Full wwPDB EM Validation Report (i)

Aug 28, 2024 – 01:12 AM JST

PDB ID	:	8WOE
EMDB ID	:	EMD-37684
Title	:	Cryo-EM structure of the intact flagellar motor-hook complex in the CW state
Authors	:	Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on	:	2023-10-07
Resolution	:	4.30 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 (i) symbol.

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

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

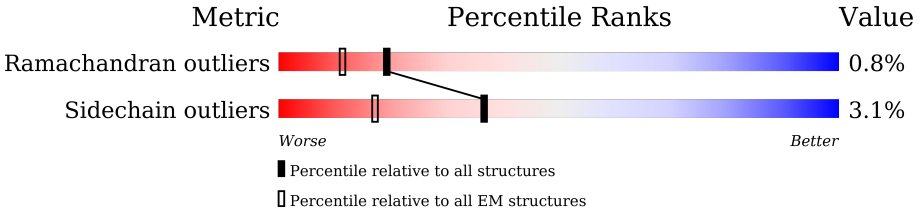
EMDB validation analysis	:	0.0.1.dev112
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	260	92% • • 5%
1	1	260	93% • •
1	2	260	98% •
1	3	260	98% •
1	4	260	97% •
1	5	260	97% •
1	6	260	97% •
1	7	260	98% •
1	8	260	98% •

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Mol	Chain	Length	Quality of chain
1	9	260	97%
1	AF	260	95%
1	AG	260	95%
1	AH	260	94%
1	AI	260	93% 5%
1	AJ	260	95%
1	AK	260	92% 7%
1	AL	260	92% 5%
1	AM	260	92% 5%
1	AN	260	93% 5%
1	ZA	260	98%
1	ZB	260	96%
1	ZC	260	98%
1	ZD	260	98%
1	ZE	260	99%
2	A	232	88% 9%
2	B	232	88% 9%
2	C	232	88% 9%
2	D	232	88% 9%
2	E	232	88% 9%
2	F	232	87% 9%
2	G	232	88% 9%
2	H	232	88% 9%
2	I	232	88% 9%
2	J	232	88% 9%

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Mol	Chain	Length	Quality of chain
2	K	232	88% 9%
2	L	232	88% 9%
2	M	232	88% 9%
2	N	232	88% 9%
2	O	232	88% 9%
2	P	232	88% 9%
2	Q	232	88% 9%
2	R	232	88% 9%
2	S	232	88% 9%
2	T	232	88% 9%
2	U	232	88% 9%
2	V	232	88% 9%
2	W	232	88% 9%
2	X	232	88% 9%
2	Y	232	88% 9%
2	Z	232	88% 9%
3	A0	138	85% 11%
3	A6	138	12% 93%
3	A7	138	7% 86% 12%
3	A8	138	8% 86% 5% 9%
3	A9	138	7% 91% 8%
4	A1	104	7% 84% 12%
4	A2	104	85% 5% 11%
4	A3	104	86% 11%
4	A4	104	86% 11%

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Mol	Chain	Length	Quality of chain
4	A5	104	85% 12%
4	Az	104	52% 5% 43%
5	AA	251	13% 96%
5	AB	251	8% 98%
5	AC	251	5% 97%
5	AD	251	99%
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%

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Mol	Chain	Length	Quality of chain
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%
6	An	560	28% 71%
6	Ao	560	28% 71%
6	Ap	560	28% 71%
6	B0	560	5% 95%
6	B3	560	5% 95%
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	28% 71%
6	BS	560	28% 71%
6	BT	560	28% 71%

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Mol	Chain	Length	Quality of chain
6	BU	560	28% 71%
6	BV	560	28% 71%
6	BW	560	28% 71%
6	BX	560	28% 71%
6	Ba	560	5% 95%
6	Bh	560	5% 95%
6	Bo	560	5% 95%
6	Bv	560	5% 95%
6	CG	560	5% 95%
6	CN	560	5% 95%
6	CU	560	5% 95%
6	Cb	560	5% 95%
6	Ci	560	5% 95%
6	Cp	560	5% 95%
6	Cw	560	5% 95%
6	DE	560	5% 95%
6	DL	560	5% 95%
6	EH	560	5% 95%
6	EO	560	5% 95%
6	EV	560	5% 95%
6	Ea	560	5% 95%
6	Eb	560	5% 95%
6	Ec	560	5% 95%
6	Ed	560	5% 95%
6	Ee	560	5% 95%

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Mol	Chain	Length	Quality of chain
6	Ef	560	5% 95%
6	Eg	560	5% 95%
6	Eh	560	5% 95%
6	Ei	560	5% 95%
6	Ej	560	5% 95%
6	Ek	560	5% 95%
6	El	560	5% 95%
6	Em	560	5% 95%
6	En	560	5% 95%
6	Eo	560	5% 95%
6	Ep	560	5% 95%
6	UI	560	25% 72%
6	UJ	560	25% 72%
6	UK	560	25% 72%
6	UL	560	25% 72%
6	UM	560	25% 72%
6	UN	560	25% 72%
6	UO	560	25% 72%
6	UP	560	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	18% 80%

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Mol	Chain	Length	Quality of chain
6	WG	560	18% 80%
6	WH	560	16% 83%
6	WI	560	15% 83%
6	WJ	560	16% 82%
6	WK	560	16% 82%
6	WL	560	14% 85%
6	WM	560	14% 85%
6	WN	560	14% 85%
6	WO	560	16% 83%
6	WP	560	16% 82%
6	WQ	560	18% 80%
6	WR	560	17% 80%
6	WS	560	18% 80%
6	WT	560	17% 80%
6	WU	560	19% 80%
6	WV	560	17% 80%
6	WW	560	18% 80%
7	Ab	89	99%
7	Aq	89	99%
7	Ar	89	100%
7	As	89	99%
8	At	264	91%
9	Au	245	81% 16%
9	Av	245	82% 15%
9	Aw	245	83% 15%

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Mol	Chain	Length	Quality of chain
9	Ax	245	82% 15%
9	Ay	245	5% 83% 15%
10	BA	134	5% 99%
10	BB	134	5% 98%
10	BC	134	99%
10	BD	134	96%
10	BE	134	96%
10	BF	134	96%
11	ZF	403	28% 97%
11	ZG	403	24% 95%
11	ZH	403	22% 97%
11	ZI	403	17% 97%
11	ZJ	403	9% 98%
11	ZK	403	5% 98%
11	ZL	403	97%
11	ZM	403	97%
11	ZN	403	97%
11	ZO	403	97%
11	ZP	403	95%
11	ZQ	403	97%
11	ZR	403	97%
11	ZS	403	98%
11	ZT	403	98%
11	ZU	403	99%
11	ZV	403	98%

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Mol	Chain	Length	Quality of chain
11	ZW	403	96%
11	ZX	403	7%, 99%
11	ZY	403	10%, 98%
11	ZZ	403	13%, 98%
11	Za	403	17%, 98%
11	Zb	403	20%, 98%
11	Zc	403	24%, 97%
11	Zd	403	29%, 98%
11	Ze	403	31%, 97%
11	Zf	403	34%, 98%
11	Zg	403	37%, 98%
11	Zh	403	38%, 98%
12	a	365	80%, 17%
12	b	365	80%, 17%
12	c	365	80%, 17%
12	d	365	80%, 17%
12	e	365	80%, 17%
12	f	365	80%, 17%
12	g	365	80%, 17%
12	h	365	80%, 17%
12	i	365	80%, 17%
12	j	365	81%, 17%
12	k	365	80%, 17%
12	l	365	80%, 17%
12	m	365	80%, 17%

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Mol	Chain	Length	Quality of chain
12	n	365	80% · 17%
12	o	365	80% · 17%
12	p	365	80% · 17%
12	q	365	80% · 17%
12	r	365	80% · 17%
12	s	365	80% · 17%
12	t	365	80% · 17%
12	u	365	80% · 17%
12	v	365	80% · 17%
12	w	365	80% · 17%
12	x	365	80% · 17%
12	y	365	80% · 17%
12	z	365	80% · 17%
13	B1	137	61% · 36%
13	B2	137	61% · 36%
13	B7	137	57% 7% 36%
13	B8	137	61% · 36%
13	B9	137	61% · 36%
13	BY	137	61% · 36%
13	BZ	137	61% · 36%
13	Be	137	57% 7% 36%
13	Bf	137	61% · 36%
13	Bg	137	61% · 36%
13	Bl	137	57% 7% 36%
13	Bm	137	61% · 36%

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Mol	Chain	Length	Quality of chain
13	Bn	137	61% · 36%
13	Bs	137	57% 7% 36%
13	Bt	137	61% · 36%
13	Bu	137	61% · 36%
13	Bz	137	57% 7% 36%
13	C1	137	57% 7% 36%
13	C2	137	61% · 36%
13	C3	137	61% · 36%
13	C4	137	57% 7% 36%
13	C5	137	61% · 36%
13	C8	137	57% 7% 36%
13	C9	137	61% · 36%
13	CD	137	57% 7% 36%
13	CE	137	61% · 36%
13	CF	137	61% · 36%
13	CK	137	57% 7% 36%
13	CL	137	61% · 36%
13	CM	137	61% · 36%
13	CR	137	57% 7% 36%
13	CS	137	61% · 36%
13	CT	137	61% · 36%
13	CY	137	57% 7% 36%
13	CZ	137	61% · 36%
13	Ca	137	61% · 36%
13	Cf	137	57% 7% 36%

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Mol	Chain	Length	Quality of chain
13	Cg	137	61% · 36%
13	Ch	137	61% · 36%
13	Cm	137	57% 7% 36%
13	Cn	137	61% · 36%
13	Co	137	61% · 36%
13	Ct	137	57% 7% 36%
13	Cu	137	61% · 36%
13	Cv	137	61% · 36%
13	D1	137	61% · 36%
13	D5	137	57% 7% 36%
13	D6	137	61% · 36%
13	D7	137	61% · 36%
13	DD	137	61% · 36%
13	DI	137	57% 7% 36%
13	DJ	137	61% · 36%
13	DK	137	61% · 36%
13	DM	137	61% · 36%
13	DN	137	61% · 36%
13	DO	137	61% · 36%
13	DP	137	61% · 36%
13	DQ	137	61% · 36%
13	DR	137	61% · 36%
13	DS	137	61% · 36%
13	DT	137	61% · 36%
13	DU	137	57% 7% 36%

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Mol	Chain	Length	Quality of chain
13	DV	137	61% · 36%
13	DW	137	61% · 36%
13	Da	137	57% 7% 36%
13	Db	137	61% · 36%
13	Dc	137	61% · 36%
13	Dg	137	57% 7% 36%
13	Dh	137	61% · 36%
13	Di	137	61% · 36%
13	Dm	137	57% 7% 36%
13	Dn	137	61% · 36%
13	Do	137	61% · 36%
13	Ds	137	57% 7% 36%
13	Dt	137	61% · 36%
13	Du	137	61% · 36%
13	Dy	137	57% 7% 36%
13	Dz	137	61% · 36%
13	EA	137	57% 7% 36%
13	EB	137	61% · 36%
13	EE	137	57% 7% 36%
13	EF	137	61% · 36%
13	EG	137	61% · 36%
13	EL	137	57% 7% 36%
13	EM	137	61% · 36%
13	EN	137	61% · 36%
13	ES	137	57% 7% 36%

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Mol	Chain	Length	Quality of chain
13	ET	137	61% · 36%
13	EU	137	61% · 36%
13	EZ	137	57% 7% 36%
13	FC	137	57% 7% 36%
13	FD	137	57% 7% 36%
13	FE	137	57% 7% 36%
13	FF	137	57% 7% 36%
13	FG	137	57% 7% 36%
13	FH	137	57% 7% 36%
13	FI	137	61% · 36%
13	FJ	137	61% · 36%
13	FK	137	61% · 36%
13	FL	137	61% · 36%
13	FM	137	61% · 36%
13	FN	137	61% · 36%
14	B5	331	91% · 6%
14	Bc	331	91% · 6%
14	Bj	331	91% · 6%
14	Bq	331	91% · 6%
14	Bx	331	91% · 6%
14	C6	331	91% · 6%
14	CB	331	91% · 6%
14	CI	331	91% · 6%
14	CP	331	91% · 6%
14	CW	331	91% · 6%

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Mol	Chain	Length	Quality of chain
14	Cd	331	91% • 6%
14	Ck	331	91% • 6%
14	Cr	331	91% • 6%
14	Cy	331	91% • 6%
14	D3	331	91% • 6%
14	D9	331	91% • 6%
14	DA	331	91% • 6%
14	DG	331	91% • 6%
14	DY	331	91% • 6%
14	De	331	91% • 6%
14	Dk	331	91% • 6%
14	Dq	331	91% • 6%
14	Dw	331	91% • 6%
14	E1	331	91% • 6%
14	E2	331	91% • 6%
14	E3	331	91% • 6%
14	E4	331	91% • 6%
14	EC	331	91% • 6%
14	EJ	331	91% • 6%
14	EQ	331	91% • 6%
14	EX	331	91% • 6%
14	Ex	331	91% • 6%
14	Ey	331	91% • 6%
14	Ez	331	91% • 6%
15	B6	129	8% 100%

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Mol	Chain	Length	Quality of chain
15	Bd	129	8% 100%
15	Bk	129	7% 100%
15	Br	129	8% 100%
15	By	129	8% 100%
15	C7	129	8% 100%
15	CC	129	8% 100%
15	CJ	129	8% 100%
15	CQ	129	8% 100%
15	CX	129	9% 100%
15	Ce	129	8% 100%
15	Cl	129	9% 100%
15	Cs	129	8% 100%
15	Cz	129	8% 100%
15	D0	129	8% 100%
15	D4	129	9% 100%
15	DB	129	9% 100%
15	DH	129	8% 100%
15	DZ	129	8% 100%
15	Df	129	8% 100%
15	Dl	129	8% 100%
15	Dr	129	8% 100%
15	Dx	129	8% 100%
15	E0	129	9% 100%
15	E6	129	8% 100%
15	E7	129	8% 100%

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Mol	Chain	Length	Quality of chain
15	E8	129	9% 100%
15	E9	129	9% 100%
15	ED	129	8% 100%
15	EK	129	8% 100%
15	ER	129	8% 100%
15	EY	129	9% 100%
15	FA	129	8% 100%
15	FB	129	9% 100%
16	B4	334	87% 10%
16	Bb	334	87% 10%
16	Bi	334	87% 10%
16	Bp	334	87% 10%
16	Bw	334	87% 10%
16	C0	334	87% 10%
16	CA	334	87% 10%
16	CH	334	87% 10%
16	CO	334	87% 10%
16	CV	334	87% 10%
16	Cc	334	87% 10%
16	Cj	334	87% 10%
16	Cq	334	87% 10%
16	Cx	334	87% 10%
16	D2	334	87% 10%
16	D8	334	87% 10%
16	DC	334	87% 10%

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Mol	Chain	Length	Quality of chain
16	DF	334	87% 10%
16	DX	334	87% 10%
16	Dd	334	87% 10%
16	Dj	334	87% 10%
16	Dp	334	87% 10%
16	Dv	334	87% 10%
16	E5	334	87% 10%
16	EI	334	87% 10%
16	EP	334	87% 10%
16	EW	334	87% 10%
16	Eq	334	87% 10%
16	Er	334	87% 10%
16	Es	334	87% 10%
16	Et	334	87% 10%
16	Eu	334	87% 10%
16	Ev	334	87% 10%
16	Ew	334	87% 10%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 614043 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 basal-body rod protein FlgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	248	1866	1154	327	379	6	0	0
1	1	252	1894	1172	331	385	6	0	0
1	2	260	1949	1202	341	400	6	0	0
1	3	260	1949	1202	341	400	6	0	0
1	4	260	1949	1202	341	400	6	0	0
1	5	260	1949	1202	341	400	6	0	0
1	6	260	1949	1202	341	400	6	0	0
1	7	260	1949	1202	341	400	6	0	0
1	8	260	1949	1202	341	400	6	0	0
1	9	260	1949	1202	341	400	6	0	0
1	AF	254	1903	1175	334	389	5	0	0
1	AG	255	1911	1181	335	390	5	0	0
1	AH	256	1919	1186	336	391	6	0	0
1	AI	254	1903	1175	334	389	5	0	0
1	AJ	255	1911	1181	335	390	5	0	0
1	AK	243	1823	1127	318	373	5	0	0
1	AL	248	1866	1154	327	379	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AM	248	1866	1154	327	379	6	0	0
			Total	C	N	O	S		
1	AN	248	1866	1154	327	379	6	0	0
			Total	C	N	O	S		
1	ZA	260	1949	1202	341	400	6	0	0
			Total	C	N	O	S		
1	ZB	260	1949	1202	341	400	6	0	0
			Total	C	N	O	S		
1	ZC	260	1949	1202	341	400	6	0	0
			Total	C	N	O	S		
1	ZD	260	1949	1202	341	400	6	0	0
			Total	C	N	O	S		
1	ZE	260	1949	1202	341	400	6	0	0

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

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

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

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

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

- Molecule 4 is a protein called Flagellar hook-basal body complex protein FliE.

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O			
6	BG	13	81	50	15	16		0	0
			Total	C	N	O			
6	BH	16	103	64	19	20		0	0
			Total	C	N	O			
6	BI	20	133	83	23	27		0	0
			Total	C	N	O			
6	BJ	16	103	64	19	20		0	0
			Total	C	N	O			
6	BK	21	140	88	24	28		0	0
			Total	C	N	O			
6	BL	16	103	64	19	20		0	0
			Total	C	N	O			
6	BM	21	140	88	24	28		0	0
			Total	C	N	O			
6	BN	16	103	64	19	20		0	0
			Total	C	N	O			
6	BO	20	133	83	23	27		0	0
			Total	C	N	O			
6	BP	16	103	64	19	20		0	0
			Total	C	N	O			
6	BQ	21	140	88	24	28		0	0
			Total	C	N	O	S		
6	BR	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
6	BS	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
6	BT	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
6	BU	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
6	BV	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
6	BW	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
6	BX	164	1275	776	237	259	3	0	0
			Total	C	N	O	S		
6	UI	155	1172	733	211	226	2	0	0
			Total	C	N	O	S		
6	UJ	155	1172	733	211	226	2	0	0
			Total	C	N	O	S		
6	UK	155	1172	733	211	226	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	UL	155	1172	733	211	226	2	0	0
			Total	C	N	O	S		
6	UM	155	1172	733	211	226	2	0	0
			Total	C	N	O	S		
6	UN	155	1172	733	211	226	2	0	0
			Total	C	N	O	S		
6	UO	155	1172	733	211	226	2	0	0
			Total	C	N	O	S		
6	UP	155	1172	733	211	226	2	0	0
			Total	C	N	O	S		
6	WA	113	849	534	148	166	1	0	0
			Total	C	N	O	S		
6	WB	111	836	526	146	163	1	0	0
			Total	C	N	O	S		
6	WC	108	812	510	142	159	1	0	0
			Total	C	N	O	S		
6	WD	110	827	522	144	160	1	0	0
			Total	C	N	O	S		
6	WE	112	843	531	147	164	1	0	0
			Total	C	N	O	S		
6	WF	111	834	526	145	162	1	0	0
			Total	C	N	O	S		
6	WG	112	843	531	147	164	1	0	0
			Total	C	N	O	S		
6	WH	95	703	439	126	137	1	0	0
			Total	C	N	O	S		
6	WI	95	703	439	126	137	1	0	0
			Total	C	N	O	S		
6	WJ	99	737	462	131	143	1	0	0
			Total	C	N	O	S		
6	WK	98	729	456	130	142	1	0	0
			Total	C	N	O	S		
6	WL	85	622	389	110	122	1	0	0
			Total	C	N	O	S		
6	WM	82	596	372	107	116	1	0	0
			Total	C	N	O	S		
6	WN	84	611	380	109	121	1	0	0
			Total	C	N	O	S		
6	WO	96	714	448	127	138	1	0	0
			Total	C	N	O	S		
6	WP	100	741	464	132	144	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	WQ	111	834	526	145	162	1	0	0
			Total	C	N	O	S		
6	WR	111	834	526	145	162	1	0	0
			Total	C	N	O	S		
6	WS	111	834	526	145	162	1	0	0
			Total	C	N	O	S		
6	WT	111	834	526	145	162	1	0	0
			Total	C	N	O	S		
6	WU	112	843	531	147	164	1	0	0
			Total	C	N	O	S		
6	WV	110	827	521	144	161	1	0	0
			Total	C	N	O	S		
6	WW	111	834	526	145	162	1	0	0
			Total	C	N	O	S		
6	DE	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	DL	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	B0	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	B3	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	EH	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	EO	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	EV	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ba	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Bh	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Bo	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Bv	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ea	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	CG	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	CN	27	224	135	44	42	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CU	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Cb	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ci	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Cp	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Cw	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Eb	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ec	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ed	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ee	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ef	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Eg	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Eh	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ei	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ej	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ek	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	El	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Em	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	En	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Eo	27	224	135	44	42	3	0	0
			Total	C	N	O	S		
6	Ep	27	224	135	44	42	3	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Au	207	1605	1072	249	272	12	0	0
9	Av	209	1626	1086	252	276	12	0	0
9	Aw	208	1614	1077	251	274	12	0	0
9	Ax	208	1614	1077	251	274	12	0	0
9	Ay	209	1623	1084	251	276	12	0	0

- Molecule 10 is a protein called Flagellar basal-body rod protein FlgC.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	BF	133	969	604	167	193	5	0	0

- Molecule 11 is a protein called Flagellar hook protein FlgE.

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

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

- Molecule 12 is a protein called Flagellar P-ring protein.

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

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

- Molecule 13 is a protein called Flagellar motor switch protein FliN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	C3	87	675	427	118	126	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	C4	87	675	427	118	126	4	0	0
13	C5	87	675	427	118	126	4	0	0
13	C8	87	675	427	118	126	4	0	0
13	C9	87	675	427	118	126	4	0	0
13	DD	87	675	427	118	126	4	0	0
13	DI	87	675	427	118	126	4	0	0
13	DJ	87	675	427	118	126	4	0	0
13	DK	87	675	427	118	126	4	0	0
13	DM	87	675	427	118	126	4	0	0
13	DN	87	675	427	118	126	4	0	0
13	DO	87	675	427	118	126	4	0	0
13	DP	87	675	427	118	126	4	0	0
13	DQ	87	675	427	118	126	4	0	0
13	DR	87	675	427	118	126	4	0	0
13	DS	87	675	427	118	126	4	0	0
13	DT	87	675	427	118	126	4	0	0
13	DU	87	675	427	118	126	4	0	0
13	DV	87	675	427	118	126	4	0	0
13	DW	87	675	427	118	126	4	0	0
13	Da	87	675	427	118	126	4	0	0
13	Db	87	675	427	118	126	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Dc	87	675	427	118	126	4	0	0
13	Dg	87	675	427	118	126	4	0	0
13	Dh	87	675	427	118	126	4	0	0
13	Di	87	675	427	118	126	4	0	0
13	Dm	87	675	427	118	126	4	0	0
13	Dn	87	675	427	118	126	4	0	0
13	Do	87	675	427	118	126	4	0	0
13	Ds	87	675	427	118	126	4	0	0
13	Dt	87	675	427	118	126	4	0	0
13	Du	87	675	427	118	126	4	0	0
13	Dy	87	675	427	118	126	4	0	0
13	Dz	87	675	427	118	126	4	0	0
13	D1	87	675	427	118	126	4	0	0
13	D5	87	675	427	118	126	4	0	0
13	D6	87	675	427	118	126	4	0	0
13	D7	87	675	427	118	126	4	0	0
13	EA	87	675	427	118	126	4	0	0
13	EB	87	675	427	118	126	4	0	0
13	B1	87	675	427	118	126	4	0	0
13	B2	87	675	427	118	126	4	0	0
13	B7	87	675	427	118	126	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	B8	87	675	427	118	126	4	0	0
13	B9	87	675	427	118	126	4	0	0
13	EE	87	675	427	118	126	4	0	0
13	EF	87	675	427	118	126	4	0	0
13	EG	87	675	427	118	126	4	0	0
13	EL	87	675	427	118	126	4	0	0
13	EM	87	675	427	118	126	4	0	0
13	EN	87	675	427	118	126	4	0	0
13	ES	87	675	427	118	126	4	0	0
13	ET	87	675	427	118	126	4	0	0
13	EU	87	675	427	118	126	4	0	0
13	EZ	87	675	427	118	126	4	0	0
13	BY	87	675	427	118	126	4	0	0
13	BZ	87	675	427	118	126	4	0	0
13	Be	87	675	427	118	126	4	0	0
13	Bf	87	675	427	118	126	4	0	0
13	Bg	87	675	427	118	126	4	0	0
13	Bl	87	675	427	118	126	4	0	0
13	Bm	87	675	427	118	126	4	0	0
13	Bn	87	675	427	118	126	4	0	0
13	Bs	87	675	427	118	126	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Bt	87	675	427	118	126	4	0	0
13	Bu	87	675	427	118	126	4	0	0
13	Bz	87	675	427	118	126	4	0	0
13	C1	87	675	427	118	126	4	0	0
13	C2	87	675	427	118	126	4	0	0
13	CD	87	675	427	118	126	4	0	0
13	CE	87	675	427	118	126	4	0	0
13	CF	87	675	427	118	126	4	0	0
13	CK	87	675	427	118	126	4	0	0
13	CL	87	675	427	118	126	4	0	0
13	CM	87	675	427	118	126	4	0	0
13	CR	87	675	427	118	126	4	0	0
13	CS	87	675	427	118	126	4	0	0
13	CT	87	675	427	118	126	4	0	0
13	CY	87	675	427	118	126	4	0	0
13	CZ	87	675	427	118	126	4	0	0
13	Ca	87	675	427	118	126	4	0	0
13	Cf	87	675	427	118	126	4	0	0
13	Cg	87	675	427	118	126	4	0	0
13	Ch	87	675	427	118	126	4	0	0
13	Cm	87	675	427	118	126	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Cn	87	675	427	118	126	4	0	0
13	Co	87	675	427	118	126	4	0	0
13	Ct	87	675	427	118	126	4	0	0
13	Cu	87	675	427	118	126	4	0	0
13	Cv	87	675	427	118	126	4	0	0
13	FC	87	675	427	118	126	4	0	0
13	FD	87	675	427	118	126	4	0	0
13	FE	87	675	427	118	126	4	0	0
13	FF	87	675	427	118	126	4	0	0
13	FG	87	675	427	118	126	4	0	0
13	FH	87	675	427	118	126	4	0	0
13	FI	87	675	427	118	126	4	0	0
13	FJ	87	675	427	118	126	4	0	0
13	FK	87	675	427	118	126	4	0	0
13	FL	87	675	427	118	126	4	0	0
13	FM	87	675	427	118	126	4	0	0
13	FN	87	675	427	118	126	4	0	0

- Molecule 14 is a protein called Flagellar motor switch protein FliG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	C6	310	2428	1515	430	474	9	0	0
14	DA	310	2428	1515	430	474	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	DG	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	DY	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	De	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	Dk	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	Dq	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	Dw	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	D3	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	D9	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	B5	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	EC	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	EJ	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	EQ	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	EX	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	Bc	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	Bj	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	Bq	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	Bx	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	CB	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	CI	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	CP	310	2428	1515	430	474	9	0	0
			Total	C	N	O	S		
14	CW	310	2428	1515	430	474	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Cd	310	2428	1515	430	474	9	0	0
14	Ck	310	2428	1515	430	474	9	0	0
14	Cr	310	2428	1515	430	474	9	0	0
14	Cy	310	2428	1515	430	474	9	0	0
14	Ex	310	2428	1515	430	474	9	0	0
14	Ey	310	2428	1515	430	474	9	0	0
14	Ez	310	2428	1515	430	474	9	0	0
14	E1	310	2428	1515	430	474	9	0	0
14	E2	310	2428	1515	430	474	9	0	0
14	E3	310	2428	1515	430	474	9	0	0
14	E4	310	2428	1515	430	474	9	0	0

- Molecule 15 is a protein called Chemotaxis protein CheY.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	C7	129	991	634	165	185	7	0	0
15	DB	129	991	634	165	185	7	0	0
15	DH	129	991	634	165	185	7	0	0
15	DZ	129	991	634	165	185	7	0	0
15	Df	129	991	634	165	185	7	0	0
15	Dl	129	991	634	165	185	7	0	0
15	Dr	129	991	634	165	185	7	0	0
15	Dx	129	991	634	165	185	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	D4	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	D0	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	B6	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	ED	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	EK	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	ER	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	EY	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	Bd	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	Bk	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	Br	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	By	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	CC	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	CJ	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	CQ	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	CX	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	Ce	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	Cl	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	Cs	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	Cz	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	E6	129	991	634	165	185	7	0	0
			Total	C	N	O	S		
15	E7	129	991	634	165	185	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	E8	129	991	634	165	185	7	0	0
15	E9	129	991	634	165	185	7	0	0
15	E0	129	991	634	165	185	7	0	0
15	FA	129	991	634	165	185	7	0	0
15	FB	129	991	634	165	185	7	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C7	13	LYS	ASP	engineered mutation	UNP P0A2D5
C7	106	TRP	TYR	engineered mutation	UNP P0A2D5
DB	13	LYS	ASP	engineered mutation	UNP P0A2D5
DB	106	TRP	TYR	engineered mutation	UNP P0A2D5
DH	13	LYS	ASP	engineered mutation	UNP P0A2D5
DH	106	TRP	TYR	engineered mutation	UNP P0A2D5
DZ	13	LYS	ASP	engineered mutation	UNP P0A2D5
DZ	106	TRP	TYR	engineered mutation	UNP P0A2D5
Df	13	LYS	ASP	engineered mutation	UNP P0A2D5
Df	106	TRP	TYR	engineered mutation	UNP P0A2D5
Dl	13	LYS	ASP	engineered mutation	UNP P0A2D5
Dl	106	TRP	TYR	engineered mutation	UNP P0A2D5
Dr	13	LYS	ASP	engineered mutation	UNP P0A2D5
Dr	106	TRP	TYR	engineered mutation	UNP P0A2D5
Dx	13	LYS	ASP	engineered mutation	UNP P0A2D5
Dx	106	TRP	TYR	engineered mutation	UNP P0A2D5
D4	13	LYS	ASP	engineered mutation	UNP P0A2D5
D4	106	TRP	TYR	engineered mutation	UNP P0A2D5
D0	13	LYS	ASP	engineered mutation	UNP P0A2D5
D0	106	TRP	TYR	engineered mutation	UNP P0A2D5
B6	13	LYS	ASP	engineered mutation	UNP P0A2D5
B6	106	TRP	TYR	engineered mutation	UNP P0A2D5
ED	13	LYS	ASP	engineered mutation	UNP P0A2D5
ED	106	TRP	TYR	engineered mutation	UNP P0A2D5
EK	13	LYS	ASP	engineered mutation	UNP P0A2D5
EK	106	TRP	TYR	engineered mutation	UNP P0A2D5
ER	13	LYS	ASP	engineered mutation	UNP P0A2D5
ER	106	TRP	TYR	engineered mutation	UNP P0A2D5
EY	13	LYS	ASP	engineered mutation	UNP P0A2D5

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Chain	Residue	Modelled	Actual	Comment	Reference
EY	106	TRP	TYR	engineered mutation	UNP P0A2D5
Bd	13	LYS	ASP	engineered mutation	UNP P0A2D5
Bd	106	TRP	TYR	engineered mutation	UNP P0A2D5
Bk	13	LYS	ASP	engineered mutation	UNP P0A2D5
Bk	106	TRP	TYR	engineered mutation	UNP P0A2D5
Br	13	LYS	ASP	engineered mutation	UNP P0A2D5
Br	106	TRP	TYR	engineered mutation	UNP P0A2D5
By	13	LYS	ASP	engineered mutation	UNP P0A2D5
By	106	TRP	TYR	engineered mutation	UNP P0A2D5
CC	13	LYS	ASP	engineered mutation	UNP P0A2D5
CC	106	TRP	TYR	engineered mutation	UNP P0A2D5
CJ	13	LYS	ASP	engineered mutation	UNP P0A2D5
CJ	106	TRP	TYR	engineered mutation	UNP P0A2D5
CQ	13	LYS	ASP	engineered mutation	UNP P0A2D5
CQ	106	TRP	TYR	engineered mutation	UNP P0A2D5
CX	13	LYS	ASP	engineered mutation	UNP P0A2D5
CX	106	TRP	TYR	engineered mutation	UNP P0A2D5
Ce	13	LYS	ASP	engineered mutation	UNP P0A2D5
Ce	106	TRP	TYR	engineered mutation	UNP P0A2D5
Cl	13	LYS	ASP	engineered mutation	UNP P0A2D5
Cl	106	TRP	TYR	engineered mutation	UNP P0A2D5
Cs	13	LYS	ASP	engineered mutation	UNP P0A2D5
Cs	106	TRP	TYR	engineered mutation	UNP P0A2D5
Cz	13	LYS	ASP	engineered mutation	UNP P0A2D5
Cz	106	TRP	TYR	engineered mutation	UNP P0A2D5
E6	13	LYS	ASP	engineered mutation	UNP P0A2D5
E6	106	TRP	TYR	engineered mutation	UNP P0A2D5
E7	13	LYS	ASP	engineered mutation	UNP P0A2D5
E7	106	TRP	TYR	engineered mutation	UNP P0A2D5
E8	13	LYS	ASP	engineered mutation	UNP P0A2D5
E8	106	TRP	TYR	engineered mutation	UNP P0A2D5
E9	13	LYS	ASP	engineered mutation	UNP P0A2D5
E9	106	TRP	TYR	engineered mutation	UNP P0A2D5
E0	13	LYS	ASP	engineered mutation	UNP P0A2D5
E0	106	TRP	TYR	engineered mutation	UNP P0A2D5
FA	13	LYS	ASP	engineered mutation	UNP P0A2D5
FA	106	TRP	TYR	engineered mutation	UNP P0A2D5
FB	13	LYS	ASP	engineered mutation	UNP P0A2D5
FB	106	TRP	TYR	engineered mutation	UNP P0A2D5

- Molecule 16 is a protein called Flagellar motor switch protein FliM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	C0	301	2431	1549	437	440	5	0	0
16	DC	301	2431	1549	437	440	5	0	0
16	DF	301	2431	1549	437	440	5	0	0
16	DX	301	2431	1549	437	440	5	0	0
16	Dd	301	2431	1549	437	440	5	0	0
16	Dj	301	2431	1549	437	440	5	0	0
16	Dp	301	2431	1549	437	440	5	0	0
16	Dv	301	2431	1549	437	440	5	0	0
16	D2	301	2431	1549	437	440	5	0	0
16	D8	301	2431	1549	437	440	5	0	0
16	B4	301	2431	1549	437	440	5	0	0
16	EI	301	2431	1549	437	440	5	0	0
16	EP	301	2431	1549	437	440	5	0	0
16	EW	301	2431	1549	437	440	5	0	0
16	Bb	301	2431	1549	437	440	5	0	0
16	Bi	301	2431	1549	437	440	5	0	0
16	Bp	301	2431	1549	437	440	5	0	0
16	Bw	301	2431	1549	437	440	5	0	0
16	CA	301	2431	1549	437	440	5	0	0
16	CH	301	2431	1549	437	440	5	0	0
16	CO	301	2431	1549	437	440	5	0	0
16	CV	301	2431	1549	437	440	5	0	0

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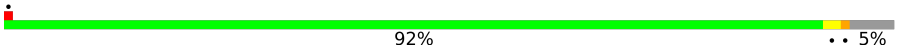
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Cc	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	Cj	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	Cq	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	Cx	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	Eq	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	Er	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	Es	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	Et	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	Eu	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	Ev	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	Ew	301	2431	1549	437	440	5	0	0
			Total	C	N	O	S		
16	E5	301	2431	1549	437	440	5	0	0

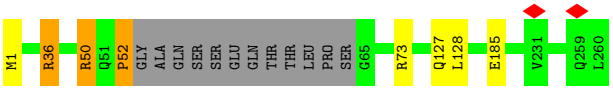
3 Residue-property plots (i)

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.

• Molecule 1: Flagellar basal-body rod protein FlgG

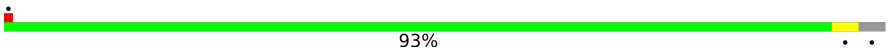
Chain 0:

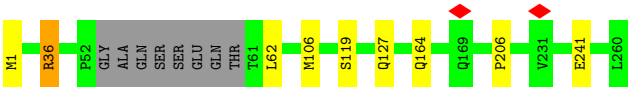




• Molecule 1: Flagellar basal-body rod protein FlgG

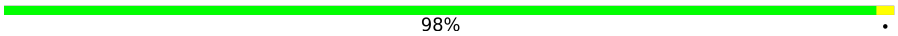
Chain 1:

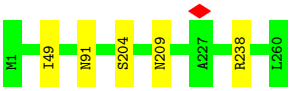




• Molecule 1: Flagellar basal-body rod protein FlgG

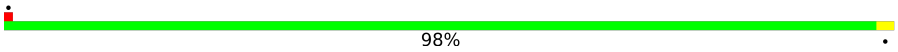
Chain 2:

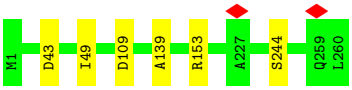




• Molecule 1: Flagellar basal-body rod protein FlgG

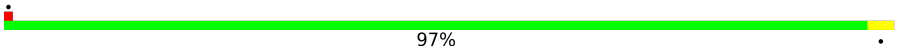
Chain 3:

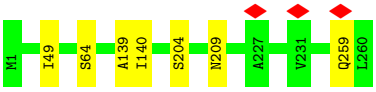




• Molecule 1: Flagellar basal-body rod protein FlgG

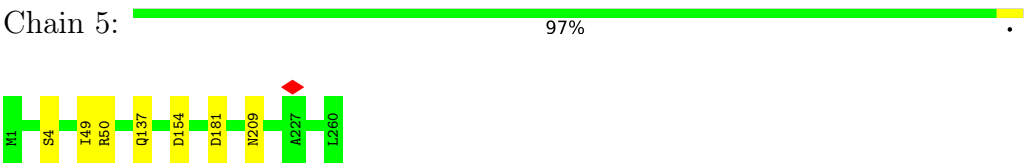
Chain 4:





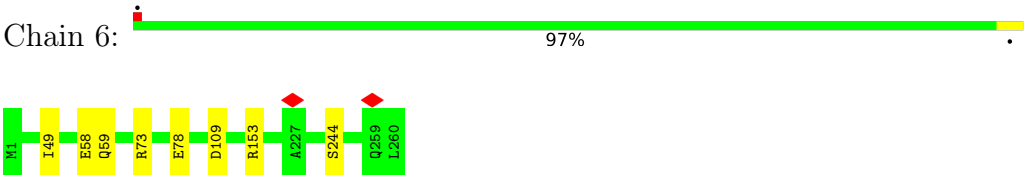
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain 5:



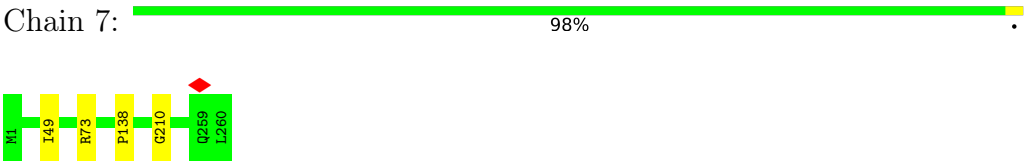
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain 6:



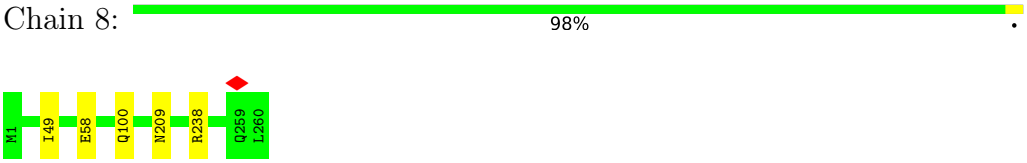
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain 7:



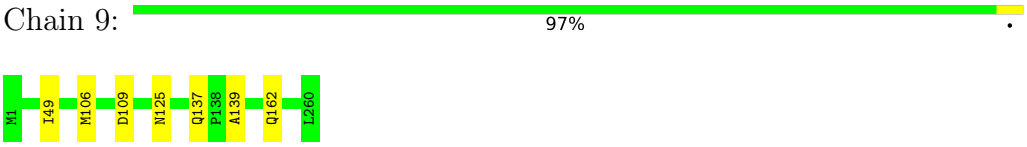
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain 8:



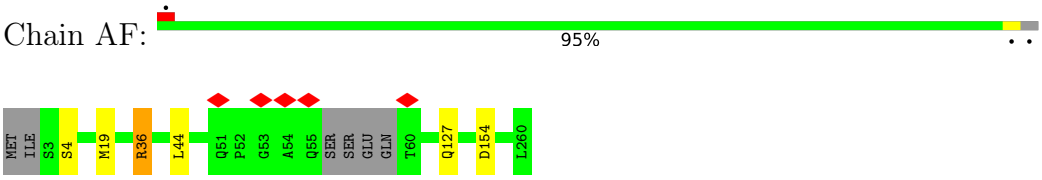
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain 9:



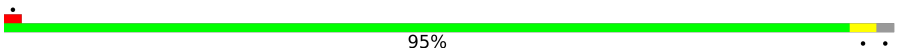
• Molecule 1: Flagellar basal-body rod protein FlgG

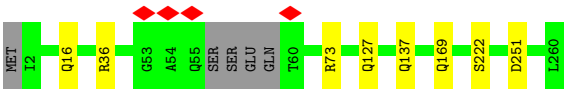
Chain AF:



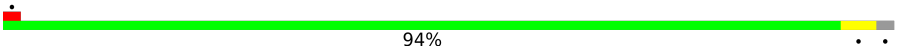
• Molecule 1: Flagellar basal-body rod protein FlgG

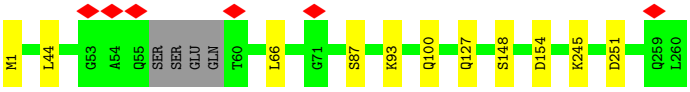
Chain AG:



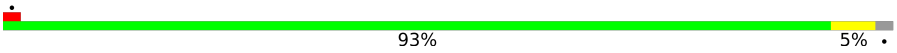


• Molecule 1: Flagellar basal-body rod protein FlgG

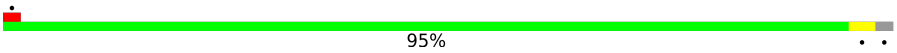
Chain AH: 



• Molecule 1: Flagellar basal-body rod protein FlgG

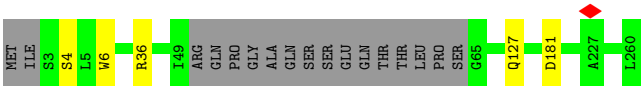
Chain AI: 

• Molecule 1: Flagellar basal-body rod protein FlgG

Chain AJ: 

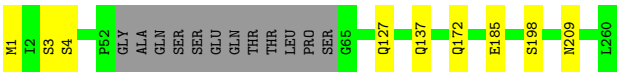
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain AK:



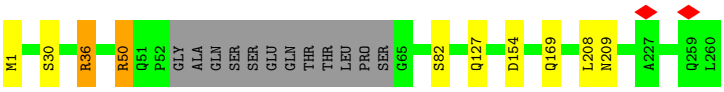
• Molecule 1: Flagellar basal-body rod protein FlgG

Chain AL:



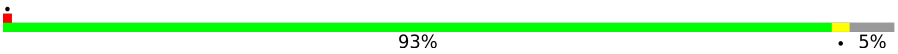
• Molecule 1: Flagellar basal-body rod protein FlgG

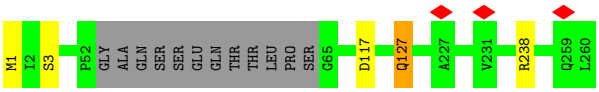
Chain AM:



• Molecule 1: Flagellar basal-body rod protein FlgG

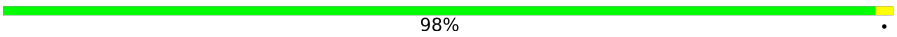
Chain AN:





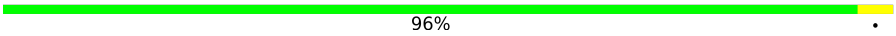
• Molecule 1: Flagellar basal-body rod protein FlgG

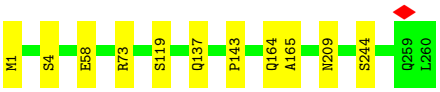
Chain ZA:



• Molecule 1: Flagellar basal-body rod protein FlgG

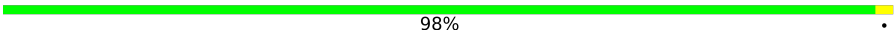
Chain ZB:

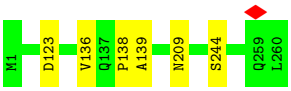




• Molecule 1: Flagellar basal-body rod protein FlgG

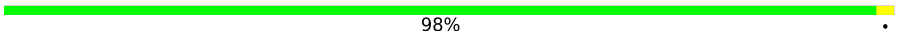
Chain ZC:

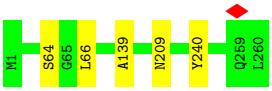




• Molecule 1: Flagellar basal-body rod protein FlgG

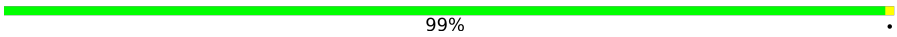
Chain ZD:

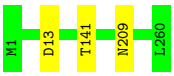




• Molecule 1: Flagellar basal-body rod protein FlgG

Chain ZE:



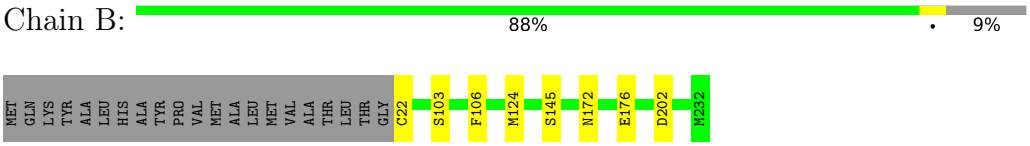


• Molecule 2: Flagellar L-ring protein

Chain A:

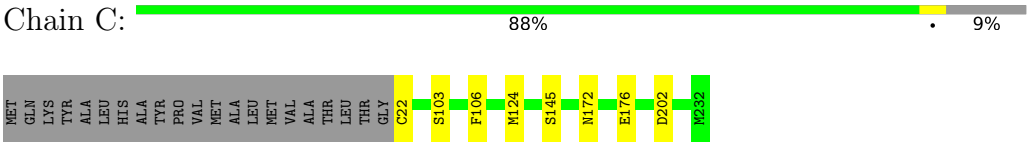
• Molecule 2: Flagellar L-ring protein

Chain B:



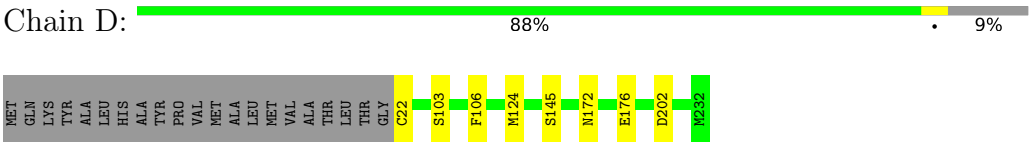
• Molecule 2: Flagellar L-ring protein

Chain C:



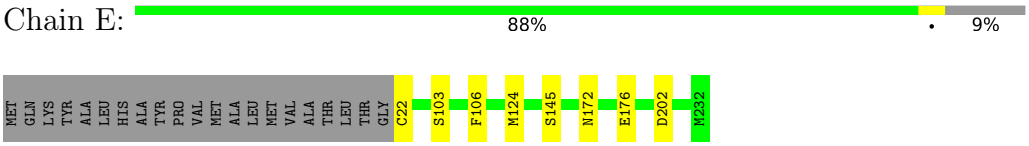
• Molecule 2: Flagellar L-ring protein

Chain D:



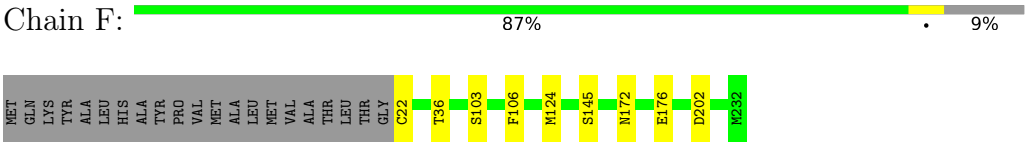
• Molecule 2: Flagellar L-ring protein

Chain E:



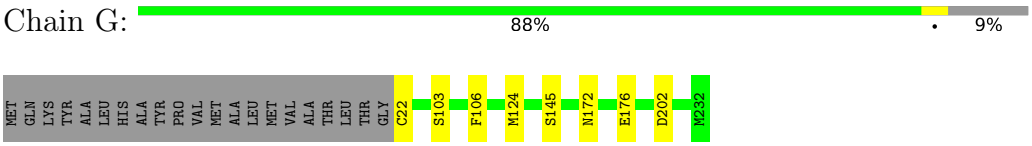
• Molecule 2: Flagellar L-ring protein

Chain F:



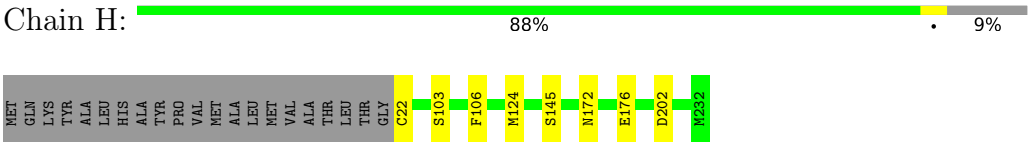
• Molecule 2: Flagellar L-ring protein

Chain G:



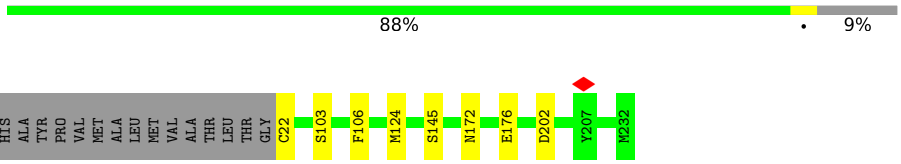
• Molecule 2: Flagellar L-ring protein

Chain H:



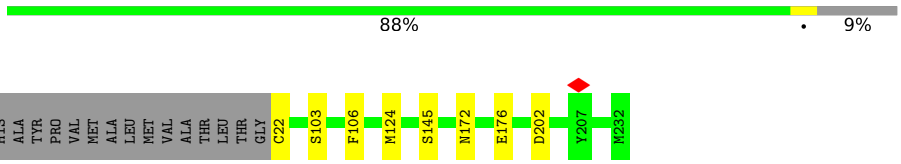
• Molecule 2: Flagellar L-ring protein

Chain I:



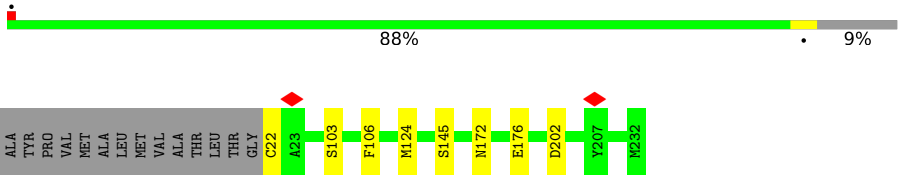
• Molecule 2: Flagellar L-ring protein

Chain J:



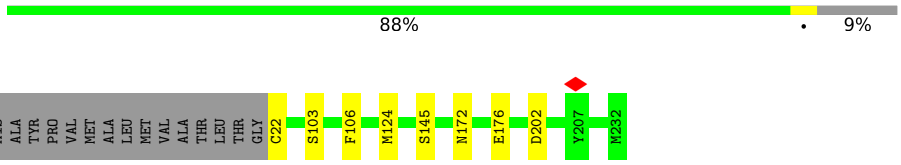
• Molecule 2: Flagellar L-ring protein

Chain K:



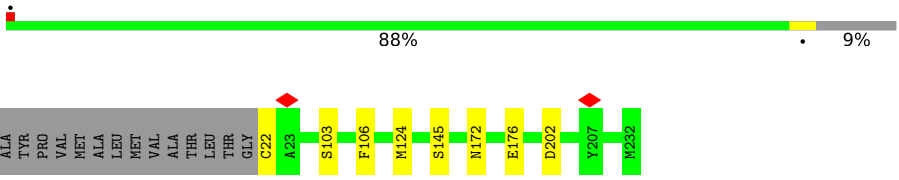
• Molecule 2: Flagellar L-ring protein

Chain L:



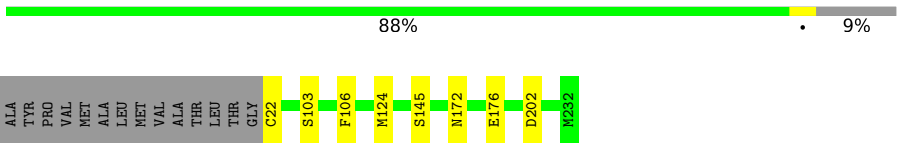
• Molecule 2: Flagellar L-ring protein

Chain M:



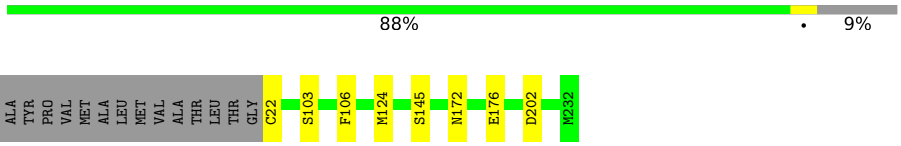
• Molecule 2: Flagellar L-ring protein

Chain N:



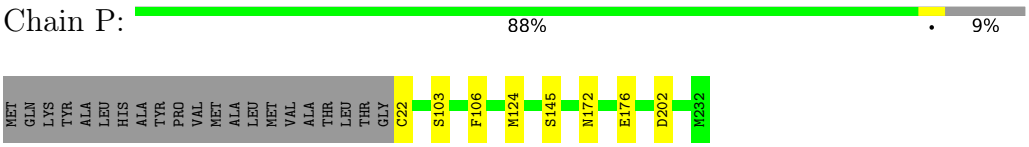
• Molecule 2: Flagellar L-ring protein

Chain O:



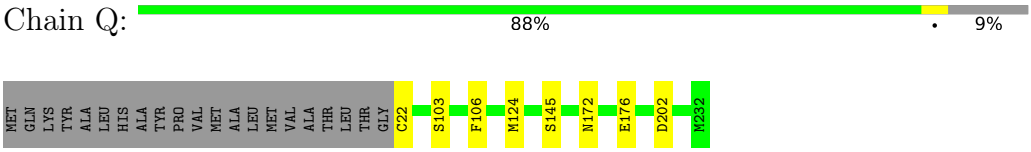
• Molecule 2: Flagellar L-ring protein

Chain P:



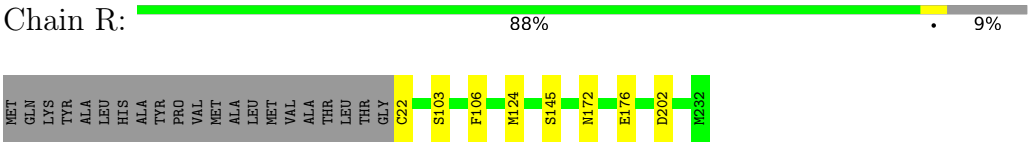
• Molecule 2: Flagellar L-ring protein

Chain Q:



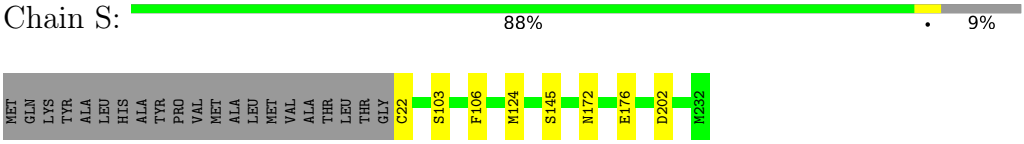
• Molecule 2: Flagellar L-ring protein

Chain R:



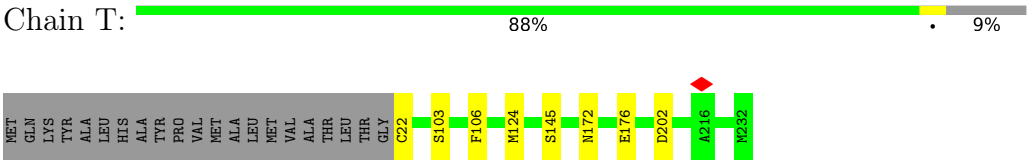
• Molecule 2: Flagellar L-ring protein

Chain S:



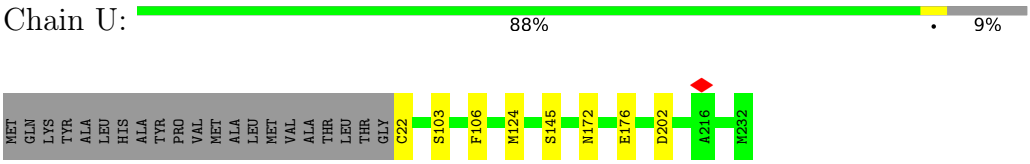
• Molecule 2: Flagellar L-ring protein

Chain T:



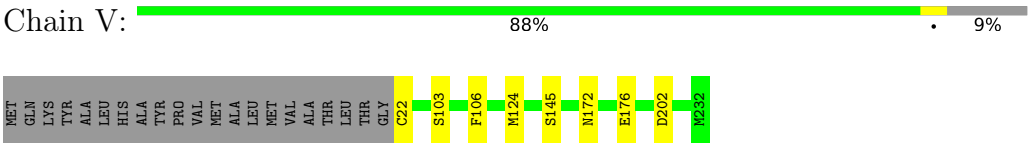
• Molecule 2: Flagellar L-ring protein

Chain U:



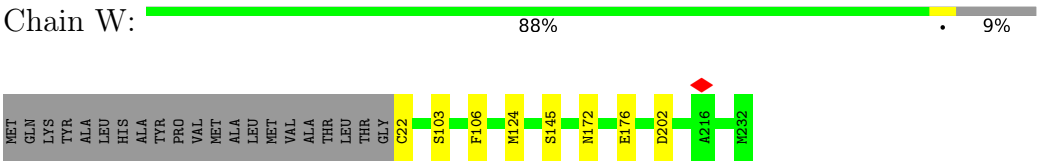
• Molecule 2: Flagellar L-ring protein

Chain V:



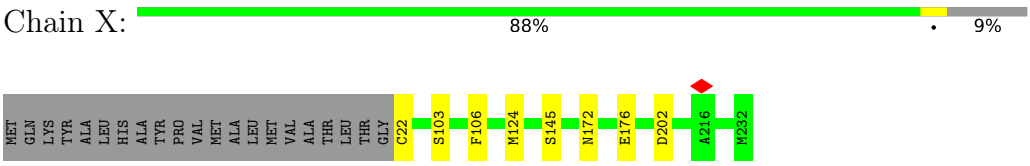
• Molecule 2: Flagellar L-ring protein

Chain W:



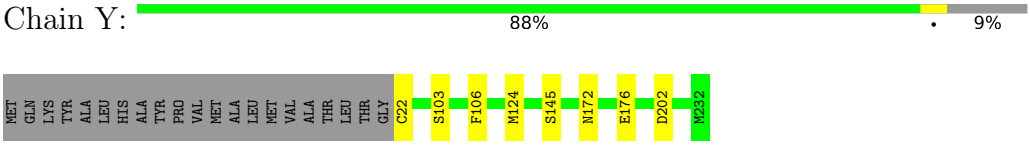
• Molecule 2: Flagellar L-ring protein

Chain X:



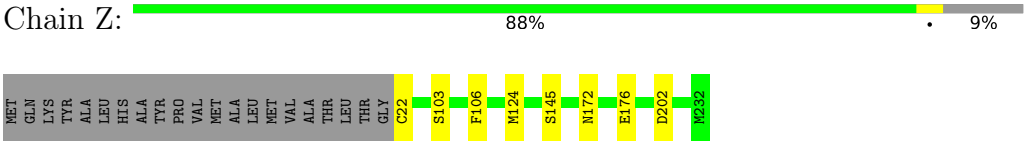
• Molecule 2: Flagellar L-ring protein

Chain Y:



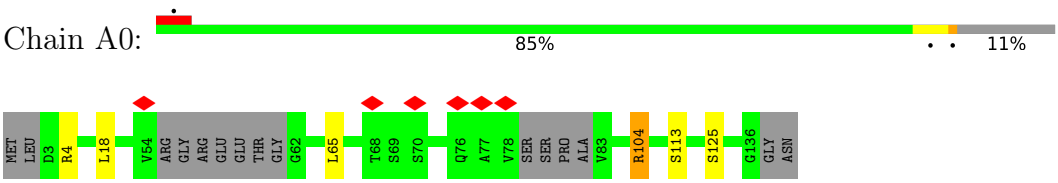
• Molecule 2: Flagellar L-ring protein

Chain Z:



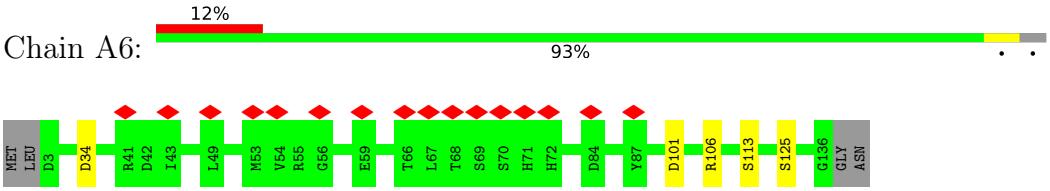
• Molecule 3: Flagellar basal body rod protein FlgB

Chain A0:



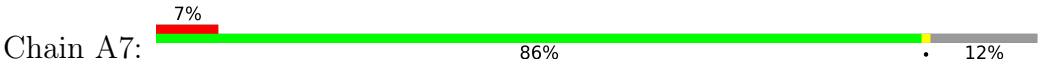
• Molecule 3: Flagellar basal body rod protein FlgB

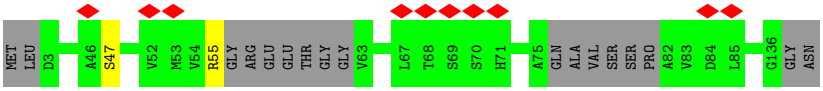
Chain A6:



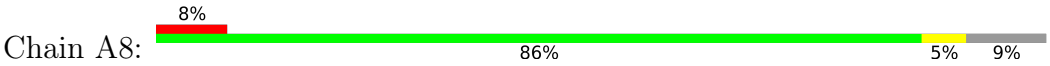
• Molecule 3: Flagellar basal body rod protein FlgB

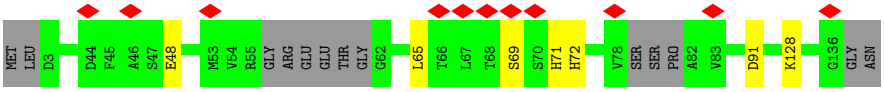
Chain A7:



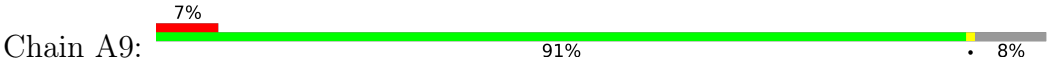


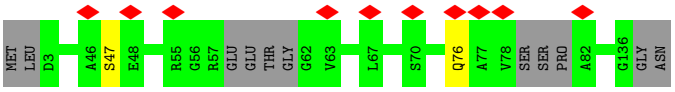
• Molecule 3: Flagellar basal body rod protein FlgB



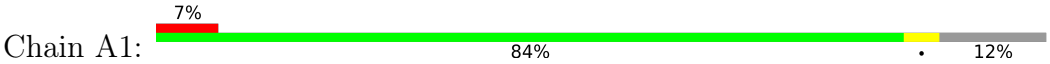


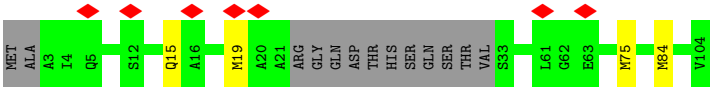
• Molecule 3: Flagellar basal body rod protein FlgB



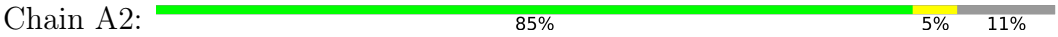


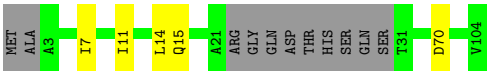
• Molecule 4: Flagellar hook-basal body complex protein FliE



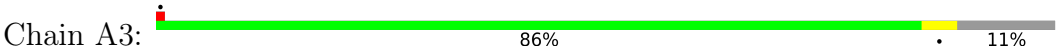


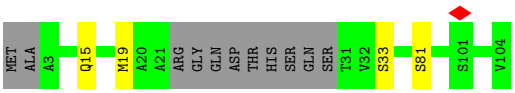
• Molecule 4: Flagellar hook-basal body complex protein FliE



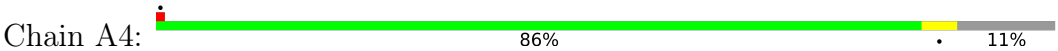


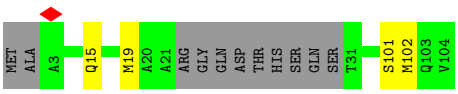
• Molecule 4: Flagellar hook-basal body complex protein FliE





• Molecule 4: Flagellar hook-basal body complex protein FliE



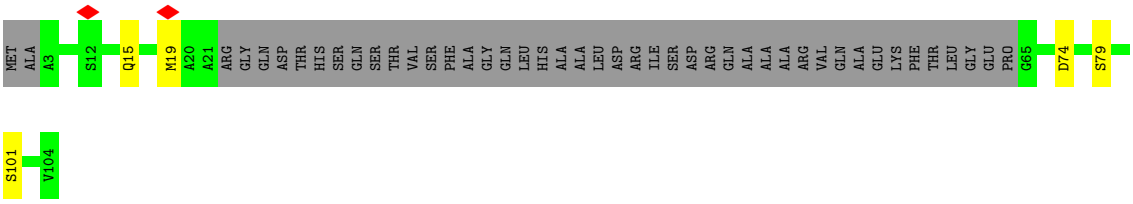


• Molecule 4: Flagellar hook-basal body complex protein FliE

Chain A5:

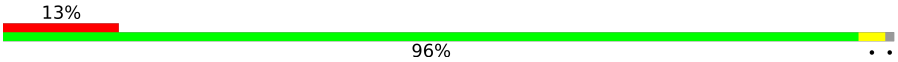
• Molecule 4: Flagellar hook-basal body complex protein FliE

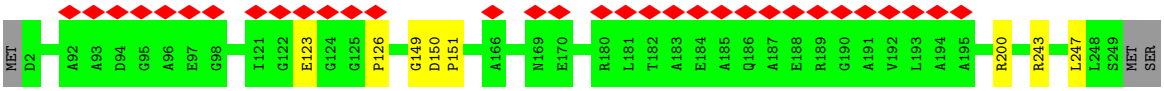
Chain Az:



• Molecule 5: Flagellar basal-body rod protein FlgF

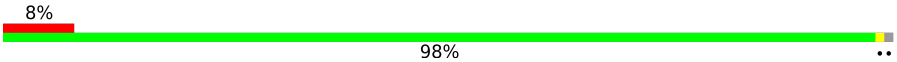
Chain AA:

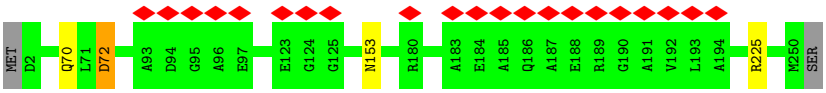




• Molecule 5: Flagellar basal-body rod protein FlgF

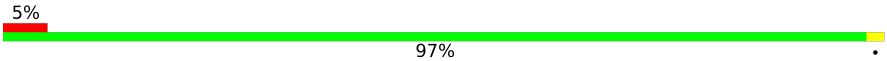
Chain AB:

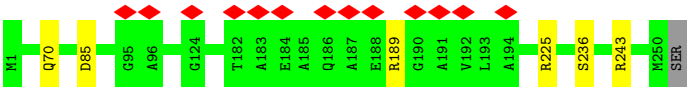




• Molecule 5: Flagellar basal-body rod protein FlgF

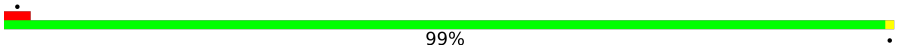
Chain AC:

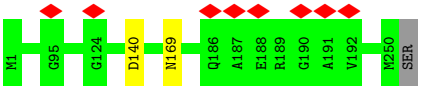




• Molecule 5: Flagellar basal-body rod protein FlgF

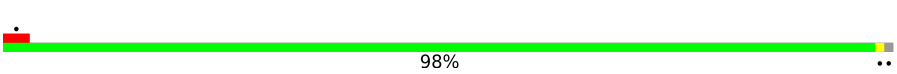
Chain AD:

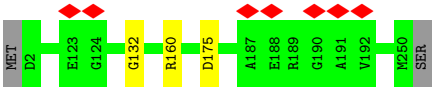




• Molecule 5: Flagellar basal-body rod protein FlgF

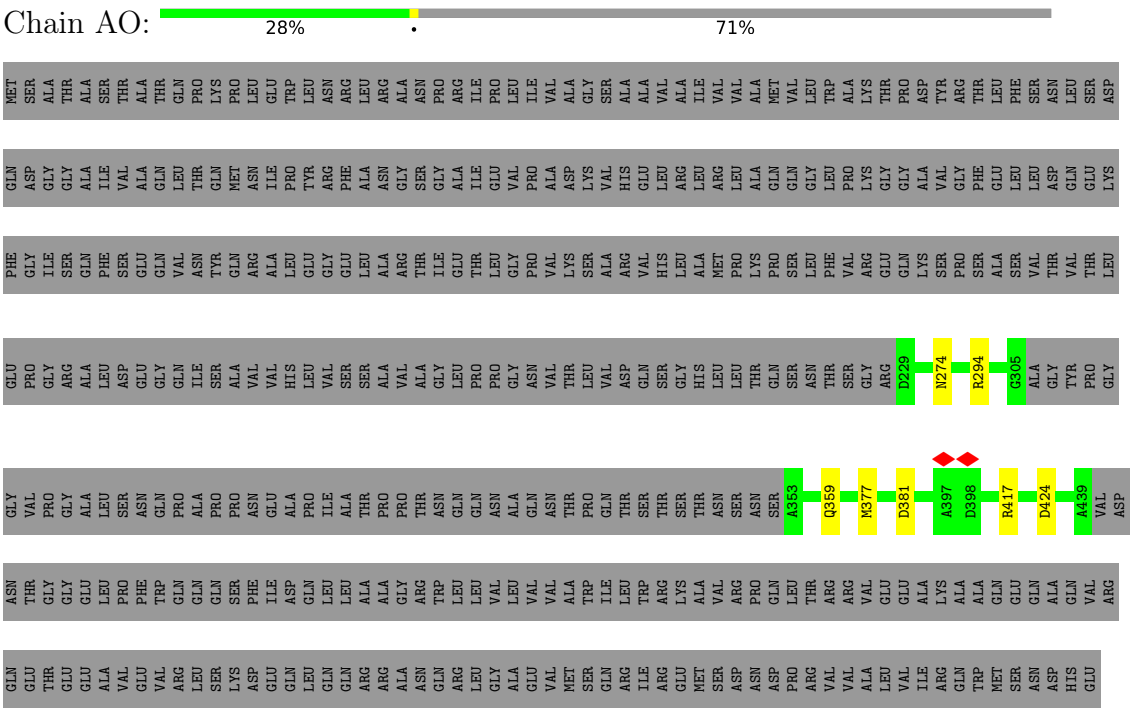
Chain AE:





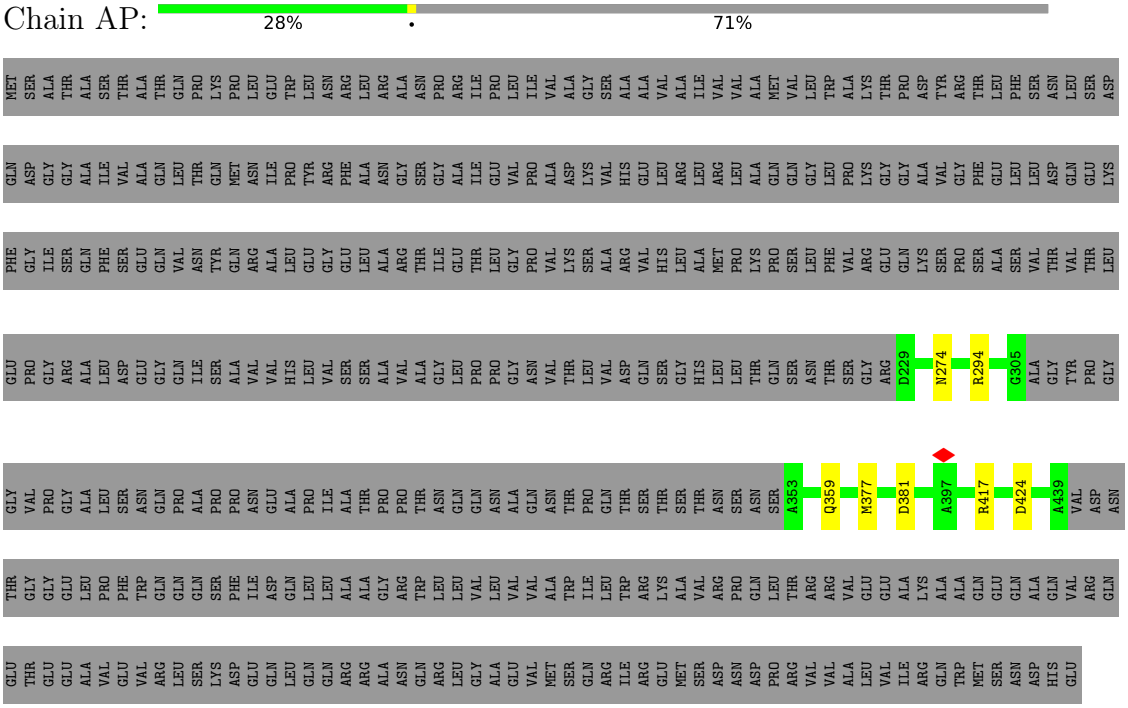
- Molecule 6: Flagellar M-ring protein

Chain AO:



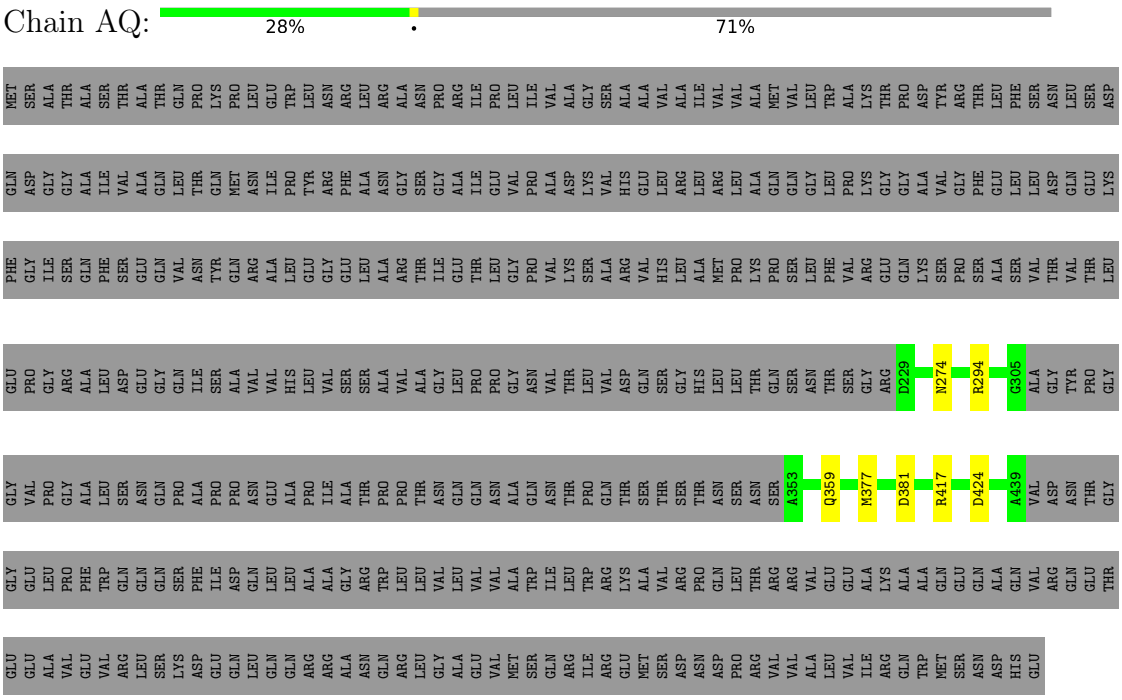
- Molecule 6: Flagellar M-ring protein

Chain AP:



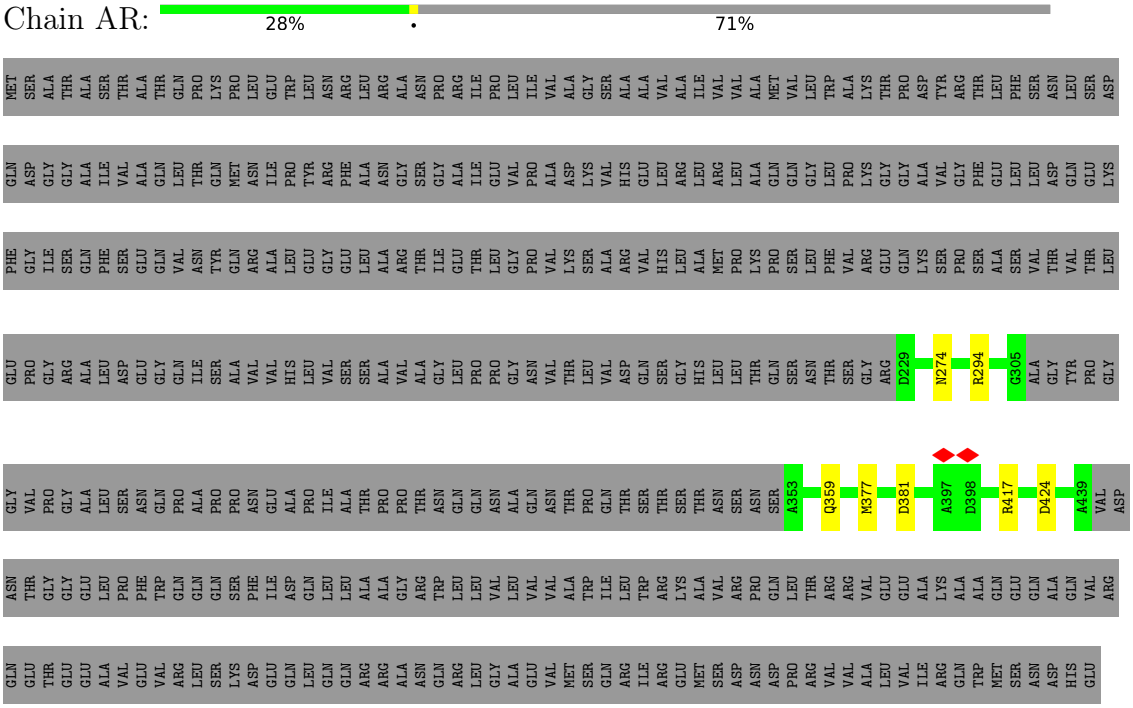
- Molecule 6: Flagellar M-ring protein

Chain AQ:



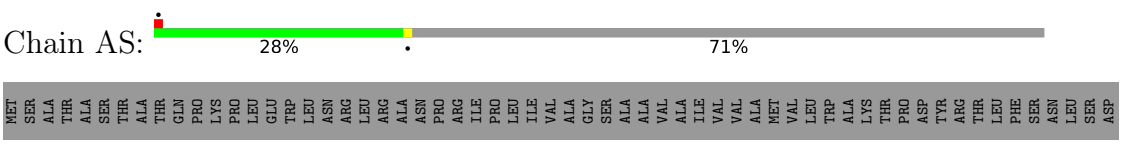
- Molecule 6: Flagellar M-ring protein

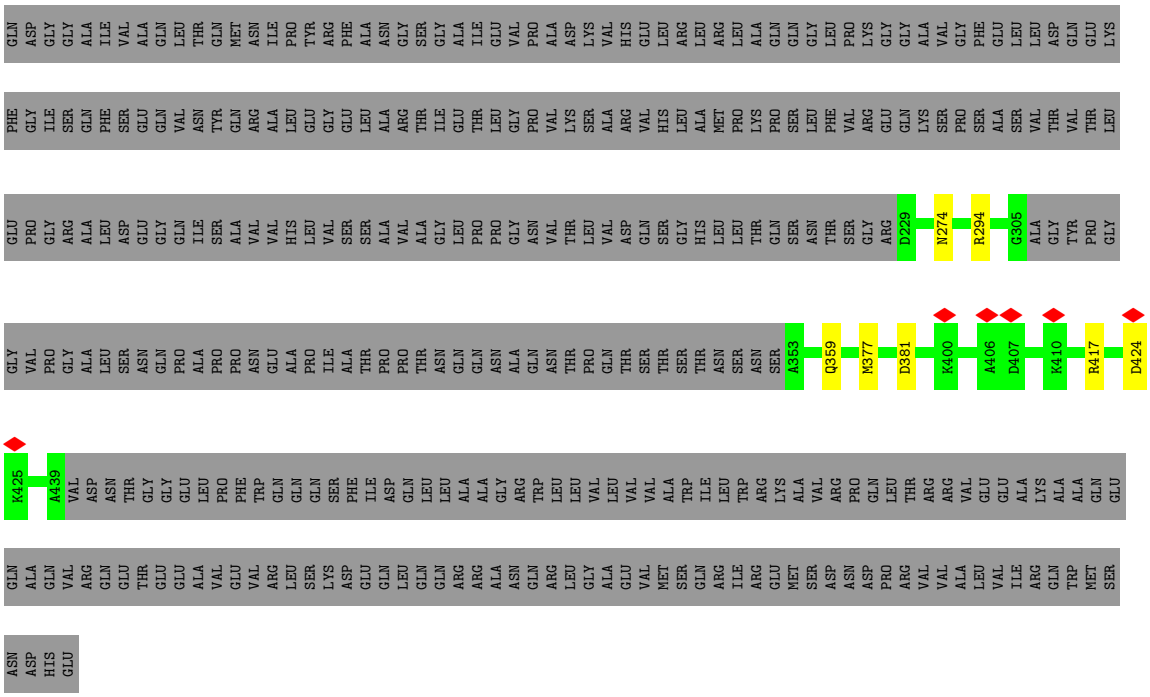
Chain AR:



- Molecule 6: Flagellar M-ring protein

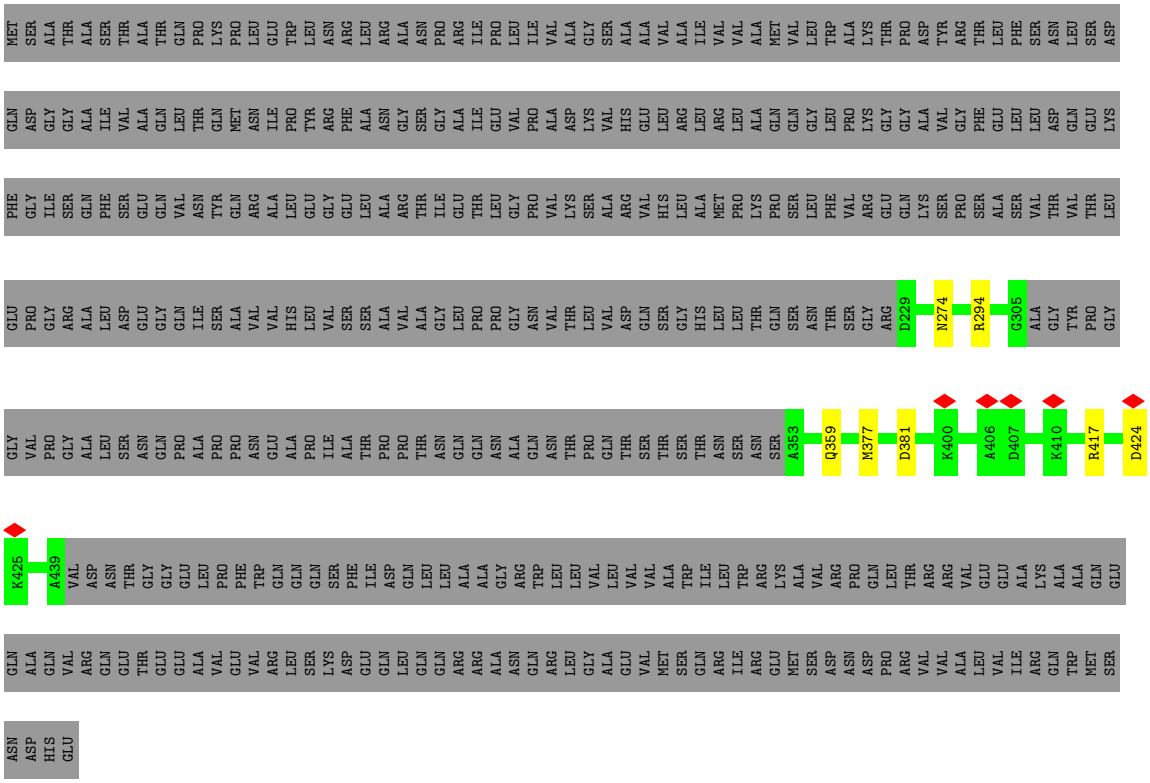
Chain AS:





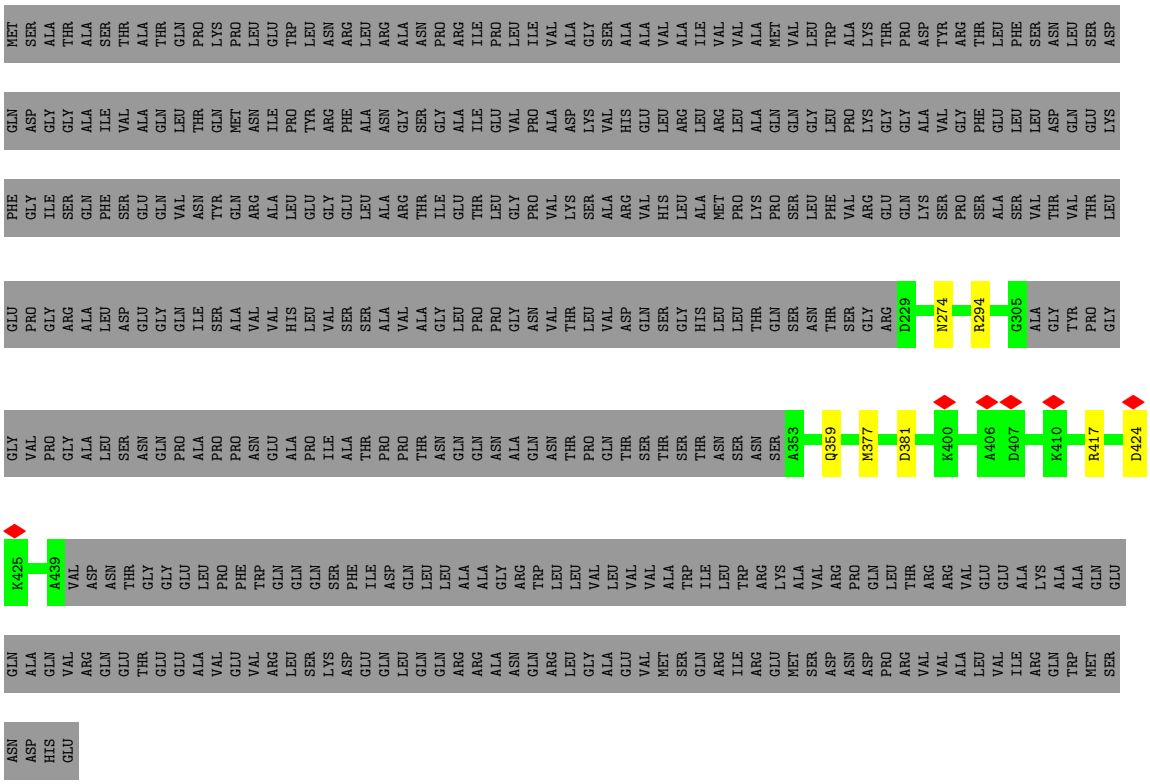
- Molecule 6: Flagellar M-ring protein

Chain AT:



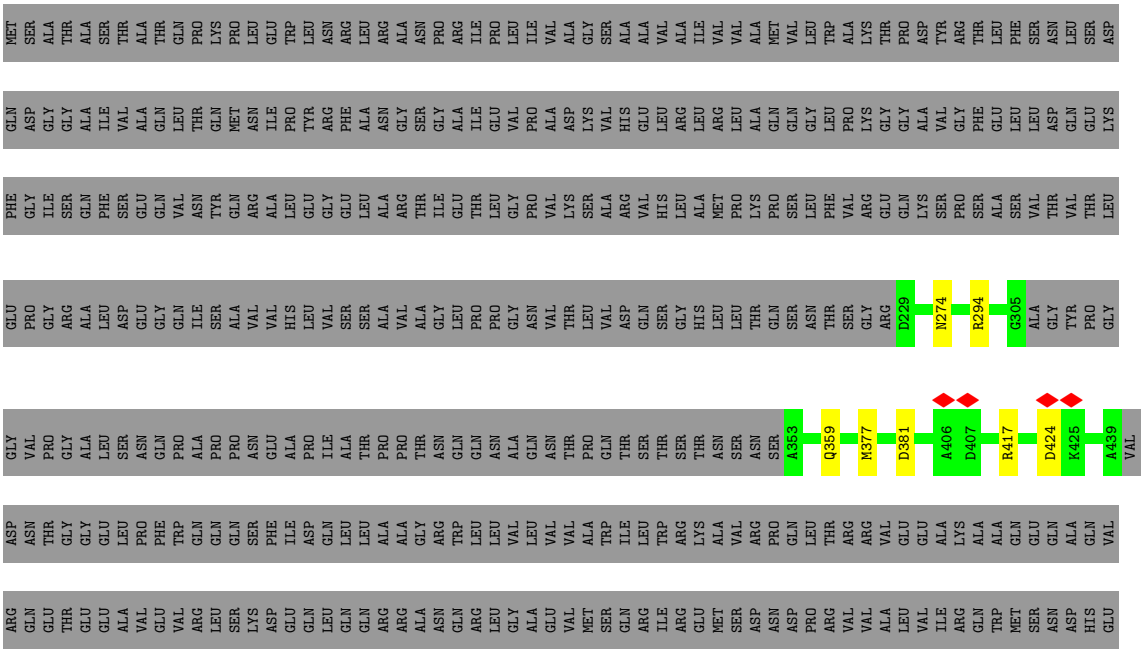
- Molecule 6: Flagellar M-ring protein

Chain AU:



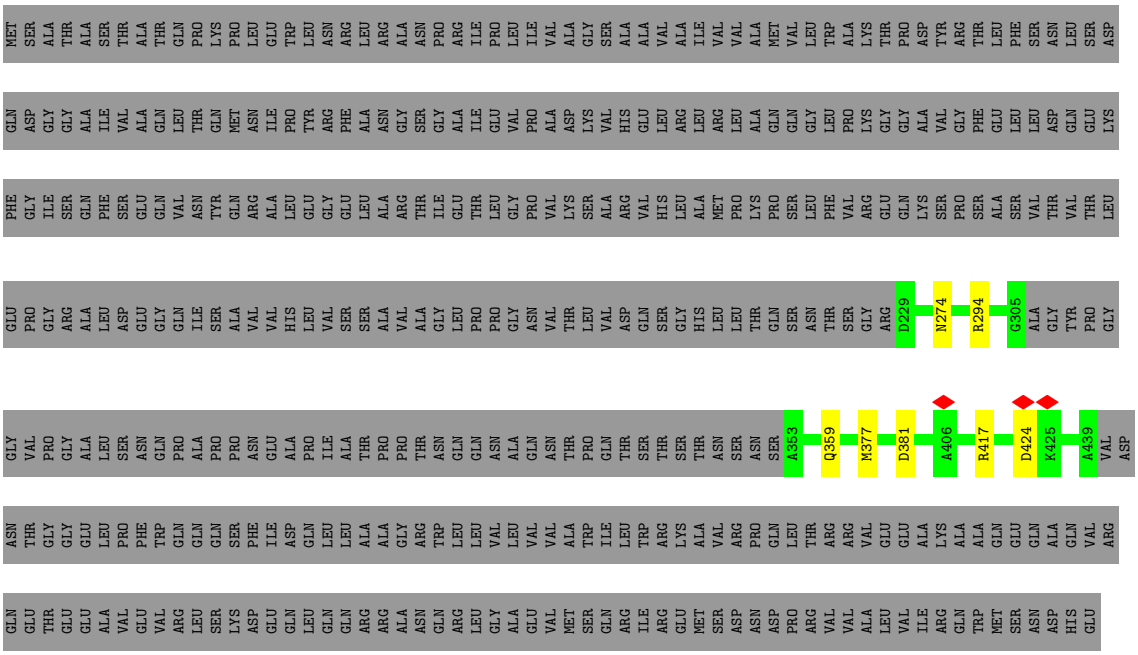
• Molecule 6: Flagellar M-ring protein

Chain AV:



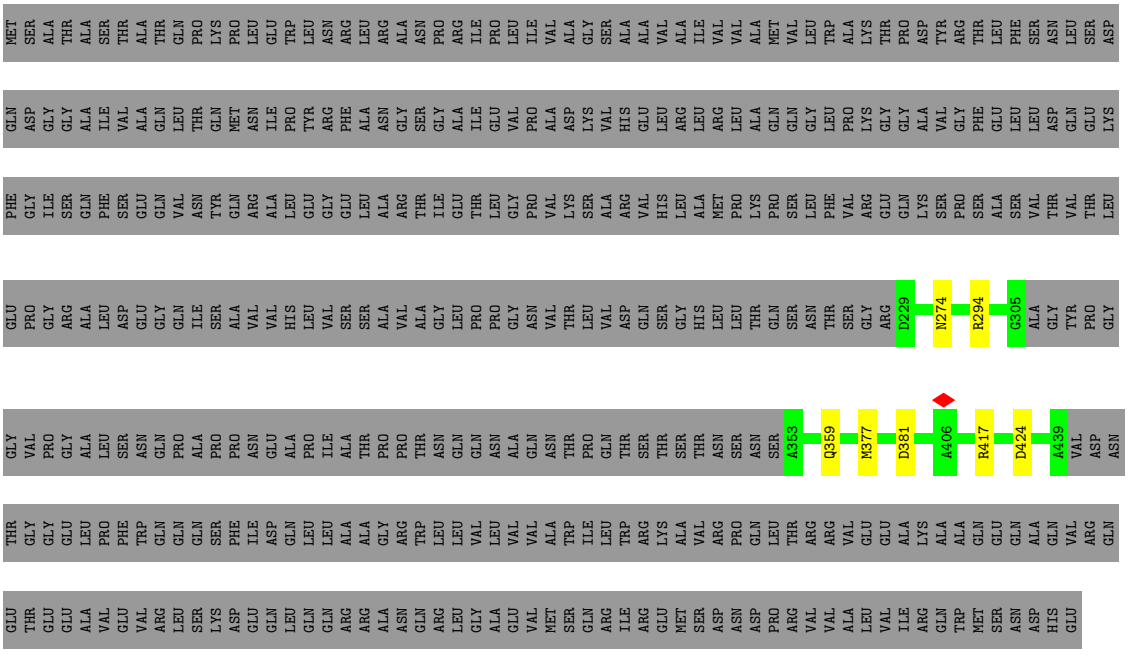
• Molecule 6: Flagellar M-ring protein

Chain AW:



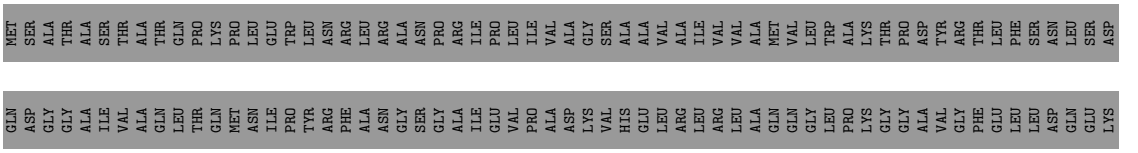
- Molecule 6: Flagellar M-ring protein

Chain AX:



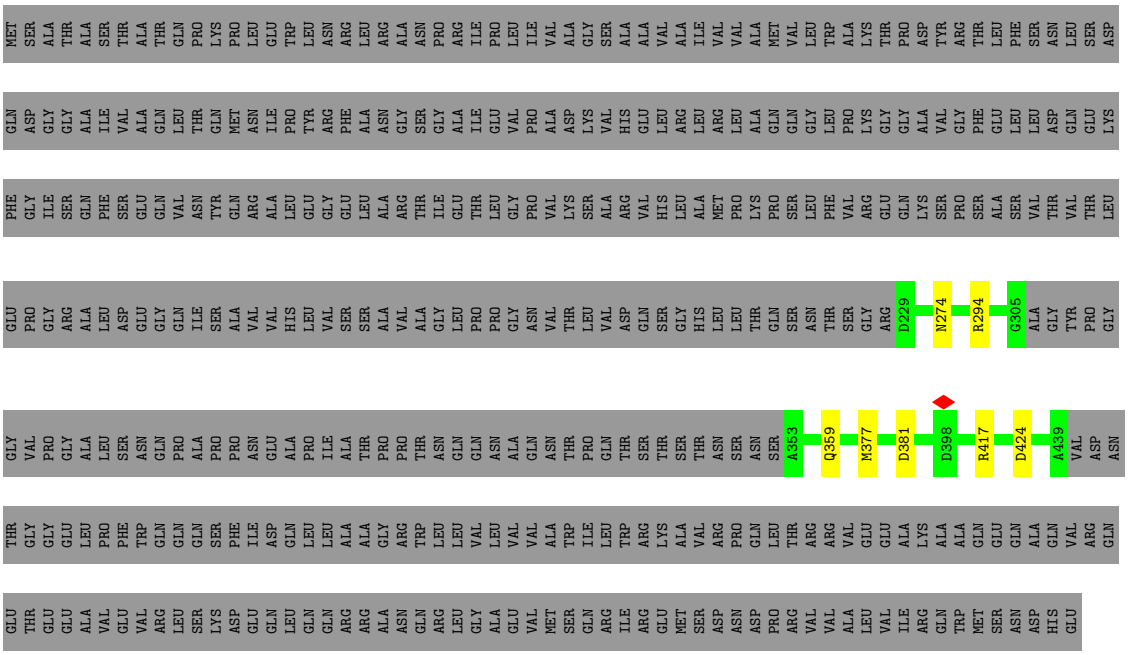
- Molecule 6: Flagellar M-ring protein

Chain AY:



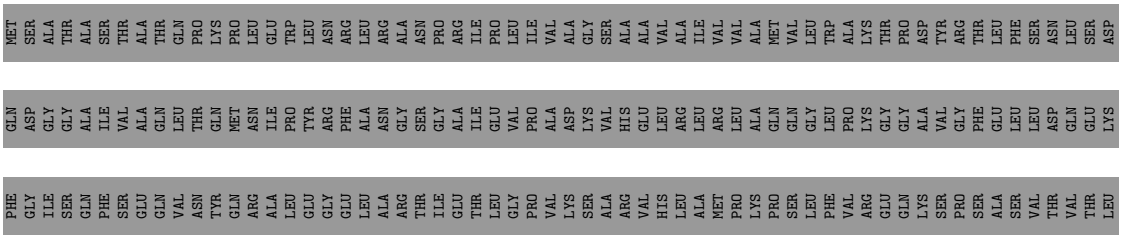
- Molecule 6: Flagellar M-ring protein

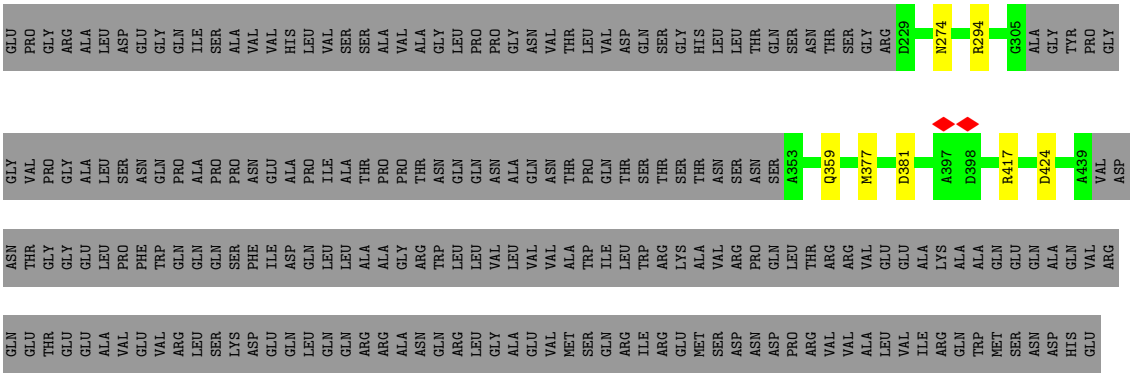
Chain AZ: 28% 71%



- Molecule 6: Flagellar M-ring protein

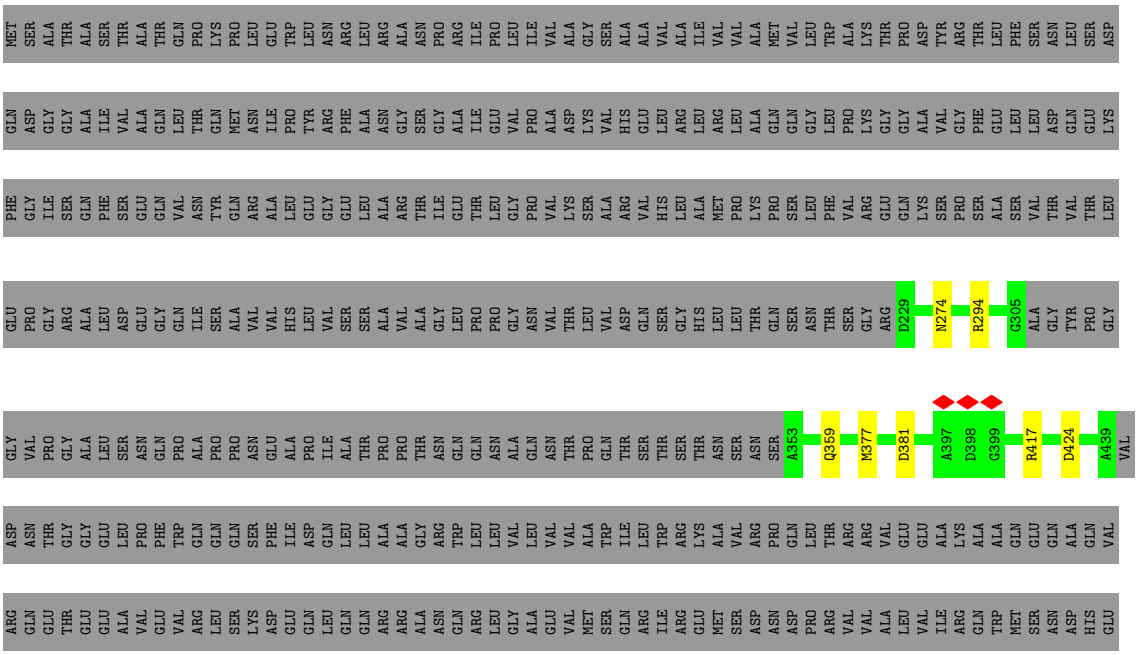
Chain Aa: 28% 71%





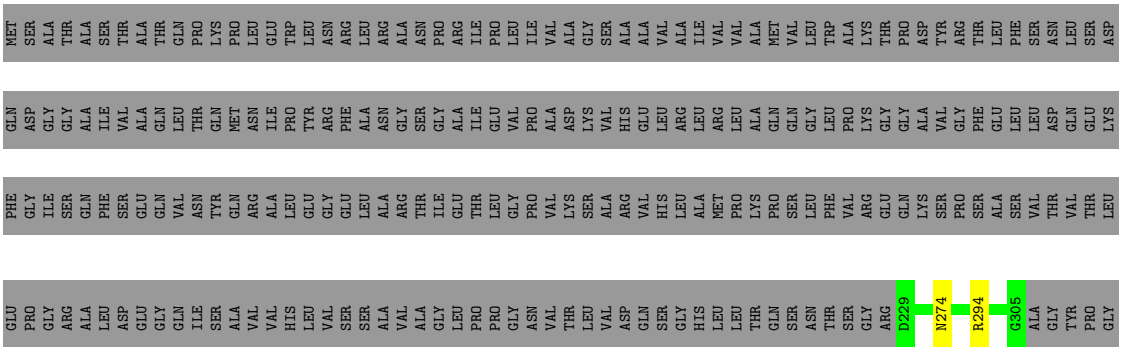
- Molecule 6: Flagellar M-ring protein

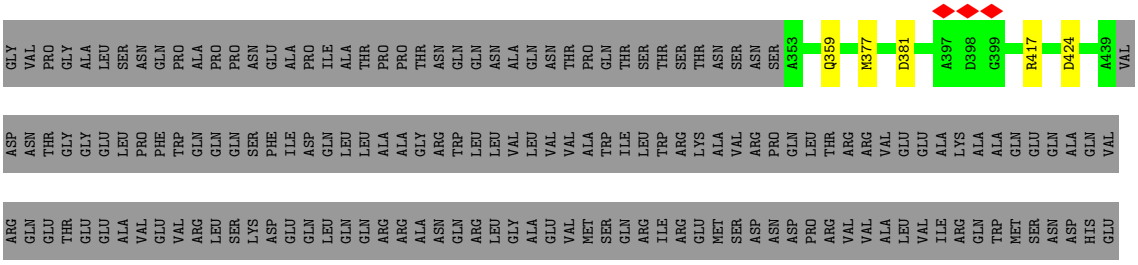
Chain Ac:



- Molecule 6: Flagellar M-ring protein

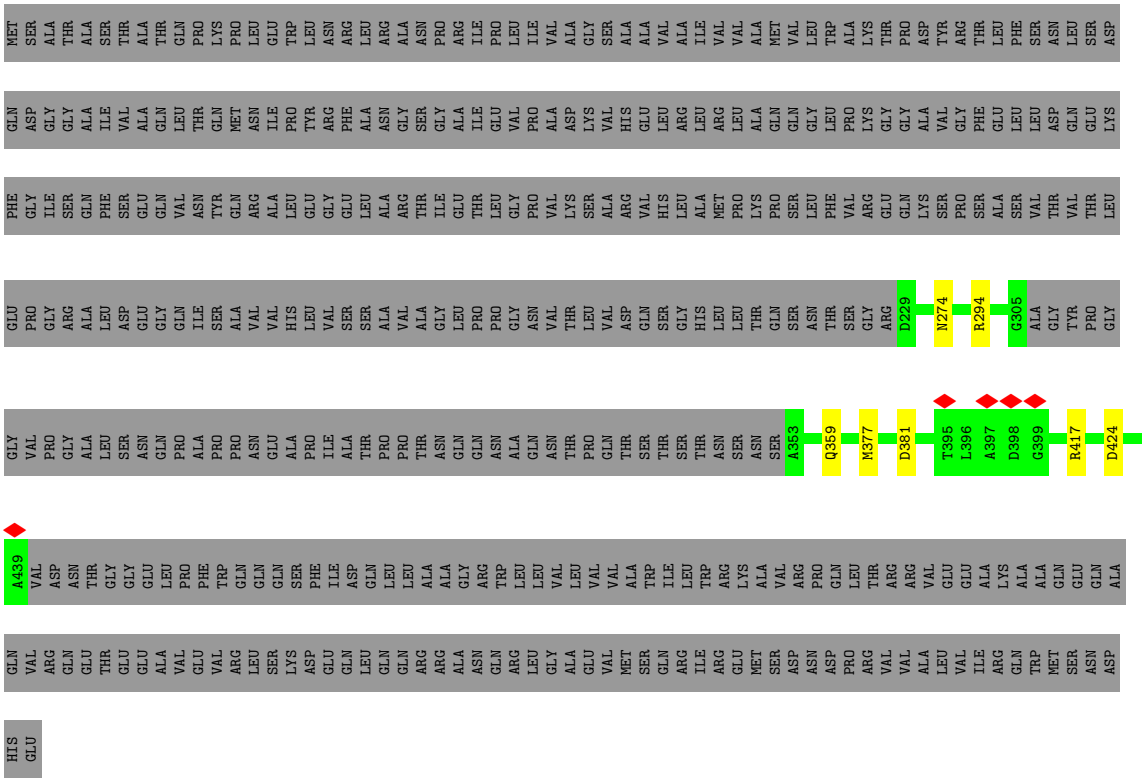
Chain Ad:





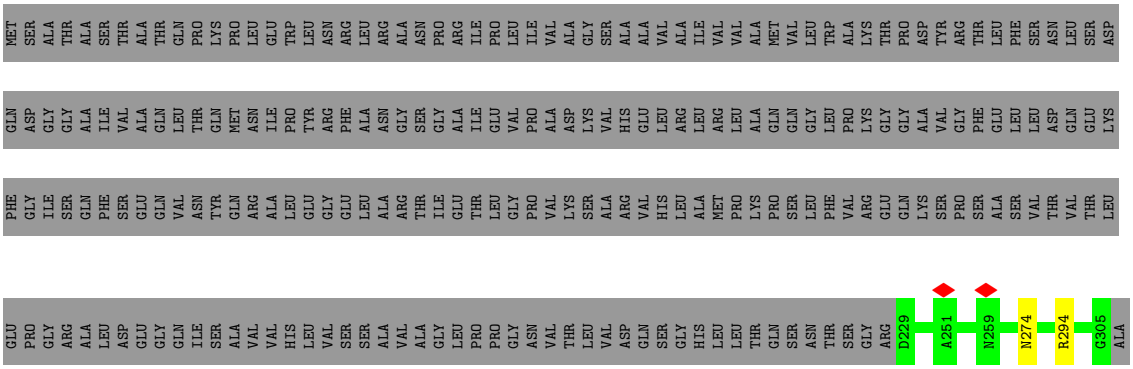
- Molecule 6: Flagellar M-ring protein

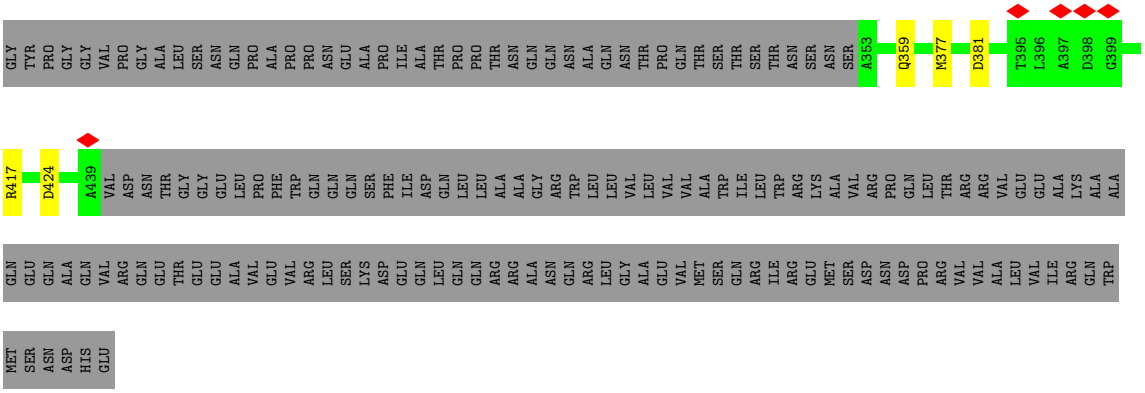
Chain Ae:



- Molecule 6: Flagellar M-ring protein

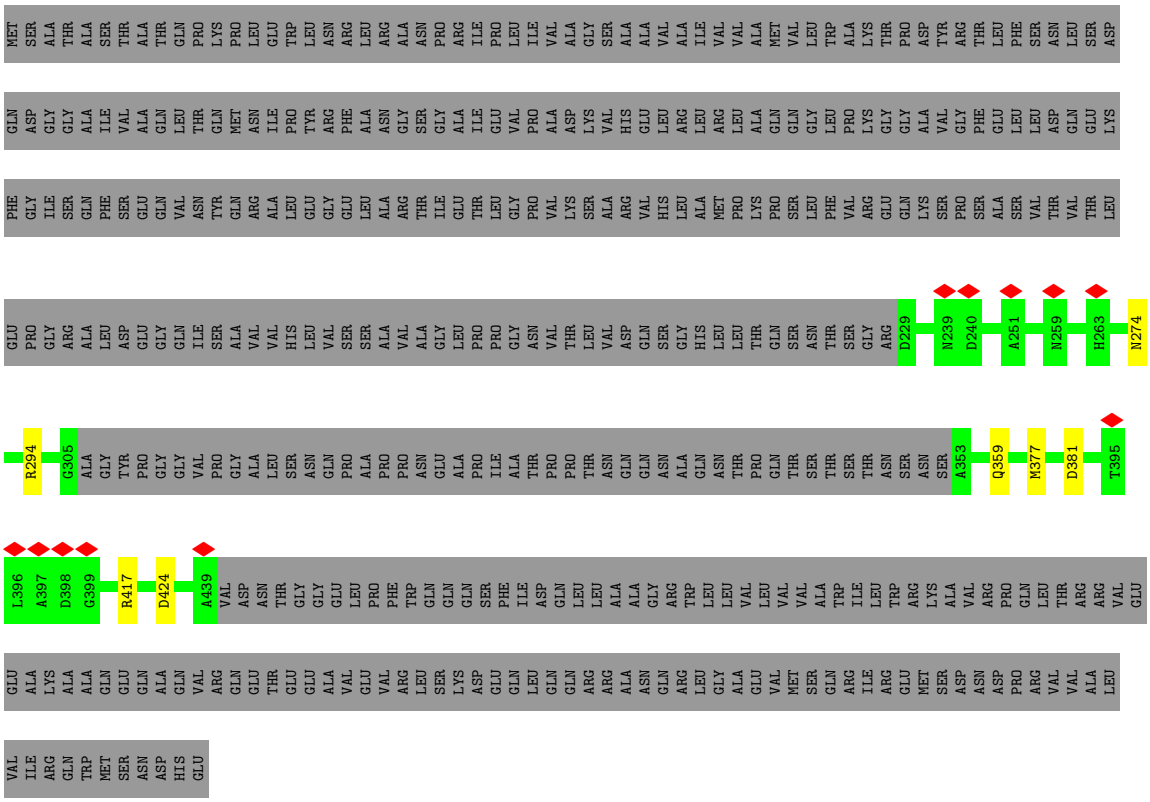
Chain Af:





- Molecule 6: Flagellar M-ring protein

Chain Ag:



- Molecule 6: Flagellar M-ring protein

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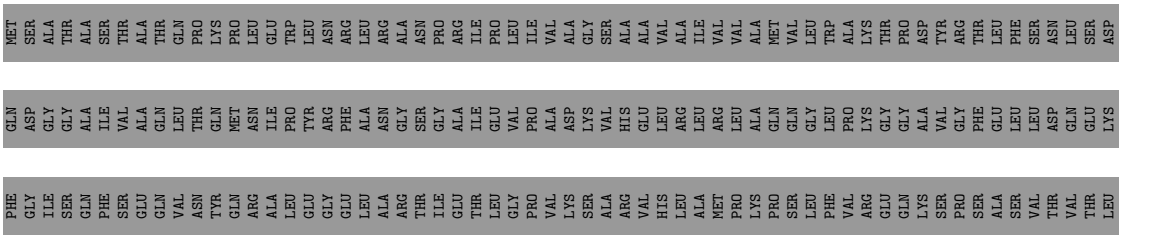
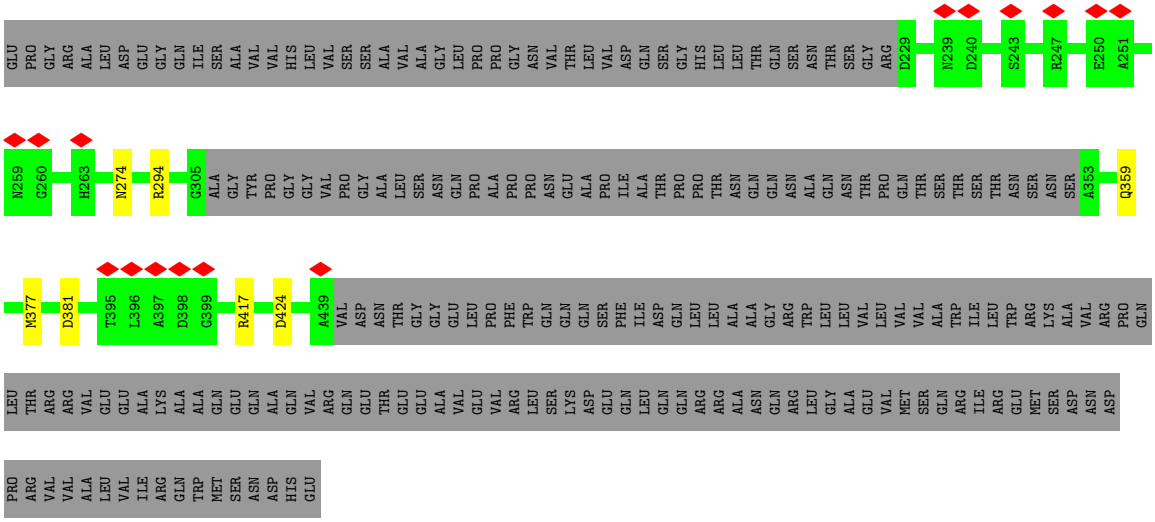
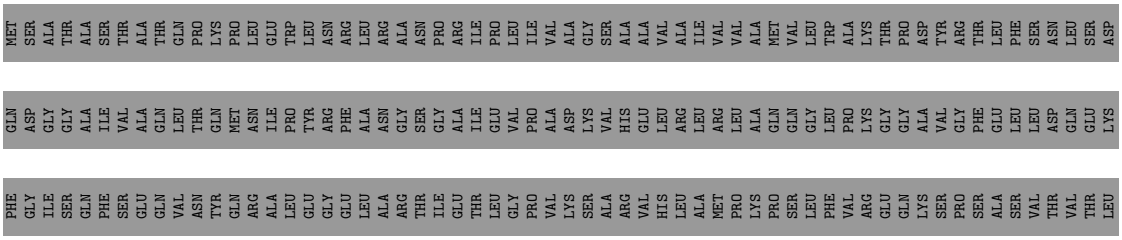
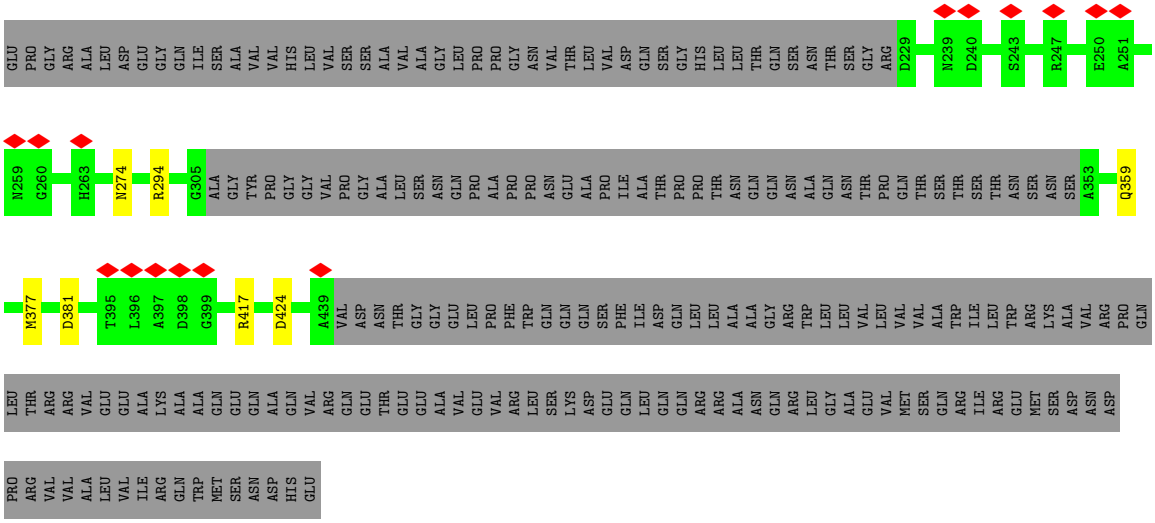




- Molecule 6: Flagellar M-ring protein

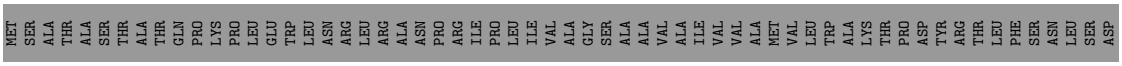
Chain Ai:

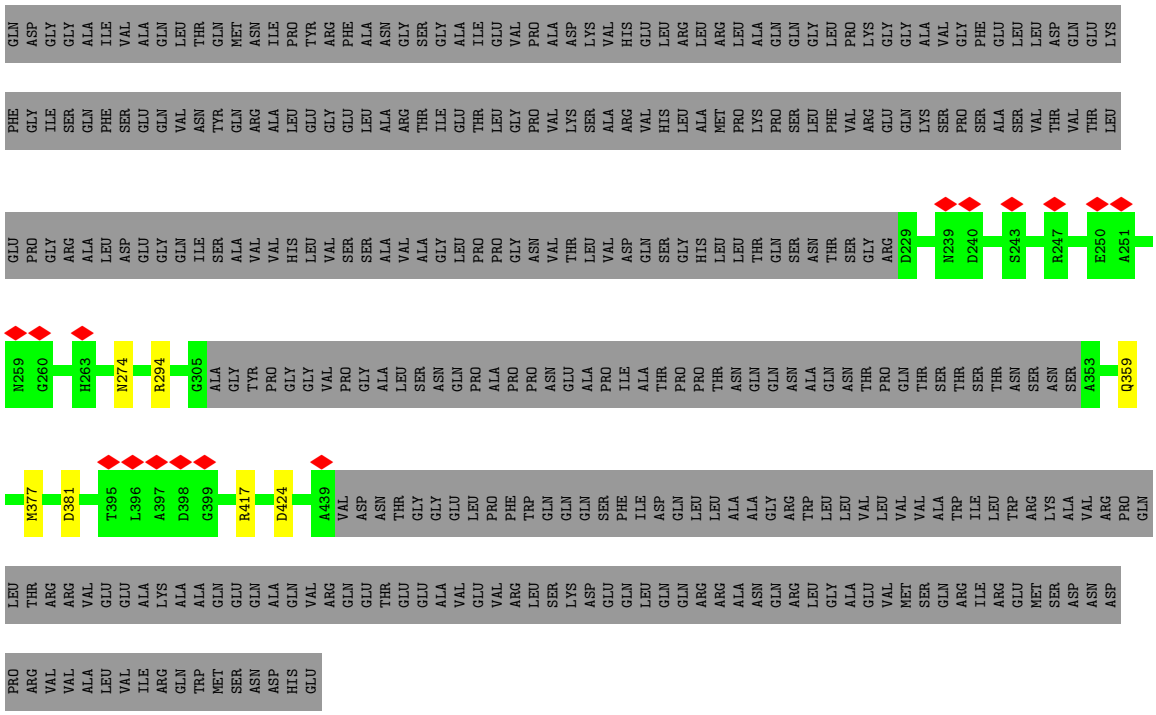




- Molecule 6: Flagellar M-ring protein

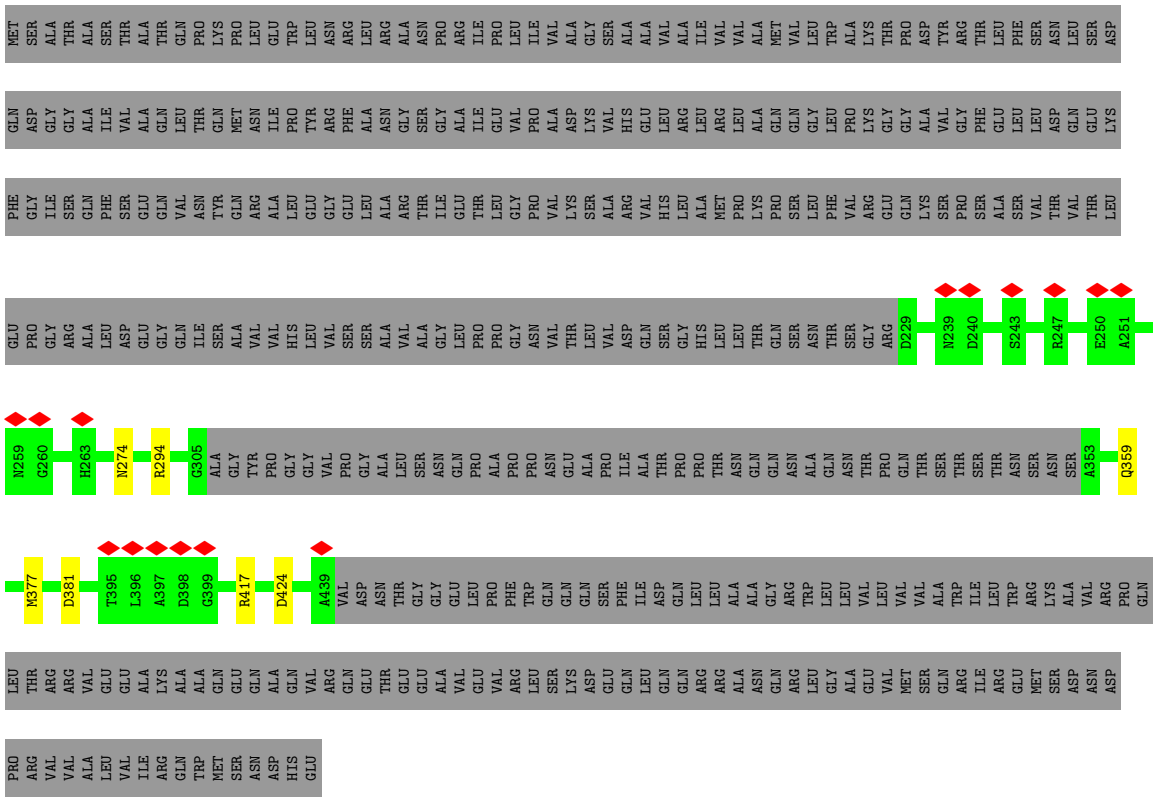
Chain Aj:





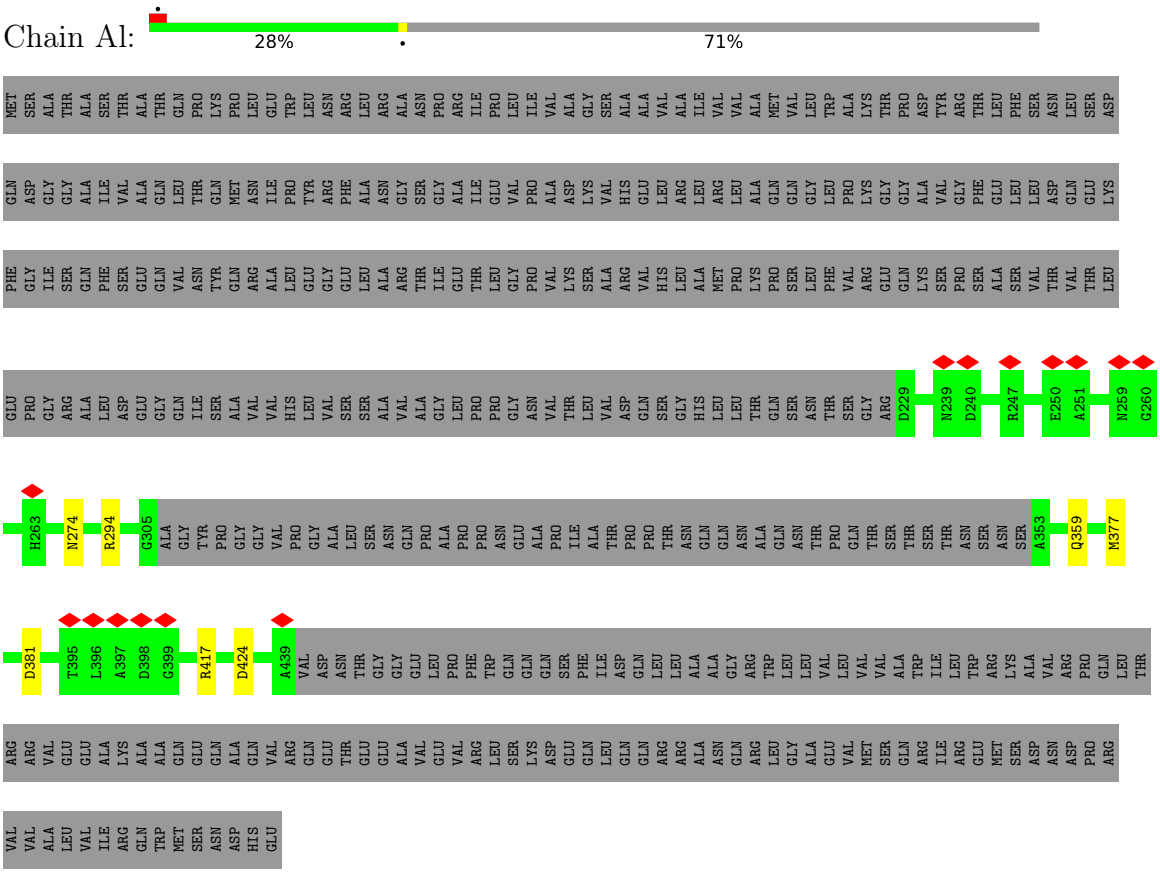
- Molecule 6: Flagellar M-ring protein

Chain Ak:



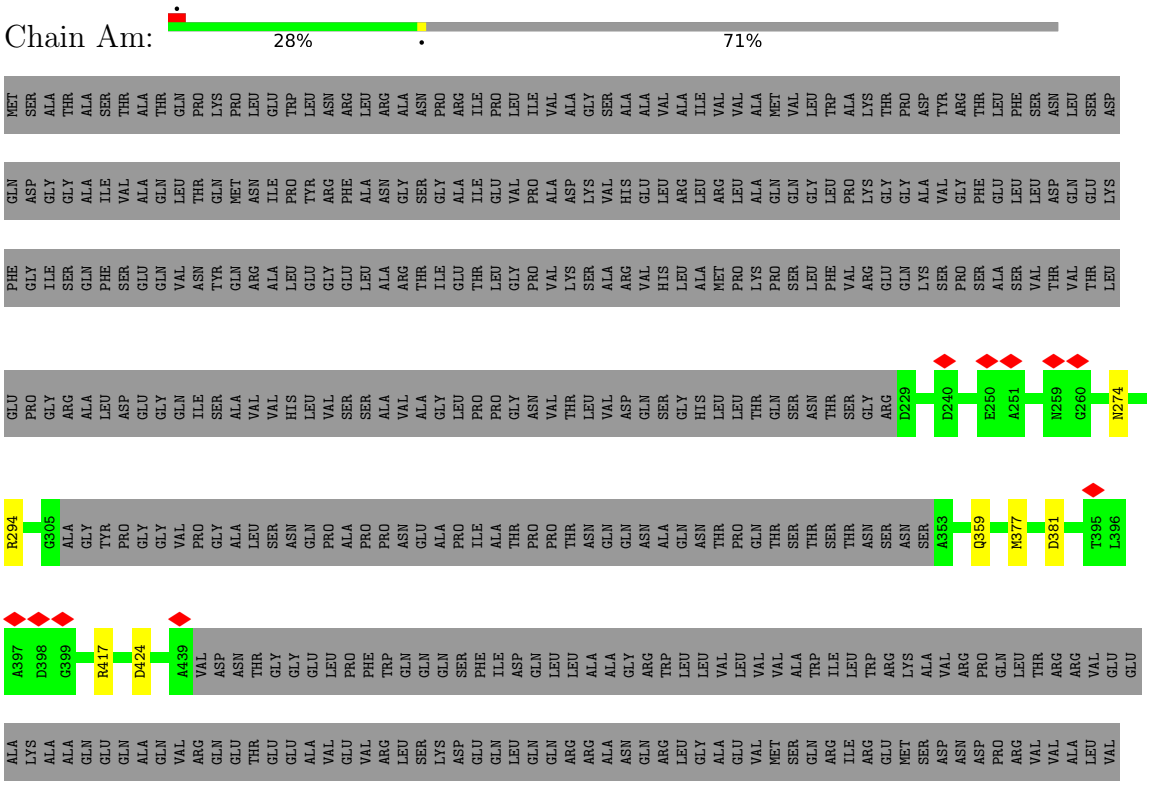
- Molecule 6: Flagellar M-ring protein

Chain Al:



• Molecule 6: Flagellar M-ring protein

Chain Am:



ILE ARG GLN TRP MET SER ASN ASP HIS GLU

• Molecule 6: Flagellar M-ring protein

Chain An:

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

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

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG D229 A251 N259 N274 R294 G305 ALA

GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER A353 Q359 M377 D381 T395 L396 A397 D398 G399

R417 D424 A439 VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA

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

MET SER ASN ASP HIS GLU

• Molecule 6: Flagellar M-ring protein

Chain Ao:

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

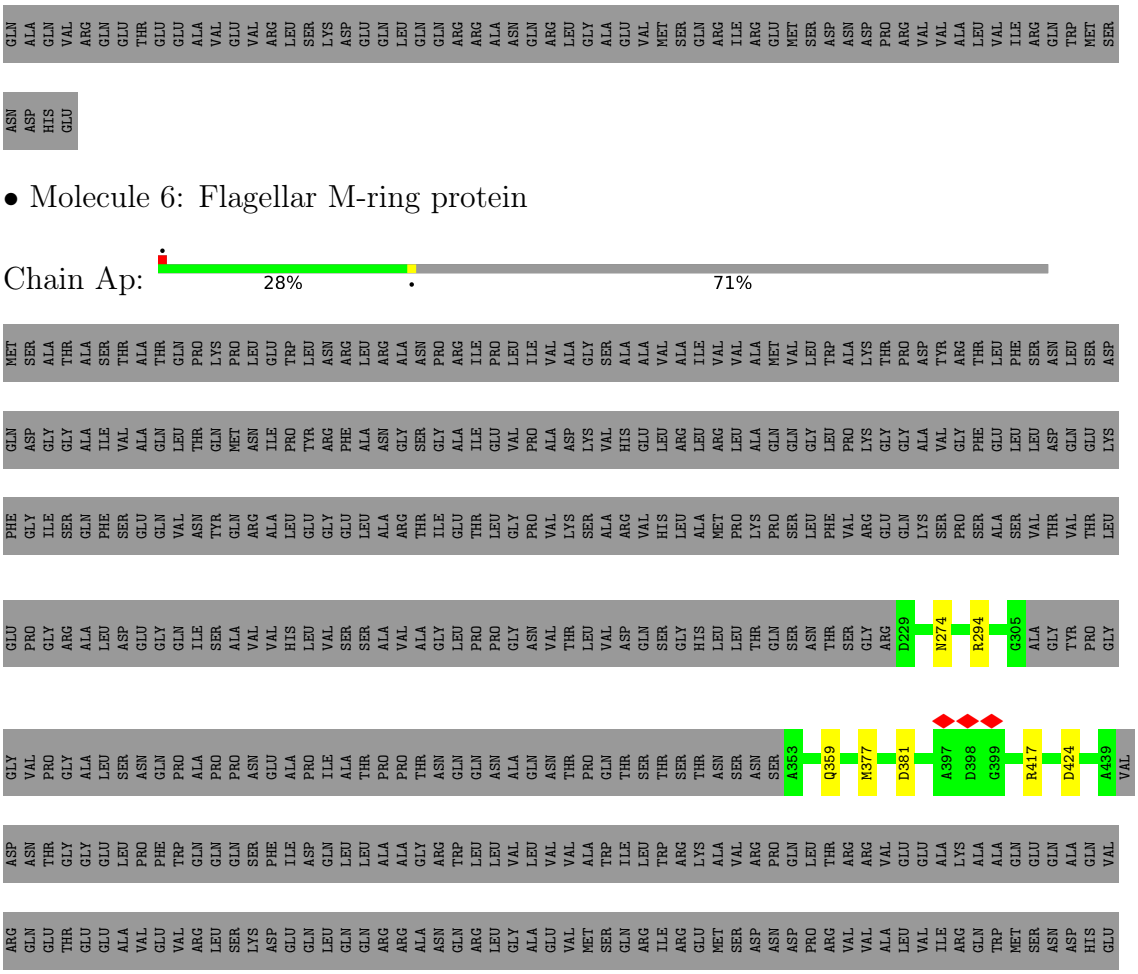
GLN ASP GLY GLY ALA ILE VAL ALA GLN LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ASN GLY SER GLY ALA ILE GLU VAL PRO ALA ASP LYS VAL HIS GLU LEU ARG LEU ARG LEU ALA VAL GLN GLN GLY LEU PRO LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU LEU ASP GLN GLU LYS

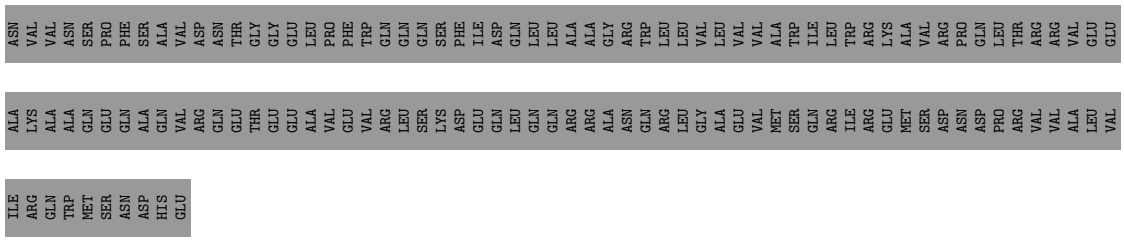
PHE GLY ILE SER GLN PHE SER GLU GLN VAL ASN TYR GLN ARG ALA LEU GLU GLY GLU LEU ALA ARG THR ILE GLU THR LEU GLY PRO VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO LYS PRO SER LEU PHE VAL ARG GLU GLN LYS SER PRO SER ALA SER VAL THR VAL THR LEU

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG D229 N259 N274 R294 G305 ALA GLY TYR

PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER A353 Q359 M377 D381 T395 L396 A397 D398 G399 R417

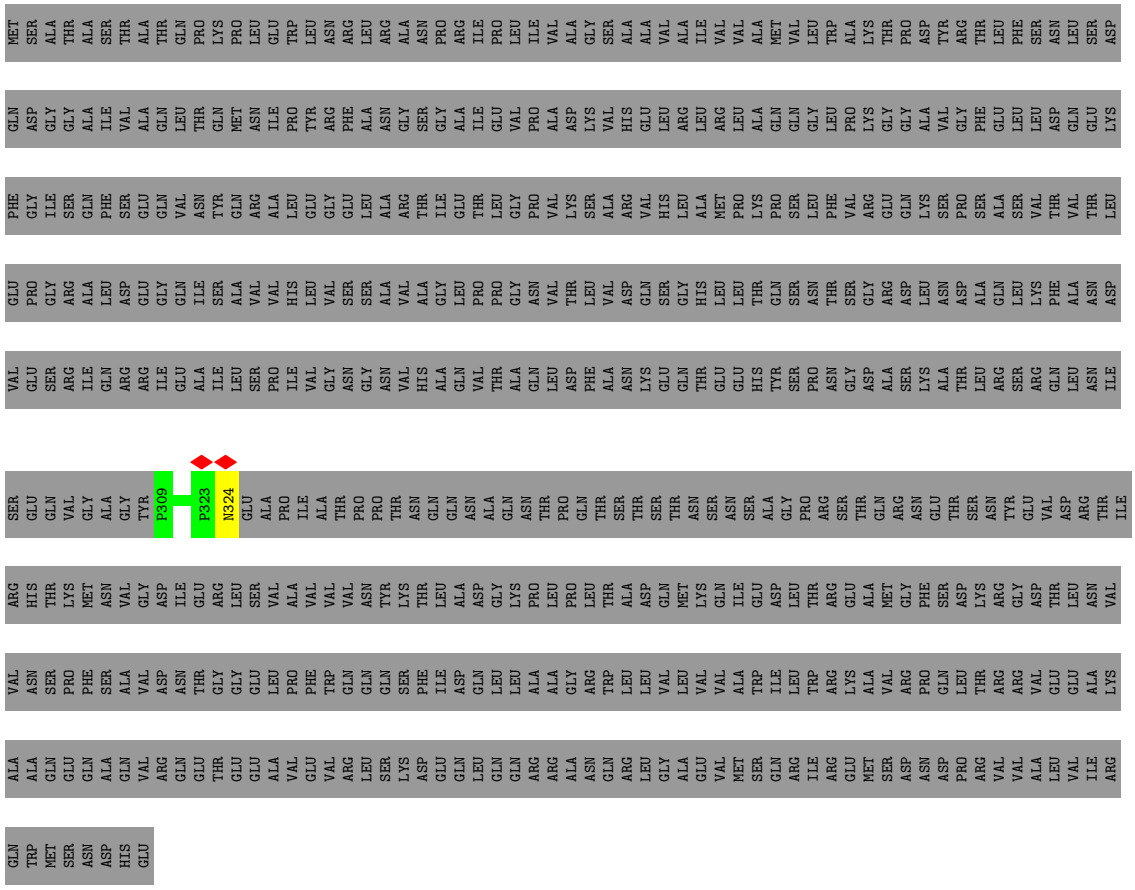
D424 A439 VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU


GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL MET SER GLN ARG ILE ARG GLU MET SER ASP ASN ASP PRO ARG VAL VAL ALA LEU VAL ILE ARG GLN TRP MET SER
ASN ASP HIS GLU
• Molecule 6: Flagellar M-ring protein
Chain Ap:
28%
71%
MET SER ALA THR ALA SER THR ALA THR GLN PRO LYS PRO LEU GLU TRP LEU ASN ARG LEU ARG ALA ASN PRO ARG ILE PRO LEU ILE VAL ALA GLY SER ALA ALA VAL ALA ILE VAL VAL ALA MET VAL LEU TRP ALA LYS THR PRO ASP TYR ARG THR LEU PHE SER ASN LEU SER ASP
GLN ASP GLY GLY ALA ILE VAL ALA GLN LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ASN GLY SER GLY ALA ILE GLU VAL PRO ALA ASP LYS VAL HIS GLU LEU ARG LEU ARG LEU ALA GLN GLN GLY LEU PRO LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU ASP GLN GLU LYS
PHE GLY ILE SER GLN PHE SER GLU GLN VAL ASN TYR GLN ARG ALA LEU GLU GLY GLU LEU ALA ARG THR ILE GLU THR LEU GLY PRO VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO LYS PRO SER LEU PHE VAL ARG GLU GLN LYS SER PRO SER ALA SER VAL THR VAL THR LEU
GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG D229 N274 R294 G305 ALA GLY TYR PRO GLY
GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER A353 Q359 M377 D381 A397 D398 G399 R417 D424 A439 VAL
ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA ASP VAL
ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL MET SER GLN ARG ILE ARG GLU MET SER ASP ASN ASP PRO ARG VAL VAL ALA LEU VAL ILE ARG GLN TRP MET SER ASN ASP HIS GLU
• Molecule 6: Flagellar M-ring protein
Chain BG:
98%
MET SER ALA THR ALA SER THR ALA THR GLN PRO LYS PRO LEU GLU TRP LEU ASN ARG LEU ARG ALA ASN PRO ARG ILE PRO LEU ILE VAL ALA GLY SER ALA ALA VAL ALA ILE VAL VAL ALA MET VAL LEU TRP ALA LYS THR PRO ASP TYR ARG THR LEU PHE SER ASN LEU SER ASP
GLN ASP GLY GLY ALA ILE VAL ALA GLN LEU THR GLN MET ASN ILE PRO TYR ARG PHE ALA ASN GLY SER GLY ALA ILE GLU VAL PRO ALA ASP LYS VAL HIS GLU LEU ARG LEU ARG LEU ALA GLN GLN GLY LEU PRO LYS GLY GLY ALA VAL GLY PHE GLU LEU LEU ASP GLN GLU LYS
PHE GLY ILE SER GLN PHE SER GLU GLN VAL ASN TYR GLN ARG ALA LEU GLU GLY GLU LEU ALA ARG THR ILE GLU THR LEU GLY PRO VAL LYS SER ALA ARG VAL HIS LEU ALA MET PRO LYS PRO SER LEU PHE VAL ARG GLU GLN LYS SER PRO SER ALA SER VAL THR VAL THR LEU
GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU ASN ASP ALA GLN LEU LYS PHE ALA ASN ASP
VAL GLU SER ARG ILE GLN ARG ARG ILE GLU ALA ILE LEU SER PRO ILE VAL GLY ASN GLY ASN VAL HIS ALA GLN VAL THR ALA GLN LEU ASP PHE ALA ASN LYS GLU GLN THR GLU GLU HIS TYR SER PRO ASN GLY ASP ALA SER LYS ALA THR LEU ARG SER ARG GLN LEU ASN ILE
SER GLU GLN VAL GLY ALA GLY TYR PRO G310 P322 PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG ASN GLU THR SER ASN TYR GLU VAL ASP ARG
THR ILE ARG HIS THR LYS MET ASN VAL GLY ASP ILE GLU ARG LEU SER VAL ALA VAL VAL VAL ASN TYR LYS THR LEU ALA ASP GLY LYS PRO LEU PRO LEU THR ALA ASP GLN MET LYS GLN ILE GLU ASP LEU THR ARG GLU ALA MET GLY PHE SER ASP LYS ARG GLY ASP THR LEU



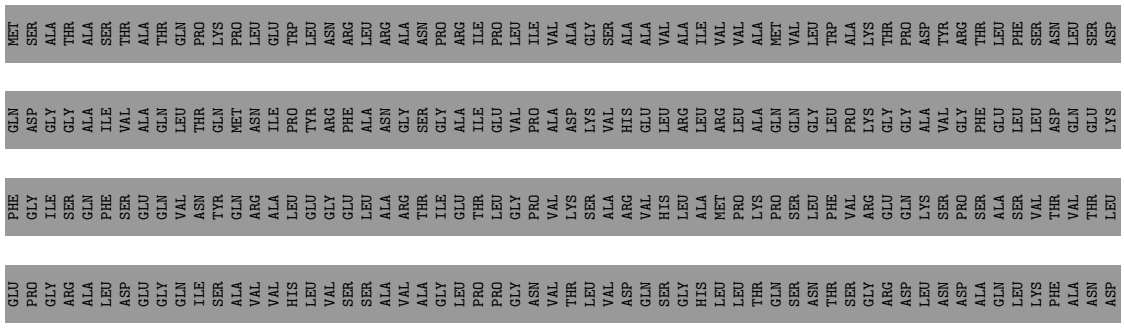
• Molecule 6: Flagellar M-ring protein

Chain BH: 97%



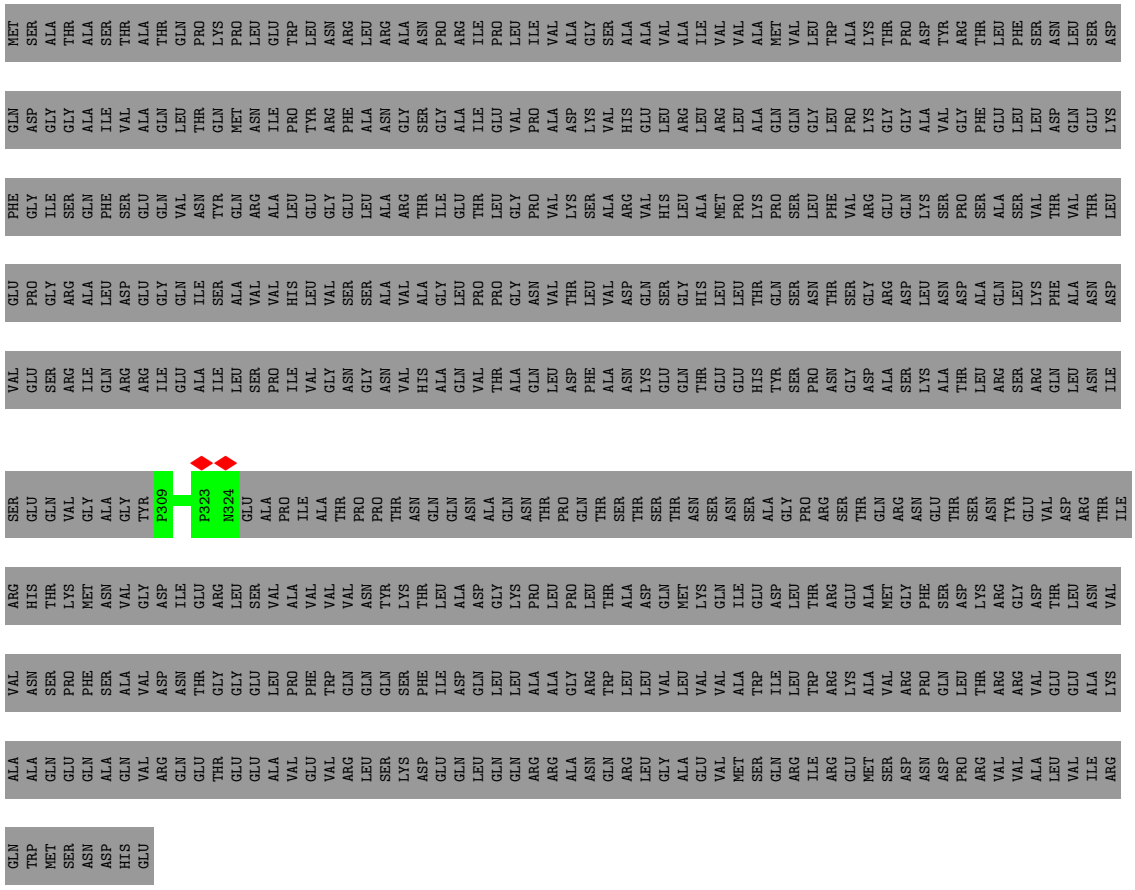
• Molecule 6: Flagellar M-ring protein

Chain BI: 96%



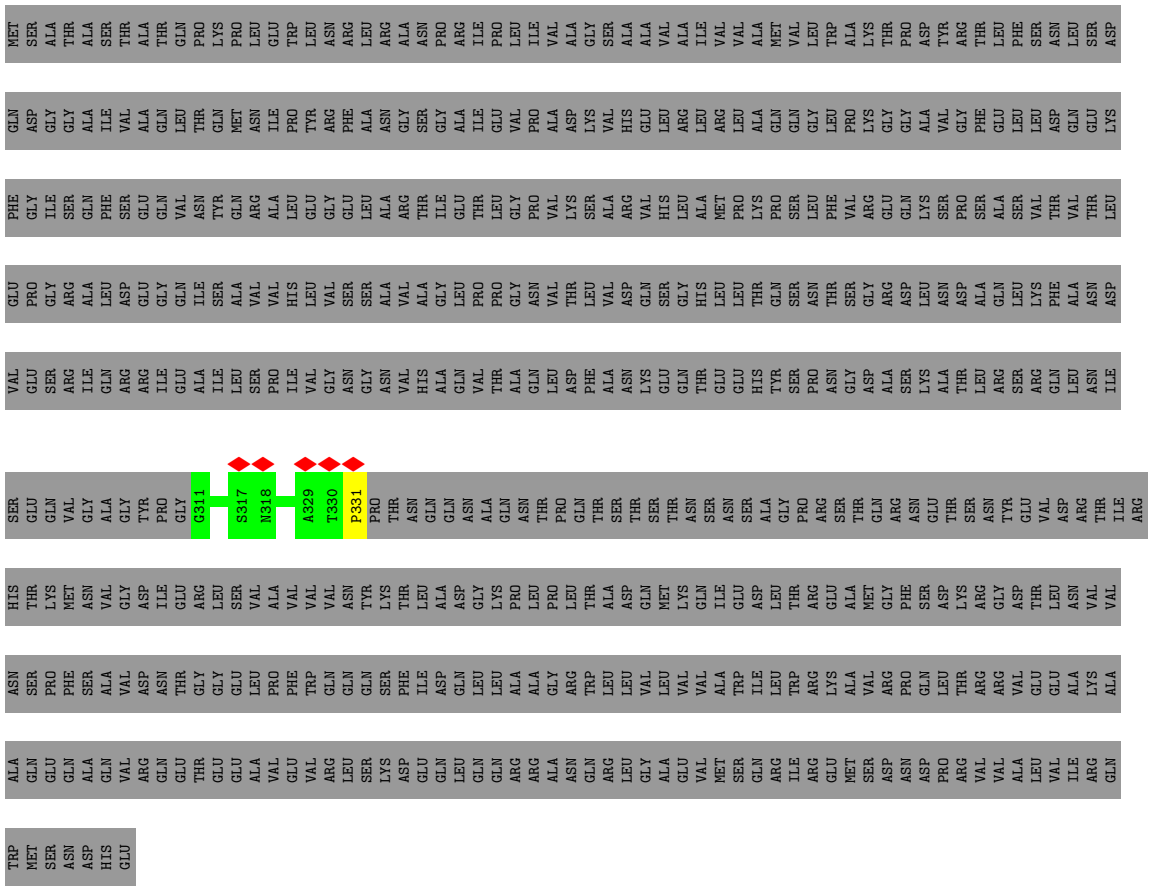
• Molecule 6: Flagellar M-ring protein

Chain BJ: 97%



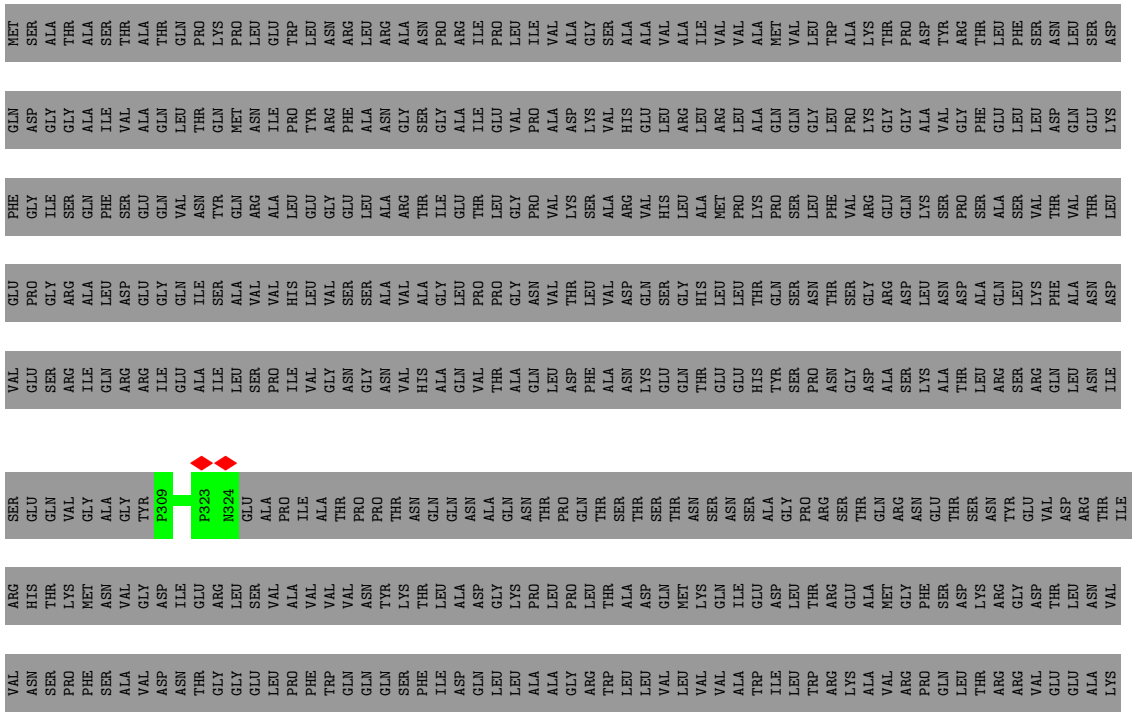
• Molecule 6: Flagellar M-ring protein

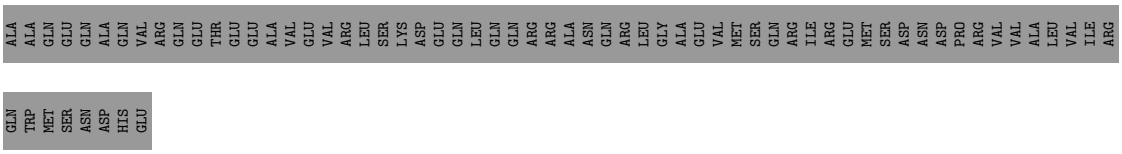
Chain BK: 96%



- Molecule 6: Flagellar M-ring protein

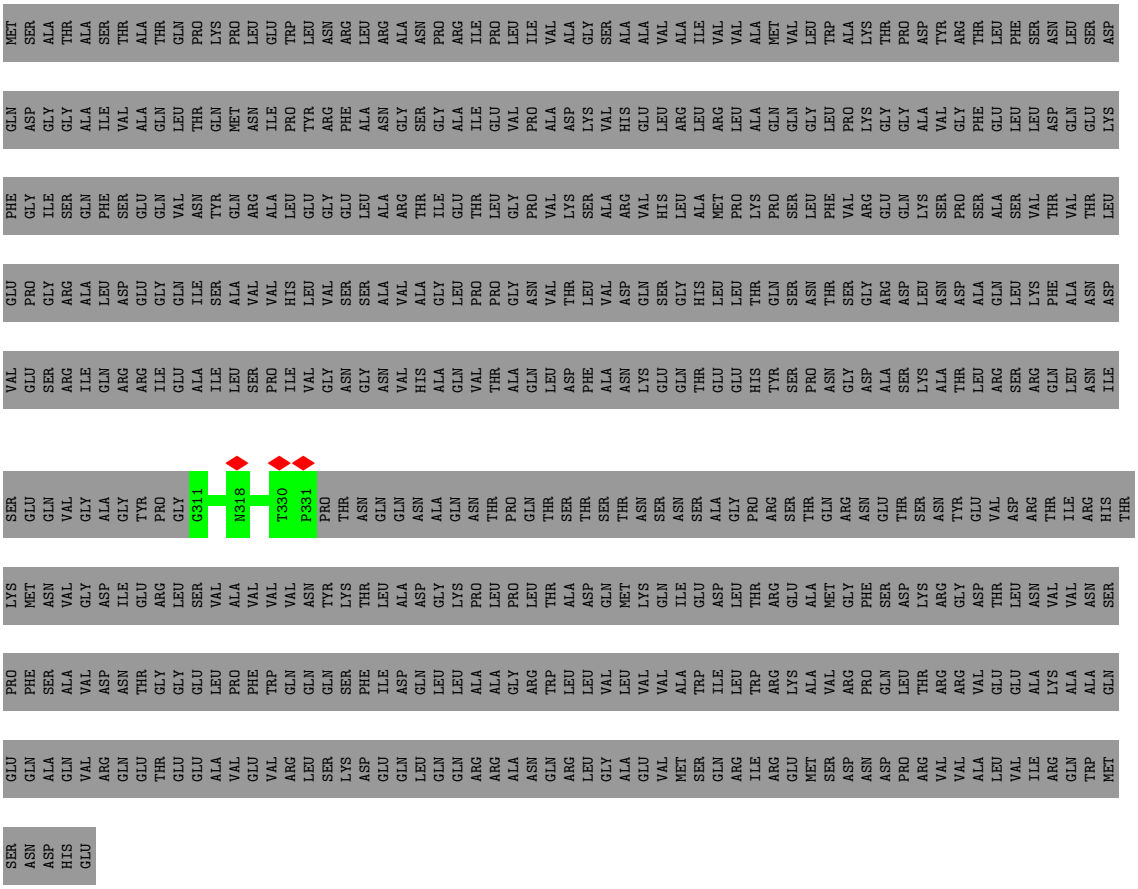
Chain BL: 97%





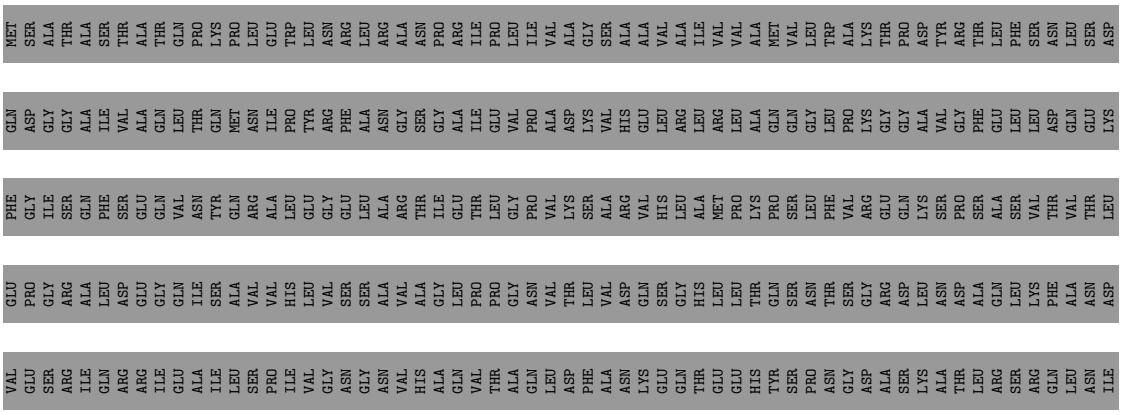
• Molecule 6: Flagellar M-ring protein

Chain BM: 96%



• Molecule 6: Flagellar M-ring protein

Chain BN: 97%

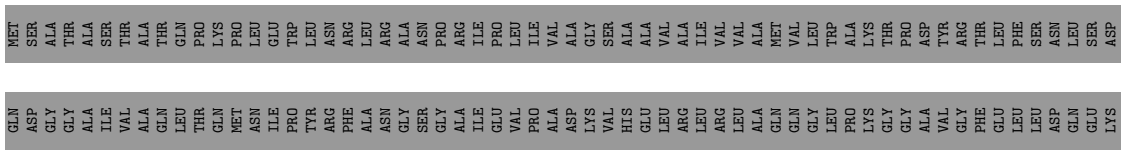


• Molecule 6: Flagellar M-ring protein

Chain BO: 96%

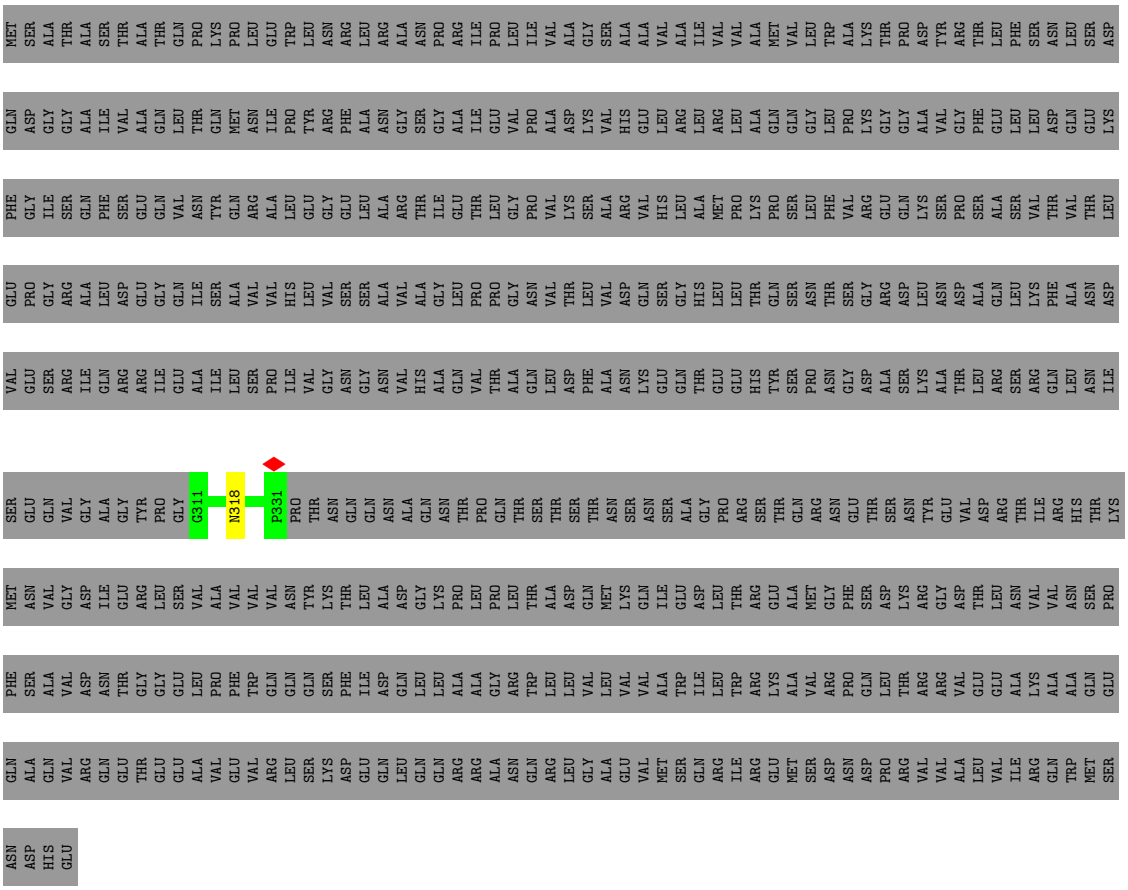
• Molecule 6: Flagellar M-ring protein

Chain BP: 97%



- Molecule 6: Flagellar M-ring protein

Chain BQ: 96%



• Molecule 6: Flagellar M-ring protein

Chain BR: 28% • 71%

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

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

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG D229 N274 R294 G305 ALA GLY TYR PRO GLY

GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER A353 Q359 M377 D381 R417 D424 A439 VAL ASP ASN THR GLY

GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR

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

• Molecule 6: Flagellar M-ring protein

Chain BS: 28% • 71%

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

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

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

GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG D229 N274 R294 G305 ALA GLY TYR PRO GLY

GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER A353 Q359 M377 D381 R417 D424 A439 VAL ASP ASN THR GLY

GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR

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

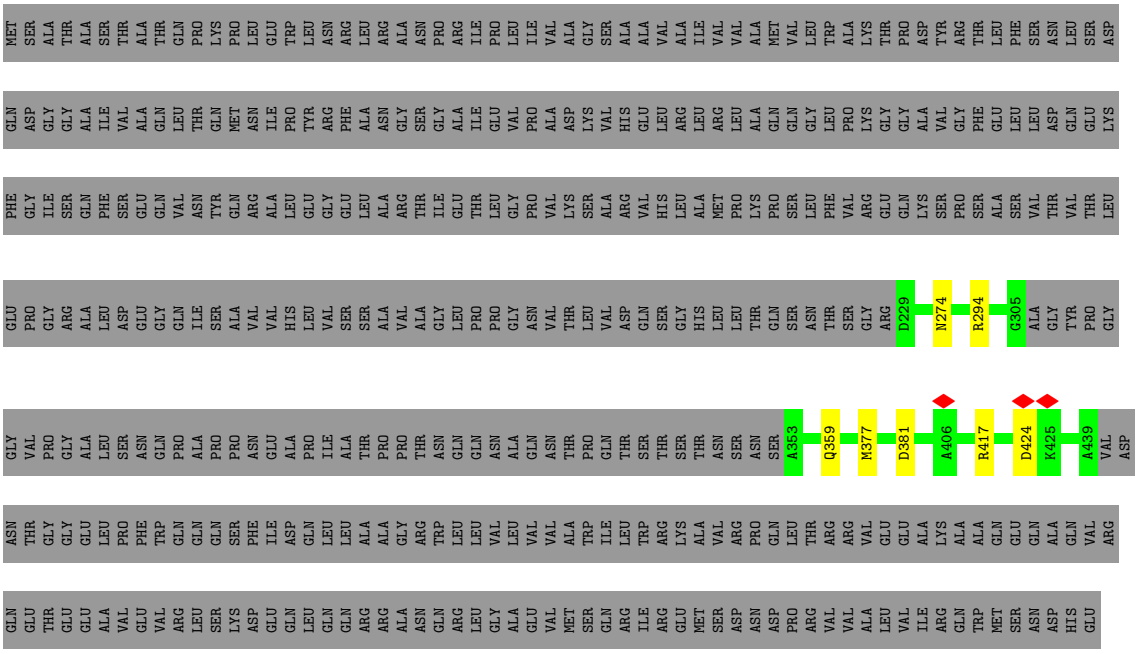
• Molecule 6: Flagellar M-ring protein

Chain BT: 28% • 71%

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

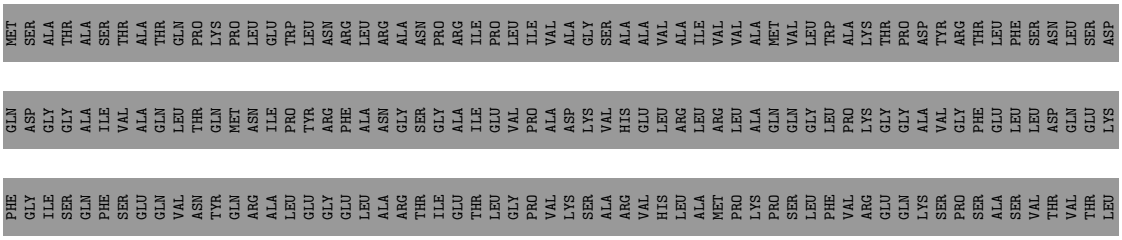
• Molecule 6: Flagellar M-ring protein

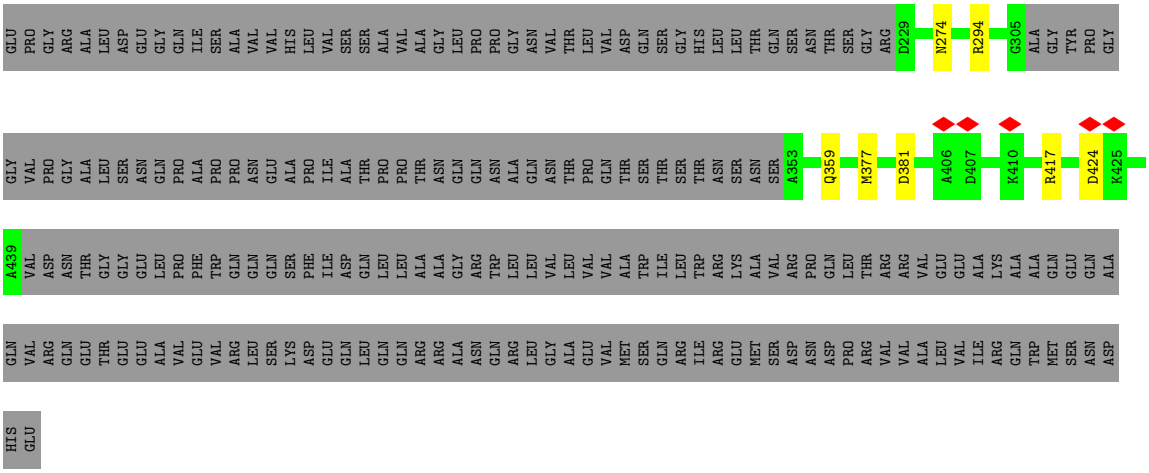
Chain BU:



• Molecule 6: Flagellar M-ring protein

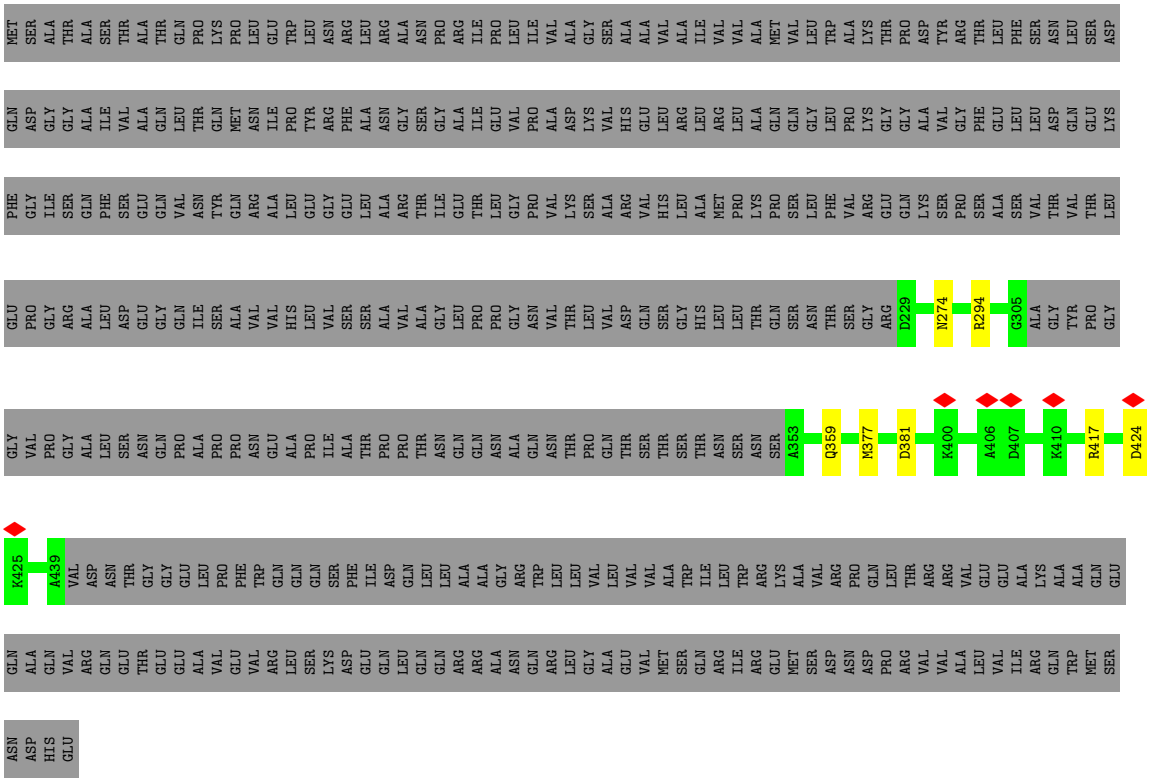
Chain BV:





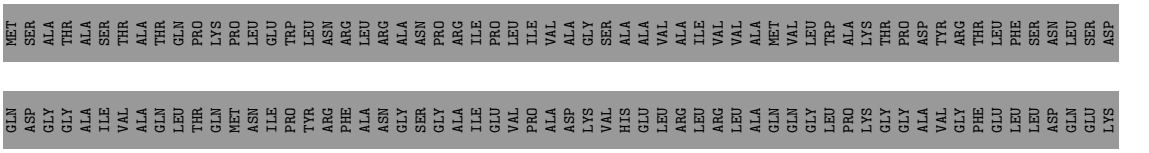
• Molecule 6: Flagellar M-ring protein

Chain BW:



• Molecule 6: Flagellar M-ring protein

Chain BX:



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GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG D229 N274 R294 G305 ALA GLY TYR PRO GLY

GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER A353 Q359 M377 D381 K400 A406 D407 K410 R417 D424

K425 A439 VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU THR ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU

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

ASN ASP HIS GLU

- Molecule 6: Flagellar M-ring protein

Chain UI: 25% 72%

MET SER ALA THR ALA SER THR ALA THR GLN PRO LYS PRO LEU GLU GLU TRP LEU ASN ARG LEU ARG ALA ASN PRO ARG ILE PRO LEU ILE VAL ALA GLY SER ALA ALA VAL ALA ILE VAL VAL ALA MET VAL LEU TRP ALA LYS THR PRO D50 L98 P106 LYS GLY GLY ALA VAL GLY

PHE GLU LEU LEU ASP GLN GLU LYS PHE GLY ILE SER Q125 F126 S127 E128 Q129 R154 M159 P162 S163 L164 F165 P172 D214 Q215 S216 G217 H218 L219 L220 T221 Q222 SER ASN THR SER GLY ARG ASP LEU ASN ASP ALA GLN LEU LYS PHE ALA ASN ASP VAL GLU SER ARG

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

GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG ASN GLU THR SER

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

LYS ARG GLY ASP THR LEU ASN VAL VAL PRO ASN SER PRO PHE SER ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL ARG PRO GLN LEU

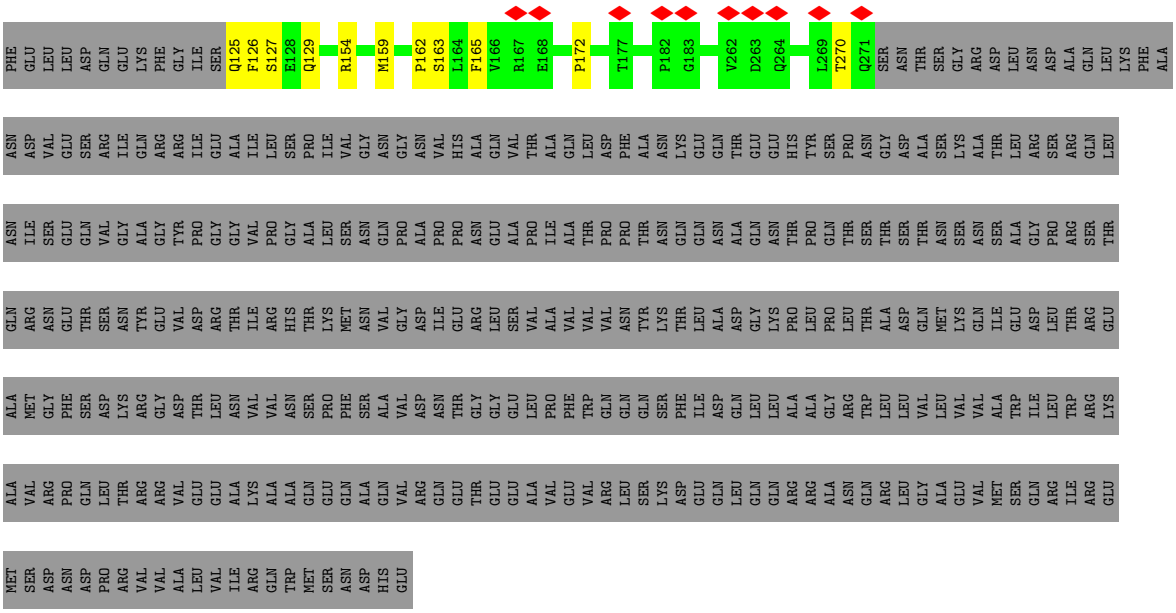
THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL MET SER GLN ARG ILE ARG GLU MET SER ASP ASN ASP PRO

ARG VAL VAL ALA LEU VAL ILE ARG GLN TRP MET SER ASN ASP HIS GLU

- Molecule 6: Flagellar M-ring protein

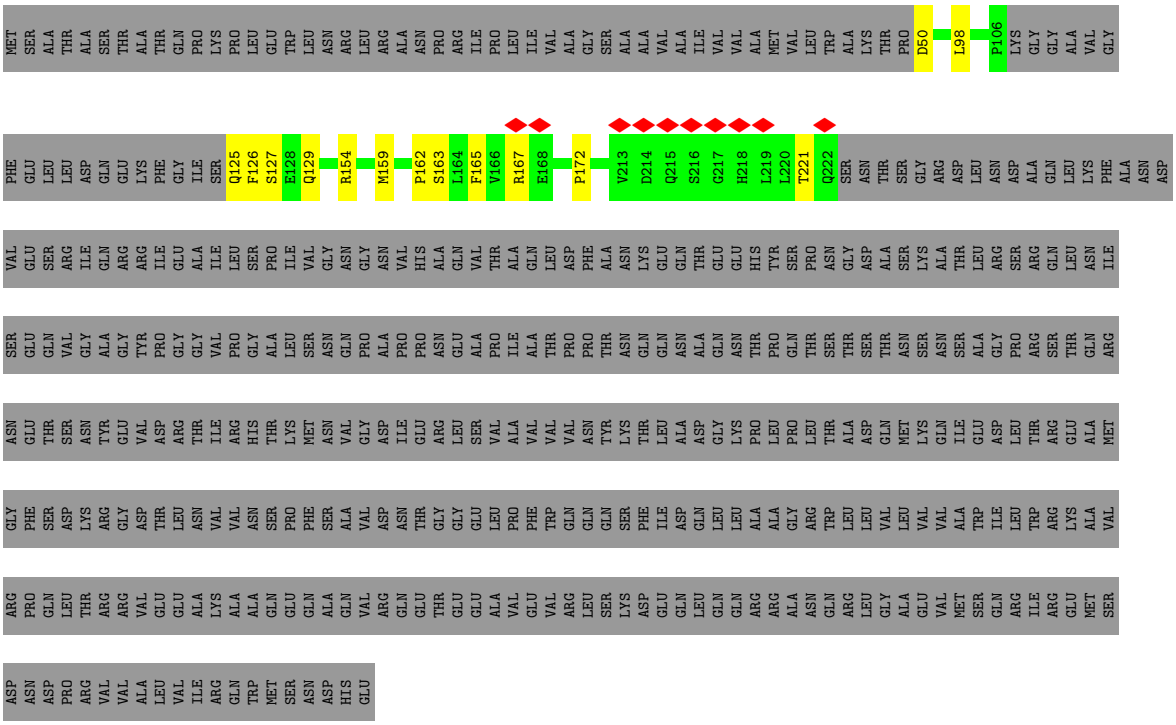
Chain UJ: 25% 72%

MET SER ALA THR ALA SER THR ALA THR GLN PRO LYS PRO LEU GLU TRP LEU ASN ARG LEU ARG ALA ASN PRO ARG ILE PRO LEU ILE VAL ALA GLY SER ALA ALA VAL ALA ILE VAL VAL ALA MET VAL LEU TRP ALA LYS THR PRO D50 L98 P106 LYS GLY GLY ALA VAL GLY



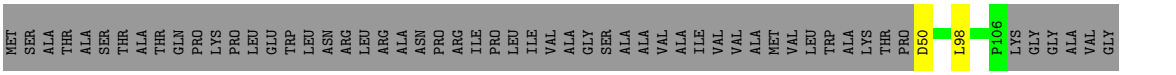
- Molecule 6: Flagellar M-ring protein

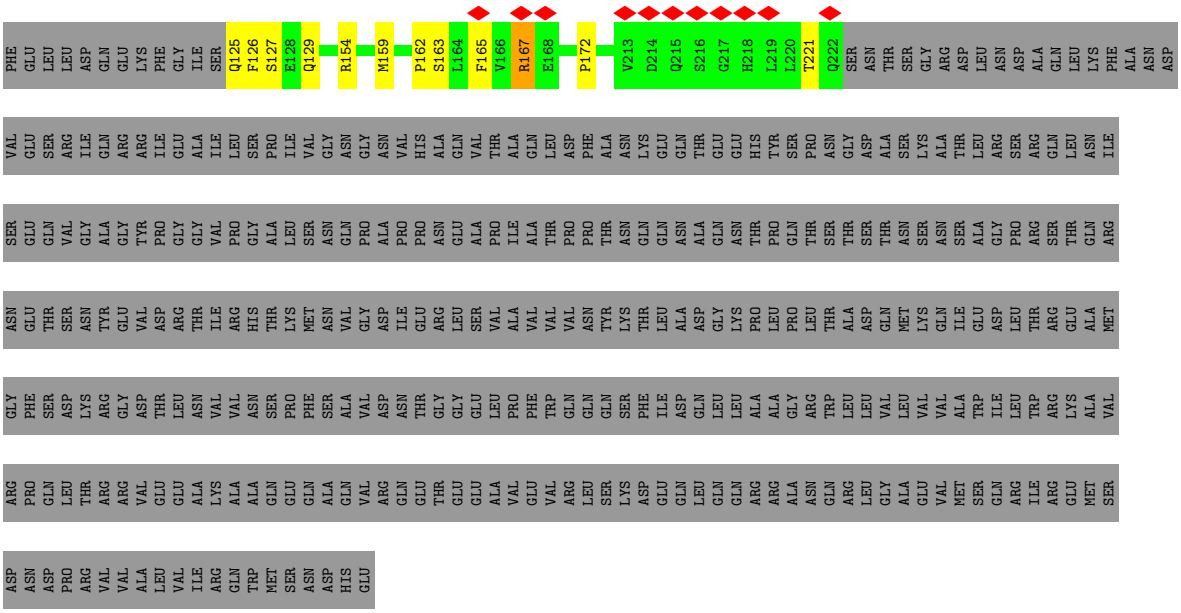
Chain UK:



- Molecule 6: Flagellar M-ring protein

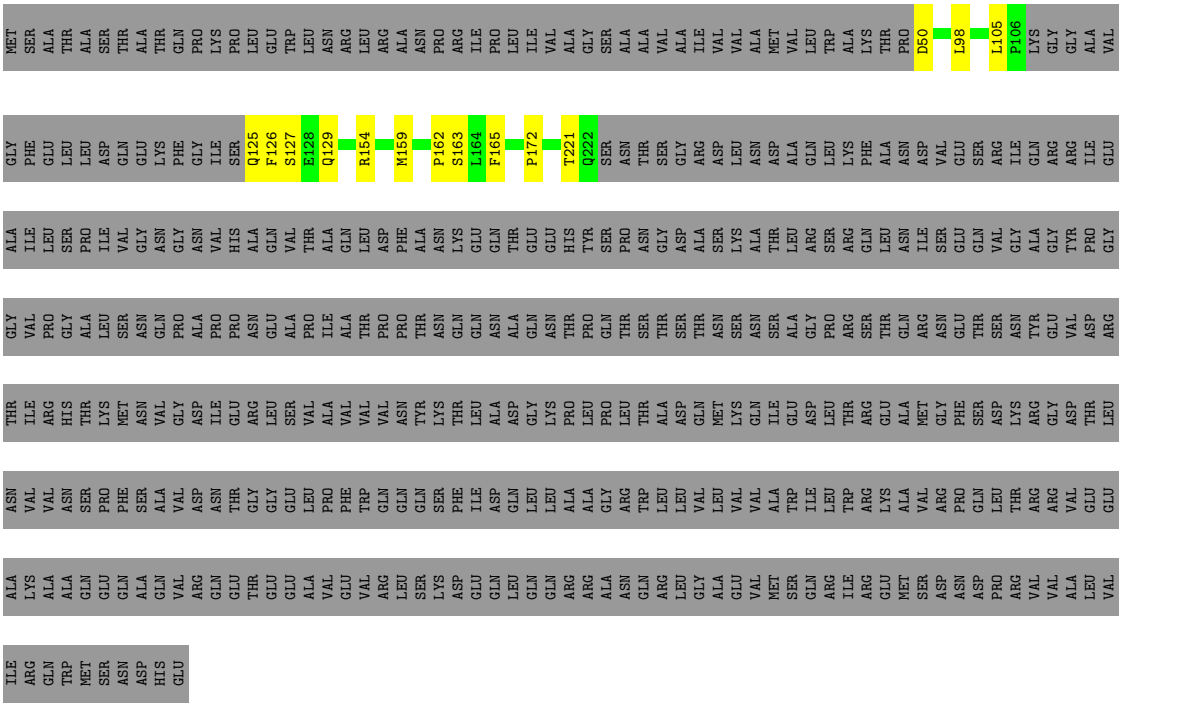
Chain UL:





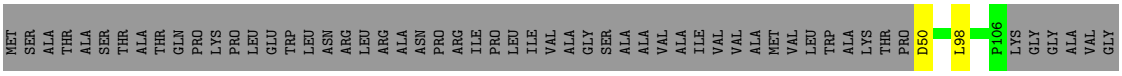
• Molecule 6: Flagellar M-ring protein

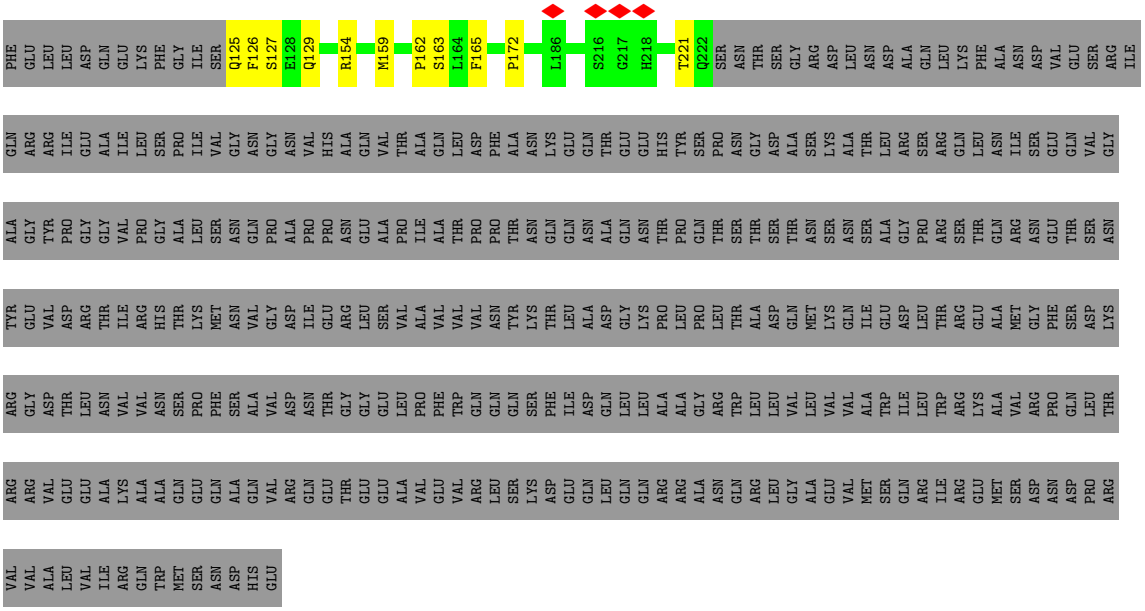
Chain UM:



• Molecule 6: Flagellar M-ring protein

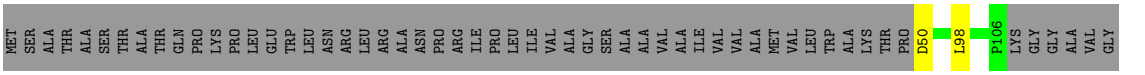
Chain UN:

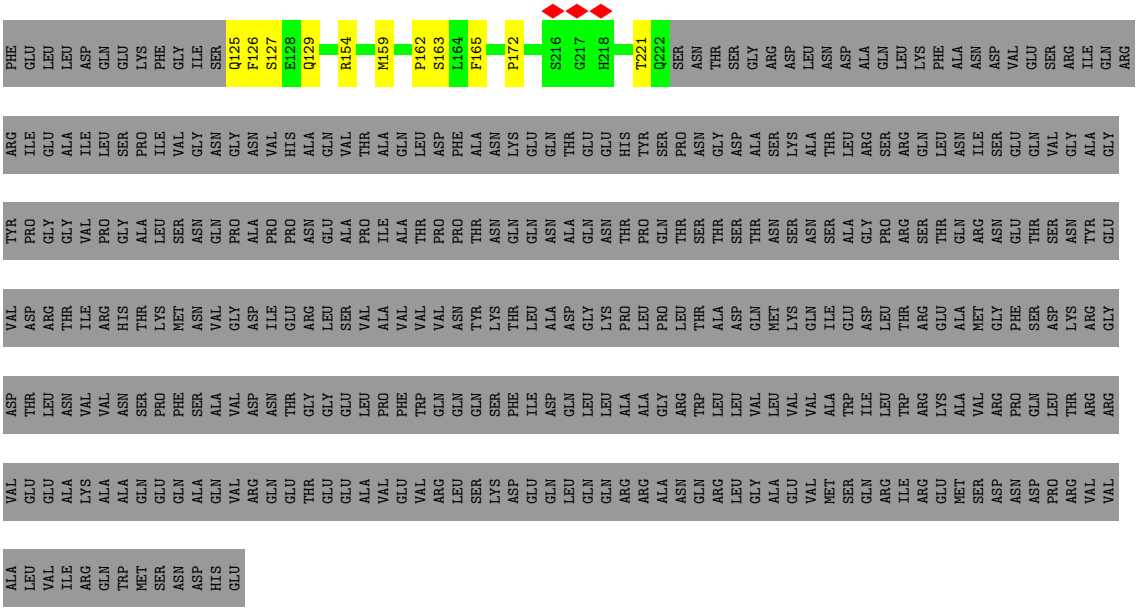




• Molecule 6: Flagellar M-ring protein

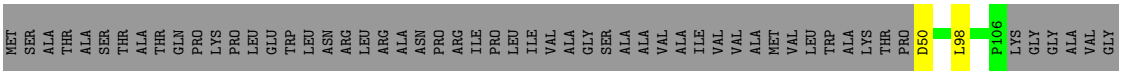
Chain UO:

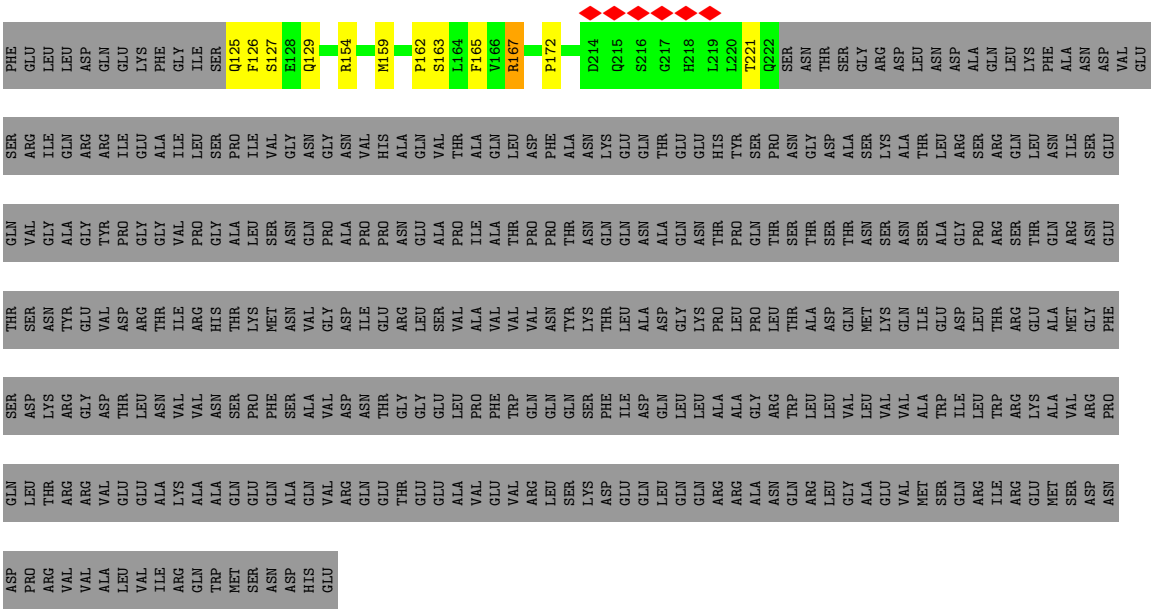




• Molecule 6: Flagellar M-ring protein

Chain UP:



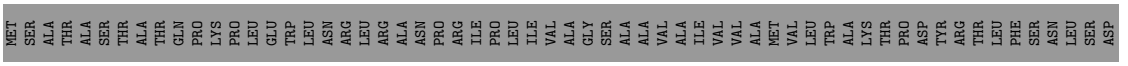


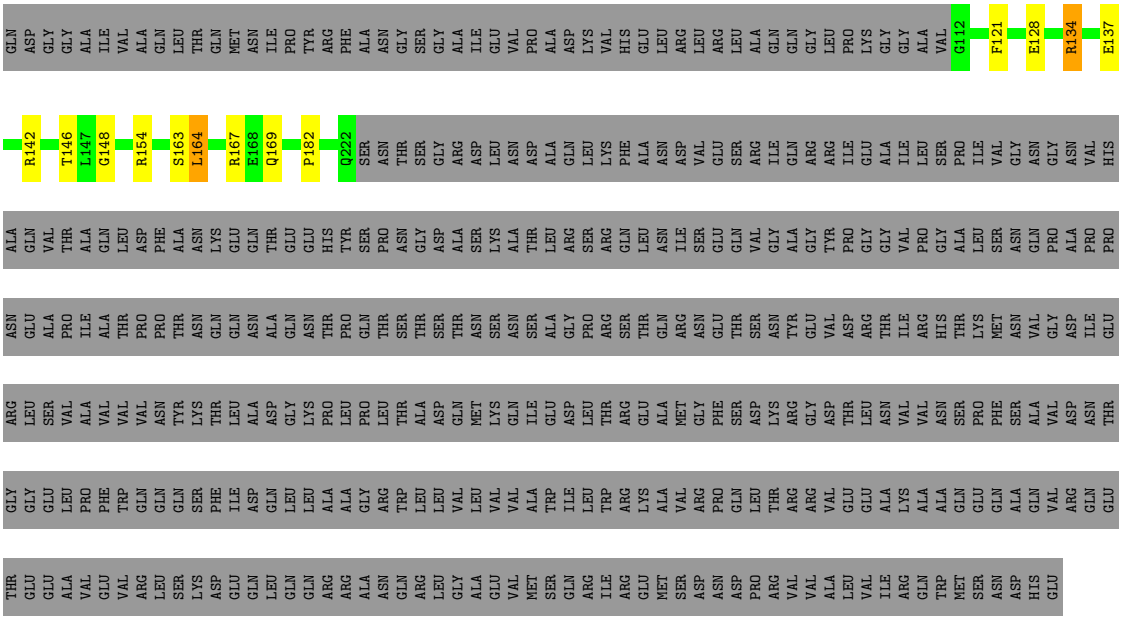
- Molecule 6: Flagellar M-ring protein

Chain WA: 18% 80%

- Molecule 6: Flagellar M-ring protein

Chain WB: 18% 80%



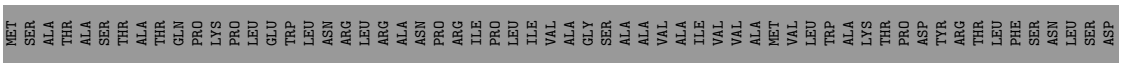


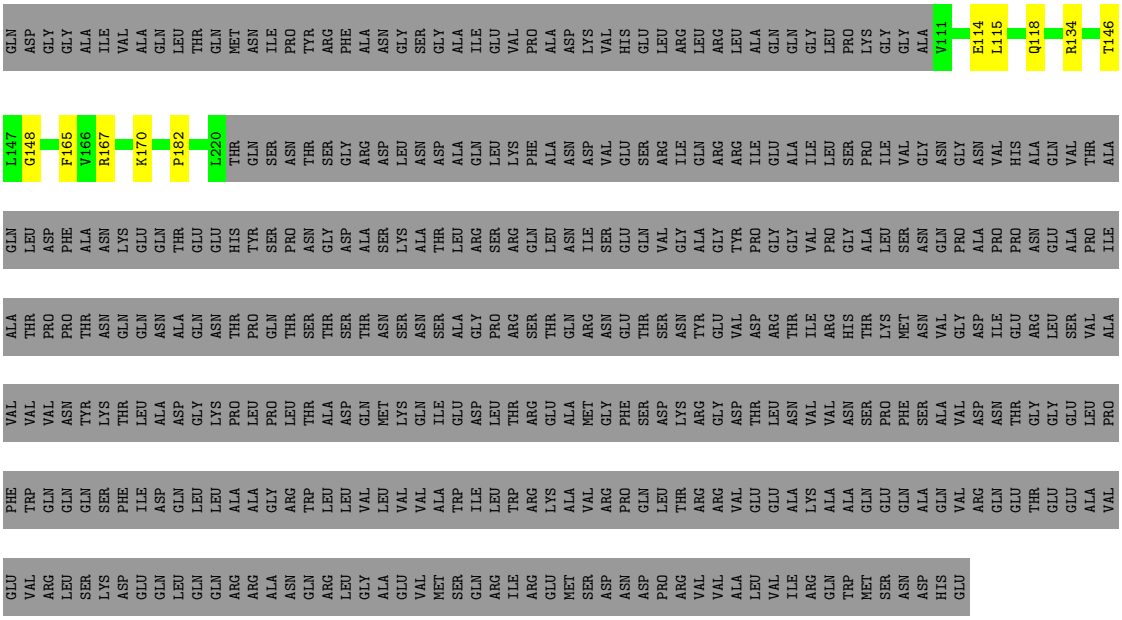
• Molecule 6: Flagellar M-ring protein

Chain WC: 17% • 81%

• Molecule 6: Flagellar M-ring protein

Chain WD: 18% • 80%



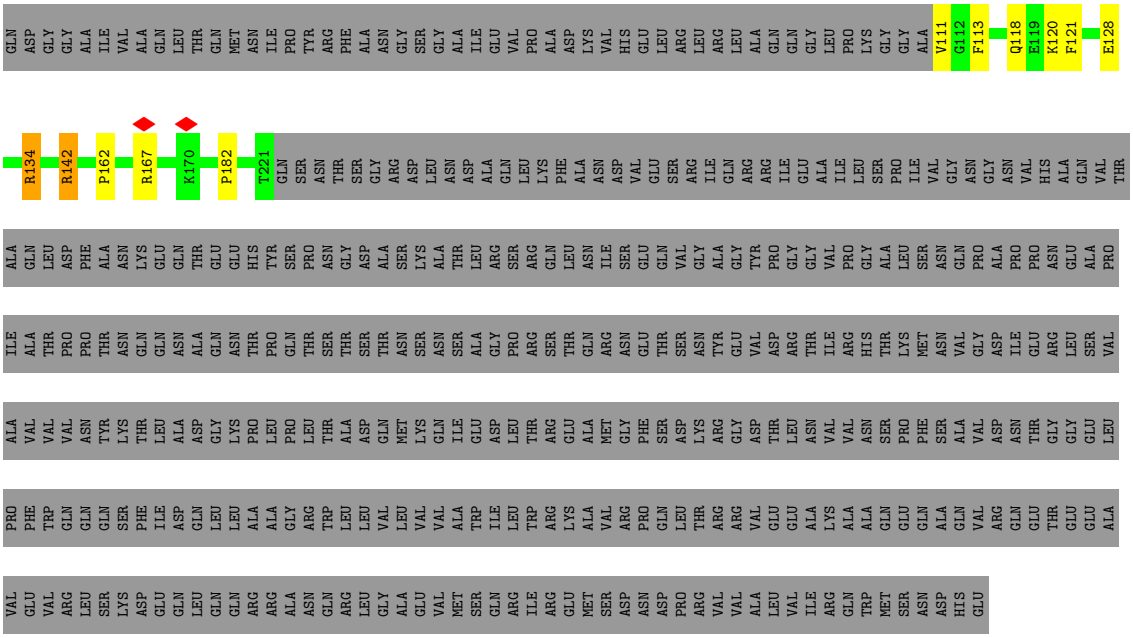


• Molecule 6: Flagellar M-ring protein

Chain WE:

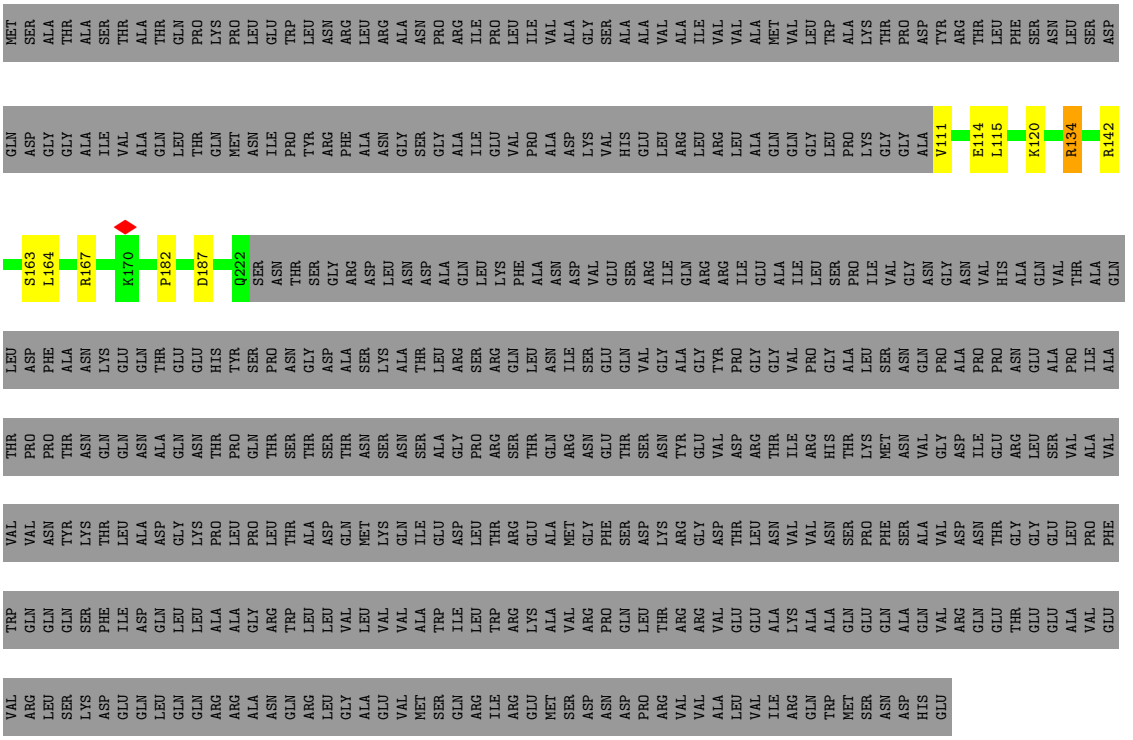
• Molecule 6: Flagellar M-ring protein

Chain WF:



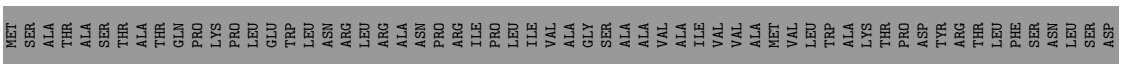
- Molecule 6: Flagellar M-ring protein

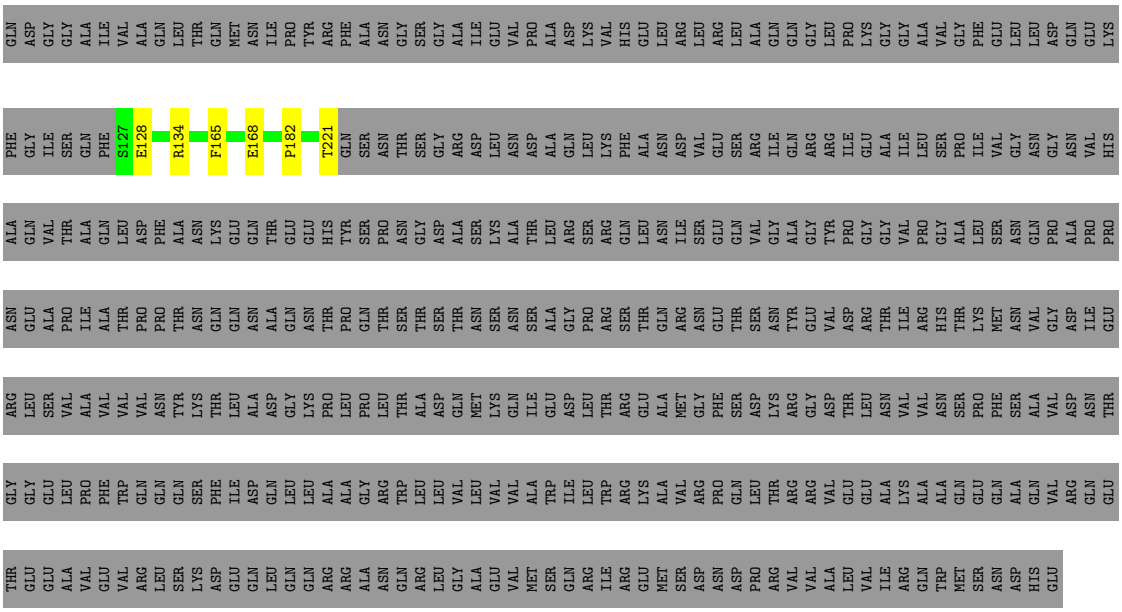
Chain WG: 18% 80%



- Molecule 6: Flagellar M-ring protein

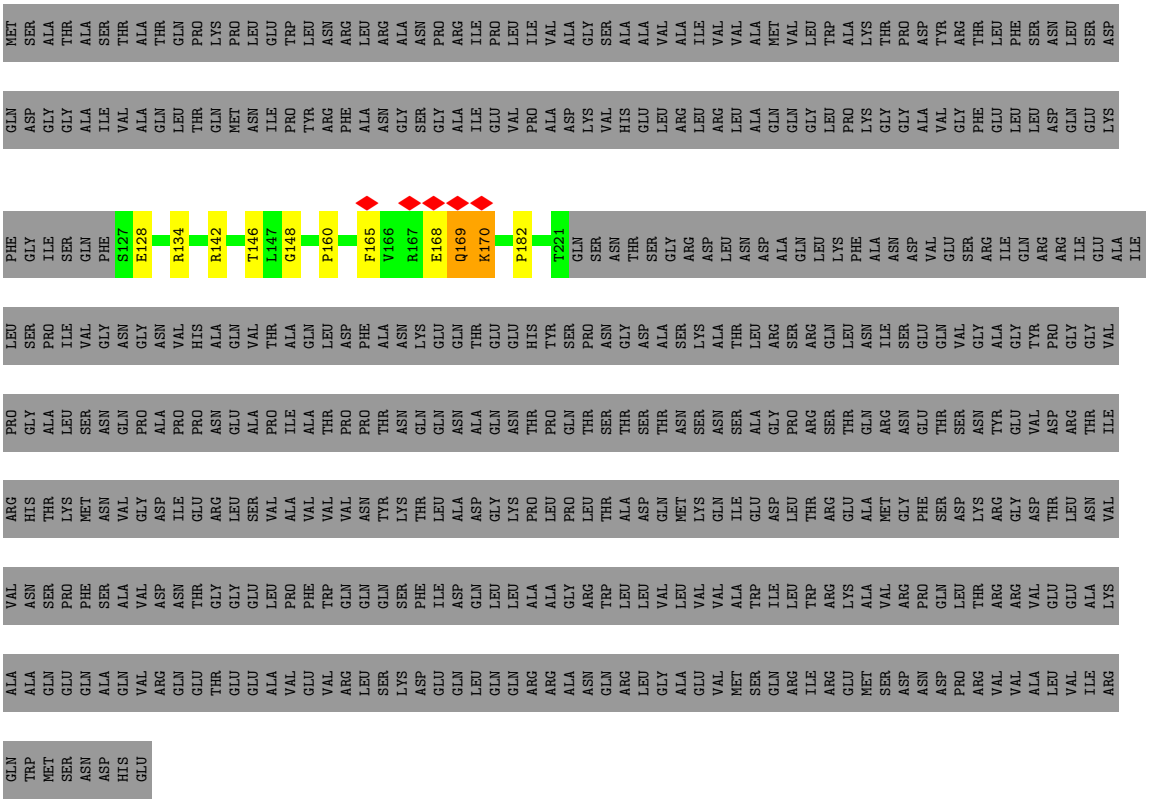
Chain WH: 16% 83%





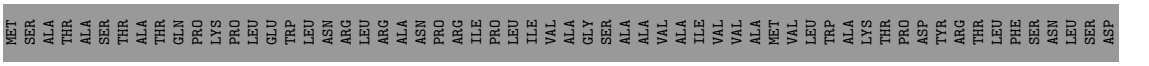
- Molecule 6: Flagellar M-ring protein

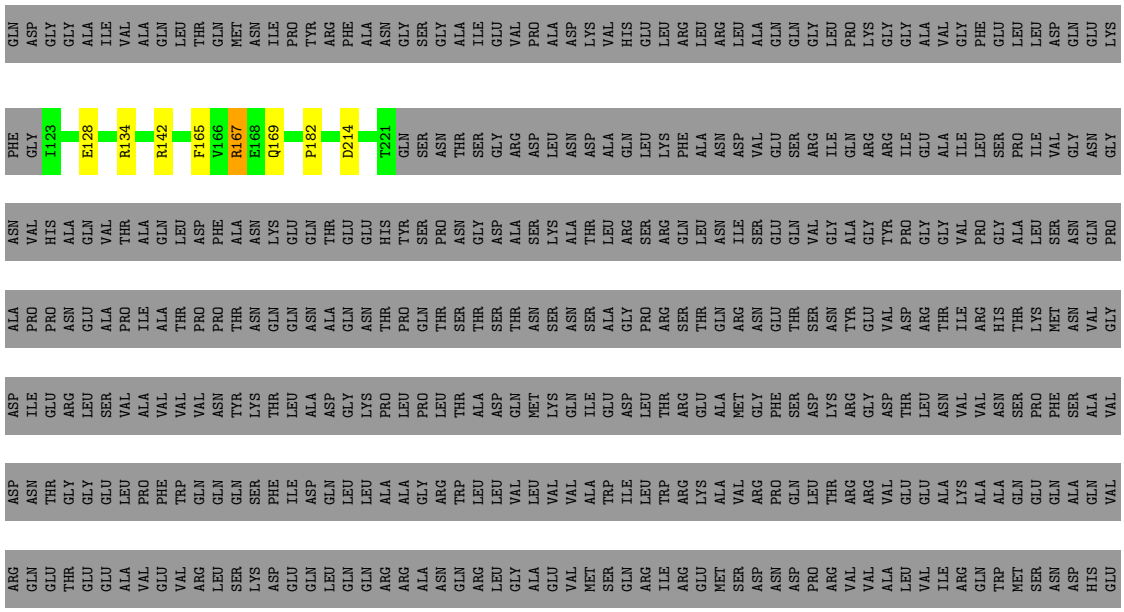
Chain WI:



- Molecule 6: Flagellar M-ring protein

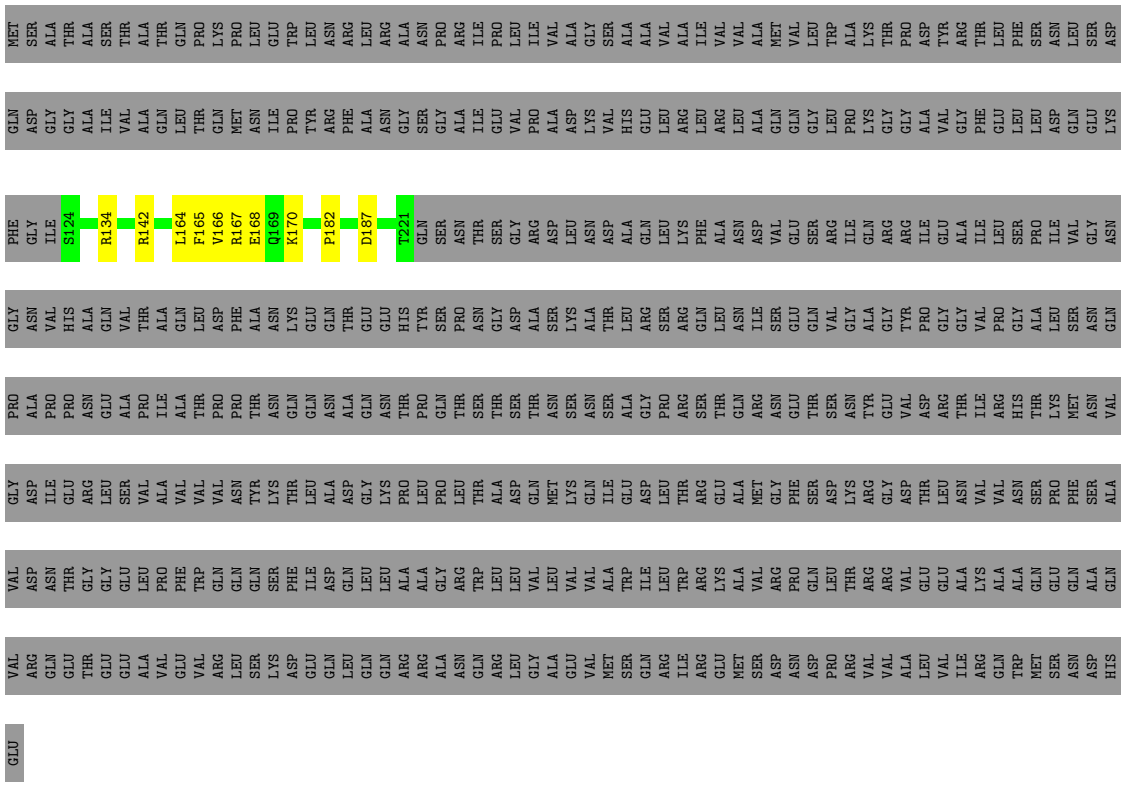
Chain WJ:





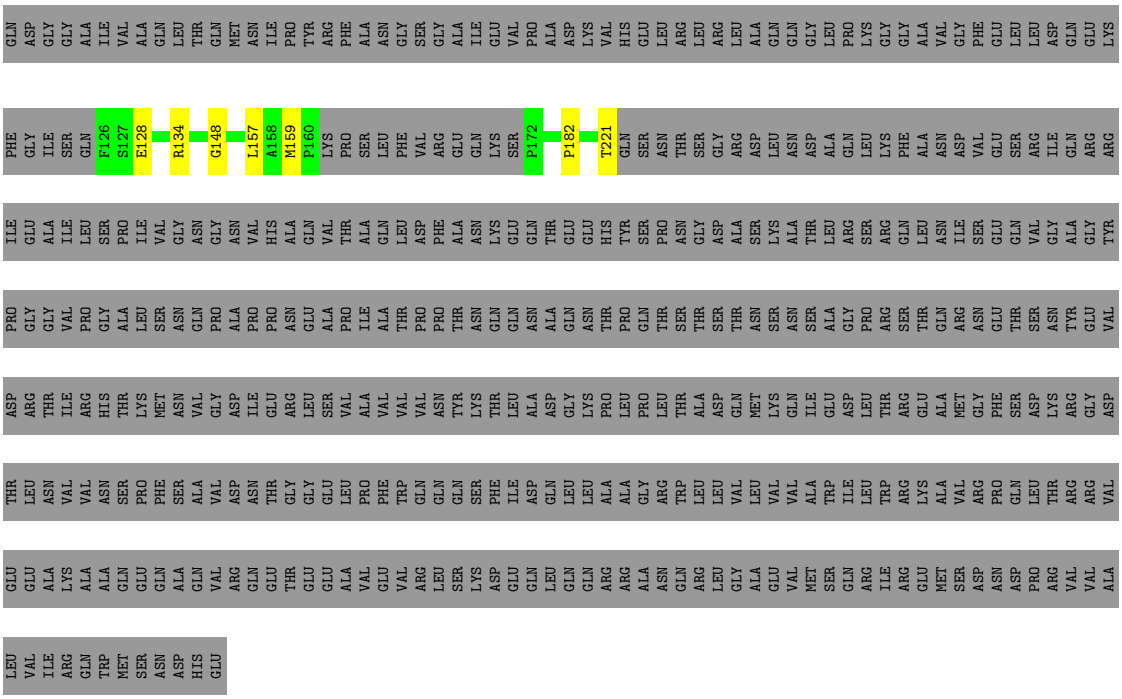
- Molecule 6: Flagellar M-ring protein

Chain WK: 16% • 82%



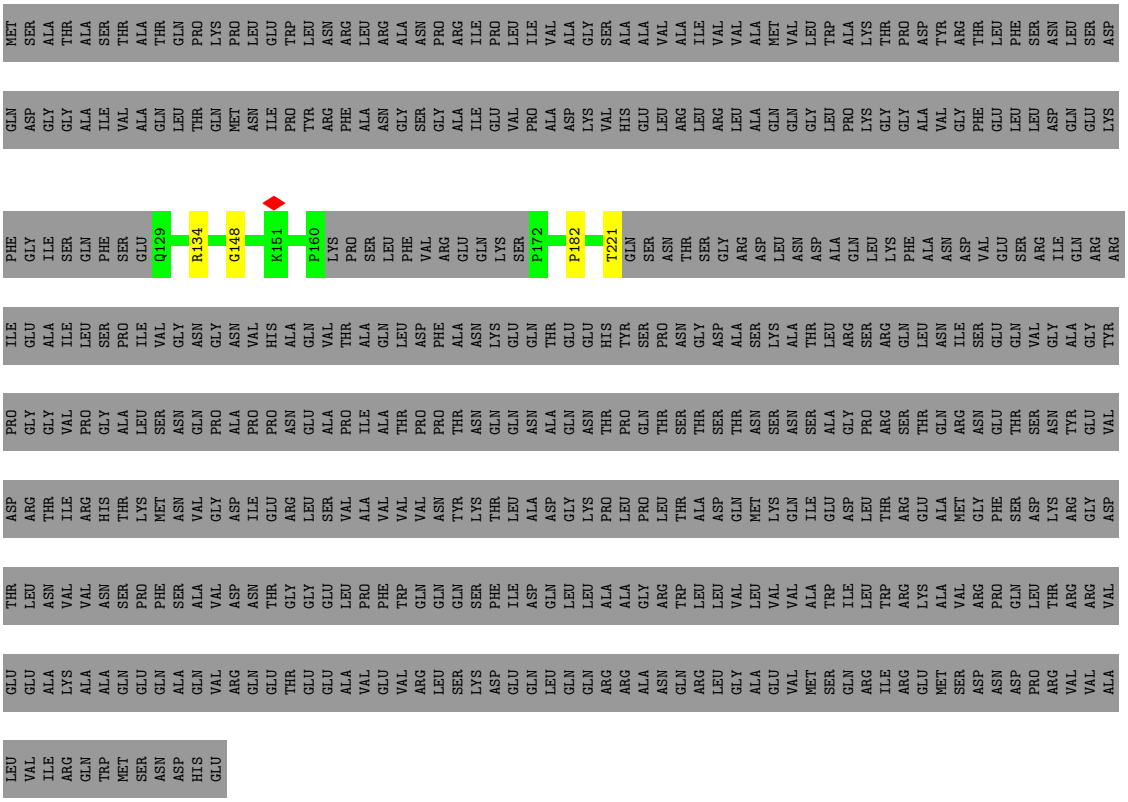
- Molecule 6: Flagellar M-ring protein

Chain WL: 14% • 85%



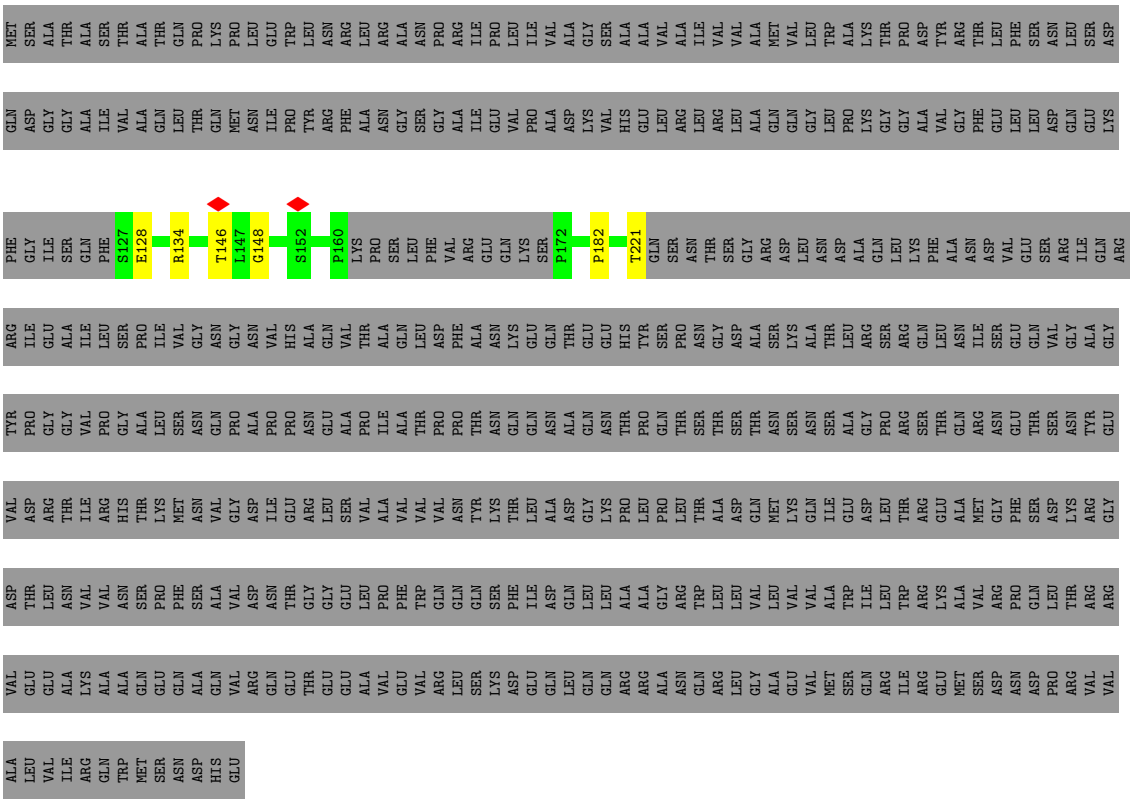
• Molecule 6: Flagellar M-ring protein

Chain WM:



• Molecule 6: Flagellar M-ring protein

Chain WN:

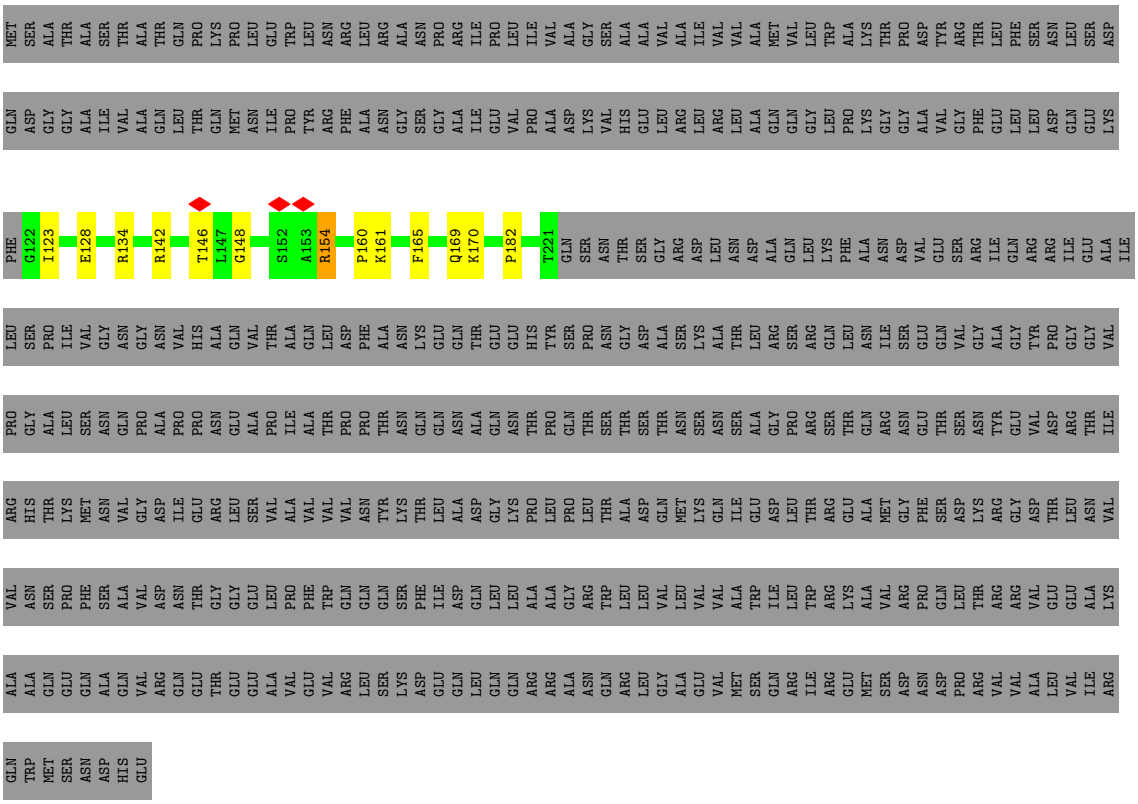


- Molecule 6: Flagellar M-ring protein

Chain WO: 16% 83%

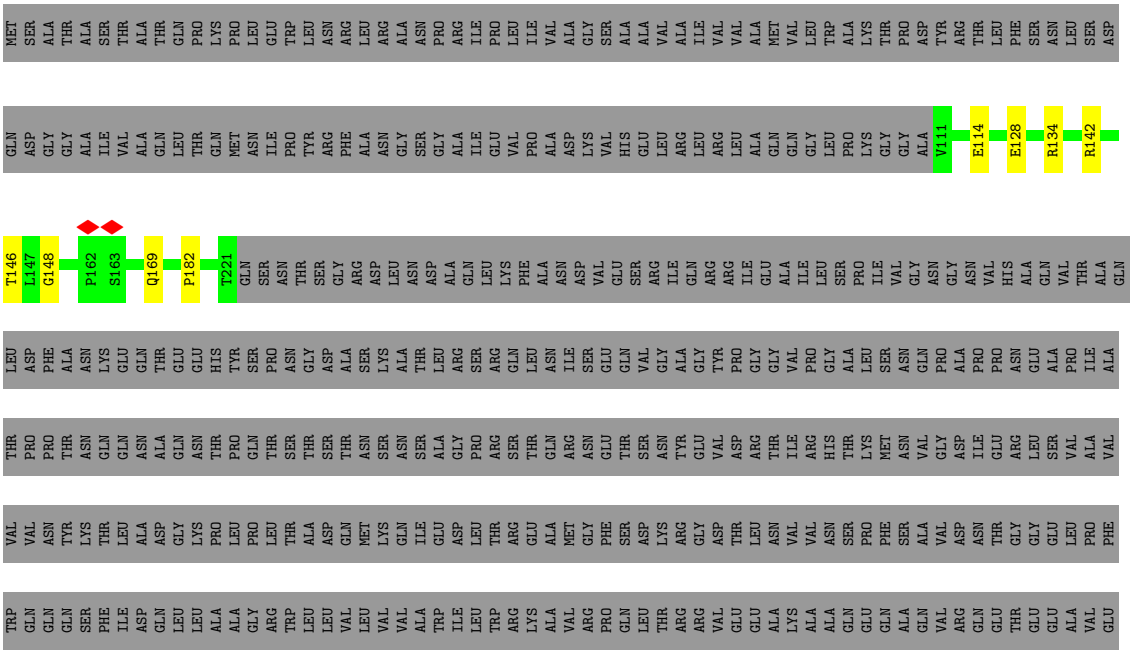
• Molecule 6: Flagellar M-ring protein

Chain WP: 16% 82%



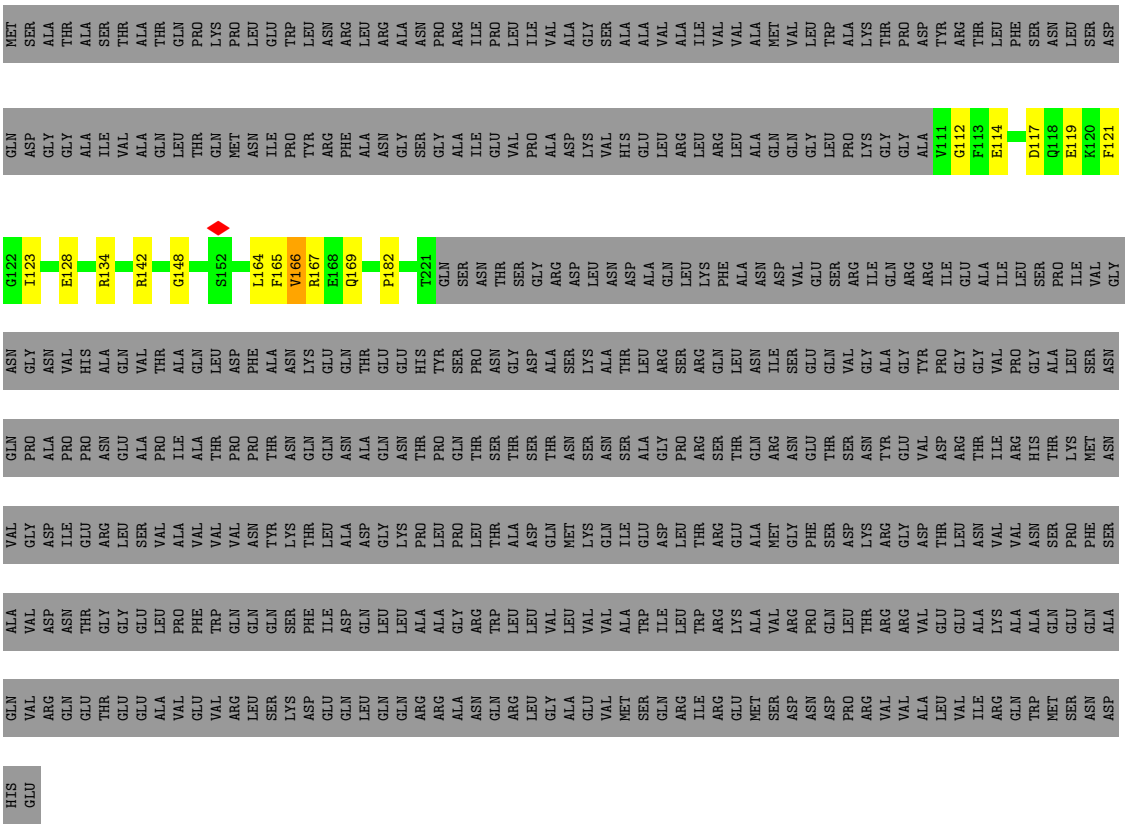
• Molecule 6: Flagellar M-ring protein

Chain WQ: 18% 80%



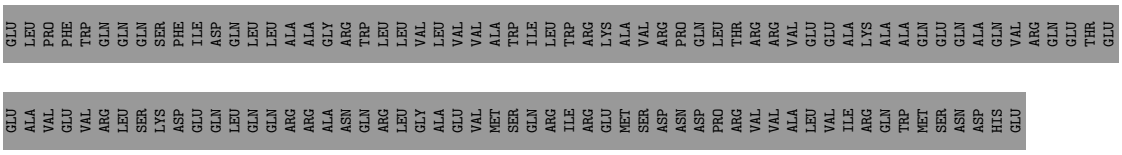
- Molecule 6: Flagellar M-ring protein

Chain WR:



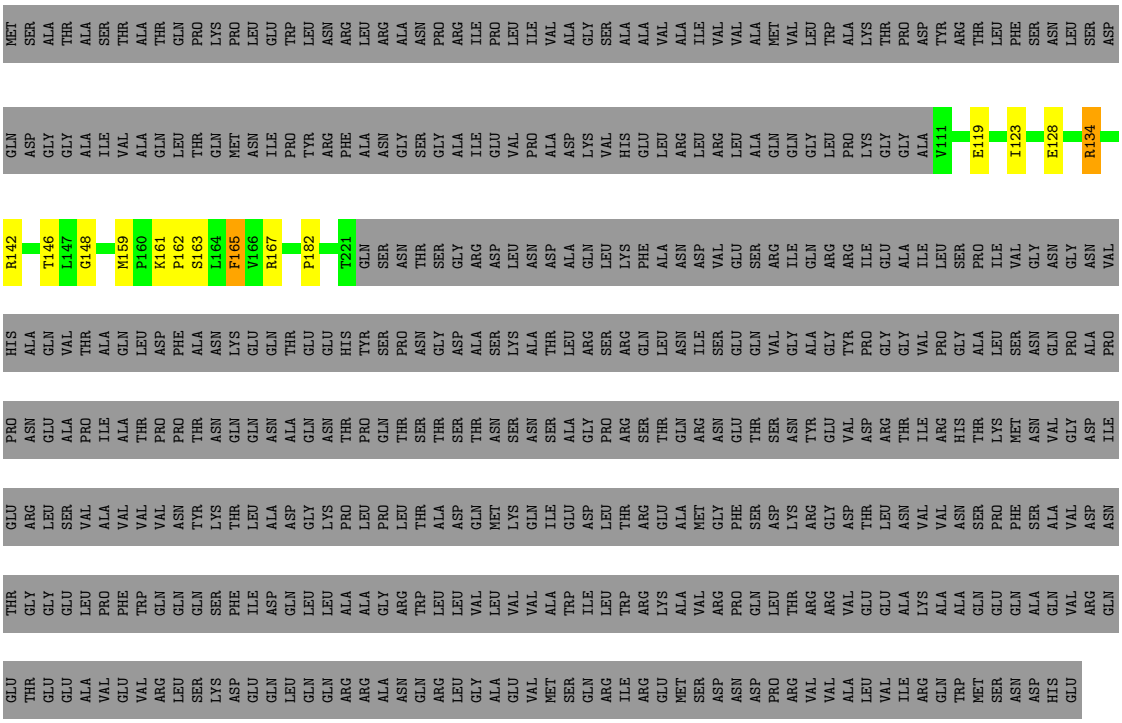
- Molecule 6: Flagellar M-ring protein

Chain WS:



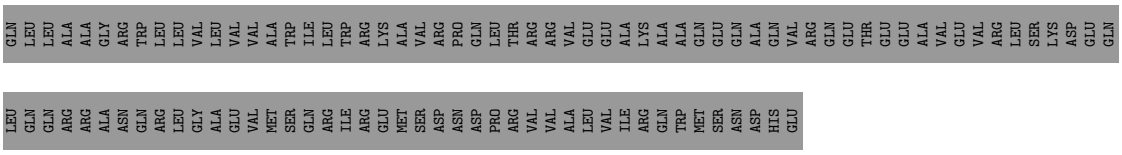
- Molecule 6: Flagellar M-ring protein

Chain WT: 17% 80%



- Molecule 6: Flagellar M-ring protein

Chain WU: 19% 80%

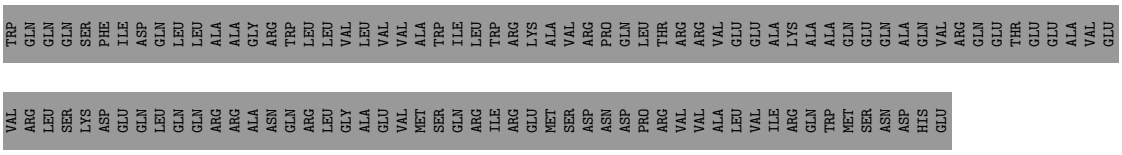


• Molecule 6: Flagellar M-ring protein

Chain WV: 17% 80%

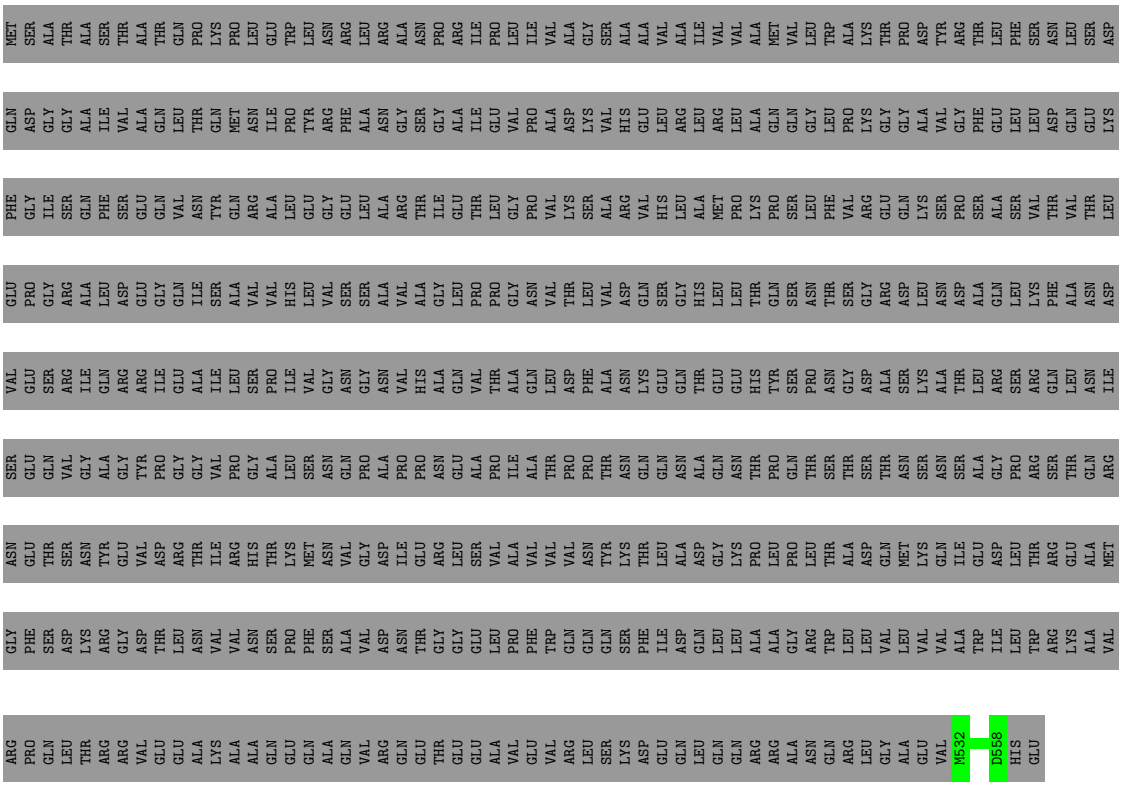
• Molecule 6: Flagellar M-ring protein

Chain WW: 18% 80%



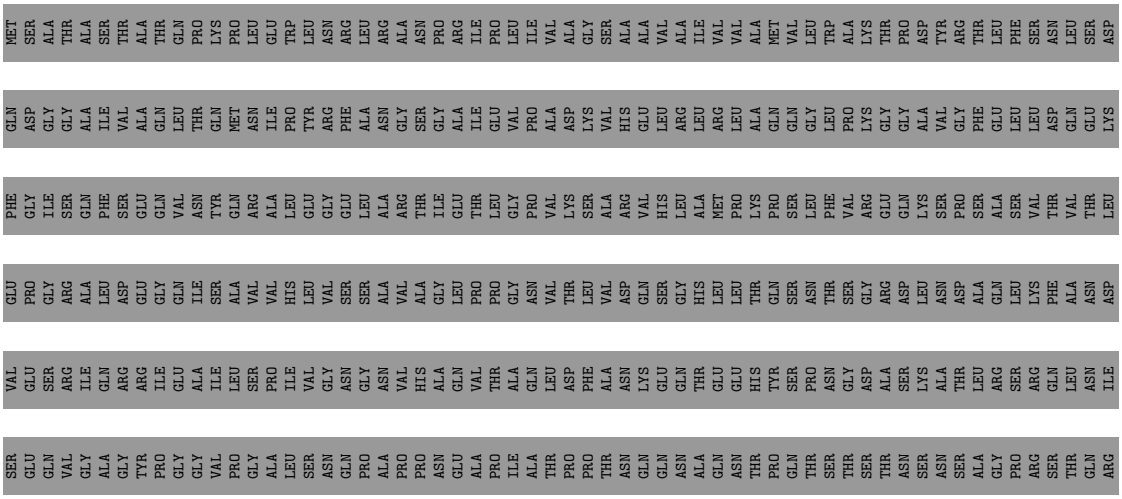
• Molecule 6: Flagellar M-ring protein

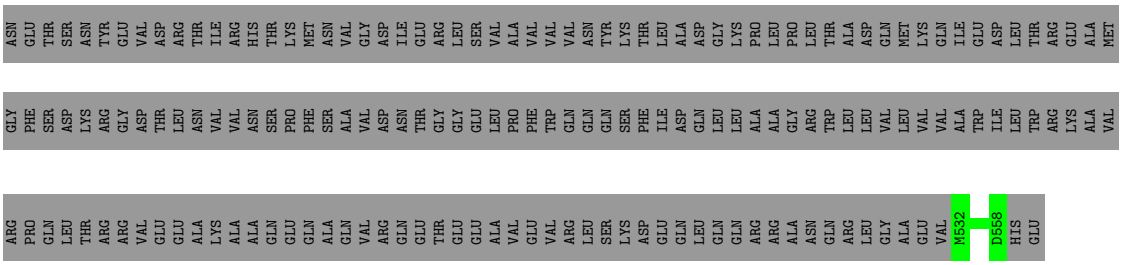
Chain DE: 5% 95%



• Molecule 6: Flagellar M-ring protein

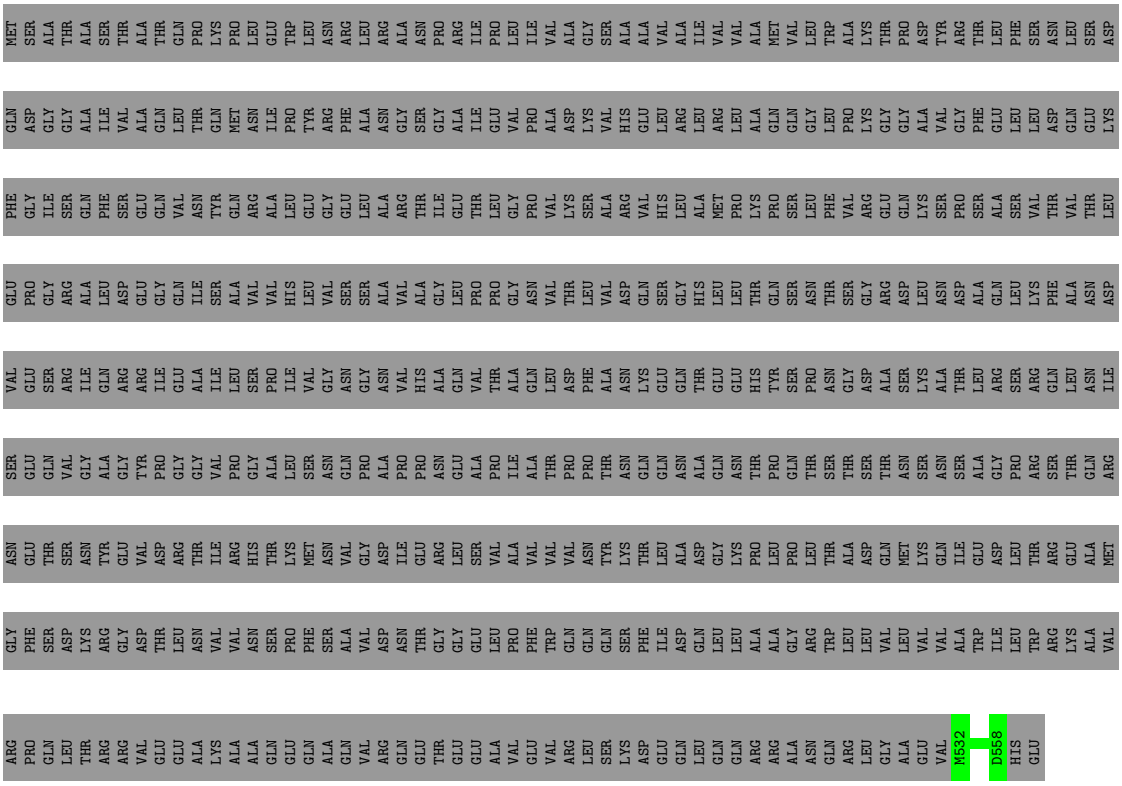
Chain DL: 5% 95%





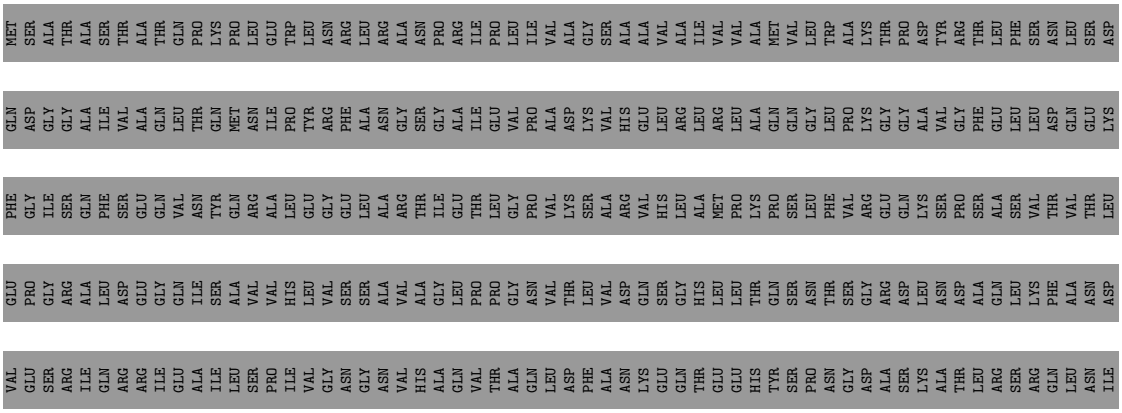
• Molecule 6: Flagellar M-ring protein

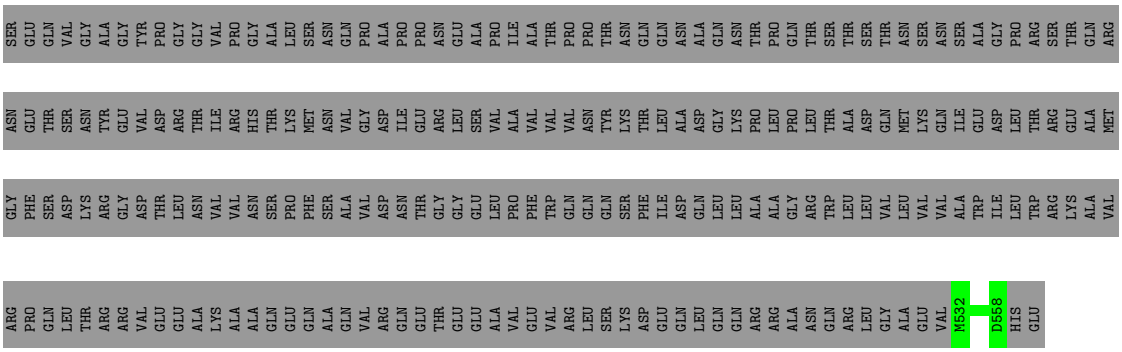
Chain B0: 5% 95%



• Molecule 6: Flagellar M-ring protein

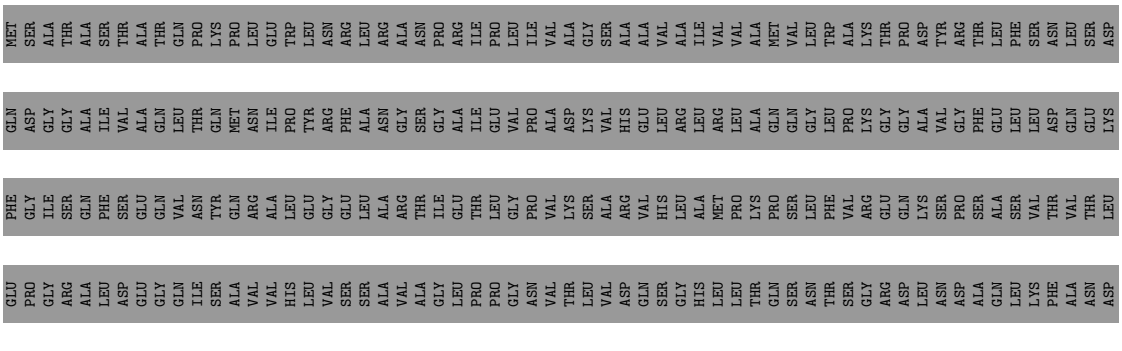
Chain B3: 5% 95%





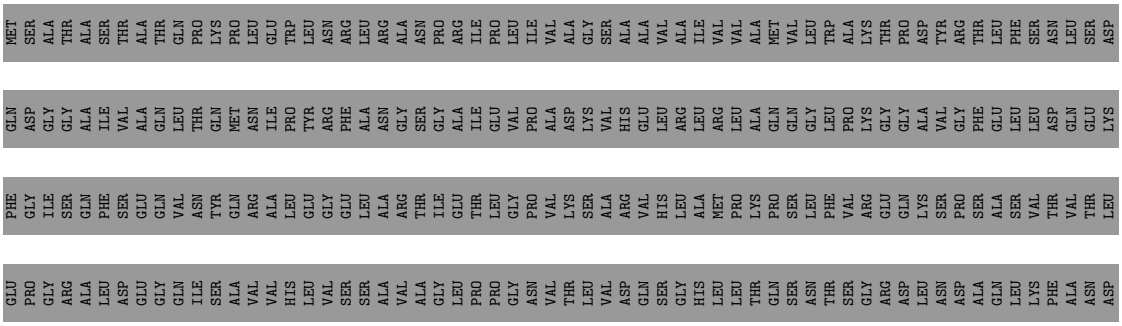
• Molecule 6: Flagellar M-ring protein

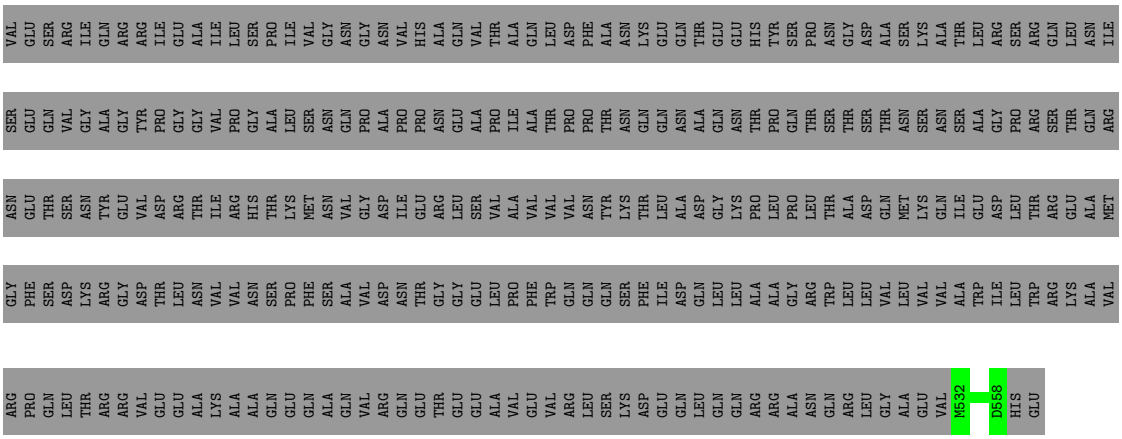
Chain EH: 5% 95%



• Molecule 6: Flagellar M-ring protein

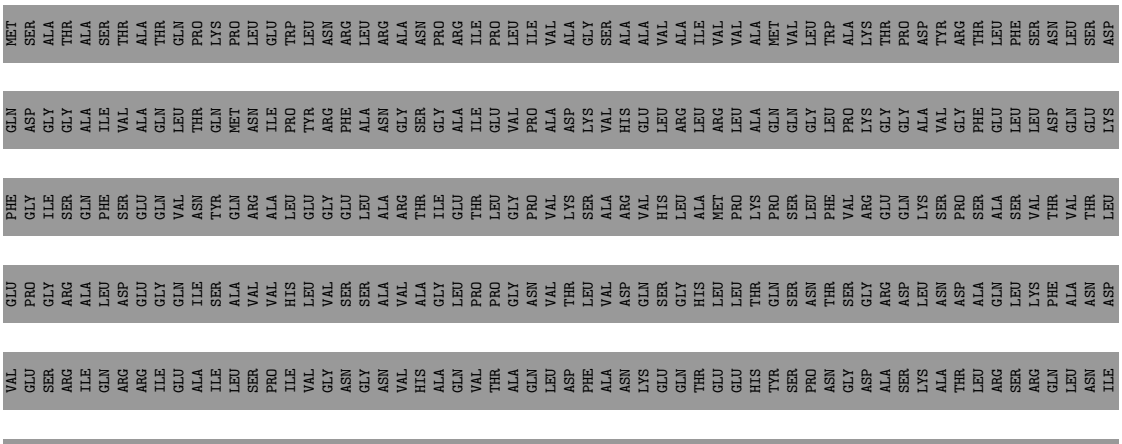
Chain EO: 5% 95%





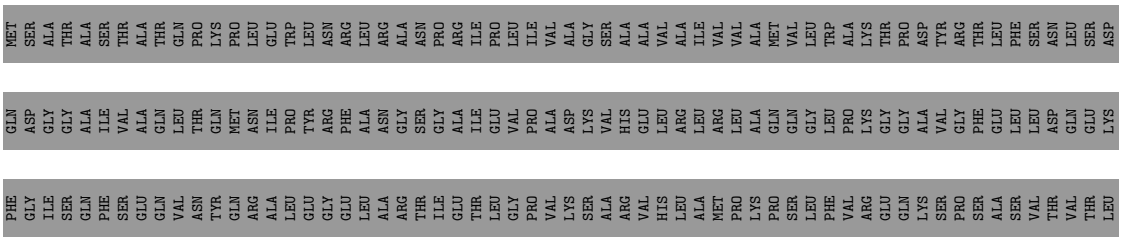
• Molecule 6: Flagellar M-ring protein

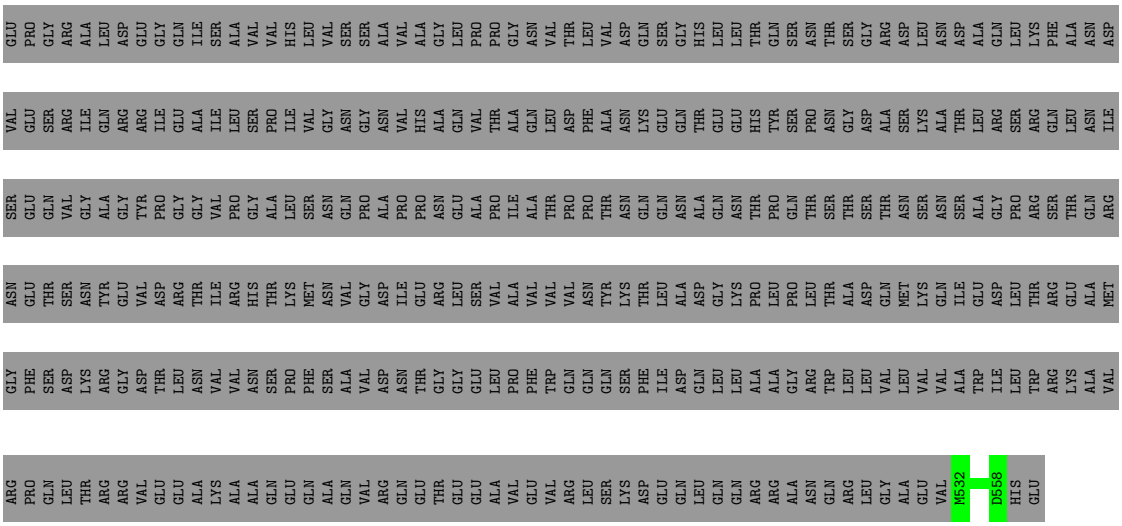
Chain EV: 5% 95%



• Molecule 6: Flagellar M-ring protein

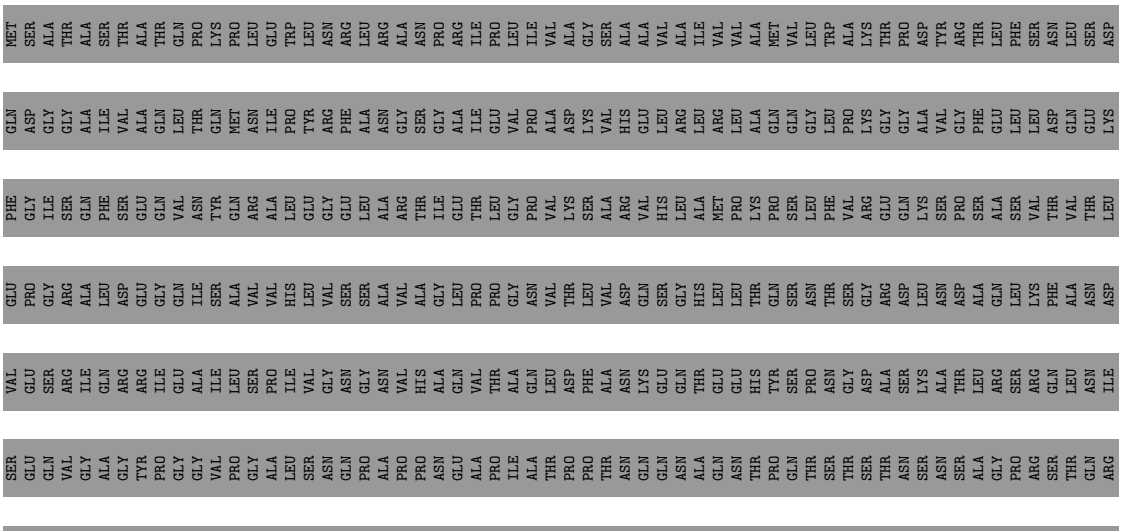
Chain Ba: 5% 95%





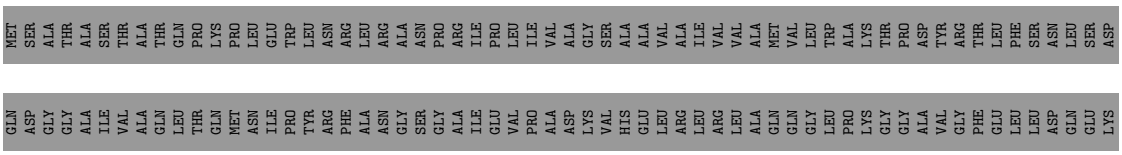
• Molecule 6: Flagellar M-ring protein

Chain Bh: 5% 95%



• Molecule 6: Flagellar M-ring protein

Chain Bo: 5% 95%



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

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

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG

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

GLY PHE SER ASP LYS ARG GLY ASP THR LEU ASN VAL VAL ASN SER PRO PHE SER ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL

ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN GLU GLN GLN ARG ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL M532 D558 HIS GLU

- Molecule 6: Flagellar M-ring protein

Chain Bv: 5% 95%

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

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

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

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

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG

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

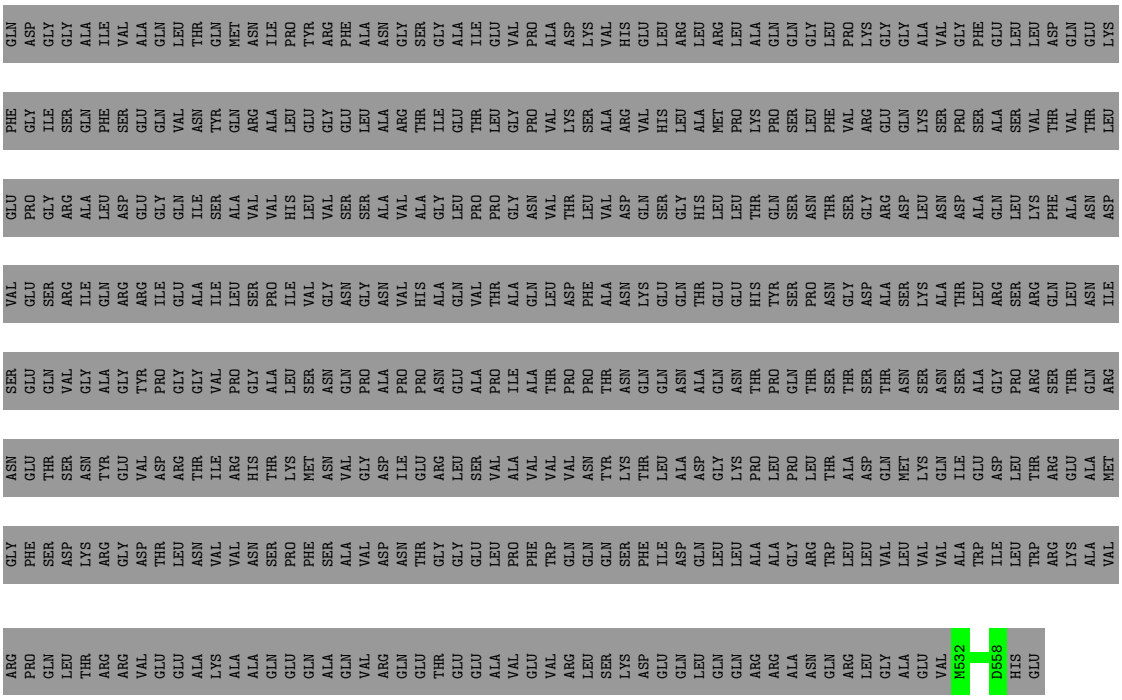
GLY PHE SER ASP LYS ARG GLY ASP THR LEU ASN VAL VAL ASN SER PRO PHE SER ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL

ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN GLU GLN GLN ARG ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL M532 D558 HIS GLU

- Molecule 6: Flagellar M-ring protein

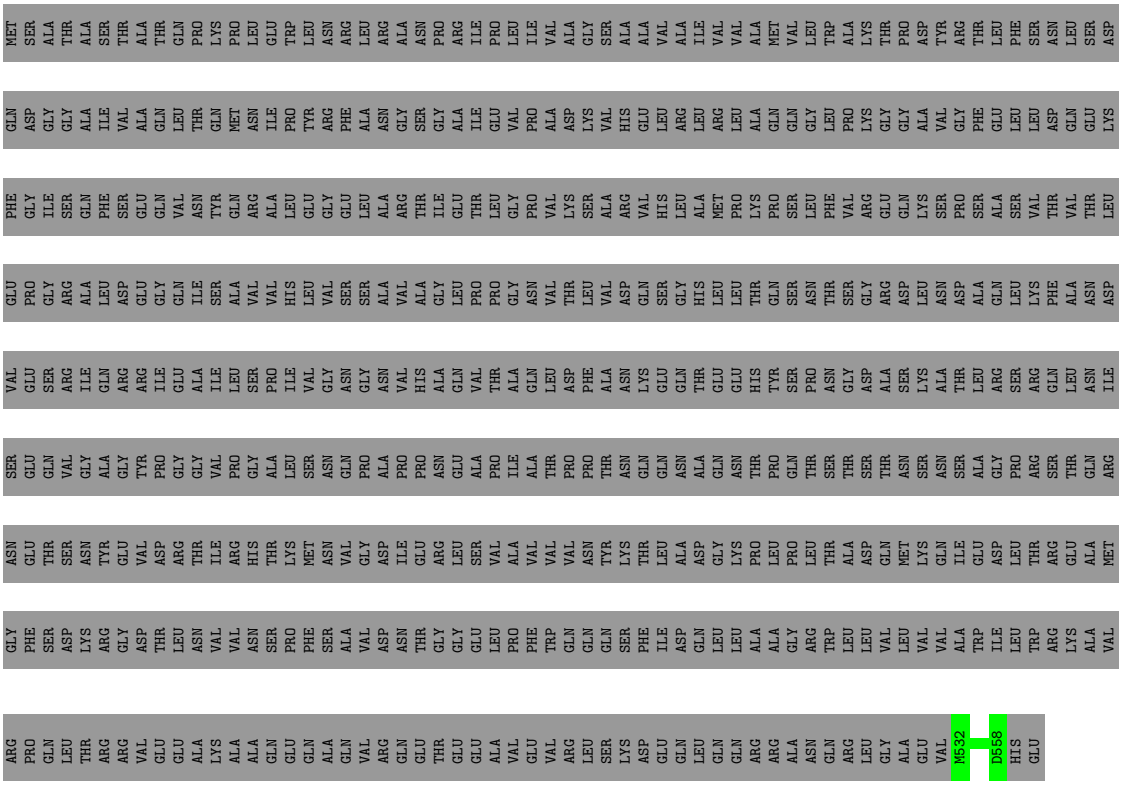
Chain Ea: 5% 95%

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



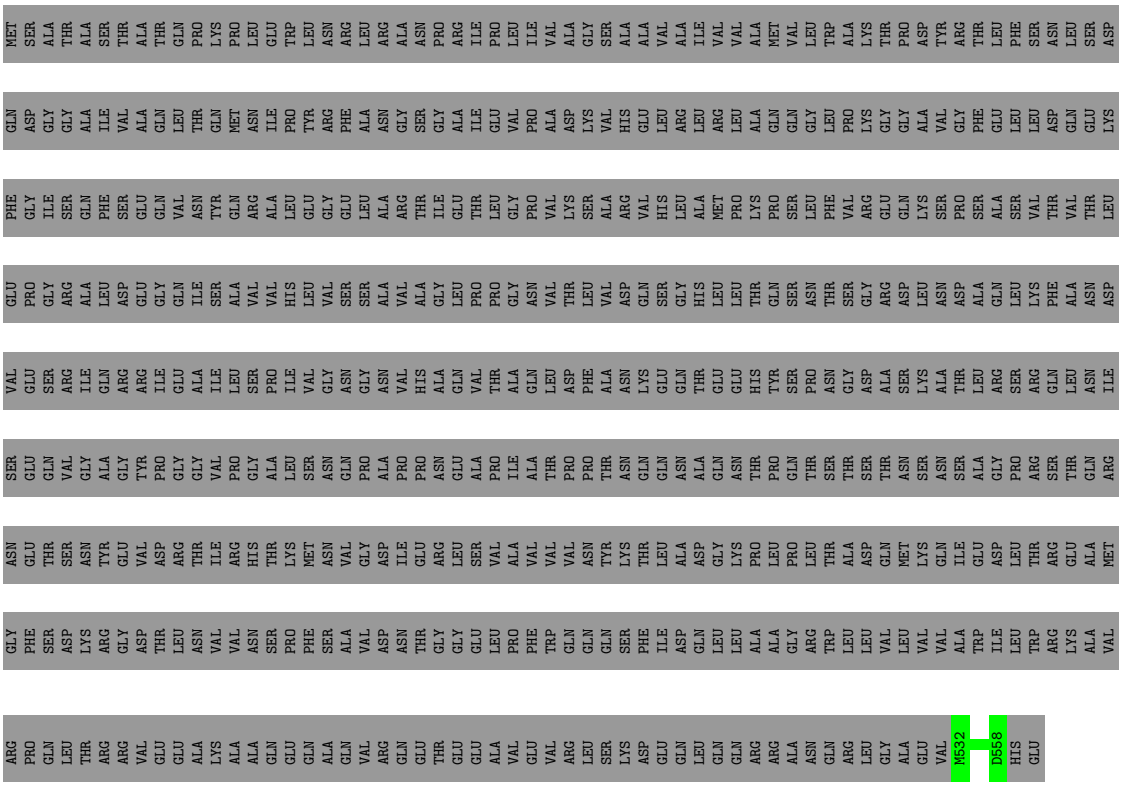
- Molecule 6: Flagellar M-ring protein

Chain CG: 5% 95%



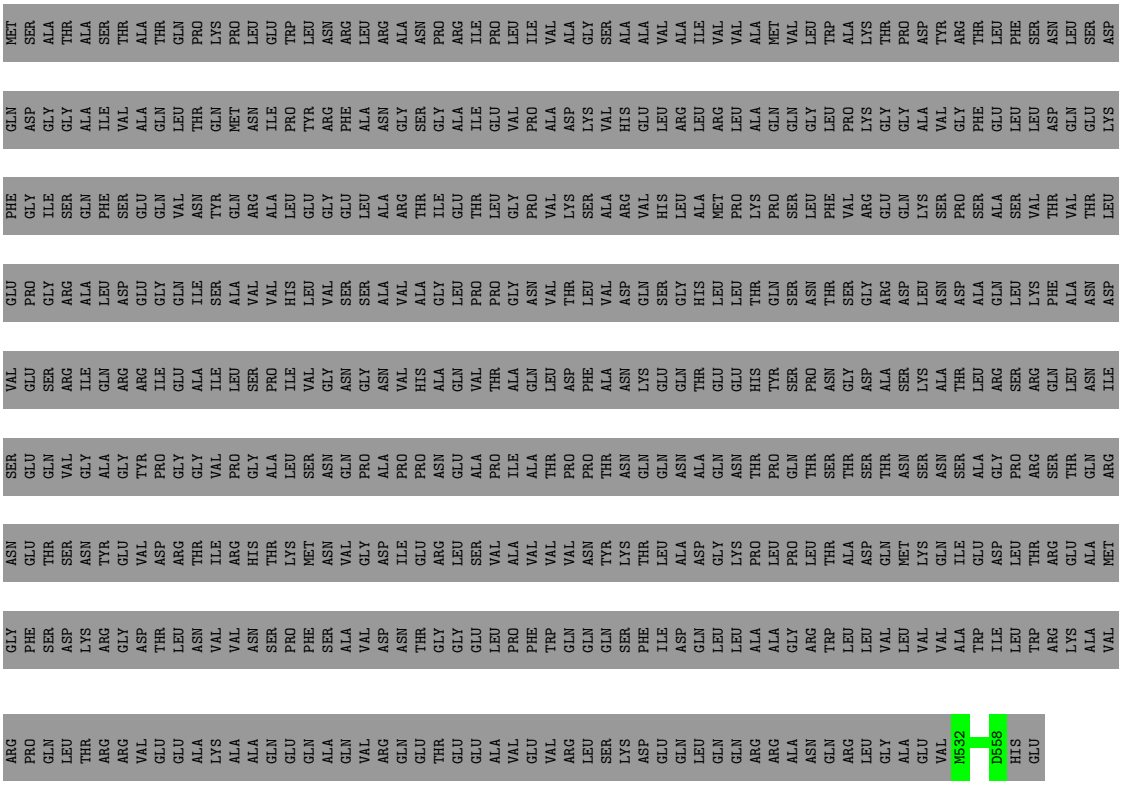
- Molecule 6: Flagellar M-ring protein

Chain CN: 5% 95%



- Molecule 6: Flagellar M-ring protein

Chain CU: 5% 95%



- Molecule 6: Flagellar M-ring protein

Chain Cb: 5% 95%

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

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

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

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

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG

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

GLY PHE SER ASP LYS ARG GLY ASP THR LEU ASN VAL VAL ASN SER PRO PHE SER ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL

ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL M532 D558 HIS GLU

- Molecule 6: Flagellar M-ring protein

Chain Ci: 5% 95%

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

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

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

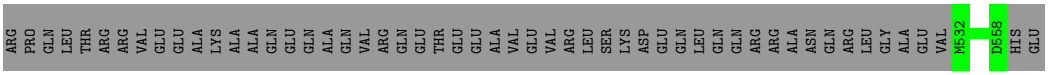
GLU PRO GLY ARG ALA LEU ASP GLU GLY GLN ILE SER ALA VAL VAL HIS LEU LEU VAL SER SER ALA VAL ALA GLY LEU PRO PRO GLY ASN VAL THR LEU VAL ASP GLN SER GLY HIS LEU LEU THR GLN SER ASN THR SER GLY ARG ASP LEU ASN ASP ALA GLN LEU LYS PHE ALA ASN ASP

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG

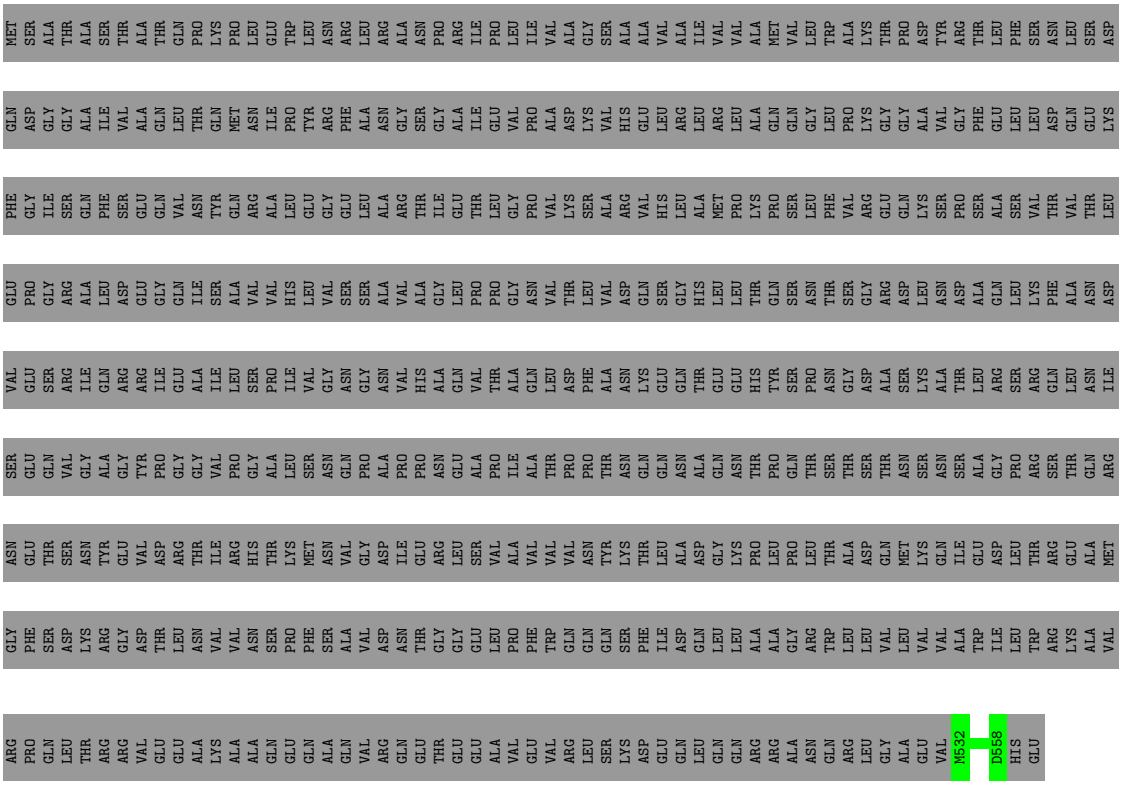
ASN GLU THR SER ASN TYR GLU VAL ASP ARG THR ILE ARG HIS THR LYS MET ASN VAL GLY ASP ILE GLU ARG LEU SER VAL ALA VAL VAL VAL ASN TYR LYS THR LEU ALA ASP GLY LYS PRO LEU PRO LEU THR ALA ASP GLN MET LYS GLN ILE GLU ASP LEU THR ARG GLU ALA MET

GLY PHE SER ASP LYS ARG GLY ASP THR LEU ASN VAL VAL ASN SER PRO PHE SER ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL



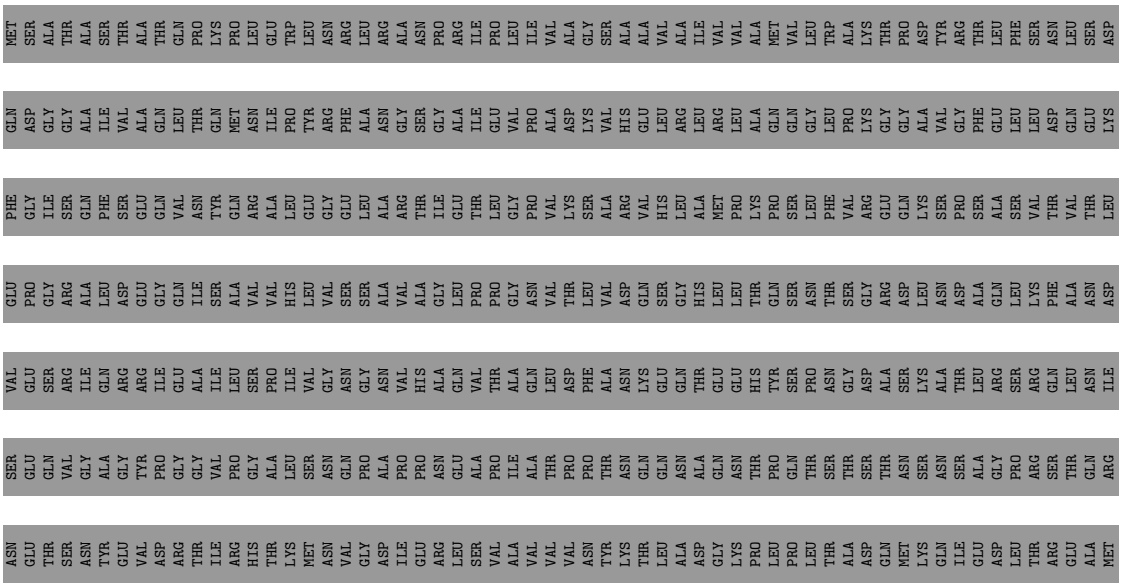
• Molecule 6: Flagellar M-ring protein

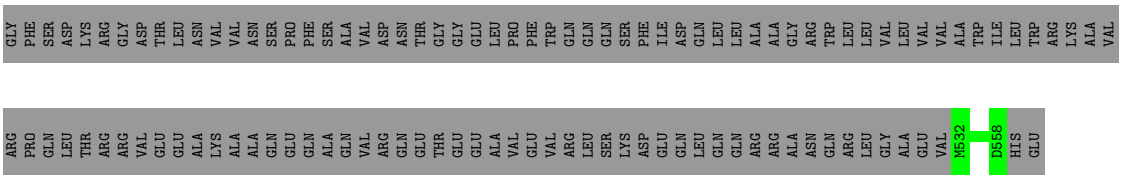
Chain Cp: 5% 95%



• Molecule 6: Flagellar M-ring protein

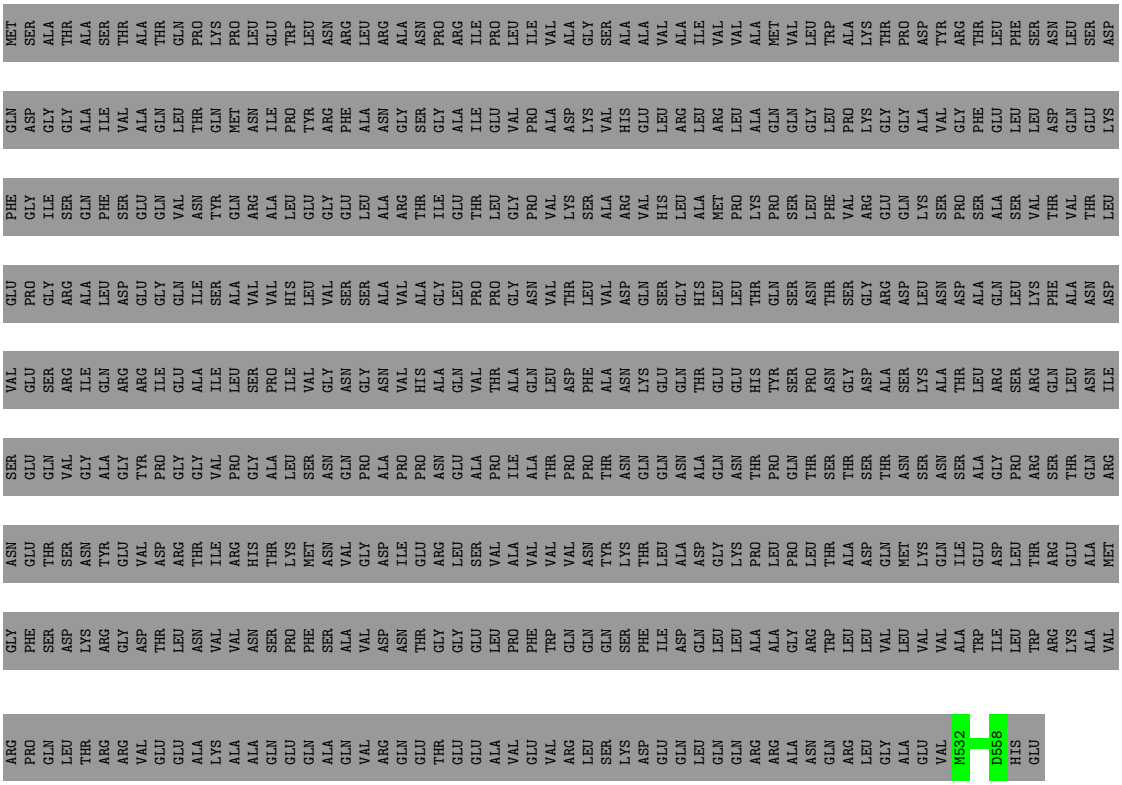
Chain Cw: 5% 95%





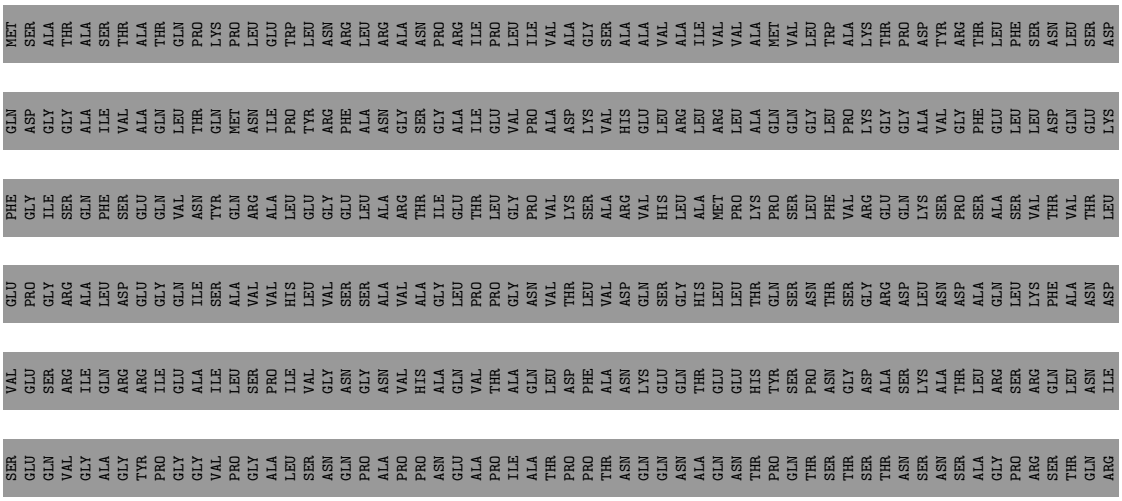
• Molecule 6: Flagellar M-ring protein

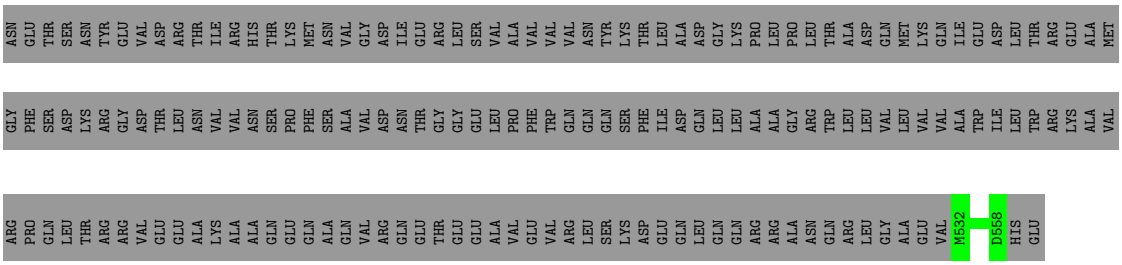
Chain Eb: 5% 95%



• Molecule 6: Flagellar M-ring protein

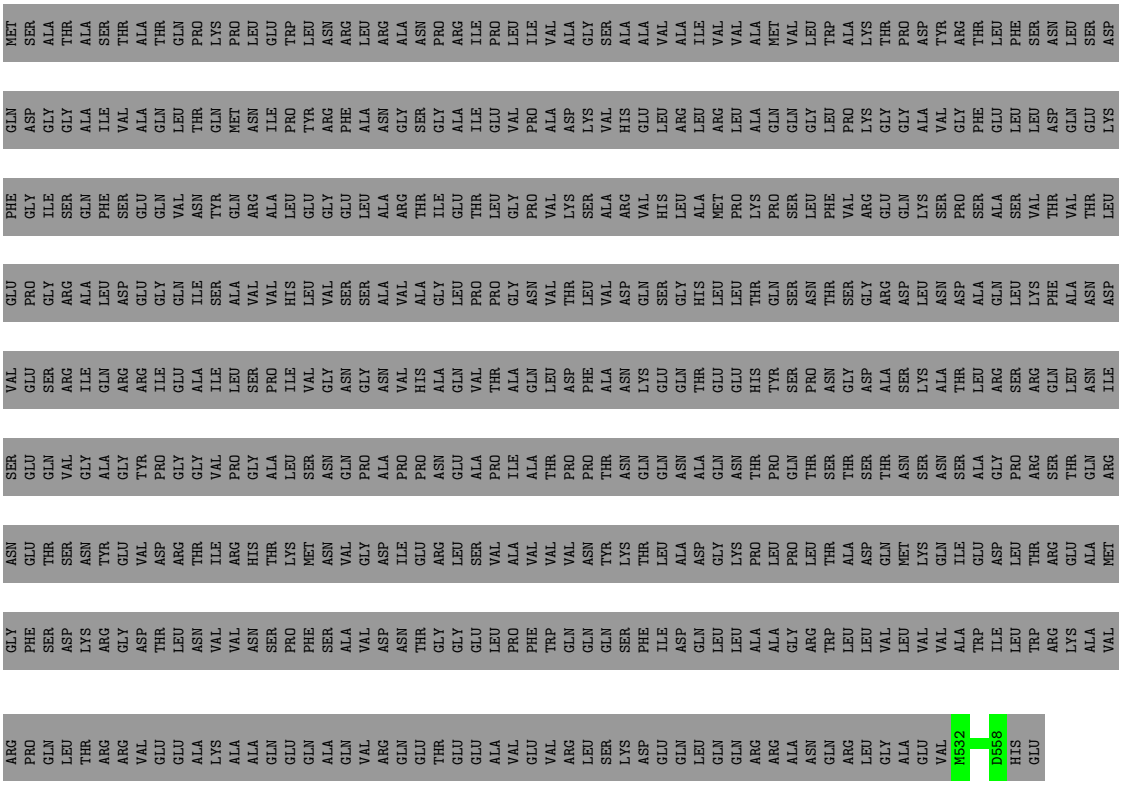
Chain Ec: 5% 95%





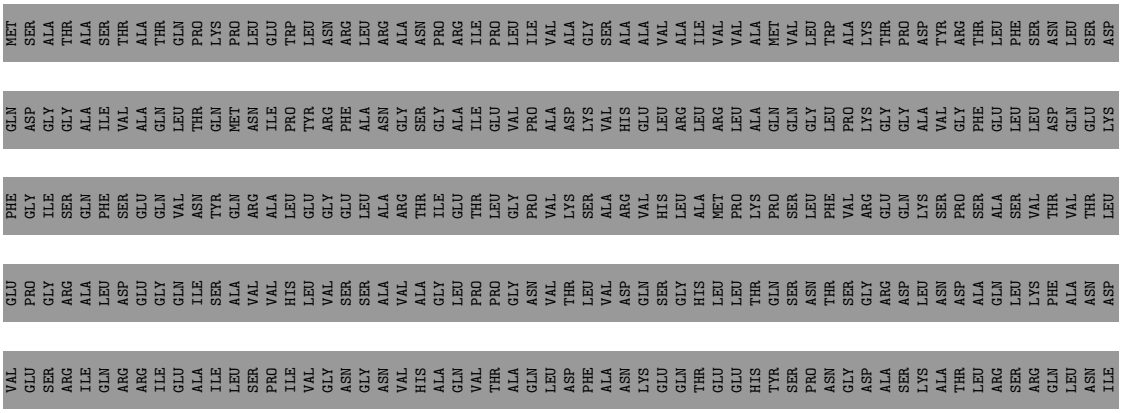
• Molecule 6: Flagellar M-ring protein

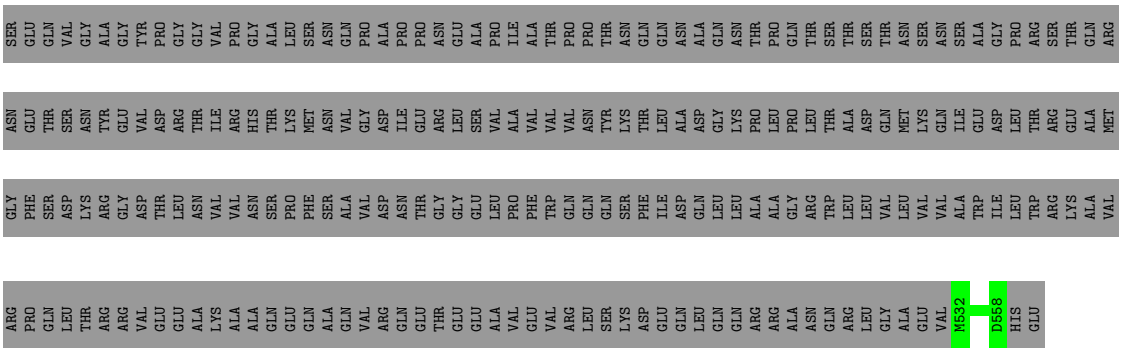
Chain Ed: 5% 95%



• Molecule 6: Flagellar M-ring protein

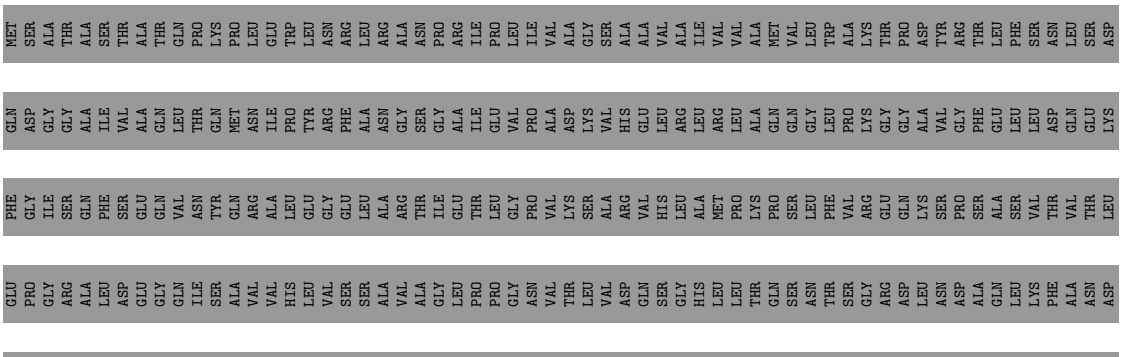
Chain Ee: 5% 95%





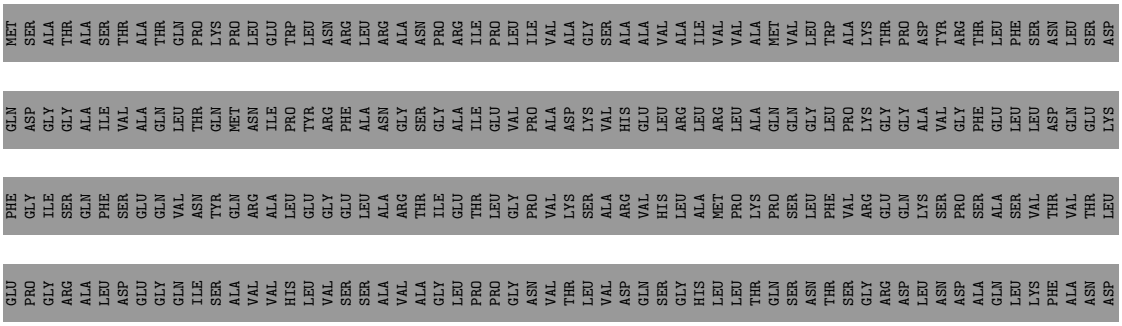
• Molecule 6: Flagellar M-ring protein

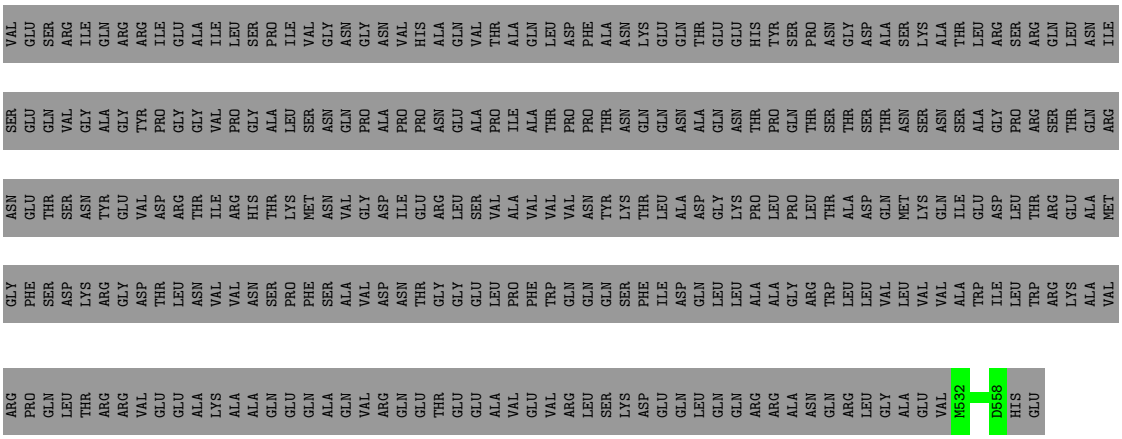
Chain Ef: 5% 95%



• Molecule 6: Flagellar M-ring protein

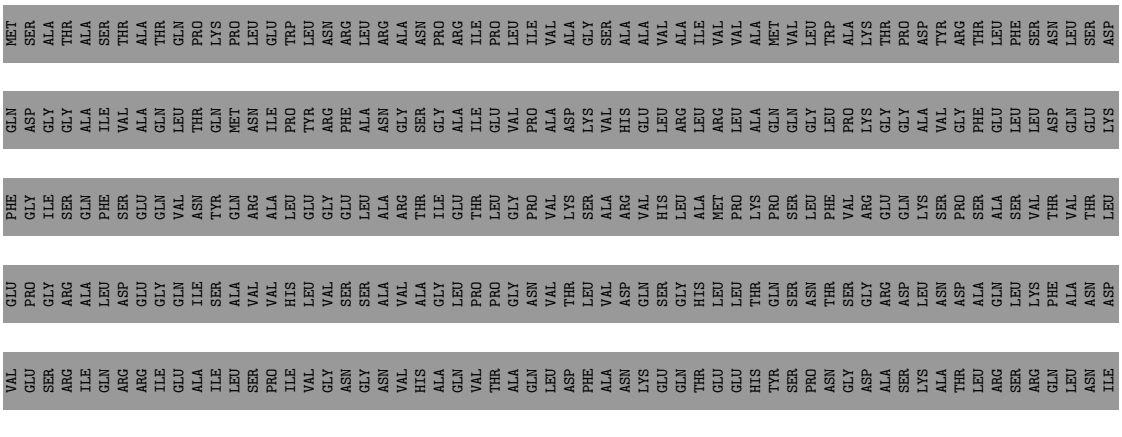
Chain Eg: 5% 95%





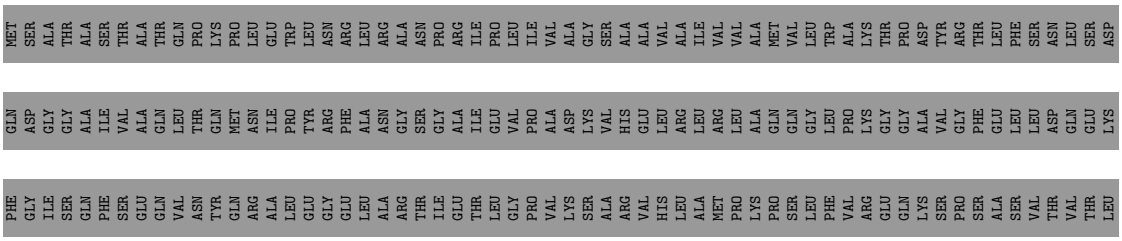
• Molecule 6: Flagellar M-ring protein

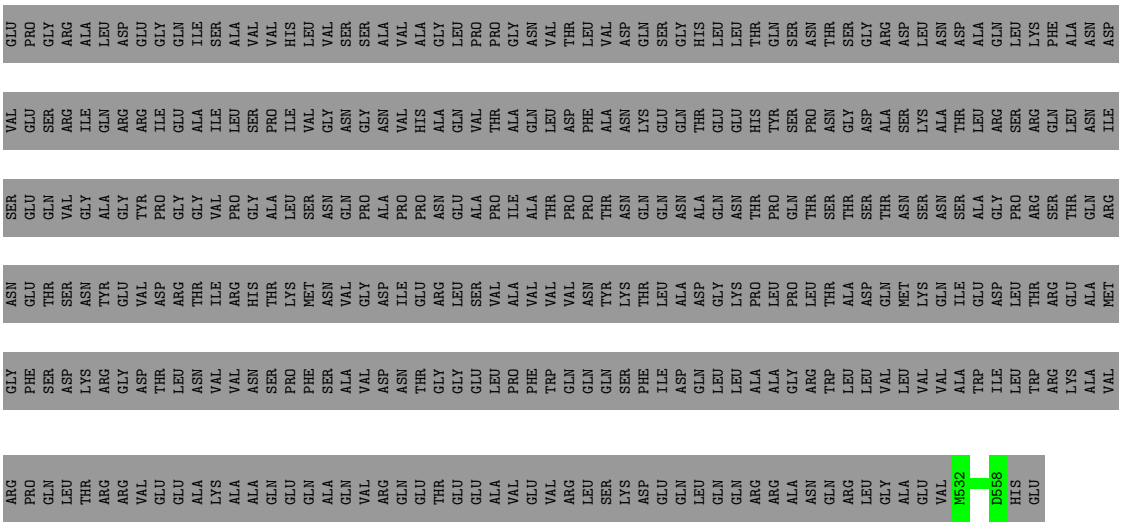
Chain Eh: 5% 95%



• Molecule 6: Flagellar M-ring protein

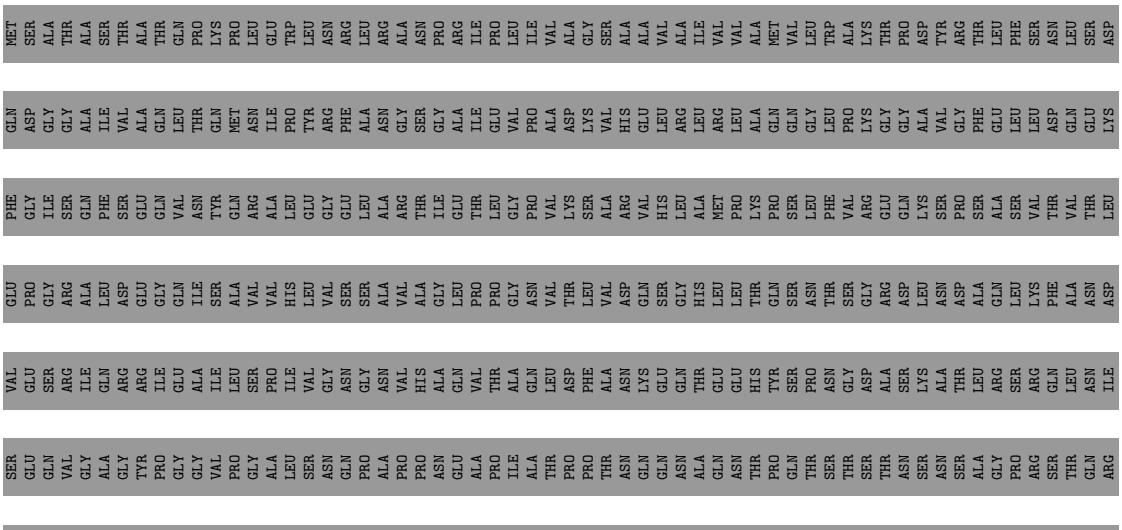
Chain Ei: 5% 95%





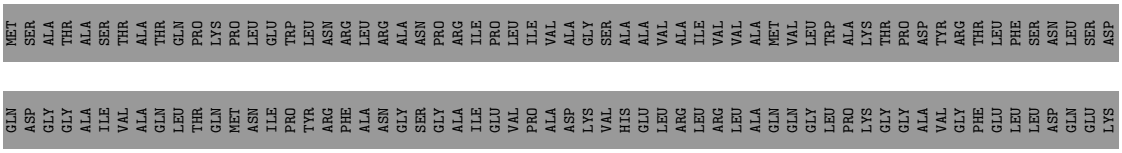
• Molecule 6: Flagellar M-ring protein

Chain Ej: 5% 95%



• Molecule 6: Flagellar M-ring protein

Chain Ek: 5% 95%



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

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

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG

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

GLY PHE SER ASP LYS ARG GLY ASP THR LEU ASN VAL VAL ASN SER PRO PHE SER ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL

ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL M532 D558 HIS GLU

- Molecule 6: Flagellar M-ring protein

Chain El: 5% 95%

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

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

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

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

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

SER GLU GLN VAL GLY ALA GLY TYR PRO GLY GLY VAL PRO GLY ALA LEU SER ASN GLN PRO ALA PRO ASN GLU ALA PRO ILE ALA THR PRO PRO THR ASN GLN GLN ASN ALA GLN ASN THR PRO GLN THR SER THR SER THR ASN SER ASN SER ALA GLY PRO ARG SER THR GLN ARG

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

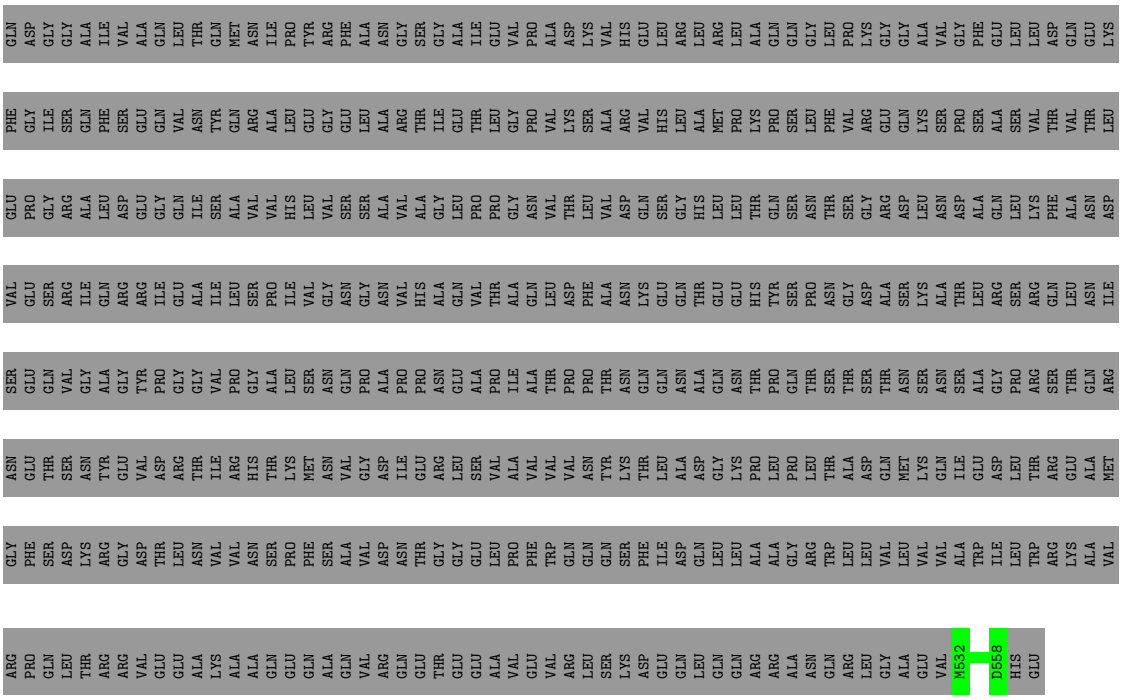
GLY PHE SER ASP LYS ARG GLY ASP THR LEU ASN VAL VAL ASN SER PRO PHE SER ALA VAL ASP ASN THR GLY GLY GLU LEU PRO PHE TRP GLN GLN GLN SER PHE ILE ASP GLN LEU LEU ALA ALA GLY ARG TRP LEU LEU VAL LEU VAL VAL ALA TRP ILE LEU TRP ARG LYS ALA VAL

ARG PRO GLN LEU THR ARG ARG VAL GLU GLU ALA LYS ALA ALA GLN GLU GLN ALA GLN VAL ARG GLN GLU THR GLU GLU ALA VAL GLU VAL ARG LEU SER LYS ASP GLU GLN LEU GLN GLN ARG ALA ASN GLN ARG LEU GLY ALA GLU VAL M532 D558 HIS GLU

- Molecule 6: Flagellar M-ring protein

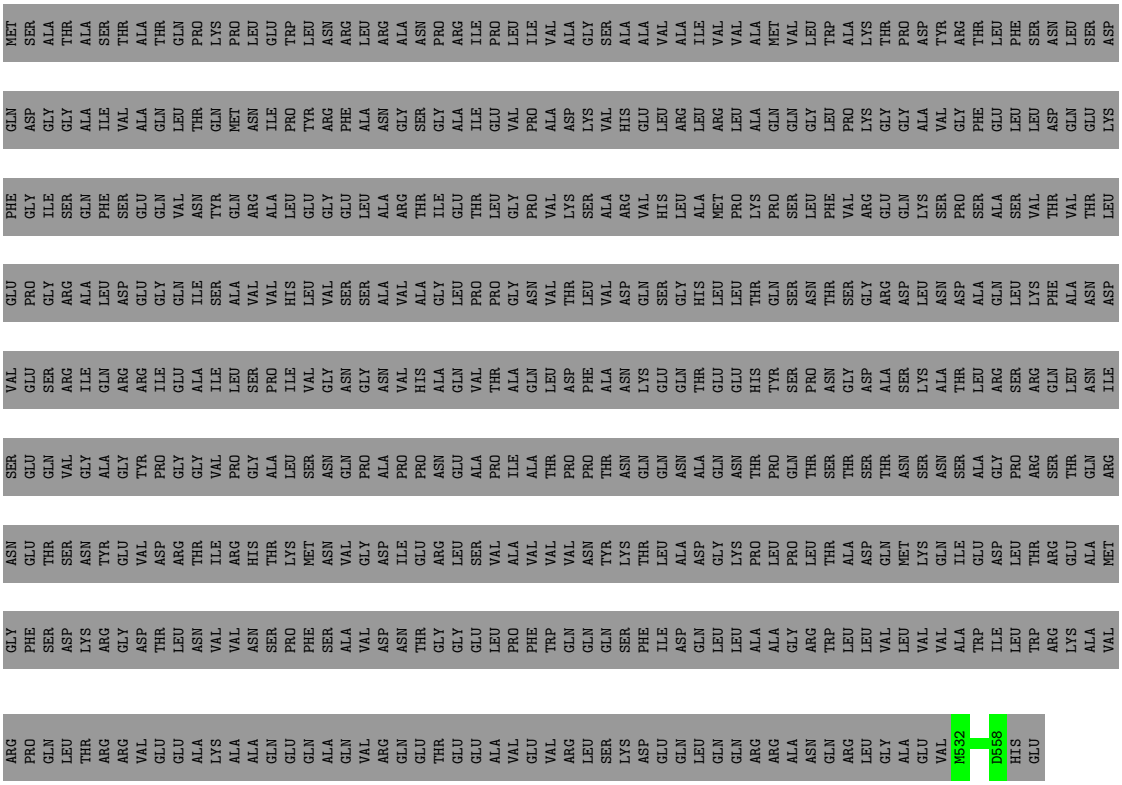
Chain Em: 5% 95%

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



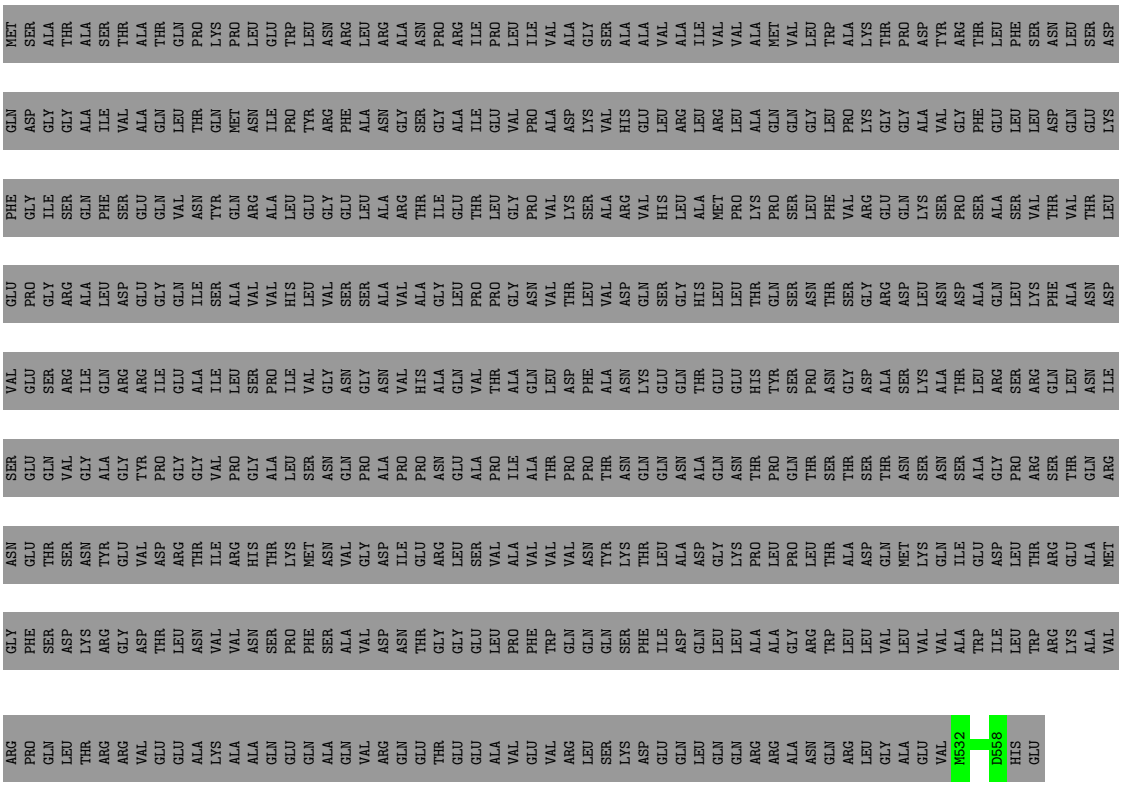
- Molecule 6: Flagellar M-ring protein

Chain En: 5% 95%



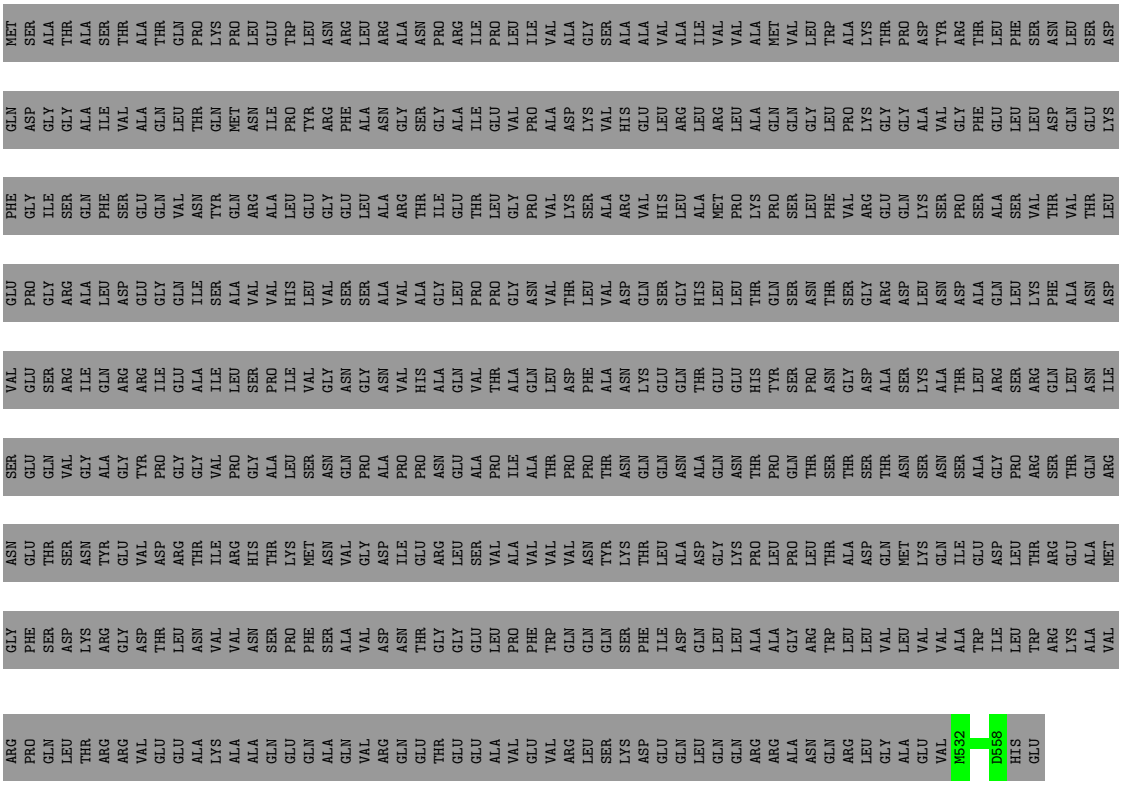
- Molecule 6: Flagellar M-ring protein

Chain Eo: 5% 95%



• Molecule 6: Flagellar M-ring protein

Chain Ep: 5% 95%



• Molecule 7: Flagellar biosynthetic protein FliQ

Chain Ab: 99%

• Molecule 7: Flagellar biosynthetic protein FliQ

Chain Aq: 99%

• Molecule 7: Flagellar biosynthetic protein FliQ

Chain Ar: 100%

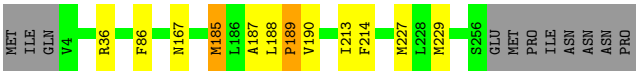
There are no outlier residues recorded for this chain.

• Molecule 7: Flagellar biosynthetic protein FliQ

Chain As: 99%

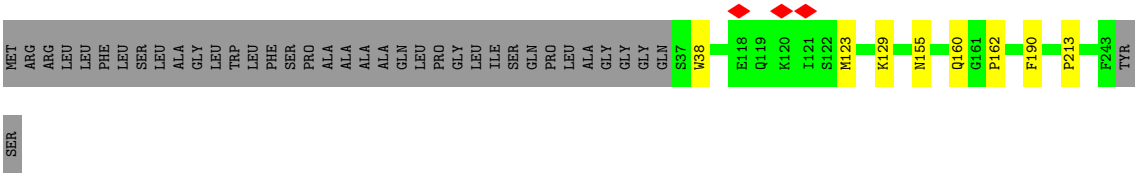
• Molecule 8: Flagellar biosynthetic protein FliR

Chain At: 91%



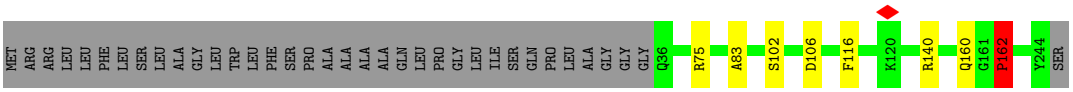
• Molecule 9: Flagellar biosynthetic protein FliP

Chain Au: 81% 16%



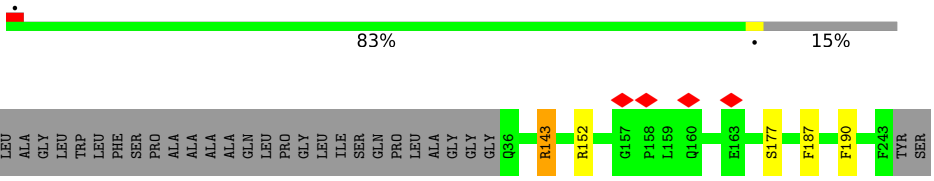
• Molecule 9: Flagellar biosynthetic protein FliP

Chain Av: 82% 15%



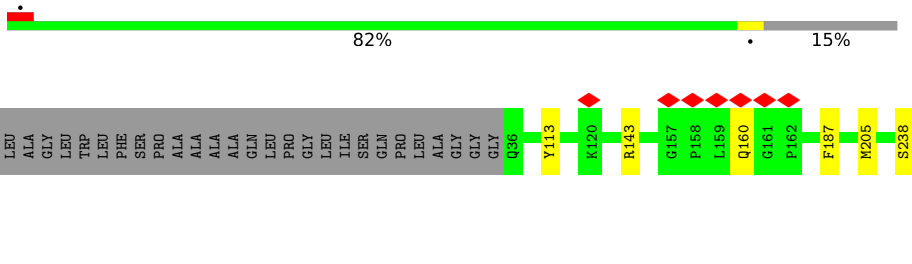
• Molecule 9: Flagellar biosynthetic protein FliP

Chain Aw:



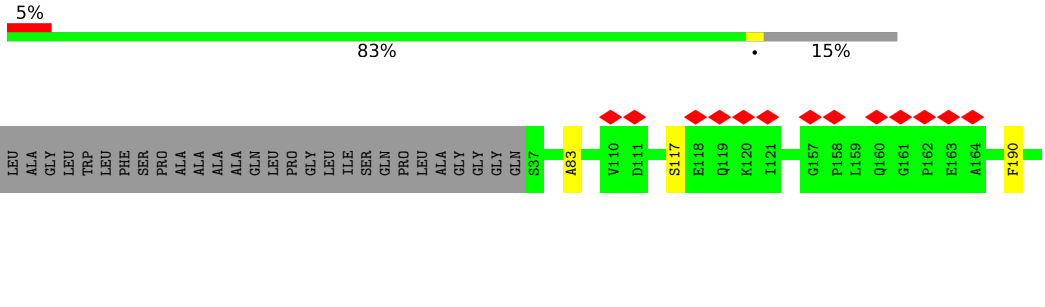
• Molecule 9: Flagellar biosynthetic protein FliP

Chain Ax:



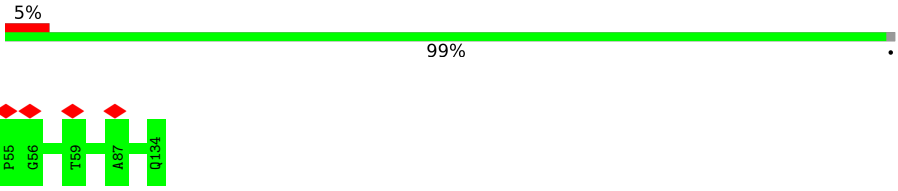
• Molecule 9: Flagellar biosynthetic protein FliP

Chain Ay:



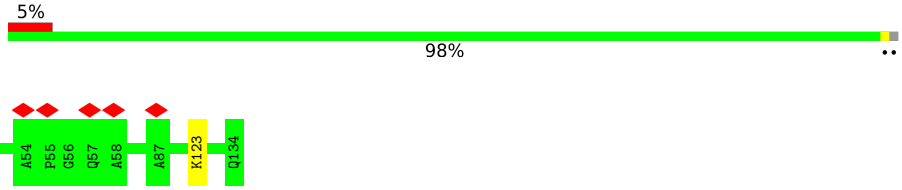
• Molecule 10: Flagellar basal-body rod protein FlgC

Chain BA:



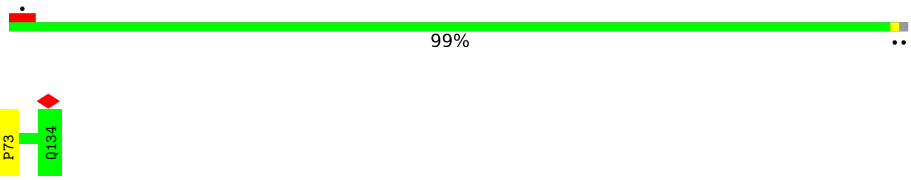
• Molecule 10: Flagellar basal-body rod protein FlgC

Chain BB:



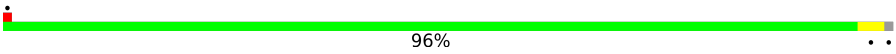
• Molecule 10: Flagellar basal-body rod protein FlgC

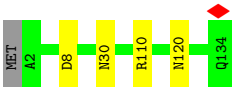
Chain BC:



• Molecule 10: Flagellar basal-body rod protein FlgC

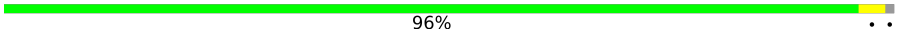
Chain BD:

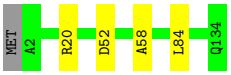




• Molecule 10: Flagellar basal-body rod protein FlgC

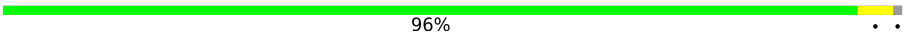
Chain BE:





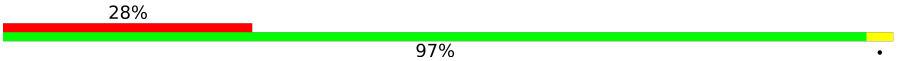
• Molecule 10: Flagellar basal-body rod protein FlgC

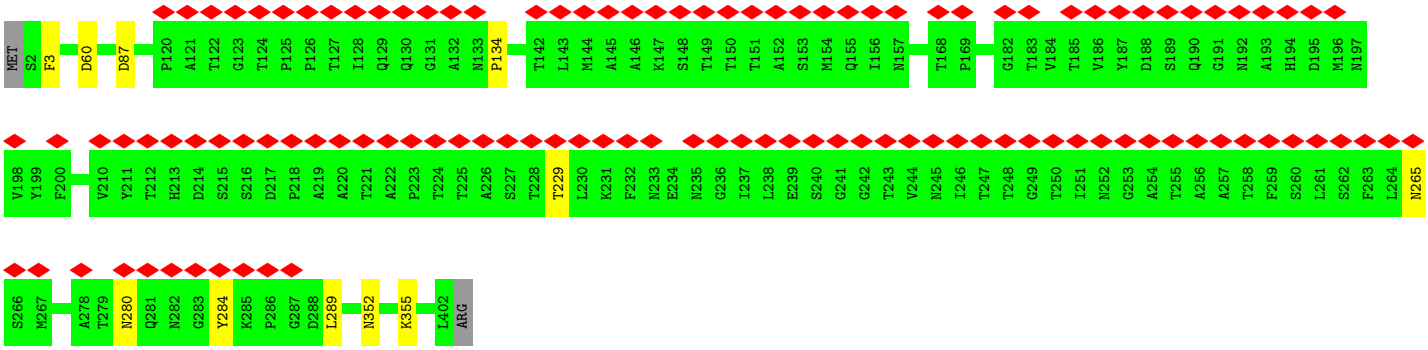
Chain BF:



• Molecule 11: Flagellar hook protein FlgE

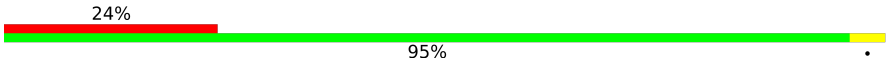
Chain ZF:

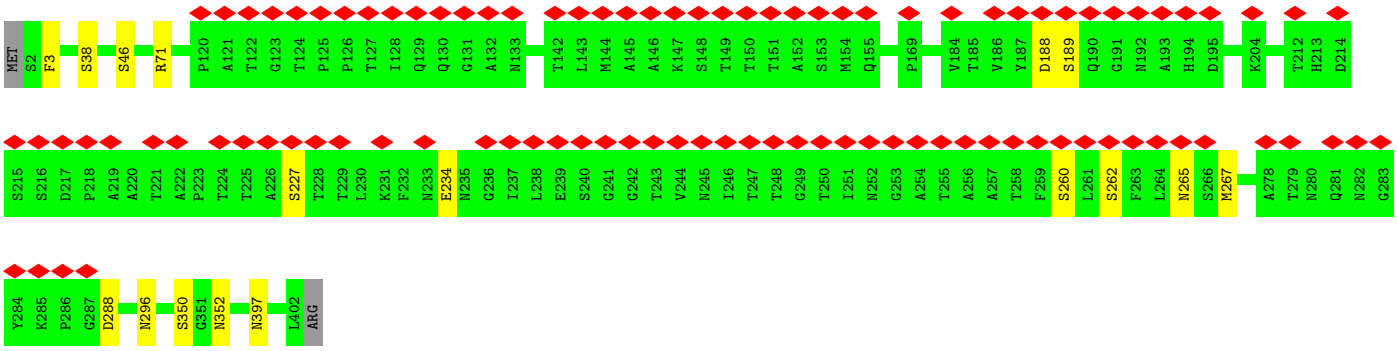




• Molecule 11: Flagellar hook protein FlgE

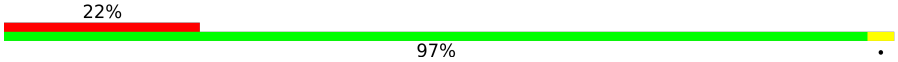
Chain ZG:

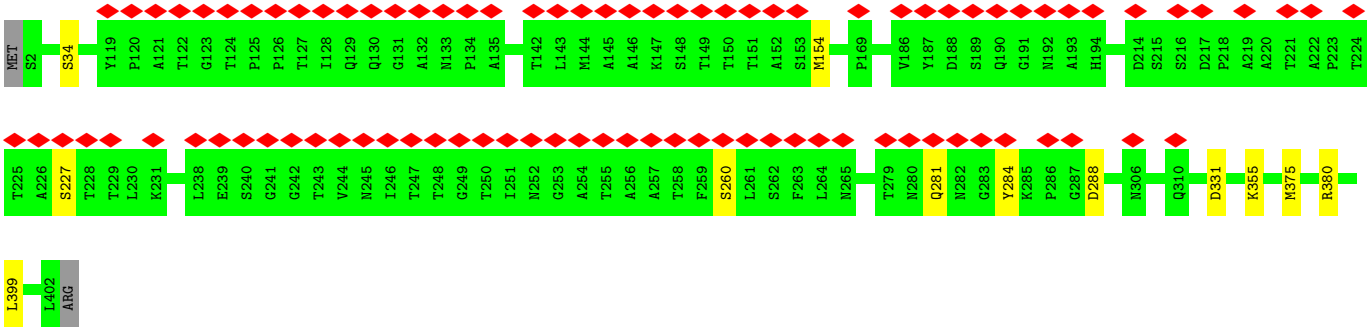




• Molecule 11: Flagellar hook protein FlgE

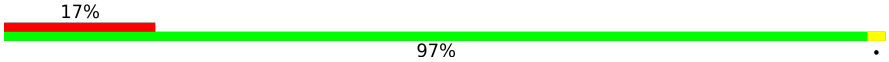
Chain ZH:

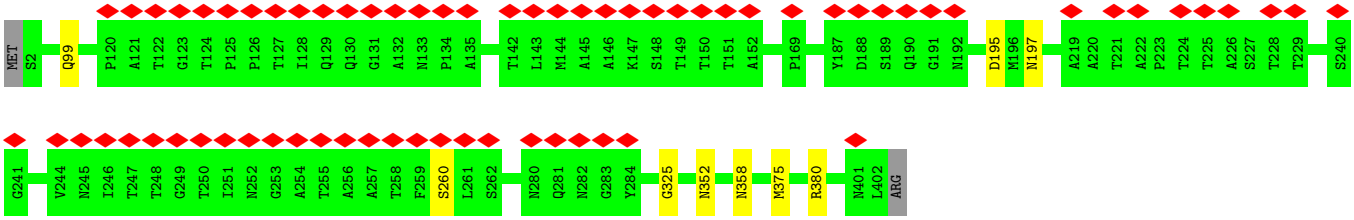




• Molecule 11: Flagellar hook protein FlgE

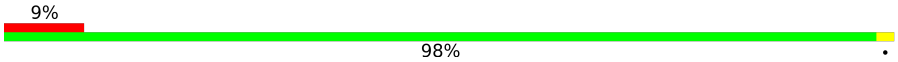
Chain ZI:

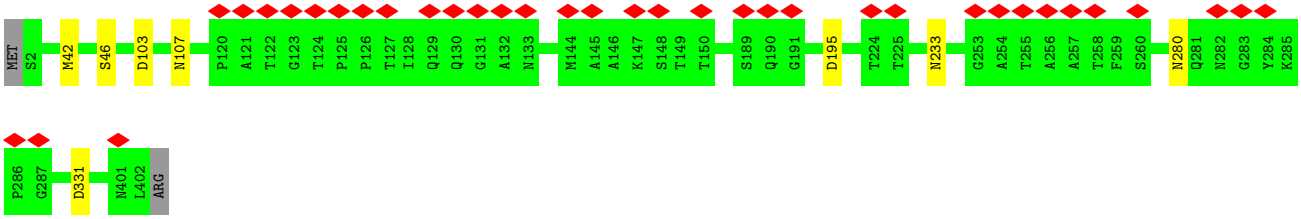




• Molecule 11: Flagellar hook protein FlgE

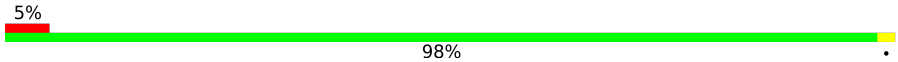
Chain ZJ:

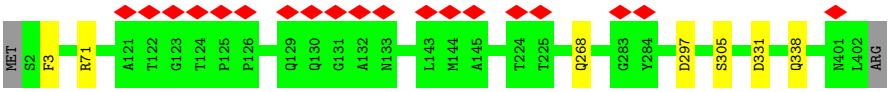




• Molecule 11: Flagellar hook protein FlgE

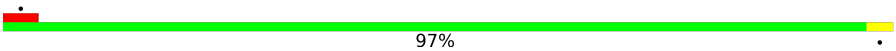
Chain ZK:

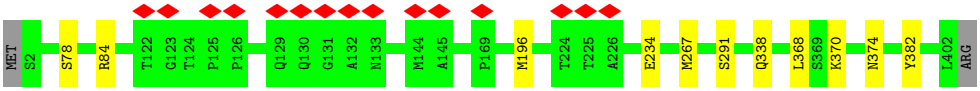




• Molecule 11: Flagellar hook protein FlgE

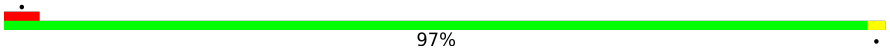
Chain ZL:

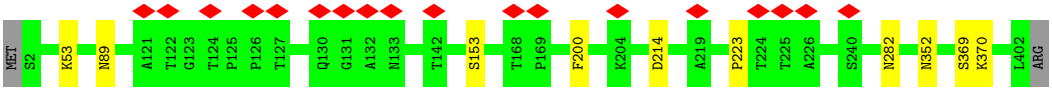




• Molecule 11: Flagellar hook protein FlgE

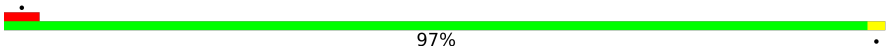
Chain ZM:

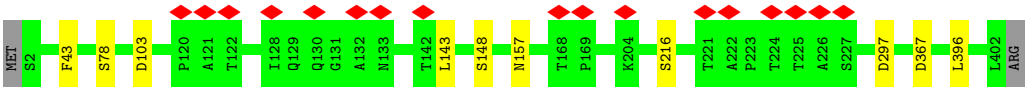




• Molecule 11: Flagellar hook protein FlgE

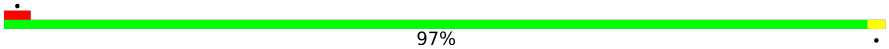
Chain ZN:

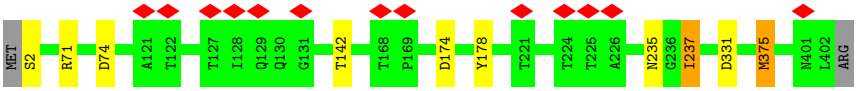




• Molecule 11: Flagellar hook protein FlgE

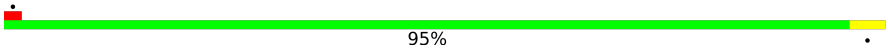
Chain ZO:

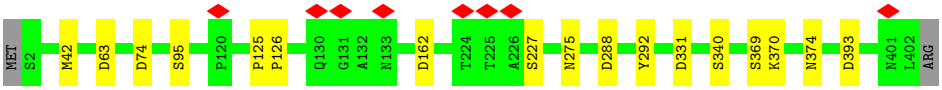




• Molecule 11: Flagellar hook protein FlgE

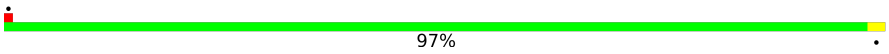
Chain ZP:

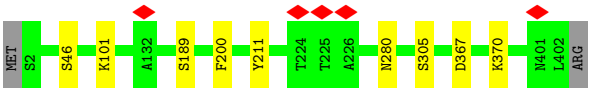




• Molecule 11: Flagellar hook protein FlgE

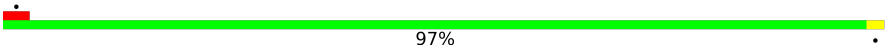
Chain ZQ:

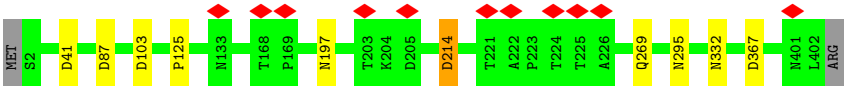




• Molecule 11: Flagellar hook protein FlgE

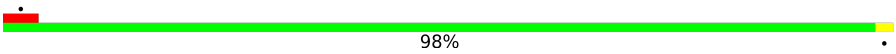
Chain ZR:

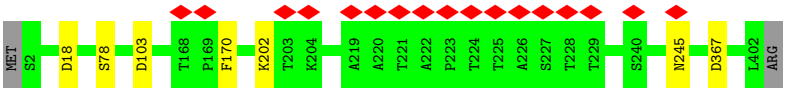




• Molecule 11: Flagellar hook protein FlgE

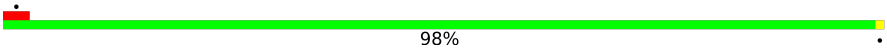
Chain ZS:

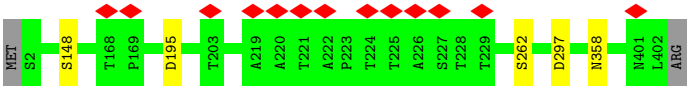




• Molecule 11: Flagellar hook protein FlgE

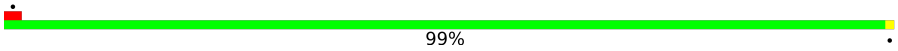
Chain ZT:

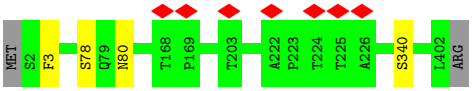




• Molecule 11: Flagellar hook protein FlgE

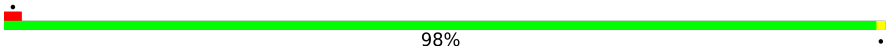
Chain ZU:

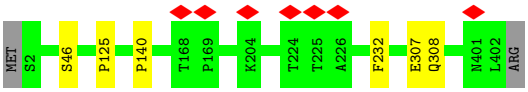




• Molecule 11: Flagellar hook protein FlgE

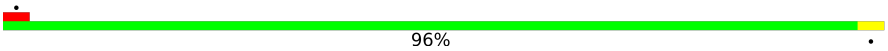
Chain ZV:

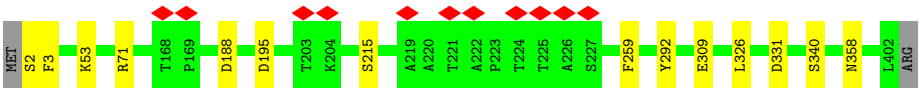




• Molecule 11: Flagellar hook protein FlgE

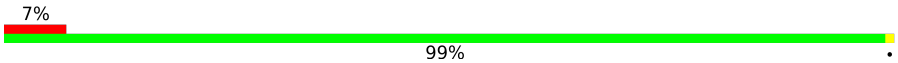
Chain ZW:

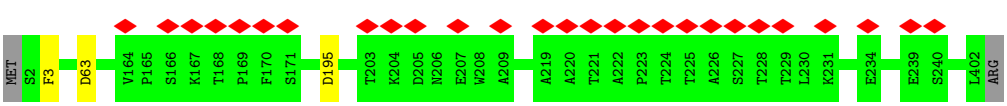




• Molecule 11: Flagellar hook protein FlgE

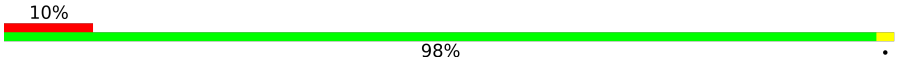
Chain ZX:

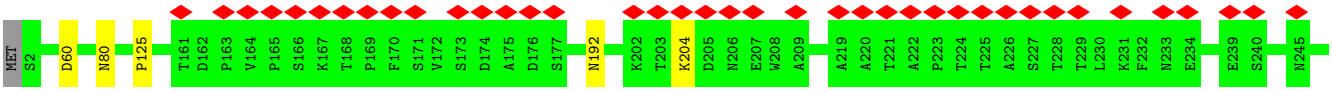


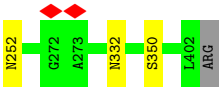


• Molecule 11: Flagellar hook protein FlgE

Chain ZY:

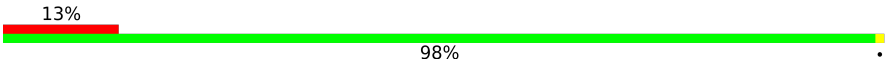


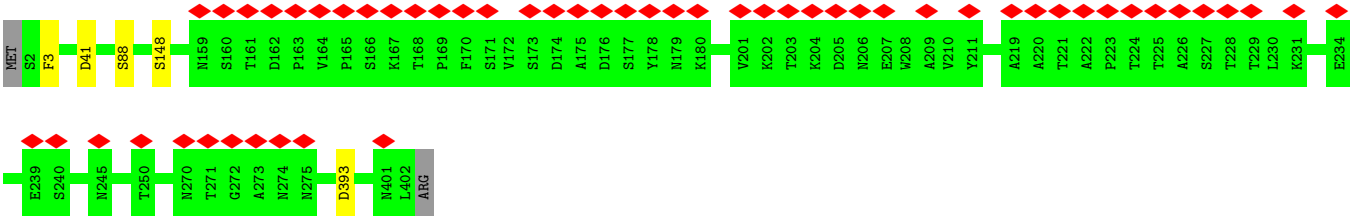




• Molecule 11: Flagellar hook protein FlgE

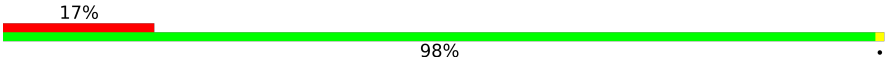
Chain ZZ:

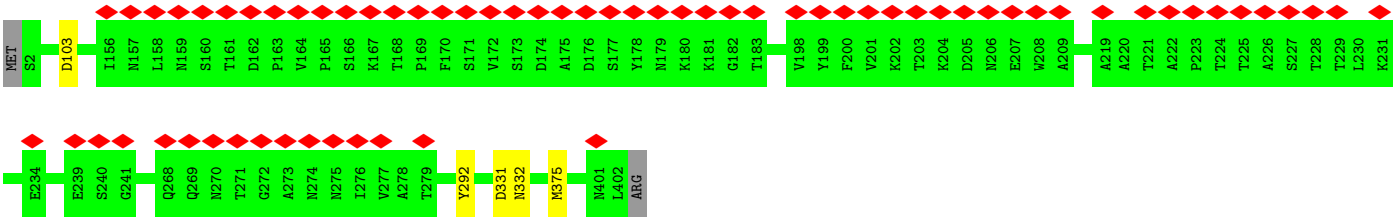




• Molecule 11: Flagellar hook protein FlgE

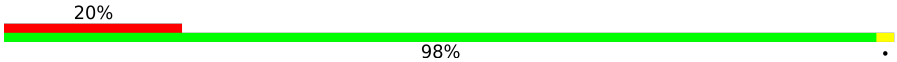
Chain Za:

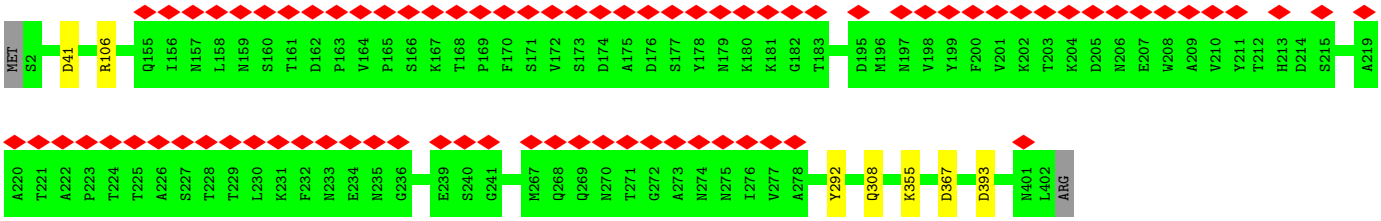




• Molecule 11: Flagellar hook protein FlgE

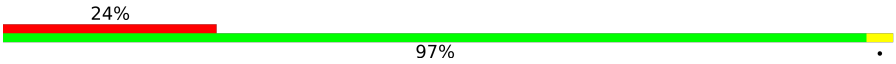
Chain Zb:

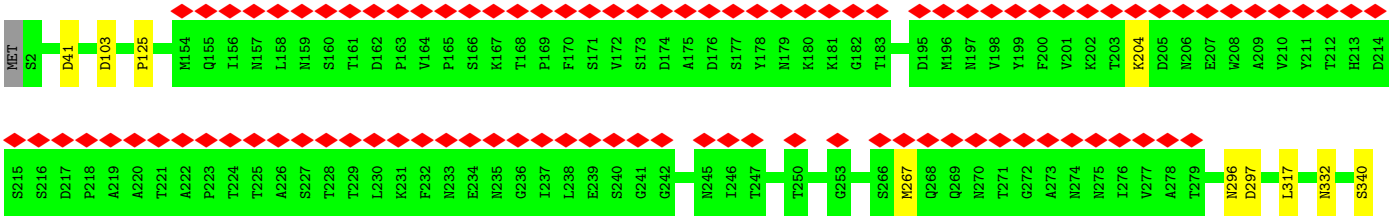




• Molecule 11: Flagellar hook protein FlgE

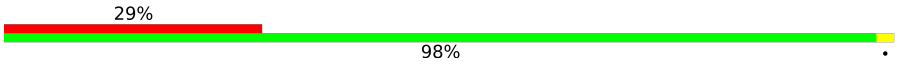
Chain Zc:

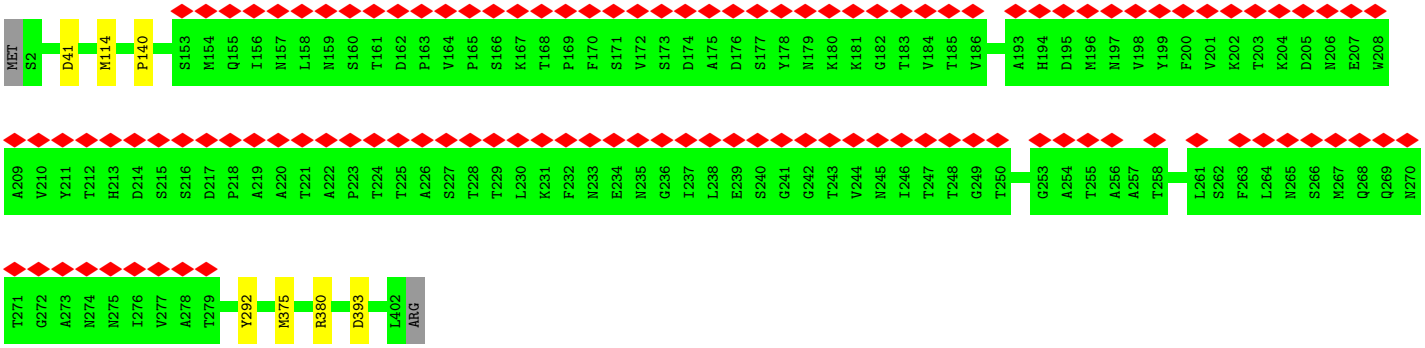




• Molecule 11: Flagellar hook protein FlgE

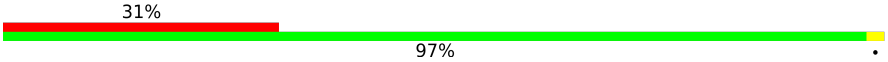
Chain Zd:

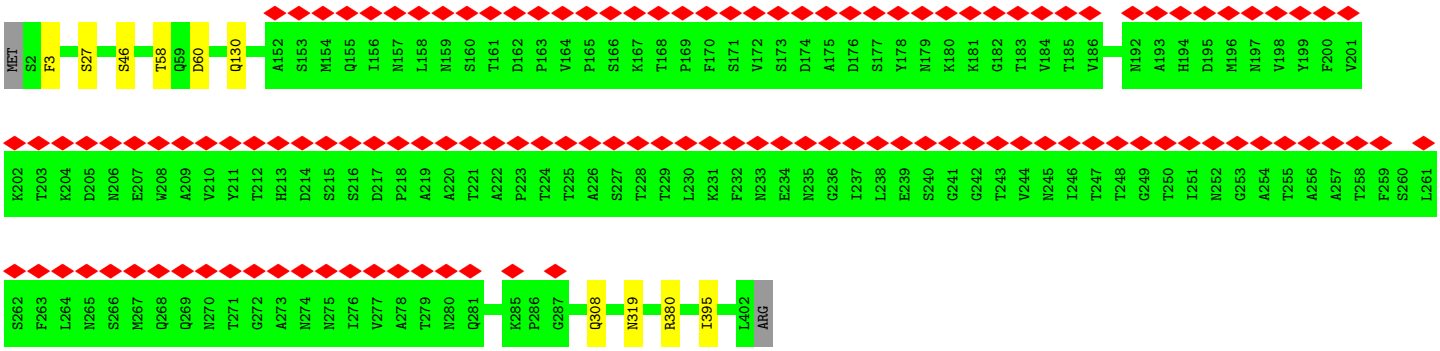




• Molecule 11: Flagellar hook protein FlgE

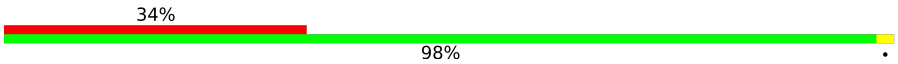
Chain Ze:

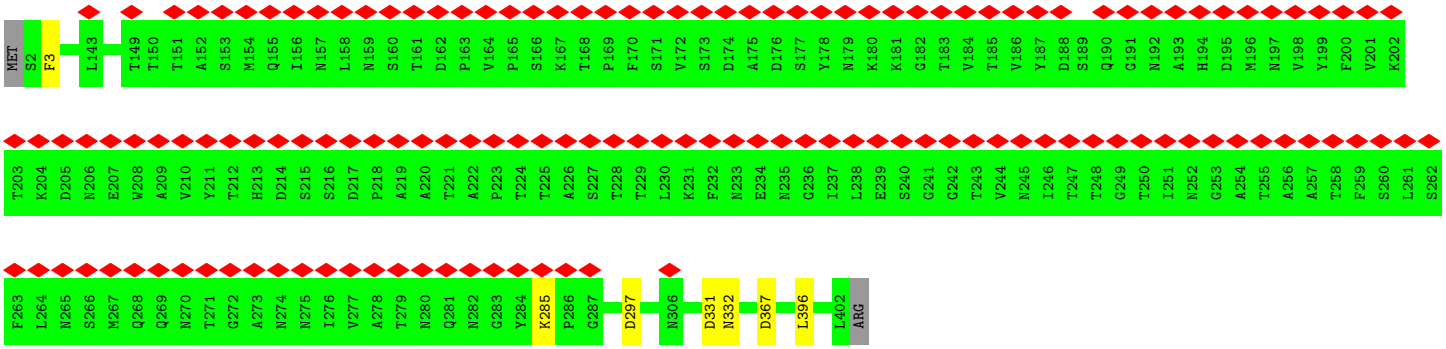




• Molecule 11: Flagellar hook protein FlgE

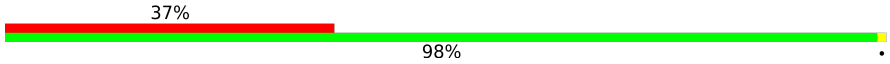
Chain Zf:

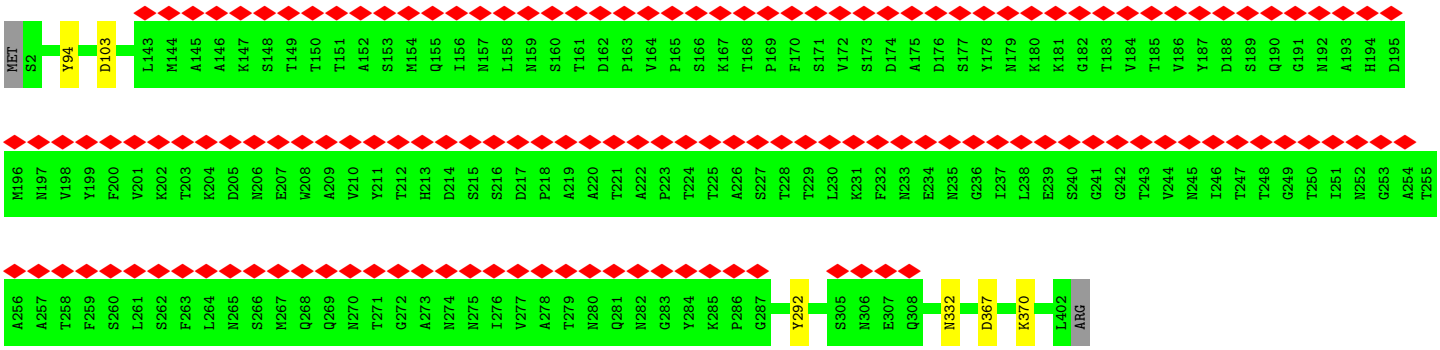




• Molecule 11: Flagellar hook protein FlgE

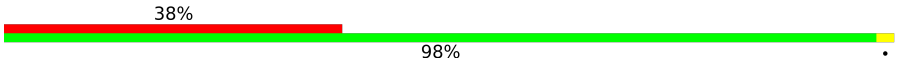
Chain Zg:

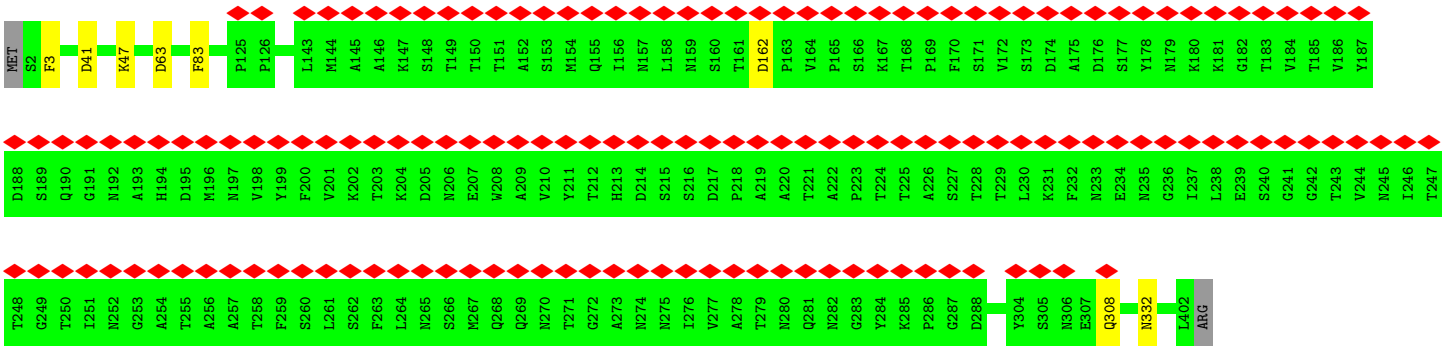




- Molecule 11: Flagellar hook protein FlgE

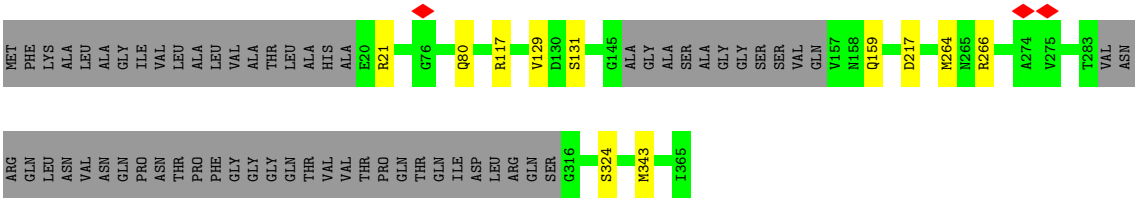
Chain Zh:





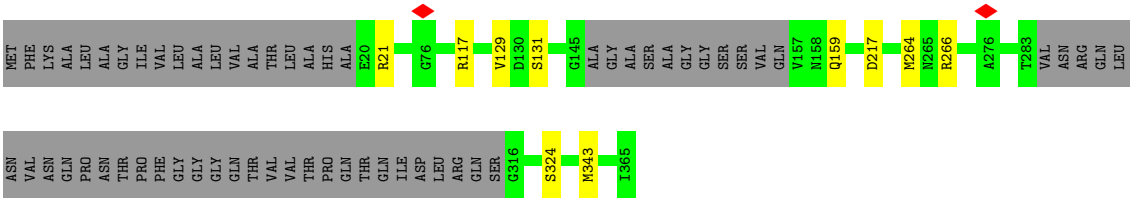
- Molecule 12: Flagellar P-ring protein

Chain a:



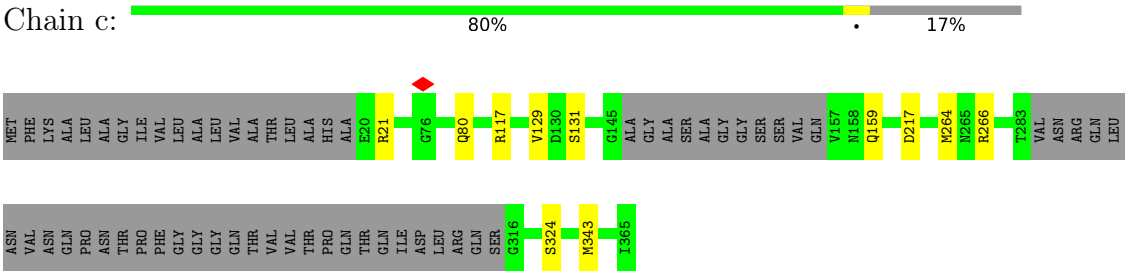
- Molecule 12: Flagellar P-ring protein

Chain b:



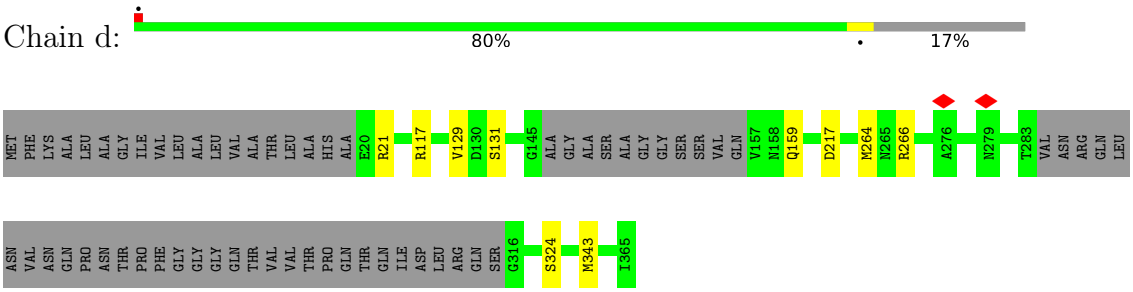
- Molecule 12: Flagellar P-ring protein

Chain c:



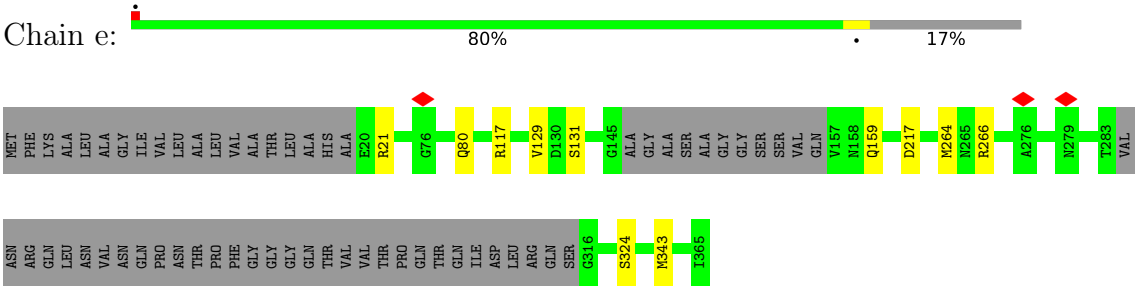
- Molecule 12: Flagellar P-ring protein

Chain d:



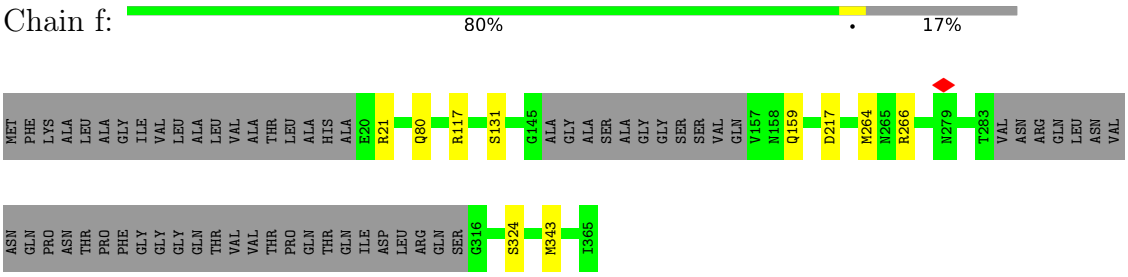
- Molecule 12: Flagellar P-ring protein

Chain e:



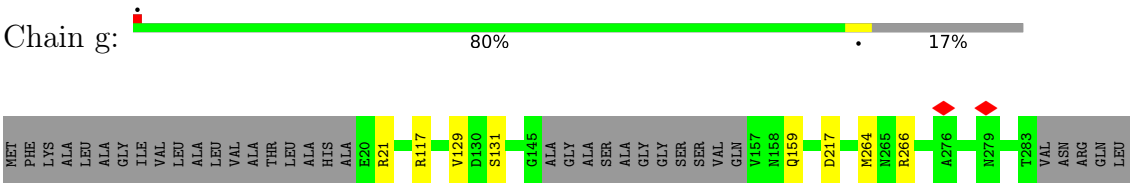
- Molecule 12: Flagellar P-ring protein

Chain f:



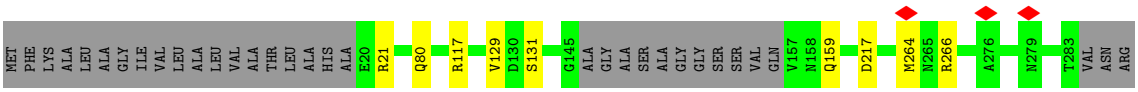
- Molecule 12: Flagellar P-ring protein

Chain g:



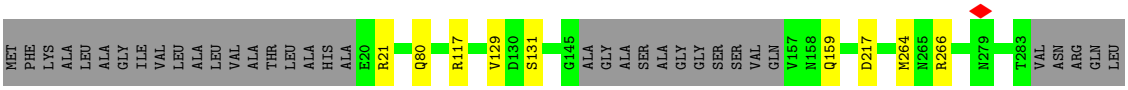
• Molecule 12: Flagellar P-ring protein

Chain h:



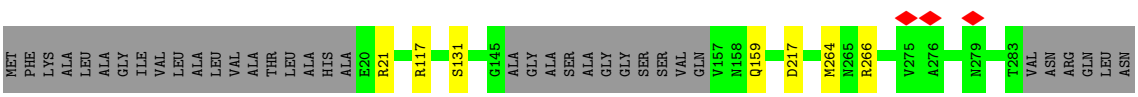
• Molecule 12: Flagellar P-ring protein

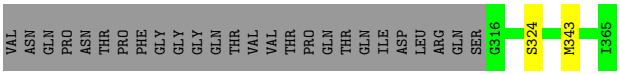
Chain i:



• Molecule 12: Flagellar P-ring protein

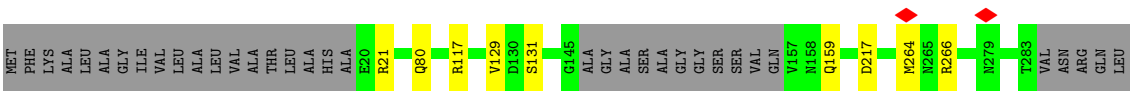
Chain j:





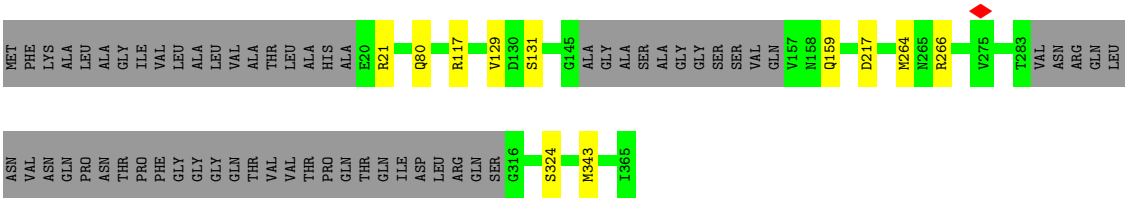
• Molecule 12: Flagellar P-ring protein

Chain k:



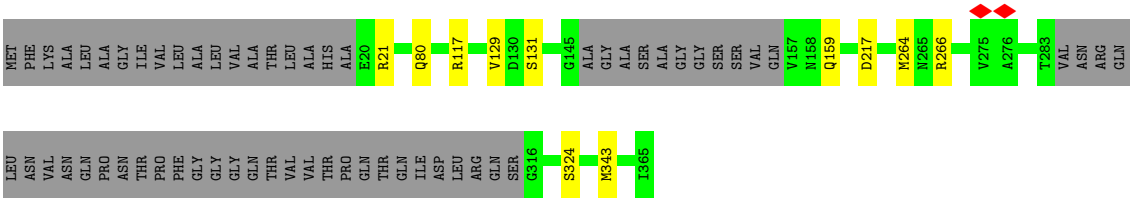
• Molecule 12: Flagellar P-ring protein

Chain l:



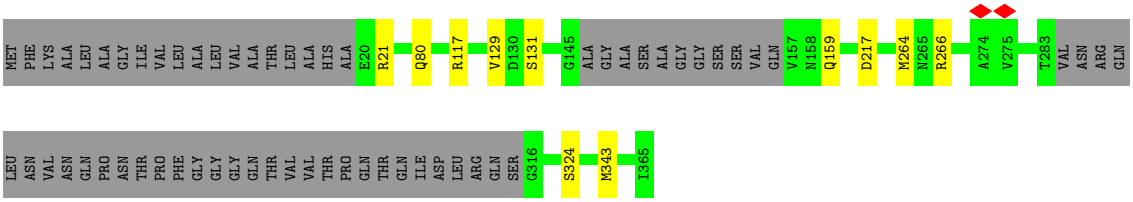
• Molecule 12: Flagellar P-ring protein

Chain m:



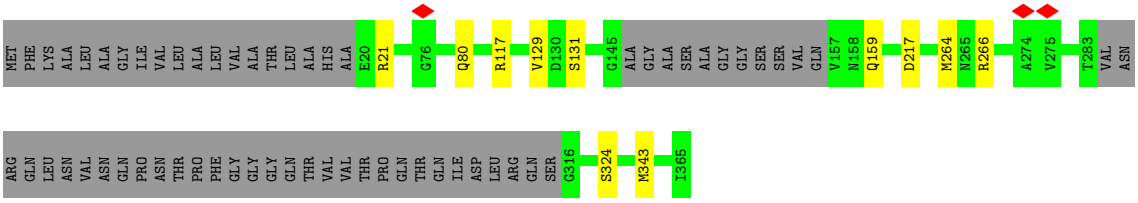
• Molecule 12: Flagellar P-ring protein

Chain n:



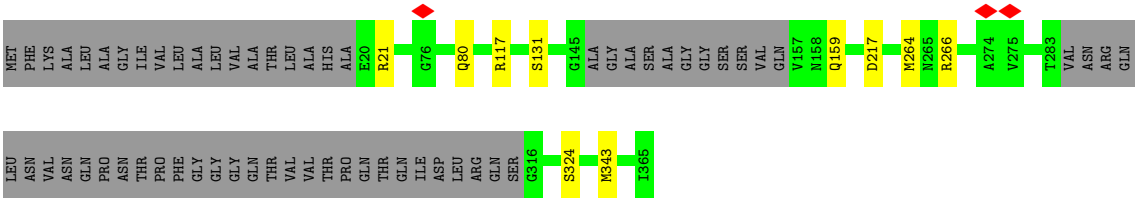
• Molecule 12: Flagellar P-ring protein

Chain o:



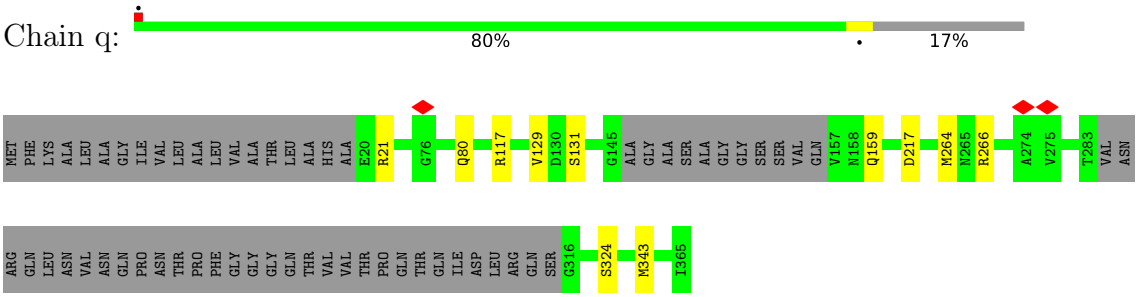
• Molecule 12: Flagellar P-ring protein

Chain p:



• Molecule 12: Flagellar P-ring protein

Chain q:



• Molecule 12: Flagellar P-ring protein

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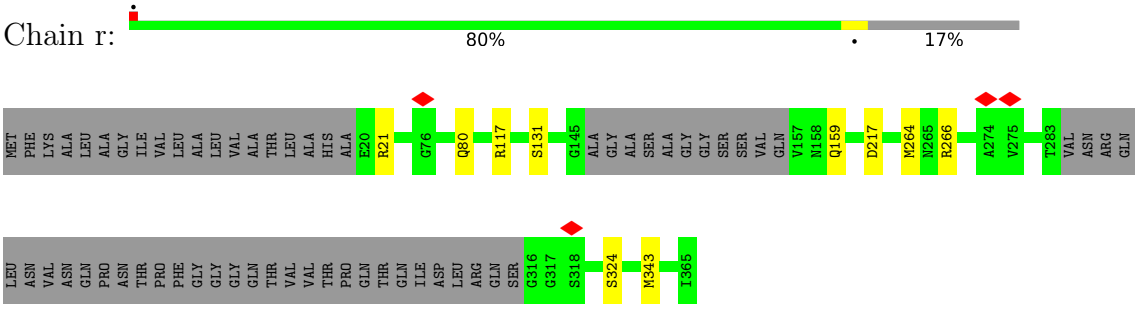
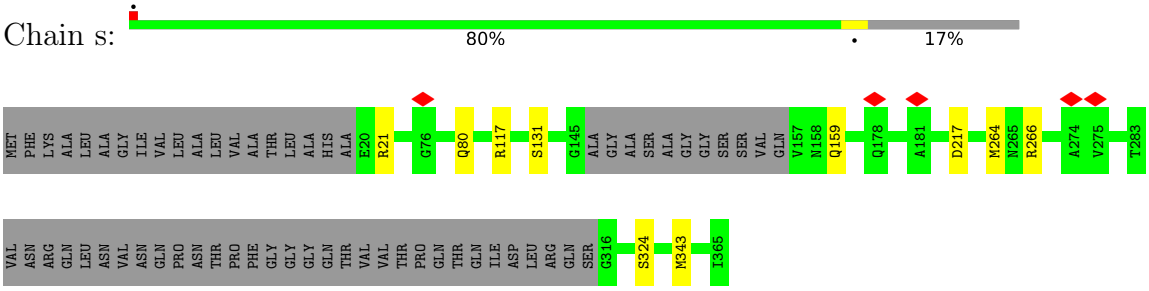


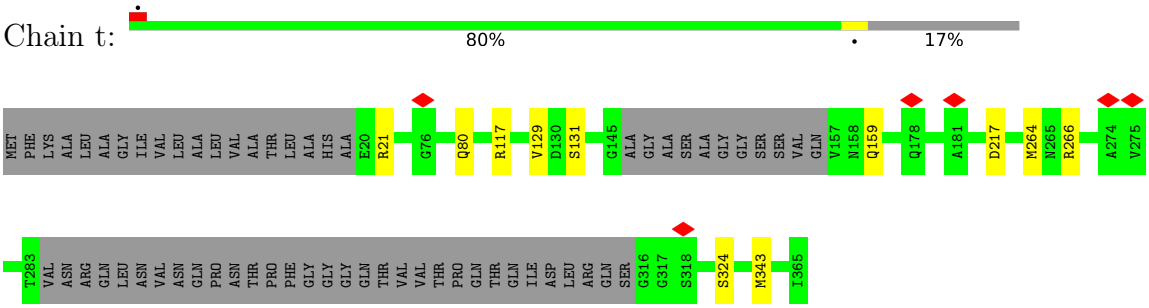
• Molecule 12: Flagellar P-ring protein

Chain s:



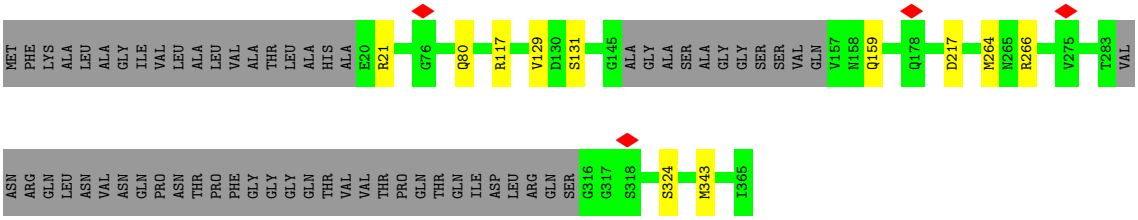
• Molecule 12: Flagellar P-ring protein

Chain t:



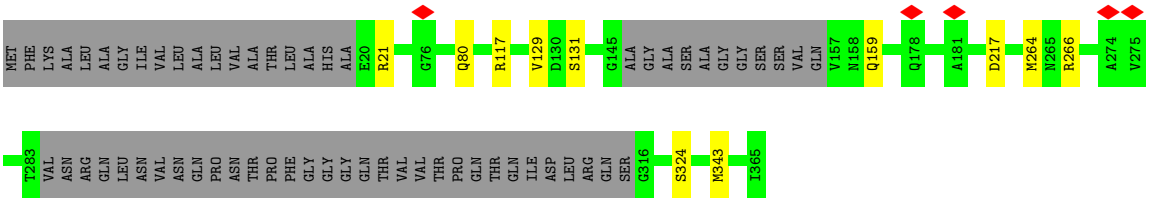
• Molecule 12: Flagellar P-ring protein

Chain u:



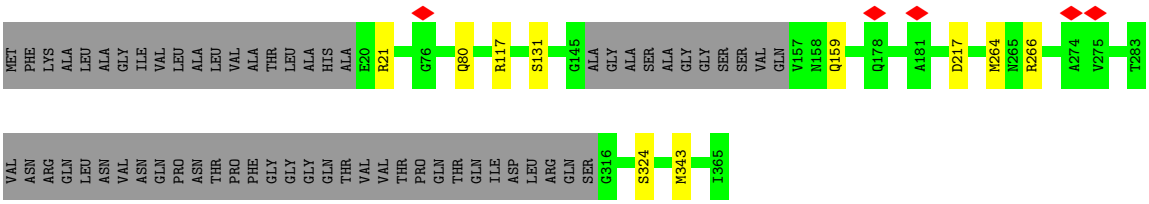
• Molecule 12: Flagellar P-ring protein

Chain v:



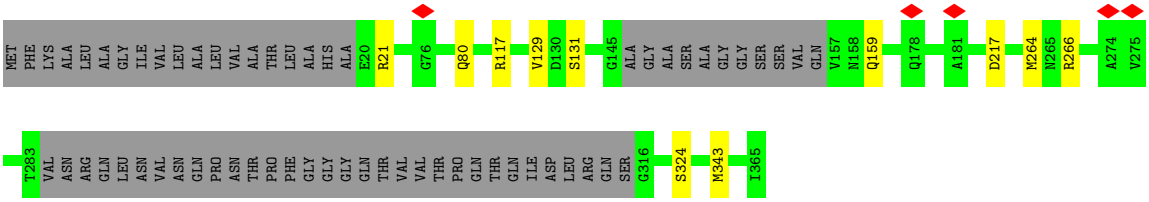
• Molecule 12: Flagellar P-ring protein

Chain w:



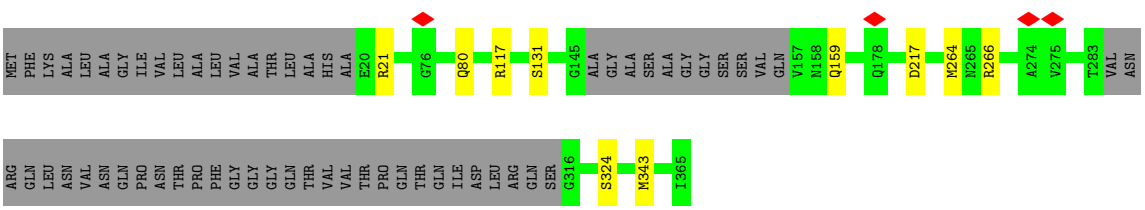
• Molecule 12: Flagellar P-ring protein

Chain x:



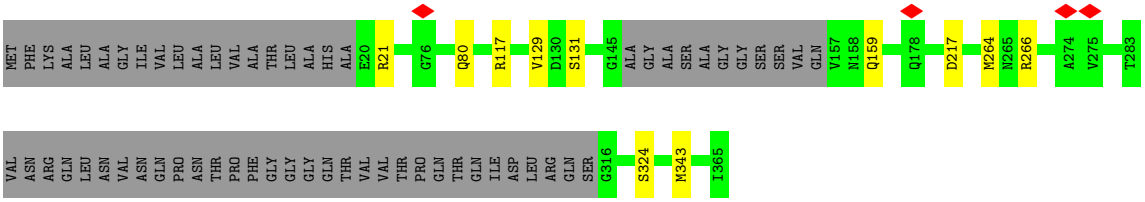
• Molecule 12: Flagellar P-ring protein

Chain y:



• Molecule 12: Flagellar P-ring protein

Chain z:

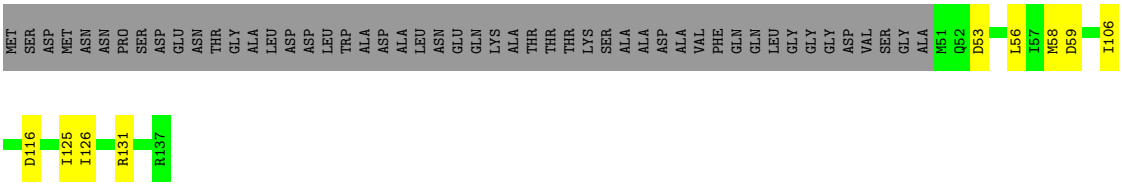


• Molecule 13: Flagellar motor switch protein FliN

Chain C3:

• Molecule 13: Flagellar motor switch protein FliN

Chain C4:



• Molecule 13: Flagellar motor switch protein FliN

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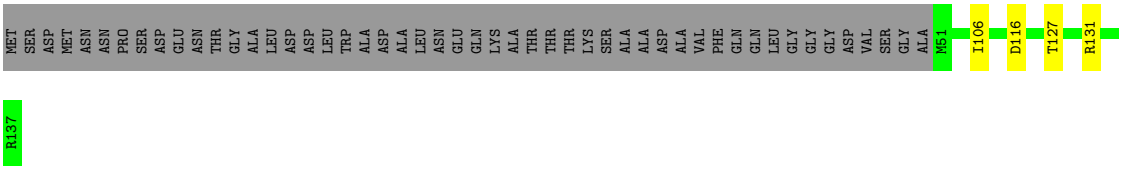
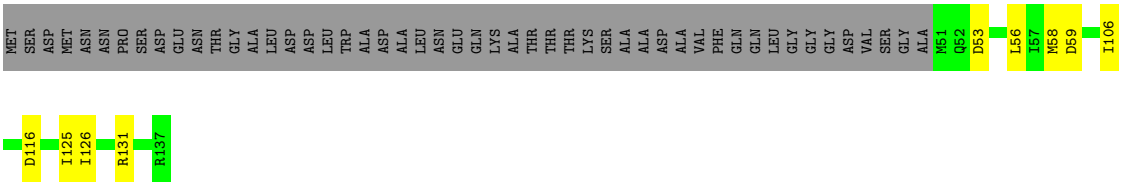


• Molecule 13: Flagellar motor switch protein FliN

Chain C8:



• Molecule 13: Flagellar motor switch protein FliN

Chain C9: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DD: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DI: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106 D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DJ: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DK: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DM: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DN: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DO: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DP: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DQ: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DR: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DS: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DT: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DU: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DV: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

• Molecule 13: Flagellar motor switch protein FliN

Chain DW: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Da: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Db: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

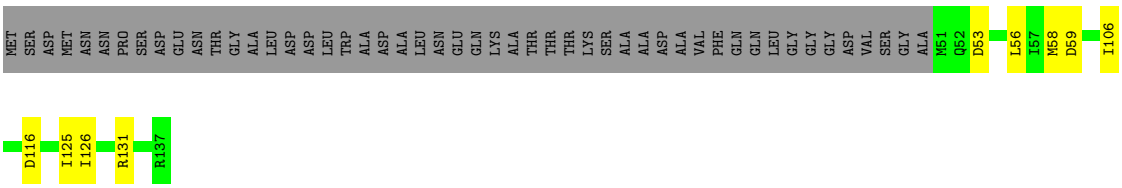
R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Dc: 61% • 36%

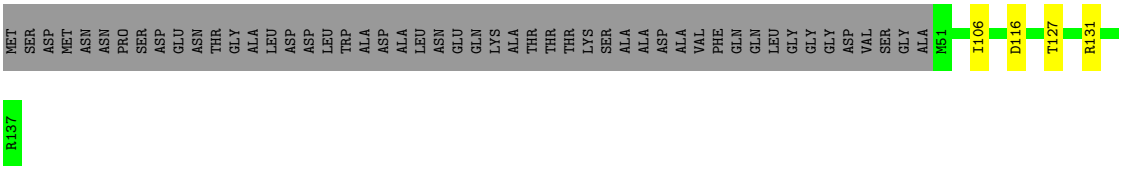
• Molecule 13: Flagellar motor switch protein FliN

Chain Dg: 57% 7% 36%



• Molecule 13: Flagellar motor switch protein FliN

Chain Dh: 61% • 36%

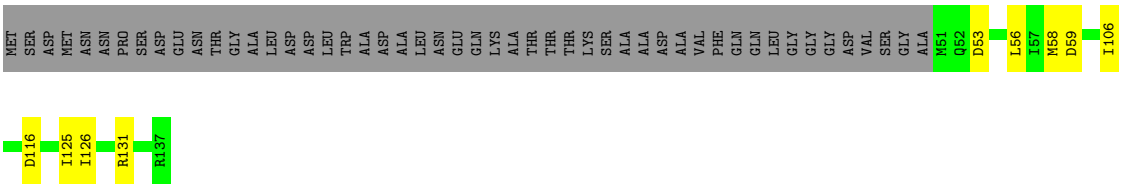


• Molecule 13: Flagellar motor switch protein FliN

Chain Di: 61% • 36%

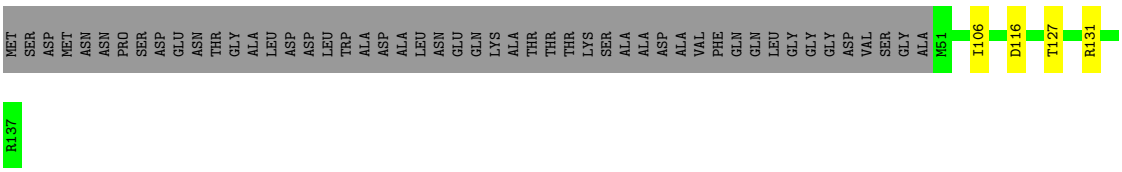
• Molecule 13: Flagellar motor switch protein FliN

Chain Dm: 57% 7% 36%



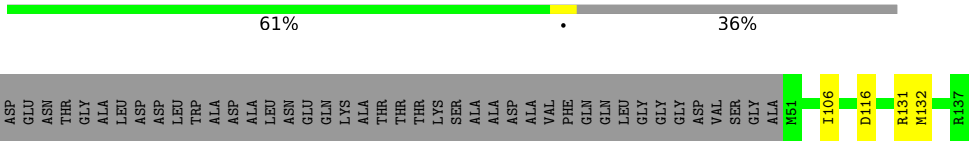
• Molecule 13: Flagellar motor switch protein FliN

Chain Dn: 61% • 36%



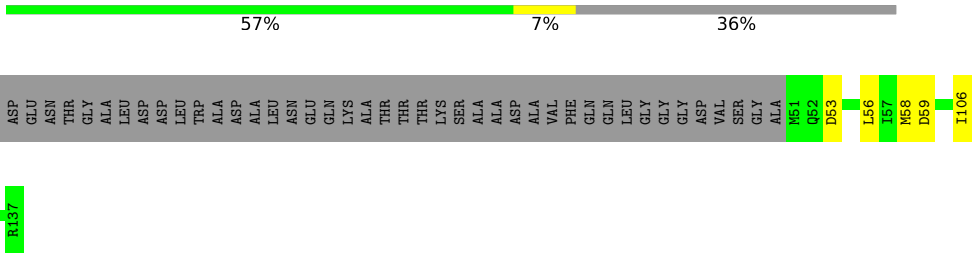
• Molecule 13: Flagellar motor switch protein FliN

Chain Do:



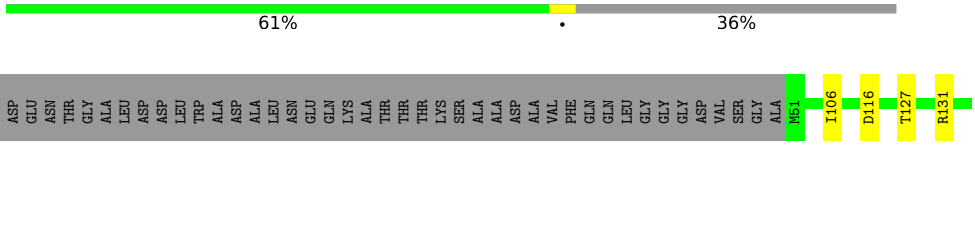
• Molecule 13: Flagellar motor switch protein FliN

Chain Ds:



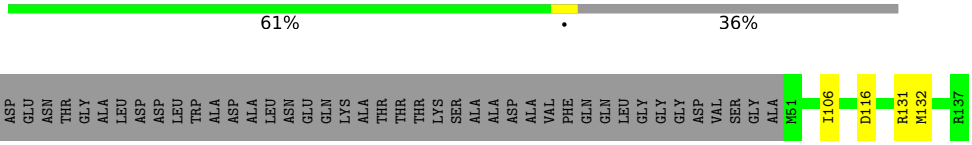
• Molecule 13: Flagellar motor switch protein FliN

Chain Dt:



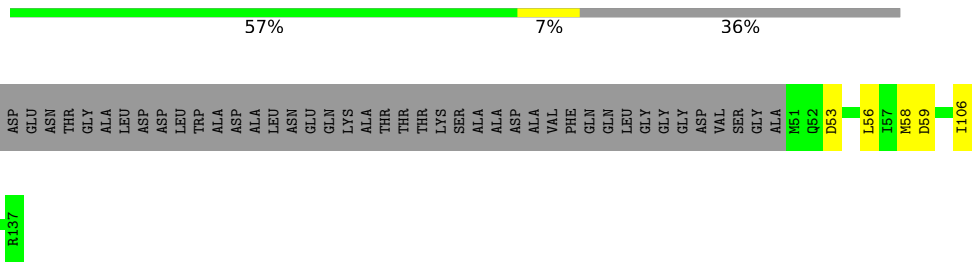
• Molecule 13: Flagellar motor switch protein FliN

Chain Du:



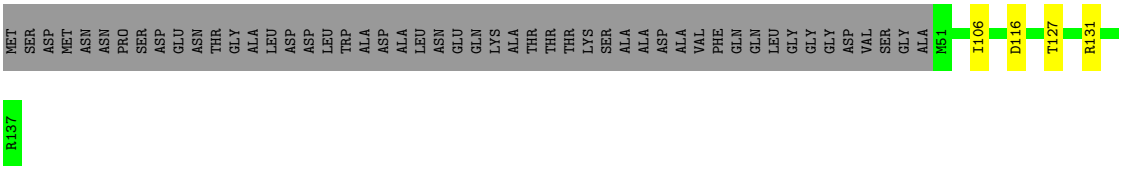
• Molecule 13: Flagellar motor switch protein FliN

Chain Dy:



• Molecule 13: Flagellar motor switch protein FliN

Chain Dz:

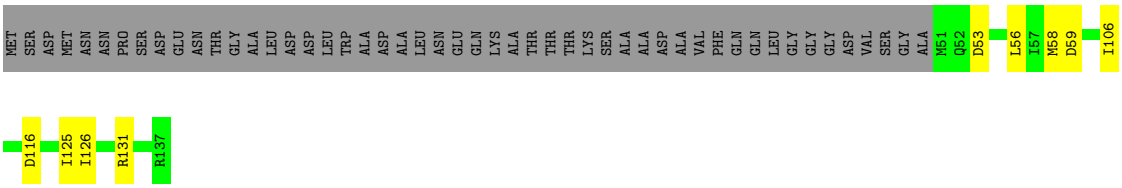


• Molecule 13: Flagellar motor switch protein FliN

Chain D1:

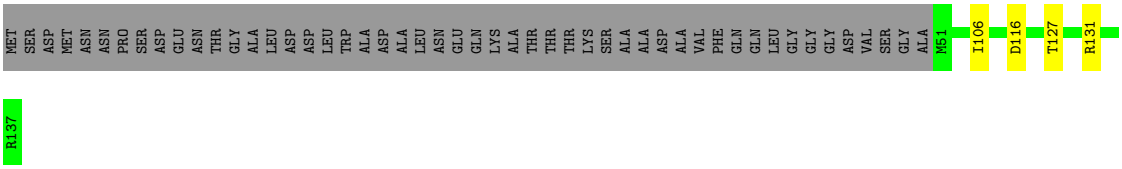
• Molecule 13: Flagellar motor switch protein FliN

Chain D5:



• Molecule 13: Flagellar motor switch protein FliN

Chain D6:

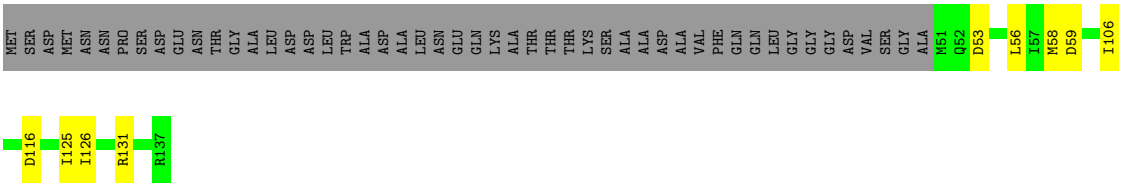


• Molecule 13: Flagellar motor switch protein FliN

Chain D7:

• Molecule 13: Flagellar motor switch protein FliN

Chain EA:



• Molecule 13: Flagellar motor switch protein FliN

• Molecule 13: Flagellar motor switch protein FliN

Chain EB: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

• Molecule 13: Flagellar motor switch protein FliN

Chain B1: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

• Molecule 13: Flagellar motor switch protein FliN

Chain B2: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain B7: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain B8: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

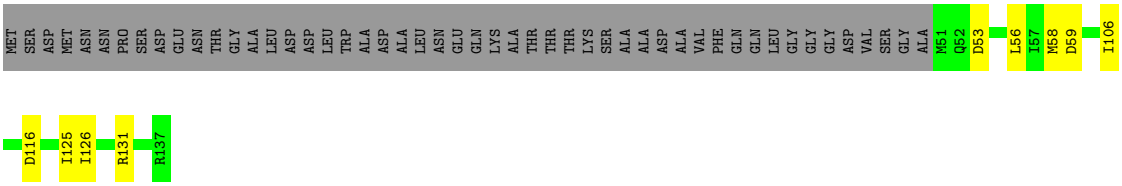
R137

• Molecule 13: Flagellar motor switch protein FliN

Chain B9: 61% • 36%

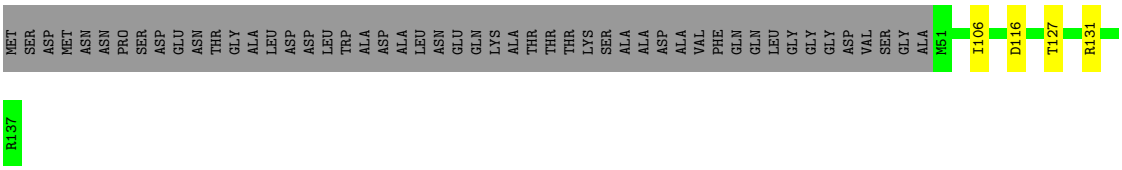
• Molecule 13: Flagellar motor switch protein FliN

Chain EE: 57% 7% 36%



• Molecule 13: Flagellar motor switch protein FliN

Chain EF: 61% • 36%

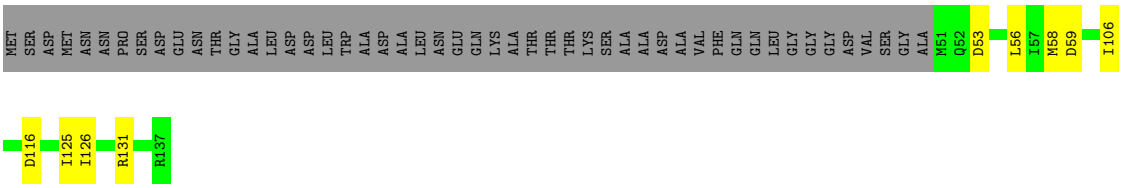


• Molecule 13: Flagellar motor switch protein FliN

Chain EG: 61% • 36%

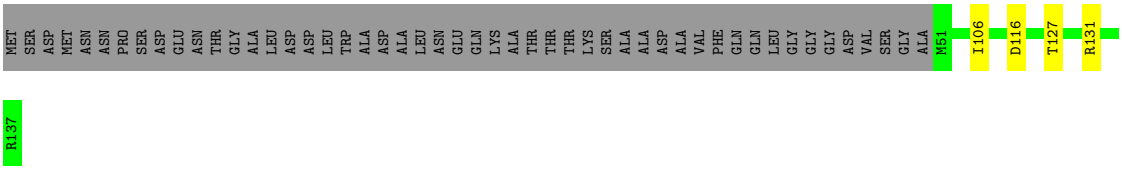
• Molecule 13: Flagellar motor switch protein FliN

Chain EL: 57% 7% 36%



• Molecule 13: Flagellar motor switch protein FliN

Chain EM: 61% • 36%



• Molecule 13: Flagellar motor switch protein FliN

Chain EN: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain ES: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain ET: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

• Molecule 13: Flagellar motor switch protein FliN

Chain EU: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain EZ: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain BY: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

• Molecule 13: Flagellar motor switch protein FliN

Chain BZ: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Be: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Bf: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Bg: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

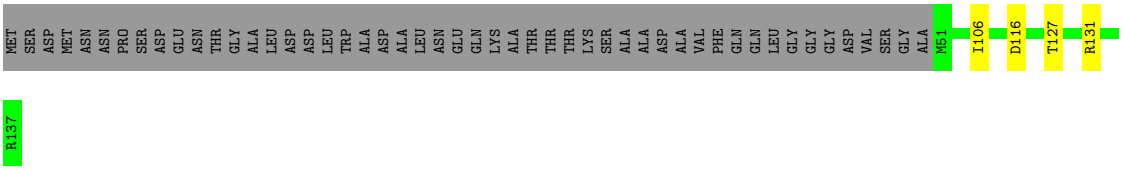
Chain Bl: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Bm: 61% • 36%

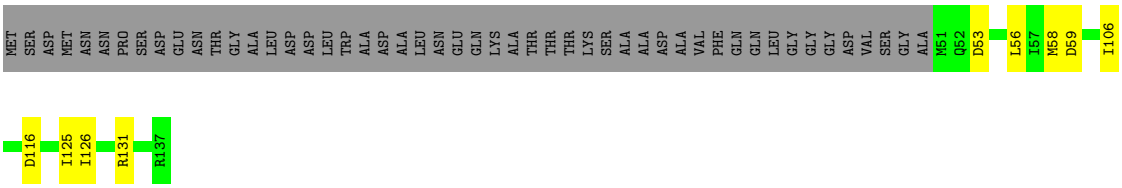


• Molecule 13: Flagellar motor switch protein FliN

Chain Bn:

• Molecule 13: Flagellar motor switch protein FliN

Chain Bs:



• Molecule 13: Flagellar motor switch protein FliN

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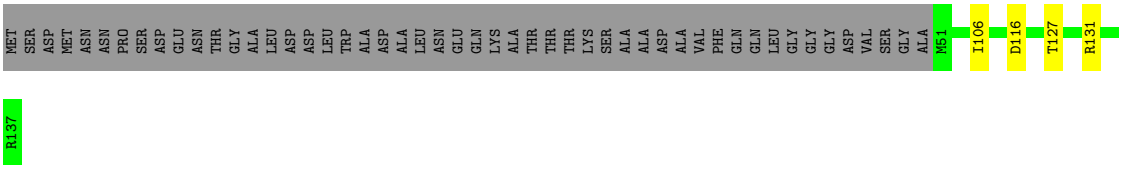
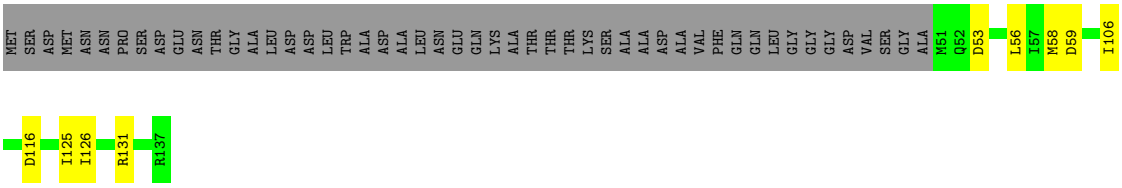


• Molecule 13: Flagellar motor switch protein FliN

Chain Bu:

• Molecule 13: Flagellar motor switch protein FliN

Chain Bz:



• Molecule 13: Flagellar motor switch protein FliN

Chain C1: 57% 7% 36%

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D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain C2: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

• Molecule 13: Flagellar motor switch protein FliN

Chain CD: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain CE: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

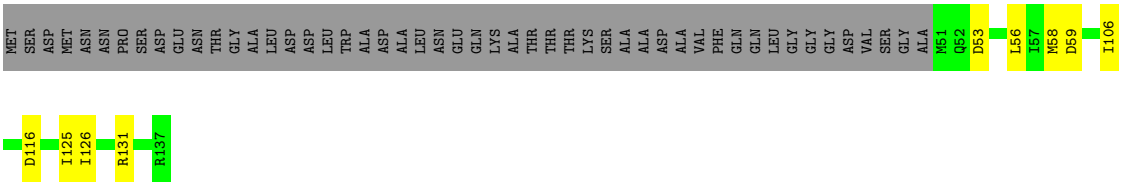
• Molecule 13: Flagellar motor switch protein FliN

Chain CF: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain CK: 57% 7% 36%



• Molecule 13: Flagellar motor switch protein FliN

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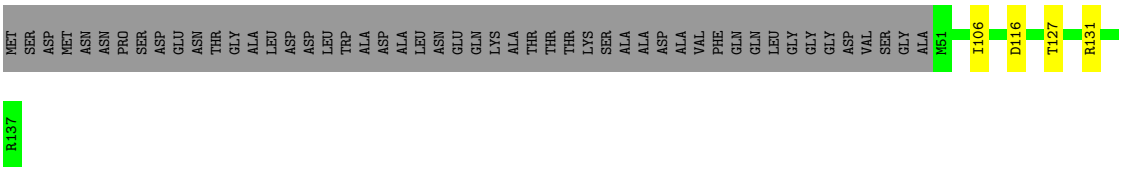
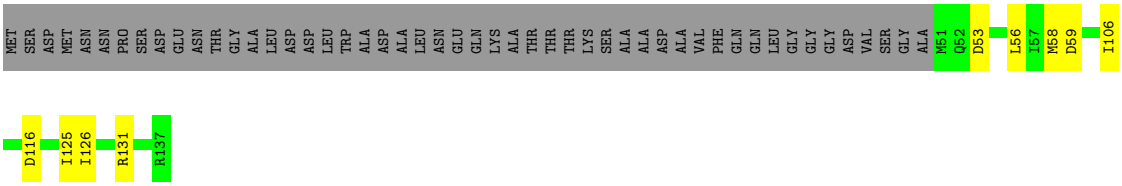


• Molecule 13: Flagellar motor switch protein FliN

Chain CM:

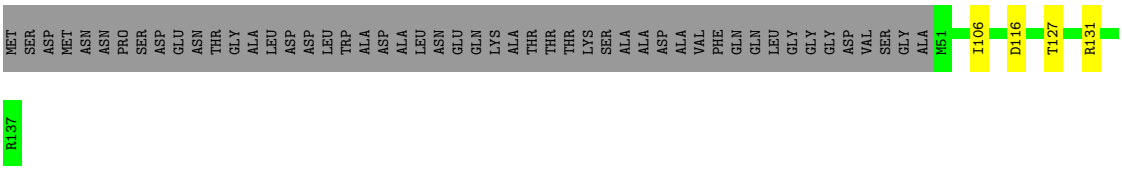
• Molecule 13: Flagellar motor switch protein FliN

Chain CR:



• Molecule 13: Flagellar motor switch protein FliN

Chain CS:



• Molecule 13: Flagellar motor switch protein FliN

Chain CT:

• Molecule 13: Flagellar motor switch protein FliN

Chain CY: 57% 7% 36%

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D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain CZ: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Ca: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 R131 M132 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Cf: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Cg: 61% • 36%

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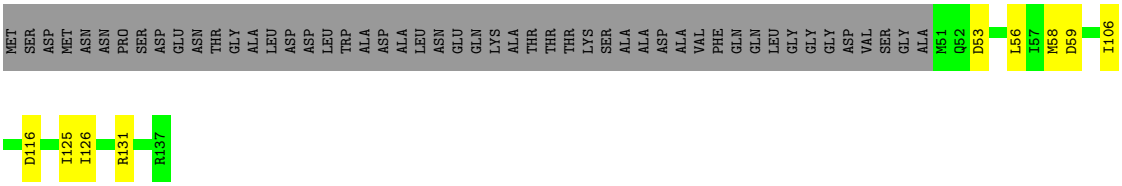
R137

• Molecule 13: Flagellar motor switch protein FliN

Chain Ch: 61% • 36%

• Molecule 13: Flagellar motor switch protein FliN

Chain Cm:



• Molecule 13: Flagellar motor switch protein FliN

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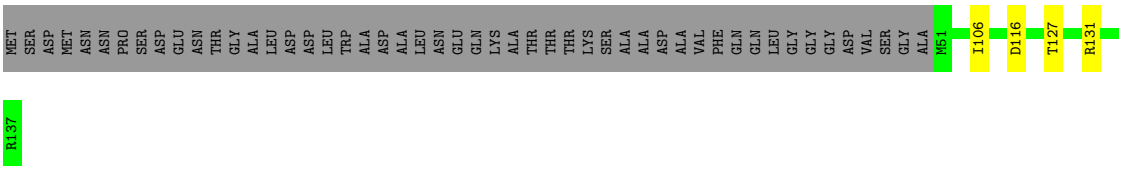
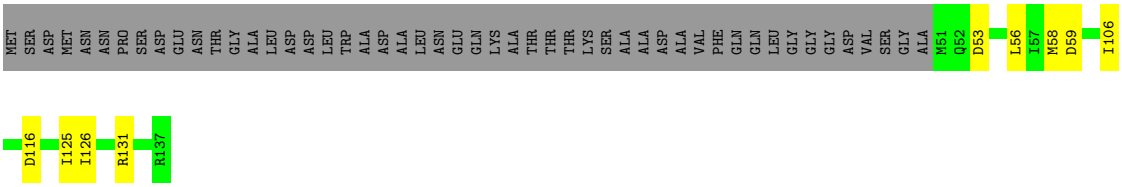


• Molecule 13: Flagellar motor switch protein FliN

Chain Co:

• Molecule 13: Flagellar motor switch protein FliN

Chain Ct:



• Molecule 13: Flagellar motor switch protein FliN

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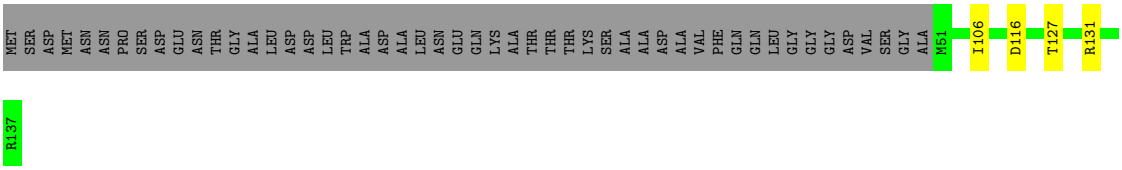

• Molecule 13: Flagellar motor switch protein FliN

Chain Cv: 61% • 36%

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• Molecule 13: Flagellar motor switch protein FliN

Chain FC: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain FD: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain FE: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain FF: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain FG: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain FH: 57% 7% 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 Q52 D53 L56 I57 M58 D59 I106

D116 I125 I126 R131 R137

• Molecule 13: Flagellar motor switch protein FliN

Chain FI: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

• Molecule 13: Flagellar motor switch protein FliN

Chain FJ: 61% • 36%

MET SER ASP MET ASN ASN PRO SER ASP GLU ASN THR GLY ALA LEU ASP ASP LEU TRP ALA ASP ALA LEU ASN GLU GLN LYS ALA THR THR THR LYS SER ALA ALA ASP ALA VAL PHE GLN GLN LEU GLY GLY GLY ASP VAL SER GLY ALA M51 I106 D116 T127 R131

R137

• Molecule 13: Flagellar motor switch protein FliN

Chain FK: 61% • 36%

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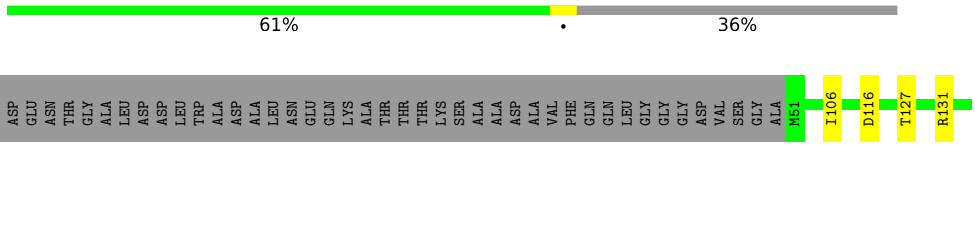
R137

• Molecule 13: Flagellar motor switch protein FliN

Chain FL:



• Molecule 13: Flagellar motor switch protein FliN

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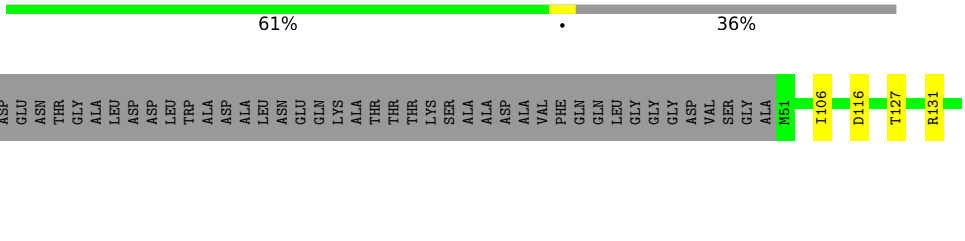

• Molecule 13: Flagellar motor switch protein FliN

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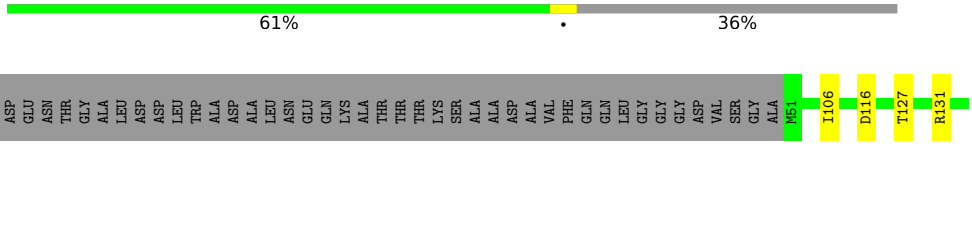
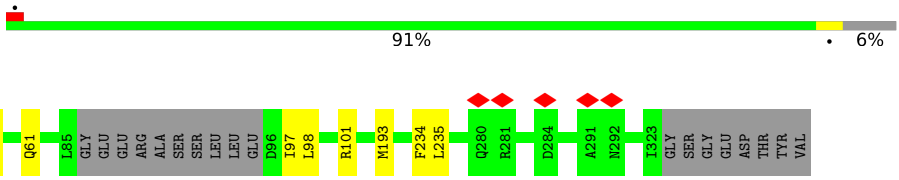


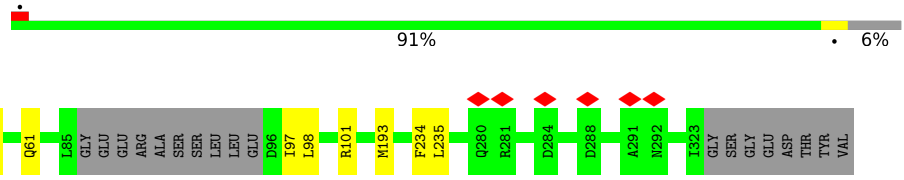
• Molecule 14: Flagellar motor switch protein FliG

Chain C6:



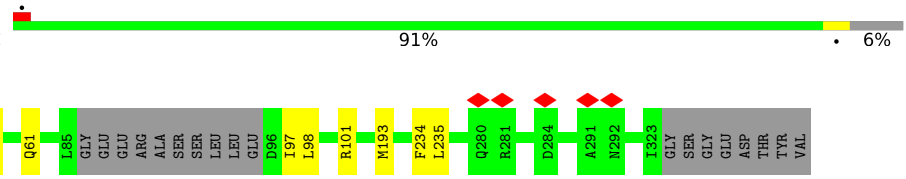
• Molecule 14: Flagellar motor switch protein FliG

Chain DA:



• Molecule 14: Flagellar motor switch protein FliG

Chain DG:



• Molecule 14: Flagellar motor switch protein FliG

Chain DY:

• Molecule 14: Flagellar motor switch protein FliG

Chain De:

• Molecule 14: Flagellar motor switch protein FliG

Chain Dk:

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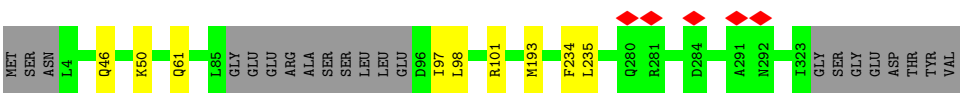
Chain Dq:

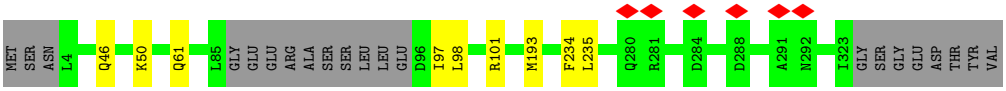


• Molecule 14: Flagellar motor switch protein FliG

Chain Dw:

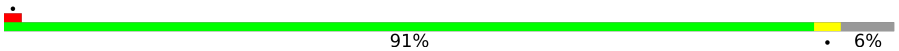
• Molecule 14: Flagellar motor switch protein FliG

Chain D3:



• Molecule 14: Flagellar motor switch protein FliG

Chain D9:

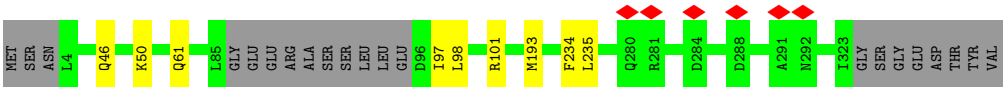


• Molecule 14: Flagellar motor switch protein FliG

Chain B5:

• Molecule 14: Flagellar motor switch protein FliG

Chain EC:

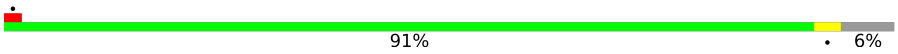


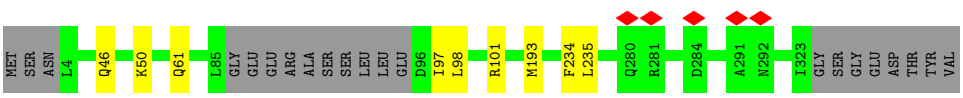
• Molecule 14: Flagellar motor switch protein FliG

Chain EJ:

• Molecule 14: Flagellar motor switch protein FliG

Chain EQ:



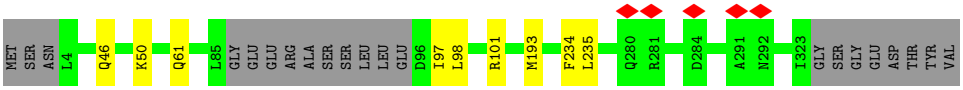


• Molecule 14: Flagellar motor switch protein FliG

Chain EX:

• Molecule 14: Flagellar motor switch protein FliG

Chain Bc:

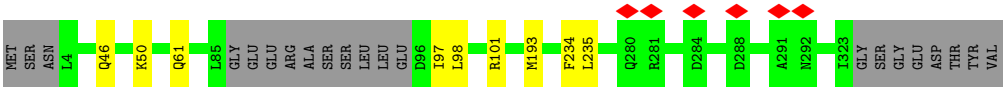


• Molecule 14: Flagellar motor switch protein FliG

Chain Bj:

• Molecule 14: Flagellar motor switch protein FliG

Chain Bq:



• Molecule 14: Flagellar motor switch protein FliG

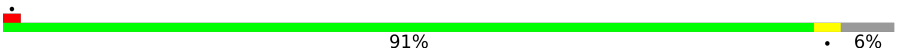
Chain Bx:

• Molecule 14: Flagellar motor switch protein FliG

Chain CB:

• Molecule 14: Flagellar motor switch protein FliG

Chain CI:

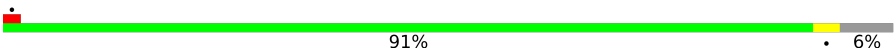


• Molecule 14: Flagellar motor switch protein FliG

Chain CP:

• Molecule 14: Flagellar motor switch protein FliG

Chain CW:



• Molecule 14: Flagellar motor switch protein FliG

Chain Cd:

• Molecule 14: Flagellar motor switch protein FliG

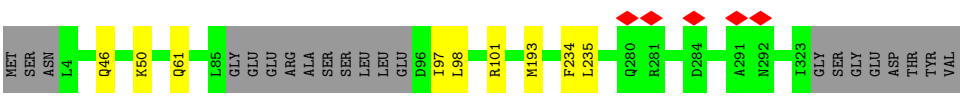
Chain Ck:

• Molecule 14: Flagellar motor switch protein FliG

Chain Cr:

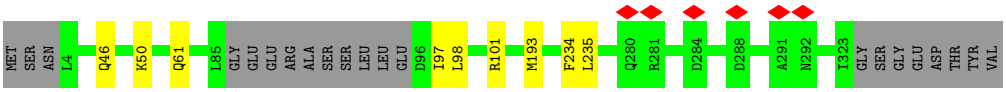
• Molecule 14: Flagellar motor switch protein FliG

Chain Cy:



• Molecule 14: Flagellar motor switch protein FliG

Chain Ex:



• Molecule 14: Flagellar motor switch protein FliG

Chain Ey:

• Molecule 14: Flagellar motor switch protein FliG

Chain Ez:

• Molecule 14: Flagellar motor switch protein FliG

Chain E1:

• Molecule 14: Flagellar motor switch protein FliG

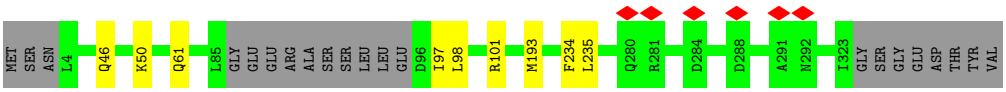
Chain E2:

• Molecule 14: Flagellar motor switch protein FliG

Chain E3:

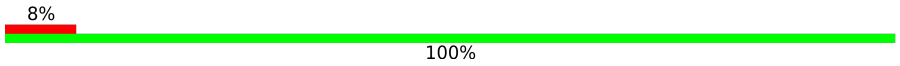
• Molecule 14: Flagellar motor switch protein FliG

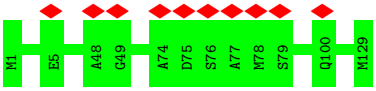
Chain E4:



• Molecule 15: Chemotaxis protein CheY

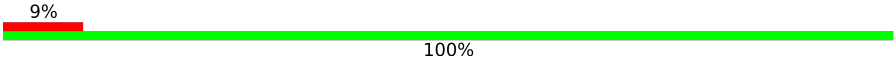
Chain C7:

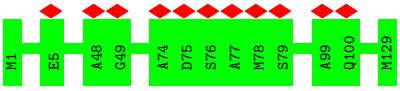




• Molecule 15: Chemotaxis protein CheY

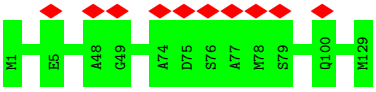
Chain DB:





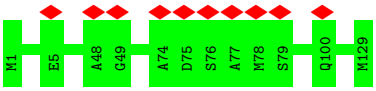
• Molecule 15: Chemotaxis protein CheY

Chain DH: 8% 100%



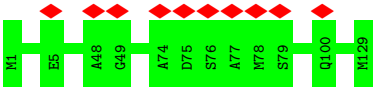
• Molecule 15: Chemotaxis protein CheY

Chain DZ: 8% 100%



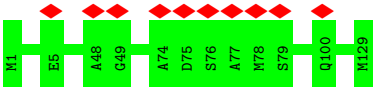
• Molecule 15: Chemotaxis protein CheY

Chain Df: 8% 100%



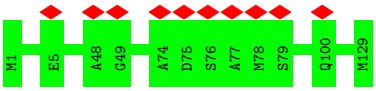
• Molecule 15: Chemotaxis protein CheY

Chain Dl: 8% 100%



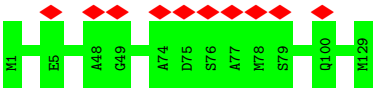
• Molecule 15: Chemotaxis protein CheY

Chain Dr: 8% 100%



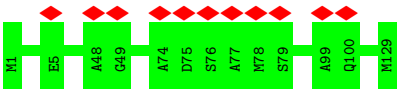
• Molecule 15: Chemotaxis protein CheY

Chain Dx: 8% 100%



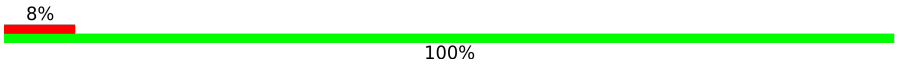
• Molecule 15: Chemotaxis protein CheY

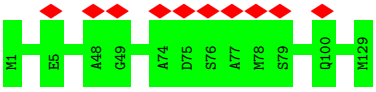
Chain D4: 9% 100%



• Molecule 15: Chemotaxis protein CheY

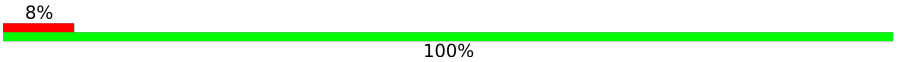
Chain D0:

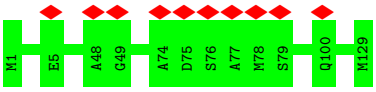




• Molecule 15: Chemotaxis protein CheY

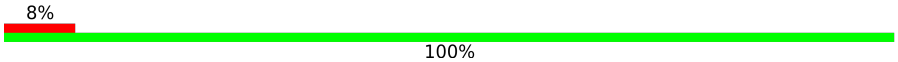
Chain B6:

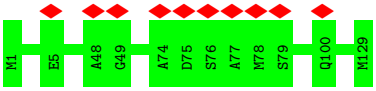




• Molecule 15: Chemotaxis protein CheY

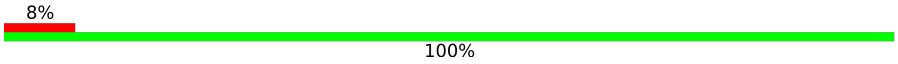
Chain ED:

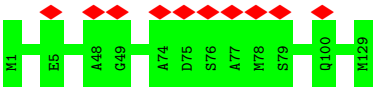




• Molecule 15: Chemotaxis protein CheY

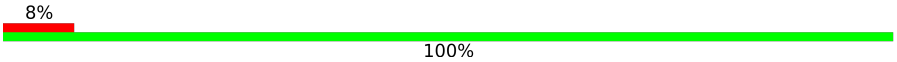
Chain EK:

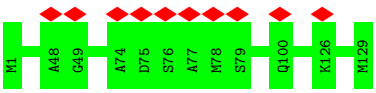




• Molecule 15: Chemotaxis protein CheY

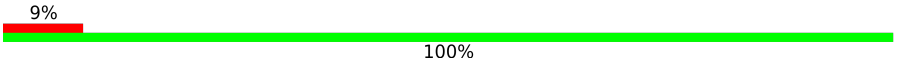
Chain ER:

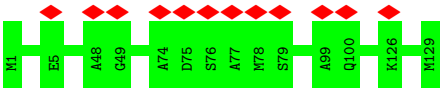




• Molecule 15: Chemotaxis protein CheY

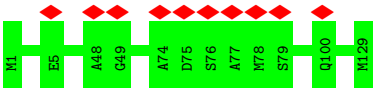
Chain EY:





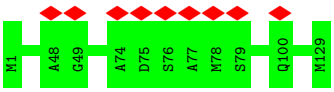
• Molecule 15: Chemotaxis protein CheY

Chain Bd: 8% 100%



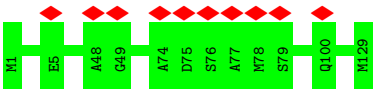
• Molecule 15: Chemotaxis protein CheY

Chain Bk: 7% 100%



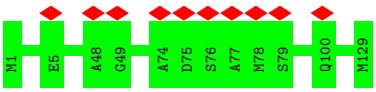
• Molecule 15: Chemotaxis protein CheY

Chain Br: 8% 100%



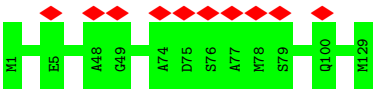
• Molecule 15: Chemotaxis protein CheY

Chain By: 8% 100%



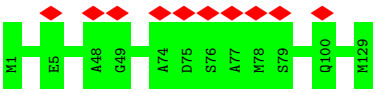
• Molecule 15: Chemotaxis protein CheY

Chain CC: 8% 100%



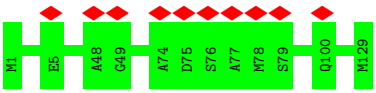
• Molecule 15: Chemotaxis protein CheY

Chain CJ: 8% 100%



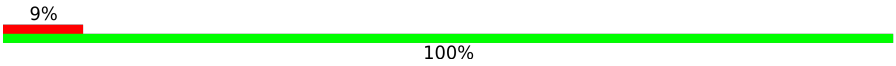
• Molecule 15: Chemotaxis protein CheY

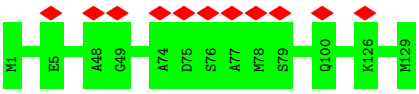
Chain CQ: 8% 100%



• Molecule 15: Chemotaxis protein CheY

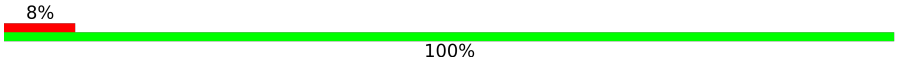
Chain CX:

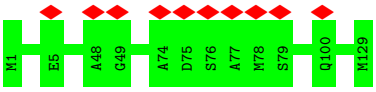




• Molecule 15: Chemotaxis protein CheY

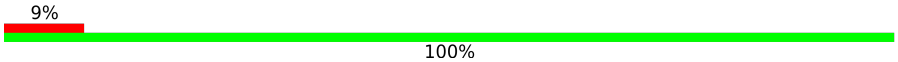
Chain Ce:

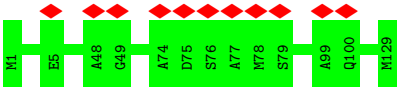




• Molecule 15: Chemotaxis protein CheY

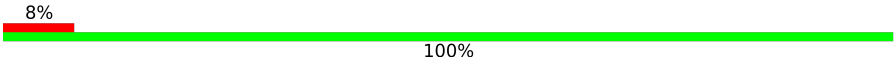
Chain Cl:

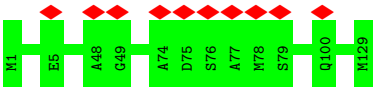




• Molecule 15: Chemotaxis protein CheY

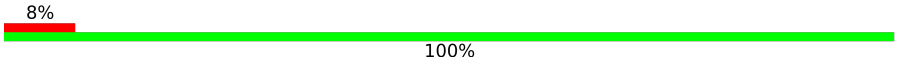
Chain Cs:

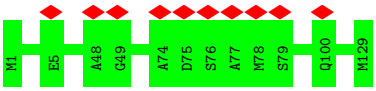




• Molecule 15: Chemotaxis protein CheY

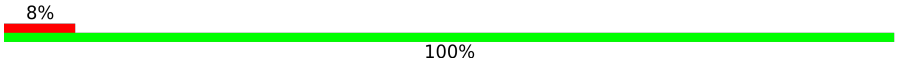
Chain Cz:

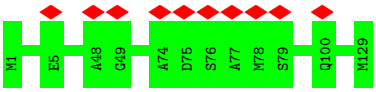




• Molecule 15: Chemotaxis protein CheY

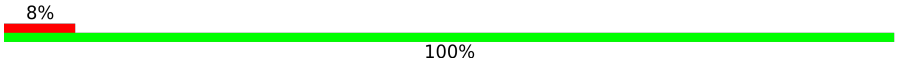
Chain E6:

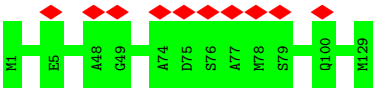




• Molecule 15: Chemotaxis protein CheY

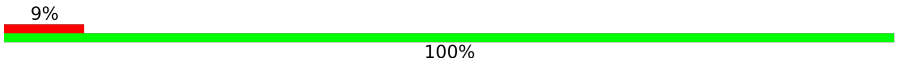
Chain E7:

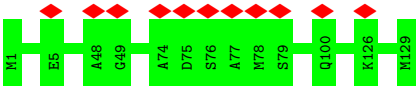




• Molecule 15: Chemotaxis protein CheY

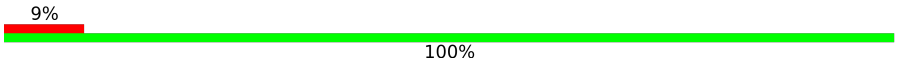
Chain E8:

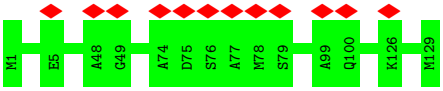




• Molecule 15: Chemotaxis protein CheY

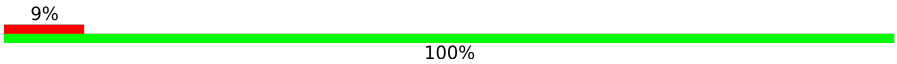
Chain E9:

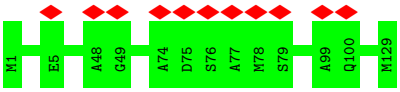




• Molecule 15: Chemotaxis protein CheY

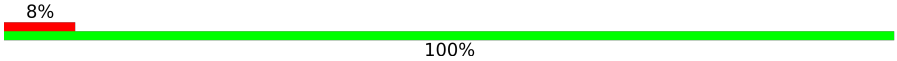
Chain E0:

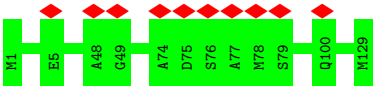




• Molecule 15: Chemotaxis protein CheY

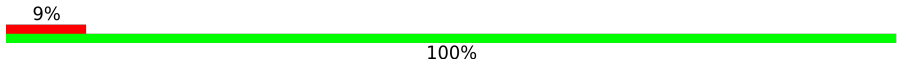
Chain FA:

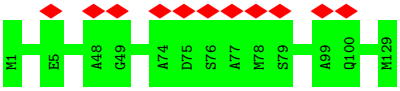




• Molecule 15: Chemotaxis protein CheY

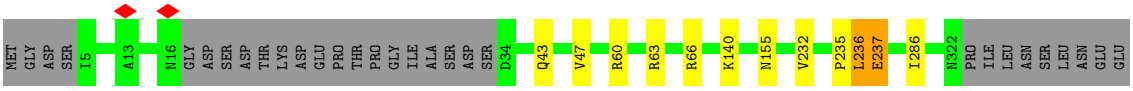
Chain FB:

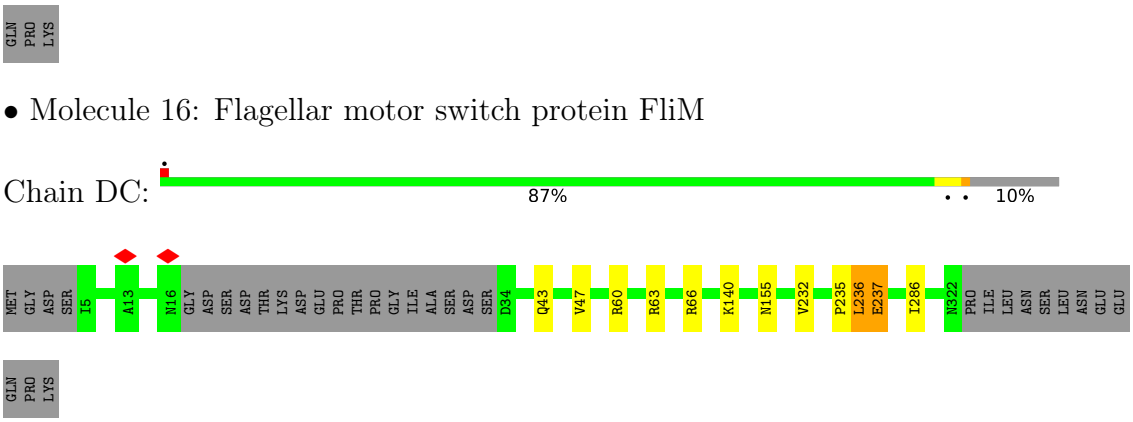




• Molecule 16: Flagellar motor switch protein FliM

Chain C0:




GLN PRO LYS
• Molecule 16: Flagellar motor switch protein FliM
Chain DC:
87%
10%
MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU
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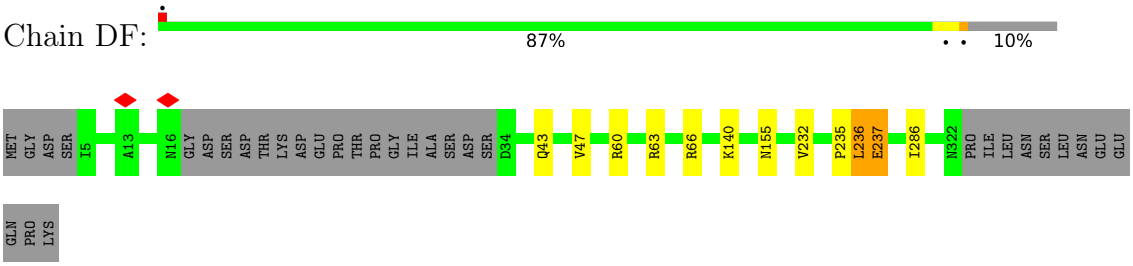
• Molecule 16: Flagellar motor switch protein FliM
Chain DF:
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10%
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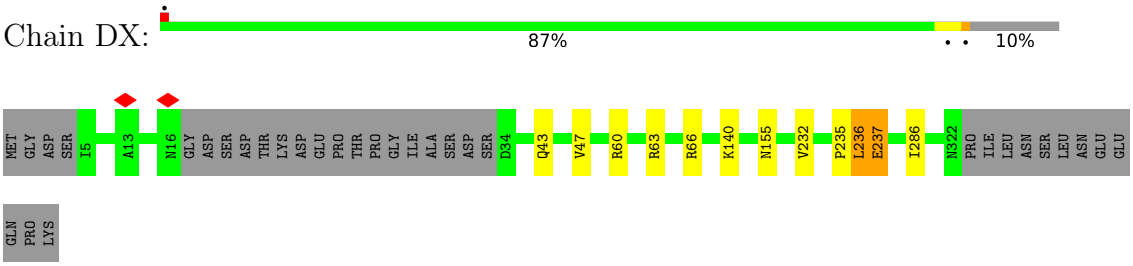
• Molecule 16: Flagellar motor switch protein FliM
Chain DX:
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10%
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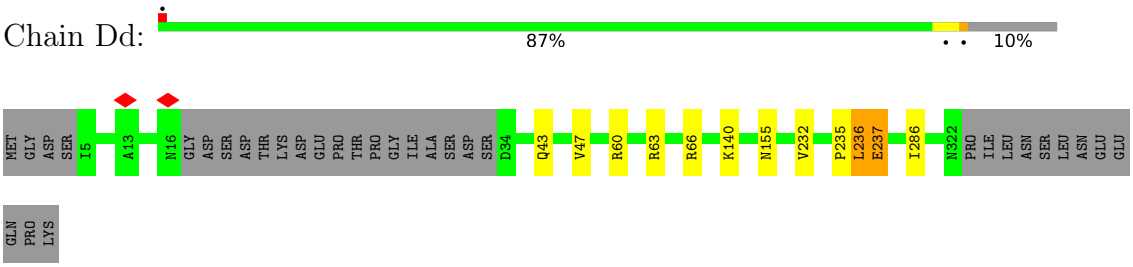
• Molecule 16: Flagellar motor switch protein FliM
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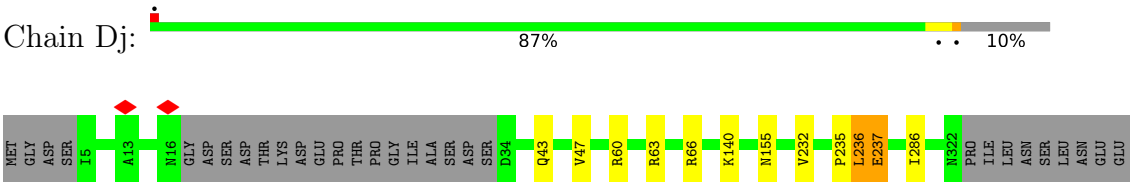
• Molecule 16: Flagellar motor switch protein FliM
Chain Dj:
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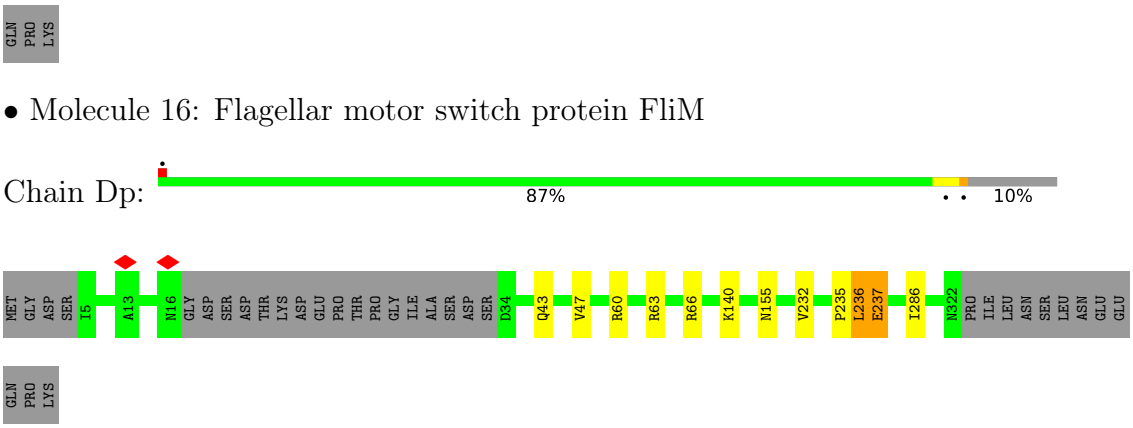
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• Molecule 16: Flagellar motor switch protein FliM
Chain Dp:
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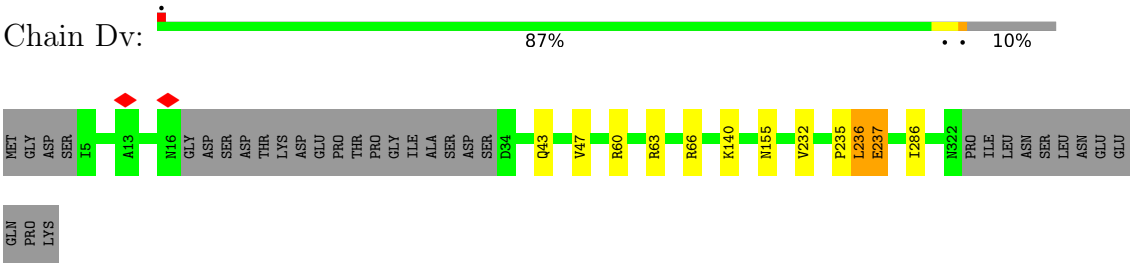
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Chain Dv:
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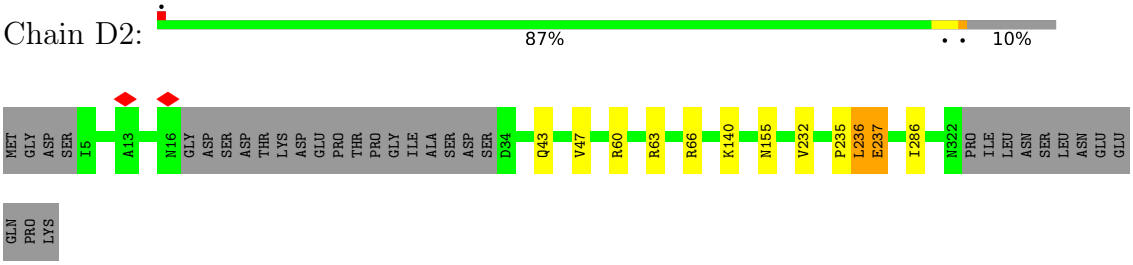
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Chain D2:
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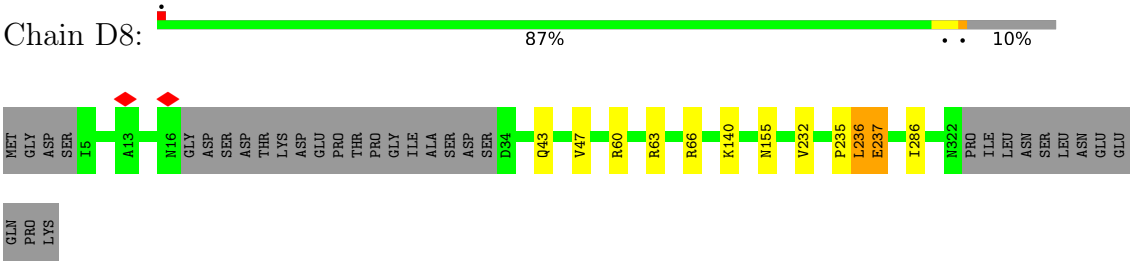
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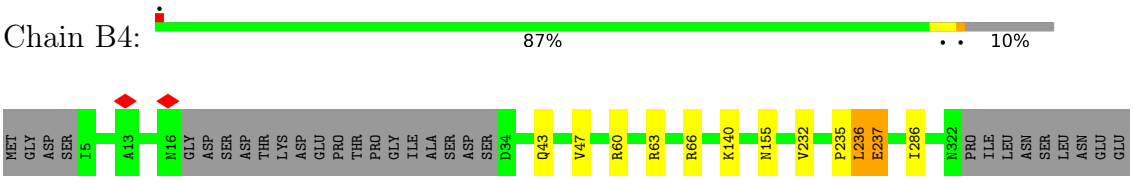
• Molecule 16: Flagellar motor switch protein FliM
Chain B4:
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10%
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GLN PRO LYS

• Molecule 16: Flagellar motor switch protein FliM

Chain EI:

MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU

GLN PRO LYS

• Molecule 16: Flagellar motor switch protein FliM

Chain EP:

MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU

GLN PRO LYS

• Molecule 16: Flagellar motor switch protein FliM

Chain EW:

MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU

GLN PRO LYS

• Molecule 16: Flagellar motor switch protein FliM

Chain Bb:

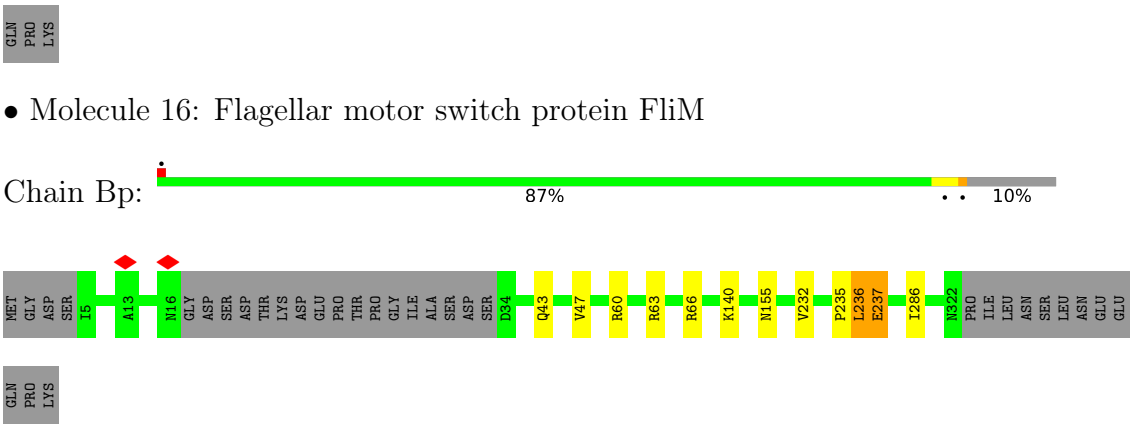
MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU

GLN PRO LYS

• Molecule 16: Flagellar motor switch protein FliM

Chain Bi:

MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU


GLN PRO LYS
• Molecule 16: Flagellar motor switch protein FliM
Chain Bp:
87%
10%
MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU
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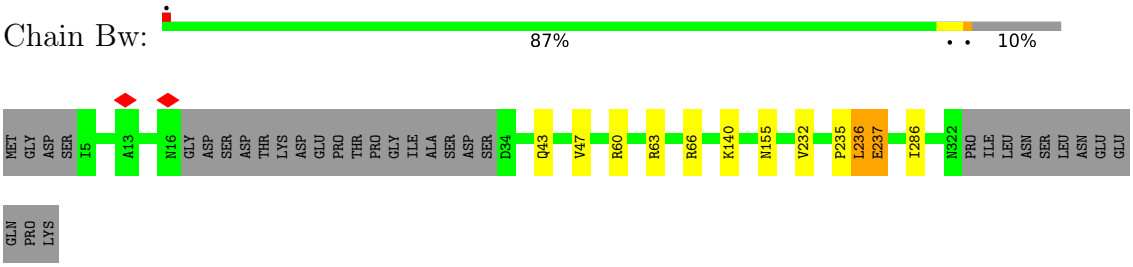
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Chain Bw:
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10%
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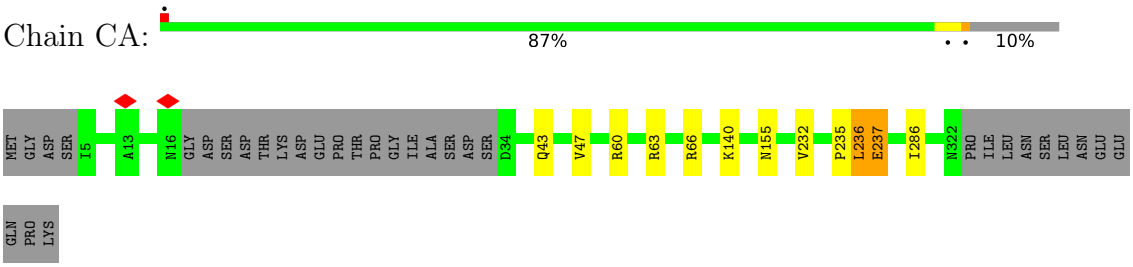
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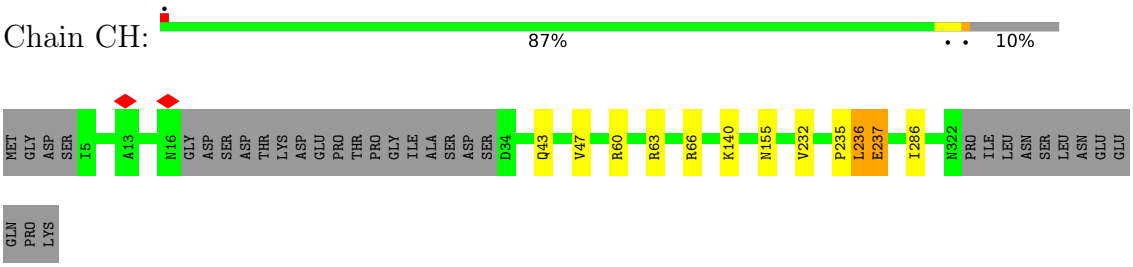
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Chain CH:
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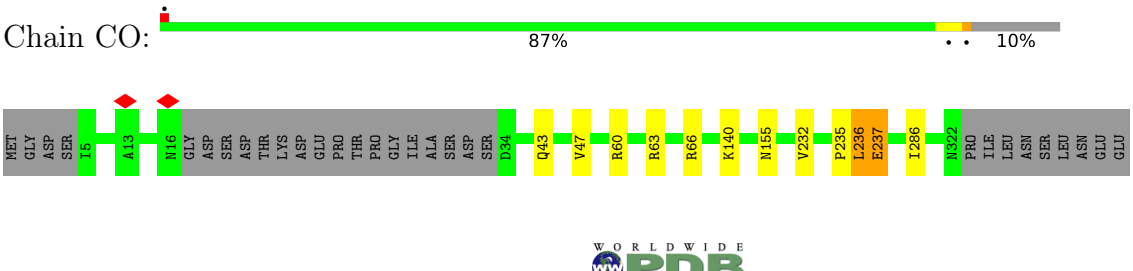
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Chain CO:
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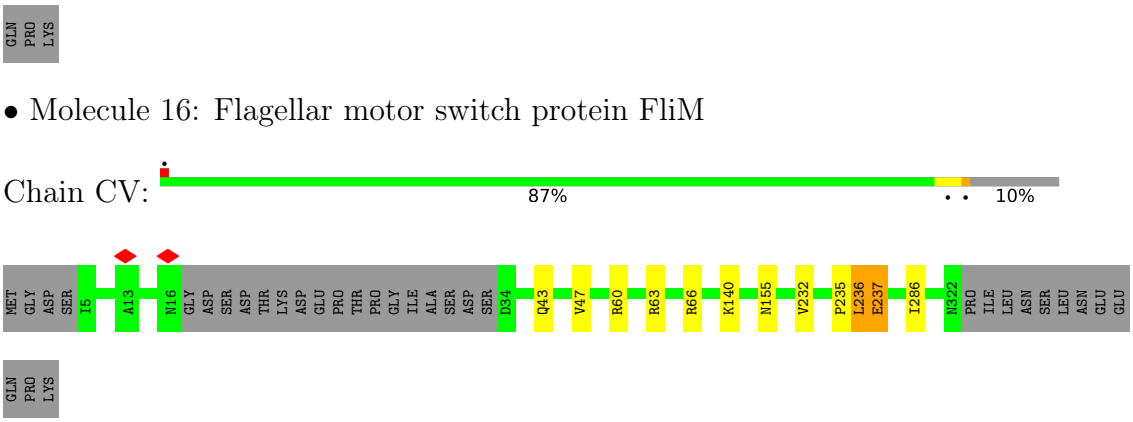
GLN PRO LYS
• Molecule 16: Flagellar motor switch protein FliM
Chain CV:
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10%
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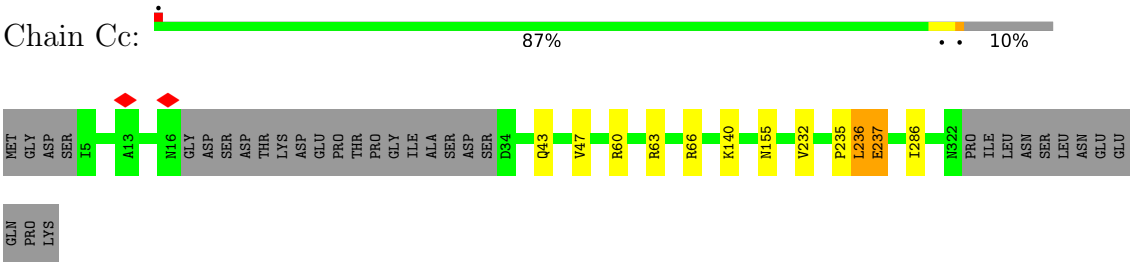
GLN PRO LYS


• Molecule 16: Flagellar motor switch protein FliM
Chain Cc:
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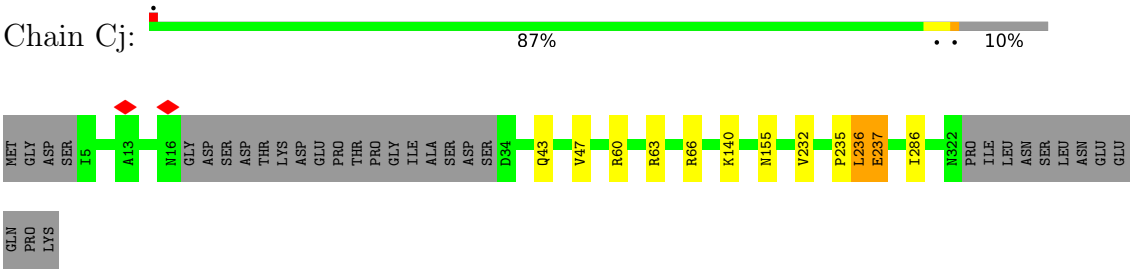
• Molecule 16: Flagellar motor switch protein FliM
Chain Cj:
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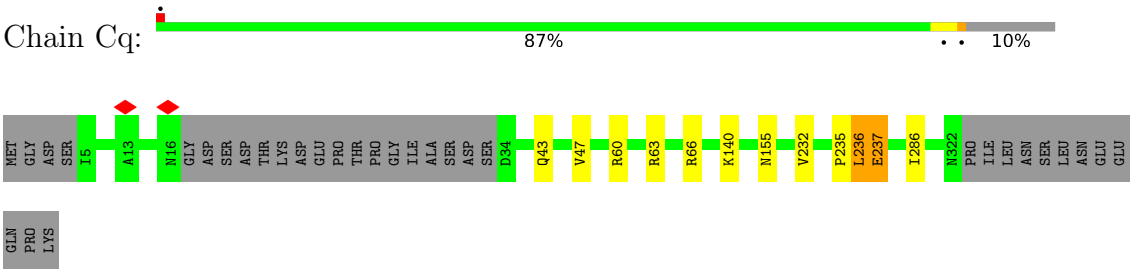
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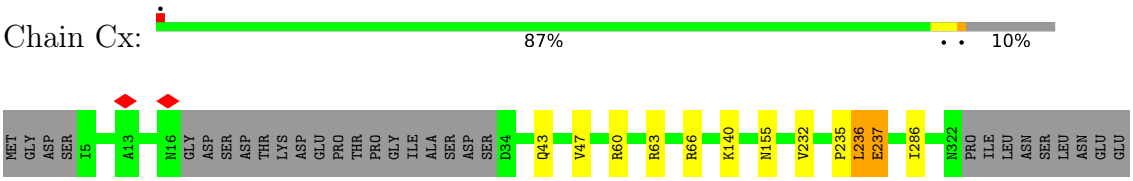
MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU
GLN PRO LYS


• Molecule 16: Flagellar motor switch protein FliM
Chain Cx:
87%
10%
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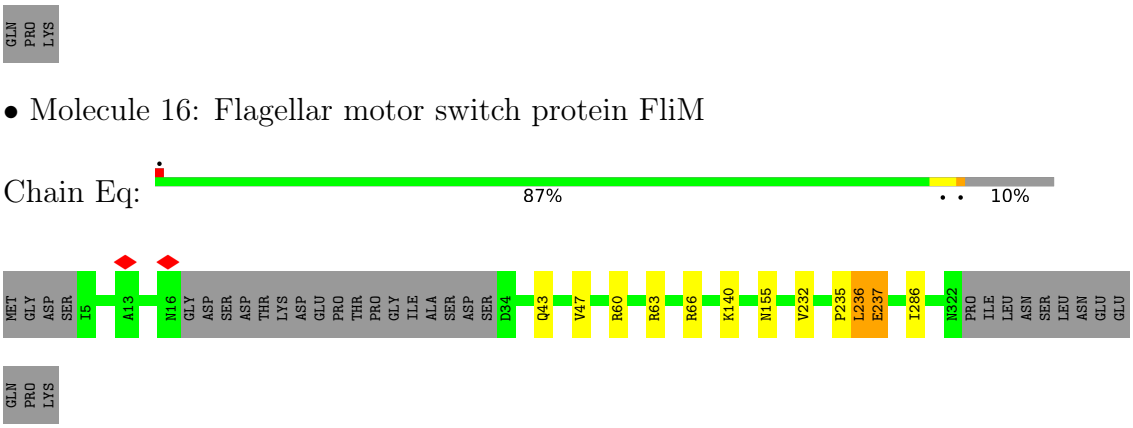
GLN PRO LYS
• Molecule 16: Flagellar motor switch protein FliM
Chain Eq:
87%
10%
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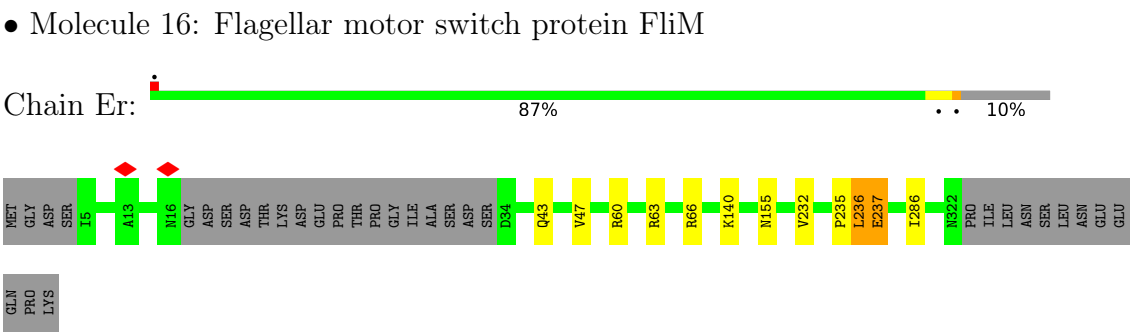
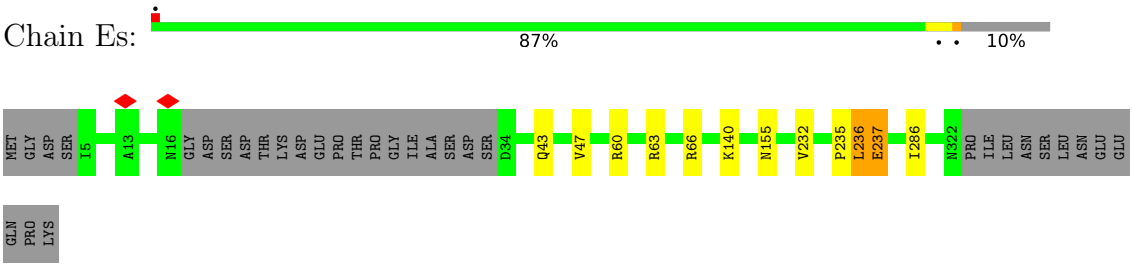
GLN PRO LYS


• Molecule 16: Flagellar motor switch protein FliM
Chain Er:
87%
10%
MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU
GLN PRO LYS


• Molecule 16: Flagellar motor switch protein FliM
Chain Es:
87%
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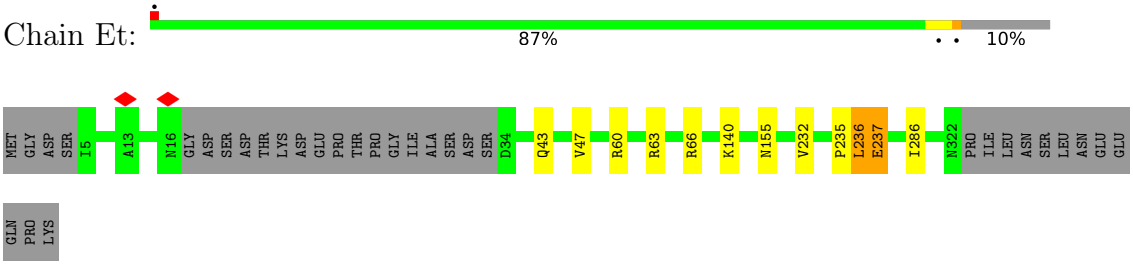
GLN PRO LYS


• Molecule 16: Flagellar motor switch protein FliM
Chain Et:
87%
10%
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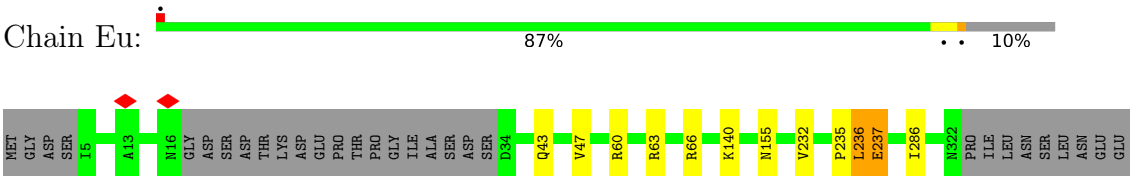
GLN PRO LYS


• Molecule 16: Flagellar motor switch protein FliM
Chain Eu:
87%
10%
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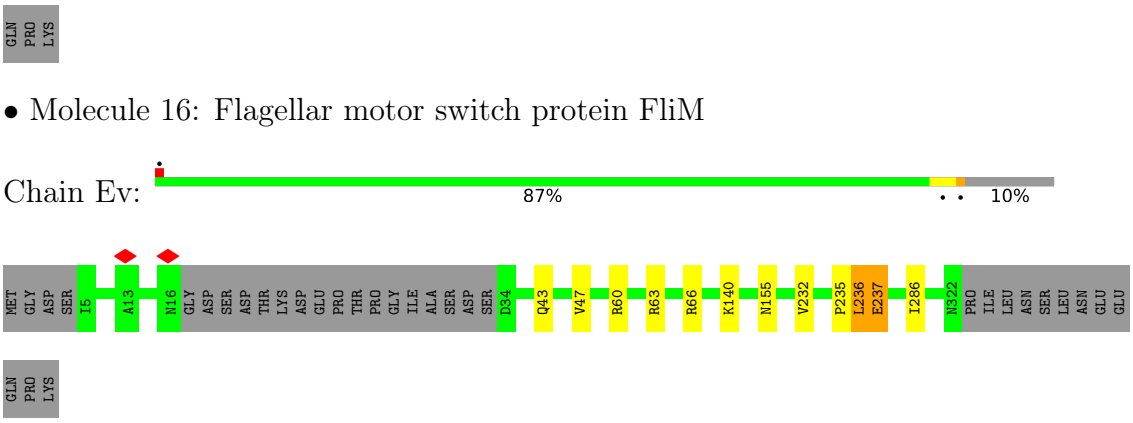
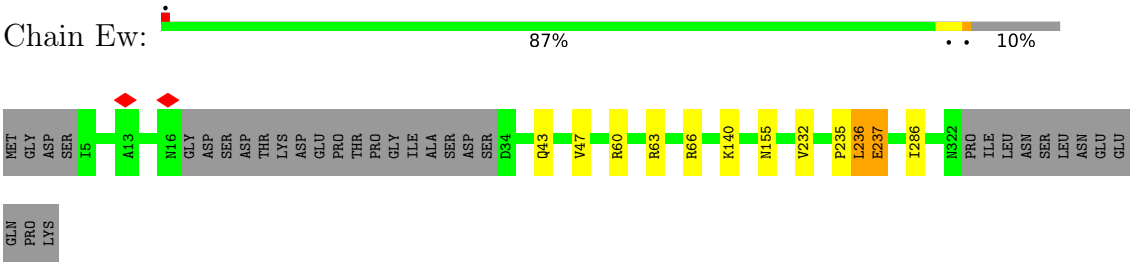

GLN PRO LYS
• Molecule 16: Flagellar motor switch protein FliM
Chain Ev:
87%
10%
MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU
GLN PRO LYS


• Molecule 16: Flagellar motor switch protein FliM
Chain Ew:
87%
10%
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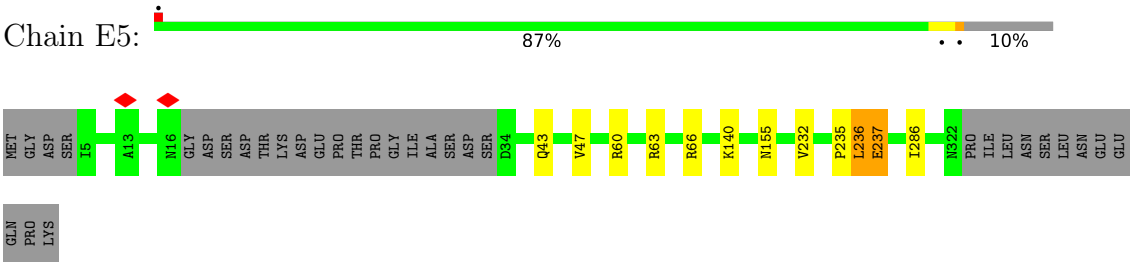
GLN PRO LYS


• Molecule 16: Flagellar motor switch protein FliM
Chain E5:
87%
10%
MET GLY ASP SER I5 A13 N16 GLY ASP SER ASP THR LYS ASP GLU PRO THR PRO GLY ILE ALA SER ASP SER D34 Q43 V47 R60 R63 R66 K140 N155 V232 P235 L236 E237 I286 N322 PRO ILE LEU ASN SER LEU ASN GLU GLU
GLN PRO LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	26921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.415	Depositor
Minimum map value	-0.224	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	1008.00006, 1008.00006, 1008.00006	wwPDB
Map dimensions	840, 840, 840	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.30	0/1888	0.52	1/2564 (0.0%)
1	1	0.31	0/1917	0.50	0/2605
1	2	0.27	0/1973	0.48	0/2682
1	3	0.28	0/1973	0.50	0/2682
1	4	0.28	0/1973	0.50	0/2682
1	5	0.32	0/1973	0.52	0/2682
1	6	0.31	0/1973	0.52	0/2682
1	7	0.28	0/1973	0.51	0/2682
1	8	0.30	0/1973	0.52	0/2682
1	9	0.29	0/1973	0.54	1/2682 (0.0%)
1	AF	0.33	0/1926	0.53	0/2618
1	AG	0.36	0/1934	0.56	0/2629
1	AH	0.33	0/1942	0.55	0/2639
1	AI	0.33	0/1926	0.57	1/2618 (0.0%)
1	AJ	0.30	0/1934	0.51	0/2629
1	AK	0.32	0/1844	0.51	0/2505
1	AL	0.31	0/1888	0.51	0/2564
1	AM	0.30	0/1888	0.54	1/2564 (0.0%)
1	AN	0.30	0/1888	0.51	0/2564
1	ZA	0.29	0/1973	0.52	0/2682
1	ZB	0.29	0/1973	0.49	0/2682
1	ZC	0.28	0/1973	0.51	0/2682
1	ZD	0.28	0/1973	0.51	0/2682
1	ZE	0.28	0/1973	0.50	1/2682 (0.0%)
2	A	0.27	0/1613	0.51	0/2194
2	B	0.27	0/1613	0.51	0/2194
2	C	0.27	0/1613	0.51	0/2194
2	D	0.27	0/1613	0.51	0/2194
2	E	0.27	0/1613	0.51	0/2194
2	F	0.27	0/1613	0.51	0/2194
2	G	0.27	0/1613	0.51	0/2194
2	H	0.27	0/1613	0.51	0/2194
2	I	0.27	0/1613	0.51	0/2194
2	J	0.27	0/1613	0.51	0/2194

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	K	0.27	0/1613	0.51	0/2194
2	L	0.27	0/1613	0.51	0/2194
2	M	0.27	0/1613	0.51	0/2194
2	N	0.27	0/1613	0.51	0/2194
2	O	0.27	0/1613	0.51	0/2194
2	P	0.27	0/1613	0.51	0/2194
2	Q	0.27	0/1613	0.51	0/2194
2	R	0.27	0/1613	0.51	0/2194
2	S	0.27	0/1613	0.51	0/2194
2	T	0.27	0/1613	0.51	0/2194
2	U	0.27	0/1613	0.51	0/2194
2	V	0.27	0/1613	0.51	0/2194
2	W	0.27	0/1613	0.51	0/2194
2	X	0.27	0/1613	0.51	0/2194
2	Y	0.27	0/1613	0.51	0/2194
2	Z	0.27	0/1613	0.51	0/2194
3	A0	0.34	0/959	0.50	0/1293
3	A6	0.36	0/1042	0.55	0/1408
3	A7	0.33	0/951	0.50	0/1282
3	A8	0.35	0/976	0.57	0/1316
3	A9	0.34	0/991	0.54	0/1335
4	A1	0.36	0/675	0.49	0/905
4	A2	0.37	0/689	0.52	0/925
4	A3	0.36	0/689	0.51	0/925
4	A4	0.37	0/689	0.53	0/925
4	A5	0.37	0/682	0.51	0/915
4	Az	0.42	0/428	0.53	0/572
5	AA	0.33	0/1828	0.56	0/2492
5	AB	0.29	0/1836	0.54	1/2502 (0.0%)
5	AC	0.28	0/1844	0.54	0/2512
5	AD	0.27	0/1844	0.53	0/2512
5	AE	0.31	0/1836	0.55	0/2502
6	AO	0.27	0/1289	0.53	0/1741
6	AP	0.27	0/1289	0.53	0/1741
6	AQ	0.27	0/1289	0.53	0/1741
6	AR	0.27	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
6	AY	0.27	0/1289	0.53	0/1741

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
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	0.27	0/1289	0.53	0/1741
6	Al	0.27	0/1289	0.53	0/1741
6	Am	0.27	0/1289	0.53	0/1741
6	An	0.27	0/1289	0.53	0/1741
6	Ao	0.27	0/1289	0.53	0/1741
6	Ap	0.26	0/1289	0.53	0/1741
6	B0	0.22	0/226	0.50	0/303
6	B3	0.22	0/226	0.48	0/303
6	BG	0.52	0/83	0.63	0/114
6	BH	0.27	0/107	0.38	0/148
6	BI	0.30	0/137	0.49	0/191
6	BJ	0.28	0/107	0.56	0/148
6	BK	1.36	1/145 (0.7%)	1.49	3/203 (1.5%)
6	BL	0.33	0/107	0.51	0/148
6	BM	0.26	0/145	0.44	0/203
6	BN	0.30	0/107	0.38	0/148
6	BO	0.30	0/137	0.57	0/191
6	BP	0.30	0/107	0.37	0/148
6	BQ	0.29	0/145	0.45	0/203
6	BR	0.27	0/1289	0.52	0/1741
6	BS	0.27	0/1289	0.53	0/1741
6	BT	0.27	0/1289	0.53	0/1741
6	BU	0.27	0/1289	0.53	0/1741
6	BV	0.27	0/1289	0.53	0/1741
6	BW	0.26	0/1289	0.53	0/1741
6	BX	0.27	0/1289	0.53	0/1741
6	Ba	0.22	0/226	0.49	0/303
6	Bh	0.22	0/226	0.49	0/303
6	Bo	0.22	0/226	0.49	0/303
6	Bv	0.22	0/226	0.49	0/303
6	CG	0.22	0/226	0.49	0/303
6	CN	0.22	0/226	0.49	0/303
6	CU	0.22	0/226	0.49	0/303

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	Cb	0.22	0/226	0.49	0/303
6	Ci	0.22	0/226	0.49	0/303
6	Cp	0.22	0/226	0.49	0/303
6	Cw	0.22	0/226	0.49	0/303
6	DE	0.22	0/226	0.49	0/303
6	DL	0.22	0/226	0.49	0/303
6	EH	0.22	0/226	0.49	0/303
6	EO	0.22	0/226	0.49	0/303
6	EV	0.22	0/226	0.49	0/303
6	Ea	0.22	0/226	0.49	0/303
6	Eb	0.22	0/226	0.48	0/303
6	Ec	0.22	0/226	0.49	0/303
6	Ed	0.22	0/226	0.49	0/303
6	Ee	0.23	0/226	0.49	0/303
6	Ef	0.22	0/226	0.48	0/303
6	Eg	0.22	0/226	0.49	0/303
6	Eh	0.22	0/226	0.49	0/303
6	Ei	0.22	0/226	0.49	0/303
6	Ej	0.22	0/226	0.50	0/303
6	Ek	0.22	0/226	0.49	0/303
6	El	0.22	0/226	0.49	0/303
6	Em	0.22	0/226	0.48	0/303
6	En	0.22	0/226	0.49	0/303
6	Eo	0.22	0/226	0.49	0/303
6	Ep	0.22	0/226	0.49	0/303
6	UI	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UJ	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UK	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UL	0.82	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UM	0.84	3/1191 (0.3%)	0.82	4/1618 (0.2%)
6	UN	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UO	0.83	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	UP	0.84	2/1191 (0.2%)	0.82	4/1618 (0.2%)
6	WA	0.61	0/863	0.72	1/1172 (0.1%)
6	WB	0.59	0/850	0.69	0/1154
6	WC	0.59	0/825	0.68	0/1121
6	WD	0.61	0/841	0.68	0/1142
6	WE	0.60	0/857	0.71	0/1164
6	WF	0.60	0/848	0.69	0/1152
6	WG	0.60	0/857	0.68	0/1164
6	WH	0.60	0/714	0.69	0/973
6	WI	0.60	0/714	0.74	0/973
6	WJ	0.61	0/749	0.72	1/1020 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
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	0.70	0/1152
6	WU	0.60	0/857	0.67	0/1164
6	WV	0.61	0/841	0.69	0/1142
6	WW	0.60	0/848	0.70	0/1152
7	Ab	0.29	0/681	0.47	0/930
7	Aq	0.26	0/681	0.49	0/930
7	Ar	0.28	0/681	0.48	0/930
7	As	0.29	0/681	0.49	0/930
8	At	0.38	1/1994 (0.1%)	0.55	1/2724 (0.0%)
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	0.29	0/1652	0.48	0/2249
9	Ax	0.28	0/1652	0.46	0/2249
9	Ay	0.31	0/1662	0.49	0/2263
10	BA	0.28	0/981	0.44	0/1334
10	BB	0.26	0/976	0.46	0/1327
10	BC	0.57	2/981 (0.2%)	0.95	3/1334 (0.2%)
10	BD	0.28	0/981	0.52	1/1334 (0.1%)
10	BE	0.26	0/981	0.47	0/1334
10	BF	0.28	0/981	0.47	0/1334
11	ZF	0.28	0/2991	0.49	0/4076
11	ZG	0.31	0/2991	0.50	0/4076
11	ZH	0.28	0/2991	0.50	0/4076
11	ZI	0.30	0/2991	0.51	0/4076
11	ZJ	0.31	0/2991	0.51	0/4076
11	ZK	0.26	0/2991	0.48	0/4076
11	ZL	0.28	0/2991	0.49	0/4076
11	ZM	0.29	0/2991	0.53	1/4076 (0.0%)
11	ZN	0.28	0/2991	0.51	0/4076
11	ZO	0.30	0/2991	0.50	0/4076
11	ZP	0.28	0/2991	0.50	1/4076 (0.0%)
11	ZQ	0.29	0/2991	0.51	0/4076
11	ZR	0.30	1/2991 (0.0%)	0.55	3/4076 (0.1%)
11	ZS	0.29	0/2991	0.52	1/4076 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
11	ZT	0.26	0/2991	0.47	0/4076
11	ZU	0.28	0/2991	0.50	0/4076
11	ZV	0.50	4/2991 (0.1%)	0.67	6/4076 (0.1%)
11	ZW	0.26	0/2991	0.48	0/4076
11	ZX	0.28	0/2991	0.48	0/4076
11	ZY	0.30	1/2991 (0.0%)	0.54	2/4076 (0.0%)
11	ZZ	0.25	0/2991	0.46	0/4076
11	Za	0.28	0/2991	0.49	0/4076
11	Zb	0.29	0/2991	0.50	0/4076
11	Zc	0.29	0/2991	0.53	2/4076 (0.0%)
11	Zd	0.29	0/2991	0.50	0/4076
11	Ze	0.27	0/2991	0.48	0/4076
11	Zf	0.27	0/2991	0.48	0/4076
11	Zg	0.27	0/2991	0.49	0/4076
11	Zh	0.26	0/2991	0.48	0/4076
12	a	0.26	0/2243	0.51	0/3041
12	b	0.26	0/2243	0.51	0/3041
12	c	0.26	0/2243	0.51	0/3041
12	d	0.26	0/2243	0.51	0/3041
12	e	0.26	0/2243	0.51	0/3041
12	f	0.26	0/2243	0.51	0/3041
12	g	0.26	0/2243	0.51	0/3041
12	h	0.26	0/2243	0.51	0/3041
12	i	0.26	0/2243	0.51	0/3041
12	j	0.26	0/2243	0.51	0/3041
12	k	0.26	0/2243	0.51	0/3041
12	l	0.26	0/2243	0.51	0/3041
12	m	0.26	0/2243	0.51	0/3041
12	n	0.26	0/2243	0.51	0/3041
12	o	0.26	0/2243	0.51	0/3041
12	p	0.26	0/2243	0.51	0/3041
12	q	0.26	0/2243	0.51	0/3041
12	r	0.26	0/2243	0.51	0/3041
12	s	0.26	0/2243	0.51	0/3041
12	t	0.26	0/2243	0.51	0/3041
12	u	0.26	0/2243	0.51	0/3041
12	v	0.26	0/2243	0.51	0/3041
12	w	0.26	0/2243	0.51	0/3041
12	x	0.26	0/2243	0.51	0/3041
12	y	0.26	0/2243	0.51	0/3041
12	z	0.26	0/2243	0.51	0/3041
13	B1	0.31	0/679	0.54	0/917
13	B2	0.29	0/679	0.53	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
13	B7	0.39	0/679	0.57	0/917
13	B8	0.31	0/679	0.55	0/917
13	B9	0.29	0/679	0.53	0/917
13	BY	0.31	0/679	0.54	0/917
13	BZ	0.29	0/679	0.53	0/917
13	Be	0.39	0/679	0.57	0/917
13	Bf	0.31	0/679	0.54	0/917
13	Bg	0.29	0/679	0.53	0/917
13	Bl	0.39	0/679	0.57	0/917
13	Bm	0.31	0/679	0.54	0/917
13	Bn	0.29	0/679	0.53	0/917
13	Bs	0.39	0/679	0.57	0/917
13	Bt	0.31	0/679	0.54	0/917
13	Bu	0.30	0/679	0.53	0/917
13	Bz	0.39	0/679	0.57	0/917
13	C1	0.39	0/679	0.57	0/917
13	C2	0.31	0/679	0.54	0/917
13	C3	0.29	0/679	0.53	0/917
13	C4	0.39	0/679	0.57	0/917
13	C5	0.31	0/679	0.54	0/917
13	C8	0.39	0/679	0.57	0/917
13	C9	0.31	0/679	0.54	0/917
13	CD	0.39	0/679	0.57	0/917
13	CE	0.31	0/679	0.54	0/917
13	CF	0.29	0/679	0.53	0/917
13	CK	0.39	0/679	0.57	0/917
13	CL	0.31	0/679	0.54	0/917
13	CM	0.29	0/679	0.53	0/917
13	CR	0.39	0/679	0.57	0/917
13	CS	0.31	0/679	0.54	0/917
13	CT	0.29	0/679	0.53	0/917
13	CY	0.39	0/679	0.57	0/917
13	CZ	0.31	0/679	0.54	0/917
13	Ca	0.29	0/679	0.53	0/917
13	Cf	0.39	0/679	0.57	0/917
13	Cg	0.31	0/679	0.54	0/917
13	Ch	0.29	0/679	0.53	0/917
13	Cm	0.39	0/679	0.57	0/917
13	Cn	0.32	0/679	0.54	0/917
13	Co	0.30	0/679	0.53	0/917
13	Ct	0.39	0/679	0.57	0/917
13	Cu	0.31	0/679	0.55	0/917
13	Cv	0.29	0/679	0.53	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
13	D1	0.29	0/679	0.53	0/917
13	D5	0.39	0/679	0.57	0/917
13	D6	0.31	0/679	0.54	0/917
13	D7	0.29	0/679	0.53	0/917
13	DD	0.30	0/679	0.53	0/917
13	DI	0.39	0/679	0.57	0/917
13	DJ	0.31	0/679	0.54	0/917
13	DK	0.29	0/679	0.53	0/917
13	DM	0.29	0/679	0.53	0/917
13	DN	0.29	0/679	0.53	0/917
13	DO	0.29	0/679	0.53	0/917
13	DP	0.29	0/679	0.53	0/917
13	DQ	0.29	0/679	0.53	0/917
13	DR	0.29	0/679	0.53	0/917
13	DS	0.29	0/679	0.53	0/917
13	DT	0.29	0/679	0.53	0/917
13	DU	0.39	0/679	0.57	0/917
13	DV	0.31	0/679	0.54	0/917
13	DW	0.29	0/679	0.53	0/917
13	Da	0.39	0/679	0.57	0/917
13	Db	0.31	0/679	0.54	0/917
13	Dc	0.29	0/679	0.53	0/917
13	Dg	0.39	0/679	0.57	0/917
13	Dh	0.31	0/679	0.54	0/917
13	Di	0.29	0/679	0.53	0/917
13	Dm	0.39	0/679	0.57	0/917
13	Dn	0.31	0/679	0.54	0/917
13	Do	0.29	0/679	0.53	0/917
13	Ds	0.39	0/679	0.57	0/917
13	Dt	0.31	0/679	0.54	0/917
13	Du	0.29	0/679	0.53	0/917
13	Dy	0.39	0/679	0.57	0/917
13	Dz	0.31	0/679	0.54	0/917
13	EA	0.39	0/679	0.57	0/917
13	EB	0.31	0/679	0.54	0/917
13	EE	0.39	0/679	0.57	0/917
13	EF	0.31	0/679	0.54	0/917
13	EG	0.30	0/679	0.53	0/917
13	EL	0.39	0/679	0.57	0/917
13	EM	0.31	0/679	0.54	0/917
13	EN	0.29	0/679	0.53	0/917
13	ES	0.39	0/679	0.57	0/917
13	ET	0.31	0/679	0.54	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
13	EU	0.29	0/679	0.53	0/917
13	EZ	0.39	0/679	0.57	0/917
13	FC	0.39	0/679	0.57	0/917
13	FD	0.39	0/679	0.57	0/917
13	FE	0.39	0/679	0.57	0/917
13	FF	0.39	0/679	0.57	0/917
13	FG	0.39	0/679	0.57	0/917
13	FH	0.39	0/679	0.57	0/917
13	FI	0.31	0/679	0.54	0/917
13	FJ	0.31	0/679	0.54	0/917
13	FK	0.31	0/679	0.54	0/917
13	FL	0.31	0/679	0.54	0/917
13	FM	0.31	0/679	0.54	0/917
13	FN	0.31	0/679	0.54	0/917
14	B5	0.24	0/2447	0.46	0/3300
14	Bc	0.23	0/2447	0.46	0/3300
14	Bj	0.23	0/2447	0.46	0/3300
14	Bq	0.23	0/2447	0.46	0/3300
14	Bx	0.24	0/2447	0.46	0/3300
14	C6	0.23	0/2447	0.46	0/3300
14	CB	0.23	0/2447	0.46	0/3300
14	CI	0.23	0/2447	0.46	0/3300
14	CP	0.23	0/2447	0.46	0/3300
14	CW	0.23	0/2447	0.46	0/3300
14	Cd	0.23	0/2447	0.46	0/3300
14	Ck	0.23	0/2447	0.46	0/3300
14	Cr	0.23	0/2447	0.46	0/3300
14	Cy	0.23	0/2447	0.46	0/3300
14	D3	0.23	0/2447	0.46	0/3300
14	D9	0.23	0/2447	0.46	0/3300
14	DA	0.24	0/2447	0.46	0/3300
14	DG	0.23	0/2447	0.46	0/3300
14	DY	0.23	0/2447	0.46	0/3300
14	De	0.23	0/2447	0.46	0/3300
14	Dk	0.23	0/2447	0.46	0/3300
14	Dq	0.23	0/2447	0.46	0/3300
14	Dw	0.24	0/2447	0.46	0/3300
14	E1	0.23	0/2447	0.46	0/3300
14	E2	0.23	0/2447	0.46	0/3300
14	E3	0.23	0/2447	0.46	0/3300
14	E4	0.23	0/2447	0.46	0/3300
14	EC	0.23	0/2447	0.46	0/3300
14	EJ	0.23	0/2447	0.46	0/3300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	EQ	0.23	0/2447	0.46	0/3300
14	EX	0.23	0/2447	0.46	0/3300
14	Ex	0.23	0/2447	0.46	0/3300
14	Ey	0.23	0/2447	0.46	0/3300
14	Ez	0.23	0/2447	0.46	0/3300
15	B6	0.24	0/1004	0.41	0/1349
15	Bd	0.24	0/1004	0.41	0/1349
15	Bk	0.24	0/1004	0.40	0/1349
15	Br	0.24	0/1004	0.41	0/1349
15	By	0.24	0/1004	0.41	0/1349
15	C7	0.24	0/1004	0.41	0/1349
15	CC	0.24	0/1004	0.41	0/1349
15	CJ	0.24	0/1004	0.40	0/1349
15	CQ	0.24	0/1004	0.41	0/1349
15	CX	0.24	0/1004	0.41	0/1349
15	Ce	0.24	0/1004	0.41	0/1349
15	Cl	0.24	0/1004	0.41	0/1349
15	Cs	0.24	0/1004	0.41	0/1349
15	Cz	0.24	0/1004	0.41	0/1349
15	D0	0.24	0/1004	0.41	0/1349
15	D4	0.24	0/1004	0.41	0/1349
15	DB	0.24	0/1004	0.41	0/1349
15	DH	0.24	0/1004	0.40	0/1349
15	DZ	0.24	0/1004	0.41	0/1349
15	Df	0.24	0/1004	0.41	0/1349
15	Dl	0.24	0/1004	0.41	0/1349
15	Dr	0.24	0/1004	0.41	0/1349
15	Dx	0.24	0/1004	0.41	0/1349
15	E0	0.24	0/1004	0.41	0/1349
15	E6	0.24	0/1004	0.41	0/1349
15	E7	0.23	0/1004	0.41	0/1349
15	E8	0.24	0/1004	0.41	0/1349
15	E9	0.24	0/1004	0.41	0/1349
15	ED	0.24	0/1004	0.41	0/1349
15	EK	0.24	0/1004	0.41	0/1349
15	ER	0.24	0/1004	0.41	0/1349
15	EY	0.24	0/1004	0.40	0/1349
15	FA	0.24	0/1004	0.40	0/1349
15	FB	0.24	0/1004	0.41	0/1349
16	B4	0.27	0/2482	0.50	0/3375
16	Bb	0.28	0/2482	0.50	0/3375
16	Bi	0.28	0/2482	0.50	0/3375
16	Bp	0.28	0/2482	0.50	0/3375

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	Bw	0.27	0/2482	0.50	0/3375
16	C0	0.27	0/2482	0.50	0/3375
16	CA	0.27	0/2482	0.50	0/3375
16	CH	0.28	0/2482	0.50	0/3375
16	CO	0.28	0/2482	0.50	0/3375
16	CV	0.28	0/2482	0.50	0/3375
16	Cc	0.28	0/2482	0.50	0/3375
16	Cj	0.28	0/2482	0.50	0/3375
16	Cq	0.27	0/2482	0.50	0/3375
16	Cx	0.28	0/2482	0.50	0/3375
16	D2	0.27	0/2482	0.50	0/3375
16	D8	0.27	0/2482	0.50	0/3375
16	DC	0.28	0/2482	0.50	0/3375
16	DF	0.28	0/2482	0.50	0/3375
16	DX	0.28	0/2482	0.50	0/3375
16	Dd	0.28	0/2482	0.50	0/3375
16	Dj	0.28	0/2482	0.50	0/3375
16	Dp	0.28	0/2482	0.50	0/3375
16	Dv	0.28	0/2482	0.50	0/3375
16	E5	0.27	0/2482	0.50	0/3375
16	EI	0.28	0/2482	0.50	0/3375
16	EP	0.28	0/2482	0.50	0/3375
16	EW	0.28	0/2482	0.50	0/3375
16	Eq	0.27	0/2482	0.50	0/3375
16	Er	0.28	0/2482	0.50	0/3375
16	Es	0.28	0/2482	0.50	0/3375
16	Et	0.27	0/2482	0.50	0/3375
16	Eu	0.27	0/2482	0.50	0/3375
16	Ev	0.27	0/2482	0.50	0/3375
16	Ew	0.28	0/2482	0.50	0/3375
All	All	0.31	27/621926 (0.0%)	0.52	68/842993 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	2
1	1	0	1
1	5	0	1
1	6	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	8	0	1
1	AF	0	1
1	AI	0	1
1	AM	0	2
1	AN	0	1
1	ZA	0	1
3	A0	0	1
3	A6	0	1
5	AA	0	2
5	AB	0	1
5	AC	0	1
5	AE	0	1
6	UI	0	2
6	UJ	0	2
6	UK	0	3
6	UL	0	3
6	UM	0	2
6	UN	0	2
6	UO	0	2
6	UP	0	3
6	WA	0	3
6	WB	0	4
6	WC	0	3
6	WD	0	1
6	WE	0	2
6	WF	0	3
6	WG	0	3
6	WI	0	1
6	WJ	0	3
6	WK	0	2
6	WL	0	2
6	WM	0	1
6	WN	0	1
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

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	Aw	0	1
10	BD	0	1
10	BF	0	1
11	ZG	0	1
11	ZI	0	1
11	ZK	0	1
11	ZO	0	1
11	ZW	0	1
11	Zb	0	1
11	Zd	0	1
11	Ze	0	1
12	a	0	1
12	b	0	1
12	c	0	1
12	d	0	1
12	e	0	1
12	f	0	1
12	g	0	1
12	h	0	1
12	i	0	1
12	j	0	1
12	k	0	1
12	l	0	1
12	m	0	1
12	n	0	1
12	o	0	1
12	p	0	1
12	q	0	1
12	r	0	1
12	s	0	1
12	t	0	1
12	u	0	1
12	v	0	1
12	w	0	1
12	x	0	1
12	y	0	1
12	z	0	1
13	B1	0	1
13	B2	0	1
13	B7	0	1
13	B8	0	1
13	B9	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	BY	0	1
13	BZ	0	1
13	Be	0	1
13	Bf	0	1
13	Bg	0	1
13	Bl	0	1
13	Bm	0	1
13	Bn	0	1
13	Bs	0	1
13	Bt	0	1
13	Bu	0	1
13	Bz	0	1
13	C1	0	1
13	C2	0	1
13	C3	0	1
13	C4	0	1
13	C5	0	1
13	C8	0	1
13	C9	0	1
13	CD	0	1
13	CE	0	1
13	CF	0	1
13	CK	0	1
13	CL	0	1
13	CM	0	1
13	CR	0	1
13	CS	0	1
13	CT	0	1
13	CY	0	1
13	CZ	0	1
13	Ca	0	1
13	Cf	0	1
13	Cg	0	1
13	Ch	0	1
13	Cm	0	1
13	Cn	0	1
13	Co	0	1
13	Ct	0	1
13	Cu	0	1
13	Cv	0	1
13	D1	0	1
13	D5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	D6	0	1
13	D7	0	1
13	DD	0	1
13	DI	0	1
13	DJ	0	1
13	DK	0	1
13	DM	0	1
13	DN	0	1
13	DO	0	1
13	DP	0	1
13	DQ	0	1
13	DR	0	1
13	DS	0	1
13	DT	0	1
13	DU	0	1
13	DV	0	1
13	DW	0	1
13	Da	0	1
13	Db	0	1
13	Dc	0	1
13	Dg	0	1
13	Dh	0	1
13	Di	0	1
13	Dm	0	1
13	Dn	0	1
13	Do	0	1
13	Ds	0	1
13	Dt	0	1
13	Du	0	1
13	Dy	0	1
13	Dz	0	1
13	EA	0	1
13	EB	0	1
13	EE	0	1
13	EF	0	1
13	EG	0	1
13	EL	0	1
13	EM	0	1
13	EN	0	1
13	ES	0	1
13	ET	0	1
13	EU	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	EZ	0	1
13	FC	0	1
13	FD	0	1
13	FE	0	1
13	FF	0	1
13	FG	0	1
13	FH	0	1
13	FI	0	1
13	FJ	0	1
13	FK	0	1
13	FL	0	1
13	FM	0	1
13	FN	0	1
16	B4	0	2
16	Bb	0	2
16	Bi	0	2
16	Bp	0	2
16	Bw	0	2
16	C0	0	2
16	CA	0	2
16	CH	0	2
16	CO	0	2
16	CV	0	2
16	Cc	0	2
16	Cj	0	2
16	Cq	0	2
16	Cx	0	2
16	D2	0	2
16	D8	0	2
16	DC	0	2
16	DF	0	2
16	DX	0	2
16	Dd	0	2
16	Dj	0	2
16	Dp	0	2
16	Dv	0	2
16	E5	0	2
16	EI	0	2
16	EP	0	2
16	EW	0	2
16	Eq	0	2
16	Er	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	Es	0	2
16	Et	0	2
16	Eu	0	2
16	Ev	0	2
16	Ew	0	2
All	All	0	293

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	ZV	140	PRO	CG-CD	-16.08	0.97	1.50
6	BK	331	PRO	CG-CD	-14.23	1.03	1.50
10	BC	73	PRO	CG-CD	-12.74	1.08	1.50
11	ZV	125	PRO	CG-CD	-10.17	1.17	1.50
6	UM	172	PRO	N-CD	-9.56	1.34	1.47
6	UL	172	PRO	N-CD	-9.54	1.34	1.47
6	UP	172	PRO	N-CD	-9.53	1.34	1.47
6	UI	172	PRO	N-CD	-9.45	1.34	1.47
6	UN	172	PRO	N-CD	-9.45	1.34	1.47
6	UK	172	PRO	N-CD	-9.44	1.34	1.47
6	UO	172	PRO	N-CD	-9.41	1.34	1.47
6	UJ	172	PRO	N-CD	-9.41	1.34	1.47
11	ZV	140	PRO	N-CD	8.33	1.59	1.47
6	UI	125	GLN	C-N	7.64	1.51	1.34
6	UP	125	GLN	C-N	7.64	1.51	1.34
6	UO	125	GLN	C-N	7.63	1.51	1.34
10	BC	73	PRO	CB-CG	-7.63	1.11	1.50
6	UJ	125	GLN	C-N	7.61	1.51	1.34
6	UK	125	GLN	C-N	7.60	1.51	1.34
6	UL	125	GLN	C-N	7.60	1.51	1.34
6	UM	125	GLN	C-N	7.59	1.51	1.34
6	UN	125	GLN	C-N	7.51	1.51	1.34
11	ZV	125	PRO	N-CD	6.66	1.57	1.47
8	At	185	MET	C-O	6.35	1.35	1.23
11	ZY	125	PRO	CG-CD	-5.46	1.32	1.50
11	ZR	125	PRO	CG-CD	-5.09	1.33	1.50
6	UM	105	LEU	C-N	-5.03	1.24	1.34

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BC	73	PRO	N-CD-CG	-18.84	74.94	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BC	73	PRO	CB-CG-CD	18.81	179.84	106.50
11	ZV	140	PRO	N-CD-CG	-17.35	77.18	103.20
6	BK	331	PRO	N-CD-CG	-16.11	79.04	103.20
10	BC	73	PRO	CA-CB-CG	-14.02	77.37	104.00
11	ZR	125	PRO	CA-N-CD	-13.98	91.93	111.50
11	ZY	125	PRO	CA-N-CD	-13.37	92.78	111.50
11	ZV	125	PRO	CA-N-CD	-13.27	92.93	111.50
9	Au	162	PRO	CA-N-CD	-12.01	94.69	111.50
11	ZV	125	PRO	N-CD-CG	-11.24	86.33	103.20
11	Zc	125	PRO	CA-N-CD	-11.22	95.79	111.50
11	ZV	140	PRO	CA-N-CD	-10.26	97.14	111.50
11	ZV	140	PRO	CA-CB-CG	-9.30	86.33	104.00
6	BK	331	PRO	CA-CB-CG	-8.99	86.92	104.00
6	UO	126	PHE	O-C-N	8.85	136.86	122.70
6	UJ	126	PHE	O-C-N	8.83	136.83	122.70
6	UL	126	PHE	O-C-N	8.82	136.81	122.70
6	UI	126	PHE	O-C-N	8.79	136.77	122.70
6	UP	126	PHE	O-C-N	8.79	136.76	122.70
6	UM	126	PHE	O-C-N	8.78	136.75	122.70
6	UK	126	PHE	O-C-N	8.77	136.73	122.70
6	UN	126	PHE	O-C-N	8.75	136.70	122.70
11	ZM	223	PRO	CA-N-CD	-8.44	99.68	111.50
11	ZR	125	PRO	N-CD-CG	-7.56	91.86	103.20
11	ZY	125	PRO	N-CD-CG	-7.45	92.03	103.20
6	BK	331	PRO	N-CA-CB	-7.03	94.87	103.30
6	UJ	126	PHE	CA-C-N	-6.81	102.22	117.20
6	UM	126	PHE	CA-C-N	-6.78	102.28	117.20
6	UO	126	PHE	CA-C-N	-6.76	102.32	117.20
6	UL	126	PHE	CA-C-N	-6.76	102.32	117.20
6	UK	126	PHE	CA-C-N	-6.76	102.33	117.20
6	UP	126	PHE	CA-C-N	-6.75	102.34	117.20
6	UN	126	PHE	CA-C-N	-6.74	102.37	117.20
6	UI	126	PHE	CA-C-N	-6.72	102.41	117.20
9	Au	162	PRO	N-CD-CG	-6.53	93.41	103.20
6	UK	129	GLN	O-C-N	6.37	132.90	122.70
6	UP	129	GLN	O-C-N	6.36	132.88	122.70
6	UO	129	GLN	O-C-N	6.35	132.86	122.70
6	UM	129	GLN	O-C-N	6.30	132.78	122.70
6	WA	162	PRO	N-CA-C	6.29	128.44	112.10
6	UL	129	GLN	O-C-N	6.28	132.75	122.70
1	AI	154	ASP	CB-CG-OD2	6.28	123.95	118.30
6	UN	129	GLN	O-C-N	6.26	132.72	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	UI	129	GLN	O-C-N	6.25	132.71	122.70
6	UJ	129	GLN	O-C-N	6.25	132.71	122.70
11	ZR	214	ASP	CB-CG-OD1	6.05	123.75	118.30
11	Zc	125	PRO	N-CD-CG	-5.88	94.38	103.20
6	UO	126	PHE	C-N-CA	-5.76	107.31	121.70
6	UP	126	PHE	C-N-CA	-5.75	107.33	121.70
6	UJ	126	PHE	C-N-CA	-5.74	107.35	121.70
6	UM	126	PHE	C-N-CA	-5.74	107.36	121.70
6	UL	126	PHE	C-N-CA	-5.74	107.36	121.70
6	UI	126	PHE	C-N-CA	-5.73	107.38	121.70
1	AM	154	ASP	CB-CG-OD1	5.72	123.45	118.30
6	UK	126	PHE	C-N-CA	-5.72	107.41	121.70
6	UN	126	PHE	C-N-CA	-5.71	107.42	121.70
1	0	52	PRO	N-CA-CB	-5.70	96.33	102.60
11	ZS	18	ASP	CB-CG-OD1	5.70	123.43	118.30
11	ZV	125	PRO	CA-CB-CG	-5.66	93.24	104.00
1	ZE	13	ASP	CB-CG-OD1	5.56	123.30	118.30
11	ZP	125	PRO	CA-N-CD	-5.55	103.73	111.50
8	At	189	PRO	CA-N-CD	-5.51	103.78	111.50
9	Av	162	PRO	N-CA-CB	-5.30	96.77	102.60
6	WJ	214	ASP	CB-CA-C	-5.21	99.97	110.40
1	9	109	ASP	CB-CG-OD2	5.21	122.99	118.30
5	AB	72	ASP	CB-CG-OD1	5.20	122.98	118.30
6	WO	168	GLU	CB-CA-C	-5.08	100.24	110.40
10	BD	8	ASP	CB-CG-OD2	5.06	122.85	118.30

There are no chirality outliers.

All (293) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	36	ARG	Sidechain
1	0	50	ARG	Sidechain
1	1	36	ARG	Sidechain
1	5	50	ARG	Sidechain
1	6	153	ARG	Sidechain
1	8	238	ARG	Sidechain
3	A0	104	ARG	Sidechain
3	A6	106	ARG	Sidechain
5	AA	200	ARG	Sidechain
5	AA	243	ARG	Sidechain
5	AB	225	ARG	Sidechain
5	AC	243	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	AE	160	ARG	Sidechain
1	AF	36	ARG	Sidechain
1	AI	116	ARG	Sidechain
1	AM	36	ARG	Sidechain
1	AM	50	ARG	Sidechain
1	AN	238	ARG	Sidechain
9	Aw	143	ARG	Sidechain
13	B1	131	ARG	Sidechain
13	B2	131	ARG	Sidechain
16	B4	60	ARG	Sidechain
16	B4	63	ARG	Sidechain
13	B7	131	ARG	Sidechain
13	B8	131	ARG	Sidechain
13	B9	131	ARG	Sidechain
10	BD	110	ARG	Sidechain
10	BF	110	ARG	Sidechain
13	BY	131	ARG	Sidechain
13	BZ	131	ARG	Sidechain
16	Bb	60	ARG	Sidechain
16	Bb	63	ARG	Sidechain
13	Be	131	ARG	Sidechain
13	Bf	131	ARG	Sidechain
13	Bg	131	ARG	Sidechain
16	Bi	60	ARG	Sidechain
16	Bi	63	ARG	Sidechain
13	Bl	131	ARG	Sidechain
13	Bm	131	ARG	Sidechain
13	Bn	131	ARG	Sidechain
16	Bp	60	ARG	Sidechain
16	Bp	63	ARG	Sidechain
13	Bs	131	ARG	Sidechain
13	Bt	131	ARG	Sidechain
13	Bu	131	ARG	Sidechain
16	Bw	60	ARG	Sidechain
16	Bw	63	ARG	Sidechain
13	Bz	131	ARG	Sidechain
16	C0	60	ARG	Sidechain
16	C0	63	ARG	Sidechain
13	C1	131	ARG	Sidechain
13	C2	131	ARG	Sidechain
13	C3	131	ARG	Sidechain
13	C4	131	ARG	Sidechain

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Mol	Chain	Res	Type	Group
13	C5	131	ARG	Sidechain
13	C8	131	ARG	Sidechain
13	C9	131	ARG	Sidechain
16	CA	60	ARG	Sidechain
16	CA	63	ARG	Sidechain
13	CD	131	ARG	Sidechain
13	CE	131	ARG	Sidechain
13	CF	131	ARG	Sidechain
16	CH	60	ARG	Sidechain
16	CH	63	ARG	Sidechain
13	CK	131	ARG	Sidechain
13	CL	131	ARG	Sidechain
13	CM	131	ARG	Sidechain
16	CO	60	ARG	Sidechain
16	CO	63	ARG	Sidechain
13	CR	131	ARG	Sidechain
13	CS	131	ARG	Sidechain
13	CT	131	ARG	Sidechain
16	CV	60	ARG	Sidechain
16	CV	63	ARG	Sidechain
13	CY	131	ARG	Sidechain
13	CZ	131	ARG	Sidechain
13	Ca	131	ARG	Sidechain
16	Cc	60	ARG	Sidechain
16	Cc	63	ARG	Sidechain
13	Cf	131	ARG	Sidechain
13	Cg	131	ARG	Sidechain
13	Ch	131	ARG	Sidechain
16	Cj	60	ARG	Sidechain
16	Cj	63	ARG	Sidechain
13	Cm	131	ARG	Sidechain
13	Cn	131	ARG	Sidechain
13	Co	131	ARG	Sidechain
16	Cq	60	ARG	Sidechain
16	Cq	63	ARG	Sidechain
13	Ct	131	ARG	Sidechain
13	Cu	131	ARG	Sidechain
13	Cv	131	ARG	Sidechain
16	Cx	60	ARG	Sidechain
16	Cx	63	ARG	Sidechain
13	D1	131	ARG	Sidechain
16	D2	60	ARG	Sidechain

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Mol	Chain	Res	Type	Group
16	D2	63	ARG	Sidechain
13	D5	131	ARG	Sidechain
13	D6	131	ARG	Sidechain
13	D7	131	ARG	Sidechain
16	D8	60	ARG	Sidechain
16	D8	63	ARG	Sidechain
16	DC	60	ARG	Sidechain
16	DC	63	ARG	Sidechain
13	DD	131	ARG	Sidechain
16	DF	60	ARG	Sidechain
16	DF	63	ARG	Sidechain
13	DI	131	ARG	Sidechain
13	DJ	131	ARG	Sidechain
13	DK	131	ARG	Sidechain
13	DM	131	ARG	Sidechain
13	DN	131	ARG	Sidechain
13	DO	131	ARG	Sidechain
13	DP	131	ARG	Sidechain
13	DQ	131	ARG	Sidechain
13	DR	131	ARG	Sidechain
13	DS	131	ARG	Sidechain
13	DT	131	ARG	Sidechain
13	DU	131	ARG	Sidechain
13	DV	131	ARG	Sidechain
13	DW	131	ARG	Sidechain
16	DX	60	ARG	Sidechain
16	DX	63	ARG	Sidechain
13	Da	131	ARG	Sidechain
13	Db	131	ARG	Sidechain
13	Dc	131	ARG	Sidechain
16	Dd	60	ARG	Sidechain
16	Dd	63	ARG	Sidechain
13	Dg	131	ARG	Sidechain
13	Dh	131	ARG	Sidechain
13	Di	131	ARG	Sidechain
16	Dj	60	ARG	Sidechain
16	Dj	63	ARG	Sidechain
13	Dm	131	ARG	Sidechain
13	Dn	131	ARG	Sidechain
13	Do	131	ARG	Sidechain
16	Dp	60	ARG	Sidechain
16	Dp	63	ARG	Sidechain

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Mol	Chain	Res	Type	Group
13	Ds	131	ARG	Sidechain
13	Dt	131	ARG	Sidechain
13	Du	131	ARG	Sidechain
16	Dv	60	ARG	Sidechain
16	Dv	63	ARG	Sidechain
13	Dy	131	ARG	Sidechain
13	Dz	131	ARG	Sidechain
16	E5	60	ARG	Sidechain
16	E5	63	ARG	Sidechain
13	EA	131	ARG	Sidechain
13	EB	131	ARG	Sidechain
13	EE	131	ARG	Sidechain
13	EF	131	ARG	Sidechain
13	EG	131	ARG	Sidechain
16	EI	60	ARG	Sidechain
16	EI	63	ARG	Sidechain
13	EL	131	ARG	Sidechain
13	EM	131	ARG	Sidechain
13	EN	131	ARG	Sidechain
16	EP	60	ARG	Sidechain
16	EP	63	ARG	Sidechain
13	ES	131	ARG	Sidechain
13	ET	131	ARG	Sidechain
13	EU	131	ARG	Sidechain
16	EW	60	ARG	Sidechain
16	EW	63	ARG	Sidechain
13	EZ	131	ARG	Sidechain
16	Eq	60	ARG	Sidechain
16	Eq	63	ARG	Sidechain
16	Er	60	ARG	Sidechain
16	Er	63	ARG	Sidechain
16	Es	60	ARG	Sidechain
16	Es	63	ARG	Sidechain
16	Et	60	ARG	Sidechain
16	Et	63	ARG	Sidechain
16	Eu	60	ARG	Sidechain
16	Eu	63	ARG	Sidechain
16	Ev	60	ARG	Sidechain
16	Ev	63	ARG	Sidechain
16	Ew	60	ARG	Sidechain
16	Ew	63	ARG	Sidechain
13	FC	131	ARG	Sidechain

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Mol	Chain	Res	Type	Group
13	FD	131	ARG	Sidechain
13	FE	131	ARG	Sidechain
13	FF	131	ARG	Sidechain
13	FG	131	ARG	Sidechain
13	FH	131	ARG	Sidechain
13	FI	131	ARG	Sidechain
13	FJ	131	ARG	Sidechain
13	FK	131	ARG	Sidechain
13	FL	131	ARG	Sidechain
13	FM	131	ARG	Sidechain
13	FN	131	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

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Mol	Chain	Res	Type	Group
6	WE	142	ARG	Sidechain
6	WF	134	ARG	Sidechain
6	WF	142	ARG	Sidechain
6	WF	167	ARG	Sidechain
6	WG	134	ARG	Sidechain
6	WG	142	ARG	Sidechain
6	WG	167	ARG	Sidechain
6	WI	142	ARG	Sidechain
6	WJ	134	ARG	Sidechain
6	WJ	142	ARG	Sidechain
6	WJ	167	ARG	Sidechain
6	WK	134	ARG	Sidechain
6	WK	142	ARG	Sidechain
6	WL	134	ARG	Sidechain
6	WL	157	LEU	Mainchain
6	WM	134	ARG	Sidechain
6	WN	134	ARG	Sidechain
6	WO	134	ARG	Sidechain
6	WP	134	ARG	Sidechain
6	WP	142	ARG	Sidechain
6	WP	154	ARG	Sidechain
6	WQ	134	ARG	Sidechain
6	WQ	142	ARG	Sidechain
6	WR	134	ARG	Sidechain
6	WR	142	ARG	Sidechain
6	WR	167	ARG	Sidechain
6	WS	167	ARG	Sidechain
6	WT	134	ARG	Sidechain
6	WT	142	ARG	Sidechain
6	WU	134	ARG	Sidechain
6	WU	142	ARG	Sidechain
6	WV	134	ARG	Sidechain
6	WV	142	ARG	Sidechain
6	WV	167	ARG	Sidechain
6	WW	134	ARG	Sidechain
6	WW	167	ARG	Sidechain
1	ZA	79	ARG	Sidechain
11	ZG	71	ARG	Sidechain
11	ZI	380	ARG	Sidechain
11	ZK	71	ARG	Sidechain
11	ZO	71	ARG	Sidechain
11	ZW	71	ARG	Sidechain

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Mol	Chain	Res	Type	Group
11	Zb	106	ARG	Sidechain
11	Zd	380	ARG	Sidechain
11	Ze	380	ARG	Sidechain
12	a	117	ARG	Sidechain
12	b	117	ARG	Sidechain
12	c	117	ARG	Sidechain
12	d	117	ARG	Sidechain
12	e	117	ARG	Sidechain
12	f	117	ARG	Sidechain
12	g	117	ARG	Sidechain
12	h	117	ARG	Sidechain
12	i	117	ARG	Sidechain
12	j	117	ARG	Sidechain
12	k	117	ARG	Sidechain
12	l	117	ARG	Sidechain
12	m	117	ARG	Sidechain
12	n	117	ARG	Sidechain
12	o	117	ARG	Sidechain
12	p	117	ARG	Sidechain
12	q	117	ARG	Sidechain
12	r	117	ARG	Sidechain
12	s	117	ARG	Sidechain
12	t	117	ARG	Sidechain
12	u	117	ARG	Sidechain
12	v	117	ARG	Sidechain
12	w	117	ARG	Sidechain
12	x	117	ARG	Sidechain
12	y	117	ARG	Sidechain
12	z	117	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	67
1	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	67
1	2	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	53
1	3	258/260 (99%)	248 (96%)	8 (3%)	2 (1%)	16	53
1	4	258/260 (99%)	248 (96%)	7 (3%)	3 (1%)	11	43
1	5	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	53
1	6	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	53
1	7	258/260 (99%)	245 (95%)	10 (4%)	3 (1%)	11	43
1	8	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	53
1	9	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	53
1	AF	250/260 (96%)	238 (95%)	11 (4%)	1 (0%)	30	67
1	AG	251/260 (96%)	237 (94%)	13 (5%)	1 (0%)	30	67
1	AH	252/260 (97%)	241 (96%)	10 (4%)	1 (0%)	30	67
1	AI	250/260 (96%)	241 (96%)	7 (3%)	2 (1%)	16	53
1	AJ	251/260 (96%)	241 (96%)	9 (4%)	1 (0%)	30	67
1	AK	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	30	67
1	AL	244/260 (94%)	237 (97%)	4 (2%)	3 (1%)	11	43
1	AM	244/260 (94%)	237 (97%)	6 (2%)	1 (0%)	30	67
1	AN	244/260 (94%)	240 (98%)	3 (1%)	1 (0%)	30	67
1	ZA	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	43
1	ZB	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	43
1	ZC	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	43
1	ZD	258/260 (99%)	244 (95%)	12 (5%)	2 (1%)	16	53
1	ZE	258/260 (99%)	245 (95%)	12 (5%)	1 (0%)	30	67
2	A	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	B	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	C	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	D	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	E	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	63
2	F	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	H	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	63
2	I	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	J	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	K	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	L	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	M	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	N	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	63
2	O	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	P	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	Q	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	R	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	S	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	T	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	U	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	V	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	W	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	X	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
2	Y	209/232 (90%)	204 (98%)	4 (2%)	1 (0%)	25	63
2	Z	209/232 (90%)	205 (98%)	3 (1%)	1 (0%)	25	63
3	A0	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
3	A6	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
3	A7	115/138 (83%)	114 (99%)	1 (1%)	0	100	100
3	A8	119/138 (86%)	116 (98%)	3 (2%)	0	100	100
3	A9	121/138 (88%)	118 (98%)	3 (2%)	0	100	100
4	A1	87/104 (84%)	87 (100%)	0	0	100	100
4	A2	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
4	A3	89/104 (86%)	89 (100%)	0	0	100	100
4	A4	89/104 (86%)	89 (100%)	0	0	100	100
4	A5	88/104 (85%)	88 (100%)	0	0	100	100
4	Az	55/104 (53%)	53 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AA	246/251 (98%)	232 (94%)	11 (4%)	3 (1%)	11	43
5	AB	247/251 (98%)	241 (98%)	6 (2%)	0	100	100
5	AC	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
5	AD	248/251 (99%)	239 (96%)	9 (4%)	0	100	100
5	AE	247/251 (98%)	233 (94%)	13 (5%)	1 (0%)	30	67
6	AO	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AP	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AQ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AR	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AS	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AT	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AU	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AV	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AW	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AX	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AY	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	AZ	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Aa	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ac	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ad	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ae	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Af	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ag	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ah	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ai	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Aj	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ak	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Al	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Am	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	An	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ao	160/560 (29%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Ap	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	B0	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	B3	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	BG	11/560 (2%)	10 (91%)	1 (9%)	0	100	100
6	BH	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
6	BI	18/560 (3%)	18 (100%)	0	0	100	100
6	BJ	14/560 (2%)	14 (100%)	0	0	100	100
6	BK	19/560 (3%)	19 (100%)	0	0	100	100
6	BL	14/560 (2%)	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
6	BO	18/560 (3%)	17 (94%)	1 (6%)	0	100	100
6	BP	14/560 (2%)	14 (100%)	0	0	100	100
6	BQ	19/560 (3%)	19 (100%)	0	0	100	100
6	BR	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BS	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BT	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BU	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BV	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BW	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	BX	160/560 (29%)	158 (99%)	2 (1%)	0	100	100
6	Ba	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Bh	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Bo	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Bv	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	CG	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	CN	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	CU	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Cb	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ci	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Cp	25/560 (4%)	24 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Cw	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	DE	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	DL	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	EH	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	EO	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	EV	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ea	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Eb	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ec	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ed	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ee	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ef	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Eg	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Eh	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ei	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ej	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ek	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	El	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Em	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	En	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Eo	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
6	Ep	25/560 (4%)	24 (96%)	1 (4%)	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	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	WB	109/560 (20%)	94 (86%)	10 (9%)	5 (5%)	2	18
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	18
6	WE	110/560 (20%)	98 (89%)	8 (7%)	4 (4%)	3	21
6	WF	109/560 (20%)	98 (90%)	8 (7%)	3 (3%)	4	25
6	WG	110/560 (20%)	98 (89%)	10 (9%)	2 (2%)	7	34
6	WH	93/560 (17%)	86 (92%)	5 (5%)	2 (2%)	5	30
6	WI	93/560 (17%)	82 (88%)	5 (5%)	6 (6%)	1	13
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	23
6	WL	81/560 (14%)	75 (93%)	4 (5%)	2 (2%)	4	27
6	WM	78/560 (14%)	72 (92%)	4 (5%)	2 (3%)	4	26
6	WN	80/560 (14%)	75 (94%)	2 (2%)	3 (4%)	2	20
6	WO	94/560 (17%)	85 (90%)	7 (7%)	2 (2%)	5	31
6	WP	98/560 (18%)	87 (89%)	6 (6%)	5 (5%)	1	16
6	WQ	109/560 (20%)	100 (92%)	5 (5%)	4 (4%)	2	21
6	WR	109/560 (20%)	94 (86%)	8 (7%)	7 (6%)	1	13
6	WS	109/560 (20%)	96 (88%)	7 (6%)	6 (6%)	1	15
6	WT	109/560 (20%)	97 (89%)	5 (5%)	7 (6%)	1	13
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	33
6	WW	109/560 (20%)	95 (87%)	9 (8%)	5 (5%)	2	18
7	Ab	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
7	Aq	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
7	Ar	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
7	As	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
8	At	251/264 (95%)	232 (92%)	13 (5%)	6 (2%)	5	28
9	Au	205/245 (84%)	195 (95%)	10 (5%)	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	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Ay	207/245 (84%)	201 (97%)	4 (2%)	2 (1%)	13	48
10	BA	131/134 (98%)	123 (94%)	8 (6%)	0	100	100
10	BB	130/134 (97%)	124 (95%)	6 (5%)	0	100	100
10	BC	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
10	BD	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
10	BE	131/134 (98%)	125 (95%)	5 (4%)	1 (1%)	16	53
10	BF	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
11	ZF	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	ZG	399/403 (99%)	392 (98%)	6 (2%)	1 (0%)	37	72
11	ZH	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25	63
11	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
11	ZK	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
11	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	72
11	ZM	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	ZN	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	ZO	399/403 (99%)	381 (96%)	15 (4%)	3 (1%)	16	53
11	ZP	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	72
11	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
11	ZR	399/403 (99%)	390 (98%)	8 (2%)	1 (0%)	37	72
11	ZS	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
11	ZT	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
11	ZU	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
11	ZV	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
11	ZW	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
11	ZX	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	ZY	399/403 (99%)	384 (96%)	15 (4%)	0	100	100
11	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
11	Za	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	Zb	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
11	Zc	399/403 (99%)	390 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Zd	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
11	Ze	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
11	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
11	Zg	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
11	Zh	399/403 (99%)	393 (98%)	6 (2%)	0	100	100
12	a	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	b	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	c	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	d	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	e	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	f	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	g	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	h	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	i	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	j	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	k	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	l	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	m	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	n	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	o	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	p	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	q	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	r	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	s	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	t	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	u	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	v	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	w	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	x	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	y	297/365 (81%)	293 (99%)	4 (1%)	0	100	100
12	z	297/365 (81%)	293 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	B1	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	B2	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	B7	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	B8	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	B9	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	BY	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	BZ	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Be	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Bf	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Bg	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Bl	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Bm	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Bn	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Bs	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Bt	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Bu	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Bz	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	C1	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	C2	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	C3	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	C4	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	C5	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	C8	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	C9	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	CD	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	CE	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	CF	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	CK	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	CL	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	CM	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	CR	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CS	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	CT	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	CY	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	CZ	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Ca	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Cf	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Cg	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Ch	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Cm	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Cn	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Co	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	Ct	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	Cu	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	Cv	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	D1	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	D5	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	D6	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	D7	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DD	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DI	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	DJ	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	DK	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DM	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DN	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DO	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DP	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DQ	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DR	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DS	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DT	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	43
13	DU	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	DV	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5 28
13	DW	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11 43
13	Da	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	Db	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5 28
13	Dc	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11 43
13	Dg	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	Dh	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5 28
13	Di	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11 43
13	Dm	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	Dn	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5 28
13	Do	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11 43
13	Ds	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	Dt	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5 28
13	Du	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11 43
13	Dy	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	Dz	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5 28
13	EA	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	EB	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5 28
13	EE	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	EF	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5 28
13	EG	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11 43
13	EL	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	EM	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5 28
13	EN	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11 43
13	ES	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	ET	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5 28
13	EU	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11 43
13	EZ	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	FC	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	FD	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17
13	FE	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	FF	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	FG	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	FH	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	17
13	FI	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	FJ	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	FK	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	FL	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	FM	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
13	FN	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	28
14	B5	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Bc	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Bj	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Bq	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Bx	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	C6	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	CB	306/331 (92%)	296 (97%)	9 (3%)	1 (0%)	37	72
14	CI	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	CP	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	CW	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Cd	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Ck	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Cr	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Cy	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	D3	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	D9	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	DA	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	DG	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	DY	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	De	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Dk	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Dq	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	Dw	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	E1	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	E2	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	E3	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	E4	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	EC	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	EJ	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	EQ	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	EX	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Ex	306/331 (92%)	296 (97%)	9 (3%)	1 (0%)	37	72
14	Ey	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
14	Ez	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
15	B6	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Bd	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Bk	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Br	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	By	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	C7	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	CC	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	CJ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	CQ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	CX	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Ce	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Cl	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Cs	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Cz	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	D0	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	D4	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	DB	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	DH	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	DZ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	Df	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Dl	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Dr	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	Dx	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	E0	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	E6	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	E7	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	E8	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	E9	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	ED	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	EK	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	ER	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	EY	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	FA	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
15	FB	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
16	B4	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Bb	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Bi	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Bp	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Bw	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	C0	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	CA	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	CH	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	CO	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	CV	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Cc	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Cj	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Cq	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Cx	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	D2	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	D8	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	DC	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	DF	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	DX	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Dd	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Dj	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Dp	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Dv	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	E5	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	EI	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	EP	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	EW	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Eq	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Er	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Es	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Et	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Eu	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Ev	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
16	Ew	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	42
All	All	79048/141237 (56%)	76302 (96%)	2146 (3%)	600 (1%)	19	53

All (600) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	209	ASN
1	5	209	ASN
1	8	209	ASN
5	AA	123	GLU
8	At	188	LEU
8	At	190	VAL
9	Ay	83	ALA
6	WO	168	GLU
6	WR	123	ILE
6	WR	165	PHE
6	WR	166	VAL
6	WS	187	ASP
1	ZA	209	ASN

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Mol	Chain	Res	Type
1	ZB	164	GLN
1	ZC	139	ALA
11	ZG	46	SER
13	C3	116	ASP
13	C4	116	ASP
13	C5	116	ASP
13	C8	116	ASP
13	C9	116	ASP
13	DD	116	ASP
13	DI	116	ASP
13	DJ	116	ASP
13	DK	116	ASP
13	DM	116	ASP
13	DN	116	ASP
13	DO	116	ASP
13	DP	116	ASP
13	DQ	116	ASP
13	DR	116	ASP
13	DS	116	ASP
13	DT	116	ASP
13	DU	116	ASP
13	DV	116	ASP
13	DW	116	ASP
13	Da	116	ASP
13	Db	116	ASP
13	Dc	116	ASP
13	Dg	116	ASP
13	Dh	116	ASP
13	Di	116	ASP
13	Dm	116	ASP
13	Dn	116	ASP
13	Do	116	ASP
13	Ds	116	ASP
13	Dt	116	ASP
13	Du	116	ASP
13	Dy	116	ASP
13	Dz	116	ASP
13	D1	116	ASP
13	D5	116	ASP
13	D6	116	ASP
13	D7	116	ASP
13	EA	116	ASP

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Mol	Chain	Res	Type
13	EB	116	ASP
13	B1	116	ASP
13	B2	116	ASP
13	B7	116	ASP
13	B8	116	ASP
13	B9	116	ASP
13	EE	116	ASP
13	EF	116	ASP
13	EG	116	ASP
13	EL	116	ASP
13	EM	116	ASP
13	EN	116	ASP
13	ES	116	ASP
13	ET	116	ASP
13	EU	116	ASP
13	EZ	116	ASP
13	BY	116	ASP
13	BZ	116	ASP
13	Be	116	ASP
13	Bf	116	ASP
13	Bg	116	ASP
13	Bl	116	ASP
13	Bm	116	ASP
13	Bn	116	ASP
13	Bs	116	ASP
13	Bt	116	ASP
13	Bu	116	ASP
13	Bz	116	ASP
13	C1	116	ASP
13	C2	116	ASP
13	CD	116	ASP
13	CE	116	ASP
13	CF	116	ASP
13	CK	116	ASP
13	CL	116	ASP
13	CM	116	ASP
13	CR	116	ASP
13	CS	116	ASP
13	CT	116	ASP
13	CY	116	ASP
13	CZ	116	ASP
13	Ca	116	ASP

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Mol	Chain	Res	Type
13	Cf	116	ASP
13	Cg	116	ASP
13	Ch	116	ASP
13	Cm	116	ASP
13	Cn	116	ASP
13	Co	116	ASP
13	Ct	116	ASP
13	Cu	116	ASP
13	Cv	116	ASP
13	FC	116	ASP
13	FD	116	ASP
13	FE	116	ASP
13	FF	116	ASP
13	FG	116	ASP
13	FH	116	ASP
13	FI	116	ASP
13	FJ	116	ASP
13	FK	116	ASP
13	FL	116	ASP
13	FM	116	ASP
13	FN	116	ASP
1	9	139	ALA
1	AI	165	ALA
1	AL	4	SER
1	AN	127	GLN
8	At	167	ASN
8	At	213	ILE
9	Av	83	ALA
9	Ax	160	GLN
6	WB	148	GLY
6	WB	163	SER
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

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Mol	Chain	Res	Type
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
1	ZB	165	ALA
1	ZB	209	ASN
1	ZC	209	ASN
1	ZD	209	ASN
1	ZE	209	ASN
11	ZI	375	MET
11	ZO	237	ILE
11	ZR	87	ASP
13	C4	125	ILE
13	C4	126	ILE
13	C8	125	ILE
13	C8	126	ILE
16	C0	232	VAL
16	DC	232	VAL
16	DF	232	VAL
13	DI	125	ILE
13	DI	126	ILE
13	DU	125	ILE
13	DU	126	ILE
16	DX	232	VAL
13	Da	125	ILE
13	Da	126	ILE
16	Dd	232	VAL
13	Dg	125	ILE
13	Dg	126	ILE
16	Dj	232	VAL
13	Dm	125	ILE
13	Dm	126	ILE
16	Dp	232	VAL
13	Ds	125	ILE
13	Ds	126	ILE
16	Dv	232	VAL
13	Dy	125	ILE
13	Dy	126	ILE

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Mol	Chain	Res	Type
16	D2	232	VAL
13	D5	125	ILE
13	D5	126	ILE
16	D8	232	VAL
13	EA	125	ILE
13	EA	126	ILE
16	B4	232	VAL
13	B7	125	ILE
13	B7	126	ILE
13	EE	125	ILE
13	EE	126	ILE
16	EI	232	VAL
13	EL	125	ILE
13	EL	126	ILE
16	EP	232	VAL
13	ES	125	ILE
13	ES	126	ILE
16	EW	232	VAL
13	EZ	125	ILE
13	EZ	126	ILE
16	Bb	232	VAL
13	Be	125	ILE
13	Be	126	ILE
16	Bi	232	VAL
13	Bl	125	ILE
13	Bl	126	ILE
16	Bp	232	VAL
13	Bs	125	ILE
13	Bs	126	ILE
16	Bw	232	VAL
13	Bz	125	ILE
13	Bz	126	ILE
13	C1	125	ILE
13	C1	126	ILE
16	CA	232	VAL
13	CD	125	ILE
13	CD	126	ILE
16	CH	232	VAL
13	CK	125	ILE
13	CK	126	ILE
16	CO	232	VAL
13	CR	125	ILE

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Mol	Chain	Res	Type
13	CR	126	ILE
16	CV	232	VAL
13	CY	125	ILE
13	CY	126	ILE
16	Cc	232	VAL
13	Cf	125	ILE
13	Cf	126	ILE
16	Cj	232	VAL
13	Cm	125	ILE
13	Cm	126	ILE
16	Cq	232	VAL
13	Ct	125	ILE
13	Ct	126	ILE
16	Cx	232	VAL
16	Eq	232	VAL
16	Er	232	VAL
16	Es	232	VAL
16	Et	232	VAL
16	Eu	232	VAL
16	Ev	232	VAL
16	Ew	232	VAL
16	E5	232	VAL
13	FC	125	ILE
13	FC	126	ILE
13	FD	125	ILE
13	FD	126	ILE
13	FE	125	ILE
13	FE	126	ILE
13	FF	125	ILE
13	FF	126	ILE
13	FG	125	ILE
13	FG	126	ILE
13	FH	125	ILE
13	FH	126	ILE
1	0	127	GLN
1	2	49	ILE
1	3	49	ILE
1	4	49	ILE
1	4	139	ALA
1	4	140	ILE
1	5	49	ILE
5	AA	151	PRO

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Mol	Chain	Res	Type
1	AF	127	GLN
1	AL	3	SER
1	AM	127	GLN
8	At	189	PRO
6	UI	162	PRO
6	UJ	162	PRO
6	UK	162	PRO
6	UL	162	PRO
6	UM	162	PRO
6	UN	162	PRO
6	UO	162	PRO
6	UP	162	PRO
6	WB	146	THR
6	WB	164	LEU
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
11	ZL	374	ASN
13	C4	59	ASP
13	C8	59	ASP
13	DI	59	ASP
13	DU	59	ASP
13	Da	59	ASP
13	Dg	59	ASP
13	Dm	59	ASP
13	Ds	59	ASP
13	Dy	59	ASP
13	D5	59	ASP
13	EA	59	ASP
13	B7	59	ASP
13	EE	59	ASP
13	EL	59	ASP
13	ES	59	ASP
13	EZ	59	ASP
13	Be	59	ASP

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Mol	Chain	Res	Type
13	Bl	59	ASP
13	Bs	59	ASP
13	Bz	59	ASP
13	C1	59	ASP
13	CD	59	ASP
13	CK	59	ASP
13	CR	59	ASP
13	CY	59	ASP
13	Cf	59	ASP
13	Cm	59	ASP
13	Ct	59	ASP
13	FC	59	ASP
13	FD	59	ASP
13	FE	59	ASP
13	FF	59	ASP
13	FG	59	ASP
13	FH	59	ASP
1	6	49	ILE
1	6	58	GLU
1	7	49	ILE
1	7	138	PRO
1	8	49	ILE
1	9	49	ILE
1	AG	127	GLN
1	AI	127	GLN
1	AK	127	GLN
1	AL	127	GLN
6	UI	163	SER
6	UJ	163	SER
6	UK	163	SER
6	UL	163	SER
6	UM	163	SER
6	UN	163	SER
6	UO	163	SER
6	UP	163	SER
6	WA	182	PRO
6	WB	182	PRO
6	WD	165	PHE
6	WD	182	PRO
6	WE	182	PRO
6	WF	182	PRO
6	WG	182	PRO

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Mol	Chain	Res	Type
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
1	ZA	49	ILE
1	ZA	139	ALA
1	ZD	139	ALA
11	ZO	142	THR
11	ZP	374	ASN
14	C6	97	ILE
16	C0	236	LEU
14	DA	97	ILE
16	DC	236	LEU
16	DF	236	LEU
14	DG	97	ILE
16	DX	236	LEU
14	DY	97	ILE
16	Dd	236	LEU
14	De	97	ILE
16	Dj	236	LEU
14	Dk	97	ILE
16	Dp	236	LEU
14	Dq	97	ILE
16	Dv	236	LEU
14	Dw	97	ILE
16	D2	236	LEU

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Mol	Chain	Res	Type
14	D3	97	ILE
16	D8	236	LEU
14	D9	97	ILE
16	B4	236	LEU
14	B5	97	ILE
14	EC	97	ILE
16	EI	236	LEU
14	EJ	97	ILE
16	EP	236	LEU
14	EQ	97	ILE
16	EW	236	LEU
14	EX	97	ILE
16	Bb	236	LEU
14	Bc	97	ILE
16	Bi	236	LEU
14	Bj	97	ILE
16	Bp	236	LEU
14	Bq	97	ILE
16	Bw	236	LEU
14	Bx	97	ILE
16	CA	236	LEU
14	CB	97	ILE
16	CH	236	LEU
14	CI	97	ILE
16	CO	236	LEU
14	CP	97	ILE
16	CV	236	LEU
14	CW	97	ILE
16	Cc	236	LEU
14	Cd	97	ILE
16	Cj	236	LEU
14	Ck	97	ILE
16	Cq	236	LEU
14	Cr	97	ILE
16	Cx	236	LEU
14	Cy	97	ILE
16	Eq	236	LEU
16	Er	236	LEU
16	Es	236	LEU
16	Et	236	LEU
16	Eu	236	LEU
16	Ev	236	LEU

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Mol	Chain	Res	Type
16	Ew	236	LEU
14	Ex	97	ILE
14	Ey	97	ILE
14	Ez	97	ILE
14	E1	97	ILE
14	E2	97	ILE
14	E3	97	ILE
14	E4	97	ILE
16	E5	236	LEU
1	1	127	GLN
1	7	210	GLY
2	A	172	ASN
1	AH	127	GLN
1	AJ	127	GLN
9	Av	162	PRO
2	B	172	ASN
2	C	172	ASN
2	D	172	ASN
2	E	172	ASN
2	F	172	ASN
2	G	172	ASN
2	H	172	ASN
2	I	172	ASN
2	J	172	ASN
2	K	172	ASN
2	L	172	ASN
2	M	172	ASN
2	N	172	ASN
2	O	172	ASN
2	P	172	ASN
2	Q	172	ASN
2	R	172	ASN
2	S	172	ASN
2	T	172	ASN
2	U	172	ASN
2	V	172	ASN
2	W	172	ASN
6	WK	168	GLU
6	WR	121	PHE
6	WT	163	SER
2	X	172	ASN
2	Y	172	ASN

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Mol	Chain	Res	Type
2	Z	172	ASN
16	DX	237	GLU
16	Dp	237	GLU
16	EW	237	GLU
16	Bb	237	GLU
16	Bi	237	GLU
16	Bw	237	GLU
16	CO	237	GLU
16	Ev	237	GLU
1	3	139	ALA
8	At	187	ALA
10	BE	58	ALA
6	WC	182	PRO
6	WE	221	THR
6	WG	163	SER
11	ZO	375	MET
13	C5	127	THR
13	C9	127	THR
16	C0	235	PRO
16	C0	237	GLU
16	DC	235	PRO
16	DC	237	GLU
16	DF	235	PRO
16	DF	237	GLU
13	DJ	127	THR
13	DV	127	THR
16	DX	235	PRO
13	Db	127	THR
16	Dd	235	PRO
16	Dd	237	GLU
13	Dh	127	THR
16	Dj	235	PRO
16	Dj	237	GLU
13	Dn	127	THR
16	Dp	235	PRO
13	Dt	127	THR
16	Dv	235	PRO
16	Dv	237	GLU
13	Dz	127	THR
16	D2	235	PRO
16	D2	237	GLU
13	D6	127	THR

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Mol	Chain	Res	Type
16	D8	235	PRO
16	D8	237	GLU
13	EB	127	THR
13	B1	127	THR
16	B4	235	PRO
16	B4	237	GLU
13	B8	127	THR
13	EF	127	THR
16	EI	235	PRO
16	EI	237	GLU
13	EM	127	THR
16	EP	235	PRO
16	EP	237	GLU
13	ET	127	THR
16	EW	235	PRO
13	BY	127	THR
16	Bb	235	PRO
13	Bf	127	THR
16	Bi	235	PRO
13	Bm	127	THR
16	Bp	235	PRO
16	Bp	237	GLU
13	Bt	127	THR
16	Bw	235	PRO
13	C2	127	THR
16	CA	235	PRO
16	CA	237	GLU
13	CE	127	THR
16	CH	235	PRO
16	CH	237	GLU
13	CL	127	THR
16	CO	235	PRO
13	CS	127	THR
16	CV	235	PRO
16	CV	237	GLU
13	CZ	127	THR
16	Cc	235	PRO
16	Cc	237	GLU
13	Cg	127	THR
16	Cj	235	PRO
16	Cj	237	GLU
13	Cn	127	THR

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Mol	Chain	Res	Type
16	Cq	235	PRO
16	Cq	237	GLU
13	Cu	127	THR
16	Cx	235	PRO
16	Cx	237	GLU
16	Eq	235	PRO
16	Eq	237	GLU
16	Er	235	PRO
16	Er	237	GLU
16	Es	235	PRO
16	Es	237	GLU
16	Et	235	PRO
16	Et	237	GLU
16	Eu	235	PRO
16	Eu	237	GLU
16	Ev	235	PRO
16	Ew	235	PRO
16	Ew	237	GLU
16	E5	235	PRO
16	E5	237	GLU
13	FI	127	THR
13	FJ	127	THR
13	FK	127	THR
13	FL	127	THR
13	FM	127	THR
13	FN	127	THR
5	AA	149	GLY
5	AE	132	GLY
6	WA	160	PRO
6	WF	162	PRO
6	WL	148	GLY
6	WS	148	GLY
6	WT	148	GLY
11	ZI	325	GLY
6	WA	148	GLY
6	WP	123	ILE
6	WR	148	GLY
9	Ay	229	VAL
6	WP	160	PRO
6	WT	161	LYS
1	ZC	138	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	205/215 (95%)	198 (97%)	7 (3%)	32	54
1	1	209/215 (97%)	201 (96%)	8 (4%)	28	50
1	2	215/215 (100%)	212 (99%)	3 (1%)	62	76
1	3	215/215 (100%)	211 (98%)	4 (2%)	52	70
1	4	215/215 (100%)	211 (98%)	4 (2%)	52	70
1	5	215/215 (100%)	211 (98%)	4 (2%)	52	70
1	6	215/215 (100%)	210 (98%)	5 (2%)	45	65
1	7	215/215 (100%)	214 (100%)	1 (0%)	86	90
1	8	215/215 (100%)	213 (99%)	2 (1%)	75	83
1	9	215/215 (100%)	211 (98%)	4 (2%)	52	70
1	AF	209/215 (97%)	204 (98%)	5 (2%)	44	64
1	AG	210/215 (98%)	203 (97%)	7 (3%)	33	55
1	AH	211/215 (98%)	201 (95%)	10 (5%)	22	45
1	AI	209/215 (97%)	200 (96%)	9 (4%)	25	48
1	AJ	210/215 (98%)	202 (96%)	8 (4%)	28	50
1	AK	200/215 (93%)	196 (98%)	4 (2%)	50	69
1	AL	205/215 (95%)	199 (97%)	6 (3%)	37	58
1	AM	205/215 (95%)	197 (96%)	8 (4%)	27	50
1	AN	205/215 (95%)	201 (98%)	4 (2%)	50	69
1	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	83
1	ZB	215/215 (100%)	207 (96%)	8 (4%)	29	51
1	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	76
1	ZD	215/215 (100%)	212 (99%)	3 (1%)	62	76
1	ZE	215/215 (100%)	214 (100%)	1 (0%)	86	90
2	A	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	B	170/186 (91%)	163 (96%)	7 (4%)	26	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	D	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	E	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	F	170/186 (91%)	162 (95%)	8 (5%)	22	45
2	G	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	H	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	I	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	J	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	K	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	L	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	M	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	N	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	O	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	P	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	Q	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	R	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	S	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	T	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	U	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	V	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	W	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	X	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	Y	170/186 (91%)	163 (96%)	7 (4%)	26	49
2	Z	170/186 (91%)	163 (96%)	7 (4%)	26	49
3	A0	102/113 (90%)	96 (94%)	6 (6%)	16	39
3	A6	110/113 (97%)	106 (96%)	4 (4%)	30	52
3	A7	101/113 (89%)	99 (98%)	2 (2%)	50	69
3	A8	103/113 (91%)	96 (93%)	7 (7%)	13	34
3	A9	104/113 (92%)	102 (98%)	2 (2%)	52	70
4	A1	68/79 (86%)	64 (94%)	4 (6%)	16	39
4	A2	70/79 (89%)	65 (93%)	5 (7%)	12	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A3	70/79 (89%)	66 (94%)	4 (6%)	17	40
4	A4	70/79 (89%)	66 (94%)	4 (6%)	17	40
4	A5	69/79 (87%)	65 (94%)	4 (6%)	17	39
4	Az	45/79 (57%)	40 (89%)	5 (11%)	5	19
5	AA	190/193 (98%)	187 (98%)	3 (2%)	58	74
5	AB	191/193 (99%)	188 (98%)	3 (2%)	58	74
5	AC	192/193 (100%)	187 (97%)	5 (3%)	41	61
5	AD	192/193 (100%)	190 (99%)	2 (1%)	73	82
5	AE	191/193 (99%)	190 (100%)	1 (0%)	86	90
6	AO	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AP	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AQ	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AR	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AS	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AT	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AU	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AV	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AW	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AX	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AY	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	AZ	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Aa	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ac	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ad	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ae	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Af	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ag	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ah	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ai	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Aj	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ak	141/467 (30%)	134 (95%)	7 (5%)	20	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Al	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Am	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	An	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ao	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ap	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	B0	26/467 (6%)	26 (100%)	0	100	100
6	B3	26/467 (6%)	26 (100%)	0	100	100
6	BG	8/467 (2%)	8 (100%)	0	100	100
6	BH	11/467 (2%)	10 (91%)	1 (9%)	7	25
6	BI	14/467 (3%)	12 (86%)	2 (14%)	2	14
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	33
6	BP	11/467 (2%)	11 (100%)	0	100	100
6	BQ	15/467 (3%)	14 (93%)	1 (7%)	13	35
6	BR	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BS	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BT	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BU	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BV	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BW	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	BX	141/467 (30%)	134 (95%)	7 (5%)	20	43
6	Ba	26/467 (6%)	26 (100%)	0	100	100
6	Bh	26/467 (6%)	26 (100%)	0	100	100
6	Bo	26/467 (6%)	26 (100%)	0	100	100
6	Bv	26/467 (6%)	26 (100%)	0	100	100
6	CG	26/467 (6%)	26 (100%)	0	100	100
6	CN	26/467 (6%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	CU	26/467 (6%)	26 (100%)	0	100	100
6	Cb	26/467 (6%)	26 (100%)	0	100	100
6	Ci	26/467 (6%)	26 (100%)	0	100	100
6	Cp	26/467 (6%)	26 (100%)	0	100	100
6	Cw	26/467 (6%)	26 (100%)	0	100	100
6	DE	26/467 (6%)	26 (100%)	0	100	100
6	DL	26/467 (6%)	26 (100%)	0	100	100
6	EH	26/467 (6%)	26 (100%)	0	100	100
6	EO	26/467 (6%)	26 (100%)	0	100	100
6	EV	26/467 (6%)	26 (100%)	0	100	100
6	Ea	26/467 (6%)	26 (100%)	0	100	100
6	Eb	26/467 (6%)	26 (100%)	0	100	100
6	Ec	26/467 (6%)	26 (100%)	0	100	100
6	Ed	26/467 (6%)	26 (100%)	0	100	100
6	Ee	26/467 (6%)	26 (100%)	0	100	100
6	Ef	26/467 (6%)	26 (100%)	0	100	100
6	Eg	26/467 (6%)	26 (100%)	0	100	100
6	Eh	26/467 (6%)	26 (100%)	0	100	100
6	Ei	26/467 (6%)	26 (100%)	0	100	100
6	Ej	26/467 (6%)	26 (100%)	0	100	100
6	Ek	26/467 (6%)	26 (100%)	0	100	100
6	El	26/467 (6%)	26 (100%)	0	100	100
6	Em	26/467 (6%)	26 (100%)	0	100	100
6	En	26/467 (6%)	26 (100%)	0	100	100
6	Eo	26/467 (6%)	26 (100%)	0	100	100
6	Ep	26/467 (6%)	26 (100%)	0	100	100
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	45
6	UM	128/467 (27%)	123 (96%)	5 (4%)	27	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	45
6	WA	95/467 (20%)	91 (96%)	4 (4%)	25	48
6	WB	93/467 (20%)	87 (94%)	6 (6%)	14	36
6	WC	91/467 (20%)	83 (91%)	8 (9%)	8	26
6	WD	92/467 (20%)	88 (96%)	4 (4%)	25	48
6	WE	94/467 (20%)	87 (93%)	7 (7%)	11	31
6	WF	93/467 (20%)	86 (92%)	7 (8%)	11	31
6	WG	94/467 (20%)	87 (93%)	7 (7%)	11	31
6	WH	79/467 (17%)	75 (95%)	4 (5%)	20	43
6	WI	79/467 (17%)	73 (92%)	6 (8%)	11	31
6	WJ	83/467 (18%)	79 (95%)	4 (5%)	21	44
6	WK	82/467 (18%)	77 (94%)	5 (6%)	15	38
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	43
6	WP	83/467 (18%)	77 (93%)	6 (7%)	12	32
6	WQ	93/467 (20%)	91 (98%)	2 (2%)	47	66
6	WR	93/467 (20%)	86 (92%)	7 (8%)	11	31
6	WS	93/467 (20%)	87 (94%)	6 (6%)	14	36
6	WT	93/467 (20%)	86 (92%)	7 (8%)	11	31
6	WU	94/467 (20%)	90 (96%)	4 (4%)	25	48
6	WV	92/467 (20%)	83 (90%)	9 (10%)	6	22
6	WW	93/467 (20%)	85 (91%)	8 (9%)	8	27
7	Ab	74/74 (100%)	73 (99%)	1 (1%)	62	76
7	Aq	74/74 (100%)	73 (99%)	1 (1%)	62	76
7	Ar	74/74 (100%)	74 (100%)	0	100	100
7	As	74/74 (100%)	73 (99%)	1 (1%)	62	76
8	At	210/221 (95%)	204 (97%)	6 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Au	177/204 (87%)	170 (96%)	7 (4%)	27	49
9	Av	179/204 (88%)	172 (96%)	7 (4%)	27	50
9	Aw	178/204 (87%)	173 (97%)	5 (3%)	38	59
9	Ax	178/204 (87%)	172 (97%)	6 (3%)	32	54
9	Ay	179/204 (88%)	175 (98%)	4 (2%)	47	66
10	BA	104/105 (99%)	104 (100%)	0	100	100
10	BB	104/105 (99%)	103 (99%)	1 (1%)	73	82
10	BC	104/105 (99%)	104 (100%)	0	100	100
10	BD	104/105 (99%)	102 (98%)	2 (2%)	52	70
10	BE	104/105 (99%)	101 (97%)	3 (3%)	37	58
10	BF	104/105 (99%)	100 (96%)	4 (4%)	28	50
11	ZF	321/323 (99%)	310 (97%)	11 (3%)	32	54
11	ZG	321/323 (99%)	306 (95%)	15 (5%)	22	45
11	ZH	321/323 (99%)	309 (96%)	12 (4%)	29	51
11	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	ZJ	321/323 (99%)	313 (98%)	8 (2%)	42	63
11	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	56
11	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	59
11	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	56
11	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	63
11	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	45
11	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	59
11	ZR	321/323 (99%)	313 (98%)	8 (2%)	42	63
11	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	ZT	321/323 (99%)	316 (98%)	5 (2%)	58	74
11	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	79
11	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	79
11	ZW	321/323 (99%)	308 (96%)	13 (4%)	27	49
11	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	83
11	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	74
11	Za	321/323 (99%)	316 (98%)	5 (2%)	58	74
11	Zb	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	54
11	Zd	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	Ze	321/323 (99%)	312 (97%)	9 (3%)	38	59
11	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	66
11	Zg	321/323 (99%)	315 (98%)	6 (2%)	52	70
11	Zh	321/323 (99%)	313 (98%)	8 (2%)	42	63
12	a	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	b	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	c	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	d	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	e	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	f	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	g	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	h	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	i	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	j	248/294 (84%)	240 (97%)	8 (3%)	34	55
12	k	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	l	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	m	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	n	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	o	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	p	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	q	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	r	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	s	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	t	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	u	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	v	248/294 (84%)	238 (96%)	10 (4%)	27	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	w	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	x	248/294 (84%)	238 (96%)	10 (4%)	27	49
12	y	248/294 (84%)	239 (96%)	9 (4%)	30	52
12	z	248/294 (84%)	238 (96%)	10 (4%)	27	49
13	B1	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	B2	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	B7	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	B8	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	B9	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	BY	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	BZ	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Be	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Bf	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Bg	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Bl	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Bm	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Bn	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Bs	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Bt	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Bu	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Bz	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	C1	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	C2	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	C3	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	C4	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	C5	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	C8	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	C9	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	CD	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	CE	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	CF	76/113 (67%)	74 (97%)	2 (3%)	41	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	CK	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	CL	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	CM	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	CR	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	CS	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	CT	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	CY	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	CZ	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Ca	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Cf	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Cg	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Ch	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Cm	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Cn	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Co	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Ct	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Cu	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Cv	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	D1	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	D5	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	D6	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	D7	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DD	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DI	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	DJ	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	DK	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DM	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DN	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DO	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DP	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DQ	76/113 (67%)	74 (97%)	2 (3%)	41	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	DR	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DS	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DT	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	DU	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	DV	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	DW	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Da	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Db	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Dc	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Dg	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Dh	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Di	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Dm	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Dn	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Do	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Ds	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Dt	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	Du	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	Dy	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	Dz	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	EA	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	EB	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	EE	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	EF	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	EG	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	EL	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	EM	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	EN	76/113 (67%)	74 (97%)	2 (3%)	41	61
13	ES	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	ET	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	EU	76/113 (67%)	74 (97%)	2 (3%)	41	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	EZ	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FC	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FD	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FE	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FF	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FG	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FH	76/113 (67%)	72 (95%)	4 (5%)	19	42
13	FI	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	FJ	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	FK	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	FL	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	FM	76/113 (67%)	75 (99%)	1 (1%)	65	77
13	FN	76/113 (67%)	75 (99%)	1 (1%)	65	77
14	B5	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Bc	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Bj	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Bq	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Bx	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	C6	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	CB	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	CI	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	CP	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	CW	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Cd	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Ck	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Cr	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Cy	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	D3	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	D9	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	DA	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	DG	265/282 (94%)	257 (97%)	8 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	DY	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	De	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Dk	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Dq	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Dw	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	E1	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	E2	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	E3	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	E4	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	EC	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	EJ	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	EQ	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	EX	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Ex	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Ey	265/282 (94%)	257 (97%)	8 (3%)	36	57
14	Ez	265/282 (94%)	257 (97%)	8 (3%)	36	57
15	B6	104/104 (100%)	104 (100%)	0	100	100
15	Bd	104/104 (100%)	104 (100%)	0	100	100
15	Bk	104/104 (100%)	104 (100%)	0	100	100
15	Br	104/104 (100%)	104 (100%)	0	100	100
15	By	104/104 (100%)	104 (100%)	0	100	100
15	C7	104/104 (100%)	104 (100%)	0	100	100
15	CC	104/104 (100%)	104 (100%)	0	100	100
15	CJ	104/104 (100%)	104 (100%)	0	100	100
15	CQ	104/104 (100%)	104 (100%)	0	100	100
15	CX	104/104 (100%)	104 (100%)	0	100	100
15	Ce	104/104 (100%)	104 (100%)	0	100	100
15	Cl	104/104 (100%)	104 (100%)	0	100	100
15	Cs	104/104 (100%)	104 (100%)	0	100	100
15	Cz	104/104 (100%)	104 (100%)	0	100	100
15	D0	104/104 (100%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	D4	104/104 (100%)	104 (100%)	0	100	100
15	DB	104/104 (100%)	104 (100%)	0	100	100
15	DH	104/104 (100%)	104 (100%)	0	100	100
15	DZ	104/104 (100%)	104 (100%)	0	100	100
15	Df	104/104 (100%)	104 (100%)	0	100	100
15	Dl	104/104 (100%)	104 (100%)	0	100	100
15	Dr	104/104 (100%)	104 (100%)	0	100	100
15	Dx	104/104 (100%)	104 (100%)	0	100	100
15	E0	104/104 (100%)	104 (100%)	0	100	100
15	E6	104/104 (100%)	104 (100%)	0	100	100
15	E7	104/104 (100%)	104 (100%)	0	100	100
15	E8	104/104 (100%)	104 (100%)	0	100	100
15	E9	104/104 (100%)	104 (100%)	0	100	100
15	ED	104/104 (100%)	104 (100%)	0	100	100
15	EK	104/104 (100%)	104 (100%)	0	100	100
15	ER	104/104 (100%)	104 (100%)	0	100	100
15	EY	104/104 (100%)	104 (100%)	0	100	100
15	FA	104/104 (100%)	104 (100%)	0	100	100
15	FB	104/104 (100%)	104 (100%)	0	100	100
16	B4	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Bb	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Bi	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Bp	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Bw	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	C0	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	CA	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	CH	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	CO	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	CV	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Cc	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Cj	272/301 (90%)	264 (97%)	8 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Cq	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Cx	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	D2	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	D8	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	DC	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	DF	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	DX	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Dd	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Dj	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Dp	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Dv	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	E5	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	EI	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	EP	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	EW	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Eq	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Er	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Es	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Et	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Eu	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Ev	272/301 (90%)	264 (97%)	8 (3%)	37	58
16	Ew	272/301 (90%)	264 (97%)	8 (3%)	37	58
All	All	67515/117432 (58%)	65434 (97%)	2081 (3%)	37	56

All (2081) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	1	MET
1	0	36	ARG
1	0	50	ARG
1	0	52	PRO
1	0	73	ARG
1	0	128	LEU
1	0	185	GLU

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Mol	Chain	Res	Type
1	1	1	MET
1	1	36	ARG
1	1	62	LEU
1	1	106	MET
1	1	119	SER
1	1	164	GLN
1	1	206	PRO
1	1	241	GLU
1	2	91	ASN
1	2	204	SER
1	2	238	ARG
1	3	43	ASP
1	3	109	ASP
1	3	153	ARG
1	3	244	SER
1	4	64	SER
1	4	204	SER
1	4	209	ASN
1	4	259	GLN
1	5	4	SER
1	5	137	GLN
1	5	154	ASP
1	5	181	ASP
1	6	59	GLN
1	6	73	ARG
1	6	78	GLU
1	6	109	ASP
1	6	244	SER
1	7	73	ARG
1	8	58	GLU
1	8	100	GLN
1	9	106	MET
1	9	125	ASN
1	9	137	GLN
1	9	162	GLN
2	A	22	CYS
2	A	103	SER
2	A	106	PHE
2	A	124	MET
2	A	145	SER
2	A	176	GLU
2	A	202	ASP

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Mol	Chain	Res	Type
3	A0	4	ARG
3	A0	18	LEU
3	A0	65	LEU
3	A0	104	ARG
3	A0	113	SER
3	A0	125	SER
4	A1	15	GLN
4	A1	19	MET
4	A1	75	MET
4	A1	84	MET
4	A2	7	ILE
4	A2	11	ILE
4	A2	14	LEU
4	A2	15	GLN
4	A2	70	ASP
4	A3	15	GLN
4	A3	19	MET
4	A3	33	SER
4	A3	81	SER
4	A4	15	GLN
4	A4	19	MET
4	A4	101	SER
4	A4	102	MET
4	A5	15	GLN
4	A5	19	MET
4	A5	57	GLU
4	A5	91	LYS
3	A6	34	ASP
3	A6	101	ASP
3	A6	113	SER
3	A6	125	SER
3	A7	47	SER
3	A7	55	ARG
3	A8	48	GLU
3	A8	65	LEU
3	A8	69	SER
3	A8	71	HIS
3	A8	72	HIS
3	A8	91	ASP
3	A8	128	LYS
3	A9	47	SER
3	A9	76	GLN

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Mol	Chain	Res	Type
5	AA	126	PRO
5	AA	150	ASP
5	AA	247	LEU
5	AB	70	GLN
5	AB	72	ASP
5	AB	153	ASN
5	AC	70	GLN
5	AC	85	ASP
5	AC	189	ARG
5	AC	225	ARG
5	AC	236	SER
5	AD	140	ASP
5	AD	169	ASN
5	AE	175	ASP
1	AF	4	SER
1	AF	19	MET
1	AF	36	ARG
1	AF	44	LEU
1	AF	154	ASP
1	AG	16	GLN
1	AG	36	ARG
1	AG	73	ARG
1	AG	137	GLN
1	AG	169	GLN
1	AG	222	SER
1	AG	251	ASP
1	AH	1	MET
1	AH	44	LEU
1	AH	66	LEU
1	AH	87	SER
1	AH	93	LYS
1	AH	100	GLN
1	AH	148	SER
1	AH	154	ASP
1	AH	245	LYS
1	AH	251	ASP
1	AI	4	SER
1	AI	30	SER
1	AI	123	ASP
1	AI	148	SER
1	AI	169	GLN
1	AI	179	MET

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

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

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

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Mol	Chain	Res	Type
6	Ac	294	ARG
6	Ac	359	GLN
6	Ac	377	MET
6	Ac	381	ASP
6	Ac	417	ARG
6	Ac	424	ASP
6	Ad	274	ASN
6	Ad	294	ARG
6	Ad	359	GLN
6	Ad	377	MET
6	Ad	381	ASP
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

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Mol	Chain	Res	Type
6	Ai	294	ARG
6	Ai	359	GLN
6	Ai	377	MET
6	Ai	381	ASP
6	Ai	417	ARG
6	Ai	424	ASP
6	Aj	274	ASN
6	Aj	294	ARG
6	Aj	359	GLN
6	Aj	377	MET
6	Aj	381	ASP
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

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Mol	Chain	Res	Type
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
7	Aq	47	MET
7	As	9	MET
8	At	36	ARG
8	At	86	PHE
8	At	185	MET
8	At	214	PHE
8	At	227	MET
8	At	229	MET
9	Au	38	TRP
9	Au	123	MET
9	Au	129	LYS
9	Au	155	ASN
9	Au	160	GLN
9	Au	190	PHE
9	Au	213	PRO
9	Av	75	ARG
9	Av	102	SER
9	Av	106	ASP
9	Av	116	PHE
9	Av	140	ARG
9	Av	160	GLN
9	Av	162	PRO
9	Aw	143	ARG
9	Aw	152	ARG
9	Aw	177	SER
9	Aw	187	PHE
9	Aw	190	PHE
9	Ax	113	TYR
9	Ax	143	ARG

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Mol	Chain	Res	Type
9	Ax	187	PHE
9	Ax	205	MET
9	Ax	238	SER
9	Ax	241	GLN
9	Ay	117	SER
9	Ay	190	PHE
9	Ay	224	MET
9	Ay	230	ASP
4	Az	15	GLN
4	Az	19	MET
4	Az	74	ASP
4	Az	79	SER
4	Az	101	SER
2	B	22	CYS
2	B	103	SER
2	B	106	PHE
2	B	124	MET
2	B	145	SER
2	B	176	GLU
2	B	202	ASP
10	BB	123	LYS
10	BD	30	ASN
10	BD	120	ASN
10	BE	20	ARG
10	BE	52	ASP
10	BE	84	LEU
10	BF	86	ASP
10	BF	88	ASN
10	BF	125	MET
10	BF	127	LEU
6	BH	324	ASN
6	BI	318	ASN
6	BI	319	GLN
6	BO	319	GLN
6	BQ	318	ASN
6	BR	274	ASN
6	BR	294	ARG
6	BR	359	GLN
6	BR	377	MET
6	BR	381	ASP
6	BR	417	ARG
6	BR	424	ASP

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	C	22	CYS
2	C	103	SER
2	C	106	PHE
2	C	124	MET
2	C	145	SER
2	C	176	GLU
2	C	202	ASP
2	D	22	CYS
2	D	103	SER
2	D	106	PHE
2	D	124	MET
2	D	145	SER
2	D	176	GLU
2	D	202	ASP
2	E	22	CYS
2	E	103	SER
2	E	106	PHE
2	E	124	MET
2	E	145	SER
2	E	176	GLU
2	E	202	ASP
2	F	22	CYS
2	F	36	THR
2	F	103	SER
2	F	106	PHE
2	F	124	MET
2	F	145	SER
2	F	176	GLU
2	F	202	ASP
2	G	22	CYS
2	G	103	SER
2	G	106	PHE
2	G	124	MET
2	G	145	SER
2	G	176	GLU
2	G	202	ASP
2	H	22	CYS
2	H	103	SER
2	H	106	PHE
2	H	124	MET
2	H	145	SER
2	H	176	GLU

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

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

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Mol	Chain	Res	Type
2	T	202	ASP
2	U	22	CYS
2	U	103	SER
2	U	106	PHE
2	U	124	MET
2	U	145	SER
2	U	176	GLU
2	U	202	ASP
6	UI	98	LEU
6	UI	127	SER
6	UI	154	ARG
6	UI	159	MET
6	UI	165	PHE
6	UJ	98	LEU
6	UJ	127	SER
6	UJ	154	ARG
6	UJ	159	MET
6	UJ	165	PHE
6	UK	98	LEU
6	UK	127	SER
6	UK	154	ARG
6	UK	159	MET
6	UK	165	PHE
6	UL	98	LEU
6	UL	127	SER
6	UL	154	ARG
6	UL	159	MET
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

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Mol	Chain	Res	Type
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
2	V	22	CYS
2	V	103	SER
2	V	106	PHE
2	V	124	MET
2	V	145	SER
2	V	176	GLU
2	V	202	ASP
2	W	22	CYS
2	W	103	SER
2	W	106	PHE
2	W	124	MET
2	W	145	SER
2	W	176	GLU
2	W	202	ASP
6	WA	114	GLU
6	WA	128	GLU
6	WA	167	ARG
6	WA	170	LYS
6	WB	121	PHE
6	WB	128	GLU
6	WB	134	ARG
6	WB	137	GLU
6	WB	164	LEU
6	WB	169	GLN
6	WC	115	LEU
6	WC	120	LYS
6	WC	128	GLU
6	WC	134	ARG
6	WC	164	LEU
6	WC	166	VAL
6	WC	168	GLU
6	WC	170	LYS
6	WD	114	GLU
6	WD	115	LEU

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

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

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Mol	Chain	Res	Type
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
2	X	22	CYS
2	X	103	SER
2	X	106	PHE
2	X	124	MET
2	X	145	SER
2	X	176	GLU
2	X	202	ASP
2	Y	22	CYS
2	Y	103	SER
2	Y	106	PHE
2	Y	124	MET
2	Y	145	SER
2	Y	176	GLU
2	Y	202	ASP
2	Z	22	CYS
2	Z	103	SER
2	Z	106	PHE
2	Z	124	MET
2	Z	145	SER
2	Z	176	GLU
2	Z	202	ASP
1	ZA	136	VAL
1	ZA	248	SER
1	ZB	1	MET
1	ZB	4	SER

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Mol	Chain	Res	Type
1	ZB	58	GLU
1	ZB	73	ARG
1	ZB	119	SER
1	ZB	137	GLN
1	ZB	143	PRO
1	ZB	244	SER
1	ZC	123	ASP
1	ZC	136	VAL
1	ZC	244	SER
1	ZD	64	SER
1	ZD	66	LEU
1	ZD	240	TYR
1	ZE	141	THR
11	ZF	3	PHE
11	ZF	60	ASP
11	ZF	87	ASP
11	ZF	134	PRO
11	ZF	229	THR
11	ZF	265	ASN
11	ZF	280	ASN
11	ZF	284	TYR
11	ZF	289	LEU
11	ZF	352	ASN
11	ZF	355	LYS
11	ZG	3	PHE
11	ZG	38	SER
11	ZG	188	ASP
11	ZG	189	SER
11	ZG	227	SER
11	ZG	234	GLU
11	ZG	260	SER
11	ZG	262	SER
11	ZG	265	ASN
11	ZG	267	MET
11	ZG	288	ASP
11	ZG	296	ASN
11	ZG	350	SER
11	ZG	352	ASN
11	ZG	397	ASN
11	ZH	34	SER
11	ZH	154	MET
11	ZH	227	SER

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Mol	Chain	Res	Type
11	ZH	260	SER
11	ZH	281	GLN
11	ZH	284	TYR
11	ZH	288	ASP
11	ZH	331	ASP
11	ZH	355	LYS
11	ZH	375	MET
11	ZH	380	ARG
11	ZH	399	LEU
11	ZI	99	GLN
11	ZI	195	ASP
11	ZI	197	ASN
11	ZI	260	SER
11	ZI	352	ASN
11	ZI	358	ASN
11	ZJ	42	MET
11	ZJ	46	SER
11	ZJ	103	ASP
11	ZJ	107	ASN
11	ZJ	195	ASP
11	ZJ	233	ASN
11	ZJ	280	ASN
11	ZJ	331	ASP
11	ZK	3	PHE
11	ZK	268	GLN
11	ZK	297	ASP
11	ZK	305	SER
11	ZK	331	ASP
11	ZK	338	GLN
11	ZL	78	SER
11	ZL	84	ARG
11	ZL	196	MET
11	ZL	234	GLU
11	ZL	267	MET
11	ZL	291	SER
11	ZL	338	GLN
11	ZL	368	LEU
11	ZL	370	LYS
11	ZL	382	TYR
11	ZM	53	LYS
11	ZM	89	ASN
11	ZM	153	SER

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Mol	Chain	Res	Type
11	ZM	200	PHE
11	ZM	214	ASP
11	ZM	282	ASN
11	ZM	352	ASN
11	ZM	369	SER
11	ZM	370	LYS
11	ZN	43	PHE
11	ZN	78	SER
11	ZN	103	ASP
11	ZN	143	LEU
11	ZN	148	SER
11	ZN	157	ASN
11	ZN	216	SER
11	ZN	297	ASP
11	ZN	367	ASP
11	ZN	396	LEU
11	ZO	2	SER
11	ZO	74	ASP
11	ZO	174	ASP
11	ZO	178	TYR
11	ZO	235	ASN
11	ZO	237	ILE
11	ZO	331	ASP
11	ZO	375	MET
11	ZP	42	MET
11	ZP	63	ASP
11	ZP	74	ASP
11	ZP	95	SER
11	ZP	126	PRO
11	ZP	162	ASP
11	ZP	227	SER
11	ZP	275	ASN
11	ZP	288	ASP
11	ZP	292	TYR
11	ZP	331	ASP
11	ZP	340	SER
11	ZP	369	SER
11	ZP	370	LYS
11	ZP	393	ASP
11	ZQ	46	SER
11	ZQ	101	LYS
11	ZQ	189	SER

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Mol	Chain	Res	Type
11	ZQ	200	PHE
11	ZQ	211	TYR
11	ZQ	280	ASN
11	ZQ	305	SER
11	ZQ	367	ASP
11	ZQ	370	LYS
11	ZR	41	ASP
11	ZR	103	ASP
11	ZR	197	ASN
11	ZR	214	ASP
11	ZR	269	GLN
11	ZR	295	ASN
11	ZR	332	ASN
11	ZR	367	ASP
11	ZS	78	SER
11	ZS	103	ASP
11	ZS	170	PHE
11	ZS	202	LYS
11	ZS	245	ASN
11	ZS	367	ASP
11	ZT	148	SER
11	ZT	195	ASP
11	ZT	262	SER
11	ZT	297	ASP
11	ZT	358	ASN
11	ZU	3	PHE
11	ZU	78	SER
11	ZU	80	ASN
11	ZU	340	SER
11	ZV	46	SER
11	ZV	232	PHE
11	ZV	307	GLU
11	ZV	308	GLN
11	ZW	2	SER
11	ZW	3	PHE
11	ZW	53	LYS
11	ZW	188	ASP
11	ZW	195	ASP
11	ZW	215	SER
11	ZW	259	PHE
11	ZW	292	TYR
11	ZW	309	GLU

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Mol	Chain	Res	Type
11	ZW	326	LEU
11	ZW	331	ASP
11	ZW	340	SER
11	ZW	358	ASN
11	ZX	3	PHE
11	ZX	63	ASP
11	ZX	195	ASP
11	ZY	60	ASP
11	ZY	80	ASN
11	ZY	192	ASN
11	ZY	204	LYS
11	ZY	252	ASN
11	ZY	332	ASN
11	ZY	350	SER
11	ZZ	3	PHE
11	ZZ	41	ASP
11	ZZ	88	SER
11	ZZ	148	SER
11	ZZ	393	ASP
11	Za	103	ASP
11	Za	292	TYR
11	Za	331	ASP
11	Za	332	ASN
11	Za	375	MET
11	Zb	41	ASP
11	Zb	292	TYR
11	Zb	308	GLN
11	Zb	355	LYS
11	Zb	367	ASP
11	Zb	393	ASP
11	Zc	41	ASP
11	Zc	103	ASP
11	Zc	204	LYS
11	Zc	267	MET
11	Zc	296	ASN
11	Zc	297	ASP
11	Zc	317	LEU
11	Zc	332	ASN
11	Zc	340	SER
11	Zc	369	SER
11	Zc	399	LEU
11	Zd	41	ASP

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Mol	Chain	Res	Type
11	Zd	114	MET
11	Zd	140	PRO
11	Zd	292	TYR
11	Zd	375	MET
11	Zd	393	ASP
11	Ze	3	PHE
11	Ze	27	SER
11	Ze	46	SER
11	Ze	58	THR
11	Ze	60	ASP
11	Ze	130	GLN
11	Ze	308	GLN
11	Ze	319	ASN
11	Ze	395	ILE
11	Zf	3	PHE
11	Zf	285	LYS
11	Zf	297	ASP
11	Zf	331	ASP
11	Zf	332	ASN
11	Zf	367	ASP
11	Zf	396	LEU
11	Zg	94	TYR
11	Zg	103	ASP
11	Zg	292	TYR
11	Zg	332	ASN
11	Zg	367	ASP
11	Zg	370	LYS
11	Zh	3	PHE
11	Zh	41	ASP
11	Zh	47	LYS
11	Zh	63	ASP
11	Zh	83	PHE
11	Zh	162	ASP
11	Zh	308	GLN
11	Zh	332	ASN
12	a	21	ARG
12	a	80	GLN
12	a	129	VAL
12	a	131	SER
12	a	159	GLN
12	a	217	ASP
12	a	264	MET

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Mol	Chain	Res	Type
12	a	266	ARG
12	a	324	SER
12	a	343	MET
12	b	21	ARG
12	b	129	VAL
12	b	131	SER
12	b	159	GLN
12	b	217	ASP
12	b	264	MET
12	b	266	ARG
12	b	324	SER
12	b	343	MET
12	c	21	ARG
12	c	80	GLN
12	c	129	VAL
12	c	131	SER
12	c	159	GLN
12	c	217	ASP
12	c	264	MET
12	c	266	ARG
12	c	324	SER
12	c	343	MET
12	d	21	ARG
12	d	129	VAL
12	d	131	SER
12	d	159	GLN
12	d	217	ASP
12	d	264	MET
12	d	266	ARG
12	d	324	SER
12	d	343	MET
12	e	21	ARG
12	e	80	GLN
12	e	129	VAL
12	e	131	SER
12	e	159	GLN
12	e	217	ASP
12	e	264	MET
12	e	266	ARG
12	e	324	SER
12	e	343	MET
12	f	21	ARG

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Mol	Chain	Res	Type
12	f	80	GLN
12	f	131	SER
12	f	159	GLN
12	f	217	ASP
12	f	264	MET
12	f	266	ARG
12	f	324	SER
12	f	343	MET
12	g	21	ARG
12	g	129	VAL
12	g	131	SER
12	g	159	GLN
12	g	217	ASP
12	g	264	MET
12	g	266	ARG
12	g	324	SER
12	g	343	MET
12	h	21	ARG
12	h	80	GLN
12	h	129	VAL
12	h	131	SER
12	h	159	GLN
12	h	217	ASP
12	h	264	MET
12	h	266	ARG
12	h	324	SER
12	h	343	MET
12	i	21	ARG
12	i	80	GLN
12	i	129	VAL
12	i	131	SER
12	i	159	GLN
12	i	217	ASP
12	i	264	MET
12	i	266	ARG
12	i	324	SER
12	i	343	MET
12	j	21	ARG
12	j	131	SER
12	j	159	GLN
12	j	217	ASP
12	j	264	MET

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Mol	Chain	Res	Type
12	j	266	ARG
12	j	324	SER
12	j	343	MET
12	k	21	ARG
12	k	80	GLN
12	k	129	VAL
12	k	131	SER
12	k	159	GLN
12	k	217	ASP
12	k	264	MET
12	k	266	ARG
12	k	324	SER
12	k	343	MET
12	l	21	ARG
12	l	80	GLN
12	l	129	VAL
12	l	131	SER
12	l	159	GLN
12	l	217	ASP
12	l	264	MET
12	l	266	ARG
12	l	324	SER
12	l	343	MET
12	m	21	ARG
12	m	80	GLN
12	m	129	VAL
12	m	131	SER
12	m	159	GLN
12	m	217	ASP
12	m	264	MET
12	m	266	ARG
12	m	324	SER
12	m	343	MET
12	n	21	ARG
12	n	80	GLN
12	n	129	VAL
12	n	131	SER
12	n	159	GLN
12	n	217	ASP
12	n	264	MET
12	n	266	ARG
12	n	324	SER

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

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Mol	Chain	Res	Type
12	s	159	GLN
12	s	217	ASP
12	s	264	MET
12	s	266	ARG
12	s	324	SER
12	s	343	MET
12	t	21	ARG
12	t	80	GLN
12	t	129	VAL
12	t	131	SER
12	t	159	GLN
12	t	217	ASP
12	t	264	MET
12	t	266	ARG
12	t	324	SER
12	t	343	MET
12	u	21	ARG
12	u	80	GLN
12	u	129	VAL
12	u	131	SER
12	u	159	GLN
12	u	217	ASP
12	u	264	MET
12	u	266	ARG
12	u	324	SER
12	u	343	MET
12	v	21	ARG
12	v	80	GLN
12	v	129	VAL
12	v	131	SER
12	v	159	GLN
12	v	217	ASP
12	v	264	MET
12	v	266	ARG
12	v	324	SER
12	v	343	MET
12	w	21	ARG
12	w	80	GLN
12	w	131	SER
12	w	159	GLN
12	w	217	ASP
12	w	264	MET

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Mol	Chain	Res	Type
12	w	266	ARG
12	w	324	SER
12	w	343	MET
12	x	21	ARG
12	x	80	GLN
12	x	129	VAL
12	x	131	SER
12	x	159	GLN
12	x	217	ASP
12	x	264	MET
12	x	266	ARG
12	x	324	SER
12	x	343	MET
12	y	21	ARG
12	y	80	GLN
12	y	131	SER
12	y	159	GLN
12	y	217	ASP
12	y	264	MET
12	y	266	ARG
12	y	324	SER
12	y	343	MET
12	z	21	ARG
12	z	80	GLN
12	z	129	VAL
12	z	131	SER
12	z	159	GLN
12	z	217	ASP
12	z	264	MET
12	z	266	ARG
12	z	324	SER
12	z	343	MET
13	C3	106	ILE
13	C3	132	MET
13	C4	53	ASP
13	C4	56	LEU
13	C4	58	MET
13	C4	106	ILE
13	C5	106	ILE
14	C6	46	GLN
14	C6	50	LYS
14	C6	61	GLN

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Mol	Chain	Res	Type
14	C6	98	LEU
14	C6	101	ARG
14	C6	193	MET
14	C6	234	PHE
14	C6	235	LEU
13	C8	53	ASP
13	C8	56	LEU
13	C8	58	MET
13	C8	106	ILE
13	C9	106	ILE
16	C0	43	GLN
16	C0	47	VAL
16	C0	66	ARG
16	C0	140	LYS
16	C0	155	ASN
16	C0	236	LEU
16	C0	237	GLU
16	C0	286	ILE
14	DA	46	GLN
14	DA	50	LYS
14	DA	61	GLN
14	DA	98	LEU
14	DA	101	ARG
14	DA	193	MET
14	DA	234	PHE
14	DA	235	LEU
16	DC	43	GLN
16	DC	47	VAL
16	DC	66	ARG
16	DC	140	LYS
16	DC	155	ASN
16	DC	236	LEU
16	DC	237	GLU
16	DC	286	ILE
13	DD	106	ILE
13	DD	132	MET
16	DF	43	GLN
16	DF	47	VAL
16	DF	66	ARG
16	DF	140	LYS
16	DF	155	ASN
16	DF	236	LEU

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Mol	Chain	Res	Type
16	DF	237	GLU
16	DF	286	ILE
14	DG	46	GLN
14	DG	50	LYS
14	DG	61	GLN
14	DG	98	LEU
14	DG	101	ARG
14	DG	193	MET
14	DG	234	PHE
14	DG	235	LEU
13	DI	53	ASP
13	DI	56	LEU
13	DI	58	MET
13	DI	106	ILE
13	DJ	106	ILE
13	DK	106	ILE
13	DK	132	MET
13	DM	106	ILE
13	DM	132	MET
13	DN	106	ILE
13	DN	132	MET
13	DO	106	ILE
13	DO	132	MET
13	DP	106	ILE
13	DP	132	MET
13	DQ	106	ILE
13	DQ	132	MET
13	DR	106	ILE
13	DR	132	MET
13	DS	106	ILE
13	DS	132	MET
13	DT	106	ILE
13	DT	132	MET
13	DU	53	ASP
13	DU	56	LEU
13	DU	58	MET
13	DU	106	ILE
13	DV	106	ILE
13	DW	106	ILE
13	DW	132	MET
16	DX	43	GLN
16	DX	47	VAL

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Mol	Chain	Res	Type
16	DX	66	ARG
16	DX	140	LYS
16	DX	155	ASN
16	DX	236	LEU
16	DX	237	GLU
16	DX	286	ILE
14	DY	46	GLN
14	DY	50	LYS
14	DY	61	GLN
14	DY	98	LEU
14	DY	101	ARG
14	DY	193	MET
14	DY	234	PHE
14	DY	235	LEU
13	Da	53	ASP
13	Da	56	LEU
13	Da	58	MET
13	Da	106	ILE
13	Db	106	ILE
13	Dc	106	ILE
13	Dc	132	MET
16	Dd	43	GLN
16	Dd	47	VAL
16	Dd	66	ARG
16	Dd	140	LYS
16	Dd	155	ASN
16	Dd	236	LEU
16	Dd	237	GLU
16	Dd	286	ILE
14	De	46	GLN
14	De	50	LYS
14	De	61	GLN
14	De	98	LEU
14	De	101	ARG
14	De	193	MET
14	De	234	PHE
14	De	235	LEU
13	Dg	53	ASP
13	Dg	56	LEU
13	Dg	58	MET
13	Dg	106	ILE
13	Dh	106	ILE

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Mol	Chain	Res	Type
13	Di	106	ILE
13	Di	132	MET
16	Dj	43	GLN
16	Dj	47	VAL
16	Dj	66	ARG
16	Dj	140	LYS
16	Dj	155	ASN
16	Dj	236	LEU
16	Dj	237	GLU
16	Dj	286	ILE
14	Dk	46	GLN
14	Dk	50	LYS
14	Dk	61	GLN
14	Dk	98	LEU
14	Dk	101	ARG
14	Dk	193	MET
14	Dk	234	PHE
14	Dk	235	LEU
13	Dm	53	ASP
13	Dm	56	LEU
13	Dm	58	MET
13	Dm	106	ILE
13	Dn	106	ILE
13	Do	106	ILE
13	Do	132	MET
16	Dp	43	GLN
16	Dp	47	VAL
16	Dp	66	ARG
16	Dp	140	LYS
16	Dp	155	ASN
16	Dp	236	LEU
16	Dp	237	GLU
16	Dp	286	ILE
14	Dq	46	GLN
14	Dq	50	LYS
14	Dq	61	GLN
14	Dq	98	LEU
14	Dq	101	ARG
14	Dq	193	MET
14	Dq	234	PHE
14	Dq	235	LEU
13	Ds	53	ASP

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Mol	Chain	Res	Type
13	Ds	56	LEU
13	Ds	58	MET
13	Ds	106	ILE
13	Dt	106	ILE
13	Du	106	ILE
13	Du	132	MET
16	Dv	43	GLN
16	Dv	47	VAL
16	Dv	66	ARG
16	Dv	140	LYS
16	Dv	155	ASN
16	Dv	236	LEU
16	Dv	237	GLU
16	Dv	286	ILE
14	Dw	46	GLN
14	Dw	50	LYS
14	Dw	61	GLN
14	Dw	98	LEU
14	Dw	101	ARG
14	Dw	193	MET
14	Dw	234	PHE
14	Dw	235	LEU
13	Dy	53	ASP
13	Dy	56	LEU
13	Dy	58	MET
13	Dy	106	ILE
13	Dz	106	ILE
13	D1	106	ILE
13	D1	132	MET
16	D2	43	GLN
16	D2	47	VAL
16	D2	66	ARG
16	D2	140	LYS
16	D2	155	ASN
16	D2	236	LEU
16	D2	237	GLU
16	D2	286	ILE
14	D3	46	GLN
14	D3	50	LYS
14	D3	61	GLN
14	D3	98	LEU
14	D3	101	ARG

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Mol	Chain	Res	Type
14	D3	193	MET
14	D3	234	PHE
14	D3	235	LEU
13	D5	53	ASP
13	D5	56	LEU
13	D5	58	MET
13	D5	106	ILE
13	D6	106	ILE
13	D7	106	ILE
13	D7	132	MET
16	D8	43	GLN
16	D8	47	VAL
16	D8	66	ARG
16	D8	140	LYS
16	D8	155	ASN
16	D8	236	LEU
16	D8	237	GLU
16	D8	286	ILE
14	D9	46	GLN
14	D9	50	LYS
14	D9	61	GLN
14	D9	98	LEU
14	D9	101	ARG
14	D9	193	MET
14	D9	234	PHE
14	D9	235	LEU
13	EA	53	ASP
13	EA	56	LEU
13	EA	58	MET
13	EA	106	ILE
13	EB	106	ILE
13	B1	106	ILE
13	B2	106	ILE
13	B2	132	MET
16	B4	43	GLN
16	B4	47	VAL
16	B4	66	ARG
16	B4	140	LYS
16	B4	155	ASN
16	B4	236	LEU
16	B4	237	GLU
16	B4	286	ILE

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Mol	Chain	Res	Type
14	B5	46	GLN
14	B5	50	LYS
14	B5	61	GLN
14	B5	98	LEU
14	B5	101	ARG
14	B5	193	MET
14	B5	234	PHE
14	B5	235	LEU
13	B7	53	ASP
13	B7	56	LEU
13	B7	58	MET
13	B7	106	ILE
13	B8	106	ILE
13	B9	106	ILE
13	B9	132	MET
14	EC	46	GLN
14	EC	50	LYS
14	EC	61	GLN
14	EC	98	LEU
14	EC	101	ARG
14	EC	193	MET
14	EC	234	PHE
14	EC	235	LEU
13	EE	53	ASP
13	EE	56	LEU
13	EE	58	MET
13	EE	106	ILE
13	EF	106	ILE
13	EG	106	ILE
13	EG	132	MET
16	EI	43	GLN
16	EI	47	VAL
16	EI	66	ARG
16	EI	140	LYS
16	EI	155	ASN
16	EI	236	LEU
16	EI	237	GLU
16	EI	286	ILE
14	EJ	46	GLN
14	EJ	50	LYS
14	EJ	61	GLN
14	EJ	98	LEU

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Mol	Chain	Res	Type
14	EJ	101	ARG
14	EJ	193	MET
14	EJ	234	PHE
14	EJ	235	LEU
13	EL	53	ASP
13	EL	56	LEU
13	EL	58	MET
13	EL	106	ILE
13	EM	106	ILE
13	EN	106	ILE
13	EN	132	MET
16	EP	43	GLN
16	EP	47	VAL
16	EP	66	ARG
16	EP	140	LYS
16	EP	155	ASN
16	EP	236	LEU
16	EP	237	GLU
16	EP	286	ILE
14	EQ	46	GLN
14	EQ	50	LYS
14	EQ	61	GLN
14	EQ	98	LEU
14	EQ	101	ARG
14	EQ	193	MET
14	EQ	234	PHE
14	EQ	235	LEU
13	ES	53	ASP
13	ES	56	LEU
13	ES	58	MET
13	ES	106	ILE
13	ET	106	ILE
13	EU	106	ILE
13	EU	132	MET
16	EW	43	GLN
16	EW	47	VAL
16	EW	66	ARG
16	EW	140	LYS
16	EW	155	ASN
16	EW	236	LEU
16	EW	237	GLU
16	EW	286	ILE

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Mol	Chain	Res	Type
14	EX	46	GLN
14	EX	50	LYS
14	EX	61	GLN
14	EX	98	LEU
14	EX	101	ARG
14	EX	193	MET
14	EX	234	PHE
14	EX	235	LEU
13	EZ	53	ASP
13	EZ	56	LEU
13	EZ	58	MET
13	EZ	106	ILE
13	BY	106	ILE
13	BZ	106	ILE
13	BZ	132	MET
16	Bb	43	GLN
16	Bb	47	VAL
16	Bb	66	ARG
16	Bb	140	LYS
16	Bb	155	ASN
16	Bb	236	LEU
16	Bb	237	GLU
16	Bb	286	ILE
14	Bc	46	GLN
14	Bc	50	LYS
14	Bc	61	GLN
14	Bc	98	LEU
14	Bc	101	ARG
14	Bc	193	MET
14	Bc	234	PHE
14	Bc	235	LEU
13	Be	53	ASP
13	Be	56	LEU
13	Be	58	MET
13	Be	106	ILE
13	Bf	106	ILE
13	Bg	106	ILE
13	Bg	132	MET
16	Bi	43	GLN
16	Bi	47	VAL
16	Bi	66	ARG
16	Bi	140	LYS

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Mol	Chain	Res	Type
16	Bi	155	ASN
16	Bi	236	LEU
16	Bi	237	GLU
16	Bi	286	ILE
14	Bj	46	GLN
14	Bj	50	LYS
14	Bj	61	GLN
14	Bj	98	LEU
14	Bj	101	ARG
14	Bj	193	MET
14	Bj	234	PHE
14	Bj	235	LEU
13	Bl	53	ASP
13	Bl	56	LEU
13	Bl	58	MET
13	Bl	106	ILE
13	Bm	106	ILE
13	Bn	106	ILE
13	Bn	132	MET
16	Bp	43	GLN
16	Bp	47	VAL
16	Bp	66	ARG
16	Bp	140	LYS
16	Bp	155	ASN
16	Bp	236	LEU
16	Bp	237	GLU
16	Bp	286	ILE
14	Bq	46	GLN
14	Bq	50	LYS
14	Bq	61	GLN
14	Bq	98	LEU
14	Bq	101	ARG
14	Bq	193	MET
14	Bq	234	PHE
14	Bq	235	LEU
13	Bs	53	ASP
13	Bs	56	LEU
13	Bs	58	MET
13	Bs	106	ILE
13	Bt	106	ILE
13	Bu	106	ILE
13	Bu	132	MET

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Mol	Chain	Res	Type
16	Bw	43	GLN
16	Bw	47	VAL
16	Bw	66	ARG
16	Bw	140	LYS
16	Bw	155	ASN
16	Bw	236	LEU
16	Bw	237	GLU
16	Bw	286	ILE
14	Bx	46	GLN
14	Bx	50	LYS
14	Bx	61	GLN
14	Bx	98	LEU
14	Bx	101	ARG
14	Bx	193	MET
14	Bx	234	PHE
14	Bx	235	LEU
13	Bz	53	ASP
13	Bz	56	LEU
13	Bz	58	MET
13	Bz	106	ILE
13	C1	53	ASP
13	C1	56	LEU
13	C1	58	MET
13	C1	106	ILE
13	C2	106	ILE
16	CA	43	GLN
16	CA	47	VAL
16	CA	66	ARG
16	CA	140	LYS
16	CA	155	ASN
16	CA	236	LEU
16	CA	237	GLU
16	CA	286	ILE
14	CB	46	GLN
14	CB	50	LYS
14	CB	61	GLN
14	CB	98	LEU
14	CB	101	ARG
14	CB	193	MET
14	CB	234	PHE
14	CB	235	LEU
13	CD	53	ASP

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Mol	Chain	Res	Type
13	CD	56	LEU
13	CD	58	MET
13	CD	106	ILE
13	CE	106	ILE
13	CF	106	ILE
13	CF	132	MET
16	CH	43	GLN
16	CH	47	VAL
16	CH	66	ARG
16	CH	140	LYS
16	CH	155	ASN
16	CH	236	LEU
16	CH	237	GLU
16	CH	286	ILE
14	CI	46	GLN
14	CI	50	LYS
14	CI	61	GLN
14	CI	98	LEU
14	CI	101	ARG
14	CI	193	MET
14	CI	234	PHE
14	CI	235	LEU
13	CK	53	ASP
13	CK	56	LEU
13	CK	58	MET
13	CK	106	ILE
13	CL	106	ILE
13	CM	106	ILE
13	CM	132	MET
16	CO	43	GLN
16	CO	47	VAL
16	CO	66	ARG
16	CO	140	LYS
16	CO	155	ASN
16	CO	236	LEU
16	CO	237	GLU
16	CO	286	ILE
14	CP	46	GLN
14	CP	50	LYS
14	CP	61	GLN
14	CP	98	LEU
14	CP	101	ARG

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Mol	Chain	Res	Type
14	CP	193	MET
14	CP	234	PHE
14	CP	235	LEU
13	CR	53	ASP
13	CR	56	LEU
13	CR	58	MET
13	CR	106	ILE
13	CS	106	ILE
13	CT	106	ILE
13	CT	132	MET
16	CV	43	GLN
16	CV	47	VAL
16	CV	66	ARG
16	CV	140	LYS
16	CV	155	ASN
16	CV	236	LEU
16	CV	237	GLU
16	CV	286	ILE
14	CW	46	GLN
14	CW	50	LYS
14	CW	61	GLN
14	CW	98	LEU
14	CW	101	ARG
14	CW	193	MET
14	CW	234	PHE
14	CW	235	LEU
13	CY	53	ASP
13	CY	56	LEU
13	CY	58	MET
13	CY	106	ILE
13	CZ	106	ILE
13	Ca	106	ILE
13	Ca	132	MET
16	Cc	43	GLN
16	Cc	47	VAL
16	Cc	66	ARG
16	Cc	140	LYS
16	Cc	155	ASN
16	Cc	236	LEU
16	Cc	237	GLU
16	Cc	286	ILE
14	Cd	46	GLN

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Mol	Chain	Res	Type
14	Cd	50	LYS
14	Cd	61	GLN
14	Cd	98	LEU
14	Cd	101	ARG
14	Cd	193	MET
14	Cd	234	PHE
14	Cd	235	LEU
13	Cf	53	ASP
13	Cf	56	LEU
13	Cf	58	MET
13	Cf	106	ILE
13	Cg	106	ILE
13	Ch	106	ILE
13	Ch	132	MET
16	Cj	43	GLN
16	Cj	47	VAL
16	Cj	66	ARG
16	Cj	140	LYS
16	Cj	155	ASN
16	Cj	236	LEU
16	Cj	237	GLU
16	Cj	286	ILE
14	Ck	46	GLN
14	Ck	50	LYS
14	Ck	61	GLN
14	Ck	98	LEU
14	Ck	101	ARG
14	Ck	193	MET
14	Ck	234	PHE
14	Ck	235	LEU
13	Cm	53	ASP
13	Cm	56	LEU
13	Cm	58	MET
13	Cm	106	ILE
13	Cn	106	ILE
13	Co	106	ILE
13	Co	132	MET
16	Cq	43	GLN
16	Cq	47	VAL
16	Cq	66	ARG
16	Cq	140	LYS
16	Cq	155	ASN

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Mol	Chain	Res	Type
16	Cq	236	LEU
16	Cq	237	GLU
16	Cq	286	ILE
14	Cr	46	GLN
14	Cr	50	LYS
14	Cr	61	GLN
14	Cr	98	LEU
14	Cr	101	ARG
14	Cr	193	MET
14	Cr	234	PHE
14	Cr	235	LEU
13	Ct	53	ASP
13	Ct	56	LEU
13	Ct	58	MET
13	Ct	106	ILE
13	Cu	106	ILE
13	Cv	106	ILE
13	Cv	132	MET
16	Cx	43	GLN
16	Cx	47	VAL
16	Cx	66	ARG
16	Cx	140	LYS
16	Cx	155	ASN
16	Cx	236	LEU
16	Cx	237	GLU
16	Cx	286	ILE
14	Cy	46	GLN
14	Cy	50	LYS
14	Cy	61	GLN
14	Cy	98	LEU
14	Cy	101	ARG
14	Cy	193	MET
14	Cy	234	PHE
14	Cy	235	LEU
16	Eq	43	GLN
16	Eq	47	VAL
16	Eq	66	ARG
16	Eq	140	LYS
16	Eq	155	ASN
16	Eq	236	LEU
16	Eq	237	GLU
16	Eq	286	ILE

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Mol	Chain	Res	Type
16	Er	43	GLN
16	Er	47	VAL
16	Er	66	ARG
16	Er	140	LYS
16	Er	155	ASN
16	Er	236	LEU
16	Er	237	GLU
16	Er	286	ILE
16	Es	43	GLN
16	Es	47	VAL
16	Es	66	ARG
16	Es	140	LYS
16	Es	155	ASN
16	Es	236	LEU
16	Es	237	GLU
16	Es	286	ILE
16	Et	43	GLN
16	Et	47	VAL
16	Et	66	ARG
16	Et	140	LYS
16	Et	155	ASN
16	Et	236	LEU
16	Et	237	GLU
16	Et	286	ILE
16	Eu	43	GLN
16	Eu	47	VAL
16	Eu	66	ARG
16	Eu	140	LYS
16	Eu	155	ASN
16	Eu	236	LEU
16	Eu	237	GLU
16	Eu	286	ILE
16	Ev	43	GLN
16	Ev	47	VAL
16	Ev	66	ARG
16	Ev	140	LYS
16	Ev	155	ASN
16	Ev	236	LEU
16	Ev	237	GLU
16	Ev	286	ILE
16	Ew	43	GLN
16	Ew	47	VAL

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Mol	Chain	Res	Type
16	Ew	66	ARG
16	Ew	140	LYS
16	Ew	155	ASN
16	Ew	236	LEU
16	Ew	237	GLU
16	Ew	286	ILE
14	Ex	46	GLN
14	Ex	50	LYS
14	Ex	61	GLN
14	Ex	98	LEU
14	Ex	101	ARG
14	Ex	193	MET
14	Ex	234	PHE
14	Ex	235	LEU
14	Ey	46	GLN
14	Ey	50	LYS
14	Ey	61	GLN
14	Ey	98	LEU
14	Ey	101	ARG
14	Ey	193	MET
14	Ey	234	PHE
14	Ey	235	LEU
14	Ez	46	GLN
14	Ez	50	LYS
14	Ez	61	GLN
14	Ez	98	LEU
14	Ez	101	ARG
14	Ez	193	MET
14	Ez	234	PHE
14	Ez	235	LEU
14	E1	46	GLN
14	E1	50	LYS
14	E1	61	GLN
14	E1	98	LEU
14	E1	101	ARG
14	E1	193	MET
14	E1	234	PHE
14	E1	235	LEU
14	E2	46	GLN
14	E2	50	LYS
14	E2	61	GLN
14	E2	98	LEU

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Mol	Chain	Res	Type
14	E2	101	ARG
14	E2	193	MET
14	E2	234	PHE
14	E2	235	LEU
14	E3	46	GLN
14	E3	50	LYS
14	E3	61	GLN
14	E3	98	LEU
14	E3	101	ARG
14	E3	193	MET
14	E3	234	PHE
14	E3	235	LEU
14	E4	46	GLN
14	E4	50	LYS
14	E4	61	GLN
14	E4	98	LEU
14	E4	101	ARG
14	E4	193	MET
14	E4	234	PHE
14	E4	235	LEU
16	E5	43	GLN
16	E5	47	VAL
16	E5	66	ARG
16	E5	140	LYS
16	E5	155	ASN
16	E5	236	LEU
16	E5	237	GLU
16	E5	286	ILE
13	FC	53	ASP
13	FC	56	LEU
13	FC	58	MET
13	FC	106	ILE
13	FD	53	ASP
13	FD	56	LEU
13	FD	58	MET
13	FD	106	ILE
13	FE	53	ASP
13	FE	56	LEU
13	FE	58	MET
13	FE	106	ILE
13	FF	53	ASP
13	FF	56	LEU

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Mol	Chain	Res	Type
13	FF	58	MET
13	FF	106	ILE
13	FG	53	ASP
13	FG	56	LEU
13	FG	58	MET
13	FG	106	ILE
13	FH	53	ASP
13	FH	56	LEU
13	FH	58	MET
13	FH	106	ILE
13	FI	106	ILE
13	FJ	106	ILE
13	FK	106	ILE
13	FL	106	ILE
13	FM	106	ILE
13	FN	106	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1341) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	88	GLN
1	0	100	GLN
1	0	135	GLN
1	0	137	GLN
1	0	180	ASN
1	0	235	GLN
1	0	237	GLN
1	0	255	GLN
1	1	47	GLN
1	1	67	GLN
1	1	91	ASN
1	1	121	GLN
1	1	135	GLN
1	1	223	ASN
1	1	252	GLN
1	2	164	GLN
1	2	255	GLN
1	3	24	ASN
1	3	67	GLN
1	3	161	GLN
1	3	190	ASN
1	3	255	GLN

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Mol	Chain	Res	Type
1	4	37	GLN
1	4	47	GLN
1	4	51	GLN
1	4	125	ASN
1	4	127	GLN
1	4	174	ASN
1	4	216	GLN
1	4	235	GLN
1	4	243	ASN
1	4	259	GLN
1	5	51	GLN
1	5	55	GLN
1	5	85	ASN
1	5	100	GLN
1	5	121	GLN
1	5	237	GLN
1	5	252	GLN
1	6	16	GLN
1	6	59	GLN
1	6	91	ASN
1	6	121	GLN
1	6	127	GLN
1	6	135	GLN
1	6	209	ASN
1	6	237	GLN
1	7	24	ASN
1	7	55	GLN
1	7	85	ASN
1	7	164	GLN
1	7	235	GLN
1	8	83	GLN
1	8	91	ASN
1	8	196	GLN
1	9	37	GLN
1	9	55	GLN
1	9	85	ASN
1	9	91	ASN
1	9	259	GLN
2	A	59	ASN
2	A	63	GLN
2	A	130	ASN
2	A	139	ASN

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Mol	Chain	Res	Type
2	A	160	ASN
2	A	172	ASN
2	A	173	GLN
2	A	185	ASN
2	A	217	GLN
3	A0	13	GLN
3	A0	72	HIS
3	A0	76	GLN
3	A0	112	ASN
4	A1	15	GLN
4	A1	90	ASN
4	A2	83	GLN
4	A2	103	GLN
4	A3	87	GLN
4	A4	39	HIS
4	A4	55	GLN
4	A4	97	GLN
4	A5	76	GLN
3	A6	17	ASN
3	A6	23	GLN
3	A7	23	GLN
3	A7	29	ASN
3	A7	92	GLN
3	A7	117	GLN
3	A8	32	ASN
3	A8	76	GLN
3	A8	92	GLN
3	A8	135	GLN
3	A9	17	ASN
3	A9	21	GLN
3	A9	32	ASN
3	A9	72	HIS
3	A9	76	GLN
3	A9	117	GLN
5	AA	102	ASN
5	AB	18	GLN
5	AB	172	GLN
5	AB	210	ASN
5	AB	223	ASN
5	AB	240	ASN
5	AC	18	GLN
5	AC	28	ASN

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Mol	Chain	Res	Type
5	AC	70	GLN
5	AC	104	ASN
5	AC	106	GLN
5	AC	186	GLN
5	AD	28	ASN
5	AD	104	ASN
5	AD	106	GLN
5	AD	153	ASN
5	AD	210	ASN
5	AD	240	ASN
5	AE	18	GLN
5	AE	37	GLN
5	AE	112	GLN
5	AE	116	GLN
1	AF	47	GLN
1	AF	83	GLN
1	AF	85	ASN
1	AF	121	GLN
1	AF	135	GLN
1	AF	164	GLN
1	AF	172	GLN
1	AF	223	ASN
1	AG	16	GLN
1	AG	28	ASN
1	AG	145	ASN
1	AG	223	ASN
1	AG	259	GLN
1	AH	47	GLN
1	AH	85	ASN
1	AH	104	GLN
1	AH	125	ASN
1	AH	127	GLN
1	AH	162	GLN
1	AH	169	GLN
1	AH	172	GLN
1	AH	259	GLN
1	AI	16	GLN
1	AI	32	ASN
1	AI	196	GLN
1	AI	209	ASN
1	AJ	47	GLN
1	AJ	90	ASN

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Mol	Chain	Res	Type
1	AJ	169	GLN
1	AJ	172	GLN
1	AJ	174	ASN
1	AJ	232	ASN
1	AK	28	ASN
1	AK	121	GLN
1	AK	125	ASN
1	AK	127	GLN
1	AK	135	GLN
1	AK	137	GLN
1	AK	196	GLN
1	AK	223	ASN
1	AK	235	GLN
1	AL	32	ASN
1	AL	104	GLN
1	AL	121	GLN
1	AL	127	GLN
1	AL	145	ASN
1	AL	209	ASN
1	AM	25	ASN
1	AM	37	GLN
1	AM	51	GLN
1	AM	67	GLN
1	AM	125	ASN
1	AM	127	GLN
1	AM	209	ASN
1	AM	223	ASN
1	AM	252	GLN
1	AN	67	GLN
1	AN	85	ASN
1	AN	125	ASN
1	AN	235	GLN
6	AO	297	GLN
6	AO	303	GLN
6	AO	374	HIS
6	AO	434	ASN
6	AP	297	GLN
6	AP	303	GLN
6	AP	359	GLN
6	AP	374	HIS
6	AP	434	ASN
6	AQ	303	GLN

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Mol	Chain	Res	Type
6	AQ	374	HIS
6	AR	303	GLN
6	AR	374	HIS
6	AS	297	GLN
6	AS	299	ASN
6	AS	303	GLN
6	AS	374	HIS
6	AT	303	GLN
6	AT	374	HIS
6	AU	303	GLN
6	AU	374	HIS
6	AV	303	GLN
6	AV	374	HIS
6	AW	299	ASN
6	AW	303	GLN
6	AW	374	HIS
6	AX	297	GLN
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	Ag	297	GLN
6	Ag	303	GLN
6	Ag	374	HIS
6	Ah	303	GLN
6	Ah	374	HIS
6	Ah	434	ASN

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Mol	Chain	Res	Type
6	Ai	303	GLN
6	Ai	374	HIS
6	Aj	303	GLN
6	Aj	374	HIS
6	Aj	434	ASN
6	Ak	303	GLN
6	Ak	374	HIS
6	Ak	434	ASN
6	Al	303	GLN
6	Al	374	HIS
6	Al	434	ASN
6	Am	303	GLN
6	Am	374	HIS
6	Am	434	ASN
6	An	303	GLN
6	An	374	HIS
6	An	434	ASN
6	Ao	374	HIS
6	Ao	434	ASN
6	Ap	374	HIS
6	Ap	434	ASN
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	160	GLN
9	Aw	233	GLN
9	Ax	160	GLN
9	Ax	184	GLN
9	Ay	114	GLN
9	Ay	155	ASN
4	Az	103	GLN
2	B	59	ASN
2	B	63	GLN
2	B	85	ASN
2	B	130	ASN
2	B	139	ASN
2	B	160	ASN
2	B	172	ASN

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Mol	Chain	Res	Type
2	B	173	GLN
2	B	185	ASN
2	B	217	GLN
10	BA	30	ASN
10	BB	22	ASN
10	BC	22	ASN
10	BC	50	GLN
10	BC	57	GLN
10	BC	134	GLN
10	BE	17	GLN
10	BF	5	ASN
10	BF	57	GLN
10	BF	115	ASN
6	BG	319	GLN
6	BO	318	ASN
6	BQ	318	ASN
6	BQ	324	ASN
6	BR	303	GLN
6	BR	374	HIS
6	BS	303	GLN
6	BS	374	HIS
6	BT	303	GLN
6	BT	374	HIS
6	BU	303	GLN
6	BU	374	HIS
6	BV	303	GLN
6	BV	374	HIS
6	BW	374	HIS
6	BX	297	GLN
6	BX	303	GLN
6	BX	374	HIS
2	C	59	ASN
2	C	63	GLN
2	C	85	ASN
2	C	130	ASN
2	C	139	ASN
2	C	160	ASN
2	C	172	ASN
2	C	173	GLN
2	C	185	ASN
2	C	217	GLN
2	D	59	ASN

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

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

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

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Mol	Chain	Res	Type
2	R	130	ASN
2	R	139	ASN
2	R	160	ASN
2	R	172	ASN
2	R	173	GLN
2	R	185	ASN
2	R	217	GLN
2	S	59	ASN
2	S	63	GLN
2	S	130	ASN
2	S	139	ASN
2	S	160	ASN
2	S	172	ASN
2	S	173	GLN
2	S	185	ASN
2	S	217	GLN
2	T	59	ASN
2	T	63	GLN
2	T	85	ASN
2	T	130	ASN
2	T	139	ASN
2	T	160	ASN
2	T	172	ASN
2	T	173	GLN
2	T	185	ASN
2	T	217	GLN
2	U	59	ASN
2	U	63	GLN
2	U	130	ASN
2	U	139	ASN
2	U	160	ASN
2	U	172	ASN
2	U	173	GLN
2	U	185	ASN
2	U	217	GLN
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

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Mol	Chain	Res	Type
6	UN	196	HIS
6	UO	196	HIS
6	UP	196	HIS
2	V	59	ASN
2	V	63	GLN
2	V	130	ASN
2	V	139	ASN
2	V	160	ASN
2	V	172	ASN
2	V	173	GLN
2	V	185	ASN
2	V	217	GLN
2	W	59	ASN
2	W	63	GLN
2	W	85	ASN
2	W	130	ASN
2	W	139	ASN
2	W	160	ASN
2	W	172	ASN
2	W	173	GLN
2	W	185	ASN
2	W	217	GLN
6	WA	209	ASN
6	WB	169	GLN
6	WE	156	HIS
6	WE	209	ASN
6	WF	118	GLN
6	WH	156	HIS
6	WI	129	GLN
6	WI	156	HIS
6	WJ	169	GLN
6	WJ	209	ASN
6	WO	209	ASN
6	WP	209	ASN
6	WT	209	ASN
6	WV	169	GLN
6	WW	169	GLN
2	X	59	ASN
2	X	63	GLN
2	X	130	ASN
2	X	139	ASN
2	X	160	ASN

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Mol	Chain	Res	Type
2	X	172	ASN
2	X	173	GLN
2	X	185	ASN
2	X	217	GLN
2	Y	59	ASN
2	Y	63	GLN
2	Y	85	ASN
2	Y	130	ASN
2	Y	139	ASN
2	Y	160	ASN
2	Y	172	ASN
2	Y	173	GLN
2	Y	185	ASN
2	Y	217	GLN
2	Z	59	ASN
2	Z	63	GLN
2	Z	85	ASN
2	Z	130	ASN
2	Z	139	ASN
2	Z	160	ASN
2	Z	172	ASN
2	Z	173	GLN
2	Z	185	ASN
2	Z	217	GLN
1	ZA	235	GLN
1	ZB	24	ASN
1	ZB	25	ASN
1	ZB	28	ASN
1	ZB	37	GLN
1	ZB	137	GLN
1	ZB	235	GLN
1	ZC	16	GLN
1	ZC	88	GLN
1	ZC	100	GLN
1	ZC	190	ASN
1	ZD	24	ASN
1	ZD	67	GLN
1	ZD	88	GLN
1	ZD	91	ASN
1	ZD	127	GLN
1	ZD	135	GLN
1	ZD	161	GLN

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Mol	Chain	Res	Type
1	ZD	235	GLN
1	ZE	37	GLN
1	ZE	67	GLN
1	ZE	121	GLN
1	ZE	252	GLN
11	ZF	5	GLN
11	ZF	16	ASN
11	ZF	107	ASN
11	ZF	155	GLN
11	ZF	197	ASN
11	ZF	358	ASN
11	ZF	385	ASN
11	ZF	401	ASN
11	ZG	89	ASN
11	ZG	130	GLN
11	ZG	133	ASN
11	ZG	332	ASN
11	ZG	387	GLN
11	ZG	397	ASN
11	ZG	401	ASN
11	ZH	5	GLN
11	ZH	155	GLN
11	ZH	206	ASN
11	ZH	270	ASN
11	ZH	296	ASN
11	ZH	352	ASN
11	ZH	365	ASN
11	ZH	379	GLN
11	ZH	392	GLN
11	ZI	197	ASN
11	ZI	269	GLN
11	ZI	323	ASN
11	ZI	385	ASN
11	ZI	387	GLN
11	ZI	392	GLN
11	ZI	394	GLN
11	ZI	401	ASN
11	ZJ	89	ASN
11	ZJ	107	ASN
11	ZJ	133	ASN
11	ZJ	159	ASN
11	ZJ	197	ASN

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Mol	Chain	Res	Type
11	ZJ	265	ASN
11	ZJ	274	ASN
11	ZJ	282	ASN
11	ZJ	379	GLN
11	ZJ	392	GLN
11	ZJ	397	ASN
11	ZJ	401	ASN
11	ZK	107	ASN
11	ZK	197	ASN
11	ZK	252	ASN
11	ZK	303	ASN
11	ZK	319	ASN
11	ZK	392	GLN
11	ZK	401	ASN
11	ZL	5	GLN
11	ZL	79	GLN
11	ZL	89	ASN
11	ZL	179	ASN
11	ZL	190	GLN
11	ZL	197	ASN
11	ZL	269	GLN
11	ZL	282	ASN
11	ZL	310	GLN
11	ZL	338	GLN
11	ZL	401	ASN
11	ZM	5	GLN
11	ZM	59	GLN
11	ZM	89	ASN
11	ZM	197	ASN
11	ZM	213	HIS
11	ZM	235	ASN
11	ZM	252	ASN
11	ZM	381	ASN
11	ZN	79	GLN
11	ZN	107	ASN
11	ZN	112	GLN
11	ZN	129	GLN
11	ZN	133	ASN
11	ZN	190	GLN
11	ZN	192	ASN
11	ZN	197	ASN
11	ZN	319	ASN

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Mol	Chain	Res	Type
11	ZN	338	GLN
11	ZN	379	GLN
11	ZN	387	GLN
11	ZN	401	ASN
11	ZO	89	ASN
11	ZO	141	ASN
11	ZO	192	ASN
11	ZO	235	ASN
11	ZO	332	ASN
11	ZP	11	ASN
11	ZP	107	ASN
11	ZP	129	GLN
11	ZP	194	HIS
11	ZP	269	GLN
11	ZP	270	ASN
11	ZP	314	GLN
11	ZP	322	ASN
11	ZP	338	GLN
11	ZP	379	GLN
11	ZP	381	ASN
11	ZP	385	ASN
11	ZQ	97	ASN
11	ZQ	133	ASN
11	ZQ	141	ASN
11	ZQ	155	GLN
11	ZQ	197	ASN
11	ZQ	233	ASN
11	ZQ	338	GLN
11	ZQ	387	GLN
11	ZR	107	ASN
11	ZR	133	ASN
11	ZR	268	GLN
11	ZR	269	GLN
11	ZR	293	GLN
11	ZR	295	ASN
11	ZR	401	ASN
11	ZS	133	ASN
11	ZS	197	ASN
11	ZS	394	GLN
11	ZT	5	GLN
11	ZT	99	GLN
11	ZT	129	GLN

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Mol	Chain	Res	Type
11	ZT	133	ASN
11	ZT	197	ASN
11	ZT	213	HIS
11	ZT	235	ASN
11	ZT	275	ASN
11	ZT	293	GLN
11	ZT	314	GLN
11	ZT	352	ASN
11	ZT	392	GLN
11	ZU	99	GLN
11	ZU	107	ASN
11	ZU	133	ASN
11	ZU	159	ASN
11	ZU	206	ASN
11	ZU	293	GLN
11	ZU	332	ASN
11	ZU	379	GLN
11	ZU	387	GLN
11	ZV	89	ASN
11	ZV	107	ASN
11	ZV	133	ASN
11	ZV	197	ASN
11	ZV	280	ASN
11	ZV	303	ASN
11	ZV	314	GLN
11	ZV	394	GLN
11	ZV	397	ASN
11	ZV	401	ASN
11	ZW	5	GLN
11	ZW	26	ASN
11	ZW	107	ASN
11	ZW	129	GLN
11	ZW	133	ASN
11	ZW	155	GLN
11	ZW	197	ASN
11	ZW	252	ASN
11	ZW	310	GLN
11	ZW	314	GLN
11	ZW	332	ASN
11	ZX	80	ASN
11	ZX	133	ASN
11	ZX	159	ASN

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Mol	Chain	Res	Type
11	ZX	314	GLN
11	ZX	352	ASN
11	ZY	5	GLN
11	ZY	115	GLN
11	ZY	159	ASN
11	ZY	197	ASN
11	ZY	268	GLN
11	ZY	392	GLN
11	ZZ	5	GLN
11	ZZ	99	GLN
11	ZZ	107	ASN
11	ZZ	133	ASN
11	ZZ	194	HIS
11	ZZ	197	ASN
11	ZZ	314	GLN
11	ZZ	332	ASN
11	ZZ	379	GLN
11	ZZ	394	GLN
11	ZZ	401	ASN
11	Za	115	GLN
11	Za	129	GLN
11	Za	133	ASN
11	Za	197	ASN
11	Za	387	GLN
11	Zb	5	GLN
11	Zb	79	GLN
11	Zb	107	ASN
11	Zb	129	GLN
11	Zb	133	ASN
11	Zb	197	ASN
11	Zb	293	GLN
11	Zb	308	GLN
11	Zb	332	ASN
11	Zb	358	ASN
11	Zb	387	GLN
11	Zc	5	GLN
11	Zc	107	ASN
11	Zc	129	GLN
11	Zc	159	ASN
11	Zc	197	ASN
11	Zc	352	ASN
11	Zc	379	GLN

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Mol	Chain	Res	Type
11	Zc	387	GLN
11	Zc	397	ASN
11	Zd	5	GLN
11	Zd	105	ASN
11	Zd	129	GLN
11	Zd	130	GLN
11	Zd	133	ASN
11	Zd	293	GLN
11	Zd	295	ASN
11	Zd	397	ASN
11	Ze	5	GLN
11	Ze	99	GLN
11	Ze	107	ASN
11	Ze	133	ASN
11	Ze	197	ASN
11	Ze	394	GLN
11	Zf	105	ASN
11	Zf	159	ASN
11	Zf	197	ASN
11	Zf	314	GLN
11	Zg	5	GLN
11	Zg	107	ASN
11	Zg	129	GLN
11	Zg	133	ASN
11	Zg	197	ASN
11	Zg	310	GLN
11	Zh	5	GLN
11	Zh	115	GLN
11	Zh	197	ASN
11	Zh	379	GLN
11	Zh	392	GLN
12	a	51	GLN
12	a	63	ASN
12	a	83	ASN
12	a	138	GLN
12	a	159	GLN
12	a	161	ASN
12	a	178	GLN
12	a	188	GLN
12	a	198	GLN
12	a	229	ASN
12	a	241	ASN

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

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Mol	Chain	Res	Type
12	e	159	GLN
12	e	161	ASN
12	e	178	GLN
12	e	188	GLN
12	e	198	GLN
12	e	229	ASN
12	e	241	ASN
12	f	51	GLN
12	f	63	ASN
12	f	83	ASN
12	f	138	GLN
12	f	140	ASN
12	f	159	GLN
12	f	161	ASN
12	f	178	GLN
12	f	188	GLN
12	f	198	GLN
12	f	229	ASN
12	f	241	ASN
12	g	51	GLN
12	g	63	ASN
12	g	80	GLN
12	g	83	ASN
12	g	138	GLN
12	g	140	ASN
12	g	159	GLN
12	g	161	ASN
12	g	178	GLN
12	g	188	GLN
12	g	198	GLN
12	g	229	ASN
12	g	241	ASN
12	g	350	GLN
12	h	51	GLN
12	h	63	ASN
12	h	83	ASN
12	h	138	GLN
12	h	140	ASN
12	h	159	GLN
12	h	161	ASN
12	h	178	GLN
12	h	188	GLN

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Mol	Chain	Res	Type
12	h	198	GLN
12	h	229	ASN
12	h	241	ASN
12	i	51	GLN
12	i	63	ASN
12	i	83	ASN
12	i	138	GLN
12	i	140	ASN
12	i	159	GLN
12	i	161	ASN
12	i	178	GLN
12	i	188	GLN
12	i	198	GLN
12	i	229	ASN
12	i	241	ASN
12	j	51	GLN
12	j	63	ASN
12	j	83	ASN
12	j	138	GLN
12	j	140	ASN
12	j	159	GLN
12	j	161	ASN
12	j	178	GLN
12	j	188	GLN
12	j	198	GLN
12	j	229	ASN
12	j	241	ASN
12	k	51	GLN
12	k	63	ASN
12	k	83	ASN
12	k	138	GLN
12	k	140	ASN
12	k	159	GLN
12	k	161	ASN
12	k	178	GLN
12	k	188	GLN
12	k	198	GLN
12	k	229	ASN
12	k	241	ASN
12	k	350	GLN
12	l	51	GLN
12	l	54	GLN

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

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Mol	Chain	Res	Type
12	o	83	ASN
12	o	138	GLN
12	o	140	ASN
12	o	159	GLN
12	o	161	ASN
12	o	178	GLN
12	o	188	GLN
12	o	198	GLN
12	o	229	ASN
12	o	241	ASN
12	p	51	GLN
12	p	63	ASN
12	p	80	GLN
12	p	83	ASN
12	p	138	GLN
12	p	140	ASN
12	p	159	GLN
12	p	161	ASN
12	p	178	GLN
12	p	188	GLN
12	p	198	GLN
12	p	229	ASN
12	p	241	ASN
12	p	350	GLN
12	q	51	GLN
12	q	63	ASN
12	q	80	GLN
12	q	83	ASN
12	q	138	GLN
12	q	140	ASN
12	q	159	GLN
12	q	161	ASN
12	q	178	GLN
12	q	188	GLN
12	q	198	GLN
12	q	229	ASN
12	q	241	ASN
12	r	51	GLN
12	r	63	ASN
12	r	80	GLN
12	r	83	ASN
12	r	138	GLN

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Mol	Chain	Res	Type
12	r	140	ASN
12	r	159	GLN
12	r	161	ASN
12	r	178	GLN
12	r	188	GLN
12	r	198	GLN
12	r	229	ASN
12	r	241	ASN
12	r	350	GLN
12	s	51	GLN
12	s	54	GLN
12	s	63	ASN
12	s	83	ASN
12	s	138	GLN
12	s	140	ASN
12	s	159	GLN
12	s	161	ASN
12	s	178	GLN
12	s	188	GLN
12	s	198	GLN
12	s	229	ASN
12	s	241	ASN
12	t	51	GLN
12	t	63	ASN
12	t	83	ASN
12	t	138	GLN
12	t	140	ASN
12	t	159	GLN
12	t	161	ASN
12	t	178	GLN
12	t	188	GLN
12	t	198	GLN
12	t	229	ASN
12	t	241	ASN
12	u	51	GLN
12	u	63	ASN
12	u	83	ASN
12	u	138	GLN
12	u	140	ASN
12	u	159	GLN
12	u	161	ASN
12	u	178	GLN

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

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Mol	Chain	Res	Type
12	y	63	ASN
12	y	83	ASN
12	y	138	GLN
12	y	140	ASN
12	y	159	GLN
12	y	161	ASN
12	y	178	GLN
12	y	188	GLN
12	y	198	GLN
12	y	229	ASN
12	y	241	ASN
12	z	51	GLN
12	z	63	ASN
12	z	83	ASN
12	z	138	GLN
12	z	140	ASN
12	z	159	GLN
12	z	161	ASN
12	z	178	GLN
12	z	188	GLN
12	z	198	GLN
12	z	229	ASN
12	z	241	ASN
14	C6	46	GLN
14	C6	186	GLN
16	C0	8	GLN
16	C0	238	ASN
16	C0	245	ASN
14	DA	46	GLN
14	DA	186	GLN
16	DC	8	GLN
16	DC	238	ASN
16	DC	245	ASN
6	DE	542	ASN
16	DF	8	GLN
16	DF	238	ASN
16	DF	245	ASN
14	DG	46	GLN
14	DG	186	GLN
6	DL	542	ASN
16	DX	8	GLN
16	DX	238	ASN

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Mol	Chain	Res	Type
16	DX	245	ASN
14	DY	46	GLN
14	DY	186	GLN
16	Dd	8	GLN
16	Dd	238	ASN
16	Dd	245	ASN
14	De	46	GLN
14	De	186	GLN
16	Dj	8	GLN
16	Dj	238	ASN
16	Dj	245	ASN
14	Dk	46	GLN
14	Dk	186	GLN
16	Dp	8	GLN
16	Dp	238	ASN
16	Dp	245	ASN
14	Dq	46	GLN
14	Dq	186	GLN
16	Dv	8	GLN
16	Dv	238	ASN
16	Dv	245	ASN
14	Dw	46	GLN
14	Dw	186	GLN
16	D2	8	GLN
16	D2	238	ASN
16	D2	245	ASN
14	D3	46	GLN
14	D3	186	GLN
16	D8	8	GLN
16	D8	238	ASN
16	D8	245	ASN
14	D9	46	GLN
14	D9	186	GLN
6	B0	542	ASN
6	B3	542	ASN
16	B4	8	GLN
16	B4	238	ASN
16	B4	245	ASN
14	B5	46	GLN
14	B5	186	GLN
14	EC	46	GLN
14	EC	186	GLN

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Mol	Chain	Res	Type
6	EH	542	ASN
16	EI	8	GLN
16	EI	238	ASN
16	EI	245	ASN
14	EJ	46	GLN
14	EJ	186	GLN
6	EO	542	ASN
16	EP	8	GLN
16	EP	238	ASN
16	EP	245	ASN
14	EQ	46	GLN
14	EQ	186	GLN
6	EV	542	ASN
16	EW	8	GLN
16	EW	238	ASN
16	EW	245	ASN
14	EX	46	GLN
14	EX	186	GLN
6	Ba	542	ASN
16	Bb	8	GLN
16	Bb	238	ASN
16	Bb	245	ASN
14	Bc	46	GLN
14	Bc	186	GLN
6	Bh	542	ASN
16	Bi	8	GLN
16	Bi	238	ASN
16	Bi	245	ASN
14	Bj	46	GLN
14	Bj	186	GLN
6	Bo	542	ASN
16	Bp	8	GLN
16	Bp	238	ASN
16	Bp	245	ASN
14	Bq	46	GLN
14	Bq	186	GLN
6	Bv	542	ASN
16	Bw	8	GLN
16	Bw	238	ASN
16	Bw	245	ASN
14	Bx	46	GLN
14	Bx	186	GLN

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Mol	Chain	Res	Type
6	Ea	542	ASN
16	CA	8	GLN
16	CA	238	ASN
16	CA	245	ASN
14	CB	46	GLN
14	CB	186	GLN
6	CG	542	ASN
16	CH	8	GLN
16	CH	238	ASN
16	CH	245	ASN
14	CI	46	GLN
14	CI	186	GLN
6	CN	542	ASN
16	CO	8	GLN
16	CO	238	ASN
16	CO	245	ASN
14	CP	46	GLN
14	CP	186	GLN
6	CU	542	ASN
16	CV	8	GLN
16	CV	238	ASN
16	CV	245	ASN
14	CW	46	GLN
14	CW	186	GLN
6	Cb	542	ASN
16	Cc	8	GLN
16	Cc	238	ASN
16	Cc	245	ASN
14	Cd	46	GLN
14	Cd	186	GLN
6	Ci	542	ASN
16	Cj	8	GLN
16	Cj	238	ASN
16	Cj	245	ASN
14	Ck	46	GLN
14	Ck	186	GLN
6	Cp	542	ASN
16	Cq	8	GLN
16	Cq	238	ASN
16	Cq	245	ASN
14	Cr	46	GLN
14	Cr	186	GLN

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Mol	Chain	Res	Type
6	Cw	542	ASN
16	Cx	8	GLN
16	Cx	238	ASN
16	Cx	245	ASN
14	Cy	46	GLN
14	Cy	186	GLN
6	Eb	542	ASN
6	Ec	542	ASN
6	Ed	542	ASN
6	Ee	542	ASN
6	Ef	542	ASN
6	Eg	542	ASN
6	Eh	542	ASN
6	Ei	542	ASN
6	Ej	542	ASN
6	Ek	542	ASN
6	El	542	ASN
6	Em	542	ASN
6	En	542	ASN
6	Eo	542	ASN
6	Ep	542	ASN
16	Eq	8	GLN
16	Eq	238	ASN
16	Eq	245	ASN
16	Er	8	GLN
16	Er	238	ASN
16	Er	245	ASN
16	Es	8	GLN
16	Es	238	ASN
16	Es	245	ASN
16	Et	8	GLN
16	Et	238	ASN
16	Et	245	ASN
16	Eu	8	GLN
16	Eu	238	ASN
16	Eu	245	ASN
16	Ev	8	GLN
16	Ev	238	ASN
16	Ev	245	ASN
16	Ew	8	GLN
16	Ew	238	ASN
16	Ew	245	ASN

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Mol	Chain	Res	Type
14	Ex	46	GLN
14	Ex	186	GLN
14	Ey	46	GLN
14	Ey	186	GLN
14	Ez	46	GLN
14	Ez	186	GLN
14	E1	46	GLN
14	E1	186	GLN
14	E2	46	GLN
14	E2	186	GLN
14	E3	46	GLN
14	E3	186	GLN
14	E4	46	GLN
14	E4	186	GLN
16	E5	8	GLN
16	E5	238	ASN
16	E5	245	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

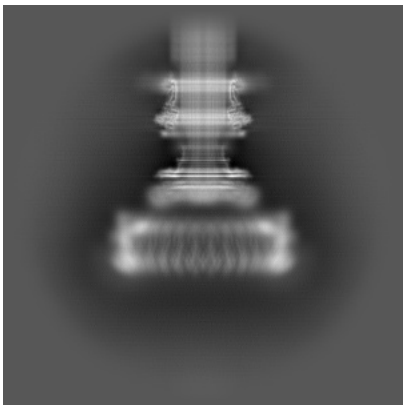
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37684. These allow visual inspection of the internal detail of the map and identification of artifacts.

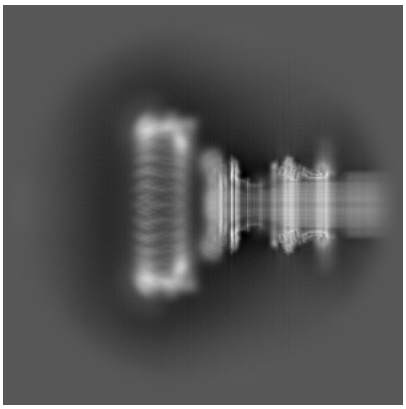
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

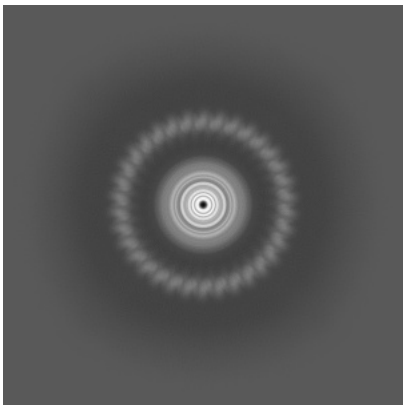
6.1.1 Primary map



X

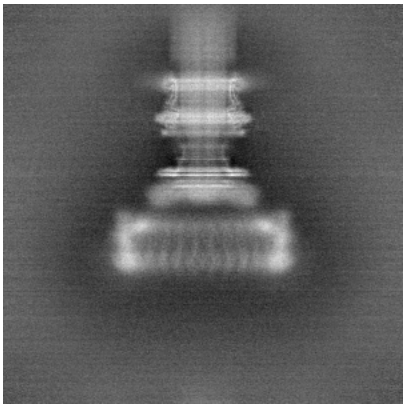


Y

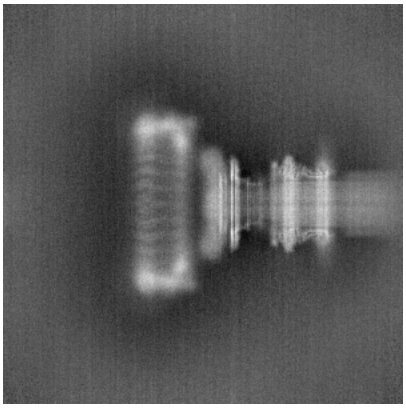


Z

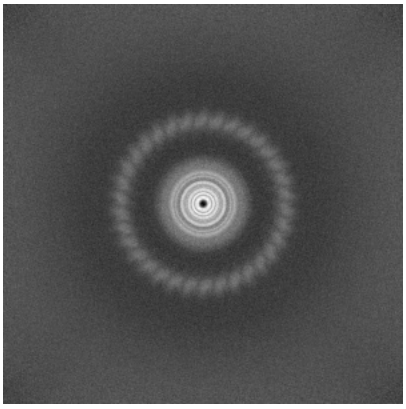
6.1.2 Raw map



X



Y

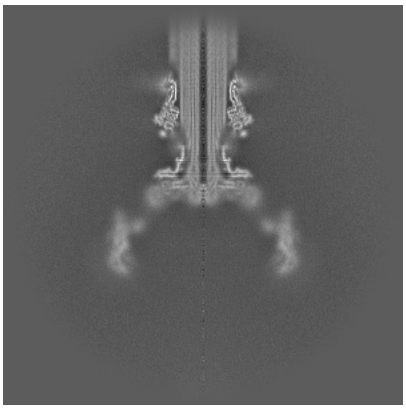


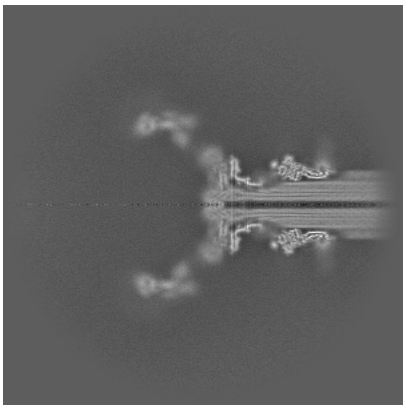
Z

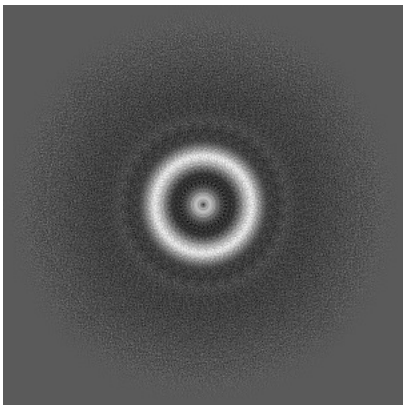
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

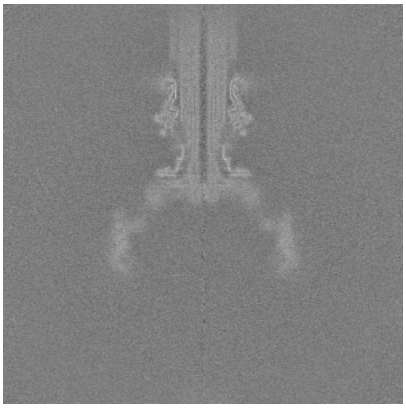
6.2.1 Primary map

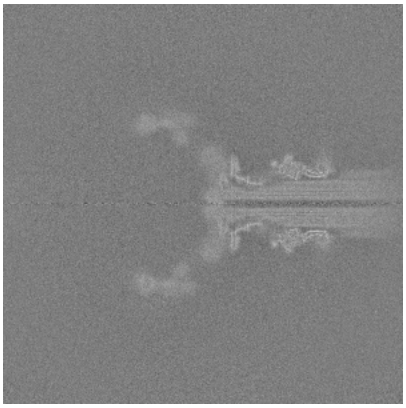

X Index: 420

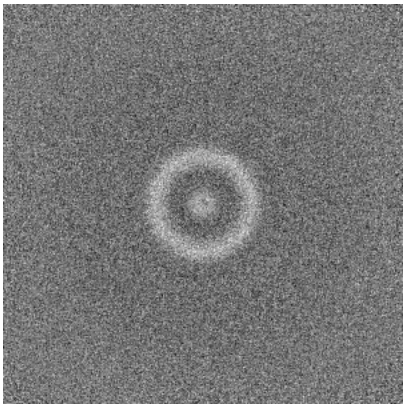

Y Index: 420


Z Index: 420

6.2.2 Raw map


X Index: 420

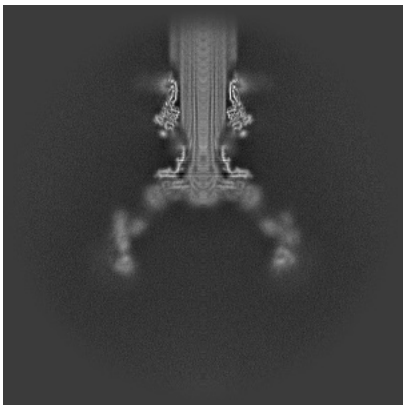

Y Index: 420

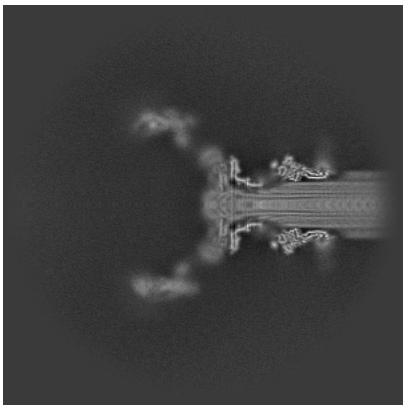

Z Index: 420

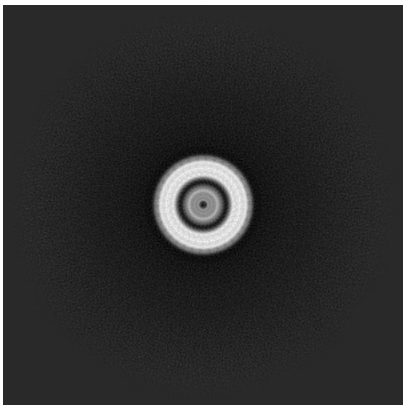
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

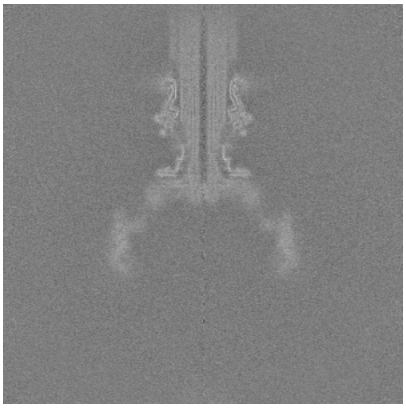
6.3.1 Primary map

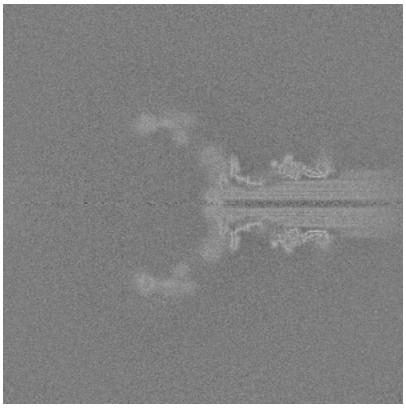

X Index: 431

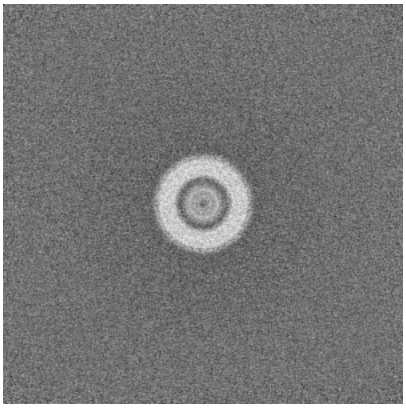

Y Index: 431


Z Index: 481

6.3.2 Raw map


X Index: 420

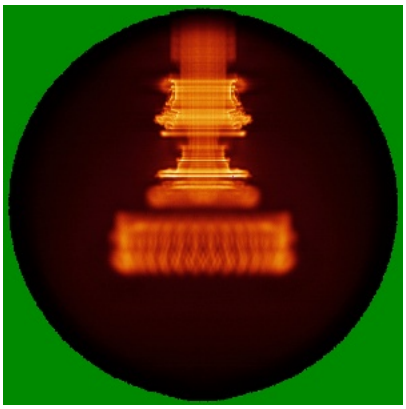

Y Index: 420

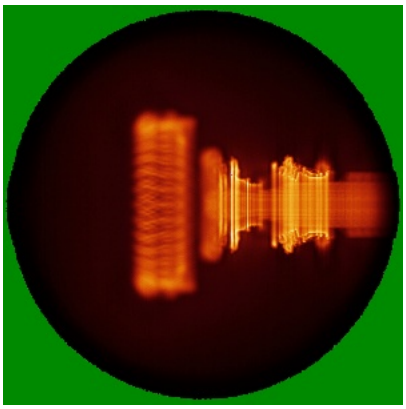

Z Index: 481

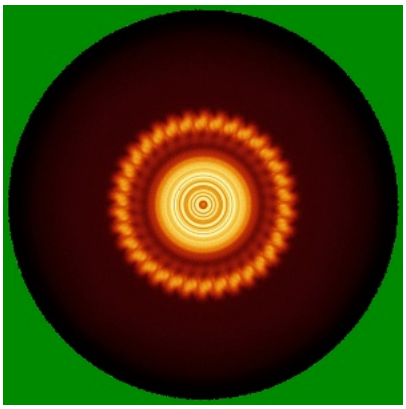
The images above show the largest variance slices of the map in three orthogonal directions.

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

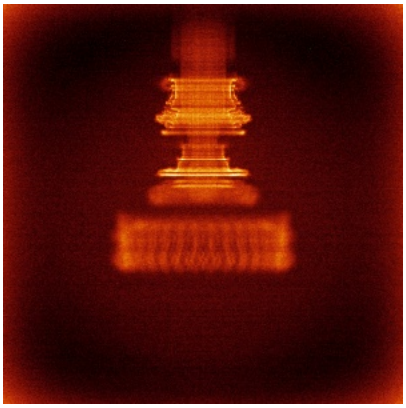
6.4.1 Primary map

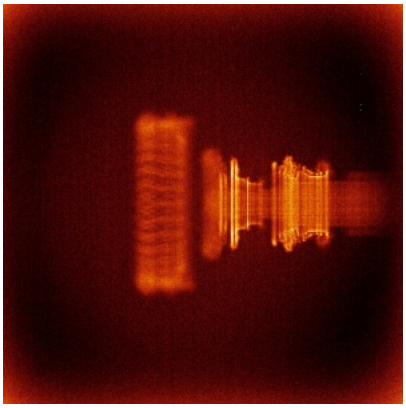

X

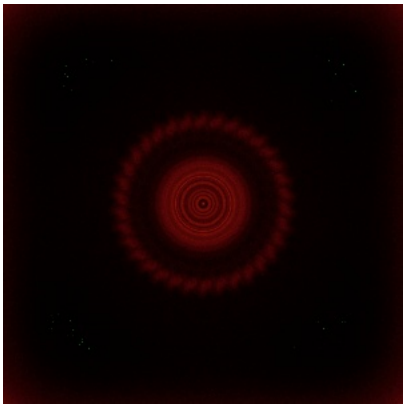

Y


Z

6.4.2 Raw map


X


Y


Z

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

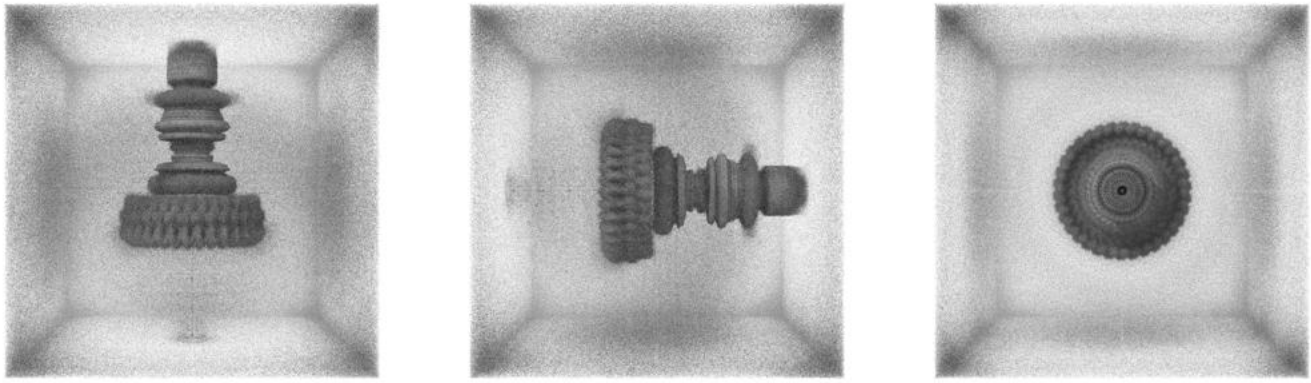
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

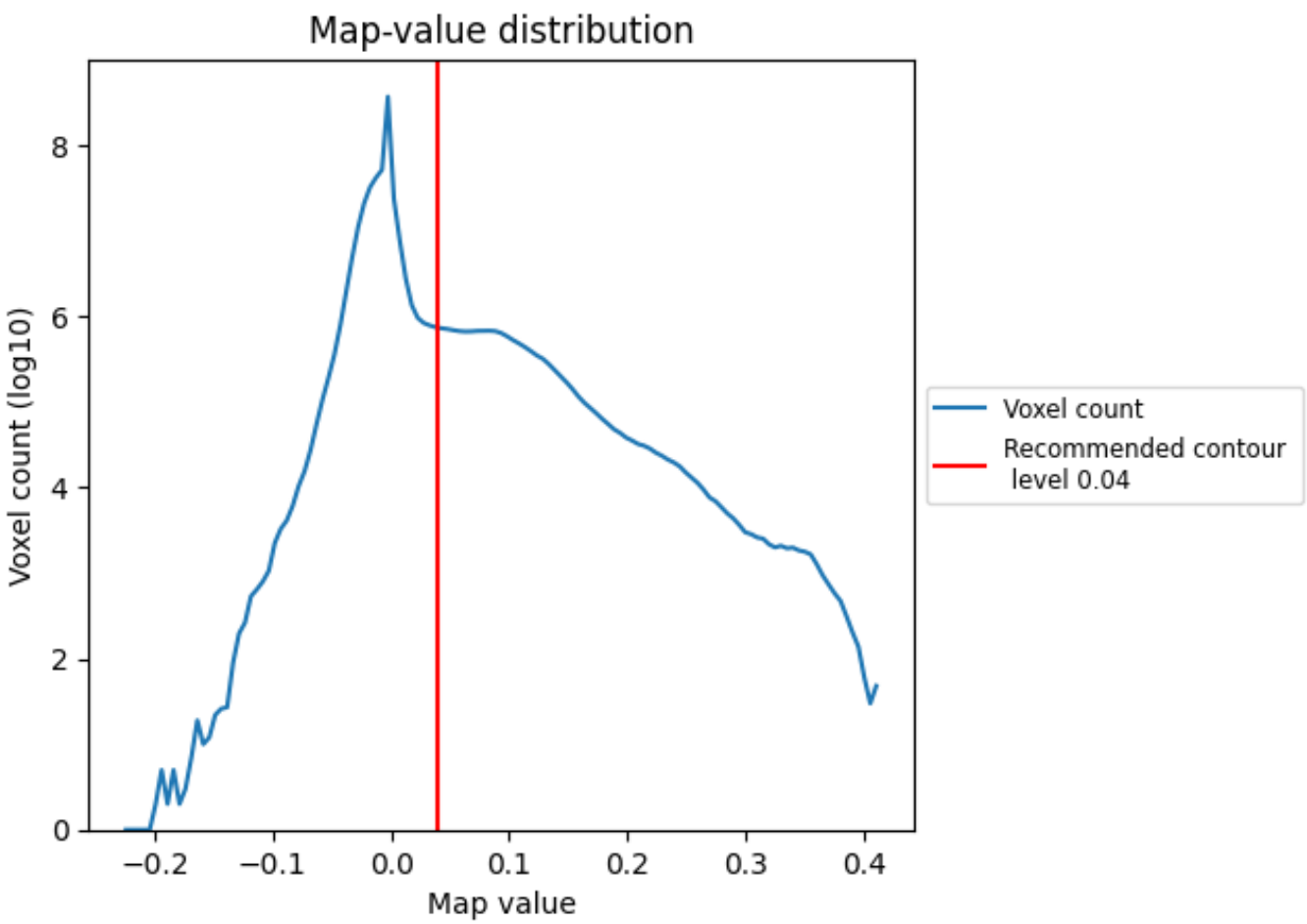
6.6 Mask visualisation (i)

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

7 Map analysis (i)

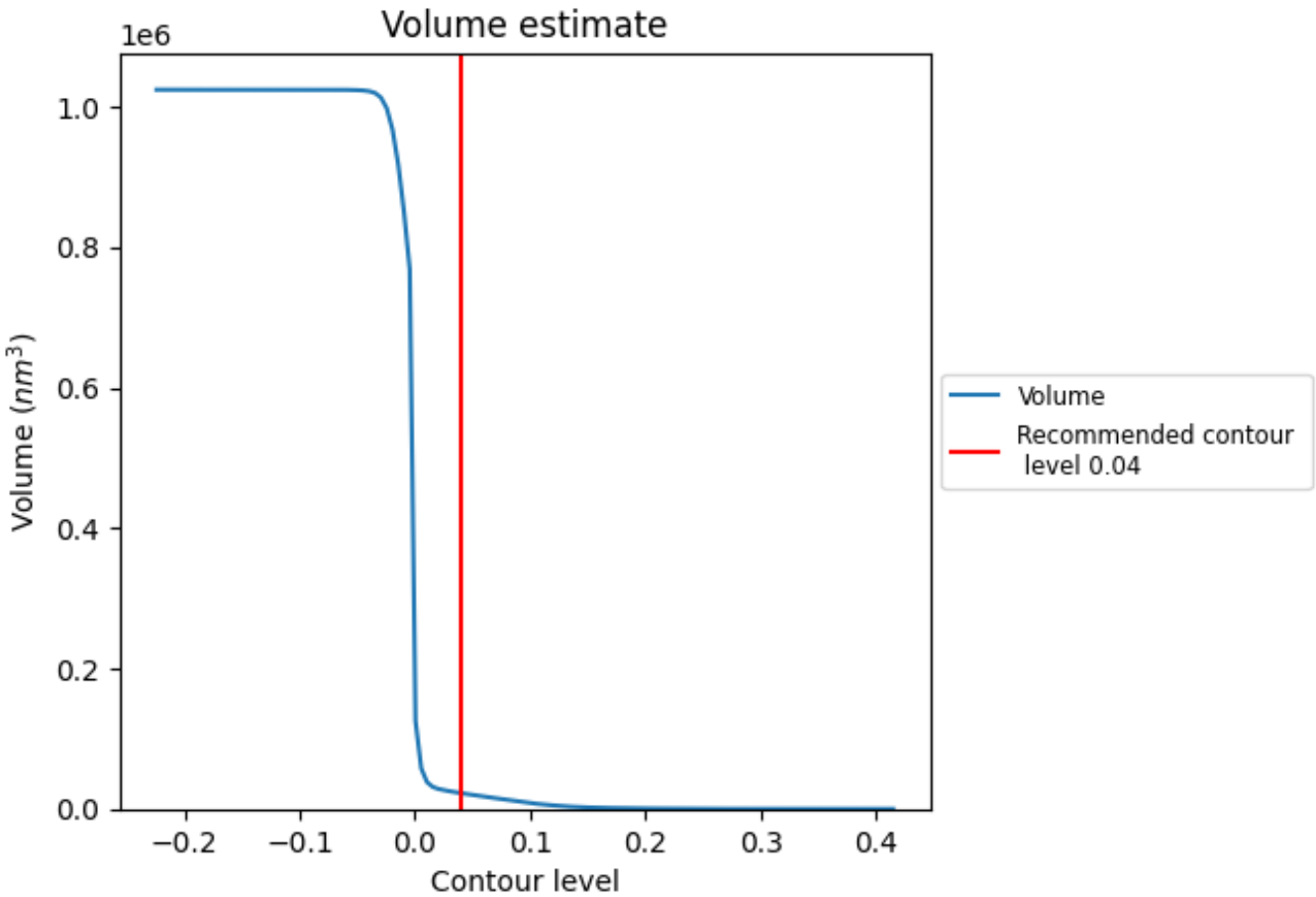
This section contains the results of statistical analysis of the map.

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.

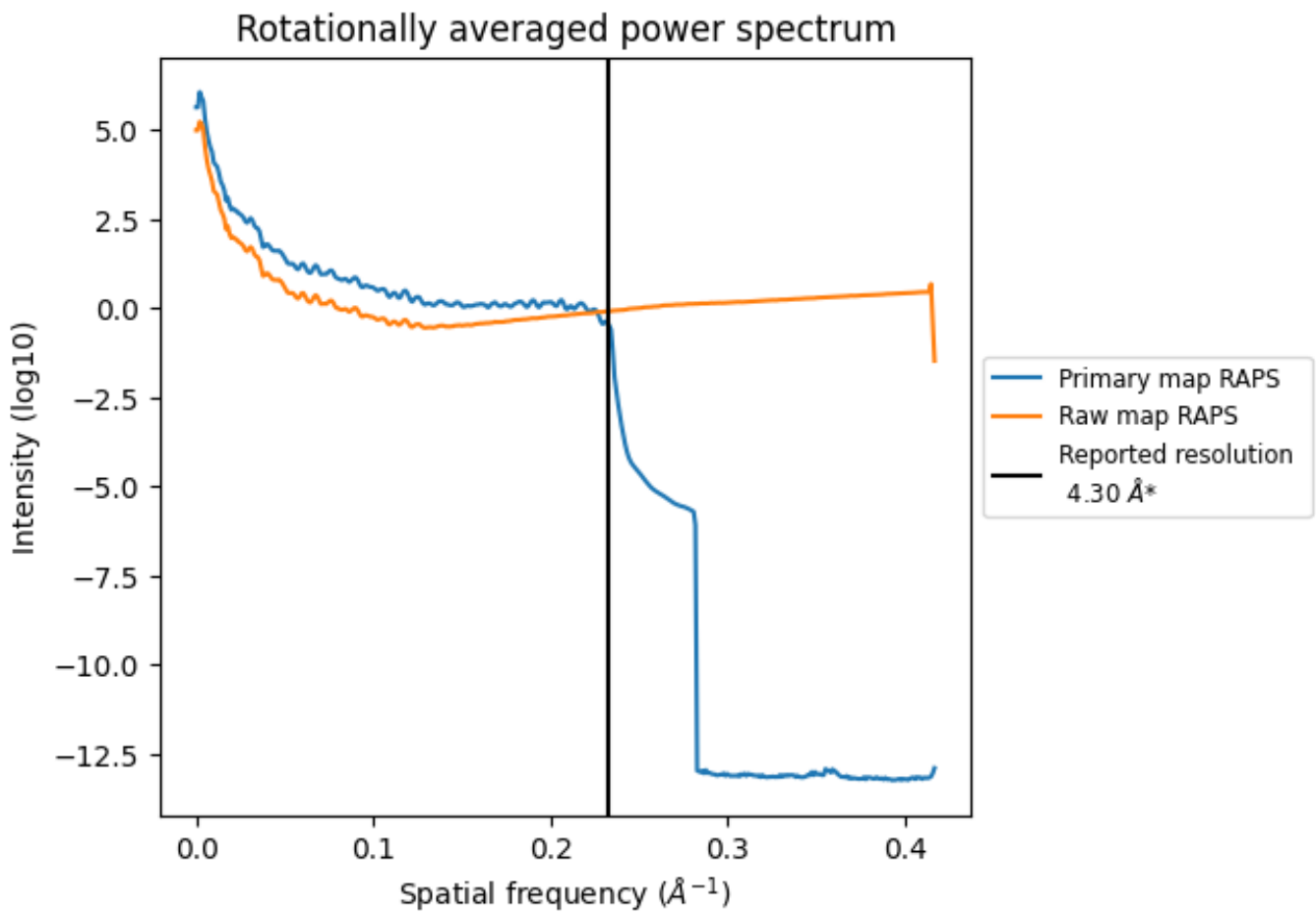
7.2 Volume estimate (i)



The volume at the recommended contour level is 22548 nm^3; this corresponds to an approximate mass of 20368 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)

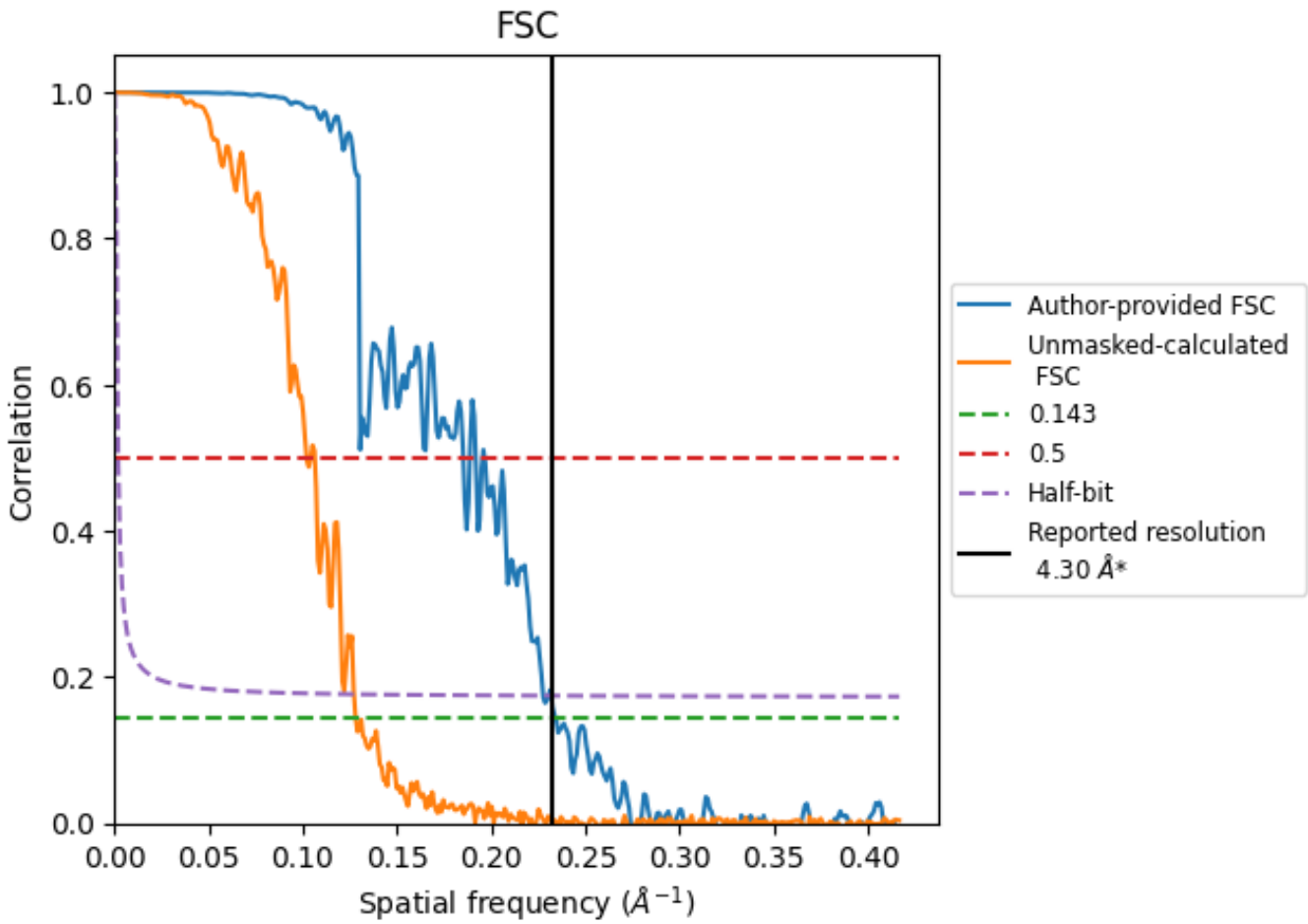


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.27	5.40	4.39
Unmasked-calculated*	7.81	9.80	7.86

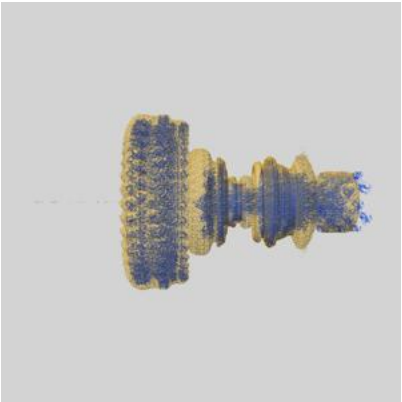
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.81 differs from the reported value 4.3 by more than 10 %

9 Map-model fit (i)

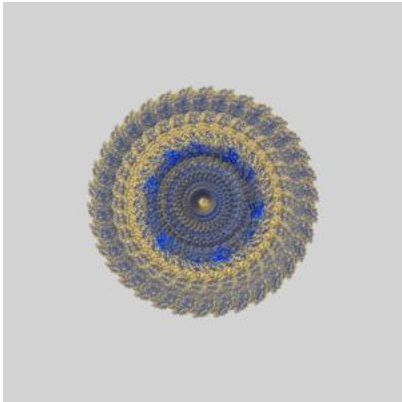
This section contains information regarding the fit between EMDB map EMD-37684 and PDB model 8WOE. Per-residue inclusion information can be found in section 3 on page 46.

9.1 Map-model overlay (i)

X



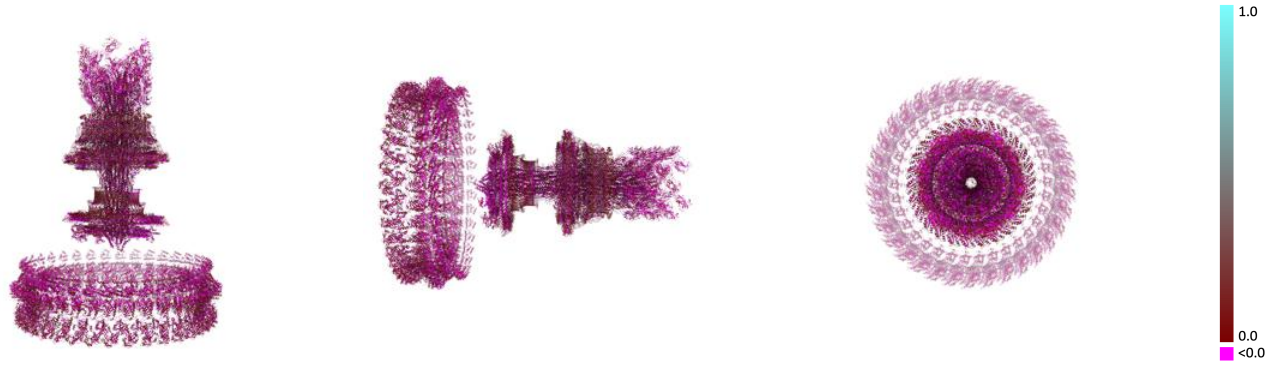
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

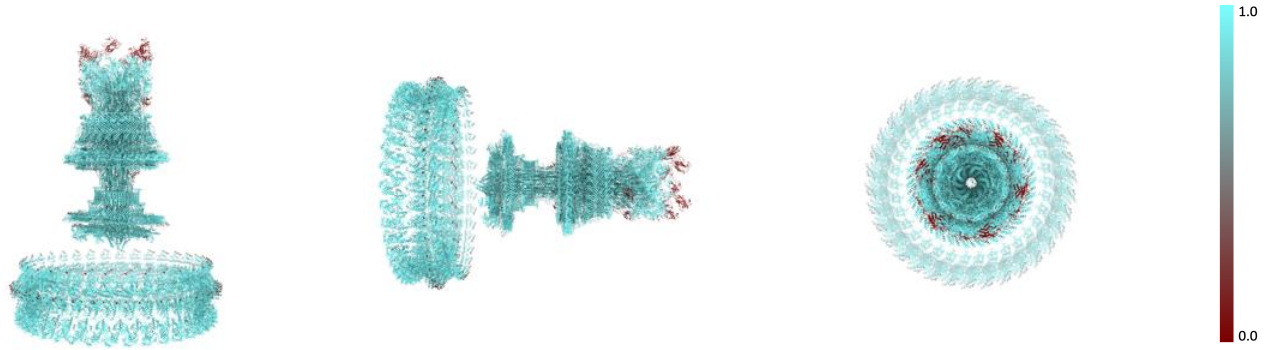
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

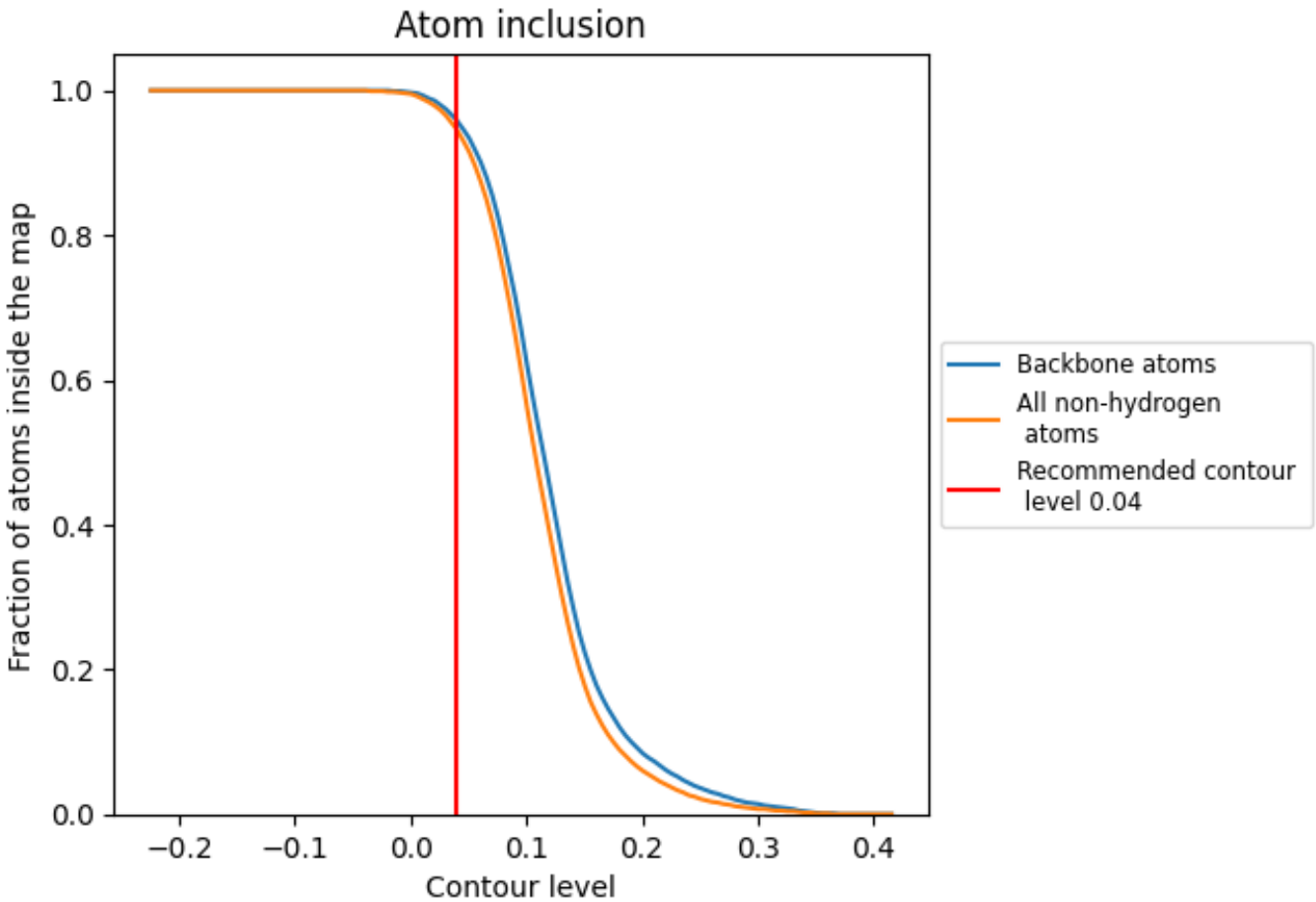
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.0660
0	0.9630	0.0640
1	0.9600	0.0700
2	0.9620	0.0710
3	0.9620	0.0670
4	0.9560	0.0560
5	0.9560	0.0480
6	0.9570	0.0700
7	0.9660	0.0710
8	0.9720	0.0770
9	0.9740	0.0690
A	0.9370	0.1470
A0	0.9020	0.0500
A1	0.8930	0.0440
A2	0.9510	0.0550
A3	0.9540	0.0720
A4	0.9590	0.1040
A5	0.9510	0.0930
A6	0.8340	0.0610
A7	0.8770	0.0350
A8	0.8850	0.0360
A9	0.8790	0.0380
AA	0.8630	0.0360
AB	0.8980	0.0310
AC	0.9290	0.0380
AD	0.9510	0.0550
AE	0.9590	0.0710
AF	0.9670	0.0760
AG	0.9660	0.0660
AH	0.9710	0.0590
AI	0.9670	0.0480
AJ	0.9690	0.0690
AK	0.9730	0.0660
AL	0.9680	0.0800
AM	0.9690	0.0620

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Chain	Atom inclusion	Q-score
AN	0.9590	0.0450
AO	0.9620	0.0790
AP	0.9750	0.1060
AQ	0.9780	0.1230
AR	0.9740	0.1190
AS	0.9290	0.0700
AT	0.9320	0.0710
AU	0.9330	0.0790
AV	0.9450	0.0910
AW	0.9550	0.1070
AX	0.9680	0.1250
AY	0.9730	0.1440
AZ	0.9770	0.1450
Aa	0.9770	0.1370
Ab	0.9870	0.0060
Ac	0.9650	0.0970
Ad	0.9540	0.0750
Ae	0.9420	0.0550
Af	0.9220	0.0390
Ag	0.9110	0.0280
Ah	0.8980	0.0200
Ai	0.8930	0.0130
Aj	0.8920	0.0120
Ak	0.8960	0.0120
Al	0.9010	0.0150
Am	0.9110	0.0190
An	0.9210	0.0240
Ao	0.9380	0.0320
Ap	0.9470	0.0510
Aq	1.0000	-0.0100
Ar	1.0000	0.0070
As	0.9940	0.0470
At	0.9950	0.0390
Au	0.9690	0.0360
Av	0.9840	0.0330
Aw	0.9770	0.0160
Ax	0.9580	0.0210
Ay	0.9240	0.0430
Az	0.9110	0.0700
B	0.9360	0.1430
B0	0.9910	0.0380
B1	0.9940	0.1100

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Chain	Atom inclusion	Q-score
B2	0.9920	0.0680
B3	0.9910	0.0420
B4	0.9880	0.0820
B5	0.9740	0.0320
B6	0.8860	0.0460
B7	0.9970	0.0820
B8	0.9940	0.1080
B9	0.9920	0.0710
BA	0.9450	0.0370
BB	0.9490	0.0440
BC	0.9530	0.0250
BD	0.9790	0.0710
BE	0.9890	0.0930
BF	0.9940	0.0690
BG	1.0000	0.0830
BH	0.8450	0.0020
BI	0.5710	-0.0320
BJ	0.8350	-0.0060
BK	0.6860	-0.0090
BL	0.8640	-0.0320
BM	0.8210	0.0250
BN	0.9710	0.0730
BO	0.9320	0.1020
BP	0.9610	0.0190
BQ	0.8570	0.0660
BR	0.9820	0.1300
BS	0.9740	0.1260
BT	0.9660	0.1160
BU	0.9480	0.1040
BV	0.9380	0.0920
BW	0.9330	0.0800
BX	0.9290	0.0720
BY	0.9940	0.1110
BZ	0.9920	0.0700
Ba	0.9910	0.0390
Bb	0.9870	0.0820
Bc	0.9730	0.0320
Bd	0.8770	0.0430
Be	0.9950	0.0790
Bf	0.9940	0.1120
Bg	0.9920	0.0670
Bh	0.9910	0.0380

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Chain	Atom inclusion	Q-score
Bi	0.9870	0.0820
Bj	0.9730	0.0320
Bk	0.8760	0.0440
Bl	0.9950	0.0790
Bm	0.9940	0.1080
Bn	0.9920	0.0690
Bo	0.9910	0.0370
Bp	0.9870	0.0830
Bq	0.9720	0.0310
Br	0.8730	0.0450
Bs	0.9970	0.0810
Bt	0.9940	0.1050
Bu	0.9920	0.0700
Bv	0.9910	0.0420
Bw	0.9870	0.0830
Bx	0.9730	0.0330
By	0.8770	0.0450
Bz	0.9950	0.0810
C	0.9410	0.1460
C0	0.9880	0.0800
C1	0.9970	0.0790
C2	0.9940	0.1060
C3	0.9920	0.0720
C4	0.9970	0.0790
C5	0.9940	0.1050
C6	0.9720	0.0320
C7	0.8770	0.0370
C8	0.9950	0.0780
C9	0.9940	0.1080
CA	0.9880	0.0820
CB	0.9740	0.0320
CC	0.8820	0.0450
CD	0.9950	0.0810
CE	0.9940	0.1100
CF	0.9920	0.0700
CG	0.9910	0.0360
CH	0.9880	0.0820
CI	0.9720	0.0300
CJ	0.8800	0.0420
CK	0.9970	0.0810
CL	0.9940	0.1100
CM	0.9920	0.0710

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Chain	Atom inclusion	Q-score
CN	0.9910	0.0410
CO	0.9880	0.0820
CP	0.9730	0.0310
CQ	0.8810	0.0420
CR	0.9970	0.0790
CS	0.9940	0.1110
CT	0.9920	0.0730
CU	0.9910	0.0430
CV	0.9870	0.0810
CW	0.9730	0.0310
CX	0.8730	0.0430
CY	0.9970	0.0820
CZ	0.9940	0.1070
Ca	0.9920	0.0710
Cb	0.9910	0.0410
Cc	0.9870	0.0810
Cd	0.9730	0.0320
Ce	0.8770	0.0420
Cf	0.9970	0.0810
Cg	0.9920	0.1080
Ch	0.9920	0.0700
Ci	0.9910	0.0380
Cj	0.9870	0.0820
Ck	0.9730	0.0310
Cl	0.8740	0.0420
Cm	0.9940	0.0780
Cn	0.9920	0.1070
Co	0.9920	0.0710
Cp	0.9910	0.0360
Cq	0.9870	0.0820
Cr	0.9730	0.0330
Cs	0.8780	0.0400
Ct	0.9950	0.0790
Cu	0.9940	0.1080
Cv	0.9920	0.0720
Cw	0.9910	0.0420
Cx	0.9870	0.0810
Cy	0.9740	0.0320
Cz	0.8770	0.0410
D	0.9350	0.1440
D0	0.8770	0.0380
D1	0.9920	0.0690

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Chain	Atom inclusion	Q-score
D2	0.9870	0.0810
D3	0.9730	0.0300
D4	0.8730	0.0380
D5	0.9940	0.0790
D6	0.9940	0.1060
D7	0.9920	0.0690
D8	0.9870	0.0820
D9	0.9730	0.0310
DA	0.9740	0.0300
DB	0.8840	0.0370
DC	0.9880	0.0810
DD	0.9920	0.0700
DE	0.9910	0.0410
DF	0.9880	0.0810
DG	0.9740	0.0310
DH	0.8800	0.0420
DI	0.9950	0.0800
DJ	0.9940	0.1070
DK	0.9920	0.0690
DL	0.9910	0.0360
DM	0.9920	0.0700
DN	0.9920	0.0720
DO	0.9920	0.0710
DP	0.9920	0.0720
DQ	0.9920	0.0690
DR	0.9920	0.0710
DS	0.9920	0.0710
DT	0.9920	0.0670
DU	0.9970	0.0800
DV	0.9940	0.1040
DW	0.9920	0.0710
DX	0.9880	0.0810
DY	0.9730	0.0300
DZ	0.8800	0.0410
Da	0.9970	0.0800
Db	0.9940	0.1060
Dc	0.9920	0.0700
Dd	0.9880	0.0810
De	0.9720	0.0290
Df	0.8810	0.0370
Dg	0.9950	0.0800
Dh	0.9940	0.1030

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Chain	Atom inclusion	Q-score
Di	0.9920	0.0700
Dj	0.9870	0.0820
Dk	0.9730	0.0300
Dl	0.8800	0.0380
Dm	0.9970	0.0820
Dn	0.9920	0.1060
Do	0.9920	0.0720
Dp	0.9870	0.0800
Dq	0.9720	0.0290
Dr	0.8760	0.0390
Ds	0.9970	0.0830
Dt	0.9940	0.1050
Du	0.9920	0.0700
Dv	0.9870	0.0790
Dw	0.9730	0.0310
Dx	0.8790	0.0380
Dy	0.9970	0.0820
Dz	0.9920	0.1060
E	0.9410	0.1370
E0	0.8750	0.0390
E1	0.9730	0.0310
E2	0.9730	0.0310
E3	0.9730	0.0310
E4	0.9720	0.0300
E5	0.9870	0.0810
E6	0.8810	0.0390
E7	0.8790	0.0390
E8	0.8780	0.0380
E9	0.8720	0.0400
EA	0.9950	0.0810
EB	0.9940	0.1080
EC	0.9720	0.0330
ED	0.8820	0.0420
EE	0.9970	0.0800
EF	0.9940	0.1080
EG	0.9920	0.0680
EH	0.9910	0.0400
EI	0.9880	0.0810
EJ	0.9720	0.0320
EK	0.8830	0.0410
EL	0.9970	0.0820
EM	0.9940	0.1080

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Chain	Atom inclusion	Q-score
EN	0.9920	0.0710
EO	0.9910	0.0380
EP	0.9880	0.0820
EQ	0.9730	0.0300
ER	0.8790	0.0430
ES	0.9970	0.0810
ET	0.9940	0.1050
EU	0.9920	0.0700
EV	0.9910	0.0380
EW	0.9870	0.0810
EX	0.9740	0.0310
EY	0.8730	0.0440
EZ	0.9970	0.0820
Ea	0.9910	0.0400
Eb	0.9910	0.0390
Ec	0.9910	0.0370
Ed	0.9910	0.0410
Ee	0.9910	0.0430
Ef	0.9910	0.0420
Eg	0.9910	0.0400
Eh	0.9910	0.0410
Ei	0.9910	0.0430
Ej	0.9910	0.0430
Ek	0.9910	0.0420
El	0.9910	0.0420
Em	0.9910	0.0370
En	0.9910	0.0390
Eo	0.9910	0.0390
Ep	0.9910	0.0410
Eq	0.9870	0.0800
Er	0.9870	0.0810
Es	0.9880	0.0820
Et	0.9870	0.0820
Eu	0.9870	0.0810
Ev	0.9870	0.0820
Ew	0.9870	0.0820
Ex	0.9720	0.0310
Ey	0.9730	0.0310
Ez	0.9730	0.0290
F	0.9400	0.1370
FA	0.8750	0.0390
FB	0.8720	0.0370

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Chain	Atom inclusion	Q-score
FC	0.9970	0.0770
FD	0.9970	0.0810
FE	0.9970	0.0780
FF	0.9970	0.0780
FG	0.9950	0.0780
FH	0.9950	0.0760
FI	0.9940	0.1080
FJ	0.9940	0.1060
FK	0.9940	0.1040
FL	0.9940	0.1060
FM	0.9940	0.1060
FN	0.9910	0.1050
G	0.9380	0.1350
H	0.9270	0.1260
I	0.9320	0.1250
J	0.9320	0.1310
K	0.9250	0.1270
L	0.9310	0.1300
M	0.9320	0.1390
N	0.9280	0.1400
O	0.9320	0.1430
P	0.9300	0.1450
Q	0.9270	0.1460
R	0.9320	0.1450
S	0.9280	0.1430
T	0.9260	0.1340
U	0.9260	0.1350
UI	0.9360	0.0490
UJ	0.8960	0.0090
UK	0.9260	0.0530
UL	0.9260	0.0540
UM	0.9890	-0.0010
UN	0.9710	0.0110
UO	0.9670	0.0410
UP	0.9440	0.0470
V	0.9310	0.1360
W	0.9290	0.1290
WA	0.9710	0.0730
WB	0.9830	0.0770
WC	0.9800	0.0500
WD	0.9770	0.0590
WE	0.9280	0.0460

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Chain	Atom inclusion	Q-score
WF	0.9610	0.0770
WG	0.9650	0.0590
WH	0.9710	0.0900
WI	0.9160	0.0950
WJ	0.9780	0.0620
WK	0.9900	0.0270
WL	0.9870	-0.0210
WM	0.9630	-0.0210
WN	0.9470	-0.0240
WO	0.9390	-0.0120
WP	0.9550	-0.0220
WQ	0.9670	-0.0370
WR	0.9790	0.0110
WS	0.9840	-0.0140
WT	0.9850	0.0440
WU	0.9930	0.0540
WV	0.9940	0.0760
WW	0.9990	0.0740
X	0.9310	0.1380
Y	0.9320	0.1400
Z	0.9380	0.1440
ZA	0.9800	0.0510
ZB	0.9730	0.0500
ZC	0.9800	0.0600
ZD	0.9840	0.0610
ZE	0.9850	0.0580
ZF	0.7050	0.0240
ZG	0.7380	0.0300
ZH	0.7700	0.0230
ZI	0.8220	0.0400
ZJ	0.9000	0.0460
ZK	0.9360	0.0390
ZL	0.9480	0.0130
ZM	0.9360	0.0410
ZN	0.9380	0.0410
ZO	0.9600	0.0390
ZP	0.9680	0.0320
ZQ	0.9760	0.0280
ZR	0.9660	0.0280
ZS	0.9540	0.0280
ZT	0.9630	0.0360
ZU	0.9720	0.0270

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Chain	Atom inclusion	Q-score
ZV	0.9710	0.0330
ZW	0.9530	0.0160
ZX	0.9180	0.0250
ZY	0.8790	0.0320
ZZ	0.8510	0.0130
Za	0.8220	0.0190
Zb	0.7790	0.0210
Zc	0.7410	0.0330
Zd	0.7020	0.0120
Ze	0.6730	0.0270
Zf	0.6350	0.0300
Zg	0.6210	0.0330
Zh	0.6050	0.0180
a	0.9660	0.1240
b	0.9680	0.1300
c	0.9660	0.1280
d	0.9640	0.1270
e	0.9650	0.1130
f	0.9640	0.1140
g	0.9650	0.1160
h	0.9610	0.1030
i	0.9630	0.1090
j	0.9620	0.1150
k	0.9620	0.1130
l	0.9670	0.1210
m	0.9640	0.1210
n	0.9620	0.1290
o	0.9640	0.1300
p	0.9620	0.1220
q	0.9660	0.1240
r	0.9610	0.1200
s	0.9580	0.1080
t	0.9570	0.1070
u	0.9580	0.1040
v	0.9550	0.0950
w	0.9550	0.0960
x	0.9630	0.1090
y	0.9590	0.1170
z	0.9620	0.1170