



Full wwPDB EM Validation Report ⓘ

Aug 27, 2024 – 05:45 PM JST

PDB ID : 8WLT
EMDB ID : EMD-37630
Title : Cryo-EM structure of the membrane-anchored part of the flagellar motor-hook complex in the CCW state
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2023-10-01
Resolution : 4.10 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:

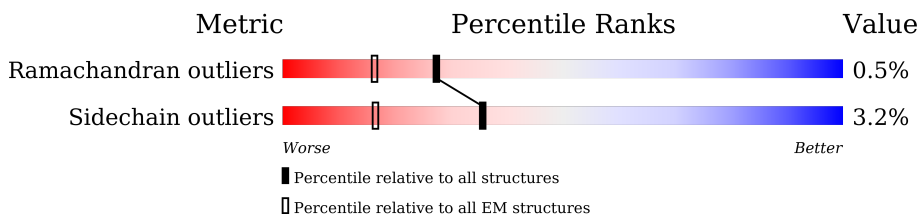
EMDB validation analysis : 0.0.1.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 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	27%	88% 9%
1	K	232	27%	88% 9%
1	L	232	28%	88% 9%
1	M	232	27%	88% 9%
1	N	232	26%	88% 9%
1	O	232	29%	88% 9%
1	P	232	26%	88% 9%
1	Q	232	27%	88% 9%
1	R	232	25%	88% 9%
1	S	232	26%	88% 9%
1	T	232	27%	88% 9%
1	U	232	24%	88% 9%
1	V	232	29%	88% 9%
1	W	232	28%	88% 9%
1	X	232	28%	88% 9%
1	Y	232	28%	88% 9%
1	Z	232	26%	88% 9%
2	a	365	37%	82% 17%
2	b	365	35%	82% 17%
2	c	365	36%	82% 17%
2	d	365	36%	82% 17%
2	e	365	39%	82% 17%
2	f	365	32%	82% 17%
2	g	365	29%	82% 17%
2	h	365	30%	82% 17%

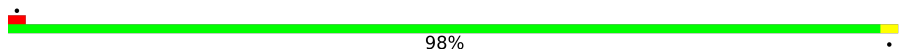
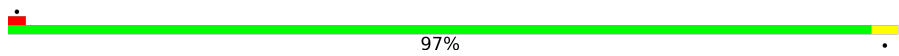
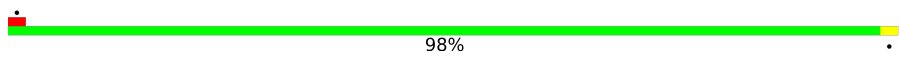
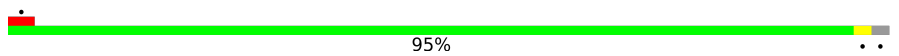
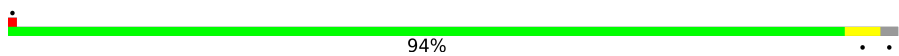
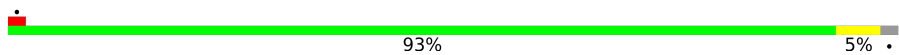
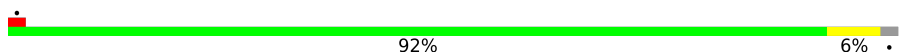
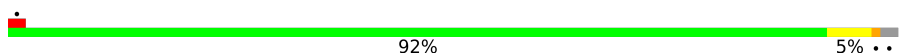
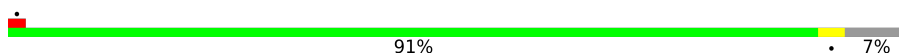

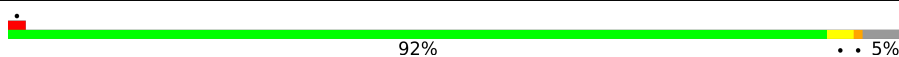
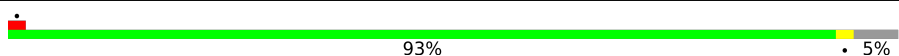
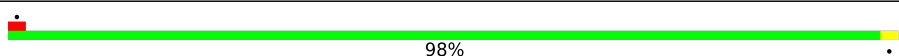
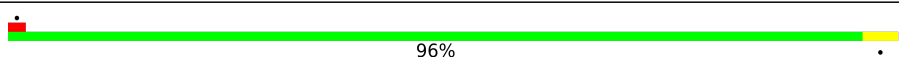
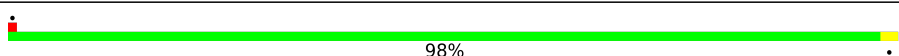
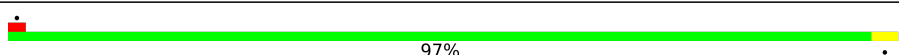
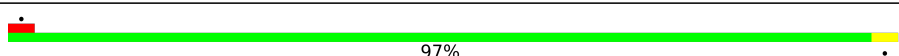
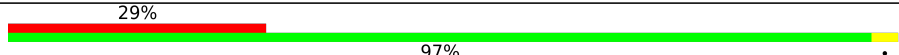
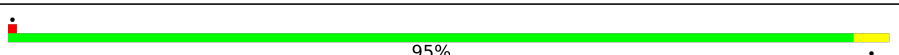
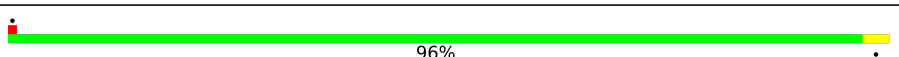
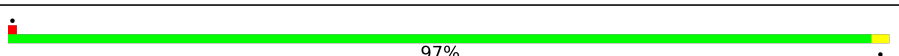
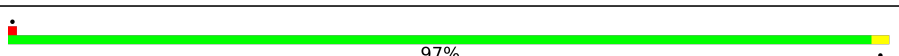
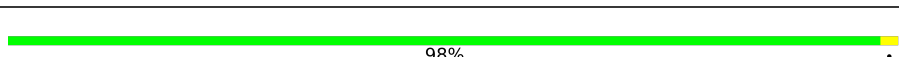
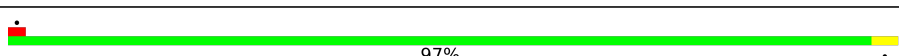
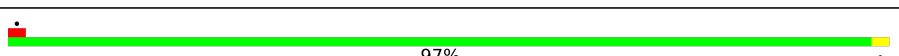
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Mol	Chain	Length	Quality of chain
2	i	365	31% 82% 17%
2	j	365	29% 82% 17%
2	k	365	29% 82% 17%
2	l	365	33% 82% 17%
2	m	365	30% 82% 17%
2	n	365	33% 82% 17%
2	o	365	32% 82% 17%
2	p	365	33% 82% 17%
2	q	365	34% 82% 17%
2	r	365	35% 82% 17%
2	s	365	34% 82% 17%
2	t	365	33% 82% 17%
2	u	365	37% 82% 17%
2	v	365	36% 82% 17%
2	w	365	34% 82% 17%
2	x	365	39% 82% 17%
2	y	365	41% 82% 17%
2	z	365	37% 82% 17%
3	0	260	92% 5%
3	1	260	93% .
3	2	260	98% .
3	3	260	98% .
3	4	260	97% .
3	5	260	97% .
3	6	260	97% .

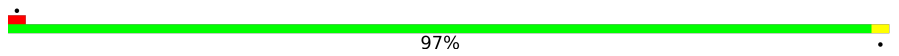
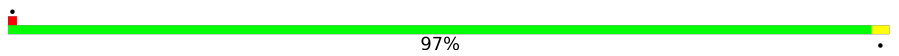
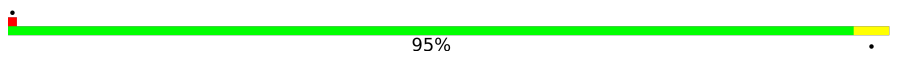
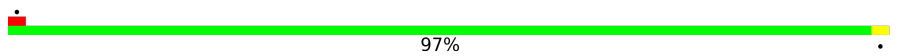
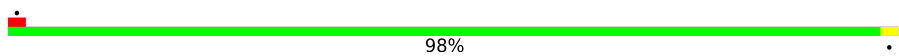
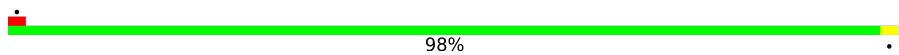
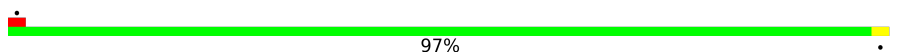
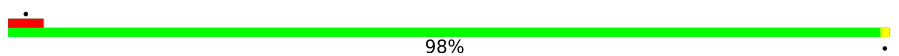
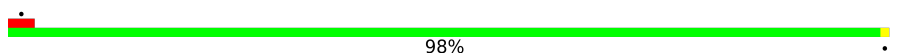
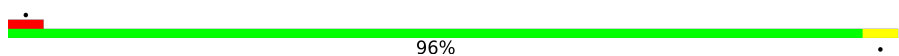
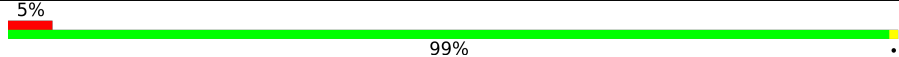
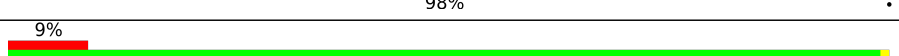
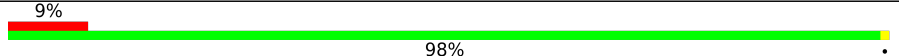
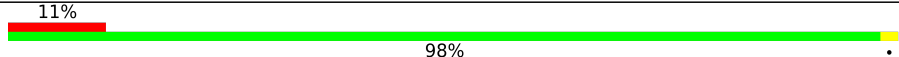
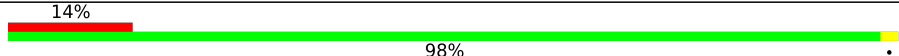
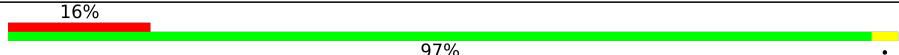
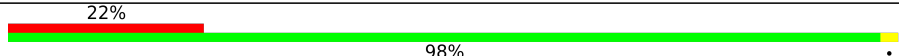
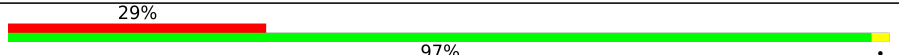
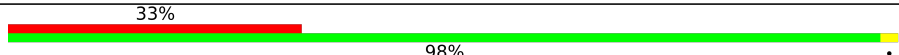
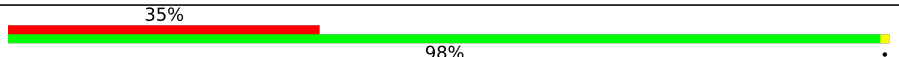
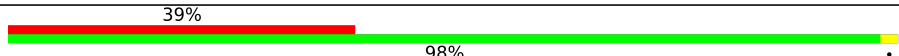
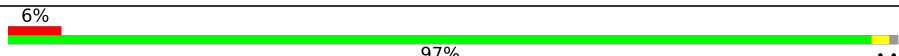
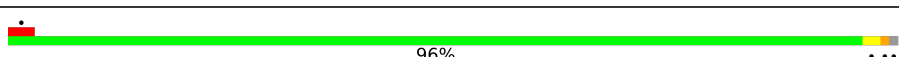
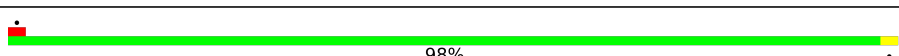
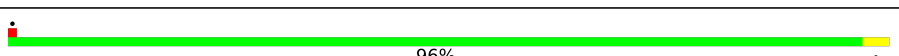
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Mol	Chain	Length	Quality of chain
3	7	260	 98%
3	8	260	 97%
3	9	260	 98%
3	AF	260	 95%
3	AG	260	 94%
3	AH	260	 93% 5%
3	AI	260	 92% 6%
3	AJ	260	 92% 5%
3	AK	260	 91% 7%
3	AL	260	 90% 5% 5%
3	AM	260	 92% 5%
3	AN	260	 93% 5%
3	ZA	260	 98%
3	ZB	260	 96%
3	ZC	260	 98%
3	ZD	260	 97%
3	ZE	260	 97%
4	ZF	403	 29% 97%
4	ZG	403	 95%
4	ZH	403	 96%
4	ZI	403	 97%
4	ZJ	403	 97%
4	ZK	403	 98%
4	ZL	403	 97%
4	ZM	403	 97%

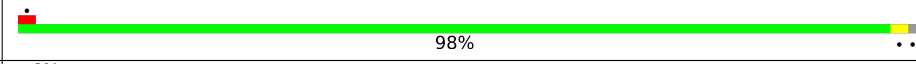






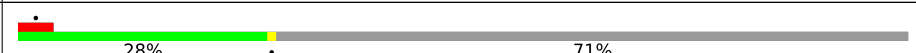

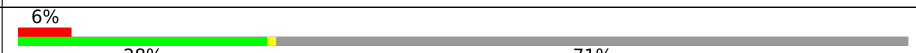
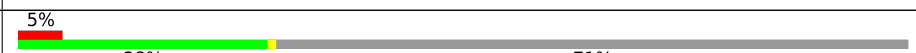





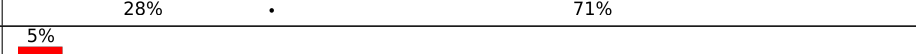








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Mol	Chain	Length	Quality of chain
4	ZN	403	 97%
4	ZO	403	 97%
4	ZP	403	 95%
4	ZQ	403	 97%
4	ZR	403	 98%
4	ZS	403	 98%
4	ZT	403	 97%
4	ZU	403	 98%
4	ZV	403	 98%
4	ZW	403	 96%
4	ZX	403	 99%
4	ZY	403	 98%
4	ZZ	403	 98%
4	Za	403	 98%
4	Zb	403	 98%
4	Zc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



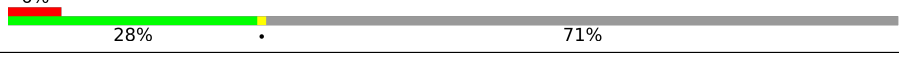
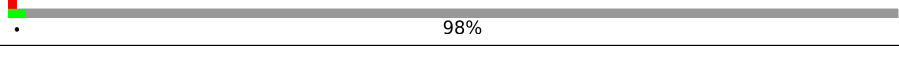
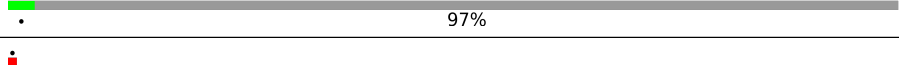
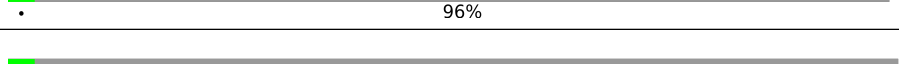
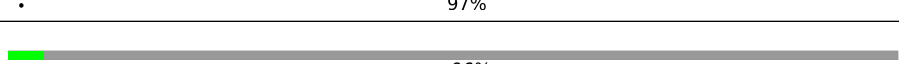
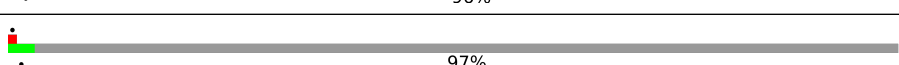
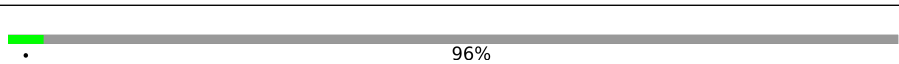
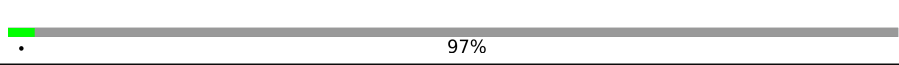
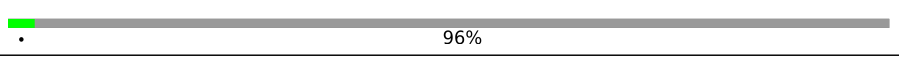
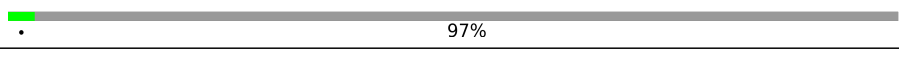
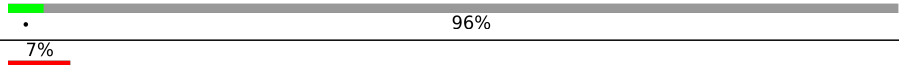


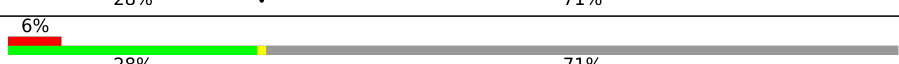
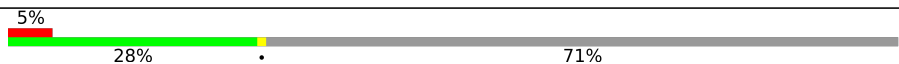








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Mol	Chain	Length	Quality of chain
5	AE	251	 98%
6	AO	560	 28% 71%
6	AP	560	 28% 71%
6	AQ	560	 28% 71%
6	AR	560	 28% 71%
6	AS	560	 28% 71%
6	AT	560	 28% 71%
6	AU	560	 28% 71%
6	AV	560	 28% 71%
6	AW	560	 28% 71%
6	AX	560	 28% 71%
6	AY	560	 28% 71%
6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

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Mol	Chain	Length	Quality of chain
6	An	560	 6% 28% 71%
6	Ao	560	 7% 28% 71%
6	Ap	560	 6% 28% 71%
6	BG	560	 98%
6	BH	560	 97%
6	BI	560	 96%
6	BJ	560	 97%
6	BK	560	 96%
6	BL	560	 97%
6	BM	560	 96%
6	BN	560	 97%
6	BO	560	 96%
6	BP	560	 97%
6	BQ	560	 96%
6	BR	560	 7% 28% 71%
6	BS	560	 6% 28% 71%
6	BT	560	 6% 28% 71%
6	BU	560	 6% 28% 71%
6	BV	560	 5% 28% 71%
6	BW	560	 28% 71%
6	BX	560	 5% 28% 71%
6	UI	560	 24% 25% 72%
6	UJ	560	 25% 25% 72%
6	UK	560	 25% 25% 72%
6	UL	560	 26% 25% 72%


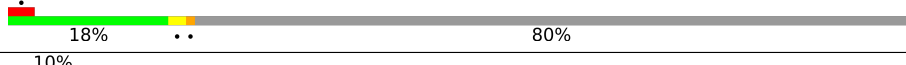
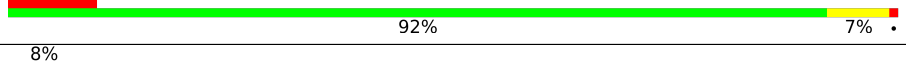
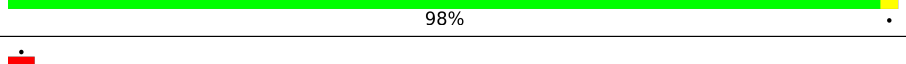
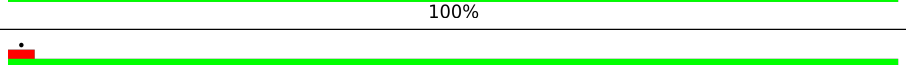
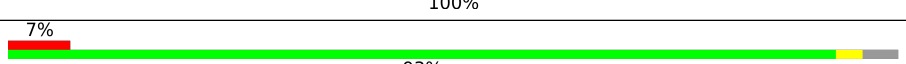
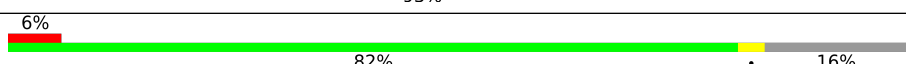
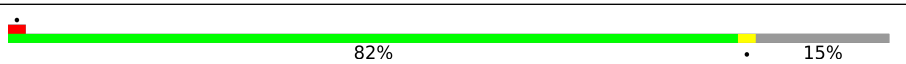


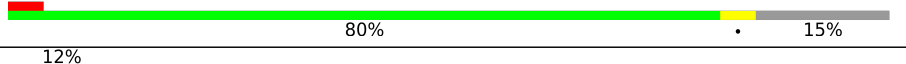
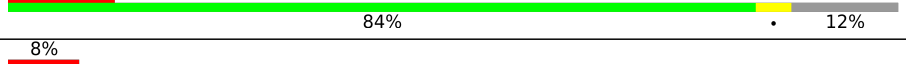

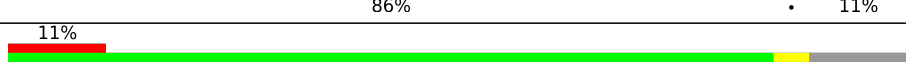
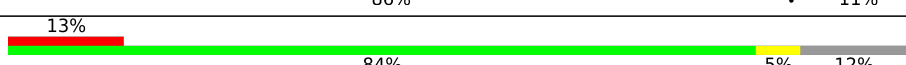
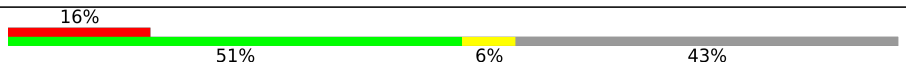

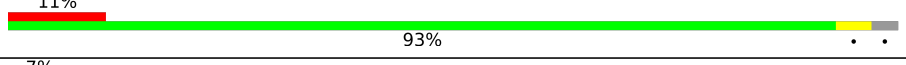


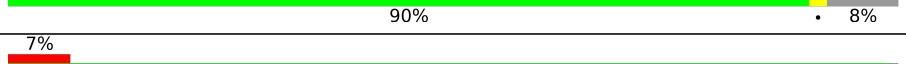
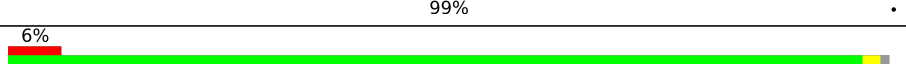
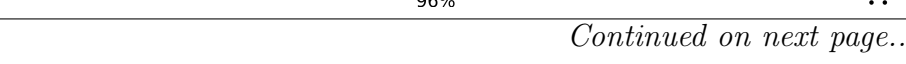


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Mol	Chain	Length	Quality of chain
6	UM	560	26% 25% 72%
6	UN	560	25% 25% 72%
6	UO	560	24% 25% 72%
6	UP	560	23% 25% 72%
6	WA	560	18% 80%
6	WB	560	18% 80%
6	WC	560	17% 81%
6	WD	560	18% 80%
6	WE	560	18% 80%
6	WF	560	5% 18% 80%
6	WG	560	7% 18% 80%
6	WH	560	7% 16% 83%
6	WI	560	7% 15% 83%
6	WJ	560	7% 16% 82%
6	WK	560	10% 16% 82%
6	WL	560	8% 14% 85%
6	WM	560	6% 14% 85%
6	WN	560	6% 14% 85%
6	WO	560	7% 16% 83%
6	WP	560	5% 16% 82%
6	WQ	560	6% 18% 80%
6	WR	560	5% 17% 80%
6	WS	560	18% 80%
6	WT	560	17% 80%
6	WU	560	19% 80%

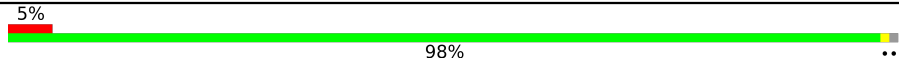
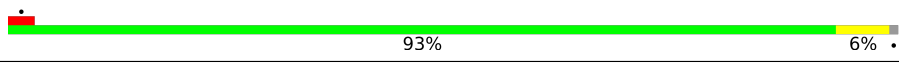
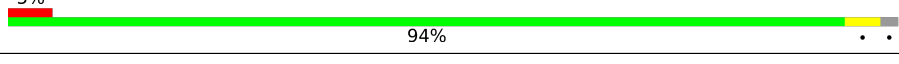
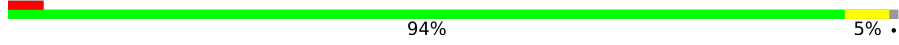
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Mol	Chain	Length	Quality of chain
6	WV	560	
6	WW	560	
7	Ab	89	
7	Aq	89	
7	Ar	89	
7	As	89	
8	At	264	
9	Au	245	
9	Av	245	
9	Aw	245	
9	Ax	245	
9	Ay	245	
10	A1	104	
10	A2	104	
10	A3	104	
10	A4	104	
10	A5	104	
10	Az	104	
11	A0	138	
11	A6	138	
11	A7	138	
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	 5% 98% ..
12	BD	134	 5% 93% 6% .
12	BE	134	 5% 94% . .
12	BF	134	 5% 94% 5% .

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 338664 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

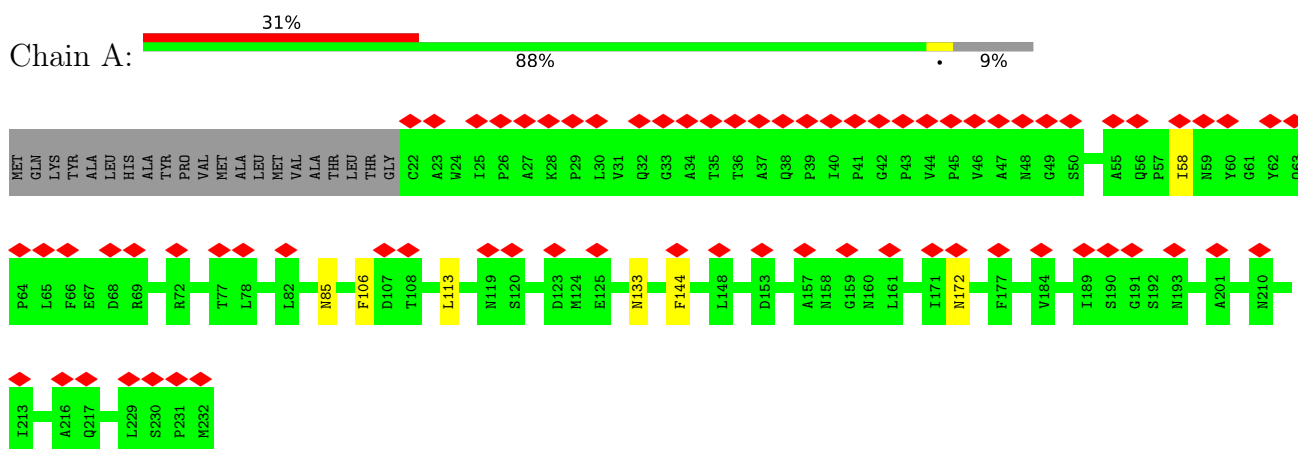
- Molecule 12 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	BA	133	Total 969	604	167	193	5	0	0
12	BB	132	Total 964	601	166	192	5	0	0
12	BC	133	Total 969	604	167	193	5	0	0
12	BD	133	Total 969	604	167	193	5	0	0
12	BE	131	Total 956	595	165	191	5	0	0
12	BF	133	Total 969	604	167	193	5	0	0

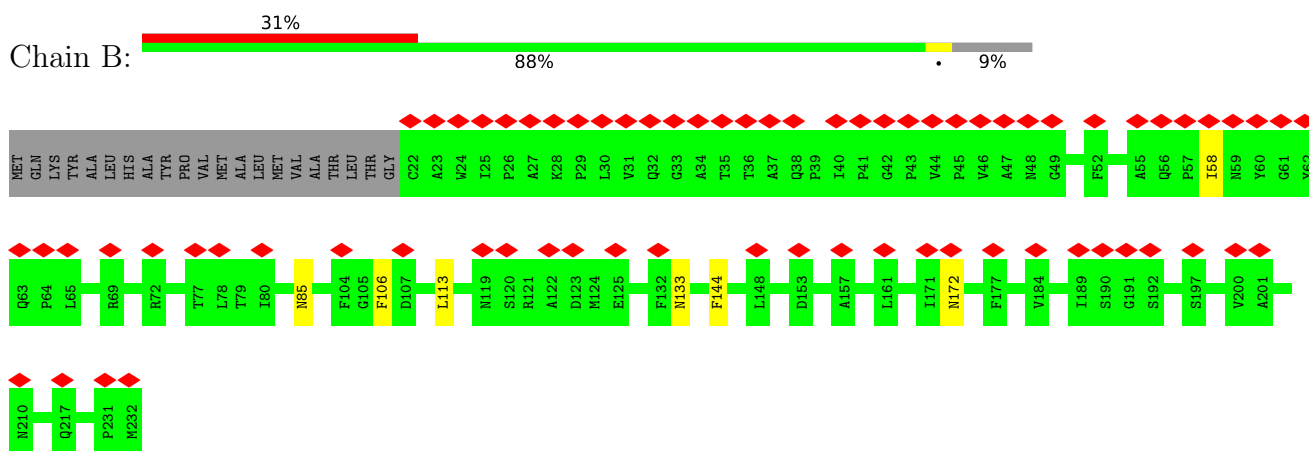
3 Residue-property plots [i](#)

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

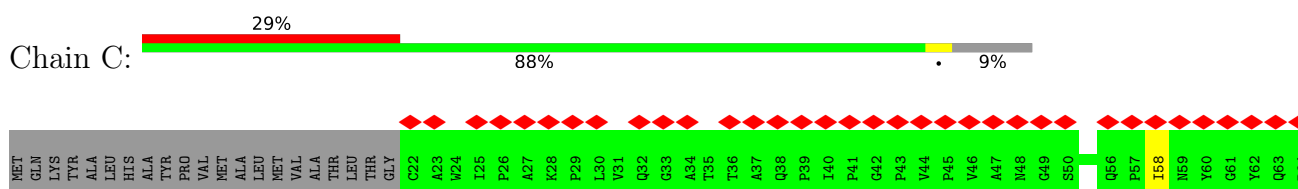
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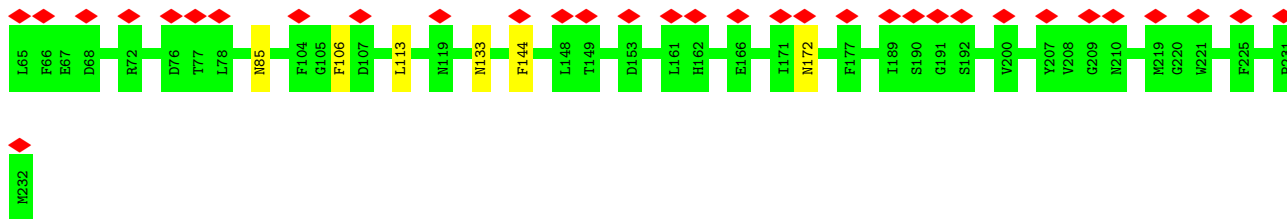


- Molecule 1: Flagellar L-ring protein

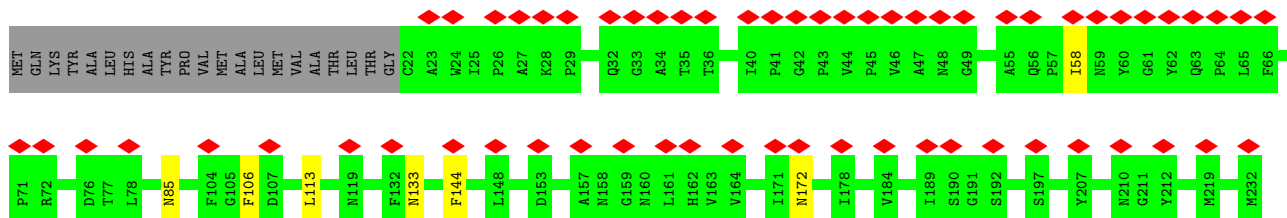
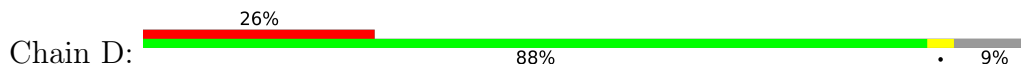


- Molecule 1: Flagellar L-ring protein

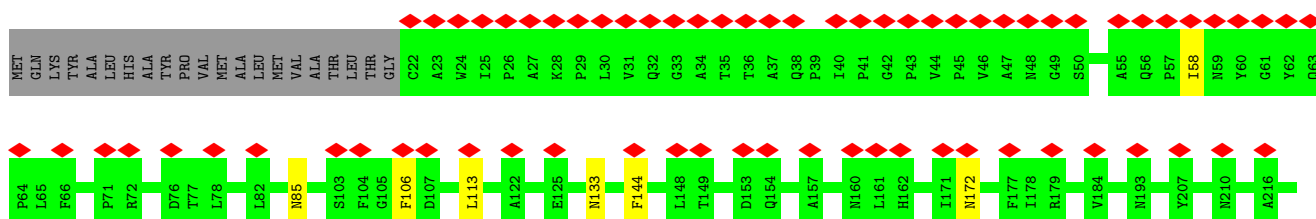
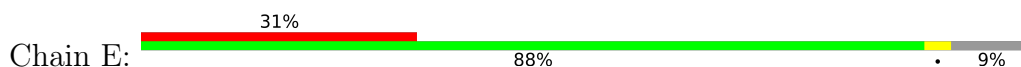




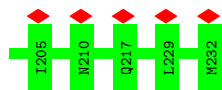
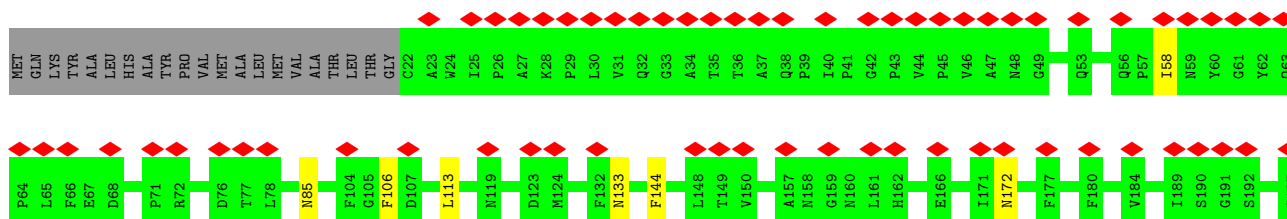
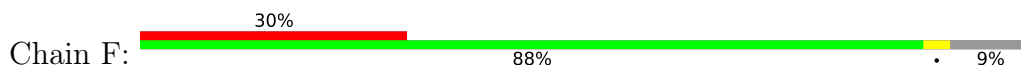
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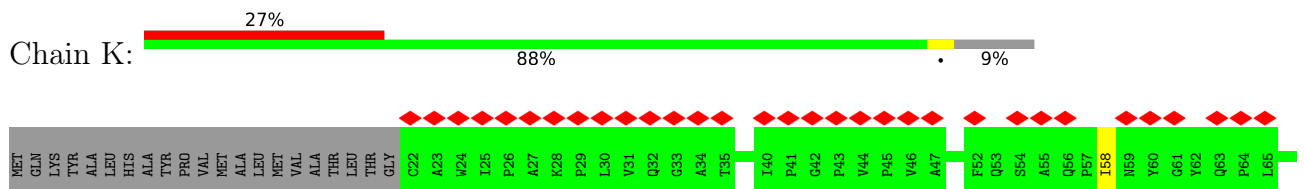
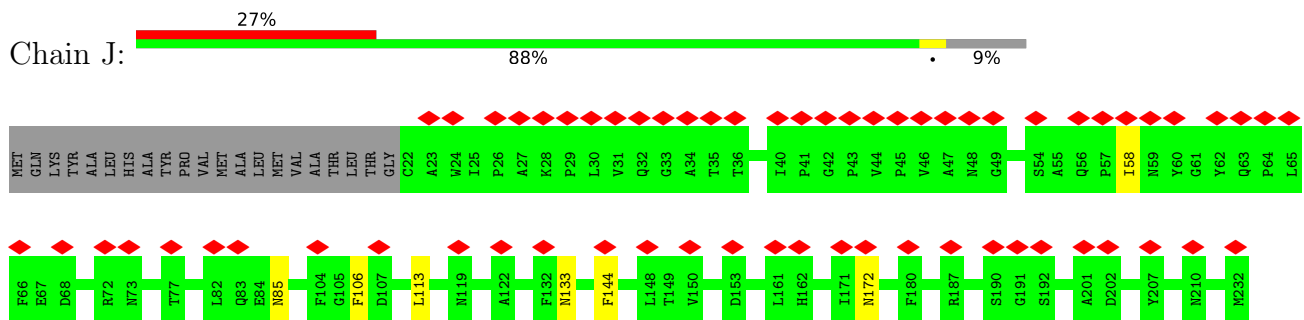
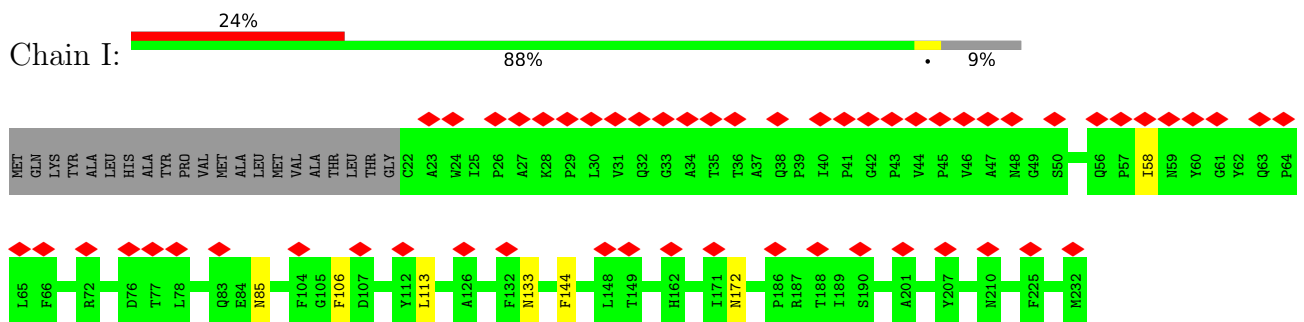
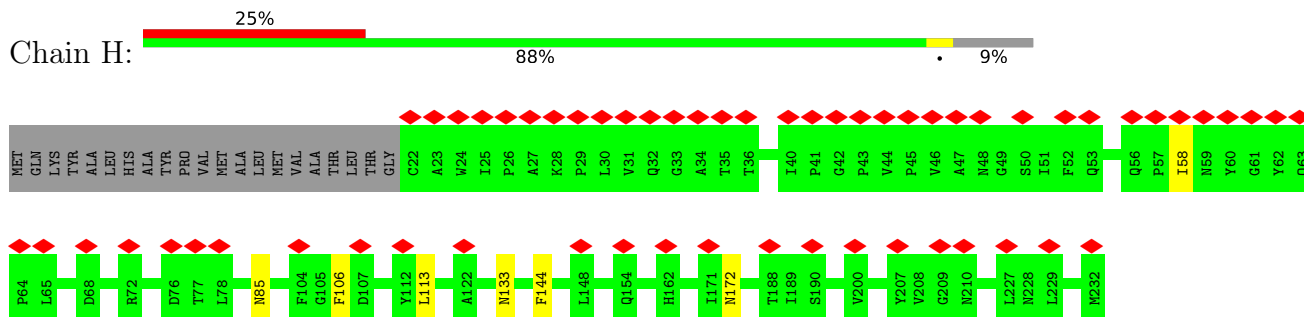
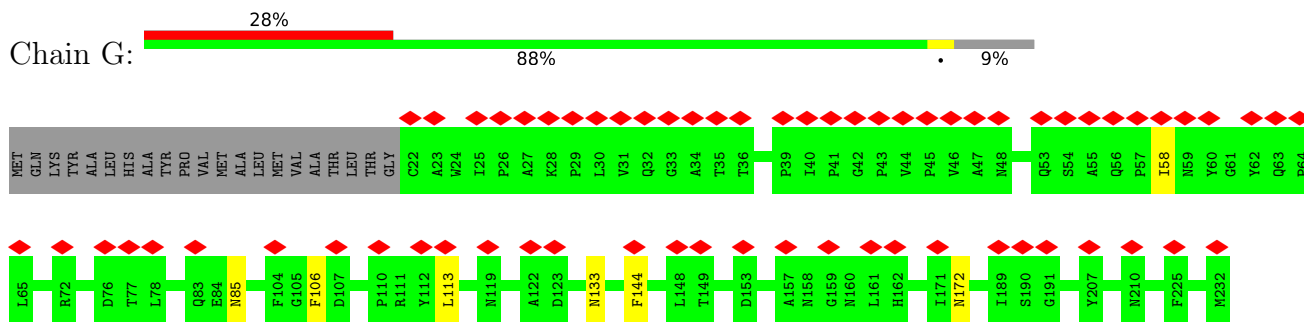
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

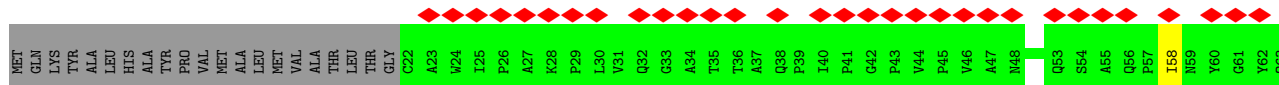
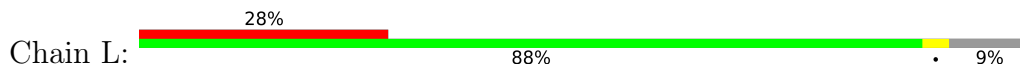


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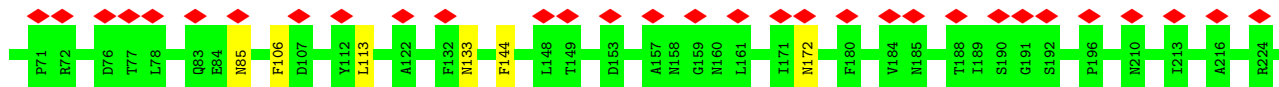
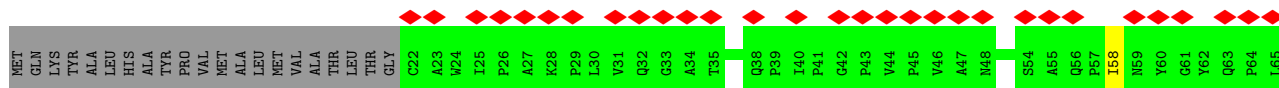
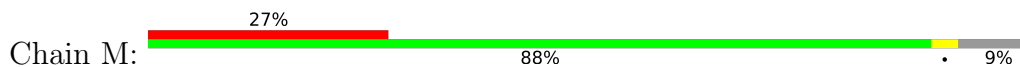




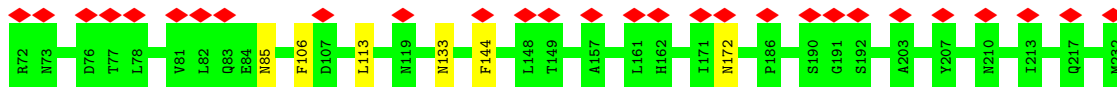
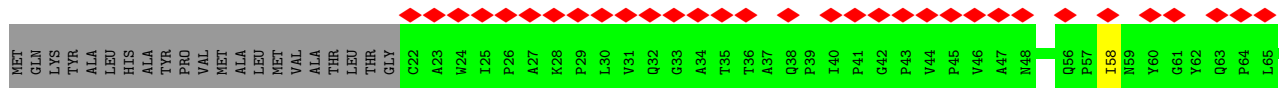
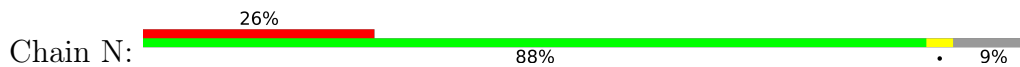
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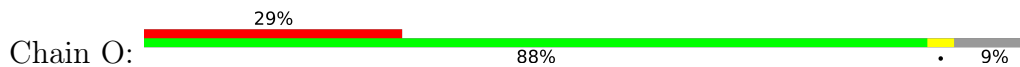
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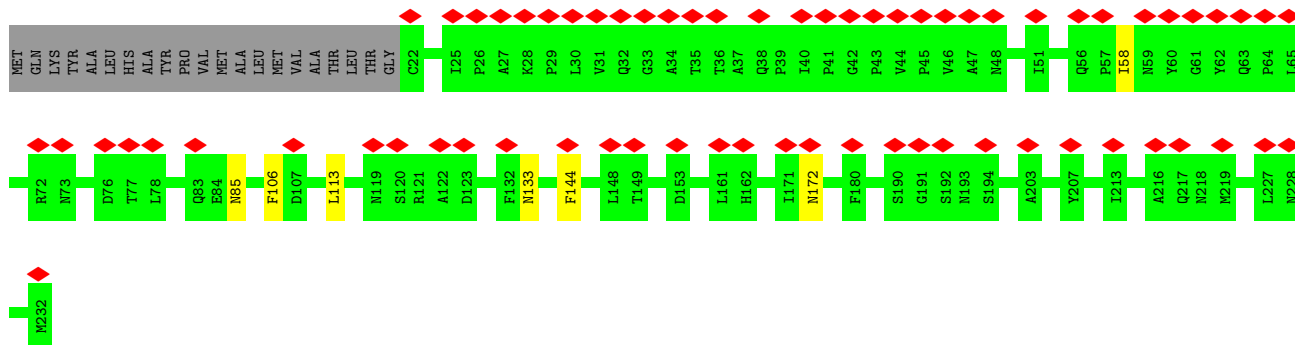


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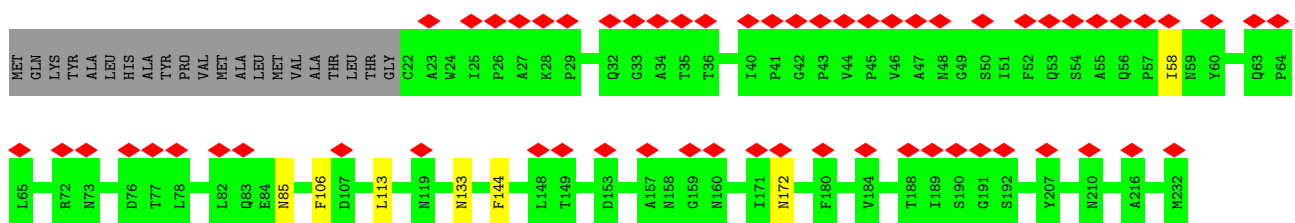
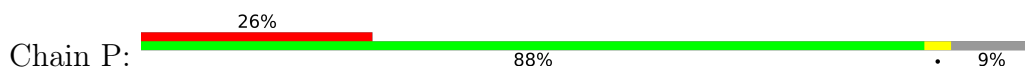


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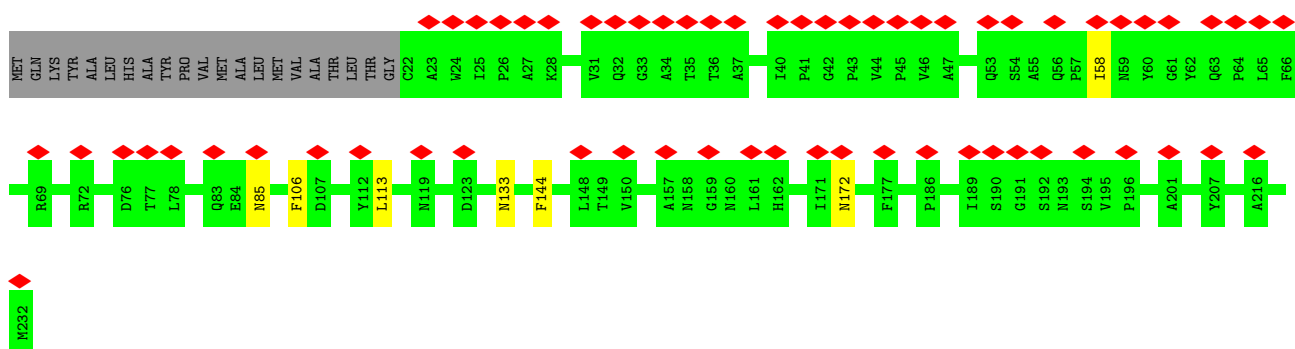
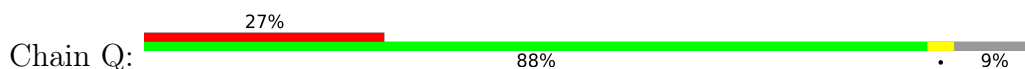




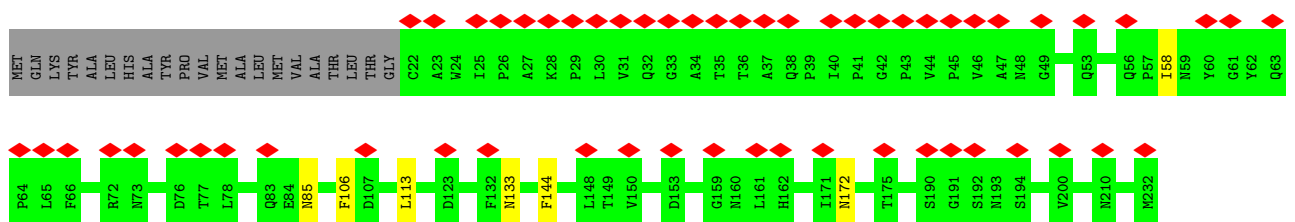
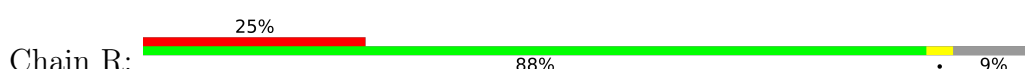
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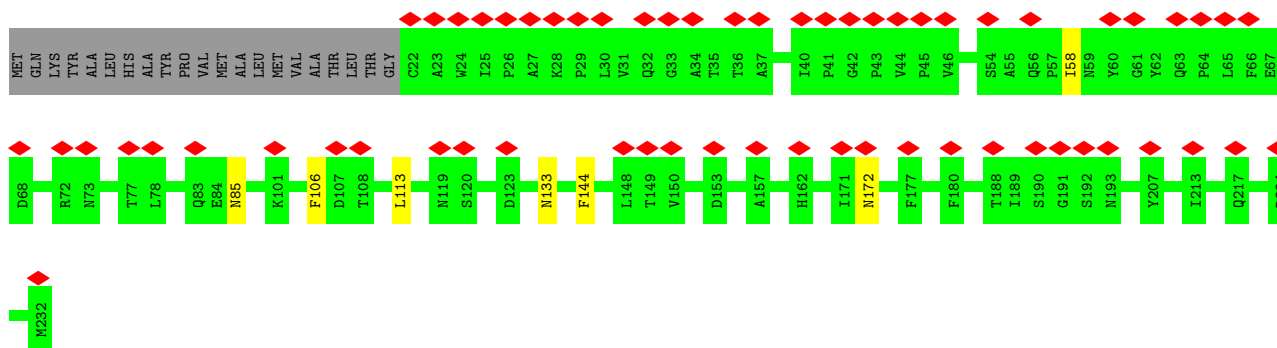
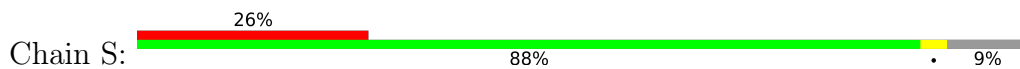
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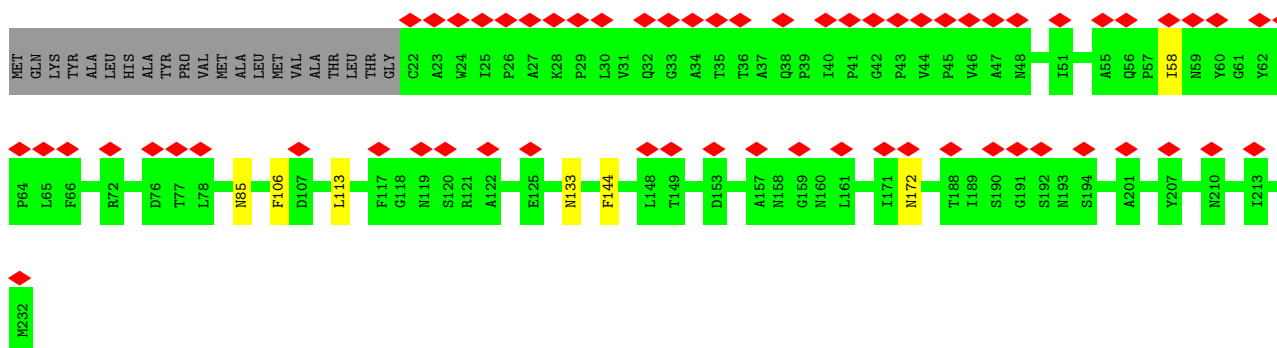
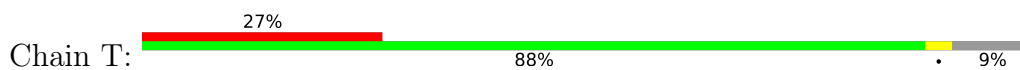
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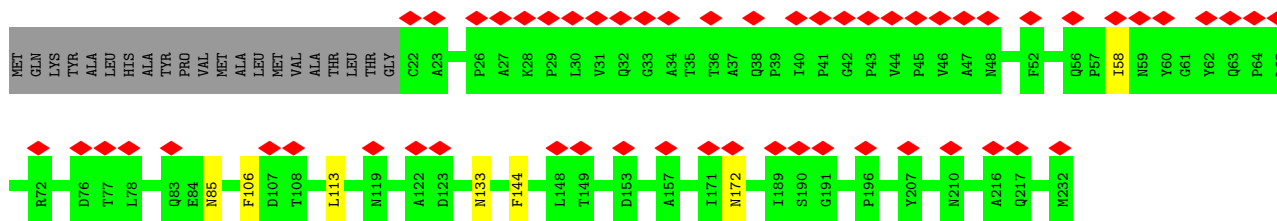
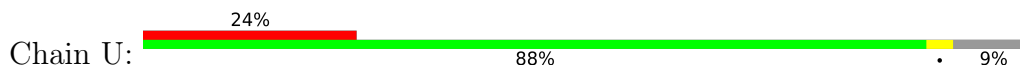
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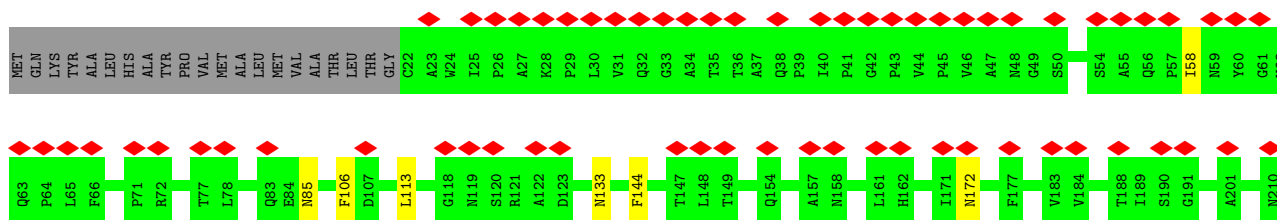
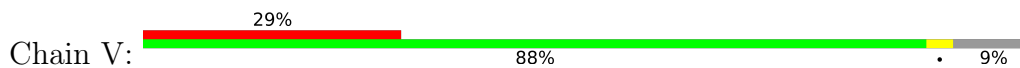
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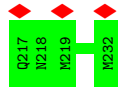


• Molecule 1: Flagellar L-ring protein

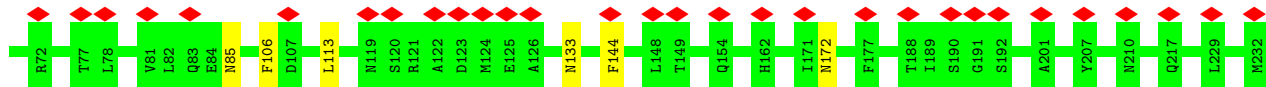
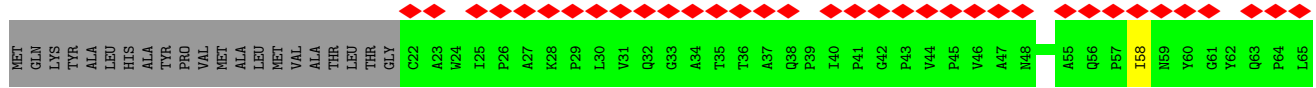
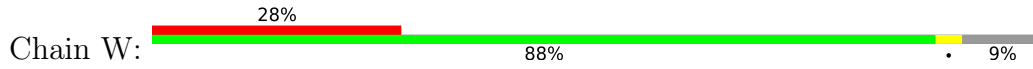


• Molecule 1: Flagellar L-ring protein

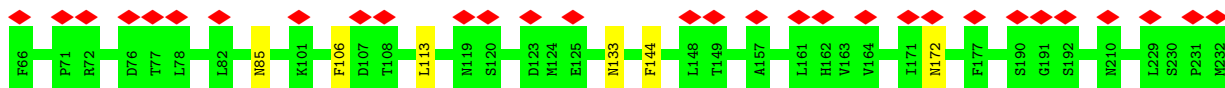
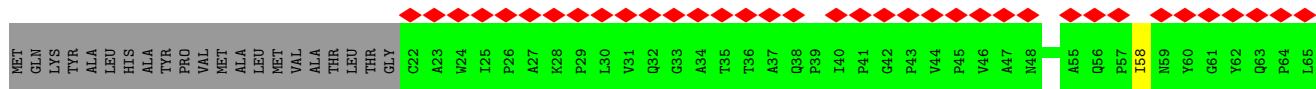
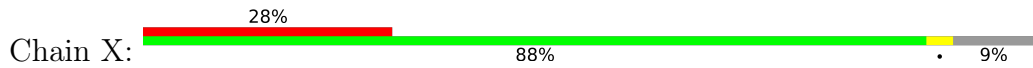




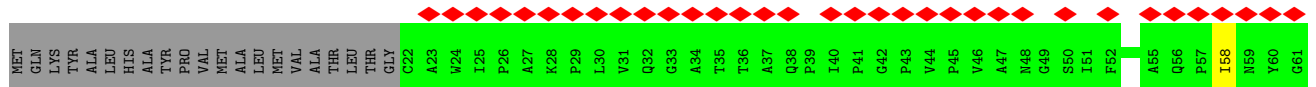
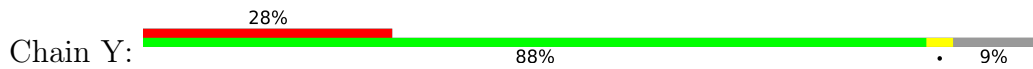
• Molecule 1: Flagellar L-ring protein



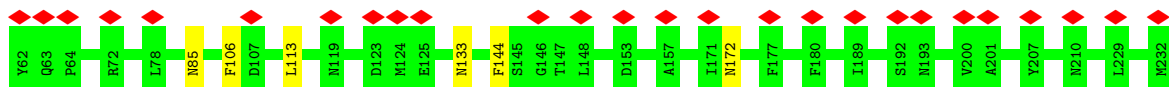
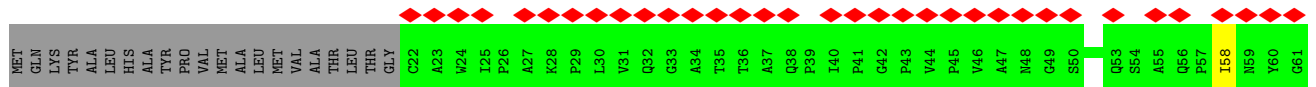
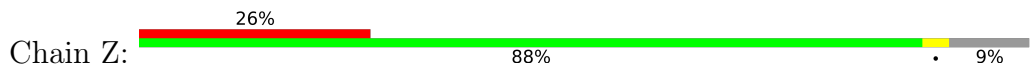
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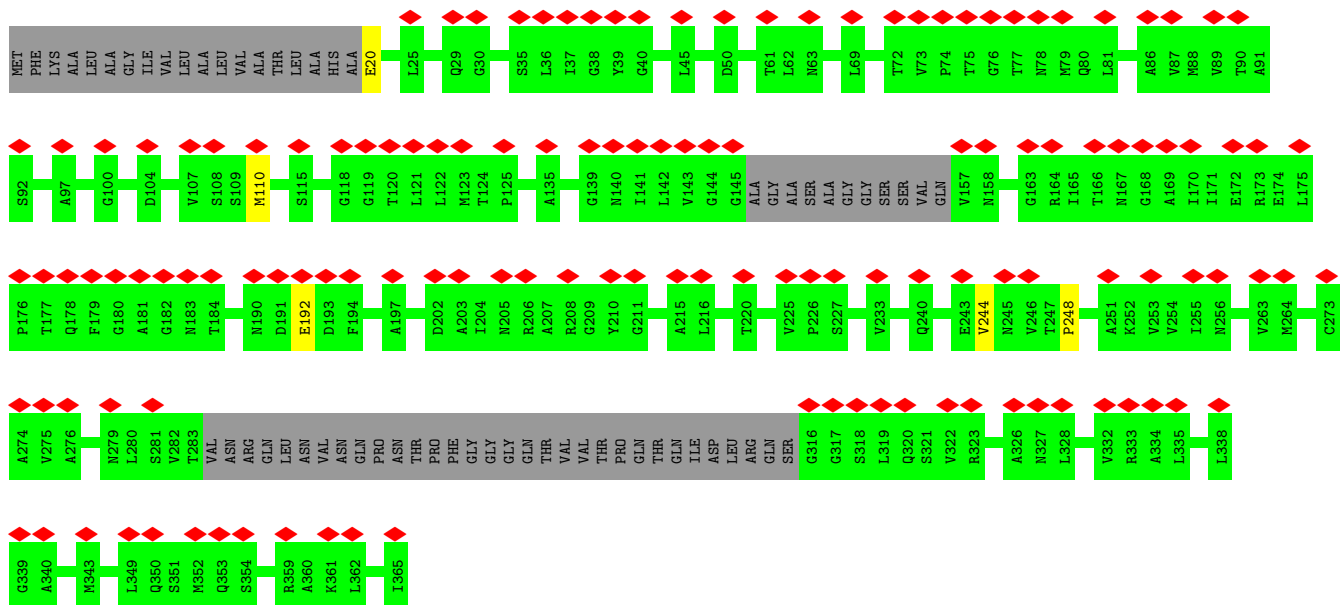
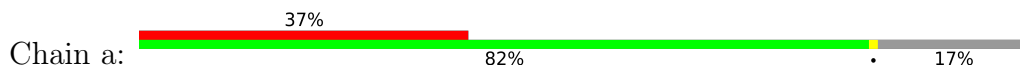
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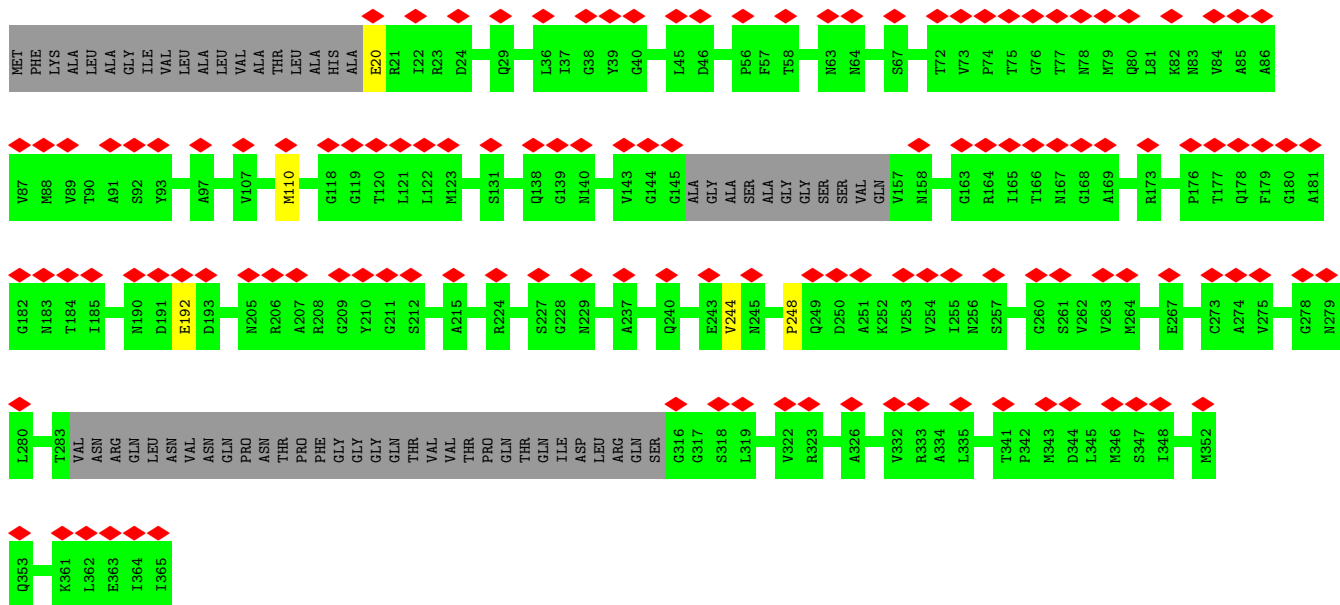
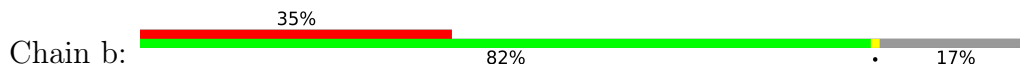
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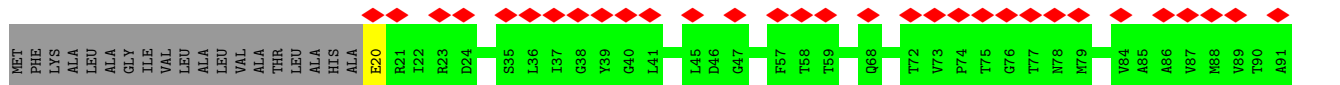
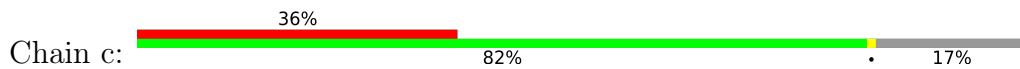
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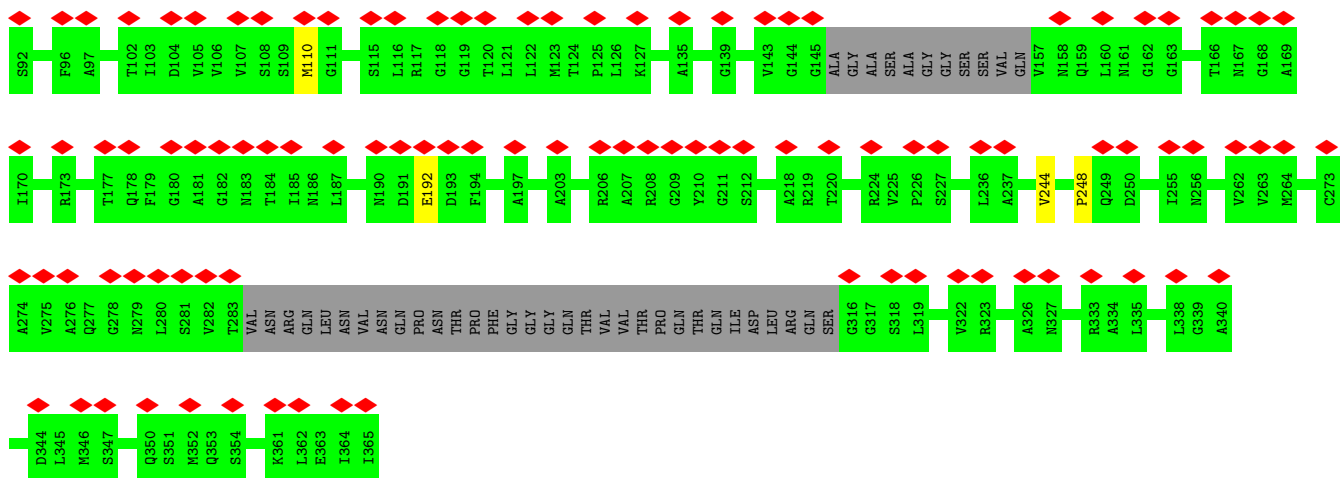


• Molecule 2: Flagellar P-ring protein

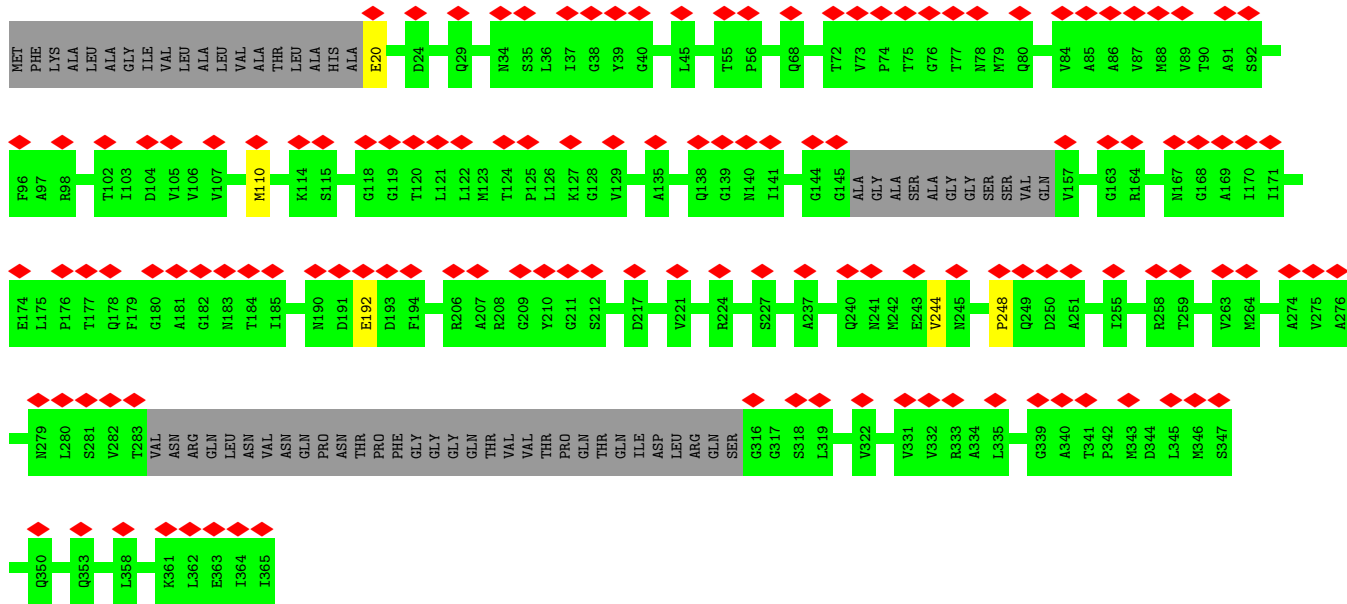
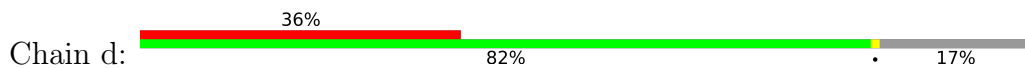


• Molecule 2: Flagellar P-ring protein

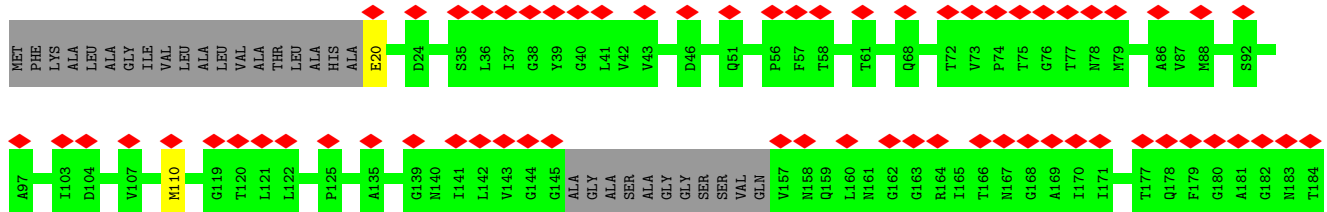
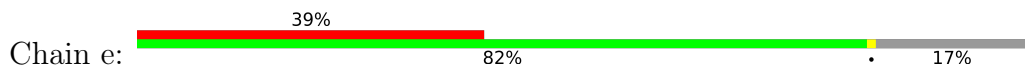


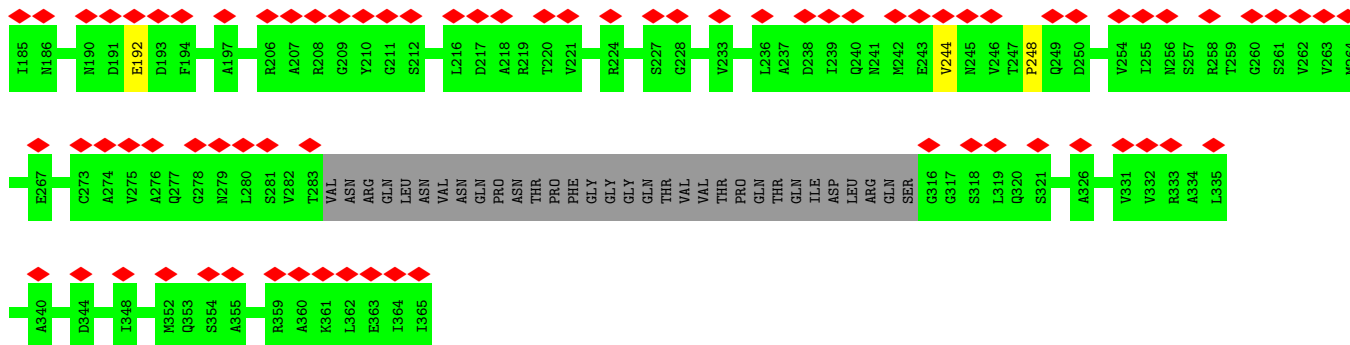


• Molecule 2: Flagellar P-ring protein

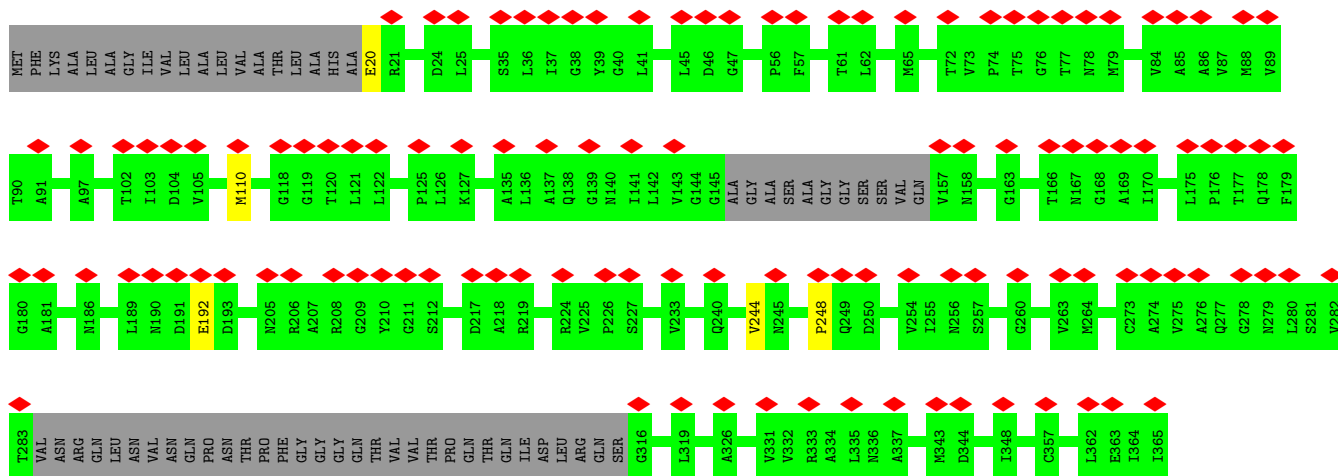
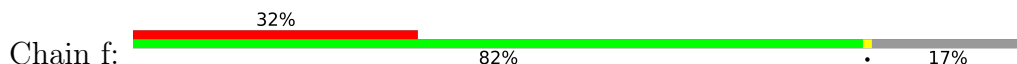


• Molecule 2: Flagellar P-ring protein

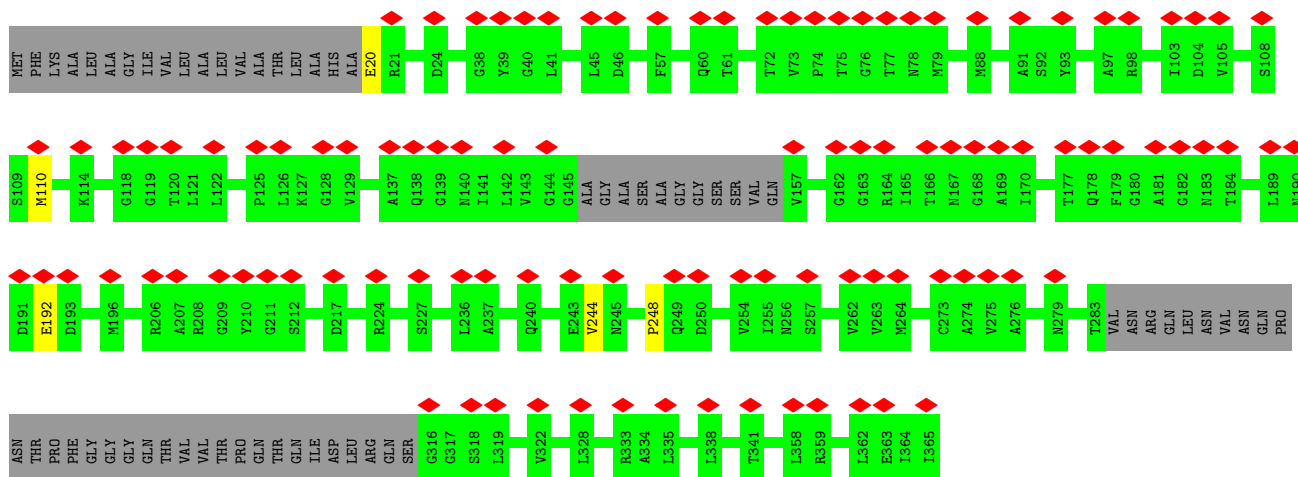
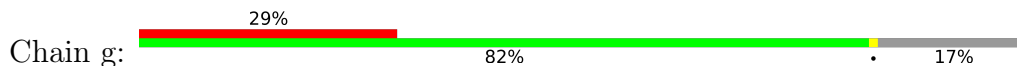




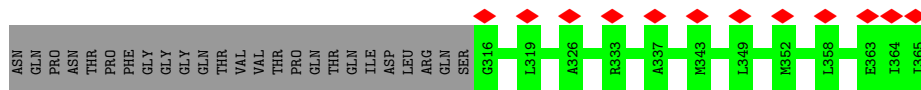
• Molecule 2: Flagellar P-ring protein



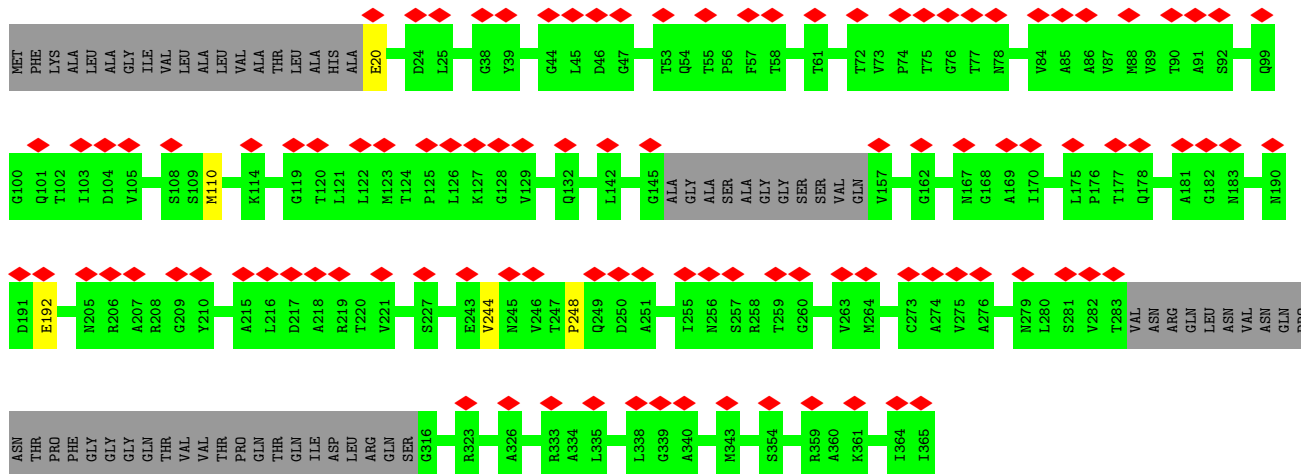
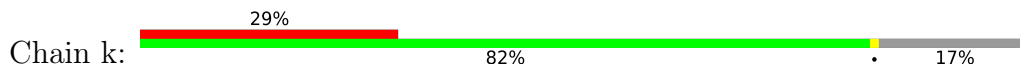
• Molecule 2: Flagellar P-ring protein



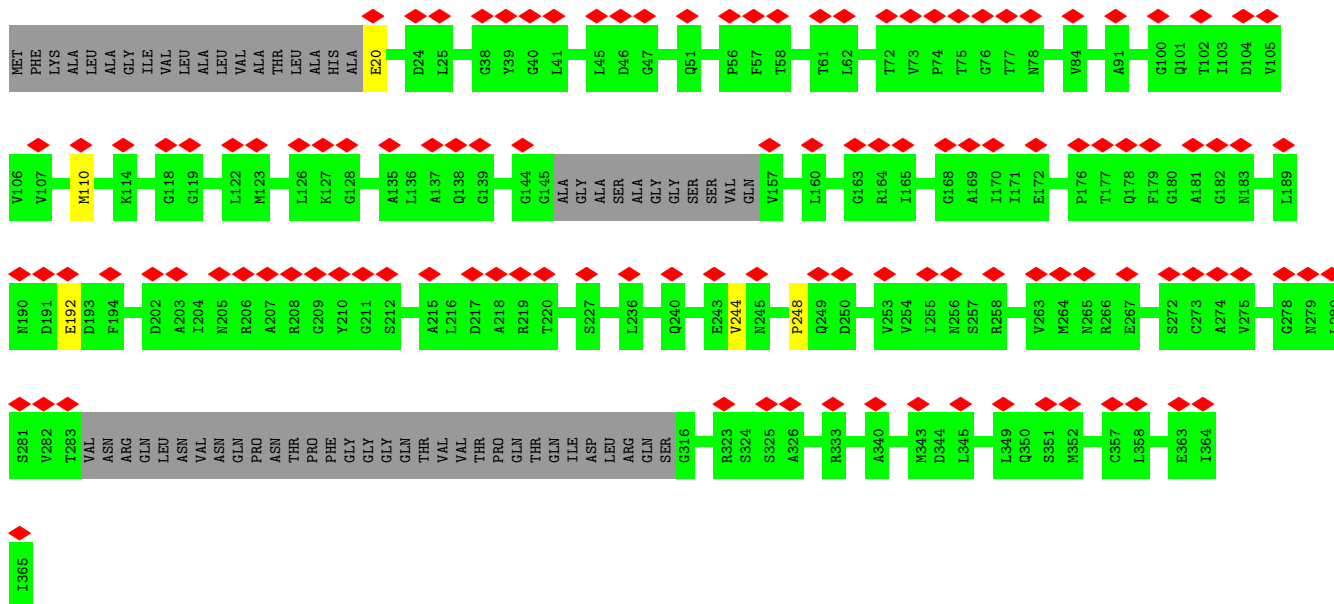
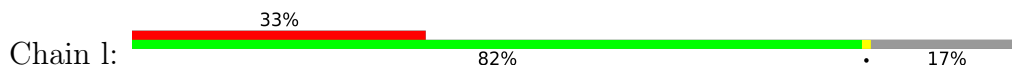
• Molecule 2: Flagellar P-ring protein



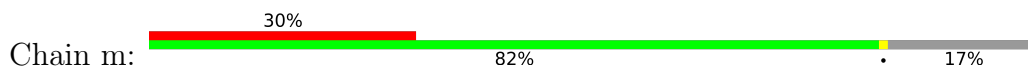
- Molecule 2: Flagellar P-ring protein

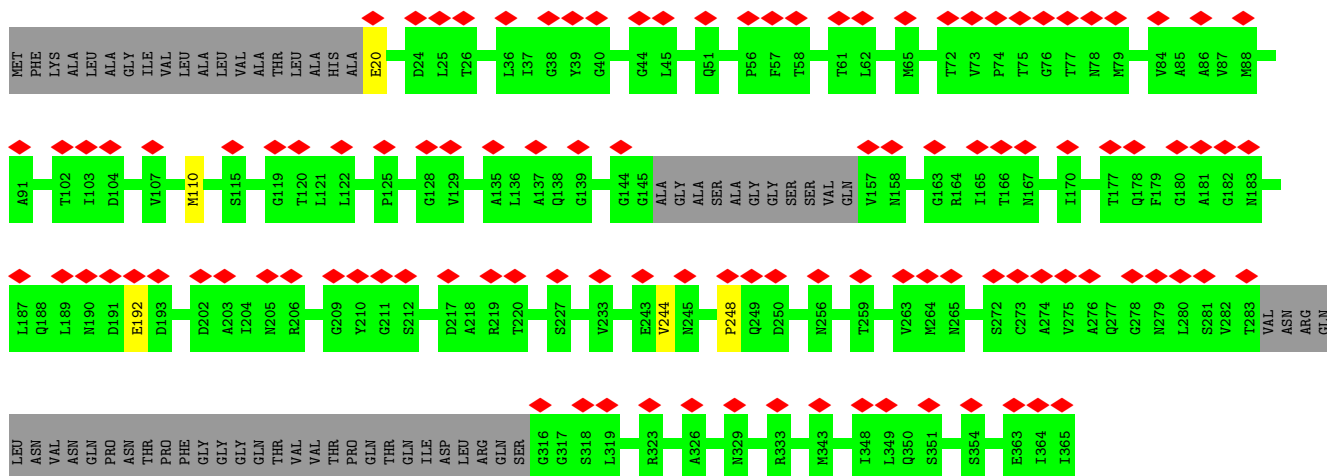


- Molecule 2: Flagellar P-ring protein

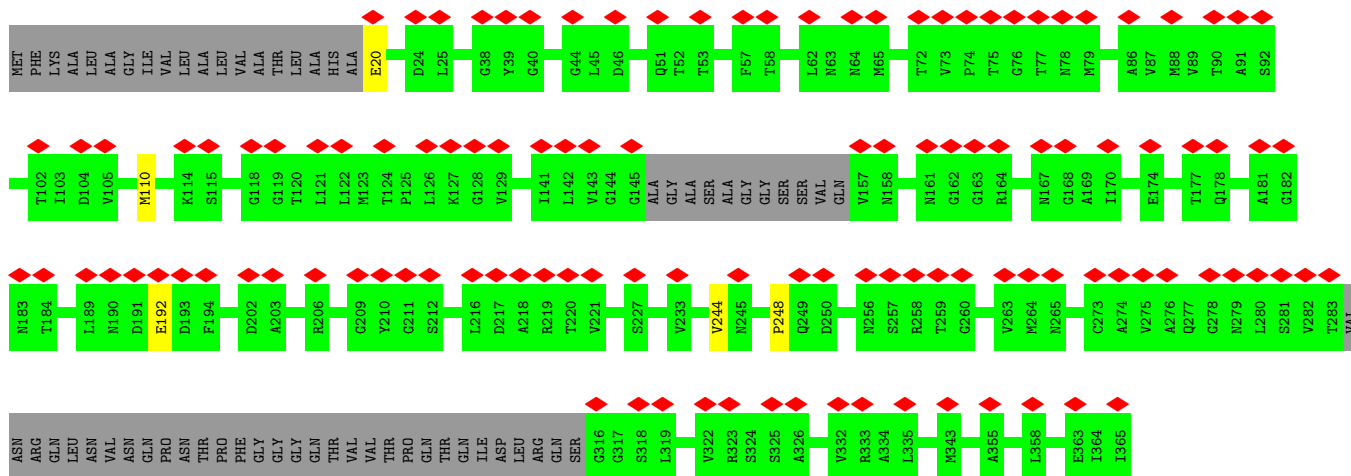
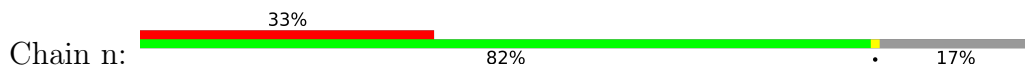


- Molecule 2: Flagellar P-ring protein

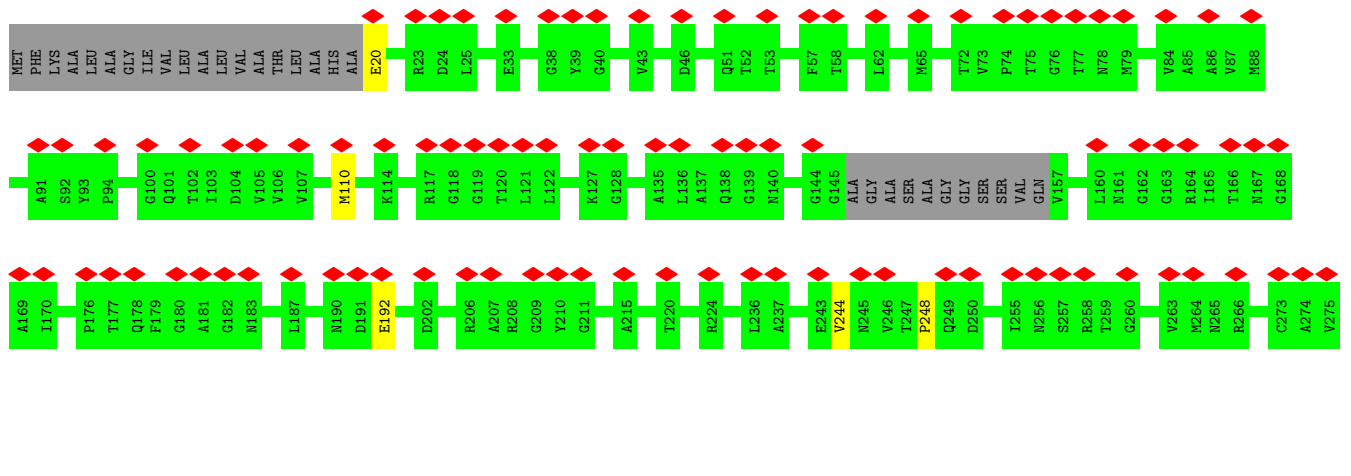
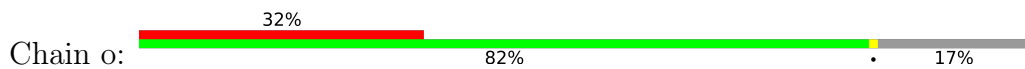


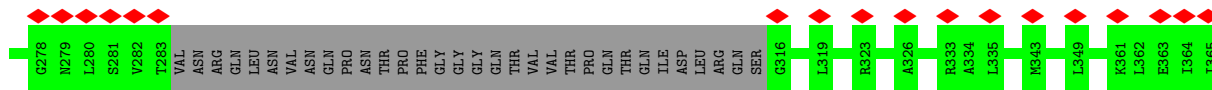


• Molecule 2: Flagellar P-ring protein

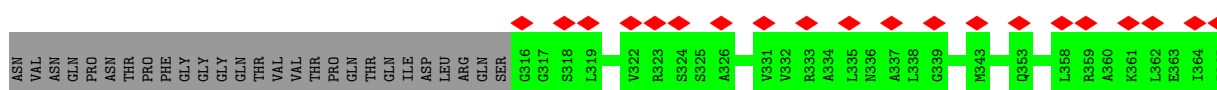
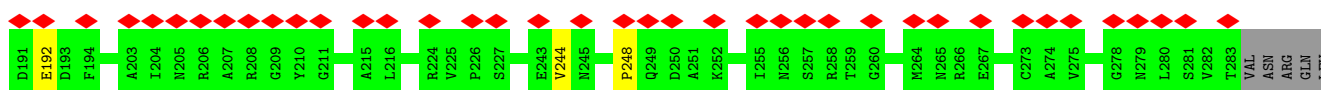
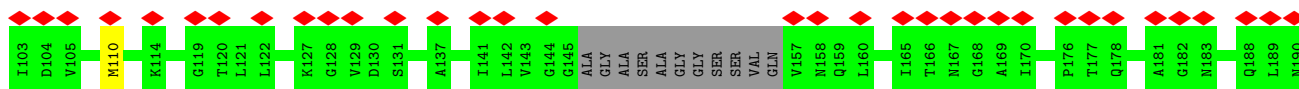
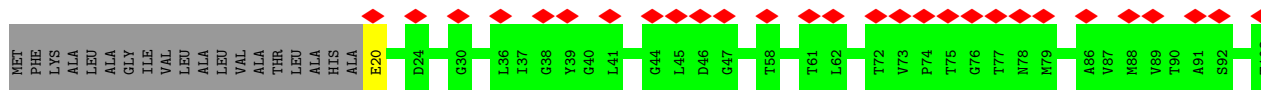
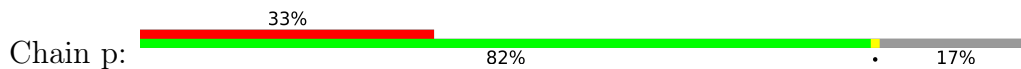


• Molecule 2: Flagellar P-ring protein

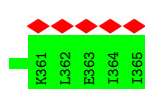
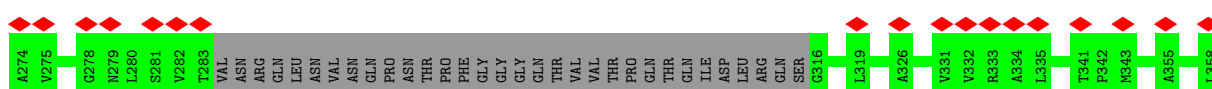
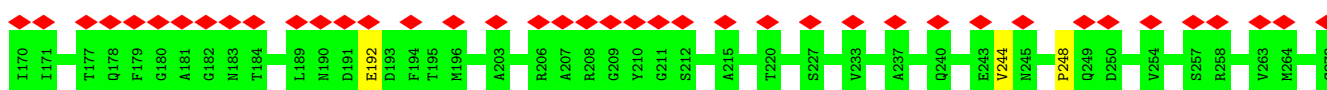
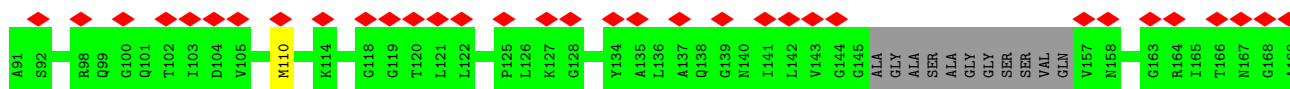
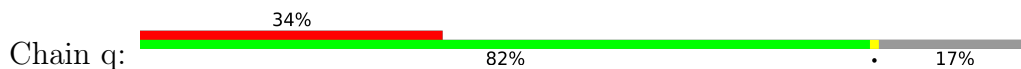




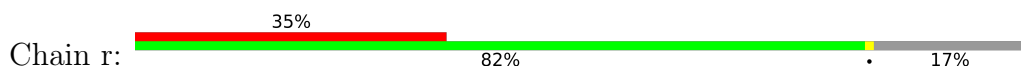
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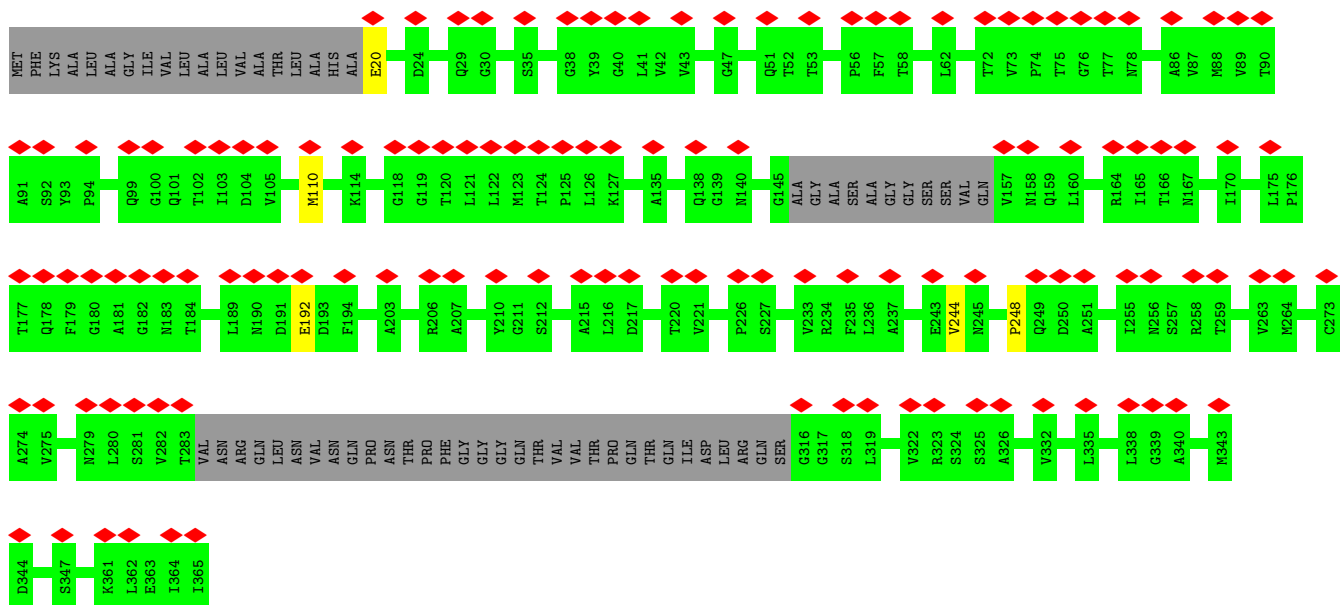


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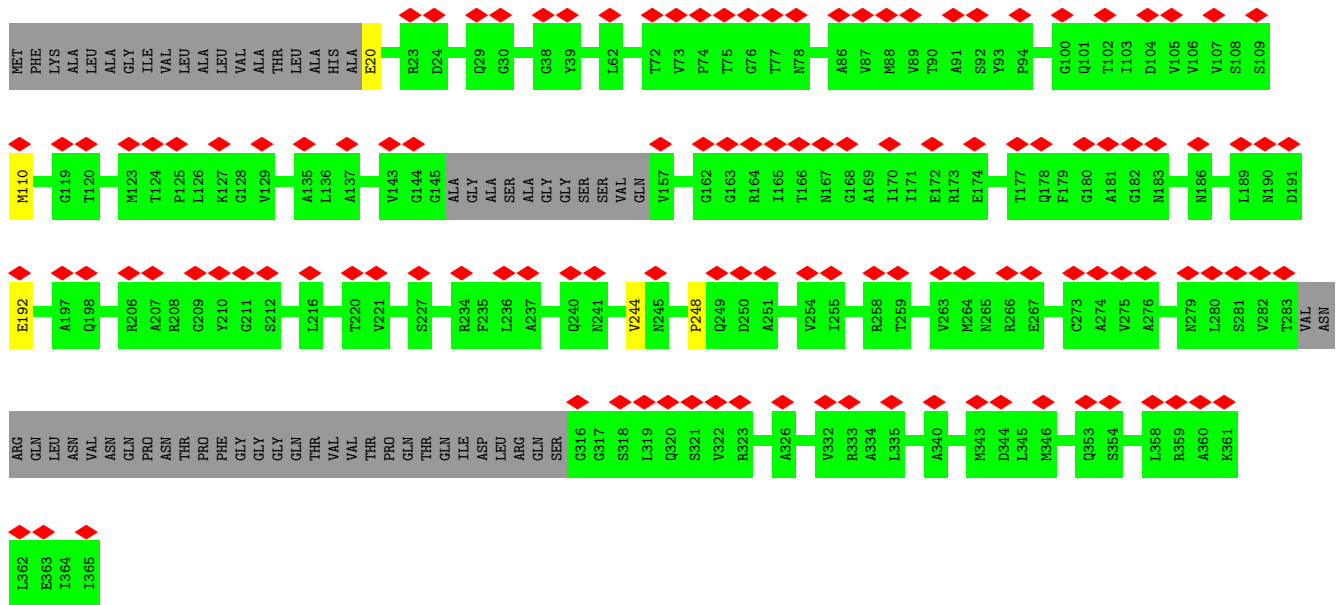
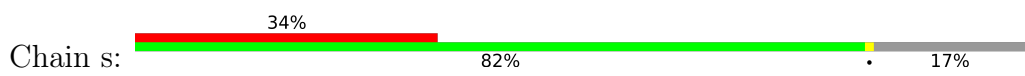


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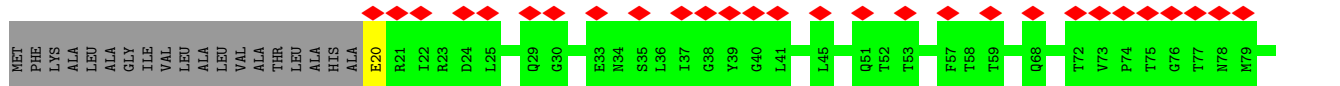
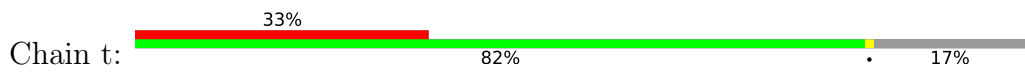


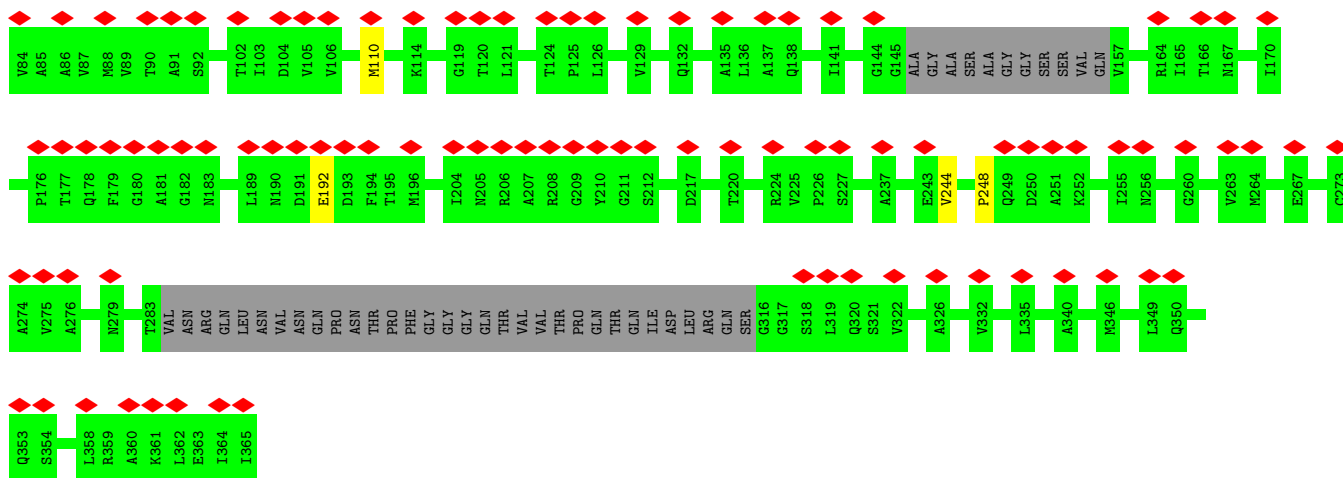


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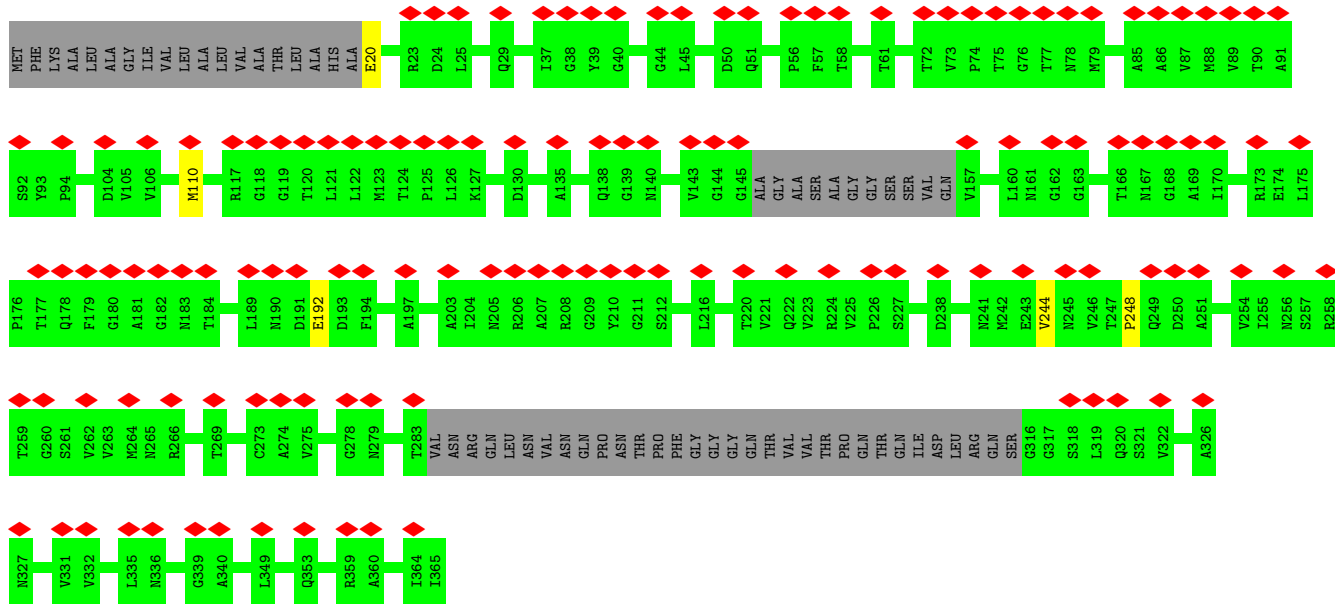
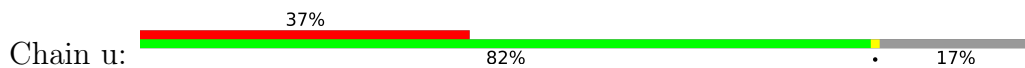


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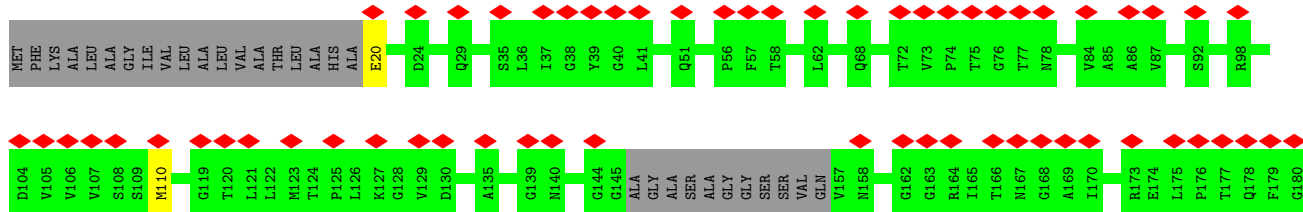
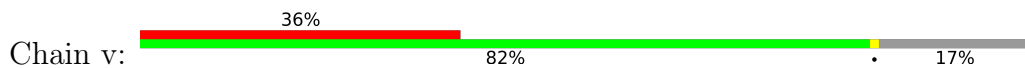


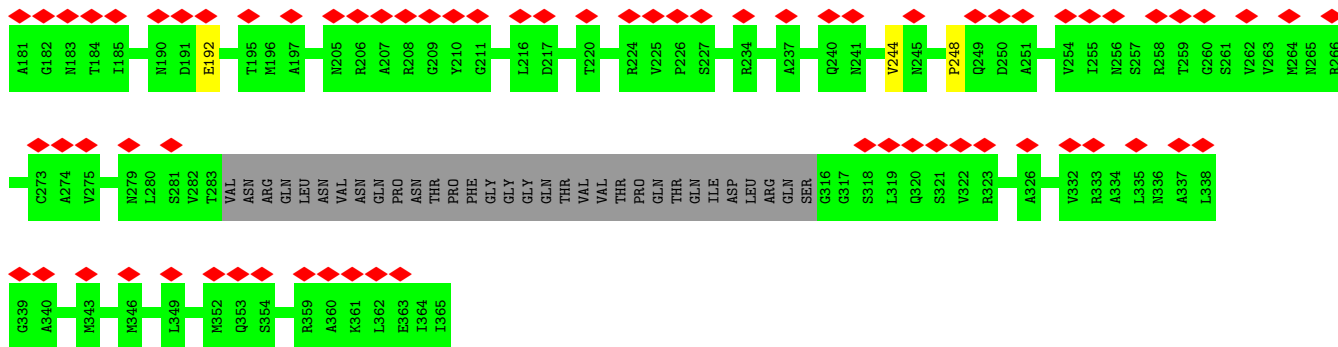


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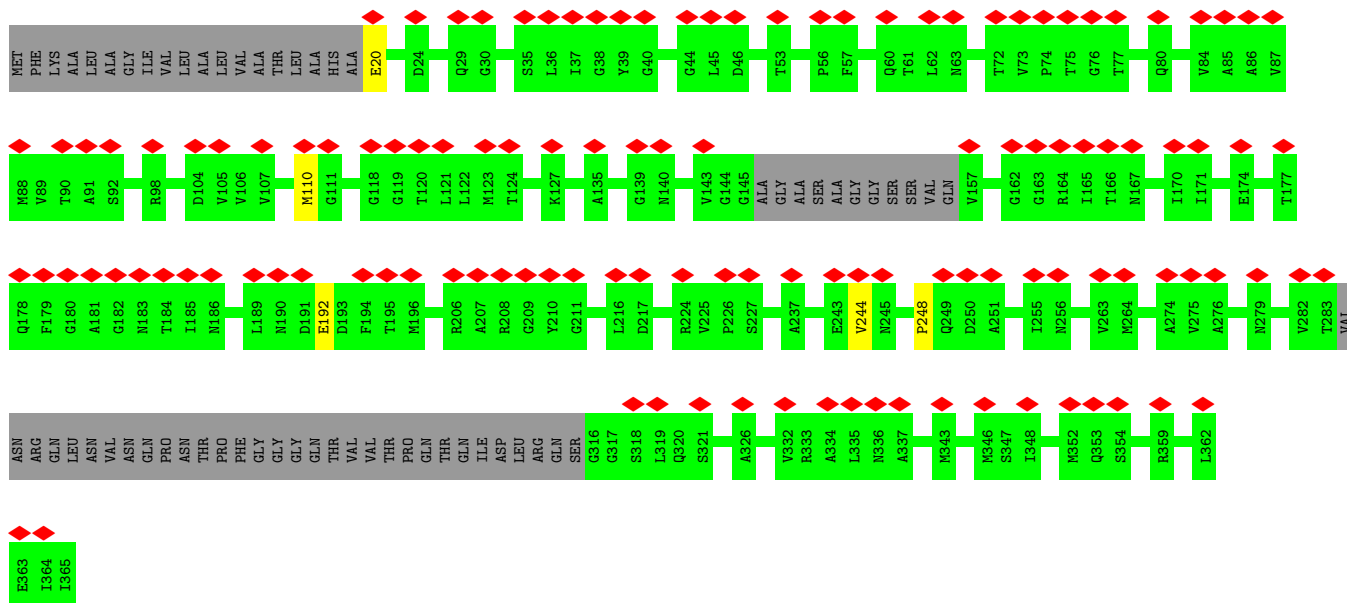
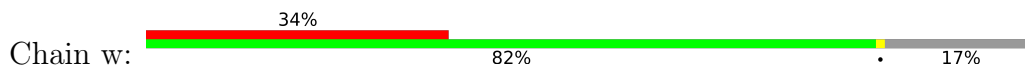


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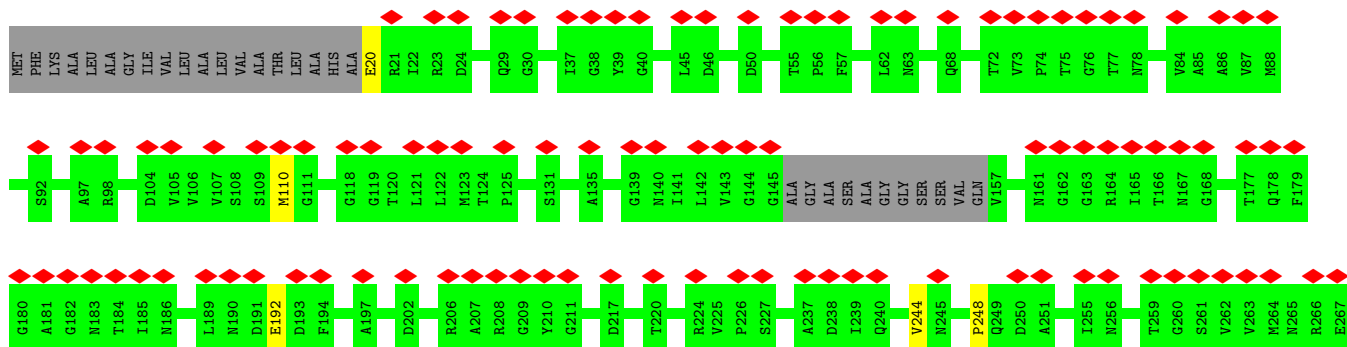
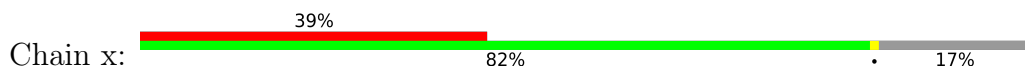


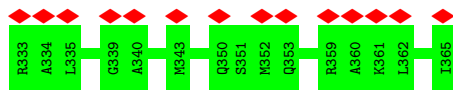


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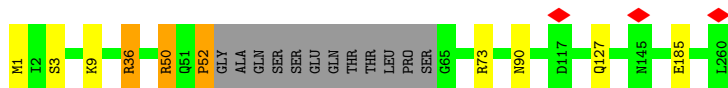
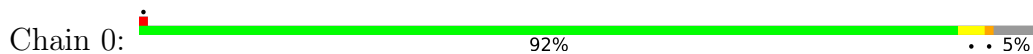


• Molecule 2: Flagellar P-ring protein

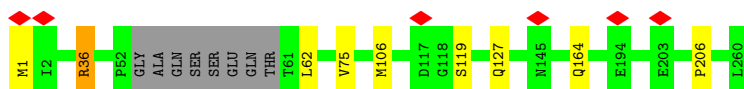




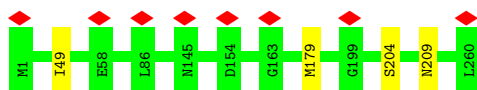
- Molecule 3: Flagellar basal-body rod protein FlgG



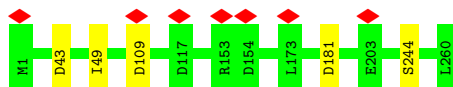
- Molecule 3: Flagellar basal-body rod protein FlgG



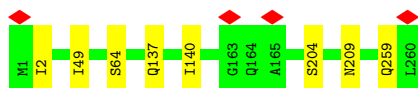
- Molecule 3: Flagellar basal-body rod protein FlgG



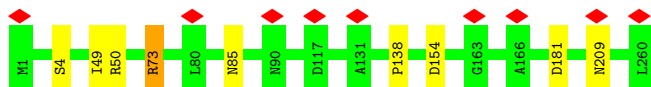
- Molecule 3: Flagellar basal-body rod protein FlgG



- Molecule 3: Flagellar basal-body rod protein FlgG

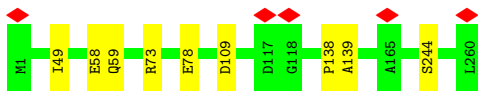


- Molecule 3: Flagellar basal-body rod protein FlgG



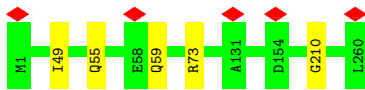
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain 6:  97%



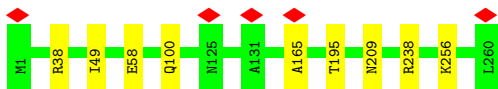
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 7:  98%



• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 8:  97%



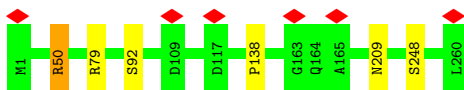
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain 9:  98%



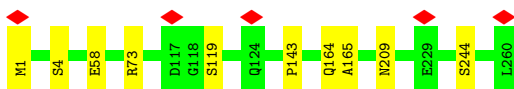
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZA:  98%



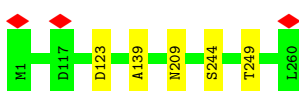
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZB:  96%



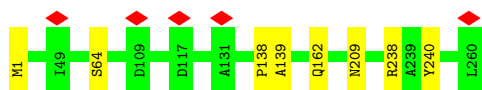
• Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZC:  98%



- Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZD:  97%



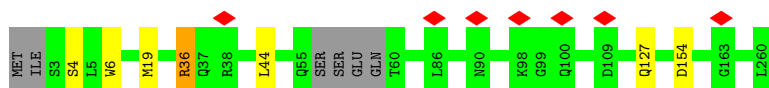
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain ZE:  97%



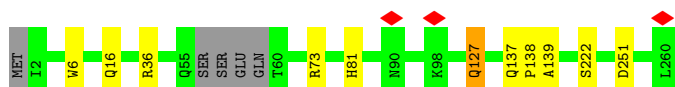
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AF:  95%



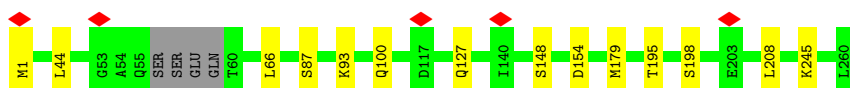
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AG:  94%

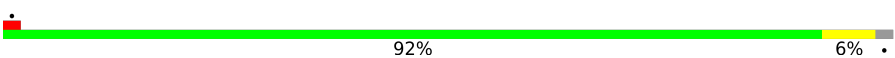


- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AH:  93% 5%



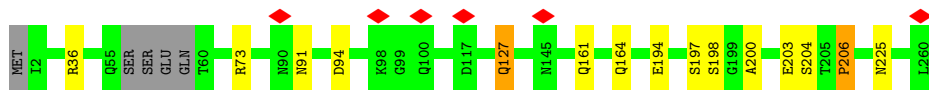
- Molecule 3: Flagellar basal-body rod protein FlgG

Chain AI:  92% 6%

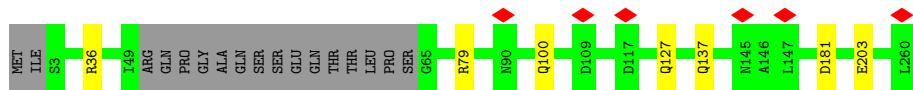


- Molecule 3: Flagellar basal-body rod protein FlgG

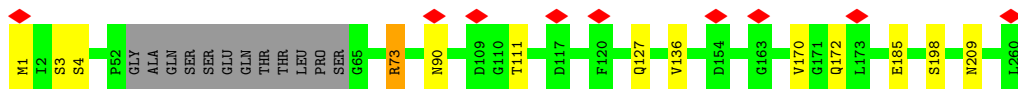
Chain AJ:  92% 5%



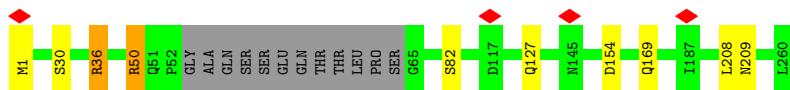
• Molecule 3: Flagellar basal-body rod protein FlgG



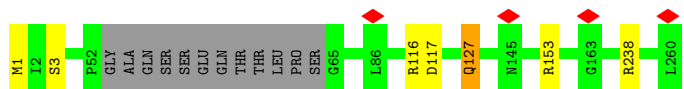
• Molecule 3: Flagellar basal-body rod protein FlgG



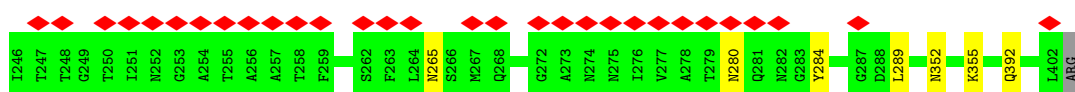
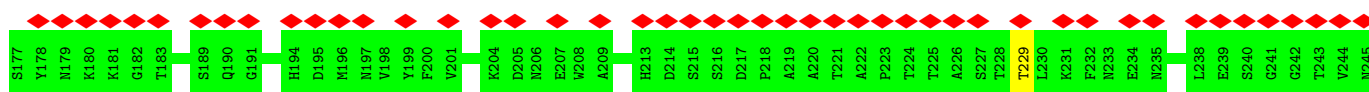
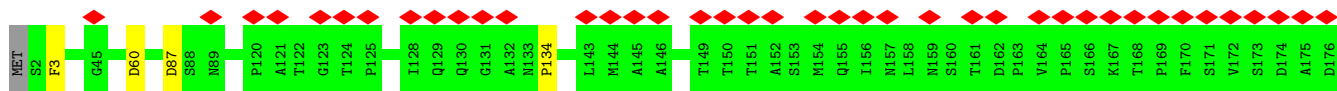
• Molecule 3: Flagellar basal-body rod protein FlgG



• Molecule 3: Flagellar basal-body rod protein FlgG



• Molecule 4: Flagellar hook protein FlgE



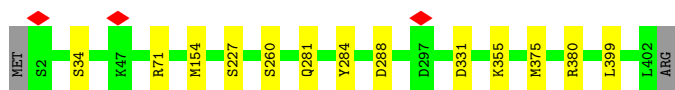
• Molecule 4: Flagellar hook protein FlgE

Chain ZG:  95%



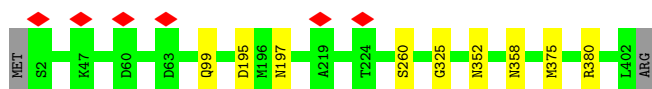
• Molecule 4: Flagellar hook protein FlgE

Chain ZH:  96%



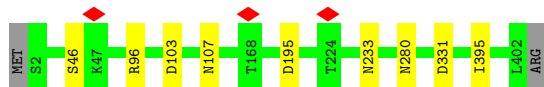
• Molecule 4: Flagellar hook protein FlgE

Chain ZI:  97%



• Molecule 4: Flagellar hook protein FlgE

Chain ZJ:  97%



• Molecule 4: Flagellar hook protein FlgE

Chain ZK:  98%



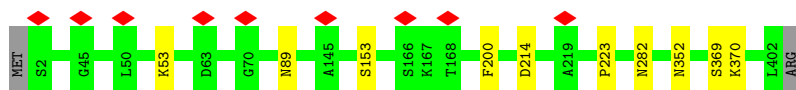
• Molecule 4: Flagellar hook protein FlgE

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%



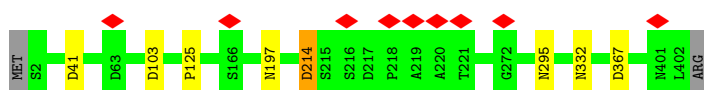
- Molecule 4: Flagellar hook protein FlgE

Chain ZQ:  97%



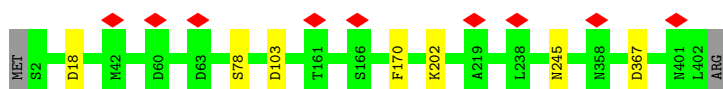
- Molecule 4: Flagellar hook protein FlgE

Chain ZR:  98%



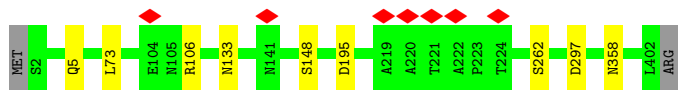
- Molecule 4: Flagellar hook protein FlgE

Chain ZS:  98%

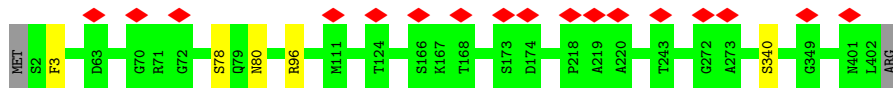


- Molecule 4: Flagellar hook protein FlgE

Chain ZT:  97%



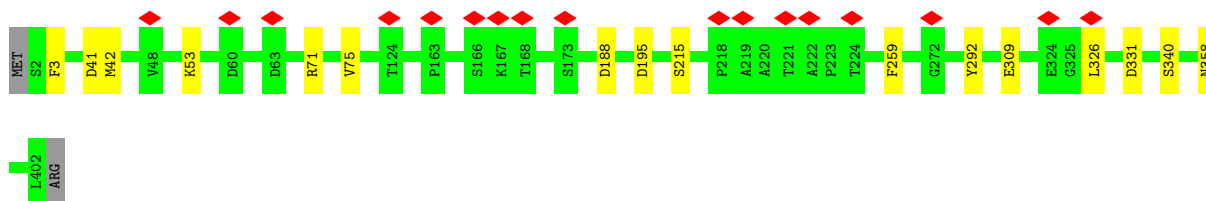
- Molecule 4: Flagellar hook protein FlgE



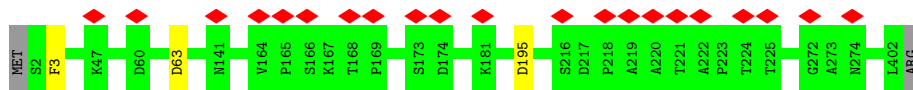
- Molecule 4: Flagellar hook protein FlgE



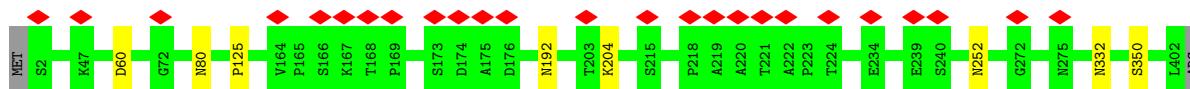
- Molecule 4: Flagellar hook protein FlgE



- Molecule 4: Flagellar hook protein FlgE

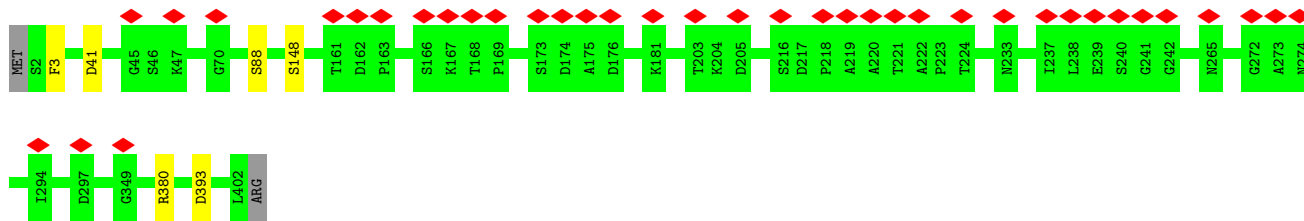


- Molecule 4: Flagellar hook protein FlgE

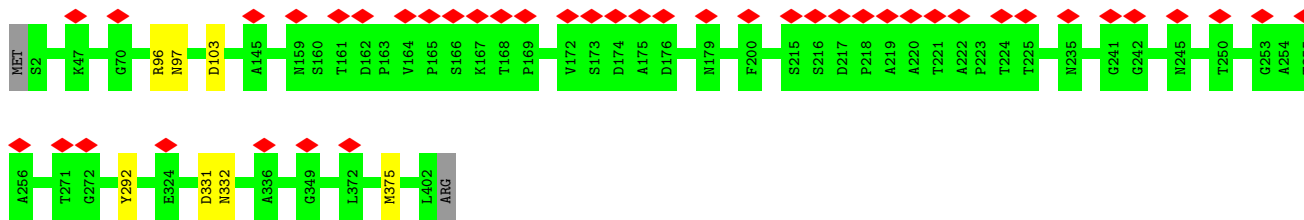


- Molecule 4: Flagellar hook protein FlgE

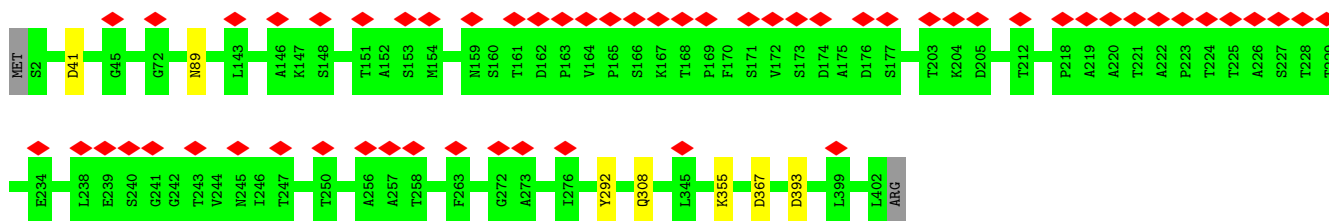




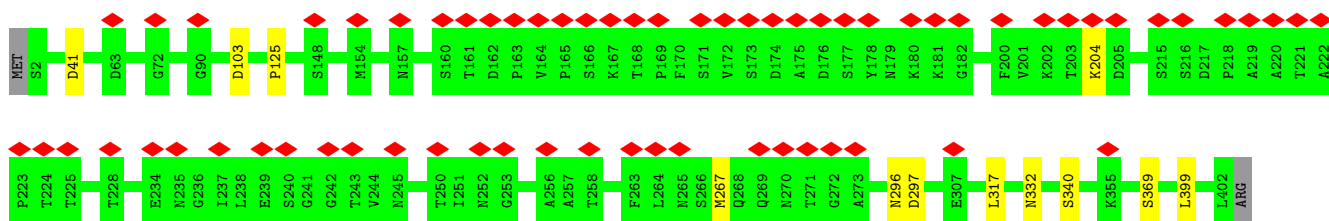
• Molecule 4: Flagellar hook protein FlgE



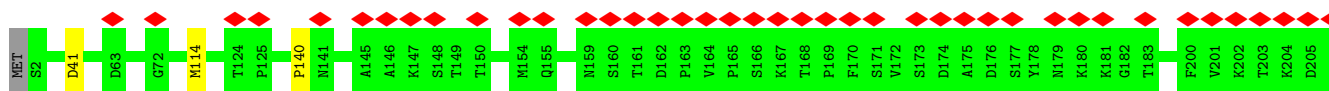
• Molecule 4: Flagellar hook protein FlgE



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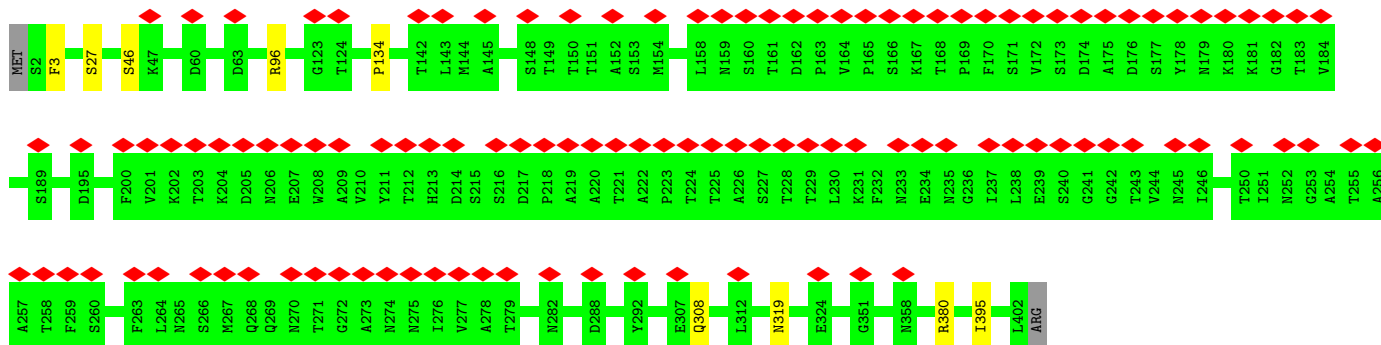


• Molecule 4: Flagellar hook protein FlgE

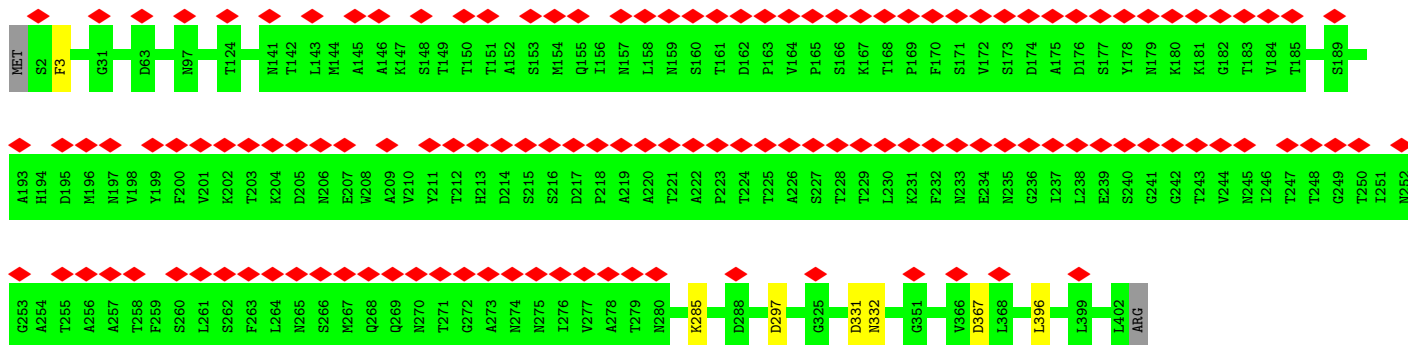




• Molecule 4: Flagellar hook protein FlgE



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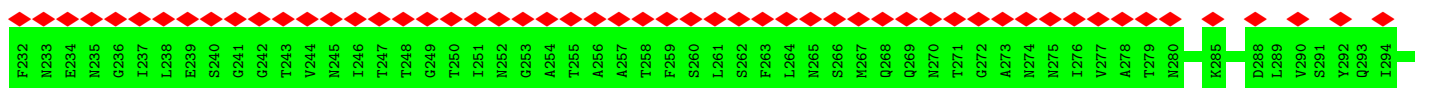
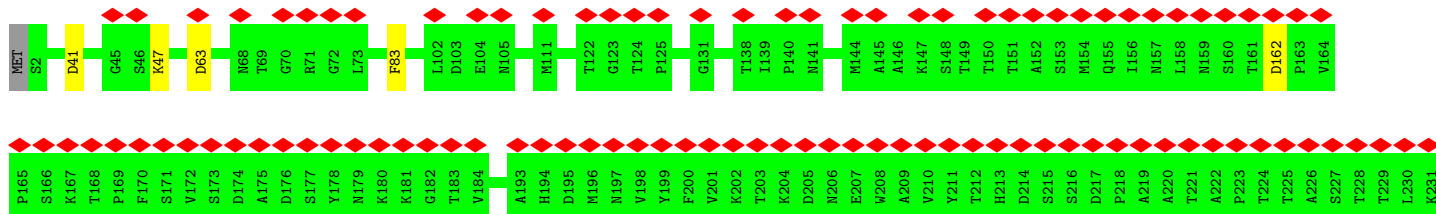
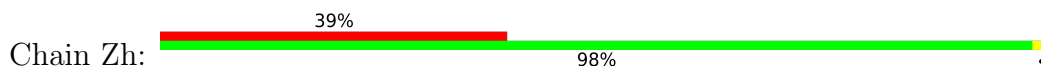


• Molecule 4: Flagellar hook protein FlgE

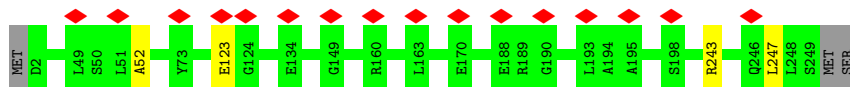




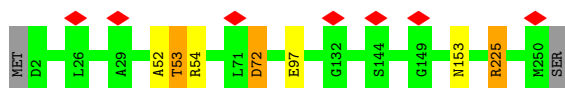
- Molecule 4: Flagellar hook protein FlgE



- Molecule 5: Flagellar basal-body rod protein FlgF



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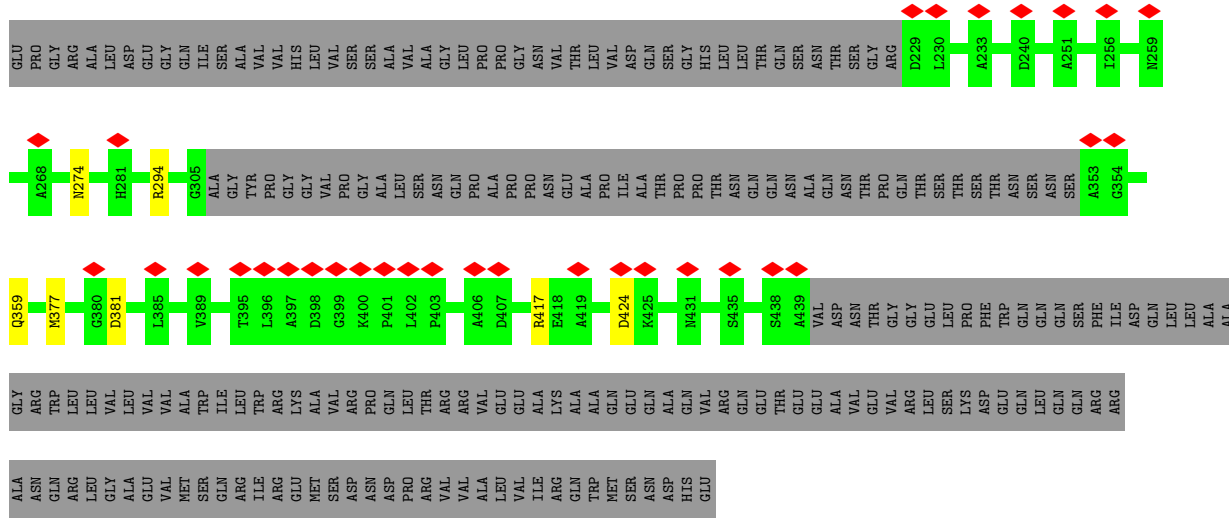


- Molecule 5: Flagellar basal-body rod protein FlgF

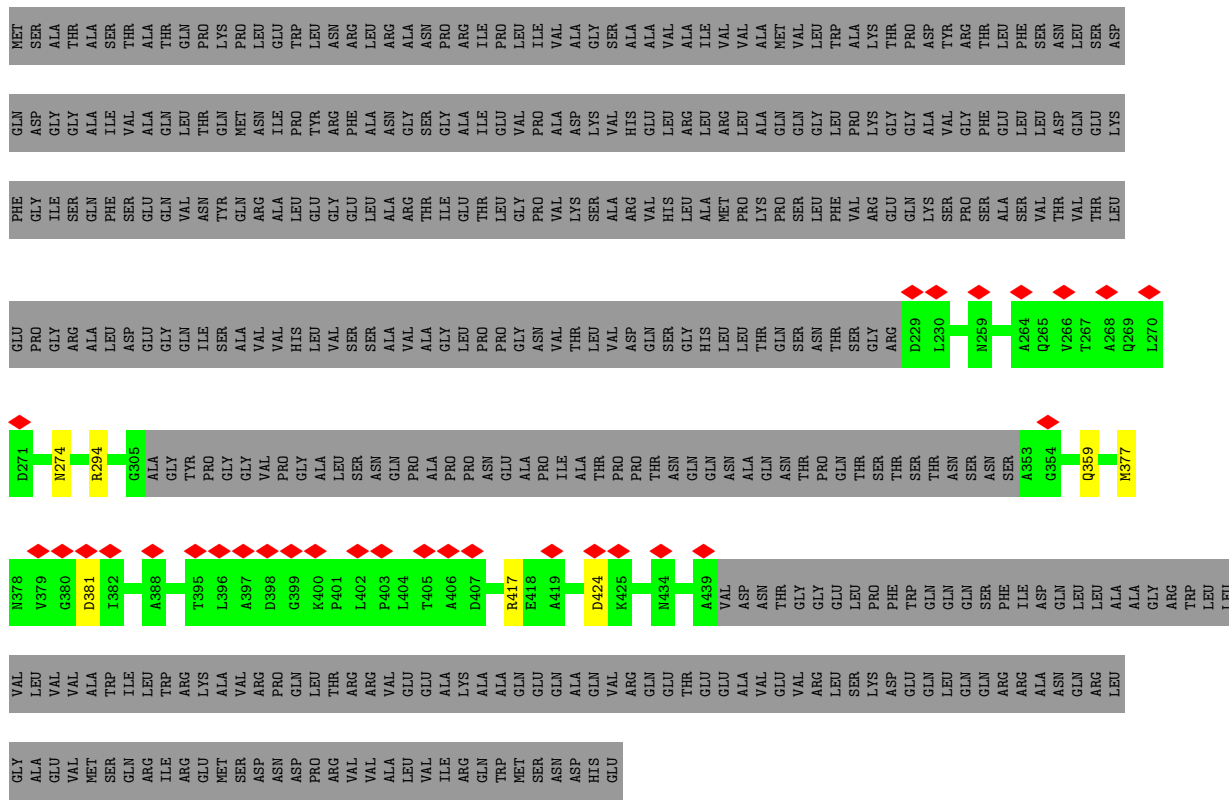


- Molecule 5: Flagellar basal-body rod protein FlgF



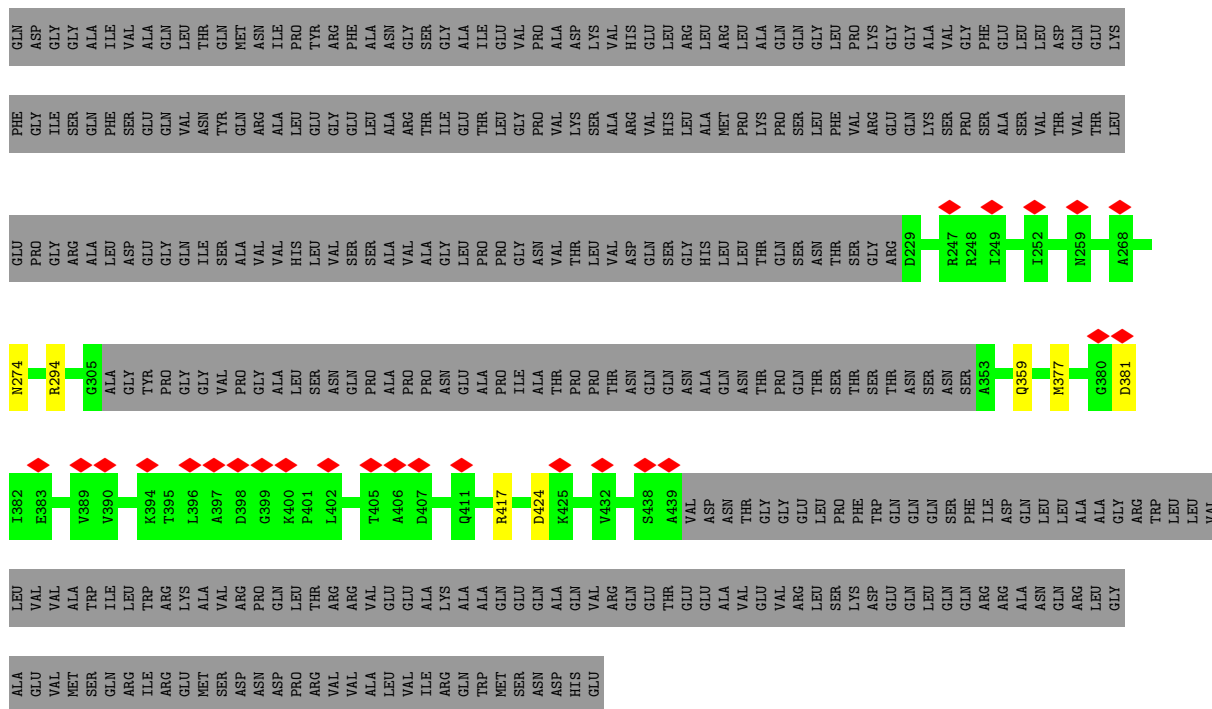


• Molecule 6: Flagellar M-ring protein

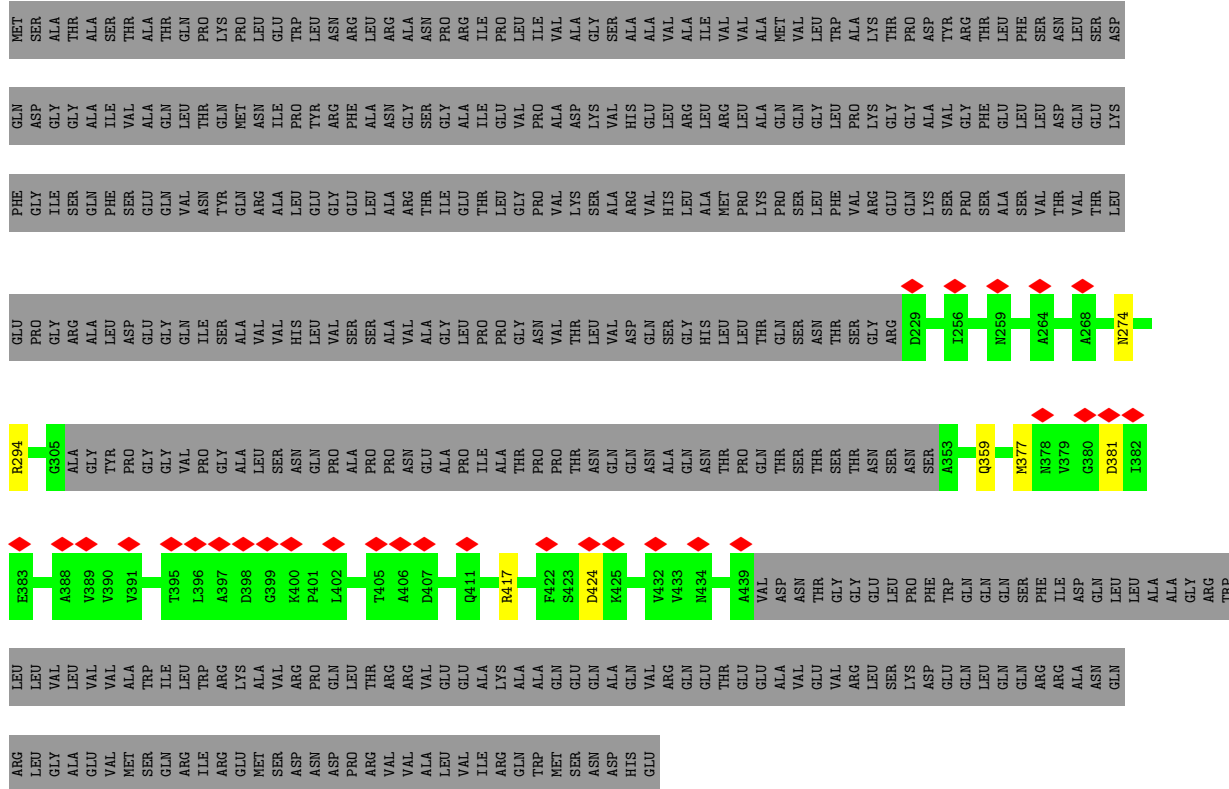


• Molecule 6: Flagellar M-ring protein

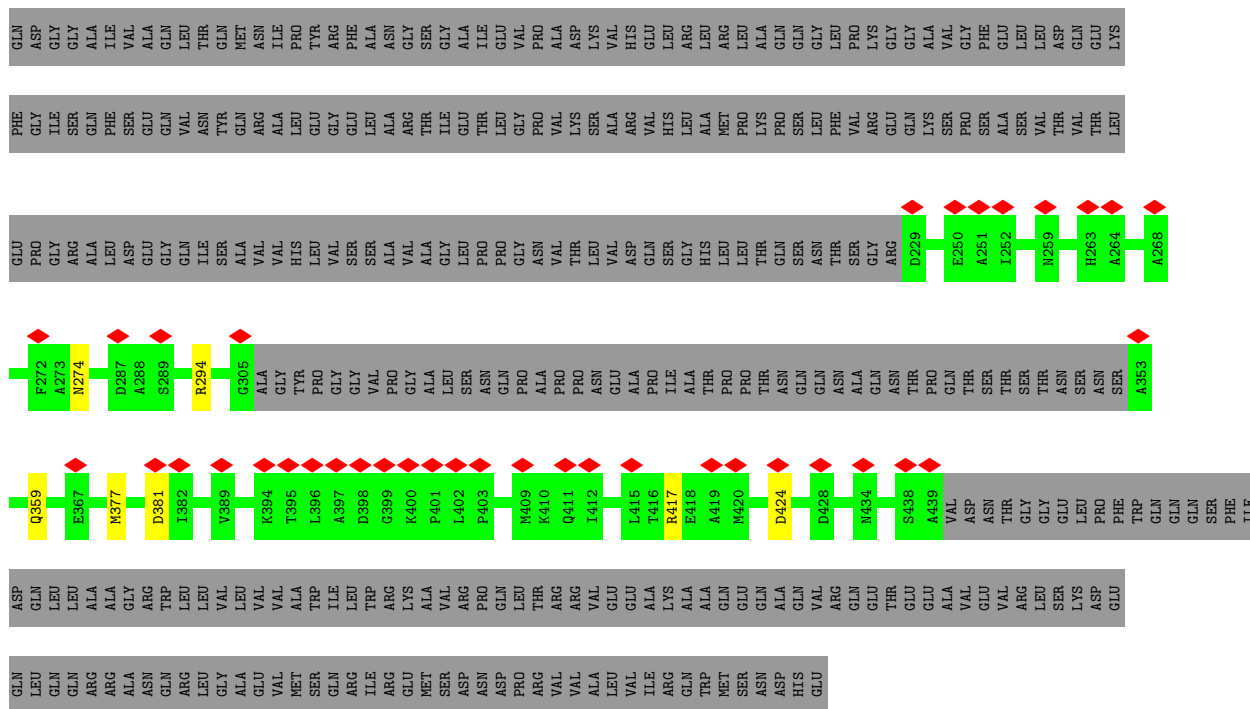




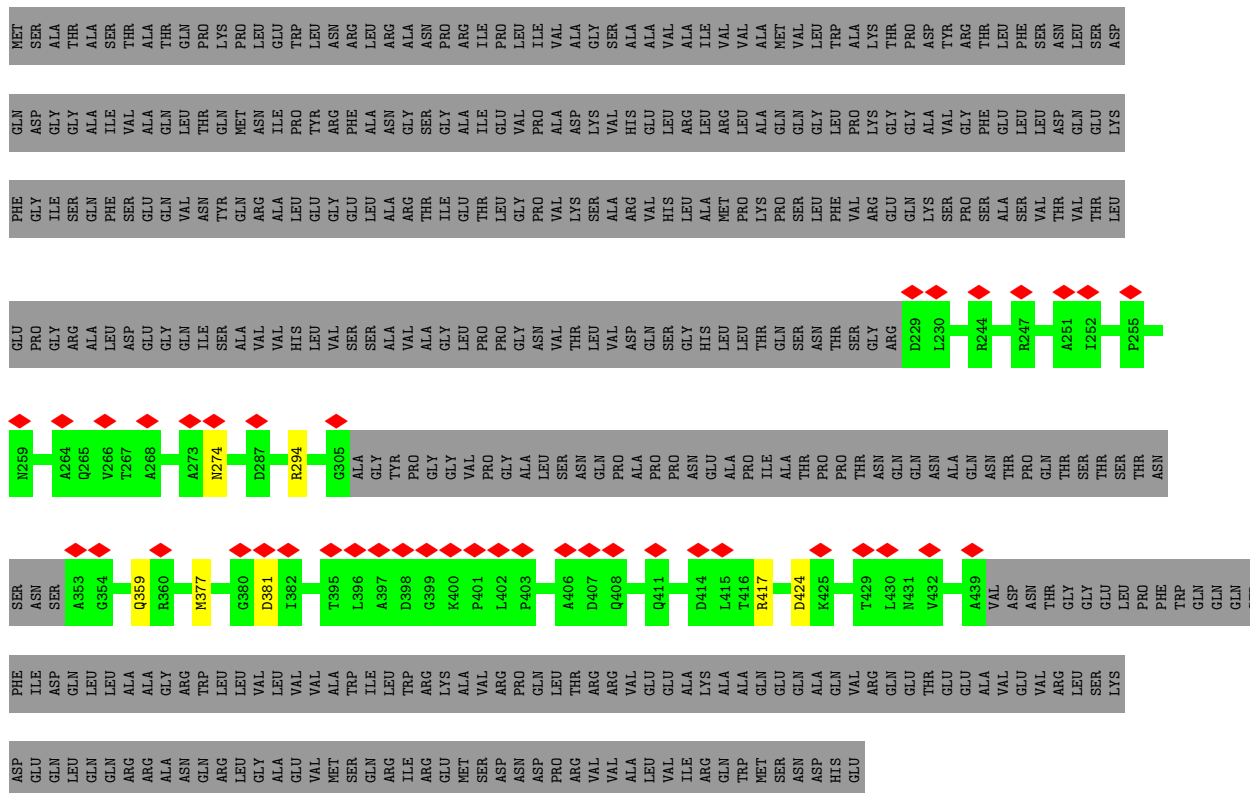
• Molecule 6: Flagellar M-ring protein



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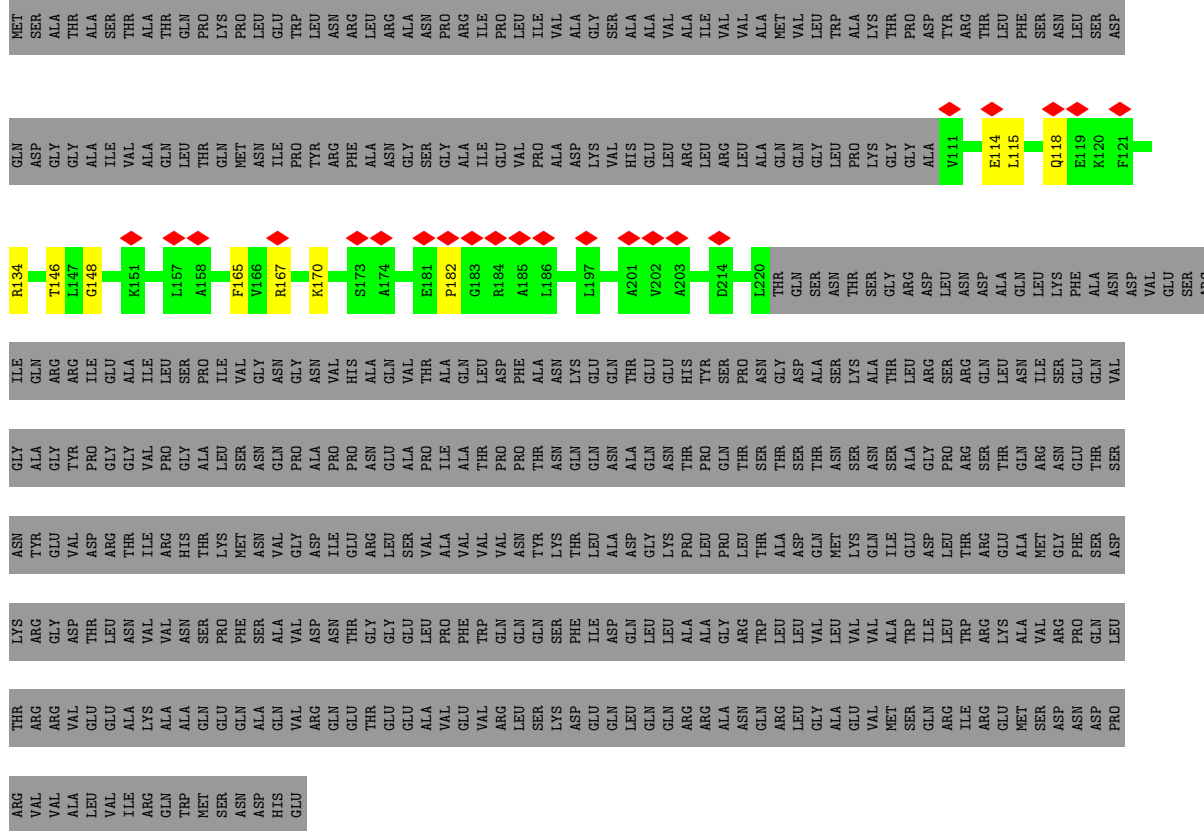


• Molecule 6: Flagellar M-ring protein

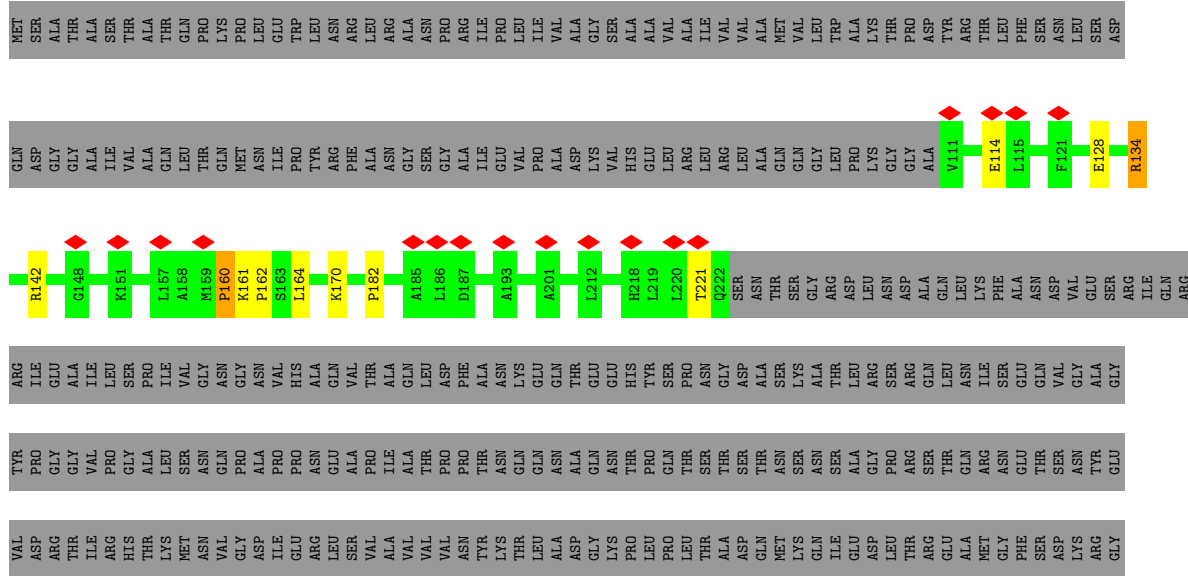


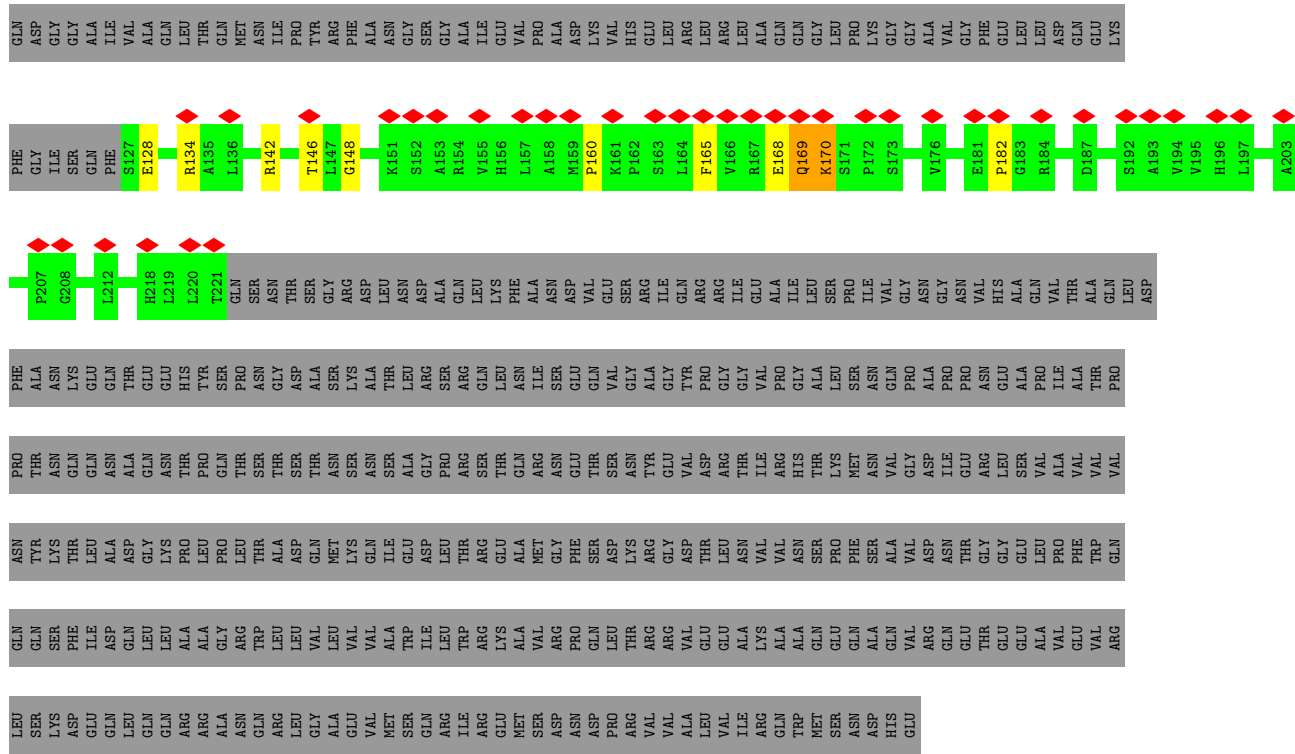
• Molecule 6: Flagellar M-ring protein

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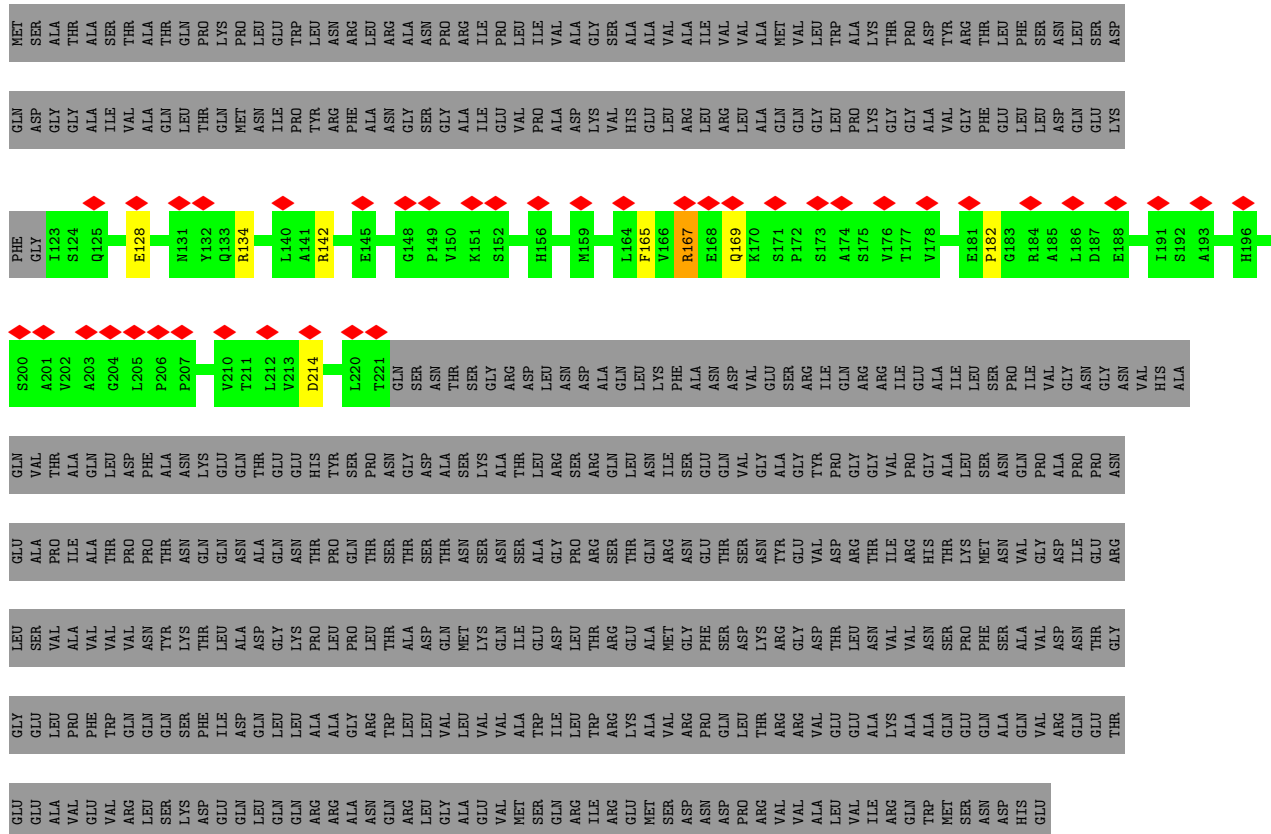


• Molecule 6: Flagellar M-ring protein



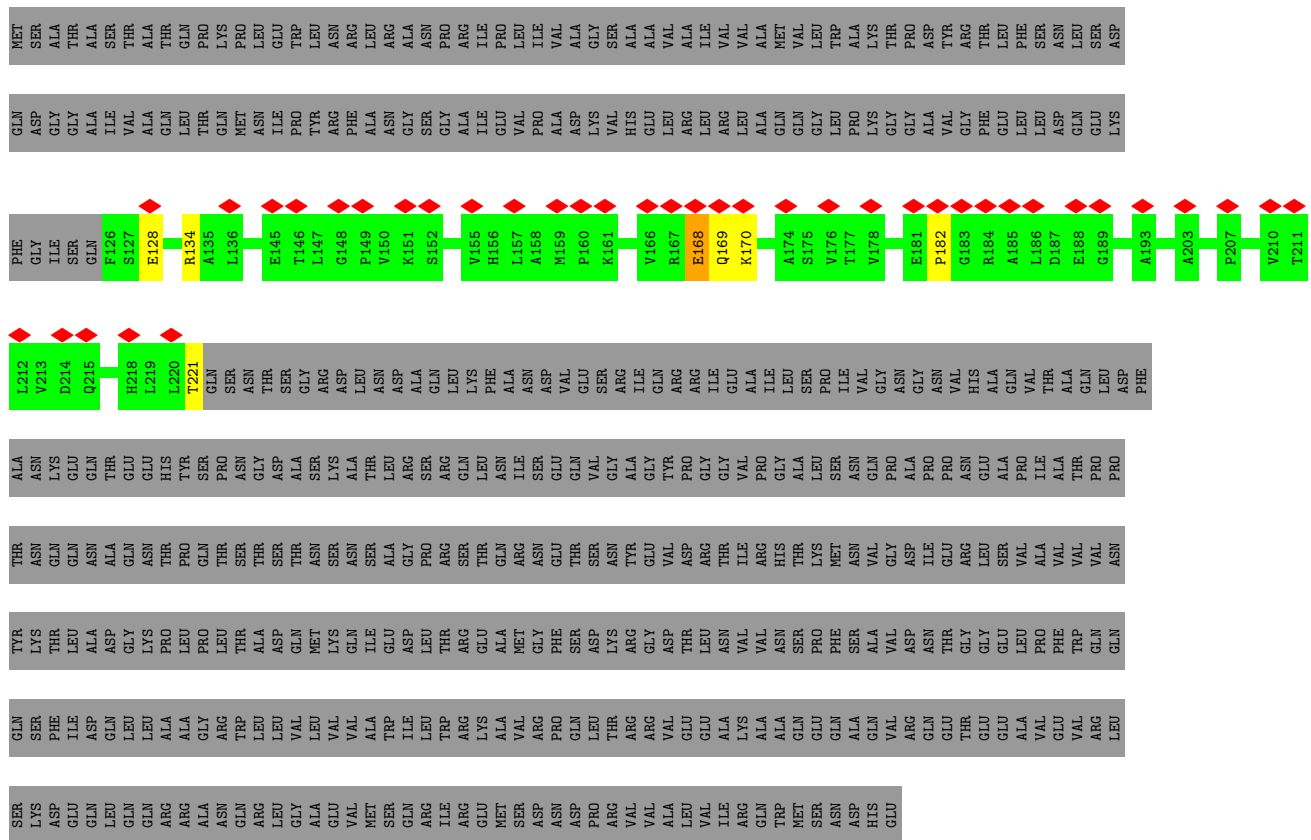


● Molecule 6: Flagellar M-ring protein

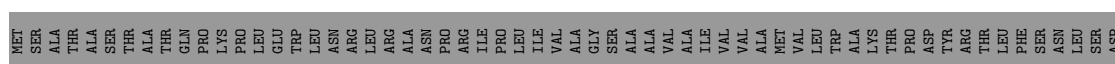


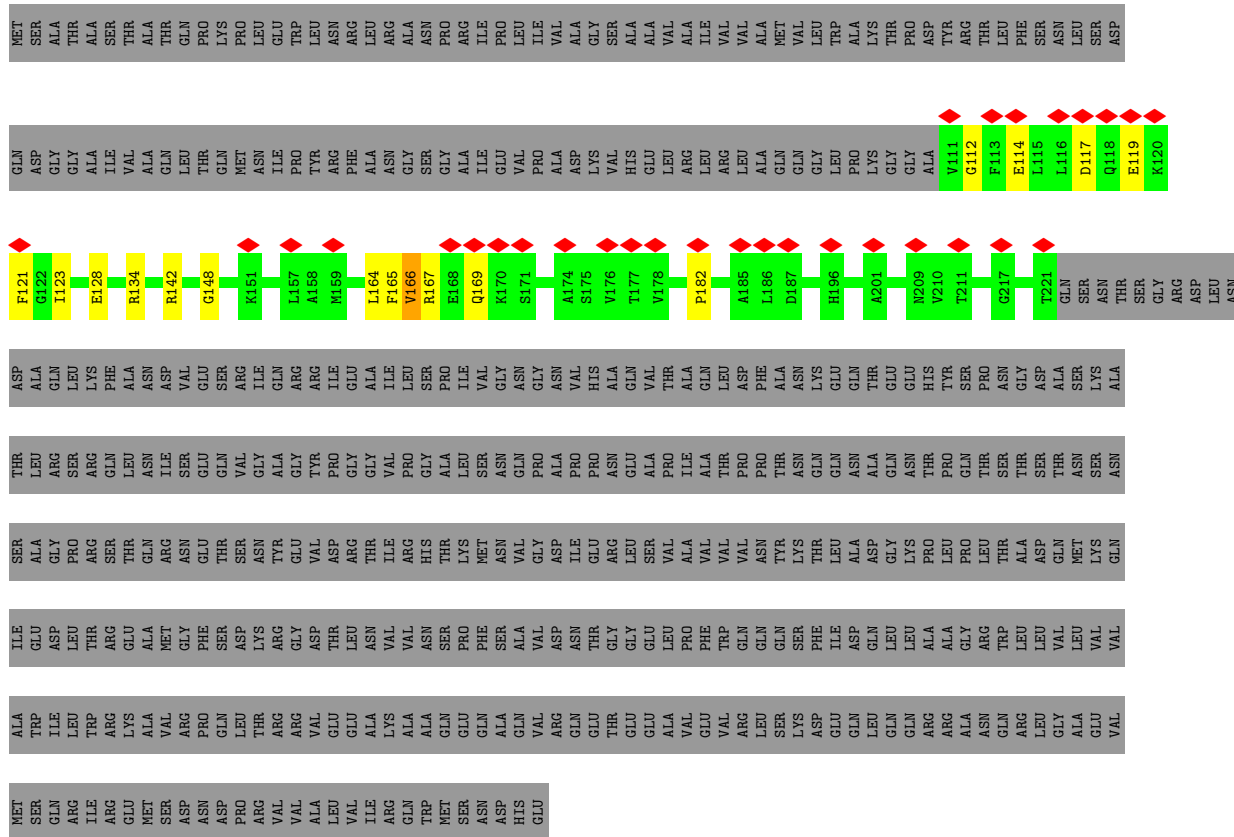


• Molecule 6: Flagellar M-ring protein

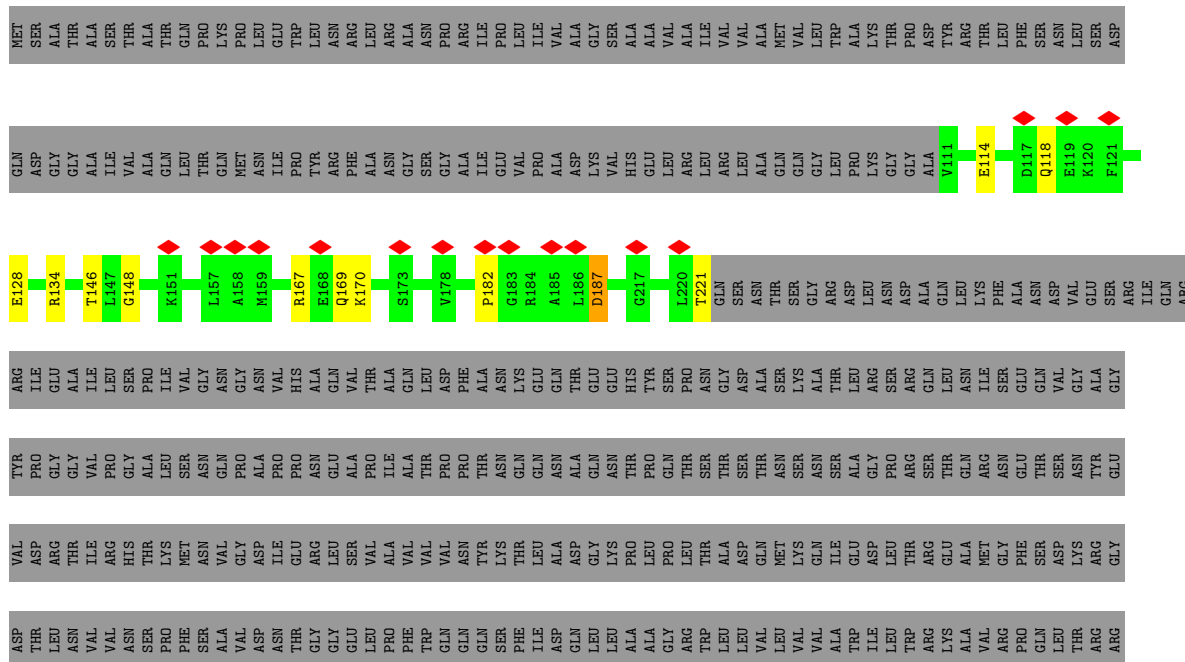


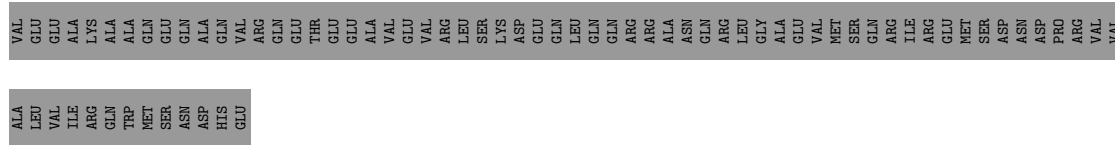
• Molecule 6: Flagellar M-ring protein



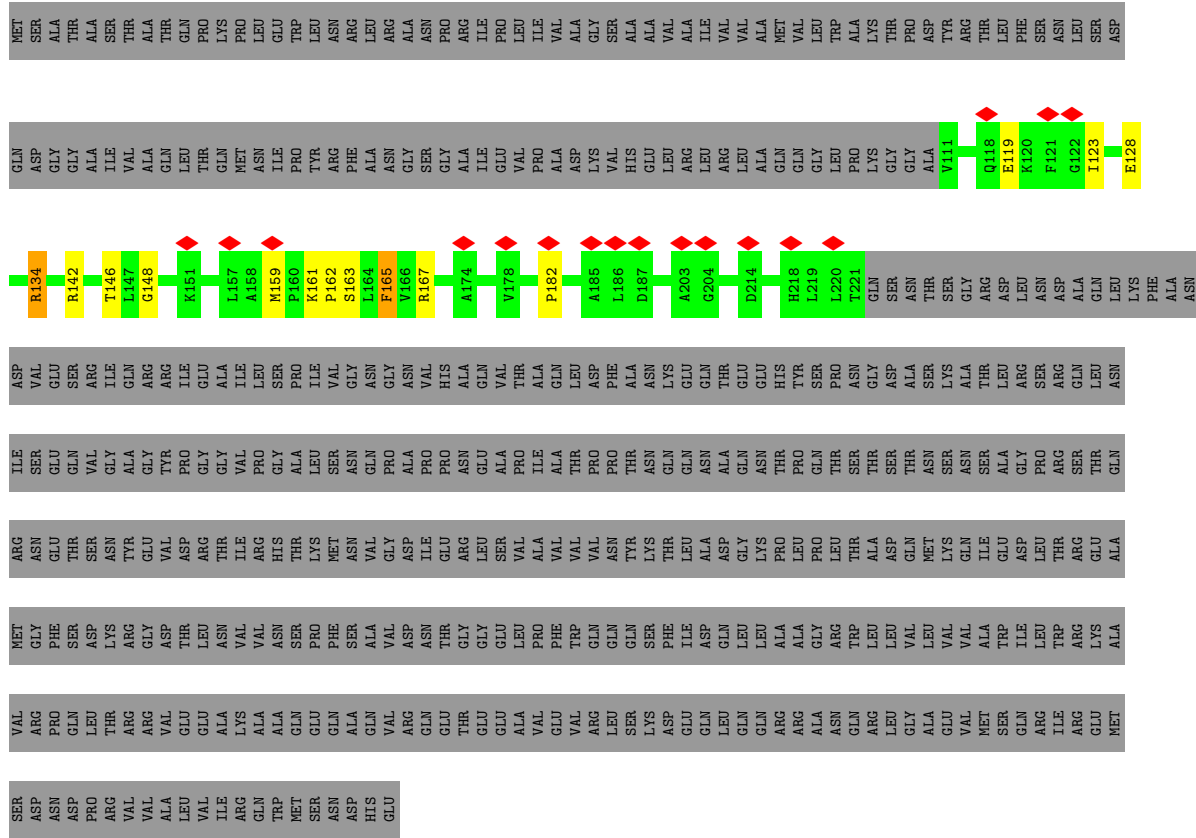


● Molecule 6: Flagellar M-ring protein

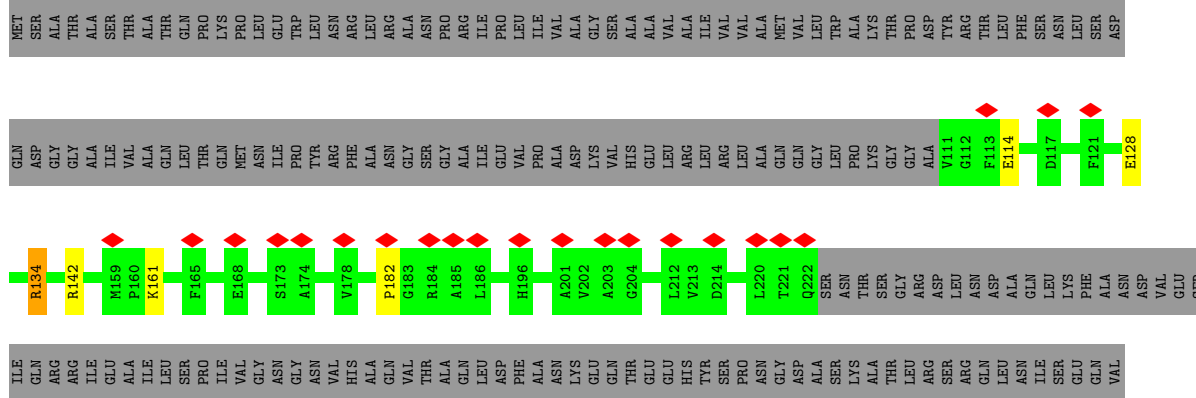


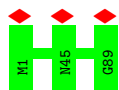


• Molecule 6: Flagellar M-ring protein

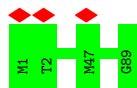


• Molecule 6: Flagellar M-ring protein

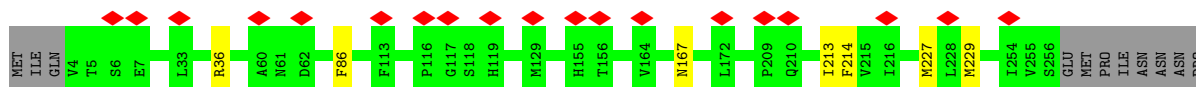




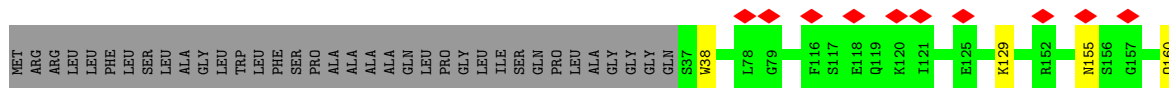
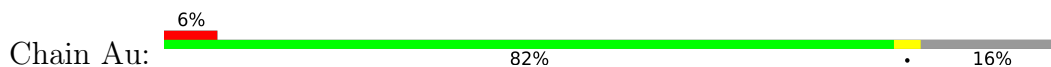
• Molecule 7: Flagellar biosynthetic protein FliQ



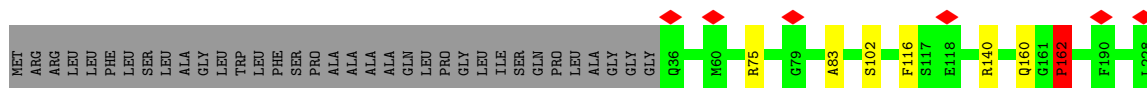
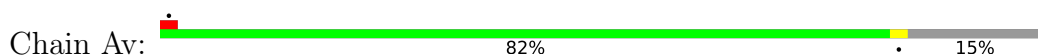
• Molecule 8: Flagellar biosynthetic protein FliR



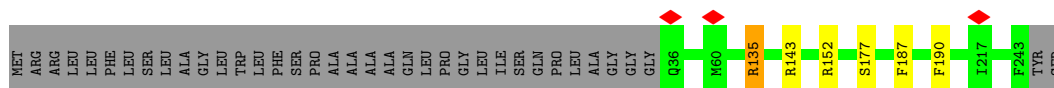
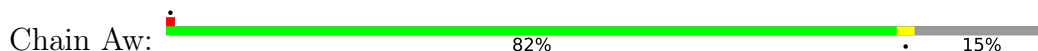
• Molecule 9: Flagellar biosynthetic protein FliP



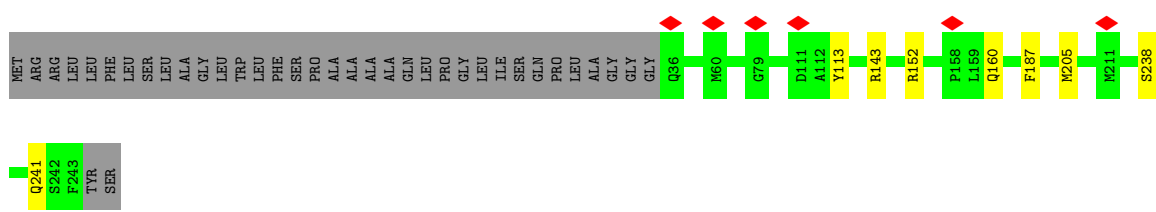
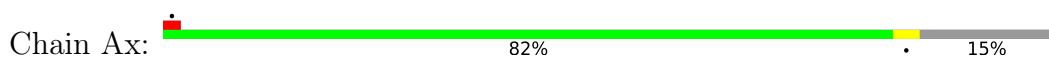
• Molecule 9: Flagellar biosynthetic protein FliP



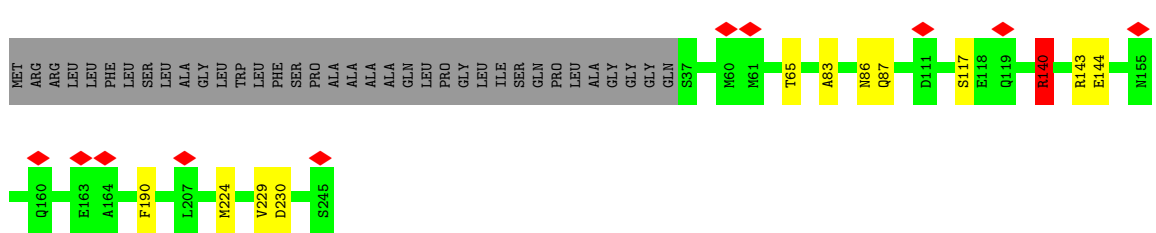
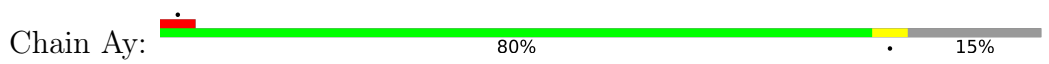
• Molecule 9: Flagellar biosynthetic protein FliP



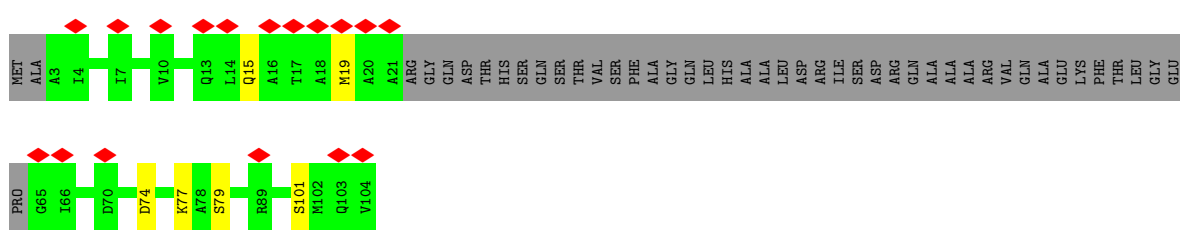
• Molecule 9: Flagellar biosynthetic protein FliP



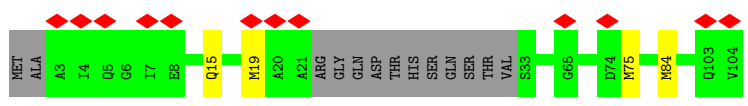
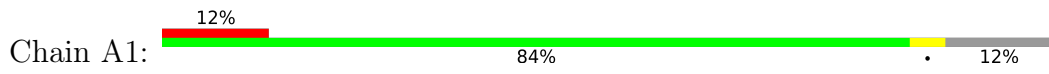
• Molecule 9: Flagellar biosynthetic protein FliP



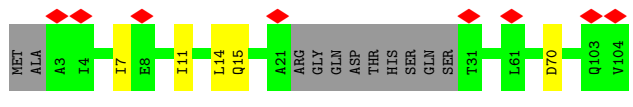
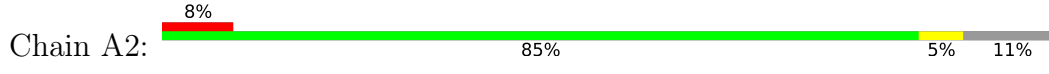
• Molecule 10: Flagellar hook-basal body complex protein FliE



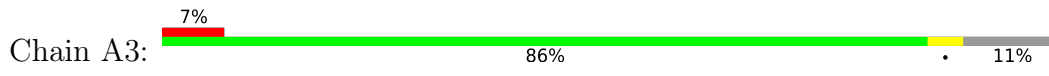
• Molecule 10: Flagellar hook-basal body complex protein FliE

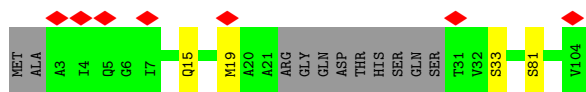


• Molecule 10: Flagellar hook-basal body complex protein FliE

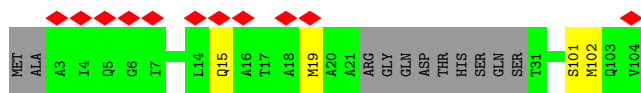
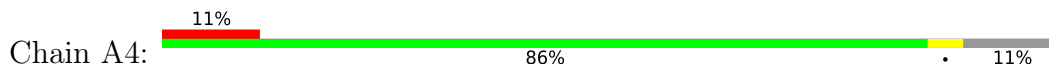


• Molecule 10: Flagellar hook-basal body complex protein FliE

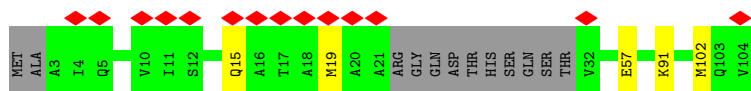
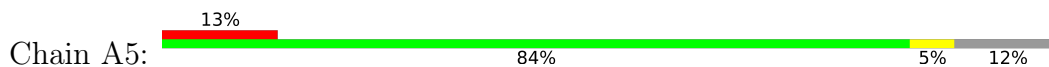




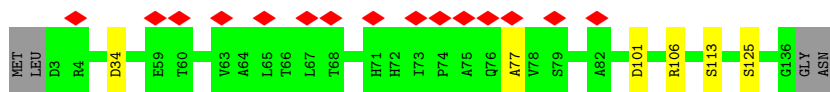
• Molecule 10: Flagellar hook-basal body complex protein FliE



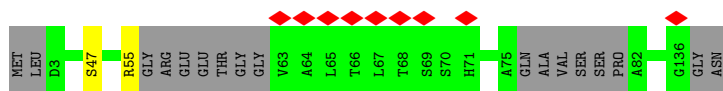
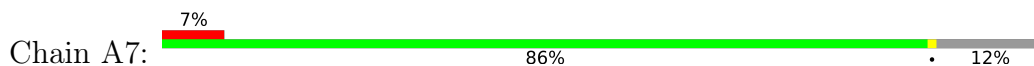
• Molecule 10: Flagellar hook-basal body complex protein FliE



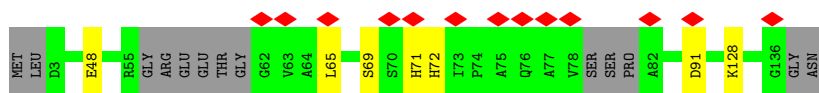
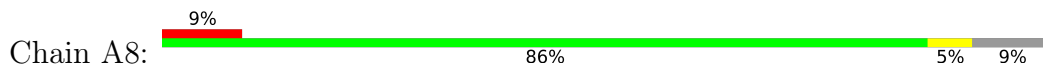
• Molecule 11: Flagellar basal body rod protein FlgB



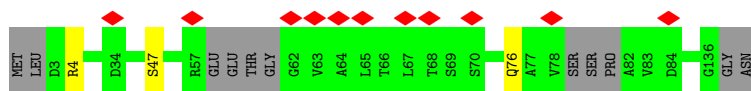
• Molecule 11: Flagellar basal body rod protein FlgB



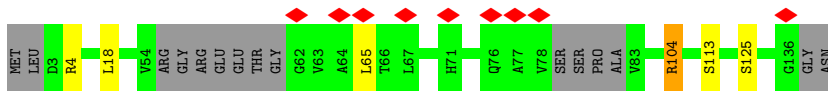
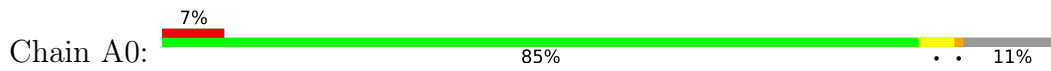
• Molecule 11: Flagellar basal body rod protein FlgB



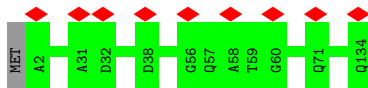
• Molecule 11: Flagellar basal body rod protein FlgB



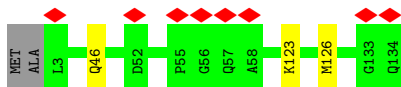
• Molecule 11: Flagellar basal body rod protein FlgB



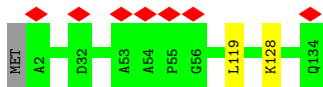
- Molecule 12: Flagellar basal-body rod protein FlgC



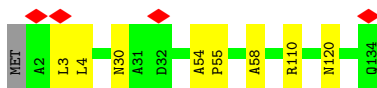
- Molecule 12: Flagellar basal-body rod protein FlgC



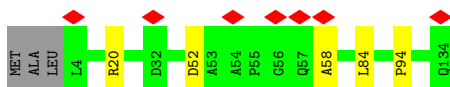
- Molecule 12: Flagellar basal-body rod protein FlgC



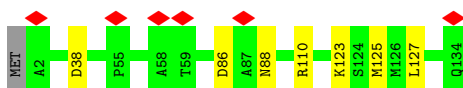
- Molecule 12: Flagellar basal-body rod protein FlgC



- 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	11858	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.637	Depositor
Minimum map value	-0.797	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	681.984, 681.984, 681.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332, 1.332, 1.332	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	0.30	0/1613	0.51	0/2194
1	B	0.30	0/1613	0.51	0/2194
1	C	0.30	0/1613	0.51	0/2194
1	D	0.29	0/1613	0.51	0/2194
1	E	0.29	0/1613	0.51	0/2194
1	F	0.30	0/1613	0.51	0/2194
1	G	0.29	0/1613	0.51	0/2194
1	H	0.29	0/1613	0.51	0/2194
1	I	0.30	0/1613	0.51	0/2194
1	J	0.30	0/1613	0.51	0/2194
1	K	0.29	0/1613	0.51	0/2194
1	L	0.30	0/1613	0.51	0/2194
1	M	0.30	0/1613	0.51	0/2194
1	N	0.29	0/1613	0.51	0/2194
1	O	0.29	0/1613	0.51	0/2194
1	P	0.30	0/1613	0.51	0/2194
1	Q	0.30	0/1613	0.51	0/2194
1	R	0.30	0/1613	0.51	0/2194
1	S	0.29	0/1613	0.51	0/2194
1	T	0.29	0/1613	0.51	0/2194
1	U	0.30	0/1613	0.51	0/2194
1	V	0.29	0/1613	0.51	0/2194
1	W	0.29	0/1613	0.51	0/2194
1	X	0.30	0/1613	0.51	0/2194
1	Y	0.30	0/1613	0.51	0/2194
1	Z	0.29	0/1613	0.51	0/2194
2	a	0.31	0/2243	0.55	0/3041
2	b	0.31	0/2243	0.54	0/3041
2	c	0.31	0/2243	0.55	0/3041
2	d	0.31	0/2243	0.55	0/3041
2	e	0.30	0/2243	0.55	0/3041
2	f	0.30	0/2243	0.55	0/3041
2	g	0.31	0/2243	0.55	0/3041
2	h	0.31	0/2243	0.55	0/3041

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	i	0.31	0/2243	0.55	0/3041
2	j	0.31	0/2243	0.55	0/3041
2	k	0.30	0/2243	0.55	0/3041
2	l	0.30	0/2243	0.55	0/3041
2	m	0.30	0/2243	0.55	0/3041
2	n	0.31	0/2243	0.55	0/3041
2	o	0.30	0/2243	0.55	0/3041
2	p	0.31	0/2243	0.55	0/3041
2	q	0.31	0/2243	0.54	0/3041
2	r	0.30	0/2243	0.54	0/3041
2	s	0.30	0/2243	0.55	0/3041
2	t	0.30	0/2243	0.55	0/3041
2	u	0.30	0/2243	0.54	0/3041
2	v	0.31	0/2243	0.55	0/3041
2	w	0.30	0/2243	0.55	0/3041
2	x	0.31	0/2243	0.55	0/3041
2	y	0.31	0/2243	0.55	0/3041
2	z	0.31	0/2243	0.55	0/3041
3	0	0.33	0/1888	0.54	1/2564 (0.0%)
3	1	0.31	0/1917	0.51	0/2605
3	2	0.29	0/1973	0.51	0/2682
3	3	0.28	0/1973	0.52	0/2682
3	4	0.28	0/1973	0.51	0/2682
3	5	0.33	0/1973	0.52	0/2682
3	6	0.32	0/1973	0.54	0/2682
3	7	0.32	0/1973	0.53	0/2682
3	8	0.33	0/1973	0.56	0/2682
3	9	0.30	0/1973	0.53	1/2682 (0.0%)
3	AF	0.34	0/1926	0.53	0/2618
3	AG	0.38	0/1934	0.59	0/2629
3	AH	0.39	0/1942	0.56	0/2639
3	AI	0.35	0/1926	0.58	1/2618 (0.0%)
3	AJ	0.34	0/1934	0.54	0/2629
3	AK	0.34	0/1844	0.51	0/2505
3	AL	0.33	0/1888	0.52	0/2564
3	AM	0.33	0/1888	0.56	1/2564 (0.0%)
3	AN	0.31	0/1888	0.51	0/2564
3	ZA	0.31	0/1973	0.53	0/2682
3	ZB	0.29	0/1973	0.49	0/2682
3	ZC	0.34	0/1973	0.54	0/2682
3	ZD	0.31	0/1973	0.52	0/2682
3	ZE	0.30	0/1973	0.51	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	0.34	0/2991	0.52	1/4076 (0.0%)
4	ZH	0.29	0/2991	0.50	0/4076
4	ZI	0.30	0/2991	0.51	0/4076
4	ZJ	0.31	0/2991	0.49	0/4076
4	ZK	0.29	0/2991	0.50	0/4076
4	ZL	0.29	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	0.29	0/2991	0.48	0/4076
4	ZU	0.29	0/2991	0.50	0/4076
4	ZV	0.50	4/2991 (0.1%)	0.67	6/4076 (0.1%)
4	ZW	0.27	0/2991	0.49	0/4076
4	ZX	0.28	0/2991	0.48	0/4076
4	ZY	0.30	1/2991 (0.0%)	0.55	2/4076 (0.0%)
4	ZZ	0.26	0/2991	0.46	0/4076
4	Za	0.28	0/2991	0.49	0/4076
4	Zb	0.30	0/2991	0.49	0/4076
4	Zc	0.29	0/2991	0.52	2/4076 (0.0%)
4	Zd	0.30	0/2991	0.51	0/4076
4	Ze	0.28	0/2991	0.48	0/4076
4	Zf	0.27	0/2991	0.48	0/4076
4	Zg	0.28	0/2991	0.49	0/4076
4	Zh	0.28	0/2991	0.48	0/4076
5	AA	0.32	0/1828	0.56	0/2492
5	AB	0.33	0/1836	0.56	2/2502 (0.1%)
5	AC	0.37	0/1844	0.57	0/2512
5	AD	0.33	0/1844	0.57	0/2512
5	AE	0.33	0/1836	0.58	0/2502
6	AO	0.27	0/1289	0.53	0/1741
6	AP	0.27	0/1289	0.53	0/1741
6	AQ	0.26	0/1289	0.53	0/1741
6	AR	0.27	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	0.27	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	0.27	0/1289	0.53	0/1741
6	BG	0.46	0/83	0.87	1/114 (0.9%)
6	BH	0.26	0/107	0.38	0/148
6	BI	0.31	0/137	0.49	0/191
6	BJ	0.28	0/107	0.57	0/148
6	BK	0.40	0/145	0.55	0/203
6	BL	0.33	0/107	0.51	0/148
6	BM	0.26	0/145	0.43	0/203
6	BN	0.30	0/107	0.38	0/148
6	BO	0.33	0/137	0.70	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	0.27	0/1289	0.53	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	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UN	0.84	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	0.60	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	0.59	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	0.61	0/848	0.69	0/1152
6	WT	0.60	0/848	0.71	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	0.45	0/681	0.67	1/930 (0.1%)
7	Aq	0.32	0/681	0.53	0/930
7	Ar	0.28	0/681	0.50	0/930
7	As	0.26	0/681	0.48	0/930
8	At	0.31	0/1994	0.52	0/2724
9	Au	0.36	0/1643	0.62	2/2237 (0.1%)
9	Av	0.30	0/1665	0.49	1/2267 (0.0%)
9	Aw	0.30	0/1652	0.50	0/2249
9	Ax	0.29	0/1652	0.47	0/2249
9	Ay	0.33	0/1662	0.52	0/2263
10	A1	0.36	0/675	0.49	0/905
10	A2	0.36	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	0.40	0/682	0.52	0/915
10	Az	0.43	0/428	0.57	0/572
11	A0	0.34	0/959	0.50	0/1293
11	A6	0.37	0/1042	0.56	0/1408
11	A7	0.33	0/951	0.50	0/1282
11	A8	0.35	0/976	0.56	0/1316

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	A9	0.35	0/991	0.54	0/1335
12	BA	0.30	0/981	0.47	0/1334
12	BB	0.29	0/976	0.50	0/1327
12	BC	0.34	0/981	0.50	0/1334
12	BD	0.33	0/981	0.62	0/1334
12	BE	0.29	0/968	0.48	0/1316
12	BF	0.36	0/981	0.52	0/1334
All	All	0.35	22/343249 (0.0%)	0.55	64/466323 (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
3	0	0	2
3	1	0	1
3	5	0	2
3	7	0	1
3	8	0	2
3	AF	0	1
3	AI	0	1
3	AK	0	1
3	AL	0	1
3	AM	0	2
3	AN	0	3
3	ZA	0	2
3	ZD	0	1
3	ZE	0	3
4	ZI	0	1
4	ZK	0	1
4	ZO	0	1
4	ZT	0	1
4	ZU	0	1
4	ZW	0	1
4	ZZ	0	1
4	Zd	0	1
4	Ze	0	1
5	AA	0	1
5	AB	0	2
5	AD	0	1
6	UI	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
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
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	2
9	Ay	0	2
11	A0	0	1
11	A6	0	1
11	A7	0	1
11	A9	0	1
12	BD	0	1
12	BF	0	1
All	All	0	113

All (22) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	ZV	140	PRO	CG-CD	-16.11	0.97	1.50
4	ZV	125	PRO	CG-CD	-10.15	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	UI	172	PRO	N-CD	-9.50	1.34	1.47
6	UO	172	PRO	N-CD	-9.50	1.34	1.47
6	UN	172	PRO	N-CD	-9.49	1.34	1.47
6	UJ	172	PRO	N-CD	-9.43	1.34	1.47
6	UP	172	PRO	N-CD	-9.43	1.34	1.47
6	UK	172	PRO	N-CD	-9.41	1.34	1.47
4	ZV	140	PRO	N-CD	8.28	1.59	1.47
6	UJ	125	GLN	C-N	7.71	1.51	1.34
6	UK	125	GLN	C-N	7.64	1.51	1.34
6	UO	125	GLN	C-N	7.62	1.51	1.34
6	UP	125	GLN	C-N	7.61	1.51	1.34
6	UI	125	GLN	C-N	7.61	1.51	1.34
6	UL	125	GLN	C-N	7.57	1.51	1.34
6	UM	125	GLN	C-N	7.55	1.51	1.34
6	UN	125	GLN	C-N	7.55	1.51	1.34
4	ZV	125	PRO	N-CD	6.62	1.57	1.47
4	ZY	125	PRO	CG-CD	-5.45	1.32	1.50
4	ZR	125	PRO	CG-CD	-5.11	1.33	1.50

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	ZV	140	PRO	N-CD-CG	-17.33	77.21	103.20
4	ZR	125	PRO	CA-N-CD	-13.96	91.96	111.50
4	ZY	125	PRO	CA-N-CD	-13.33	92.84	111.50
4	ZV	125	PRO	CA-N-CD	-13.27	92.93	111.50
9	Au	162	PRO	CA-N-CD	-11.97	94.75	111.50
4	Zc	125	PRO	CA-N-CD	-11.26	95.73	111.50
4	ZV	125	PRO	N-CD-CG	-11.25	86.32	103.20
4	ZV	140	PRO	CA-N-CD	-10.22	97.19	111.50
4	ZV	140	PRO	CA-CB-CG	-9.29	86.34	104.00
6	UL	126	PHE	O-C-N	8.83	136.83	122.70
6	UO	126	PHE	O-C-N	8.82	136.82	122.70
6	UI	126	PHE	O-C-N	8.80	136.78	122.70
6	UK	126	PHE	O-C-N	8.79	136.76	122.70
6	UN	126	PHE	O-C-N	8.78	136.75	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	UJ	126	PHE	O-C-N	8.78	136.74	122.70
6	UP	126	PHE	O-C-N	8.77	136.74	122.70
6	UM	126	PHE	O-C-N	8.77	136.73	122.70
4	ZM	223	PRO	CA-N-CD	-8.38	99.77	111.50
4	ZR	125	PRO	N-CD-CG	-7.59	91.82	103.20
4	ZY	125	PRO	N-CD-CG	-7.44	92.05	103.20
6	UL	126	PHE	CA-C-N	-6.79	102.25	117.20
6	UO	126	PHE	CA-C-N	-6.76	102.33	117.20
6	UK	126	PHE	CA-C-N	-6.76	102.33	117.20
6	UJ	126	PHE	CA-C-N	-6.75	102.35	117.20
6	UM	126	PHE	CA-C-N	-6.75	102.36	117.20
6	UI	126	PHE	CA-C-N	-6.75	102.36	117.20
6	UP	126	PHE	CA-C-N	-6.73	102.38	117.20
6	UN	126	PHE	CA-C-N	-6.72	102.42	117.20
9	Au	162	PRO	N-CD-CG	-6.59	93.31	103.20
6	UP	129	GLN	O-C-N	6.41	132.95	122.70
6	UK	129	GLN	O-C-N	6.39	132.93	122.70
6	UO	129	GLN	O-C-N	6.37	132.89	122.70
6	UJ	129	GLN	O-C-N	6.31	132.80	122.70
6	UN	129	GLN	O-C-N	6.30	132.77	122.70
6	UM	129	GLN	O-C-N	6.29	132.77	122.70
6	UI	129	GLN	O-C-N	6.29	132.76	122.70
6	WA	162	PRO	N-CA-C	6.28	128.44	112.10
6	UL	129	GLN	O-C-N	6.28	132.75	122.70
3	AI	154	ASP	CB-CG-OD2	6.24	123.92	118.30
4	ZG	297	ASP	CB-CG-OD2	6.13	123.81	118.30
4	ZR	214	ASP	CB-CG-OD1	6.01	123.71	118.30
7	Ab	85	PRO	CA-N-CD	-5.88	103.28	111.50
4	Zc	125	PRO	N-CD-CG	-5.83	94.46	103.20
3	AM	154	ASP	CB-CG-OD1	5.80	123.52	118.30
6	UL	126	PHE	C-N-CA	-5.76	107.30	121.70
6	UM	126	PHE	C-N-CA	-5.74	107.35	121.70
3	0	52	PRO	N-CA-CB	-5.73	96.30	102.60
6	UO	126	PHE	C-N-CA	-5.73	107.38	121.70
6	UP	126	PHE	C-N-CA	-5.73	107.39	121.70
4	ZS	18	ASP	CB-CG-OD1	5.72	123.45	118.30
6	UJ	126	PHE	C-N-CA	-5.72	107.39	121.70
6	UN	126	PHE	C-N-CA	-5.72	107.40	121.70
6	UK	126	PHE	C-N-CA	-5.72	107.40	121.70
6	UI	126	PHE	C-N-CA	-5.71	107.42	121.70
4	ZV	125	PRO	CA-CB-CG	-5.68	93.20	104.00
5	AB	53	THR	CB-CA-C	-5.62	96.43	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	ZP	125	PRO	CA-N-CD	-5.56	103.71	111.50
3	ZE	13	ASP	CB-CG-OD1	5.51	123.26	118.30
9	Av	162	PRO	N-CA-CB	-5.31	96.76	102.60
5	AB	72	ASP	CB-CG-OD1	5.28	123.05	118.30
6	BG	322	PRO	N-CA-CB	-5.24	96.83	102.60
6	WJ	214	ASP	CB-CA-C	-5.21	99.98	110.40
3	9	109	ASP	CB-CG-OD2	5.19	122.97	118.30
6	WO	168	GLU	CB-CA-C	-5.04	100.33	110.40

There are no chirality outliers.

All (113) 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
3	5	50	ARG	Sidechain
3	5	73	ARG	Sidechain
3	7	73	ARG	Sidechain
3	8	238	ARG	Sidechain
3	8	38	ARG	Sidechain
11	A0	104	ARG	Sidechain
11	A6	106	ARG	Sidechain
11	A7	55	ARG	Sidechain
11	A9	4	ARG	Sidechain
5	AA	243	ARG	Sidechain
5	AB	225	ARG	Sidechain
5	AB	54	ARG	Sidechain
5	AD	200	ARG	Sidechain
3	AF	36	ARG	Sidechain
3	AI	116	ARG	Sidechain
3	AK	79	ARG	Sidechain
3	AL	73	ARG	Sidechain
3	AM	36	ARG	Sidechain
3	AM	50	ARG	Sidechain
3	AN	116	ARG	Sidechain
3	AN	153	ARG	Sidechain
3	AN	238	ARG	Sidechain
9	Aw	135	ARG	Sidechain
9	Aw	143	ARG	Sidechain
9	Ay	140	ARG	Sidechain
9	Ay	143	ARG	Sidechain

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
6	WW	167	ARG	Sidechain
3	ZA	50	ARG	Sidechain
3	ZA	79	ARG	Sidechain
3	ZD	238	ARG	Sidechain
3	ZE	238	ARG	Sidechain
3	ZE	50	ARG	Sidechain
3	ZE	79	ARG	Sidechain
4	ZI	380	ARG	Sidechain
4	ZK	71	ARG	Sidechain
4	ZO	71	ARG	Sidechain
4	ZT	106	ARG	Sidechain
4	ZU	96	ARG	Sidechain
4	ZW	71	ARG	Sidechain
4	ZZ	380	ARG	Sidechain
4	Zd	380	ARG	Sidechain
4	Ze	380	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	B	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	C	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	D	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	E	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	F	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	G	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	H	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	I	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	J	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	K	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	L	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	M	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	N	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	O	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	P	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	Q	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	R	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	S	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	T	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	U	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	W	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	X	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	Y	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
1	Z	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	62
2	a	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	b	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	c	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	d	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	e	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	f	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	g	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	h	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	i	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	j	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	k	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	l	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	m	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	n	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	o	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	p	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	q	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	r	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	s	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	t	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	u	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	v	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	w	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	x	297/365 (81%)	288 (97%)	9 (3%)	0	100	100
2	y	297/365 (81%)	289 (97%)	8 (3%)	0	100	100
2	z	297/365 (81%)	288 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	0	244/260 (94%)	236 (97%)	5 (2%)	3 (1%)	11	44
3	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	67
3	2	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	53
3	3	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	53
3	4	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	53
3	5	258/260 (99%)	240 (93%)	15 (6%)	3 (1%)	11	44
3	6	258/260 (99%)	244 (95%)	10 (4%)	4 (2%)	8	39
3	7	258/260 (99%)	244 (95%)	11 (4%)	3 (1%)	11	44
3	8	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	44
3	9	258/260 (99%)	244 (95%)	13 (5%)	1 (0%)	30	67
3	AF	250/260 (96%)	238 (95%)	11 (4%)	1 (0%)	30	67
3	AG	251/260 (96%)	234 (93%)	14 (6%)	3 (1%)	11	44
3	AH	252/260 (97%)	234 (93%)	16 (6%)	2 (1%)	16	53
3	AI	250/260 (96%)	239 (96%)	9 (4%)	2 (1%)	16	53
3	AJ	251/260 (96%)	235 (94%)	10 (4%)	6 (2%)	5	30
3	AK	239/260 (92%)	231 (97%)	7 (3%)	1 (0%)	30	67
3	AL	244/260 (94%)	229 (94%)	10 (4%)	5 (2%)	6	34
3	AM	244/260 (94%)	234 (96%)	9 (4%)	1 (0%)	30	67
3	AN	244/260 (94%)	239 (98%)	4 (2%)	1 (0%)	30	67
3	ZA	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	44
3	ZB	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	11	44
3	ZC	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	53
3	ZD	258/260 (99%)	237 (92%)	18 (7%)	3 (1%)	11	44
3	ZE	258/260 (99%)	243 (94%)	14 (5%)	1 (0%)	30	67
4	ZF	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
4	ZG	399/403 (99%)	388 (97%)	10 (2%)	1 (0%)	37	71
4	ZH	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
4	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25	62
4	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
4	ZK	399/403 (99%)	387 (97%)	11 (3%)	1 (0%)	37	71
4	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	53
4	ZP	399/403 (99%)	386 (97%)	12 (3%)	1 (0%)	37	71
4	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
4	ZR	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
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%)	380 (95%)	18 (4%)	1 (0%)	37	71
4	ZX	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
4	ZY	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
4	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
4	Za	399/403 (99%)	386 (97%)	12 (3%)	1 (0%)	37	71
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%)	384 (96%)	15 (4%)	0	100	100
4	Ze	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	71
4	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
4	Zg	399/403 (99%)	383 (96%)	16 (4%)	0	100	100
4	Zh	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
5	AA	246/251 (98%)	238 (97%)	7 (3%)	1 (0%)	30	67
5	AB	247/251 (98%)	242 (98%)	4 (2%)	1 (0%)	30	67
5	AC	248/251 (99%)	233 (94%)	13 (5%)	2 (1%)	16	53
5	AD	248/251 (99%)	235 (95%)	13 (5%)	0	100	100
5	AE	247/251 (98%)	236 (96%)	9 (4%)	2 (1%)	16	53
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AS	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AT	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AU	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AV	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AW	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AX	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AY	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AZ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Aa	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ac	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ad	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ae	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Af	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ag	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ah	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ai	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Aj	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ak	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Al	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Am	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	An	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ao	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ap	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BG	11/560 (2%)	9 (82%)	2 (18%)	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%)	17 (90%)	2 (10%)	0	100	100
6	BL	14/560 (2%)	13 (93%)	1 (7%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BO	18/560 (3%)	18 (100%)	0	0	100	100
6	BP	14/560 (2%)	14 (100%)	0	0	100	100
6	BQ	19/560 (3%)	19 (100%)	0	0	100	100
6	BR	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BS	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BT	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BU	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BV	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BW	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BX	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	UI	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UJ	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UK	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UL	151/560 (27%)	142 (94%)	7 (5%)	2 (1%)	10	42
6	UM	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UN	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UO	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	UP	151/560 (27%)	146 (97%)	3 (2%)	2 (1%)	10	42
6	WA	111/560 (20%)	99 (89%)	9 (8%)	3 (3%)	4	28
6	WB	109/560 (20%)	94 (86%)	10 (9%)	5 (5%)	2	20
6	WC	106/560 (19%)	96 (91%)	9 (8%)	1 (1%)	14	50
6	WD	108/560 (19%)	99 (92%)	4 (4%)	5 (5%)	2	20
6	WE	110/560 (20%)	98 (89%)	8 (7%)	4 (4%)	3	23
6	WF	109/560 (20%)	98 (90%)	8 (7%)	3 (3%)	4	27
6	WG	110/560 (20%)	98 (89%)	10 (9%)	2 (2%)	7	36
6	WH	93/560 (17%)	86 (92%)	5 (5%)	2 (2%)	5	32
6	WI	93/560 (17%)	82 (88%)	5 (5%)	6 (6%)	1	15
6	WJ	97/560 (17%)	89 (92%)	7 (7%)	1 (1%)	13	48
6	WK	96/560 (17%)	84 (88%)	9 (9%)	3 (3%)	3	26
6	WL	81/560 (14%)	75 (93%)	4 (5%)	2 (2%)	4	30
6	WM	78/560 (14%)	72 (92%)	4 (5%)	2 (3%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	WN	80/560 (14%)	75 (94%)	2 (2%)	3 (4%)	2	22
6	WO	94/560 (17%)	85 (90%)	7 (7%)	2 (2%)	5	33
6	WP	98/560 (18%)	87 (89%)	6 (6%)	5 (5%)	1	18
6	WQ	109/560 (20%)	100 (92%)	5 (5%)	4 (4%)	2	23
6	WR	109/560 (20%)	94 (86%)	8 (7%)	7 (6%)	1	15
6	WS	109/560 (20%)	96 (88%)	7 (6%)	6 (6%)	1	18
6	WT	109/560 (20%)	97 (89%)	5 (5%)	7 (6%)	1	15
6	WU	110/560 (20%)	101 (92%)	8 (7%)	1 (1%)	14	50
6	WV	108/560 (19%)	97 (90%)	9 (8%)	2 (2%)	6	35
6	WW	109/560 (20%)	95 (87%)	9 (8%)	5 (5%)	2	20
7	Ab	87/89 (98%)	81 (93%)	4 (5%)	2 (2%)	5	31
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%)	233 (93%)	16 (6%)	2 (1%)	16	53
9	Au	205/245 (84%)	197 (96%)	8 (4%)	0	100	100
9	Av	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13	48
9	Aw	206/245 (84%)	201 (98%)	5 (2%)	0	100	100
9	Ax	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25	62
9	Ay	207/245 (84%)	192 (93%)	10 (5%)	5 (2%)	5	30
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%)	52 (94%)	3 (6%)	0	100	100
11	A0	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
11	A6	132/138 (96%)	127 (96%)	4 (3%)	1 (1%)	16	53
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%)	119 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	BA	131/134 (98%)	122 (93%)	9 (7%)	0	100	100
12	BB	130/134 (97%)	123 (95%)	7 (5%)	0	100	100
12	BC	131/134 (98%)	124 (95%)	7 (5%)	0	100	100
12	BD	131/134 (98%)	121 (92%)	7 (5%)	3 (2%)	5	31
12	BE	129/134 (96%)	123 (95%)	5 (4%)	1 (1%)	16	53
12	BF	131/134 (98%)	124 (95%)	7 (5%)	0	100	100
All	All	44706/81227 (55%)	43140 (96%)	1350 (3%)	216 (0%)	27	62

All (216) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	209	ASN
3	4	140	ILE
3	5	209	ASN
3	6	139	ALA
3	8	209	ASN
3	ZA	92	SER
3	ZA	209	ASN
3	ZB	164	GLN
4	ZG	46	SER
5	AE	155	VAL
3	AL	90	ASN
7	Ab	84	LEU
9	Ay	83	ALA
9	Ay	87	GLN
6	WB	163	SER
6	WO	168	GLU
6	WR	123	ILE
6	WR	165	PHE
6	WR	166	VAL
6	WS	187	ASP
3	0	90	ASN
3	8	165	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

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Mol	Chain	Res	Type
5	AC	50	SER
5	AE	53	THR
3	AI	127	GLN
3	AI	165	ALA
3	AJ	204	SER
3	AL	4	SER
3	AN	127	GLN
8	At	167	ASN
8	At	213	ILE
9	Av	83	ALA
9	Ax	160	GLN
9	Ay	86	ASN
6	WB	148	GLY
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
12	BD	54	ALA
3	0	3	SER
3	0	127	GLN
3	2	49	ILE
3	3	49	ILE
3	3	181	ASP
3	4	49	ILE
3	5	49	ILE
3	6	138	PRO
3	7	55	GLN

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Mol	Chain	Res	Type
4	ZK	375	MET
4	ZL	374	ASN
3	AF	127	GLN
3	AH	198	SER
3	AJ	164	GLN
3	AJ	206	PRO
3	AL	3	SER
3	AL	127	GLN
3	AM	127	GLN
9	Ay	140	ARG
11	A6	77	ALA
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
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
12	BD	58	ALA
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

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Mol	Chain	Res	Type
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
1	Y	172	ASN
1	Z	172	ASN
3	6	49	ILE
3	6	58	GLU
3	7	49	ILE
3	8	49	ILE
3	9	49	ILE
3	ZA	138	PRO
4	ZO	142	THR
4	ZP	374	ASN
3	AG	81	HIS
3	AG	127	GLN
3	AJ	203	GLU
3	AK	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

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Mol	Chain	Res	Type
6	WG	182	PRO
6	WH	165	PHE
6	WH	182	PRO
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
12	BD	55	PRO
3	1	127	GLN
3	7	210	GLY
3	ZC	139	ALA
3	ZD	139	ALA
5	AB	52	ALA
5	AC	52	ALA
3	AG	139	ALA
3	AH	127	GLN
3	AJ	127	GLN
7	Ab	85	PRO
9	Av	162	PRO
6	WK	168	GLU
6	WR	121	PHE
6	WT	163	SER
4	ZO	375	MET
4	Za	97	ASN
4	Ze	134	PRO
5	AA	52	ALA
3	AJ	200	ALA
6	WC	182	PRO

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Mol	Chain	Res	Type
6	WE	221	THR
6	WF	162	PRO
6	WG	163	SER
12	BE	58	ALA
4	ZI	325	GLY
6	WA	160	PRO
6	WL	148	GLY
6	WS	148	GLY
6	WT	148	GLY
4	ZW	75	VAL
6	WA	148	GLY
6	WP	123	ILE
6	WR	148	GLY
3	5	138	PRO
3	AL	136	VAL
9	Ay	229	VAL
6	WP	160	PRO
6	WT	161	LYS
3	ZD	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%)	164 (96%)	6 (4%)	31 53
1	B	170/186 (91%)	164 (96%)	6 (4%)	31 53
1	C	170/186 (91%)	164 (96%)	6 (4%)	31 53
1	D	170/186 (91%)	164 (96%)	6 (4%)	31 53
1	E	170/186 (91%)	164 (96%)	6 (4%)	31 53
1	F	170/186 (91%)	164 (96%)	6 (4%)	31 53
1	G	170/186 (91%)	164 (96%)	6 (4%)	31 53
1	H	170/186 (91%)	164 (96%)	6 (4%)	31 53
1	I	170/186 (91%)	164 (96%)	6 (4%)	31 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	K	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	L	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	M	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	N	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	O	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	P	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	Q	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	R	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	S	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	T	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	U	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	V	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	W	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	X	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	Y	170/186 (91%)	164 (96%)	6 (4%)	31	53
1	Z	170/186 (91%)	164 (96%)	6 (4%)	31	53
2	a	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	b	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	c	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	d	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	e	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	f	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	g	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	h	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	i	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	j	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	k	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	l	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	m	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	n	248/294 (84%)	243 (98%)	5 (2%)	50	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	o	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	p	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	q	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	r	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	s	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	t	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	u	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	v	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	w	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	x	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	y	248/294 (84%)	243 (98%)	5 (2%)	50	68
2	z	248/294 (84%)	243 (98%)	5 (2%)	50	68
3	0	205/215 (95%)	198 (97%)	7 (3%)	32	54
3	1	209/215 (97%)	201 (96%)	8 (4%)	28	51
3	2	215/215 (100%)	213 (99%)	2 (1%)	75	83
3	3	215/215 (100%)	212 (99%)	3 (1%)	62	76
3	4	215/215 (100%)	209 (97%)	6 (3%)	38	59
3	5	215/215 (100%)	210 (98%)	5 (2%)	45	64
3	6	215/215 (100%)	210 (98%)	5 (2%)	45	64
3	7	215/215 (100%)	214 (100%)	1 (0%)	86	90
3	8	215/215 (100%)	211 (98%)	4 (2%)	52	69
3	9	215/215 (100%)	212 (99%)	3 (1%)	62	76
3	AF	209/215 (97%)	203 (97%)	6 (3%)	37	58
3	AG	210/215 (98%)	201 (96%)	9 (4%)	25	48
3	AH	211/215 (98%)	199 (94%)	12 (6%)	17	41
3	AI	209/215 (97%)	198 (95%)	11 (5%)	19	43
3	AJ	210/215 (98%)	199 (95%)	11 (5%)	19	43
3	AK	200/215 (93%)	195 (98%)	5 (2%)	42	62
3	AL	205/215 (95%)	197 (96%)	8 (4%)	27	50
3	AM	205/215 (95%)	197 (96%)	8 (4%)	27	50
3	AN	205/215 (95%)	201 (98%)	4 (2%)	50	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	83
3	ZB	215/215 (100%)	208 (97%)	7 (3%)	33	55
3	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	76
3	ZD	215/215 (100%)	211 (98%)	4 (2%)	52	69
3	ZE	215/215 (100%)	210 (98%)	5 (2%)	45	64
4	ZF	321/323 (99%)	309 (96%)	12 (4%)	29	52
4	ZG	321/323 (99%)	305 (95%)	16 (5%)	20	44
4	ZH	321/323 (99%)	308 (96%)	13 (4%)	27	50
4	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	69
4	ZJ	321/323 (99%)	312 (97%)	9 (3%)	38	59
4	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	69
4	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	56
4	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	59
4	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	56
4	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	62
4	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	46
4	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	59
4	ZR	321/323 (99%)	314 (98%)	7 (2%)	47	65
4	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	69
4	ZT	321/323 (99%)	313 (98%)	8 (2%)	42	62
4	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	79
4	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	79
4	ZW	321/323 (99%)	307 (96%)	14 (4%)	24	47
4	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	83
4	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	65
4	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	74
4	Za	321/323 (99%)	315 (98%)	6 (2%)	52	69
4	Zb	321/323 (99%)	314 (98%)	7 (2%)	47	65
4	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	54
4	Zd	321/323 (99%)	314 (98%)	7 (2%)	47	65
4	Ze	321/323 (99%)	314 (98%)	7 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	65
4	Zg	321/323 (99%)	315 (98%)	6 (2%)	52	69
4	Zh	321/323 (99%)	314 (98%)	7 (2%)	47	65
5	AA	190/193 (98%)	188 (99%)	2 (1%)	70	80
5	AB	191/193 (99%)	186 (97%)	5 (3%)	41	61
5	AC	192/193 (100%)	189 (98%)	3 (2%)	58	74
5	AD	192/193 (100%)	185 (96%)	7 (4%)	30	53
5	AE	191/193 (99%)	189 (99%)	2 (1%)	73	81
6	AO	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AP	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AQ	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AR	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AS	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AT	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AU	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AV	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AW	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AX	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AY	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	AZ	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Aa	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Ac	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Ad	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Ae	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Af	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Ag	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Ah	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Ai	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Aj	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Ak	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Al	141/467 (30%)	134 (95%)	7 (5%)	20	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Am	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	An	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Ao	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	Ap	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	BG	8/467 (2%)	6 (75%)	2 (25%)	0	3
6	BH	11/467 (2%)	10 (91%)	1 (9%)	7	26
6	BI	14/467 (3%)	12 (86%)	2 (14%)	2	15
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	34
6	BP	11/467 (2%)	11 (100%)	0	100	100
6	BQ	15/467 (3%)	14 (93%)	1 (7%)	13	36
6	BR	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	BS	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	BT	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	BU	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	BV	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	BW	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	BX	141/467 (30%)	134 (95%)	7 (5%)	20	44
6	UI	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UJ	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UK	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UL	128/467 (27%)	122 (95%)	6 (5%)	22	46
6	UM	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UN	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UO	128/467 (27%)	123 (96%)	5 (4%)	27	50
6	UP	128/467 (27%)	122 (95%)	6 (5%)	22	46
6	WA	95/467 (20%)	91 (96%)	4 (4%)	25	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	WB	93/467 (20%)	87 (94%)	6 (6%)	14	37
6	WC	91/467 (20%)	83 (91%)	8 (9%)	8	28
6	WD	92/467 (20%)	88 (96%)	4 (4%)	25	48
6	WE	94/467 (20%)	87 (93%)	7 (7%)	11	33
6	WF	93/467 (20%)	86 (92%)	7 (8%)	11	33
6	WG	94/467 (20%)	87 (93%)	7 (7%)	11	33
6	WH	79/467 (17%)	75 (95%)	4 (5%)	20	43
6	WI	79/467 (17%)	73 (92%)	6 (8%)	11	32
6	WJ	83/467 (18%)	79 (95%)	4 (5%)	21	45
6	WK	82/467 (18%)	77 (94%)	5 (6%)	15	39
6	WL	69/467 (15%)	66 (96%)	3 (4%)	25	48
6	WM	66/467 (14%)	65 (98%)	1 (2%)	60	75
6	WN	68/467 (15%)	66 (97%)	2 (3%)	37	58
6	WO	80/467 (17%)	76 (95%)	4 (5%)	20	44
6	WP	83/467 (18%)	77 (93%)	6 (7%)	12	34
6	WQ	93/467 (20%)	91 (98%)	2 (2%)	47	65
6	WR	93/467 (20%)	86 (92%)	7 (8%)	11	33
6	WS	93/467 (20%)	87 (94%)	6 (6%)	14	37
6	WT	93/467 (20%)	86 (92%)	7 (8%)	11	33
6	WU	94/467 (20%)	90 (96%)	4 (4%)	25	48
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%)	68 (92%)	6 (8%)	9	31
7	Aq	74/74 (100%)	72 (97%)	2 (3%)	40	61
7	Ar	74/74 (100%)	74 (100%)	0	100	100
7	As	74/74 (100%)	74 (100%)	0	100	100
8	At	210/221 (95%)	205 (98%)	5 (2%)	44	63
9	Au	177/204 (87%)	171 (97%)	6 (3%)	32	54
9	Av	179/204 (88%)	173 (97%)	6 (3%)	32	54
9	Aw	178/204 (87%)	173 (97%)	5 (3%)	38	59
9	Ax	178/204 (87%)	171 (96%)	7 (4%)	27	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Ay	179/204 (88%)	172 (96%)	7 (4%)	27	50
10	A1	68/79 (86%)	64 (94%)	4 (6%)	16	40
10	A2	70/79 (89%)	65 (93%)	5 (7%)	12	34
10	A3	70/79 (89%)	66 (94%)	4 (6%)	17	41
10	A4	70/79 (89%)	66 (94%)	4 (6%)	17	41
10	A5	69/79 (87%)	64 (93%)	5 (7%)	12	34
10	Az	45/79 (57%)	39 (87%)	6 (13%)	3	17
11	A0	102/113 (90%)	96 (94%)	6 (6%)	16	40
11	A6	110/113 (97%)	106 (96%)	4 (4%)	30	53
11	A7	101/113 (89%)	100 (99%)	1 (1%)	73	81
11	A8	103/113 (91%)	96 (93%)	7 (7%)	13	36
11	A9	104/113 (92%)	102 (98%)	2 (2%)	52	69
12	BA	104/105 (99%)	104 (100%)	0	100	100
12	BB	104/105 (99%)	101 (97%)	3 (3%)	37	58
12	BC	104/105 (99%)	102 (98%)	2 (2%)	52	69
12	BD	104/105 (99%)	100 (96%)	4 (4%)	28	51
12	BE	103/105 (98%)	99 (96%)	4 (4%)	27	50
12	BF	104/105 (99%)	98 (94%)	6 (6%)	17	40
All	All	37084/66670 (56%)	35882 (97%)	1202 (3%)	36	55

All (1202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ILE
1	A	85	ASN
1	A	106	PHE
1	A	113	LEU
1	A	133	ASN
1	A	144	PHE
1	B	58	ILE
1	B	85	ASN
1	B	106	PHE
1	B	113	LEU
1	B	133	ASN
1	B	144	PHE
1	C	58	ILE

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Mol	Chain	Res	Type
1	C	85	ASN
1	C	106	PHE
1	C	113	LEU
1	C	133	ASN
1	C	144	PHE
1	D	58	ILE
1	D	85	ASN
1	D	106	PHE
1	D	113	LEU
1	D	133	ASN
1	D	144	PHE
1	E	58	ILE
1	E	85	ASN
1	E	106	PHE
1	E	113	LEU
1	E	133	ASN
1	E	144	PHE
1	F	58	ILE
1	F	85	ASN
1	F	106	PHE
1	F	113	LEU
1	F	133	ASN
1	F	144	PHE
1	G	58	ILE
1	G	85	ASN
1	G	106	PHE
1	G	113	LEU
1	G	133	ASN
1	G	144	PHE
1	H	58	ILE
1	H	85	ASN
1	H	106	PHE
1	H	113	LEU
1	H	133	ASN
1	H	144	PHE
1	I	58	ILE
1	I	85	ASN
1	I	106	PHE
1	I	113	LEU
1	I	133	ASN
1	I	144	PHE
1	J	58	ILE

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Mol	Chain	Res	Type
1	J	85	ASN
1	J	106	PHE
1	J	113	LEU
1	J	133	ASN
1	J	144	PHE
1	K	58	ILE
1	K	85	ASN
1	K	106	PHE
1	K	113	LEU
1	K	133	ASN
1	K	144	PHE
1	L	58	ILE
1	L	85	ASN
1	L	106	PHE
1	L	113	LEU
1	L	133	ASN
1	L	144	PHE
1	M	58	ILE
1	M	85	ASN
1	M	106	PHE
1	M	113	LEU
1	M	133	ASN
1	M	144	PHE
1	N	58	ILE
1	N	85	ASN
1	N	106	PHE
1	N	113	LEU
1	N	133	ASN
1	N	144	PHE
1	O	58	ILE
1	O	85	ASN
1	O	106	PHE
1	O	113	LEU
1	O	133	ASN
1	O	144	PHE
1	P	58	ILE
1	P	85	ASN
1	P	106	PHE
1	P	113	LEU
1	P	133	ASN
1	P	144	PHE
1	Q	58	ILE

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Mol	Chain	Res	Type
1	Q	85	ASN
1	Q	106	PHE
1	Q	113	LEU
1	Q	133	ASN
1	Q	144	PHE
1	R	58	ILE
1	R	85	ASN
1	R	106	PHE
1	R	113	LEU
1	R	133	ASN
1	R	144	PHE
1	S	58	ILE
1	S	85	ASN
1	S	106	PHE
1	S	113	LEU
1	S	133	ASN
1	S	144	PHE
1	T	58	ILE
1	T	85	ASN
1	T	106	PHE
1	T	113	LEU
1	T	133	ASN
1	T	144	PHE
1	U	58	ILE
1	U	85	ASN
1	U	106	PHE
1	U	113	LEU
1	U	133	ASN
1	U	144	PHE
1	V	58	ILE
1	V	85	ASN
1	V	106	PHE
1	V	113	LEU
1	V	133	ASN
1	V	144	PHE
1	W	58	ILE
1	W	85	ASN
1	W	106	PHE
1	W	113	LEU
1	W	133	ASN
1	W	144	PHE
1	X	58	ILE

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Mol	Chain	Res	Type
1	X	85	ASN
1	X	106	PHE
1	X	113	LEU
1	X	133	ASN
1	X	144	PHE
1	Y	58	ILE
1	Y	85	ASN
1	Y	106	PHE
1	Y	113	LEU
1	Y	133	ASN
1	Y	144	PHE
1	Z	58	ILE
1	Z	85	ASN
1	Z	106	PHE
1	Z	113	LEU
1	Z	133	ASN
1	Z	144	PHE
2	a	20	GLU
2	a	110	MET
2	a	192	GLU
2	a	244	VAL
2	a	248	PRO
2	b	20	GLU
2	b	110	MET
2	b	192	GLU
2	b	244	VAL
2	b	248	PRO
2	c	20	GLU
2	c	110	MET
2	c	192	GLU
2	c	244	VAL
2	c	248	PRO
2	d	20	GLU
2	d	110	MET
2	d	192	GLU
2	d	244	VAL
2	d	248	PRO
2	e	20	GLU
2	e	110	MET
2	e	192	GLU
2	e	244	VAL
2	e	248	PRO

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Mol	Chain	Res	Type
2	f	20	GLU
2	f	110	MET
2	f	192	GLU
2	f	244	VAL
2	f	248	PRO
2	g	20	GLU
2	g	110	MET
2	g	192	GLU
2	g	244	VAL
2	g	248	PRO
2	h	20	GLU
2	h	110	MET
2	h	192	GLU
2	h	244	VAL
2	h	248	PRO
2	i	20	GLU
2	i	110	MET
2	i	192	GLU
2	i	244	VAL
2	i	248	PRO
2	j	20	GLU
2	j	110	MET
2	j	192	GLU
2	j	244	VAL
2	j	248	PRO
2	k	20	GLU
2	k	110	MET
2	k	192	GLU
2	k	244	VAL
2	k	248	PRO
2	l	20	GLU
2	l	110	MET
2	l	192	GLU
2	l	244	VAL
2	l	248	PRO
2	m	20	GLU
2	m	110	MET
2	m	192	GLU
2	m	244	VAL
2	m	248	PRO
2	n	20	GLU
2	n	110	MET

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Mol	Chain	Res	Type
2	n	192	GLU
2	n	244	VAL
2	n	248	PRO
2	o	20	GLU
2	o	110	MET
2	o	192	GLU
2	o	244	VAL
2	o	248	PRO
2	p	20	GLU
2	p	110	MET
2	p	192	GLU
2	p	244	VAL
2	p	248	PRO
2	q	20	GLU
2	q	110	MET
2	q	192	GLU
2	q	244	VAL
2	q	248	PRO
2	r	20	GLU
2	r	110	MET
2	r	192	GLU
2	r	244	VAL
2	r	248	PRO
2	s	20	GLU
2	s	110	MET
2	s	192	GLU
2	s	244	VAL
2	s	248	PRO
2	t	20	GLU
2	t	110	MET
2	t	192	GLU
2	t	244	VAL
2	t	248	PRO
2	u	20	GLU
2	u	110	MET
2	u	192	GLU
2	u	244	VAL
2	u	248	PRO
2	v	20	GLU
2	v	110	MET
2	v	192	GLU
2	v	244	VAL

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Mol	Chain	Res	Type
2	v	248	PRO
2	w	20	GLU
2	w	110	MET
2	w	192	GLU
2	w	244	VAL
2	w	248	PRO
2	x	20	GLU
2	x	110	MET
2	x	192	GLU
2	x	244	VAL
2	x	248	PRO
2	y	20	GLU
2	y	110	MET
2	y	192	GLU
2	y	244	VAL
2	y	248	PRO
2	z	20	GLU
2	z	110	MET
2	z	192	GLU
2	z	244	VAL
2	z	248	PRO
3	0	1	MET
3	0	9	LYS
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	75	VAL
3	1	106	MET
3	1	119	SER
3	1	164	GLN
3	1	206	PRO
3	2	179	MET
3	2	204	SER
3	3	43	ASP
3	3	109	ASP
3	3	244	SER
3	4	2	ILE

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Mol	Chain	Res	Type
3	4	64	SER
3	4	137	GLN
3	4	204	SER
3	4	209	ASN
3	4	259	GLN
3	5	4	SER
3	5	73	ARG
3	5	85	ASN
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	59	GLN
3	8	58	GLU
3	8	100	GLN
3	8	195	THR
3	8	256	LYS
3	9	106	MET
3	9	125	ASN
3	9	162	GLN
3	ZA	50	ARG
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	143	PRO
3	ZB	244	SER
3	ZC	123	ASP
3	ZC	244	SER
3	ZC	249	THR
3	ZD	1	MET
3	ZD	64	SER
3	ZD	162	GLN
3	ZD	240	TYR
3	ZE	37	GLN
3	ZE	50	ARG
3	ZE	137	GLN

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Mol	Chain	Res	Type
3	ZE	141	THR
3	ZE	259	GLN
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	ZF	392	GLN
4	ZG	3	PHE
4	ZG	38	SER
4	ZG	103	ASP
4	ZG	104	GLU
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	350	SER
4	ZG	352	ASN
4	ZG	395	ILE
4	ZH	34	SER
4	ZH	71	ARG
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

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Mol	Chain	Res	Type
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	46	SER
4	ZJ	96	ARG
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	ZJ	395	ILE
4	ZK	3	PHE
4	ZK	268	GLN
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
4	ZR	103	ASP
4	ZR	197	ASN
4	ZR	214	ASP
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	5	GLN
4	ZT	73	LEU
4	ZT	133	ASN
4	ZT	148	SER
4	ZT	195	ASP
4	ZT	262	SER
4	ZT	297	ASP
4	ZT	358	ASN
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	3	PHE
4	ZW	41	ASP
4	ZW	42	MET
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

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Mol	Chain	Res	Type
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	96	ARG
4	Za	103	ASP
4	Za	292	TYR
4	Za	331	ASP
4	Za	332	ASN
4	Za	375	MET
4	Zb	41	ASP
4	Zb	89	ASN
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

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Mol	Chain	Res	Type
4	Zd	292	TYR
4	Zd	375	MET
4	Zd	393	ASP
4	Zd	397	ASN
4	Ze	3	PHE
4	Ze	27	SER
4	Ze	46	SER
4	Ze	96	ARG
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	308	GLN
4	Zg	332	ASN
4	Zg	370	LYS
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	123	GLU
5	AA	247	LEU
5	AB	53	THR
5	AB	72	ASP
5	AB	97	GLU
5	AB	153	ASN
5	AB	225	ARG
5	AC	189	ARG
5	AC	200	ARG
5	AC	225	ARG
5	AD	47	ASP

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Mol	Chain	Res	Type
5	AD	49	LEU
5	AD	72	ASP
5	AD	140	ASP
5	AD	160	ARG
5	AD	169	ASN
5	AD	189	ARG
5	AE	51	LEU
5	AE	175	ASP
3	AF	4	SER
3	AF	6	TRP
3	AF	19	MET
3	AF	36	ARG
3	AF	44	LEU
3	AF	154	ASP
3	AG	6	TRP
3	AG	16	GLN
3	AG	36	ARG
3	AG	73	ARG
3	AG	127	GLN
3	AG	137	GLN
3	AG	138	PRO
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
3	AH	148	SER
3	AH	154	ASP
3	AH	179	MET
3	AH	195	THR
3	AH	208	LEU
3	AH	245	LYS
3	AI	4	SER
3	AI	30	SER
3	AI	123	ASP
3	AI	148	SER
3	AI	169	GLN
3	AI	173	LEU
3	AI	179	MET

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Mol	Chain	Res	Type
3	AI	195	THR
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	161	GLN
3	AJ	194	GLU
3	AJ	197	SER
3	AJ	198	SER
3	AJ	206	PRO
3	AJ	225	ASN
3	AK	36	ARG
3	AK	100	GLN
3	AK	137	GLN
3	AK	181	ASP
3	AK	203	GLU
3	AL	1	MET
3	AL	73	ARG
3	AL	111	THR
3	AL	170	VAL
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
3	AN	127	GLN
6	AR	274	ASN
6	AR	294	ARG

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Mol	Chain	Res	Type
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
6	AW	424	ASP
6	AX	274	ASN
6	AX	294	ARG

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Mol	Chain	Res	Type
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
7	Ab	69	MET
7	Ab	73	LEU
7	Ab	75	ASP
7	Ab	85	PRO
7	Ab	87	ILE
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

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Mol	Chain	Res	Type
6	Ad	377	MET
6	Ad	381	ASP
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

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Mol	Chain	Res	Type
6	Aj	377	MET
6	Aj	381	ASP
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

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Mol	Chain	Res	Type
6	Ap	377	MET
6	Ap	381	ASP
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	2	THR
7	Aq	47	MET
8	At	36	ARG
8	At	86	PHE
8	At	214	PHE
8	At	227	MET
8	At	229	MET
9	Au	38	TRP
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	116	PHE
9	Av	140	ARG

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Mol	Chain	Res	Type
9	Av	160	GLN
9	Av	162	PRO
9	Aw	135	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	152	ARG
9	Ax	187	PHE
9	Ax	205	MET
9	Ax	238	SER
9	Ax	241	GLN
9	Ay	65	THR
9	Ay	117	SER
9	Ay	140	ARG
9	Ay	144	GLU
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	77	LYS
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

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Mol	Chain	Res	Type
10	A4	101	SER
10	A4	102	MET
10	A5	15	GLN
10	A5	19	MET
10	A5	57	GLU
10	A5	91	LYS
10	A5	102	MET
11	A6	34	ASP
11	A6	101	ASP
11	A6	113	SER
11	A6	125	SER
11	A7	47	SER
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

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Mol	Chain	Res	Type
6	UL	98	LEU
6	UL	127	SER
6	UL	154	ARG
6	UL	159	MET
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	46	GLN
12	BB	123	LYS
12	BB	126	MET
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

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Mol	Chain	Res	Type
6	WC	128	GLU
6	WC	134	ARG
6	WC	164	LEU
6	WC	166	VAL
6	WC	168	GLU
6	WC	170	LYS
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

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Mol	Chain	Res	Type
6	WJ	165	PHE
6	WJ	167	ARG
6	WJ	169	GLN
6	WK	164	LEU
6	WK	165	PHE
6	WK	167	ARG
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

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Mol	Chain	Res	Type
6	WT	134	ARG
6	WT	159	MET
6	WT	165	PHE
6	WT	167	ARG
6	WU	114	GLU
6	WU	128	GLU
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	BC	119	LEU
12	BC	128	LYS
12	BD	3	LEU
12	BD	4	LEU
12	BD	30	ASN
12	BD	120	ASN
12	BE	20	ARG
12	BE	52	ASP
12	BE	84	LEU
12	BE	94	PRO
12	BF	38	ASP
12	BF	86	ASP
12	BF	88	ASN
12	BF	123	LYS
12	BF	125	MET
12	BF	127	LEU
6	BG	317	SER

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Mol	Chain	Res	Type
6	BG	322	PRO
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
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

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Mol	Chain	Res	Type
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 (984) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	142	ASN
1	A	160	ASN
1	A	173	GLN
1	A	214	ASN
1	A	217	GLN
1	A	223	GLN
1	B	130	ASN
1	B	142	ASN
1	B	160	ASN
1	B	173	GLN
1	B	214	ASN
1	B	217	GLN
1	B	223	GLN
1	C	130	ASN
1	C	142	ASN
1	C	160	ASN
1	C	173	GLN
1	C	214	ASN
1	C	217	GLN
1	C	223	GLN
1	D	130	ASN
1	D	142	ASN
1	D	160	ASN
1	D	173	GLN

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Mol	Chain	Res	Type
1	D	214	ASN
1	D	217	GLN
1	D	223	GLN
1	E	130	ASN
1	E	142	ASN
1	E	160	ASN
1	E	173	GLN
1	E	214	ASN
1	E	217	GLN
1	E	223	GLN
1	F	130	ASN
1	F	142	ASN
1	F	160	ASN
1	F	173	GLN
1	F	214	ASN
1	F	217	GLN
1	F	223	GLN
1	G	130	ASN
1	G	142	ASN
1	G	160	ASN
1	G	173	GLN
1	G	214	ASN
1	G	217	GLN
1	G	223	GLN
1	H	130	ASN
1	H	142	ASN
1	H	160	ASN
1	H	173	GLN
1	H	214	ASN
1	H	217	GLN
1	H	223	GLN
1	I	130	ASN
1	I	142	ASN
1	I	160	ASN
1	I	173	GLN
1	I	214	ASN
1	I	217	GLN
1	I	223	GLN
1	J	130	ASN
1	J	142	ASN
1	J	160	ASN
1	J	173	GLN

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Mol	Chain	Res	Type
1	J	214	ASN
1	J	217	GLN
1	J	223	GLN
1	K	130	ASN
1	K	142	ASN
1	K	160	ASN
1	K	173	GLN
1	K	214	ASN
1	K	217	GLN
1	K	223	GLN
1	L	130	ASN
1	L	142	ASN
1	L	160	ASN
1	L	173	GLN
1	L	214	ASN
1	L	217	GLN
1	M	130	ASN
1	M	142	ASN
1	M	160	ASN
1	M	173	GLN
1	M	214	ASN
1	M	217	GLN
1	M	223	GLN
1	N	130	ASN
1	N	142	ASN
1	N	160	ASN
1	N	173	GLN
1	N	214	ASN
1	N	217	GLN
1	N	223	GLN
1	O	130	ASN
1	O	142	ASN
1	O	160	ASN
1	O	173	GLN
1	O	214	ASN
1	O	217	GLN
1	O	223	GLN
1	P	130	ASN
1	P	139	ASN
1	P	142	ASN
1	P	160	ASN
1	P	173	GLN

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Mol	Chain	Res	Type
1	P	214	ASN
1	P	217	GLN
1	P	223	GLN
1	Q	130	ASN
1	Q	142	ASN
1	Q	160	ASN
1	Q	173	GLN
1	Q	214	ASN
1	Q	217	GLN
1	R	130	ASN
1	R	142	ASN
1	R	160	ASN
1	R	173	GLN
1	R	214	ASN
1	R	217	GLN
1	R	223	GLN
1	S	130	ASN
1	S	142	ASN
1	S	160	ASN
1	S	173	GLN
1	S	214	ASN
1	S	217	GLN
1	S	223	GLN
1	T	130	ASN
1	T	142	ASN
1	T	160	ASN
1	T	173	GLN
1	T	214	ASN
1	T	217	GLN
1	T	223	GLN
1	U	130	ASN
1	U	142	ASN
1	U	160	ASN
1	U	173	GLN
1	U	214	ASN
1	U	217	GLN
1	U	223	GLN
1	V	130	ASN
1	V	142	ASN
1	V	160	ASN
1	V	173	GLN
1	V	214	ASN

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Mol	Chain	Res	Type
1	V	217	GLN
1	V	223	GLN
1	W	130	ASN
1	W	142	ASN
1	W	160	ASN
1	W	173	GLN
1	W	214	ASN
1	W	217	GLN
1	W	223	GLN
1	X	130	ASN
1	X	142	ASN
1	X	160	ASN
1	X	173	GLN
1	X	214	ASN
1	X	217	GLN
1	Y	130	ASN
1	Y	142	ASN
1	Y	160	ASN
1	Y	173	GLN
1	Y	214	ASN
1	Y	217	GLN
1	Y	223	GLN
1	Z	130	ASN
1	Z	142	ASN
1	Z	160	ASN
1	Z	173	GLN
1	Z	214	ASN
1	Z	217	GLN
1	Z	223	GLN
2	a	63	ASN
2	a	80	GLN
2	a	140	ASN
2	a	159	GLN
2	a	178	GLN
2	a	188	GLN
2	a	350	GLN
2	b	54	GLN
2	b	63	ASN
2	b	140	ASN
2	b	159	GLN
2	b	178	GLN
2	b	188	GLN

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Mol	Chain	Res	Type
2	b	350	GLN
2	c	54	GLN
2	c	63	ASN
2	c	80	GLN
2	c	140	ASN
2	c	159	GLN
2	c	178	GLN
2	c	188	GLN
2	c	350	GLN
2	d	63	ASN
2	d	80	GLN
2	d	140	ASN
2	d	159	GLN
2	d	178	GLN
2	d	188	GLN
2	d	350	GLN
2	e	63	ASN
2	e	80	GLN
2	e	140	ASN
2	e	159	GLN
2	e	178	GLN
2	e	188	GLN
2	e	350	GLN
2	f	63	ASN
2	f	80	GLN
2	f	140	ASN
2	f	159	GLN
2	f	178	GLN
2	f	188	GLN
2	f	350	GLN
2	g	54	GLN
2	g	63	ASN
2	g	80	GLN
2	g	140	ASN
2	g	159	GLN
2	g	178	GLN
2	g	188	GLN
2	g	350	GLN
2	h	54	GLN
2	h	63	ASN
2	h	140	ASN
2	h	159	GLN

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Mol	Chain	Res	Type
2	h	178	GLN
2	h	188	GLN
2	h	350	GLN
2	i	54	GLN
2	i	63	ASN
2	i	80	GLN
2	i	140	ASN
2	i	159	GLN
2	i	178	GLN
2	i	188	GLN
2	i	350	GLN
2	j	63	ASN
2	j	80	GLN
2	j	140	ASN
2	j	159	GLN
2	j	178	GLN
2	j	188	GLN
2	j	350	GLN
2	k	54	GLN
2	k	63	ASN
2	k	140	ASN
2	k	159	GLN
2	k	178	GLN
2	k	188	GLN
2	k	350	GLN
2	l	63	ASN
2	l	140	ASN
2	l	159	GLN
2	l	178	GLN
2	l	188	GLN
2	l	350	GLN
2	m	63	ASN
2	m	140	ASN
2	m	159	GLN
2	m	178	GLN
2	m	188	GLN
2	m	350	GLN
2	n	54	GLN
2	n	63	ASN
2	n	140	ASN
2	n	159	GLN
2	n	178	GLN

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Mol	Chain	Res	Type
2	n	188	GLN
2	n	350	GLN
2	o	54	GLN
2	o	63	ASN
2	o	80	GLN
2	o	140	ASN
2	o	159	GLN
2	o	178	GLN
2	o	188	GLN
2	o	350	GLN
2	p	54	GLN
2	p	63	ASN
2	p	140	ASN
2	p	159	GLN
2	p	178	GLN
2	p	188	GLN
2	p	350	GLN
2	q	63	ASN
2	q	140	ASN
2	q	159	GLN
2	q	178	GLN
2	q	188	GLN
2	q	350	GLN
2	r	63	ASN
2	r	140	ASN
2	r	159	GLN
2	r	178	GLN
2	r	188	GLN
2	r	350	GLN
2	s	63	ASN
2	s	80	GLN
2	s	140	ASN
2	s	159	GLN
2	s	178	GLN
2	s	188	GLN
2	s	350	GLN
2	t	54	GLN
2	t	63	ASN
2	t	80	GLN
2	t	140	ASN
2	t	159	GLN
2	t	178	GLN

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Mol	Chain	Res	Type
2	t	188	GLN
2	t	350	GLN
2	u	54	GLN
2	u	63	ASN
2	u	140	ASN
2	u	159	GLN
2	u	178	GLN
2	u	188	GLN
2	u	350	GLN
2	v	63	ASN
2	v	140	ASN
2	v	159	GLN
2	v	178	GLN
2	v	188	GLN
2	v	350	GLN
2	w	63	ASN
2	w	80	GLN
2	w	140	ASN
2	w	159	GLN
2	w	178	GLN
2	w	188	GLN
2	w	350	GLN
2	x	51	GLN
2	x	63	ASN
2	x	80	GLN
2	x	140	ASN
2	x	159	GLN
2	x	178	GLN
2	x	188	GLN
2	x	350	GLN
2	y	54	GLN
2	y	63	ASN
2	y	80	GLN
2	y	140	ASN
2	y	159	GLN
2	y	178	GLN
2	y	188	GLN
2	y	350	GLN
2	z	54	GLN
2	z	63	ASN
2	z	80	GLN
2	z	140	ASN

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Mol	Chain	Res	Type
2	z	159	GLN
2	z	178	GLN
2	z	188	GLN
2	z	350	GLN
3	0	16	GLN
3	0	47	GLN
3	0	100	GLN
3	0	135	GLN
3	0	196	GLN
3	0	235	GLN
3	0	255	GLN
3	1	47	GLN
3	1	67	GLN
3	1	83	GLN
3	1	85	ASN
3	1	91	ASN
3	1	121	GLN
3	1	223	ASN
3	1	252	GLN
3	2	51	GLN
3	2	145	ASN
3	2	164	GLN
3	2	232	ASN
3	2	235	GLN
3	2	255	GLN
3	3	67	GLN
3	3	121	GLN
3	3	161	GLN
3	3	255	GLN
3	4	32	ASN
3	4	37	GLN
3	4	47	GLN
3	4	51	GLN
3	4	125	ASN
3	4	127	GLN
3	4	137	GLN
3	4	174	ASN
3	4	216	GLN
3	4	235	GLN
3	4	243	ASN
3	4	259	GLN
3	5	16	GLN

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Mol	Chain	Res	Type
3	5	55	GLN
3	5	100	GLN
3	5	121	GLN
3	5	237	GLN
3	6	59	GLN
3	6	121	GLN
3	6	127	GLN
3	6	135	GLN
3	6	137	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	24	ASN
3	8	28	ASN
3	8	83	GLN
3	8	91	ASN
3	9	37	GLN
3	9	55	GLN
3	9	85	ASN
3	9	91	ASN
3	9	127	GLN
3	9	259	GLN
3	ZA	37	GLN
3	ZA	137	GLN
3	ZA	235	GLN
3	ZB	24	ASN
3	ZB	25	ASN
3	ZB	28	ASN
3	ZB	37	GLN
3	ZB	104	GLN
3	ZB	135	GLN
3	ZB	137	GLN
3	ZB	237	GLN
3	ZC	16	GLN
3	ZC	37	GLN
3	ZC	88	GLN
3	ZC	100	GLN
3	ZC	137	GLN
3	ZD	24	ASN

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Mol	Chain	Res	Type
3	ZD	67	GLN
3	ZD	88	GLN
3	ZD	91	ASN
3	ZD	135	GLN
3	ZD	235	GLN
3	ZD	237	GLN
3	ZE	24	ASN
3	ZE	37	GLN
3	ZE	67	GLN
3	ZE	121	GLN
3	ZE	235	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	392	GLN
4	ZF	401	ASN
4	ZG	107	ASN
4	ZG	112	GLN
4	ZG	130	GLN
4	ZG	133	ASN
4	ZG	332	ASN
4	ZG	387	GLN
4	ZG	394	GLN
4	ZH	5	GLN
4	ZH	155	GLN
4	ZH	157	ASN
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	ZI	79	GLN
4	ZI	89	ASN
4	ZI	197	ASN
4	ZI	269	GLN
4	ZI	310	GLN
4	ZI	385	ASN

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Mol	Chain	Res	Type
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	ZK	89	ASN
4	ZK	107	ASN
4	ZK	197	ASN
4	ZK	252	ASN
4	ZK	270	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
4	ZL	310	GLN
4	ZL	338	GLN
4	ZL	394	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

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Mol	Chain	Res	Type
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	197	ASN
4	ZN	319	ASN
4	ZN	332	ASN
4	ZN	379	GLN
4	ZN	401	ASN
4	ZO	5	GLN
4	ZO	141	ASN
4	ZO	235	ASN
4	ZO	268	GLN
4	ZO	332	ASN
4	ZP	5	GLN
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	5	GLN
4	ZQ	89	ASN
4	ZQ	97	ASN
4	ZQ	133	ASN
4	ZQ	141	ASN
4	ZQ	155	GLN
4	ZQ	157	ASN
4	ZQ	197	ASN
4	ZQ	233	ASN
4	ZQ	338	GLN
4	ZQ	387	GLN
4	ZR	5	GLN
4	ZR	89	ASN

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Mol	Chain	Res	Type
4	ZR	107	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	192	ASN
4	ZS	197	ASN
4	ZS	387	GLN
4	ZS	394	GLN
4	ZT	99	GLN
4	ZT	129	GLN
4	ZT	190	GLN
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	97	ASN
4	ZU	99	GLN
4	ZU	107	ASN
4	ZU	133	ASN
4	ZU	159	ASN
4	ZU	190	GLN
4	ZU	268	GLN
4	ZU	269	GLN
4	ZU	293	GLN
4	ZU	379	GLN
4	ZV	5	GLN
4	ZV	107	ASN
4	ZV	133	ASN
4	ZV	197	ASN
4	ZV	280	ASN
4	ZV	303	ASN
4	ZV	314	GLN
4	ZV	381	ASN
4	ZV	387	GLN
4	ZV	394	GLN

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Mol	Chain	Res	Type
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	11	ASN
4	ZX	80	ASN
4	ZX	133	ASN
4	ZX	159	ASN
4	ZX	314	GLN
4	ZX	352	ASN
4	ZX	387	GLN
4	ZX	401	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	26	ASN
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	401	ASN
4	Za	115	GLN
4	Za	129	GLN
4	Za	157	ASN
4	Za	190	GLN
4	Za	197	ASN
4	Za	332	ASN
4	Za	385	ASN

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Mol	Chain	Res	Type
4	Zb	5	GLN
4	Zb	79	GLN
4	Zb	107	ASN
4	Zb	129	GLN
4	Zb	130	GLN
4	Zb	190	GLN
4	Zb	197	ASN
4	Zb	293	GLN
4	Zb	308	GLN
4	Zb	322	ASN
4	Zb	332	ASN
4	Zb	358	ASN
4	Zb	381	ASN
4	Zb	387	GLN
4	Zc	5	GLN
4	Zc	107	ASN
4	Zc	129	GLN
4	Zc	133	ASN
4	Zc	159	ASN
4	Zc	197	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	293	GLN
4	Zd	295	ASN
4	Zd	322	ASN
4	Zd	397	ASN
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	133	ASN
4	Zf	159	ASN
4	Zf	197	ASN
4	Zf	252	ASN
4	Zf	314	GLN

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Mol	Chain	Res	Type
4	Zf	397	ASN
4	Zg	5	GLN
4	Zg	107	ASN
4	Zg	129	GLN
4	Zg	133	ASN
4	Zg	197	ASN
4	Zg	310	GLN
4	Zh	5	GLN
4	Zh	115	GLN
4	Zh	129	GLN
4	Zh	197	ASN
4	Zh	379	GLN
4	Zh	392	GLN
5	AA	102	ASN
5	AB	18	GLN
5	AB	70	GLN
5	AB	106	GLN
5	AB	116	GLN
5	AB	172	GLN
5	AB	210	ASN
5	AB	223	ASN
5	AB	240	ASN
5	AC	14	GLN
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	AC	230	GLN
5	AD	17	ASN
5	AD	28	ASN
5	AD	104	ASN
5	AD	106	GLN
5	AD	210	ASN
5	AD	240	ASN
5	AE	18	GLN
5	AE	37	GLN
5	AE	104	ASN
5	AE	106	GLN
5	AE	112	GLN
5	AE	116	GLN

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Mol	Chain	Res	Type
5	AE	118	HIS
5	AE	153	ASN
5	AE	240	ASN
3	AF	47	GLN
3	AF	121	GLN
3	AF	135	GLN
3	AF	169	GLN
3	AF	172	GLN
3	AF	180	ASN
3	AF	223	ASN
3	AG	16	GLN
3	AG	28	ASN
3	AG	88	GLN
3	AG	145	ASN
3	AG	180	ASN
3	AG	259	GLN
3	AH	85	ASN
3	AH	104	GLN
3	AH	127	GLN
3	AH	137	GLN
3	AH	172	GLN
3	AH	174	ASN
3	AH	196	GLN
3	AH	259	GLN
3	AI	16	GLN
3	AI	32	ASN
3	AI	47	GLN
3	AI	67	GLN
3	AI	104	GLN
3	AI	162	GLN
3	AI	209	ASN
3	AI	235	GLN
3	AJ	47	GLN
3	AJ	67	GLN
3	AJ	90	ASN
3	AJ	125	ASN
3	AJ	127	GLN
3	AJ	137	GLN
3	AJ	169	GLN
3	AJ	172	GLN
3	AJ	174	ASN
3	AJ	232	ASN

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Mol	Chain	Res	Type
3	AJ	252	GLN
3	AK	28	ASN
3	AK	47	GLN
3	AK	104	GLN
3	AK	121	GLN
3	AK	135	GLN
3	AK	145	ASN
3	AK	174	ASN
3	AK	196	GLN
3	AK	202	ASN
3	AK	223	ASN
3	AK	235	GLN
3	AL	32	ASN
3	AL	47	GLN
3	AL	83	GLN
3	AL	127	GLN
3	AL	145	ASN
3	AL	209	ASN
3	AM	25	ASN
3	AM	37	GLN
3	AM	51	GLN
3	AM	67	GLN
3	AM	125	ASN
3	AM	127	GLN
3	AM	137	GLN
3	AM	209	ASN
3	AM	223	ASN
3	AM	252	GLN
3	AN	67	GLN
3	AN	125	ASN
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

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Mol	Chain	Res	Type
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
6	Af	303	GLN
6	Af	365	ASN
6	Af	374	HIS
6	Af	434	ASN
6	Ag	297	GLN
6	Ag	303	GLN
6	Ag	374	HIS
6	Ag	434	ASN
6	Ah	303	GLN
6	Ah	374	HIS
6	Ai	303	GLN
6	Ai	374	HIS
6	Ai	434	ASN
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

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Mol	Chain	Res	Type
6	Am	374	HIS
6	Am	434	ASN
6	An	303	GLN
6	An	374	HIS
6	An	434	ASN
6	Ao	374	HIS
6	Ao	434	ASN
6	Ap	374	HIS
6	AO	297	GLN
6	AO	303	GLN
6	AO	374	HIS
6	AP	297	GLN
6	AP	299	ASN
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
8	At	182	ASN
8	At	205	ASN
9	Au	119	GLN
9	Au	141	GLN
9	Aw	36	GLN
9	Aw	132	GLN
9	Aw	160	GLN
9	Aw	233	GLN
9	Ax	160	GLN
9	Ax	184	GLN
9	Ax	233	GLN
9	Ay	114	GLN
9	Ay	155	ASN
9	Ay	241	GLN
10	Az	69	ASN
10	Az	83	GLN
10	Az	103	GLN
10	A1	15	GLN
10	A1	87	GLN
10	A1	90	ASN
10	A2	103	GLN
10	A3	87	GLN

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Mol	Chain	Res	Type
10	A4	55	GLN
11	A6	17	ASN
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	A9	17	ASN
11	A9	21	GLN
11	A9	32	ASN
11	A9	72	HIS
11	A9	76	GLN
11	A9	117	GLN
11	A0	72	HIS
11	A0	76	GLN
11	A0	112	ASN
6	UI	196	HIS
6	UJ	245	HIS
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	5	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

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Mol	Chain	Res	Type
6	WP	209	ASN
6	WT	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	BD	22	ASN
12	BE	17	GLN
12	BE	30	ASN
12	BF	57	GLN
12	BF	115	ASN
6	BG	318	ASN
6	BG	319	GLN
6	BI	319	GLN
6	BJ	324	ASN
6	BO	318	ASN
6	BQ	319	GLN
6	BQ	324	ASN
6	BR	303	GLN
6	BR	374	HIS
6	BS	303	GLN
6	BS	374	HIS
6	BT	303	GLN
6	BT	374	HIS
6	BU	303	GLN
6	BU	374	HIS
6	BV	303	GLN
6	BV	374	HIS
6	BW	303	GLN
6	BW	374	HIS
6	BX	297	GLN
6	BX	303	GLN
6	BX	374	HIS

5.3.3 RNA

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.

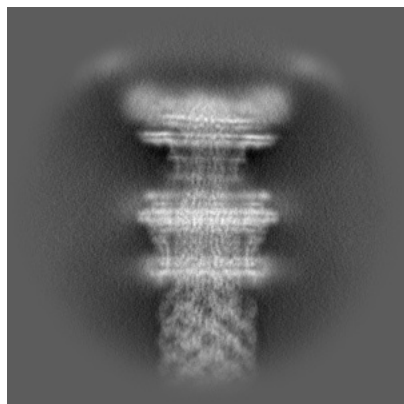
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37630. These allow visual inspection of the internal detail of the map and identification of artifacts.

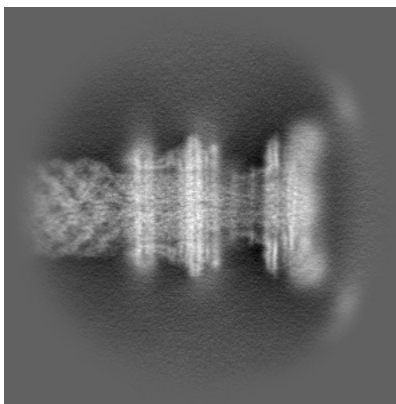
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

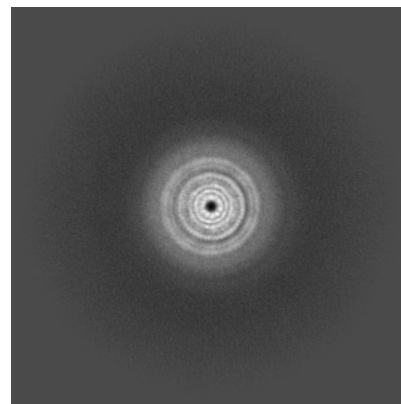
6.1.1 Primary map



X

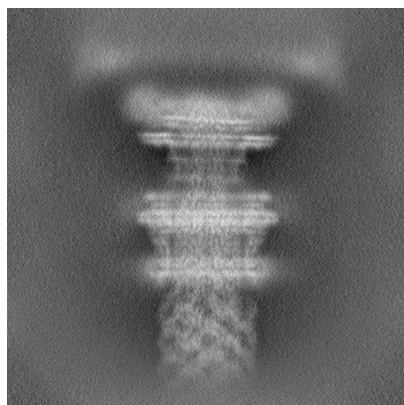


Y

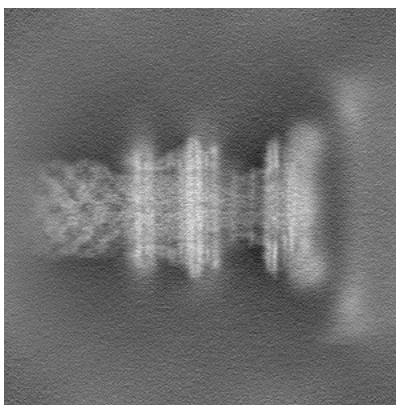


Z

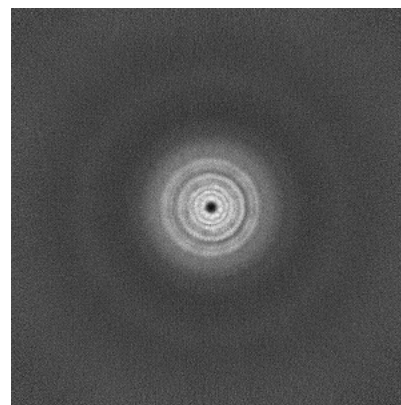
6.1.2 Raw map



X



Y

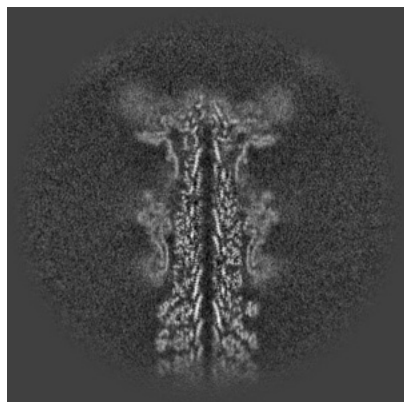


Z

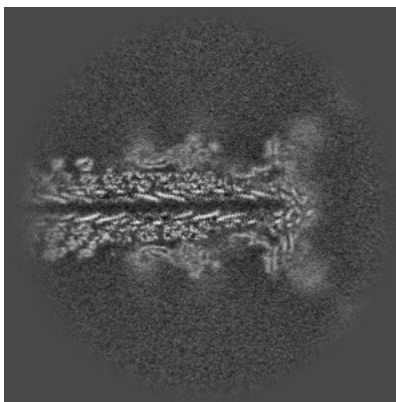
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

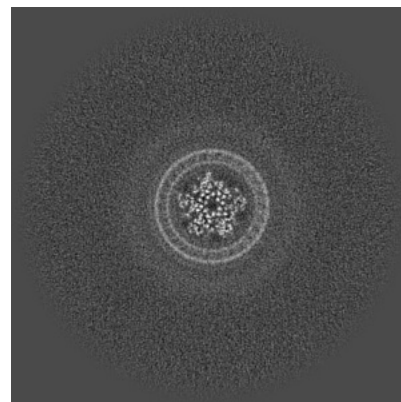
6.2.1 Primary map



X Index: 256

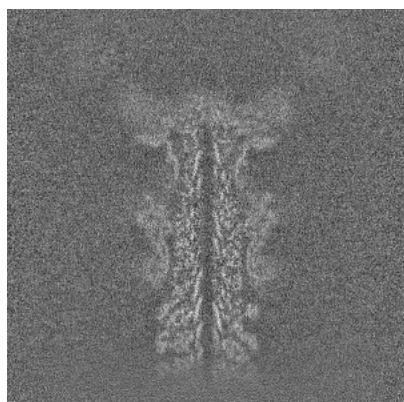


Y Index: 256

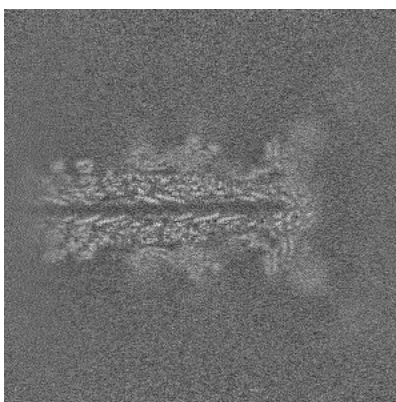


Z Index: 256

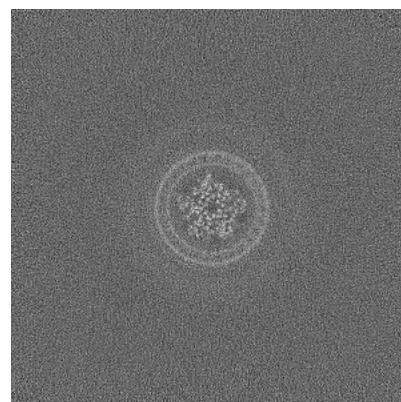
6.2.2 Raw map



X Index: 256



Y Index: 256

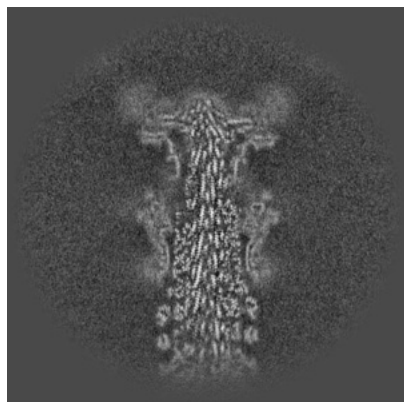


Z Index: 256

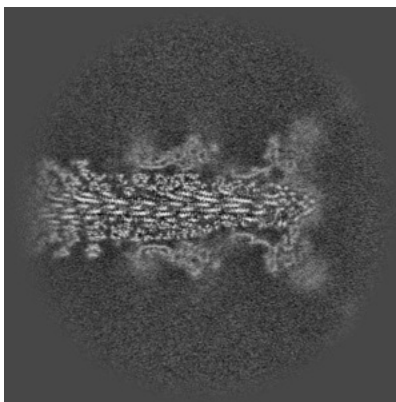
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

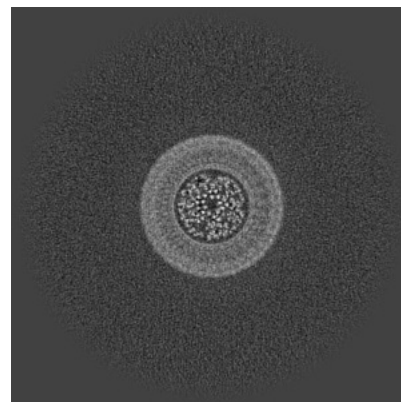
6.3.1 Primary map



X Index: 247

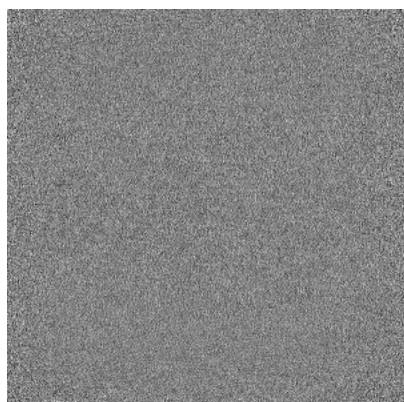


Y Index: 246

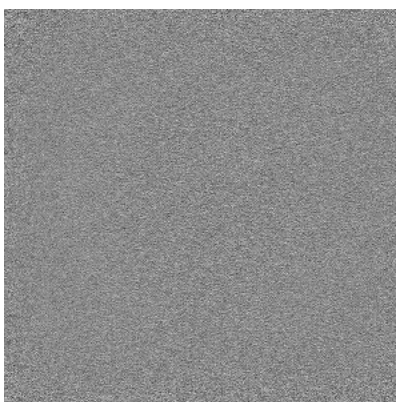


Z Index: 239

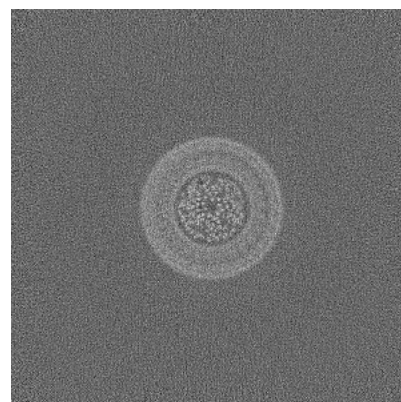
6.3.2 Raw map



X Index: 0



Y Index: 0

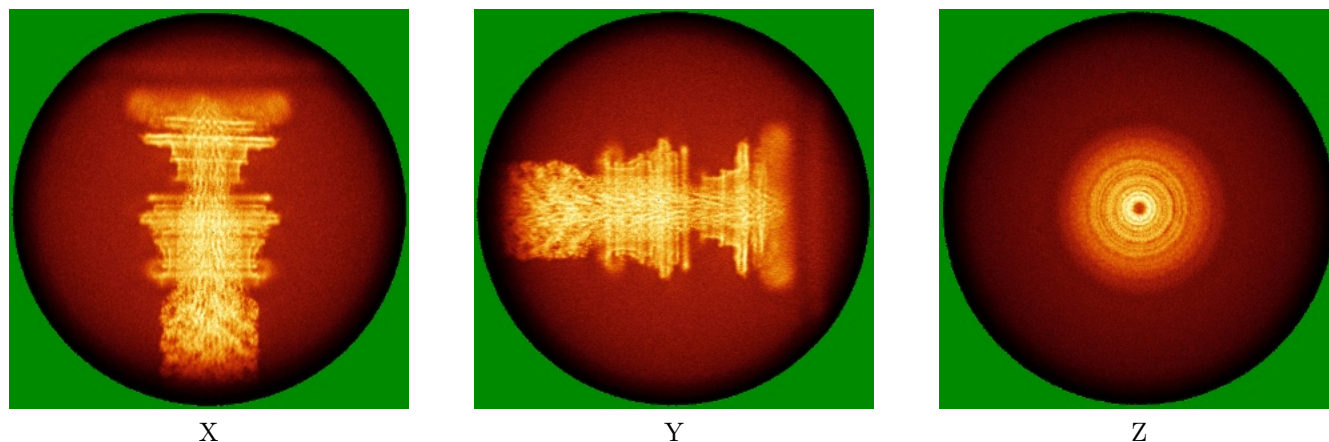


Z Index: 240

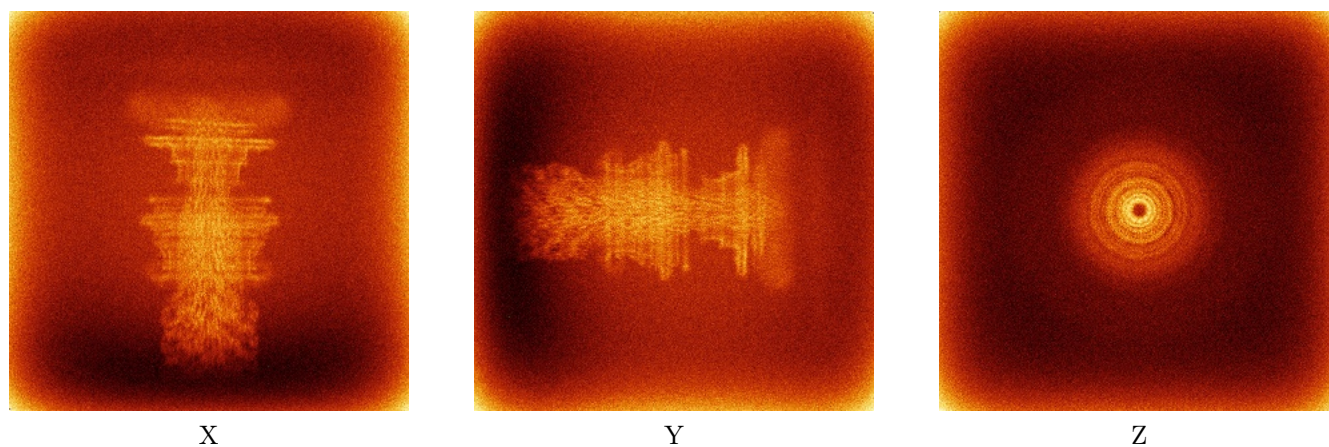
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



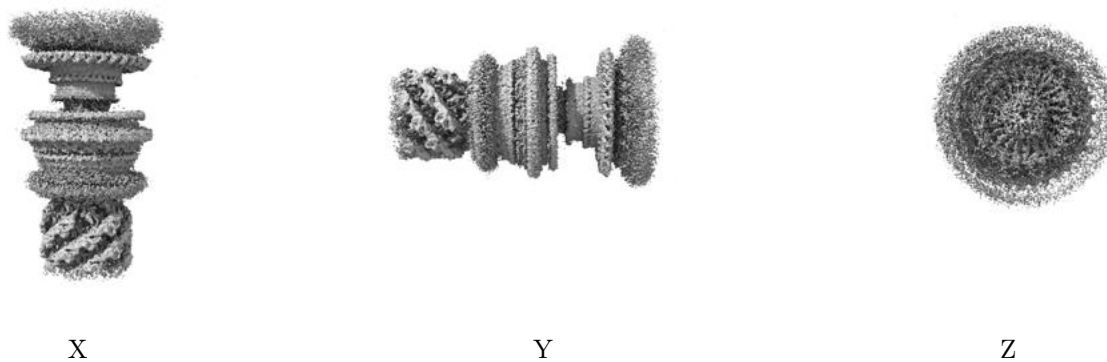
6.4.2 Raw map



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

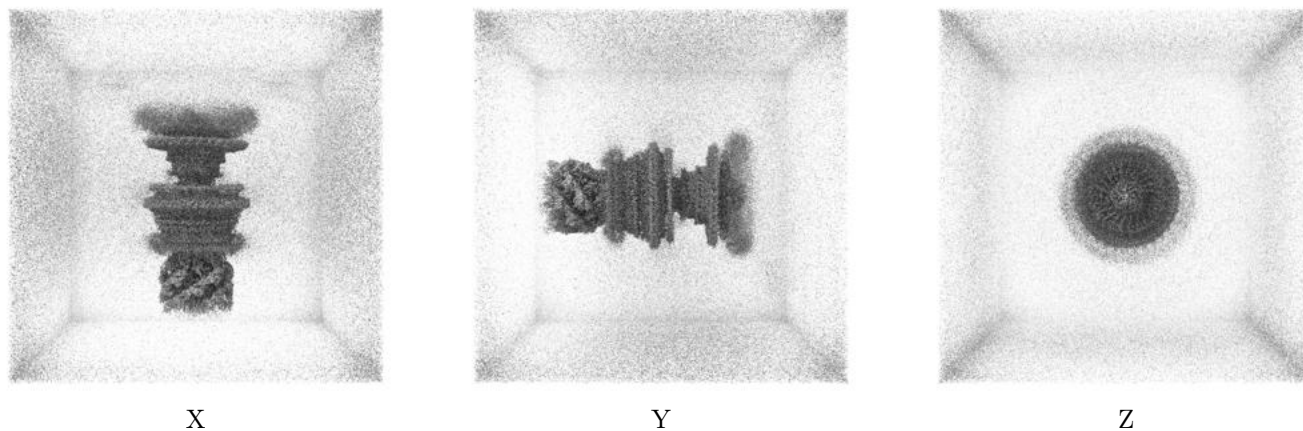
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

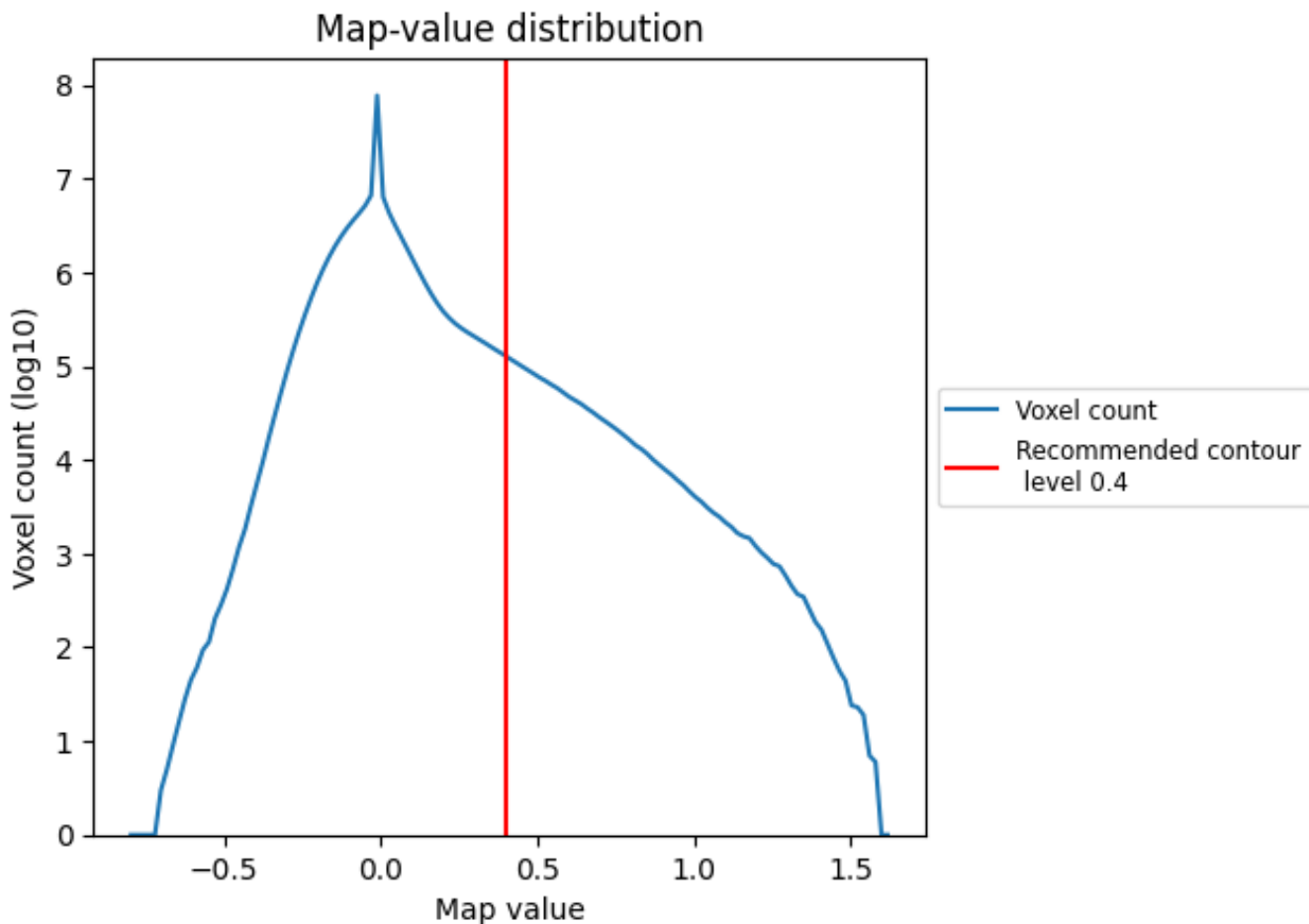
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

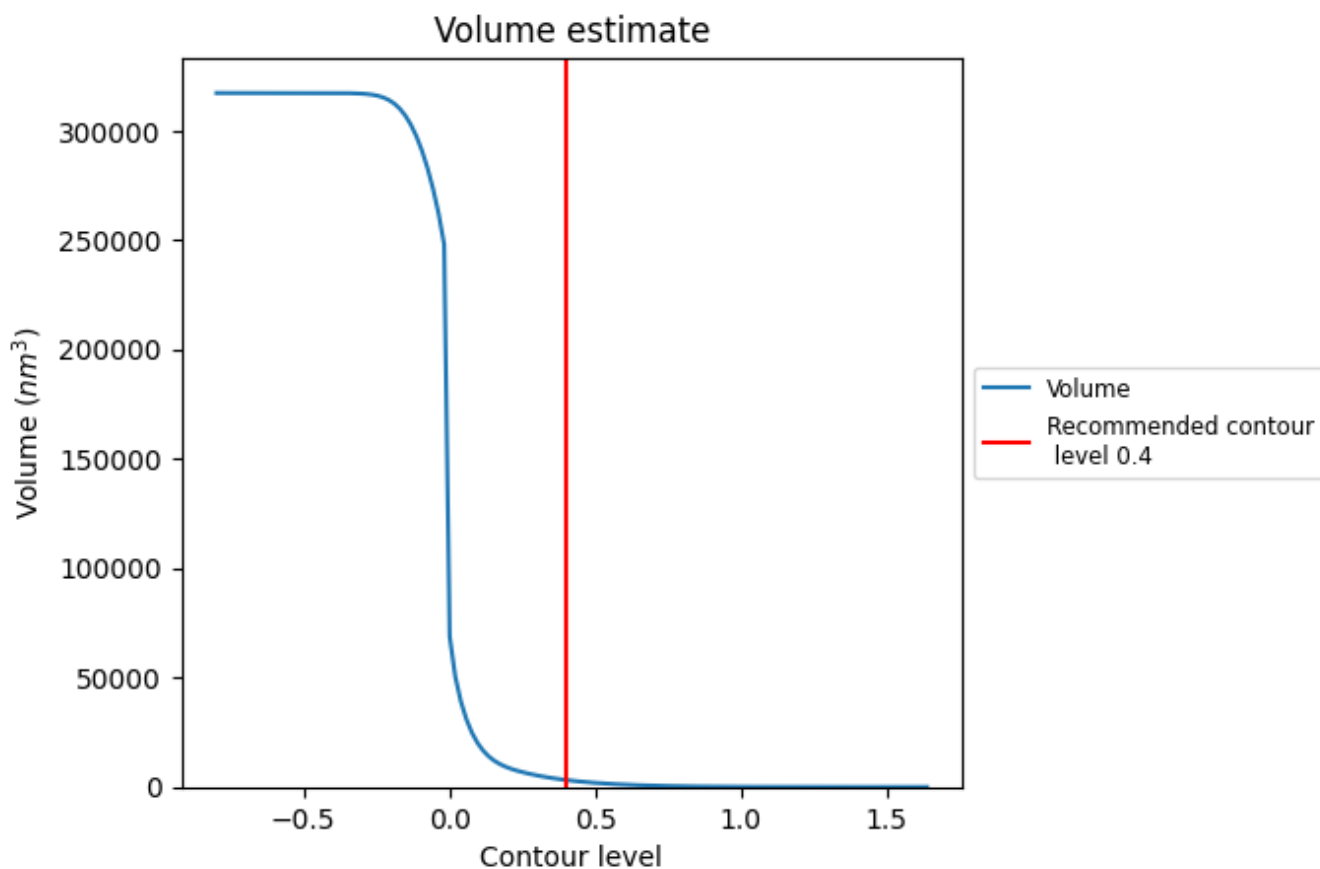
This section contains the results of statistical analysis of the map.

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.

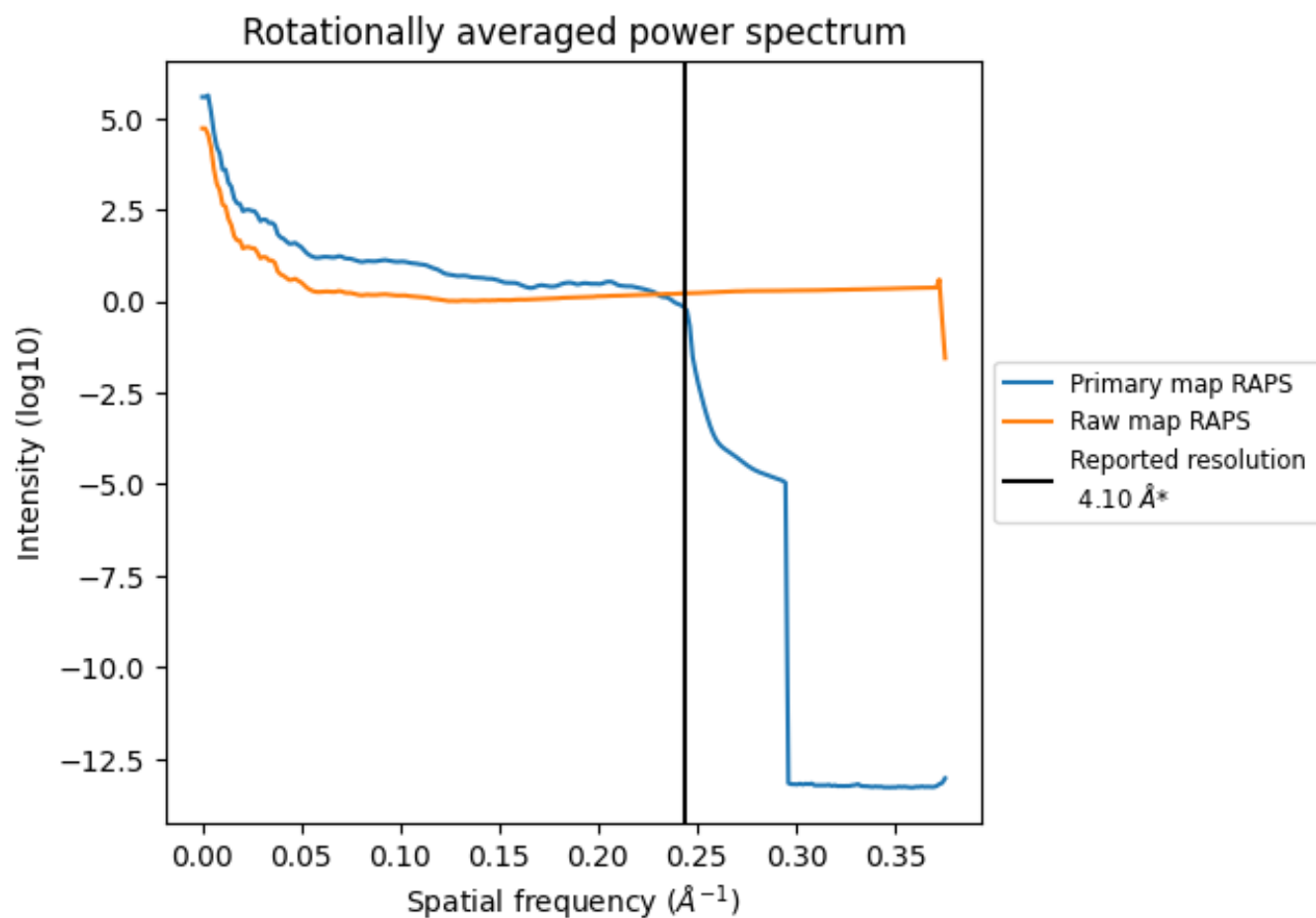
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3185 nm³; this corresponds to an approximate mass of 2877 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

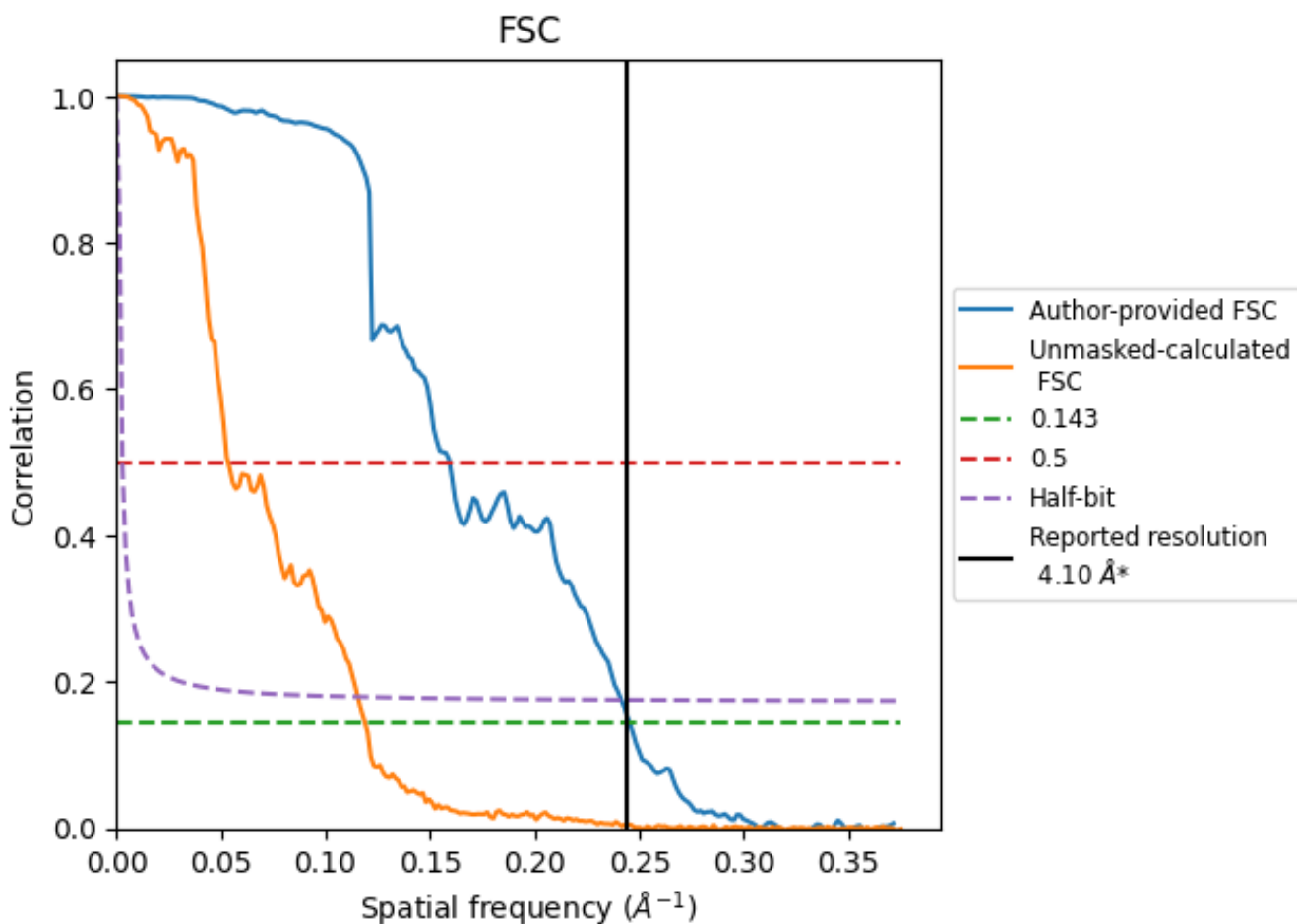


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

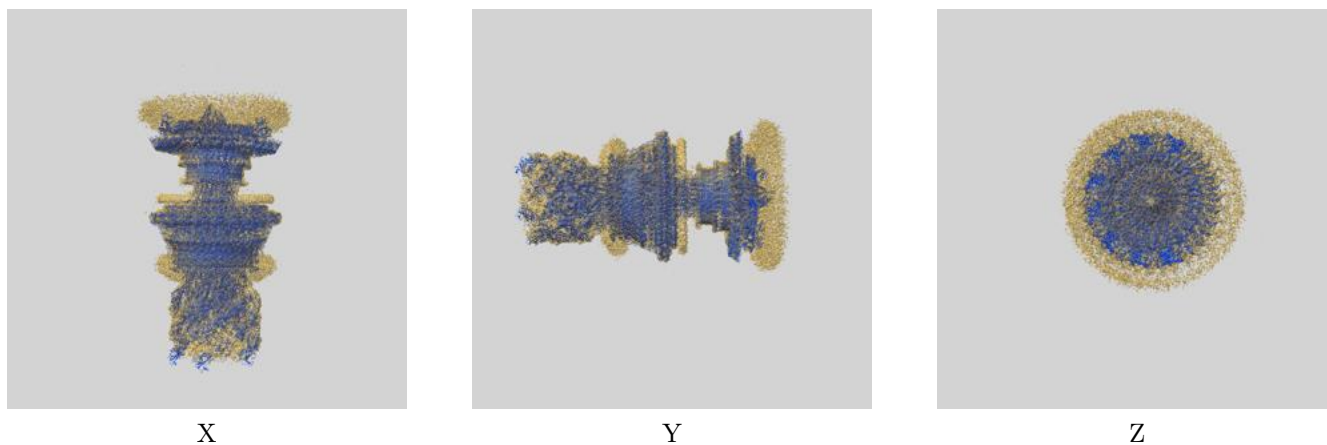
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.07	6.28	4.14
Unmasked-calculated*	8.41	18.73	8.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.41 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

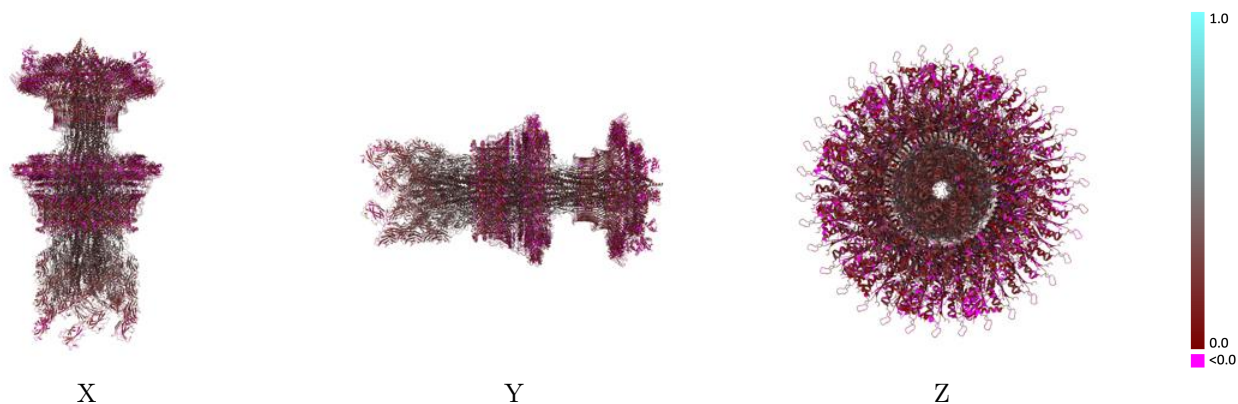
This section contains information regarding the fit between EMDB map EMD-37630 and PDB model 8WLT. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



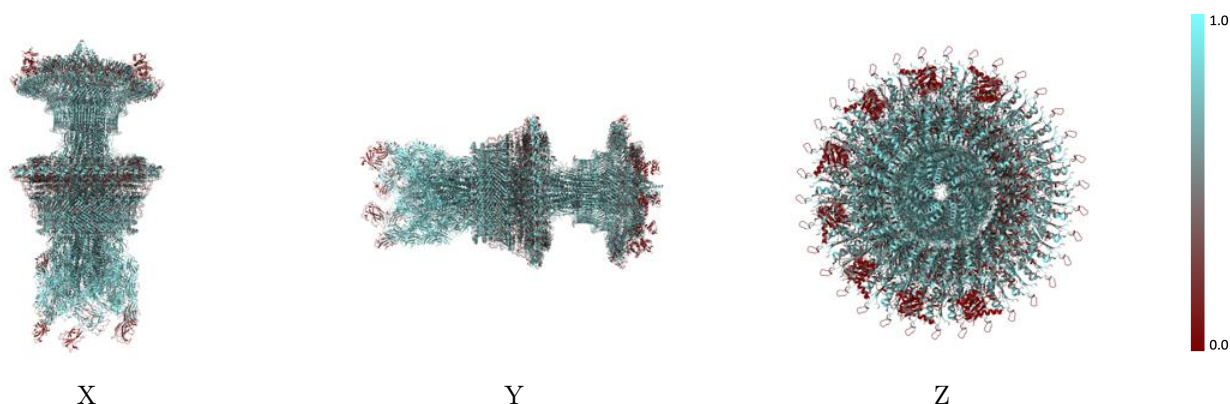
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



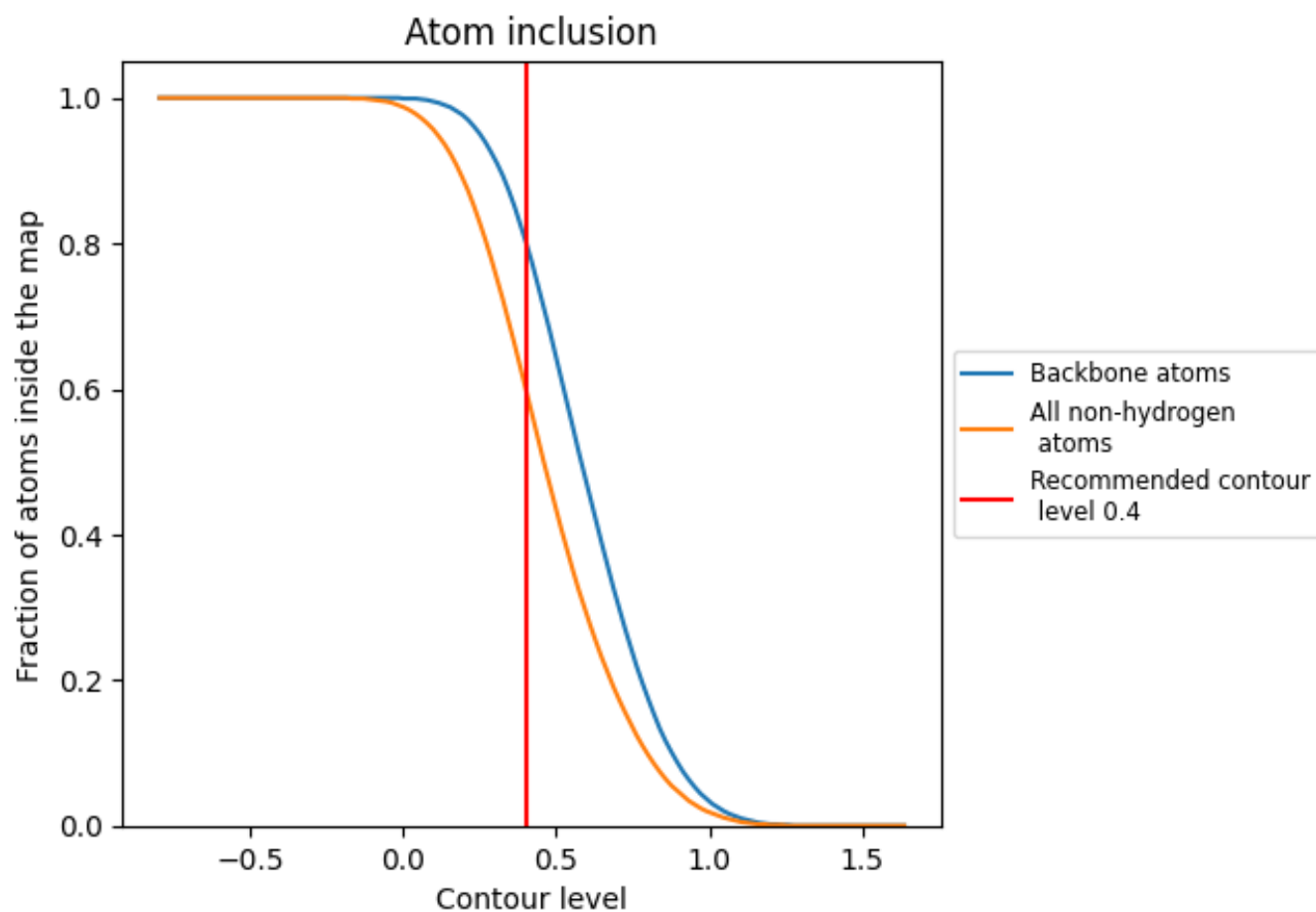
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 60% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6010	 0.2210
0	 0.6940	 0.3430
1	 0.6920	 0.3390
2	 0.6780	 0.3430
3	 0.6990	 0.3360
4	 0.7050	 0.3390
5	 0.6890	 0.3410
6	 0.7000	 0.3430
7	 0.7050	 0.3460
8	 0.7000	 0.3440
9	 0.6990	 0.3440
A	 0.5000	 0.1420
A0	 0.6570	 0.3040
A1	 0.6240	 0.2630
A2	 0.6620	 0.2750
A3	 0.6410	 0.2660
A4	 0.6090	 0.2540
A5	 0.6020	 0.2560
A6	 0.6260	 0.2980
A7	 0.6680	 0.2990
A8	 0.6560	 0.2990
A9	 0.6780	 0.2950
AA	 0.6770	 0.3340
AB	 0.7270	 0.3410
AC	 0.7260	 0.3560
AD	 0.7180	 0.3410
AE	 0.7100	 0.3340
AF	 0.6820	 0.3310
AG	 0.7090	 0.3440
AH	 0.7040	 0.3490
AI	 0.7050	 0.3470
AJ	 0.6920	 0.3430
AK	 0.6950	 0.3430
AL	 0.6840	 0.3310
AM	 0.6980	 0.3480























































































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Chain	Atom inclusion	Q-score
AN	0.6980	0.3400
AO	0.6000	0.1490
AP	0.5970	0.1380
AQ	0.5990	0.1500
AR	0.6430	0.1560
AS	0.6100	0.1490
AT	0.6400	0.1730
AU	0.6380	0.1670
AV	0.6220	0.1490
AW	0.6150	0.1550
AX	0.6250	0.1600
AY	0.6250	0.1370
AZ	0.6350	0.1560
Aa	0.6330	0.1520
Ab	0.5990	0.2220
Ac	0.6450	0.1550
Ad	0.6390	0.1510
Ae	0.6260	0.1520
Af	0.6320	0.1300
Ag	0.6360	0.1470
Ah	0.6350	0.1320
Ai	0.6330	0.1440
Aj	0.6180	0.1450
Ak	0.6020	0.1370
Al	0.6030	0.1530
Am	0.6070	0.1450
An	0.6020	0.1370
Ao	0.5850	0.1270
Ap	0.5980	0.1500
Aq	0.6660	0.2410
Ar	0.6660	0.2290
As	0.6500	0.2090
At	0.6460	0.2490
Au	0.6580	0.2420
Av	0.6730	0.2690
Aw	0.6880	0.2770
Ax	0.6800	0.2750
Ay	0.6610	0.2730
Az	0.5230	0.2200
B	0.4930	0.1220
BA	0.6650	0.3090
BB	0.6940	0.3290

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Chain	Atom inclusion	Q-score
BC	 0.7000	 0.3350
BD	 0.6860	 0.3390
BE	 0.6960	 0.3350
BF	 0.6890	 0.3090
BG	 0.5430	 0.3200
BH	 0.6410	 0.3630
BI	 0.6240	 0.3380
BJ	 0.7670	 0.3940
BK	 0.7360	 0.3660
BL	 0.6800	 0.3550
BM	 0.7290	 0.3910
BN	 0.6800	 0.3410
BO	 0.7520	 0.4020
BP	 0.6700	 0.3130
BQ	 0.6500	 0.3280
BR	 0.5940	 0.1420
BS	 0.5910	 0.1320
BT	 0.6110	 0.1480
BU	 0.6150	 0.1570
BV	 0.6070	 0.1450
BW	 0.6270	 0.1610
BX	 0.6100	 0.1560
C	 0.5140	 0.1440
D	 0.5180	 0.1420
E	 0.5030	 0.1370
F	 0.5050	 0.1320
G	 0.5180	 0.1380
H	 0.5290	 0.1420
I	 0.5420	 0.1350
J	 0.5330	 0.1450
K	 0.5290	 0.1490
L	 0.5400	 0.1490
M	 0.5420	 0.1610
N	 0.5320	 0.1480
O	 0.5220	 0.1300
P	 0.5240	 0.1450
Q	 0.5360	 0.1470
R	 0.5220	 0.1420
S	 0.5400	 0.1290
T	 0.5110	 0.1390
U	 0.5270	 0.1470
UI	 0.1300	 0.0680





















































































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Chain	Atom inclusion	Q-score
UJ	0.1340	0.0770
UK	0.1080	0.0850
UL	0.1020	0.0320
UM	0.0690	0.0500
UN	0.1330	0.0700
UO	0.1360	0.0810
UP	0.1950	0.0760
V	0.5270	0.1490
W	0.5200	0.1430
WA	0.6210	0.1920
WB	0.6410	0.2010
WC	0.6490	0.2210
WD	0.6120	0.1780
WE	0.6320	0.1860
WF	0.5930	0.1650
WG	0.5140	0.1550
WH	0.4740	0.1420
WI	0.4840	0.1480
WJ	0.4820	0.1460
WK	0.3380	0.1160
WL	0.3880	0.1150
WM	0.4870	0.1190
WN	0.4520	0.1200
WO	0.4240	0.1050
WP	0.5660	0.1610
WQ	0.5480	0.1810
WR	0.5700	0.1690
WS	0.6120	0.2160
WT	0.6190	0.1870
WU	0.5990	0.2010
WV	0.6180	0.2050
WW	0.6090	0.1940
X	0.5190	0.1620
Y	0.5070	0.1390
Z	0.5150	0.1530
ZA	0.7070	0.3440
ZB	0.7120	0.3440
ZC	0.7230	0.3510
ZD	0.7050	0.3420
ZE	0.6980	0.3410
ZF	0.5380	0.2920
ZG	0.7300	0.3270

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Chain	Atom inclusion	Q-score
ZH	 0.7480	 0.3250
ZI	 0.7530	 0.3290
ZJ	 0.7500	 0.3260
ZK	 0.7630	 0.3230
ZL	 0.7550	 0.3280
ZM	 0.7440	 0.3180
ZN	 0.7530	 0.3170
ZO	 0.7570	 0.3160
ZP	 0.7510	 0.3160
ZQ	 0.7460	 0.3080
ZR	 0.7440	 0.3050
ZS	 0.7540	 0.3060
ZT	 0.7450	 0.3010
ZU	 0.7320	 0.2980
ZV	 0.7400	 0.2950
ZW	 0.7290	 0.2830
ZX	 0.7140	 0.2830
ZY	 0.7090	 0.2760
ZZ	 0.6810	 0.2700
Za	 0.6710	 0.2720
Zb	 0.6320	 0.2480
Zc	 0.6290	 0.2530
Zd	 0.5790	 0.2460
Ze	 0.5240	 0.2320
Zf	 0.5060	 0.2320
Zg	 0.4670	 0.2100
Zh	 0.4390	 0.2040
a	 0.4680	 0.1160
b	 0.4770	 0.1300
c	 0.4540	 0.1230
d	 0.4850	 0.1250
e	 0.4730	 0.1230
f	 0.4860	 0.1360
g	 0.5150	 0.1260
h	 0.5190	 0.1440
i	 0.5260	 0.1450
j	 0.5220	 0.1390
k	 0.5320	 0.1400
l	 0.5100	 0.1340
m	 0.5050	 0.1400
n	 0.4890	 0.1230
o	 0.5040	 0.1430

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Chain	Atom inclusion	Q-score
p	█ 0.5020	█ 0.1290
q	█ 0.4840	█ 0.1170
r	█ 0.4790	█ 0.1220
s	█ 0.4910	█ 0.1180
t	█ 0.4890	█ 0.1330
u	█ 0.4570	█ 0.1090
v	█ 0.4730	█ 0.1200
w	█ 0.4790	█ 0.1150
x	█ 0.4520	█ 0.1060
y	█ 0.4510	█ 0.1040
z	█ 0.4600	█ 0.1200