



Full wwPDB EM Validation Report ⓘ

Mar 18, 2025 – 11:27 PM JST

PDB ID : 8WIW
EMDB ID : EMD-37570
Title : Cryo-EM structure of the flagellar C ring in the CW state
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2023-09-25
Resolution : 5.60 Å(reported)
Based on initial model : 8XP1

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

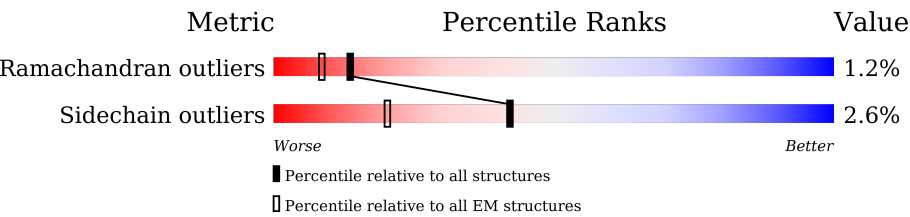
EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.60 Å.

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









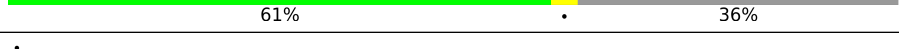
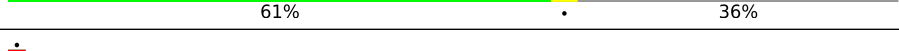
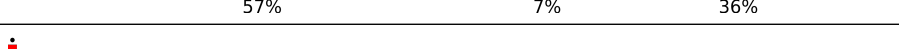
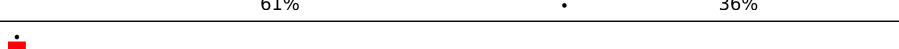
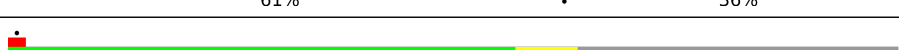

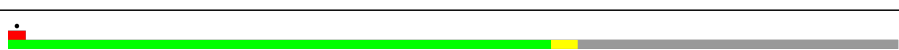

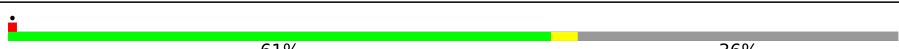





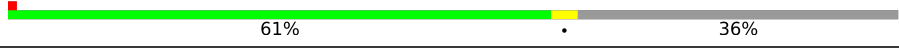
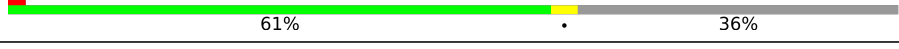



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	0	137	
1	1	137	
1	2	137	
1	5	137	
1	6	137	
1	A1	137	
1	A6	137	
1	A7	137	
1	A8	137	







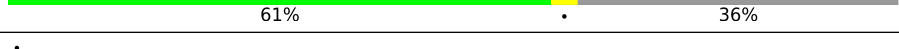
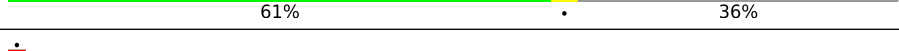
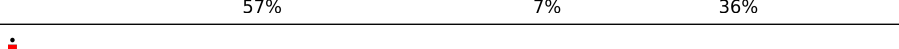
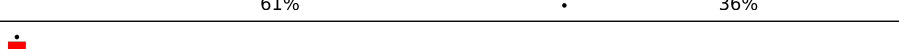
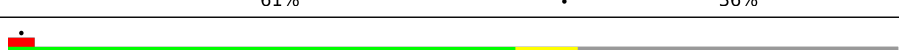

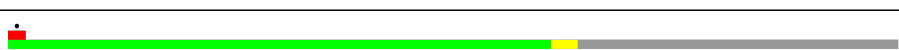

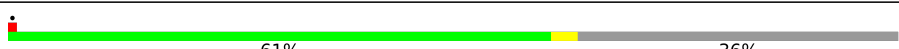





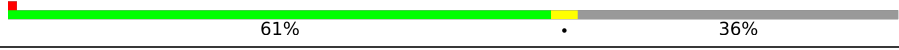
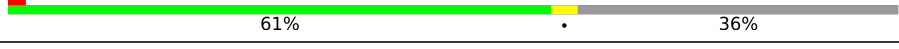



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Mol	Chain	Length	Quality of chain
1	AA	137	
1	AB	137	
1	AC	137	
1	AD	137	
1	AE	137	
1	AF	137	
1	AG	137	
1	AH	137	
1	AI	137	
1	AJ	137	
1	AK	137	
1	AO	137	
1	AP	137	
1	AQ	137	
1	AU	137	
1	AV	137	
1	AW	137	
1	Aa	137	
1	Ab	137	
1	Ac	137	
1	Ag	137	
1	Ah	137	
1	Ai	137	
1	Am	137	
1	An	137	







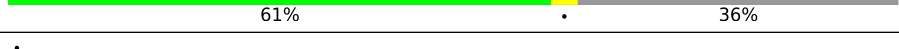
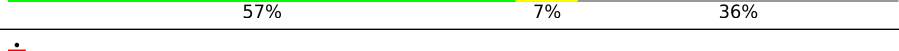
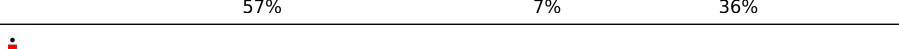
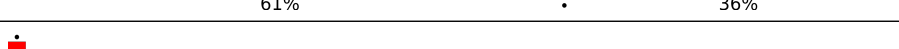
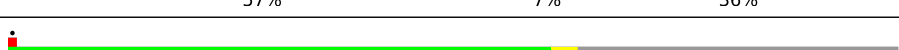

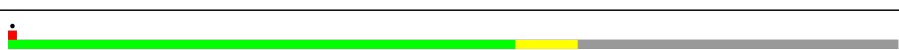

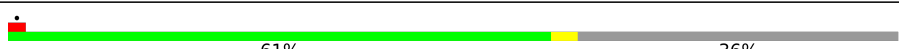





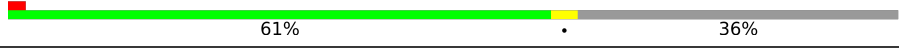
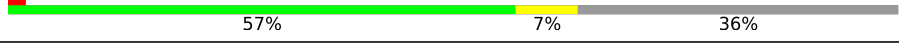



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Mol	Chain	Length	Quality of chain
1	Ao	137	
1	As	137	
1	At	137	
1	Au	137	
1	Ay	137	
1	Az	137	
1	B1	137	
1	B2	137	
1	B7	137	
1	B8	137	
1	B9	137	
1	BC	137	
1	BD	137	
1	BE	137	
1	BJ	137	
1	BK	137	
1	BL	137	
1	BQ	137	
1	BR	137	
1	BS	137	
1	BX	137	
1	BY	137	
1	BZ	137	
1	Be	137	
1	Bf	137	







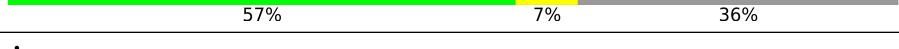
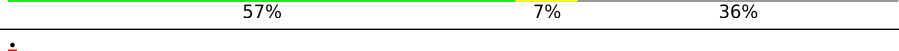
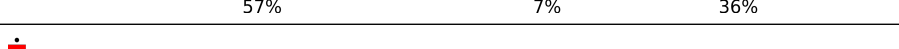
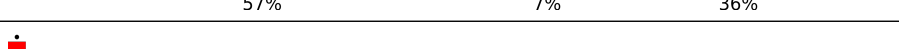
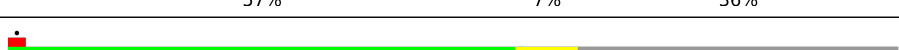

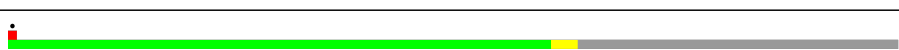

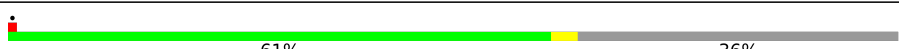


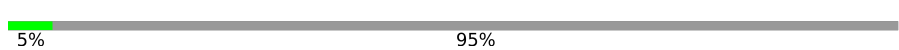
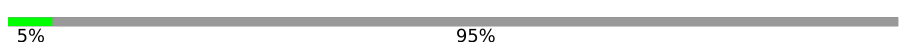
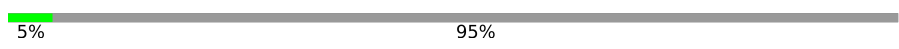
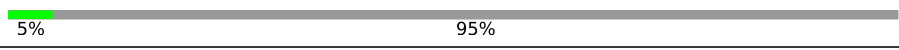
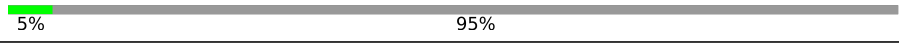
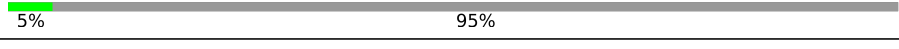
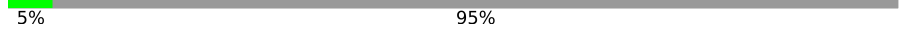

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Mol	Chain	Length	Quality of chain
1	Bg	137	
1	Bl	137	
1	Bm	137	
1	Bn	137	
1	Bs	137	
1	Bt	137	
1	Bu	137	
1	Bz	137	
1	C1	137	
1	C2	137	
1	CD	137	
1	CE	137	
1	CF	137	
1	CK	137	
1	CL	137	
1	CM	137	
1	CR	137	
1	CS	137	
1	CT	137	
1	CY	137	
1	CZ	137	
1	Ca	137	
1	Cf	137	
1	Cg	137	
1	Ch	137	

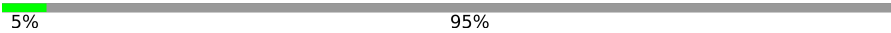
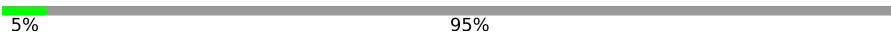
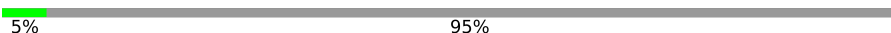
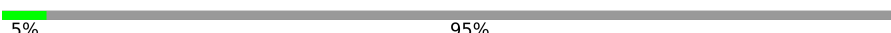

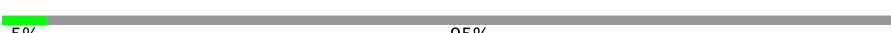









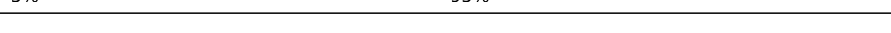
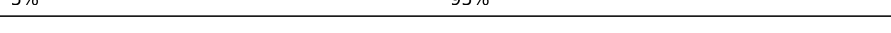
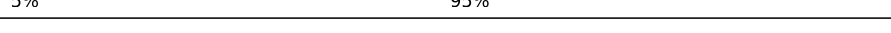
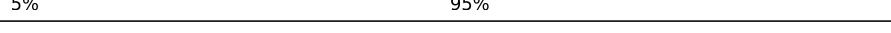
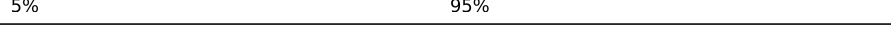
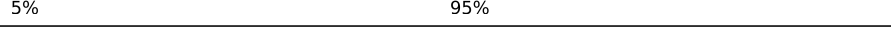
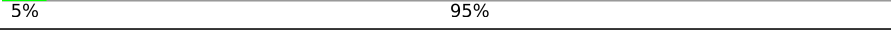

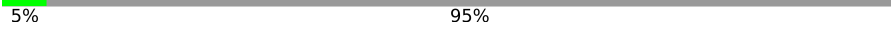

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Mol	Chain	Length	Quality of chain
1	Cm	137	
1	Cn	137	
1	Co	137	
1	Ct	137	
1	Cu	137	
1	Cv	137	
1	o	137	
1	p	137	
1	q	137	
1	r	137	
1	s	137	
1	t	137	
1	u	137	
1	v	137	
1	w	137	
1	x	137	
1	y	137	
1	z	137	
2	A2	560	
2	A9	560	
2	B0	560	
2	B3	560	
2	BF	560	
2	BM	560	
2	BT	560	

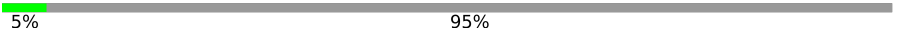
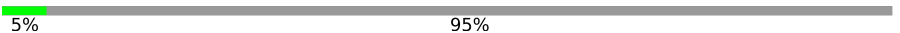























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Mol	Chain	Length	Quality of chain	
2	Ba	560		
2	Bh	560		
2	Bo	560		
2	Bv	560		
2	C	560		
2	CG	560		
2	CN	560		
2	CU	560		
2	Cb	560		
2	Ci	560		
2	Cp	560		
2	Cw	560		
2	D	560		
2	E	560		
2	F	560		
2	G	560		
2	H	560		
2	I	560		
2	J	560		
2	K	560		
2	L	560		
2	M	560		
2	N	560		
2	O	560		
2	P	560		







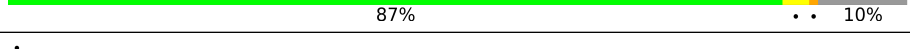
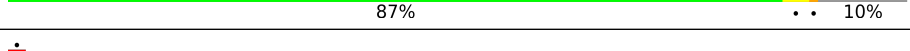
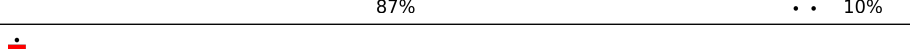
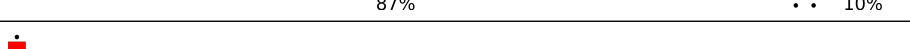
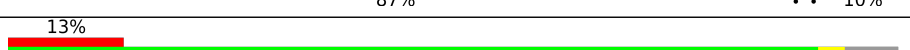
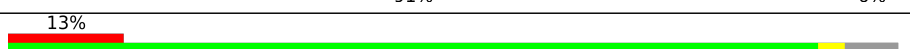
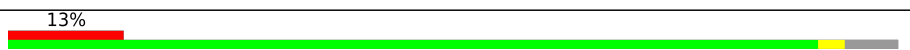

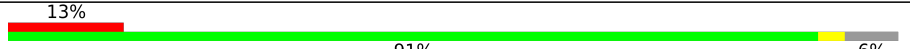

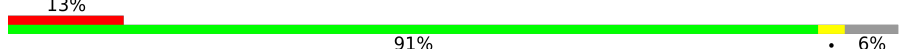



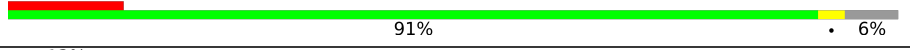
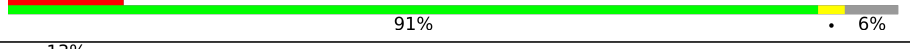



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Mol	Chain	Length	Quality of chain
2	Q	560	 5% 95%
2	R	560	 5% 95%
3	7	334	 87% 10%
3	A0	334	 87% 10%
3	A3	334	 87% 10%
3	AL	334	 87% 10%
3	AR	334	 87% 10%
3	AX	334	 87% 10%
3	Ad	334	 87% 10%
3	Aj	334	 87% 10%
3	Ap	334	 87% 10%
3	Av	334	 87% 10%
3	B4	334	 87% 10%
3	BG	334	 87% 10%
3	BN	334	 87% 10%
3	BU	334	 87% 10%
3	Bb	334	 87% 10%
3	Bi	334	 87% 10%
3	Bp	334	 87% 10%
3	Bw	334	 87% 10%
3	CA	334	 87% 10%
3	CH	334	 87% 10%
3	CO	334	 87% 10%
3	CV	334	 87% 10%
3	Cc	334	 87% 10%

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Mol	Chain	Length	Quality of chain
3	Cj	334	
3	Cq	334	
3	Cx	334	
3	S	334	
3	T	334	
3	U	334	
3	V	334	
3	W	334	
3	X	334	
3	Y	334	
3	g	334	
4	3	331	
4	8	331	
4	A4	331	
4	AM	331	
4	AS	331	
4	AY	331	
4	Ae	331	
4	Ak	331	
4	Aq	331	
4	Aw	331	
4	B5	331	
4	BA	331	
4	BH	331	
4	BO	331	

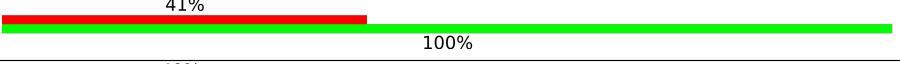
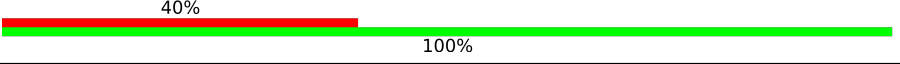
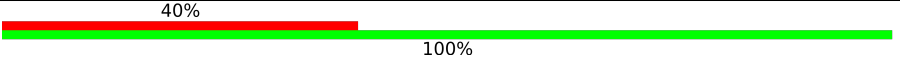
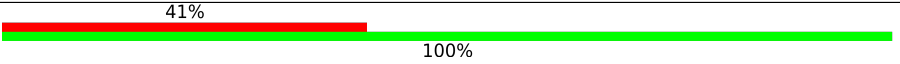
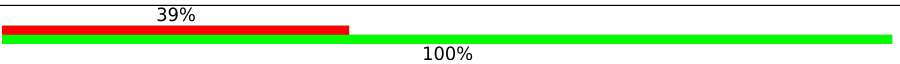
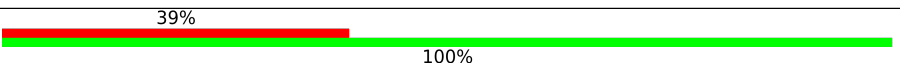
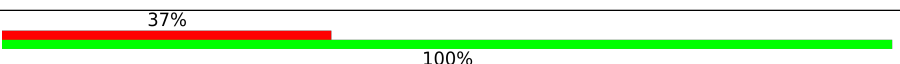
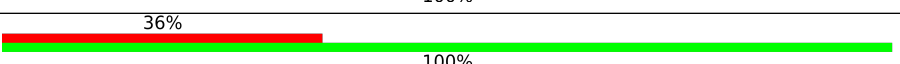
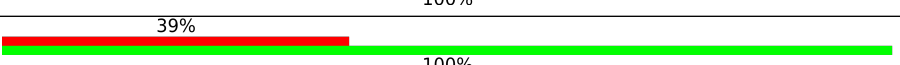
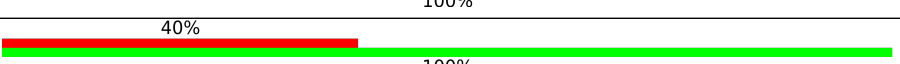
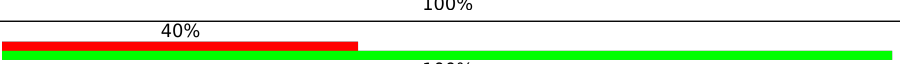
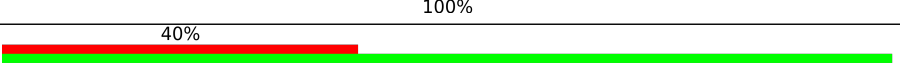
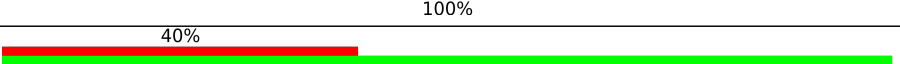
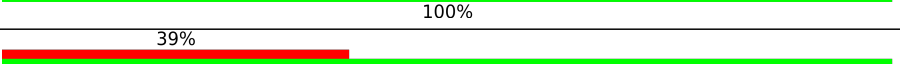
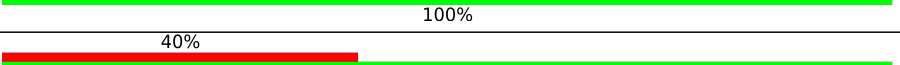
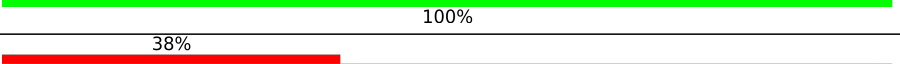
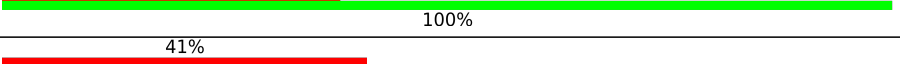
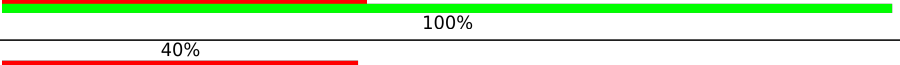
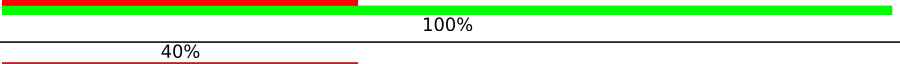
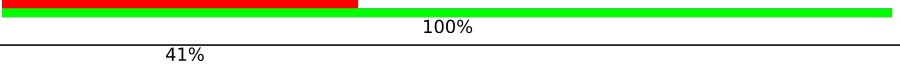
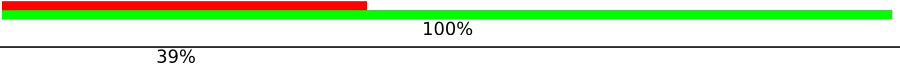
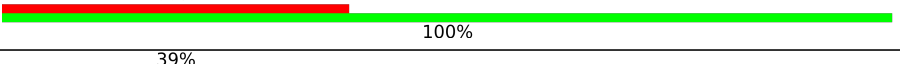
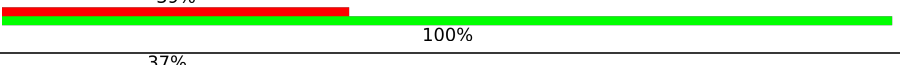
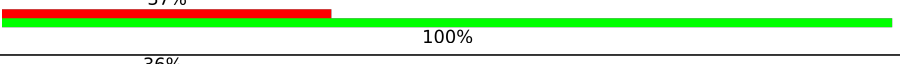
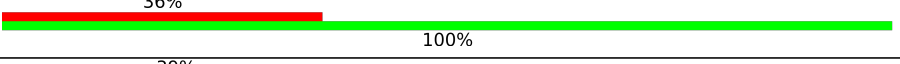
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Mol	Chain	Length	Quality of chain
4	BV	331	
4	Bc	331	
4	Bj	331	
4	Bq	331	
4	Bx	331	
4	CB	331	
4	CI	331	
4	CP	331	
4	CW	331	
4	Cd	331	
4	Ck	331	
4	Cr	331	
4	Cy	331	
4	Z	331	
4	a	331	
4	b	331	
4	c	331	
4	d	331	
4	e	331	
4	f	331	
5	4	129	
5	9	129	
5	A5	129	
5	AN	129	
5	AT	129	

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Mol	Chain	Length	Quality of chain
5	AZ	129	41% 
5	Af	129	40% 
5	Al	129	40% 
5	Ar	129	41% 
5	Ax	129	39% 
5	B6	129	39% 
5	BB	129	37% 
5	BI	129	36% 
5	BP	129	39% 
5	BW	129	40% 
5	Bd	129	40% 
5	Bk	129	40% 
5	Br	129	40% 
5	By	129	39% 
5	CC	129	40% 
5	CJ	129	38% 
5	CQ	129	41% 
5	CX	129	40% 
5	Ce	129	40% 
5	Cl	129	41% 
5	Cs	129	39% 
5	Cz	129	39% 
5	h	129	37% 
5	i	129	36% 
5	j	129	39% 

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Mol	Chain	Length	Quality of chain
5	k	129	<div><div>40%</div><div></div><div>100%</div></div>
5	l	129	<div><div>40%</div><div></div><div>100%</div></div>
5	m	129	<div><div>40%</div><div></div><div>100%</div></div>
5	n	129	<div><div>40%</div><div></div><div>100%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 275366 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 motor switch protein FliN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	o	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	u	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AA	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	p	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	v	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AB	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	q	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	w	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AC	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	r	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	x	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AD	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	s	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	y	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AE	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	t	87	Total 675	C 427	N 118	O 126	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	z	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AF	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	1	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	2	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AG	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	5	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	6	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AH	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AI	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AJ	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AK	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AO	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AP	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AQ	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AU	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AV	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	AW	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Aa	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Ab	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Ac	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Ag	87	Total 675	C 427	N 118	O 126	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ah	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Ai	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Am	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	An	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Ao	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	As	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	At	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Au	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Ay	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Az	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	A1	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	A6	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	A7	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	A8	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BC	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BD	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BE	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BJ	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BK	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BL	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BQ	87	Total 675	C 427	N 118	O 126	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BR	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BS	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BX	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BY	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	BZ	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Be	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Bf	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Bg	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Bl	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Bm	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Bn	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Bs	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Bt	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Bu	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Bz	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	B1	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	B2	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	B7	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	B8	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	B9	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	CD	87	Total 675	C 427	N 118	O 126	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CE	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	CF	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	CK	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	CL	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	CM	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	CR	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	CS	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	CT	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	CY	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	CZ	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Ca	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Cf	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Cg	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Ch	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Cm	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Cn	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Co	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Ct	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Cu	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	Cv	87	Total 675	C 427	N 118	O 126	S 4	0	0
1	C1	87	Total 675	C 427	N 118	O 126	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	C2	87	Total	C	N	O	S	0	0
			675	427	118	126	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	D	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	E	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	F	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	G	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	H	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	I	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	J	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	K	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	L	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	M	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	N	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	O	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	P	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Q	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	R	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	A2	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	A9	27	Total	C	N	O	S	0	0
			224	135	44	42	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BF	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	BM	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	BT	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Ba	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Bh	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Bo	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Bv	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	B3	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	B0	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	CG	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	CN	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	CU	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Cb	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Ci	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Cp	27	Total	C	N	O	S	0	0
			224	135	44	42	3		
2	Cw	27	Total	C	N	O	S	0	0
			224	135	44	42	3		

- Molecule 3 is a protein called Flagellar motor switch protein FliM.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	T	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	U	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	W	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	X	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Y	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	g	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	7	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	AL	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	AR	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	AX	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Ad	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Aj	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Ap	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Av	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	A3	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	A0	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	BG	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	BN	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	BU	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Bb	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Bi	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Bp	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Bw	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	B4	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	CA	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	CH	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	CO	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	CV	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Cc	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Cj	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Cq	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		
3	Cx	301	Total	C	N	O	S	0	0
			2431	1549	437	440	5		

- Molecule 4 is a protein called Flagellar motor switch protein FliG.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	a	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	b	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	c	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	d	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	e	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	f	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	3	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	8	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	AM	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	AS	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	AY	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Ae	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Ak	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Aq	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Aw	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	A4	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	BA	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	BH	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	BO	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	BV	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Bc	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Bj	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Bq	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Bx	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	B5	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	CB	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	CI	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	CP	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	CW	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Cd	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Ck	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Cr	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		
4	Cy	310	Total	C	N	O	S	0	0
			2428	1515	430	474	9		

- Molecule 5 is a protein called Chemotaxis protein CheY.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	i	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	j	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	k	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	l	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	m	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	n	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	4	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	9	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	AN	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	AT	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	AZ	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	Af	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	Al	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	Ar	129	Total	C	N	O	S	0	0
			991	634	165	185	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ax	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	A5	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	BB	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	BI	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	BP	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	BW	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	Bd	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	Bk	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	Br	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	By	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	B6	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	CC	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	CJ	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	CQ	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	CX	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	Ce	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	Cl	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	Cs	129	Total	C	N	O	S	0	0
			991	634	165	185	7		
5	Cz	129	Total	C	N	O	S	0	0
			991	634	165	185	7		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	13	LYS	ASP	engineered mutation	UNP P0A2D5

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Chain	Residue	Modelled	Actual	Comment	Reference
h	106	TRP	TYR	engineered mutation	UNP P0A2D5
i	13	LYS	ASP	engineered mutation	UNP P0A2D5
i	106	TRP	TYR	engineered mutation	UNP P0A2D5
j	13	LYS	ASP	engineered mutation	UNP P0A2D5
j	106	TRP	TYR	engineered mutation	UNP P0A2D5
k	13	LYS	ASP	engineered mutation	UNP P0A2D5
k	106	TRP	TYR	engineered mutation	UNP P0A2D5
l	13	LYS	ASP	engineered mutation	UNP P0A2D5
l	106	TRP	TYR	engineered mutation	UNP P0A2D5
m	13	LYS	ASP	engineered mutation	UNP P0A2D5
m	106	TRP	TYR	engineered mutation	UNP P0A2D5
n	13	LYS	ASP	engineered mutation	UNP P0A2D5
n	106	TRP	TYR	engineered mutation	UNP P0A2D5
4	13	LYS	ASP	engineered mutation	UNP P0A2D5
4	106	TRP	TYR	engineered mutation	UNP P0A2D5
9	13	LYS	ASP	engineered mutation	UNP P0A2D5
9	106	TRP	TYR	engineered mutation	UNP P0A2D5
AN	13	LYS	ASP	engineered mutation	UNP P0A2D5
AN	106	TRP	TYR	engineered mutation	UNP P0A2D5
AT	13	LYS	ASP	engineered mutation	UNP P0A2D5
AT	106	TRP	TYR	engineered mutation	UNP P0A2D5
AZ	13	LYS	ASP	engineered mutation	UNP P0A2D5
AZ	106	TRP	TYR	engineered mutation	UNP P0A2D5
Af	13	LYS	ASP	engineered mutation	UNP P0A2D5
Af	106	TRP	TYR	engineered mutation	UNP P0A2D5
Al	13	LYS	ASP	engineered mutation	UNP P0A2D5
Al	106	TRP	TYR	engineered mutation	UNP P0A2D5
Ar	13	LYS	ASP	engineered mutation	UNP P0A2D5
Ar	106	TRP	TYR	engineered mutation	UNP P0A2D5
Ax	13	LYS	ASP	engineered mutation	UNP P0A2D5
Ax	106	TRP	TYR	engineered mutation	UNP P0A2D5
A5	13	LYS	ASP	engineered mutation	UNP P0A2D5
A5	106	TRP	TYR	engineered mutation	UNP P0A2D5
BB	13	LYS	ASP	engineered mutation	UNP P0A2D5
BB	106	TRP	TYR	engineered mutation	UNP P0A2D5
BI	13	LYS	ASP	engineered mutation	UNP P0A2D5
BI	106	TRP	TYR	engineered mutation	UNP P0A2D5
BP	13	LYS	ASP	engineered mutation	UNP P0A2D5
BP	106	TRP	TYR	engineered mutation	UNP P0A2D5
BW	13	LYS	ASP	engineered mutation	UNP P0A2D5
BW	106	TRP	TYR	engineered mutation	UNP P0A2D5
Bd	13	LYS	ASP	engineered mutation	UNP P0A2D5

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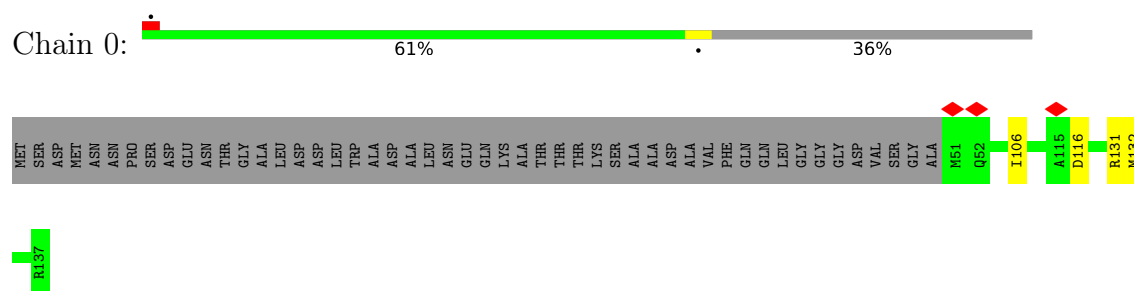
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Chain	Residue	Modelled	Actual	Comment	Reference
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Bk	13	LYS	ASP	engineered mutation	UNP P0A2D5
Bk	106	TRP	TYR	engineered mutation	UNP P0A2D5
Br	13	LYS	ASP	engineered mutation	UNP P0A2D5
Br	106	TRP	TYR	engineered mutation	UNP P0A2D5
By	13	LYS	ASP	engineered mutation	UNP P0A2D5
By	106	TRP	TYR	engineered mutation	UNP P0A2D5
B6	13	LYS	ASP	engineered mutation	UNP P0A2D5
B6	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

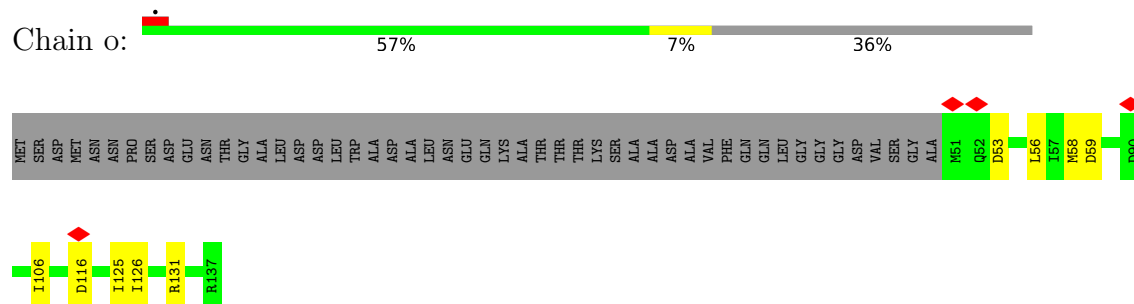
3 Residue-property plots [i](#)

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.

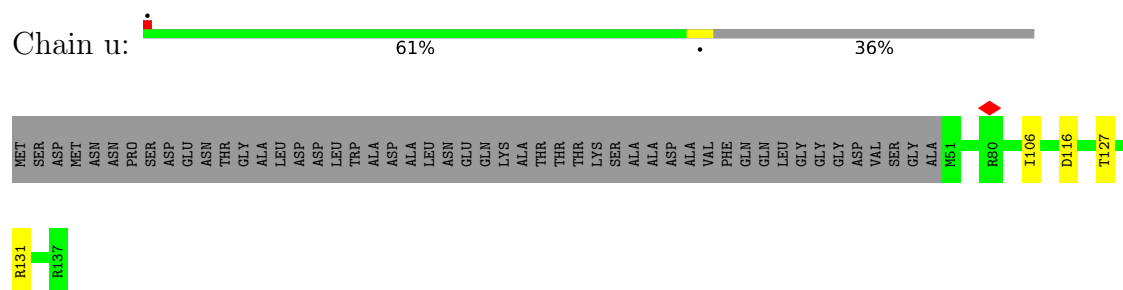
- Molecule 1: Flagellar motor switch protein FliN



- Molecule 1: Flagellar motor switch protein FliN

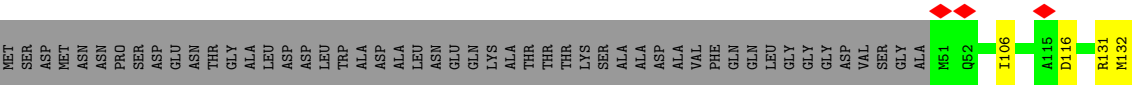


- Molecule 1: Flagellar motor switch protein FliN

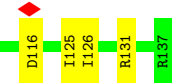
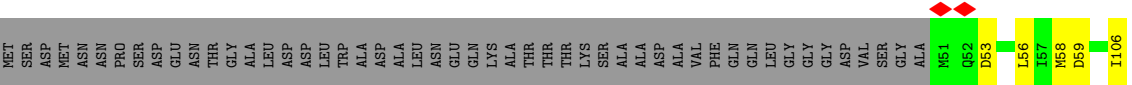


- Molecule 1: Flagellar motor switch protein FliN

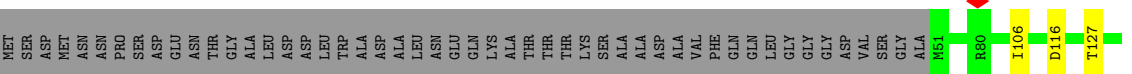




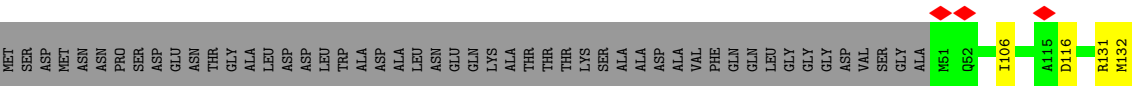
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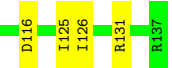
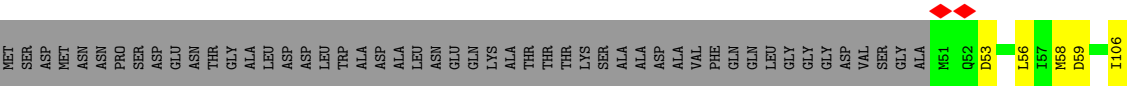
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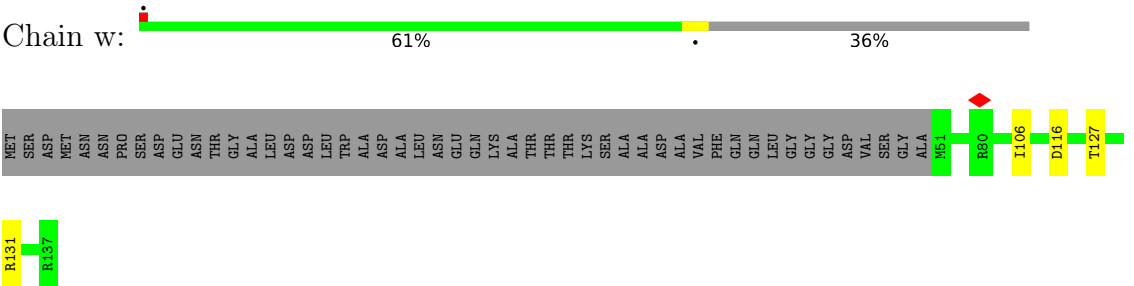
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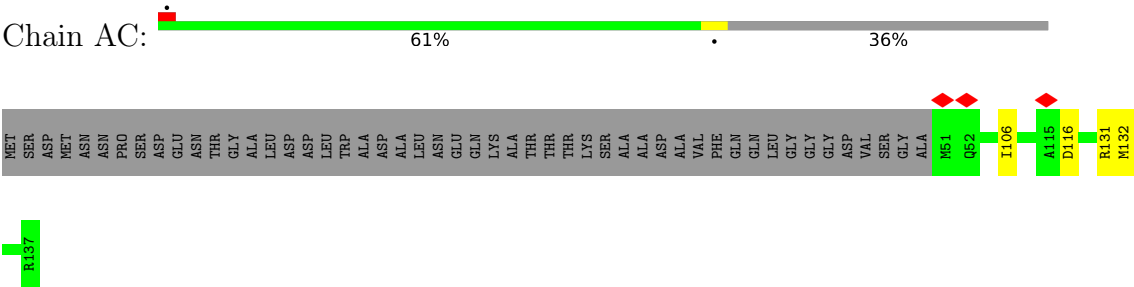
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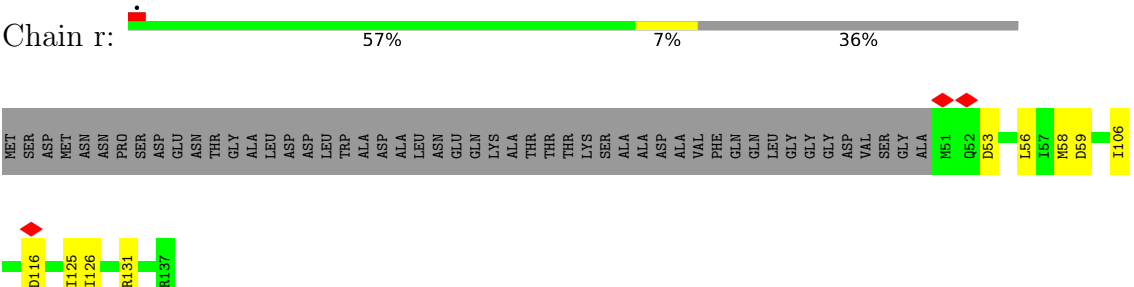
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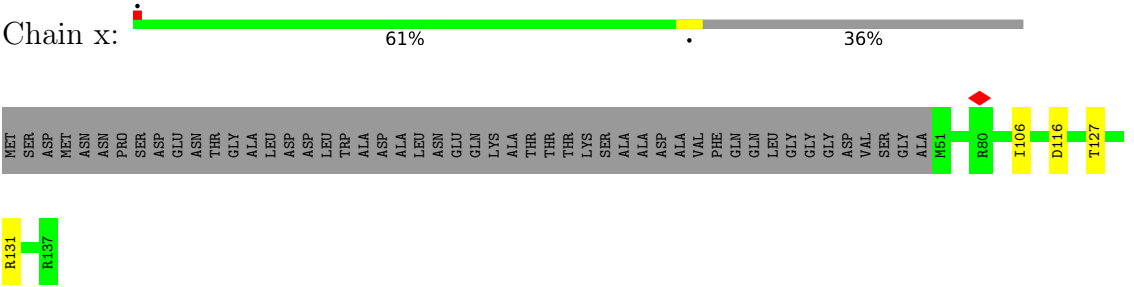
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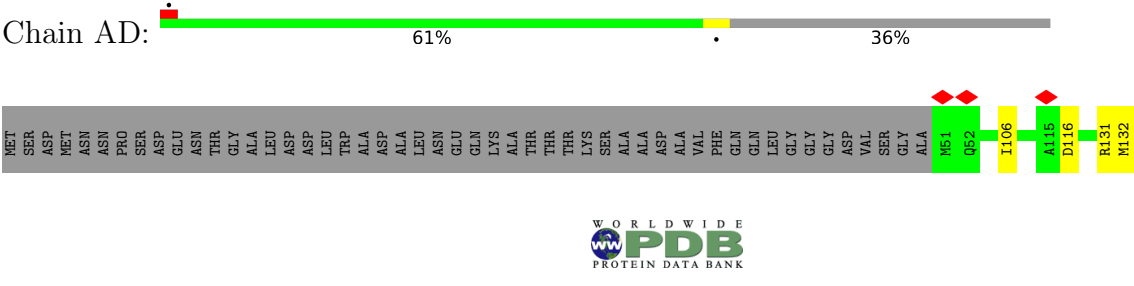
• Molecule 1: Flagellar motor switch protein FliN



• Molecule 1: Flagellar motor switch protein FliN

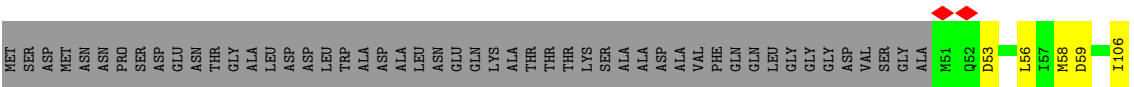


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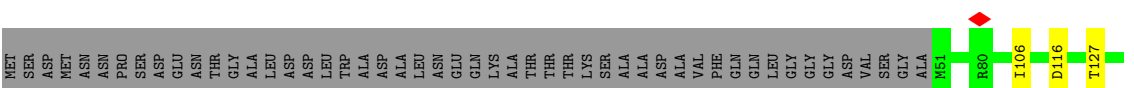




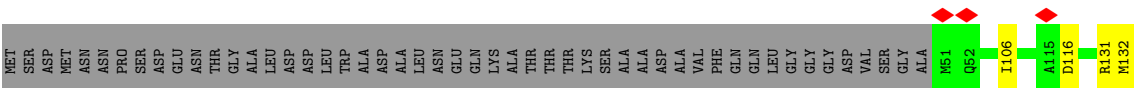
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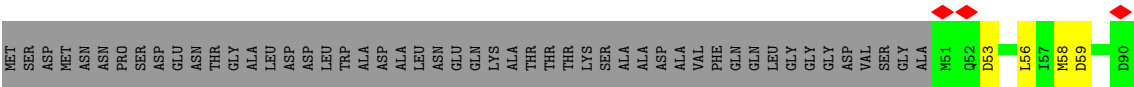
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• Molecule 1: Flagellar motor switch protein FliN

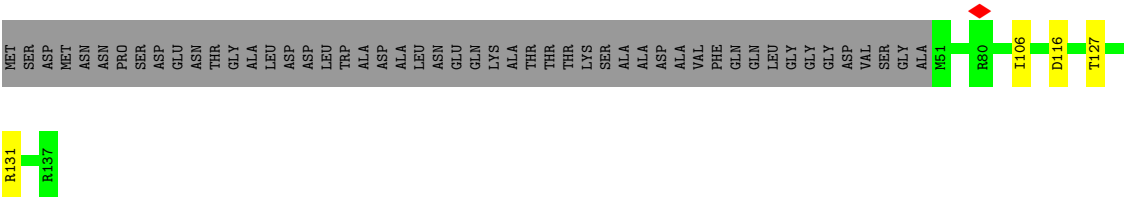


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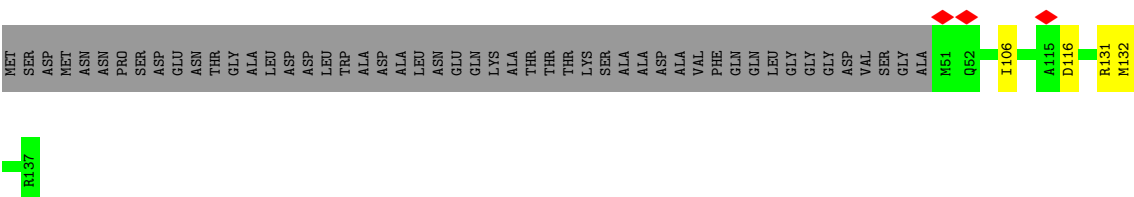


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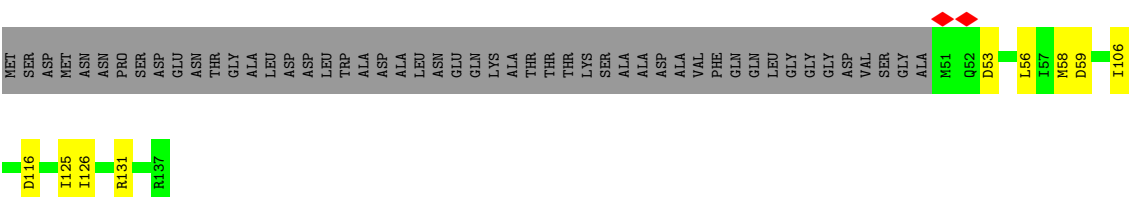




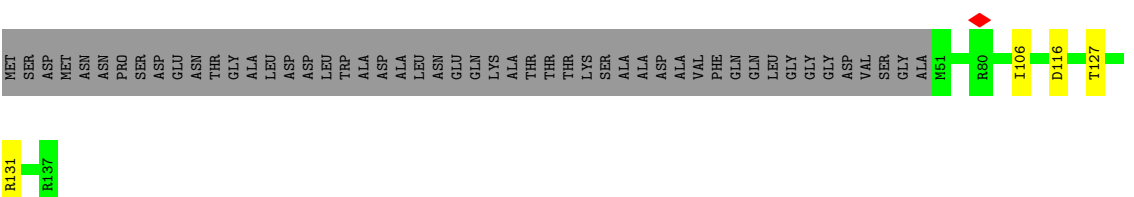
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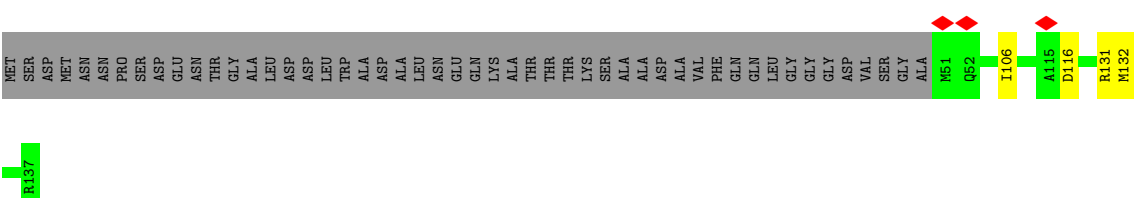
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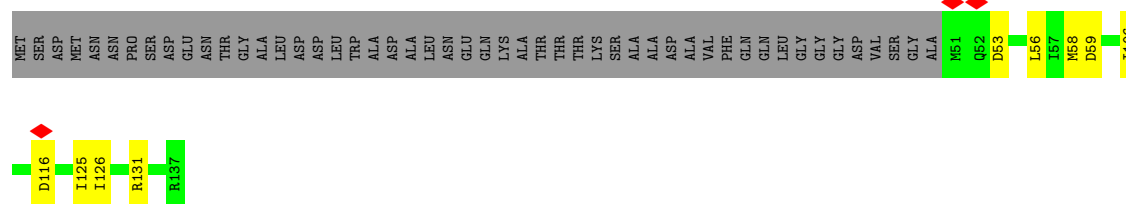
• Molecule 1: Flagellar motor switch protein FliN



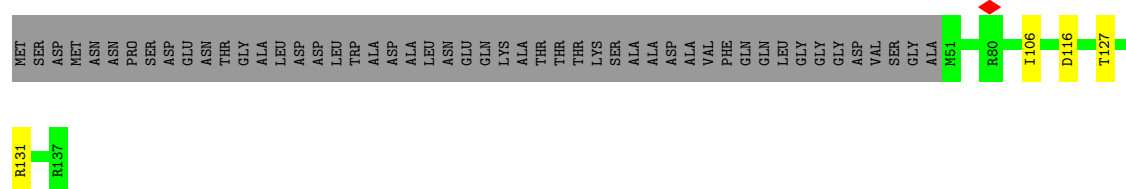
• Molecule 1: Flagellar motor switch protein FliN



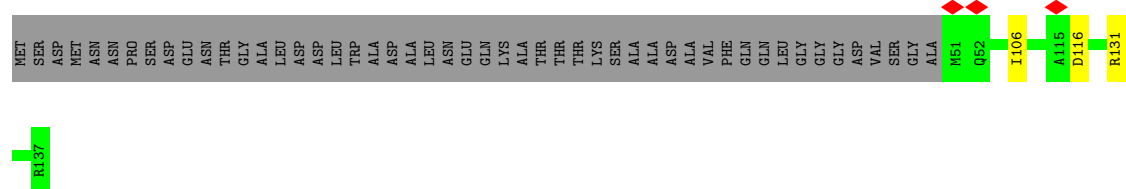
• Molecule 1: Flagellar motor switch protein FliN



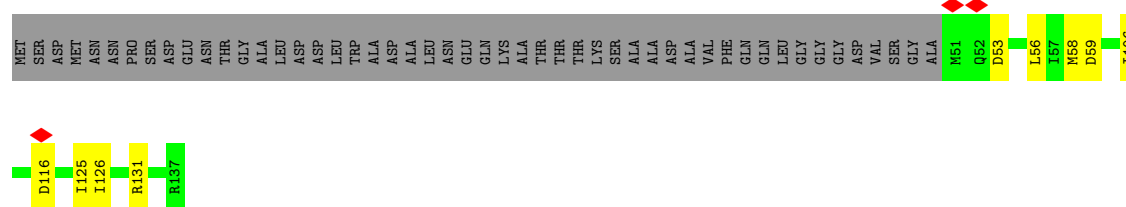
- Molecule 1: Flagellar motor switch protein FliN



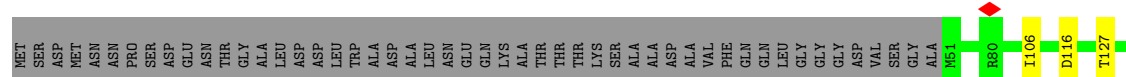
- Molecule 1: Flagellar motor switch protein FliN



- Molecule 1: Flagellar motor switch protein FliN



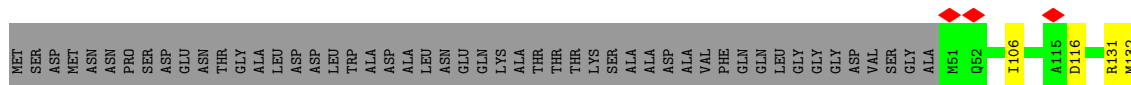
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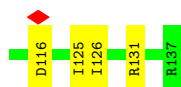
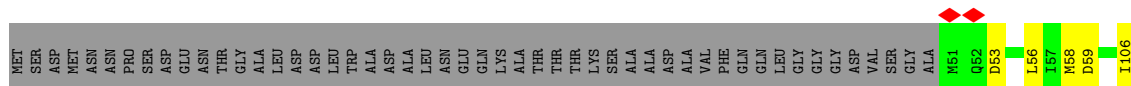
- Molecule 1: Flagellar motor switch protein FliN

Chain AK: 61% 36%



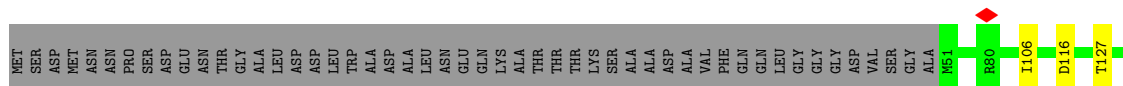
- Molecule 1: Flagellar motor switch protein FliN

Chain AO: 57% 7% 36%



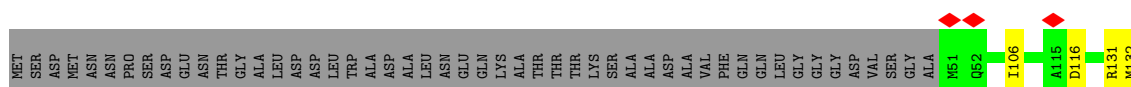
- Molecule 1: Flagellar motor switch protein FliN

Chain AP: 61% 36%



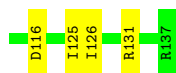
- Molecule 1: Flagellar motor switch protein FliN

Chain AQ: 61% 36%

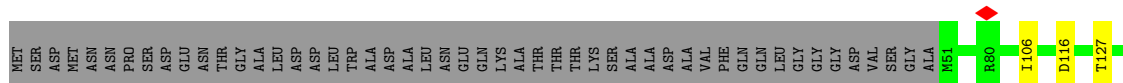


- Molecule 1: Flagellar motor switch protein FliN

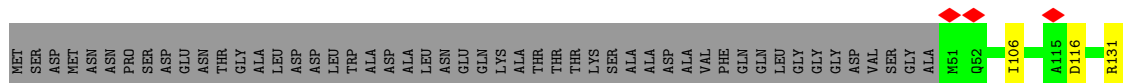
Chain AU: 57% 7% 36%



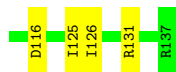
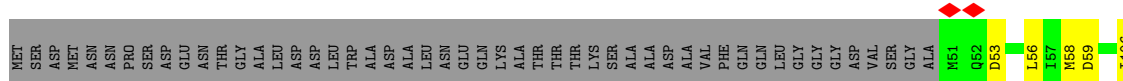
- Molecule 1: Flagellar motor switch protein FliN



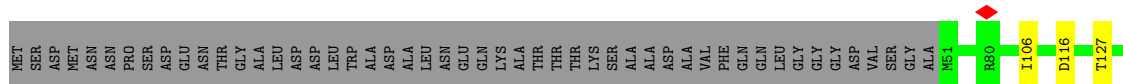
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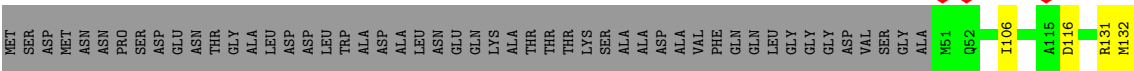
- Molecule 1: Flagellar motor switch protein FliN



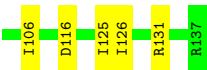
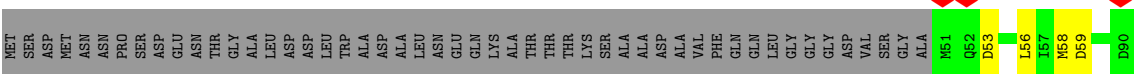
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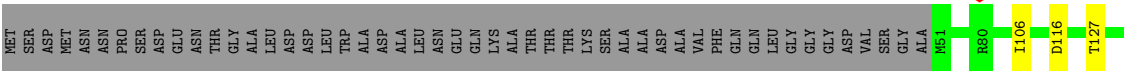
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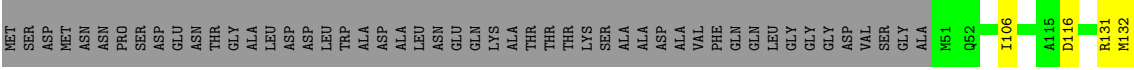
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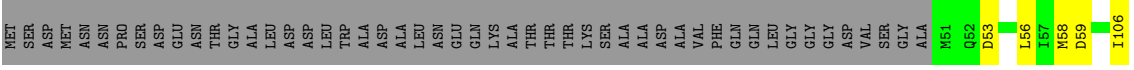
• Molecule 1: Flagellar motor switch protein FliN

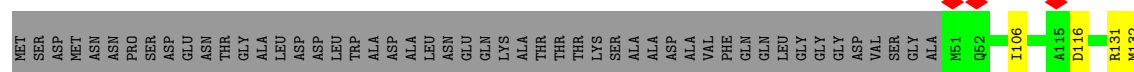


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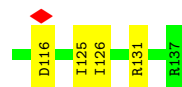
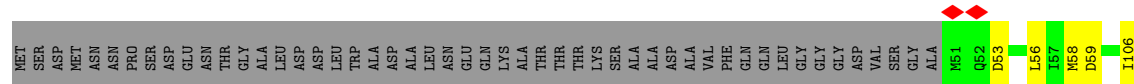


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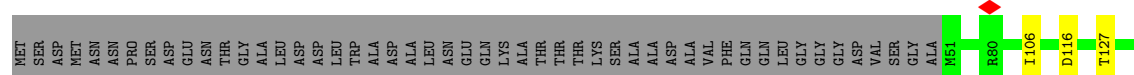




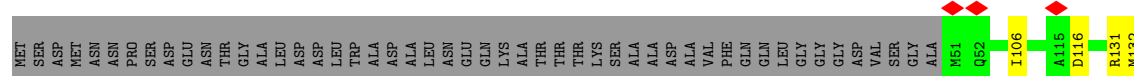
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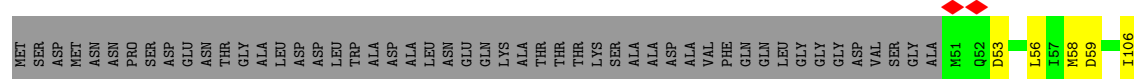
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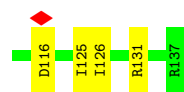


- Molecule 1: Flagellar motor switch protein FliN

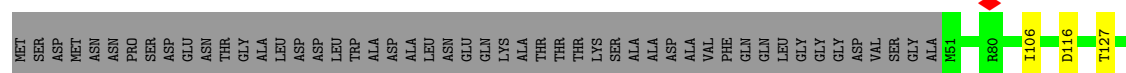


- Molecule 1: Flagellar motor switch protein FliN

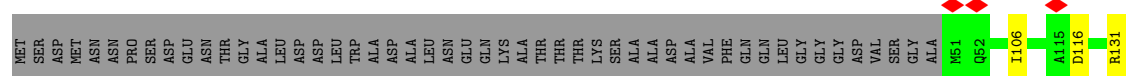




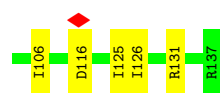
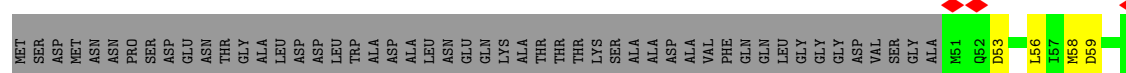
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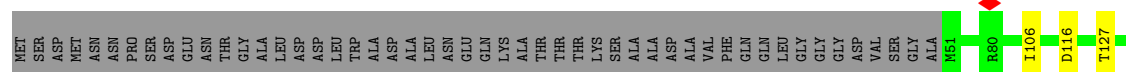
- Molecule 1: Flagellar motor switch protein FliN



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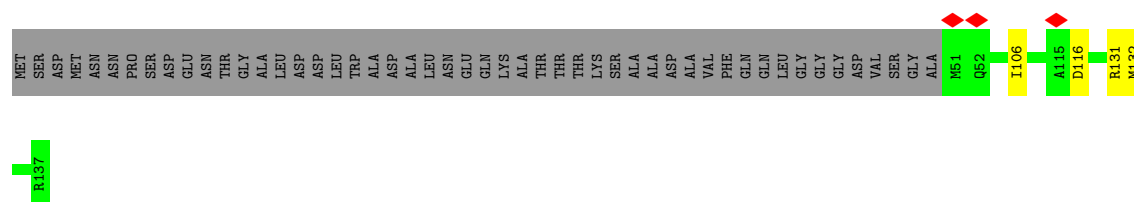


- Molecule 1: Flagellar motor switch protein FliN

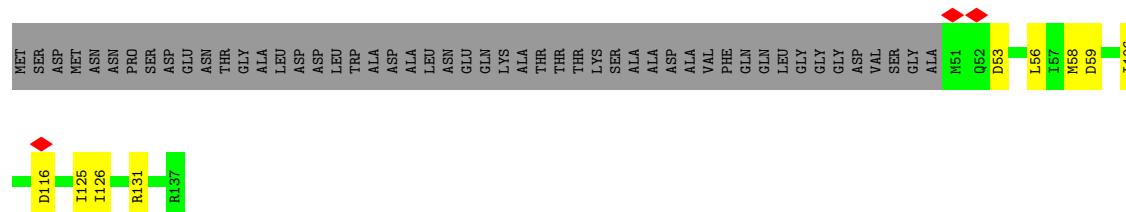


- Molecule 1: Flagellar motor switch protein FliN

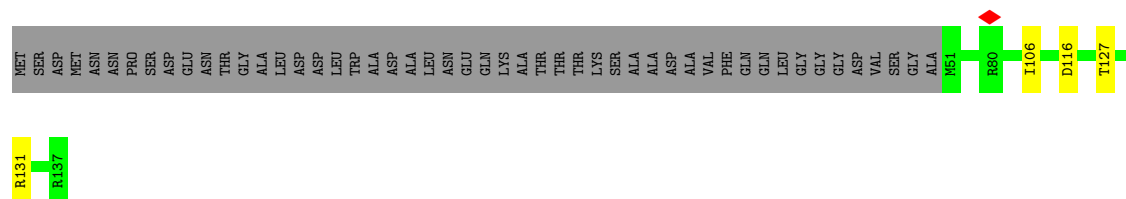




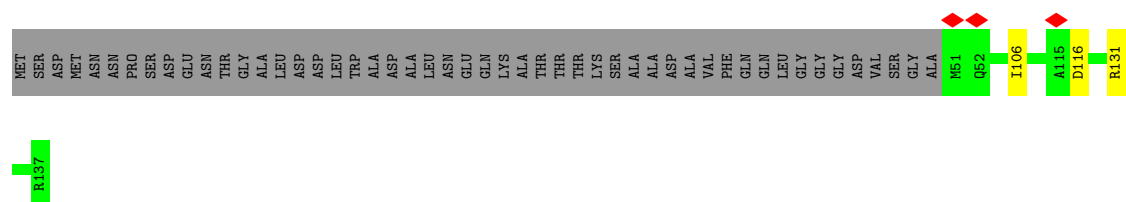
- Molecule 1: Flagellar motor switch protein FliN



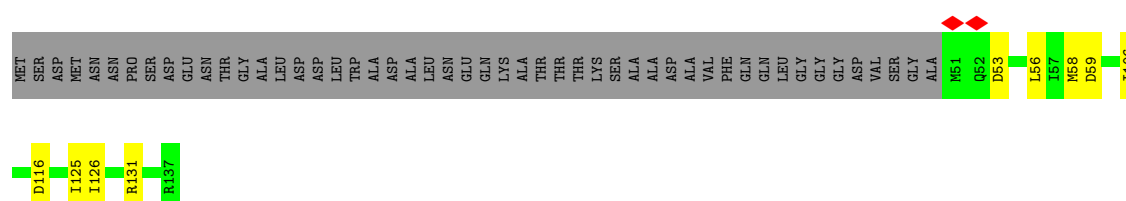
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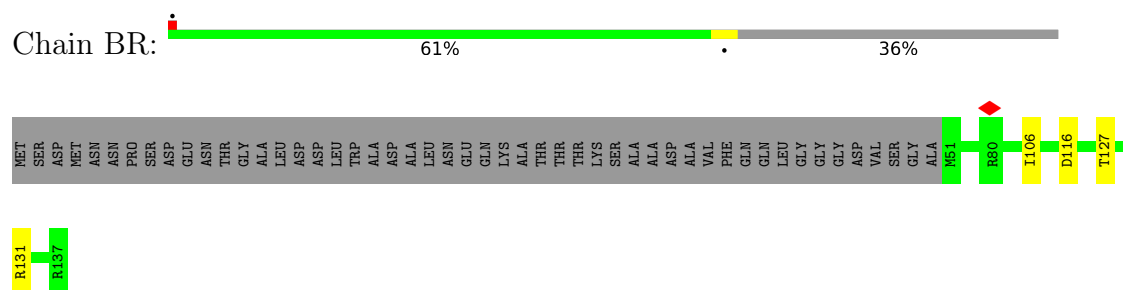
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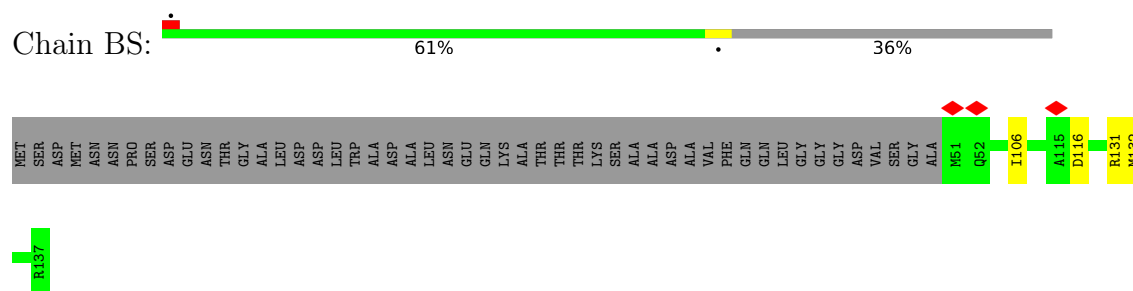
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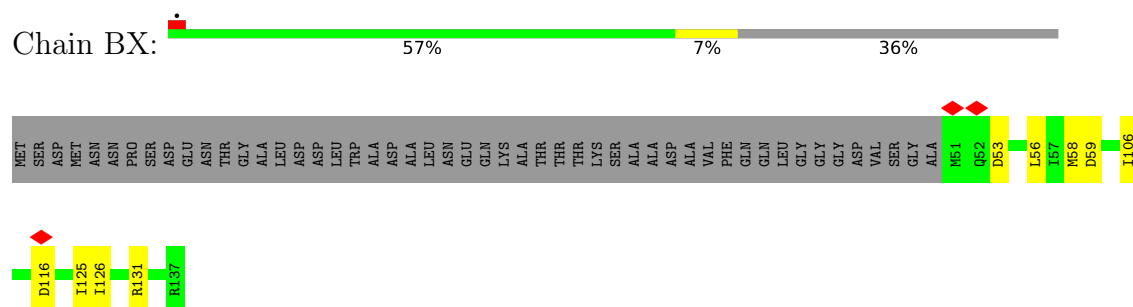
- Molecule 1: Flagellar motor switch protein FliN



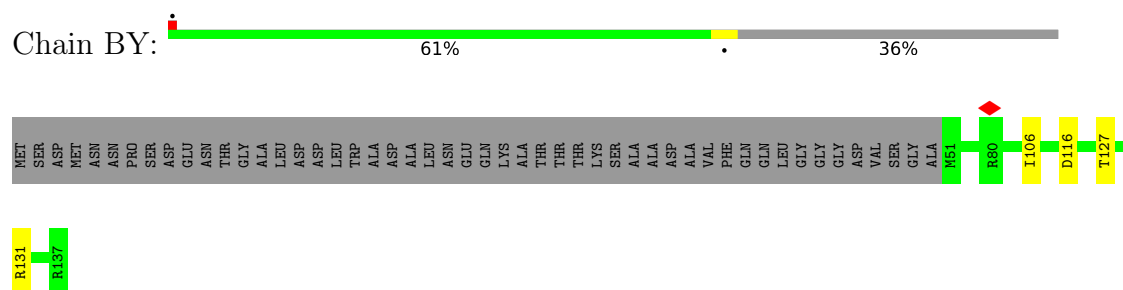
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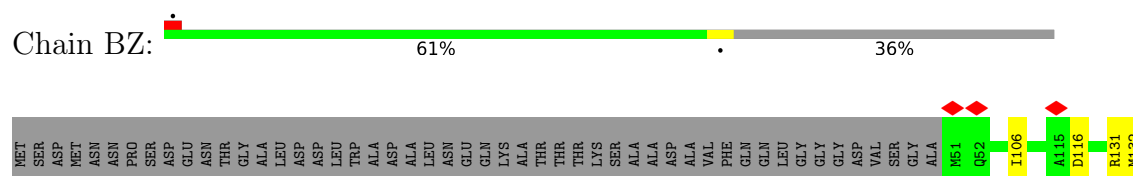
- Molecule 1: Flagellar motor switch protein FliN



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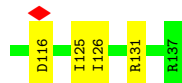
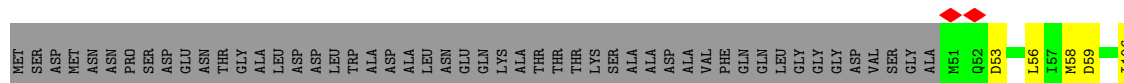


- Molecule 1: Flagellar motor switch protein FliN

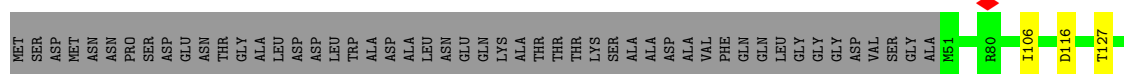




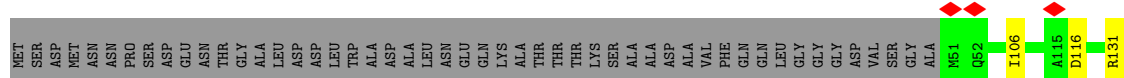
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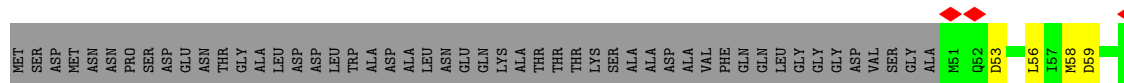
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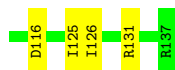




- Chain Bn:  61% 36%



- Chain Bs: 



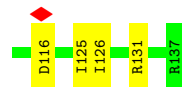
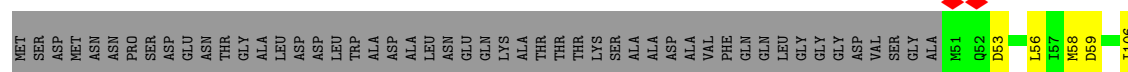
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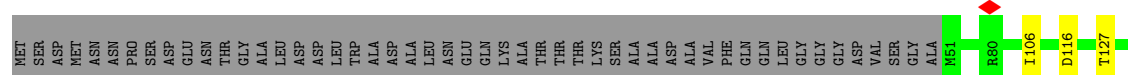
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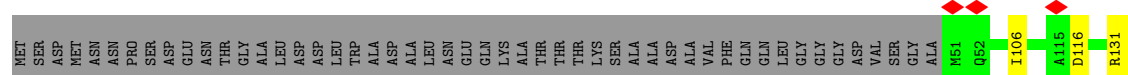
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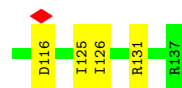
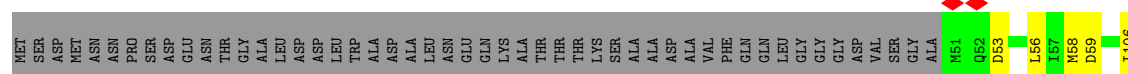
- Molecule 1: Flagellar motor switch protein FliN



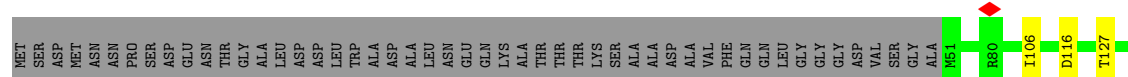
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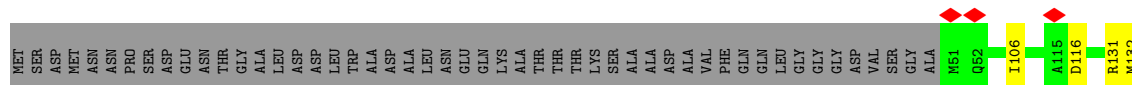


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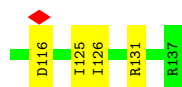
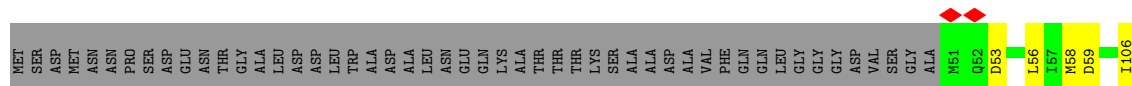




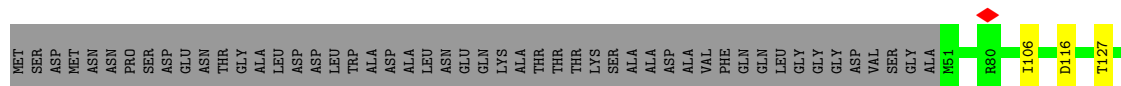
- Molecule 1: Flagellar motor switch protein FliN



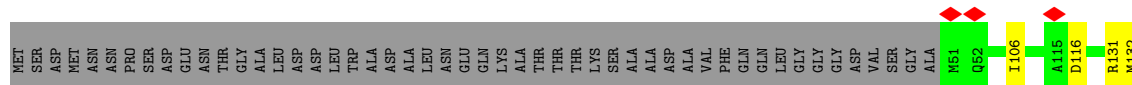
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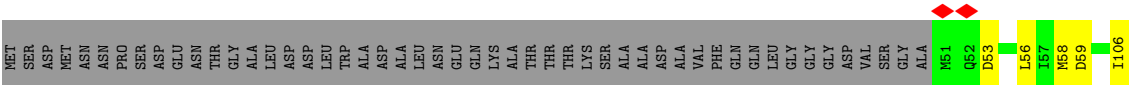


- Molecule 1: Flagellar motor switch protein FliN

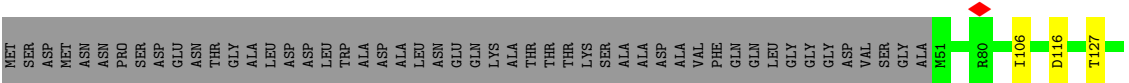


- Molecule 1: Flagellar motor switch protein FliN

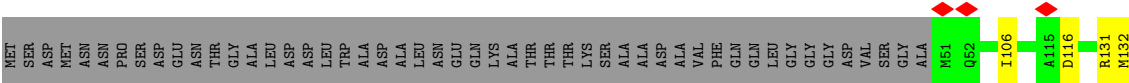




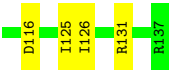
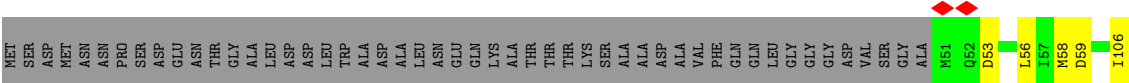
• Molecule 1: Flagellar motor switch protein FliN



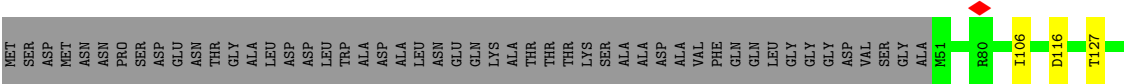
• Molecule 1: Flagellar motor switch protein FliN



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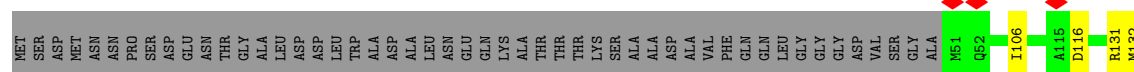


• Molecule 1: Flagellar motor switch protein FliN



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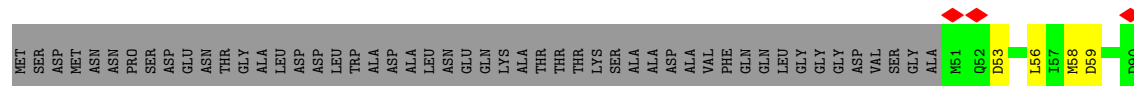
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 R137

- Molecule 1: Flagellar motor switch protein FliN

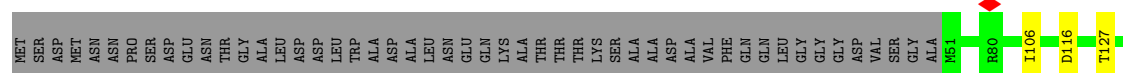
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- Molecule 1: Flagellar motor switch protein FliN

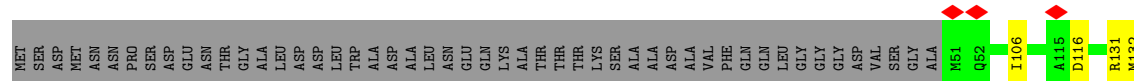
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- Molecule 1: Flagellar motor switch protein FliN

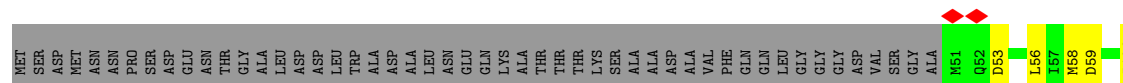
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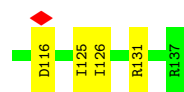


 R137

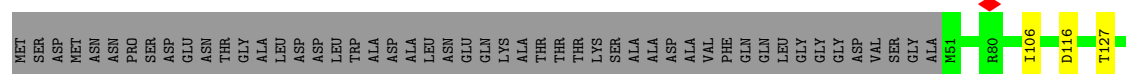
- Molecule 1: Flagellar motor switch protein FliN

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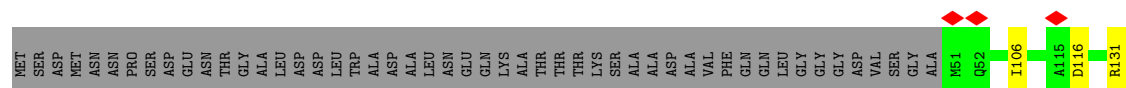




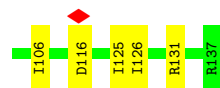
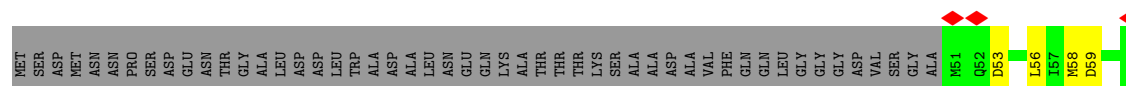
- Molecule 1: Flagellar motor switch protein FliN



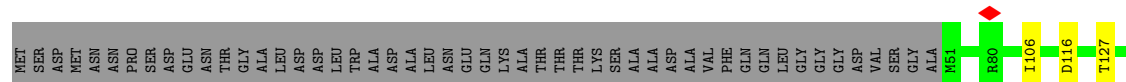
- Molecule 1: Flagellar motor switch protein FliN



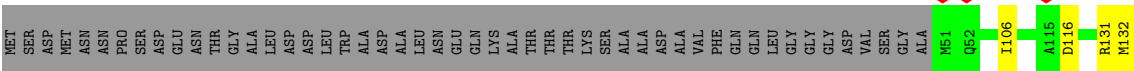
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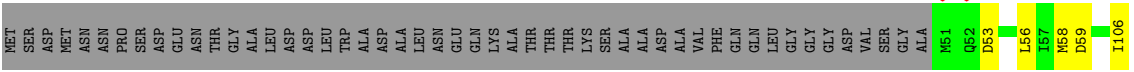
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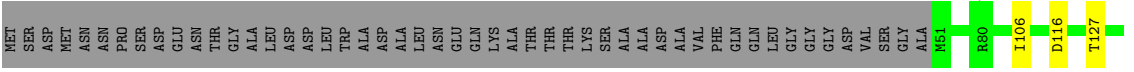
- Molecule 1: Flagellar motor switch protein FliN



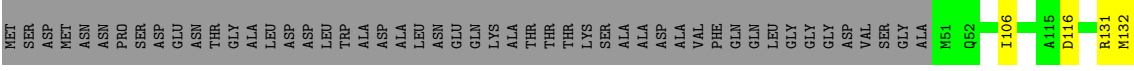
• Molecule 1: Flagellar motor switch protein FliN



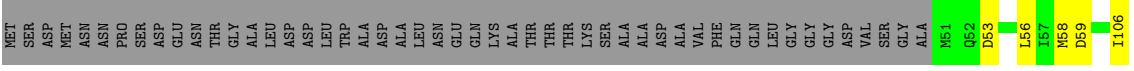
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ARG	GLY	ASN	SER	VAL	GLU	PHE	GLY
PRO	PHE	GLU	GLN	GLN	GLU	GLY	PRO
GLN	SER	THR	GLN	GLN	SER	GLY	ILE
LEU	ASP	SER	VAL	ARG	ARG	ALA	GLN
THR	LYS	ASN	GLY	ILE	ILE	ALA	PHE
ARG	ARG	TYR	ALA	GLN	ASP	LEU	SER
GLY	GLY	GLU	GLY	GLY	ARG	ASP	GLN
VAL	ASP	GLU	TYR	ARG	ILE	GLY	VAL
GLU	THR	ASP	PRO	GLY	GLU	ILE	ASN
GLU	LEU	ARG	GLY	GLY	GLY	ALA	TYR
ALA	ASN	THR	GLY	VAL	ILE	ILE	ASN
LYS	VAL	ILE	PRO	VAL	ILE	ILE	GLN
ALA	VAL	ARG	PRO	LEU	GLY	VAL	GLY
ALA	VAL	ASN	ASN	ASN	ASN	VAL	LEU
ALA	VAL	ASN	GLN	GLN	ASN	GLY	GLY
ALA	ASN	HIS	GLY	SER	VAL	SER	LEU
GLN	SER	THR	ALA	PRO	HIS	ALA	ARG
GLU	PHE	MET	SER	VAL	VAL	ALA	THR
GLN	PRO	ASN	ASN	GLY	GLY	ALA	ILE
ALA	SER	ASN	ASN	GLY	GLN	GLY	ILE
ALA	VAL	VAL	GLN	GLY	GLN	GLY	GLY
GLN	VAL	GLY	PRO	GLY	VAL	PRO	LEU
VAL	VAL	ILE	ALA	VAL	THR	THR	LEU
GLN	ASN	ASN	ALA	ASN	ASN	ASN	GLY
GLU	THR	GLY	PRO	ASN	ASN	ASN	PRO
THR	GLY	ARG	ASN	ASN	ASN	VAL	GLY
GLY	GLY	LEU	GLY	GLY	GLN	GLY	GLY
GLU	GLU	SER	ALA	PRO	THR	THR	LEU
GLU	LEU	VAL	PRO	PRO	THR	GLY	GLY
VAL	PRO	ALA	ILE	ALA	GLN	GLY	GLY
GLU	PHE	VAL	VAL	ALA	GLN	GLY	GLY
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GLN	LEU	LYS	ASN	ASN	ASN	GLY	GLY
ARG	ALA	PRO	THR	THR	HIS	THR	GLN
ARG	ALA	LEU	PRO	PRO	TYR	GLN	GLN
ALA	GLY	PRO	GLN	THR	SER	THR	GLY
ASN	ARG	LEU	THR	THR	ASN	SER	VAL
GLN	GLY	VAL	THR	THR	ASP	ARG	ARG
GLU	VAL	LEU	GLN	THR	ALA	ALA	GLY
ALA	LEU	MET	ASN	SER	ALA	ARG	GLY
GLU	VAL	LYS	LYS	LYS	LYS	LYS	GLN
GLU	VAL	VAL	GLN	VAL	THR	THR	ASN
M632	ALA	ILE	ILE	ILE	THR	ALA	ASN
S633	LEU	ASP	GLY	ARG	ASP	LEU	ASN
Q634	ILE	LEU	GLY	GLY	GLY	ALA	GLN
D858	LEU	THR	THR	THR	THR	ARG	ALA
HIS	THR	ARG	THR	ARG	ARG	THR	ALA
GLU	VAL	LYS	GLY	LYS	GLY	GLY	THR
	VAL	VAL	ALA	ALA	ASN	ASN	ASN

- Molecule 2: Flagellar M-ring protein

Chain E:  5% 95%

[illegible]

- Molecule 2: Flagellar M-ring protein

Chain F: 5% 95%

- Molecule 2: Flagellar M-ring protein

[illegible]

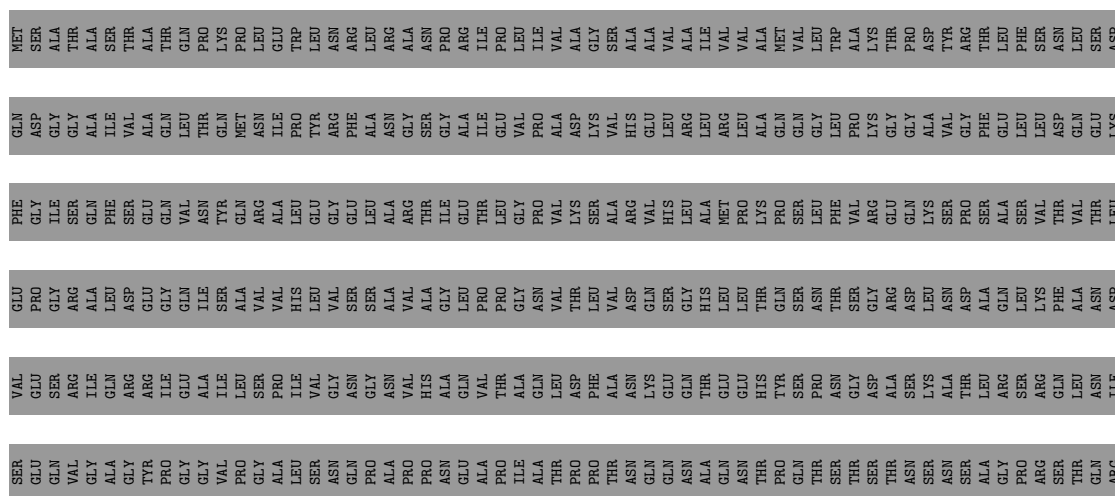


- Molecule 2: Flagellar M-ring protein

Chain J: 5% 95%

- Molecule 2: Flagellar M-ring protein

Chain K:  5% 95%





[illegible]

- Molecule 2: Flagellar M-ring protein

Chain P: 

[illegible]

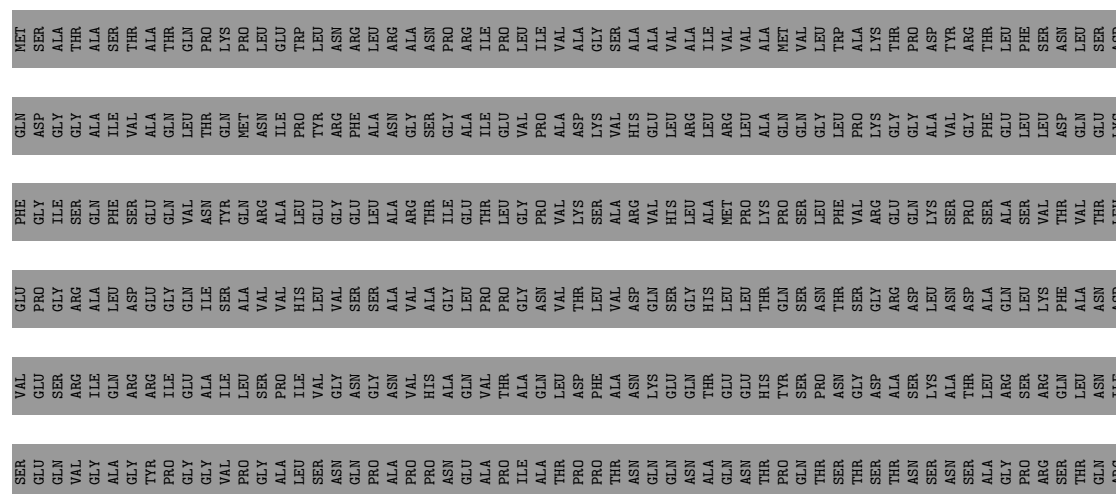
- Molecule 2: Flagellar M-ring protein

Chain Q: 5% 95%

- Molecule 2: Flagellar M-ring protein



- Molecule 2: Flagellar M-ring protein





[illegible]

- Molecule 2: Flagellar M-ring protein

Chain Bv: 5% 95%

[illegible]

- Molecule 2: Flagellar M-ring protein

Chain B3: 5% 95%






[illegible]

- Molecule 2: Flagellar M-ring protein

Chain Cw:  5% 95%

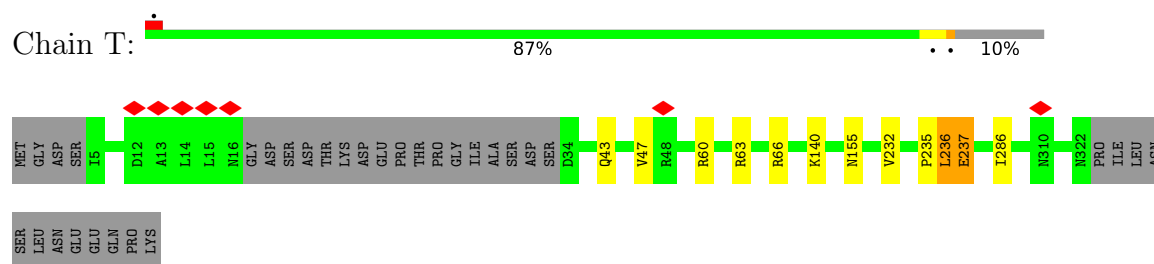
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LEU	THR	ARG	ASN	TYR	ASN	GLY	ALA	GLN	ARG	ILE	ALA	ALA	GLN	THR	ALA	ALA
ARG	ARG	ARG	TYR	GLU	GLY	GLY	GLY	TYR	PHE	GLN	ASP	LEU	PHE	SER	THR	SER
ARG	VAL	ASP	VAL	VAL	VAL	TYR	ARG	VAL	ARG	ARG	ARG	GLU	GLU	GLU	ALA	ALA
GLU	GLU	THR	ASP	ARG	GLY	PRO	GLY	ILE	GLN	GLY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

- Molecule 3: Flagellar motor switch protein FliM

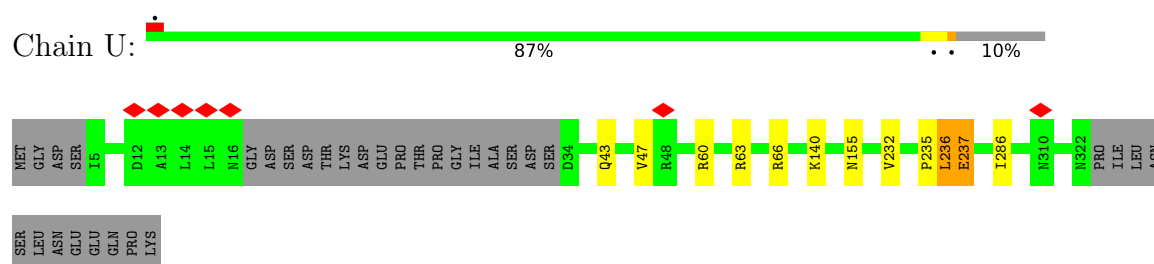
Chain S:  87% 10%

[illegible]

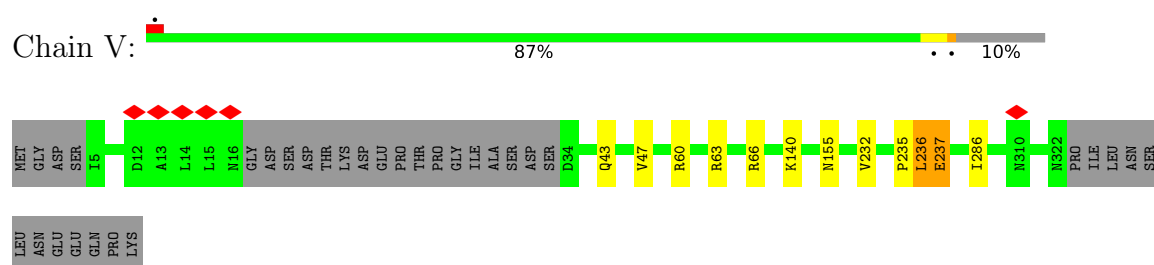
• Molecule 3: Flagellar motor switch protein FliM



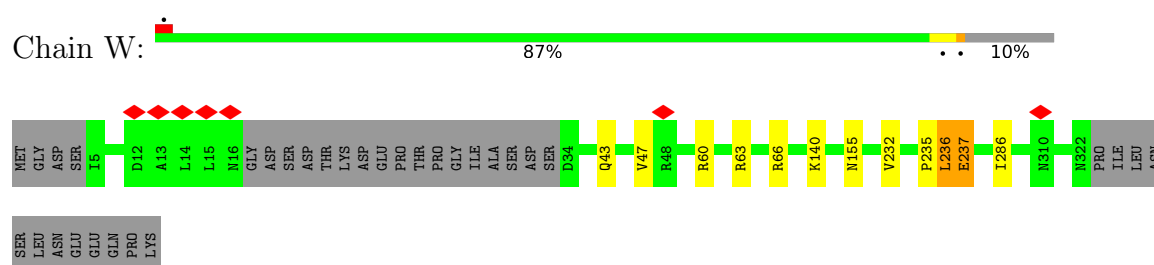
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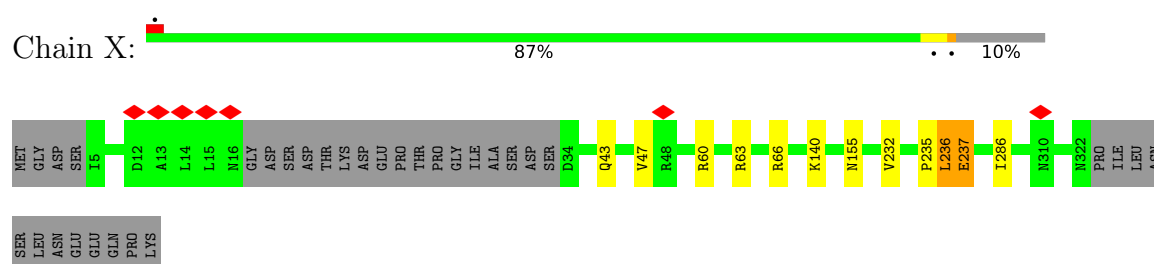
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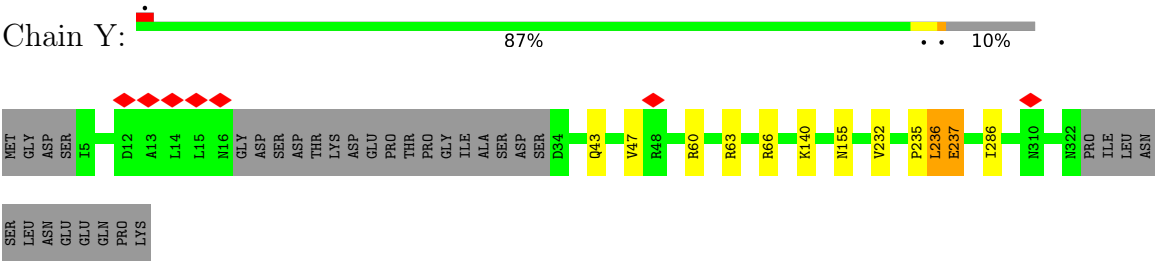
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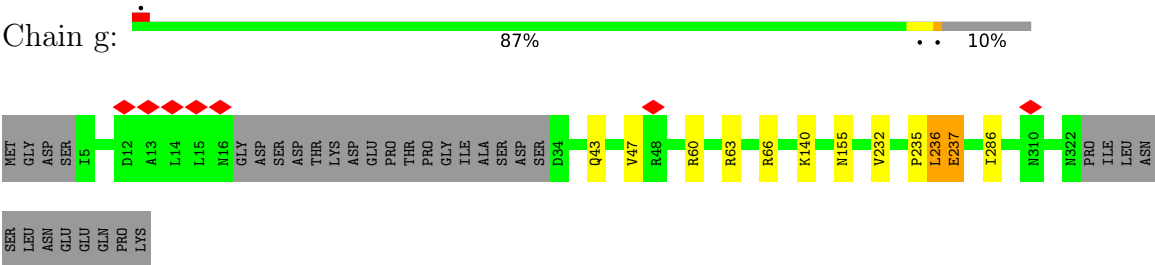
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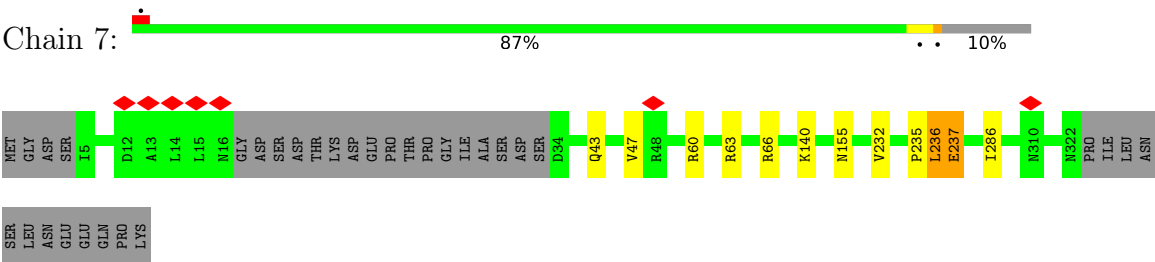
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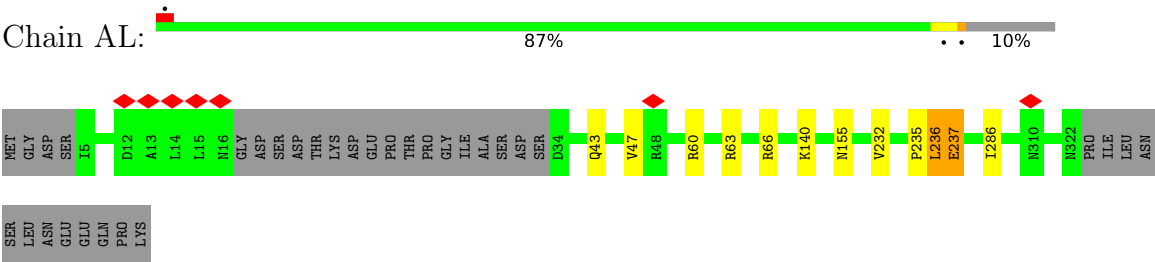
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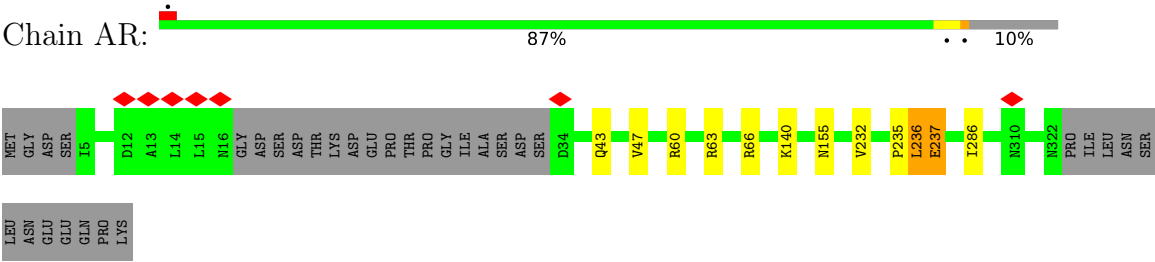
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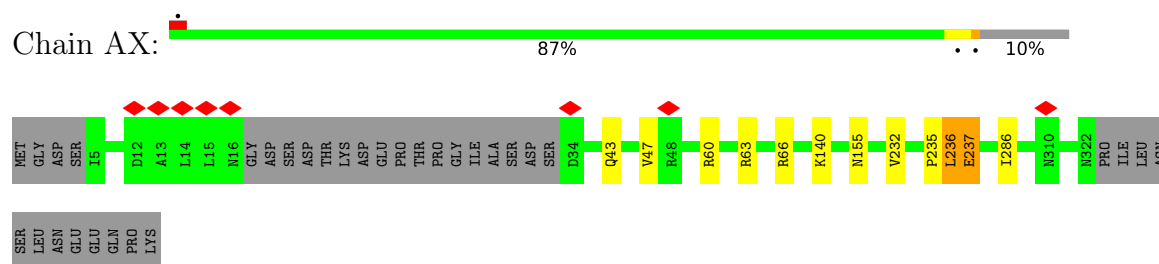
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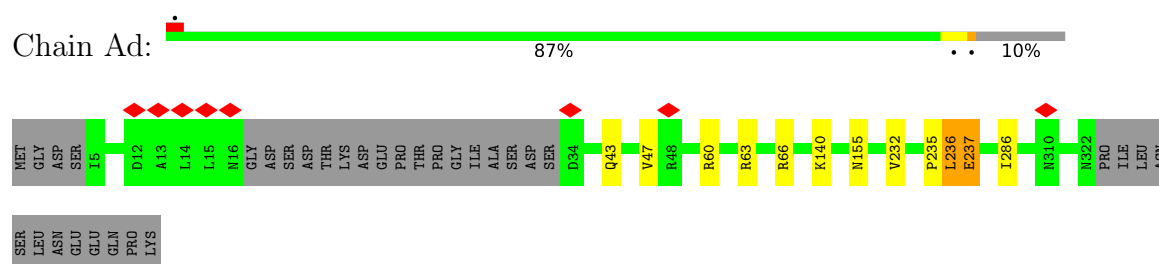
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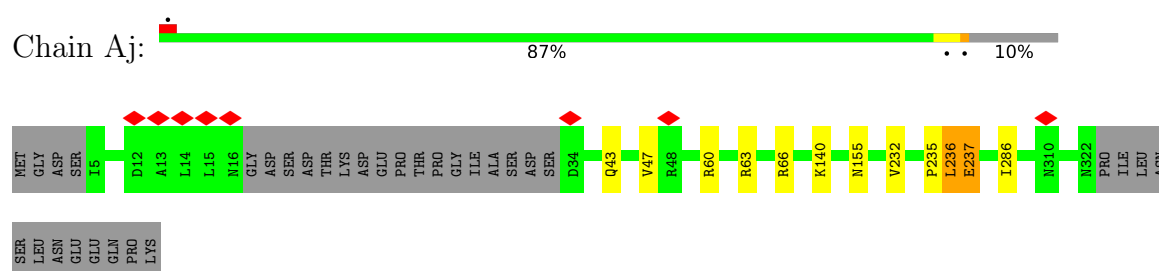
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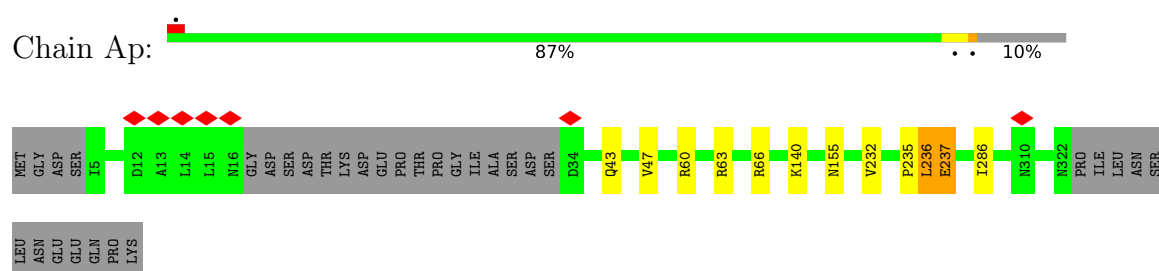
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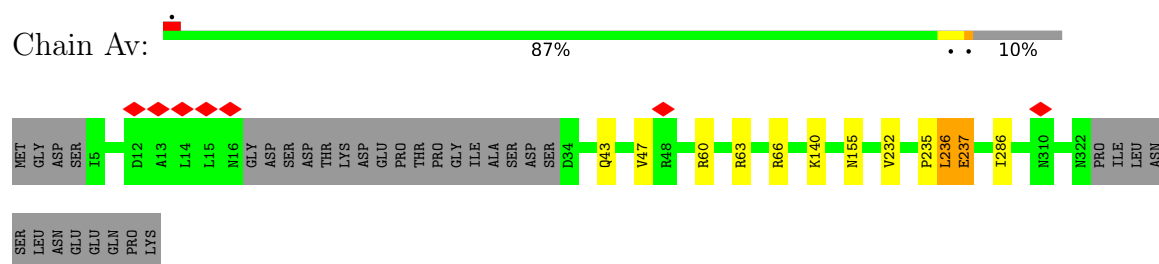
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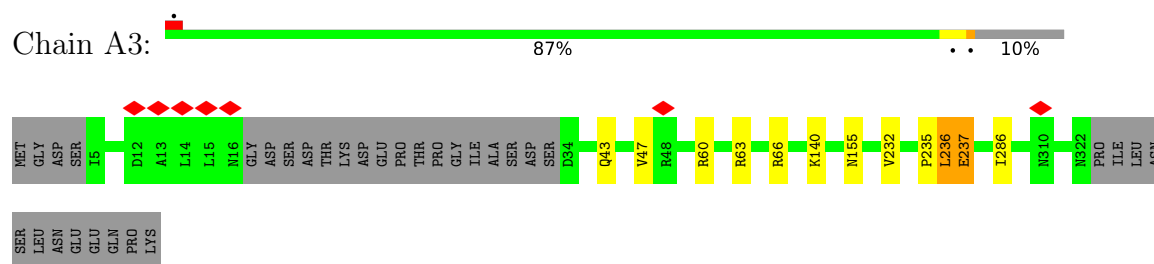
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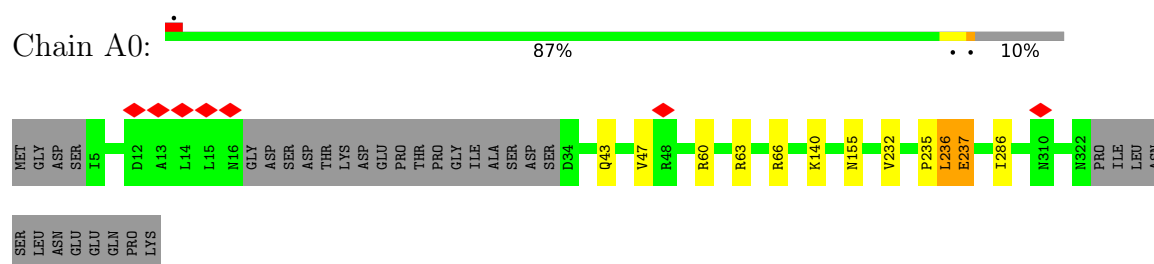
• Molecule 3: Flagellar motor switch protein FliM



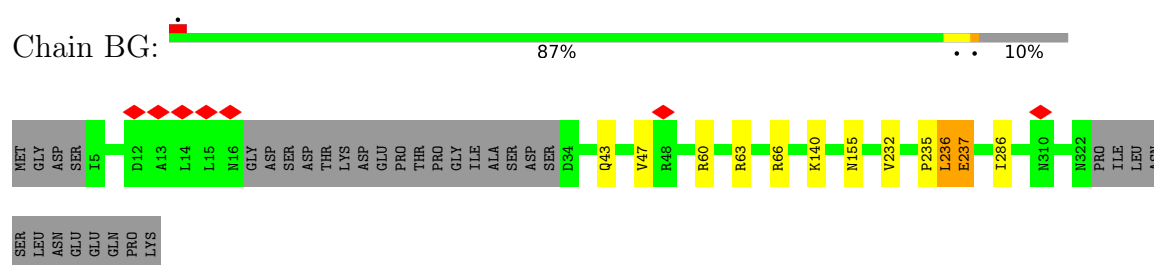
• Molecule 3: Flagellar motor switch protein FliM



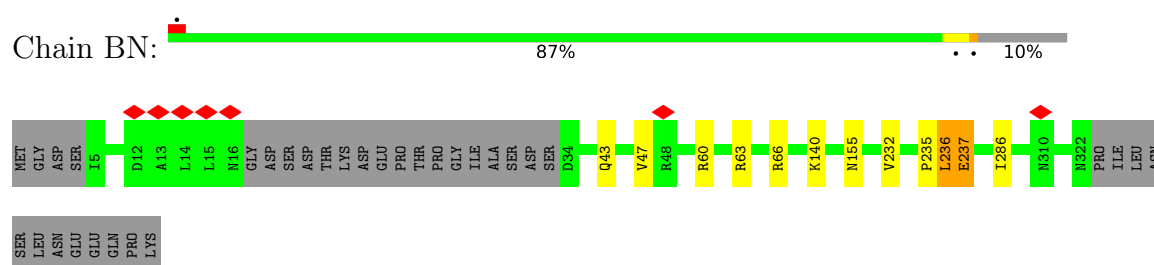
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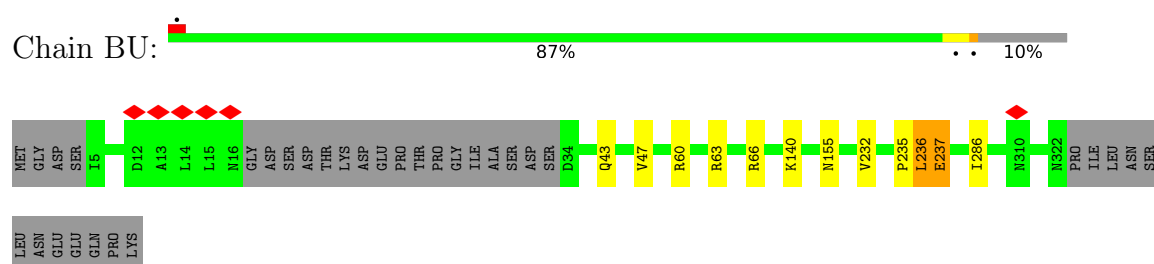
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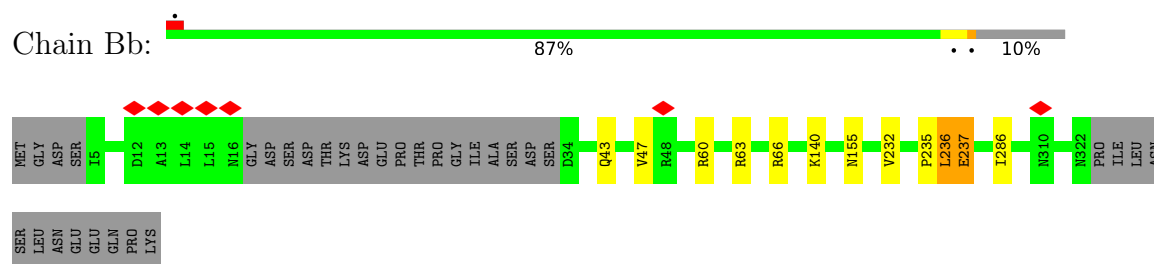
• Molecule 3: Flagellar motor switch protein FliM



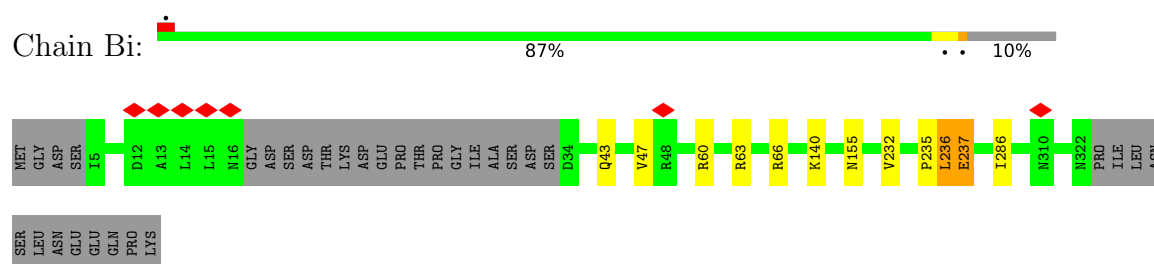
• Molecule 3: Flagellar motor switch protein FliM



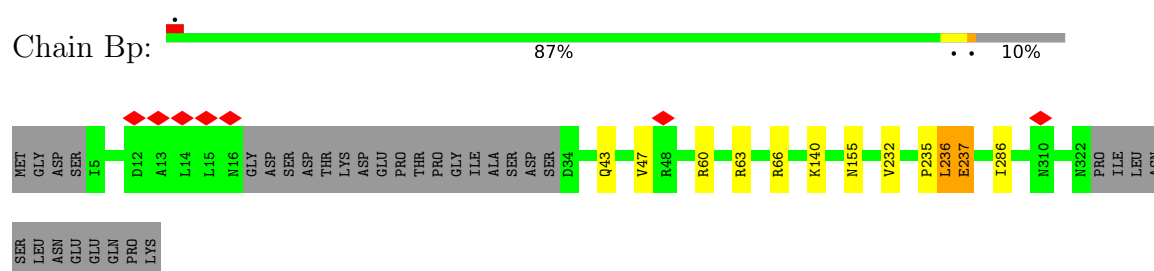
● Molecule 3: Flagellar motor switch protein FliM



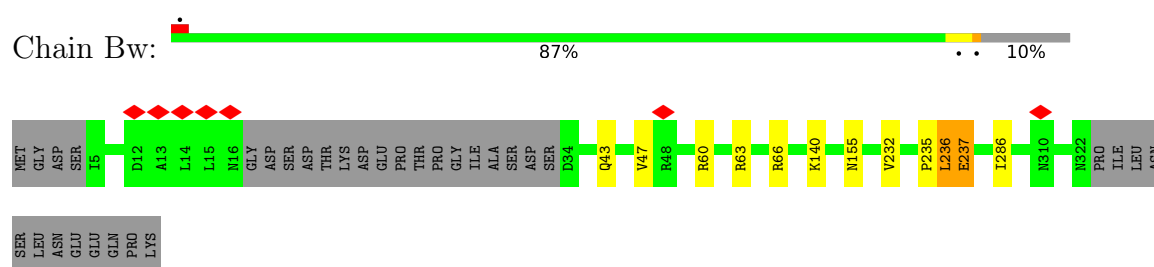
● Molecule 3: Flagellar motor switch protein FliM



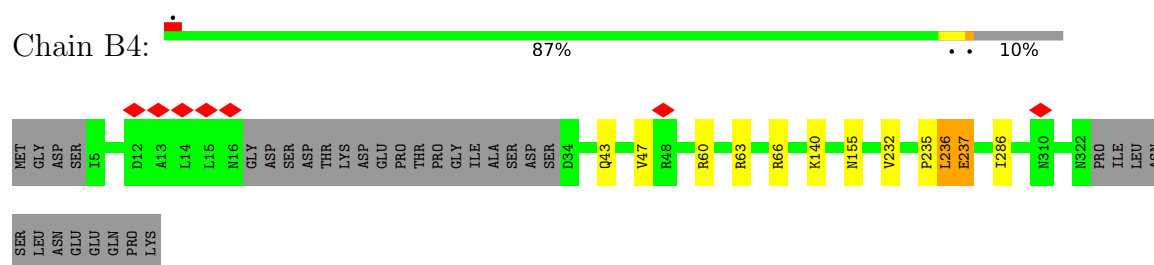
● Molecule 3: Flagellar motor switch protein FliM




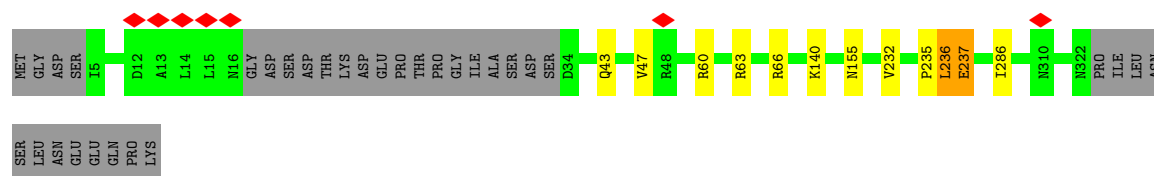
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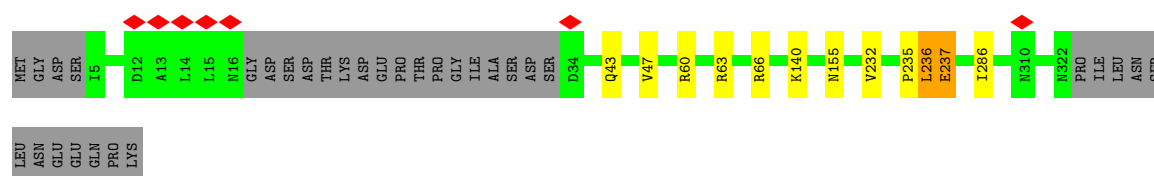
● Molecule 3: Flagellar motor switch protein FliM




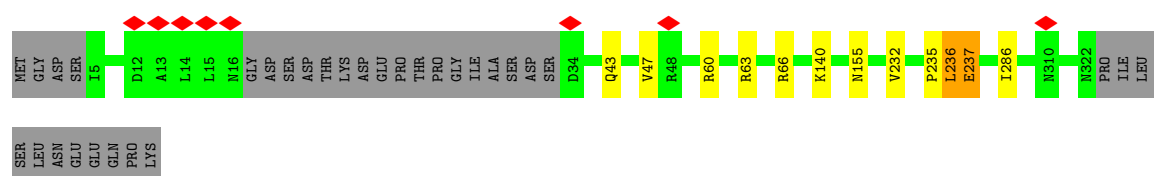
• Molecule 3: Flagellar motor switch protein FliM

Chain CA:  87% 10%


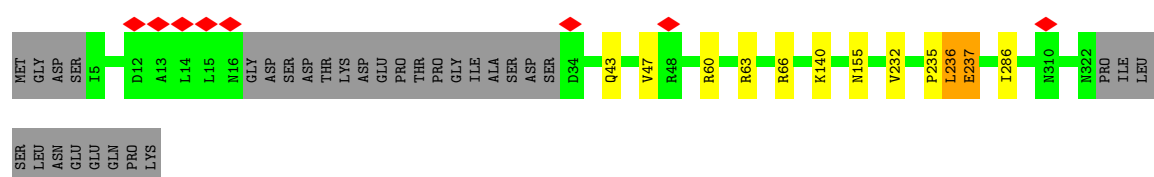
• Molecule 3: Flagellar motor switch protein FliM

Chain CH:  87% 10%


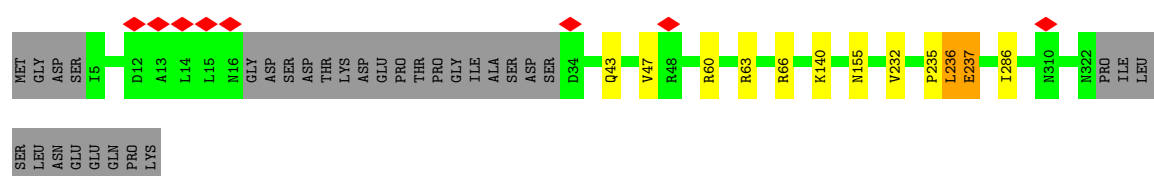
• Molecule 3: Flagellar motor switch protein FliM

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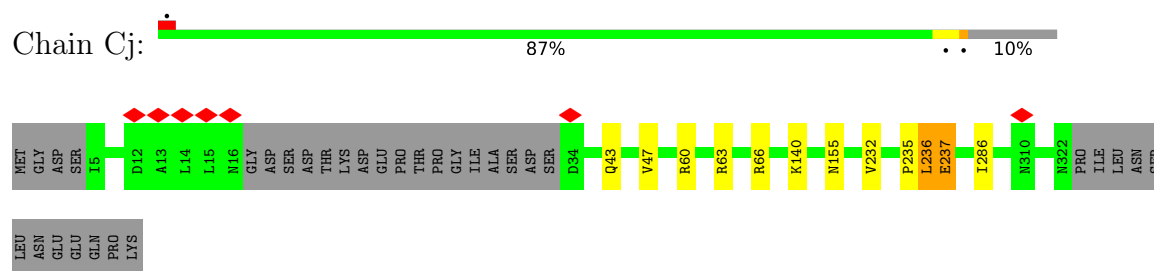
• Molecule 3: Flagellar motor switch protein FliM

Chain CV:  87% 10%

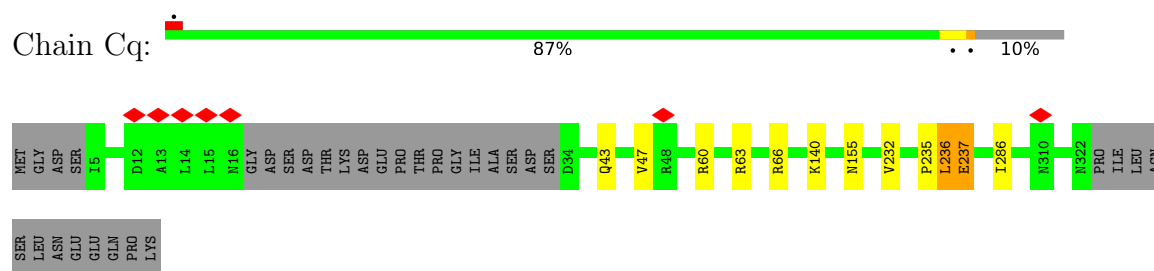
• Molecule 3: Flagellar motor switch protein FliM

Chain Cc:  87% 10%

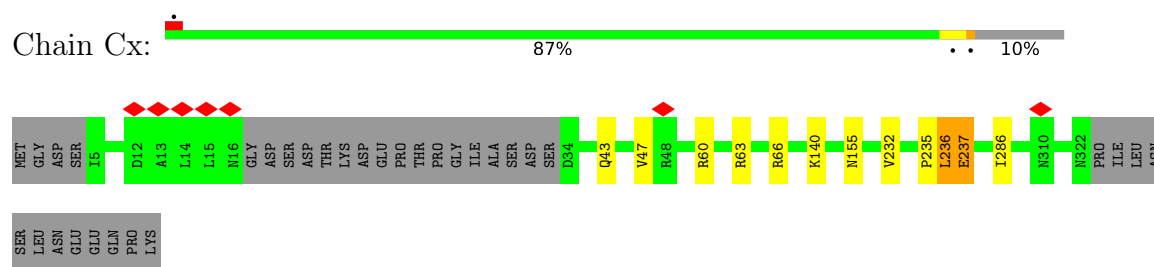
- Molecule 3: Flagellar motor switch protein FliM



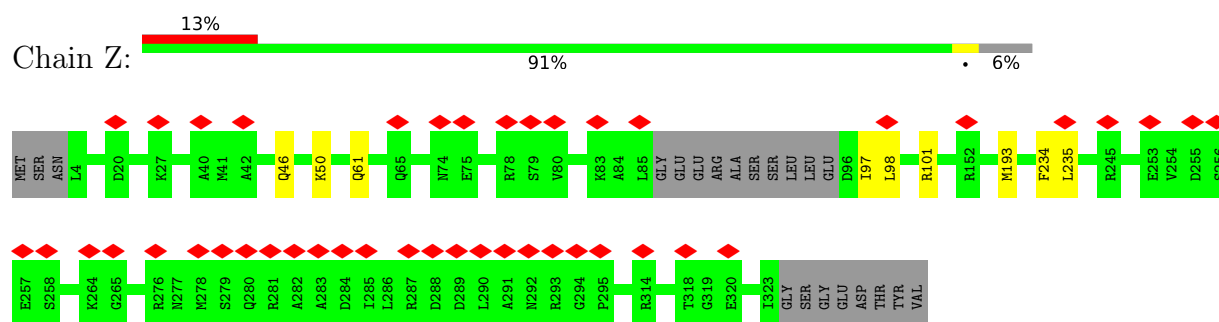
- Molecule 3: Flagellar motor switch protein FliM



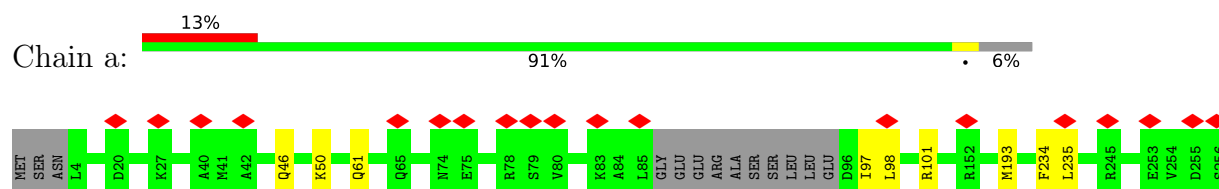
- Molecule 3: Flagellar motor switch protein FliM

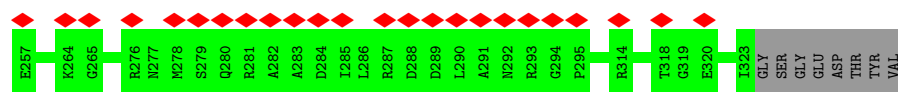


- Molecule 4: Flagellar motor switch protein FliG



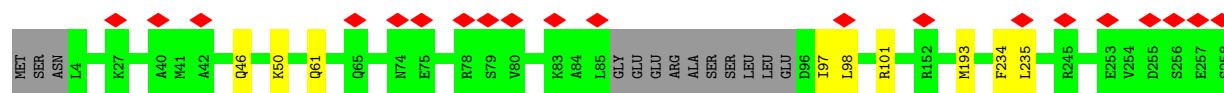
- Molecule 4: Flagellar motor switch protein FliG





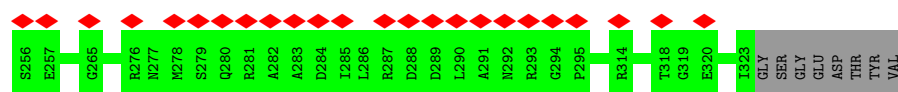
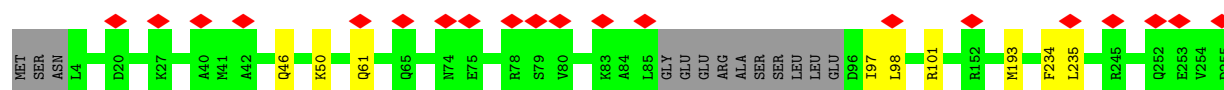
- Molecule 4: Flagellar motor switch protein FlIG

Chain b: 13% 91% 6%



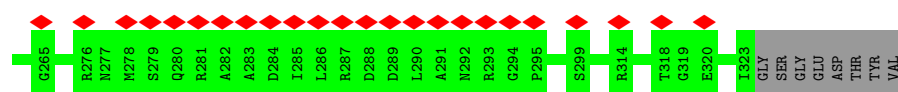
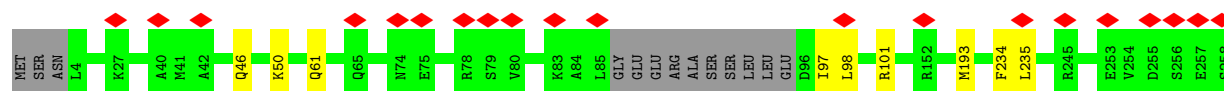
- Molecule 4: Flagellar motor switch protein FlIG

Chain c: 13% 91% 6%



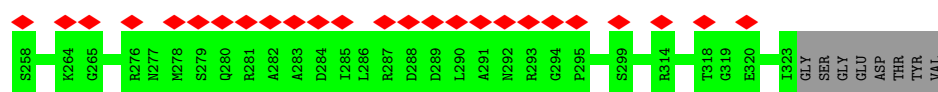
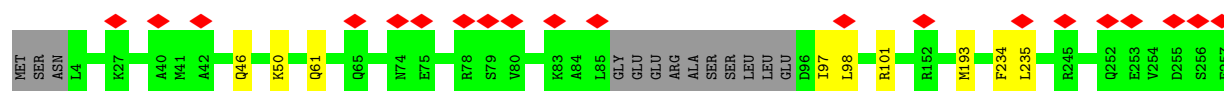
- Molecule 4: Flagellar motor switch protein FlIG

Chain d: 13% 91% 6%

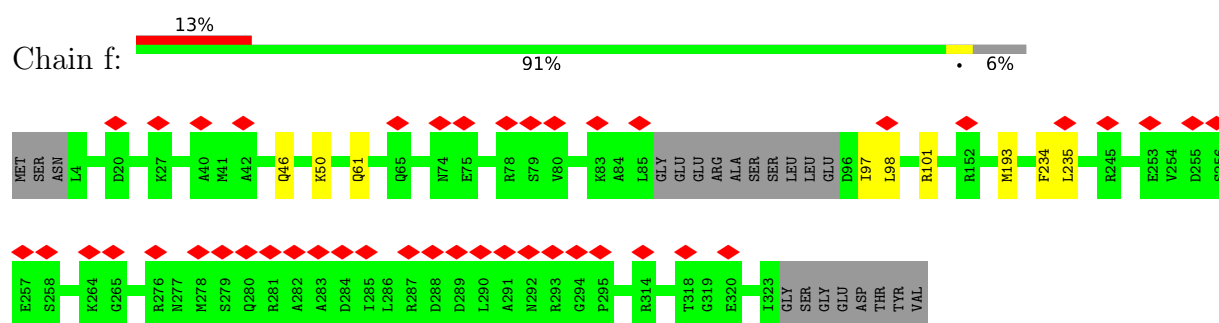


- Molecule 4: Flagellar motor switch protein FlIG

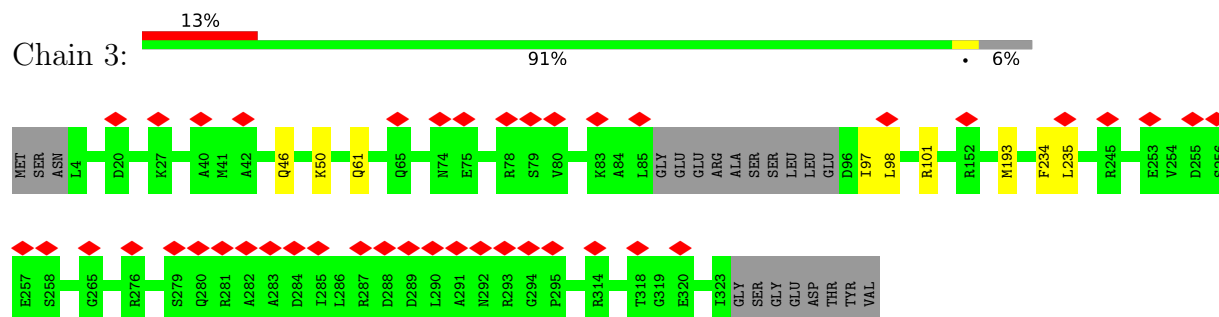
Chain e: 14% 91% 6%



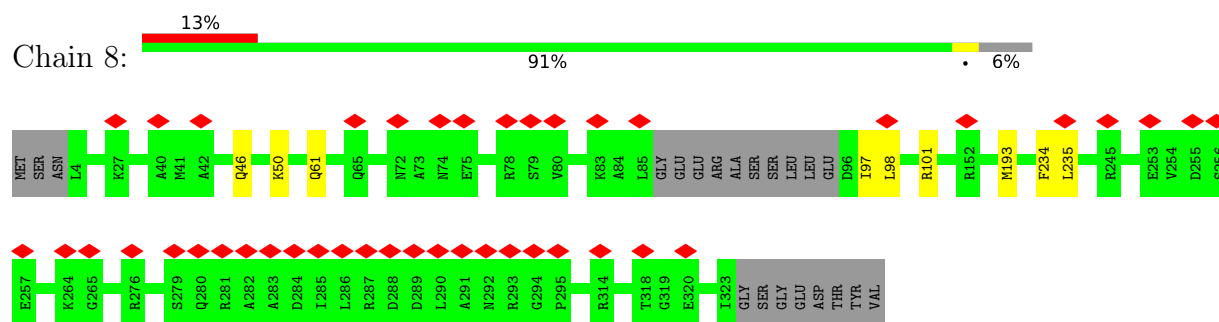
- Molecule 4: Flagellar motor switch protein FlIG



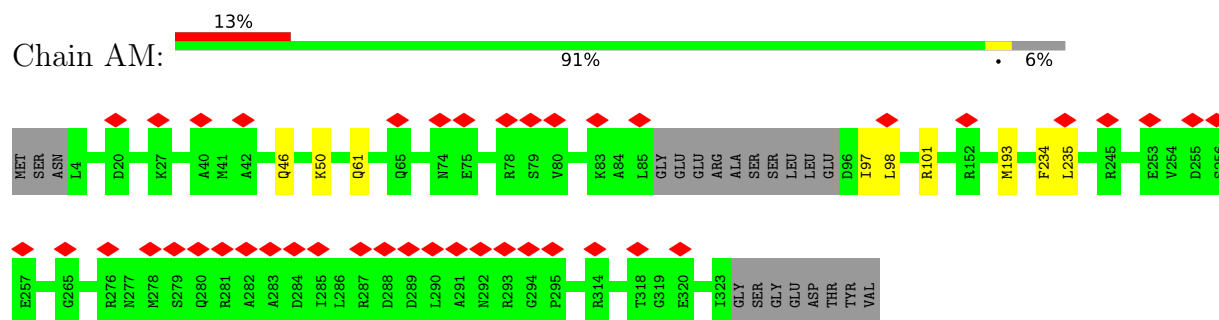
• Molecule 4: Flagellar motor switch protein Flig



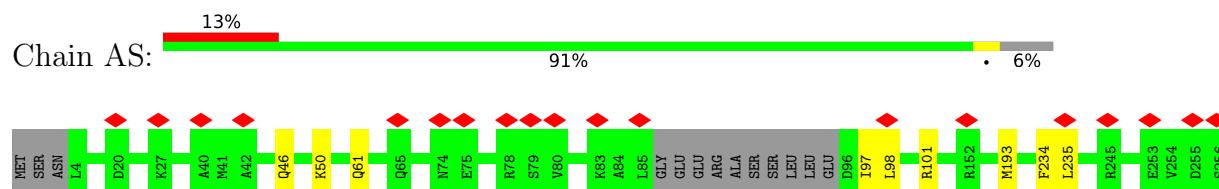
• Molecule 4: Flagellar motor switch protein Flig

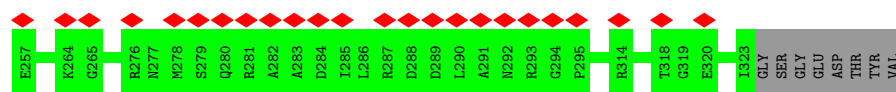


• Molecule 4: Flagellar motor switch protein Flig



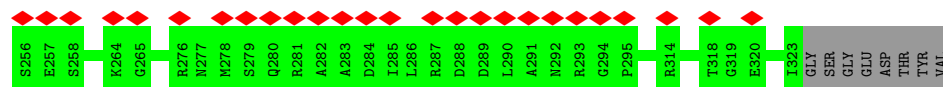
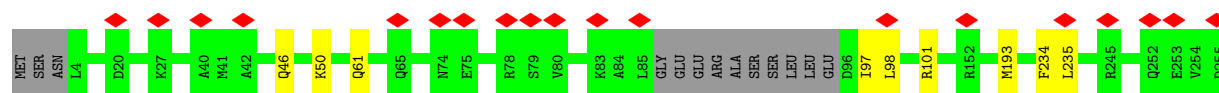
• Molecule 4: Flagellar motor switch protein Flig





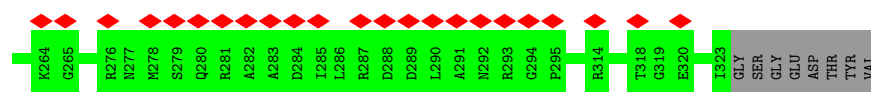
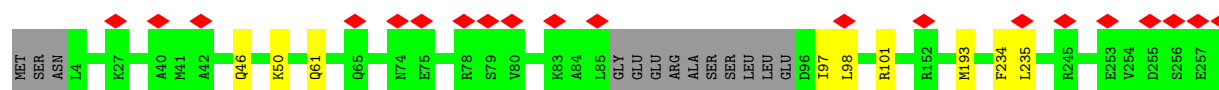
- Molecule 4: Flagellar motor switch protein Flig

Chain AY: 14% 91% 6%



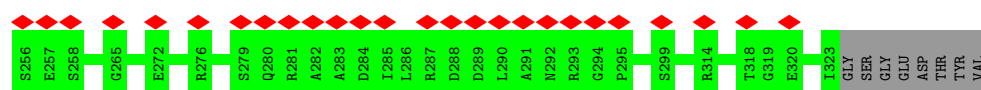
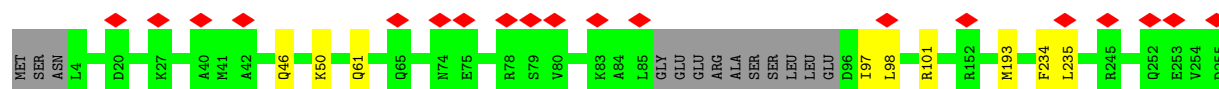
- Molecule 4: Flagellar motor switch protein Flig

Chain Ae: 13% 91% 6%



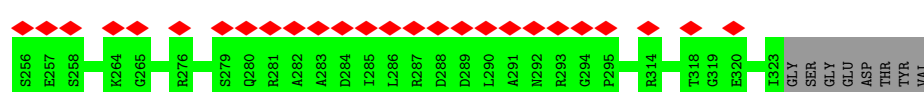
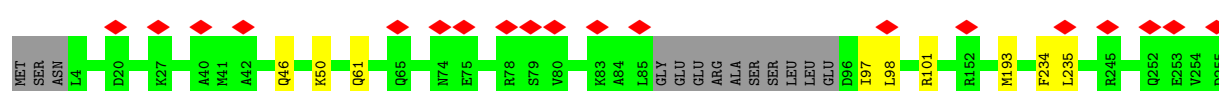
- Molecule 4: Flagellar motor switch protein Flig

Chain Ak: 14% 91% 6%

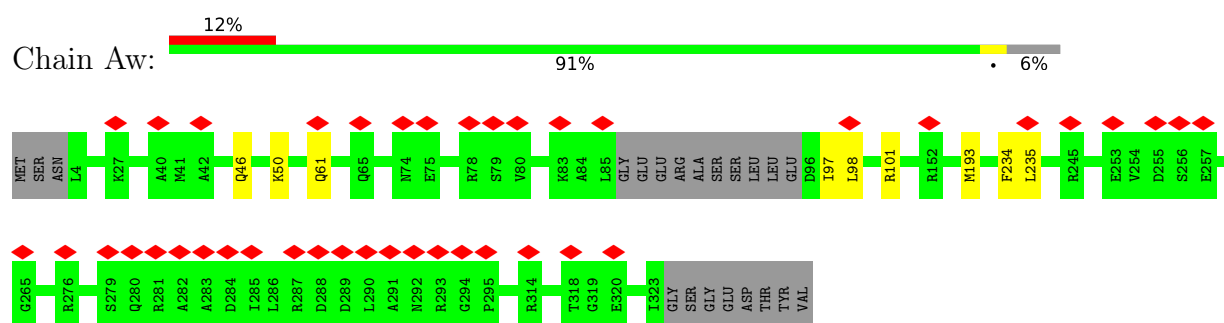


- Molecule 4: Flagellar motor switch protein Flig

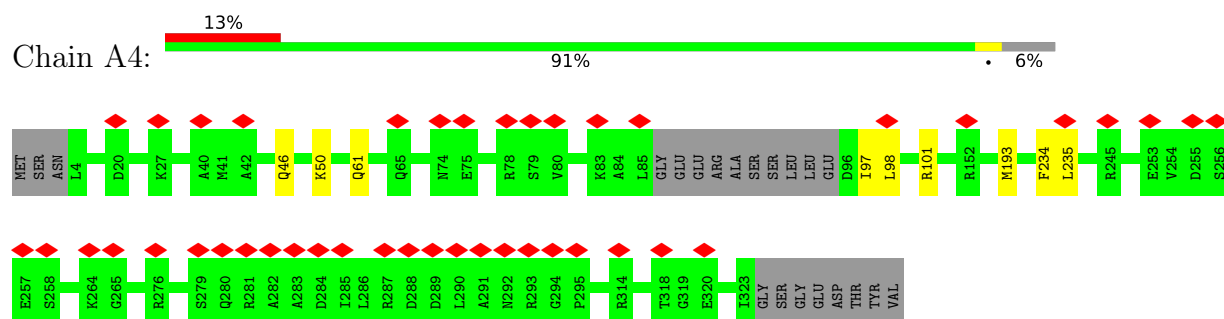
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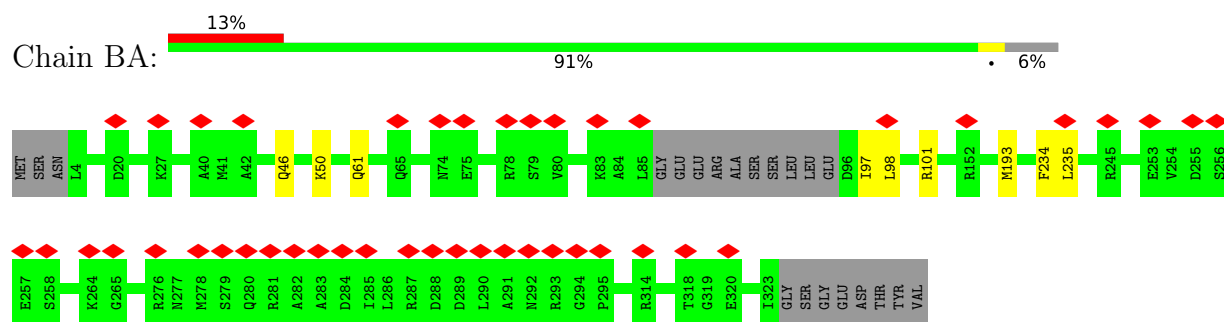
- Molecule 4: Flagellar motor switch protein Flig



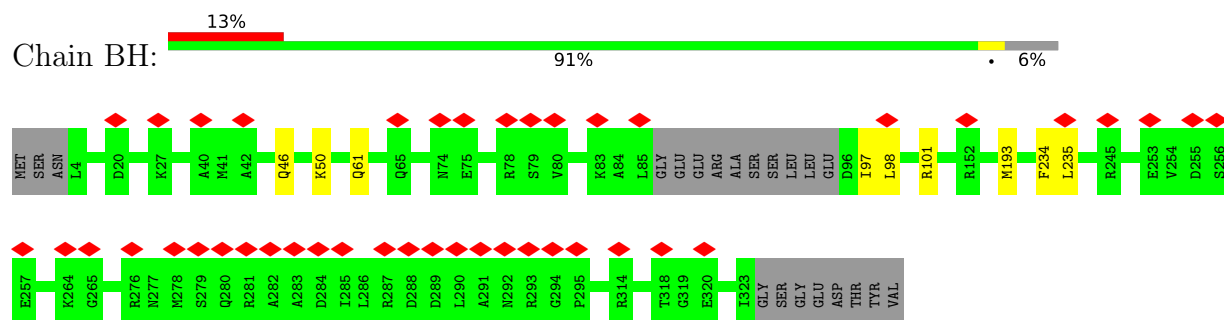
- Molecule 4: Flagellar motor switch protein Flig



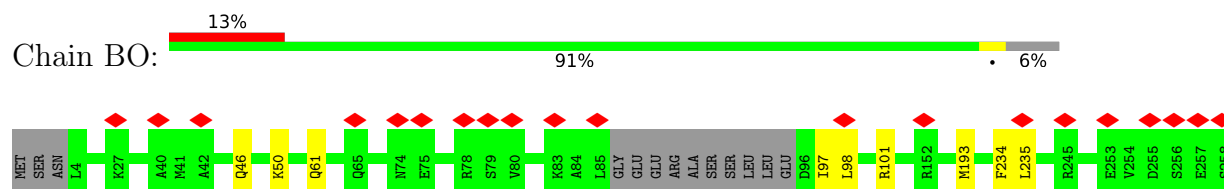
- Molecule 4: Flagellar motor switch protein Flig

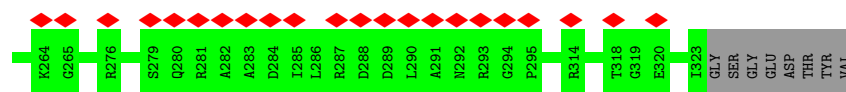


- Molecule 4: Flagellar motor switch protein Flig

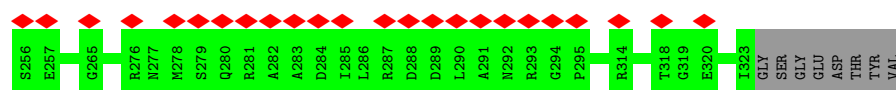
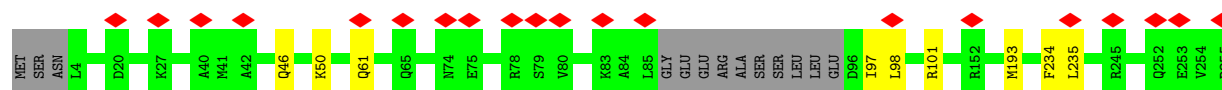


- Molecule 4: Flagellar motor switch protein Flig

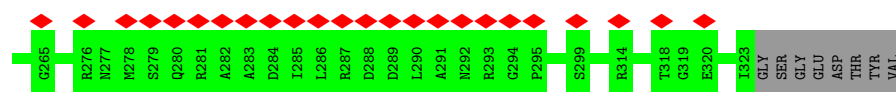
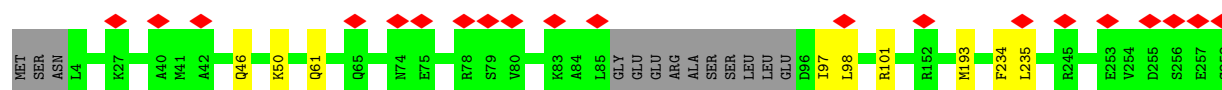




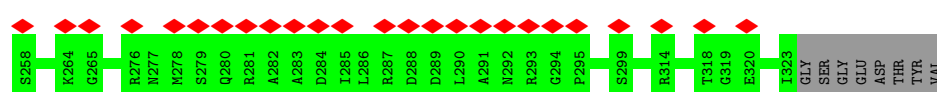
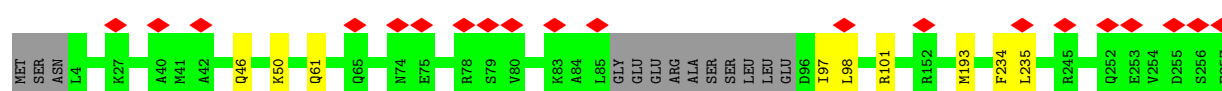
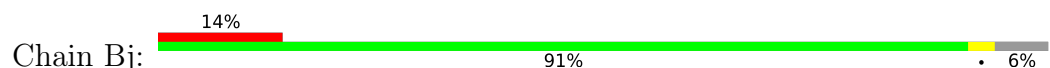
• Molecule 4: Flagellar motor switch protein FlIG



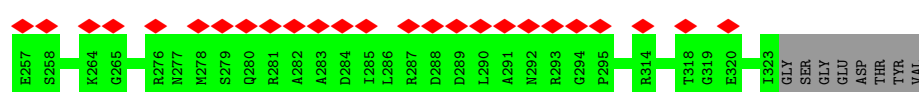
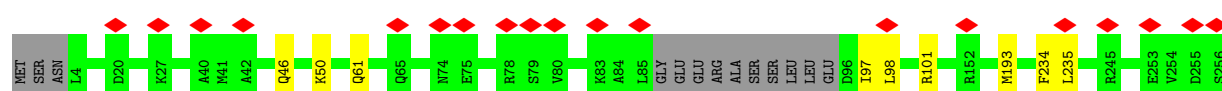
• Molecule 4: Flagellar motor switch protein FlIG



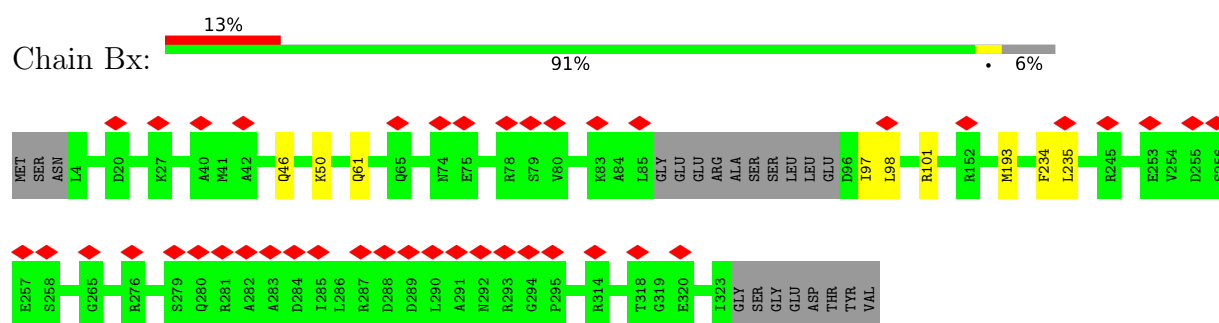
• Molecule 4: Flagellar motor switch protein FlIG



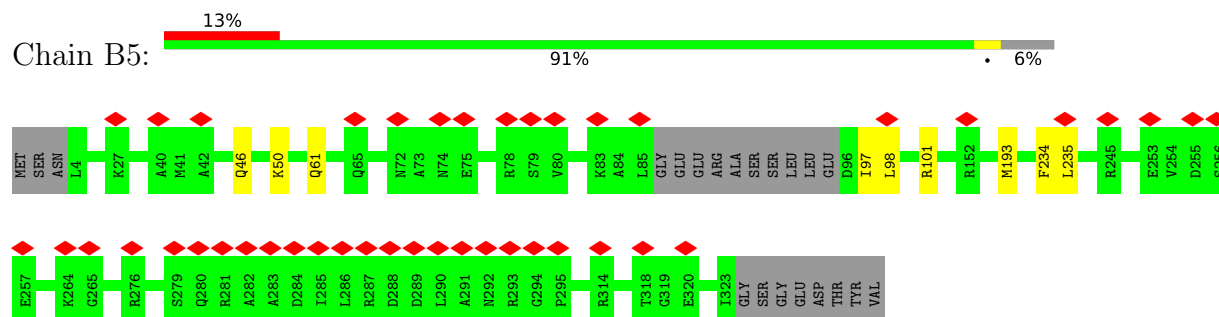
• Molecule 4: Flagellar motor switch protein FlIG



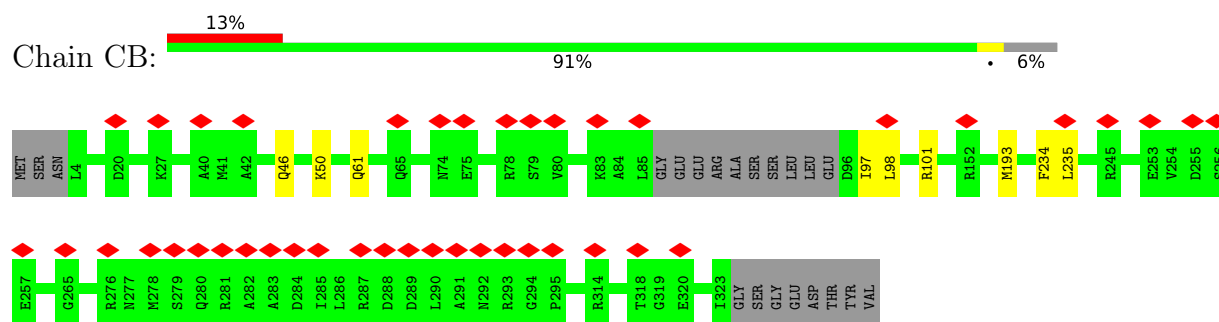
• Molecule 4: Flagellar motor switch protein FlIG



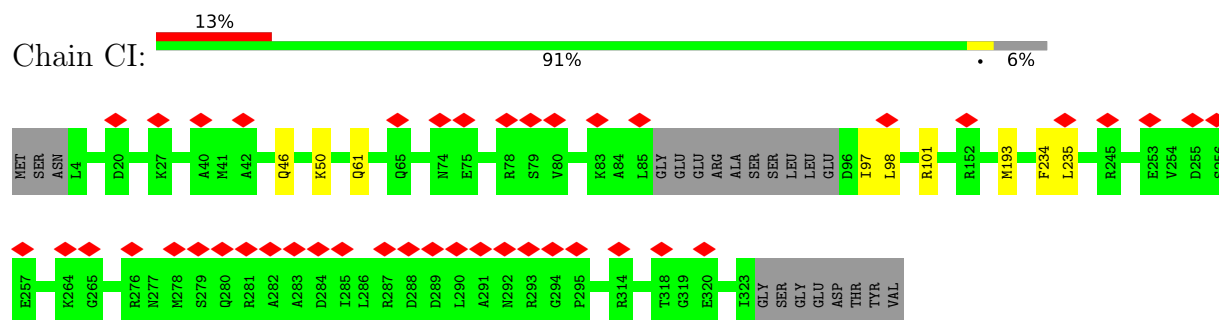
- Molecule 4: Flagellar motor switch protein FlgG



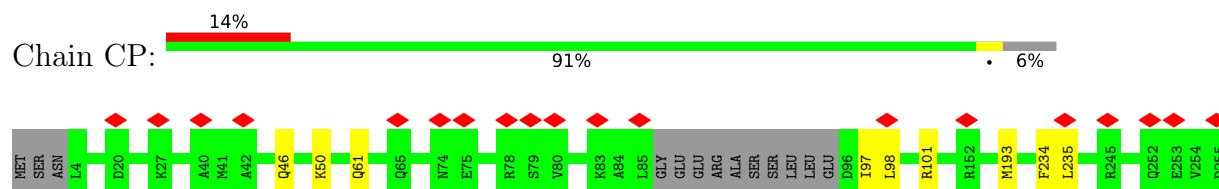
- Molecule 4: Flagellar motor switch protein FlgG

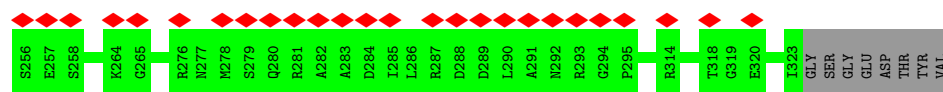


- Molecule 4: Flagellar motor switch protein FlgG

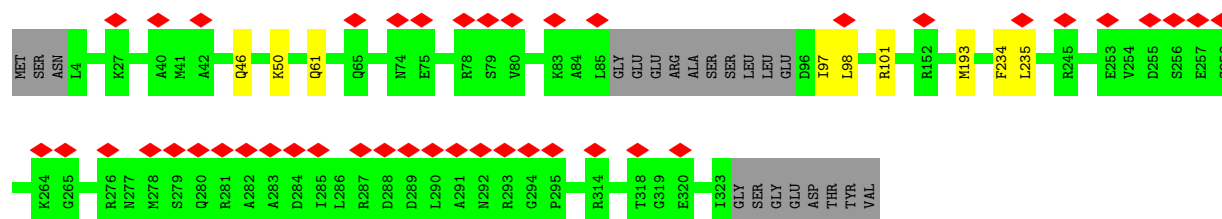


- Molecule 4: Flagellar motor switch protein FlgG

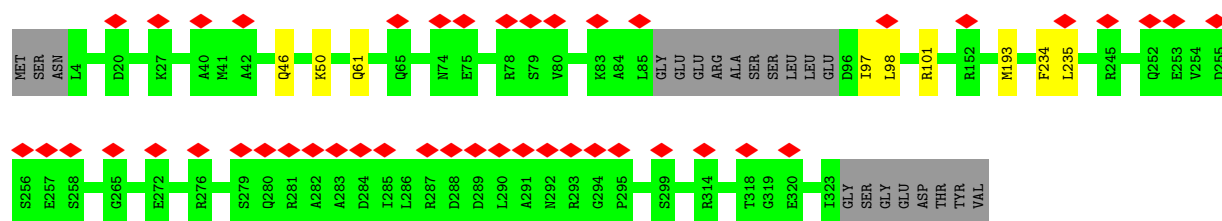
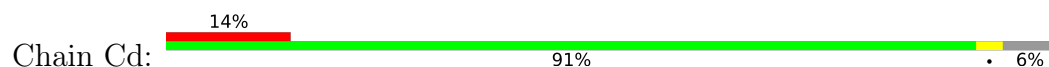




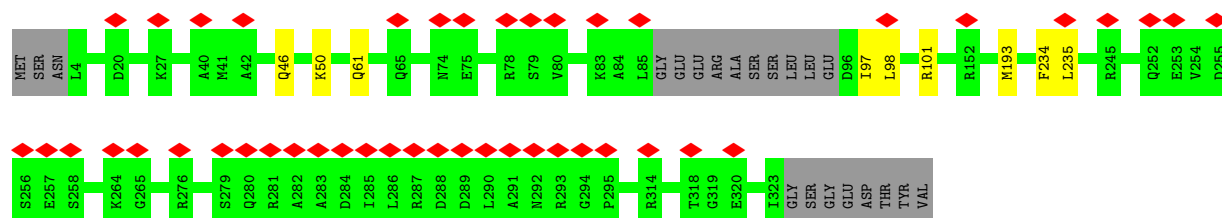
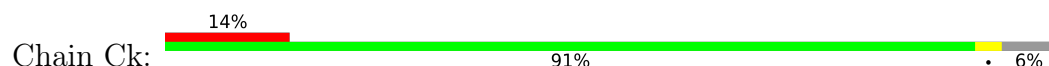
- Molecule 4: Flagellar motor switch protein Flig



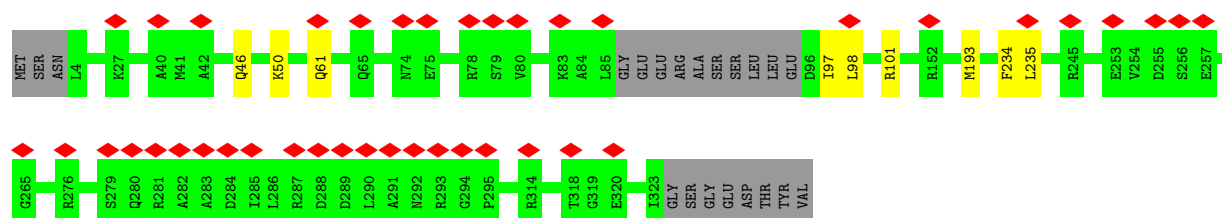
- Molecule 4: Flagellar motor switch protein Flig



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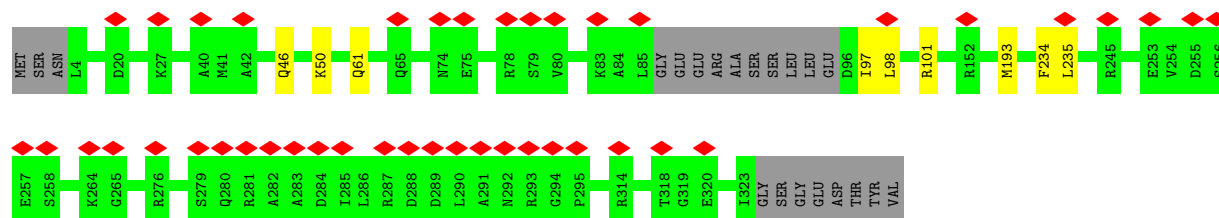


- Molecule 4: Flagellar motor switch protein Flig



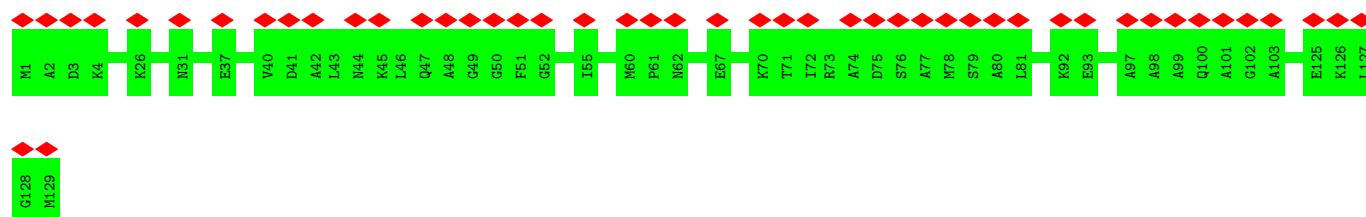
- Molecule 4: Flagellar motor switch protein Flig

Chain Cy: 13% 91% 6%



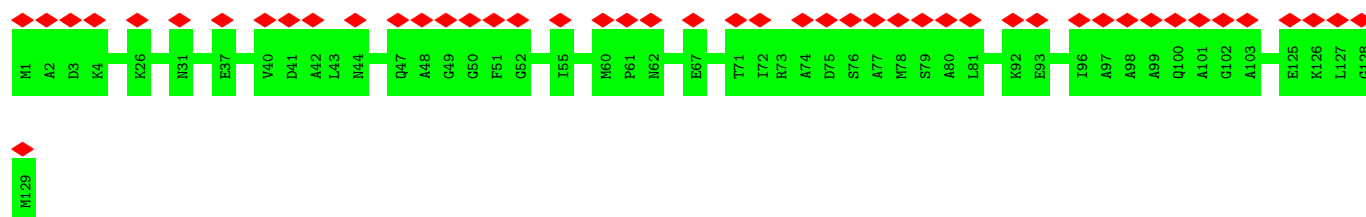
• Molecule 5: Chemotaxis protein CheY

Chain h: 37% 100%



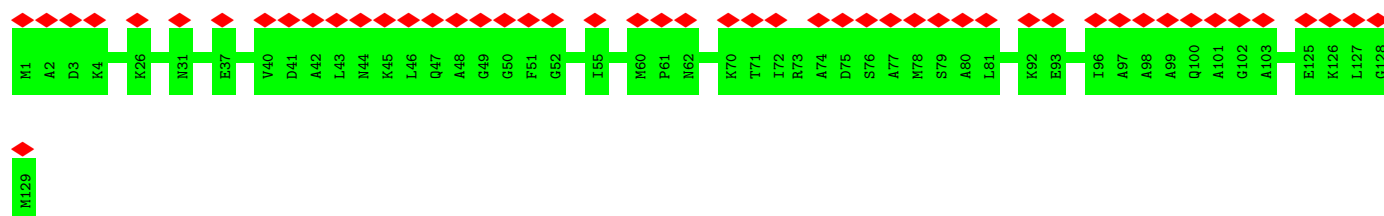
• Molecule 5: Chemotaxis protein CheY

Chain i: 36% 100%



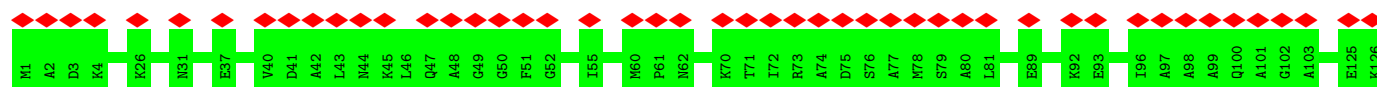
• Molecule 5: Chemotaxis protein CheY

Chain j: 39% 100%



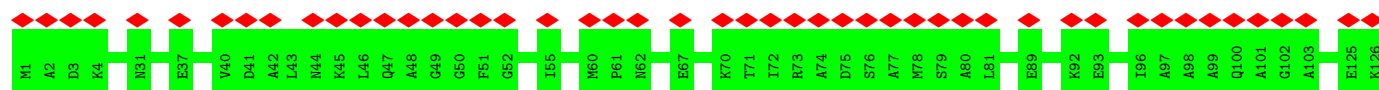
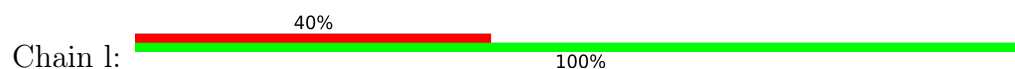
• Molecule 5: Chemotaxis protein CheY

Chain k: 40% 100%





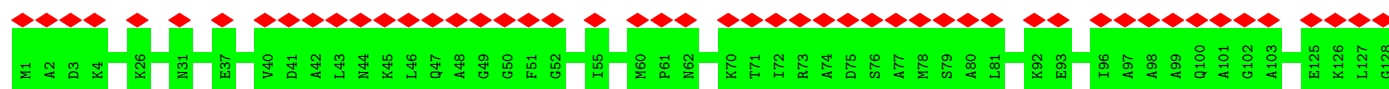
- Molecule 5: Chemotaxis protein CheY



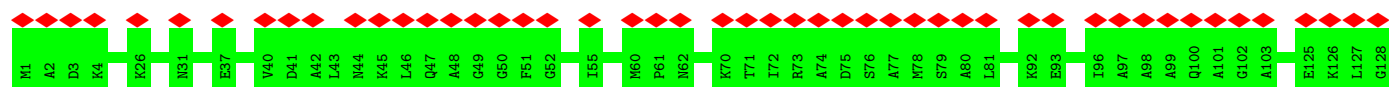
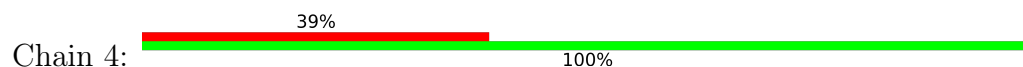
- Molecule 5: Chemotaxis protein CheY



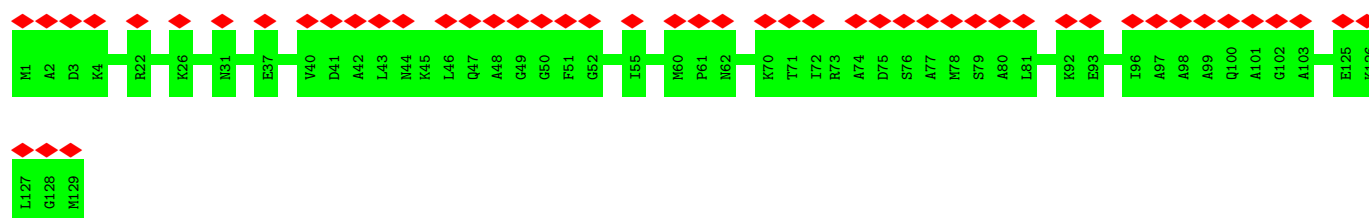
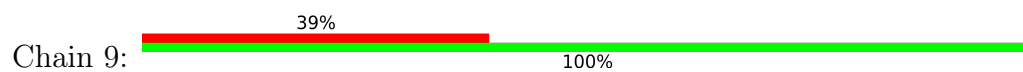
- Molecule 5: Chemotaxis protein CheY



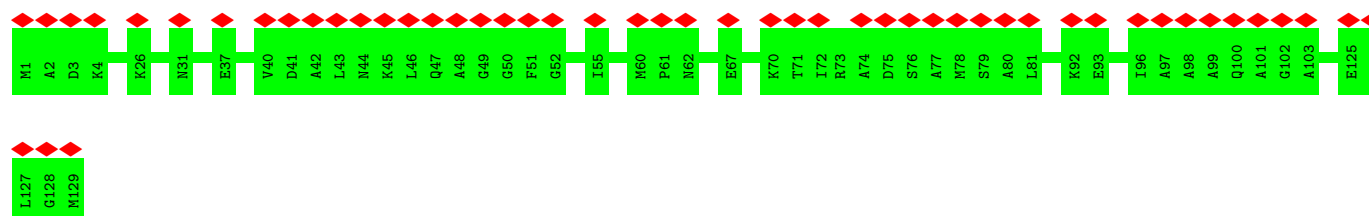
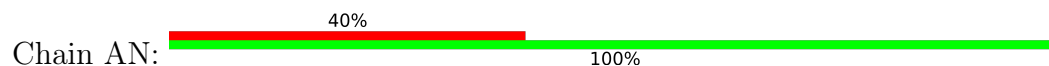
- Molecule 5: Chemotaxis protein CheY



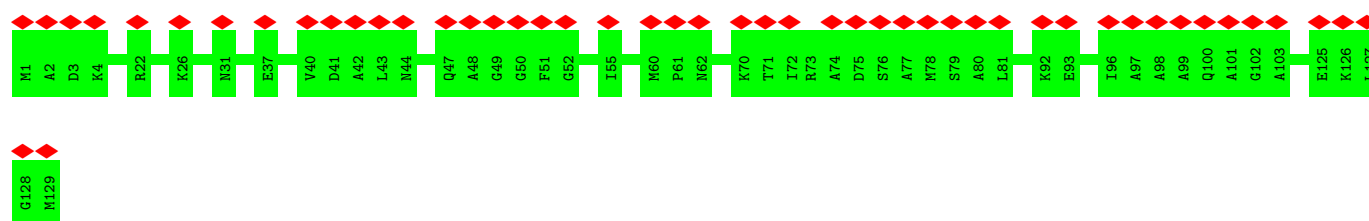
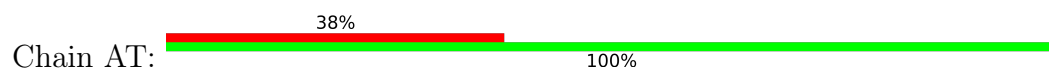
- Molecule 5: Chemotaxis protein CheY



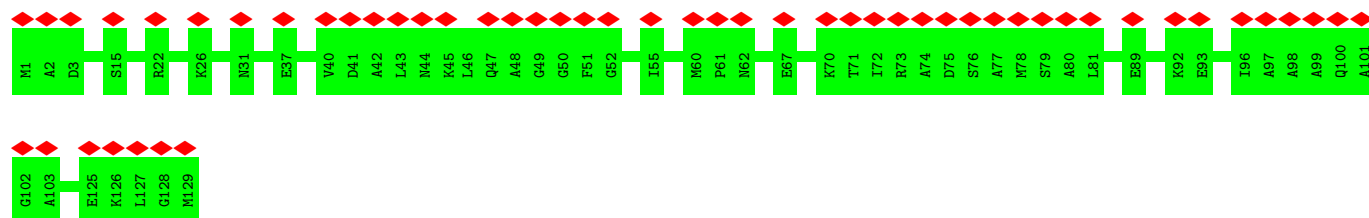
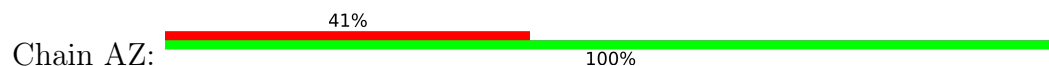
- Molecule 5: Chemotaxis protein CheY



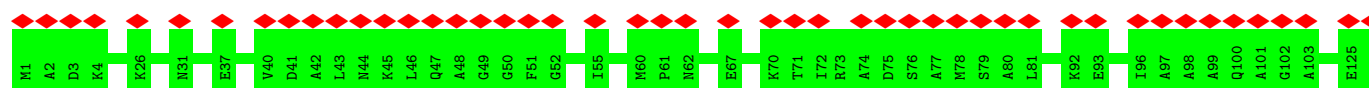
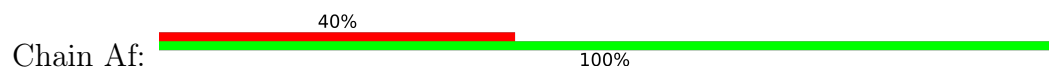
- Molecule 5: Chemotaxis protein CheY



- Molecule 5: Chemotaxis protein CheY

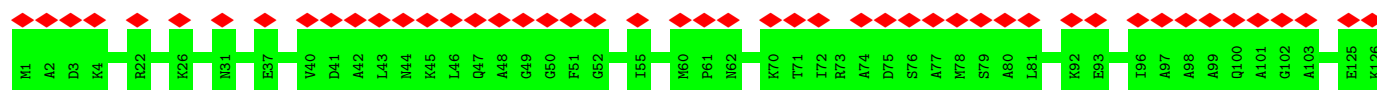
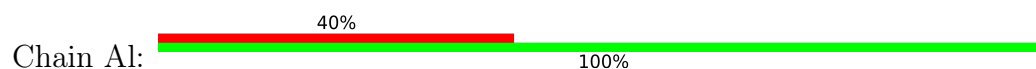


- Molecule 5: Chemotaxis protein CheY

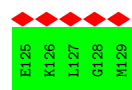
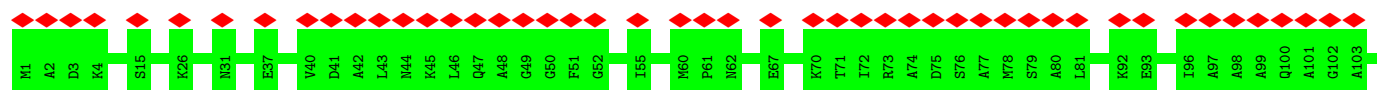
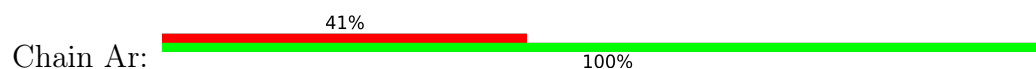




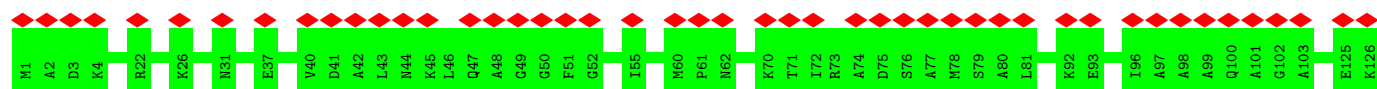
- Molecule 5: Chemotaxis protein CheY



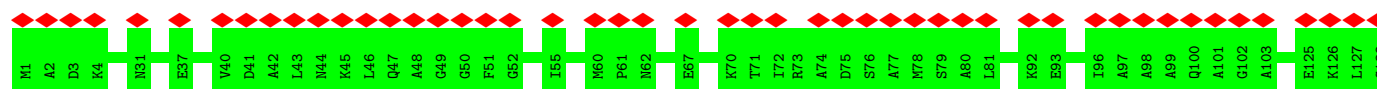
- Molecule 5: Chemotaxis protein CheY



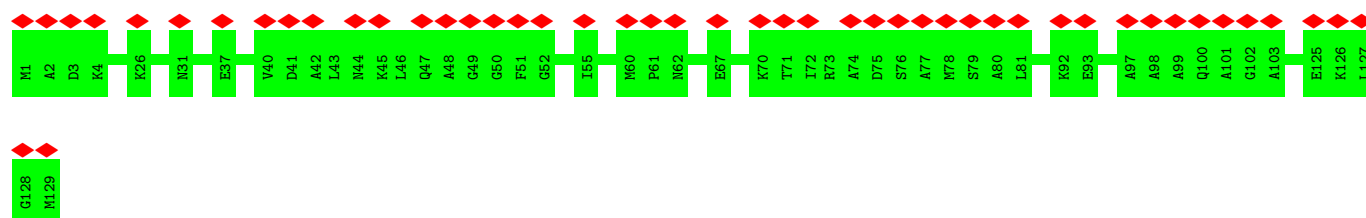
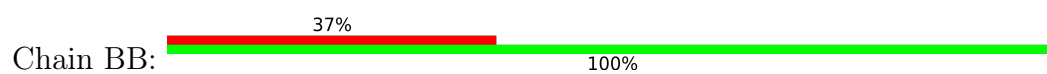
- Molecule 5: Chemotaxis protein CheY



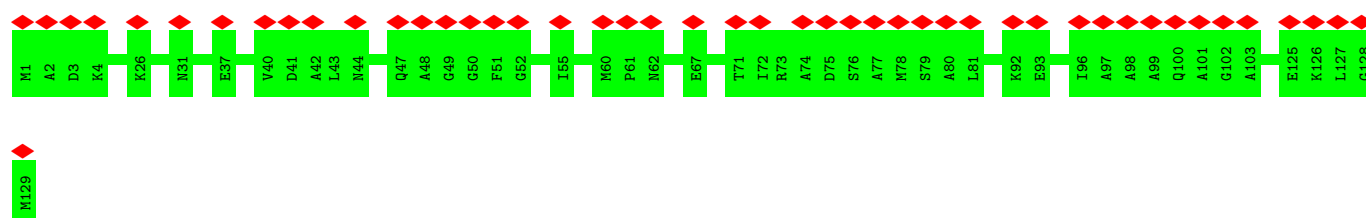
- Molecule 5: Chemotaxis protein CheY



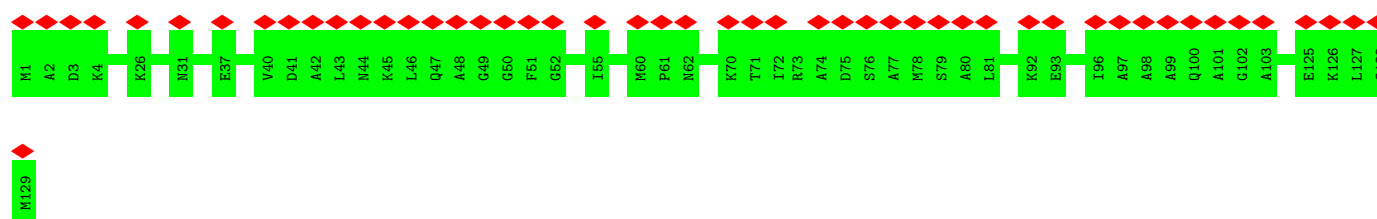
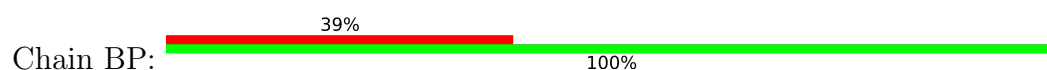
- Molecule 5: Chemotaxis protein CheY



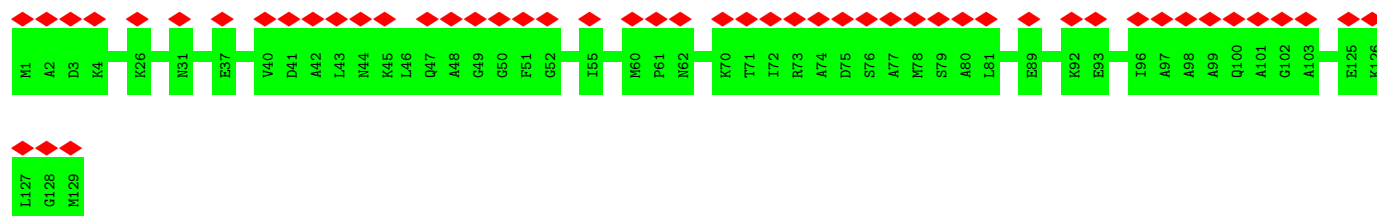
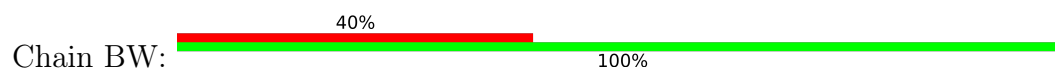
- Molecule 5: Chemotaxis protein CheY



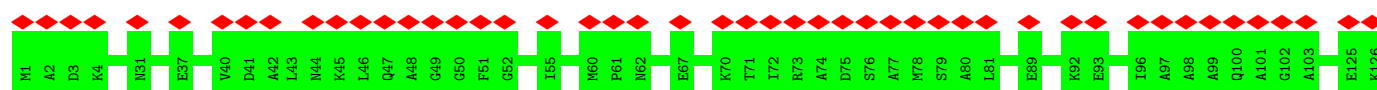
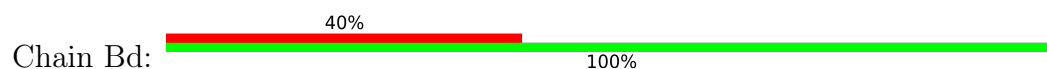
- Molecule 5: Chemotaxis protein CheY



- Molecule 5: Chemotaxis protein CheY

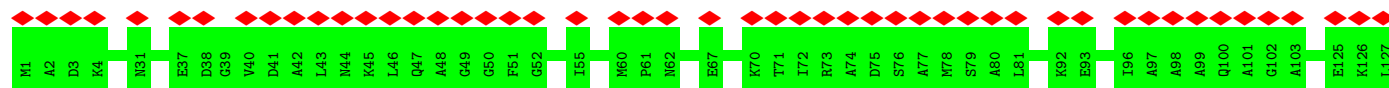
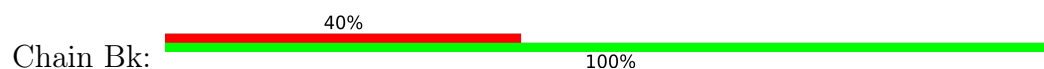


- Molecule 5: Chemotaxis protein CheY

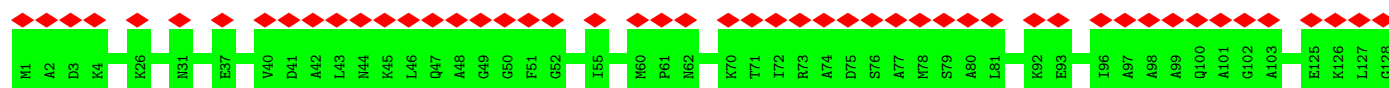
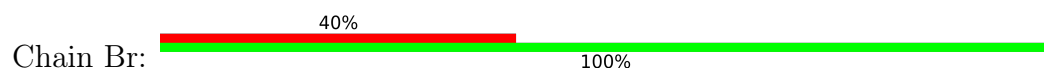




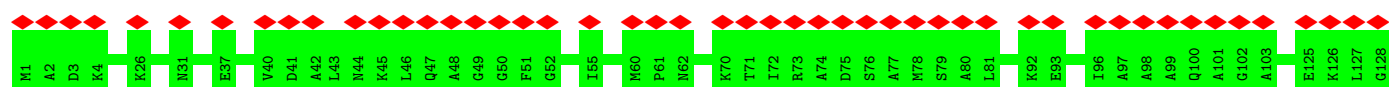
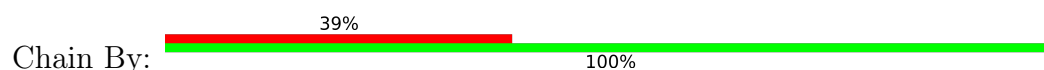
- Molecule 5: Chemotaxis protein CheY



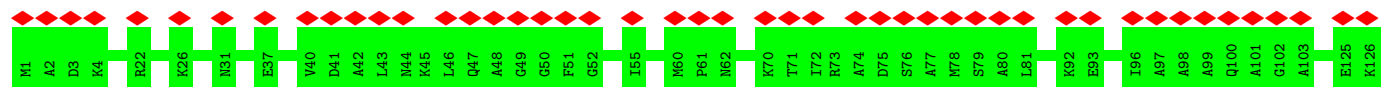
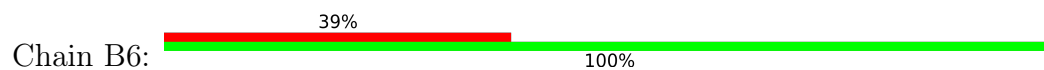
- Molecule 5: Chemotaxis protein CheY



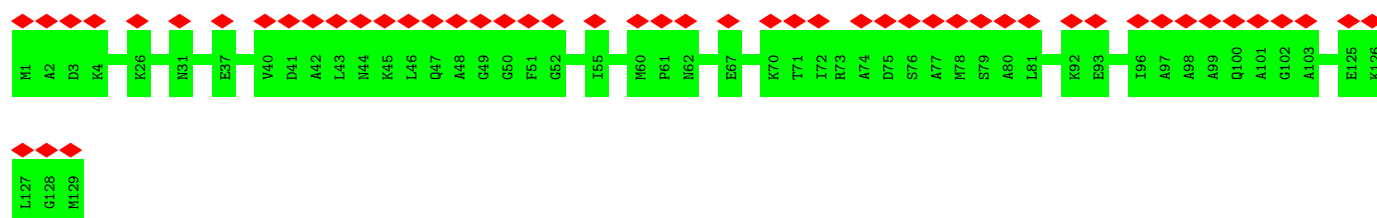
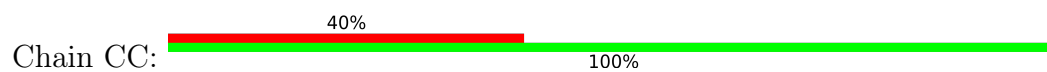
- Molecule 5: Chemotaxis protein CheY



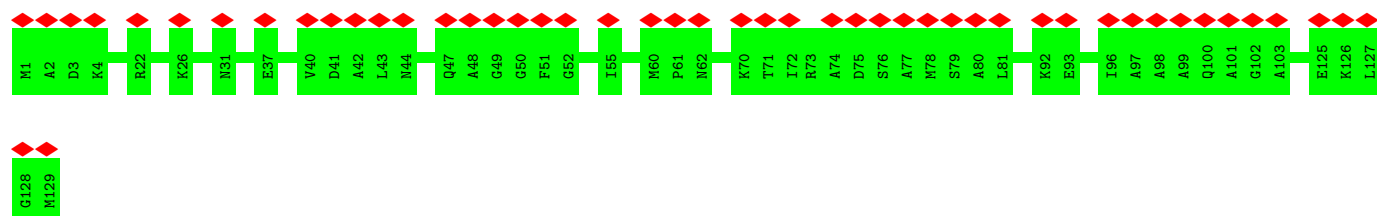
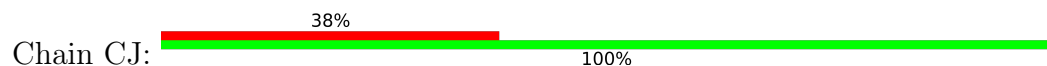
- Molecule 5: Chemotaxis protein CheY



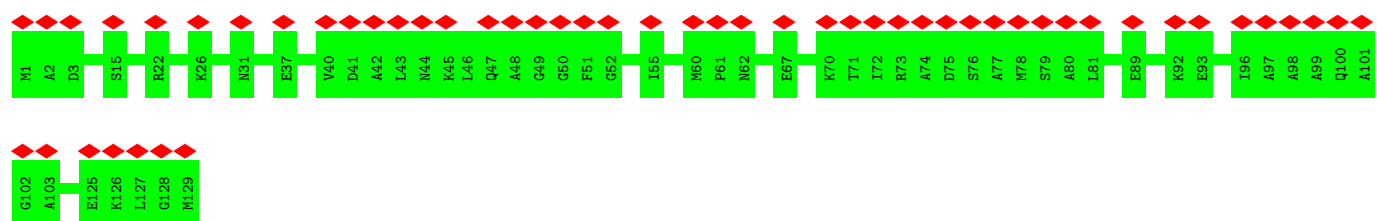
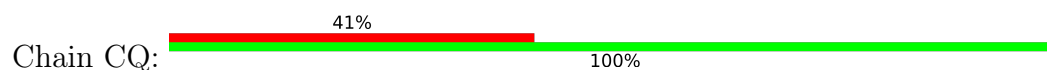
- Molecule 5: Chemotaxis protein CheY



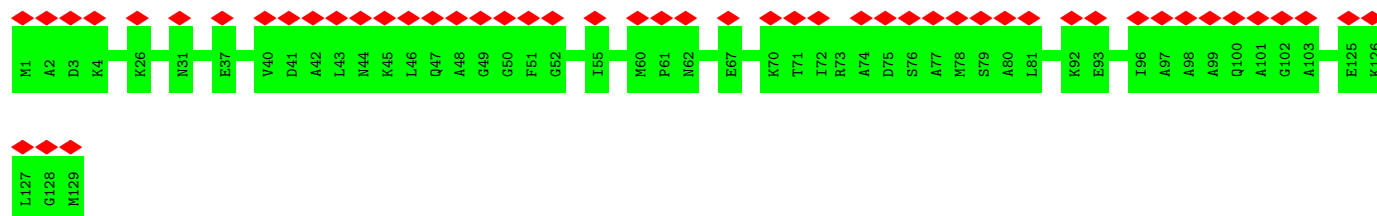
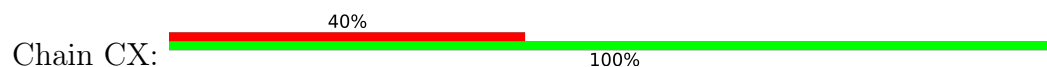
- Molecule 5: Chemotaxis protein CheY



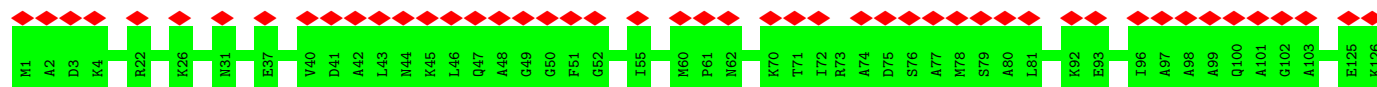
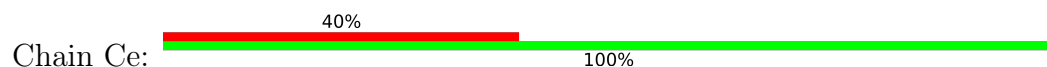
- Molecule 5: Chemotaxis protein CheY



- Molecule 5: Chemotaxis protein CheY

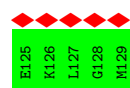
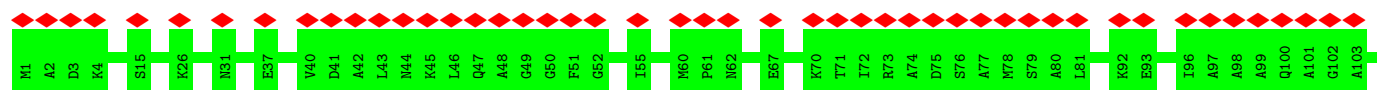


- Molecule 5: Chemotaxis protein CheY

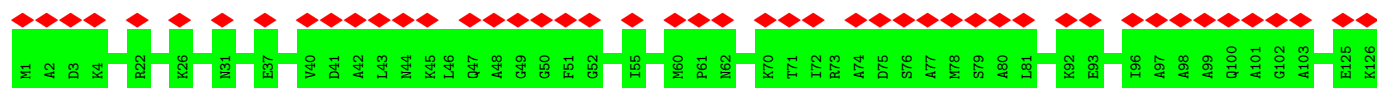
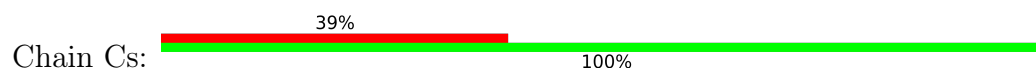




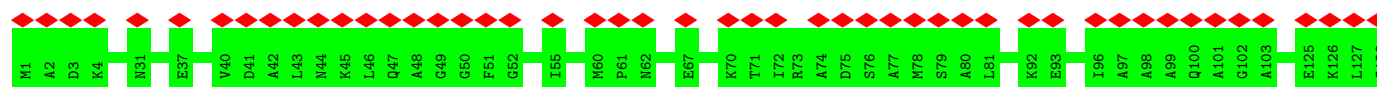
- Molecule 5: Chemotaxis protein CheY



- Molecule 5: Chemotaxis protein CheY



- Molecule 5: Chemotaxis protein CheY



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C34	Depositor
Number of particles used	28119	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.438	Depositor
Minimum map value	-0.222	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	720.0, 720.0, 720.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.29	0/679	0.53	0/917
1	1	0.39	0/679	0.57	0/917
1	2	0.31	0/679	0.54	0/917
1	5	0.39	0/679	0.57	0/917
1	6	0.31	0/679	0.54	0/917
1	A1	0.29	0/679	0.53	0/917
1	A6	0.39	0/679	0.57	0/917
1	A7	0.31	0/679	0.54	0/917
1	A8	0.29	0/679	0.53	0/917
1	AA	0.29	0/679	0.53	0/917
1	AB	0.29	0/679	0.53	0/917
1	AC	0.29	0/679	0.53	0/917
1	AD	0.29	0/679	0.53	0/917
1	AE	0.29	0/679	0.53	0/917
1	AF	0.29	0/679	0.53	0/917
1	AG	0.29	0/679	0.53	0/917
1	AH	0.29	0/679	0.53	0/917
1	AI	0.39	0/679	0.57	0/917
1	AJ	0.31	0/679	0.54	0/917
1	AK	0.29	0/679	0.53	0/917
1	AO	0.39	0/679	0.57	0/917
1	AP	0.31	0/679	0.54	0/917
1	AQ	0.29	0/679	0.53	0/917
1	AU	0.39	0/679	0.57	0/917
1	AV	0.31	0/679	0.54	0/917
1	AW	0.29	0/679	0.53	0/917
1	Aa	0.39	0/679	0.57	0/917
1	Ab	0.31	0/679	0.54	0/917
1	Ac	0.29	0/679	0.53	0/917
1	Ag	0.39	0/679	0.57	0/917
1	Ah	0.31	0/679	0.54	0/917
1	Ai	0.29	0/679	0.53	0/917
1	Am	0.39	0/679	0.57	0/917
1	An	0.31	0/679	0.54	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ao	0.29	0/679	0.53	0/917
1	As	0.39	0/679	0.57	0/917
1	At	0.31	0/679	0.54	0/917
1	Au	0.29	0/679	0.53	0/917
1	Ay	0.39	0/679	0.57	0/917
1	Az	0.31	0/679	0.54	0/917
1	B1	0.31	0/679	0.54	0/917
1	B2	0.29	0/679	0.53	0/917
1	B7	0.39	0/679	0.57	0/917
1	B8	0.31	0/679	0.54	0/917
1	B9	0.29	0/679	0.53	0/917
1	BC	0.39	0/679	0.57	0/917
1	BD	0.31	0/679	0.54	0/917
1	BE	0.29	0/679	0.53	0/917
1	BJ	0.39	0/679	0.57	0/917
1	BK	0.31	0/679	0.54	0/917
1	BL	0.29	0/679	0.53	0/917
1	BQ	0.39	0/679	0.57	0/917
1	BR	0.31	0/679	0.54	0/917
1	BS	0.29	0/679	0.53	0/917
1	BX	0.39	0/679	0.57	0/917
1	BY	0.31	0/679	0.54	0/917
1	BZ	0.29	0/679	0.53	0/917
1	Be	0.39	0/679	0.57	0/917
1	Bf	0.31	0/679	0.54	0/917
1	Bg	0.29	0/679	0.53	0/917
1	Bl	0.39	0/679	0.57	0/917
1	Bm	0.31	0/679	0.54	0/917
1	Bn	0.29	0/679	0.53	0/917
1	Bs	0.39	0/679	0.57	0/917
1	Bt	0.31	0/679	0.54	0/917
1	Bu	0.29	0/679	0.53	0/917
1	Bz	0.39	0/679	0.57	0/917
1	C1	0.39	0/679	0.57	0/917
1	C2	0.31	0/679	0.54	0/917
1	CD	0.39	0/679	0.57	0/917
1	CE	0.31	0/679	0.54	0/917
1	CF	0.29	0/679	0.53	0/917
1	CK	0.39	0/679	0.57	0/917
1	CL	0.31	0/679	0.54	0/917
1	CM	0.29	0/679	0.53	0/917
1	CR	0.39	0/679	0.57	0/917
1	CS	0.31	0/679	0.54	0/917

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CT	0.29	0/679	0.53	0/917
1	CY	0.39	0/679	0.57	0/917
1	CZ	0.31	0/679	0.54	0/917
1	Ca	0.29	0/679	0.53	0/917
1	Cf	0.39	0/679	0.57	0/917
1	Cg	0.31	0/679	0.54	0/917
1	Ch	0.29	0/679	0.53	0/917
1	Cm	0.39	0/679	0.57	0/917
1	Cn	0.31	0/679	0.54	0/917
1	Co	0.29	0/679	0.53	0/917
1	Ct	0.39	0/679	0.57	0/917
1	Cu	0.31	0/679	0.54	0/917
1	Cv	0.29	0/679	0.53	0/917
1	o	0.39	0/679	0.57	0/917
1	p	0.39	0/679	0.57	0/917
1	q	0.39	0/679	0.57	0/917
1	r	0.39	0/679	0.57	0/917
1	s	0.39	0/679	0.57	0/917
1	t	0.39	0/679	0.57	0/917
1	u	0.31	0/679	0.54	0/917
1	v	0.31	0/679	0.54	0/917
1	w	0.31	0/679	0.54	0/917
1	x	0.31	0/679	0.54	0/917
1	y	0.31	0/679	0.54	0/917
1	z	0.31	0/679	0.54	0/917
2	A2	0.22	0/226	0.49	0/303
2	A9	0.22	0/226	0.49	0/303
2	B0	0.22	0/226	0.49	0/303
2	B3	0.22	0/226	0.49	0/303
2	BF	0.22	0/226	0.49	0/303
2	BM	0.22	0/226	0.49	0/303
2	BT	0.22	0/226	0.49	0/303
2	Ba	0.22	0/226	0.49	0/303
2	Bh	0.22	0/226	0.49	0/303
2	Bo	0.22	0/226	0.49	0/303
2	Bv	0.22	0/226	0.49	0/303
2	C	0.22	0/226	0.49	0/303
2	CG	0.22	0/226	0.49	0/303
2	CN	0.22	0/226	0.49	0/303
2	CU	0.22	0/226	0.49	0/303
2	Cb	0.22	0/226	0.49	0/303
2	Ci	0.22	0/226	0.49	0/303
2	Cp	0.22	0/226	0.49	0/303

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Cw	0.22	0/226	0.49	0/303
2	D	0.22	0/226	0.49	0/303
2	E	0.22	0/226	0.49	0/303
2	F	0.22	0/226	0.49	0/303
2	G	0.22	0/226	0.49	0/303
2	H	0.22	0/226	0.49	0/303
2	I	0.22	0/226	0.49	0/303
2	J	0.22	0/226	0.49	0/303
2	K	0.22	0/226	0.49	0/303
2	L	0.22	0/226	0.49	0/303
2	M	0.22	0/226	0.49	0/303
2	N	0.22	0/226	0.49	0/303
2	O	0.22	0/226	0.49	0/303
2	P	0.22	0/226	0.49	0/303
2	Q	0.22	0/226	0.49	0/303
2	R	0.22	0/226	0.49	0/303
3	7	0.27	0/2482	0.50	0/3375
3	A0	0.27	0/2482	0.50	0/3375
3	A3	0.27	0/2482	0.50	0/3375
3	AL	0.27	0/2482	0.50	0/3375
3	AR	0.27	0/2482	0.50	0/3375
3	AX	0.28	0/2482	0.50	0/3375
3	Ad	0.28	0/2482	0.50	0/3375
3	Aj	0.27	0/2482	0.50	0/3375
3	Ap	0.27	0/2482	0.50	0/3375
3	Av	0.27	0/2482	0.50	0/3375
3	B4	0.27	0/2482	0.50	0/3375
3	BG	0.28	0/2482	0.50	0/3375
3	BN	0.28	0/2482	0.50	0/3375
3	BU	0.27	0/2482	0.50	0/3375
3	Bb	0.27	0/2482	0.50	0/3375
3	Bi	0.27	0/2482	0.50	0/3375
3	Bp	0.28	0/2482	0.50	0/3375
3	Bw	0.27	0/2482	0.50	0/3375
3	CA	0.27	0/2482	0.50	0/3375
3	CH	0.27	0/2482	0.50	0/3375
3	CO	0.28	0/2482	0.50	0/3375
3	CV	0.28	0/2482	0.50	0/3375
3	Cc	0.27	0/2482	0.50	0/3375
3	Cj	0.27	0/2482	0.50	0/3375
3	Cq	0.27	0/2482	0.50	0/3375
3	Cx	0.27	0/2482	0.50	0/3375
3	S	0.27	0/2482	0.50	0/3375

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	T	0.28	0/2482	0.50	0/3375
3	U	0.28	0/2482	0.50	0/3375
3	V	0.27	0/2482	0.50	0/3375
3	W	0.27	0/2482	0.50	0/3375
3	X	0.27	0/2482	0.50	0/3375
3	Y	0.28	0/2482	0.50	0/3375
3	g	0.27	0/2482	0.50	0/3375
4	3	0.23	0/2447	0.46	0/3300
4	8	0.23	0/2447	0.46	0/3300
4	A4	0.23	0/2447	0.46	0/3300
4	AM	0.23	0/2447	0.46	0/3300
4	AS	0.23	0/2447	0.46	0/3300
4	AY	0.23	0/2447	0.46	0/3300
4	Ae	0.23	0/2447	0.46	0/3300
4	Ak	0.23	0/2447	0.46	0/3300
4	Aq	0.23	0/2447	0.46	0/3300
4	Aw	0.23	0/2447	0.46	0/3300
4	B5	0.23	0/2447	0.46	0/3300
4	BA	0.23	0/2447	0.46	0/3300
4	BH	0.23	0/2447	0.46	0/3300
4	BO	0.23	0/2447	0.46	0/3300
4	BV	0.23	0/2447	0.46	0/3300
4	Bc	0.23	0/2447	0.46	0/3300
4	Bj	0.23	0/2447	0.46	0/3300
4	Bq	0.23	0/2447	0.46	0/3300
4	Bx	0.23	0/2447	0.46	0/3300
4	CB	0.23	0/2447	0.46	0/3300
4	CI	0.23	0/2447	0.46	0/3300
4	CP	0.23	0/2447	0.46	0/3300
4	CW	0.23	0/2447	0.46	0/3300
4	Cd	0.23	0/2447	0.46	0/3300
4	Ck	0.23	0/2447	0.46	0/3300
4	Cr	0.23	0/2447	0.46	0/3300
4	Cy	0.23	0/2447	0.46	0/3300
4	Z	0.23	0/2447	0.46	0/3300
4	a	0.23	0/2447	0.46	0/3300
4	b	0.23	0/2447	0.46	0/3300
4	c	0.23	0/2447	0.46	0/3300
4	d	0.23	0/2447	0.46	0/3300
4	e	0.23	0/2447	0.46	0/3300
4	f	0.23	0/2447	0.46	0/3300
5	4	0.24	0/1004	0.41	0/1349
5	9	0.24	0/1004	0.41	0/1349

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	A5	0.24	0/1004	0.40	0/1349
5	AN	0.24	0/1004	0.41	0/1349
5	AT	0.24	0/1004	0.41	0/1349
5	AZ	0.24	0/1004	0.41	0/1349
5	Af	0.24	0/1004	0.41	0/1349
5	Al	0.24	0/1004	0.41	0/1349
5	Ar	0.24	0/1004	0.41	0/1349
5	Ax	0.24	0/1004	0.41	0/1349
5	B6	0.24	0/1004	0.41	0/1349
5	BB	0.24	0/1004	0.41	0/1349
5	BI	0.24	0/1004	0.41	0/1349
5	BP	0.24	0/1004	0.41	0/1349
5	BW	0.24	0/1004	0.40	0/1349
5	Bd	0.24	0/1004	0.41	0/1349
5	Bk	0.24	0/1004	0.40	0/1349
5	Br	0.24	0/1004	0.41	0/1349
5	By	0.24	0/1004	0.41	0/1349
5	CC	0.24	0/1004	0.41	0/1349
5	CJ	0.24	0/1004	0.41	0/1349
5	CQ	0.24	0/1004	0.41	0/1349
5	CX	0.24	0/1004	0.41	0/1349
5	Ce	0.24	0/1004	0.41	0/1349
5	Cl	0.24	0/1004	0.41	0/1349
5	Cs	0.24	0/1004	0.41	0/1349
5	Cz	0.24	0/1004	0.40	0/1349
5	h	0.24	0/1004	0.41	0/1349
5	i	0.24	0/1004	0.41	0/1349
5	j	0.24	0/1004	0.41	0/1349
5	k	0.24	0/1004	0.40	0/1349
5	l	0.24	0/1004	0.41	0/1349
5	m	0.24	0/1004	0.40	0/1349
5	n	0.24	0/1004	0.41	0/1349
All	All	0.27	0/278664	0.49	0/376652

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	1
1	1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	1
1	5	0	1
1	6	0	1
1	A1	0	1
1	A6	0	1
1	A7	0	1
1	A8	0	1
1	AA	0	1
1	AB	0	1
1	AC	0	1
1	AD	0	1
1	AE	0	1
1	AF	0	1
1	AG	0	1
1	AH	0	1
1	AI	0	1
1	AJ	0	1
1	AK	0	1
1	AO	0	1
1	AP	0	1
1	AQ	0	1
1	AU	0	1
1	AV	0	1
1	AW	0	1
1	Aa	0	1
1	Ab	0	1
1	Ac	0	1
1	Ag	0	1
1	Ah	0	1
1	Ai	0	1
1	Am	0	1
1	An	0	1
1	Ao	0	1
1	As	0	1
1	At	0	1
1	Au	0	1
1	Ay	0	1
1	Az	0	1
1	B1	0	1
1	B2	0	1
1	B7	0	1
1	B8	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B9	0	1
1	BC	0	1
1	BD	0	1
1	BE	0	1
1	BJ	0	1
1	BK	0	1
1	BL	0	1
1	BQ	0	1
1	BR	0	1
1	BS	0	1
1	BX	0	1
1	BY	0	1
1	BZ	0	1
1	Be	0	1
1	Bf	0	1
1	Bg	0	1
1	Bl	0	1
1	Bm	0	1
1	Bn	0	1
1	Bs	0	1
1	Bt	0	1
1	Bu	0	1
1	Bz	0	1
1	C1	0	1
1	C2	0	1
1	CD	0	1
1	CE	0	1
1	CF	0	1
1	CK	0	1
1	CL	0	1
1	CM	0	1
1	CR	0	1
1	CS	0	1
1	CT	0	1
1	CY	0	1
1	CZ	0	1
1	Ca	0	1
1	Cf	0	1
1	Cg	0	1
1	Ch	0	1
1	Cm	0	1
1	Cn	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Co	0	1
1	Ct	0	1
1	Cu	0	1
1	Cv	0	1
1	o	0	1
1	p	0	1
1	q	0	1
1	r	0	1
1	s	0	1
1	t	0	1
1	u	0	1
1	v	0	1
1	w	0	1
1	x	0	1
1	y	0	1
1	z	0	1
3	7	0	2
3	A0	0	2
3	A3	0	2
3	AL	0	2
3	AR	0	2
3	AX	0	2
3	Ad	0	2
3	Aj	0	2
3	Ap	0	2
3	Av	0	2
3	B4	0	2
3	BG	0	2
3	BN	0	2
3	BU	0	2
3	Bb	0	2
3	Bi	0	2
3	Bp	0	2
3	Bw	0	2
3	CA	0	2
3	CH	0	2
3	CO	0	2
3	CV	0	2
3	Cc	0	2
3	Cj	0	2
3	Cq	0	2
3	Cx	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	S	0	2
3	T	0	2
3	U	0	2
3	V	0	2
3	W	0	2
3	X	0	2
3	Y	0	2
3	g	0	2
All	All	0	170

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (170) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	131	ARG	Sidechain
1	1	131	ARG	Sidechain
1	2	131	ARG	Sidechain
1	5	131	ARG	Sidechain
1	6	131	ARG	Sidechain
3	7	60	ARG	Sidechain
3	7	63	ARG	Sidechain
3	A0	60	ARG	Sidechain
3	A0	63	ARG	Sidechain
1	A1	131	ARG	Sidechain
3	A3	60	ARG	Sidechain
3	A3	63	ARG	Sidechain
1	A6	131	ARG	Sidechain
1	A7	131	ARG	Sidechain
1	A8	131	ARG	Sidechain
1	AA	131	ARG	Sidechain
1	AB	131	ARG	Sidechain
1	AC	131	ARG	Sidechain
1	AD	131	ARG	Sidechain
1	AE	131	ARG	Sidechain
1	AF	131	ARG	Sidechain
1	AG	131	ARG	Sidechain
1	AH	131	ARG	Sidechain
1	AI	131	ARG	Sidechain
1	AJ	131	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	AK	131	ARG	Sidechain
3	AL	60	ARG	Sidechain
3	AL	63	ARG	Sidechain
1	AO	131	ARG	Sidechain
1	AP	131	ARG	Sidechain
1	AQ	131	ARG	Sidechain
3	AR	60	ARG	Sidechain
3	AR	63	ARG	Sidechain
1	AU	131	ARG	Sidechain
1	AV	131	ARG	Sidechain
1	AW	131	ARG	Sidechain
3	AX	60	ARG	Sidechain
3	AX	63	ARG	Sidechain
1	Aa	131	ARG	Sidechain
1	Ab	131	ARG	Sidechain
1	Ac	131	ARG	Sidechain
3	Ad	60	ARG	Sidechain
3	Ad	63	ARG	Sidechain
1	Ag	131	ARG	Sidechain
1	Ah	131	ARG	Sidechain
1	Ai	131	ARG	Sidechain
3	Aj	60	ARG	Sidechain
3	Aj	63	ARG	Sidechain
1	Am	131	ARG	Sidechain
1	An	131	ARG	Sidechain
1	Ao	131	ARG	Sidechain
3	Ap	60	ARG	Sidechain
3	Ap	63	ARG	Sidechain
1	As	131	ARG	Sidechain
1	At	131	ARG	Sidechain
1	Au	131	ARG	Sidechain
3	Av	60	ARG	Sidechain
3	Av	63	ARG	Sidechain
1	Ay	131	ARG	Sidechain
1	Az	131	ARG	Sidechain
1	B1	131	ARG	Sidechain
1	B2	131	ARG	Sidechain
3	B4	60	ARG	Sidechain
3	B4	63	ARG	Sidechain
1	B7	131	ARG	Sidechain
1	B8	131	ARG	Sidechain
1	B9	131	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	BC	131	ARG	Sidechain
1	BD	131	ARG	Sidechain
1	BE	131	ARG	Sidechain
3	BG	60	ARG	Sidechain
3	BG	63	ARG	Sidechain
1	BJ	131	ARG	Sidechain
1	BK	131	ARG	Sidechain
1	BL	131	ARG	Sidechain
3	BN	60	ARG	Sidechain
3	BN	63	ARG	Sidechain
1	BQ	131	ARG	Sidechain
1	BR	131	ARG	Sidechain
1	BS	131	ARG	Sidechain
3	BU	60	ARG	Sidechain
3	BU	63	ARG	Sidechain
1	BX	131	ARG	Sidechain
1	BY	131	ARG	Sidechain
1	BZ	131	ARG	Sidechain
3	Bb	60	ARG	Sidechain
3	Bb	63	ARG	Sidechain
1	Be	131	ARG	Sidechain
1	Bf	131	ARG	Sidechain
1	Bg	131	ARG	Sidechain
3	Bi	60	ARG	Sidechain
3	Bi	63	ARG	Sidechain
1	Bl	131	ARG	Sidechain
1	Bm	131	ARG	Sidechain
1	Bn	131	ARG	Sidechain
3	Bp	60	ARG	Sidechain
3	Bp	63	ARG	Sidechain
1	Bs	131	ARG	Sidechain
1	Bt	131	ARG	Sidechain
1	Bu	131	ARG	Sidechain
3	Bw	60	ARG	Sidechain
3	Bw	63	ARG	Sidechain
1	Bz	131	ARG	Sidechain
1	C1	131	ARG	Sidechain
1	C2	131	ARG	Sidechain
3	CA	60	ARG	Sidechain
3	CA	63	ARG	Sidechain
1	CD	131	ARG	Sidechain
1	CE	131	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	CF	131	ARG	Sidechain
3	CH	60	ARG	Sidechain
3	CH	63	ARG	Sidechain
1	CK	131	ARG	Sidechain
1	CL	131	ARG	Sidechain
1	CM	131	ARG	Sidechain
3	CO	60	ARG	Sidechain
3	CO	63	ARG	Sidechain
1	CR	131	ARG	Sidechain
1	CS	131	ARG	Sidechain
1	CT	131	ARG	Sidechain
3	CV	60	ARG	Sidechain
3	CV	63	ARG	Sidechain
1	CY	131	ARG	Sidechain
1	CZ	131	ARG	Sidechain
1	Ca	131	ARG	Sidechain
3	Cc	60	ARG	Sidechain
3	Cc	63	ARG	Sidechain
1	Cf	131	ARG	Sidechain
1	Cg	131	ARG	Sidechain
1	Ch	131	ARG	Sidechain
3	Cj	60	ARG	Sidechain
3	Cj	63	ARG	Sidechain
1	Cm	131	ARG	Sidechain
1	Cn	131	ARG	Sidechain
1	Co	131	ARG	Sidechain
3	Cq	60	ARG	Sidechain
3	Cq	63	ARG	Sidechain
1	Ct	131	ARG	Sidechain
1	Cu	131	ARG	Sidechain
1	Cv	131	ARG	Sidechain
3	Cx	60	ARG	Sidechain
3	Cx	63	ARG	Sidechain
3	S	60	ARG	Sidechain
3	S	63	ARG	Sidechain
3	T	60	ARG	Sidechain
3	T	63	ARG	Sidechain
3	U	60	ARG	Sidechain
3	U	63	ARG	Sidechain
3	V	60	ARG	Sidechain
3	V	63	ARG	Sidechain
3	W	60	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	W	63	ARG	Sidechain
3	X	60	ARG	Sidechain
3	X	63	ARG	Sidechain
3	Y	60	ARG	Sidechain
3	Y	63	ARG	Sidechain
3	g	60	ARG	Sidechain
3	g	63	ARG	Sidechain
1	o	131	ARG	Sidechain
1	p	131	ARG	Sidechain
1	q	131	ARG	Sidechain
1	r	131	ARG	Sidechain
1	s	131	ARG	Sidechain
1	t	131	ARG	Sidechain
1	u	131	ARG	Sidechain
1	v	131	ARG	Sidechain
1	w	131	ARG	Sidechain
1	x	131	ARG	Sidechain
1	y	131	ARG	Sidechain
1	z	131	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	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	1	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	2	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	5	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	A1	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	A6	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	A7	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	A8	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AA	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AB	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AC	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AD	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AE	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AF	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AG	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AH	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AI	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	AJ	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	AK	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AO	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	AP	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	AQ	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	AU	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	AV	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	AW	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	Aa	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	Ab	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Ac	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	Ag	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	Ah	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Ai	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	Am	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	An	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Ao	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	As	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	At	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Au	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	Ay	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	Az	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	B1	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	B2	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	B7	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	B8	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	B9	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	BC	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	BD	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	BE	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	BJ	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	BK	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	BL	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	BQ	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	BR	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	BS	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	BX	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	BY	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	BZ	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	Be	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	Bf	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Bg	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	Bl	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	Bm	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Bn	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	Bs	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	Bt	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Bu	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bz	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	C1	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	C2	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	CD	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	CE	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	CF	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	CK	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	CL	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	CM	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	CR	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	CS	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	CT	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	CY	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	CZ	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Ca	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	Cf	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	Cg	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Ch	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	Cm	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	Cn	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Co	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	Ct	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	Cu	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	Cv	85/137 (62%)	80 (94%)	4 (5%)	1 (1%)	11	44
1	o	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	p	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	q	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	r	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	s	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	t	85/137 (62%)	78 (92%)	3 (4%)	4 (5%)	2	16
1	u	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	w	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	x	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	y	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
1	z	85/137 (62%)	81 (95%)	2 (2%)	2 (2%)	5	27
2	A2	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	A9	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	B0	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	B3	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	BF	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	BM	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	BT	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Ba	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Bh	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Bo	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Bv	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	C	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	CG	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	CN	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	CU	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Cb	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Ci	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Cp	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Cw	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	D	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	E	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	F	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	G	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	H	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	I	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	J	25/560 (4%)	24 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	L	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	M	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	N	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	O	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	P	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	Q	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
2	R	25/560 (4%)	24 (96%)	1 (4%)	0	100	100
3	7	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	A0	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	A3	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	AL	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	AR	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	AX	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Ad	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Aj	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Ap	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Av	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	B4	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	BG	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	BN	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	BU	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Bb	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Bi	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Bp	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Bw	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	CA	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	CH	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	CO	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	CV	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Cc	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Cj	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Cq	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Cx	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	S	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	T	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	U	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	V	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	W	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	X	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	Y	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
3	g	297/334 (89%)	285 (96%)	8 (3%)	4 (1%)	10	41
4	3	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	8	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	A4	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	AM	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	AS	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	AY	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Ae	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Ak	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Aq	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Aw	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	B5	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	BA	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	BH	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	BO	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	BV	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Bc	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Bj	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Bq	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Bx	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	CB	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CI	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	CP	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	CW	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Cd	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Ck	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Cr	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Cy	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	Z	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	a	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	b	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	c	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	d	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	e	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
4	f	306/331 (92%)	295 (96%)	10 (3%)	1 (0%)	37	72
5	4	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	9	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	A5	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	AN	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	AT	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	AZ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	Af	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	Al	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	Ar	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	Ax	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	B6	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	BB	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	BI	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	BP	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	BW	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	Bd	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	Bk	127/129 (98%)	125 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Br	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	By	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	CC	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	CJ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	CQ	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	CX	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	Ce	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	Cl	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	Cs	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	Cz	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	h	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	i	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	j	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	k	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	l	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	m	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
5	n	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
All	All	34340/60010 (57%)	32912 (96%)	1020 (3%)	408 (1%)	14	44

All (408) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	116	ASP
1	o	116	ASP
1	u	116	ASP
1	AA	116	ASP
1	p	116	ASP
1	v	116	ASP
1	AB	116	ASP
1	q	116	ASP
1	w	116	ASP
1	AC	116	ASP
1	r	116	ASP
1	x	116	ASP
1	AD	116	ASP
1	s	116	ASP

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Mol	Chain	Res	Type
1	y	116	ASP
1	AE	116	ASP
1	t	116	ASP
1	z	116	ASP
1	AF	116	ASP
1	1	116	ASP
1	2	116	ASP
1	AG	116	ASP
1	5	116	ASP
1	6	116	ASP
1	AH	116	ASP
1	AI	116	ASP
1	AJ	116	ASP
1	AK	116	ASP
1	AO	116	ASP
1	AP	116	ASP
1	AQ	116	ASP
1	AU	116	ASP
1	AV	116	ASP
1	AW	116	ASP
1	Aa	116	ASP
1	Ab	116	ASP
1	Ac	116	ASP
1	Ag	116	ASP
1	Ah	116	ASP
1	Ai	116	ASP
1	Am	116	ASP
1	An	116	ASP
1	Ao	116	ASP
1	As	116	ASP
1	At	116	ASP
1	Au	116	ASP
1	Ay	116	ASP
1	Az	116	ASP
1	A1	116	ASP
1	A6	116	ASP
1	A7	116	ASP
1	A8	116	ASP
1	BC	116	ASP
1	BD	116	ASP
1	BE	116	ASP
1	BJ	116	ASP

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Mol	Chain	Res	Type
1	BK	116	ASP
1	BL	116	ASP
1	BQ	116	ASP
1	BR	116	ASP
1	BS	116	ASP
1	BX	116	ASP
1	BY	116	ASP
1	BZ	116	ASP
1	Be	116	ASP
1	Bf	116	ASP
1	Bg	116	ASP
1	Bl	116	ASP
1	Bm	116	ASP
1	Bn	116	ASP
1	Bs	116	ASP
1	Bt	116	ASP
1	Bu	116	ASP
1	Bz	116	ASP
1	B1	116	ASP
1	B2	116	ASP
1	B7	116	ASP
1	B8	116	ASP
1	B9	116	ASP
1	CD	116	ASP
1	CE	116	ASP
1	CF	116	ASP
1	CK	116	ASP
1	CL	116	ASP
1	CM	116	ASP
1	CR	116	ASP
1	CS	116	ASP
1	CT	116	ASP
1	CY	116	ASP
1	CZ	116	ASP
1	Ca	116	ASP
1	Cf	116	ASP
1	Cg	116	ASP
1	Ch	116	ASP
1	Cm	116	ASP
1	Cn	116	ASP
1	Co	116	ASP
1	Ct	116	ASP

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Mol	Chain	Res	Type
1	Cu	116	ASP
1	Cv	116	ASP
1	C1	116	ASP
1	C2	116	ASP
3	S	232	VAL
1	o	125	ILE
1	o	126	ILE
3	T	232	VAL
1	p	125	ILE
1	p	126	ILE
3	U	232	VAL
1	q	125	ILE
1	q	126	ILE
3	V	232	VAL
1	r	125	ILE
1	r	126	ILE
3	W	232	VAL
1	s	125	ILE
1	s	126	ILE
3	X	232	VAL
1	t	125	ILE
1	t	126	ILE
3	Y	232	VAL
1	l	125	ILE
1	l	126	ILE
3	g	232	VAL
1	5	125	ILE
1	5	126	ILE
3	7	232	VAL
1	AI	125	ILE
1	AI	126	ILE
3	AL	232	VAL
1	AO	125	ILE
1	AO	126	ILE
3	AR	232	VAL
1	AU	125	ILE
1	AU	126	ILE
3	AX	232	VAL
1	Aa	125	ILE
1	Aa	126	ILE
3	Ad	232	VAL
1	Ag	125	ILE

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Mol	Chain	Res	Type
1	Ag	126	ILE
3	Aj	232	VAL
1	Am	125	ILE
1	Am	126	ILE
3	Ap	232	VAL
1	As	125	ILE
1	As	126	ILE
3	Av	232	VAL
1	Ay	125	ILE
1	Ay	126	ILE
3	A3	232	VAL
1	A6	125	ILE
1	A6	126	ILE
3	A0	232	VAL
1	BC	125	ILE
1	BC	126	ILE
3	BG	232	VAL
1	BJ	125	ILE
1	BJ	126	ILE
3	BN	232	VAL
1	BQ	125	ILE
1	BQ	126	ILE
3	BU	232	VAL
1	BX	125	ILE
1	BX	126	ILE
3	Bb	232	VAL
1	Be	125	ILE
1	Be	126	ILE
3	Bi	232	VAL
1	Bl	125	ILE
1	Bl	126	ILE
3	Bp	232	VAL
1	Bs	125	ILE
1	Bs	126	ILE
3	Bw	232	VAL
1	Bz	125	ILE
1	Bz	126	ILE
3	B4	232	VAL
1	B7	125	ILE
1	B7	126	ILE
3	CA	232	VAL
1	CD	125	ILE

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Mol	Chain	Res	Type
1	CD	126	ILE
3	CH	232	VAL
1	CK	125	ILE
1	CK	126	ILE
3	CO	232	VAL
1	CR	125	ILE
1	CR	126	ILE
3	CV	232	VAL
1	CY	125	ILE
1	CY	126	ILE
3	Cc	232	VAL
1	Cf	125	ILE
1	Cf	126	ILE
3	Cj	232	VAL
1	Cm	125	ILE
1	Cm	126	ILE
3	Cq	232	VAL
1	Ct	125	ILE
1	Ct	126	ILE
3	Cx	232	VAL
1	C1	125	ILE
1	C1	126	ILE
1	o	59	ASP
1	p	59	ASP
1	q	59	ASP
1	r	59	ASP
1	s	59	ASP
1	t	59	ASP
1	1	59	ASP
1	5	59	ASP
1	AI	59	ASP
1	AO	59	ASP
1	AU	59	ASP
1	Aa	59	ASP
1	Ag	59	ASP
1	Am	59	ASP
1	As	59	ASP
1	Ay	59	ASP
1	A6	59	ASP
1	BC	59	ASP
1	BJ	59	ASP
1	BQ	59	ASP

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Mol	Chain	Res	Type
1	BX	59	ASP
1	Be	59	ASP
1	Bl	59	ASP
1	Bs	59	ASP
1	Bz	59	ASP
1	B7	59	ASP
1	CD	59	ASP
1	CK	59	ASP
1	CR	59	ASP
1	CY	59	ASP
1	Cf	59	ASP
1	Cm	59	ASP
1	Ct	59	ASP
1	C1	59	ASP
3	S	236	LEU
4	Z	97	ILE
3	T	236	LEU
4	a	97	ILE
3	U	236	LEU
4	b	97	ILE
3	V	236	LEU
4	c	97	ILE
3	W	236	LEU
4	d	97	ILE
3	X	236	LEU
4	e	97	ILE
3	Y	236	LEU
4	f	97	ILE
3	g	236	LEU
4	3	97	ILE
3	7	236	LEU
4	8	97	ILE
3	AL	236	LEU
4	AM	97	ILE
3	AR	236	LEU
4	AS	97	ILE
3	AX	236	LEU
4	AY	97	ILE
3	Ad	236	LEU
4	Ae	97	ILE
3	Aj	236	LEU
4	Ak	97	ILE

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Mol	Chain	Res	Type
3	Ap	236	LEU
4	Aq	97	ILE
3	Av	236	LEU
4	Aw	97	ILE
3	A3	236	LEU
4	A4	97	ILE
3	A0	236	LEU
4	BA	97	ILE
3	BG	236	LEU
4	BH	97	ILE
3	BN	236	LEU
4	BO	97	ILE
3	BU	236	LEU
4	BV	97	ILE
3	Bb	236	LEU
4	Bc	97	ILE
3	Bi	236	LEU
4	Bj	97	ILE
3	Bp	236	LEU
4	Bq	97	ILE
3	Bw	236	LEU
4	Bx	97	ILE
3	B4	236	LEU
4	B5	97	ILE
3	CA	236	LEU
4	CB	97	ILE
3	CH	236	LEU
4	CI	97	ILE
3	CO	236	LEU
4	CP	97	ILE
3	CV	236	LEU
4	CW	97	ILE
3	Cc	236	LEU
4	Cd	97	ILE
3	Cj	236	LEU
4	Ck	97	ILE
3	Cq	236	LEU
4	Cr	97	ILE
3	Cx	236	LEU
4	Cy	97	ILE
3	T	237	GLU
3	V	237	GLU

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Mol	Chain	Res	Type
3	X	237	GLU
3	g	237	GLU
3	AX	237	GLU
3	BG	237	GLU
3	BU	237	GLU
3	Bi	237	GLU
3	Bw	237	GLU
3	CO	237	GLU
3	S	235	PRO
3	S	237	GLU
1	u	127	THR
3	T	235	PRO
1	v	127	THR
3	U	235	PRO
3	U	237	GLU
1	w	127	THR
3	V	235	PRO
1	x	127	THR
3	W	235	PRO
3	W	237	GLU
1	y	127	THR
3	X	235	PRO
1	z	127	THR
3	Y	235	PRO
3	Y	237	GLU
1	2	127	THR
3	g	235	PRO
1	6	127	THR
3	7	235	PRO
3	7	237	GLU
1	AJ	127	THR
3	AL	235	PRO
3	AL	237	GLU
1	AP	127	THR
3	AR	235	PRO
3	AR	237	GLU
1	AV	127	THR
3	AX	235	PRO
1	Ab	127	THR
3	Ad	235	PRO
3	Ad	237	GLU
1	Ah	127	THR

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Mol	Chain	Res	Type
3	Aj	235	PRO
3	Aj	237	GLU
1	An	127	THR
3	Ap	235	PRO
3	Ap	237	GLU
1	At	127	THR
3	Av	235	PRO
3	Av	237	GLU
1	Az	127	THR
3	A3	235	PRO
3	A3	237	GLU
1	A7	127	THR
3	A0	235	PRO
3	A0	237	GLU
1	BD	127	THR
3	BG	235	PRO
1	BK	127	THR
3	BN	235	PRO
3	BN	237	GLU
1	BR	127	THR
3	BU	235	PRO
1	BY	127	THR
3	Bb	235	PRO
3	Bb	237	GLU
1	Bf	127	THR
3	Bi	235	PRO
1	Bm	127	THR
3	Bp	235	PRO
3	Bp	237	GLU
1	Bt	127	THR
3	Bw	235	PRO
1	B1	127	THR
3	B4	235	PRO
3	B4	237	GLU
1	B8	127	THR
3	CA	235	PRO
3	CA	237	GLU
1	CE	127	THR
3	CH	235	PRO
3	CH	237	GLU
1	CL	127	THR
3	CO	235	PRO

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Mol	Chain	Res	Type
1	CS	127	THR
3	CV	235	PRO
3	CV	237	GLU
1	CZ	127	THR
3	Cc	235	PRO
3	Cc	237	GLU
1	Cg	127	THR
3	Cj	235	PRO
3	Cj	237	GLU
1	Cn	127	THR
3	Cq	235	PRO
3	Cq	237	GLU
1	Cu	127	THR
3	Cx	235	PRO
3	Cx	237	GLU
1	C2	127	THR

5.3.2 Protein sidechains ⓘ

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	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	1	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	2	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	5	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	6	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	A1	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	A6	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	A7	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	A8	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	AA	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	AB	76/113 (67%)	74 (97%)	2 (3%)	41	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	AD	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	AE	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	AF	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	AG	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	AH	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	AI	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	AJ	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	AK	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	AO	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	AP	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	AQ	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	AU	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	AV	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	AW	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Aa	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	Ab	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Ac	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Ag	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	Ah	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Ai	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Am	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	An	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Ao	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	As	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	At	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Au	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Ay	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	Az	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	B1	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	B2	76/113 (67%)	74 (97%)	2 (3%)	41	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B7	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	B8	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	B9	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	BC	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	BD	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	BE	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	BJ	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	BK	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	BL	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	BQ	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	BR	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	BS	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	BX	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	BY	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	BZ	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Be	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	Bf	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Bg	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Bl	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	Bm	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Bn	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Bs	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	Bt	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Bu	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Bz	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	C1	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	C2	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	CD	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	CE	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	CF	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	CK	76/113 (67%)	72 (95%)	4 (5%)	19	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CL	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	CM	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	CR	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	CS	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	CT	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	CY	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	CZ	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Ca	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Cf	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	Cg	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Ch	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Cm	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	Cn	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Co	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	Ct	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	Cu	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	Cv	76/113 (67%)	74 (97%)	2 (3%)	41	59
1	o	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	p	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	q	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	r	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	s	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	t	76/113 (67%)	72 (95%)	4 (5%)	19	40
1	u	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	v	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	w	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	x	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	y	76/113 (67%)	75 (99%)	1 (1%)	65	76
1	z	76/113 (67%)	75 (99%)	1 (1%)	65	76
2	A2	26/467 (6%)	26 (100%)	0	100	100
2	A9	26/467 (6%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B0	26/467 (6%)	26 (100%)	0	100	100
2	B3	26/467 (6%)	26 (100%)	0	100	100
2	BF	26/467 (6%)	26 (100%)	0	100	100
2	BM	26/467 (6%)	26 (100%)	0	100	100
2	BT	26/467 (6%)	26 (100%)	0	100	100
2	Ba	26/467 (6%)	26 (100%)	0	100	100
2	Bh	26/467 (6%)	26 (100%)	0	100	100
2	Bo	26/467 (6%)	26 (100%)	0	100	100
2	Bv	26/467 (6%)	26 (100%)	0	100	100
2	C	26/467 (6%)	26 (100%)	0	100	100
2	CG	26/467 (6%)	26 (100%)	0	100	100
2	CN	26/467 (6%)	26 (100%)	0	100	100
2	CU	26/467 (6%)	26 (100%)	0	100	100
2	Cb	26/467 (6%)	26 (100%)	0	100	100
2	Ci	26/467 (6%)	26 (100%)	0	100	100
2	Cp	26/467 (6%)	26 (100%)	0	100	100
2	Cw	26/467 (6%)	26 (100%)	0	100	100
2	D	26/467 (6%)	26 (100%)	0	100	100
2	E	26/467 (6%)	26 (100%)	0	100	100
2	F	26/467 (6%)	26 (100%)	0	100	100
2	G	26/467 (6%)	26 (100%)	0	100	100
2	H	26/467 (6%)	26 (100%)	0	100	100
2	I	26/467 (6%)	26 (100%)	0	100	100
2	J	26/467 (6%)	26 (100%)	0	100	100
2	K	26/467 (6%)	26 (100%)	0	100	100
2	L	26/467 (6%)	26 (100%)	0	100	100
2	M	26/467 (6%)	26 (100%)	0	100	100
2	N	26/467 (6%)	26 (100%)	0	100	100
2	O	26/467 (6%)	26 (100%)	0	100	100
2	P	26/467 (6%)	26 (100%)	0	100	100
2	Q	26/467 (6%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	26/467 (6%)	26 (100%)	0	100	100
3	7	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	A0	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	A3	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	AL	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	AR	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	AX	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Ad	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Aj	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Ap	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Av	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	B4	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	BG	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	BN	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	BU	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Bb	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Bi	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Bp	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Bw	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	CA	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	CH	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	CO	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	CV	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Cc	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Cj	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Cq	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Cx	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	S	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	T	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	U	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	V	272/301 (90%)	264 (97%)	8 (3%)	37	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	W	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	X	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	Y	272/301 (90%)	264 (97%)	8 (3%)	37	56
3	g	272/301 (90%)	264 (97%)	8 (3%)	37	56
4	3	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	8	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	A4	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	AM	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	AS	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	AY	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Ae	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Ak	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Aq	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Aw	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	B5	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	BA	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	BH	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	BO	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	BV	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Bc	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Bj	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Bq	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Bx	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	CB	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	CI	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	CP	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	CW	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Cd	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Ck	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Cr	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	Cy	265/282 (94%)	257 (97%)	8 (3%)	36	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Z	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	a	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	b	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	c	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	d	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	e	265/282 (94%)	257 (97%)	8 (3%)	36	55
4	f	265/282 (94%)	257 (97%)	8 (3%)	36	55
5	4	104/104 (100%)	104 (100%)	0	100	100
5	9	104/104 (100%)	104 (100%)	0	100	100
5	A5	104/104 (100%)	104 (100%)	0	100	100
5	AN	104/104 (100%)	104 (100%)	0	100	100
5	AT	104/104 (100%)	104 (100%)	0	100	100
5	AZ	104/104 (100%)	104 (100%)	0	100	100
5	Af	104/104 (100%)	104 (100%)	0	100	100
5	Al	104/104 (100%)	104 (100%)	0	100	100
5	Ar	104/104 (100%)	104 (100%)	0	100	100
5	Ax	104/104 (100%)	104 (100%)	0	100	100
5	B6	104/104 (100%)	104 (100%)	0	100	100
5	BB	104/104 (100%)	104 (100%)	0	100	100
5	BI	104/104 (100%)	104 (100%)	0	100	100
5	BP	104/104 (100%)	104 (100%)	0	100	100
5	BW	104/104 (100%)	104 (100%)	0	100	100
5	Bd	104/104 (100%)	104 (100%)	0	100	100
5	Bk	104/104 (100%)	104 (100%)	0	100	100
5	Br	104/104 (100%)	104 (100%)	0	100	100
5	By	104/104 (100%)	104 (100%)	0	100	100
5	CC	104/104 (100%)	104 (100%)	0	100	100
5	CJ	104/104 (100%)	104 (100%)	0	100	100
5	CQ	104/104 (100%)	104 (100%)	0	100	100
5	CX	104/104 (100%)	104 (100%)	0	100	100
5	Ce	104/104 (100%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Cl	104/104 (100%)	104 (100%)	0	100	100
5	Cs	104/104 (100%)	104 (100%)	0	100	100
5	Cz	104/104 (100%)	104 (100%)	0	100	100
5	h	104/104 (100%)	104 (100%)	0	100	100
5	i	104/104 (100%)	104 (100%)	0	100	100
5	j	104/104 (100%)	104 (100%)	0	100	100
5	k	104/104 (100%)	104 (100%)	0	100	100
5	l	104/104 (100%)	104 (100%)	0	100	100
5	m	104/104 (100%)	104 (100%)	0	100	100
5	n	104/104 (100%)	104 (100%)	0	100	100
All	All	30430/50762 (60%)	29648 (97%)	782 (3%)	42	59

All (782) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	106	ILE
1	0	132	MET
3	S	43	GLN
3	S	47	VAL
3	S	66	ARG
3	S	140	LYS
3	S	155	ASN
3	S	236	LEU
3	S	237	GLU
3	S	286	ILE
4	Z	46	GLN
4	Z	50	LYS
4	Z	61	GLN
4	Z	98	LEU
4	Z	101	ARG
4	Z	193	MET
4	Z	234	PHE
4	Z	235	LEU
1	o	53	ASP
1	o	56	LEU
1	o	58	MET
1	o	106	ILE
1	u	106	ILE

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Mol	Chain	Res	Type
1	AA	106	ILE
1	AA	132	MET
3	T	43	GLN
3	T	47	VAL
3	T	66	ARG
3	T	140	LYS
3	T	155	ASN
3	T	236	LEU
3	T	237	GLU
3	T	286	ILE
4	a	46	GLN
4	a	50	LYS
4	a	61	GLN
4	a	98	LEU
4	a	101	ARG
4	a	193	MET
4	a	234	PHE
4	a	235	LEU
1	p	53	ASP
1	p	56	LEU
1	p	58	MET
1	p	106	ILE
1	v	106	ILE
1	AB	106	ILE
1	AB	132	MET
3	U	43	GLN
3	U	47	VAL
3	U	66	ARG
3	U	140	LYS
3	U	155	ASN
3	U	236	LEU
3	U	237	GLU
3	U	286	ILE
4	b	46	GLN
4	b	50	LYS
4	b	61	GLN
4	b	98	LEU
4	b	101	ARG
4	b	193	MET
4	b	234	PHE
4	b	235	LEU
1	q	53	ASP

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Mol	Chain	Res	Type
1	q	56	LEU
1	q	58	MET
1	q	106	ILE
1	w	106	ILE
1	AC	106	ILE
1	AC	132	MET
3	V	43	GLN
3	V	47	VAL
3	V	66	ARG
3	V	140	LYS
3	V	155	ASN
3	V	236	LEU
3	V	237	GLU
3	V	286	ILE
4	c	46	GLN
4	c	50	LYS
4	c	61	GLN
4	c	98	LEU
4	c	101	ARG
4	c	193	MET
4	c	234	PHE
4	c	235	LEU
1	r	53	ASP
1	r	56	LEU
1	r	58	MET
1	r	106	ILE
1	x	106	ILE
1	AD	106	ILE
1	AD	132	MET
3	W	43	GLN
3	W	47	VAL
3	W	66	ARG
3	W	140	LYS
3	W	155	ASN
3	W	236	LEU
3	W	237	GLU
3	W	286	ILE
4	d	46	GLN
4	d	50	LYS
4	d	61	GLN
4	d	98	LEU
4	d	101	ARG

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Mol	Chain	Res	Type
4	d	193	MET
4	d	234	PHE
4	d	235	LEU
1	s	53	ASP
1	s	56	LEU
1	s	58	MET
1	s	106	ILE
1	y	106	ILE
1	AE	106	ILE
1	AE	132	MET
3	X	43	GLN
3	X	47	VAL
3	X	66	ARG
3	X	140	LYS
3	X	155	ASN
3	X	236	LEU
3	X	237	GLU
3	X	286	ILE
4	e	46	GLN
4	e	50	LYS
4	e	61	GLN
4	e	98	LEU
4	e	101	ARG
4	e	193	MET
4	e	234	PHE
4	e	235	LEU
1	t	53	ASP
1	t	56	LEU
1	t	58	MET
1	t	106	ILE
1	z	106	ILE
1	AF	106	ILE
1	AF	132	MET
3	Y	43	GLN
3	Y	47	VAL
3	Y	66	ARG
3	Y	140	LYS
3	Y	155	ASN
3	Y	236	LEU
3	Y	237	GLU
3	Y	286	ILE
4	f	46	GLN

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Mol	Chain	Res	Type
4	f	50	LYS
4	f	61	GLN
4	f	98	LEU
4	f	101	ARG
4	f	193	MET
4	f	234	PHE
4	f	235	LEU
1	1	53	ASP
1	1	56	LEU
1	1	58	MET
1	1	106	ILE
1	2	106	ILE
1	AG	106	ILE
1	AG	132	MET
3	g	43	GLN
3	g	47	VAL
3	g	66	ARG
3	g	140	LYS
3	g	155	ASN
3	g	236	LEU
3	g	237	GLU
3	g	286	ILE
4	3	46	GLN
4	3	50	LYS
4	3	61	GLN
4	3	98	LEU
4	3	101	ARG
4	3	193	MET
4	3	234	PHE
4	3	235	LEU
1	5	53	ASP
1	5	56	LEU
1	5	58	MET
1	5	106	ILE
1	6	106	ILE
1	AH	106	ILE
1	AH	132	MET
3	7	43	GLN
3	7	47	VAL
3	7	66	ARG
3	7	140	LYS
3	7	155	ASN

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Mol	Chain	Res	Type
3	7	236	LEU
3	7	237	GLU
3	7	286	ILE
4	8	46	GLN
4	8	50	LYS
4	8	61	GLN
4	8	98	LEU
4	8	101	ARG
4	8	193	MET
4	8	234	PHE
4	8	235	LEU
1	AI	53	ASP
1	AI	56	LEU
1	AI	58	MET
1	AI	106	ILE
1	AJ	106	ILE
1	AK	106	ILE
1	AK	132	MET
3	AL	43	GLN
3	AL	47	VAL
3	AL	66	ARG
3	AL	140	LYS
3	AL	155	ASN
3	AL	236	LEU
3	AL	237	GLU
3	AL	286	ILE
4	AM	46	GLN
4	AM	50	LYS
4	AM	61	GLN
4	AM	98	LEU
4	AM	101	ARG
4	AM	193	MET
4	AM	234	PHE
4	AM	235	LEU
1	AO	53	ASP
1	AO	56	LEU
1	AO	58	MET
1	AO	106	ILE
1	AP	106	ILE
1	AQ	106	ILE
1	AQ	132	MET
3	AR	43	GLN

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Mol	Chain	Res	Type
3	AR	47	VAL
3	AR	66	ARG
3	AR	140	LYS
3	AR	155	ASN
3	AR	236	LEU
3	AR	237	GLU
3	AR	286	ILE
4	AS	46	GLN
4	AS	50	LYS
4	AS	61	GLN
4	AS	98	LEU
4	AS	101	ARG
4	AS	193	MET
4	AS	234	PHE
4	AS	235	LEU
1	AU	53	ASP
1	AU	56	LEU
1	AU	58	MET
1	AU	106	ILE
1	AV	106	ILE
1	AW	106	ILE
1	AW	132	MET
3	AX	43	GLN
3	AX	47	VAL
3	AX	66	ARG
3	AX	140	LYS
3	AX	155	ASN
3	AX	236	LEU
3	AX	237	GLU
3	AX	286	ILE
4	AY	46	GLN
4	AY	50	LYS
4	AY	61	GLN
4	AY	98	LEU
4	AY	101	ARG
4	AY	193	MET
4	AY	234	PHE
4	AY	235	LEU
1	Aa	53	ASP
1	Aa	56	LEU
1	Aa	58	MET
1	Aa	106	ILE

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Mol	Chain	Res	Type
1	Ab	106	ILE
1	Ac	106	ILE
1	Ac	132	MET
3	Ad	43	GLN
3	Ad	47	VAL
3	Ad	66	ARG
3	Ad	140	LYS
3	Ad	155	ASN
3	Ad	236	LEU
3	Ad	237	GLU
3	Ad	286	ILE
4	Ae	46	GLN
4	Ae	50	LYS
4	Ae	61	GLN
4	Ae	98	LEU
4	Ae	101	ARG
4	Ae	193	MET
4	Ae	234	PHE
4	Ae	235	LEU
1	Ag	53	ASP
1	Ag	56	LEU
1	Ag	58	MET
1	Ag	106	ILE
1	Ah	106	ILE
1	Ai	106	ILE
1	Ai	132	MET
3	Aj	43	GLN
3	Aj	47	VAL
3	Aj	66	ARG
3	Aj	140	LYS
3	Aj	155	ASN
3	Aj	236	LEU
3	Aj	237	GLU
3	Aj	286	ILE
4	Ak	46	GLN
4	Ak	50	LYS
4	Ak	61	GLN
4	Ak	98	LEU
4	Ak	101	ARG
4	Ak	193	MET
4	Ak	234	PHE
4	Ak	235	LEU

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Mol	Chain	Res	Type
1	Am	53	ASP
1	Am	56	LEU
1	Am	58	MET
1	Am	106	ILE
1	An	106	ILE
1	Ao	106	ILE
1	Ao	132	MET
3	Ap	43	GLN
3	Ap	47	VAL
3	Ap	66	ARG
3	Ap	140	LYS
3	Ap	155	ASN
3	Ap	236	LEU
3	Ap	237	GLU
3	Ap	286	ILE
4	Aq	46	GLN
4	Aq	50	LYS
4	Aq	61	GLN
4	Aq	98	LEU
4	Aq	101	ARG
4	Aq	193	MET
4	Aq	234	PHE
4	Aq	235	LEU
1	As	53	ASP
1	As	56	LEU
1	As	58	MET
1	As	106	ILE
1	At	106	ILE
1	Au	106	ILE
1	Au	132	MET
3	Av	43	GLN
3	Av	47	VAL
3	Av	66	ARG
3	Av	140	LYS
3	Av	155	ASN
3	Av	236	LEU
3	Av	237	GLU
3	Av	286	ILE
4	Aw	46	GLN
4	Aw	50	LYS
4	Aw	61	GLN
4	Aw	98	LEU

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Mol	Chain	Res	Type
4	Aw	101	ARG
4	Aw	193	MET
4	Aw	234	PHE
4	Aw	235	LEU
1	Ay	53	ASP
1	Ay	56	LEU
1	Ay	58	MET
1	Ay	106	ILE
1	Az	106	ILE
1	A1	106	ILE
1	A1	132	MET
3	A3	43	GLN
3	A3	47	VAL
3	A3	66	ARG
3	A3	140	LYS
3	A3	155	ASN
3	A3	236	LEU
3	A3	237	GLU
3	A3	286	ILE
4	A4	46	GLN
4	A4	50	LYS
4	A4	61	GLN
4	A4	98	LEU
4	A4	101	ARG
4	A4	193	MET
4	A4	234	PHE
4	A4	235	LEU
1	A6	53	ASP
1	A6	56	LEU
1	A6	58	MET
1	A6	106	ILE
1	A7	106	ILE
1	A8	106	ILE
1	A8	132	MET
3	A0	43	GLN
3	A0	47	VAL
3	A0	66	ARG
3	A0	140	LYS
3	A0	155	ASN
3	A0	236	LEU
3	A0	237	GLU
3	A0	286	ILE

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Mol	Chain	Res	Type
4	BA	46	GLN
4	BA	50	LYS
4	BA	61	GLN
4	BA	98	LEU
4	BA	101	ARG
4	BA	193	MET
4	BA	234	PHE
4	BA	235	LEU
1	BC	53	ASP
1	BC	56	LEU
1	BC	58	MET
1	BC	106	ILE
1	BD	106	ILE
1	BE	106	ILE
1	BE	132	MET
3	BG	43	GLN
3	BG	47	VAL
3	BG	66	ARG
3	BG	140	LYS
3	BG	155	ASN
3	BG	236	LEU
3	BG	237	GLU
3	BG	286	ILE
4	BH	46	GLN
4	BH	50	LYS
4	BH	61	GLN
4	BH	98	LEU
4	BH	101	ARG
4	BH	193	MET
4	BH	234	PHE
4	BH	235	LEU
1	BJ	53	ASP
1	BJ	56	LEU
1	BJ	58	MET
1	BJ	106	ILE
1	BK	106	ILE
1	BL	106	ILE
1	BL	132	MET
3	BN	43	GLN
3	BN	47	VAL
3	BN	66	ARG
3	BN	140	LYS

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Mol	Chain	Res	Type
3	BN	155	ASN
3	BN	236	LEU
3	BN	237	GLU
3	BN	286	ILE
4	BO	46	GLN
4	BO	50	LYS
4	BO	61	GLN
4	BO	98	LEU
4	BO	101	ARG
4	BO	193	MET
4	BO	234	PHE
4	BO	235	LEU
1	BQ	53	ASP
1	BQ	56	LEU
1	BQ	58	MET
1	BQ	106	ILE
1	BR	106	ILE
1	BS	106	ILE
1	BS	132	MET
3	BU	43	GLN
3	BU	47	VAL
3	BU	66	ARG
3	BU	140	LYS
3	BU	155	ASN
3	BU	236	LEU
3	BU	237	GLU
3	BU	286	ILE
4	BV	46	GLN
4	BV	50	LYS
4	BV	61	GLN
4	BV	98	LEU
4	BV	101	ARG
4	BV	193	MET
4	BV	234	PHE
4	BV	235	LEU
1	BX	53	ASP
1	BX	56	LEU
1	BX	58	MET
1	BX	106	ILE
1	BY	106	ILE
1	BZ	106	ILE
1	BZ	132	MET

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Mol	Chain	Res	Type
3	Bb	43	GLN
3	Bb	47	VAL
3	Bb	66	ARG
3	Bb	140	LYS
3	Bb	155	ASN
3	Bb	236	LEU
3	Bb	237	GLU
3	Bb	286	ILE
4	Bc	46	GLN
4	Bc	50	LYS
4	Bc	61	GLN
4	Bc	98	LEU
4	Bc	101	ARG
4	Bc	193	MET
4	Bc	234	PHE
4	Bc	235	LEU
1	Be	53	ASP
1	Be	56	LEU
1	Be	58	MET
1	Be	106	ILE
1	Bf	106	ILE
1	Bg	106	ILE
1	Bg	132	MET
3	Bi	43	GLN
3	Bi	47	VAL
3	Bi	66	ARG
3	Bi	140	LYS
3	Bi	155	ASN
3	Bi	236	LEU
3	Bi	237	GLU
3	Bi	286	ILE
4	Bj	46	GLN
4	Bj	50	LYS
4	Bj	61	GLN
4	Bj	98	LEU
4	Bj	101	ARG
4	Bj	193	MET
4	Bj	234	PHE
4	Bj	235	LEU
1	Bl	53	ASP
1	Bl	56	LEU
1	Bl	58	MET

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

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Mol	Chain	Res	Type
4	Bx	235	LEU
1	Bz	53	ASP
1	Bz	56	LEU
1	Bz	58	MET
1	Bz	106	ILE
1	B1	106	ILE
1	B2	106	ILE
1	B2	132	MET
3	B4	43	GLN
3	B4	47	VAL
3	B4	66	ARG
3	B4	140	LYS
3	B4	155	ASN
3	B4	236	LEU
3	B4	237	GLU
3	B4	286	ILE
4	B5	46	GLN
4	B5	50	LYS
4	B5	61	GLN
4	B5	98	LEU
4	B5	101	ARG
4	B5	193	MET
4	B5	234	PHE
4	B5	235	LEU
1	B7	53	ASP
1	B7	56	LEU
1	B7	58	MET
1	B7	106	ILE
1	B8	106	ILE
1	B9	106	ILE
1	B9	132	MET
3	CA	43	GLN
3	CA	47	VAL
3	CA	66	ARG
3	CA	140	LYS
3	CA	155	ASN
3	CA	236	LEU
3	CA	237	GLU
3	CA	286	ILE
4	CB	46	GLN
4	CB	50	LYS
4	CB	61	GLN

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

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

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

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Mol	Chain	Res	Type
1	Co	132	MET
3	Cq	43	GLN
3	Cq	47	VAL
3	Cq	66	ARG
3	Cq	140	LYS
3	Cq	155	ASN
3	Cq	236	LEU
3	Cq	237	GLU
3	Cq	286	ILE
4	Cr	46	GLN
4	Cr	50	LYS
4	Cr	61	GLN
4	Cr	98	LEU
4	Cr	101	ARG
4	Cr	193	MET
4	Cr	234	PHE
4	Cr	235	LEU
1	Ct	53	ASP
1	Ct	56	LEU
1	Ct	58	MET
1	Ct	106	ILE
1	Cu	106	ILE
1	Cv	106	ILE
1	Cv	132	MET
3	Cx	43	GLN
3	Cx	47	VAL
3	Cx	66	ARG
3	Cx	140	LYS
3	Cx	155	ASN
3	Cx	236	LEU
3	Cx	237	GLU
3	Cx	286	ILE
4	Cy	46	GLN
4	Cy	50	LYS
4	Cy	61	GLN
4	Cy	98	LEU
4	Cy	101	ARG
4	Cy	193	MET
4	Cy	234	PHE
4	Cy	235	LEU
1	C1	53	ASP
1	C1	56	LEU

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Mol	Chain	Res	Type
1	C1	58	MET
1	C1	106	ILE
1	C2	106	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (204) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	542	ASN
3	S	8	GLN
3	S	238	ASN
3	S	245	ASN
4	Z	46	GLN
4	Z	186	GLN
2	D	542	ASN
3	T	8	GLN
3	T	238	ASN
3	T	245	ASN
4	a	46	GLN
4	a	186	GLN
2	E	542	ASN
3	U	8	GLN
3	U	238	ASN
3	U	245	ASN
4	b	46	GLN
4	b	186	GLN
2	F	542	ASN
3	V	8	GLN
3	V	238	ASN
3	V	245	ASN
4	c	46	GLN
4	c	186	GLN
2	G	542	ASN
3	W	8	GLN
3	W	238	ASN
3	W	245	ASN
4	d	46	GLN
4	d	186	GLN
2	H	542	ASN
3	X	8	GLN
3	X	238	ASN
3	X	245	ASN
4	e	46	GLN

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Mol	Chain	Res	Type
4	e	186	GLN
2	I	542	ASN
3	Y	8	GLN
3	Y	238	ASN
3	Y	245	ASN
4	f	46	GLN
4	f	186	GLN
2	J	542	ASN
3	g	8	GLN
3	g	238	ASN
3	g	245	ASN
4	3	46	GLN
4	3	186	GLN
2	K	542	ASN
3	7	8	GLN
3	7	238	ASN
3	7	245	ASN
4	8	46	GLN
4	8	186	GLN
2	L	542	ASN
3	AL	8	GLN
3	AL	238	ASN
3	AL	245	ASN
4	AM	46	GLN
4	AM	186	GLN
2	M	542	ASN
3	AR	8	GLN
3	AR	238	ASN
3	AR	245	ASN
4	AS	46	GLN
4	AS	186	GLN
2	N	542	ASN
3	AX	8	GLN
3	AX	238	ASN
3	AX	245	ASN
4	AY	46	GLN
4	AY	186	GLN
2	O	542	ASN
3	Ad	8	GLN
3	Ad	238	ASN
3	Ad	245	ASN
4	Ae	46	GLN

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Mol	Chain	Res	Type
4	Ae	186	GLN
2	P	542	ASN
3	Aj	8	GLN
3	Aj	238	ASN
3	Aj	245	ASN
4	Ak	46	GLN
4	Ak	186	GLN
2	Q	542	ASN
3	Ap	8	GLN
3	Ap	238	ASN
3	Ap	245	ASN
4	Aq	46	GLN
4	Aq	186	GLN
2	R	542	ASN
3	Av	8	GLN
3	Av	238	ASN
3	Av	245	ASN
4	Aw	46	GLN
4	Aw	186	GLN
2	A2	542	ASN
3	A3	8	GLN
3	A3	238	ASN
3	A3	245	ASN
4	A4	46	GLN
4	A4	186	GLN
2	A9	542	ASN
3	A0	8	GLN
3	A0	238	ASN
3	A0	245	ASN
4	BA	46	GLN
4	BA	186	GLN
2	BF	542	ASN
3	BG	8	GLN
3	BG	238	ASN
3	BG	245	ASN
4	BH	46	GLN
4	BH	186	GLN
2	BM	542	ASN
3	BN	8	GLN
3	BN	238	ASN
3	BN	245	ASN
4	BO	46	GLN

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Mol	Chain	Res	Type
4	BO	186	GLN
2	BT	542	ASN
3	BU	8	GLN
3	BU	238	ASN
3	BU	245	ASN
4	BV	46	GLN
4	BV	186	GLN
2	Ba	542	ASN
3	Bb	8	GLN
3	Bb	238	ASN
3	Bb	245	ASN
4	Bc	46	GLN
4	Bc	186	GLN
2	Bh	542	ASN
3	Bi	8	GLN
3	Bi	238	ASN
3	Bi	245	ASN
4	Bj	46	GLN
4	Bj	186	GLN
2	Bo	542	ASN
3	Bp	8	GLN
3	Bp	238	ASN
3	Bp	245	ASN
4	Bq	46	GLN
4	Bq	186	GLN
2	Bv	542	ASN
3	Bw	8	GLN
3	Bw	238	ASN
3	Bw	245	ASN
4	Bx	46	GLN
4	Bx	186	GLN
2	B3	542	ASN
3	B4	8	GLN
3	B4	238	ASN
3	B4	245	ASN
4	B5	46	GLN
4	B5	186	GLN
2	B0	542	ASN
3	CA	8	GLN
3	CA	238	ASN
3	CA	245	ASN
4	CB	46	GLN

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Mol	Chain	Res	Type
4	CB	186	GLN
2	CG	542	ASN
3	CH	8	GLN
3	CH	238	ASN
3	CH	245	ASN
4	CI	46	GLN
4	CI	186	GLN
2	CN	542	ASN
3	CO	8	GLN
3	CO	238	ASN
3	CO	245	ASN
4	CP	46	GLN
4	CP	186	GLN
2	CU	542	ASN
3	CV	8	GLN
3	CV	238	ASN
3	CV	245	ASN
4	CW	46	GLN
4	CW	186	GLN
2	Cb	542	ASN
3	Cc	8	GLN
3	Cc	238	ASN
3	Cc	245	ASN
4	Cd	46	GLN
4	Cd	186	GLN
2	Ci	542	ASN
3	Cj	8	GLN
3	Cj	238	ASN
3	Cj	245	ASN
4	Ck	46	GLN
4	Ck	186	GLN
2	Cp	542	ASN
3	Cq	8	GLN
3	Cq	238	ASN
3	Cq	245	ASN
4	Cr	46	GLN
4	Cr	186	GLN
2	Cw	542	ASN
3	Cx	8	GLN
3	Cx	238	ASN
3	Cx	245	ASN
4	Cy	46	GLN

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Mol	Chain	Res	Type
4	Cy	186	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

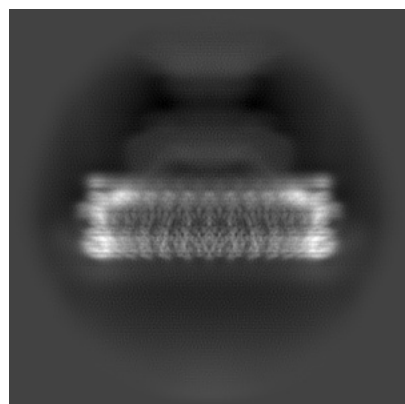
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37570. These allow visual inspection of the internal detail of the map and identification of artifacts.

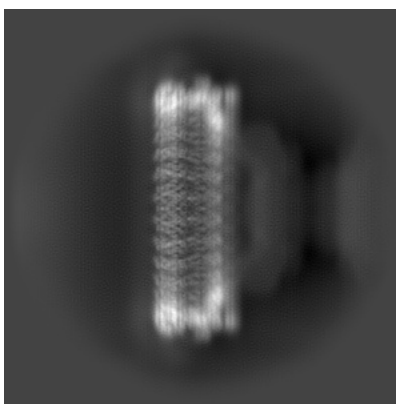
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

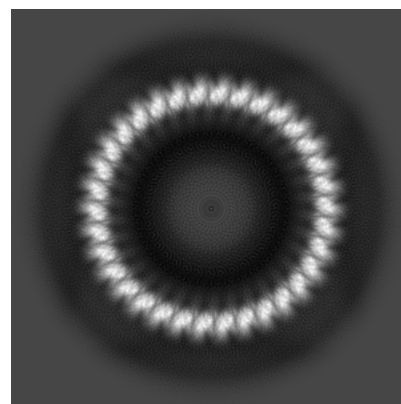
6.1.1 Primary map



X

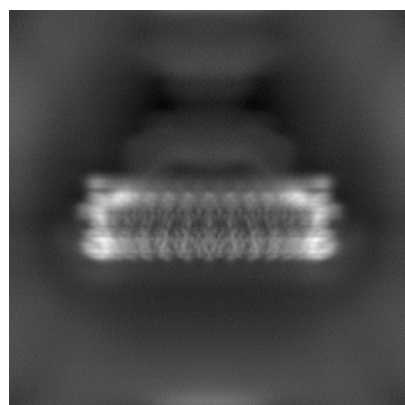


Y

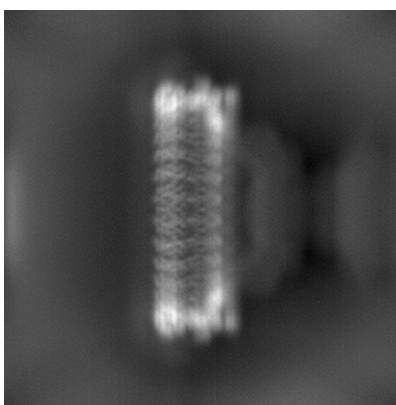


Z

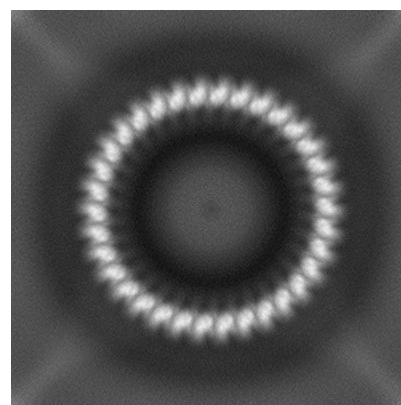
6.1.2 Raw map



X



Y

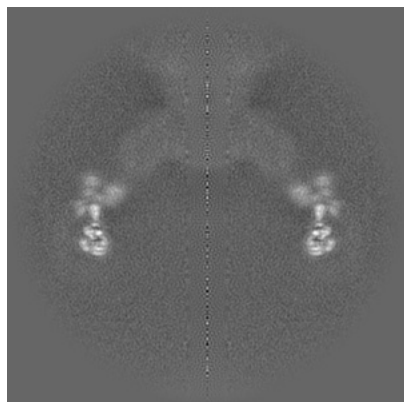


Z

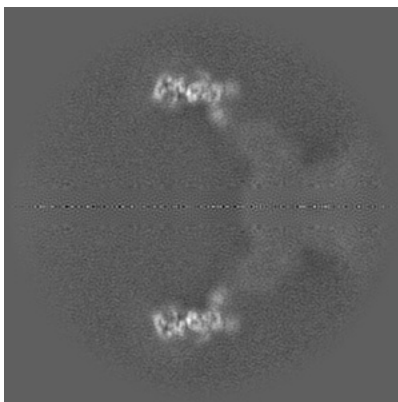
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

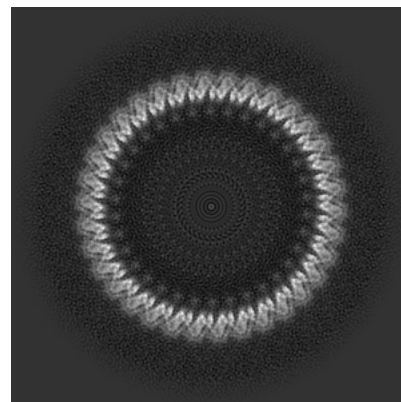
6.2.1 Primary map



X Index: 300



Y Index: 300

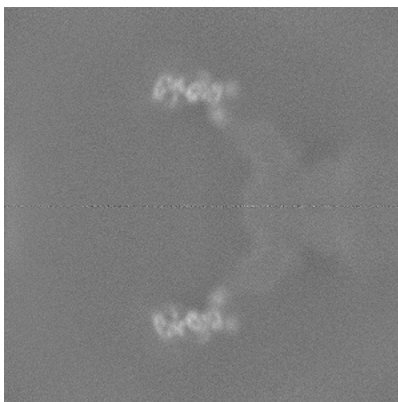


Z Index: 300

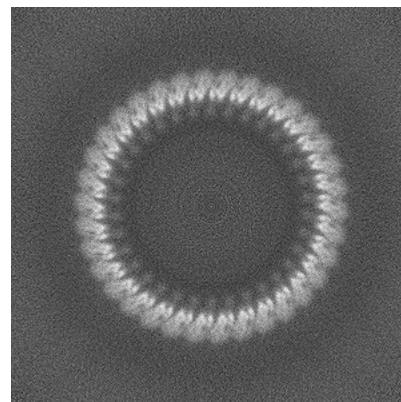
6.2.2 Raw map



X Index: 300



Y Index: 300

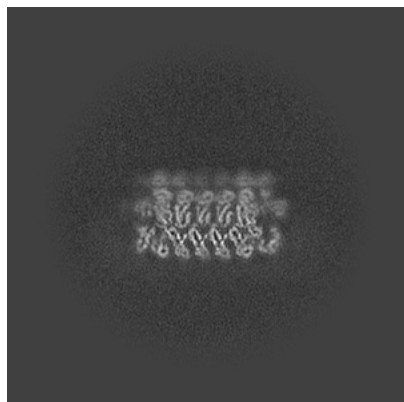


Z Index: 300

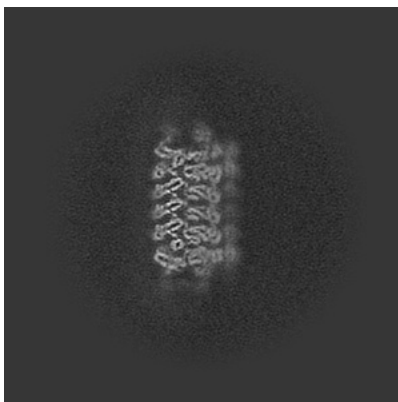
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

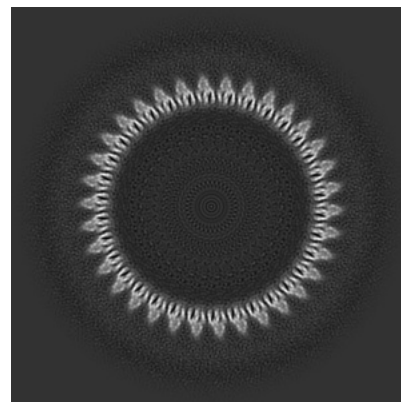
6.3.1 Primary map



X Index: 138

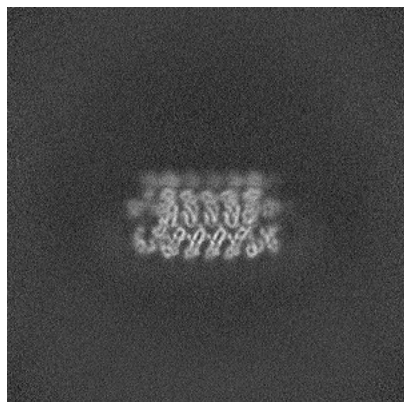


Y Index: 138

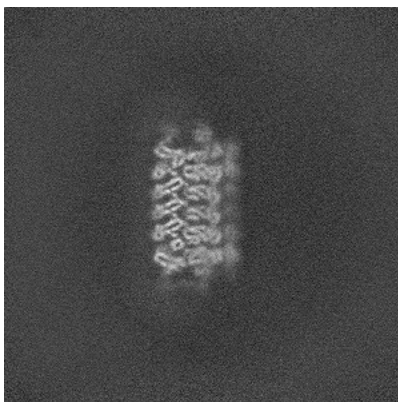


Z Index: 256

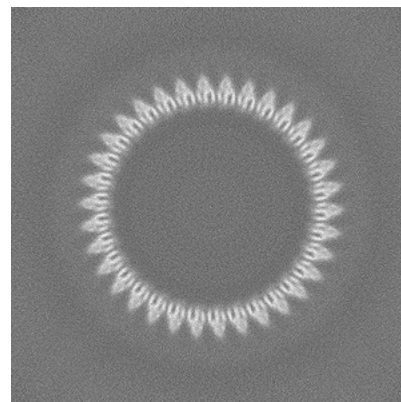
6.3.2 Raw map



X Index: 463



Y Index: 138

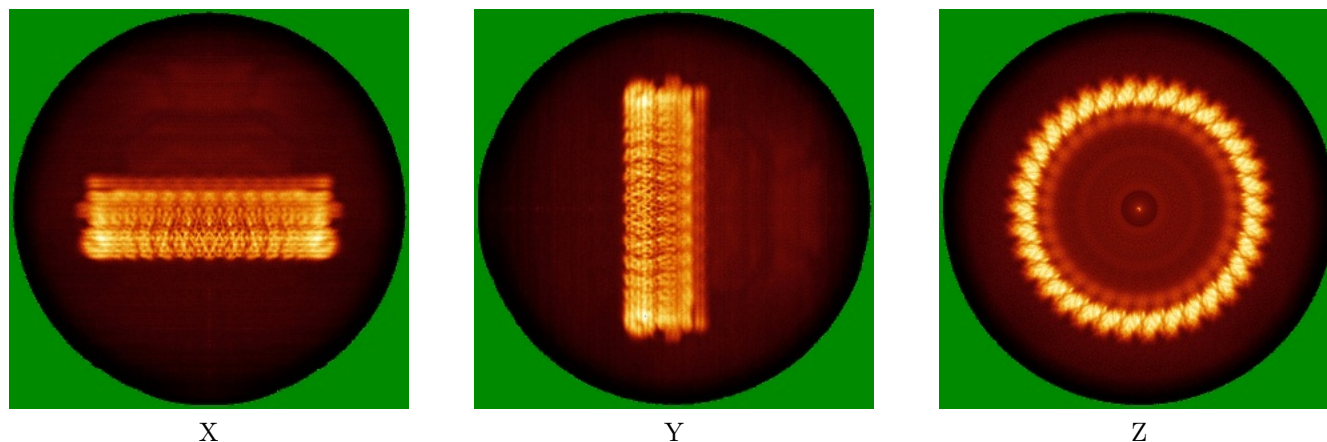


Z Index: 256

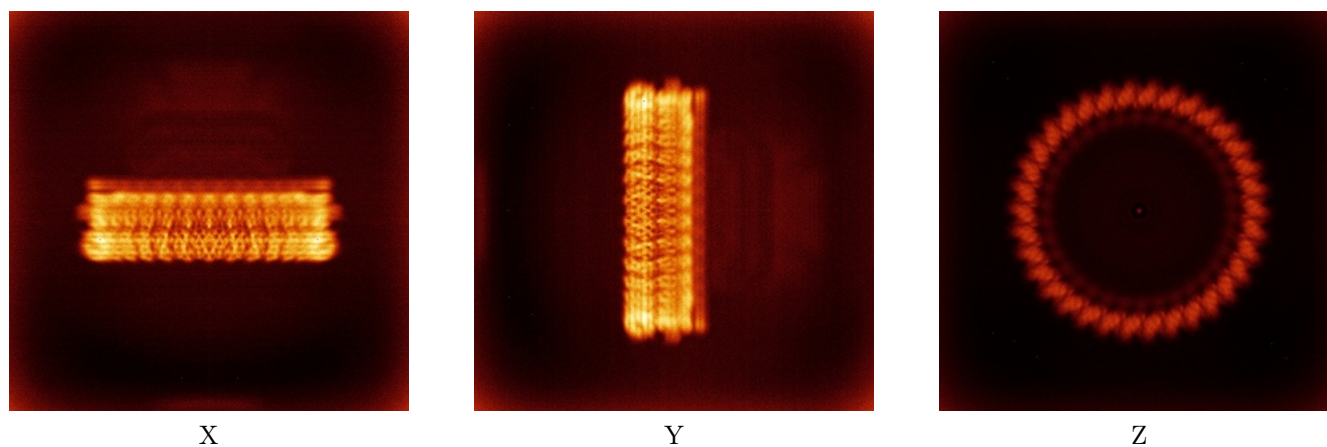
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



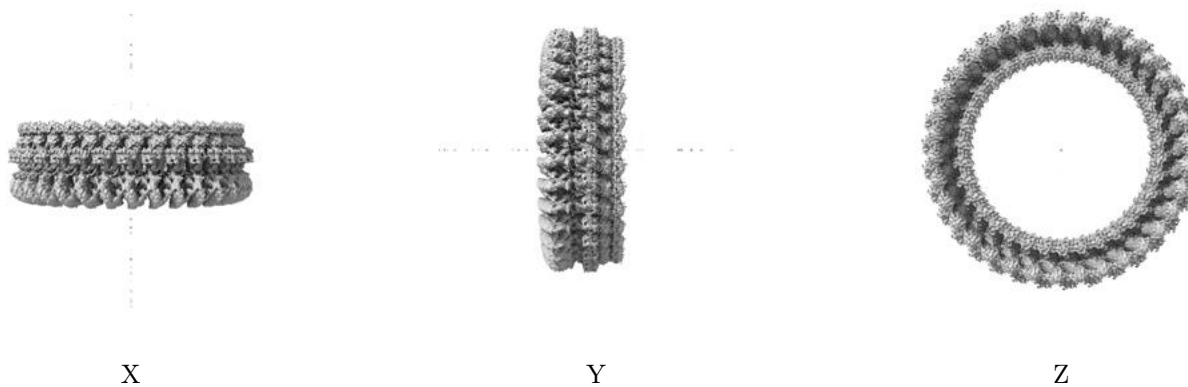
6.4.2 Raw map



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

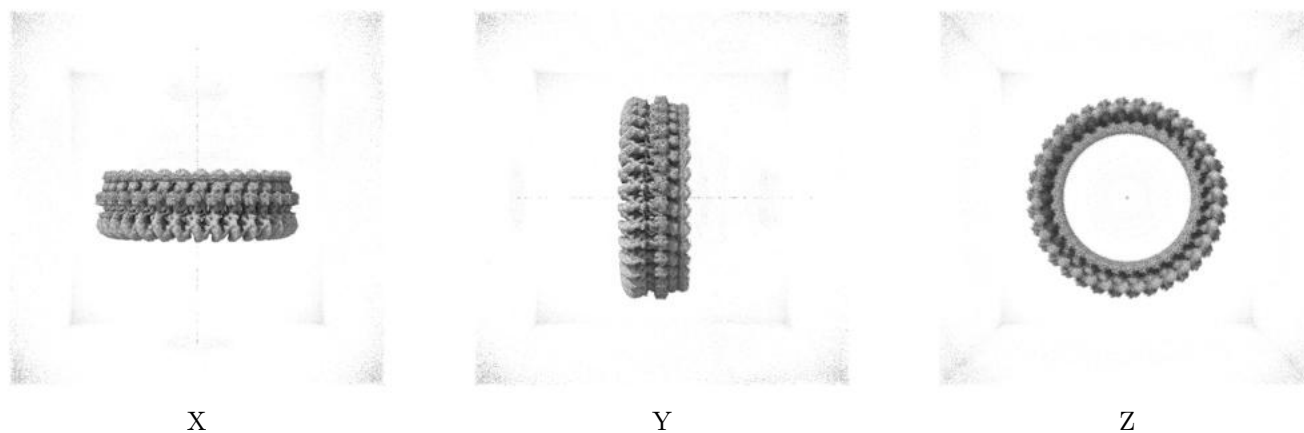
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

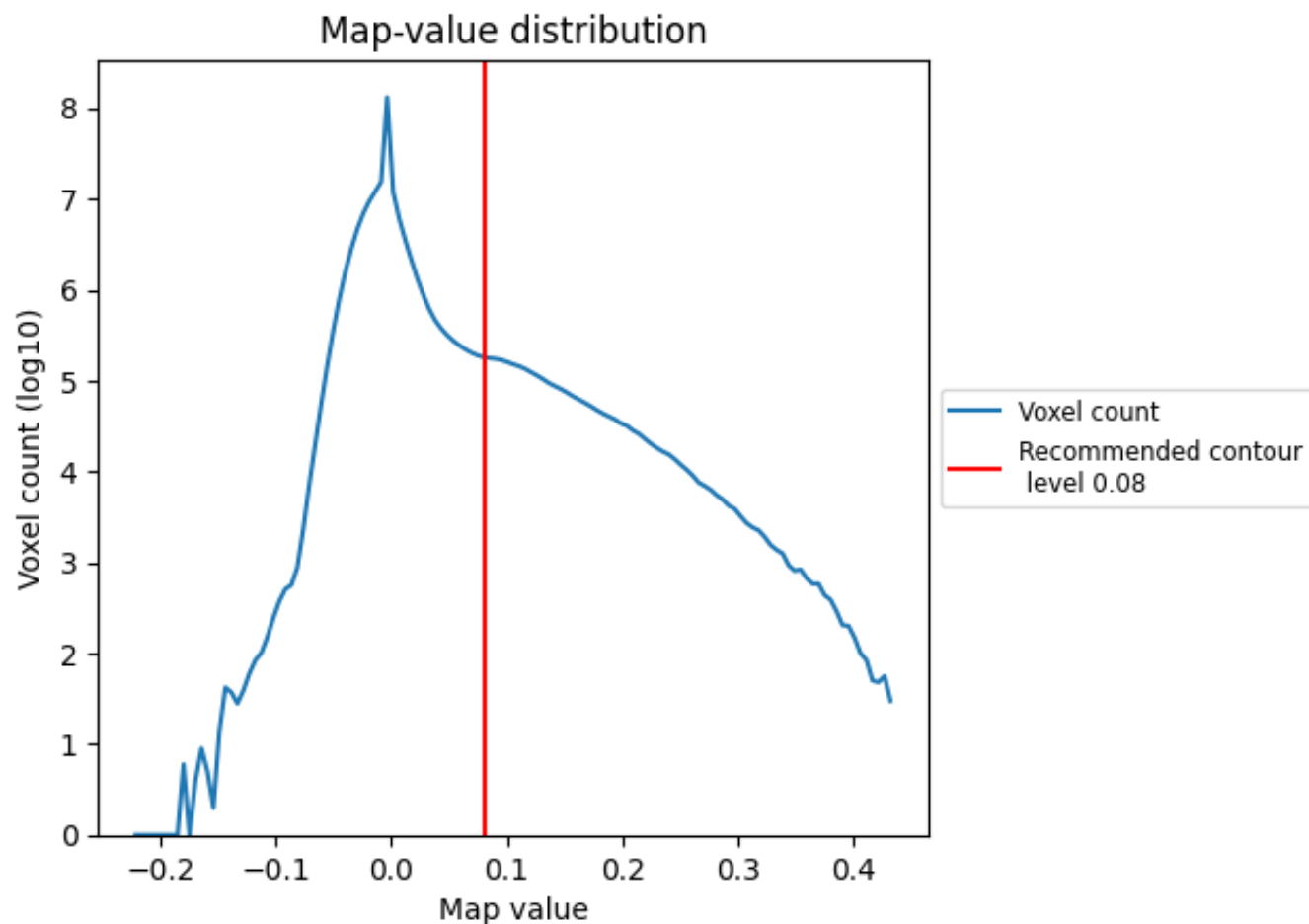
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

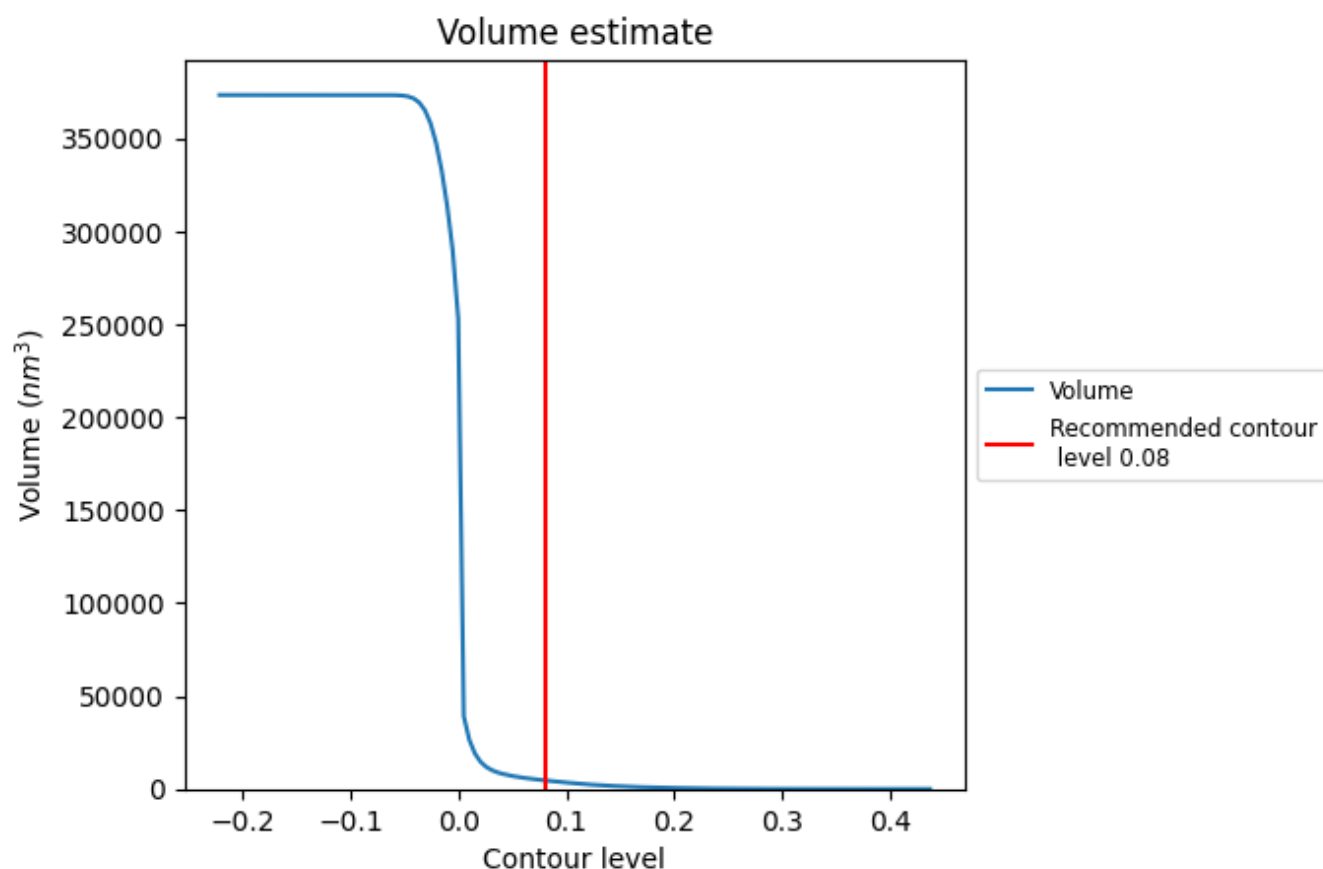
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

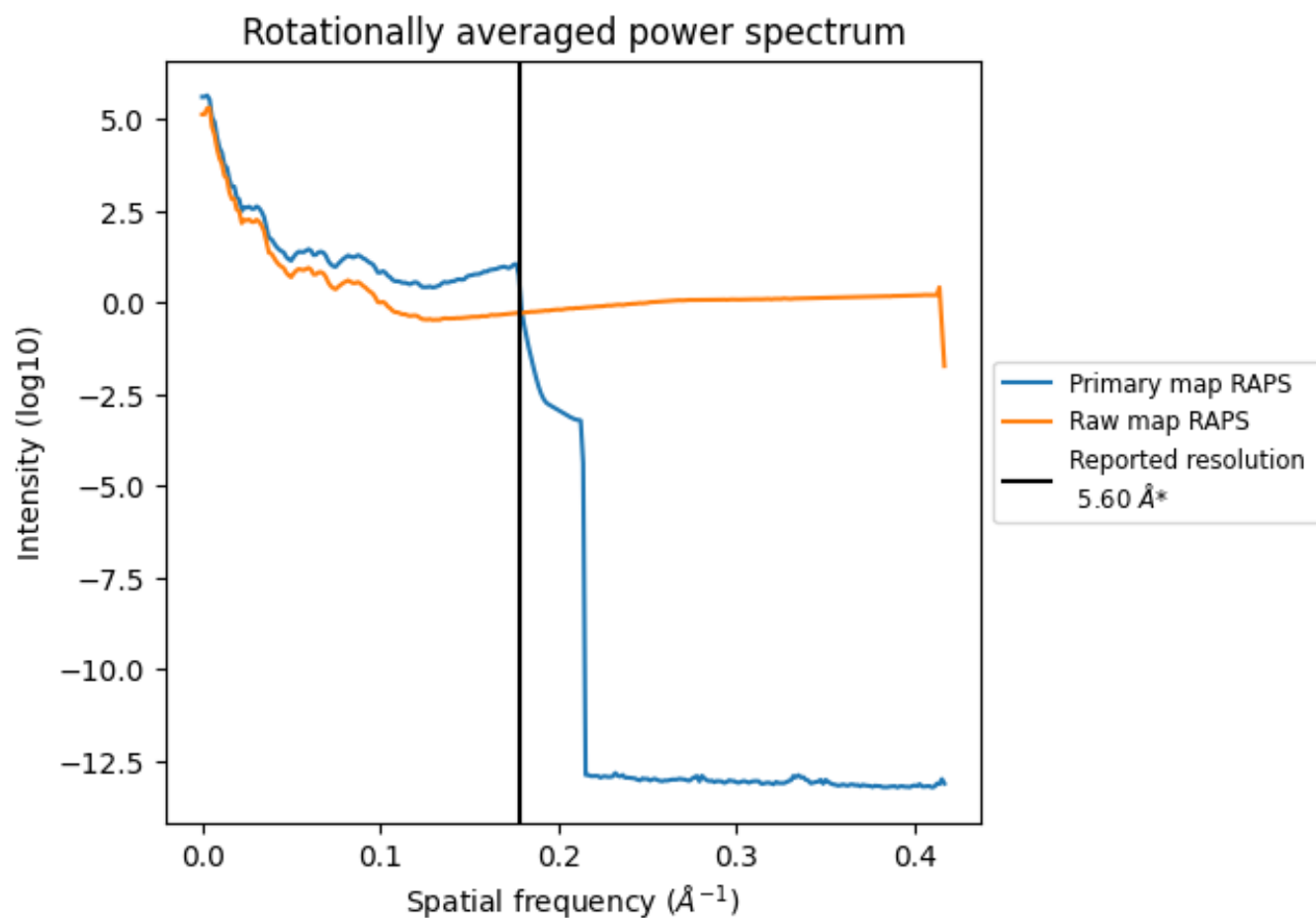
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4620 nm³; this corresponds to an approximate mass of 4173 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

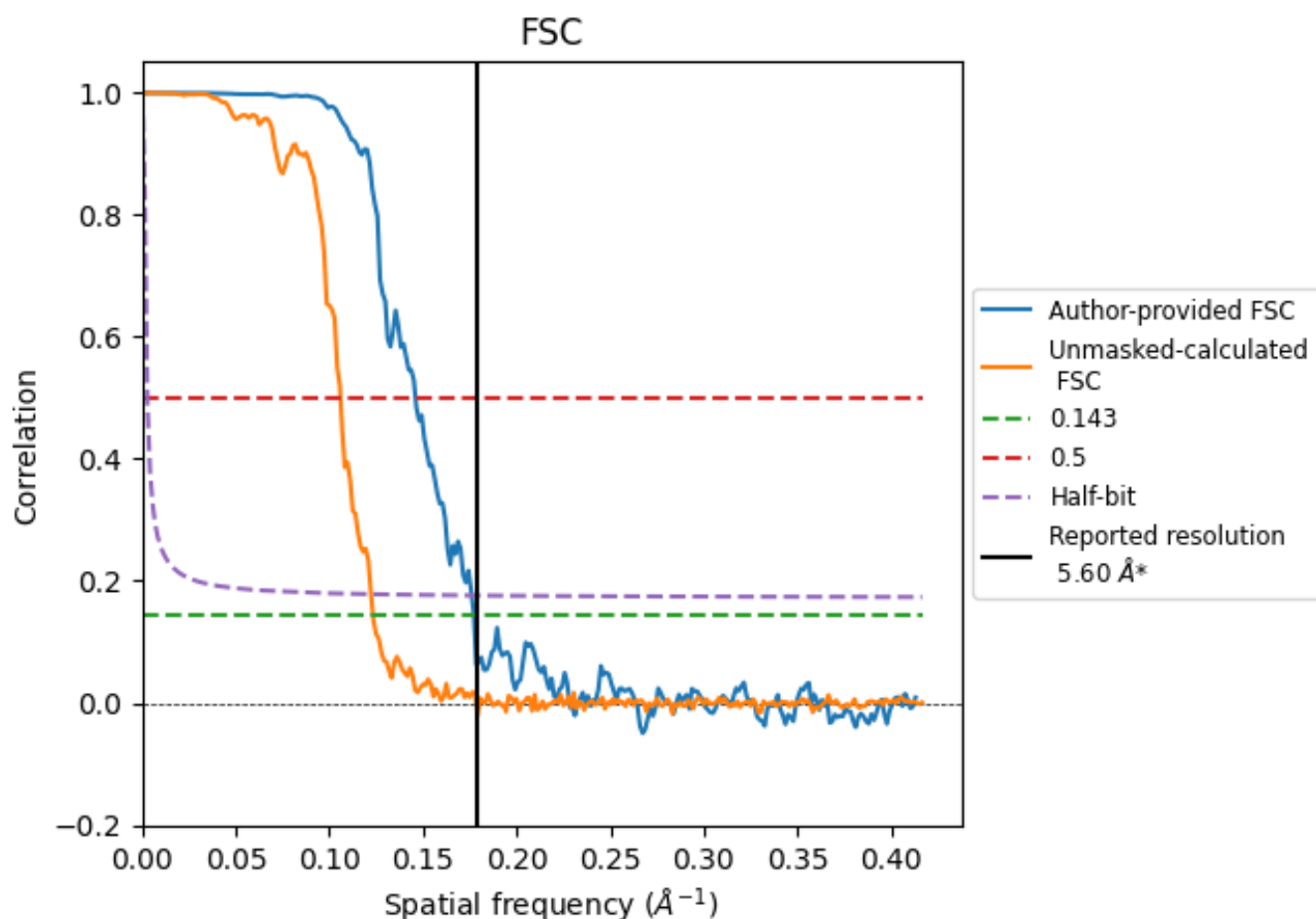


*Reported resolution corresponds to spatial frequency of 0.179 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.179 \AA^{-1}

8.2 Resolution estimates [i](#)

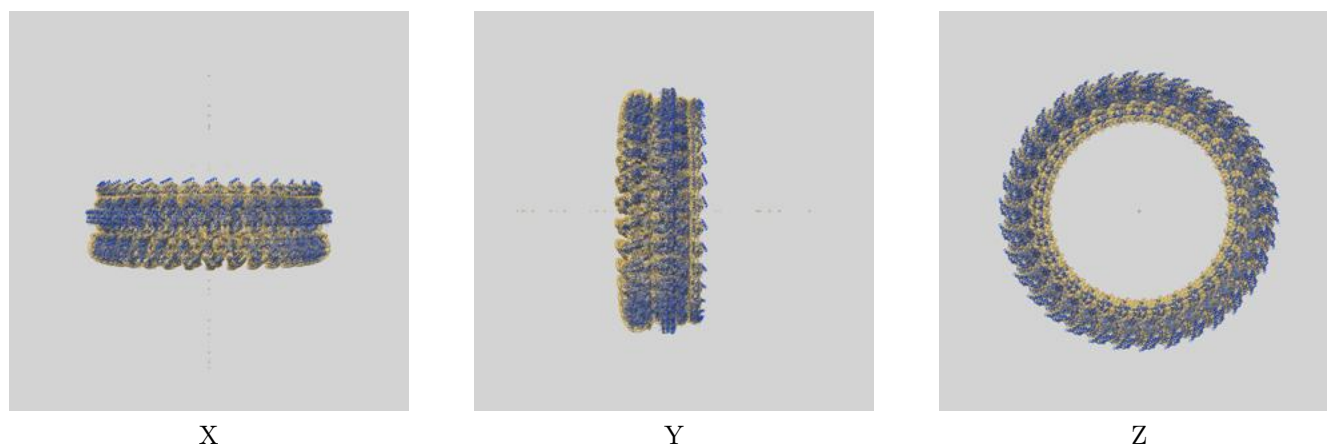
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.60	-	-
Author-provided FSC curve	5.64	6.85	5.68
Unmasked-calculated*	8.11	9.44	8.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.11 differs from the reported value 5.6 by more than 10 %

9 Map-model fit [i](#)

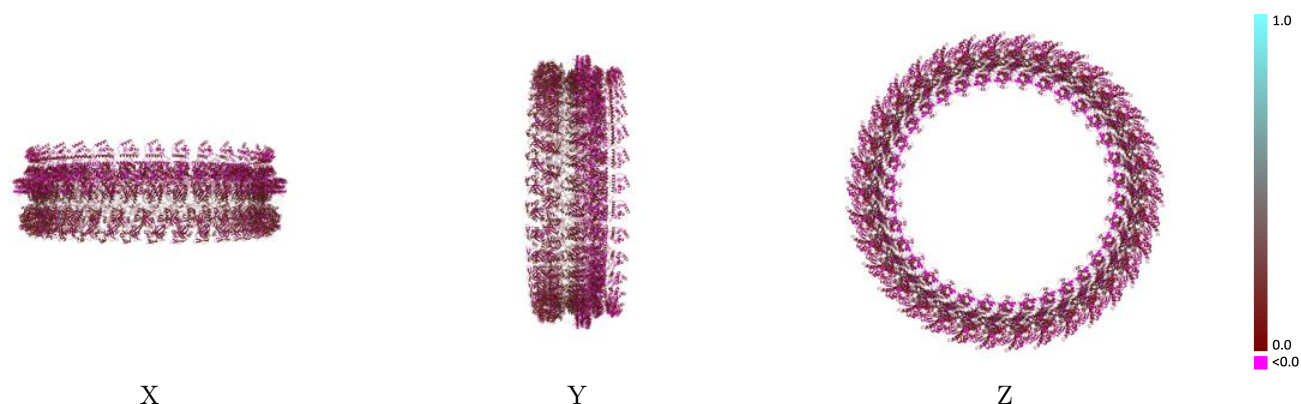
This section contains information regarding the fit between EMDB map EMD-37570 and PDB model 8WIW. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



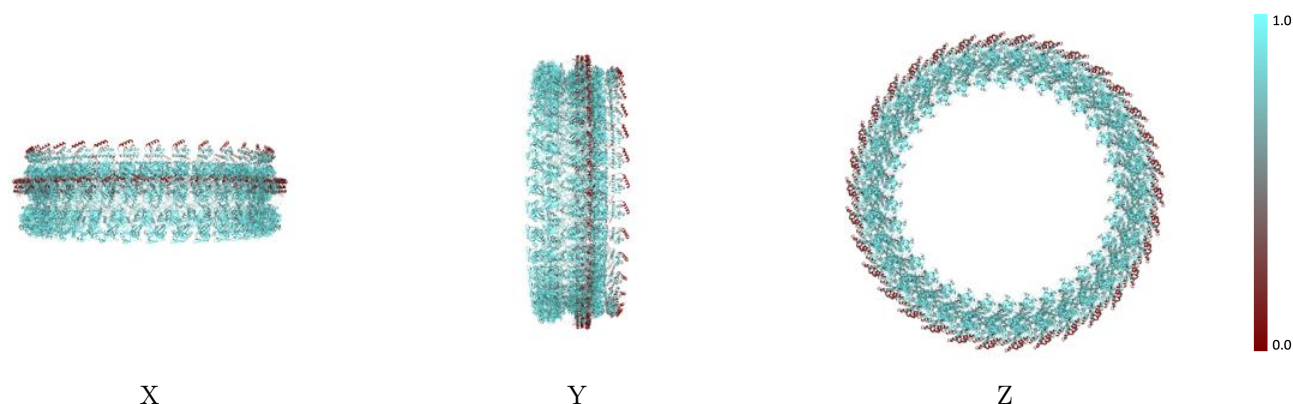
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



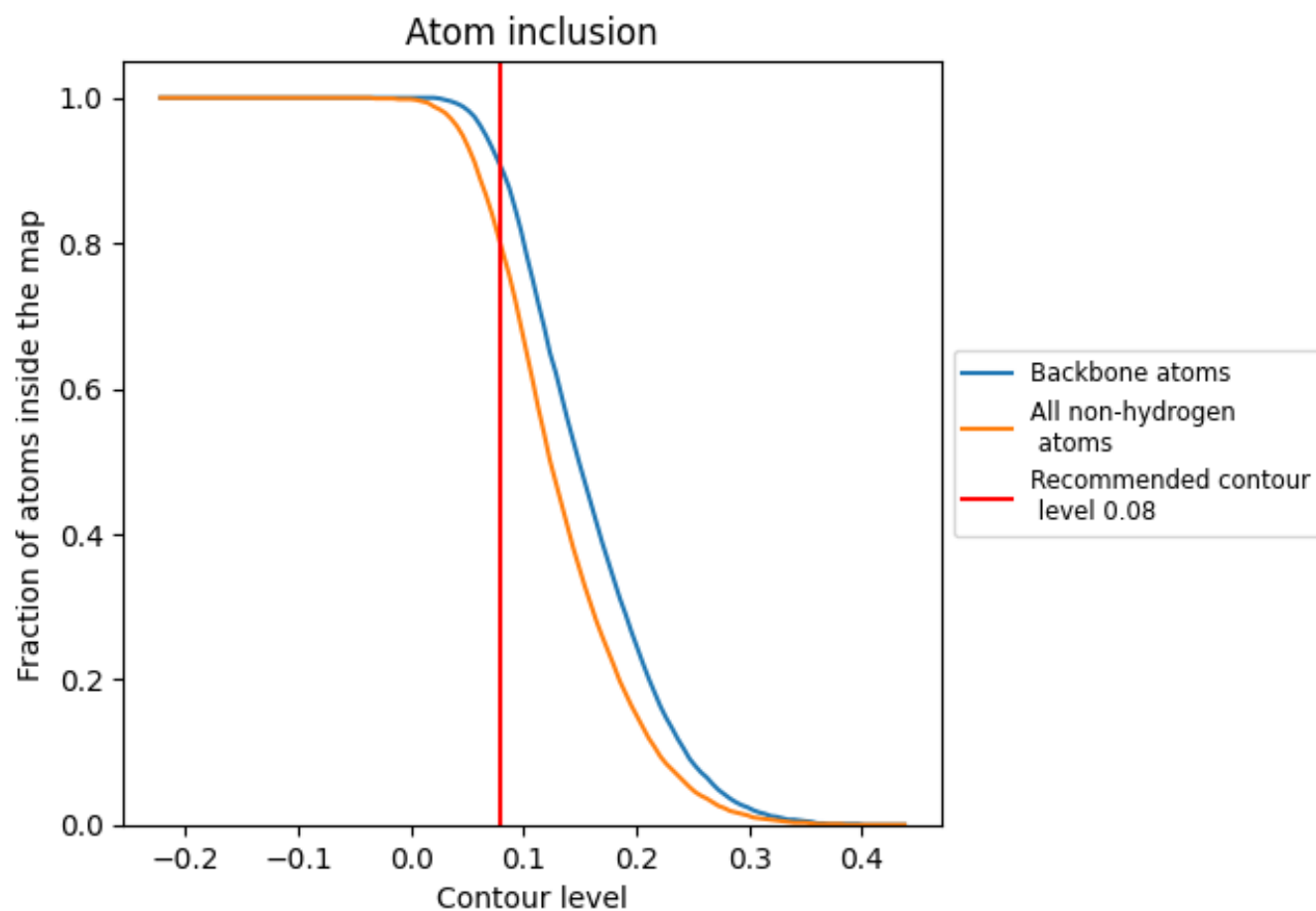
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7970	 0.1300
0	 0.8680	 0.1720
1	 0.8660	 0.1660
2	 0.8750	 0.1640
3	 0.7770	 0.0820
4	 0.5350	 0.1050
5	 0.8660	 0.1670
6	 0.8780	 0.1620
7	 0.8670	 0.1670
8	 0.7720	 0.0800
9	 0.5430	 0.1070
A0	 0.8690	 0.1670
A1	 0.8690	 0.1710
A2	 0.8470	 0.0510
A3	 0.8680	 0.1670
A4	 0.7750	 0.0820
A5	 0.5410	 0.1050
A6	 0.8620	 0.1650
A7	 0.8740	 0.1650
A8	 0.8680	 0.1730
A9	 0.8370	 0.0510
AA	 0.8680	 0.1690
AB	 0.8660	 0.1700
AC	 0.8660	 0.1700
AD	 0.8600	 0.1680
AE	 0.8680	 0.1680
AF	 0.8660	 0.1690
AG	 0.8680	 0.1680
AH	 0.8680	 0.1690
AI	 0.8660	 0.1660
AJ	 0.8780	 0.1640
AK	 0.8650	 0.1690
AL	 0.8690	 0.1670
AM	 0.7740	 0.0780
AN	 0.5340	 0.1050























































































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Chain	Atom inclusion	Q-score
AO	 0.8650	 0.1650
AP	 0.8800	 0.1650
AQ	 0.8650	 0.1710
AR	 0.8690	 0.1670
AS	 0.7740	 0.0810
AT	 0.5410	 0.1040
AU	 0.8660	 0.1660
AV	 0.8780	 0.1630
AW	 0.8650	 0.1710
AX	 0.8670	 0.1660
AY	 0.7740	 0.0800
AZ	 0.5290	 0.1030
Aa	 0.8630	 0.1630
Ab	 0.8750	 0.1650
Ac	 0.8710	 0.1700
Ad	 0.8670	 0.1660
Ae	 0.7730	 0.0790
Af	 0.5210	 0.1040
Ag	 0.8630	 0.1640
Ah	 0.8720	 0.1630
Ai	 0.8630	 0.1710
Aj	 0.8660	 0.1680
Ak	 0.7700	 0.0800
Al	 0.5220	 0.1030
Am	 0.8600	 0.1660
An	 0.8660	 0.1640
Ao	 0.8660	 0.1700
Ap	 0.8680	 0.1660
Aq	 0.7730	 0.0810
Ar	 0.5220	 0.1030
As	 0.8600	 0.1640
At	 0.8750	 0.1660
Au	 0.8680	 0.1690
Av	 0.8680	 0.1670
Aw	 0.7730	 0.0800
Ax	 0.5290	 0.1040
Ay	 0.8660	 0.1650
Az	 0.8780	 0.1660
B0	 0.8560	 0.0530
B1	 0.8780	 0.1640
B2	 0.8680	 0.1740
B3	 0.8470	 0.0530





















































































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Chain	Atom inclusion	Q-score
B4	 0.8670	 0.1670
B5	 0.7720	 0.0820
B6	 0.5430	 0.1050
B7	 0.8660	 0.1680
B8	 0.8780	 0.1630
B9	 0.8650	 0.1720
BA	 0.7710	 0.0800
BB	 0.5400	 0.1030
BC	 0.8620	 0.1670
BD	 0.8800	 0.1640
BE	 0.8680	 0.1710
BF	 0.8510	 0.0510
BG	 0.8660	 0.1660
BH	 0.7710	 0.0800
BI	 0.5410	 0.1030
BJ	 0.8660	 0.1670
BK	 0.8770	 0.1620
BL	 0.8660	 0.1740
BM	 0.8420	 0.0560
BN	 0.8690	 0.1660
BO	 0.7750	 0.0810
BP	 0.5280	 0.1020
BQ	 0.8650	 0.1690
BR	 0.8740	 0.1650
BS	 0.8660	 0.1750
BT	 0.8560	 0.0570
BU	 0.8670	 0.1660
BV	 0.7750	 0.0820
BW	 0.5180	 0.1030
BX	 0.8650	 0.1670
BY	 0.8720	 0.1650
BZ	 0.8600	 0.1710
Ba	 0.8510	 0.0560
Bb	 0.8650	 0.1670
Bc	 0.7740	 0.0810
Bd	 0.5270	 0.1030
Be	 0.8630	 0.1650
Bf	 0.8710	 0.1670
Bg	 0.8680	 0.1710
Bh	 0.8510	 0.0520
Bi	 0.8670	 0.1660
Bj	 0.7710	 0.0810





















































































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Chain	Atom inclusion	Q-score
Bk	 0.5200	 0.1070
Bl	 0.8630	 0.1650
Bm	 0.8740	 0.1640
Bn	 0.8660	 0.1720
Bo	 0.8420	 0.0520
Bp	 0.8700	 0.1660
Bq	 0.7740	 0.0810
Br	 0.5240	 0.1080
Bs	 0.8660	 0.1660
Bt	 0.8750	 0.1650
Bu	 0.8680	 0.1720
Bv	 0.8510	 0.0530
Bw	 0.8680	 0.1670
Bx	 0.7770	 0.0820
By	 0.5350	 0.1050
Bz	 0.8660	 0.1690
C	 0.8370	 0.0560
C1	 0.8620	 0.1630
C2	 0.8740	 0.1620
CA	 0.8690	 0.1660
CB	 0.7740	 0.0820
CC	 0.5340	 0.1030
CD	 0.8650	 0.1650
CE	 0.8800	 0.1650
CF	 0.8650	 0.1720
CG	 0.8560	 0.0580
CH	 0.8690	 0.1650
CI	 0.7740	 0.0830
CJ	 0.5410	 0.1040
CK	 0.8660	 0.1650
CL	 0.8780	 0.1640
CM	 0.8650	 0.1730
CN	 0.8370	 0.0570
CO	 0.8670	 0.1640
CP	 0.7740	 0.0820
CQ	 0.5290	 0.1030
CR	 0.8630	 0.1620
CS	 0.8750	 0.1650
CT	 0.8710	 0.1710
CU	 0.8510	 0.0530
CV	 0.8670	 0.1640
CW	 0.7730	 0.0810









































































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Chain	Atom inclusion	Q-score
CX	 0.5210	 0.1050
CY	 0.8630	 0.1620
CZ	 0.8720	 0.1620
Ca	 0.8630	 0.1710
Cb	 0.8510	 0.0520
Cc	 0.8660	 0.1660
Cd	 0.7700	 0.0810
Ce	 0.5220	 0.1050
Cf	 0.8600	 0.1650
Cg	 0.8660	 0.1630
Ch	 0.8660	 0.1730
Ci	 0.8560	 0.0560
Cj	 0.8680	 0.1660
Ck	 0.7730	 0.0820
Cl	 0.5220	 0.1040
Cm	 0.8600	 0.1640
Cn	 0.8750	 0.1630
Co	 0.8680	 0.1720
Cp	 0.8420	 0.0560
Cq	 0.8680	 0.1670
Cr	 0.7730	 0.0810
Cs	 0.5290	 0.1040
Ct	 0.8660	 0.1640
Cu	 0.8780	 0.1610
Cv	 0.8690	 0.1710
Cw	 0.8470	 0.0540
Cx	 0.8680	 0.1670
Cy	 0.7750	 0.0820
Cz	 0.5410	 0.1050
D	 0.8510	 0.0530
E	 0.8420	 0.0550
F	 0.8560	 0.0600
G	 0.8510	 0.0580
H	 0.8510	 0.0510
I	 0.8420	 0.0510
J	 0.8510	 0.0510
K	 0.8470	 0.0550
L	 0.8560	 0.0550
M	 0.8560	 0.0550
N	 0.8370	 0.0550
O	 0.8510	 0.0520
P	 0.8510	 0.0490

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Chain	Atom inclusion	Q-score
Q	 0.8560	 0.0560
R	 0.8420	 0.0540
S	 0.8690	 0.1660
T	 0.8660	 0.1660
U	 0.8690	 0.1650
V	 0.8670	 0.1670
W	 0.8650	 0.1690
X	 0.8670	 0.1680
Y	 0.8700	 0.1670
Z	 0.7710	 0.0810
a	 0.7710	 0.0820
b	 0.7750	 0.0820
c	 0.7750	 0.0820
d	 0.7740	 0.0790
e	 0.7710	 0.0810
f	 0.7740	 0.0800
g	 0.8680	 0.1680
h	 0.5400	 0.1040
i	 0.5410	 0.1030
j	 0.5280	 0.1020
k	 0.5180	 0.1010
l	 0.5270	 0.1040
m	 0.5200	 0.1050
n	 0.5240	 0.1080
o	 0.8620	 0.1630
p	 0.8660	 0.1650
q	 0.8650	 0.1650
r	 0.8650	 0.1630
s	 0.8630	 0.1630
t	 0.8630	 0.1630
u	 0.8800	 0.1620
v	 0.8770	 0.1610
w	 0.8740	 0.1640
x	 0.8720	 0.1630
y	 0.8710	 0.1630
z	 0.8740	 0.1630