



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 09:50 PM EDT

PDB ID : 7TNQ
EMDB ID : EMD-26018
Title : The symmetry-released subpellicular microtubule map from detergent-extracted Toxoplasma cells
Authors : Sun, S.Y.; Pintilie, G.D.; Chen, M.
Deposited on : 2022-01-21
Resolution : 8.40 Å(reported)
Based on initial model : 7MIZ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

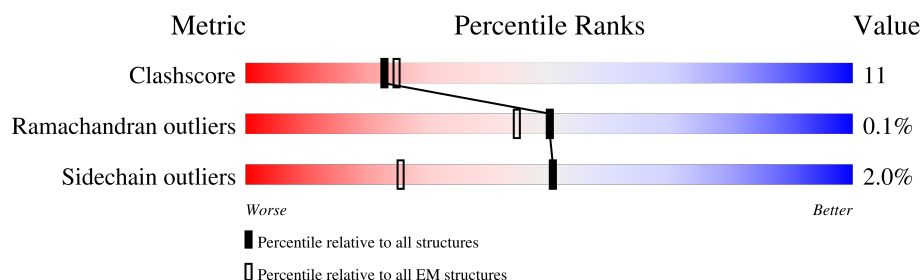
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.40 Å.

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



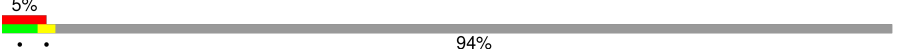
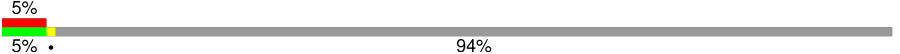

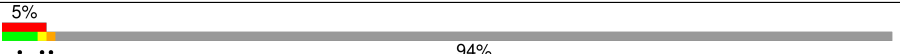
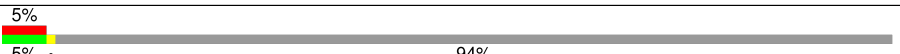
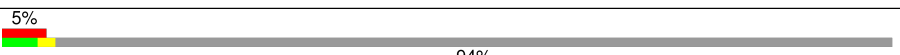
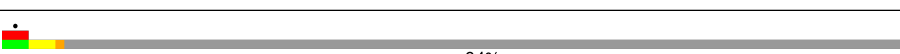
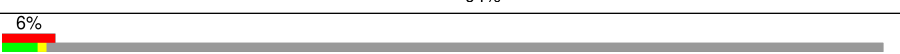
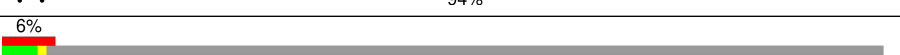
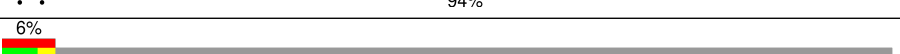
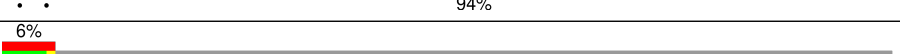
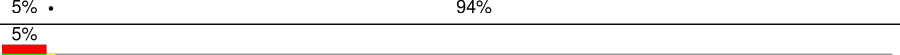
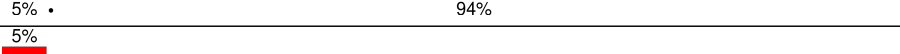
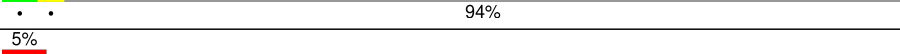
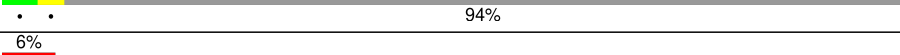
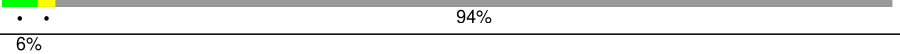


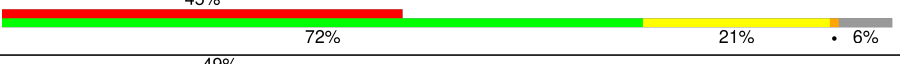
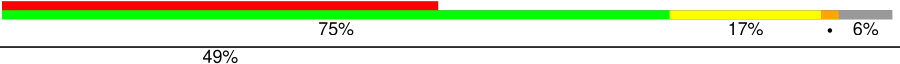





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	351	<div> <div>5%</div> <div>5%</div> <div>94%</div> </div>
1	1	351	<div> <div>6%</div> <div>94%</div> </div>
1	10	351	<div> <div>6%</div> <div>94%</div> </div>
1	11	351	<div> <div>6%</div> <div>94%</div> </div>
1	12	351	<div> <div>5%</div> <div>94%</div> </div>
1	13	351	<div> <div>5%</div> <div>94%</div> </div>
1	14	351	<div> <div>6%</div> <div>94%</div> </div>
1	15	351	<div> <div>5%</div> <div>94%</div> </div>

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Mol	Chain	Length	Quality of chain
1	16	351	
1	17	351	
1	18	351	
1	19	351	
1	2	351	
1	20	351	
1	21	351	
1	22	351	
1	23	351	
1	3	351	
1	4	351	
1	5	351	
1	6	351	
1	7	351	
1	8	351	
1	9	351	
2	A0	453	
2	A2	453	
2	A4	453	
2	A6	453	
2	A8	453	
2	B0	453	
2	B2	453	
2	B4	453	
2	B6	453	

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Mol	Chain	Length	Quality of chain
2	B8	453	
2	C0	453	
2	C2	453	
2	C4	453	
2	C6	453	
2	C8	453	
2	D0	453	
2	D2	453	
2	D4	453	
2	D6	453	
2	D8	453	
2	E0	453	
2	E2	453	
2	E4	453	
2	E6	453	
2	E8	453	
2	F0	453	
3	A1	449	
3	A3	449	
3	A5	449	
3	A7	449	
3	A9	449	
3	B1	449	
3	B3	449	
3	B5	449	

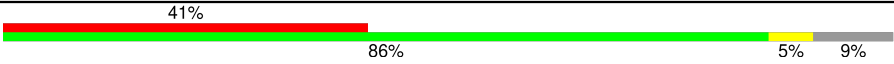

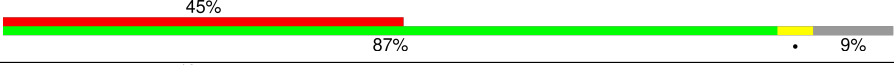



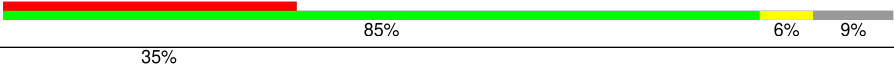

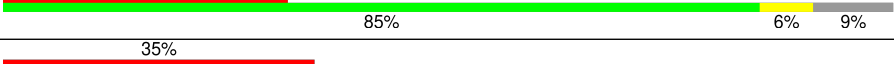


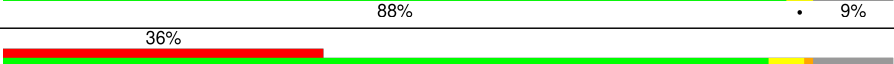

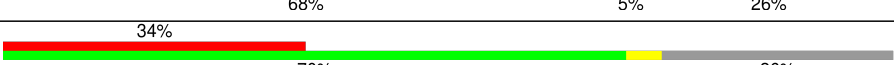

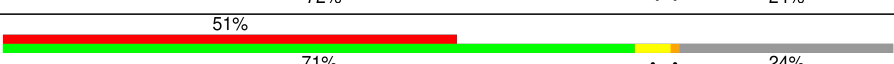
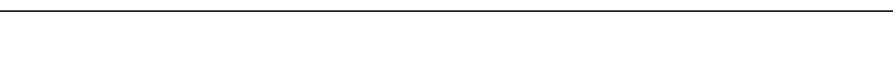
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Mol	Chain	Length	Quality of chain
3	B7	449	
3	B9	449	
3	C1	449	
3	C3	449	
3	C5	449	
3	C7	449	
3	C9	449	
3	D1	449	
3	D3	449	
3	D5	449	
3	D7	449	
3	D9	449	
3	E1	449	
3	E3	449	
3	E5	449	
3	E7	449	
3	E9	449	
3	F1	449	
4	a	220	
4	b	220	
4	c	220	
4	d	220	
4	e	220	
4	f	220	
4	g	220	

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Mol	Chain	Length	Quality of chain
4	h	220	
4	i	220	
4	j	220	
4	m	220	
4	n	220	
4	o	220	
4	p	220	
4	q	220	
4	r	220	
4	s	220	
4	t	220	
4	u	220	
4	v	220	
5	k	189	
5	l	189	
5	w	189	
5	x	189	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 213168 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 Microtubule associated protein SPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	1	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	10	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	11	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	12	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	13	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	14	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	15	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	16	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	17	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	18	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	19	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	2	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	20	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	21	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	22	20	Total	C	N	O	S	0	0
			160	105	26	28	1		
1	23	20	Total	C	N	O	S	0	0
			160	105	26	28	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	22	Total 174	C 114	N 28	O 31	S 1	0	0
1	4	22	Total 174	C 114	N 28	O 31	S 1	0	0
1	5	22	Total 174	C 114	N 28	O 31	S 1	0	0
1	6	22	Total 174	C 114	N 28	O 31	S 1	0	0
1	7	22	Total 174	C 114	N 28	O 31	S 1	0	0
1	8	22	Total 174	C 114	N 28	O 31	S 1	0	0
1	9	22	Total 174	C 114	N 28	O 31	S 1	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	263	ALA	VAL	conflict	UNP S8F1Y1
1	263	ALA	VAL	conflict	UNP S8F1Y1
10	263	ALA	VAL	conflict	UNP S8F1Y1
11	263	ALA	VAL	conflict	UNP S8F1Y1
12	263	ALA	VAL	conflict	UNP S8F1Y1
13	263	ALA	VAL	conflict	UNP S8F1Y1
14	263	ALA	VAL	conflict	UNP S8F1Y1
15	263	ALA	VAL	conflict	UNP S8F1Y1
16	263	ALA	VAL	conflict	UNP S8F1Y1
17	263	ALA	VAL	conflict	UNP S8F1Y1
18	263	ALA	VAL	conflict	UNP S8F1Y1
19	263	ALA	VAL	conflict	UNP S8F1Y1
2	263	ALA	VAL	conflict	UNP S8F1Y1
20	263	ALA	VAL	conflict	UNP S8F1Y1
21	263	ALA	VAL	conflict	UNP S8F1Y1
22	263	ALA	VAL	conflict	UNP S8F1Y1
23	263	ALA	VAL	conflict	UNP S8F1Y1
3	263	ALA	VAL	conflict	UNP S8F1Y1
4	263	ALA	VAL	conflict	UNP S8F1Y1
5	263	ALA	VAL	conflict	UNP S8F1Y1
6	263	ALA	VAL	conflict	UNP S8F1Y1
7	263	ALA	VAL	conflict	UNP S8F1Y1
8	263	ALA	VAL	conflict	UNP S8F1Y1
9	263	ALA	VAL	conflict	UNP S8F1Y1

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	A2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	A4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	A6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	A8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	B0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	B2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	B4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	B6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	B8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	C0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	C2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	C4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	C6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	C8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	D0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	D2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	D4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	D6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	D8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
2	E0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	E2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	F0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	D1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	D3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	D5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	D7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	D9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	E1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	E3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	E5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	E7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	E9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
3	F1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

- Molecule 4 is a protein called PDI family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	150	Total 1198	C 763	N 213	O 217	S 5	0	0
4	b	150	Total 1198	C 763	N 213	O 217	S 5	0	0
4	c	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	d	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	e	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	f	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	g	201	Total 1608	C 1021	N 283	O 297	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	h	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	i	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	j	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	m	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	n	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	o	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	p	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	q	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	r	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	s	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	t	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	u	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	v	201	Total 1608	C 1021	N 283	O 297	S 7	0	0

- Molecule 5 is a protein called PDI family protein.

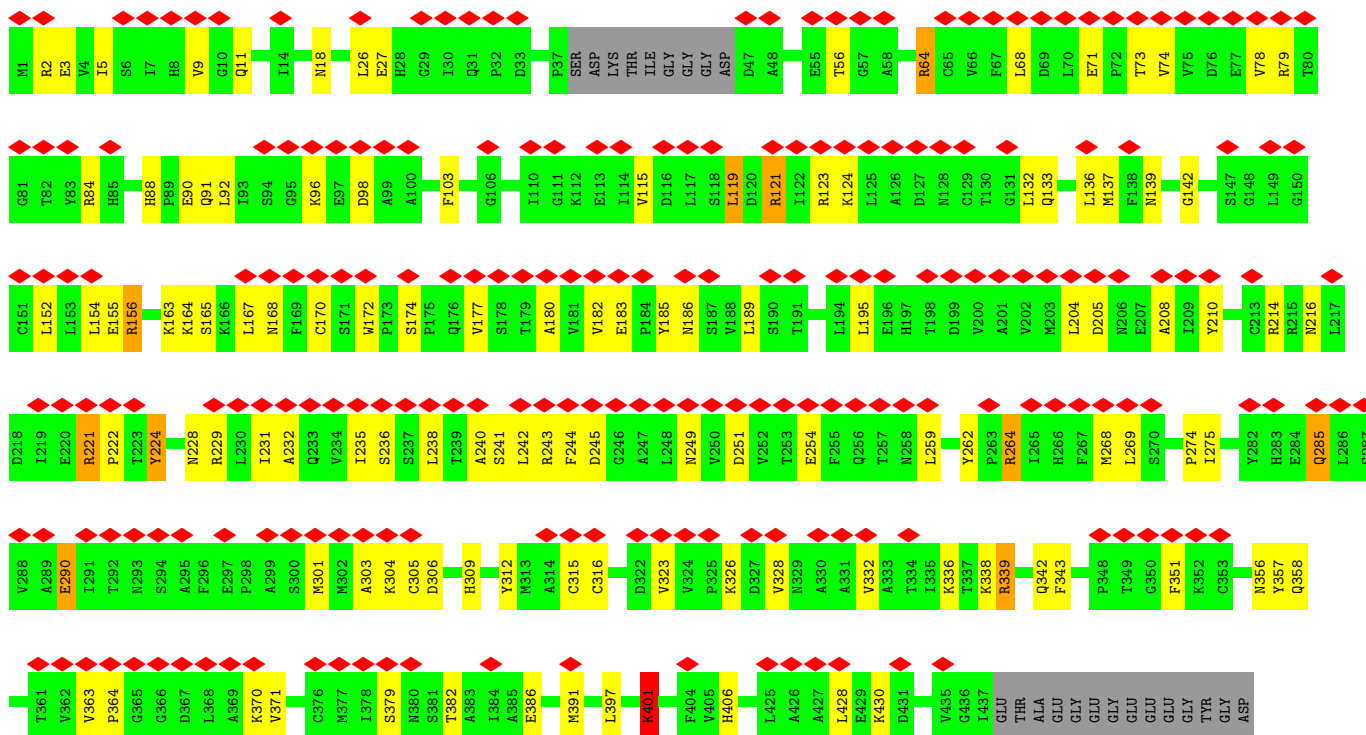
Mol	Chain	Residues	Atoms					AltConf	Trace
5	k	139	Total 1140	C 738	N 203	O 195	S 4	0	0
5	l	139	Total 1140	C 738	N 203	O 195	S 4	0	0
5	w	143	Total 1172	C 755	N 207	O 205	S 5	0	0
5	x	143	Total 1172	C 755	N 207	O 205	S 5	0	0



[illegible]



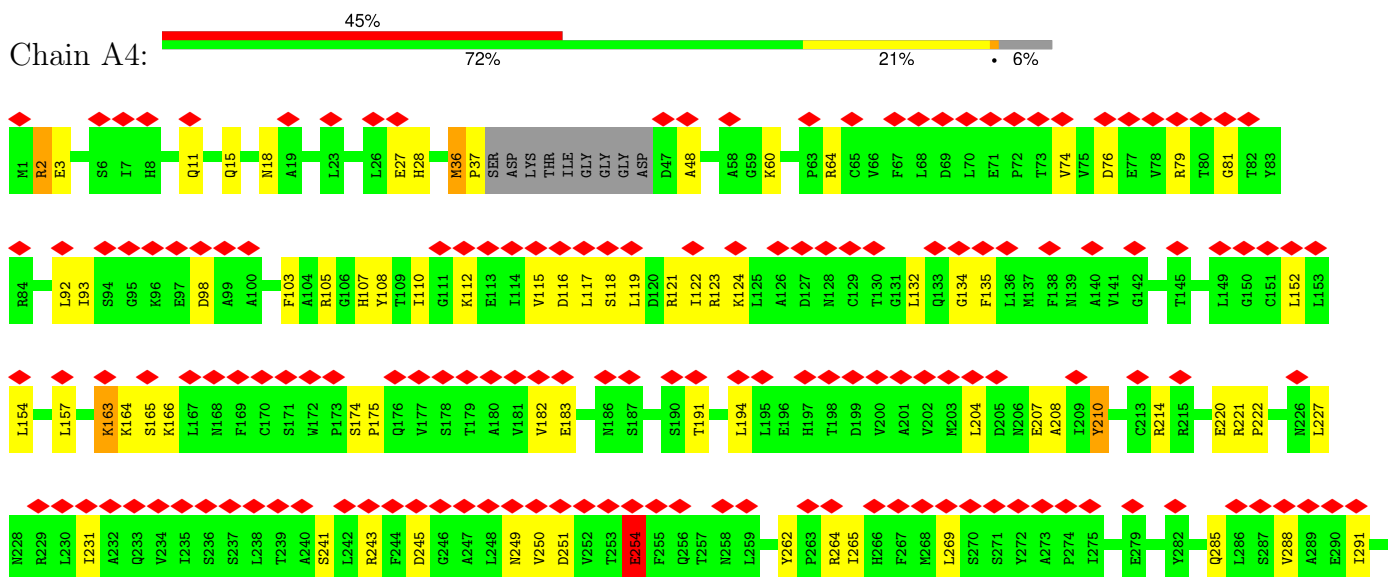
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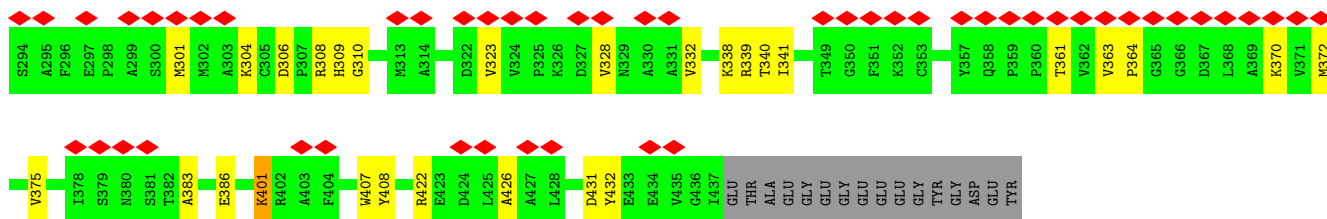


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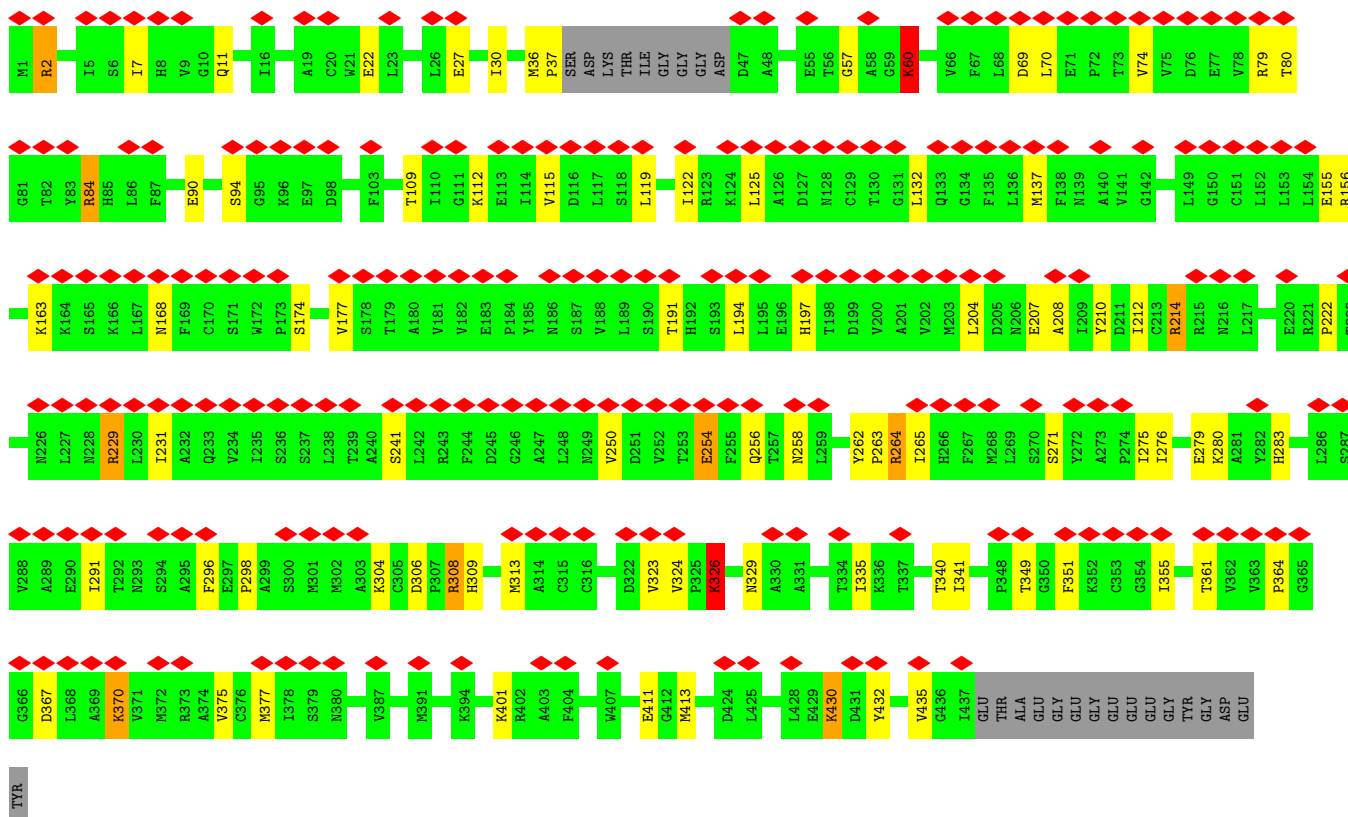
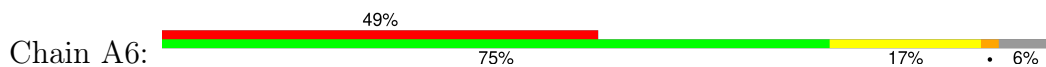


Chain A4:

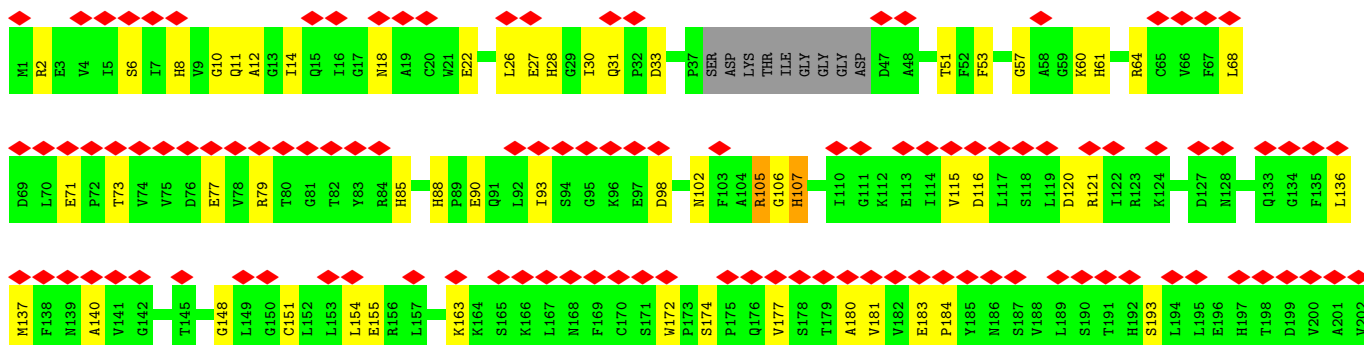


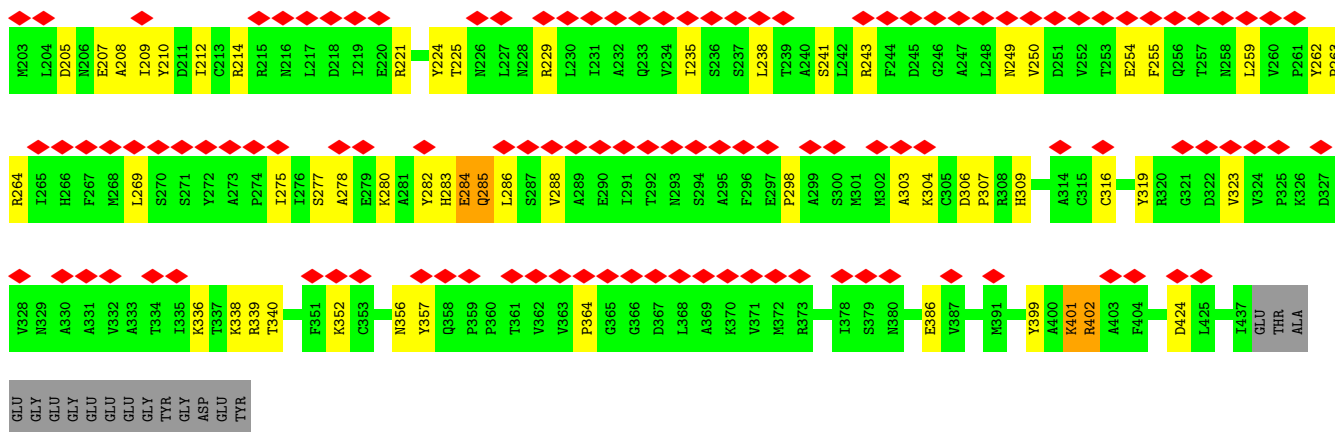


• Molecule 2: Tubulin alpha chain

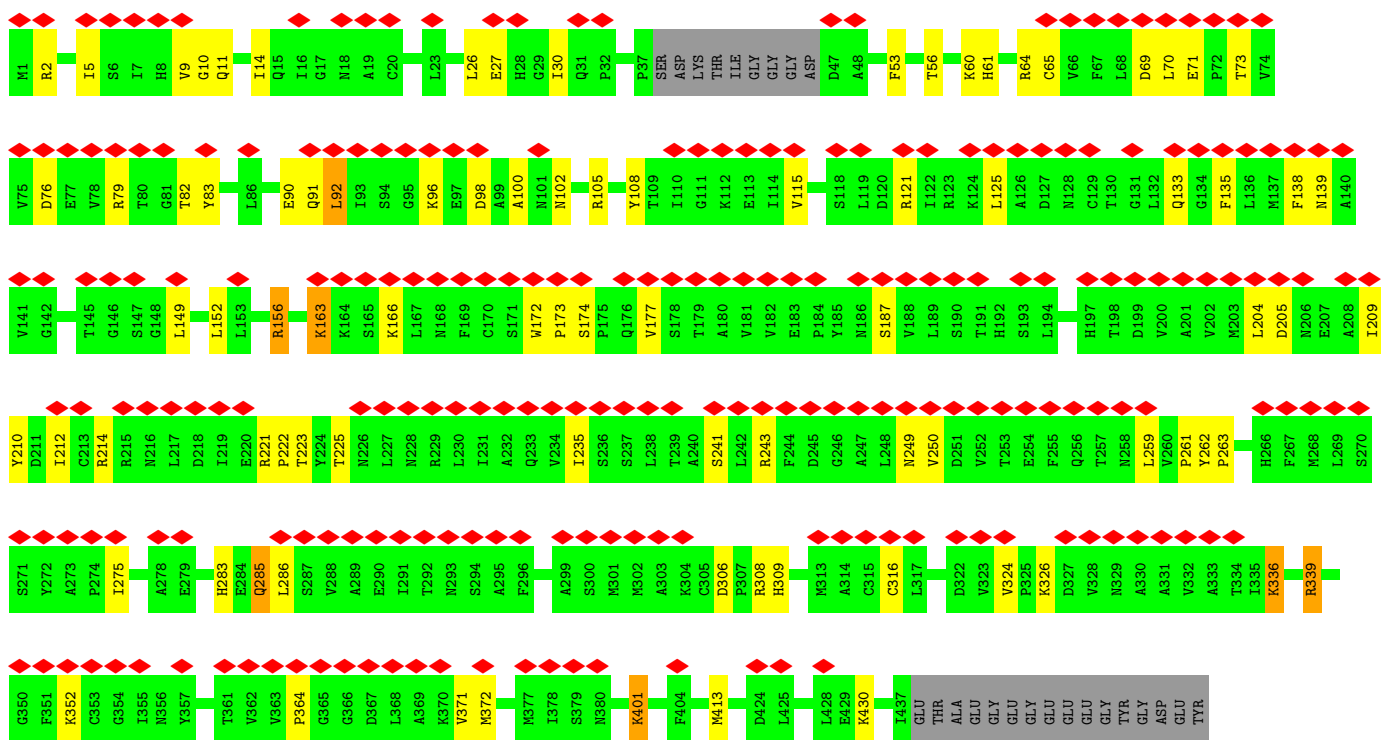
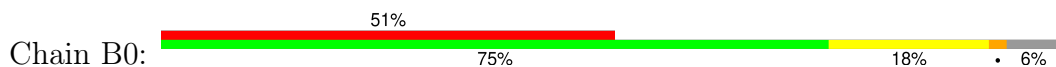


• Molecule 2: Tubulin alpha chain

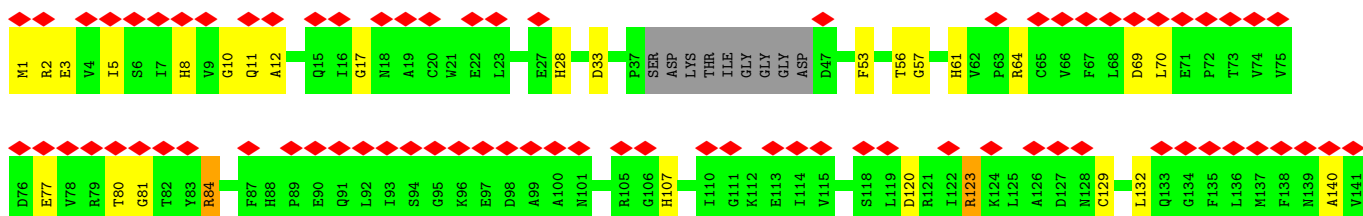
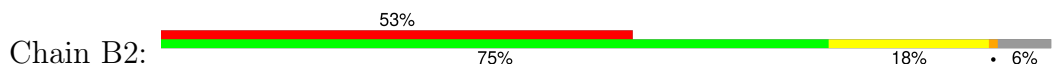


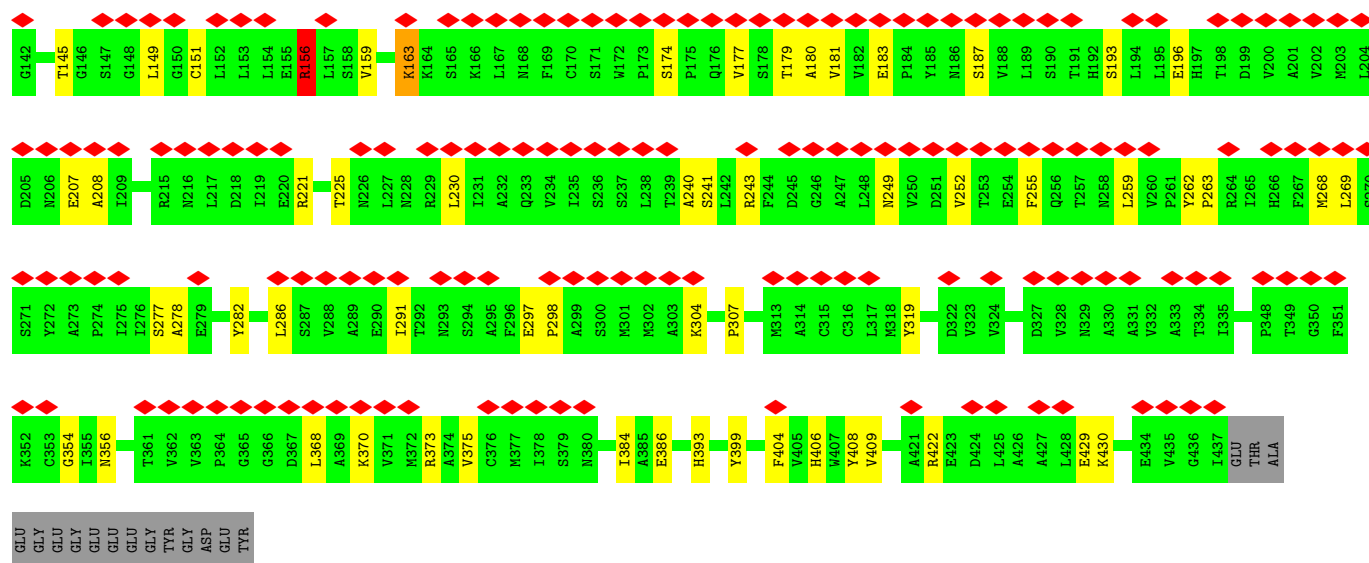


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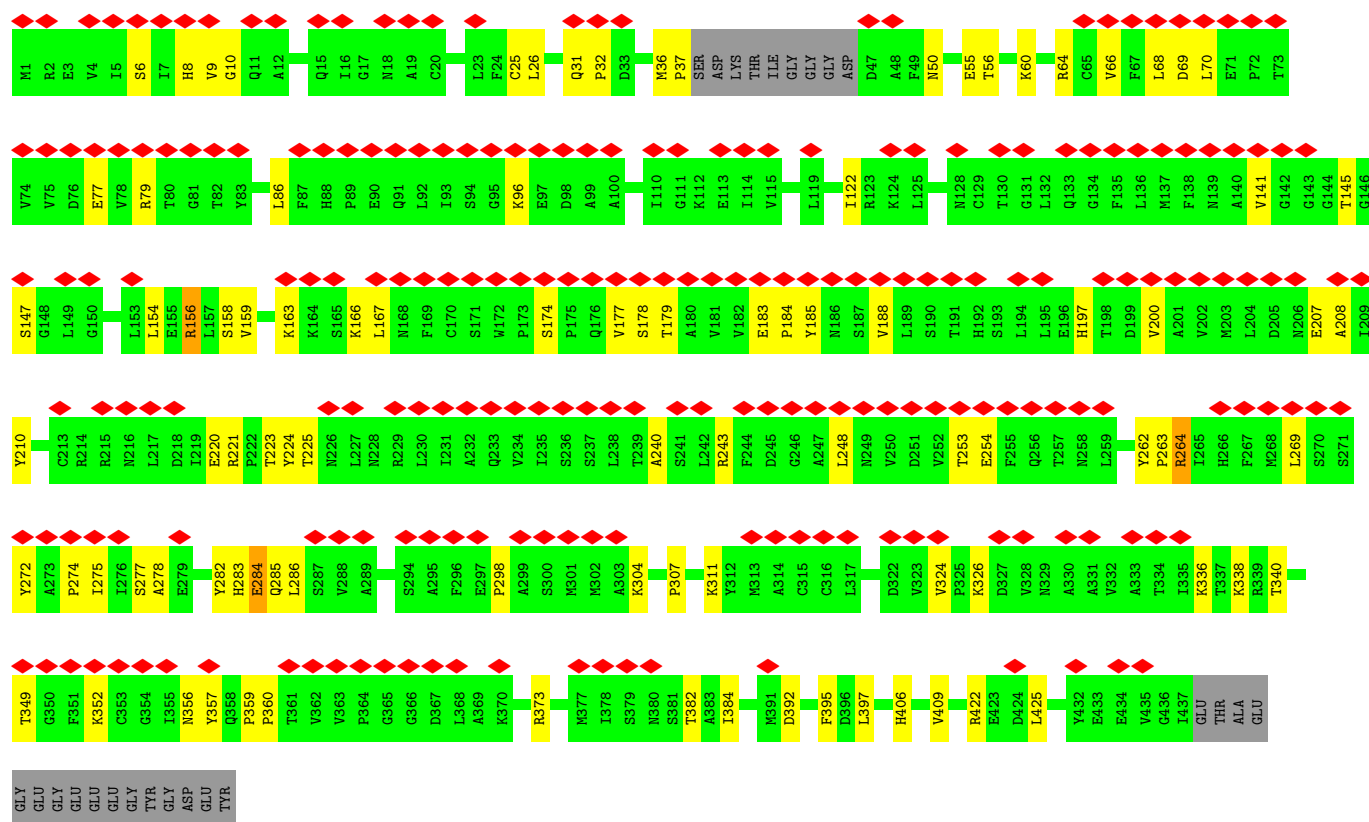


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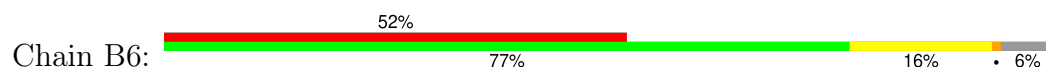


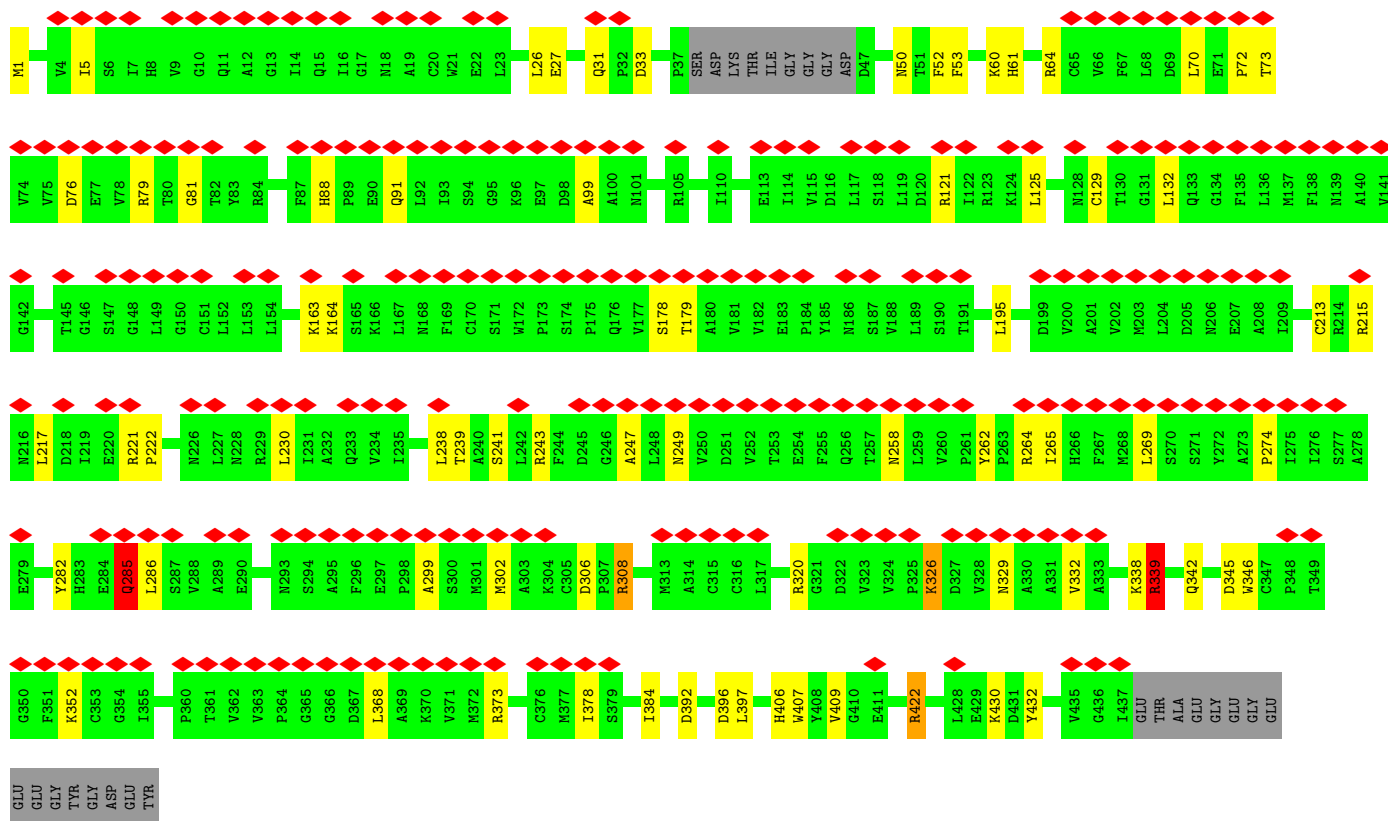


• Molecule 2: Tubulin alpha chain

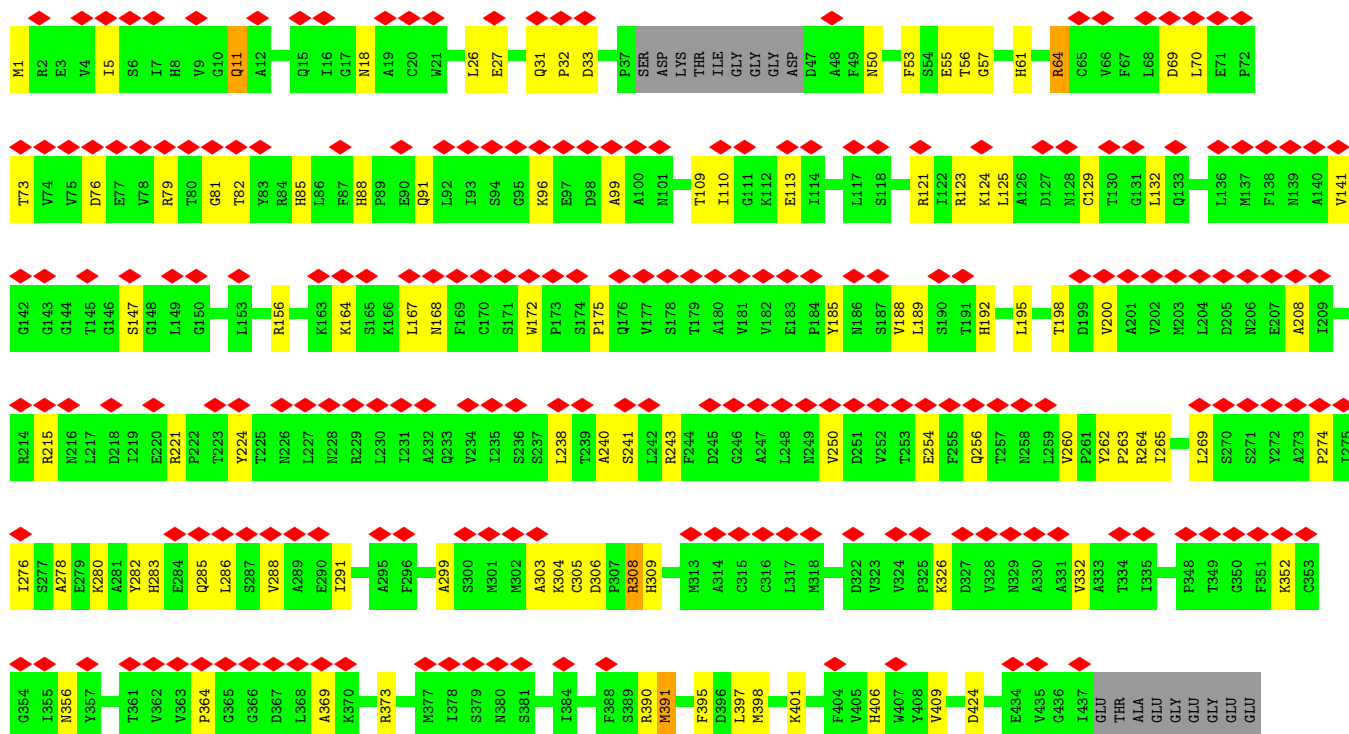


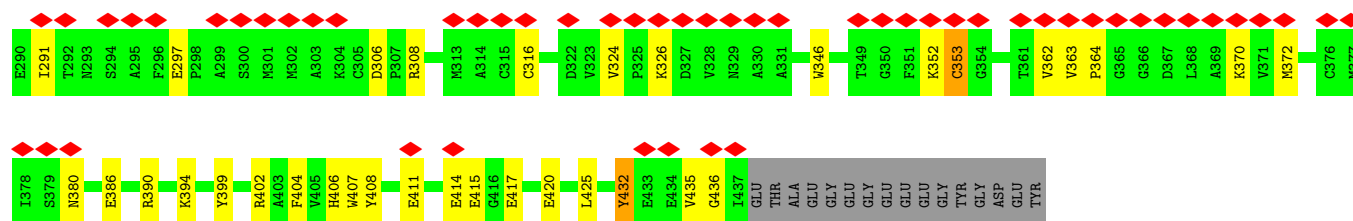
• Molecule 2: Tubulin alpha chain



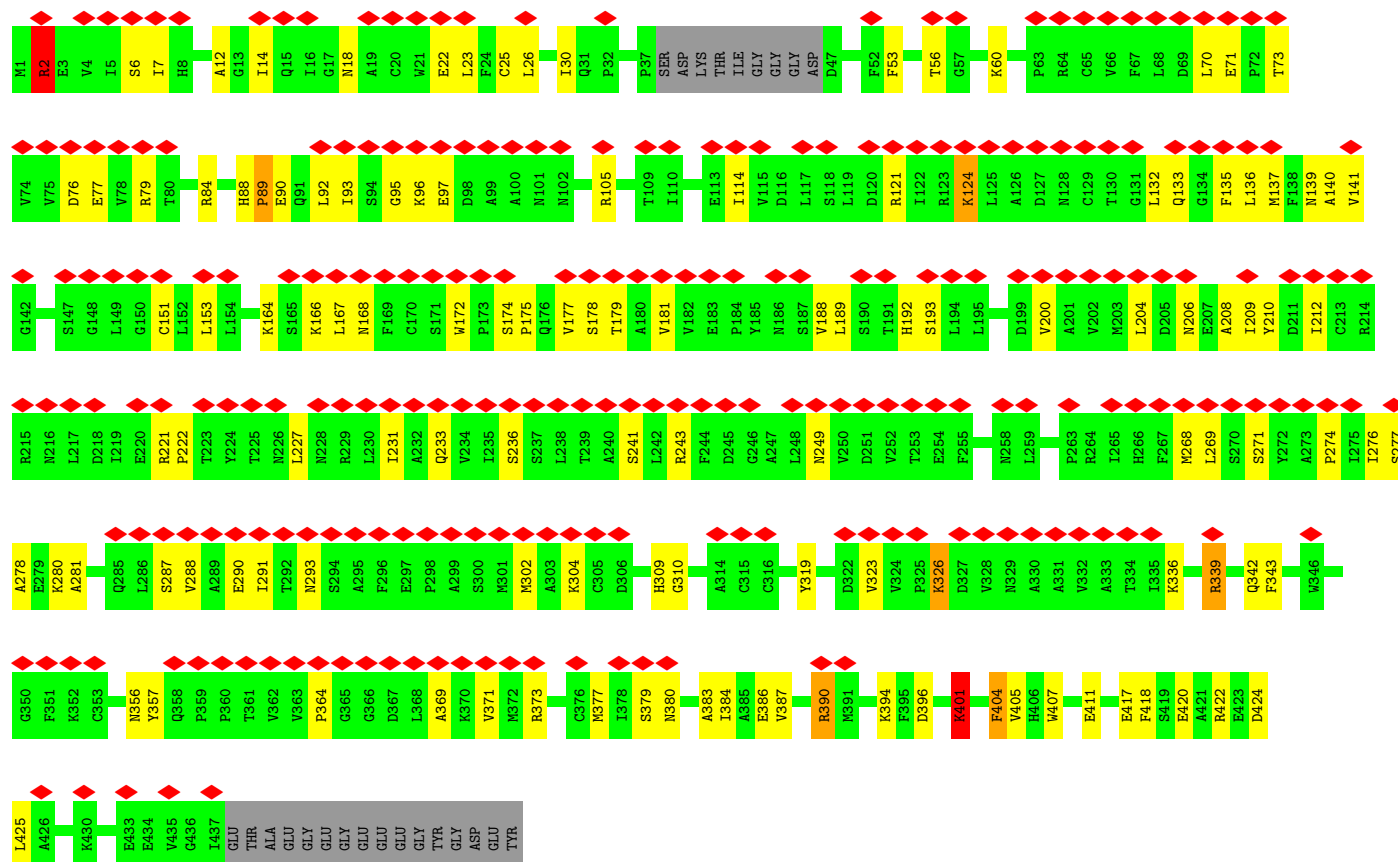


• Molecule 2: Tubulin alpha chain

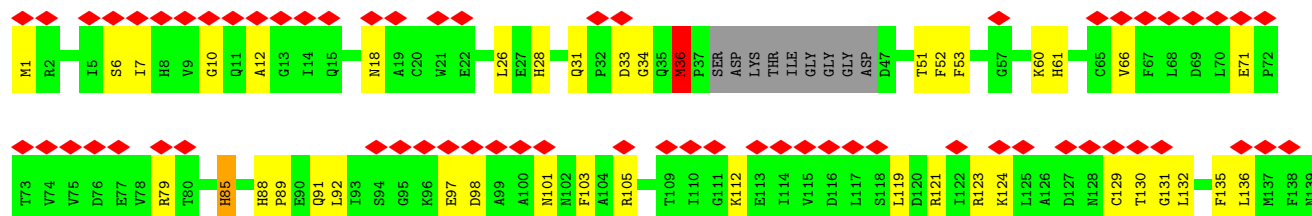


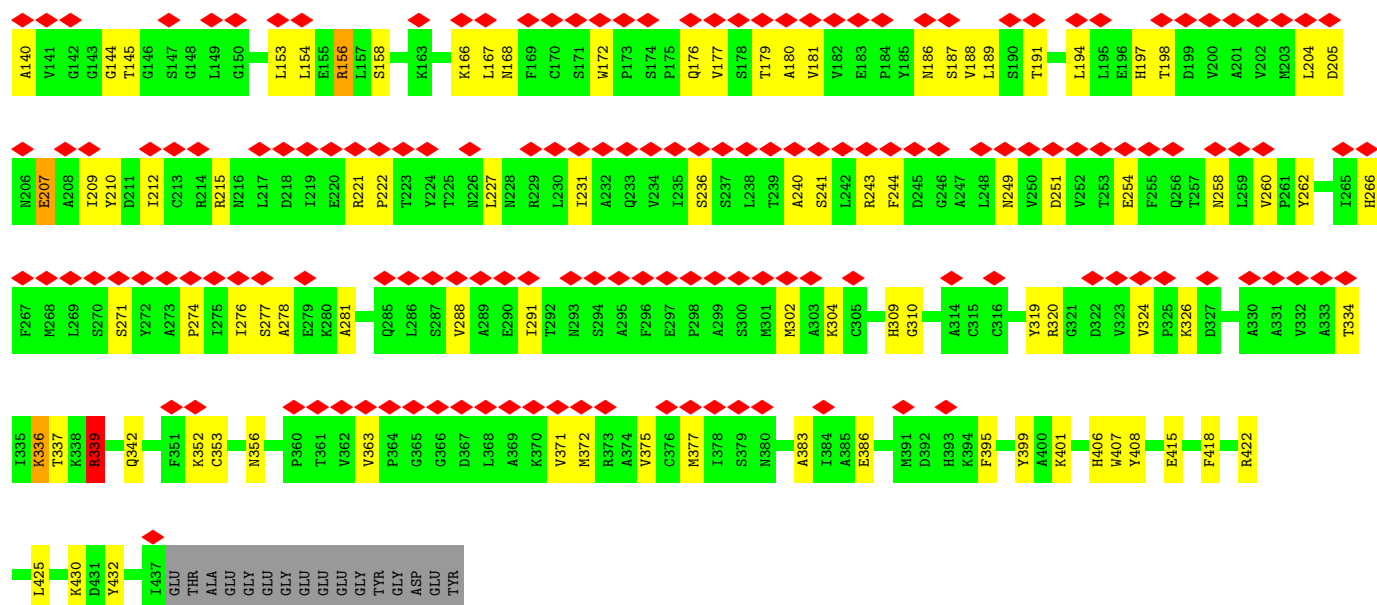


• Molecule 2: Tubulin alpha chain

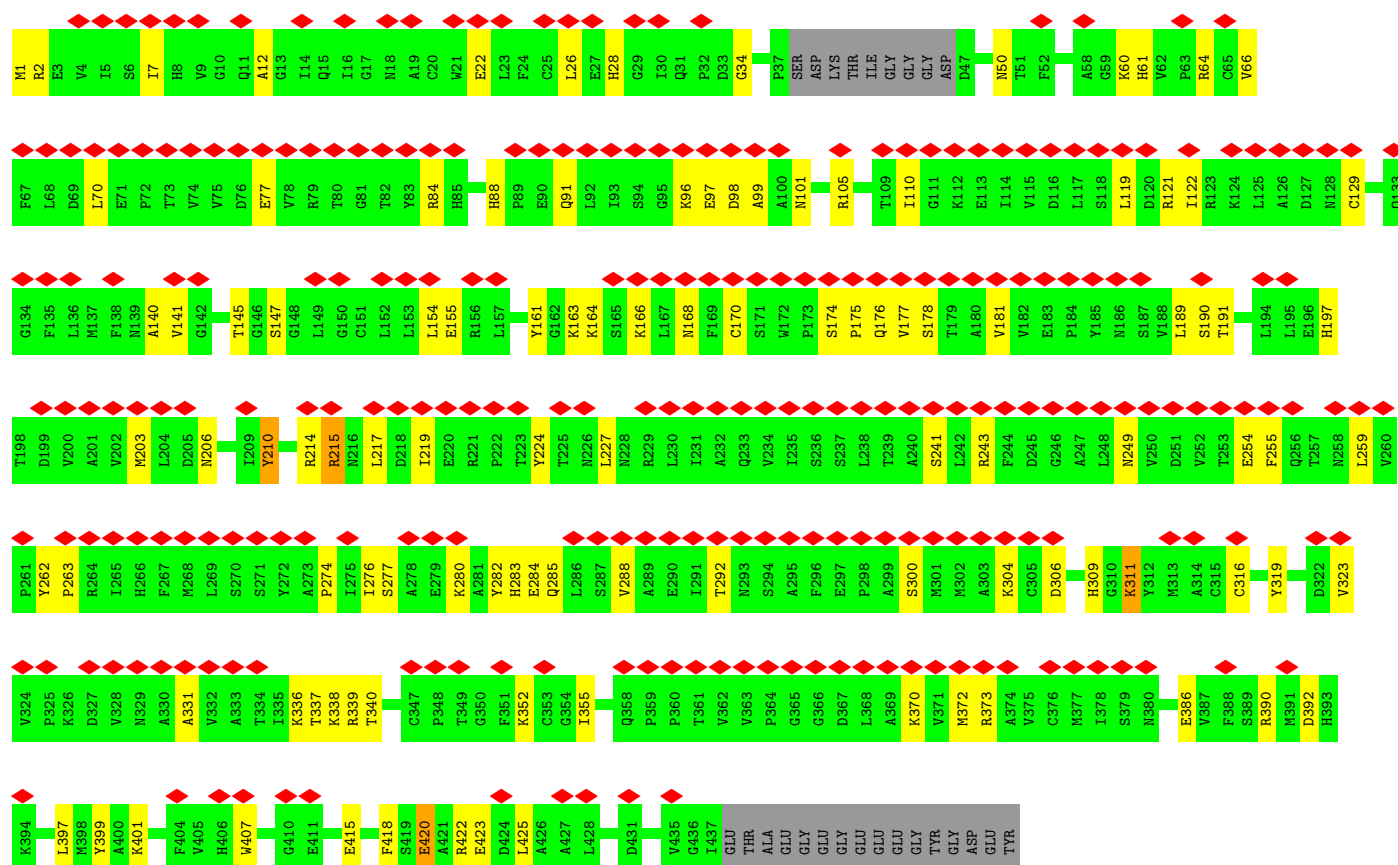
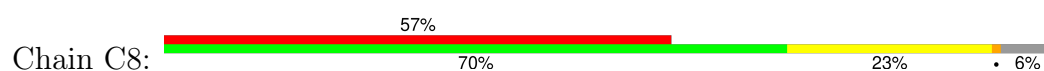


• Molecule 2: Tubulin alpha chain

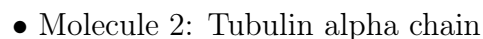




• Molecule 2: Tubulin alpha chain

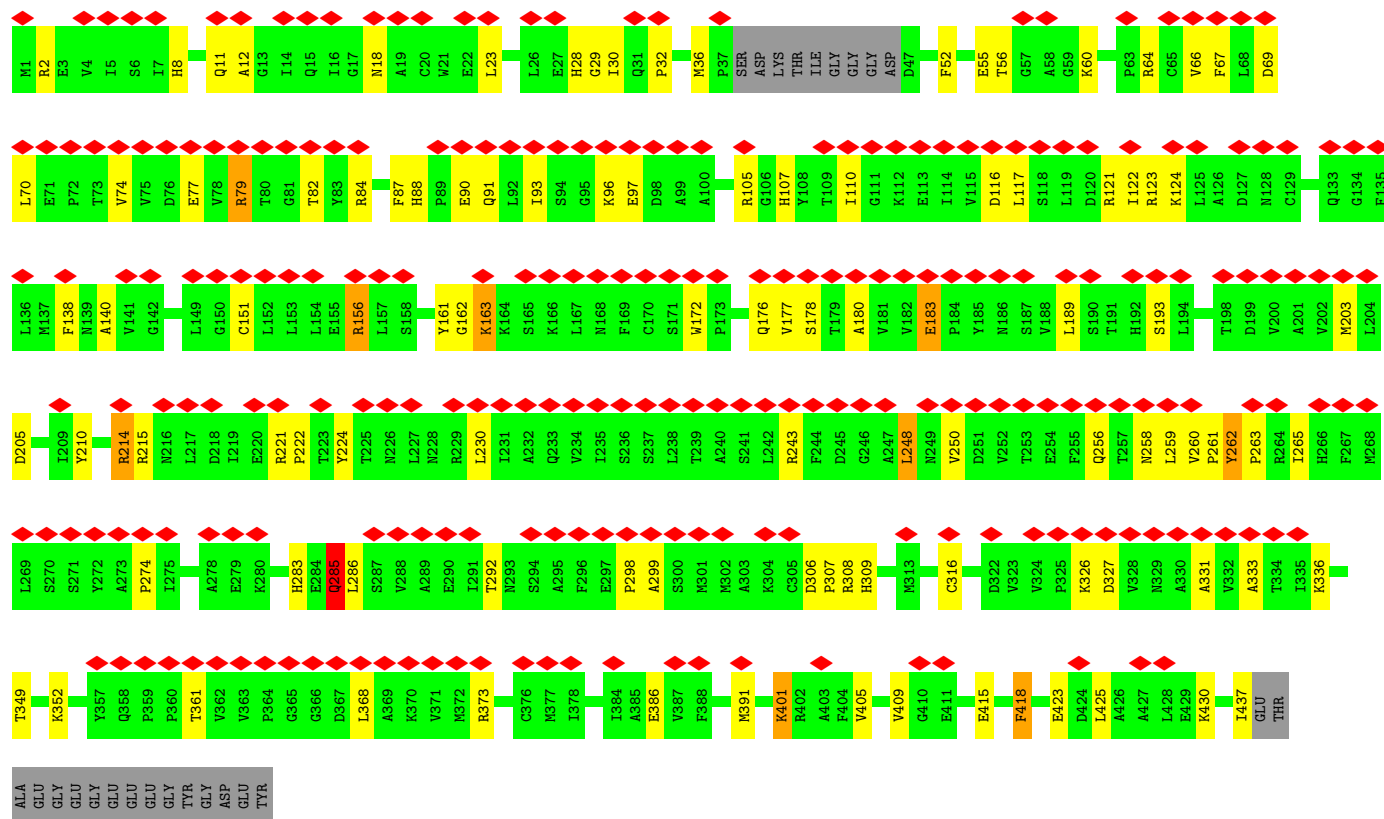
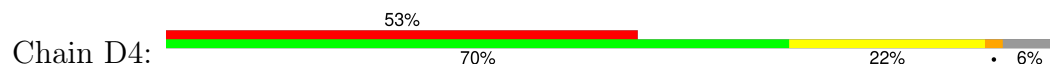


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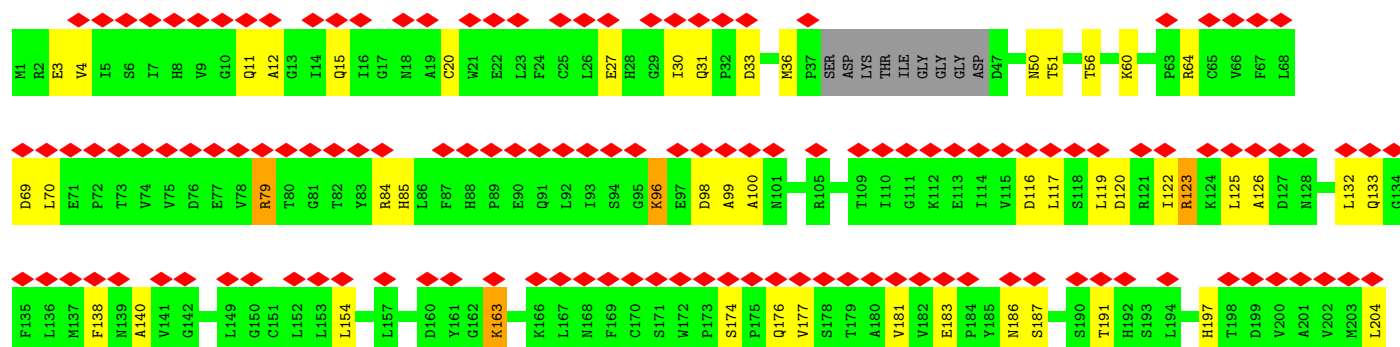
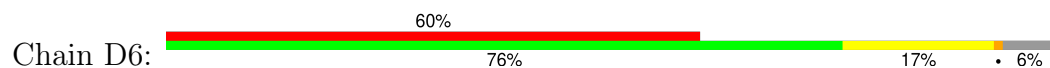


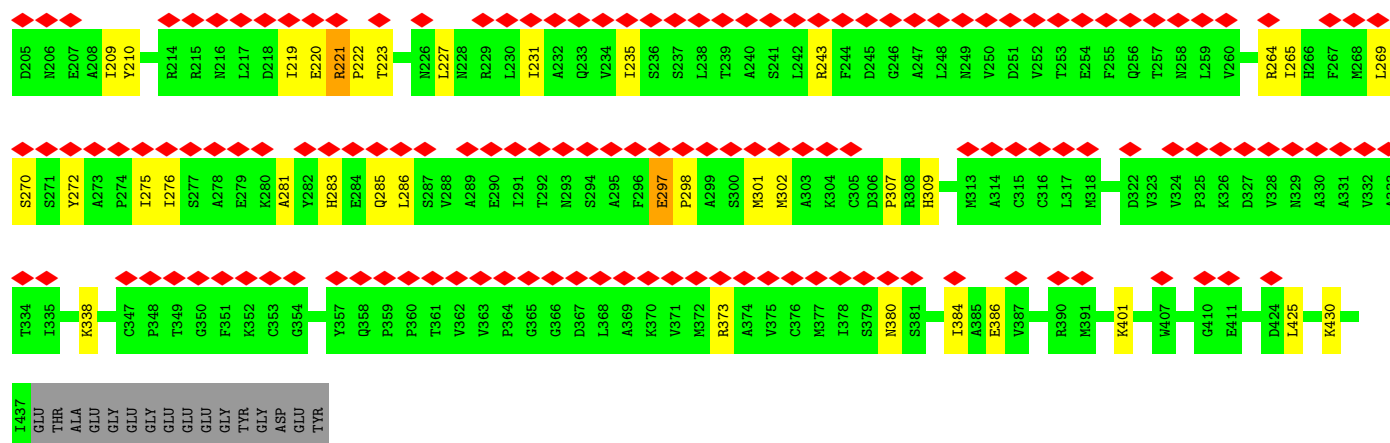


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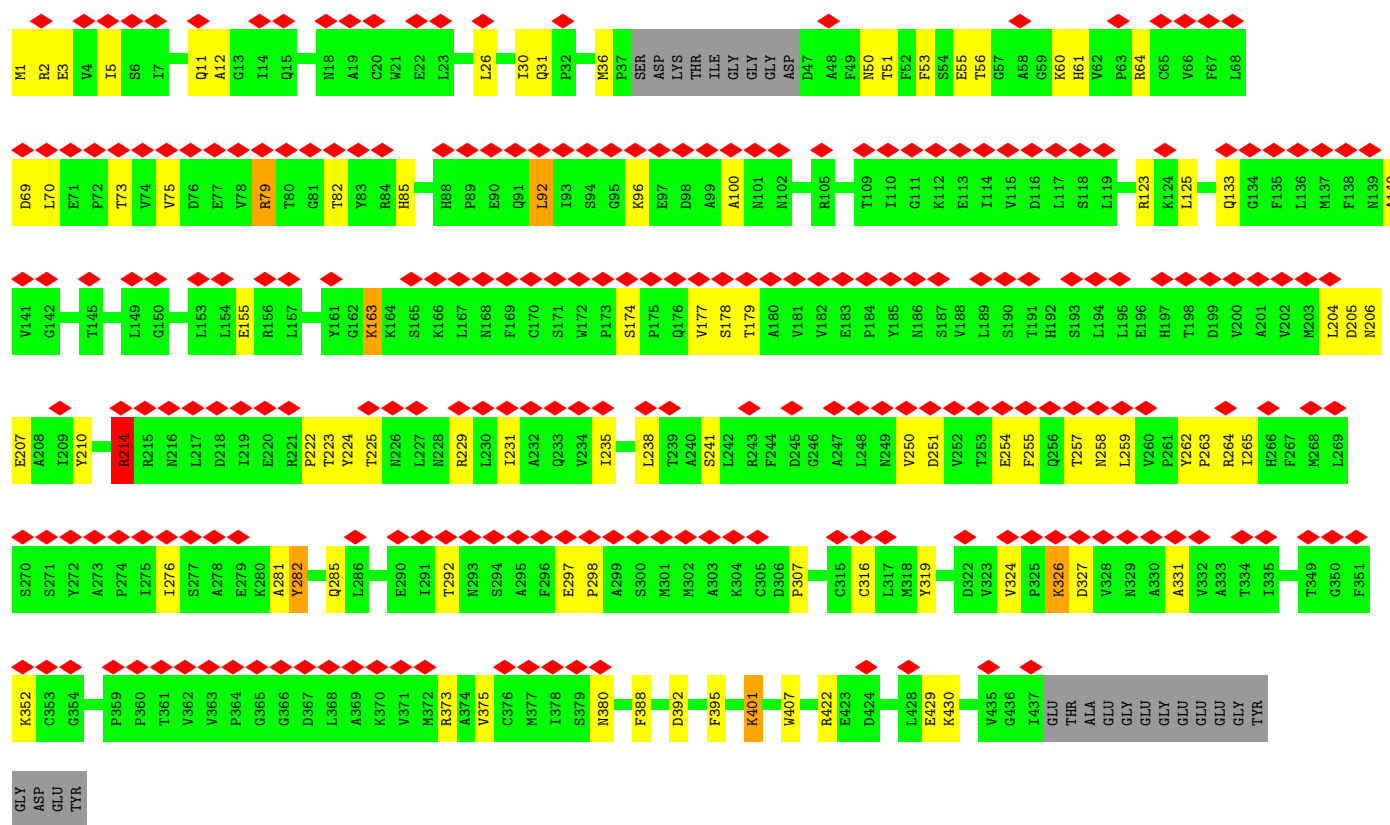
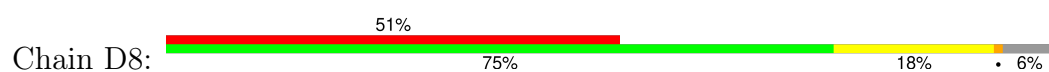


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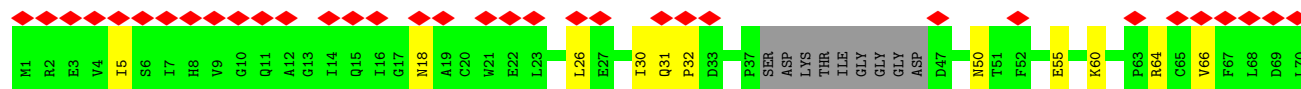
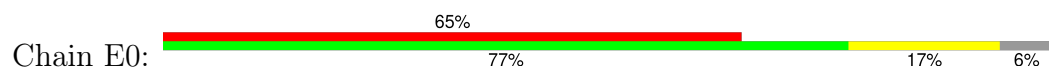


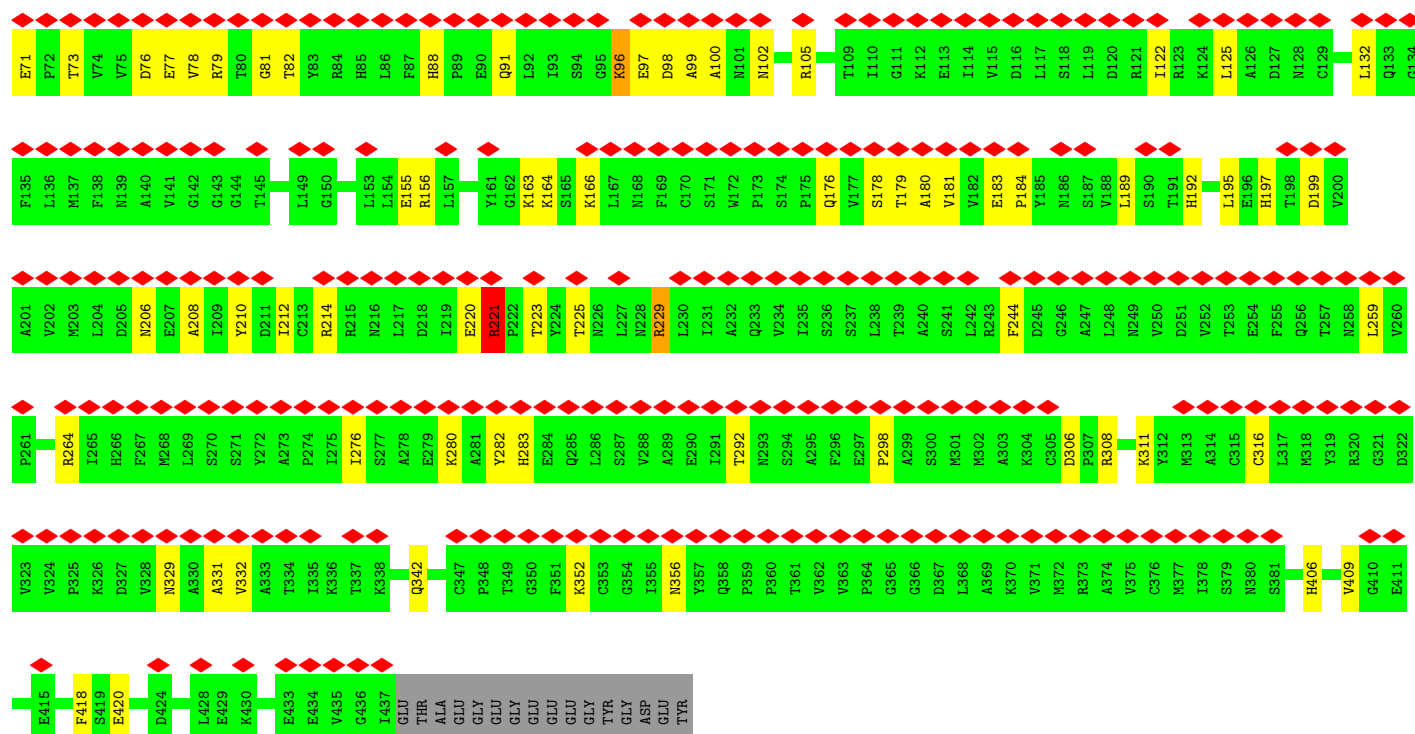


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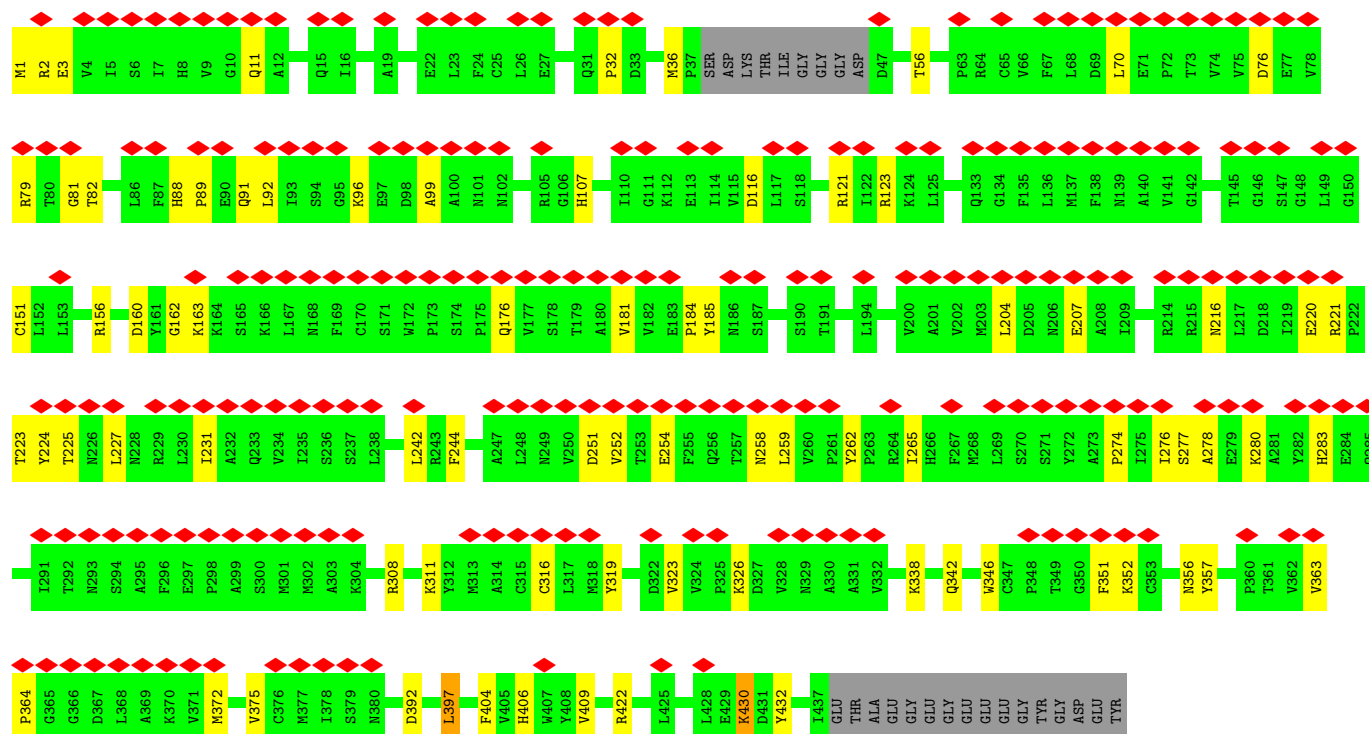
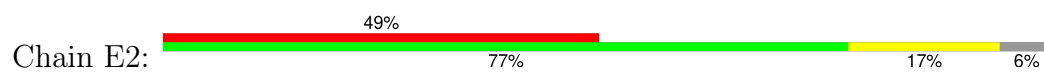


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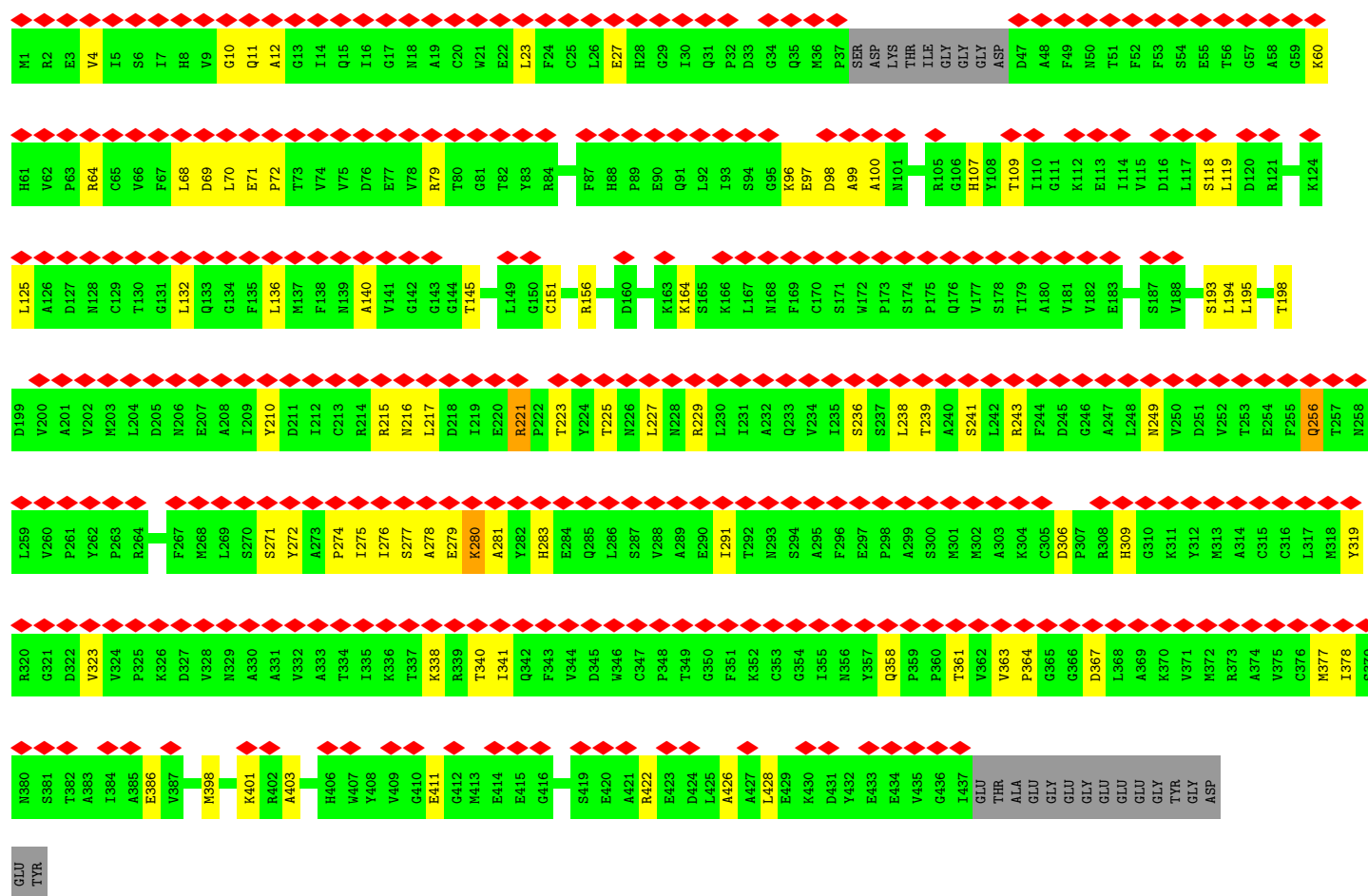


Molecule 2: Tubulin alpha chain




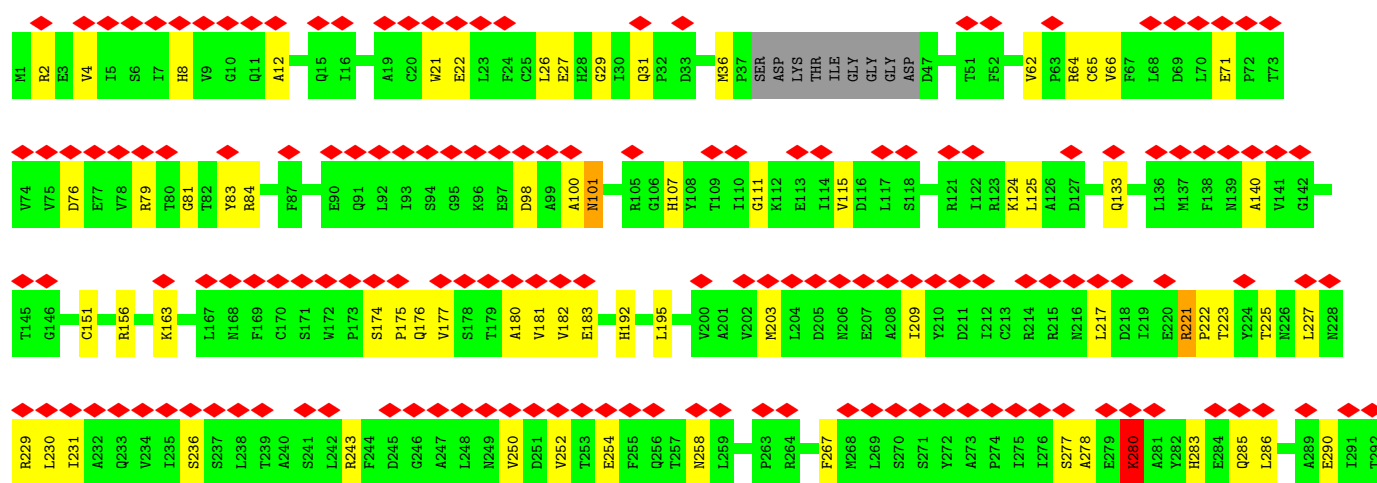
Molecule 2: Tubulin alpha chain

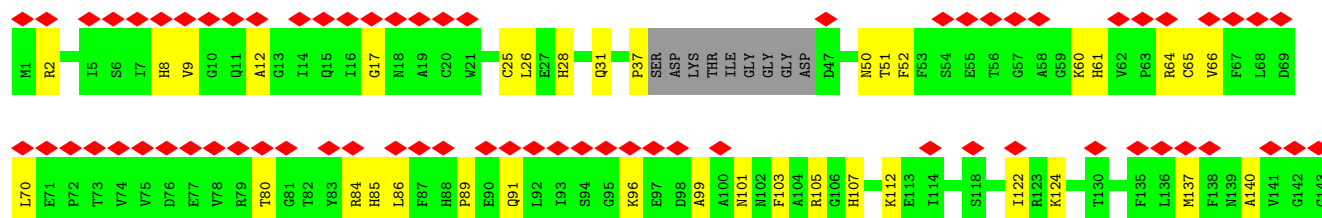
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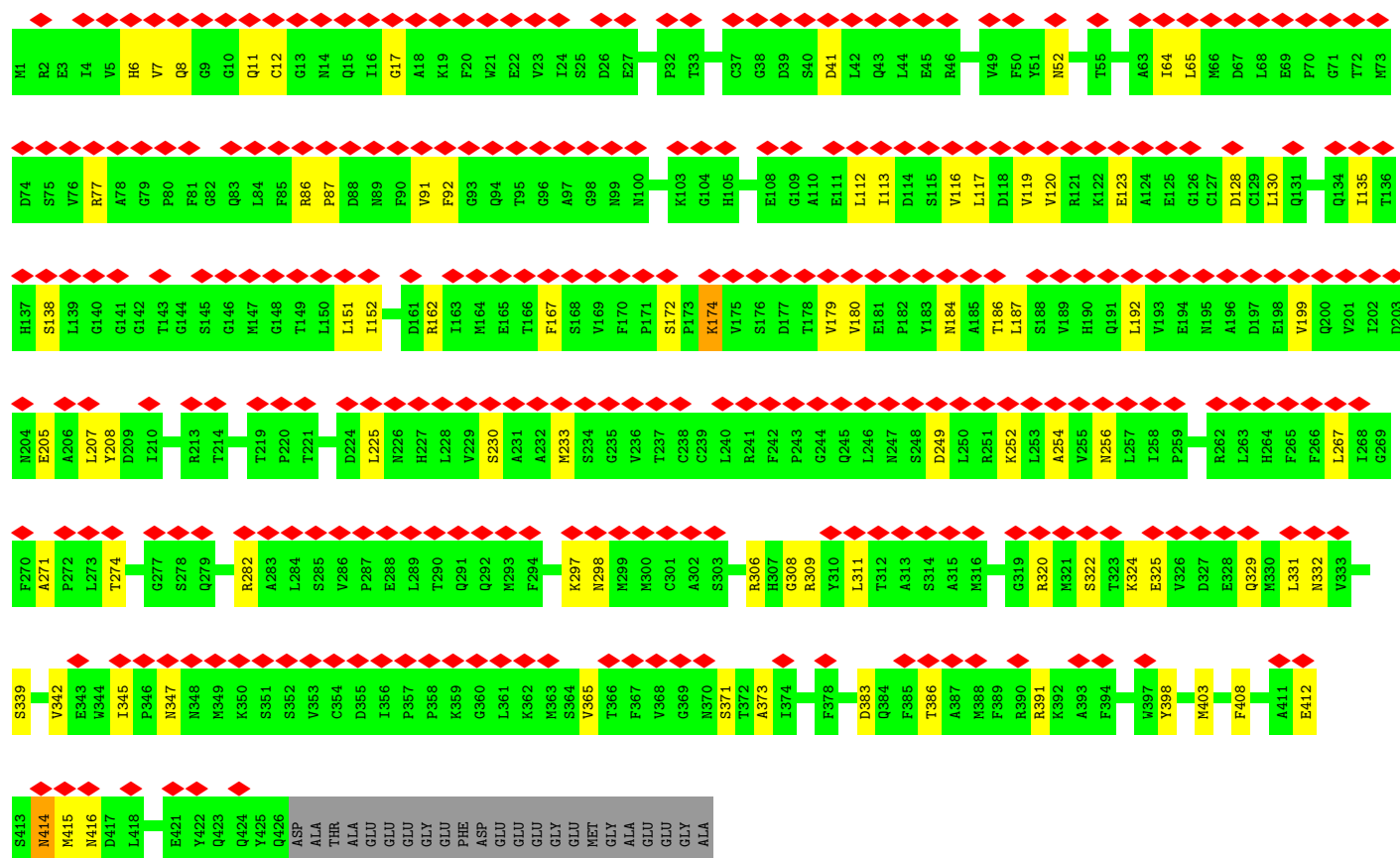
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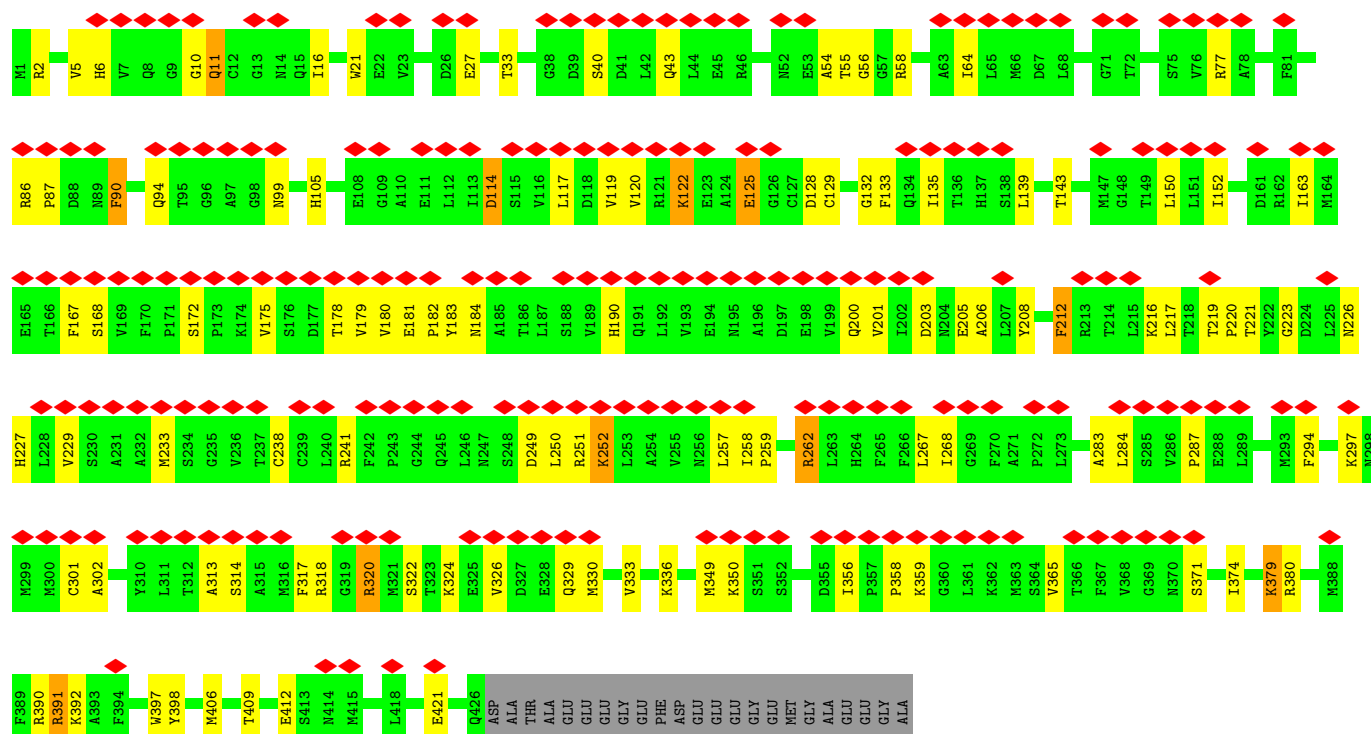






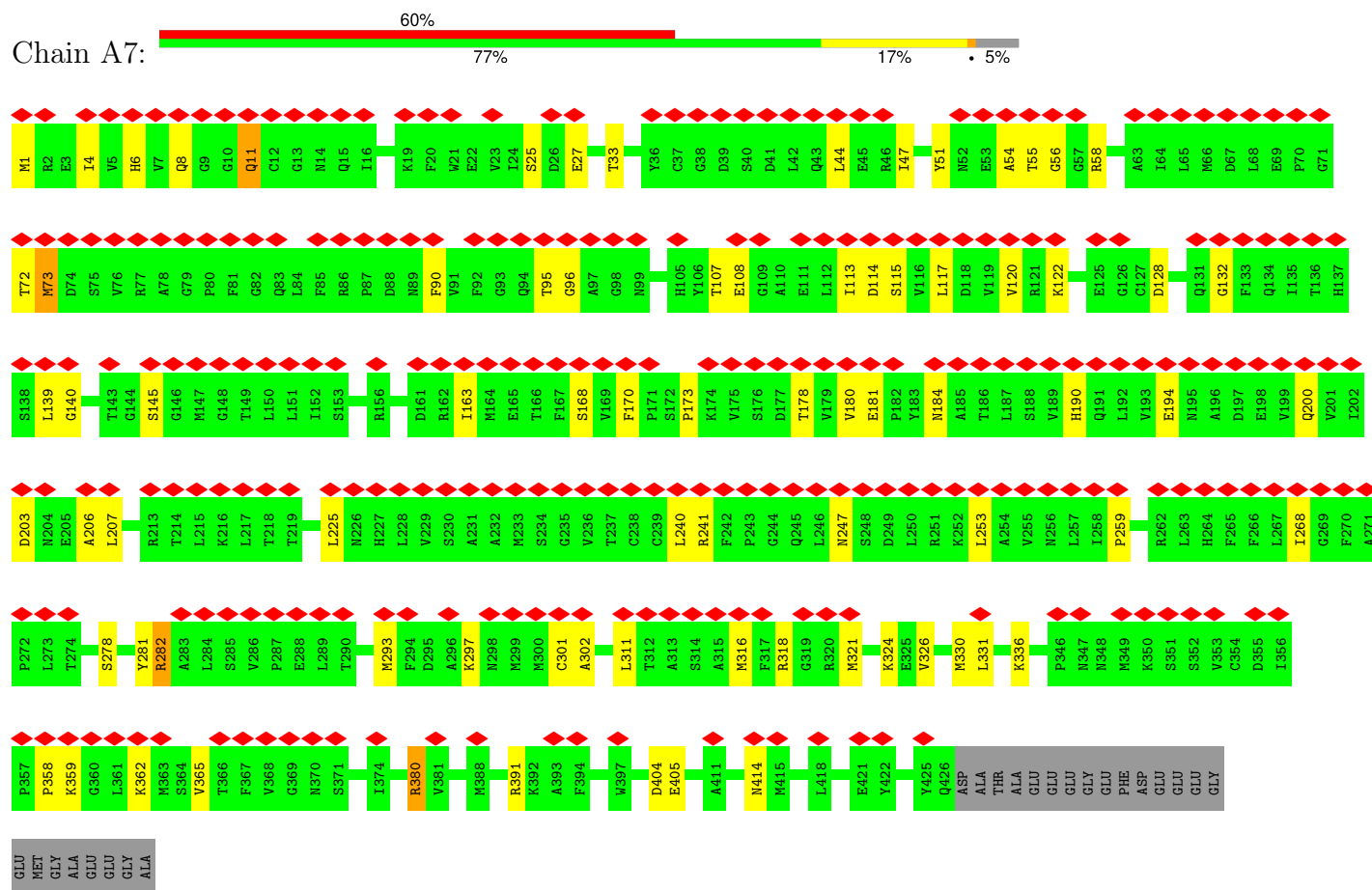


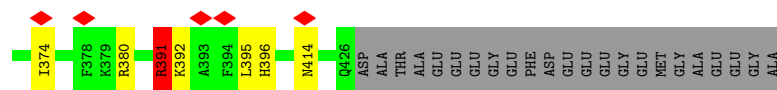
• Molecule 3: Tubulin beta chain



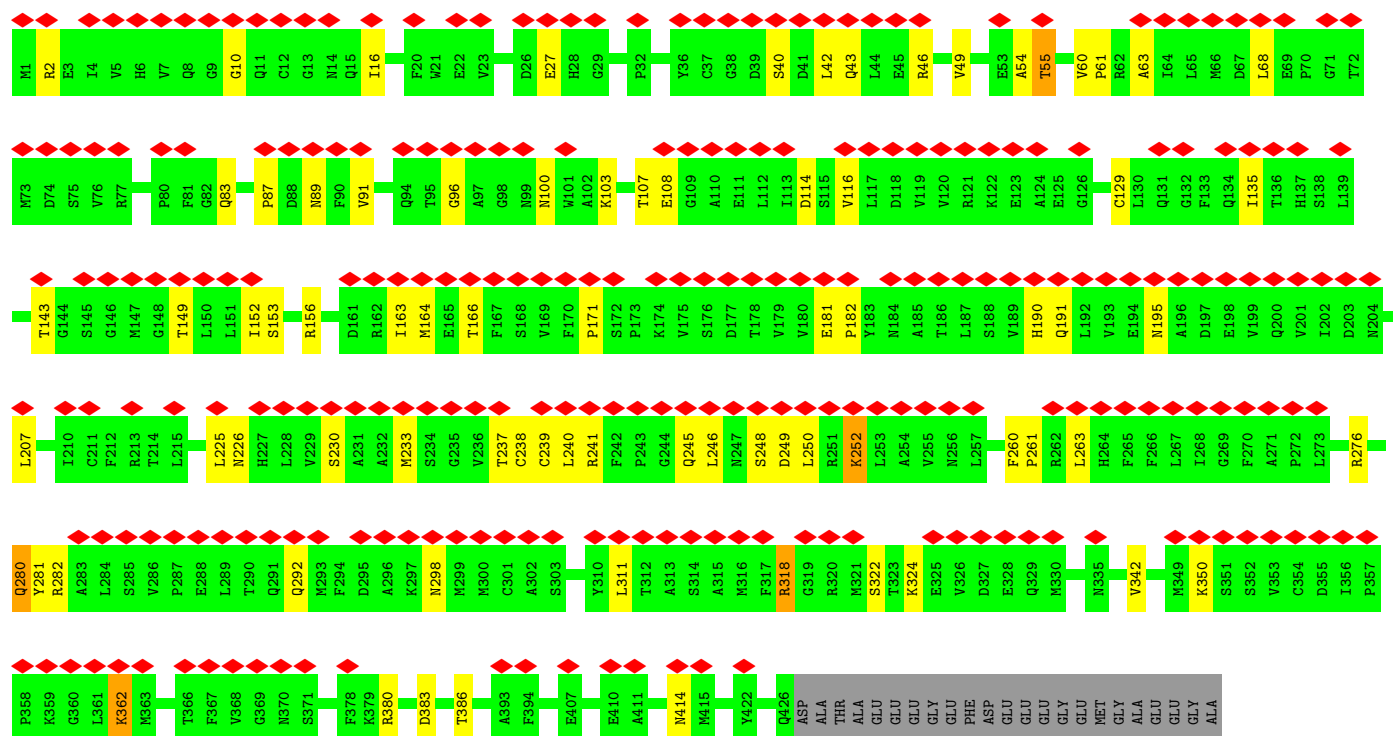
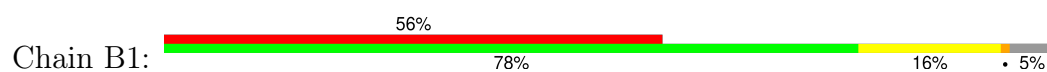
- Molecule 3: Tubulin beta chain

Chain A7:

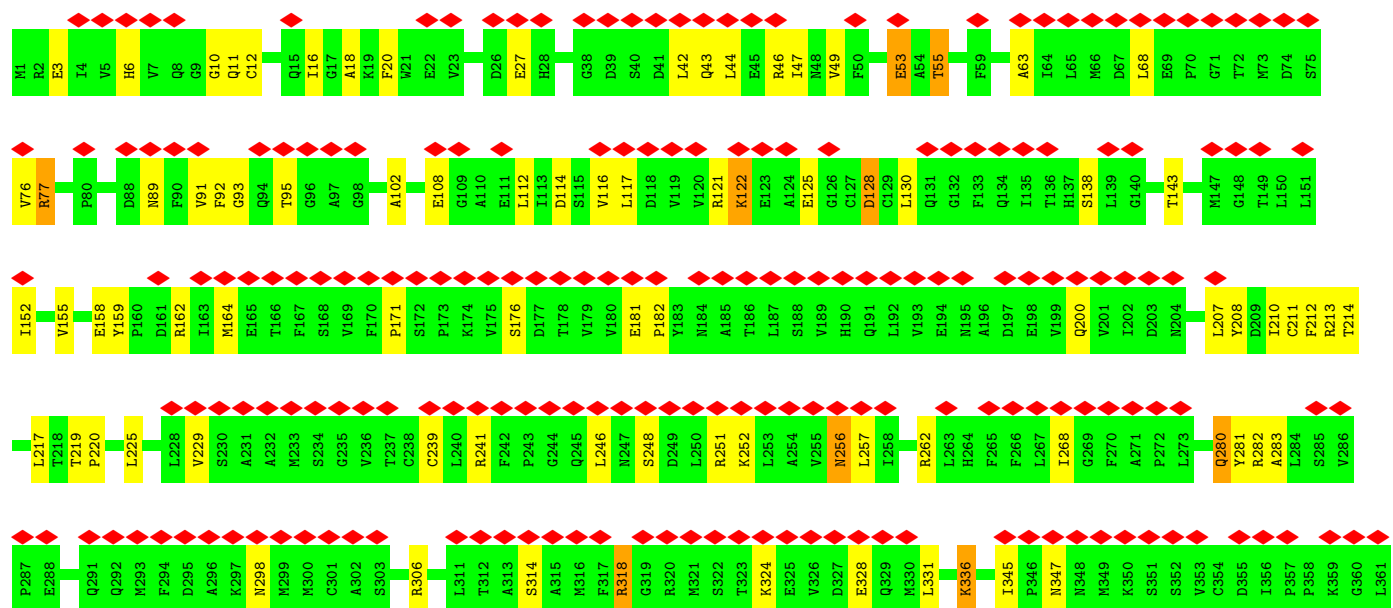
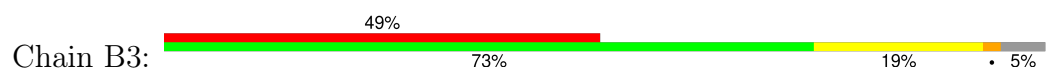


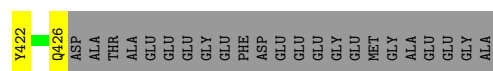


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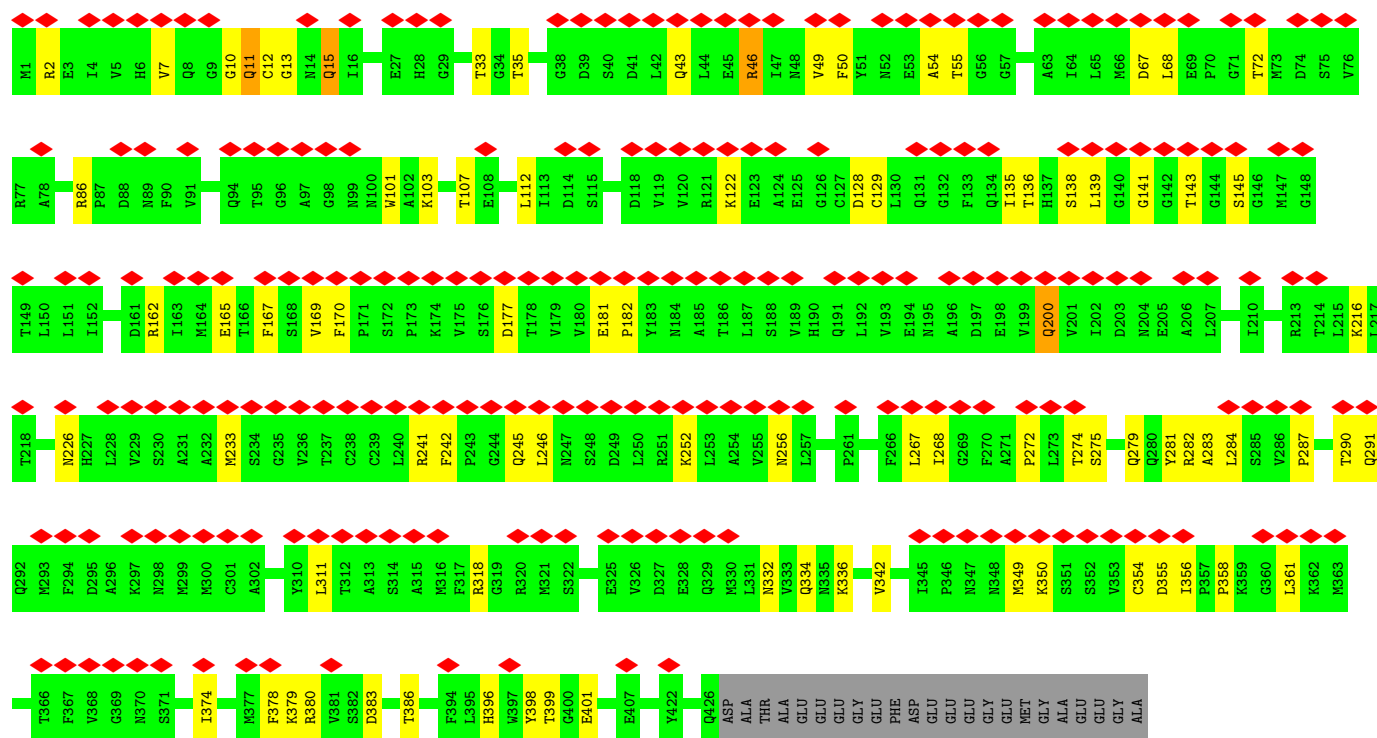
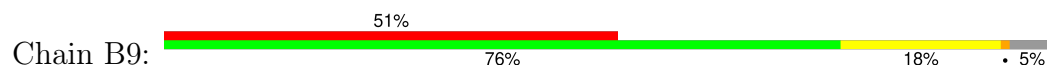


• Molecule 3: Tubulin beta chain

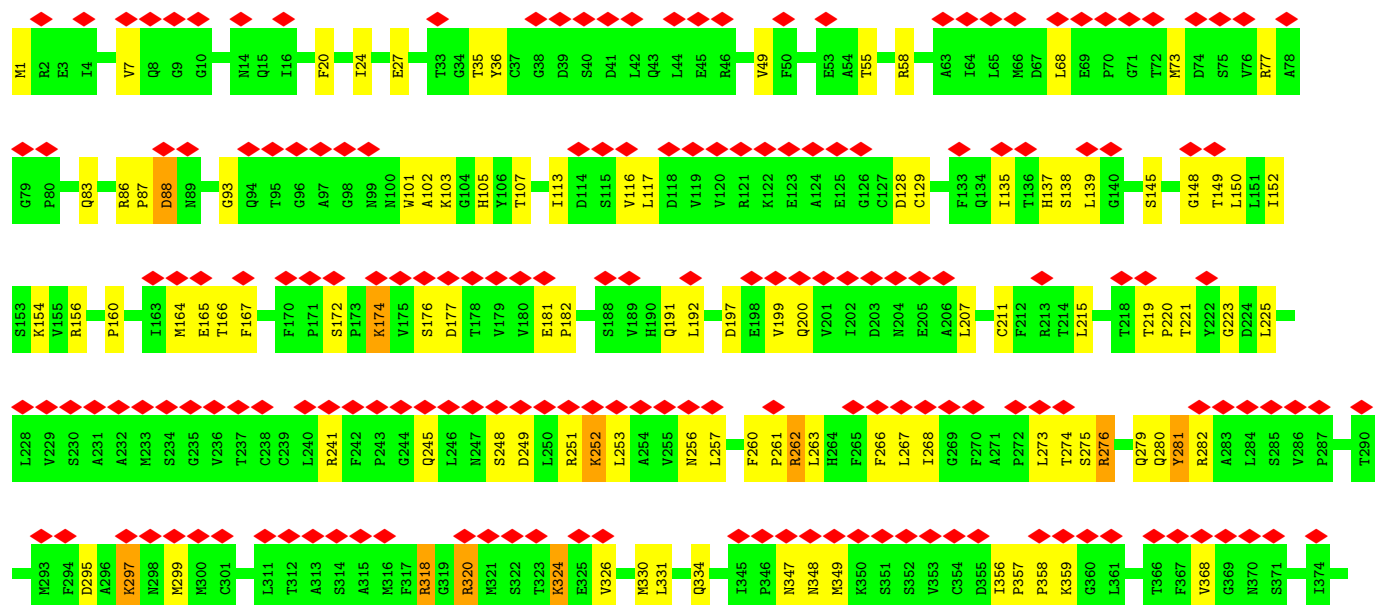
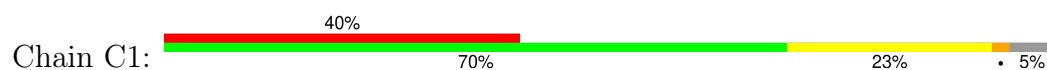


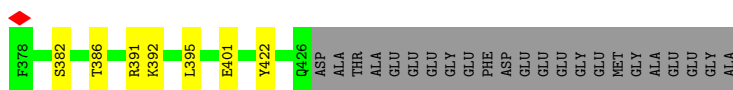


• Molecule 3: Tubulin beta chain

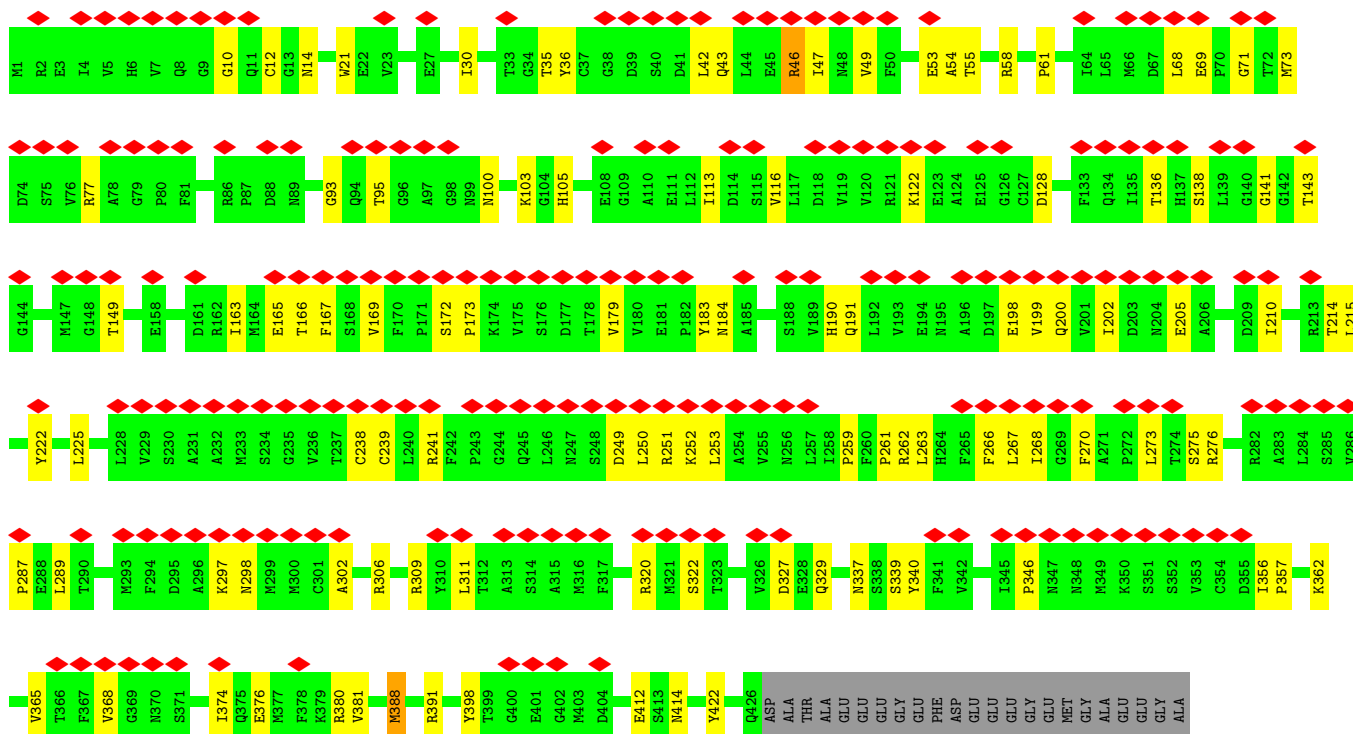
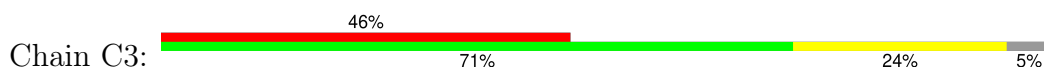


• Molecule 3: Tubulin beta chain

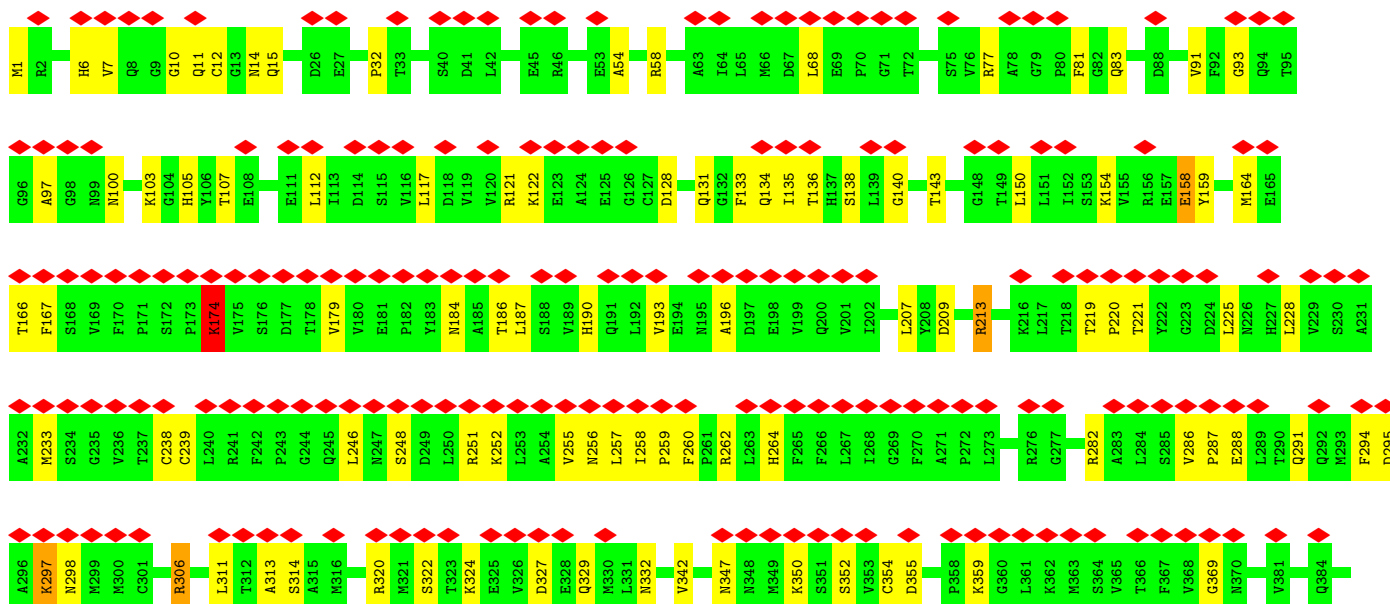
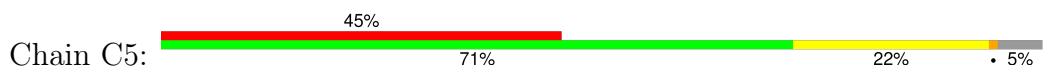


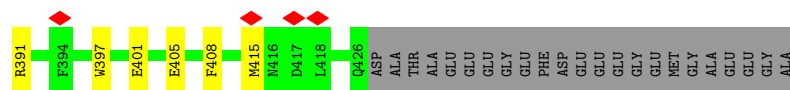


• Molecule 3: Tubulin beta chain

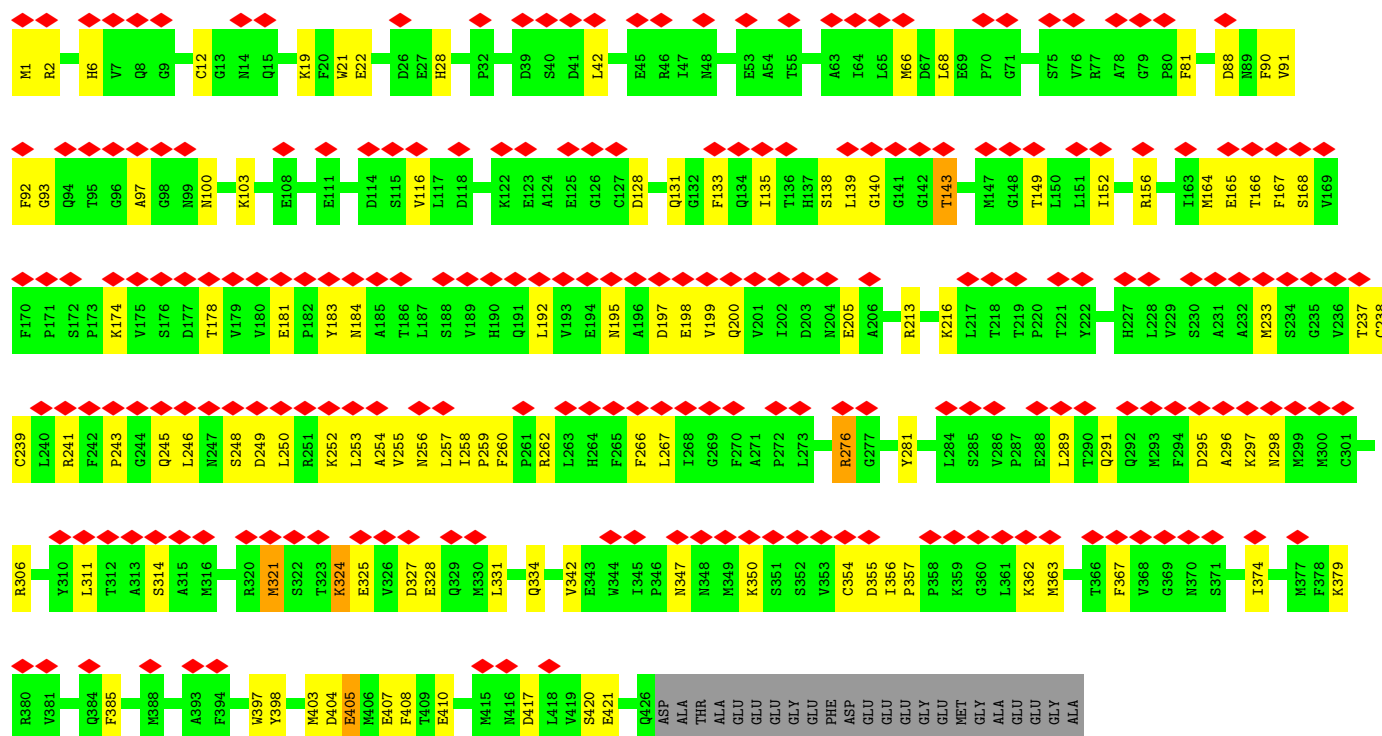


• Molecule 3: Tubulin beta chain

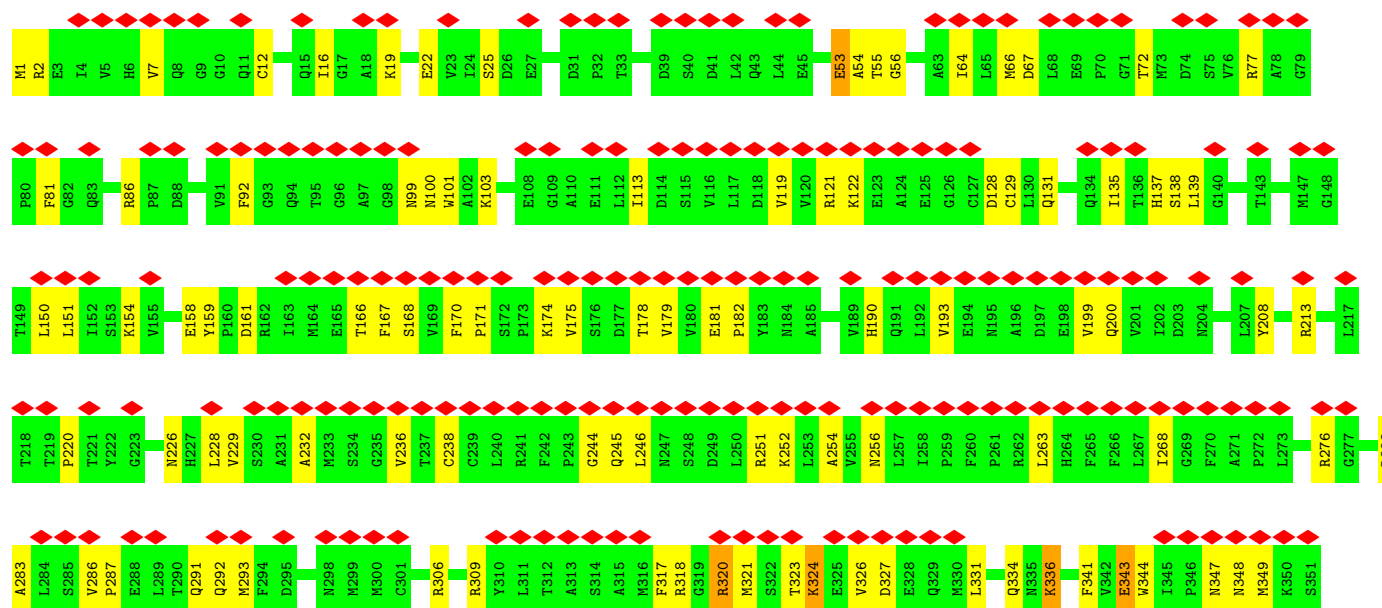


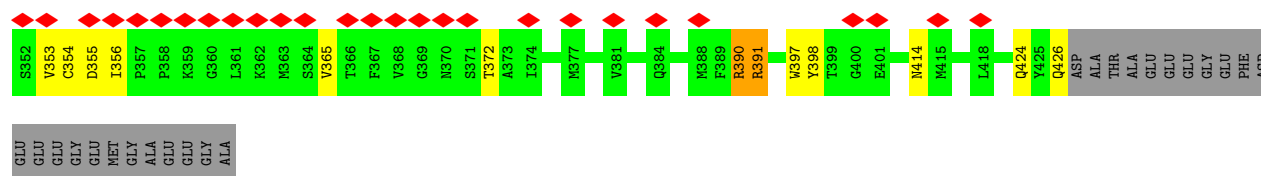


• Molecule 3: Tubulin beta chain



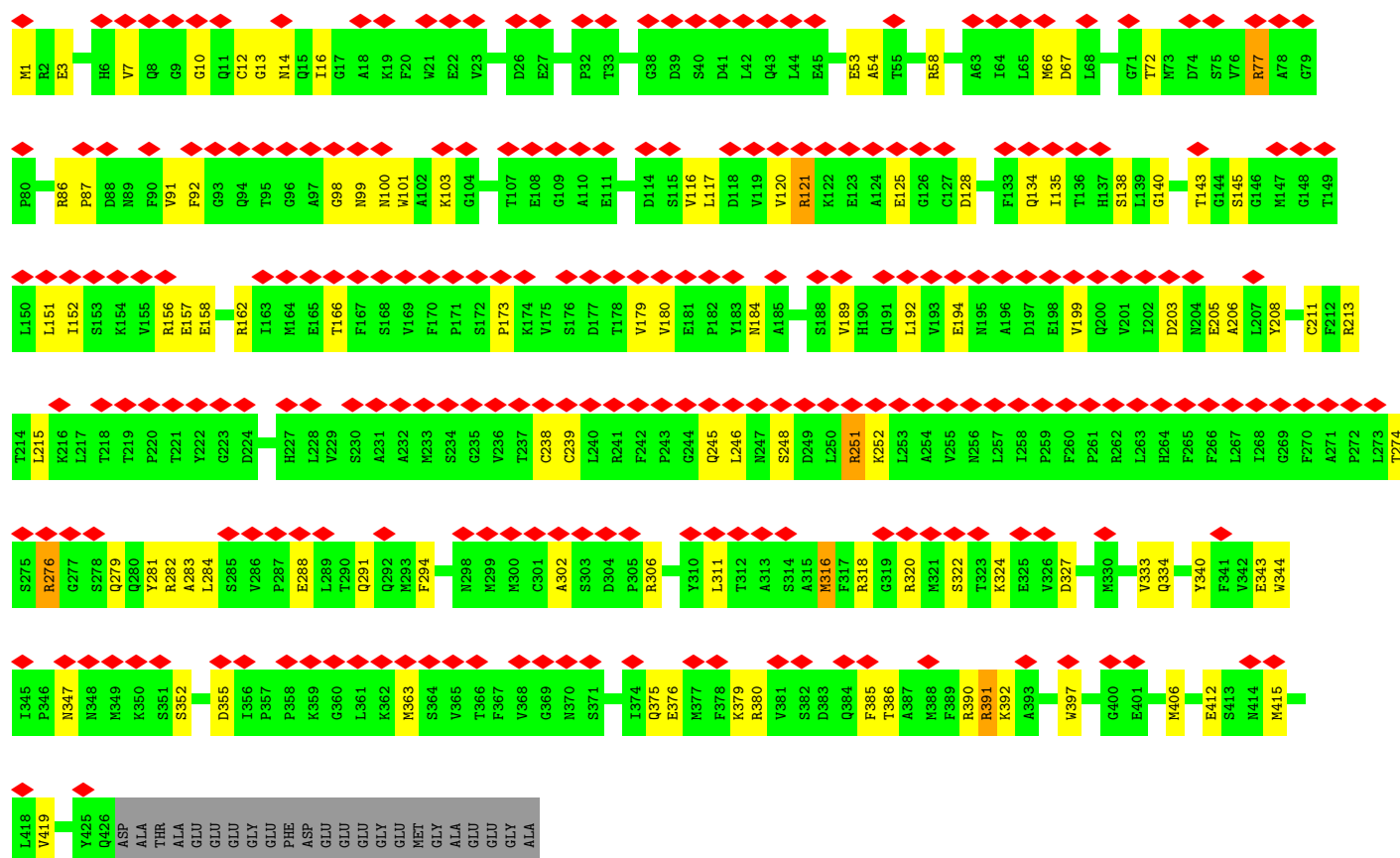
• Molecule 3: Tubulin beta chain





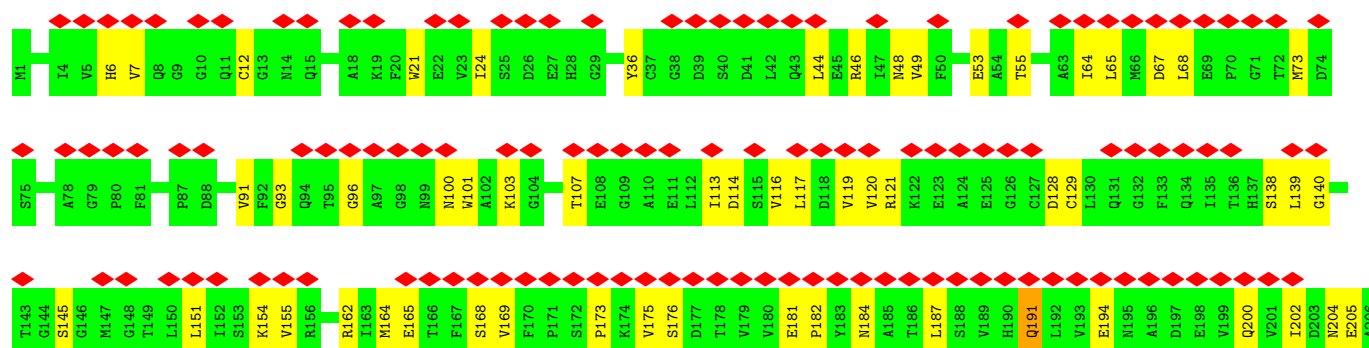
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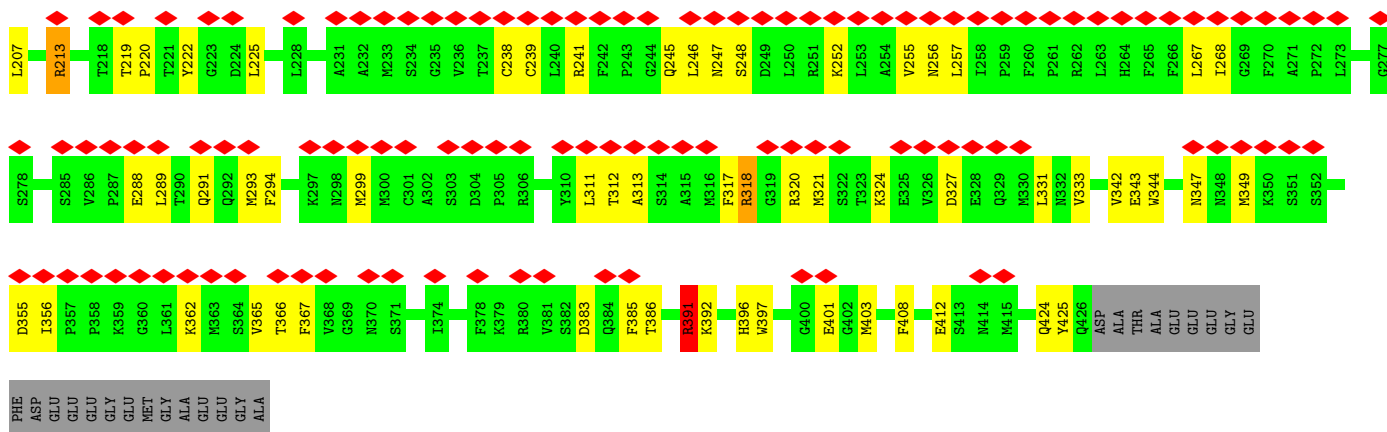
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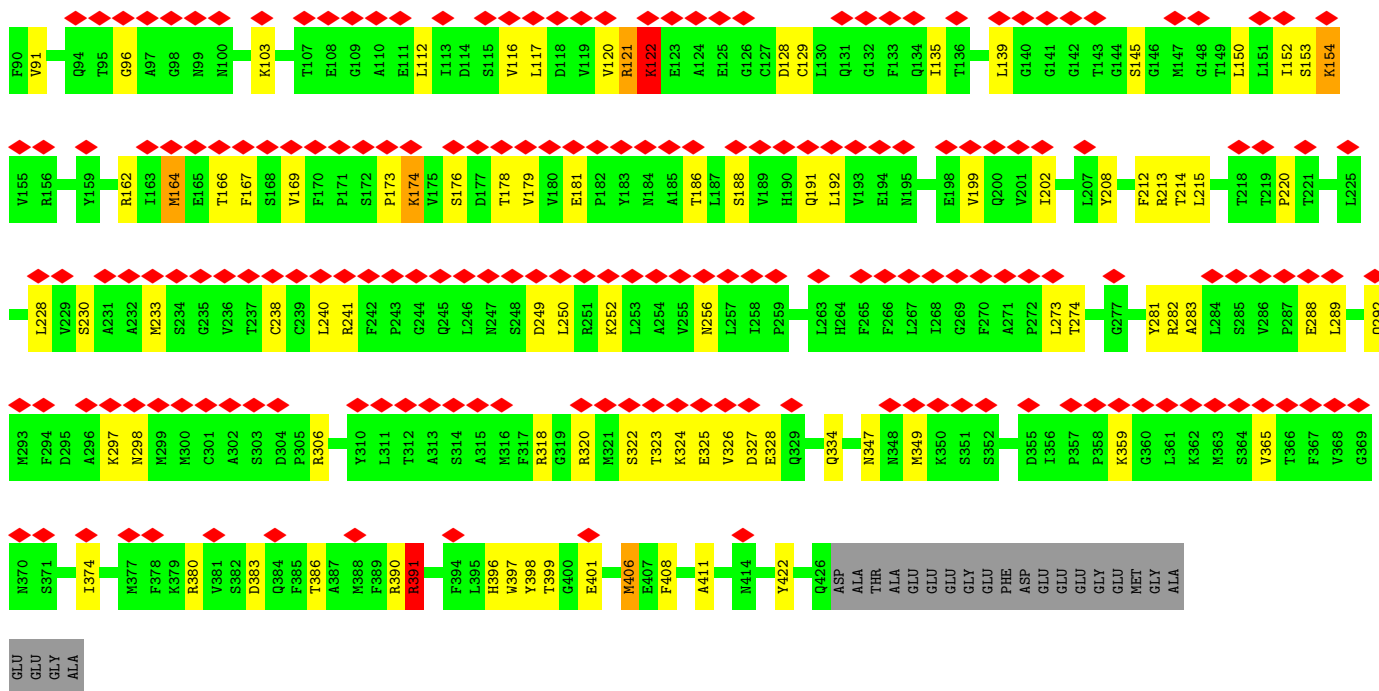


• Molecule 3: Tubulin beta chain

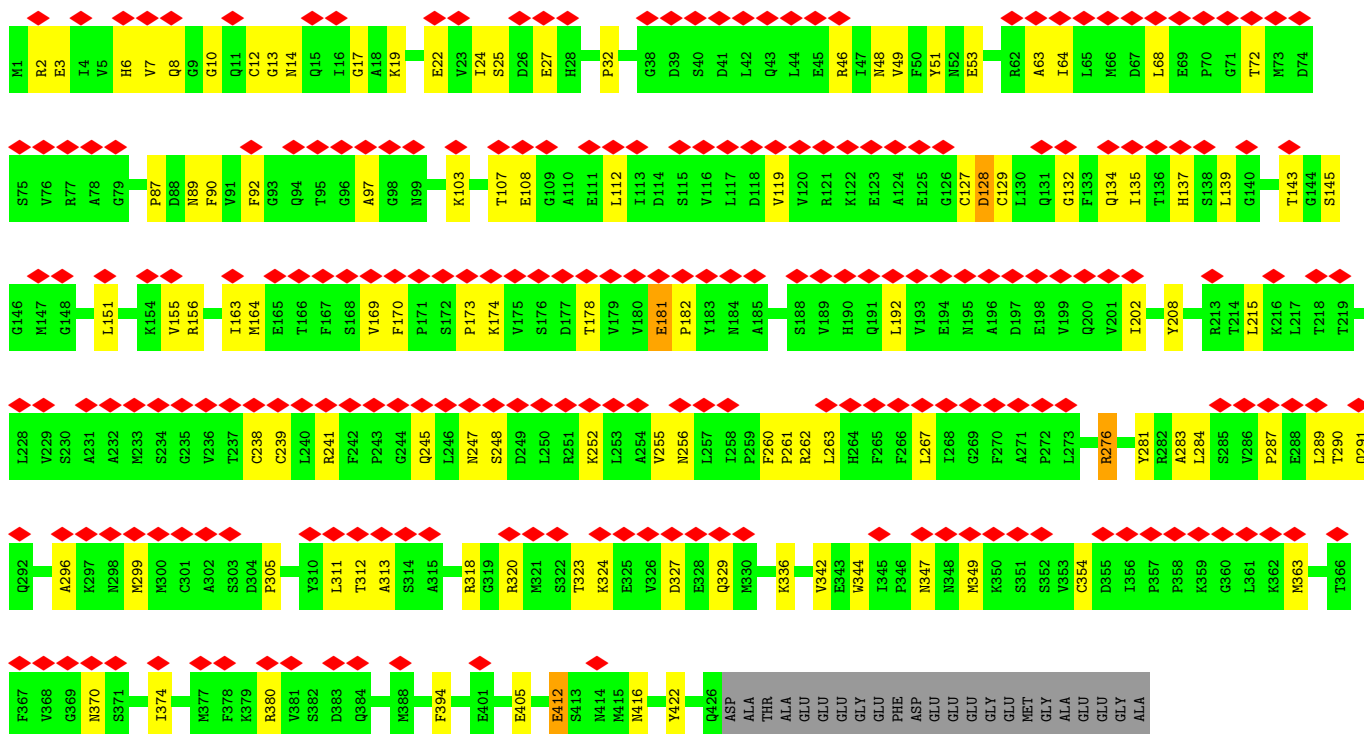
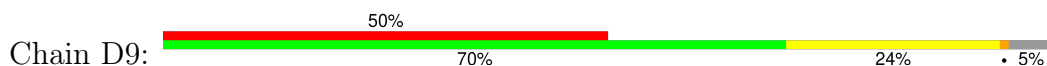
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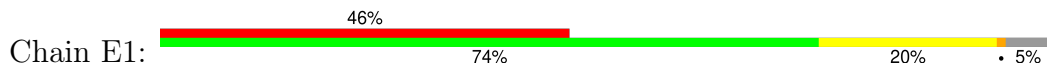


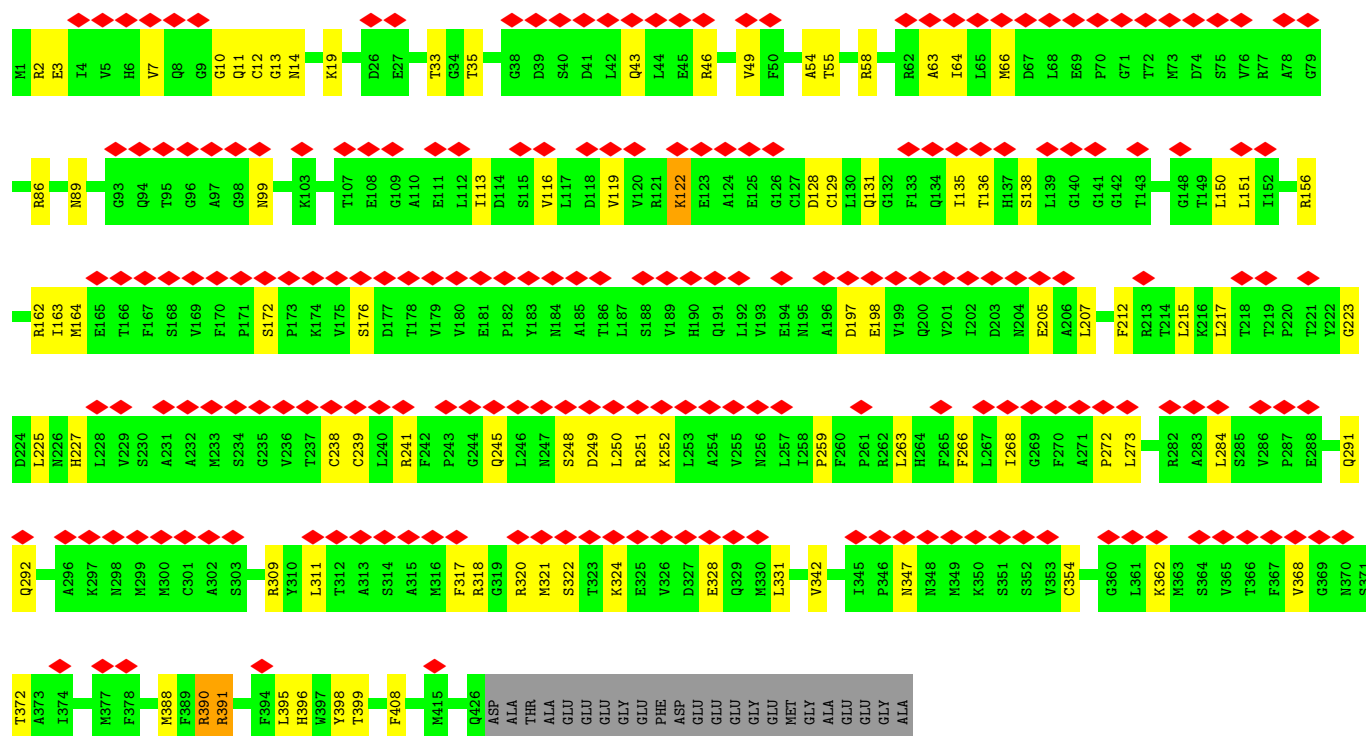


- Molecule 3: Tubulin beta chain

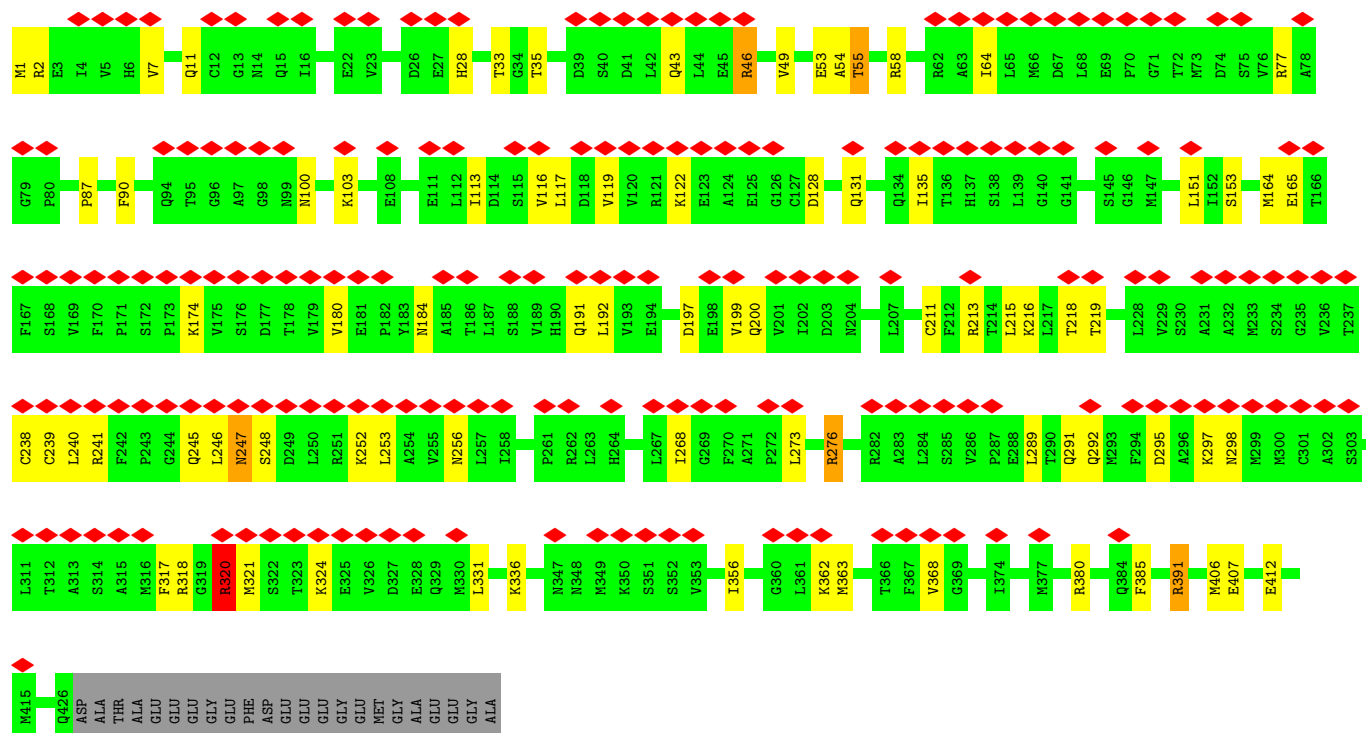
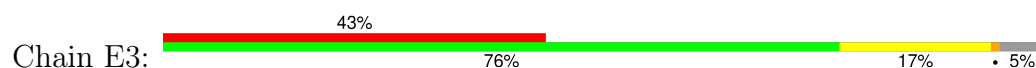


- Molecule 3: Tubulin beta chain

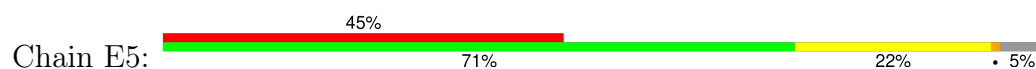




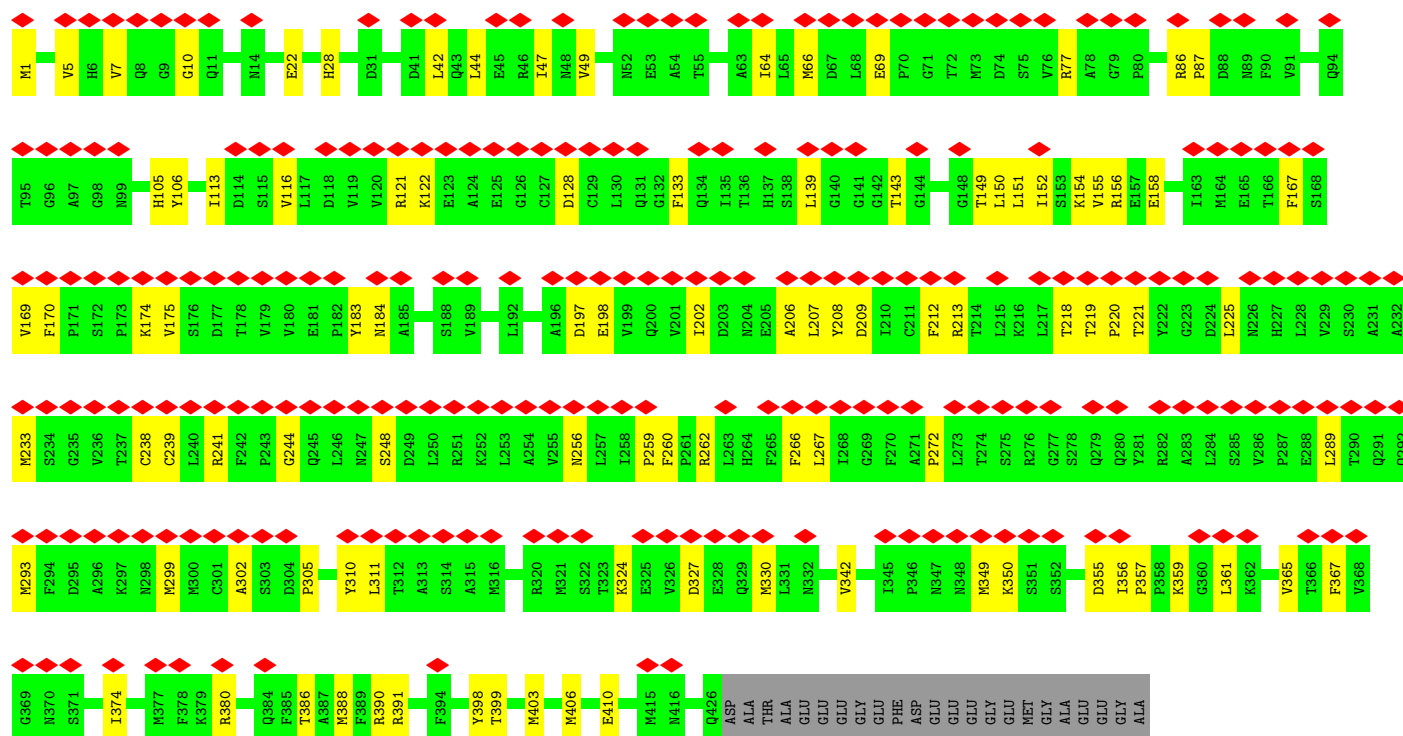
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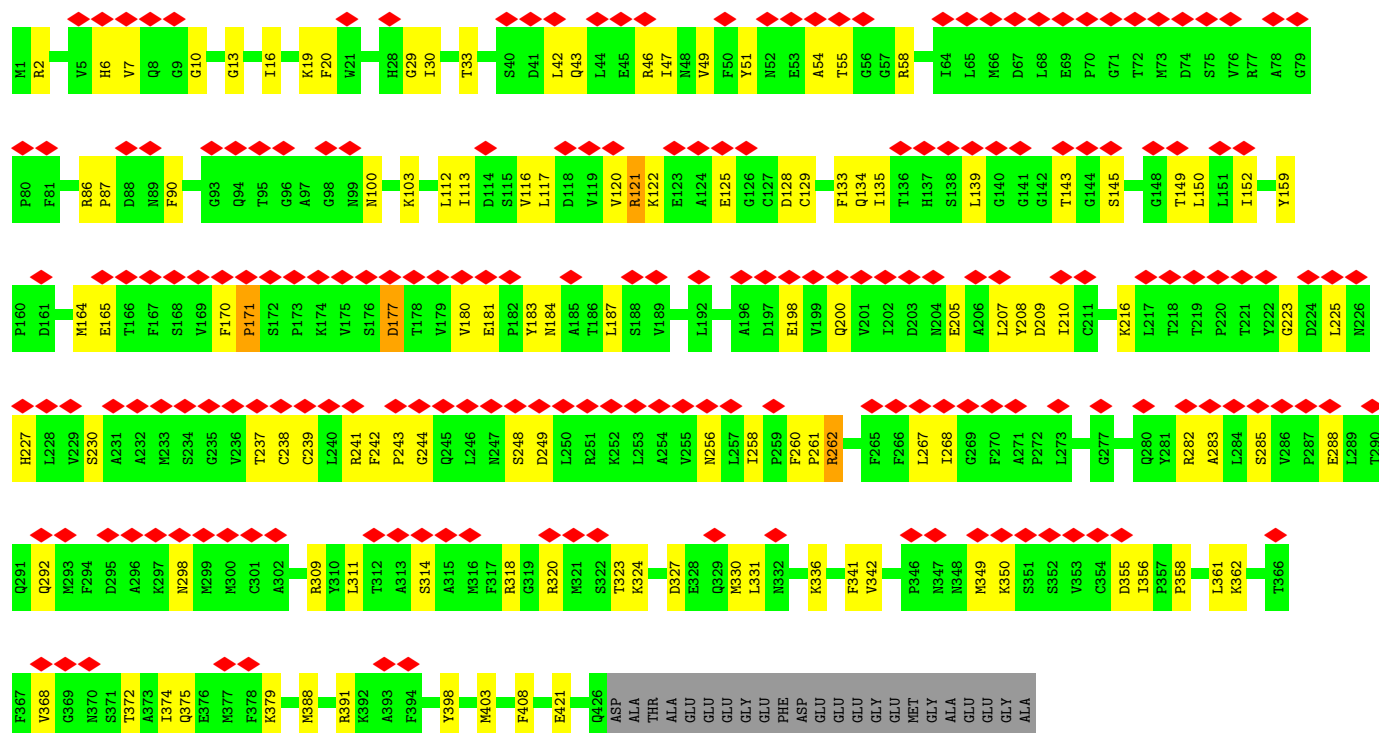
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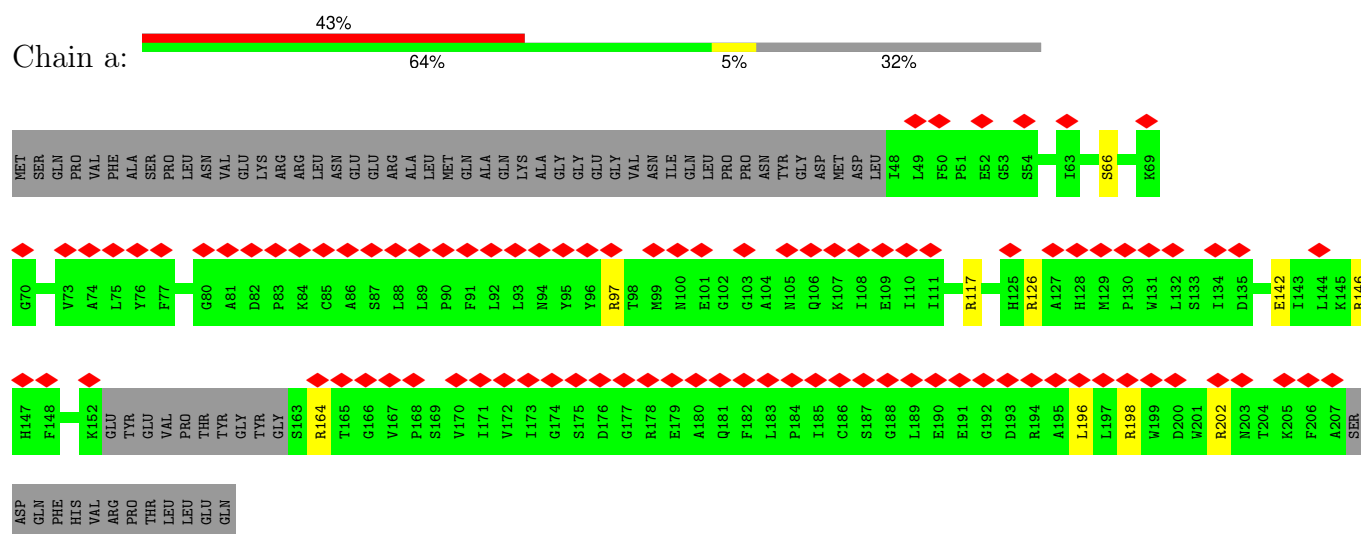




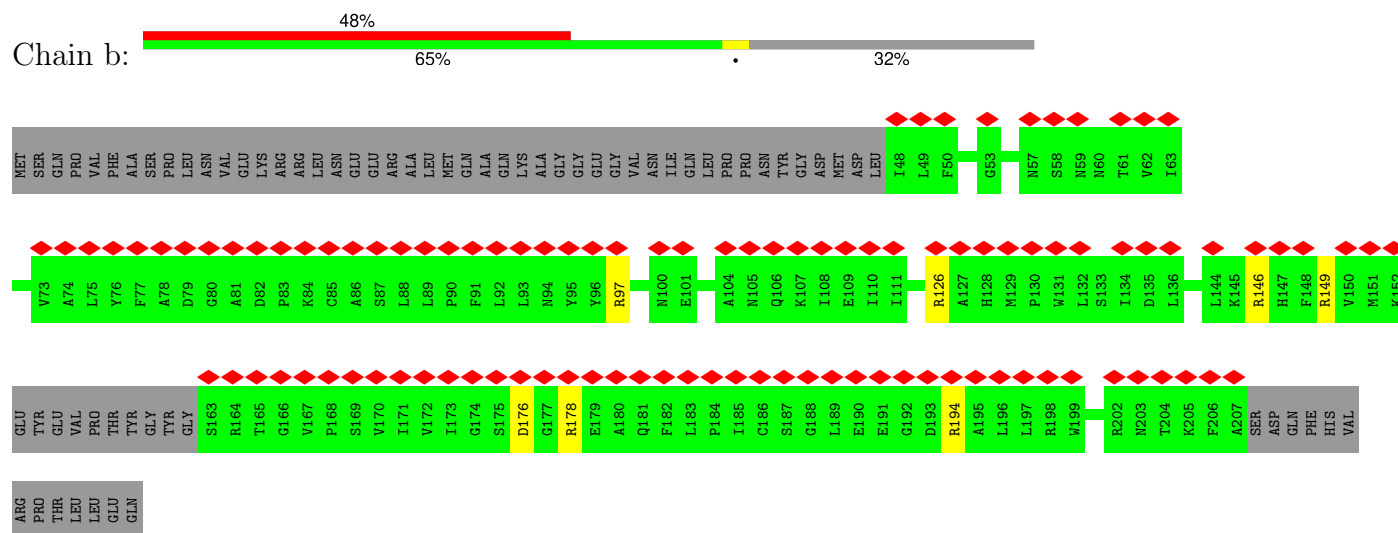
• Molecule 3: Tubulin beta chain



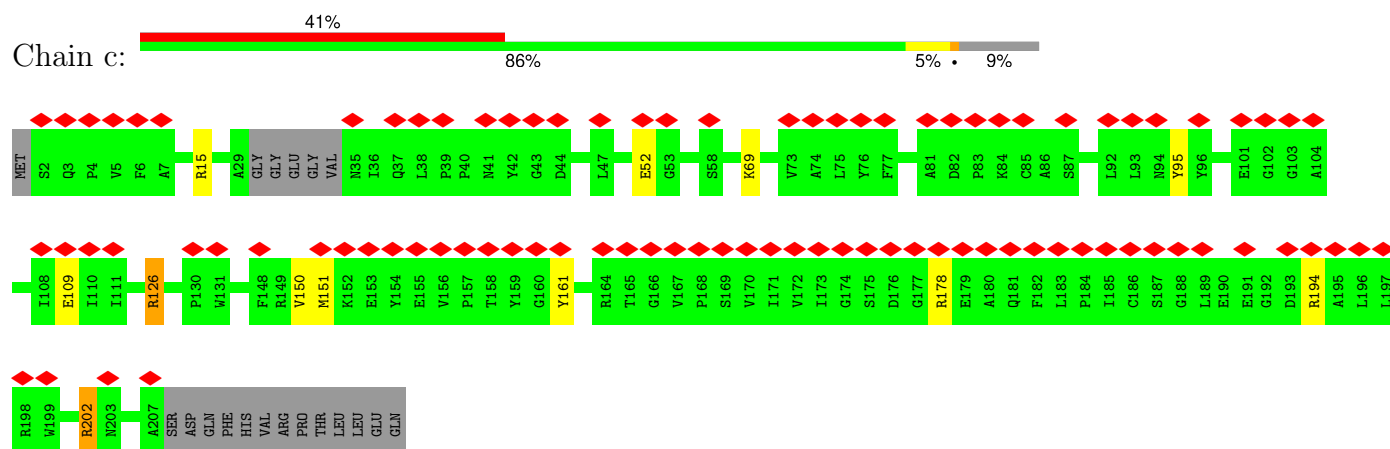
• Molecule 4: PDI family protein



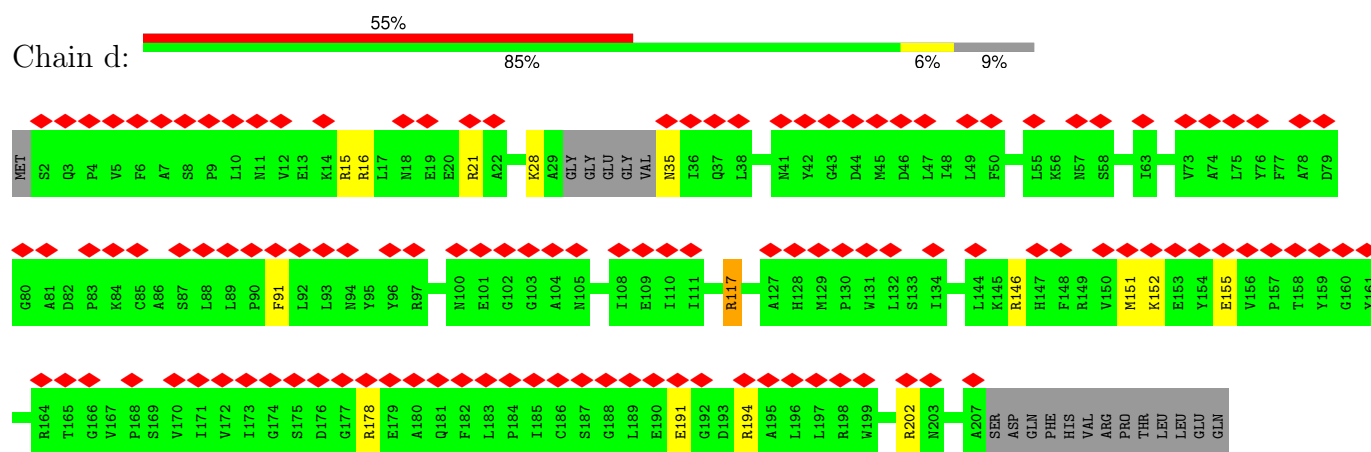
• Molecule 4: PDI family protein



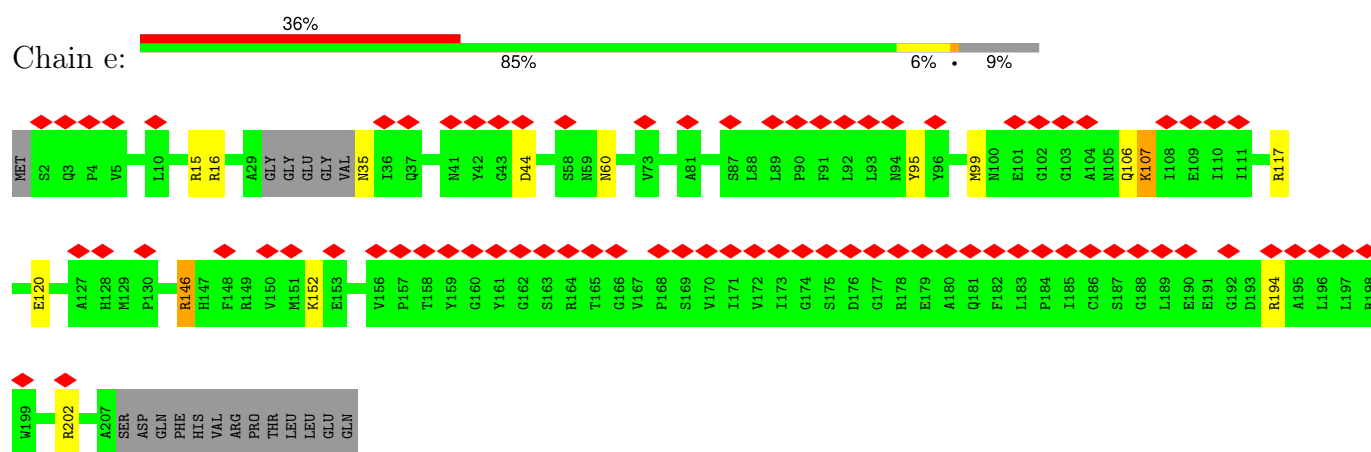
• Molecule 4: PDI family protein



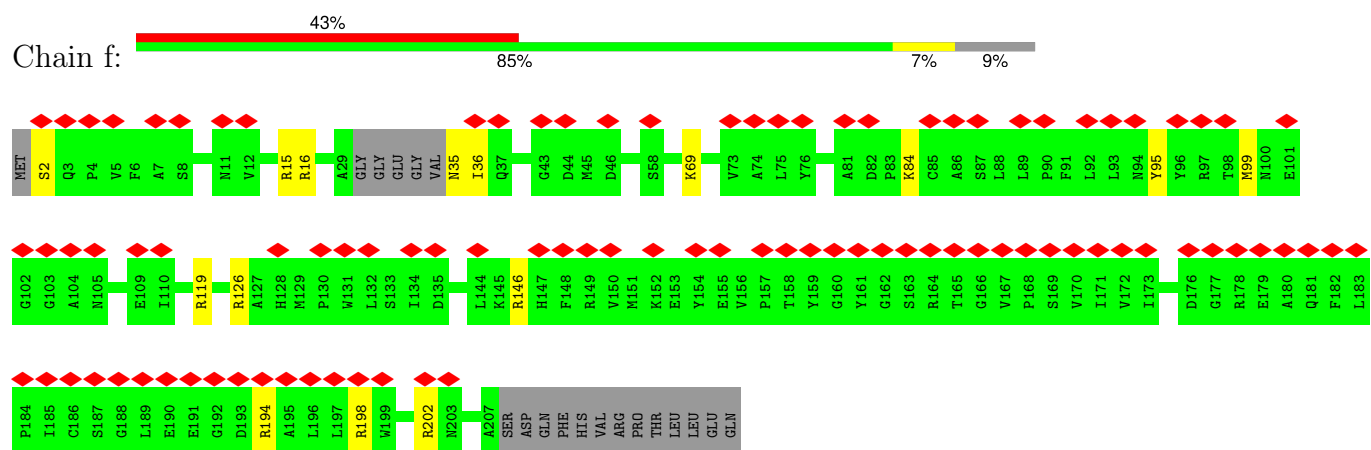
• Molecule 4: PDI family protein



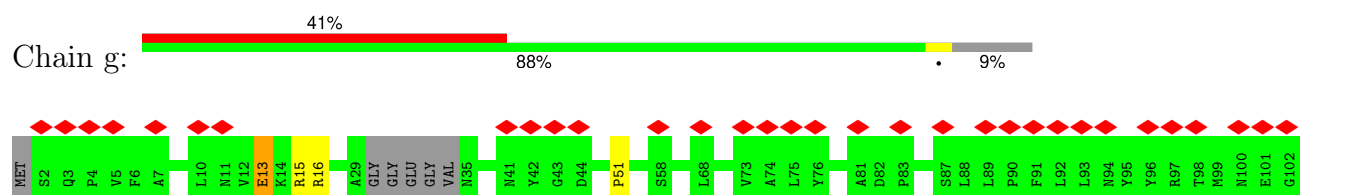
• Molecule 4: PDI family protein

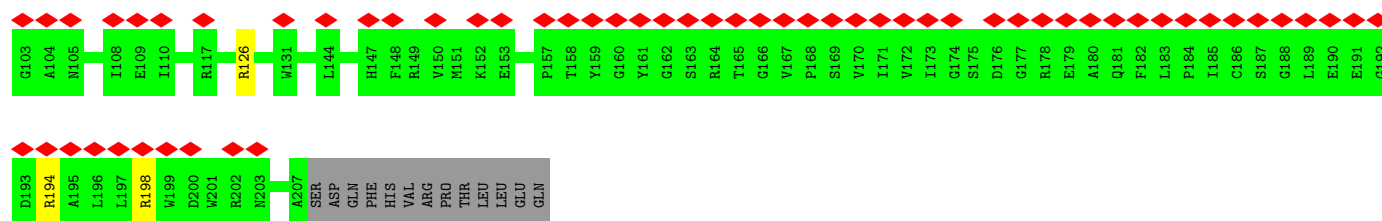


• Molecule 4: PDI family protein

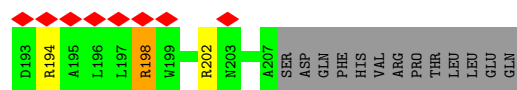
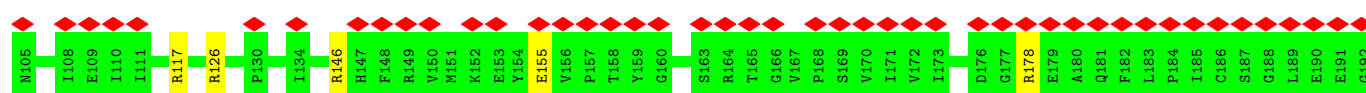
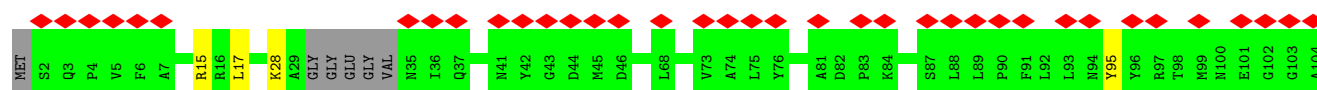
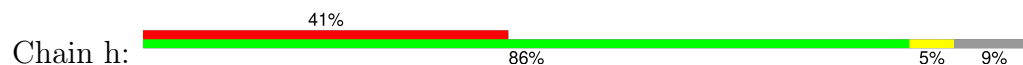


• Molecule 4: PDI family protein

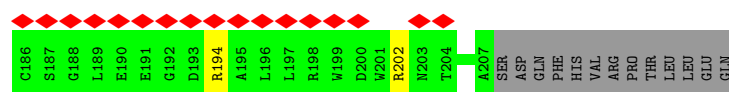
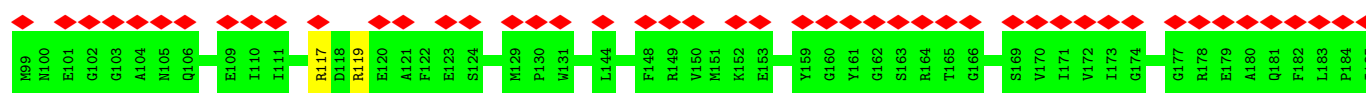
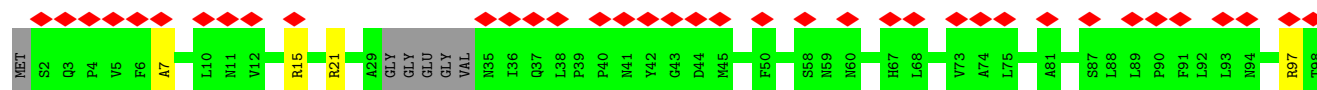
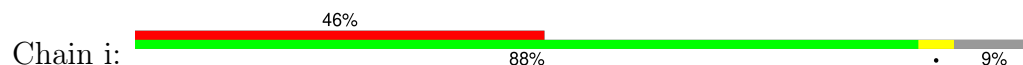




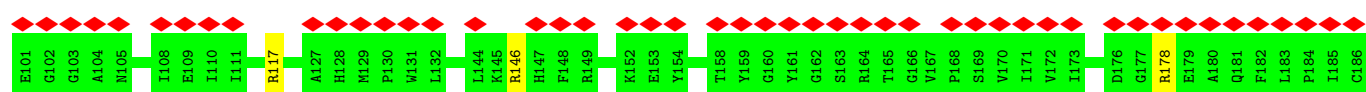
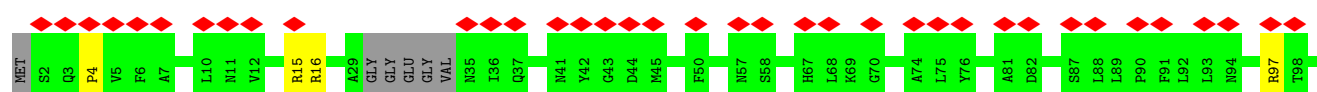
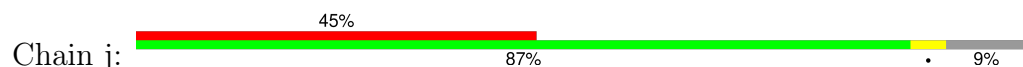
• Molecule 4: PDI family protein

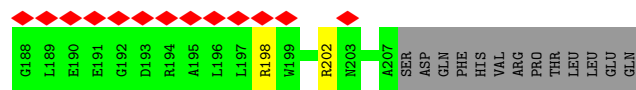


• Molecule 4: PDI family protein

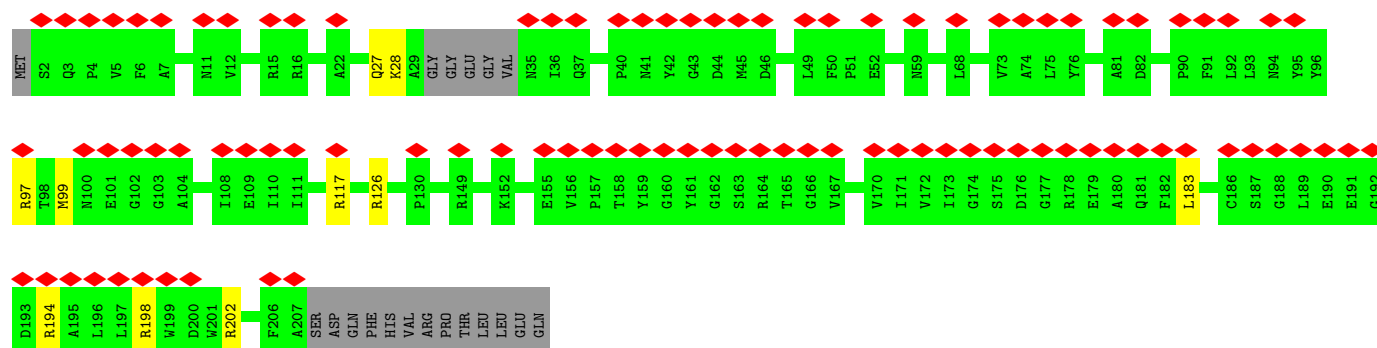
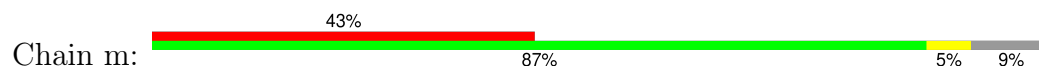


• Molecule 4: PDI family protein

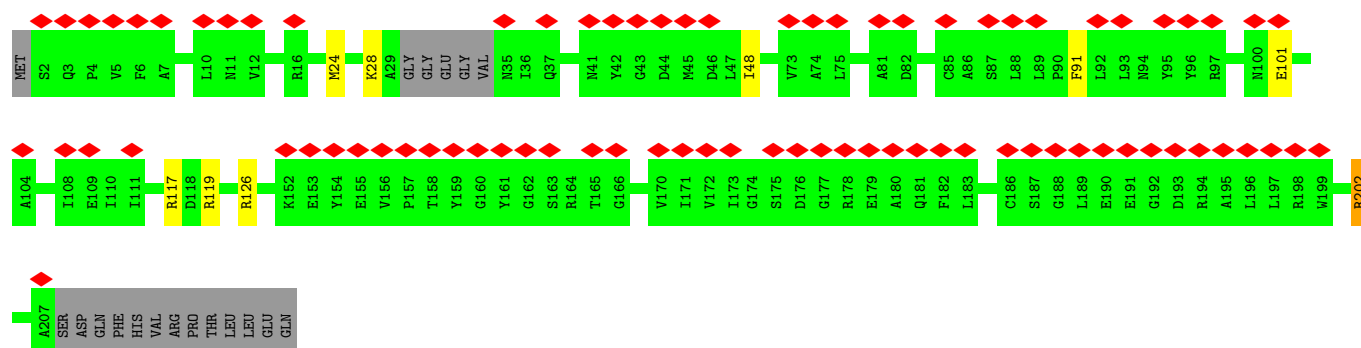
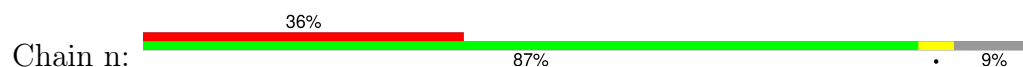




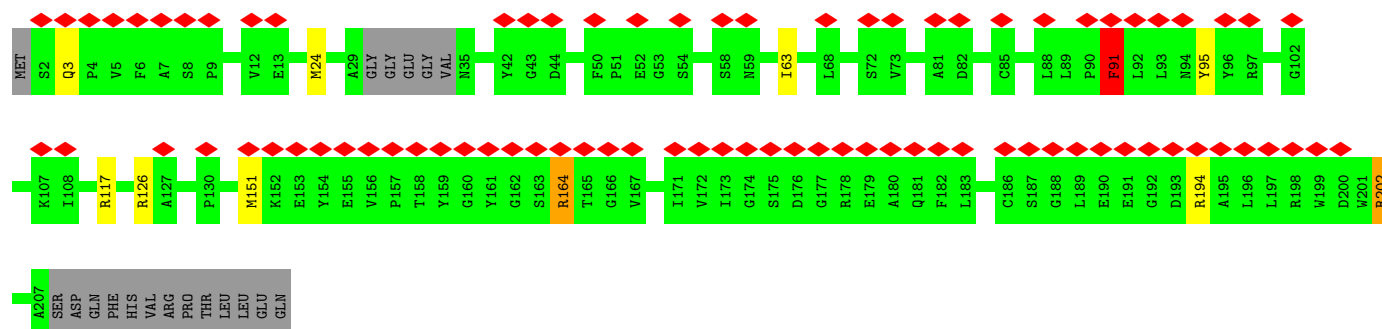
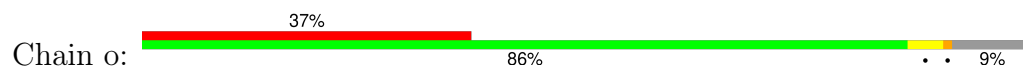
• Molecule 4: PDI family protein



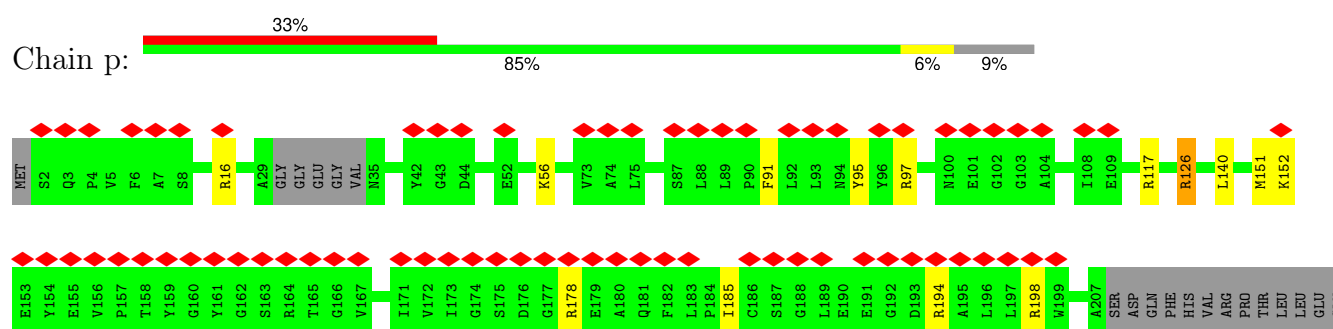
• Molecule 4: PDI family protein



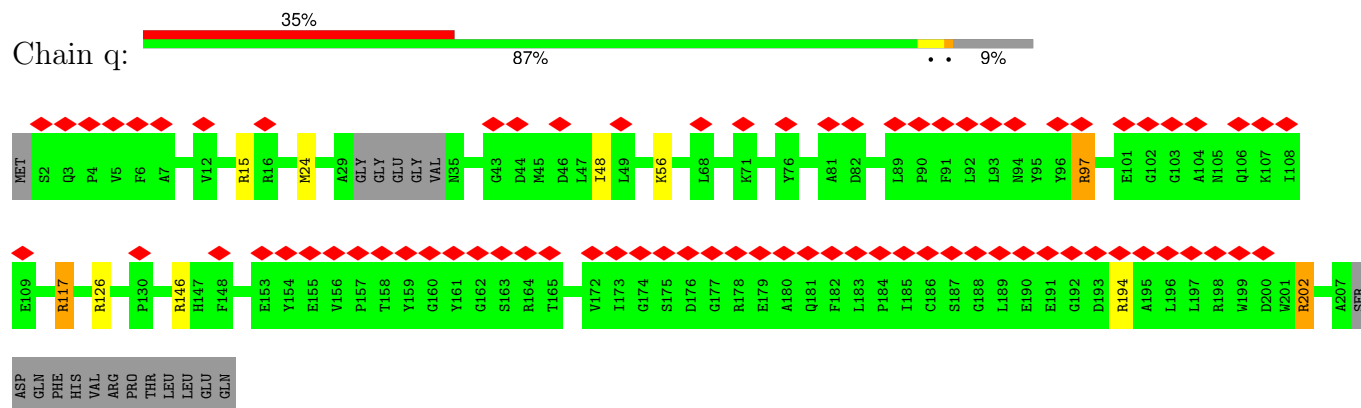
• Molecule 4: PDI family protein



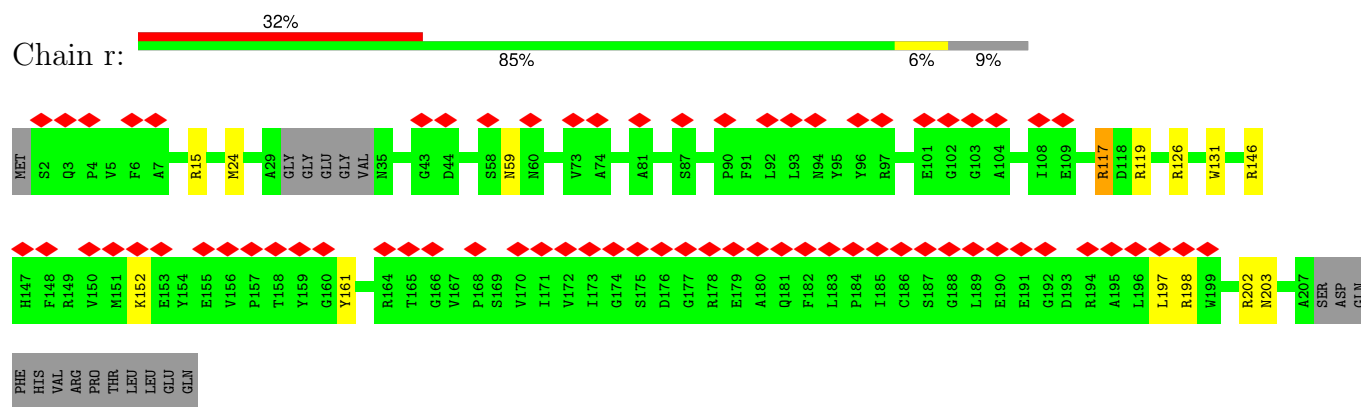
• Molecule 4: PDI family protein



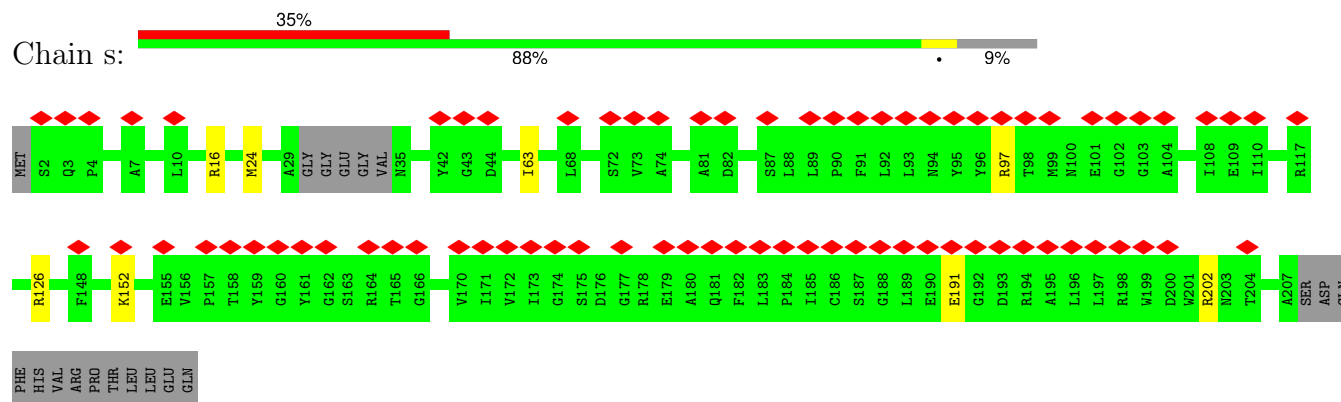
- Molecule 4: PDI family protein



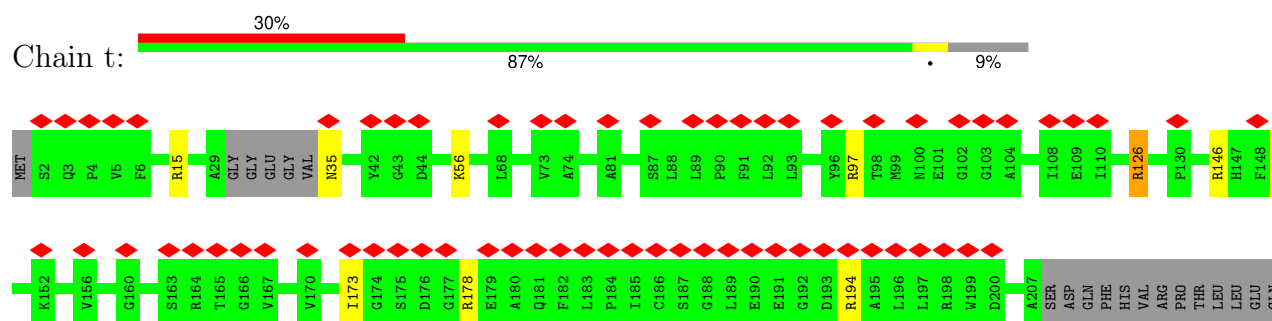
- Molecule 4: PDI family protein



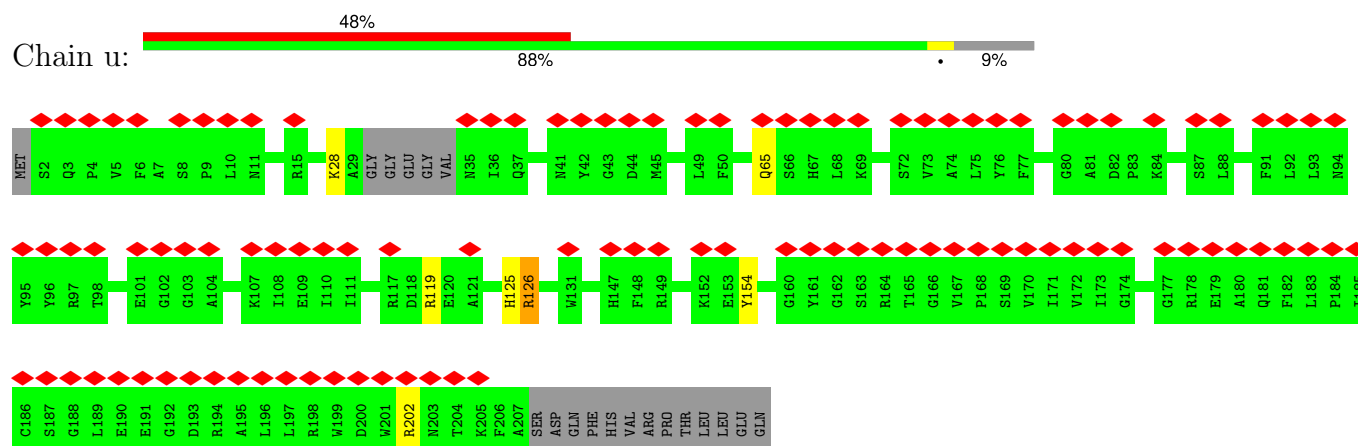
- Molecule 4: PDI family protein



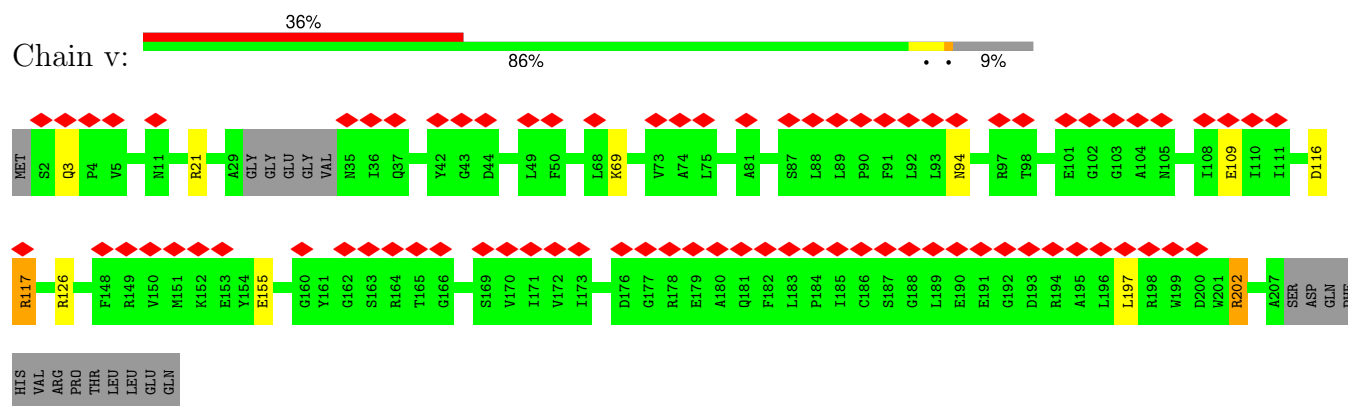
- Molecule 4: PDI family protein



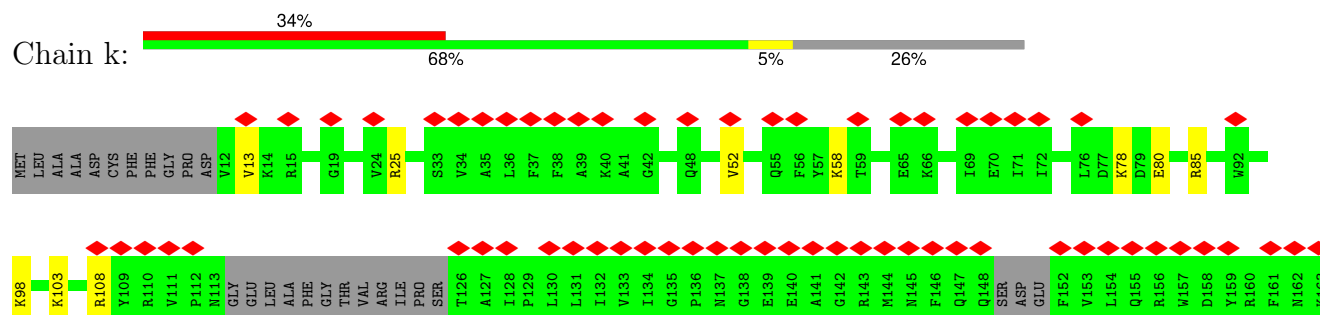
- Molecule 4: PDI family protein

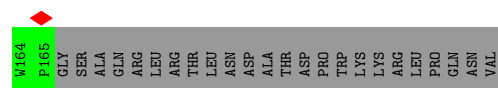


- Molecule 4: PDI family protein

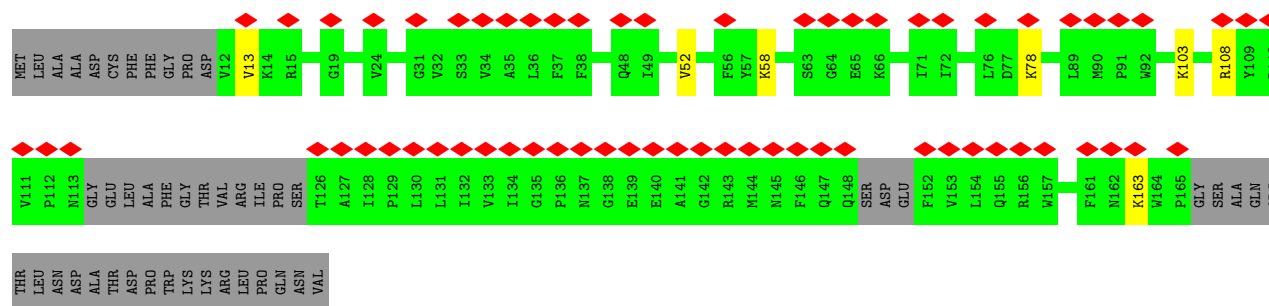


- Molecule 5: PDI family protein

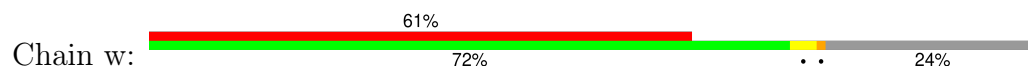




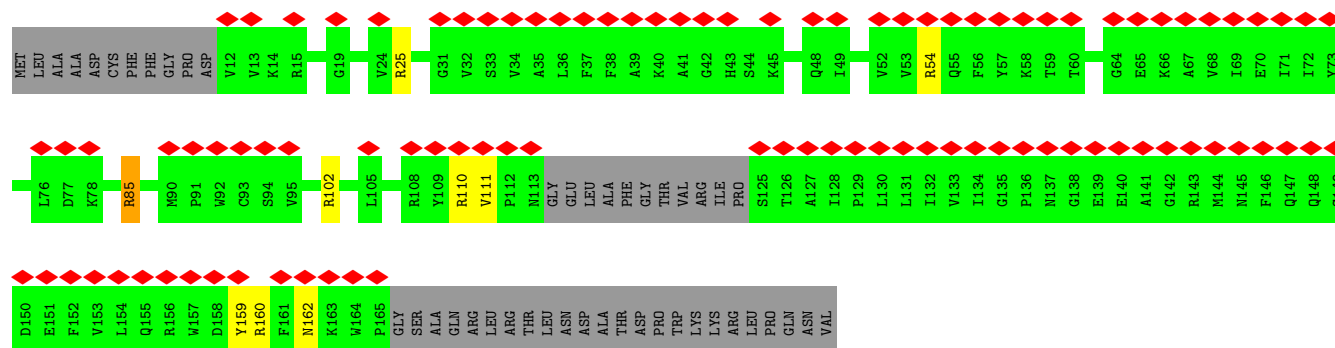
• Molecule 5: PDI family protein



• Molecule 5: PDI family protein



• Molecule 5: PDI family protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	39122	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	132	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.004	Depositor
Minimum map value	-8.373	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.892	Depositor
Recommended contour level	2	Depositor
Map size (\AA)	447.444, 447.444, 447.444	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.0715, 2.0715, 2.0715	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.50	0/181	0.96	0/248
1	1	0.52	0/181	0.99	1/248 (0.4%)
1	10	0.41	0/181	0.99	0/248
1	11	0.53	0/181	1.39	3/248 (1.2%)
1	12	0.60	0/181	1.43	2/248 (0.8%)
1	13	0.52	0/181	1.13	0/248
1	14	0.45	0/181	0.88	0/248
1	15	0.60	0/181	1.32	1/248 (0.4%)
1	16	0.53	0/181	0.94	1/248 (0.4%)
1	17	0.60	0/181	1.20	1/248 (0.4%)
1	18	0.46	0/181	0.99	0/248
1	19	0.86	2/181 (1.1%)	1.13	2/248 (0.8%)
1	2	0.57	0/181	1.28	1/248 (0.4%)
1	20	0.45	0/181	0.76	0/248
1	21	0.57	0/181	1.11	1/248 (0.4%)
1	22	0.61	0/166	1.19	1/227 (0.4%)
1	23	0.46	0/166	0.89	0/227
1	3	0.50	0/181	0.94	0/248
1	4	0.45	0/181	1.12	1/248 (0.4%)
1	5	0.44	0/181	1.06	1/248 (0.4%)
1	6	0.45	0/181	1.11	1/248 (0.4%)
1	7	0.44	0/181	0.91	0/248
1	8	0.48	0/181	1.12	1/248 (0.4%)
1	9	0.52	0/181	0.96	0/248
2	A0	0.57	1/3398 (0.0%)	1.11	22/4606 (0.5%)
2	A2	0.51	1/3398 (0.0%)	0.99	15/4606 (0.3%)
2	A4	0.77	4/3398 (0.1%)	1.14	15/4606 (0.3%)
2	A6	0.54	2/3398 (0.1%)	1.01	13/4606 (0.3%)
2	A8	0.68	5/3398 (0.1%)	1.15	21/4606 (0.5%)
2	B0	0.53	0/3398	0.97	11/4606 (0.2%)
2	B2	0.59	2/3398 (0.1%)	1.02	8/4606 (0.2%)
2	B4	0.51	2/3398 (0.1%)	0.92	5/4606 (0.1%)
2	B6	0.51	2/3398 (0.1%)	0.88	5/4606 (0.1%)
2	B8	0.46	0/3398	0.88	9/4606 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	C0	0.47	2/3398 (0.1%)	0.87	4/4606 (0.1%)
2	C2	0.47	0/3398	0.91	7/4606 (0.2%)
2	C4	0.63	6/3398 (0.2%)	0.97	12/4606 (0.3%)
2	C6	0.53	1/3398 (0.0%)	1.00	8/4606 (0.2%)
2	C8	0.58	2/3398 (0.1%)	0.99	11/4606 (0.2%)
2	D0	0.57	2/3398 (0.1%)	1.06	21/4606 (0.5%)
2	D2	0.51	1/3398 (0.0%)	0.96	13/4606 (0.3%)
2	D4	0.64	3/3398 (0.1%)	1.20	25/4606 (0.5%)
2	D6	0.51	0/3398	0.91	12/4606 (0.3%)
2	D8	0.59	1/3398 (0.0%)	1.07	16/4606 (0.3%)
2	E0	0.40	0/3398	0.76	5/4606 (0.1%)
2	E2	0.51	2/3398 (0.1%)	0.93	10/4606 (0.2%)
2	E4	0.39	0/3398	0.73	4/4606 (0.1%)
2	E6	0.47	0/3398	0.87	4/4606 (0.1%)
2	E8	0.35	0/3398	0.70	0/4606
2	F0	0.54	2/3398 (0.1%)	0.90	13/4606 (0.3%)
3	A1	0.58	3/3404 (0.1%)	0.99	10/4606 (0.2%)
3	A3	0.45	0/3404	0.85	2/4606 (0.0%)
3	A5	0.66	3/3404 (0.1%)	1.07	18/4606 (0.4%)
3	A7	0.48	1/3404 (0.0%)	0.86	5/4606 (0.1%)
3	A9	0.59	2/3404 (0.1%)	0.99	9/4606 (0.2%)
3	B1	0.50	0/3404	0.90	3/4606 (0.1%)
3	B3	0.55	3/3404 (0.1%)	1.01	11/4606 (0.2%)
3	B5	0.52	1/3404 (0.0%)	0.95	5/4606 (0.1%)
3	B7	0.49	1/3404 (0.0%)	0.92	7/4606 (0.2%)
3	B9	0.46	0/3404	0.87	6/4606 (0.1%)
3	C1	0.48	1/3404 (0.0%)	0.92	7/4606 (0.2%)
3	C3	0.50	3/3404 (0.1%)	0.90	5/4606 (0.1%)
3	C5	0.54	2/3404 (0.1%)	0.93	10/4606 (0.2%)
3	C7	0.59	4/3404 (0.1%)	1.00	10/4606 (0.2%)
3	C9	0.56	3/3404 (0.1%)	1.02	17/4606 (0.4%)
3	D1	0.75	10/3404 (0.3%)	1.23	29/4606 (0.6%)
3	D3	0.59	1/3404 (0.0%)	1.10	19/4606 (0.4%)
3	D5	0.74	4/3404 (0.1%)	1.23	26/4606 (0.6%)
3	D7	0.55	2/3404 (0.1%)	0.96	7/4606 (0.2%)
3	D9	0.61	3/3404 (0.1%)	1.06	14/4606 (0.3%)
3	E1	0.45	0/3404	0.83	4/4606 (0.1%)
3	E3	0.52	0/3404	0.95	11/4606 (0.2%)
3	E5	0.45	1/3404 (0.0%)	0.88	10/4606 (0.2%)
3	E7	0.52	1/3404 (0.0%)	0.97	11/4606 (0.2%)
3	E9	0.48	2/3404 (0.1%)	0.85	5/4606 (0.1%)
3	F1	0.52	0/3404	1.02	14/4606 (0.3%)
4	a	0.67	4/1225 (0.3%)	1.07	4/1654 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	b	0.60	3/1225 (0.2%)	1.02	9/1654 (0.5%)
4	c	0.97	4/1645 (0.2%)	1.66	12/2225 (0.5%)
4	d	0.64	2/1645 (0.1%)	1.12	15/2225 (0.7%)
4	e	0.55	0/1645	1.06	12/2225 (0.5%)
4	f	0.54	0/1645	1.03	11/2225 (0.5%)
4	g	0.58	1/1645 (0.1%)	1.06	6/2225 (0.3%)
4	h	0.57	1/1645 (0.1%)	1.09	9/2225 (0.4%)
4	i	0.63	2/1645 (0.1%)	1.03	7/2225 (0.3%)
4	j	0.67	2/1645 (0.1%)	1.02	10/2225 (0.4%)
4	m	0.50	0/1645	0.96	9/2225 (0.4%)
4	n	0.65	4/1645 (0.2%)	1.11	9/2225 (0.4%)
4	o	0.55	0/1645	1.01	8/2225 (0.4%)
4	p	0.82	2/1645 (0.1%)	1.20	16/2225 (0.7%)
4	q	0.67	2/1645 (0.1%)	1.03	9/2225 (0.4%)
4	r	0.57	0/1645	1.07	10/2225 (0.4%)
4	s	0.51	1/1645 (0.1%)	0.97	2/2225 (0.1%)
4	t	0.68	2/1645 (0.1%)	1.13	9/2225 (0.4%)
4	u	0.49	0/1645	0.92	3/2225 (0.1%)
4	v	0.68	4/1645 (0.2%)	1.14	9/2225 (0.4%)
5	k	0.54	1/1168 (0.1%)	1.10	5/1578 (0.3%)
5	l	0.55	2/1168 (0.2%)	0.99	2/1578 (0.1%)
5	w	0.48	1/1201 (0.1%)	0.89	2/1623 (0.1%)
5	x	0.60	0/1201	1.15	7/1623 (0.4%)
All	All	0.56	132/217964 (0.1%)	0.99	777/295182 (0.3%)

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	13	0	1
1	15	0	2
1	18	0	1
1	23	0	2
1	4	0	1
1	7	0	1
2	A0	0	1
2	A2	0	2
2	A4	0	2
2	A8	0	3
2	B0	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B4	0	1
2	B6	0	1
2	C4	0	1
2	C8	0	1
2	D0	0	2
2	D2	0	1
2	E2	0	1
3	B3	0	1
3	B9	0	1
3	E5	0	2
4	c	0	1
4	e	0	1
4	o	0	1
4	t	0	1
5	k	0	1
5	l	0	1
All	All	0	35

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	178	ARG	NE-CZ	24.25	1.64	1.33
4	p	97	ARG	NE-CZ	22.41	1.62	1.33
4	c	178	ARG	CZ-NH1	17.44	1.55	1.33
2	A4	254	GLU	CG-CD	16.52	1.76	1.51
3	D5	3	GLU	CD-OE1	16.43	1.43	1.25

The worst 5 of 777 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	178	ARG	NE-CZ-NH1	43.97	142.28	120.30
4	c	178	ARG	NE-CZ-NH2	-27.43	106.59	120.30
2	C4	2	ARG	CG-CD-NE	18.40	150.43	111.80
4	t	97	ARG	NE-CZ-NH1	17.48	129.04	120.30
3	D1	213	ARG	CG-CD-NE	-15.65	78.93	111.80

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	13	255	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	15	237	PRO	Peptide
1	15	240	PRO	Peptide
1	18	242	ASN	Peptide
1	23	239	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	174	0	171	18	0
1	1	174	0	171	6	0
1	10	174	0	171	24	0
1	11	174	0	171	20	0
1	12	174	0	171	9	0
1	13	174	0	171	10	0
1	14	174	0	171	6	0
1	15	174	0	171	17	0
1	16	174	0	171	18	0
1	17	174	0	171	8	0
1	18	174	0	171	8	0
1	19	174	0	171	24	0
1	2	174	0	171	13	0
1	20	174	0	171	13	0
1	21	174	0	171	20	0
1	22	160	0	156	8	0
1	23	160	0	156	5	0
1	3	174	0	171	8	0
1	4	174	0	171	10	0
1	5	174	0	171	13	0
1	6	174	0	171	15	0
1	7	174	0	171	18	0
1	8	174	0	171	29	0
1	9	174	0	171	32	0
2	A0	3325	0	3252	86	0
2	A2	3325	0	3252	74	0
2	A4	3325	0	3252	81	0
2	A6	3325	0	3252	78	0
2	A8	3325	0	3252	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B0	3325	0	3252	80	0
2	B2	3325	0	3252	73	0
2	B4	3325	0	3252	83	0
2	B6	3325	0	3252	69	0
2	B8	3325	0	3252	93	0
2	C0	3325	0	3252	73	0
2	C2	3325	0	3252	91	0
2	C4	3325	0	3252	91	0
2	C6	3325	0	3252	107	0
2	C8	3325	0	3252	78	0
2	D0	3325	0	3252	86	0
2	D2	3325	0	3252	76	0
2	D4	3325	0	3252	118	0
2	D6	3325	0	3252	63	0
2	D8	3325	0	3252	97	0
2	E0	3325	0	3252	78	0
2	E2	3325	0	3252	56	0
2	E4	3325	0	3252	64	0
2	E6	3325	0	3252	83	0
2	E8	3325	0	3252	72	0
2	F0	3325	0	3252	97	0
3	A1	3331	0	3207	98	0
3	A3	3331	0	3209	54	0
3	A5	3331	0	3207	99	0
3	A7	3331	0	3207	66	0
3	A9	3331	0	3207	79	0
3	B1	3331	0	3209	70	0
3	B3	3331	0	3207	82	0
3	B5	3331	0	3207	56	0
3	B7	3331	0	3209	62	0
3	B9	3331	0	3209	59	0
3	C1	3331	0	3209	110	0
3	C3	3331	0	3209	91	0
3	C5	3331	0	3209	77	0
3	C7	3331	0	3209	93	0
3	C9	3331	0	3209	101	0
3	D1	3331	0	3209	83	0
3	D3	3331	0	3207	106	0
3	D5	3331	0	3207	107	0
3	D7	3331	0	3207	86	0
3	D9	3331	0	3207	80	0
3	E1	3331	0	3207	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E3	3331	0	3209	61	0
3	E5	3331	0	3207	76	0
3	E7	3331	0	3207	86	0
3	E9	3331	0	3207	76	0
3	F1	3331	0	3207	85	0
4	a	1198	0	1194	0	0
4	b	1198	0	1194	0	0
4	c	1608	0	1590	0	0
4	d	1608	0	1590	0	0
4	e	1608	0	1590	0	0
4	f	1608	0	1590	0	0
4	g	1608	0	1590	0	0
4	h	1608	0	1590	0	0
4	i	1608	0	1590	0	0
4	j	1608	0	1590	0	0
4	m	1608	0	1590	0	0
4	n	1608	0	1590	0	0
4	o	1608	0	1590	0	0
4	p	1608	0	1590	0	0
4	q	1608	0	1590	0	0
4	r	1608	0	1590	0	0
4	s	1608	0	1590	0	0
4	t	1608	0	1590	0	0
4	u	1608	0	1590	0	0
4	v	1608	0	1588	0	0
5	k	1140	0	1143	0	0
5	l	1140	0	1143	0	0
5	w	1172	0	1171	0	0
5	x	1172	0	1171	0	0
All	All	213168	0	207664	3610	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 3610 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:19:241:PHE:CZ	3:E7:356:ILE:HG23	1.28	1.68
2:C4:2:ARG:CG	2:C4:2:ARG:CD	1.76	1.56
3:A9:252:LYS:CG	3:A9:252:LYS:CD	1.84	1.55
1:19:241:PHE:HZ	3:E7:356:ILE:CG2	1.03	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C4:2:ARG:CD	2:C4:2:ARG:NE	1.70	1.54

There are no symmetry-related clashes.

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	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	1	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	10	20/351 (6%)	17 (85%)	3 (15%)	0	100	100
1	11	20/351 (6%)	16 (80%)	4 (20%)	0	100	100
1	12	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	13	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	14	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	15	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	16	20/351 (6%)	20 (100%)	0	0	100	100
1	17	20/351 (6%)	20 (100%)	0	0	100	100
1	18	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	19	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	2	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	20	20/351 (6%)	17 (85%)	3 (15%)	0	100	100
1	21	20/351 (6%)	18 (90%)	1 (5%)	1 (5%)	1	16
1	22	18/351 (5%)	16 (89%)	2 (11%)	0	100	100
1	23	18/351 (5%)	15 (83%)	3 (17%)	0	100	100
1	3	20/351 (6%)	18 (90%)	1 (5%)	1 (5%)	1	16
1	4	20/351 (6%)	20 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	6	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	7	20/351 (6%)	20 (100%)	0	0	100	100
1	8	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	9	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
2	A0	424/453 (94%)	398 (94%)	26 (6%)	0	100	100
2	A2	424/453 (94%)	405 (96%)	18 (4%)	1 (0%)	44	78
2	A4	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
2	A6	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	A8	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	B0	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
2	B2	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
2	B4	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
2	B6	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
2	B8	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
2	C0	424/453 (94%)	402 (95%)	21 (5%)	1 (0%)	44	78
2	C2	424/453 (94%)	399 (94%)	24 (6%)	1 (0%)	44	78
2	C4	424/453 (94%)	386 (91%)	37 (9%)	1 (0%)	44	78
2	C6	424/453 (94%)	397 (94%)	27 (6%)	0	100	100
2	C8	424/453 (94%)	396 (93%)	28 (7%)	0	100	100
2	D0	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	D2	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	D4	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	D6	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
2	D8	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
2	E0	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	E2	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	E4	424/453 (94%)	399 (94%)	25 (6%)	0	100	100
2	E6	424/453 (94%)	399 (94%)	24 (6%)	1 (0%)	44	78
2	E8	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	F0	424/453 (94%)	401 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A1	424/449 (94%)	397 (94%)	27 (6%)	0	100	100
3	A3	424/449 (94%)	399 (94%)	24 (6%)	1 (0%)	44	78
3	A5	424/449 (94%)	388 (92%)	34 (8%)	2 (0%)	25	64
3	A7	424/449 (94%)	397 (94%)	26 (6%)	1 (0%)	44	78
3	A9	424/449 (94%)	400 (94%)	23 (5%)	1 (0%)	44	78
3	B1	424/449 (94%)	401 (95%)	22 (5%)	1 (0%)	44	78
3	B3	424/449 (94%)	400 (94%)	22 (5%)	2 (0%)	25	64
3	B5	424/449 (94%)	394 (93%)	28 (7%)	2 (0%)	25	64
3	B7	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	B9	424/449 (94%)	407 (96%)	17 (4%)	0	100	100
3	C1	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	C3	424/449 (94%)	396 (93%)	27 (6%)	1 (0%)	44	78
3	C5	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	C7	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	C9	424/449 (94%)	396 (93%)	27 (6%)	1 (0%)	44	78
3	D1	424/449 (94%)	399 (94%)	24 (6%)	1 (0%)	44	78
3	D3	424/449 (94%)	395 (93%)	28 (7%)	1 (0%)	44	78
3	D5	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	D7	424/449 (94%)	399 (94%)	24 (6%)	1 (0%)	44	78
3	D9	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	E1	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	E3	424/449 (94%)	402 (95%)	21 (5%)	1 (0%)	44	78
3	E5	424/449 (94%)	392 (92%)	32 (8%)	0	100	100
3	E7	424/449 (94%)	397 (94%)	26 (6%)	1 (0%)	44	78
3	E9	424/449 (94%)	388 (92%)	36 (8%)	0	100	100
3	F1	424/449 (94%)	389 (92%)	34 (8%)	1 (0%)	44	78
4	a	146/220 (66%)	135 (92%)	11 (8%)	0	100	100
4	b	146/220 (66%)	137 (94%)	9 (6%)	0	100	100
4	c	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
4	d	197/220 (90%)	179 (91%)	18 (9%)	0	100	100
4	e	197/220 (90%)	183 (93%)	13 (7%)	1 (0%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	f	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	g	197/220 (90%)	185 (94%)	11 (6%)	1 (0%)	25	64
4	h	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
4	i	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	j	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	m	197/220 (90%)	180 (91%)	17 (9%)	0	100	100
4	n	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	o	197/220 (90%)	179 (91%)	18 (9%)	0	100	100
4	p	197/220 (90%)	182 (92%)	15 (8%)	0	100	100
4	q	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
4	r	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	s	197/220 (90%)	179 (91%)	18 (9%)	0	100	100
4	t	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	u	197/220 (90%)	189 (96%)	7 (4%)	1 (0%)	25	64
4	v	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
5	k	133/189 (70%)	127 (96%)	6 (4%)	0	100	100
5	l	133/189 (70%)	128 (96%)	5 (4%)	0	100	100
5	w	139/189 (74%)	133 (96%)	6 (4%)	0	100	100
5	x	139/189 (74%)	129 (93%)	10 (7%)	0	100	100
All	All	26906/37032 (73%)	25298 (94%)	1580 (6%)	28 (0%)	50	83

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A3	179	VAL
3	A5	55	THR
3	A7	55	THR
3	B3	55	THR
3	C3	179	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	20/304 (7%)	20 (100%)	0	100	100
1	1	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	10	20/304 (7%)	20 (100%)	0	100	100
1	11	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	12	20/304 (7%)	18 (90%)	2 (10%)	6	20
1	13	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	14	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	15	20/304 (7%)	20 (100%)	0	100	100
1	16	20/304 (7%)	20 (100%)	0	100	100
1	17	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	18	20/304 (7%)	18 (90%)	2 (10%)	6	20
1	19	20/304 (7%)	17 (85%)	3 (15%)	2	11
1	2	20/304 (7%)	20 (100%)	0	100	100
1	20	20/304 (7%)	20 (100%)	0	100	100
1	21	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	22	18/304 (6%)	17 (94%)	1 (6%)	17	38
1	23	18/304 (6%)	18 (100%)	0	100	100
1	3	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	4	20/304 (7%)	18 (90%)	2 (10%)	6	20
1	5	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	6	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	7	20/304 (7%)	20 (100%)	0	100	100
1	8	20/304 (7%)	20 (100%)	0	100	100
1	9	20/304 (7%)	20 (100%)	0	100	100
2	A0	359/379 (95%)	349 (97%)	10 (3%)	38	57
2	A2	359/379 (95%)	354 (99%)	5 (1%)	62	75
2	A4	359/379 (95%)	350 (98%)	9 (2%)	42	61
2	A6	359/379 (95%)	349 (97%)	10 (3%)	38	57
2	A8	359/379 (95%)	356 (99%)	3 (1%)	79	85
2	B0	359/379 (95%)	350 (98%)	9 (2%)	42	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B2	359/379 (95%)	351 (98%)	8 (2%)	47	65
2	B4	359/379 (95%)	354 (99%)	5 (1%)	62	75
2	B6	359/379 (95%)	355 (99%)	4 (1%)	70	80
2	B8	359/379 (95%)	353 (98%)	6 (2%)	56	72
2	C0	359/379 (95%)	355 (99%)	4 (1%)	70	80
2	C2	359/379 (95%)	354 (99%)	5 (1%)	62	75
2	C4	359/379 (95%)	352 (98%)	7 (2%)	52	69
2	C6	359/379 (95%)	351 (98%)	8 (2%)	47	65
2	C8	359/379 (95%)	352 (98%)	7 (2%)	52	69
2	D0	359/379 (95%)	352 (98%)	7 (2%)	52	69
2	D2	359/379 (95%)	351 (98%)	8 (2%)	47	65
2	D4	359/379 (95%)	350 (98%)	9 (2%)	42	61
2	D6	359/379 (95%)	353 (98%)	6 (2%)	56	72
2	D8	359/379 (95%)	351 (98%)	8 (2%)	47	65
2	E0	359/379 (95%)	357 (99%)	2 (1%)	84	88
2	E2	359/379 (95%)	352 (98%)	7 (2%)	52	69
2	E4	359/379 (95%)	354 (99%)	5 (1%)	62	75
2	E6	359/379 (95%)	351 (98%)	8 (2%)	47	65
2	E8	359/379 (95%)	357 (99%)	2 (1%)	84	88
2	F0	359/379 (95%)	353 (98%)	6 (2%)	56	72
3	A1	364/381 (96%)	360 (99%)	4 (1%)	70	80
3	A3	364/381 (96%)	358 (98%)	6 (2%)	58	73
3	A5	364/381 (96%)	356 (98%)	8 (2%)	47	65
3	A7	364/381 (96%)	357 (98%)	7 (2%)	52	69
3	A9	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	B1	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	B3	364/381 (96%)	358 (98%)	6 (2%)	58	73
3	B5	364/381 (96%)	358 (98%)	6 (2%)	58	73
3	B7	364/381 (96%)	358 (98%)	6 (2%)	58	73
3	B9	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	C1	364/381 (96%)	357 (98%)	7 (2%)	52	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C3	364/381 (96%)	360 (99%)	4 (1%)	70	80
3	C5	364/381 (96%)	356 (98%)	8 (2%)	47	65
3	C7	364/381 (96%)	354 (97%)	10 (3%)	40	58
3	C9	364/381 (96%)	358 (98%)	6 (2%)	58	73
3	D1	364/381 (96%)	356 (98%)	8 (2%)	47	65
3	D3	364/381 (96%)	358 (98%)	6 (2%)	58	73
3	D5	364/381 (96%)	351 (96%)	13 (4%)	30	50
3	D7	364/381 (96%)	356 (98%)	8 (2%)	47	65
3	D9	364/381 (96%)	357 (98%)	7 (2%)	52	69
3	E1	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	E3	364/381 (96%)	354 (97%)	10 (3%)	40	58
3	E5	364/381 (96%)	361 (99%)	3 (1%)	79	85
3	E7	364/381 (96%)	358 (98%)	6 (2%)	58	73
3	E9	364/381 (96%)	361 (99%)	3 (1%)	79	85
3	F1	364/381 (96%)	360 (99%)	4 (1%)	70	80
4	a	130/190 (68%)	125 (96%)	5 (4%)	28	49
4	b	130/190 (68%)	128 (98%)	2 (2%)	60	75
4	c	174/190 (92%)	170 (98%)	4 (2%)	45	64
4	d	174/190 (92%)	168 (97%)	6 (3%)	32	51
4	e	174/190 (92%)	169 (97%)	5 (3%)	37	56
4	f	174/190 (92%)	169 (97%)	5 (3%)	37	56
4	g	174/190 (92%)	171 (98%)	3 (2%)	56	72
4	h	174/190 (92%)	168 (97%)	6 (3%)	32	51
4	i	174/190 (92%)	171 (98%)	3 (2%)	56	72
4	j	174/190 (92%)	171 (98%)	3 (2%)	56	72
4	m	174/190 (92%)	169 (97%)	5 (3%)	37	56
4	n	174/190 (92%)	169 (97%)	5 (3%)	37	56
4	o	174/190 (92%)	165 (95%)	9 (5%)	19	40
4	p	174/190 (92%)	170 (98%)	4 (2%)	45	64
4	q	174/190 (92%)	168 (97%)	6 (3%)	32	51
4	r	174/190 (92%)	167 (96%)	7 (4%)	27	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	s	174/190 (92%)	169 (97%)	5 (3%)	37	56
4	t	174/190 (92%)	171 (98%)	3 (2%)	56	72
4	u	174/190 (92%)	170 (98%)	4 (2%)	45	64
4	v	174/190 (92%)	167 (96%)	7 (4%)	27	47
5	k	122/164 (74%)	118 (97%)	4 (3%)	33	52
5	l	122/164 (74%)	119 (98%)	3 (2%)	42	61
5	w	127/164 (77%)	122 (96%)	5 (4%)	27	48
5	x	127/164 (77%)	124 (98%)	3 (2%)	44	62
All	All	23164/31512 (74%)	22699 (98%)	465 (2%)	50	68

5 of 465 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D2	311	LYS
4	t	126	ARG
3	D9	32	PRO
4	s	24	MET
5	l	52	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
2	E6	101	ASN
4	m	94	ASN
3	E9	204	ASN
4	f	18	ASN
4	p	203	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

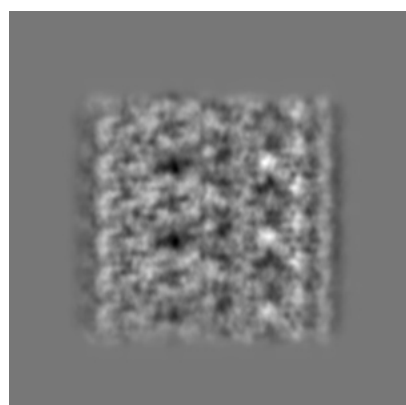
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26018. These allow visual inspection of the internal detail of the map and identification of artifacts.

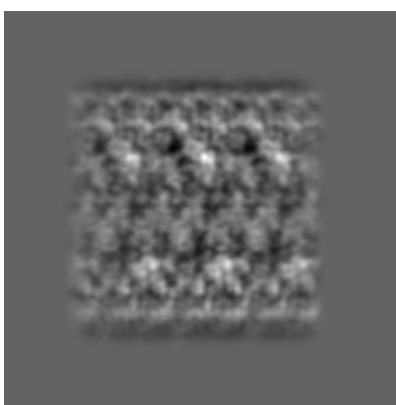
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

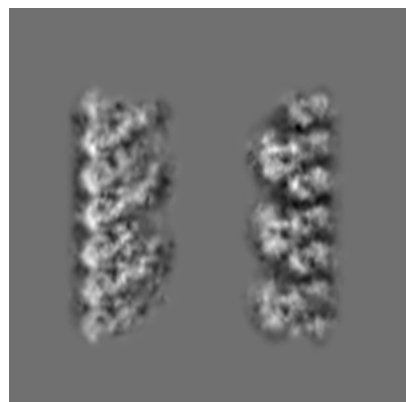


Z

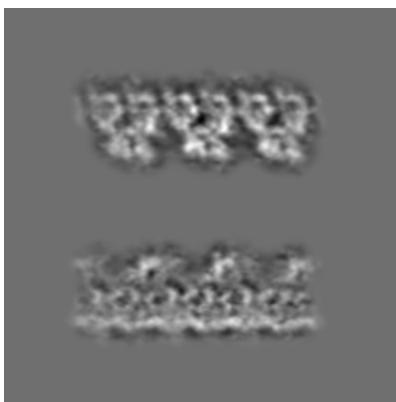
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 108



Y Index: 108

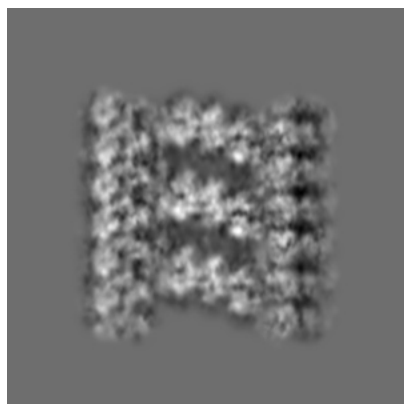


Z Index: 108

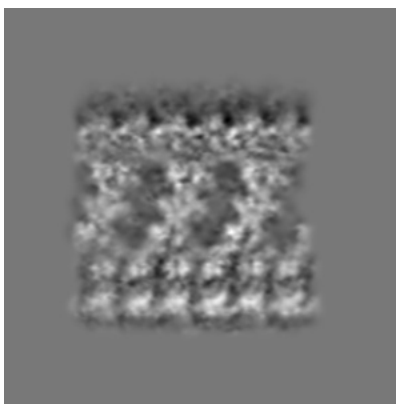
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 137



Y Index: 139

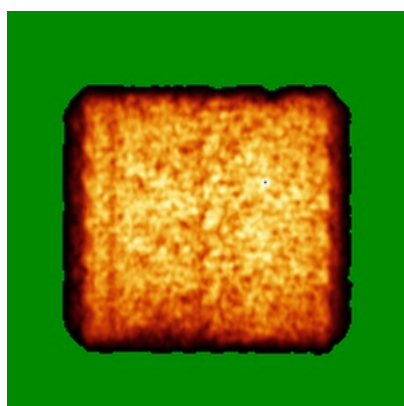


Z Index: 114

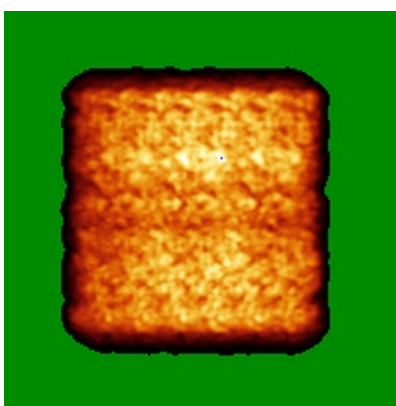
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

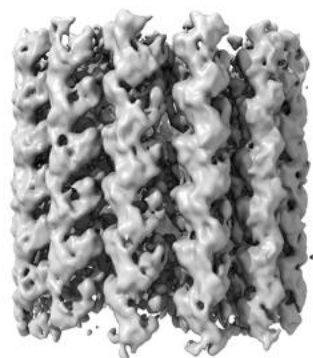


Z

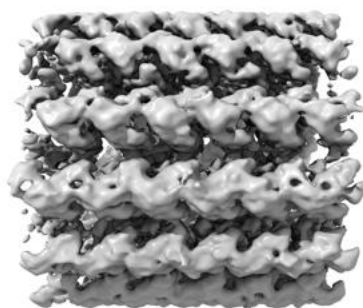
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

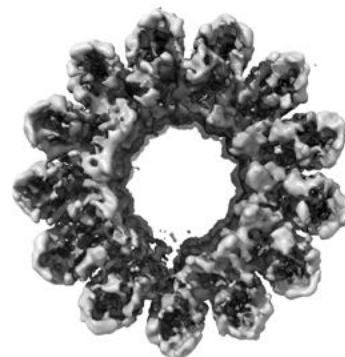
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

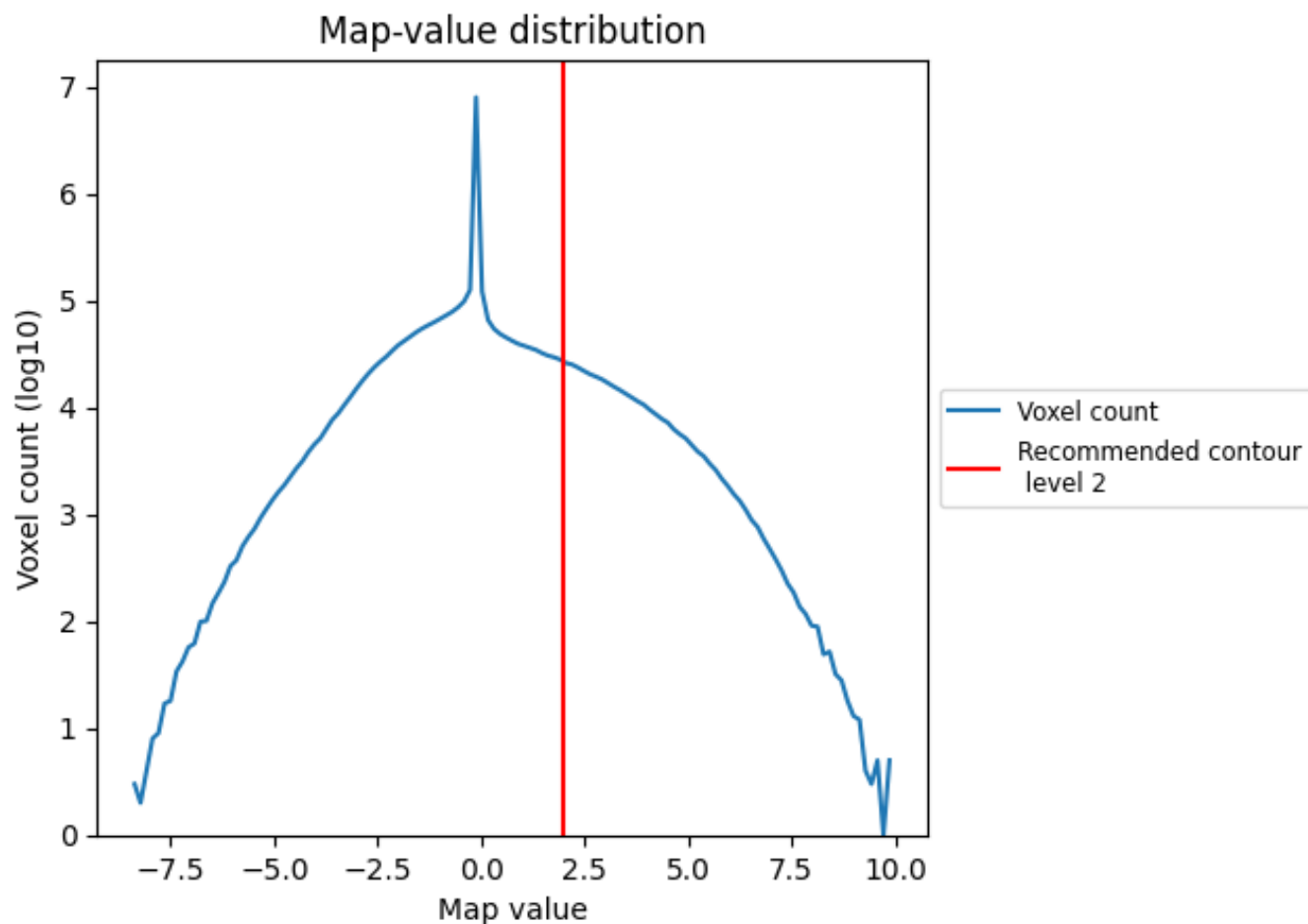
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

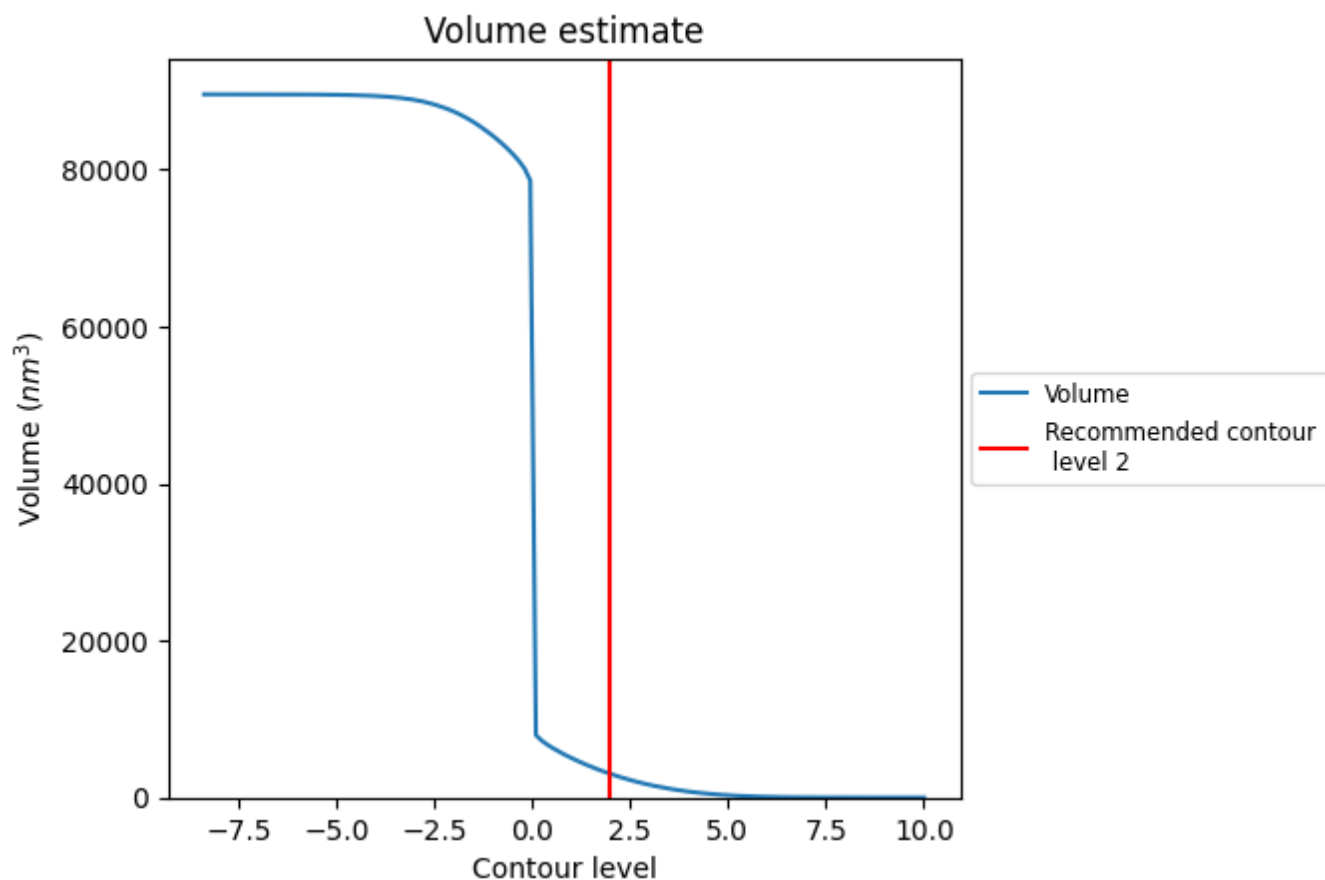
This section contains the results of statistical analysis of the map.

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.

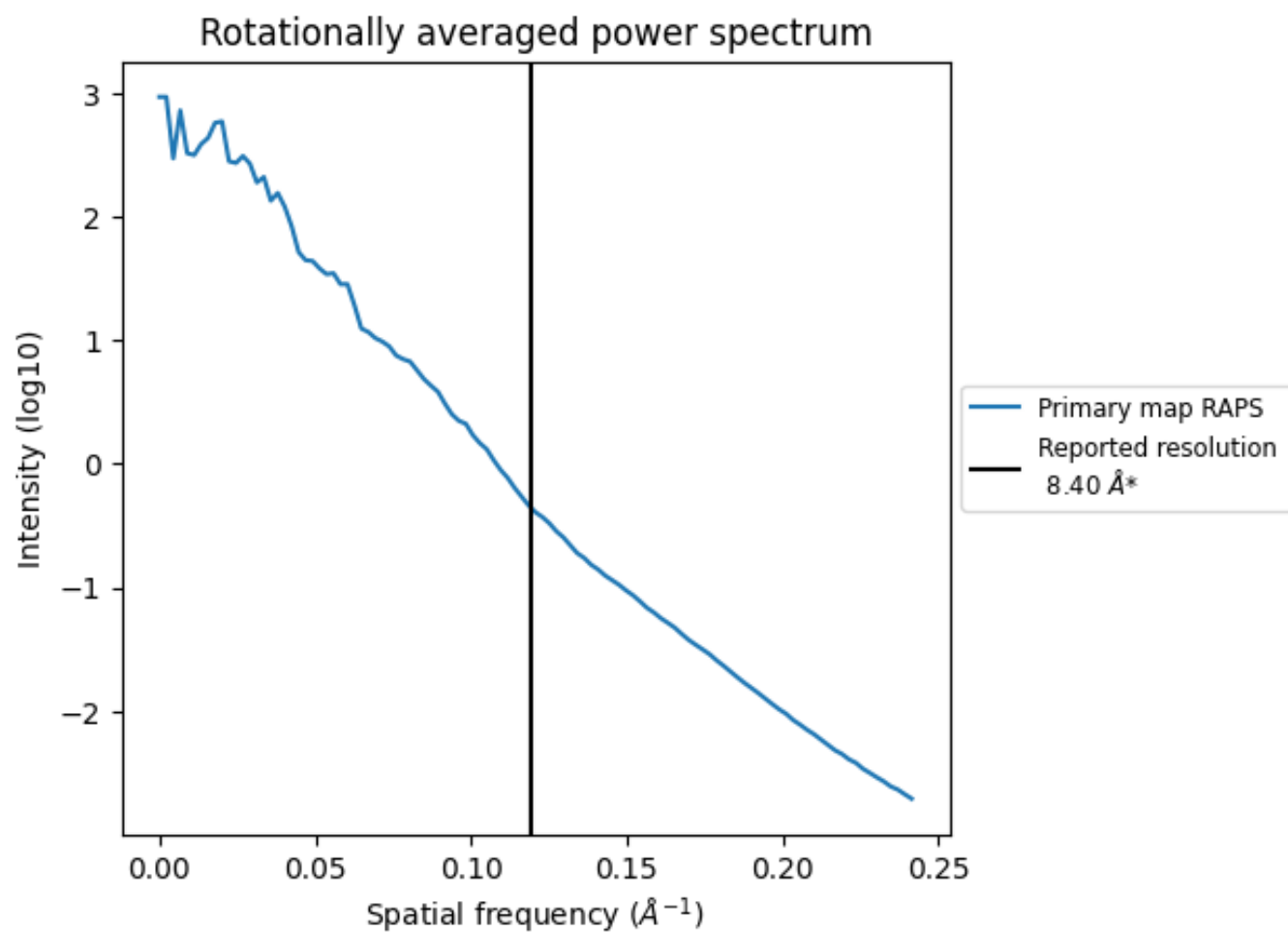
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3015 nm³; this corresponds to an approximate mass of 2724 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.119 Å⁻¹

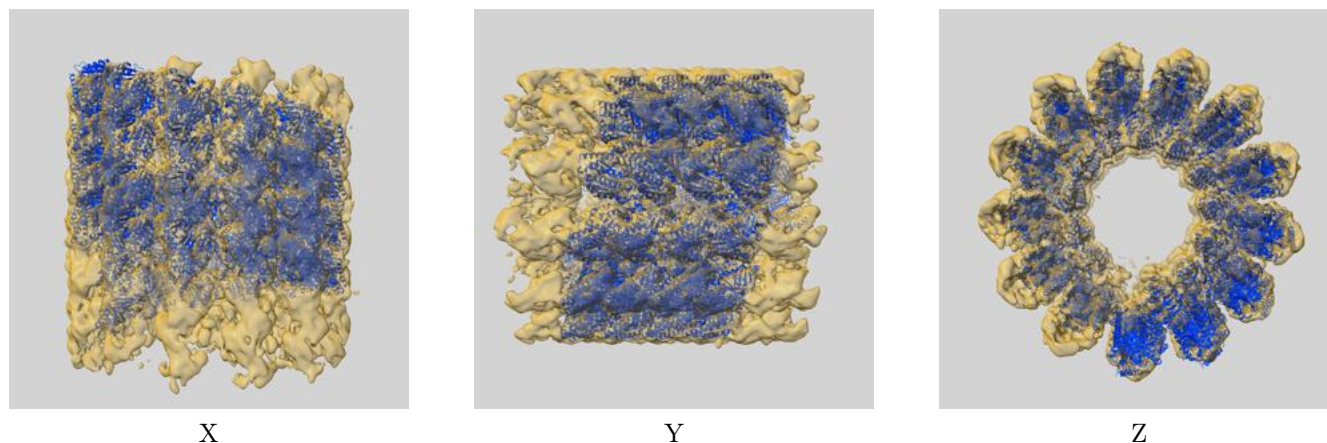
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

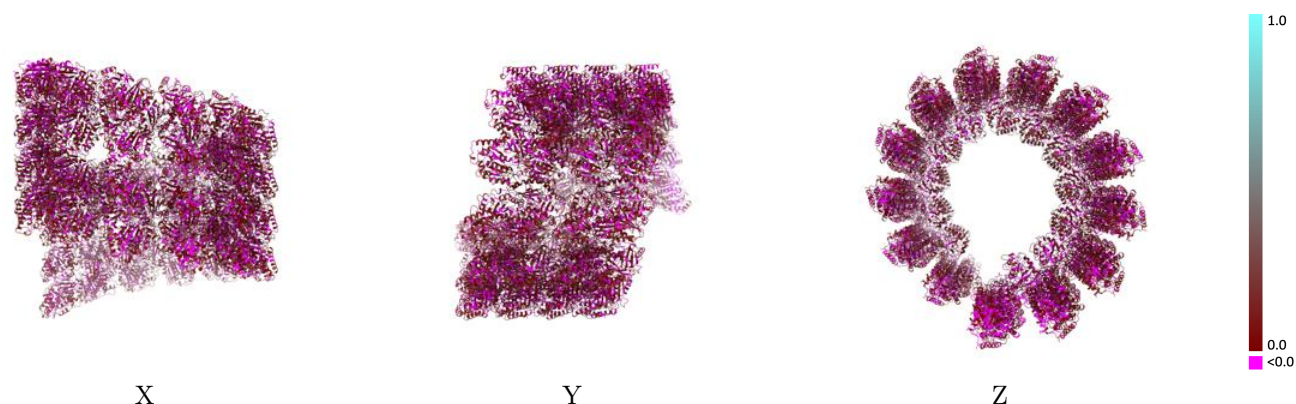
This section contains information regarding the fit between EMDB map EMD-26018 and PDB model 7TNQ. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



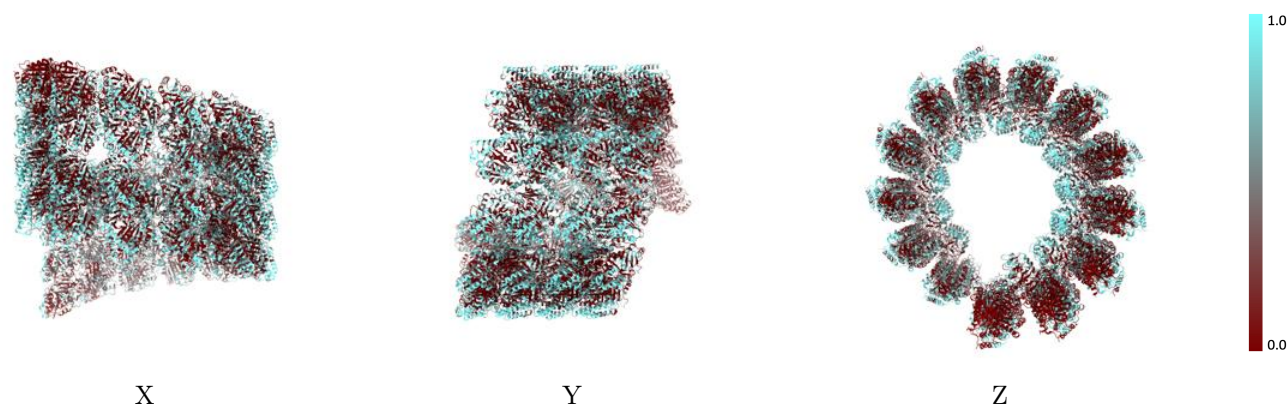
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



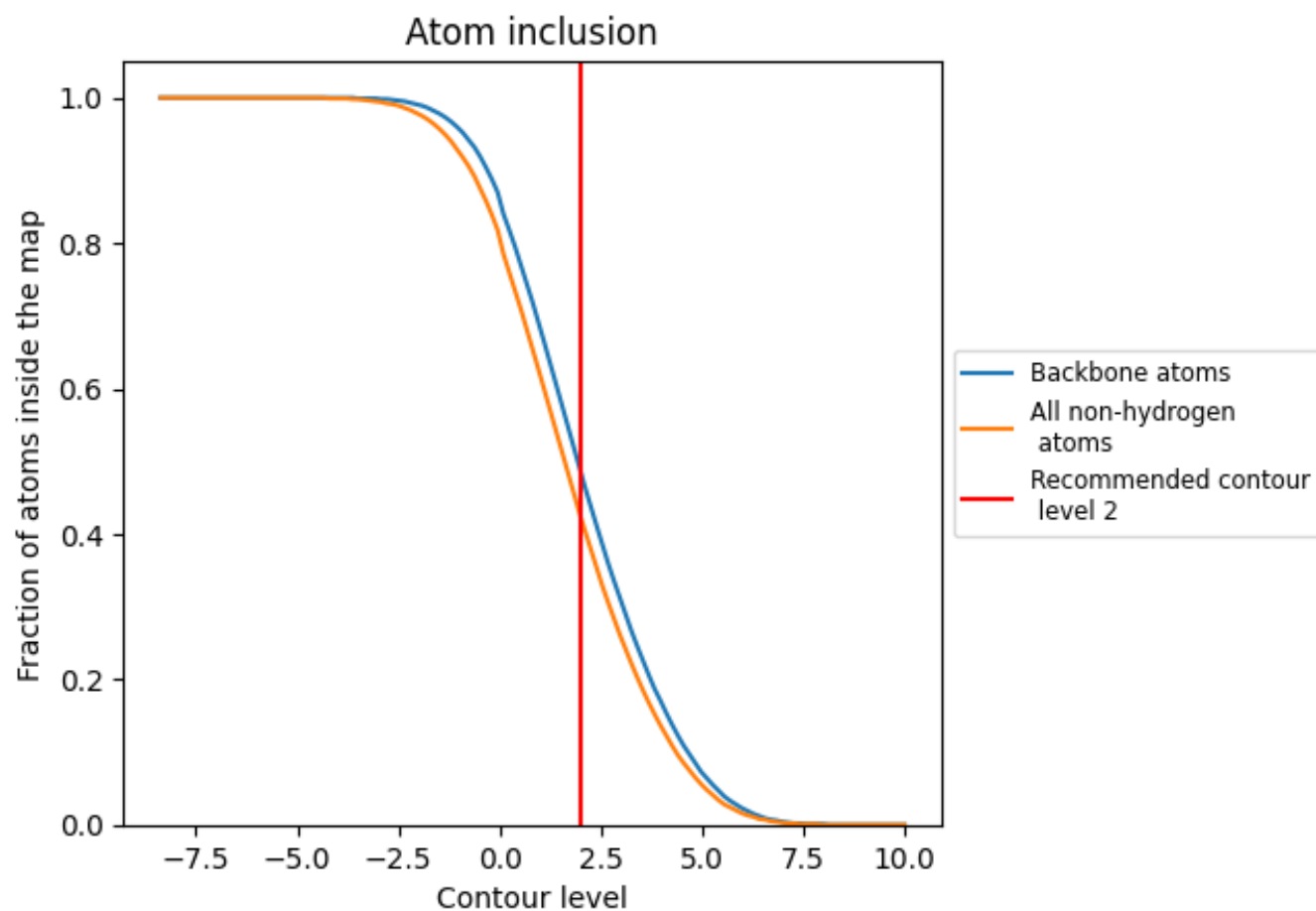
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 42% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4240	0.0760
0	0.1290	0.1680
1	0.0000	0.0940
10	0.0820	0.0720
11	0.0470	0.1110
12	0.1710	0.1250
13	0.1470	0.1000
14	0.0180	0.0900
15	0.0940	0.1000
16	0.1350	0.1160
17	0.2590	0.1140
18	0.1820	0.0380
19	0.2410	0.0440
2	0.1120	0.1250
20	0.1410	0.0080
21	0.4230	0.0670
22	0.0190	0.0960
23	0.0130	0.1160
3	0.0650	0.1040
4	0.1290	0.1020
5	0.1180	0.1400
6	0.1290	0.0710
7	0.1470	0.1150
8	0.0760	0.0500
9	0.0290	0.0540
A0	0.4570	0.0780
A1	0.4220	0.0750
A2	0.4210	0.0760
A3	0.2960	0.0730
A4	0.4700	0.0730
A5	0.4630	0.0750
A6	0.4380	0.0780
A7	0.3430	0.0670
A8	0.4370	0.0720
A9	0.4450	0.0830



















































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Chain	Atom inclusion	Q-score
B0	0.4220	0.0810
B1	0.3690	0.0780
B2	0.4200	0.0800
B3	0.4480	0.0790
B4	0.4340	0.0810
B5	0.3970	0.0760
B6	0.4140	0.0790
B7	0.5220	0.0920
B8	0.4770	0.0920
B9	0.4330	0.0850
C0	0.4230	0.0770
C1	0.5340	0.0910
C2	0.4690	0.0920
C3	0.4730	0.0890
C4	0.4010	0.0880
C5	0.4720	0.0910
C6	0.4550	0.0830
C7	0.4460	0.0890
C8	0.3750	0.0630
C9	0.4450	0.0740
D0	0.4290	0.0600
D1	0.3940	0.0560
D2	0.3460	0.0480
D3	0.4020	0.0600
D4	0.4090	0.0630
D5	0.3920	0.0520
D6	0.3360	0.0680
D7	0.4160	0.0710
D8	0.4200	0.0730
D9	0.4310	0.0690
E0	0.2840	0.0700
E1	0.4700	0.0890
E2	0.4410	0.0810
E3	0.4960	0.0820
E4	0.1810	0.0390
E5	0.4740	0.0670
E6	0.4780	0.0800
E7	0.5310	0.0850
E8	0.1180	-0.0050
E9	0.4120	0.0750
F0	0.4420	0.0840
F1	0.5000	0.0860

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Chain	Atom inclusion	Q-score
a	 0.3480	 0.1010
b	 0.2640	 0.0810
c	 0.4900	 0.1010
d	 0.3900	 0.0780
e	 0.5520	 0.0950
f	 0.4870	 0.0930
g	 0.5360	 0.0850
h	 0.5170	 0.0850
i	 0.4540	 0.0550
j	 0.4620	 0.0640
k	 0.4650	 0.0850
l	 0.4770	 0.0960
m	 0.4800	 0.0800
n	 0.5180	 0.1010
o	 0.5300	 0.0910
p	 0.5650	 0.1010
q	 0.5510	 0.0870
r	 0.5860	 0.1040
s	 0.5570	 0.0850
t	 0.6030	 0.0800
u	 0.4430	 0.0570
v	 0.5680	 0.0740
w	 0.1920	 0.0270
x	 0.2870	 0.0190