



## wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 09:14 PM EDT

PDB ID : 9NW3 / pdb\_00009nw3  
EMDB ID : EMD-49872  
Title : Ciliary tip central pair  
Authors : Legal, T.L.; Bui, K.H.  
Deposited on : 2025-03-21  
Resolution : 3.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
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) : 2.45.1

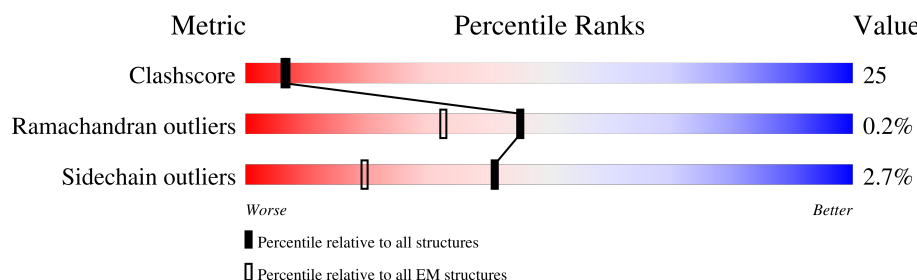
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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  $\geq 3$ , 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	AA	449	<div> <div>21%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
1	AC	449	<div> <div>22%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
1	AE	449	<div> <div>25%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
1	BA	449	<div> <div>15%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
1	BC	449	<div> <div>13%</div> <div>69%</div> <div>26%</div> <div>.</div> </div>
1	BE	449	<div> <div>13%</div> <div>69%</div> <div>26%</div> <div>.</div> </div>
1	CA	449	<div> <div>10%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
1	CC	449	<div> <div>8%</div> <div>69%</div> <div>26%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	CE	449	<div> <div>9%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
1	DA	449	<div> <div>18%</div> <div>70%</div> <div>25%</div> <div>.</div> </div>
1	DC	449	<div> <div>16%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	DE	449	<div> <div>11%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	EA	449	<div> <div>33%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
1	EC	449	<div> <div>29%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	EE	449	<div> <div>26%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
1	FA	449	<div> <div>46%</div> <div>68%</div> <div>27%</div> <div>.</div> </div>
1	FC	449	<div> <div>42%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
1	FE	449	<div> <div>39%</div> <div>67%</div> <div>28%</div> <div>.</div> </div>
1	GA	449	<div> <div>49%</div> <div>73%</div> <div>22%</div> <div>.</div> </div>
1	GC	449	<div> <div>49%</div> <div>70%</div> <div>25%</div> <div>.</div> </div>
1	GE	449	<div> <div>51%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
1	HA	449	<div> <div>49%</div> <div>71%</div> <div>24%</div> <div>.</div> </div>
1	HC	449	<div> <div>47%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
1	HE	449	<div> <div>49%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
1	IA	449	<div> <div>49%</div> <div>71%</div> <div>24%</div> <div>.</div> </div>
1	IC	449	<div> <div>47%</div> <div>68%</div> <div>27%</div> <div>.</div> </div>
1	IE	449	<div> <div>49%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	JA	449	<div> <div>50%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
1	JC	449	<div> <div>52%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
1	JE	449	<div> <div>55%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
1	KA	449	<div> <div>56%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
1	KC	449	<div> <div>56%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
1	KE	449	<div> <div>57%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	LA	449	
1	LC	449	
1	LE	449	
1	MA	449	
1	MC	449	
1	ME	449	
2	AB	443	
2	AD	443	
2	AF	443	
2	BB	443	
2	BD	443	
2	BF	443	
2	CB	443	
2	CD	443	
2	CF	443	
2	DB	443	
2	DD	443	
2	DF	443	
2	EB	443	
2	ED	443	
2	EF	443	
2	FB	443	
2	FD	443	
2	FF	443	
2	GB	443	

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Mol	Chain	Length	Quality of chain
2	GD	443	<div> <div>50%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
2	GF	443	<div> <div>51%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
2	HB	443	<div> <div>48%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
2	HD	443	<div> <div>49%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
2	HF	443	<div> <div>52%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
2	IB	443	<div> <div>50%</div> <div>69%</div> <div>27%</div> <div>.</div> </div>
2	ID	443	<div> <div>50%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
2	IF	443	<div> <div>49%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
2	JB	443	<div> <div>53%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>
2	JD	443	<div> <div>55%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
2	JF	443	<div> <div>61%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
2	KB	443	<div> <div>54%</div> <div>65%</div> <div>32%</div> <div>.</div> </div>
2	KD	443	<div> <div>53%</div> <div>66%</div> <div>31%</div> <div>.</div> </div>
2	KF	443	<div> <div>51%</div> <div>68%</div> <div>28%</div> <div>..</div> </div>
2	LB	443	<div> <div>45%</div> <div>64%</div> <div>33%</div> <div>.</div> </div>
2	LD	443	<div> <div>43%</div> <div>65%</div> <div>32%</div> <div>.</div> </div>
2	LF	443	<div> <div>42%</div> <div>66%</div> <div>30%</div> <div>.</div> </div>
2	MB	443	<div> <div>37%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>
2	MD	443	<div> <div>35%</div> <div>69%</div> <div>28%</div> <div>.</div> </div>
2	MF	443	<div> <div>35%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
3	1A	213	<div> <div>45%</div> <div>60%</div> <div>6%</div> <div>34%</div> </div>
3	1B	213	<div> <div>44%</div> <div>61%</div> <div>5%</div> <div>34%</div> </div>
3	1C	213	<div> <div>44%</div> <div>61%</div> <div>5%</div> <div>34%</div> </div>
4	2A	742	<div> <div>14%</div> <div>17%</div> <div>6%</div> <div>74%</div> </div>
4	2B	742	<div> <div>13%</div> <div>17%</div> <div>7%</div> <div>74%</div> </div>

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Mol	Chain	Length	Quality of chain
4	2C	742	
5	3A	495	
5	3B	495	
5	3C	495	
6	4A	317	
6	4B	317	
6	4C	317	
6	4D	317	
7	5A	1754	
7	5B	1754	
7	5C	1754	
8	6A	346	
8	6B	346	
8	6C	346	
9	7A	101	
9	7B	101	
9	7C	101	
9	7D	101	
9	7E	101	
9	7F	101	
10	8A	38	
10	8B	38	
10	8C	38	
10	8D	38	
10	8E	38	

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Mol	Chain	Length	Quality of chain
10	8F	38	
10	8G	38	
10	8H	38	
10	8I	38	
10	8J	38	
10	8K	38	
10	8L	38	
10	8M	38	
10	8N	38	
10	8O	38	
10	8P	38	
10	8Q	38	
10	8R	38	
10	8S	38	
10	8T	38	
10	8U	38	
10	8V	38	
10	8W	38	
10	8X	38	
10	8Y	38	
10	8Z	38	
10	9A	38	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 318666 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	AC	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	AE	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	BA	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	BC	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	BE	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	CA	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	CC	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	CE	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	DA	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	DC	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	DE	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	EA	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	EC	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	EE	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	FA	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		
1	FC	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FE	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	GA	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	GC	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	GE	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	HA	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	HC	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	HE	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	IA	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	IC	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	IE	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	JA	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	JC	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	JE	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	KA	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	KC	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	KE	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	LA	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	LC	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	LE	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	MA	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
1	MC	430	Total 3350	C 2122	N 569	O 637	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ME	430	Total	C	N	O	S	0	0
			3350	2122	569	637	22		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	AD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	AF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	BB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	BD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	BF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	CB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	CD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	CF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	DB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	DD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	DF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	EB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	ED	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	EF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	FB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	FD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	FF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	GB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	GD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	GF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	HB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	HD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	HF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	IB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	ID	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	IF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	JB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	JD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	JF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	KB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	KD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	KF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	LB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	LD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	LF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	MB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	MD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
2	MF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

- Molecule 3 is a protein called Sperm flagellar protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1A	140	Total	C	N	O	S	0	0
			1141	717	200	215	9		
3	1B	140	Total	C	N	O	S	0	0
			1141	717	200	215	9		
3	1C	140	Total	C	N	O	S	0	0
			1141	717	200	215	9		

- Molecule 4 is a protein called TLP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2A	190	Total	C	N	O	S	0	0
			1615	1046	279	283	7		
4	2B	190	Total	C	N	O	S	0	0
			1615	1046	279	283	7		
4	2C	190	Total	C	N	O	S	0	0
			1615	1046	279	283	7		

- Molecule 5 is a protein called C2 domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3A	335	Total	C	N	O	S	0	0
			2752	1754	470	518	10		
5	3B	335	Total	C	N	O	S	0	0
			2752	1754	470	518	10		
5	3C	335	Total	C	N	O	S	0	0
			2752	1754	470	518	10		

- Molecule 6 is a protein called CFAP213.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4A	189	Total	C	N	O	S	0	0
			1587	981	298	303	5		
6	4B	189	Total	C	N	O	S	0	0
			1587	981	298	303	5		
6	4C	189	Total	C	N	O	S	0	0
			1587	981	298	303	5		
6	4D	189	Total	C	N	O	S	0	0
			1587	981	298	303	5		

- Molecule 7 is a protein called TLP2.



Mol	Chain	Residues	Atoms					AltConf	Trace
7	5A	705	Total	C	N	O	S	0	0
			5953	3778	1021	1141	13		
7	5B	705	Total	C	N	O	S	0	0
			5953	3778	1021	1141	13		
7	5C	705	Total	C	N	O	S	0	0
			5953	3778	1021	1141	13		

- Molecule 8 is a protein called Cation channel family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6A	256	Total	C	N	O	S	0	0
			2077	1352	338	380	7		
8	6B	256	Total	C	N	O	S	0	0
			2077	1352	338	380	7		
8	6C	256	Total	C	N	O	S	0	0
			2077	1352	338	380	7		

- Molecule 9 is a protein called Dpy-30 motif protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	7A	46	Total	C	N	O	0	0
			383	247	66	70		
9	7B	46	Total	C	N	O	0	0
			383	247	66	70		
9	7C	46	Total	C	N	O	0	0
			383	247	66	70		
9	7D	46	Total	C	N	O	0	0
			383	247	66	70		
9	7E	46	Total	C	N	O	0	0
			383	247	66	70		
9	7F	46	Total	C	N	O	0	0
			383	247	66	70		

- Molecule 10 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	8A	38	Total	C	N	O	0	0
			189	114	38	37		
10	8B	38	Total	C	N	O	0	0
			189	114	38	37		
10	8C	38	Total	C	N	O	0	0
			189	114	38	37		

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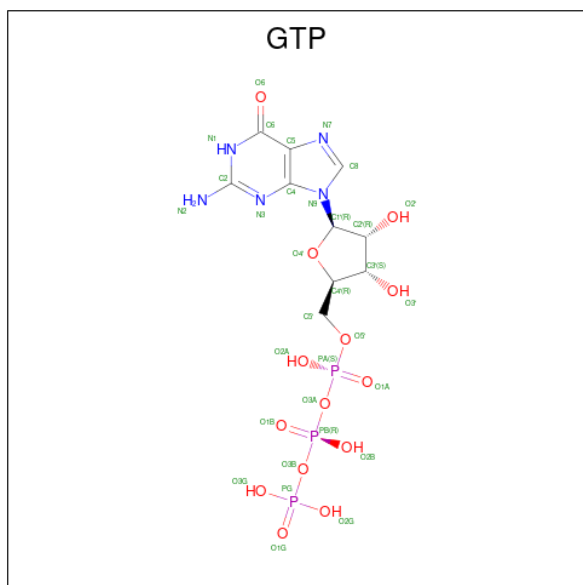
Mol	Chain	Residues	Atoms				AltConf	Trace
10	8D	38	Total	C	N	O	0	0
			189	114	38	37		
10	8E	38	Total	C	N	O	0	0
			189	114	38	37		
10	8F	38	Total	C	N	O	0	0
			189	114	38	37		
10	8G	38	Total	C	N	O	0	0
			189	114	38	37		
10	8H	38	Total	C	N	O	0	0
			189	114	38	37		
10	8I	38	Total	C	N	O	0	0
			189	114	38	37		
10	8J	38	Total	C	N	O	0	0
			189	114	38	37		
10	8K	38	Total	C	N	O	0	0
			189	114	38	37		
10	8L	38	Total	C	N	O	0	0
			189	114	38	37		
10	8M	38	Total	C	N	O	0	0
			189	114	38	37		
10	8N	38	Total	C	N	O	0	0
			189	114	38	37		
10	8O	38	Total	C	N	O	0	0
			189	114	38	37		
10	8P	38	Total	C	N	O	0	0
			189	114	38	37		
10	8Q	38	Total	C	N	O	0	0
			189	114	38	37		
10	8R	38	Total	C	N	O	0	0
			189	114	38	37		
10	8S	38	Total	C	N	O	0	0
			189	114	38	37		
10	8T	38	Total	C	N	O	0	0
			189	114	38	37		
10	8U	38	Total	C	N	O	0	0
			189	114	38	37		
10	8V	38	Total	C	N	O	0	0
			189	114	38	37		
10	8W	38	Total	C	N	O	0	0
			189	114	38	37		
10	8X	38	Total	C	N	O	0	0
			189	114	38	37		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	8Y	38	Total	C	N	O	0	0
			189	114	38	37		
10	8Z	38	Total	C	N	O	0	0
			189	114	38	37		
10	9A	38	Total	C	N	O	0	0
			189	114	38	37		

- Molecule 11 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
11	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	AC	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	BA	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	BC	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	CA	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	CC	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
11	CE	1	Total 32	C 10	N 5	O 14	P 3	0
11	DA	1	Total 32	C 10	N 5	O 14	P 3	0
11	DC	1	Total 32	C 10	N 5	O 14	P 3	0
11	DE	1	Total 32	C 10	N 5	O 14	P 3	0
11	EA	1	Total 32	C 10	N 5	O 14	P 3	0
11	EC	1	Total 32	C 10	N 5	O 14	P 3	0
11	EE	1	Total 32	C 10	N 5	O 14	P 3	0
11	FA	1	Total 32	C 10	N 5	O 14	P 3	0
11	FC	1	Total 32	C 10	N 5	O 14	P 3	0
11	FE	1	Total 32	C 10	N 5	O 14	P 3	0
11	GA	1	Total 32	C 10	N 5	O 14	P 3	0
11	GC	1	Total 32	C 10	N 5	O 14	P 3	0
11	GE	1	Total 32	C 10	N 5	O 14	P 3	0
11	HA	1	Total 32	C 10	N 5	O 14	P 3	0
11	HC	1	Total 32	C 10	N 5	O 14	P 3	0
11	HE	1	Total 32	C 10	N 5	O 14	P 3	0
11	IA	1	Total 32	C 10	N 5	O 14	P 3	0
11	IC	1	Total 32	C 10	N 5	O 14	P 3	0
11	IE	1	Total 32	C 10	N 5	O 14	P 3	0
11	JA	1	Total 32	C 10	N 5	O 14	P 3	0
11	JC	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
11	JE	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	KA	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	KC	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	KE	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	LA	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	LC	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	LE	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	MA	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	MC	1	Total	C	N	O	P	0
			32	10	5	14	3	
11	ME	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
12	AA	1	Total	Mg	0
			1	1	
12	AC	1	Total	Mg	0
			1	1	
12	AE	1	Total	Mg	0
			1	1	
12	BA	1	Total	Mg	0
			1	1	
12	BC	1	Total	Mg	0
			1	1	
12	BE	1	Total	Mg	0
			1	1	
12	CA	1	Total	Mg	0
			1	1	
12	CC	1	Total	Mg	0
			1	1	
12	CE	1	Total	Mg	0
			1	1	

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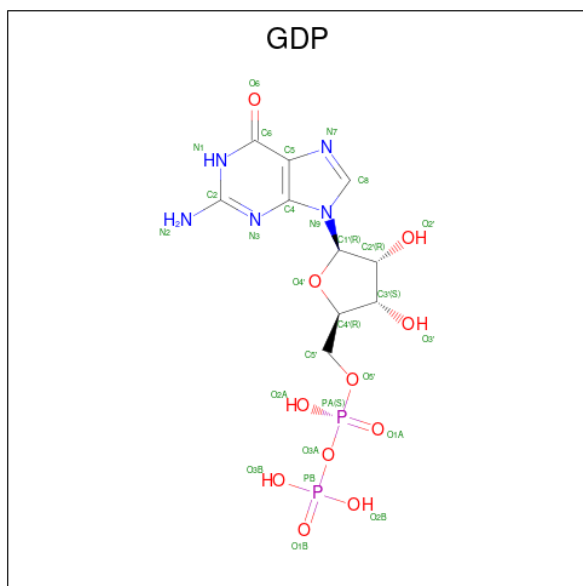
Mol	Chain	Residues	Atoms		AltConf
12	DA	1	Total 1	Mg 1	0
12	DC	1	Total 1	Mg 1	0
12	DE	1	Total 1	Mg 1	0
12	EA	1	Total 1	Mg 1	0
12	ED	1	Total 1	Mg 1	0
12	EE	1	Total 1	Mg 1	0
12	FB	1	Total 1	Mg 1	0
12	FD	1	Total 1	Mg 1	0
12	FE	1	Total 1	Mg 1	0
12	GA	1	Total 1	Mg 1	0
12	GC	1	Total 1	Mg 1	0
12	GE	1	Total 1	Mg 1	0
12	HA	1	Total 1	Mg 1	0
12	HC	1	Total 1	Mg 1	0
12	HE	1	Total 1	Mg 1	0
12	IA	1	Total 1	Mg 1	0
12	IC	1	Total 1	Mg 1	0
12	IE	1	Total 1	Mg 1	0
12	JA	1	Total 1	Mg 1	0
12	JC	1	Total 1	Mg 1	0
12	JE	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
12	KA	1	Total	Mg	0
			1	1	
12	KC	1	Total	Mg	0
			1	1	
12	KE	1	Total	Mg	0
			1	1	
12	LA	1	Total	Mg	0
			1	1	
12	LC	1	Total	Mg	0
			1	1	
12	LE	1	Total	Mg	0
			1	1	
12	MB	1	Total	Mg	0
			1	1	
12	MD	1	Total	Mg	0
			1	1	
12	MF	1	Total	Mg	0
			1	1	

- Molecule 13 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
13	AB	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	AD	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
13	AF	1	Total 28	C 10	N 5	O 11	P 2	0
13	BB	1	Total 28	C 10	N 5	O 11	P 2	0
13	BD	1	Total 28	C 10	N 5	O 11	P 2	0
13	BF	1	Total 28	C 10	N 5	O 11	P 2	0
13	CB	1	Total 28	C 10	N 5	O 11	P 2	0
13	CD	1	Total 28	C 10	N 5	O 11	P 2	0
13	CF	1	Total 28	C 10	N 5	O 11	P 2	0
13	DB	1	Total 28	C 10	N 5	O 11	P 2	0
13	DD	1	Total 28	C 10	N 5	O 11	P 2	0
13	DF	1	Total 28	C 10	N 5	O 11	P 2	0
13	EB	1	Total 28	C 10	N 5	O 11	P 2	0
13	ED	1	Total 28	C 10	N 5	O 11	P 2	0
13	EF	1	Total 28	C 10	N 5	O 11	P 2	0
13	FB	1	Total 28	C 10	N 5	O 11	P 2	0
13	FD	1	Total 28	C 10	N 5	O 11	P 2	0
13	FF	1	Total 28	C 10	N 5	O 11	P 2	0
13	GB	1	Total 28	C 10	N 5	O 11	P 2	0
13	GD	1	Total 28	C 10	N 5	O 11	P 2	0
13	GF	1	Total 28	C 10	N 5	O 11	P 2	0
13	HB	1	Total 28	C 10	N 5	O 11	P 2	0
13	HD	1	Total 28	C 10	N 5	O 11	P 2	0

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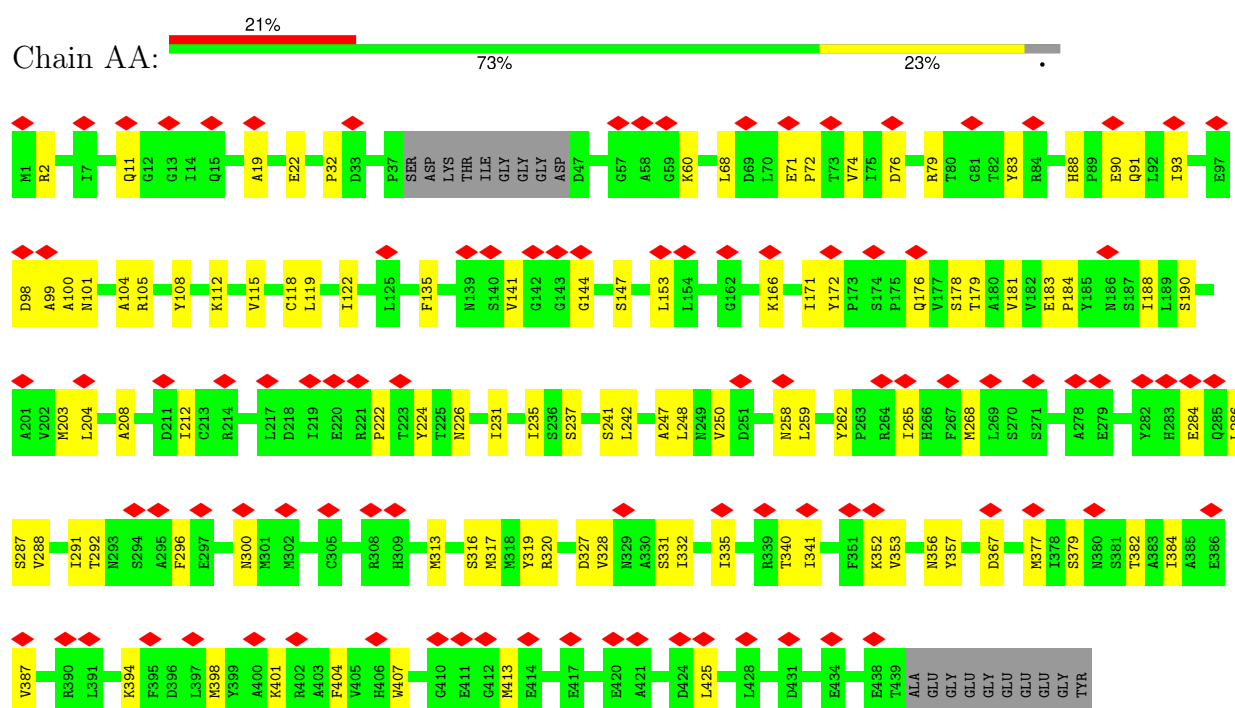
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Mol	Chain	Residues	Atoms					AltConf
13	HF	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	IB	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	ID	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	IF	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	JB	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	JD	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	JF	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	KB	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	KD	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	KF	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	LB	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	LD	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	LF	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	MB	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	MD	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	MF	1	Total	C	N	O	P	0
			28	10	5	11	2	

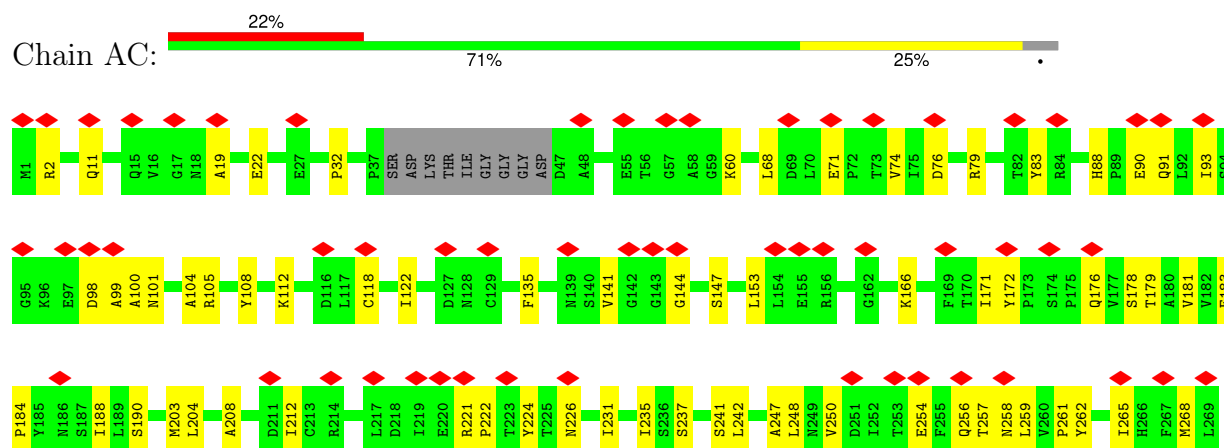
### 3 Residue-property plots [i](#)

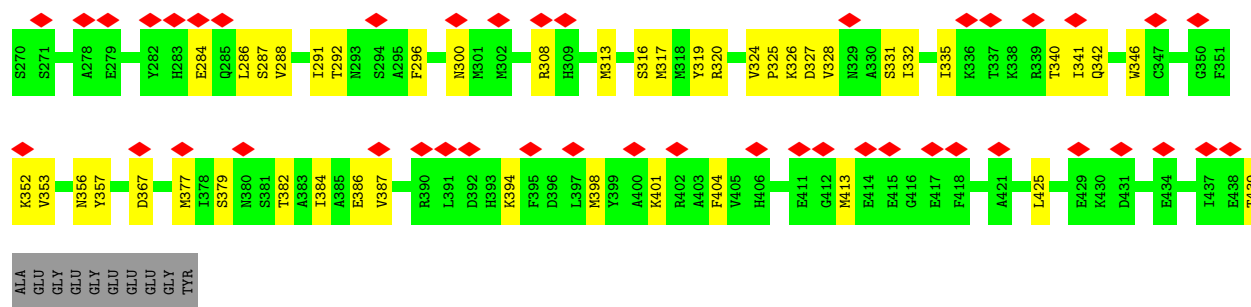
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Tubulin alpha chain

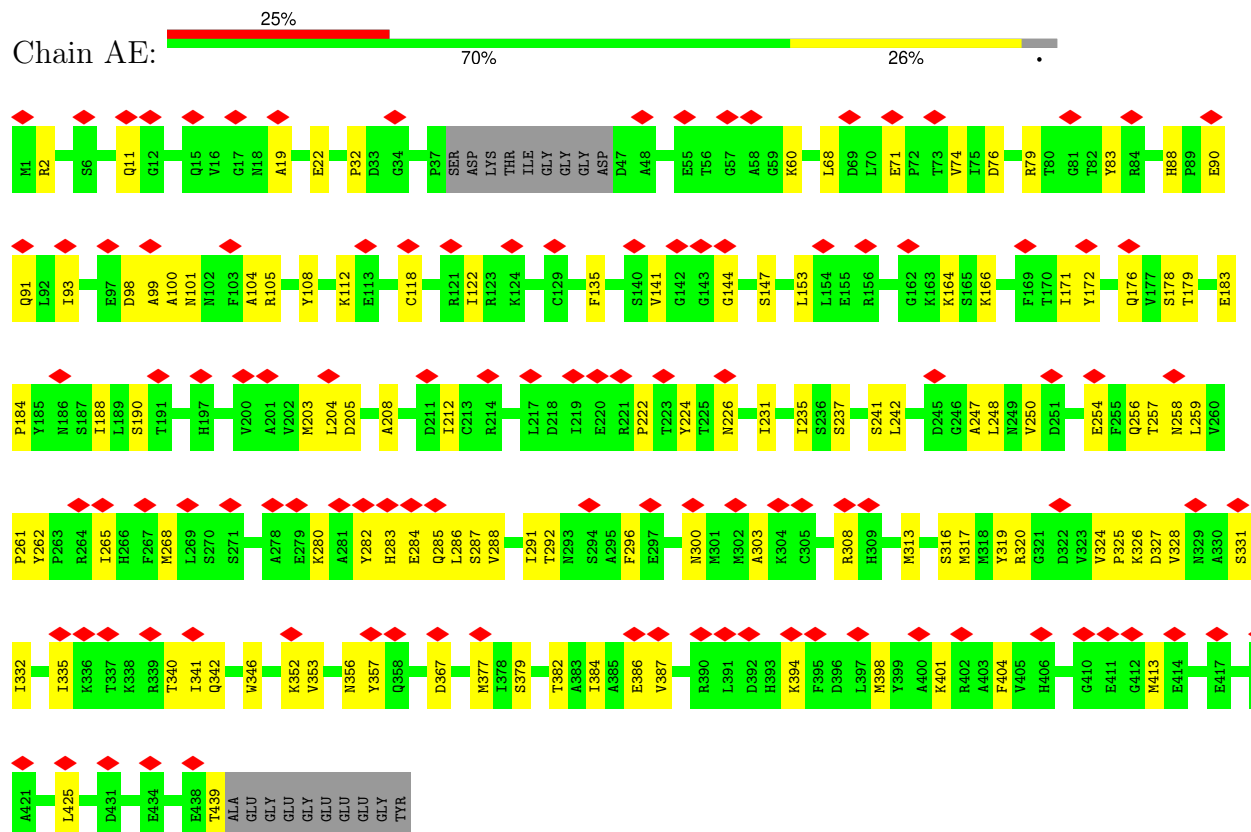


#### • Molecule 1: Tubulin alpha chain

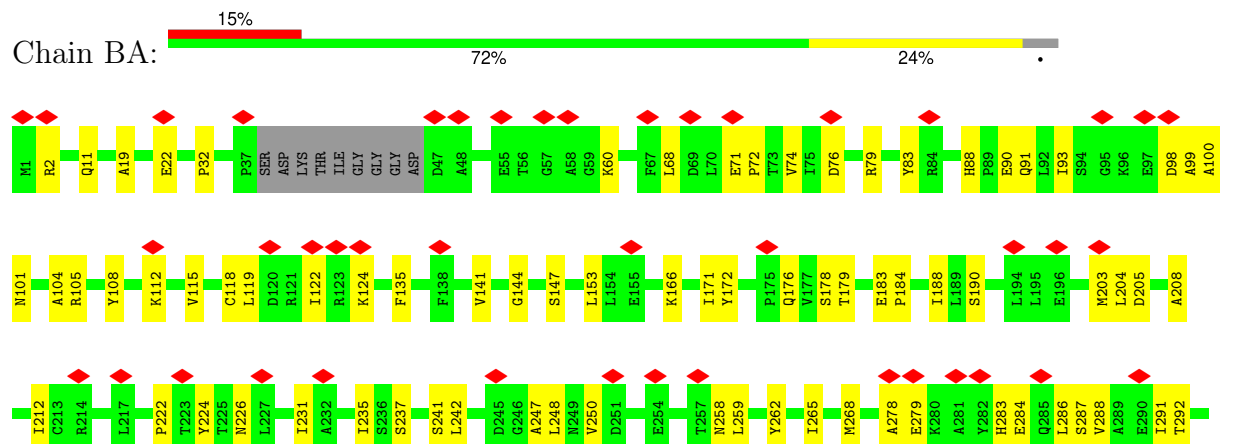


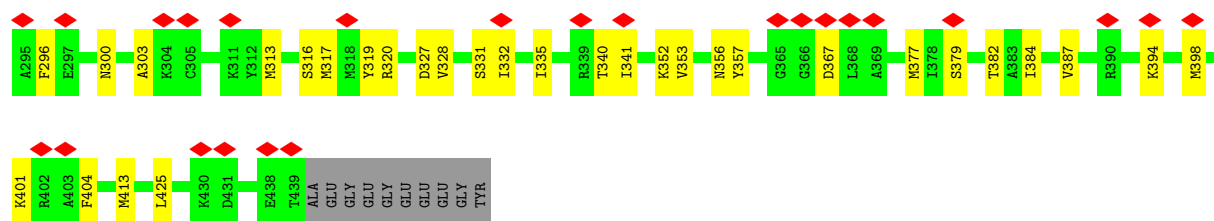


• Molecule 1: Tubulin alpha chain

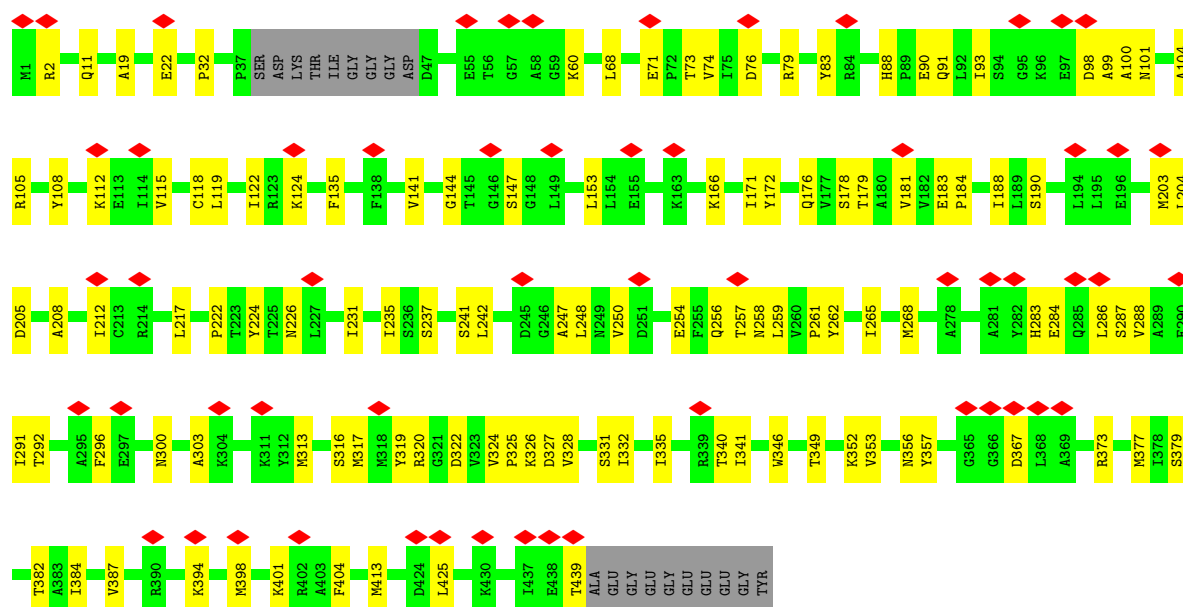


• Molecule 1: Tubulin alpha chain

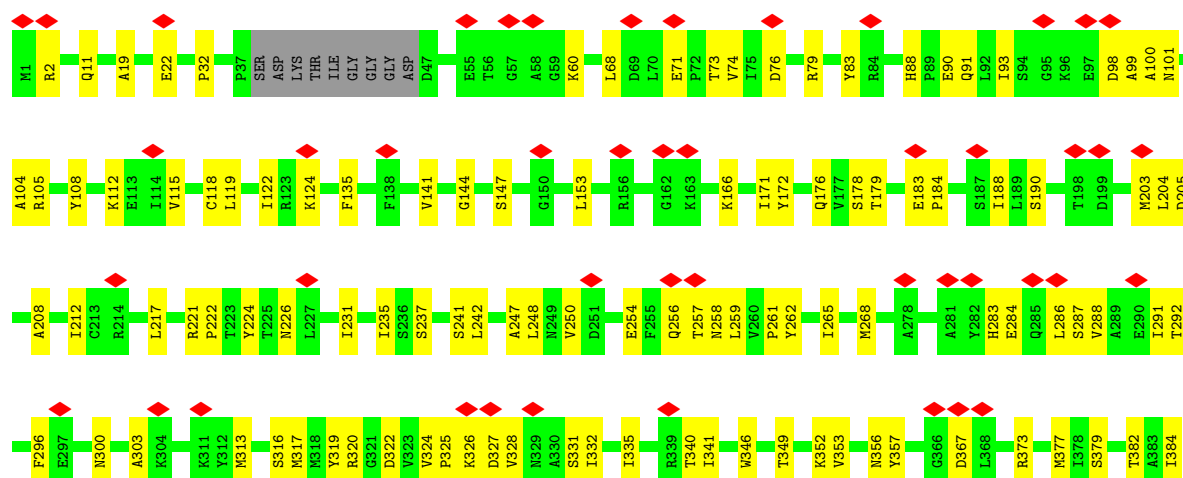


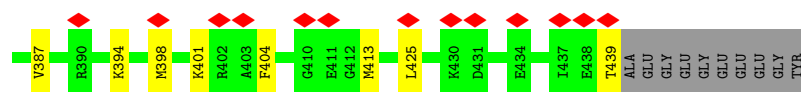


• Molecule 1: Tubulin alpha chain

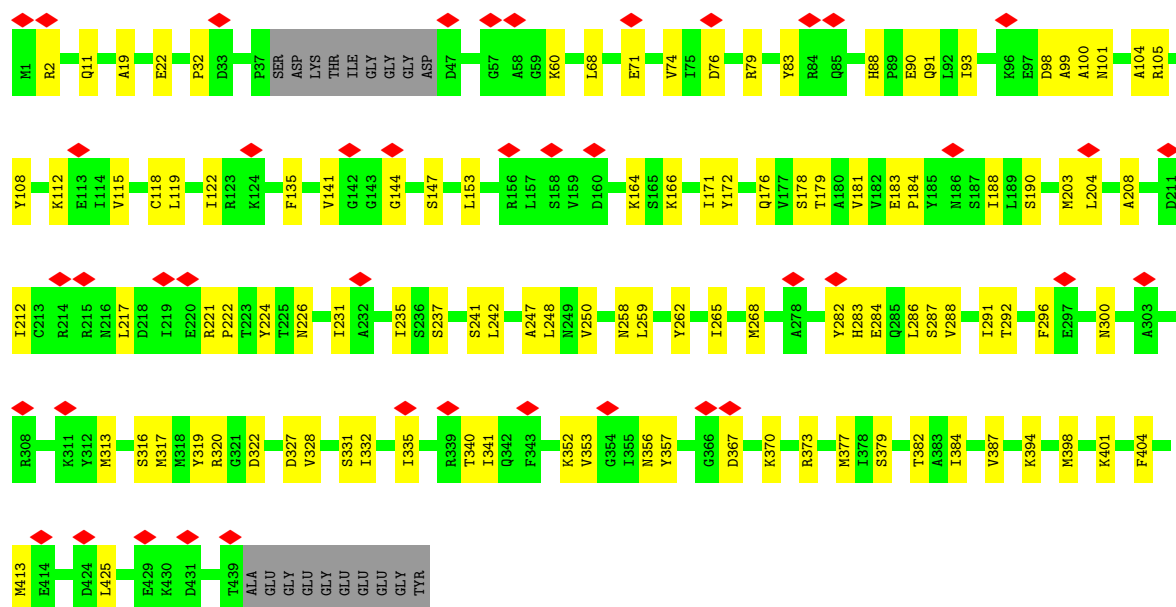
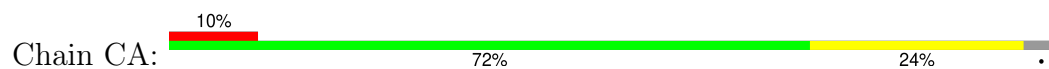


• Molecule 1: Tubulin alpha chain

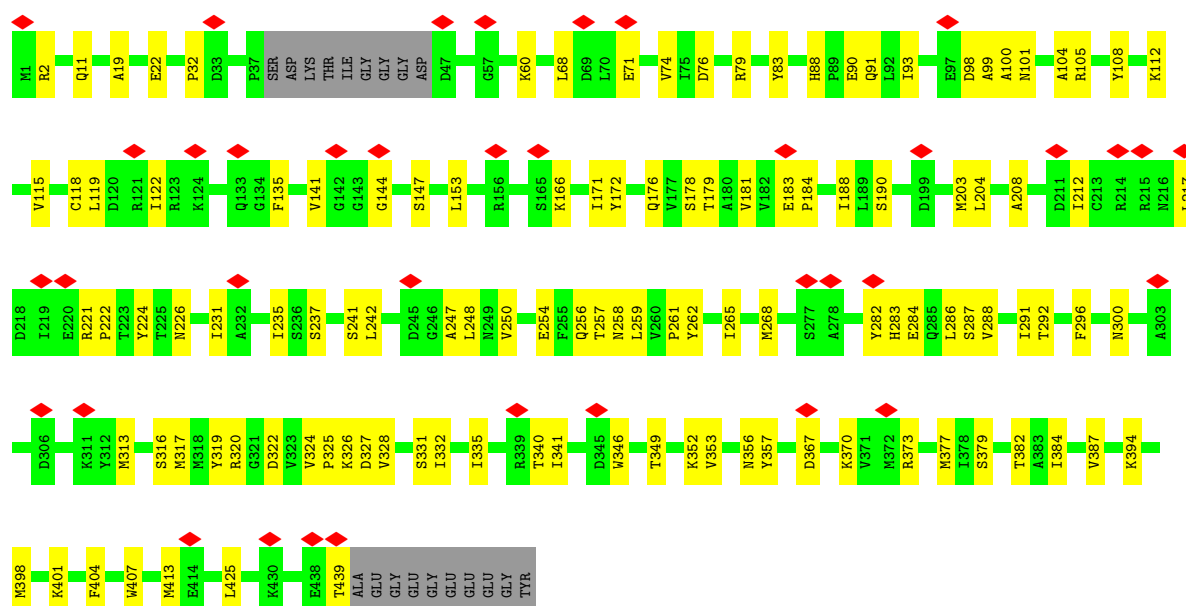




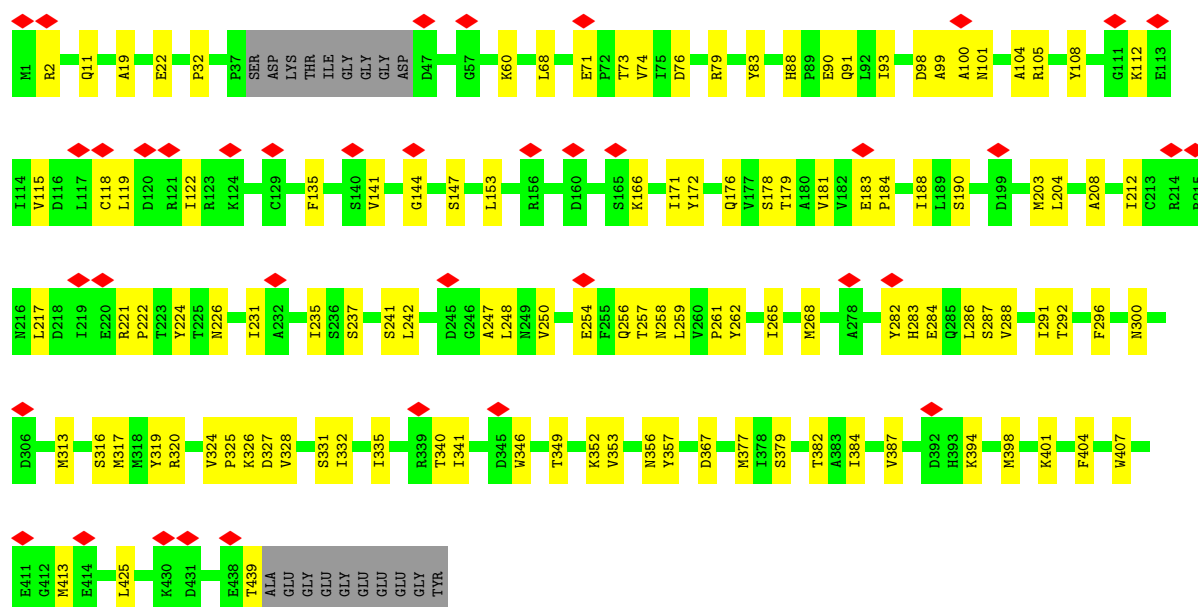
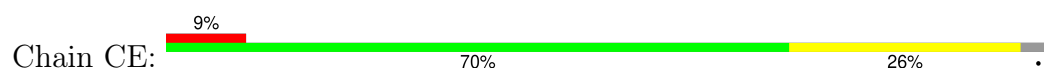
• Molecule 1: Tubulin alpha chain



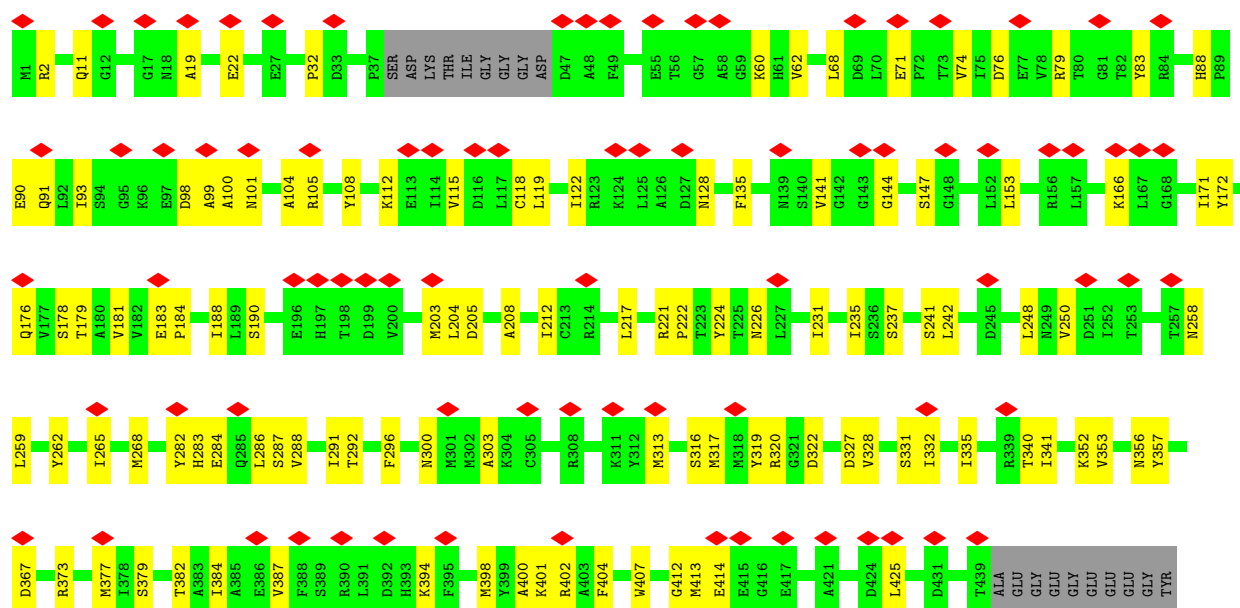
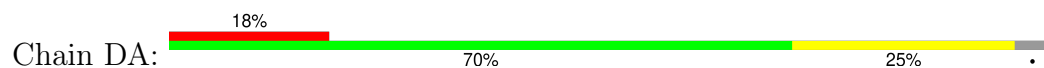
• Molecule 1: Tubulin alpha chain



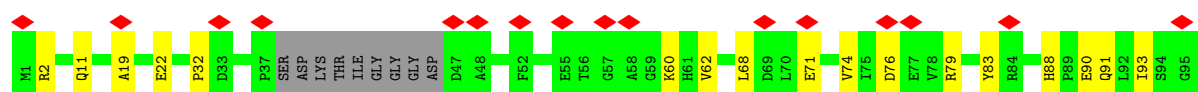
• Molecule 1: Tubulin alpha chain

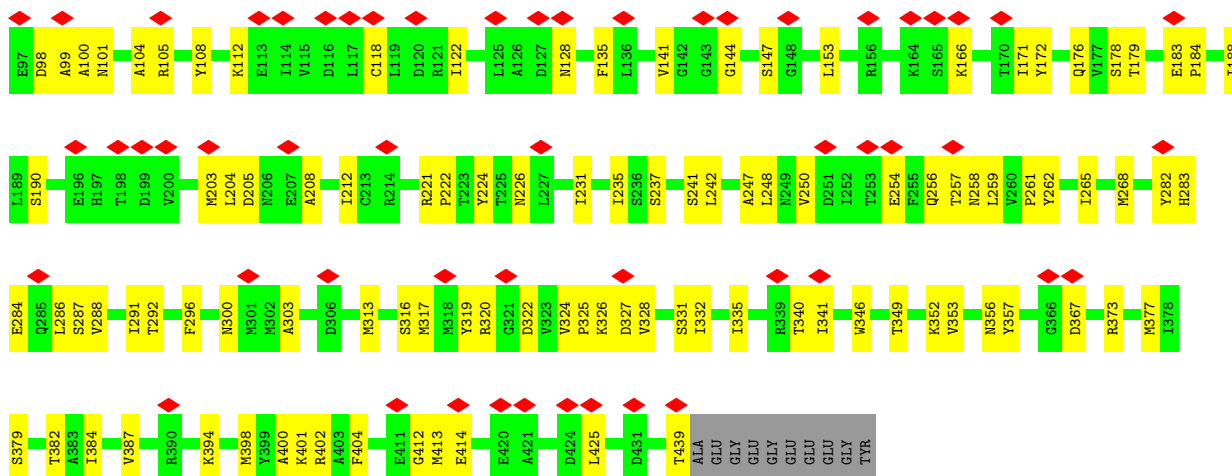


• Molecule 1: Tubulin alpha chain

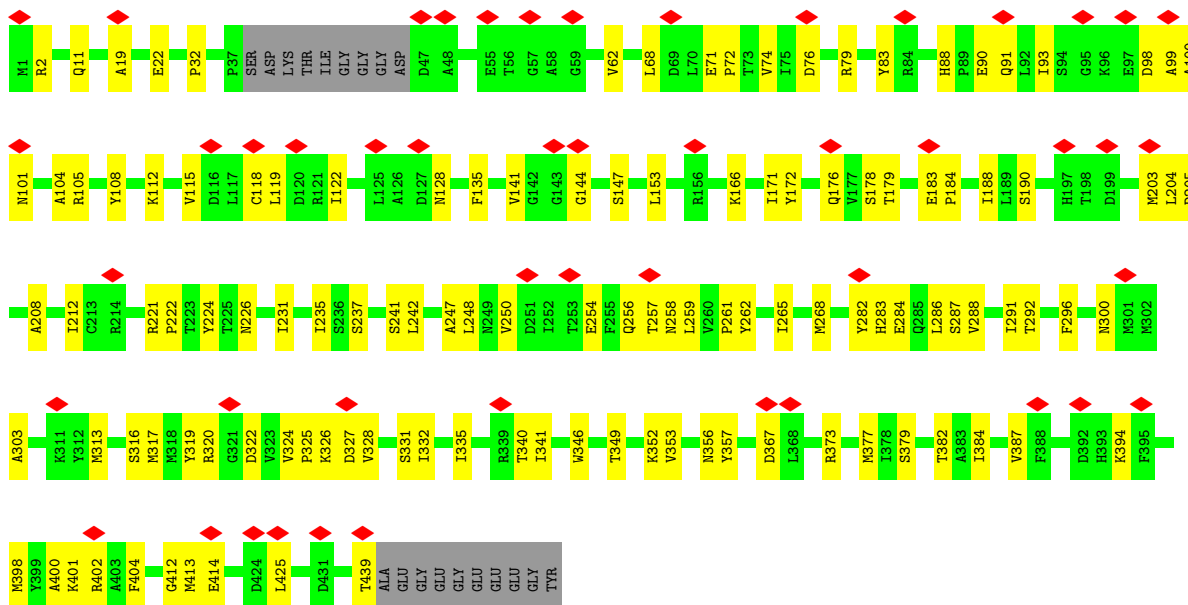


• Molecule 1: Tubulin alpha chain

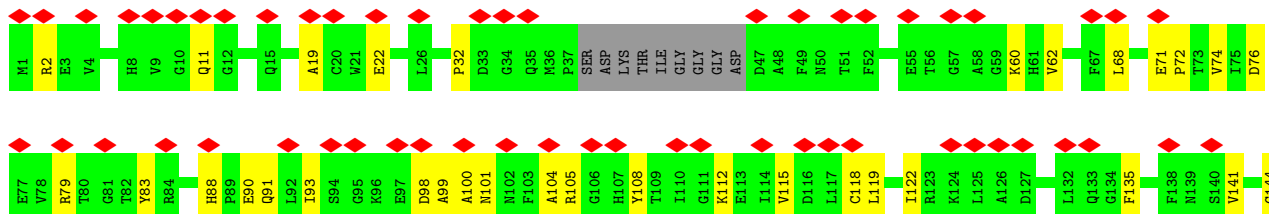
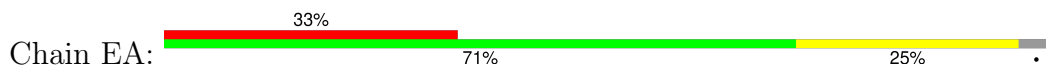


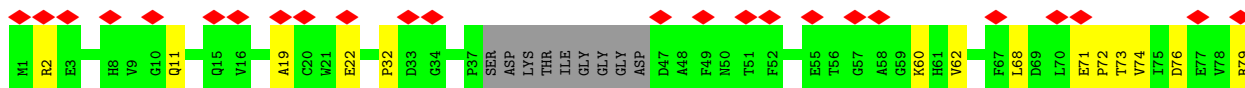


• Molecule 1: Tubulin alpha chain

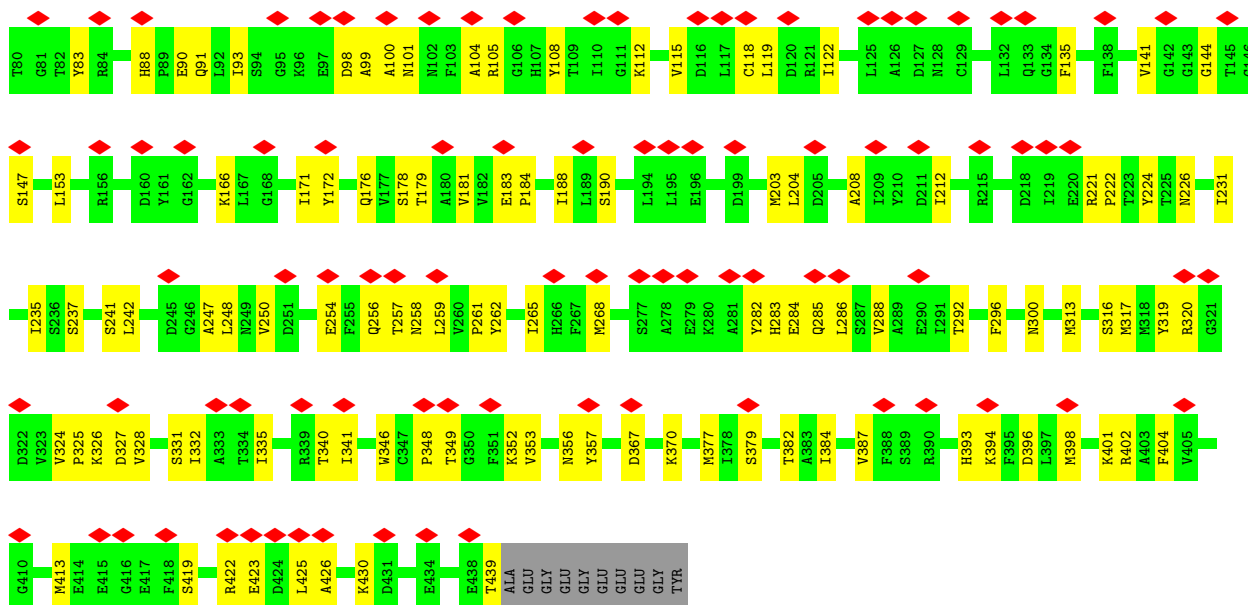


• Molecule 1: Tubulin alpha chain

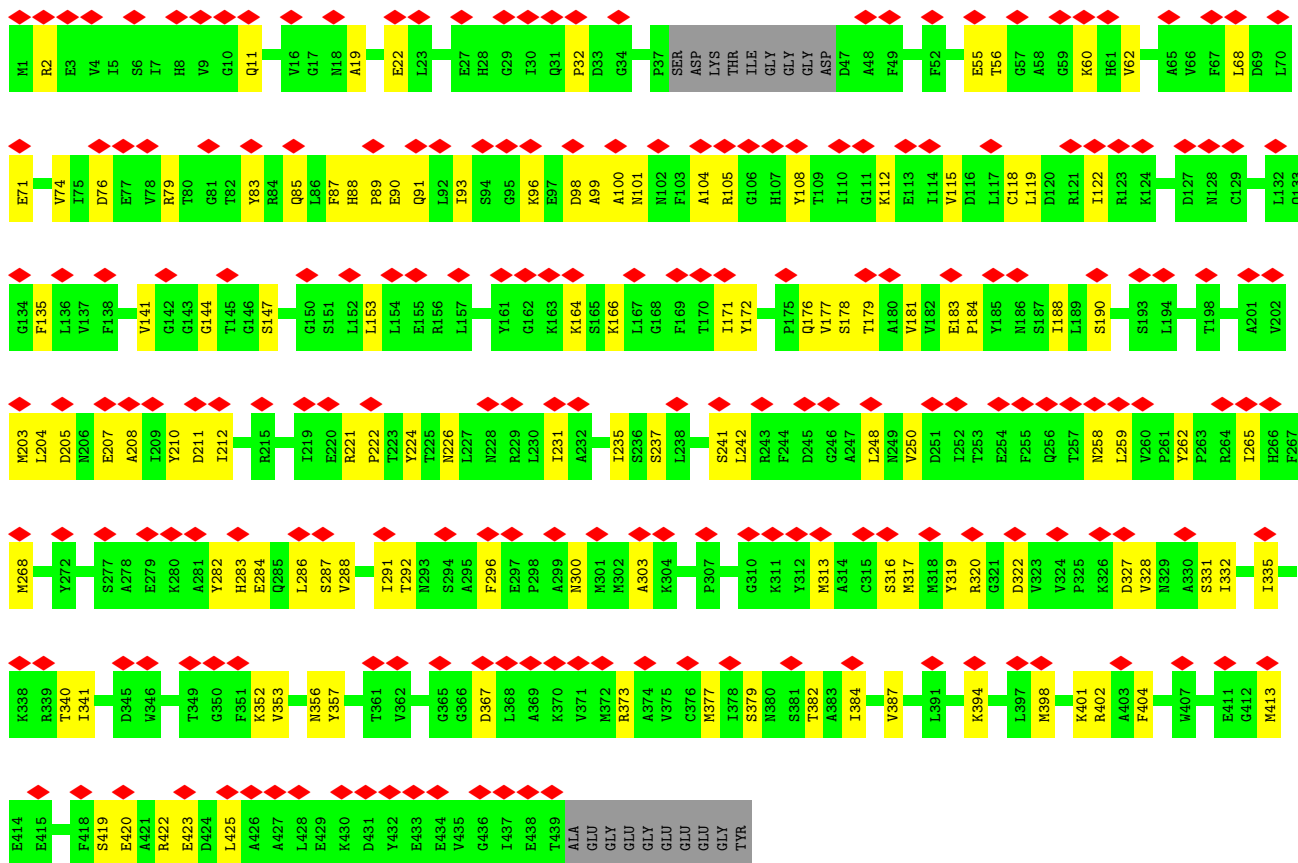




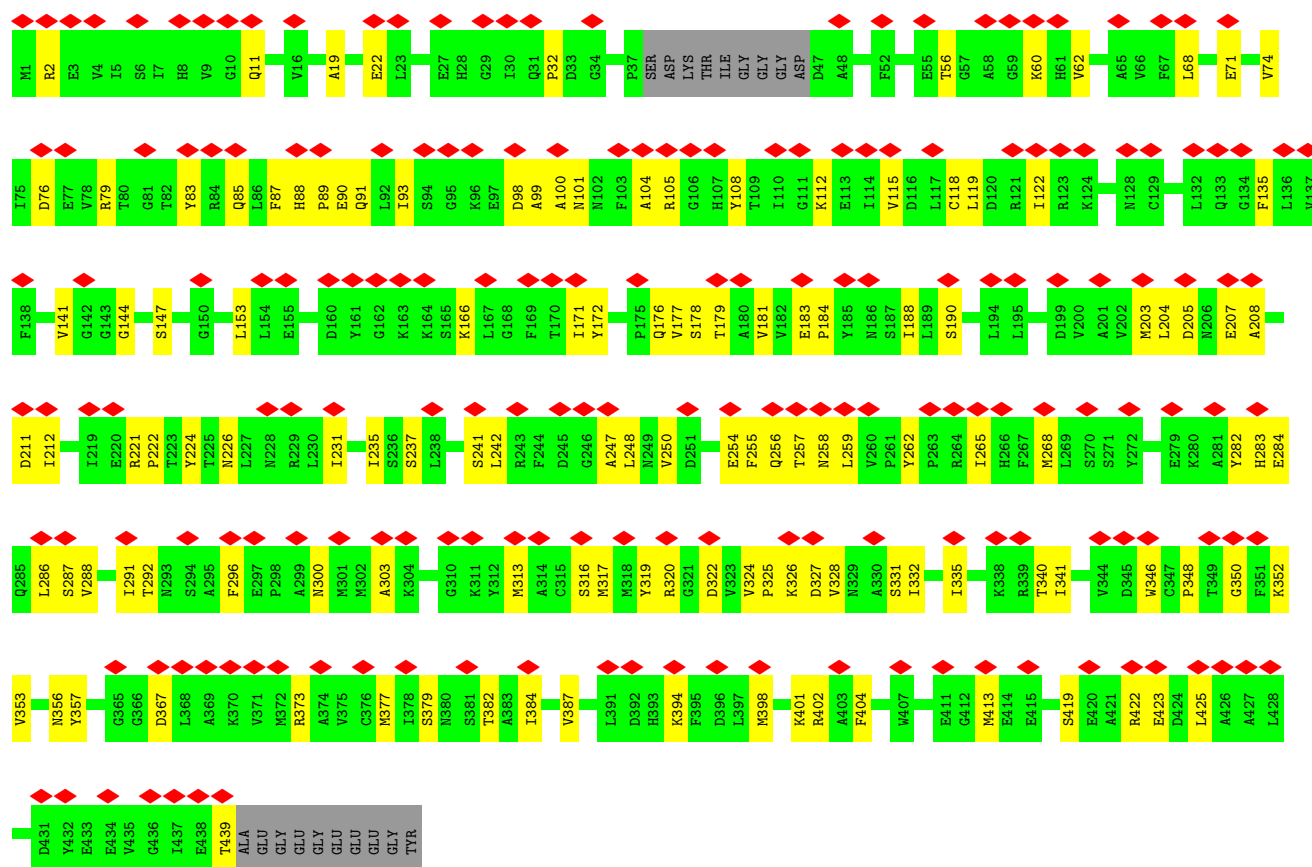
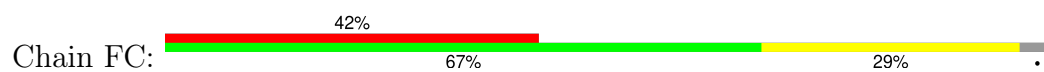




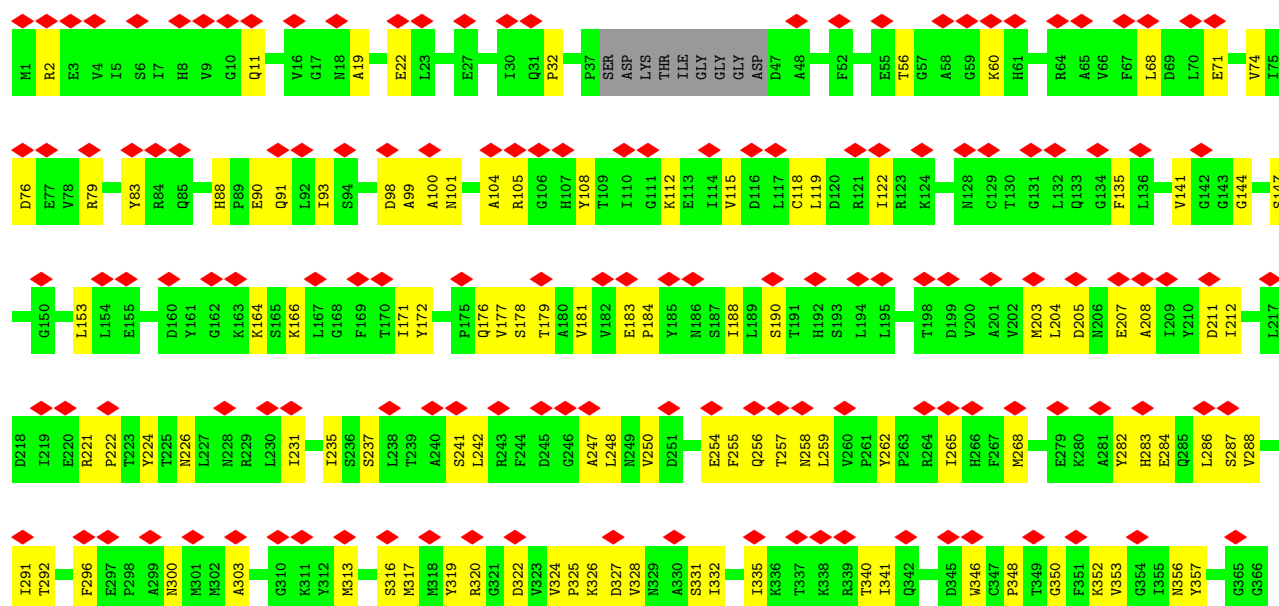
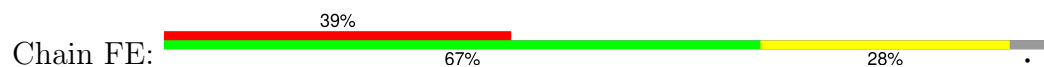
• Molecule 1: Tubulin alpha chain

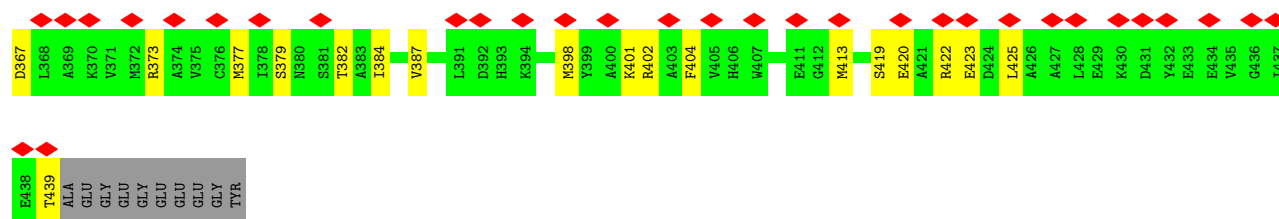


• Molecule 1: Tubulin alpha chain

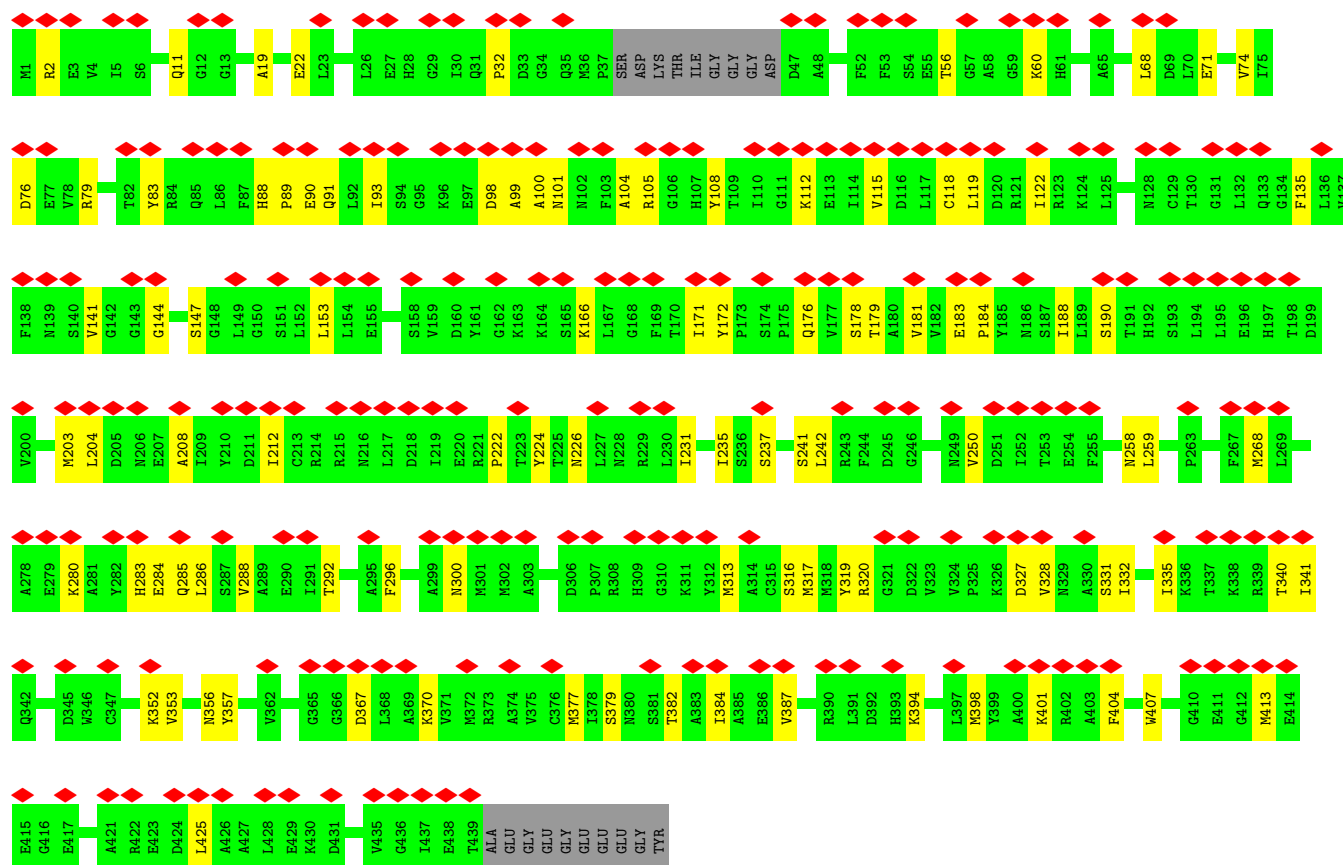
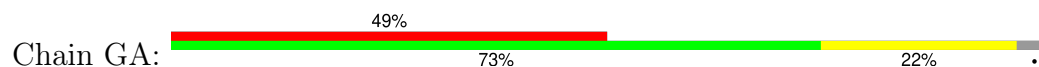


• Molecule 1: Tubulin alpha chain

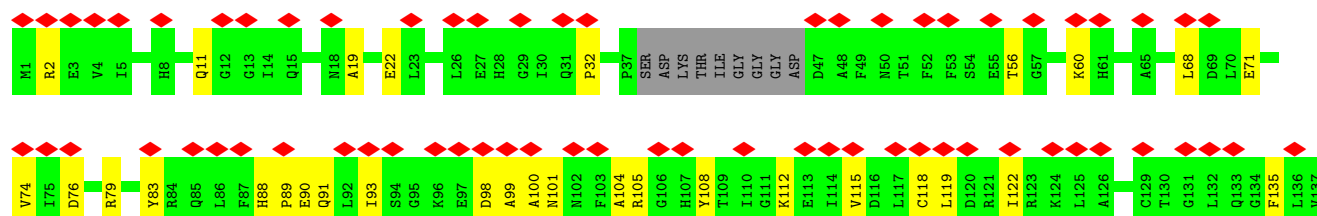


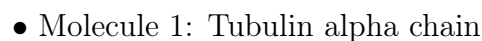


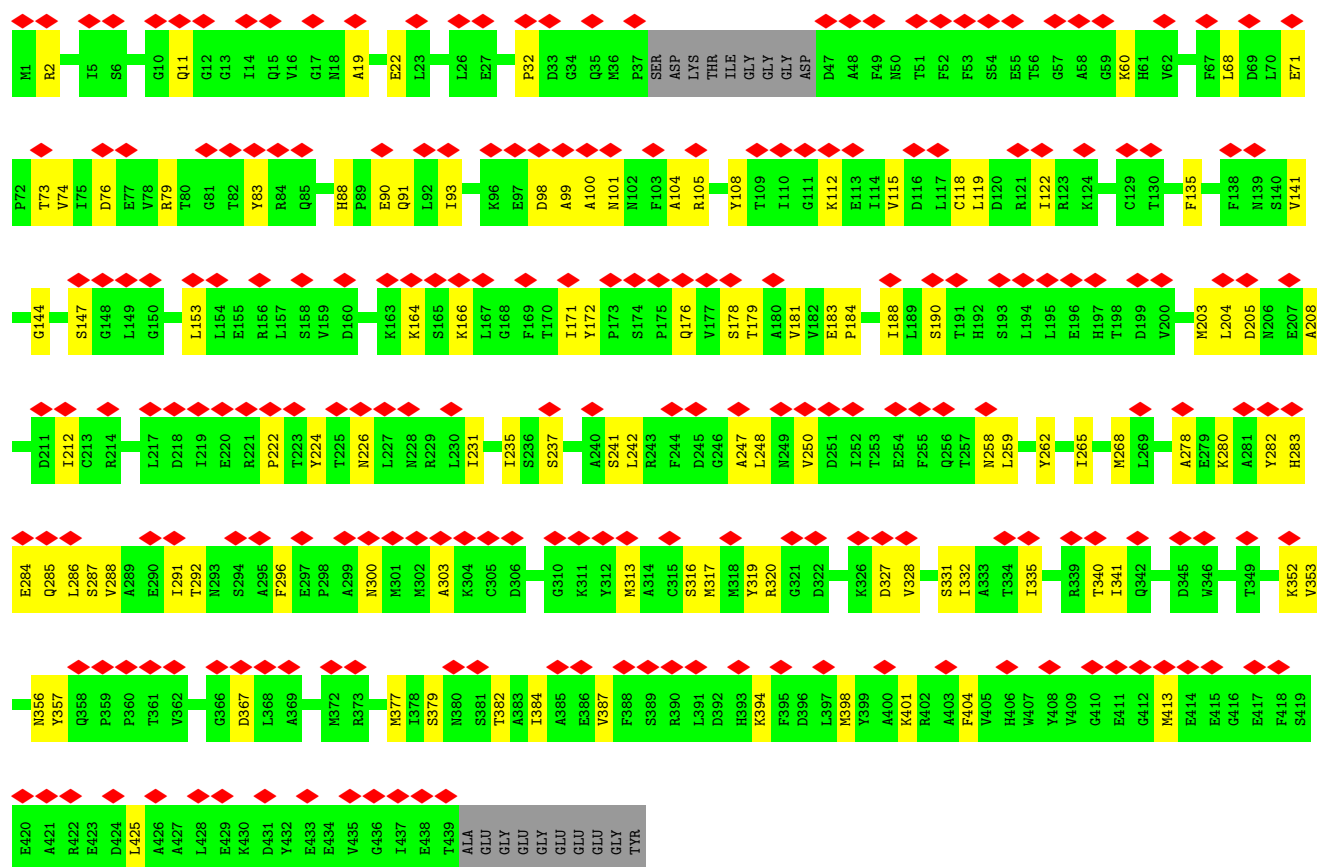
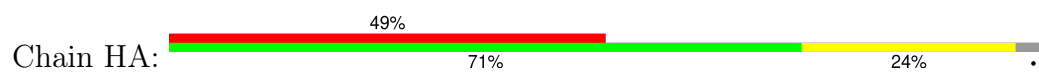
• Molecule 1: Tubulin alpha chain



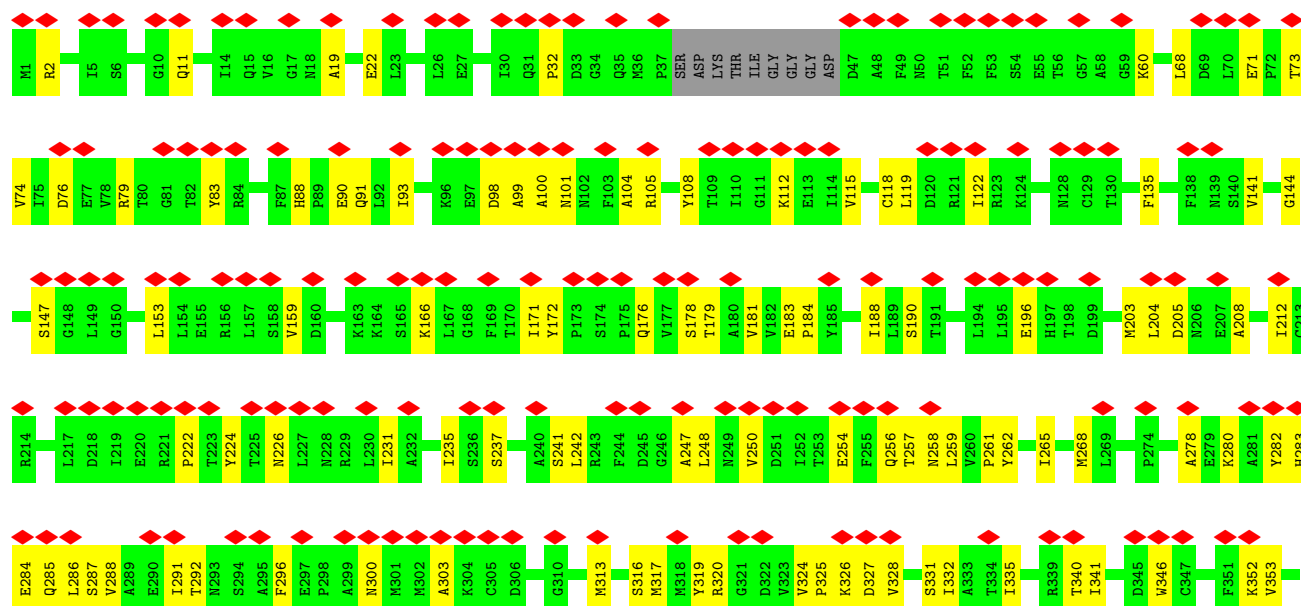
• Molecule 1: Tubulin alpha chain

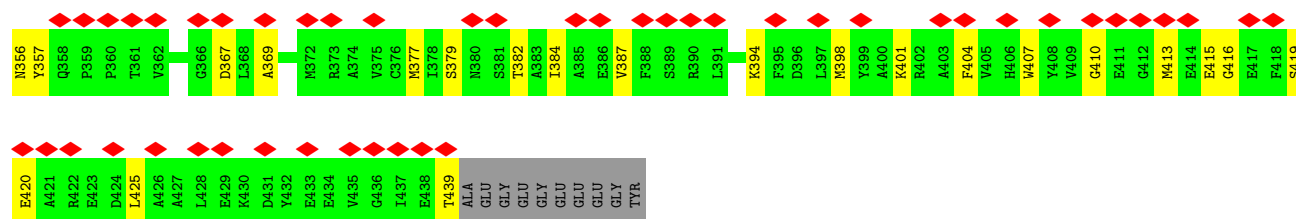




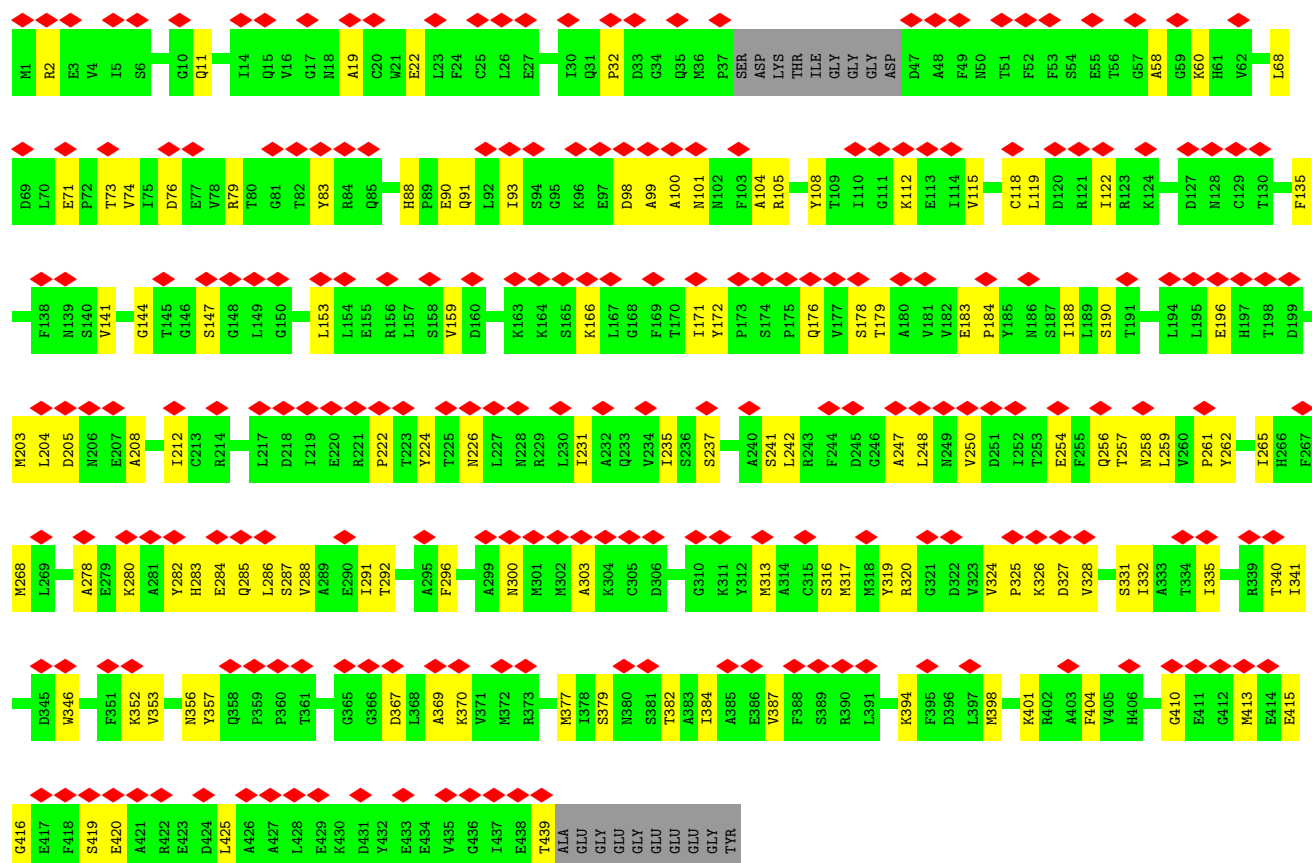


• Molecule 1: Tubulin alpha chain

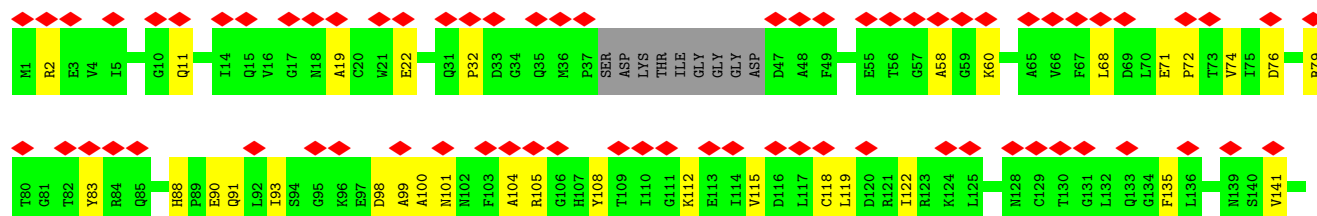


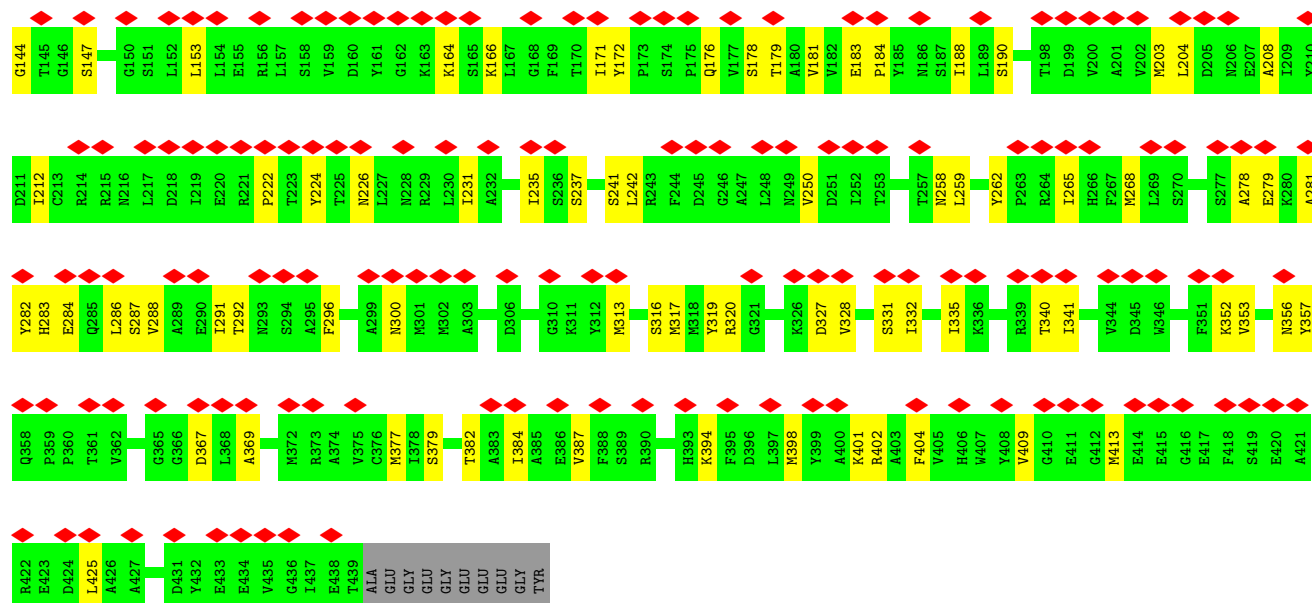


• Molecule 1: Tubulin alpha chain

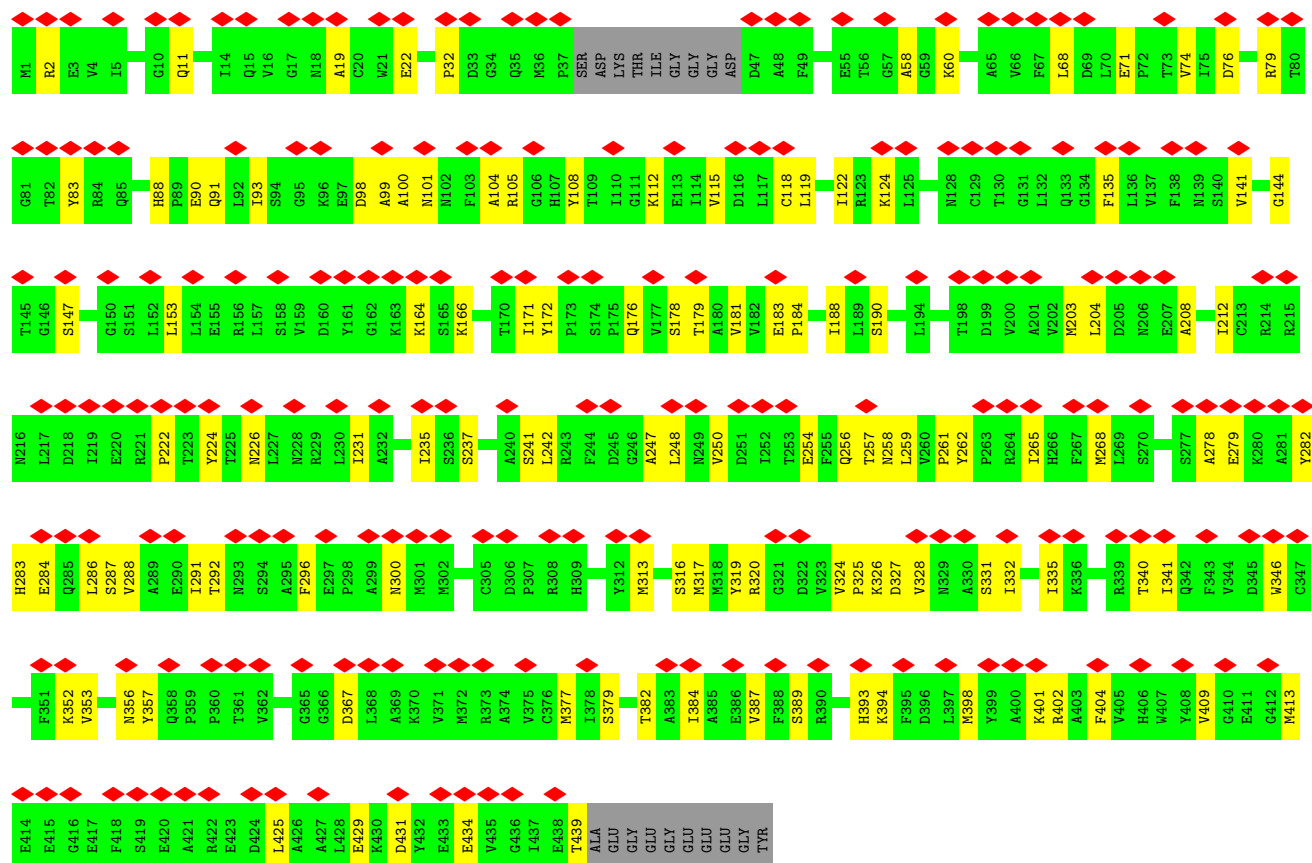


• Molecule 1: Tubulin alpha chain

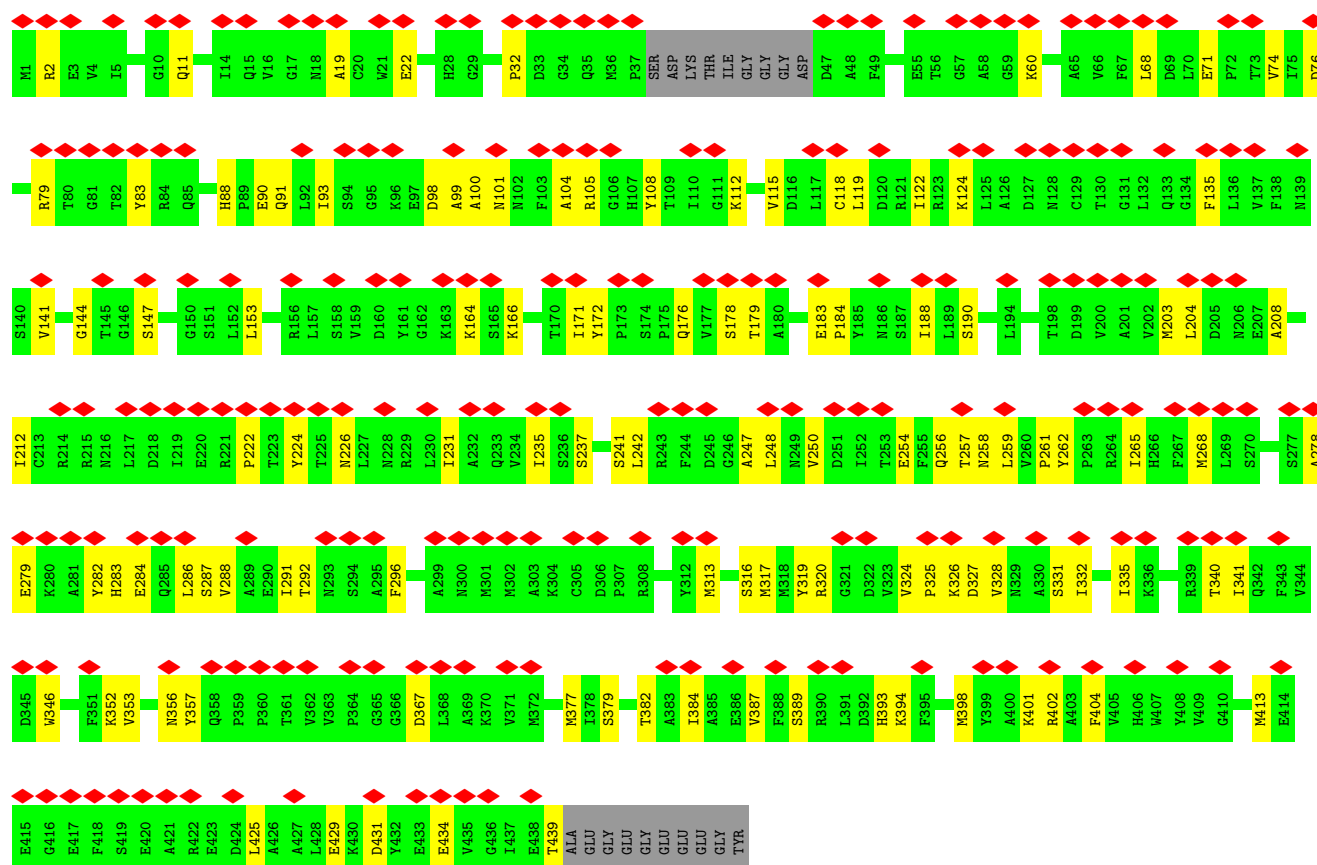




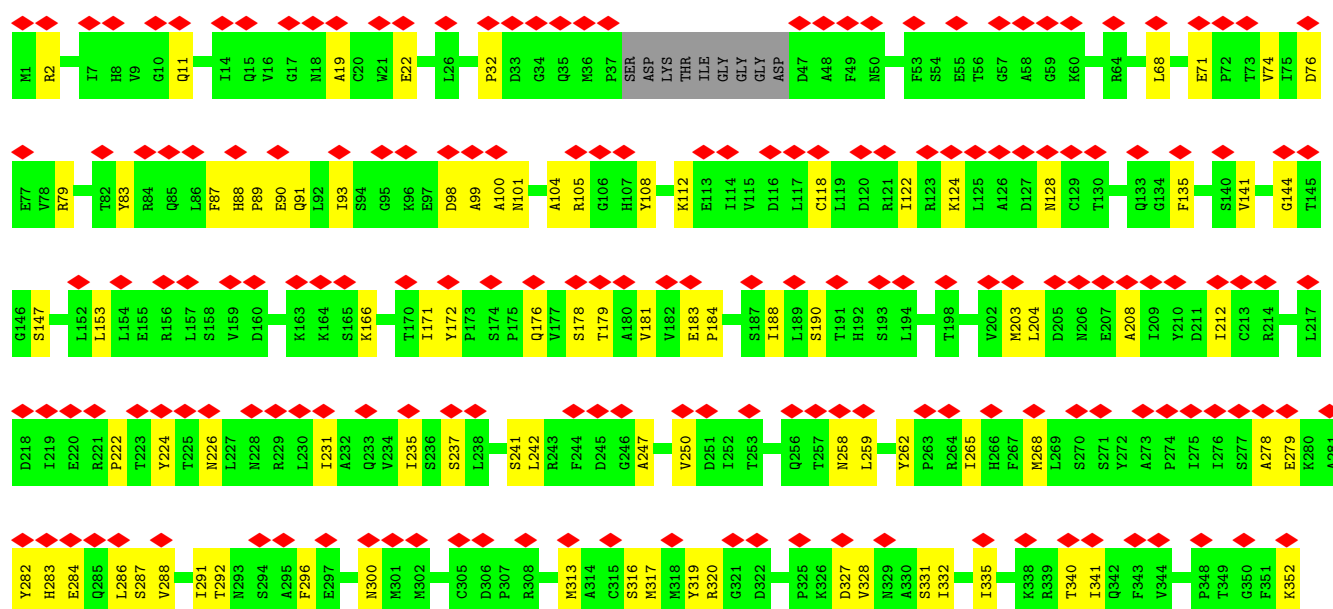
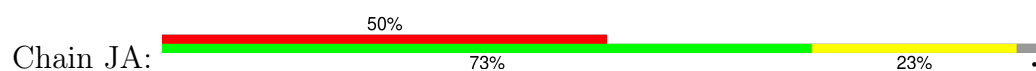
• Molecule 1: Tubulin alpha chain



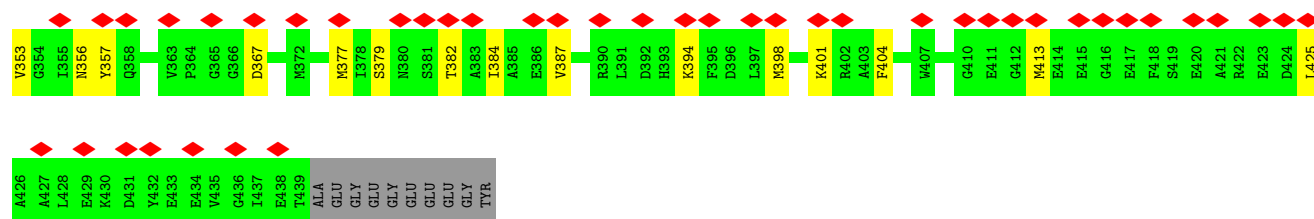
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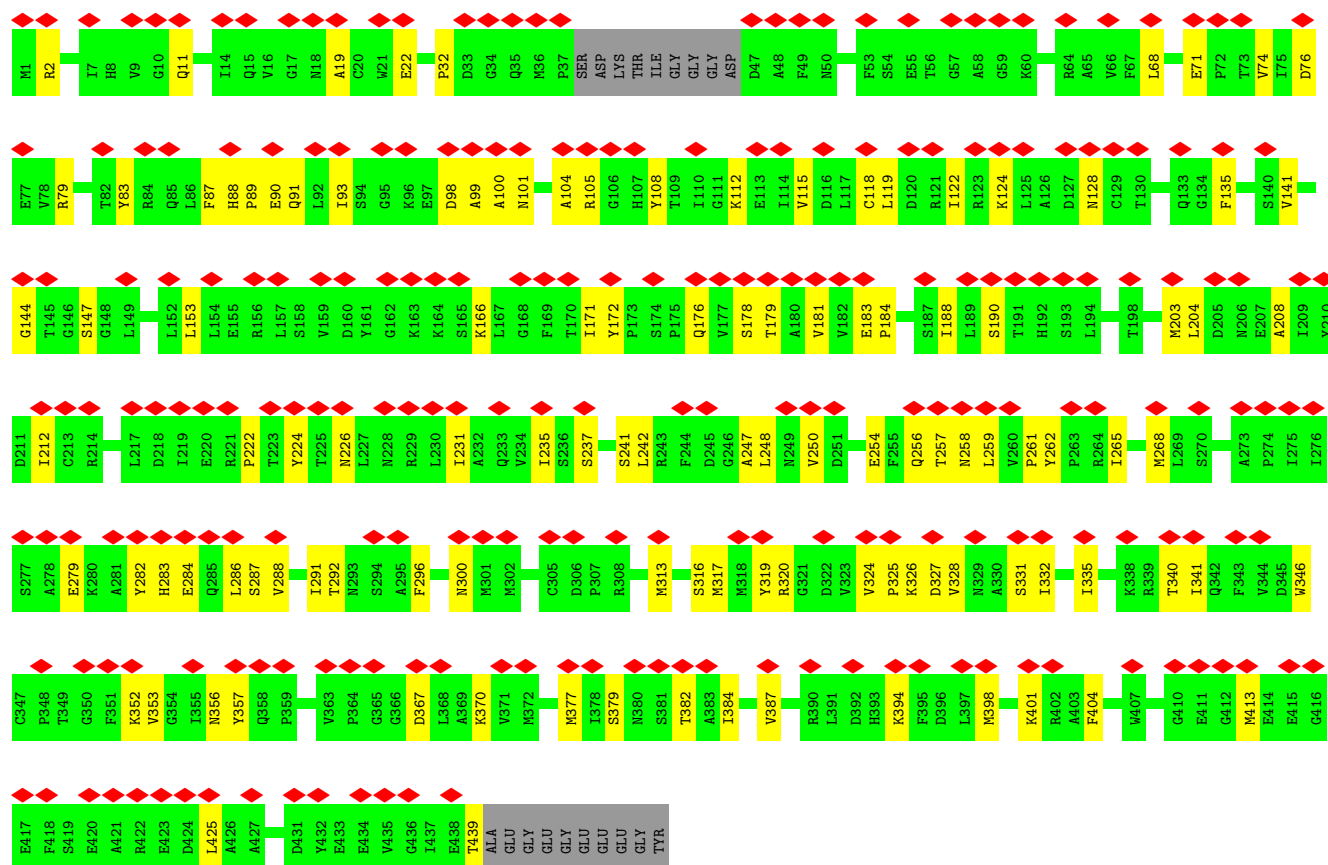
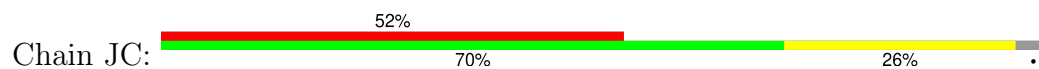
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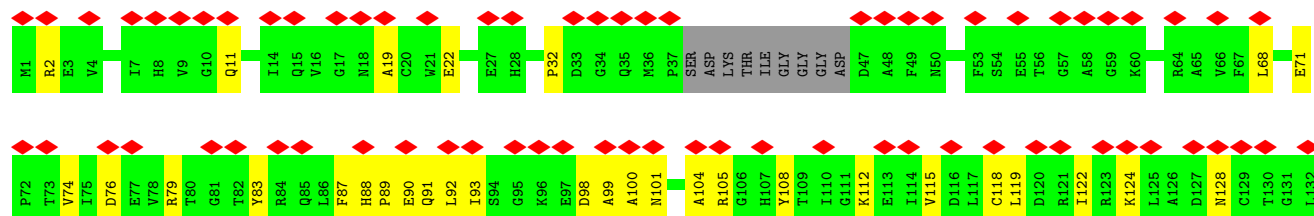


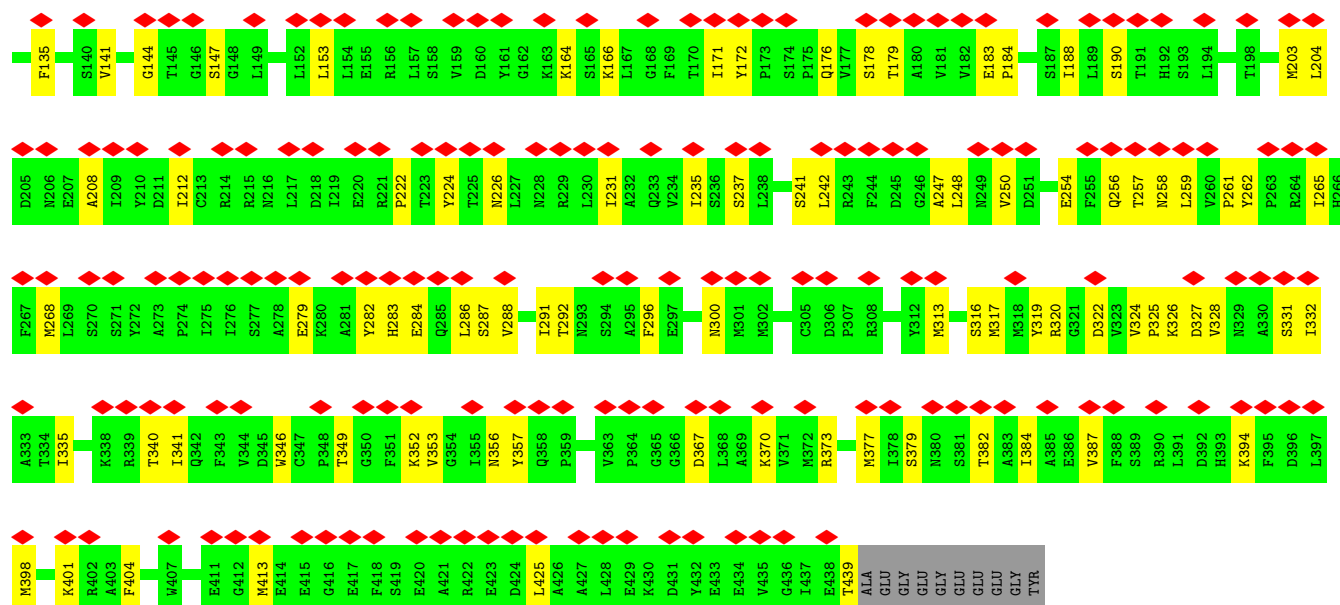


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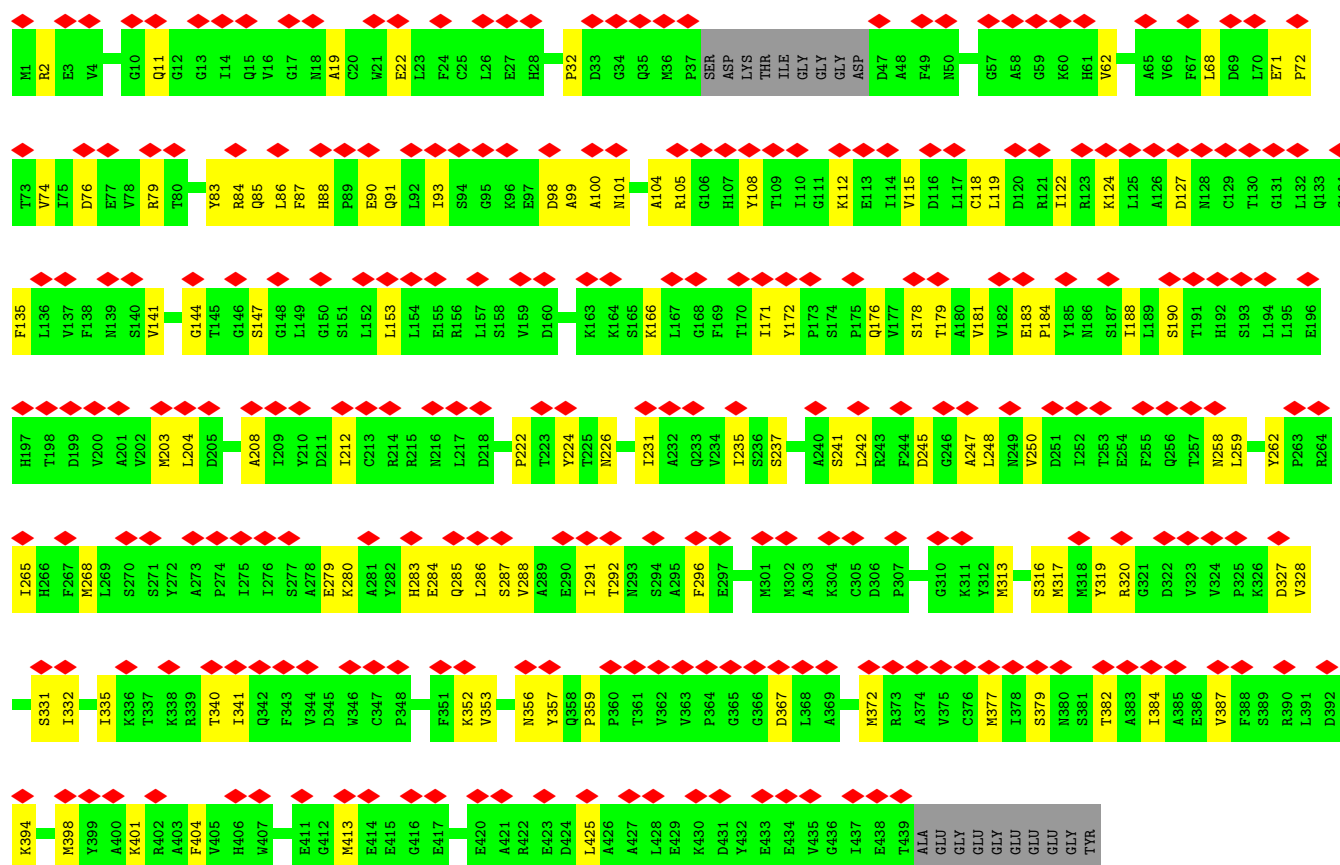
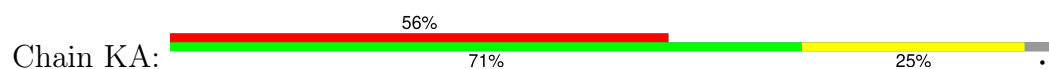


• Molecule 1: Tubulin alpha chain

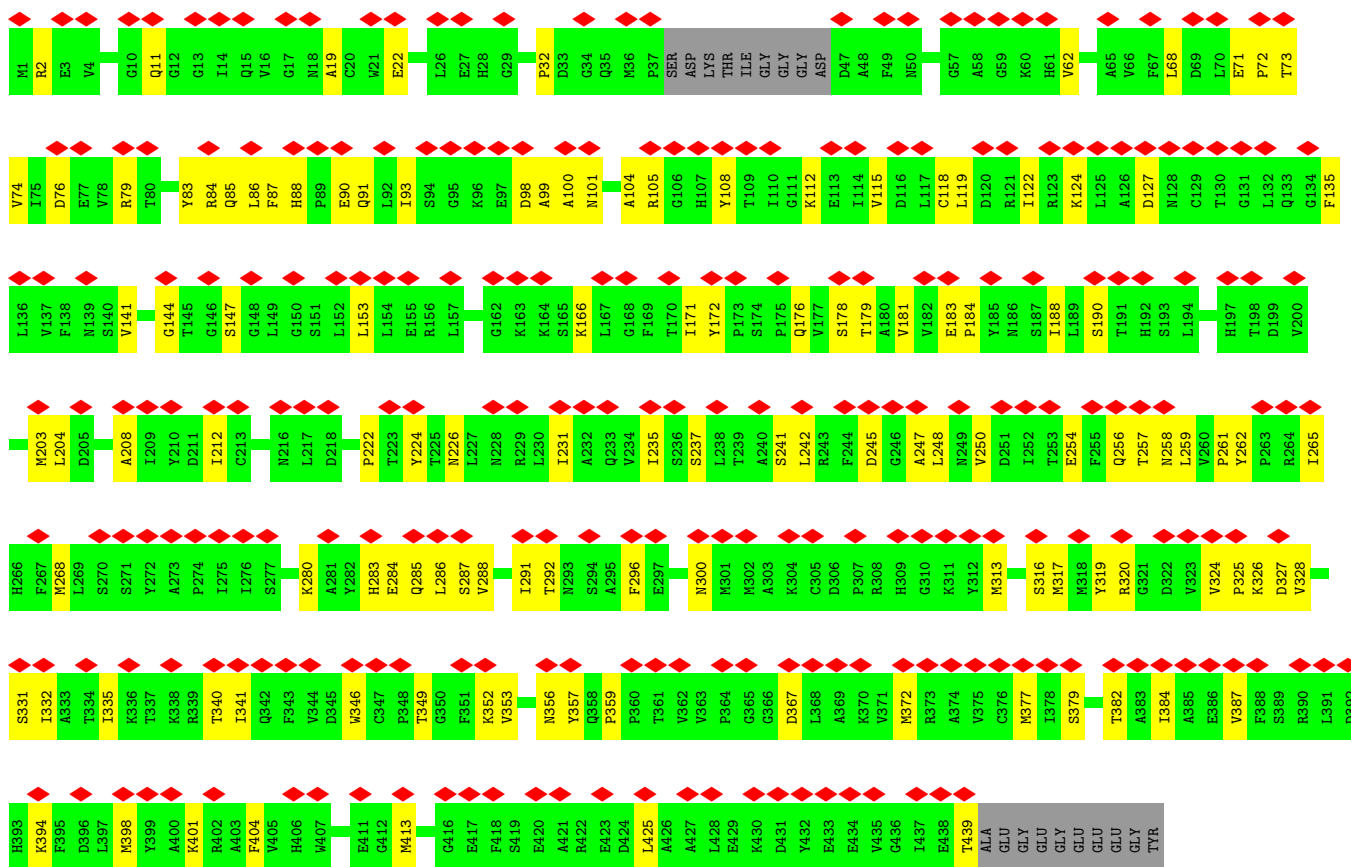




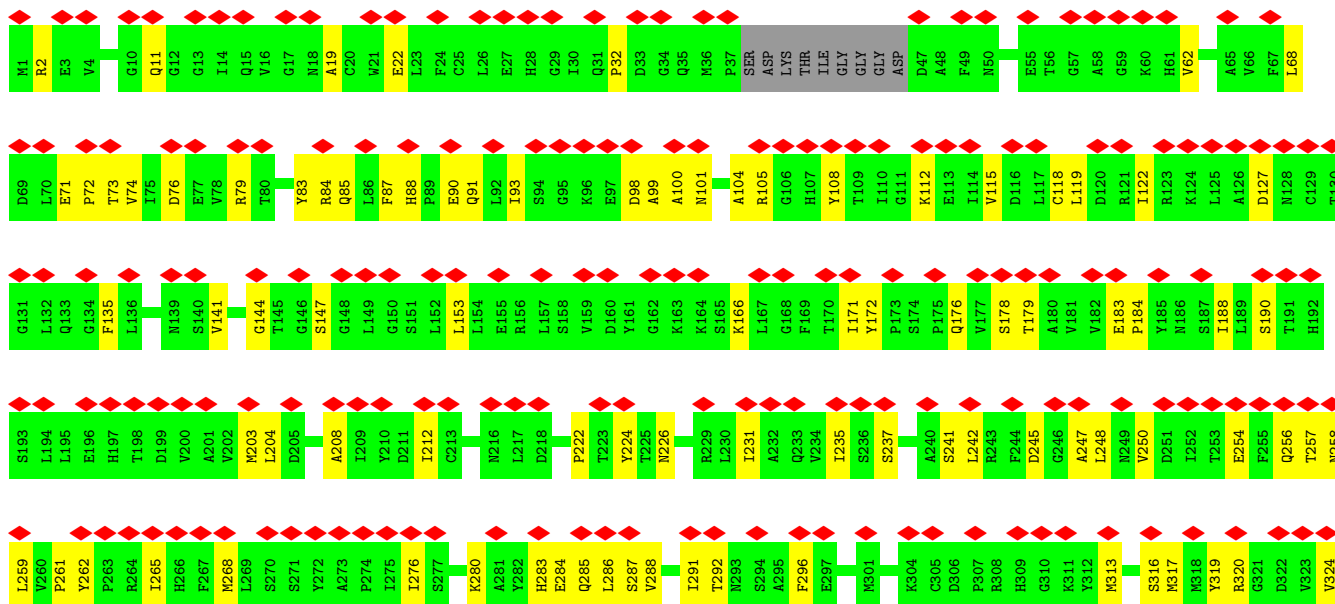
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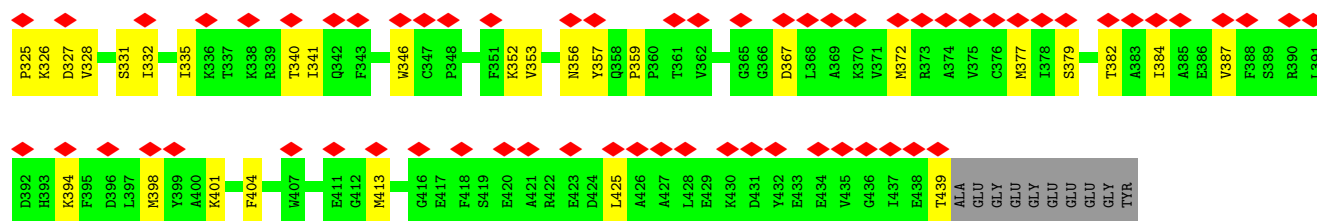


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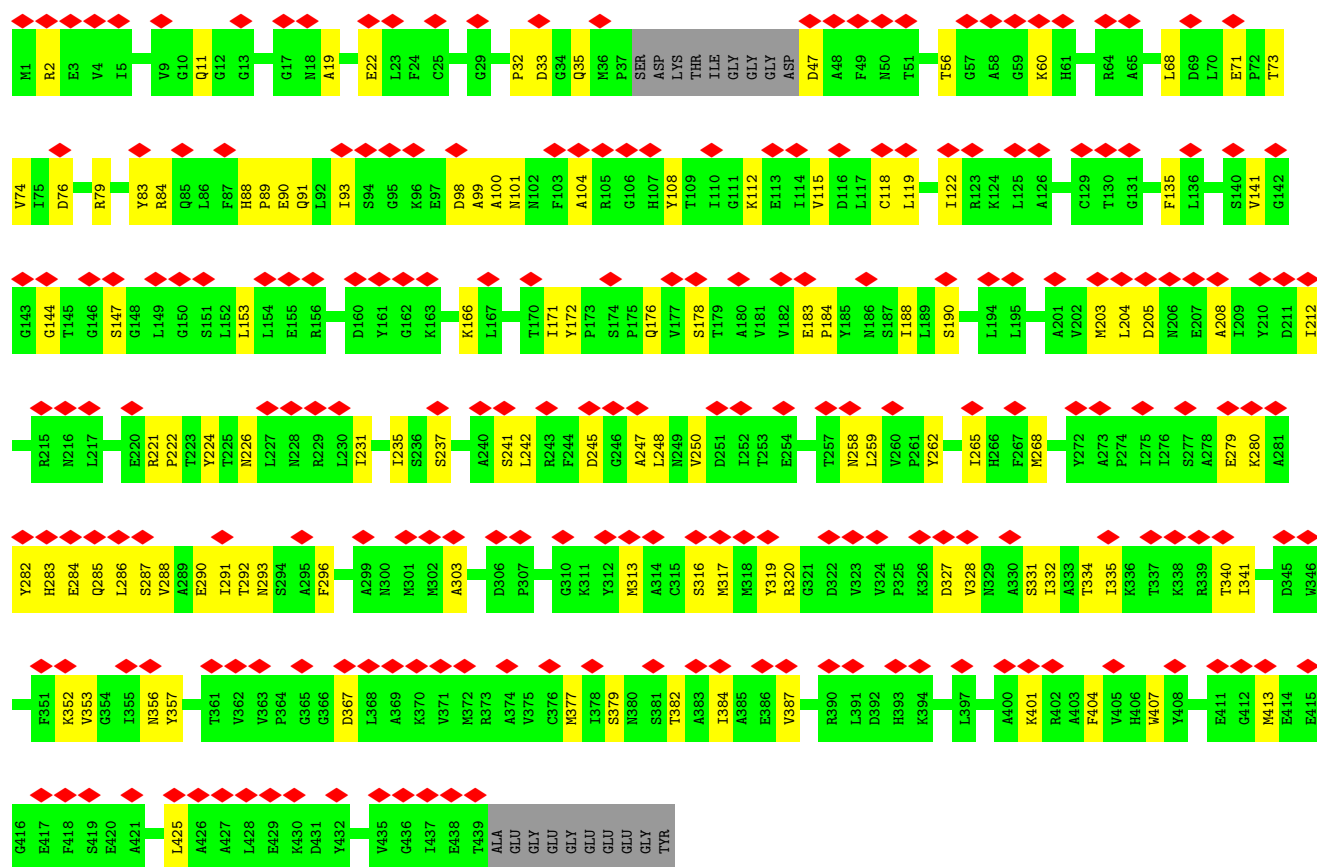
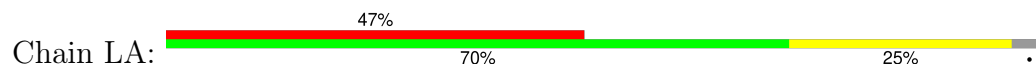


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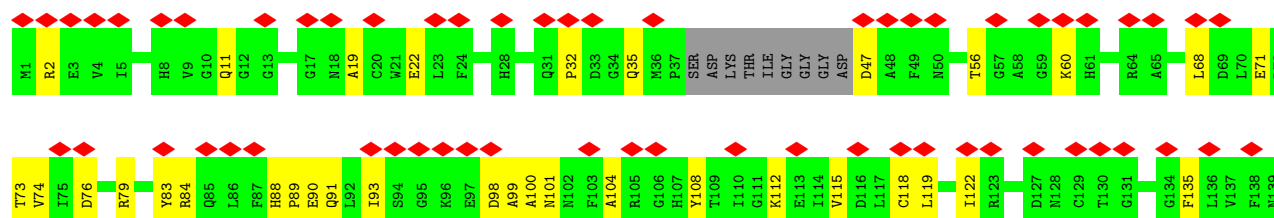


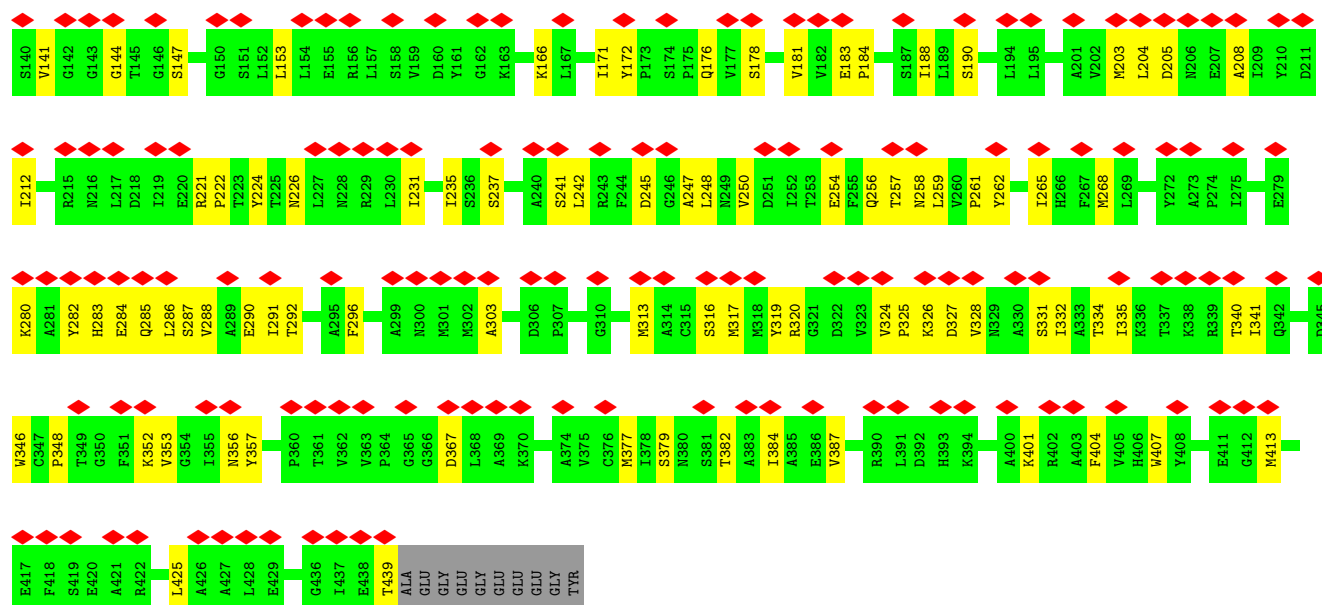


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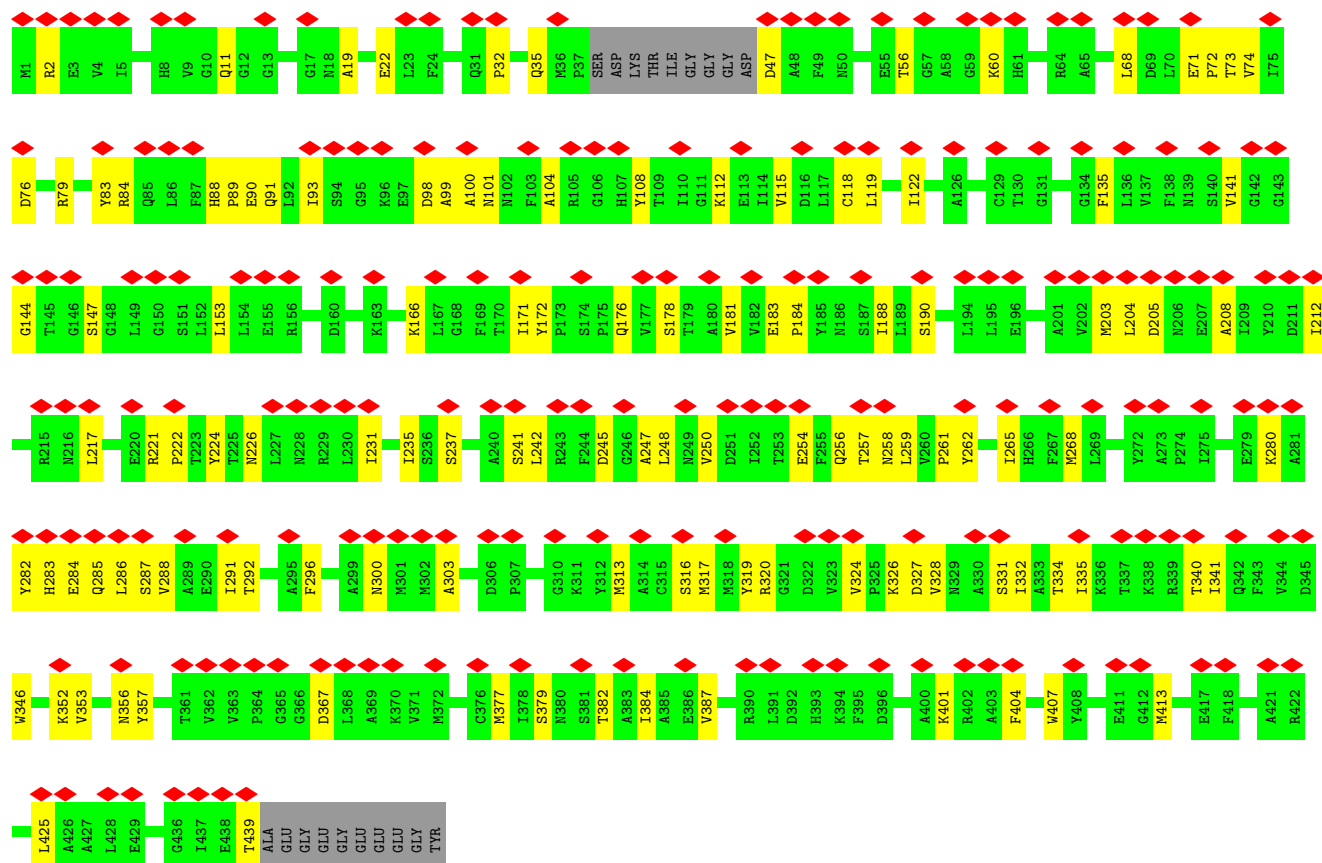


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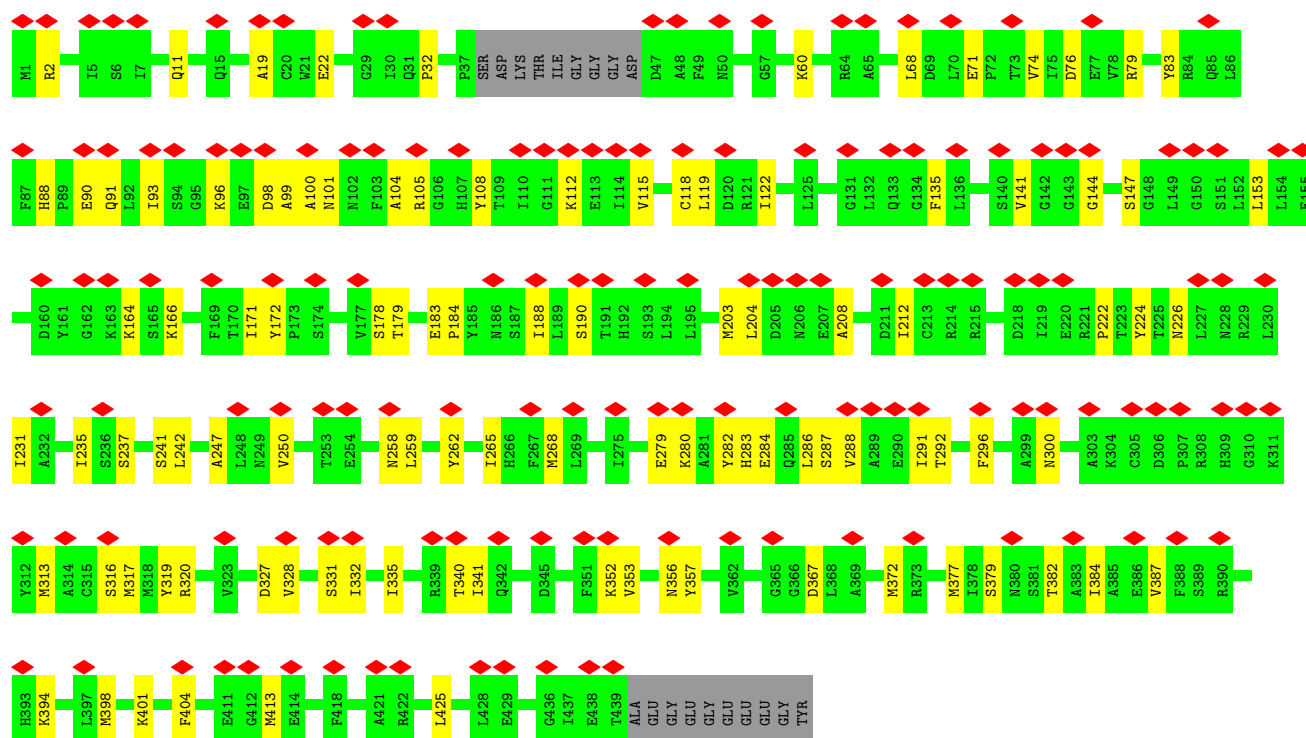
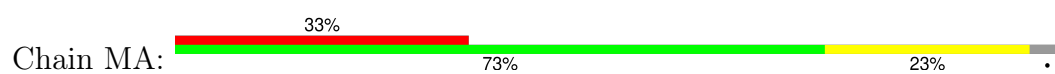




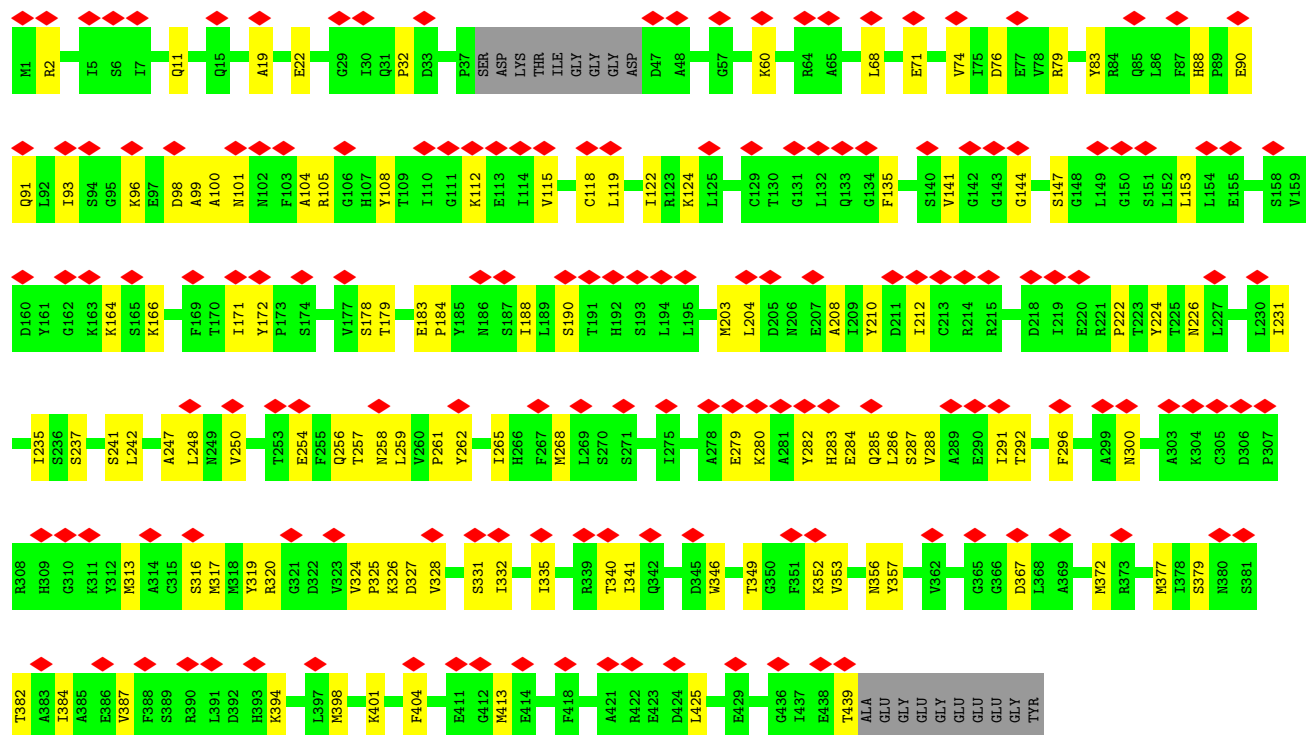
• Molecule 1: Tubulin alpha chain



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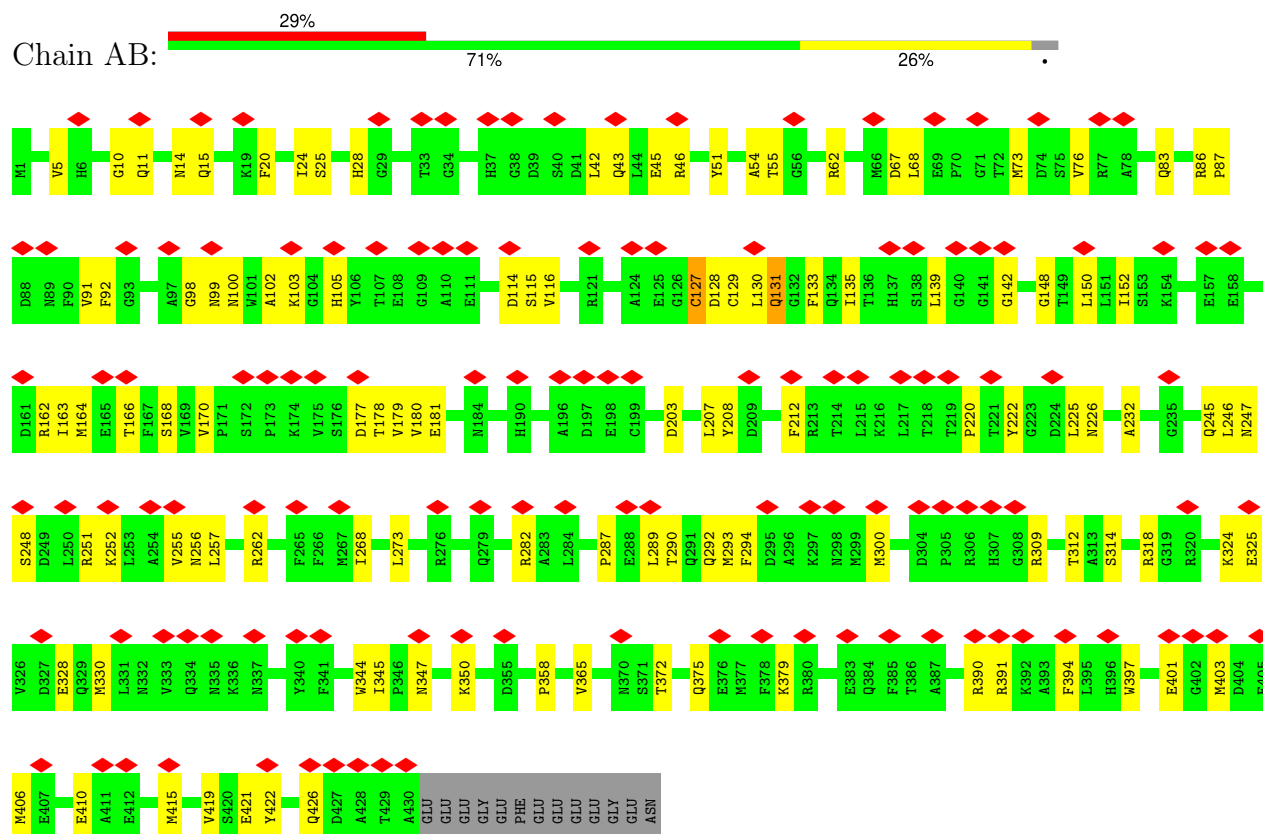
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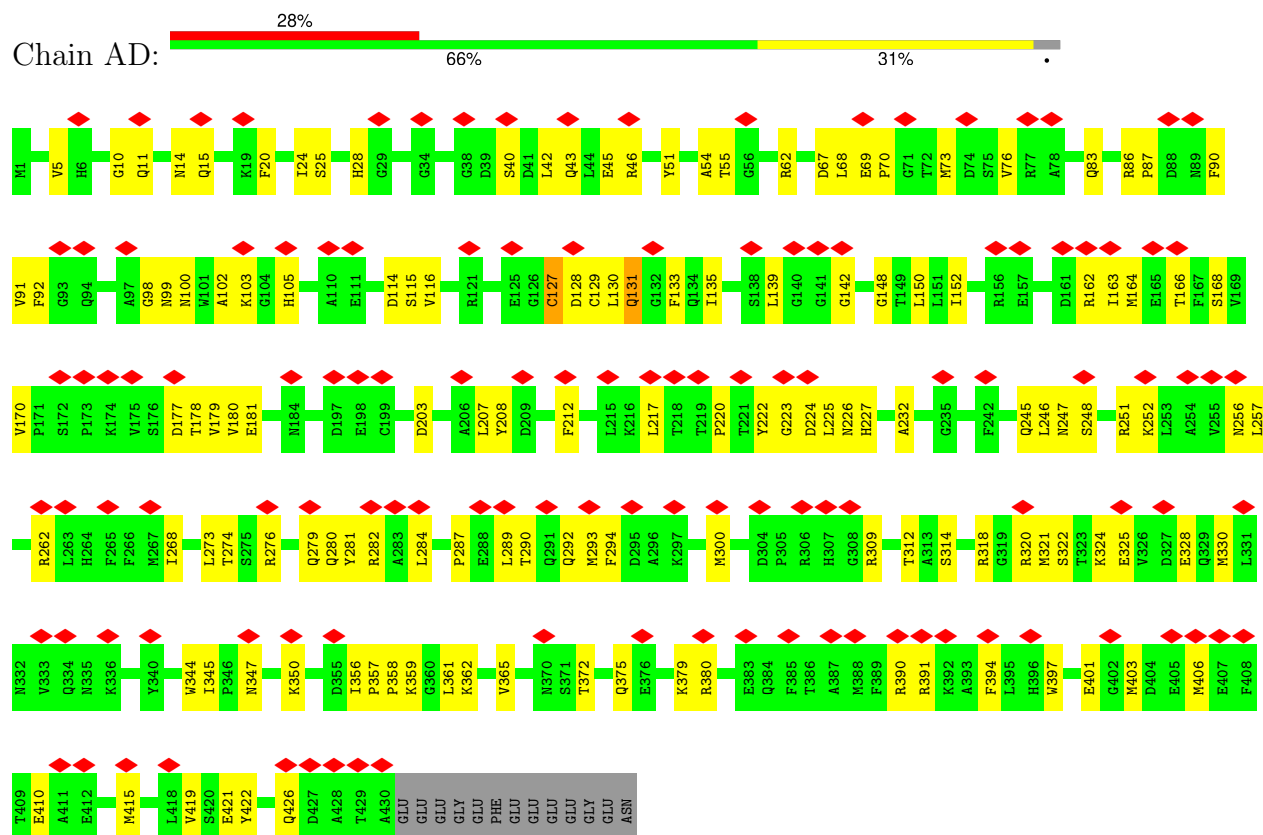
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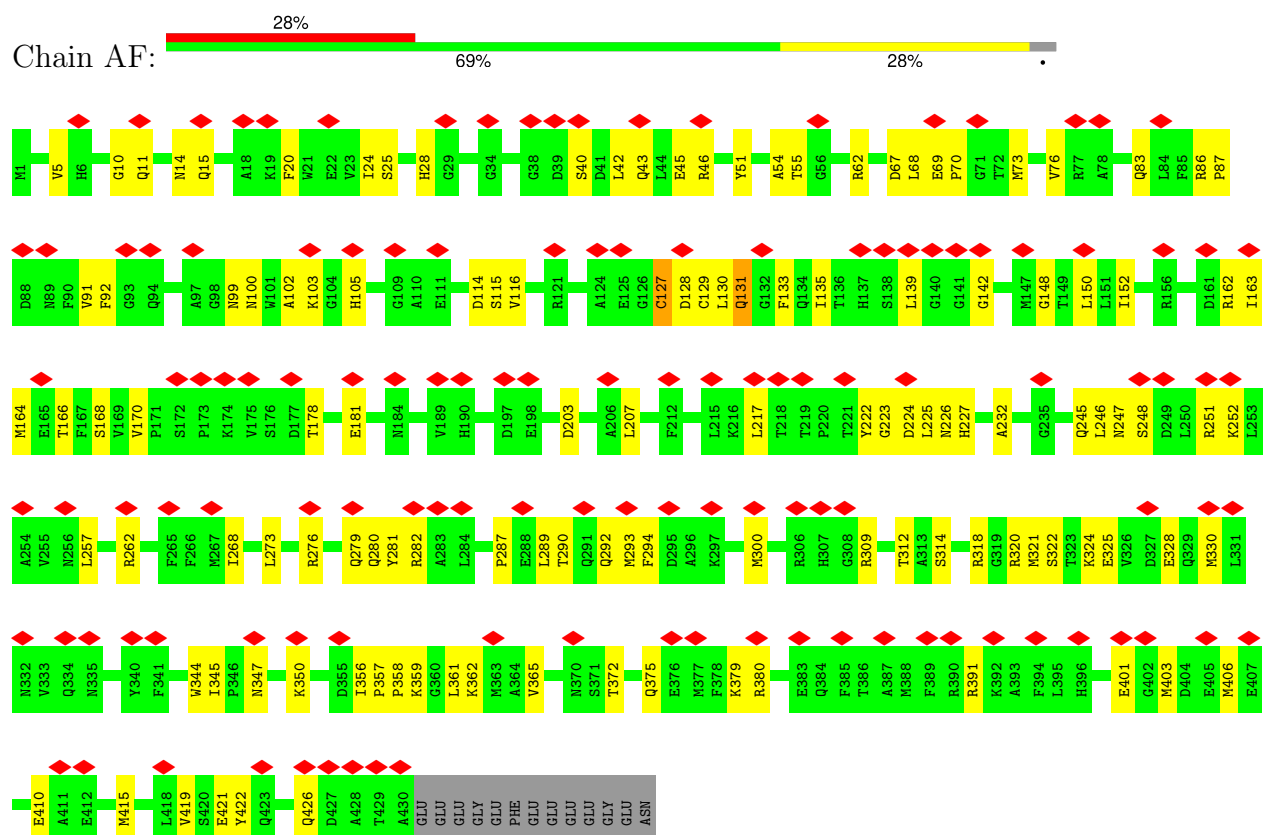
- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain

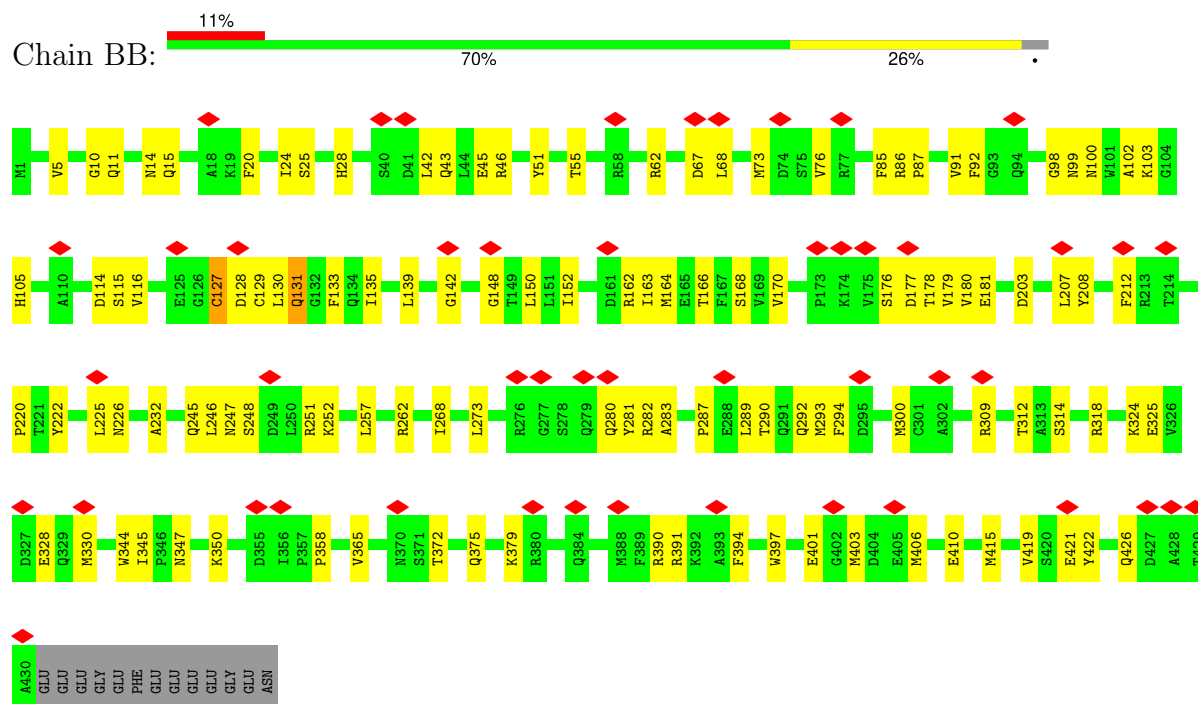


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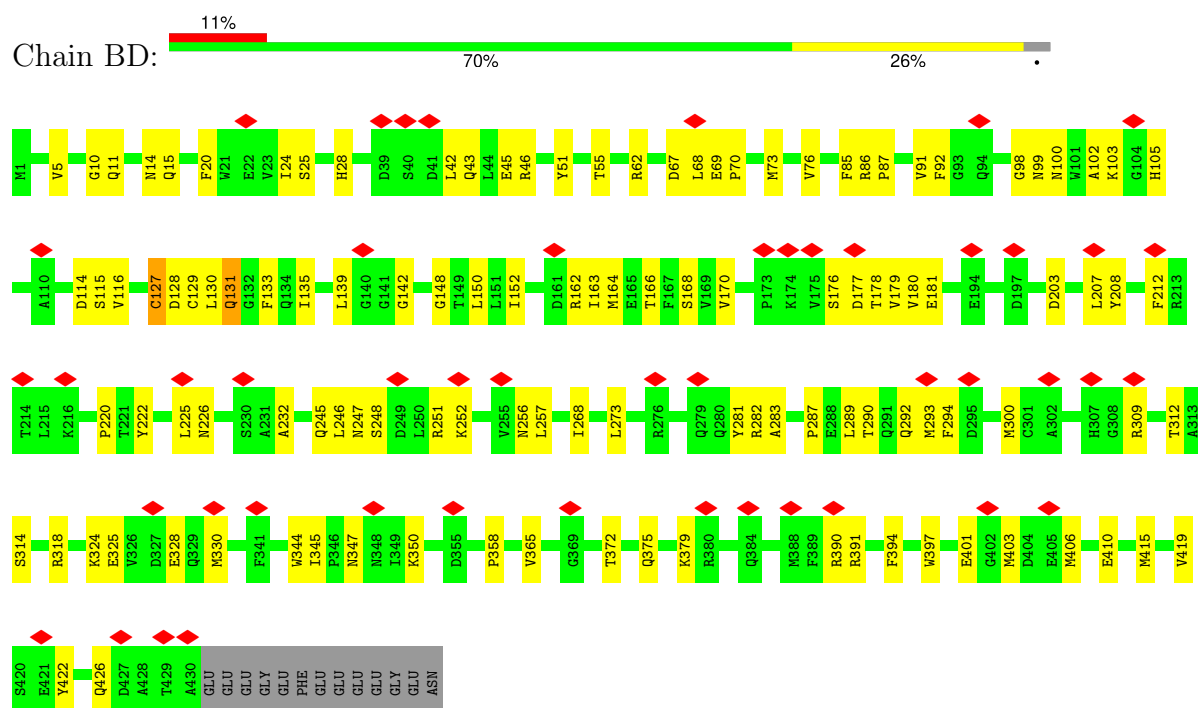




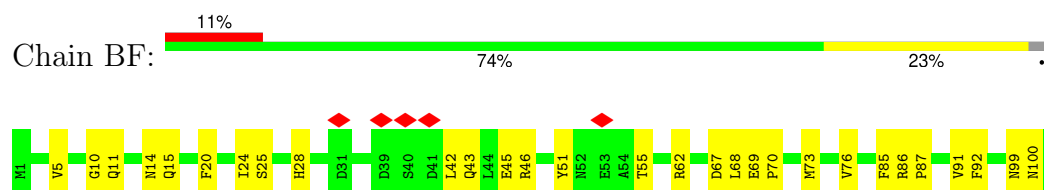
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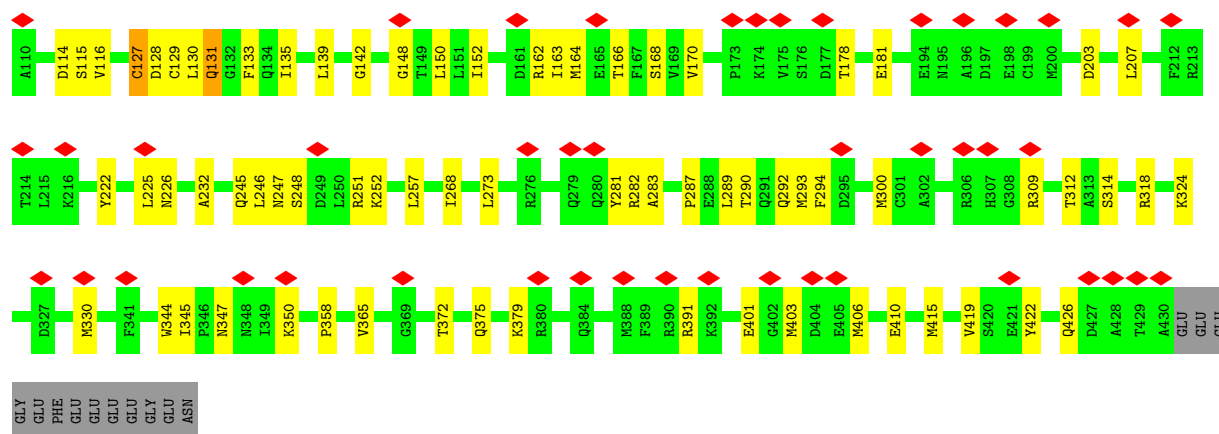


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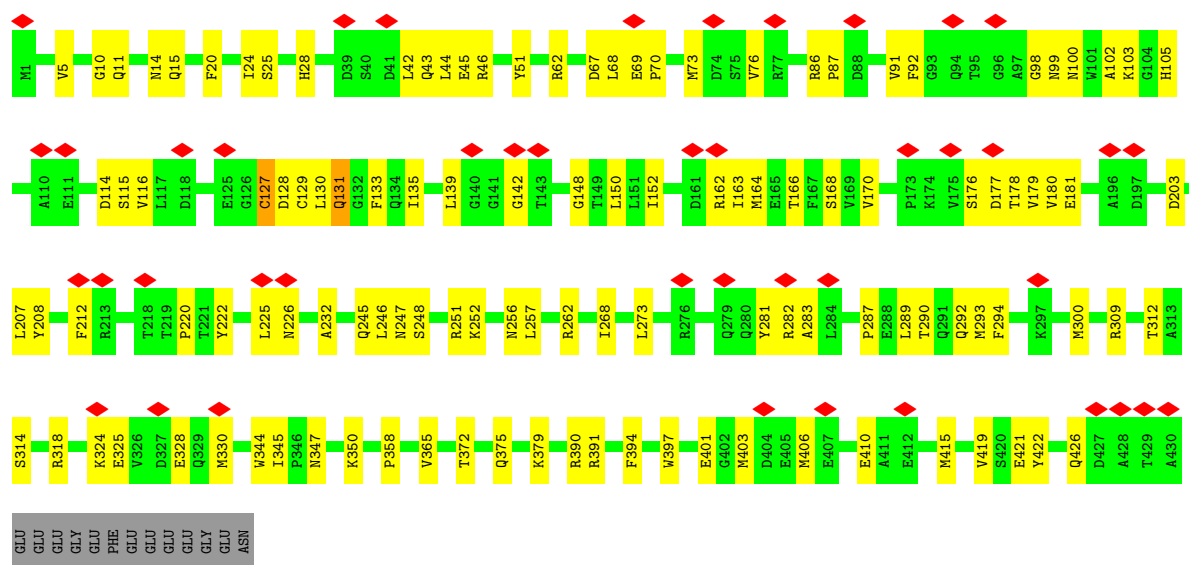
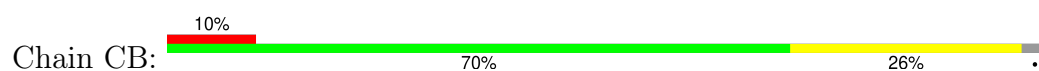


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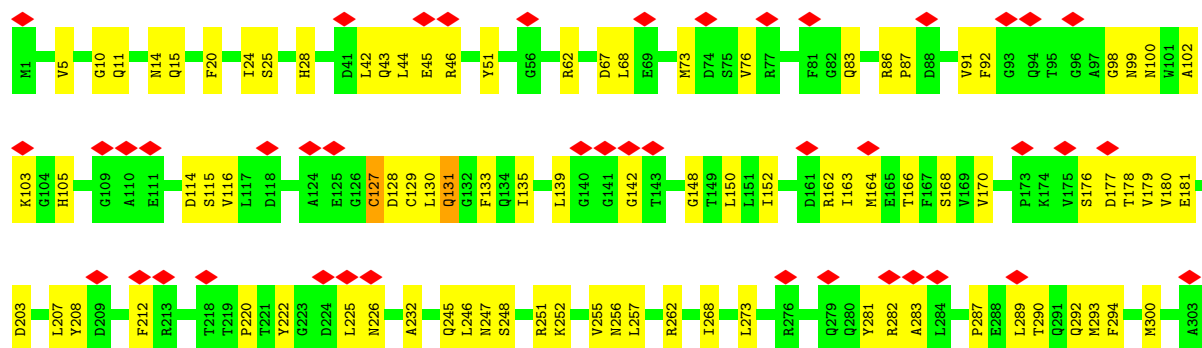
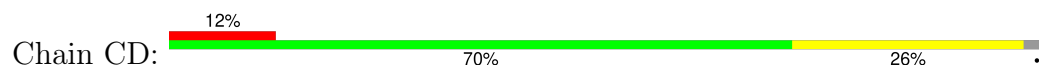


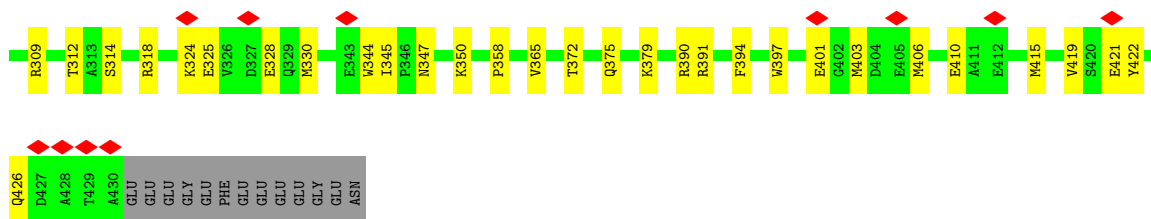


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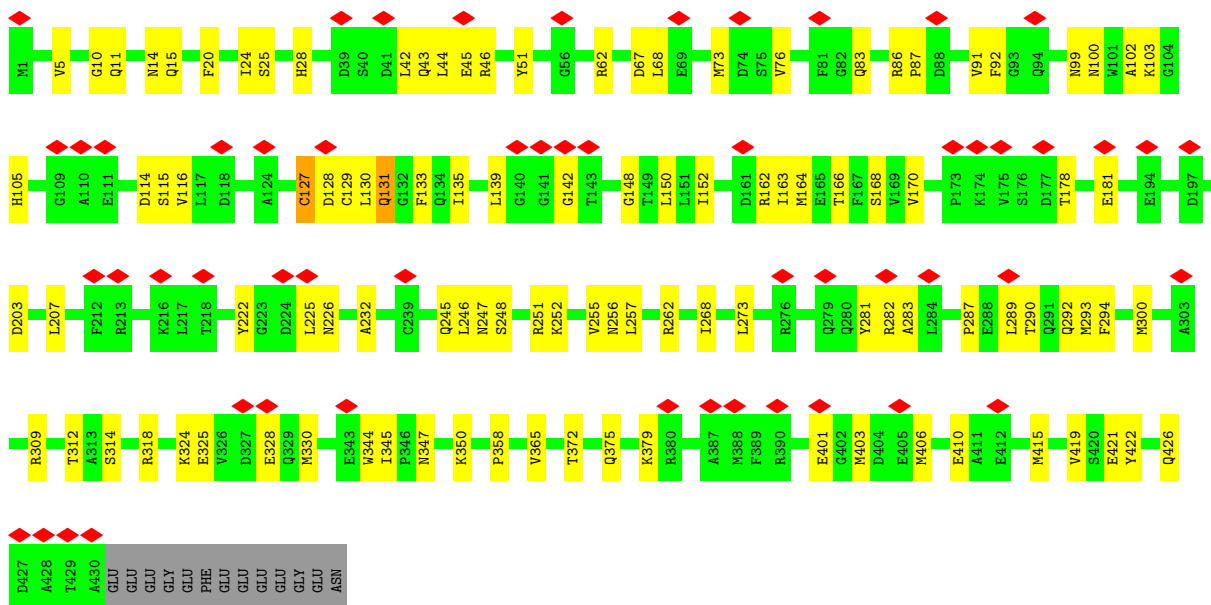
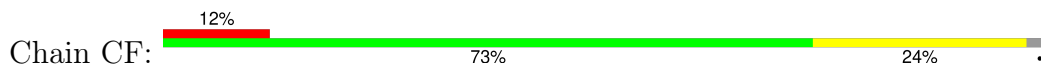


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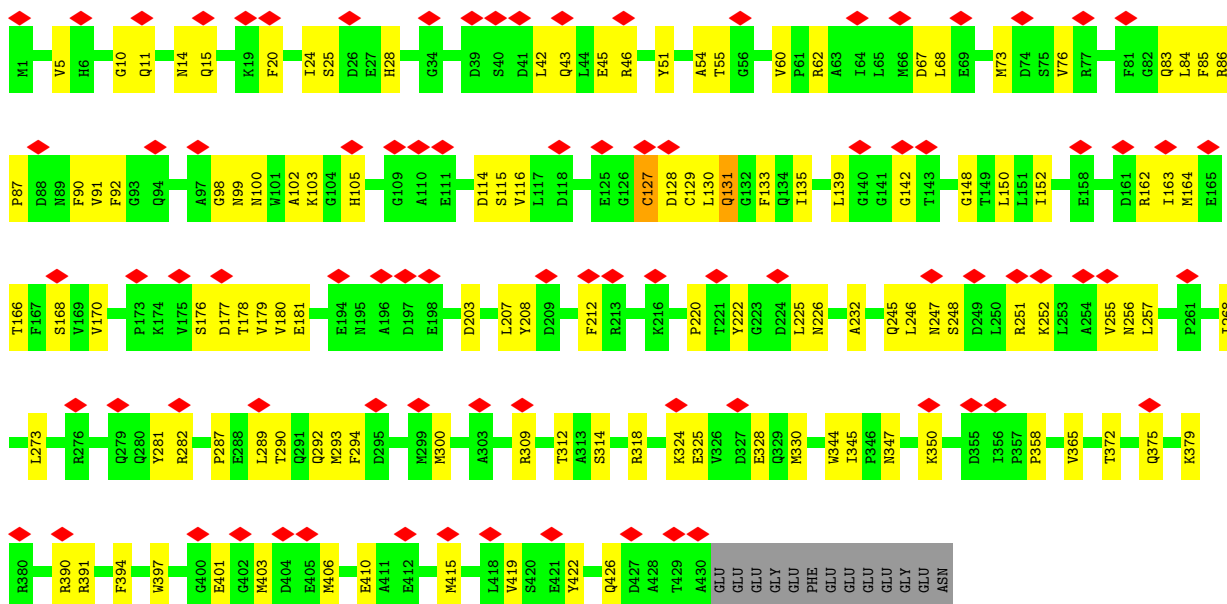




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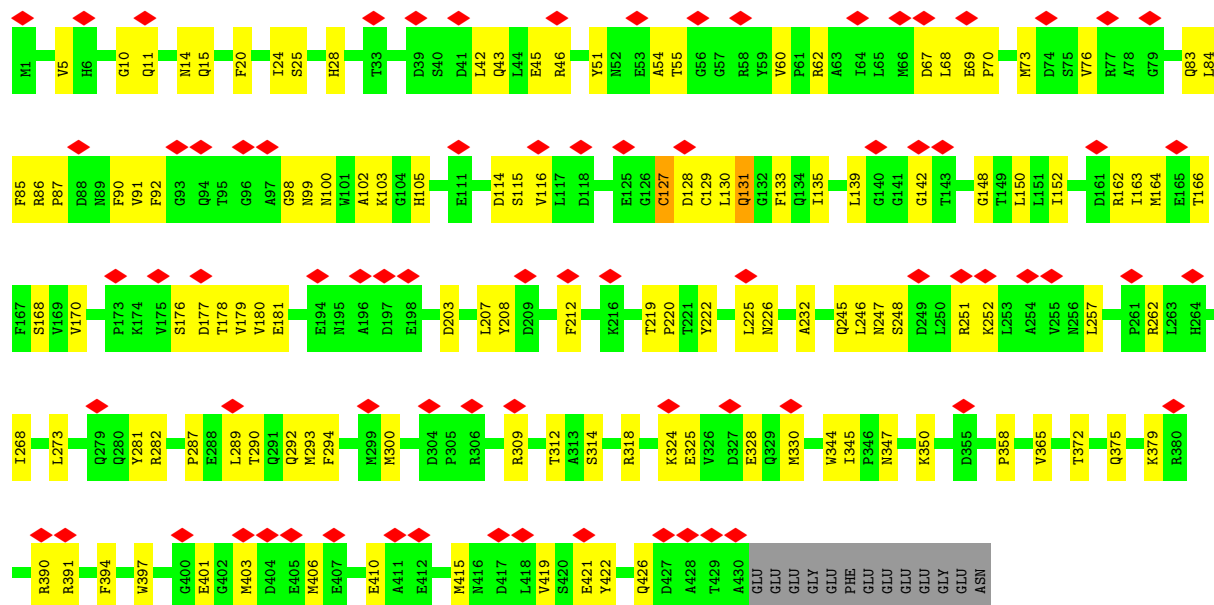


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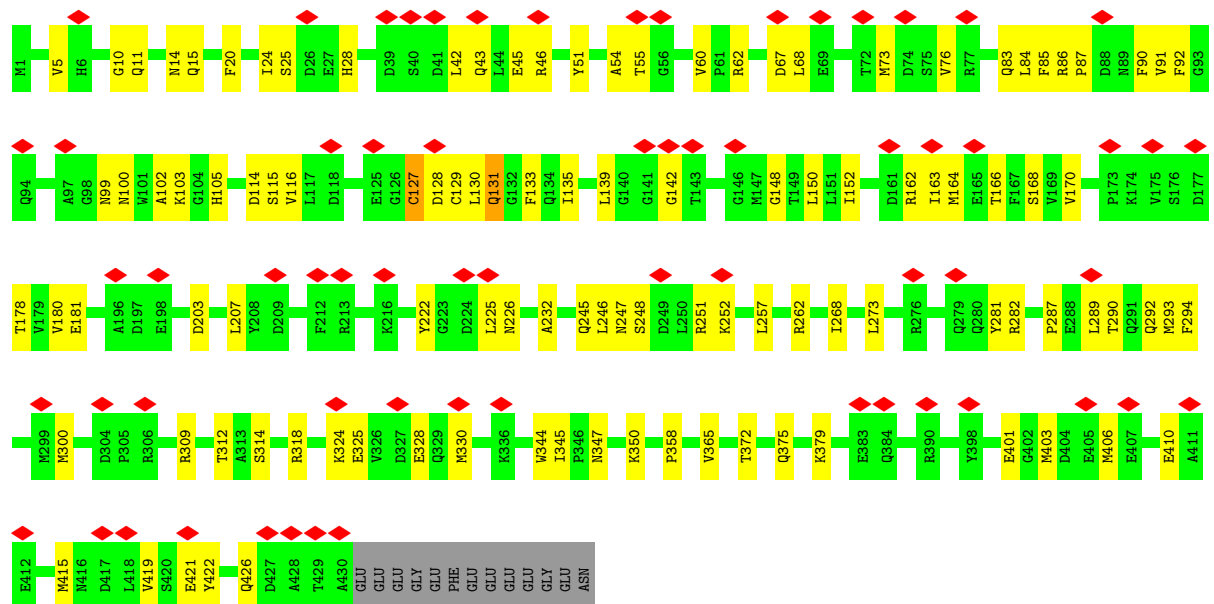
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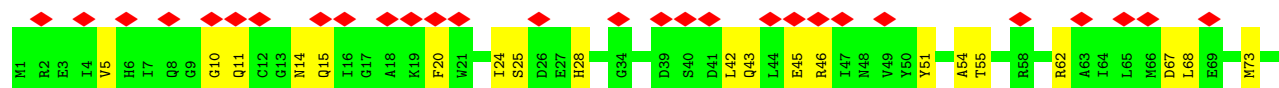
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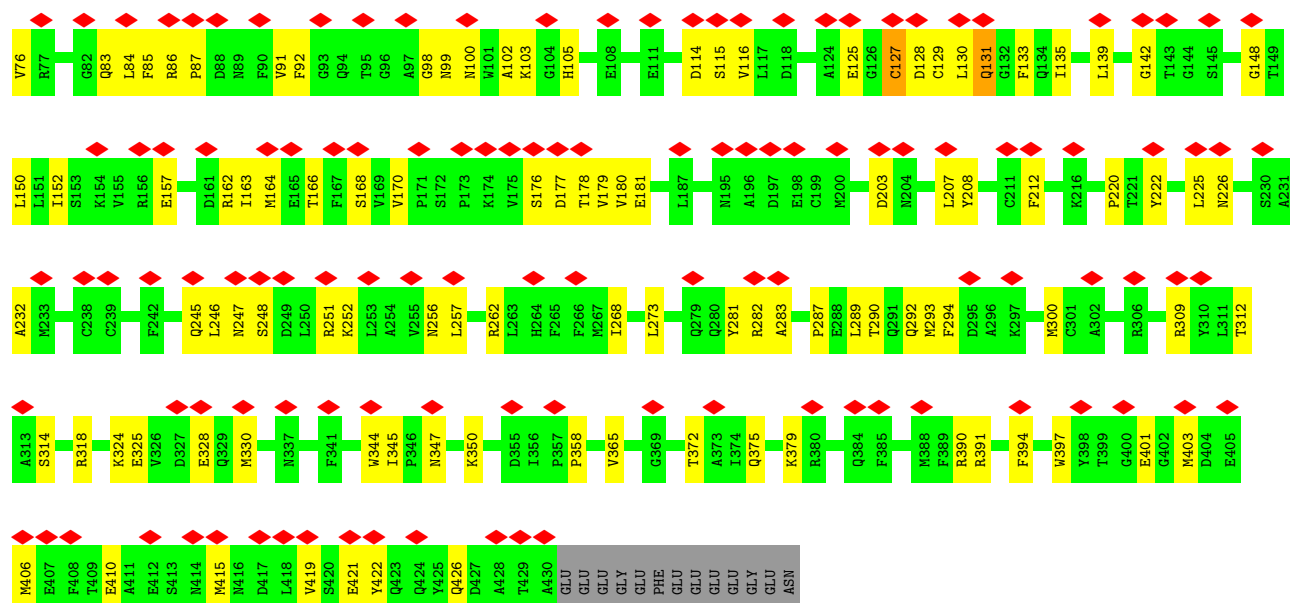
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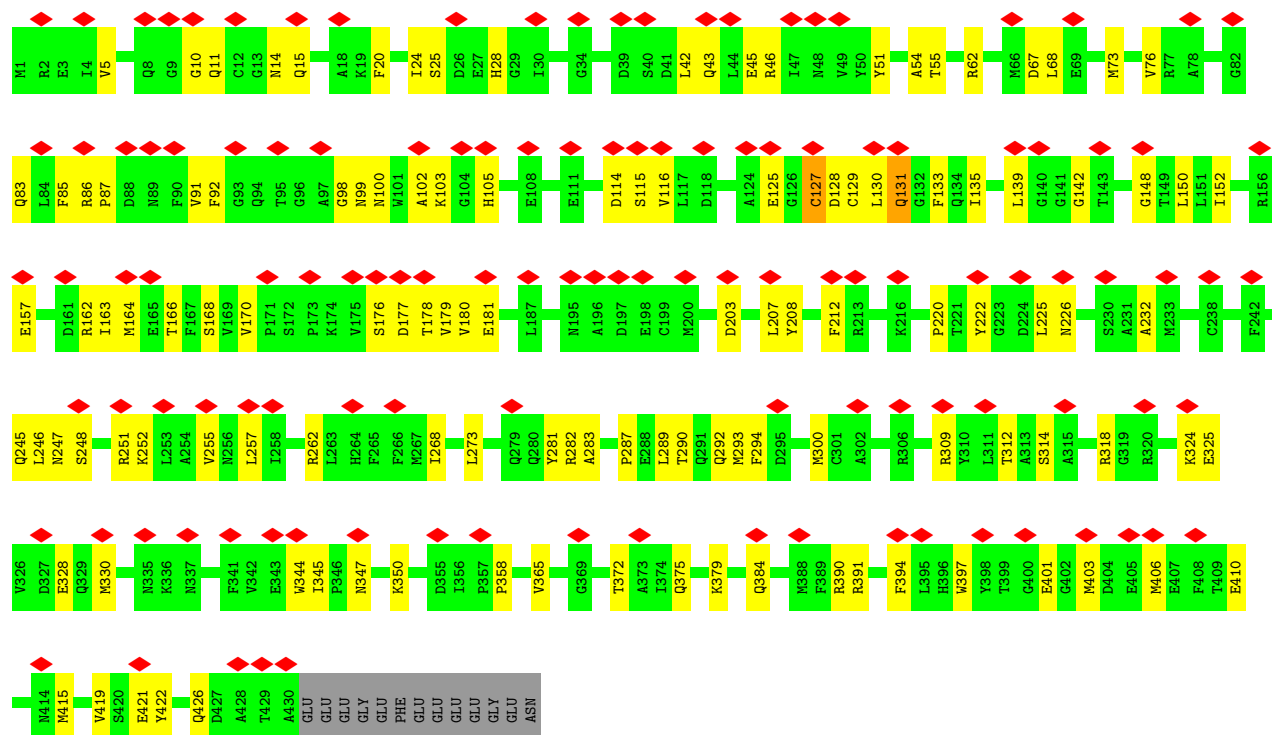
- Molecule 2: Tubulin beta chain

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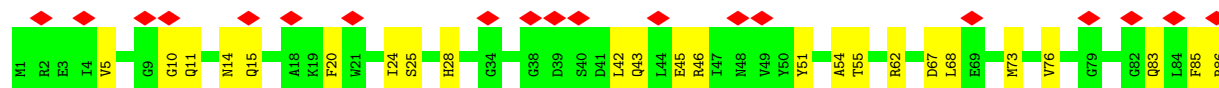
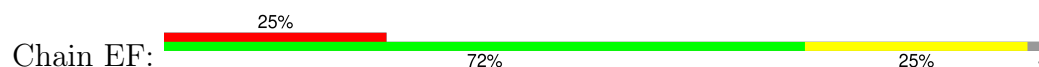


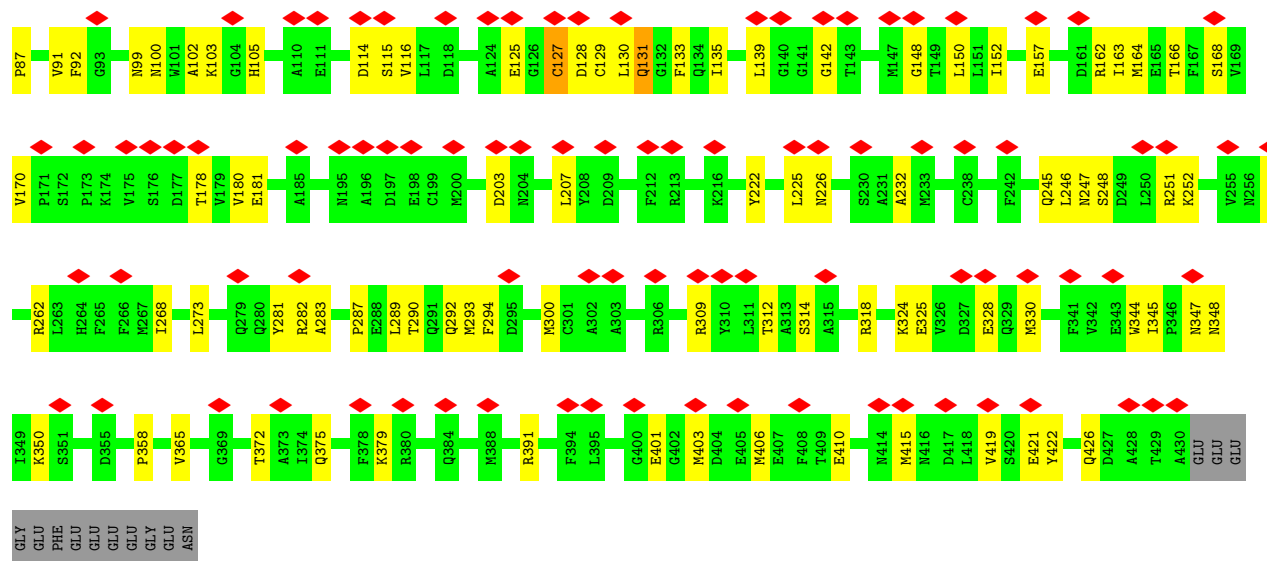


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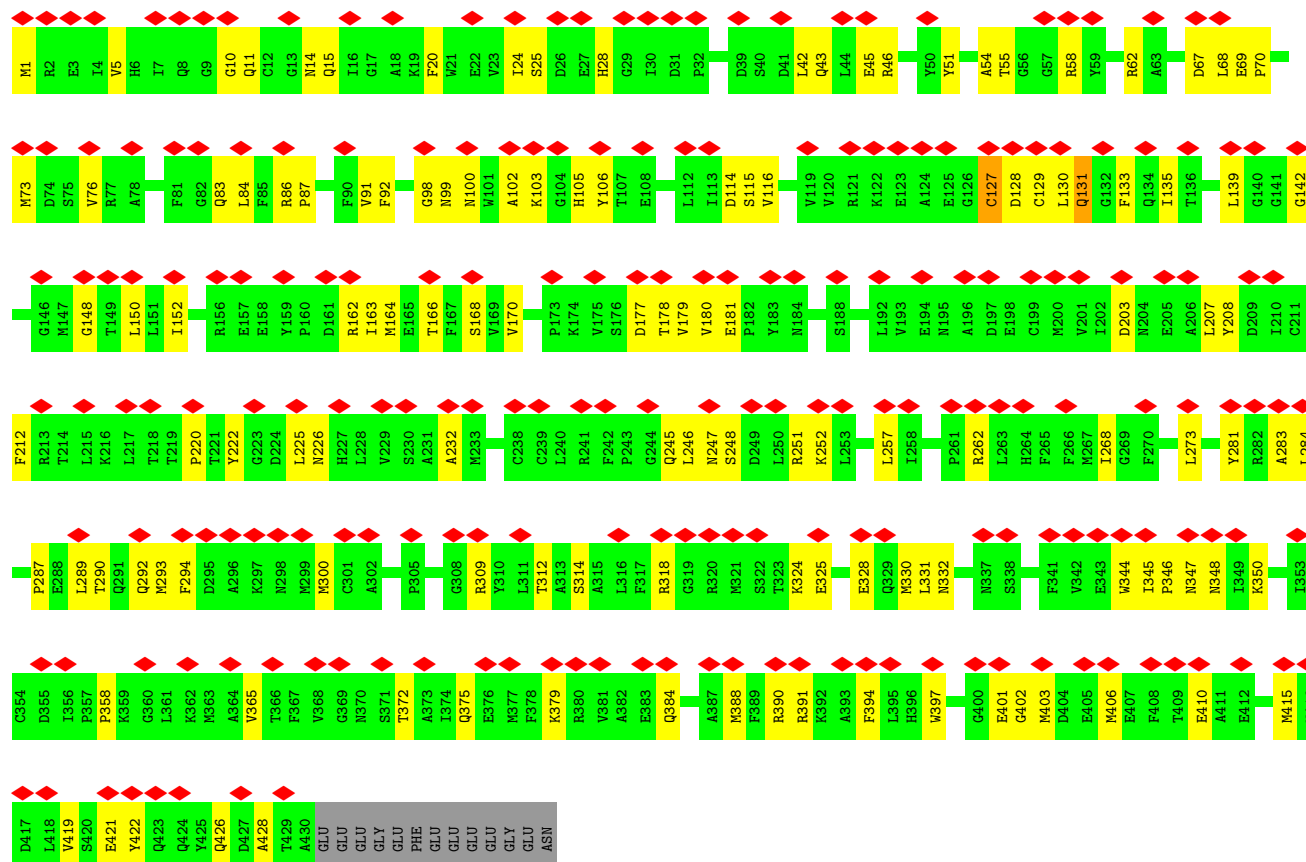


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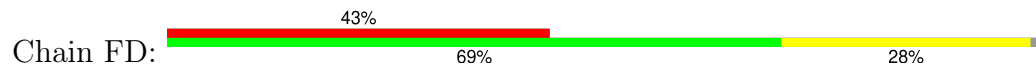


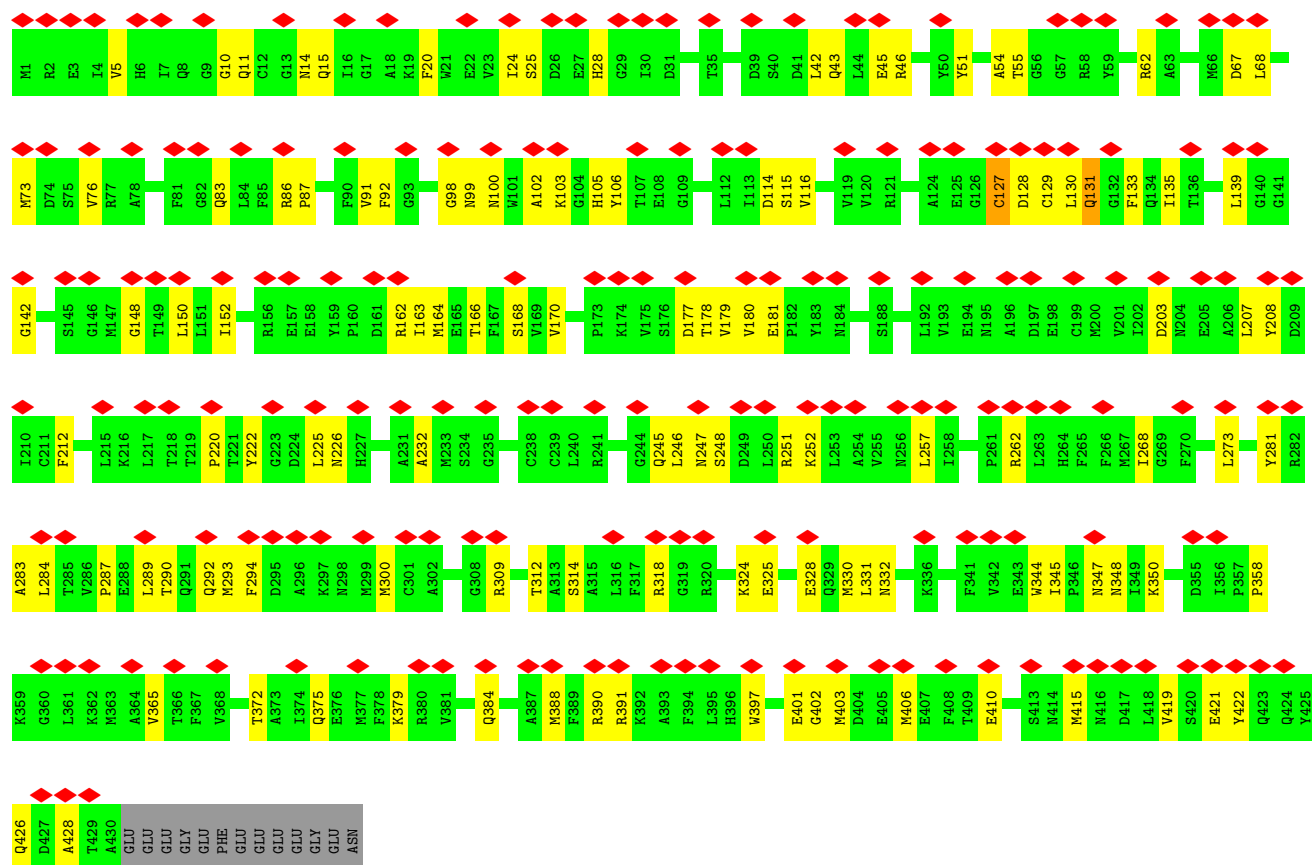


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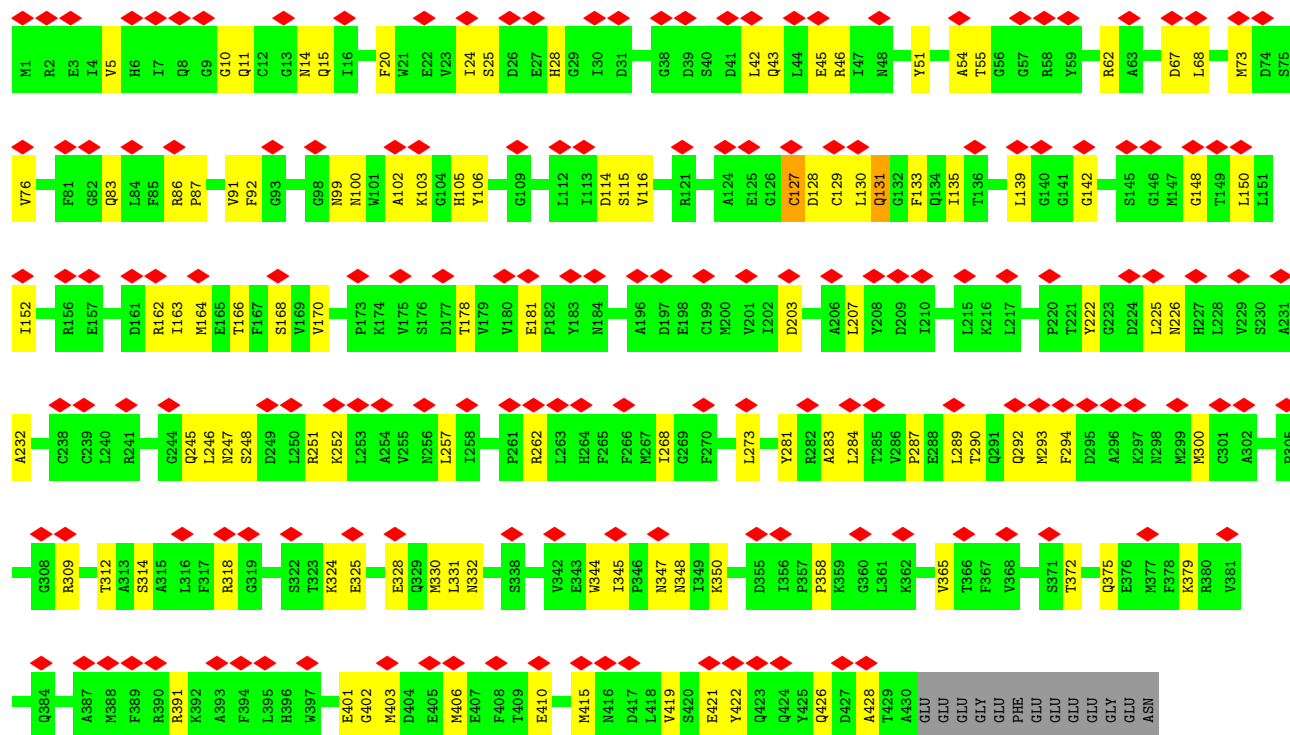
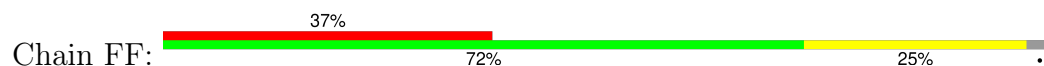


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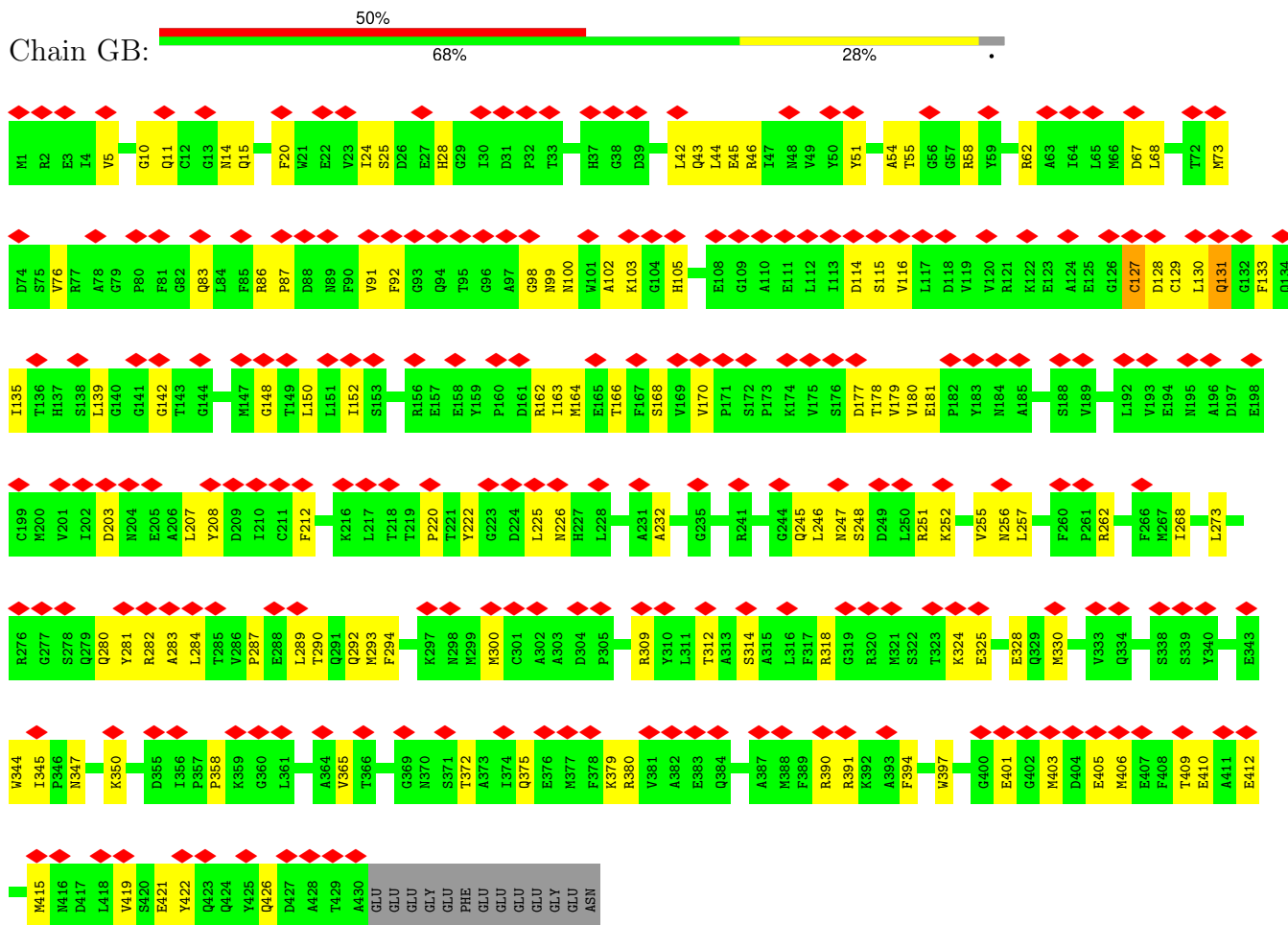


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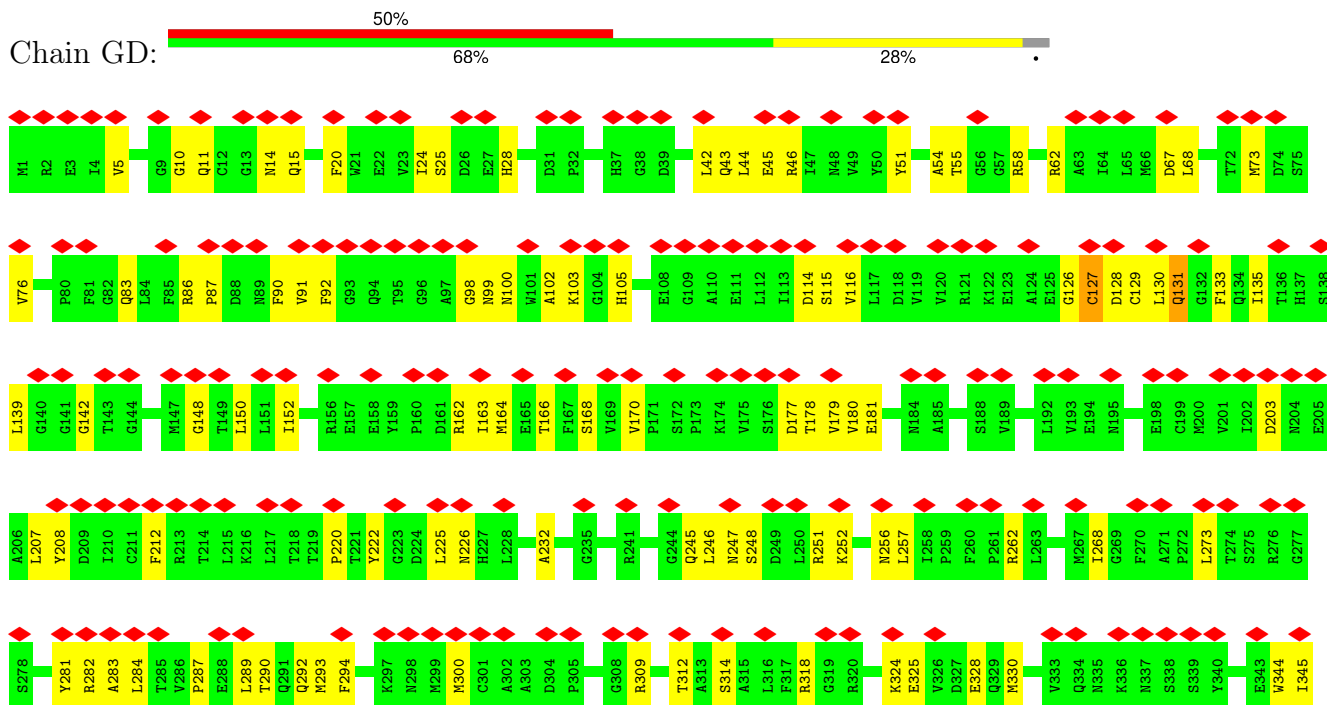
- Molecule 2: Tubulin beta chain

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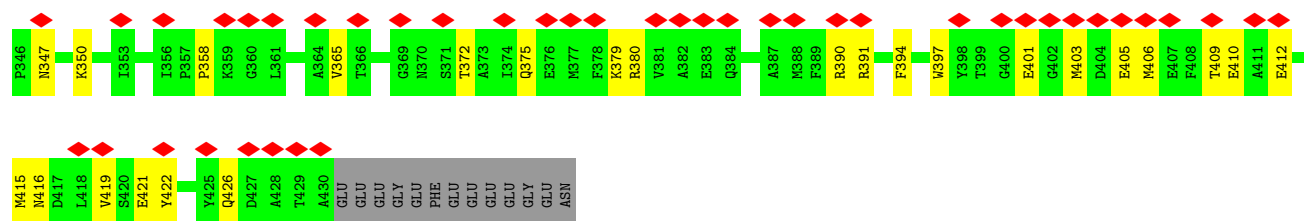


- Molecule 2: Tubulin beta chain

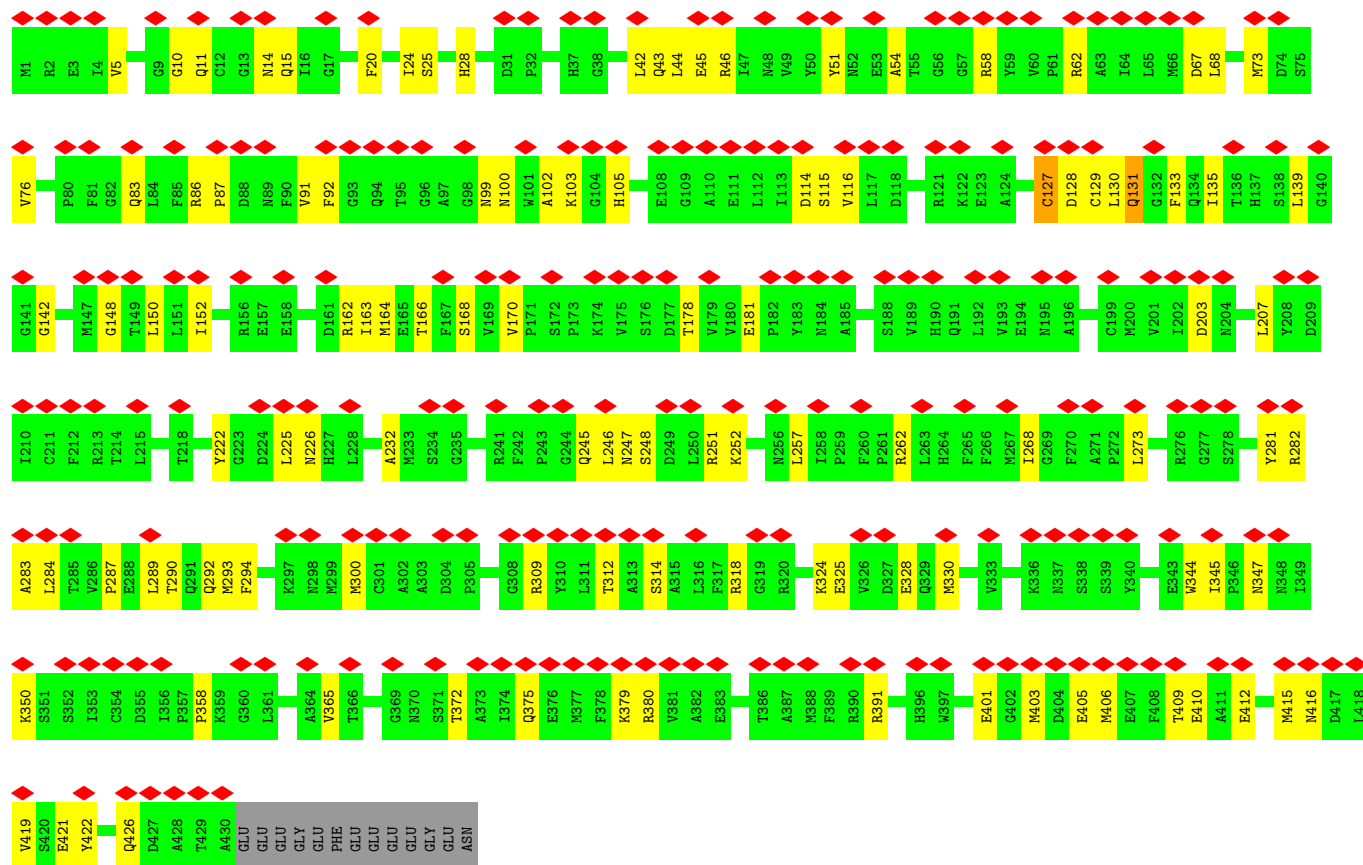
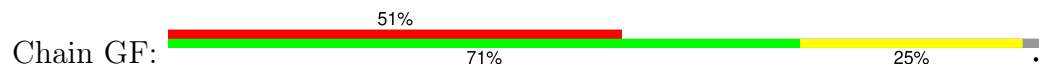
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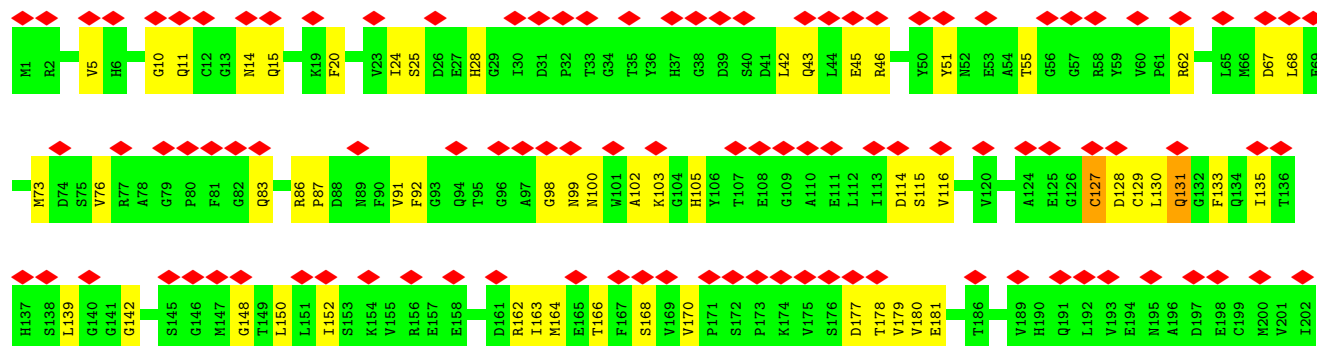
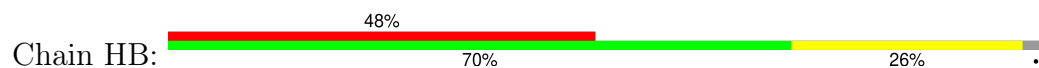


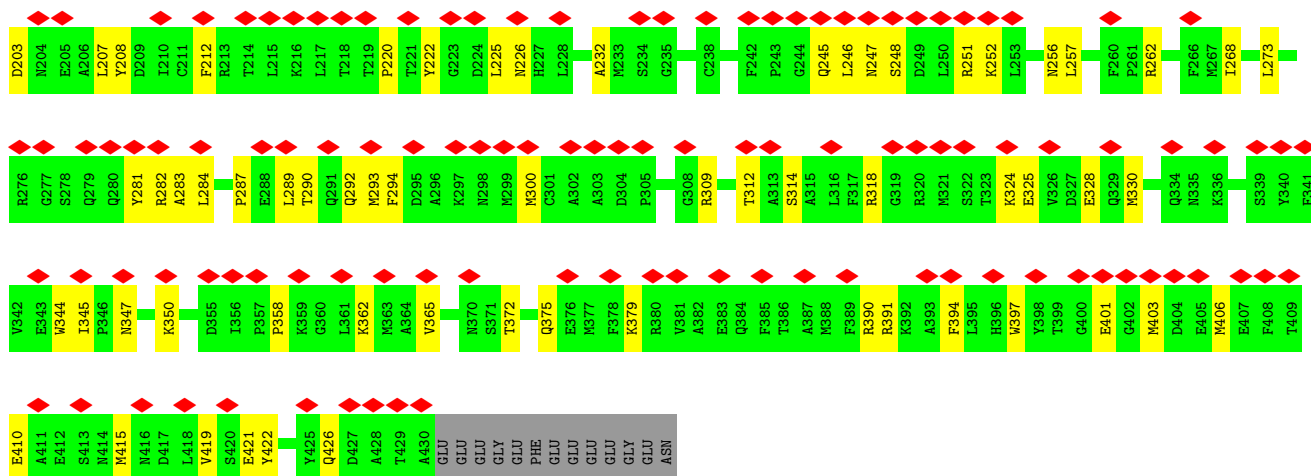


• Molecule 2: Tubulin beta chain

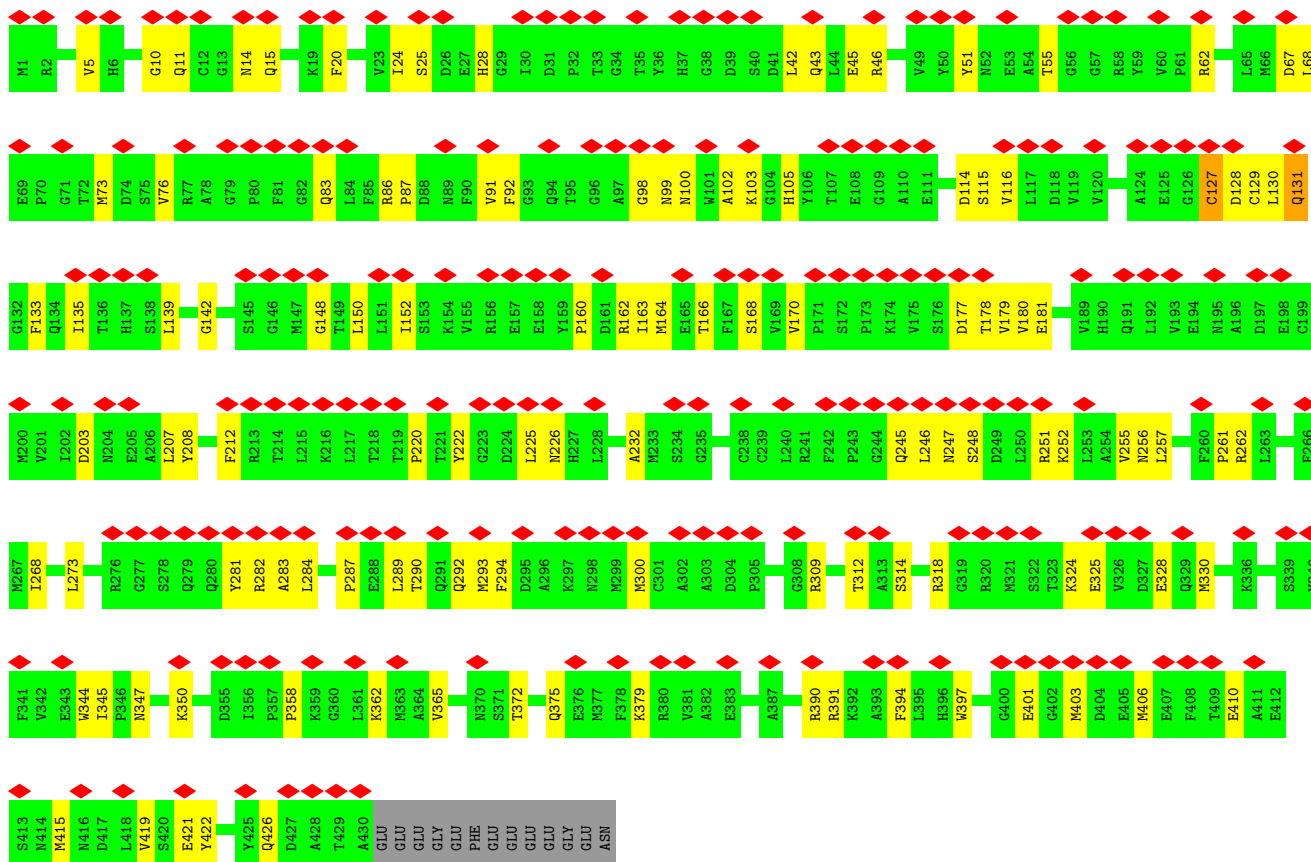
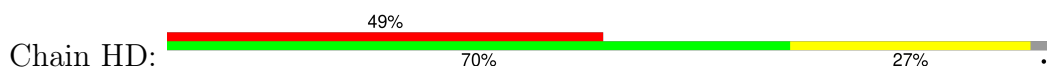


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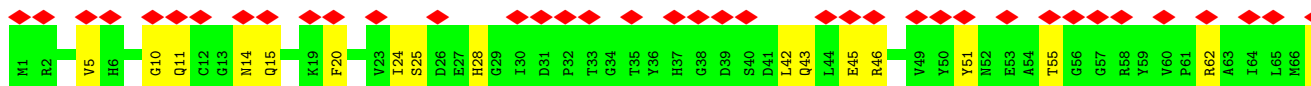
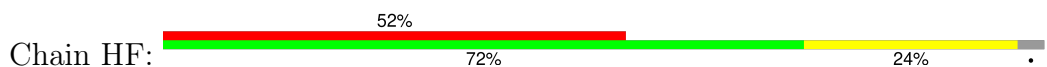


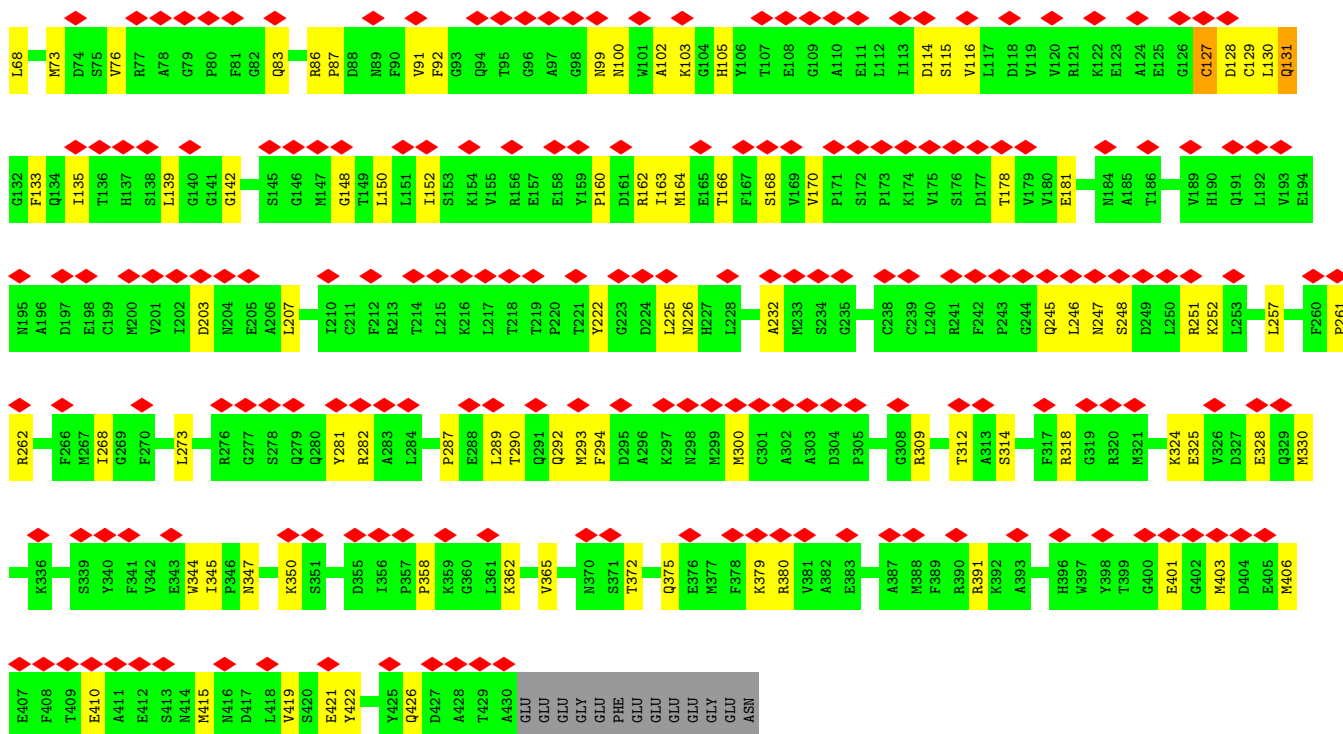


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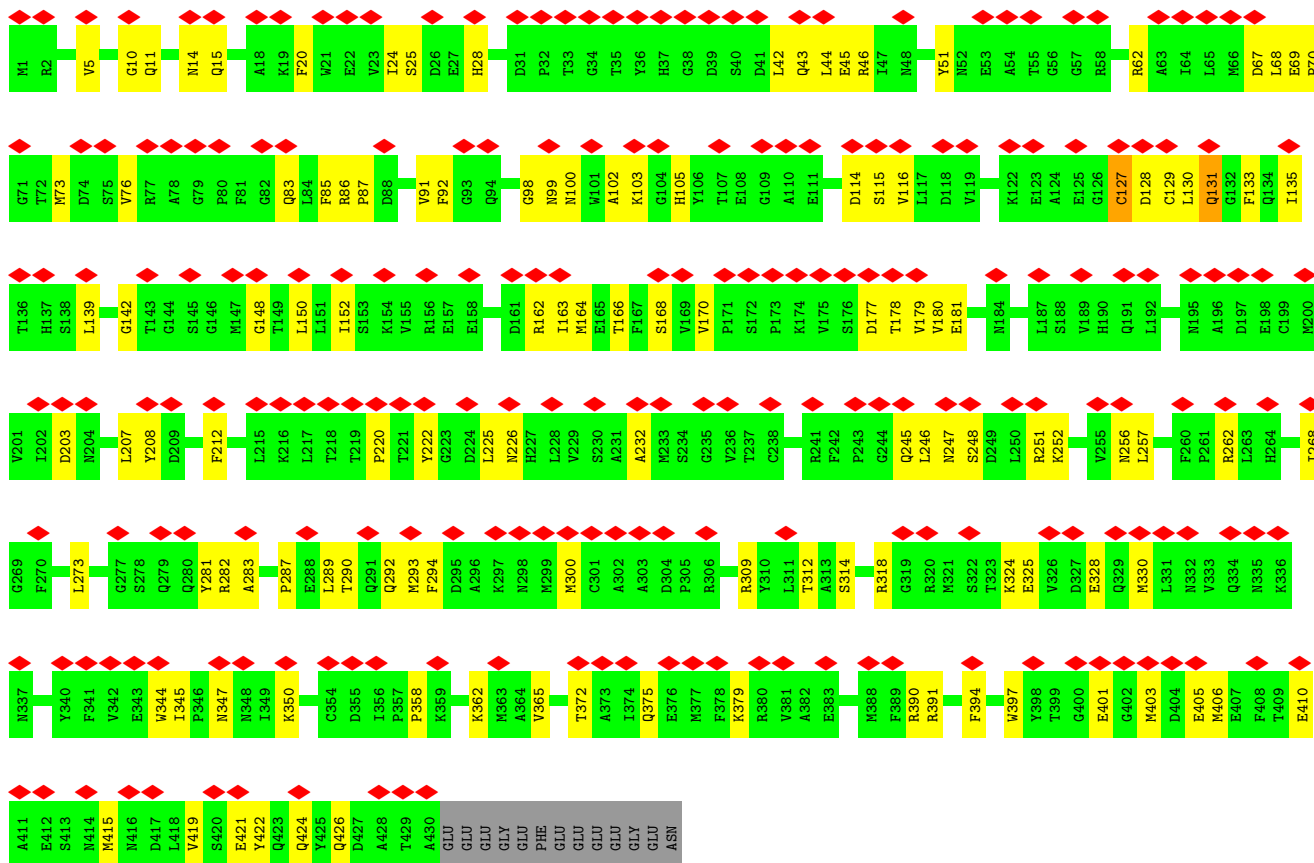


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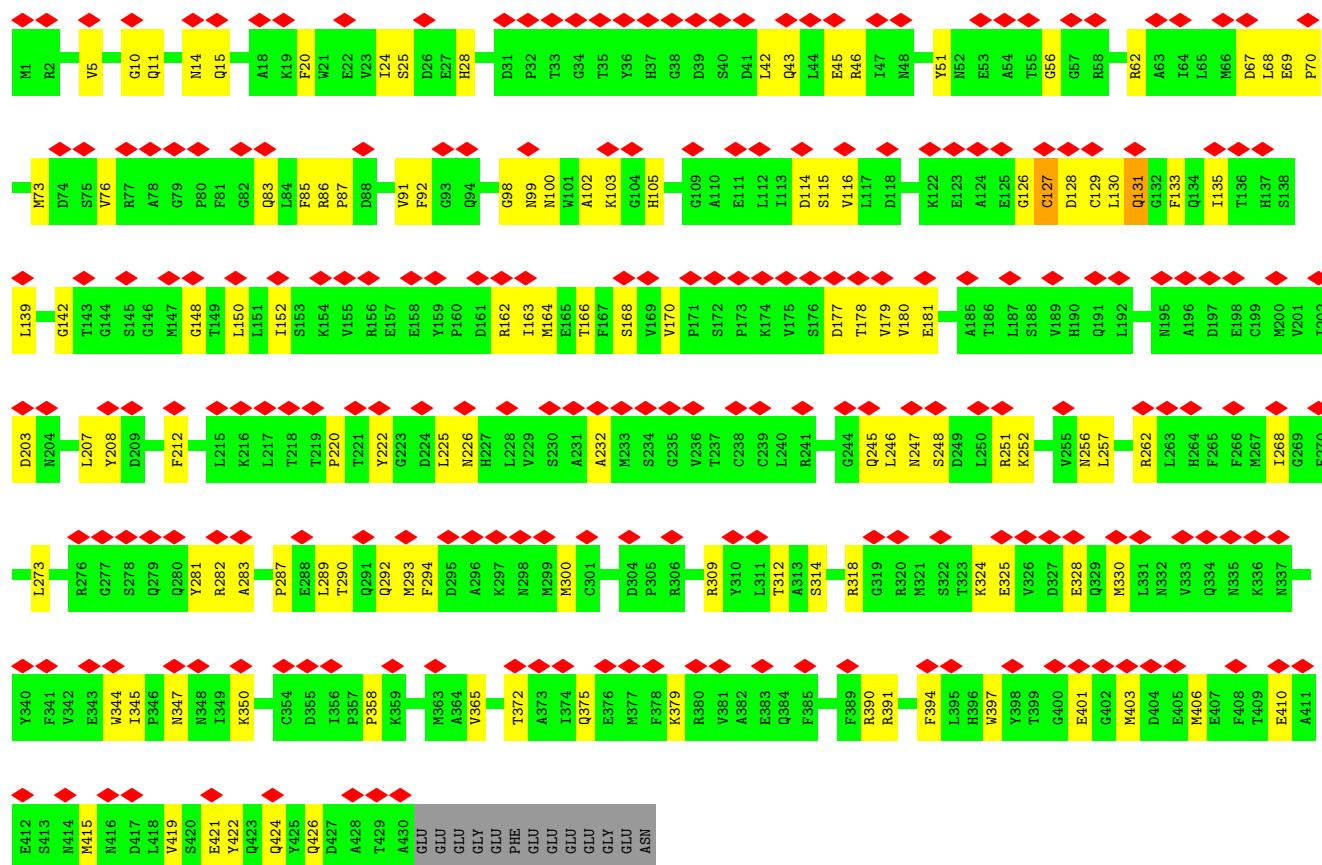




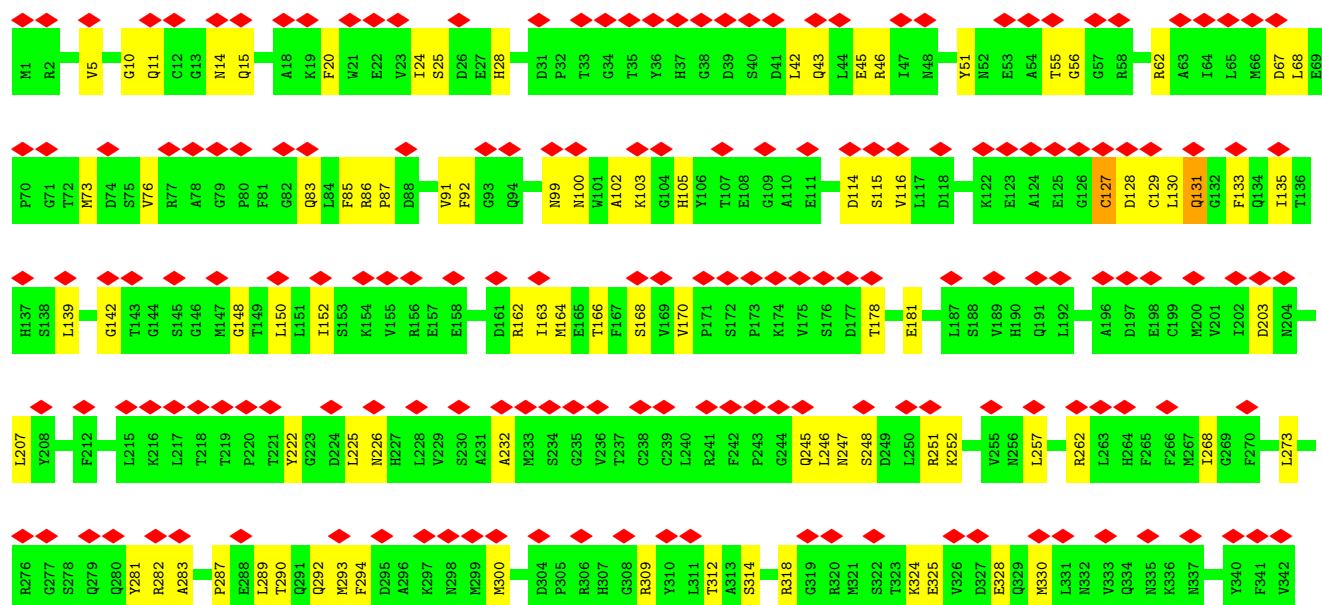
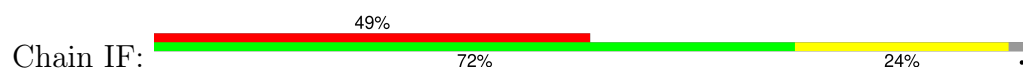
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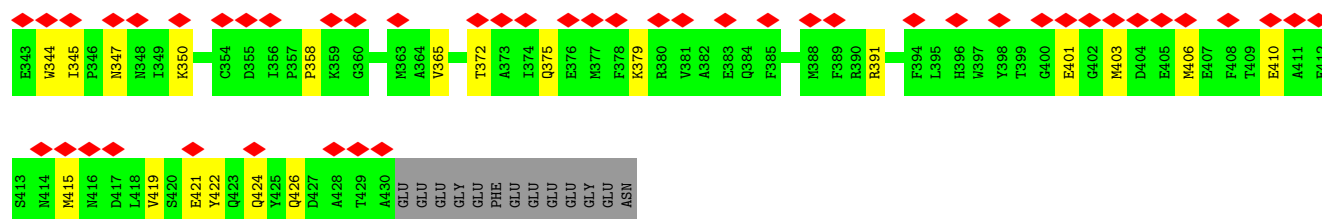


- Molecule 2: Tubulin beta chain

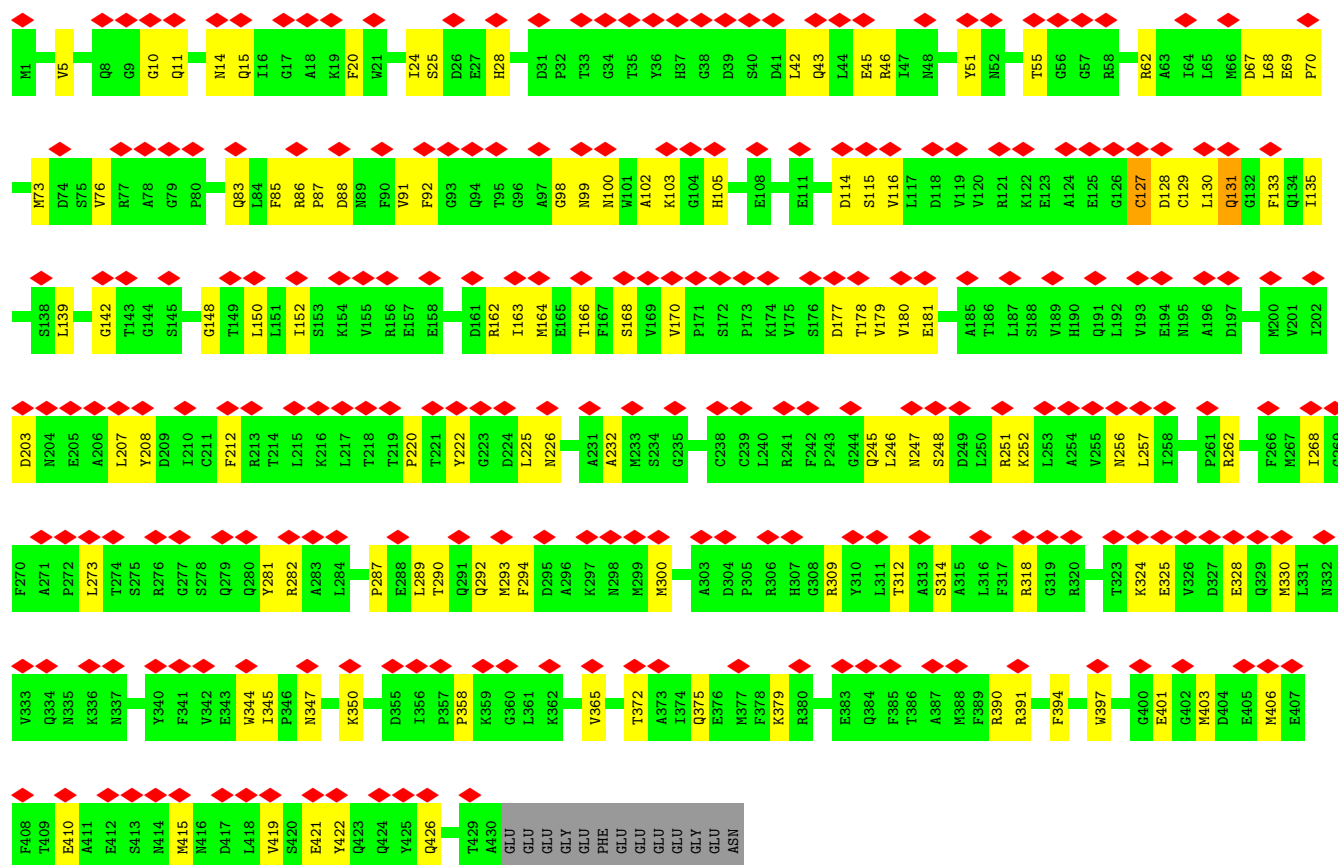


- Molecule 2: Tubulin beta chain

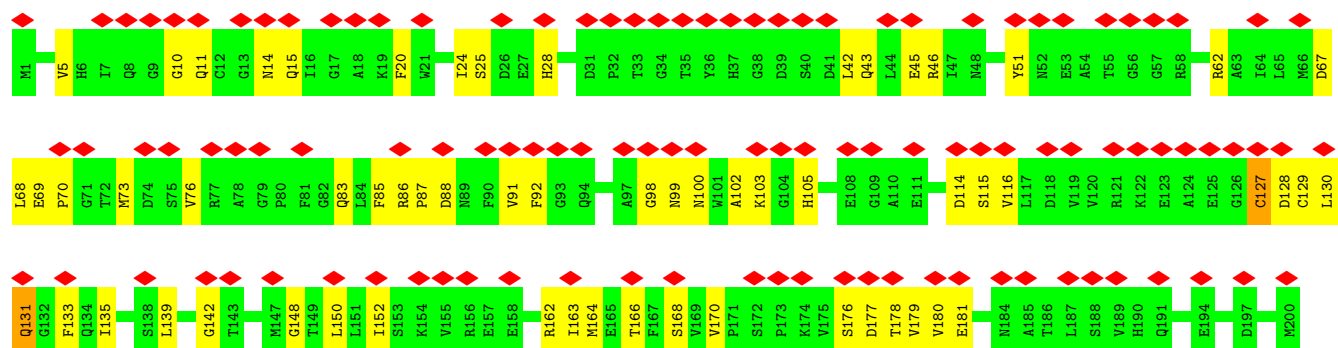
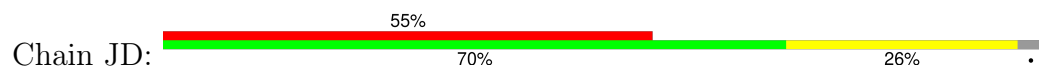


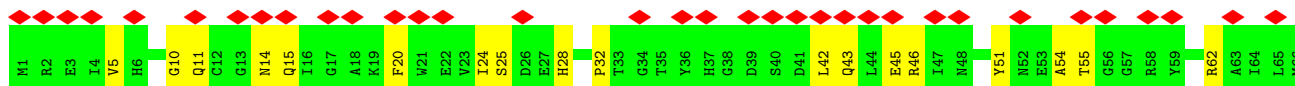


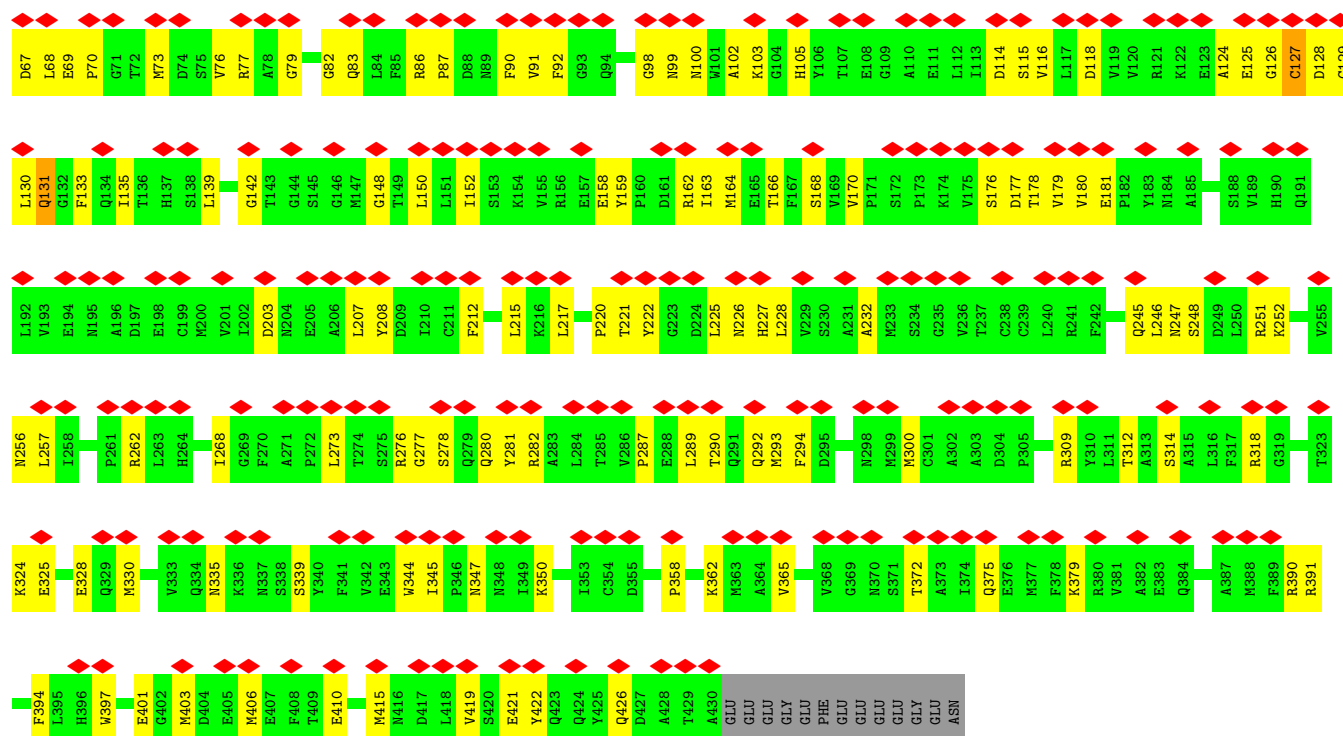
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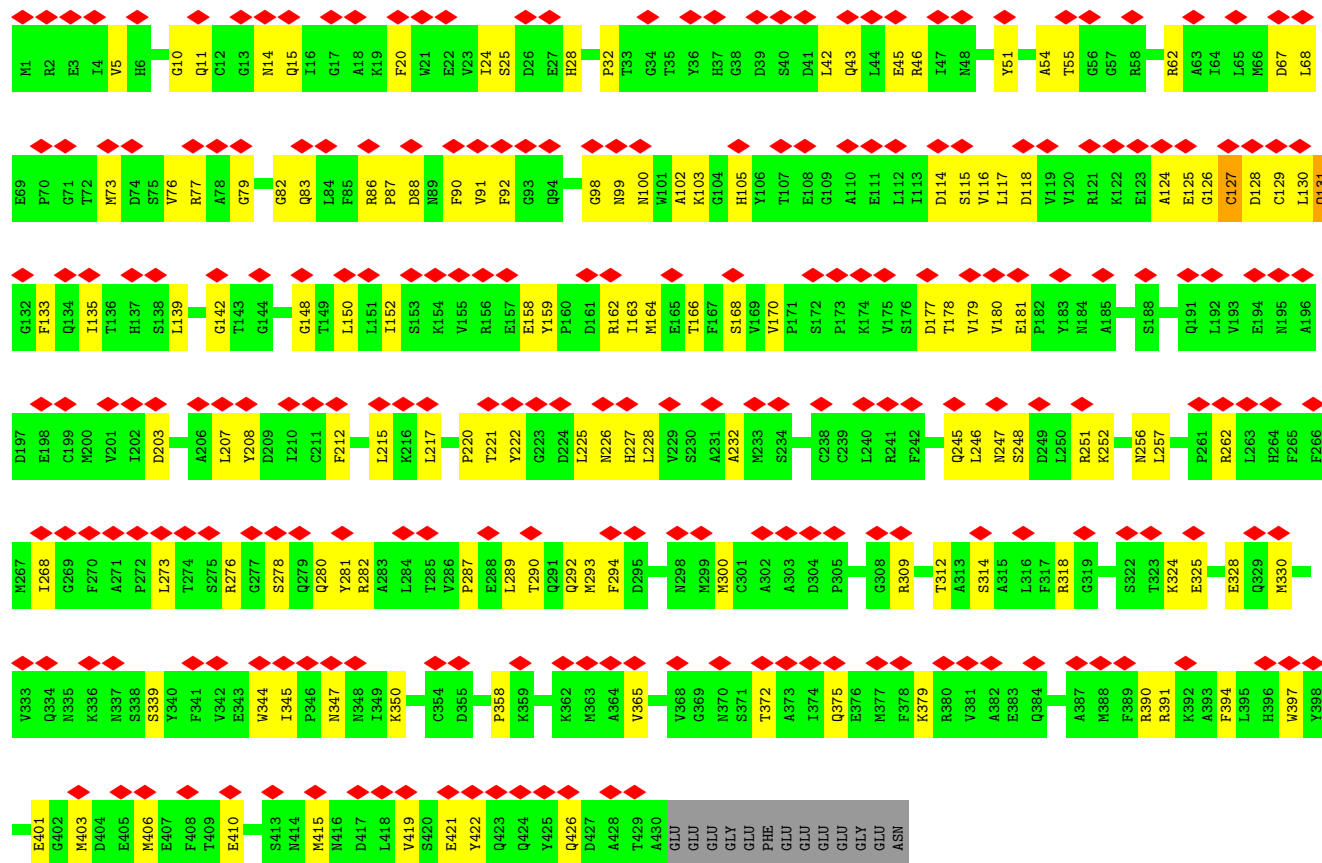
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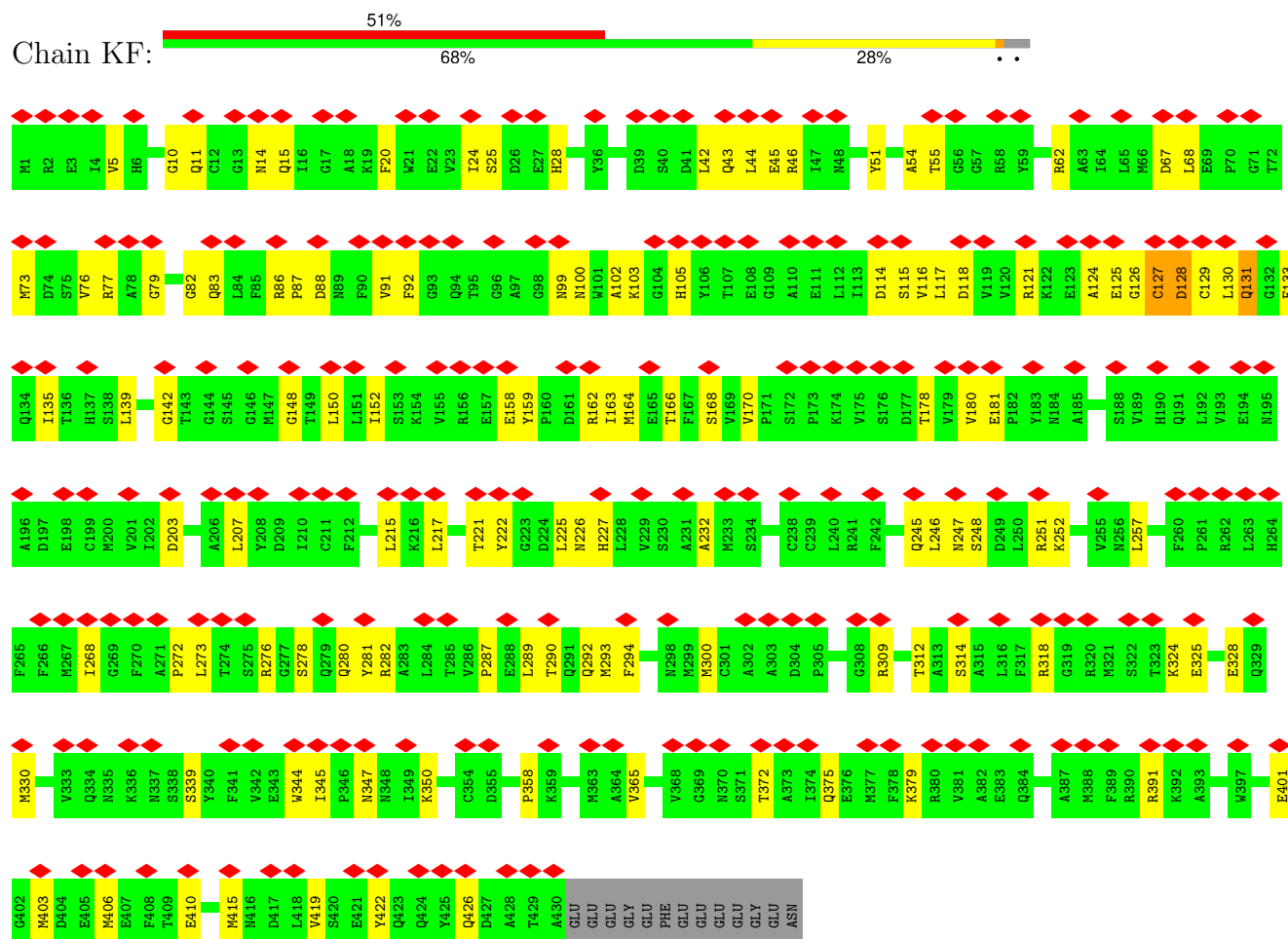




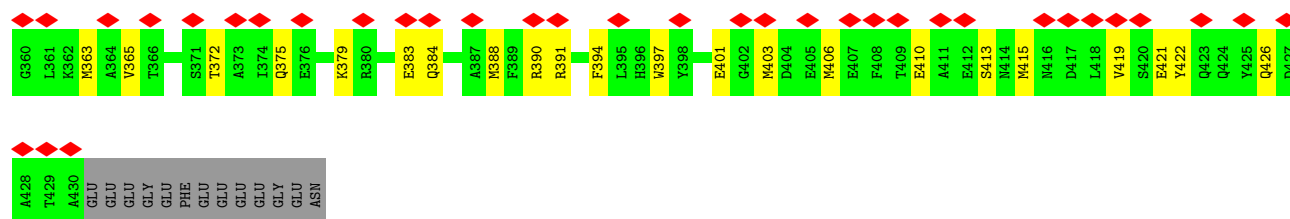
• Molecule 2: Tubulin beta chain



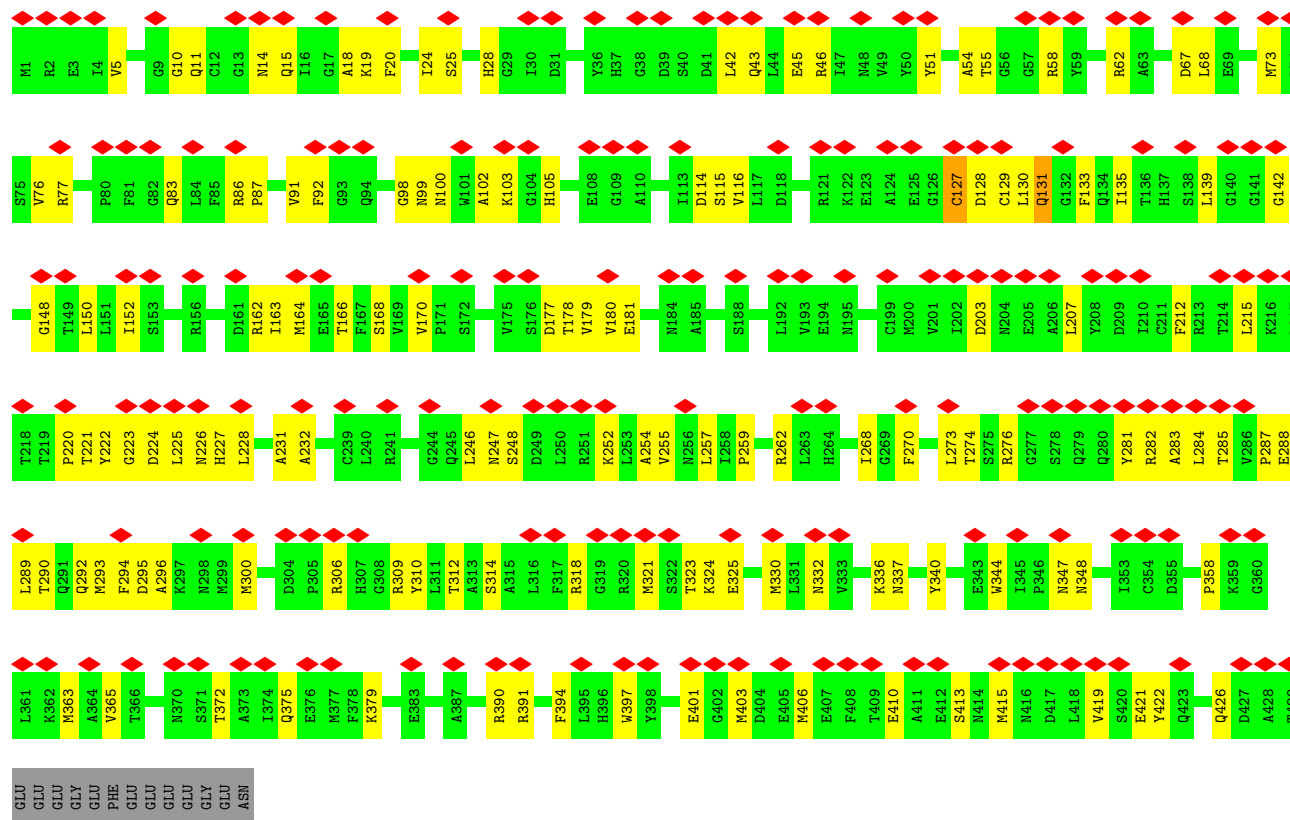
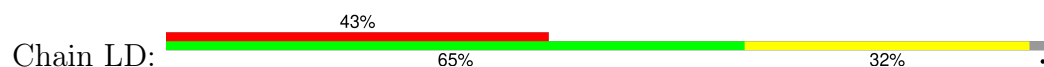
- Molecule 2: Tubulin beta chain



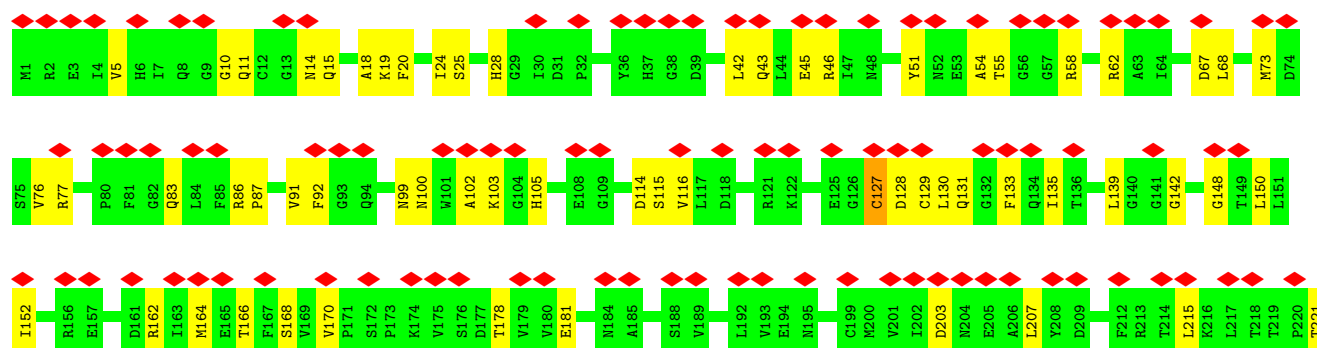
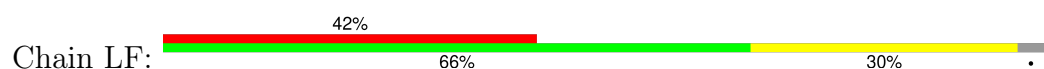


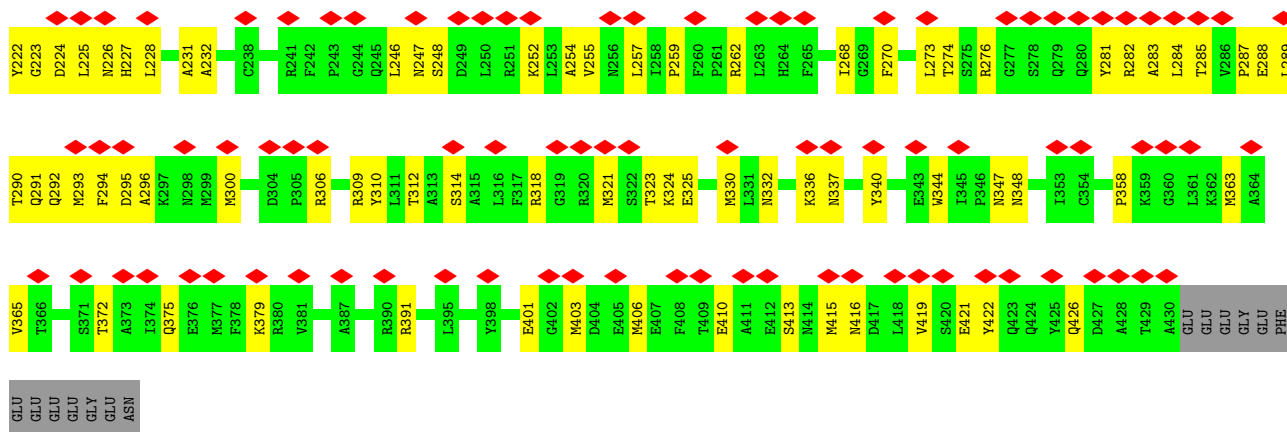


• Molecule 2: Tubulin beta chain

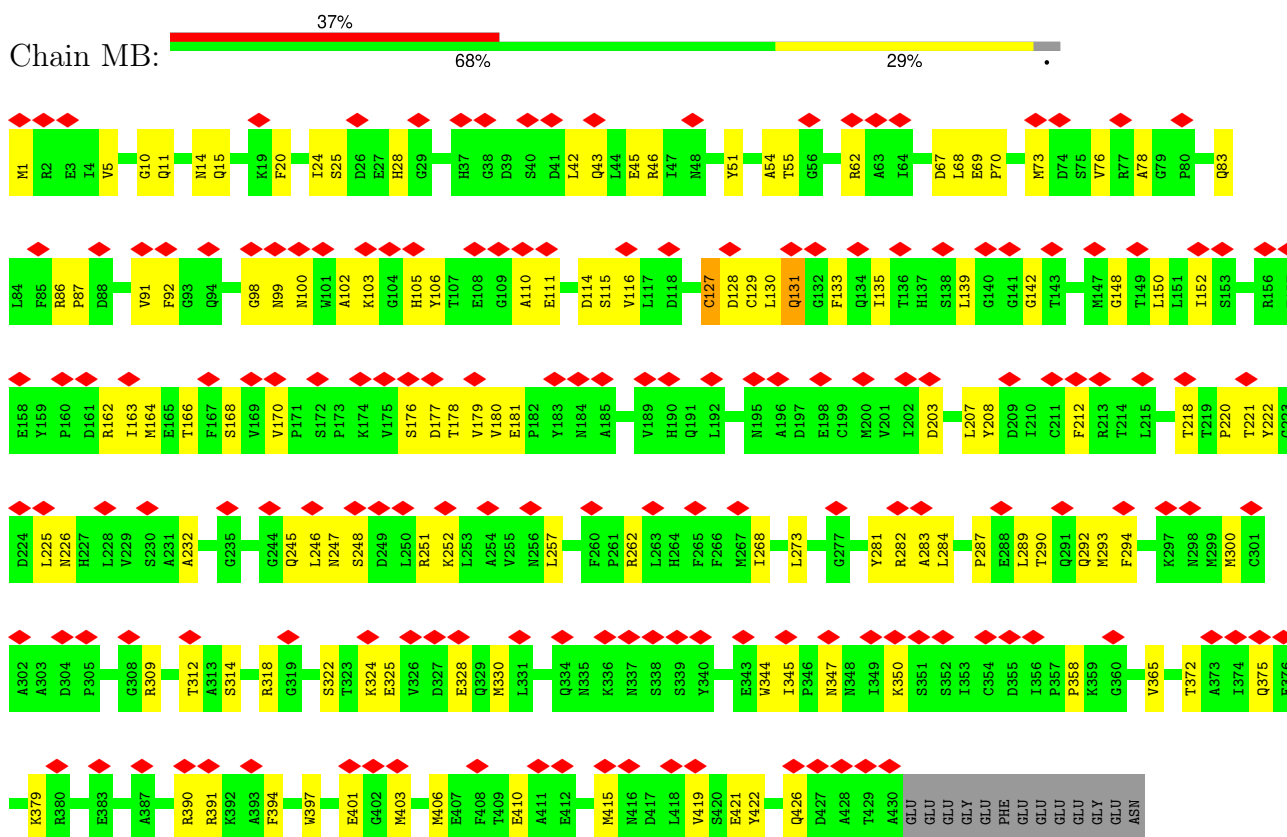


• Molecule 2: Tubulin beta chain

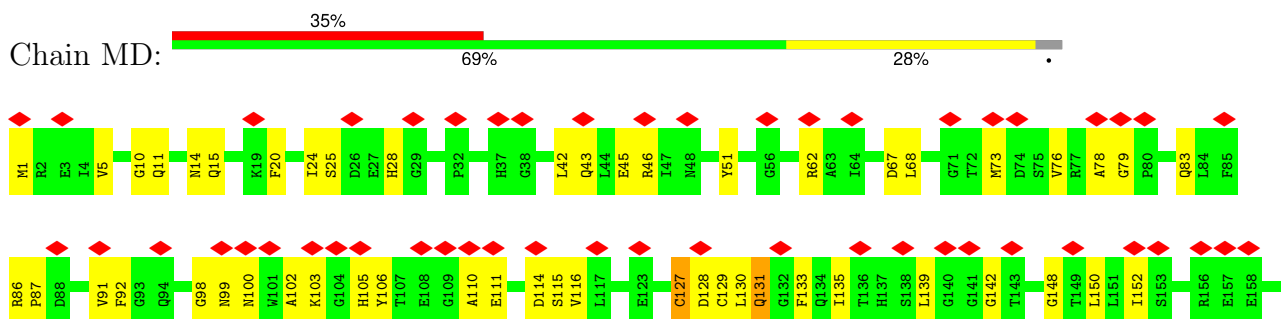


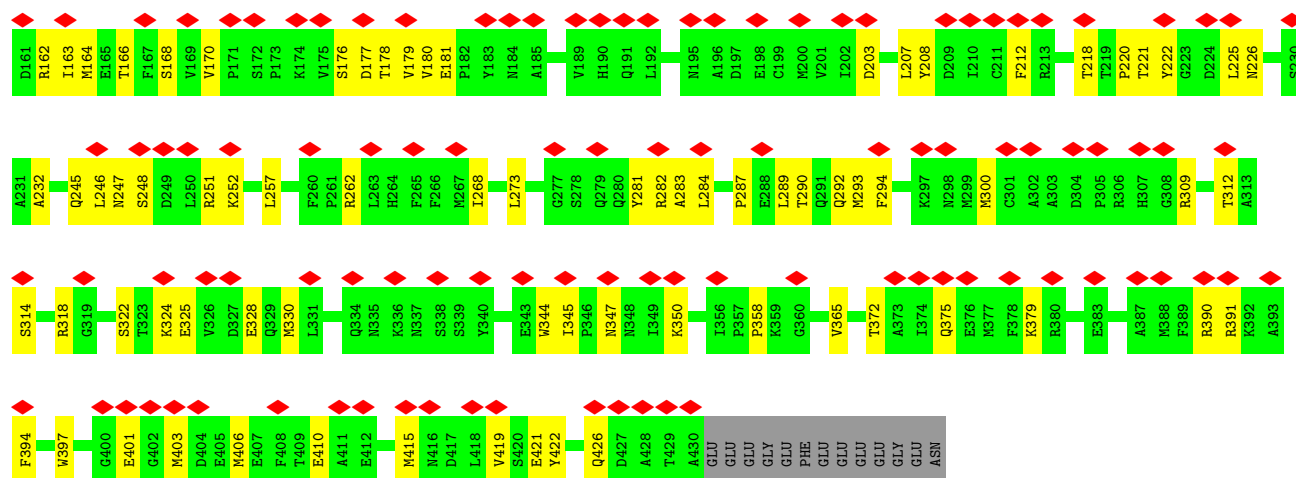


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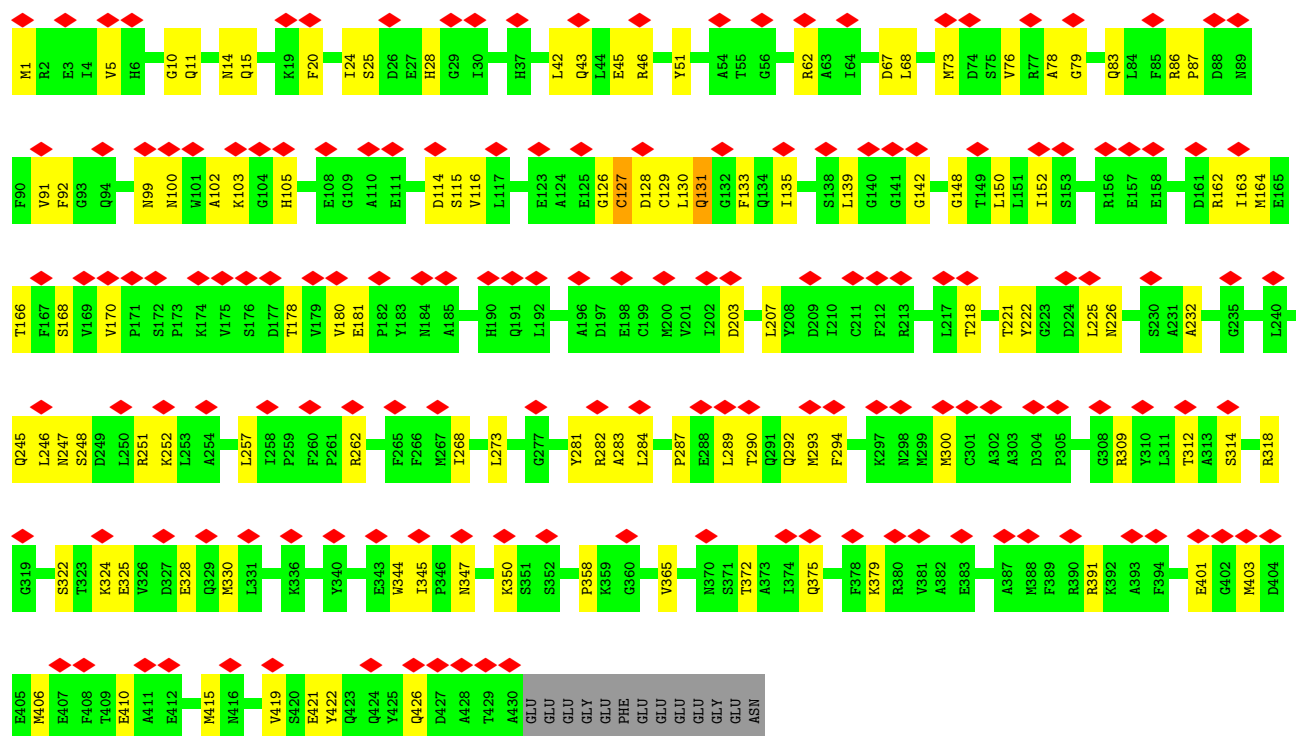
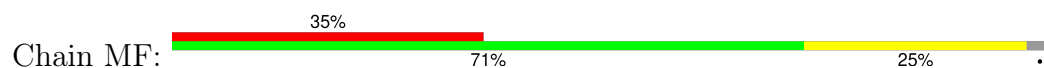


• Molecule 2: Tubulin beta chain

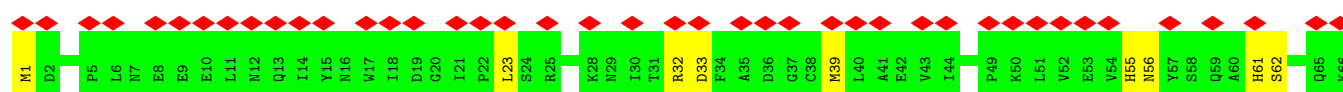


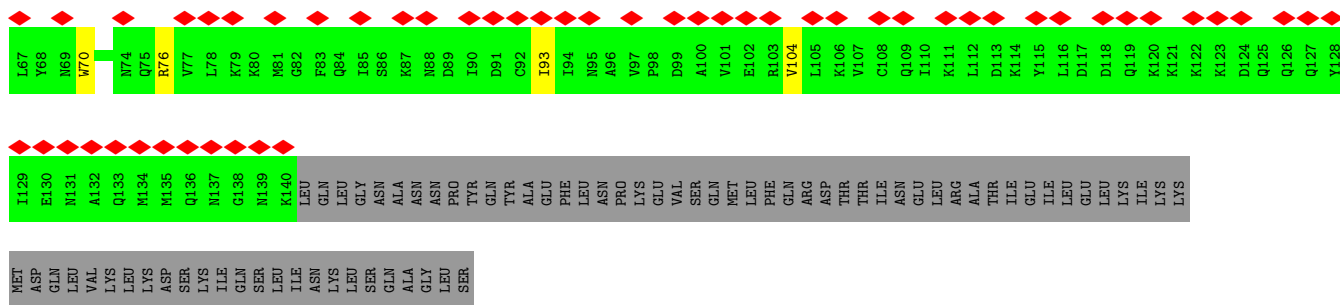


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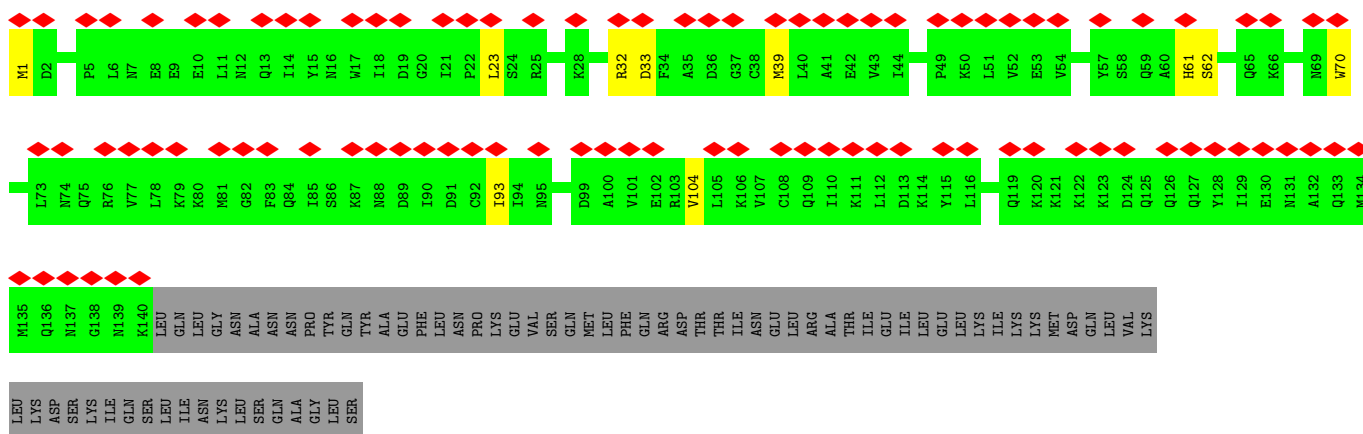


• Molecule 3: Sperm flagellar protein

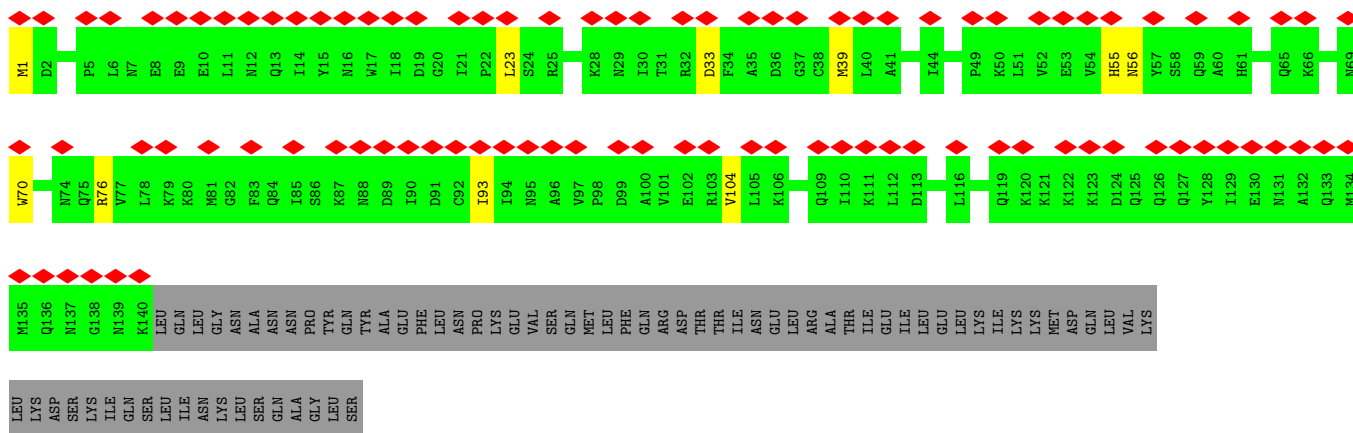




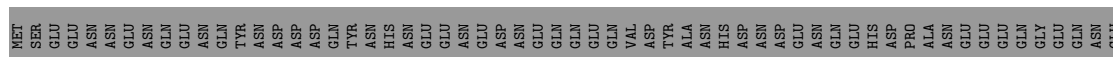
- Molecule 3: Sperm flagellar protein

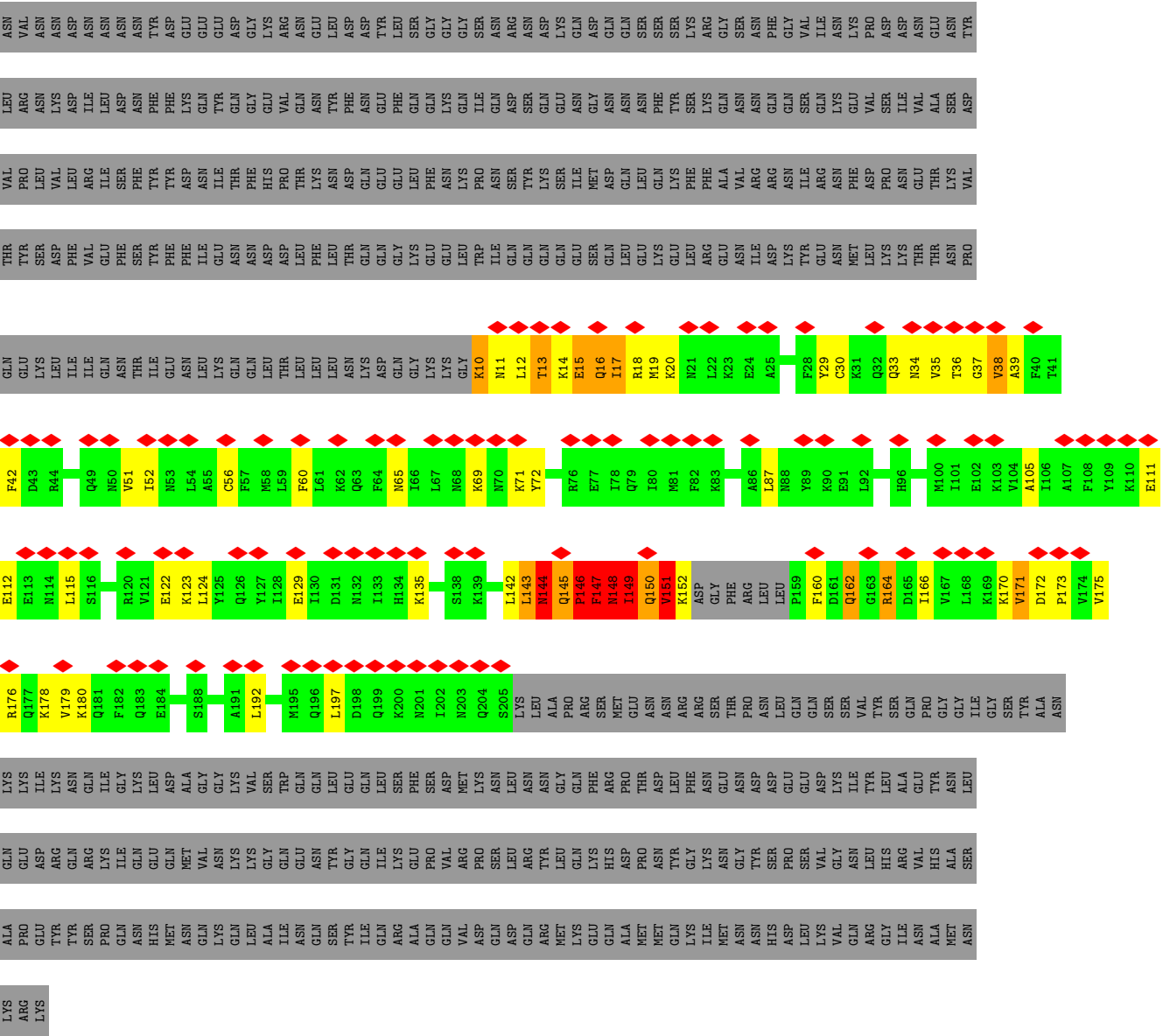


- Molecule 3: Sperm flagellar protein

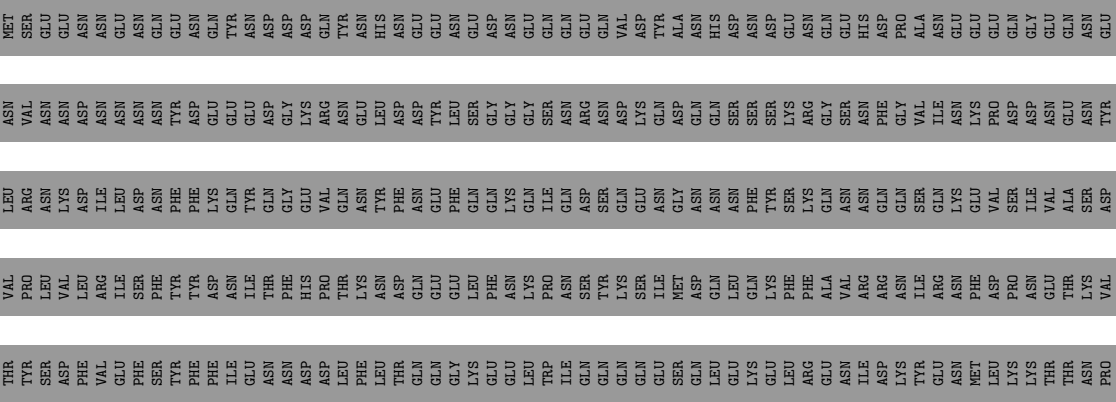


- Molecule 4: TLP1

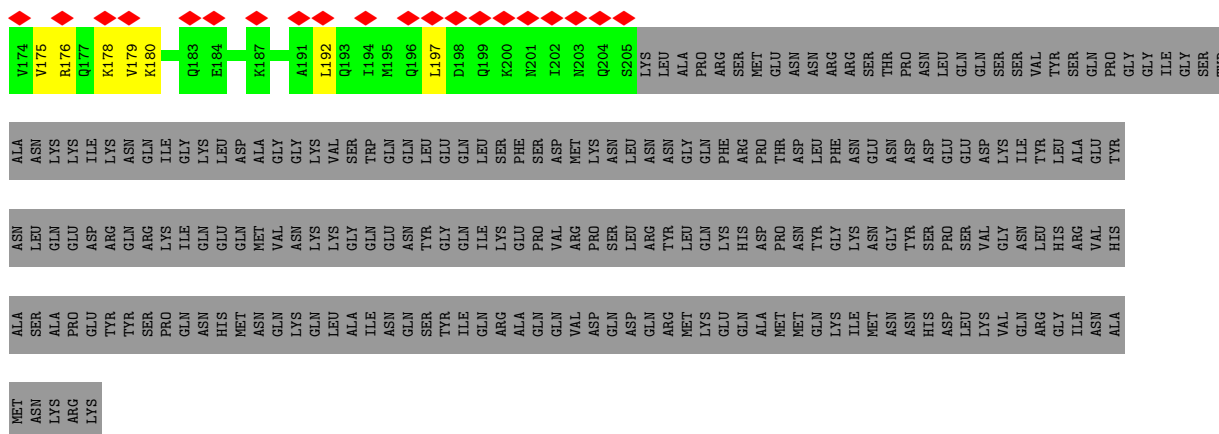




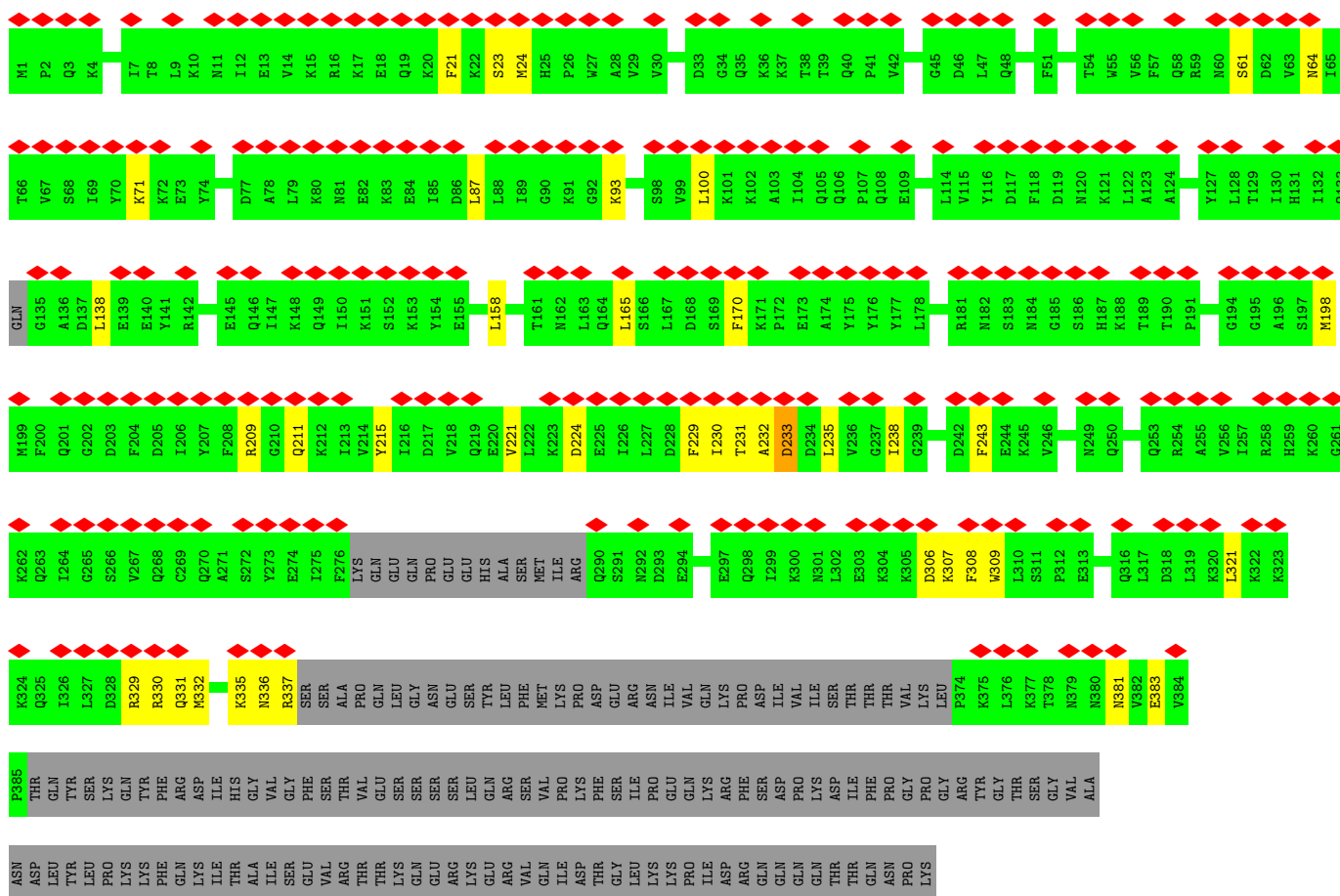
● Molecule 4: TLP1







- Molecule 5: C2 domain protein

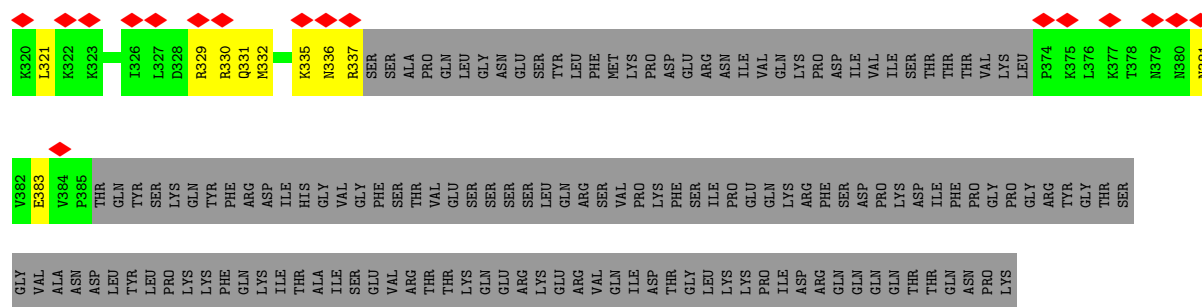


- Molecule 5: C2 domain protein

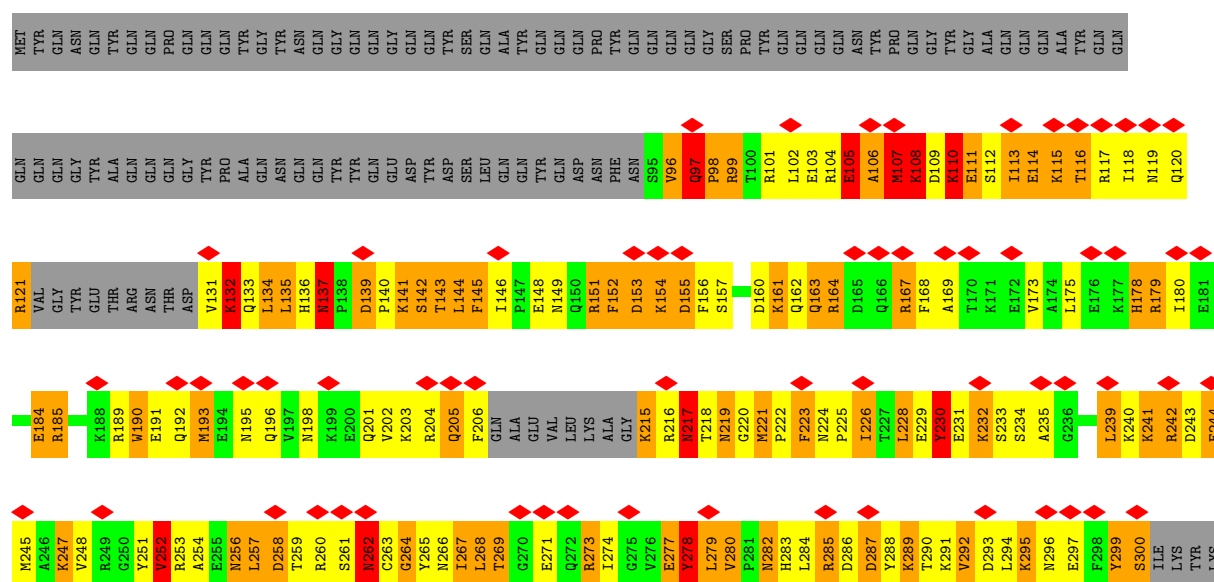




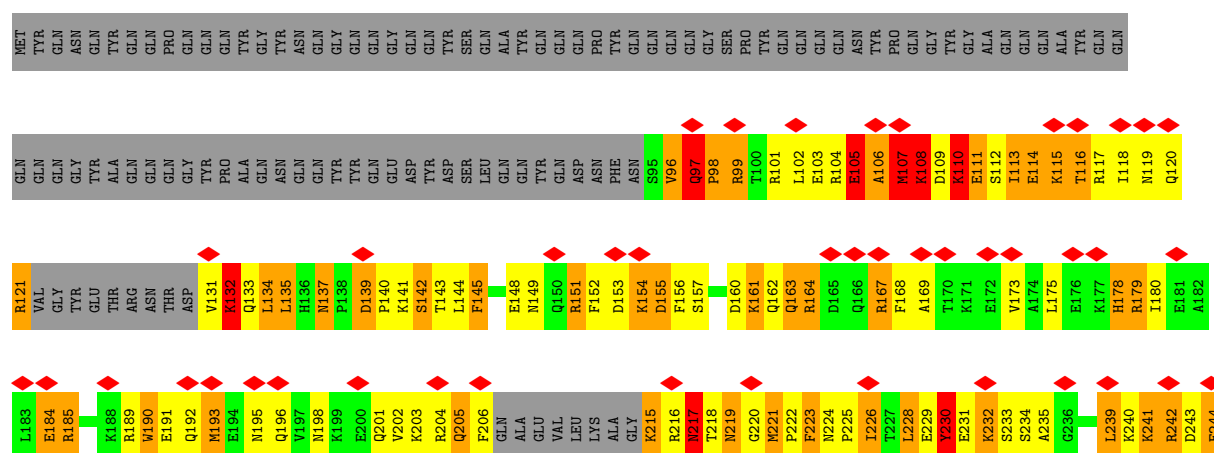


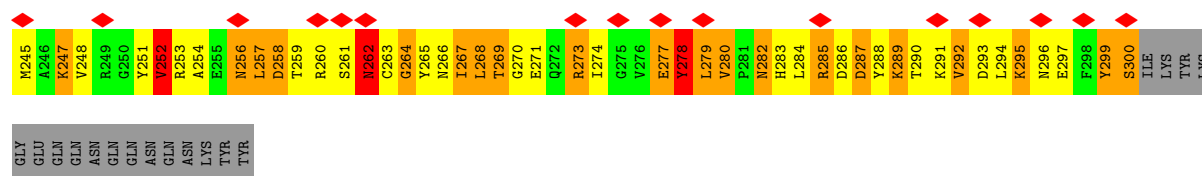


## • Molecule 6: CFAP213

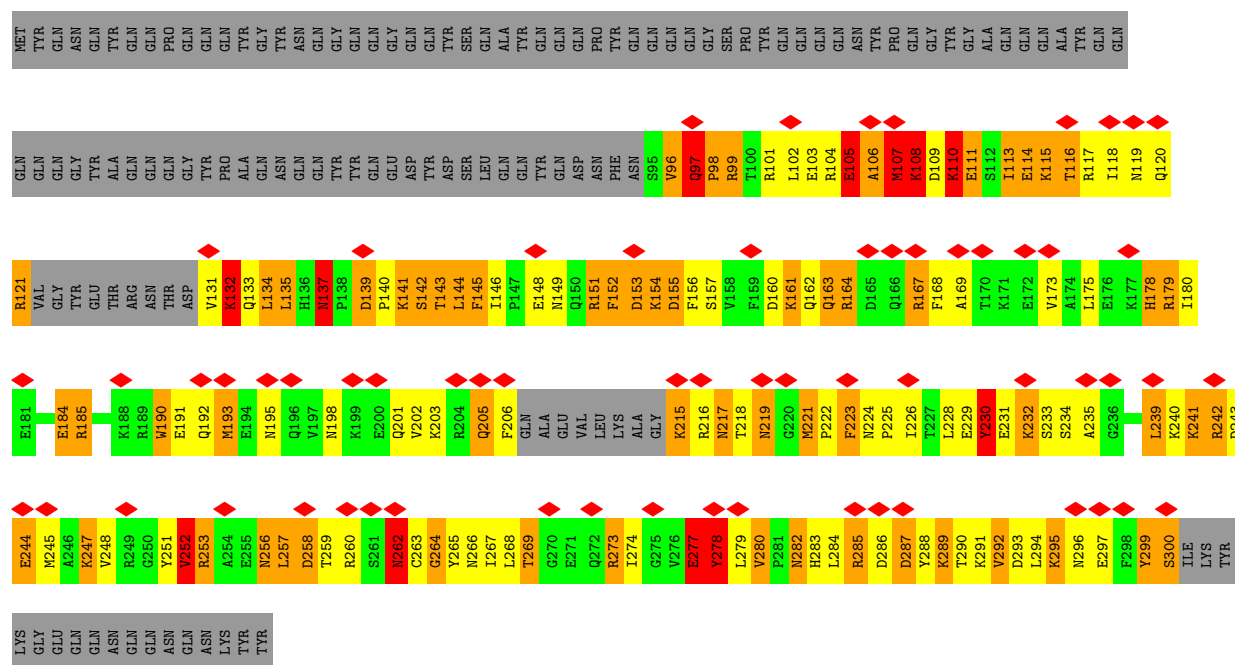


## • Molecule 6: CFAP213

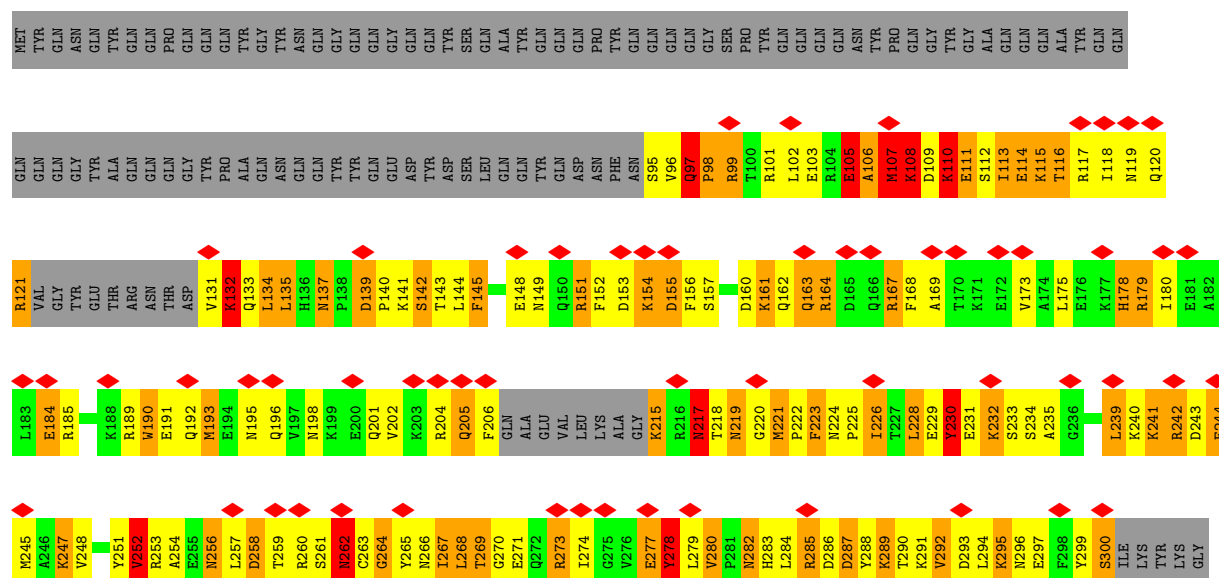




## ● Molecule 6: CFAP213



## ● Molecule 6: CFAP213









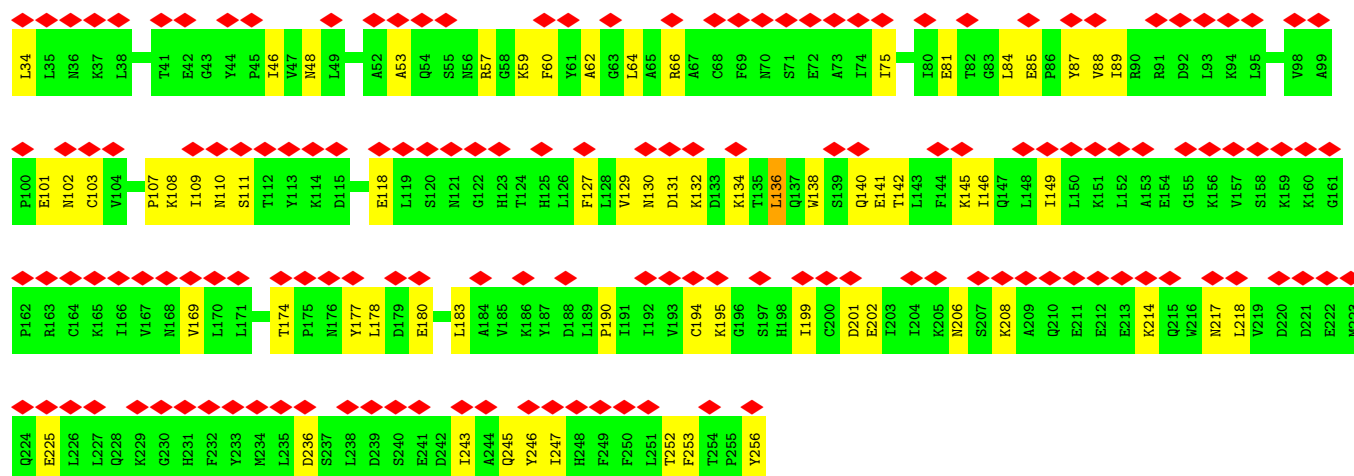




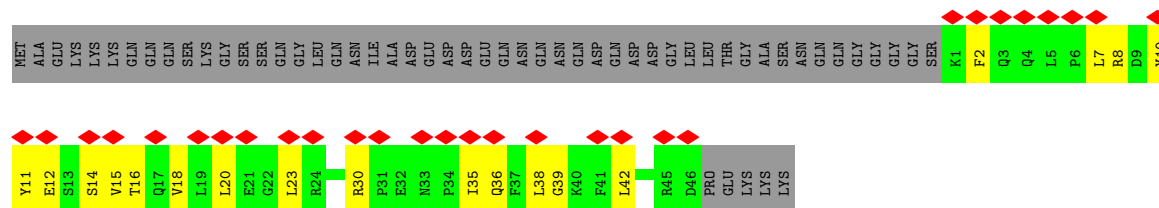
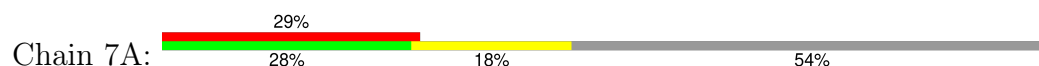




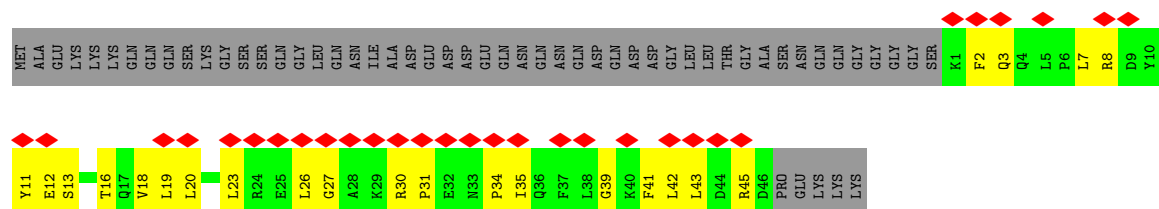
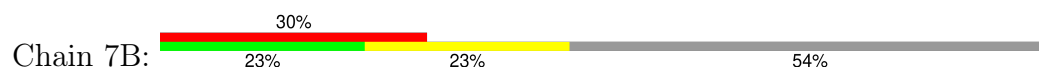




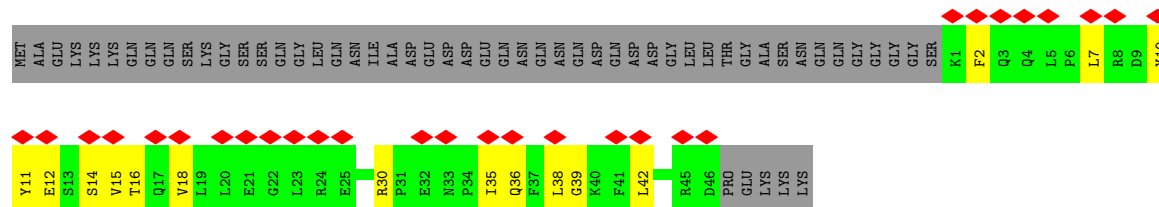
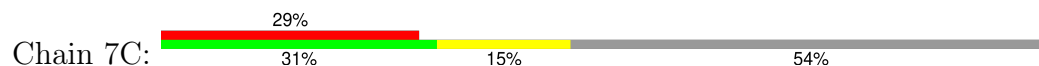
- Molecule 9: Dpy-30 motif protein



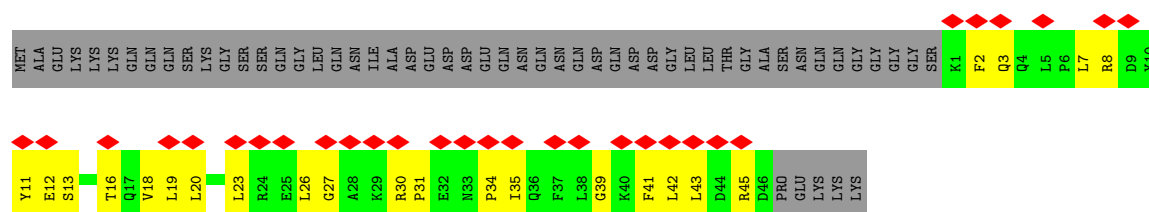
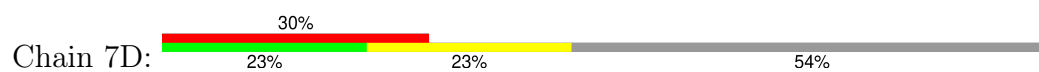
- Molecule 9: Dpy-30 motif protein



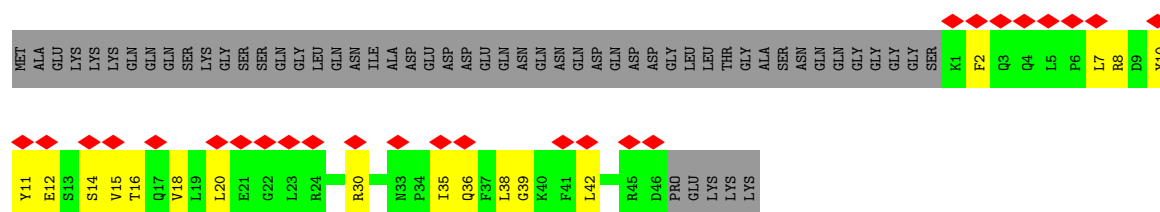
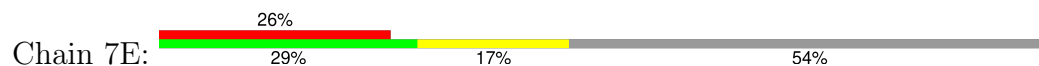
- Molecule 9: Dpy-30 motif protein



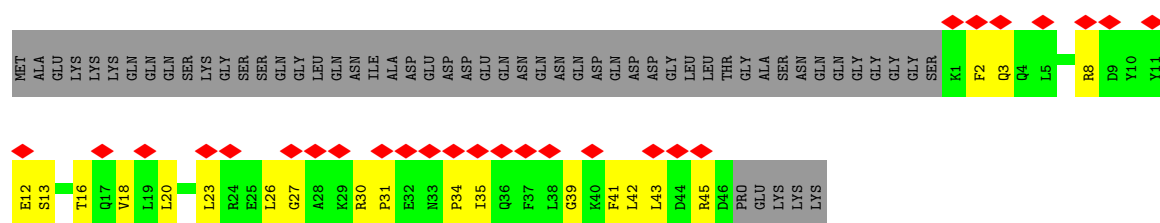
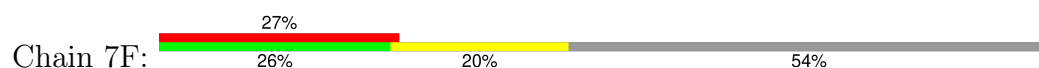
- Molecule 9: Dpy-30 motif protein



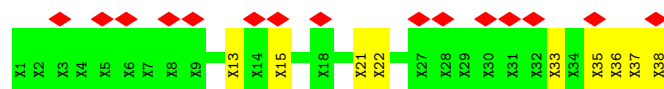
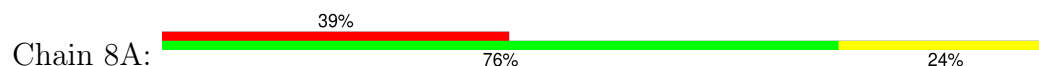
- Molecule 9: Dpy-30 motif protein



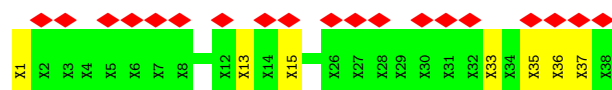
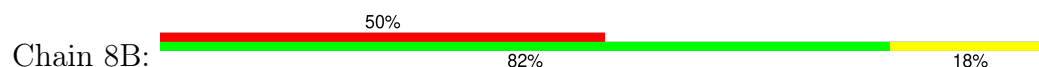
- Molecule 9: Dpy-30 motif protein



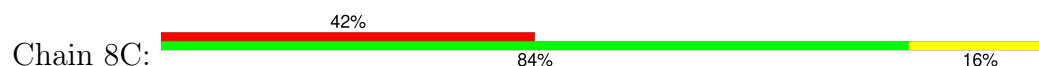
- Molecule 10: Unknown



- Molecule 10: Unknown

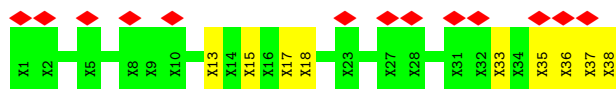
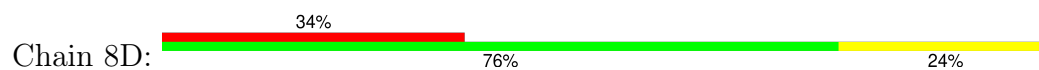


- Molecule 10: Unknown

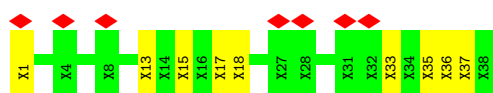
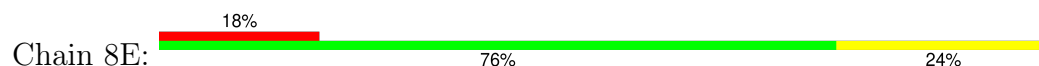




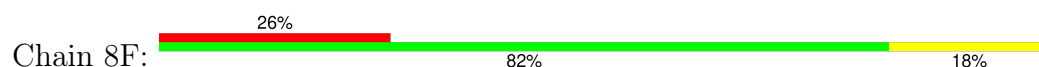
- Molecule 10: Unknown



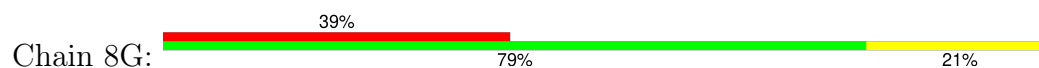
- Molecule 10: Unknown



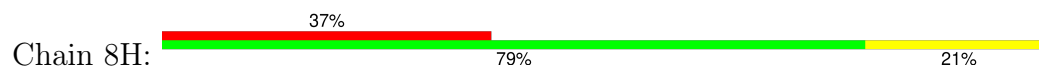
- Molecule 10: Unknown



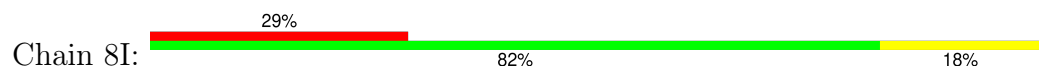
- Molecule 10: Unknown



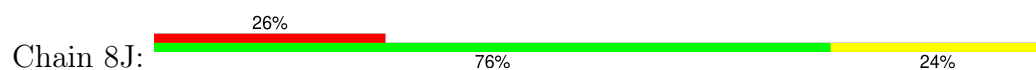
- Molecule 10: Unknown



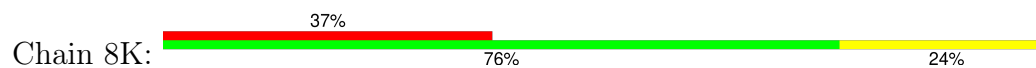
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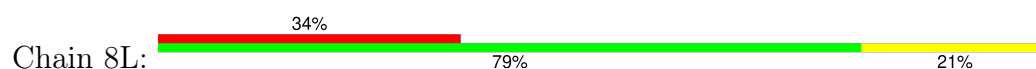
- Molecule 10: Unknown



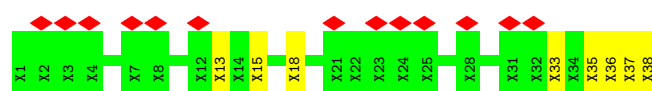
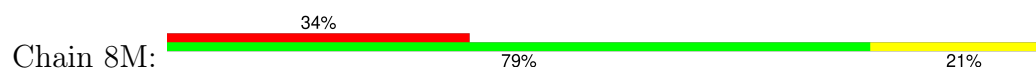
• Molecule 10: Unknown



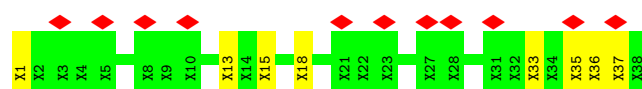
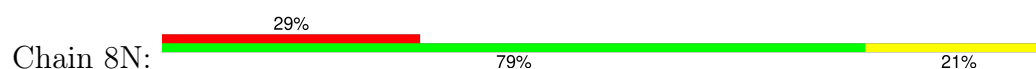
• Molecule 10: Unknown



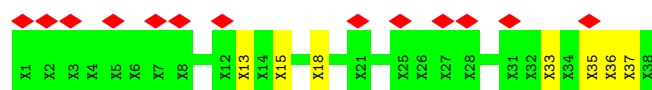
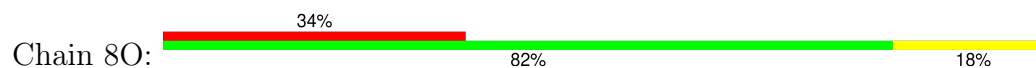
• Molecule 10: Unknown



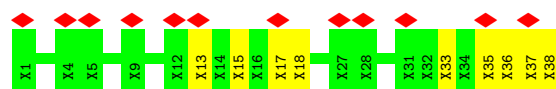
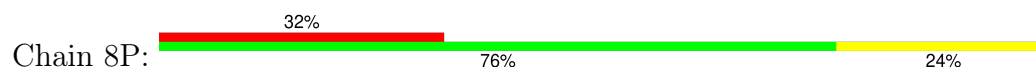
• Molecule 10: Unknown



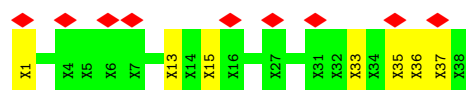
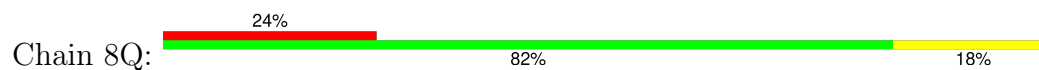
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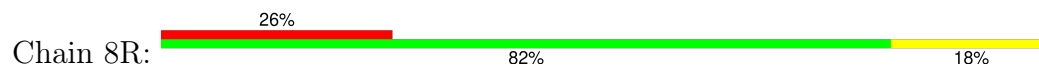
• Molecule 10: Unknown



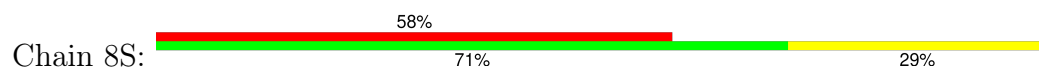
## ● Molecule 10: Unknown



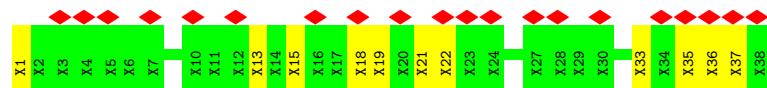
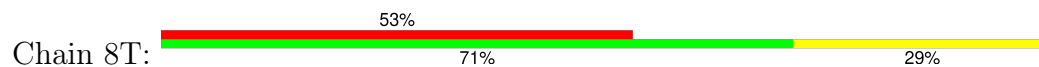
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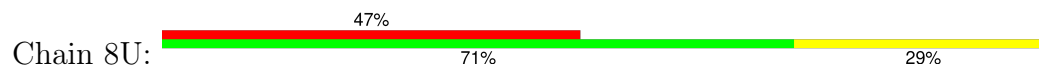
## ● Molecule 10: Unknown



## ● Molecule 10: Unknown



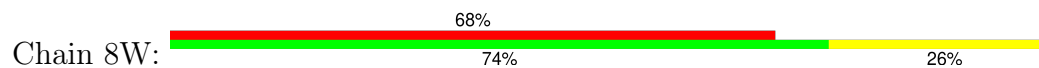
## ● Molecule 10: Unknown



## ● Molecule 10: Unknown

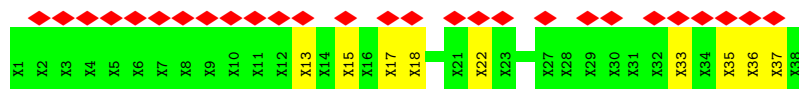
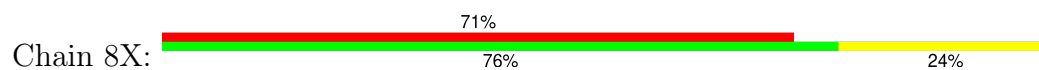


## ● Molecule 10: Unknown

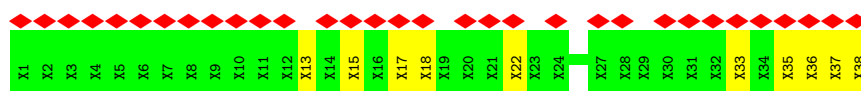
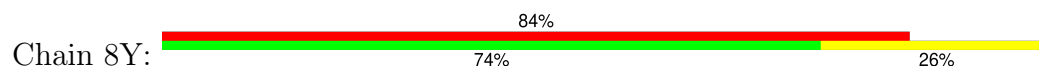




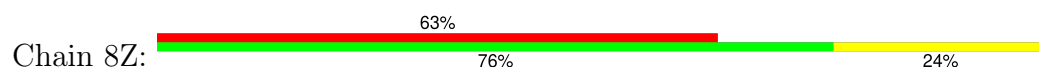
• Molecule 10: Unknown



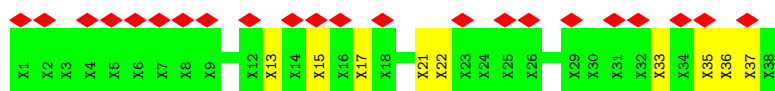
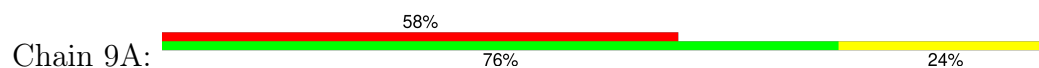
• Molecule 10: Unknown



• Molecule 10: Unknown



• Molecule 10: Unknown



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66174	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.798	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	931.6, 931.6, 931.6	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, GTP

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	AA	0.19	0/3421	0.45	0/4636
1	AC	0.19	0/3421	0.45	0/4636
1	AE	0.19	0/3421	0.45	0/4636
1	BA	0.19	0/3421	0.45	0/4636
1	BC	0.19	0/3421	0.45	0/4636
1	BE	0.19	0/3421	0.45	0/4636
1	CA	0.19	0/3421	0.45	0/4636
1	CC	0.19	0/3421	0.45	0/4636
1	CE	0.19	0/3421	0.45	0/4636
1	DA	0.19	0/3421	0.45	0/4636
1	DC	0.19	0/3421	0.45	0/4636
1	DE	0.19	0/3421	0.45	0/4636
1	EA	0.19	0/3421	0.45	0/4636
1	EC	0.19	0/3421	0.45	0/4636
1	EE	0.19	0/3421	0.45	0/4636
1	FA	0.19	0/3421	0.45	0/4636
1	FC	0.19	0/3421	0.45	0/4636
1	FE	0.19	0/3421	0.45	0/4636
1	GA	0.19	0/3421	0.45	0/4636
1	GC	0.19	0/3421	0.45	0/4636
1	GE	0.19	0/3421	0.45	0/4636
1	HA	0.19	0/3421	0.45	0/4636
1	HC	0.19	0/3421	0.45	0/4636
1	HE	0.19	0/3421	0.45	0/4636
1	IA	0.19	0/3421	0.45	0/4636
1	IC	0.19	0/3421	0.45	0/4636
1	IE	0.19	0/3421	0.45	0/4636
1	JA	0.19	0/3421	0.45	0/4636
1	JC	0.19	0/3421	0.45	0/4636
1	JE	0.19	0/3421	0.45	0/4636
1	KA	0.19	0/3421	0.45	0/4636
1	KC	0.19	0/3421	0.45	0/4636

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	KE	0.19	0/3421	0.45	0/4636
1	LA	0.19	0/3421	0.45	0/4636
1	LC	0.19	0/3421	0.45	0/4636
1	LE	0.19	0/3421	0.45	0/4636
1	MA	0.19	0/3421	0.45	0/4636
1	MC	0.19	0/3421	0.45	0/4636
1	ME	0.19	0/3421	0.45	0/4636
2	AB	0.21	0/3439	0.47	4/4655 (0.1%)
2	AD	0.21	0/3439	0.47	4/4655 (0.1%)
2	AF	0.21	0/3439	0.46	4/4655 (0.1%)
2	BB	0.21	0/3439	0.47	4/4655 (0.1%)
2	BD	0.21	0/3439	0.47	4/4655 (0.1%)
2	BF	0.21	0/3439	0.47	4/4655 (0.1%)
2	CB	0.21	0/3439	0.47	4/4655 (0.1%)
2	CD	0.21	0/3439	0.47	4/4655 (0.1%)
2	CF	0.21	0/3439	0.46	4/4655 (0.1%)
2	DB	0.21	0/3439	0.47	4/4655 (0.1%)
2	DD	0.21	0/3439	0.47	4/4655 (0.1%)
2	DF	0.21	0/3439	0.47	4/4655 (0.1%)
2	EB	0.21	0/3439	0.47	4/4655 (0.1%)
2	ED	0.21	0/3439	0.46	4/4655 (0.1%)
2	EF	0.21	0/3439	0.47	4/4655 (0.1%)
2	FB	0.21	0/3439	0.47	4/4655 (0.1%)
2	FD	0.21	0/3439	0.47	4/4655 (0.1%)
2	FF	0.21	0/3439	0.47	4/4655 (0.1%)
2	GB	0.21	0/3439	0.47	4/4655 (0.1%)
2	GD	0.21	0/3439	0.47	5/4655 (0.1%)
2	GF	0.21	0/3439	0.46	4/4655 (0.1%)
2	HB	0.21	0/3439	0.46	4/4655 (0.1%)
2	HD	0.21	0/3439	0.47	4/4655 (0.1%)
2	HF	0.21	0/3439	0.47	4/4655 (0.1%)
2	IB	0.21	0/3439	0.47	4/4655 (0.1%)
2	ID	0.21	0/3439	0.47	5/4655 (0.1%)
2	IF	0.21	0/3439	0.47	4/4655 (0.1%)
2	JB	0.21	0/3439	0.46	4/4655 (0.1%)
2	JD	0.21	0/3439	0.47	4/4655 (0.1%)
2	JF	0.21	0/3439	0.46	4/4655 (0.1%)
2	KB	0.21	0/3439	0.47	4/4655 (0.1%)
2	KD	0.21	0/3439	0.47	4/4655 (0.1%)
2	KF	0.21	0/3439	0.47	4/4655 (0.1%)
2	LB	0.21	0/3439	0.47	4/4655 (0.1%)
2	LD	0.21	0/3439	0.47	4/4655 (0.1%)
2	LF	0.21	0/3439	0.47	4/4655 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	MB	0.21	0/3439	0.47	4/4655 (0.1%)
2	MD	0.21	0/3439	0.47	4/4655 (0.1%)
2	MF	0.21	0/3439	0.46	5/4655 (0.1%)
3	1A	0.68	0/1161	1.23	0/1566
3	1B	0.68	0/1161	1.23	0/1566
3	1C	0.68	0/1161	1.23	0/1566
4	2A	0.76	1/1642 (0.1%)	1.29	13/2193 (0.6%)
4	2B	0.76	1/1642 (0.1%)	1.29	13/2193 (0.6%)
4	2C	0.76	1/1642 (0.1%)	1.29	13/2193 (0.6%)
5	3A	0.65	0/2795	1.13	1/3751 (0.0%)
5	3B	0.65	0/2795	1.13	1/3751 (0.0%)
5	3C	0.65	0/2795	1.13	1/3751 (0.0%)
6	4A	0.99	2/1610 (0.1%)	1.50	35/2151 (1.6%)
6	4B	0.99	2/1610 (0.1%)	1.50	35/2151 (1.6%)
6	4C	0.99	2/1610 (0.1%)	1.50	35/2151 (1.6%)
6	4D	0.99	2/1610 (0.1%)	1.50	35/2151 (1.6%)
7	5A	1.02	31/6042 (0.5%)	1.37	68/8049 (0.8%)
7	5B	1.02	31/6042 (0.5%)	1.37	68/8049 (0.8%)
7	5C	1.02	31/6042 (0.5%)	1.37	68/8049 (0.8%)
8	6A	0.71	0/2126	1.03	0/2877
8	6B	0.71	0/2126	1.03	0/2877
8	6C	0.71	0/2126	1.03	0/2877
9	7A	0.58	0/390	0.66	0/524
9	7B	0.59	0/390	0.68	0/524
9	7C	0.58	0/390	0.67	0/524
9	7D	0.59	0/390	0.68	0/524
9	7E	0.58	0/390	0.66	0/524
9	7F	0.59	0/390	0.68	0/524
All	All	0.39	104/317618 (0.0%)	0.65	545/429405 (0.1%)

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
4	2A	0	1
4	2B	0	1
4	2C	0	2
7	5A	0	7
7	5B	0	7
7	5C	0	7
All	All	0	25

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	5C	1372	VAL	CA-C	14.89	1.71	1.52
7	5B	1372	VAL	CA-C	14.89	1.71	1.52
7	5A	1372	VAL	CA-C	14.88	1.71	1.52
7	5B	1372	VAL	N-CA	14.51	1.64	1.46
7	5C	1372	VAL	N-CA	14.50	1.64	1.46

The worst 5 of 545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	5A	1283	ALA	O-C-N	-18.60	96.86	121.97
7	5B	1283	ALA	O-C-N	-18.59	96.87	121.97
7	5C	1283	ALA	O-C-N	-18.55	96.93	121.97
4	2C	17	ILE	N-CA-C	-15.81	94.97	110.30
4	2A	17	ILE	N-CA-C	-15.75	95.02	110.30

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	2A	142	LEU	Mainchain
4	2B	142	LEU	Mainchain
4	2C	142	LEU	Mainchain
4	2C	144	ASN	Peptide
7	5A	1253	ILE	Mainchain

## 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	AA	3350	0	3287	97	0
1	AC	3350	0	3284	169	0
1	AE	3350	0	3282	192	0
1	BA	3350	0	3285	101	0
1	BC	3350	0	3282	168	0
1	BE	3350	0	3281	171	0
1	CA	3350	0	3284	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CC	3350	0	3280	189	0
1	CE	3350	0	3280	190	0
1	DA	3350	0	3278	138	0
1	DC	3350	0	3276	211	0
1	DE	3350	0	3275	212	0
1	EA	3350	0	3281	157	0
1	EC	3350	0	3279	216	0
1	EE	3350	0	3279	226	0
1	FA	3350	0	3277	235	0
1	FC	3350	0	3274	277	0
1	FE	3350	0	3276	269	0
1	GA	3350	0	3284	181	0
1	GC	3350	0	3279	234	0
1	GE	3350	0	3278	227	0
1	HA	3350	0	3286	144	0
1	HC	3350	0	3283	243	0
1	HE	3350	0	3283	259	0
1	IA	3350	0	3282	169	0
1	IC	3350	0	3279	247	0
1	IE	3350	0	3279	215	0
1	JA	3350	0	3283	158	0
1	JC	3350	0	3278	221	0
1	JE	3350	0	3278	231	0
1	KA	3350	0	3283	219	0
1	KC	3350	0	3282	283	0
1	KE	3350	0	3281	266	0
1	LA	3350	0	3281	234	0
1	LC	3350	0	3277	315	0
1	LE	3350	0	3277	275	0
1	MA	3350	0	3286	176	0
1	MC	3350	0	3283	235	0
1	ME	3350	0	3283	231	0
2	AB	3366	0	3252	166	0
2	AD	3366	0	3246	262	0
2	AF	3366	0	3248	182	0
2	BB	3366	0	3254	182	0
2	BD	3366	0	3254	181	0
2	BF	3366	0	3254	109	0
2	CB	3366	0	3255	204	0
2	CD	3366	0	3255	205	0
2	CF	3366	0	3255	129	0
2	DB	3366	0	3252	214	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DD	3366	0	3252	221	0
2	DF	3366	0	3252	137	0
2	EB	3366	0	3253	240	0
2	ED	3366	0	3252	242	0
2	EF	3366	0	3252	165	0
2	FB	3366	0	3250	254	0
2	FD	3366	0	3250	242	0
2	FF	3366	0	3250	170	0
2	GB	3366	0	3251	242	0
2	GD	3366	0	3251	220	0
2	GF	3366	0	3252	147	0
2	HB	3366	0	3255	197	0
2	HD	3366	0	3255	190	0
2	HF	3366	0	3255	120	0
2	IB	3366	0	3254	194	0
2	ID	3366	0	3254	185	0
2	IF	3366	0	3255	123	0
2	JB	3366	0	3254	209	0
2	JD	3366	0	3254	198	0
2	JF	3366	0	3254	138	0
2	KB	3366	0	3248	356	0
2	KD	3366	0	3246	348	0
2	KF	3366	0	3246	290	0
2	LB	3366	0	3241	435	0
2	LD	3366	0	3244	399	0
2	LF	3366	0	3249	355	0
2	MB	3366	0	3255	242	0
2	MD	3366	0	3256	225	0
2	MF	3366	0	3256	145	0
3	1A	1141	0	1144	37	0
3	1B	1141	0	1145	23	0
3	1C	1141	0	1144	14	0
4	2A	1615	0	1664	170	0
4	2B	1615	0	1665	183	0
4	2C	1615	0	1662	215	0
5	3A	2752	0	2802	129	0
5	3B	2752	0	2807	46	0
5	3C	2752	0	2802	129	0
6	4A	1587	0	1558	487	0
6	4B	1587	0	1561	408	0
6	4C	1587	0	1562	349	0
6	4D	1587	0	1569	339	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	5A	5953	0	6017	966	0
7	5B	5953	0	6016	943	0
7	5C	5953	0	6016	953	0
8	6A	2077	0	2097	86	0
8	6B	2077	0	2098	87	0
8	6C	2077	0	2099	93	0
9	7A	383	0	390	151	0
9	7B	383	0	392	155	0
9	7C	383	0	390	131	0
9	7D	383	0	392	155	0
9	7E	383	0	391	105	0
9	7F	383	0	392	109	0
10	8A	189	0	41	8	0
10	8B	189	0	41	7	0
10	8C	189	0	40	3	0
10	8D	189	0	41	18	0
10	8E	189	0	41	16	0
10	8F	189	0	40	10	0
10	8G	189	0	41	9	0
10	8H	189	0	41	9	0
10	8I	189	0	40	6	0
10	8J	189	0	41	14	0
10	8K	189	0	41	14	0
10	8L	189	0	40	11	0
10	8M	189	0	41	10	0
10	8N	189	0	41	10	0
10	8O	189	0	40	7	0
10	8P	189	0	41	10	0
10	8Q	189	0	41	6	0
10	8R	189	0	40	5	0
10	8S	189	0	41	20	0
10	8T	189	0	40	23	0
10	8U	189	0	39	33	0
10	8V	189	0	41	45	0
10	8W	189	0	41	34	0
10	8X	189	0	40	19	0
10	8Y	189	0	40	25	0
10	8Z	189	0	40	31	0
10	9A	189	0	38	26	0
11	AA	32	0	12	0	0
11	AC	32	0	12	0	0
11	AE	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	BA	32	0	12	0	0
11	BC	32	0	12	0	0
11	BE	32	0	12	0	0
11	CA	32	0	12	0	0
11	CC	32	0	12	0	0
11	CE	32	0	12	0	0
11	DA	32	0	12	0	0
11	DC	32	0	12	0	0
11	DE	32	0	12	0	0
11	EA	32	0	12	0	0
11	EC	32	0	12	0	0
11	EE	32	0	12	0	0
11	FA	32	0	12	0	0
11	FC	32	0	12	0	0
11	FE	32	0	12	0	0
11	GA	32	0	12	0	0
11	GC	32	0	12	0	0
11	GE	32	0	12	0	0
11	HA	32	0	12	0	0
11	HC	32	0	12	0	0
11	HE	32	0	12	0	0
11	IA	32	0	12	0	0
11	IC	32	0	12	0	0
11	IE	32	0	12	0	0
11	JA	32	0	12	0	0
11	JC	32	0	12	0	0
11	JE	32	0	12	0	0
11	KA	32	0	12	0	0
11	KC	32	0	12	0	0
11	KE	32	0	12	0	0
11	LA	32	0	12	0	0
11	LC	32	0	12	0	0
11	LE	32	0	12	0	0
11	MA	32	0	12	1	0
11	MC	32	0	12	1	0
11	ME	32	0	12	0	0
12	AA	1	0	0	0	0
12	AC	1	0	0	0	0
12	AE	1	0	0	0	0
12	BA	1	0	0	0	0
12	BC	1	0	0	0	0
12	BE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	CA	1	0	0	0	0
12	CC	1	0	0	0	0
12	CE	1	0	0	0	0
12	DA	1	0	0	0	0
12	DC	1	0	0	0	0
12	DE	1	0	0	0	0
12	EA	1	0	0	0	0
12	ED	1	0	0	0	0
12	EE	1	0	0	0	0
12	FB	1	0	0	0	0
12	FD	1	0	0	0	0
12	FE	1	0	0	0	0
12	GA	1	0	0	0	0
12	GC	1	0	0	0	0
12	GE	1	0	0	0	0
12	HA	1	0	0	0	0
12	HC	1	0	0	0	0
12	HE	1	0	0	0	0
12	IA	1	0	0	0	0
12	IC	1	0	0	0	0
12	IE	1	0	0	0	0
12	JA	1	0	0	0	0
12	JC	1	0	0	0	0
12	JE	1	0	0	0	0
12	KA	1	0	0	0	0
12	KC	1	0	0	0	0
12	KE	1	0	0	0	0
12	LA	1	0	0	0	0
12	LC	1	0	0	0	0
12	LE	1	0	0	0	0
12	MB	1	0	0	0	0
12	MD	1	0	0	0	0
12	MF	1	0	0	0	0
13	AB	28	0	12	2	0
13	AD	28	0	12	2	0
13	AF	28	0	12	1	0
13	BB	28	0	12	3	0
13	BD	28	0	12	3	0
13	BF	28	0	12	2	0
13	CB	28	0	12	3	0
13	CD	28	0	12	3	0
13	CF	28	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	DB	28	0	12	3	0
13	DD	28	0	12	3	0
13	DF	28	0	12	2	0
13	EB	28	0	12	4	0
13	ED	28	0	12	4	0
13	EF	28	0	12	2	0
13	FB	28	0	12	4	0
13	FD	28	0	12	4	0
13	FF	28	0	12	2	0
13	GB	28	0	12	3	0
13	GD	28	0	12	3	0
13	GF	28	0	12	2	0
13	HB	28	0	12	3	0
13	HD	28	0	12	3	0
13	HF	28	0	12	2	0
13	IB	28	0	12	3	0
13	ID	28	0	12	3	0
13	IF	28	0	12	2	0
13	JB	28	0	12	3	0
13	JD	28	0	12	3	0
13	JF	28	0	12	2	0
13	KB	28	0	12	3	0
13	KD	28	0	12	3	0
13	KF	28	0	12	2	0
13	LB	28	0	12	2	0
13	LD	28	0	12	2	0
13	LF	28	0	12	2	0
13	MB	28	0	12	2	0
13	MD	28	0	12	2	0
13	MF	28	0	12	2	0
All	All	318666	0	306569	15548	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 25.

The worst 5 of 15548 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:DD:212:PHE:CZ	1:DE:326:LYS:HD3	1.22	1.73
2:KB:217:LEU:HD22	6:4A:263:CYS:SG	1.30	1.72
2:DB:212:PHE:CZ	1:DC:326:LYS:HD3	1.24	1.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:ED:125:GLU:CA	7:5A:903:PHE:CE2	1.76	1.67
2:ED:212:PHE:CZ	1:EE:326:LYS:HD3	1.27	1.67

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	AA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	AC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	AE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	BA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	BC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	BE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	CA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	CC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	CE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	DA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	DC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	DE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	EA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	EC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	EE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	FA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	FC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	FE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	GC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	GE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	HA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	HC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	HE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	IA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	IC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	IE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	JA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	JC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	JE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	KA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	KC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	KE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	LA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	LC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	LE	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	MA	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	MC	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
1	ME	426/449 (95%)	416 (98%)	10 (2%)	0	100	100
2	AB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	AD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	AF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	BB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	BD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	BF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	CB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	CD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	CF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	DB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	DD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	DF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	EB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	ED	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	EF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	FB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	FD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	FF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	GB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	GD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	GF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	HB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	HD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	HF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	IB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	ID	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	IF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	JB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	JD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	JF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	KB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	KD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	KF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	LB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	LD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	LF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	MB	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	MD	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
2	MF	428/443 (97%)	423 (99%)	5 (1%)	0	100	100
3	1A	138/213 (65%)	136 (99%)	2 (1%)	0	100	100
3	1B	138/213 (65%)	136 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1C	138/213 (65%)	136 (99%)	2 (1%)	0	100	100
4	2A	186/742 (25%)	172 (92%)	9 (5%)	5 (3%)	4	29
4	2B	186/742 (25%)	172 (92%)	9 (5%)	5 (3%)	4	29
4	2C	186/742 (25%)	172 (92%)	9 (5%)	5 (3%)	4	29
5	3A	327/495 (66%)	316 (97%)	10 (3%)	1 (0%)	37	67
5	3B	327/495 (66%)	316 (97%)	10 (3%)	1 (0%)	37	67
5	3C	327/495 (66%)	316 (97%)	10 (3%)	1 (0%)	37	67
6	4A	183/317 (58%)	176 (96%)	4 (2%)	3 (2%)	8	37
6	4B	183/317 (58%)	176 (96%)	4 (2%)	3 (2%)	8	37
6	4C	183/317 (58%)	176 (96%)	4 (2%)	3 (2%)	8	37
6	4D	183/317 (58%)	176 (96%)	4 (2%)	3 (2%)	8	37
7	5A	695/1754 (40%)	650 (94%)	33 (5%)	12 (2%)	7	36
7	5B	695/1754 (40%)	650 (94%)	33 (5%)	12 (2%)	7	36
7	5C	695/1754 (40%)	650 (94%)	33 (5%)	12 (2%)	7	36
8	6A	254/346 (73%)	247 (97%)	7 (3%)	0	100	100
8	6B	254/346 (73%)	247 (97%)	7 (3%)	0	100	100
8	6C	254/346 (73%)	247 (97%)	7 (3%)	0	100	100
9	7A	44/101 (44%)	44 (100%)	0	0	100	100
9	7B	44/101 (44%)	44 (100%)	0	0	100	100
9	7C	44/101 (44%)	44 (100%)	0	0	100	100
9	7D	44/101 (44%)	44 (100%)	0	0	100	100
9	7E	44/101 (44%)	44 (100%)	0	0	100	100
9	7F	44/101 (44%)	44 (100%)	0	0	100	100
All	All	39102/47312 (83%)	38252 (98%)	784 (2%)	66 (0%)	45	72

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	2A	146	PRO
4	2A	147	PHE
4	2A	150	GLN
4	2B	146	PRO
4	2B	147	PHE

### 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	AA	364/376 (97%)	364 (100%)	0	100	100
1	AC	364/376 (97%)	364 (100%)	0	100	100
1	AE	364/376 (97%)	364 (100%)	0	100	100
1	BA	364/376 (97%)	364 (100%)	0	100	100
1	BC	364/376 (97%)	364 (100%)	0	100	100
1	BE	364/376 (97%)	364 (100%)	0	100	100
1	CA	364/376 (97%)	364 (100%)	0	100	100
1	CC	364/376 (97%)	364 (100%)	0	100	100
1	CE	364/376 (97%)	364 (100%)	0	100	100
1	DA	364/376 (97%)	364 (100%)	0	100	100
1	DC	364/376 (97%)	364 (100%)	0	100	100
1	DE	364/376 (97%)	364 (100%)	0	100	100
1	EA	364/376 (97%)	364 (100%)	0	100	100
1	EC	364/376 (97%)	364 (100%)	0	100	100
1	EE	364/376 (97%)	364 (100%)	0	100	100
1	FA	364/376 (97%)	364 (100%)	0	100	100
1	FC	364/376 (97%)	364 (100%)	0	100	100
1	FE	364/376 (97%)	364 (100%)	0	100	100
1	GA	364/376 (97%)	364 (100%)	0	100	100
1	GC	364/376 (97%)	364 (100%)	0	100	100
1	GE	364/376 (97%)	364 (100%)	0	100	100
1	HA	364/376 (97%)	364 (100%)	0	100	100
1	HC	364/376 (97%)	364 (100%)	0	100	100
1	HE	364/376 (97%)	364 (100%)	0	100	100
1	IA	364/376 (97%)	364 (100%)	0	100	100
1	IC	364/376 (97%)	364 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	IE	364/376 (97%)	364 (100%)	0	100	100
1	JA	364/376 (97%)	364 (100%)	0	100	100
1	JC	364/376 (97%)	364 (100%)	0	100	100
1	JE	364/376 (97%)	364 (100%)	0	100	100
1	KA	364/376 (97%)	364 (100%)	0	100	100
1	KC	364/376 (97%)	364 (100%)	0	100	100
1	KE	364/376 (97%)	364 (100%)	0	100	100
1	LA	364/376 (97%)	364 (100%)	0	100	100
1	LC	364/376 (97%)	364 (100%)	0	100	100
1	LE	364/376 (97%)	364 (100%)	0	100	100
1	MA	364/376 (97%)	364 (100%)	0	100	100
1	MC	364/376 (97%)	364 (100%)	0	100	100
1	ME	364/376 (97%)	364 (100%)	0	100	100
2	AB	365/376 (97%)	365 (100%)	0	100	100
2	AD	365/376 (97%)	365 (100%)	0	100	100
2	AF	365/376 (97%)	365 (100%)	0	100	100
2	BB	365/376 (97%)	365 (100%)	0	100	100
2	BD	365/376 (97%)	365 (100%)	0	100	100
2	BF	365/376 (97%)	365 (100%)	0	100	100
2	CB	365/376 (97%)	365 (100%)	0	100	100
2	CD	365/376 (97%)	365 (100%)	0	100	100
2	CF	365/376 (97%)	365 (100%)	0	100	100
2	DB	365/376 (97%)	365 (100%)	0	100	100
2	DD	365/376 (97%)	365 (100%)	0	100	100
2	DF	365/376 (97%)	365 (100%)	0	100	100
2	EB	365/376 (97%)	365 (100%)	0	100	100
2	ED	365/376 (97%)	365 (100%)	0	100	100
2	EF	365/376 (97%)	365 (100%)	0	100	100
2	FB	365/376 (97%)	365 (100%)	0	100	100
2	FD	365/376 (97%)	365 (100%)	0	100	100
2	FF	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	GB	365/376 (97%)	365 (100%)	0	100	100
2	GD	365/376 (97%)	365 (100%)	0	100	100
2	GF	365/376 (97%)	365 (100%)	0	100	100
2	HB	365/376 (97%)	365 (100%)	0	100	100
2	HD	365/376 (97%)	365 (100%)	0	100	100
2	HF	365/376 (97%)	365 (100%)	0	100	100
2	IB	365/376 (97%)	365 (100%)	0	100	100
2	ID	365/376 (97%)	365 (100%)	0	100	100
2	IF	365/376 (97%)	365 (100%)	0	100	100
2	JB	365/376 (97%)	365 (100%)	0	100	100
2	JD	365/376 (97%)	365 (100%)	0	100	100
2	JF	365/376 (97%)	365 (100%)	0	100	100
2	KB	365/376 (97%)	365 (100%)	0	100	100
2	KD	365/376 (97%)	365 (100%)	0	100	100
2	KF	365/376 (97%)	365 (100%)	0	100	100
2	LB	365/376 (97%)	365 (100%)	0	100	100
2	LD	365/376 (97%)	365 (100%)	0	100	100
2	LF	365/376 (97%)	365 (100%)	0	100	100
2	MB	365/376 (97%)	365 (100%)	0	100	100
2	MD	365/376 (97%)	365 (100%)	0	100	100
2	MF	365/376 (97%)	365 (100%)	0	100	100
3	1A	129/196 (66%)	128 (99%)	1 (1%)	79	85
3	1B	129/196 (66%)	128 (99%)	1 (1%)	79	85
3	1C	129/196 (66%)	128 (99%)	1 (1%)	79	85
4	2A	180/692 (26%)	162 (90%)	18 (10%)	6	26
4	2B	180/692 (26%)	162 (90%)	18 (10%)	6	26
4	2C	180/692 (26%)	162 (90%)	18 (10%)	6	26
5	3A	309/457 (68%)	305 (99%)	4 (1%)	65	77
5	3B	309/457 (68%)	305 (99%)	4 (1%)	65	77
5	3C	309/457 (68%)	305 (99%)	4 (1%)	65	77
6	4A	176/286 (62%)	92 (52%)	84 (48%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	4B	176/286 (62%)	92 (52%)	84 (48%)	0	0
6	4C	176/286 (62%)	92 (52%)	84 (48%)	0	0
6	4D	176/286 (62%)	92 (52%)	84 (48%)	0	0
7	5A	663/1625 (41%)	501 (76%)	162 (24%)	0	4
7	5B	663/1625 (41%)	501 (76%)	162 (24%)	0	4
7	5C	663/1625 (41%)	500 (75%)	163 (25%)	0	4
8	6A	229/316 (72%)	225 (98%)	4 (2%)	56	73
8	6B	229/316 (72%)	225 (98%)	4 (2%)	56	73
8	6C	229/316 (72%)	225 (98%)	4 (2%)	56	73
9	7A	42/86 (49%)	42 (100%)	0	100	100
9	7B	42/86 (49%)	42 (100%)	0	100	100
9	7C	42/86 (49%)	42 (100%)	0	100	100
9	7D	42/86 (49%)	42 (100%)	0	100	100
9	7E	42/86 (49%)	42 (100%)	0	100	100
9	7F	42/86 (49%)	42 (100%)	0	100	100
All	All	33917/40846 (83%)	33013 (97%)	904 (3%)	41	61

5 of 904 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	5A	1323	MET
7	5C	1491	LEU
7	5B	803	VAL
7	5C	1469	VAL
7	5C	1343	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 386 such sidechains are listed below:

Mol	Chain	Res	Type
1	LC	249	ASN
5	3A	192	GLN
1	LE	101	ASN
1	ME	192	HIS
5	3C	290	GLN

### 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 117 ligands modelled in this entry, 39 are monoatomic - leaving 78 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
11	GTP	AA	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
13	GDP	LB	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.04	2 (6%)
11	GTP	DC	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
13	GDP	JB	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.04	2 (6%)
11	GTP	MC	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
13	GDP	KB	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.03	2 (6%)
11	GTP	LE	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
13	GDP	DD	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.03	2 (6%)
11	GTP	LA	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
13	GDP	BB	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.04	2 (6%)
13	GDP	AB	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.04	2 (6%)
13	GDP	BD	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.04	2 (6%)
13	GDP	FF	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.04	2 (6%)
13	GDP	BF	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.03	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	GTP	GA	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	KA	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
13	GDP	CF	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.03	2 (6%)
11	GTP	JC	501	12	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
11	GTP	AC	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
11	GTP	CC	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	MA	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	ME	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
13	GDP	KD	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.03	2 (6%)
13	GDP	JD	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.03	2 (6%)
11	GTP	BA	501	12	29,34,34	1.18	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	HC	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
13	GDP	CD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.03	1 (3%)
11	GTP	KE	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
13	GDP	MF	502	-	25,30,30	1.01	1 (4%)	30,47,47	1.03	2 (6%)
11	GTP	IC	501	12	29,34,34	1.18	2 (6%)	35,54,54	1.28	4 (11%)
13	GDP	EB	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.03	2 (6%)
13	GDP	LD	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.03	2 (6%)
13	GDP	FB	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.04	2 (6%)
13	GDP	ID	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.03	2 (6%)
13	GDP	HD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.02	1 (3%)
11	GTP	DE	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
11	GTP	HE	501	12	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
13	GDP	FD	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.03	2 (6%)
13	GDP	MD	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.03	2 (6%)
13	GDP	IF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.03	1 (3%)
13	GDP	AD	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.03	2 (6%)
13	GDP	CB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.03	1 (3%)
13	GDP	GD	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.02	2 (6%)
13	GDP	LF	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.03	2 (6%)
11	GTP	JE	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
11	GTP	BE	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	GE	501	12	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
13	GDP	AF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.03	1 (3%)
11	GTP	GC	501	12	29,34,34	1.20	2 (6%)	35,54,54	1.29	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	GDP	DF	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.04	2 (6%)
13	GDP	DB	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.04	2 (6%)
13	GDP	GB	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.04	2 (6%)
11	GTP	FC	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
11	GTP	HA	501	12	29,34,34	1.20	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	EA	501	12	29,34,34	1.18	2 (6%)	35,54,54	1.28	4 (11%)
13	GDP	IB	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.04	2 (6%)
13	GDP	EF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.04	2 (6%)
11	GTP	LC	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	BC	501	12	29,34,34	1.18	2 (6%)	35,54,54	1.29	4 (11%)
13	GDP	KF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.04	2 (6%)
11	GTP	FE	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
13	GDP	HB	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.04	2 (6%)
11	GTP	IE	501	12	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
11	GTP	CE	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
13	GDP	HF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.04	2 (6%)
13	GDP	JF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.04	2 (6%)
13	GDP	GF	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.03	2 (6%)
11	GTP	CA	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
13	GDP	MB	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.03	2 (6%)
11	GTP	DA	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
13	GDP	ED	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.03	2 (6%)
11	GTP	EC	501	12	29,34,34	1.18	2 (6%)	35,54,54	1.28	4 (11%)
11	GTP	AE	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
11	GTP	JA	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	IA	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	EE	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	KC	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
11	GTP	FA	501	12	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	GTP	AA	501	12	-	8/18/38/38	0/3/3/3
13	GDP	LB	501	-	-	0/12/32/32	0/3/3/3
11	GTP	DC	501	12	-	8/18/38/38	0/3/3/3
13	GDP	JB	501	-	-	0/12/32/32	0/3/3/3
11	GTP	MC	501	12	-	8/18/38/38	0/3/3/3
13	GDP	KB	501	-	-	0/12/32/32	0/3/3/3
11	GTP	LE	501	12	-	8/18/38/38	0/3/3/3
13	GDP	DD	501	-	-	1/12/32/32	0/3/3/3
11	GTP	LA	501	12	-	8/18/38/38	0/3/3/3
13	GDP	BB	501	-	-	0/12/32/32	0/3/3/3
13	GDP	AB	501	-	-	0/12/32/32	0/3/3/3
13	GDP	BD	501	-	-	0/12/32/32	0/3/3/3
13	GDP	FF	501	-	-	1/12/32/32	0/3/3/3
13	GDP	BF	501	-	-	1/12/32/32	0/3/3/3
11	GTP	GA	501	12	-	8/18/38/38	0/3/3/3
11	GTP	KA	501	12	-	8/18/38/38	0/3/3/3
13	GDP	CF	501	-	-	1/12/32/32	0/3/3/3
11	GTP	JC	501	12	-	8/18/38/38	0/3/3/3
11	GTP	AC	501	12	-	8/18/38/38	0/3/3/3
11	GTP	CC	501	12	-	8/18/38/38	0/3/3/3
11	GTP	MA	501	12	-	8/18/38/38	0/3/3/3
11	GTP	ME	501	12	-	8/18/38/38	0/3/3/3
13	GDP	KD	501	-	-	0/12/32/32	0/3/3/3
13	GDP	JD	501	-	-	0/12/32/32	0/3/3/3
11	GTP	BA	501	12	-	8/18/38/38	0/3/3/3
11	GTP	HC	501	12	-	8/18/38/38	0/3/3/3
13	GDP	CD	501	-	-	1/12/32/32	0/3/3/3
11	GTP	KE	501	12	-	8/18/38/38	0/3/3/3
13	GDP	MF	502	-	-	0/12/32/32	0/3/3/3
11	GTP	IC	501	12	-	8/18/38/38	0/3/3/3
13	GDP	EB	501	-	-	0/12/32/32	0/3/3/3
13	GDP	LD	501	-	-	1/12/32/32	0/3/3/3
13	GDP	FB	502	-	-	1/12/32/32	0/3/3/3
13	GDP	ID	501	-	-	0/12/32/32	0/3/3/3
13	GDP	HD	501	-	-	0/12/32/32	0/3/3/3
11	GTP	DE	501	12	-	8/18/38/38	0/3/3/3
11	GTP	HE	501	12	-	8/18/38/38	0/3/3/3
13	GDP	FD	502	-	-	0/12/32/32	0/3/3/3
13	GDP	MD	502	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GDP	IF	501	-	-	1/12/32/32	0/3/3/3
13	GDP	AD	501	-	-	0/12/32/32	0/3/3/3
13	GDP	CB	501	-	-	1/12/32/32	0/3/3/3
13	GDP	GD	501	-	-	0/12/32/32	0/3/3/3
13	GDP	LF	501	-	-	0/12/32/32	0/3/3/3
11	GTP	JE	501	12	-	8/18/38/38	0/3/3/3
11	GTP	BE	501	12	-	8/18/38/38	0/3/3/3
11	GTP	GE	501	12	-	8/18/38/38	0/3/3/3
13	GDP	AF	501	-	-	1/12/32/32	0/3/3/3
11	GTP	GC	501	12	-	8/18/38/38	0/3/3/3
13	GDP	DF	501	-	-	1/12/32/32	0/3/3/3
13	GDP	DB	501	-	-	0/12/32/32	0/3/3/3
13	GDP	GB	501	-	-	1/12/32/32	0/3/3/3
11	GTP	FC	501	12	-	8/18/38/38	0/3/3/3
11	GTP	HA	501	12	-	8/18/38/38	0/3/3/3
11	GTP	EA	501	12	-	8/18/38/38	0/3/3/3
13	GDP	IB	501	-	-	0/12/32/32	0/3/3/3
13	GDP	EF	501	-	-	0/12/32/32	0/3/3/3
11	GTP	LC	501	12	-	8/18/38/38	0/3/3/3
11	GTP	BC	501	12	-	8/18/38/38	0/3/3/3
13	GDP	KF	501	-	-	0/12/32/32	0/3/3/3
11	GTP	FE	501	12	-	8/18/38/38	0/3/3/3
13	GDP	HB	501	-	-	0/12/32/32	0/3/3/3
11	GTP	IE	501	12	-	8/18/38/38	0/3/3/3
11	GTP	CE	501	12	-	8/18/38/38	0/3/3/3
13	GDP	HF	501	-	-	0/12/32/32	0/3/3/3
13	GDP	JF	501	-	-	1/12/32/32	0/3/3/3
13	GDP	GF	501	-	-	1/12/32/32	0/3/3/3
11	GTP	CA	501	12	-	8/18/38/38	0/3/3/3
13	GDP	MB	502	-	-	0/12/32/32	0/3/3/3
11	GTP	DA	501	12	-	8/18/38/38	0/3/3/3
13	GDP	ED	502	-	-	0/12/32/32	0/3/3/3
11	GTP	EC	501	12	-	8/18/38/38	0/3/3/3
11	GTP	AE	501	12	-	8/18/38/38	0/3/3/3
11	GTP	JA	501	12	-	8/18/38/38	0/3/3/3
11	GTP	IA	501	12	-	8/18/38/38	0/3/3/3
11	GTP	EE	501	12	-	8/18/38/38	0/3/3/3
11	GTP	KC	501	12	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	GTP	FA	501	12	-	8/18/38/38	0/3/3/3

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	CE	501	GTP	C5-C6	-4.15	1.39	1.47
11	CC	501	GTP	C5-C6	-4.14	1.39	1.47
11	JC	501	GTP	C5-C6	-4.13	1.39	1.47
11	GC	501	GTP	C5-C6	-4.13	1.39	1.47
11	HA	501	GTP	C5-C6	-4.13	1.39	1.47

The worst 5 of 229 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	LC	501	GTP	C8-N7-C5	3.58	108.64	102.55
11	CE	501	GTP	C8-N7-C5	3.57	108.63	102.55
11	BE	501	GTP	C8-N7-C5	3.57	108.62	102.55
11	LE	501	GTP	C8-N7-C5	3.57	108.62	102.55
11	MA	501	GTP	C8-N7-C5	3.57	108.62	102.55

There are no chirality outliers.

5 of 327 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	AA	501	GTP	C5'-O5'-PA-O3A
11	AA	501	GTP	C5'-O5'-PA-O1A
11	AA	501	GTP	C5'-O5'-PA-O2A
11	AC	501	GTP	C5'-O5'-PA-O3A
11	AC	501	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

41 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	LB	501	GDP	2	0
13	JB	501	GDP	3	0
11	MC	501	GTP	1	0
13	KB	501	GDP	3	0
13	DD	501	GDP	3	0
13	BB	501	GDP	3	0
13	AB	501	GDP	2	0

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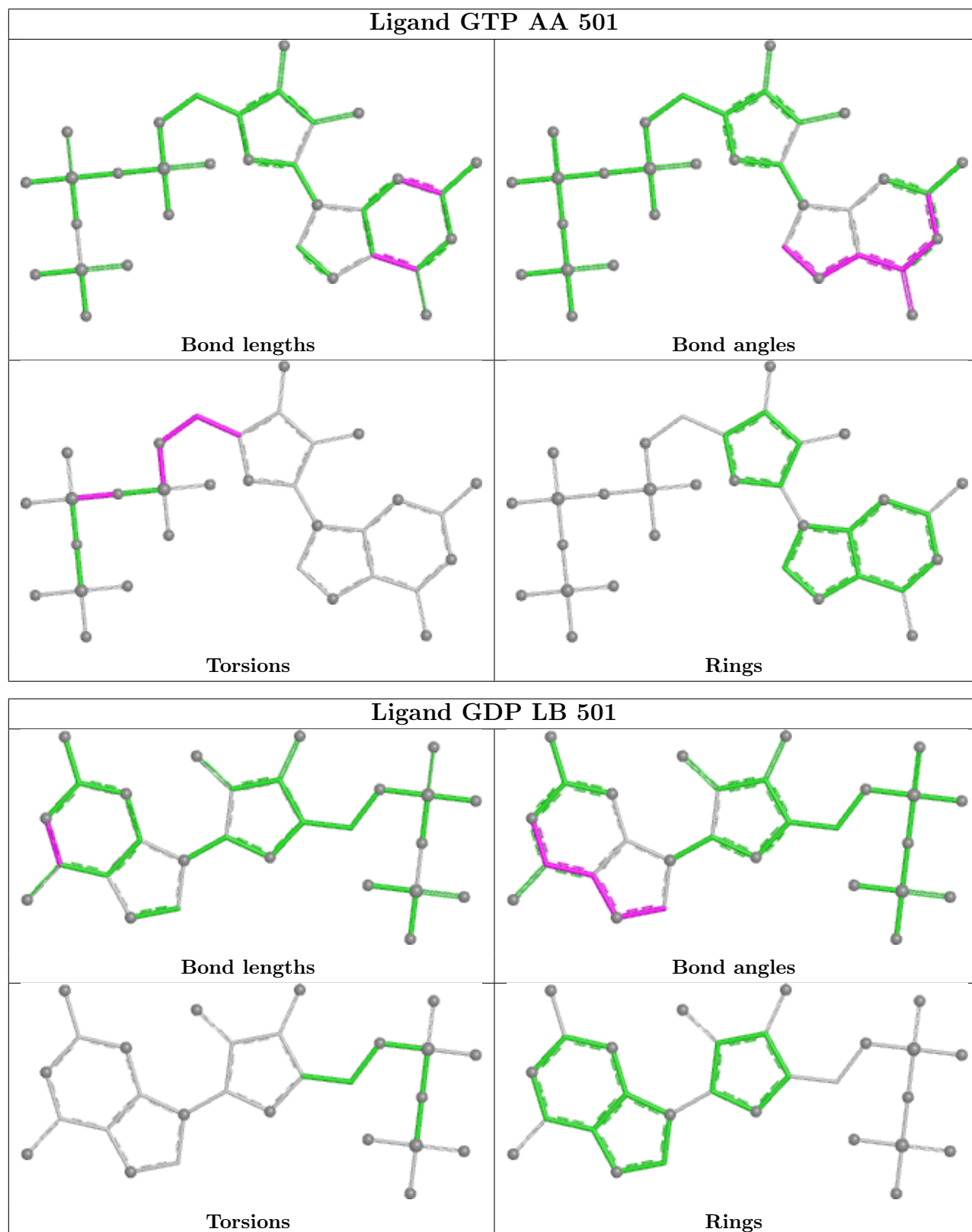


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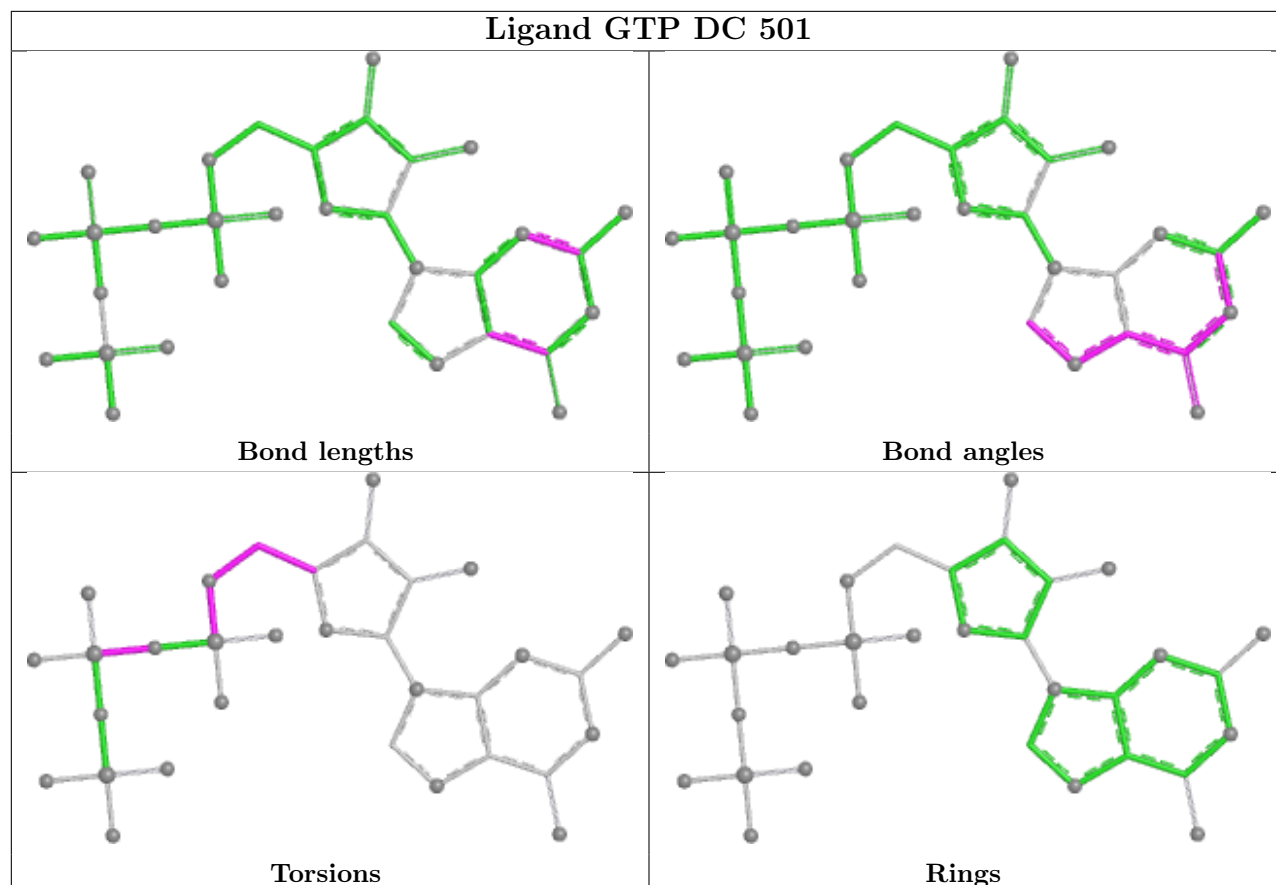
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	BD	501	GDP	3	0
13	FF	501	GDP	2	0
13	BF	501	GDP	2	0
13	CF	501	GDP	2	0
11	MA	501	GTP	1	0
13	KD	501	GDP	3	0
13	JD	501	GDP	3	0
13	CD	501	GDP	3	0
13	MF	502	GDP	2	0
13	EB	501	GDP	4	0
13	LD	501	GDP	2	0
13	FB	502	GDP	4	0
13	ID	501	GDP	3	0
13	HD	501	GDP	3	0
13	FD	502	GDP	4	0
13	MD	502	GDP	2	0
13	IF	501	GDP	2	0
13	AD	501	GDP	2	0
13	CB	501	GDP	3	0
13	GD	501	GDP	3	0
13	LF	501	GDP	2	0
13	AF	501	GDP	1	0
13	DF	501	GDP	2	0
13	DB	501	GDP	3	0
13	GB	501	GDP	3	0
13	IB	501	GDP	3	0
13	EF	501	GDP	2	0
13	KF	501	GDP	2	0
13	HB	501	GDP	3	0
13	HF	501	GDP	2	0
13	JF	501	GDP	2	0
13	GF	501	GDP	2	0
13	MB	502	GDP	2	0
13	ED	502	GDP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

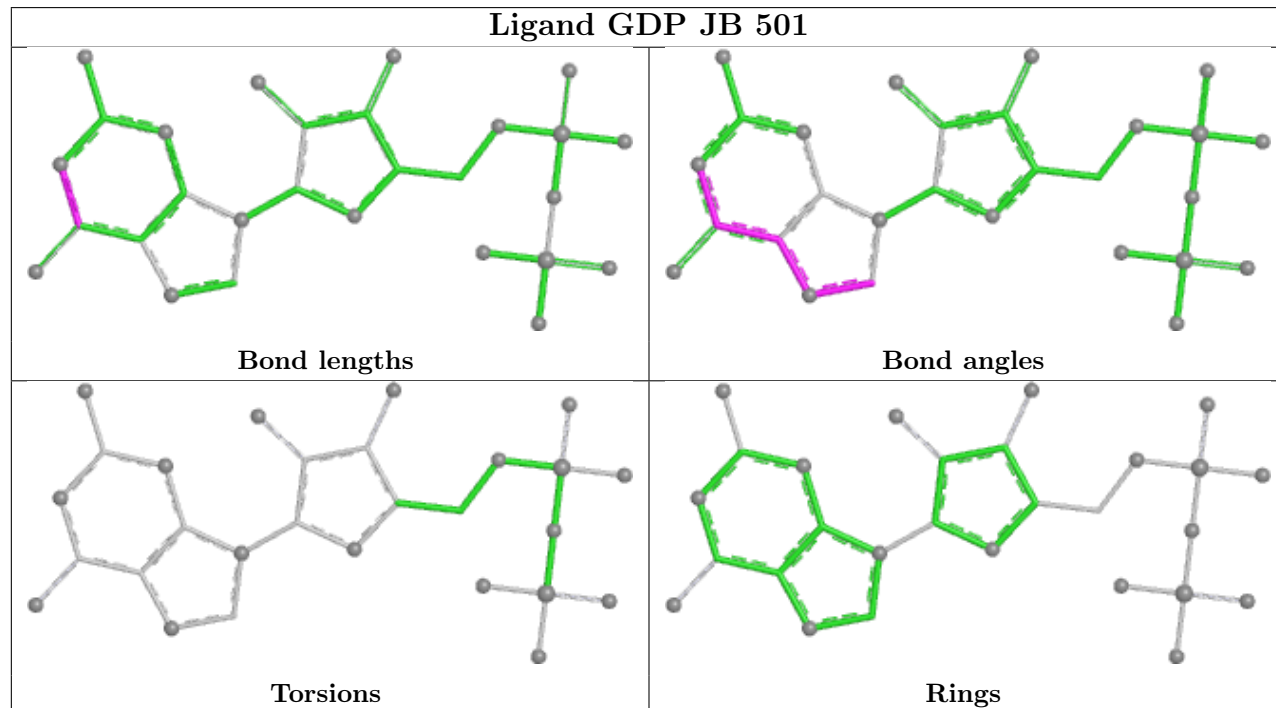
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



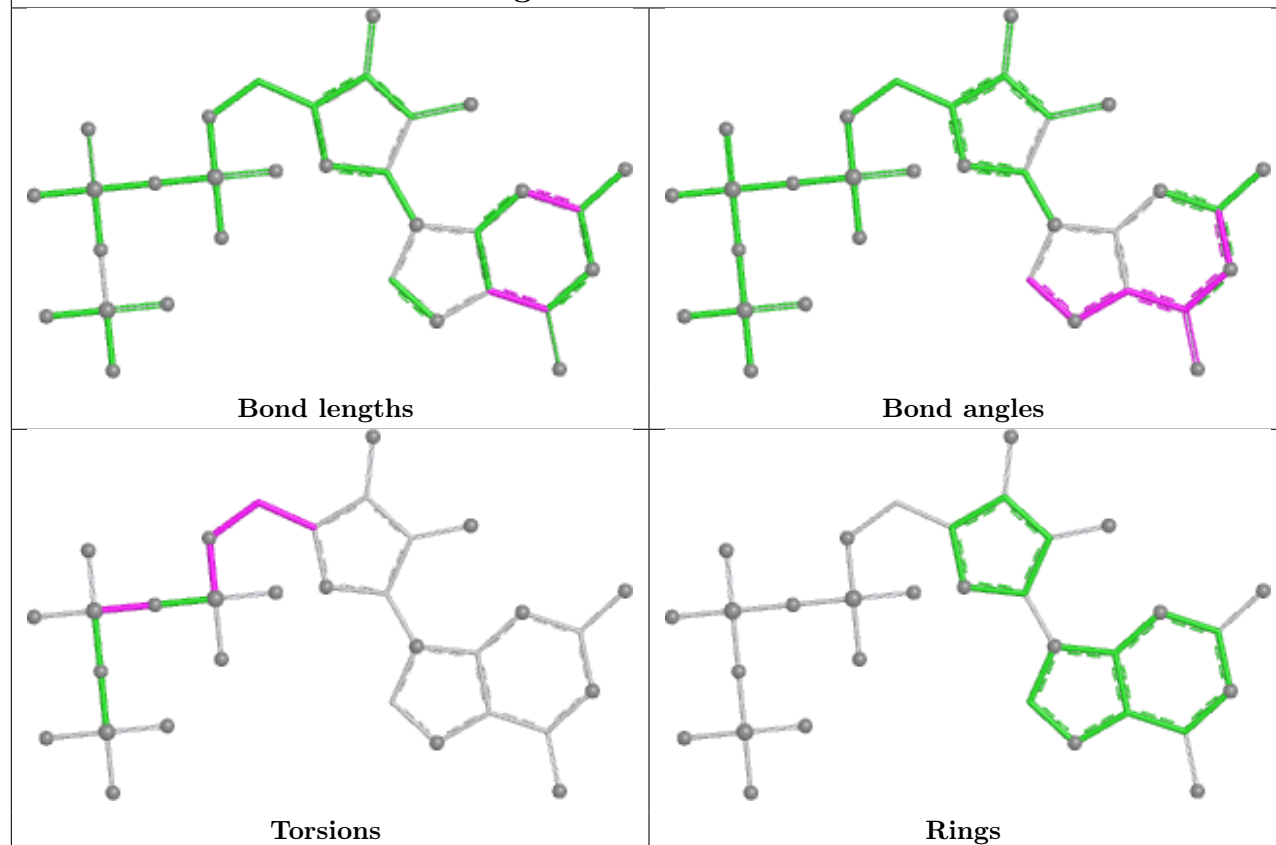
## Ligand GTP DC 501



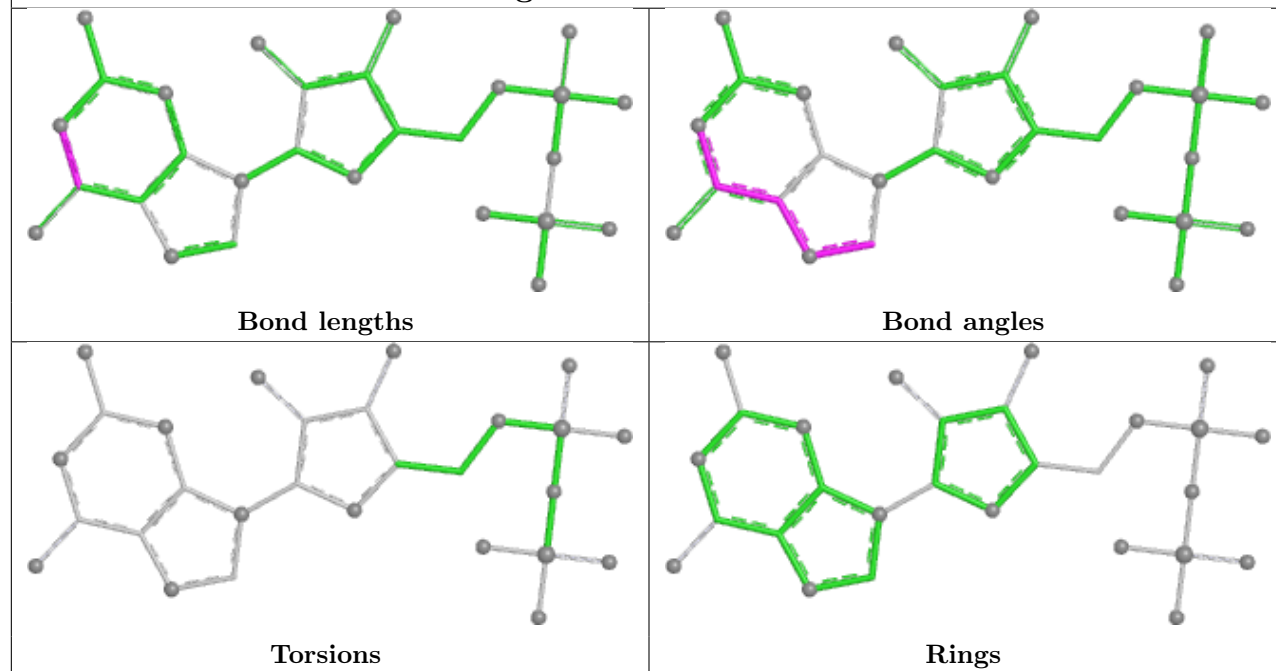
## Ligand GDP JB 501

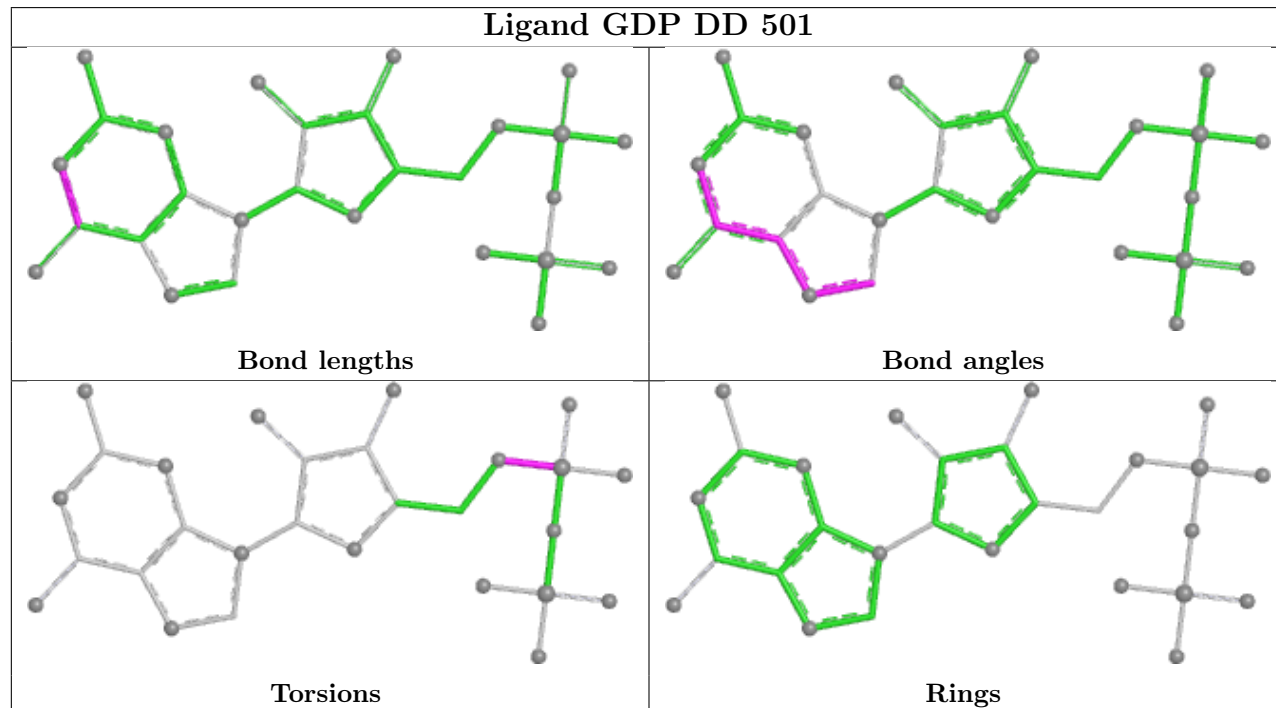
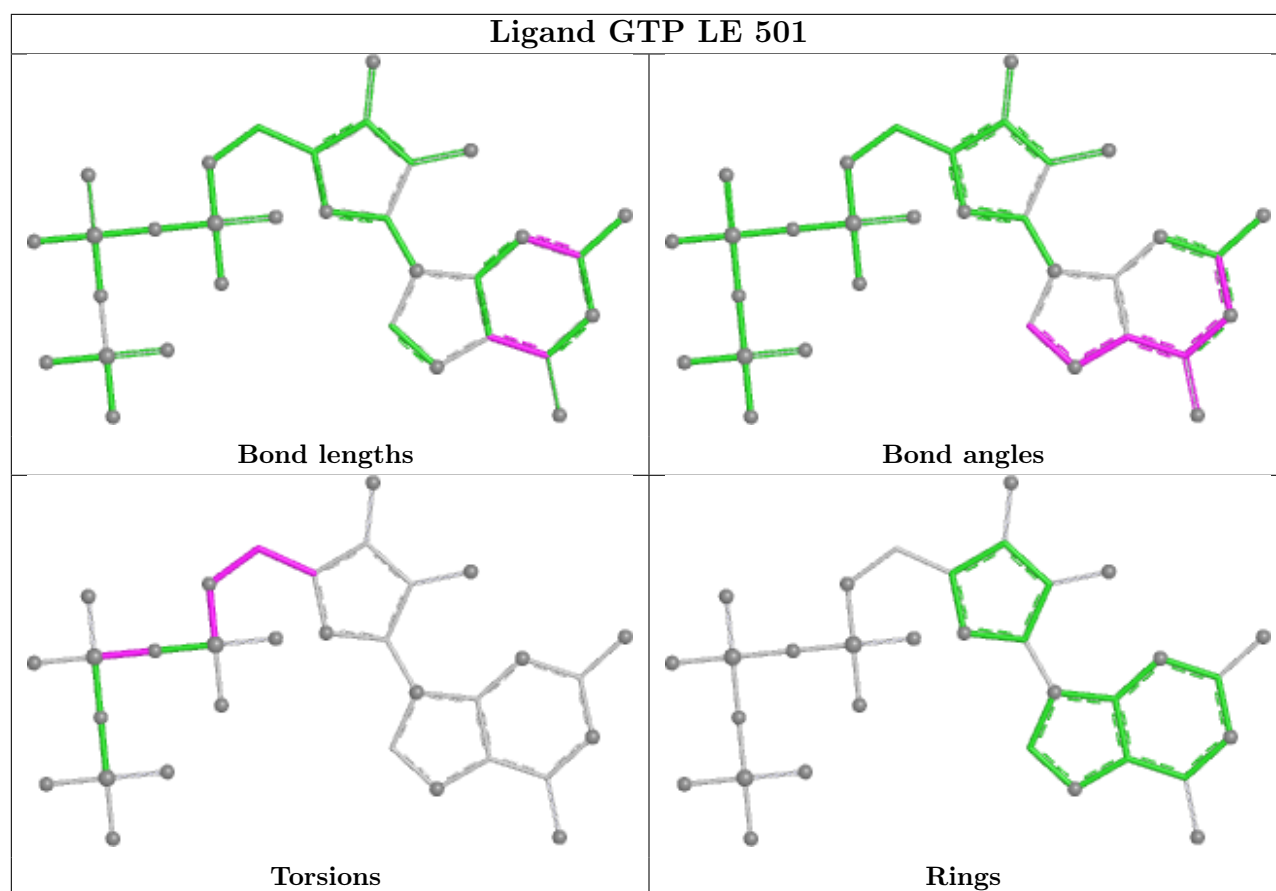


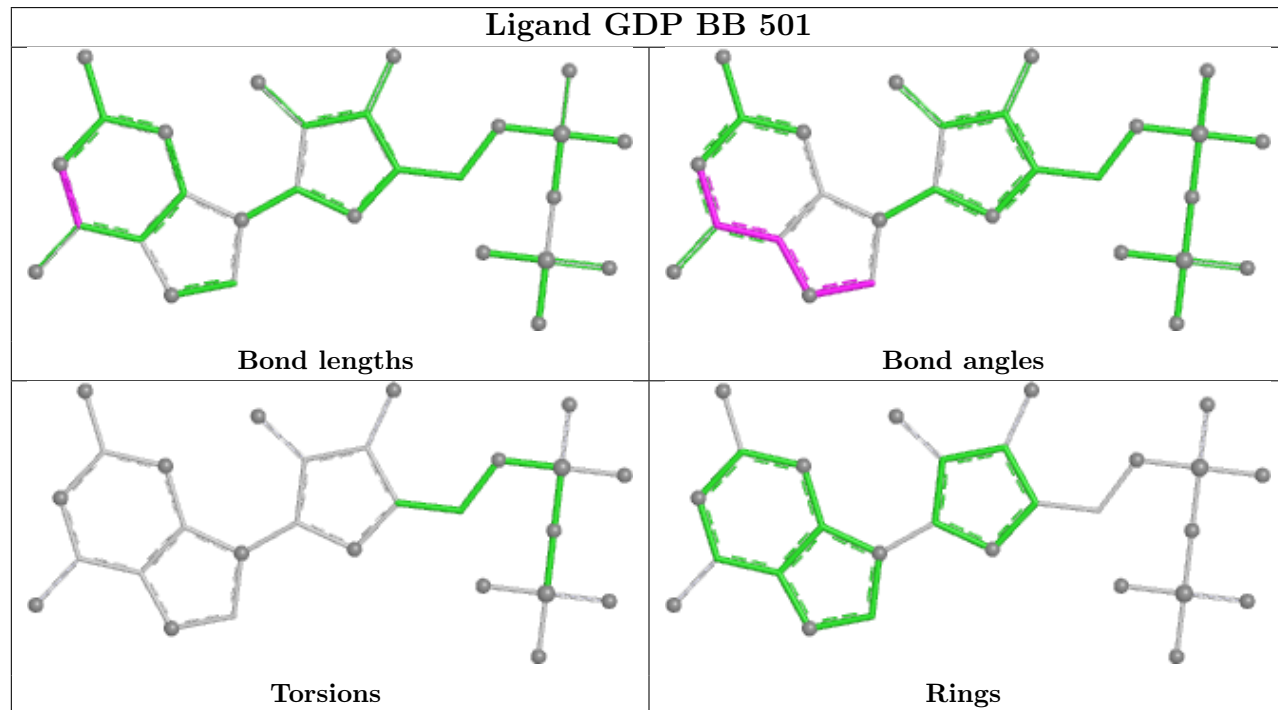
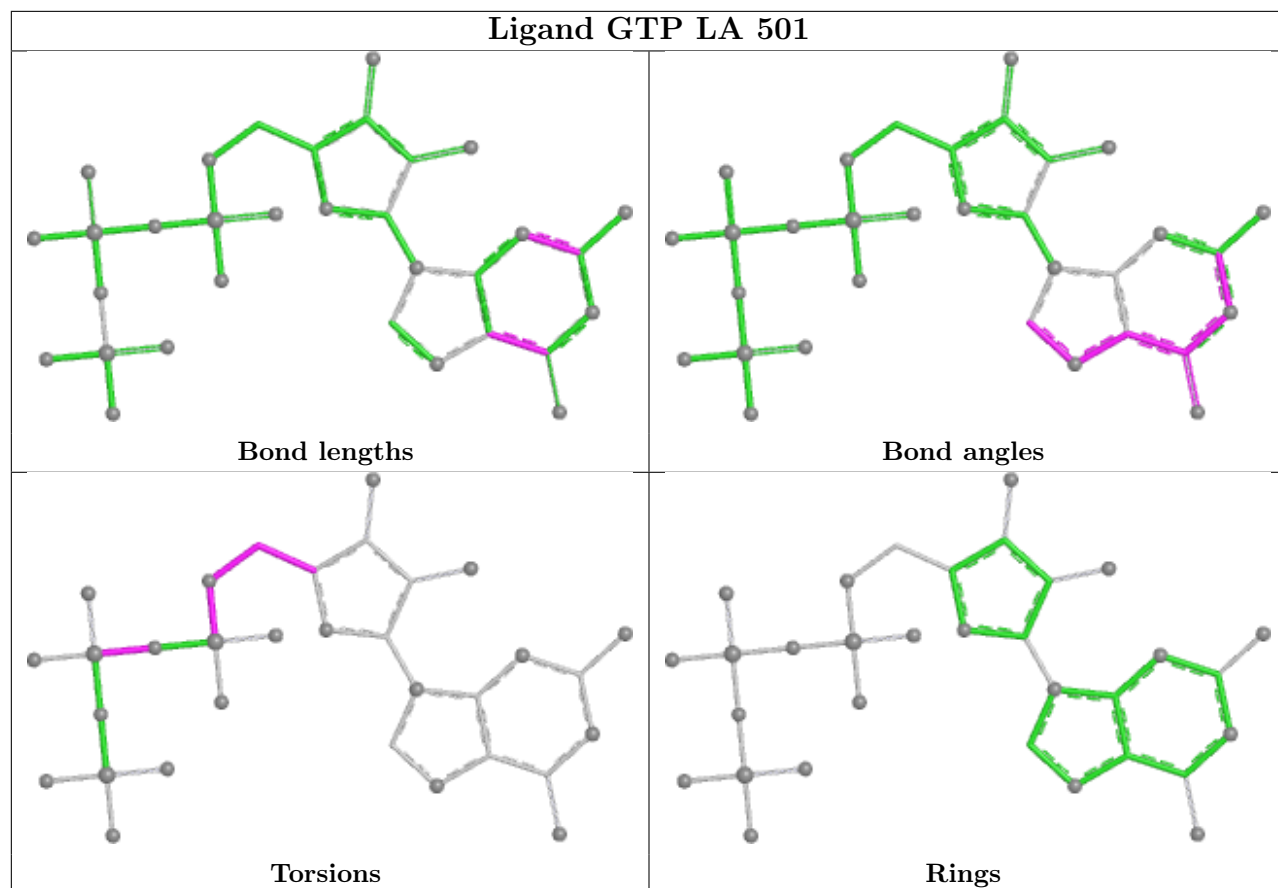
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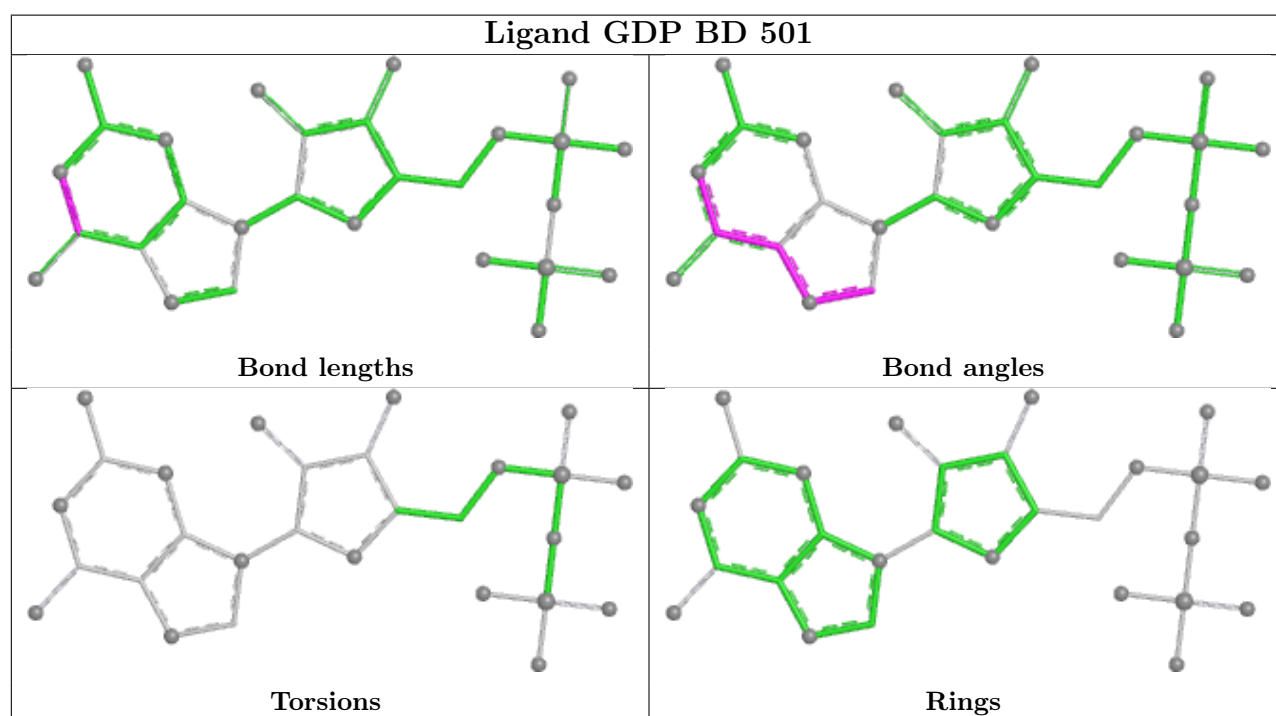
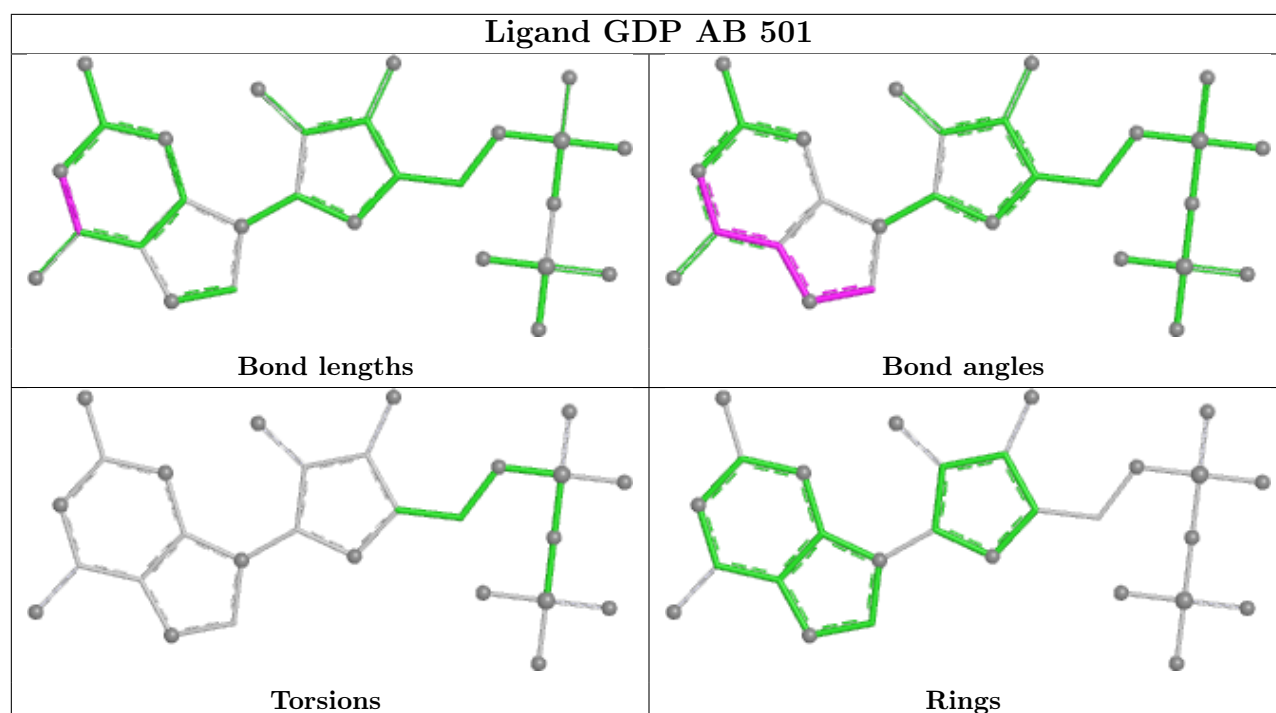


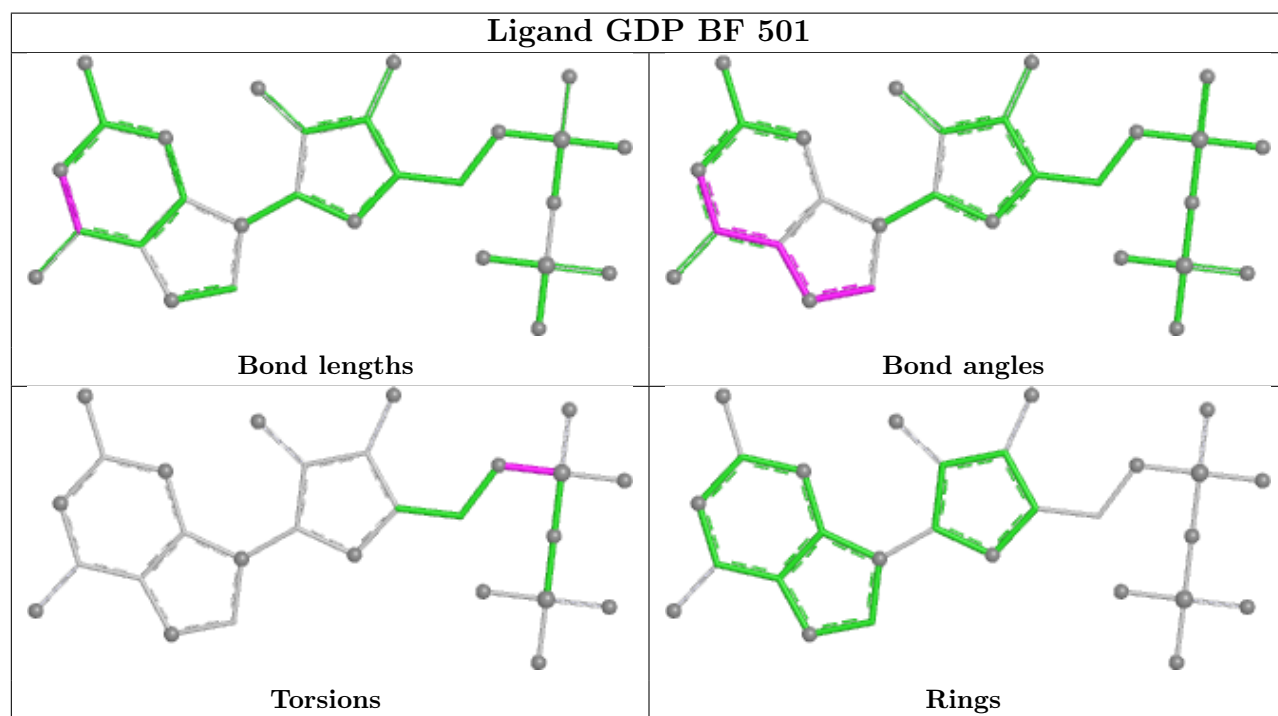
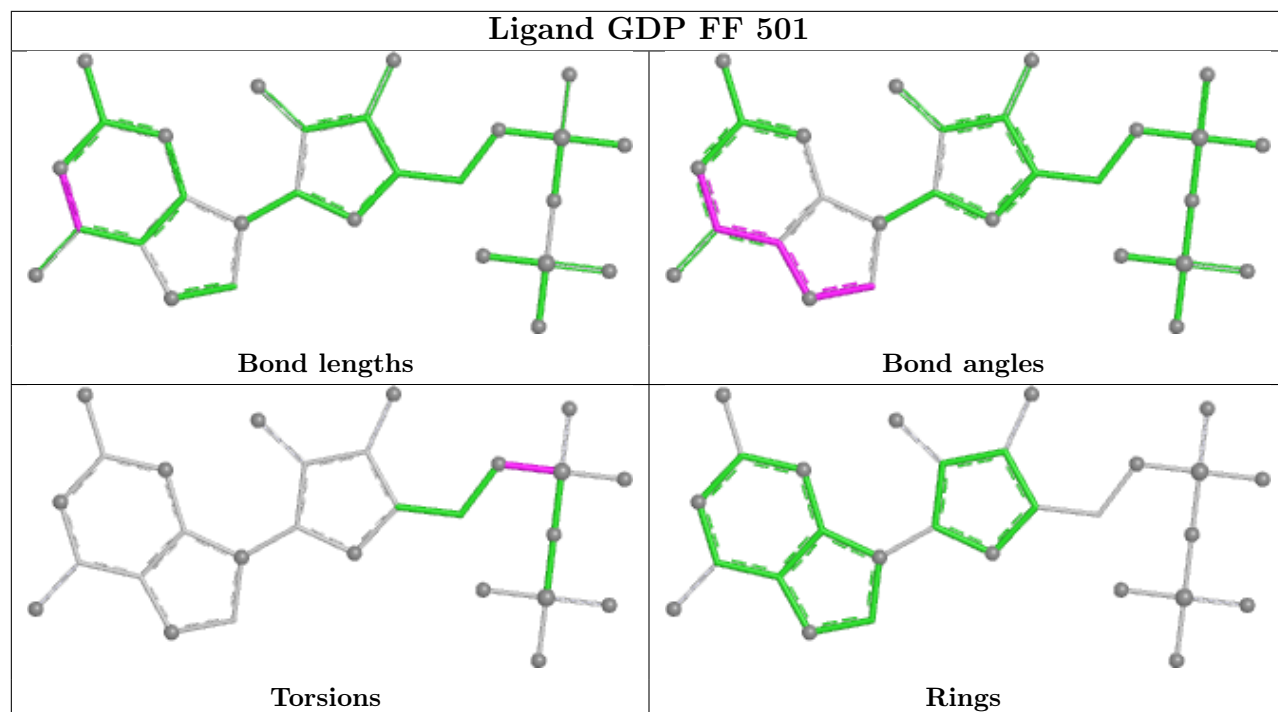
## Ligand GDP KB 501





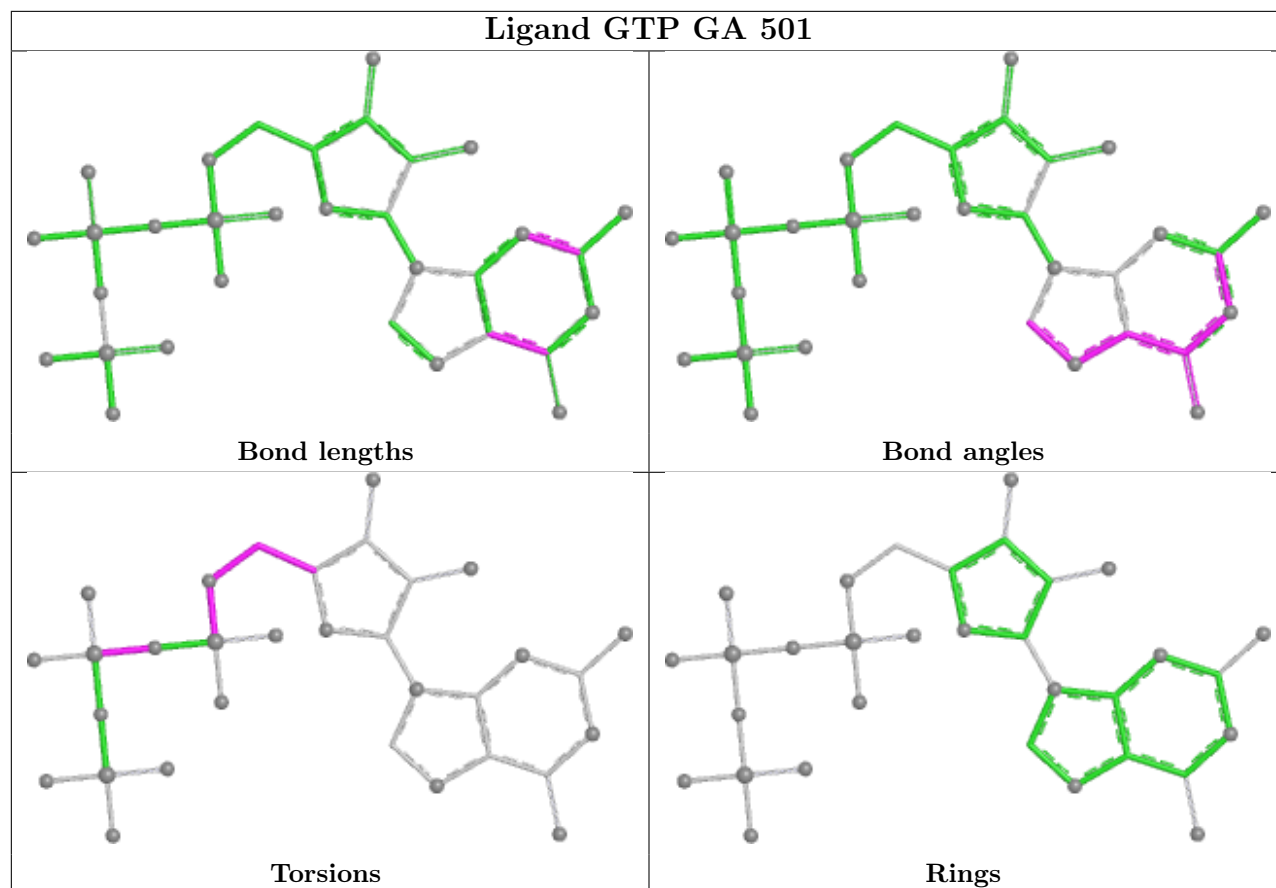




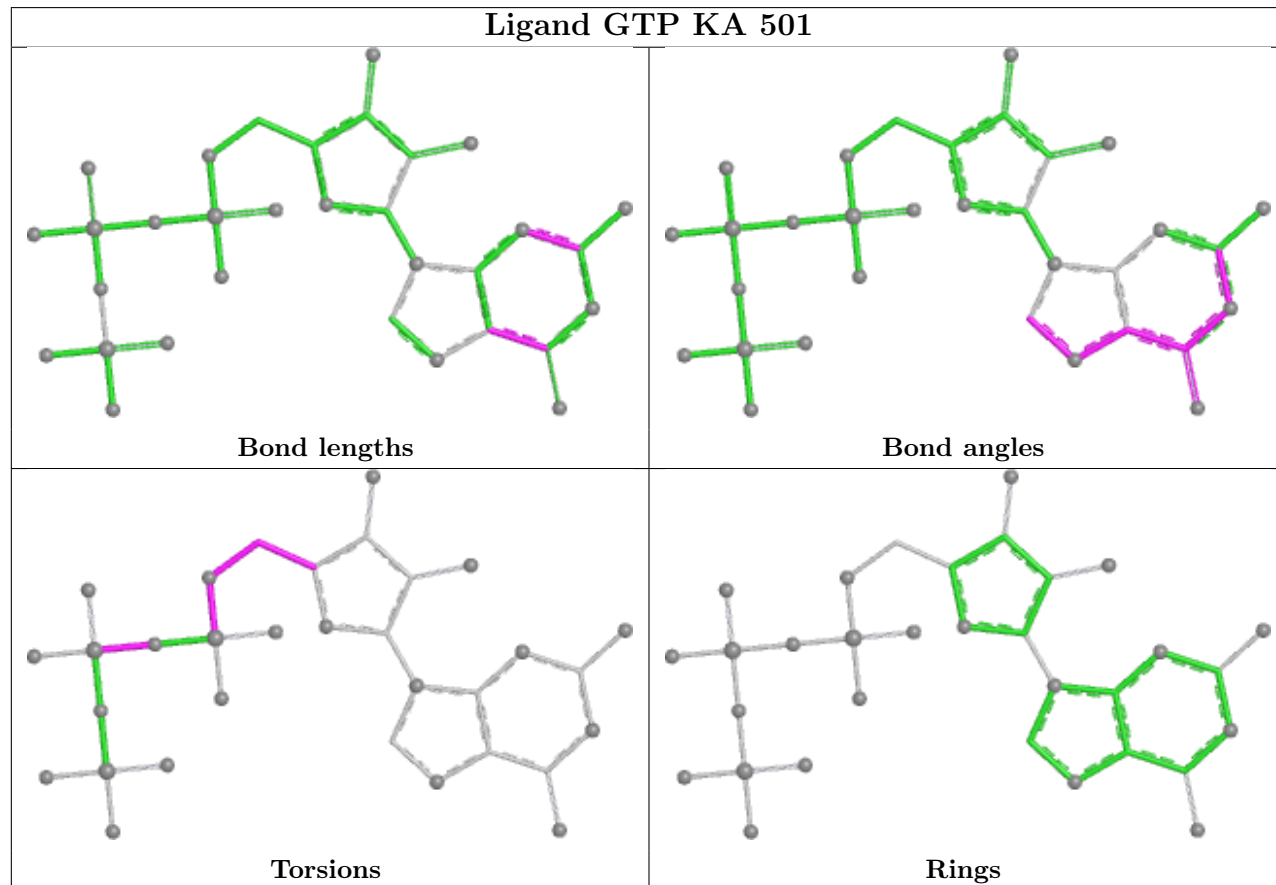


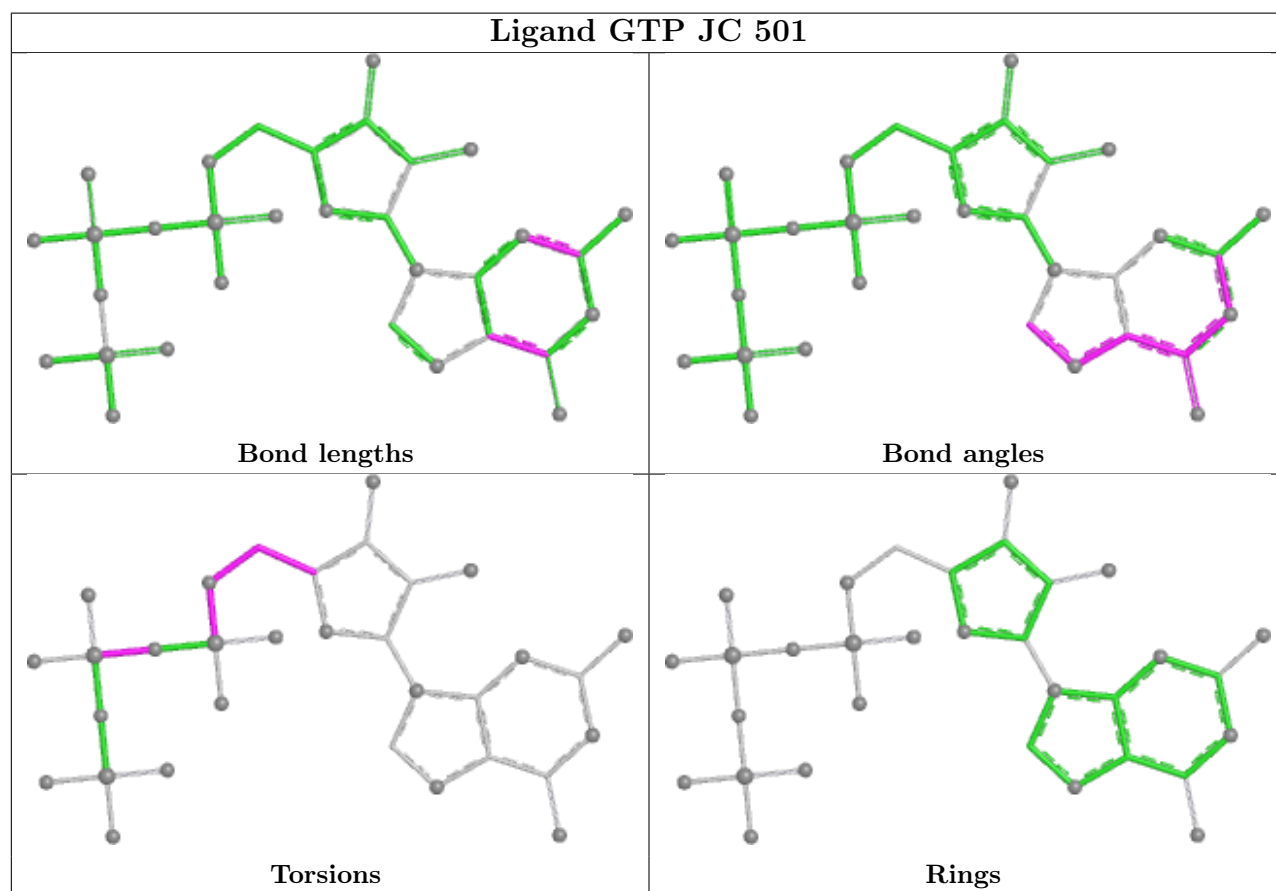
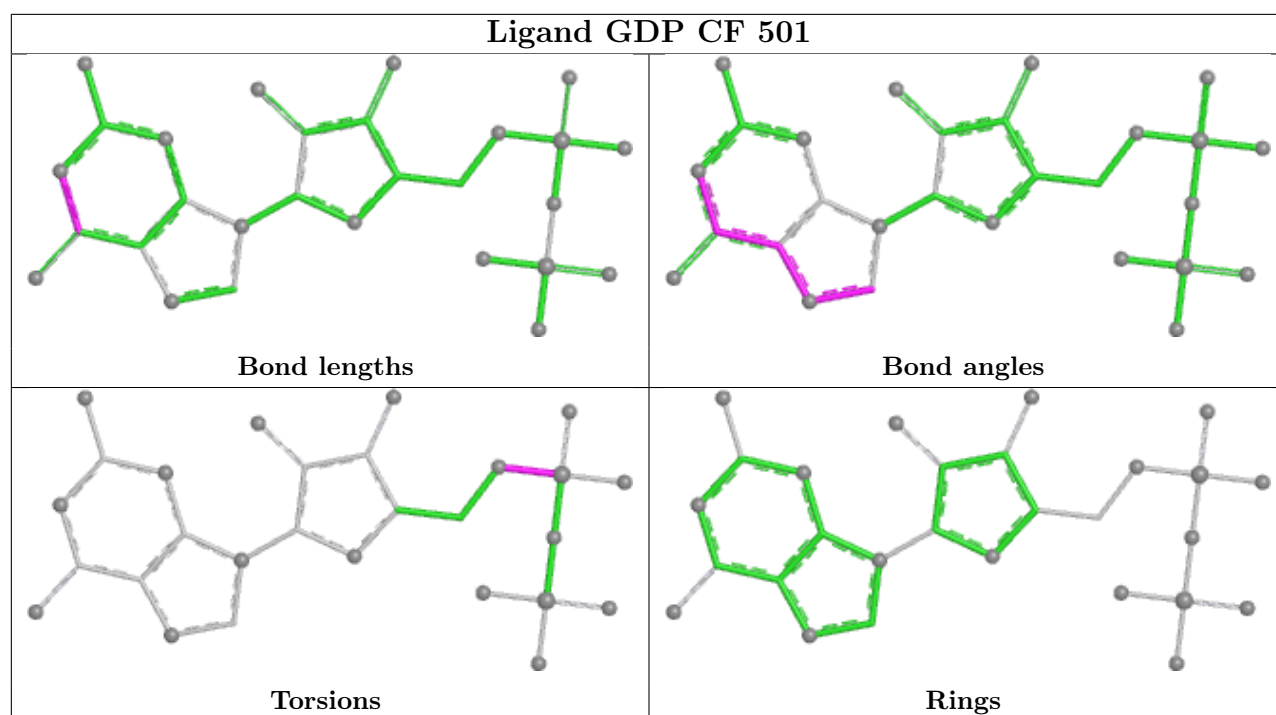


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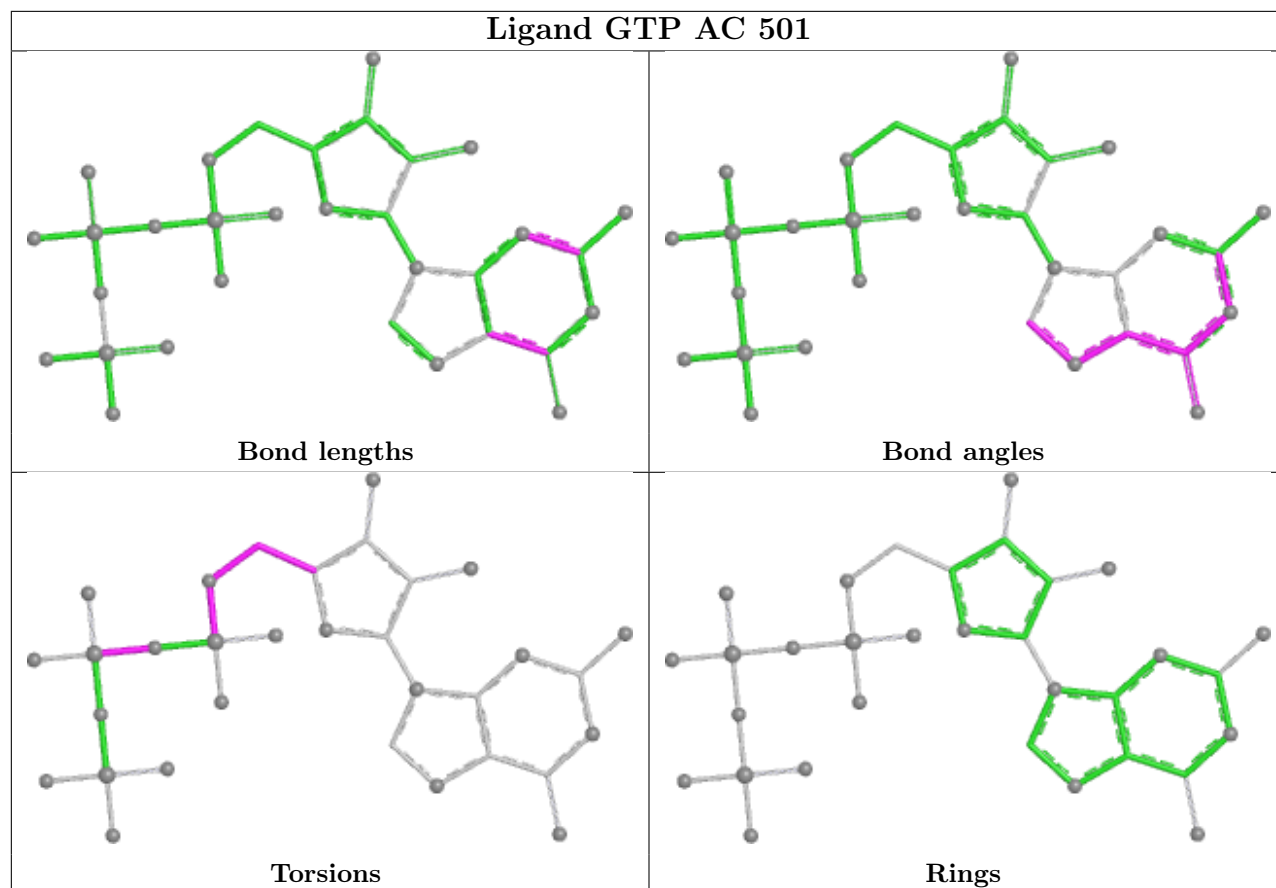


## Ligand GTP KA 501

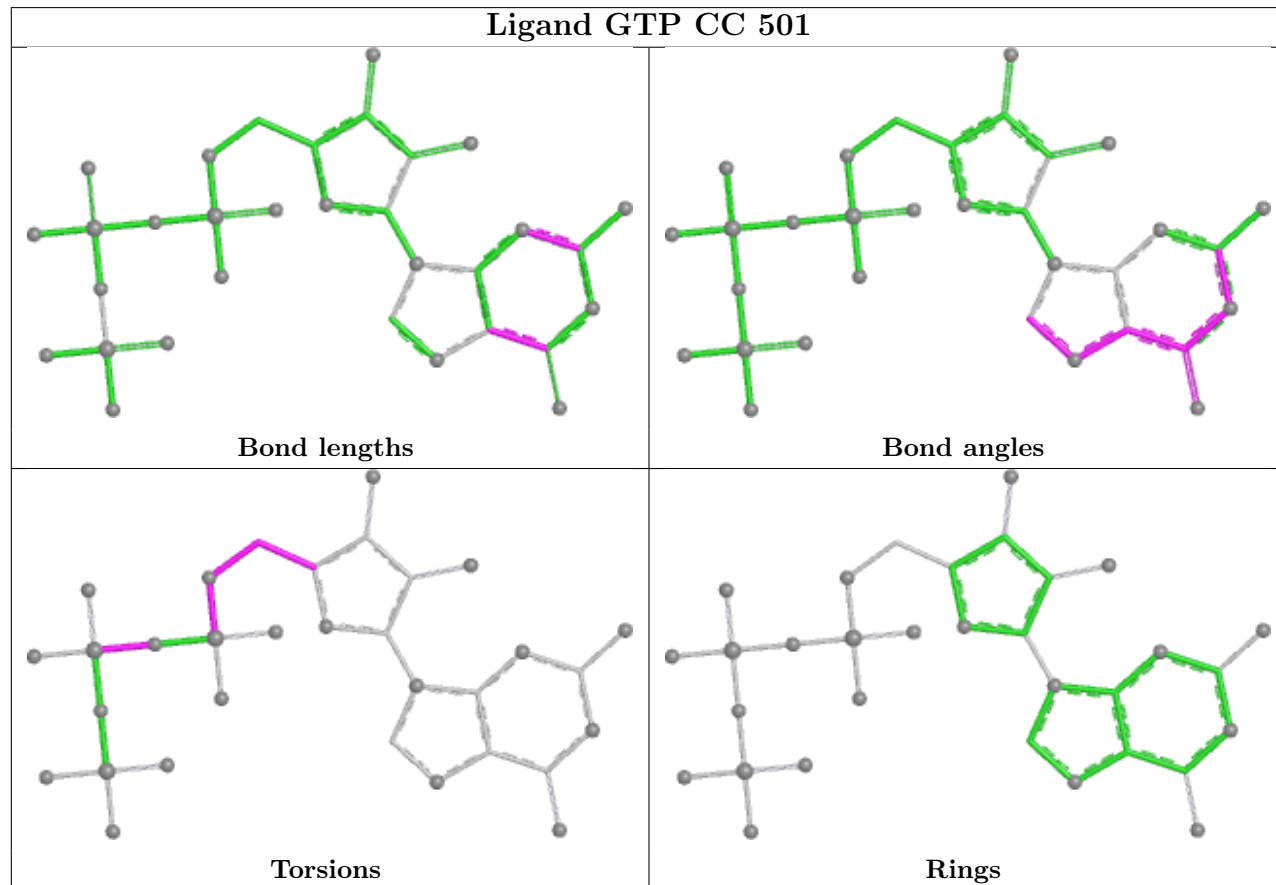




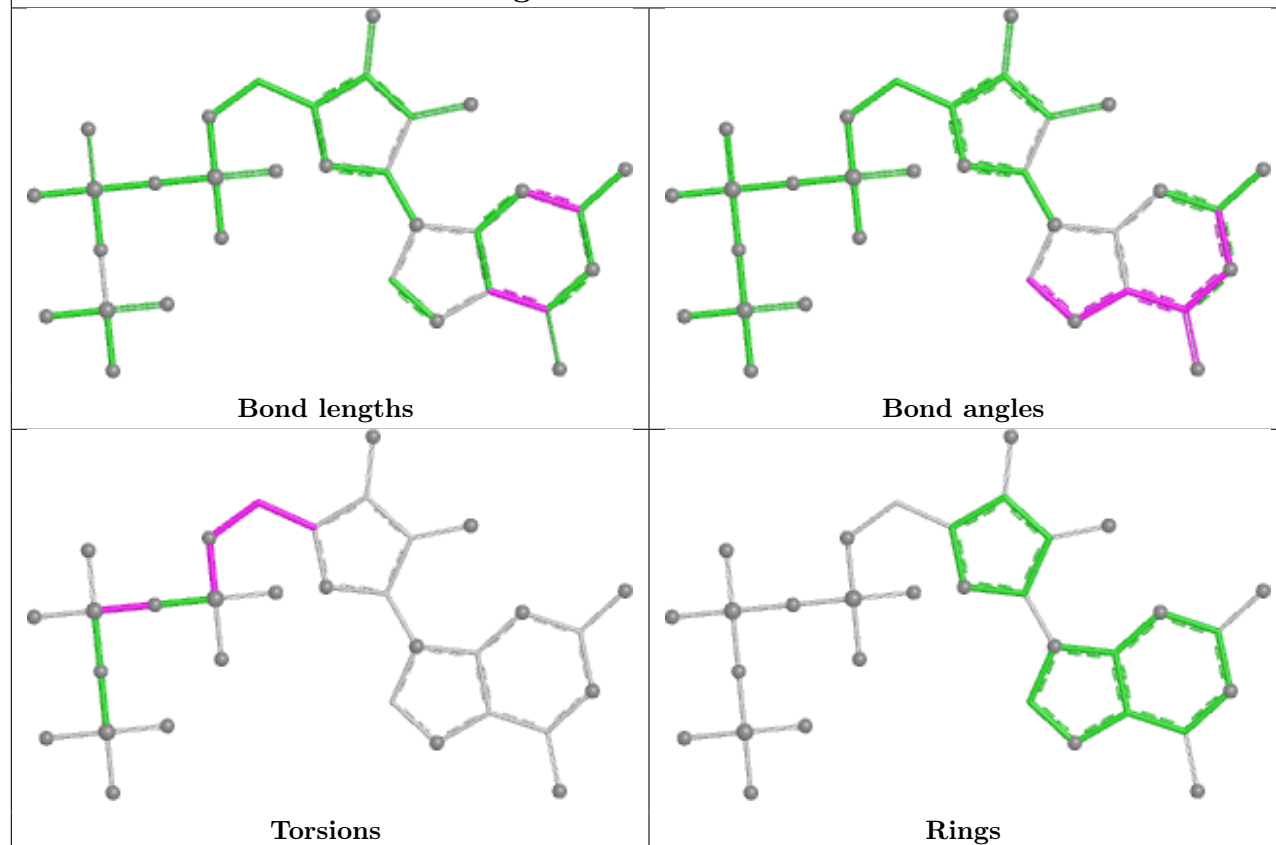
## Ligand GTP AC 501



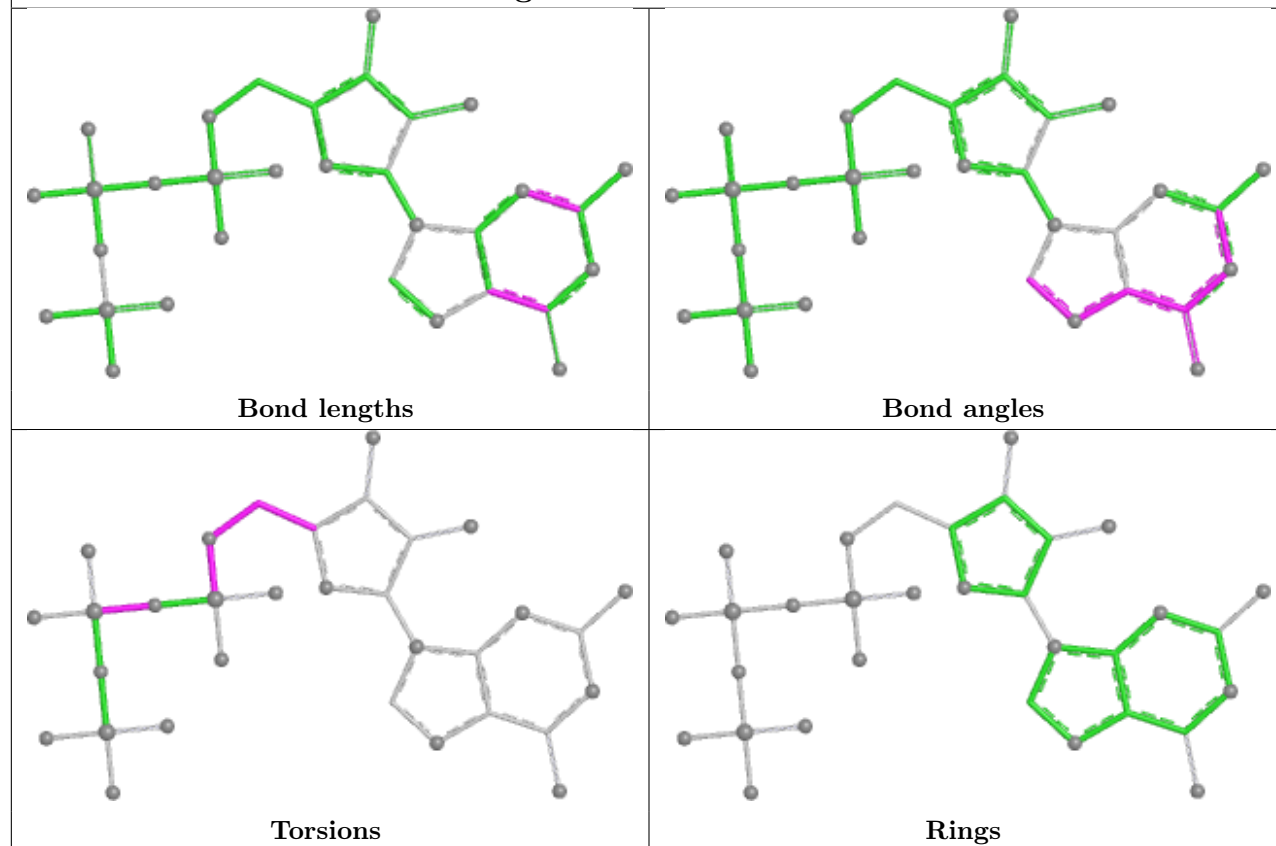
## Ligand GTP CC 501

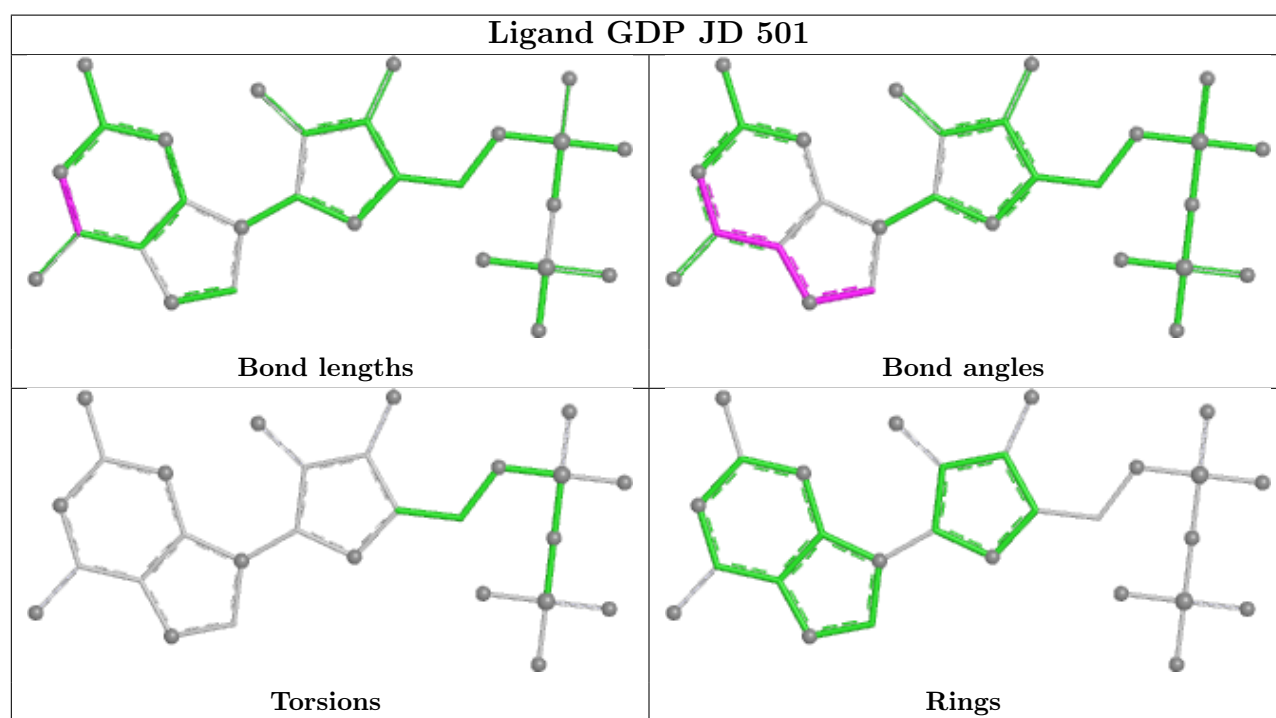
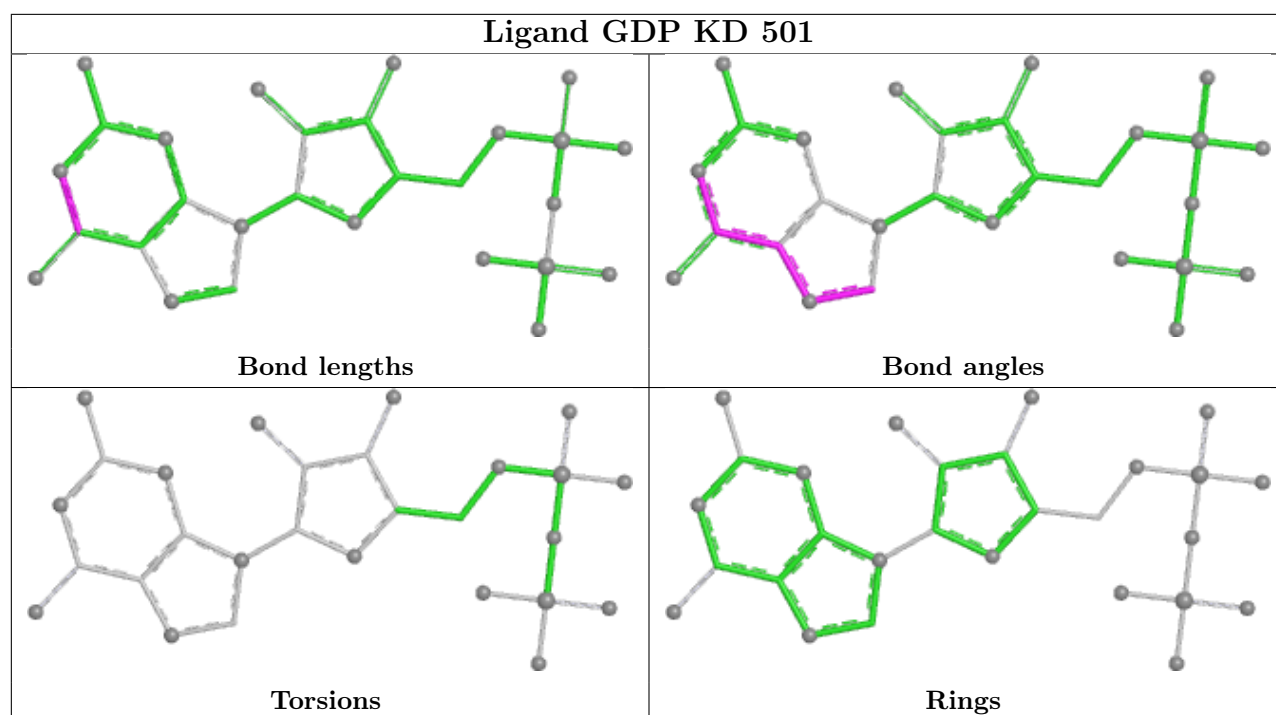


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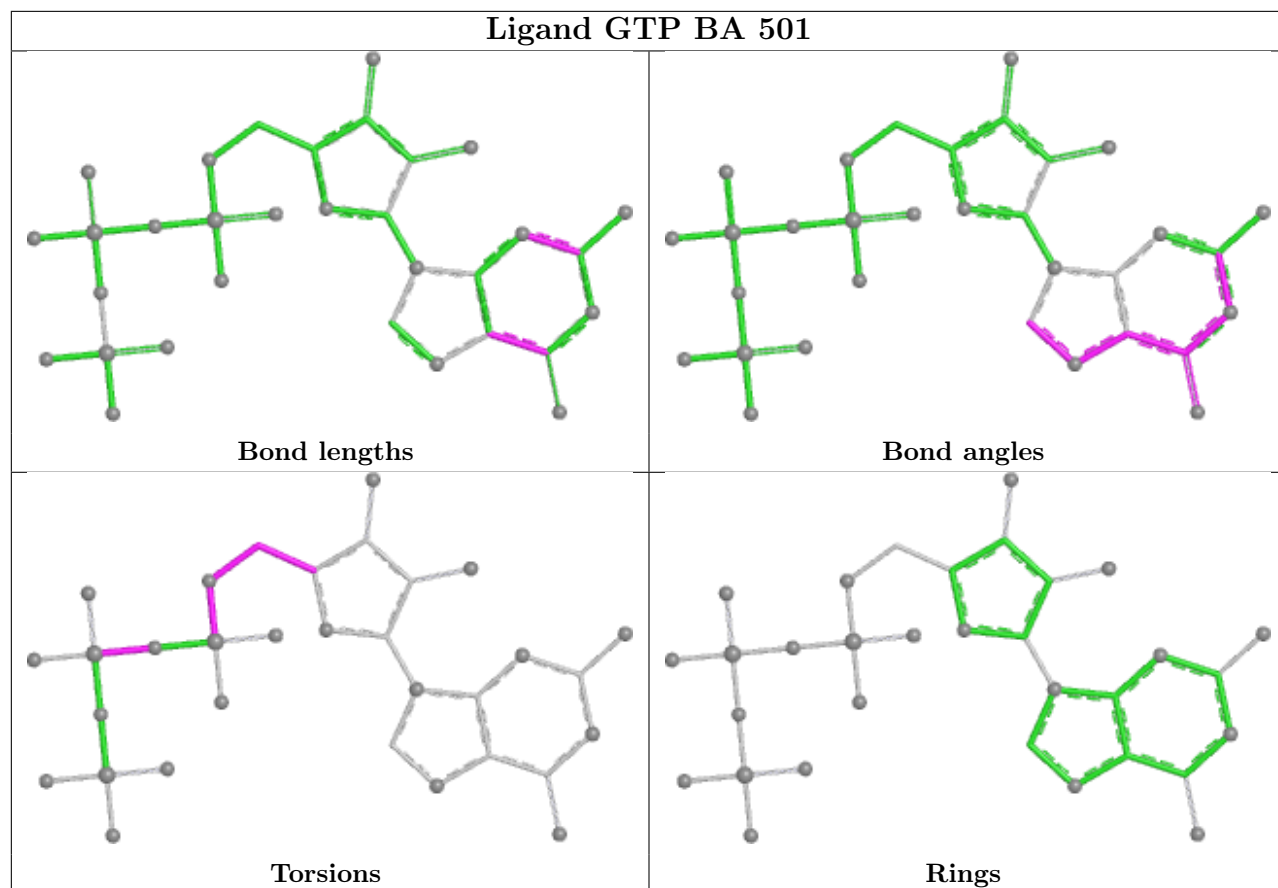


## Ligand GTP ME 501

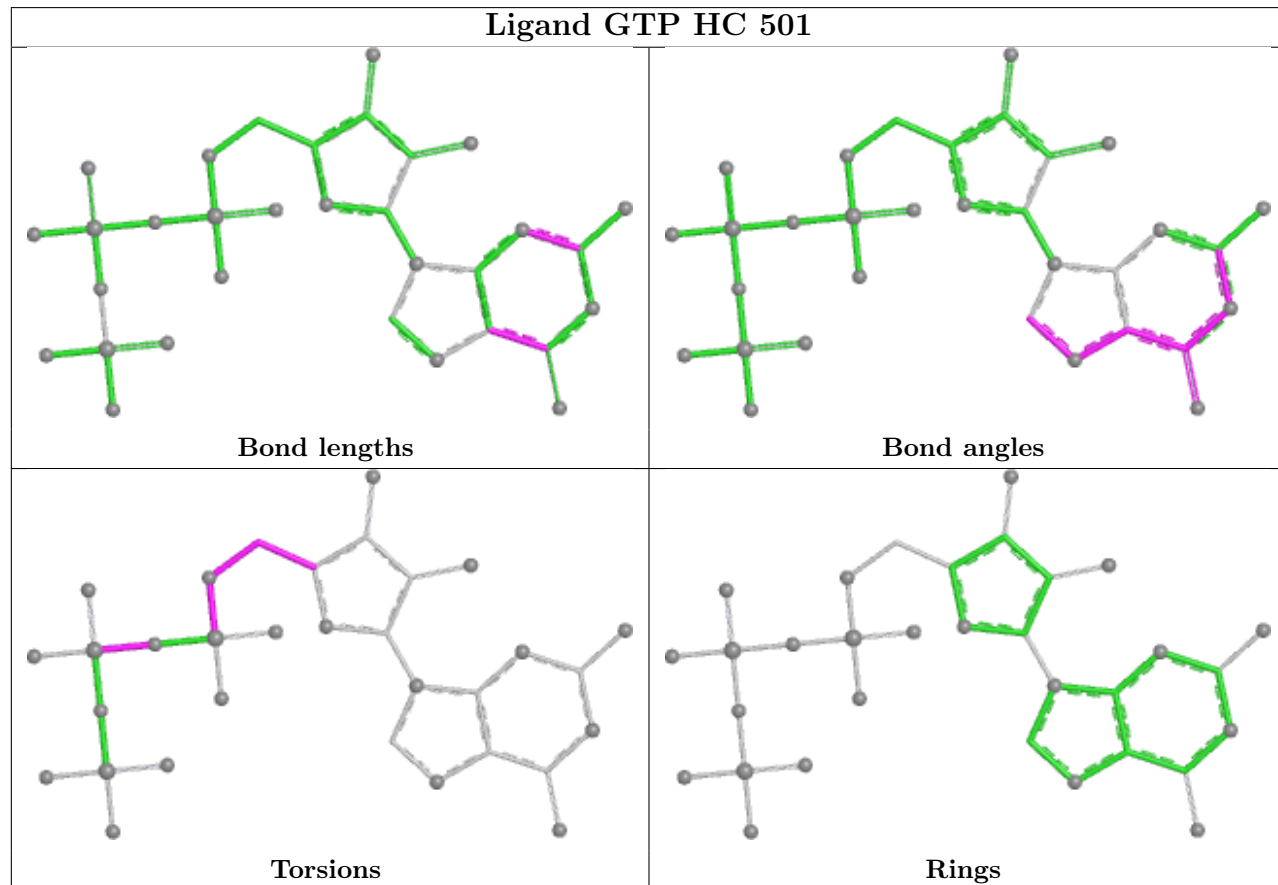


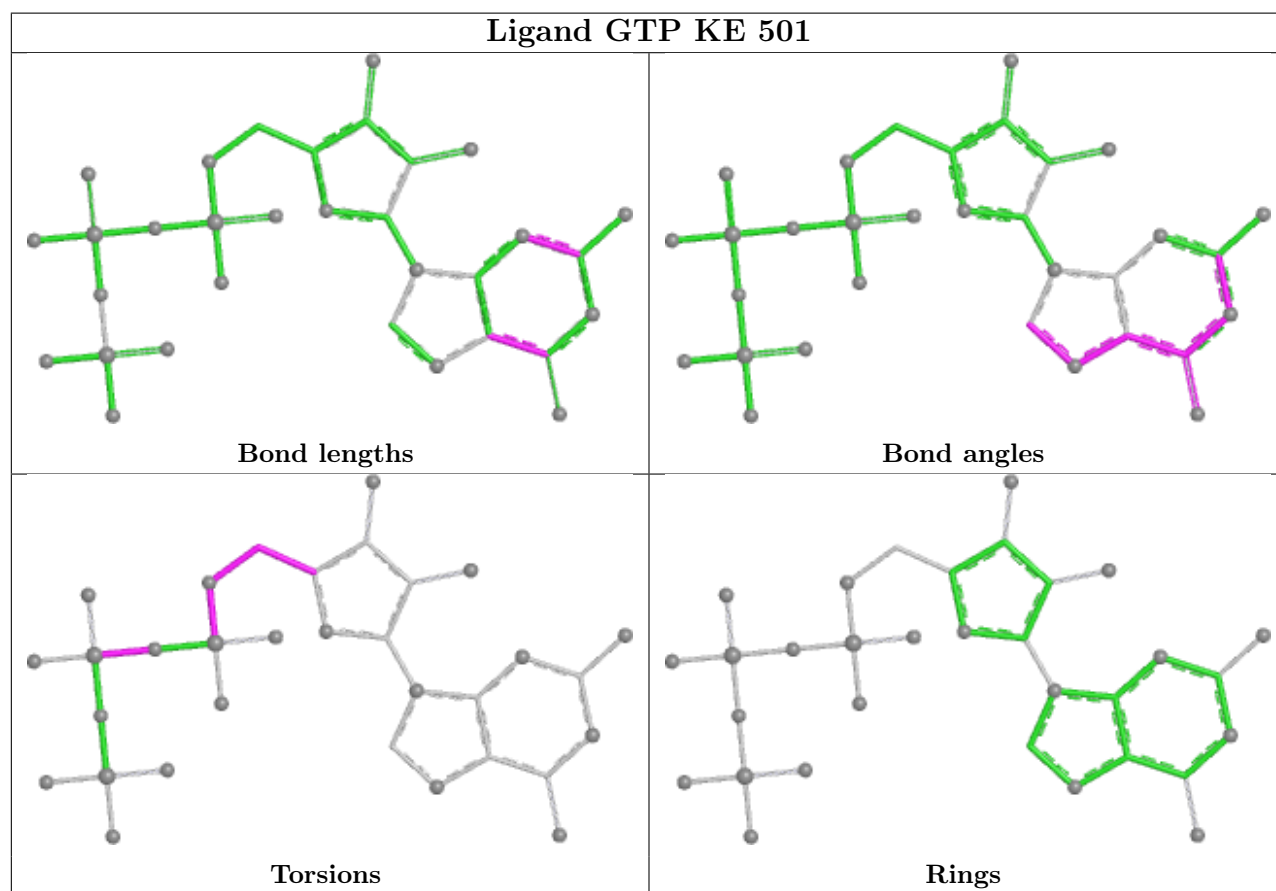
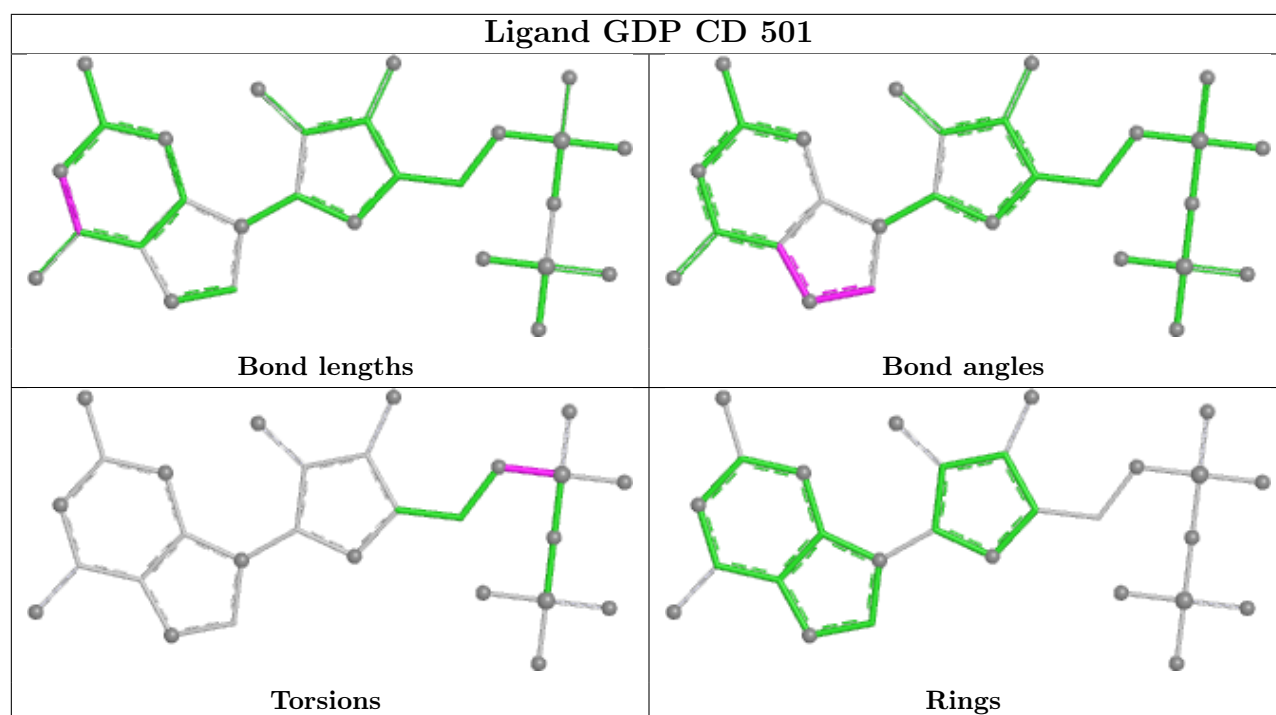


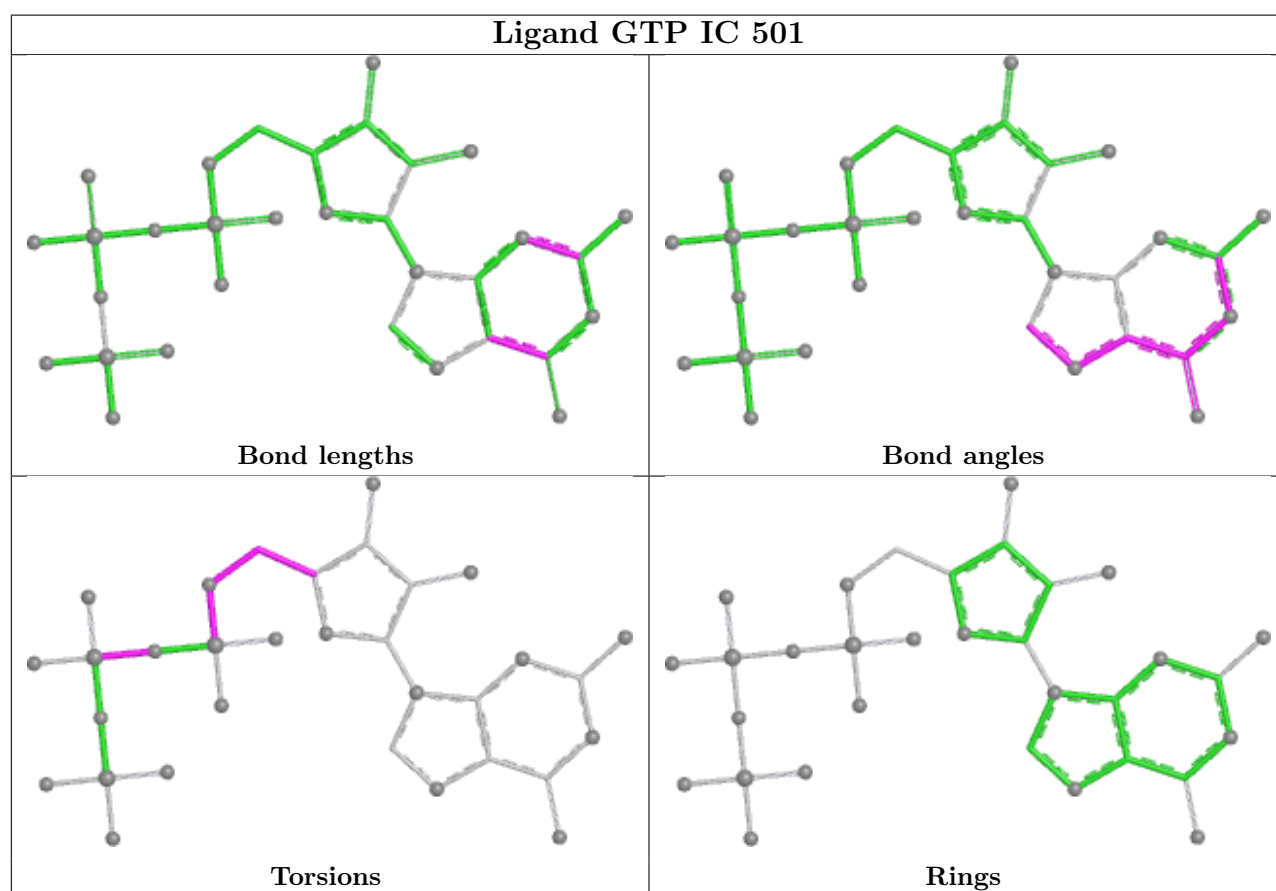
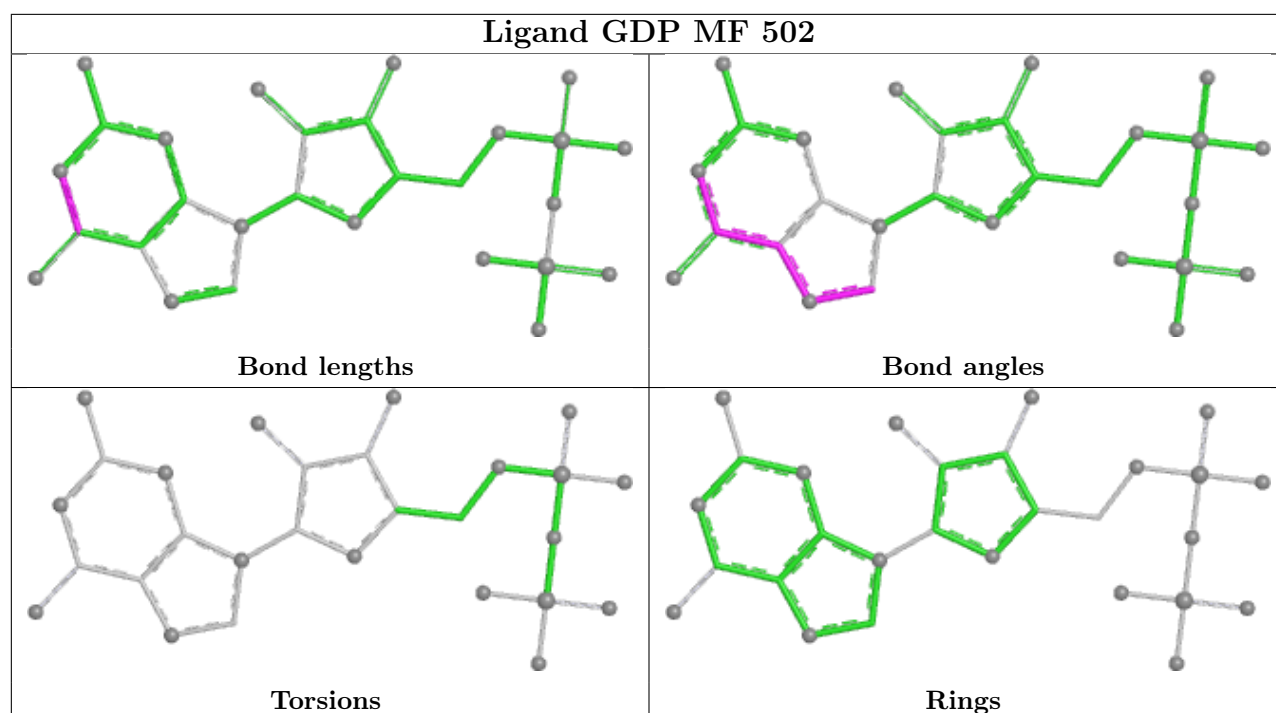
## Ligand GTP BA 501



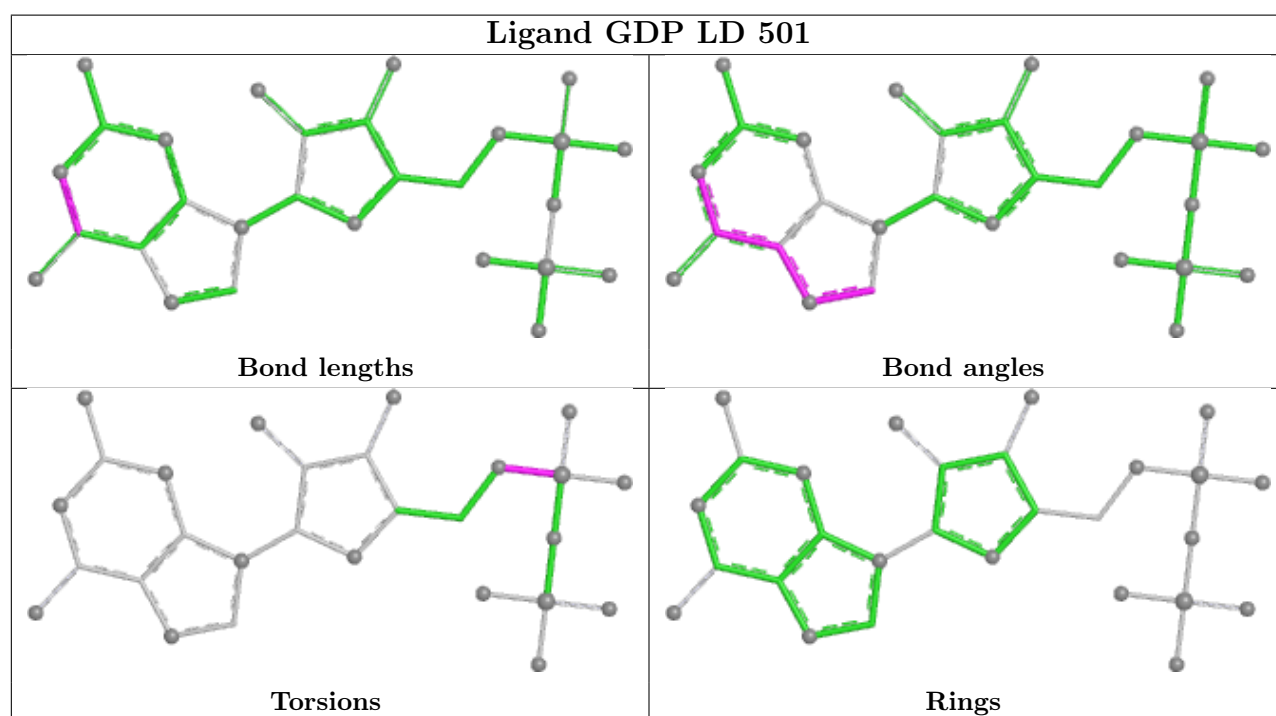
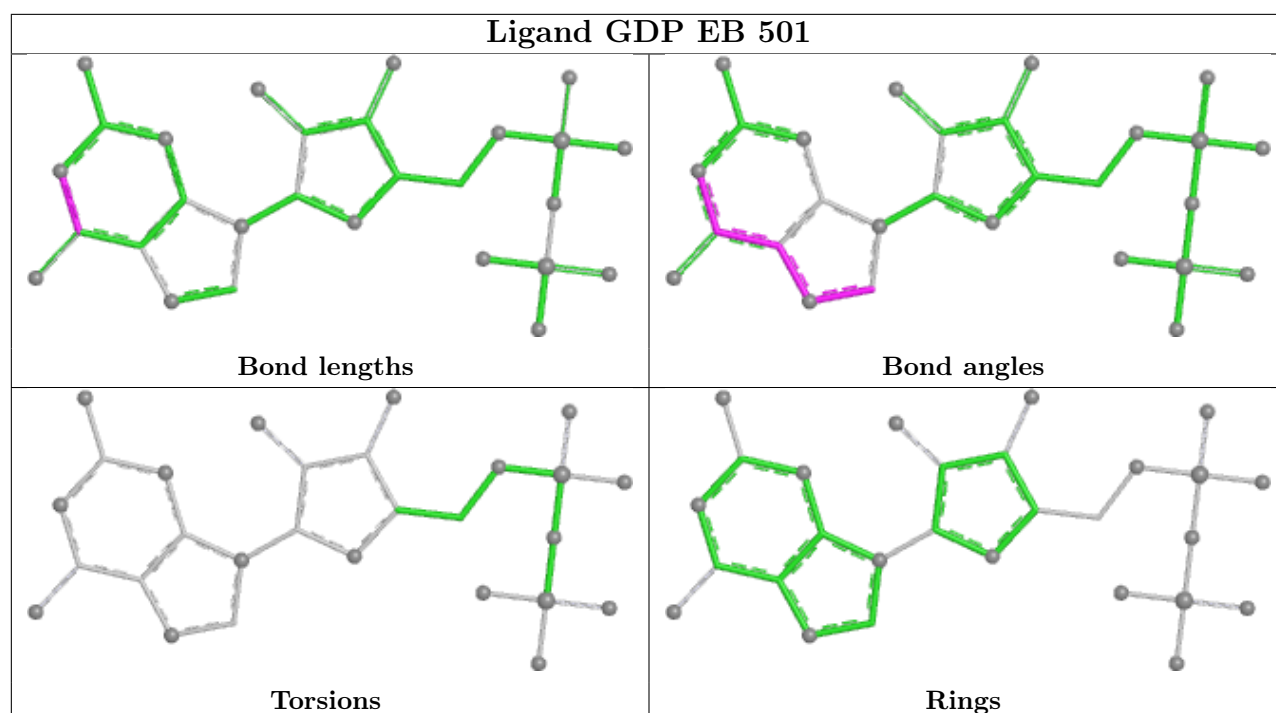
## Ligand GTP HC 501

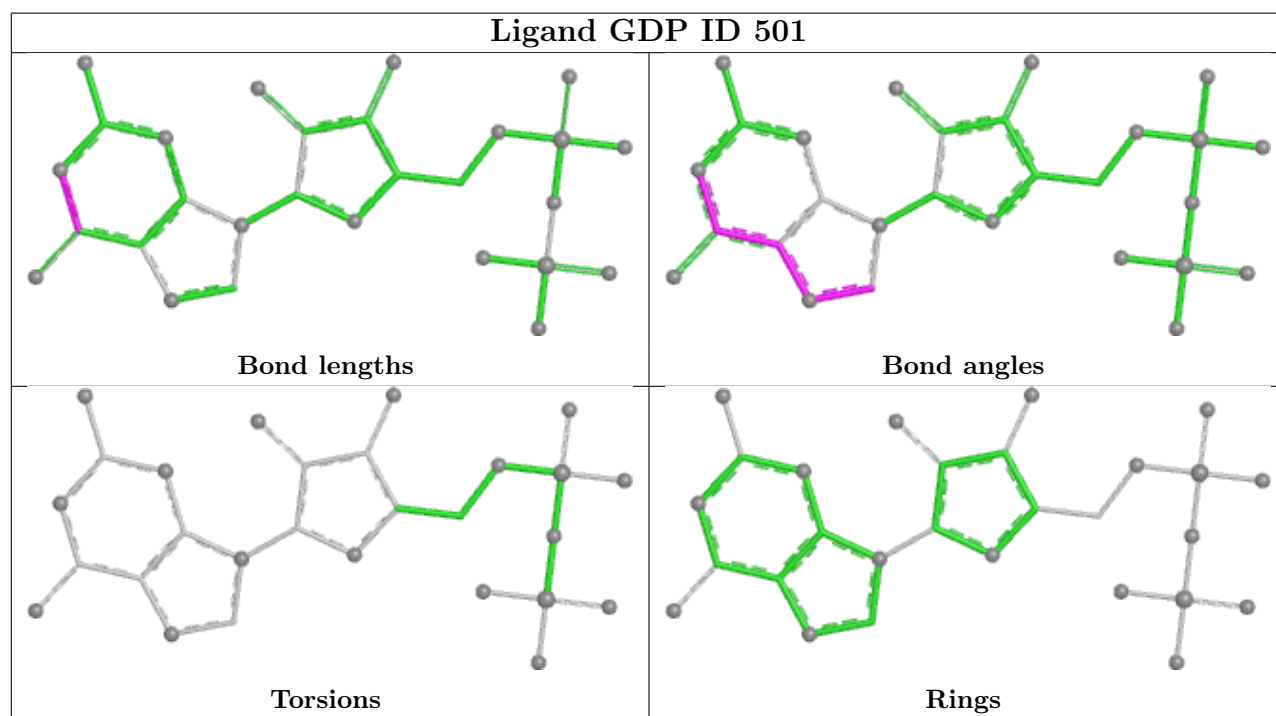
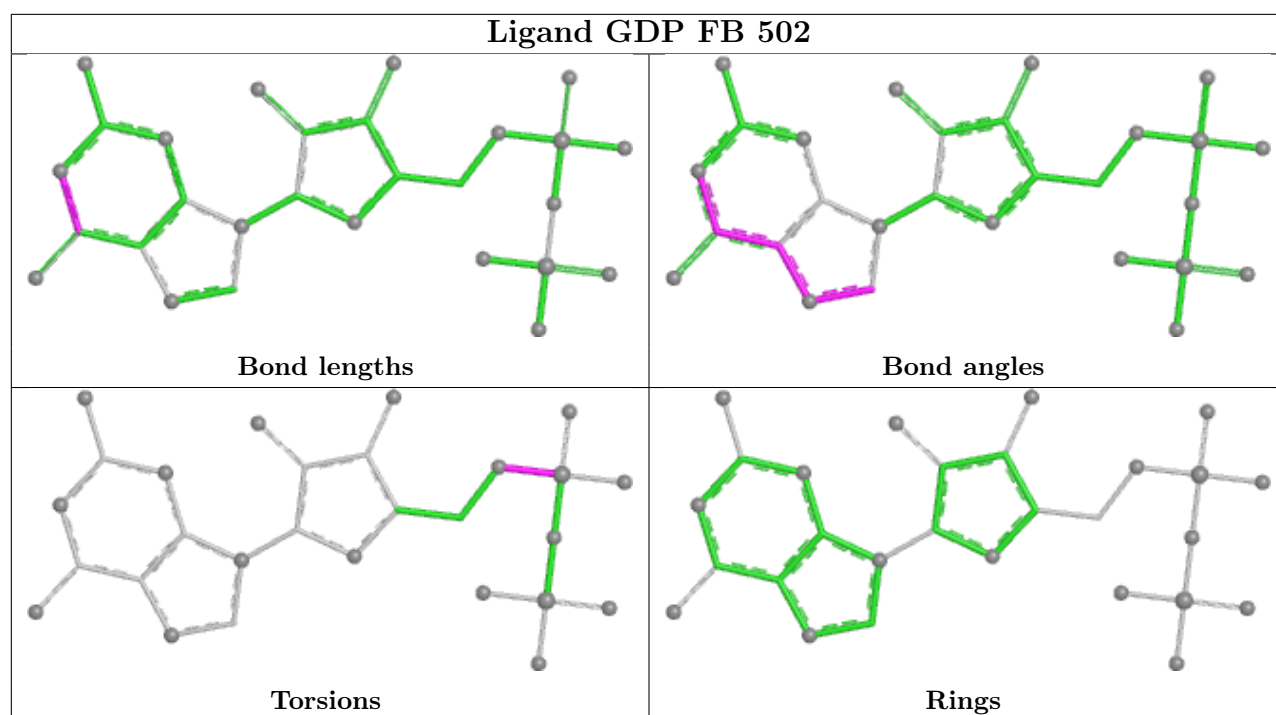


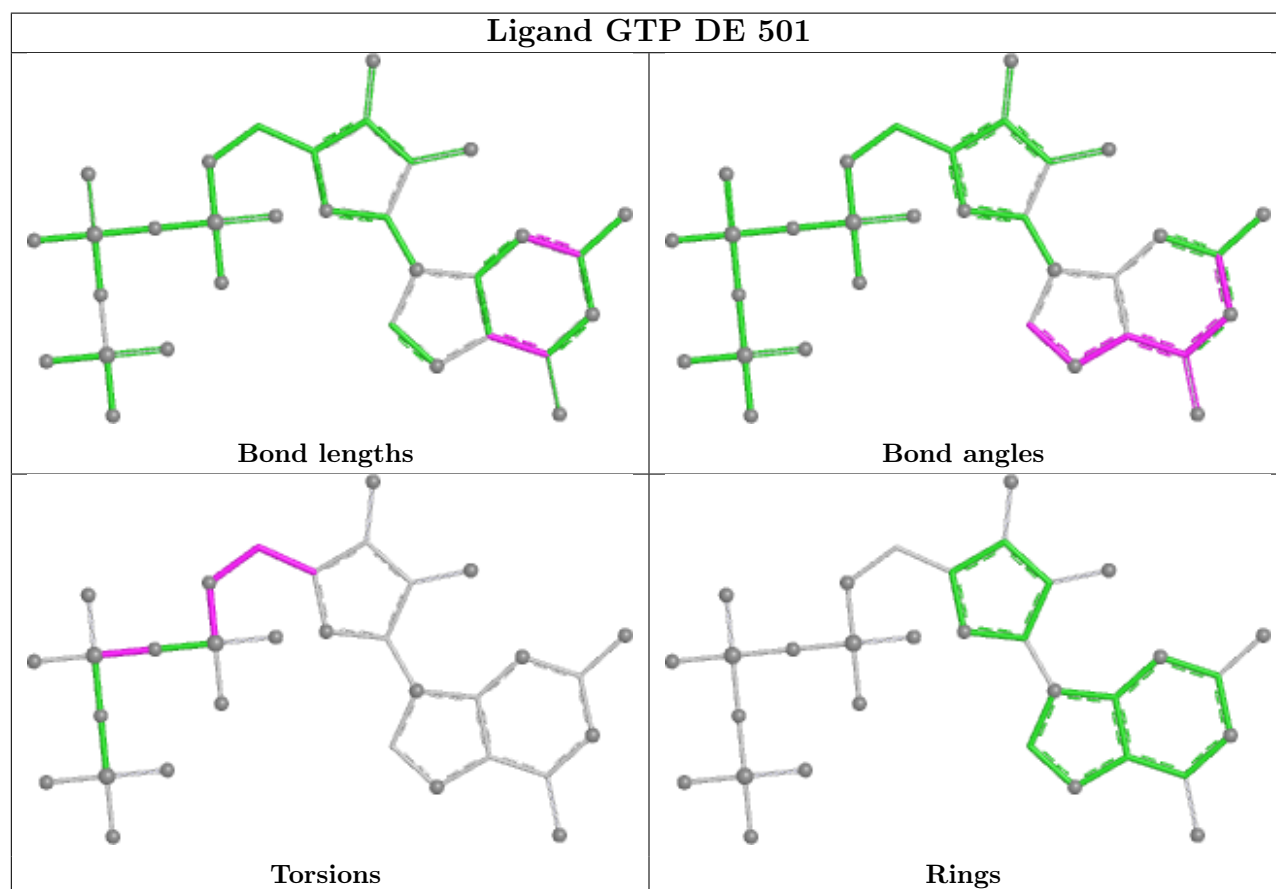
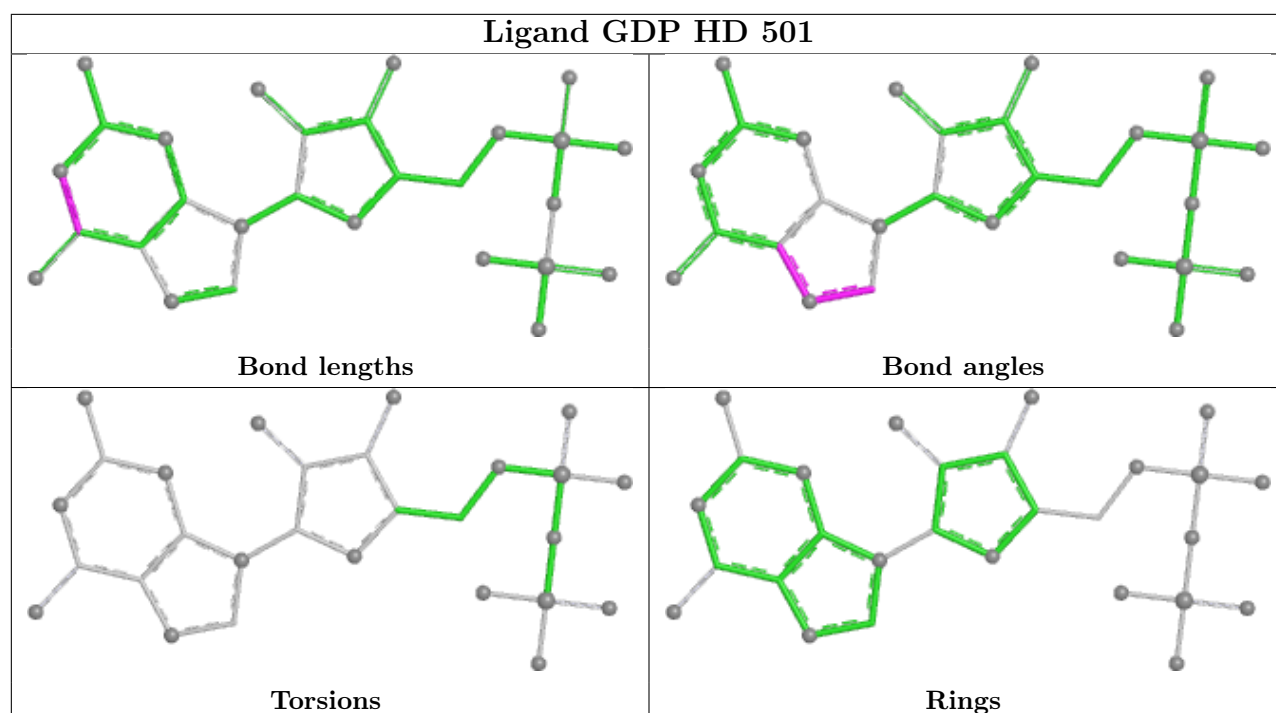


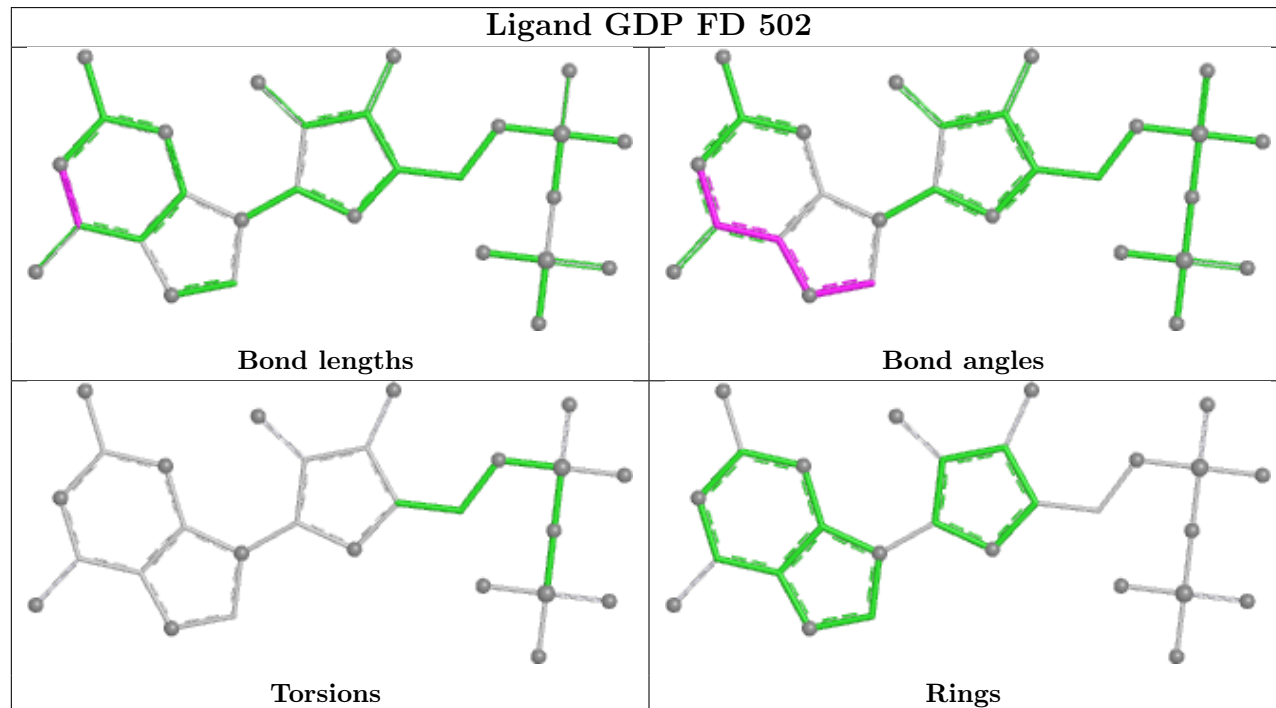
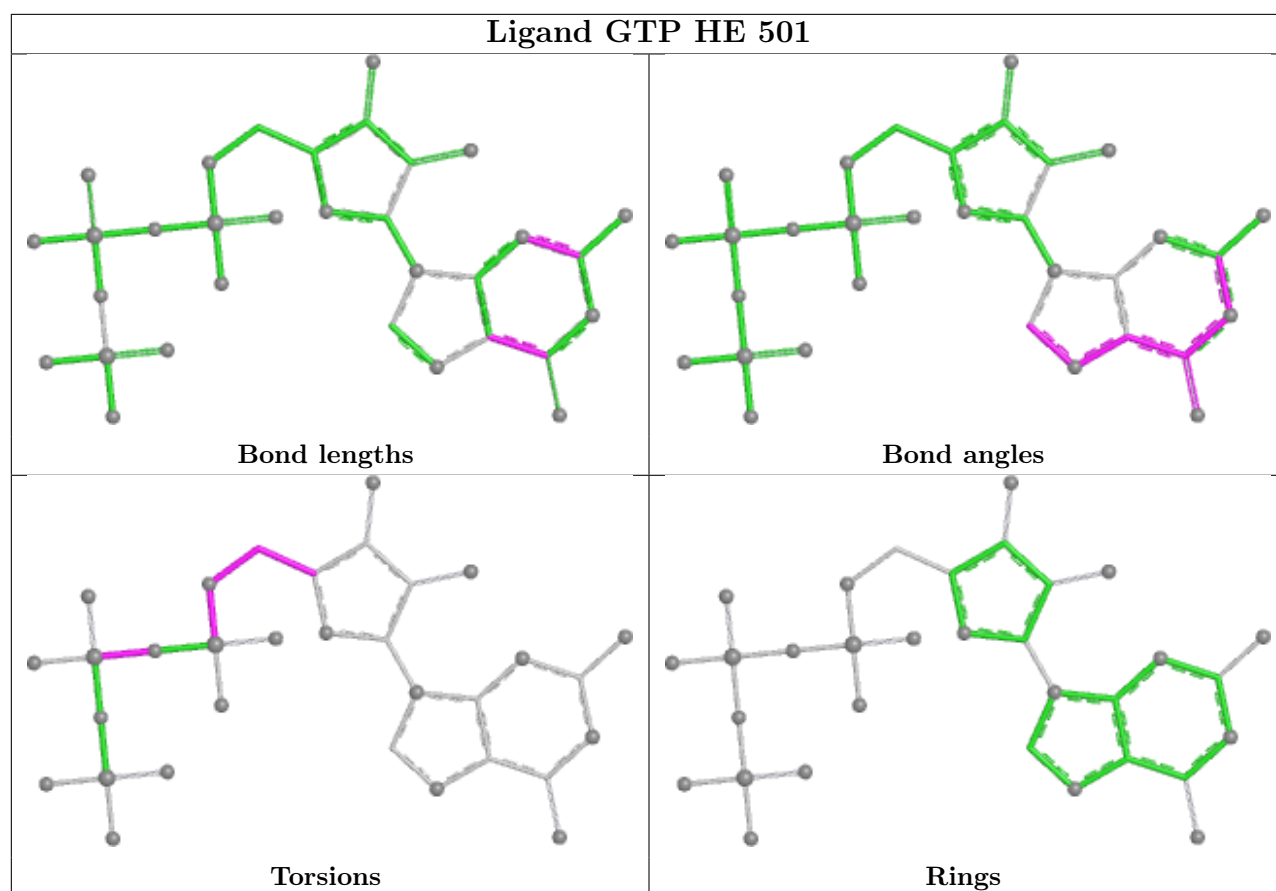


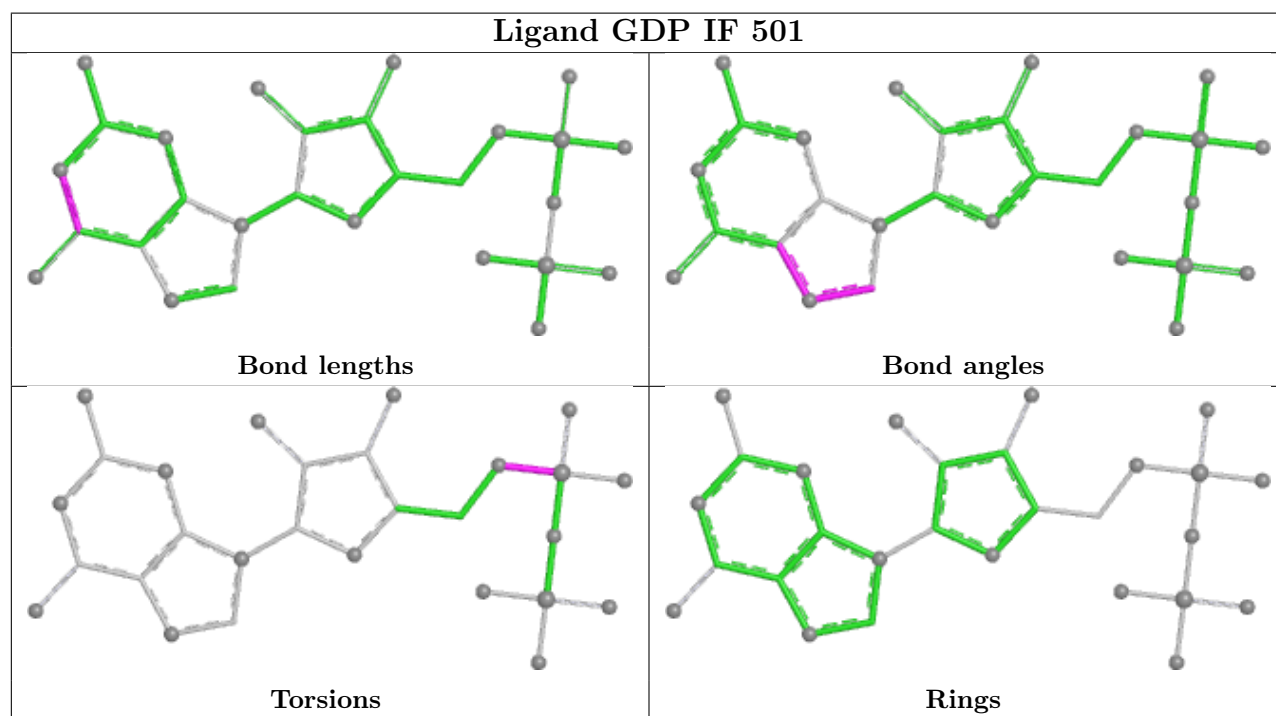
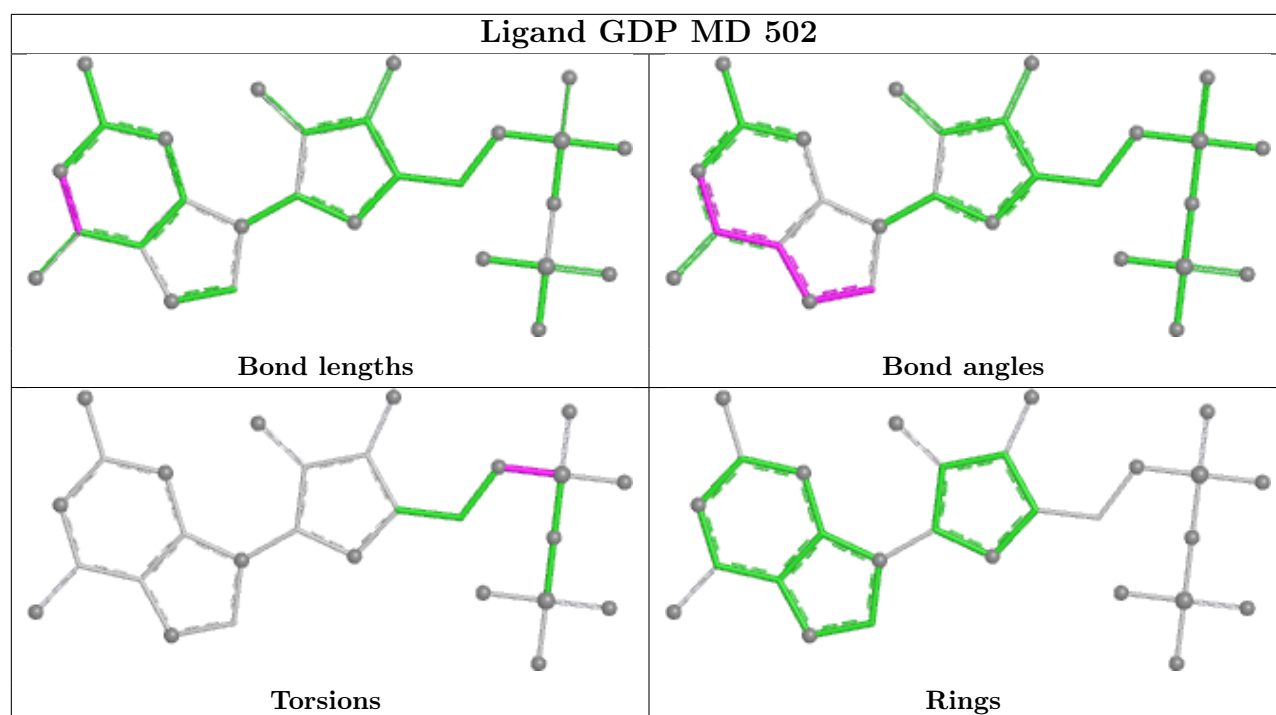


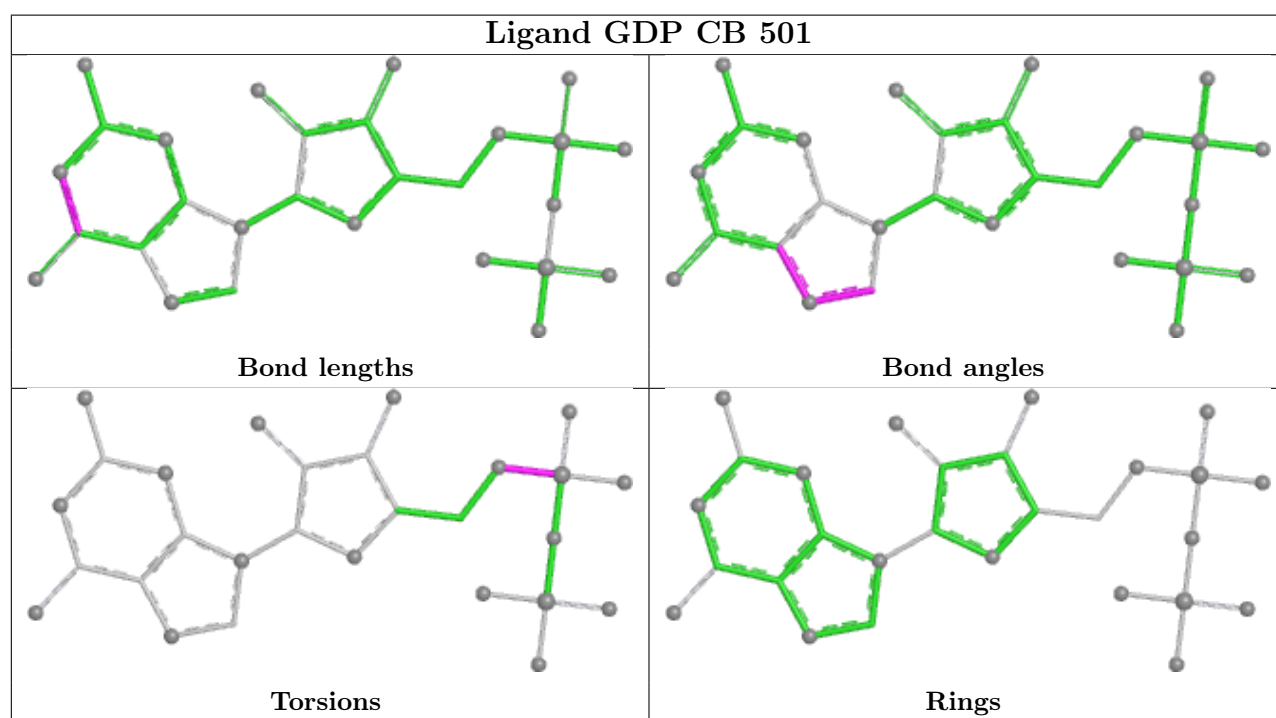
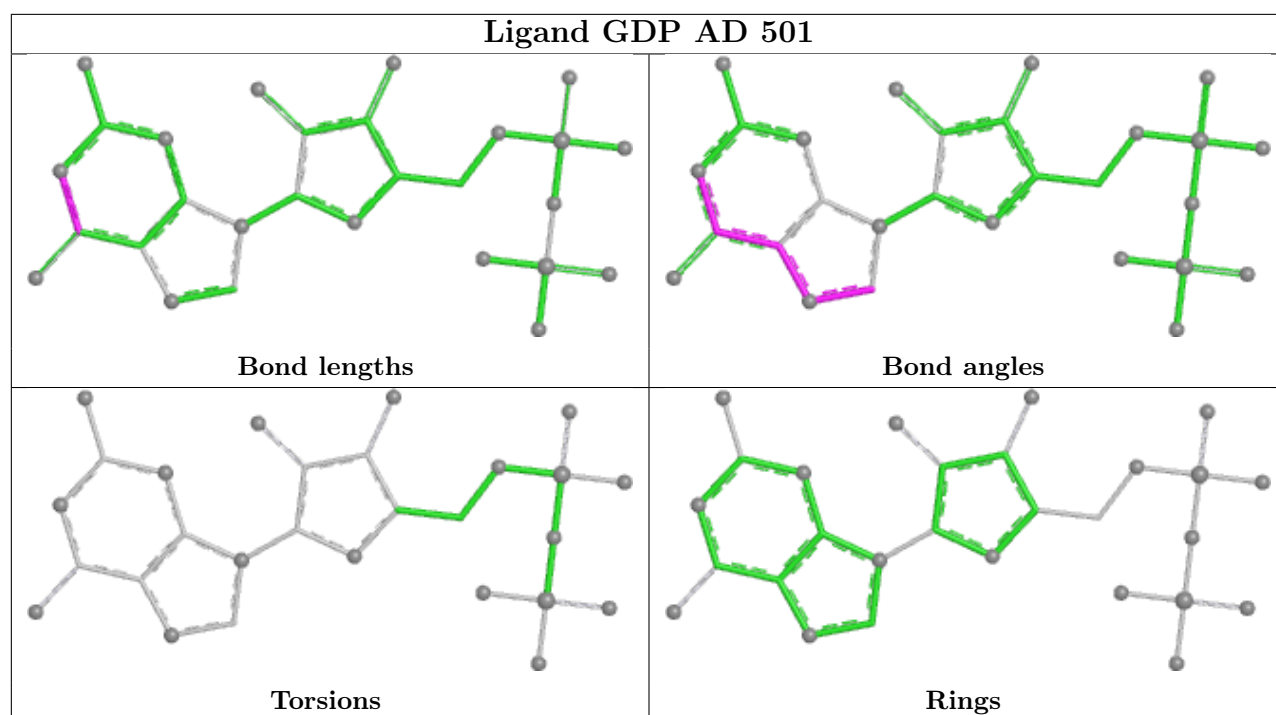


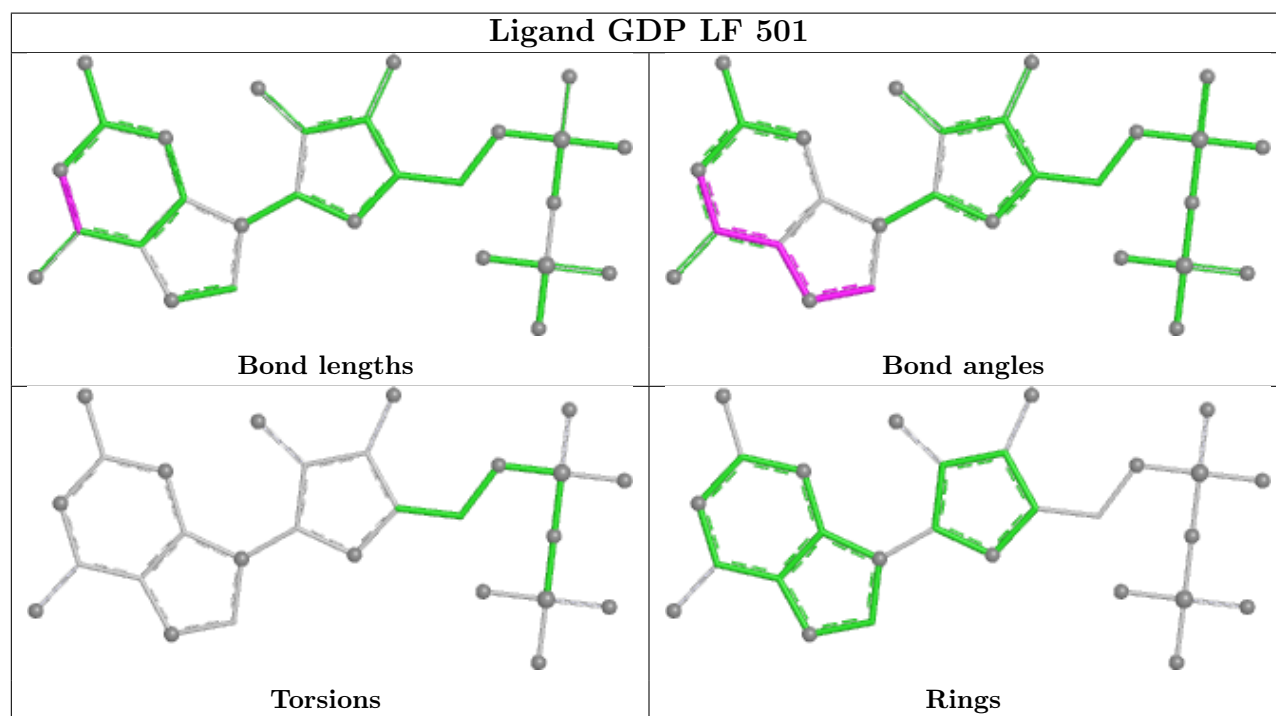
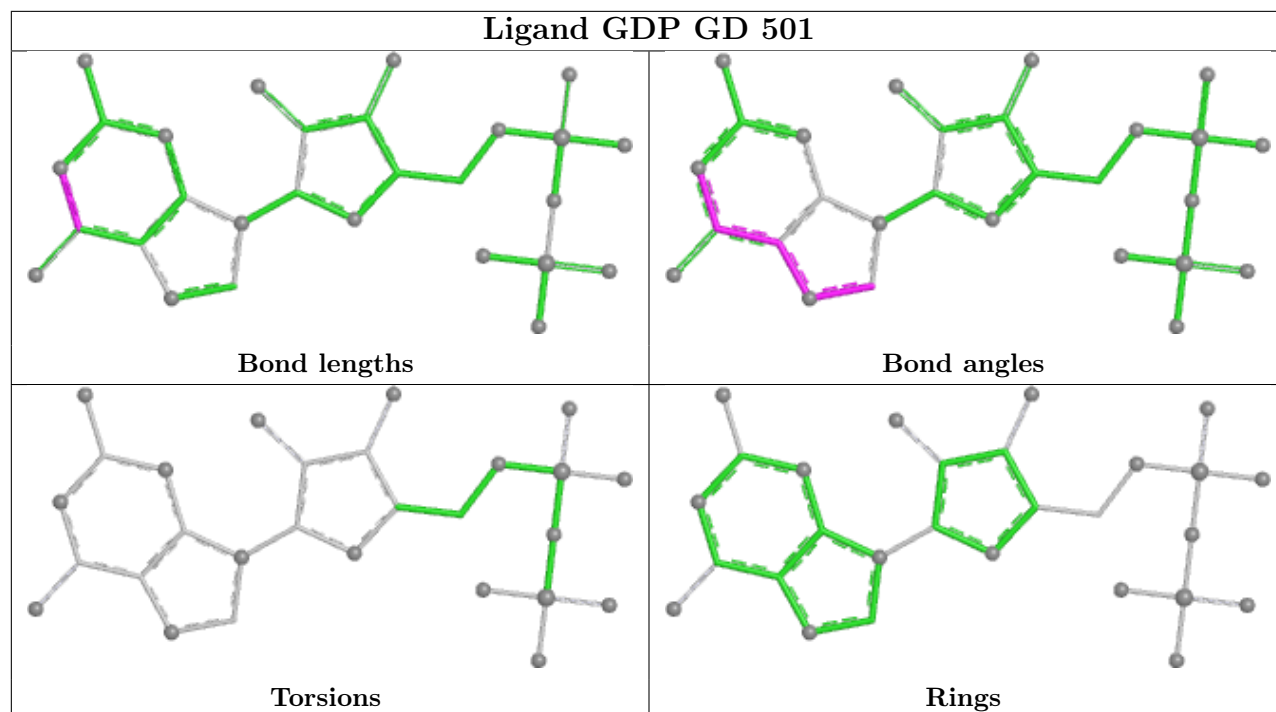




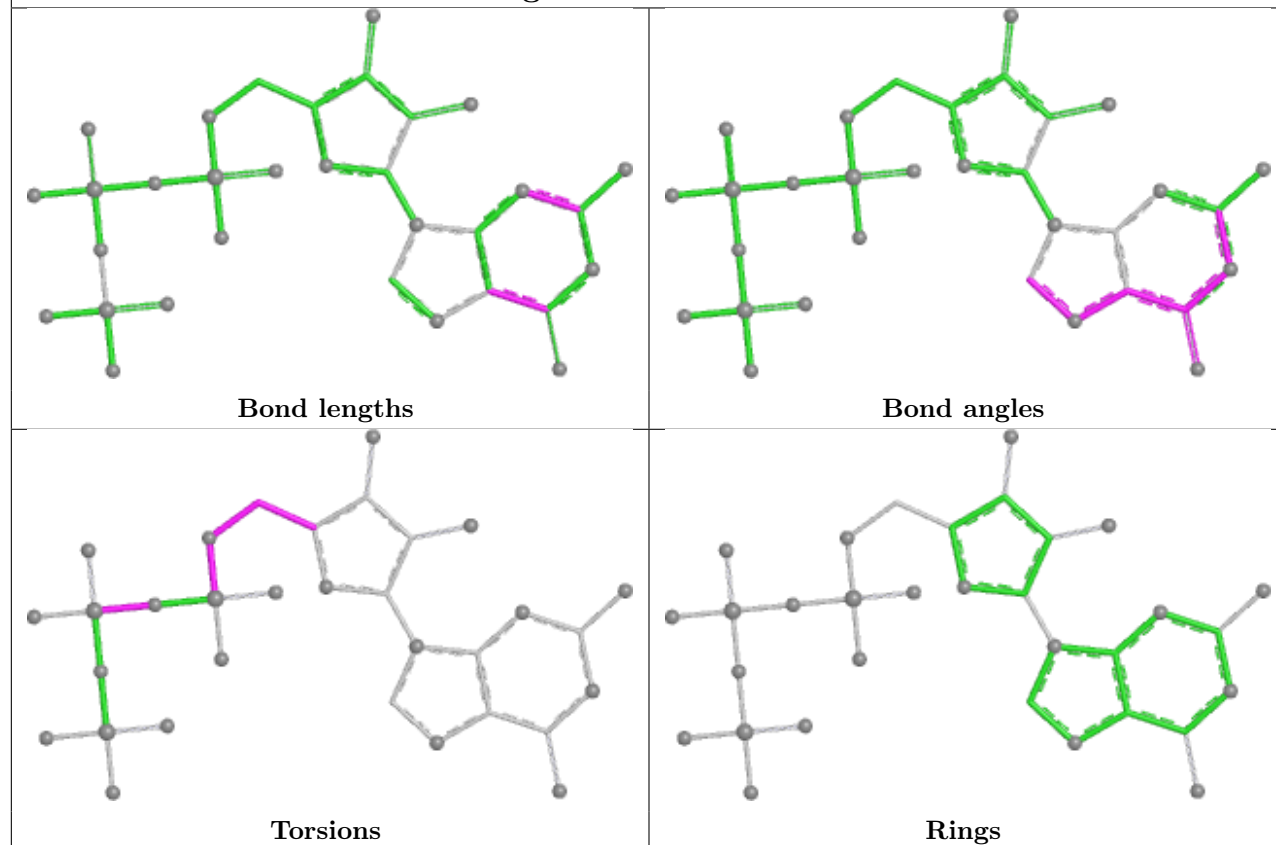




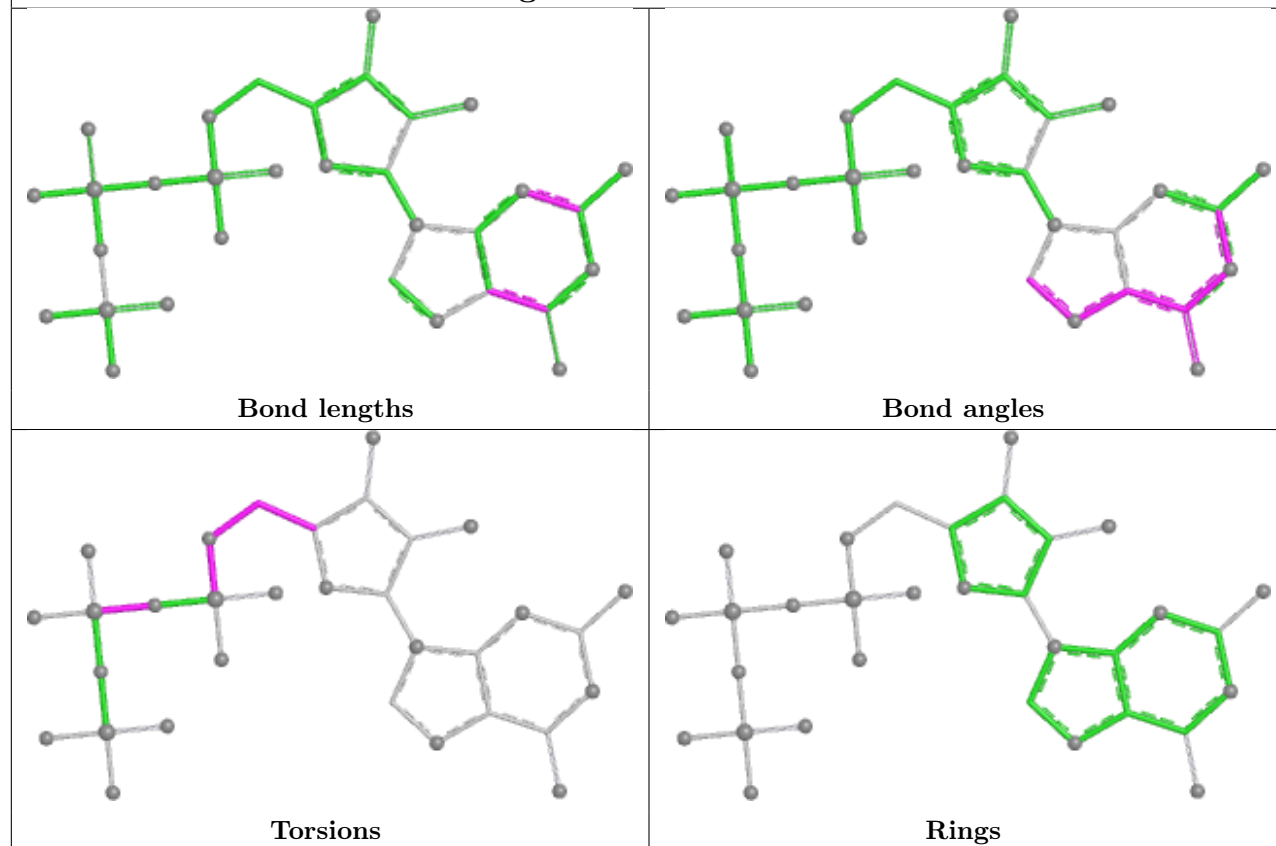




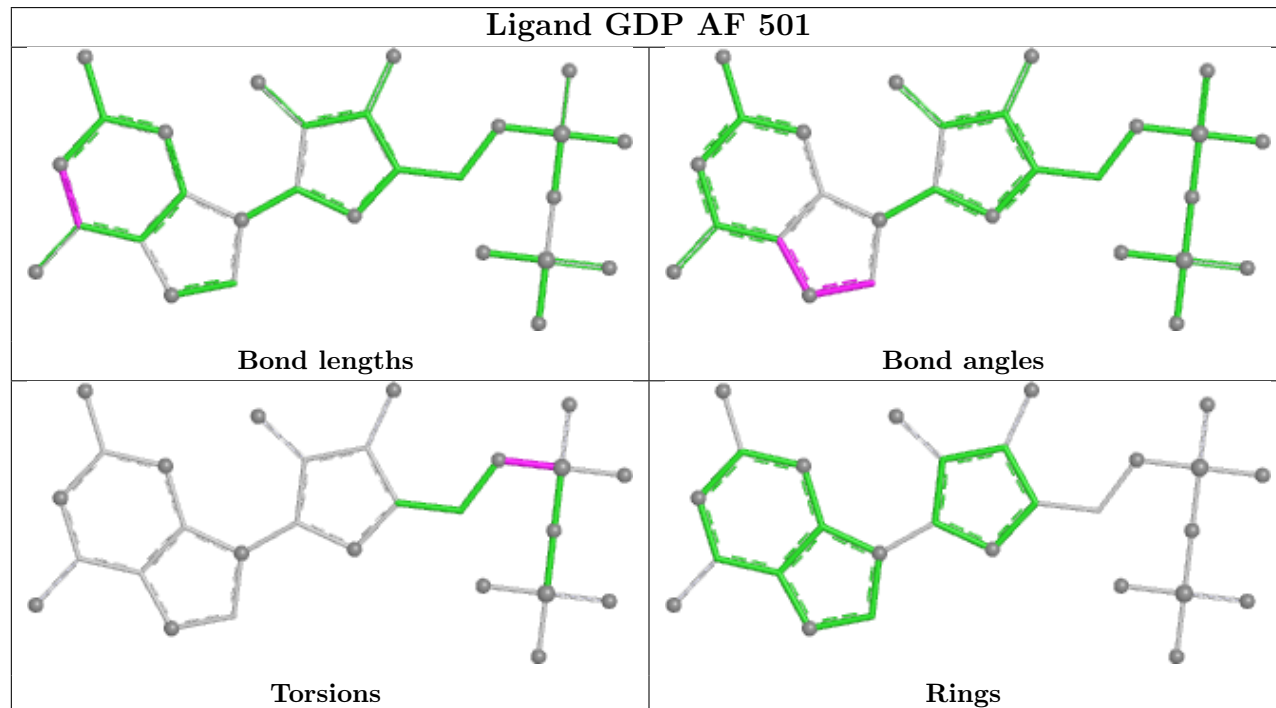
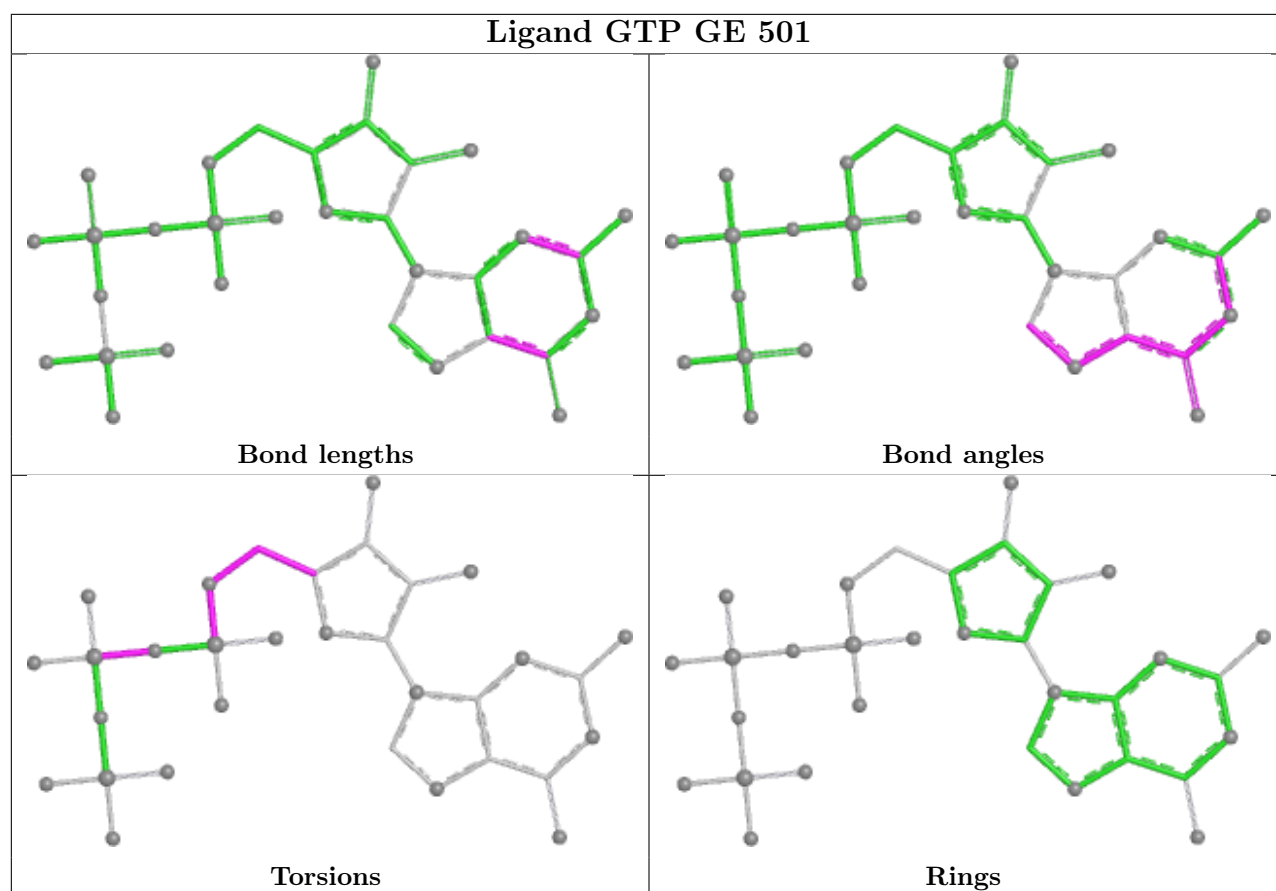
## Ligand GTP JE 501

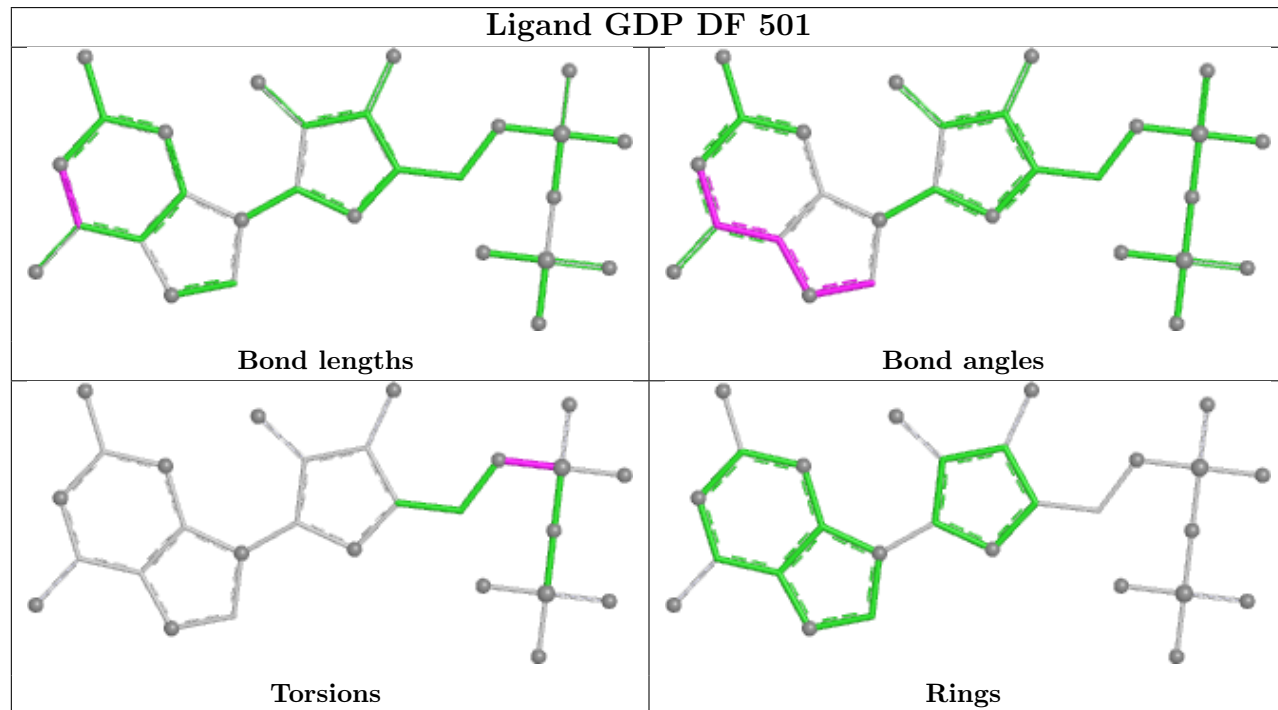
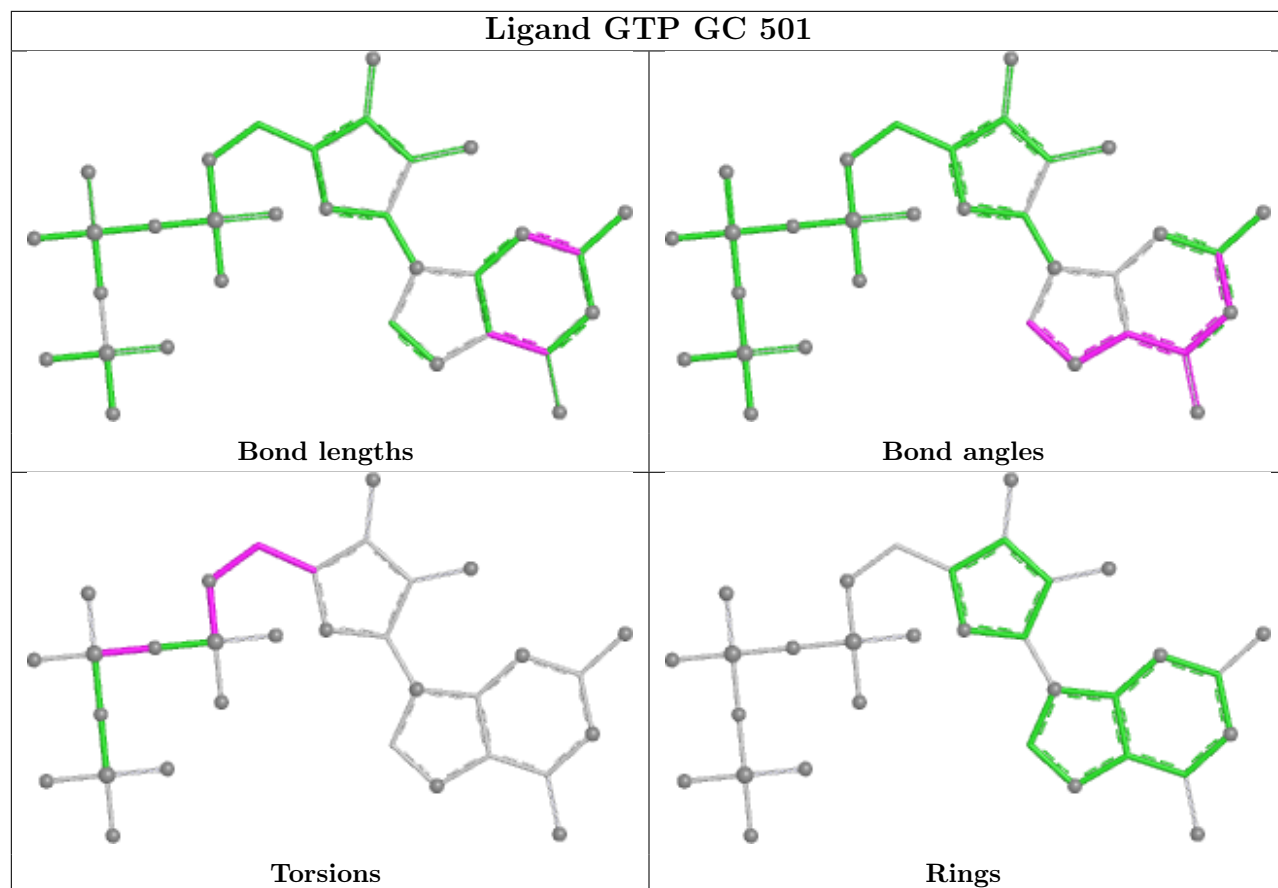


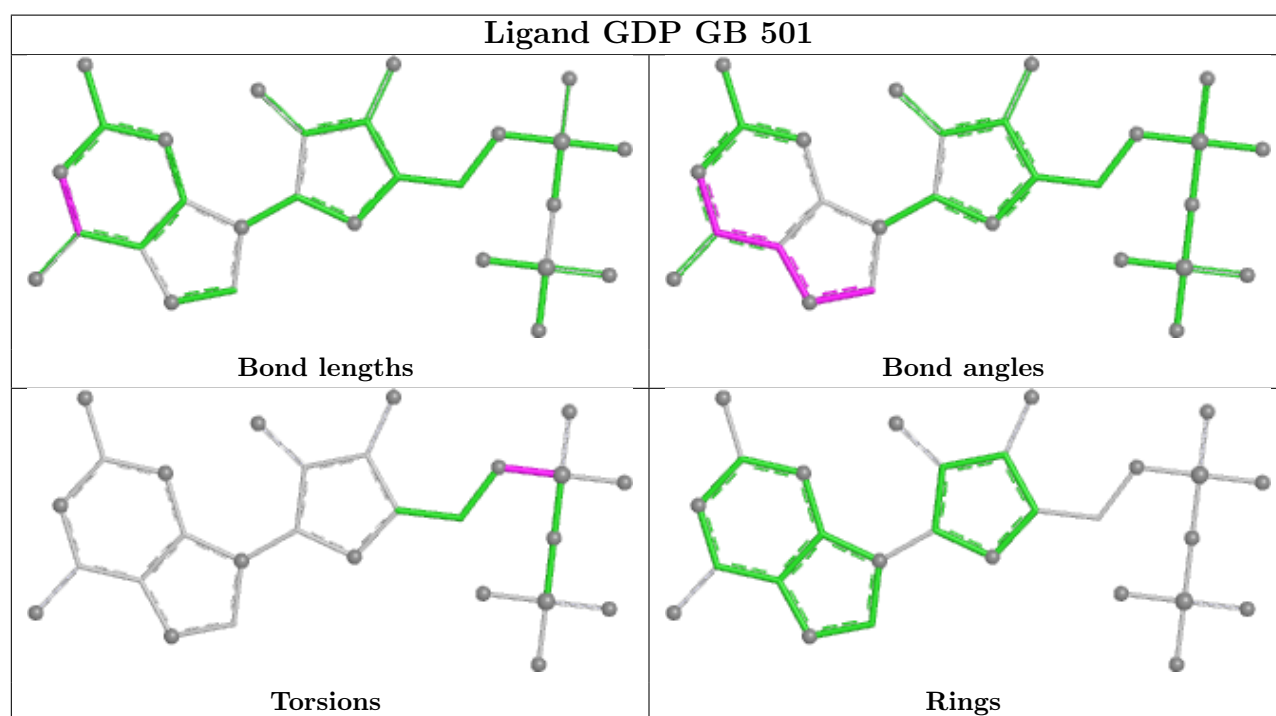
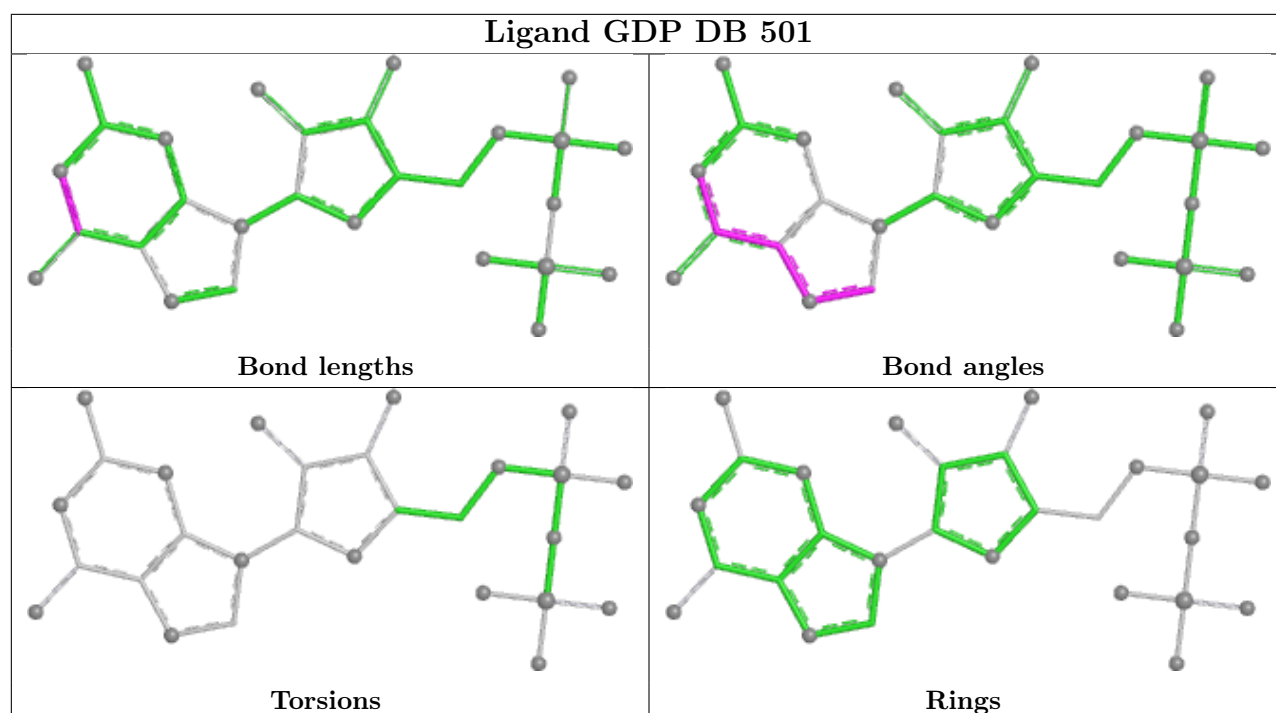
## Ligand GTP BE 501



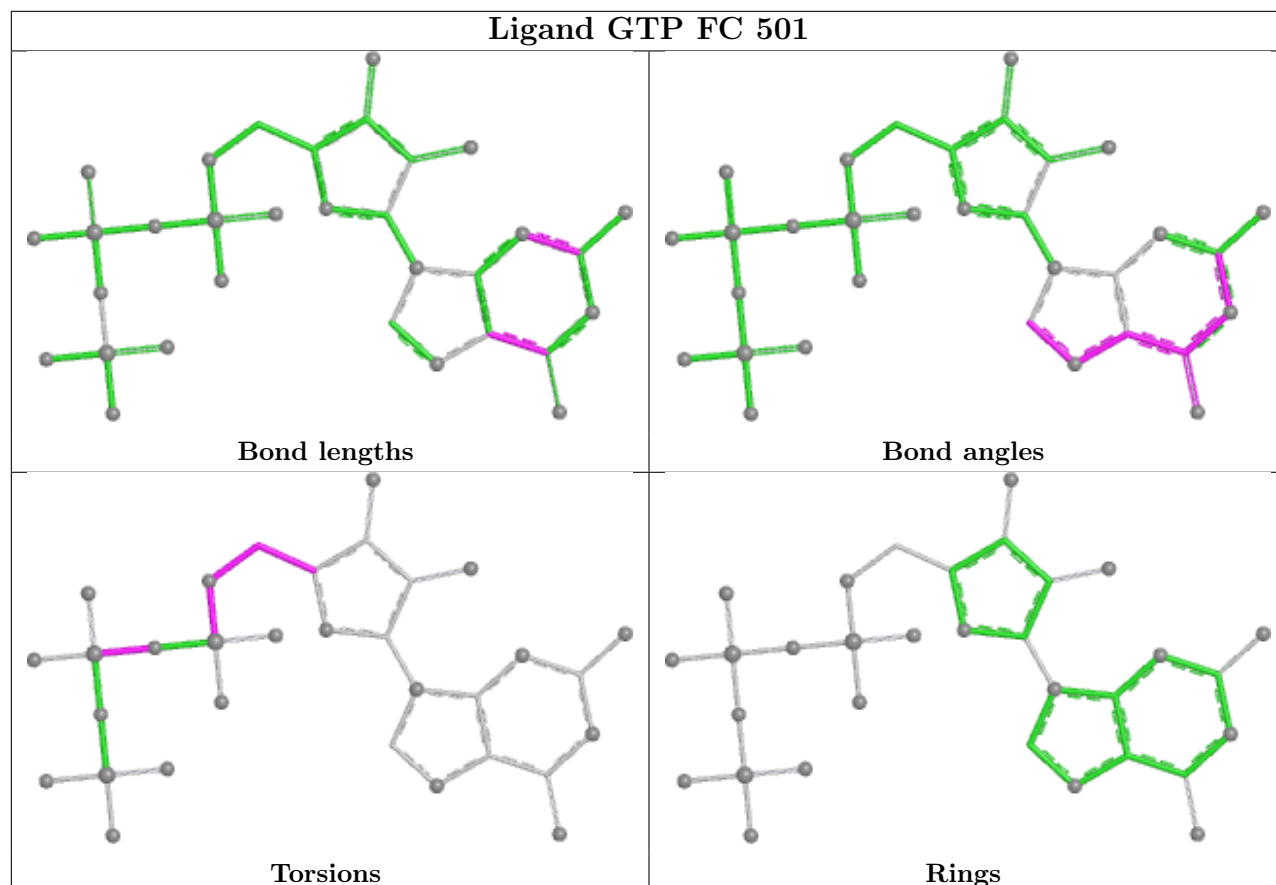




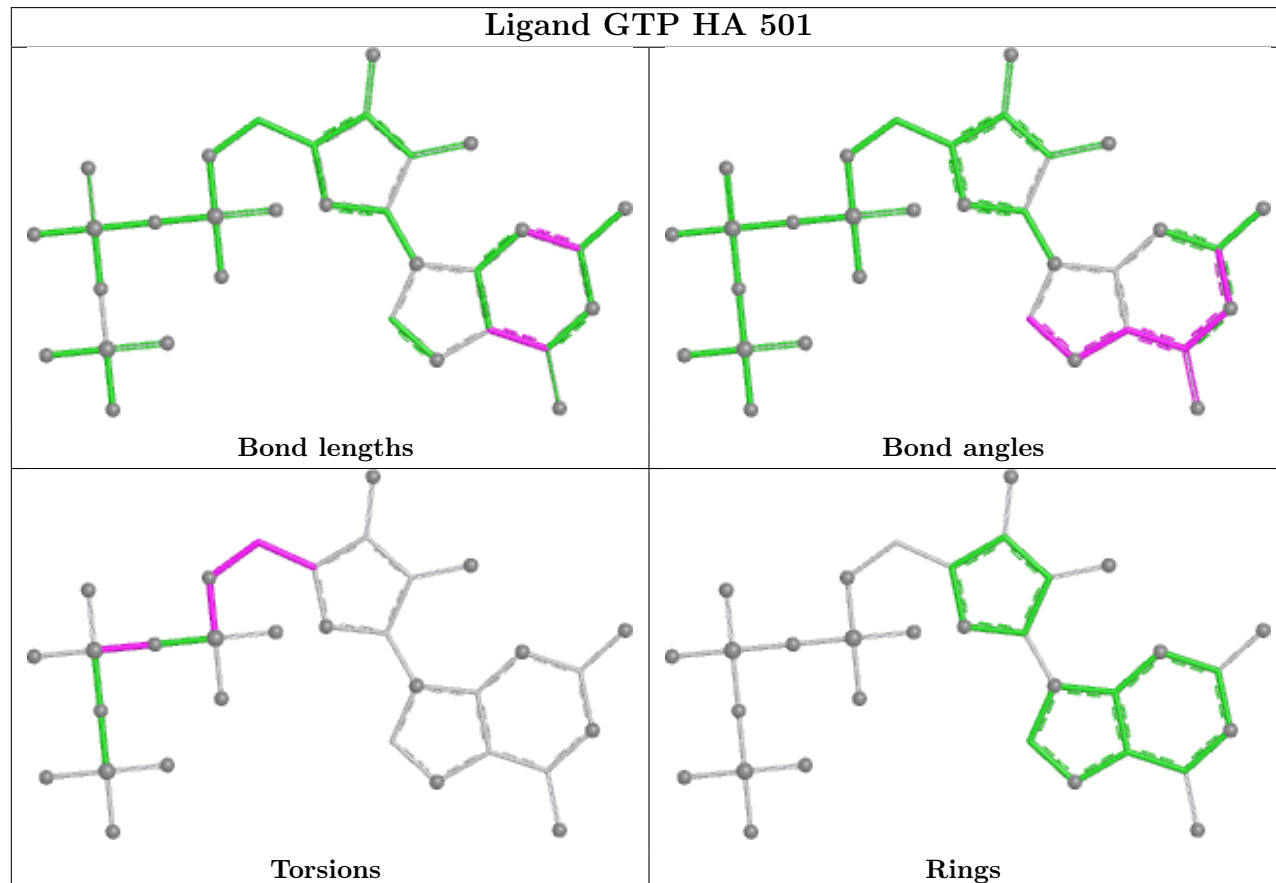


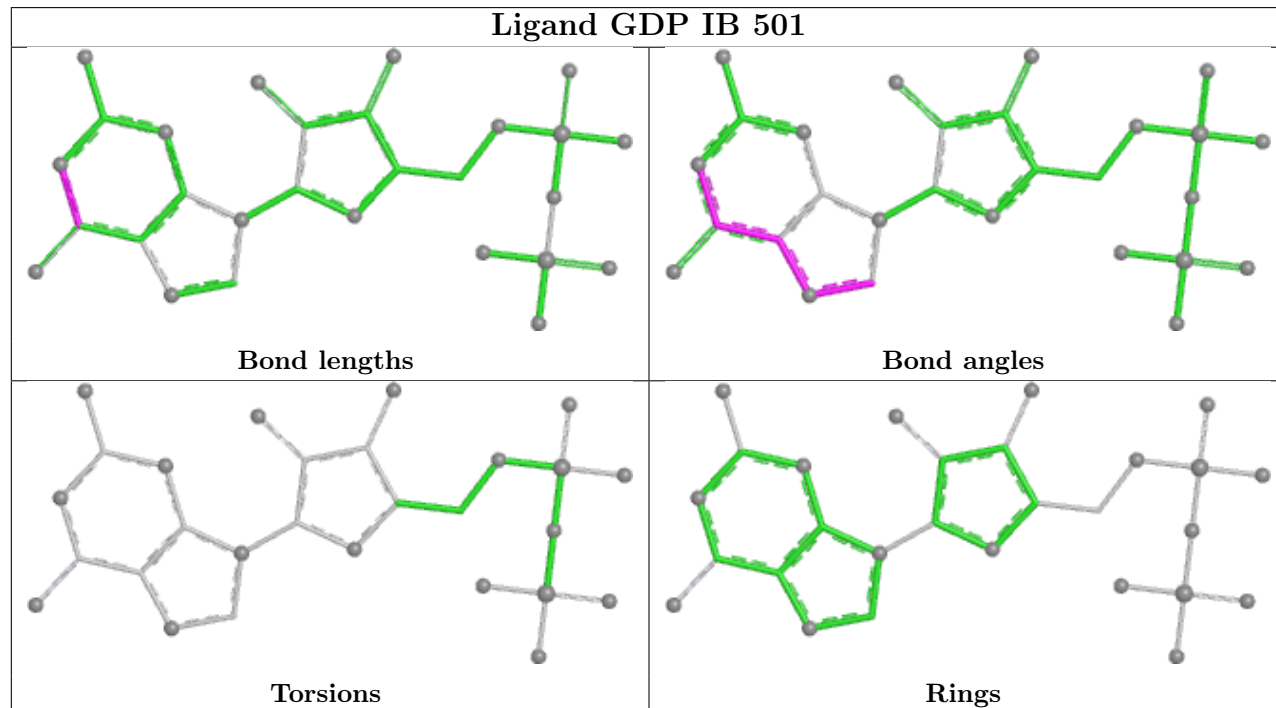
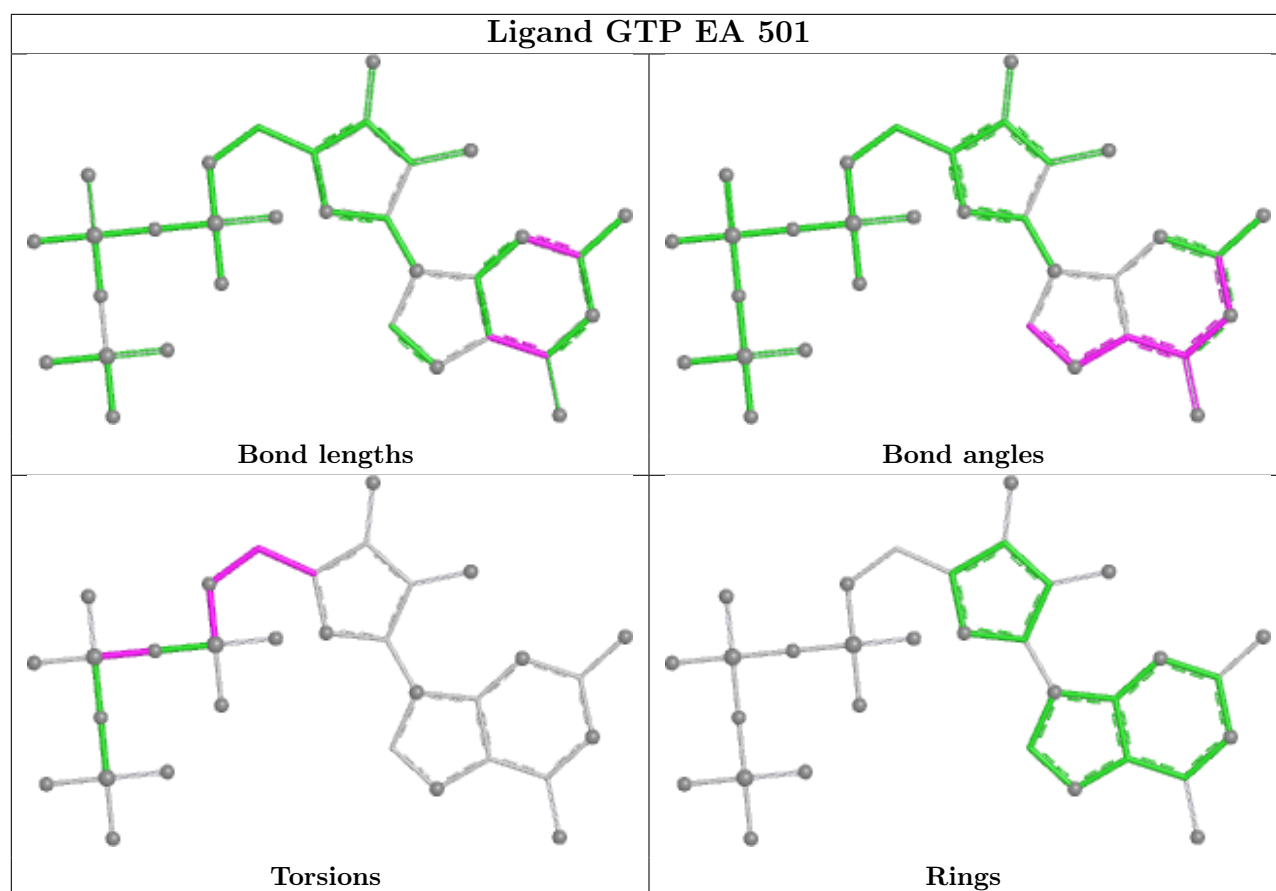


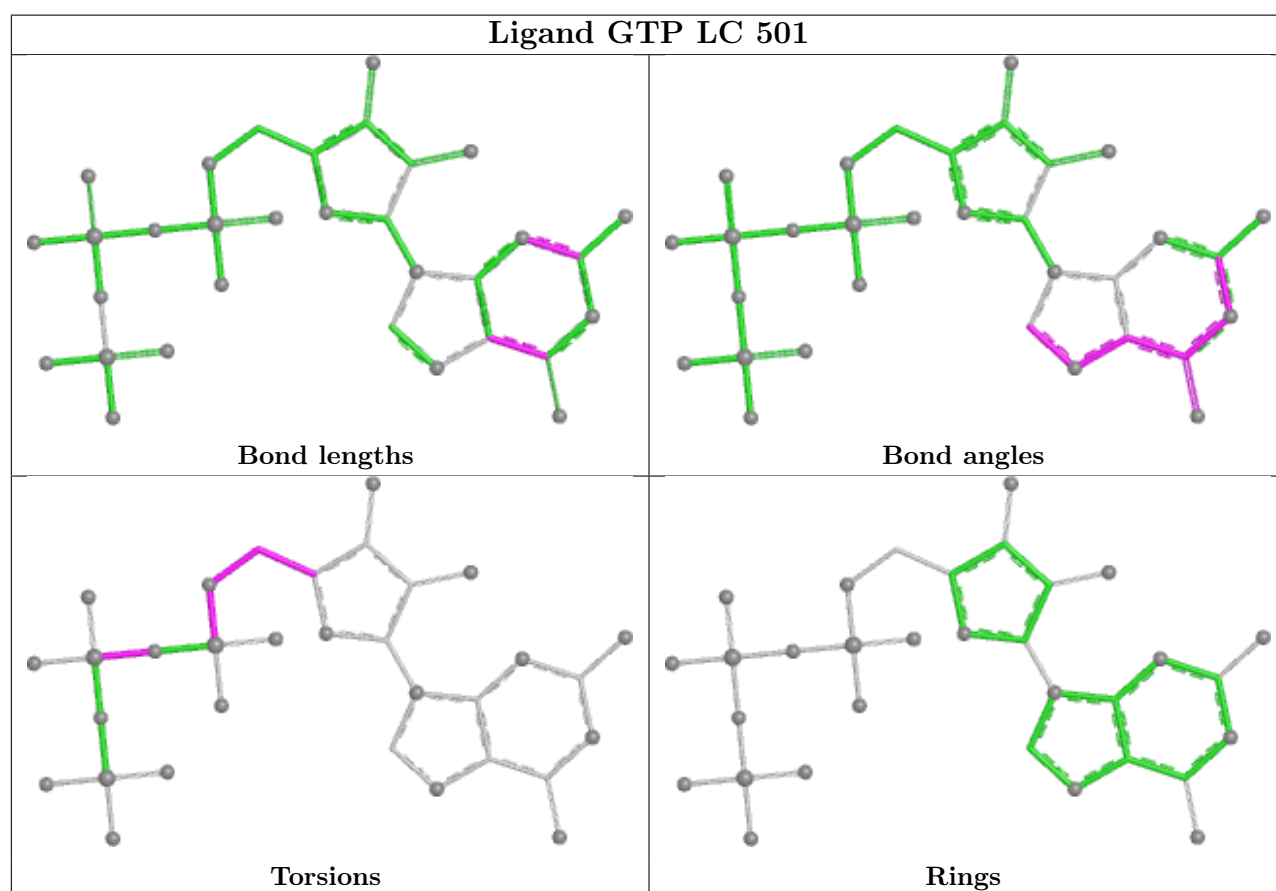
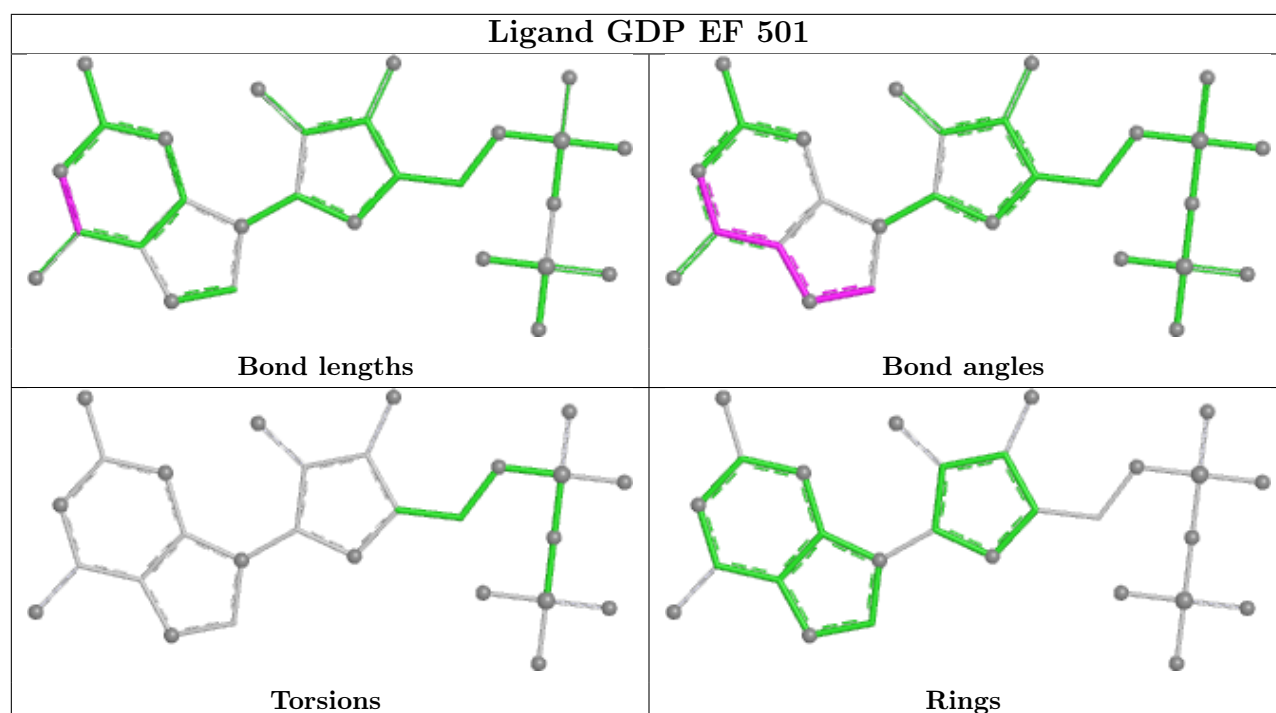
## Ligand GTP FC 501



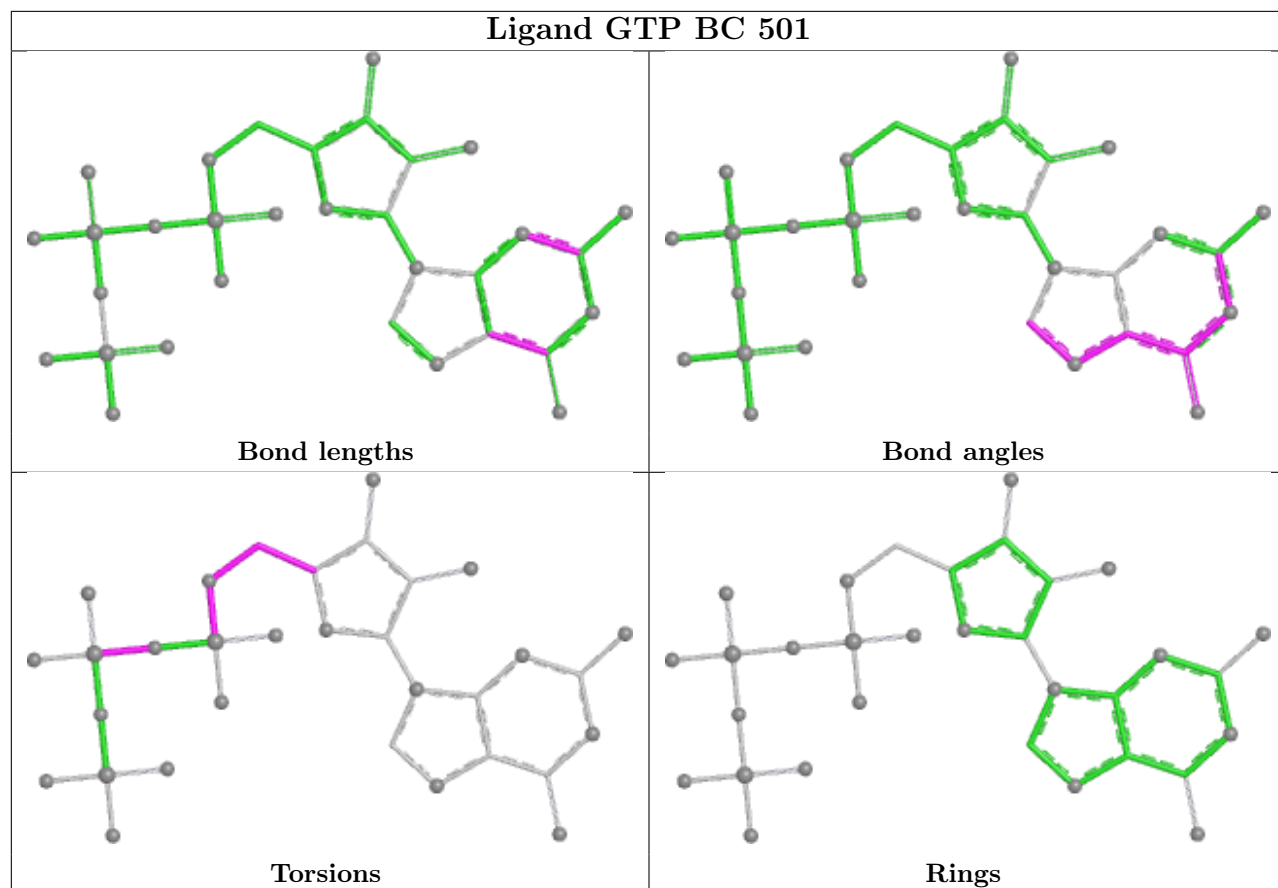
## Ligand GTP HA 501



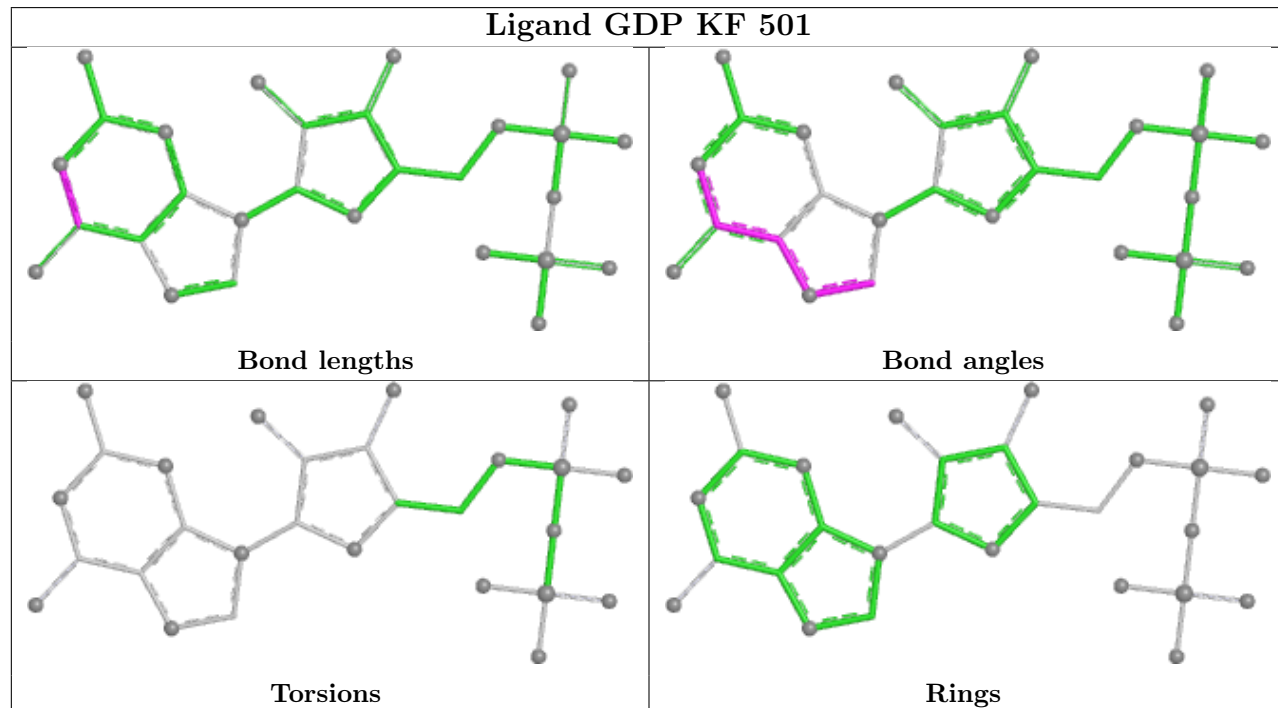


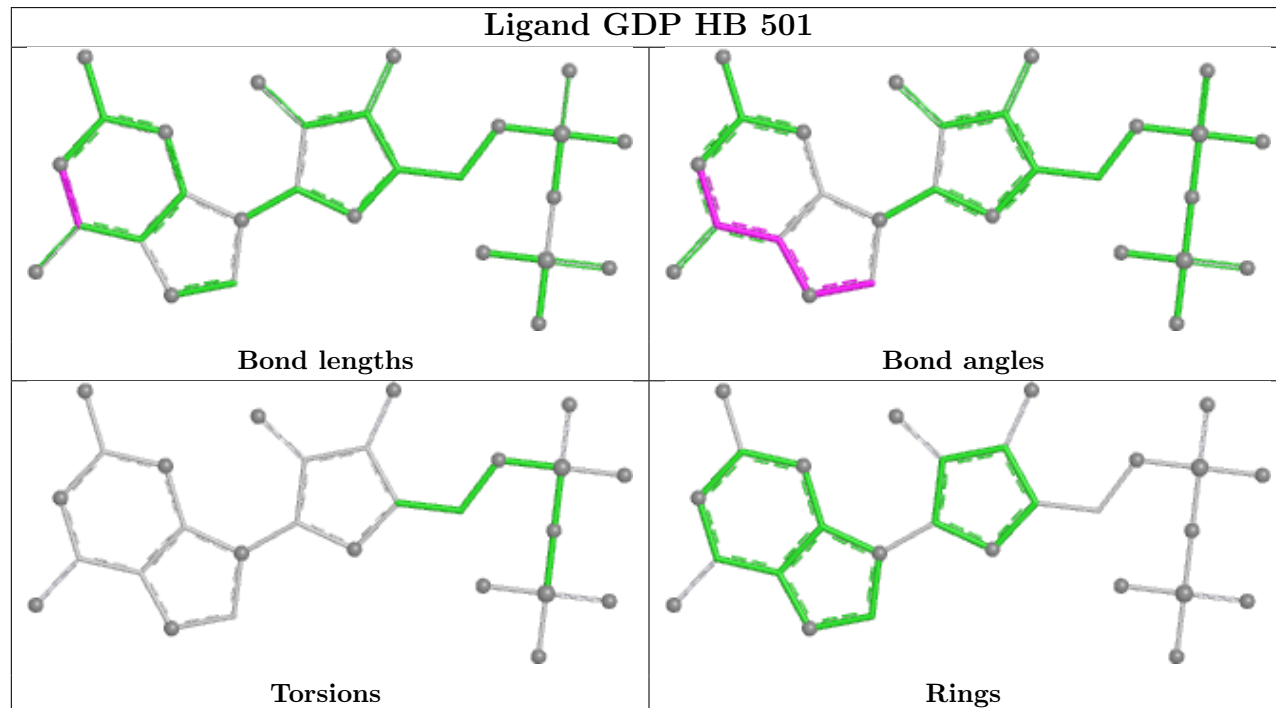
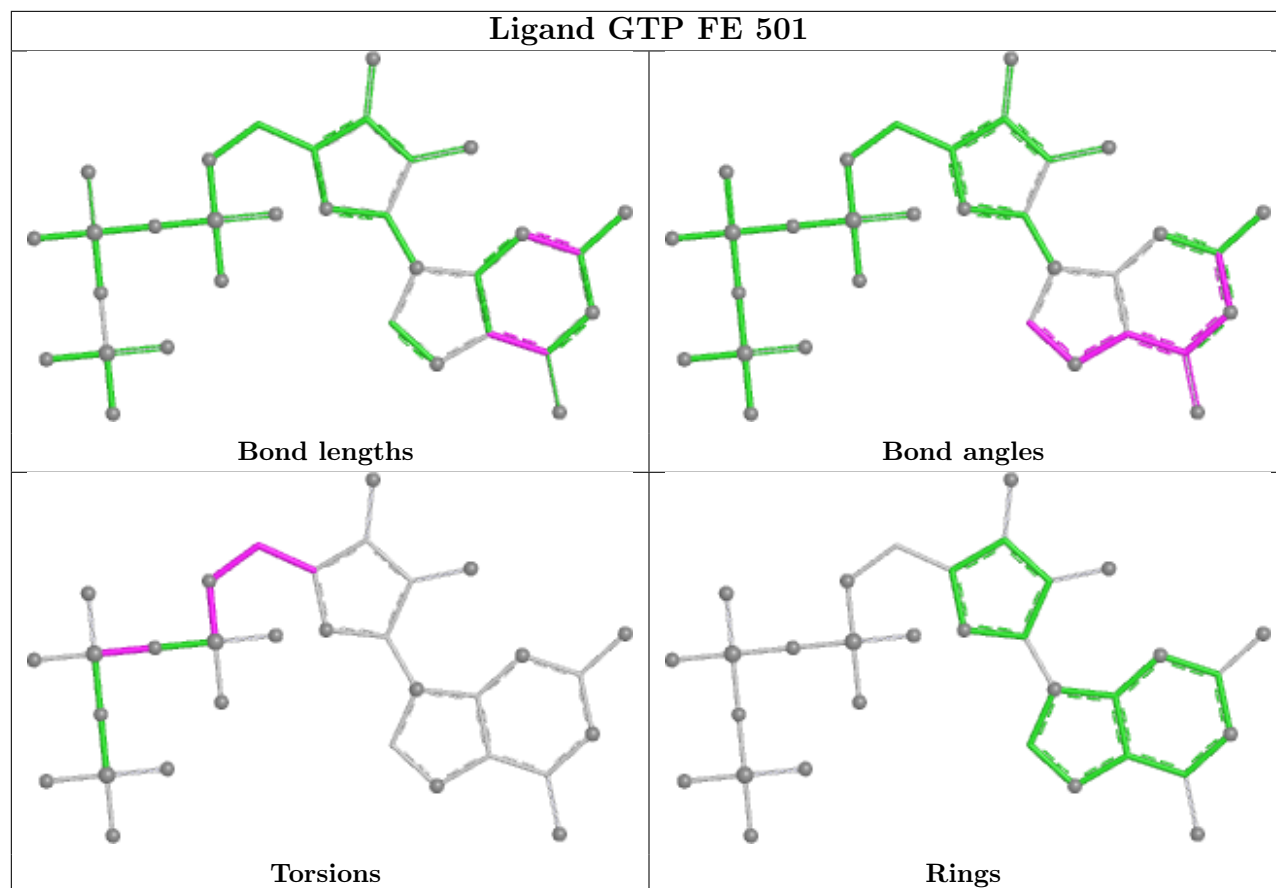


## Ligand GTP BC 501

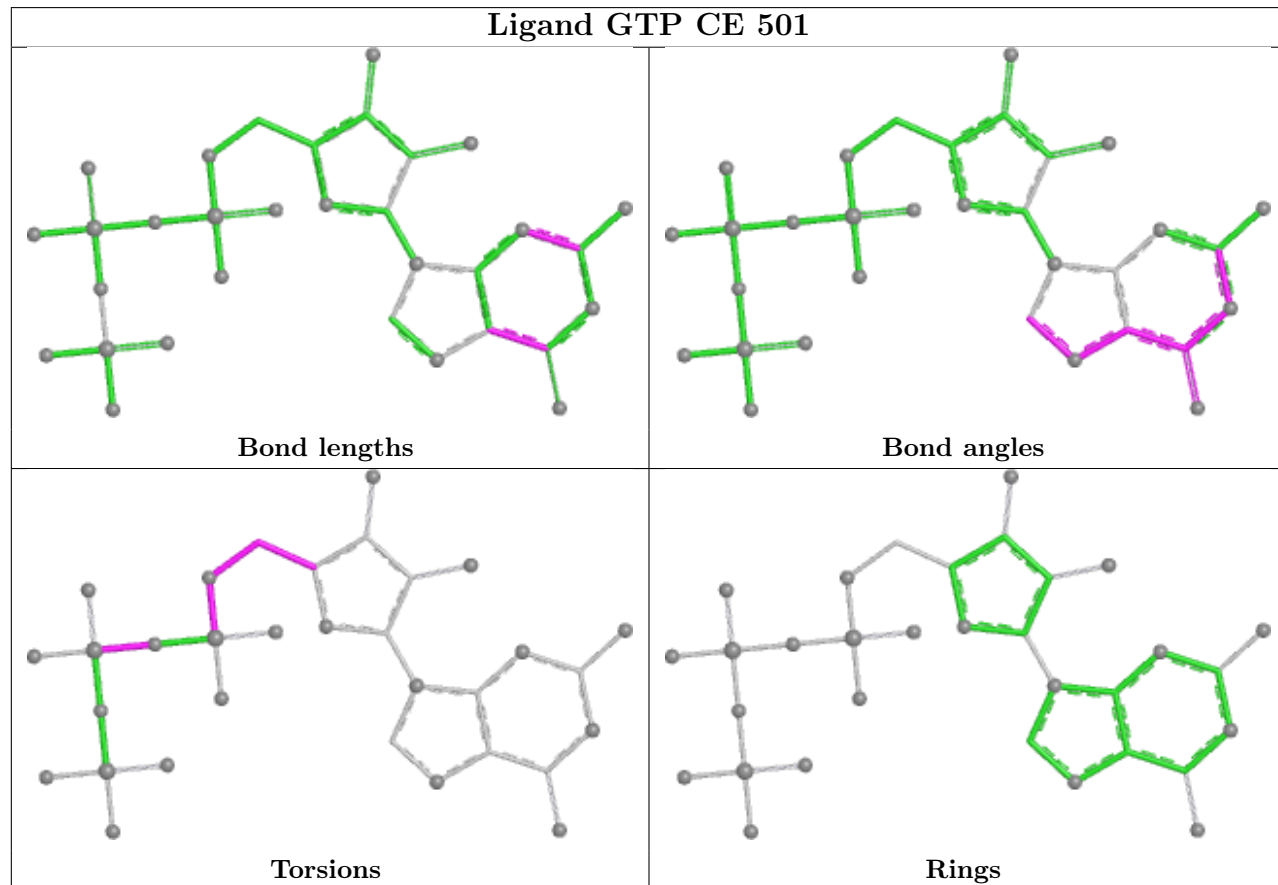
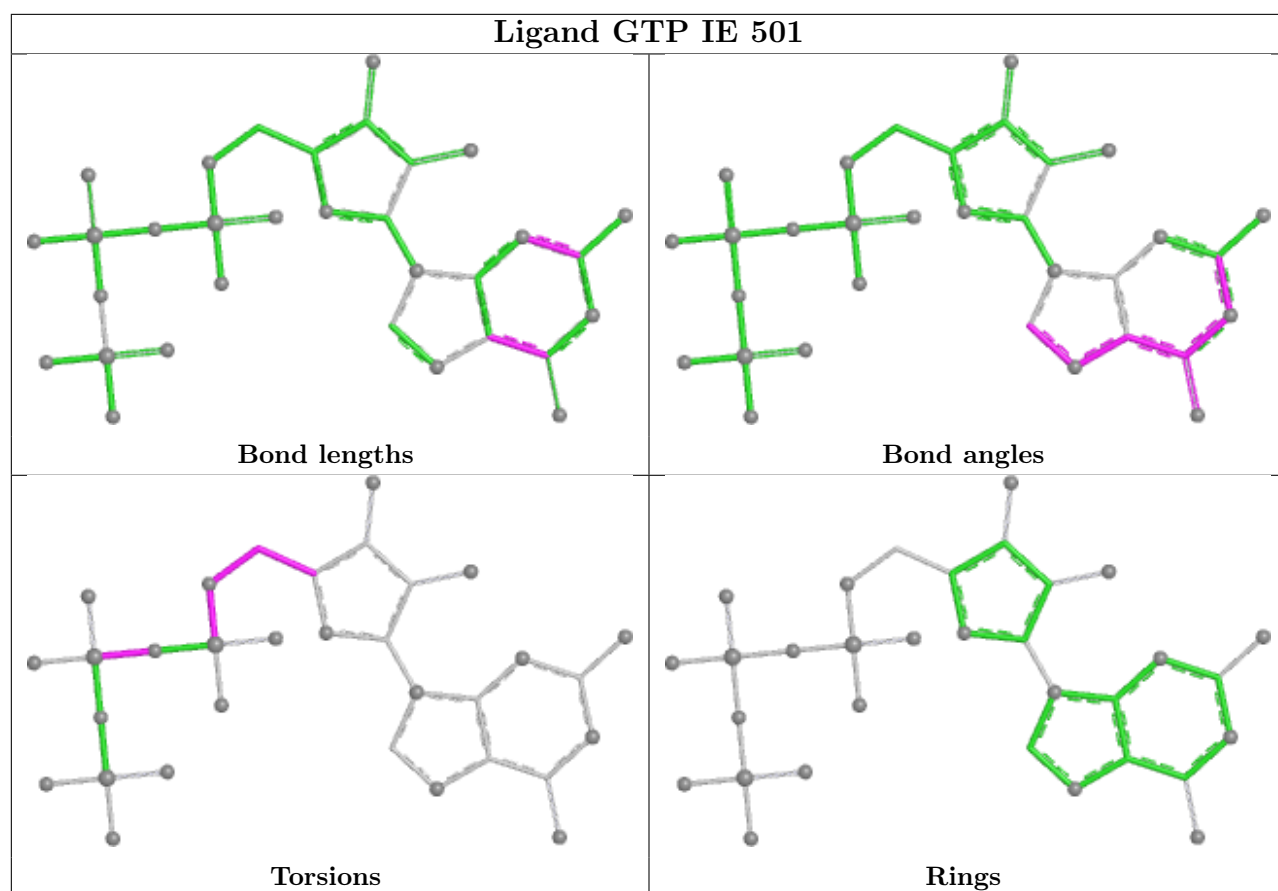


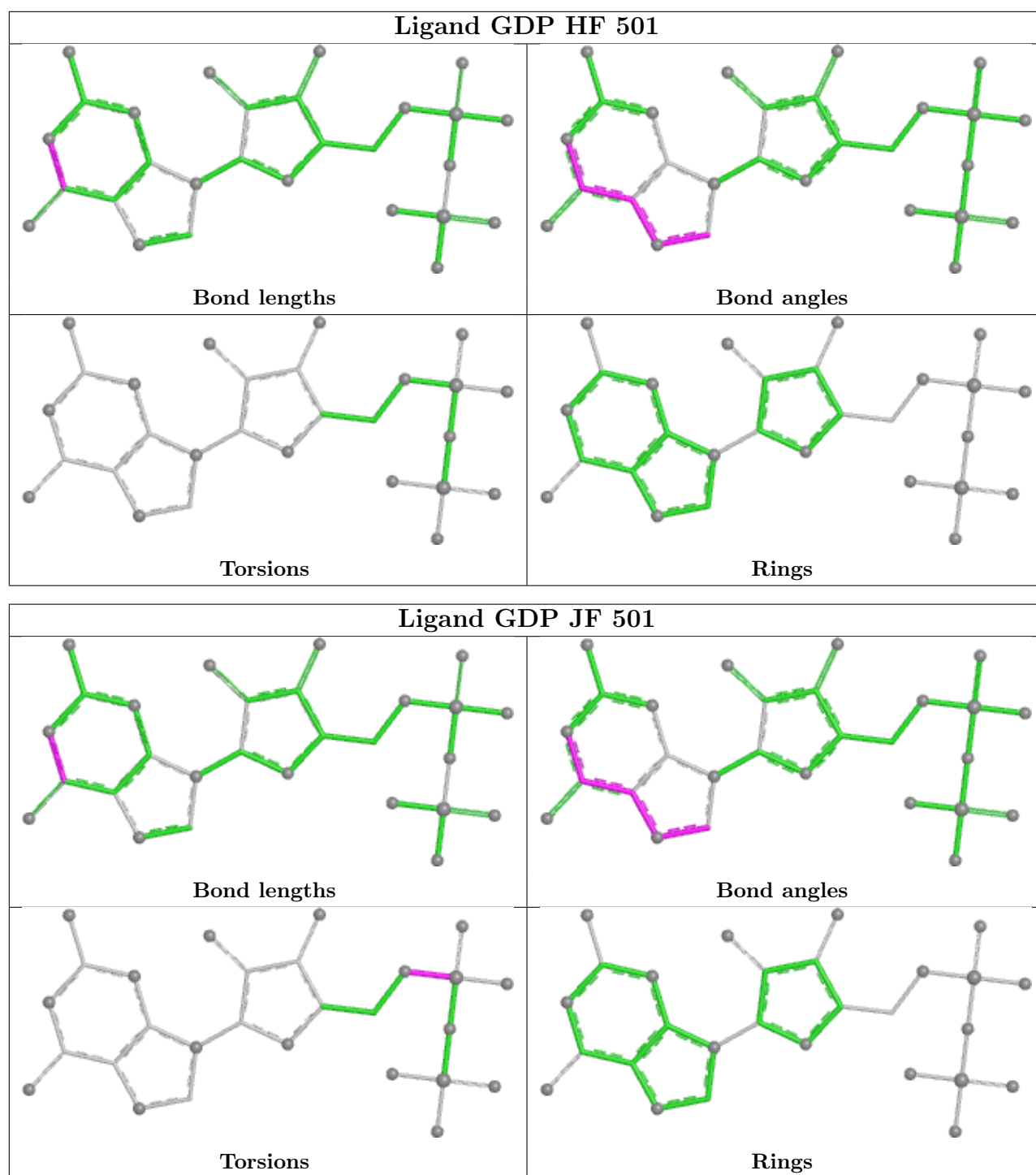
## Ligand GDP KF 501

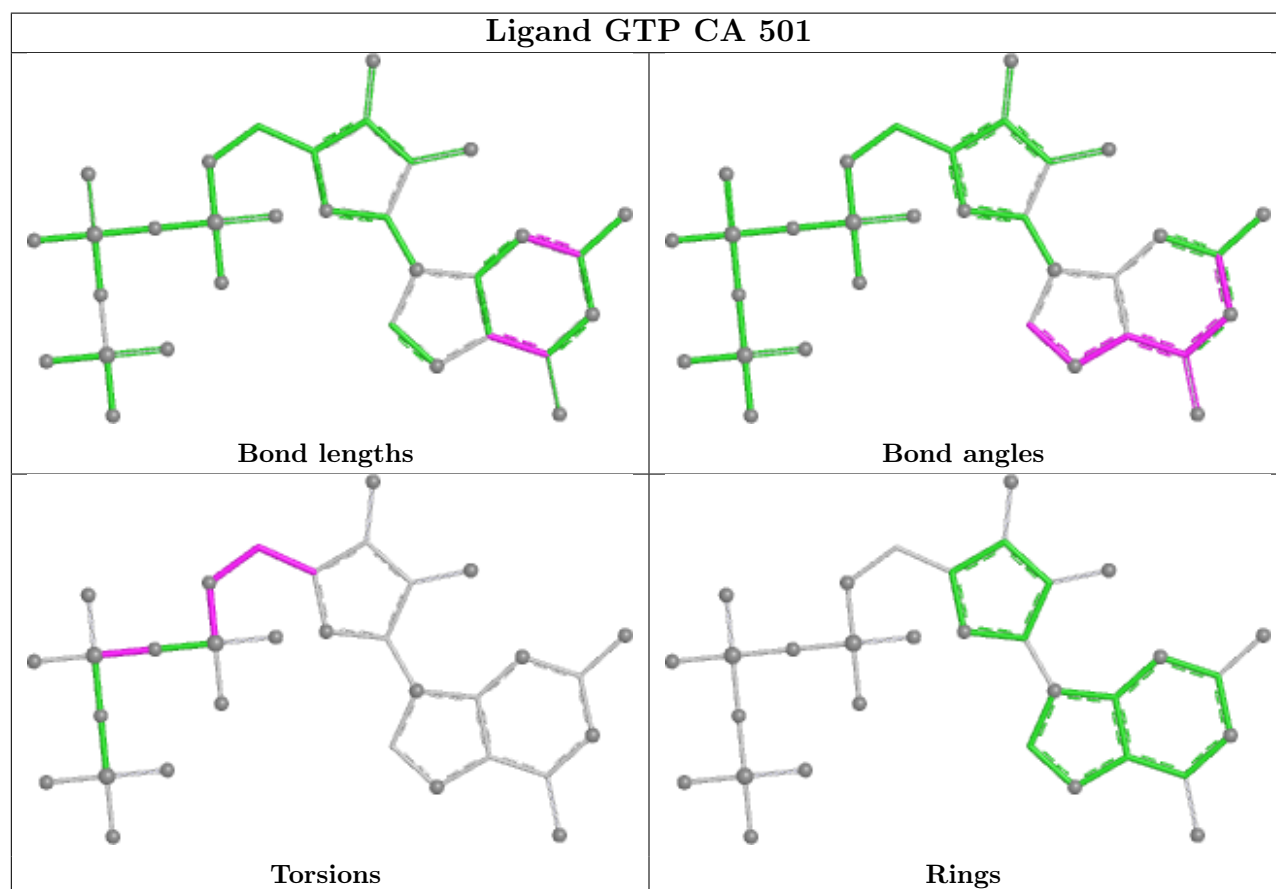
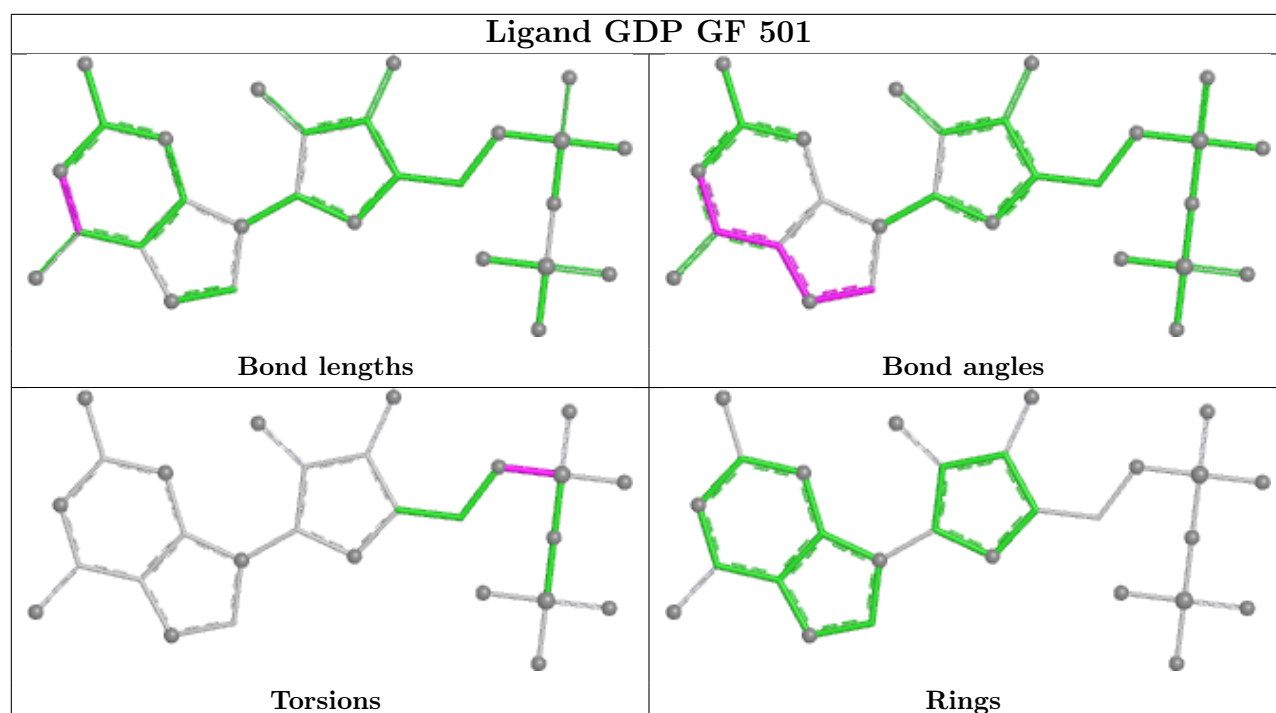


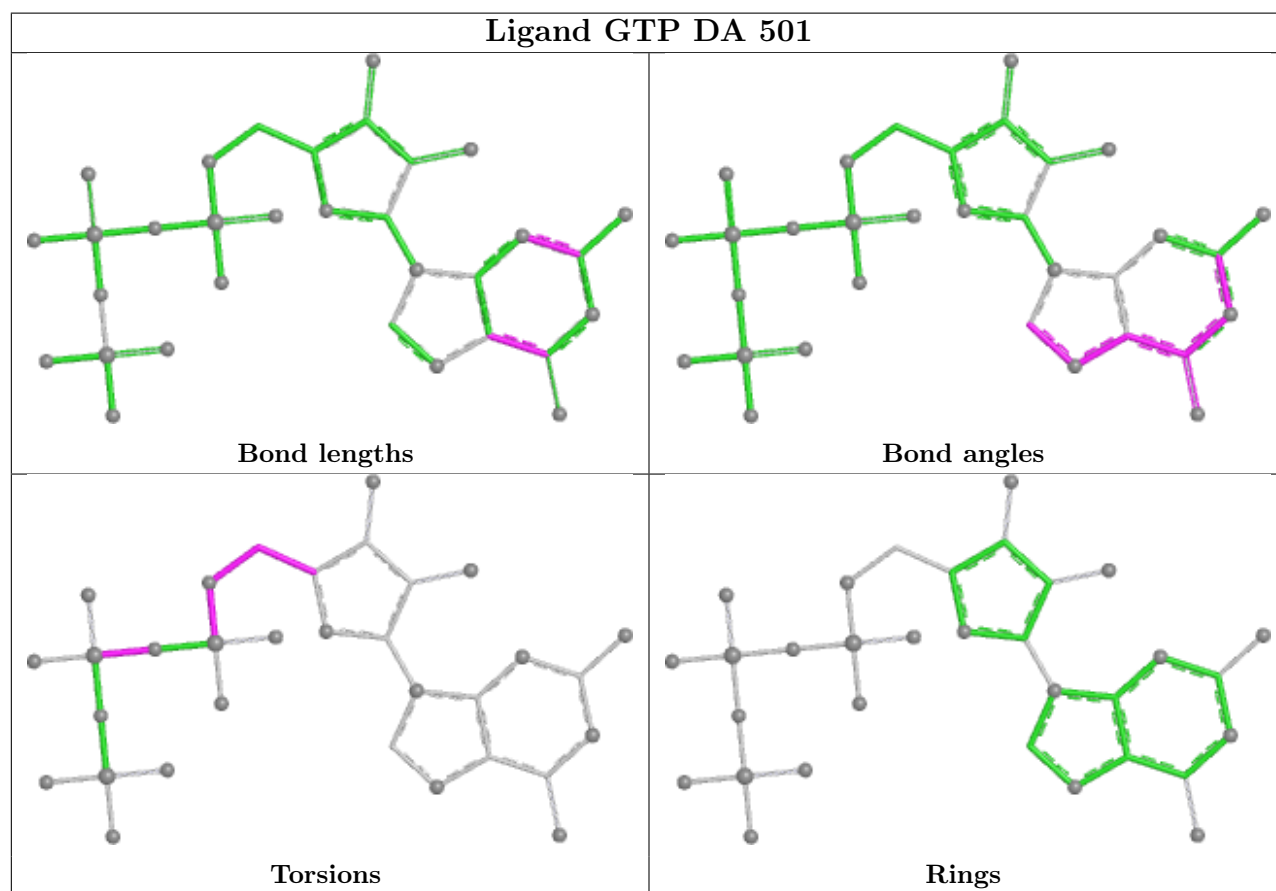
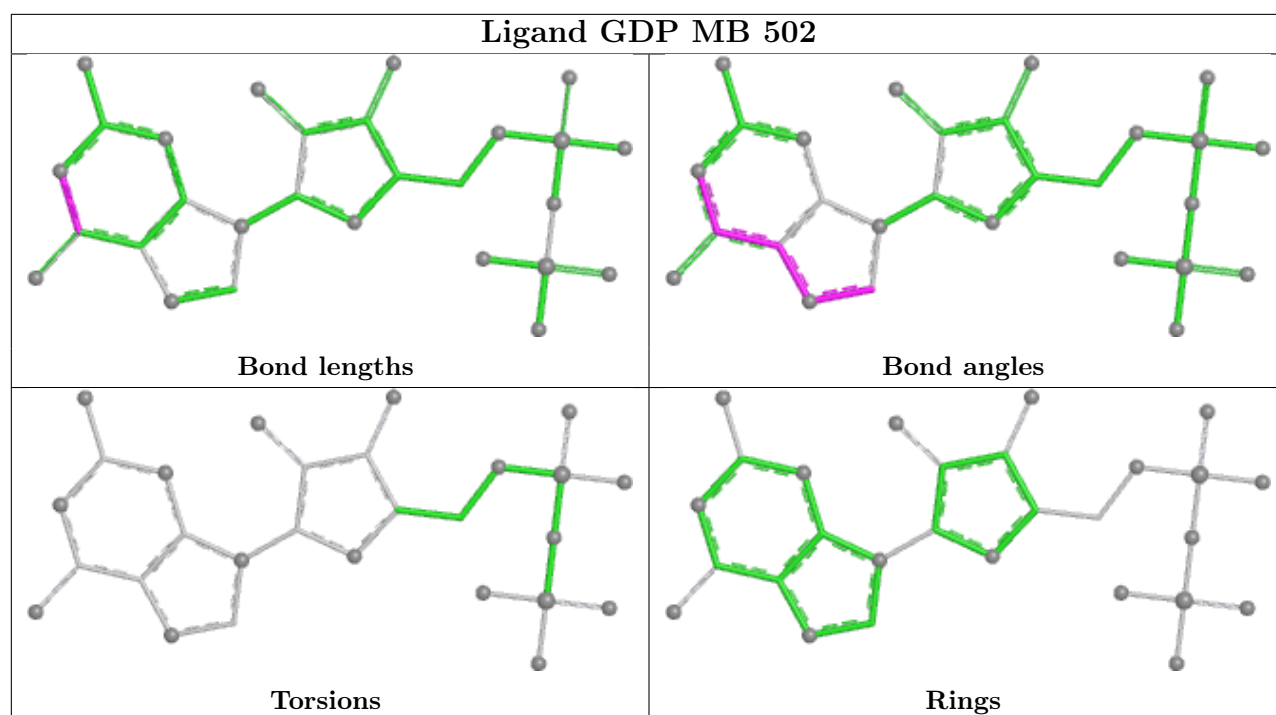


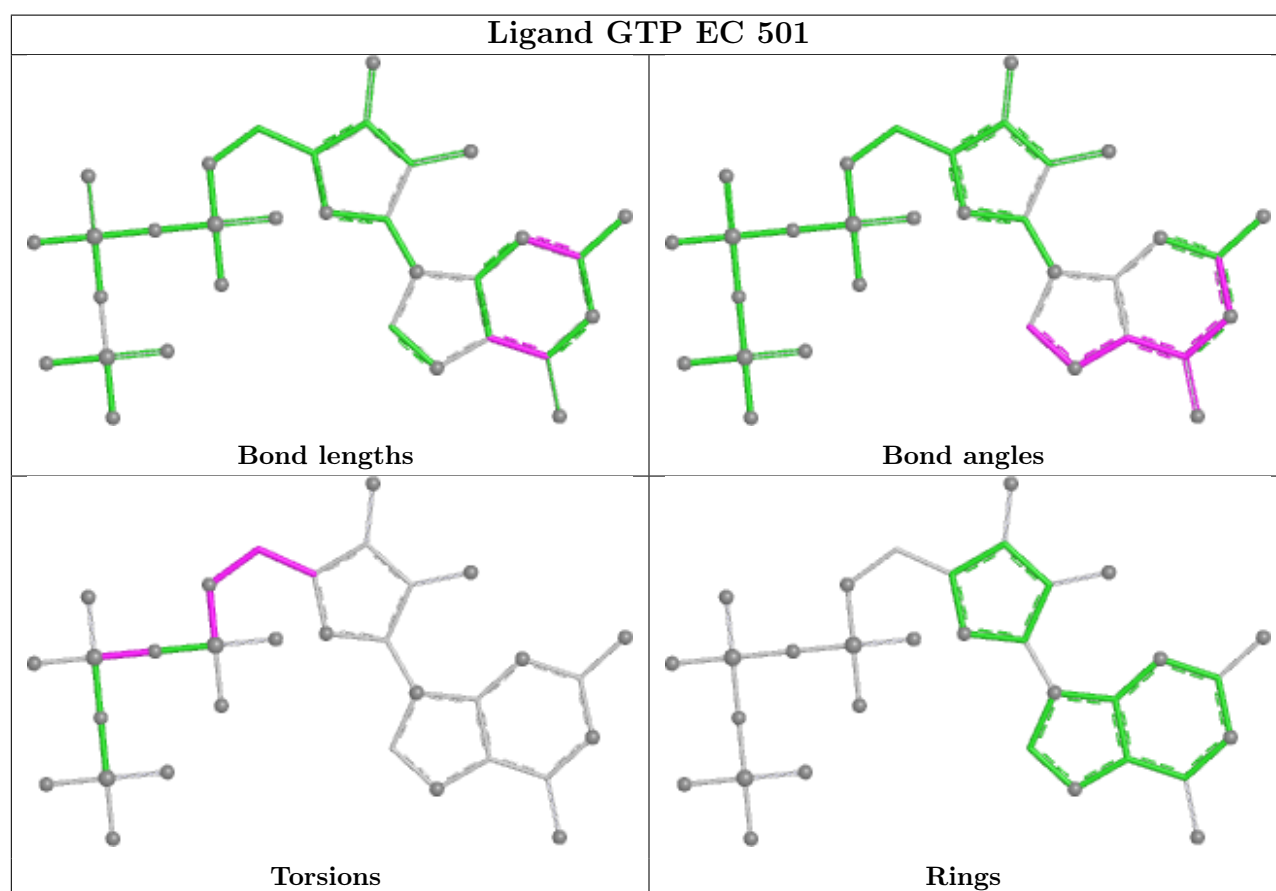
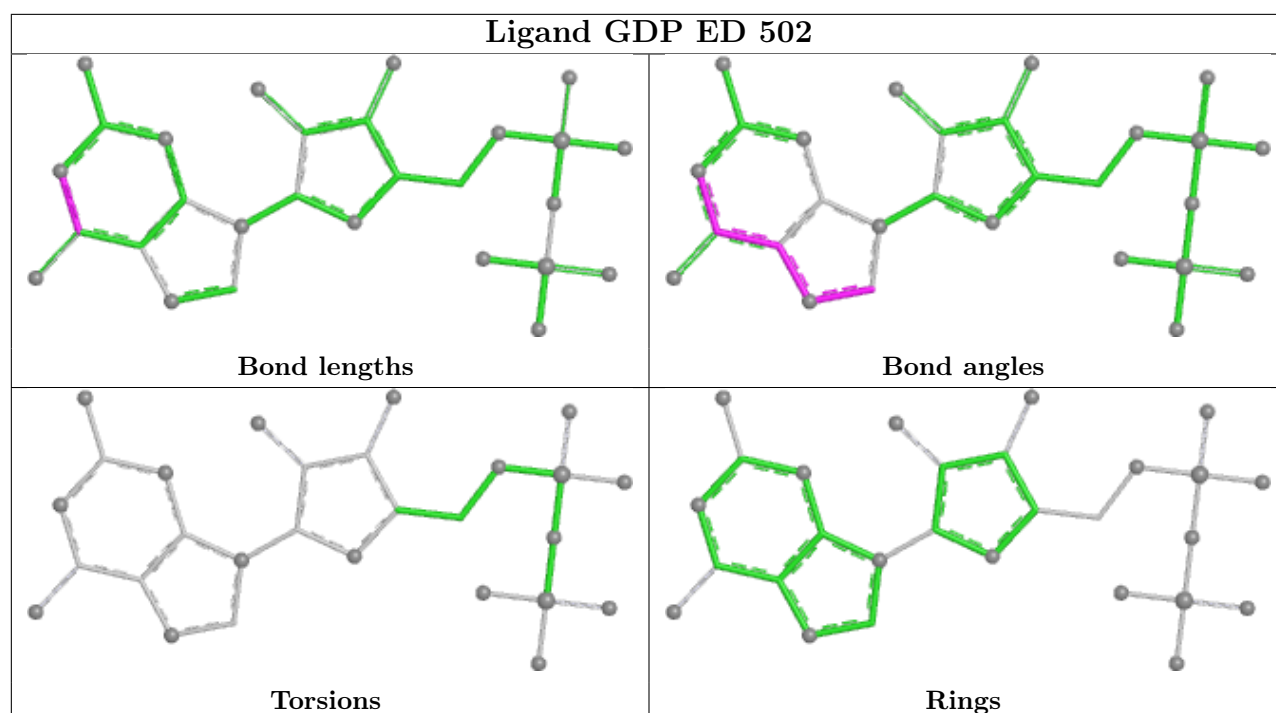




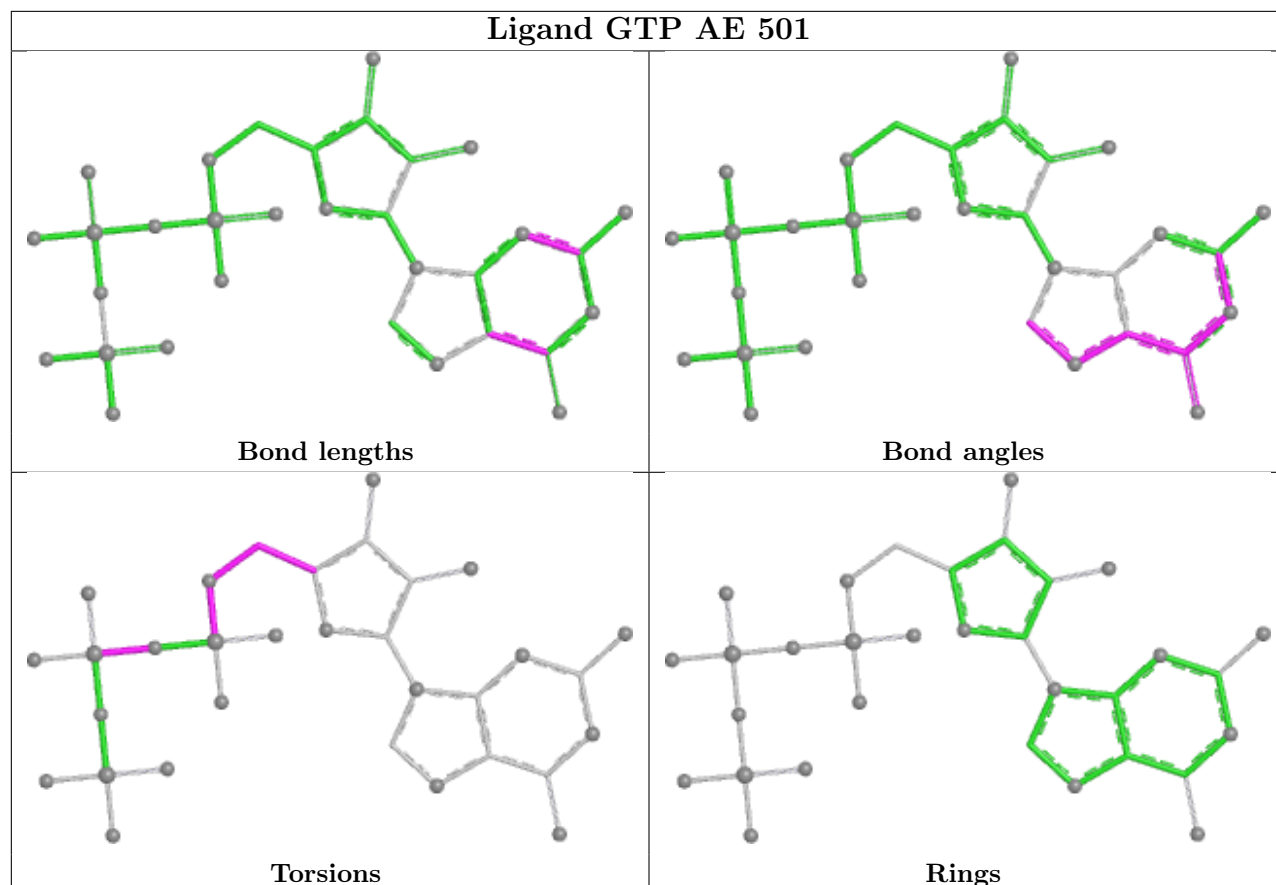




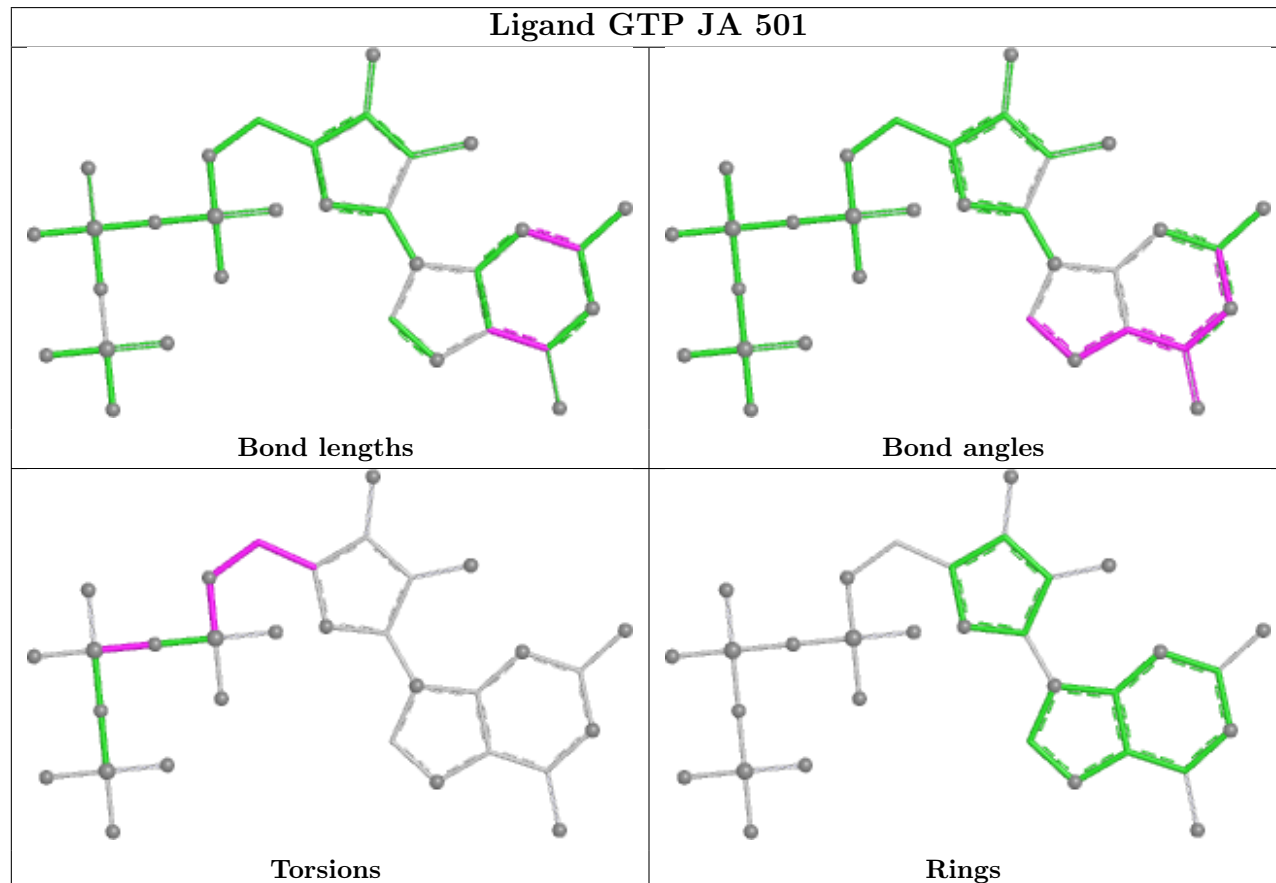


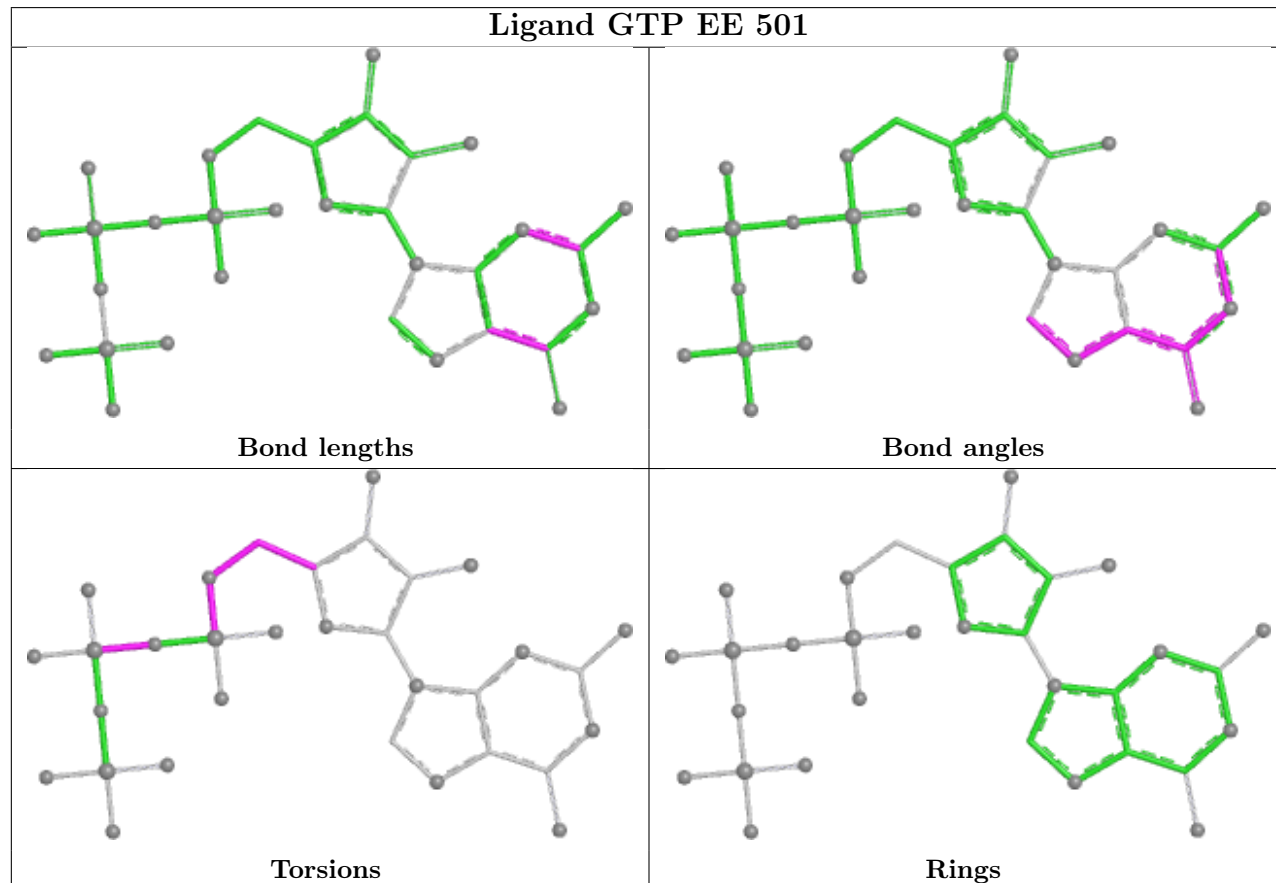
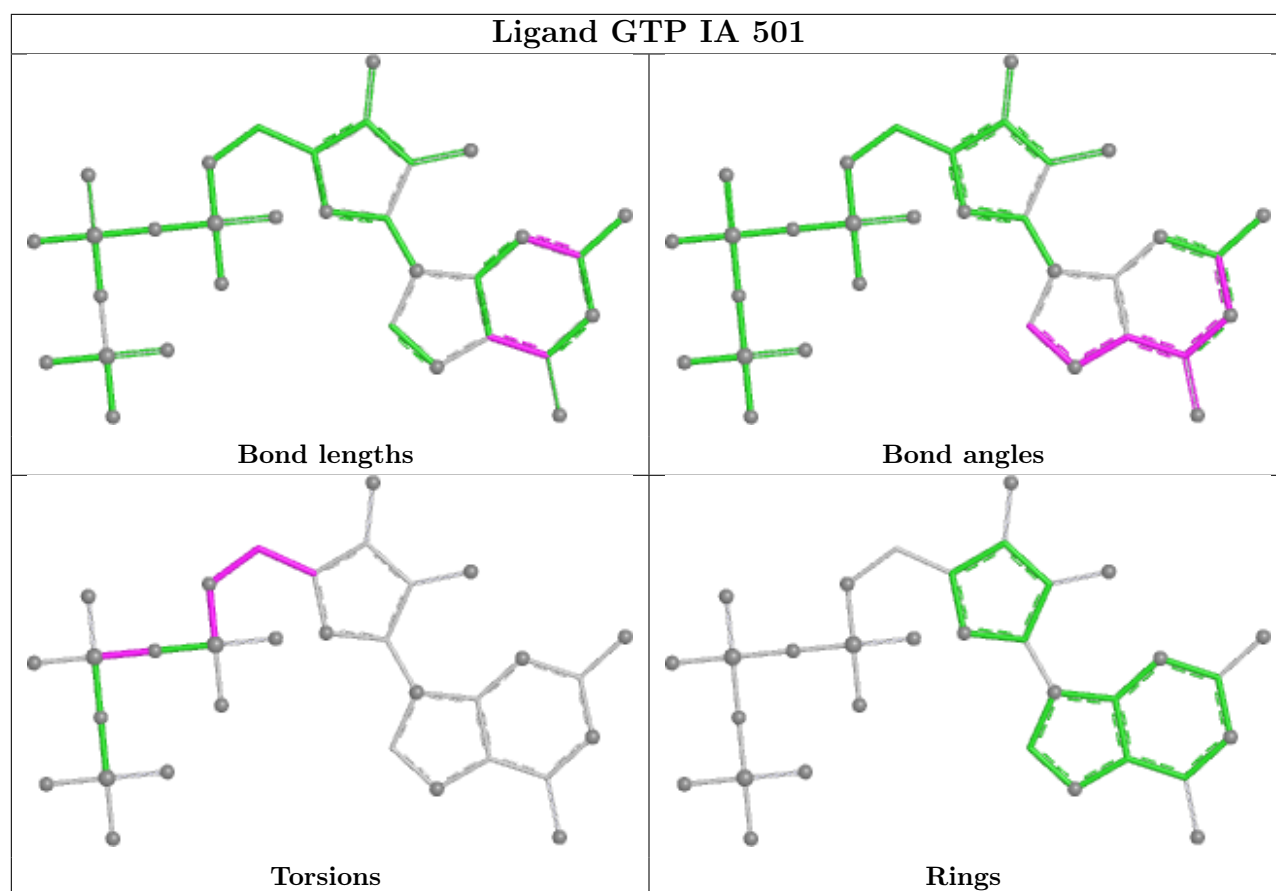


## Ligand GTP AE 501

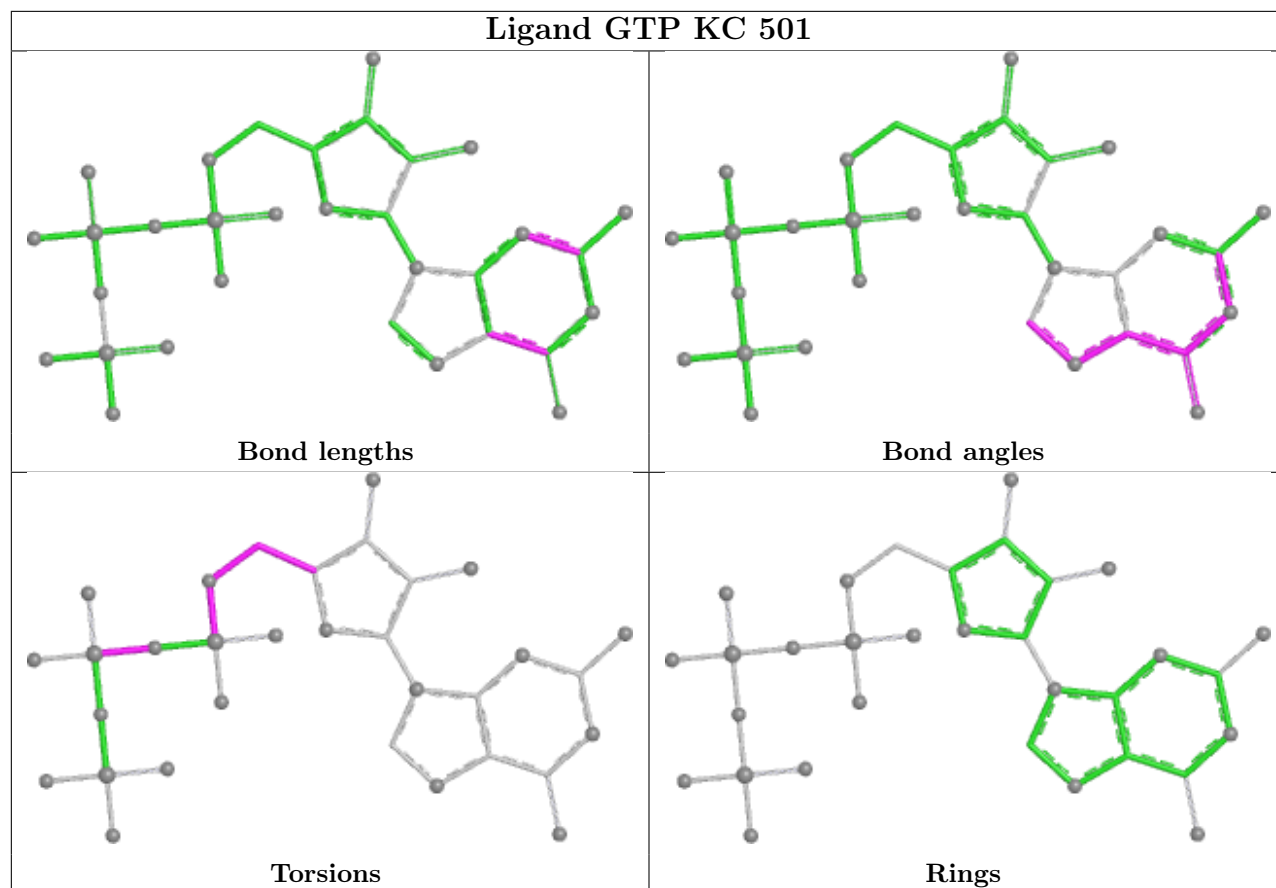


## Ligand GTP JA 501

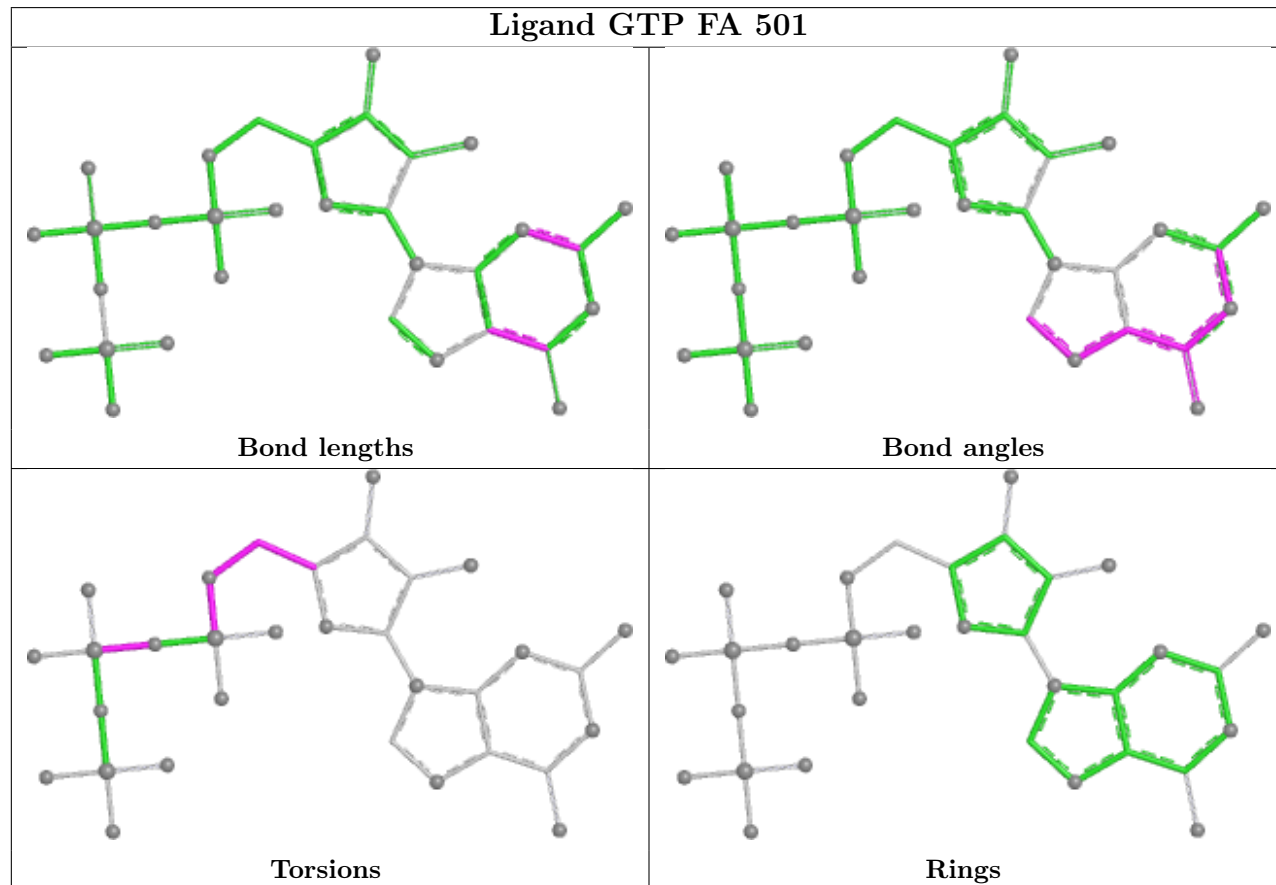




## Ligand GTP KC 501



## Ligand GTP FA 501





## 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.

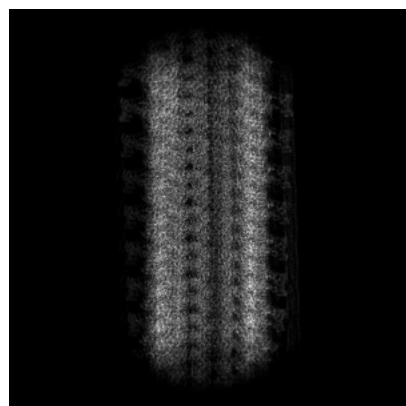
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49872. These allow visual inspection of the internal detail of the map and identification of artifacts.

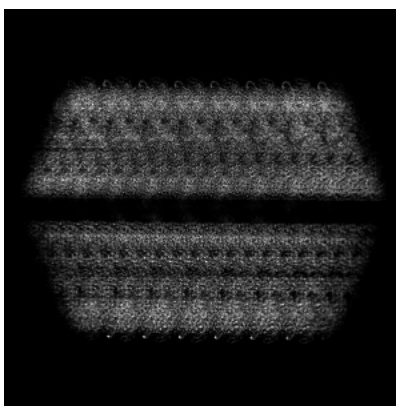
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

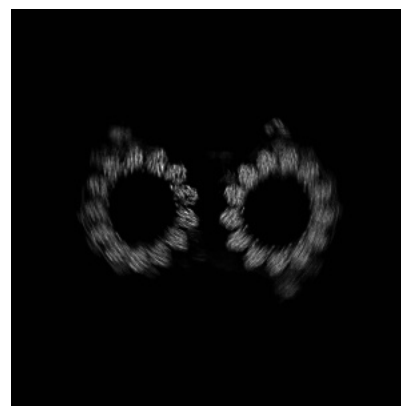
#### 6.1.1 Primary map



X

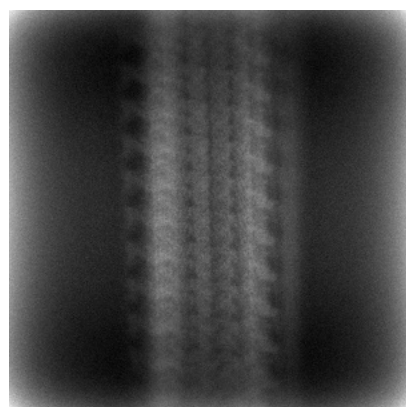


Y

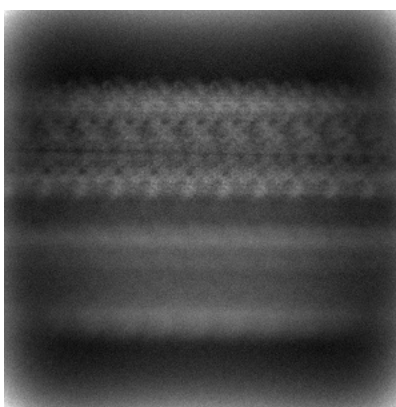


Z

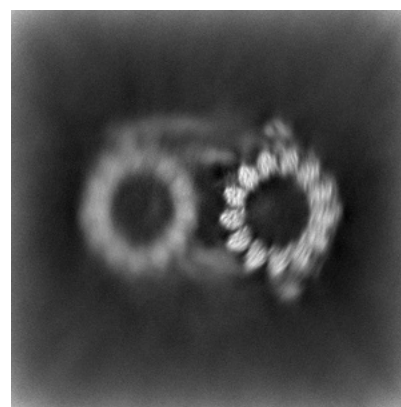
#### 6.1.2 Raw map



X



Y

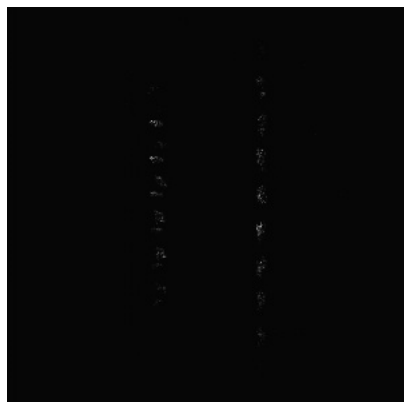


Z

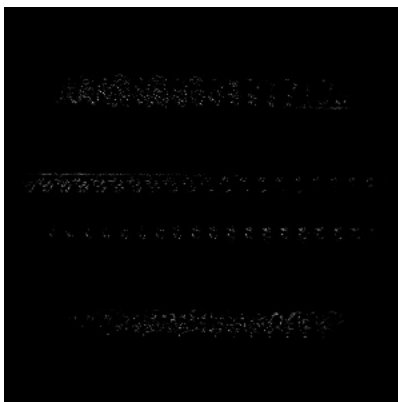
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 340

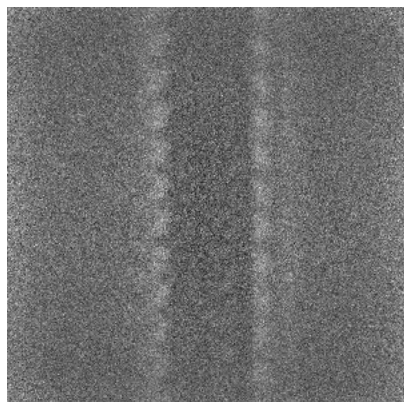


Y Index: 340

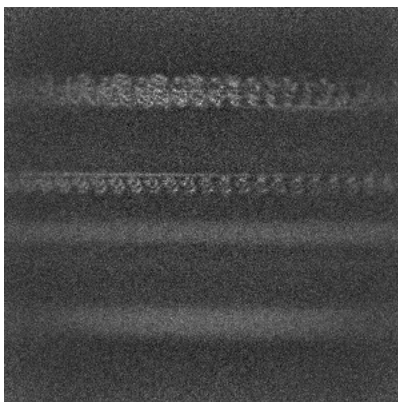


Z Index: 340

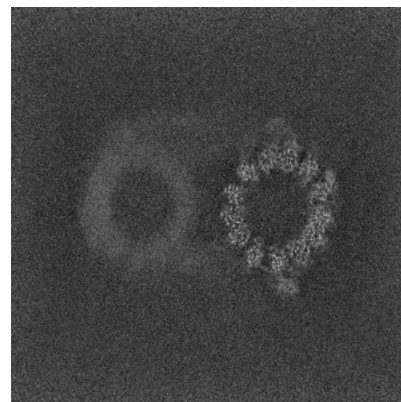
### 6.2.2 Raw map



X Index: 340



Y Index: 340

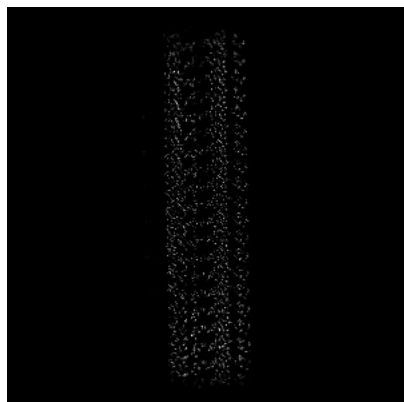


Z Index: 340

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

## 6.3 Largest variance slices [i](#)

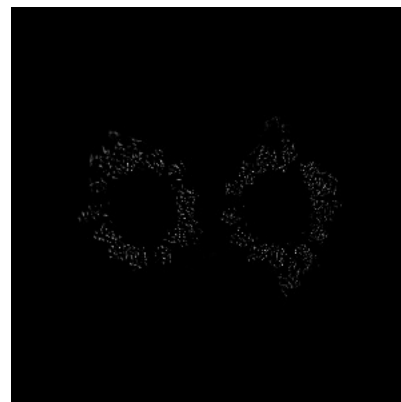
### 6.3.1 Primary map



X Index: 388

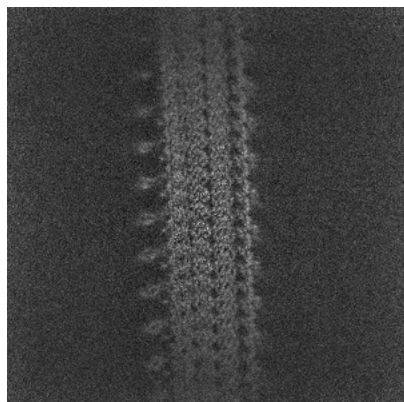


Y Index: 410

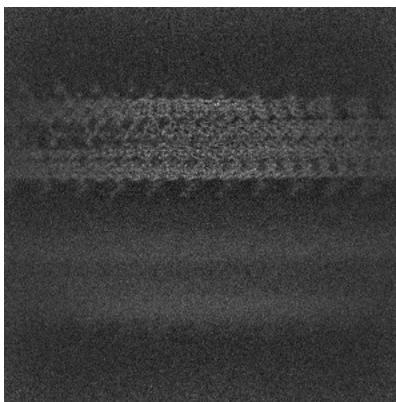


Z Index: 207

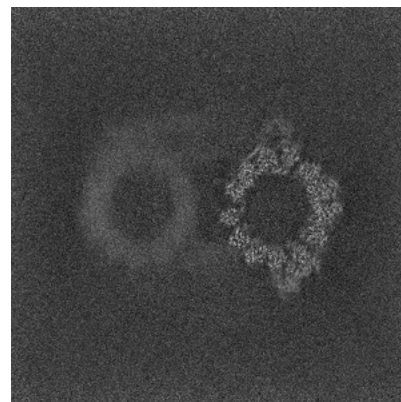
### 6.3.2 Raw map



X Index: 520



Y Index: 408

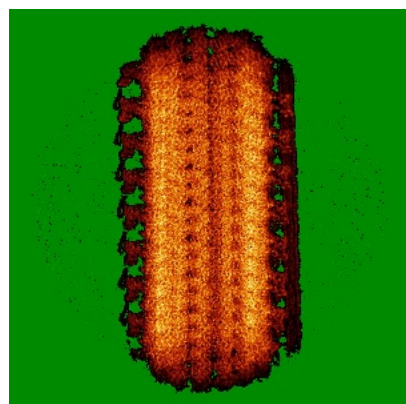


Z Index: 327

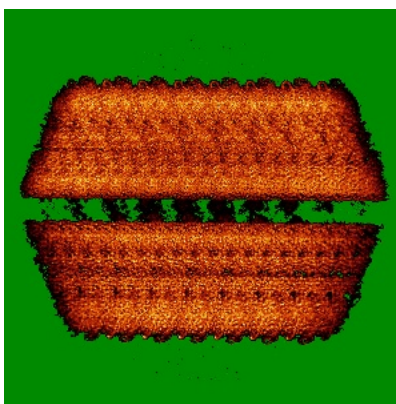
The images above show the largest variance slices of the map in three orthogonal directions.

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

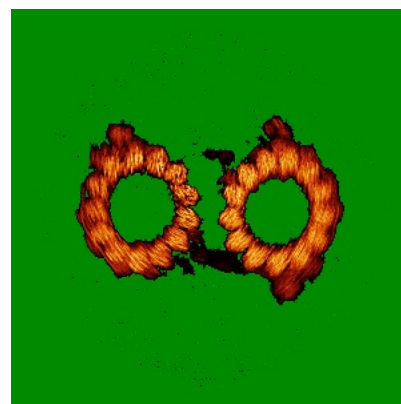
### 6.4.1 Primary map



X

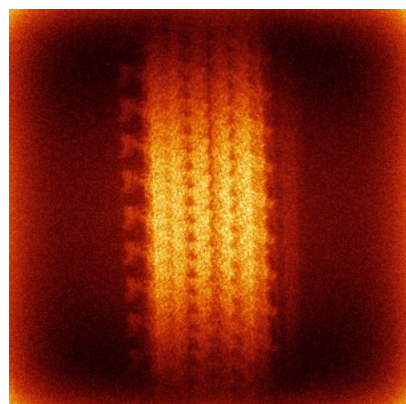


Y

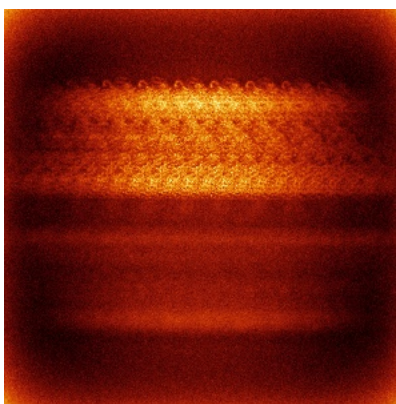


Z

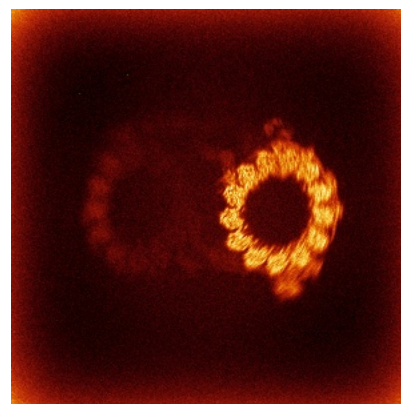
### 6.4.2 Raw map



X



Y



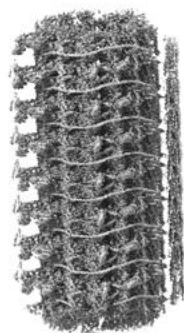
Z

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

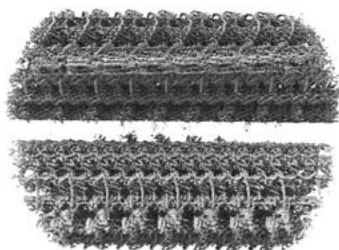


## 6.5 Orthogonal surface views [i](#)

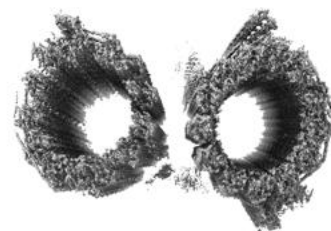
### 6.5.1 Primary map



X



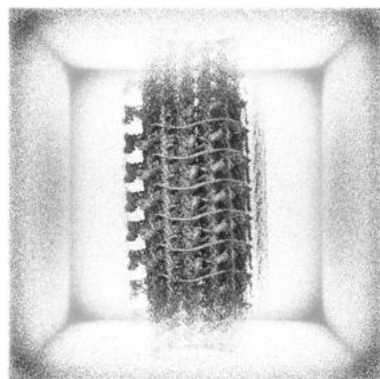
Y



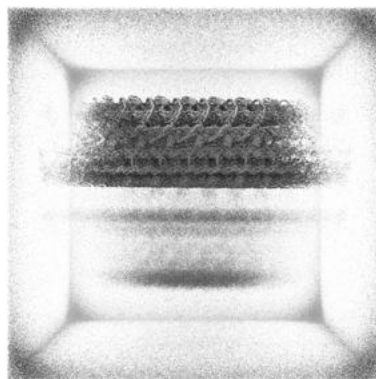
Z

The images above show the 3D surface view of the map at the recommended contour level 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

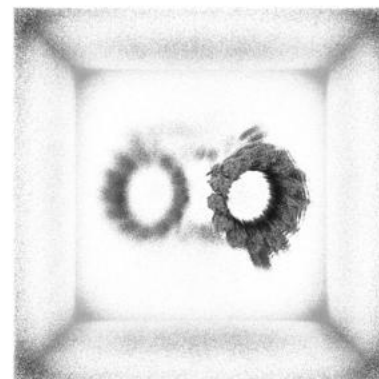
### 6.5.2 Raw map



X



Y



Z

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

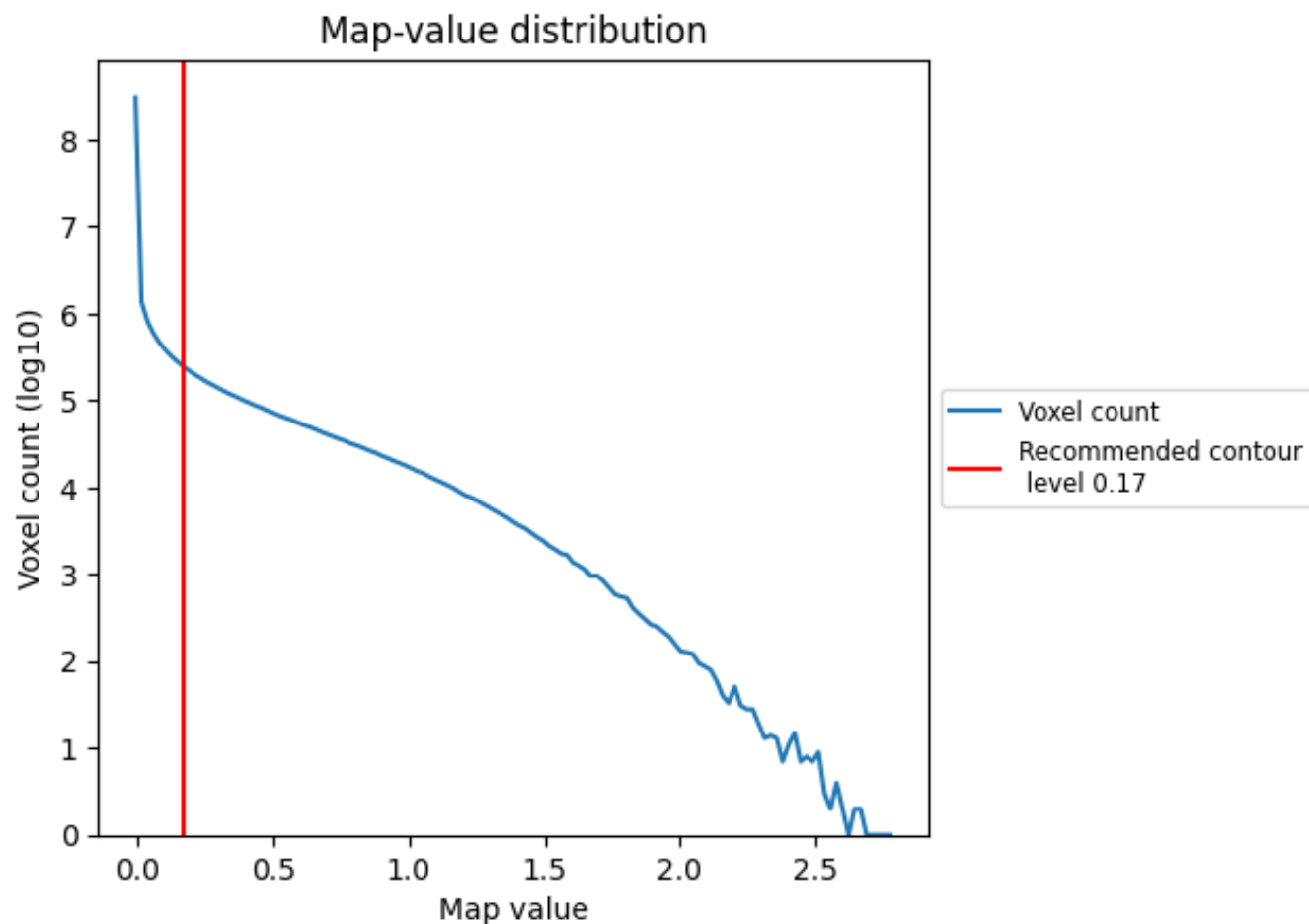
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

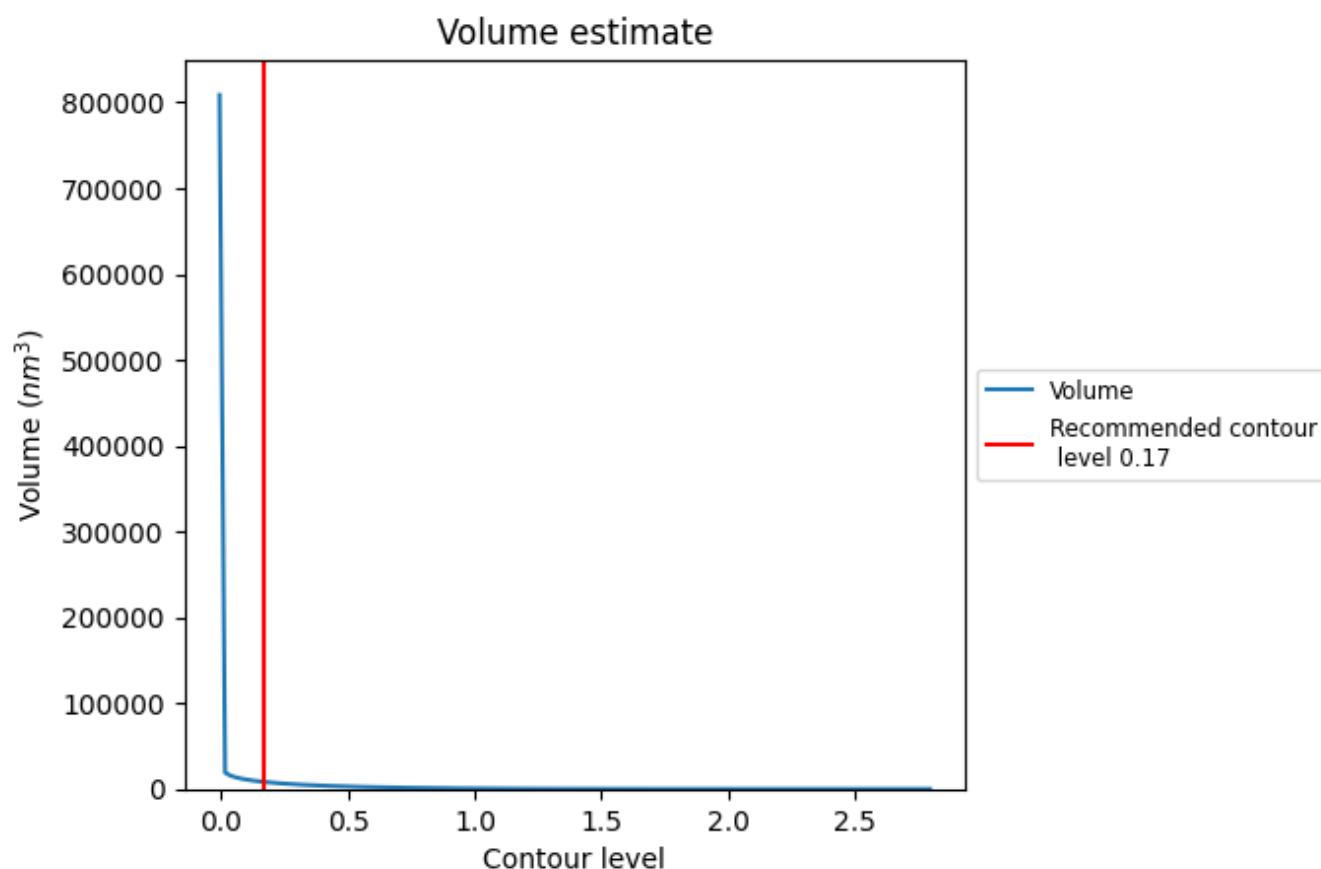
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

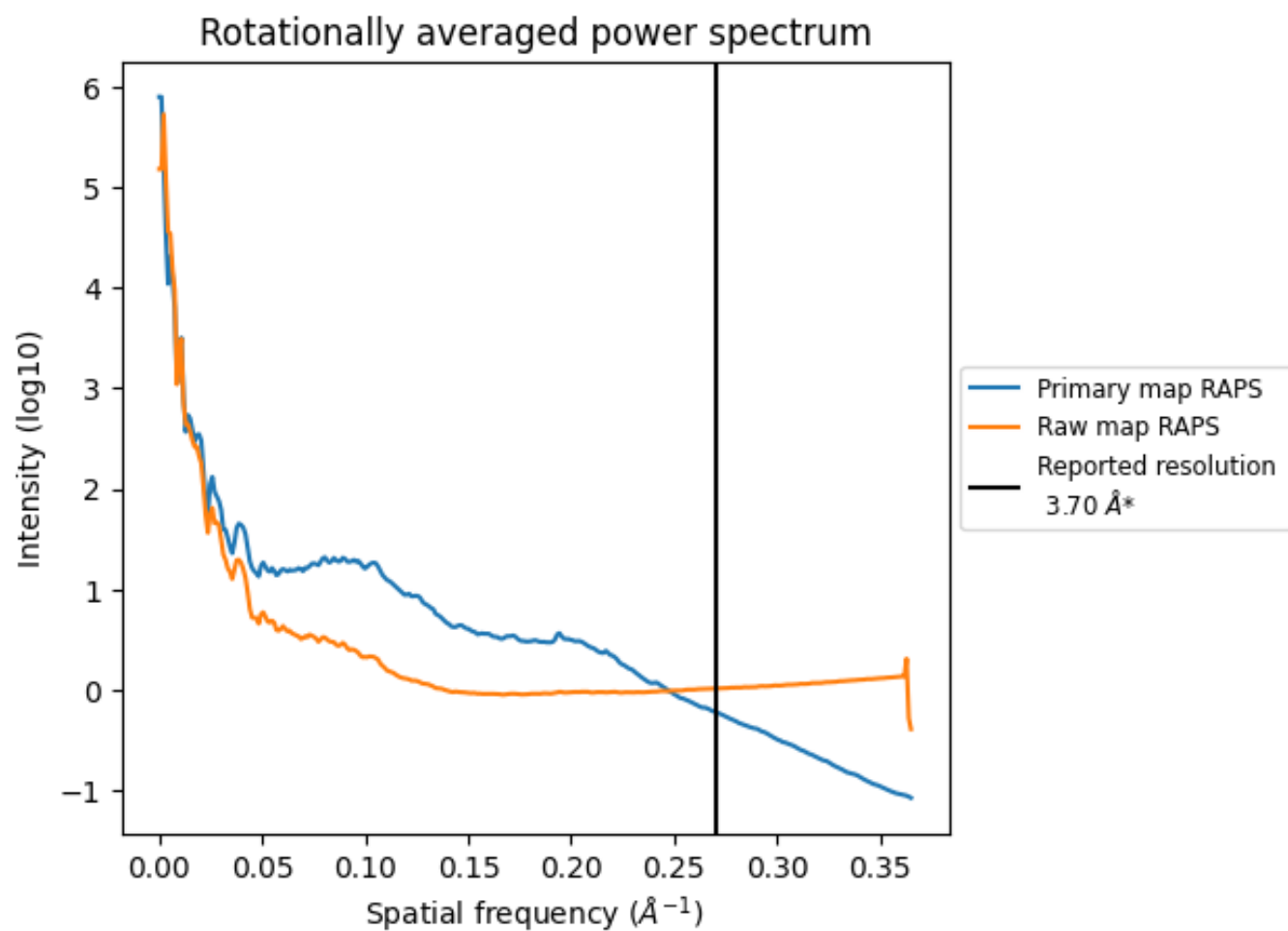


The volume at the recommended contour level is 8171 nm<sup>3</sup>; this corresponds to an approximate mass of 7381 kDa.

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 ⓘ

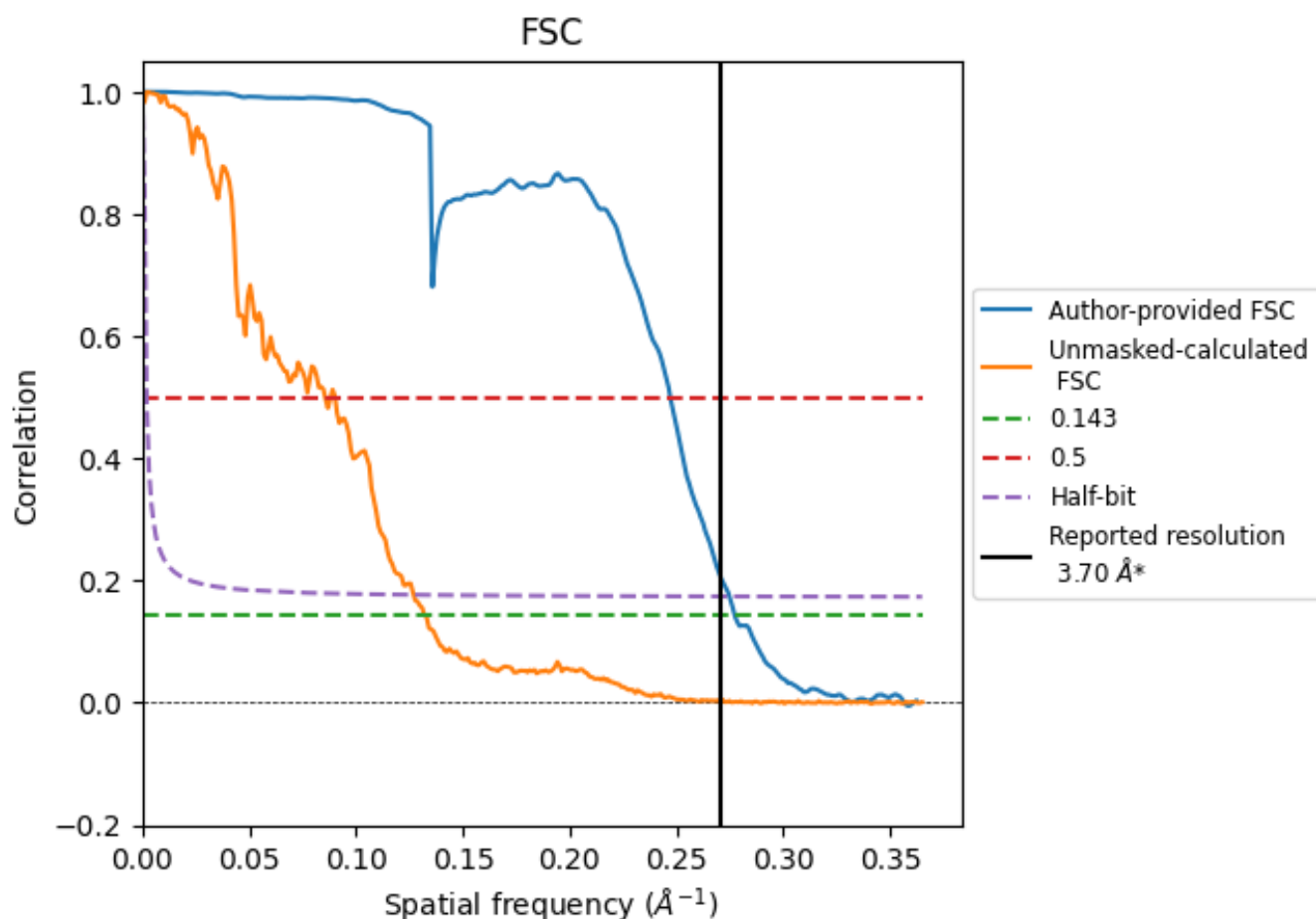


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

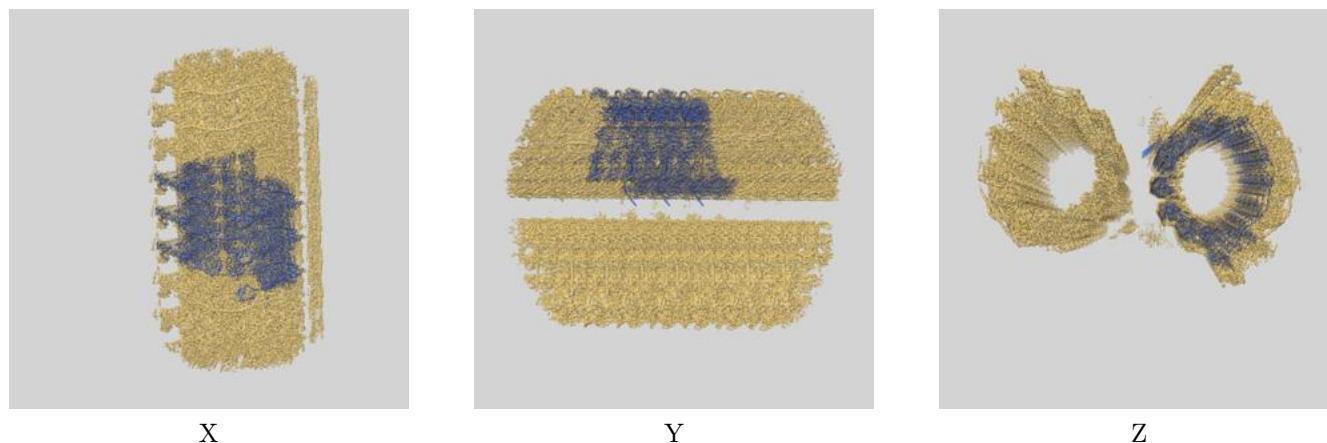
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.61	4.05	3.64
Unmasked-calculated*	7.56	11.68	7.87

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.56 differs from the reported value 3.7 by more than 10 %

## 9 Map-model fit [i](#)

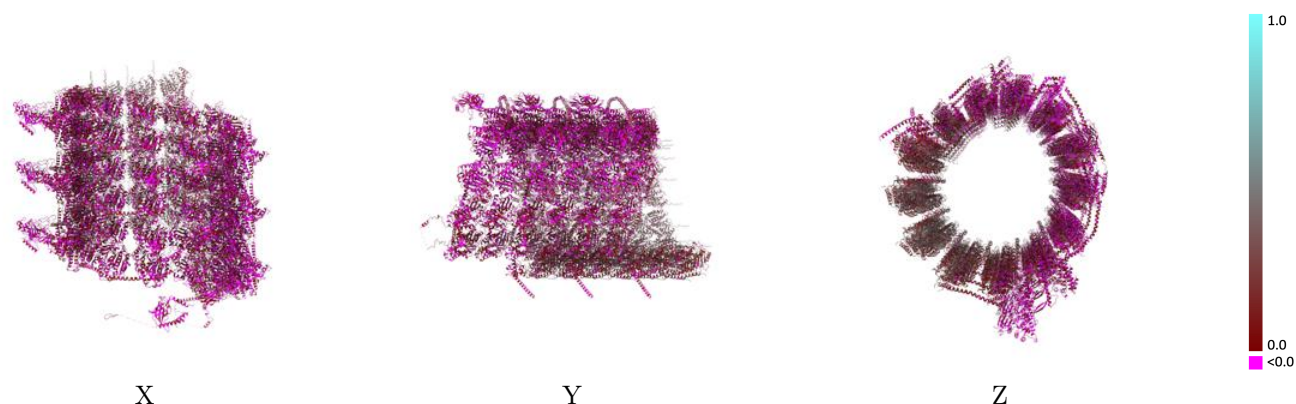
This section contains information regarding the fit between EMDB map EMD-49872 and PDB model 9NW3. Per-residue inclusion information can be found in section [3](#) on page [22](#).

### 9.1 Map-model overlay [i](#)



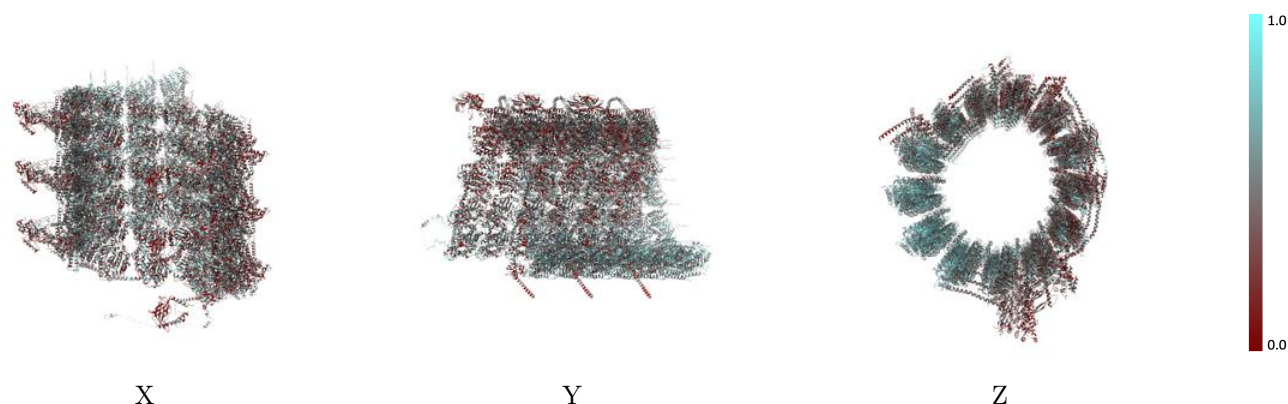
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



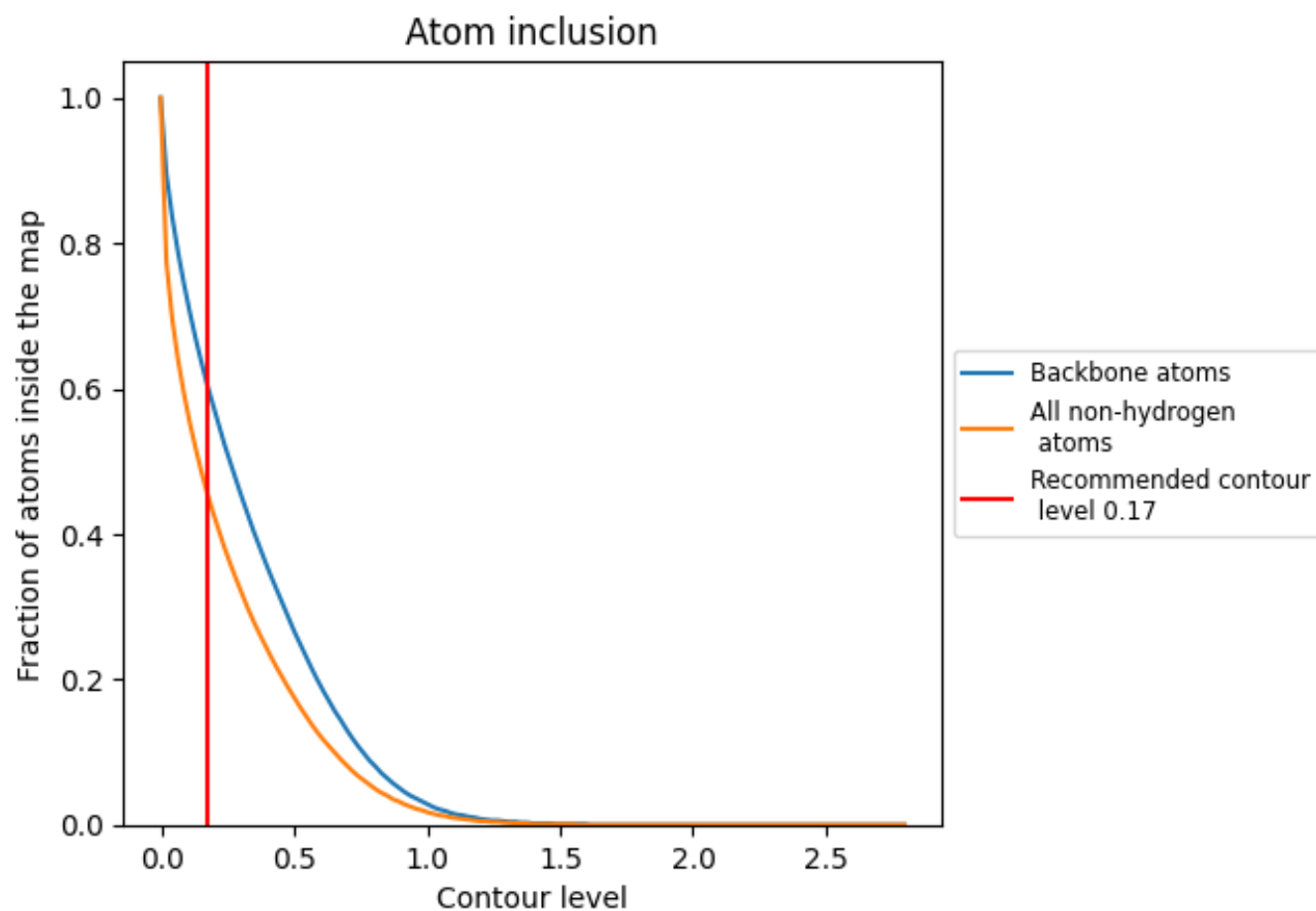
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.17).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 60% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4550	0.1370
1A	0.2930	0.0820
1B	0.2820	0.0750
1C	0.3090	0.0770
2A	0.3760	0.0670
2B	0.3770	0.0590
2C	0.3700	0.0770
3A	0.2760	0.0160
3B	0.2780	0.0100
3C	0.2670	0.0100
4A	0.5490	0.2790
4B	0.5460	0.2330
4C	0.5210	0.2260
4D	0.5490	0.1840
5A	0.3430	0.0690
5B	0.3440	0.0600
5C	0.3330	0.0520
6A	0.2950	0.0020
6B	0.3240	0.0110
6C	0.2940	-0.0160
7A	0.3110	0.0210
7B	0.3240	0.0160
7C	0.3320	0.0460
7D	0.2980	0.0160
7E	0.3240	0.0440
7F	0.3060	0.0270
8A	0.5560	0.2440
8B	0.4600	0.2670
8C	0.5180	0.2650
8D	0.5820	0.3310
8E	0.6300	0.3780
8F	0.6090	0.3700
8G	0.5770	0.3190
8H	0.5820	0.3340
8I	0.5820	0.3400



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Chain	Atom inclusion	Q-score
8J	 0.6140	 0.2900
8K	 0.5930	 0.2960
8L	 0.5560	 0.2870
8M	 0.6190	 0.2670
8N	 0.6450	 0.2700
8O	 0.5980	 0.2560
8P	 0.6090	 0.2170
8Q	 0.6090	 0.2400
8R	 0.6140	 0.2470
8S	 0.4390	 0.1840
8T	 0.4920	 0.2080
8U	 0.4920	 0.2010
8V	 0.4020	 0.1670
8W	 0.3230	 0.1630
8X	 0.3180	 0.1780
8Y	 0.2590	 0.0830
8Z	 0.4340	 0.1630
9A	 0.4340	 0.1580
AA	 0.5470	 0.2130
AB	 0.5180	 0.1970
AC	 0.5490	 0.2330
AD	 0.5180	 0.2090
AE	 0.5410	 0.2300
AF	 0.5170	 0.2090
BA	 0.5930	 0.2920
BB	 0.6010	 0.3000
BC	 0.6040	 0.3080
BD	 0.5960	 0.2990
BE	 0.6010	 0.3070
BF	 0.5950	 0.3010
CA	 0.6260	 0.3110
CB	 0.6220	 0.3150
CC	 0.6320	 0.3320
CD	 0.6150	 0.3200
CE	 0.6300	 0.3330
CF	 0.6100	 0.3180
DA	 0.5770	 0.2440
DB	 0.5780	 0.2570
DC	 0.5930	 0.2760
DD	 0.5840	 0.2740
DE	 0.6070	 0.2910
DF	 0.5910	 0.2810

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Chain	Atom inclusion	Q-score
EA	 0.4910	 0.1470
EB	 0.4920	 0.1590
EC	 0.5110	 0.1740
ED	 0.5160	 0.1840
EE	 0.5280	 0.1930
EF	 0.5370	 0.1920
FA	 0.4420	 0.0830
FB	 0.4360	 0.0790
FC	 0.4550	 0.1020
FD	 0.4540	 0.0930
FE	 0.4710	 0.1180
FF	 0.4690	 0.1070
GA	 0.4110	 0.0660
GB	 0.3980	 0.0560
GC	 0.3960	 0.0590
GD	 0.4050	 0.0600
GE	 0.3990	 0.0610
GF	 0.4020	 0.0600
HA	 0.4130	 0.0920
HB	 0.4100	 0.0860
HC	 0.4060	 0.0940
HD	 0.4010	 0.0810
HE	 0.3880	 0.0820
HF	 0.3920	 0.0700
IA	 0.4020	 0.0900
IB	 0.4040	 0.1020
IC	 0.4120	 0.0990
ID	 0.4030	 0.0910
IE	 0.3970	 0.0860
IF	 0.3970	 0.0790
JA	 0.3890	 0.0790
JB	 0.3830	 0.0710
JC	 0.3810	 0.0730
JD	 0.3620	 0.0510
JE	 0.3660	 0.0600
JF	 0.3490	 0.0390
KA	 0.3580	 0.0460
KB	 0.3710	 0.0480
KC	 0.3560	 0.0400
KD	 0.3740	 0.0360
KE	 0.3550	 0.0260
KF	 0.3780	 0.0200

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Chain	Atom inclusion	Q-score
LA	 0.4220	 0.0710
LB	 0.4300	 0.0830
LC	 0.4260	 0.0750
LD	 0.4330	 0.0810
LE	 0.4340	 0.0670
LF	 0.4380	 0.0680
MA	 0.4860	 0.1590
MB	 0.4740	 0.1390
MC	 0.4840	 0.1490
MD	 0.4750	 0.1330
ME	 0.4740	 0.1310
MF	 0.4850	 0.1170