



wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 06:36 AM EDT

PDB ID : 7TNS
EMDB ID : EMD-26019
Title : Subpellicular microtubule from detergent-extract *Toxoplasma gondii* cells
Authors : Sun, S.Y.; Pintilie, G.D.; Chen, M.; Chiu, W.
Deposited on : 2022-01-21
Resolution : 6.70 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

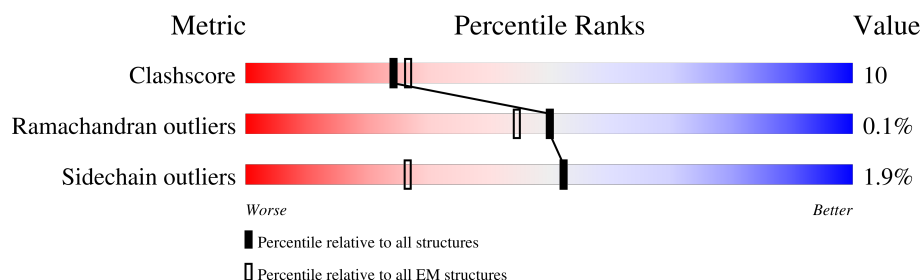
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 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	 5% • 94%
1	1	351	 5% • 94%
1	10	351	 • • 94%
1	11	351	 • • 94%
1	12	351	 5% • 94%
1	13	351	 5% • 94%
1	14	351	 5% 6% 94%
1	15	351	 5% • 94%

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Mol	Chain	Length	Quality of chain
1	16	351	 5% 5% 94%
1	17	351	 5% 5% 94%
1	18	351	 6% 6% 94%
1	19	351	 6% 6% 94%
1	2	351	 5% 5% 94%
1	20	351	 6% 6% 94%
1	21	351	 5% 5% 94%
1	22	351	 5% 5% 94%
1	23	351	 5% 5% 94%
1	3	351	 5% 5% 94%
1	4	351	 5% 5% 94%
1	5	351	 6% 6% 94%
1	6	351	 5% 5% 94%
1	7	351	 5% 5% 94%
1	8	351	 5% 5% 94%
1	9	351	 5% 5% 94%
2	A0	453	 31% 70% 23% 6%
2	A2	453	 30% 73% 20% 6%
2	A4	453	 29% 76% 17% 6%
2	A6	453	 29% 74% 19% 6%
2	A8	453	 28% 73% 21% 6%
2	B0	453	 28% 73% 20% 6%
2	B2	453	 30% 77% 17% 6%
2	B4	453	 29% 71% 23% 6%
2	B6	453	 28% 77% 17% 6%

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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	k	220	
4	l	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	
4	x	220	
4	y	220	
5	w	189	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 216148 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	C	N	O	S	0	0
			174	114	28	31	1		
1	4	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	5	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	6	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	7	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	8	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	9	22	Total	C	N	O	S	0	0
			174	114	28	31	1		

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

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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

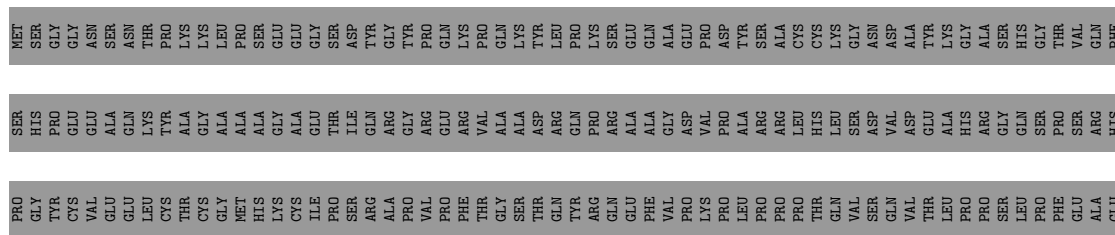
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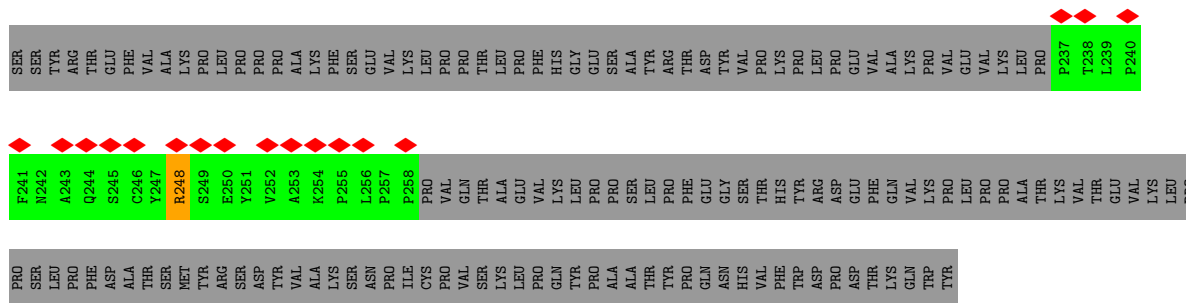
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	h	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	i	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	j	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	k	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4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

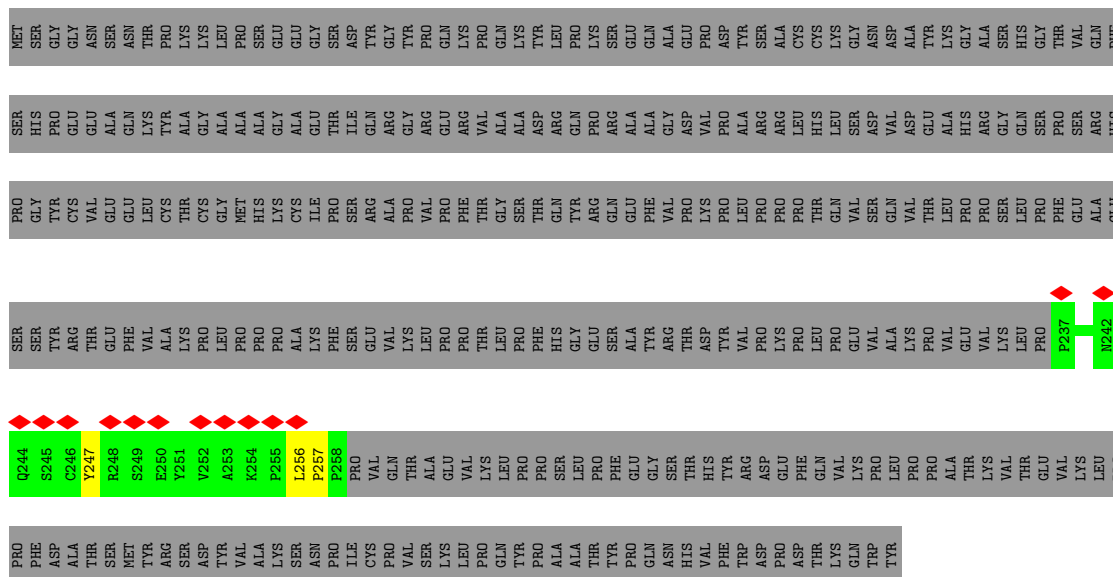
- Molecule 5 is a protein called PDI family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	w	143	Total	C	N	O	S	0	0
			1172	755	207	205	5		

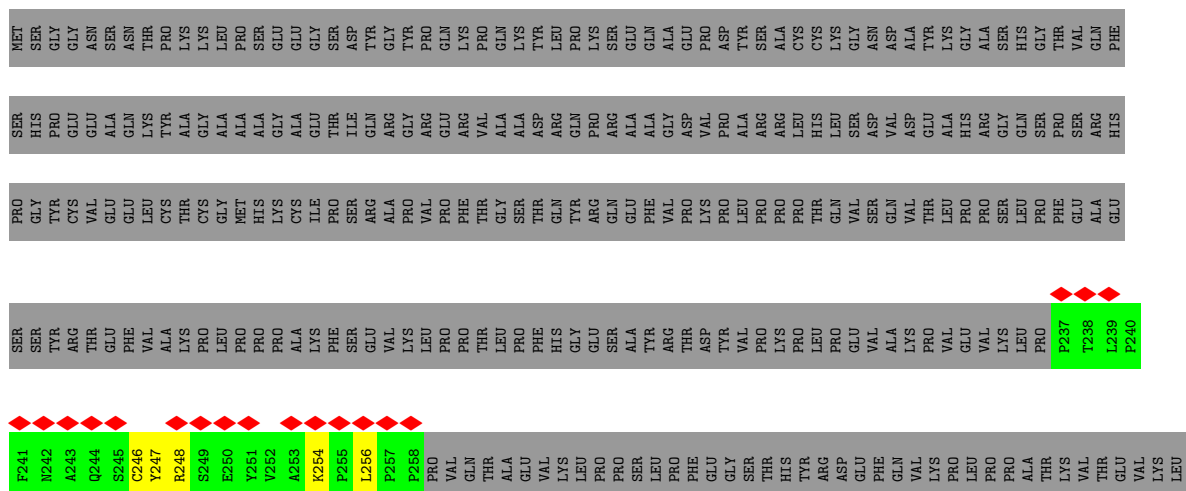


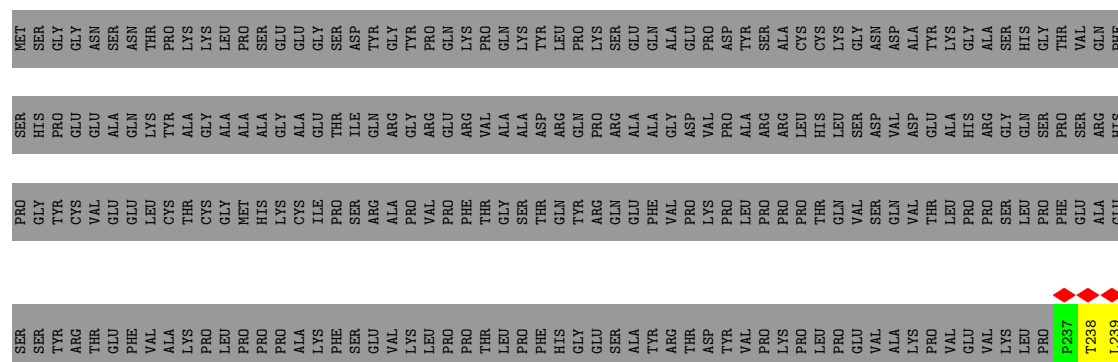


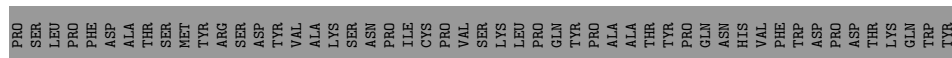
- Molecule 1: Microtubule associated protein SPM1

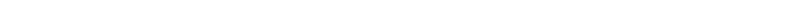


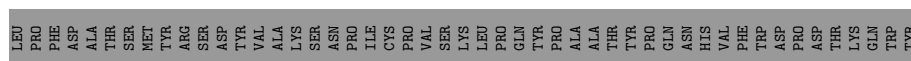
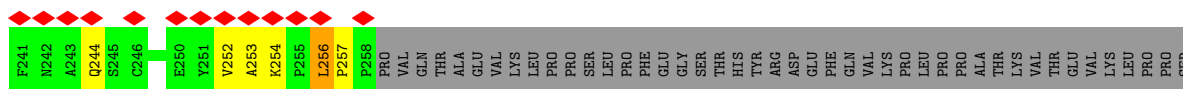
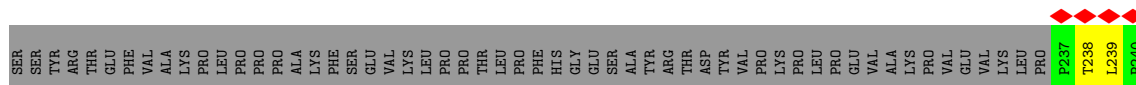
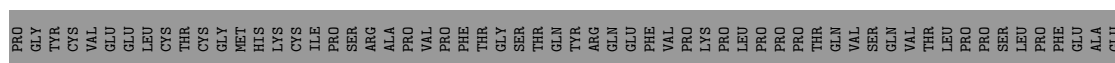
- Molecule 1: Microtubule associated protein SPM1

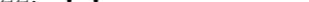


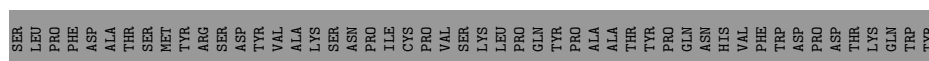
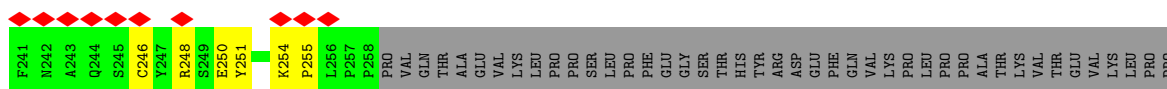
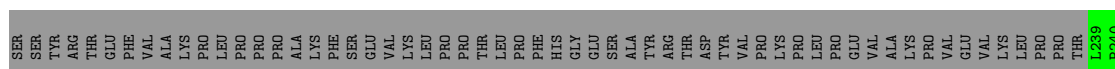
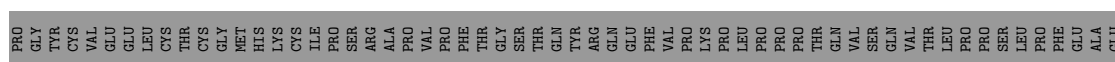
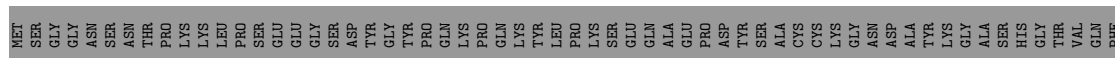




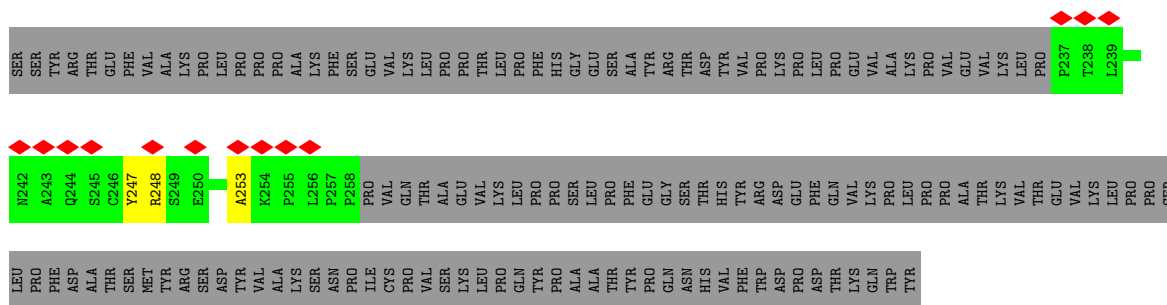
Chain 21: 



Chain 22:  94%



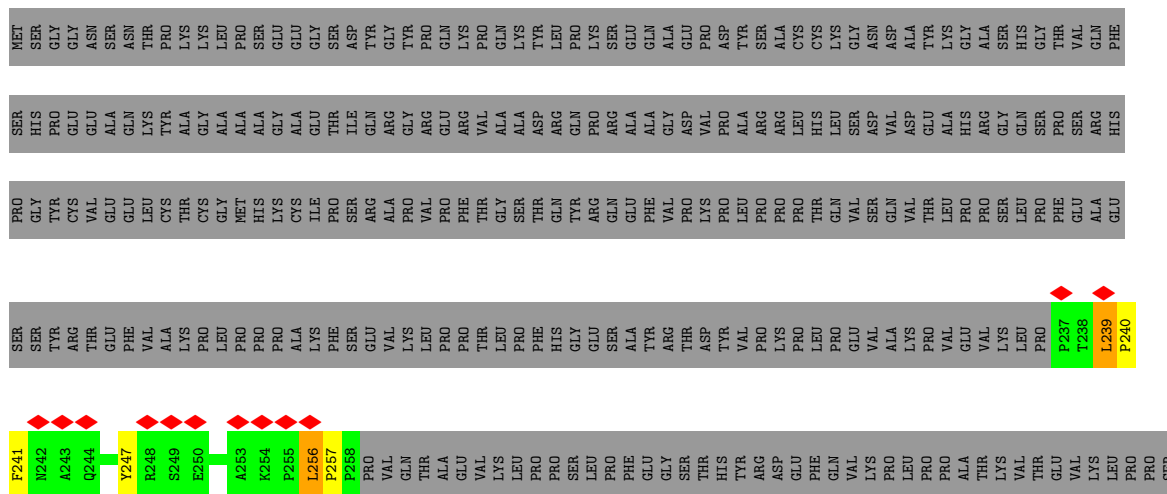
Chain 23: 94%



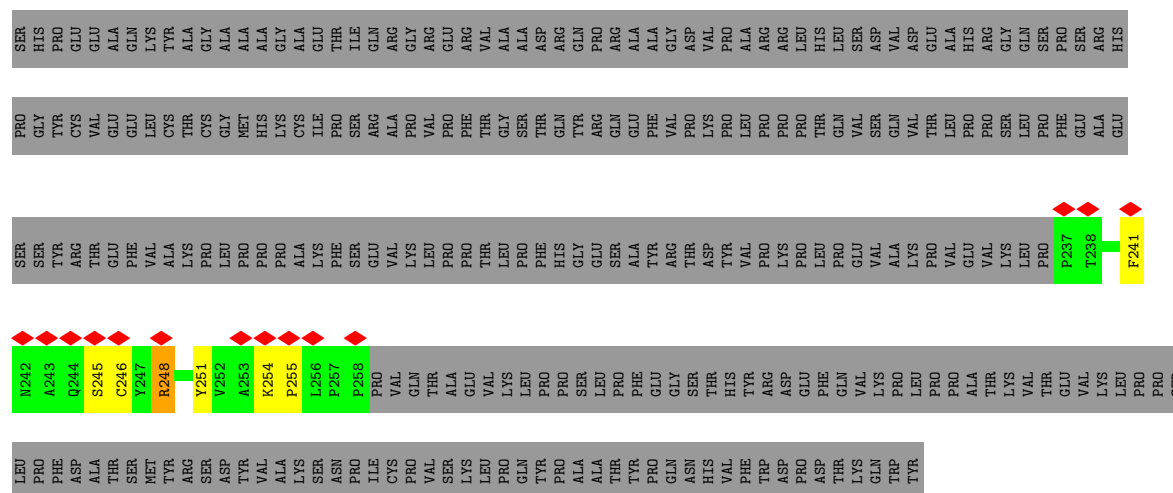
- Molecule 1: Microtubule associated protein SPM1



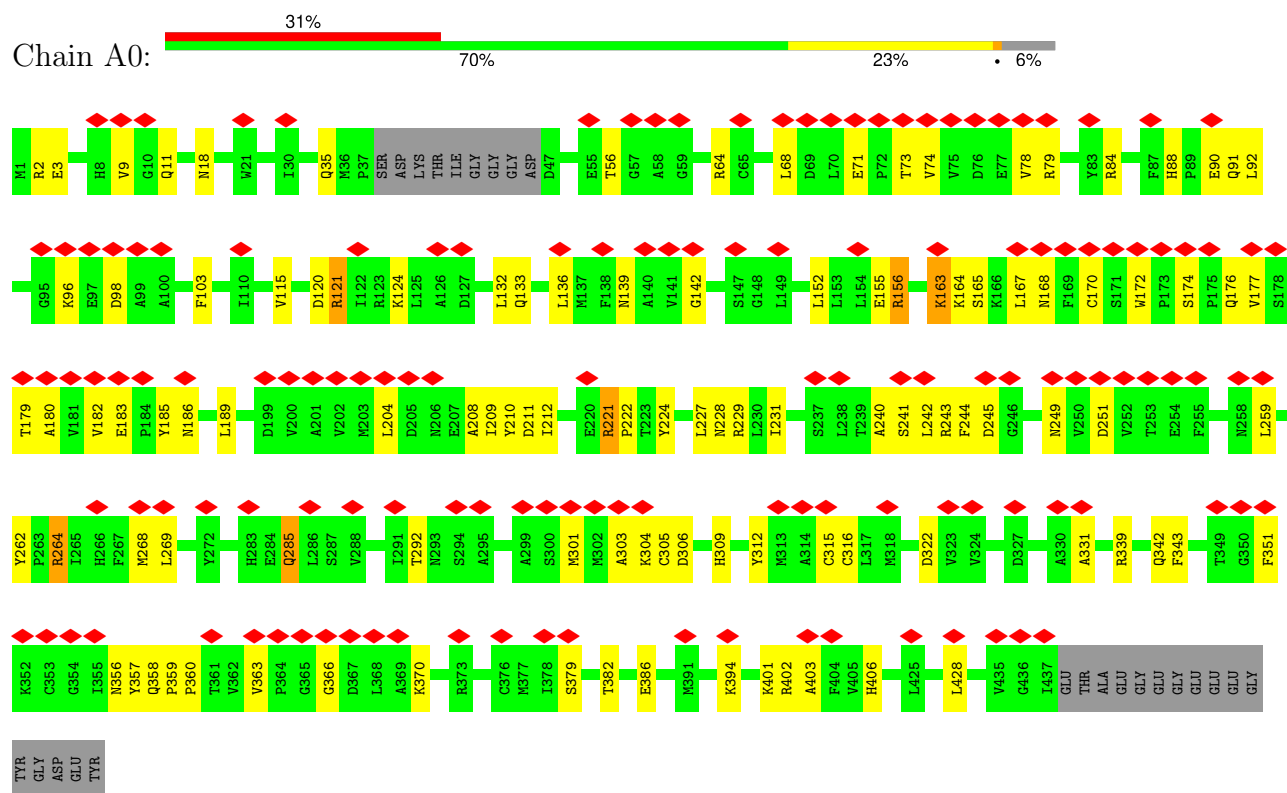
- Molecule 1: Microtubule associated protein SPM1



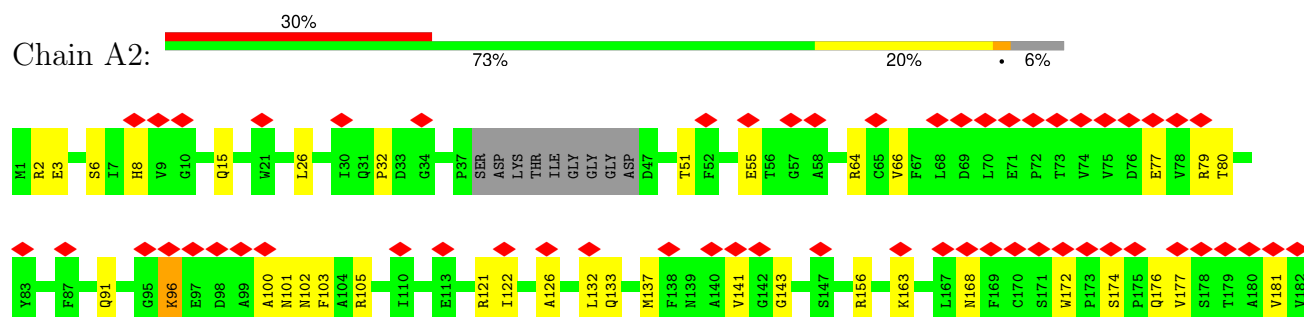
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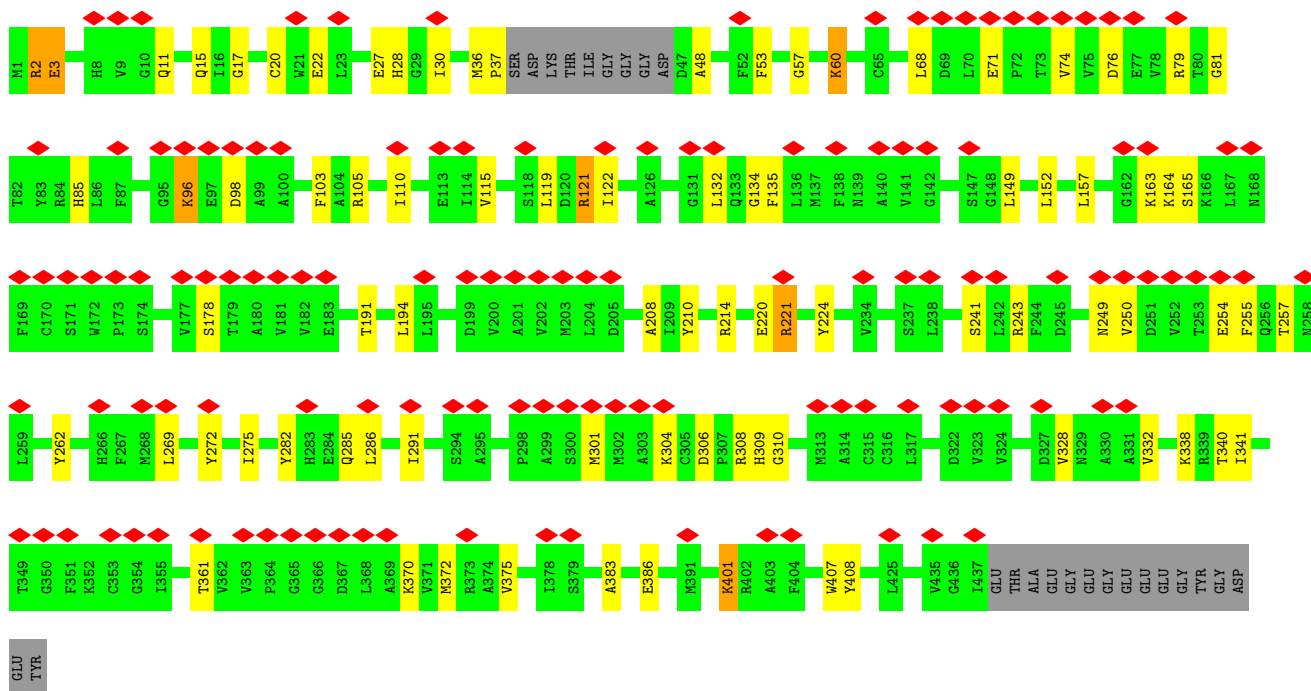
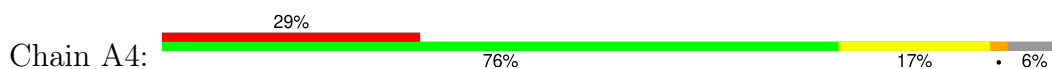
• Molecule 2: Tubulin alpha chain



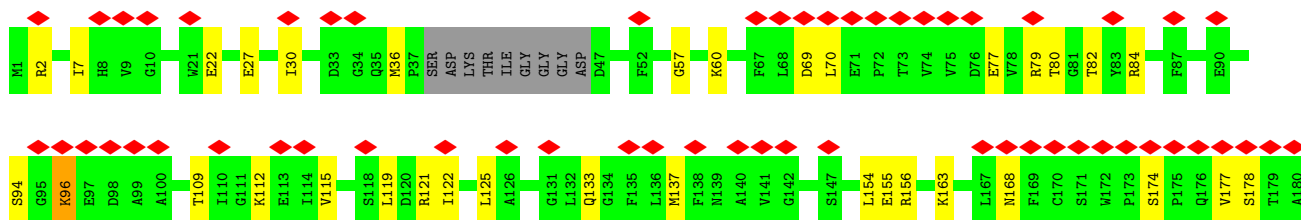
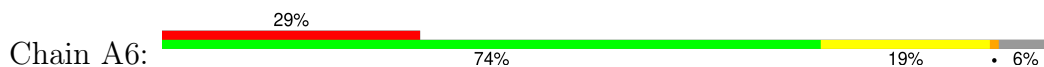
• Molecule 2: Tubulin alpha chain

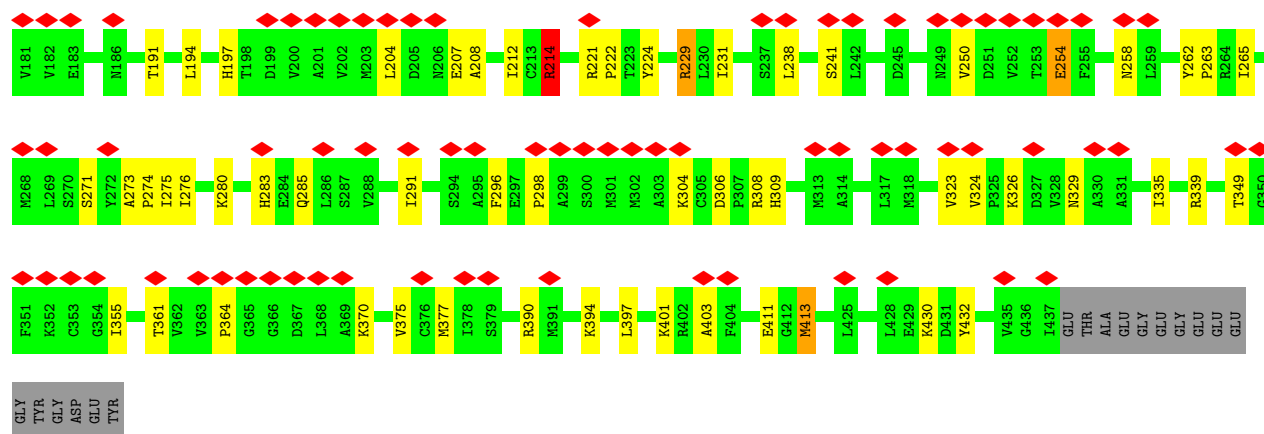


- Molecule 2: Tubulin alpha chain

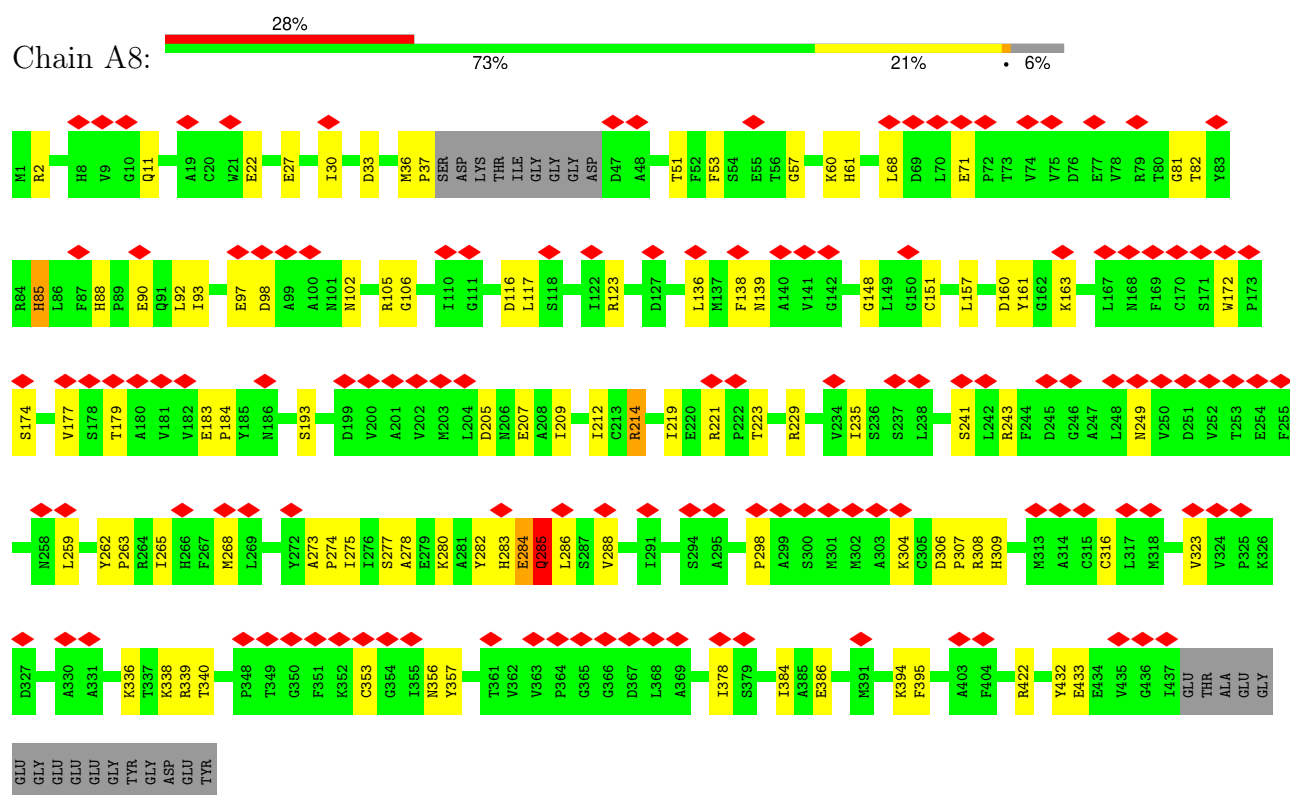


- Molecule 2: Tubulin alpha chain

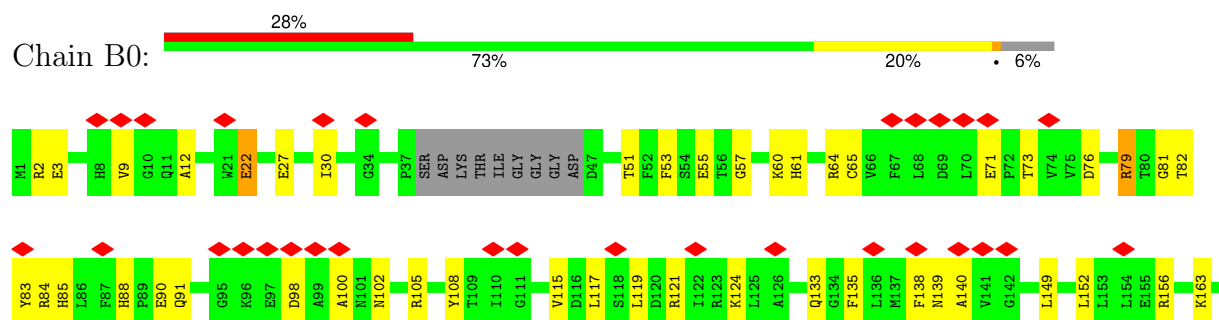


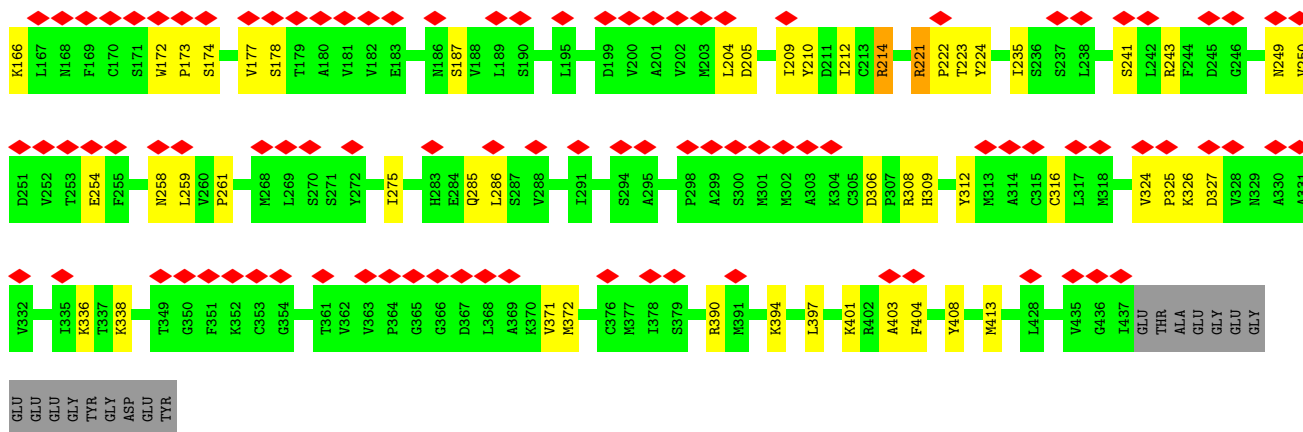


• Molecule 2: Tubulin alpha chain

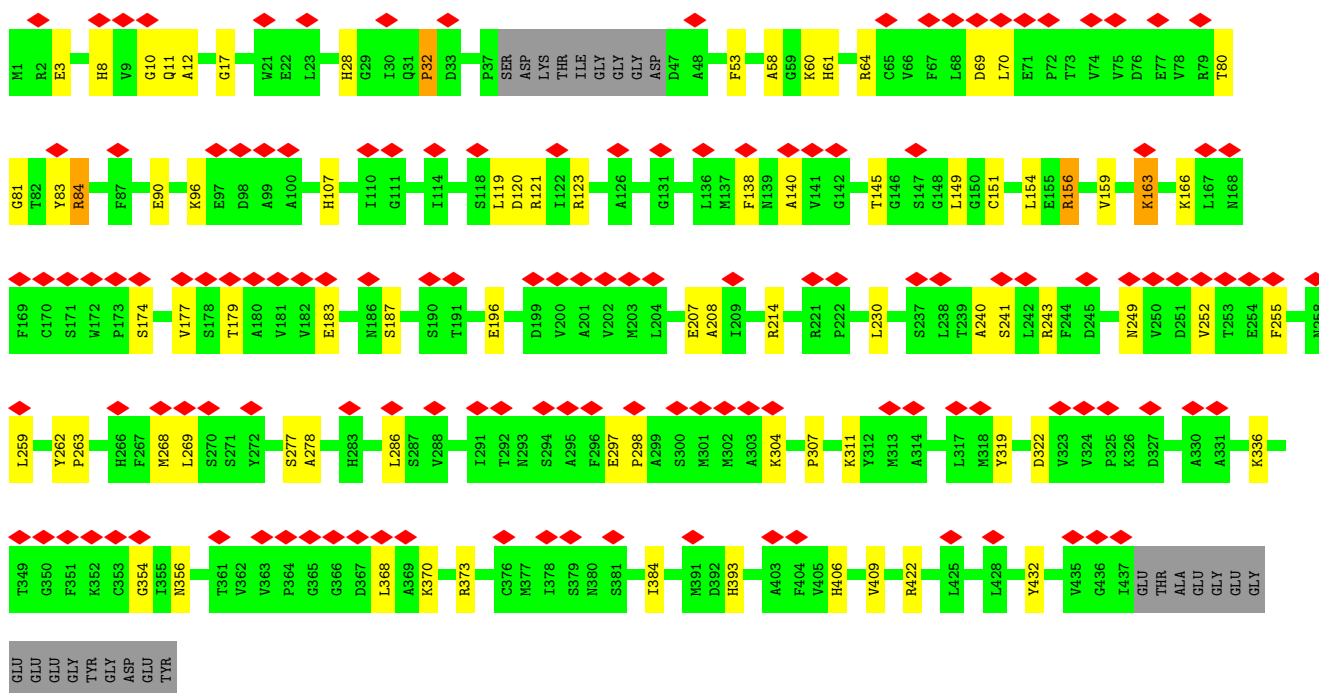
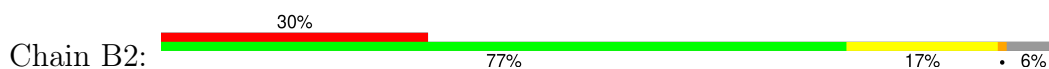


• Molecule 2: Tubulin alpha chain

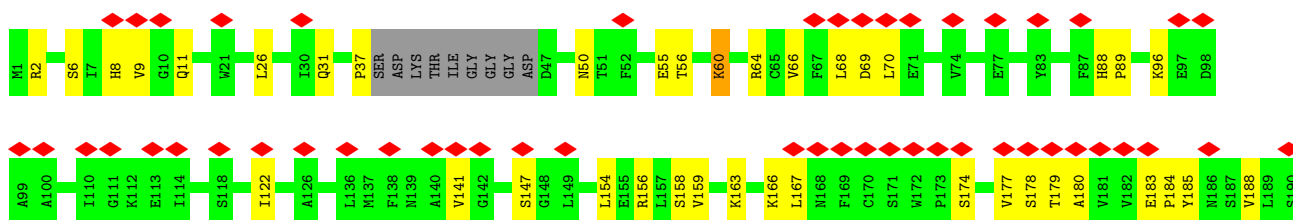


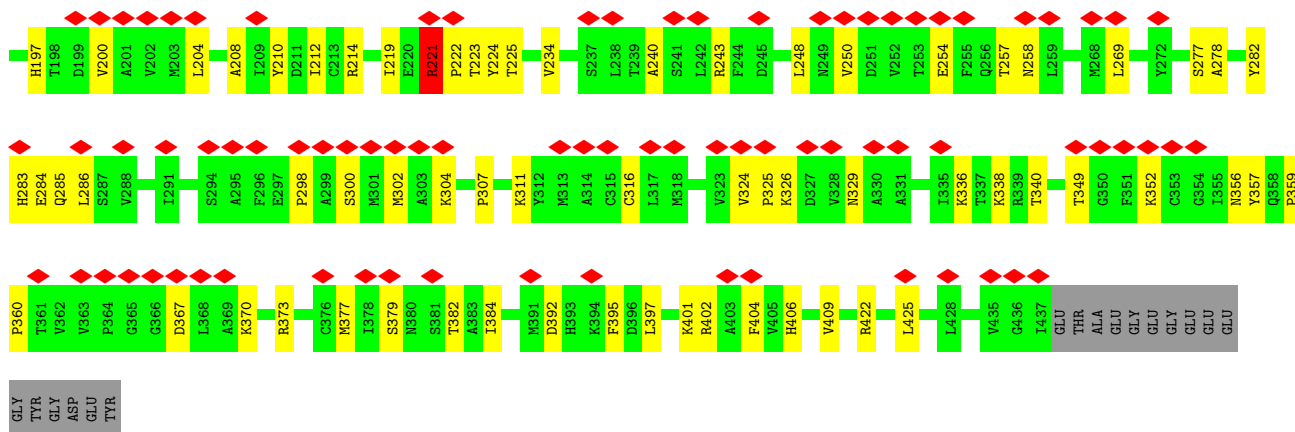


• Molecule 2: Tubulin alpha chain

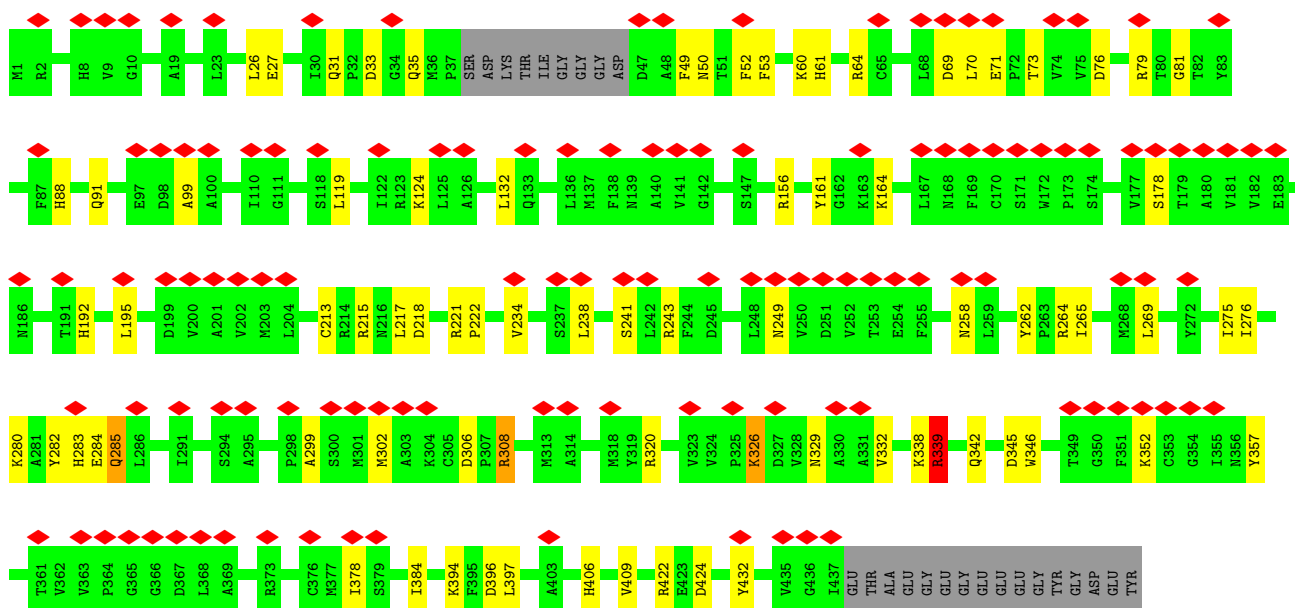
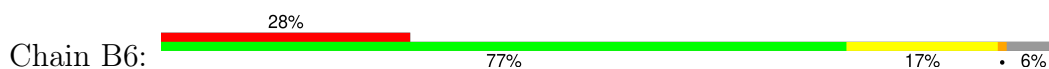


• Molecule 2: Tubulin alpha chain

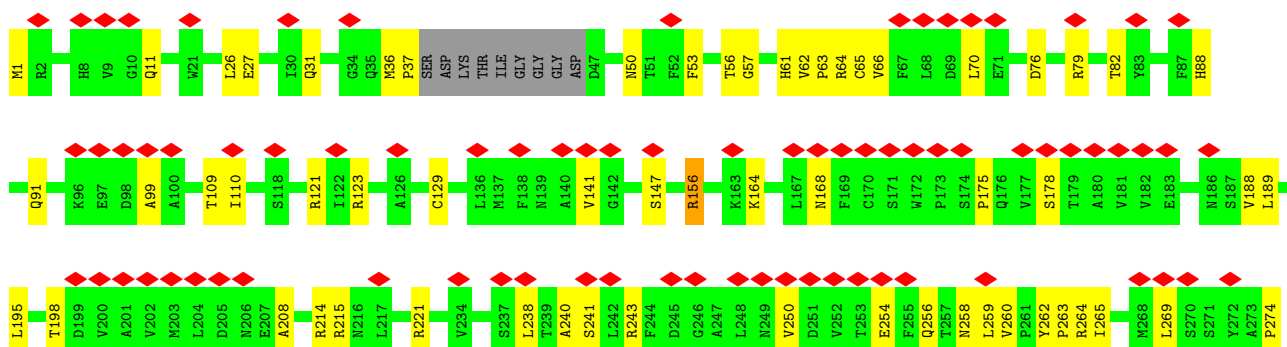
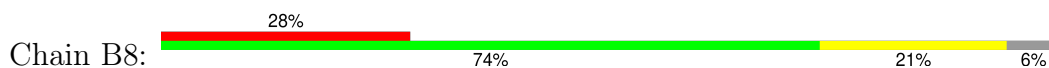


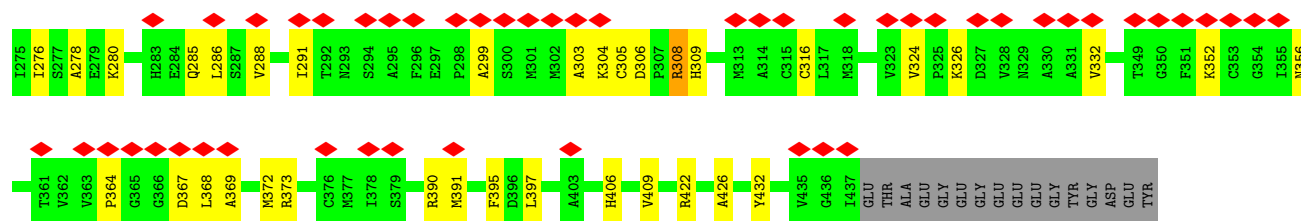


• Molecule 2: Tubulin alpha chain

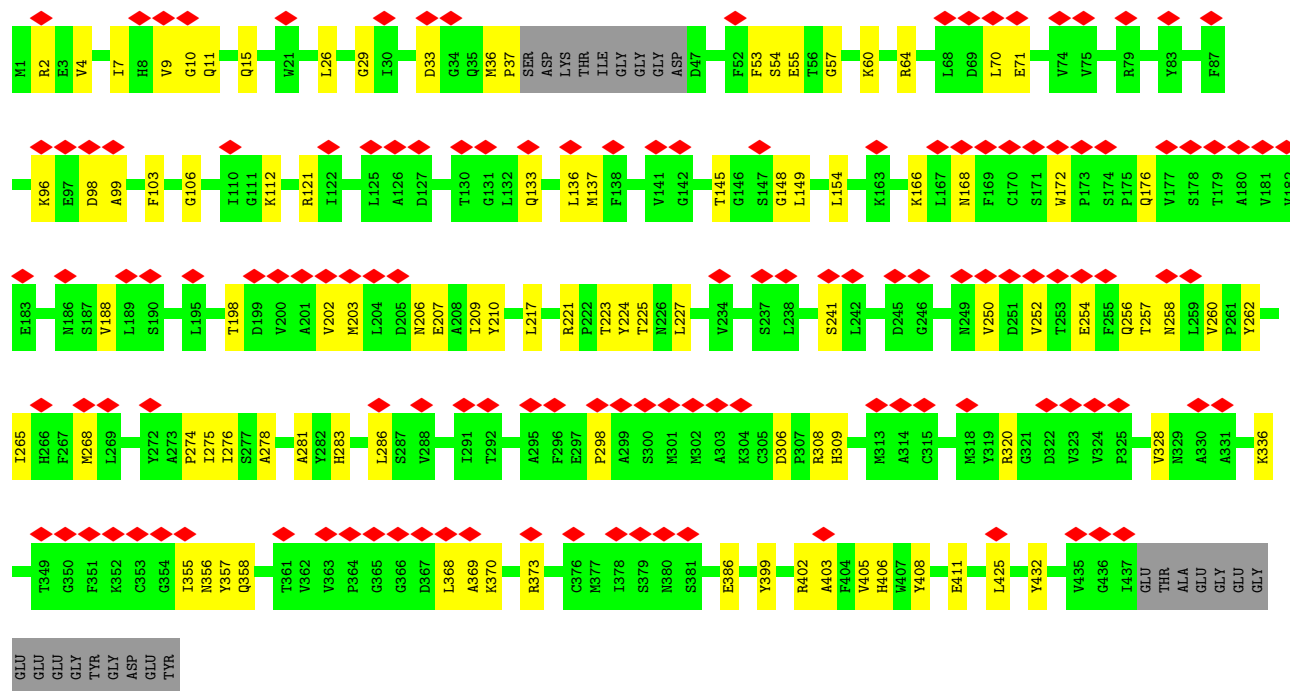
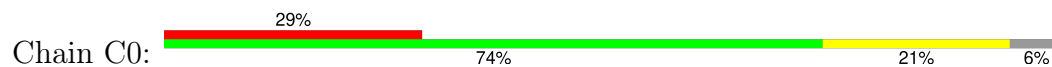


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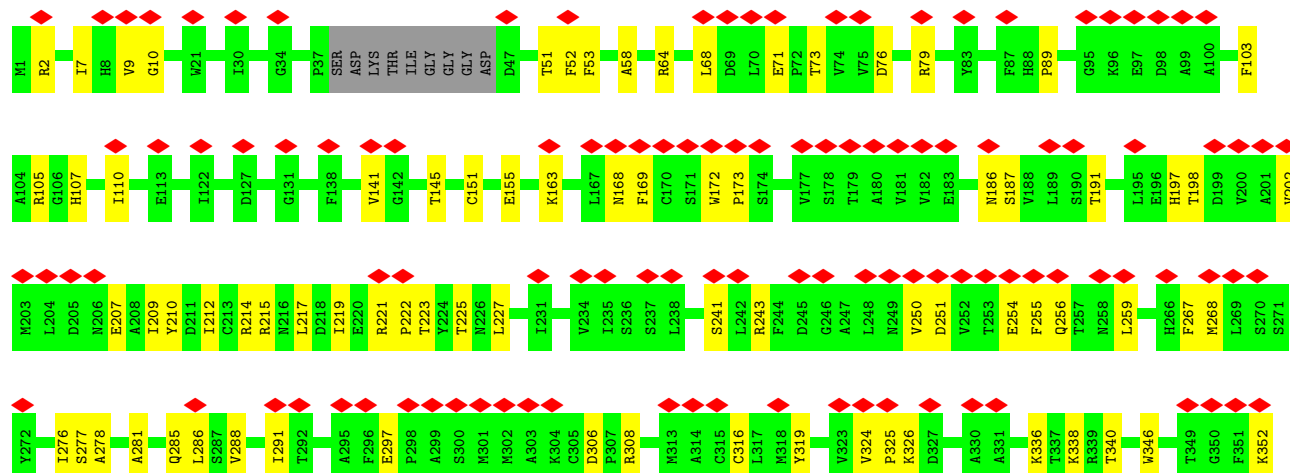
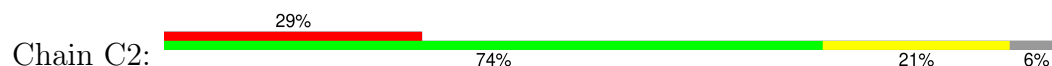


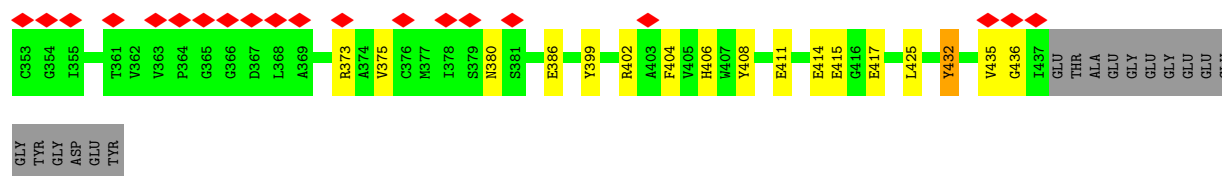


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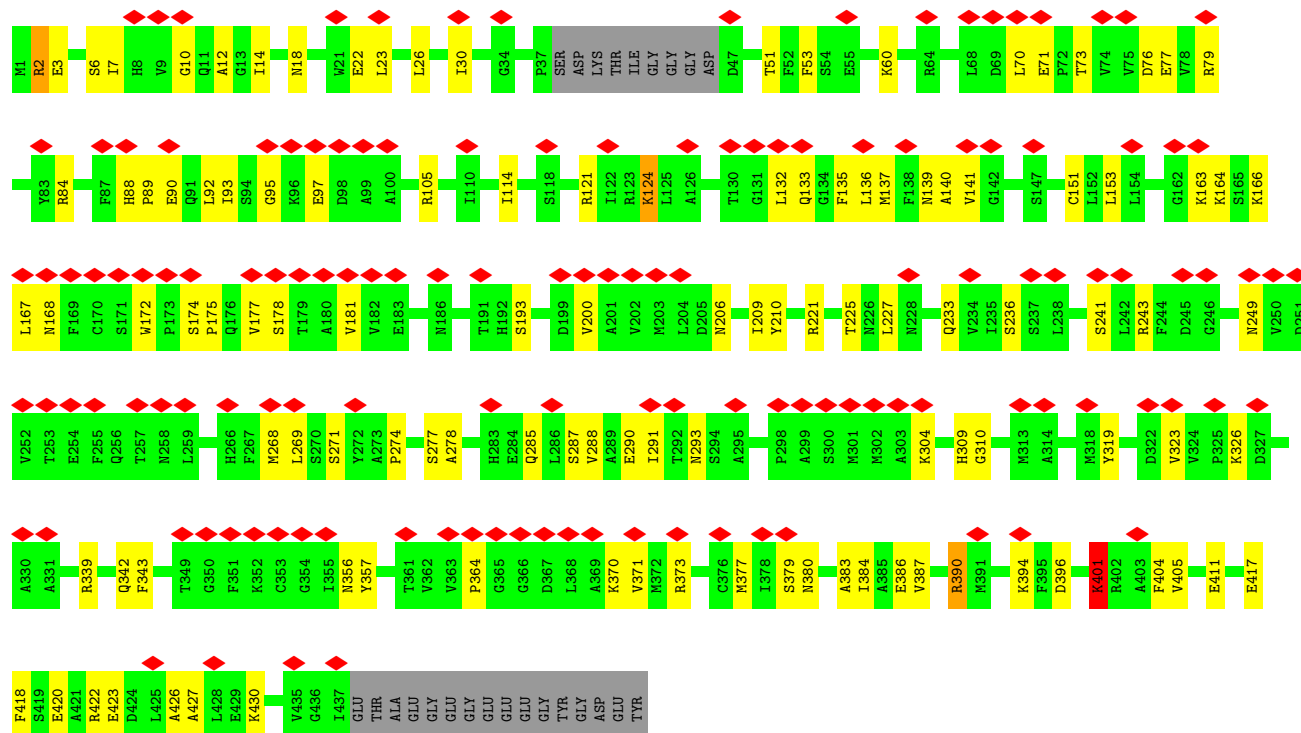


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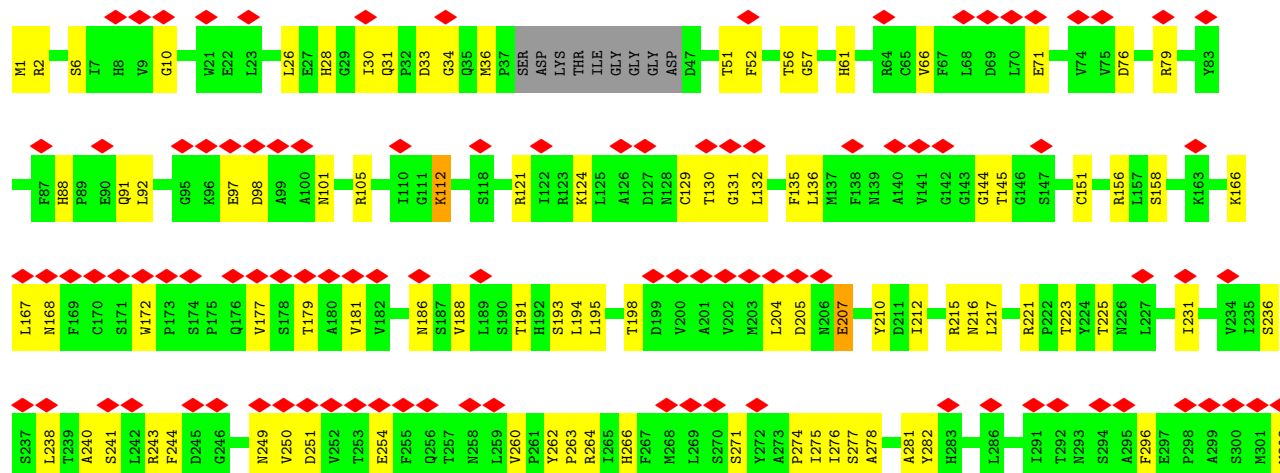


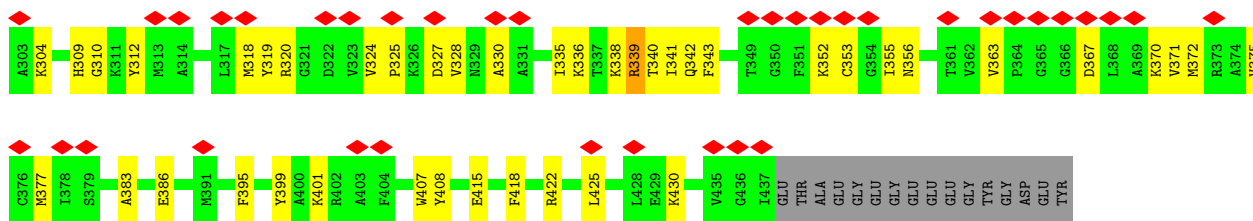


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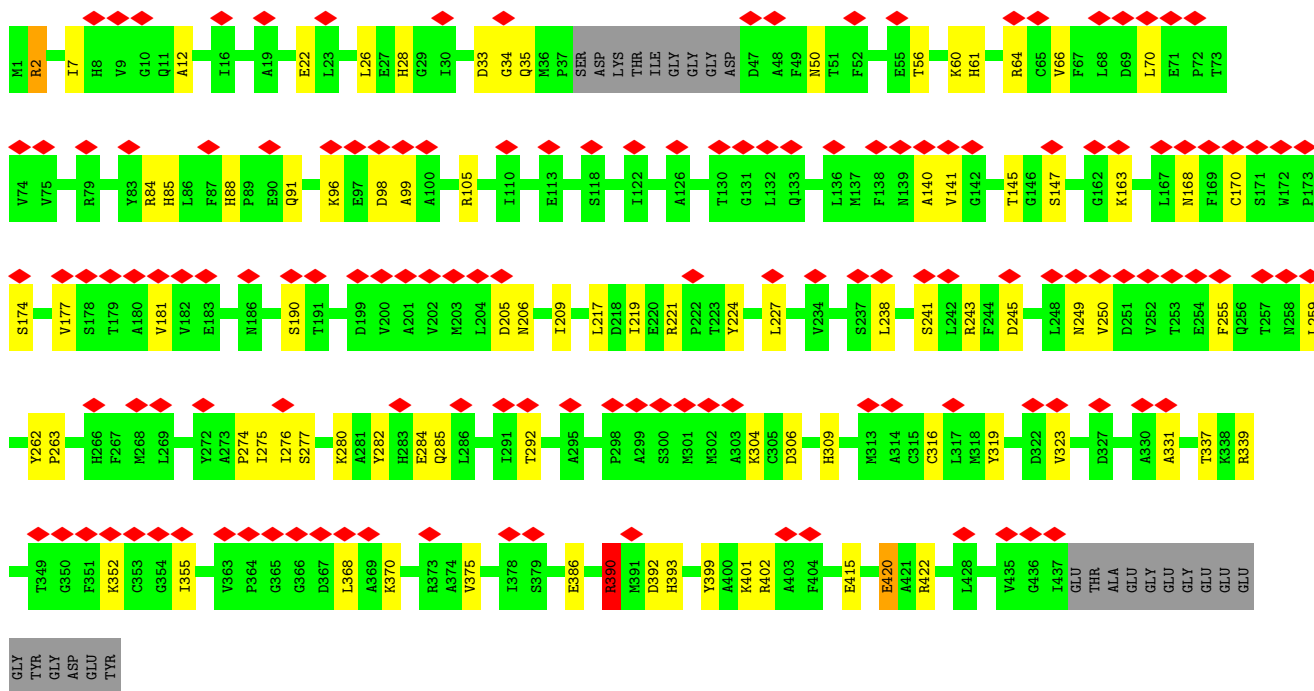
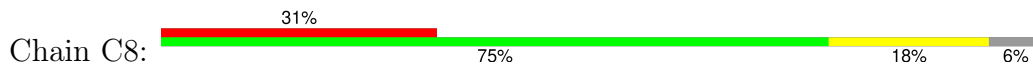


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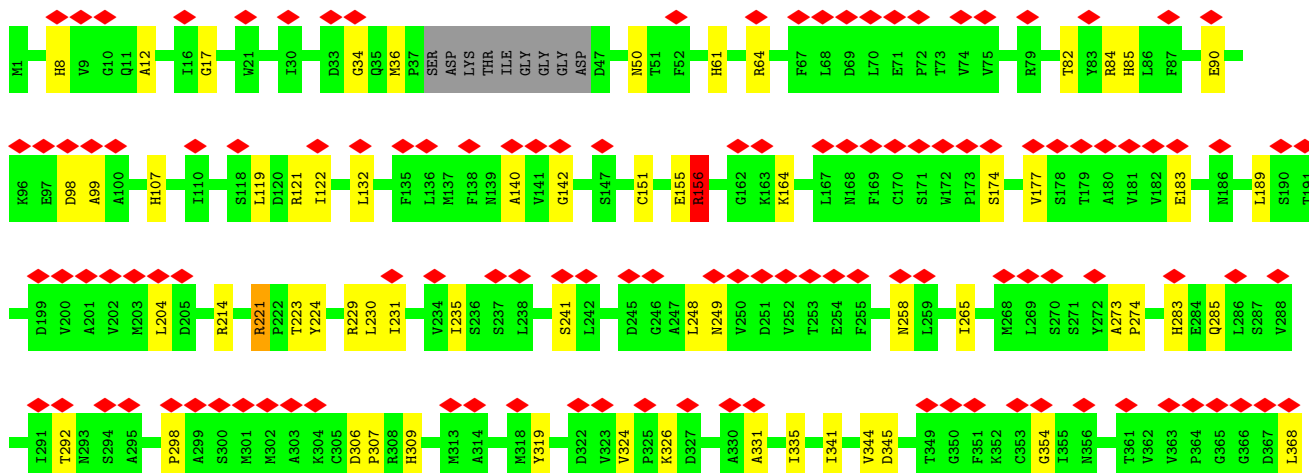
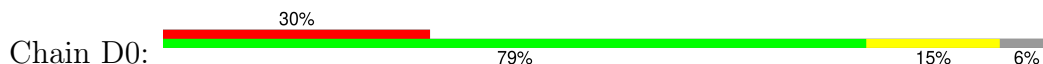


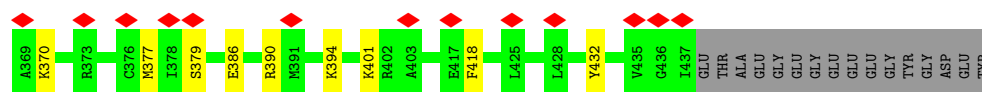


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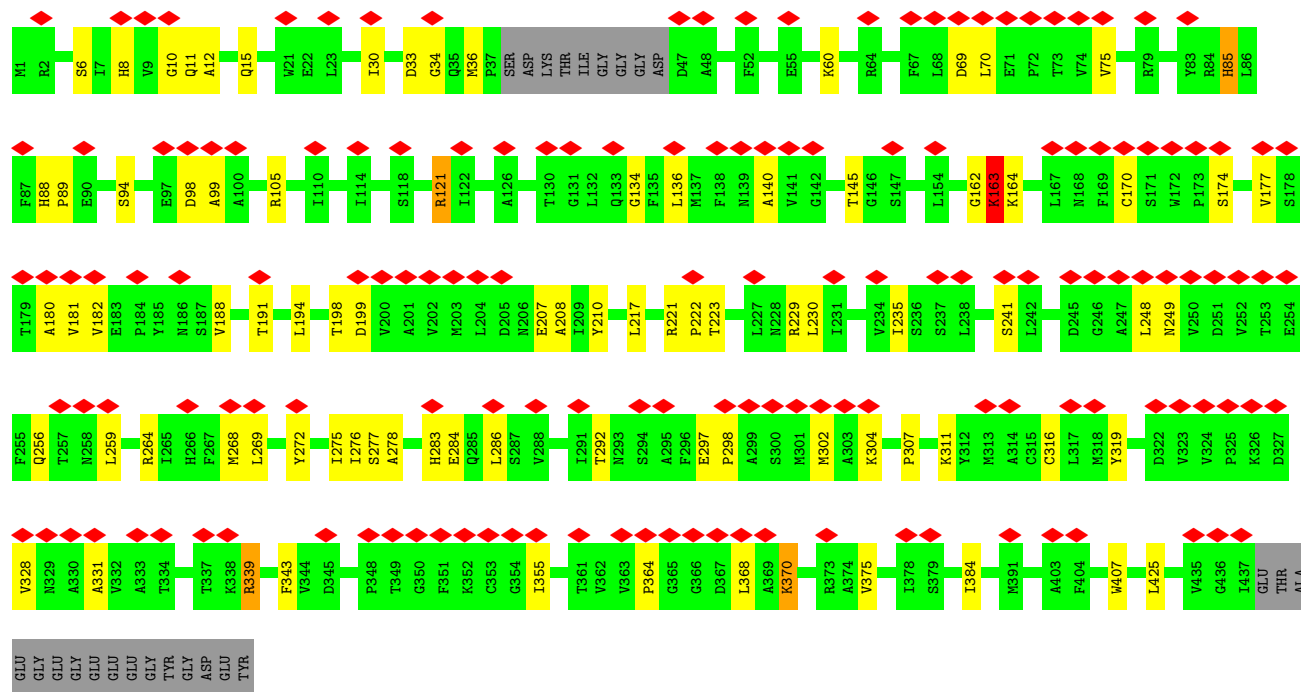
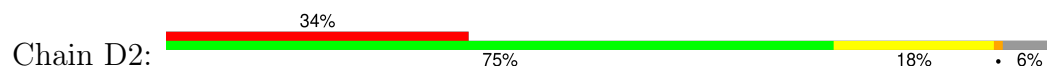


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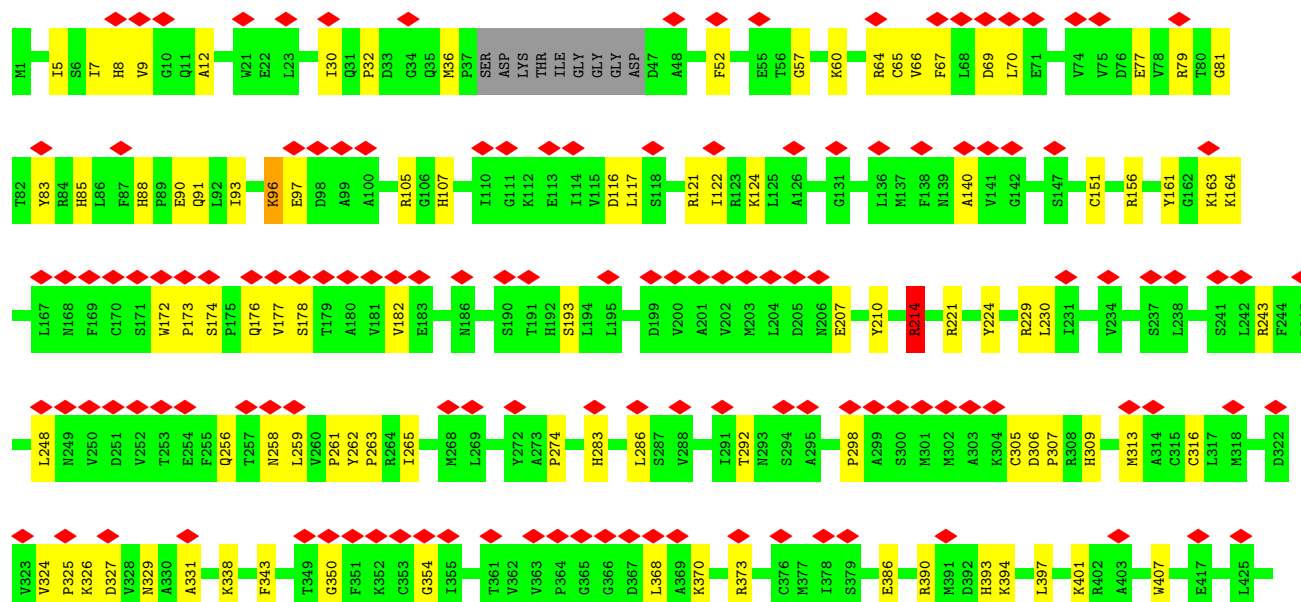
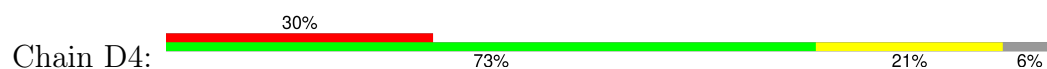


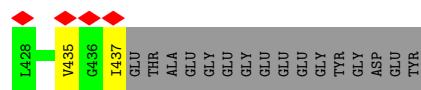


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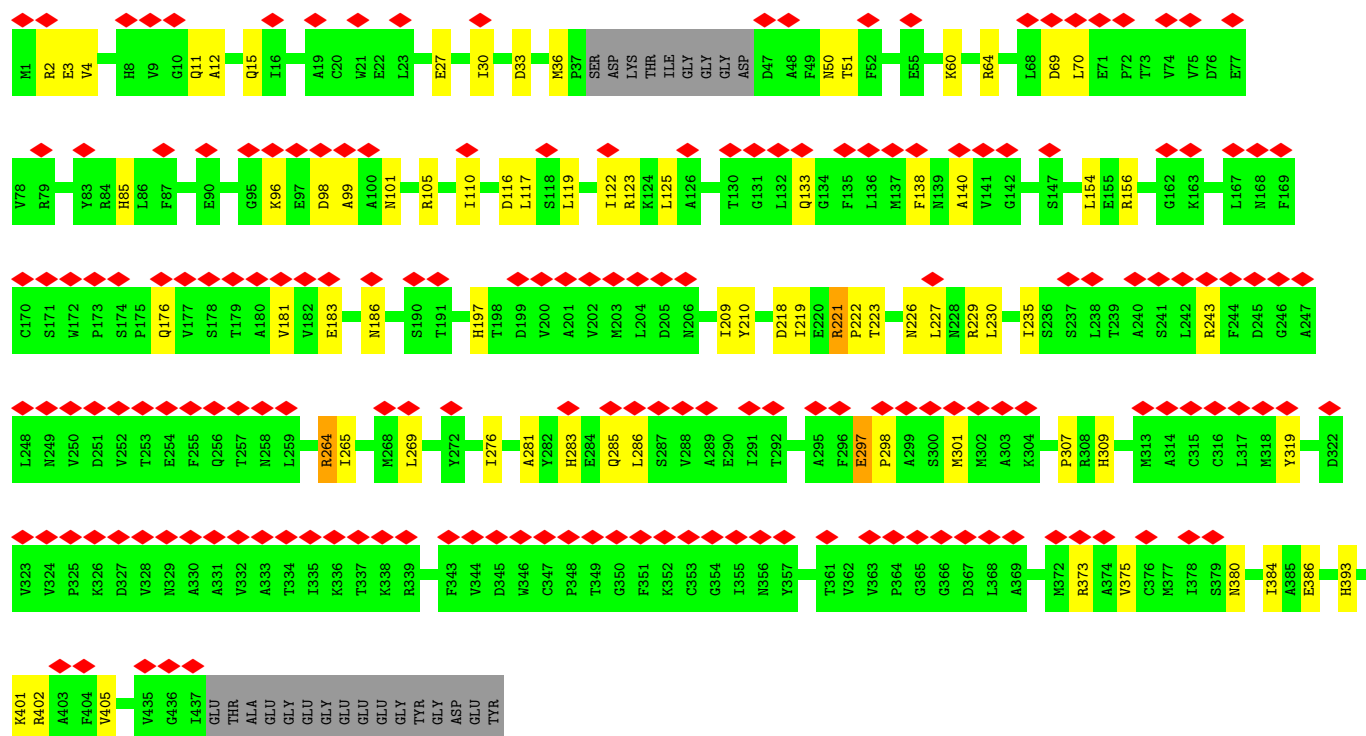
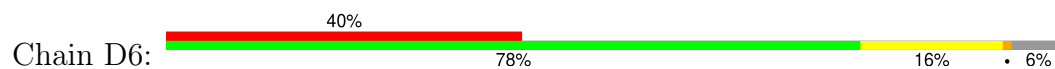


• Molecule 2: Tubulin alpha chain

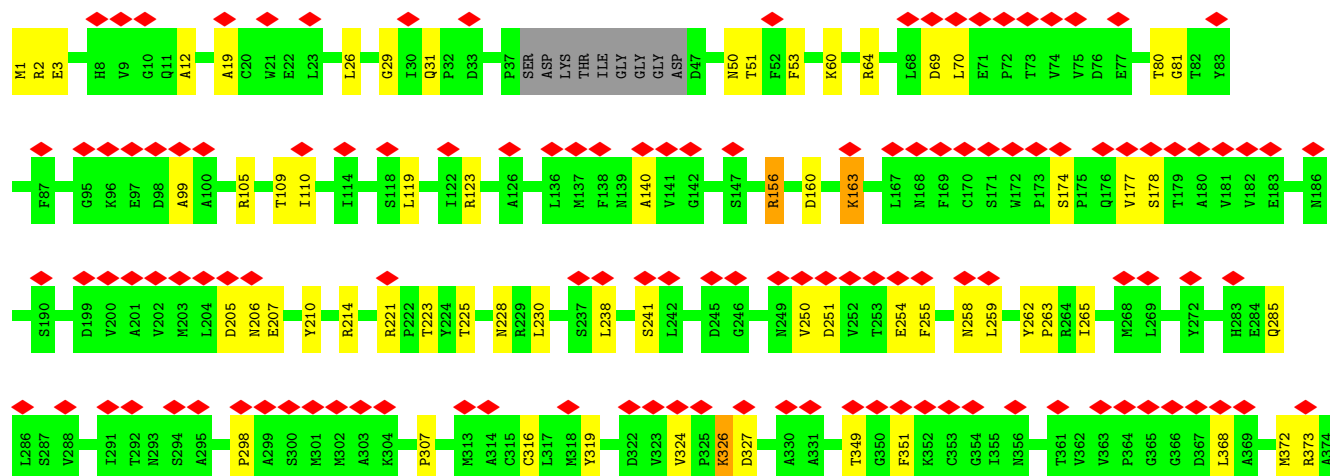
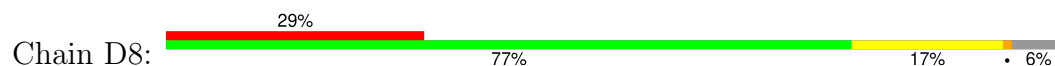




• Molecule 2: Tubulin alpha chain

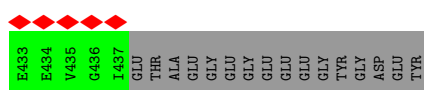
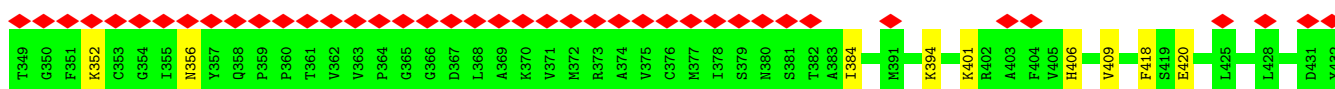
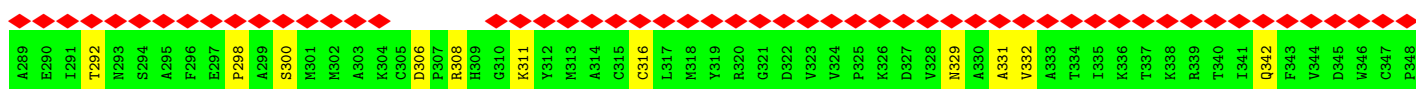
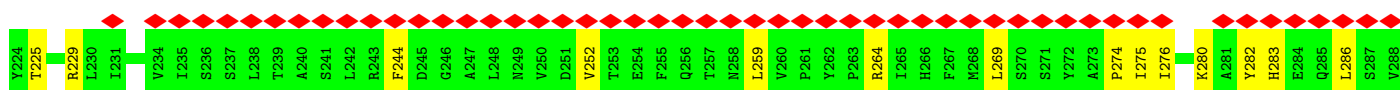
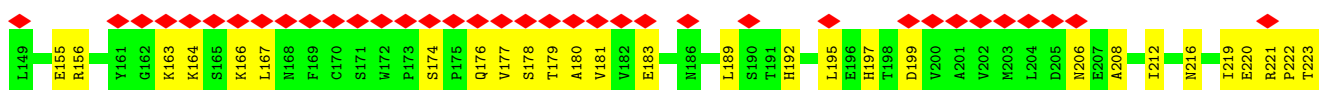
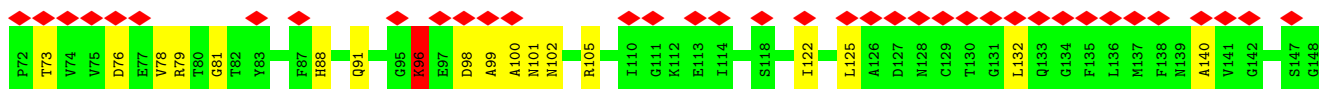
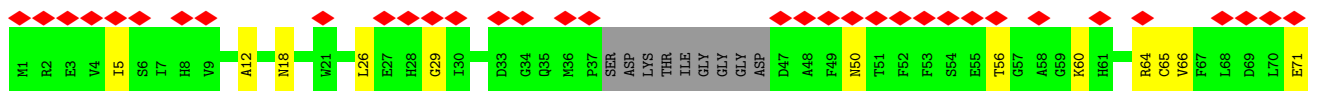
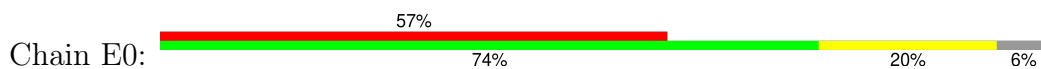


• Molecule 2: Tubulin alpha chain

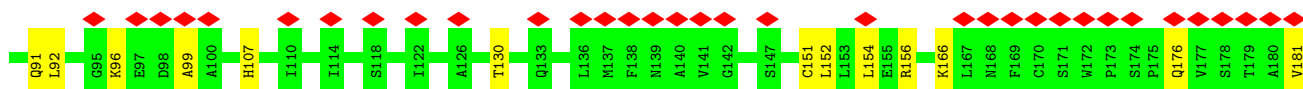
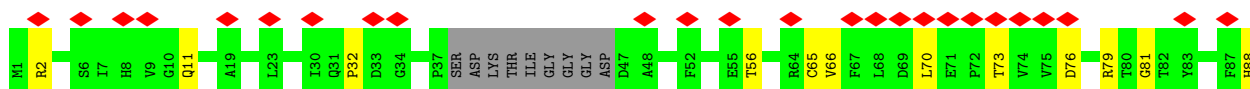
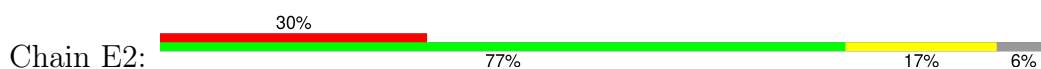


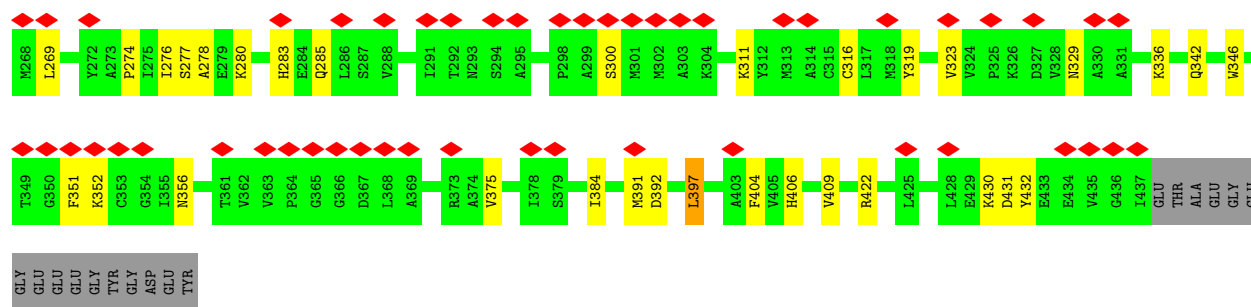


• Molecule 2: Tubulin alpha chain

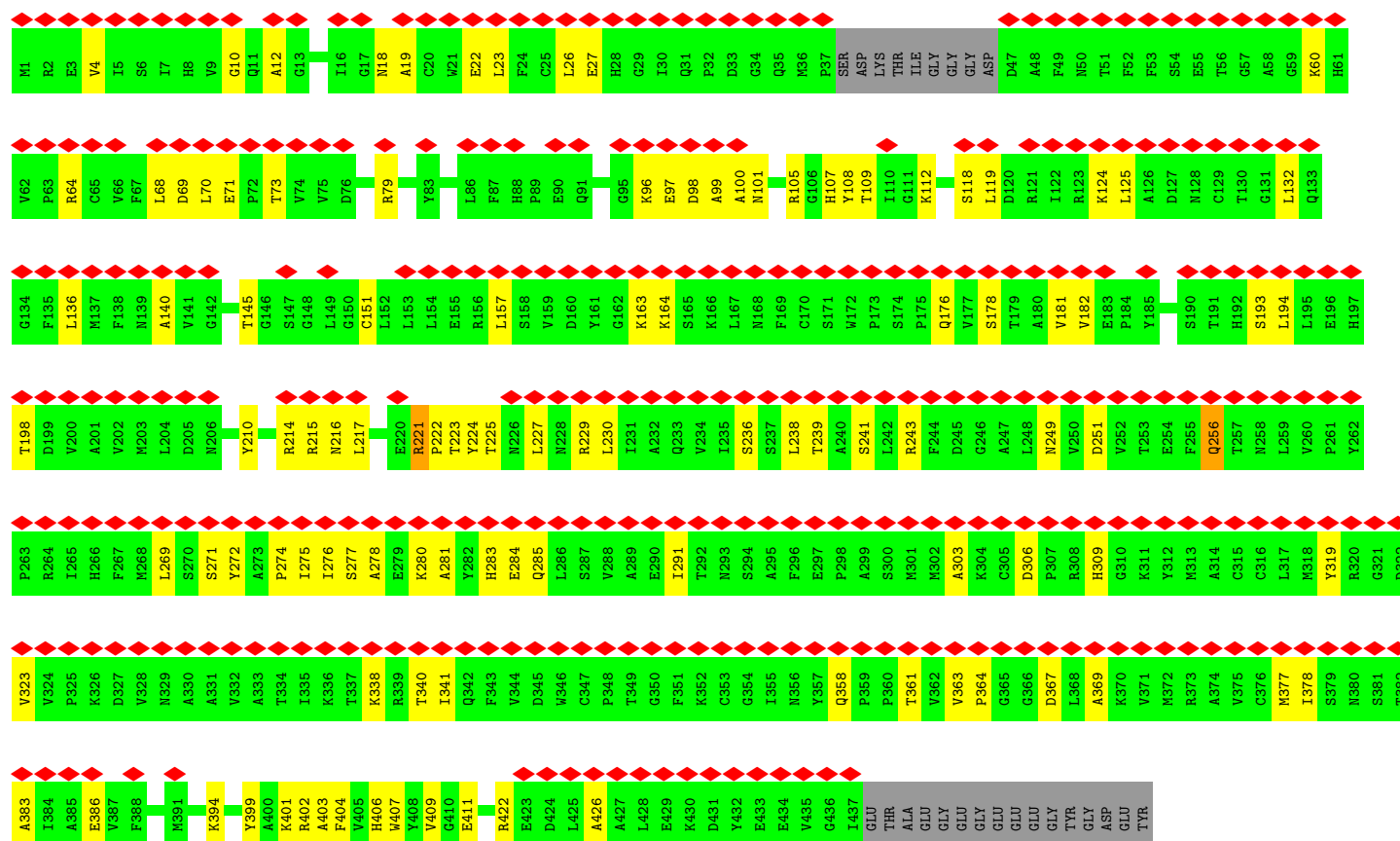
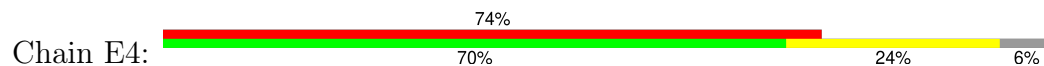


• Molecule 2: Tubulin alpha chain

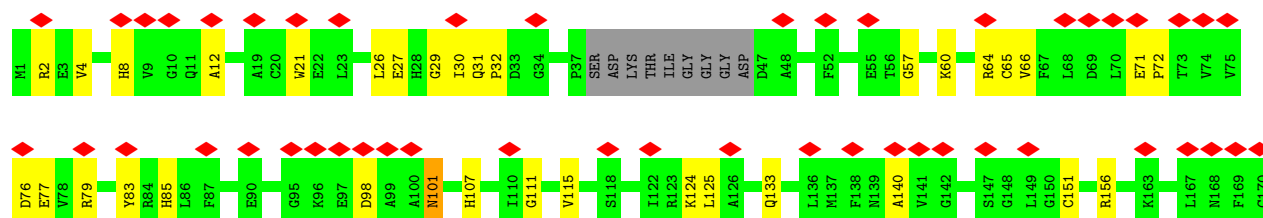
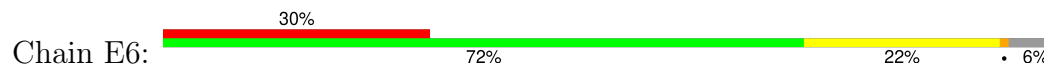


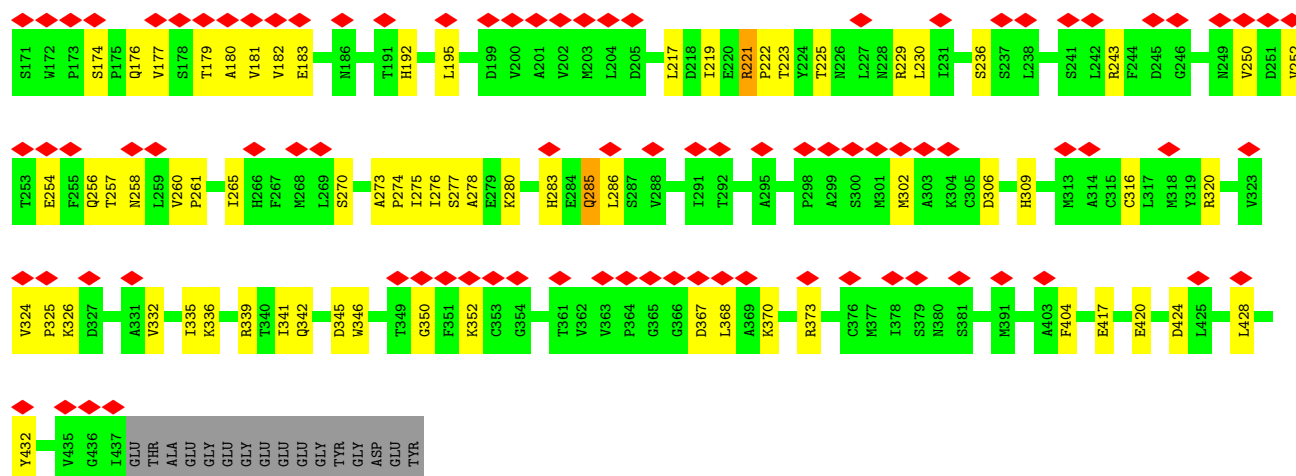


• Molecule 2: Tubulin alpha chain

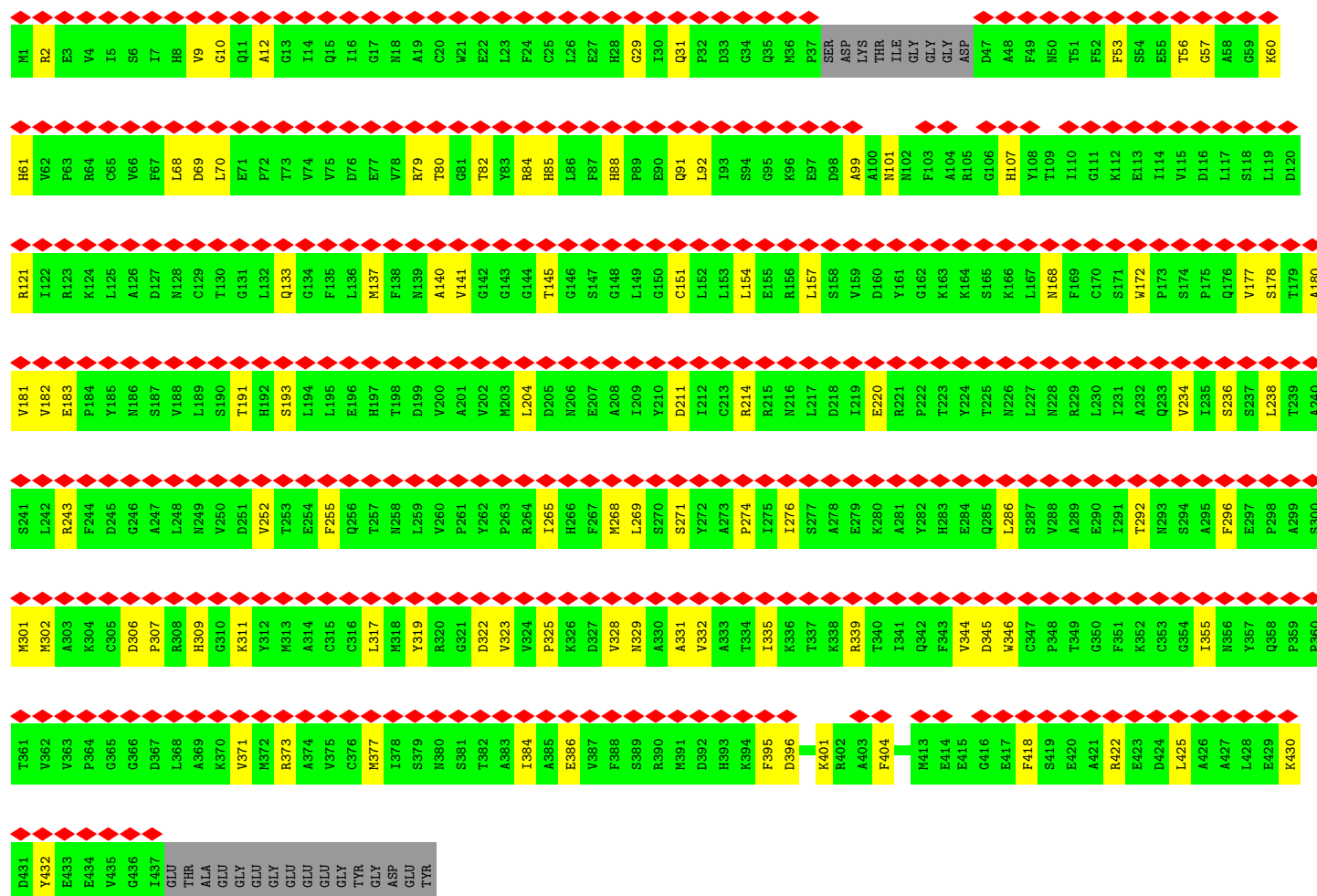
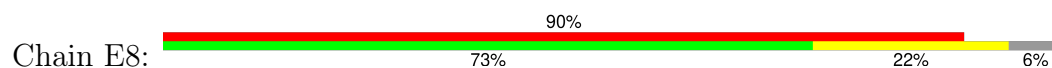


• Molecule 2: Tubulin alpha chain



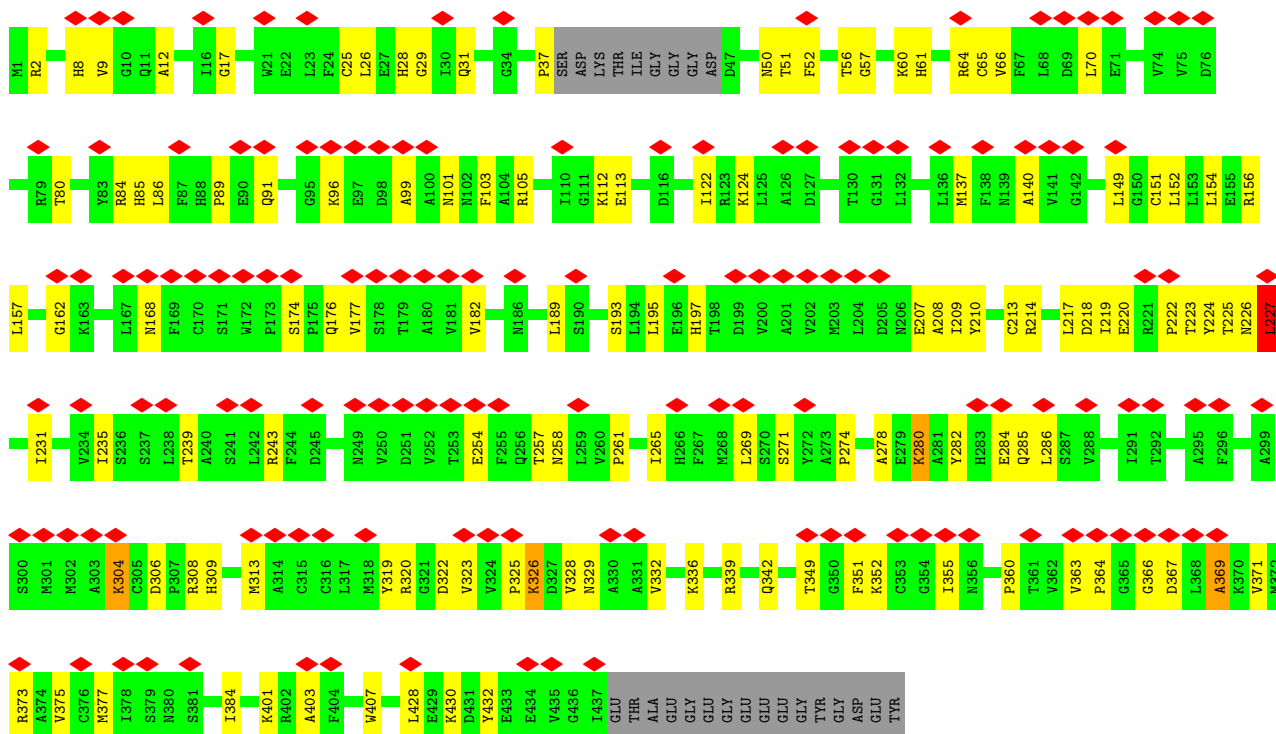


• Molecule 2: Tubulin alpha chain

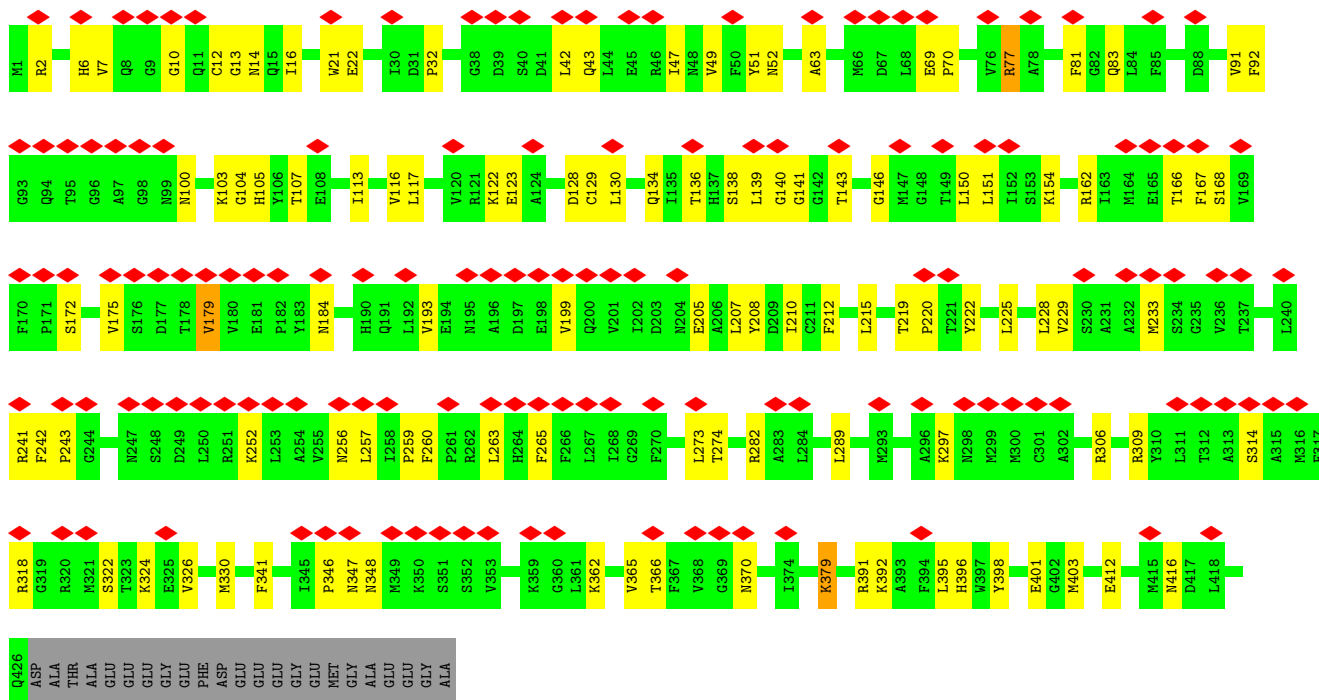


• Molecule 2: Tubulin alpha chain

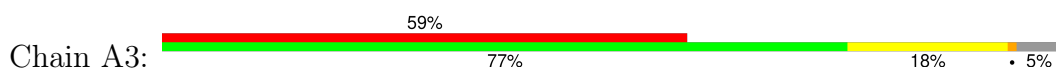




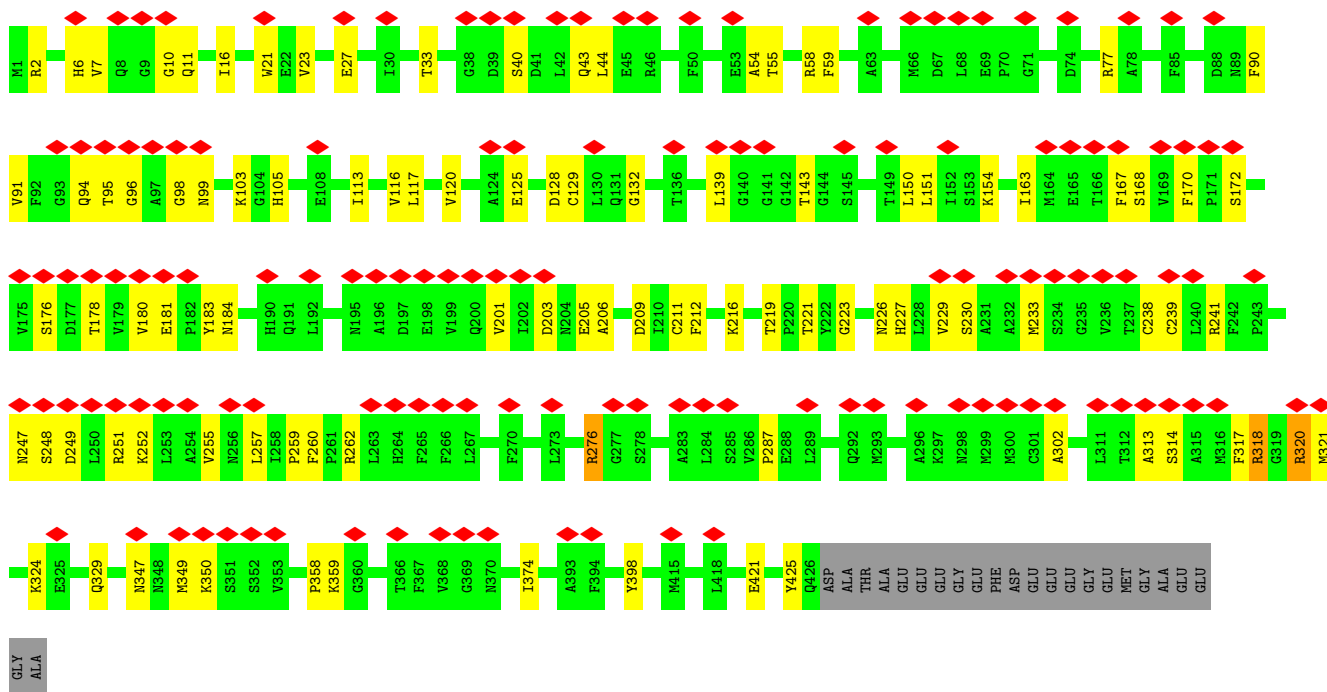
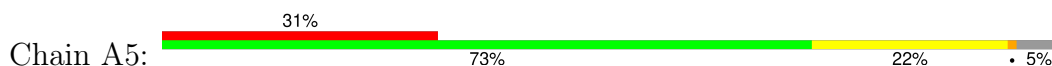
• Molecule 3: Tubulin beta chain




• Molecule 3: Tubulin beta chain

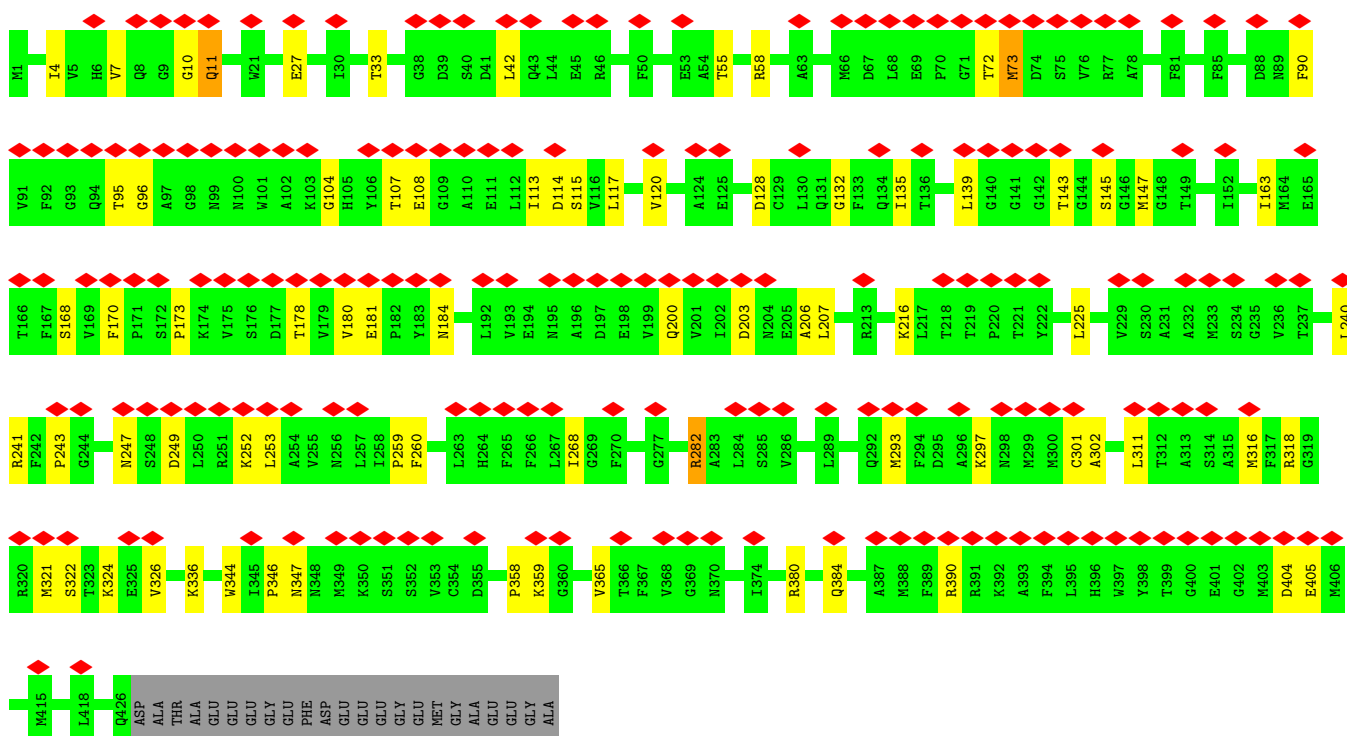


- Molecule 3: Tubulin beta chain




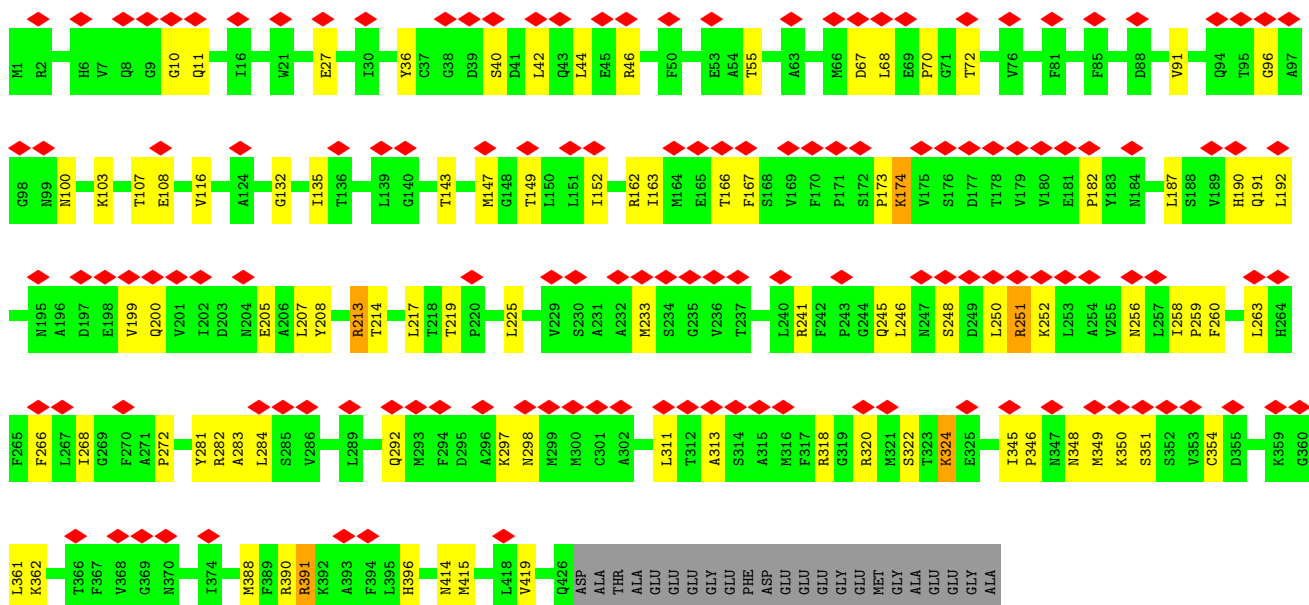
- Molecule 3: Tubulin beta chain

Chain A7: 




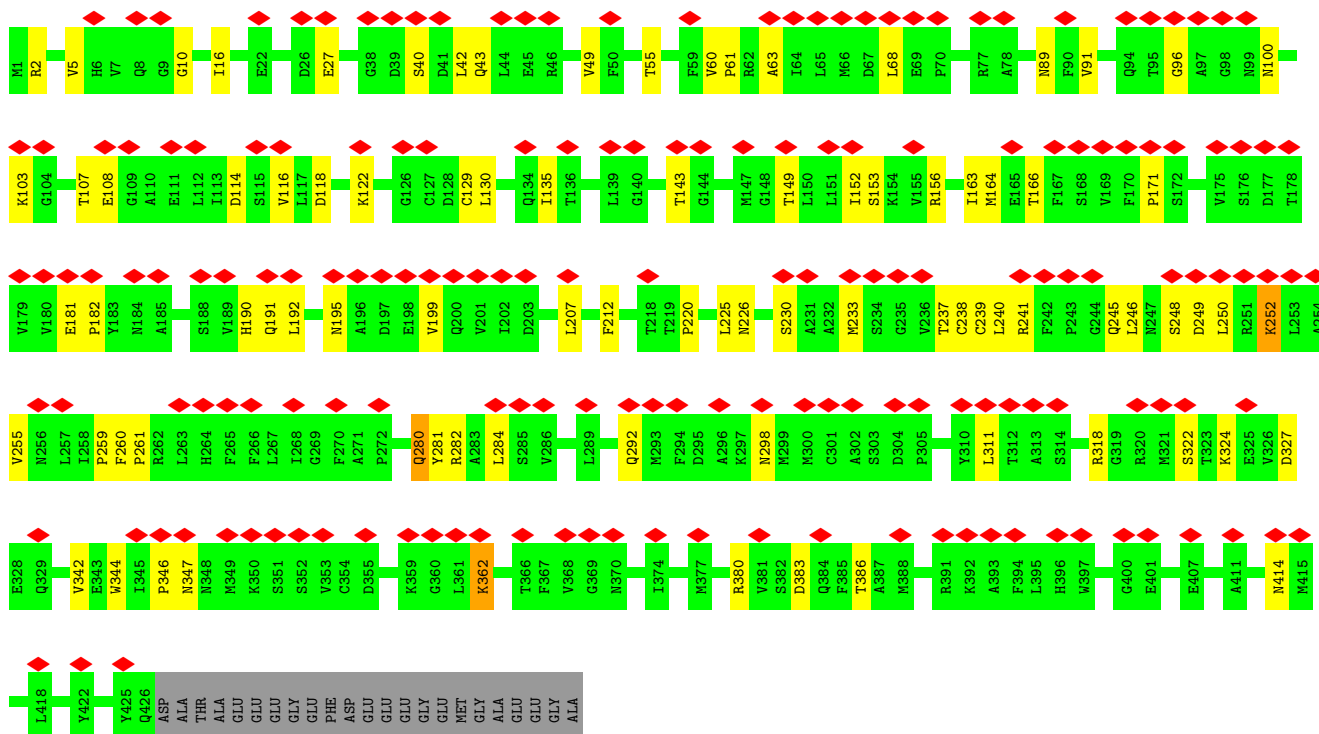
• Molecule 3: Tubulin beta chain

Chain A9: 

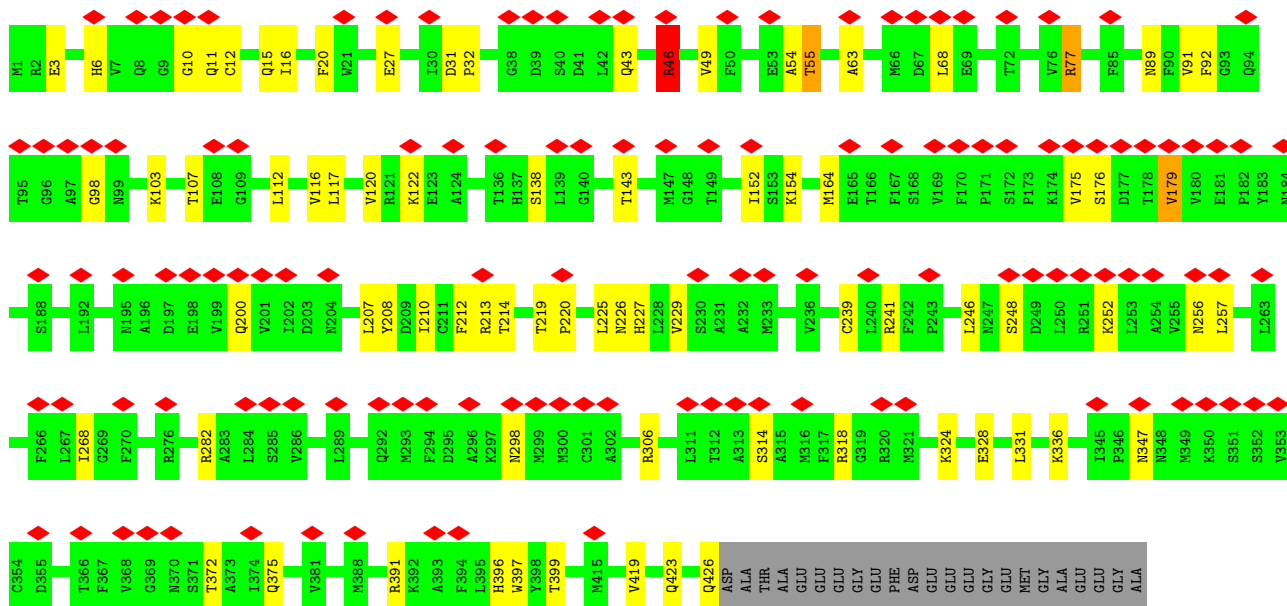
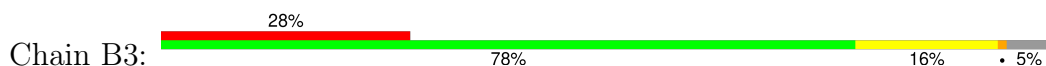


• Molecule 3: Tubulin beta chain

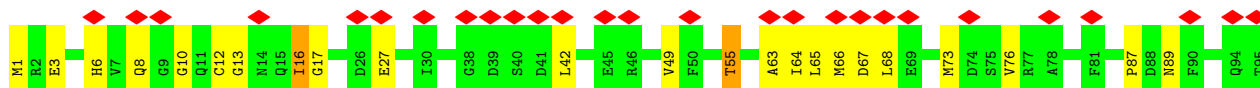
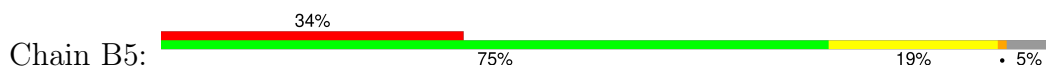
Chain B1: 

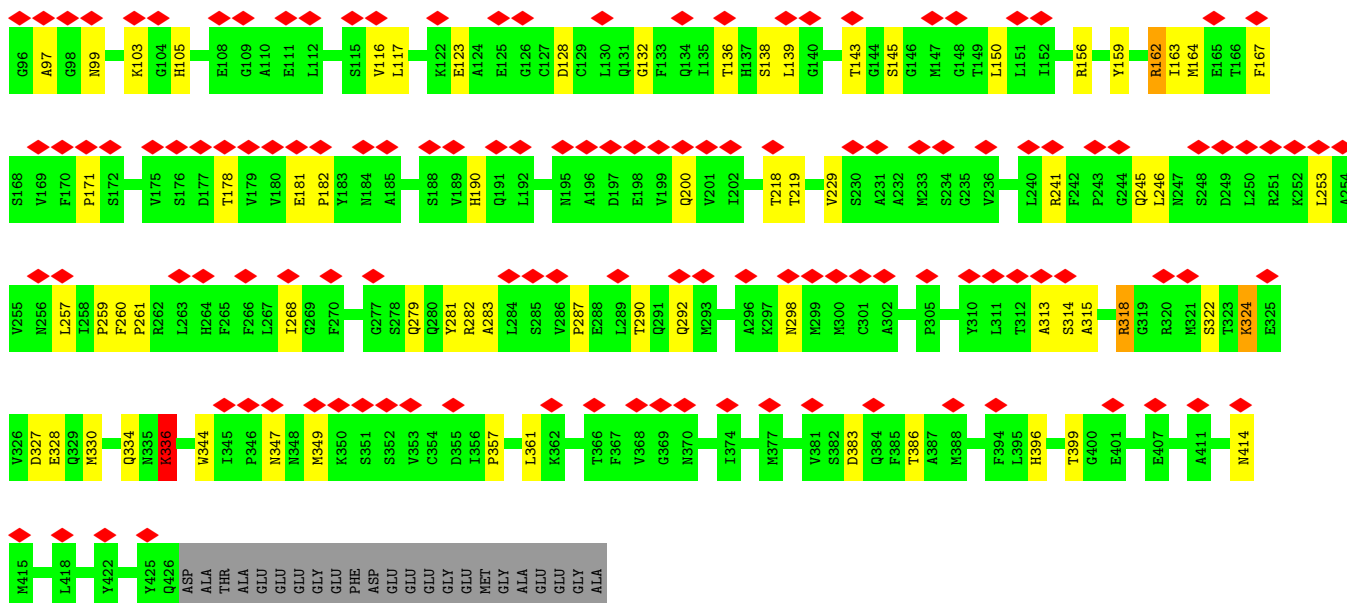


• Molecule 3: Tubulin beta chain

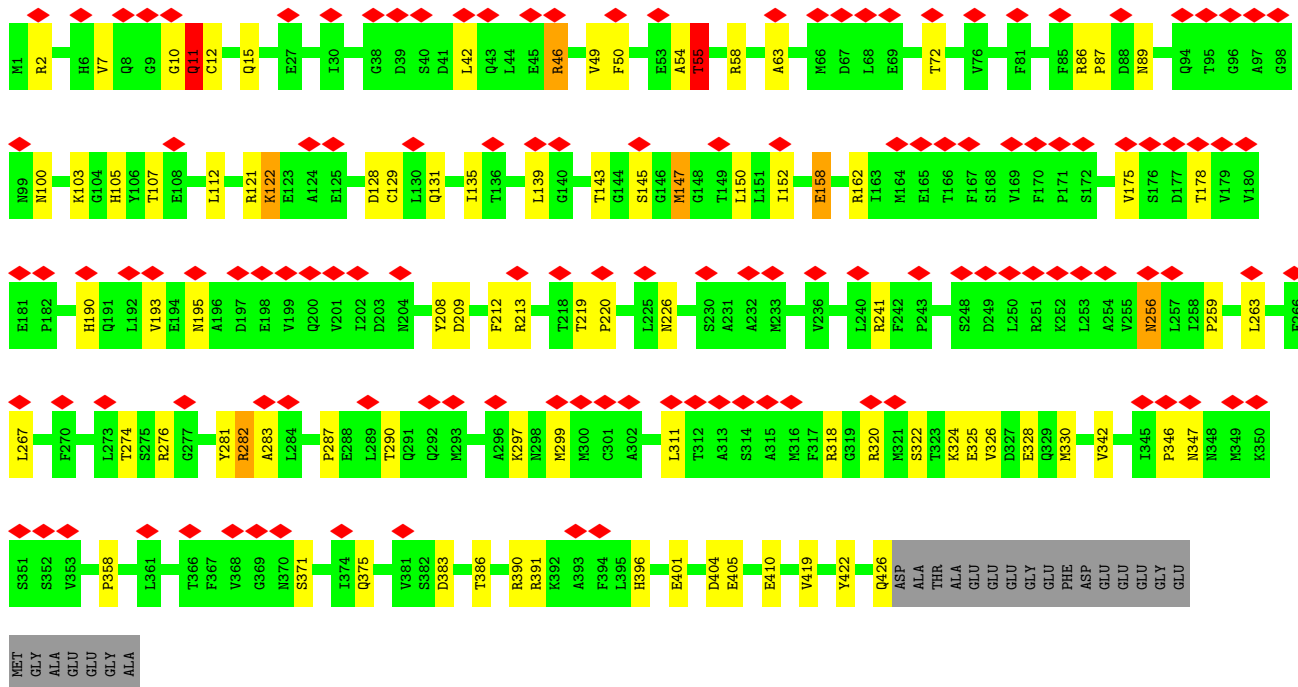
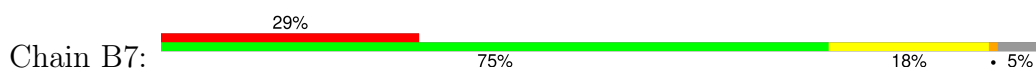


• Molecule 3: Tubulin beta chain

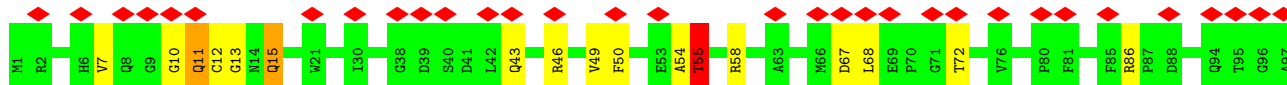
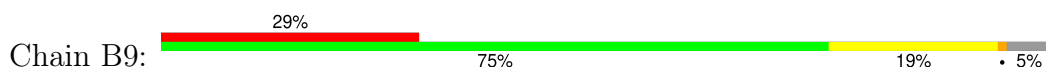


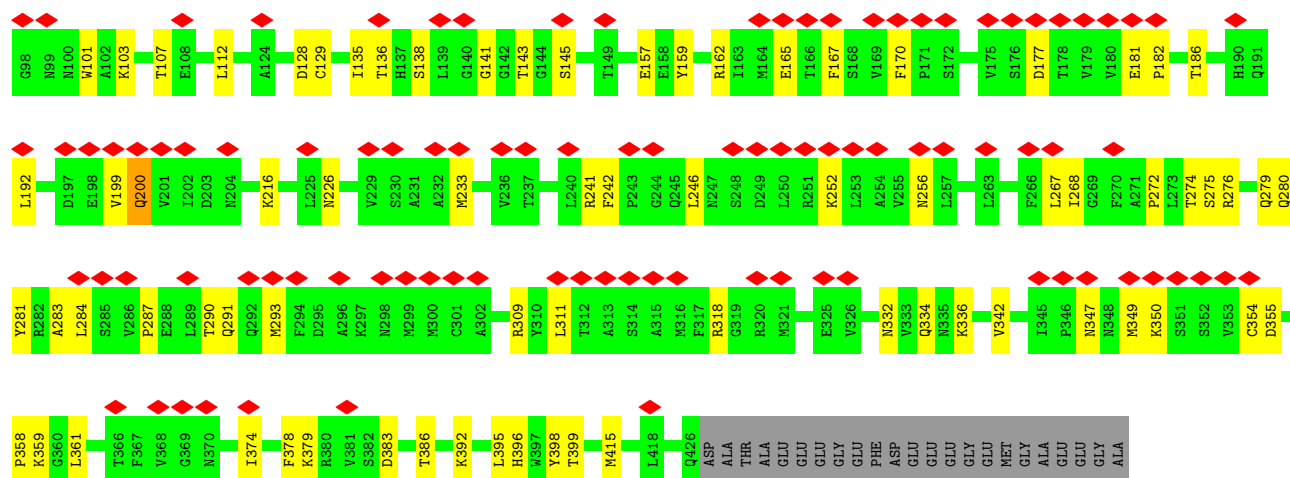


• Molecule 3: Tubulin beta chain

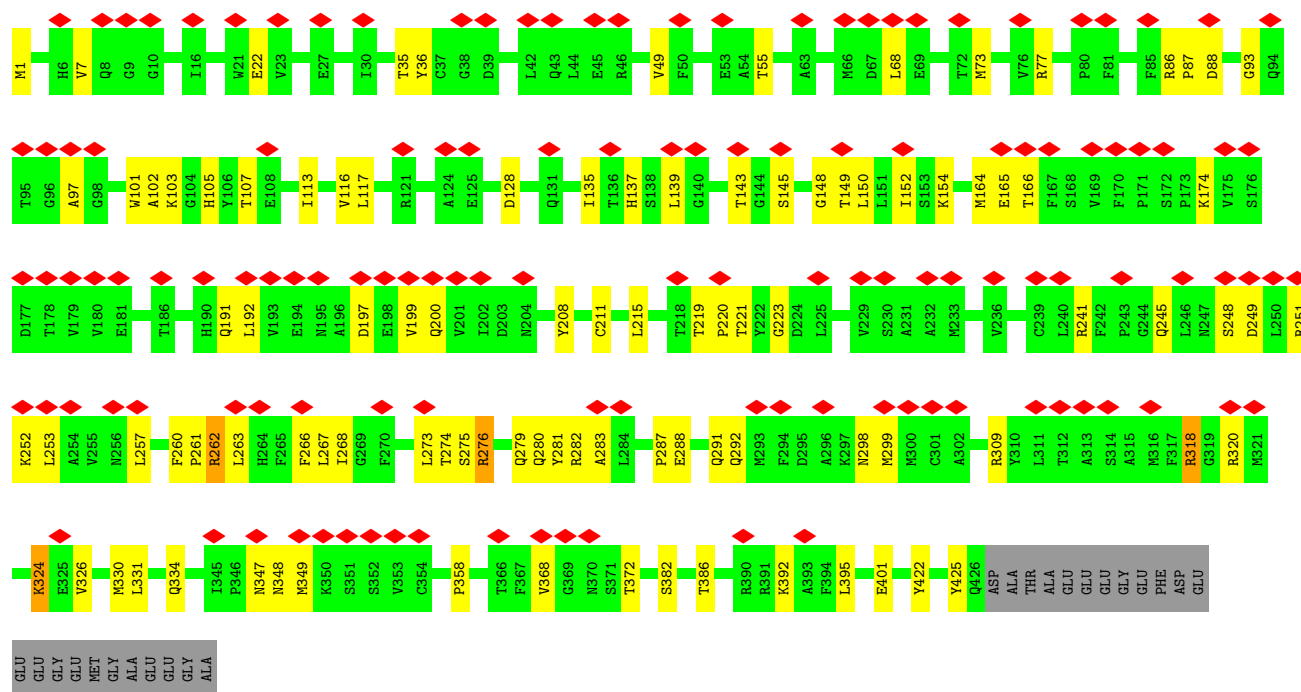
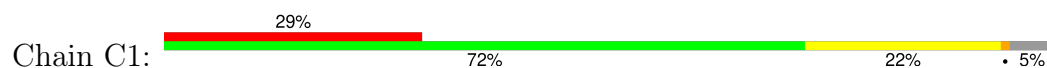


• Molecule 3: Tubulin beta chain

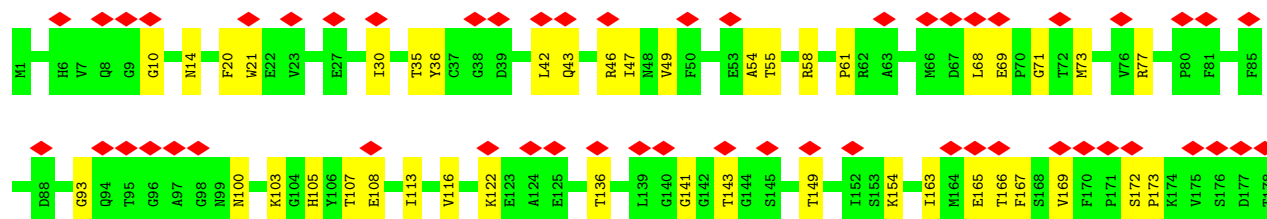


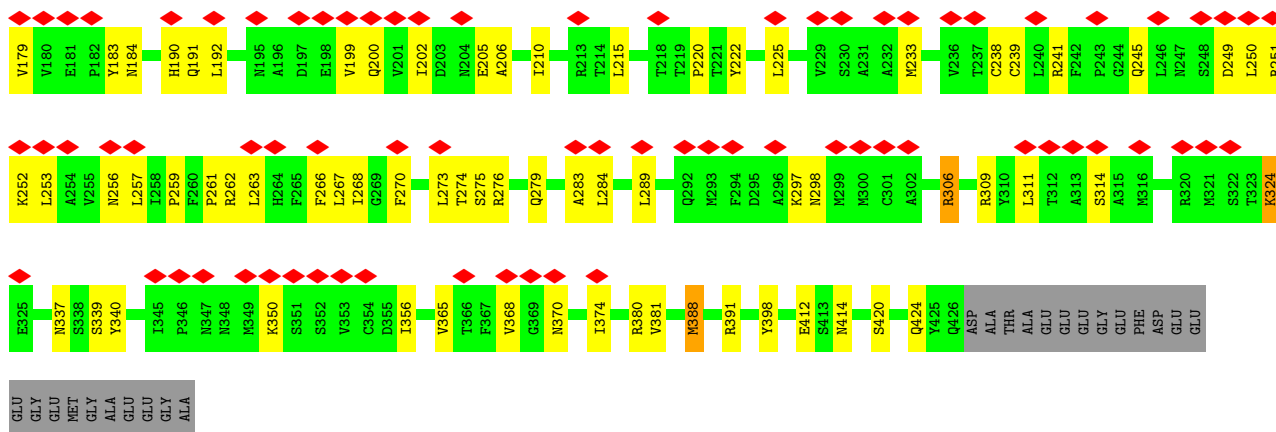


• Molecule 3: Tubulin beta chain

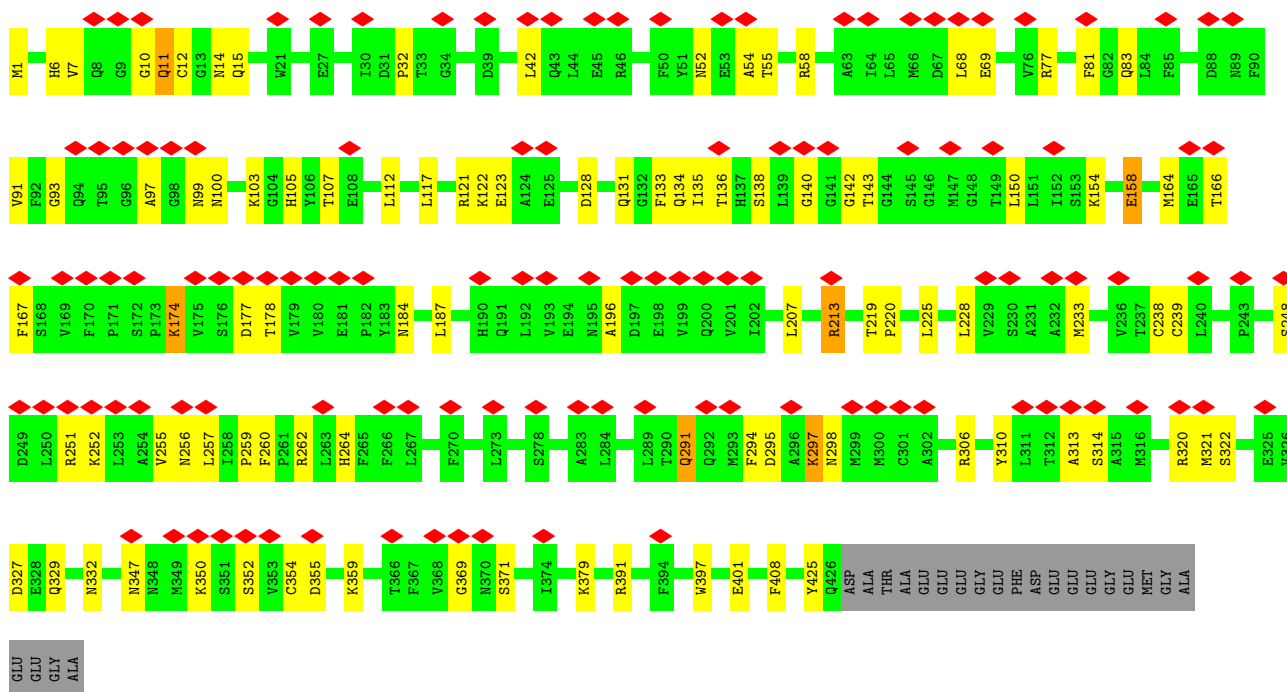
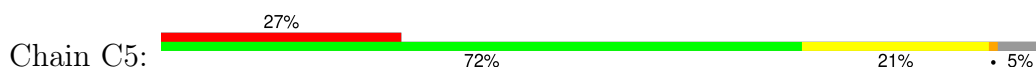


• Molecule 3: Tubulin beta chain

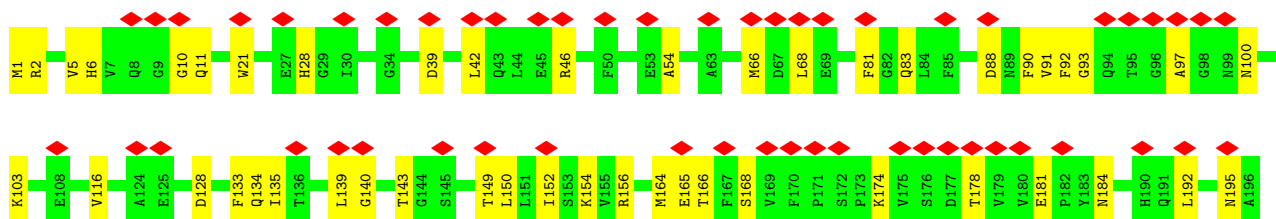
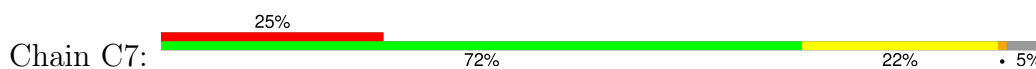


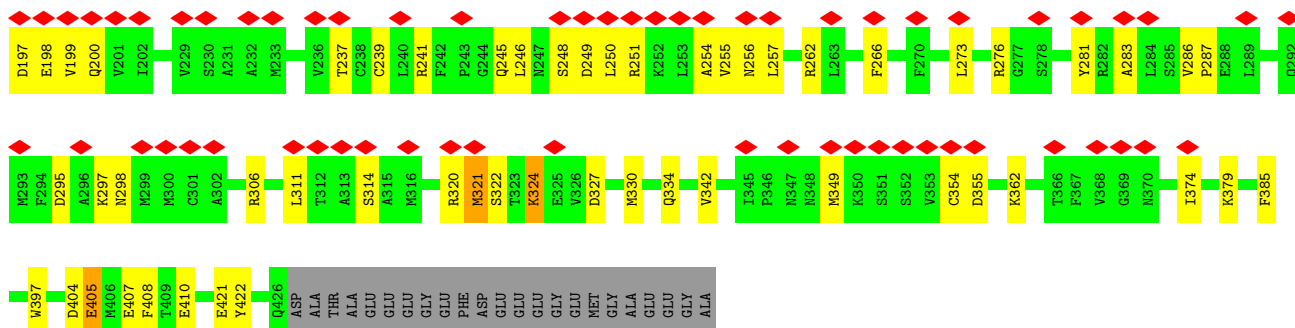


• Molecule 3: Tubulin beta chain

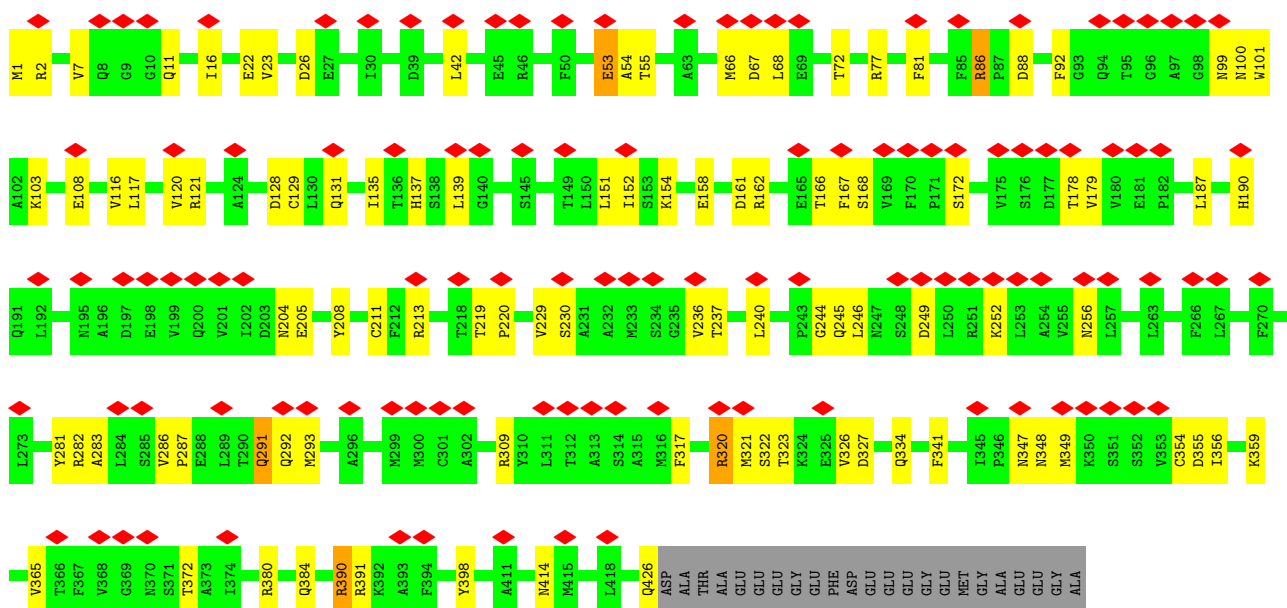


• Molecule 3: Tubulin beta chain

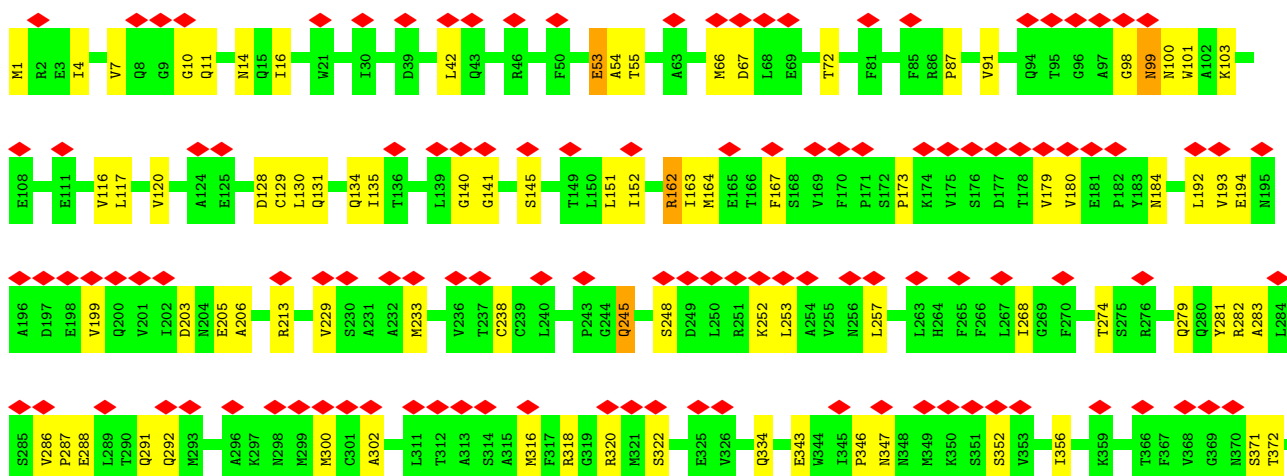
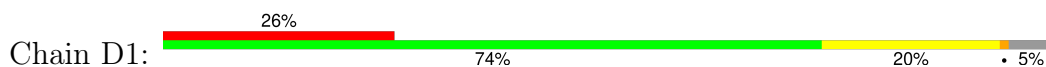


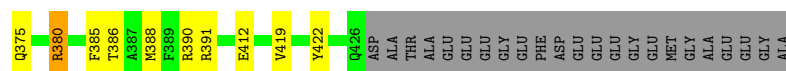


• Molecule 3: Tubulin beta chain

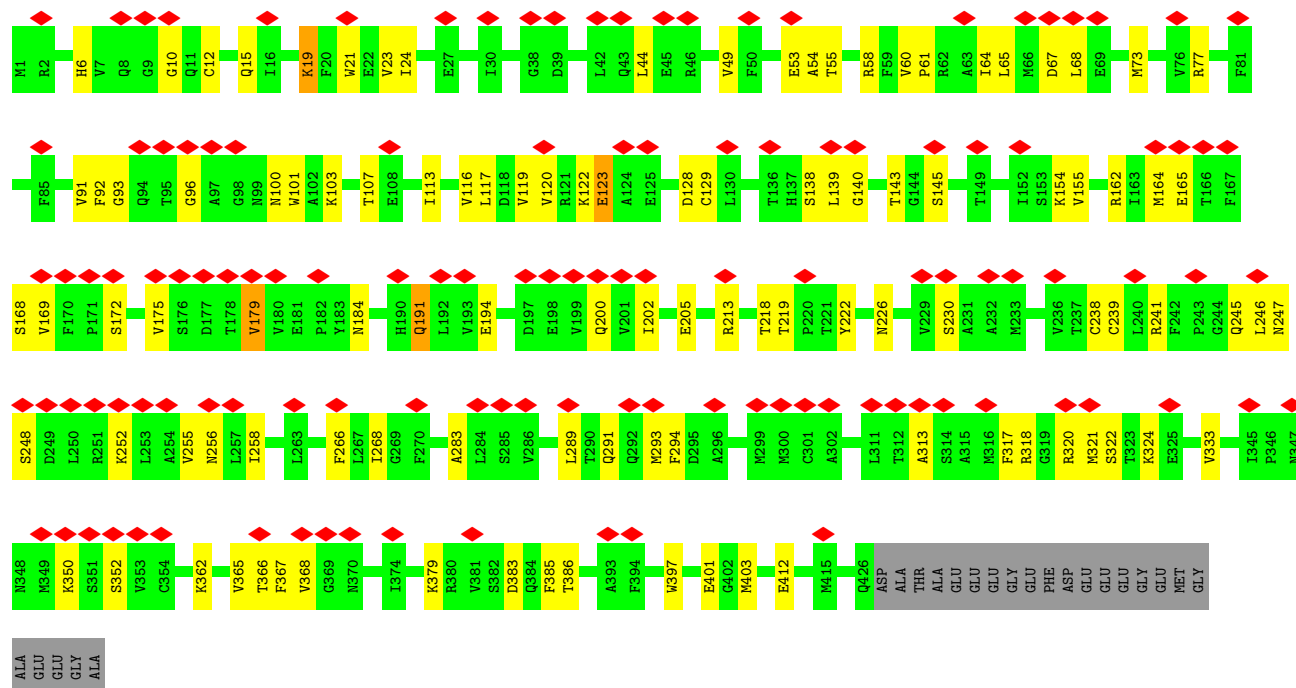


• Molecule 3: Tubulin beta chain

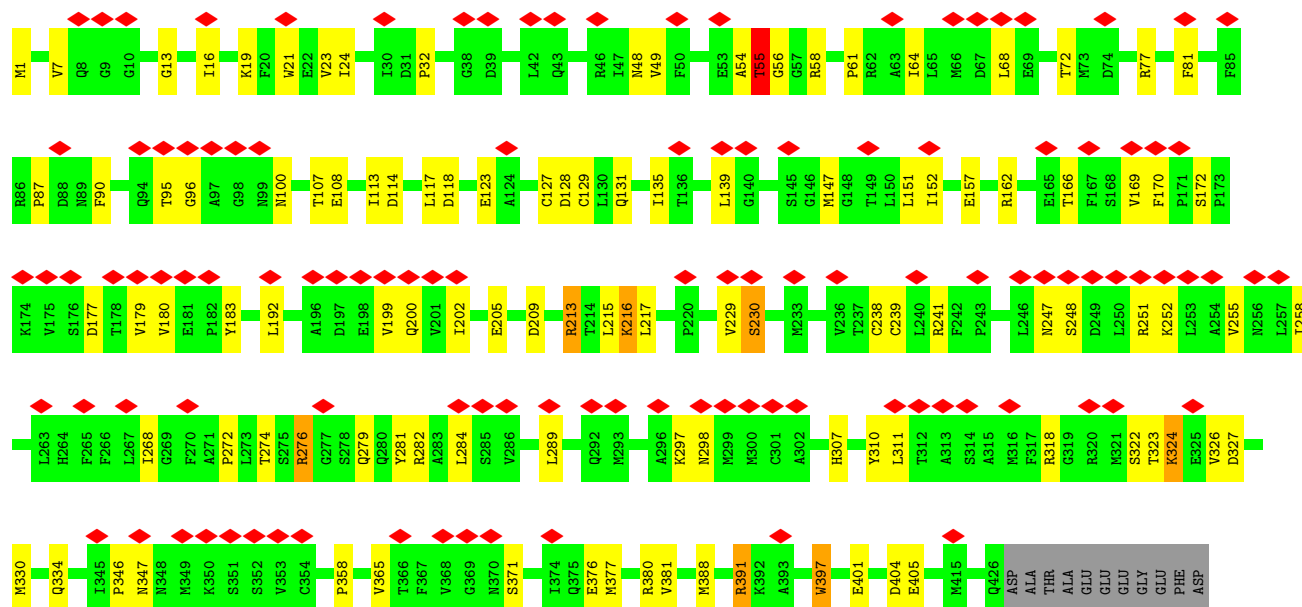




• Molecule 3: Tubulin beta chain




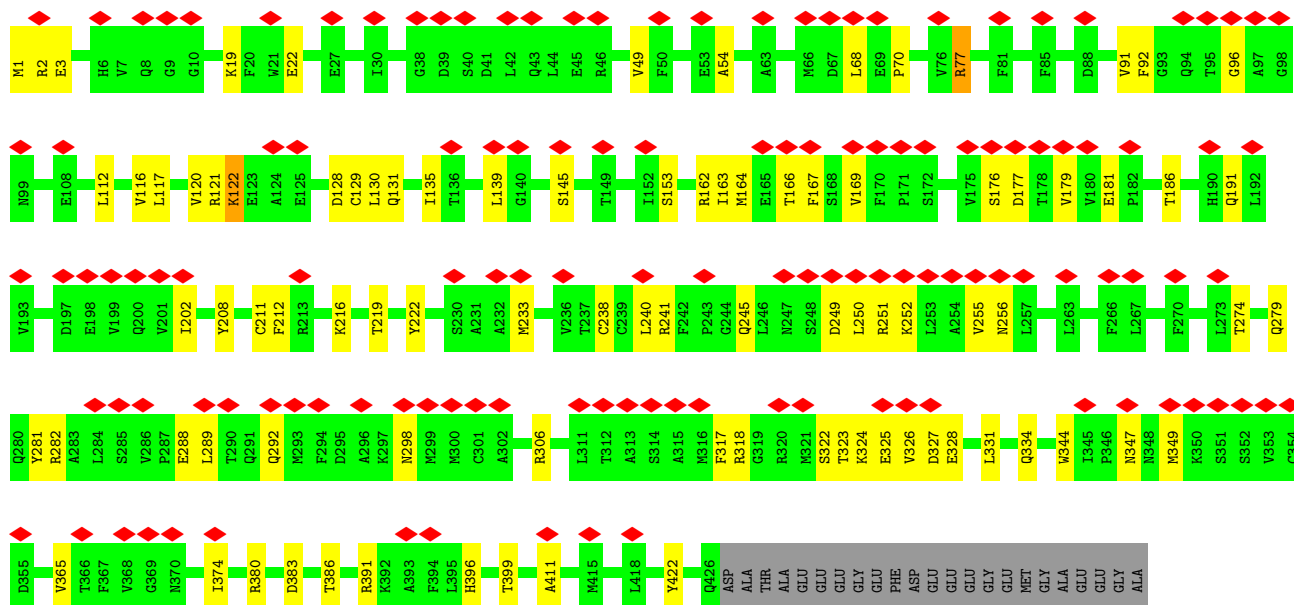
• Molecule 3: Tubulin beta chain




GLU
GLU
GLU
GLU
MET
GLY
ALA
GLU
GLY
ALA

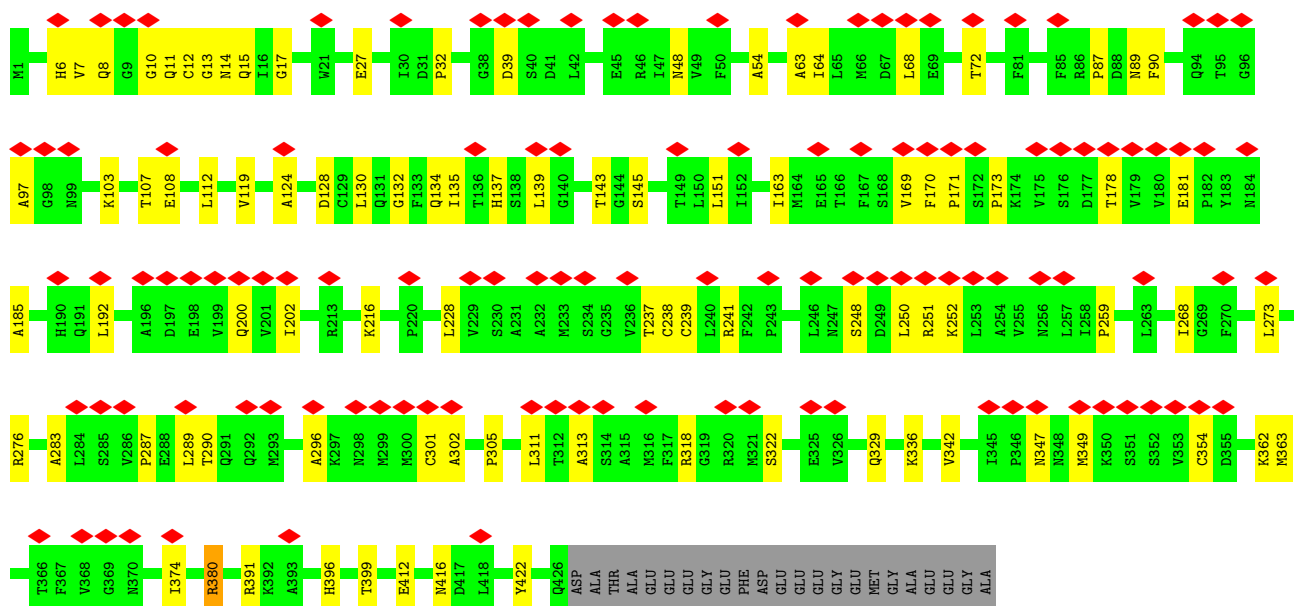
• Molecule 3: Tubulin beta chain

Chain D7: 




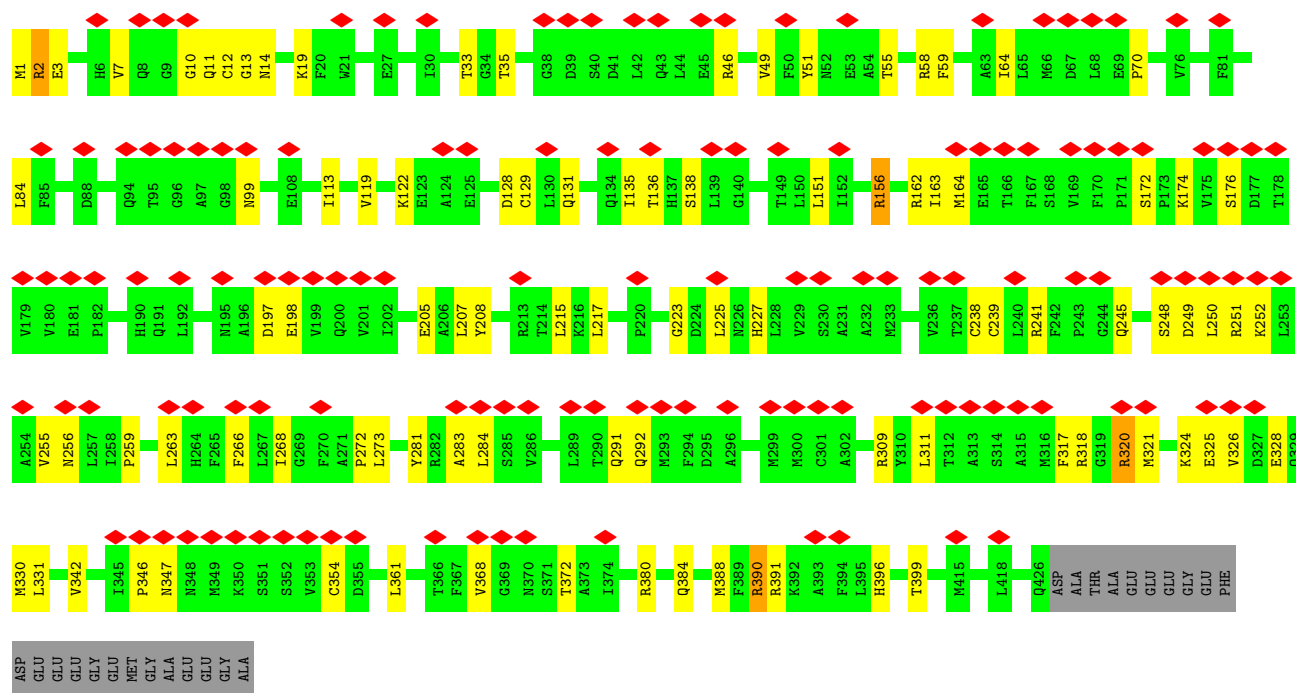
• Molecule 3: Tubulin beta chain

Chain D9: 

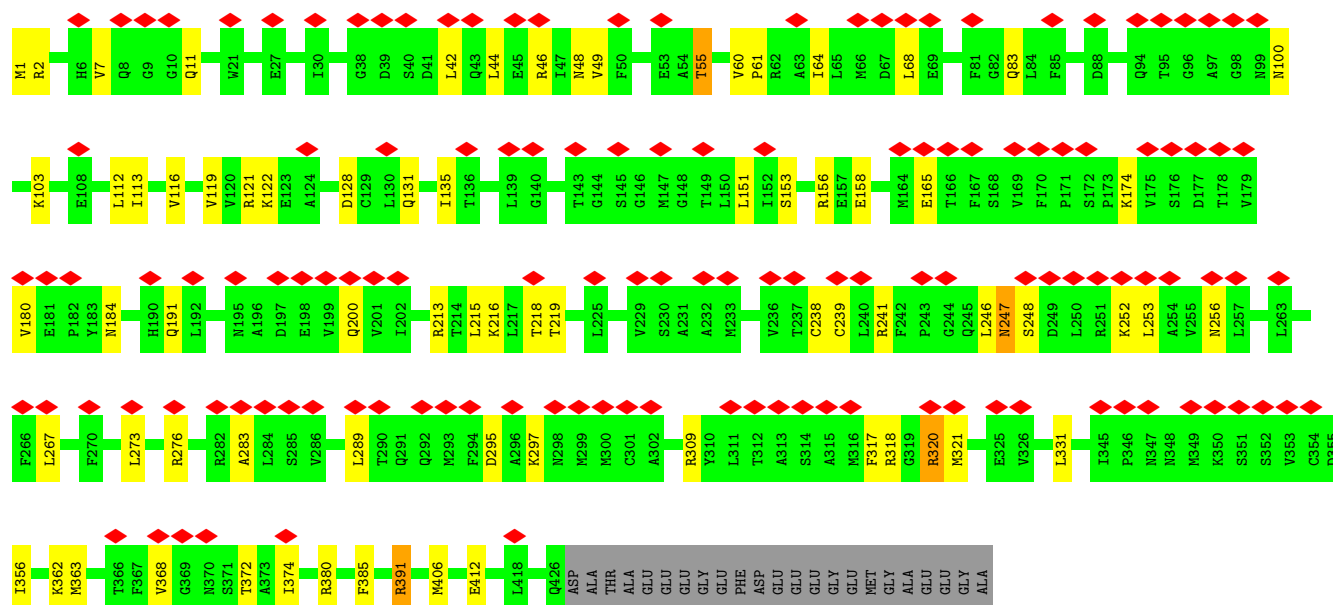
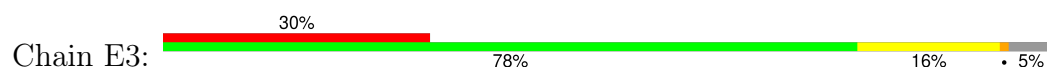


• Molecule 3: Tubulin beta chain

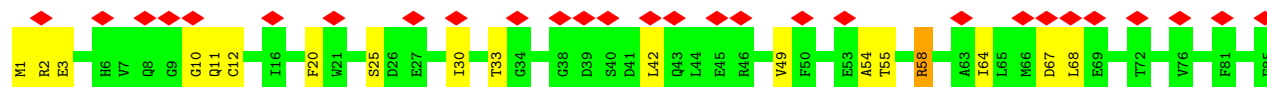
Chain E1: 

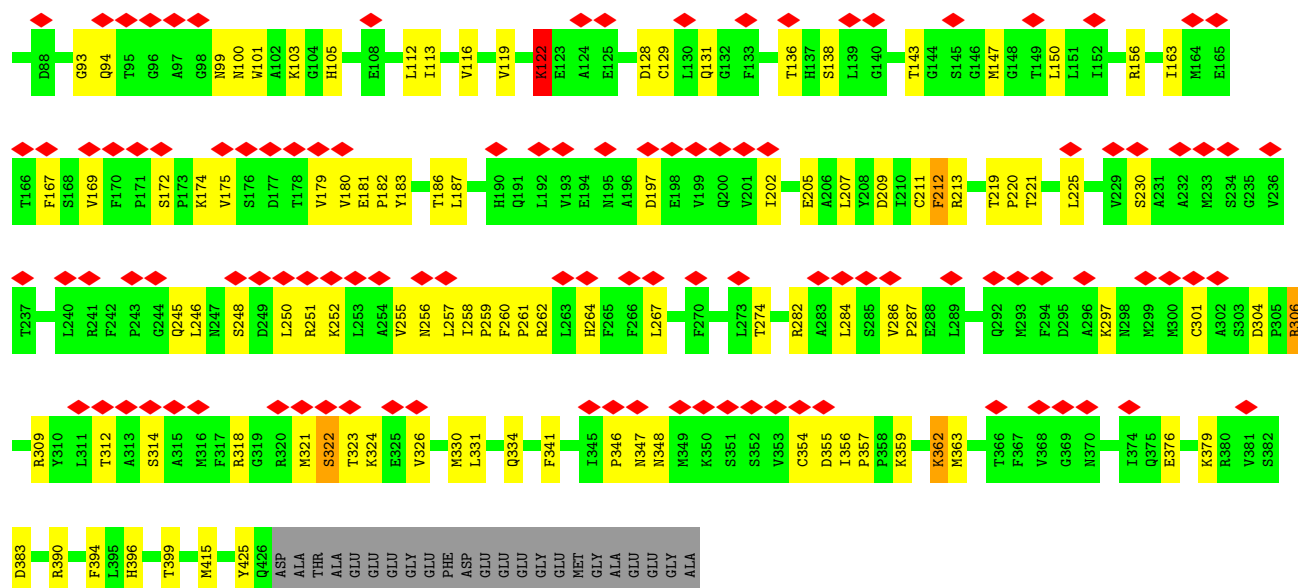


• Molecule 3: Tubulin beta chain

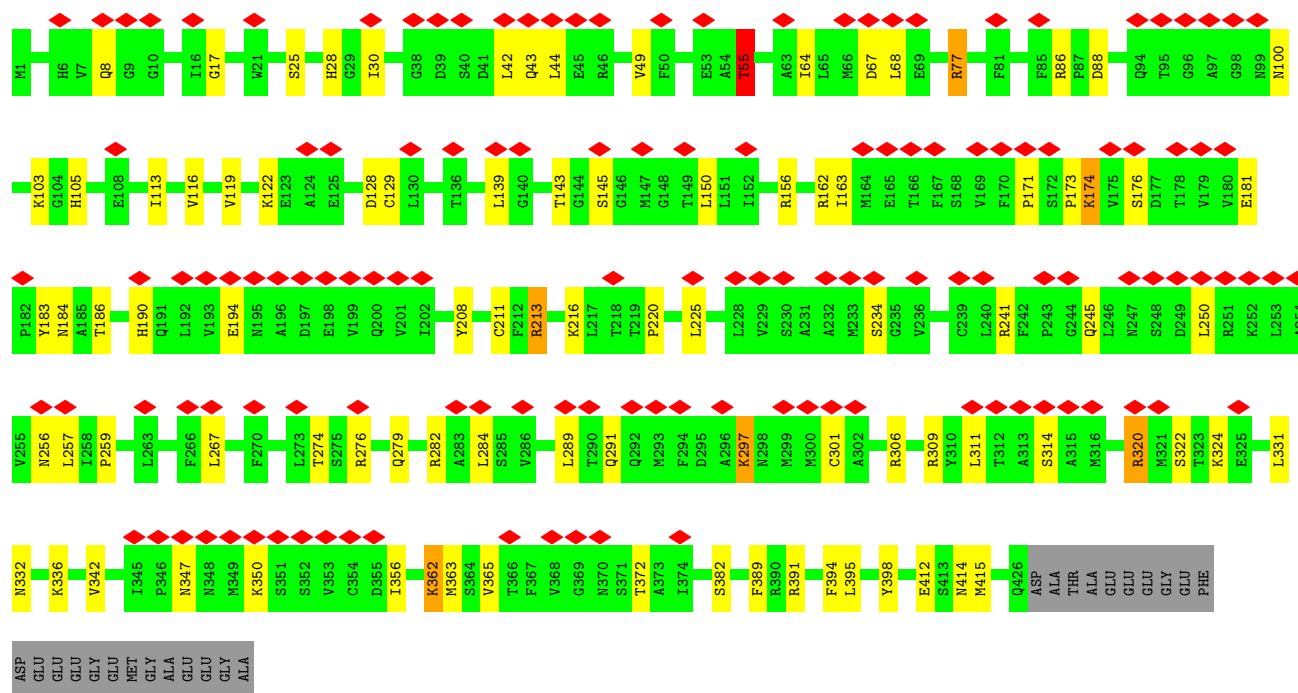
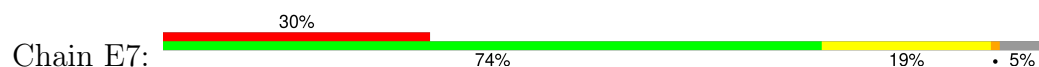


• Molecule 3: Tubulin beta chain

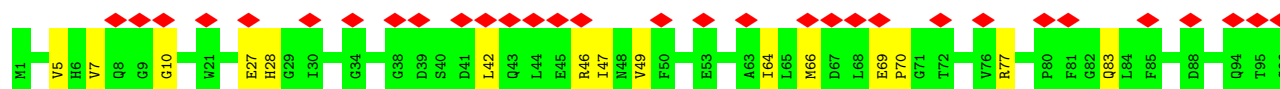
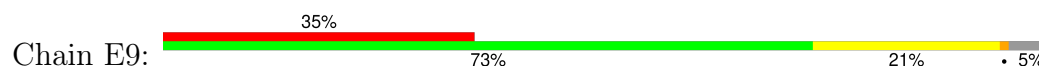


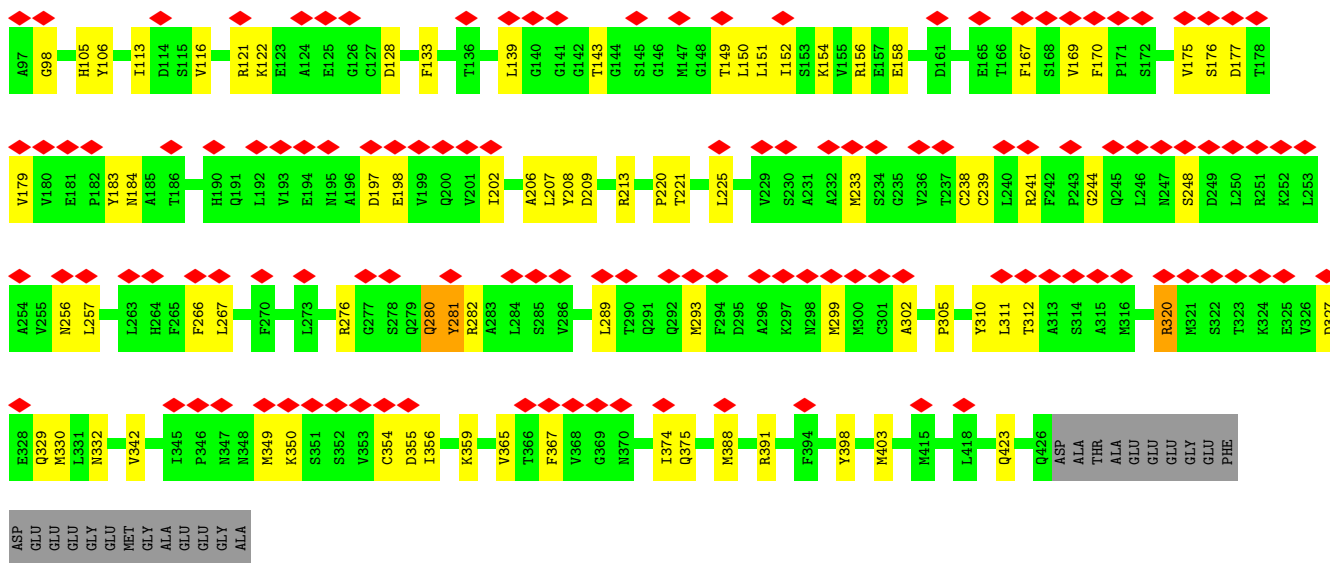


• Molecule 3: Tubulin beta chain

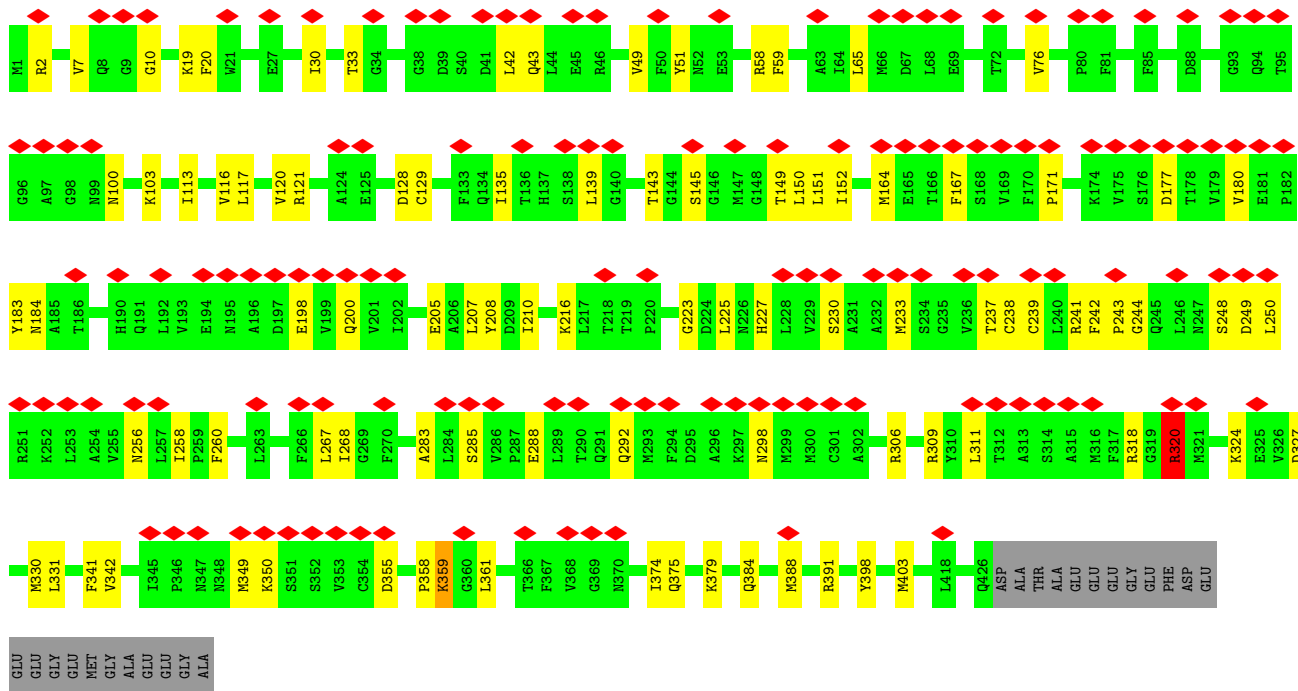
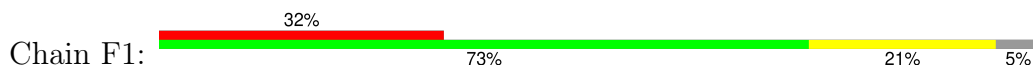


• Molecule 3: Tubulin beta chain

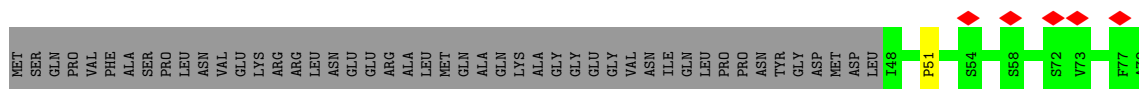


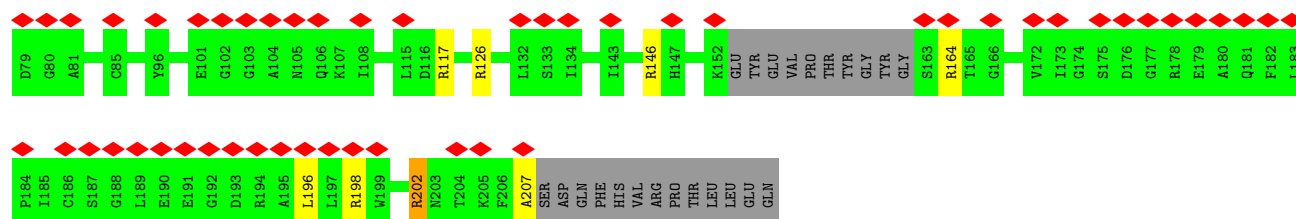


- Molecule 3: Tubulin beta chain

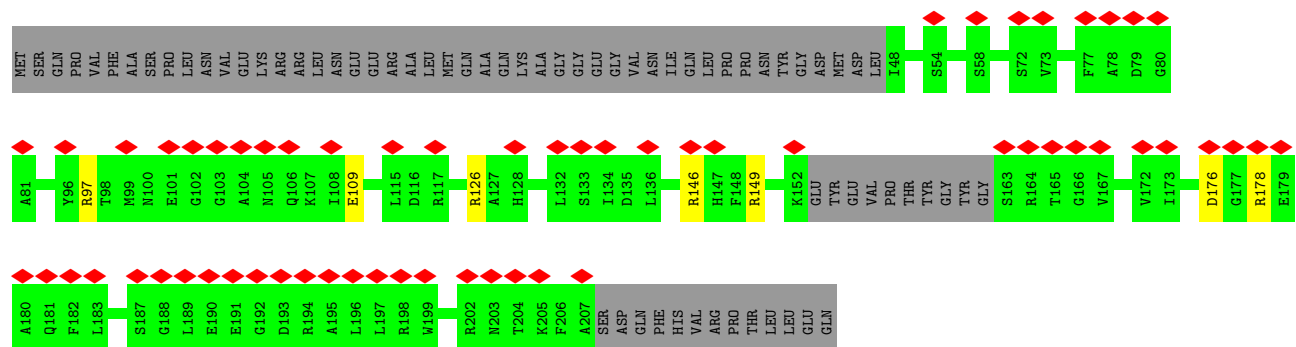


- Molecule 4: PDI family protein

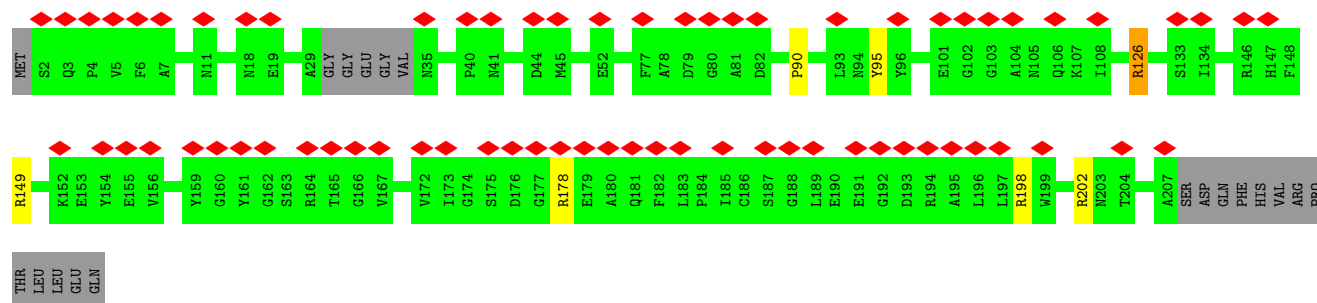
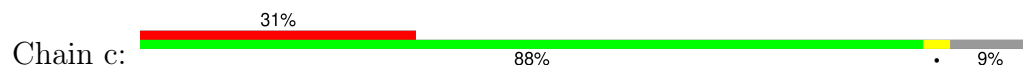




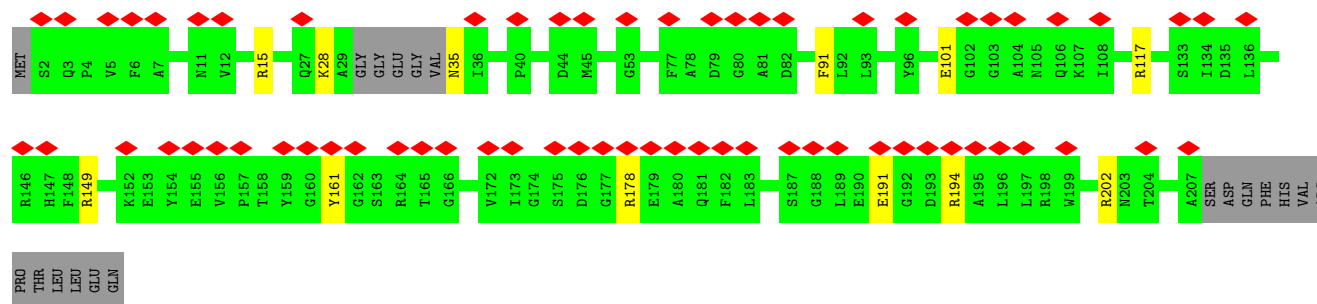
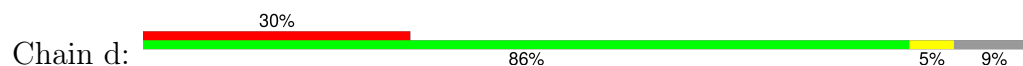
• Molecule 4: PDI family protein



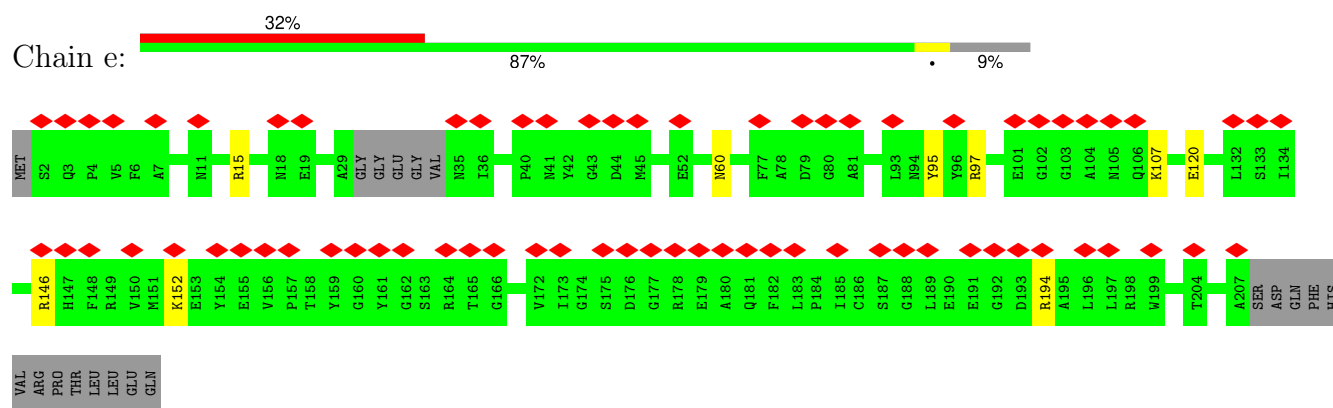
• Molecule 4: PDI family protein



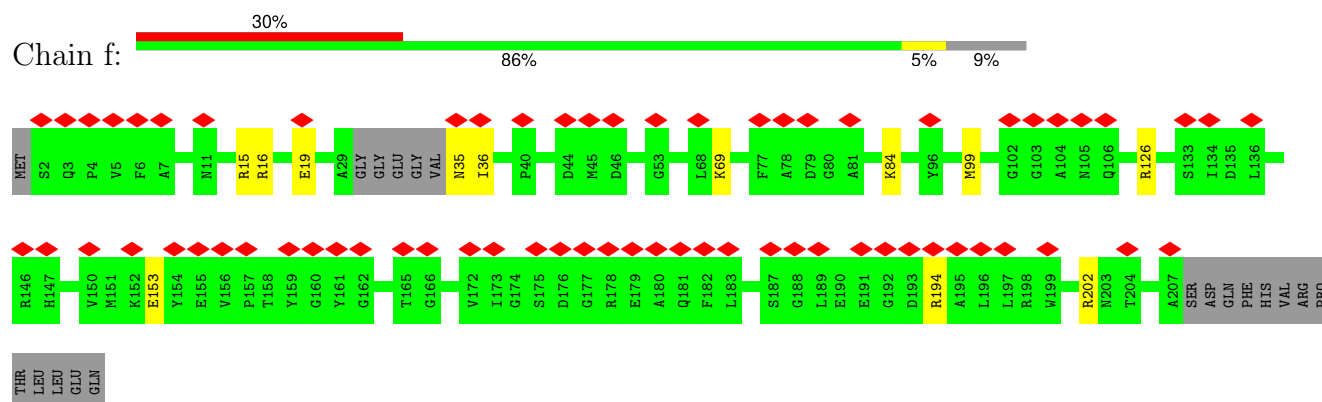
• Molecule 4: PDI family protein



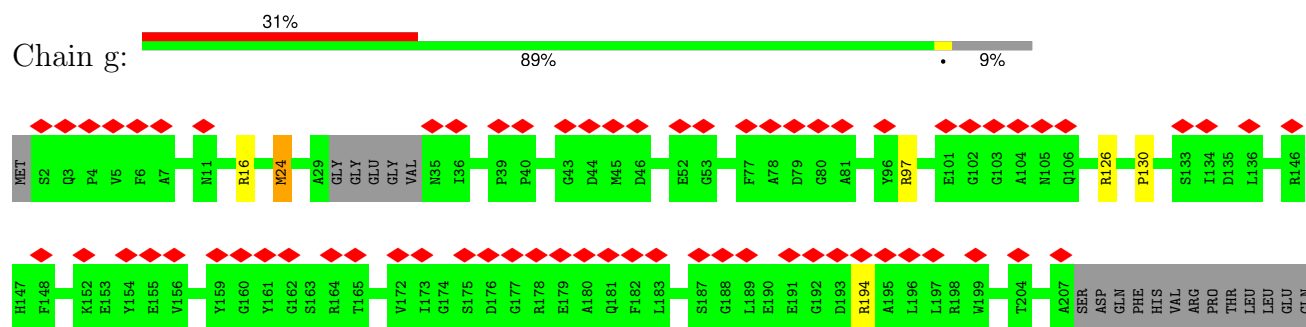
• Molecule 4: PDI family protein



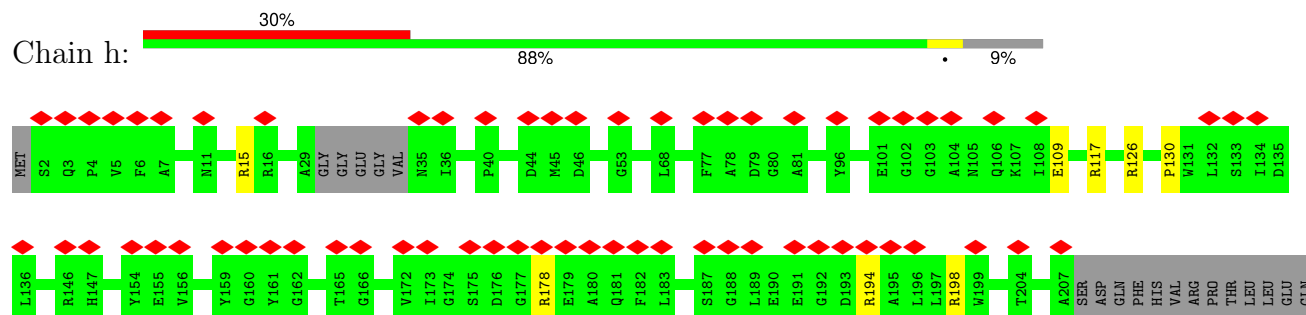
- Molecule 4: PDI family protein



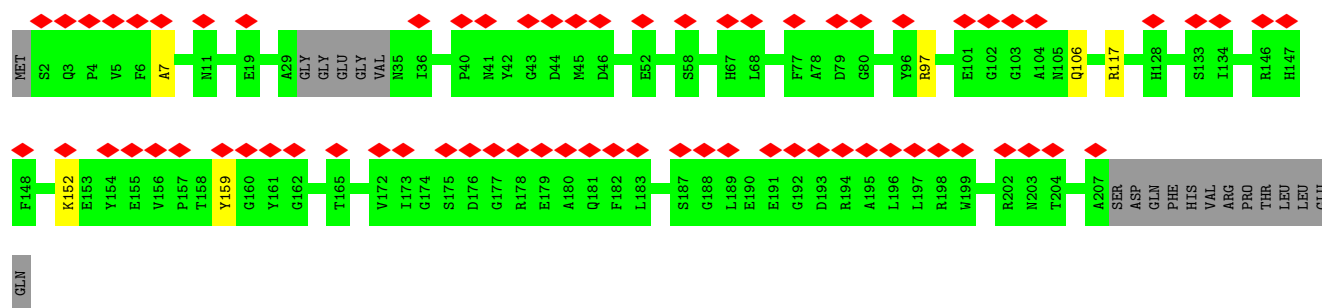
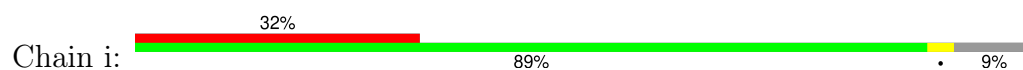
- Molecule 4: PDI family protein



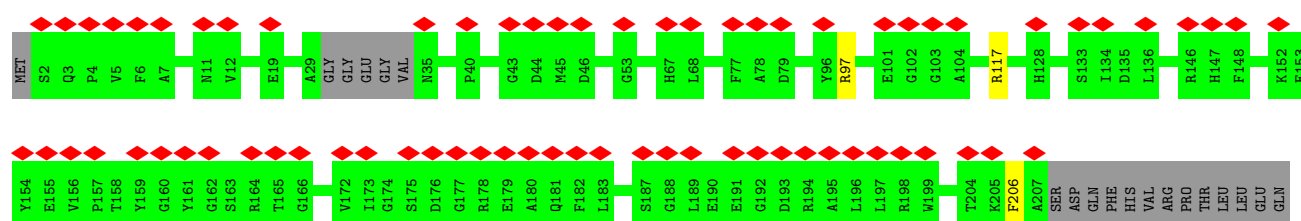
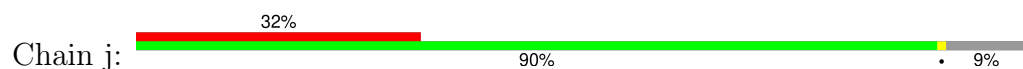
- Molecule 4: PDI family protein



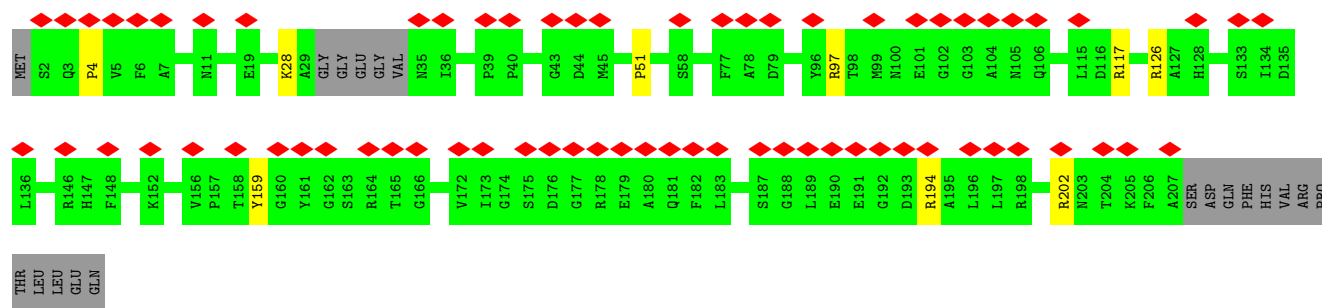
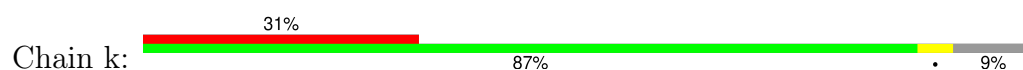
- Molecule 4: PDI family protein



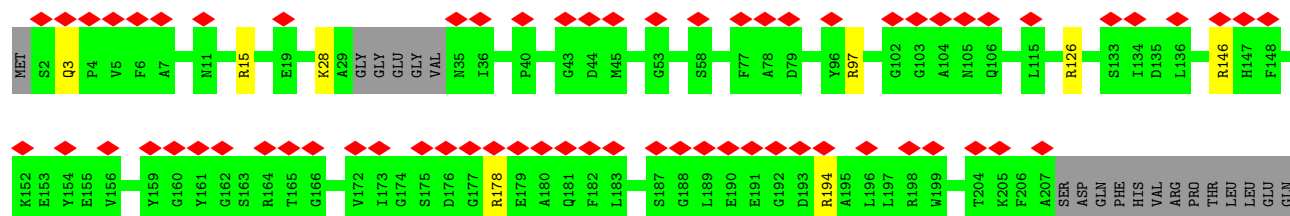
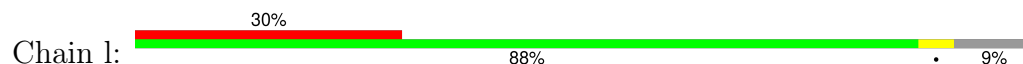
- Molecule 4: PDI family protein



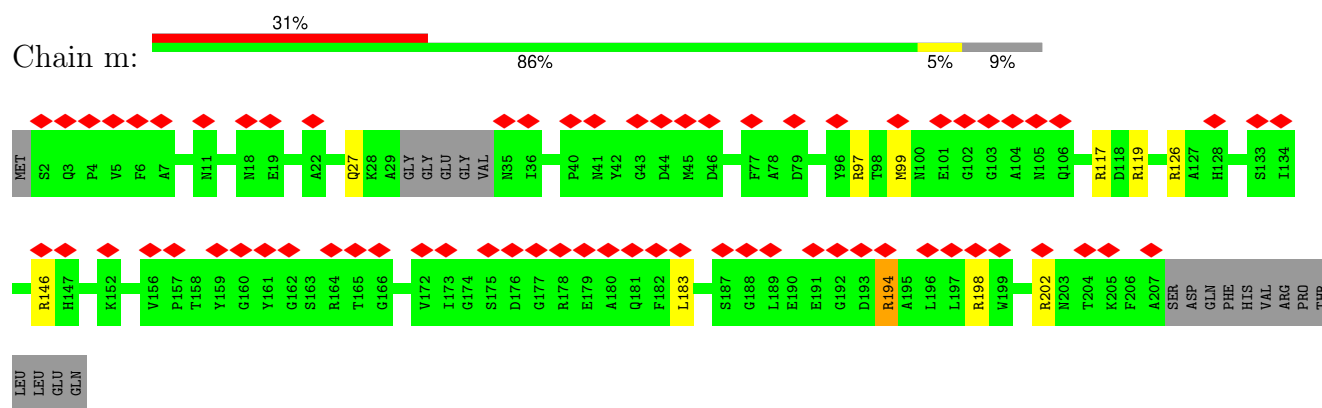
- Molecule 4: PDI family protein



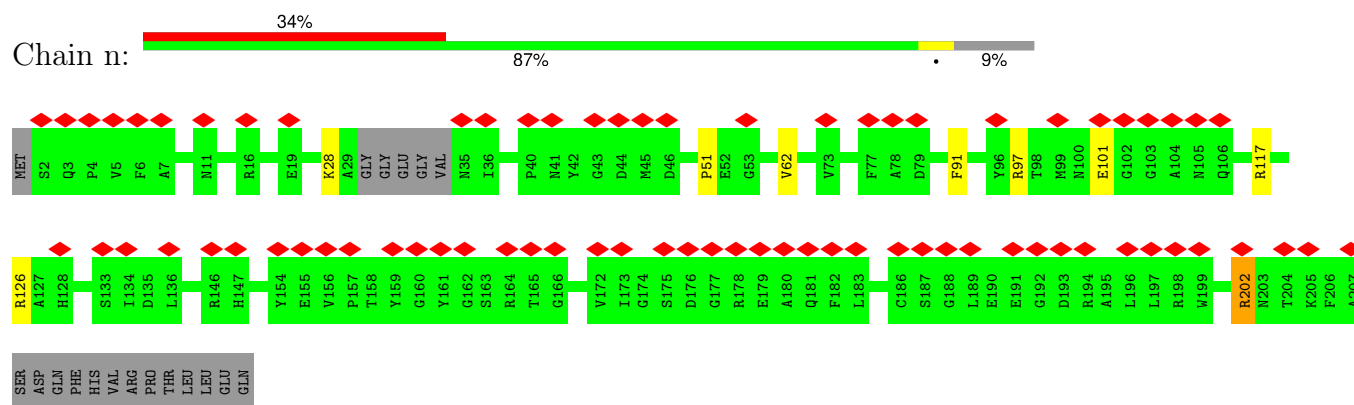
- Molecule 4: PDI family protein



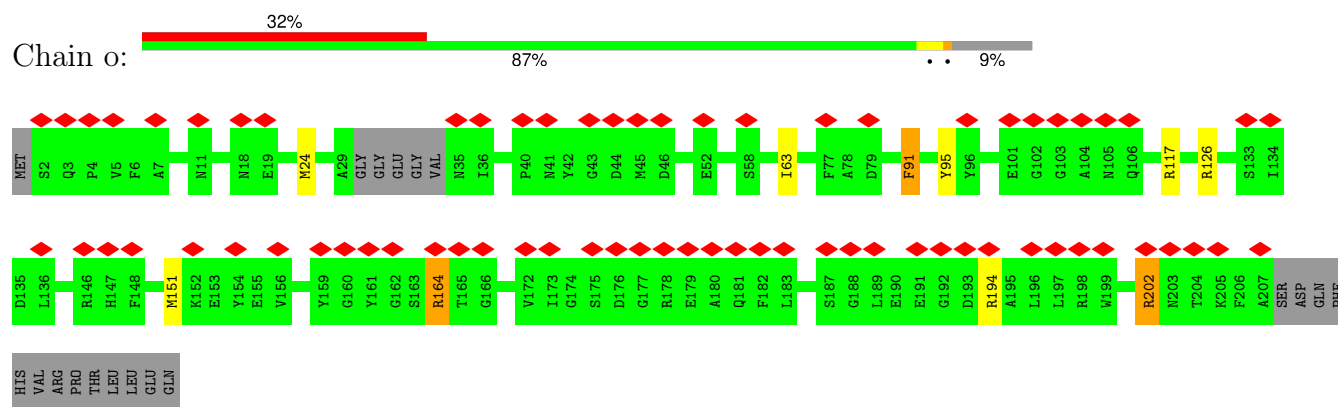
- Molecule 4: PDI family protein



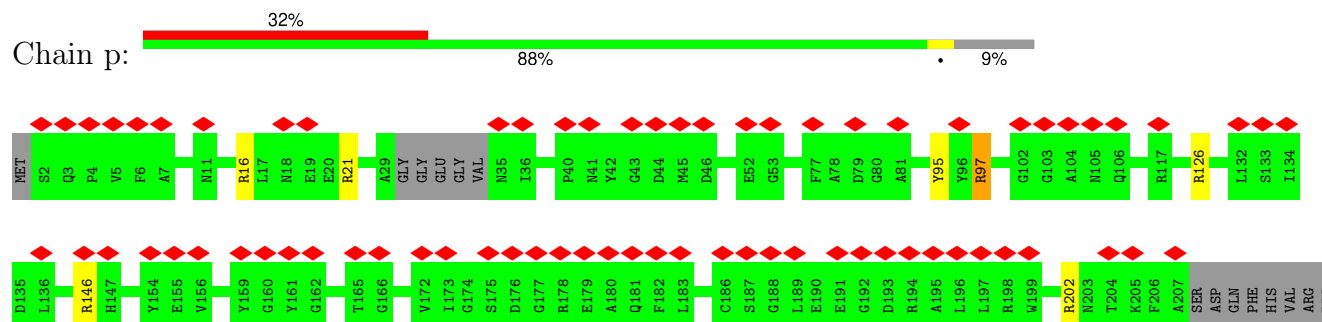
- Molecule 4: PDI family protein



- Molecule 4: PDI family protein

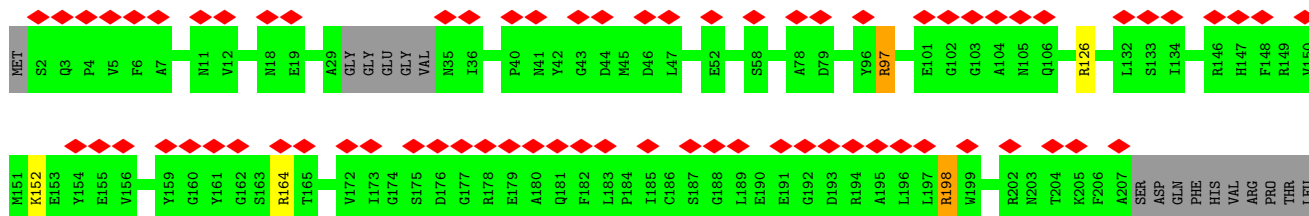
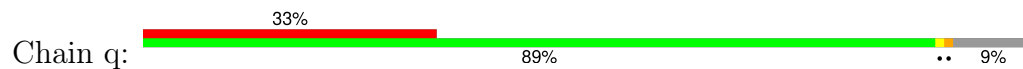


- Molecule 4: PDI family protein



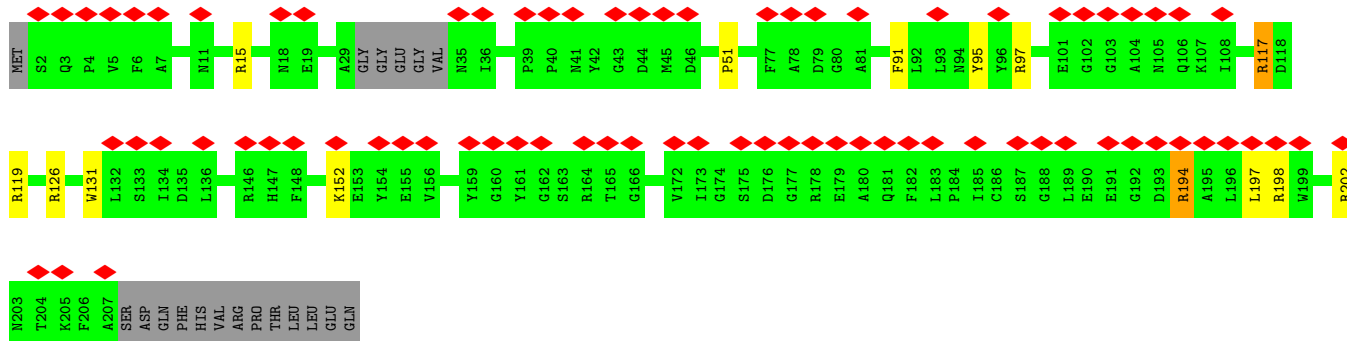
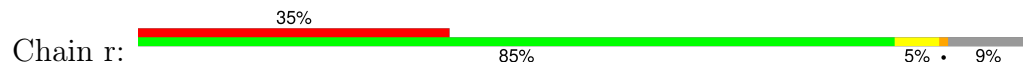
THR
LEU
LEU
GLU
GLN

• Molecule 4: PDI family protein

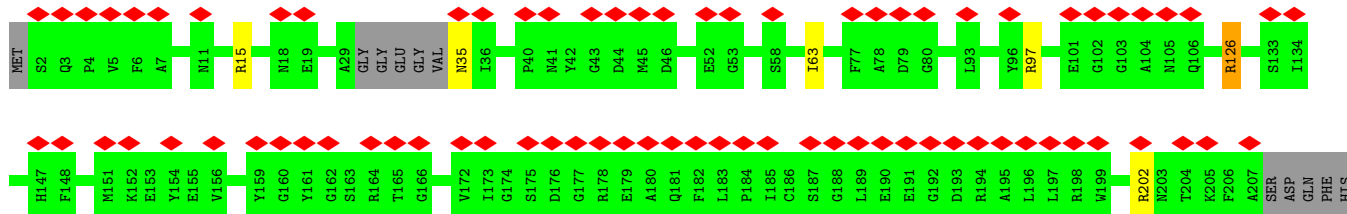
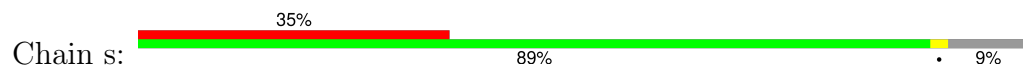


LEU
GLU
GLN

• Molecule 4: PDI family protein

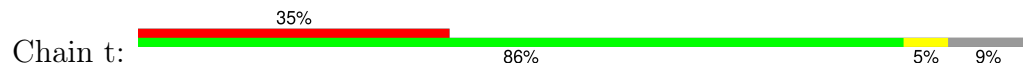


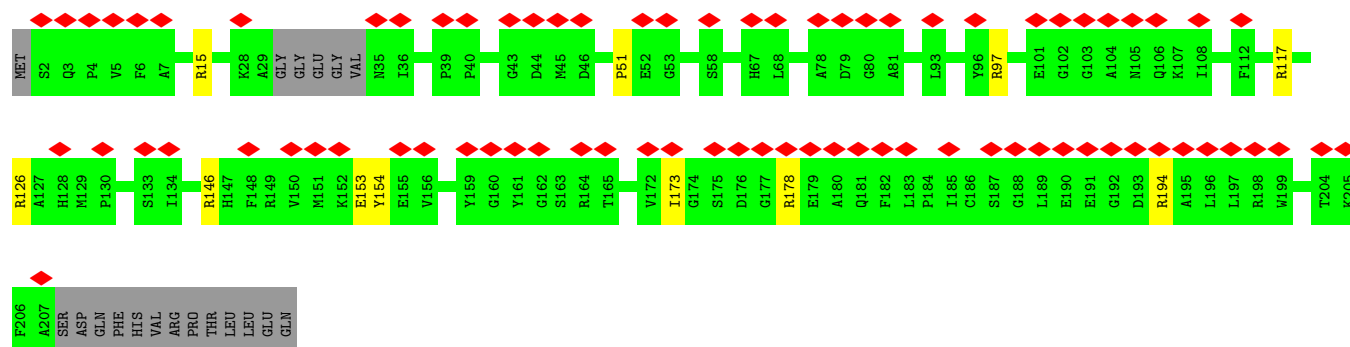
• Molecule 4: PDI family protein



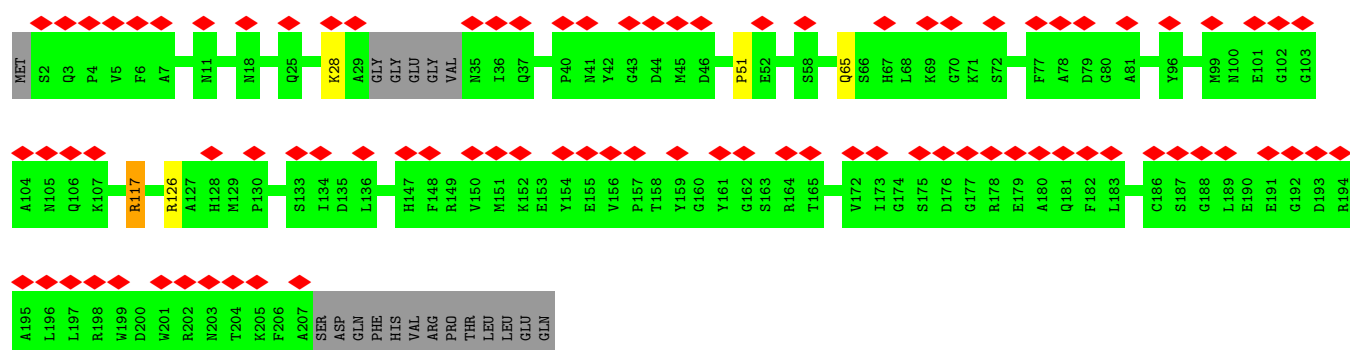
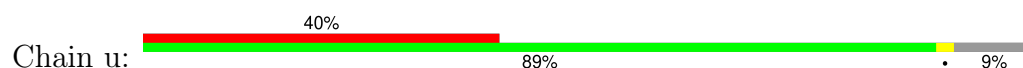
VAL
ARG
PRO
THR
LEU
LEU
GLU
GLN

• Molecule 4: PDI family protein

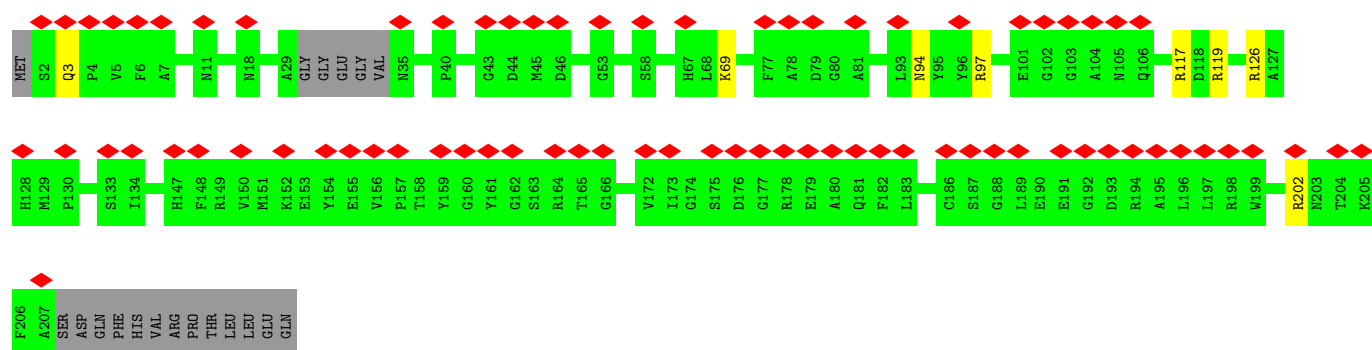
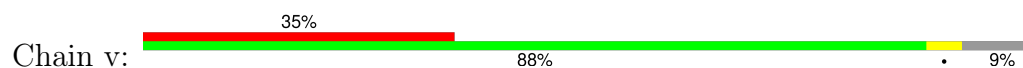




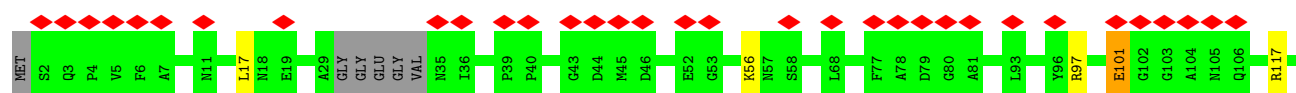
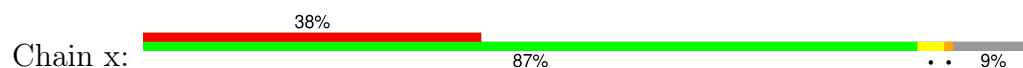
• Molecule 4: PDI family protein

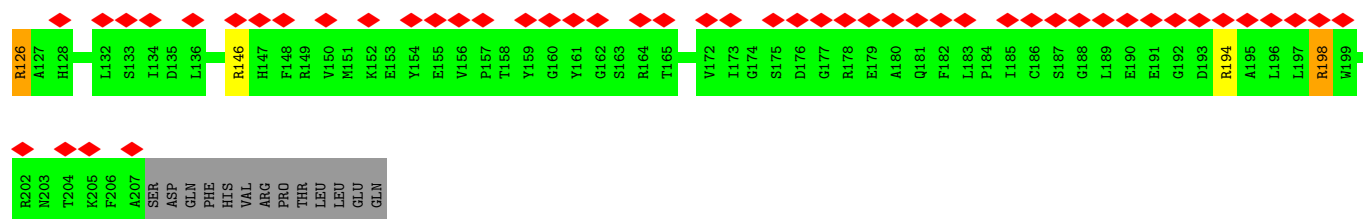


• Molecule 4: PDI family protein

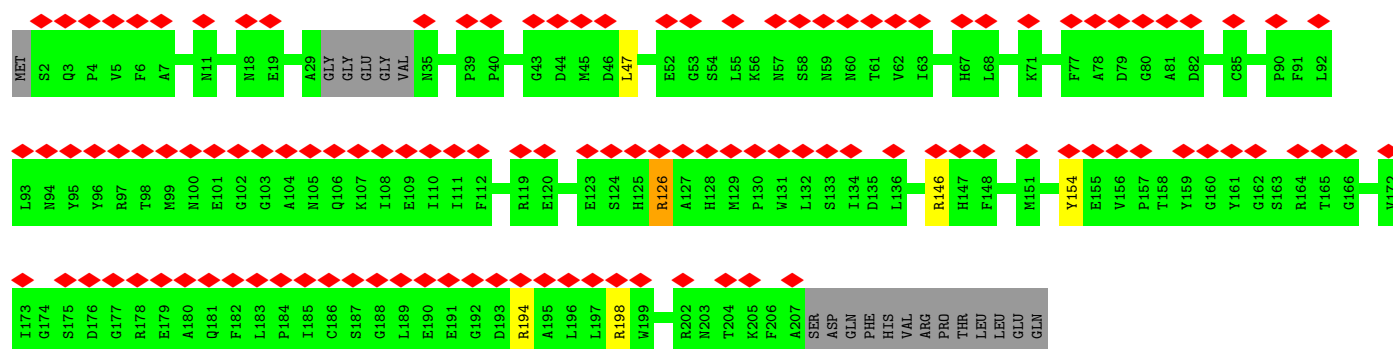
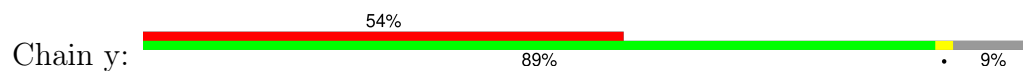


• Molecule 4: PDI family protein

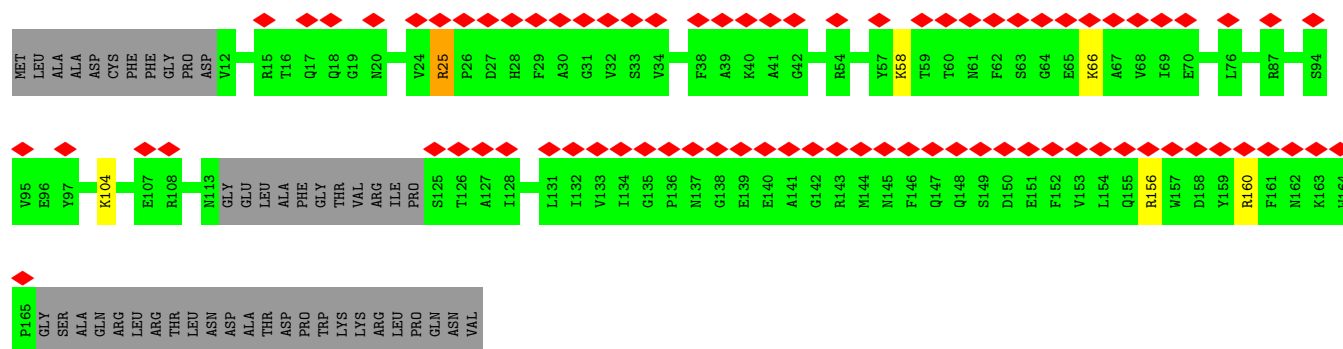
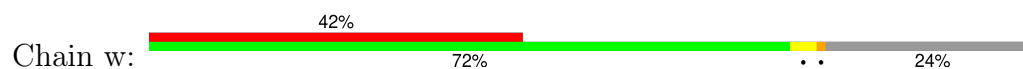




• Molecule 4: PDI family protein



• Molecule 5: PDI family protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	HELICAL, twist=27.7°, rise=80 Å, axial sym=C13	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	16.064	Depositor
Minimum map value	-13.513	Depositor
Average map value	0.056	Depositor
Map value standard deviation	0.986	Depositor
Recommended contour level	2	Depositor
Map size (Å)	447.444, 447.444, 447.444	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.46	0/181	0.93	0/248
1	1	0.46	0/181	0.90	0/248
1	10	0.41	0/181	1.04	0/248
1	11	0.47	0/181	1.20	1/248 (0.4%)
1	12	0.46	0/181	1.03	0/248
1	13	0.46	0/181	1.10	0/248
1	14	0.39	0/181	0.83	1/248 (0.4%)
1	15	0.48	0/181	1.15	0/248
1	16	0.46	0/181	0.98	1/248 (0.4%)
1	17	0.82	2/181 (1.1%)	1.30	5/248 (2.0%)
1	18	0.46	0/181	0.80	0/248
1	19	0.57	0/181	1.06	0/248
1	2	0.46	0/181	1.11	0/248
1	20	0.49	0/181	0.84	0/248
1	21	0.48	0/181	0.99	0/248
1	22	0.69	0/166	1.34	3/227 (1.3%)
1	23	0.49	0/166	1.08	0/227
1	3	0.41	0/181	0.93	0/248
1	4	0.42	0/181	1.04	1/248 (0.4%)
1	5	0.43	0/181	1.10	2/248 (0.8%)
1	6	0.39	0/181	1.03	0/248
1	7	0.36	0/181	0.80	0/248
1	8	0.44	0/181	1.01	0/248
1	9	0.46	0/181	1.04	2/248 (0.8%)
2	A0	0.50	1/3398 (0.0%)	0.95	9/4606 (0.2%)
2	A2	0.47	2/3398 (0.1%)	0.91	6/4606 (0.1%)
2	A4	0.64	5/3398 (0.1%)	1.00	7/4606 (0.2%)
2	A6	0.47	1/3398 (0.0%)	0.92	8/4606 (0.2%)
2	A8	0.58	2/3398 (0.1%)	1.00	6/4606 (0.1%)
2	B0	0.48	2/3398 (0.1%)	0.93	11/4606 (0.2%)
2	B2	0.50	0/3398	0.95	9/4606 (0.2%)
2	B4	0.45	2/3398 (0.1%)	0.87	5/4606 (0.1%)
2	B6	0.43	0/3398	0.84	3/4606 (0.1%)
2	B8	0.43	0/3398	0.85	7/4606 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	C0	0.48	3/3398 (0.1%)	0.85	5/4606 (0.1%)
2	C2	0.48	2/3398 (0.1%)	0.84	3/4606 (0.1%)
2	C4	0.62	2/3398 (0.1%)	1.10	10/4606 (0.2%)
2	C6	0.48	1/3398 (0.0%)	0.94	9/4606 (0.2%)
2	C8	0.46	0/3398	0.88	9/4606 (0.2%)
2	D0	0.47	1/3398 (0.0%)	0.95	9/4606 (0.2%)
2	D2	0.43	0/3398	0.84	8/4606 (0.2%)
2	D4	0.49	1/3398 (0.0%)	0.90	7/4606 (0.2%)
2	D6	0.42	0/3398	0.83	8/4606 (0.2%)
2	D8	0.46	0/3398	0.89	5/4606 (0.1%)
2	E0	0.38	0/3398	0.74	3/4606 (0.1%)
2	E2	0.45	1/3398 (0.0%)	0.83	1/4606 (0.0%)
2	E4	0.38	0/3398	0.78	4/4606 (0.1%)
2	E6	0.42	0/3398	0.81	1/4606 (0.0%)
2	E8	0.34	0/3398	0.68	0/4606
2	F0	0.49	1/3398 (0.0%)	0.87	5/4606 (0.1%)
3	A1	0.48	1/3404 (0.0%)	0.90	3/4606 (0.1%)
3	A3	0.39	0/3404	0.77	1/4606 (0.0%)
3	A5	0.49	0/3404	0.94	6/4606 (0.1%)
3	A7	0.44	1/3404 (0.0%)	0.85	2/4606 (0.0%)
3	A9	0.47	0/3404	0.90	5/4606 (0.1%)
3	B1	0.47	0/3404	0.87	2/4606 (0.0%)
3	B3	0.46	0/3404	0.88	7/4606 (0.2%)
3	B5	0.47	1/3404 (0.0%)	0.89	4/4606 (0.1%)
3	B7	0.46	1/3404 (0.0%)	0.88	7/4606 (0.2%)
3	B9	0.43	0/3404	0.83	5/4606 (0.1%)
3	C1	0.48	2/3404 (0.1%)	0.88	3/4606 (0.1%)
3	C3	0.46	1/3404 (0.0%)	0.85	4/4606 (0.1%)
3	C5	0.49	1/3404 (0.0%)	0.88	6/4606 (0.1%)
3	C7	0.46	0/3404	0.90	6/4606 (0.1%)
3	C9	0.48	1/3404 (0.0%)	0.94	14/4606 (0.3%)
3	D1	0.51	1/3404 (0.0%)	0.94	8/4606 (0.2%)
3	D3	0.47	2/3404 (0.1%)	0.87	4/4606 (0.1%)
3	D5	0.56	1/3404 (0.0%)	1.04	16/4606 (0.3%)
3	D7	0.46	1/3404 (0.0%)	0.84	5/4606 (0.1%)
3	D9	0.48	0/3404	0.93	8/4606 (0.2%)
3	E1	0.42	0/3404	0.82	5/4606 (0.1%)
3	E3	0.51	4/3404 (0.1%)	0.90	8/4606 (0.2%)
3	E5	0.45	1/3404 (0.0%)	0.81	3/4606 (0.1%)
3	E7	0.48	1/3404 (0.0%)	0.89	6/4606 (0.1%)
3	E9	0.44	0/3404	0.88	7/4606 (0.2%)
3	F1	0.47	1/3404 (0.0%)	0.96	7/4606 (0.2%)
4	a	0.58	1/1225 (0.1%)	1.05	4/1654 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	b	0.56	2/1225 (0.2%)	1.00	7/1654 (0.4%)
4	c	0.70	2/1645 (0.1%)	1.28	10/2225 (0.4%)
4	d	0.54	0/1645	1.08	9/2225 (0.4%)
4	e	0.51	0/1645	1.00	3/2225 (0.1%)
4	f	0.59	4/1645 (0.2%)	0.99	8/2225 (0.4%)
4	g	0.49	0/1645	1.00	4/2225 (0.2%)
4	h	0.48	1/1645 (0.1%)	0.92	2/2225 (0.1%)
4	i	0.47	0/1645	0.92	2/2225 (0.1%)
4	j	0.46	0/1645	0.90	1/2225 (0.0%)
4	k	0.50	1/1645 (0.1%)	0.98	5/2225 (0.2%)
4	l	0.45	0/1645	0.92	4/2225 (0.2%)
4	m	0.60	3/1645 (0.2%)	1.04	12/2225 (0.5%)
4	n	0.53	0/1645	1.03	5/2225 (0.2%)
4	o	0.48	0/1645	1.01	5/2225 (0.2%)
4	p	0.54	0/1645	1.10	8/2225 (0.4%)
4	q	0.56	2/1645 (0.1%)	0.98	3/2225 (0.1%)
4	r	0.55	0/1645	1.09	10/2225 (0.4%)
4	s	0.43	0/1645	0.91	2/2225 (0.1%)
4	t	0.49	0/1645	1.04	7/2225 (0.3%)
4	u	0.47	0/1645	0.86	3/2225 (0.1%)
4	v	0.46	0/1645	0.89	0/2225
4	x	0.43	0/1645	0.91	5/2225 (0.2%)
4	y	0.41	0/1645	0.89	3/2225 (0.1%)
5	w	0.43	0/1201	0.90	5/1623 (0.3%)
All	All	0.48	66/221007 (0.0%)	0.91	453/299303 (0.2%)

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	12	0	1
1	19	0	1
1	2	0	1
1	20	0	2
1	21	0	1
1	23	0	1
1	7	0	1
1	8	0	1
2	A0	0	1
2	A2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	A4	0	1
2	A8	0	1
2	B4	0	1
2	B6	0	2
2	C4	0	1
2	C8	0	1
2	D2	0	2
2	D8	0	1
2	E4	0	1
2	F0	0	1
3	B3	0	1
3	B9	0	1
3	E5	0	2
3	E9	0	1
4	o	0	1
4	s	0	1
All	All	0	31

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C4	2	ARG	NE-CZ	19.02	1.57	1.33
2	C4	2	ARG	CD-NE	16.25	1.74	1.46
2	A4	254	GLU	CD-OE2	16.25	1.43	1.25
4	c	178	ARG	NE-CZ	14.78	1.52	1.33
2	F0	284	GLU	CD-OE1	12.40	1.39	1.25

The worst 5 of 453 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C4	2	ARG	NE-CZ-NH1	37.15	138.88	120.30
4	c	178	ARG	NE-CZ-NH1	21.23	130.91	120.30
2	C4	2	ARG	CD-NE-CZ	20.60	152.44	123.60
3	F1	391	ARG	NE-CZ-NH1	19.42	130.01	120.30
4	c	178	ARG	CD-NE-CZ	18.04	148.85	123.60

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	12	255	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	19	257	PRO	Peptide
1	2	239	LEU	Peptide
1	20	238	THR	Peptide
1	20	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	10	0
1	1	174	0	171	6	0
1	10	174	0	171	14	0
1	11	174	0	171	6	0
1	12	174	0	171	4	0
1	13	174	0	171	7	0
1	14	174	0	171	0	0
1	15	174	0	171	9	0
1	16	174	0	171	9	0
1	17	174	0	171	4	0
1	18	174	0	171	29	0
1	19	174	0	171	28	0
1	2	174	0	171	7	0
1	20	174	0	171	8	0
1	21	174	0	171	23	0
1	22	160	0	156	8	0
1	23	160	0	156	10	0
1	3	174	0	171	5	0
1	4	174	0	171	7	0
1	5	174	0	171	3	0
1	6	174	0	171	13	0
1	7	174	0	171	7	0
1	8	174	0	171	10	0
1	9	174	0	171	6	0
2	A0	3325	0	3252	76	0
2	A2	3325	0	3252	87	0
2	A4	3325	0	3252	56	0
2	A6	3325	0	3252	79	0
2	A8	3325	0	3252	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B0	3325	0	3252	91	0
2	B2	3325	0	3252	52	0
2	B4	3325	0	3252	80	0
2	B6	3325	0	3252	65	0
2	B8	3325	0	3252	72	0
2	C0	3325	0	3252	69	0
2	C2	3325	0	3252	66	0
2	C4	3325	0	3252	82	0
2	C6	3325	0	3252	99	0
2	C8	3325	0	3252	56	0
2	D0	3325	0	3252	71	0
2	D2	3325	0	3252	60	0
2	D4	3325	0	3252	91	0
2	D6	3325	0	3252	55	0
2	D8	3325	0	3252	61	0
2	E0	3325	0	3252	92	0
2	E2	3325	0	3252	62	0
2	E4	3325	0	3252	147	0
2	E6	3325	0	3252	93	0
2	E8	3325	0	3252	70	0
2	F0	3325	0	3252	104	0
3	A1	3331	0	3207	84	0
3	A3	3331	0	3209	66	0
3	A5	3331	0	3207	66	0
3	A7	3331	0	3207	55	0
3	A9	3331	0	3207	75	0
3	B1	3331	0	3209	89	0
3	B3	3331	0	3207	56	0
3	B5	3331	0	3207	71	0
3	B7	3331	0	3209	73	0
3	B9	3331	0	3209	56	0
3	C1	3331	0	3209	83	0
3	C3	3331	0	3209	76	0
3	C5	3331	0	3209	75	0
3	C7	3331	0	3209	64	0
3	C9	3331	0	3209	82	0
3	D1	3331	0	3209	67	0
3	D3	3331	0	3207	90	0
3	D5	3331	0	3207	81	0
3	D7	3331	0	3207	72	0
3	D9	3331	0	3207	65	0
3	E1	3331	0	3207	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E3	3331	0	3209	51	0
3	E5	3331	0	3207	154	0
3	E7	3331	0	3207	70	0
3	E9	3331	0	3207	64	0
3	F1	3331	0	3207	67	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	k	1608	0	1590	0	0
4	l	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	1590	0	0
4	x	1608	0	1590	0	0
4	y	1608	0	1590	0	0
5	w	1172	0	1171	0	0
All	All	216148	0	210569	3331	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 10.

The worst 5 of 3331 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)
2:C4:2:ARG:NE	2:C4:2:ARG:CD	1.74	1.46
1:13:247:TYR:OH	2:D4:81:GLY:HA3	1.22	1.27
3:A1:219:THR:CG2	2:A2:324:VAL:HG21	1.69	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:15:247:TYR:OH	2:D8:81:GLY:CA	1.88	1.20
1:15:247:TYR:OH	2:D8:81:GLY:HA3	1.09	1.19

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%)	15 (75%)	5 (25%)	0	100	100
1	12	20/351 (6%)	18 (90%)	2 (10%)	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%)	19 (95%)	1 (5%)	0	100	100
1	16	20/351 (6%)	19 (95%)	1 (5%)	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%)	17 (85%)	3 (15%)	0	100	100
1	2	20/351 (6%)	17 (85%)	3 (15%)	0	100	100
1	20	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	21	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	22	18/351 (5%)	14 (78%)	4 (22%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	20/351 (6%)	20 (100%)	0	0	100	100
1	5	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	6	20/351 (6%)	20 (100%)	0	0	100	100
1	7	20/351 (6%)	20 (100%)	0	0	100	100
1	8	20/351 (6%)	17 (85%)	3 (15%)	0	100	100
1	9	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
2	A0	424/453 (94%)	397 (94%)	27 (6%)	0	100	100
2	A2	424/453 (94%)	406 (96%)	17 (4%)	1 (0%)	44	78
2	A4	424/453 (94%)	398 (94%)	26 (6%)	0	100	100
2	A6	424/453 (94%)	399 (94%)	25 (6%)	0	100	100
2	A8	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
2	B0	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	B2	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
2	B4	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
2	B6	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	B8	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	C0	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
2	C2	424/453 (94%)	395 (93%)	28 (7%)	1 (0%)	44	78
2	C4	424/453 (94%)	390 (92%)	33 (8%)	1 (0%)	44	78
2	C6	424/453 (94%)	396 (93%)	28 (7%)	0	100	100
2	C8	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
2	D0	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
2	D2	424/453 (94%)	405 (96%)	18 (4%)	1 (0%)	44	78
2	D4	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
2	D6	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	D8	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	E0	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	E2	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	E4	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	E6	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	E8	424/453 (94%)	400 (94%)	24 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F0	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
3	A1	424/449 (94%)	390 (92%)	34 (8%)	0	100	100
3	A3	424/449 (94%)	402 (95%)	21 (5%)	1 (0%)	44	78
3	A5	424/449 (94%)	388 (92%)	34 (8%)	2 (0%)	25	64
3	A7	424/449 (94%)	394 (93%)	29 (7%)	1 (0%)	44	78
3	A9	424/449 (94%)	395 (93%)	28 (7%)	1 (0%)	44	78
3	B1	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	B3	424/449 (94%)	397 (94%)	25 (6%)	2 (0%)	25	64
3	B5	424/449 (94%)	394 (93%)	28 (7%)	2 (0%)	25	64
3	B7	424/449 (94%)	399 (94%)	24 (6%)	1 (0%)	44	78
3	B9	424/449 (94%)	405 (96%)	18 (4%)	1 (0%)	44	78
3	C1	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
3	C3	424/449 (94%)	398 (94%)	25 (6%)	1 (0%)	44	78
3	C5	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
3	C7	424/449 (94%)	394 (93%)	29 (7%)	1 (0%)	44	78
3	C9	424/449 (94%)	395 (93%)	28 (7%)	1 (0%)	44	78
3	D1	424/449 (94%)	398 (94%)	25 (6%)	1 (0%)	44	78
3	D3	424/449 (94%)	394 (93%)	28 (7%)	2 (0%)	25	64
3	D5	424/449 (94%)	396 (93%)	26 (6%)	2 (0%)	25	64
3	D7	424/449 (94%)	404 (95%)	20 (5%)	0	100	100
3	D9	424/449 (94%)	398 (94%)	25 (6%)	1 (0%)	44	78
3	E1	424/449 (94%)	402 (95%)	21 (5%)	1 (0%)	44	78
3	E3	424/449 (94%)	400 (94%)	23 (5%)	1 (0%)	44	78
3	E5	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	E7	424/449 (94%)	400 (94%)	23 (5%)	1 (0%)	44	78
3	E9	424/449 (94%)	393 (93%)	31 (7%)	0	100	100
3	F1	424/449 (94%)	391 (92%)	32 (8%)	1 (0%)	44	78
4	a	146/220 (66%)	134 (92%)	11 (8%)	1 (1%)	19	57
4	b	146/220 (66%)	134 (92%)	12 (8%)	0	100	100
4	c	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	d	197/220 (90%)	180 (91%)	17 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	e	197/220 (90%)	185 (94%)	11 (6%)	1 (0%)	25	64
4	f	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	g	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	h	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
4	i	197/220 (90%)	182 (92%)	14 (7%)	1 (0%)	25	64
4	j	197/220 (90%)	182 (92%)	15 (8%)	0	100	100
4	k	197/220 (90%)	183 (93%)	13 (7%)	1 (0%)	25	64
4	l	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	m	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
4	n	197/220 (90%)	182 (92%)	14 (7%)	1 (0%)	25	64
4	o	197/220 (90%)	180 (91%)	17 (9%)	0	100	100
4	p	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	q	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	r	197/220 (90%)	184 (93%)	12 (6%)	1 (0%)	25	64
4	s	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
4	t	197/220 (90%)	188 (95%)	7 (4%)	2 (1%)	13	49
4	u	197/220 (90%)	188 (95%)	8 (4%)	1 (0%)	25	64
4	v	197/220 (90%)	180 (91%)	17 (9%)	0	100	100
4	x	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	y	197/220 (90%)	184 (93%)	12 (6%)	1 (0%)	25	64
5	w	139/189 (74%)	133 (96%)	6 (4%)	0	100	100
All	All	27289/37345 (73%)	25630 (94%)	1620 (6%)	39 (0%)	50	83

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A3	179	VAL
3	A5	55	THR
3	A7	55	THR
3	A9	55	THR
3	B3	55	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	1	20/304 (7%)	20 (100%)	0	100	100
1	10	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	11	20/304 (7%)	18 (90%)	2 (10%)	6	20
1	12	20/304 (7%)	19 (95%)	1 (5%)	20	41
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%)	20 (100%)	0	100	100
1	18	20/304 (7%)	19 (95%)	1 (5%)	20	41
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%)	18 (100%)	0	100	100
1	23	18/304 (6%)	18 (100%)	0	100	100
1	3	20/304 (7%)	18 (90%)	2 (10%)	6	20
1	4	20/304 (7%)	20 (100%)	0	100	100
1	5	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	6	20/304 (7%)	18 (90%)	2 (10%)	6	20
1	7	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	8	20/304 (7%)	19 (95%)	1 (5%)	20	41
1	9	20/304 (7%)	20 (100%)	0	100	100
2	A0	359/379 (95%)	353 (98%)	6 (2%)	56	72
2	A2	359/379 (95%)	352 (98%)	7 (2%)	52	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A4	359/379 (95%)	348 (97%)	11 (3%)	35	54
2	A6	359/379 (95%)	351 (98%)	8 (2%)	47	65
2	A8	359/379 (95%)	354 (99%)	5 (1%)	62	75
2	B0	359/379 (95%)	349 (97%)	10 (3%)	38	57
2	B2	359/379 (95%)	351 (98%)	8 (2%)	47	65
2	B4	359/379 (95%)	352 (98%)	7 (2%)	52	69
2	B6	359/379 (95%)	354 (99%)	5 (1%)	62	75
2	B8	359/379 (95%)	356 (99%)	3 (1%)	79	85
2	C0	359/379 (95%)	355 (99%)	4 (1%)	70	80
2	C2	359/379 (95%)	356 (99%)	3 (1%)	79	85
2	C4	359/379 (95%)	353 (98%)	6 (2%)	56	72
2	C6	359/379 (95%)	351 (98%)	8 (2%)	47	65
2	C8	359/379 (95%)	350 (98%)	9 (2%)	42	61
2	D0	359/379 (95%)	355 (99%)	4 (1%)	70	80
2	D2	359/379 (95%)	352 (98%)	7 (2%)	52	69
2	D4	359/379 (95%)	350 (98%)	9 (2%)	42	61
2	D6	359/379 (95%)	354 (99%)	5 (1%)	62	75
2	D8	359/379 (95%)	355 (99%)	4 (1%)	70	80
2	E0	359/379 (95%)	356 (99%)	3 (1%)	79	85
2	E2	359/379 (95%)	353 (98%)	6 (2%)	56	72
2	E4	359/379 (95%)	354 (99%)	5 (1%)	62	75
2	E6	359/379 (95%)	355 (99%)	4 (1%)	70	80
2	E8	359/379 (95%)	357 (99%)	2 (1%)	84	88
2	F0	359/379 (95%)	349 (97%)	10 (3%)	38	57
3	A1	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	A3	364/381 (96%)	358 (98%)	6 (2%)	58	74
3	A5	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	A7	364/381 (96%)	358 (98%)	6 (2%)	58	74
3	A9	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	B1	364/381 (96%)	361 (99%)	3 (1%)	79	85
3	B3	364/381 (96%)	359 (99%)	5 (1%)	62	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B5	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	B7	364/381 (96%)	356 (98%)	8 (2%)	47	65
3	B9	364/381 (96%)	357 (98%)	7 (2%)	52	69
3	C1	364/381 (96%)	361 (99%)	3 (1%)	79	85
3	C3	364/381 (96%)	360 (99%)	4 (1%)	70	80
3	C5	364/381 (96%)	355 (98%)	9 (2%)	42	61
3	C7	364/381 (96%)	351 (96%)	13 (4%)	30	50
3	C9	364/381 (96%)	360 (99%)	4 (1%)	70	80
3	D1	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	D3	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	D5	364/381 (96%)	354 (97%)	10 (3%)	40	58
3	D7	364/381 (96%)	358 (98%)	6 (2%)	58	74
3	D9	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	E1	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	E3	364/381 (96%)	357 (98%)	7 (2%)	52	69
3	E5	364/381 (96%)	357 (98%)	7 (2%)	52	69
3	E7	364/381 (96%)	355 (98%)	9 (2%)	42	61
3	E9	364/381 (96%)	359 (99%)	5 (1%)	62	75
3	F1	364/381 (96%)	358 (98%)	6 (2%)	58	74
4	a	130/190 (68%)	126 (97%)	4 (3%)	35	54
4	b	130/190 (68%)	128 (98%)	2 (2%)	60	75
4	c	174/190 (92%)	172 (99%)	2 (1%)	70	80
4	d	174/190 (92%)	169 (97%)	5 (3%)	37	56
4	e	174/190 (92%)	168 (97%)	6 (3%)	32	51
4	f	174/190 (92%)	170 (98%)	4 (2%)	45	64
4	g	174/190 (92%)	170 (98%)	4 (2%)	45	64
4	h	174/190 (92%)	169 (97%)	5 (3%)	37	56
4	i	174/190 (92%)	171 (98%)	3 (2%)	56	72
4	j	174/190 (92%)	172 (99%)	2 (1%)	70	80
4	k	174/190 (92%)	169 (97%)	5 (3%)	37	56
4	l	174/190 (92%)	170 (98%)	4 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	m	174/190 (92%)	169 (97%)	5 (3%)	37	56
4	n	174/190 (92%)	168 (97%)	6 (3%)	32	51
4	o	174/190 (92%)	166 (95%)	8 (5%)	23	44
4	p	174/190 (92%)	171 (98%)	3 (2%)	56	72
4	q	174/190 (92%)	169 (97%)	5 (3%)	37	56
4	r	174/190 (92%)	168 (97%)	6 (3%)	32	51
4	s	174/190 (92%)	170 (98%)	4 (2%)	45	64
4	t	174/190 (92%)	171 (98%)	3 (2%)	56	72
4	u	174/190 (92%)	171 (98%)	3 (2%)	56	72
4	v	174/190 (92%)	166 (95%)	8 (5%)	23	44
4	x	174/190 (92%)	167 (96%)	7 (4%)	27	47
4	y	174/190 (92%)	170 (98%)	4 (2%)	45	64
5	w	127/164 (77%)	123 (97%)	4 (3%)	35	54
All	All	23489/31780 (74%)	23041 (98%)	448 (2%)	52	69

5 of 448 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D4	214	ARG
4	x	198	ARG
3	E3	391	ARG
4	x	56	LYS
4	o	164	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 185 such sidechains are listed below:

Mol	Chain	Res	Type
2	E2	258	ASN
4	d	35	ASN
3	E3	291	GLN
3	E7	245	GLN
4	j	67	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

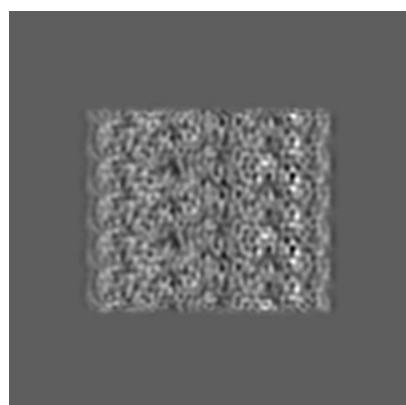
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26019. These allow visual inspection of the internal detail of the map and identification of artifacts.

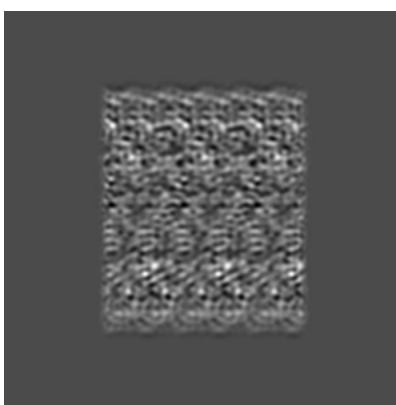
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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: 156



Y Index: 153

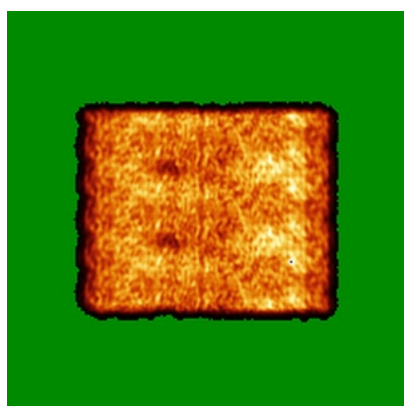


Z Index: 155

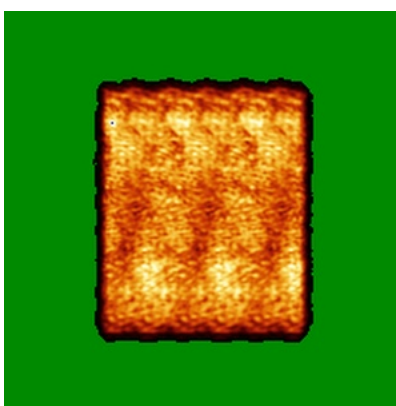
The images above show the largest variance slices of the map in three orthogonal directions.

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

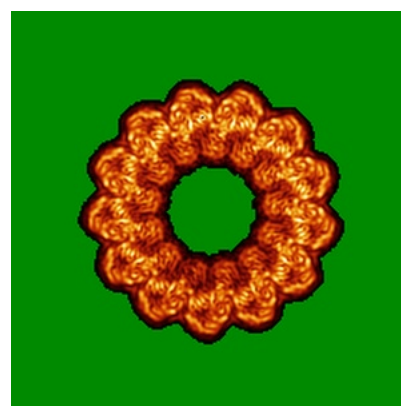
6.4.1 Primary map



X



Y

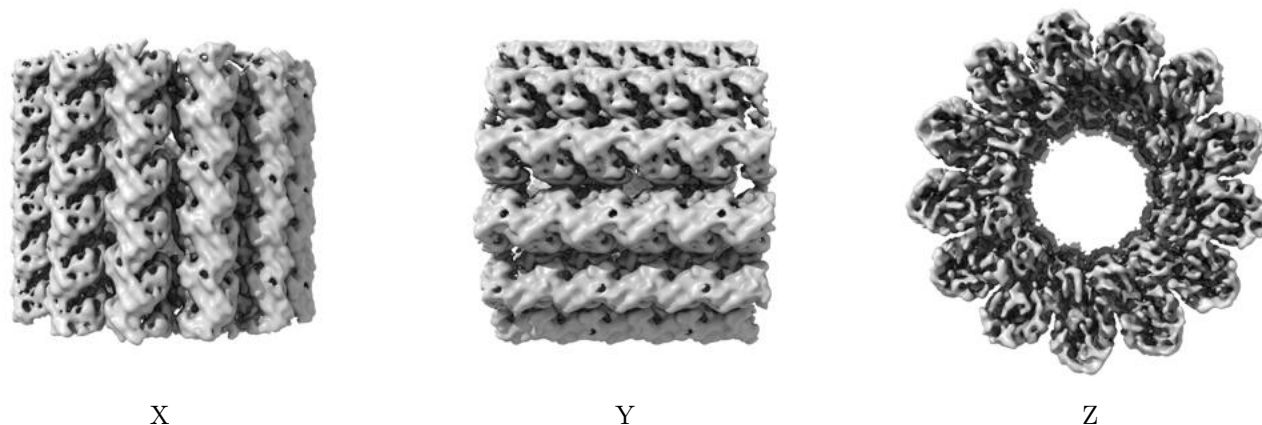


Z

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



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.

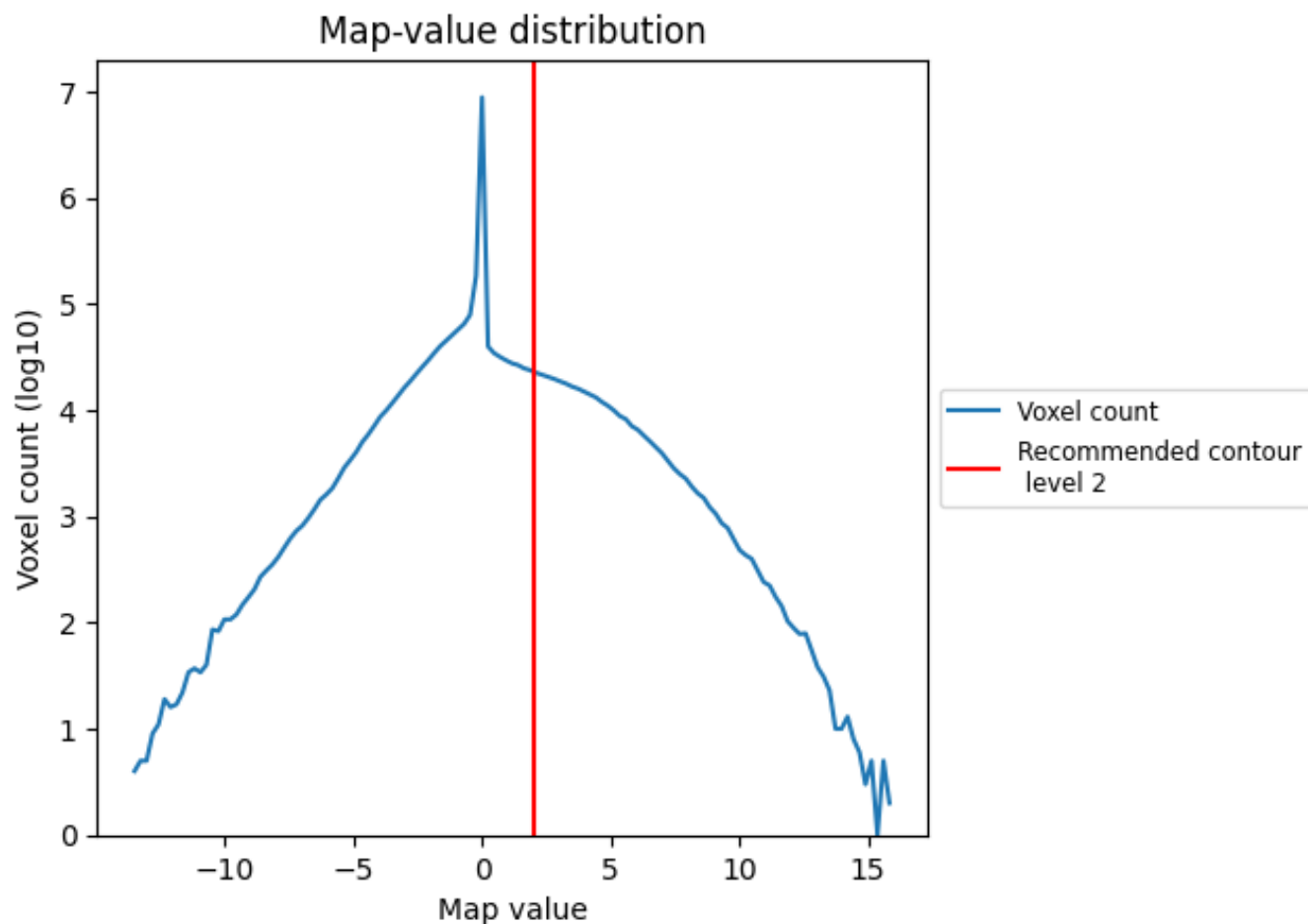
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

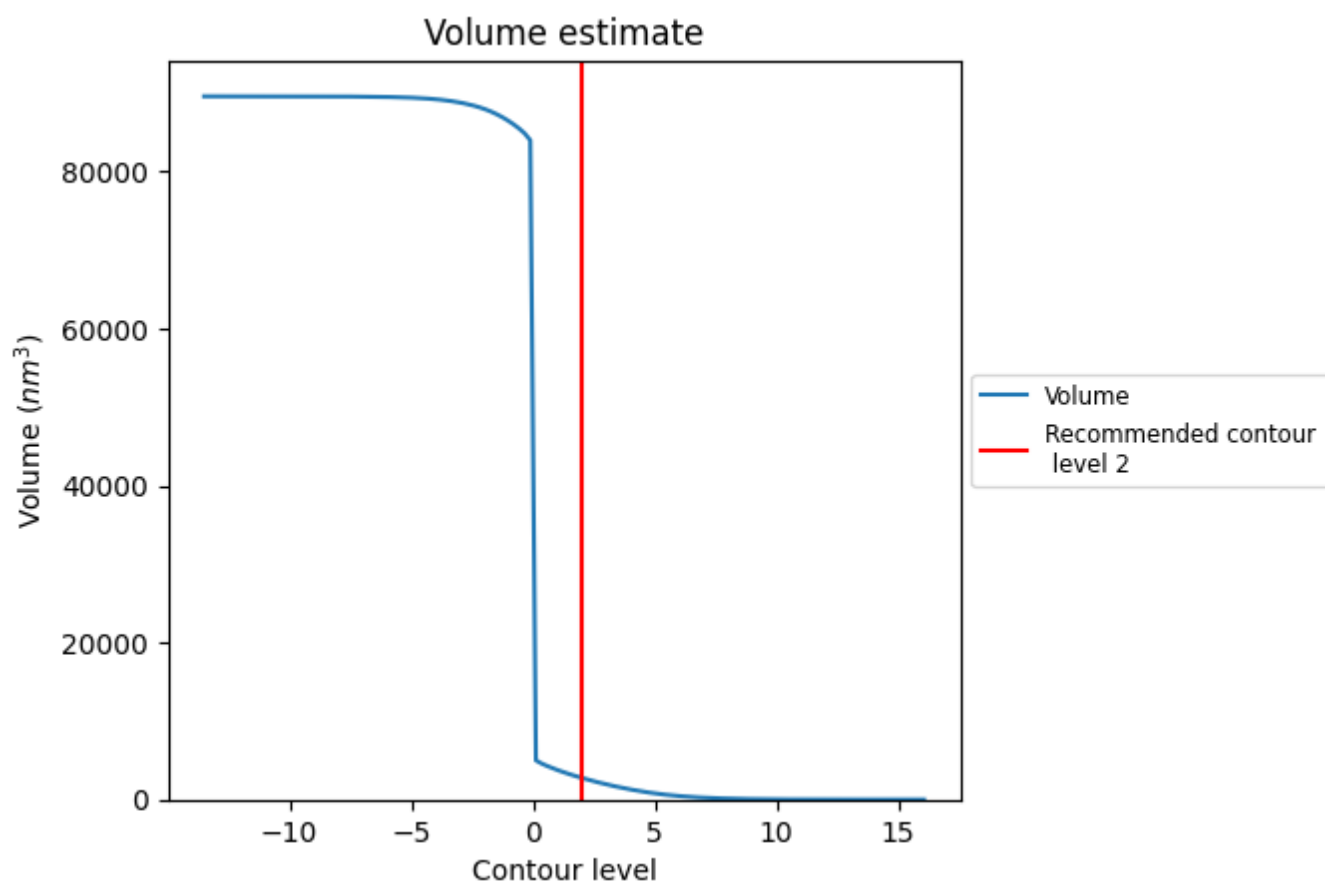
This section contains the results of statistical analysis of the map.

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.

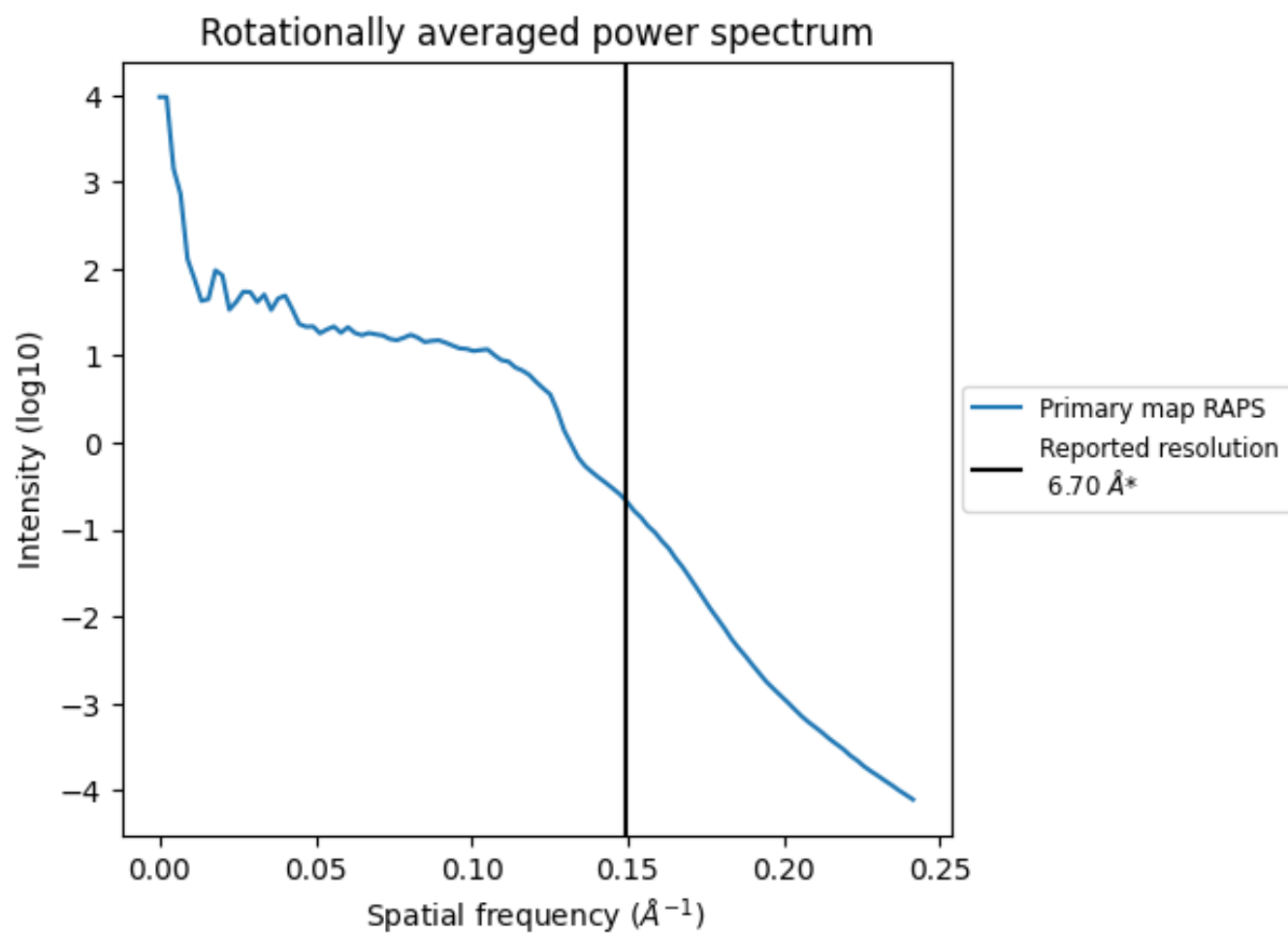
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2760 nm³; this corresponds to an approximate mass of 2494 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 0.149 Å⁻¹

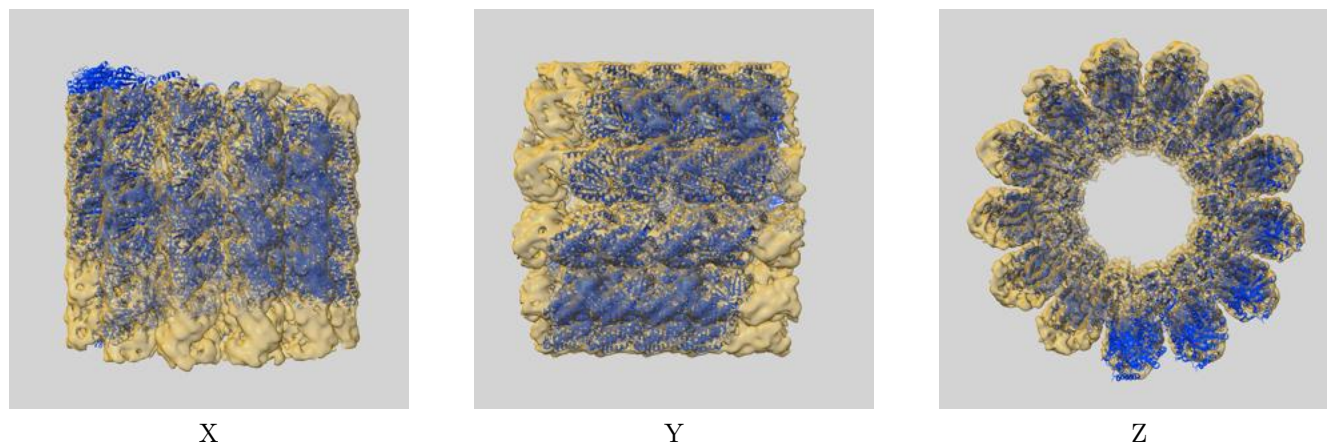
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

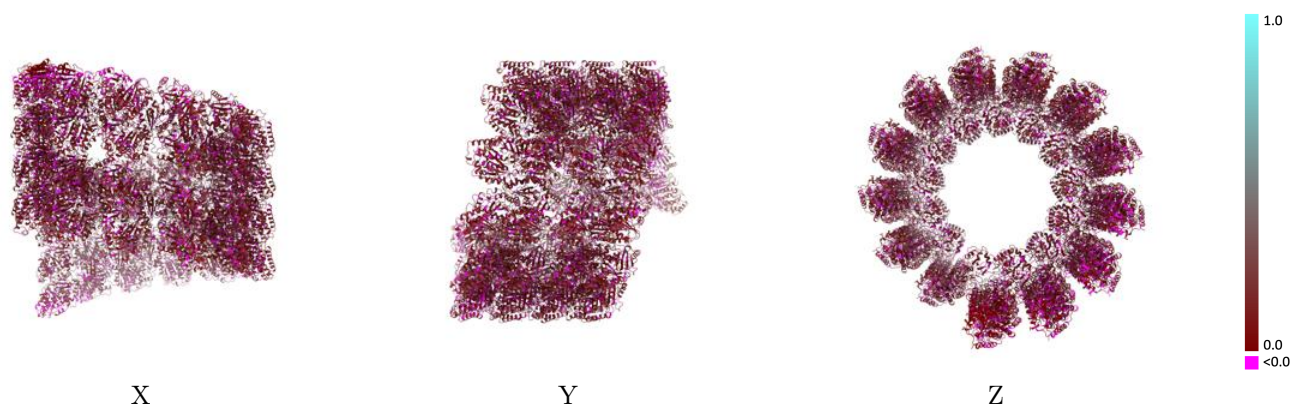
This section contains information regarding the fit between EMDB map EMD-26019 and PDB model 7TNS. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



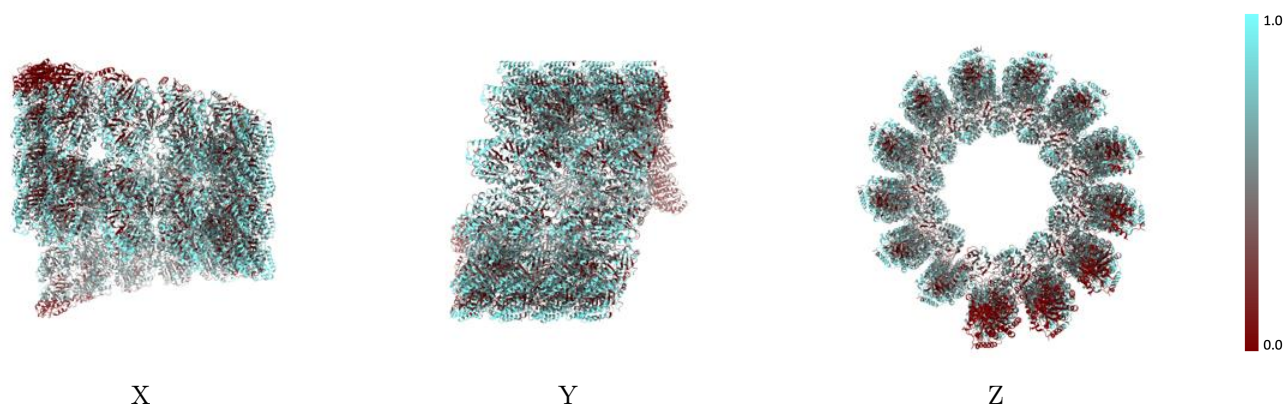
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



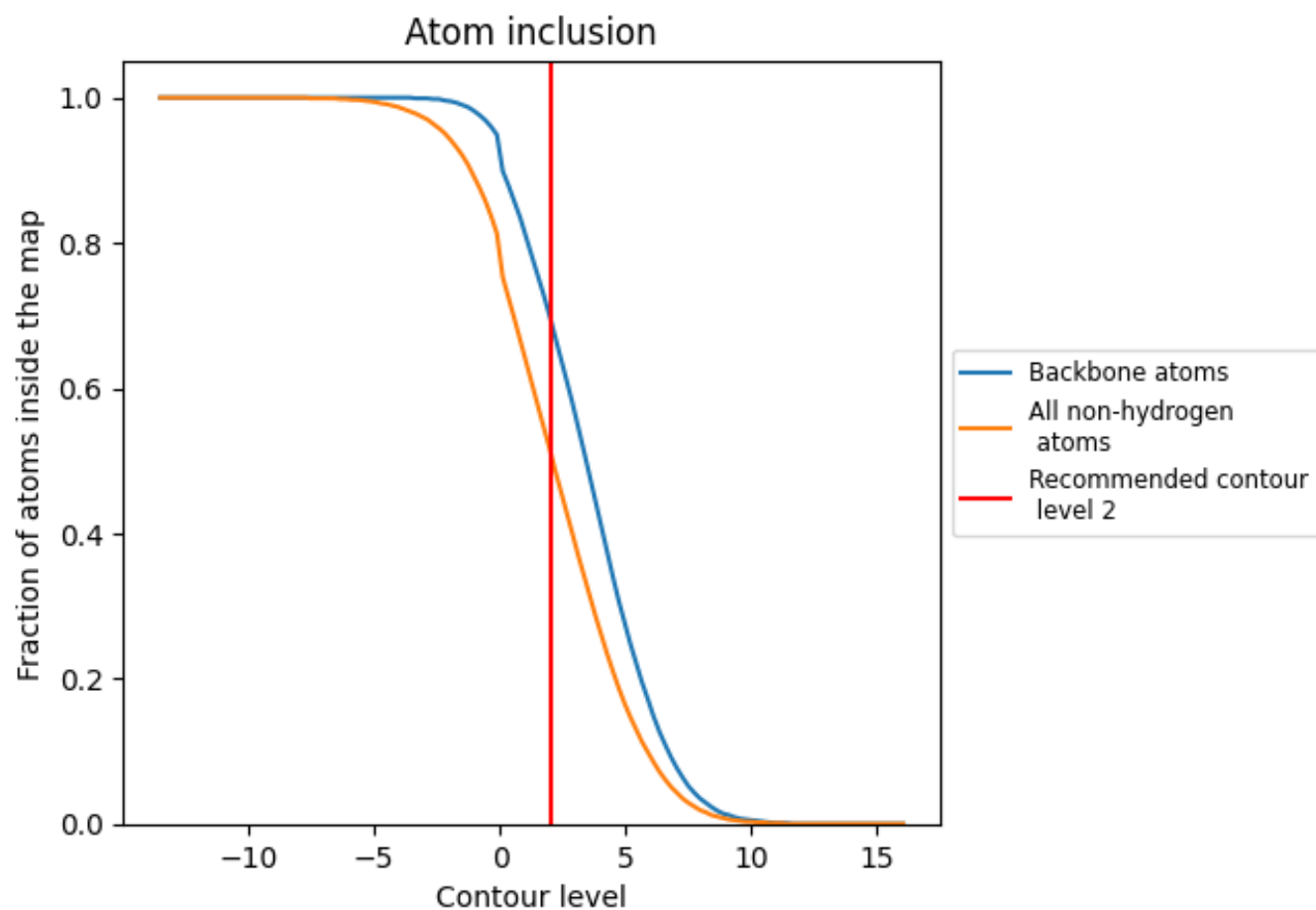
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 70% of all backbone atoms, 52% 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	 0.5150	 0.1180
0	 0.2880	 0.1450
1	 0.3000	 0.1410
10	 0.3880	 0.1250
11	 0.3770	 0.1420
12	 0.3710	 0.1570
13	 0.3470	 0.1610
14	 0.2770	 0.1400
15	 0.3350	 0.1650
16	 0.2120	 0.1180
17	 0.3000	 0.1450
18	 0.0470	 0.0790
19	 0.1000	 0.0800
2	 0.3240	 0.1350
20	 0.0000	 0.0600
21	 0.1710	 0.0210
22	 0.3650	 0.1020
23	 0.3590	 0.1330
3	 0.3410	 0.1590
4	 0.3350	 0.1460
5	 0.3880	 0.1640
6	 0.3710	 0.1390
7	 0.3180	 0.1220
8	 0.3470	 0.1410
9	 0.3180	 0.1130
A0	 0.5410	 0.1270
A1	 0.5410	 0.1220
A2	 0.5450	 0.1240
A3	 0.3160	 0.0720
A4	 0.5640	 0.1300
A5	 0.5420	 0.1250
A6	 0.5610	 0.1270
A7	 0.4440	 0.0970
A8	 0.5680	 0.1290
A9	 0.5510	 0.1270





















































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Chain	Atom inclusion	Q-score
B0	 0.5640	 0.1260
B1	 0.4770	 0.0940
B2	 0.5620	 0.1280
B3	 0.5590	 0.1210
B4	 0.5620	 0.1260
B5	 0.5190	 0.1020
B6	 0.5520	 0.1200
B7	 0.5630	 0.1200
B8	 0.5570	 0.1190
B9	 0.5680	 0.1170
C0	 0.5670	 0.1310
C1	 0.5730	 0.1230
C2	 0.5620	 0.1300
C3	 0.5730	 0.1200
C4	 0.5620	 0.1310
C5	 0.5810	 0.1280
C6	 0.5520	 0.1250
C7	 0.5840	 0.1230
C8	 0.5470	 0.1270
C9	 0.5890	 0.1300
D0	 0.5540	 0.1270
D1	 0.5910	 0.1260
D2	 0.5270	 0.1210
D3	 0.5800	 0.1270
D4	 0.5520	 0.1280
D5	 0.5880	 0.1260
D6	 0.4660	 0.1050
D7	 0.5750	 0.1290
D8	 0.5500	 0.1300
D9	 0.5760	 0.1250
E0	 0.3190	 0.0770
E1	 0.5510	 0.1200
E2	 0.5540	 0.1280
E3	 0.5630	 0.1200
E4	 0.1930	 0.0440
E5	 0.5400	 0.1200
E6	 0.5510	 0.1250
E7	 0.5400	 0.1200
E8	 0.0500	 0.0060
E9	 0.5170	 0.1160
F0	 0.5540	 0.1250
F1	 0.5370	 0.1200

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Chain	Atom inclusion	Q-score
a	 0.4960	 0.1230
b	 0.4710	 0.1120
c	 0.4990	 0.1250
d	 0.5070	 0.1220
e	 0.5110	 0.1290
f	 0.5110	 0.1280
g	 0.5130	 0.1210
h	 0.5280	 0.1240
i	 0.5250	 0.1290
j	 0.5190	 0.1320
k	 0.5070	 0.1260
l	 0.5190	 0.1290
m	 0.5110	 0.1300
n	 0.5060	 0.1300
o	 0.4990	 0.1310
p	 0.4990	 0.1290
q	 0.4920	 0.1250
r	 0.4930	 0.1310
s	 0.4880	 0.1280
t	 0.4650	 0.1220
u	 0.4320	 0.1110
v	 0.4830	 0.1240
w	 0.3220	 0.0780
x	 0.4590	 0.1250
y	 0.3440	 0.1120