



Full wwPDB EM Validation Report ⓘ

Aug 27, 2024 – 05:03 PM JST

PDB ID : 8WLQ
EMDB ID : EMD-37628
Title : Cryo-EM structure of the whole rod-export apparatus with hook within the flagellar motor-hook complex in the CCW state.
Authors : Tan, J.X.; Zhang, L.; Zhou, Y.; Zhu, Y.Q.
Deposited on : 2023-09-30
Resolution : 3.80 Å(reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

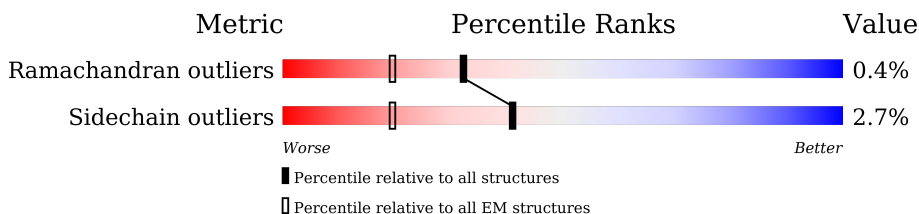
EMDB validation analysis : 0.0.1.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	260	
1	1	260	
1	2	260	
1	3	260	
1	4	260	
1	5	260	
1	6	260	
1	7	260	
1	8	260	

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Mol	Chain	Length	Quality of chain
1	9	260	13% 98% .
1	ZA	260	12% 98% .
1	ZB	260	13% 96% .
1	ZC	260	8% 98% .
1	ZD	260	11% 97% .
1	ZE	260	13% 97% .
1	r	260	18% 95% ..
1	s	260	10% 94% ..
1	t	260	11% 93% 5% .
1	u	260	10% 92% 6% .
1	v	260	12% 92% 5% ..
1	w	260	11% 91% . 7%
1	x	260	11% 90% 5% 5%
1	y	260	11% 92% .. 5%
1	z	260	12% 93% . 5%
2	ZF	403	47% 97% .
2	ZG	403	20% 95% .
2	ZH	403	14% 96% .
2	ZI	403	13% 97% .
2	ZJ	403	12% 97% .
2	ZK	403	14% 98% .
2	ZL	403	12% 97% .
2	ZM	403	13% 97% .
2	ZN	403	13% 97% .
2	ZO	403	12% 97% .

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Mol	Chain	Length	Quality of chain
2	ZP	403	12% 95%
2	ZQ	403	13% 97%
2	ZR	403	15% 98%
2	ZS	403	16% 98%
2	ZT	403	16% 97%
2	ZU	403	18% 98%
2	ZV	403	18% 98%
2	ZW	403	23% 96%
2	ZX	403	22% 99%
2	ZY	403	30% 98%
2	ZZ	403	31% 98%
2	Za	403	38% 98%
2	Zb	403	42% 98%
2	Zc	403	44% 97%
2	Zd	403	46% 98%
2	Ze	403	52% 97%
2	Zf	403	54% 98%
2	Zg	403	57% 98%
2	Zh	403	58% 98%
3	A	89	84% 92% 7%
3	B	89	58% 98%
3	C	89	49% 100%
3	D	89	61% 100%
4	E	264	63% 93%
5	F	245	46% 82% 16%

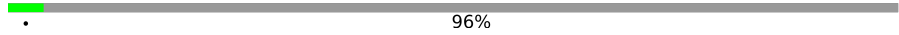
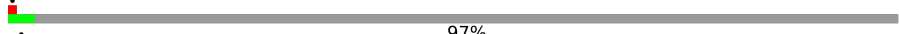
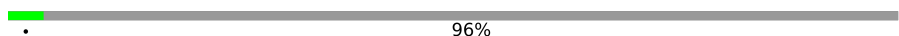
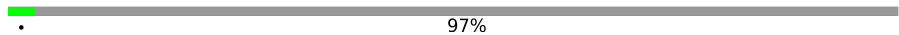
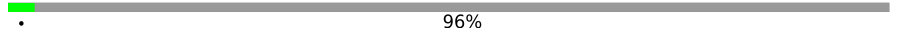



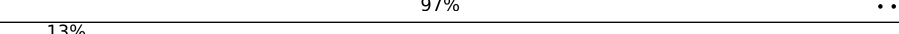
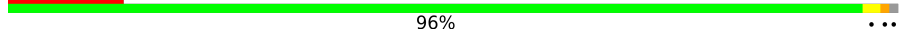

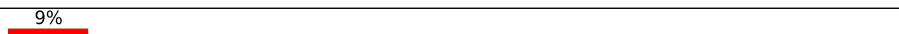
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Mol	Chain	Length	Quality of chain
5	G	245	36% 82% 15%
5	H	245	30% 82% 15%
5	I	245	31% 82% 15%
5	J	245	40% 80% 15%
6	K	104	15% 35% 62%
6	L	104	16% 67% 31%
6	M	104	15% 70% 29%
6	N	104	15% 69% 29%
6	O	104	18% 69% 29%
6	P	104	14% 67% 30%
7	Q	138	23% 83% 14%
7	R	138	12% 77% 22%
7	S	138	10% 76% 22%
7	T	138	9% 78% 20%
7	U	138	12% 73% 23%
8	V	134	25% 99%
8	W	134	16% 96%
8	X	134	12% 98%
8	Y	134	12% 93% 6%
8	Z	134	9% 95%
8	a	134	13% 94% 5%
9	b	560	98%
9	c	560	97%
9	d	560	96%
9	e	560	97%

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Mol	Chain	Length	Quality of chain
9	f	560	 96%
9	g	560	 97%
9	h	560	 96%
9	i	560	 97%
9	j	560	 96%
9	k	560	 97%
9	l	560	 96%
10	m	251	 23% 97%
10	n	251	 13% 96%
10	o	251	 9% 98%
10	p	251	 9% 96%
10	q	251	 13% 98%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 167758 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Flagellar basal-body rod protein FlgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	248	Total 1866	C 1154	N 327	O 379	S 6	0	0
1	1	252	Total 1894	C 1172	N 331	O 385	S 6	0	0
1	2	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	3	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	4	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	5	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	6	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	7	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	8	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	9	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	ZA	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	ZB	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	ZC	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	ZD	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	ZE	260	Total 1949	C 1202	N 341	O 400	S 6	0	0
1	r	254	Total 1903	C 1175	N 334	O 389	S 5	0	0
1	s	255	Total 1911	C 1181	N 335	O 390	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	t	256	Total	C	N	O	S	0	0
			1919	1186	336	391	6		
1	u	254	Total	C	N	O	S	0	0
			1903	1175	334	389	5		
1	v	255	Total	C	N	O	S	0	0
			1911	1181	335	390	5		
1	w	243	Total	C	N	O	S	0	0
			1823	1127	318	373	5		
1	x	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
1	y	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		
1	z	248	Total	C	N	O	S	0	0
			1866	1154	327	379	6		

- Molecule 2 is a protein called Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	ZF	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZG	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZH	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZI	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZJ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZK	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZL	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZM	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZN	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZO	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZP	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZQ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	ZR	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZS	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZT	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZU	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZV	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZW	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZX	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZY	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	ZZ	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	Za	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	Zb	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	Zc	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	Zd	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	Ze	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	Zf	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	Zg	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		
2	Zh	401	Total	C	N	O	S	0	0
			2947	1814	507	618	8		

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

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

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

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

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

- Molecule 5 is a protein called Flagellar biosynthetic protein FliP.

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

- Molecule 6 is a protein called Flagellar hook-basal body complex protein FliE.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	40	Total	C	N	O	S	0	0
			300	185	52	57	6		
6	L	72	Total	C	N	O	S	0	0
			543	335	99	103	6		
6	M	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
6	N	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
6	O	74	Total	C	N	O	S	0	0
			557	344	101	106	6		
6	P	73	Total	C	N	O	S	0	0
			550	340	100	104	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	119	Total	C	N	O	S	0	0
			922	565	169	183	5		
7	R	108	Total	C	N	O	S	0	0
			848	523	155	165	5		
7	S	108	Total	C	N	O	S	0	0
			848	523	155	165	5		
7	T	110	Total	C	N	O	S	0	0
			863	531	160	167	5		
7	U	106	Total	C	N	O	S	0	0
			832	514	150	163	5		

- Molecule 8 is a protein called Flagellar basal-body rod protein FlgC.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
8	W	132	Total	C	N	O	S	0	0
			964	601	166	192	5		
8	X	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
8	Y	133	Total	C	N	O	S	0	0
			969	604	167	193	5		
8	Z	131	Total	C	N	O	S	0	0
			956	595	165	191	5		
8	a	133	Total	C	N	O	S	0	0
			969	604	167	193	5		

- Molecule 9 is a protein called Flagellar M-ring protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	b	13	Total	C	N	O	0	0
			81	50	15	16		
9	c	16	Total	C	N	O	0	0
			103	64	19	20		
9	d	20	Total	C	N	O	0	0
			133	83	23	27		
9	e	16	Total	C	N	O	0	0
			103	64	19	20		
9	f	21	Total	C	N	O	0	0
			140	88	24	28		
9	g	16	Total	C	N	O	0	0
			103	64	19	20		
9	h	21	Total	C	N	O	0	0
			140	88	24	28		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	i	16	Total	C	N	O	0	0
			103	64	19	20		
9	j	20	Total	C	N	O	0	0
			133	83	23	27		
9	k	16	Total	C	N	O	0	0
			103	64	19	20		
9	l	21	Total	C	N	O	0	0
			140	88	24	28		

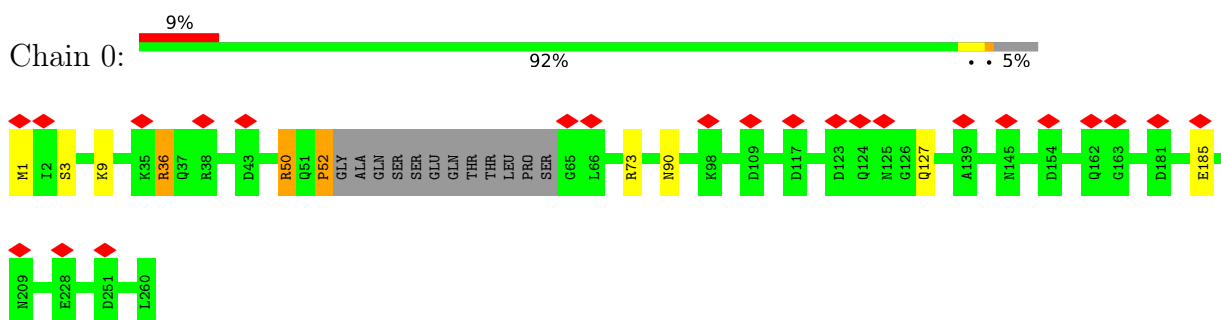
- Molecule 10 is a protein called Flagellar basal-body rod protein FlgF.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	248	Total	C	N	O	S	0	0
			1804	1106	324	367	7		
10	n	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		
10	o	250	Total	C	N	O	S	0	0
			1820	1116	326	369	9		
10	p	250	Total	C	N	O	S	0	0
			1820	1116	326	369	9		
10	q	249	Total	C	N	O	S	0	0
			1812	1111	325	368	8		

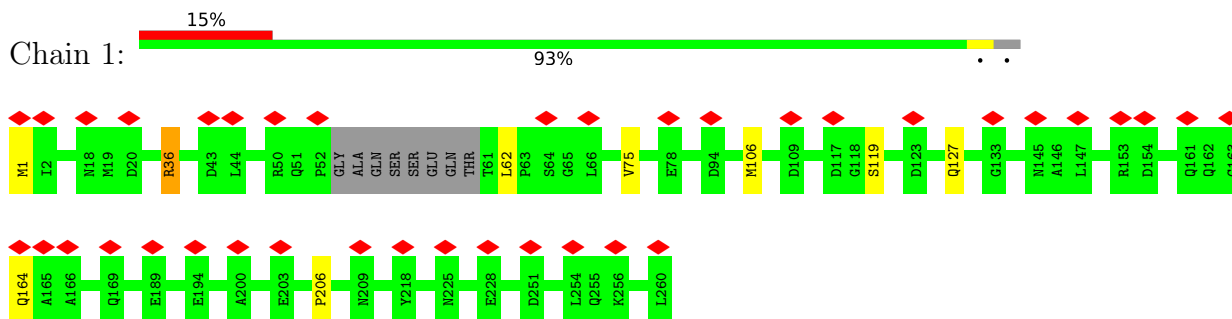
3 Residue-property plots [i](#)

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

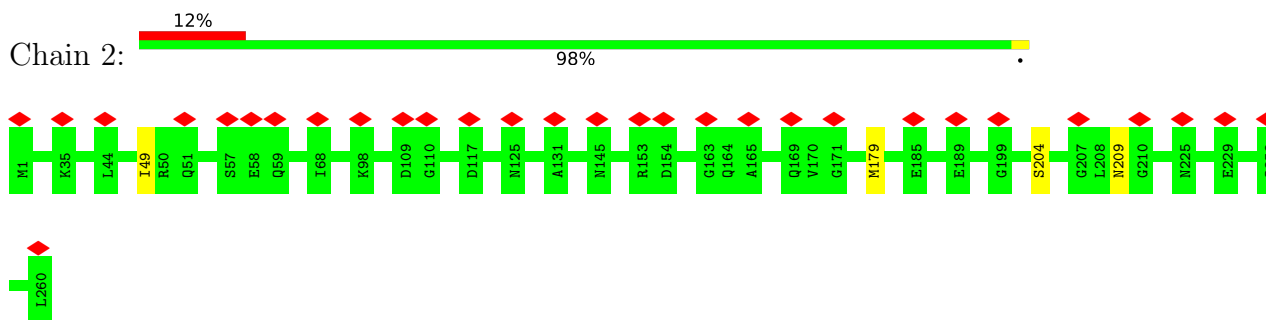
- Molecule 1: Flagellar basal-body rod protein FlgG



- Molecule 1: Flagellar basal-body rod protein FlgG

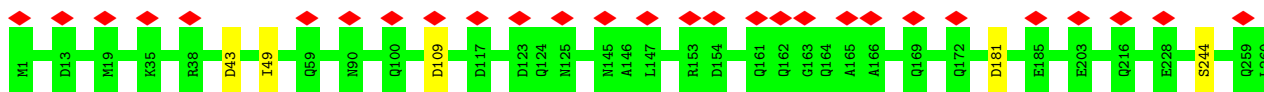


- Molecule 1: Flagellar basal-body rod protein FlgG

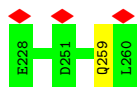
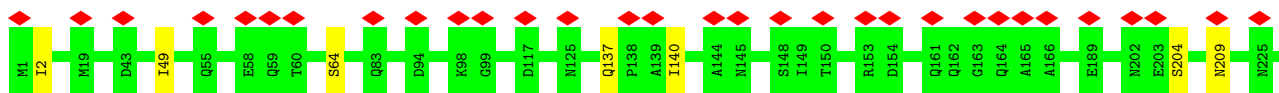


- Molecule 1: Flagellar basal-body rod protein FlgG

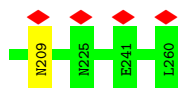
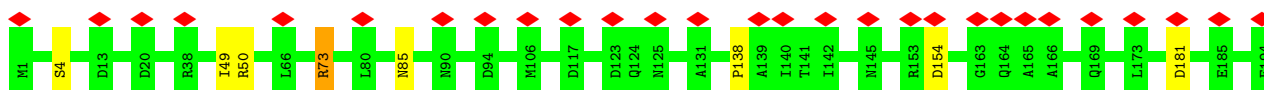




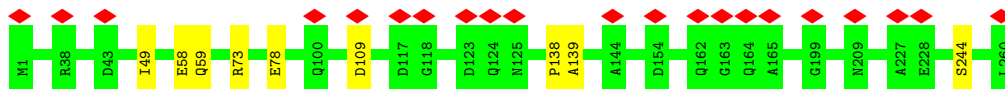
- Molecule 1: Flagellar basal-body rod protein FlgG



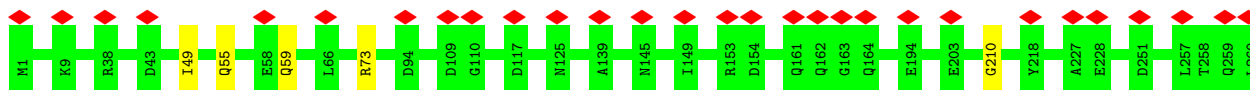
- Molecule 1: Flagellar basal-body rod protein FlgG



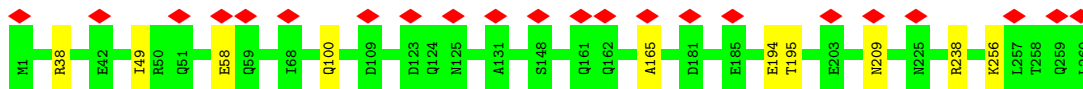
- Molecule 1: Flagellar basal-body rod protein FlgG



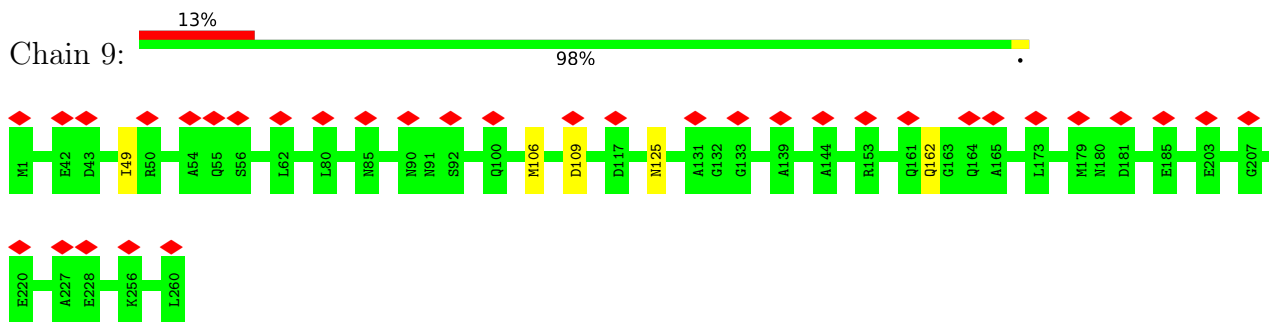
- Molecule 1: Flagellar basal-body rod protein FlgG



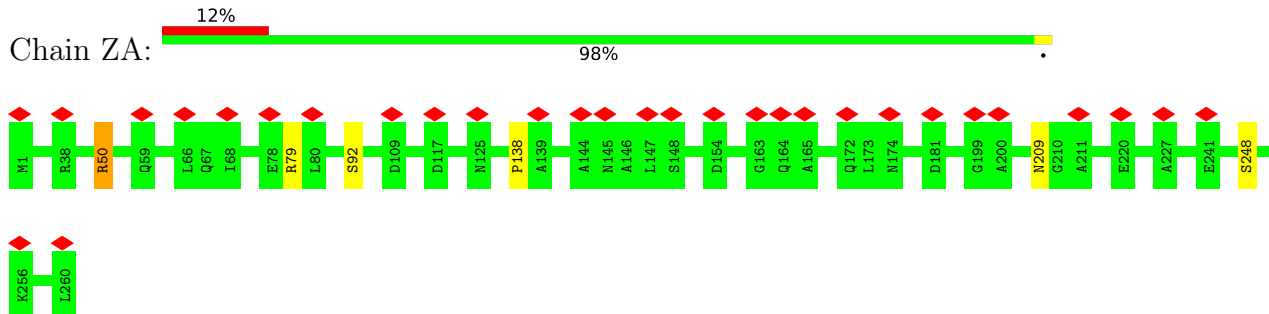
- Molecule 1: Flagellar basal-body rod protein FlgG



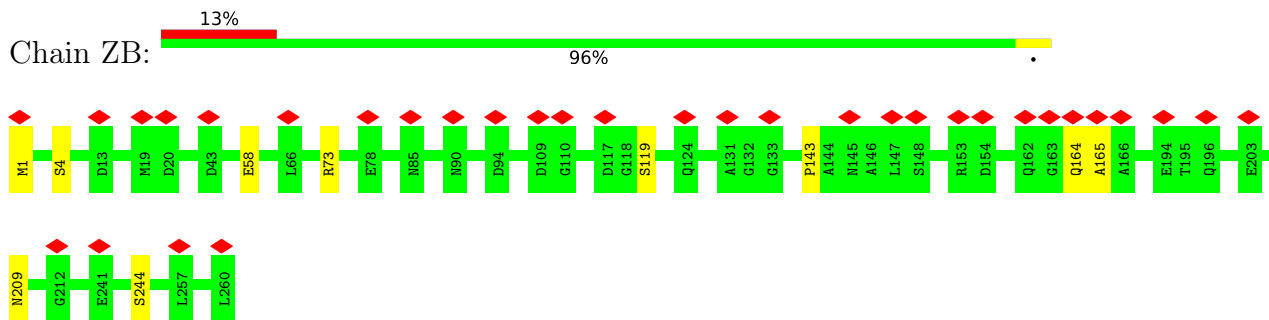
- Molecule 1: Flagellar basal-body rod protein FlgG



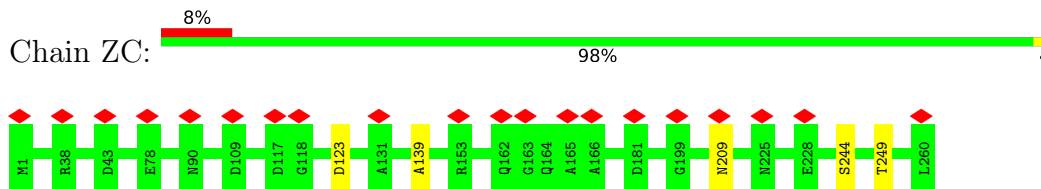
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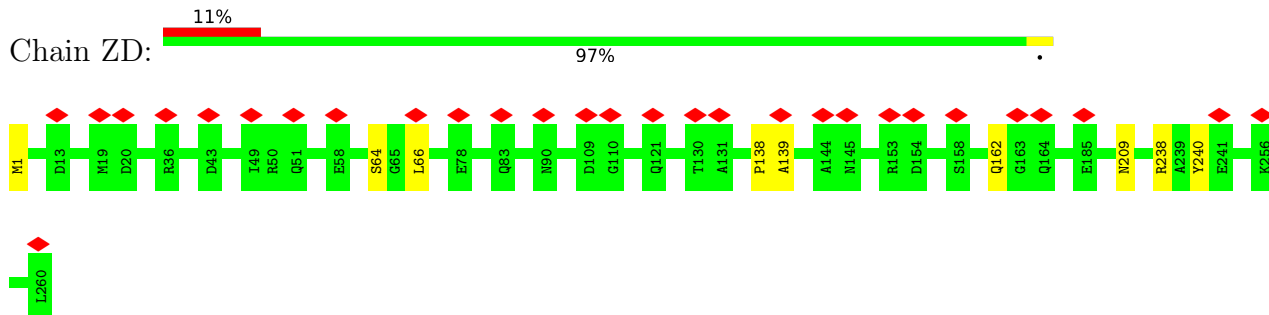
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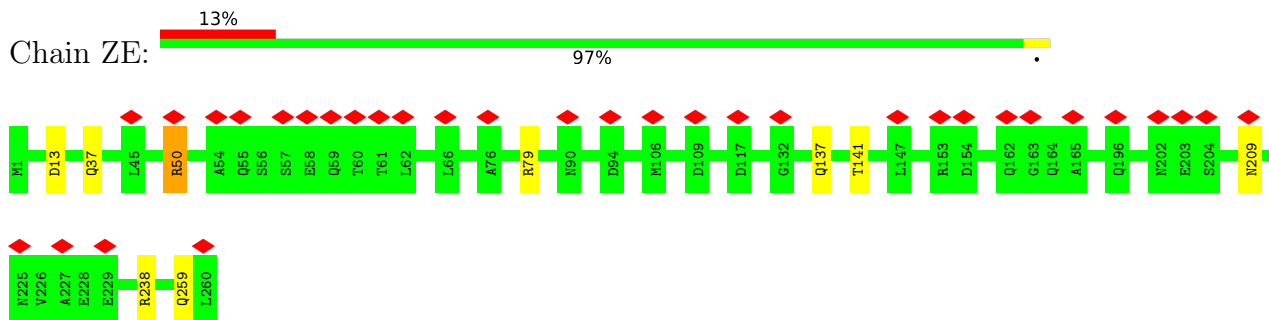
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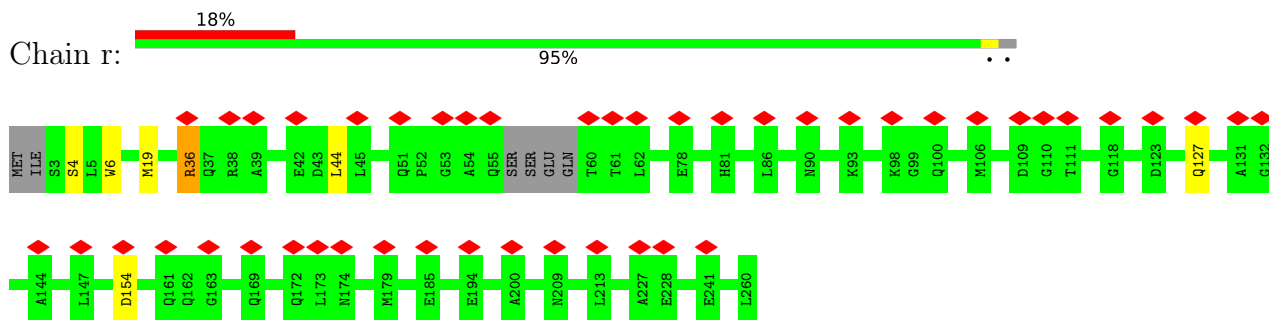
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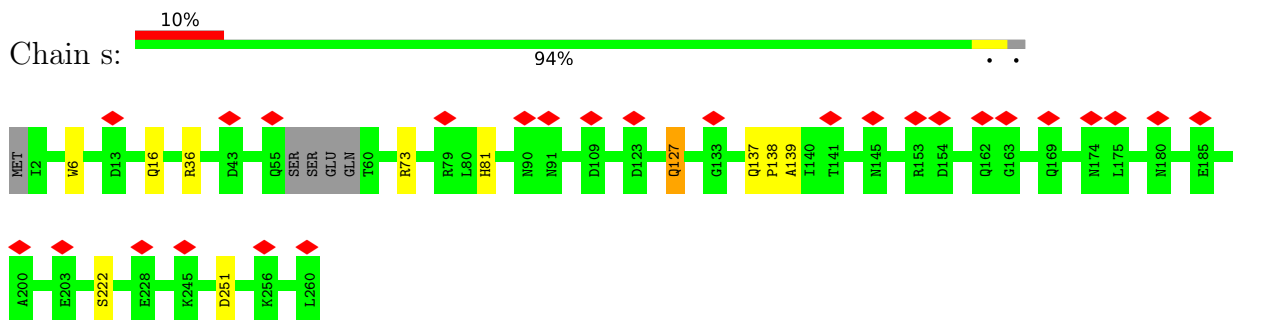
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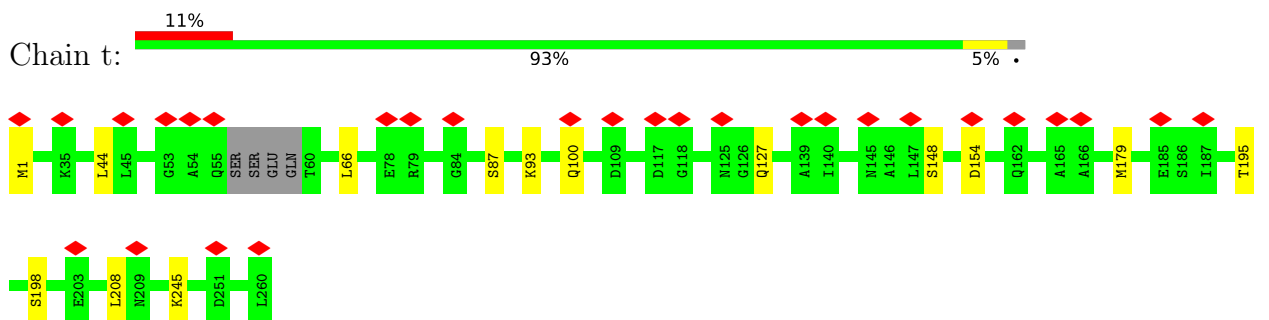
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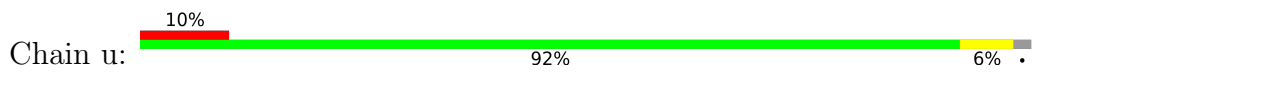
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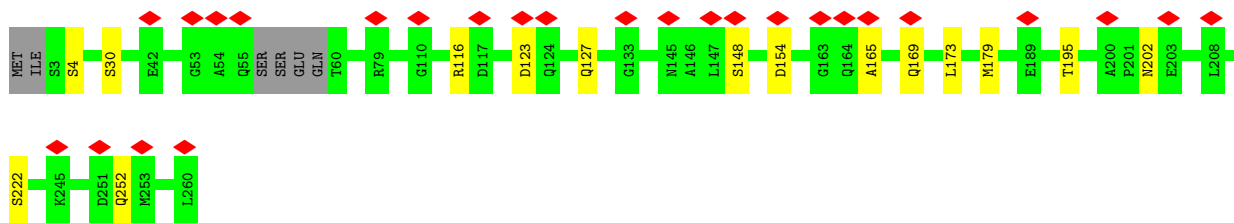


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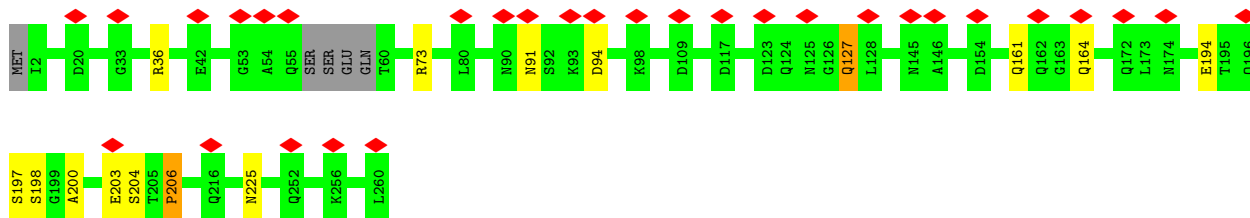
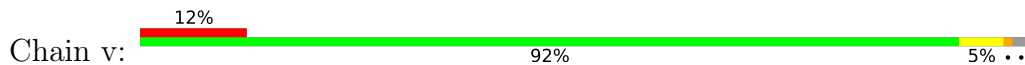


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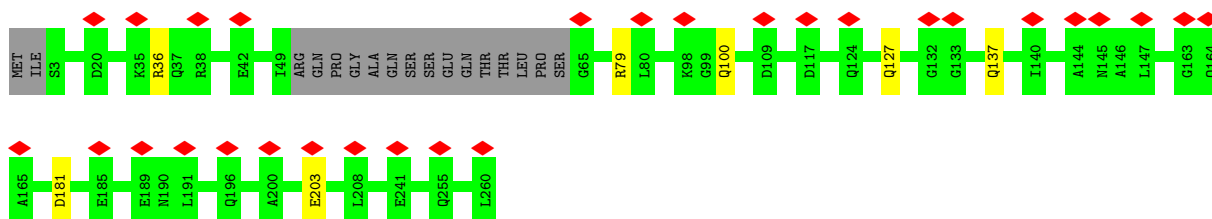
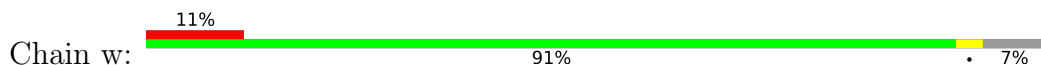




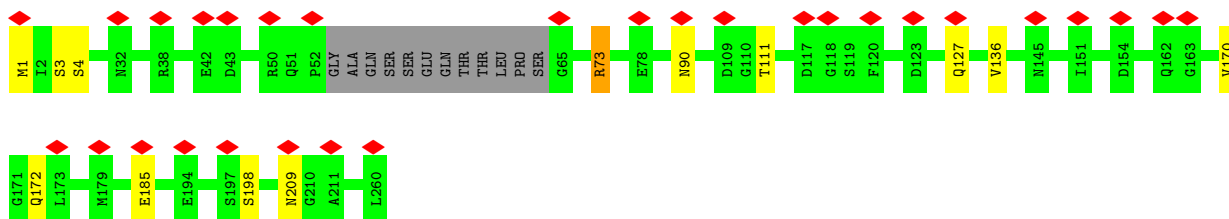
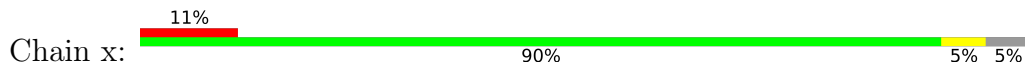
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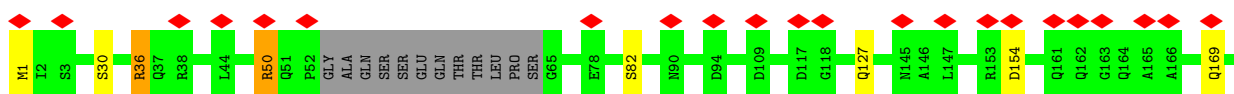
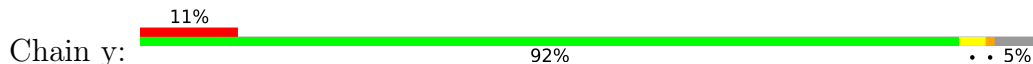
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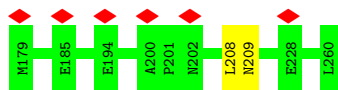


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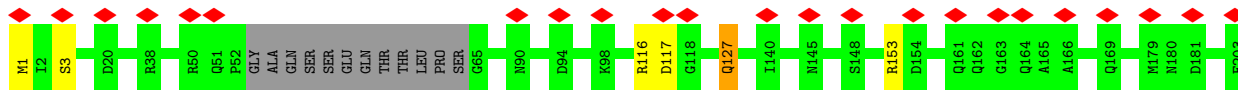
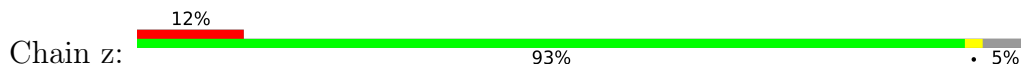


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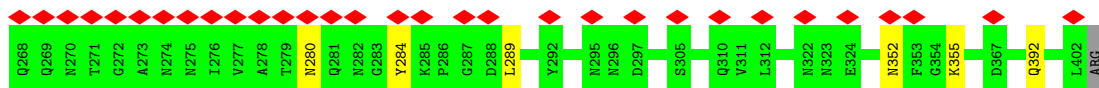
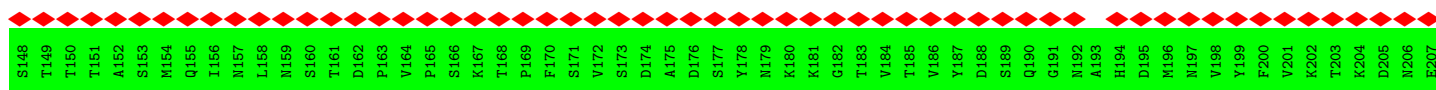
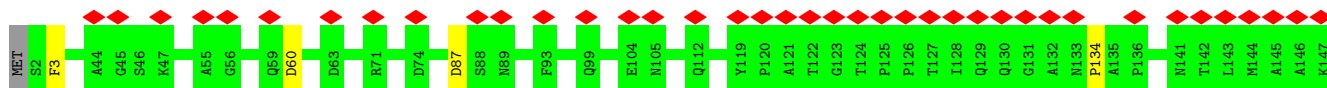




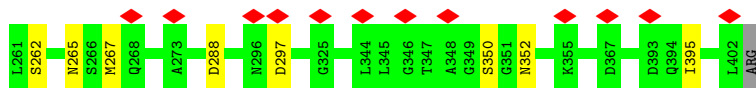
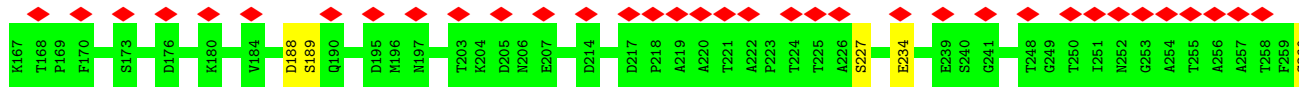
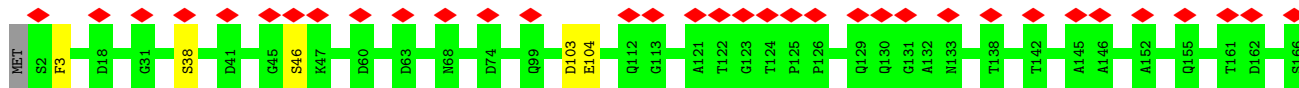
• Molecule 1: Flagellar basal-body rod protein FlgG



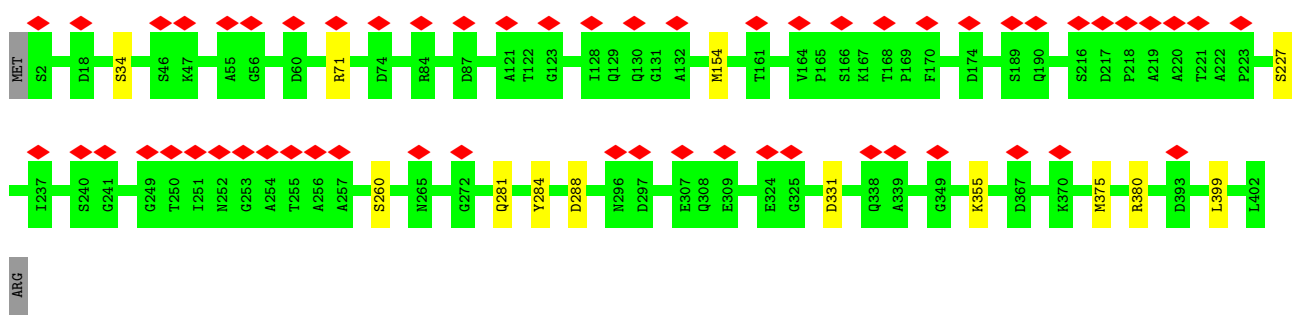
• Molecule 2: Flagellar hook protein FlgE



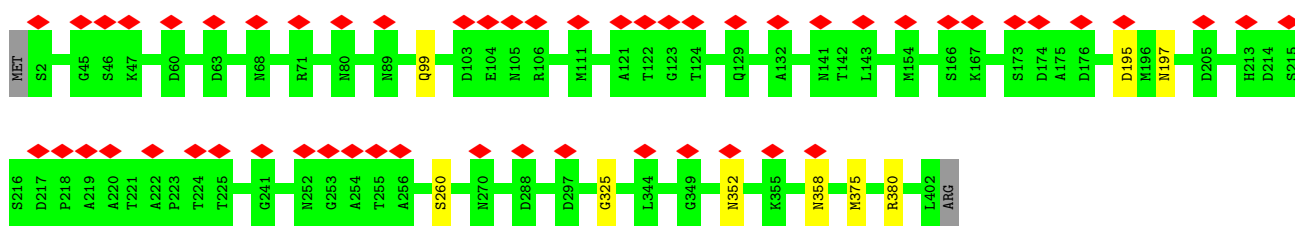
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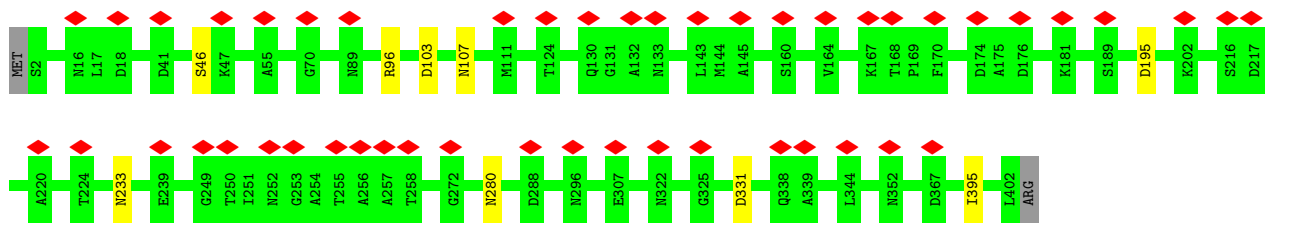
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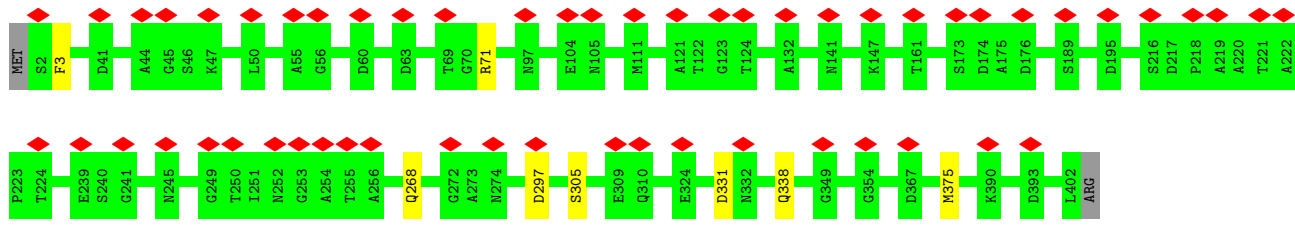
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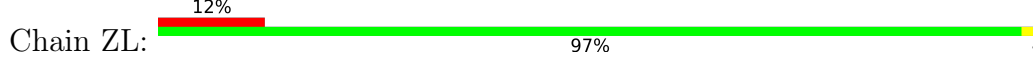
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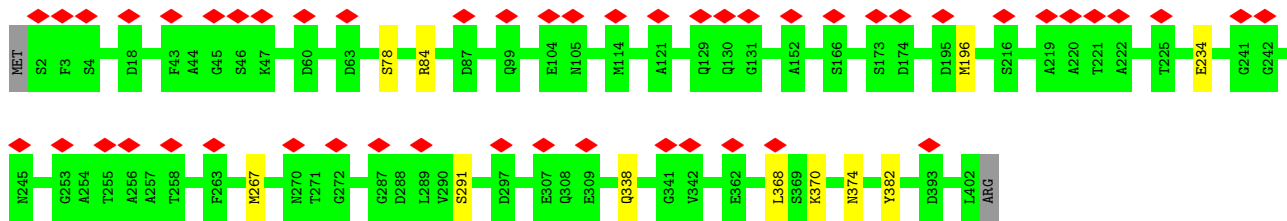


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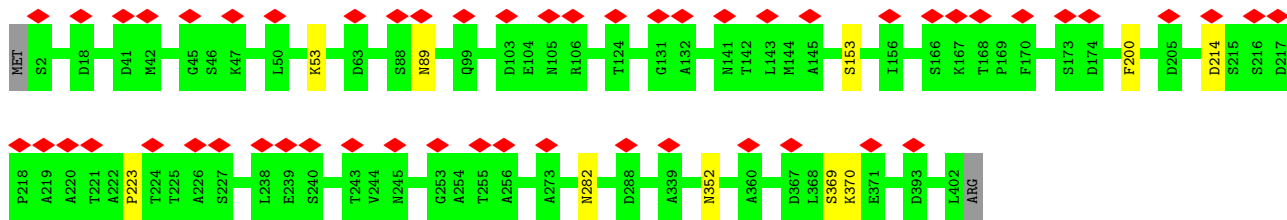


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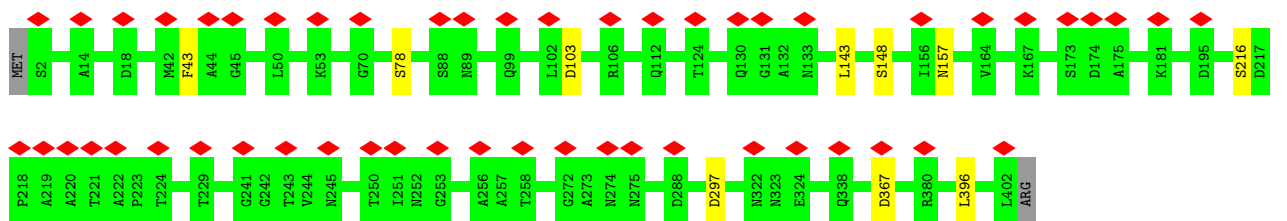




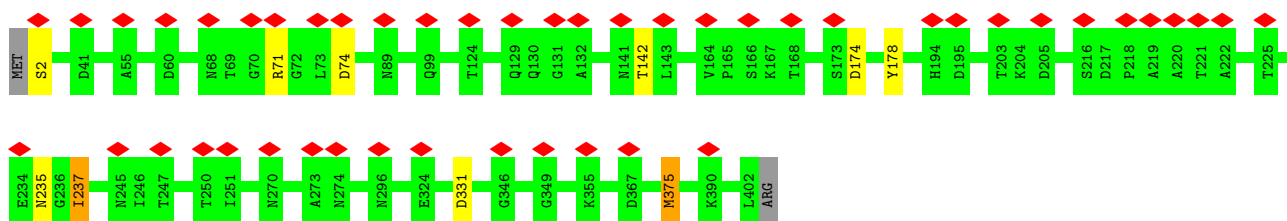
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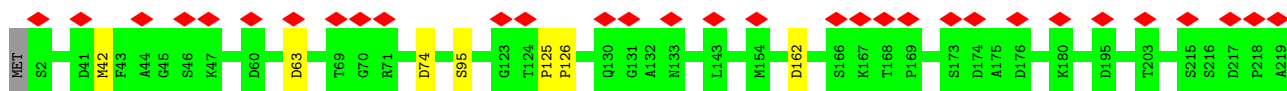
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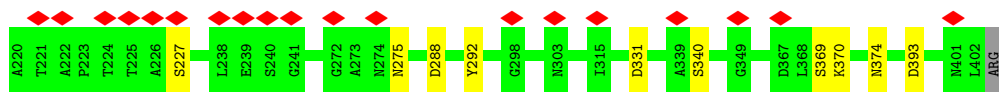


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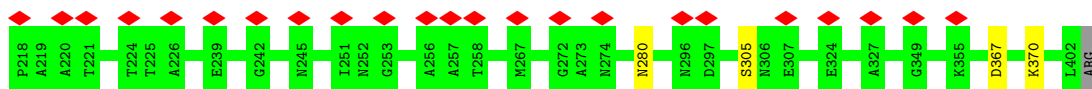
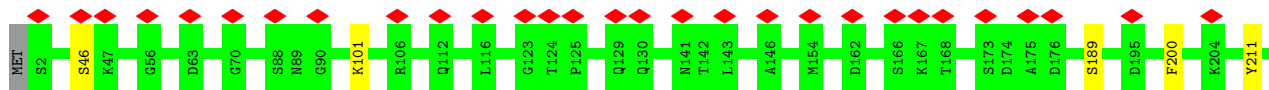


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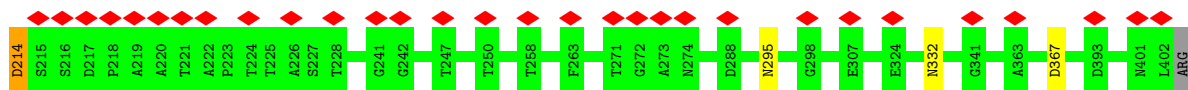
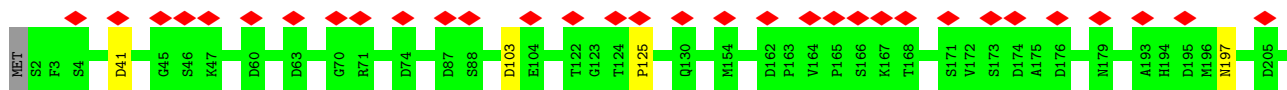




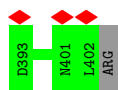
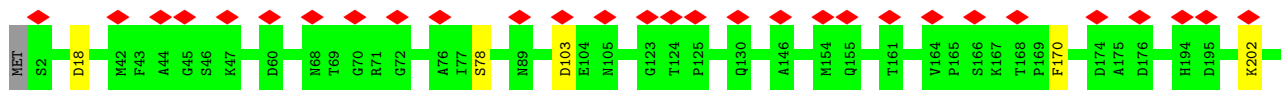
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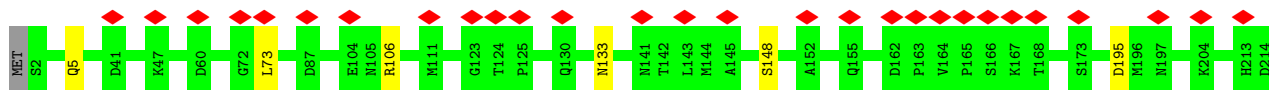
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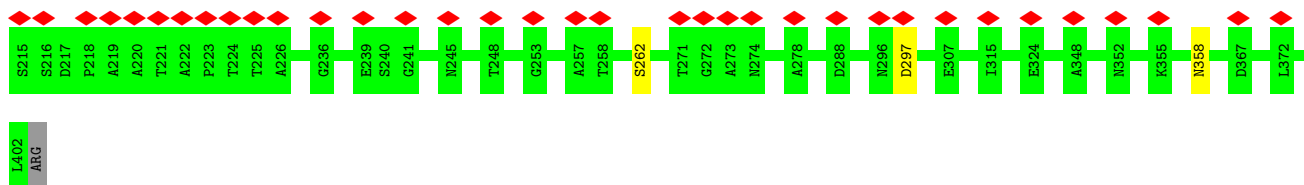


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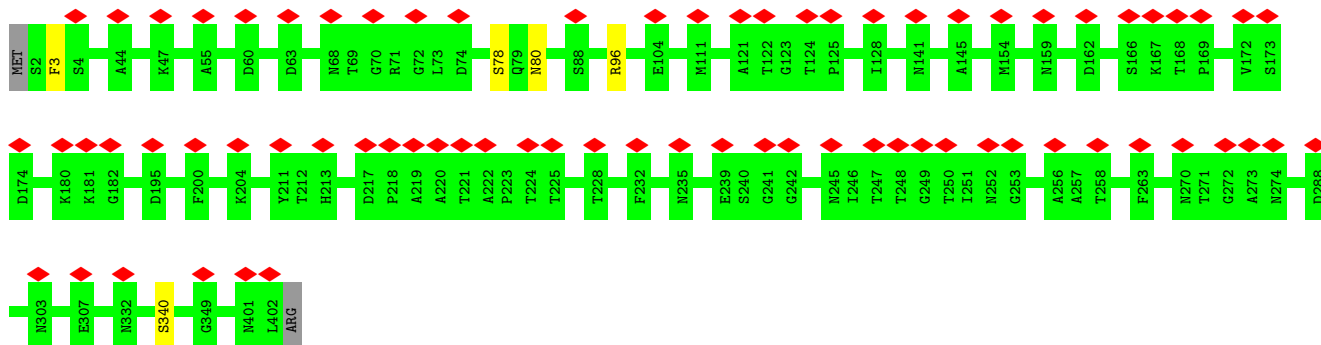


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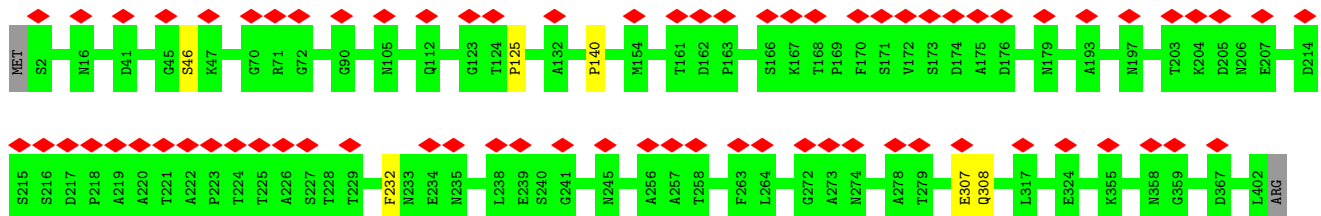




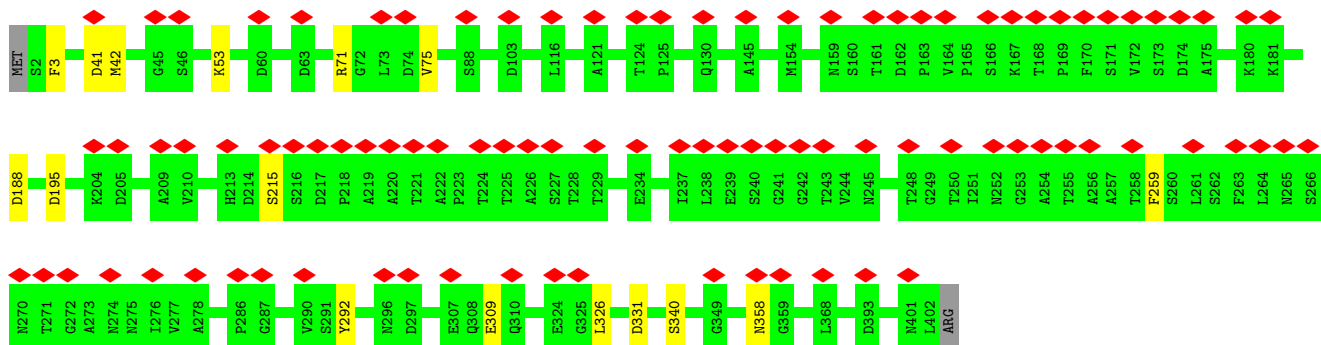
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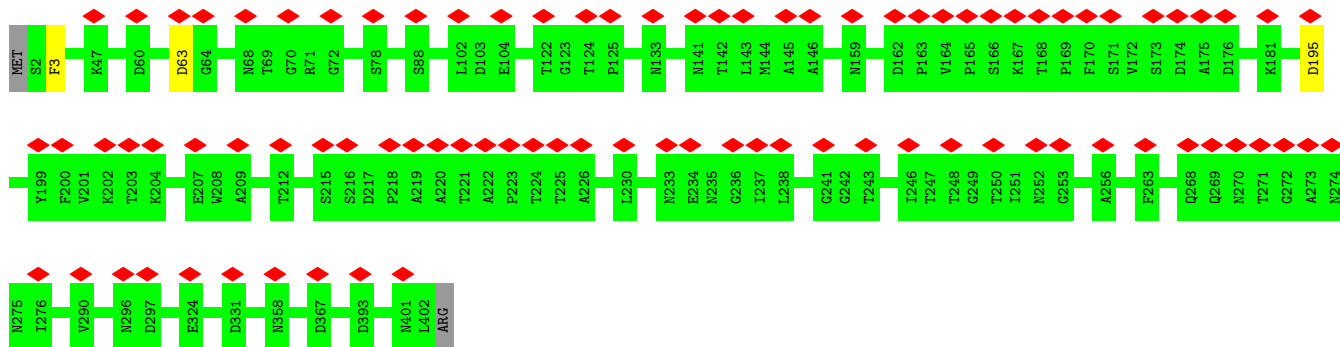


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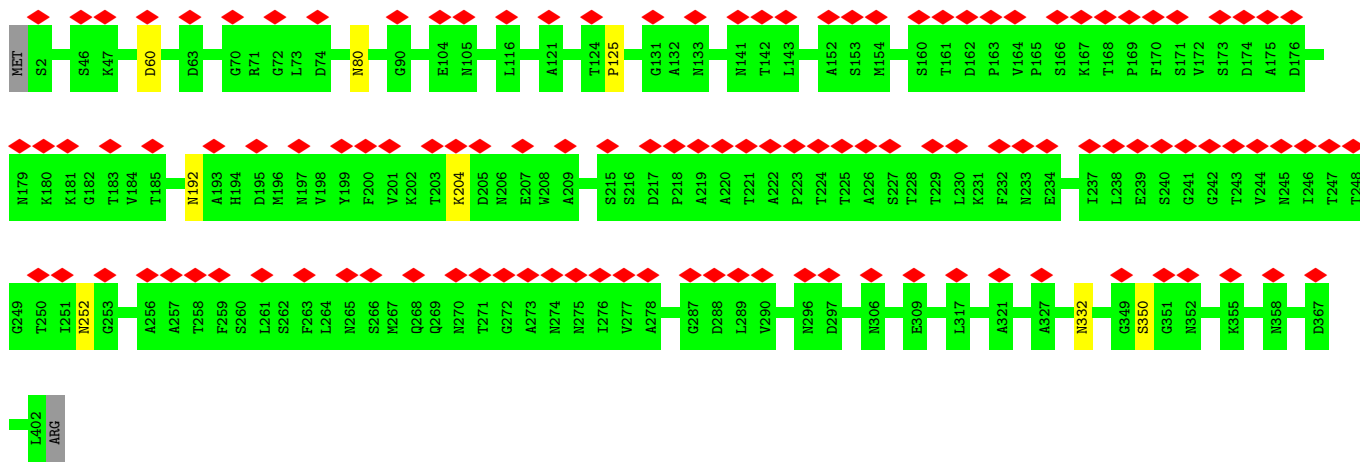


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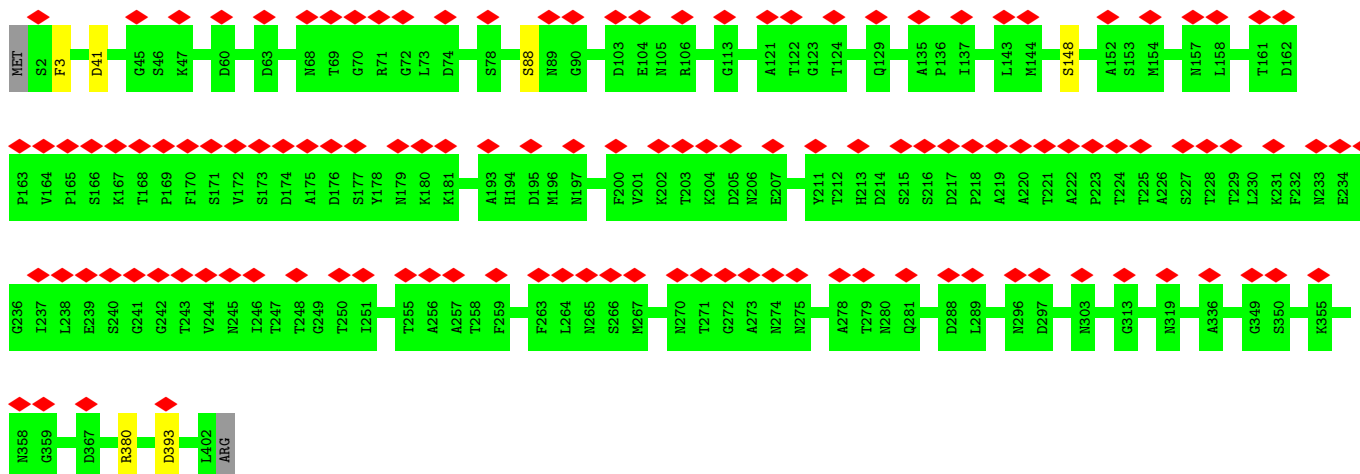




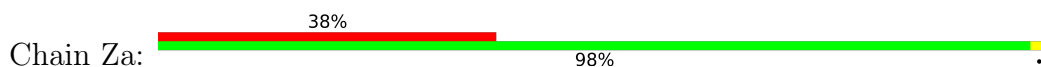
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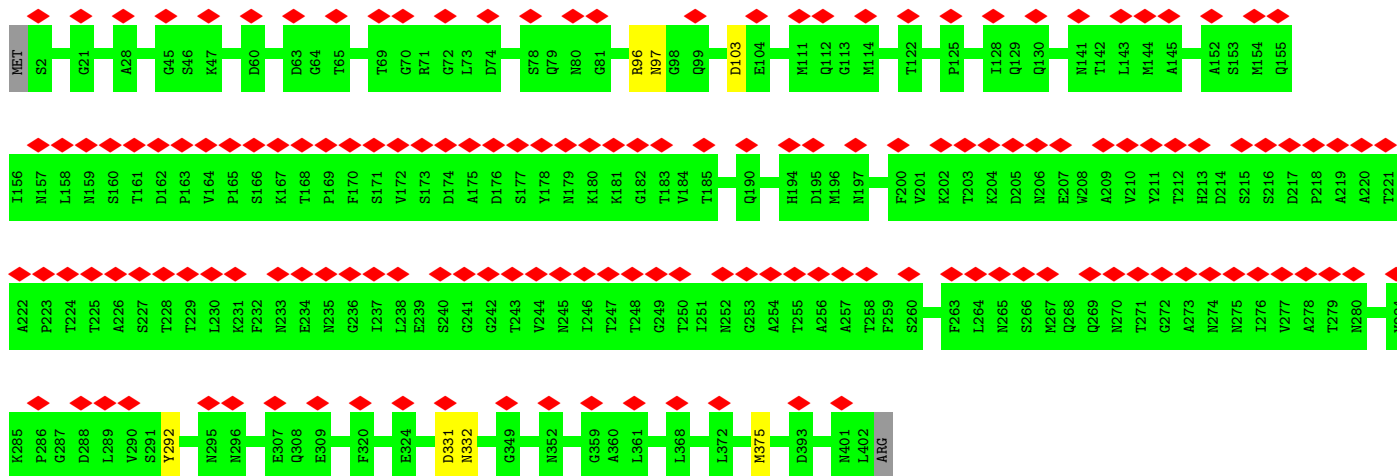


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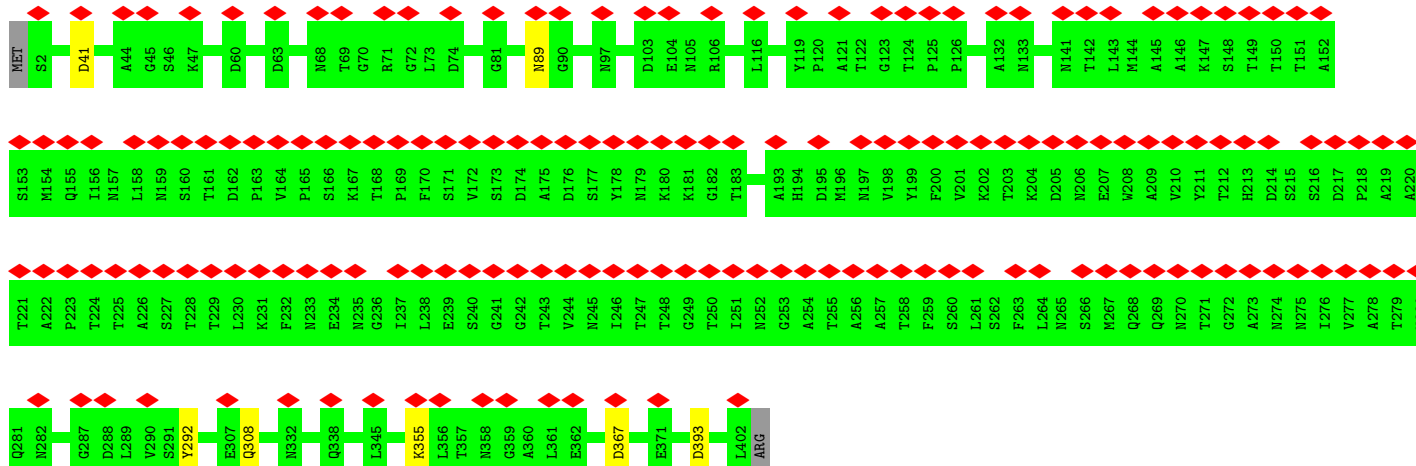


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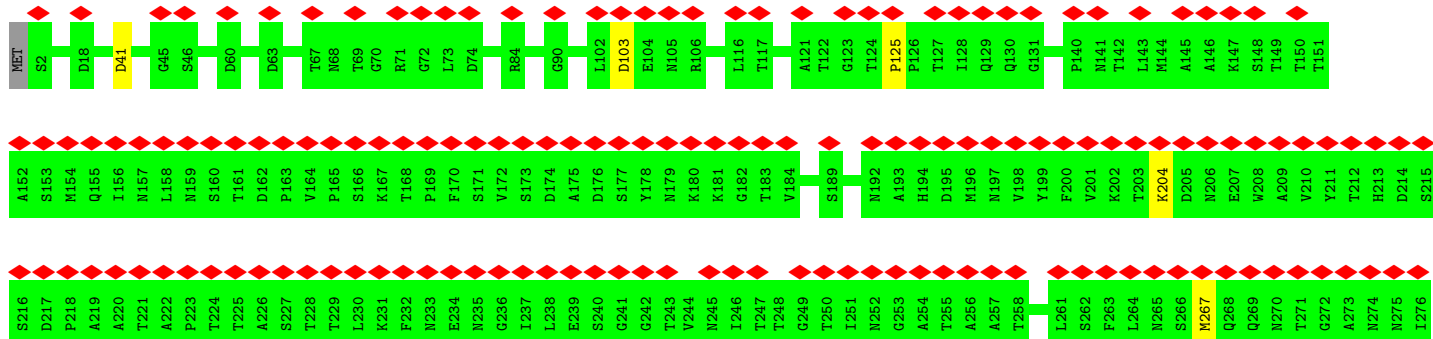
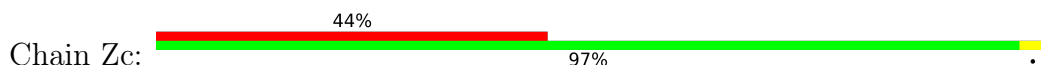


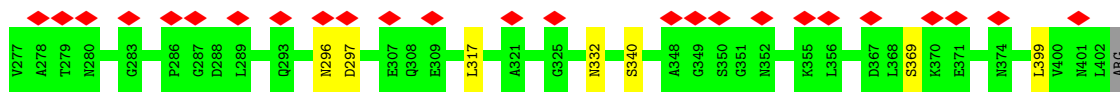


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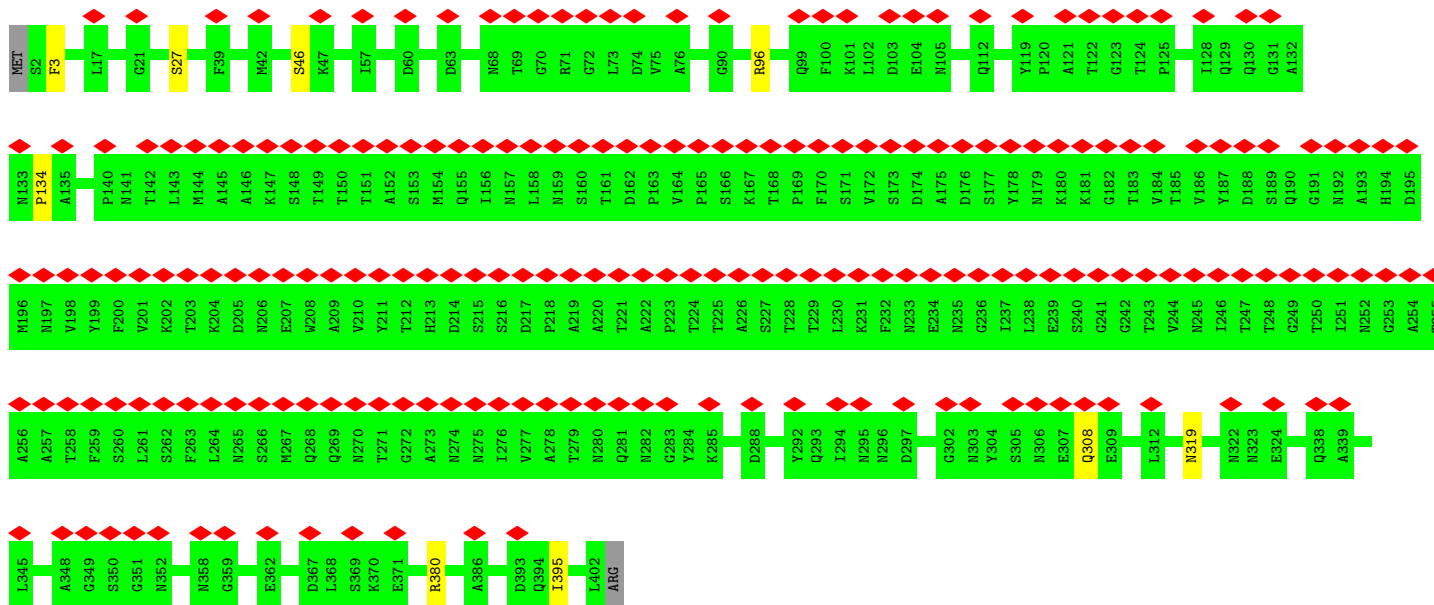




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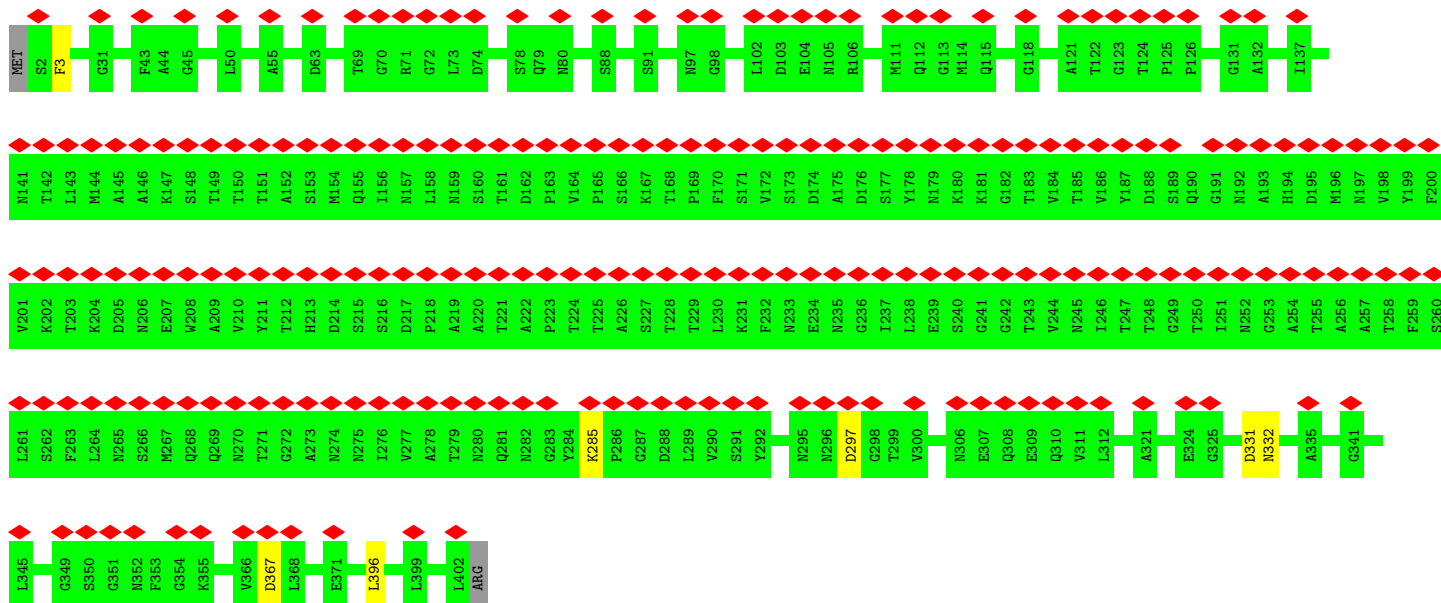


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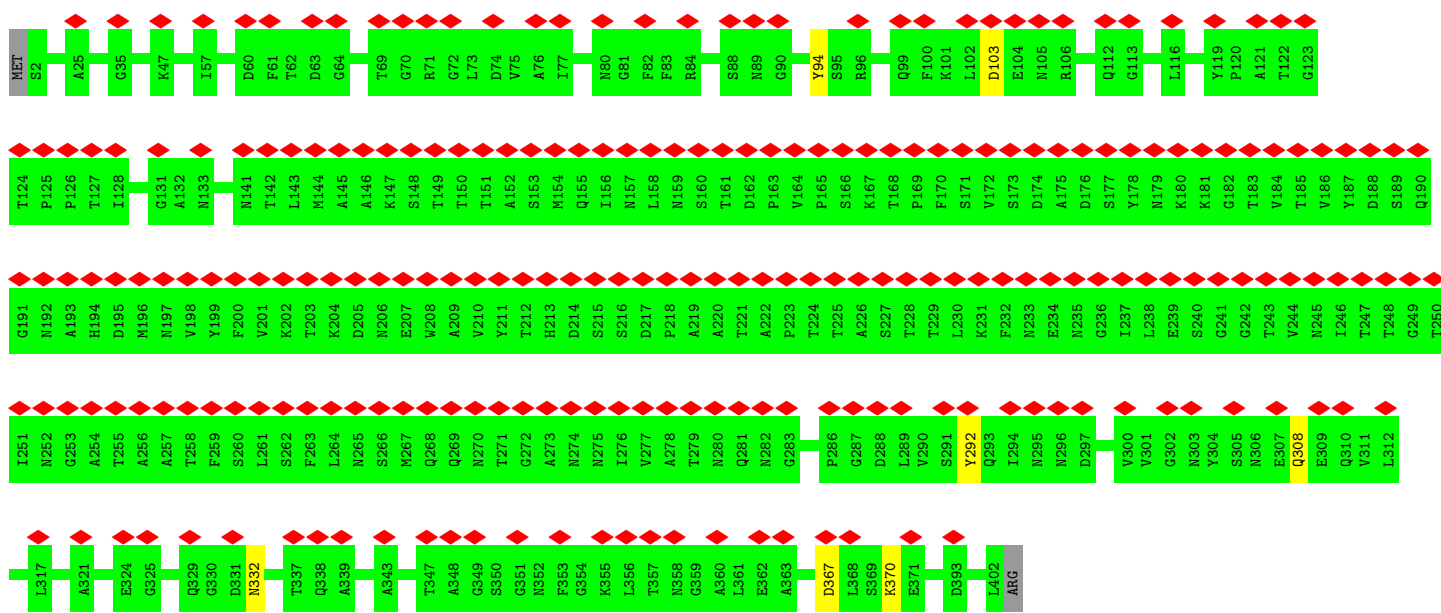


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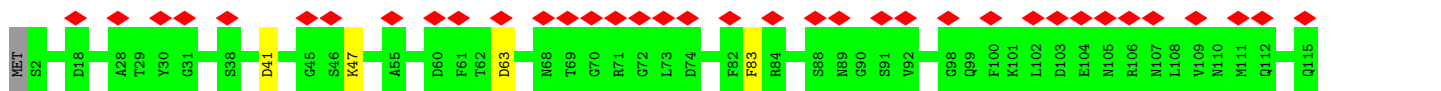


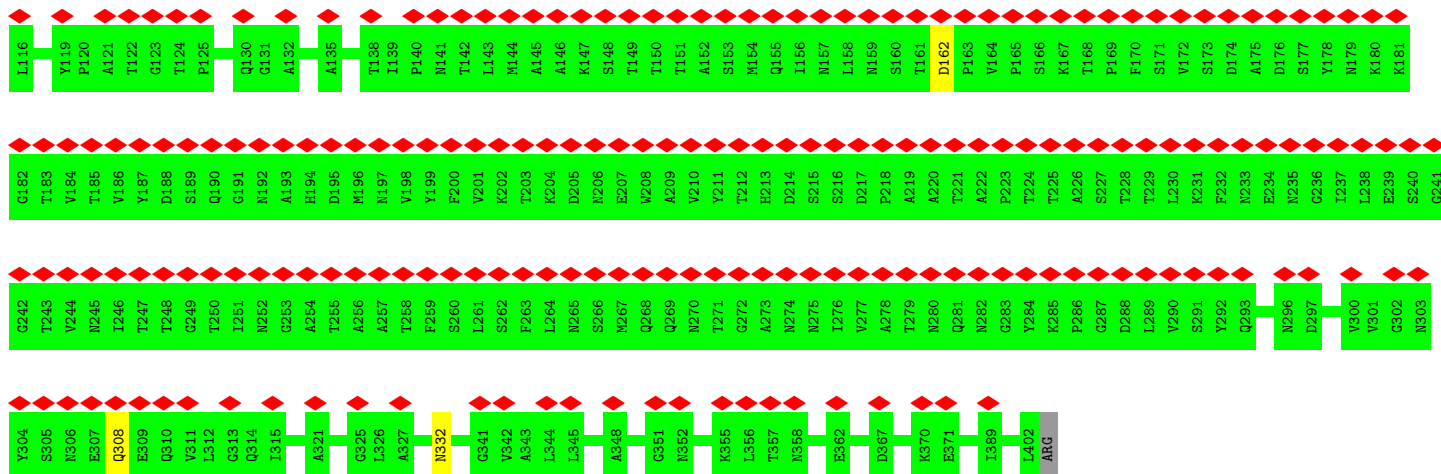


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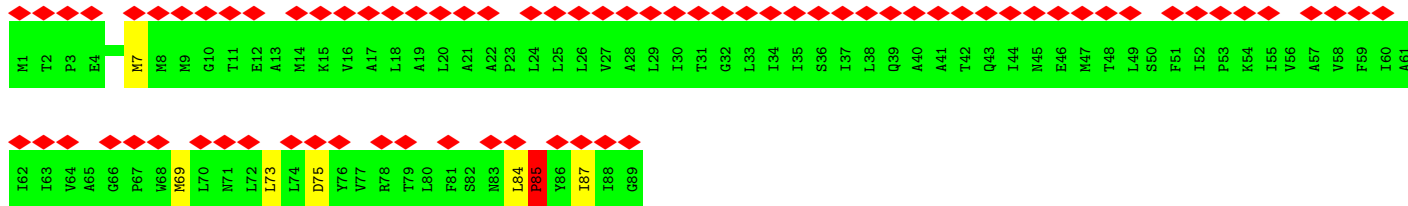
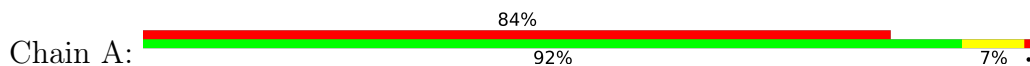


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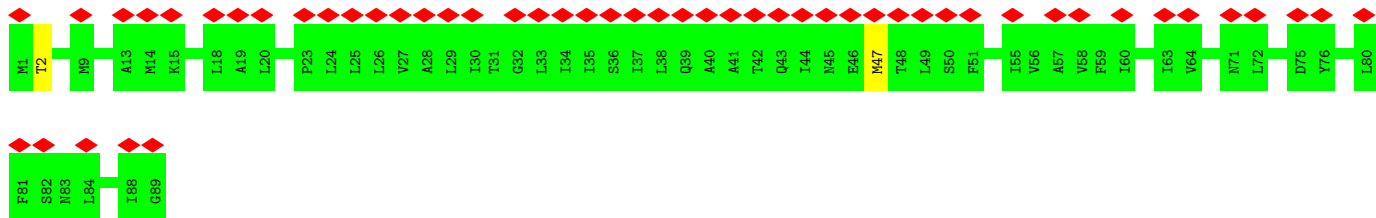




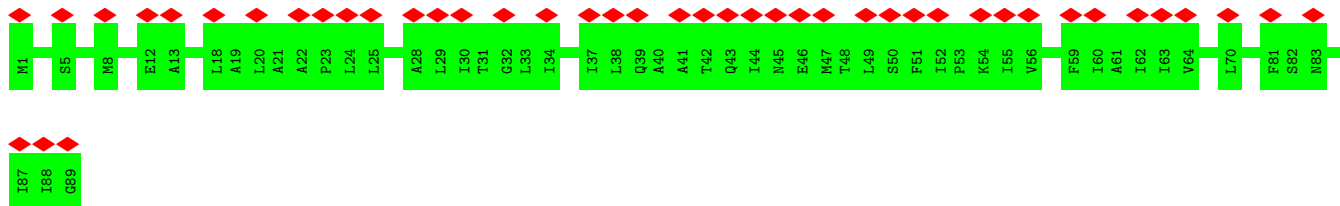
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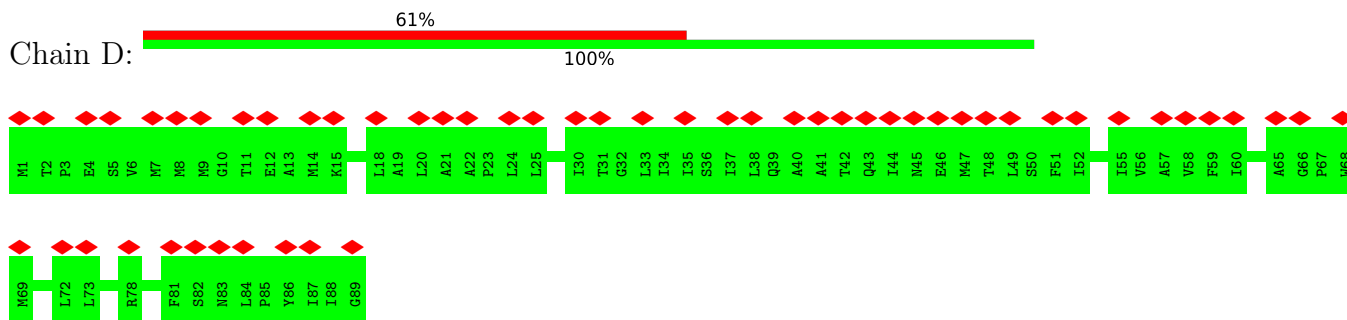
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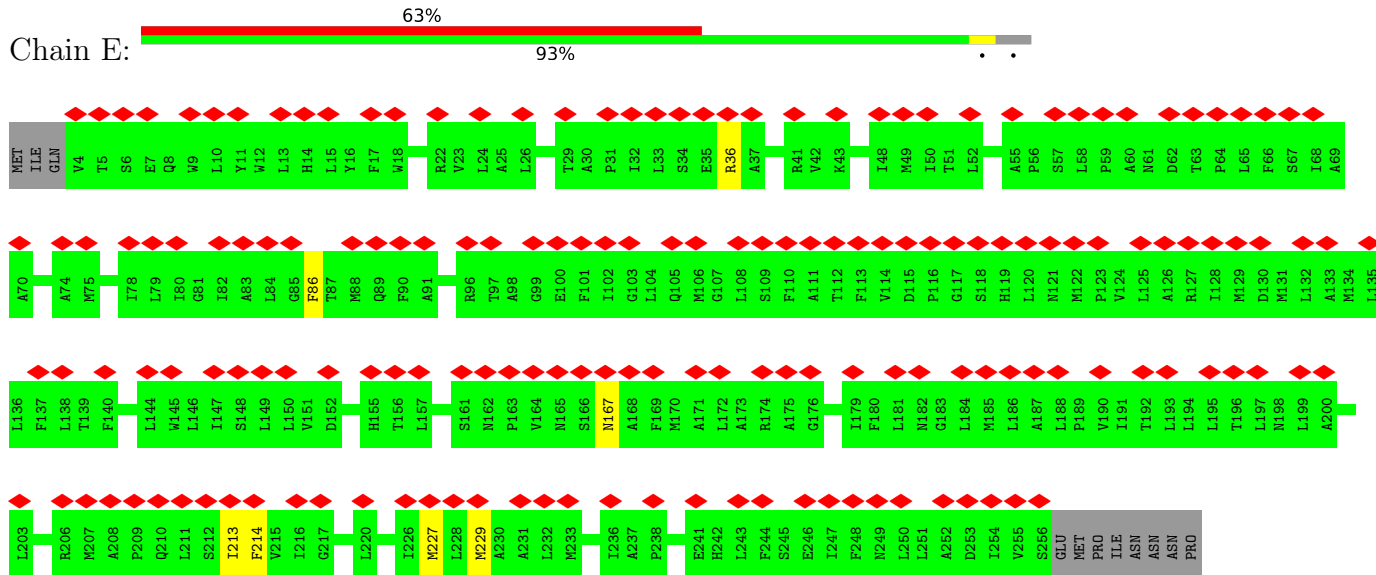
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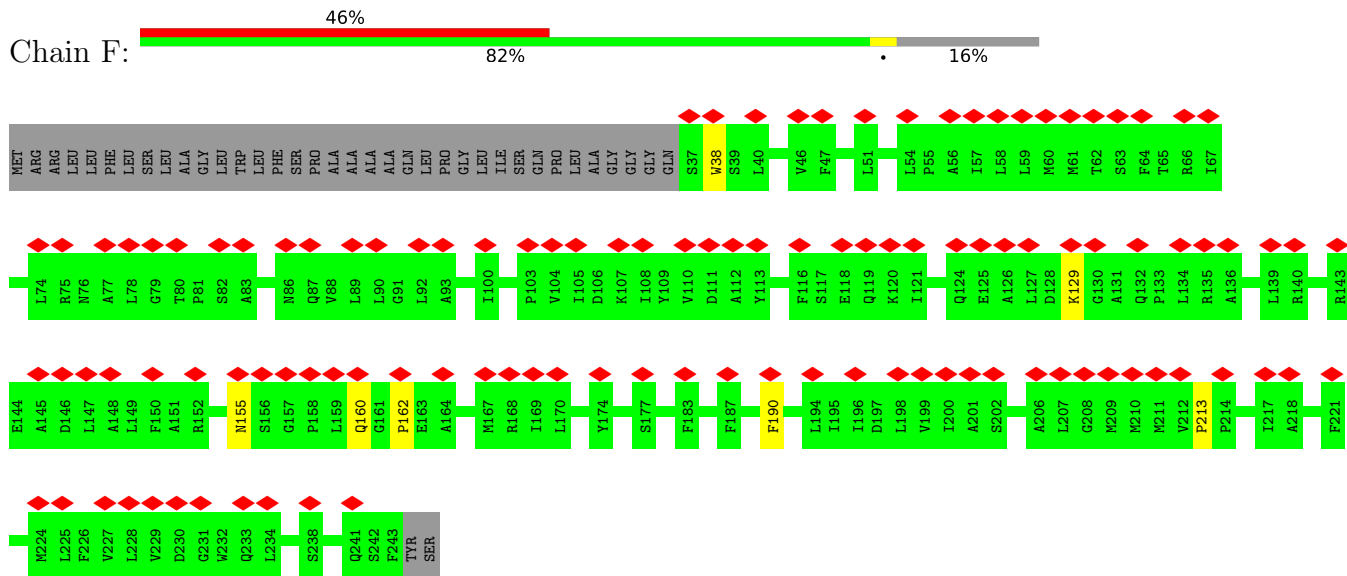
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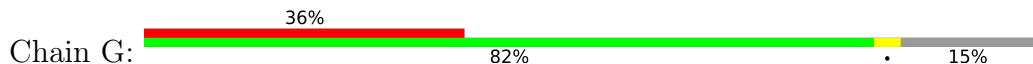
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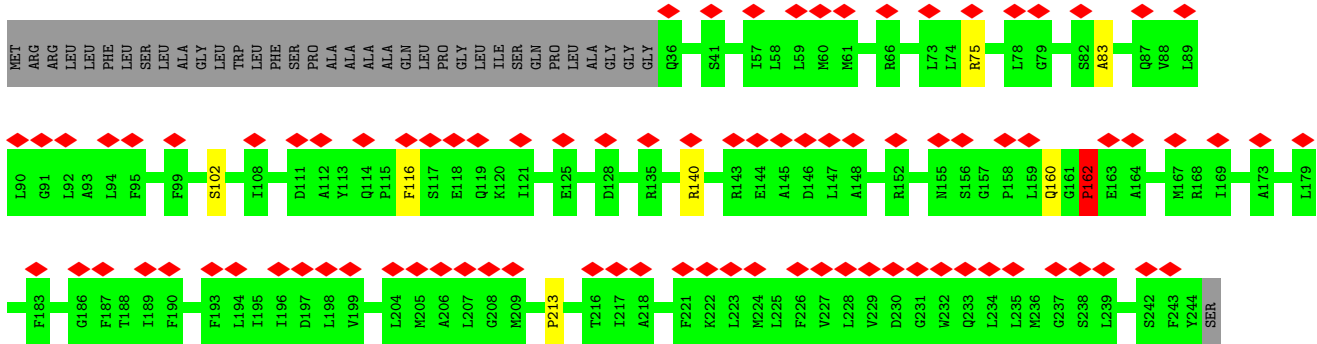


• Molecule 5: Flagellar biosynthetic protein FliP

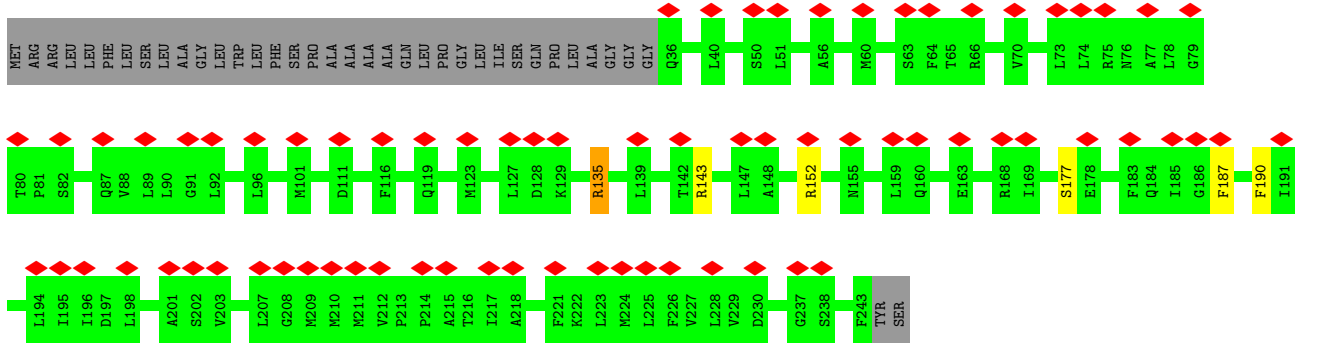
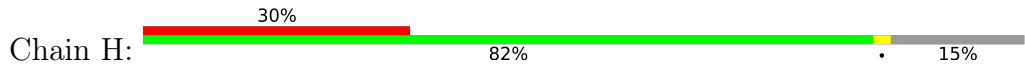


• Molecule 5: Flagellar biosynthetic protein FliP

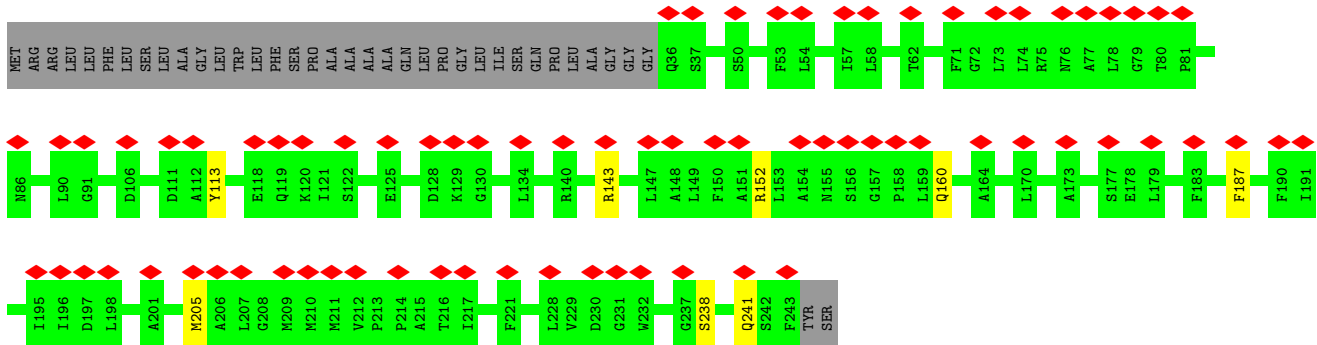
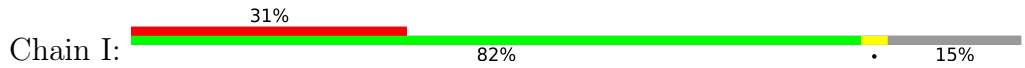




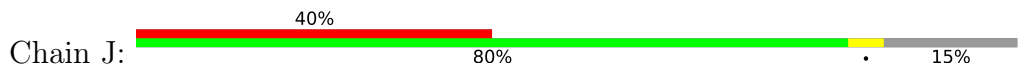
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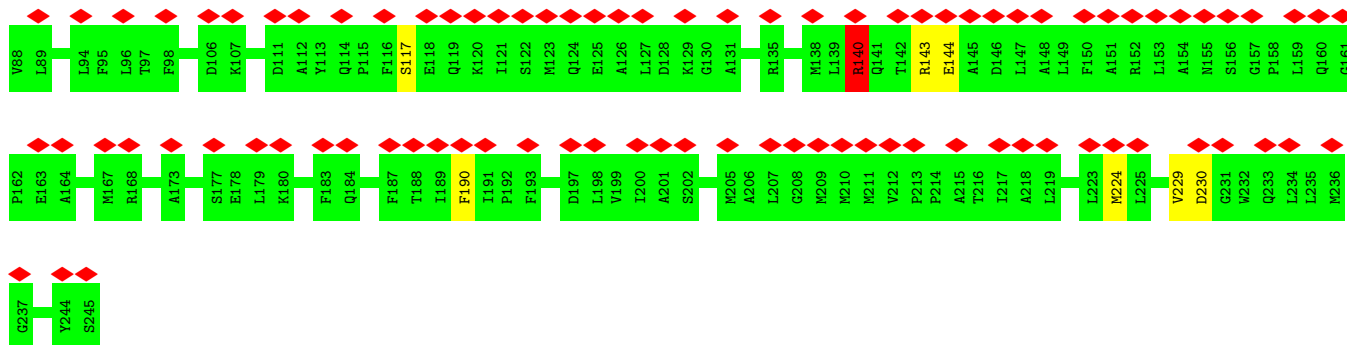


• Molecule 5: Flagellar biosynthetic protein FliP

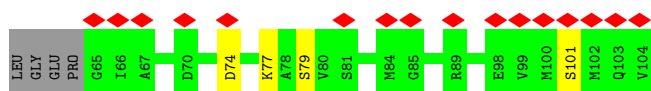
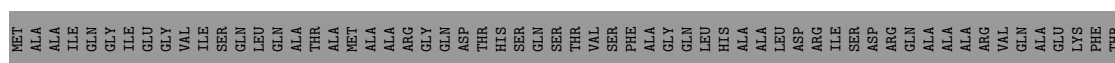


• Molecule 5: Flagellar biosynthetic protein FliP

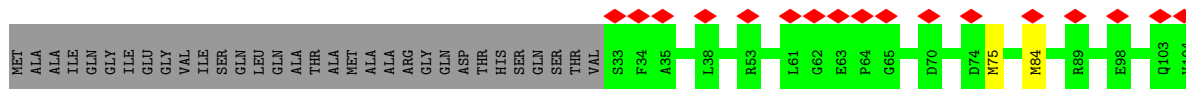




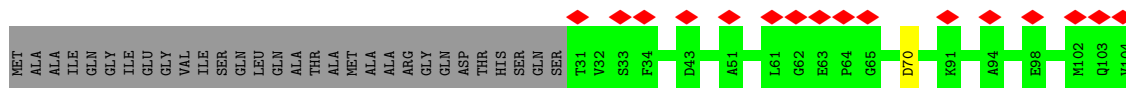
• Molecule 6: Flagellar hook-basal body complex protein FliE



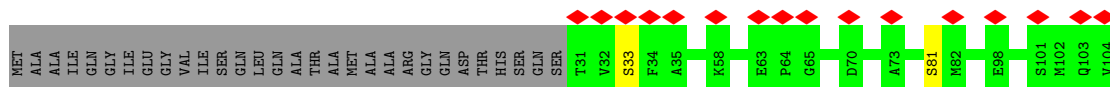
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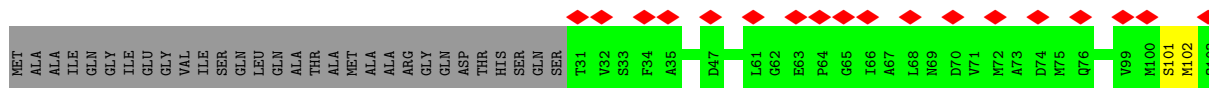
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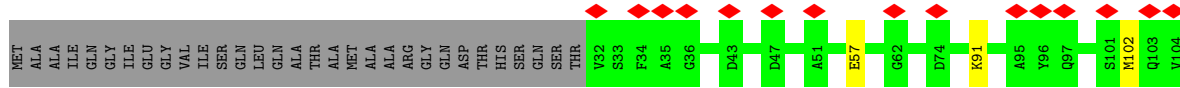


• Molecule 6: Flagellar hook-basal body complex protein FliE

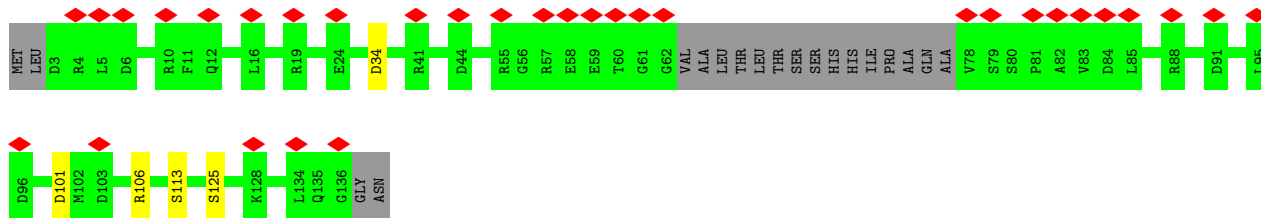
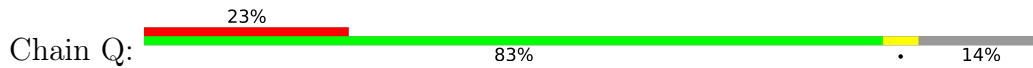


V104

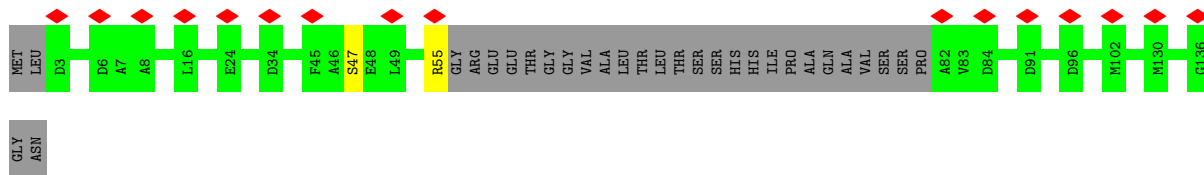
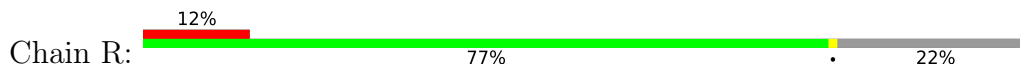
• Molecule 6: Flagellar hook-basal body complex protein FliE



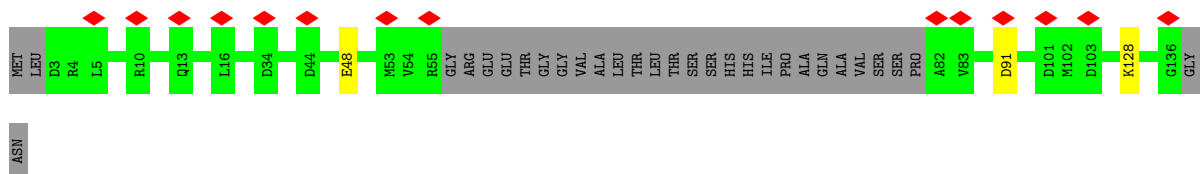
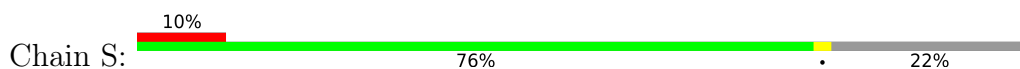
• Molecule 7: Flagellar basal body rod protein FlgB



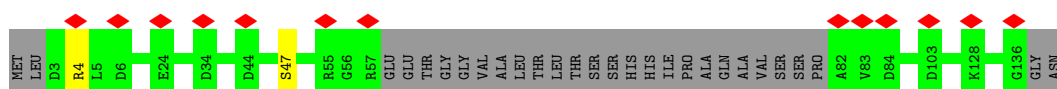
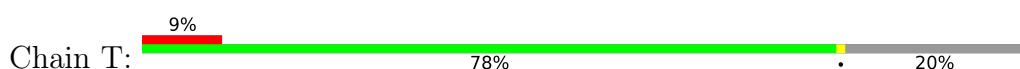
• Molecule 7: Flagellar basal body rod protein FlgB



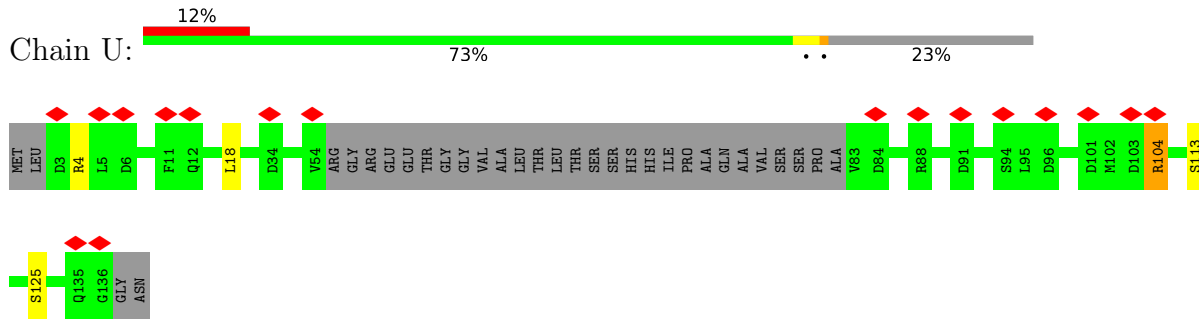
• Molecule 7: Flagellar basal body rod protein FlgB



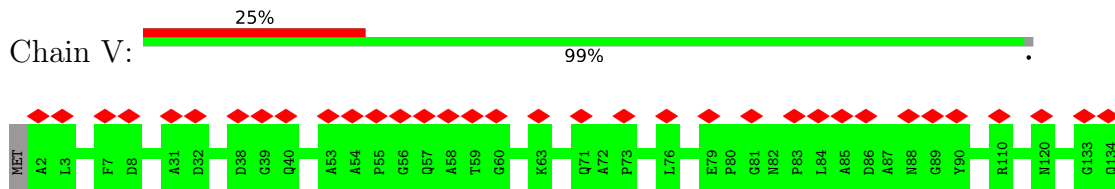
• Molecule 7: Flagellar basal body rod protein FlgB



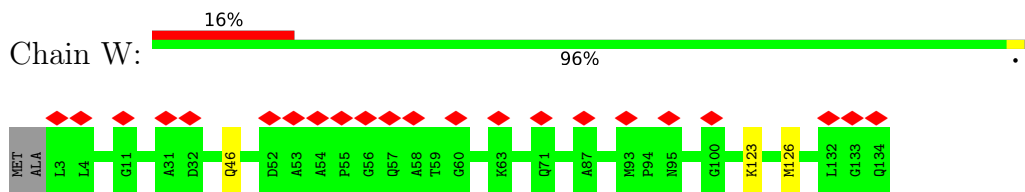
- Molecule 7: Flagellar basal body rod protein FlgB



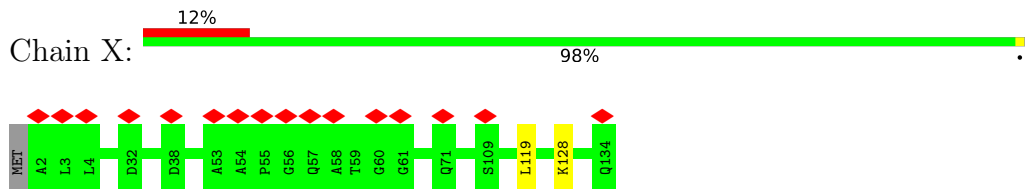
- Molecule 8: Flagellar basal-body rod protein FlgC



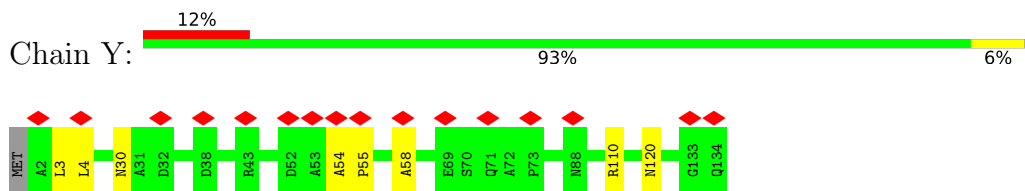
- Molecule 8: Flagellar basal-body rod protein FlgC



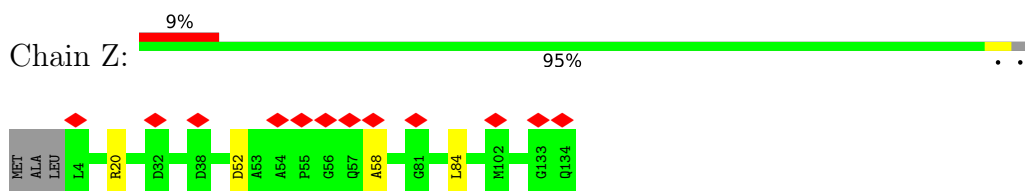
- Molecule 8: Flagellar basal-body rod protein FlgC



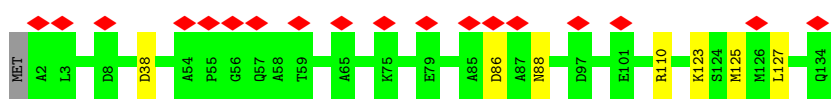
- Molecule 8: Flagellar basal-body rod protein FlgC



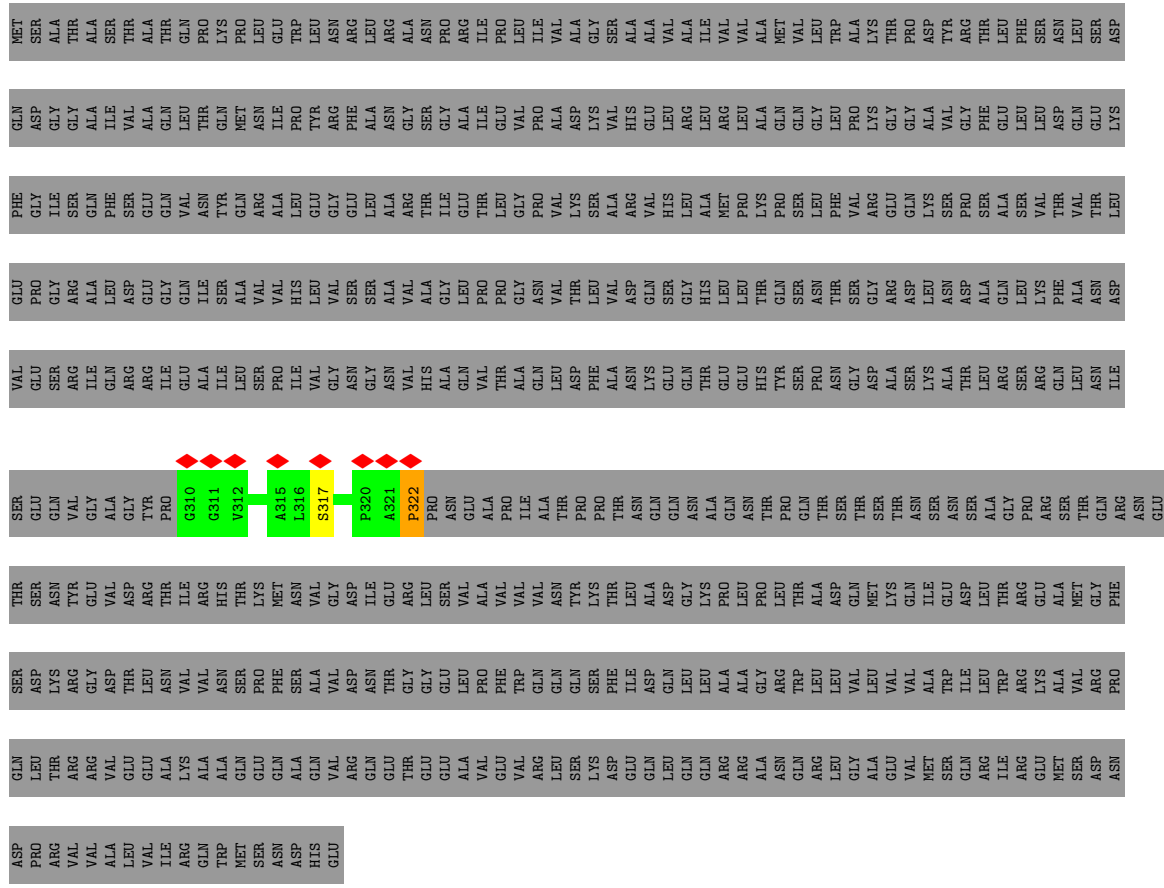
- Molecule 8: Flagellar basal-body rod protein FlgC



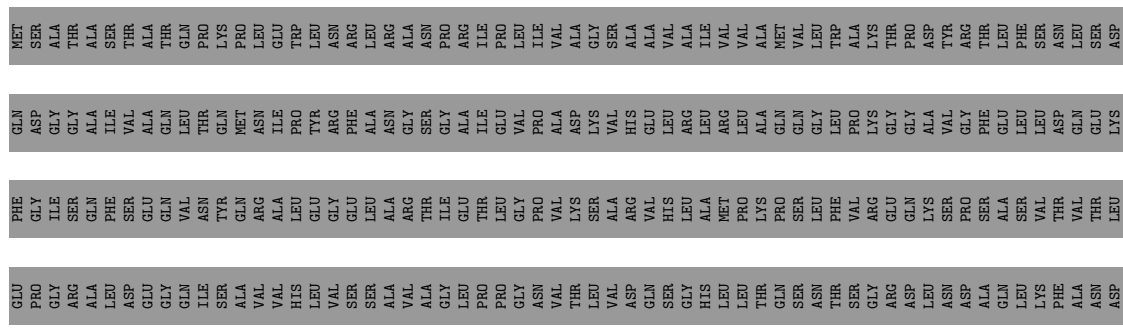
- Molecule 8: Flagellar basal-body rod protein FlgC



• Molecule 9: Flagellar M-ring protein



• Molecule 9: Flagellar M-ring protein



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

• Molecule 9: Flagellar M-ring protein

Chain l:  96%

MET SER
SER ALA
THR ARG
ALA LEU
ALA VAL
SER ILE
THR ARG
ALA GLN
GLN GLN
PRO PRO
LYS LYS
PRO PRO
LEU LEU

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

PHE GLY
ILE ILE
SER ARG
GLN SER
PHE THR
SER SER
GLU VAL
GLN VAL
ALA GLN
THR THR
ARG ARG

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

VAL GLU
SER SER
ARG ILE
GLN ILE
ARG ARG
GLY GLY
VAL VAL
SER SER
ASN ASN
GLY GLY

SER SER
GLU GLU
GLN GLN
VAL VAL
GLY GLY
TYR TYR
GLY GLY
PRO PRO
G311
G316
S317
N318
E325
A329
T330
P331

THR THR
ILE ILE
ARG ARG
HIS HIS
THR THR
LYS LYS
MET MET
ASN ASN
VAL VAL
GLY GLY
ILE ILE
ARG ARG

ASN VAL
VAL VAL
ALA ALA
GLN GLN
PRO PRO
PHE PHE
SER SER
ALA ALA
GLY GLY
THR THR
GLU GLU

ALA LYS
ALA ALA
ALA ALA
GLN GLN
GLU GLU
GLN GLN
ALA ALA
VAL VAL
VAL VAL
VAL VAL
PHE PHE
TRP TRP

ILE ARG
GLN GLN
TRP TRP
MET MET
SER SER
ASN ASN
HIS HIS
GLU GLU

• Molecule 10: Flagellar basal-body rod protein FlgF

Chain m:  97%

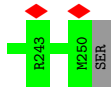
MET D2
G19
L38
L49
S50
L51
A52
D72
Y73
T74
S75
R76
L82
D85
L88
Q91
A92
A93
D94
G95
A96
E97
G111
Q116
E123
G124
E131
G132
S133
E134
A138
A139
D140
P148
G149
D150
R160
L161
K162
L163
V164
K165
A166
E167

G168
N169
E170
D175
D176
G177
L178
L181
T182
A183
E184
A185
E188
R189
G190
A191
D192
V192
L193
A194
A195
D196
P197
S198
I199
R200
E207
E241
G242
R243
Q246
L247
L248
S249
MET
SER

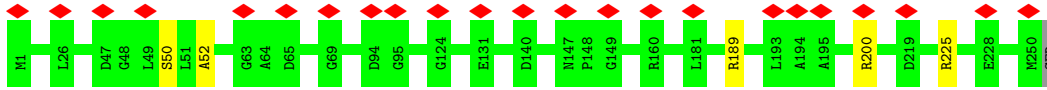
• Molecule 10: Flagellar basal-body rod protein FlgF

Chain n:  96%

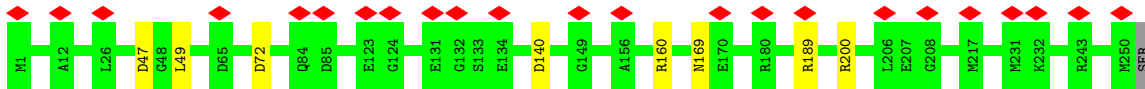
MET D2
L26
G48
L49
A53
T53
R54
Q70
L71
D72
Y73
A92
A93
D94
G95
A96
E97
G122
E123
G124
E131
G132
S133
E134
S144
G149
M153
R160
E167
G168
D175
D176
E188
L193
D196
D219
R225
E228
D238



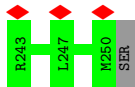
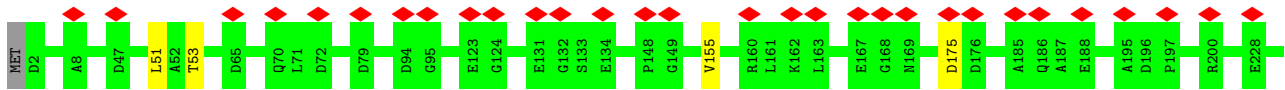
- Molecule 10: Flagellar basal-body rod protein FlgF



- Molecule 10: Flagellar basal-body rod protein FlgF



- Molecule 10: Flagellar basal-body rod protein FlgF



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11858	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.384	Depositor
Minimum map value	-1.313	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.124	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	681.984, 681.984, 681.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332, 1.332, 1.332	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.33	0/1888	0.54	1/2564 (0.0%)
1	1	0.31	0/1917	0.51	0/2605
1	2	0.29	0/1973	0.51	0/2682
1	3	0.28	0/1973	0.52	0/2682
1	4	0.28	0/1973	0.51	0/2682
1	5	0.33	0/1973	0.52	0/2682
1	6	0.32	0/1973	0.54	0/2682
1	7	0.32	0/1973	0.53	0/2682
1	8	0.33	0/1973	0.56	0/2682
1	9	0.30	0/1973	0.53	1/2682 (0.0%)
1	ZA	0.31	0/1973	0.53	0/2682
1	ZB	0.29	0/1973	0.49	0/2682
1	ZC	0.34	0/1973	0.54	0/2682
1	ZD	0.31	0/1973	0.52	0/2682
1	ZE	0.30	0/1973	0.51	1/2682 (0.0%)
1	r	0.34	0/1926	0.53	0/2618
1	s	0.38	0/1934	0.59	0/2629
1	t	0.39	0/1942	0.56	0/2639
1	u	0.35	0/1926	0.58	1/2618 (0.0%)
1	v	0.35	0/1934	0.54	0/2629
1	w	0.34	0/1844	0.51	0/2505
1	x	0.33	0/1888	0.52	0/2564
1	y	0.33	0/1888	0.56	1/2564 (0.0%)
1	z	0.31	0/1888	0.51	0/2564
2	ZF	0.28	0/2991	0.49	0/4076
2	ZG	0.34	0/2991	0.52	1/4076 (0.0%)
2	ZH	0.29	0/2991	0.50	0/4076
2	ZI	0.30	0/2991	0.51	0/4076
2	ZJ	0.31	0/2991	0.49	0/4076
2	ZK	0.29	0/2991	0.50	0/4076
2	ZL	0.29	0/2991	0.49	0/4076
2	ZM	0.29	0/2991	0.53	1/4076 (0.0%)
2	ZN	0.28	0/2991	0.51	0/4076
2	ZO	0.30	0/2991	0.50	0/4076

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	ZP	0.28	0/2991	0.50	1/4076 (0.0%)
2	ZQ	0.29	0/2991	0.51	0/4076
2	ZR	0.30	1/2991 (0.0%)	0.55	3/4076 (0.1%)
2	ZS	0.29	0/2991	0.52	1/4076 (0.0%)
2	ZT	0.29	0/2991	0.48	0/4076
2	ZU	0.29	0/2991	0.50	0/4076
2	ZV	0.50	4/2991 (0.1%)	0.67	6/4076 (0.1%)
2	ZW	0.27	0/2991	0.49	0/4076
2	ZX	0.28	0/2991	0.48	0/4076
2	ZY	0.30	1/2991 (0.0%)	0.54	2/4076 (0.0%)
2	ZZ	0.26	0/2991	0.46	0/4076
2	Za	0.28	0/2991	0.49	0/4076
2	Zb	0.30	0/2991	0.49	0/4076
2	Zc	0.29	0/2991	0.52	2/4076 (0.0%)
2	Zd	0.30	0/2991	0.51	0/4076
2	Ze	0.28	0/2991	0.48	0/4076
2	Zf	0.27	0/2991	0.48	0/4076
2	Zg	0.28	0/2991	0.49	0/4076
2	Zh	0.28	0/2991	0.48	0/4076
3	A	0.45	0/681	0.67	1/930 (0.1%)
3	B	0.33	0/681	0.53	0/930
3	C	0.28	0/681	0.50	0/930
3	D	0.26	0/681	0.48	0/930
4	E	0.31	0/1994	0.52	0/2724
5	F	0.36	0/1643	0.62	2/2237 (0.1%)
5	G	0.30	0/1665	0.49	1/2267 (0.0%)
5	H	0.29	0/1652	0.50	0/2249
5	I	0.29	0/1652	0.47	0/2249
5	J	0.33	0/1662	0.52	0/2263
6	K	0.28	0/300	0.52	0/400
6	L	0.25	0/547	0.44	0/733
6	M	0.26	0/561	0.44	0/753
6	N	0.25	0/561	0.46	0/753
6	O	0.27	0/561	0.49	0/753
6	P	0.31	0/554	0.48	0/743
7	Q	0.29	0/930	0.56	0/1251
7	R	0.26	0/855	0.49	0/1150
7	S	0.28	0/855	0.53	0/1150
7	T	0.26	0/870	0.49	0/1169
7	U	0.26	0/839	0.47	0/1129
8	V	0.30	0/981	0.47	0/1334
8	W	0.29	0/976	0.50	0/1327
8	X	0.34	0/981	0.50	0/1334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	Y	0.33	0/981	0.62	0/1334
8	Z	0.29	0/968	0.48	0/1316
8	a	0.36	0/981	0.52	0/1334
9	b	0.46	0/83	0.86	1/114 (0.9%)
9	c	0.27	0/107	0.38	0/148
9	d	0.31	0/137	0.49	0/191
9	e	0.28	0/107	0.57	0/148
9	f	0.39	0/145	0.55	0/203
9	g	0.33	0/107	0.51	0/148
9	h	0.26	0/145	0.43	0/203
9	i	0.29	0/107	0.38	0/148
9	j	0.33	0/137	0.70	0/191
9	k	0.30	0/107	0.37	0/148
9	l	0.29	0/145	0.45	0/203
10	m	0.32	0/1828	0.56	0/2492
10	n	0.33	0/1836	0.56	2/2502 (0.1%)
10	o	0.37	0/1844	0.57	0/2512
10	p	0.33	0/1844	0.57	0/2512
10	q	0.33	0/1836	0.58	0/2502
All	All	0.31	6/170171 (0.0%)	0.52	29/231606 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	2
1	1	0	1
1	5	0	2
1	7	0	1
1	8	0	2
1	ZA	0	2
1	ZD	0	1
1	ZE	0	3
1	r	0	1
1	u	0	1
1	w	0	1
1	x	0	1
1	y	0	2
1	z	0	3
2	ZI	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	ZK	0	1
2	ZO	0	1
2	ZT	0	1
2	ZU	0	1
2	ZW	0	1
2	ZZ	0	1
2	Zd	0	1
2	Ze	0	1
5	H	0	2
5	J	0	2
7	Q	0	1
7	R	0	1
7	T	0	1
7	U	0	1
8	Y	0	1
8	a	0	1
10	m	0	1
10	n	0	2
10	p	0	1
All	All	0	46

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	ZV	140	PRO	CG-CD	-16.12	0.97	1.50
2	ZV	125	PRO	CG-CD	-10.14	1.17	1.50
2	ZV	140	PRO	N-CD	8.29	1.59	1.47
2	ZV	125	PRO	N-CD	6.59	1.57	1.47
2	ZY	125	PRO	CG-CD	-5.45	1.32	1.50
2	ZR	125	PRO	CG-CD	-5.12	1.33	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	ZV	140	PRO	N-CD-CG	-17.34	77.19	103.20
2	ZR	125	PRO	CA-N-CD	-13.94	91.98	111.50
2	ZY	125	PRO	CA-N-CD	-13.33	92.84	111.50
2	ZV	125	PRO	CA-N-CD	-13.25	92.95	111.50
5	F	162	PRO	CA-N-CD	-11.93	94.80	111.50
2	Zc	125	PRO	CA-N-CD	-11.28	95.70	111.50
2	ZV	125	PRO	N-CD-CG	-11.26	86.32	103.20
2	ZV	140	PRO	CA-N-CD	-10.23	97.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	ZV	140	PRO	CA-CB-CG	-9.30	86.32	104.00
2	ZM	223	PRO	CA-N-CD	-8.39	99.76	111.50
2	ZR	125	PRO	N-CD-CG	-7.57	91.85	103.20
2	ZY	125	PRO	N-CD-CG	-7.45	92.02	103.20
5	F	162	PRO	N-CD-CG	-6.60	93.31	103.20
1	u	154	ASP	CB-CG-OD2	6.25	123.92	118.30
2	ZG	297	ASP	CB-CG-OD2	6.12	123.81	118.30
2	ZR	214	ASP	CB-CG-OD1	6.04	123.74	118.30
3	A	85	PRO	CA-N-CD	-5.88	103.26	111.50
2	Zc	125	PRO	N-CD-CG	-5.85	94.43	103.20
1	y	154	ASP	CB-CG-OD1	5.76	123.48	118.30
2	ZS	18	ASP	CB-CG-OD1	5.72	123.45	118.30
1	0	52	PRO	N-CA-CB	-5.71	96.32	102.60
2	ZV	125	PRO	CA-CB-CG	-5.67	93.22	104.00
10	n	53	THR	CB-CA-C	-5.62	96.43	111.60
2	ZP	125	PRO	CA-N-CD	-5.56	103.72	111.50
1	ZE	13	ASP	CB-CG-OD1	5.51	123.26	118.30
10	n	72	ASP	CB-CG-OD1	5.27	123.04	118.30
5	G	162	PRO	N-CA-CB	-5.26	96.82	102.60
1	9	109	ASP	CB-CG-OD2	5.19	122.97	118.30
9	b	322	PRO	N-CA-CB	-5.19	96.89	102.60

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	36	ARG	Sidechain
1	0	50	ARG	Sidechain
1	1	36	ARG	Sidechain
1	5	50	ARG	Sidechain
1	5	73	ARG	Sidechain
1	7	73	ARG	Sidechain
1	8	238	ARG	Sidechain
1	8	38	ARG	Sidechain
5	H	135	ARG	Sidechain
5	H	143	ARG	Sidechain
5	J	140	ARG	Sidechain
5	J	143	ARG	Sidechain
7	Q	106	ARG	Sidechain
7	R	55	ARG	Sidechain
7	T	4	ARG	Sidechain
7	U	104	ARG	Sidechain

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Mol	Chain	Res	Type	Group
8	Y	110	ARG	Sidechain
1	ZA	50	ARG	Sidechain
1	ZA	79	ARG	Sidechain
1	ZD	238	ARG	Sidechain
1	ZE	238	ARG	Sidechain
1	ZE	50	ARG	Sidechain
1	ZE	79	ARG	Sidechain
2	ZI	380	ARG	Sidechain
2	ZK	71	ARG	Sidechain
2	ZO	71	ARG	Sidechain
2	ZT	106	ARG	Sidechain
2	ZU	96	ARG	Sidechain
2	ZW	71	ARG	Sidechain
2	ZZ	380	ARG	Sidechain
2	Zd	380	ARG	Sidechain
2	Ze	380	ARG	Sidechain
8	a	110	ARG	Sidechain
10	m	243	ARG	Sidechain
10	n	225	ARG	Sidechain
10	n	54	ARG	Sidechain
10	p	200	ARG	Sidechain
1	r	36	ARG	Sidechain
1	u	116	ARG	Sidechain
1	w	79	ARG	Sidechain
1	x	73	ARG	Sidechain
1	y	36	ARG	Sidechain
1	y	50	ARG	Sidechain
1	z	116	ARG	Sidechain
1	z	153	ARG	Sidechain
1	z	238	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	244/260 (94%)	236 (97%)	5 (2%)	3 (1%)	11	40
1	1	248/260 (95%)	238 (96%)	9 (4%)	1 (0%)	30	63
1	2	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	49
1	3	258/260 (99%)	247 (96%)	9 (4%)	2 (1%)	16	49
1	4	258/260 (99%)	245 (95%)	11 (4%)	2 (1%)	16	49
1	5	258/260 (99%)	240 (93%)	15 (6%)	3 (1%)	11	40
1	6	258/260 (99%)	244 (95%)	10 (4%)	4 (2%)	8	36
1	7	258/260 (99%)	244 (95%)	11 (4%)	3 (1%)	11	40
1	8	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	40
1	9	258/260 (99%)	244 (95%)	13 (5%)	1 (0%)	30	63
1	ZA	258/260 (99%)	242 (94%)	13 (5%)	3 (1%)	11	40
1	ZB	258/260 (99%)	243 (94%)	12 (5%)	3 (1%)	11	40
1	ZC	258/260 (99%)	242 (94%)	14 (5%)	2 (1%)	16	49
1	ZD	258/260 (99%)	237 (92%)	18 (7%)	3 (1%)	11	40
1	ZE	258/260 (99%)	242 (94%)	15 (6%)	1 (0%)	30	63
1	r	250/260 (96%)	238 (95%)	11 (4%)	1 (0%)	30	63
1	s	251/260 (96%)	234 (93%)	14 (6%)	3 (1%)	11	40
1	t	252/260 (97%)	234 (93%)	16 (6%)	2 (1%)	16	49
1	u	250/260 (96%)	239 (96%)	9 (4%)	2 (1%)	16	49
1	v	251/260 (96%)	235 (94%)	10 (4%)	6 (2%)	5	29
1	w	239/260 (92%)	231 (97%)	7 (3%)	1 (0%)	30	63
1	x	244/260 (94%)	229 (94%)	10 (4%)	5 (2%)	6	32
1	y	244/260 (94%)	234 (96%)	9 (4%)	1 (0%)	30	63
1	z	244/260 (94%)	239 (98%)	4 (2%)	1 (0%)	30	63
2	ZF	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
2	ZG	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	69
2	ZH	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
2	ZI	399/403 (99%)	387 (97%)	10 (2%)	2 (0%)	25	58
2	ZJ	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
2	ZK	399/403 (99%)	387 (97%)	11 (3%)	1 (0%)	37	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	ZL	399/403 (99%)	389 (98%)	9 (2%)	1 (0%)	37	69
2	ZM	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
2	ZN	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
2	ZO	399/403 (99%)	381 (96%)	15 (4%)	3 (1%)	16	49
2	ZP	399/403 (99%)	386 (97%)	12 (3%)	1 (0%)	37	69
2	ZQ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
2	ZR	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
2	ZS	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
2	ZT	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
2	ZU	399/403 (99%)	387 (97%)	12 (3%)	0	100	100
2	ZV	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
2	ZW	399/403 (99%)	380 (95%)	18 (4%)	1 (0%)	37	69
2	ZX	399/403 (99%)	388 (97%)	11 (3%)	0	100	100
2	ZY	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
2	ZZ	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
2	Za	399/403 (99%)	386 (97%)	12 (3%)	1 (0%)	37	69
2	Zb	399/403 (99%)	392 (98%)	7 (2%)	0	100	100
2	Zc	399/403 (99%)	390 (98%)	9 (2%)	0	100	100
2	Zd	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
2	Ze	399/403 (99%)	385 (96%)	13 (3%)	1 (0%)	37	69
2	Zf	399/403 (99%)	386 (97%)	13 (3%)	0	100	100
2	Zg	399/403 (99%)	383 (96%)	16 (4%)	0	100	100
2	Zh	399/403 (99%)	391 (98%)	8 (2%)	0	100	100
3	A	87/89 (98%)	81 (93%)	4 (5%)	2 (2%)	5	30
3	B	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
3	C	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
3	D	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
4	E	251/264 (95%)	234 (93%)	15 (6%)	2 (1%)	16	49
5	F	205/245 (84%)	197 (96%)	8 (4%)	0	100	100
5	G	207/245 (84%)	199 (96%)	6 (3%)	2 (1%)	13	44
5	H	206/245 (84%)	201 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	206/245 (84%)	199 (97%)	6 (3%)	1 (0%)	25	58
5	J	207/245 (84%)	192 (93%)	10 (5%)	5 (2%)	5	29
6	K	38/104 (36%)	35 (92%)	3 (8%)	0	100	100
6	L	70/104 (67%)	70 (100%)	0	0	100	100
6	M	72/104 (69%)	70 (97%)	2 (3%)	0	100	100
6	N	72/104 (69%)	72 (100%)	0	0	100	100
6	O	72/104 (69%)	72 (100%)	0	0	100	100
6	P	71/104 (68%)	71 (100%)	0	0	100	100
7	Q	115/138 (83%)	114 (99%)	1 (1%)	0	100	100
7	R	104/138 (75%)	103 (99%)	1 (1%)	0	100	100
7	S	104/138 (75%)	103 (99%)	1 (1%)	0	100	100
7	T	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
7	U	102/138 (74%)	101 (99%)	1 (1%)	0	100	100
8	V	131/134 (98%)	122 (93%)	9 (7%)	0	100	100
8	W	130/134 (97%)	123 (95%)	7 (5%)	0	100	100
8	X	131/134 (98%)	124 (95%)	7 (5%)	0	100	100
8	Y	131/134 (98%)	121 (92%)	7 (5%)	3 (2%)	5	30
8	Z	129/134 (96%)	123 (95%)	5 (4%)	1 (1%)	16	49
8	a	131/134 (98%)	124 (95%)	7 (5%)	0	100	100
9	b	11/560 (2%)	9 (82%)	2 (18%)	0	100	100
9	c	14/560 (2%)	12 (86%)	2 (14%)	0	100	100
9	d	18/560 (3%)	18 (100%)	0	0	100	100
9	e	14/560 (2%)	14 (100%)	0	0	100	100
9	f	19/560 (3%)	18 (95%)	1 (5%)	0	100	100
9	g	14/560 (2%)	13 (93%)	1 (7%)	0	100	100
9	h	19/560 (3%)	19 (100%)	0	0	100	100
9	i	14/560 (2%)	14 (100%)	0	0	100	100
9	j	18/560 (3%)	18 (100%)	0	0	100	100
9	k	14/560 (2%)	14 (100%)	0	0	100	100
9	l	19/560 (3%)	19 (100%)	0	0	100	100
10	m	246/251 (98%)	238 (97%)	7 (3%)	1 (0%)	30	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	n	247/251 (98%)	242 (98%)	4 (2%)	1 (0%)	30	63
10	o	248/251 (99%)	233 (94%)	13 (5%)	2 (1%)	16	49
10	p	248/251 (99%)	235 (95%)	13 (5%)	0	100	100
10	q	247/251 (98%)	236 (96%)	9 (4%)	2 (1%)	16	49
All	All	22391/29305 (76%)	21536 (96%)	763 (3%)	92 (0%)	32	63

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	209	ASN
1	4	140	ILE
1	5	209	ASN
1	6	139	ALA
1	8	209	ASN
1	ZA	92	SER
1	ZA	209	ASN
1	ZB	164	GLN
2	ZG	46	SER
1	x	90	ASN
3	A	84	LEU
5	J	83	ALA
5	J	87	GLN
10	q	155	VAL
1	0	90	ASN
1	8	165	ALA
1	ZB	165	ALA
1	ZB	209	ASN
1	ZC	209	ASN
1	ZD	209	ASN
1	ZE	209	ASN
2	ZI	375	MET
2	ZO	237	ILE
1	u	127	GLN
1	u	165	ALA
1	v	204	SER
1	x	4	SER
1	z	127	GLN
4	E	167	ASN
4	E	213	ILE
5	G	83	ALA
5	I	160	GLN

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Mol	Chain	Res	Type
5	J	86	ASN
8	Y	54	ALA
10	o	50	SER
10	q	53	THR
1	0	3	SER
1	0	127	GLN
1	2	49	ILE
1	3	49	ILE
1	3	181	ASP
1	4	49	ILE
1	5	49	ILE
1	6	138	PRO
1	7	55	GLN
2	ZK	375	MET
2	ZL	374	ASN
1	r	127	GLN
1	t	198	SER
1	v	164	GLN
1	v	206	PRO
1	x	3	SER
1	x	127	GLN
1	y	127	GLN
5	J	140	ARG
8	Y	58	ALA
1	6	49	ILE
1	6	58	GLU
1	7	49	ILE
1	8	49	ILE
1	9	49	ILE
1	ZA	138	PRO
2	ZO	142	THR
2	ZP	374	ASN
1	s	81	HIS
1	s	127	GLN
1	v	203	GLU
1	w	127	GLN
8	Y	55	PRO
1	1	127	GLN
1	7	210	GLY
1	ZC	139	ALA
1	ZD	139	ALA
1	s	139	ALA

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Mol	Chain	Res	Type
1	t	127	GLN
1	v	127	GLN
3	A	85	PRO
5	G	162	PRO
10	o	52	ALA
2	ZO	375	MET
2	Za	97	ASN
2	Ze	134	PRO
1	v	200	ALA
8	Z	58	ALA
10	m	52	ALA
10	n	52	ALA
2	ZI	325	GLY
2	ZW	75	VAL
1	5	138	PRO
1	x	136	VAL
5	J	229	VAL
1	ZD	138	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	205/215 (95%)	198 (97%)	7 (3%)	32	55
1	1	209/215 (97%)	201 (96%)	8 (4%)	28	52
1	2	215/215 (100%)	213 (99%)	2 (1%)	75	82
1	3	215/215 (100%)	212 (99%)	3 (1%)	62	75
1	4	215/215 (100%)	209 (97%)	6 (3%)	38	59
1	5	215/215 (100%)	210 (98%)	5 (2%)	45	63
1	6	215/215 (100%)	210 (98%)	5 (2%)	45	63
1	7	215/215 (100%)	214 (100%)	1 (0%)	86	90
1	8	215/215 (100%)	210 (98%)	5 (2%)	45	63
1	9	215/215 (100%)	212 (99%)	3 (1%)	62	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ZA	215/215 (100%)	213 (99%)	2 (1%)	75	82
1	ZB	215/215 (100%)	208 (97%)	7 (3%)	33	56
1	ZC	215/215 (100%)	212 (99%)	3 (1%)	62	75
1	ZD	215/215 (100%)	210 (98%)	5 (2%)	45	63
1	ZE	215/215 (100%)	210 (98%)	5 (2%)	45	63
1	r	209/215 (97%)	203 (97%)	6 (3%)	37	58
1	s	210/215 (98%)	201 (96%)	9 (4%)	25	49
1	t	211/215 (98%)	199 (94%)	12 (6%)	17	43
1	u	209/215 (97%)	198 (95%)	11 (5%)	19	44
1	v	210/215 (98%)	199 (95%)	11 (5%)	19	44
1	w	200/215 (93%)	195 (98%)	5 (2%)	42	62
1	x	205/215 (95%)	197 (96%)	8 (4%)	27	51
1	y	205/215 (95%)	197 (96%)	8 (4%)	27	51
1	z	205/215 (95%)	201 (98%)	4 (2%)	50	68
2	ZF	321/323 (99%)	309 (96%)	12 (4%)	29	53
2	ZG	321/323 (99%)	305 (95%)	16 (5%)	20	45
2	ZH	321/323 (99%)	308 (96%)	13 (4%)	27	50
2	ZI	321/323 (99%)	315 (98%)	6 (2%)	52	69
2	ZJ	321/323 (99%)	312 (97%)	9 (3%)	38	59
2	ZK	321/323 (99%)	315 (98%)	6 (2%)	52	69
2	ZL	321/323 (99%)	311 (97%)	10 (3%)	35	56
2	ZM	321/323 (99%)	312 (97%)	9 (3%)	38	59
2	ZN	321/323 (99%)	311 (97%)	10 (3%)	35	56
2	ZO	321/323 (99%)	313 (98%)	8 (2%)	42	62
2	ZP	321/323 (99%)	306 (95%)	15 (5%)	22	46
2	ZQ	321/323 (99%)	312 (97%)	9 (3%)	38	59
2	ZR	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	ZS	321/323 (99%)	315 (98%)	6 (2%)	52	69
2	ZT	321/323 (99%)	313 (98%)	8 (2%)	42	62
2	ZU	321/323 (99%)	317 (99%)	4 (1%)	67	77
2	ZV	321/323 (99%)	317 (99%)	4 (1%)	67	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	ZW	321/323 (99%)	307 (96%)	14 (4%)	24	48
2	ZX	321/323 (99%)	318 (99%)	3 (1%)	75	82
2	ZY	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	ZZ	321/323 (99%)	316 (98%)	5 (2%)	58	73
2	Za	321/323 (99%)	315 (98%)	6 (2%)	52	69
2	Zb	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	Zc	321/323 (99%)	310 (97%)	11 (3%)	32	55
2	Zd	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	Ze	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	Zf	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	Zg	321/323 (99%)	314 (98%)	7 (2%)	47	64
2	Zh	321/323 (99%)	314 (98%)	7 (2%)	47	64
3	A	74/74 (100%)	68 (92%)	6 (8%)	9	32
3	B	74/74 (100%)	72 (97%)	2 (3%)	40	60
3	C	74/74 (100%)	74 (100%)	0	100	100
3	D	74/74 (100%)	74 (100%)	0	100	100
4	E	210/221 (95%)	205 (98%)	5 (2%)	44	62
5	F	177/204 (87%)	171 (97%)	6 (3%)	32	55
5	G	179/204 (88%)	172 (96%)	7 (4%)	27	51
5	H	178/204 (87%)	173 (97%)	5 (3%)	38	59
5	I	178/204 (87%)	171 (96%)	7 (4%)	27	51
5	J	179/204 (88%)	172 (96%)	7 (4%)	27	51
6	K	33/79 (42%)	29 (88%)	4 (12%)	4	19
6	L	56/79 (71%)	54 (96%)	2 (4%)	30	54
6	M	58/79 (73%)	57 (98%)	1 (2%)	56	72
6	N	58/79 (73%)	56 (97%)	2 (3%)	32	55
6	O	58/79 (73%)	56 (97%)	2 (3%)	32	55
6	P	57/79 (72%)	54 (95%)	3 (5%)	19	44
7	Q	98/113 (87%)	94 (96%)	4 (4%)	26	50
7	R	90/113 (80%)	89 (99%)	1 (1%)	70	79
7	S	90/113 (80%)	87 (97%)	3 (3%)	33	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	91/113 (80%)	90 (99%)	1 (1%)	70	79
7	U	89/113 (79%)	84 (94%)	5 (6%)	17	43
8	V	104/105 (99%)	104 (100%)	0	100	100
8	W	104/105 (99%)	101 (97%)	3 (3%)	37	58
8	X	104/105 (99%)	102 (98%)	2 (2%)	52	69
8	Y	104/105 (99%)	100 (96%)	4 (4%)	28	52
8	Z	103/105 (98%)	100 (97%)	3 (3%)	37	58
8	a	104/105 (99%)	98 (94%)	6 (6%)	17	42
9	b	8/467 (2%)	6 (75%)	2 (25%)	0	3
9	c	11/467 (2%)	10 (91%)	1 (9%)	7	28
9	d	14/467 (3%)	12 (86%)	2 (14%)	2	16
9	e	11/467 (2%)	11 (100%)	0	100	100
9	f	15/467 (3%)	15 (100%)	0	100	100
9	g	11/467 (2%)	11 (100%)	0	100	100
9	h	15/467 (3%)	15 (100%)	0	100	100
9	i	11/467 (2%)	11 (100%)	0	100	100
9	j	14/467 (3%)	13 (93%)	1 (7%)	12	36
9	k	11/467 (2%)	11 (100%)	0	100	100
9	l	15/467 (3%)	14 (93%)	1 (7%)	13	38
10	m	190/193 (98%)	188 (99%)	2 (1%)	70	79
10	n	191/193 (99%)	186 (97%)	5 (3%)	41	61
10	o	192/193 (100%)	189 (98%)	3 (2%)	58	73
10	p	192/193 (100%)	185 (96%)	7 (4%)	30	54
10	q	191/193 (99%)	189 (99%)	2 (1%)	73	80
All	All	18272/23835 (77%)	17774 (97%)	498 (3%)	41	60

All (498) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	1	MET
1	0	9	LYS
1	0	36	ARG
1	0	50	ARG
1	0	52	PRO

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Mol	Chain	Res	Type
1	0	73	ARG
1	0	185	GLU
1	1	1	MET
1	1	36	ARG
1	1	62	LEU
1	1	75	VAL
1	1	106	MET
1	1	119	SER
1	1	164	GLN
1	1	206	PRO
1	2	179	MET
1	2	204	SER
1	3	43	ASP
1	3	109	ASP
1	3	244	SER
1	4	2	ILE
1	4	64	SER
1	4	137	GLN
1	4	204	SER
1	4	209	ASN
1	4	259	GLN
1	5	4	SER
1	5	73	ARG
1	5	85	ASN
1	5	154	ASP
1	5	181	ASP
1	6	59	GLN
1	6	73	ARG
1	6	78	GLU
1	6	109	ASP
1	6	244	SER
1	7	59	GLN
1	8	58	GLU
1	8	100	GLN
1	8	194	GLU
1	8	195	THR
1	8	256	LYS
1	9	106	MET
1	9	125	ASN
1	9	162	GLN
1	ZA	50	ARG
1	ZA	248	SER

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Mol	Chain	Res	Type
1	ZB	1	MET
1	ZB	4	SER
1	ZB	58	GLU
1	ZB	73	ARG
1	ZB	119	SER
1	ZB	143	PRO
1	ZB	244	SER
1	ZC	123	ASP
1	ZC	244	SER
1	ZC	249	THR
1	ZD	1	MET
1	ZD	64	SER
1	ZD	66	LEU
1	ZD	162	GLN
1	ZD	240	TYR
1	ZE	37	GLN
1	ZE	50	ARG
1	ZE	137	GLN
1	ZE	141	THR
1	ZE	259	GLN
2	ZF	3	PHE
2	ZF	60	ASP
2	ZF	87	ASP
2	ZF	134	PRO
2	ZF	229	THR
2	ZF	265	ASN
2	ZF	280	ASN
2	ZF	284	TYR
2	ZF	289	LEU
2	ZF	352	ASN
2	ZF	355	LYS
2	ZF	392	GLN
2	ZG	3	PHE
2	ZG	38	SER
2	ZG	103	ASP
2	ZG	104	GLU
2	ZG	188	ASP
2	ZG	189	SER
2	ZG	227	SER
2	ZG	234	GLU
2	ZG	260	SER
2	ZG	262	SER

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Mol	Chain	Res	Type
2	ZG	265	ASN
2	ZG	267	MET
2	ZG	288	ASP
2	ZG	350	SER
2	ZG	352	ASN
2	ZG	395	ILE
2	ZH	34	SER
2	ZH	71	ARG
2	ZH	154	MET
2	ZH	227	SER
2	ZH	260	SER
2	ZH	281	GLN
2	ZH	284	TYR
2	ZH	288	ASP
2	ZH	331	ASP
2	ZH	355	LYS
2	ZH	375	MET
2	ZH	380	ARG
2	ZH	399	LEU
2	ZI	99	GLN
2	ZI	195	ASP
2	ZI	197	ASN
2	ZI	260	SER
2	ZI	352	ASN
2	ZI	358	ASN
2	ZJ	46	SER
2	ZJ	96	ARG
2	ZJ	103	ASP
2	ZJ	107	ASN
2	ZJ	195	ASP
2	ZJ	233	ASN
2	ZJ	280	ASN
2	ZJ	331	ASP
2	ZJ	395	ILE
2	ZK	3	PHE
2	ZK	268	GLN
2	ZK	297	ASP
2	ZK	305	SER
2	ZK	331	ASP
2	ZK	338	GLN
2	ZL	78	SER
2	ZL	84	ARG

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Mol	Chain	Res	Type
2	ZL	196	MET
2	ZL	234	GLU
2	ZL	267	MET
2	ZL	291	SER
2	ZL	338	GLN
2	ZL	368	LEU
2	ZL	370	LYS
2	ZL	382	TYR
2	ZM	53	LYS
2	ZM	89	ASN
2	ZM	153	SER
2	ZM	200	PHE
2	ZM	214	ASP
2	ZM	282	ASN
2	ZM	352	ASN
2	ZM	369	SER
2	ZM	370	LYS
2	ZN	43	PHE
2	ZN	78	SER
2	ZN	103	ASP
2	ZN	143	LEU
2	ZN	148	SER
2	ZN	157	ASN
2	ZN	216	SER
2	ZN	297	ASP
2	ZN	367	ASP
2	ZN	396	LEU
2	ZO	2	SER
2	ZO	74	ASP
2	ZO	174	ASP
2	ZO	178	TYR
2	ZO	235	ASN
2	ZO	237	ILE
2	ZO	331	ASP
2	ZO	375	MET
2	ZP	42	MET
2	ZP	63	ASP
2	ZP	74	ASP
2	ZP	95	SER
2	ZP	126	PRO
2	ZP	162	ASP
2	ZP	227	SER

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Mol	Chain	Res	Type
2	ZP	275	ASN
2	ZP	288	ASP
2	ZP	292	TYR
2	ZP	331	ASP
2	ZP	340	SER
2	ZP	369	SER
2	ZP	370	LYS
2	ZP	393	ASP
2	ZQ	46	SER
2	ZQ	101	LYS
2	ZQ	189	SER
2	ZQ	200	PHE
2	ZQ	211	TYR
2	ZQ	280	ASN
2	ZQ	305	SER
2	ZQ	367	ASP
2	ZQ	370	LYS
2	ZR	41	ASP
2	ZR	103	ASP
2	ZR	197	ASN
2	ZR	214	ASP
2	ZR	295	ASN
2	ZR	332	ASN
2	ZR	367	ASP
2	ZS	78	SER
2	ZS	103	ASP
2	ZS	170	PHE
2	ZS	202	LYS
2	ZS	245	ASN
2	ZS	367	ASP
2	ZT	5	GLN
2	ZT	73	LEU
2	ZT	133	ASN
2	ZT	148	SER
2	ZT	195	ASP
2	ZT	262	SER
2	ZT	297	ASP
2	ZT	358	ASN
2	ZU	3	PHE
2	ZU	78	SER
2	ZU	80	ASN
2	ZU	340	SER

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Mol	Chain	Res	Type
2	ZV	46	SER
2	ZV	232	PHE
2	ZV	307	GLU
2	ZV	308	GLN
2	ZW	3	PHE
2	ZW	41	ASP
2	ZW	42	MET
2	ZW	53	LYS
2	ZW	188	ASP
2	ZW	195	ASP
2	ZW	215	SER
2	ZW	259	PHE
2	ZW	292	TYR
2	ZW	309	GLU
2	ZW	326	LEU
2	ZW	331	ASP
2	ZW	340	SER
2	ZW	358	ASN
2	ZX	3	PHE
2	ZX	63	ASP
2	ZX	195	ASP
2	ZY	60	ASP
2	ZY	80	ASN
2	ZY	192	ASN
2	ZY	204	LYS
2	ZY	252	ASN
2	ZY	332	ASN
2	ZY	350	SER
2	ZZ	3	PHE
2	ZZ	41	ASP
2	ZZ	88	SER
2	ZZ	148	SER
2	ZZ	393	ASP
2	Za	96	ARG
2	Za	103	ASP
2	Za	292	TYR
2	Za	331	ASP
2	Za	332	ASN
2	Za	375	MET
2	Zb	41	ASP
2	Zb	89	ASN
2	Zb	292	TYR

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Mol	Chain	Res	Type
2	Zb	308	GLN
2	Zb	355	LYS
2	Zb	367	ASP
2	Zb	393	ASP
2	Zc	41	ASP
2	Zc	103	ASP
2	Zc	204	LYS
2	Zc	267	MET
2	Zc	296	ASN
2	Zc	297	ASP
2	Zc	317	LEU
2	Zc	332	ASN
2	Zc	340	SER
2	Zc	369	SER
2	Zc	399	LEU
2	Zd	41	ASP
2	Zd	114	MET
2	Zd	140	PRO
2	Zd	292	TYR
2	Zd	375	MET
2	Zd	393	ASP
2	Zd	397	ASN
2	Ze	3	PHE
2	Ze	27	SER
2	Ze	46	SER
2	Ze	96	ARG
2	Ze	308	GLN
2	Ze	319	ASN
2	Ze	395	ILE
2	Zf	3	PHE
2	Zf	285	LYS
2	Zf	297	ASP
2	Zf	331	ASP
2	Zf	332	ASN
2	Zf	367	ASP
2	Zf	396	LEU
2	Zg	94	TYR
2	Zg	103	ASP
2	Zg	292	TYR
2	Zg	308	GLN
2	Zg	332	ASN
2	Zg	367	ASP

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Mol	Chain	Res	Type
2	Zg	370	LYS
2	Zh	41	ASP
2	Zh	47	LYS
2	Zh	63	ASP
2	Zh	83	PHE
2	Zh	162	ASP
2	Zh	308	GLN
2	Zh	332	ASN
1	r	4	SER
1	r	6	TRP
1	r	19	MET
1	r	36	ARG
1	r	44	LEU
1	r	154	ASP
1	s	6	TRP
1	s	16	GLN
1	s	36	ARG
1	s	73	ARG
1	s	127	GLN
1	s	137	GLN
1	s	138	PRO
1	s	222	SER
1	s	251	ASP
1	t	1	MET
1	t	44	LEU
1	t	66	LEU
1	t	87	SER
1	t	93	LYS
1	t	100	GLN
1	t	148	SER
1	t	154	ASP
1	t	179	MET
1	t	195	THR
1	t	208	LEU
1	t	245	LYS
1	u	4	SER
1	u	30	SER
1	u	123	ASP
1	u	148	SER
1	u	169	GLN
1	u	173	LEU
1	u	179	MET

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Mol	Chain	Res	Type
1	u	195	THR
1	u	202	ASN
1	u	222	SER
1	u	252	GLN
1	v	36	ARG
1	v	73	ARG
1	v	91	ASN
1	v	94	ASP
1	v	127	GLN
1	v	161	GLN
1	v	194	GLU
1	v	197	SER
1	v	198	SER
1	v	206	PRO
1	v	225	ASN
1	w	36	ARG
1	w	100	GLN
1	w	137	GLN
1	w	181	ASP
1	w	203	GLU
1	x	1	MET
1	x	73	ARG
1	x	111	THR
1	x	170	VAL
1	x	172	GLN
1	x	185	GLU
1	x	198	SER
1	x	209	ASN
1	y	1	MET
1	y	30	SER
1	y	36	ARG
1	y	50	ARG
1	y	82	SER
1	y	169	GLN
1	y	208	LEU
1	y	209	ASN
1	z	1	MET
1	z	3	SER
1	z	117	ASP
1	z	127	GLN
3	A	7	MET
3	A	69	MET

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Mol	Chain	Res	Type
3	A	73	LEU
3	A	75	ASP
3	A	85	PRO
3	A	87	ILE
3	B	2	THR
3	B	47	MET
4	E	36	ARG
4	E	86	PHE
4	E	214	PHE
4	E	227	MET
4	E	229	MET
5	F	38	TRP
5	F	129	LYS
5	F	155	ASN
5	F	160	GLN
5	F	190	PHE
5	F	213	PRO
5	G	75	ARG
5	G	102	SER
5	G	116	PHE
5	G	140	ARG
5	G	160	GLN
5	G	162	PRO
5	G	213	PRO
5	H	135	ARG
5	H	152	ARG
5	H	177	SER
5	H	187	PHE
5	H	190	PHE
5	I	113	TYR
5	I	143	ARG
5	I	152	ARG
5	I	187	PHE
5	I	205	MET
5	I	238	SER
5	I	241	GLN
5	J	65	THR
5	J	117	SER
5	J	140	ARG
5	J	144	GLU
5	J	190	PHE
5	J	224	MET

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Mol	Chain	Res	Type
5	J	230	ASP
6	K	74	ASP
6	K	77	LYS
6	K	79	SER
6	K	101	SER
6	L	75	MET
6	L	84	MET
6	M	70	ASP
6	N	33	SER
6	N	81	SER
6	O	101	SER
6	O	102	MET
6	P	57	GLU
6	P	91	LYS
6	P	102	MET
7	Q	34	ASP
7	Q	101	ASP
7	Q	113	SER
7	Q	125	SER
7	R	47	SER
7	S	48	GLU
7	S	91	ASP
7	S	128	LYS
7	T	47	SER
7	U	4	ARG
7	U	18	LEU
7	U	104	ARG
7	U	113	SER
7	U	125	SER
8	W	46	GLN
8	W	123	LYS
8	W	126	MET
8	X	119	LEU
8	X	128	LYS
8	Y	3	LEU
8	Y	4	LEU
8	Y	30	ASN
8	Y	120	ASN
8	Z	20	ARG
8	Z	52	ASP
8	Z	84	LEU
8	a	38	ASP

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Mol	Chain	Res	Type
8	a	86	ASP
8	a	88	ASN
8	a	123	LYS
8	a	125	MET
8	a	127	LEU
9	b	317	SER
9	b	322	PRO
9	c	324	ASN
9	d	318	ASN
9	d	319	GLN
9	j	319	GLN
9	l	318	ASN
10	m	123	GLU
10	m	247	LEU
10	n	53	THR
10	n	72	ASP
10	n	97	GLU
10	n	153	ASN
10	n	225	ARG
10	o	189	ARG
10	o	200	ARG
10	o	225	ARG
10	p	47	ASP
10	p	49	LEU
10	p	72	ASP
10	p	140	ASP
10	p	160	ARG
10	p	169	ASN
10	p	189	ARG
10	q	51	LEU
10	q	175	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (487) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	16	GLN
1	0	47	GLN
1	0	100	GLN
1	0	135	GLN
1	0	196	GLN
1	0	235	GLN
1	0	255	GLN

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Mol	Chain	Res	Type
1	1	47	GLN
1	1	67	GLN
1	1	83	GLN
1	1	85	ASN
1	1	91	ASN
1	1	121	GLN
1	1	223	ASN
1	1	252	GLN
1	2	51	GLN
1	2	145	ASN
1	2	164	GLN
1	2	232	ASN
1	2	235	GLN
1	2	255	GLN
1	3	67	GLN
1	3	121	GLN
1	3	161	GLN
1	3	255	GLN
1	4	32	ASN
1	4	37	GLN
1	4	47	GLN
1	4	51	GLN
1	4	125	ASN
1	4	127	GLN
1	4	137	GLN
1	4	174	ASN
1	4	216	GLN
1	4	235	GLN
1	4	243	ASN
1	4	259	GLN
1	5	16	GLN
1	5	55	GLN
1	5	100	GLN
1	5	121	GLN
1	5	237	GLN
1	6	59	GLN
1	6	121	GLN
1	6	127	GLN
1	6	135	GLN
1	6	137	GLN
1	6	209	ASN
1	6	237	GLN

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Mol	Chain	Res	Type
1	7	24	ASN
1	7	55	GLN
1	7	164	GLN
1	7	235	GLN
1	8	24	ASN
1	8	28	ASN
1	8	83	GLN
1	8	91	ASN
1	9	37	GLN
1	9	55	GLN
1	9	85	ASN
1	9	91	ASN
1	9	127	GLN
1	9	259	GLN
1	ZA	37	GLN
1	ZA	137	GLN
1	ZA	235	GLN
1	ZB	24	ASN
1	ZB	25	ASN
1	ZB	28	ASN
1	ZB	37	GLN
1	ZB	104	GLN
1	ZB	135	GLN
1	ZB	137	GLN
1	ZB	237	GLN
1	ZC	16	GLN
1	ZC	37	GLN
1	ZC	88	GLN
1	ZC	100	GLN
1	ZC	137	GLN
1	ZD	24	ASN
1	ZD	67	GLN
1	ZD	88	GLN
1	ZD	91	ASN
1	ZD	135	GLN
1	ZD	235	GLN
1	ZD	237	GLN
1	ZE	24	ASN
1	ZE	37	GLN
1	ZE	67	GLN
1	ZE	121	GLN
1	ZE	235	GLN

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Mol	Chain	Res	Type
1	ZE	252	GLN
2	ZF	5	GLN
2	ZF	16	ASN
2	ZF	107	ASN
2	ZF	155	GLN
2	ZF	197	ASN
2	ZF	358	ASN
2	ZF	392	GLN
2	ZF	401	ASN
2	ZG	107	ASN
2	ZG	112	GLN
2	ZG	130	GLN
2	ZG	133	ASN
2	ZG	332	ASN
2	ZG	387	GLN
2	ZG	394	GLN
2	ZH	5	GLN
2	ZH	155	GLN
2	ZH	157	ASN
2	ZH	206	ASN
2	ZH	270	ASN
2	ZH	296	ASN
2	ZH	352	ASN
2	ZH	365	ASN
2	ZH	379	GLN
2	ZI	79	GLN
2	ZI	89	ASN
2	ZI	197	ASN
2	ZI	269	GLN
2	ZI	310	GLN
2	ZI	385	ASN
2	ZI	392	GLN
2	ZI	394	GLN
2	ZI	401	ASN
2	ZJ	89	ASN
2	ZJ	107	ASN
2	ZJ	133	ASN
2	ZJ	159	ASN
2	ZJ	197	ASN
2	ZJ	265	ASN
2	ZJ	274	ASN
2	ZJ	282	ASN

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Mol	Chain	Res	Type
2	ZJ	379	GLN
2	ZJ	392	GLN
2	ZK	89	ASN
2	ZK	107	ASN
2	ZK	197	ASN
2	ZK	252	ASN
2	ZK	270	ASN
2	ZK	303	ASN
2	ZK	319	ASN
2	ZK	392	GLN
2	ZK	401	ASN
2	ZL	5	GLN
2	ZL	79	GLN
2	ZL	89	ASN
2	ZL	179	ASN
2	ZL	190	GLN
2	ZL	197	ASN
2	ZL	269	GLN
2	ZL	282	ASN
2	ZL	310	GLN
2	ZL	338	GLN
2	ZL	394	GLN
2	ZL	401	ASN
2	ZM	5	GLN
2	ZM	59	GLN
2	ZM	89	ASN
2	ZM	197	ASN
2	ZM	213	HIS
2	ZM	235	ASN
2	ZM	252	ASN
2	ZM	381	ASN
2	ZN	79	GLN
2	ZN	107	ASN
2	ZN	112	GLN
2	ZN	129	GLN
2	ZN	133	ASN
2	ZN	190	GLN
2	ZN	197	ASN
2	ZN	319	ASN
2	ZN	332	ASN
2	ZN	379	GLN
2	ZN	401	ASN

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Mol	Chain	Res	Type
2	ZO	5	GLN
2	ZO	141	ASN
2	ZO	235	ASN
2	ZO	268	GLN
2	ZO	332	ASN
2	ZP	5	GLN
2	ZP	11	ASN
2	ZP	107	ASN
2	ZP	129	GLN
2	ZP	194	HIS
2	ZP	269	GLN
2	ZP	270	ASN
2	ZP	314	GLN
2	ZP	322	ASN
2	ZP	338	GLN
2	ZP	379	GLN
2	ZP	381	ASN
2	ZP	385	ASN
2	ZQ	5	GLN
2	ZQ	89	ASN
2	ZQ	97	ASN
2	ZQ	133	ASN
2	ZQ	141	ASN
2	ZQ	155	GLN
2	ZQ	157	ASN
2	ZQ	197	ASN
2	ZQ	233	ASN
2	ZQ	338	GLN
2	ZQ	387	GLN
2	ZR	5	GLN
2	ZR	89	ASN
2	ZR	107	ASN
2	ZR	268	GLN
2	ZR	269	GLN
2	ZR	293	GLN
2	ZR	295	ASN
2	ZR	401	ASN
2	ZS	133	ASN
2	ZS	192	ASN
2	ZS	197	ASN
2	ZS	387	GLN
2	ZS	394	GLN

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Mol	Chain	Res	Type
2	ZT	99	GLN
2	ZT	129	GLN
2	ZT	190	GLN
2	ZT	197	ASN
2	ZT	213	HIS
2	ZT	235	ASN
2	ZT	275	ASN
2	ZT	293	GLN
2	ZT	314	GLN
2	ZT	352	ASN
2	ZT	392	GLN
2	ZU	97	ASN
2	ZU	99	GLN
2	ZU	107	ASN
2	ZU	133	ASN
2	ZU	159	ASN
2	ZU	190	GLN
2	ZU	268	GLN
2	ZU	269	GLN
2	ZU	293	GLN
2	ZU	379	GLN
2	ZV	5	GLN
2	ZV	107	ASN
2	ZV	133	ASN
2	ZV	197	ASN
2	ZV	280	ASN
2	ZV	303	ASN
2	ZV	314	GLN
2	ZV	381	ASN
2	ZV	387	GLN
2	ZV	394	GLN
2	ZW	5	GLN
2	ZW	26	ASN
2	ZW	107	ASN
2	ZW	129	GLN
2	ZW	133	ASN
2	ZW	155	GLN
2	ZW	197	ASN
2	ZW	252	ASN
2	ZW	310	GLN
2	ZW	314	GLN
2	ZW	332	ASN

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Mol	Chain	Res	Type
2	ZX	11	ASN
2	ZX	80	ASN
2	ZX	133	ASN
2	ZX	159	ASN
2	ZX	314	GLN
2	ZX	352	ASN
2	ZX	387	GLN
2	ZX	401	ASN
2	ZY	5	GLN
2	ZY	115	GLN
2	ZY	159	ASN
2	ZY	197	ASN
2	ZY	268	GLN
2	ZY	392	GLN
2	ZZ	5	GLN
2	ZZ	26	ASN
2	ZZ	99	GLN
2	ZZ	107	ASN
2	ZZ	133	ASN
2	ZZ	194	HIS
2	ZZ	197	ASN
2	ZZ	314	GLN
2	ZZ	332	ASN
2	ZZ	401	ASN
2	Za	115	GLN
2	Za	129	GLN
2	Za	157	ASN
2	Za	190	GLN
2	Za	197	ASN
2	Za	332	ASN
2	Za	385	ASN
2	Zb	5	GLN
2	Zb	79	GLN
2	Zb	107	ASN
2	Zb	129	GLN
2	Zb	130	GLN
2	Zb	190	GLN
2	Zb	197	ASN
2	Zb	293	GLN
2	Zb	308	GLN
2	Zb	322	ASN
2	Zb	332	ASN

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Mol	Chain	Res	Type
2	Zb	358	ASN
2	Zb	381	ASN
2	Zb	387	GLN
2	Zc	5	GLN
2	Zc	107	ASN
2	Zc	129	GLN
2	Zc	133	ASN
2	Zc	159	ASN
2	Zc	197	ASN
2	Zc	379	GLN
2	Zc	387	GLN
2	Zc	397	ASN
2	Zd	5	GLN
2	Zd	105	ASN
2	Zd	129	GLN
2	Zd	130	GLN
2	Zd	293	GLN
2	Zd	295	ASN
2	Zd	322	ASN
2	Zd	397	ASN
2	Ze	99	GLN
2	Ze	107	ASN
2	Ze	133	ASN
2	Ze	197	ASN
2	Ze	394	GLN
2	Zf	105	ASN
2	Zf	133	ASN
2	Zf	159	ASN
2	Zf	197	ASN
2	Zf	252	ASN
2	Zf	314	GLN
2	Zf	397	ASN
2	Zg	5	GLN
2	Zg	107	ASN
2	Zg	129	GLN
2	Zg	133	ASN
2	Zg	197	ASN
2	Zg	310	GLN
2	Zh	5	GLN
2	Zh	115	GLN
2	Zh	129	GLN
2	Zh	197	ASN

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Mol	Chain	Res	Type
2	Zh	379	GLN
2	Zh	392	GLN
1	r	47	GLN
1	r	121	GLN
1	r	135	GLN
1	r	169	GLN
1	r	172	GLN
1	r	180	ASN
1	r	223	ASN
1	s	16	GLN
1	s	28	ASN
1	s	88	GLN
1	s	169	GLN
1	s	180	ASN
1	s	259	GLN
1	t	85	ASN
1	t	104	GLN
1	t	127	GLN
1	t	137	GLN
1	t	196	GLN
1	t	259	GLN
1	u	16	GLN
1	u	32	ASN
1	u	47	GLN
1	u	67	GLN
1	u	104	GLN
1	u	162	GLN
1	u	235	GLN
1	v	47	GLN
1	v	67	GLN
1	v	90	ASN
1	v	127	GLN
1	v	169	GLN
1	v	172	GLN
1	v	232	ASN
1	v	252	GLN
1	w	28	ASN
1	w	47	GLN
1	w	121	GLN
1	w	135	GLN
1	w	145	ASN
1	w	196	GLN

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Mol	Chain	Res	Type
1	w	223	ASN
1	w	235	GLN
1	x	32	ASN
1	x	47	GLN
1	x	83	GLN
1	x	127	GLN
1	x	145	ASN
1	x	209	ASN
1	y	25	ASN
1	y	37	GLN
1	y	51	GLN
1	y	67	GLN
1	y	125	ASN
1	y	127	GLN
1	y	137	GLN
1	y	209	ASN
1	y	223	ASN
1	y	252	GLN
1	z	67	GLN
1	z	125	ASN
3	D	39	GLN
4	E	162	ASN
4	E	182	ASN
4	E	205	ASN
5	F	119	GLN
5	F	141	GLN
5	H	36	GLN
5	H	132	GLN
5	H	233	GLN
5	I	160	GLN
5	I	184	GLN
5	J	114	GLN
5	J	155	ASN
6	K	69	ASN
6	K	83	GLN
6	K	103	GLN
6	L	87	GLN
6	L	90	ASN
6	M	103	GLN
6	N	87	GLN
6	O	55	GLN
7	Q	17	ASN

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Mol	Chain	Res	Type
7	R	23	GLN
7	R	29	ASN
7	R	92	GLN
7	R	117	GLN
7	S	32	ASN
7	S	92	GLN
7	T	17	ASN
7	T	21	GLN
7	T	32	ASN
7	T	117	GLN
7	U	112	ASN
8	V	30	ASN
8	W	5	ASN
8	W	22	ASN
8	W	120	ASN
8	X	22	ASN
8	X	50	GLN
8	X	57	GLN
8	X	134	GLN
8	Y	22	ASN
8	Z	17	GLN
8	Z	30	ASN
8	a	57	GLN
8	a	115	ASN
9	b	318	ASN
9	b	319	GLN
9	e	324	ASN
9	l	324	ASN
10	m	102	ASN
10	n	18	GLN
10	n	70	GLN
10	n	106	GLN
10	n	116	GLN
10	n	172	GLN
10	n	210	ASN
10	n	223	ASN
10	n	240	ASN
10	o	14	GLN
10	o	18	GLN
10	o	28	ASN
10	o	70	GLN
10	o	104	ASN

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Mol	Chain	Res	Type
10	o	106	GLN
10	o	186	GLN
10	o	230	GLN
10	p	17	ASN
10	p	28	ASN
10	p	104	ASN
10	p	106	GLN
10	p	210	ASN
10	p	240	ASN
10	q	18	GLN
10	q	37	GLN
10	q	104	ASN
10	q	106	GLN
10	q	112	GLN
10	q	116	GLN
10	q	118	HIS
10	q	153	ASN
10	q	240	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

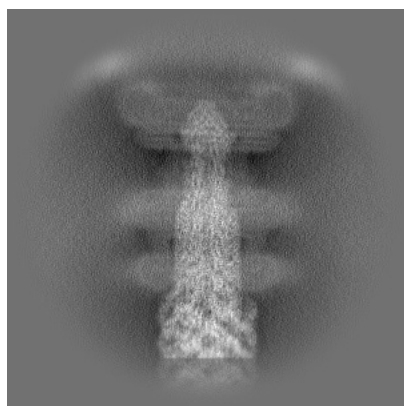
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37628. These allow visual inspection of the internal detail of the map and identification of artifacts.

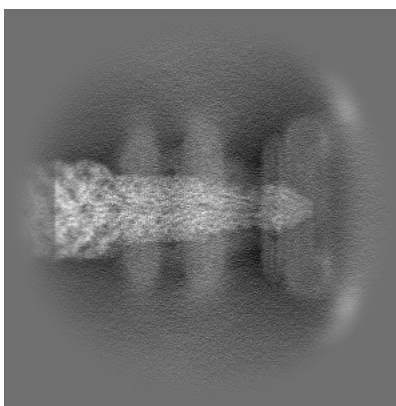
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

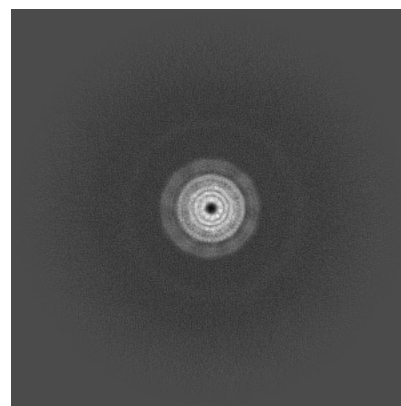
6.1.1 Primary map



X

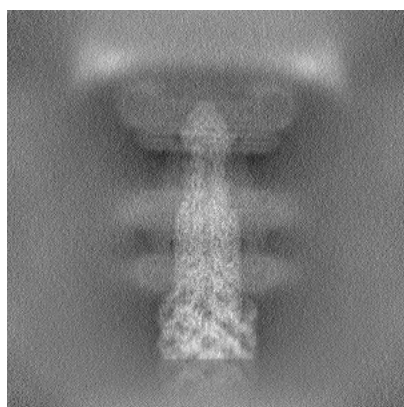


Y

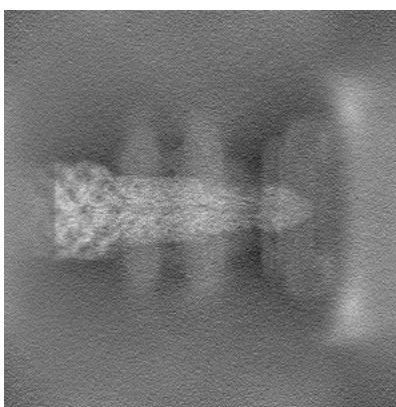


Z

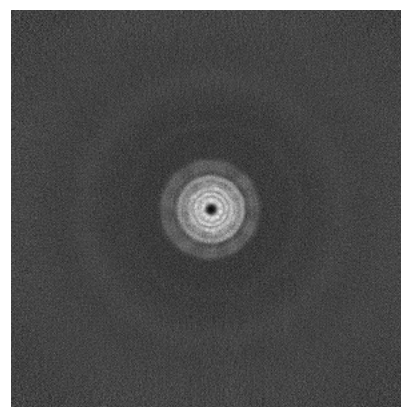
6.1.2 Raw map



X



Y

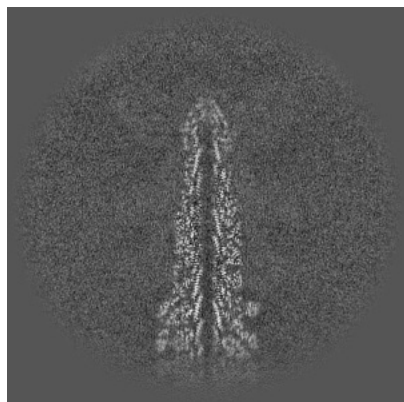


Z

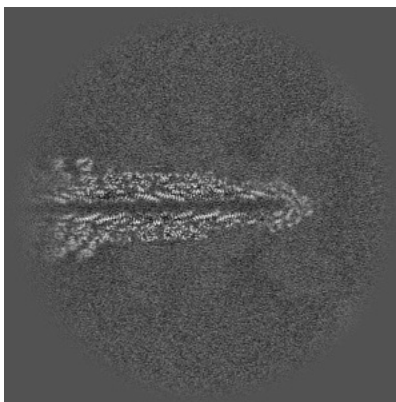
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

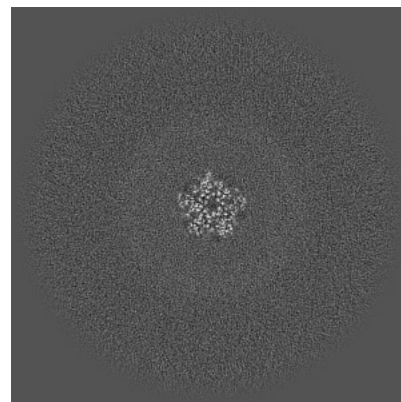
6.2.1 Primary map



X Index: 256

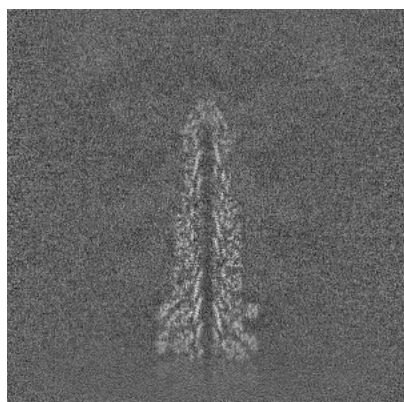


Y Index: 256

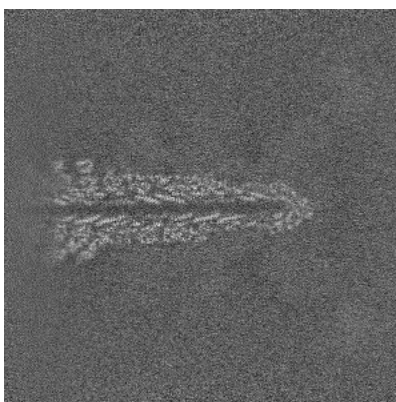


Z Index: 256

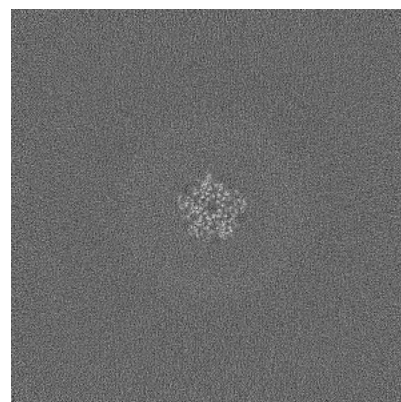
6.2.2 Raw map



X Index: 256



Y Index: 256

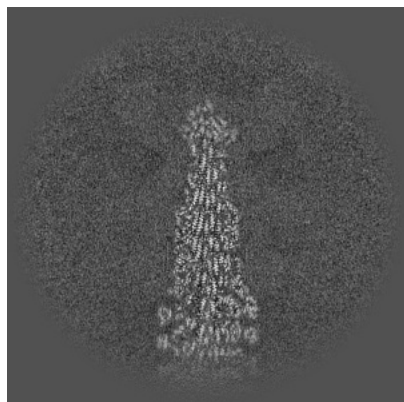


Z Index: 256

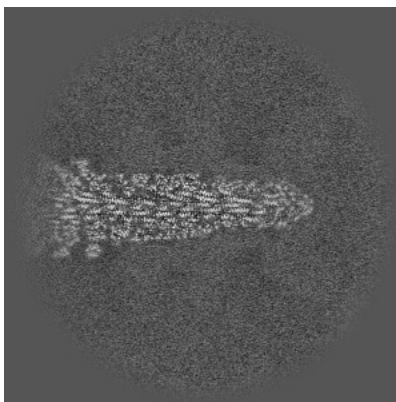
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

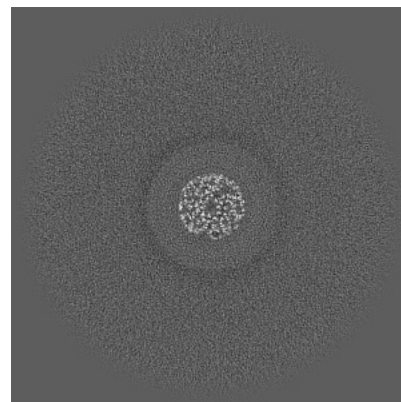
6.3.1 Primary map



X Index: 245

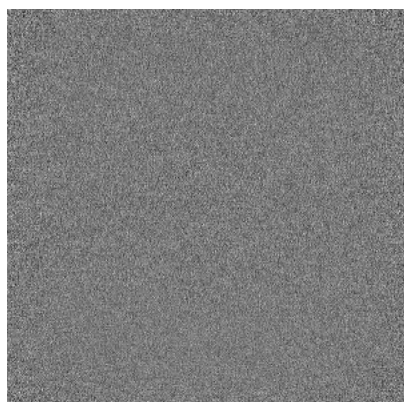


Y Index: 246

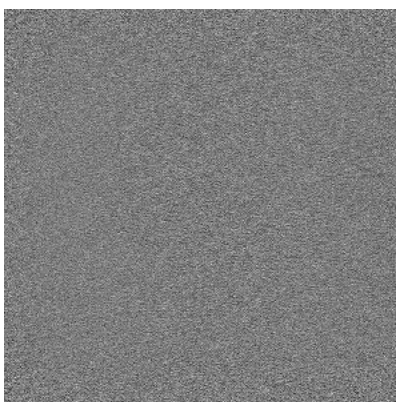


Z Index: 229

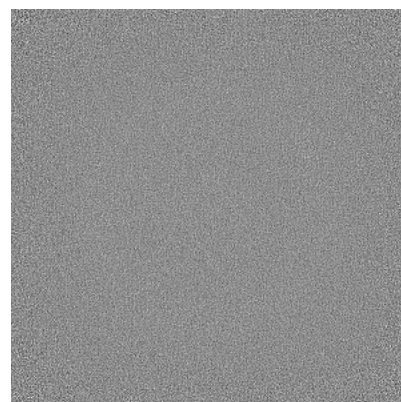
6.3.2 Raw map



X Index: 0



Y Index: 0

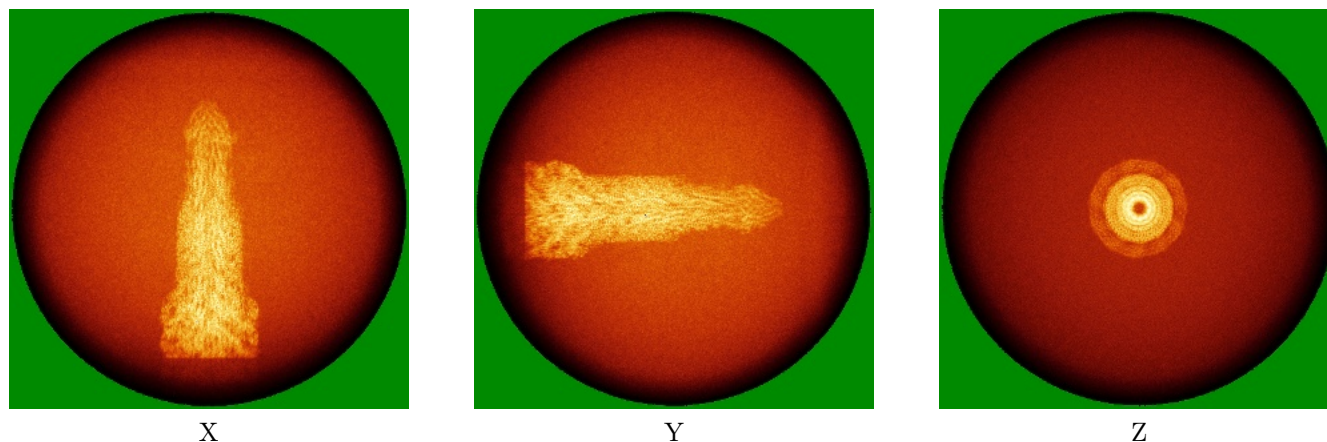


Z Index: 511

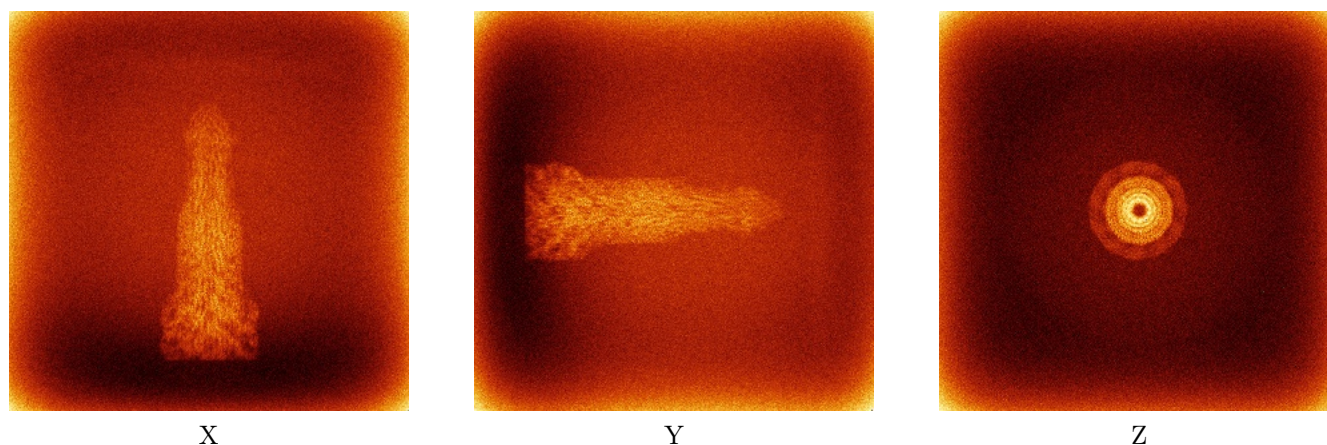
The images above show the largest variance slices of the map in three orthogonal directions.

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



X



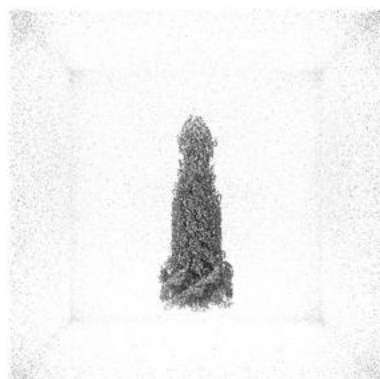
Y



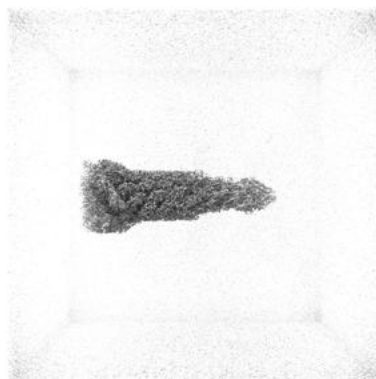
Z

The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

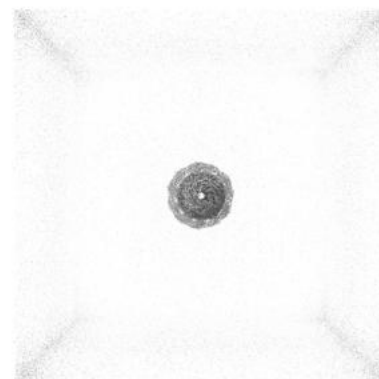
6.5.2 Raw map



X



Y



Z

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

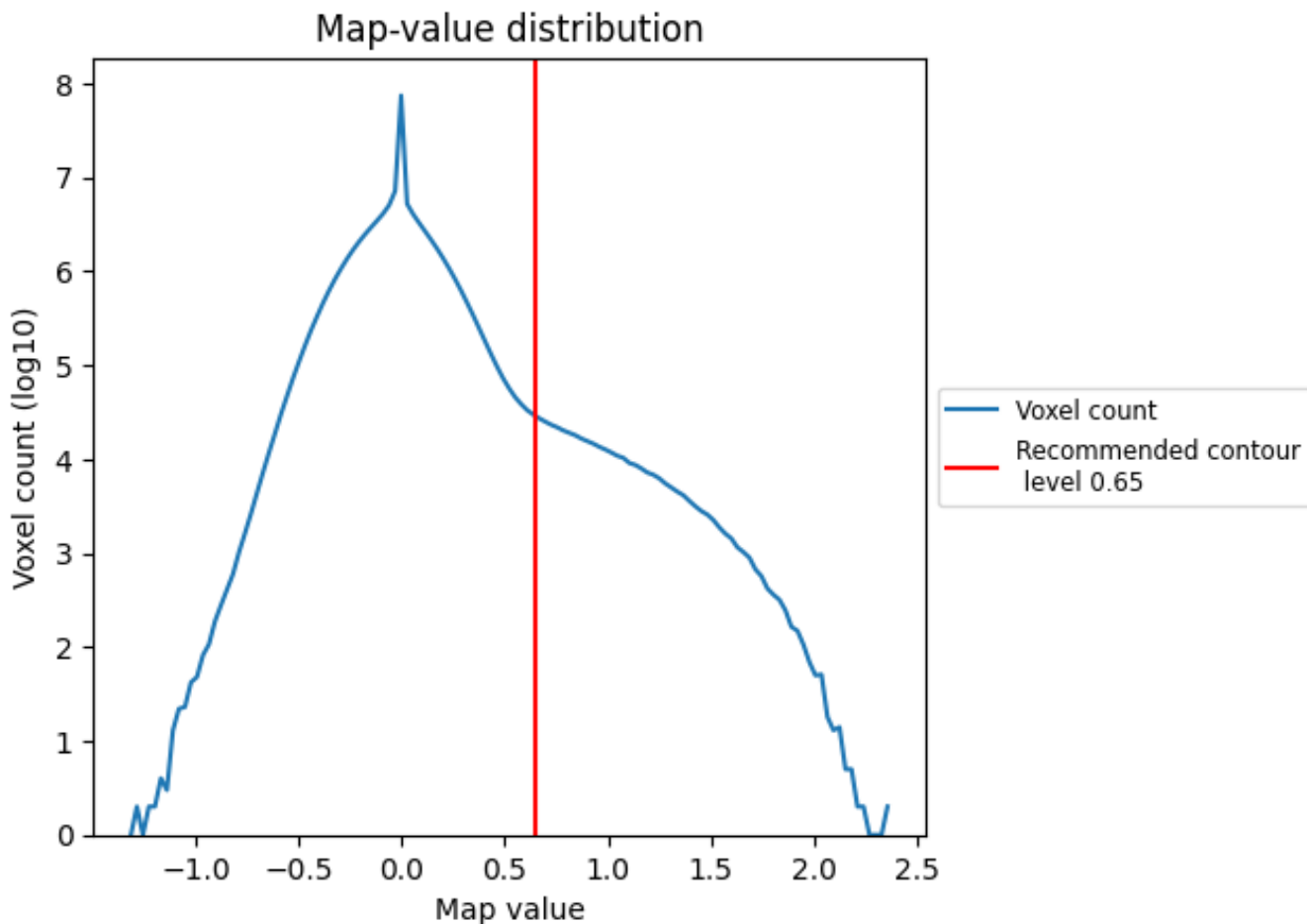
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

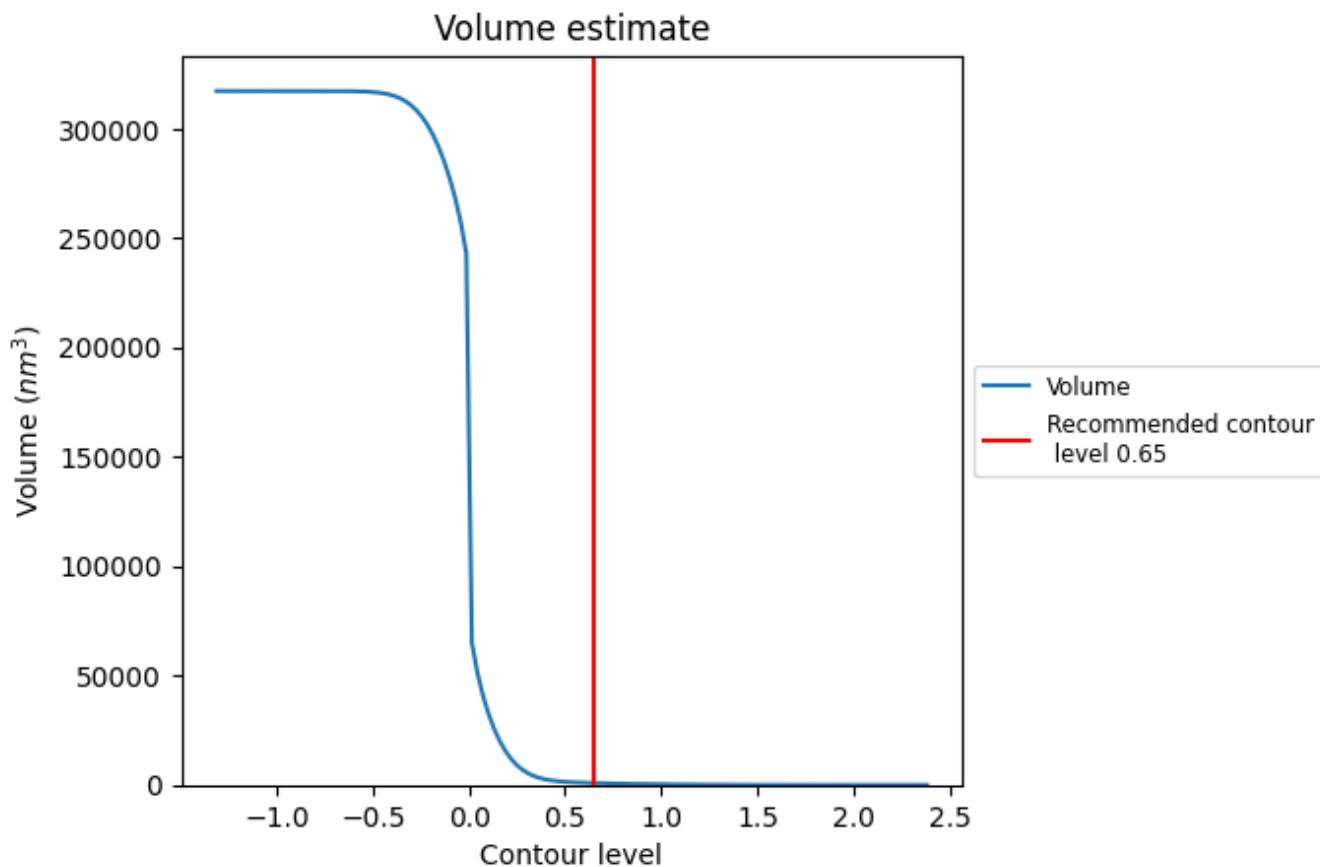
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

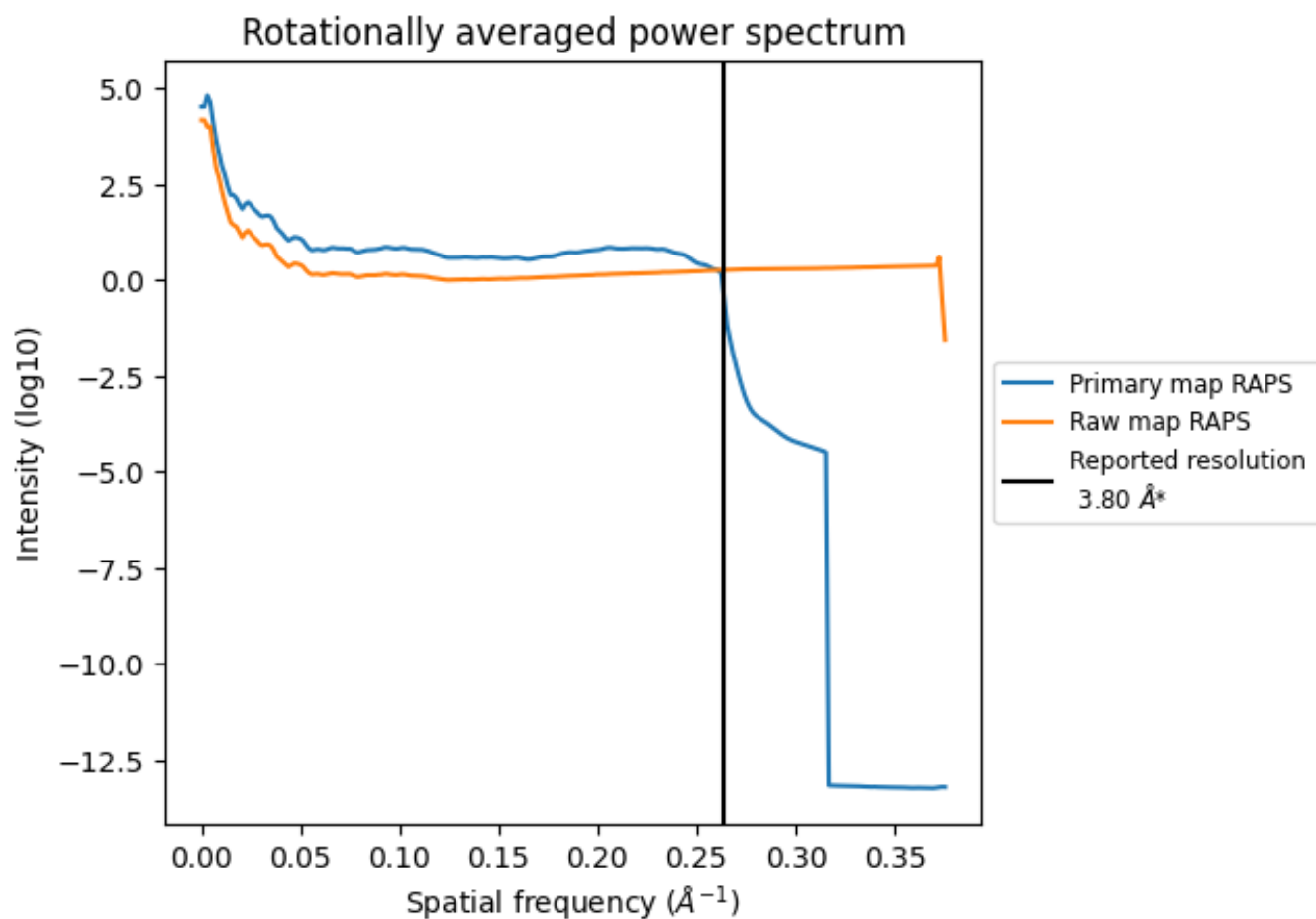
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 871 nm^3 ; this corresponds to an approximate mass of 787 kDa.

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

7.3 Rotationally averaged power spectrum i

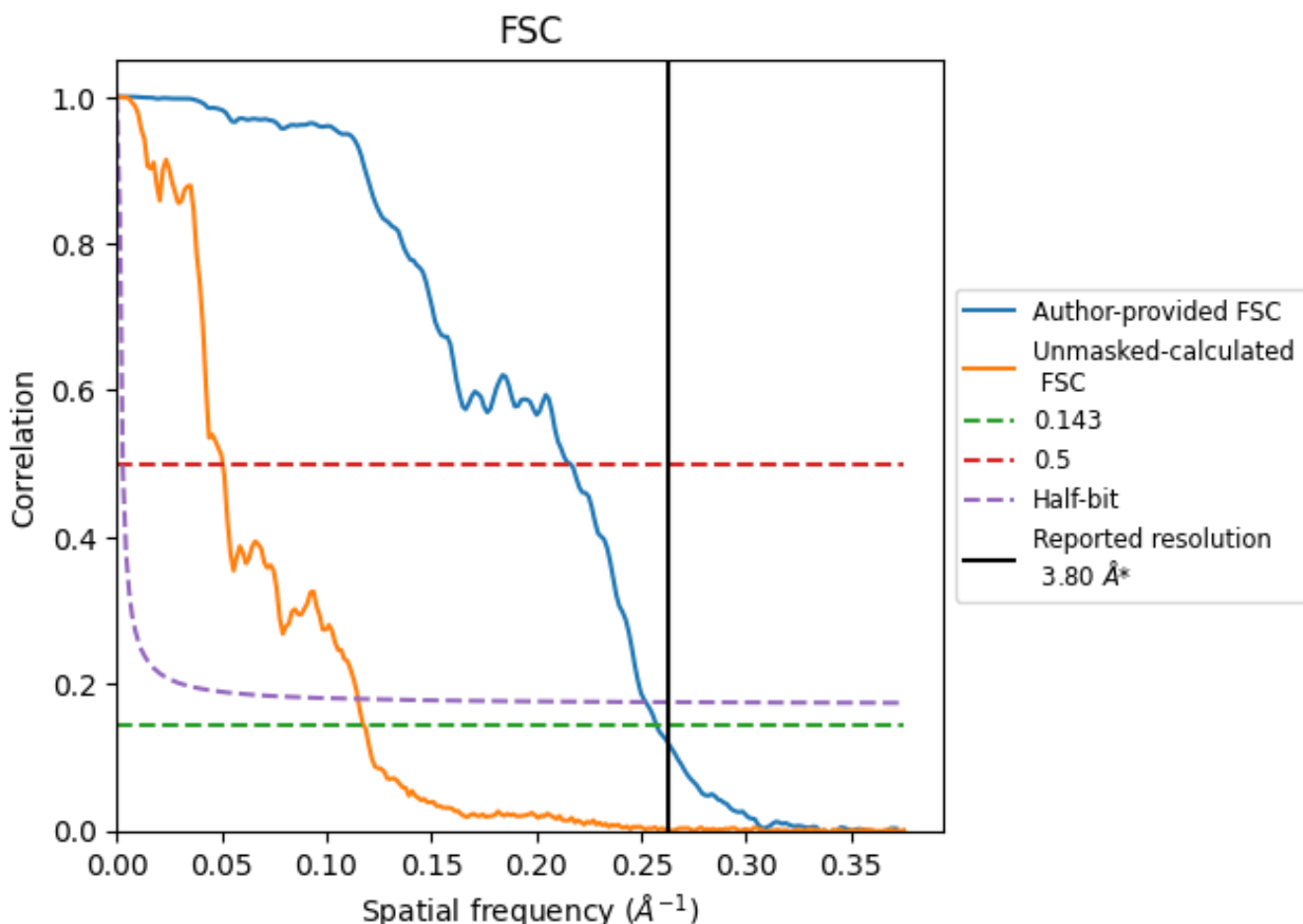


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

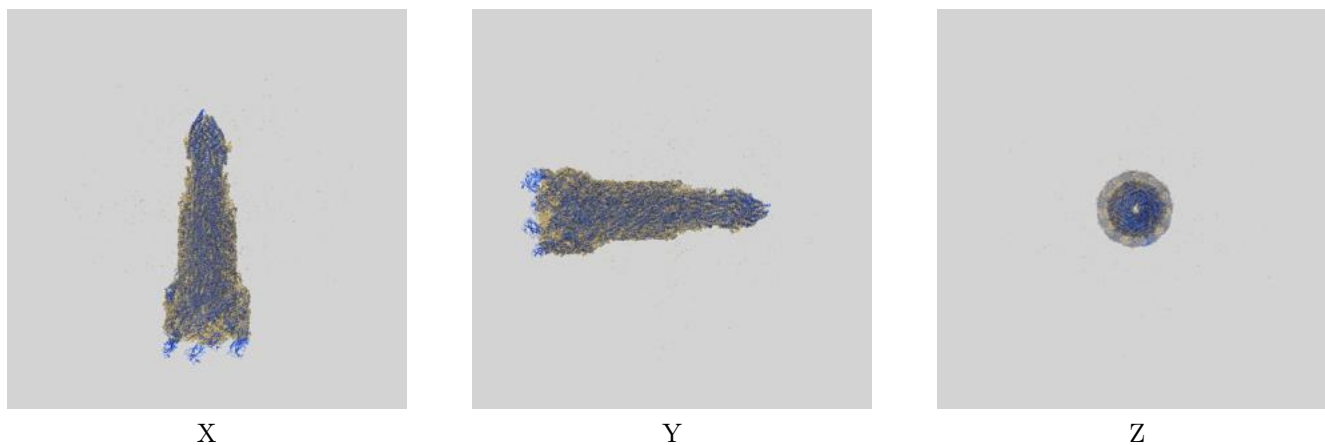
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.89	4.63	3.97
Unmasked-calculated*	8.49	19.80	8.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.49 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

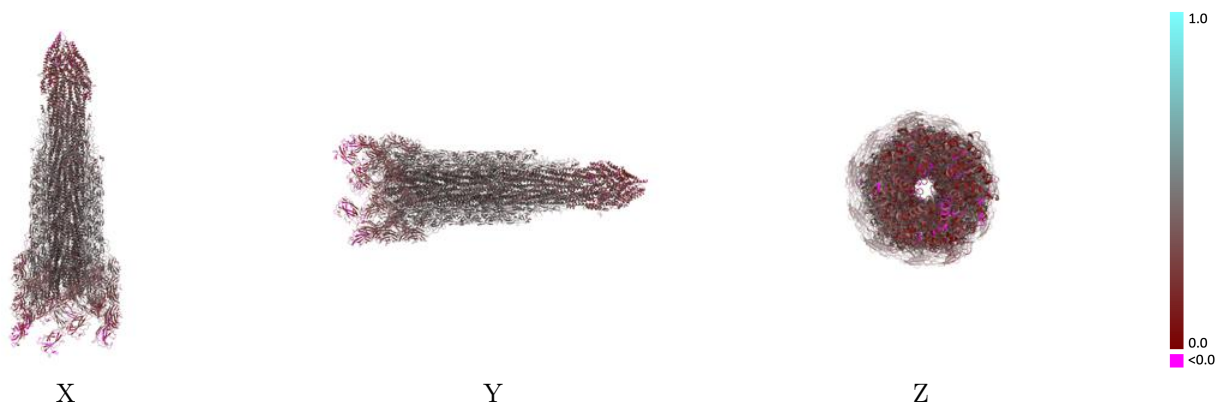
This section contains information regarding the fit between EMDB map EMD-37628 and PDB model 8WLQ. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



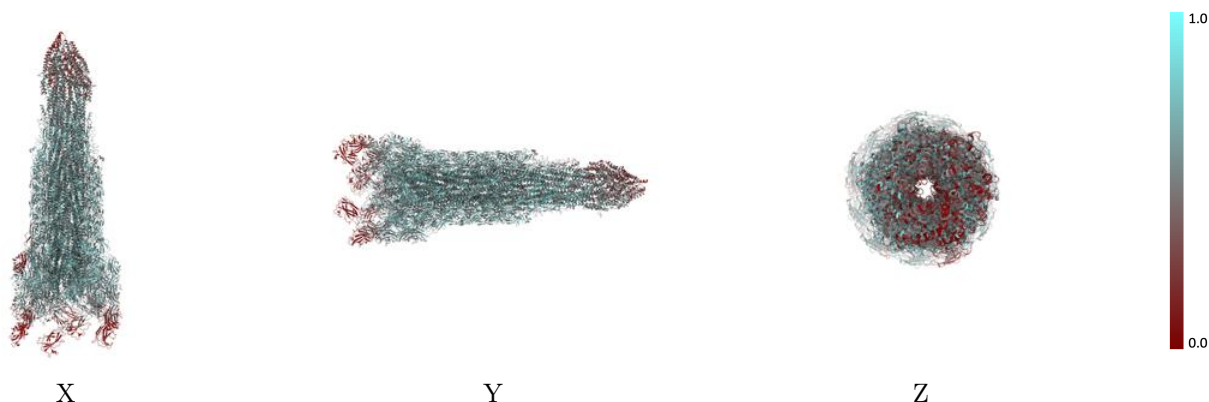
The images above show the 3D surface view of the map at the recommended contour level 0.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



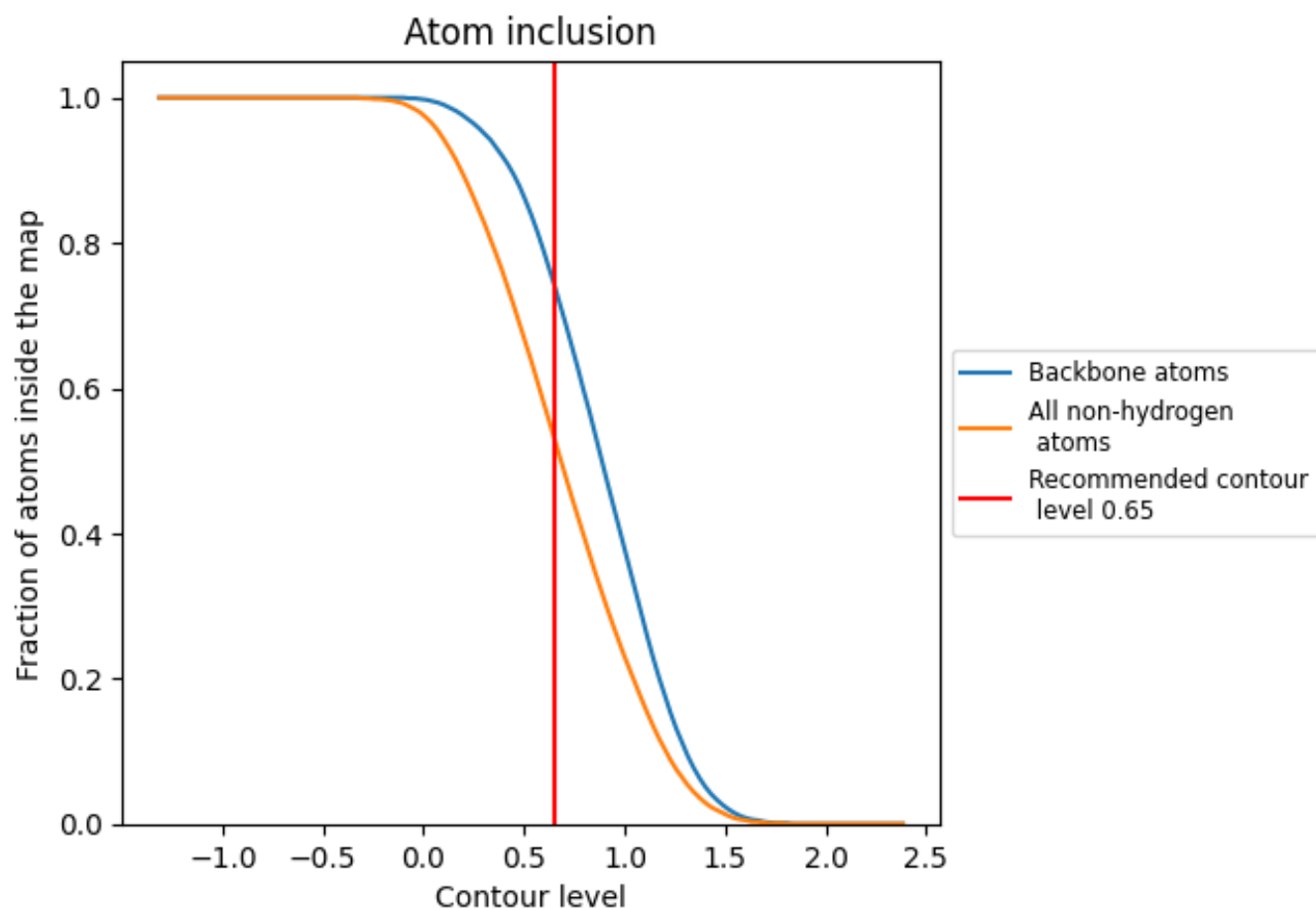
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.65).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 53% 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 (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5300	 0.3500
0	 0.6070	 0.4090
1	 0.5800	 0.4020
2	 0.5900	 0.4060
3	 0.5980	 0.3990
4	 0.6000	 0.3950
5	 0.5870	 0.4010
6	 0.6040	 0.4060
7	 0.5970	 0.4070
8	 0.5940	 0.4040
9	 0.5740	 0.3940
A	 0.1730	 0.1850
B	 0.3560	 0.2400
C	 0.3900	 0.2320
D	 0.3590	 0.1900
E	 0.3230	 0.2250
F	 0.3730	 0.2390
G	 0.4440	 0.2750
H	 0.4670	 0.2980
I	 0.4650	 0.2870
J	 0.4240	 0.2890
K	 0.4440	 0.2800
L	 0.5070	 0.3100
M	 0.5330	 0.3380
N	 0.5530	 0.3390
O	 0.5200	 0.3260
P	 0.5320	 0.3370
Q	 0.4940	 0.3360
R	 0.5870	 0.3710
S	 0.5930	 0.3730
T	 0.6070	 0.3750
U	 0.5700	 0.3680
V	 0.5200	 0.3610
W	 0.5610	 0.3730
X	 0.5850	 0.4010











































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Chain	Atom inclusion	Q-score
Y	0.5810	0.4000
Z	0.6090	0.3980
ZA	0.5780	0.3920
ZB	0.5910	0.3970
ZC	0.6080	0.4120
ZD	0.5910	0.4090
ZE	0.5700	0.3960
ZF	0.3840	0.3220
ZG	0.5490	0.3670
ZH	0.5850	0.3690
ZI	0.6000	0.3760
ZJ	0.6020	0.3740
ZK	0.5880	0.3660
ZL	0.5930	0.3710
ZM	0.5910	0.3750
ZN	0.6010	0.3710
ZO	0.6000	0.3650
ZP	0.6030	0.3630
ZQ	0.5830	0.3570
ZR	0.5800	0.3520
ZS	0.5890	0.3550
ZT	0.5660	0.3490
ZU	0.5590	0.3420
ZV	0.5520	0.3350
ZW	0.5380	0.3290
ZX	0.5310	0.3240
ZY	0.5000	0.3190
ZZ	0.4900	0.3060
Za	0.4610	0.3080
Zb	0.4190	0.2820
Zc	0.4030	0.2900
Zd	0.3780	0.2790
Ze	0.3450	0.2630
Zf	0.3370	0.2470
Zg	0.3130	0.2380
Zh	0.2950	0.2350
a	0.5650	0.3790
b	0.3210	0.3210
c	0.4470	0.3630
d	0.3990	0.3370
e	0.6210	0.4010
f	0.5500	0.3570

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Chain	Atom inclusion	Q-score
g	 0.5240	 0.3350
h	 0.6000	 0.4050
i	 0.5530	 0.3420
j	 0.5870	 0.3990
k	 0.4560	 0.2680
l	 0.4860	 0.3280
m	 0.5430	 0.3860
n	 0.6180	 0.4010
o	 0.6160	 0.4150
p	 0.6110	 0.4030
q	 0.5920	 0.3880
r	 0.5490	 0.3830
s	 0.5910	 0.4050
t	 0.6130	 0.4110
u	 0.5920	 0.4070
v	 0.5820	 0.4080
w	 0.5950	 0.4020
x	 0.5890	 0.3990
y	 0.5950	 0.4080
z	 0.5810	 0.3980