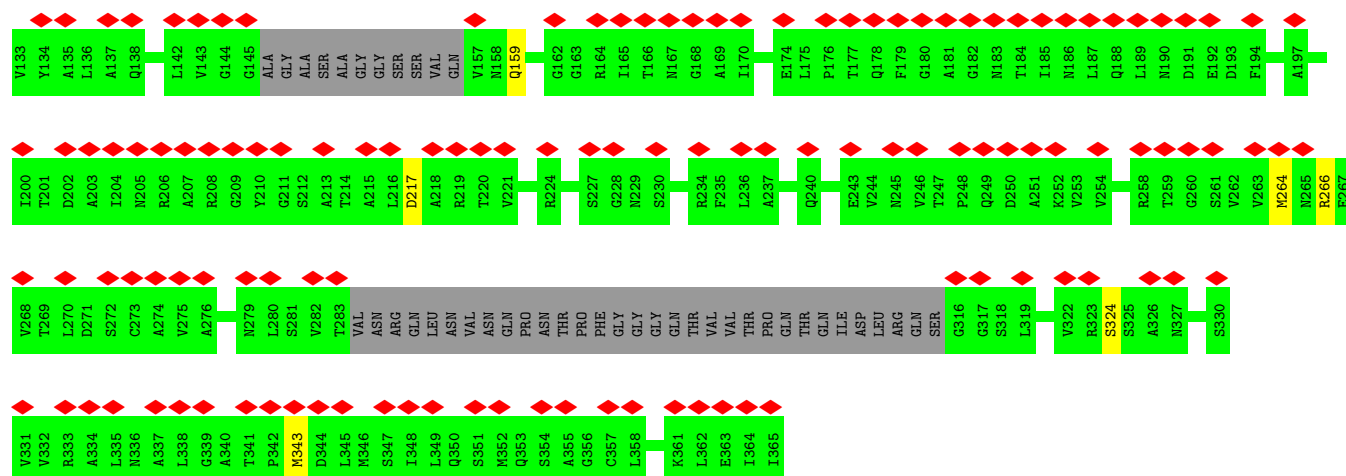


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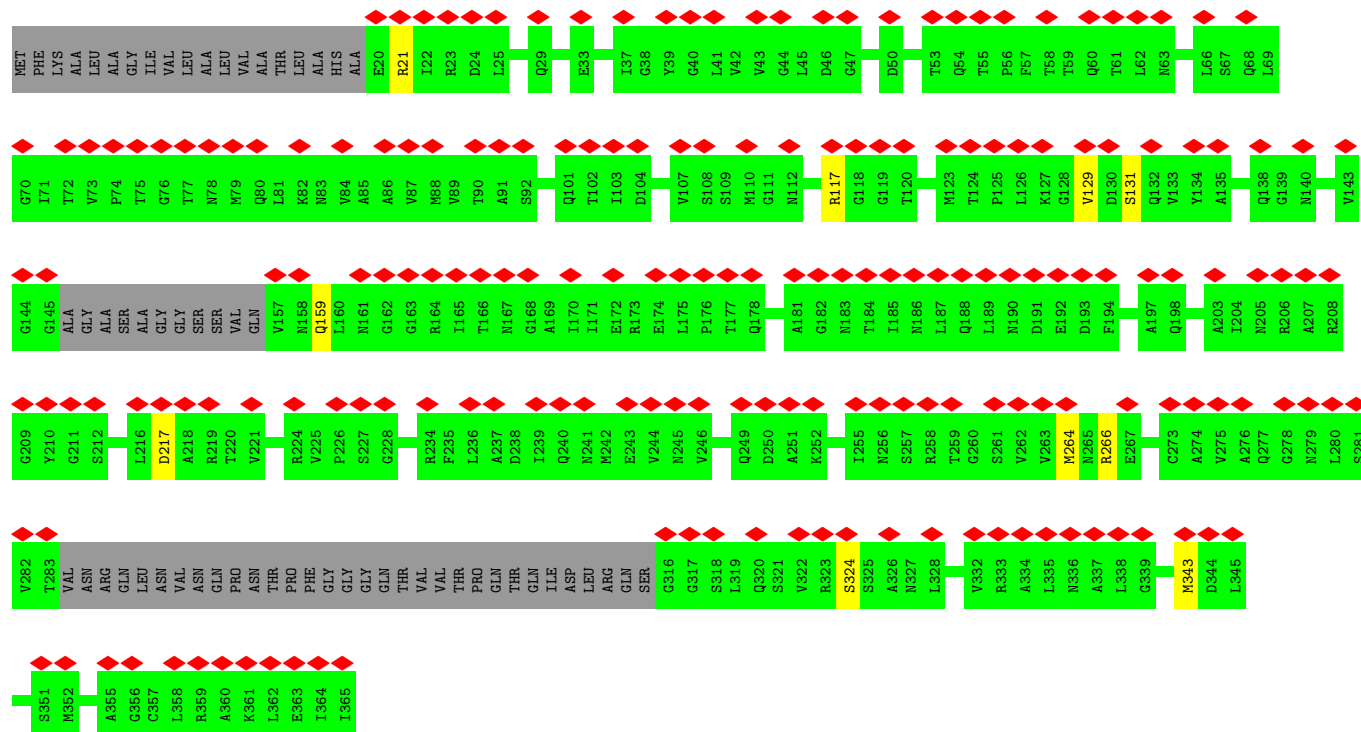
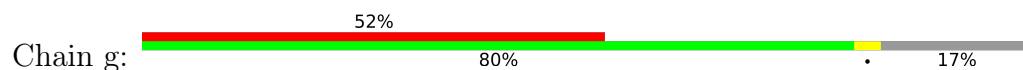


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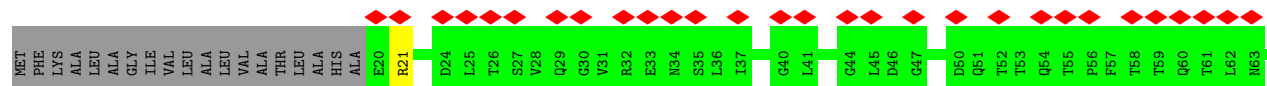
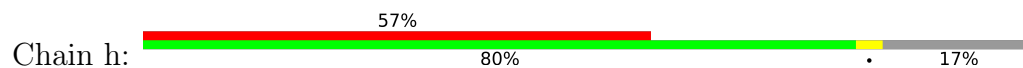




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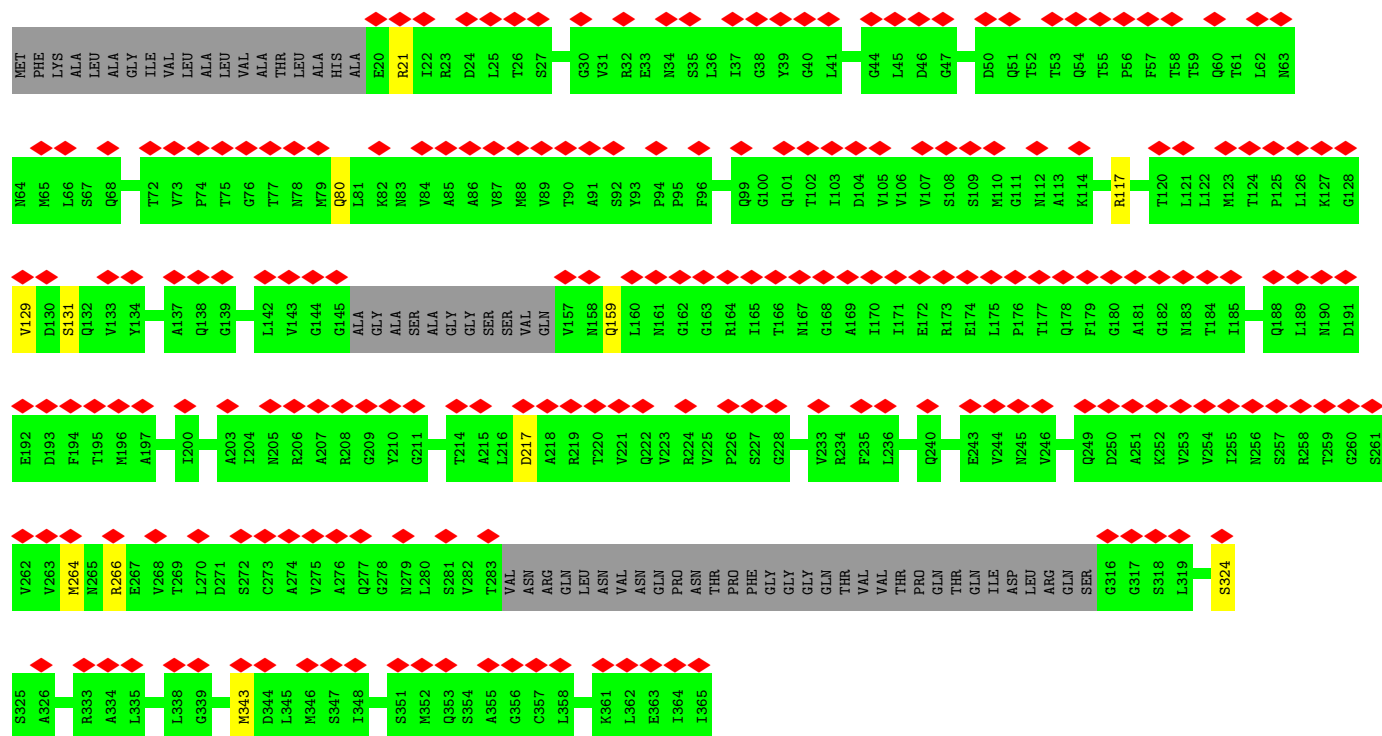
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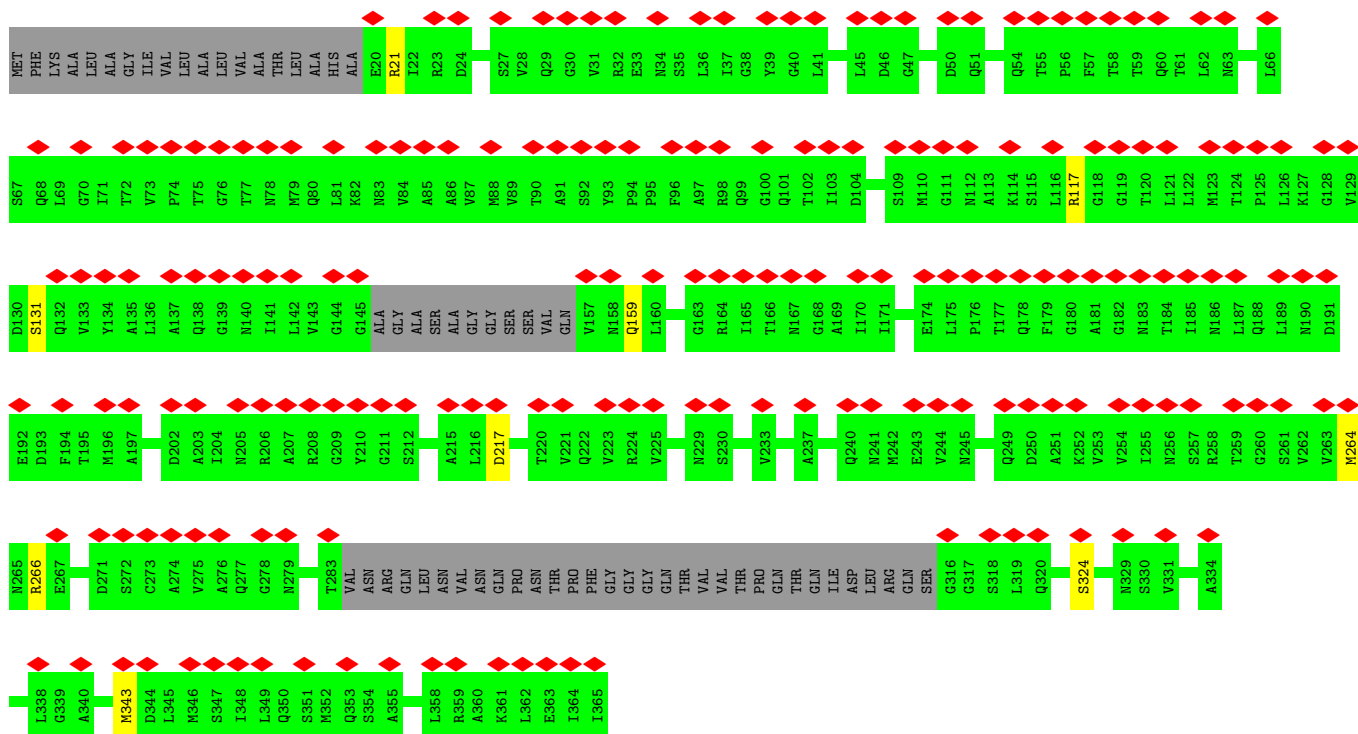
• Molecule 2: Flagellar P-ring protein

Chain i: 57% 80% 17%

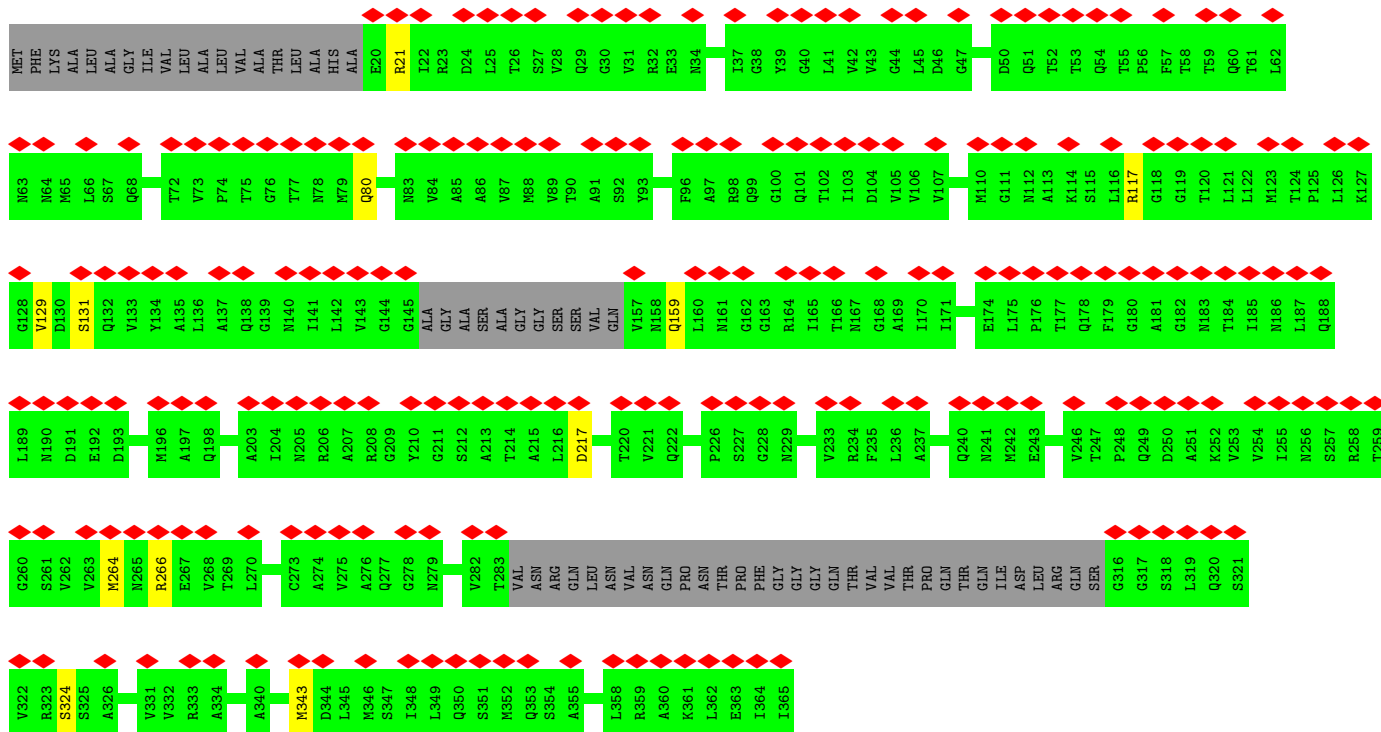
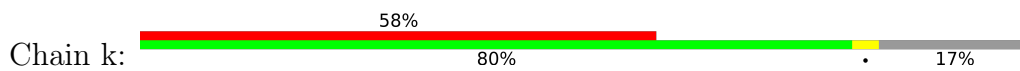


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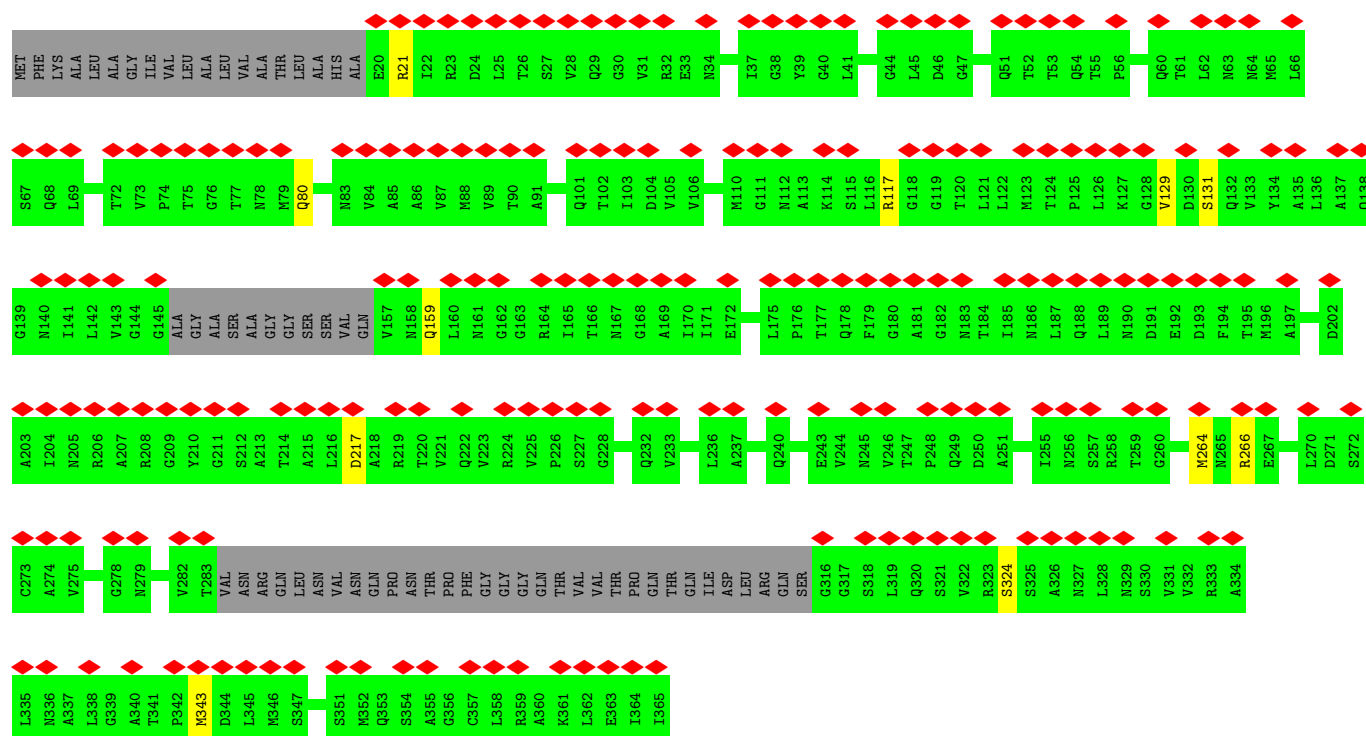
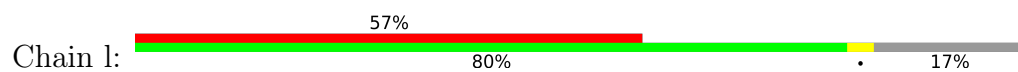
Chain j: 53% 81% 17%



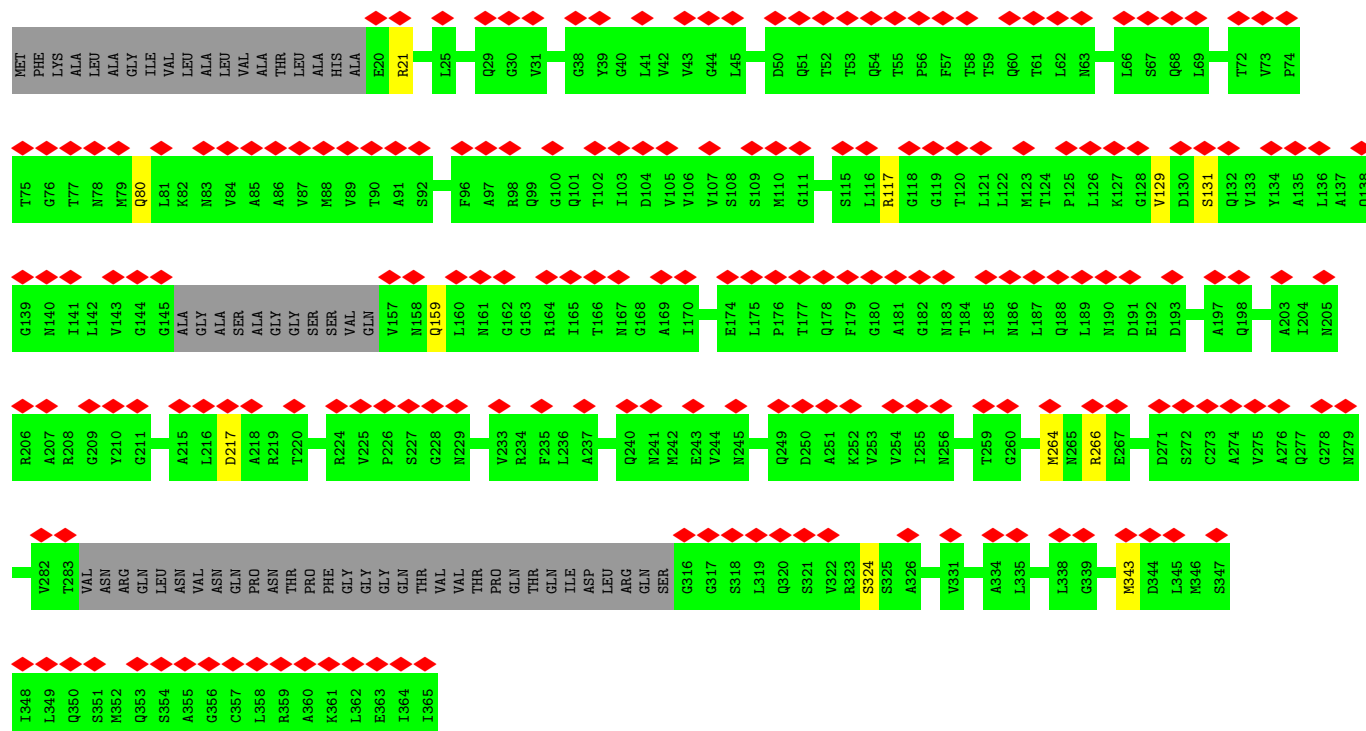
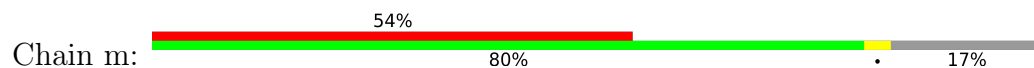
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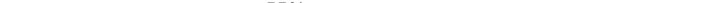


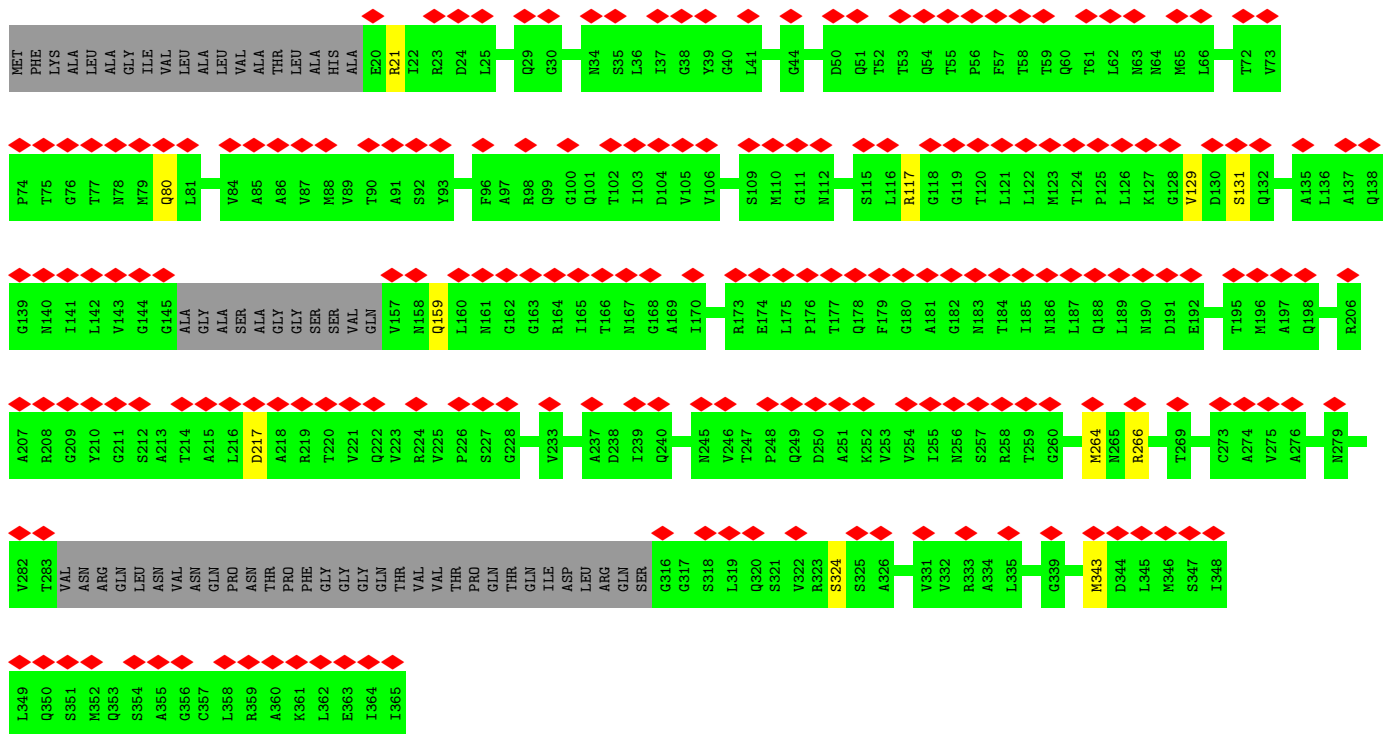
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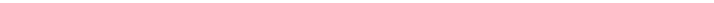


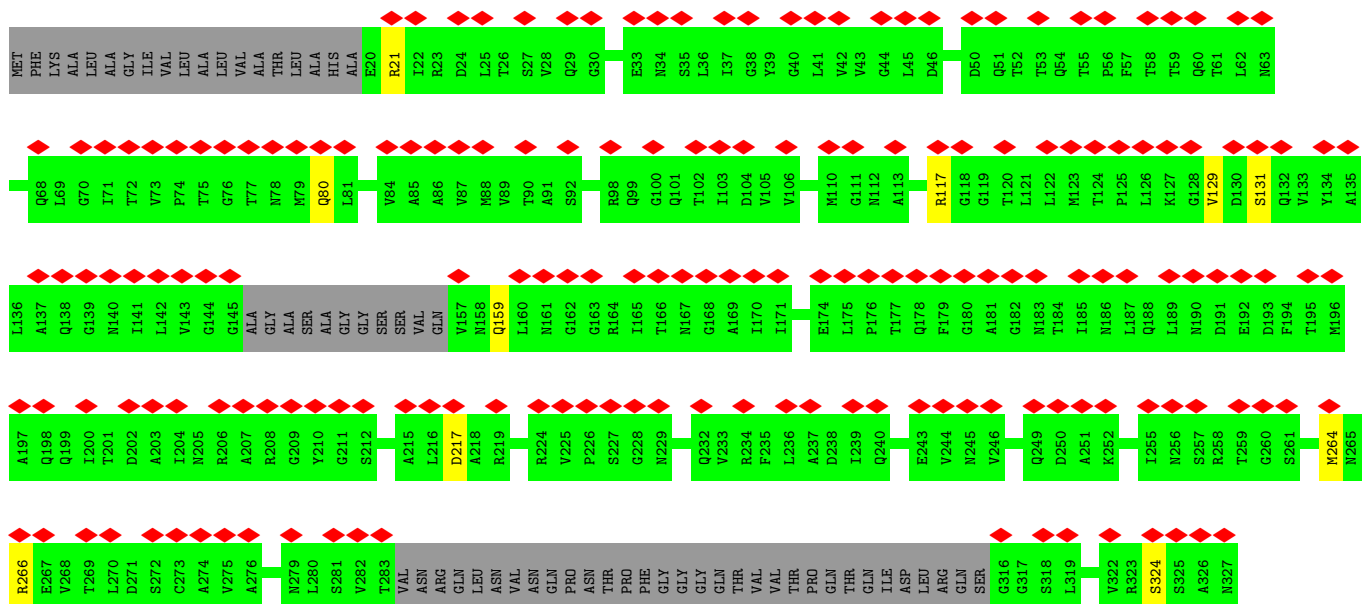
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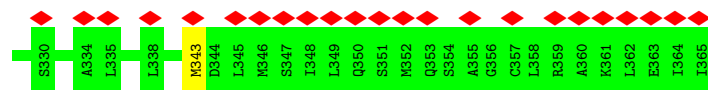


Chain n:  55% 80% 17%

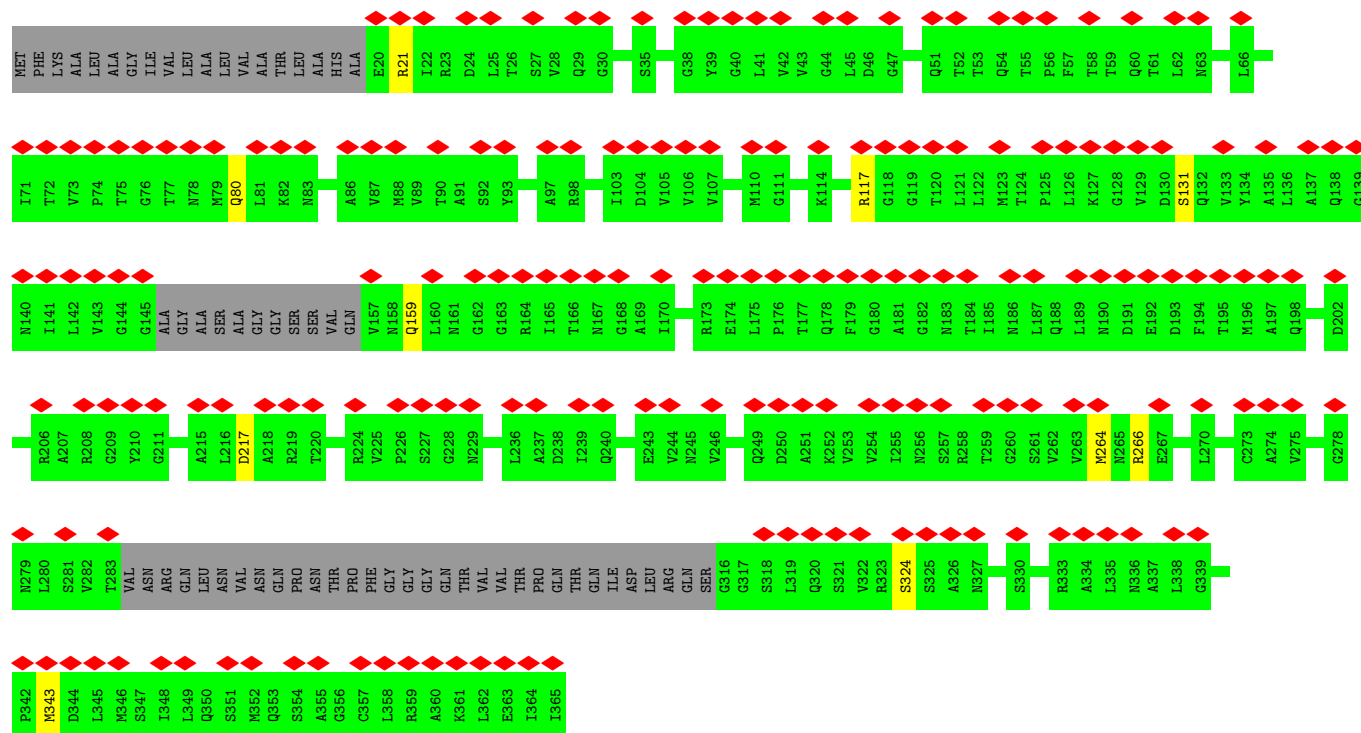
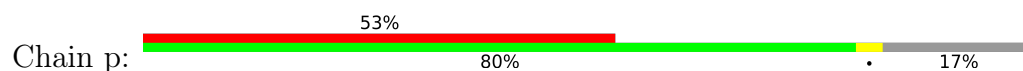


Chain o:  55% 80% 17%

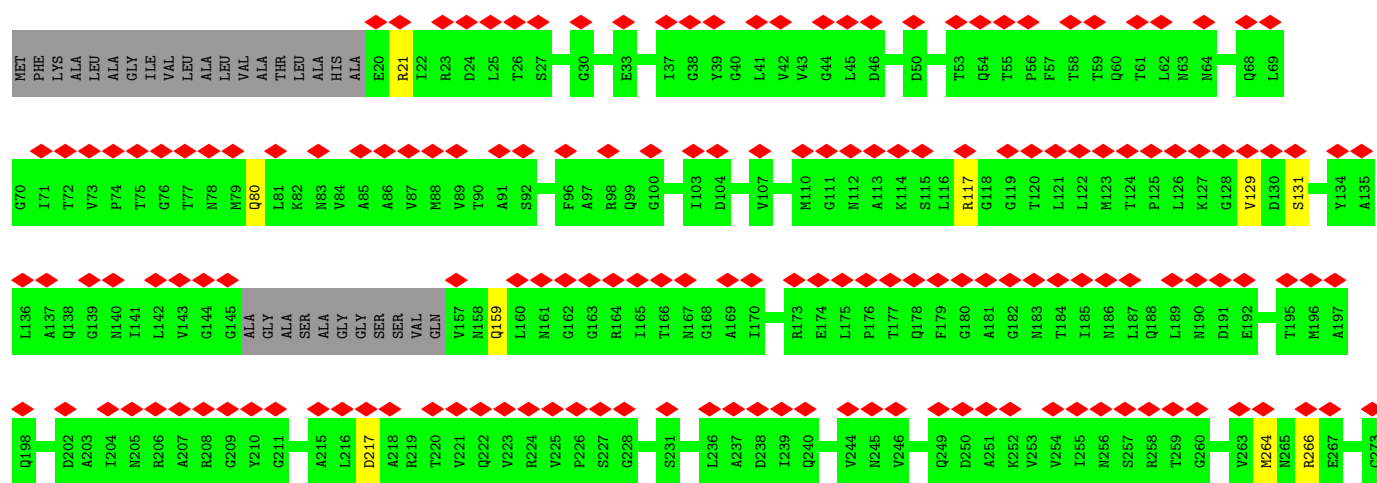
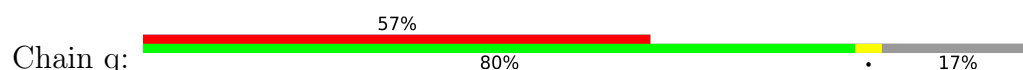


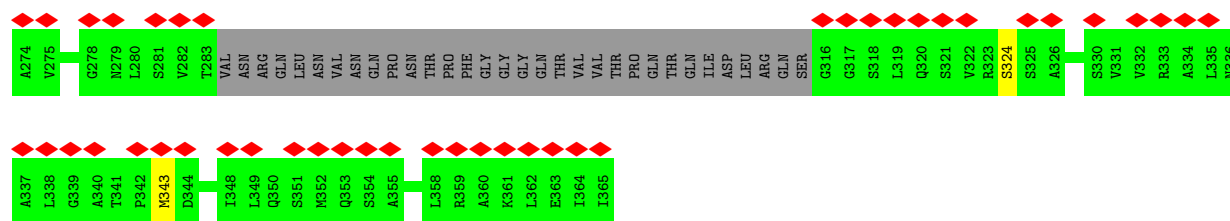


• Molecule 2: Flagellar P-ring protein

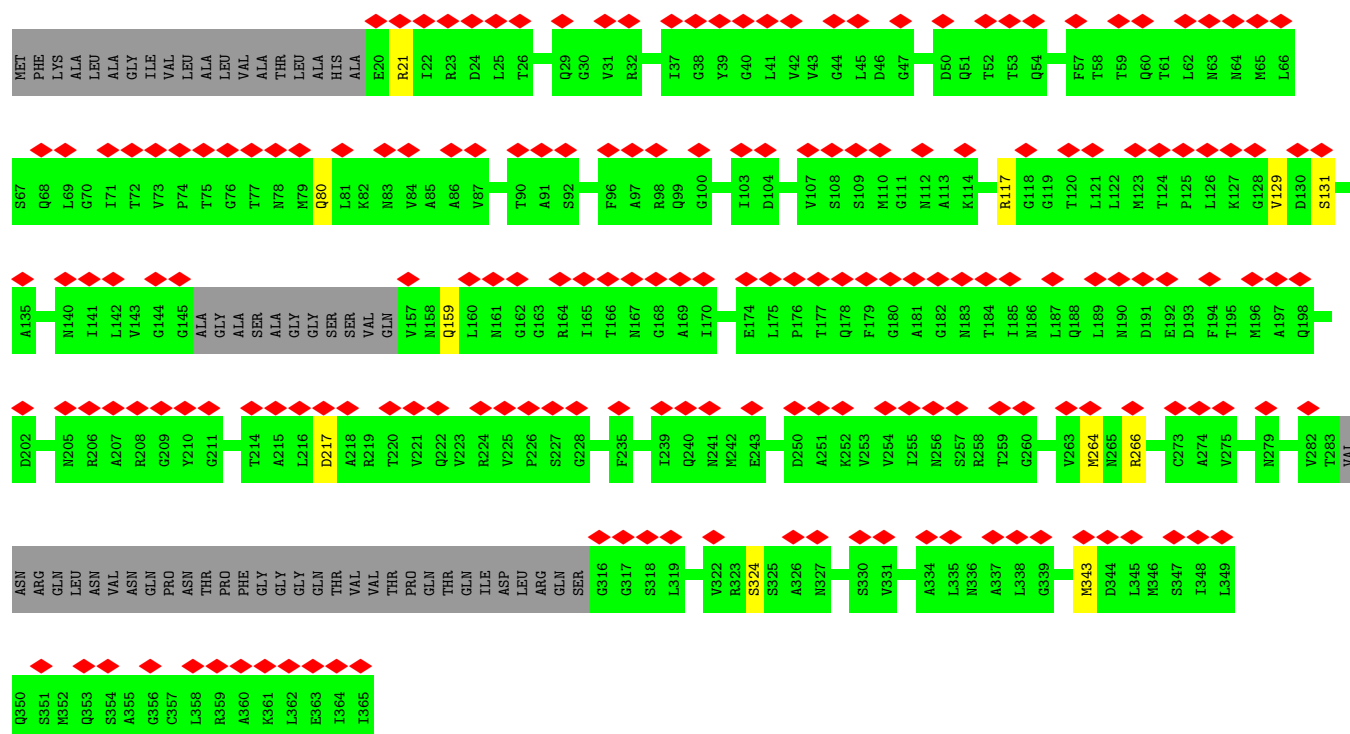
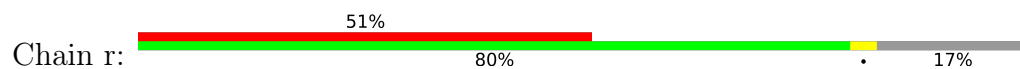


• Molecule 2: Flagellar P-ring protein

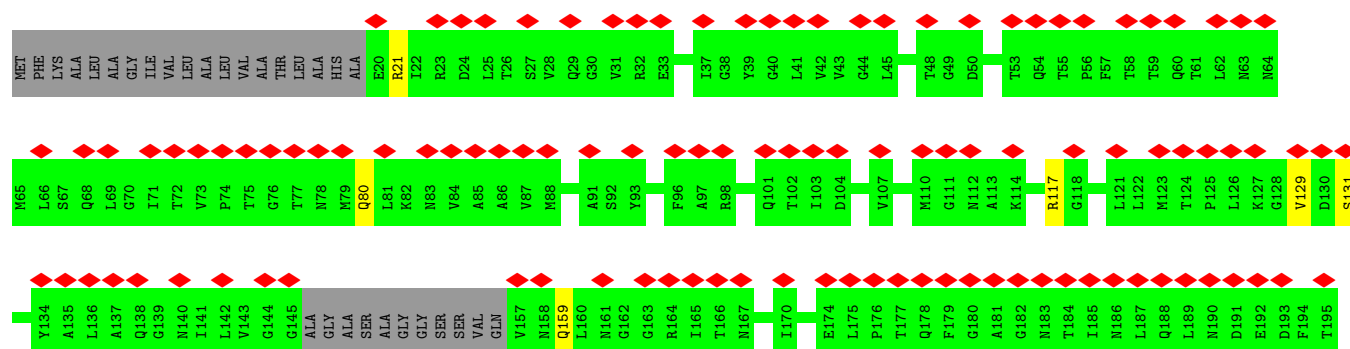


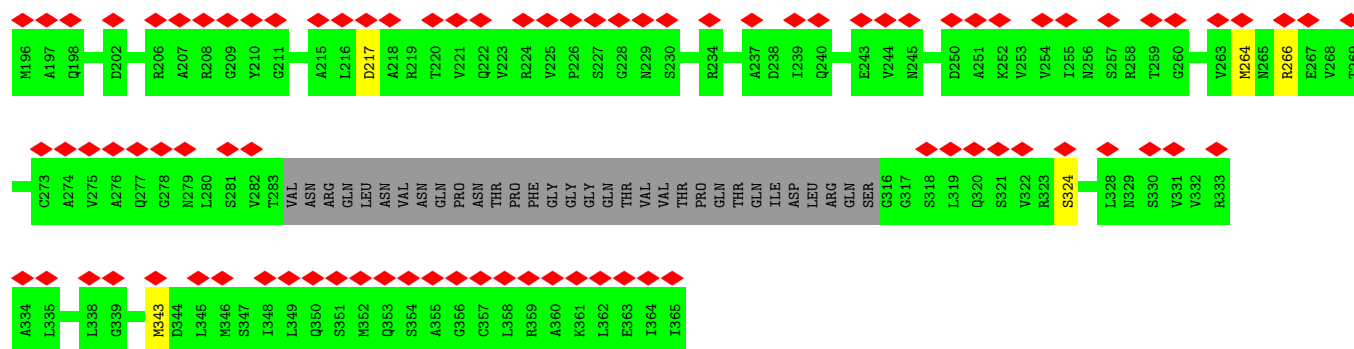


• Molecule 2: Flagellar P-ring protein

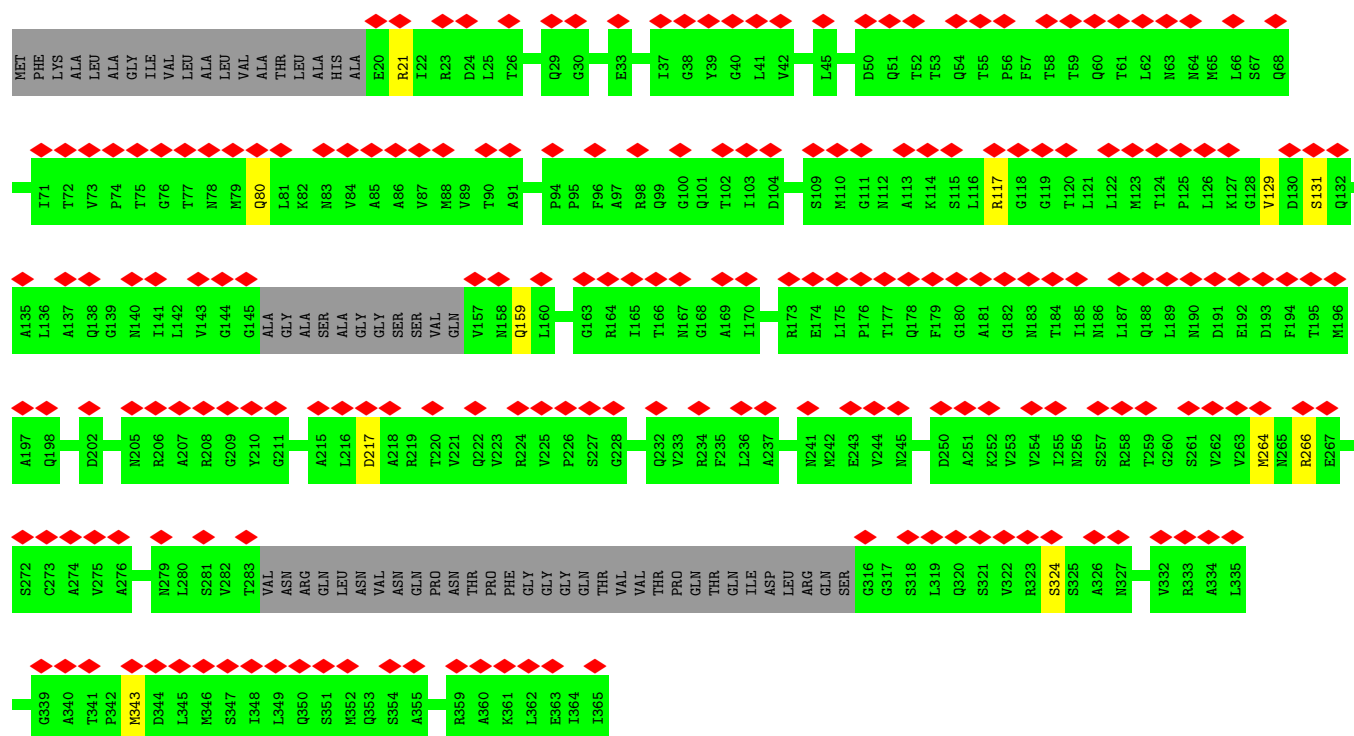


• Molecule 2: Flagellar P-ring protein

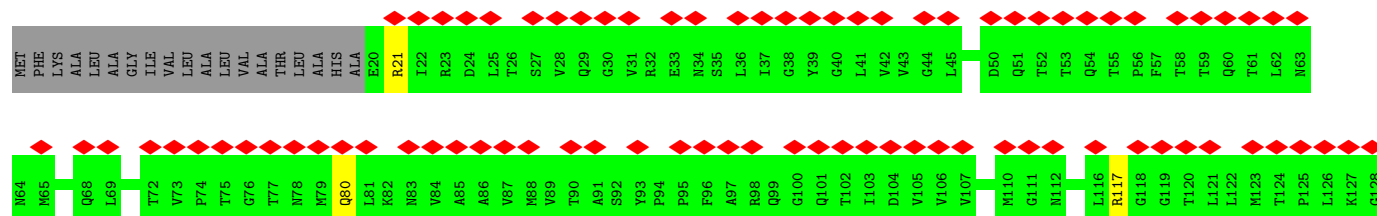
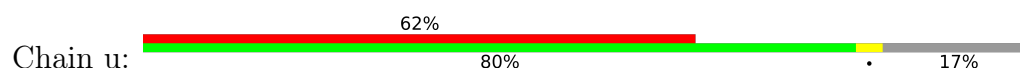


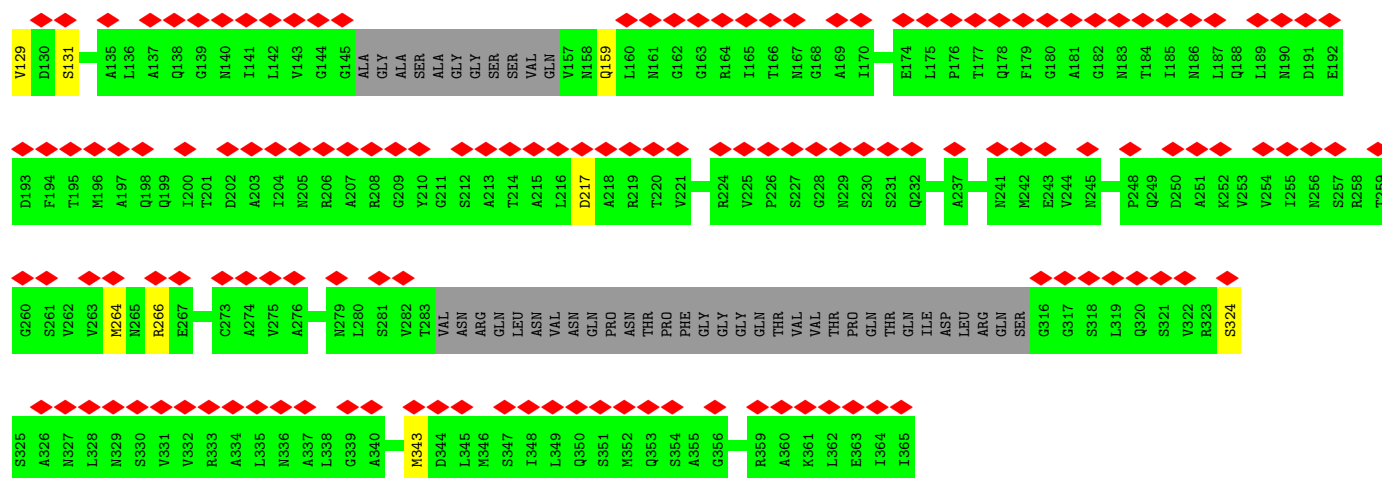


• Molecule 2: Flagellar P-ring protein

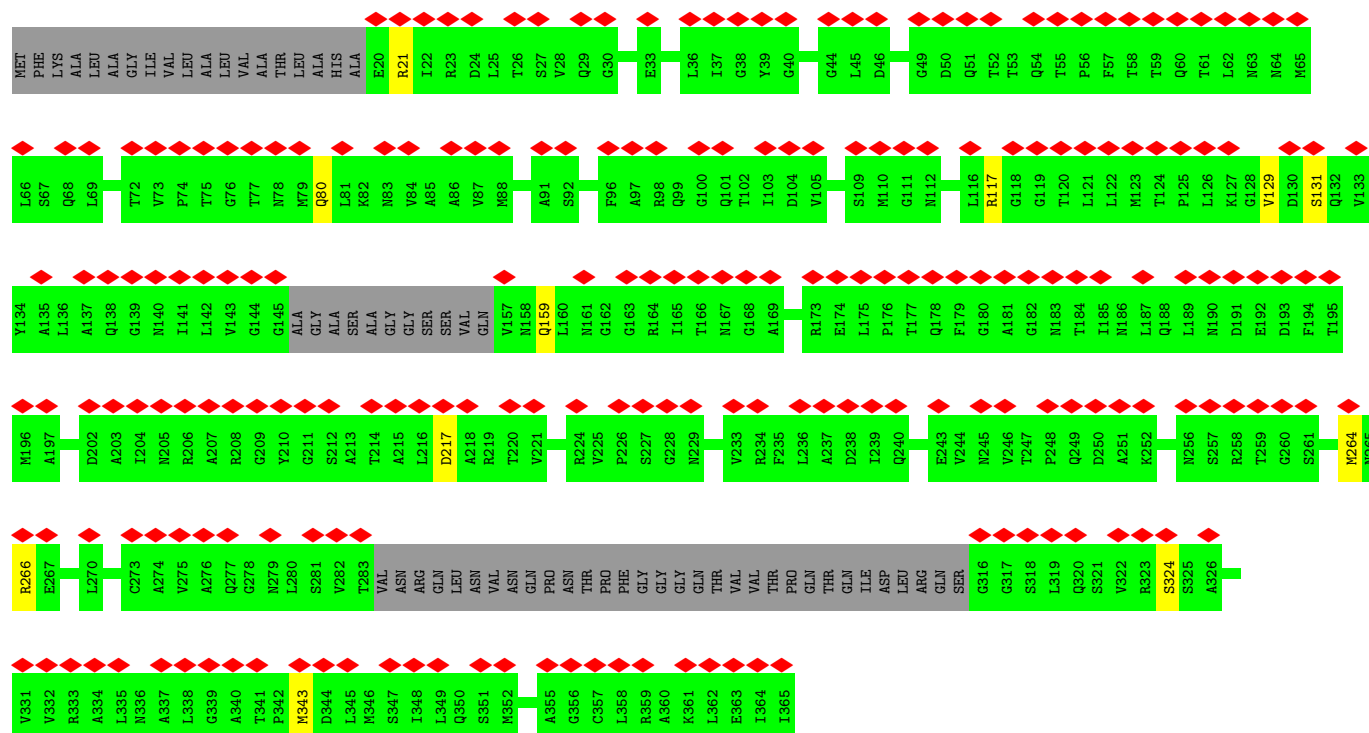
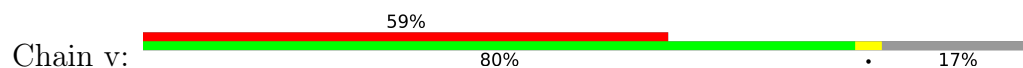


• Molecule 2: Flagellar P-ring protein

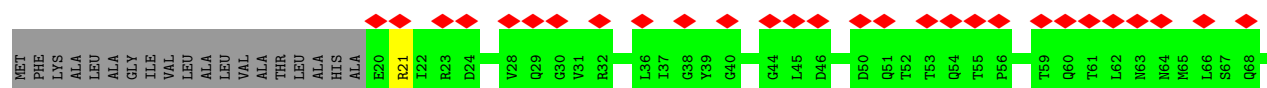
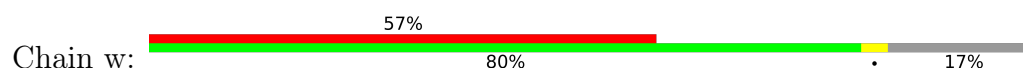


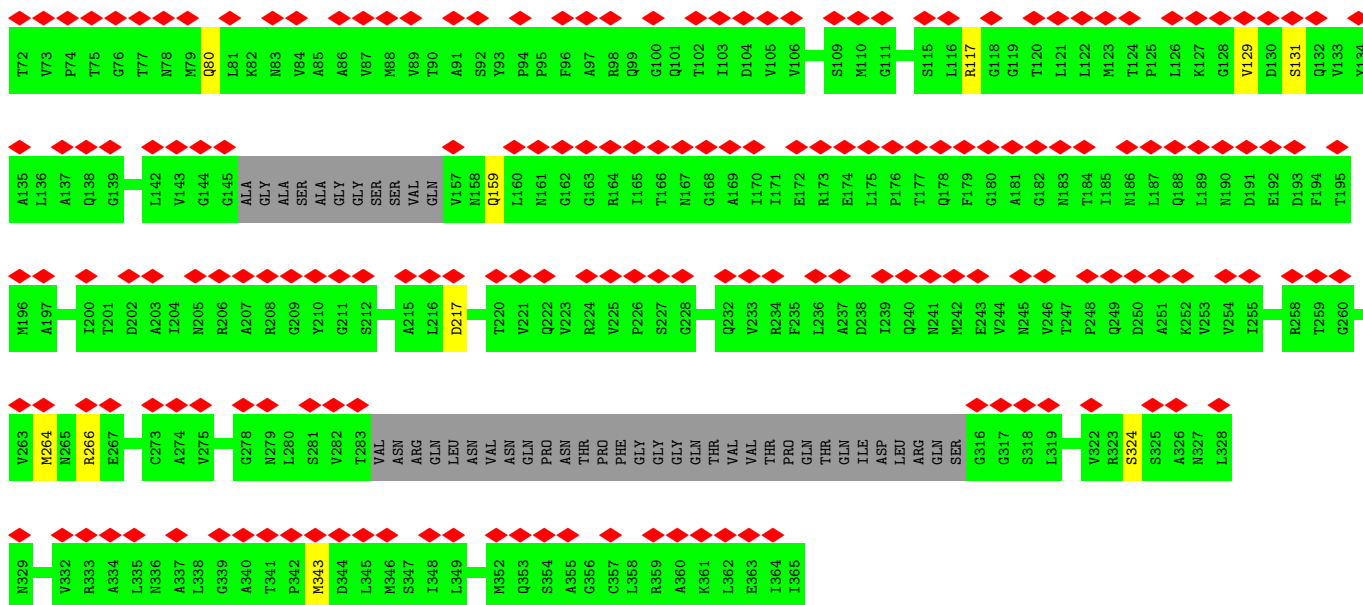


• Molecule 2: Flagellar P-ring protein

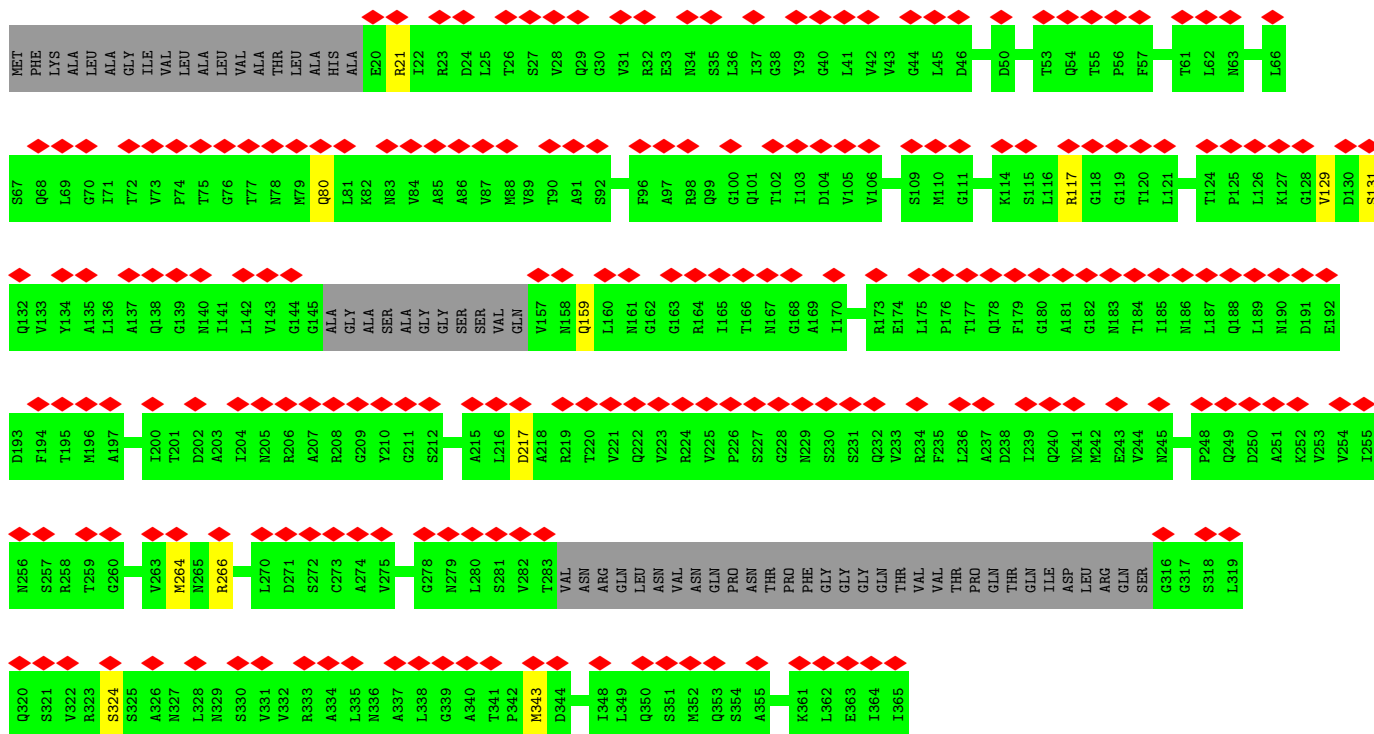
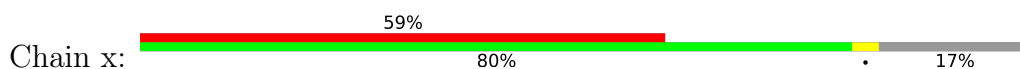


• Molecule 2: Flagellar P-ring protein

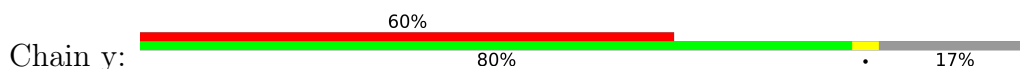


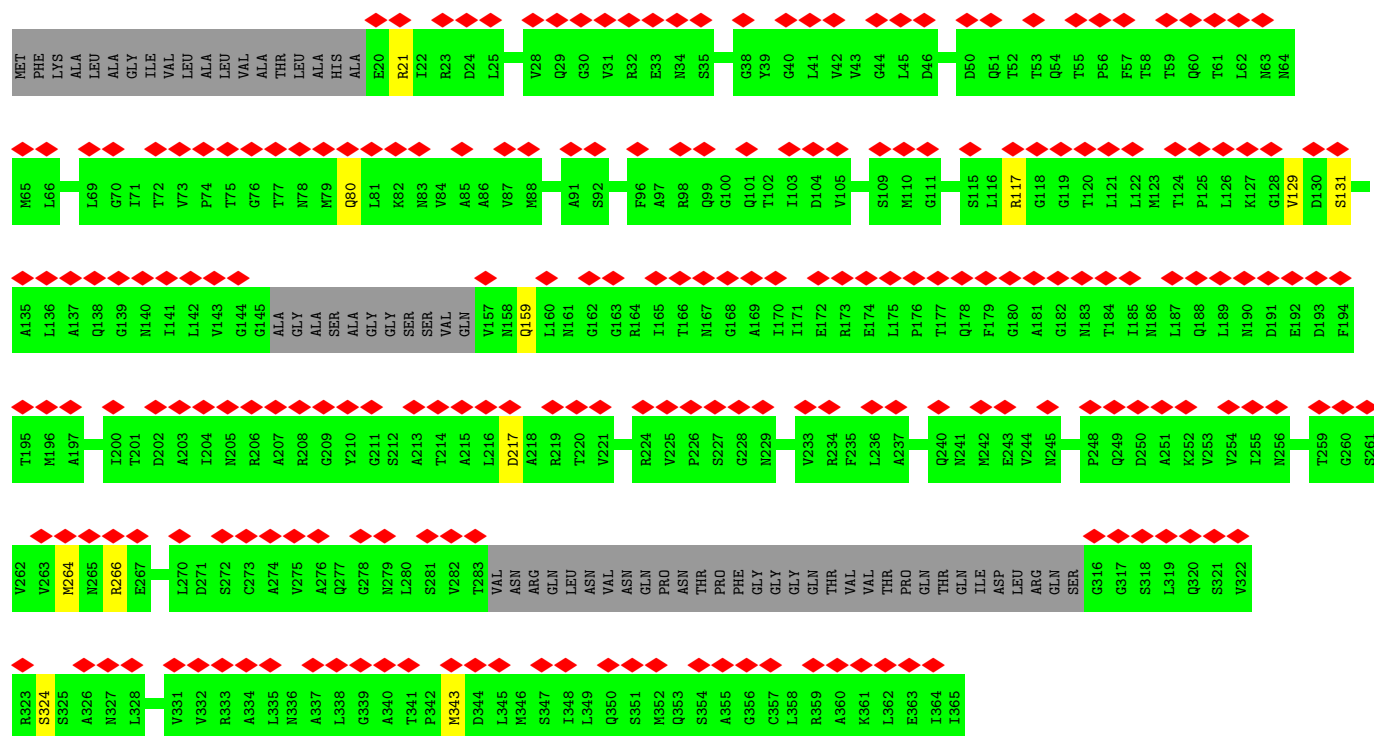


- Molecule 2: Flagellar P-ring protein

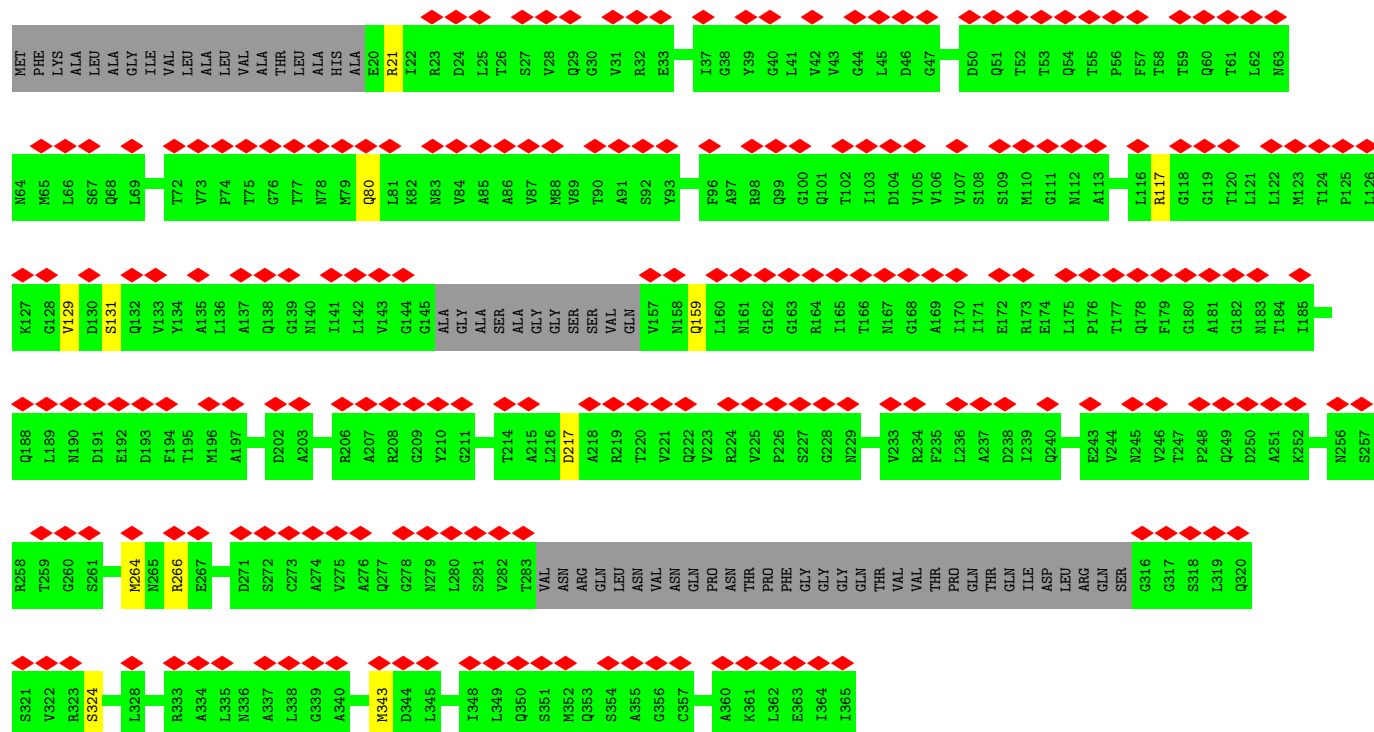
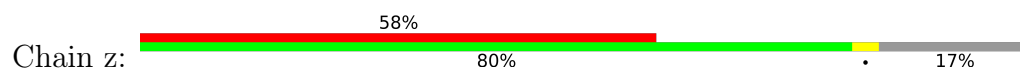


- Molecule 2: Flagellar P-ring protein



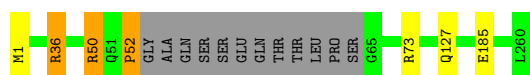


• Molecule 2: Flagellar P-ring protein



• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 0:  93% .. 5%



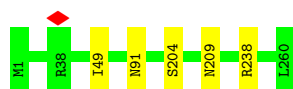
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain 1:  93% ..



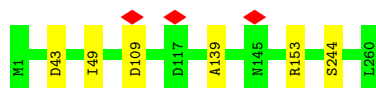
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain 2:  98% .



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain 3:  98% .



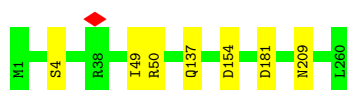
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain 4:  97% .



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain 5:  97% .



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain 6:  97% .



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain 7:  98% .



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain 8:  98% .



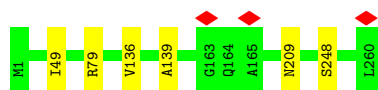
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain 9:  97% .



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZA:  98% .



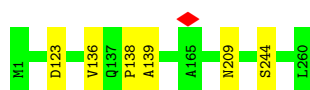
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZB:  96% .



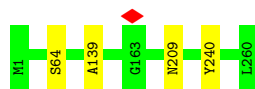
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZC:  98% .



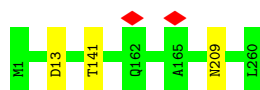
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZD:  98% .



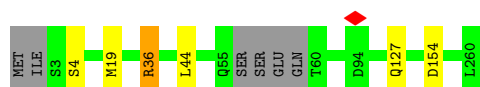
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZE:  99%



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AF:  95%



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AG:  95%



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AH:  94%



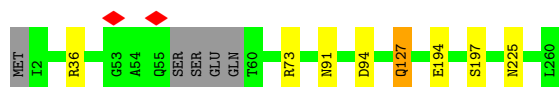
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AI:  93%



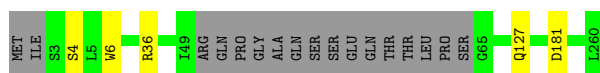
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AJ:  95%



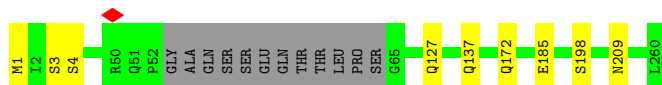
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AK:  92%



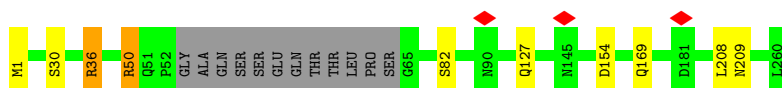
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AL: 92% 5%



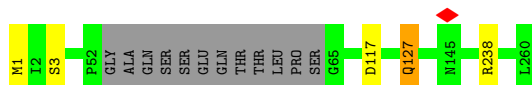
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AM: 92% 5%



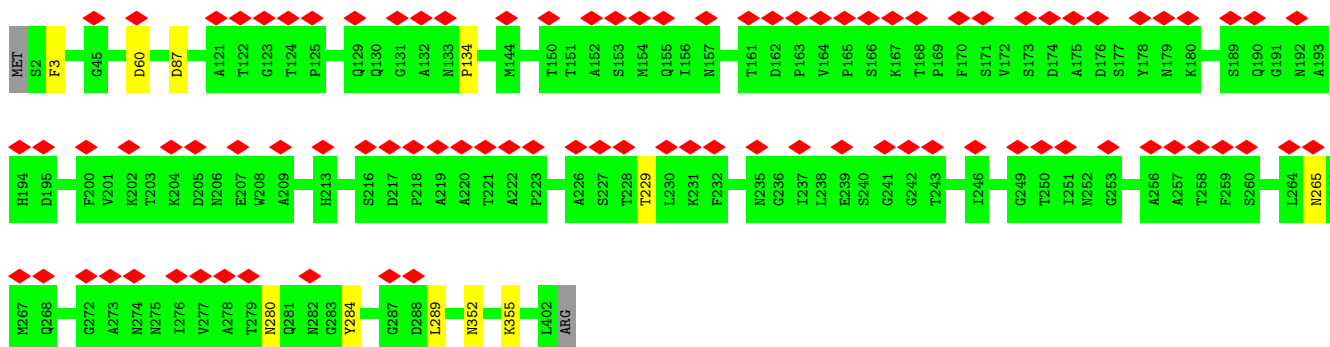
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AN: 93% 5%



- Molecule 4: Flagellar hook protein FlgE

Chain ZF: 23% 97% 5%



- Molecule 4: Flagellar hook protein FlgE

Chain ZG: 95% 5%



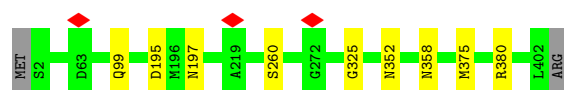
- Molecule 4: Flagellar hook protein FlgE

Chain ZH:  97%



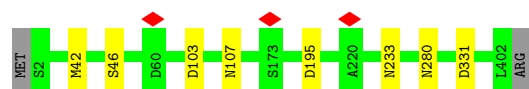
- Molecule 4: Flagellar hook protein FlgE

Chain ZI:  97%



- Molecule 4: Flagellar hook protein FlgE

Chain ZJ:  98%



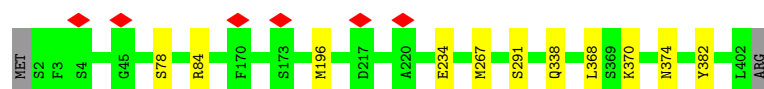
- Molecule 4: Flagellar hook protein FlgE

Chain ZK:  98%



- Molecule 4: Flagellar hook protein FlgE

Chain ZL:  97%



- Molecule 4: Flagellar hook protein FlgE

Chain ZM:  97%



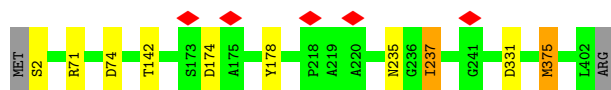
- Molecule 4: Flagellar hook protein FlgE

Chain ZN:  97%



- Molecule 4: Flagellar hook protein FlgE

Chain ZO:  97%



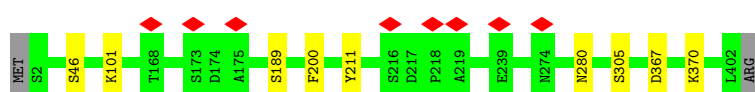
- Molecule 4: Flagellar hook protein FlgE

Chain ZP:  95%



- Molecule 4: Flagellar hook protein FlgE

Chain ZQ:  97%



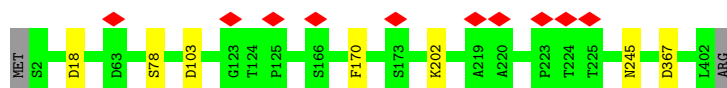
- Molecule 4: Flagellar hook protein FlgE

Chain ZR:  97%



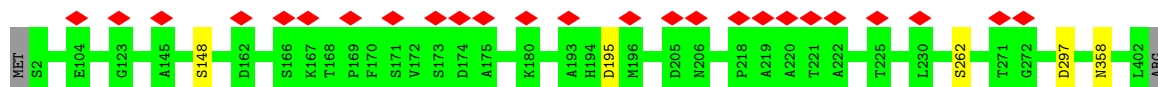
- Molecule 4: Flagellar hook protein FlgE

Chain ZS:  98%



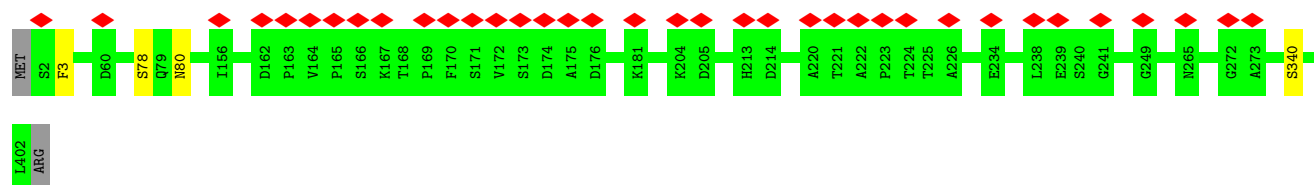
- Molecule 4: Flagellar hook protein FlgE

Chain ZT:  98%

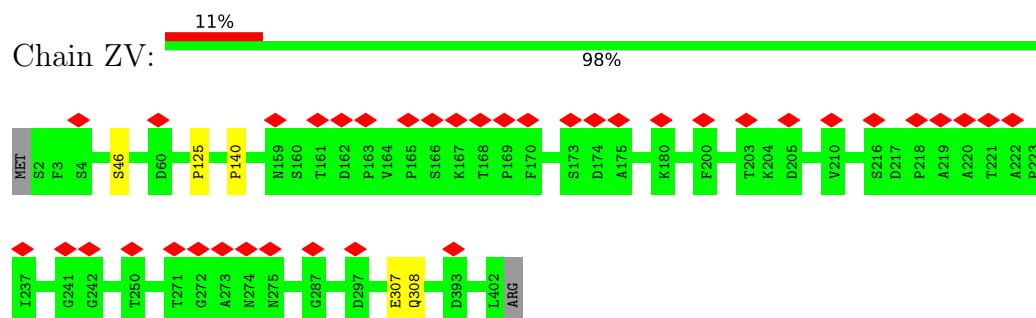


- Molecule 4: Flagellar hook protein FlgE

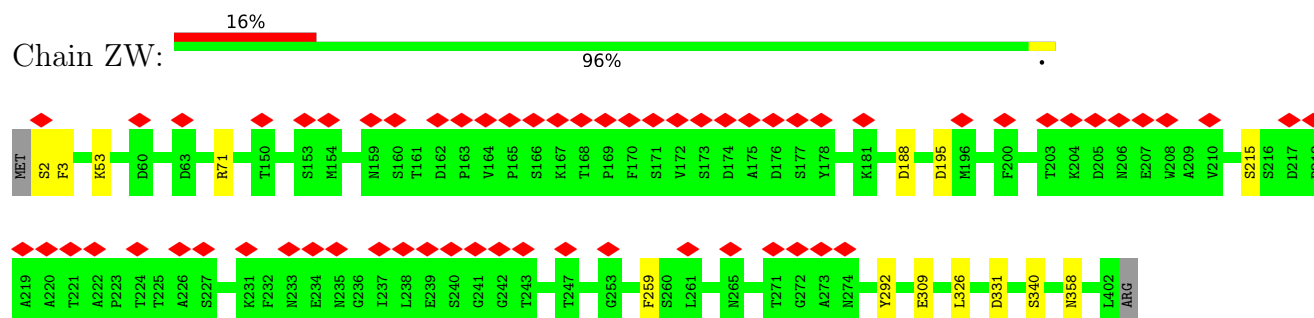
Chain ZU:  99%



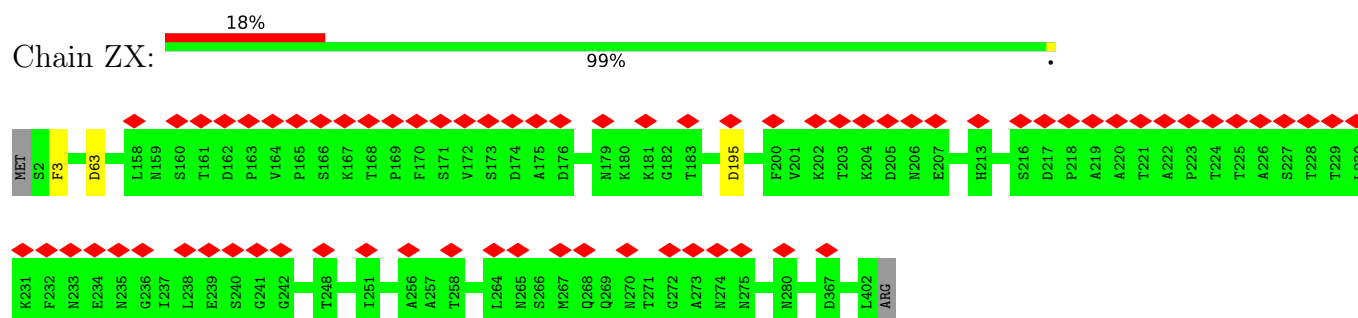
• Molecule 4: Flagellar hook protein FlgE



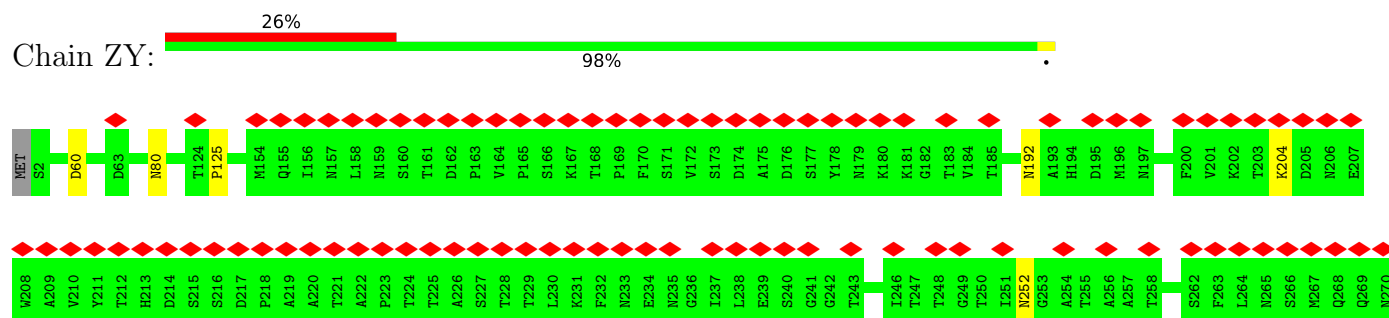
• Molecule 4: Flagellar hook protein FlgE

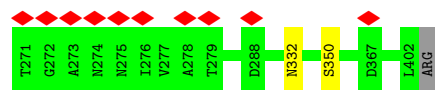


• Molecule 4: Flagellar hook protein FlgE

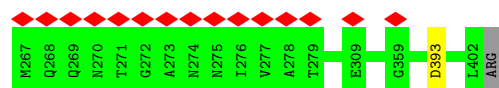
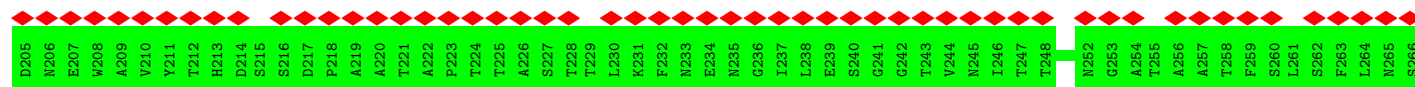
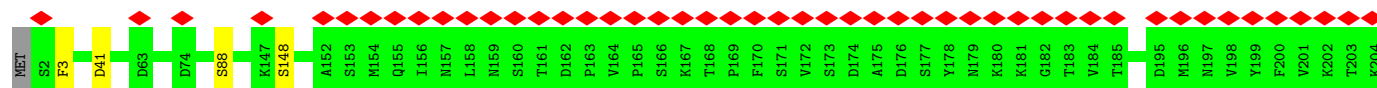


• Molecule 4: Flagellar hook protein FlgE

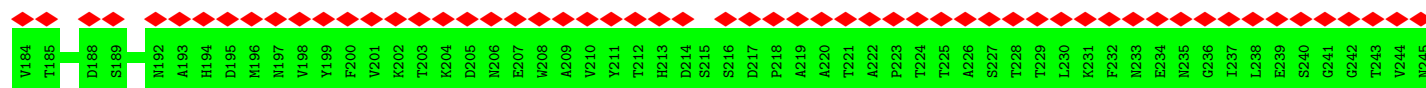
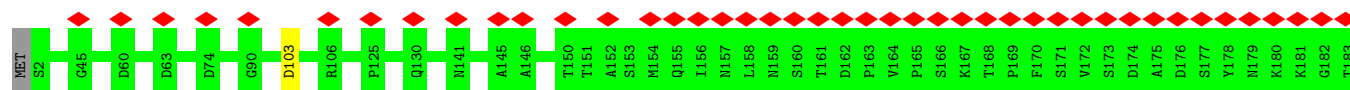




• Molecule 4: Flagellar hook protein FlgE



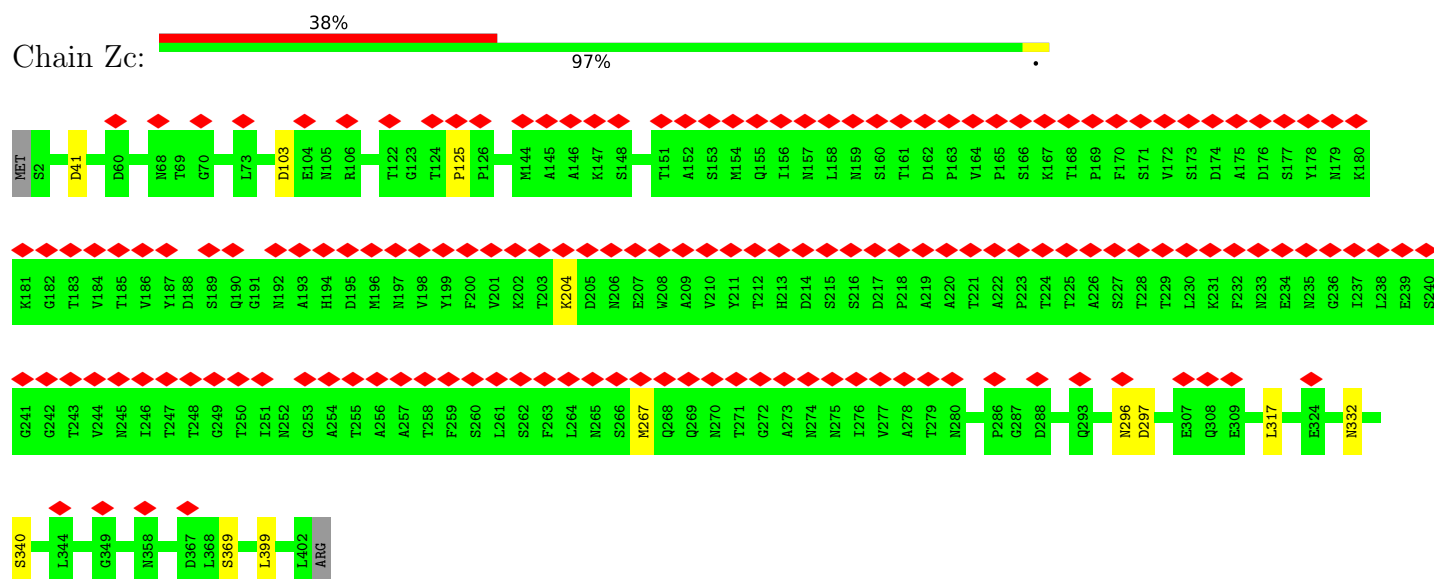
• Molecule 4: Flagellar hook protein FlgE



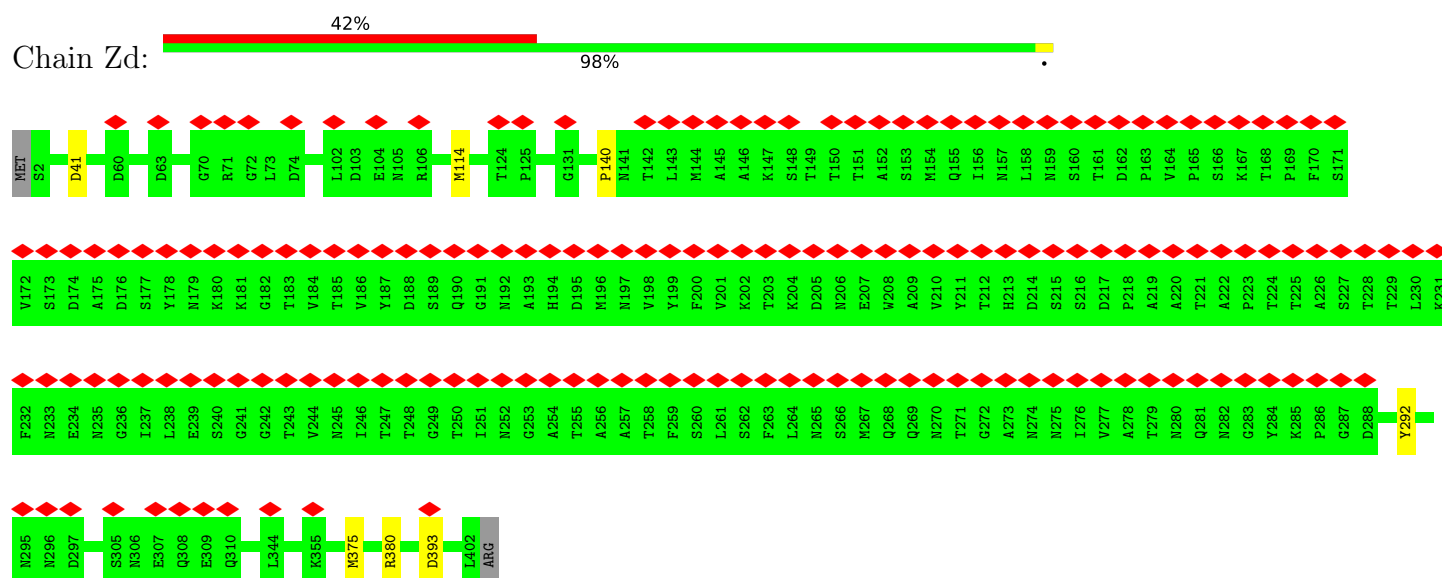
• Molecule 4: Flagellar hook protein FlgE



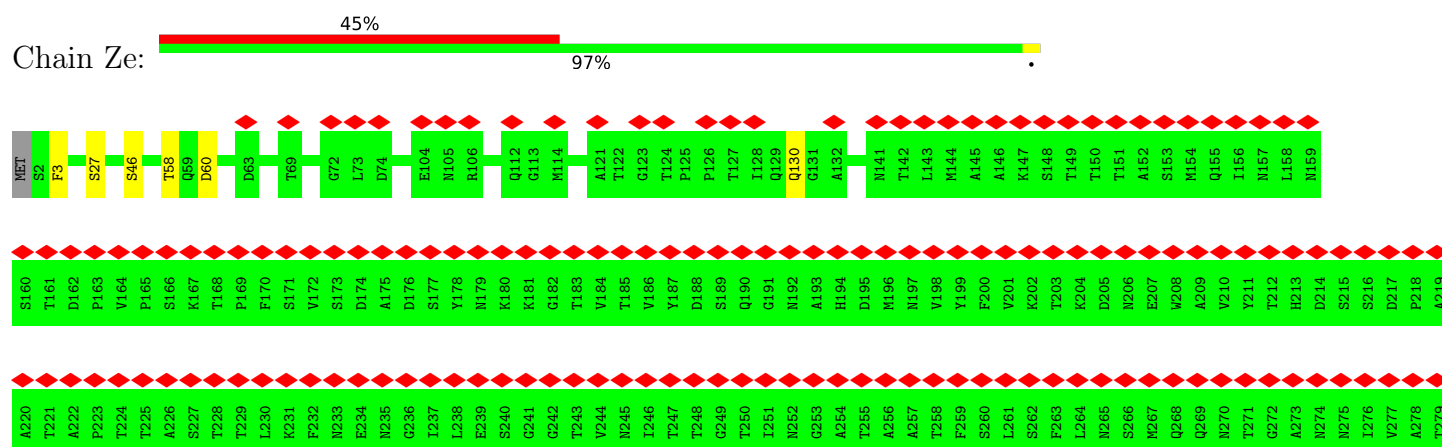
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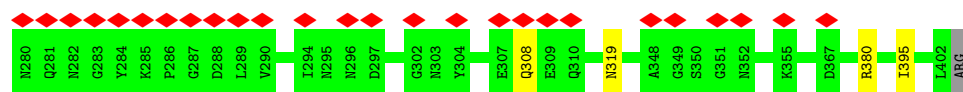


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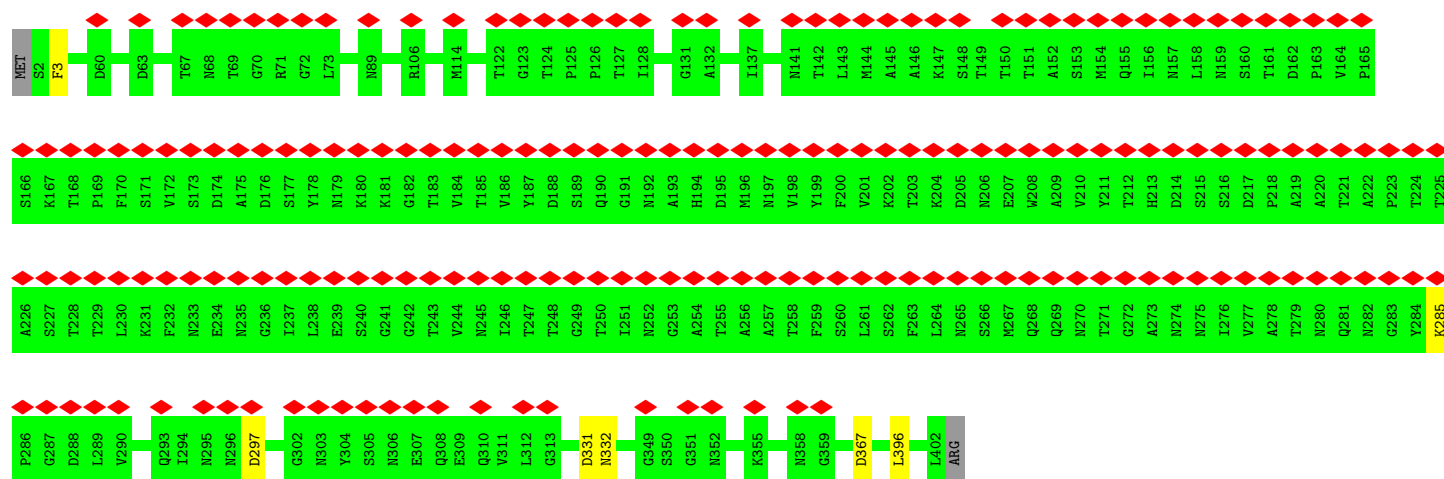


• Molecule 4: Flagellar hook protein FlgE

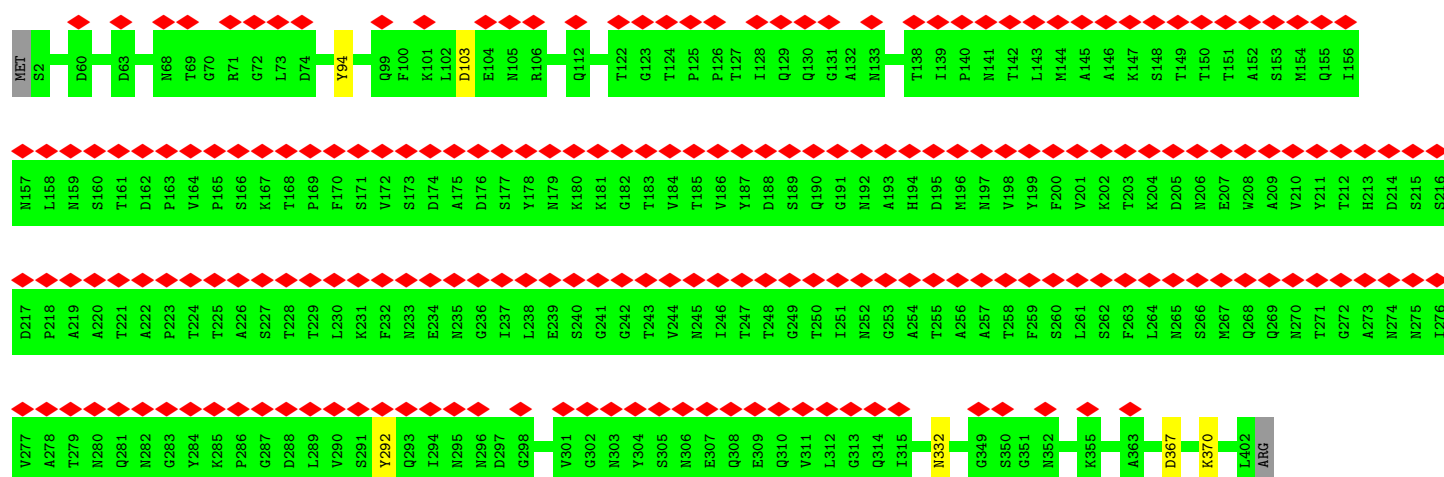




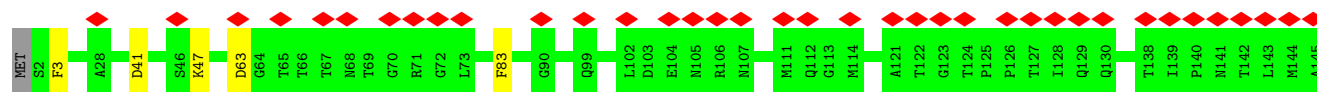
• Molecule 4: Flagellar hook protein FlgE

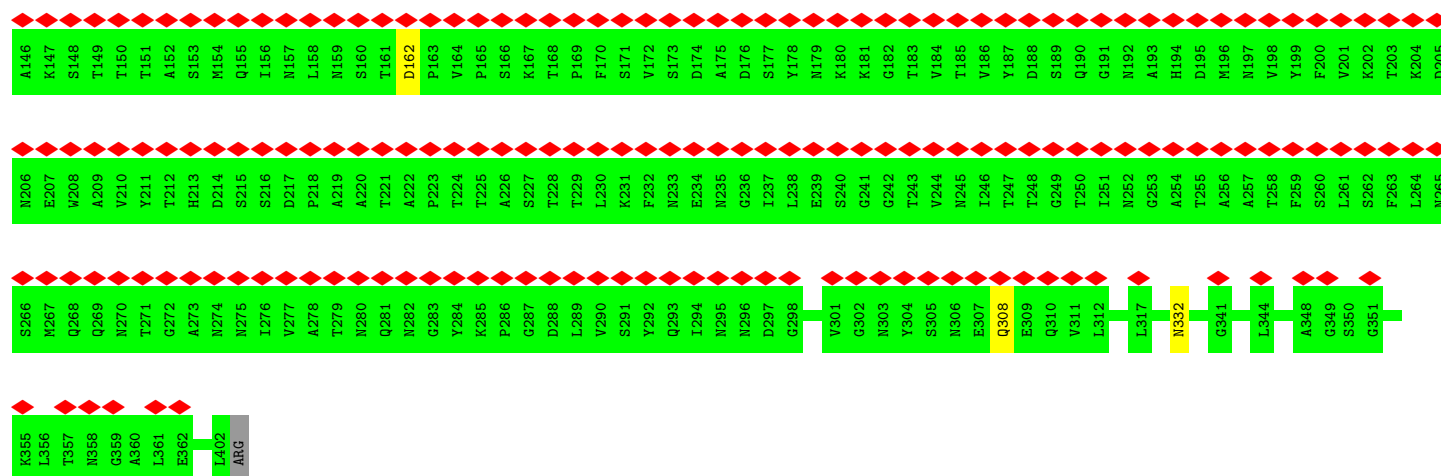


• Molecule 4: Flagellar hook protein FlgE



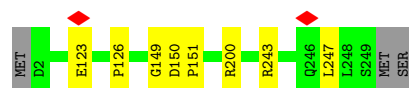
• Molecule 4: Flagellar hook protein FlgE





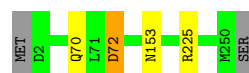
- Molecule 5: Flagellar basal-body rod protein FlgF

Chain AA: 96%



- Molecule 5: Flagellar basal-body rod protein FlgF

Chain AB: 98%



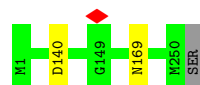
- Molecule 5: Flagellar basal-body rod protein FlgF

Chain AC: 97%



- Molecule 5: Flagellar basal-body rod protein FlgF

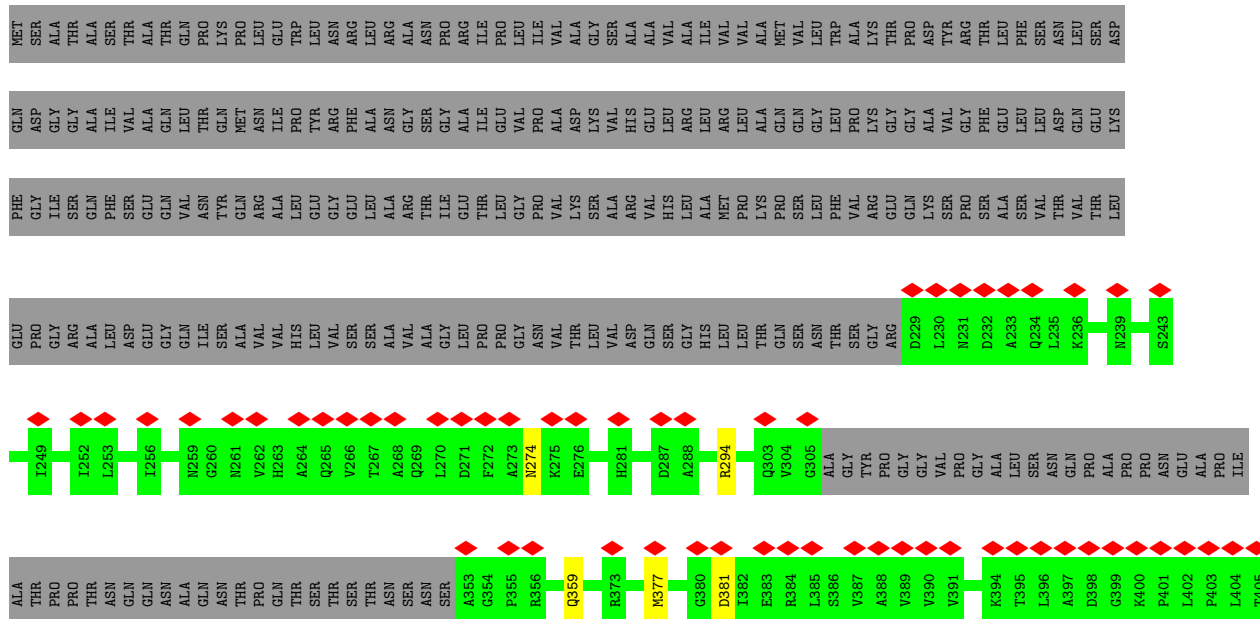
Chain AD: 99%



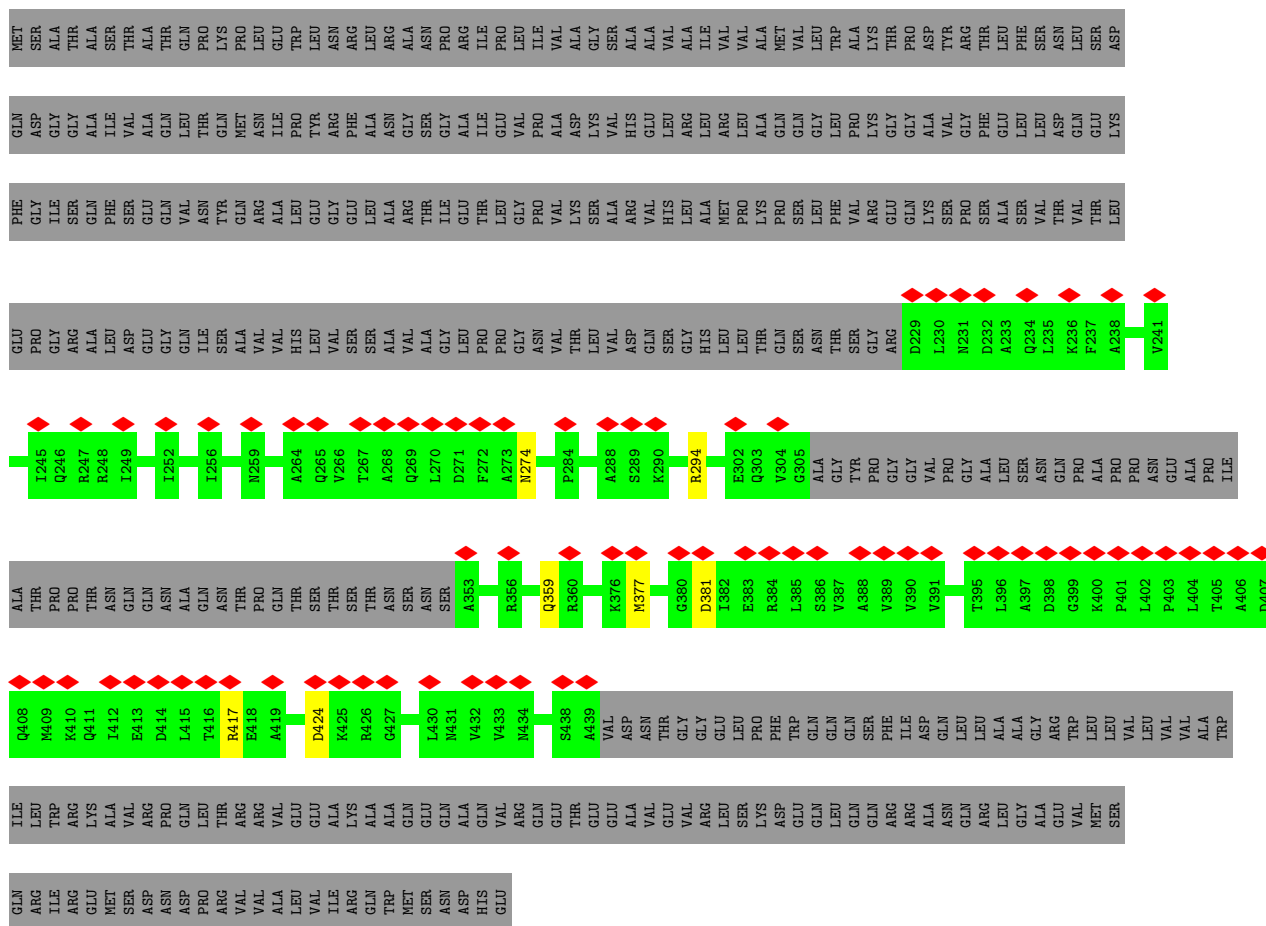
- Molecule 5: Flagellar basal-body rod protein FlgF

Chain AE: 98%

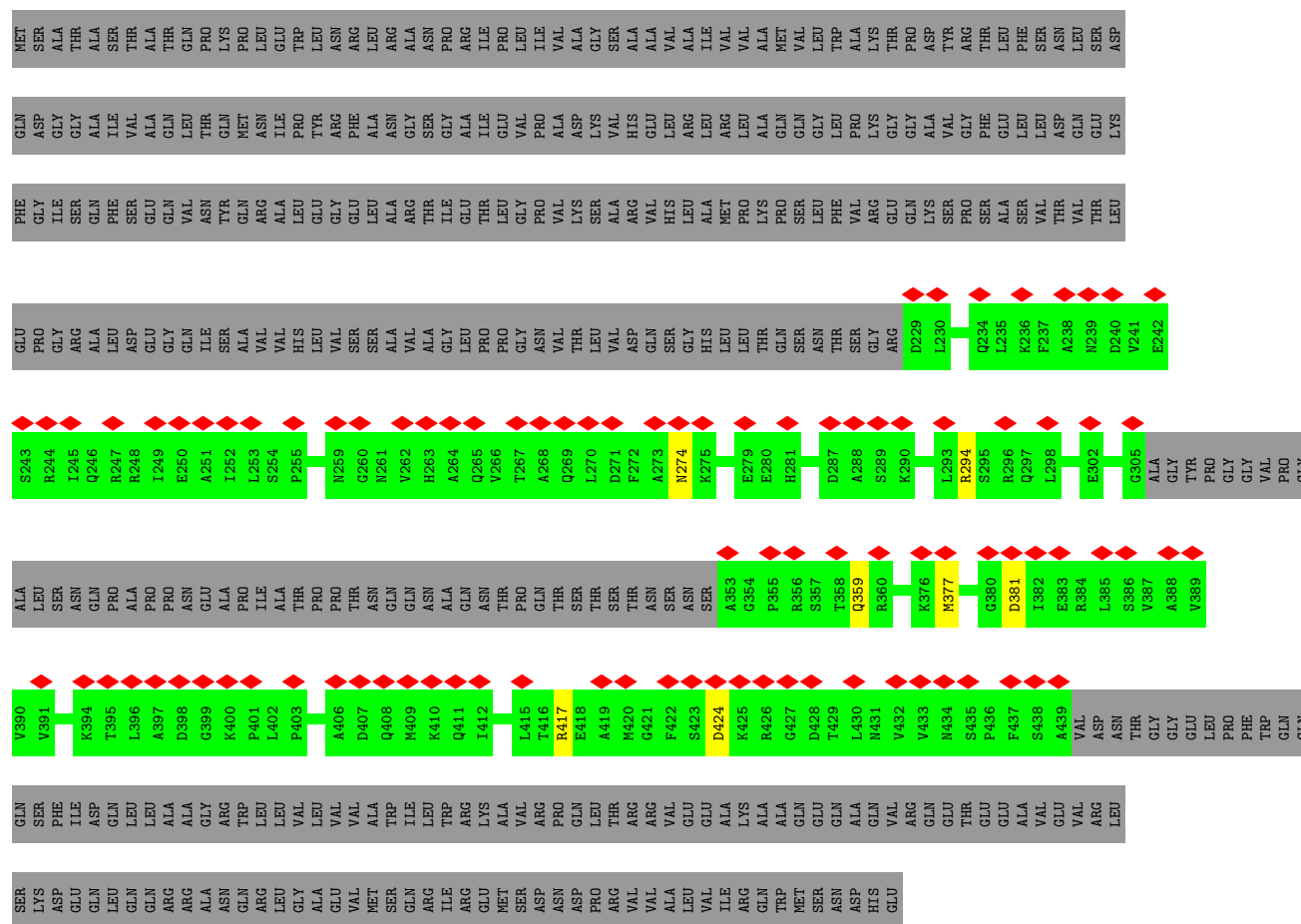




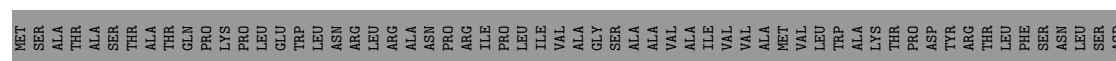
- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein





- Molecule 6: Flagellar M-ring protein



PHE	GLY	ILE	SER	GLN	PHE	SER	GLU	GLN	VAL	ASN	TYR	GLN	ARG	ALA	LEU	GLU	GLY	GLU	LEU	ALA	ARG	THR	ILE	GLU	THR	LEU	GLY	PRO	VAL	LYS	SER	ALA	ARG	VAL	HIS	LEU	ALA	MET	PRO	LYS	PRO	SER	SER	PHE	VAL	ARG	GLU	GLN	LYS	LEU	LEU	THR	THR	THR	THR	LEU
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[illegible]

E242	S243	R244	T245	Q246	R247		A251	T252	L253	S254	P255	T256	N259	Q260	N261	V262	H263	A264	O265	V266	T267	A268	Q269	L270	D271	F272	A273	N274	K275	E279	S283	D287	A288	S289	K290	A291	R294	L298	N299	I300	S301	F302	Q303	V304	G305	ALA	GLY	TYR	PRO	GLY	GLY	VAL	PRO
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GLY	ALA	LEU	SER	ASN	GLN	PRO	ALA	PRO	PRO	ASN	GLU	ALA	PRO	ILE	ALA	THR	PRO	PRO	THR	ASN	GLN	GLN	ASN	ALA	GLN	ASN	THR	PRO	GLN	THR	SER	THR	THR	ASN	SER	ASN	SER	A353	R356	S357	T358	Q359	R360	N361	E362	R370	T371	I372	M377	N378	V379	C380	D381	I382	R383
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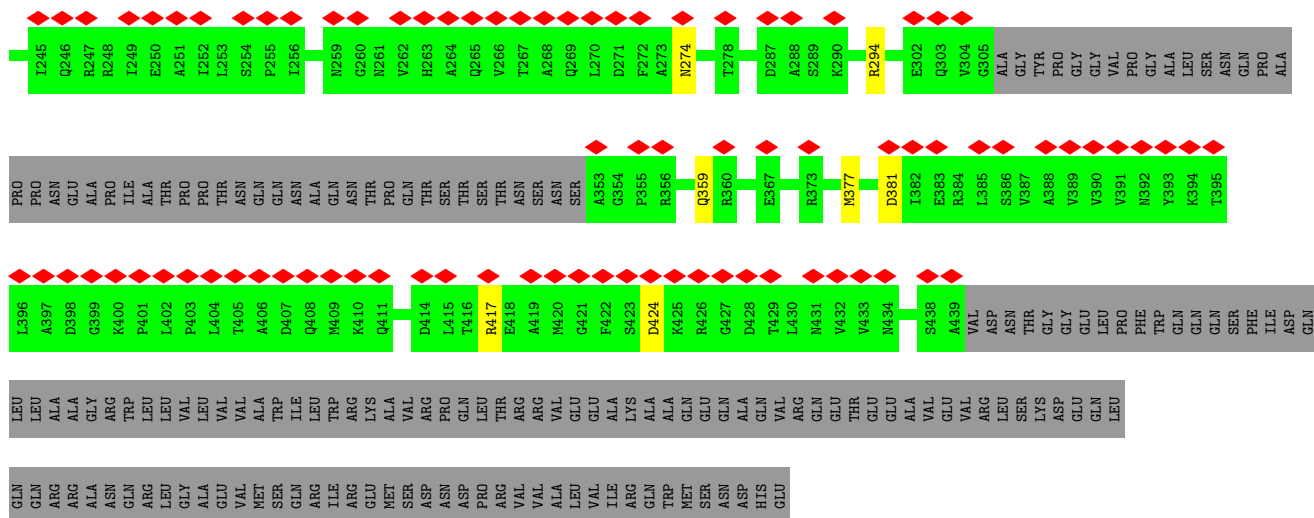
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- Molecule 6: Flagellar M-ring protein

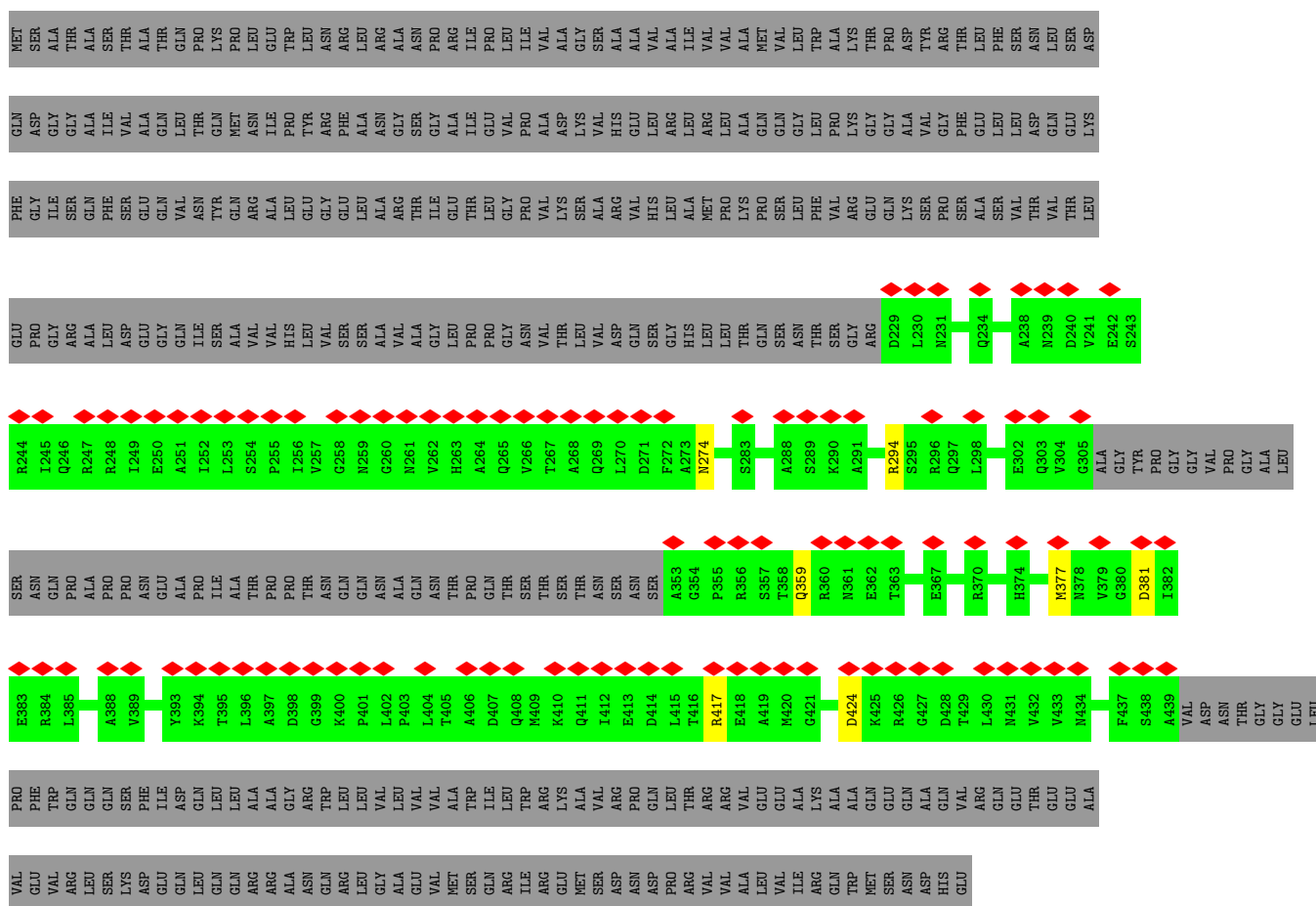
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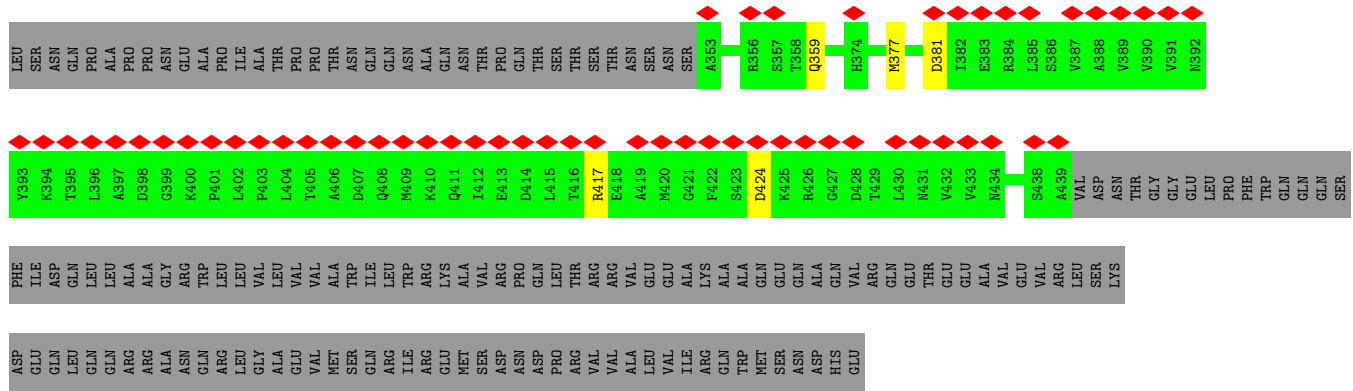


- Molecule 6: Flagellar M-ring protein

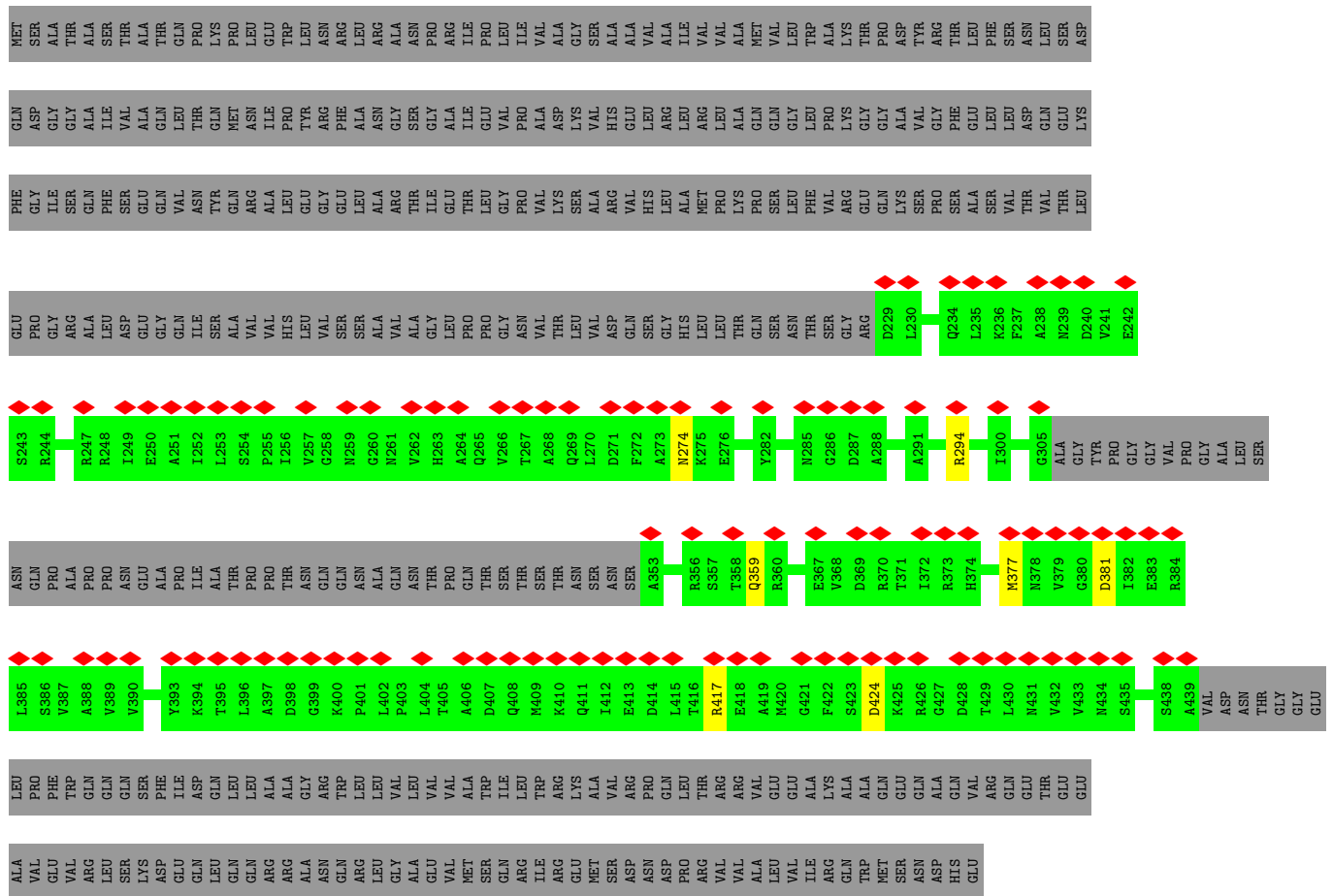


- Molecule 6: Flagellar M-ring protein

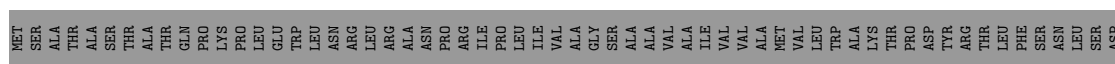


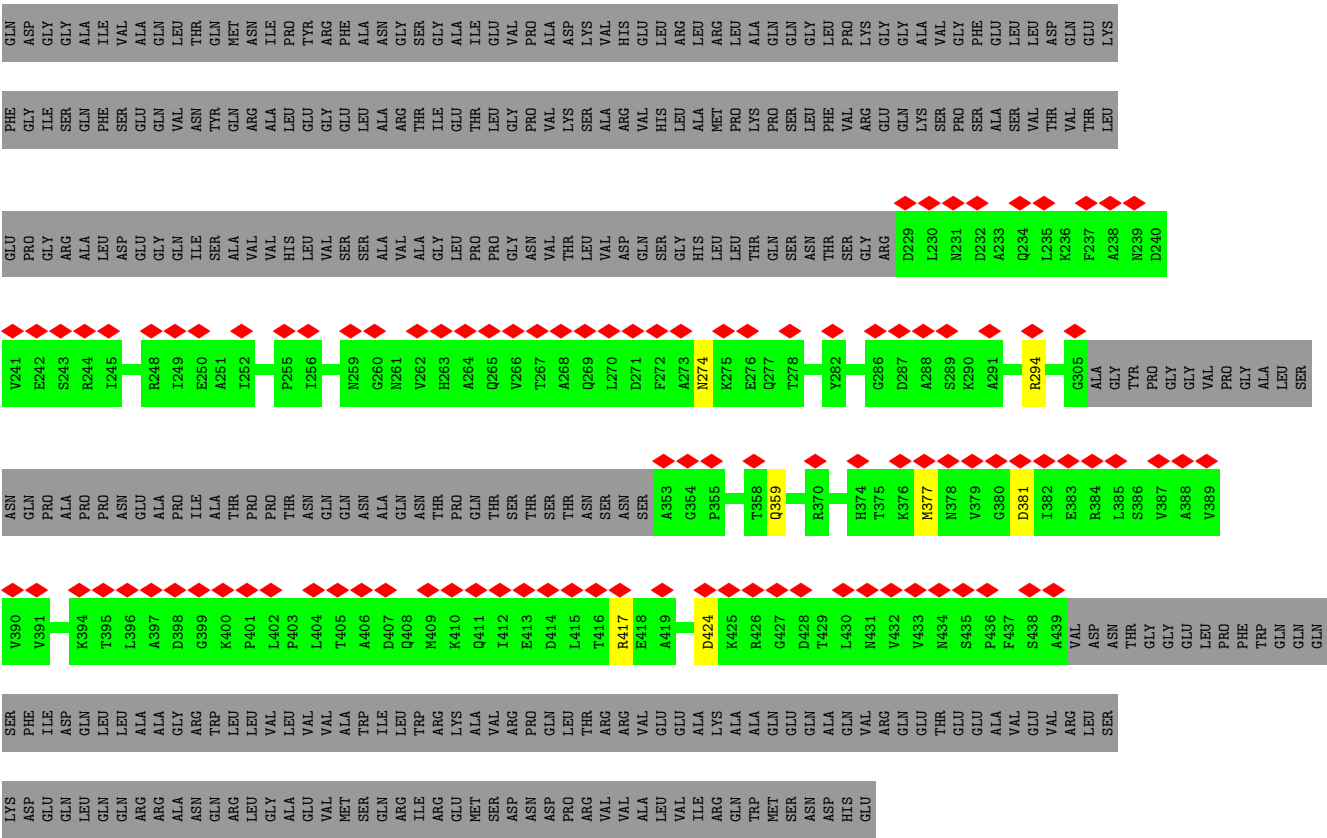


- Molecule 6: Flagellar M-ring protein

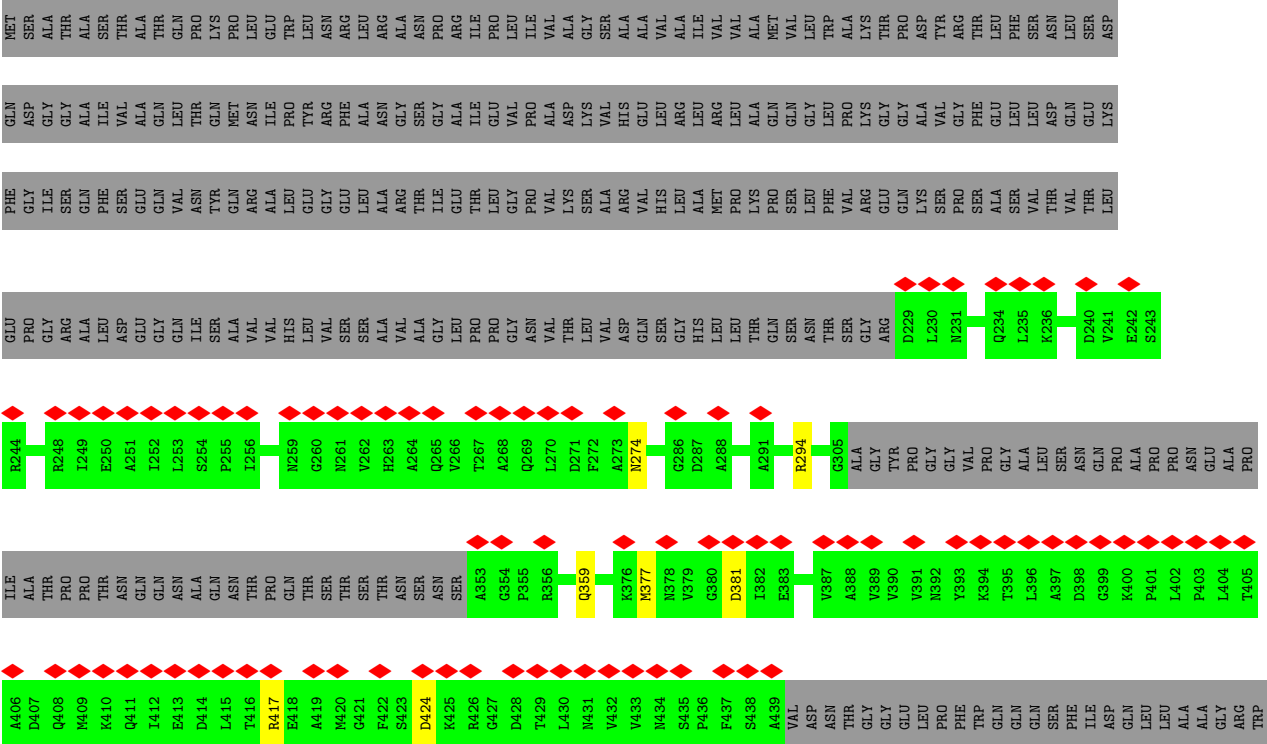


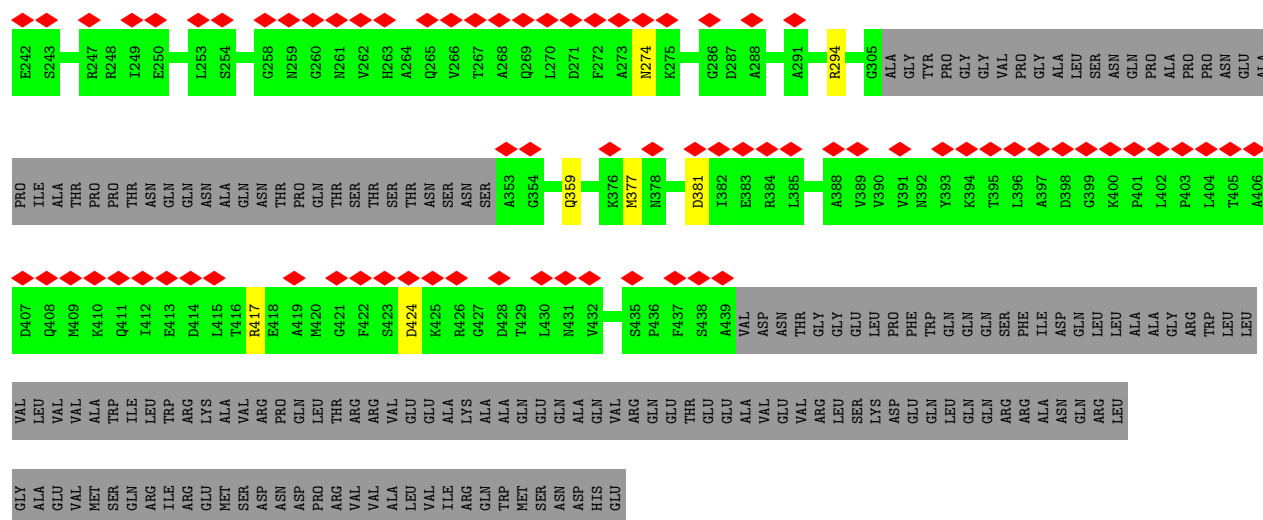
- Molecule 6: Flagellar M-ring protein



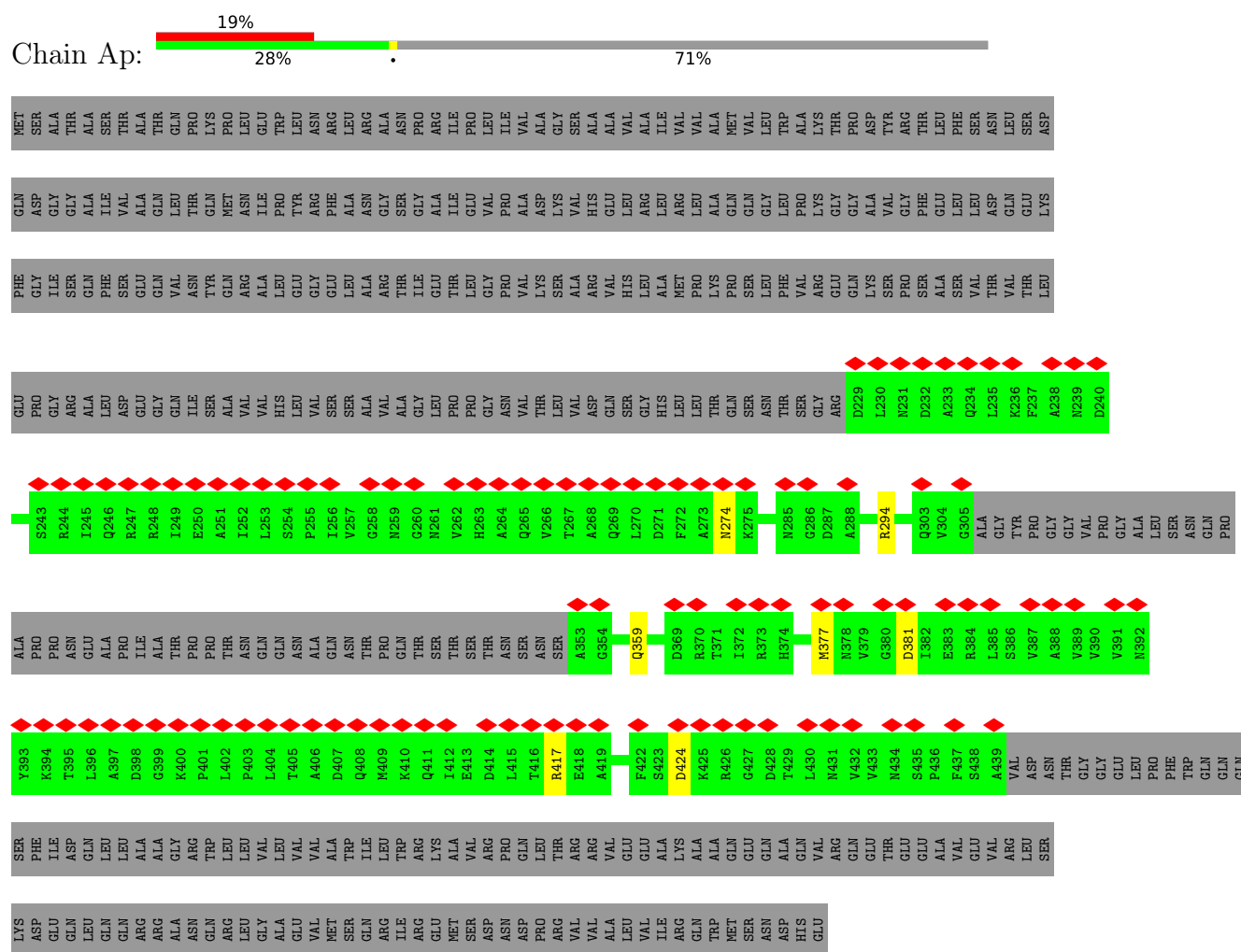


• Molecule 6: Flagellar M-ring protein



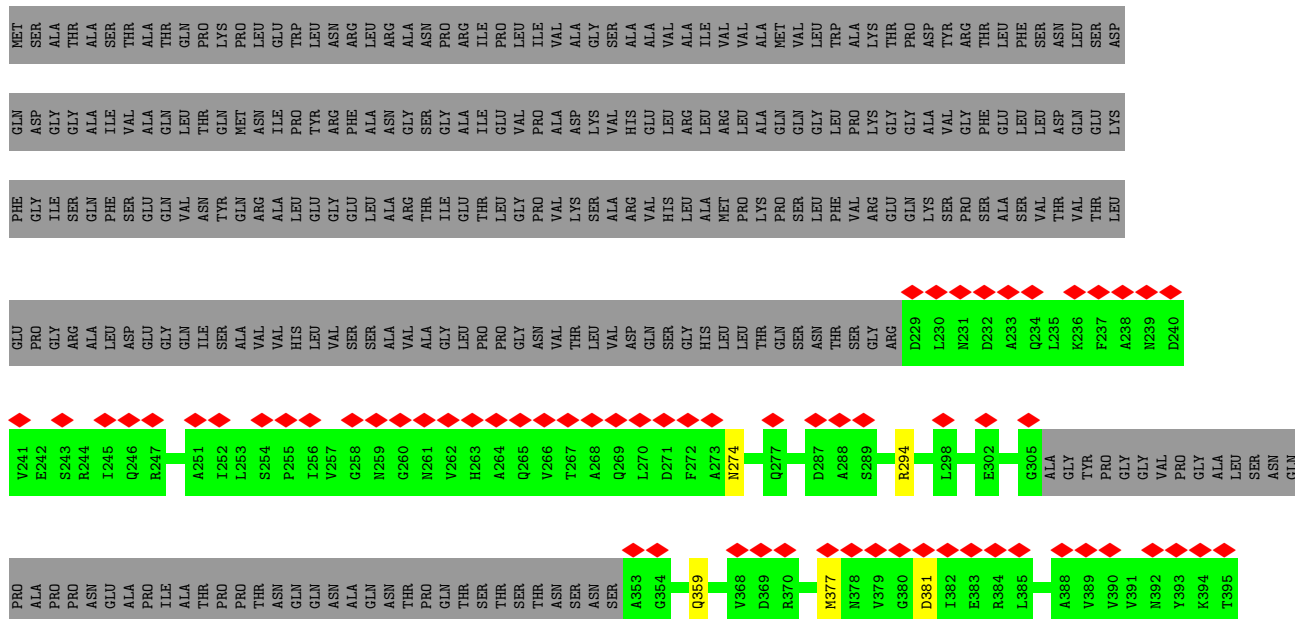


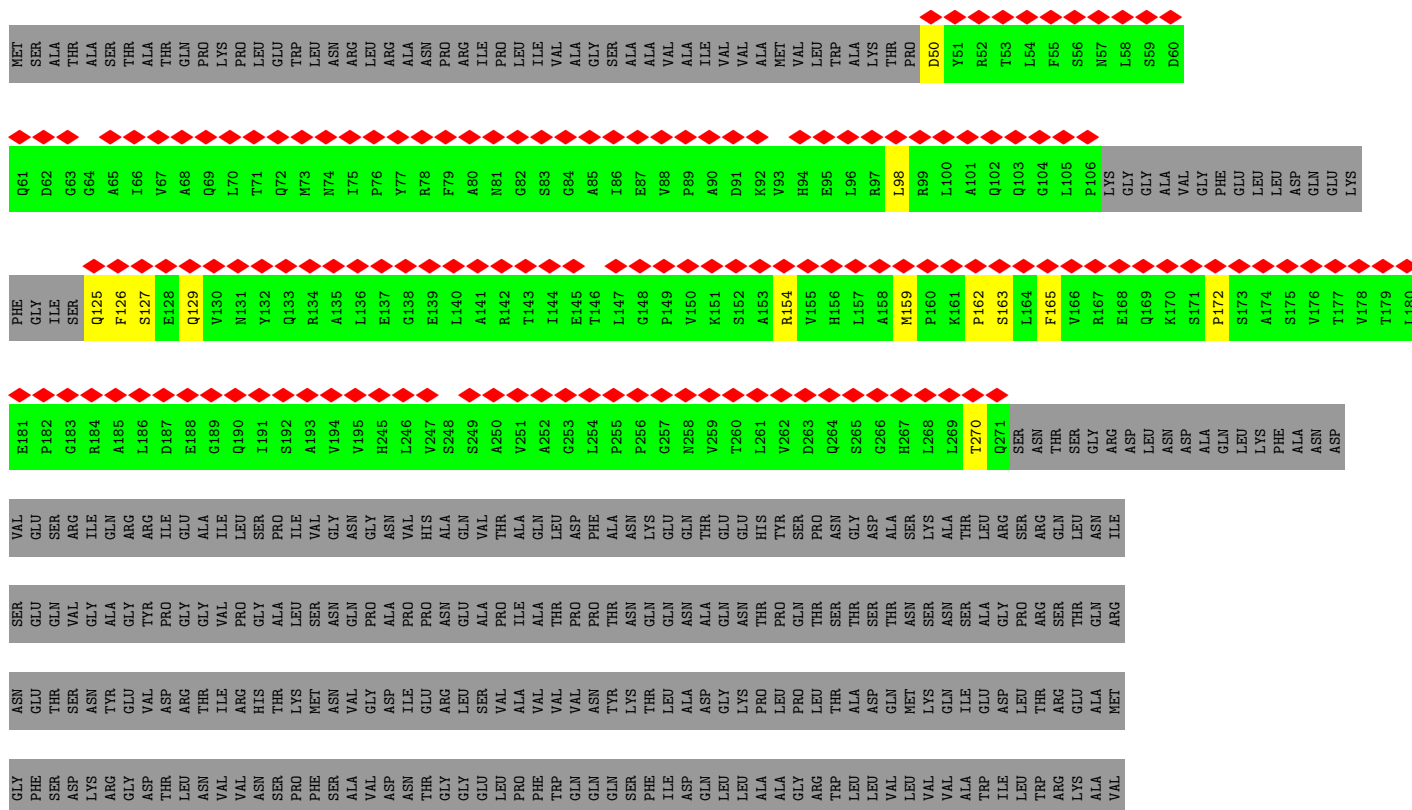
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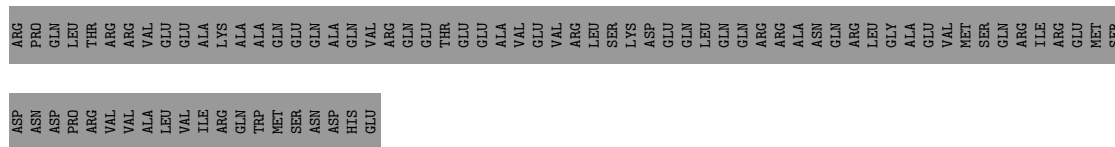


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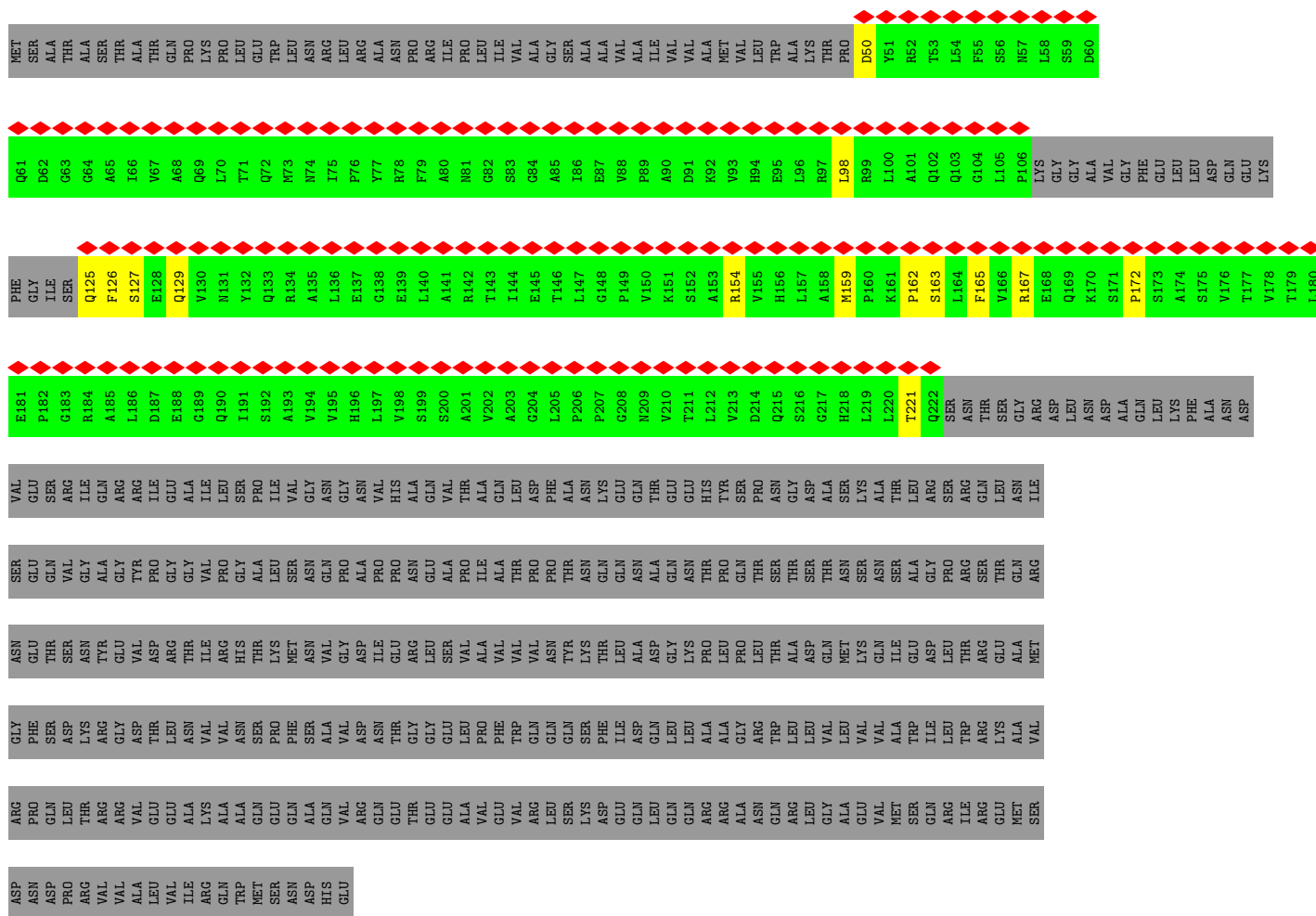




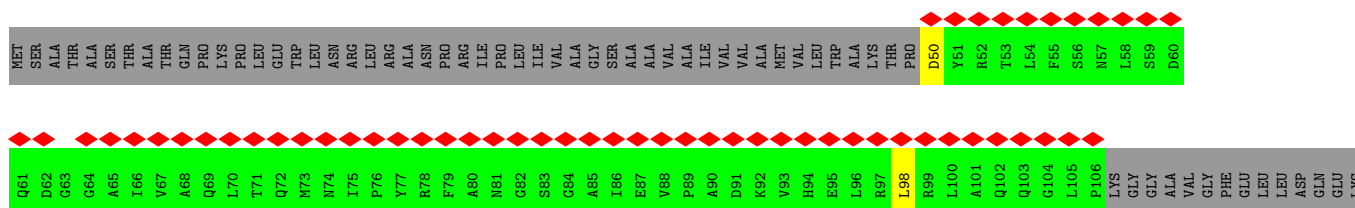


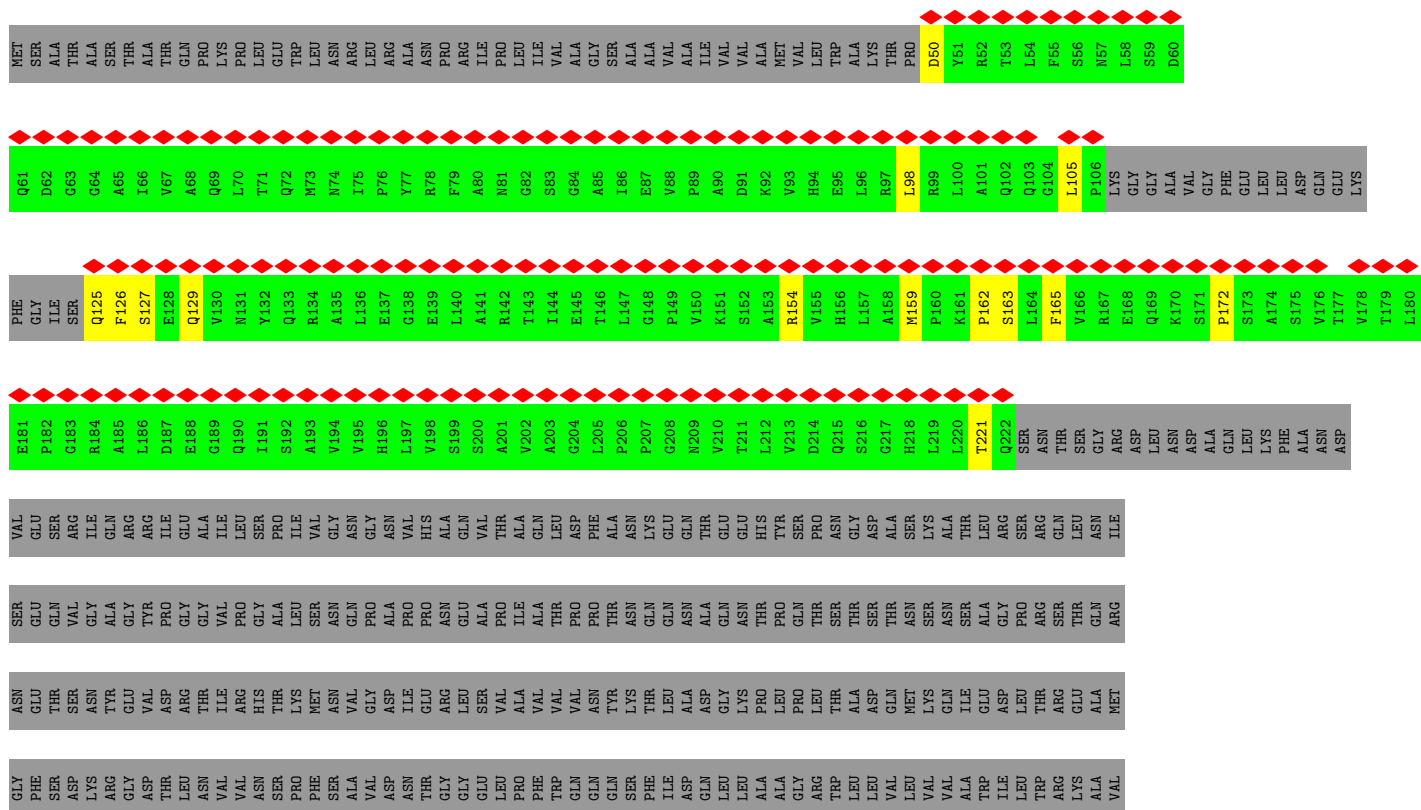


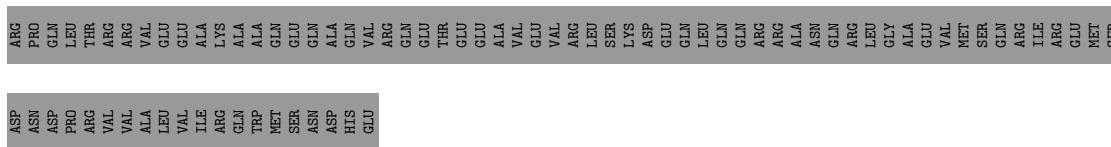
- Molecule 6: Flagellar M-ring protein



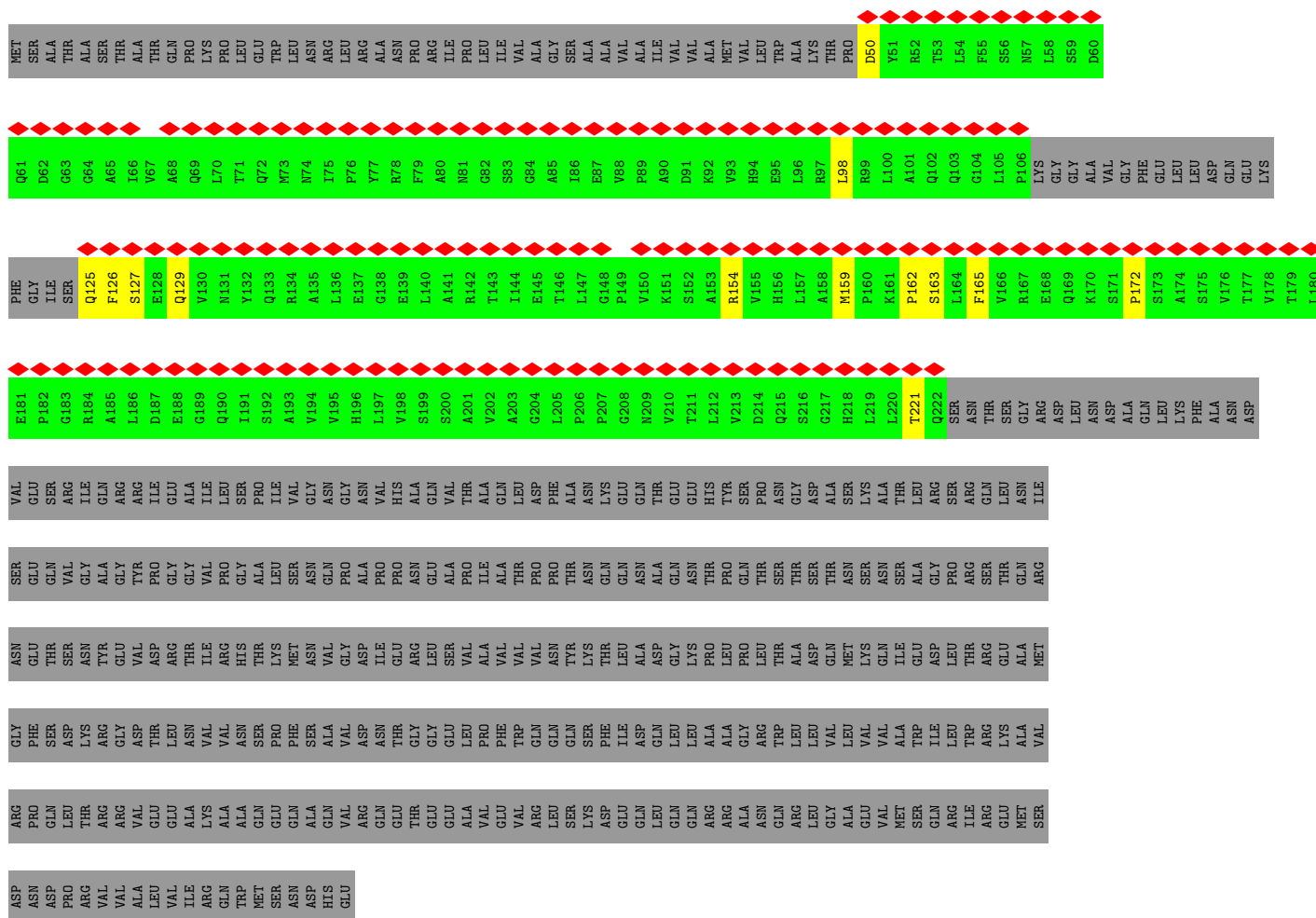
- Molecule 6: Flagellar M-ring protein



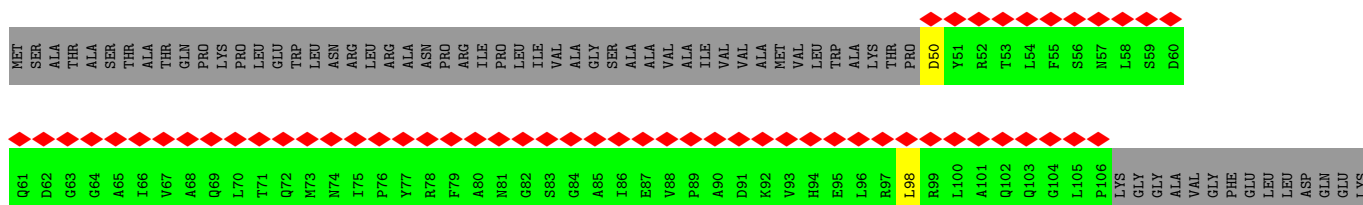




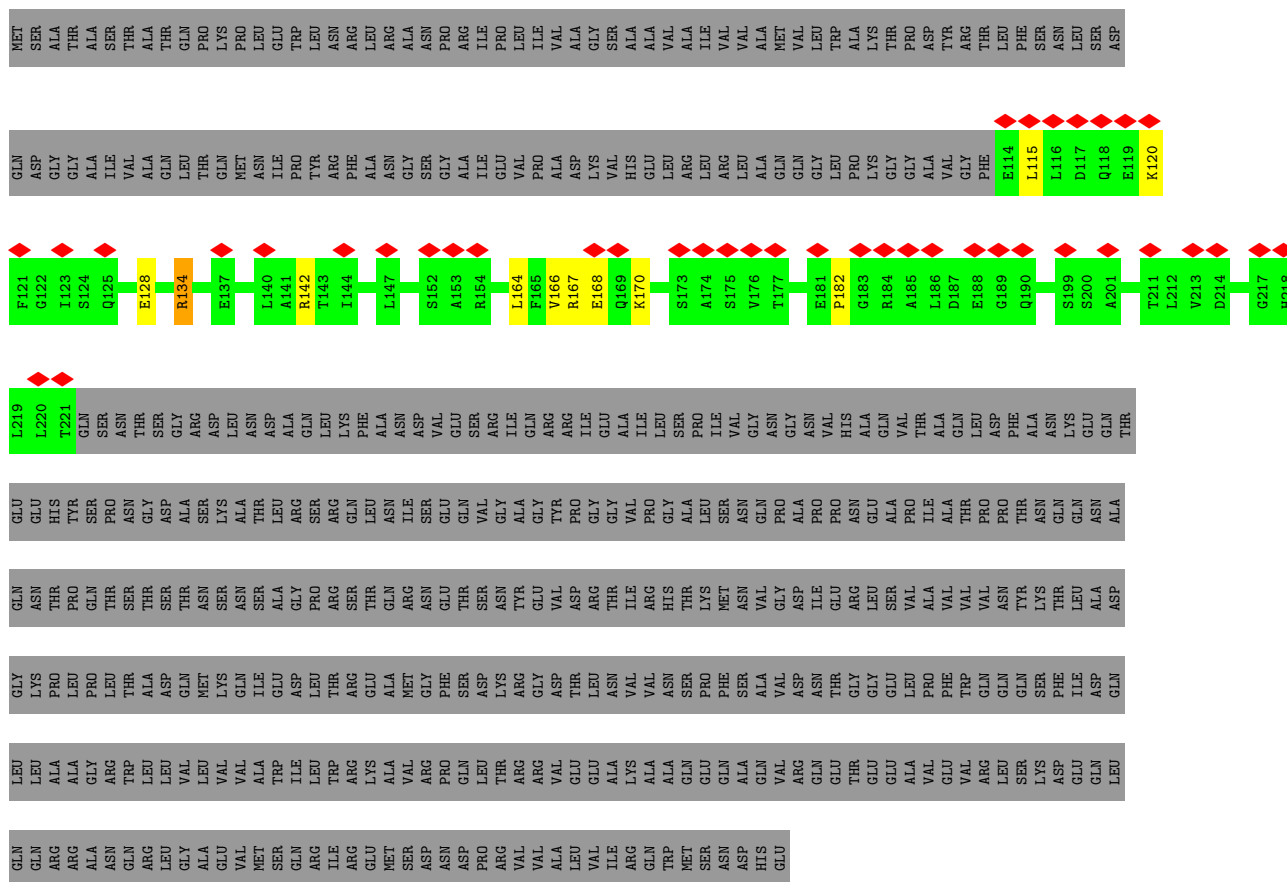
- Molecule 6: Flagellar M-ring protein



- Molecule 6: Flagellar M-ring protein

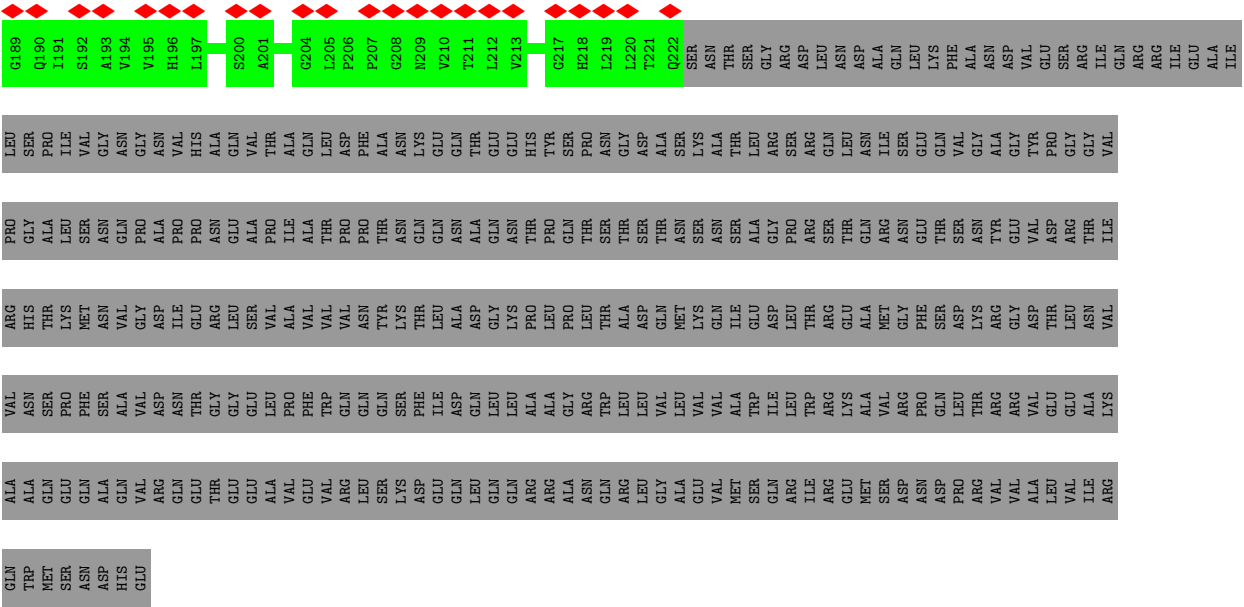


- Molecule 6: Flagellar M-ring protein

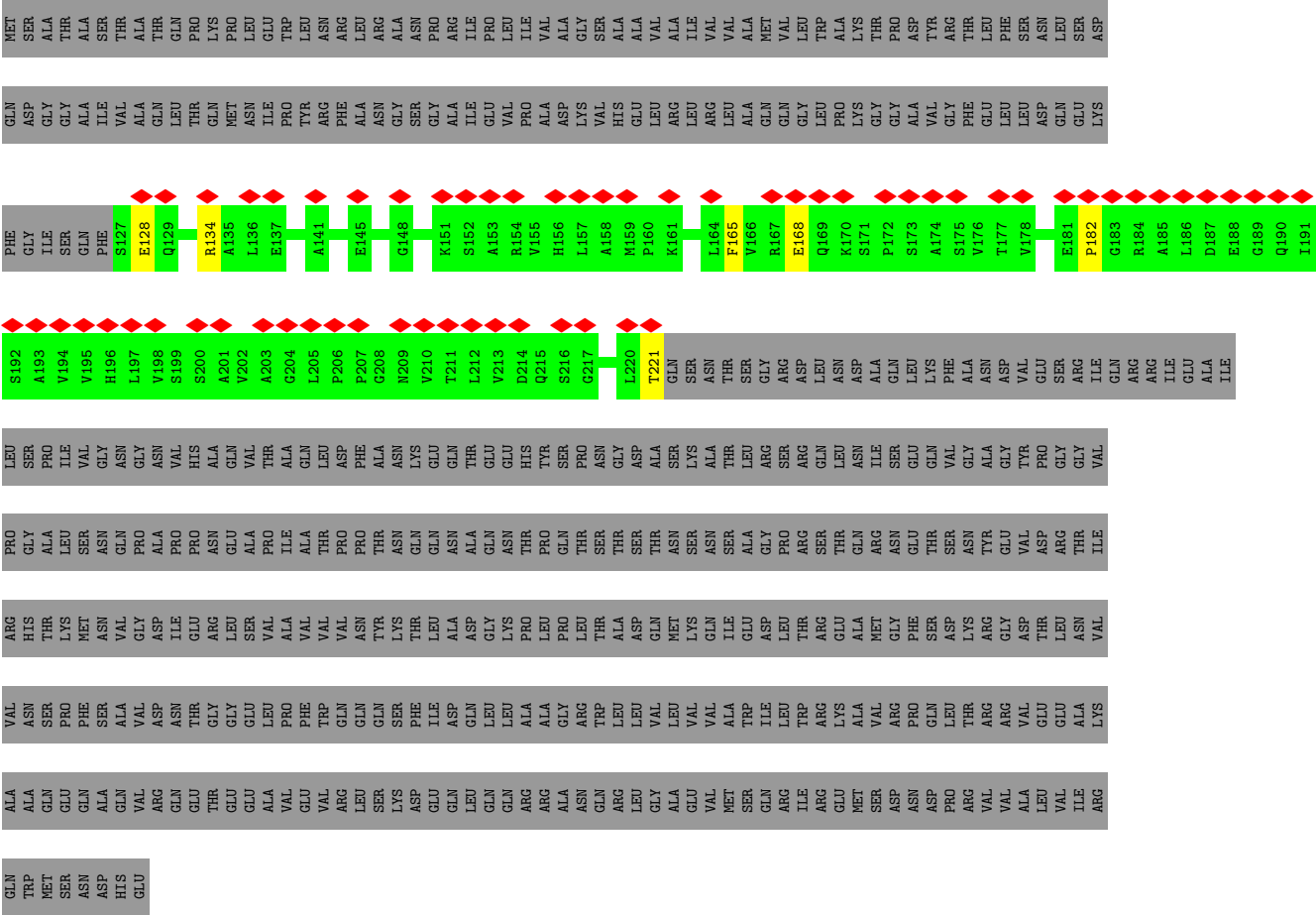


- Molecule 6: Flagellar M-ring protein

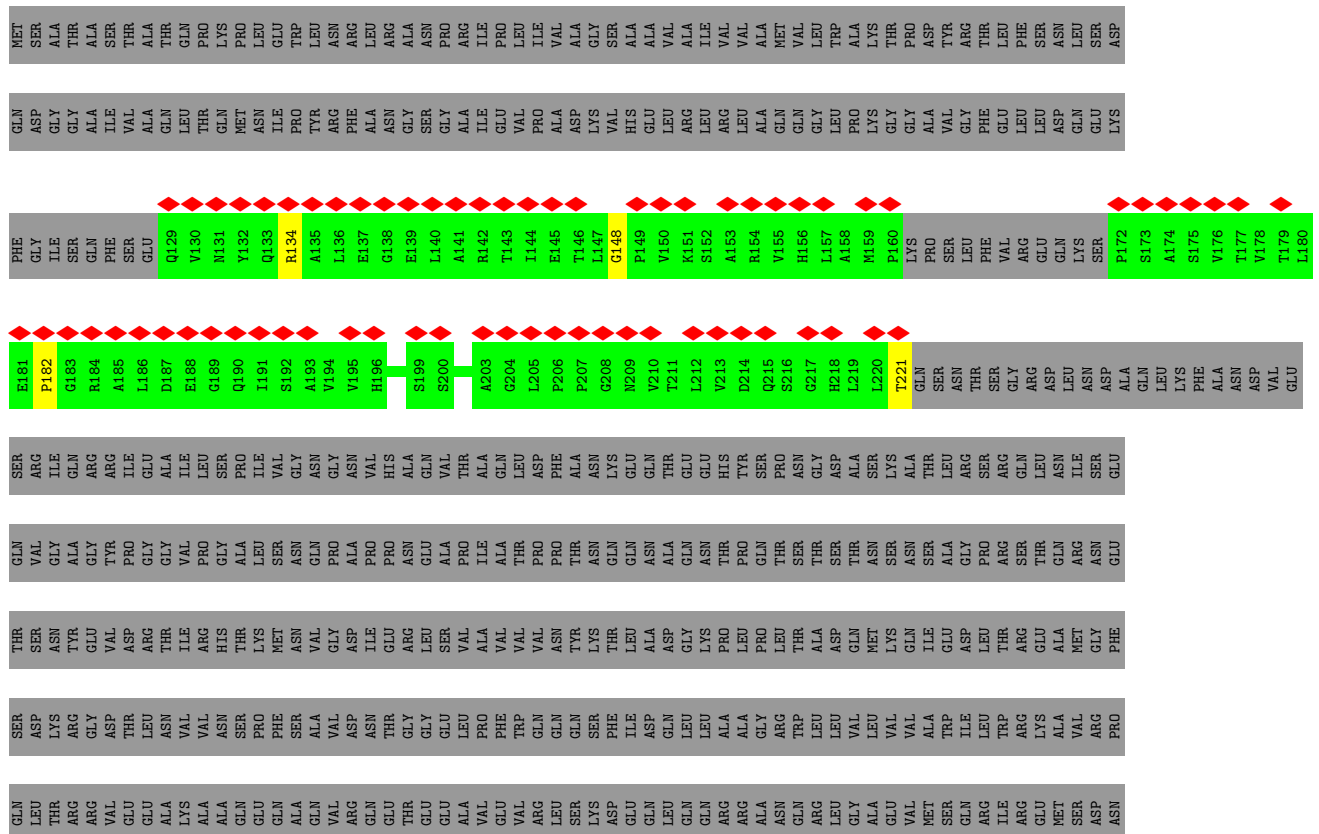


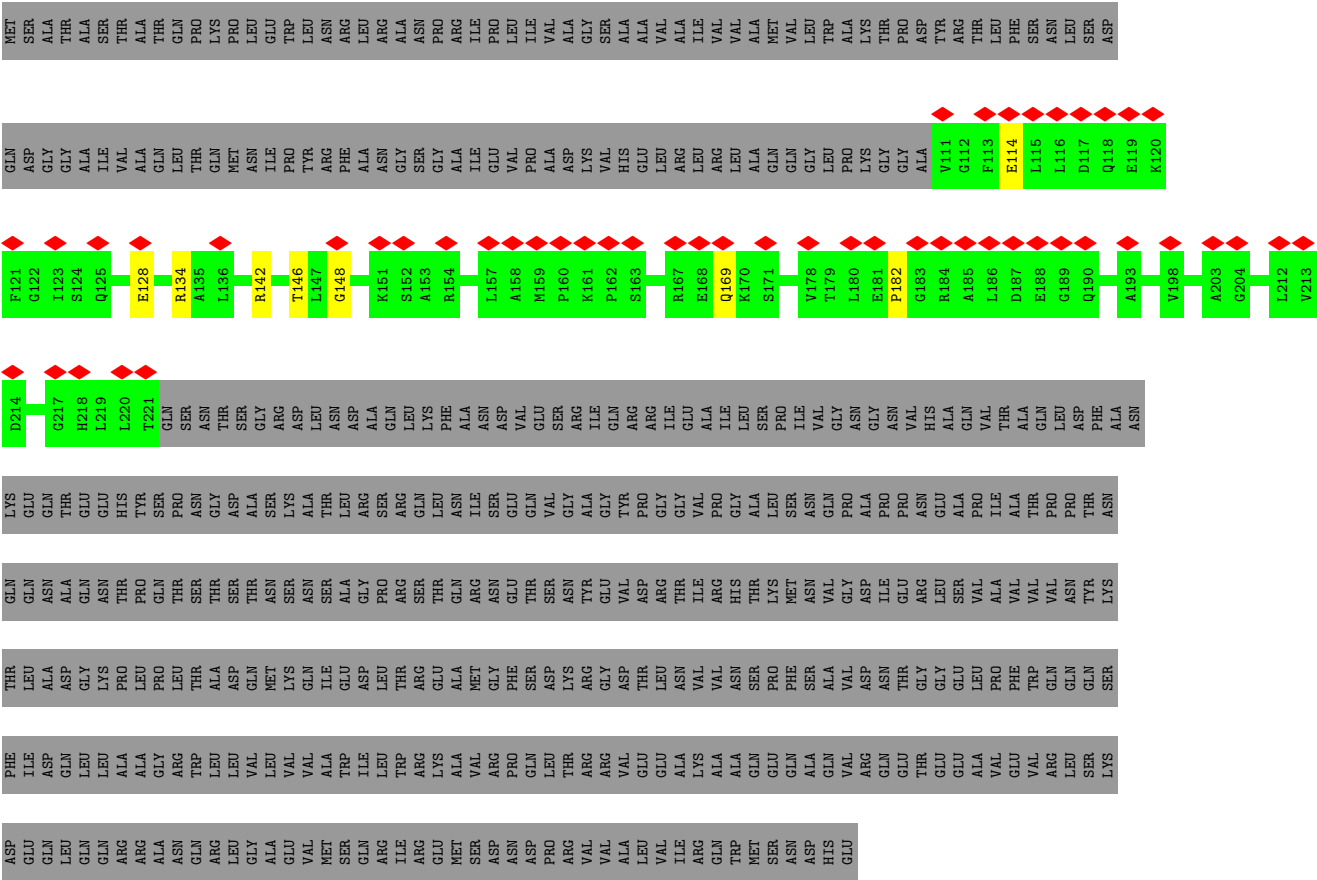


● Molecule 6: Flagellar M-ring protein

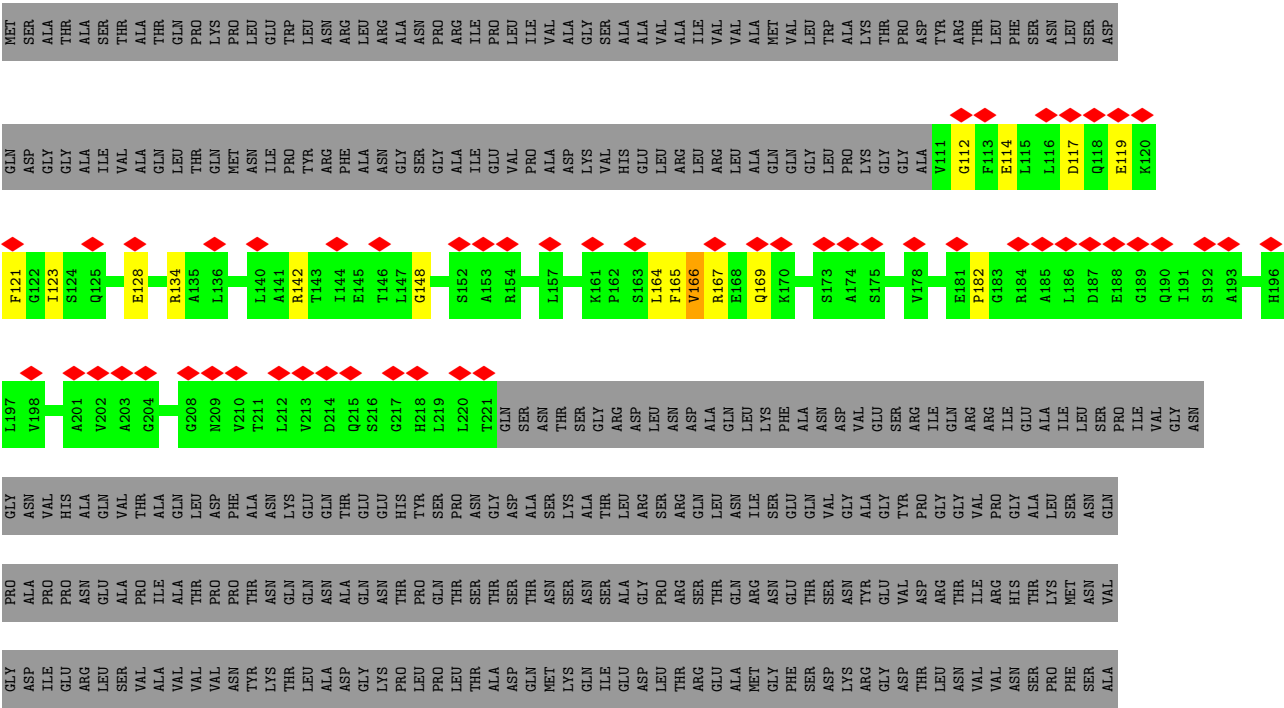


● Molecule 6: Flagellar M-ring protein





● Molecule 6: Flagellar M-ring protein



GLU

- Molecule 6: Flagellar M-ring protein



GLN	ASP	GLY	GLY	ILE	VAL	ALA	GLN	LEU	THR	GLN	MET	ASN	ILE	PRO	TYR	ARG	PHE	ALA	ALA	ASN	GLY	SSR	GLY	ALA	ILE	GLU	VAL	PRO	ALA	ASP	LYS	VAL	HIS	GLU	LEU	ARG	LEU	ARG	LEU	ALA	GLN	GLN	GLY	LEU	PRO	GLY	GLY	ALA	V111	G112	F113	E114	D117	Q118	E119	K120	F121
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G217	H218	T221	GLN	SER	ASN	THR	SER	GLY	ARG	ASP	LEU	LEU	ASP	ALA	GLN	LEU	PHE	LYS	ALA	ASN	ASP	VAL	GLU	SER	ARG	TLE	GLN	ARG	ARG	TLE	GLU	ALA	TLE	LEU	SER	PRO	TLE	VAL	GLY	ASN	GLY	ASN	ASN	VAL	HIS	ALA	GLN	VAL	THR	ALA	ALA	GLN	LEU	ASP	PHE	ALA	ALA	ASN	LYS	ASN	GLU
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THR GLU GLU HIS TYR SER SER PRO PRO GLY ASP ALA SER SER GLN LEU THR THR ARG SER ARG GLN LEU ASN TLE SER SER GLU GLN VAL GLY GLY TYR PRO GLY VAL VAL PRO PRO GLY GLY ALA ALA SER SER ASN GLN GLN PRO PRO ALA ALA PRO ASN GLU ALA THR THR PRO THR THR ASN GLN GLN ASN

GLN	GLN	ASN	THR	PRO	GLN	THR	THR	THR	SER	THR	ASN	SER	SER	ALA	GLY	PRO	ARG	SER	THR	THR	GLN	ARG	ASN	GLU	THR	SER	SER	ASN	TYR	GLU	VAL	ASP	ARG	THR	THR	ILE	ARG	HIS	THR	LYS	MET	THR	ASN	VAL	VAL	GLY	ASP	ILE	GLU	ARG	LEU	SER	VAL	VAL	ALA	ALA	VAL	VAL	VAL	ASN	TYR	THR	LYS	THR	LEU	ALA
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GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL VAL VAL VAL ALA ALA TRP TRP THR LEU LEU ARG ARG ARG VAL GLU GLU GLY LYS LYS ALA ALA ALA ALA GLN GLN GLN GLN ALA ALA VAL VAL VAL VAL ARG ARG GLN GLU THR GLU GLU GLU GLU LYS ASP LYS ASP GLU GLN

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- Molecule 6: Flagellar M-ring protein



NET	SER	ALA	THR	ALA	SER	THR	THR	ALA	THR	GLN	PRO	LYS	PRO	PRO	LEU	LEU	GLU	TRP	LEU	ASN	ARG	ARG	LEU	ALA	ALA	ASN	PRO	PRO	ARG	ILE	LEU	LEU	ILE	VAL	VAL	ALA	GLY	SER	ALA	ALA	ALA	VAL	VAL	ILE	VAL	VAL	ALA	ALA	VAL	VAL	VAL	TRP	ALA	LYS	THR	PRO	ASP	TYR	ARG	THR	LEU	PHE	SER	ASN	LEU	LEU	SER	ASN
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GLN	ASP	GLY	GLY	ALA	ILE	VAL	ALA	GLN	LEU	THR	GLN	MET	ASN	ILE	PRO	TYR	PHE	ARG	ASN	GLY	SER	GLY	ILE	GLU	VAL	PRO	ALA	ASP	LYS	VAL	HIS	GLU	LEU	ARG	LEU	ARG	LEU	ALA	GLN	GLN	GLY	LEU	PRO	LYS	GLY	GLY	ALA	VAL11	G112	L116	D117	Q118	E119	K120	F121	G122
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Chain BL: . 97%

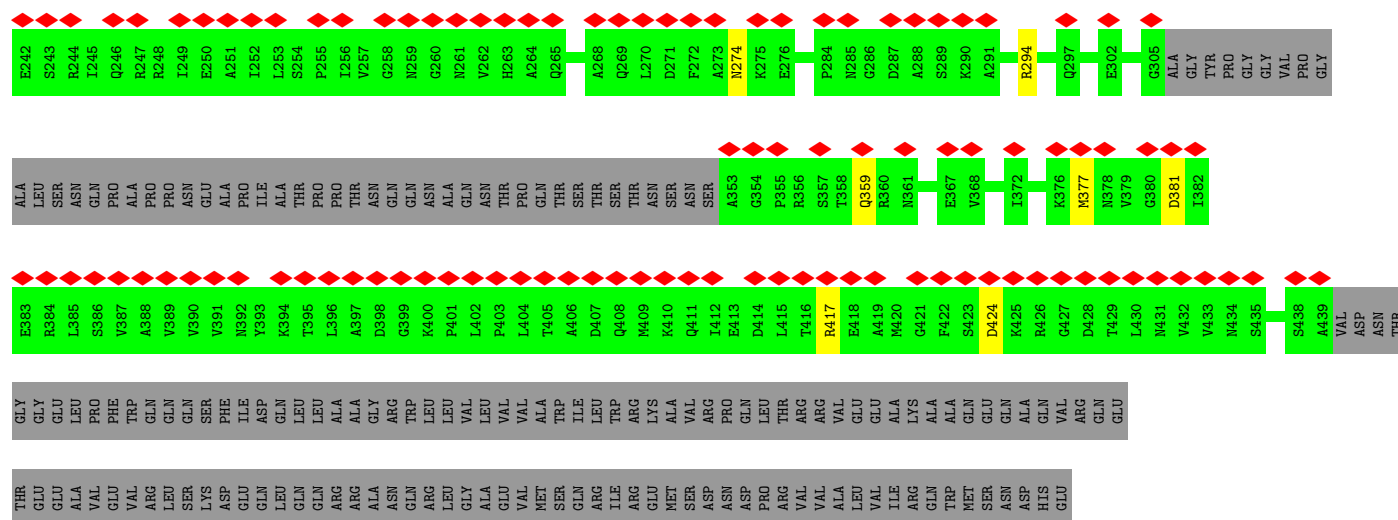
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PHE	GLY	ILE	SER	GLY	PHE	GLY	ASP	GLY	GLY	ASN	ARG	GLN	GLY	GLY	GLY	GLY	GLY	THR	THR	LEU	GLY	VAL	VAL	LYS	SER	ALA	ALA	VAL	ARG	VAL	PRO	SER	THR	THR	LEU		
GLU	PRO	GLY	ARG	ALA	LEU	ASP	GLY	GLY	GLY	ASN	VAL	ALA	VAL	VAL	VAL	VAL	VAL	THR	THR	LEU	PRO	HIS	VAL	VAL	THR	LEU	VAL	VAL	GLY	GLY	GLY	GLY	GLY	GLY	ASP		
VAL	GLU	SER	ARG	ILE	GLN	ARG	ILE	GLU	ALA	ILE	SER	LEU	SER	PRO	ILE	VAL	GLY	ASN	GLY	ASN	GLY	VAL	VAL	GLN	VAL	PHE	ALA	VAL	ASN	PHE	ALA	THR	THR	ILE	ARG		
SER	GLU	GLN	VAL	VAL	ALA	TYR	P309	K324	GLU	ALA	PRO	ILE	ALA	THR	VAL	ARG	PRO	PRO	THR	ASN	GLN	ASN	ALA	GLN	VAL	THR	GLN	ASN	THR	THR	THR	THR	THR	THR	ARG		
HIS	THR	LYS	MET	ASN	VAL	GLY	ASP	GLY	LEU	SER	VAL	VAL	ALA	VAL	VAL	VAL	ASN	TYR	THR	THR	GLN	ASN	ALA	ASP	GLY	GLY	LYS	GLN	ILE	GLU	GLY	GLY	THR	THR	VAL		
ASN	SER	PRO	PHE	GLN	ALA	VAL	ASP	ASP	GLY	GLY	GLY	LEU	LEU	VAL	PHE	TRP	GLN	GLN	GLY	ASP	GLN	LEU	LEU	LEU	TRP	TRP	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ALA		
ALA	GLN	GLY	GLN	GLN	GLN	VAL	ARG	GLN	GLY	GLY	ALA	GLY	VAL	VAL	VAL	VAL	LEU	SER	LYS	ASP	GLY	GLN	GLN	GLN	ARG	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLN			
TRP	MET	SER	ASN	HIS	GLU																																

● Molecule 6: Flagellar M-ring protein

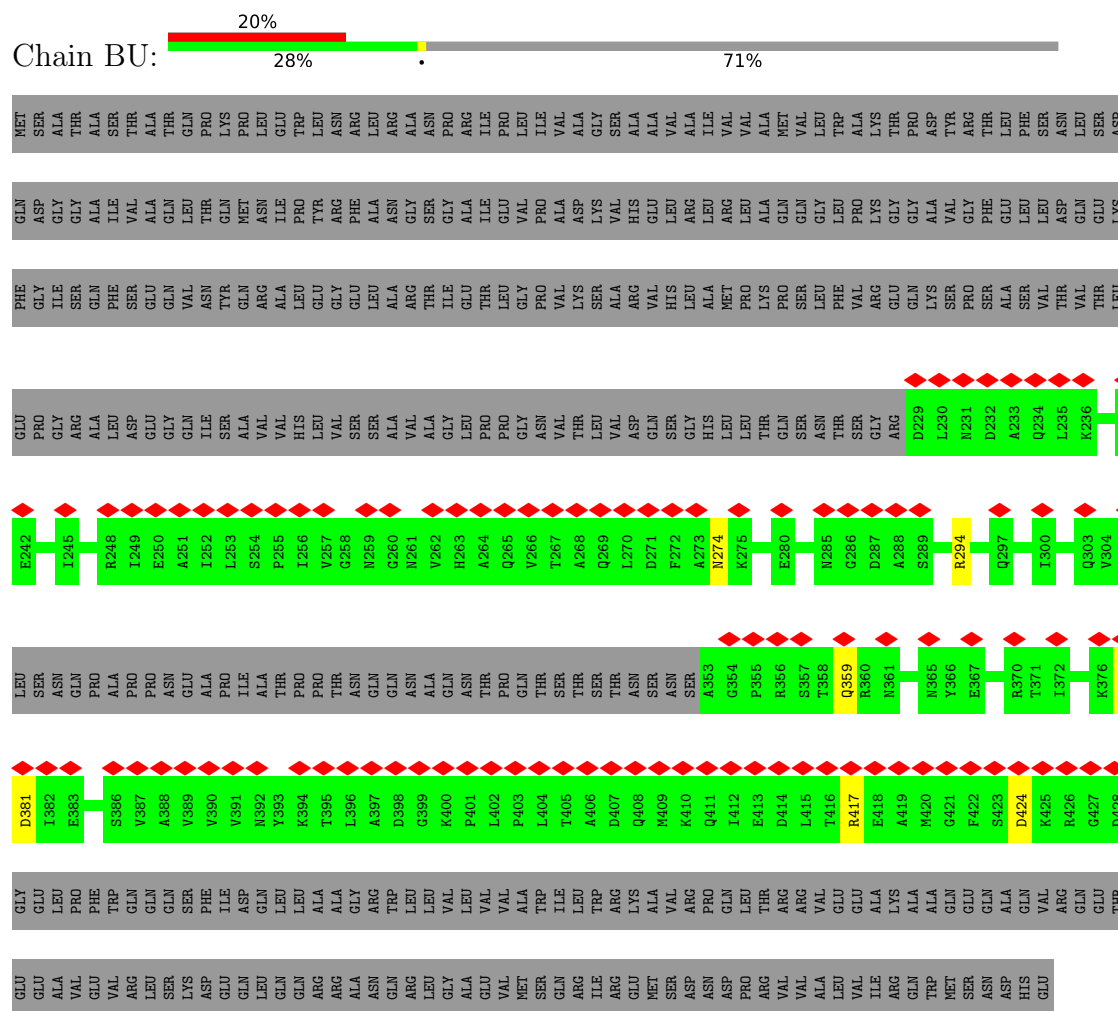
Chain BM: . 96%

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GLN	ASP	GLY	THR	GLY	ILE	VAL	ASP	GLN	TYR	ASN	ASN	GLN	GLY	ALA	GLY	ILE	GLY	ILE	GLY	VAL	PRO	ALA	ALA	ASP	LYS	VAL	ALA	VAL	GLY	VAL	GLY	GLY	GLY	GLY	LYS	
PHE	GLY	ILE	SER	GLY	PHE	GLY	ASP	GLY	GLY	GLN	ARG	GLN	GLY	GLY	GLY	GLY	GLY	THR	THR	LEU	GLY	VAL	VAL	LYS	SER	ALA	ALA	VAL	ARG	VAL	PRO	SER	THR	THR	LEU	
GLU	PRO	ARG	ALA	LEU	LEU	ASP	GLY	GLY	GLY	ASN	VAL	ALA	VAL	VAL	VAL	VAL	SER	SER	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	
VAL	GLU	SER	ARG	GLN	ILE	ARG	ILE	GLU	ALA	ILE	SER	LEU	SER	PRO	ILE	VAL	GLY	ASN	GLY	ASN	GLY	VAL	VAL	HIS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	ILE	
SER	GLU	GLN	VAL	GLY	TYR	GLY	G311	G311	P333	PRO	THR	THR	ASN	GLN	GLY	VAL	GLY	GLN	GLN	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN	
VAL	GLY	ASP	ILE	ARG	GLN	GLY	THR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	SER	



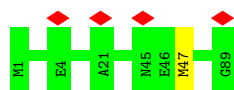


• Molecule 6: Flagellar M-ring protein

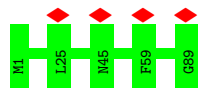


• Molecule 6: Flagellar M-ring protein

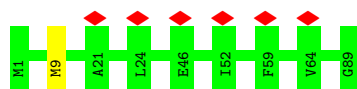




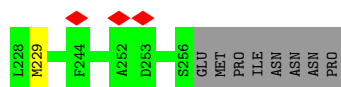
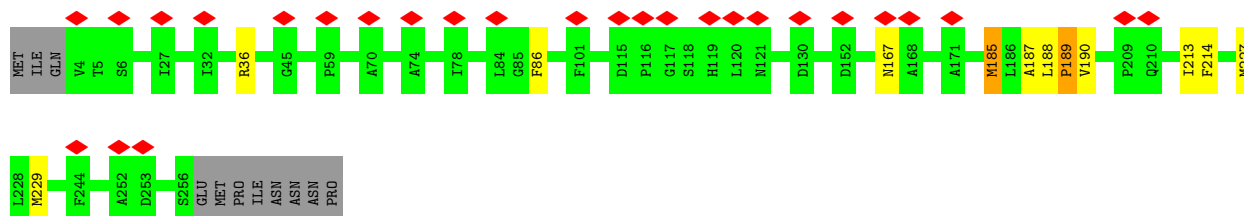
- Molecule 7: Flagellar biosynthetic protein FliQ



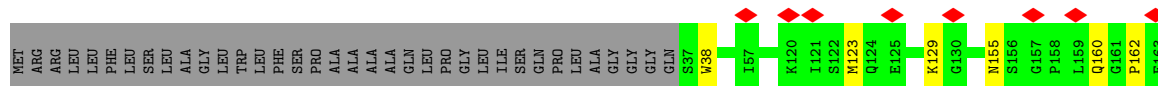
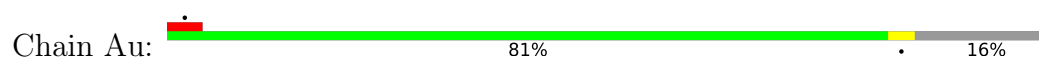
- Molecule 7: Flagellar biosynthetic protein FliQ



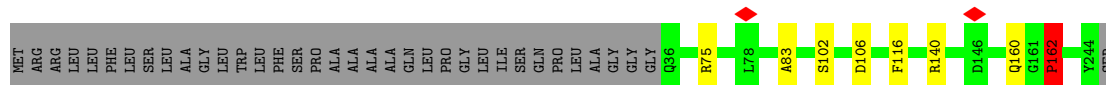
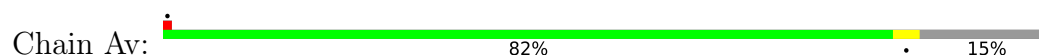
- Molecule 8: Flagellar biosynthetic protein FliR




- Molecule 9: Flagellar biosynthetic protein FliP

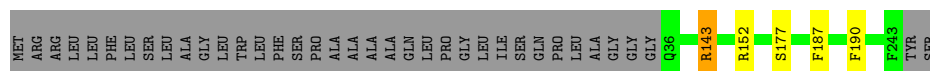


- Molecule 9: Flagellar biosynthetic protein FliP




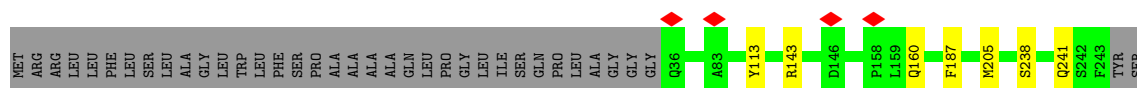
- Molecule 9: Flagellar biosynthetic protein FliP

Chain Aw:  83% 15%




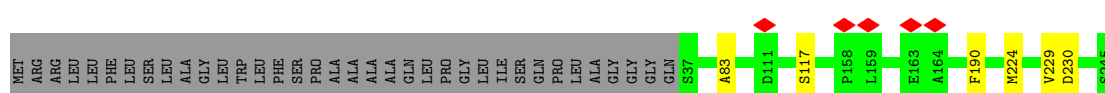
- Molecule 9: Flagellar biosynthetic protein FliP

Chain Ax:  82% 15%



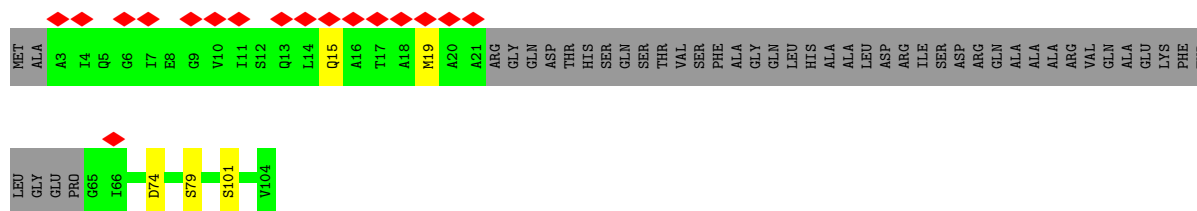
- Molecule 9: Flagellar biosynthetic protein FliP

Chain Ay:  83% 15%




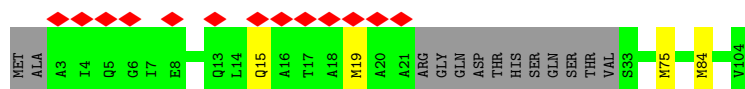
- Molecule 10: Flagellar hook-basal body complex protein FliE

Chain Az:  16% 52% 5% 43%




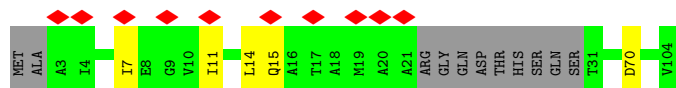
- Molecule 10: Flagellar hook-basal body complex protein FliE

Chain A1:  12% 84% 12%




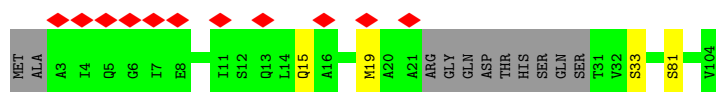
- Molecule 10: Flagellar hook-basal body complex protein FliE

Chain A2:  10% 85% 5% 11%

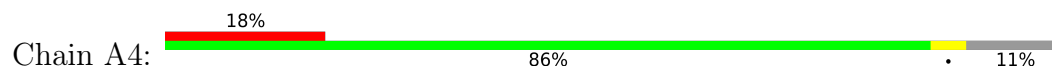


- Molecule 10: Flagellar hook-basal body complex protein FliE

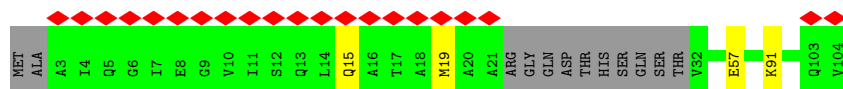
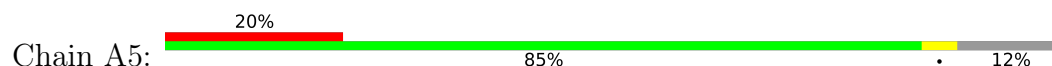
Chain A3:  11% 86% 11%



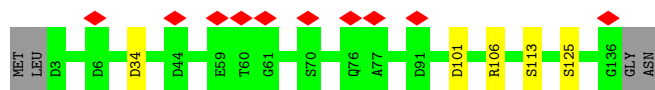
- Molecule 10: Flagellar hook-basal body complex protein FliE



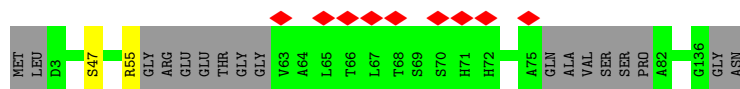
- Molecule 10: Flagellar hook-basal body complex protein FliE



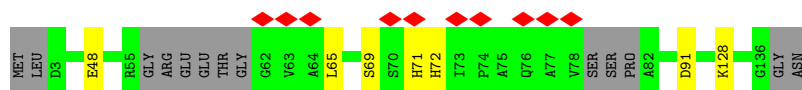
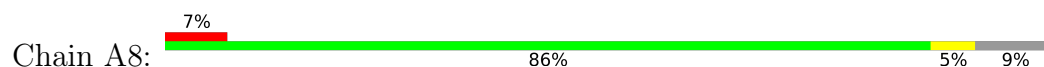
- Molecule 11: Flagellar basal body rod protein FlgB



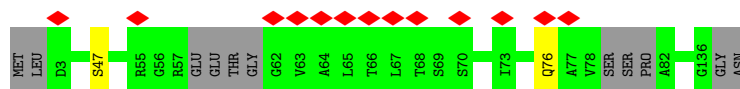
- Molecule 11: Flagellar basal body rod protein FlgB



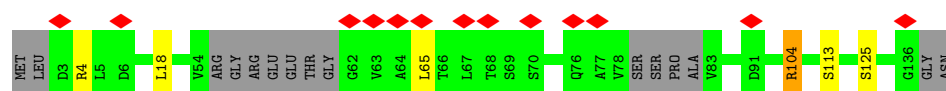
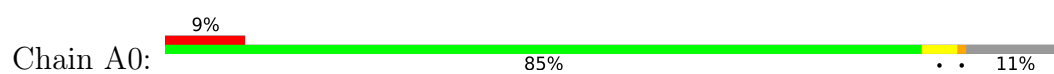
- Molecule 11: Flagellar basal body rod protein FlgB



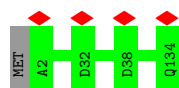
- Molecule 11: Flagellar basal body rod protein FlgB



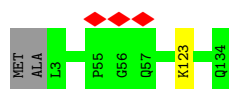
- Molecule 11: Flagellar basal body rod protein FlgB



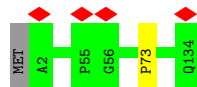
- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC



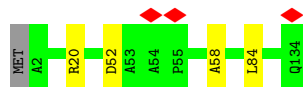
- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC



- Molecule 12: Flagellar basal-body rod protein FlgC



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.118	Depositor
Minimum map value	-0.684	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.18	Depositor
Map size (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	A	0.27	0/1613	0.51	0/2194
1	B	0.27	0/1613	0.51	0/2194
1	C	0.27	0/1613	0.51	0/2194
1	D	0.27	0/1613	0.51	0/2194
1	E	0.27	0/1613	0.51	0/2194
1	F	0.27	0/1613	0.51	0/2194
1	G	0.27	0/1613	0.51	0/2194
1	H	0.27	0/1613	0.51	0/2194
1	I	0.27	0/1613	0.51	0/2194
1	J	0.27	0/1613	0.51	0/2194
1	K	0.27	0/1613	0.51	0/2194
1	L	0.27	0/1613	0.51	0/2194
1	M	0.27	0/1613	0.51	0/2194
1	N	0.27	0/1613	0.51	0/2194
1	O	0.27	0/1613	0.51	0/2194
1	P	0.27	0/1613	0.51	0/2194
1	Q	0.27	0/1613	0.51	0/2194
1	R	0.27	0/1613	0.51	0/2194
1	S	0.27	0/1613	0.51	0/2194
1	T	0.27	0/1613	0.51	0/2194
1	U	0.27	0/1613	0.51	0/2194
1	V	0.27	0/1613	0.51	0/2194
1	W	0.27	0/1613	0.51	0/2194
1	X	0.27	0/1613	0.51	0/2194
1	Y	0.27	0/1613	0.51	0/2194
1	Z	0.27	0/1613	0.51	0/2194
2	a	0.26	0/2243	0.51	0/3041
2	b	0.26	0/2243	0.51	0/3041
2	c	0.26	0/2243	0.51	0/3041
2	d	0.26	0/2243	0.51	0/3041
2	e	0.26	0/2243	0.51	0/3041
2	f	0.26	0/2243	0.51	0/3041
2	g	0.26	0/2243	0.51	0/3041
2	h	0.26	0/2243	0.51	0/3041

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

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	A9	0.34	0/991	0.54	0/1335
12	BA	0.28	0/981	0.44	0/1334
12	BB	0.26	0/976	0.46	0/1327
12	BC	0.57	2/981 (0.2%)	0.95	3/1334 (0.2%)
12	BD	0.28	0/981	0.52	1/1334 (0.1%)
12	BE	0.26	0/981	0.47	0/1334
12	BF	0.28	0/981	0.47	0/1334
All	All	0.34	27/343262 (0.0%)	0.54	68/466341 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	a	0	1
2	b	0	1
2	c	0	1
2	d	0	1
2	e	0	1
2	f	0	1
2	g	0	1
2	h	0	1
2	i	0	1
2	j	0	1
2	k	0	1
2	l	0	1
2	m	0	1
2	n	0	1
2	o	0	1
2	p	0	1
2	q	0	1
2	r	0	1
2	s	0	1
2	t	0	1
2	u	0	1
2	v	0	1
2	w	0	1
2	x	0	1
2	y	0	1
2	z	0	1
3	0	0	2

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

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

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	ZV	140	PRO	CG-CD	-16.09	0.97	1.50
6	BK	331	PRO	CG-CD	-14.22	1.03	1.50
12	BC	73	PRO	CG-CD	-12.75	1.08	1.50
4	ZV	125	PRO	CG-CD	-10.16	1.17	1.50
6	UM	172	PRO	N-CD	-9.55	1.34	1.47
6	UL	172	PRO	N-CD	-9.54	1.34	1.47
6	UP	172	PRO	N-CD	-9.53	1.34	1.47
6	UN	172	PRO	N-CD	-9.47	1.34	1.47
6	UJ	172	PRO	N-CD	-9.46	1.34	1.47
6	UO	172	PRO	N-CD	-9.45	1.34	1.47
6	UK	172	PRO	N-CD	-9.45	1.34	1.47
6	UI	172	PRO	N-CD	-9.43	1.34	1.47
4	ZV	140	PRO	N-CD	8.31	1.59	1.47
6	UP	125	GLN	C-N	7.65	1.51	1.34
6	UJ	125	GLN	C-N	7.63	1.51	1.34
12	BC	73	PRO	CB-CG	-7.62	1.11	1.50
6	UO	125	GLN	C-N	7.62	1.51	1.34
6	UI	125	GLN	C-N	7.61	1.51	1.34
6	UL	125	GLN	C-N	7.60	1.51	1.34
6	UK	125	GLN	C-N	7.59	1.51	1.34
6	UM	125	GLN	C-N	7.59	1.51	1.34
6	UN	125	GLN	C-N	7.54	1.51	1.34
4	ZV	125	PRO	N-CD	6.61	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	At	185	MET	C-O	6.34	1.35	1.23
4	ZY	125	PRO	CG-CD	-5.45	1.32	1.50
4	ZR	125	PRO	CG-CD	-5.08	1.33	1.50
6	UM	105	LEU	C-N	-5.02	1.24	1.34

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	BC	73	PRO	N-CD-CG	-18.82	74.97	103.20
12	BC	73	PRO	CB-CG-CD	18.82	179.88	106.50
4	ZV	140	PRO	N-CD-CG	-17.33	77.21	103.20
6	BK	331	PRO	N-CD-CG	-16.14	78.99	103.20
12	BC	73	PRO	CA-CB-CG	-14.02	77.37	104.00
4	ZR	125	PRO	CA-N-CD	-13.95	91.97	111.50
4	ZY	125	PRO	CA-N-CD	-13.36	92.80	111.50
4	ZV	125	PRO	CA-N-CD	-13.25	92.95	111.50
9	Au	162	PRO	CA-N-CD	-12.03	94.65	111.50
4	Zc	125	PRO	CA-N-CD	-11.23	95.77	111.50
4	ZV	125	PRO	N-CD-CG	-11.23	86.36	103.20
4	ZV	140	PRO	CA-N-CD	-10.27	97.13	111.50
4	ZV	140	PRO	CA-CB-CG	-9.30	86.34	104.00
6	BK	331	PRO	CA-CB-CG	-9.00	86.90	104.00
6	UO	126	PHE	O-C-N	8.85	136.86	122.70
6	UJ	126	PHE	O-C-N	8.83	136.82	122.70
6	UL	126	PHE	O-C-N	8.82	136.81	122.70
6	UK	126	PHE	O-C-N	8.80	136.78	122.70
6	UN	126	PHE	O-C-N	8.79	136.76	122.70
6	UP	126	PHE	O-C-N	8.78	136.75	122.70
6	UM	126	PHE	O-C-N	8.77	136.73	122.70
6	UI	126	PHE	O-C-N	8.76	136.72	122.70
4	ZM	223	PRO	CA-N-CD	-8.44	99.69	111.50
4	ZR	125	PRO	N-CD-CG	-7.57	91.84	103.20
4	ZY	125	PRO	N-CD-CG	-7.45	92.02	103.20
6	BK	331	PRO	N-CA-CB	-7.03	94.86	103.30
6	UJ	126	PHE	CA-C-N	-6.79	102.26	117.20
6	UK	126	PHE	CA-C-N	-6.78	102.29	117.20
6	UM	126	PHE	CA-C-N	-6.77	102.31	117.20
6	UO	126	PHE	CA-C-N	-6.77	102.30	117.20
6	UL	126	PHE	CA-C-N	-6.77	102.31	117.20
6	UN	126	PHE	CA-C-N	-6.75	102.36	117.20
6	UP	126	PHE	CA-C-N	-6.74	102.38	117.20
6	UI	126	PHE	CA-C-N	-6.72	102.42	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Au	162	PRO	N-CD-CG	-6.54	93.40	103.20
6	UP	129	GLN	O-C-N	6.39	132.92	122.70
6	UK	129	GLN	O-C-N	6.38	132.91	122.70
6	UO	129	GLN	O-C-N	6.32	132.80	122.70
6	UM	129	GLN	O-C-N	6.31	132.79	122.70
6	WA	162	PRO	N-CA-C	6.29	128.46	112.10
6	UJ	129	GLN	O-C-N	6.29	132.76	122.70
6	UL	129	GLN	O-C-N	6.28	132.74	122.70
6	UI	129	GLN	O-C-N	6.27	132.73	122.70
6	UN	129	GLN	O-C-N	6.25	132.71	122.70
3	AI	154	ASP	CB-CG-OD2	6.24	123.92	118.30
4	ZR	214	ASP	CB-CG-OD1	6.05	123.74	118.30
4	Zc	125	PRO	N-CD-CG	-5.88	94.37	103.20
3	AM	154	ASP	CB-CG-OD1	5.76	123.48	118.30
6	UO	126	PHE	C-N-CA	-5.75	107.32	121.70
6	UJ	126	PHE	C-N-CA	-5.74	107.36	121.70
6	UL	126	PHE	C-N-CA	-5.74	107.36	121.70
6	UP	126	PHE	C-N-CA	-5.74	107.36	121.70
6	UM	126	PHE	C-N-CA	-5.73	107.37	121.70
6	UN	126	PHE	C-N-CA	-5.72	107.39	121.70
6	UK	126	PHE	C-N-CA	-5.72	107.39	121.70
3	0	52	PRO	N-CA-CB	-5.71	96.32	102.60
6	UI	126	PHE	C-N-CA	-5.71	107.43	121.70
4	ZS	18	ASP	CB-CG-OD1	5.67	123.40	118.30
4	ZV	125	PRO	CA-CB-CG	-5.66	93.25	104.00
4	ZP	125	PRO	CA-N-CD	-5.58	103.69	111.50
3	ZE	13	ASP	CB-CG-OD1	5.53	123.28	118.30
8	At	189	PRO	CA-N-CD	-5.50	103.80	111.50
9	Av	162	PRO	N-CA-CB	-5.29	96.78	102.60
5	AB	72	ASP	CB-CG-OD1	5.22	123.00	118.30
6	WJ	214	ASP	CB-CA-C	-5.20	99.99	110.40
3	9	109	ASP	CB-CG-OD2	5.16	122.95	118.30
12	BD	8	ASP	CB-CG-OD2	5.08	122.87	118.30
6	WO	168	GLU	CB-CA-C	-5.07	100.25	110.40

There are no chirality outliers.

All (123) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	0	36	ARG	Sidechain
3	0	50	ARG	Sidechain
3	1	36	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	5	50	ARG	Sidechain
3	6	153	ARG	Sidechain
3	8	238	ARG	Sidechain
11	A0	104	ARG	Sidechain
11	A6	106	ARG	Sidechain
5	AA	200	ARG	Sidechain
5	AA	243	ARG	Sidechain
5	AB	225	ARG	Sidechain
5	AC	243	ARG	Sidechain
5	AE	160	ARG	Sidechain
3	AF	36	ARG	Sidechain
3	AI	116	ARG	Sidechain
3	AM	36	ARG	Sidechain
3	AM	50	ARG	Sidechain
3	AN	238	ARG	Sidechain
9	Aw	143	ARG	Sidechain
12	BD	110	ARG	Sidechain
12	BF	110	ARG	Sidechain
6	UI	221	THR	Mainchain
6	UI	50	ASP	Mainchain
6	UJ	270	THR	Mainchain
6	UJ	50	ASP	Mainchain
6	UK	167	ARG	Sidechain
6	UK	221	THR	Mainchain
6	UK	50	ASP	Mainchain
6	UL	167	ARG	Sidechain
6	UL	221	THR	Mainchain
6	UL	50	ASP	Mainchain
6	UM	221	THR	Mainchain
6	UM	50	ASP	Mainchain
6	UN	221	THR	Mainchain
6	UN	50	ASP	Mainchain
6	UO	221	THR	Mainchain
6	UO	50	ASP	Mainchain
6	UP	167	ARG	Sidechain
6	UP	221	THR	Mainchain
6	UP	50	ASP	Mainchain
6	WA	134	ARG	Sidechain
6	WA	142	ARG	Sidechain
6	WA	167	ARG	Sidechain
6	WB	134	ARG	Sidechain
6	WB	142	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	WB	154	ARG	Sidechain
6	WB	167	ARG	Sidechain
6	WC	134	ARG	Sidechain
6	WC	142	ARG	Sidechain
6	WC	167	ARG	Sidechain
6	WD	134	ARG	Sidechain
6	WE	134	ARG	Sidechain
6	WE	142	ARG	Sidechain
6	WF	134	ARG	Sidechain
6	WF	142	ARG	Sidechain
6	WF	167	ARG	Sidechain
6	WG	134	ARG	Sidechain
6	WG	142	ARG	Sidechain
6	WG	167	ARG	Sidechain
6	WI	142	ARG	Sidechain
6	WJ	134	ARG	Sidechain
6	WJ	142	ARG	Sidechain
6	WJ	167	ARG	Sidechain
6	WK	134	ARG	Sidechain
6	WK	142	ARG	Sidechain
6	WL	134	ARG	Sidechain
6	WL	157	LEU	Mainchain
6	WM	134	ARG	Sidechain
6	WN	134	ARG	Sidechain
6	WO	134	ARG	Sidechain
6	WP	134	ARG	Sidechain
6	WP	142	ARG	Sidechain
6	WP	154	ARG	Sidechain
6	WQ	134	ARG	Sidechain
6	WQ	142	ARG	Sidechain
6	WR	134	ARG	Sidechain
6	WR	142	ARG	Sidechain
6	WR	167	ARG	Sidechain
6	WS	167	ARG	Sidechain
6	WT	134	ARG	Sidechain
6	WT	142	ARG	Sidechain
6	WU	134	ARG	Sidechain
6	WU	142	ARG	Sidechain
6	WV	134	ARG	Sidechain
6	WV	142	ARG	Sidechain
6	WV	167	ARG	Sidechain
6	WW	134	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	WW	167	ARG	Sidechain
3	ZA	79	ARG	Sidechain
4	ZG	71	ARG	Sidechain
4	ZI	380	ARG	Sidechain
4	ZK	71	ARG	Sidechain
4	ZO	71	ARG	Sidechain
4	ZW	71	ARG	Sidechain
4	Zb	106	ARG	Sidechain
4	Zd	380	ARG	Sidechain
4	Ze	380	ARG	Sidechain
2	a	117	ARG	Sidechain
2	b	117	ARG	Sidechain
2	c	117	ARG	Sidechain
2	d	117	ARG	Sidechain
2	e	117	ARG	Sidechain
2	f	117	ARG	Sidechain
2	g	117	ARG	Sidechain
2	h	117	ARG	Sidechain
2	i	117	ARG	Sidechain
2	j	117	ARG	Sidechain
2	k	117	ARG	Sidechain
2	l	117	ARG	Sidechain
2	m	117	ARG	Sidechain
2	n	117	ARG	Sidechain
2	o	117	ARG	Sidechain
2	p	117	ARG	Sidechain
2	q	117	ARG	Sidechain
2	r	117	ARG	Sidechain
2	s	117	ARG	Sidechain
2	t	117	ARG	Sidechain
2	u	117	ARG	Sidechain
2	v	117	ARG	Sidechain
2	w	117	ARG	Sidechain
2	x	117	ARG	Sidechain
2	y	117	ARG	Sidechain
2	z	117	ARG	Sidechain

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	54
2	a	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	b	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	c	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	d	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	e	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	f	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	g	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	h	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	i	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	j	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	k	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	l	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	m	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	n	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	o	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	p	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	q	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	r	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	s	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	t	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	u	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	v	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	w	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	x	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	y	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
2	z	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
3	0	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	60
3	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	60
3	2	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	44
3	3	258/260 (99%)	248 (96%)	8 (3%)	2 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	4	258/260 (99%)	248 (96%)	7 (3%)	3 (1%)	11	35
3	5	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	44
3	6	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	44
3	7	258/260 (99%)	245 (95%)	10 (4%)	3 (1%)	11	35
3	8	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	44
3	9	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	44
3	AF	250/260 (96%)	237 (95%)	12 (5%)	1 (0%)	30	60
3	AG	251/260 (96%)	237 (94%)	13 (5%)	1 (0%)	30	60
3	AH	252/260 (97%)	241 (96%)	10 (4%)	1 (0%)	30	60
3	AI	250/260 (96%)	242 (97%)	6 (2%)	2 (1%)	16	44
3	AJ	251/260 (96%)	241 (96%)	9 (4%)	1 (0%)	30	60
3	AK	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	30	60
3	AL	244/260 (94%)	237 (97%)	4 (2%)	3 (1%)	11	35
3	AM	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	60
3	AN	244/260 (94%)	240 (98%)	3 (1%)	1 (0%)	30	60
3	ZA	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	11	35
3	ZB	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	35
3	ZC	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	35
3	ZD	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	44
3	ZE	258/260 (99%)	245 (95%)	12 (5%)	1 (0%)	30	60
4	ZF	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	ZG	399/403 (99%)	392 (98%)	6 (2%)	1 (0%)	37	66
4	ZH	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25	54
4	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
4	ZK	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
4	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	66
4	ZM	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	ZN	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	ZO	399/403 (99%)	381 (96%)	15 (4%)	3 (1%)	16	44
4	ZP	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
4	ZR	399/403 (99%)	390 (98%)	8 (2%)	1 (0%)	37	66
4	ZS	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
4	ZT	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
4	ZU	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
4	ZV	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
4	ZW	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
4	ZX	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	ZY	399/403 (99%)	384 (96%)	15 (4%)	0	100	100
4	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
4	Za	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	Zb	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
4	Zc	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
4	Zd	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	Ze	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
4	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
4	Zg	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
4	Zh	399/403 (99%)	393 (98%)	6 (2%)	0	100	100
5	AA	246/251 (98%)	232 (94%)	11 (4%)	3 (1%)	11	35
5	AB	247/251 (98%)	241 (98%)	6 (2%)	0	100	100
5	AC	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
5	AD	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
5	AE	247/251 (98%)	233 (94%)	13 (5%)	1 (0%)	30	60
6	AO	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AP	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AQ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AR	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AS	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AT	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AU	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AV	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AW	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AX	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AY	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AZ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Aa	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ac	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ad	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ae	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Af	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ag	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ah	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ai	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Aj	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ak	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Al	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Am	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	An	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ao	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ap	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BG	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
6	BH	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
6	BI	18/560 (3%)	18 (100%)	0	0	100	100
6	BJ	14/560 (2%)	14 (100%)	0	0	100	100
6	BK	19/560 (3%)	19 (100%)	0	0	100	100
6	BL	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
6	BM	19/560 (3%)	19 (100%)	0	0	100	100
6	BN	14/560 (2%)	14 (100%)	0	0	100	100
6	BO	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
6	BP	14/560 (2%)	14 (100%)	0	0	100	100
6	BQ	19/560 (3%)	19 (100%)	0	0	100	100
6	BR	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BS	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BT	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BU	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BV	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BW	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BX	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	UI	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UJ	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UK	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UL	151/560 (27%)	142 (94%)	7 (5%)	2 (1%)	10	33
6	UM	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UN	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UO	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	UP	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	33
6	WA	111/560 (20%)	99 (89%)	9 (8%)	3 (3%)	4	21
6	WB	109/560 (20%)	94 (86%)	10 (9%)	5 (5%)	2	12
6	WC	106/560 (19%)	96 (91%)	9 (8%)	1 (1%)	14	41
6	WD	108/560 (19%)	99 (92%)	4 (4%)	5 (5%)	2	12
6	WE	110/560 (20%)	98 (89%)	8 (7%)	4 (4%)	3	16
6	WF	109/560 (20%)	98 (90%)	8 (7%)	3 (3%)	4	20
6	WG	110/560 (20%)	98 (89%)	10 (9%)	2 (2%)	7	27
6	WH	93/560 (17%)	86 (92%)	5 (5%)	2 (2%)	5	24
6	WI	93/560 (17%)	82 (88%)	5 (5%)	6 (6%)	1	7
6	WJ	97/560 (17%)	89 (92%)	7 (7%)	1 (1%)	13	39
6	WK	96/560 (17%)	84 (88%)	9 (9%)	3 (3%)	3	18
6	WL	81/560 (14%)	75 (93%)	4 (5%)	2 (2%)	4	22
6	WM	78/560 (14%)	72 (92%)	4 (5%)	2 (3%)	4	22
6	WN	80/560 (14%)	75 (94%)	2 (2%)	3 (4%)	2	15
6	WO	94/560 (17%)	85 (90%)	7 (7%)	2 (2%)	5	24
6	WP	98/560 (18%)	87 (89%)	6 (6%)	5 (5%)	1	11
6	WQ	109/560 (20%)	100 (92%)	5 (5%)	4 (4%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	WR	109/560 (20%)	94 (86%)	8 (7%)	7 (6%)	1	7
6	WS	109/560 (20%)	96 (88%)	7 (6%)	6 (6%)	1	10
6	WT	109/560 (20%)	97 (89%)	5 (5%)	7 (6%)	1	7
6	WU	110/560 (20%)	101 (92%)	8 (7%)	1 (1%)	14	41
6	WV	108/560 (19%)	97 (90%)	9 (8%)	2 (2%)	6	26
6	WW	109/560 (20%)	95 (87%)	9 (8%)	5 (5%)	2	12
7	Ab	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
7	Aq	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
7	Ar	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
7	As	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
8	At	251/264 (95%)	231 (92%)	14 (6%)	6 (2%)	5	23
9	Au	205/245 (84%)	195 (95%)	10 (5%)	0	100	100
9	Av	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13	39
9	Aw	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
9	Ax	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25	54
9	Ay	207/245 (84%)	201 (97%)	4 (2%)	2 (1%)	13	39
10	A1	87/104 (84%)	87 (100%)	0	0	100	100
10	A2	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
10	A3	89/104 (86%)	89 (100%)	0	0	100	100
10	A4	89/104 (86%)	89 (100%)	0	0	100	100
10	A5	88/104 (85%)	88 (100%)	0	0	100	100
10	Az	55/104 (53%)	53 (96%)	2 (4%)	0	100	100
11	A0	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
11	A6	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
11	A7	115/138 (83%)	114 (99%)	1 (1%)	0	100	100
11	A8	119/138 (86%)	116 (98%)	3 (2%)	0	100	100
11	A9	121/138 (88%)	118 (98%)	3 (2%)	0	100	100
12	BA	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
12	BB	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
12	BC	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
12	BD	131/134 (98%)	127 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	BE	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16	44
12	BF	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
All	All	44708/81227 (55%)	43390 (97%)	1126 (2%)	192 (0%)	32	60

All (192) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	209	ASN
3	5	209	ASN
3	8	209	ASN
3	ZA	209	ASN
3	ZB	164	GLN
3	ZC	139	ALA
4	ZG	46	SER
5	AA	123	GLU
8	At	188	LEU
8	At	190	VAL
9	Ay	83	ALA
6	WO	168	GLU
6	WR	123	ILE
6	WR	165	PHE
6	WR	166	VAL
6	WS	187	ASP
3	9	139	ALA
3	ZB	165	ALA
3	ZB	209	ASN
3	ZC	209	ASN
3	ZD	209	ASN
3	ZE	209	ASN
4	ZI	375	MET
4	ZO	237	ILE
4	ZR	87	ASP
3	AI	165	ALA
3	AL	4	SER
3	AN	127	GLN
8	At	167	ASN
8	At	213	ILE
9	Av	83	ALA
9	Ax	160	GLN
6	WB	148	GLY
6	WB	163	SER

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Mol	Chain	Res	Type
6	WD	146	THR
6	WD	148	GLY
6	WF	118	GLN
6	WI	146	THR
6	WI	160	PRO
6	WI	170	LYS
6	WK	166	VAL
6	WM	148	GLY
6	WN	146	THR
6	WN	148	GLY
6	WP	146	THR
6	WQ	146	THR
6	WQ	148	GLY
6	WQ	169	GLN
6	WS	146	THR
6	WT	146	THR
6	WT	162	PRO
6	WW	146	THR
6	WW	148	GLY
3	0	127	GLN
3	2	49	ILE
3	3	49	ILE
3	4	49	ILE
3	4	139	ALA
3	4	140	ILE
3	5	49	ILE
4	ZL	374	ASN
5	AA	151	PRO
3	AF	127	GLN
3	AL	3	SER
3	AM	127	GLN
8	At	189	PRO
6	UI	162	PRO
6	UJ	162	PRO
6	UK	162	PRO
6	UL	162	PRO
6	UM	162	PRO
6	UN	162	PRO
6	UO	162	PRO
6	UP	162	PRO
6	WB	146	THR
6	WB	164	LEU

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Mol	Chain	Res	Type
6	WD	118	GLN
6	WE	160	PRO
6	WE	162	PRO
6	WI	148	GLY
6	WP	148	GLY
6	WS	118	GLN
6	WS	169	GLN
6	WT	165	PHE
6	WW	118	GLN
6	WW	168	GLU
3	6	49	ILE
3	6	58	GLU
3	7	49	ILE
3	7	138	PRO
3	8	49	ILE
3	9	49	ILE
3	ZA	49	ILE
3	ZA	139	ALA
3	ZD	139	ALA
4	ZO	142	THR
4	ZP	374	ASN
3	AG	127	GLN
3	AI	127	GLN
3	AK	127	GLN
3	AL	127	GLN
6	UI	163	SER
6	UJ	163	SER
6	UK	163	SER
6	UL	163	SER
6	UM	163	SER
6	UN	163	SER
6	UO	163	SER
6	UP	163	SER
6	WA	182	PRO
6	WB	182	PRO
6	WD	165	PHE
6	WD	182	PRO
6	WE	182	PRO
6	WF	182	PRO
6	WG	182	PRO
6	WH	165	PHE
6	WH	182	PRO

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Mol	Chain	Res	Type
6	WI	169	GLN
6	WI	182	PRO
6	WJ	182	PRO
6	WK	182	PRO
6	WL	182	PRO
6	WM	182	PRO
6	WN	182	PRO
6	WO	182	PRO
6	WP	182	PRO
6	WQ	182	PRO
6	WR	112	GLY
6	WR	182	PRO
6	WS	182	PRO
6	WT	182	PRO
6	WU	182	PRO
6	WV	148	GLY
6	WV	182	PRO
6	WW	182	PRO
1	A	172	ASN
1	B	172	ASN
1	C	172	ASN
1	D	172	ASN
1	E	172	ASN
1	F	172	ASN
1	G	172	ASN
1	H	172	ASN
1	I	172	ASN
1	J	172	ASN
1	K	172	ASN
1	L	172	ASN
1	M	172	ASN
1	N	172	ASN
1	O	172	ASN
1	P	172	ASN
1	Q	172	ASN
1	R	172	ASN
1	S	172	ASN
1	T	172	ASN
1	U	172	ASN
1	V	172	ASN
1	W	172	ASN
1	X	172	ASN

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Mol	Chain	Res	Type
1	Y	172	ASN
1	Z	172	ASN
3	1	127	GLN
3	7	210	GLY
3	AH	127	GLN
3	AJ	127	GLN
9	Av	162	PRO
6	WK	168	GLU
6	WR	121	PHE
6	WT	163	SER
3	3	139	ALA
4	ZO	375	MET
8	At	187	ALA
6	WC	182	PRO
6	WE	221	THR
6	WG	163	SER
12	BE	58	ALA
4	ZI	325	GLY
5	AA	149	GLY
5	AE	132	GLY
6	WA	160	PRO
6	WF	162	PRO
6	WL	148	GLY
6	WS	148	GLY
6	WT	148	GLY
6	WA	148	GLY
6	WP	123	ILE
6	WR	148	GLY
9	Ay	229	VAL
6	WP	160	PRO
6	WT	161	LYS
3	ZC	138	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	B	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	C	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	D	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	E	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	F	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	G	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	H	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	I	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	J	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	K	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	L	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	M	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	N	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	O	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	P	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	Q	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	R	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	S	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	T	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	U	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	V	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	W	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	X	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	Y	170/186 (91%)	163 (96%)	7 (4%)	26	51
1	Z	170/186 (91%)	163 (96%)	7 (4%)	26	51
2	a	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	b	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	c	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	d	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	e	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	f	248/294 (84%)	239 (96%)	9 (4%)	30	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	g	248/294 (84%)	239 (96%)	9 (4%)	30	56
2	h	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	i	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	j	248/294 (84%)	240 (97%)	8 (3%)	34	59
2	k	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	l	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	m	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	n	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	o	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	p	248/294 (84%)	239 (96%)	9 (4%)	30	56
2	q	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	r	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	s	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	t	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	u	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	v	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	w	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	x	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	y	248/294 (84%)	238 (96%)	10 (4%)	27	52
2	z	248/294 (84%)	238 (96%)	10 (4%)	27	52
3	0	205/215 (95%)	199 (97%)	6 (3%)	37	61
3	1	209/215 (97%)	201 (96%)	8 (4%)	28	54
3	2	215/215 (100%)	212 (99%)	3 (1%)	62	77
3	3	215/215 (100%)	211 (98%)	4 (2%)	52	71
3	4	215/215 (100%)	211 (98%)	4 (2%)	52	71
3	5	215/215 (100%)	211 (98%)	4 (2%)	52	71
3	6	215/215 (100%)	210 (98%)	5 (2%)	45	67
3	7	215/215 (100%)	214 (100%)	1 (0%)	86	91
3	8	215/215 (100%)	213 (99%)	2 (1%)	75	86
3	9	215/215 (100%)	211 (98%)	4 (2%)	52	71
3	AF	209/215 (97%)	204 (98%)	5 (2%)	44	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AG	210/215 (98%)	203 (97%)	7 (3%)	33	58
3	AH	211/215 (98%)	201 (95%)	10 (5%)	22	49
3	AI	209/215 (97%)	200 (96%)	9 (4%)	25	50
3	AJ	210/215 (98%)	202 (96%)	8 (4%)	28	54
3	AK	200/215 (93%)	196 (98%)	4 (2%)	50	70
3	AL	205/215 (95%)	199 (97%)	6 (3%)	37	61
3	AM	205/215 (95%)	197 (96%)	8 (4%)	27	53
3	AN	205/215 (95%)	201 (98%)	4 (2%)	50	70
3	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	86
3	ZB	215/215 (100%)	207 (96%)	8 (4%)	29	54
3	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	77
3	ZD	215/215 (100%)	213 (99%)	2 (1%)	75	86
3	ZE	215/215 (100%)	214 (100%)	1 (0%)	86	91
4	ZF	321/323 (99%)	310 (97%)	11 (3%)	32	57
4	ZG	321/323 (99%)	306 (95%)	15 (5%)	22	49
4	ZH	321/323 (99%)	309 (96%)	12 (4%)	29	54
4	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	ZJ	321/323 (99%)	313 (98%)	8 (2%)	42	65
4	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	60
4	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	62
4	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	60
4	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	65
4	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	49
4	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	62
4	ZR	321/323 (99%)	313 (98%)	8 (2%)	42	65
4	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	ZT	321/323 (99%)	316 (98%)	5 (2%)	58	75
4	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	80
4	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	80
4	ZW	321/323 (99%)	308 (96%)	13 (4%)	27	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	86
4	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	68
4	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	75
4	Za	321/323 (99%)	316 (98%)	5 (2%)	58	75
4	Zb	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	57
4	Zd	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	Ze	321/323 (99%)	312 (97%)	9 (3%)	38	62
4	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	68
4	Zg	321/323 (99%)	315 (98%)	6 (2%)	52	71
4	Zh	321/323 (99%)	313 (98%)	8 (2%)	42	65
5	AA	190/193 (98%)	187 (98%)	3 (2%)	58	75
5	AB	191/193 (99%)	188 (98%)	3 (2%)	58	75
5	AC	192/193 (100%)	187 (97%)	5 (3%)	41	64
5	AD	192/193 (100%)	190 (99%)	2 (1%)	73	83
5	AE	191/193 (99%)	190 (100%)	1 (0%)	86	91
6	AO	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AP	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AQ	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AR	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AS	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AT	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AU	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AV	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AW	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AX	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AY	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	AZ	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Aa	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ac	141/467 (30%)	134 (95%)	7 (5%)	20	46
6	Ad	141/467 (30%)	134 (95%)	7 (5%)	20	46

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Aq	74/74 (100%)	73 (99%)	1 (1%)	62	77
7	Ar	74/74 (100%)	74 (100%)	0	100	100
7	As	74/74 (100%)	73 (99%)	1 (1%)	62	77
8	At	210/221 (95%)	204 (97%)	6 (3%)	37	61
9	Au	177/204 (87%)	170 (96%)	7 (4%)	27	52
9	Av	179/204 (88%)	172 (96%)	7 (4%)	27	53
9	Aw	178/204 (87%)	173 (97%)	5 (3%)	38	62
9	Ax	178/204 (87%)	172 (97%)	6 (3%)	32	57
9	Ay	179/204 (88%)	175 (98%)	4 (2%)	47	68
10	A1	68/79 (86%)	64 (94%)	4 (6%)	16	41
10	A2	70/79 (89%)	65 (93%)	5 (7%)	12	37
10	A3	70/79 (89%)	66 (94%)	4 (6%)	17	43
10	A4	70/79 (89%)	66 (94%)	4 (6%)	17	43
10	A5	69/79 (87%)	65 (94%)	4 (6%)	17	42
10	Az	45/79 (57%)	40 (89%)	5 (11%)	5	18
11	A0	102/113 (90%)	96 (94%)	6 (6%)	16	41
11	A6	110/113 (97%)	106 (96%)	4 (4%)	30	56
11	A7	101/113 (89%)	99 (98%)	2 (2%)	50	70
11	A8	103/113 (91%)	96 (93%)	7 (7%)	13	38
11	A9	104/113 (92%)	102 (98%)	2 (2%)	52	71
12	BA	104/105 (99%)	104 (100%)	0	100	100
12	BB	104/105 (99%)	103 (99%)	1 (1%)	73	83
12	BC	104/105 (99%)	104 (100%)	0	100	100
12	BD	104/105 (99%)	102 (98%)	2 (2%)	52	71
12	BE	104/105 (99%)	101 (97%)	3 (3%)	37	61
12	BF	104/105 (99%)	100 (96%)	4 (4%)	28	54
All	All	37085/66670 (56%)	35783 (96%)	1302 (4%)	33	56

All (1302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	CYS
1	A	103	SER

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Mol	Chain	Res	Type
1	A	106	PHE
1	A	124	MET
1	A	145	SER
1	A	176	GLU
1	A	202	ASP
1	B	22	CYS
1	B	103	SER
1	B	106	PHE
1	B	124	MET
1	B	145	SER
1	B	176	GLU
1	B	202	ASP
1	C	22	CYS
1	C	103	SER
1	C	106	PHE
1	C	124	MET
1	C	145	SER
1	C	176	GLU
1	C	202	ASP
1	D	22	CYS
1	D	103	SER
1	D	106	PHE
1	D	124	MET
1	D	145	SER
1	D	176	GLU
1	D	202	ASP
1	E	22	CYS
1	E	103	SER
1	E	106	PHE
1	E	124	MET
1	E	145	SER
1	E	176	GLU
1	E	202	ASP
1	F	22	CYS
1	F	103	SER
1	F	106	PHE
1	F	124	MET
1	F	145	SER
1	F	176	GLU
1	F	202	ASP
1	G	22	CYS
1	G	103	SER

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Mol	Chain	Res	Type
1	G	106	PHE
1	G	124	MET
1	G	145	SER
1	G	176	GLU
1	G	202	ASP
1	H	22	CYS
1	H	103	SER
1	H	106	PHE
1	H	124	MET
1	H	145	SER
1	H	176	GLU
1	H	202	ASP
1	I	22	CYS
1	I	103	SER
1	I	106	PHE
1	I	124	MET
1	I	145	SER
1	I	176	GLU
1	I	202	ASP
1	J	22	CYS
1	J	103	SER
1	J	106	PHE
1	J	124	MET
1	J	145	SER
1	J	176	GLU
1	J	202	ASP
1	K	22	CYS
1	K	103	SER
1	K	106	PHE
1	K	124	MET
1	K	145	SER
1	K	176	GLU
1	K	202	ASP
1	L	22	CYS
1	L	103	SER
1	L	106	PHE
1	L	124	MET
1	L	145	SER
1	L	176	GLU
1	L	202	ASP
1	M	22	CYS
1	M	103	SER

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Mol	Chain	Res	Type
1	M	106	PHE
1	M	124	MET
1	M	145	SER
1	M	176	GLU
1	M	202	ASP
1	N	22	CYS
1	N	103	SER
1	N	106	PHE
1	N	124	MET
1	N	145	SER
1	N	176	GLU
1	N	202	ASP
1	O	22	CYS
1	O	103	SER
1	O	106	PHE
1	O	124	MET
1	O	145	SER
1	O	176	GLU
1	O	202	ASP
1	P	22	CYS
1	P	103	SER
1	P	106	PHE
1	P	124	MET
1	P	145	SER
1	P	176	GLU
1	P	202	ASP
1	Q	22	CYS
1	Q	103	SER
1	Q	106	PHE
1	Q	124	MET
1	Q	145	SER
1	Q	176	GLU
1	Q	202	ASP
1	R	22	CYS
1	R	103	SER
1	R	106	PHE
1	R	124	MET
1	R	145	SER
1	R	176	GLU
1	R	202	ASP
1	S	22	CYS
1	S	103	SER

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Mol	Chain	Res	Type
1	S	106	PHE
1	S	124	MET
1	S	145	SER
1	S	176	GLU
1	S	202	ASP
1	T	22	CYS
1	T	103	SER
1	T	106	PHE
1	T	124	MET
1	T	145	SER
1	T	176	GLU
1	T	202	ASP
1	U	22	CYS
1	U	103	SER
1	U	106	PHE
1	U	124	MET
1	U	145	SER
1	U	176	GLU
1	U	202	ASP
1	V	22	CYS
1	V	103	SER
1	V	106	PHE
1	V	124	MET
1	V	145	SER
1	V	176	GLU
1	V	202	ASP
1	W	22	CYS
1	W	103	SER
1	W	106	PHE
1	W	124	MET
1	W	145	SER
1	W	176	GLU
1	W	202	ASP
1	X	22	CYS
1	X	103	SER
1	X	106	PHE
1	X	124	MET
1	X	145	SER
1	X	176	GLU
1	X	202	ASP
1	Y	22	CYS
1	Y	103	SER

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Mol	Chain	Res	Type
1	Y	106	PHE
1	Y	124	MET
1	Y	145	SER
1	Y	176	GLU
1	Y	202	ASP
1	Z	22	CYS
1	Z	103	SER
1	Z	106	PHE
1	Z	124	MET
1	Z	145	SER
1	Z	176	GLU
1	Z	202	ASP
2	a	21	ARG
2	a	80	GLN
2	a	129	VAL
2	a	131	SER
2	a	159	GLN
2	a	217	ASP
2	a	264	MET
2	a	266	ARG
2	a	324	SER
2	a	343	MET
2	b	21	ARG
2	b	80	GLN
2	b	129	VAL
2	b	131	SER
2	b	159	GLN
2	b	217	ASP
2	b	264	MET
2	b	266	ARG
2	b	324	SER
2	b	343	MET
2	c	21	ARG
2	c	80	GLN
2	c	129	VAL
2	c	131	SER
2	c	159	GLN
2	c	217	ASP
2	c	264	MET
2	c	266	ARG
2	c	324	SER
2	c	343	MET

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Mol	Chain	Res	Type
2	d	21	ARG
2	d	80	GLN
2	d	129	VAL
2	d	131	SER
2	d	159	GLN
2	d	217	ASP
2	d	264	MET
2	d	266	ARG
2	d	324	SER
2	d	343	MET
2	e	21	ARG
2	e	80	GLN
2	e	129	VAL
2	e	131	SER
2	e	159	GLN
2	e	217	ASP
2	e	264	MET
2	e	266	ARG
2	e	324	SER
2	e	343	MET
2	f	21	ARG
2	f	80	GLN
2	f	131	SER
2	f	159	GLN
2	f	217	ASP
2	f	264	MET
2	f	266	ARG
2	f	324	SER
2	f	343	MET
2	g	21	ARG
2	g	129	VAL
2	g	131	SER
2	g	159	GLN
2	g	217	ASP
2	g	264	MET
2	g	266	ARG
2	g	324	SER
2	g	343	MET
2	h	21	ARG
2	h	80	GLN
2	h	129	VAL
2	h	131	SER

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Mol	Chain	Res	Type
2	h	159	GLN
2	h	217	ASP
2	h	264	MET
2	h	266	ARG
2	h	324	SER
2	h	343	MET
2	i	21	ARG
2	i	80	GLN
2	i	129	VAL
2	i	131	SER
2	i	159	GLN
2	i	217	ASP
2	i	264	MET
2	i	266	ARG
2	i	324	SER
2	i	343	MET
2	j	21	ARG
2	j	131	SER
2	j	159	GLN
2	j	217	ASP
2	j	264	MET
2	j	266	ARG
2	j	324	SER
2	j	343	MET
2	k	21	ARG
2	k	80	GLN
2	k	129	VAL
2	k	131	SER
2	k	159	GLN
2	k	217	ASP
2	k	264	MET
2	k	266	ARG
2	k	324	SER
2	k	343	MET
2	l	21	ARG
2	l	80	GLN
2	l	129	VAL
2	l	131	SER
2	l	159	GLN
2	l	217	ASP
2	l	264	MET
2	l	266	ARG

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Mol	Chain	Res	Type
2	l	324	SER
2	l	343	MET
2	m	21	ARG
2	m	80	GLN
2	m	129	VAL
2	m	131	SER
2	m	159	GLN
2	m	217	ASP
2	m	264	MET
2	m	266	ARG
2	m	324	SER
2	m	343	MET
2	n	21	ARG
2	n	80	GLN
2	n	129	VAL
2	n	131	SER
2	n	159	GLN
2	n	217	ASP
2	n	264	MET
2	n	266	ARG
2	n	324	SER
2	n	343	MET
2	o	21	ARG
2	o	80	GLN
2	o	129	VAL
2	o	131	SER
2	o	159	GLN
2	o	217	ASP
2	o	264	MET
2	o	266	ARG
2	o	324	SER
2	o	343	MET
2	p	21	ARG
2	p	80	GLN
2	p	131	SER
2	p	159	GLN
2	p	217	ASP
2	p	264	MET
2	p	266	ARG
2	p	324	SER
2	p	343	MET
2	q	21	ARG

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Mol	Chain	Res	Type
2	q	80	GLN
2	q	129	VAL
2	q	131	SER
2	q	159	GLN
2	q	217	ASP
2	q	264	MET
2	q	266	ARG
2	q	324	SER
2	q	343	MET
2	r	21	ARG
2	r	80	GLN
2	r	129	VAL
2	r	131	SER
2	r	159	GLN
2	r	217	ASP
2	r	264	MET
2	r	266	ARG
2	r	324	SER
2	r	343	MET
2	s	21	ARG
2	s	80	GLN
2	s	129	VAL
2	s	131	SER
2	s	159	GLN
2	s	217	ASP
2	s	264	MET
2	s	266	ARG
2	s	324	SER
2	s	343	MET
2	t	21	ARG
2	t	80	GLN
2	t	129	VAL
2	t	131	SER
2	t	159	GLN
2	t	217	ASP
2	t	264	MET
2	t	266	ARG
2	t	324	SER
2	t	343	MET
2	u	21	ARG
2	u	80	GLN
2	u	129	VAL

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Mol	Chain	Res	Type
2	u	131	SER
2	u	159	GLN
2	u	217	ASP
2	u	264	MET
2	u	266	ARG
2	u	324	SER
2	u	343	MET
2	v	21	ARG
2	v	80	GLN
2	v	129	VAL
2	v	131	SER
2	v	159	GLN
2	v	217	ASP
2	v	264	MET
2	v	266	ARG
2	v	324	SER
2	v	343	MET
2	w	21	ARG
2	w	80	GLN
2	w	129	VAL
2	w	131	SER
2	w	159	GLN
2	w	217	ASP
2	w	264	MET
2	w	266	ARG
2	w	324	SER
2	w	343	MET
2	x	21	ARG
2	x	80	GLN
2	x	129	VAL
2	x	131	SER
2	x	159	GLN
2	x	217	ASP
2	x	264	MET
2	x	266	ARG
2	x	324	SER
2	x	343	MET
2	y	21	ARG
2	y	80	GLN
2	y	129	VAL
2	y	131	SER
2	y	159	GLN

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Mol	Chain	Res	Type
2	y	217	ASP
2	y	264	MET
2	y	266	ARG
2	y	324	SER
2	y	343	MET
2	z	21	ARG
2	z	80	GLN
2	z	129	VAL
2	z	131	SER
2	z	159	GLN
2	z	217	ASP
2	z	264	MET
2	z	266	ARG
2	z	324	SER
2	z	343	MET
3	0	1	MET
3	0	36	ARG
3	0	50	ARG
3	0	52	PRO
3	0	73	ARG
3	0	185	GLU
3	1	1	MET
3	1	36	ARG
3	1	62	LEU
3	1	106	MET
3	1	119	SER
3	1	164	GLN
3	1	206	PRO
3	1	241	GLU
3	2	91	ASN
3	2	204	SER
3	2	238	ARG
3	3	43	ASP
3	3	109	ASP
3	3	153	ARG
3	3	244	SER
3	4	64	SER
3	4	204	SER
3	4	209	ASN
3	4	259	GLN
3	5	4	SER
3	5	137	GLN

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Mol	Chain	Res	Type
3	5	154	ASP
3	5	181	ASP
3	6	59	GLN
3	6	73	ARG
3	6	78	GLU
3	6	109	ASP
3	6	244	SER
3	7	73	ARG
3	8	58	GLU
3	8	100	GLN
3	9	106	MET
3	9	125	ASN
3	9	137	GLN
3	9	162	GLN
3	ZA	136	VAL
3	ZA	248	SER
3	ZB	1	MET
3	ZB	4	SER
3	ZB	58	GLU
3	ZB	73	ARG
3	ZB	119	SER
3	ZB	137	GLN
3	ZB	143	PRO
3	ZB	244	SER
3	ZC	123	ASP
3	ZC	136	VAL
3	ZC	244	SER
3	ZD	64	SER
3	ZD	240	TYR
3	ZE	141	THR
4	ZF	3	PHE
4	ZF	60	ASP
4	ZF	87	ASP
4	ZF	134	PRO
4	ZF	229	THR
4	ZF	265	ASN
4	ZF	280	ASN
4	ZF	284	TYR
4	ZF	289	LEU
4	ZF	352	ASN
4	ZF	355	LYS
4	ZG	3	PHE

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Mol	Chain	Res	Type
4	ZG	38	SER
4	ZG	188	ASP
4	ZG	189	SER
4	ZG	227	SER
4	ZG	234	GLU
4	ZG	260	SER
4	ZG	262	SER
4	ZG	265	ASN
4	ZG	267	MET
4	ZG	288	ASP
4	ZG	296	ASN
4	ZG	350	SER
4	ZG	352	ASN
4	ZG	397	ASN
4	ZH	34	SER
4	ZH	154	MET
4	ZH	227	SER
4	ZH	260	SER
4	ZH	281	GLN
4	ZH	284	TYR
4	ZH	288	ASP
4	ZH	331	ASP
4	ZH	355	LYS
4	ZH	375	MET
4	ZH	380	ARG
4	ZH	399	LEU
4	ZI	99	GLN
4	ZI	195	ASP
4	ZI	197	ASN
4	ZI	260	SER
4	ZI	352	ASN
4	ZI	358	ASN
4	ZJ	42	MET
4	ZJ	46	SER
4	ZJ	103	ASP
4	ZJ	107	ASN
4	ZJ	195	ASP
4	ZJ	233	ASN
4	ZJ	280	ASN
4	ZJ	331	ASP
4	ZK	3	PHE
4	ZK	268	GLN

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Mol	Chain	Res	Type
4	ZK	297	ASP
4	ZK	305	SER
4	ZK	331	ASP
4	ZK	338	GLN
4	ZL	78	SER
4	ZL	84	ARG
4	ZL	196	MET
4	ZL	234	GLU
4	ZL	267	MET
4	ZL	291	SER
4	ZL	338	GLN
4	ZL	368	LEU
4	ZL	370	LYS
4	ZL	382	TYR
4	ZM	53	LYS
4	ZM	89	ASN
4	ZM	153	SER
4	ZM	200	PHE
4	ZM	214	ASP
4	ZM	282	ASN
4	ZM	352	ASN
4	ZM	369	SER
4	ZM	370	LYS
4	ZN	43	PHE
4	ZN	78	SER
4	ZN	103	ASP
4	ZN	143	LEU
4	ZN	148	SER
4	ZN	157	ASN
4	ZN	216	SER
4	ZN	297	ASP
4	ZN	367	ASP
4	ZN	396	LEU
4	ZO	2	SER
4	ZO	74	ASP
4	ZO	174	ASP
4	ZO	178	TYR
4	ZO	235	ASN
4	ZO	237	ILE
4	ZO	331	ASP
4	ZO	375	MET
4	ZP	42	MET

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Mol	Chain	Res	Type
4	ZP	63	ASP
4	ZP	74	ASP
4	ZP	95	SER
4	ZP	126	PRO
4	ZP	162	ASP
4	ZP	227	SER
4	ZP	275	ASN
4	ZP	288	ASP
4	ZP	292	TYR
4	ZP	331	ASP
4	ZP	340	SER
4	ZP	369	SER
4	ZP	370	LYS
4	ZP	393	ASP
4	ZQ	46	SER
4	ZQ	101	LYS
4	ZQ	189	SER
4	ZQ	200	PHE
4	ZQ	211	TYR
4	ZQ	280	ASN
4	ZQ	305	SER
4	ZQ	367	ASP
4	ZQ	370	LYS
4	ZR	41	ASP
4	ZR	103	ASP
4	ZR	197	ASN
4	ZR	214	ASP
4	ZR	269	GLN
4	ZR	295	ASN
4	ZR	332	ASN
4	ZR	367	ASP
4	ZS	78	SER
4	ZS	103	ASP
4	ZS	170	PHE
4	ZS	202	LYS
4	ZS	245	ASN
4	ZS	367	ASP
4	ZT	148	SER
4	ZT	195	ASP
4	ZT	262	SER
4	ZT	297	ASP
4	ZT	358	ASN

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Mol	Chain	Res	Type
4	ZU	3	PHE
4	ZU	78	SER
4	ZU	80	ASN
4	ZU	340	SER
4	ZV	46	SER
4	ZV	232	PHE
4	ZV	307	GLU
4	ZV	308	GLN
4	ZW	2	SER
4	ZW	3	PHE
4	ZW	53	LYS
4	ZW	188	ASP
4	ZW	195	ASP
4	ZW	215	SER
4	ZW	259	PHE
4	ZW	292	TYR
4	ZW	309	GLU
4	ZW	326	LEU
4	ZW	331	ASP
4	ZW	340	SER
4	ZW	358	ASN
4	ZX	3	PHE
4	ZX	63	ASP
4	ZX	195	ASP
4	ZY	60	ASP
4	ZY	80	ASN
4	ZY	192	ASN
4	ZY	204	LYS
4	ZY	252	ASN
4	ZY	332	ASN
4	ZY	350	SER
4	ZZ	3	PHE
4	ZZ	41	ASP
4	ZZ	88	SER
4	ZZ	148	SER
4	ZZ	393	ASP
4	Za	103	ASP
4	Za	292	TYR
4	Za	331	ASP
4	Za	332	ASN
4	Za	375	MET
4	Zb	41	ASP

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Mol	Chain	Res	Type
4	Zb	292	TYR
4	Zb	308	GLN
4	Zb	355	LYS
4	Zb	367	ASP
4	Zb	393	ASP
4	Zc	41	ASP
4	Zc	103	ASP
4	Zc	204	LYS
4	Zc	267	MET
4	Zc	296	ASN
4	Zc	297	ASP
4	Zc	317	LEU
4	Zc	332	ASN
4	Zc	340	SER
4	Zc	369	SER
4	Zc	399	LEU
4	Zd	41	ASP
4	Zd	114	MET
4	Zd	140	PRO
4	Zd	292	TYR
4	Zd	375	MET
4	Zd	393	ASP
4	Ze	3	PHE
4	Ze	27	SER
4	Ze	46	SER
4	Ze	58	THR
4	Ze	60	ASP
4	Ze	130	GLN
4	Ze	308	GLN
4	Ze	319	ASN
4	Ze	395	ILE
4	Zf	3	PHE
4	Zf	285	LYS
4	Zf	297	ASP
4	Zf	331	ASP
4	Zf	332	ASN
4	Zf	367	ASP
4	Zf	396	LEU
4	Zg	94	TYR
4	Zg	103	ASP
4	Zg	292	TYR
4	Zg	332	ASN

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Mol	Chain	Res	Type
4	Zg	367	ASP
4	Zg	370	LYS
4	Zh	3	PHE
4	Zh	41	ASP
4	Zh	47	LYS
4	Zh	63	ASP
4	Zh	83	PHE
4	Zh	162	ASP
4	Zh	308	GLN
4	Zh	332	ASN
5	AA	126	PRO
5	AA	150	ASP
5	AA	247	LEU
5	AB	70	GLN
5	AB	72	ASP
5	AB	153	ASN
5	AC	70	GLN
5	AC	85	ASP
5	AC	189	ARG
5	AC	225	ARG
5	AC	236	SER
5	AD	140	ASP
5	AD	169	ASN
5	AE	175	ASP
3	AF	4	SER
3	AF	19	MET
3	AF	36	ARG
3	AF	44	LEU
3	AF	154	ASP
3	AG	16	GLN
3	AG	36	ARG
3	AG	73	ARG
3	AG	137	GLN
3	AG	169	GLN
3	AG	222	SER
3	AG	251	ASP
3	AH	1	MET
3	AH	44	LEU
3	AH	66	LEU
3	AH	87	SER
3	AH	93	LYS
3	AH	100	GLN

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Mol	Chain	Res	Type
3	AH	148	SER
3	AH	154	ASP
3	AH	245	LYS
3	AH	251	ASP
3	AI	4	SER
3	AI	30	SER
3	AI	123	ASP
3	AI	148	SER
3	AI	169	GLN
3	AI	179	MET
3	AI	202	ASN
3	AI	222	SER
3	AI	252	GLN
3	AJ	36	ARG
3	AJ	73	ARG
3	AJ	91	ASN
3	AJ	94	ASP
3	AJ	127	GLN
3	AJ	194	GLU
3	AJ	197	SER
3	AJ	225	ASN
3	AK	4	SER
3	AK	6	TRP
3	AK	36	ARG
3	AK	181	ASP
3	AL	1	MET
3	AL	137	GLN
3	AL	172	GLN
3	AL	185	GLU
3	AL	198	SER
3	AL	209	ASN
3	AM	1	MET
3	AM	30	SER
3	AM	36	ARG
3	AM	50	ARG
3	AM	82	SER
3	AM	169	GLN
3	AM	208	LEU
3	AM	209	ASN
3	AN	1	MET
3	AN	3	SER
3	AN	117	ASP

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Mol	Chain	Res	Type
3	AN	127	GLN
6	AR	274	ASN
6	AR	294	ARG
6	AR	359	GLN
6	AR	377	MET
6	AR	381	ASP
6	AR	417	ARG
6	AR	424	ASP
6	AS	274	ASN
6	AS	294	ARG
6	AS	359	GLN
6	AS	377	MET
6	AS	381	ASP
6	AS	417	ARG
6	AS	424	ASP
6	AT	274	ASN
6	AT	294	ARG
6	AT	359	GLN
6	AT	377	MET
6	AT	381	ASP
6	AT	417	ARG
6	AT	424	ASP
6	AU	274	ASN
6	AU	294	ARG
6	AU	359	GLN
6	AU	377	MET
6	AU	381	ASP
6	AU	417	ARG
6	AU	424	ASP
6	AV	274	ASN
6	AV	294	ARG
6	AV	359	GLN
6	AV	377	MET
6	AV	381	ASP
6	AV	417	ARG
6	AV	424	ASP
6	AW	274	ASN
6	AW	294	ARG
6	AW	359	GLN
6	AW	377	MET
6	AW	381	ASP
6	AW	417	ARG

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Mol	Chain	Res	Type
6	AW	424	ASP
6	AX	274	ASN
6	AX	294	ARG
6	AX	359	GLN
6	AX	377	MET
6	AX	381	ASP
6	AX	417	ARG
6	AX	424	ASP
6	AY	274	ASN
6	AY	294	ARG
6	AY	359	GLN
6	AY	377	MET
6	AY	381	ASP
6	AY	417	ARG
6	AY	424	ASP
6	AZ	274	ASN
6	AZ	294	ARG
6	AZ	359	GLN
6	AZ	377	MET
6	AZ	381	ASP
6	AZ	417	ARG
6	AZ	424	ASP
6	Aa	274	ASN
6	Aa	294	ARG
6	Aa	359	GLN
6	Aa	377	MET
6	Aa	381	ASP
6	Aa	417	ARG
6	Aa	424	ASP
7	Ab	7	MET
6	Ac	274	ASN
6	Ac	294	ARG
6	Ac	359	GLN
6	Ac	377	MET
6	Ac	381	ASP
6	Ac	417	ARG
6	Ac	424	ASP
6	Ad	274	ASN
6	Ad	294	ARG
6	Ad	359	GLN
6	Ad	377	MET
6	Ad	381	ASP

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Mol	Chain	Res	Type
6	Ad	417	ARG
6	Ad	424	ASP
6	Ae	274	ASN
6	Ae	294	ARG
6	Ae	359	GLN
6	Ae	377	MET
6	Ae	381	ASP
6	Ae	417	ARG
6	Ae	424	ASP
6	Af	274	ASN
6	Af	294	ARG
6	Af	359	GLN
6	Af	377	MET
6	Af	381	ASP
6	Af	417	ARG
6	Af	424	ASP
6	Ag	274	ASN
6	Ag	294	ARG
6	Ag	359	GLN
6	Ag	377	MET
6	Ag	381	ASP
6	Ag	417	ARG
6	Ag	424	ASP
6	Ah	274	ASN
6	Ah	294	ARG
6	Ah	359	GLN
6	Ah	377	MET
6	Ah	381	ASP
6	Ah	417	ARG
6	Ah	424	ASP
6	Ai	274	ASN
6	Ai	294	ARG
6	Ai	359	GLN
6	Ai	377	MET
6	Ai	381	ASP
6	Ai	417	ARG
6	Ai	424	ASP
6	Aj	274	ASN
6	Aj	294	ARG
6	Aj	359	GLN
6	Aj	377	MET
6	Aj	381	ASP

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Mol	Chain	Res	Type
6	Aj	417	ARG
6	Aj	424	ASP
6	Ak	274	ASN
6	Ak	294	ARG
6	Ak	359	GLN
6	Ak	377	MET
6	Ak	381	ASP
6	Ak	417	ARG
6	Ak	424	ASP
6	Al	274	ASN
6	Al	294	ARG
6	Al	359	GLN
6	Al	377	MET
6	Al	381	ASP
6	Al	417	ARG
6	Al	424	ASP
6	Am	274	ASN
6	Am	294	ARG
6	Am	359	GLN
6	Am	377	MET
6	Am	381	ASP
6	Am	417	ARG
6	Am	424	ASP
6	An	274	ASN
6	An	294	ARG
6	An	359	GLN
6	An	377	MET
6	An	381	ASP
6	An	417	ARG
6	An	424	ASP
6	Ao	274	ASN
6	Ao	294	ARG
6	Ao	359	GLN
6	Ao	377	MET
6	Ao	381	ASP
6	Ao	417	ARG
6	Ao	424	ASP
6	Ap	274	ASN
6	Ap	294	ARG
6	Ap	359	GLN
6	Ap	377	MET
6	Ap	381	ASP

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Mol	Chain	Res	Type
6	Ap	417	ARG
6	Ap	424	ASP
6	AO	274	ASN
6	AO	294	ARG
6	AO	359	GLN
6	AO	377	MET
6	AO	381	ASP
6	AO	417	ARG
6	AO	424	ASP
6	AP	274	ASN
6	AP	294	ARG
6	AP	359	GLN
6	AP	377	MET
6	AP	381	ASP
6	AP	417	ARG
6	AP	424	ASP
6	AQ	274	ASN
6	AQ	294	ARG
6	AQ	359	GLN
6	AQ	377	MET
6	AQ	381	ASP
6	AQ	417	ARG
6	AQ	424	ASP
7	Aq	47	MET
7	As	9	MET
8	At	36	ARG
8	At	86	PHE
8	At	185	MET
8	At	214	PHE
8	At	227	MET
8	At	229	MET
9	Au	38	TRP
9	Au	123	MET
9	Au	129	LYS
9	Au	155	ASN
9	Au	160	GLN
9	Au	190	PHE
9	Au	213	PRO
9	Av	75	ARG
9	Av	102	SER
9	Av	106	ASP
9	Av	116	PHE

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Mol	Chain	Res	Type
9	Av	140	ARG
9	Av	160	GLN
9	Av	162	PRO
9	Aw	143	ARG
9	Aw	152	ARG
9	Aw	177	SER
9	Aw	187	PHE
9	Aw	190	PHE
9	Ax	113	TYR
9	Ax	143	ARG
9	Ax	187	PHE
9	Ax	205	MET
9	Ax	238	SER
9	Ax	241	GLN
9	Ay	117	SER
9	Ay	190	PHE
9	Ay	224	MET
9	Ay	230	ASP
10	Az	15	GLN
10	Az	19	MET
10	Az	74	ASP
10	Az	79	SER
10	Az	101	SER
10	A1	15	GLN
10	A1	19	MET
10	A1	75	MET
10	A1	84	MET
10	A2	7	ILE
10	A2	11	ILE
10	A2	14	LEU
10	A2	15	GLN
10	A2	70	ASP
10	A3	15	GLN
10	A3	19	MET
10	A3	33	SER
10	A3	81	SER
10	A4	15	GLN
10	A4	19	MET
10	A4	101	SER
10	A4	102	MET
10	A5	15	GLN
10	A5	19	MET

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Mol	Chain	Res	Type
10	A5	57	GLU
10	A5	91	LYS
11	A6	34	ASP
11	A6	101	ASP
11	A6	113	SER
11	A6	125	SER
11	A7	47	SER
11	A7	55	ARG
11	A8	48	GLU
11	A8	65	LEU
11	A8	69	SER
11	A8	71	HIS
11	A8	72	HIS
11	A8	91	ASP
11	A8	128	LYS
11	A9	47	SER
11	A9	76	GLN
11	A0	4	ARG
11	A0	18	LEU
11	A0	65	LEU
11	A0	104	ARG
11	A0	113	SER
11	A0	125	SER
6	UI	98	LEU
6	UI	127	SER
6	UI	154	ARG
6	UI	159	MET
6	UI	165	PHE
6	UJ	98	LEU
6	UJ	127	SER
6	UJ	154	ARG
6	UJ	159	MET
6	UJ	165	PHE
6	UK	98	LEU
6	UK	127	SER
6	UK	154	ARG
6	UK	159	MET
6	UK	165	PHE
6	UL	98	LEU
6	UL	127	SER
6	UL	154	ARG
6	UL	159	MET

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Mol	Chain	Res	Type
6	UL	165	PHE
6	UL	167	ARG
6	UM	98	LEU
6	UM	127	SER
6	UM	154	ARG
6	UM	159	MET
6	UM	165	PHE
6	UN	98	LEU
6	UN	127	SER
6	UN	154	ARG
6	UN	159	MET
6	UN	165	PHE
6	UO	98	LEU
6	UO	127	SER
6	UO	154	ARG
6	UO	159	MET
6	UO	165	PHE
6	UP	98	LEU
6	UP	127	SER
6	UP	154	ARG
6	UP	159	MET
6	UP	165	PHE
6	UP	167	ARG
12	BB	123	LYS
6	WA	114	GLU
6	WA	128	GLU
6	WA	167	ARG
6	WA	170	LYS
6	WB	121	PHE
6	WB	128	GLU
6	WB	134	ARG
6	WB	137	GLU
6	WB	164	LEU
6	WB	169	GLN
6	WC	115	LEU
6	WC	120	LYS
6	WC	128	GLU
6	WC	134	ARG
6	WC	164	LEU
6	WC	166	VAL
6	WC	168	GLU
6	WC	170	LYS

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

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

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Mol	Chain	Res	Type
6	WU	134	ARG
6	WU	161	LYS
6	WV	114	GLU
6	WV	117	ASP
6	WV	120	LYS
6	WV	128	GLU
6	WV	134	ARG
6	WV	164	LEU
6	WV	166	VAL
6	WV	169	GLN
6	WV	187	ASP
6	WW	114	GLU
6	WW	115	LEU
6	WW	128	GLU
6	WW	134	ARG
6	WW	167	ARG
6	WW	168	GLU
6	WW	169	GLN
6	WW	221	THR
12	BD	30	ASN
12	BD	120	ASN
12	BE	20	ARG
12	BE	52	ASP
12	BE	84	LEU
12	BF	86	ASP
12	BF	88	ASN
12	BF	125	MET
12	BF	127	LEU
6	BH	324	ASN
6	BI	318	ASN
6	BI	319	GLN
6	BO	319	GLN
6	BQ	318	ASN
6	BR	274	ASN
6	BR	294	ARG
6	BR	359	GLN
6	BR	377	MET
6	BR	381	ASP
6	BR	417	ARG
6	BR	424	ASP
6	BS	274	ASN
6	BS	294	ARG

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Mol	Chain	Res	Type
6	BS	359	GLN
6	BS	377	MET
6	BS	381	ASP
6	BS	417	ARG
6	BS	424	ASP
6	BT	274	ASN
6	BT	294	ARG
6	BT	359	GLN
6	BT	377	MET
6	BT	381	ASP
6	BT	417	ARG
6	BT	424	ASP
6	BU	274	ASN
6	BU	294	ARG
6	BU	359	GLN
6	BU	377	MET
6	BU	381	ASP
6	BU	417	ARG
6	BU	424	ASP
6	BV	274	ASN
6	BV	294	ARG
6	BV	359	GLN
6	BV	377	MET
6	BV	381	ASP
6	BV	417	ARG
6	BV	424	ASP
6	BW	274	ASN
6	BW	294	ARG
6	BW	359	GLN
6	BW	377	MET
6	BW	381	ASP
6	BW	417	ARG
6	BW	424	ASP
6	BX	274	ASN
6	BX	294	ARG
6	BX	359	GLN
6	BX	377	MET
6	BX	381	ASP
6	BX	417	ARG
6	BX	424	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	63	GLN
1	A	85	ASN
1	A	130	ASN
1	A	160	ASN
1	A	172	ASN
1	A	173	GLN
1	A	185	ASN
1	A	217	GLN
1	B	59	ASN
1	B	63	GLN
1	B	85	ASN
1	B	130	ASN
1	B	139	ASN
1	B	160	ASN
1	B	172	ASN
1	B	173	GLN
1	B	185	ASN
1	B	217	GLN
1	C	59	ASN
1	C	63	GLN
1	C	85	ASN
1	C	130	ASN
1	C	139	ASN
1	C	160	ASN
1	C	172	ASN
1	C	173	GLN
1	C	185	ASN
1	C	217	GLN
1	D	59	ASN
1	D	63	GLN
1	D	85	ASN
1	D	130	ASN
1	D	139	ASN
1	D	160	ASN
1	D	173	GLN
1	D	185	ASN
1	D	217	GLN
1	E	59	ASN
1	E	63	GLN
1	E	85	ASN
1	E	130	ASN
1	E	139	ASN

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Mol	Chain	Res	Type
1	E	160	ASN
1	E	172	ASN
1	E	173	GLN
1	E	185	ASN
1	E	217	GLN
1	F	59	ASN
1	F	63	GLN
1	F	85	ASN
1	F	130	ASN
1	F	139	ASN
1	F	160	ASN
1	F	173	GLN
1	F	185	ASN
1	F	217	GLN
1	G	59	ASN
1	G	63	GLN
1	G	85	ASN
1	G	130	ASN
1	G	139	ASN
1	G	160	ASN
1	G	173	GLN
1	G	185	ASN
1	G	217	GLN
1	H	59	ASN
1	H	63	GLN
1	H	85	ASN
1	H	130	ASN
1	H	139	ASN
1	H	160	ASN
1	H	172	ASN
1	H	173	GLN
1	H	185	ASN
1	H	217	GLN
1	I	59	ASN
1	I	63	GLN
1	I	85	ASN
1	I	130	ASN
1	I	139	ASN
1	I	160	ASN
1	I	172	ASN
1	I	173	GLN
1	I	185	ASN

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Mol	Chain	Res	Type
1	I	217	GLN
1	J	59	ASN
1	J	63	GLN
1	J	130	ASN
1	J	139	ASN
1	J	160	ASN
1	J	172	ASN
1	J	173	GLN
1	J	185	ASN
1	J	217	GLN
1	K	59	ASN
1	K	63	GLN
1	K	85	ASN
1	K	130	ASN
1	K	139	ASN
1	K	160	ASN
1	K	172	ASN
1	K	173	GLN
1	K	185	ASN
1	K	217	GLN
1	L	59	ASN
1	L	63	GLN
1	L	130	ASN
1	L	139	ASN
1	L	160	ASN
1	L	172	ASN
1	L	173	GLN
1	L	185	ASN
1	L	217	GLN
1	M	59	ASN
1	M	63	GLN
1	M	85	ASN
1	M	130	ASN
1	M	160	ASN
1	M	172	ASN
1	M	173	GLN
1	M	185	ASN
1	M	217	GLN
1	N	59	ASN
1	N	63	GLN
1	N	85	ASN
1	N	130	ASN

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Mol	Chain	Res	Type
1	N	160	ASN
1	N	172	ASN
1	N	173	GLN
1	N	185	ASN
1	N	217	GLN
1	O	59	ASN
1	O	63	GLN
1	O	85	ASN
1	O	130	ASN
1	O	160	ASN
1	O	173	GLN
1	O	185	ASN
1	O	217	GLN
1	P	59	ASN
1	P	63	GLN
1	P	85	ASN
1	P	130	ASN
1	P	160	ASN
1	P	172	ASN
1	P	173	GLN
1	P	185	ASN
1	P	217	GLN
1	Q	59	ASN
1	Q	63	GLN
1	Q	85	ASN
1	Q	130	ASN
1	Q	139	ASN
1	Q	160	ASN
1	Q	172	ASN
1	Q	173	GLN
1	Q	185	ASN
1	Q	217	GLN
1	R	59	ASN
1	R	63	GLN
1	R	85	ASN
1	R	130	ASN
1	R	139	ASN
1	R	160	ASN
1	R	172	ASN
1	R	173	GLN
1	R	185	ASN
1	R	217	GLN

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Mol	Chain	Res	Type
1	S	59	ASN
1	S	63	GLN
1	S	85	ASN
1	S	130	ASN
1	S	139	ASN
1	S	160	ASN
1	S	172	ASN
1	S	173	GLN
1	S	185	ASN
1	S	217	GLN
1	T	59	ASN
1	T	63	GLN
1	T	85	ASN
1	T	130	ASN
1	T	139	ASN
1	T	160	ASN
1	T	172	ASN
1	T	173	GLN
1	T	185	ASN
1	T	217	GLN
1	U	59	ASN
1	U	63	GLN
1	U	130	ASN
1	U	160	ASN
1	U	172	ASN
1	U	173	GLN
1	U	185	ASN
1	U	217	GLN
1	V	59	ASN
1	V	63	GLN
1	V	85	ASN
1	V	130	ASN
1	V	160	ASN
1	V	172	ASN
1	V	173	GLN
1	V	185	ASN
1	V	217	GLN
1	W	59	ASN
1	W	63	GLN
1	W	85	ASN
1	W	130	ASN
1	W	139	ASN

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Mol	Chain	Res	Type
1	W	160	ASN
1	W	172	ASN
1	W	173	GLN
1	W	185	ASN
1	W	217	GLN
1	X	59	ASN
1	X	63	GLN
1	X	85	ASN
1	X	130	ASN
1	X	160	ASN
1	X	172	ASN
1	X	173	GLN
1	X	185	ASN
1	X	217	GLN
1	Y	59	ASN
1	Y	63	GLN
1	Y	85	ASN
1	Y	130	ASN
1	Y	160	ASN
1	Y	172	ASN
1	Y	173	GLN
1	Y	185	ASN
1	Y	217	GLN
1	Z	59	ASN
1	Z	63	GLN
1	Z	85	ASN
1	Z	130	ASN
1	Z	139	ASN
1	Z	160	ASN
1	Z	172	ASN
1	Z	173	GLN
1	Z	185	ASN
1	Z	217	GLN
2	a	51	GLN
2	a	63	ASN
2	a	83	ASN
2	a	138	GLN
2	a	159	GLN
2	a	161	ASN
2	a	178	GLN
2	a	188	GLN
2	a	198	GLN

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Mol	Chain	Res	Type
2	a	229	ASN
2	a	241	ASN
2	b	51	GLN
2	b	63	ASN
2	b	83	ASN
2	b	138	GLN
2	b	140	ASN
2	b	159	GLN
2	b	161	ASN
2	b	178	GLN
2	b	188	GLN
2	b	198	GLN
2	b	229	ASN
2	b	241	ASN
2	b	350	GLN
2	c	51	GLN
2	c	63	ASN
2	c	80	GLN
2	c	83	ASN
2	c	138	GLN
2	c	140	ASN
2	c	159	GLN
2	c	161	ASN
2	c	178	GLN
2	c	188	GLN
2	c	198	GLN
2	c	229	ASN
2	c	241	ASN
2	c	350	GLN
2	d	51	GLN
2	d	63	ASN
2	d	83	ASN
2	d	138	GLN
2	d	140	ASN
2	d	159	GLN
2	d	161	ASN
2	d	178	GLN
2	d	188	GLN
2	d	198	GLN
2	d	229	ASN
2	d	241	ASN
2	e	51	GLN

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Mol	Chain	Res	Type
2	e	63	ASN
2	e	83	ASN
2	e	138	GLN
2	e	140	ASN
2	e	159	GLN
2	e	161	ASN
2	e	178	GLN
2	e	188	GLN
2	e	198	GLN
2	e	229	ASN
2	e	241	ASN
2	f	51	GLN
2	f	63	ASN
2	f	83	ASN
2	f	138	GLN
2	f	140	ASN
2	f	159	GLN
2	f	161	ASN
2	f	178	GLN
2	f	188	GLN
2	f	198	GLN
2	f	229	ASN
2	f	241	ASN
2	g	51	GLN
2	g	63	ASN
2	g	83	ASN
2	g	138	GLN
2	g	140	ASN
2	g	159	GLN
2	g	161	ASN
2	g	178	GLN
2	g	188	GLN
2	g	198	GLN
2	g	229	ASN
2	g	241	ASN
2	h	51	GLN
2	h	63	ASN
2	h	83	ASN
2	h	138	GLN
2	h	140	ASN
2	h	159	GLN
2	h	161	ASN

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Mol	Chain	Res	Type
2	h	178	GLN
2	h	188	GLN
2	h	198	GLN
2	h	229	ASN
2	h	241	ASN
2	i	51	GLN
2	i	63	ASN
2	i	83	ASN
2	i	138	GLN
2	i	140	ASN
2	i	159	GLN
2	i	161	ASN
2	i	178	GLN
2	i	188	GLN
2	i	198	GLN
2	i	229	ASN
2	i	241	ASN
2	j	51	GLN
2	j	63	ASN
2	j	83	ASN
2	j	138	GLN
2	j	140	ASN
2	j	159	GLN
2	j	161	ASN
2	j	178	GLN
2	j	188	GLN
2	j	198	GLN
2	j	229	ASN
2	j	241	ASN
2	k	51	GLN
2	k	63	ASN
2	k	83	ASN
2	k	138	GLN
2	k	159	GLN
2	k	161	ASN
2	k	178	GLN
2	k	188	GLN
2	k	198	GLN
2	k	229	ASN
2	k	241	ASN
2	l	51	GLN
2	l	54	GLN

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Mol	Chain	Res	Type
2	l	63	ASN
2	l	80	GLN
2	l	83	ASN
2	l	138	GLN
2	l	140	ASN
2	l	159	GLN
2	l	161	ASN
2	l	178	GLN
2	l	188	GLN
2	l	198	GLN
2	l	229	ASN
2	l	241	ASN
2	l	350	GLN
2	m	51	GLN
2	m	54	GLN
2	m	63	ASN
2	m	83	ASN
2	m	138	GLN
2	m	140	ASN
2	m	159	GLN
2	m	161	ASN
2	m	178	GLN
2	m	188	GLN
2	m	198	GLN
2	m	229	ASN
2	m	241	ASN
2	n	51	GLN
2	n	63	ASN
2	n	83	ASN
2	n	138	GLN
2	n	140	ASN
2	n	159	GLN
2	n	161	ASN
2	n	178	GLN
2	n	188	GLN
2	n	198	GLN
2	n	229	ASN
2	n	241	ASN
2	n	350	GLN
2	o	51	GLN
2	o	63	ASN
2	o	78	ASN

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Mol	Chain	Res	Type
2	o	83	ASN
2	o	138	GLN
2	o	140	ASN
2	o	159	GLN
2	o	161	ASN
2	o	178	GLN
2	o	188	GLN
2	o	198	GLN
2	o	229	ASN
2	o	241	ASN
2	p	51	GLN
2	p	63	ASN
2	p	80	GLN
2	p	83	ASN
2	p	138	GLN
2	p	140	ASN
2	p	159	GLN
2	p	161	ASN
2	p	178	GLN
2	p	188	GLN
2	p	198	GLN
2	p	229	ASN
2	p	241	ASN
2	q	51	GLN
2	q	63	ASN
2	q	80	GLN
2	q	83	ASN
2	q	138	GLN
2	q	140	ASN
2	q	159	GLN
2	q	161	ASN
2	q	178	GLN
2	q	188	GLN
2	q	198	GLN
2	q	229	ASN
2	q	241	ASN
2	r	51	GLN
2	r	63	ASN
2	r	80	GLN
2	r	83	ASN
2	r	138	GLN
2	r	140	ASN

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Mol	Chain	Res	Type
2	r	159	GLN
2	r	161	ASN
2	r	178	GLN
2	r	188	GLN
2	r	198	GLN
2	r	229	ASN
2	r	241	ASN
2	s	51	GLN
2	s	54	GLN
2	s	63	ASN
2	s	83	ASN
2	s	138	GLN
2	s	140	ASN
2	s	159	GLN
2	s	161	ASN
2	s	178	GLN
2	s	188	GLN
2	s	198	GLN
2	s	229	ASN
2	s	241	ASN
2	t	51	GLN
2	t	63	ASN
2	t	83	ASN
2	t	138	GLN
2	t	140	ASN
2	t	159	GLN
2	t	161	ASN
2	t	178	GLN
2	t	188	GLN
2	t	198	GLN
2	t	229	ASN
2	t	241	ASN
2	u	51	GLN
2	u	63	ASN
2	u	80	GLN
2	u	83	ASN
2	u	138	GLN
2	u	140	ASN
2	u	159	GLN
2	u	161	ASN
2	u	178	GLN
2	u	188	GLN

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Mol	Chain	Res	Type
2	u	198	GLN
2	u	229	ASN
2	u	241	ASN
2	v	51	GLN
2	v	54	GLN
2	v	63	ASN
2	v	80	GLN
2	v	83	ASN
2	v	138	GLN
2	v	140	ASN
2	v	159	GLN
2	v	161	ASN
2	v	178	GLN
2	v	188	GLN
2	v	198	GLN
2	v	229	ASN
2	v	241	ASN
2	w	51	GLN
2	w	63	ASN
2	w	80	GLN
2	w	83	ASN
2	w	138	GLN
2	w	159	GLN
2	w	161	ASN
2	w	178	GLN
2	w	188	GLN
2	w	198	GLN
2	w	229	ASN
2	w	241	ASN
2	x	51	GLN
2	x	63	ASN
2	x	80	GLN
2	x	83	ASN
2	x	138	GLN
2	x	140	ASN
2	x	159	GLN
2	x	161	ASN
2	x	178	GLN
2	x	188	GLN
2	x	198	GLN
2	x	229	ASN
2	x	241	ASN

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Mol	Chain	Res	Type
2	y	51	GLN
2	y	63	ASN
2	y	83	ASN
2	y	138	GLN
2	y	140	ASN
2	y	159	GLN
2	y	161	ASN
2	y	178	GLN
2	y	188	GLN
2	y	198	GLN
2	y	229	ASN
2	y	241	ASN
2	z	51	GLN
2	z	63	ASN
2	z	83	ASN
2	z	138	GLN
2	z	140	ASN
2	z	159	GLN
2	z	161	ASN
2	z	178	GLN
2	z	188	GLN
2	z	198	GLN
2	z	229	ASN
2	z	241	ASN
3	0	88	GLN
3	0	100	GLN
3	0	135	GLN
3	0	137	GLN
3	0	180	ASN
3	0	235	GLN
3	0	237	GLN
3	0	255	GLN
3	1	47	GLN
3	1	67	GLN
3	1	91	ASN
3	1	121	GLN
3	1	135	GLN
3	1	223	ASN
3	1	252	GLN
3	2	164	GLN
3	2	180	ASN
3	2	255	GLN

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Mol	Chain	Res	Type
3	3	24	ASN
3	3	67	GLN
3	3	161	GLN
3	3	190	ASN
3	3	255	GLN
3	4	37	GLN
3	4	47	GLN
3	4	51	GLN
3	4	125	ASN
3	4	127	GLN
3	4	174	ASN
3	4	216	GLN
3	4	235	GLN
3	4	243	ASN
3	4	259	GLN
3	5	51	GLN
3	5	55	GLN
3	5	85	ASN
3	5	100	GLN
3	5	121	GLN
3	5	237	GLN
3	5	252	GLN
3	6	16	GLN
3	6	59	GLN
3	6	91	ASN
3	6	121	GLN
3	6	127	GLN
3	6	135	GLN
3	6	209	ASN
3	6	237	GLN
3	7	24	ASN
3	7	55	GLN
3	7	164	GLN
3	7	235	GLN
3	8	59	GLN
3	8	83	GLN
3	8	91	ASN
3	8	196	GLN
3	9	37	GLN
3	9	55	GLN
3	9	85	ASN
3	9	91	ASN

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Mol	Chain	Res	Type
3	9	259	GLN
3	ZA	37	GLN
3	ZA	235	GLN
3	ZB	24	ASN
3	ZB	25	ASN
3	ZB	28	ASN
3	ZB	37	GLN
3	ZB	137	GLN
3	ZB	235	GLN
3	ZC	16	GLN
3	ZC	88	GLN
3	ZC	100	GLN
3	ZC	190	ASN
3	ZD	24	ASN
3	ZD	67	GLN
3	ZD	88	GLN
3	ZD	91	ASN
3	ZD	127	GLN
3	ZD	135	GLN
3	ZD	161	GLN
3	ZD	235	GLN
3	ZE	37	GLN
3	ZE	67	GLN
3	ZE	121	GLN
3	ZE	252	GLN
4	ZF	5	GLN
4	ZF	16	ASN
4	ZF	107	ASN
4	ZF	155	GLN
4	ZF	197	ASN
4	ZF	358	ASN
4	ZF	385	ASN
4	ZF	401	ASN
4	ZG	89	ASN
4	ZG	130	GLN
4	ZG	133	ASN
4	ZG	332	ASN
4	ZG	387	GLN
4	ZG	397	ASN
4	ZG	401	ASN
4	ZH	5	GLN
4	ZH	155	GLN

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Mol	Chain	Res	Type
4	ZH	206	ASN
4	ZH	270	ASN
4	ZH	296	ASN
4	ZH	352	ASN
4	ZH	365	ASN
4	ZH	379	GLN
4	ZH	392	GLN
4	ZI	197	ASN
4	ZI	269	GLN
4	ZI	323	ASN
4	ZI	385	ASN
4	ZI	387	GLN
4	ZI	392	GLN
4	ZI	394	GLN
4	ZI	401	ASN
4	ZJ	89	ASN
4	ZJ	107	ASN
4	ZJ	133	ASN
4	ZJ	159	ASN
4	ZJ	197	ASN
4	ZJ	265	ASN
4	ZJ	274	ASN
4	ZJ	282	ASN
4	ZJ	379	GLN
4	ZJ	392	GLN
4	ZJ	397	ASN
4	ZJ	401	ASN
4	ZK	107	ASN
4	ZK	197	ASN
4	ZK	252	ASN
4	ZK	303	ASN
4	ZK	319	ASN
4	ZK	392	GLN
4	ZK	401	ASN
4	ZL	5	GLN
4	ZL	79	GLN
4	ZL	89	ASN
4	ZL	179	ASN
4	ZL	190	GLN
4	ZL	197	ASN
4	ZL	269	GLN
4	ZL	282	ASN

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Mol	Chain	Res	Type
4	ZL	310	GLN
4	ZL	338	GLN
4	ZL	401	ASN
4	ZM	5	GLN
4	ZM	59	GLN
4	ZM	89	ASN
4	ZM	197	ASN
4	ZM	213	HIS
4	ZM	235	ASN
4	ZM	252	ASN
4	ZM	381	ASN
4	ZN	79	GLN
4	ZN	107	ASN
4	ZN	112	GLN
4	ZN	129	GLN
4	ZN	133	ASN
4	ZN	190	GLN
4	ZN	192	ASN
4	ZN	197	ASN
4	ZN	319	ASN
4	ZN	338	GLN
4	ZN	379	GLN
4	ZN	387	GLN
4	ZN	401	ASN
4	ZO	89	ASN
4	ZO	141	ASN
4	ZO	192	ASN
4	ZO	235	ASN
4	ZO	332	ASN
4	ZP	11	ASN
4	ZP	107	ASN
4	ZP	129	GLN
4	ZP	194	HIS
4	ZP	269	GLN
4	ZP	270	ASN
4	ZP	314	GLN
4	ZP	322	ASN
4	ZP	338	GLN
4	ZP	379	GLN
4	ZP	381	ASN
4	ZP	385	ASN
4	ZQ	89	ASN

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Mol	Chain	Res	Type
4	ZQ	97	ASN
4	ZQ	133	ASN
4	ZQ	141	ASN
4	ZQ	155	GLN
4	ZQ	197	ASN
4	ZQ	233	ASN
4	ZQ	338	GLN
4	ZQ	387	GLN
4	ZR	107	ASN
4	ZR	133	ASN
4	ZR	268	GLN
4	ZR	269	GLN
4	ZR	293	GLN
4	ZR	295	ASN
4	ZR	401	ASN
4	ZS	133	ASN
4	ZS	197	ASN
4	ZS	394	GLN
4	ZT	5	GLN
4	ZT	99	GLN
4	ZT	129	GLN
4	ZT	133	ASN
4	ZT	197	ASN
4	ZT	213	HIS
4	ZT	235	ASN
4	ZT	275	ASN
4	ZT	293	GLN
4	ZT	314	GLN
4	ZT	352	ASN
4	ZT	392	GLN
4	ZU	99	GLN
4	ZU	107	ASN
4	ZU	133	ASN
4	ZU	159	ASN
4	ZU	206	ASN
4	ZU	293	GLN
4	ZU	332	ASN
4	ZU	379	GLN
4	ZU	387	GLN
4	ZV	107	ASN
4	ZV	133	ASN
4	ZV	197	ASN

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Mol	Chain	Res	Type
4	ZV	280	ASN
4	ZV	303	ASN
4	ZV	314	GLN
4	ZV	394	GLN
4	ZV	397	ASN
4	ZV	401	ASN
4	ZW	5	GLN
4	ZW	26	ASN
4	ZW	107	ASN
4	ZW	129	GLN
4	ZW	133	ASN
4	ZW	155	GLN
4	ZW	197	ASN
4	ZW	252	ASN
4	ZW	310	GLN
4	ZW	314	GLN
4	ZW	332	ASN
4	ZX	80	ASN
4	ZX	133	ASN
4	ZX	314	GLN
4	ZX	352	ASN
4	ZY	5	GLN
4	ZY	115	GLN
4	ZY	159	ASN
4	ZY	197	ASN
4	ZY	268	GLN
4	ZY	392	GLN
4	ZZ	5	GLN
4	ZZ	99	GLN
4	ZZ	107	ASN
4	ZZ	133	ASN
4	ZZ	194	HIS
4	ZZ	197	ASN
4	ZZ	314	GLN
4	ZZ	332	ASN
4	ZZ	379	GLN
4	ZZ	394	GLN
4	ZZ	401	ASN
4	Za	115	GLN
4	Za	129	GLN
4	Za	133	ASN
4	Za	197	ASN

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Mol	Chain	Res	Type
4	Za	387	GLN
4	Zb	5	GLN
4	Zb	79	GLN
4	Zb	107	ASN
4	Zb	129	GLN
4	Zb	133	ASN
4	Zb	197	ASN
4	Zb	293	GLN
4	Zb	308	GLN
4	Zb	332	ASN
4	Zb	358	ASN
4	Zb	387	GLN
4	Zc	5	GLN
4	Zc	107	ASN
4	Zc	129	GLN
4	Zc	159	ASN
4	Zc	197	ASN
4	Zc	352	ASN
4	Zc	379	GLN
4	Zc	387	GLN
4	Zc	397	ASN
4	Zd	5	GLN
4	Zd	105	ASN
4	Zd	129	GLN
4	Zd	130	GLN
4	Zd	133	ASN
4	Zd	293	GLN
4	Zd	295	ASN
4	Zd	397	ASN
4	Ze	5	GLN
4	Ze	99	GLN
4	Ze	107	ASN
4	Ze	133	ASN
4	Ze	197	ASN
4	Ze	394	GLN
4	Zf	105	ASN
4	Zf	159	ASN
4	Zf	197	ASN
4	Zf	314	GLN
4	Zg	5	GLN
4	Zg	107	ASN
4	Zg	129	GLN

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Mol	Chain	Res	Type
4	Zg	133	ASN
4	Zg	197	ASN
4	Zg	310	GLN
4	Zh	5	GLN
4	Zh	115	GLN
4	Zh	197	ASN
4	Zh	379	GLN
4	Zh	392	GLN
5	AA	102	ASN
5	AB	18	GLN
5	AB	172	GLN
5	AB	210	ASN
5	AB	223	ASN
5	AB	240	ASN
5	AC	18	GLN
5	AC	28	ASN
5	AC	70	GLN
5	AC	104	ASN
5	AC	106	GLN
5	AC	186	GLN
5	AD	17	ASN
5	AD	28	ASN
5	AD	104	ASN
5	AD	106	GLN
5	AD	153	ASN
5	AD	210	ASN
5	AD	240	ASN
5	AE	18	GLN
5	AE	37	GLN
5	AE	112	GLN
5	AE	116	GLN
3	AF	47	GLN
3	AF	83	GLN
3	AF	85	ASN
3	AF	121	GLN
3	AF	135	GLN
3	AF	164	GLN
3	AF	172	GLN
3	AF	174	ASN
3	AF	223	ASN
3	AG	16	GLN
3	AG	28	ASN

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Mol	Chain	Res	Type
3	AG	145	ASN
3	AG	223	ASN
3	AG	259	GLN
3	AH	47	GLN
3	AH	85	ASN
3	AH	104	GLN
3	AH	125	ASN
3	AH	127	GLN
3	AH	162	GLN
3	AH	169	GLN
3	AH	172	GLN
3	AH	259	GLN
3	AI	16	GLN
3	AI	32	ASN
3	AI	196	GLN
3	AI	209	ASN
3	AJ	47	GLN
3	AJ	90	ASN
3	AJ	161	GLN
3	AJ	164	GLN
3	AJ	169	GLN
3	AJ	172	GLN
3	AJ	174	ASN
3	AJ	223	ASN
3	AJ	232	ASN
3	AK	28	ASN
3	AK	121	GLN
3	AK	125	ASN
3	AK	127	GLN
3	AK	135	GLN
3	AK	137	GLN
3	AK	196	GLN
3	AK	223	ASN
3	AK	235	GLN
3	AL	32	ASN
3	AL	104	GLN
3	AL	121	GLN
3	AL	127	GLN
3	AL	145	ASN
3	AL	209	ASN
3	AM	25	ASN
3	AM	37	GLN

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Mol	Chain	Res	Type
3	AM	51	GLN
3	AM	67	GLN
3	AM	125	ASN
3	AM	127	GLN
3	AM	209	ASN
3	AM	223	ASN
3	AM	252	GLN
3	AN	67	GLN
3	AN	85	ASN
3	AN	125	ASN
3	AN	235	GLN
6	AR	303	GLN
6	AR	374	HIS
6	AS	297	GLN
6	AS	299	ASN
6	AS	303	GLN
6	AS	374	HIS
6	AT	303	GLN
6	AT	374	HIS
6	AU	303	GLN
6	AU	374	HIS
6	AV	303	GLN
6	AV	374	HIS
6	AW	299	ASN
6	AW	303	GLN
6	AW	374	HIS
6	AX	303	GLN
6	AX	374	HIS
6	AY	299	ASN
6	AY	303	GLN
6	AY	374	HIS
6	AZ	303	GLN
6	AZ	374	HIS
6	Aa	303	GLN
6	Aa	374	HIS
6	Ac	303	GLN
6	Ad	265	GLN
6	Ad	303	GLN
6	Ad	374	HIS
6	Ae	303	GLN
6	Ae	374	HIS
6	Af	297	GLN

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Mol	Chain	Res	Type
6	Af	303	GLN
6	Af	365	ASN
6	Af	374	HIS
6	Ag	297	GLN
6	Ag	303	GLN
6	Ag	374	HIS
6	Ah	303	GLN
6	Ah	374	HIS
6	Ai	303	GLN
6	Ai	374	HIS
6	Aj	303	GLN
6	Aj	374	HIS
6	Aj	434	ASN
6	Ak	303	GLN
6	Ak	374	HIS
6	Ak	434	ASN
6	Al	303	GLN
6	Al	374	HIS
6	Al	434	ASN
6	Am	303	GLN
6	Am	374	HIS
6	Am	434	ASN
6	An	303	GLN
6	An	374	HIS
6	An	434	ASN
6	Ao	303	GLN
6	Ao	374	HIS
6	Ao	434	ASN
6	Ap	374	HIS
6	Ap	434	ASN
6	AO	297	GLN
6	AO	303	GLN
6	AO	374	HIS
6	AO	434	ASN
6	AP	297	GLN
6	AP	303	GLN
6	AP	359	GLN
6	AP	374	HIS
6	AQ	303	GLN
6	AQ	374	HIS
7	As	39	GLN
8	At	162	ASN

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Mol	Chain	Res	Type
8	At	182	ASN
8	At	205	ASN
9	Au	119	GLN
9	Au	141	GLN
9	Aw	36	GLN
9	Aw	160	GLN
9	Aw	233	GLN
9	Ax	160	GLN
9	Ax	184	GLN
9	Ay	114	GLN
9	Ay	155	ASN
10	Az	103	GLN
10	A1	15	GLN
10	A1	90	ASN
10	A2	83	GLN
10	A2	103	GLN
10	A3	87	GLN
10	A4	39	HIS
10	A4	55	GLN
10	A4	97	GLN
10	A5	76	GLN
11	A6	17	ASN
11	A6	23	GLN
11	A7	23	GLN
11	A7	29	ASN
11	A7	92	GLN
11	A7	117	GLN
11	A8	32	ASN
11	A8	76	GLN
11	A8	92	GLN
11	A8	135	GLN
11	A9	21	GLN
11	A9	32	ASN
11	A9	72	HIS
11	A9	76	GLN
11	A9	117	GLN
11	A0	13	GLN
11	A0	72	HIS
11	A0	76	GLN
11	A0	112	ASN
6	UI	196	HIS
6	UJ	245	HIS

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Mol	Chain	Res	Type
6	UK	196	HIS
6	UL	69	GLN
6	UL	196	HIS
6	UM	196	HIS
6	UN	69	GLN
6	UN	196	HIS
6	UO	196	HIS
6	UP	196	HIS
12	BA	30	ASN
12	BB	22	ASN
12	BB	120	ASN
6	WB	169	GLN
6	WE	156	HIS
6	WE	209	ASN
6	WF	118	GLN
6	WH	156	HIS
6	WI	129	GLN
6	WI	156	HIS
6	WJ	169	GLN
6	WJ	209	ASN
6	WO	209	ASN
6	WP	209	ASN
6	WV	169	GLN
6	WW	169	GLN
12	BC	22	ASN
12	BC	50	GLN
12	BC	57	GLN
12	BC	134	GLN
12	BE	17	GLN
12	BF	5	ASN
12	BF	57	GLN
12	BF	115	ASN
6	BG	319	GLN
6	BM	324	ASN
6	BO	318	ASN
6	BQ	318	ASN
6	BQ	324	ASN
6	BR	303	GLN
6	BR	374	HIS
6	BS	303	GLN
6	BS	374	HIS
6	BT	303	GLN

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Mol	Chain	Res	Type
6	BT	374	HIS
6	BU	303	GLN
6	BU	374	HIS
6	BV	303	GLN
6	BV	374	HIS
6	BW	374	HIS
6	BX	297	GLN
6	BX	303	GLN
6	BX	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.

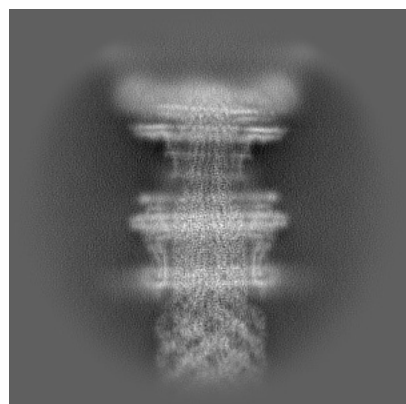
6 Map visualisation [i](#)

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

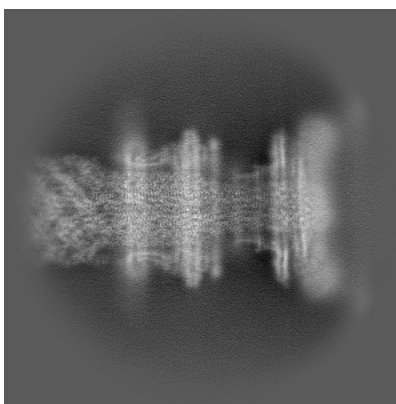
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

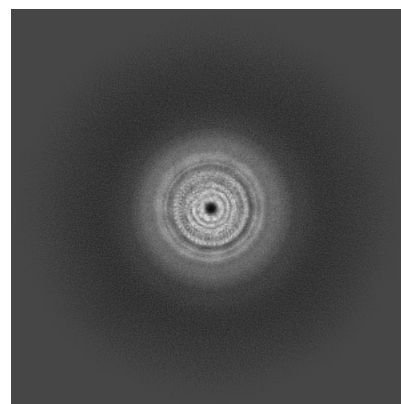
6.1.1 Primary map



X

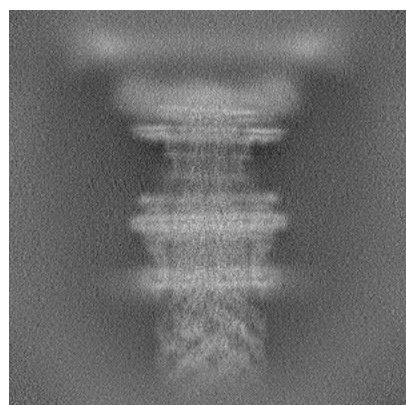


Y

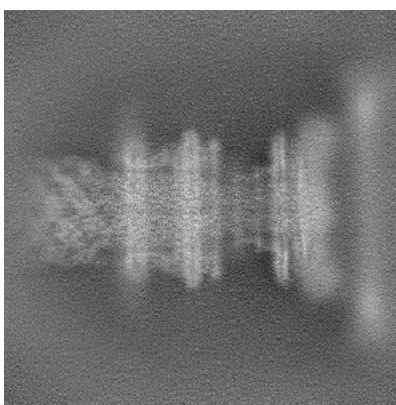


Z

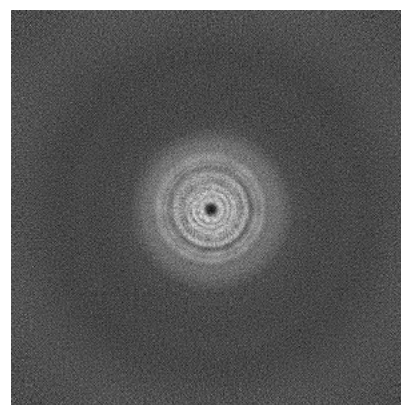
6.1.2 Raw map



X



Y

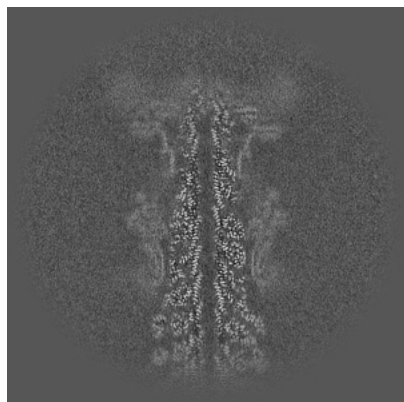


Z

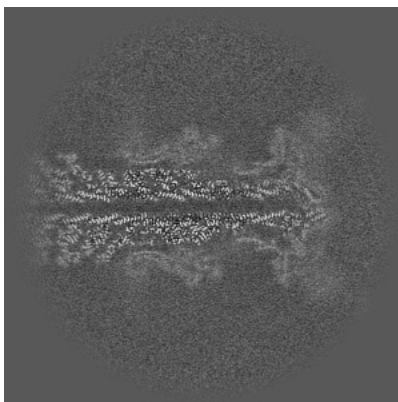
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

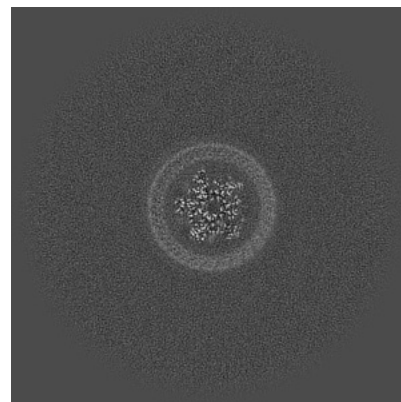
6.2.1 Primary map



X Index: 256

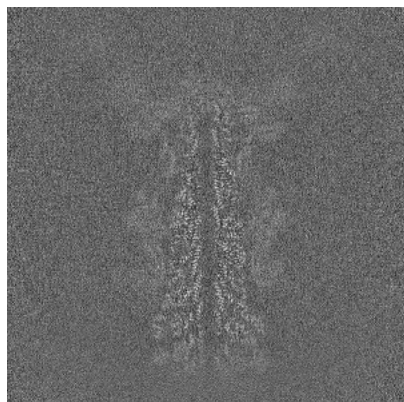


Y Index: 256

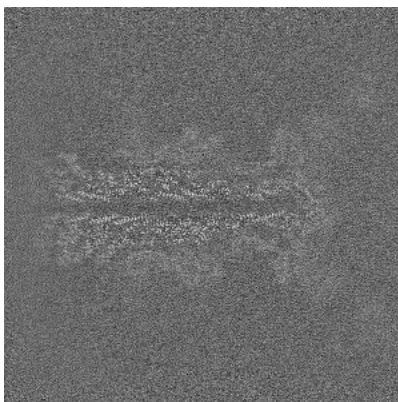


Z Index: 256

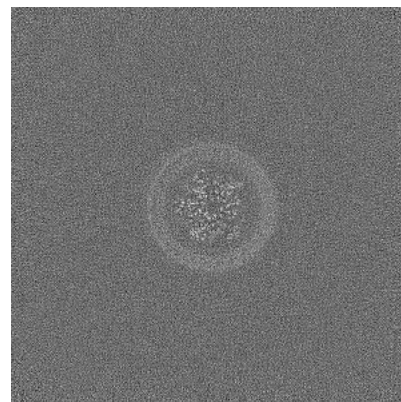
6.2.2 Raw map



X Index: 256



Y Index: 256

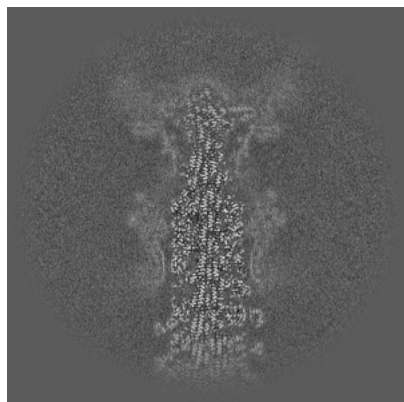


Z Index: 256

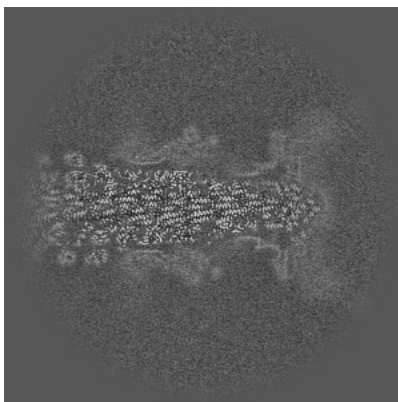
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

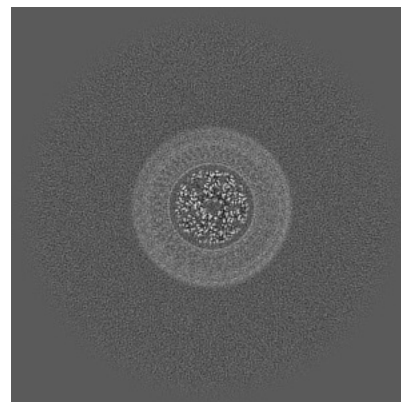
6.3.1 Primary map



X Index: 242

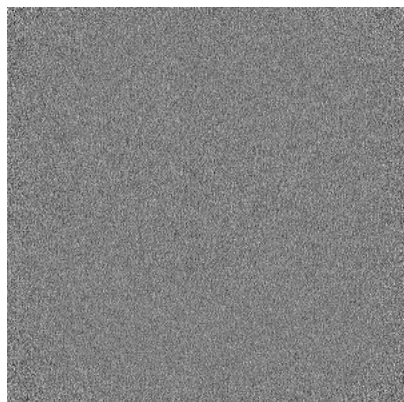


Y Index: 268

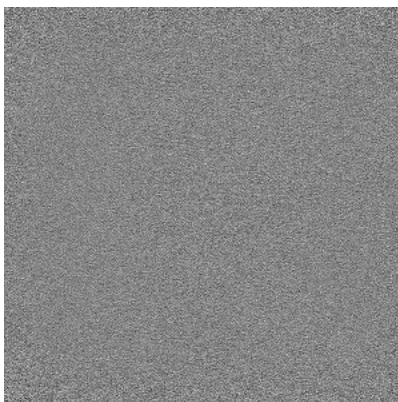


Z Index: 234

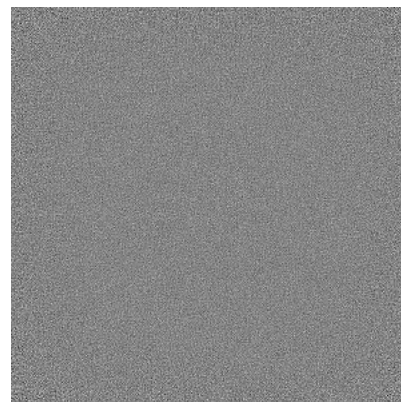
6.3.2 Raw map



X Index: 0



Y Index: 0

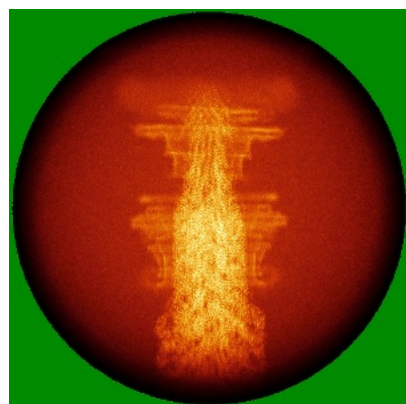


Z Index: 0

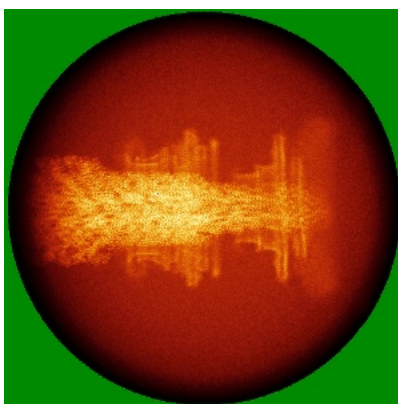
The images above show the largest variance slices of the map in three orthogonal directions.

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

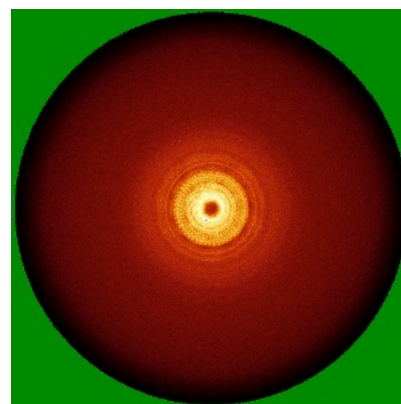
6.4.1 Primary map



X

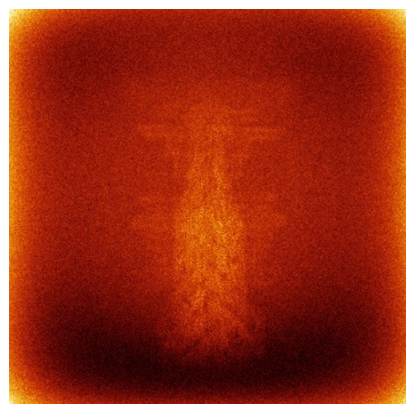


Y

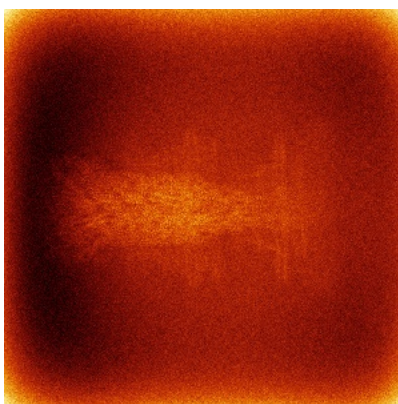


Z

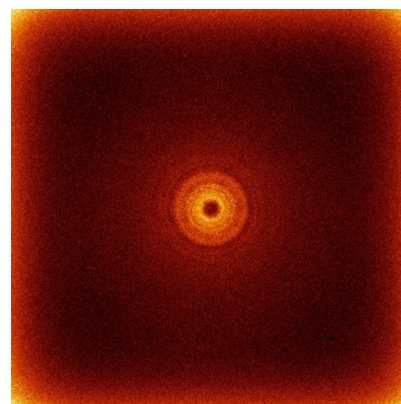
6.4.2 Raw map



X



Y

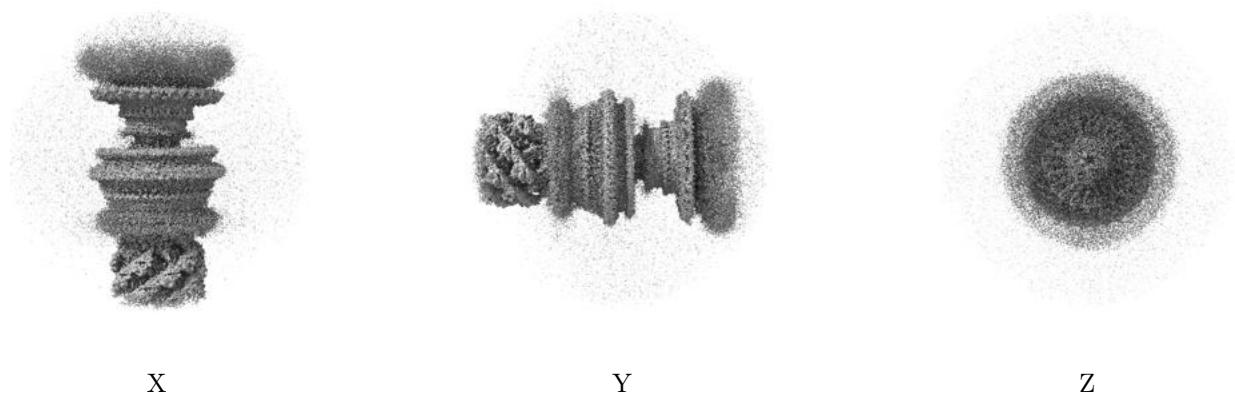


Z

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.

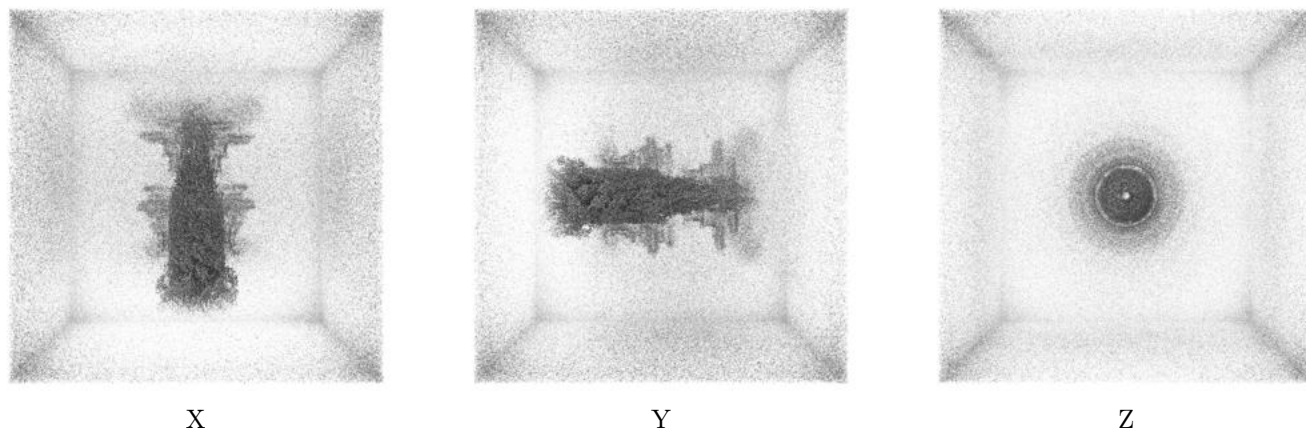
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

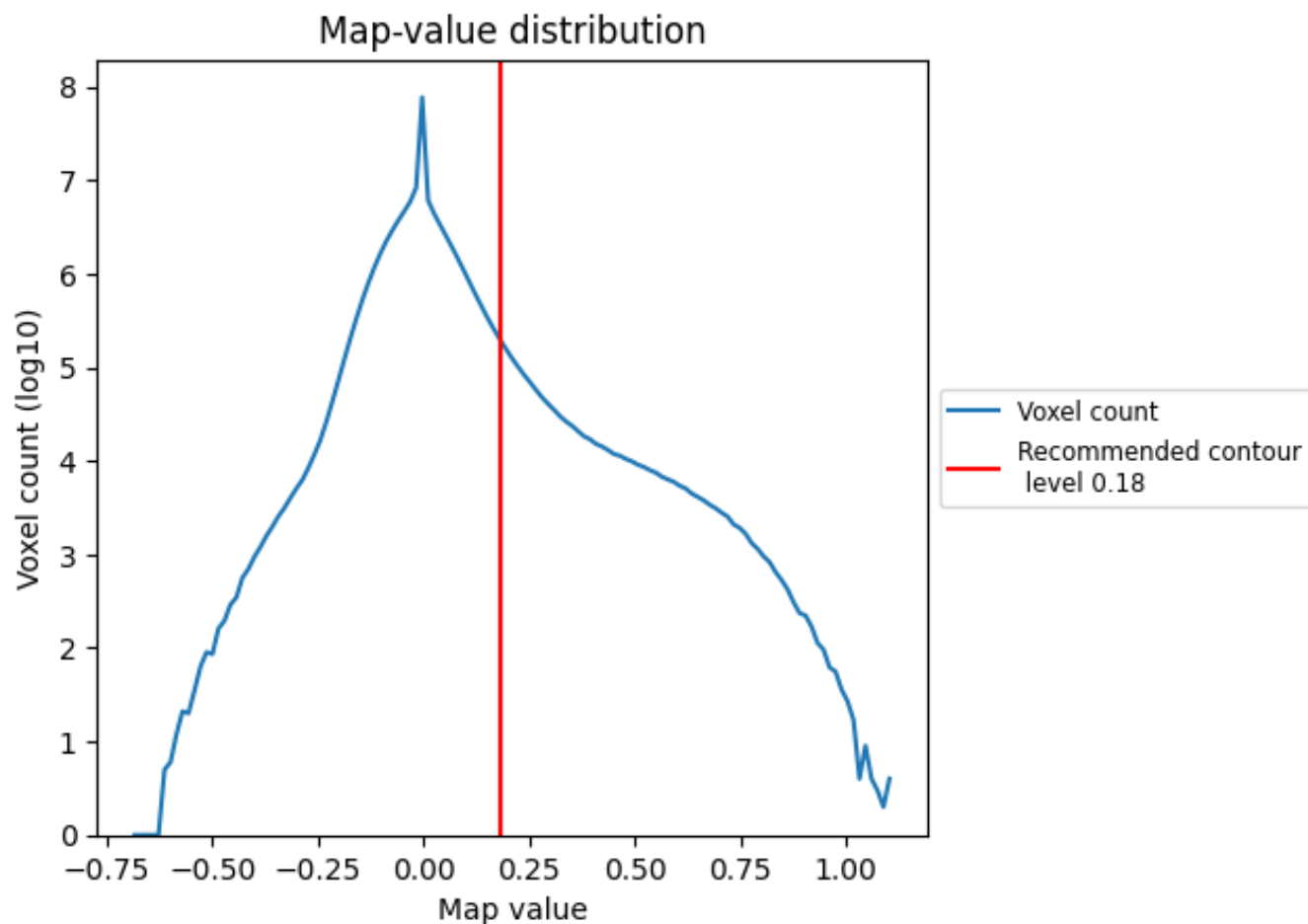
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

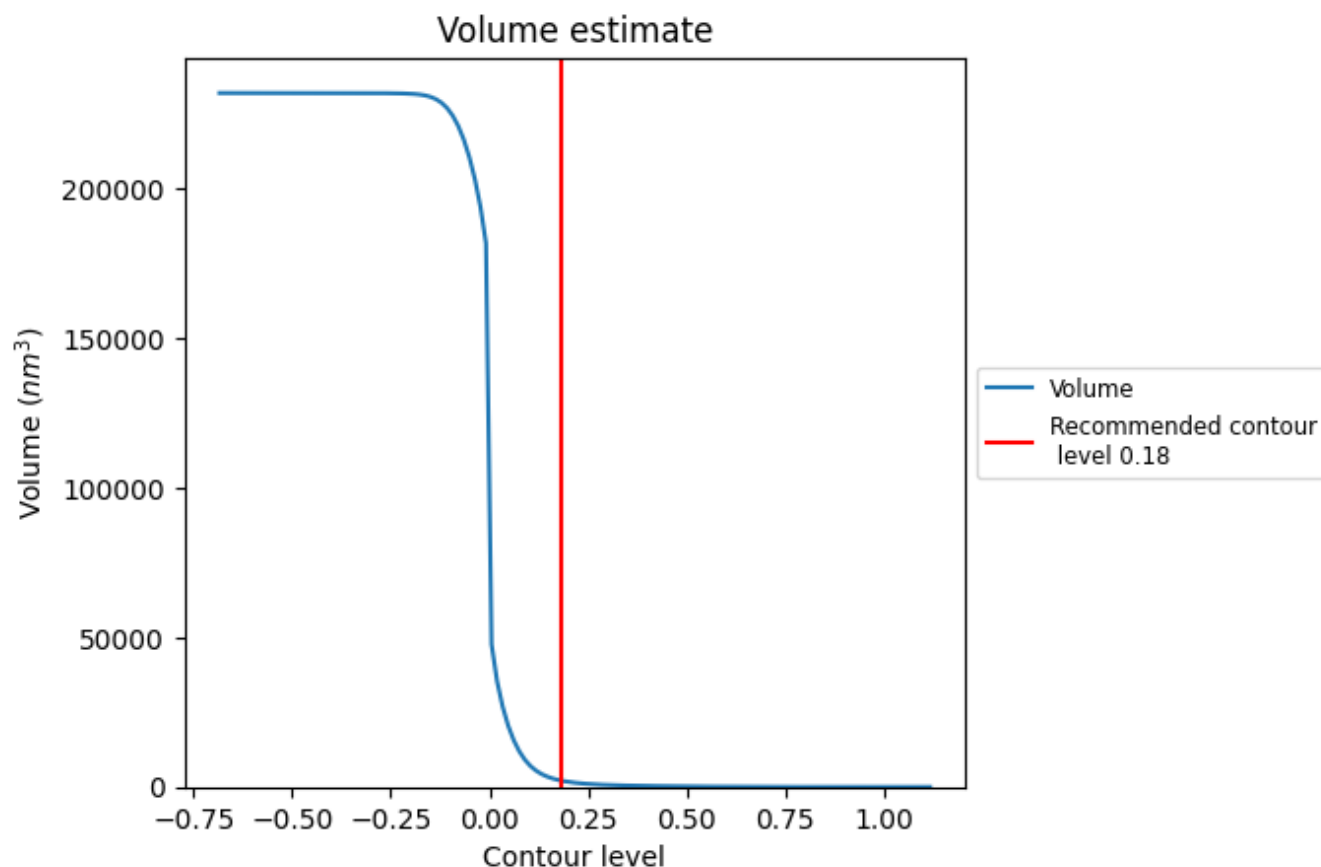
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

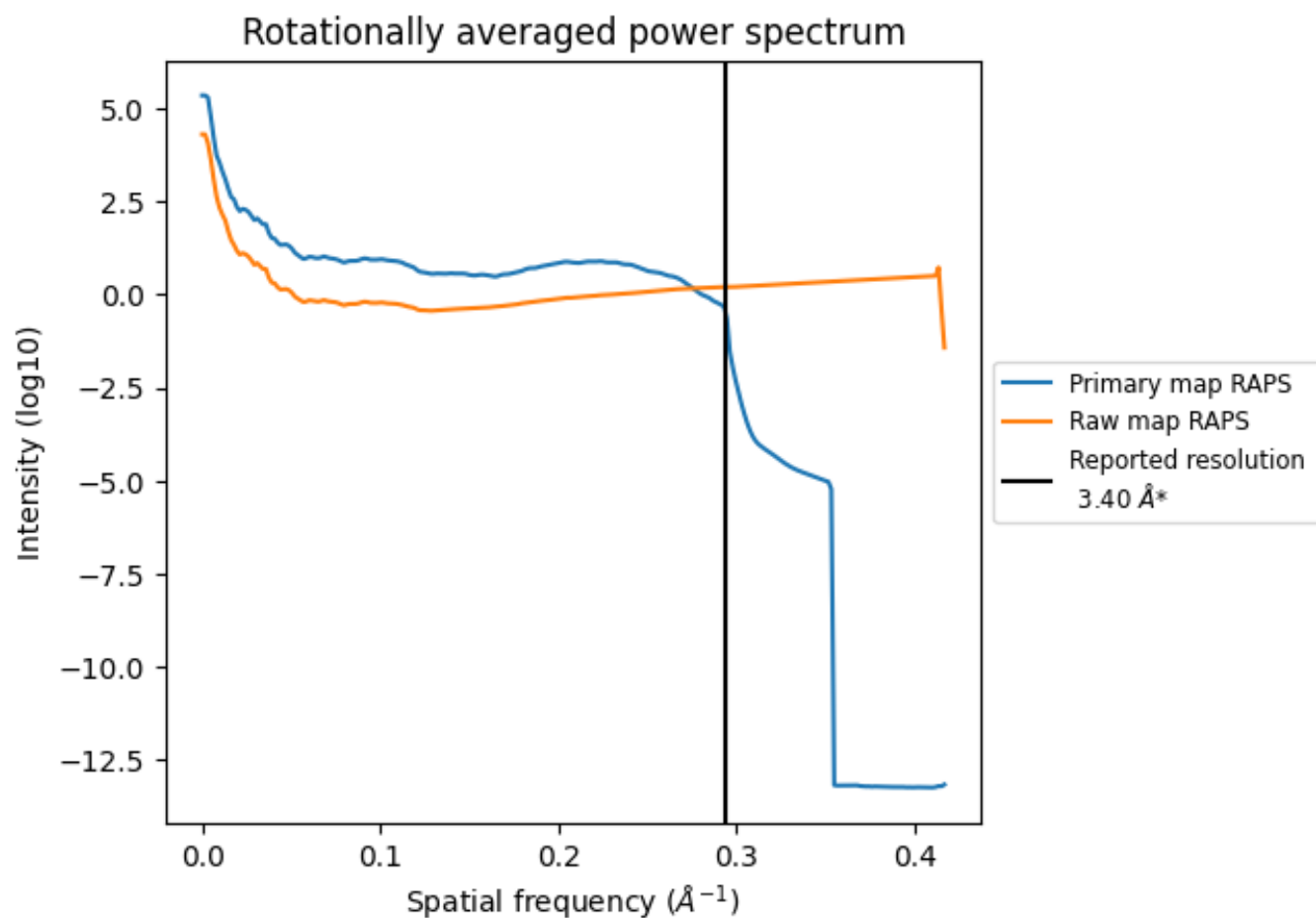
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2188 nm³; this corresponds to an approximate mass of 1977 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

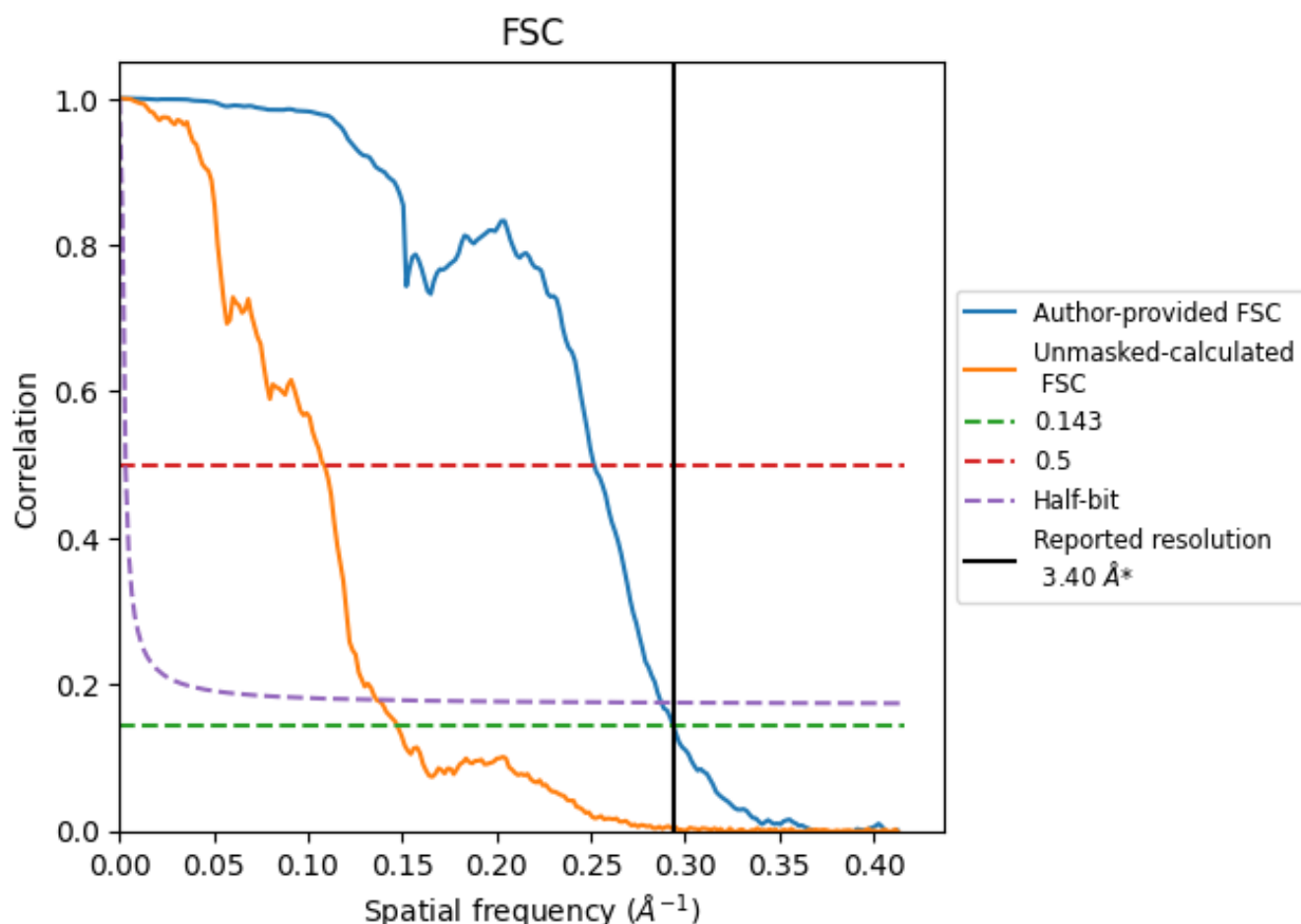


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

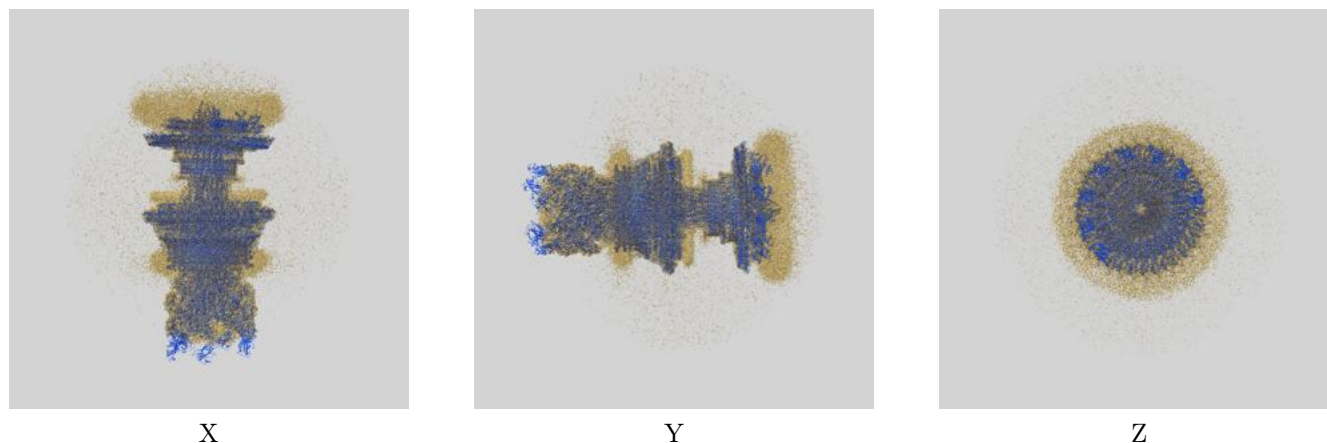
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.97	3.48
Unmasked-calculated*	6.78	9.23	7.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.78 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

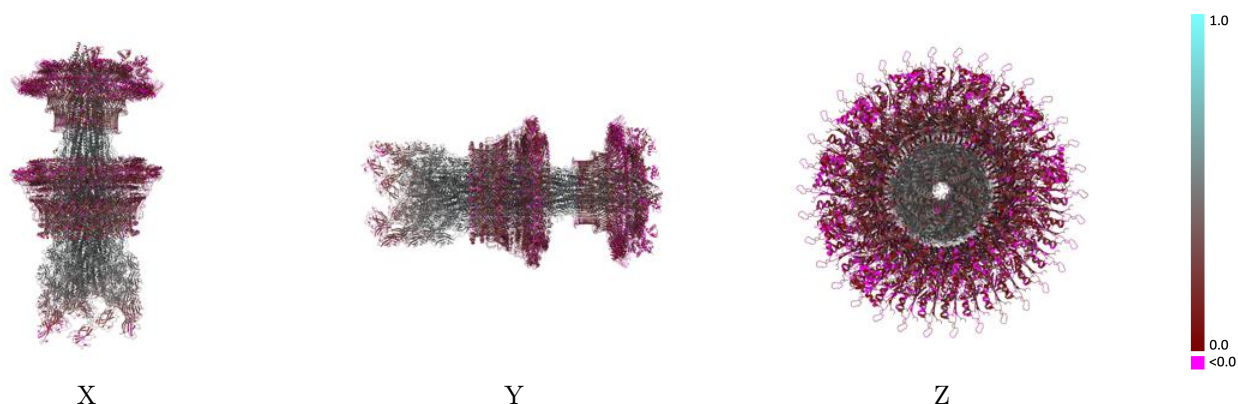
This section contains information regarding the fit between EMDB map EMD-37611 and PDB model 8WL2. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



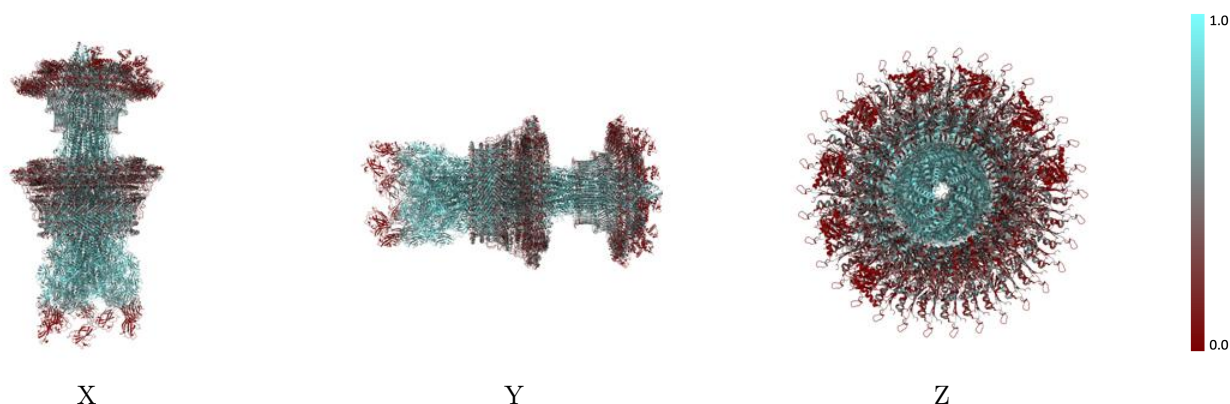
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



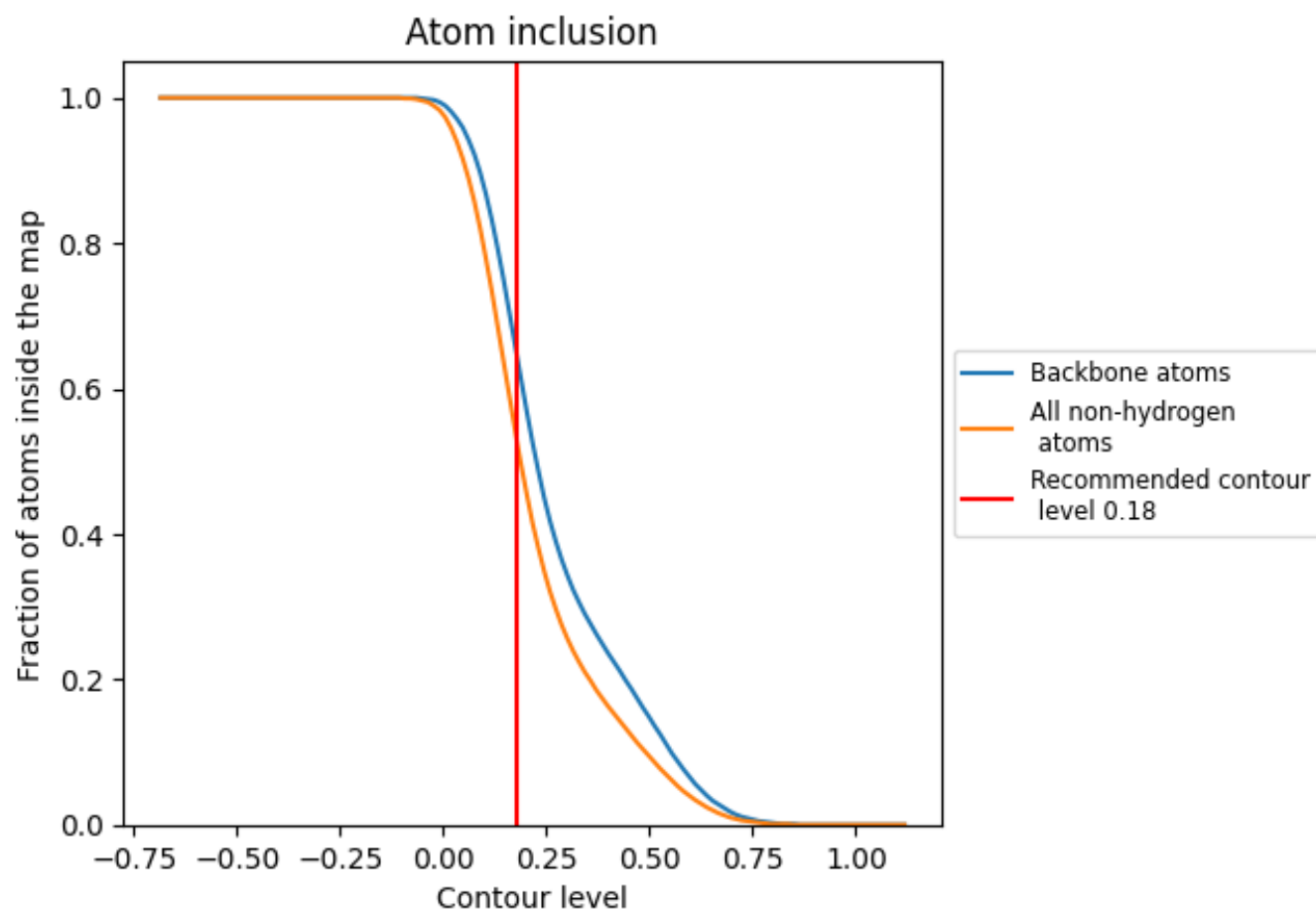
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ





















































































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

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























































































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





















































































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





















































































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























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

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