



## wwPDB EM Validation Summary Report ⓘ

Mar 18, 2025 – 09:27 PM EDT

PDB ID : 9E2G  
EMDB ID : EMD-47451  
Title : Cryo-EM structure of 48 nm repeat of microtubule doublet from *T. brucei* flagellum  
Authors : Xia, X.; Shimogawa, M.M.; Wang, H.; Liu, S.; Wijono, A.; Langousis, G.; Kassem, A.M.; Wohlschlegel, J.A.; Hill, K.; Zhou, Z.H.  
Deposited on : 2024-10-22  
Resolution : 2.80 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>.

---

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.41.4

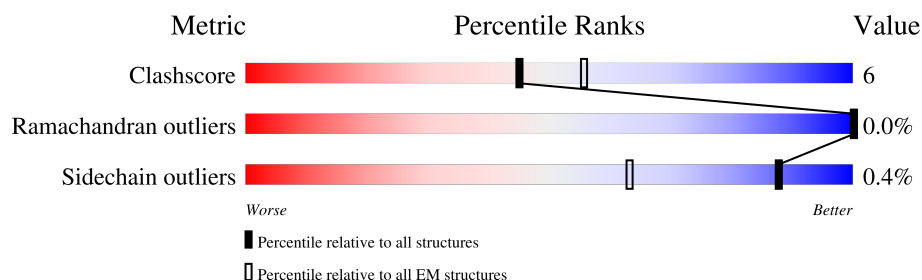
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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














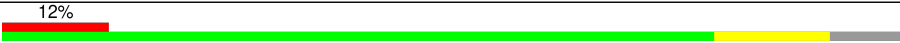




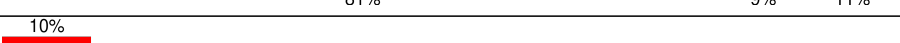
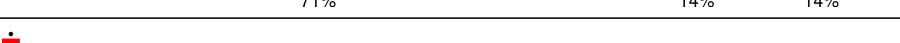



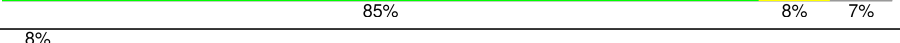



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	0A	752	<div> <div>16%</div> <div>77%</div> <div>10%</div> <div>12%</div> </div>
1	0B	752	<div> <div>24%</div> <div>87%</div> <div>10%</div> <div>•</div> </div>
1	0C	752	<div> <div>18%</div> <div>88%</div> <div>10%</div> <div>•</div> </div>
1	0D	752	<div> <div>16%</div> <div>83%</div> <div>•</div> </div>
2	0E	779	<div> <div>16%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div>
3	0F	724	<div> <div>8%</div> <div>77%</div> <div>15%</div> <div>8%</div> </div>
4	0G	779	<div> <div>22%</div> <div>83%</div> <div>14%</div> <div>•</div> </div>
5	0H	385	<div> <div>•</div> <div>59%</div> <div>9%</div> <div>32%</div> </div>





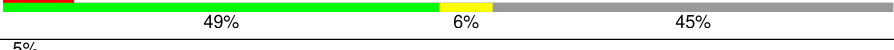
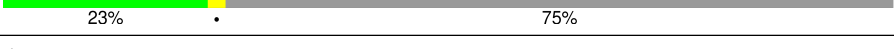

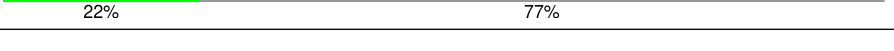
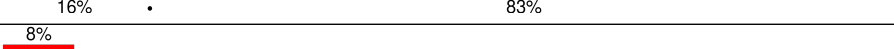
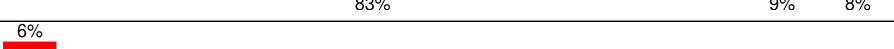
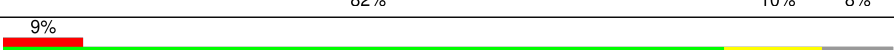

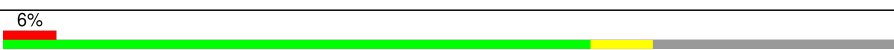

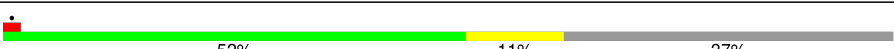





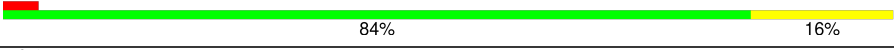
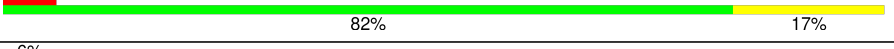



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	0I	385	
5	0J	385	
5	0K	385	
6	0M	483	
6	0N	483	
7	0O	436	
7	0P	436	
8	0Q	334	
9	0R	349	
10	0S	422	
11	0T	422	
12	0U	331	
13	0V	219	
14	0W	130	
15	0X	270	
16	0Y	301	
17	0Z	552	
18	1A	359	
19	1B	297	
20	1C	282	
21	1D	320	
22	1E	249	
23	1F	254	
24	1G	182	
25	1H	386	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
26	1I	417	
26	1J	417	
27	1K	415	
27	1L	415	
28	1M	415	
28	1N	415	
29	1O	247	
29	1P	247	
29	4X	247	
30	1Q	300	
30	1R	300	
30	1S	300	
31	1T	312	
31	1U	312	
32	1V	294	
32	1W	294	
32	1X	294	
32	1Y	294	
32	1Z	294	
32	2A	294	
33	2B	629	
33	2C	629	
33	2D	629	
34	2E	274	
34	2F	274	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
35	2G	374	
35	2H	374	
36	2I	369	
36	2J	369	
36	2K	369	
37	2L	272	
37	2M	272	
38	2N	262	
39	2O	483	
39	2P	483	
39	2Q	483	
39	2R	483	
40	2S	515	
40	2T	515	
40	2U	515	
41	2V	348	
41	2W	348	
41	2X	348	
41	2Y	348	
41	2Z	348	
41	3A	348	
41	3B	348	
41	3C	348	
41	3D	348	
42	3E	266	

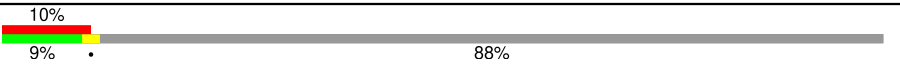


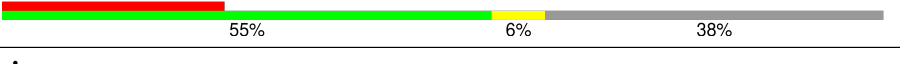

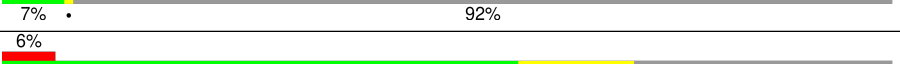




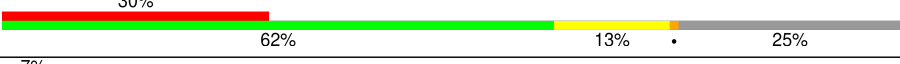




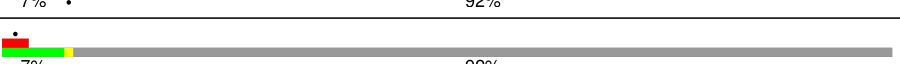
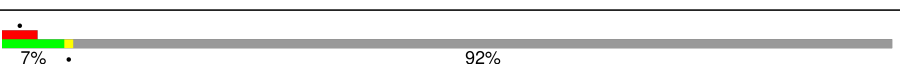
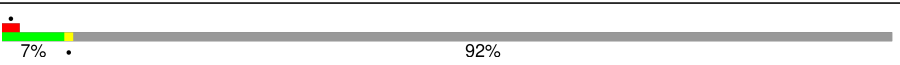


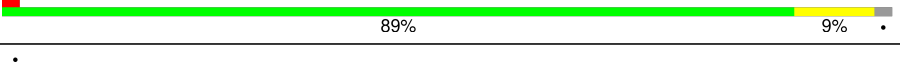

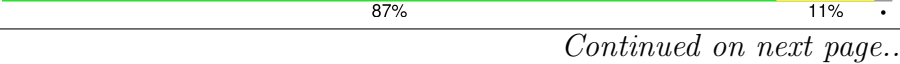


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
42	3F	266	
42	3G	266	
42	3H	266	
42	3I	266	
42	3J	266	
42	3K	266	
42	3L	266	
42	3M	266	
42	3N	266	
42	3O	266	
42	3P	266	
43	3Q	270	
44	3R	325	
45	3S	191	
46	3T	320	
46	3U	320	
47	3V	278	
47	3W	278	
47	3X	278	
48	3Y	269	
48	3Z	269	
48	4A	269	
49	4B	420	
49	4C	420	
49	4D	420	



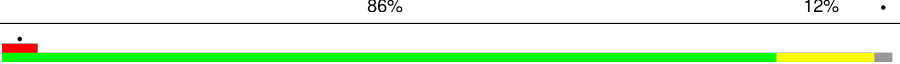
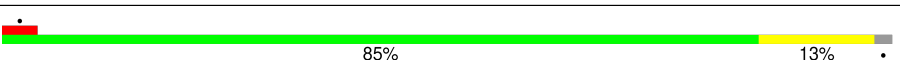


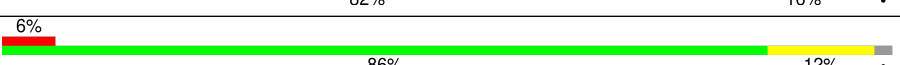

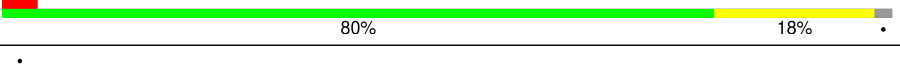




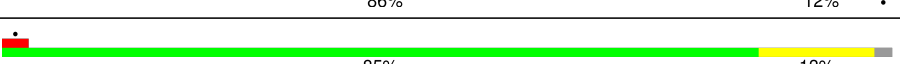

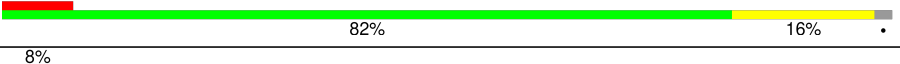

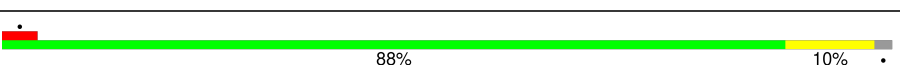





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
50	4E	337	
50	4F	337	
50	4G	337	
51	4H	329	
52	4I	350	
52	4J	350	
53	4K	286	
53	4L	286	
54	4M	193	
54	4N	193	
54	4O	193	
55	4P	191	
56	4Q	166	
57	4R	161	
57	4S	161	
57	4Y	161	
58	4T	867	
58	4U	867	
58	4V	867	
58	4W	867	
59	AA	451	
59	AC	451	
59	AE	451	
59	AG	451	
59	AI	451	







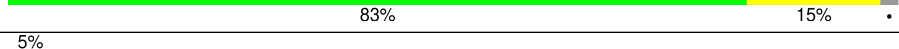
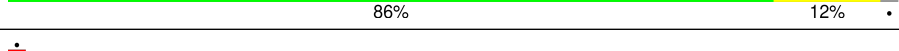
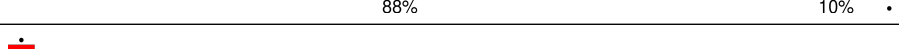
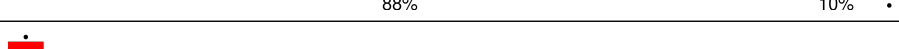
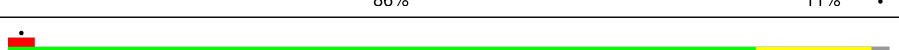

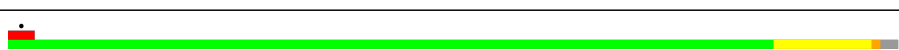

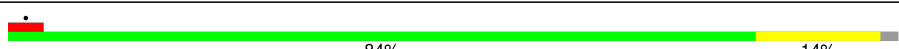





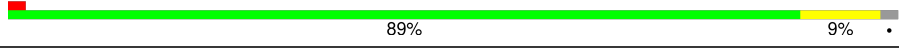
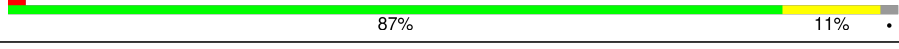



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	AK	451	
59	AM	451	
59	AO	451	
59	AQ	451	
59	AS	451	
59	AU	451	
59	AW	451	
59	AY	451	
59	BA	451	
59	BC	451	
59	BE	451	
59	BG	451	
59	BI	451	
59	BK	451	
59	BM	451	
59	BO	451	
59	BQ	451	
59	BS	451	
59	BU	451	
59	BW	451	
59	BX	451	
59	BZ	451	
59	CB	451	
59	CD	451	
59	CF	451	







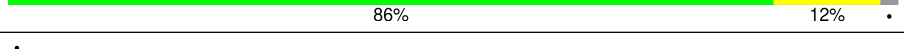
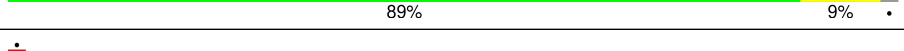
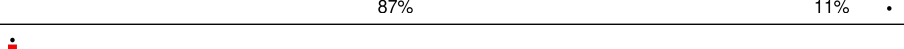
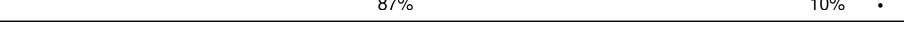
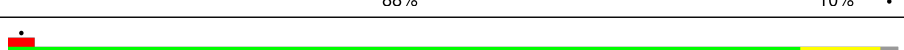

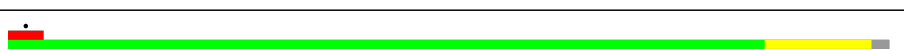

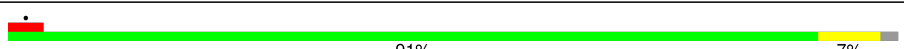





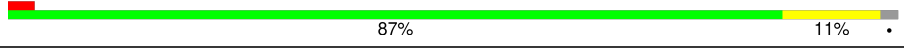
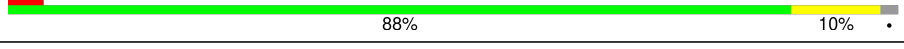



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	CH	451	
59	CJ	451	
59	CM	451	
59	CO	451	
59	CQ	451	
59	CS	451	
59	CU	451	
59	CW	451	
59	CY	451	
59	DA	451	
59	DC	451	
59	DE	451	
59	DG	451	
59	DI	451	
59	DK	451	
59	DM	451	
59	DO	451	
59	DQ	451	
59	DS	451	
59	DU	451	
59	DX	451	
59	DZ	451	
59	EB	451	
59	ED	451	
59	EF	451	






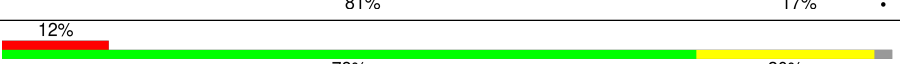
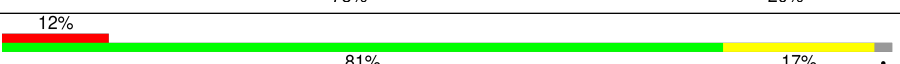
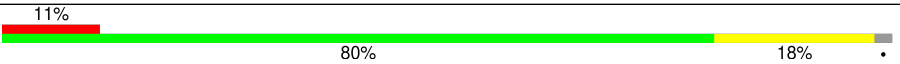


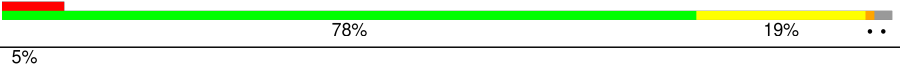
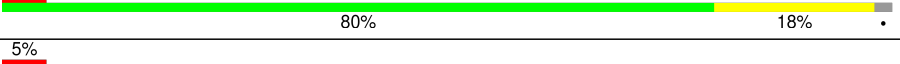

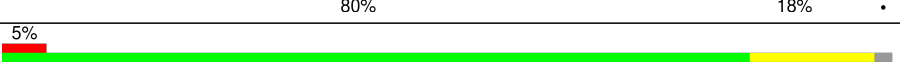
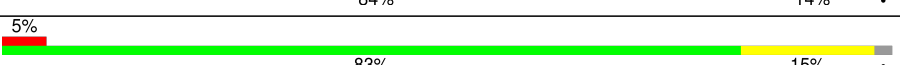










Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
59	EH	451	 89% 9%
59	EJ	451	 88% 10%
59	EL	451	 87% 11%
59	EN	451	 85% 13%
59	EP	451	 84% 14%
59	ER	451	 82% 15%
59	ET	451	 86% 12%
59	EV	451	 89% 9%
59	EX	451	 87% 11%
59	EZ	451	 87% 10%
59	FB	451	 88% 10%
59	FD	451	 89% 9%
59	FF	451	 90% 8%
59	FH	451	 85% 12%
59	FJ	451	 88% 10%
59	FL	451	 91% 7%
59	FN	451	 90% 8%
59	FP	451	 88% 10%
59	FR	451	 89% 9%
59	FT	451	 88% 10% 5%
59	FU	451	 84% 14%
59	FW	451	 87% 11%
59	FY	451	 88% 10%
59	GA	451	 88% 10%
59	GC	451	 85% 13%




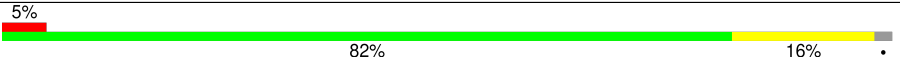
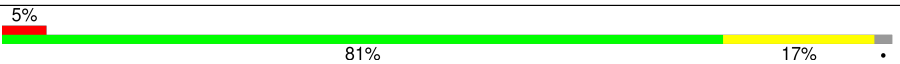

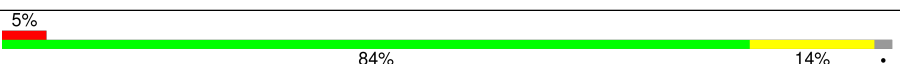
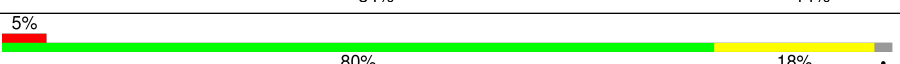
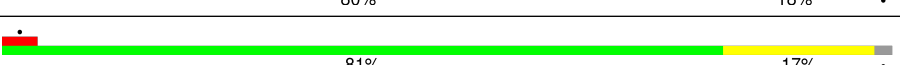
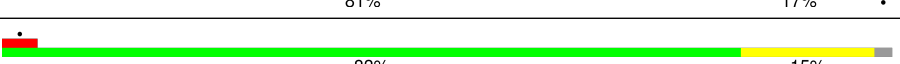
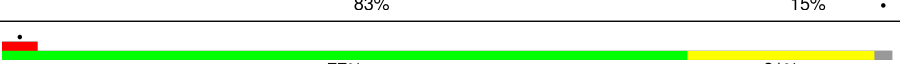
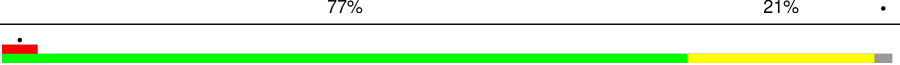

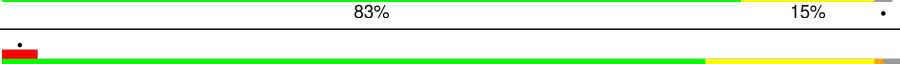



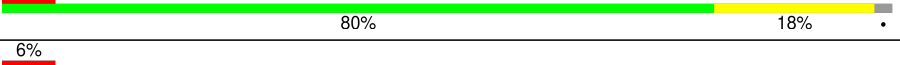

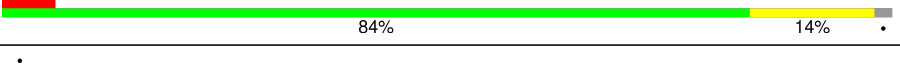
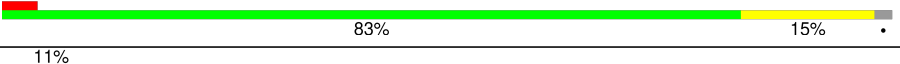


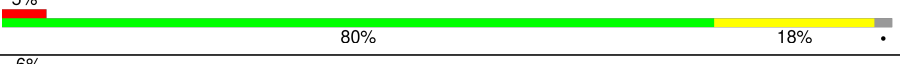

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
59	GE	451	
59	GG	451	
59	GH	451	
59	GJ	451	
59	GL	451	
59	GN	451	
59	GP	451	
59	GR	451	
59	GT	451	
59	GU	451	
59	GW	451	
59	GY	451	
59	HA	451	
59	HC	451	
59	HE	451	
59	HG	451	
59	HI	451	
59	HK	451	
59	HM	451	
59	HO	451	
59	HQ	451	
59	HT	451	
59	HV	451	
59	HX	451	
59	HZ	451	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	IB	451	
59	ID	451	
59	IG	451	
59	II	451	
59	IK	451	
59	IM	451	
59	IO	451	
59	IQ	451	
59	IT	451	
59	IV	451	
59	IX	451	
59	IZ	451	
59	JB	451	
59	JD	451	
59	JF	451	
59	JH	451	
59	JJ	451	
59	JL	451	
59	JN	451	
59	JP	451	
59	JQ	451	
59	JS	451	
59	JU	451	
59	JW	451	
59	JY	451	

Continued on next page...







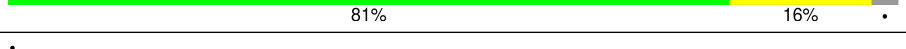
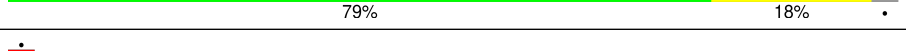
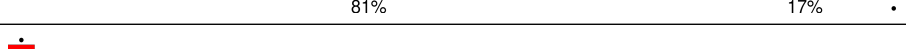
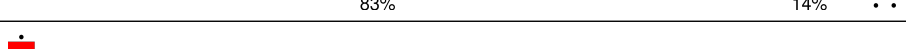
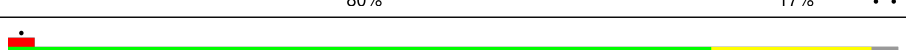

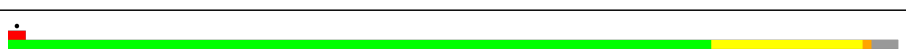

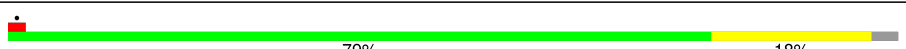





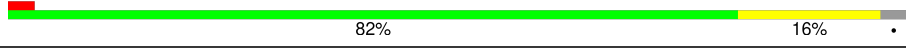
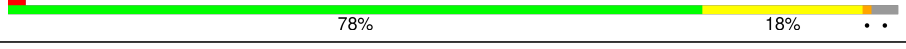





Continued from previous page...

Mol	Chain	Length	Quality of chain
59	KA	451	
59	KC	451	
59	KD	451	
59	KF	451	
59	KH	451	
59	KJ	451	
59	KL	451	
59	KN	451	
59	KP	451	
59	KQ	451	
59	KS	451	
59	KU	451	
59	KW	451	
59	KY	451	
59	LA	451	
60	AB	442	
60	AD	442	
60	AF	442	
60	AH	442	
60	AJ	442	
60	AL	442	
60	AN	442	
60	AP	442	
60	AR	442	
60	AT	442	







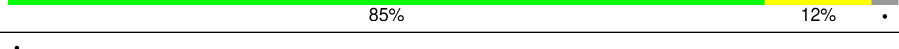
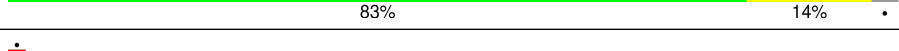
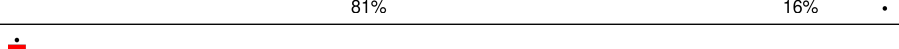
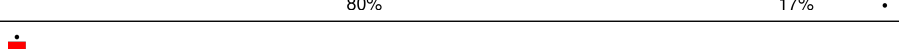
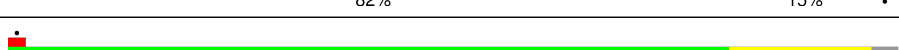

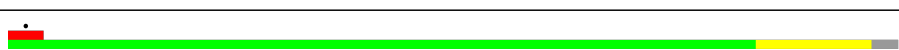

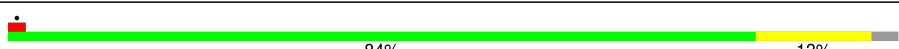





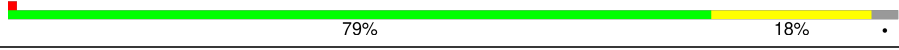
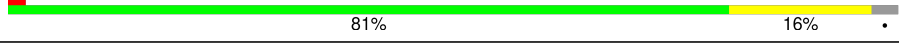



Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
60	AV	442	
60	AX	442	
60	AZ	442	
60	BB	442	
60	BD	442	
60	BF	442	
60	BH	442	
60	BJ	442	
60	BL	442	
60	BN	442	
60	BP	442	
60	BR	442	
60	BT	442	
60	BV	442	
60	BY	442	
60	CA	442	
60	CC	442	
60	CE	442	
60	CG	442	
60	CI	442	
60	CL	442	
60	CN	442	
60	CP	442	
60	CR	442	
60	CT	442	







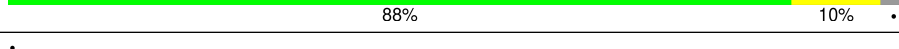
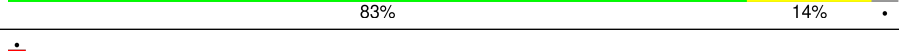
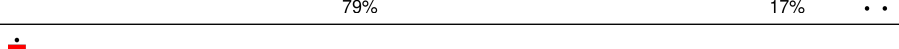
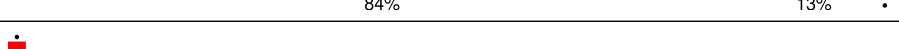
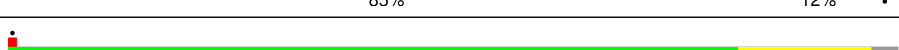

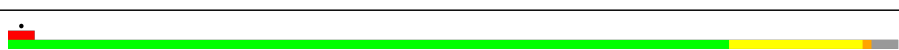

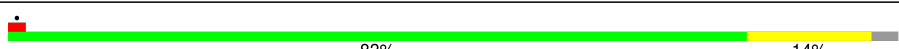





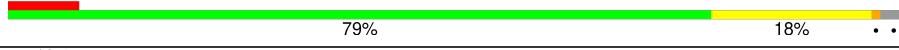
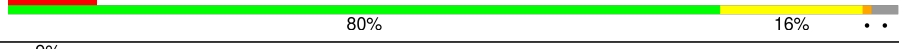



*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
60	CV	442	
60	CX	442	
60	CZ	442	
60	DB	442	
60	DD	442	
60	DF	442	
60	DH	442	
60	DJ	442	
60	DL	442	
60	DN	442	
60	DP	442	
60	DR	442	
60	DT	442	
60	DV	442	
60	DW	442	
60	DY	442	
60	EA	442	
60	EC	442	
60	EE	442	
60	EG	442	
60	EI	442	
60	EK	442	
60	EM	442	
60	EO	442	
60	EQ	442	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
60	ES	442	
60	EU	442	
60	EW	442	
60	EY	442	
60	FA	442	
60	FC	442	
60	FE	442	
60	FG	442	
60	FI	442	
60	FK	442	
60	FM	442	
60	FO	442	
60	FQ	442	
60	FS	442	
60	FV	442	
60	FX	442	
60	FZ	442	
60	GB	442	
60	GD	442	
60	GF	442	
60	GI	442	
60	GK	442	
60	GM	442	
60	GO	442	
60	GQ	442	






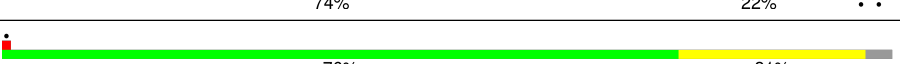
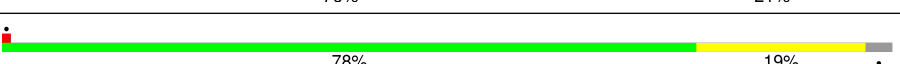
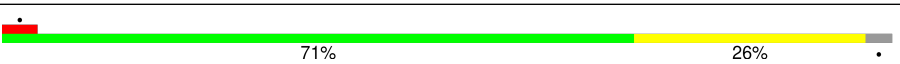


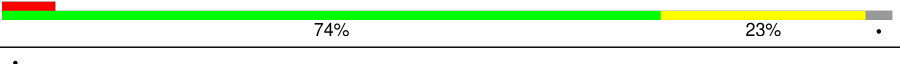
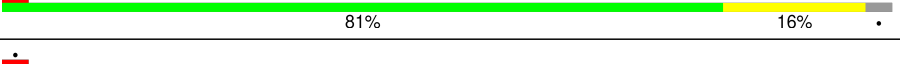

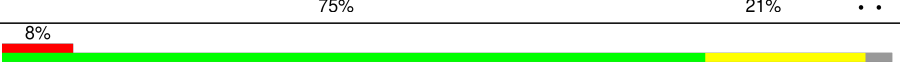
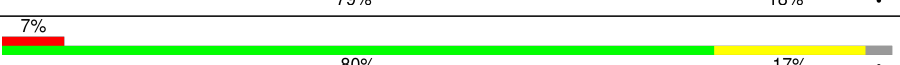










*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
60	GS	442	
60	GV	442	
60	GX	442	
60	GZ	442	
60	HB	442	
60	HD	442	
60	HF	442	
60	HH	442	
60	HJ	442	
60	HL	442	
60	HN	442	
60	HP	442	
60	HR	442	
60	HS	442	
60	HU	442	
60	HW	442	
60	HY	442	
60	IA	442	
60	IC	442	
60	IE	442	
60	IF	442	
60	IH	442	
60	IJ	442	
60	IL	442	
60	IN	442	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
60	IP	442	
60	IR	442	
60	IS	442	
60	IU	442	
60	IW	442	
60	IY	442	
60	JA	442	
60	JC	442	
60	JE	442	
60	JG	442	
60	JI	442	
60	JK	442	
60	JM	442	
60	JO	442	
60	JR	442	
60	JT	442	
60	JV	442	
60	JX	442	
60	JZ	442	
60	KB	442	
60	KE	442	
60	KG	442	
60	KI	442	
60	KK	442	
60	KM	442	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
60	KO	442	
60	KR	442	
60	KT	442	
60	KV	442	
60	KX	442	
60	KZ	442	
60	LB	442	

## 2 Entry composition [i](#)

There are 64 unique types of molecules in this entry. The entry contains 1215524 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 EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0A	662	Total	C	N	O	S	0	0
			5390	3423	929	1014	24		
1	0B	730	Total	C	N	O	S	0	0
			5933	3757	1026	1121	29		
1	0C	734	Total	C	N	O	S	0	0
			5972	3782	1036	1125	29		
1	0D	131	Total	C	N	O	S	0	0
			1064	685	176	200	3		

- Molecule 2 is a protein called EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0E	730	Total	C	N	O	S	0	0
			5862	3718	1025	1088	31		

- Molecule 3 is a protein called Rib72 protein-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0F	665	Total	C	N	O	S	0	0
			5389	3412	938	1011	28		

- Molecule 4 is a protein called CMF34/CARP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	0G	758	Total	C	N	O	S	0	0
			6157	3875	1093	1162	27		

- Molecule 5 is a protein called Flagellar protofilament ribbon protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	0H	263	Total	C	N	O	S	0	0
			2274	1382	453	430	9		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
5	0I	119	Total	C	N	O	S	0	0
			1052	644	205	196	7		
5	0J	44	Total	C	N	O	S	0	0
			376	228	80	64	4		
5	0K	363	Total	C	N	O	S	0	0
			3130	1907	616	593	14		

- Molecule 6 is a protein called Cilia- and flagella-associated protein 53.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	0M	304	Total	C	N	O	S	0	0
			2576	1553	530	482	11		
6	0N	169	Total	C	N	O	S	0	0
			1449	889	293	263	4		

- Molecule 7 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	0O	154	Total	C	N	O	S	0	0
			1288	780	255	247	6		
7	0P	303	Total	C	N	O	S	0	0
			2584	1574	505	502	3		

- Molecule 8 is a protein called Nucleoside diphosphate kinase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	0Q	332	Total	C	N	O	S	0	0
			2587	1637	446	484	20		

- Molecule 9 is a protein called Nucleoside diphosphate kinase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0R	343	Total	C	N	O	S	0	0
			2685	1703	472	493	17		

- Molecule 10 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	0S	419	Total	C	N	O	S	0	0
			3331	2094	584	638	15		

- Molecule 11 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	0T	414	Total	C	N	O	S	0	0
			3295	2050	603	624	18		

- Molecule 12 is a protein called Cyclic nucleotide-binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	0U	306	Total	C	N	O	S	0	0
			2446	1557	422	454	13		

- Molecule 13 is a protein called TbMIP23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	0V	170	Total	C	N	O	S	0	0
			1262	795	219	241	7		

- Molecule 14 is a protein called FAP141.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	0W	105	Total	C	N	O	S	0	0
			836	503	167	161	5		

- Molecule 15 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	0X	181	Total	C	N	O	S	0	0
			1457	935	250	267	5		

- Molecule 16 is a protein called Calpain-like cysteine peptidase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	0Y	269	Total	C	N	O	S	0	0
			2100	1327	366	392	15		

- Molecule 17 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	0Z	472	Total	C	N	O	S	0	0
			3717	2352	651	692	22		

- Molecule 18 is a protein called Calcium-binding protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1A	357	Total	C	N	O	S	0	0
			2920	1842	511	551	16		

- Molecule 19 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1B	276	Total	C	N	O	S	0	0
			2252	1422	411	408	11		

- Molecule 20 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1C	247	Total	C	N	O	S	0	0
			1908	1188	346	360	14		

- Molecule 21 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1D	298	Total	C	N	O	S	0	0
			2371	1516	415	427	13		

- Molecule 22 is a protein called FAP107/MC11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1E	237	Total	C	N	O	S	0	0
			1880	1180	325	363	12		

- Molecule 23 is a protein called T. brucei spp.-specific protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1F	234	Total	C	N	O	S	0	0
			1861	1148	338	365	10		

- Molecule 24 is a protein called FAP95/MC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1G	165	Total	C	N	O	S	0	0
			1287	808	234	239	6		

- Molecule 25 is a protein called FAP129.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1H	258	Total	C	N	O	S	0	0
			2005	1242	371	379	13		

- Molecule 26 is a protein called T. brucei spp.-specific protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1I	320	Total	C	N	O	S	0	0
			2535	1574	465	490	6		
26	1J	89	Total	C	N	O	S	0	0
			707	444	129	132	2		

- Molecule 27 is a protein called FAP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1K	269	Total	C	N	O	S	0	0
			2119	1307	411	387	14		
27	1L	138	Total	C	N	O	S	0	0
			1103	680	209	204	10		

- Molecule 28 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1M	227	Total	C	N	O	S	0	0
			1778	1109	330	331	8		
28	1N	105	Total	C	N	O	S	0	0
			814	506	150	156	2		

- Molecule 29 is a protein called TbRib26b.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1O	120	Total	C	N	O	S	0	0
			953	598	170	182	3		
29	1P	56	Total	C	N	O		0	0
			423	271	72	80			
29	4X	42	Total	C	N	O	S	0	0
			348	221	60	65	2		

- Molecule 30 is a protein called PACRGA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1Q	277	Total	C	N	O	S	0	0
			2223	1425	399	393	6		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1R	277	Total	C	N	O	S	0	0
			2223	1425	399	393	6		
30	1S	277	Total	C	N	O	S	0	0
			2223	1425	399	393	6		

- Molecule 31 is a protein called PACRGB.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1T	226	Total	C	N	O	S	0	0
			1819	1174	311	329	5		
31	1U	226	Total	C	N	O	S	0	0
			1819	1174	311	329	5		

- Molecule 32 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1V	185	Total	C	N	O	S	0	0
			1537	985	271	273	8		
32	1W	185	Total	C	N	O	S	0	0
			1537	985	271	273	8		
32	1X	185	Total	C	N	O	S	0	0
			1537	985	271	273	8		
32	1Y	185	Total	C	N	O	S	0	0
			1537	985	271	273	8		
32	1Z	185	Total	C	N	O	S	0	0
			1537	985	271	273	8		
32	2A	185	Total	C	N	O	S	0	0
			1537	985	271	273	8		

- Molecule 33 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2B	620	Total	C	N	O	S	0	0
			4671	2918	821	901	31		
33	2C	627	Total	C	N	O	S	0	0
			4727	2953	829	914	31		
33	2D	627	Total	C	N	O	S	0	0
			4727	2953	829	914	31		

- Molecule 34 is a protein called Enkurin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	2E	240	Total	C	N	O	S	0	0
			1867	1166	339	358	4		
34	2F	240	Total	C	N	O	S	0	0
			1867	1166	339	358	4		

- Molecule 35 is a protein called Enkurin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2G	175	Total	C	N	O	S	0	0
			1456	927	258	266	5		
35	2H	150	Total	C	N	O	S	0	0
			1248	786	225	232	5		

- Molecule 36 is a protein called MC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2I	279	Total	C	N	O	S	0	0
			2217	1384	418	404	11		
36	2J	275	Total	C	N	O	S	0	0
			2186	1366	412	398	10		
36	2K	275	Total	C	N	O	S	0	0
			2186	1366	412	398	10		

- Molecule 37 is a protein called MC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2L	238	Total	C	N	O	S	0	0
			1900	1188	349	355	8		
37	2M	238	Total	C	N	O	S	0	0
			1900	1188	349	355	8		

- Molecule 38 is a protein called CCDC81 HU domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2N	239	Total	C	N	O	S	0	0
			1911	1207	342	348	14		

- Molecule 39 is a protein called Cilia- and flagella-associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	2O	193	Total	C	N	O	S	0	0
			1599	965	306	315	13		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
39	2P	303	Total	C	N	O	S	0	0
			2590	1566	517	496	11		
39	2Q	321	Total	C	N	O	S	0	0
			2678	1615	524	524	15		
39	2R	189	Total	C	N	O	S	0	0
			1613	968	325	311	9		

- Molecule 40 is a protein called Trichohyalin-pectin-homology domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	2S	79	Total	C	N	O	S	0	0
			647	394	122	128	3		
40	2T	437	Total	C	N	O	S	0	0
			3667	2228	713	707	19		
40	2U	66	Total	C	N	O	S	0	0
			564	346	105	110	3		

- Molecule 41 is a protein called Trichohyalin-pectin-homology domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	2V	126	Total	C	N	O	S	0	0
			1062	658	206	195	3		
41	2W	233	Total	C	N	O	S	0	0
			1977	1201	383	381	12		
41	2X	52	Total	C	N	O	S	0	0
			441	274	87	79	1		
41	2Y	333	Total	C	N	O	S	0	0
			2808	1716	549	530	13		
41	2Z	272	Total	C	N	O	S	0	0
			2259	1382	441	424	12		
41	3A	110	Total	C	N	O	S	0	0
			954	580	188	182	4		
41	3B	173	Total	C	N	O	S	0	0
			1421	877	275	263	6		
41	3C	213	Total	C	N	O	S	0	0
			1797	1088	349	348	12		
41	3D	253	Total	C	N	O	S	0	0
			2146	1307	417	410	12		

- Molecule 42 is a protein called STOP axonemal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3E	66	Total	C	N	O	S	0	0
			517	329	91	94	3		
42	3F	186	Total	C	N	O	S	0	0
			1483	940	261	273	9		
42	3G	174	Total	C	N	O	S	0	0
			1388	889	242	251	6		
42	3H	80	Total	C	N	O	S	0	0
			638	404	110	118	6		
42	3I	112	Total	C	N	O	S	0	0
			890	566	156	163	5		
42	3J	147	Total	C	N	O	S	0	0
			1184	745	214	218	7		
42	3K	51	Total	C	N	O	S	0	0
			401	253	75	71	2		
42	3L	188	Total	C	N	O	S	0	0
			1496	947	260	279	10		
42	3M	191	Total	C	N	O	S	0	0
			1526	974	267	279	6		
42	3N	63	Total	C	N	O	S	0	0
			497	312	86	93	6		
42	3O	123	Total	C	N	O	S	0	0
			977	620	172	180	5		
42	3P	121	Total	C	N	O	S	0	0
			967	612	173	176	6		

- Molecule 43 is a protein called MC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3Q	154	Total	C	N	O	S	0	0
			1293	822	224	238	9		

- Molecule 44 is a protein called MC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3R	163	Total	C	N	O	S	0	0
			1338	844	232	252	10		

- Molecule 45 is a protein called FAP90.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3S	161	Total	C	N	O	S	0	0
			1281	794	235	244	8		



- Molecule 46 is a protein called PBP36.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3T	174	Total	C	N	O	S	0	0
			1398	895	257	241	5		
46	3U	137	Total	C	N	O	S	0	0
			1120	704	212	199	5		

- Molecule 47 is a protein called Enkurin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3V	239	Total	C	N	O	S	0	0
			1919	1191	366	351	11		
47	3W	238	Total	C	N	O	S	0	0
			1905	1183	363	346	13		
47	3X	231	Total	C	N	O	S	0	0
			1843	1145	349	336	13		

- Molecule 48 is a protein called Enkurin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3Y	249	Total	C	N	O	S	0	0
			2017	1253	377	376	11		
48	3Z	120	Total	C	N	O	S	0	0
			990	609	183	193	5		
48	4A	239	Total	C	N	O	S	0	0
			1937	1202	360	364	11		

- Molecule 49 is a protein called PON3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	4B	104	Total	C	N	O	S	0	0
			858	528	167	155	8		
49	4C	108	Total	C	N	O	S	0	0
			889	548	171	162	8		
49	4D	101	Total	C	N	O	S	0	0
			831	513	159	151	8		

- Molecule 50 is a protein called PON4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4E	40	Total	C	N	O	S	0	0
			327	199	60	67	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4F	131	Total	C	N	O	S	0	0
			1054	633	203	208	10		
50	4G	40	Total	C	N	O	S	0	0
			327	199	60	67	1		

- Molecule 51 is a protein called MC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4H	203	Total	C	N	O	S	0	0
			1642	1020	321	293	8		

- Molecule 52 is a protein called FAP96C/MC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4I	130	Total	C	N	O	S	0	0
			1013	639	175	193	6		
52	4J	28	Total	C	N	O	S	0	0
			222	143	39	38	2		

- Molecule 53 is a protein called FAP96B.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4K	202	Total	C	N	O	S	0	0
			1650	1067	289	286	8		
53	4L	107	Total	C	N	O	S	0	0
			882	563	157	158	4		

- Molecule 54 is a protein called MOP23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4M	160	Total	C	N	O	S	0	0
			1380	847	261	270	2		
54	4N	160	Total	C	N	O	S	0	0
			1380	847	261	270	2		
54	4O	159	Total	C	N	O	S	0	0
			1373	843	260	268	2		

- Molecule 55 is a protein called MOP23B.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4P	144	Total	C	N	O	S	0	0
			1193	730	230	229	4		

- Molecule 56 is a protein called MOP23C.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4Q	71	Total	C	N	O	S	0	0
			583	368	100	113	2		

- Molecule 57 is a protein called KIAA1430 homologue.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4R	129	Total	C	N	O	S	0	0
			1116	682	225	204	5		
57	4S	134	Total	C	N	O	S	0	0
			1155	706	234	210	5		
57	4Y	38	Total	C	N	O	S	0	0
			327	201	67	58	1		

- Molecule 58 is a protein called Starmaker.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	4T	72	Total	C	N	O	S	0	0
			643	395	130	116	2		
58	4U	72	Total	C	N	O	S	0	0
			643	395	130	116	2		
58	4V	72	Total	C	N	O	S	0	0
			643	395	130	116	2		
58	4W	72	Total	C	N	O	S	0	0
			643	395	130	116	2		

- Molecule 59 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AA	442	Total	C	N	O	S	0	0
			3421	2158	582	660	21		
59	AC	442	Total	C	N	O	S	0	0
			3421	2158	582	660	21		
59	AE	442	Total	C	N	O	S	0	0
			3421	2158	582	660	21		
59	AG	442	Total	C	N	O	S	0	0
			3421	2158	582	660	21		
59	AI	442	Total	C	N	O	S	0	0
			3421	2158	582	660	21		
59	AK	442	Total	C	N	O	S	0	0
			3421	2158	582	660	21		
59	AM	442	Total	C	N	O	S	0	0
			3421	2158	582	660	21		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AO	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	AQ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	AS	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	AU	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	AW	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	AY	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BA	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BC	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BE	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BG	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BI	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BK	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BM	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BO	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BQ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BS	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BU	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BW	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BX	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	BZ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CB	442	Total 3421	C 2158	N 582	O 660	S 21	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CD	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CF	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CH	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CJ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CM	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CO	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CQ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CS	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CU	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CW	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	CY	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DA	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DC	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DE	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DG	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DI	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DK	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DM	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DO	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DQ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DS	442	Total 3421	C 2158	N 582	O 660	S 21	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
59	DU	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DX	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	DZ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	EB	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	ED	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	EF	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	EH	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	EJ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	EL	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	EN	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	EP	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	ER	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	ET	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	EV	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	EX	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	EZ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FB	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FD	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FF	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FH	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FJ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
59	FL	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FN	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FP	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FR	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FT	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FU	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FW	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	FY	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GA	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GC	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GE	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GG	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GH	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GJ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GL	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GN	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GP	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GR	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GT	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GU	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	GW	442	Total 3421	C 2158	N 582	O 660	S 21	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
59	GY	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HA	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HC	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HE	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HG	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HI	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HK	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HM	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HO	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HQ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HT	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HV	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HX	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	HZ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	IB	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	ID	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	IG	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	II	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	IK	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	IM	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	IO	442	Total 3421	C 2158	N 582	O 660	S 21	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
59	IQ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	IT	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	IV	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	IX	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	IZ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JB	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JD	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JF	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JH	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JJ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JL	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JN	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JP	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JQ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JS	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JU	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JW	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	JY	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KA	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KC	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KD	442	Total 3421	C 2158	N 582	O 660	S 21	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
59	KF	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KH	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KJ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KL	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KN	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KP	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KQ	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KS	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KU	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KW	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	KY	442	Total 3421	C 2158	N 582	O 660	S 21	0	0
59	LA	442	Total 3421	C 2158	N 582	O 660	S 21	0	0

- Molecule 60 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AB	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AD	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AF	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AH	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AJ	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AL	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AN	430	Total 3372	C 2114	N 575	O 652	S 31	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AP	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AR	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AT	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AV	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AX	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	AZ	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BB	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BD	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BF	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BH	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BJ	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BL	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BN	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BP	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BR	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BT	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BV	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	BY	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CA	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CC	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CE	430	Total 3372	C 2114	N 575	O 652	S 31	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CG	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CI	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CL	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CN	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CP	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CR	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CT	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CV	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CX	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	CZ	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DB	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DD	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DF	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DH	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DJ	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DL	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DN	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DP	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DR	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DT	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DV	430	Total 3372	C 2114	N 575	O 652	S 31	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
60	DW	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	DY	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EA	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EC	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EE	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EG	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EI	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EK	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EM	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EO	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EQ	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	ES	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EU	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EW	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	EY	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	FA	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	FC	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	FE	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	FG	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	FI	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	FK	430	Total 3372	C 2114	N 575	O 652	S 31	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
60	FM	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	FO	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	FQ	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	FS	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	FV	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	FX	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	FZ	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GB	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GD	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GF	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GI	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GK	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GM	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GO	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GQ	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GS	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GV	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GX	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	GZ	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	HB	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	HD	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
60	HF	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	HH	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	HJ	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	HL	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	HN	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	HP	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	HR	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	HS	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	HU	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	HW	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	HY	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IA	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IC	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IE	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IF	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IH	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IJ	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IL	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IN	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IP	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IR	430	Total 3372	C 2114	N 575	O 652	S 31	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
60	IS	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IU	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IW	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	IY	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JA	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JC	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JE	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JG	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JI	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JK	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JM	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JO	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JR	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JT	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JV	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JX	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	JZ	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	KB	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	KE	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	KG	430	Total 3372	C 2114	N 575	O 652	S 31	0	0
60	KI	430	Total 3372	C 2114	N 575	O 652	S 31	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
60	KK	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	KM	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	KO	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	KR	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	KT	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	KV	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	KX	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	KZ	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		
60	LB	430	Total	C	N	O	S	0	0
			3372	2114	575	652	31		

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

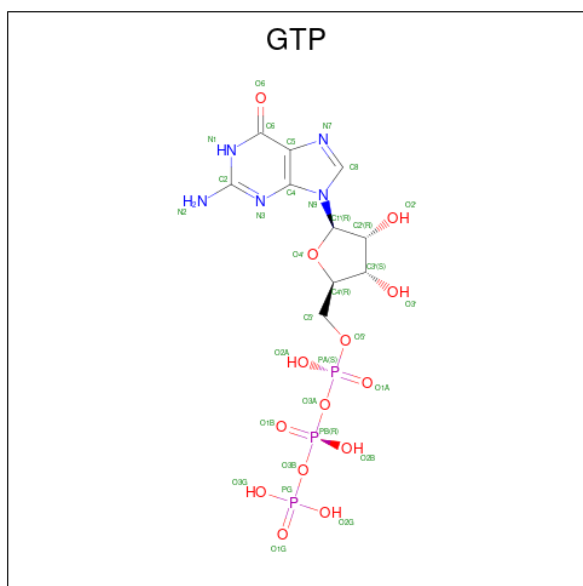
Mol	Chain	Residues	Atoms		AltConf
61	2I	2	Total	Zn	0
			2	2	
61	2K	1	Total	Zn	0
			1	1	
61	2N	1	Total	Zn	0
			1	1	
61	3V	2	Total	Zn	0
			2	2	
61	3W	2	Total	Zn	0
			2	2	
61	3X	3	Total	Zn	0
			3	3	
61	3Y	2	Total	Zn	0
			2	2	
61	4A	1	Total	Zn	0
			1	1	
61	4B	1	Total	Zn	0
			1	1	
61	4C	1	Total	Zn	0
			1	1	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
61	4D	1	Total	Zn	0
			1	1	
61	4F	3	Total	Zn	0
			3	3	
61	FB	1	Total	Zn	0
			1	1	
61	FN	1	Total	Zn	0
			1	1	
61	FP	1	Total	Zn	0
			1	1	
61	FR	1	Total	Zn	0
			1	1	

- Molecule 62 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
62	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	AC	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	AI	1	Total	C	N	O	P	0
			32	10	5	14	3	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
62	AK	1	Total 32	C 10	N 5	O 14	P 3	0
62	AM	1	Total 32	C 10	N 5	O 14	P 3	0
62	AO	1	Total 32	C 10	N 5	O 14	P 3	0
62	AQ	1	Total 32	C 10	N 5	O 14	P 3	0
62	AS	1	Total 32	C 10	N 5	O 14	P 3	0
62	AU	1	Total 32	C 10	N 5	O 14	P 3	0
62	AW	1	Total 32	C 10	N 5	O 14	P 3	0
62	AY	1	Total 32	C 10	N 5	O 14	P 3	0
62	BA	1	Total 32	C 10	N 5	O 14	P 3	0
62	BC	1	Total 32	C 10	N 5	O 14	P 3	0
62	BE	1	Total 32	C 10	N 5	O 14	P 3	0
62	BG	1	Total 32	C 10	N 5	O 14	P 3	0
62	BI	1	Total 32	C 10	N 5	O 14	P 3	0
62	BK	1	Total 32	C 10	N 5	O 14	P 3	0
62	BM	1	Total 32	C 10	N 5	O 14	P 3	0
62	BO	1	Total 32	C 10	N 5	O 14	P 3	0
62	BQ	1	Total 32	C 10	N 5	O 14	P 3	0
62	BS	1	Total 32	C 10	N 5	O 14	P 3	0
62	BU	1	Total 32	C 10	N 5	O 14	P 3	0
62	BW	1	Total 32	C 10	N 5	O 14	P 3	0
62	BX	1	Total 32	C 10	N 5	O 14	P 3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
62	BZ	1	Total 32	C 10	N 5	O 14	P 3	0
62	CB	1	Total 32	C 10	N 5	O 14	P 3	0
62	CD	1	Total 32	C 10	N 5	O 14	P 3	0
62	CF	1	Total 32	C 10	N 5	O 14	P 3	0
62	CH	1	Total 32	C 10	N 5	O 14	P 3	0
62	CJ	1	Total 32	C 10	N 5	O 14	P 3	0
62	CM	1	Total 32	C 10	N 5	O 14	P 3	0
62	CO	1	Total 32	C 10	N 5	O 14	P 3	0
62	CQ	1	Total 32	C 10	N 5	O 14	P 3	0
62	CS	1	Total 32	C 10	N 5	O 14	P 3	0
62	CU	1	Total 32	C 10	N 5	O 14	P 3	0
62	CW	1	Total 32	C 10	N 5	O 14	P 3	0
62	CY	1	Total 32	C 10	N 5	O 14	P 3	0
62	DA	1	Total 32	C 10	N 5	O 14	P 3	0
62	DC	1	Total 32	C 10	N 5	O 14	P 3	0
62	DE	1	Total 32	C 10	N 5	O 14	P 3	0
62	DG	1	Total 32	C 10	N 5	O 14	P 3	0
62	DI	1	Total 32	C 10	N 5	O 14	P 3	0
62	DK	1	Total 32	C 10	N 5	O 14	P 3	0
62	DM	1	Total 32	C 10	N 5	O 14	P 3	0
62	DO	1	Total 32	C 10	N 5	O 14	P 3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
62	DQ	1	Total 32	C 10	N 5	O 14	P 3	0
62	DS	1	Total 32	C 10	N 5	O 14	P 3	0
62	DU	1	Total 32	C 10	N 5	O 14	P 3	0
62	DX	1	Total 32	C 10	N 5	O 14	P 3	0
62	DZ	1	Total 32	C 10	N 5	O 14	P 3	0
62	EB	1	Total 32	C 10	N 5	O 14	P 3	0
62	ED	1	Total 32	C 10	N 5	O 14	P 3	0
62	EF	1	Total 32	C 10	N 5	O 14	P 3	0
62	EH	1	Total 32	C 10	N 5	O 14	P 3	0
62	EJ	1	Total 32	C 10	N 5	O 14	P 3	0
62	EL	1	Total 32	C 10	N 5	O 14	P 3	0
62	EN	1	Total 32	C 10	N 5	O 14	P 3	0
62	EP	1	Total 32	C 10	N 5	O 14	P 3	0
62	ER	1	Total 32	C 10	N 5	O 14	P 3	0
62	ET	1	Total 32	C 10	N 5	O 14	P 3	0
62	EV	1	Total 32	C 10	N 5	O 14	P 3	0
62	EX	1	Total 32	C 10	N 5	O 14	P 3	0
62	EZ	1	Total 32	C 10	N 5	O 14	P 3	0
62	FB	1	Total 32	C 10	N 5	O 14	P 3	0
62	FD	1	Total 32	C 10	N 5	O 14	P 3	0
62	FF	1	Total 32	C 10	N 5	O 14	P 3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
62	FH	1	Total 32	C 10	N 5	O 14	P 3	0
62	FJ	1	Total 32	C 10	N 5	O 14	P 3	0
62	FL	1	Total 32	C 10	N 5	O 14	P 3	0
62	FN	1	Total 32	C 10	N 5	O 14	P 3	0
62	FP	1	Total 32	C 10	N 5	O 14	P 3	0
62	FR	1	Total 32	C 10	N 5	O 14	P 3	0
62	FT	1	Total 32	C 10	N 5	O 14	P 3	0
62	FU	1	Total 32	C 10	N 5	O 14	P 3	0
62	FW	1	Total 32	C 10	N 5	O 14	P 3	0
62	FY	1	Total 32	C 10	N 5	O 14	P 3	0
62	GA	1	Total 32	C 10	N 5	O 14	P 3	0
62	GC	1	Total 32	C 10	N 5	O 14	P 3	0
62	GE	1	Total 32	C 10	N 5	O 14	P 3	0
62	GG	1	Total 32	C 10	N 5	O 14	P 3	0
62	GH	1	Total 32	C 10	N 5	O 14	P 3	0
62	GJ	1	Total 32	C 10	N 5	O 14	P 3	0
62	GL	1	Total 32	C 10	N 5	O 14	P 3	0
62	GN	1	Total 32	C 10	N 5	O 14	P 3	0
62	GP	1	Total 32	C 10	N 5	O 14	P 3	0
62	GR	1	Total 32	C 10	N 5	O 14	P 3	0
62	GT	1	Total 32	C 10	N 5	O 14	P 3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
62	GU	1	Total 32	C 10	N 5	O 14	P 3	0
62	GW	1	Total 32	C 10	N 5	O 14	P 3	0
62	GY	1	Total 32	C 10	N 5	O 14	P 3	0
62	HA	1	Total 32	C 10	N 5	O 14	P 3	0
62	HC	1	Total 32	C 10	N 5	O 14	P 3	0
62	HE	1	Total 32	C 10	N 5	O 14	P 3	0
62	HG	1	Total 32	C 10	N 5	O 14	P 3	0
62	HI	1	Total 32	C 10	N 5	O 14	P 3	0
62	HK	1	Total 32	C 10	N 5	O 14	P 3	0
62	HM	1	Total 32	C 10	N 5	O 14	P 3	0
62	HO	1	Total 32	C 10	N 5	O 14	P 3	0
62	HQ	1	Total 32	C 10	N 5	O 14	P 3	0
62	HT	1	Total 32	C 10	N 5	O 14	P 3	0
62	HV	1	Total 32	C 10	N 5	O 14	P 3	0
62	HX	1	Total 32	C 10	N 5	O 14	P 3	0
62	HZ	1	Total 32	C 10	N 5	O 14	P 3	0
62	IB	1	Total 32	C 10	N 5	O 14	P 3	0
62	ID	1	Total 32	C 10	N 5	O 14	P 3	0
62	IG	1	Total 32	C 10	N 5	O 14	P 3	0
62	II	1	Total 32	C 10	N 5	O 14	P 3	0
62	IK	1	Total 32	C 10	N 5	O 14	P 3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
62	IM	1	Total 32	C 10	N 5	O 14	P 3	0
62	IO	1	Total 32	C 10	N 5	O 14	P 3	0
62	IQ	1	Total 32	C 10	N 5	O 14	P 3	0
62	IT	1	Total 32	C 10	N 5	O 14	P 3	0
62	IV	1	Total 32	C 10	N 5	O 14	P 3	0
62	IX	1	Total 32	C 10	N 5	O 14	P 3	0
62	IZ	1	Total 32	C 10	N 5	O 14	P 3	0
62	JB	1	Total 32	C 10	N 5	O 14	P 3	0
62	JD	1	Total 32	C 10	N 5	O 14	P 3	0
62	JF	1	Total 32	C 10	N 5	O 14	P 3	0
62	JH	1	Total 32	C 10	N 5	O 14	P 3	0
62	JJ	1	Total 32	C 10	N 5	O 14	P 3	0
62	JL	1	Total 32	C 10	N 5	O 14	P 3	0
62	JN	1	Total 32	C 10	N 5	O 14	P 3	0
62	JP	1	Total 32	C 10	N 5	O 14	P 3	0
62	JQ	1	Total 32	C 10	N 5	O 14	P 3	0
62	JS	1	Total 32	C 10	N 5	O 14	P 3	0
62	JU	1	Total 32	C 10	N 5	O 14	P 3	0
62	JW	1	Total 32	C 10	N 5	O 14	P 3	0
62	JY	1	Total 32	C 10	N 5	O 14	P 3	0
62	KA	1	Total 32	C 10	N 5	O 14	P 3	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
62	KC	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KD	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KF	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KH	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KJ	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KL	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KN	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KP	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KS	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KU	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KW	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	KY	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	LA	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
63	AA	1	Total	Mg	0
			1	1	
63	AC	1	Total	Mg	0
			1	1	
63	AE	1	Total	Mg	0
			1	1	
63	AG	1	Total	Mg	0
			1	1	
63	AI	1	Total	Mg	0
			1	1	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
63	AK	1	Total 1	Mg 1	0
63	AM	1	Total 1	Mg 1	0
63	AO	1	Total 1	Mg 1	0
63	AQ	1	Total 1	Mg 1	0
63	AS	1	Total 1	Mg 1	0
63	AU	1	Total 1	Mg 1	0
63	AW	1	Total 1	Mg 1	0
63	AY	1	Total 1	Mg 1	0
63	BA	1	Total 1	Mg 1	0
63	BC	1	Total 1	Mg 1	0
63	BE	1	Total 1	Mg 1	0
63	BG	1	Total 1	Mg 1	0
63	BI	1	Total 1	Mg 1	0
63	BK	1	Total 1	Mg 1	0
63	BM	1	Total 1	Mg 1	0
63	BO	1	Total 1	Mg 1	0
63	BQ	1	Total 1	Mg 1	0
63	BS	1	Total 1	Mg 1	0
63	BU	1	Total 1	Mg 1	0
63	BW	1	Total 1	Mg 1	0
63	BX	1	Total 1	Mg 1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
63	CA	1	Total 1	Mg 1	0
63	CB	1	Total 1	Mg 1	0
63	CD	1	Total 1	Mg 1	0
63	CF	1	Total 1	Mg 1	0
63	CH	1	Total 1	Mg 1	0
63	CJ	1	Total 1	Mg 1	0
63	CM	1	Total 1	Mg 1	0
63	CO	1	Total 1	Mg 1	0
63	CQ	1	Total 1	Mg 1	0
63	CS	1	Total 1	Mg 1	0
63	CU	1	Total 1	Mg 1	0
63	CW	1	Total 1	Mg 1	0
63	CY	1	Total 1	Mg 1	0
63	DA	1	Total 1	Mg 1	0
63	DC	1	Total 1	Mg 1	0
63	DE	1	Total 1	Mg 1	0
63	DG	1	Total 1	Mg 1	0
63	DI	1	Total 1	Mg 1	0
63	DK	1	Total 1	Mg 1	0
63	DM	1	Total 1	Mg 1	0
63	DO	1	Total 1	Mg 1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
63	DQ	1	Total 1	Mg 1	0
63	DS	1	Total 1	Mg 1	0
63	DU	1	Total 1	Mg 1	0
63	DX	1	Total 1	Mg 1	0
63	DZ	1	Total 1	Mg 1	0
63	EB	1	Total 1	Mg 1	0
63	ED	1	Total 1	Mg 1	0
63	EF	1	Total 1	Mg 1	0
63	EH	1	Total 1	Mg 1	0
63	EJ	1	Total 1	Mg 1	0
63	EL	1	Total 1	Mg 1	0
63	EN	1	Total 1	Mg 1	0
63	EP	1	Total 1	Mg 1	0
63	ER	1	Total 1	Mg 1	0
63	ET	1	Total 1	Mg 1	0
63	EV	1	Total 1	Mg 1	0
63	EX	1	Total 1	Mg 1	0
63	EZ	1	Total 1	Mg 1	0
63	FB	1	Total 1	Mg 1	0
63	FD	1	Total 1	Mg 1	0
63	FF	1	Total 1	Mg 1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
63	FH	1	Total 1	Mg 1	0
63	FJ	1	Total 1	Mg 1	0
63	FL	1	Total 1	Mg 1	0
63	FN	1	Total 1	Mg 1	0
63	FP	1	Total 1	Mg 1	0
63	FR	1	Total 1	Mg 1	0
63	FT	1	Total 1	Mg 1	0
63	FU	1	Total 1	Mg 1	0
63	FW	1	Total 1	Mg 1	0
63	FY	1	Total 1	Mg 1	0
63	GA	1	Total 1	Mg 1	0
63	GC	1	Total 1	Mg 1	0
63	GE	1	Total 1	Mg 1	0
63	GG	1	Total 1	Mg 1	0
63	GH	1	Total 1	Mg 1	0
63	GJ	1	Total 1	Mg 1	0
63	GL	1	Total 1	Mg 1	0
63	GN	1	Total 1	Mg 1	0
63	GP	1	Total 1	Mg 1	0
63	GR	1	Total 1	Mg 1	0
63	GT	1	Total 1	Mg 1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
63	GU	1	Total 1	Mg 1	0
63	GW	1	Total 1	Mg 1	0
63	GY	1	Total 1	Mg 1	0
63	HA	1	Total 1	Mg 1	0
63	HC	1	Total 1	Mg 1	0
63	HE	1	Total 1	Mg 1	0
63	HG	1	Total 1	Mg 1	0
63	HI	1	Total 1	Mg 1	0
63	HK	1	Total 1	Mg 1	0
63	HM	1	Total 1	Mg 1	0
63	HO	1	Total 1	Mg 1	0
63	HQ	1	Total 1	Mg 1	0
63	HT	1	Total 1	Mg 1	0
63	HV	1	Total 1	Mg 1	0
63	HX	1	Total 1	Mg 1	0
63	HZ	1	Total 1	Mg 1	0
63	IB	1	Total 1	Mg 1	0
63	ID	1	Total 1	Mg 1	0
63	IG	1	Total 1	Mg 1	0
63	II	1	Total 1	Mg 1	0
63	IK	1	Total 1	Mg 1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
63	IM	1	Total 1	Mg 1	0
63	IO	1	Total 1	Mg 1	0
63	IQ	1	Total 1	Mg 1	0
63	IT	1	Total 1	Mg 1	0
63	IV	1	Total 1	Mg 1	0
63	IX	1	Total 1	Mg 1	0
63	IZ	1	Total 1	Mg 1	0
63	JB	1	Total 1	Mg 1	0
63	JD	1	Total 1	Mg 1	0
63	JF	1	Total 1	Mg 1	0
63	JH	1	Total 1	Mg 1	0
63	JJ	1	Total 1	Mg 1	0
63	JL	1	Total 1	Mg 1	0
63	JN	1	Total 1	Mg 1	0
63	JP	1	Total 1	Mg 1	0
63	JQ	1	Total 1	Mg 1	0
63	JS	1	Total 1	Mg 1	0
63	JU	1	Total 1	Mg 1	0
63	JW	1	Total 1	Mg 1	0
63	JY	1	Total 1	Mg 1	0
63	KA	1	Total 1	Mg 1	0

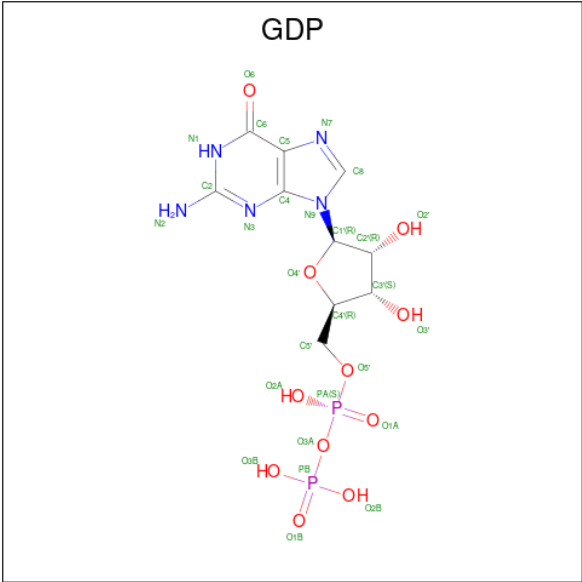
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
63	KC	1	Total	Mg	0
			1	1	
63	KD	1	Total	Mg	0
			1	1	
63	KF	1	Total	Mg	0
			1	1	
63	KH	1	Total	Mg	0
			1	1	
63	KJ	1	Total	Mg	0
			1	1	
63	KL	1	Total	Mg	0
			1	1	
63	KN	1	Total	Mg	0
			1	1	
63	KP	1	Total	Mg	0
			1	1	
63	KQ	1	Total	Mg	0
			1	1	
63	KS	1	Total	Mg	0
			1	1	
63	KU	1	Total	Mg	0
			1	1	
63	KW	1	Total	Mg	0
			1	1	
63	KY	1	Total	Mg	0
			1	1	
63	LA	1	Total	Mg	0
			1	1	

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					AltConf
64	AB	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AD	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AF	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AH	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AL	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AN	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AP	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AR	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AT	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AV	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AX	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	AZ	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	BB	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
64	BD	1	Total 28	C 10	N 5	O 11	P 2	0
64	BF	1	Total 28	C 10	N 5	O 11	P 2	0
64	BH	1	Total 28	C 10	N 5	O 11	P 2	0
64	BJ	1	Total 28	C 10	N 5	O 11	P 2	0
64	BL	1	Total 28	C 10	N 5	O 11	P 2	0
64	BN	1	Total 28	C 10	N 5	O 11	P 2	0
64	BP	1	Total 28	C 10	N 5	O 11	P 2	0
64	BR	1	Total 28	C 10	N 5	O 11	P 2	0
64	BT	1	Total 28	C 10	N 5	O 11	P 2	0
64	BV	1	Total 28	C 10	N 5	O 11	P 2	0
64	BY	1	Total 28	C 10	N 5	O 11	P 2	0
64	CA	1	Total 28	C 10	N 5	O 11	P 2	0
64	CC	1	Total 28	C 10	N 5	O 11	P 2	0
64	CE	1	Total 28	C 10	N 5	O 11	P 2	0
64	CG	1	Total 28	C 10	N 5	O 11	P 2	0
64	CI	1	Total 28	C 10	N 5	O 11	P 2	0
64	CL	1	Total 28	C 10	N 5	O 11	P 2	0
64	CN	1	Total 28	C 10	N 5	O 11	P 2	0
64	CP	1	Total 28	C 10	N 5	O 11	P 2	0
64	CR	1	Total 28	C 10	N 5	O 11	P 2	0
64	CT	1	Total 28	C 10	N 5	O 11	P 2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
64	CV	1	Total 28	C 10	N 5	O 11	P 2	0
64	CX	1	Total 28	C 10	N 5	O 11	P 2	0
64	CZ	1	Total 28	C 10	N 5	O 11	P 2	0
64	DB	1	Total 28	C 10	N 5	O 11	P 2	0
64	DD	1	Total 28	C 10	N 5	O 11	P 2	0
64	DF	1	Total 28	C 10	N 5	O 11	P 2	0
64	DH	1	Total 28	C 10	N 5	O 11	P 2	0
64	DJ	1	Total 28	C 10	N 5	O 11	P 2	0
64	DL	1	Total 28	C 10	N 5	O 11	P 2	0
64	DN	1	Total 28	C 10	N 5	O 11	P 2	0
64	DP	1	Total 28	C 10	N 5	O 11	P 2	0
64	DR	1	Total 28	C 10	N 5	O 11	P 2	0
64	DT	1	Total 28	C 10	N 5	O 11	P 2	0
64	DV	1	Total 28	C 10	N 5	O 11	P 2	0
64	DW	1	Total 28	C 10	N 5	O 11	P 2	0
64	DY	1	Total 28	C 10	N 5	O 11	P 2	0
64	EA	1	Total 28	C 10	N 5	O 11	P 2	0
64	EC	1	Total 28	C 10	N 5	O 11	P 2	0
64	EE	1	Total 28	C 10	N 5	O 11	P 2	0
64	EG	1	Total 28	C 10	N 5	O 11	P 2	0
64	EI	1	Total 28	C 10	N 5	O 11	P 2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
64	EK	1	Total 28	C 10	N 5	O 11	P 2	0
64	EM	1	Total 28	C 10	N 5	O 11	P 2	0
64	EO	1	Total 28	C 10	N 5	O 11	P 2	0
64	EQ	1	Total 28	C 10	N 5	O 11	P 2	0
64	ES	1	Total 28	C 10	N 5	O 11	P 2	0
64	EU	1	Total 28	C 10	N 5	O 11	P 2	0
64	EW	1	Total 28	C 10	N 5	O 11	P 2	0
64	EY	1	Total 28	C 10	N 5	O 11	P 2	0
64	FA	1	Total 28	C 10	N 5	O 11	P 2	0
64	FC	1	Total 28	C 10	N 5	O 11	P 2	0
64	FE	1	Total 28	C 10	N 5	O 11	P 2	0
64	FG	1	Total 28	C 10	N 5	O 11	P 2	0
64	FI	1	Total 28	C 10	N 5	O 11	P 2	0
64	FK	1	Total 28	C 10	N 5	O 11	P 2	0
64	FM	1	Total 28	C 10	N 5	O 11	P 2	0
64	FO	1	Total 28	C 10	N 5	O 11	P 2	0
64	FQ	1	Total 28	C 10	N 5	O 11	P 2	0
64	FS	1	Total 28	C 10	N 5	O 11	P 2	0
64	FV	1	Total 28	C 10	N 5	O 11	P 2	0
64	FX	1	Total 28	C 10	N 5	O 11	P 2	0
64	FZ	1	Total 28	C 10	N 5	O 11	P 2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
64	GB	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GD	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GF	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GI	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GK	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GM	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GO	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GS	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GV	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GX	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	GZ	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	HB	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	HD	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	HF	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	HH	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	HJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	HL	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	HN	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	HP	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	HR	1	Total	C	N	O	P	0
			28	10	5	11	2	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
64	HS	1	Total 28	C 10	N 5	O 11	P 2	0
64	HU	1	Total 28	C 10	N 5	O 11	P 2	0
64	HW	1	Total 28	C 10	N 5	O 11	P 2	0
64	HY	1	Total 28	C 10	N 5	O 11	P 2	0
64	IA	1	Total 28	C 10	N 5	O 11	P 2	0
64	IC	1	Total 28	C 10	N 5	O 11	P 2	0
64	IE	1	Total 28	C 10	N 5	O 11	P 2	0
64	IF	1	Total 28	C 10	N 5	O 11	P 2	0
64	IH	1	Total 28	C 10	N 5	O 11	P 2	0
64	IJ	1	Total 28	C 10	N 5	O 11	P 2	0
64	IL	1	Total 28	C 10	N 5	O 11	P 2	0
64	IN	1	Total 28	C 10	N 5	O 11	P 2	0
64	IP	1	Total 28	C 10	N 5	O 11	P 2	0
64	IR	1	Total 28	C 10	N 5	O 11	P 2	0
64	IS	1	Total 28	C 10	N 5	O 11	P 2	0
64	IU	1	Total 28	C 10	N 5	O 11	P 2	0
64	IW	1	Total 28	C 10	N 5	O 11	P 2	0
64	IY	1	Total 28	C 10	N 5	O 11	P 2	0
64	JA	1	Total 28	C 10	N 5	O 11	P 2	0
64	JC	1	Total 28	C 10	N 5	O 11	P 2	0
64	JE	1	Total 28	C 10	N 5	O 11	P 2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
64	JG	1	Total 28	C 10	N 5	O 11	P 2	0
64	JI	1	Total 28	C 10	N 5	O 11	P 2	0
64	JK	1	Total 28	C 10	N 5	O 11	P 2	0
64	JM	1	Total 28	C 10	N 5	O 11	P 2	0
64	JO	1	Total 28	C 10	N 5	O 11	P 2	0
64	JR	1	Total 28	C 10	N 5	O 11	P 2	0
64	JT	1	Total 28	C 10	N 5	O 11	P 2	0
64	JV	1	Total 28	C 10	N 5	O 11	P 2	0
64	JX	1	Total 28	C 10	N 5	O 11	P 2	0
64	JZ	1	Total 28	C 10	N 5	O 11	P 2	0
64	KB	1	Total 28	C 10	N 5	O 11	P 2	0
64	KE	1	Total 28	C 10	N 5	O 11	P 2	0
64	KG	1	Total 28	C 10	N 5	O 11	P 2	0
64	KI	1	Total 28	C 10	N 5	O 11	P 2	0
64	KK	1	Total 28	C 10	N 5	O 11	P 2	0
64	KM	1	Total 28	C 10	N 5	O 11	P 2	0
64	KO	1	Total 28	C 10	N 5	O 11	P 2	0
64	KR	1	Total 28	C 10	N 5	O 11	P 2	0
64	KT	1	Total 28	C 10	N 5	O 11	P 2	0
64	KV	1	Total 28	C 10	N 5	O 11	P 2	0
64	KX	1	Total 28	C 10	N 5	O 11	P 2	0

*Continued on next page...*

*Continued from previous page...*

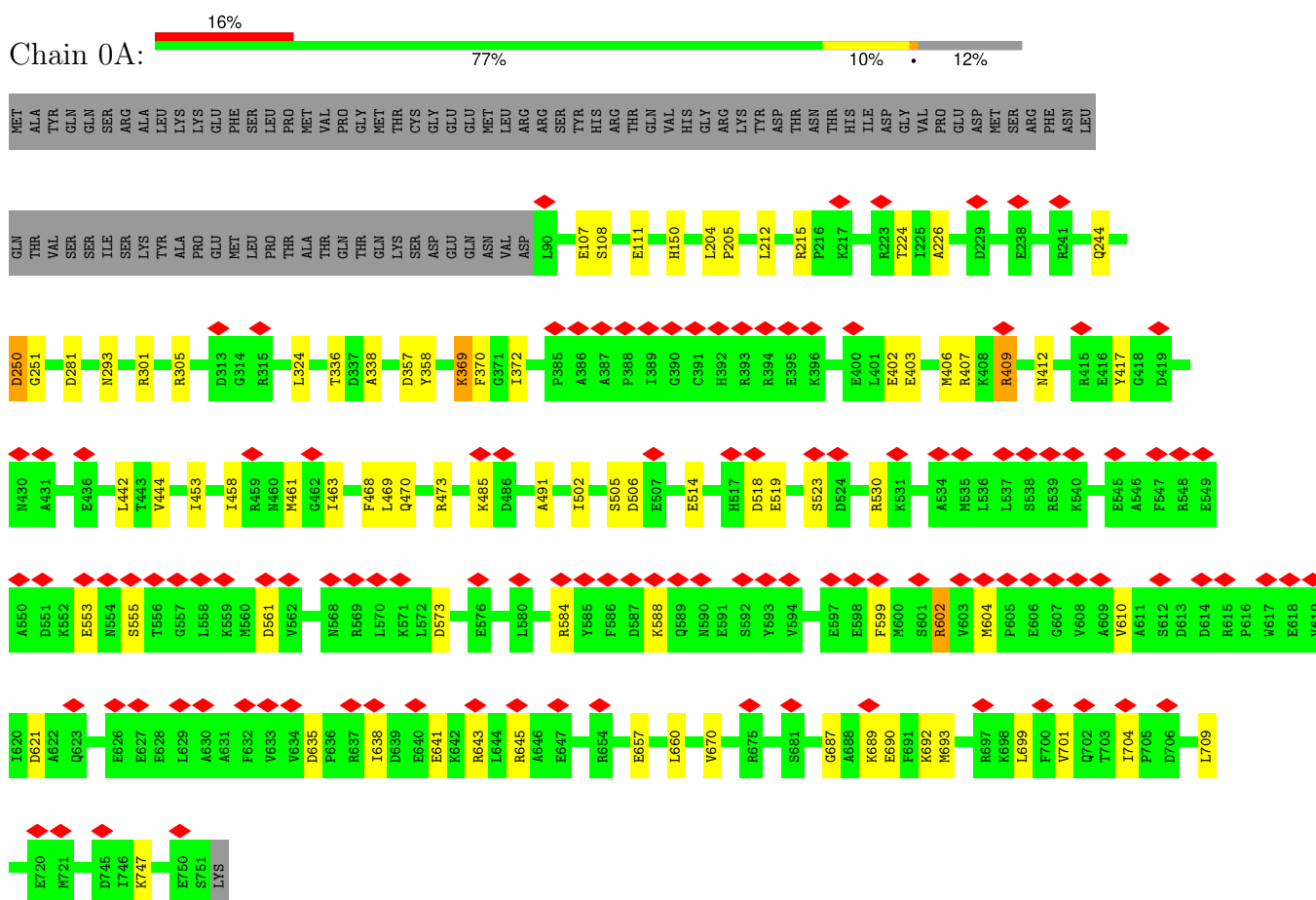
Mol	Chain	Residues	Atoms					AltConf
64	KZ	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	LB	1	Total	C	N	O	P	0
			28	10	5	11	2	



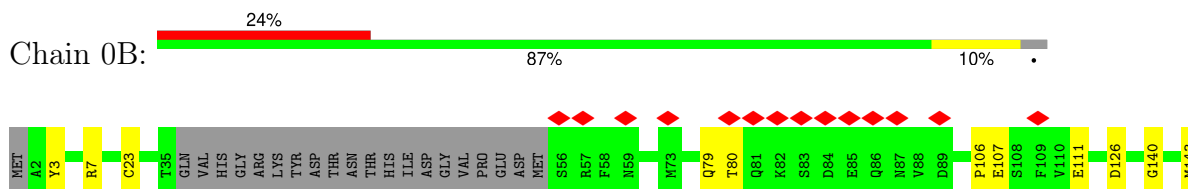
### 3 Residue-property plots

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: EF-hand domain-containing family member C2

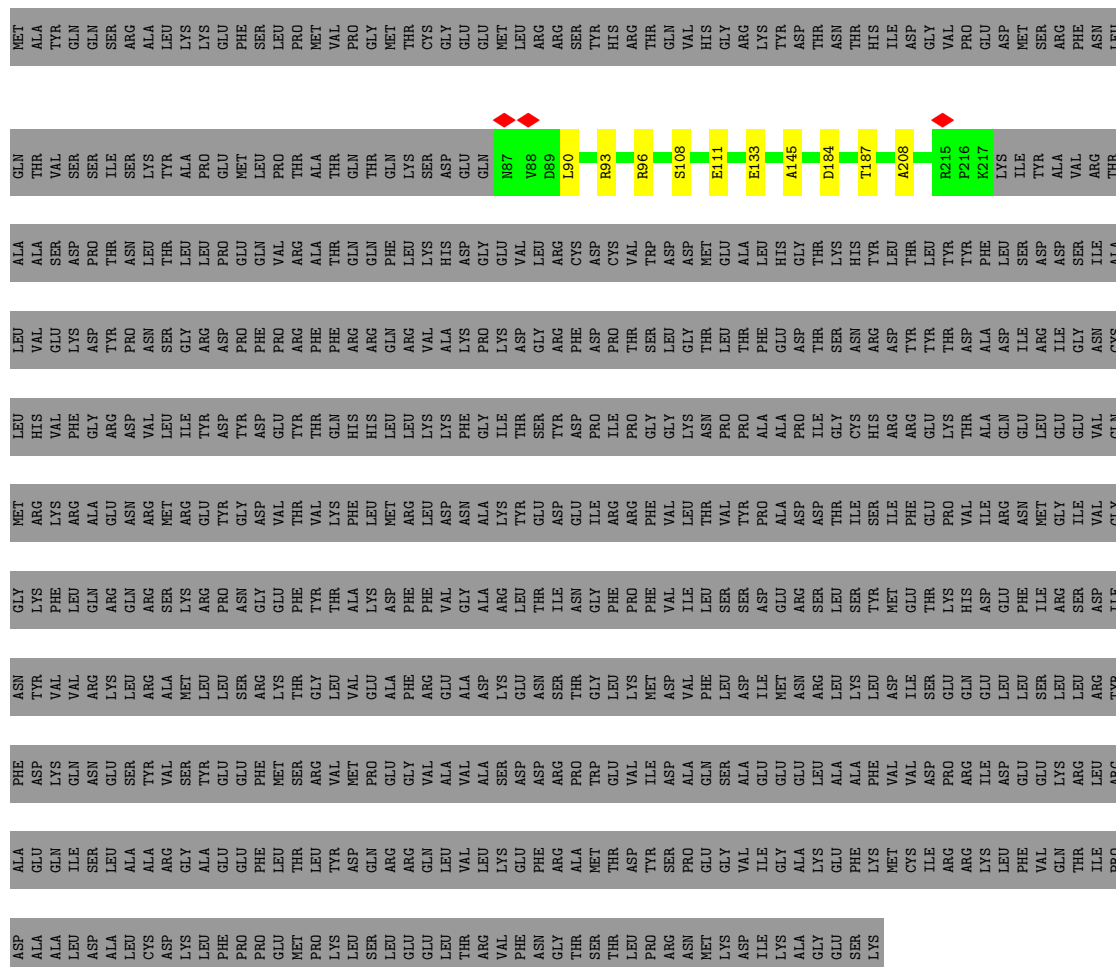


- Molecule 1: EF-hand domain-containing family member C2




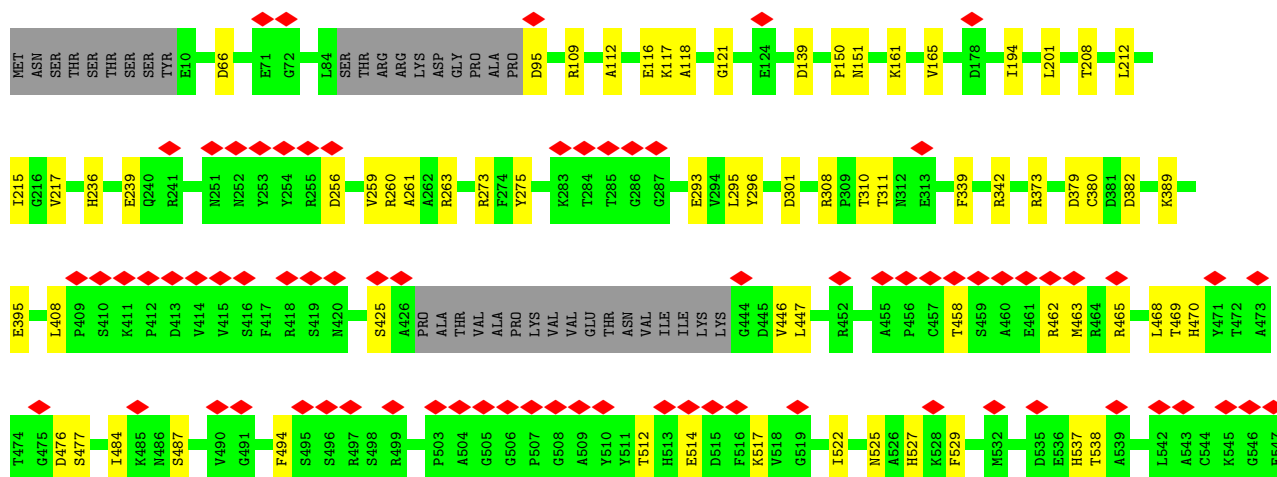
- Molecule 1: EF-hand domain-containing family member C2

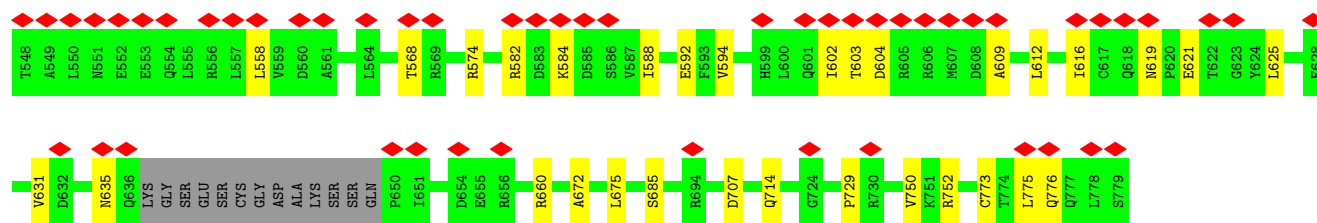
Chain 0D:  16% 83%



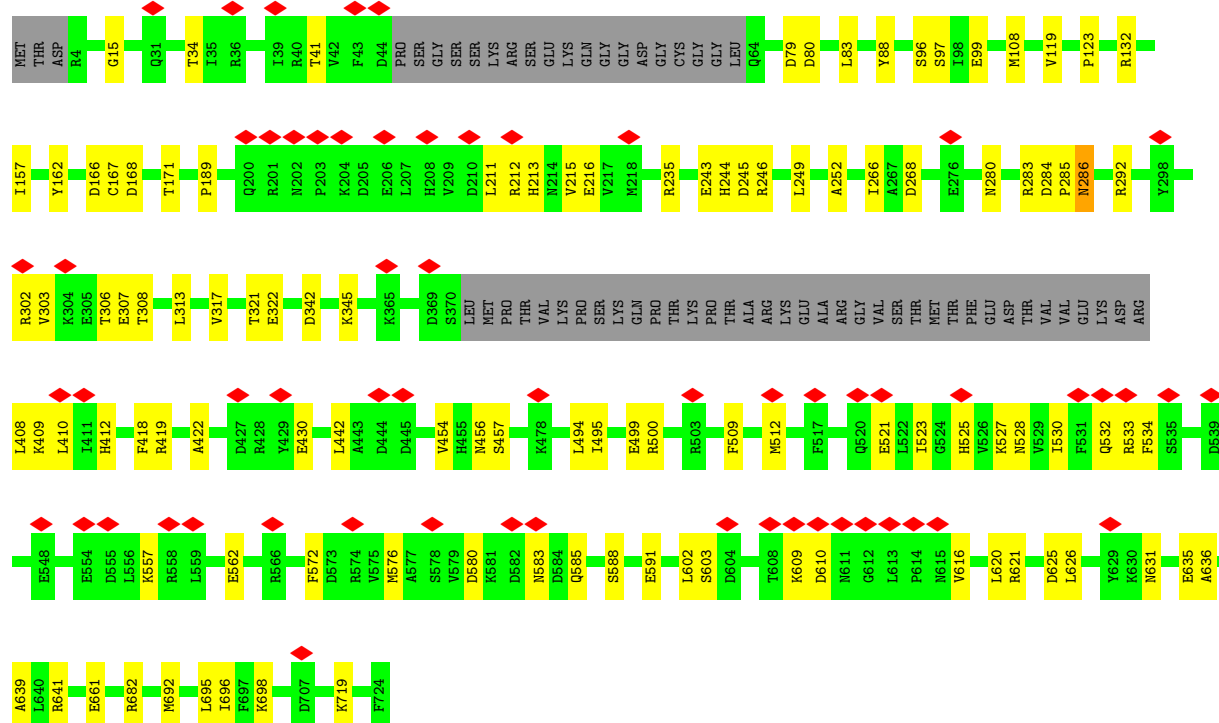
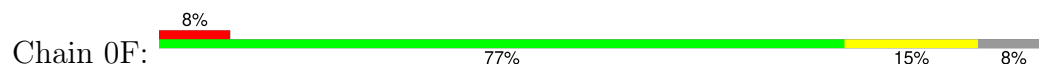
• Molecule 2: EF-hand domain-containing family member C2

Chain 0E:  16% 81% 13% 6%

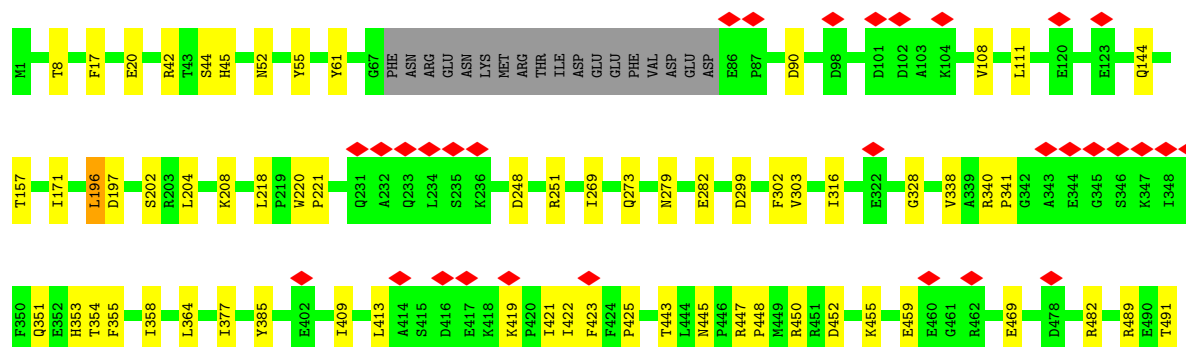
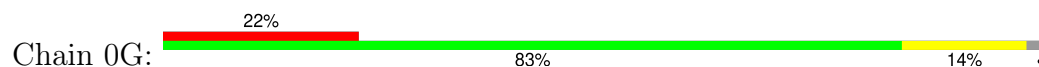


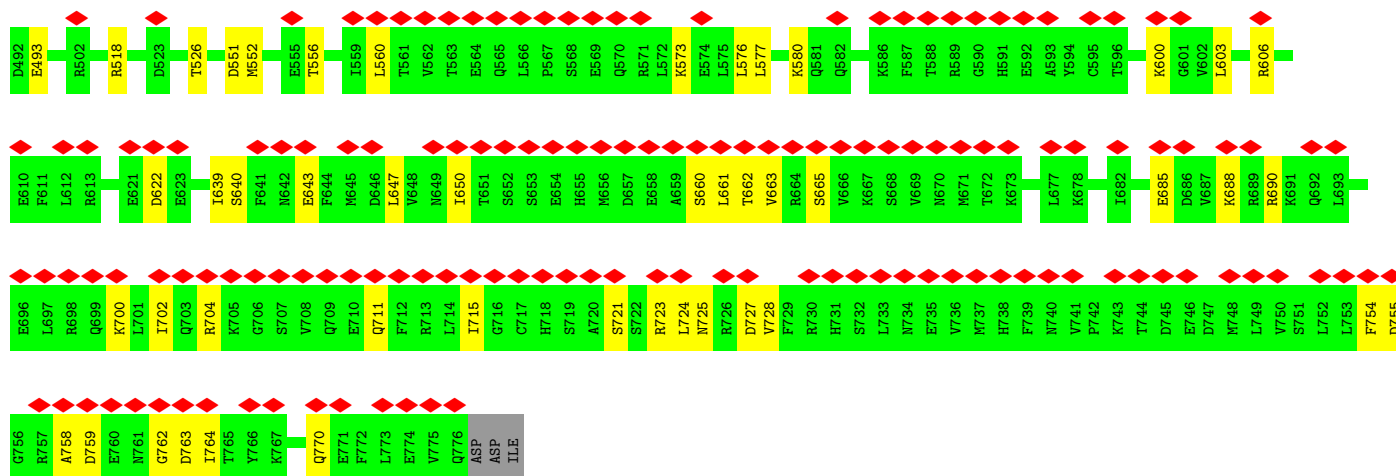


• Molecule 3: Rib72 protein-like protein



• Molecule 4: CMF34/CARP4



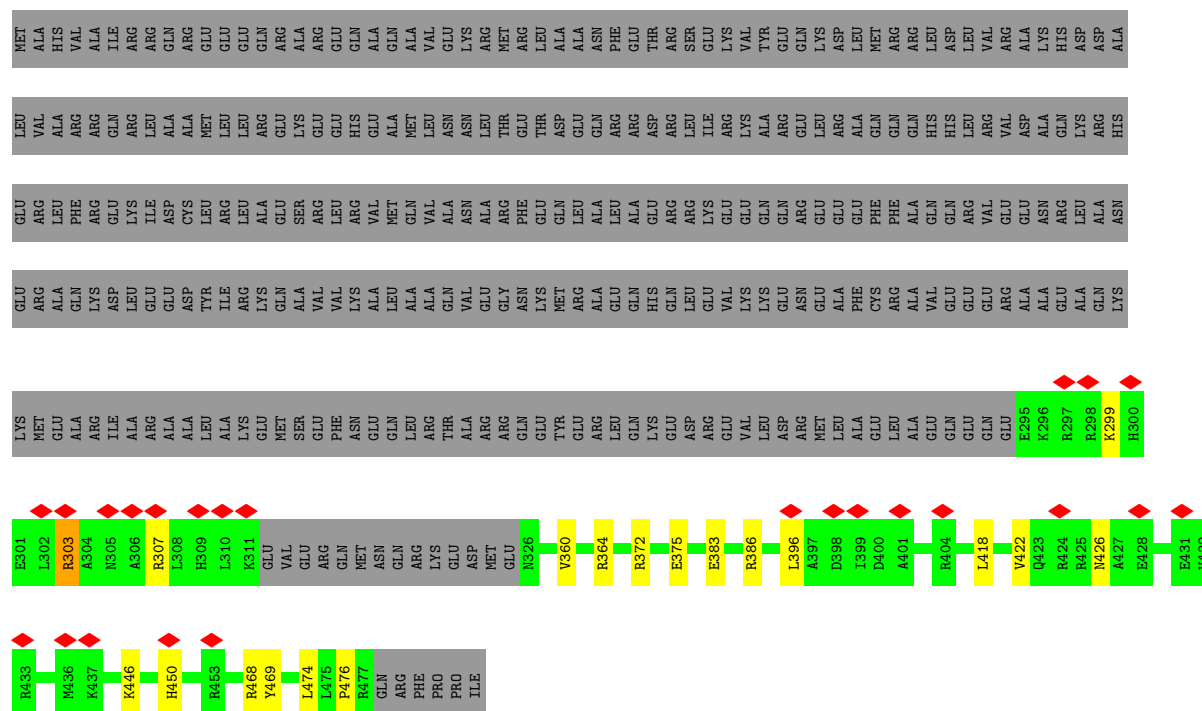


ARG	GLU	TLE	LYS	ASN	ASN	MET
ARG	ARG	HIS	ASN	ASN	ASN	GLU
ALA	TYR	GLN	ASN	ARG	GLU	ARG
GLU	LYS	ASN	ALA	ALA	LYS	ALA
ARG	GLY	GLN	ALA	ALA	LEU	ALA
LEU	MET	ALA	ALA	GLN	THR	GLU
THR	THR	GLU	GLN	GLN	LEU	THR
ILE	GLU	PHE	GLN	ILE	ASP	ILE
ALA	GLU	ASN	LYS	ASN	TYR	ASN
ALA	GLN	LYS	GLN	GLN	ARG	VAL
GLU	ARG	LYS	GLN	GLN	GLU	ALA
GLN	ARG	LEU	ARG	THR	THR	SER
MET	LYS	ALA	GLU	GLU	TYR	ASN
GLN	LYS	ALA	GLU	THR	GLN	SER
LYS	PHE	GLN	GLU	TRP	LYS	SER
GLN	LEU	GLN	ALA	ALA	LYS	SER
LYS	GLU	LYS	LYS	GLN	LYS	LYS
ARG	GLU	ARG	GLN	GLN	LEU	LEU
GLU	ASP	ARG	ARG	GLN	THR	PRO
ALA	ARG	ARG	ARG	GLN	THR	PRO
SER	ALA	GLU	GLU	THR	GLN	LEU
GLN	ARG	ALA	GLU	GLU	ARG	LEU
ILE	GLN	ILE	GLU	GLU	GLU	GLU
ARG	ARG	ARG	LYS	LYS	TRP	THR
LYS	ASP	ASP	ASP	LEU	ASP	A23
LYS	LEU	LYS	ALA	ALA	LEU	
GLN	LEU	GLU	LYS	LYS	ASN	R39
LEU	ARG	GLU	LYS	ASP	ASP	
LEU	ARG	THR	MET	TRP	PRO	re6
THR	PHE	ARG	GLU	GLU	HIS	
THR	THR	LYS	GLU	GLU	GLN	
THR	MET	ALA	GLU	GLU	LEU	
ASN	GLU	LEU	ALA	LYS	LYS	GLU
GLN	VAL	GLU	ASN	ASN	ARG	GLU
VAL	GLU	GLU	GLN	LEU	ASP	ASN
ASP	GLU	ILE	VAL	PRO	ASN	ASN
GLU	GLU	ARG	PHE	GLY	ASP	PHE
ASP	ARG	PHE	ASN	ARG	TYR	THR
TYR	ARG	HIS	GLU	VAL	ASP	ASP
LYS	ALA	MET	ARG	GLY	ARG	GLN
TYR	GLN	GLY	ASN	ASN	ASN	ALA
TRP	GLN	ASP	GLU	ASP	ASP	LEU
ASP	ASP	PHE	THR	THR	PRO	LEU
LEU	ASN	LEU	THR	THR	THR	LEU
LEU	ASN	VAL	ILE	ILE	GLN	LEU
CYS	LEU	SER	GLN	GLN	LYS	GLN
MET	GLU	LEU	GLY	PHE	LYS	LYS
	GLU	LEU	ILE	GLU	GLU	GLU
	ARG	GLY	ALA	ALA	GLY	VAL
	GLN	LYS	GLN	GLU	ASP	ASN
	GLU	LYS	GLN	GLN	GLU	GLU
	GLU	VAL	VAL	ARG	LEU	ILE
	ARG	LYS	LYS	MET	ASP	ARG
	GLU	ALA	ALA	THR	TRP	ALA

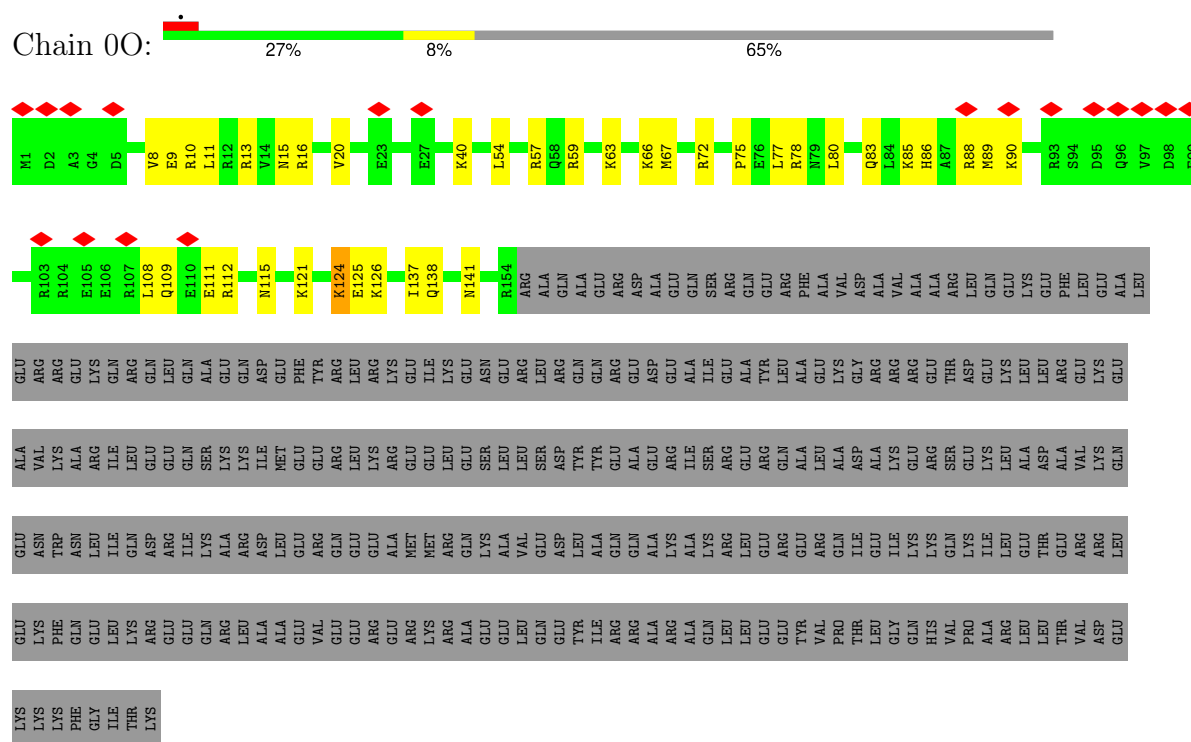
Amino Acid	Category	Value
MET	Amino acid types	123
GLU	Amino acid types	123
PRO	Amino acid types	123
ALA	Amino acid types	123
ALA	Amino acid types	123
GLU	Amino acid types	123
THR	Amino acid types	123
ILE	Amino acid types	123
ASN	Amino acid types	123
VAL	Amino acid types	123
ALA	Amino acid types	123
SER	Amino acid types	123
ASN	Amino acid types	123
SER	Amino acid types	123
SER	Amino acid types	123
LEU	Amino acid types	123
PRO	Amino acid types	123
GLN	Amino acid types	123
LEU	Amino acid types	123
GLU	Amino acid types	123
THR	Amino acid types	123
H257	Amino acid types	123
G260	Amino acid types	123
N264	Amino acid types	123
E288	Amino acid types	123
R291	Amino acid types	123
R297	Amino acid types	123
R307	Amino acid types	123
M310	Amino acid types	123
E314	Amino acid types	123
E315	Amino acid types	123
R316	Amino acid types	123
R334	Amino acid types	123
L365	Amino acid types	123
N371	Amino acid types	123
Q372	Amino acid types	123
V373	Amino acid types	123
D374	Amino acid types	123
E375	Amino acid types	123
D376	Amino acid types	123
Y377	Amino acid types	123
K385	Amino acid types	123
R39	Amino acid types	123
L40	Amino acid types	123
K41	Amino acid types	123
K44	Amino acid types	123
K52	Amino acid types	123
R57	Amino acid types	123
R60	Amino acid types	123
R61	Amino acid types	123
R62	Amino acid types	123
Q118	Amino acid types	123
R119	Amino acid types	123
T144	Amino acid types	123
Q150	Amino acid types	123
Q167	Amino acid types	123
W186	Amino acid types	123
M187	Amino acid types	123
E188	Amino acid types	123
V194	Amino acid types	123
E197	Amino acid types	123
R198	Amino acid types	123
R218	Amino acid types	123
E253	Amino acid types	123

ARG	GLN	VAL	K220	MET
MET	GLN	GLU	E224	ALA
ALA	GLU	ARG		HIS
MET	LYS	GLN		VAL
LYS	GLU	MET	R228	ALA
THR	ALA	ASN		ILE
ALA	VAL	GLN	Q239	ARG
LEU	GLU	ARG	K240	R8
THR	ARG	LYS	K241	Q9
GLU	ALA	GLU	M242	R10
GLU	GLU	ASP		E11
GLN	VAL	MET		E12
GLU	GLU	GLU	R245	E13
LYS	ARG	ASN	I246	Q14
GLU	GLN	GLU	A247	R15
LYS	GLU	ASP	R248	E16
VAL	PHE	ASP		
HIS	ARG	LEU		R17
ALA	ASN	THR	L251	E18
GLU	MET	GLU	A252	
ARG	ILE	GLU	K253	V23
ILE	ALA	GLU		
GLY	GLY	ASN		H27
LEU	LEU	ASN	E257	
ARG	ASP	LYS		S37
GLU	ALA	VAL	E260	V40
ILE	ILE	TRP		Y41
ASN	ASP	GLU	R263	E42
LEU	ALA	LYS	T264	Q43
GLU	MET	GLU	A265	K44
ARG	GLU	ARG	R266	
ALA	ARG	ALA	R267	L73
LYS	ALA	HIS		L83
PRO	GLN	TRP	Q268	
GLU	ARG	ARG	E269	
ARG	PHE	ALA	Y270	L86
TYR	ALA	ASP	E271	R137
LYS	VAL	GLU		M141
ASP	ALA	GLU	K275	R147
VAL	LYS	LYS		K158
PRO	GLU	ARG	R278	Q161
LEU	ASN	ARG		E174
LEU	GLN	LYS	R283	R177
PRO	LYS	LEU		R182
ARG	TYR	ARG		Y191
GLN	LEU	ARG	Q293	I192
ARG	GLU	ASN	E294	R193
PHE	SER	VAL	E295	K194
PRO	GLN	LEU	K296	
PRO	VAL	ILE	R297	
ILE	GLN	VAL	R298	
	ARG	ARG	K299	
	ASN	GLN	H300	
	ALA	VAL	E301	
	GLU	VAL	L302	
	LYS	LEU	R303	
	GLU	ASP	A304	
	GLU	LYS	N305	
	VAL	ARG	A306	
			R307	
			L308	
			H309	
			L310	
			K311	

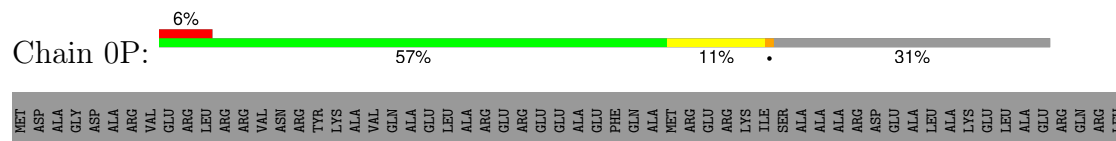
Chain 0N: 

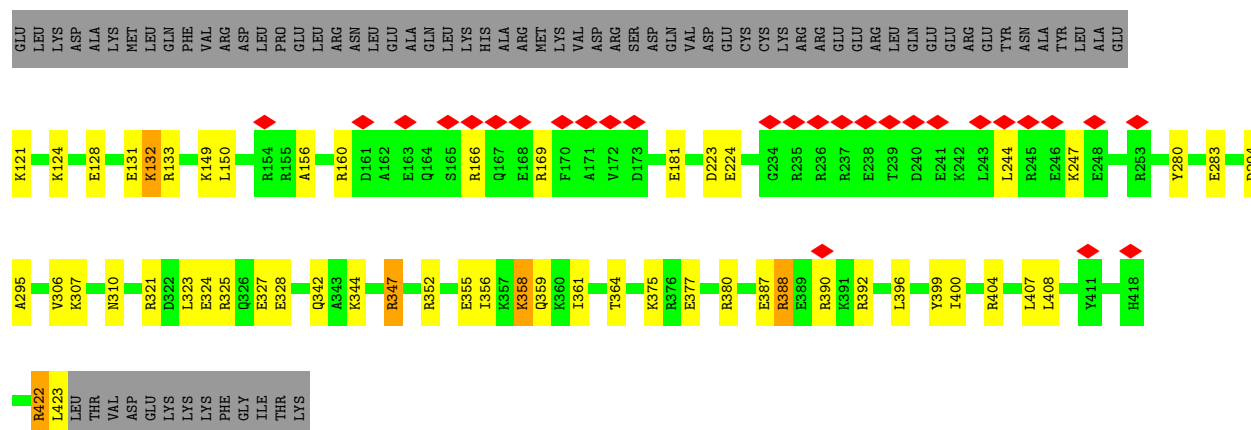


- Molecule 7: Meiosis-specific nuclear structural protein 1



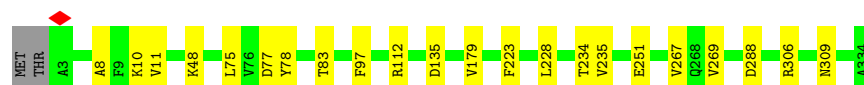
- Molecule 7: Meiosis-specific nuclear structural protein 1





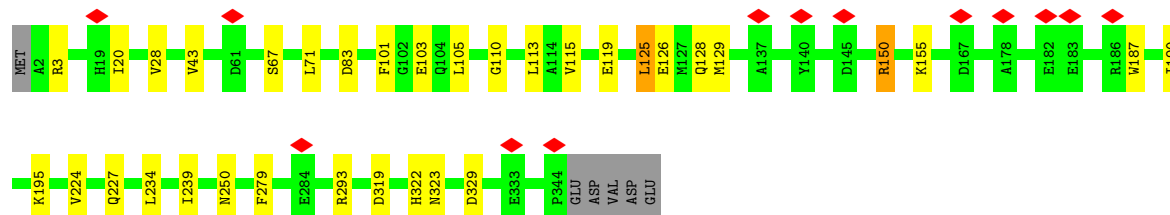
- Molecule 8: Nucleoside diphosphate kinase, putative

Chain 0Q: 93% 7%



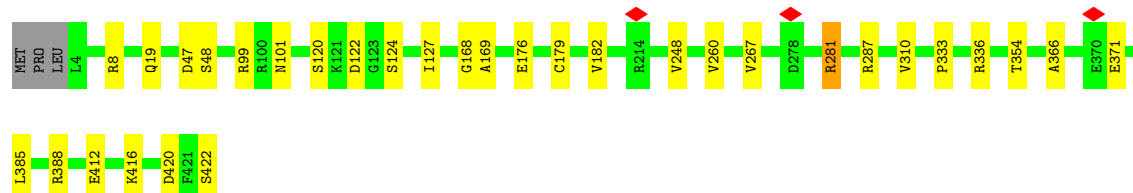
- Molecule 9: Nucleoside diphosphate kinase, putative

Chain 0R: 89% 9%



- Molecule 10: EF-hand domain-containing protein

Chain 0S: 92% 7%

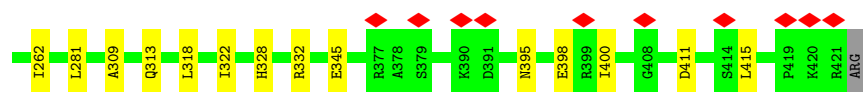


- Molecule 11: EF-hand domain-containing protein

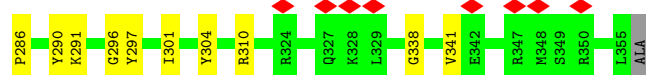
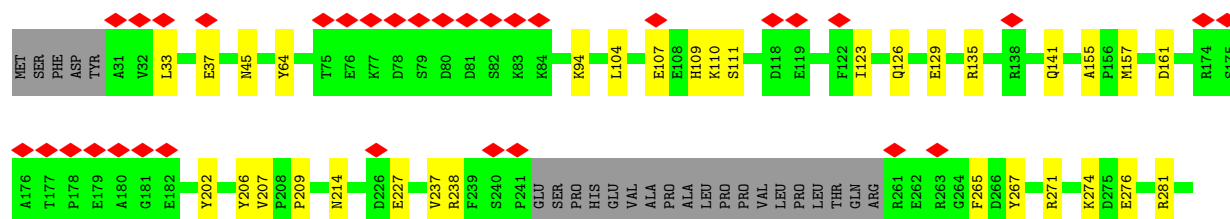
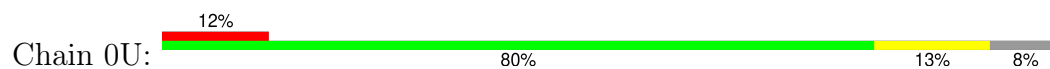
Chain 0T: 6% 91% 7%



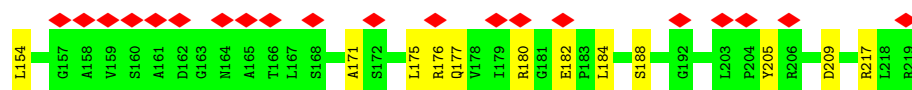
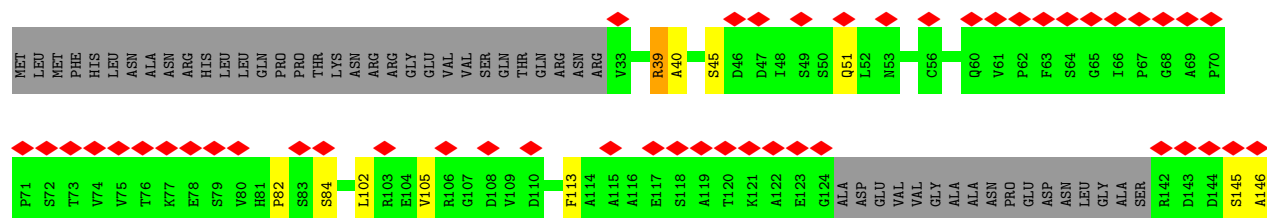




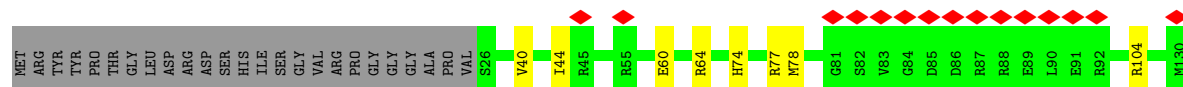
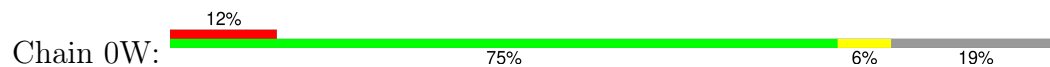
• Molecule 12: Cyclic nucleotide-binding domain-containing protein



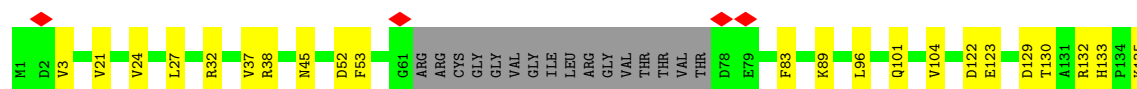
• Molecule 13: TbMIP23

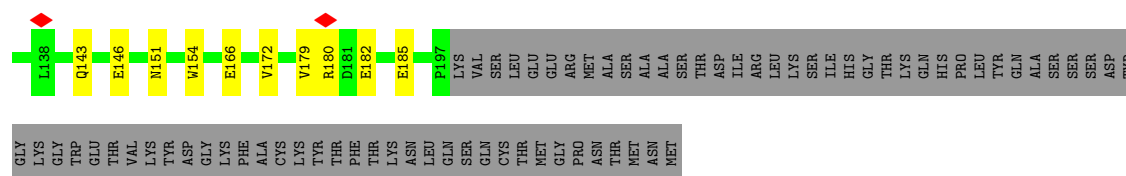


• Molecule 14: FAP141

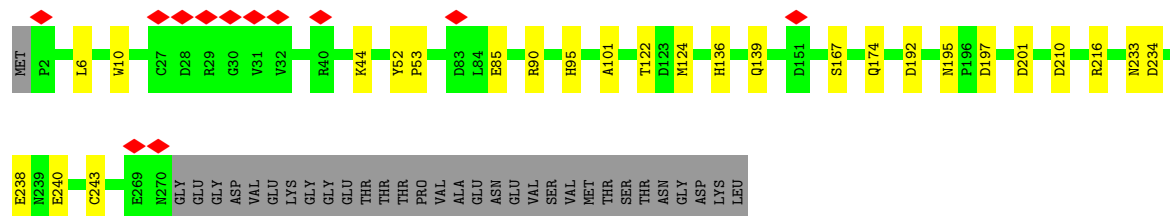
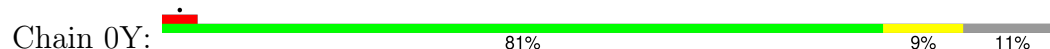


• Molecule 15: EF-hand domain-containing protein

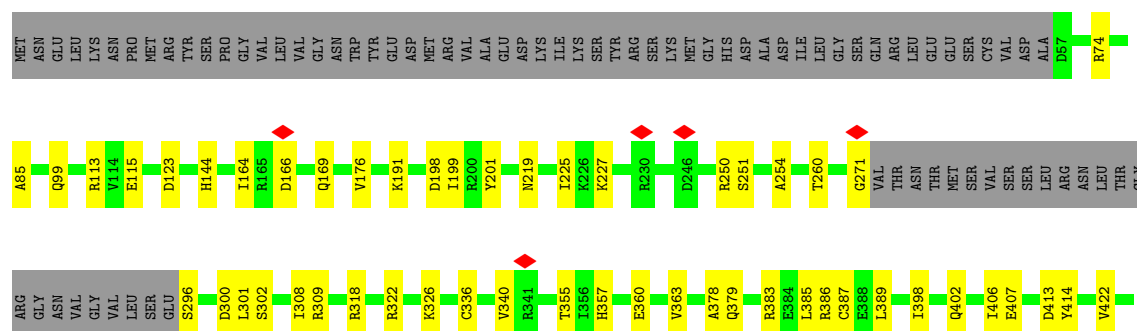
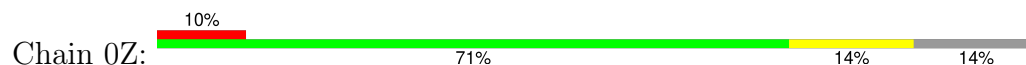




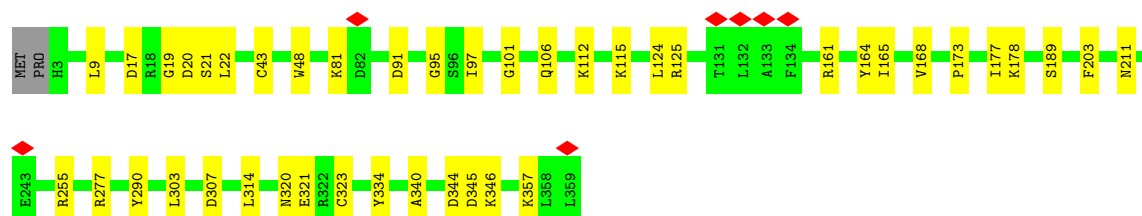
- Molecule 16: Calpain-like cysteine peptidase, putative




- Molecule 17: EF-hand domain-containing protein

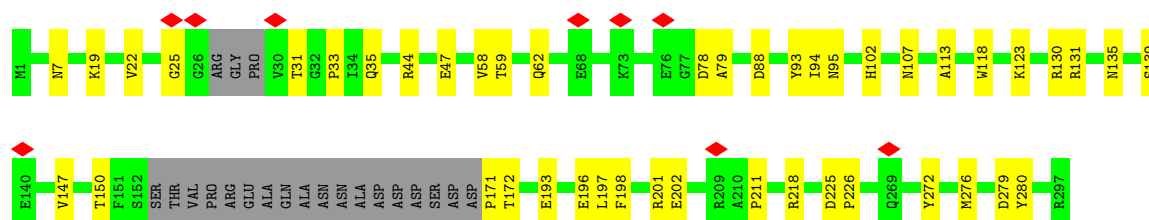


- Molecule 18: Calcium-binding protein, putative




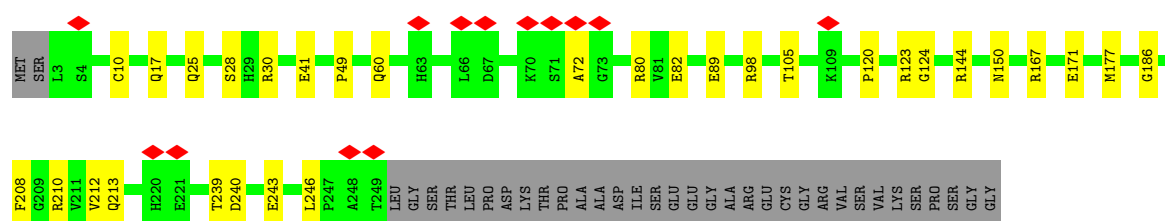
- Molecule 19: EF-hand domain-containing protein

Chain 1B: 




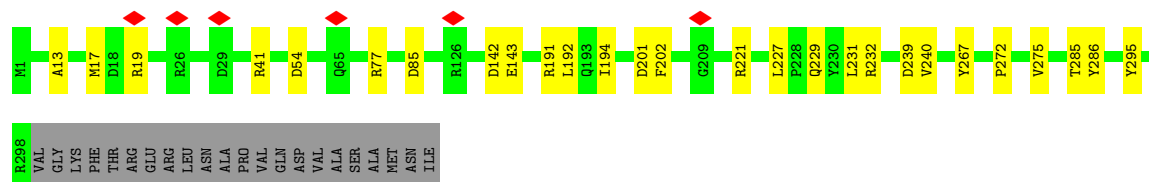
- Molecule 20: Peptidyl-prolyl cis-trans isomerase

Chain 1C: 




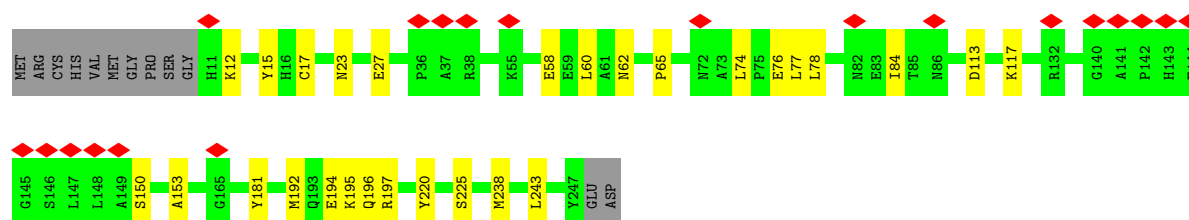
- Molecule 21: EF-hand domain-containing protein

Chain 1D: 




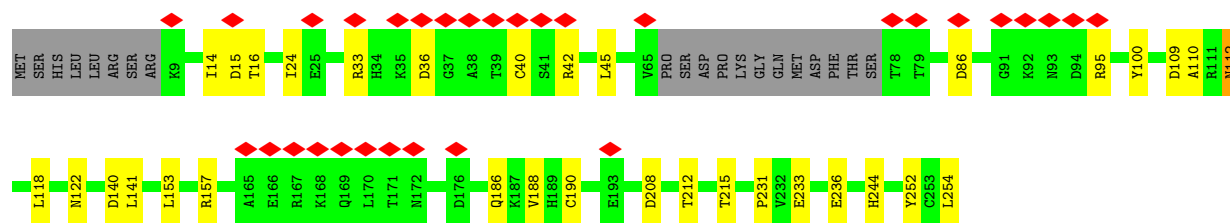
- Molecule 22: FAP107/MC11

Chain 1E: 

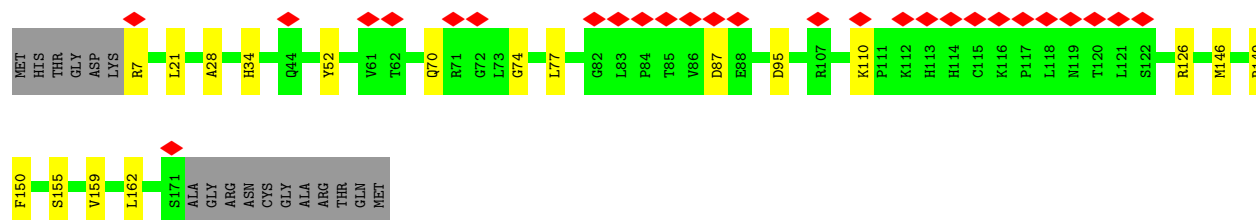
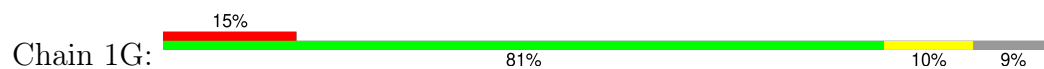


- Molecule 23: T. brucei spp.-specific protein

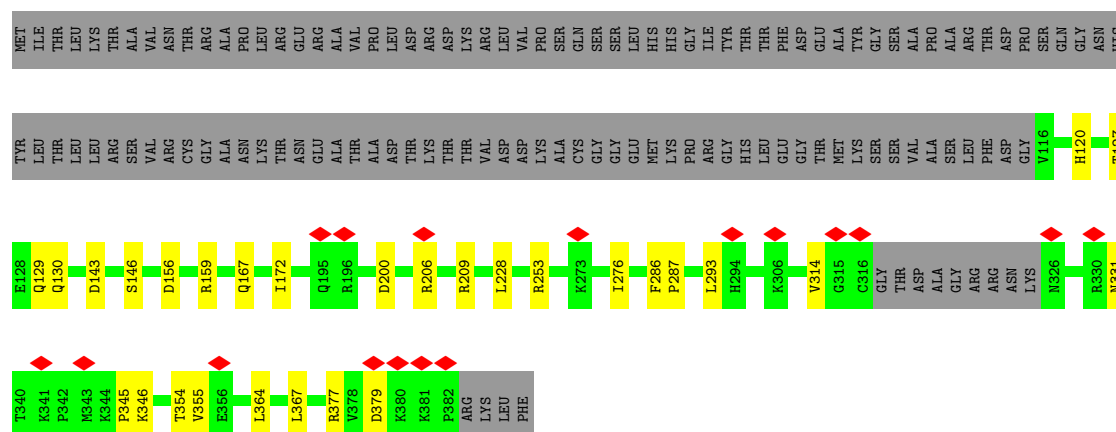
Chain 1F: 



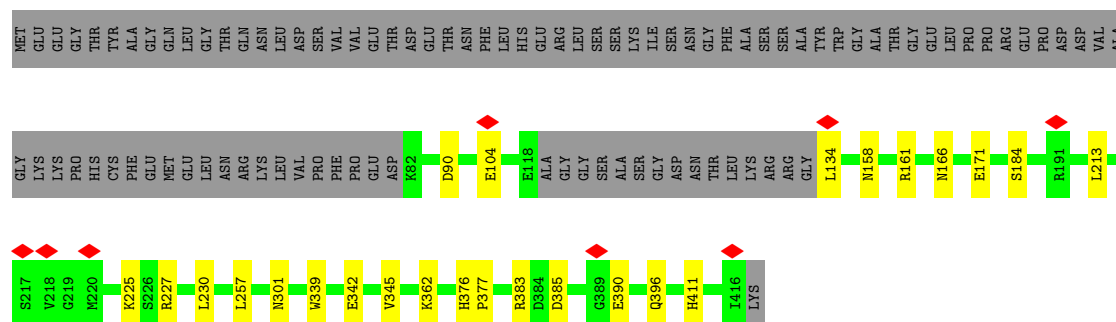
• Molecule 24: FAP95/MC6



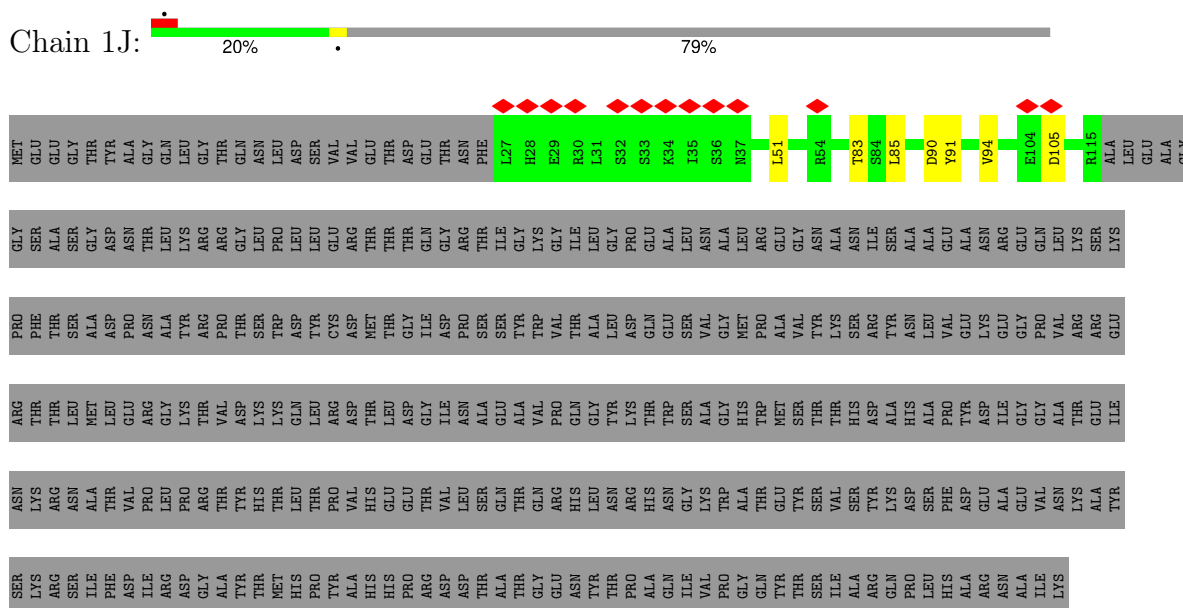
• Molecule 25: FAP129



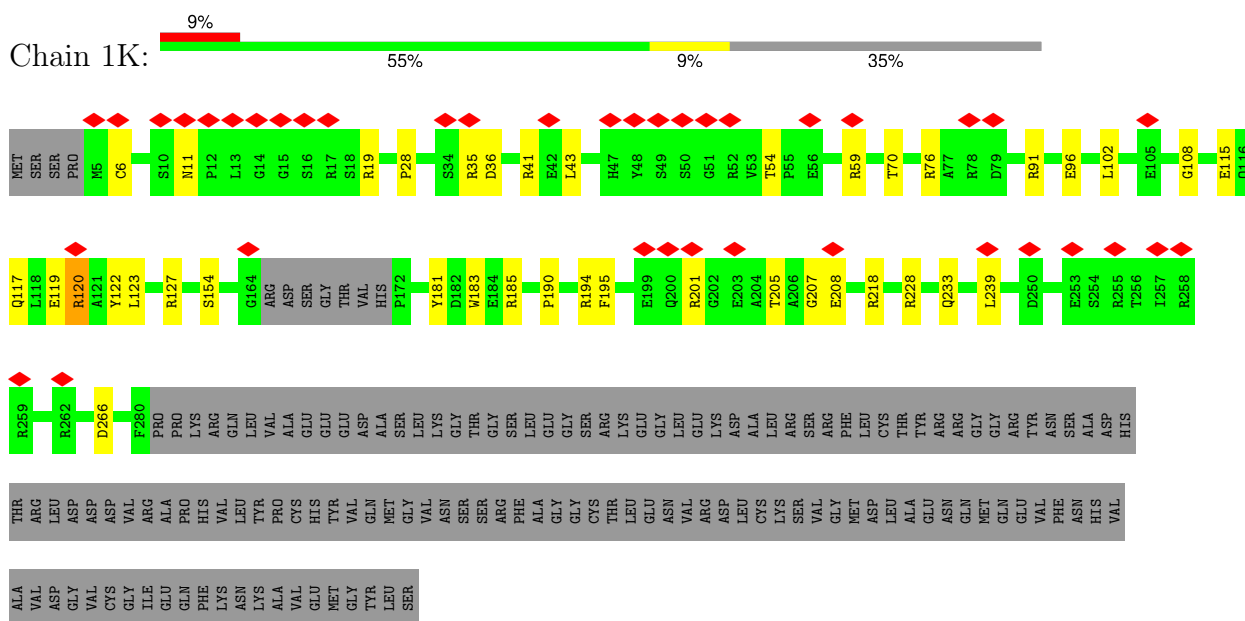
• Molecule 26: T. brucei spp.-specific protein



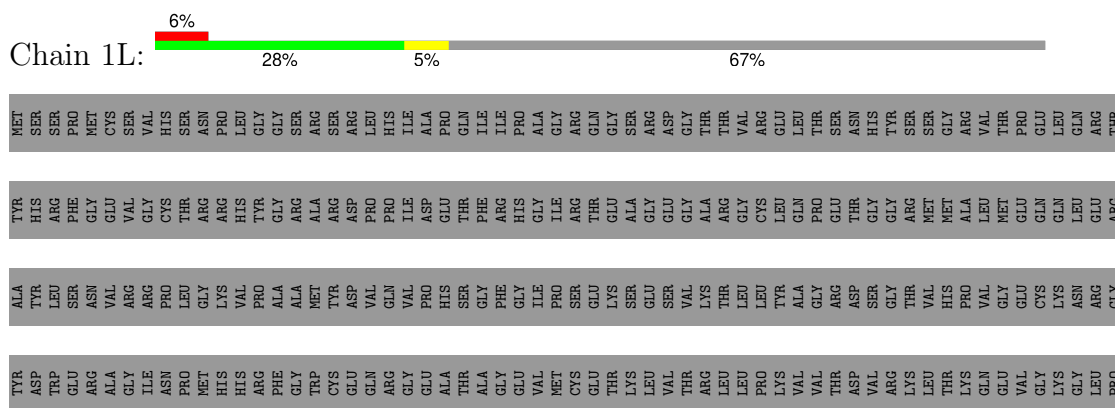
• Molecule 26: T. brucei spp.-specific protein



- Molecule 27: FAP21



- Molecule 27: FAP21

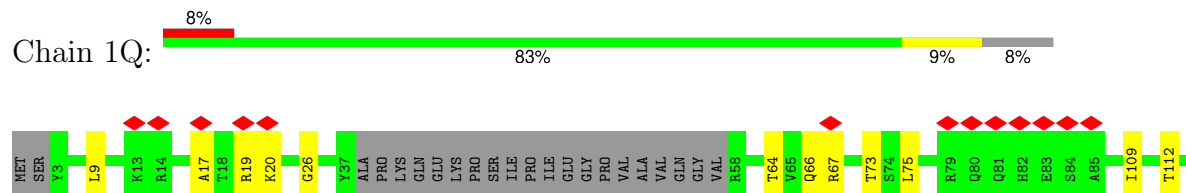




- Molecule 29: TbRib26b

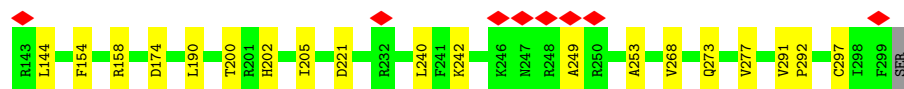
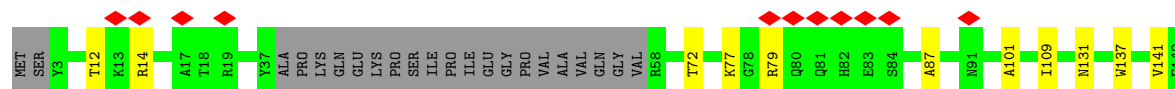
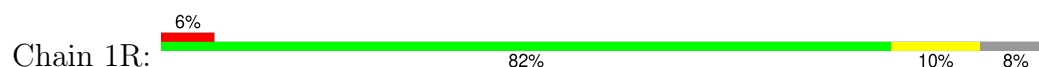
- Molecule 29: TbRib26b

- Molecule 30: PACRGA

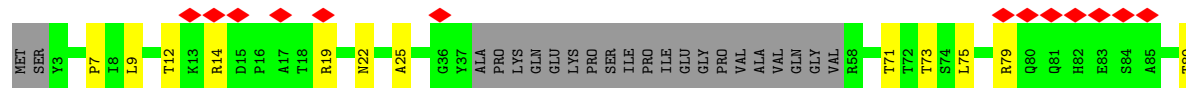
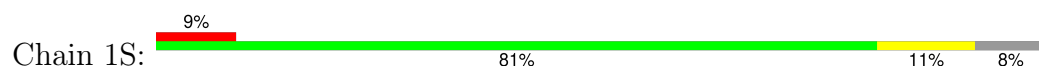




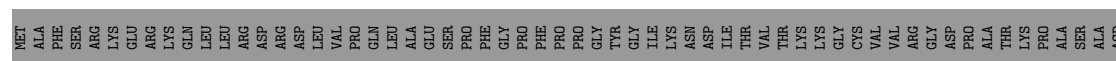
- Molecule 30: PACRGA



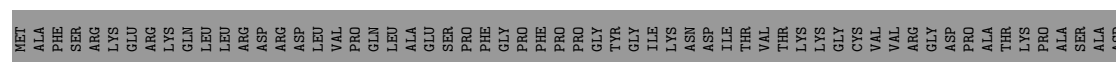
- Molecule 30: PACRGA



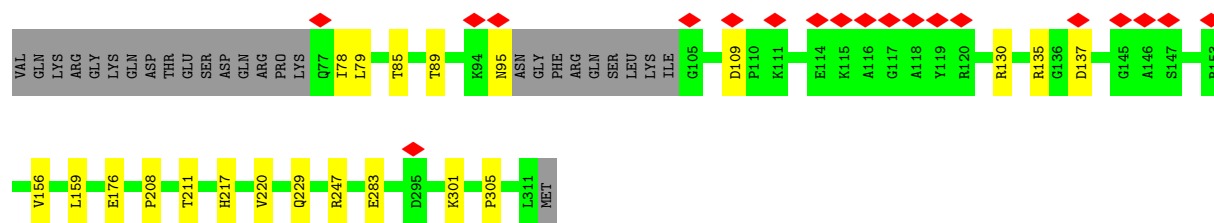
- Molecule 31: PACRGB



- Molecule 31: PACRGB

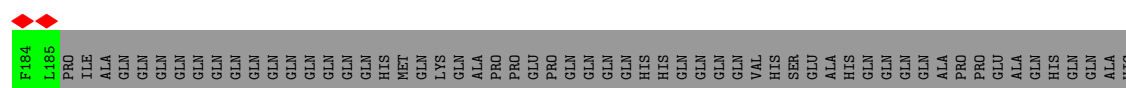
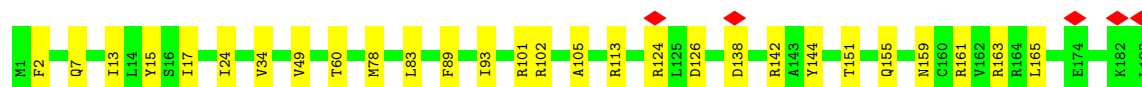






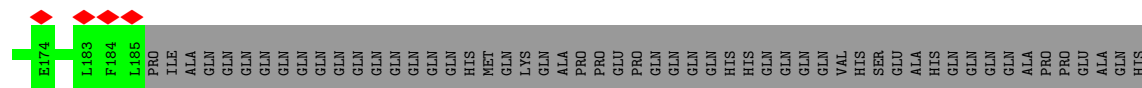
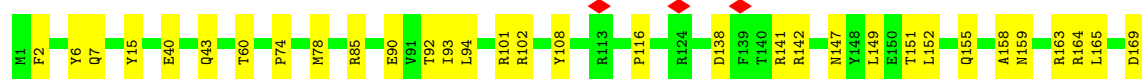
• Molecule 32: Cilia- and flagella-associated protein 20

Chain 1V: 53% 10% 37%



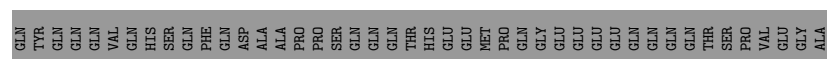
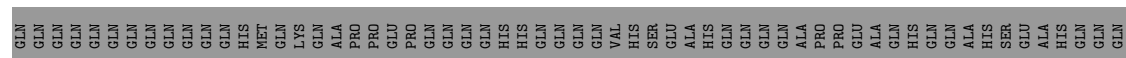
• Molecule 32: Cilia- and flagella-associated protein 20

Chain 1W: 52% 11% 37%



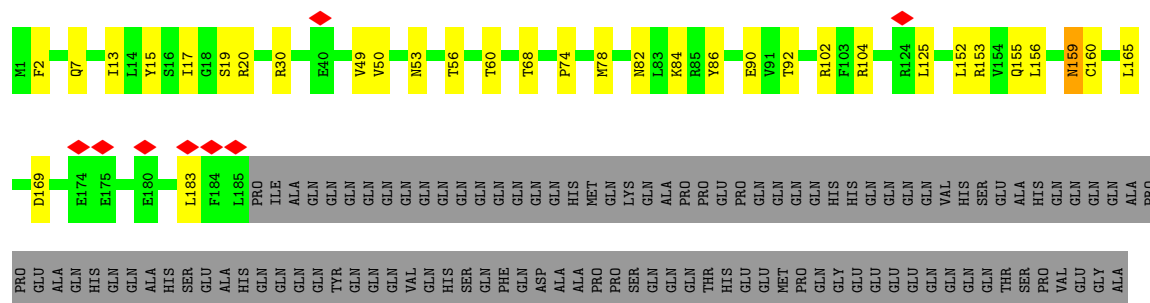
• Molecule 32: Cilia- and flagella-associated protein 20

Chain 1X: 54% 9% 37%



• Molecule 32: Cilia- and flagella-associated protein 20

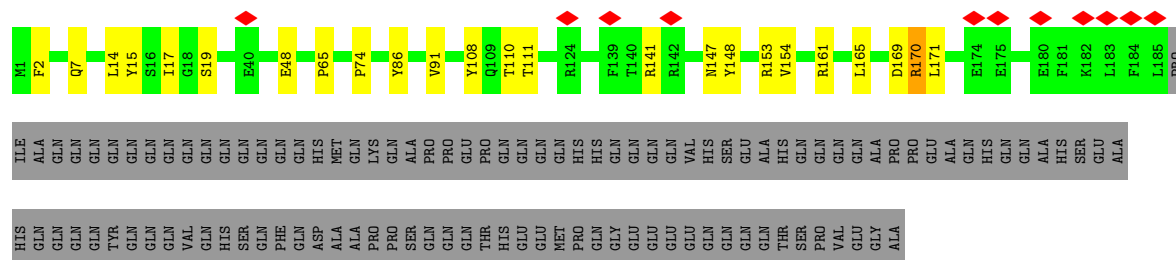
Chain 1Y: 52% 11% 37%



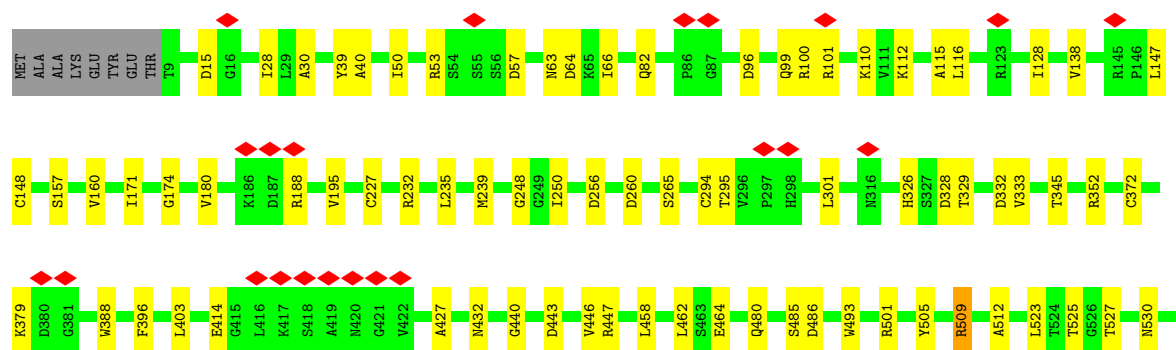
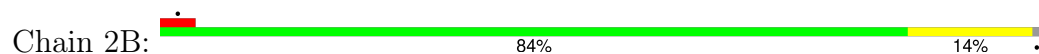
• Molecule 32: Cilia- and flagella-associated protein 20

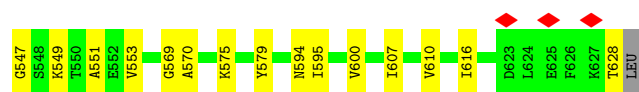


• Molecule 32: Cilia- and flagella-associated protein 20

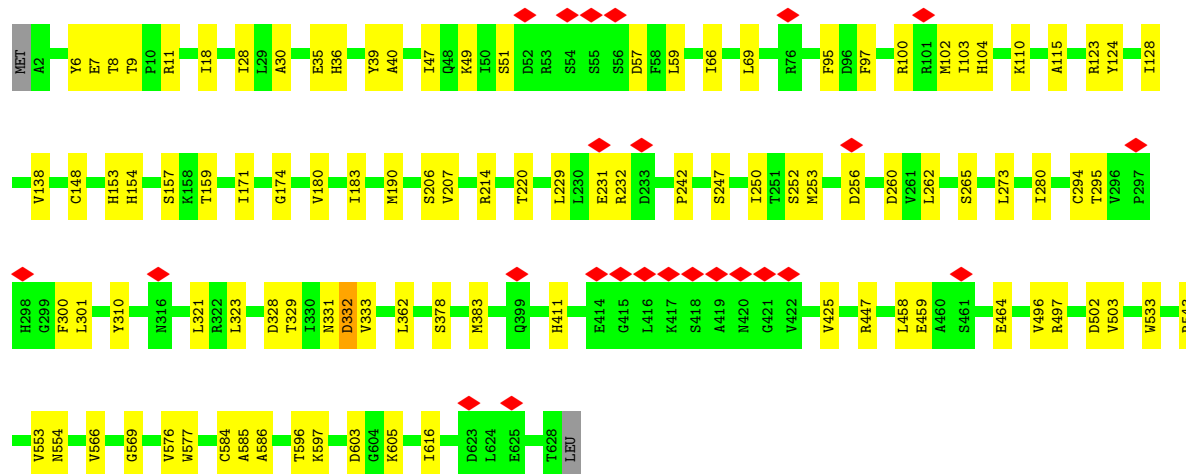
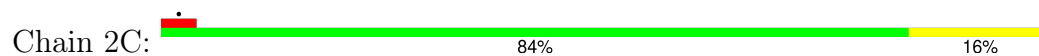


• Molecule 33: Cilia- and flagella-associated protein 52

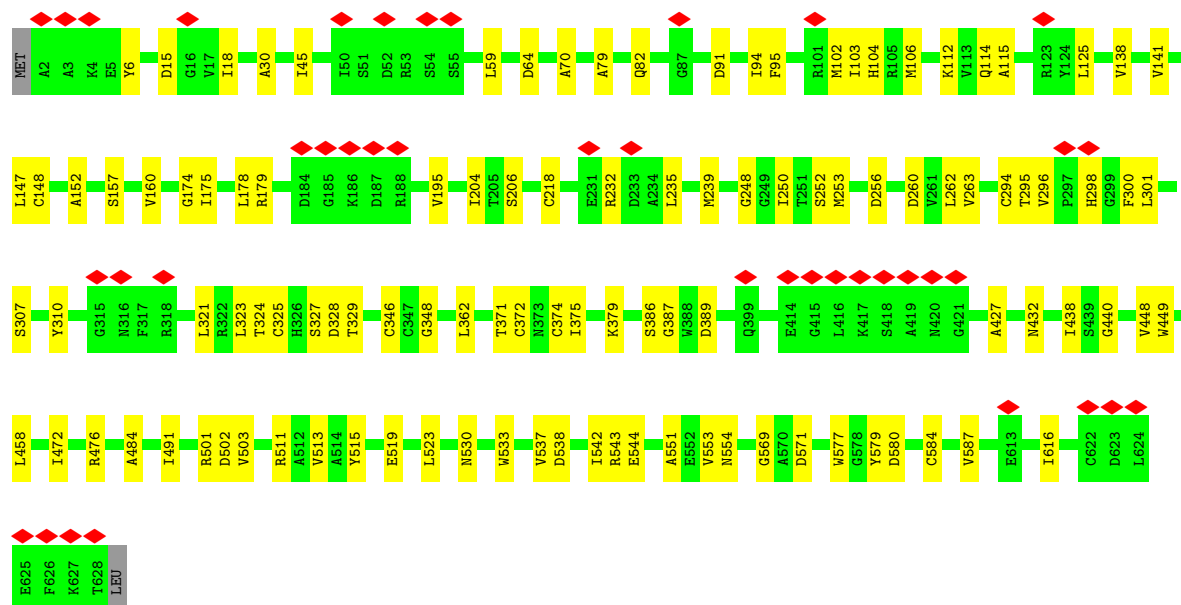
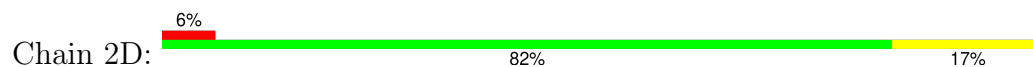




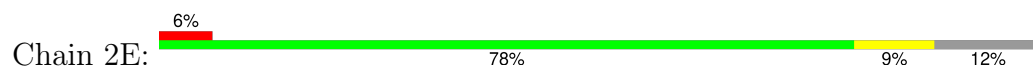
- Molecule 33: Cilia- and flagella-associated protein 52

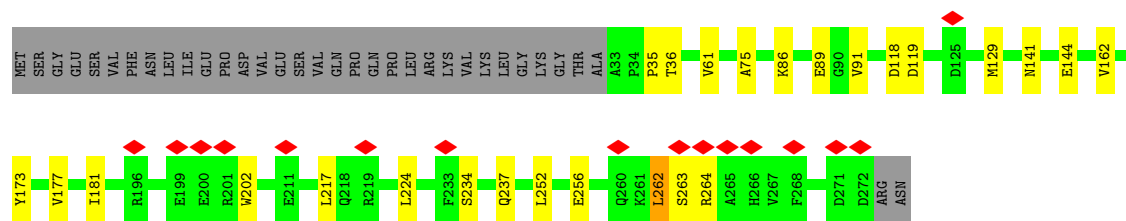


- Molecule 33: Cilia- and flagella-associated protein 52

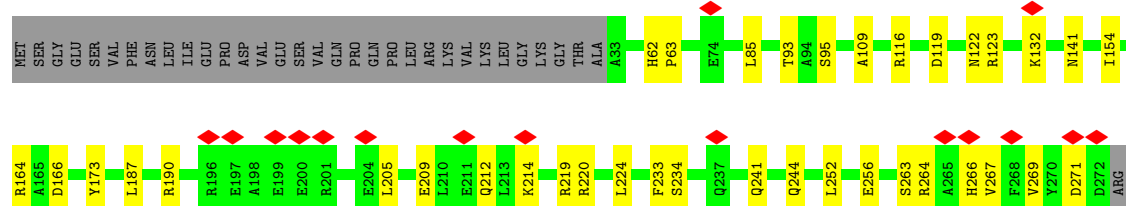
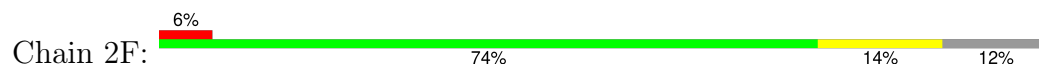


- Molecule 34: Enkurin domain-containing protein

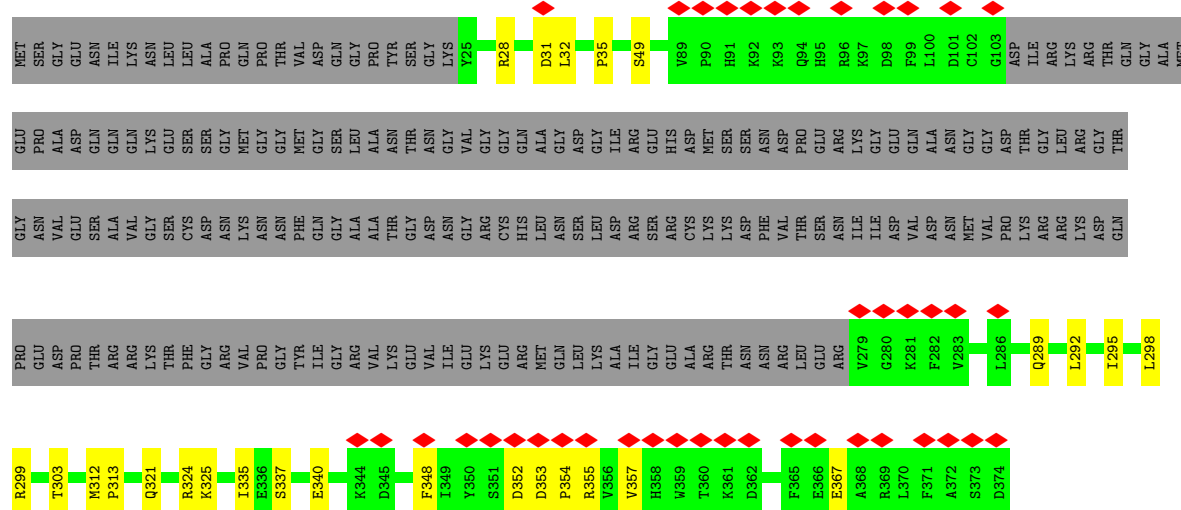
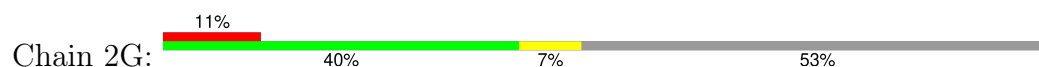




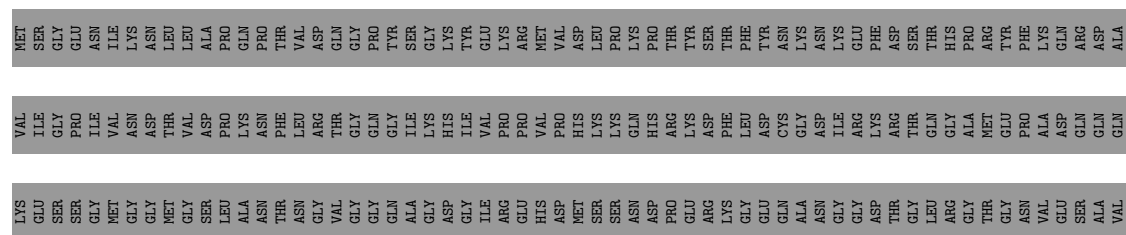
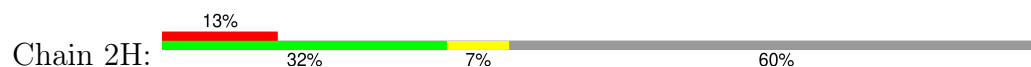
• Molecule 34: Enkurin domain-containing protein

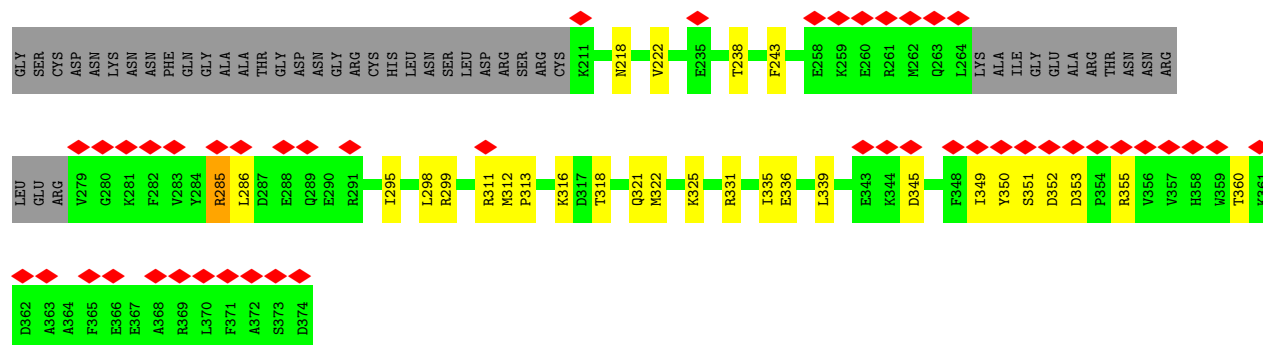


• Molecule 35: Enkurin domain-containing protein

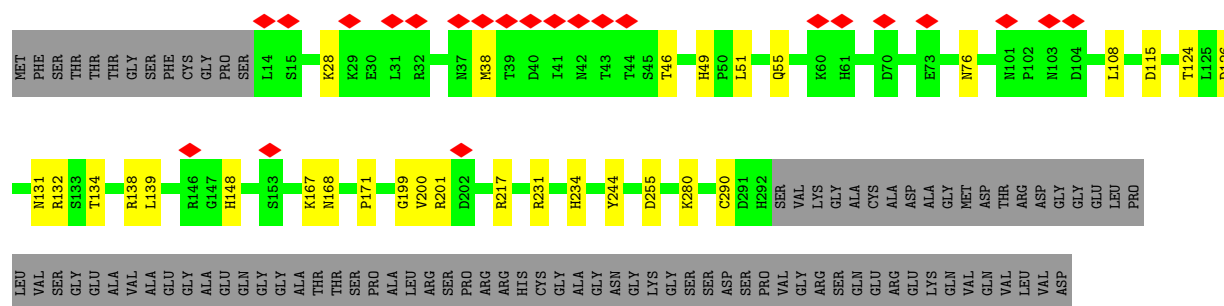


• Molecule 35: Enkurin domain-containing protein

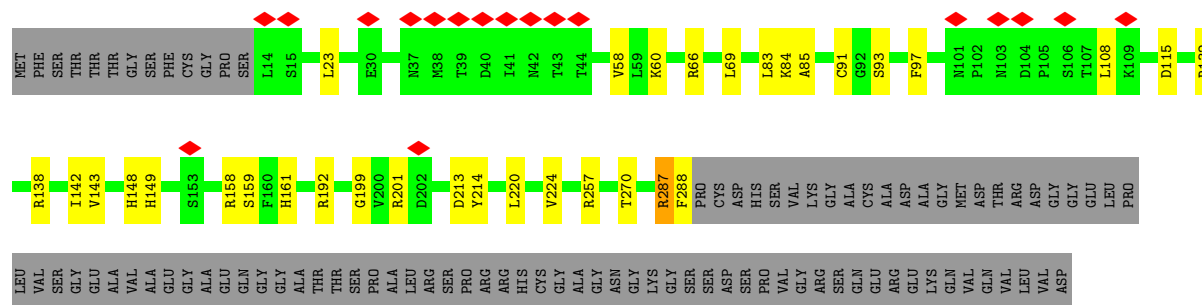




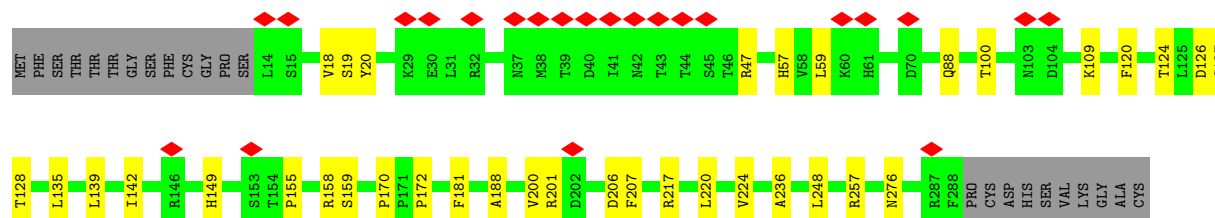
• Molecule 36: MC4



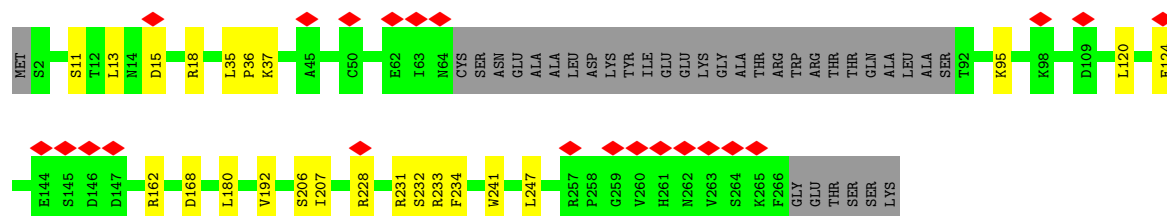
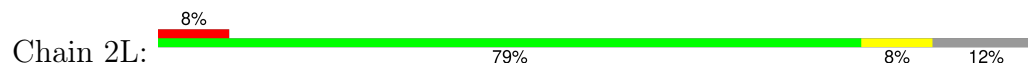
• Molecule 36: MC4



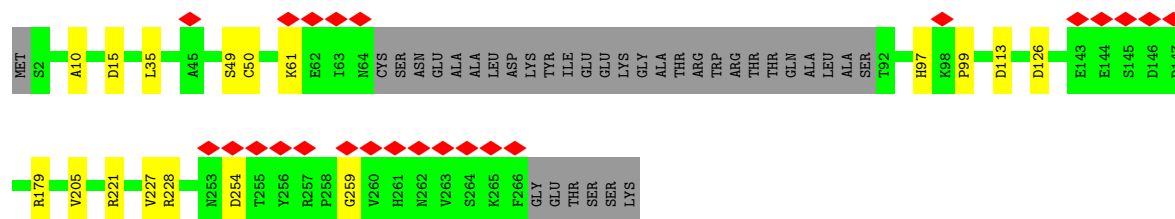
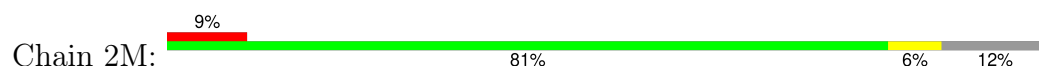
• Molecule 36: MC4



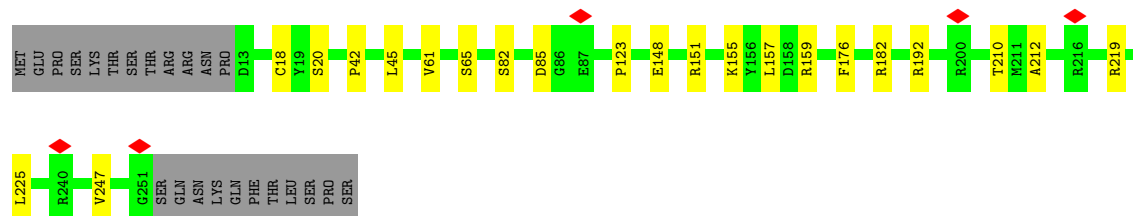
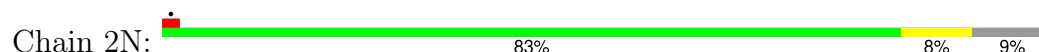
- Molecule 37: MC5



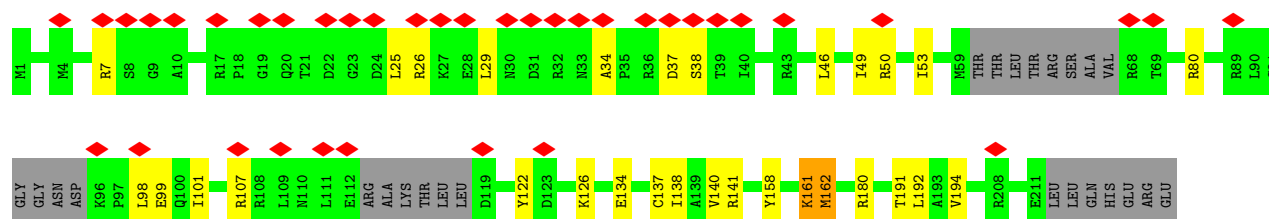
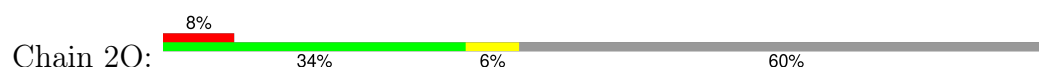
- Molecule 37: MC5

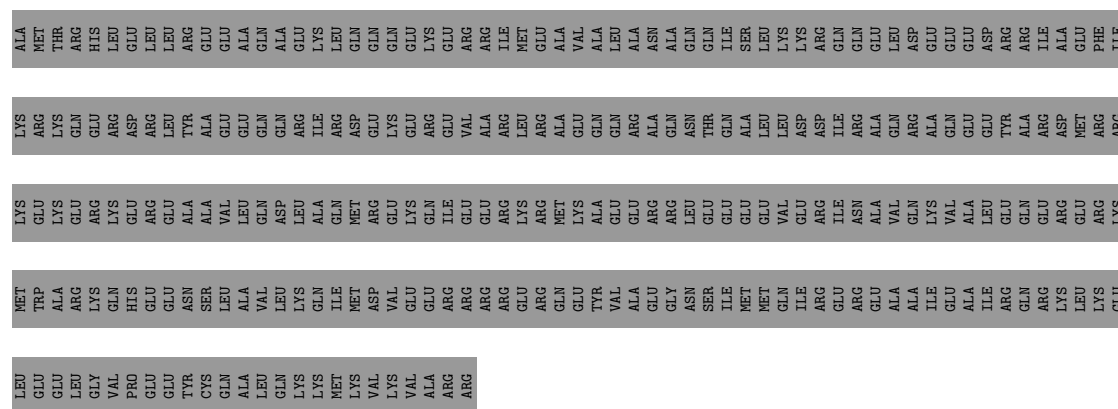


- Molecule 38: CCDC81 HU domain-containing protein

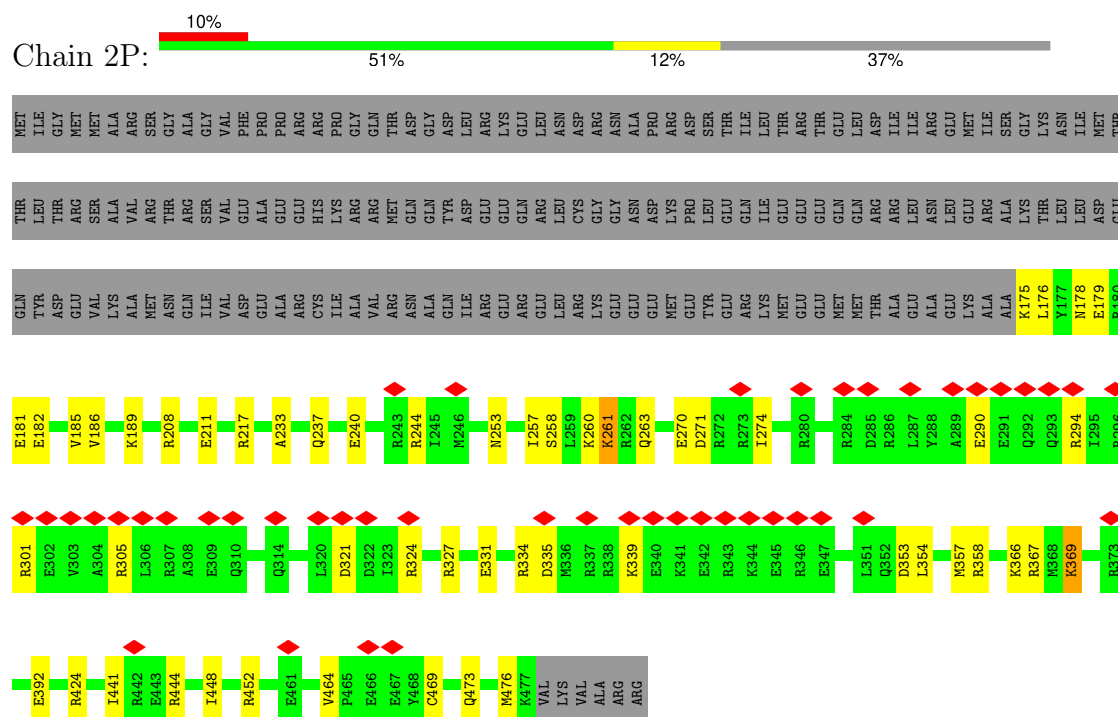


- Molecule 39: Cilia- and flagella-associated protein 45

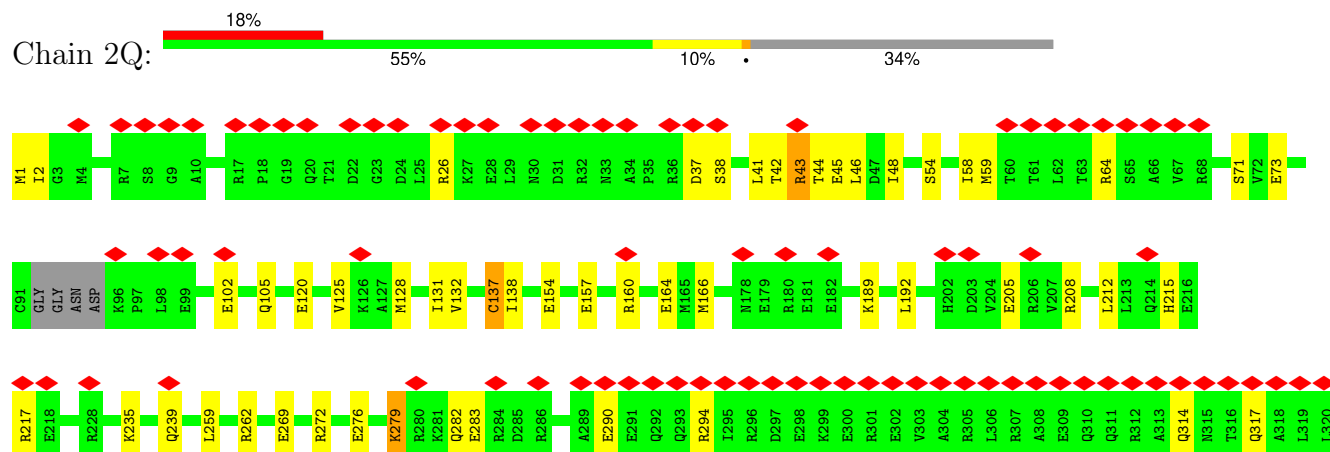




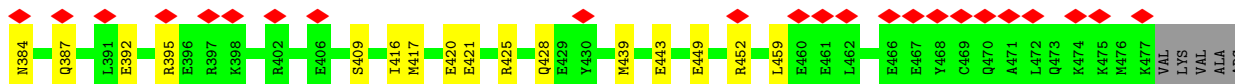
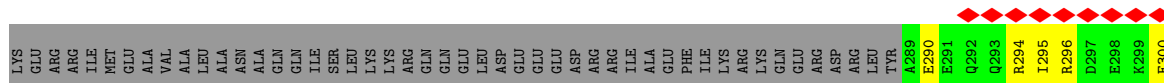
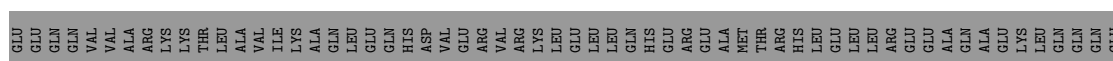
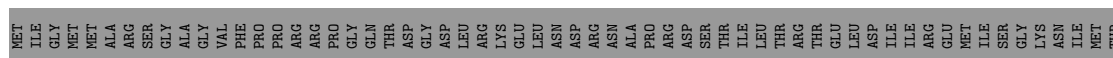
- Molecule 39: Cilia- and flagella-associated protein 45



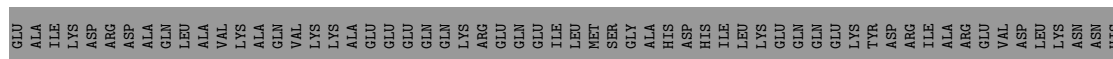
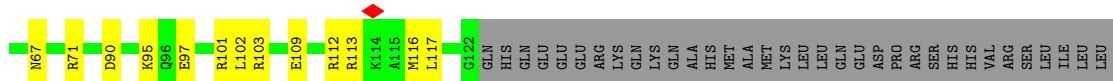
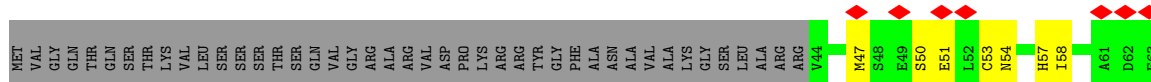
- Molecule 39: Cilia- and flagella-associated protein 45



- Molecule 39: Cilia- and flagella-associated protein 45



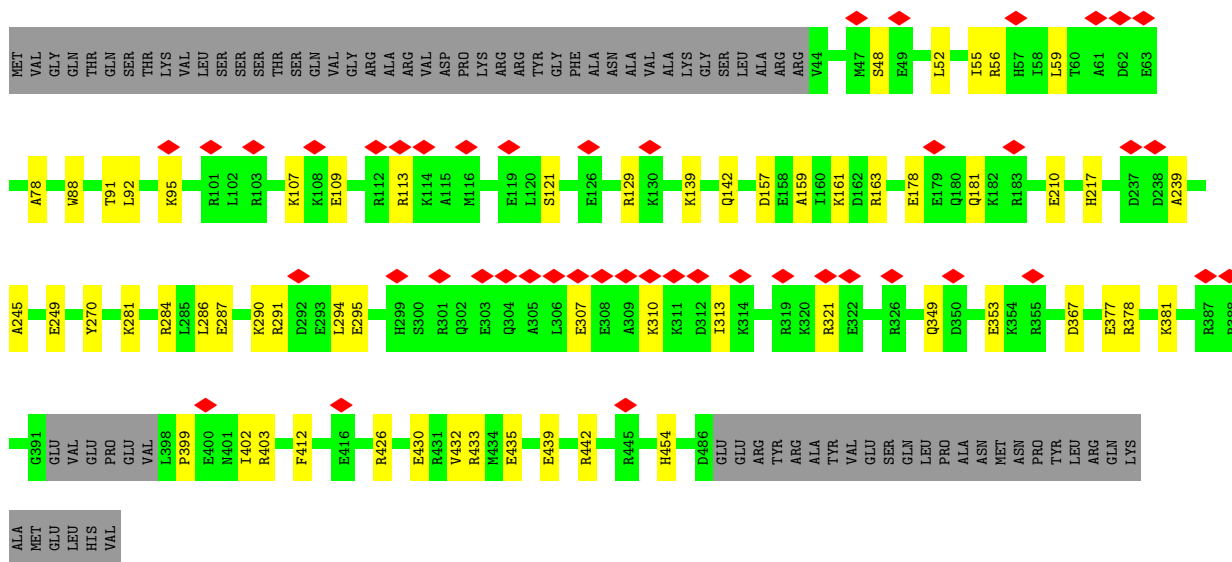
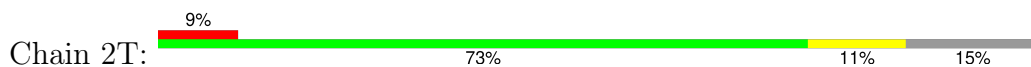
- Molecule 40: Trichohyalin-plectin-homology domain-containing protein





[illegible]

- Molecule 40: Trichohyalin-plectin-homology domain-containing protein

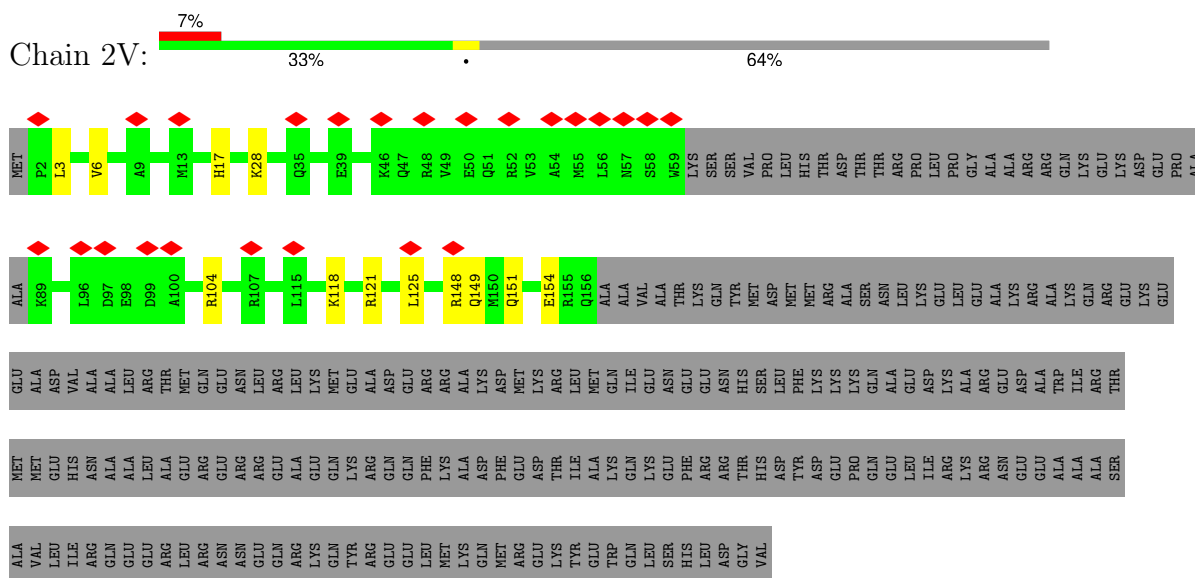


- Molecule 40: Trichohyalin-plectin-homology domain-containing protein

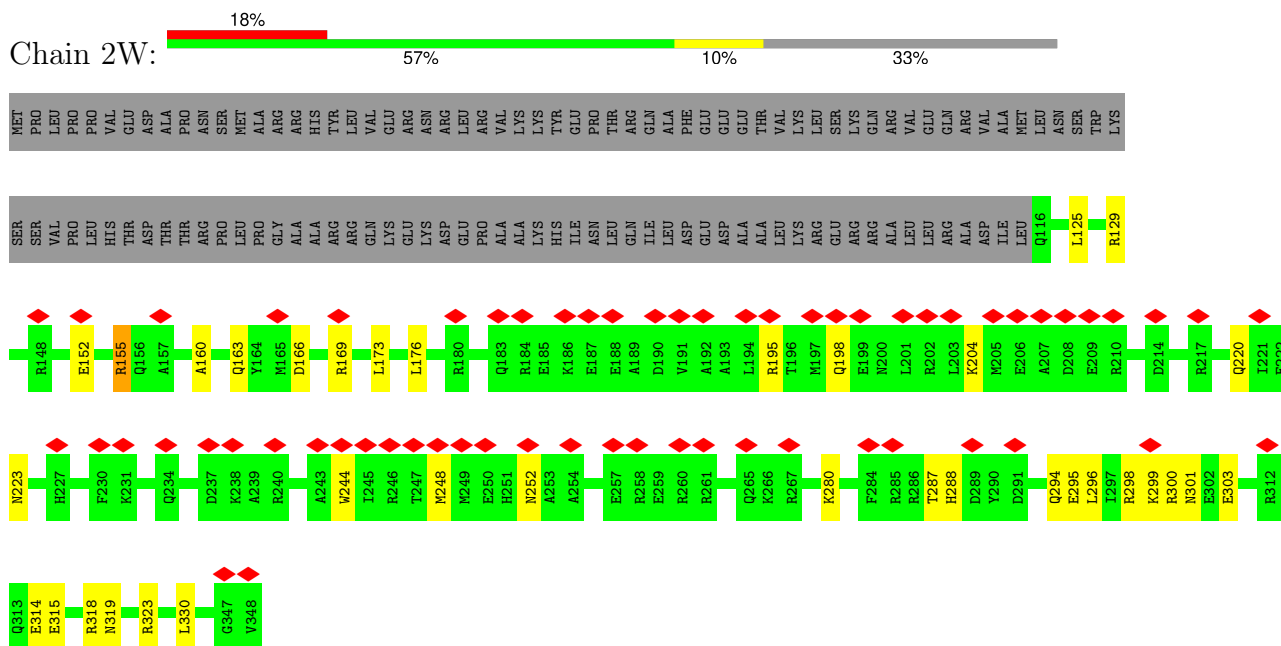


GLU	ALA	GLN	SER	ALA	MET
ALA	LYS	LYS	GLY	ASP	VAL
LYS	ARG	GLN	GLN	GLU	GLY
ARG	GLU	HIS	ASP	GLN	GLN
ALA	GLN	GLN	SER	THR	THR
ALA	GLU	GLU	GLU	TVR	GLN
GLU	ILE	ILE	GLU	ASN	SER
GLU	LEU	LEU	GLU	ALA	THR
GLU	MET	ARG	TVR	LYS	VAL
GLU	SER	LYS	ARG	ARG	LEU
GLN	GLY	GLN	ARG	GLN	SER
ALA	HIS	LYS	HIS	VAL	SER
ASN	ASP	GLN	ALA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

- Molecule 41: Trichohyalin-plectin-homology domain-containing protein

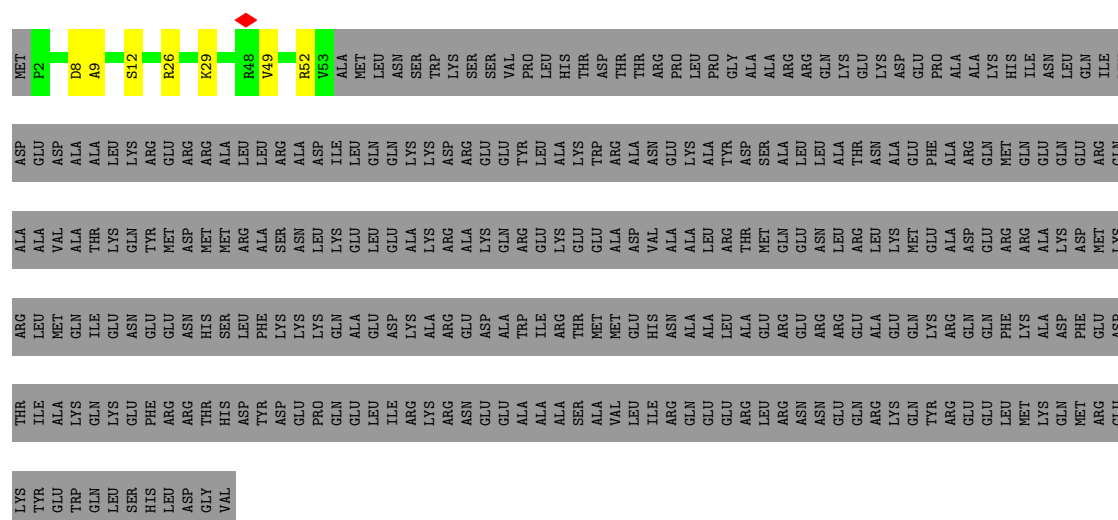


- Molecule 41: Trichohyalin-plectin-homology domain-containing protein

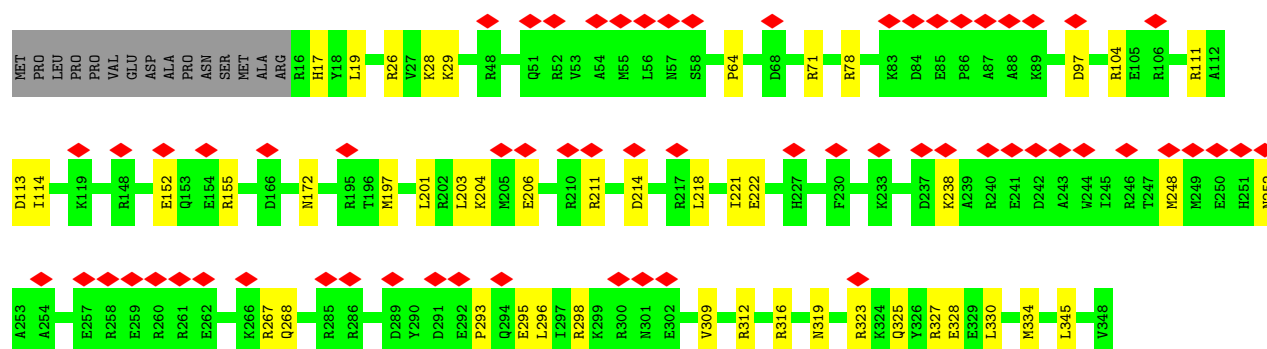
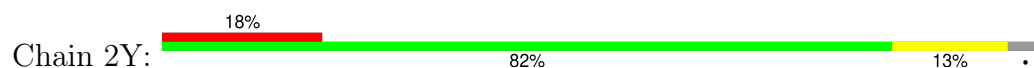


- Molecule 41: Trichohyalin-plectin-homology domain-containing protein

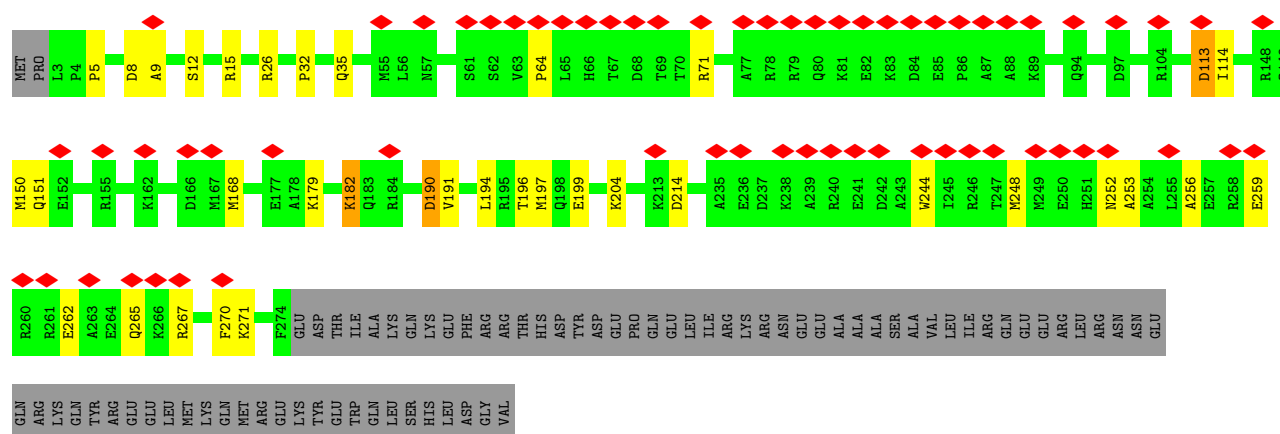




• Molecule 41: Trichohyalin-plectin-homology domain-containing protein

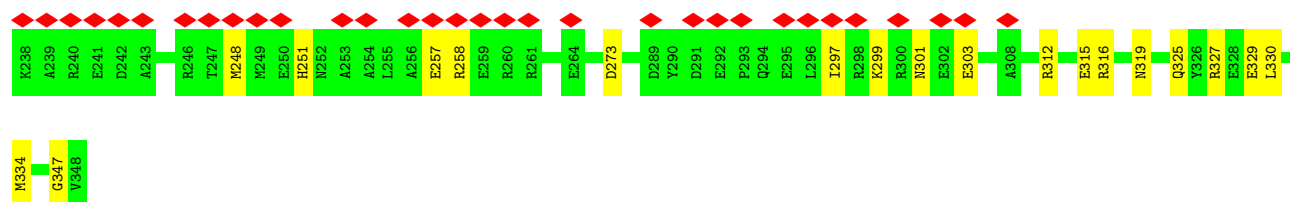


• Molecule 41: Trichohyalin-plectin-homology domain-containing protein

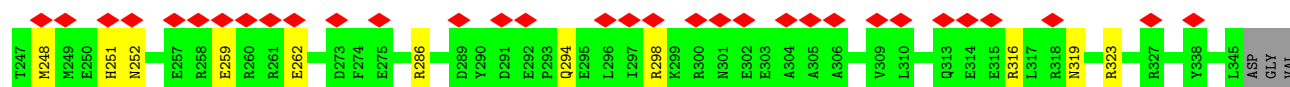
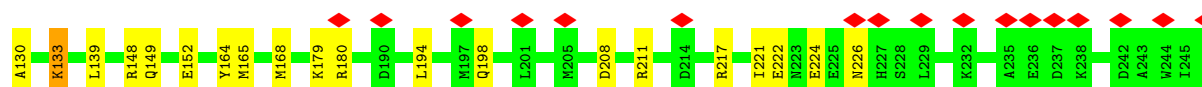
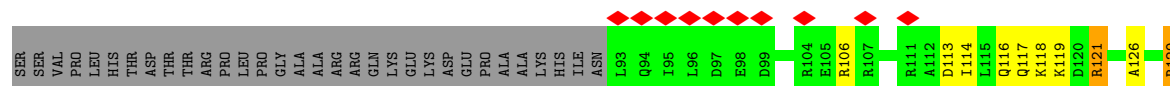
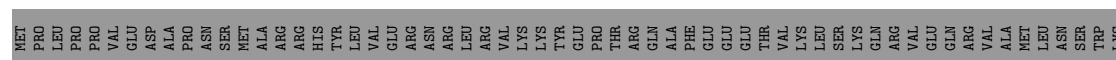


• Molecule 41: Trichohyalin-plectin-homology domain-containing protein

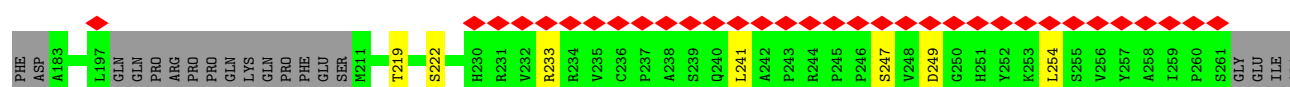
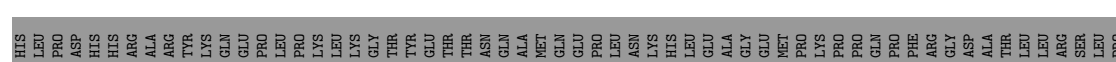
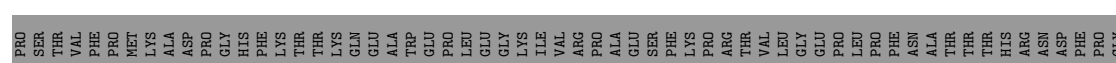




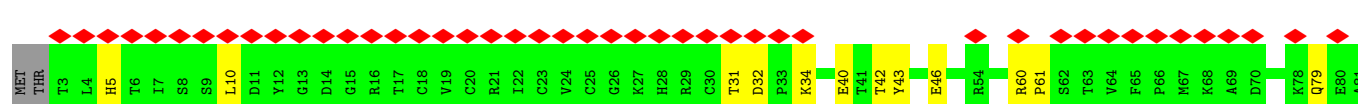
• Molecule 41: Trichohyalin-plectin-homology domain-containing protein



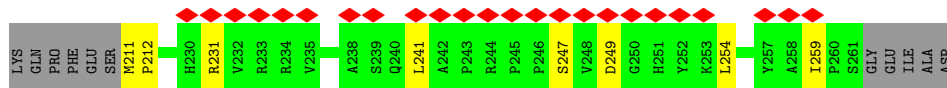
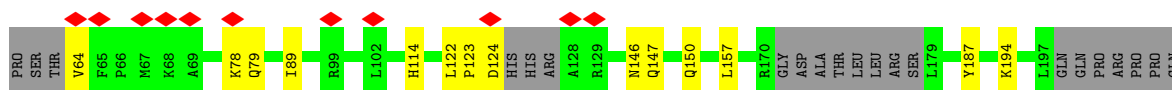
• Molecule 42: STOP axonemal protein



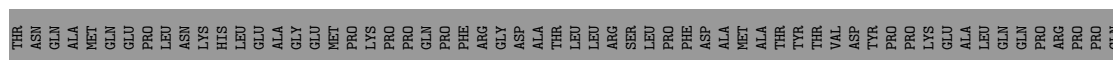
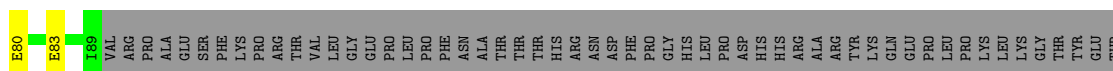
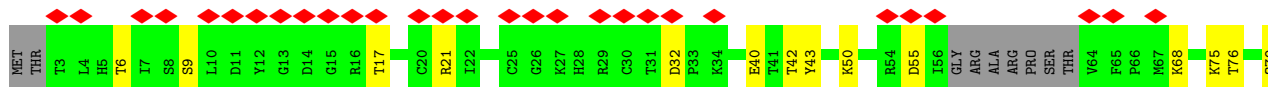
• Molecule 42: STOP axonemal protein



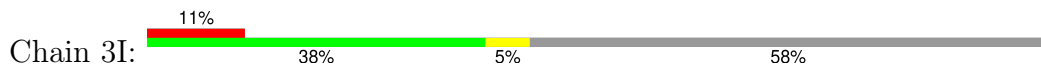
- Molecule 42: STOP axonemal protein

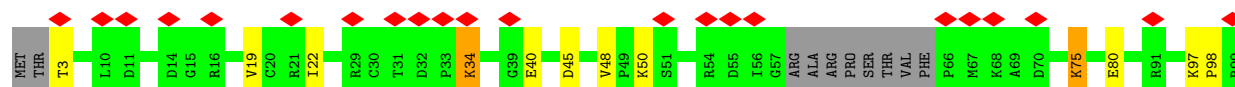


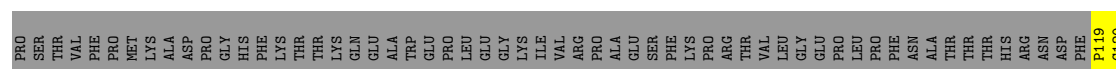
- Molecule 42: STOP axonemal protein



- Molecule 42: STOP axonemal protein

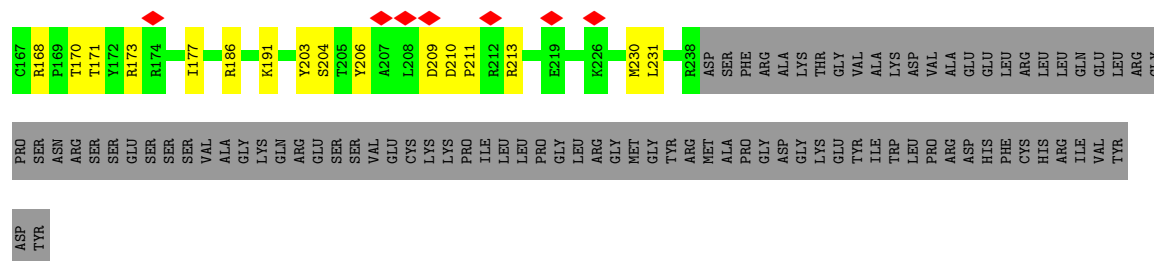




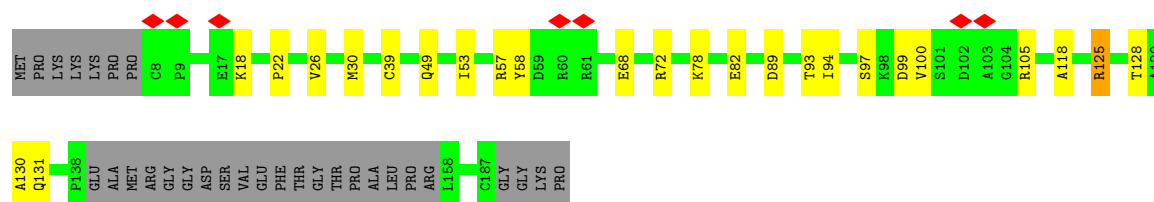




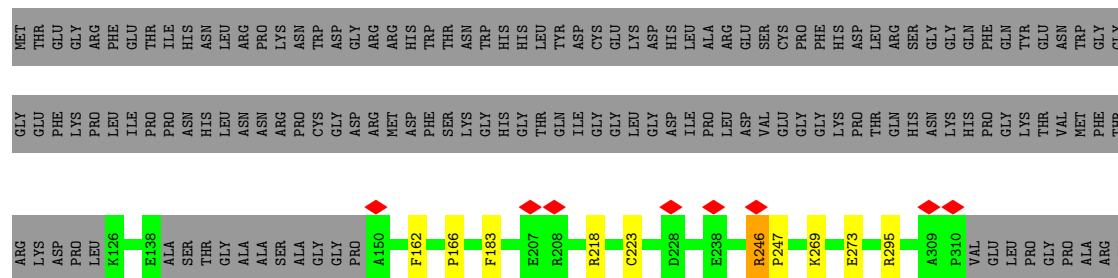




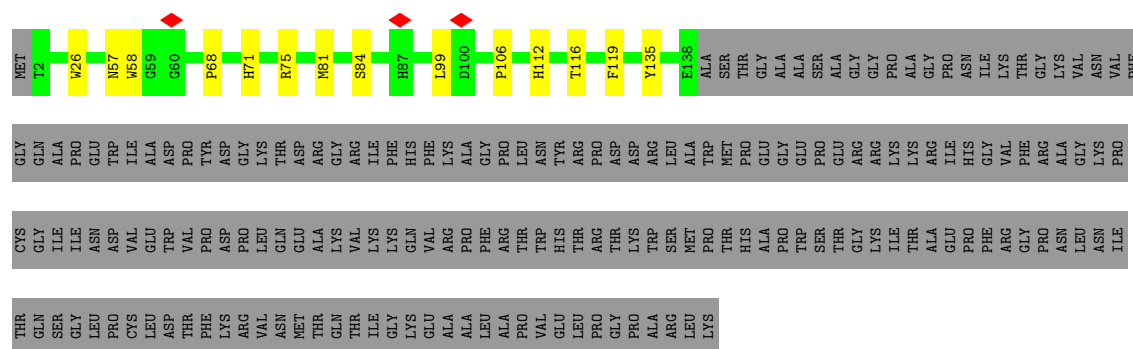
- Molecule 45: FAP90



- Molecule 46: PBP36

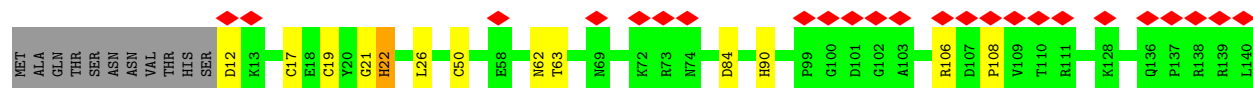


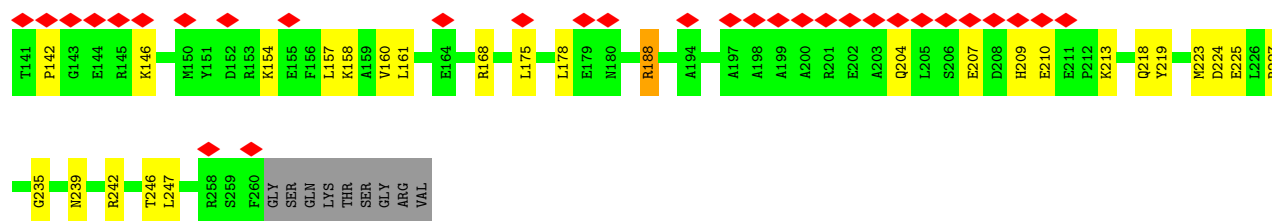
- Molecule 46: PBP36



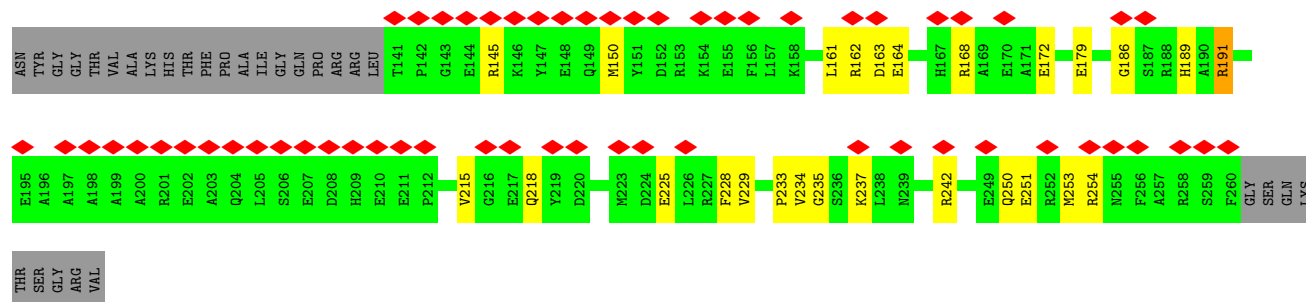
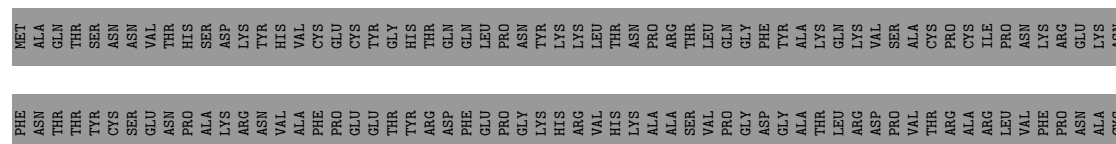
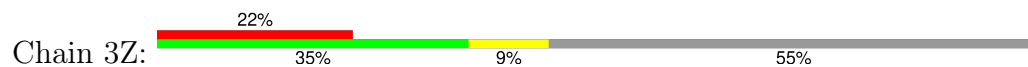
- Molecule 47: Enkurin domain-containing protein



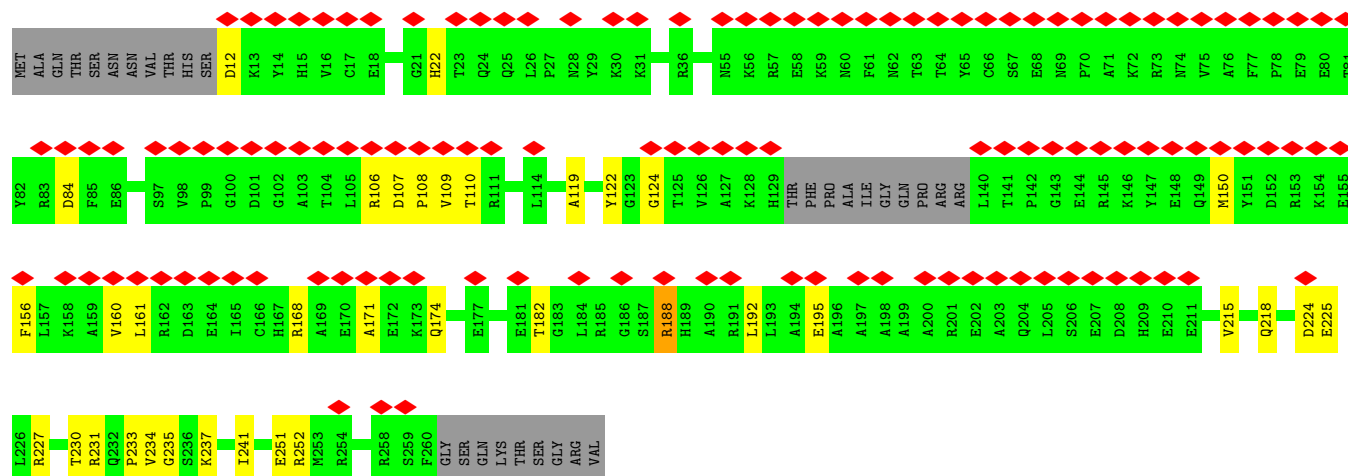
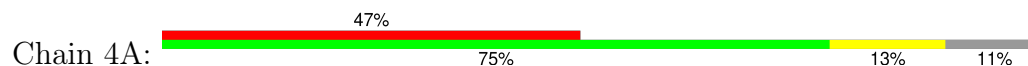




• Molecule 48: Enkurin domain-containing protein

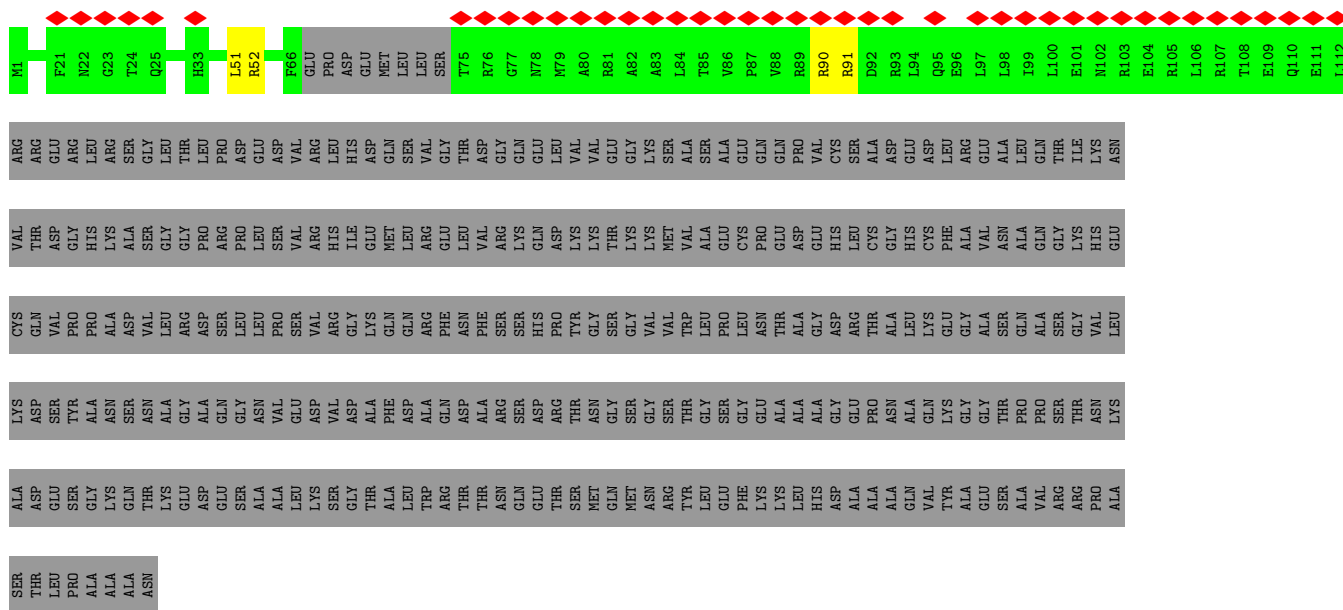


• Molecule 48: Enkurin domain-containing protein

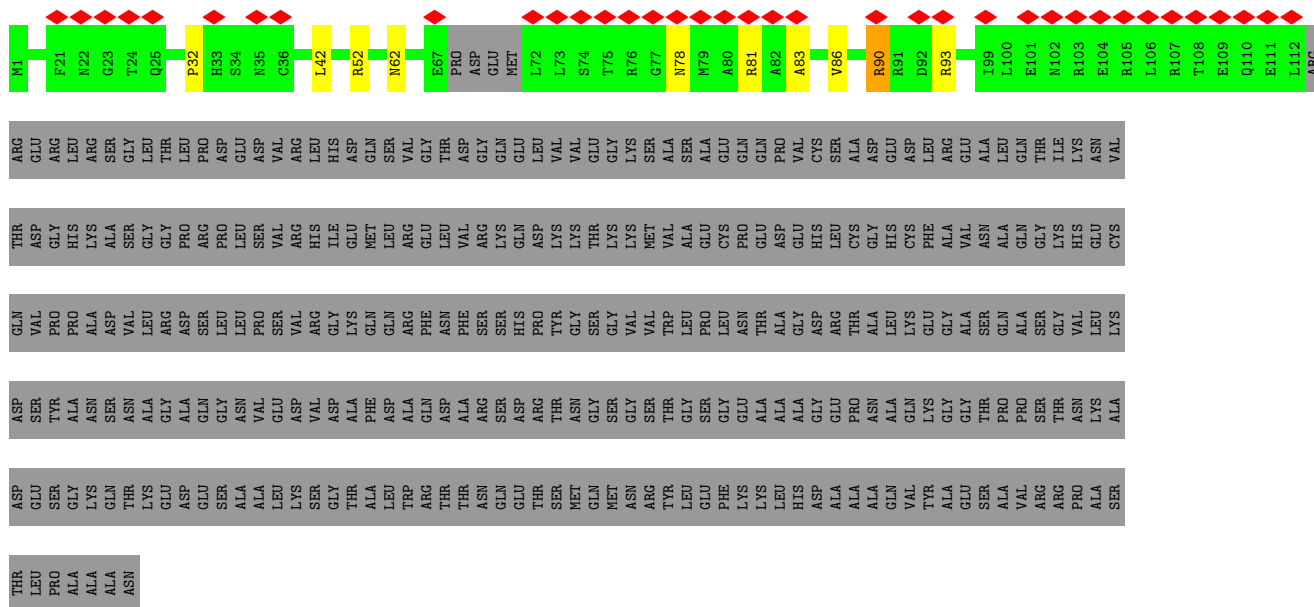


• Molecule 49: PON3

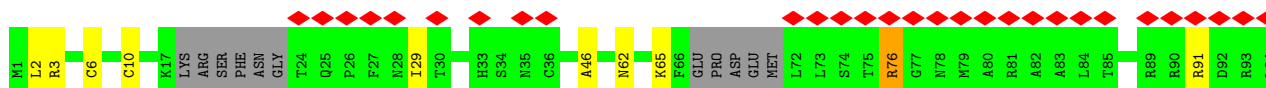


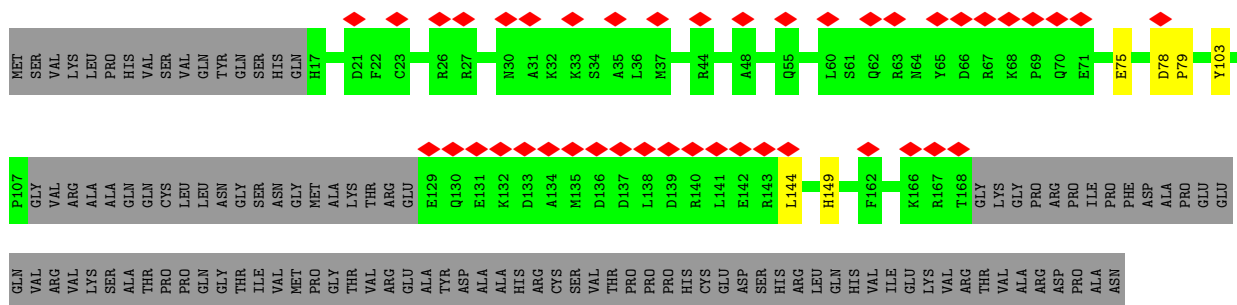


- Molecule 49: PON3



- Molecule 49: PON3





ARG ASP  
ASN  
ALA  
ALA  
LEU  
GLY  
ALA  
VAL  
ALA  
HIS  
ARG  
GLN  
CYS  
GLY  
ASP  
ALA  
GLY  
THR  
PRO  
VAL  
SER  
CYS  
GLY  
THR  
ASN  
GLN  
ARG  
THR  
PRO  
LEU  
TRP  
VAL  
SER  
CYS  
GLY  
THR  
ASN  
GLN  
PRO  
ILE  
GLY  
MET  
MET  
LYS  
THR  
ILE  
GLY  
THR  
SER  
ASN  
THR  
TVR  
GLY  
PRO  
ARG  
PRO  
GLU  
GLY  
ALA  
GLY  
VAL  
VAL  
TRP  
CYS  
ARG  
GLY  
ASN

ALA  
VAL  
VAL  
ASP  
ASP  
GLY  
ILE  
GLY  
THR  
SER  
ALA  
ALA  
LEU  
ALA  
HIS  
ARG  
GLN  
CYS  
THR  
ASN  
ASP  
ALA  
GLY  
THR  
PRO  
LEU  
TRP  
VAL  
SER  
CYS  
GLY  
THR  
ASN

• Molecule 50: PON4



MET  
SER  
VAL  
LYS  
LEU  
PRO  
HIS  
VAL  
SER  
VAL  
GLN  
TVR  
HIS  
ALA  
LEU  
SER  
GLN  
SER  
HIS  
GLN  
CYS  
ASP  
GLY  
THR  
PRO  
GLU  
CYS  
PHE  
VAL  
SER  
CYS  
ASN  
SER  
ARG  
GLY  
THR  
ASN  
LEU  
ASN  
GLN  
ALA  
PRO  
ILE  
LYS  
GLY  
SER  
ALA  
LEU  
MET  
LYS  
THR  
ASN

SER  
GLN  
ARG  
ASN  
LYS  
ASP  
ARG  
LYS  
PRO  
GLU  
GLN  
GLY  
VAL  
PRO  
SER  
PHE  
GLU  
LEU  
GLY  
ASP  
GLY  
THR  
GLN  
THR  
GLY  
LEU  
ASN  
ALA  
LEU  
MET  
LYS  
GLY  
ARG  
ASN  
GLY  
LEU  
GLN  
HIS  
GLY  
GLY  
SER  
GLY  
HIS  
LEU  
THR  
ARG  
GLY  
PRO  
GLN  
VAL  
VAL  
ARG  
ALA  
ALA  
GLN  
CYS  
GLN  
CYS  
LEU  
LEU  
ASN  
GLY  
SER

ASN  
GLY  
MET  
ALA  
LYS  
THR  
ARG  
GLY  
E129  
Q130  
E131  
K132  
D133  
A134  
M135  
D136  
D137  
L138  
R140  
L141  
E142  
R143  
L144  
V146  
L147  
E148  
H149  
S151  
R152  
A155  
A156  
A157  
D158  
M161  
F162  
E163  
T164  
L165  
K166  
R167  
T168  
GLY  
LYS  
GLY  
PRO  
ARG  
PRO  
ILE  
PHE  
ASP  
ALA  
PRO  
GLU

GLN  
VAL  
VAL  
VAL  
SER  
ALA  
THR  
PRO  
ALA  
PRO  
GLN  
GLY  
THR  
ILE  
VAL  
MET  
GLY  
PRO  
GLY  
THR  
VAL  
ARG  
GLY  
THR  
ASP  
ALA  
HIS  
ARG  
CYS  
SER  
THR  
GLY  
THR  
VAL  
SER  
GLY  
THR  
ASN

ARG  
ASP  
ASN  
ALA  
ALA  
LEU  
GLY  
ALA  
THR  
ALA  
VAL  
LEU  
HIS  
HIS  
GLN  
CYS  
GLY  
ALA  
THR  
PRO  
VAL  
SER  
ARG  
GLY  
GLY  
VAL  
ALA  
HIS  
THR  
PRO  
CYS  
GLY  
SER  
ILE  
GLY  
THR  
MET  
LYS  
THR  
ILE  
GLY  
THR  
LEU  
ASN  
THR  
TYR  
GLY  
PRO  
ARG  
GLY  
GLY  
ALA  
VAL  
VAL  
TRP  
CYS  
ARG  
GLY  
LEU  
ASN

ALA  
VAL  
VAL  
ASP  
ASP  
GLY  
ILE  
GLY  
THR  
THR  
SER  
ALA  
LEU  
LEU  
LEU  
GLY  
THR  
THR  
ASN

• Molecule 51: MC7



MET  
VAL  
ARG  
W4  
G5  
G6  
P7  
R8  
F9  
E10  
F11  
Y12  
F13  
T14  
R15  
D16  
F17  
L18  
Y22  
L23  
I24  
K25  
A32  
A33  
H36  
S37  
K38  
R39  
E40  
H41  
E42  
R43  
A44  
K45  
E46  
D47  
A48  
R49  
F50  
A51  
E52  
A53  
E54  
L60  
Q61  
E62  
E63  
A64  
Q65  
R66  
E71  
V72  
A76  
R77

R78  
A79  
A80  
A81  
E82  
A83  
A84  
A85  
Q86  
A89  
H90  
A91  
R92  
R93  
L94  
R95  
V104  
I105  
R106  
G107  
K125  
R135  
D170  
K171  
D174  
V175  
Q176  
K177  
Q178  
Y179  
Y180  
K183  
S184  
K185  
R186  
P187  
A188  
E189  
T190  
L191  
R192  
E193  
R194  
R195  
A196  
C197  
I198  
D199  
K200  
M201  
E202  
R203  
C204

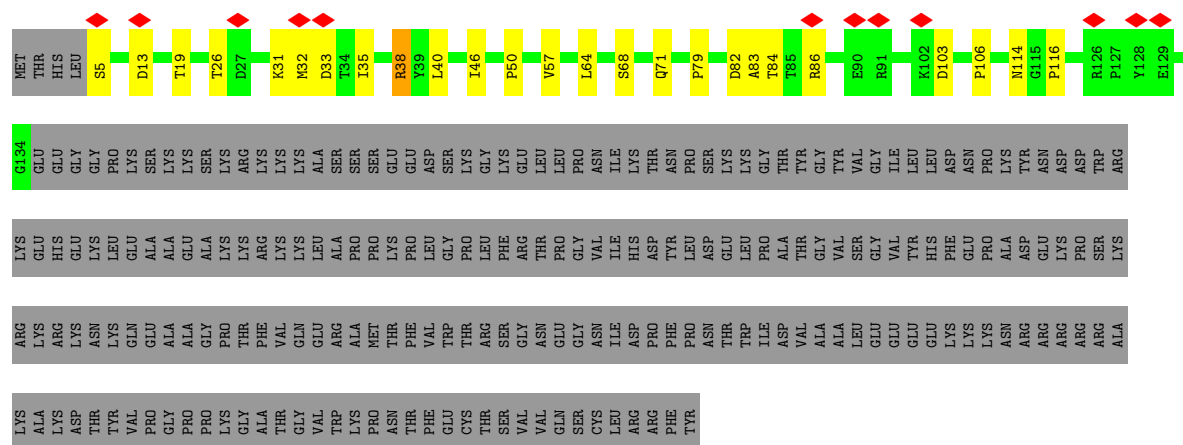
H205  
T206  
ASN  
GLY  
ALA  
ALA  
LYS  
PRO  
PRO  
VAL  
GLN  
ASN  
ASP  
GLY  
SER  
GLY  
PHE  
ALA  
ASN  
ASP  
GLN  
ARG  
GLY  
ILE  
PRO  
PHE  
GLY  
THR  
GLY  
ARG  
GLY  
ARG  
K38  
HIS  
ASP  
MET  
GLY  
SER  
SER  
ARG  
PRO  
LEU  
SER  
ILE  
PHE  
SER  
HIS  
GLY  
SER  
SER  
ASN  
ALA  
PRO  
ILE  
ARG

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

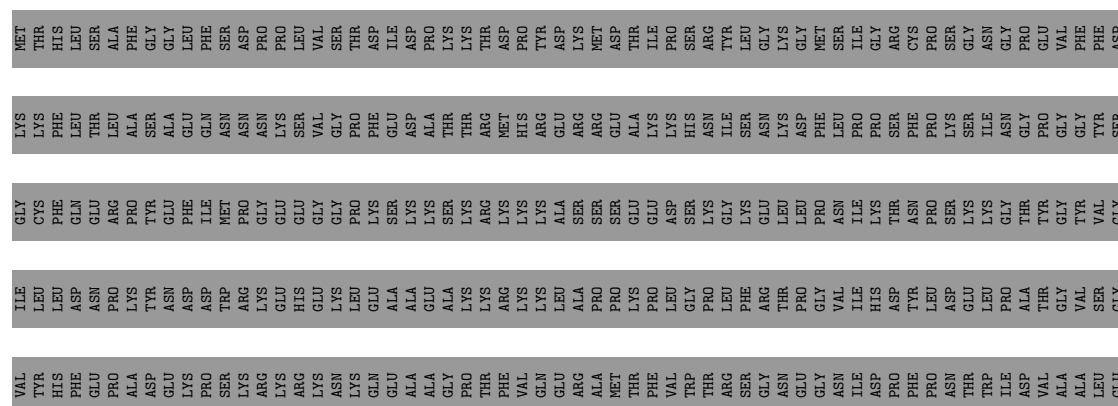
CYS  
GLY  
GLY  
HIS  
PRO

• Molecule 52: FAP96C/MC15

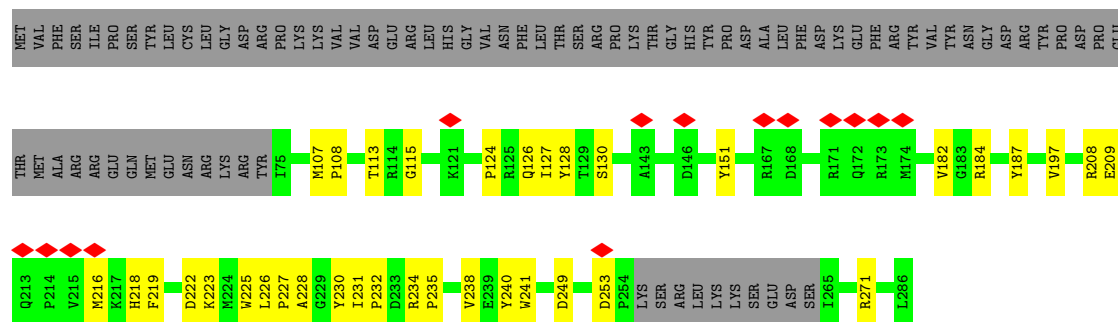




• Molecule 52: FAP96C/MC15



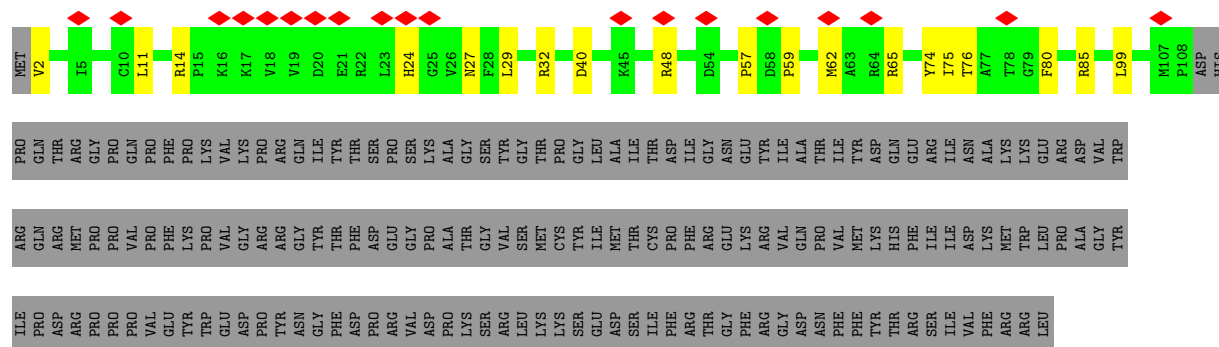
• Molecule 53: FAP96B



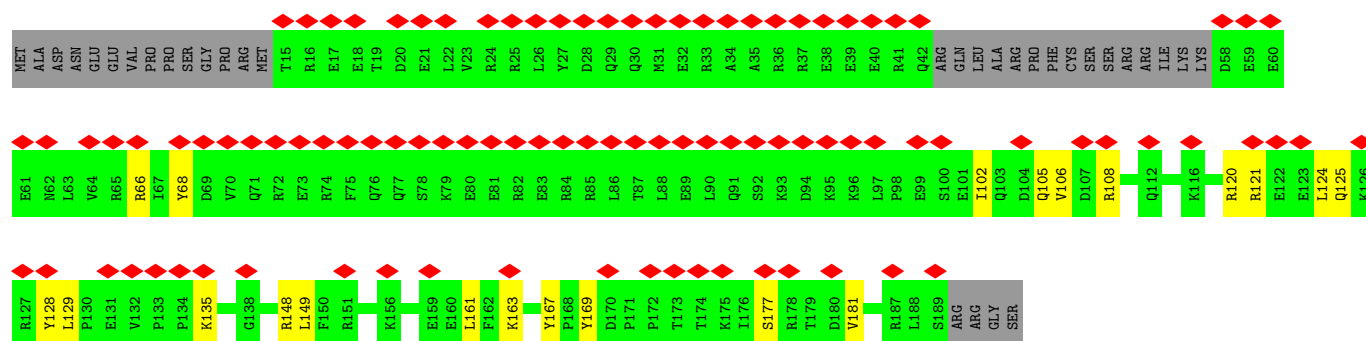
• Molecule 53: FAP96B



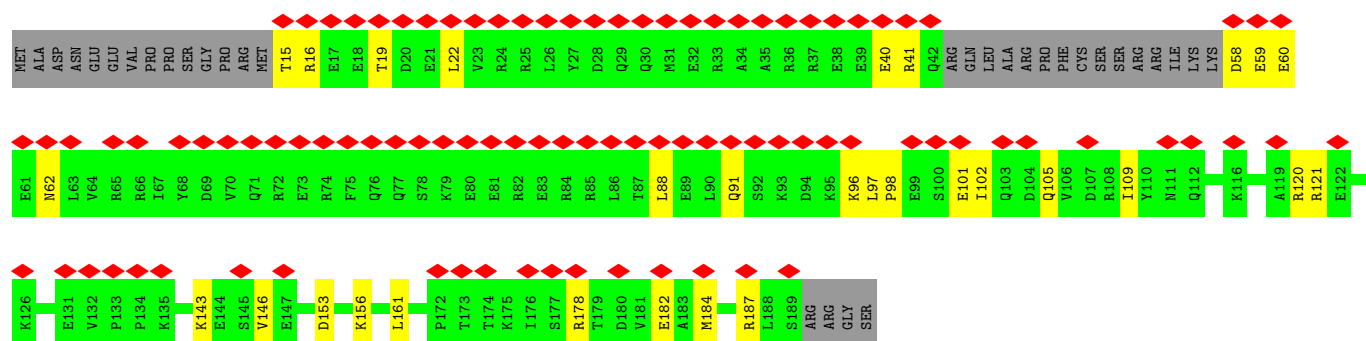




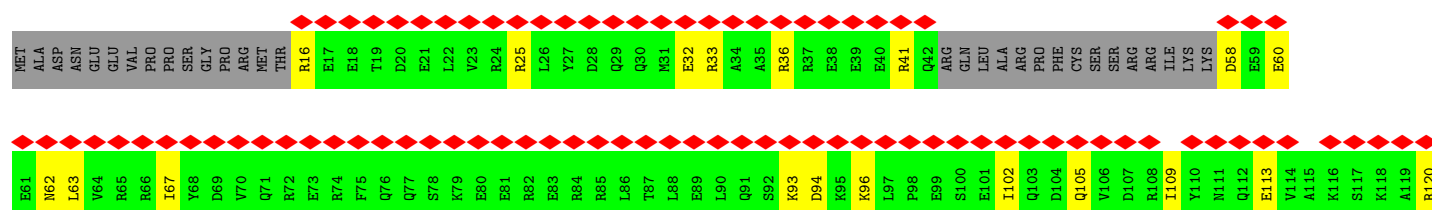
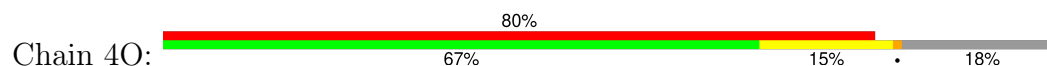
• Molecule 54: MOP23A

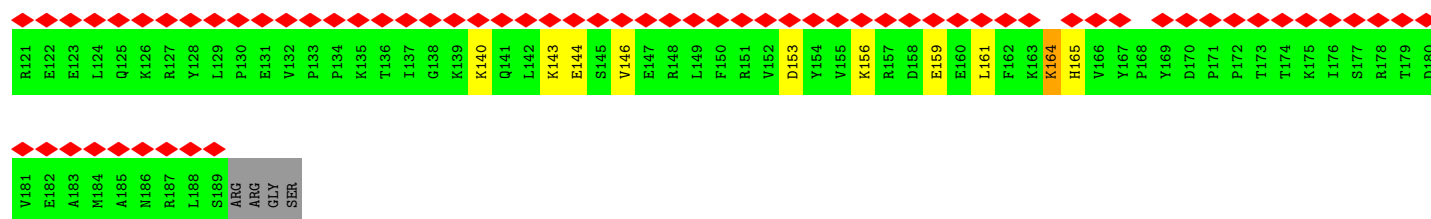


• Molecule 54: MOP23A

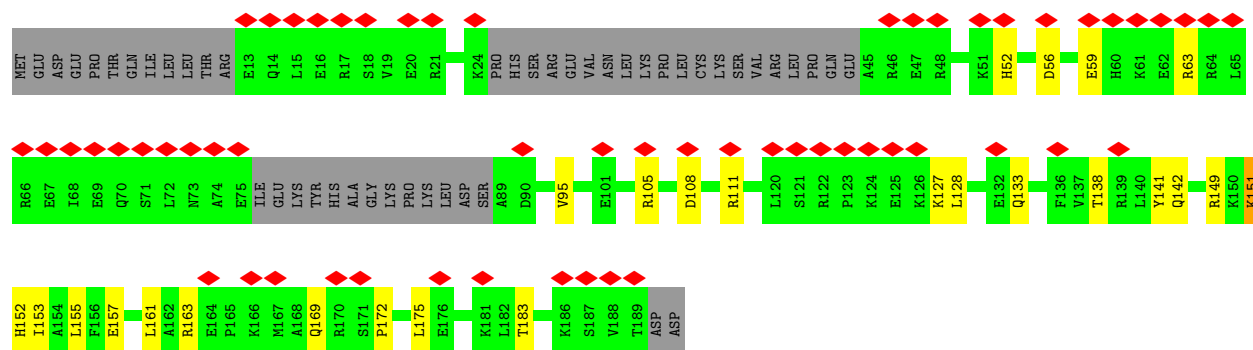


• Molecule 54: MOP23A

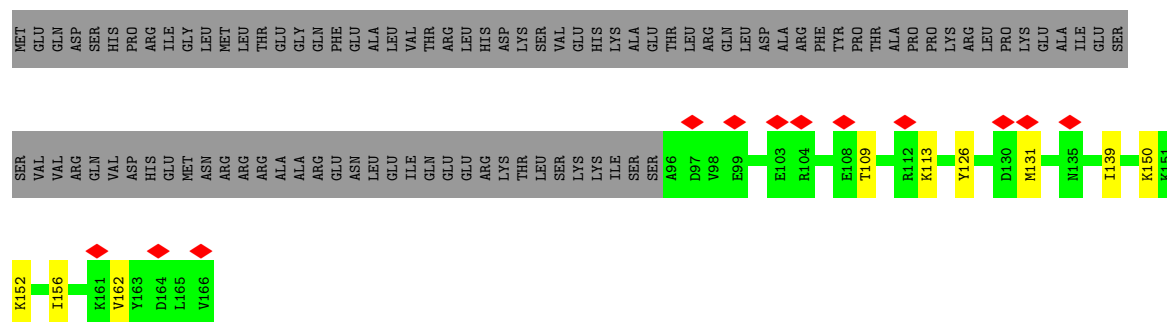
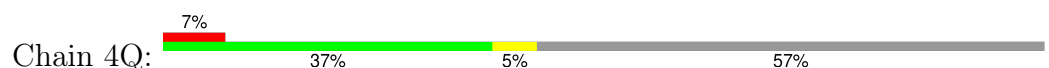




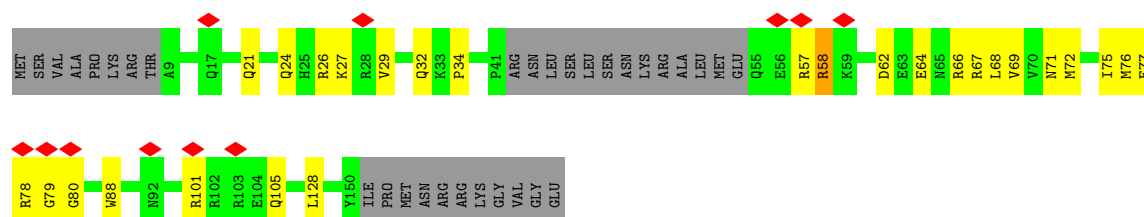
• Molecule 55: MOP23B



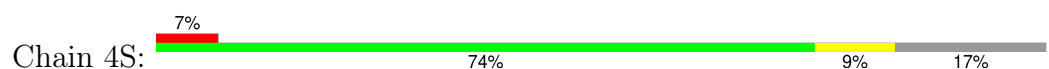
• Molecule 56: MOP23C

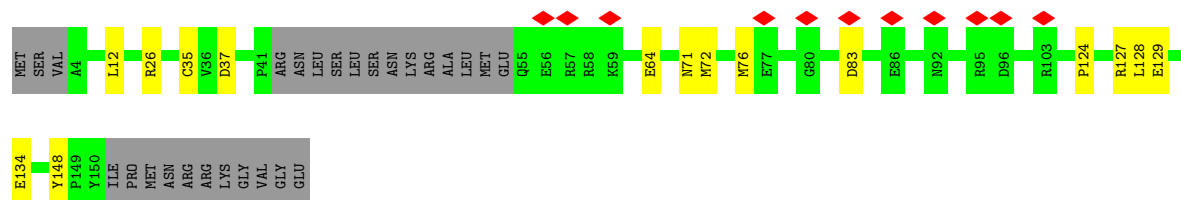


• Molecule 57: KIAA1430 homologue

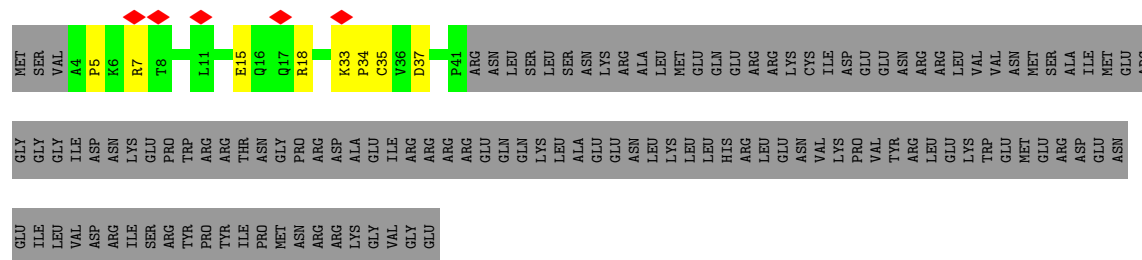


• Molecule 57: KIAA1430 homologue

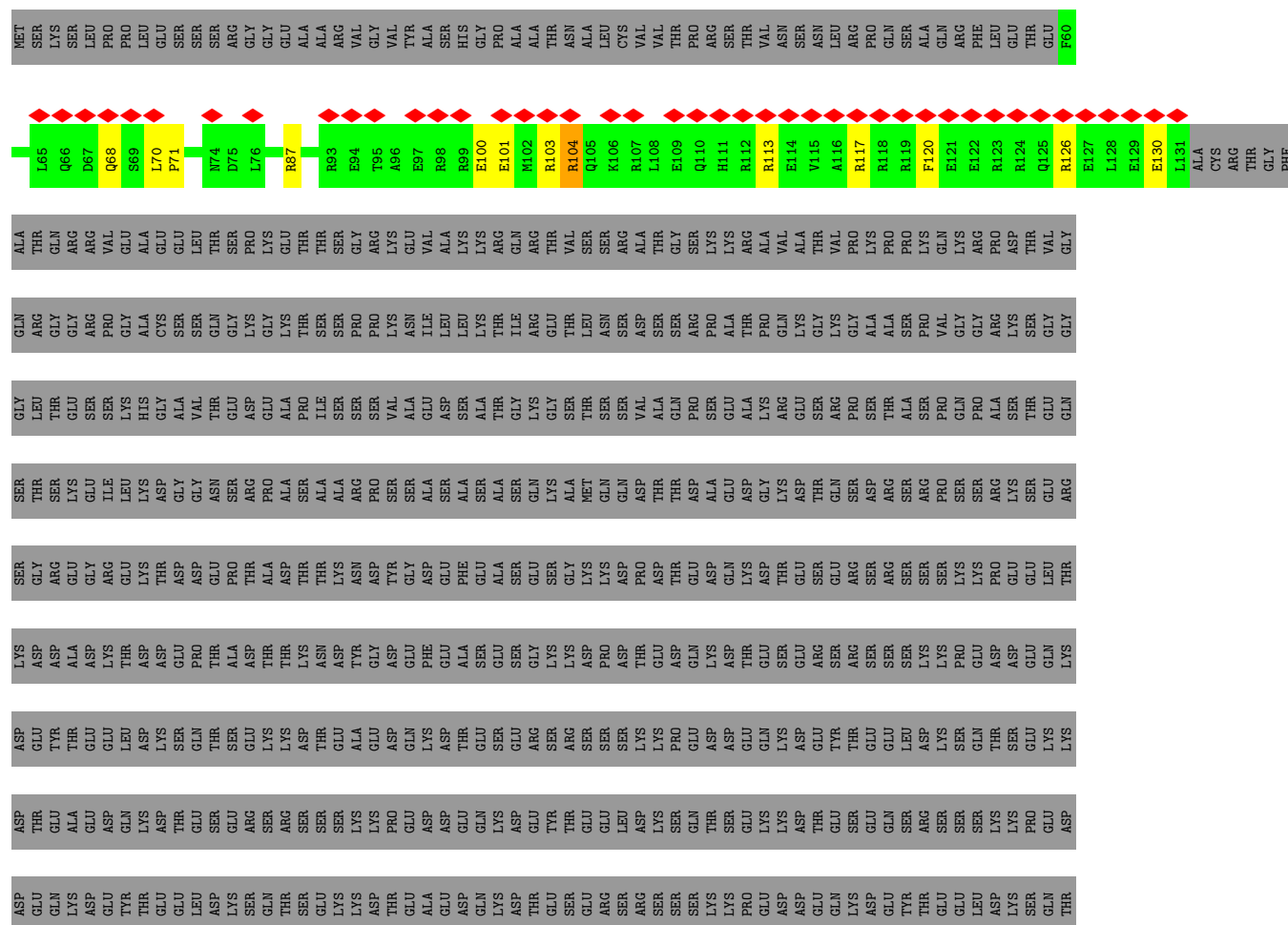




• Molecule 57: KIAA1430 homologue



• Molecule 58: Starmaker

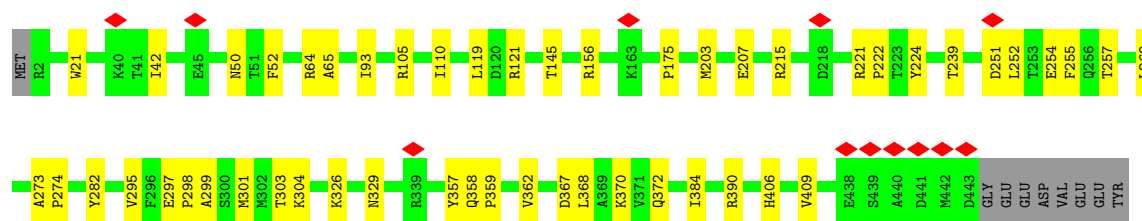


- Molecule 58: Starmaker

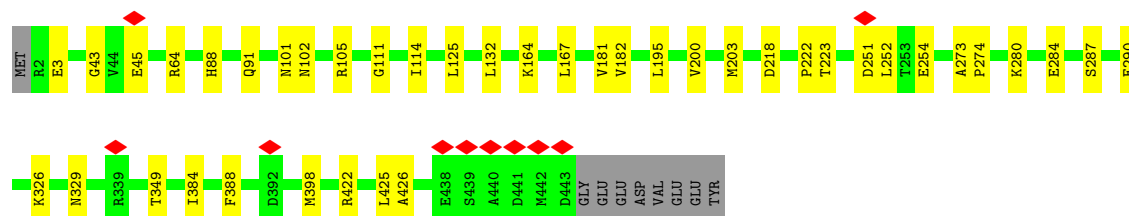
[illegible]



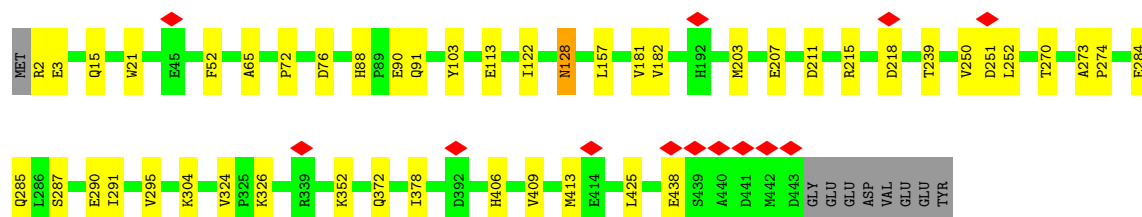




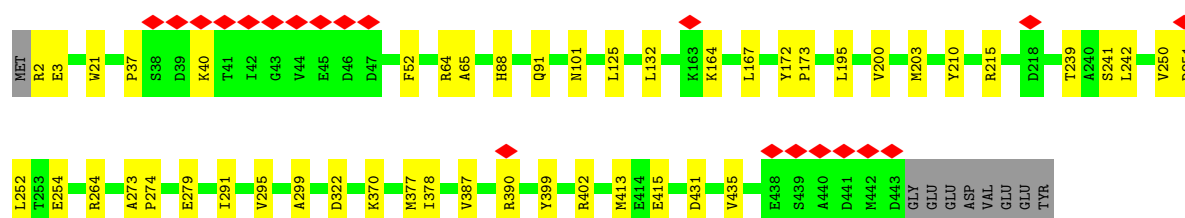
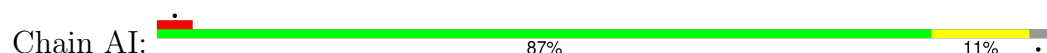
- Molecule 59: Tubulin alpha chain



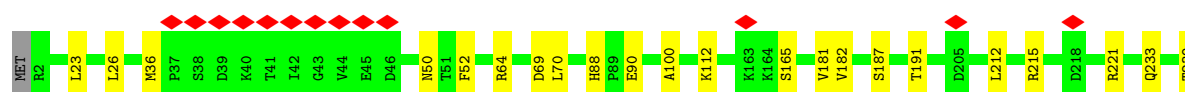
- Molecule 59: Tubulin alpha chain

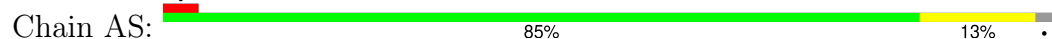
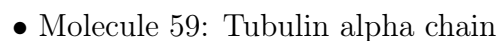
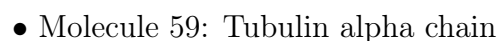


- Molecule 59: Tubulin alpha chain

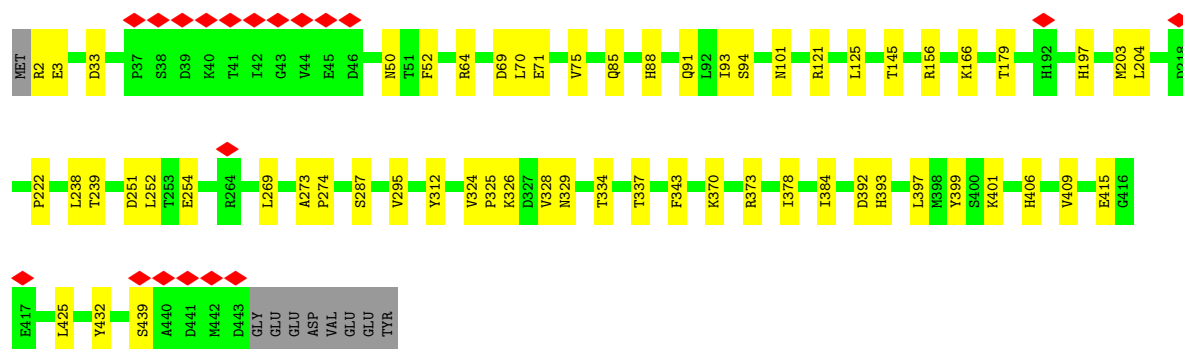


- Molecule 59: Tubulin alpha chain

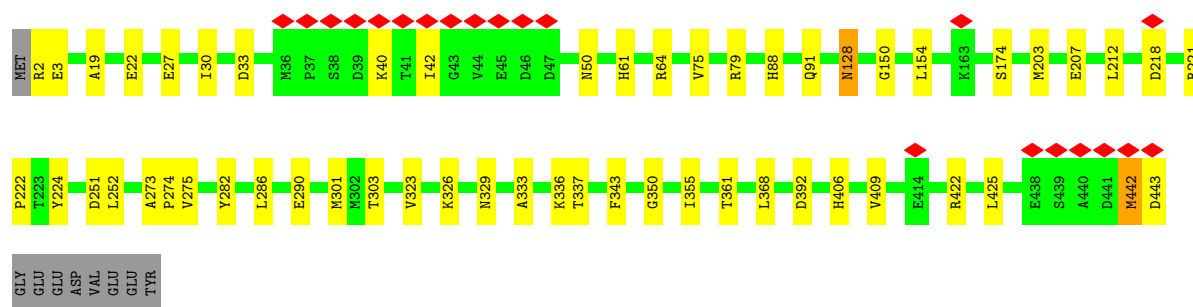
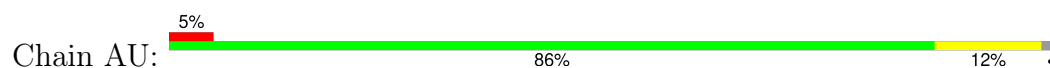




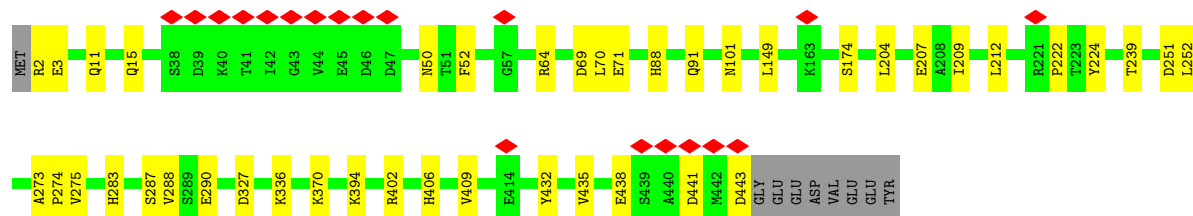




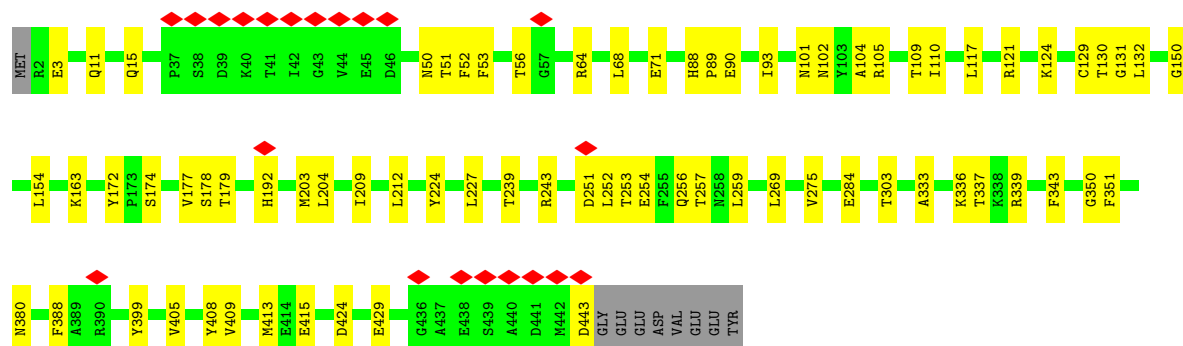
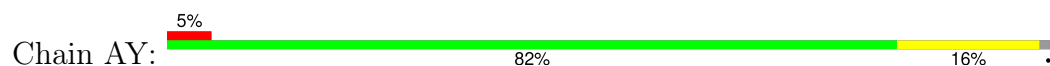
• Molecule 59: Tubulin alpha chain



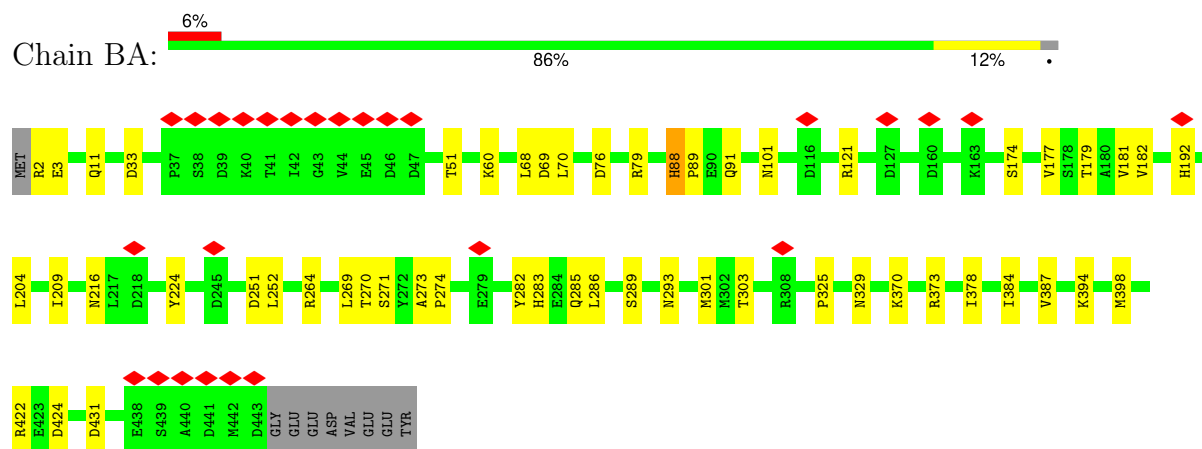
• Molecule 59: Tubulin alpha chain



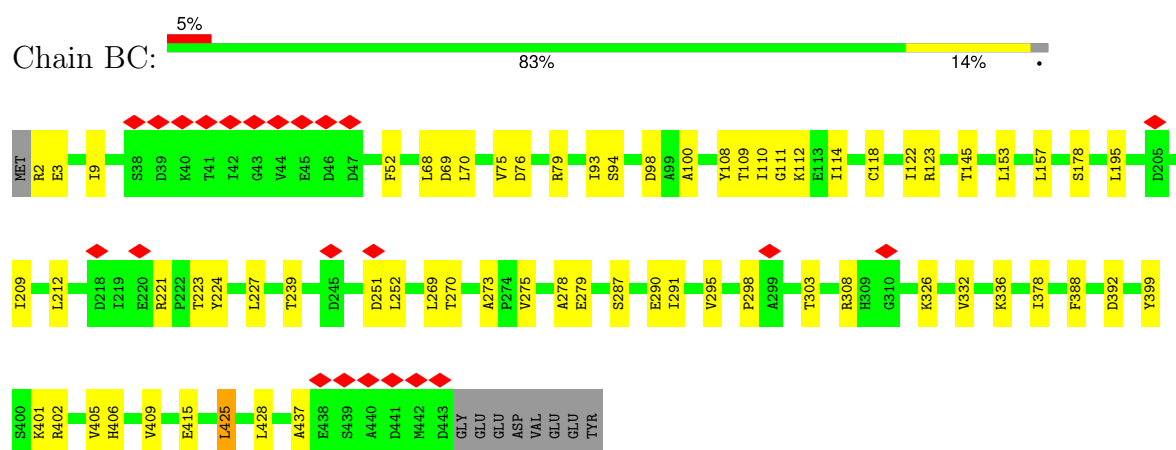
• Molecule 59: Tubulin alpha chain



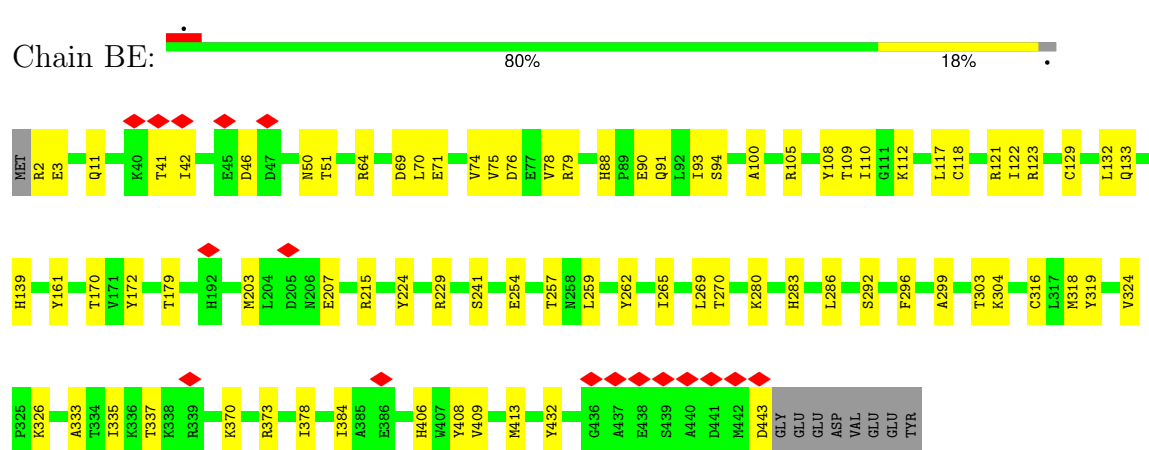
- Molecule 59: Tubulin alpha chain



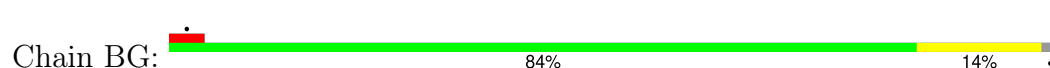
- Molecule 59: Tubulin alpha chain

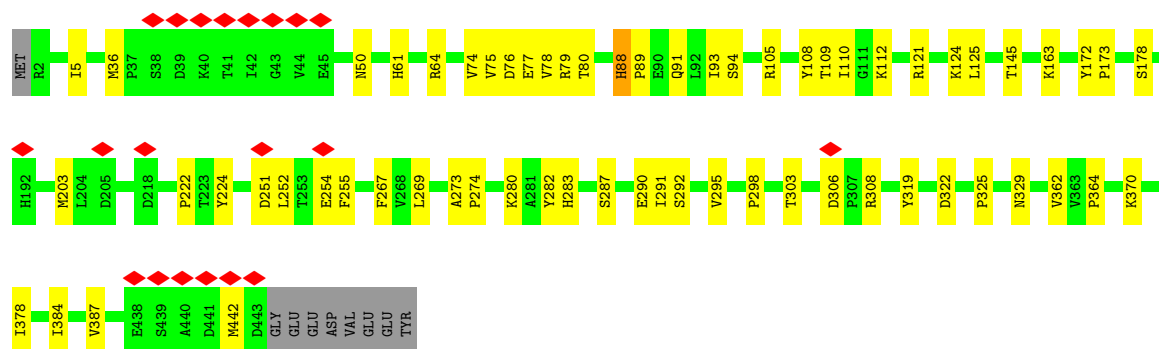


- Molecule 59: Tubulin alpha chain

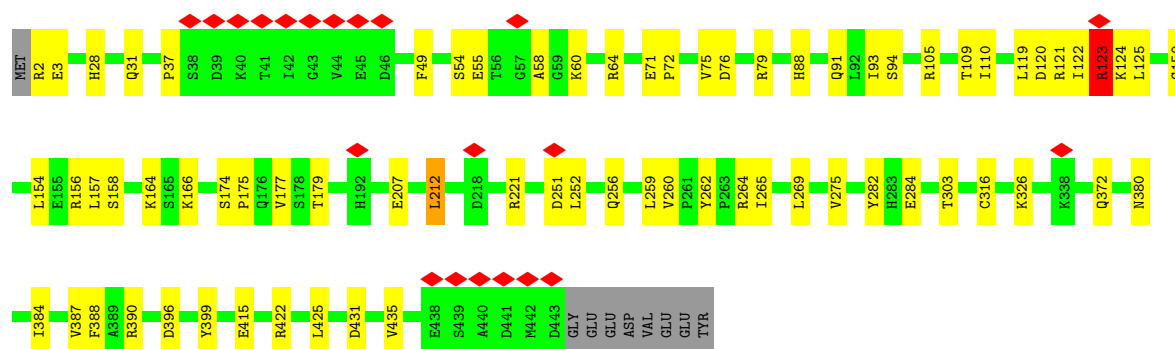
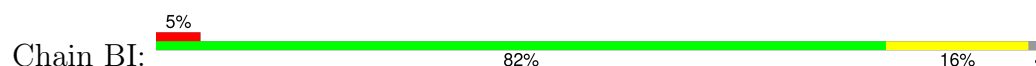


- Molecule 59: Tubulin alpha chain

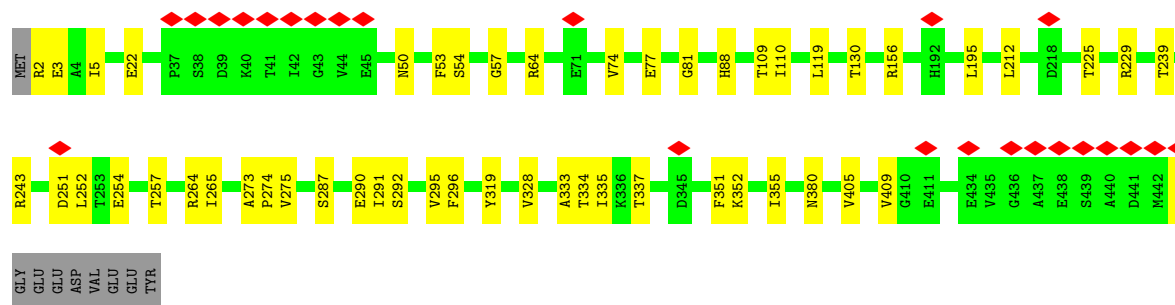




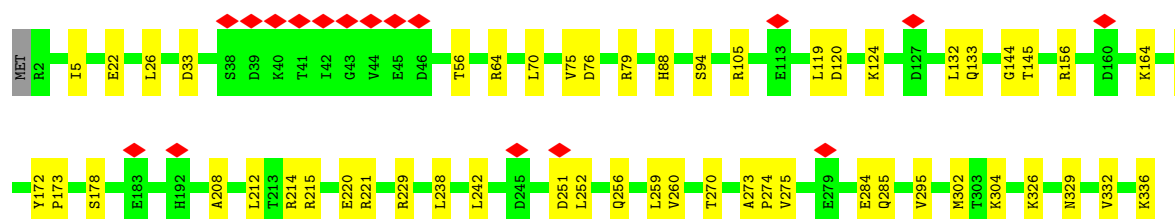
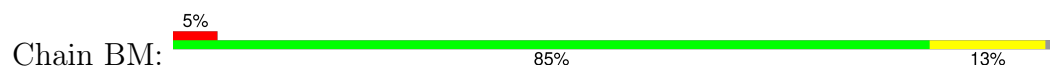
• Molecule 59: Tubulin alpha chain

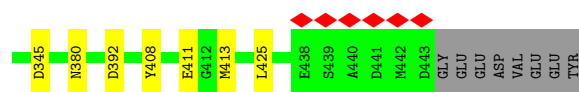


• Molecule 59: Tubulin alpha chain

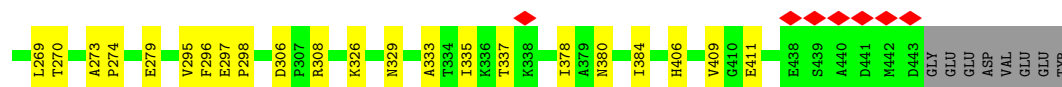
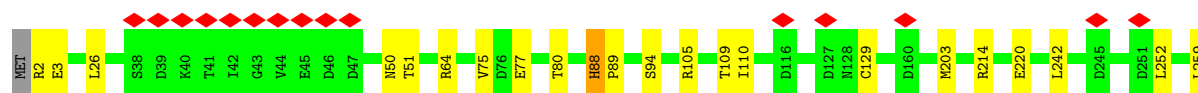
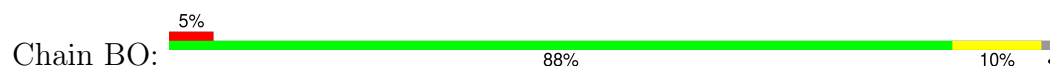


• Molecule 59: Tubulin alpha chain

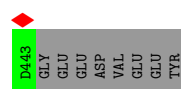
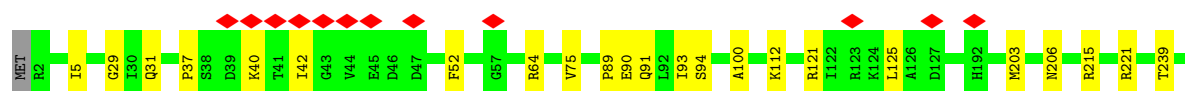
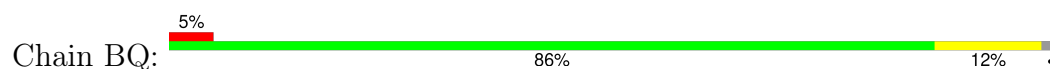




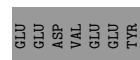
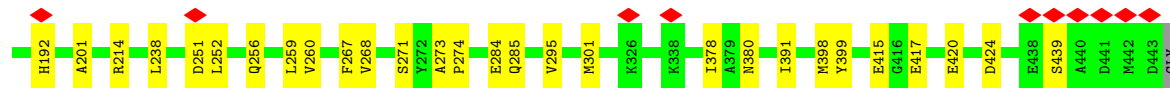
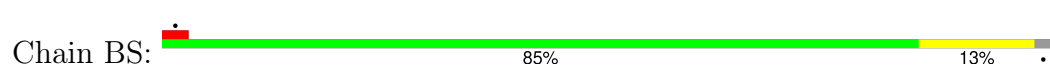
- Molecule 59: Tubulin alpha chain



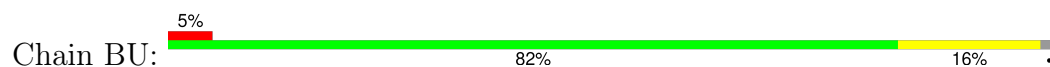
- Molecule 59: Tubulin alpha chain

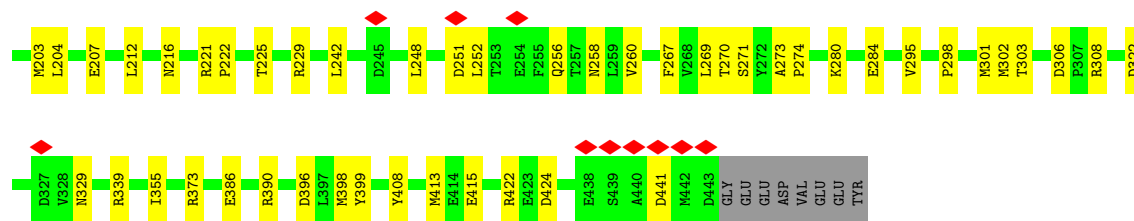


- Molecule 59: Tubulin alpha chain

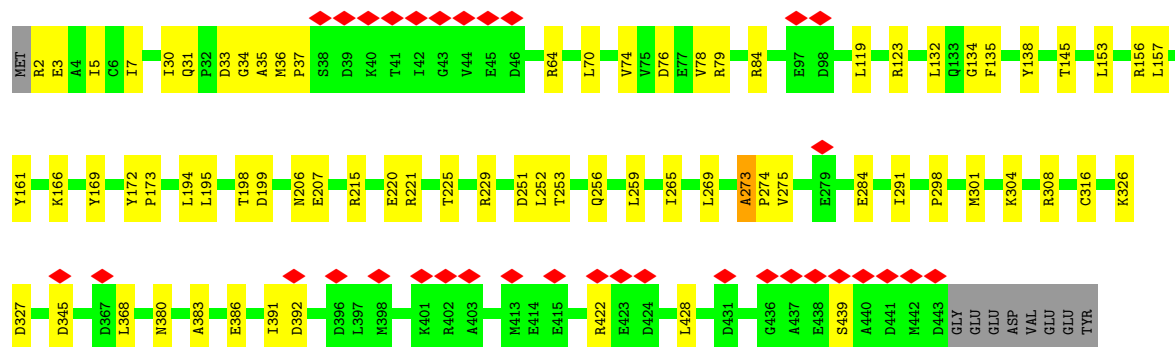
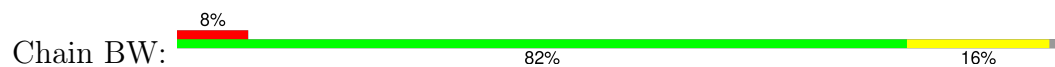


- Molecule 59: Tubulin alpha chain

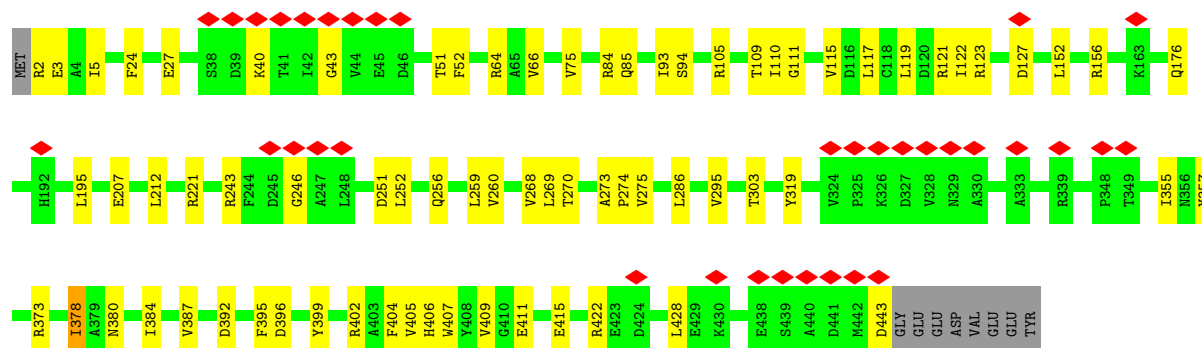
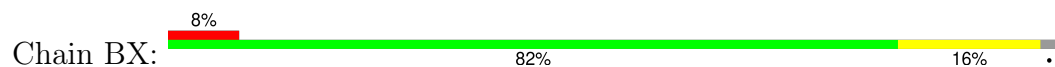




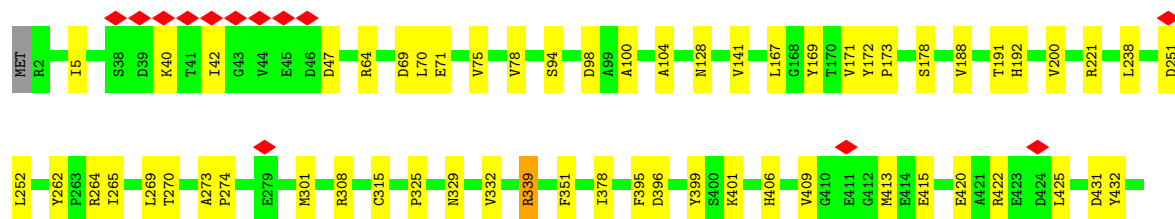
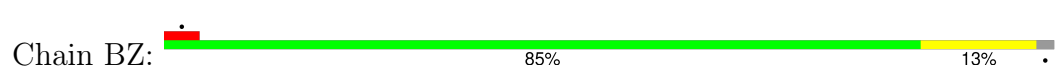
• Molecule 59: Tubulin alpha chain

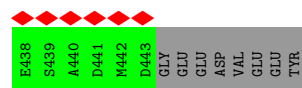


• Molecule 59: Tubulin alpha chain

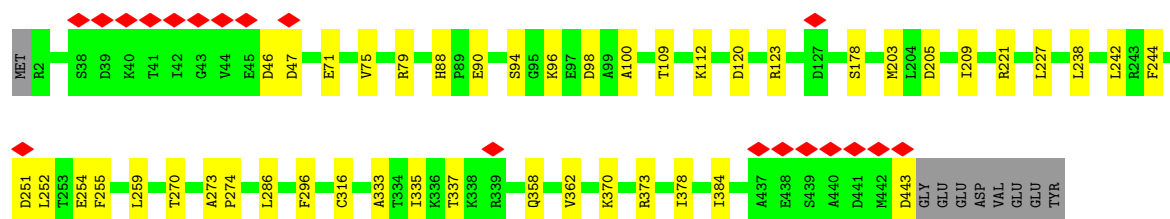
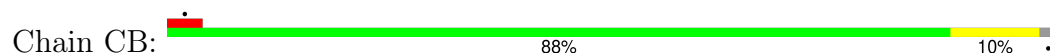


• Molecule 59: Tubulin alpha chain

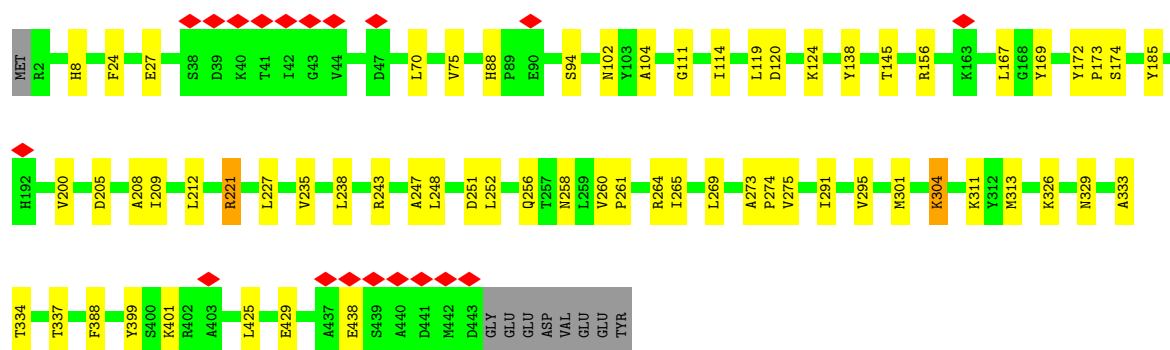
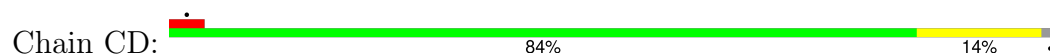




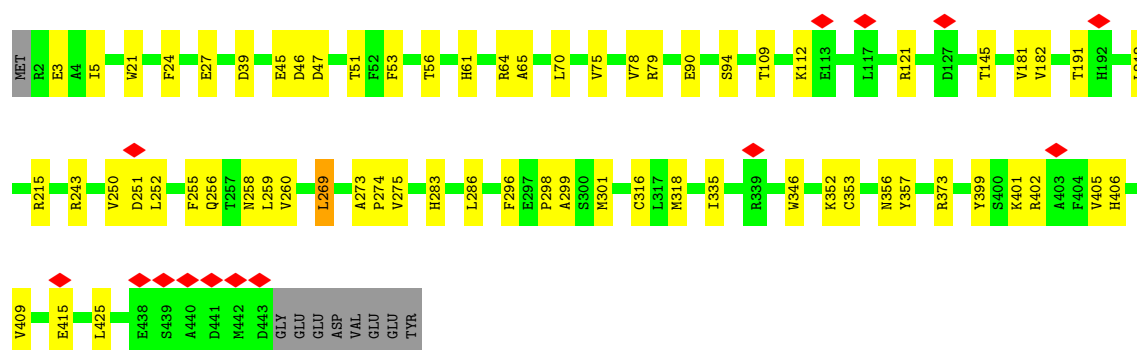
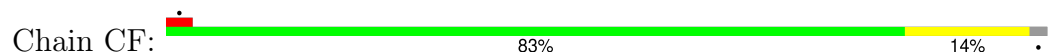
- Molecule 59: Tubulin alpha chain



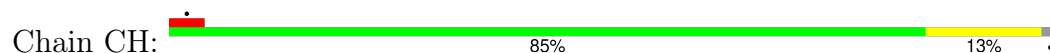
- Molecule 59: Tubulin alpha chain

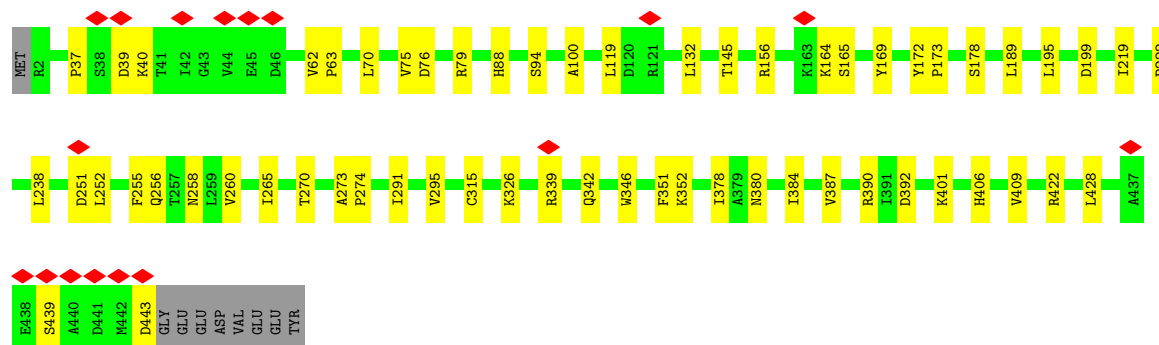


- Molecule 59: Tubulin alpha chain



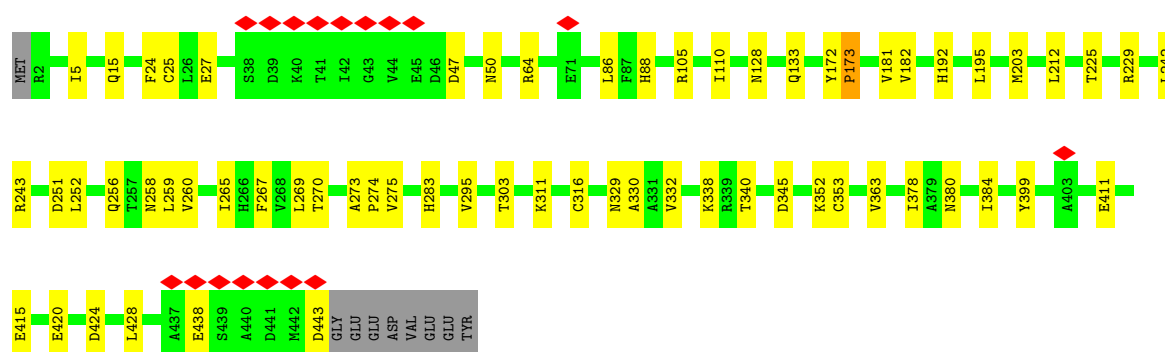
- Molecule 59: Tubulin alpha chain





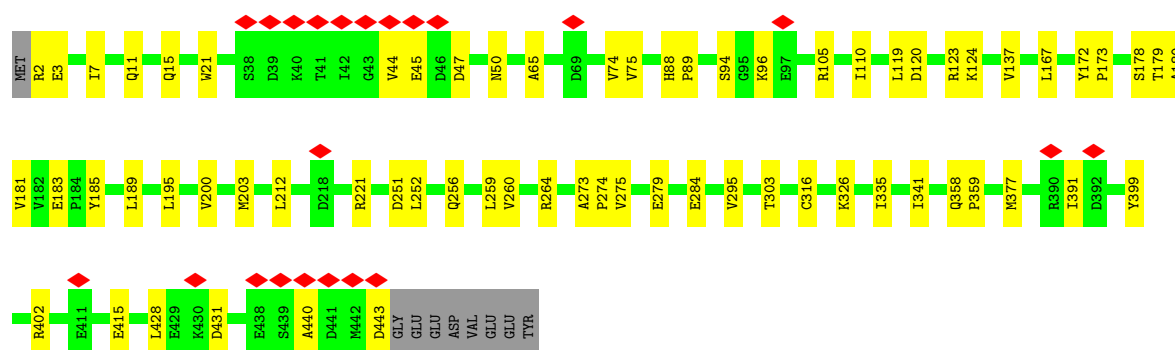
- Molecule 59: Tubulin alpha chain

Chain CJ: 84% 14%



- Molecule 59: Tubulin alpha chain

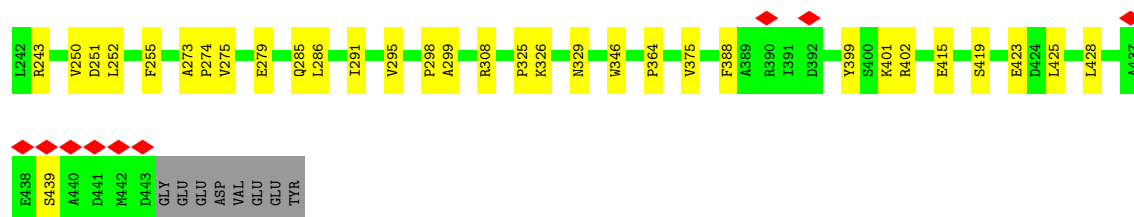
Chain CM: 5% 83% 15%



- Molecule 59: Tubulin alpha chain

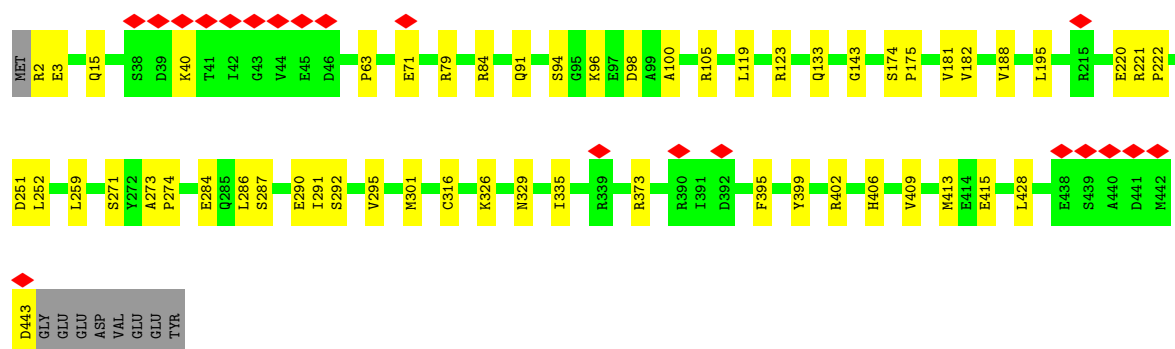
Chain CO: 5% 85% 13%





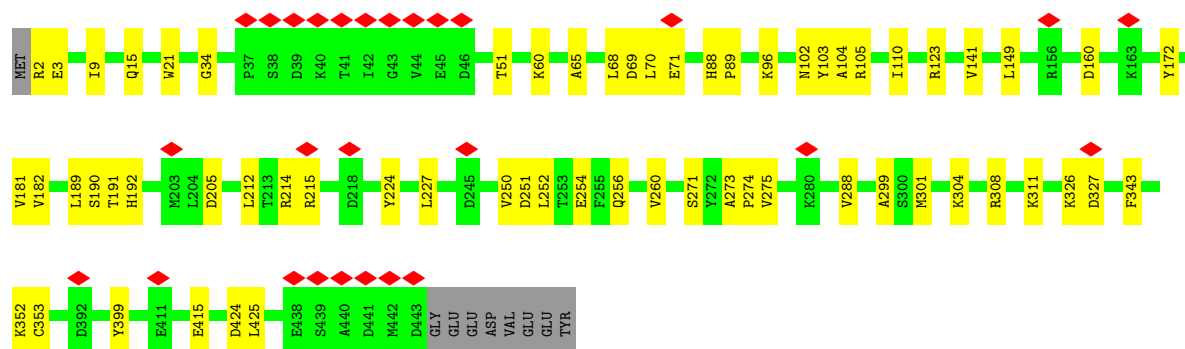
• Molecule 59: Tubulin alpha chain

Chain CQ: 86% 12%



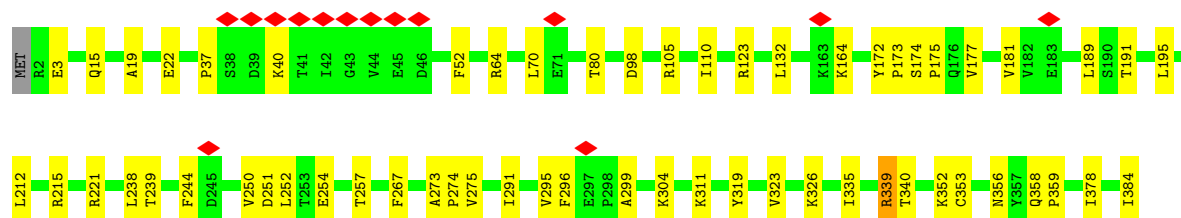
• Molecule 59: Tubulin alpha chain

Chain CS: 6% 84% 14%

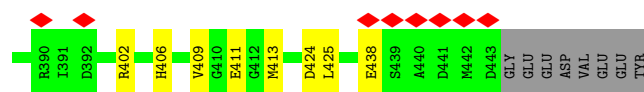


• Molecule 59: Tubulin alpha chain

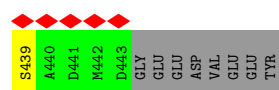
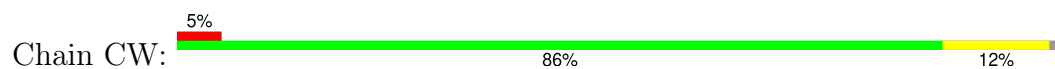
Chain CU: 5% 83% 15%



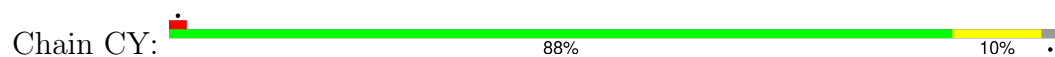




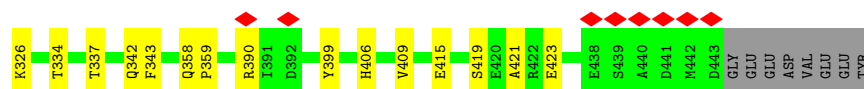
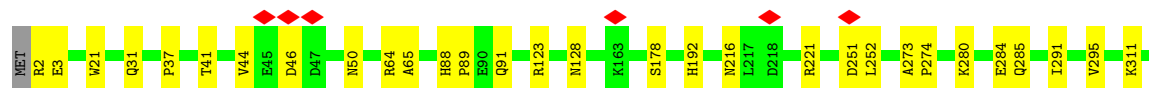
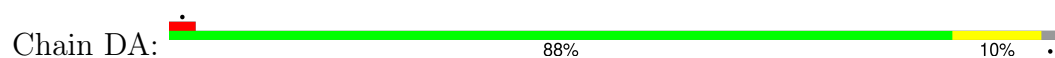
• Molecule 59: Tubulin alpha chain



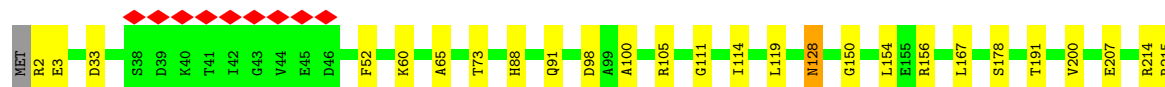
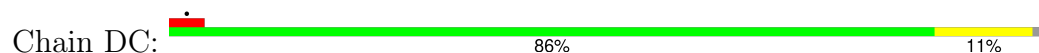
• Molecule 59: Tubulin alpha chain



• Molecule 59: Tubulin alpha chain

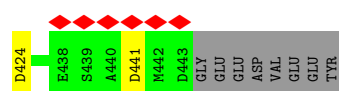
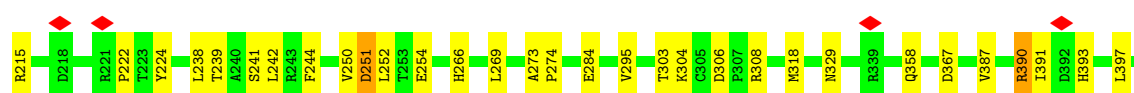


• Molecule 59: Tubulin alpha chain

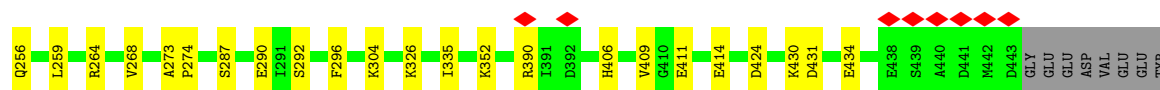




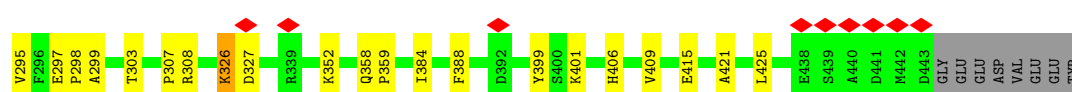
• Molecule 59: Tubulin alpha chain



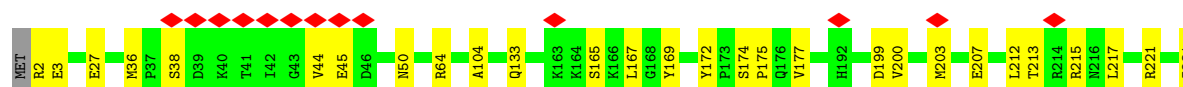
• Molecule 59: Tubulin alpha chain



• Molecule 59: Tubulin alpha chain

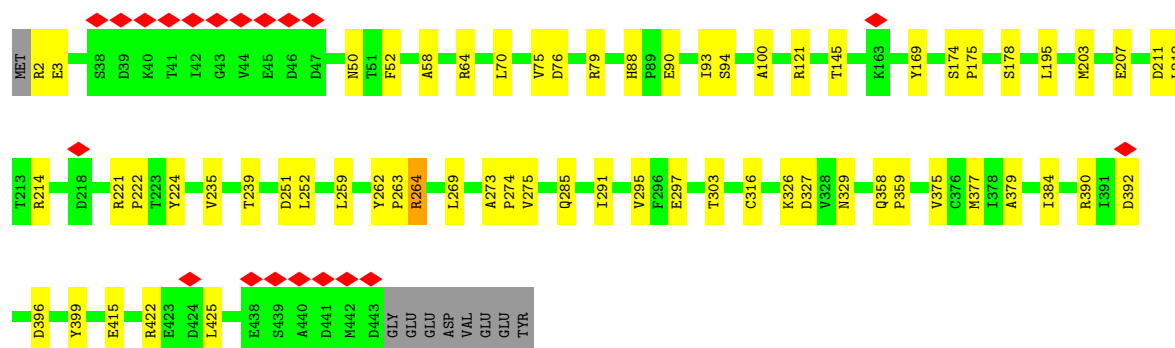
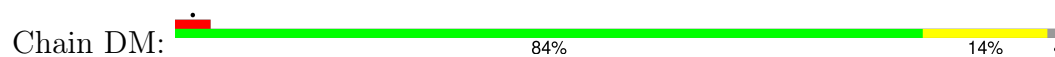


• Molecule 59: Tubulin alpha chain

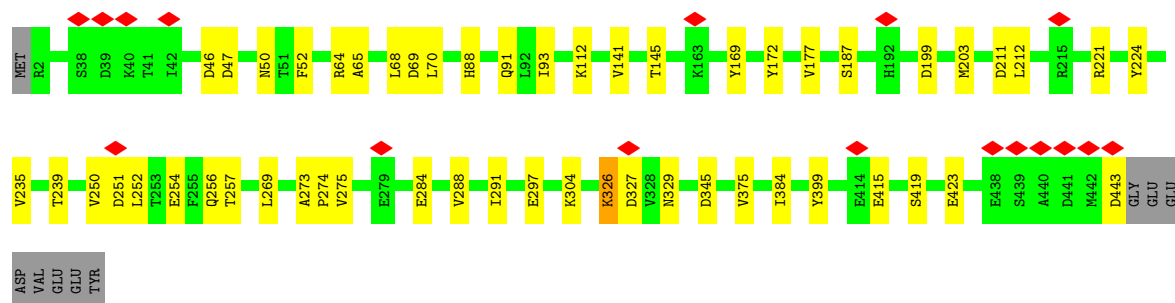




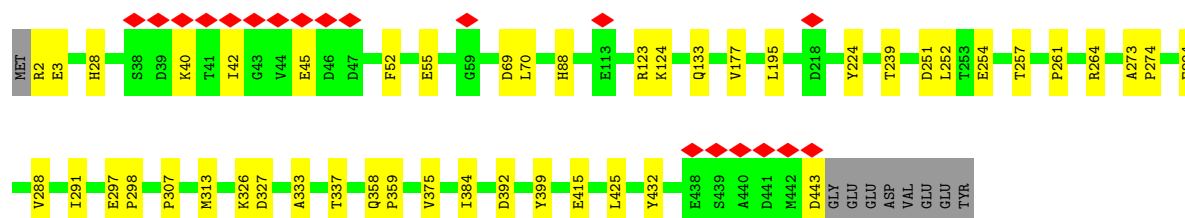
• Molecule 59: Tubulin alpha chain



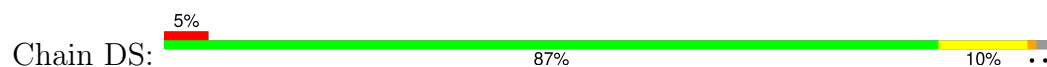
• Molecule 59: Tubulin alpha chain

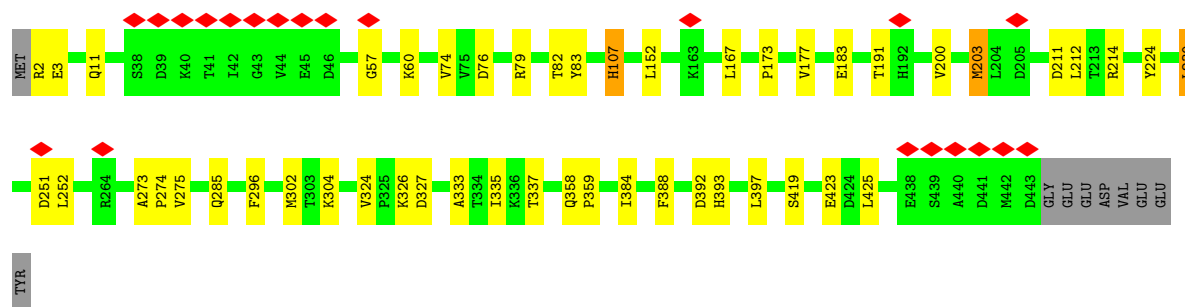


• Molecule 59: Tubulin alpha chain

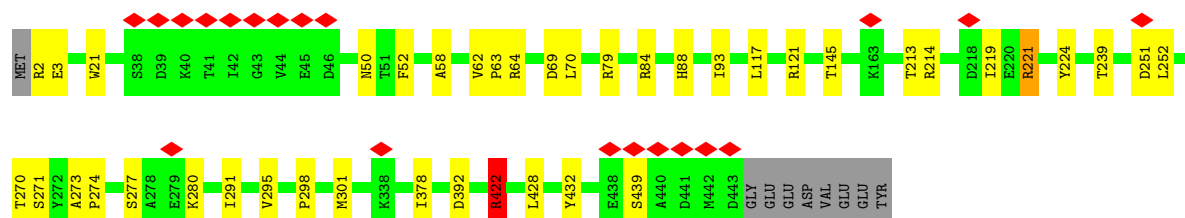


• Molecule 59: Tubulin alpha chain

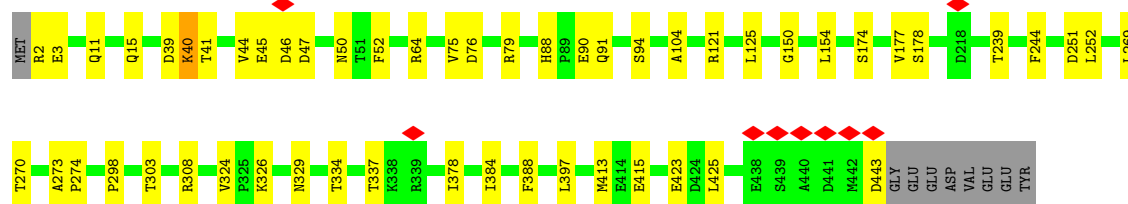
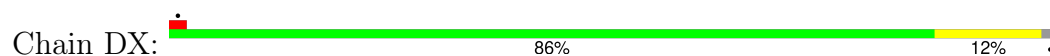




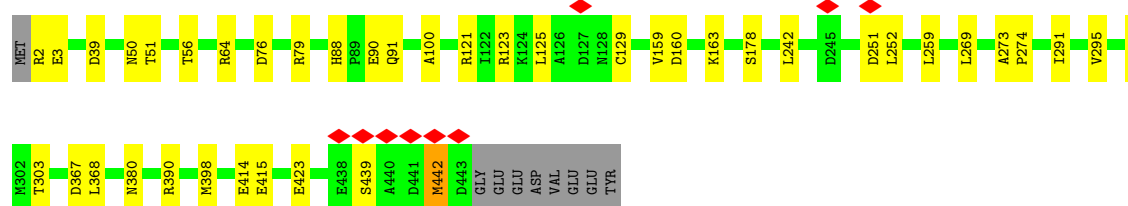
- Molecule 59: Tubulin alpha chain



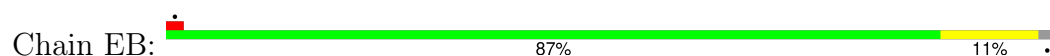
- Molecule 59: Tubulin alpha chain



- Molecule 59: Tubulin alpha chain

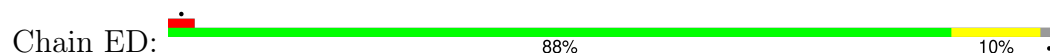


- Molecule 59: Tubulin alpha chain

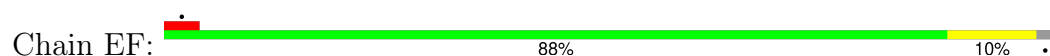




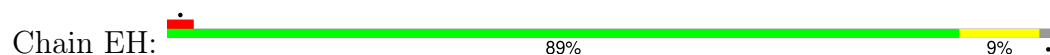
- Molecule 59: Tubulin alpha chain



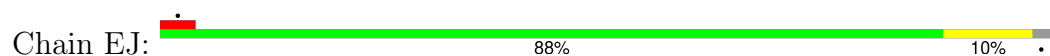
- Molecule 59: Tubulin alpha chain




- Molecule 59: Tubulin alpha chain

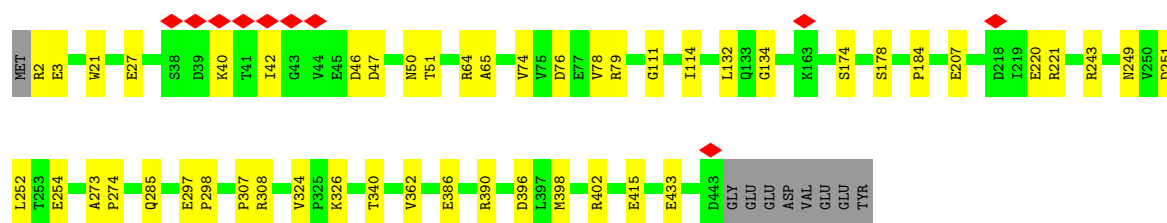


- Molecule 59: Tubulin alpha chain




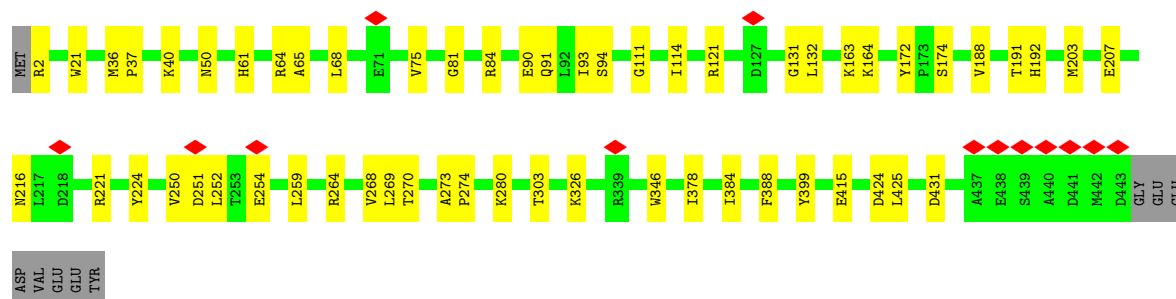
- Molecule 59: Tubulin alpha chain

Chain EL:  87% 11%




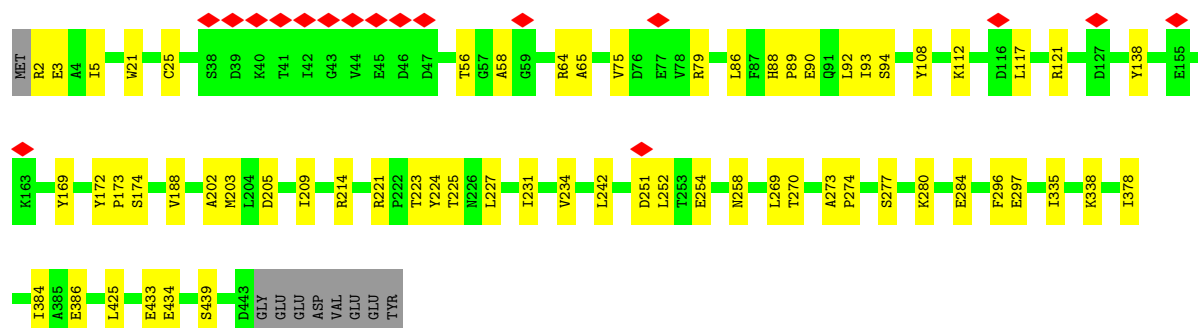
• Molecule 59: Tubulin alpha chain

Chain EN:  85% 13%




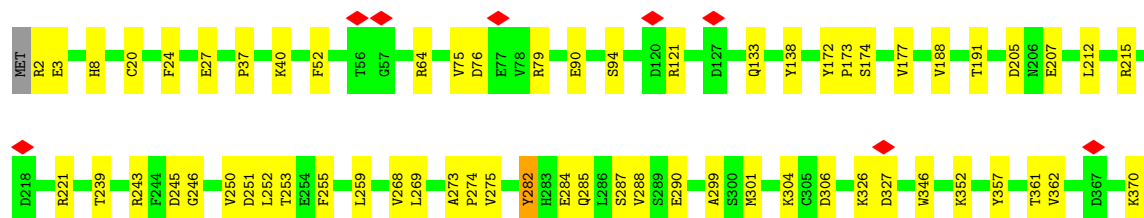
• Molecule 59: Tubulin alpha chain

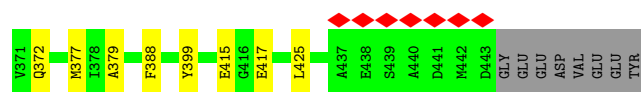
Chain EP:  84% 14%



• Molecule 59: Tubulin alpha chain

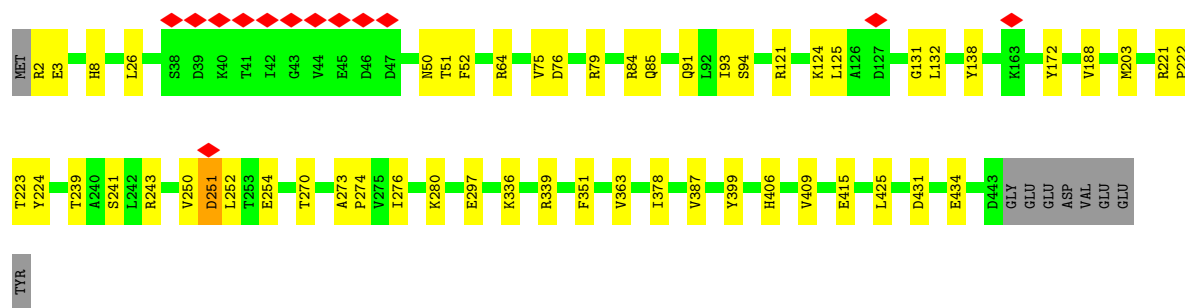
Chain ER:  82% 15%





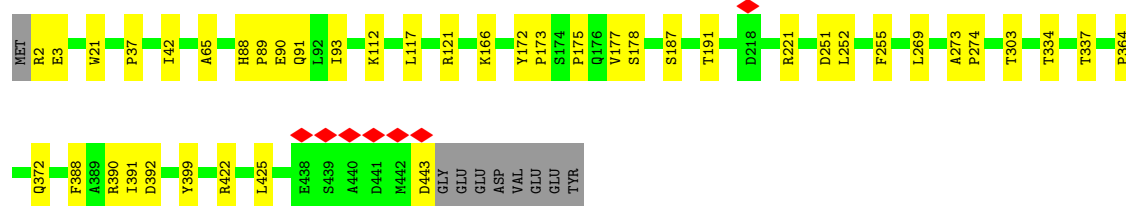
- Molecule 59: Tubulin alpha chain

Chain ET: 86% 12%



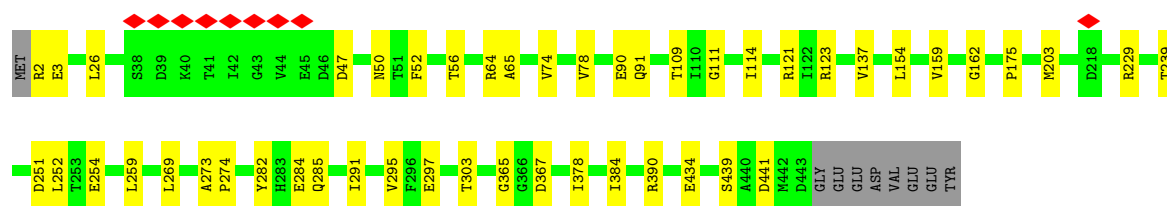
- Molecule 59: Tubulin alpha chain

Chain EV: 89% 9%



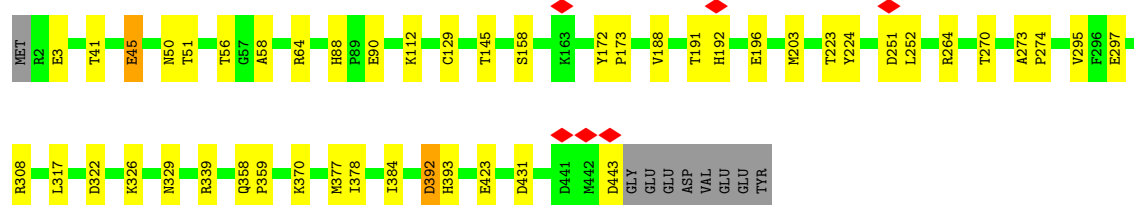
- Molecule 59: Tubulin alpha chain

Chain EX: 87% 11%




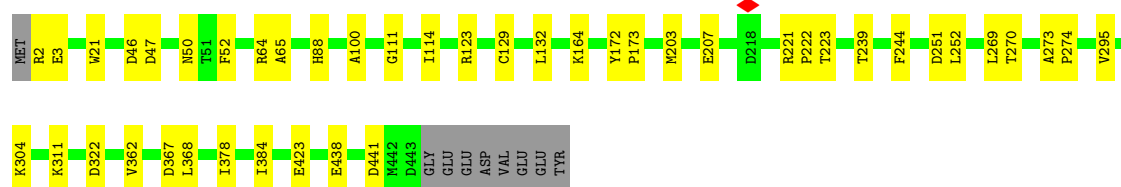
- Molecule 59: Tubulin alpha chain

Chain EZ: 87% 10%



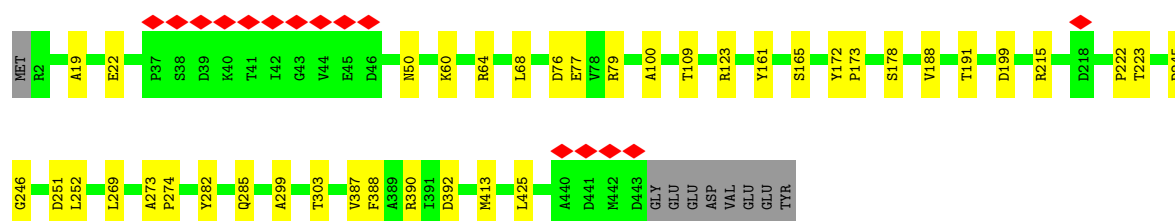
- Molecule 59: Tubulin alpha chain

Chain FB:  88% 10%



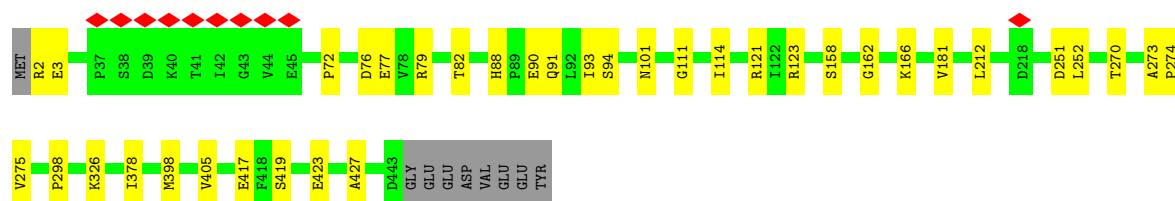
- Molecule 59: Tubulin alpha chain

Chain FD:  89% 9%




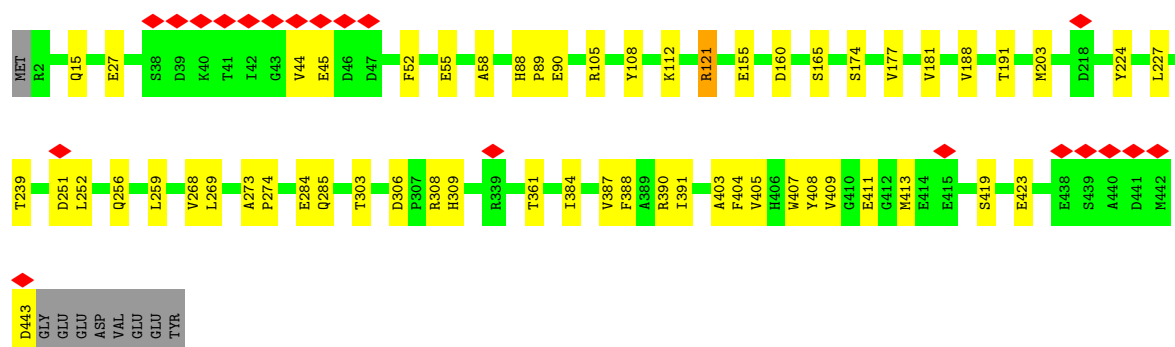
- Molecule 59: Tubulin alpha chain

Chain FF:  90% 8%




- Molecule 59: Tubulin alpha chain

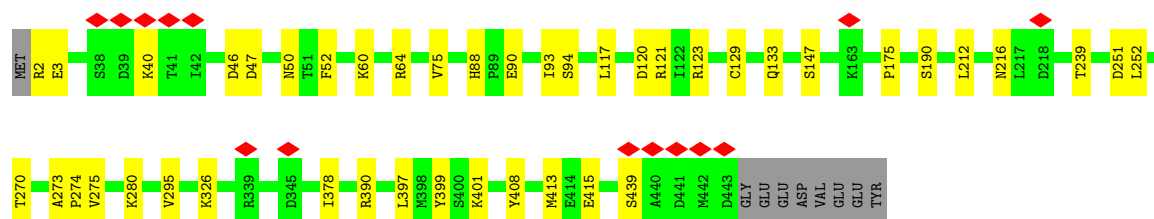
Chain FH:  85% 12%



- Molecule 59: Tubulin alpha chain

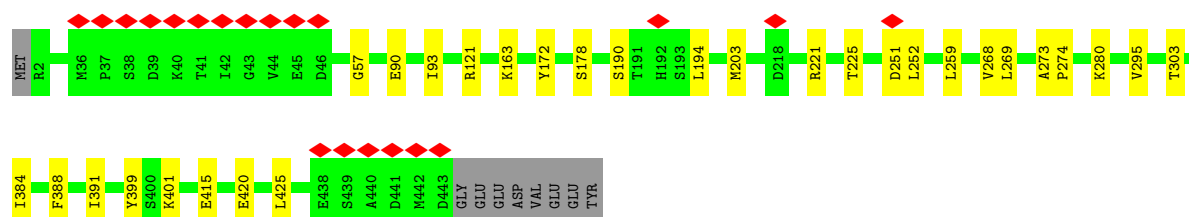
Chain FJ:  88% 10%





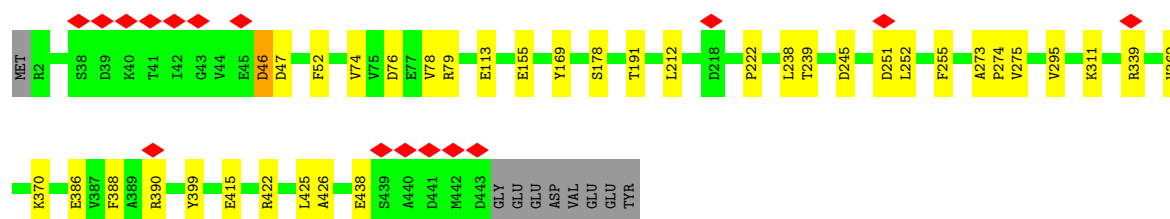
- Molecule 59: Tubulin alpha chain

Chain FL: 91% 7% •



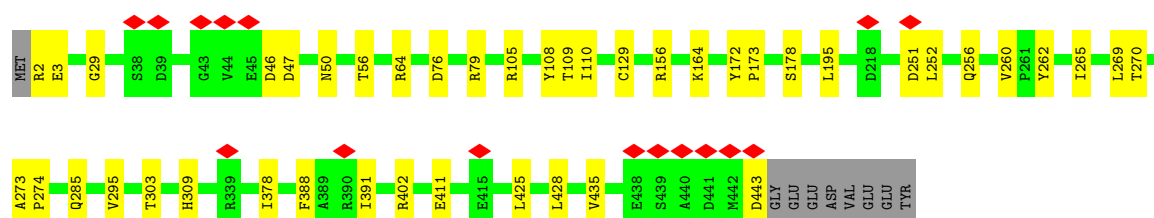
- Molecule 59: Tubulin alpha chain

Chain FN: 90% 8% •



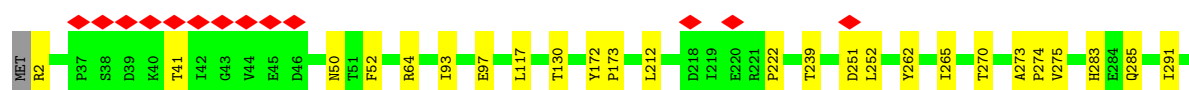
- Molecule 59: Tubulin alpha chain

Chain FP: 88% 10% •



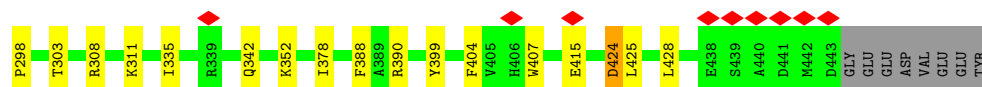
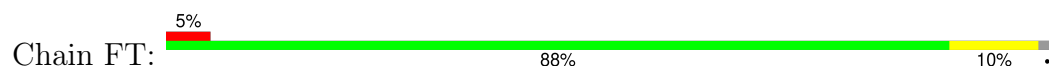
- Molecule 59: Tubulin alpha chain

Chain FR: 89% 9% •

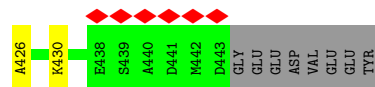
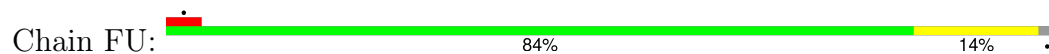




- Molecule 59: Tubulin alpha chain



- Molecule 59: Tubulin alpha chain



- Molecule 59: Tubulin alpha chain

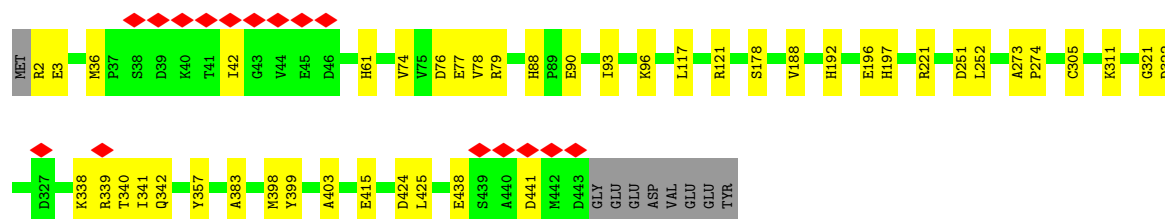


- Molecule 59: Tubulin alpha chain

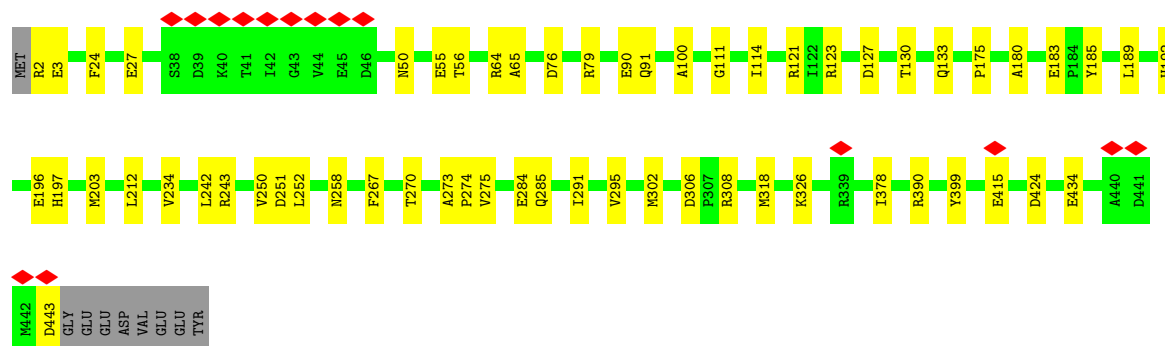
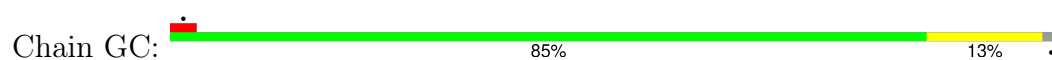




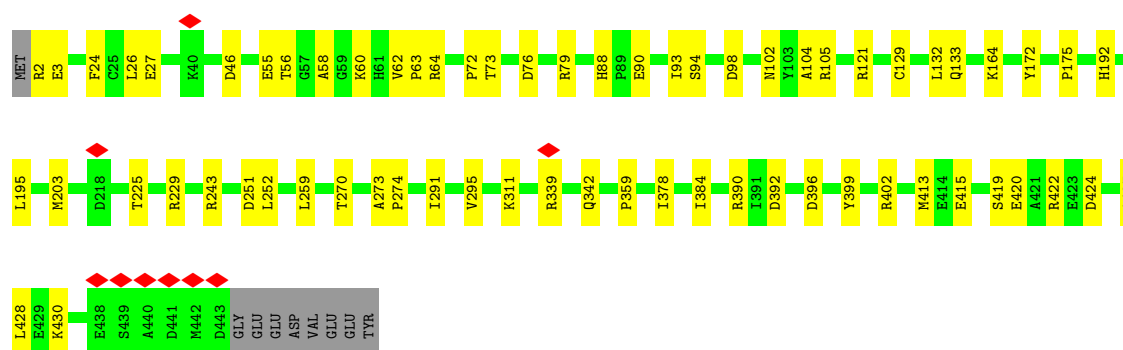
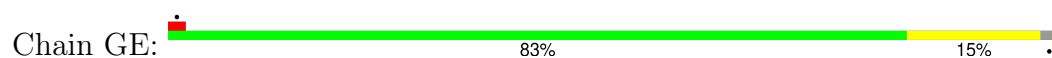
- Molecule 59: Tubulin alpha chain



- Molecule 59: Tubulin alpha chain

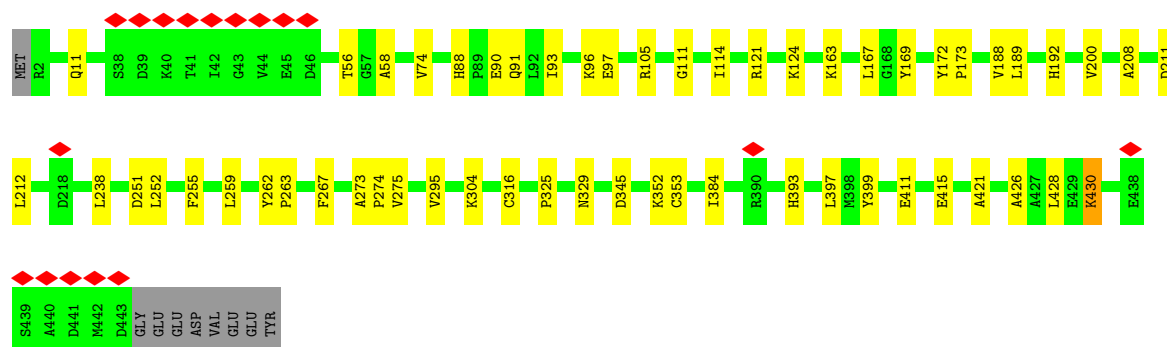


- Molecule 59: Tubulin alpha chain

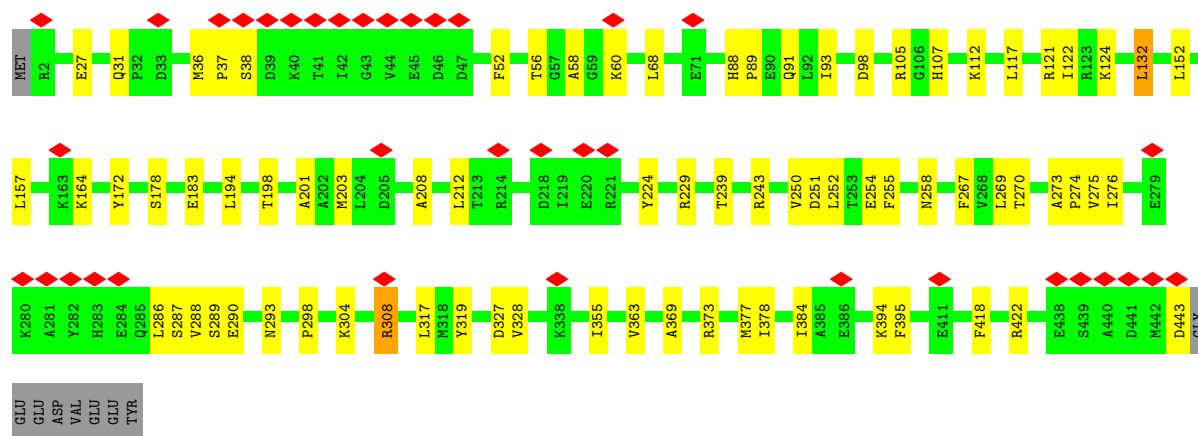
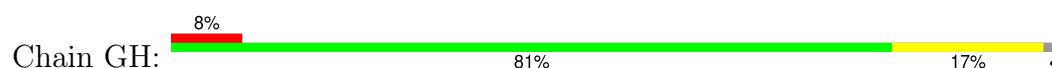


- Molecule 59: Tubulin alpha chain

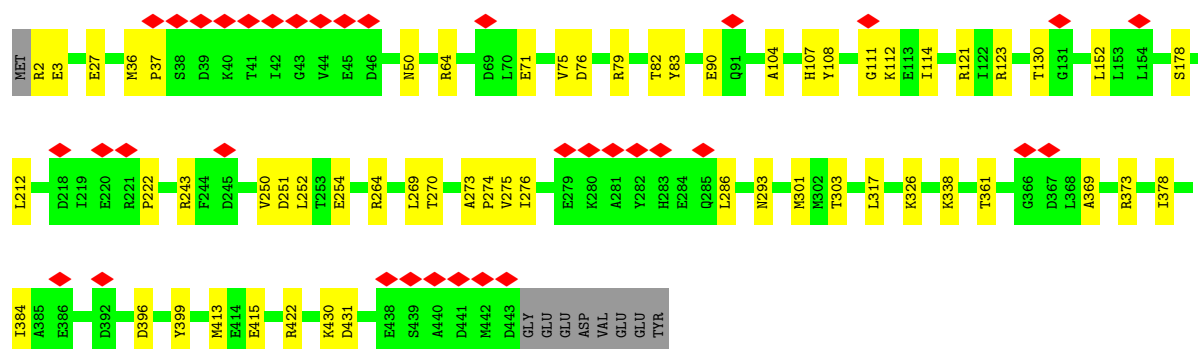
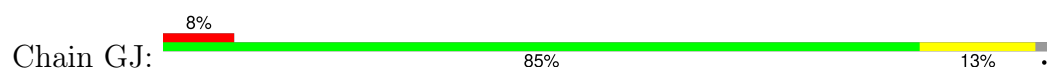




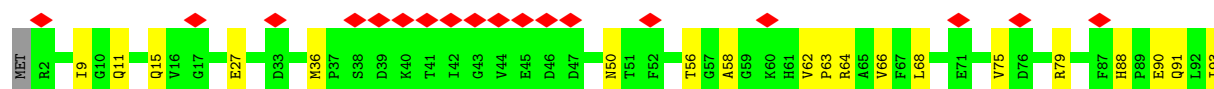
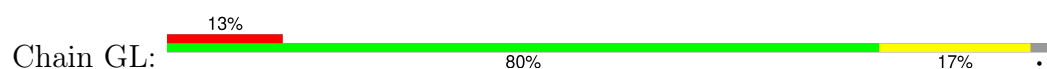
• Molecule 59: Tubulin alpha chain

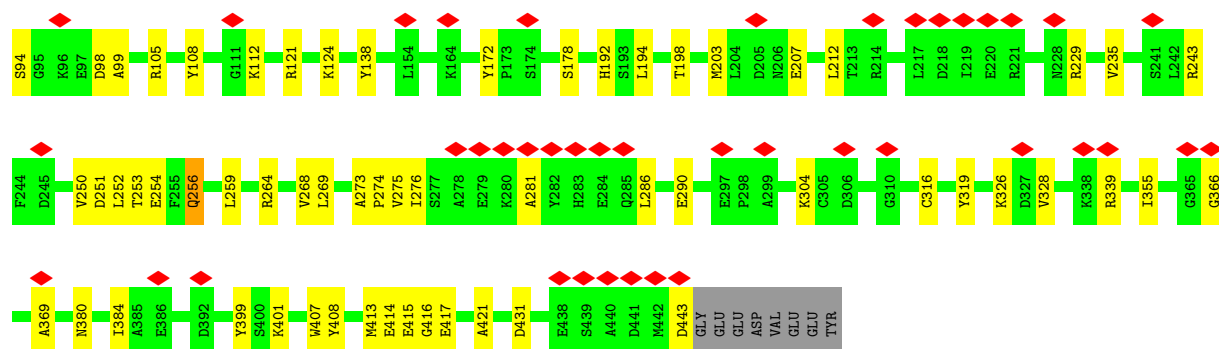


• Molecule 59: Tubulin alpha chain

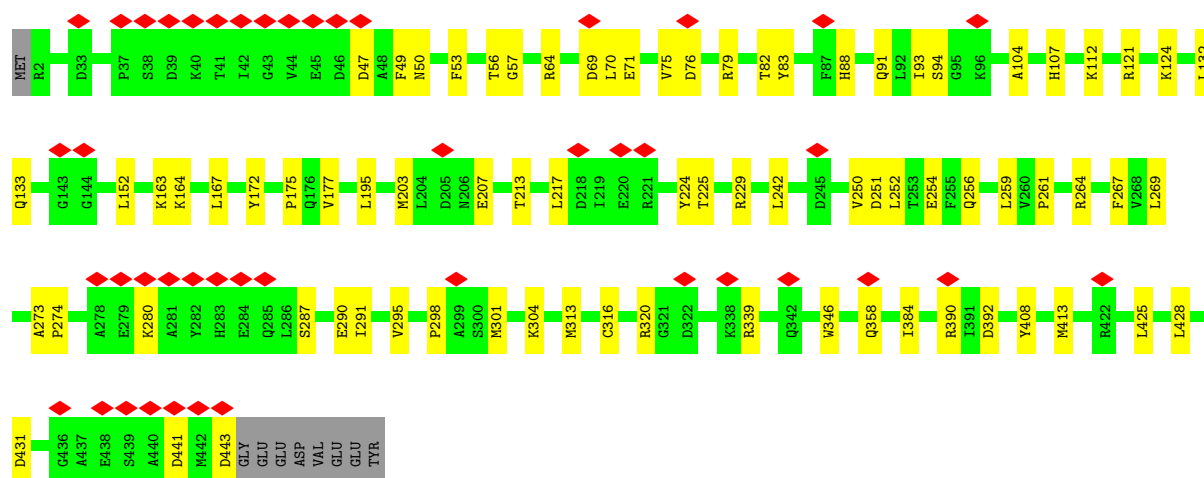
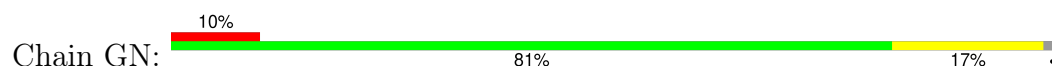


• Molecule 59: Tubulin alpha chain

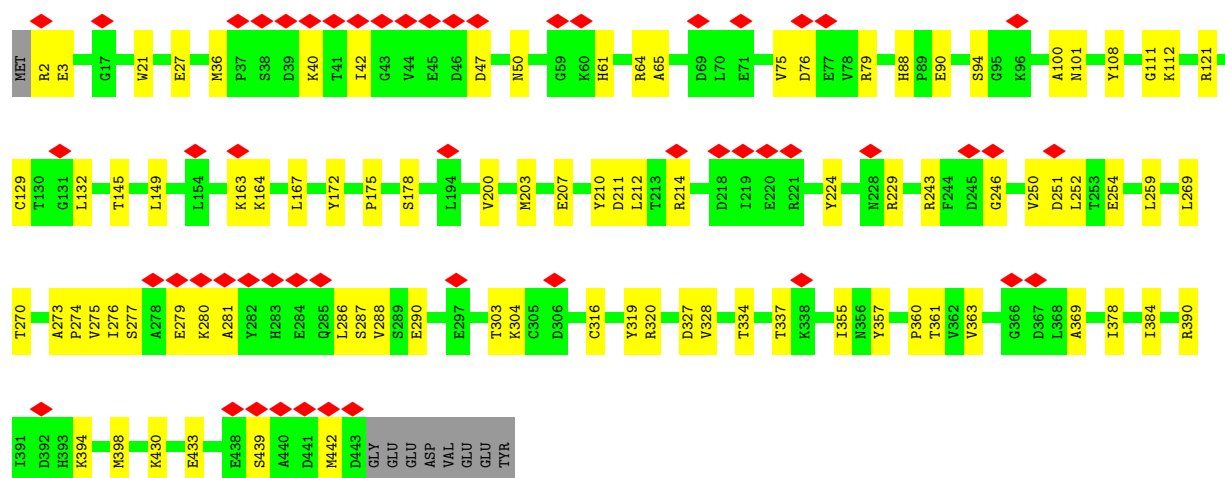
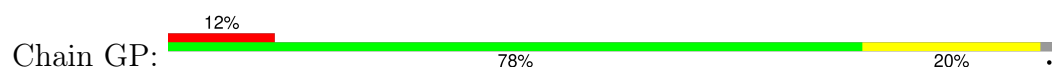




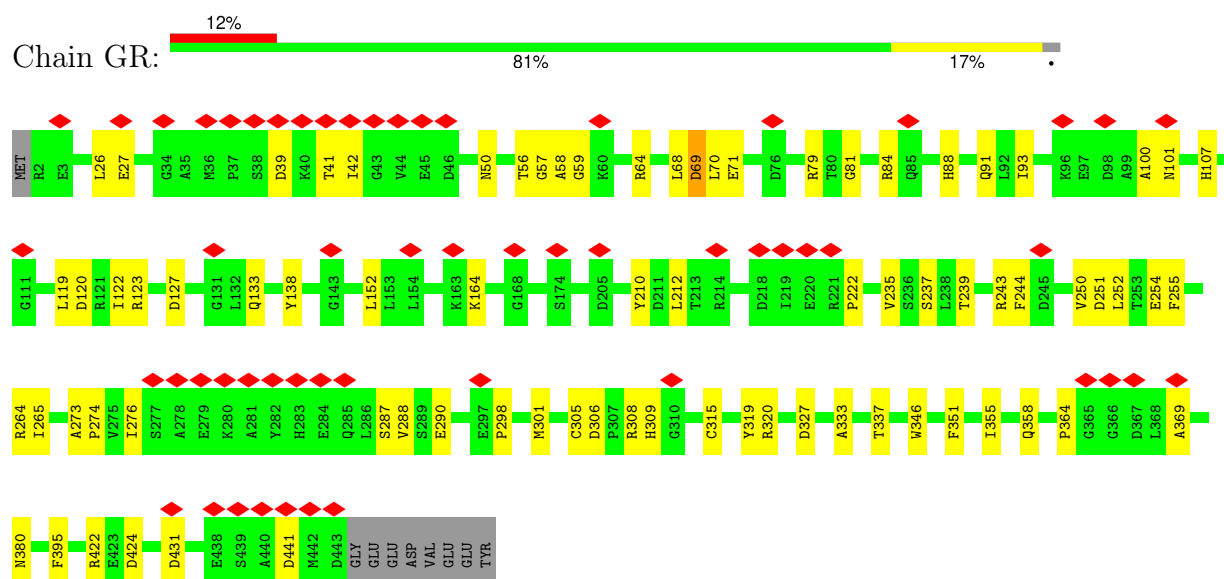
• Molecule 59: Tubulin alpha chain



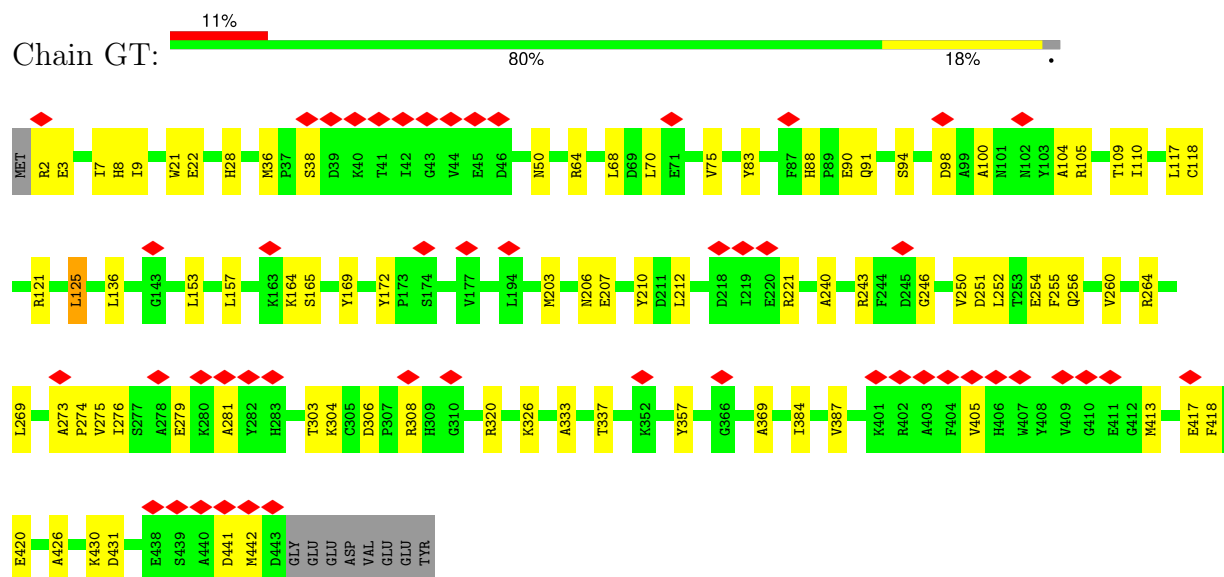
• Molecule 59: Tubulin alpha chain



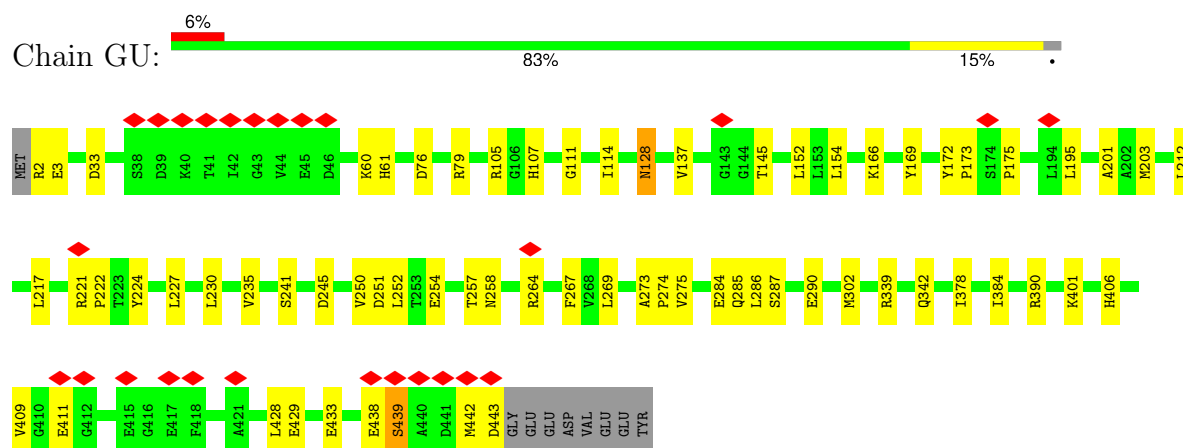
• Molecule 59: Tubulin alpha chain



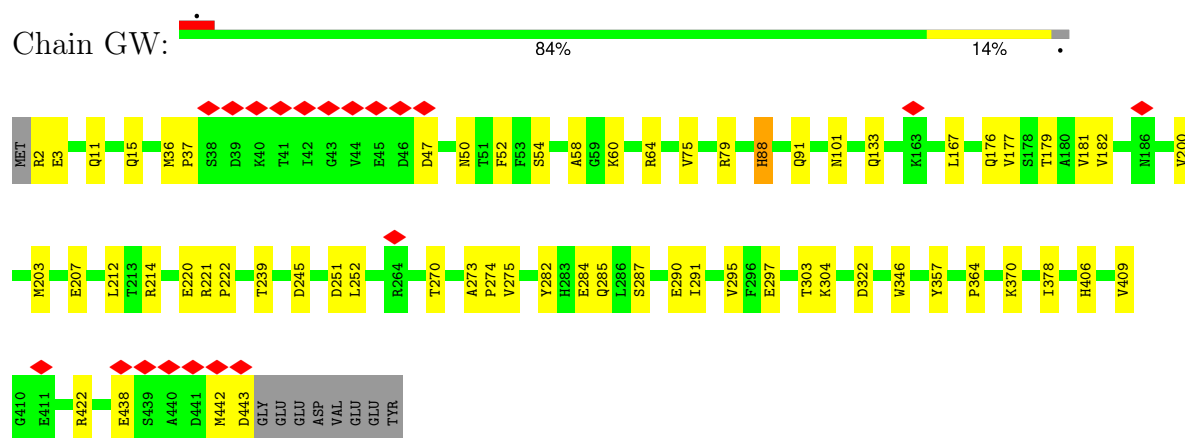
• Molecule 59: Tubulin alpha chain



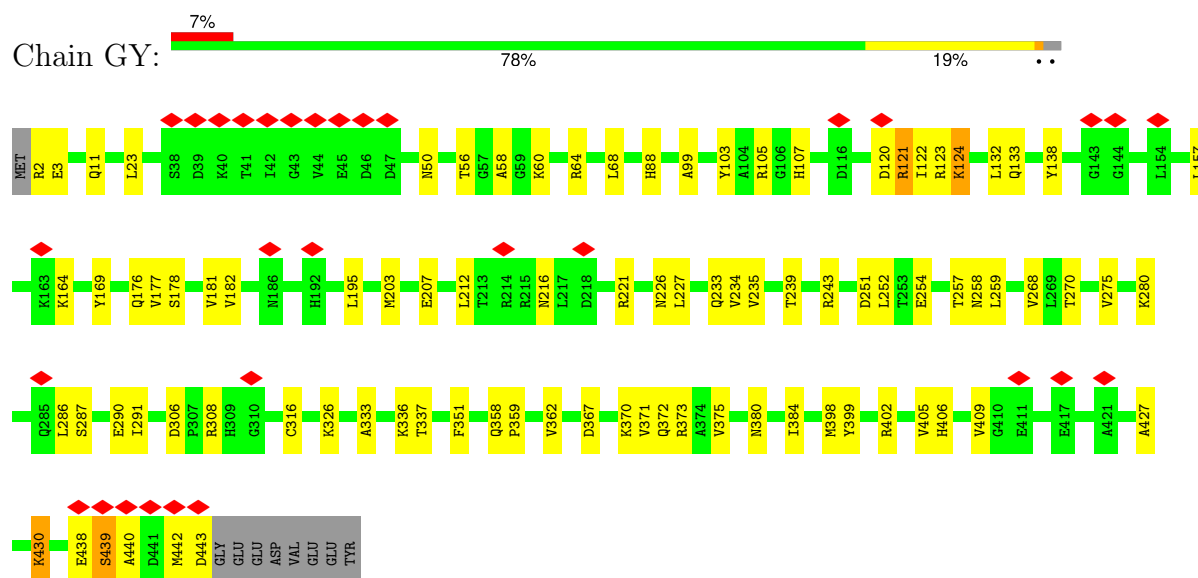
• Molecule 59: Tubulin alpha chain



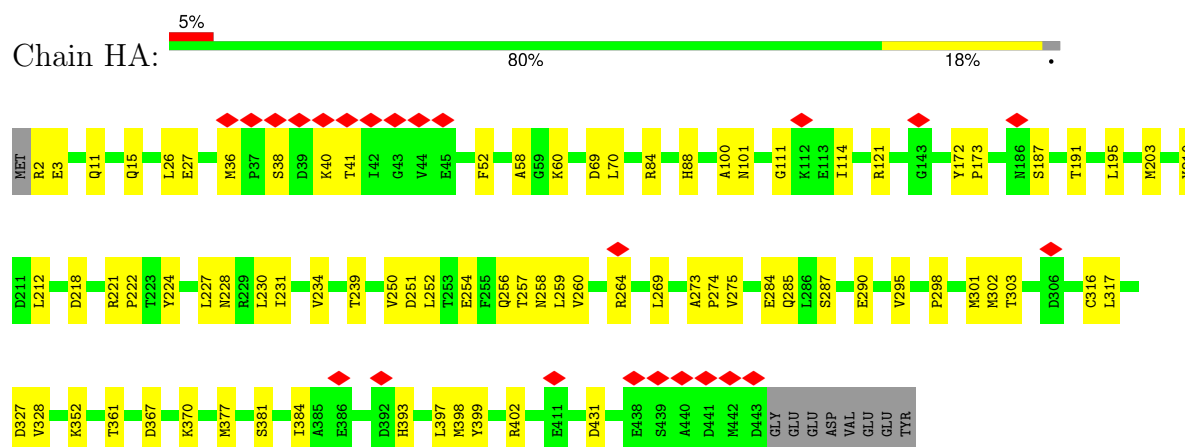
- Molecule 59: Tubulin alpha chain



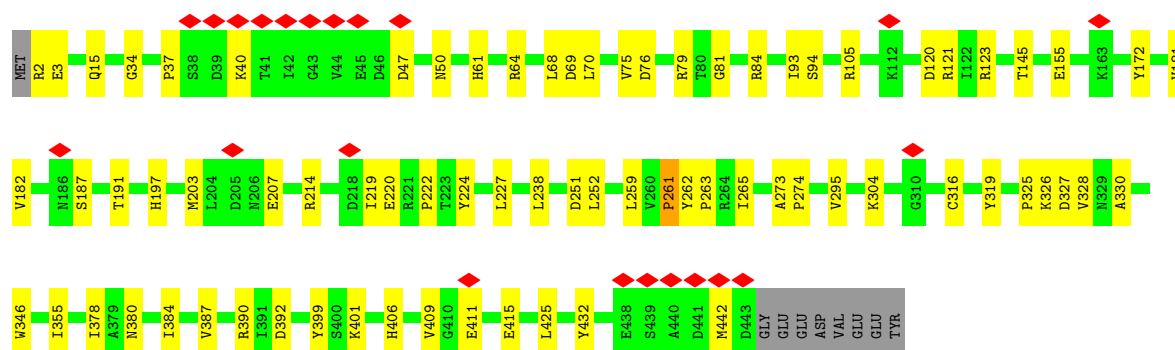
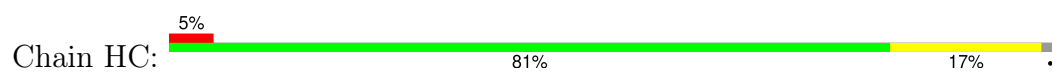
- Molecule 59: Tubulin alpha chain



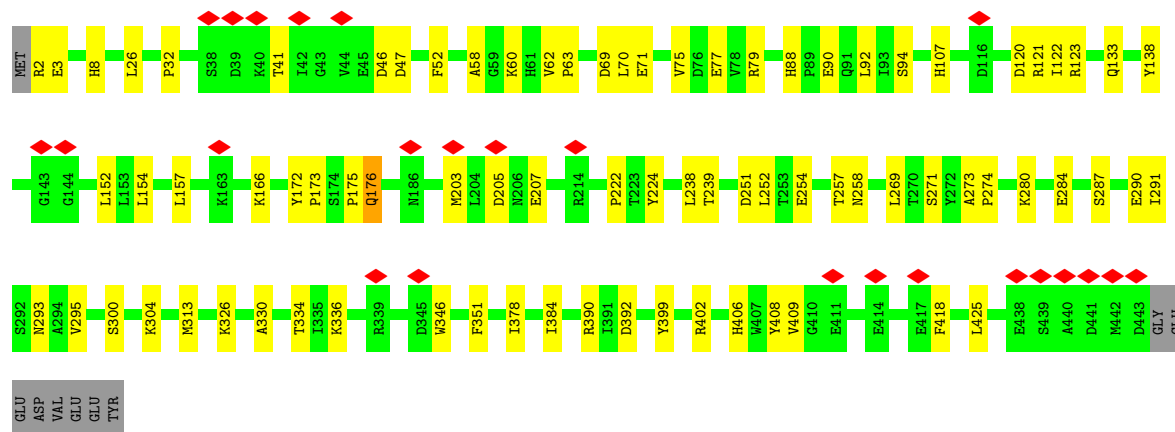
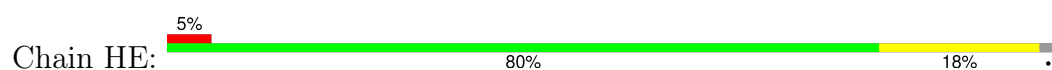
- Molecule 59: Tubulin alpha chain



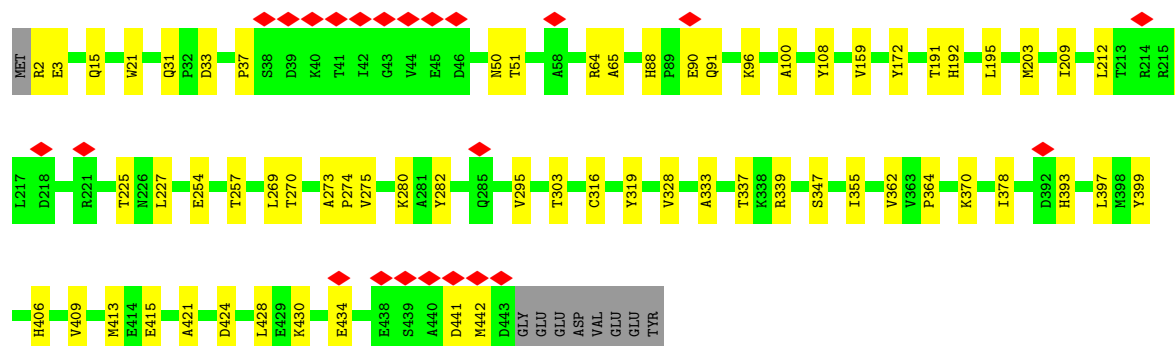
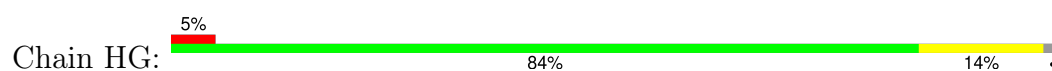
- Molecule 59: Tubulin alpha chain



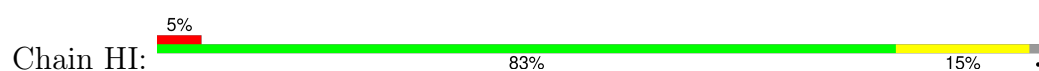
• Molecule 59: Tubulin alpha chain



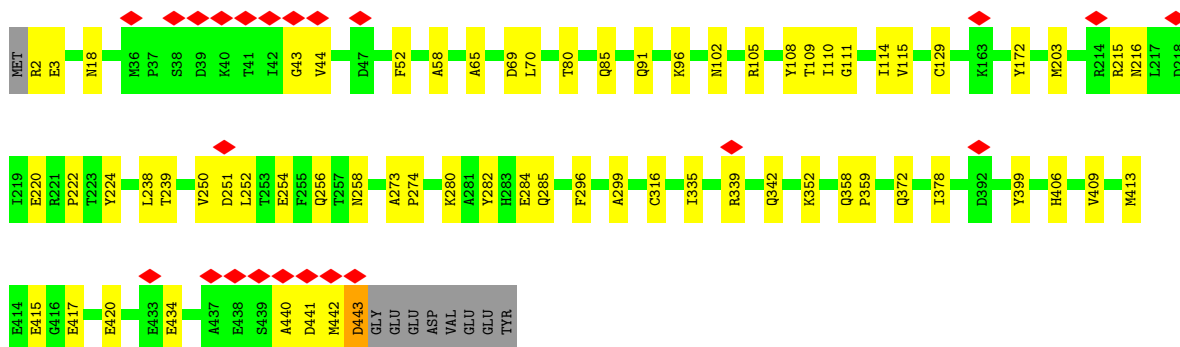
• Molecule 59: Tubulin alpha chain



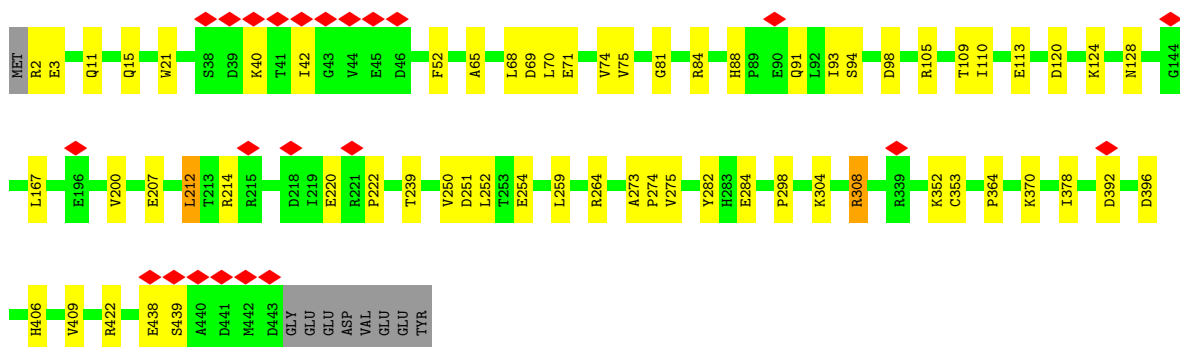
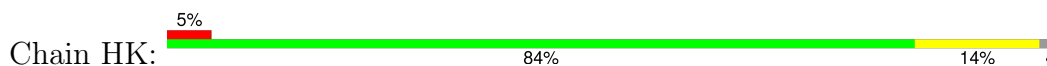
• Molecule 59: Tubulin alpha chain



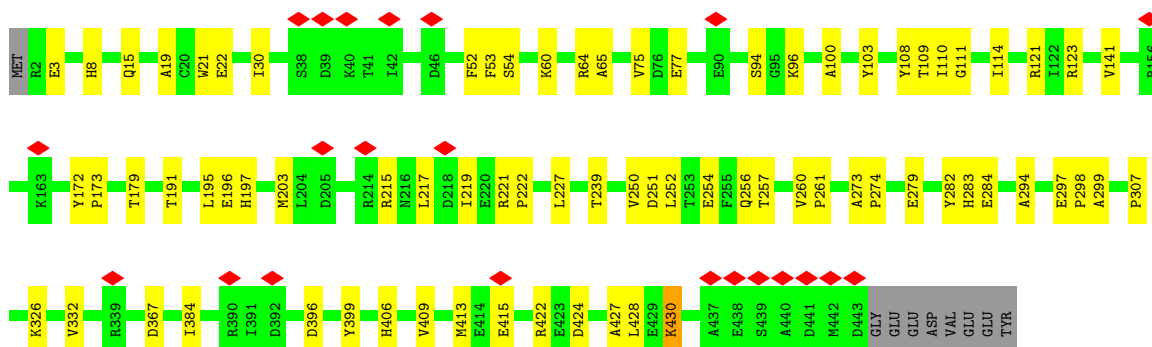
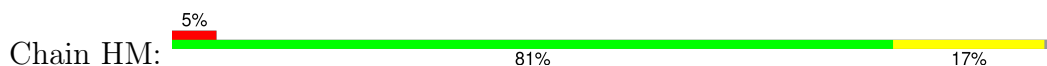




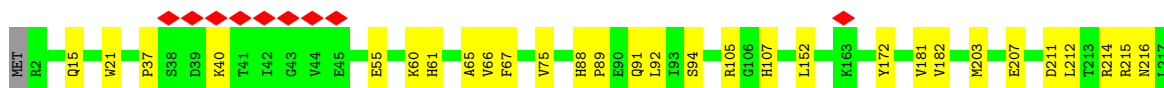
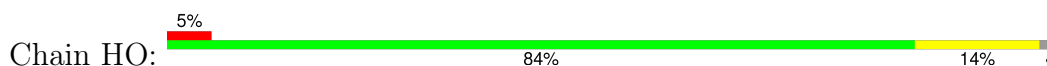
• Molecule 59: Tubulin alpha chain

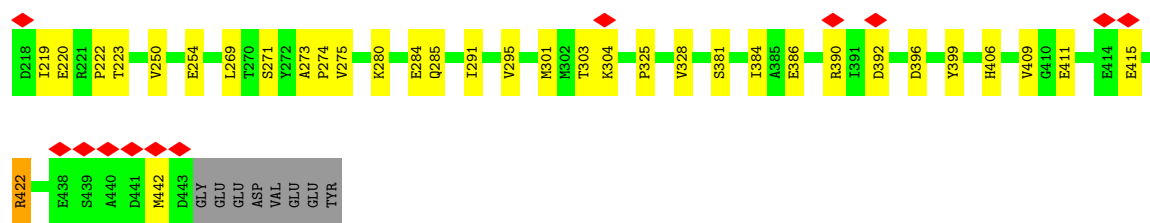


• Molecule 59: Tubulin alpha chain

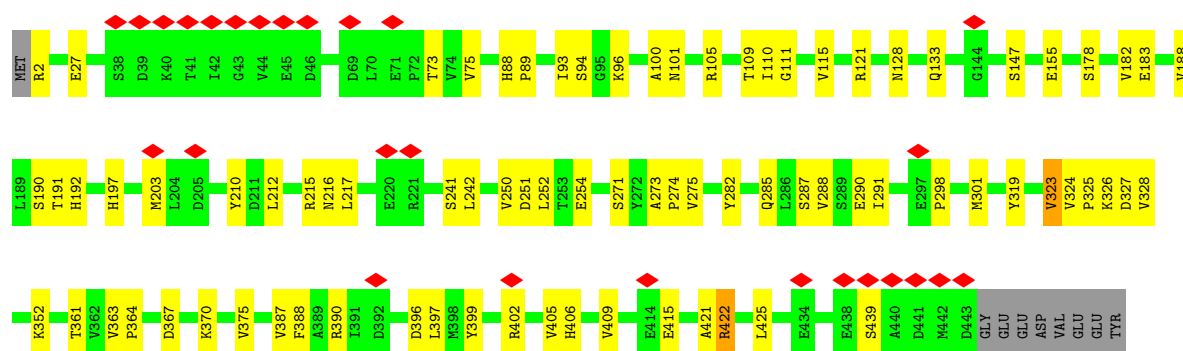
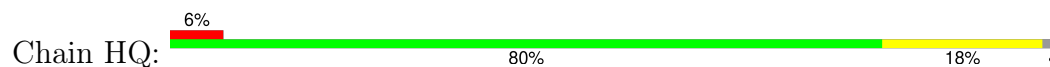


• Molecule 59: Tubulin alpha chain

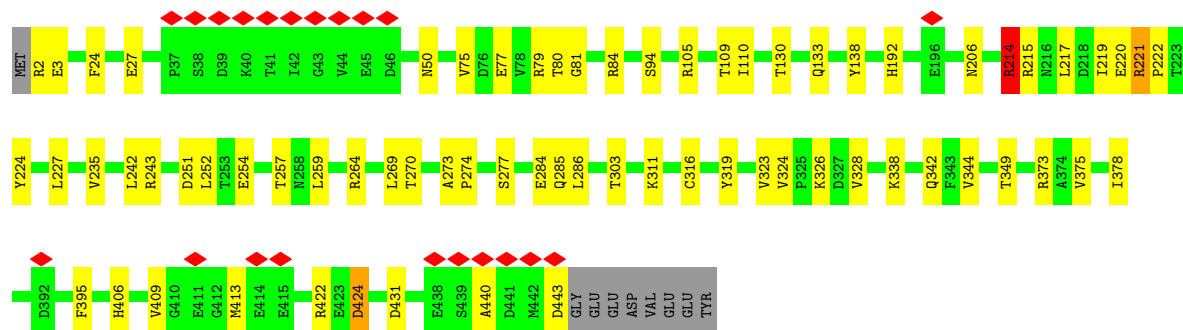
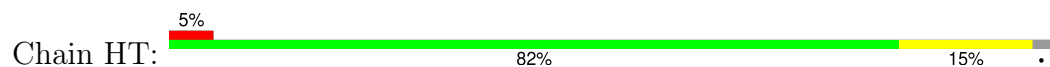




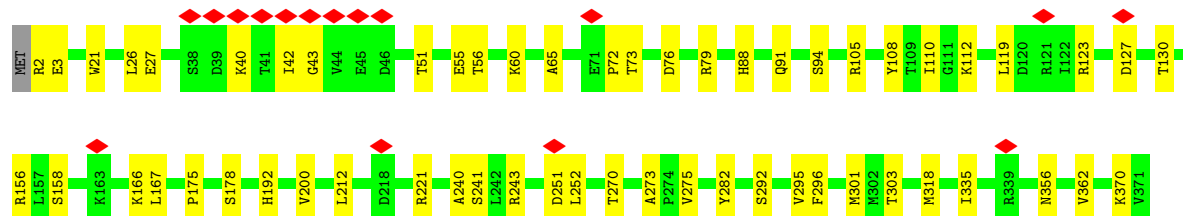
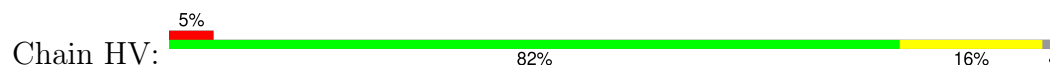
• Molecule 59: Tubulin alpha chain



• Molecule 59: Tubulin alpha chain

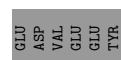
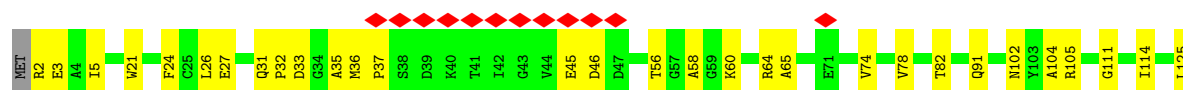
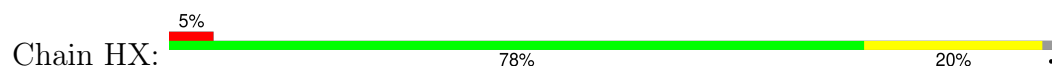


• Molecule 59: Tubulin alpha chain

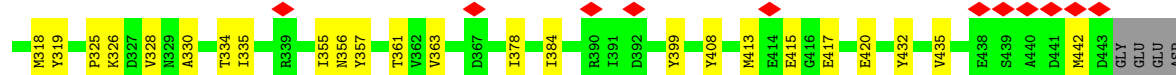
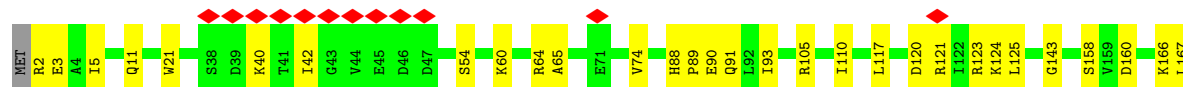
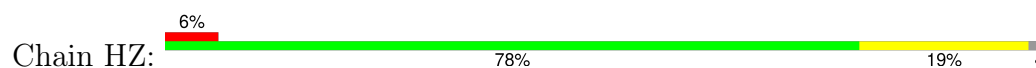




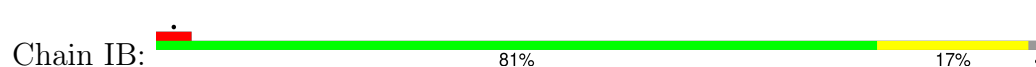
• Molecule 59: Tubulin alpha chain



• Molecule 59: Tubulin alpha chain

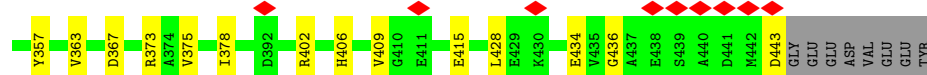
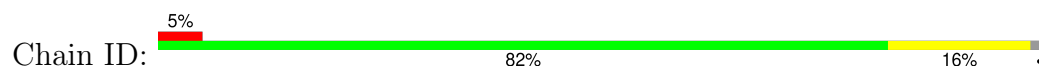


• Molecule 59: Tubulin alpha chain

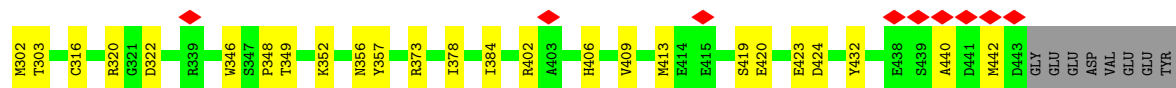
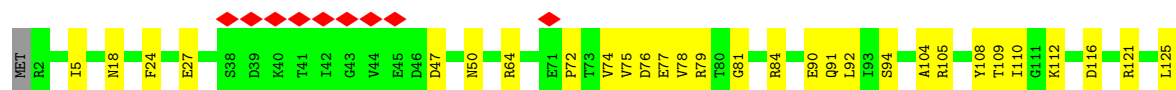
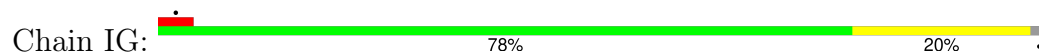




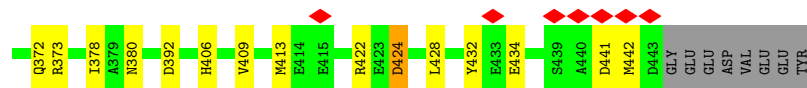
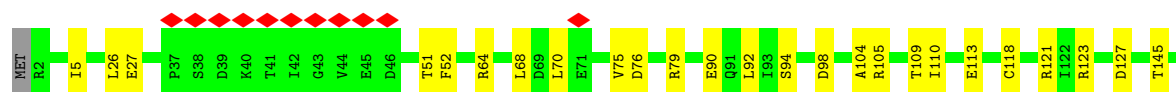
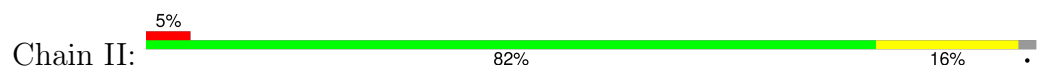
- Molecule 59: Tubulin alpha chain



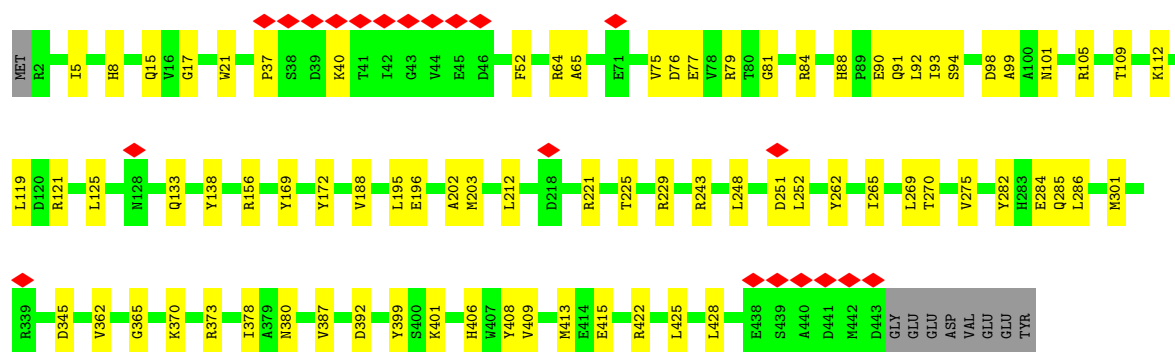
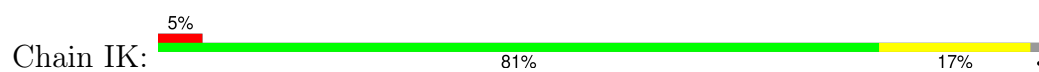
- Molecule 59: Tubulin alpha chain



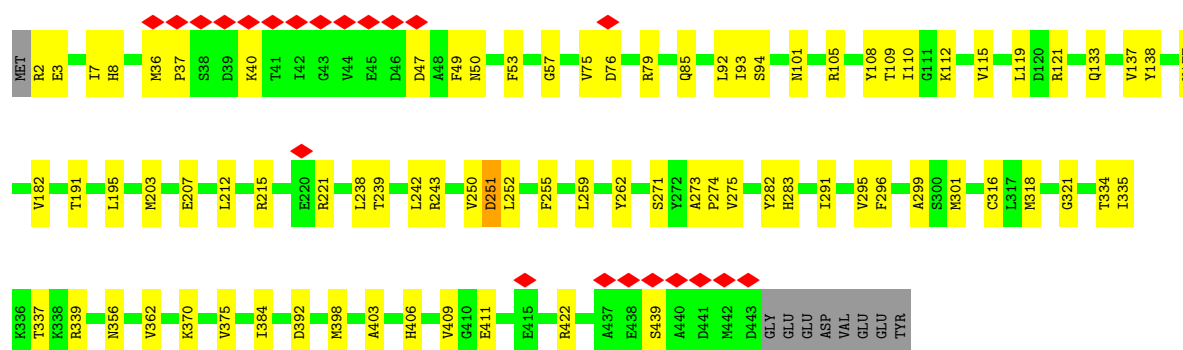
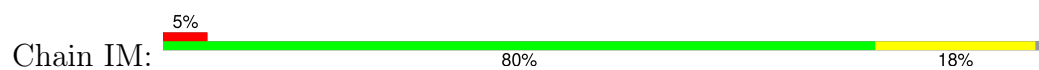
- Molecule 59: Tubulin alpha chain



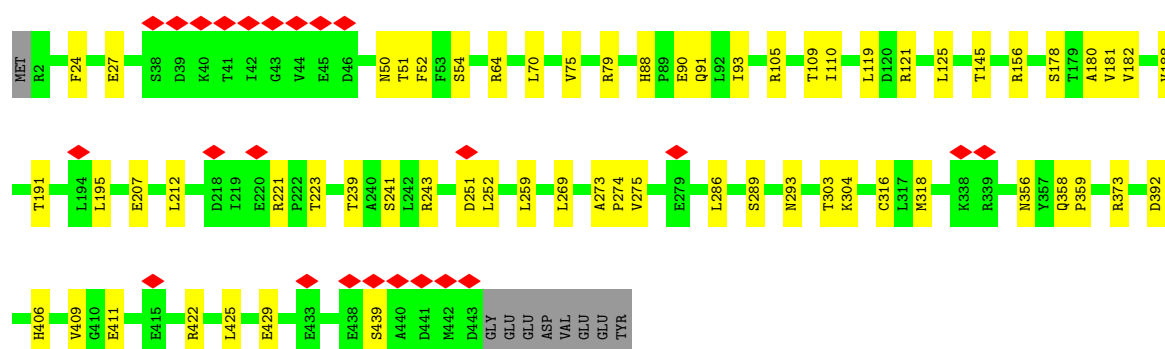
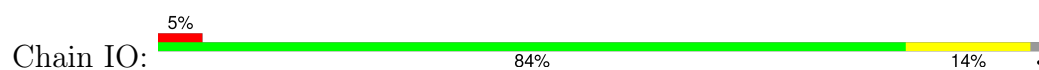
- Molecule 59: Tubulin alpha chain



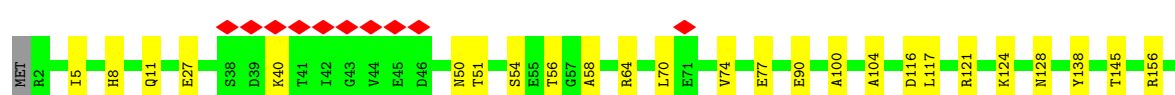
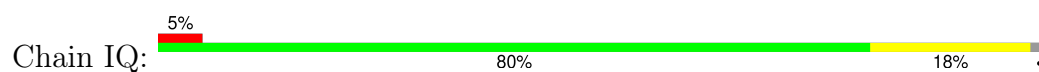
• Molecule 59: Tubulin alpha chain

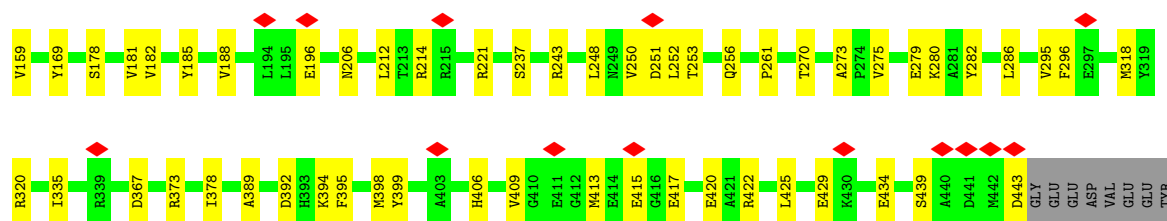


• Molecule 59: Tubulin alpha chain

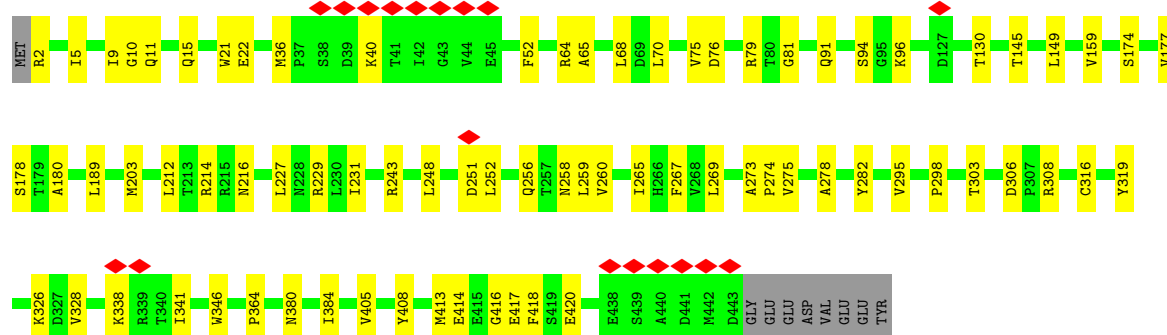
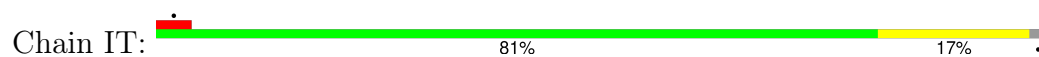


• Molecule 59: Tubulin alpha chain

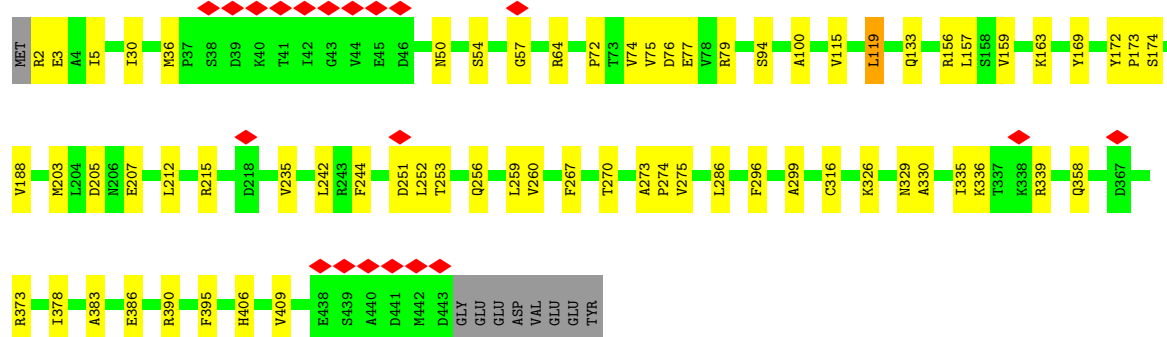
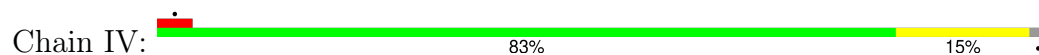




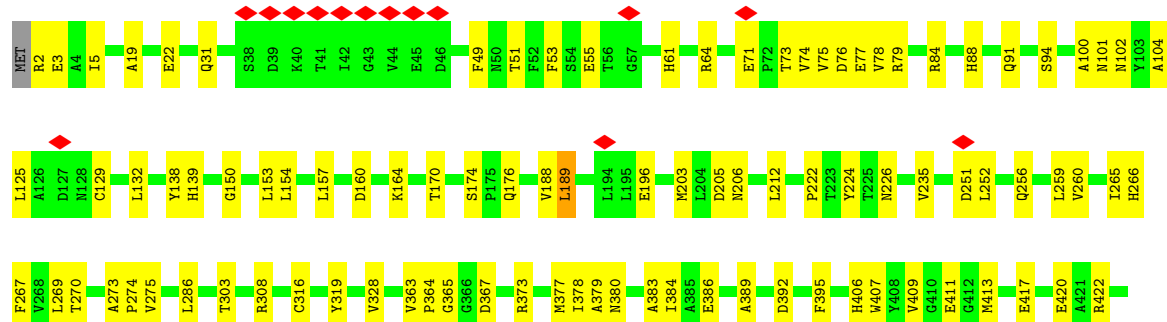
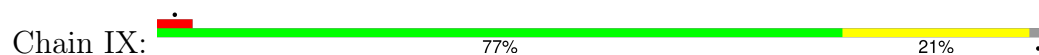
• Molecule 59: Tubulin alpha chain

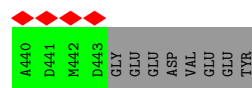


• Molecule 59: Tubulin alpha chain



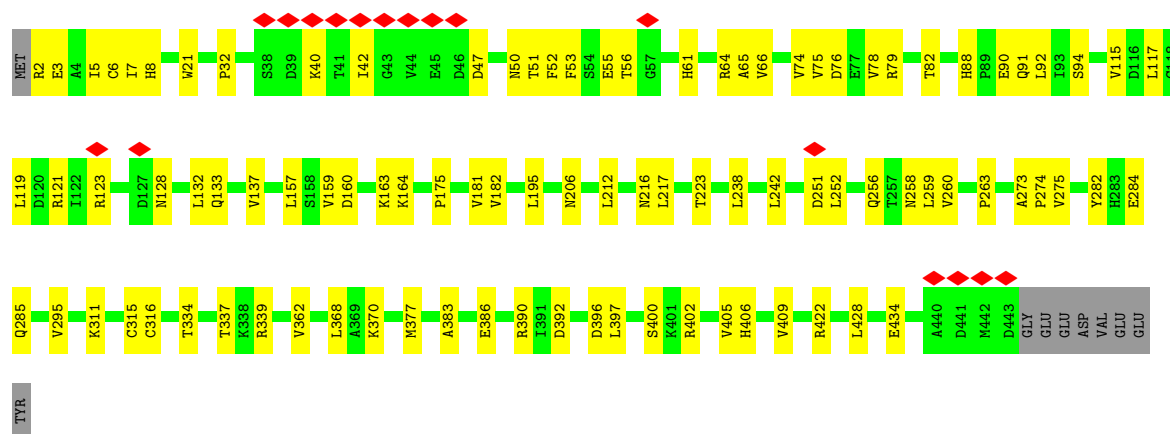
• Molecule 59: Tubulin alpha chain





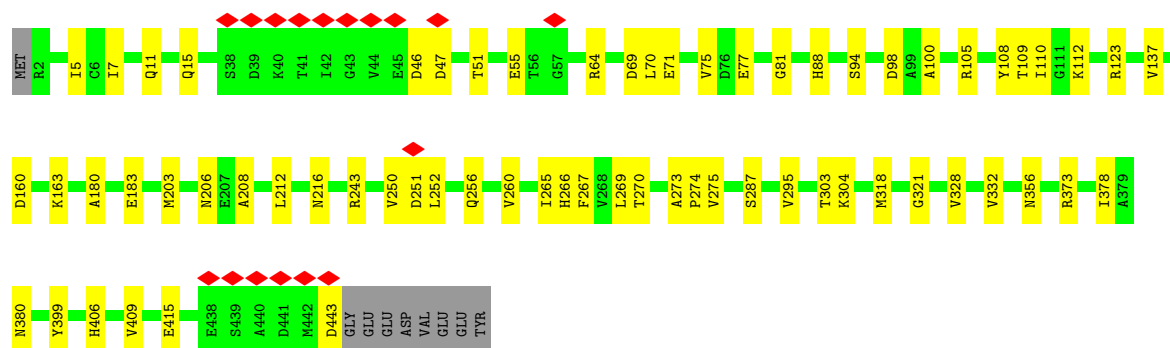
• Molecule 59: Tubulin alpha chain

Chain IZ: 77% 21%



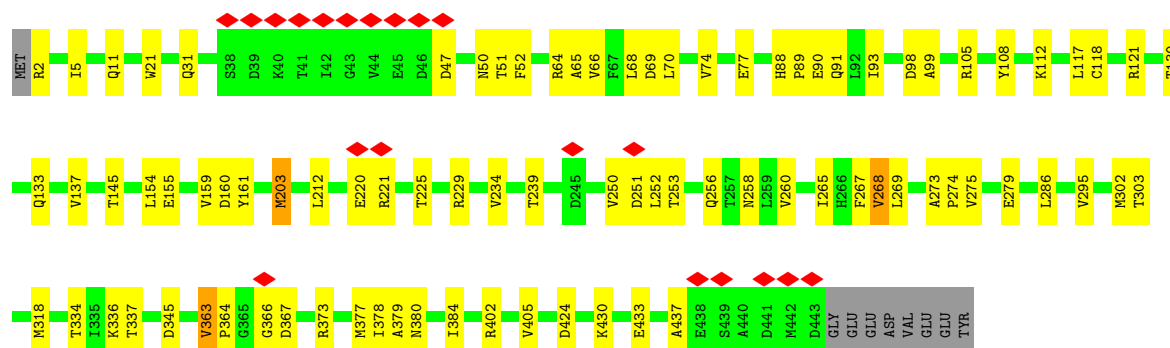
• Molecule 59: Tubulin alpha chain

Chain JB: 83% 15%

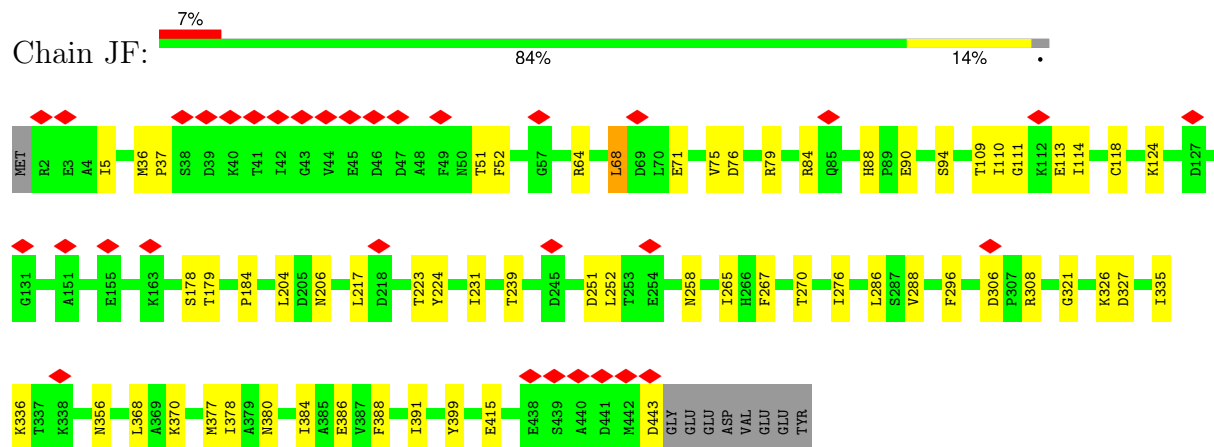


• Molecule 59: Tubulin alpha chain

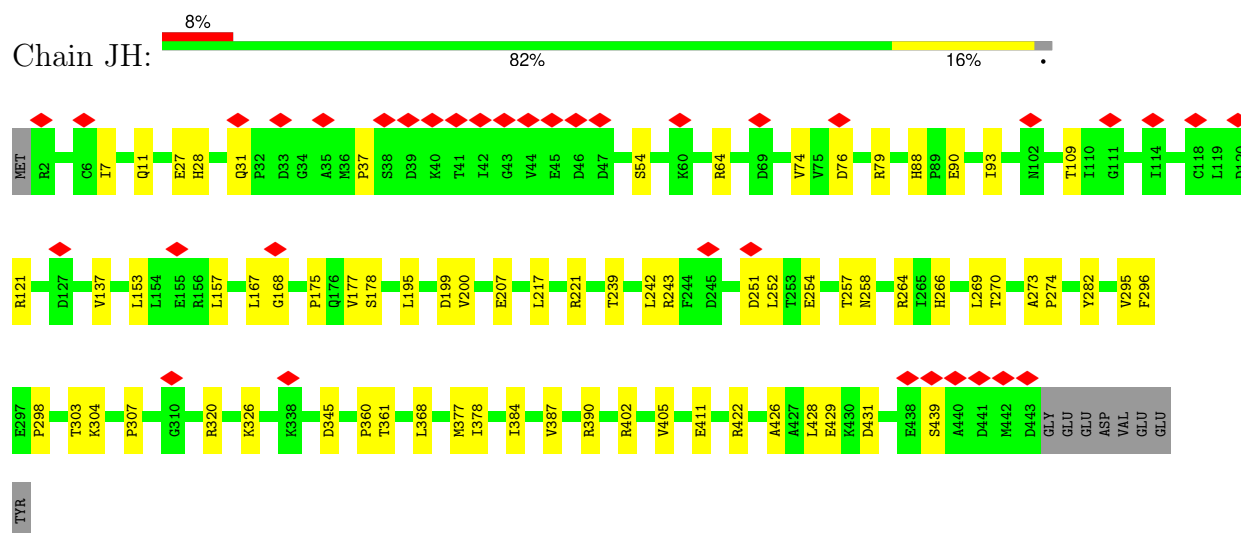
Chain JD: 79% 19%



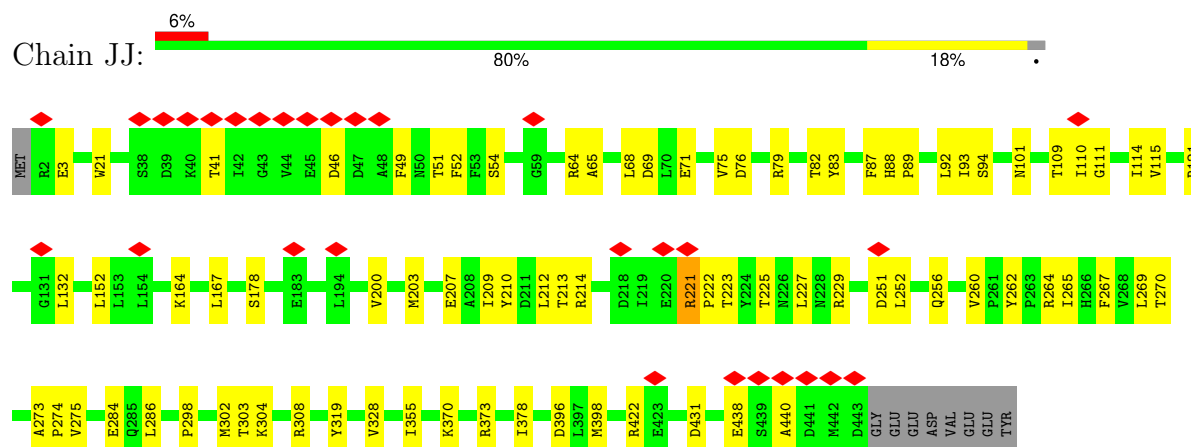
- Molecule 59: Tubulin alpha chain



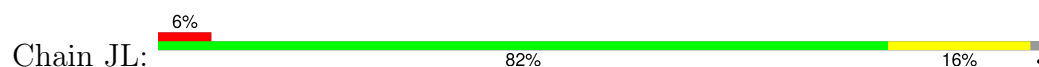
- Molecule 59: Tubulin alpha chain



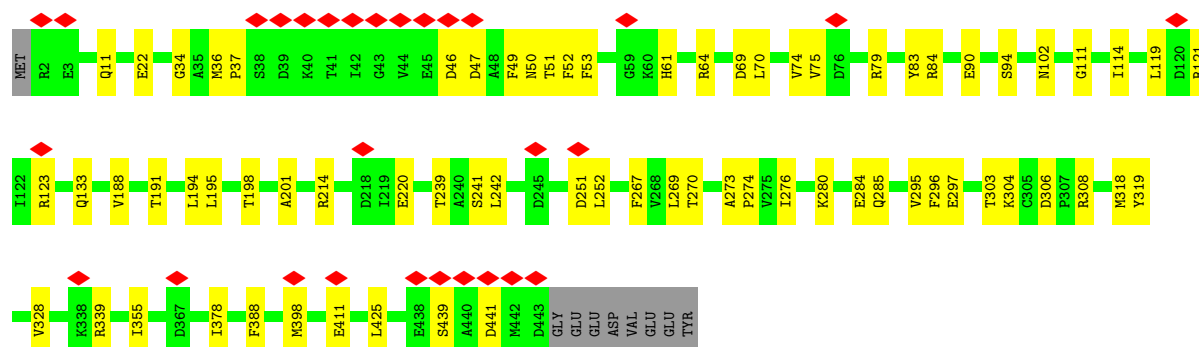
- Molecule 59: Tubulin alpha chain



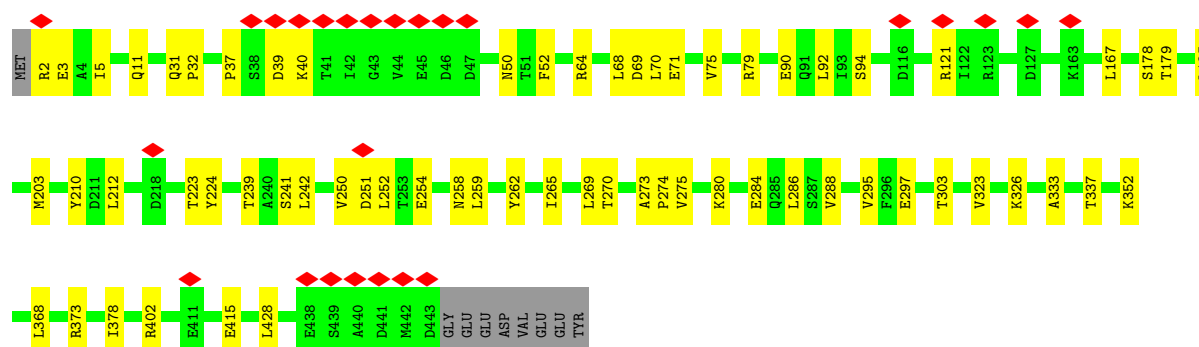
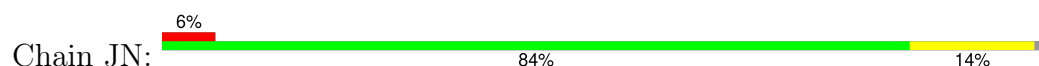
- Molecule 59: Tubulin alpha chain



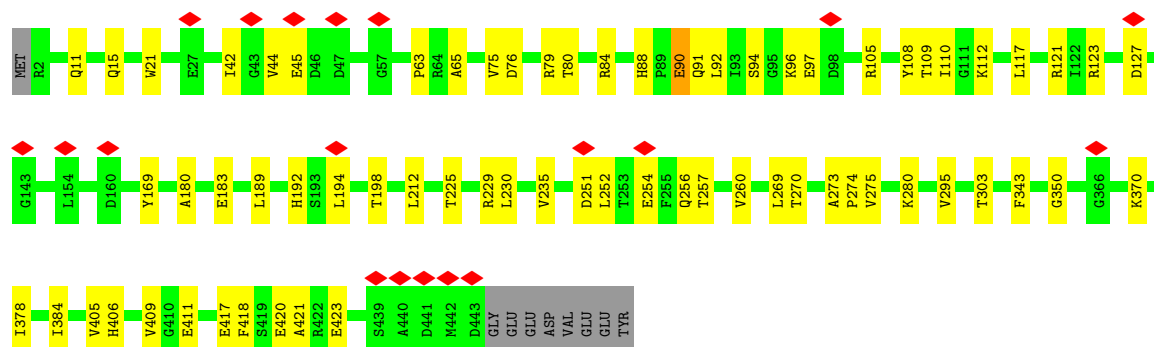
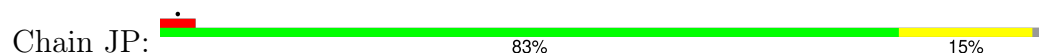




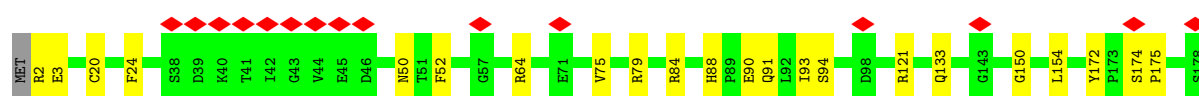
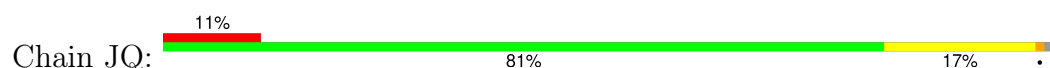
• Molecule 59: Tubulin alpha chain

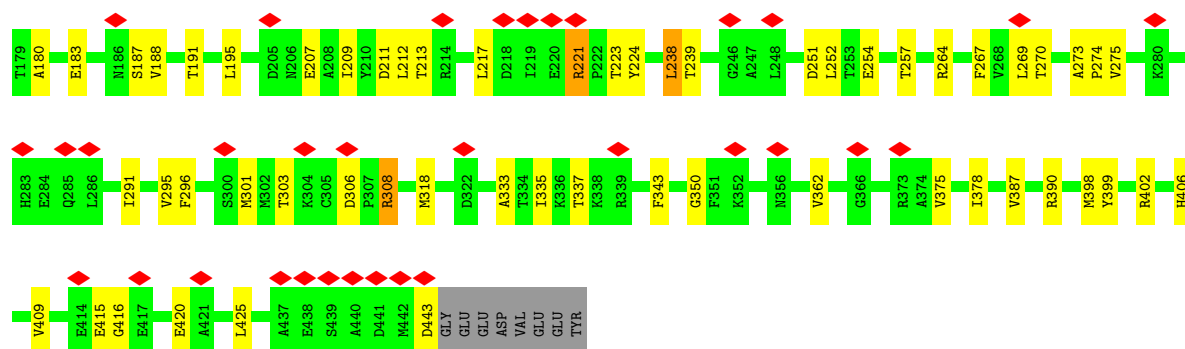


• Molecule 59: Tubulin alpha chain

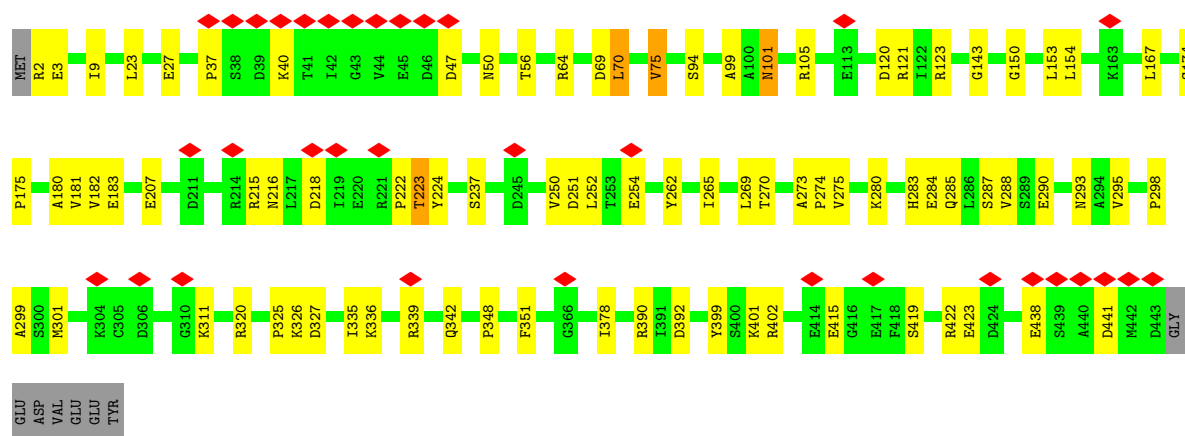
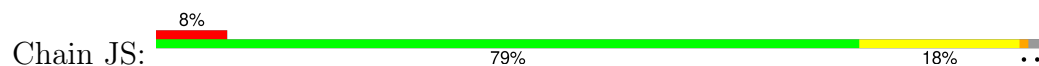


• Molecule 59: Tubulin alpha chain

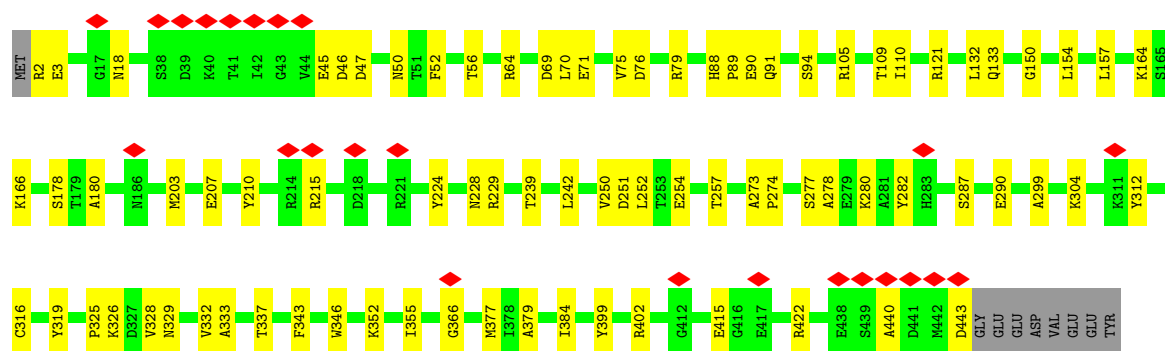
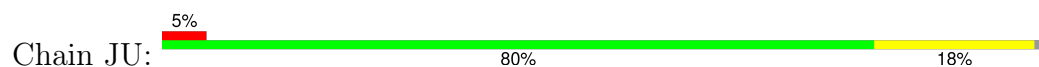




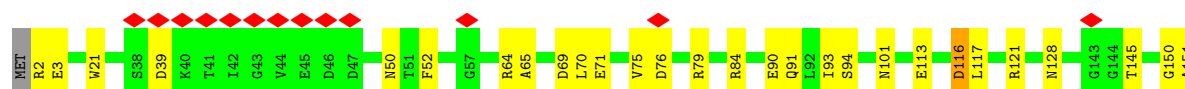
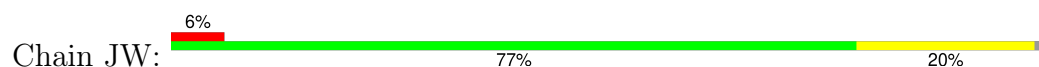
• Molecule 59: Tubulin alpha chain

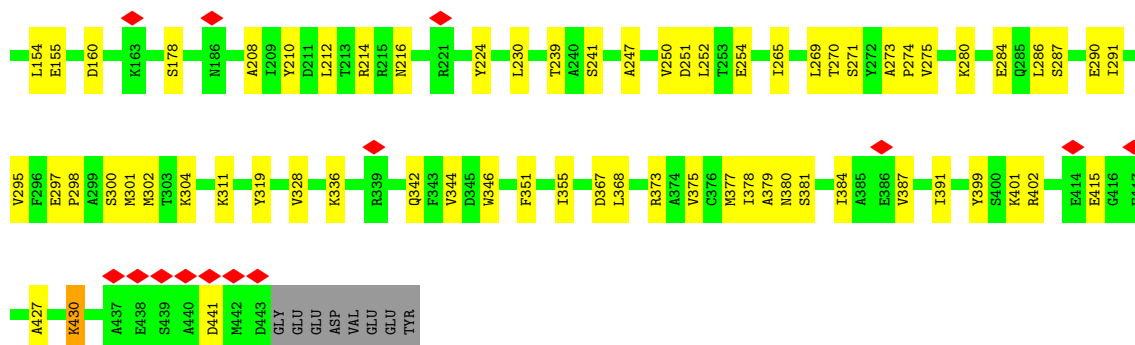


• Molecule 59: Tubulin alpha chain

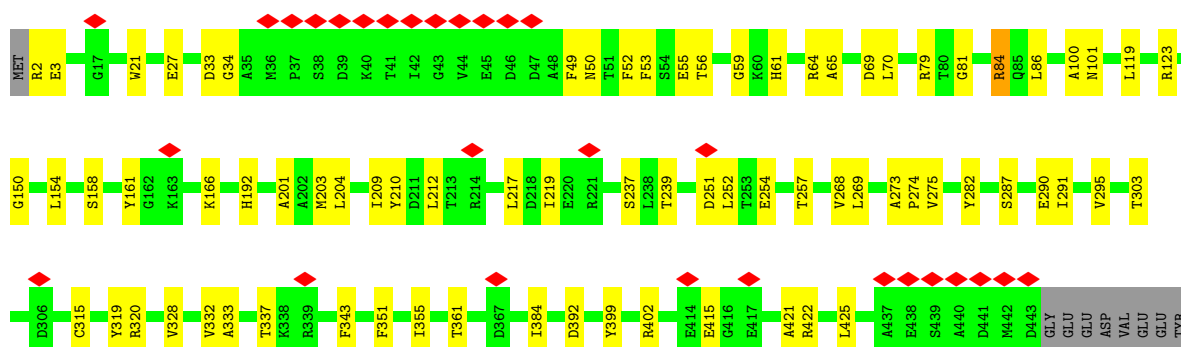
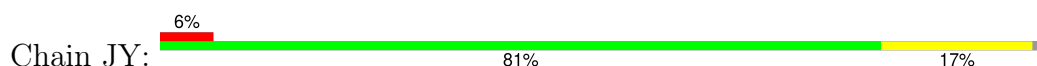


• Molecule 59: Tubulin alpha chain

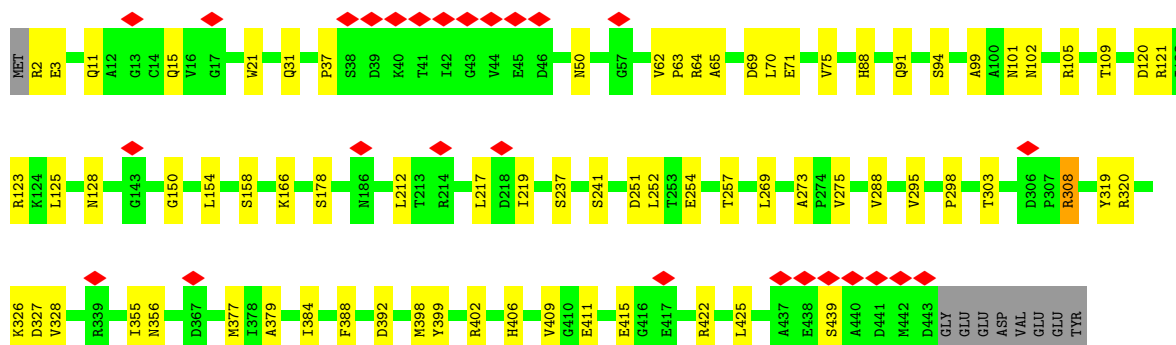
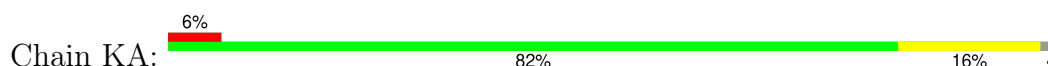




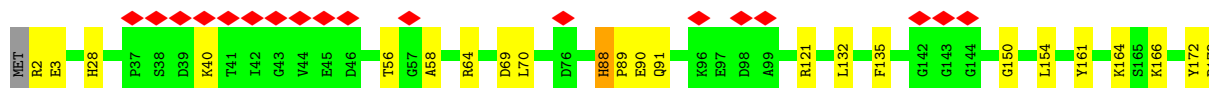
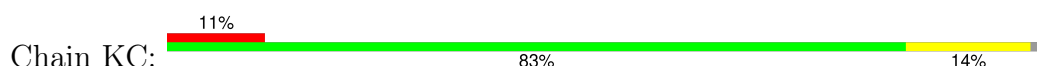
• Molecule 59: Tubulin alpha chain

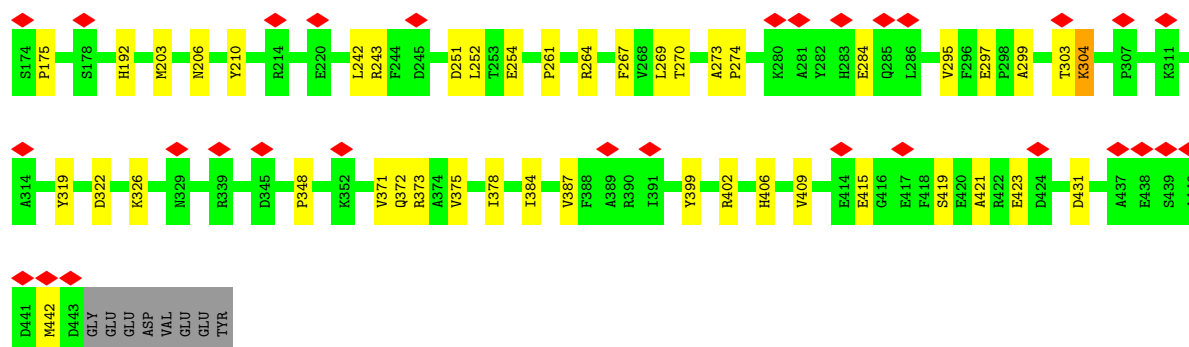


• Molecule 59: Tubulin alpha chain

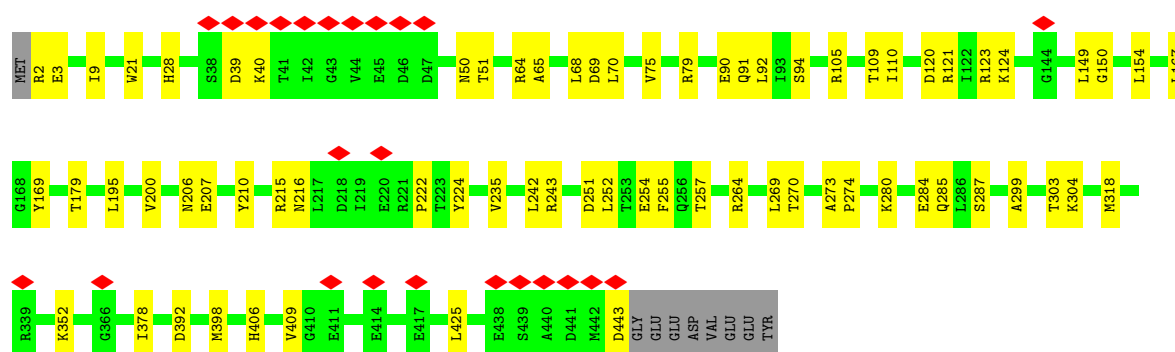
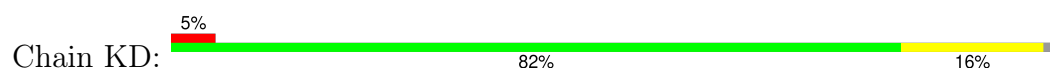


• Molecule 59: Tubulin alpha chain

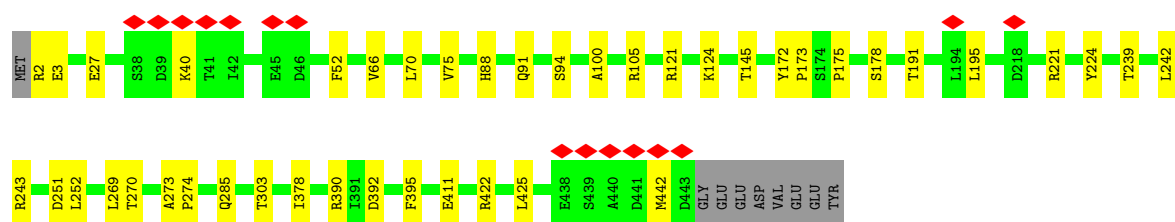




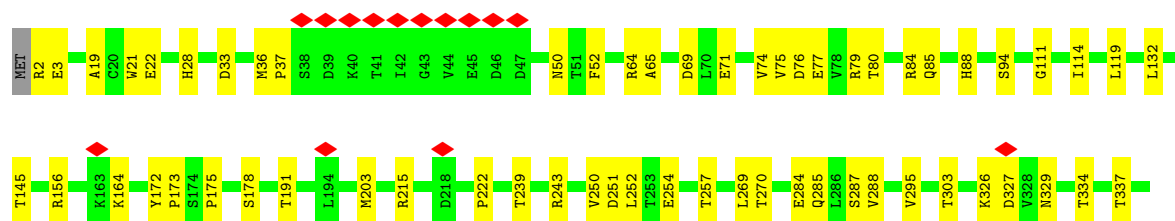
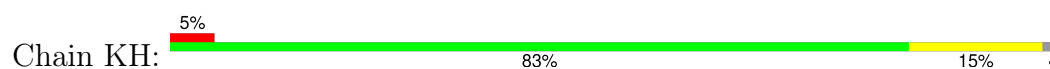
• Molecule 59: Tubulin alpha chain

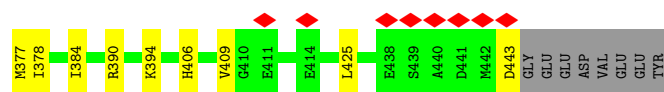


• Molecule 59: Tubulin alpha chain

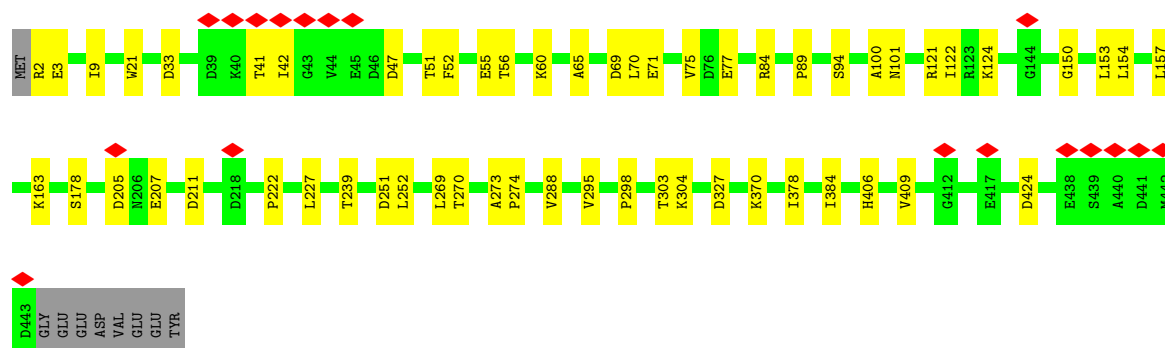
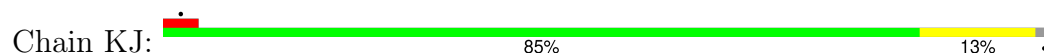


• Molecule 59: Tubulin alpha chain

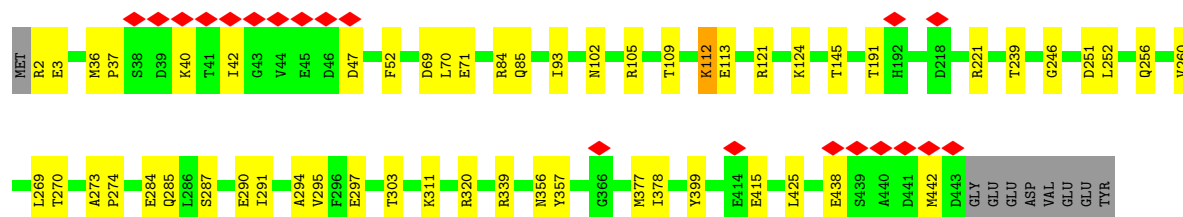
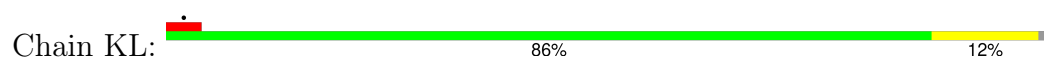




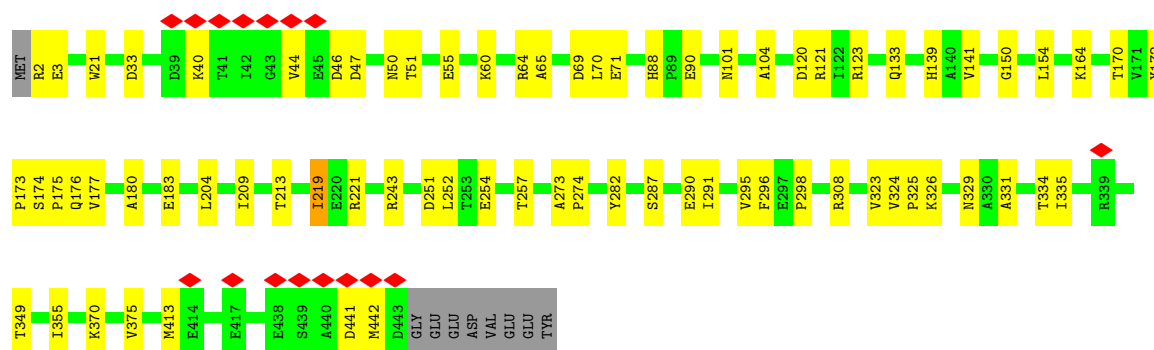
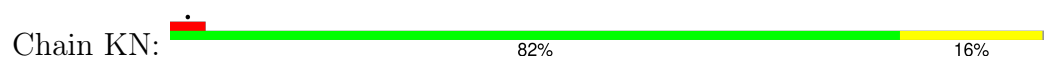
- Molecule 59: Tubulin alpha chain



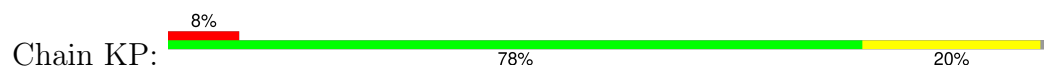
- Molecule 59: Tubulin alpha chain

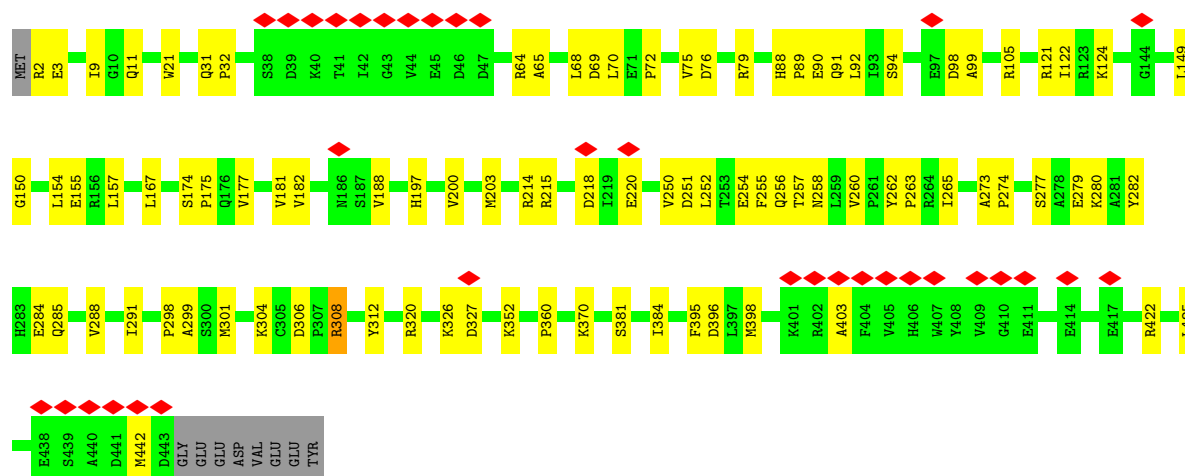


- Molecule 59: Tubulin alpha chain



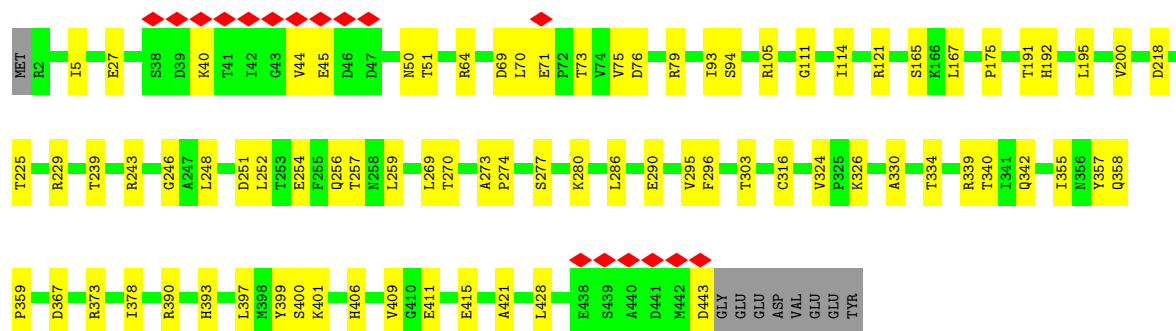
- Molecule 59: Tubulin alpha chain





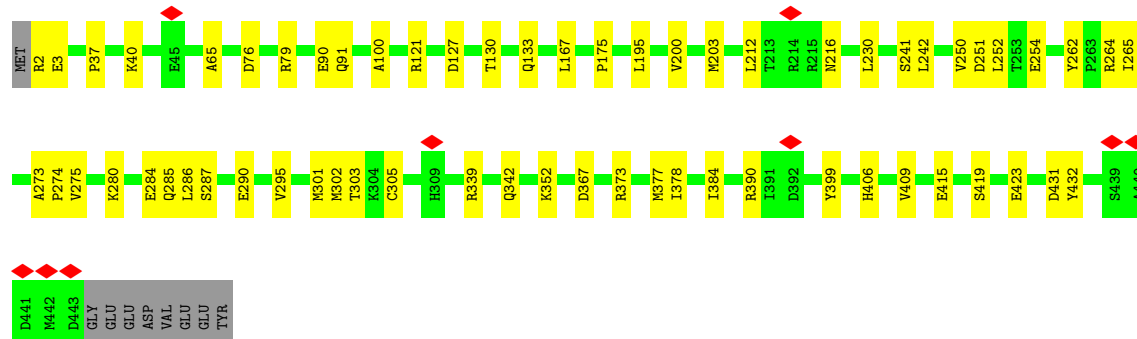
- Molecule 59: Tubulin alpha chain

Chain KQ: 80% 18% .



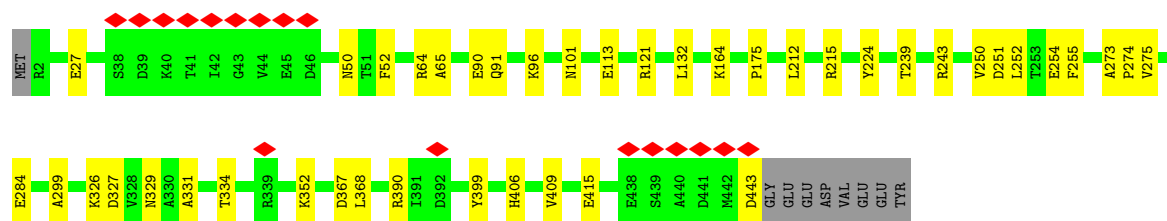
- Molecule 59: Tubulin alpha chain

Chain KS: 84% 14% .



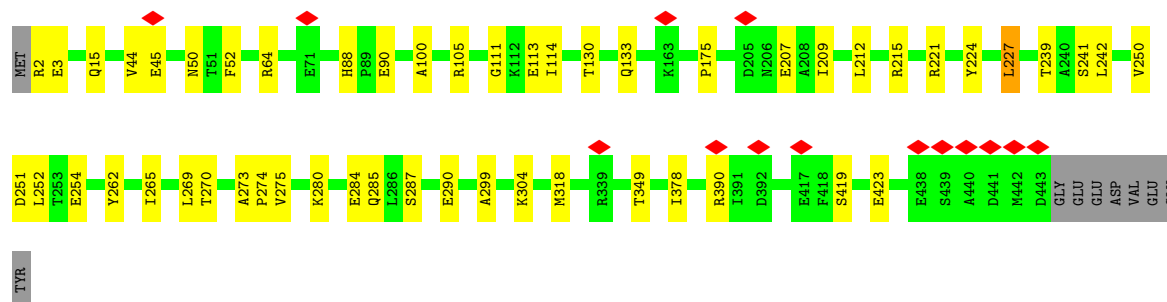
- Molecule 59: Tubulin alpha chain

Chain KU: 88% 10% .



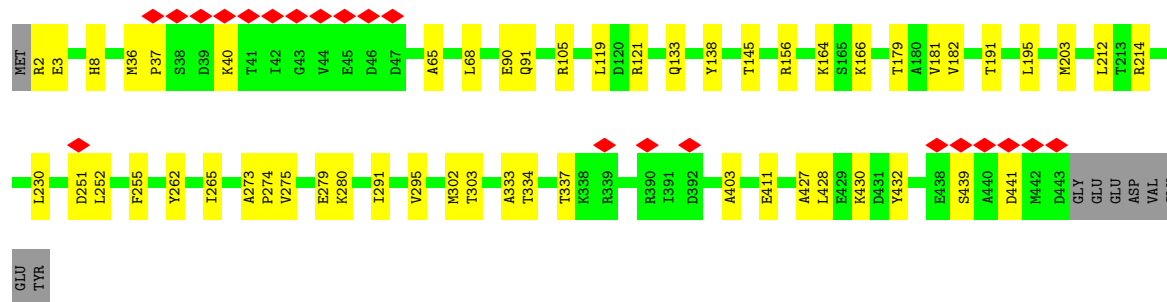
- Molecule 59: Tubulin alpha chain

Chain KW: 86% 11%



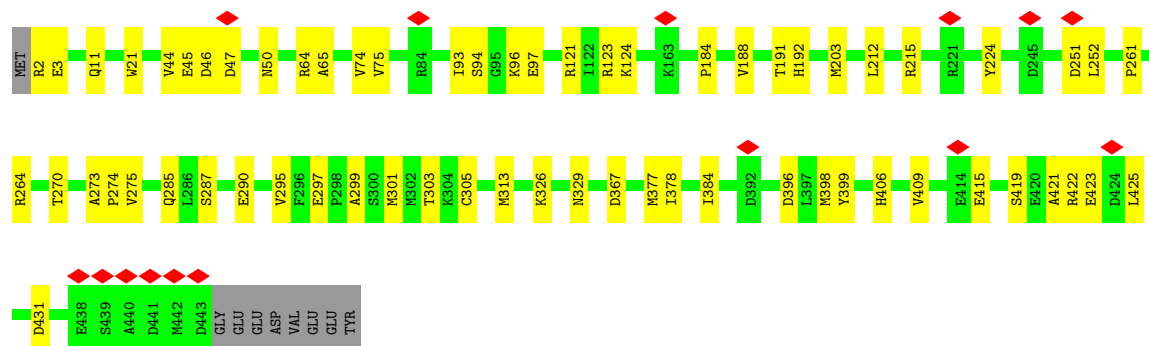
- Molecule 59: Tubulin alpha chain

Chain KY: 5% 86% 12%




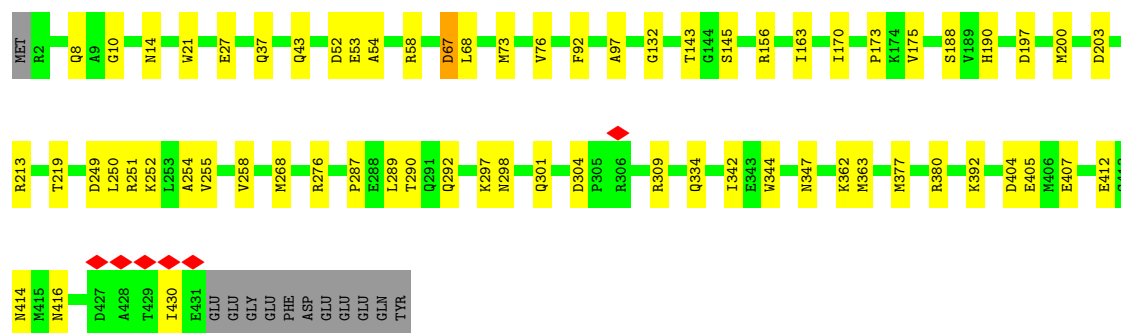
- Molecule 59: Tubulin alpha chain

Chain LA: 84% 14%




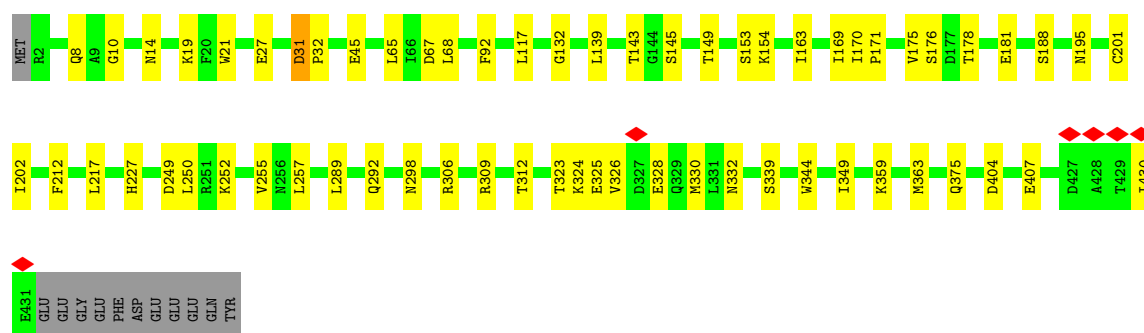
- Molecule 60: Tubulin beta chain

Chain AB:  82% 15%




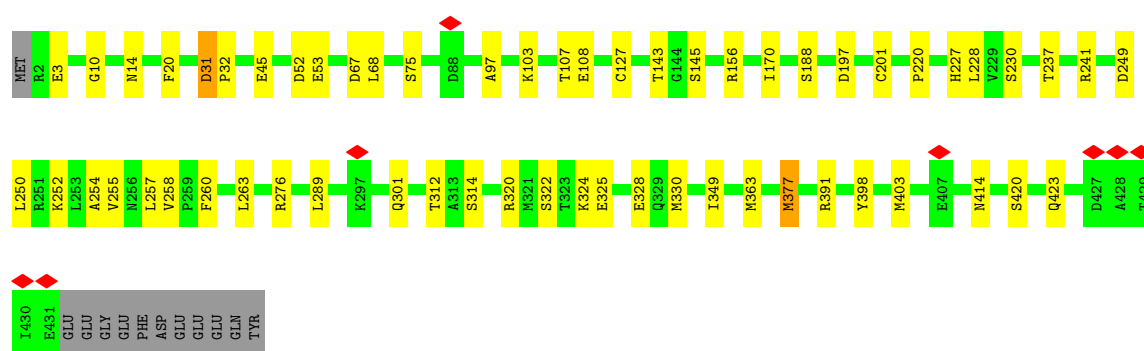
• Molecule 60: Tubulin beta chain

Chain AD:  83% 14%



• Molecule 60: Tubulin beta chain

Chain AF:  84% 13%



• Molecule 60: Tubulin beta chain

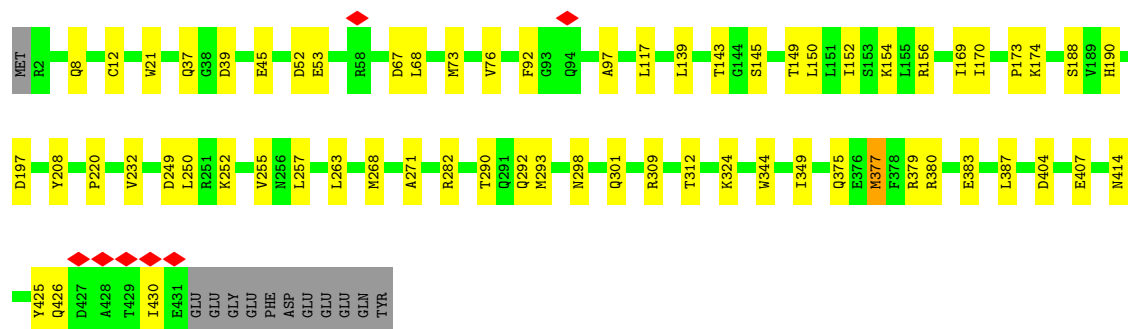
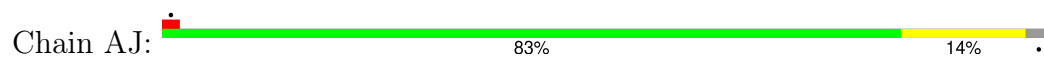
Chain AH:  86% 11%



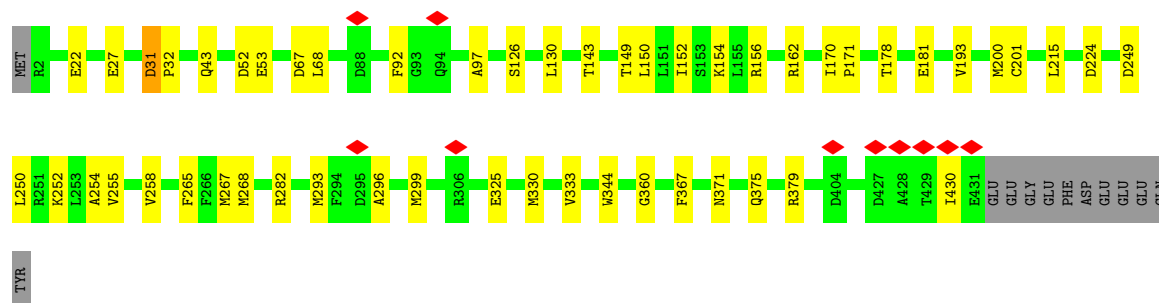




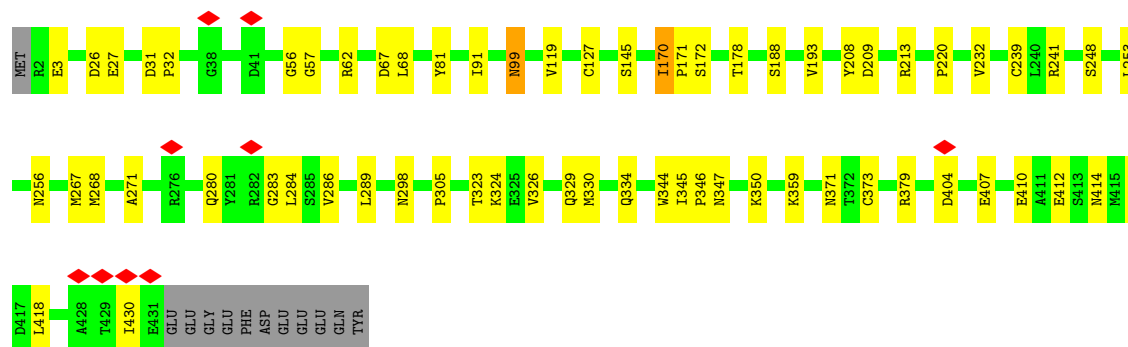
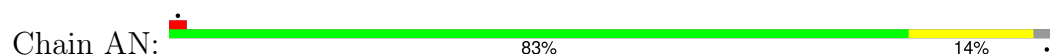
- Molecule 60: Tubulin beta chain



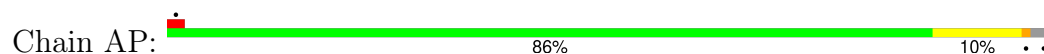
- Molecule 60: Tubulin beta chain

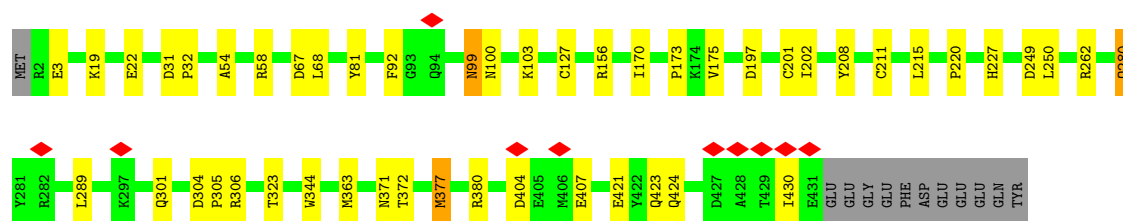


- Molecule 60: Tubulin beta chain



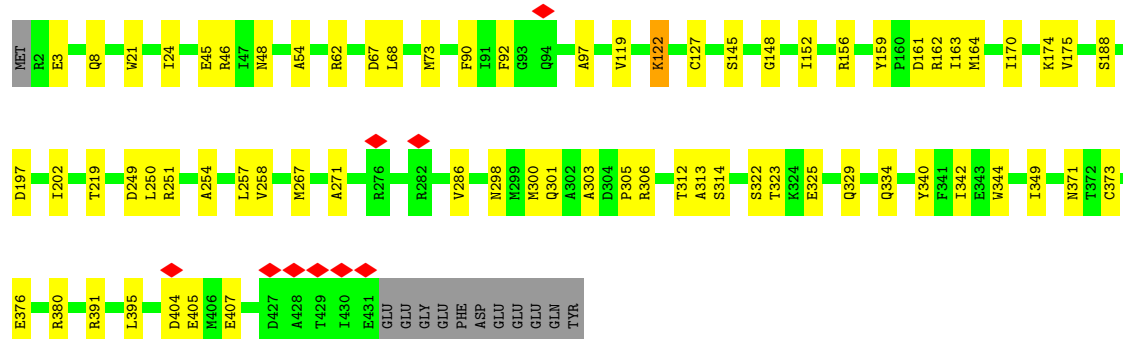
- Molecule 60: Tubulin beta chain





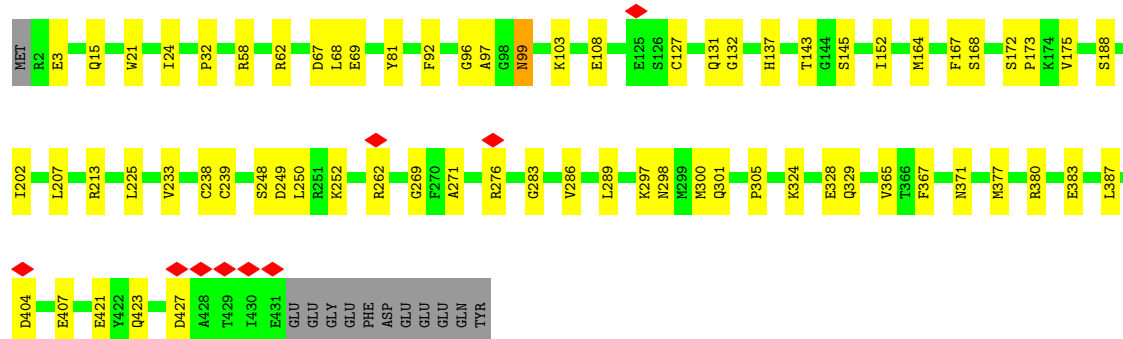
• Molecule 60: Tubulin beta chain

Chain AR: 81% 16%



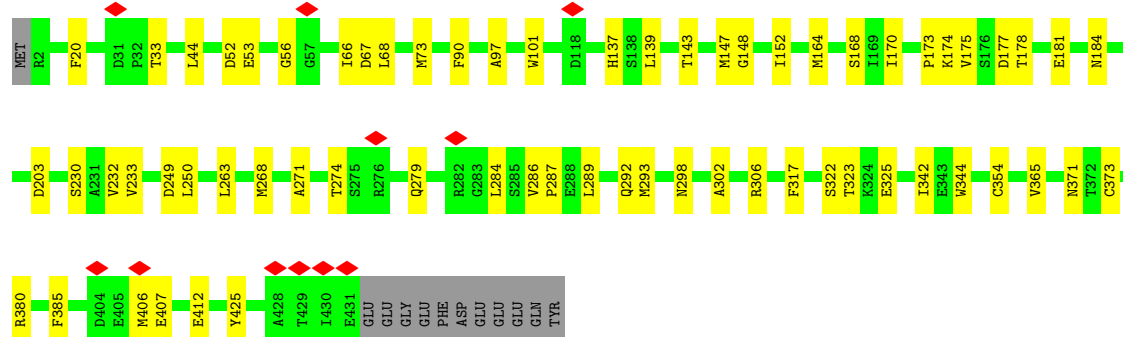
• Molecule 60: Tubulin beta chain

Chain AT: 82% 15%



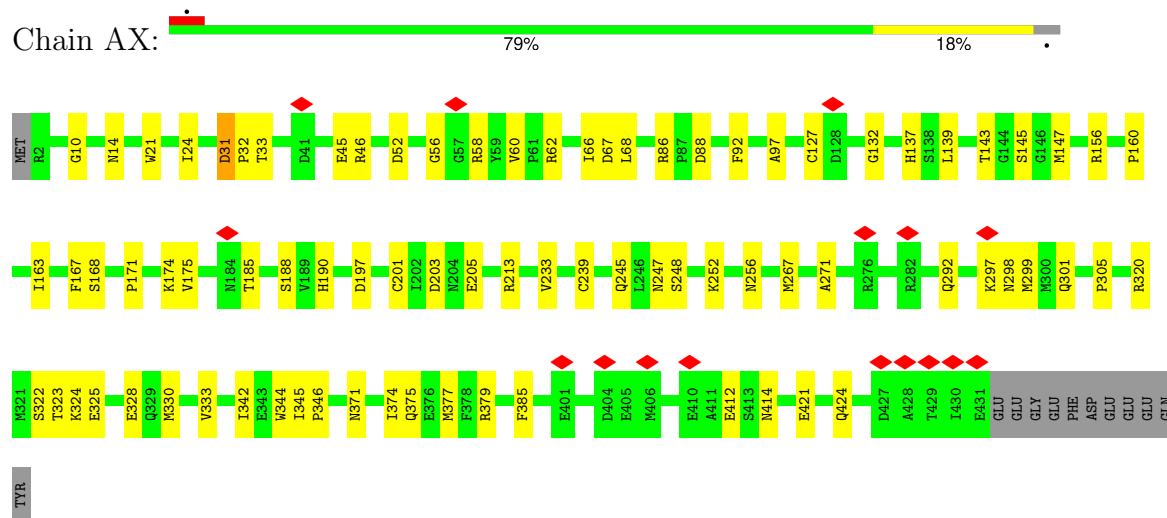
• Molecule 60: Tubulin beta chain

Chain AV: 82% 15%



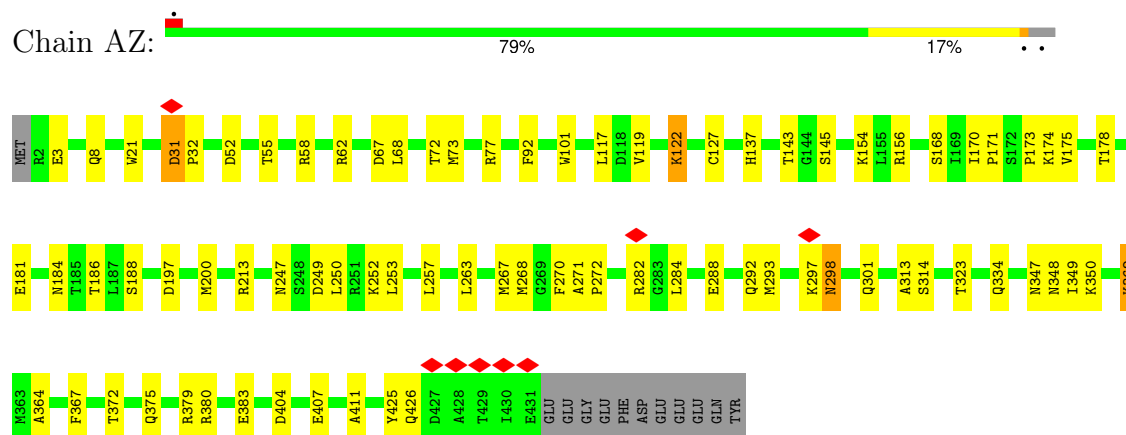
- Molecule 60: Tubulin beta chain

Chain AX:



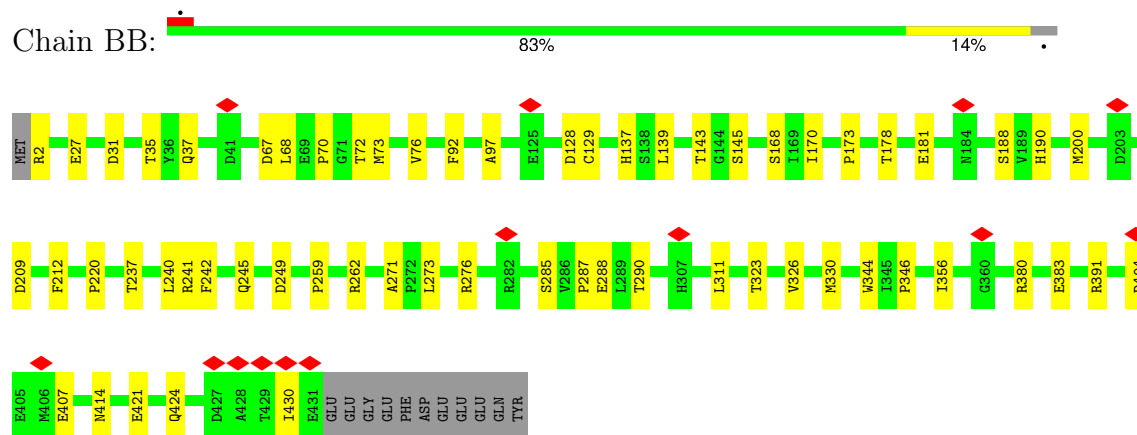
- Molecule 60: Tubulin beta chain

Chain AZ:



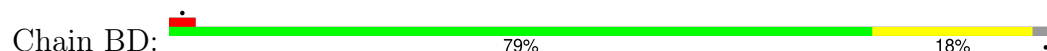
- Molecule 60: Tubulin beta chain

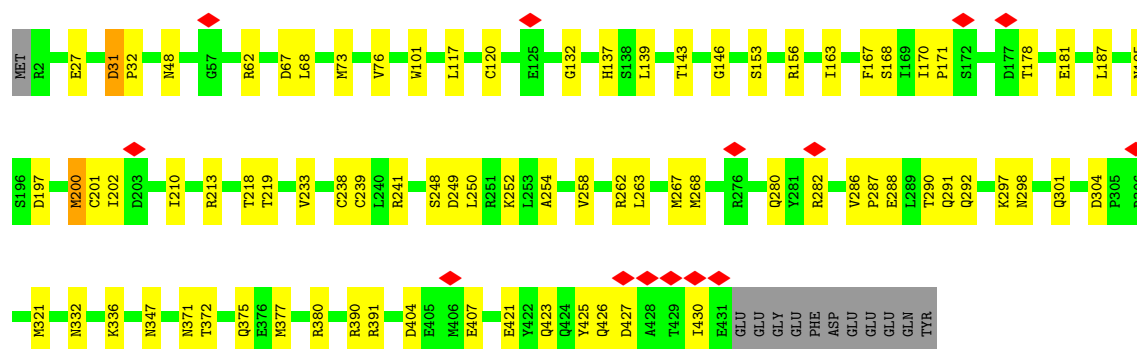
Chain BB:



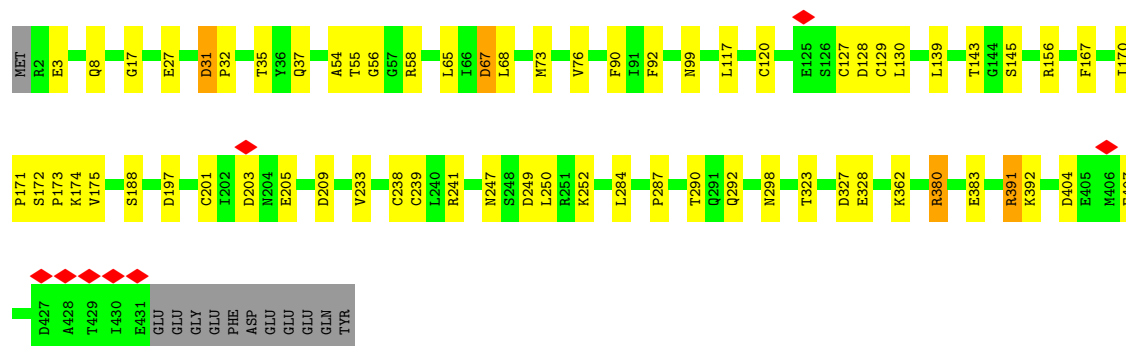
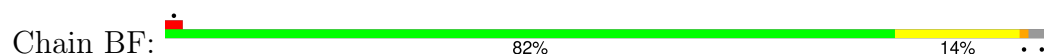
- Molecule 60: Tubulin beta chain

Chain BD:

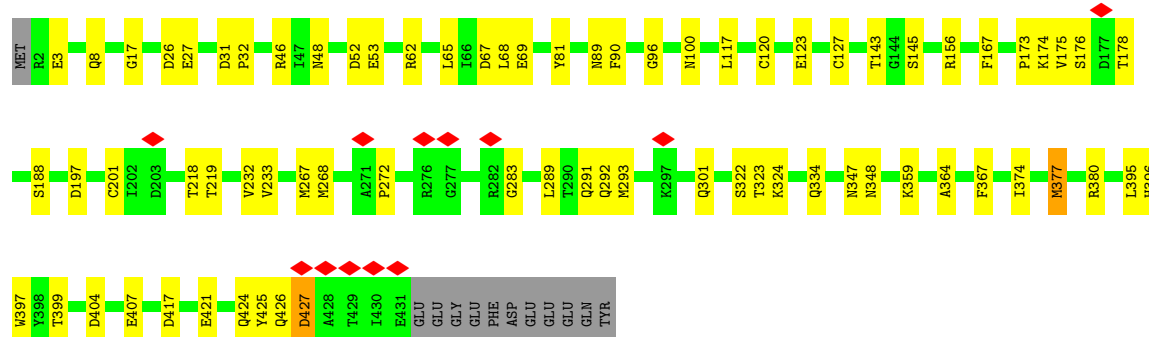
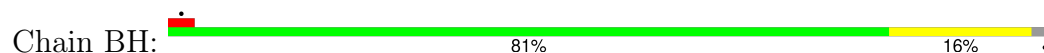




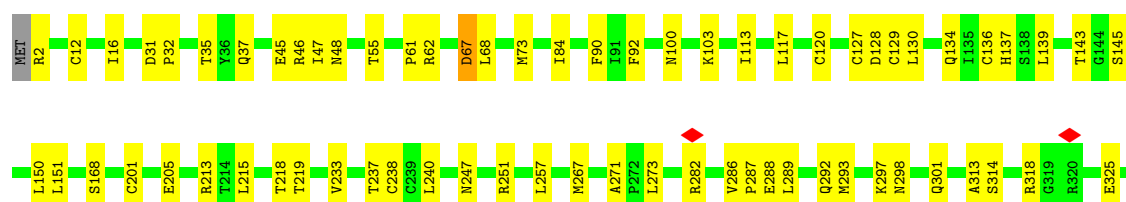
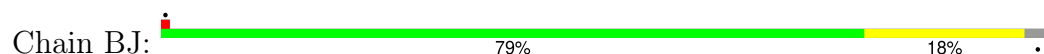
• Molecule 60: Tubulin beta chain



• Molecule 60: Tubulin beta chain

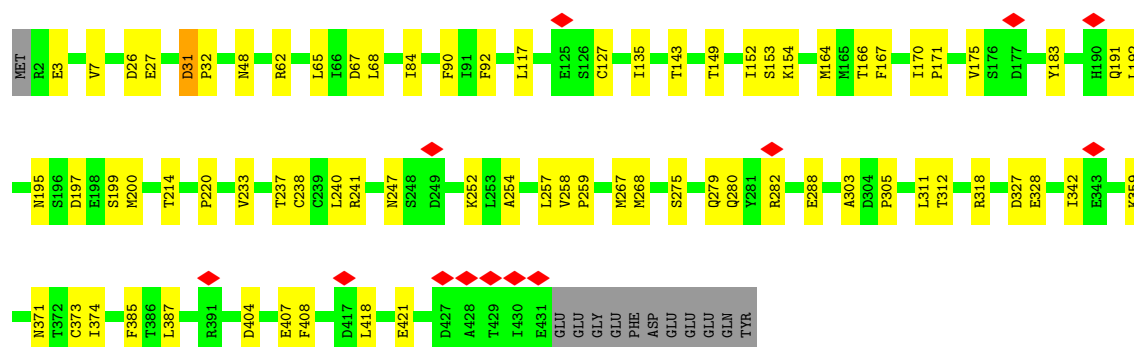
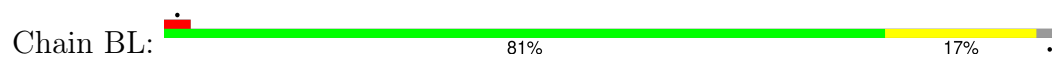


• Molecule 60: Tubulin beta chain

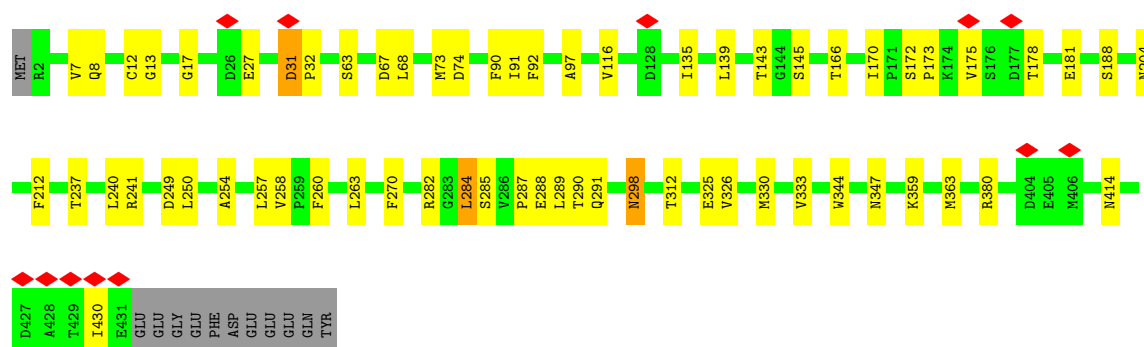
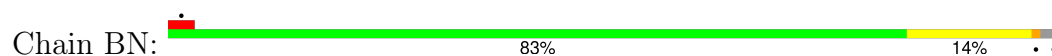




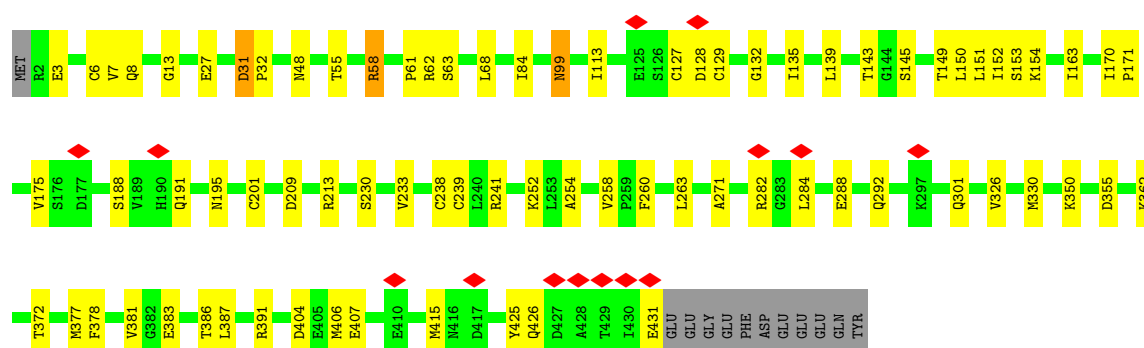
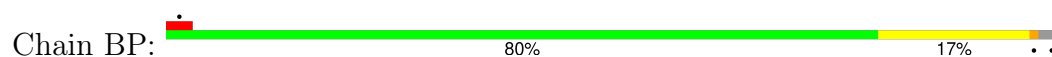
- Molecule 60: Tubulin beta chain




- Molecule 60: Tubulin beta chain

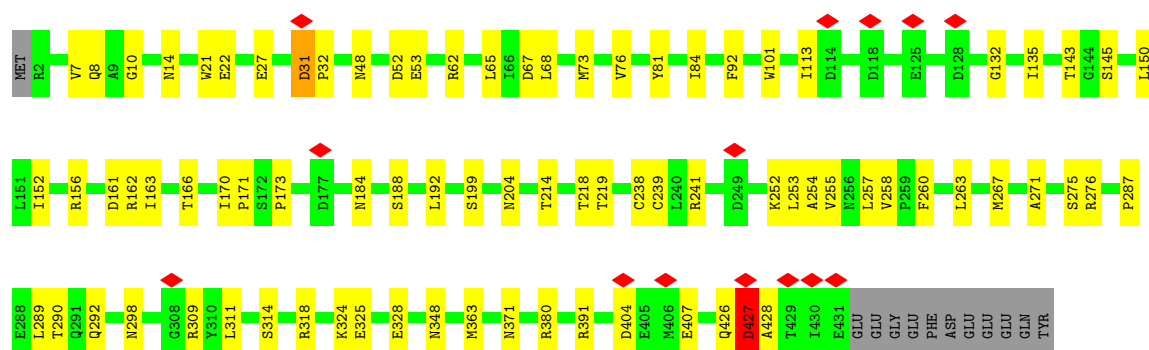


- Molecule 60: Tubulin beta chain




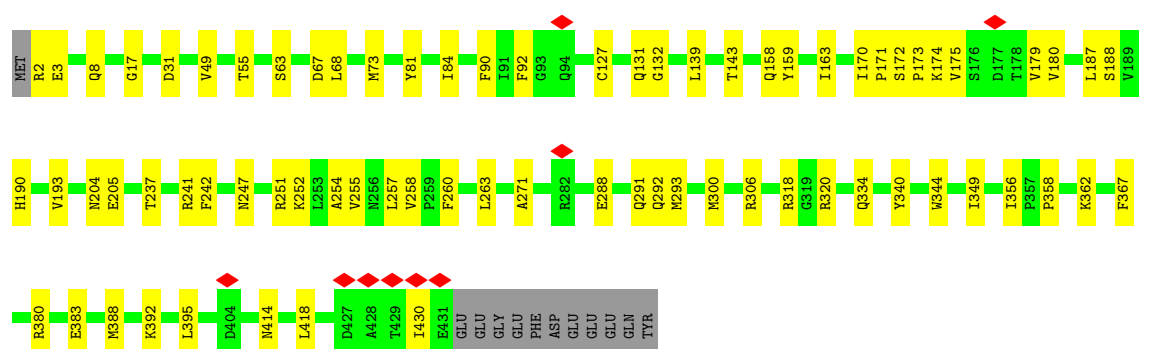
- Molecule 60: Tubulin beta chain

Chain BR: 




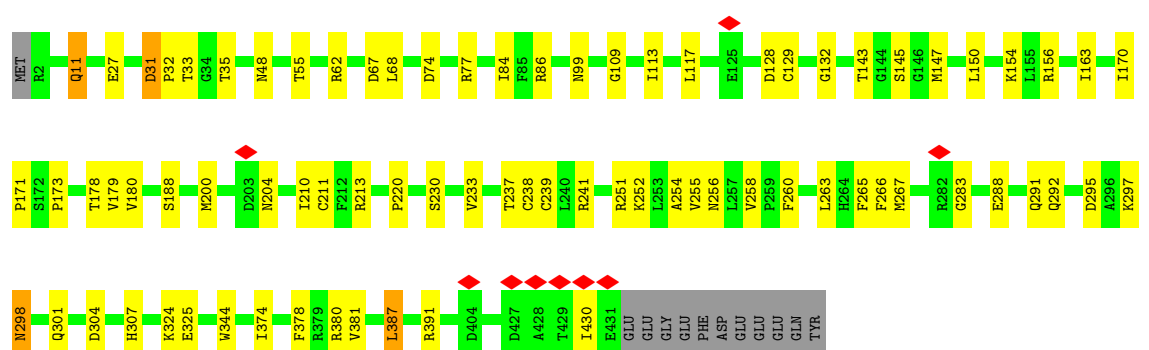
• Molecule 60: Tubulin beta chain

Chain BT: 




• Molecule 60: Tubulin beta chain

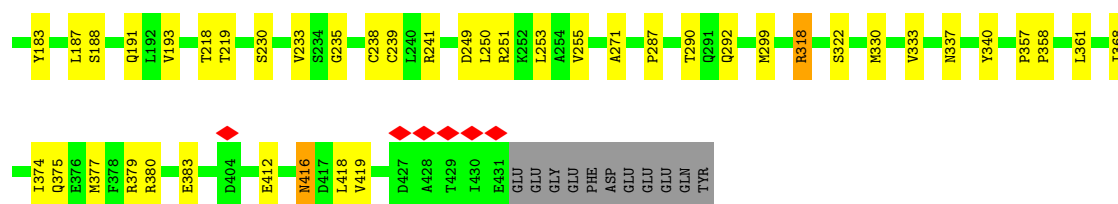
Chain BV: 



• Molecule 60: Tubulin beta chain

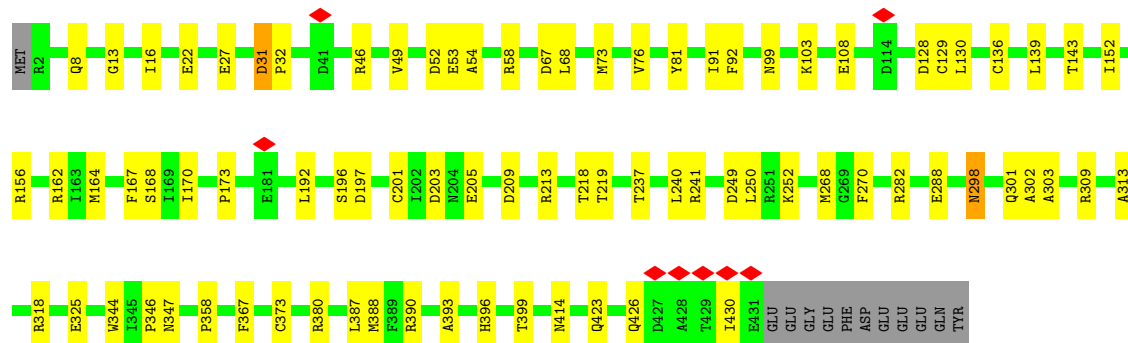
Chain BY: 





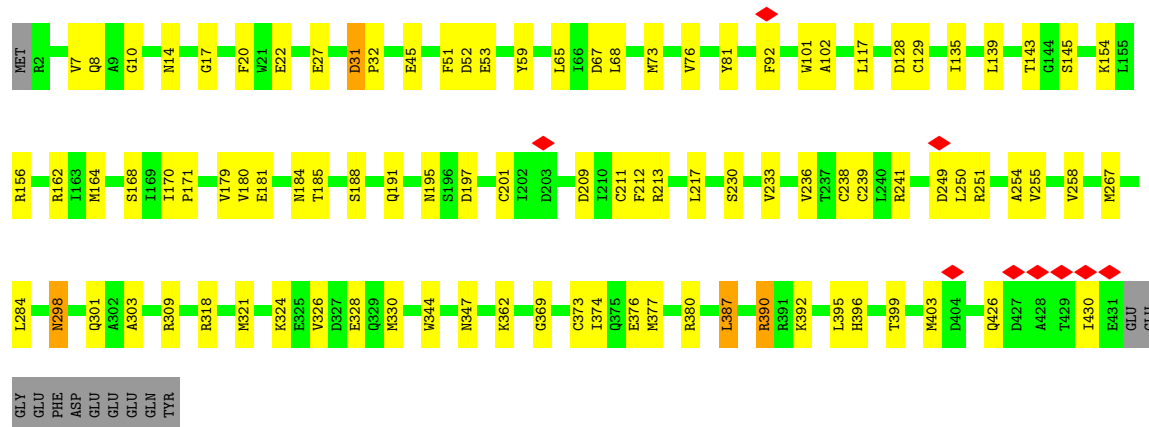
• Molecule 60: Tubulin beta chain

Chain CA: 79% 18%



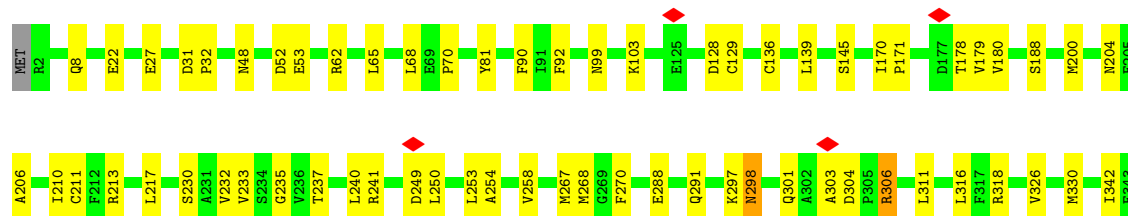
• Molecule 60: Tubulin beta chain

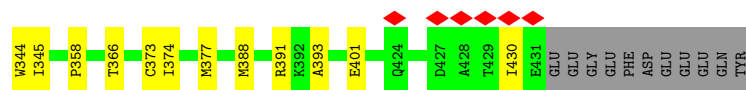
Chain CC: 76% 21%



• Molecule 60: Tubulin beta chain

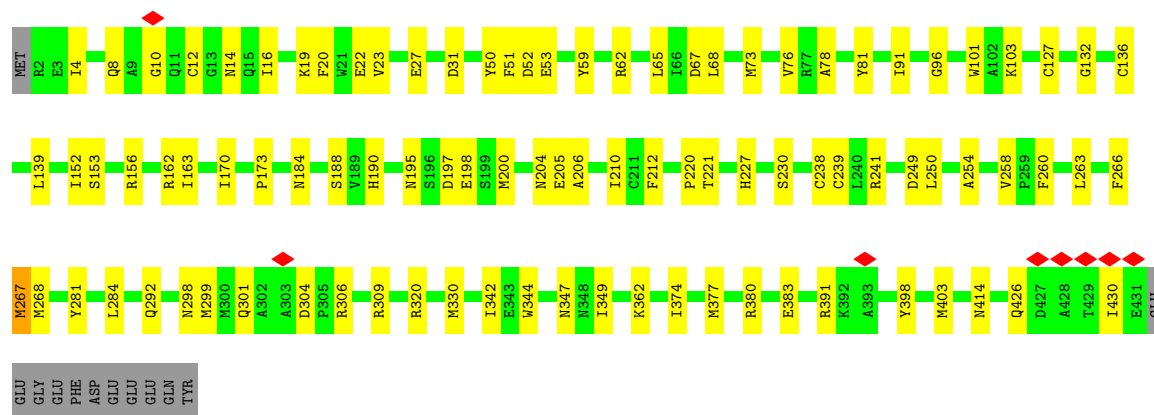
Chain CE: 80% 17%





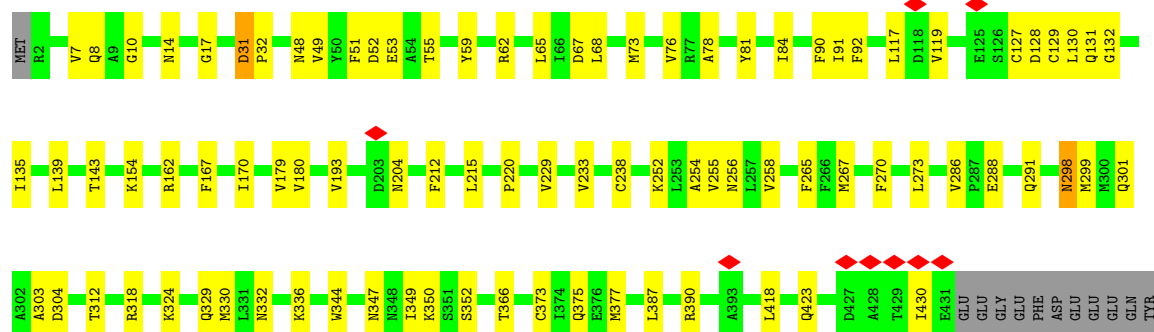
- Molecule 60: Tubulin beta chain

Chain CG: 76% 21%



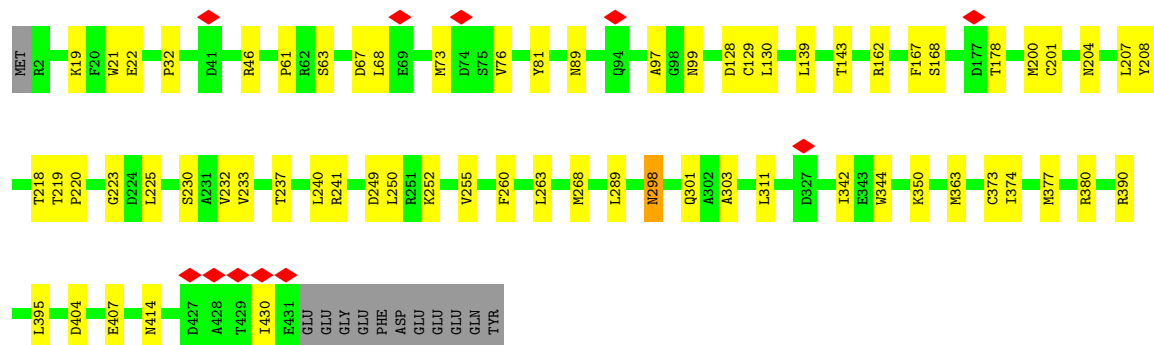
- Molecule 60: Tubulin beta chain

Chain CI: 77% 20%



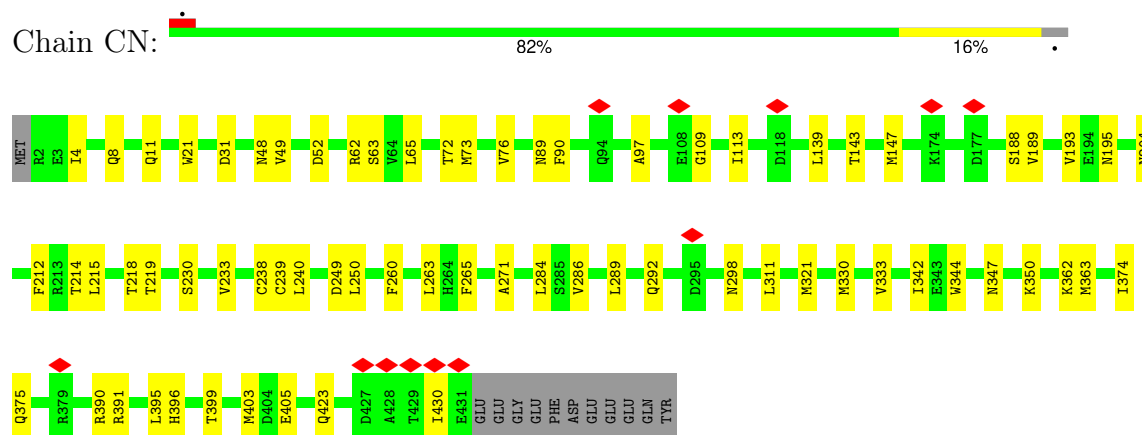
- Molecule 60: Tubulin beta chain

Chain CL: 82% 15%

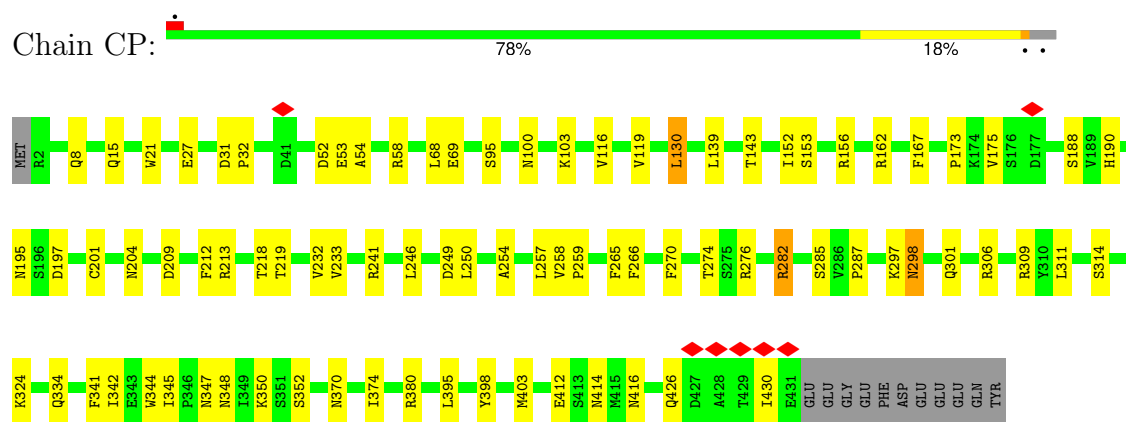


- Molecule 60: Tubulin beta chain

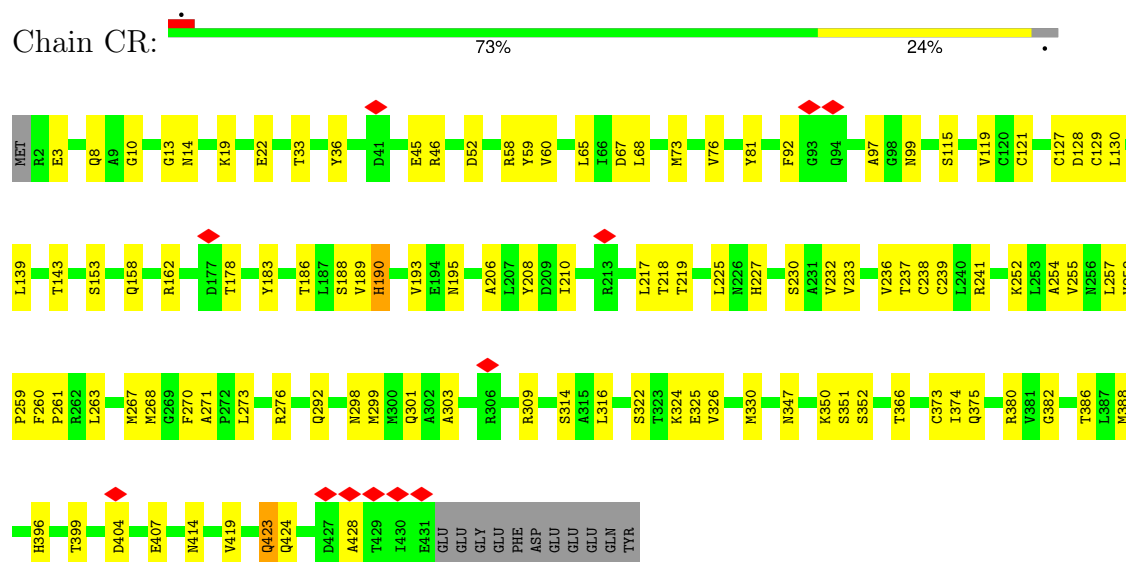




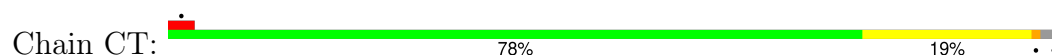
• Molecule 60: Tubulin beta chain

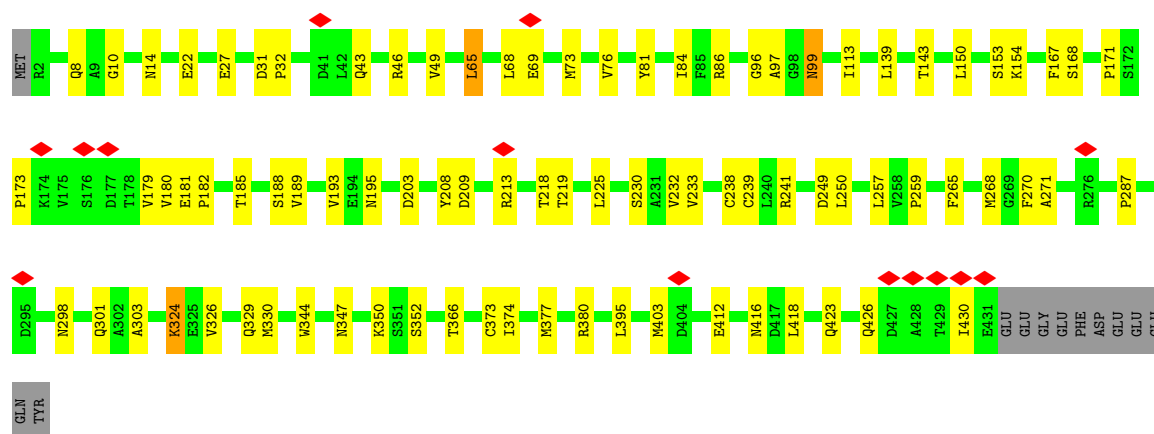


• Molecule 60: Tubulin beta chain

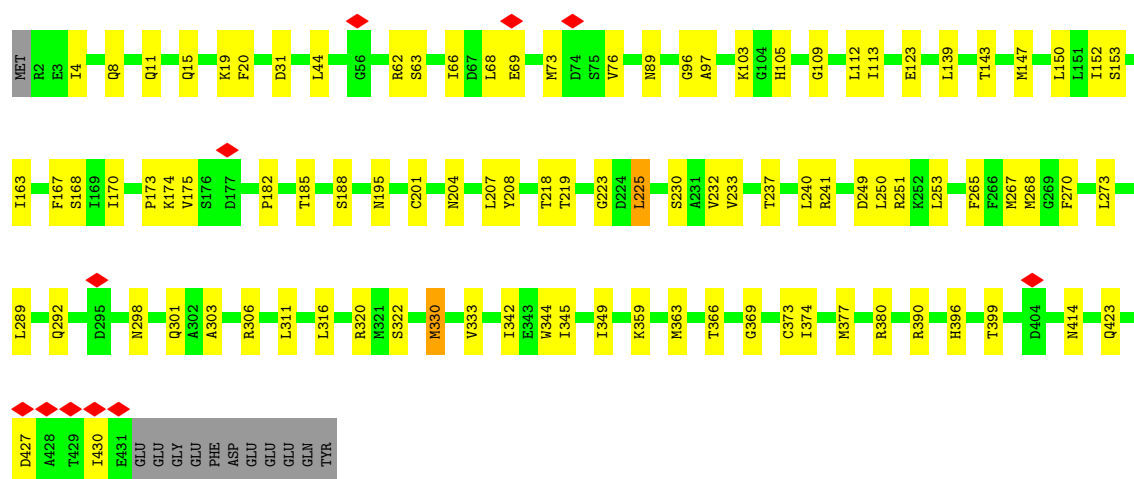
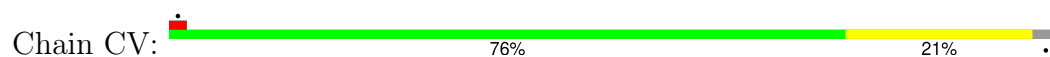


• Molecule 60: Tubulin beta chain

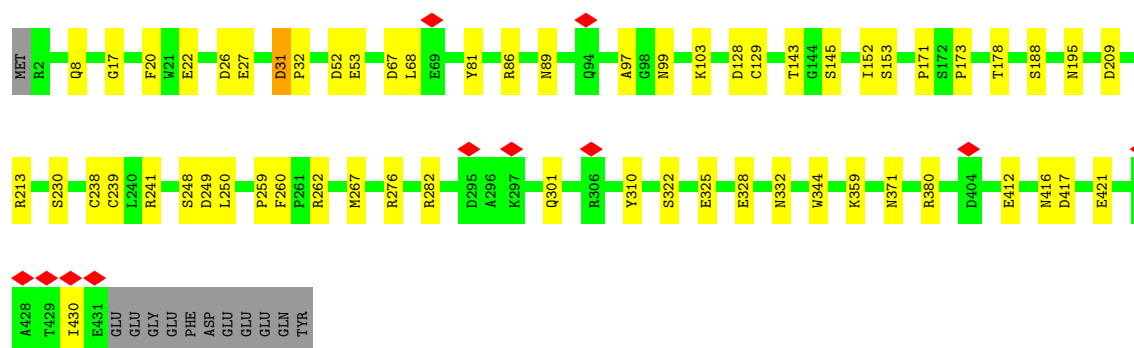
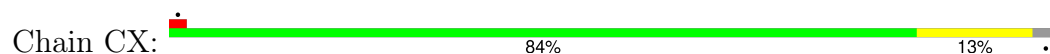




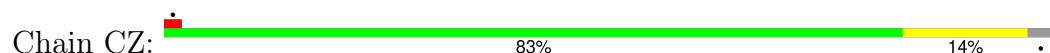
• Molecule 60: Tubulin beta chain

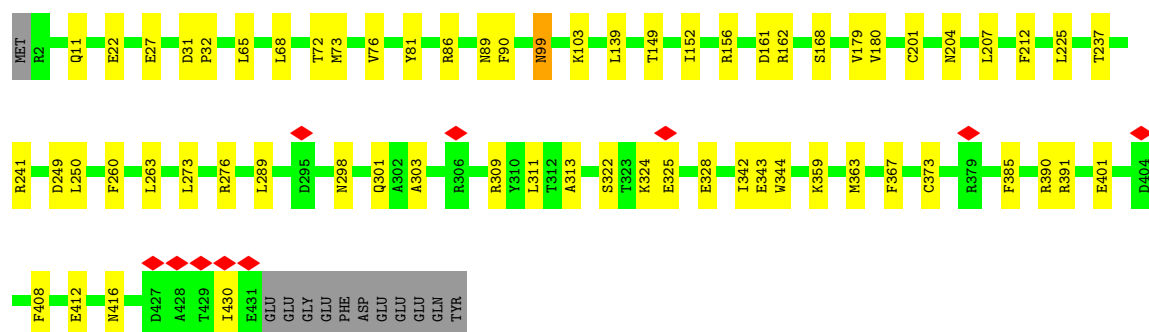


• Molecule 60: Tubulin beta chain

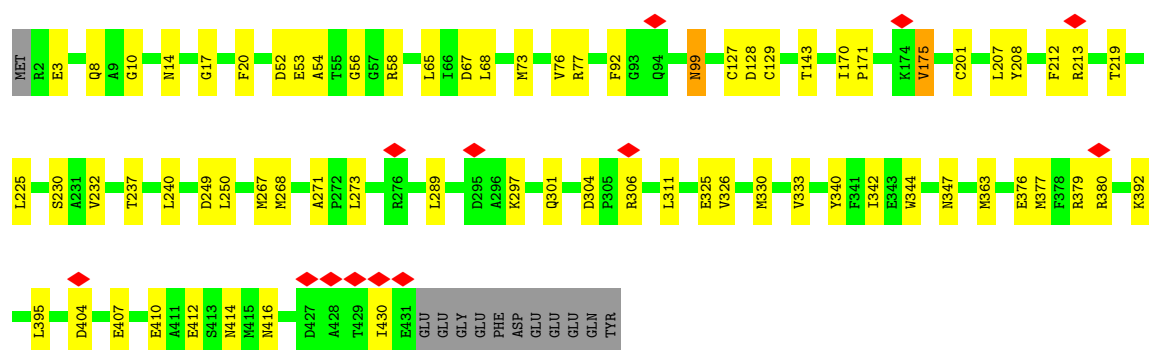
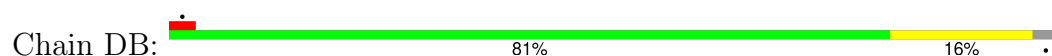


• Molecule 60: Tubulin beta chain

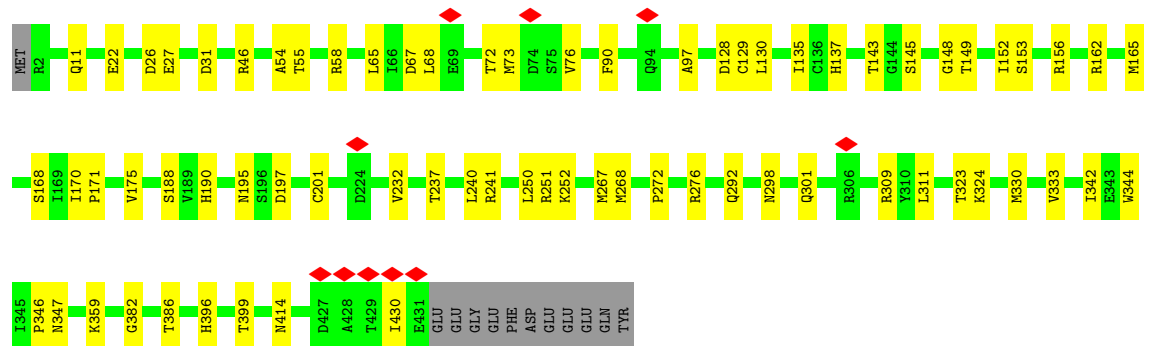
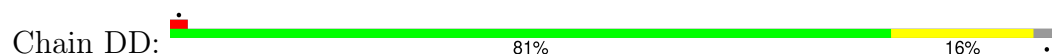




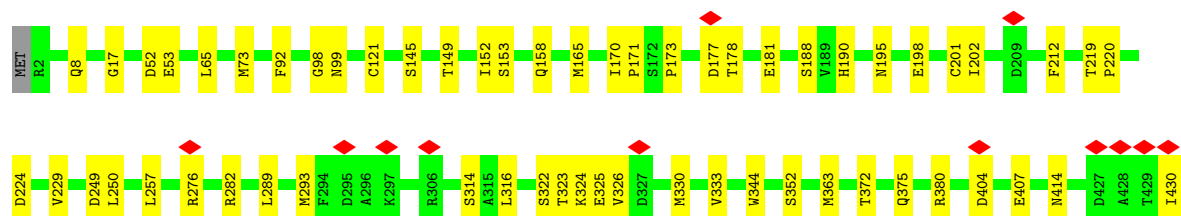
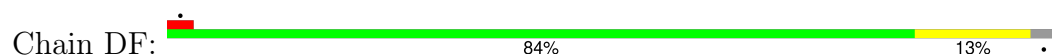
• Molecule 60: Tubulin beta chain

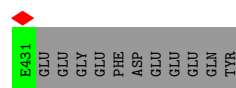


• Molecule 60: Tubulin beta chain

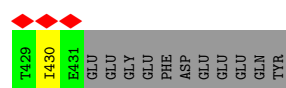
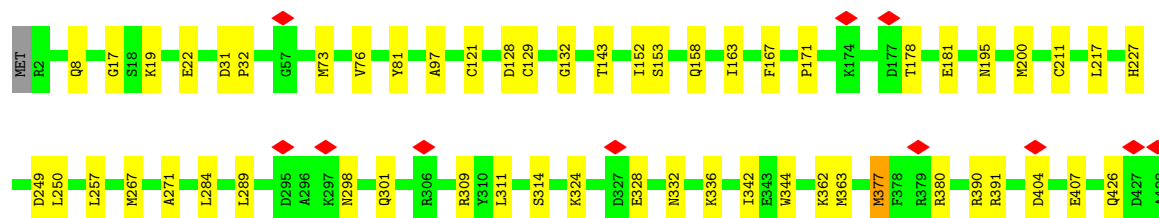
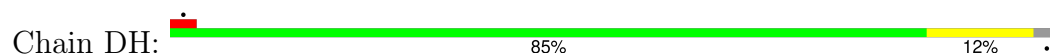


• Molecule 60: Tubulin beta chain

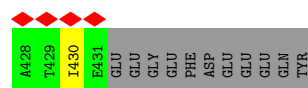
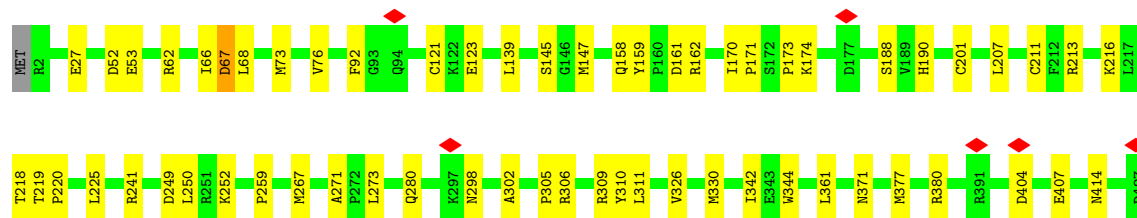
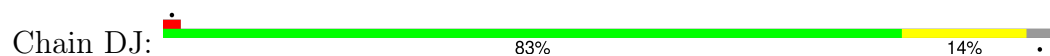




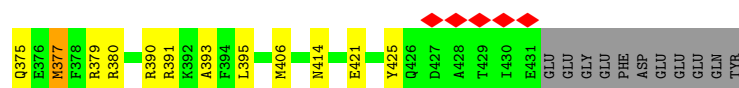
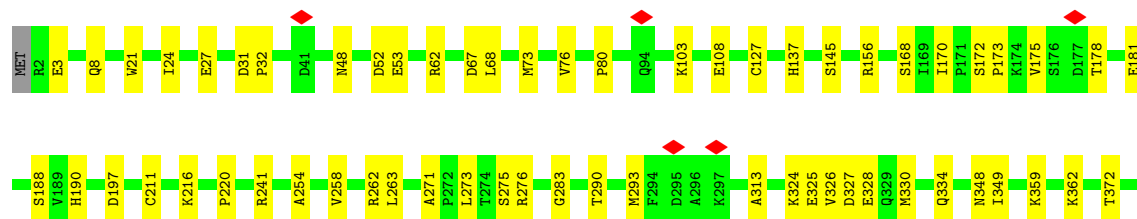
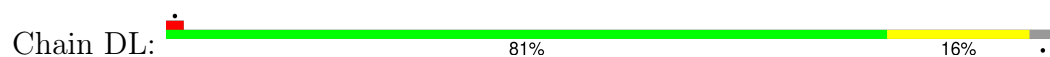
- Molecule 60: Tubulin beta chain




- Molecule 60: Tubulin beta chain

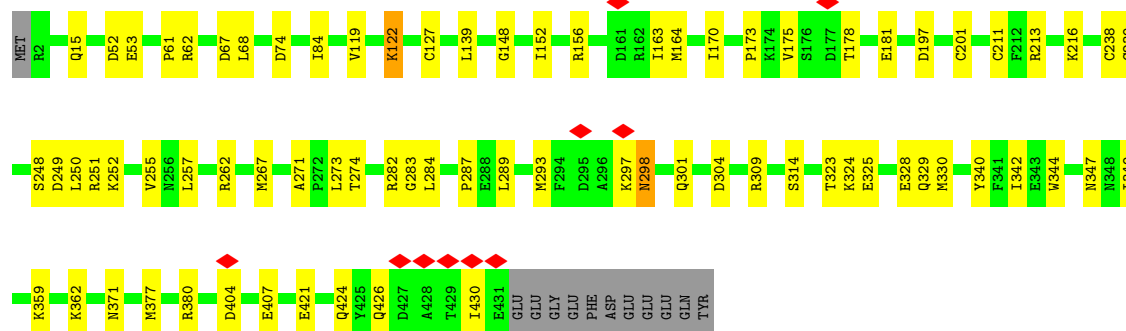


- Molecule 60: Tubulin beta chain




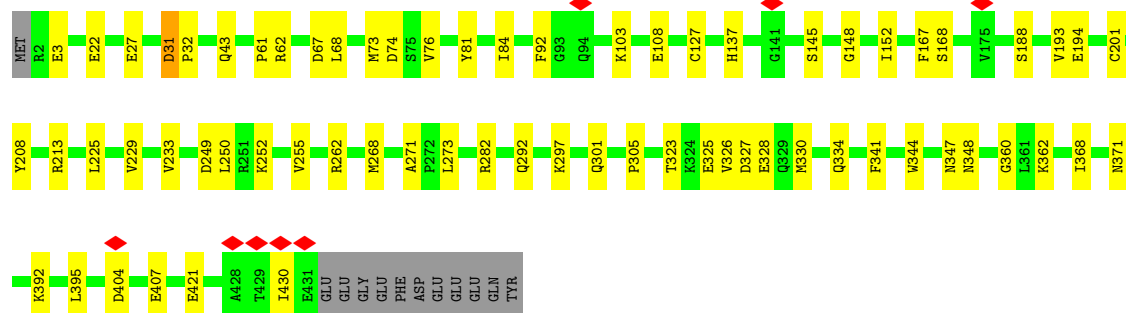
- Molecule 60: Tubulin beta chain

Chain DN: 




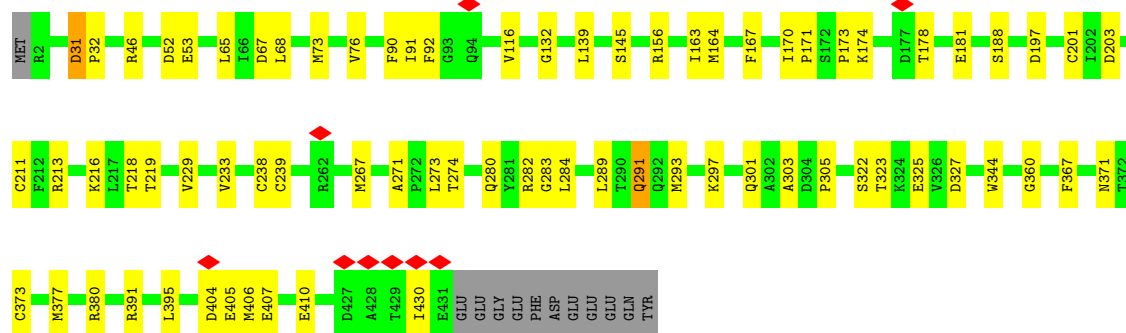
• Molecule 60: Tubulin beta chain

Chain DP: 




• Molecule 60: Tubulin beta chain

Chain DR: 



• Molecule 60: Tubulin beta chain

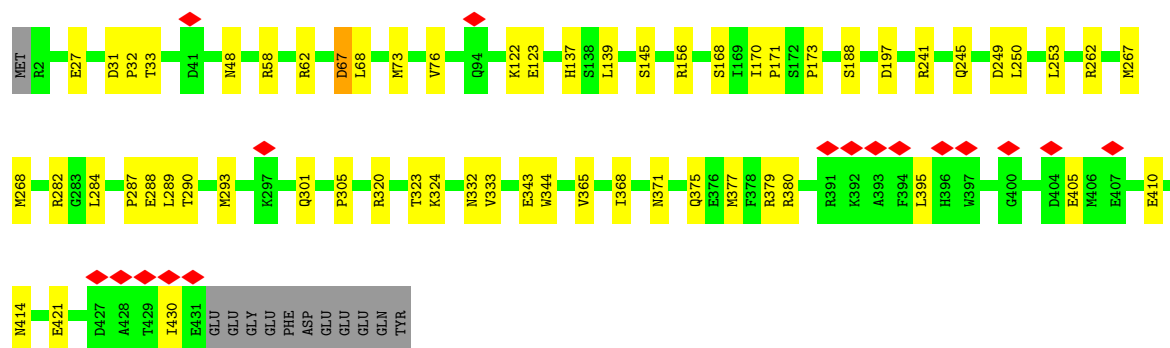
Chain DT: 





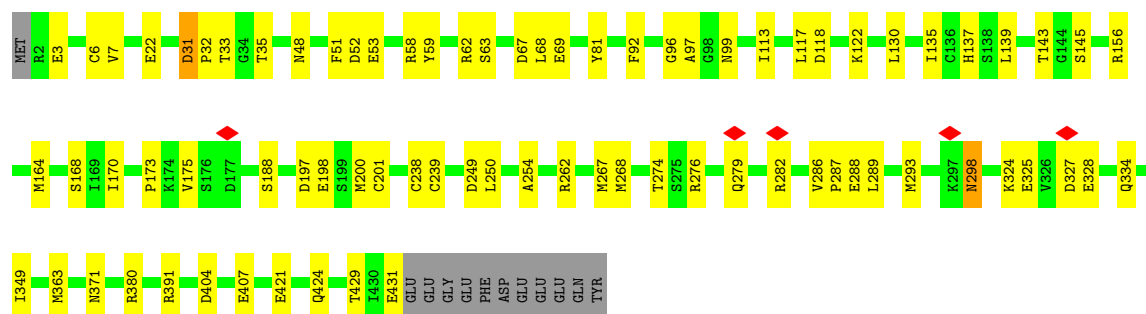
- Molecule 60: Tubulin beta chain

Chain DV: 84% 13%



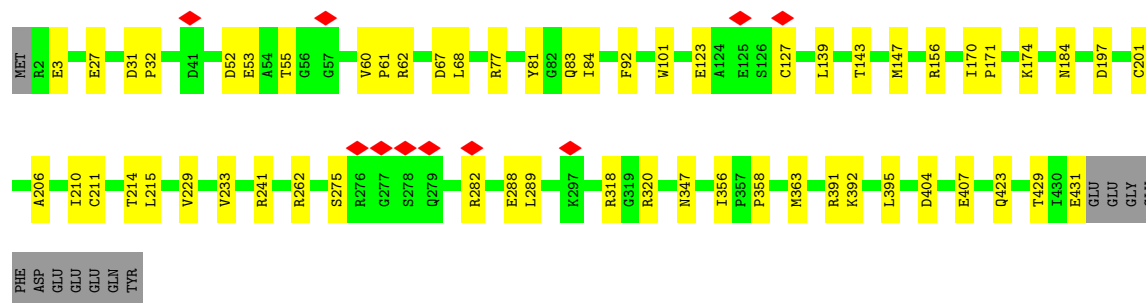
- Molecule 60: Tubulin beta chain

Chain DW: 79% 17%




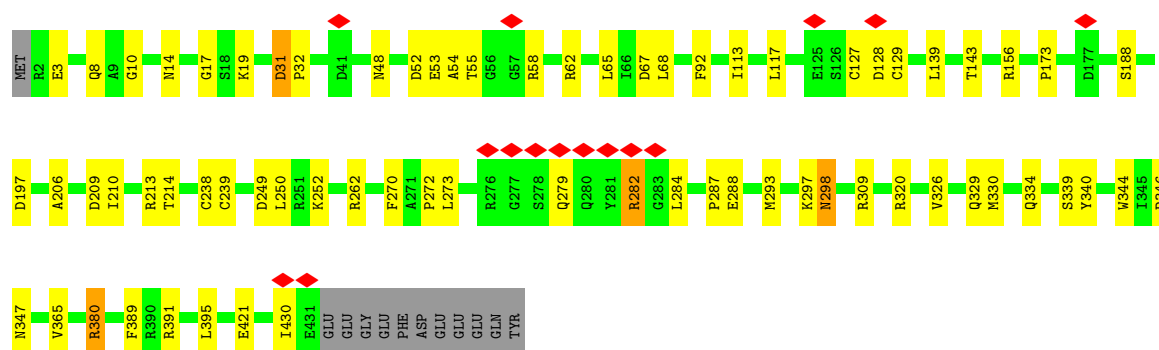
- Molecule 60: Tubulin beta chain

Chain DY: 84% 13%




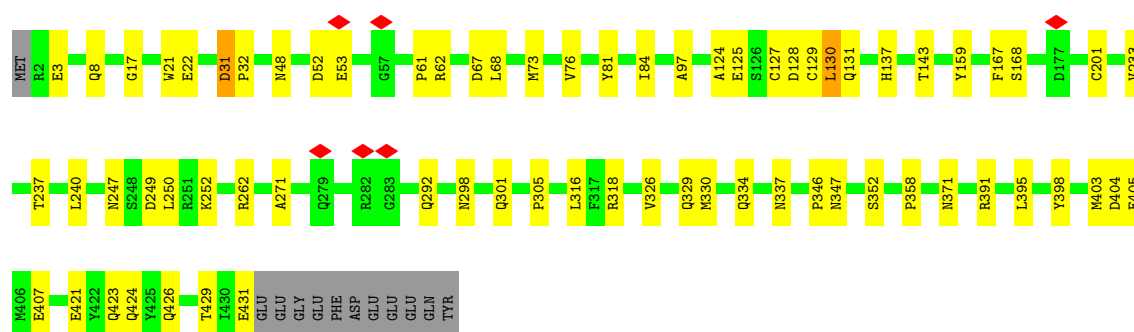
- Molecule 60: Tubulin beta chain

Chain EA:  81% 15%




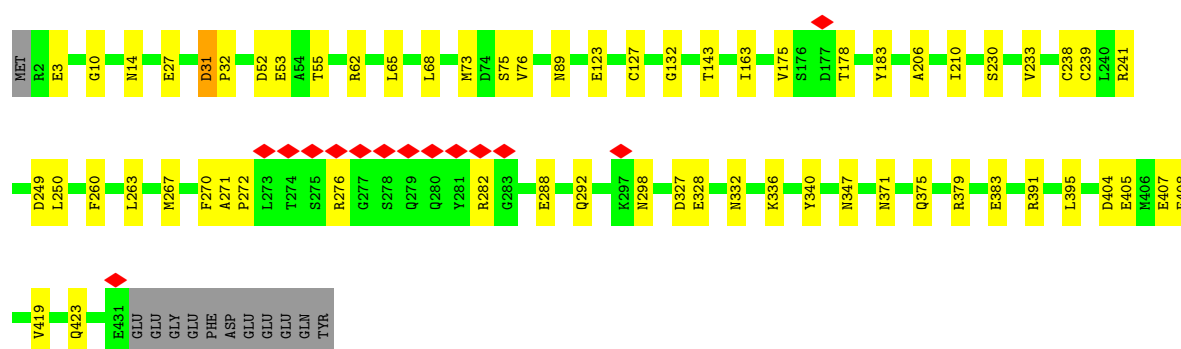
• Molecule 60: Tubulin beta chain

Chain EC:  81% 15%




• Molecule 60: Tubulin beta chain

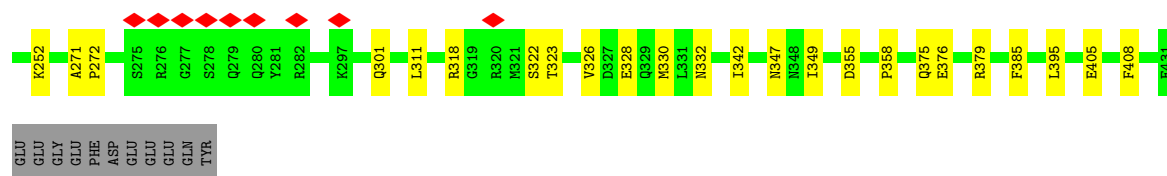
Chain EE:  83% 14%



• Molecule 60: Tubulin beta chain

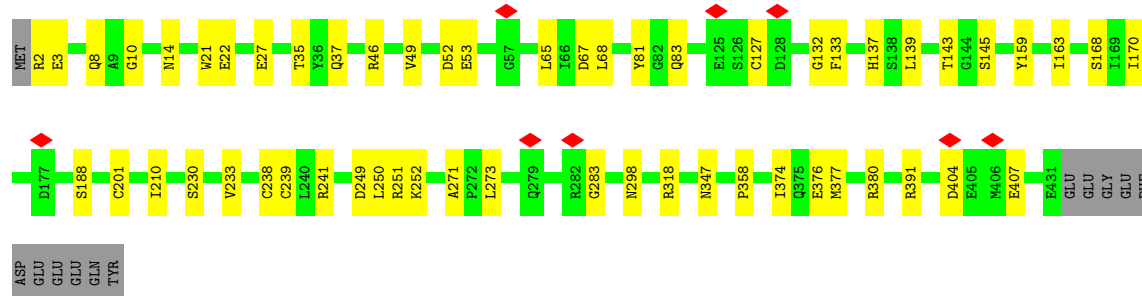
Chain EG:  85% 12%





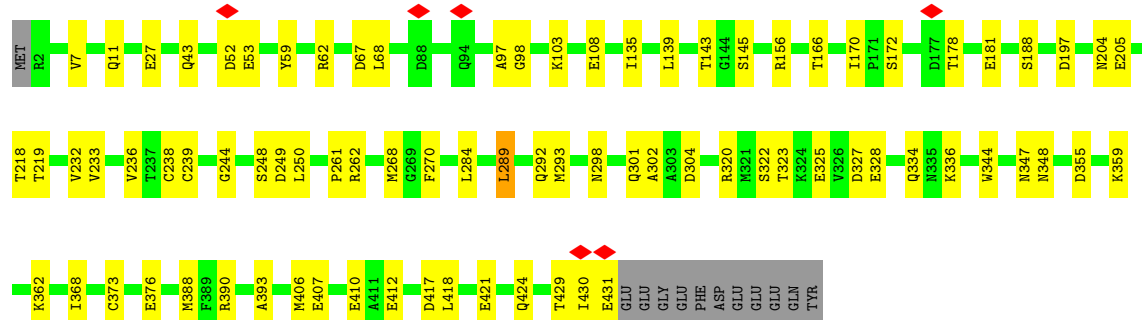
- Molecule 60: Tubulin beta chain

Chain EI: 85% 13%



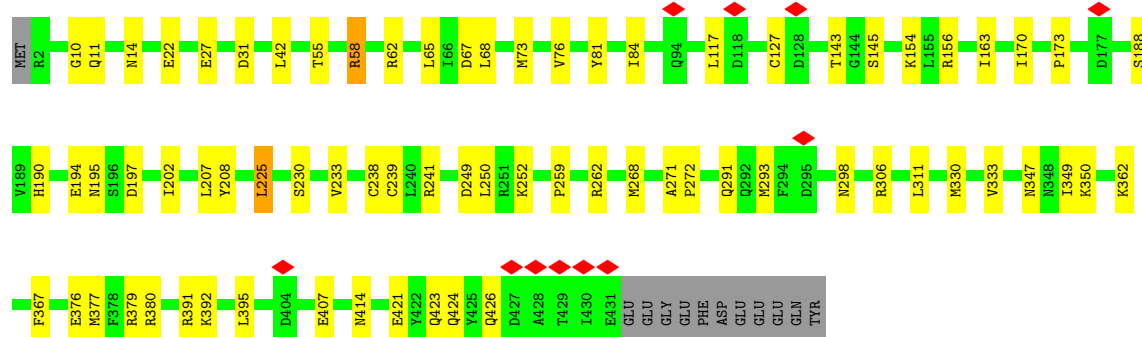
- Molecule 60: Tubulin beta chain

Chain EK: 79% 18%



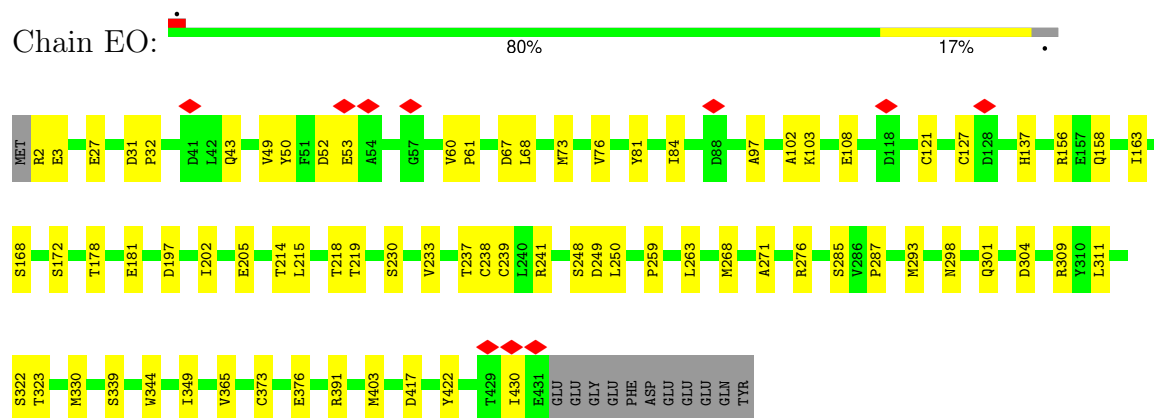
- Molecule 60: Tubulin beta chain

Chain EM: 81% 16%

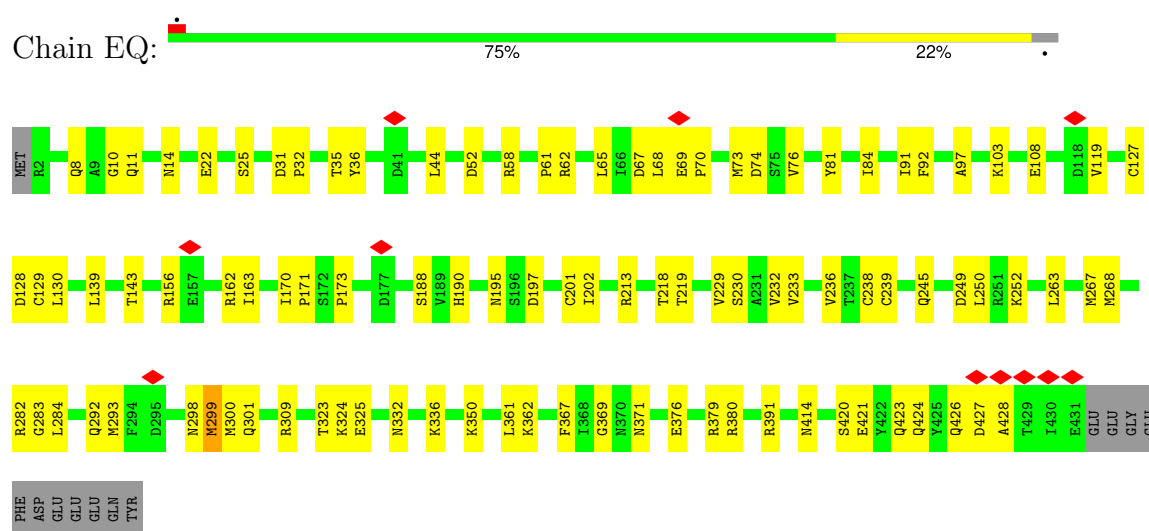


- Molecule 60: Tubulin beta chain

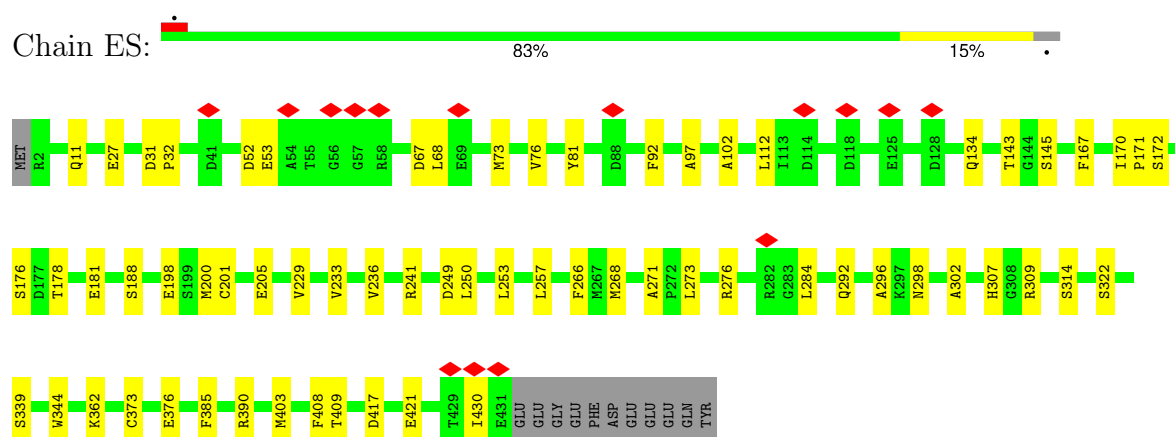




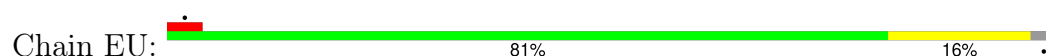
• Molecule 60: Tubulin beta chain

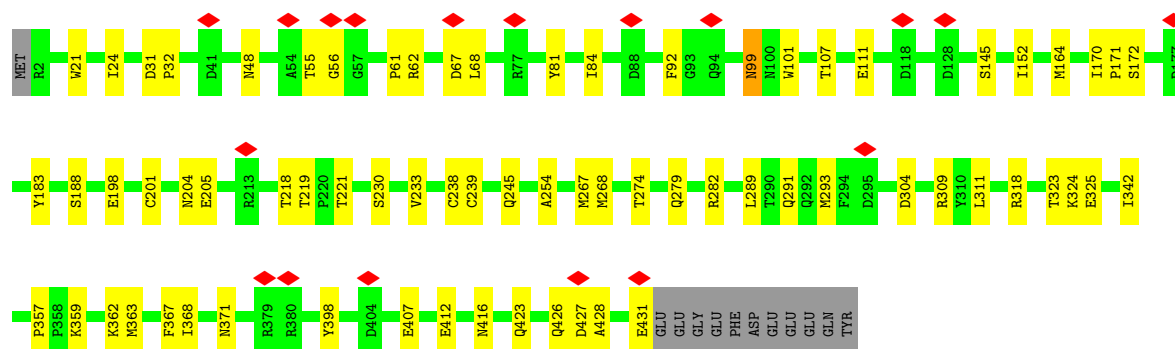


• Molecule 60: Tubulin beta chain



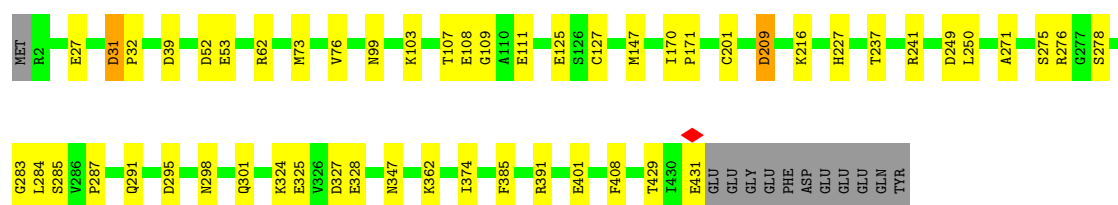
• Molecule 60: Tubulin beta chain





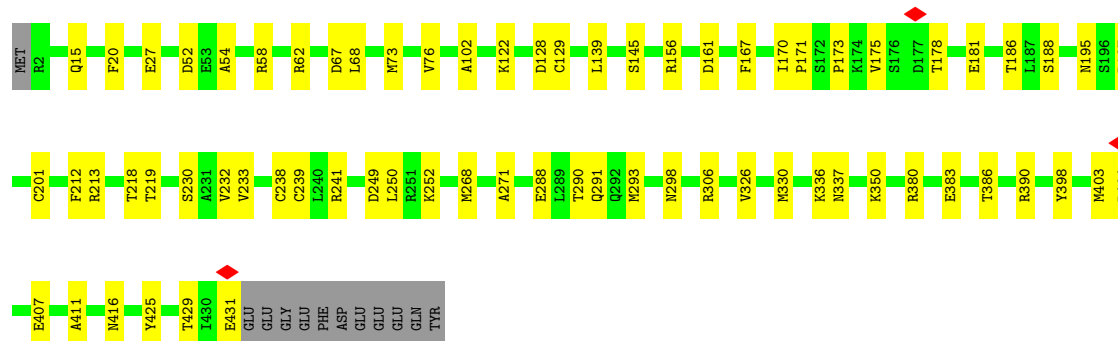
- Molecule 60: Tubulin beta chain

Chain EW: 85% 12% .



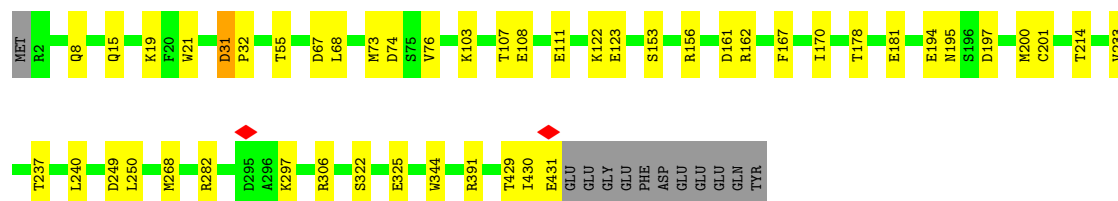
- Molecule 60: Tubulin beta chain

Chain EY: 81% 16% .



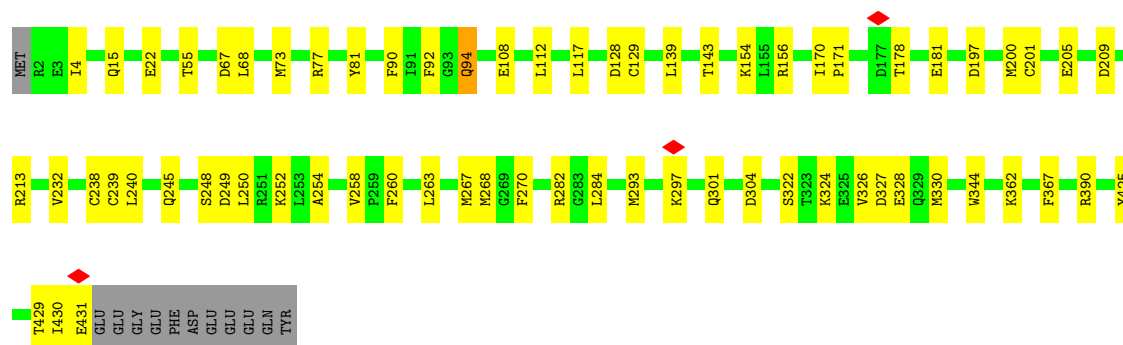
- Molecule 60: Tubulin beta chain

Chain FA: 86% 11% .



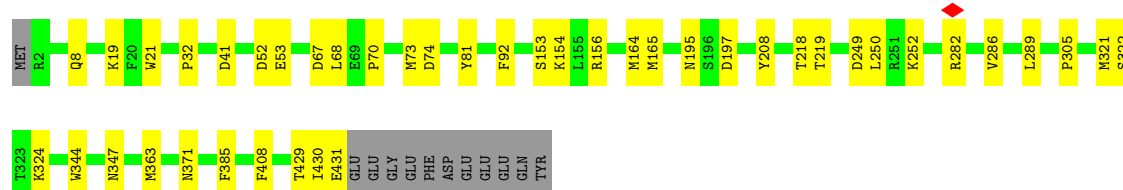
- Molecule 60: Tubulin beta chain

Chain FC: 82% 15% .



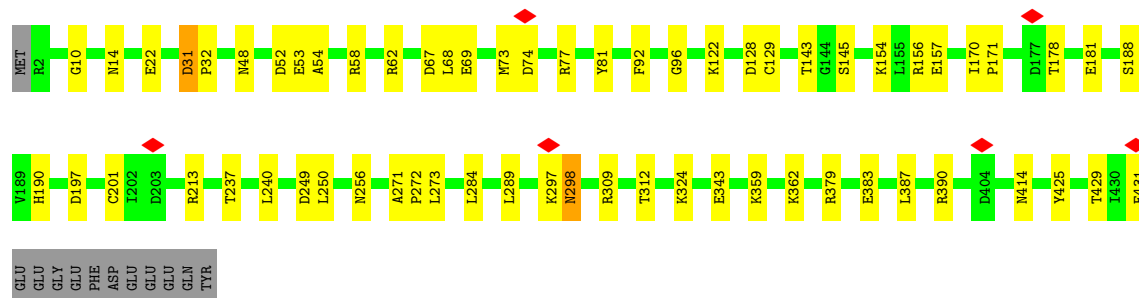
- Molecule 60: Tubulin beta chain

Chain FE: 88% 10% .



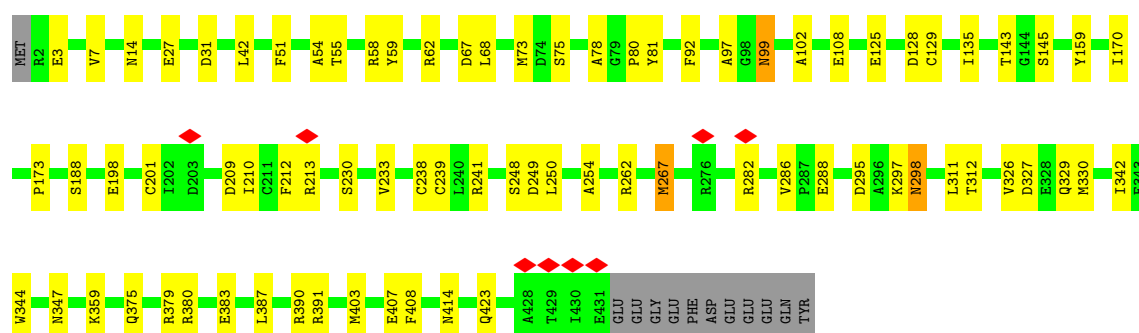
- Molecule 60: Tubulin beta chain

Chain FG: 83% 14% .

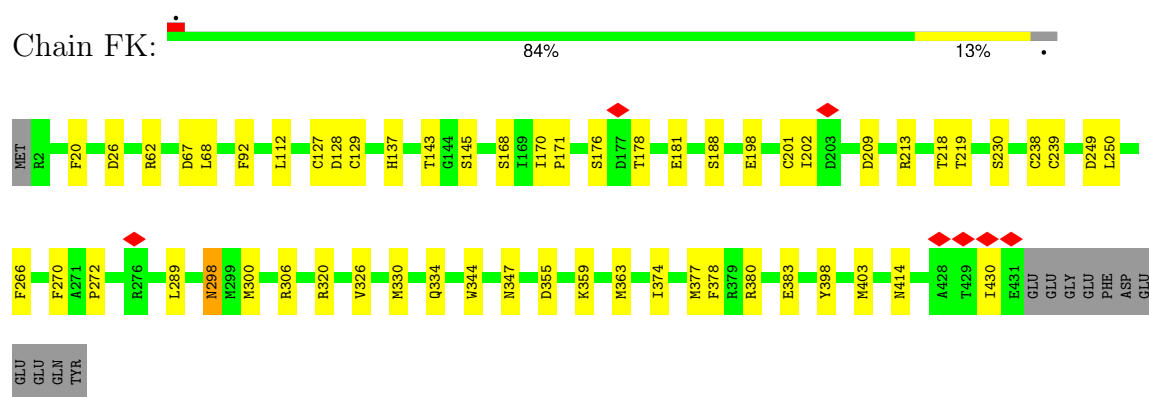


- Molecule 60: Tubulin beta chain

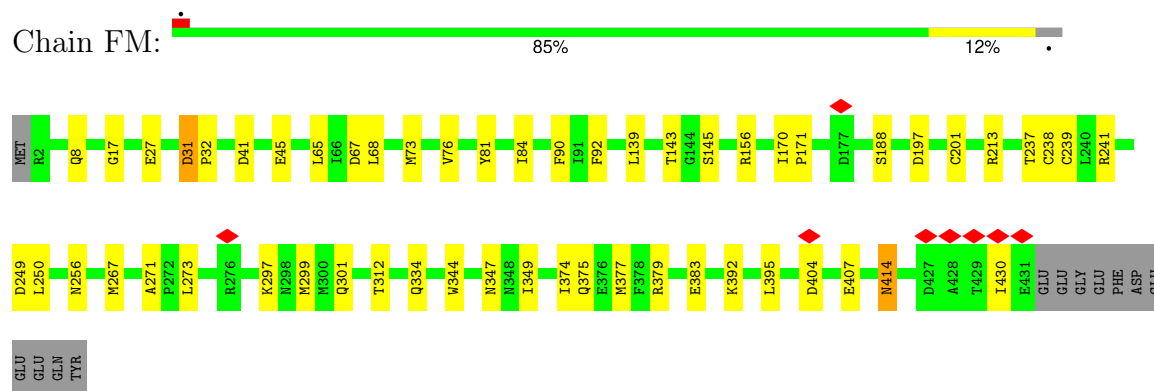
Chain FI: 79% 17% . .



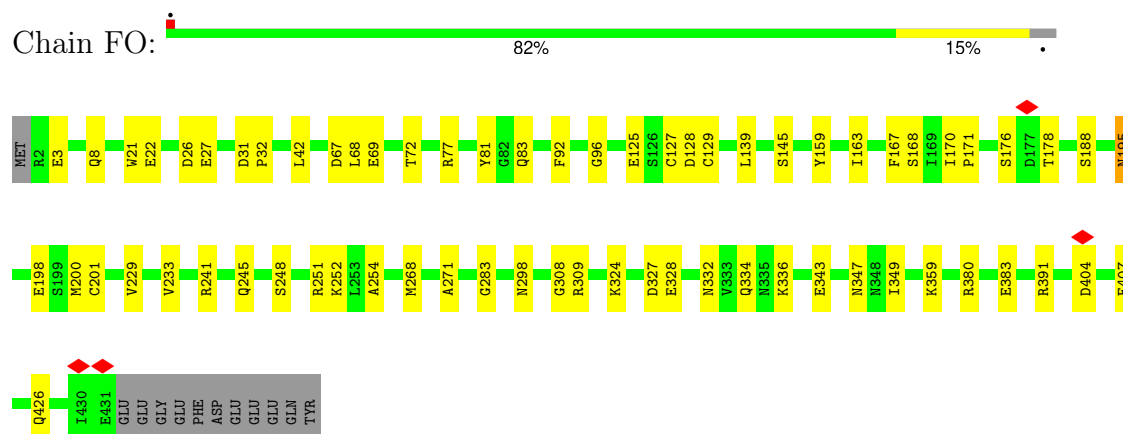
- Molecule 60: Tubulin beta chain



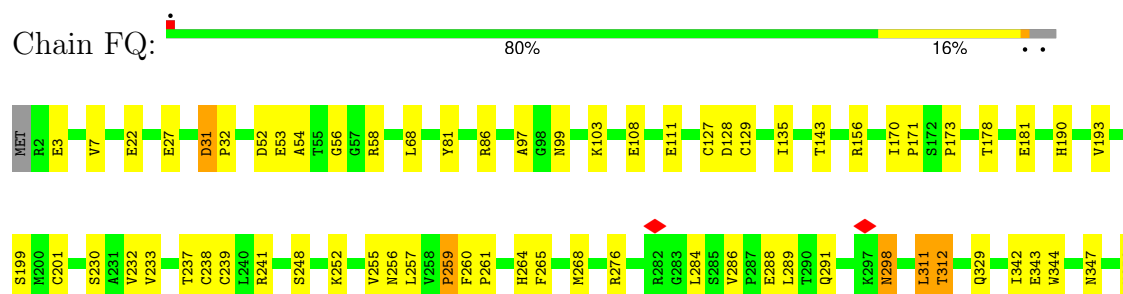
- Molecule 60: Tubulin beta chain



- Molecule 60: Tubulin beta chain

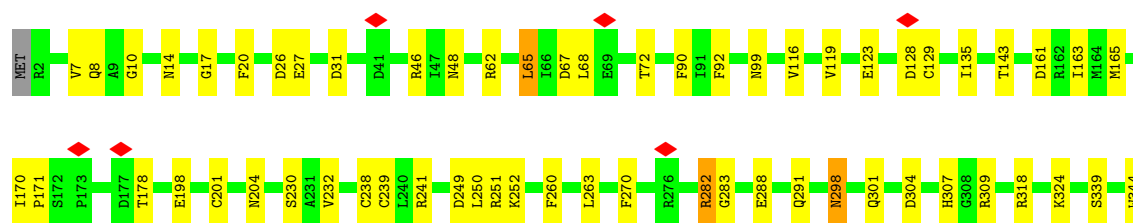
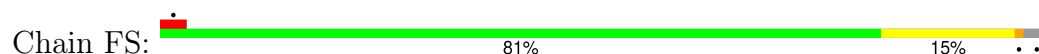


- Molecule 60: Tubulin beta chain

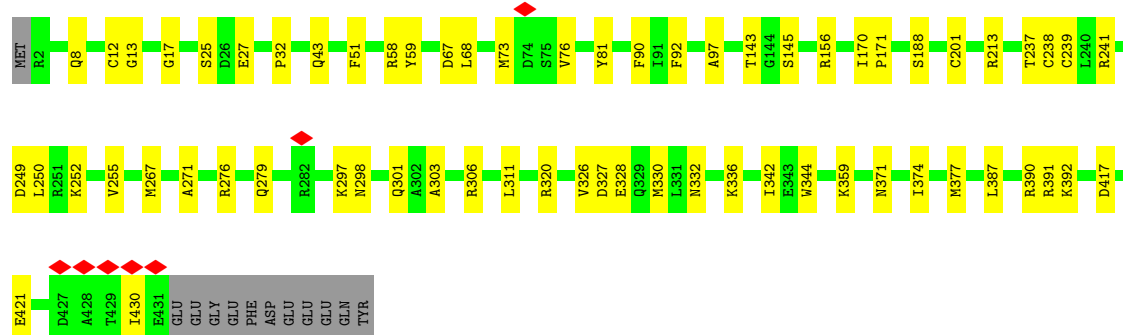
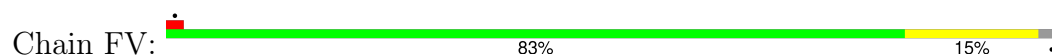




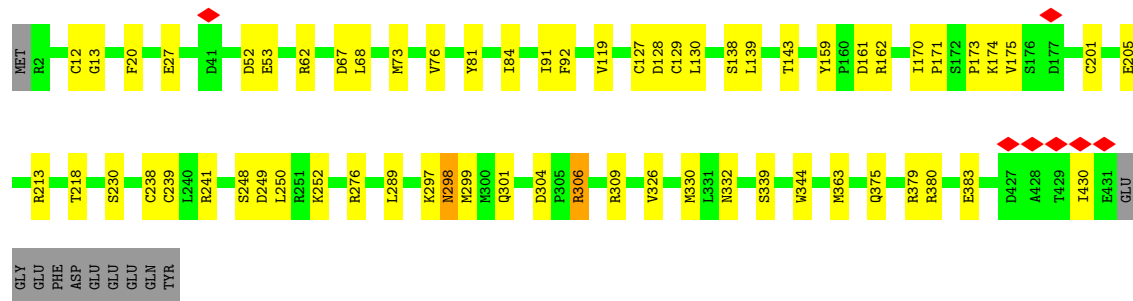
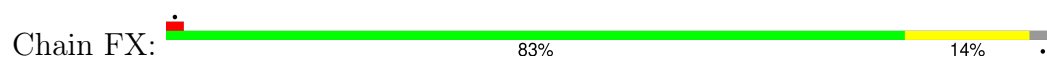
• Molecule 60: Tubulin beta chain



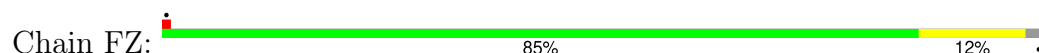
• Molecule 60: Tubulin beta chain

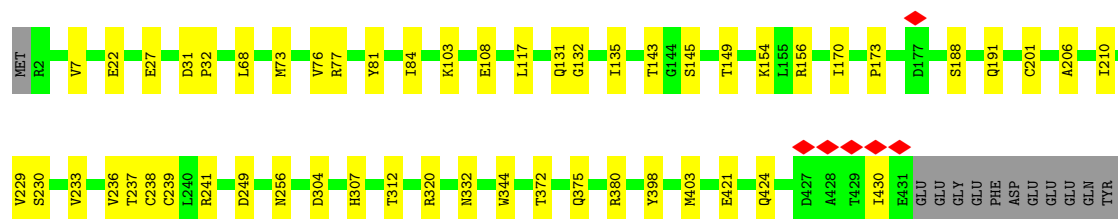


• Molecule 60: Tubulin beta chain

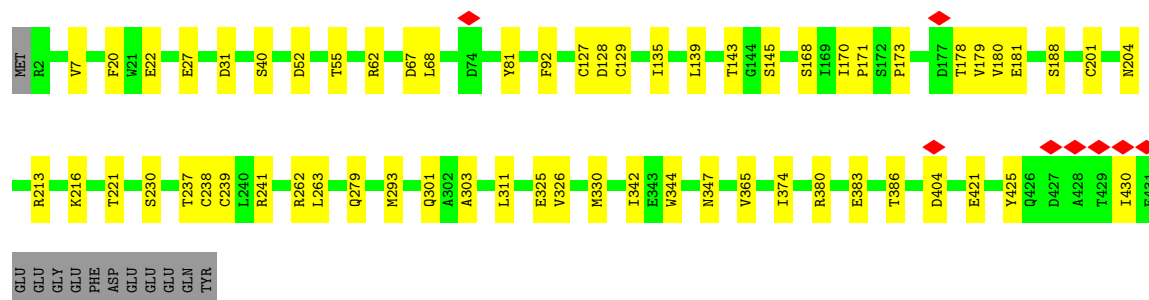
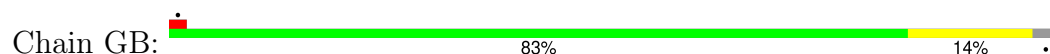


• Molecule 60: Tubulin beta chain

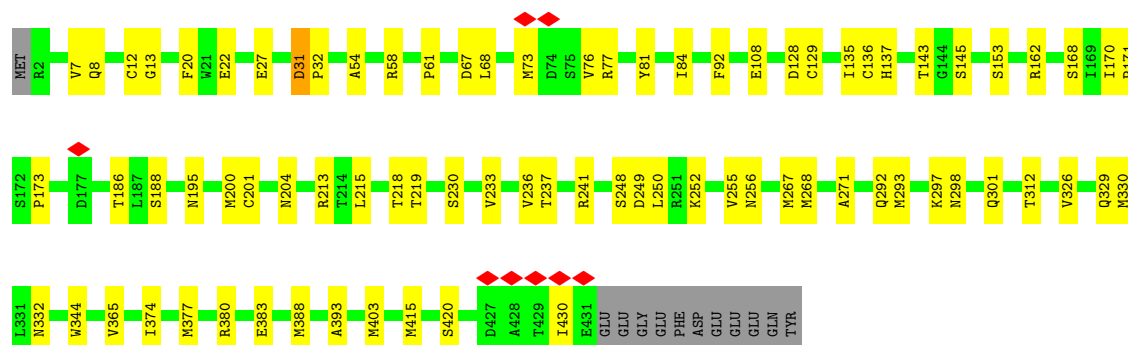
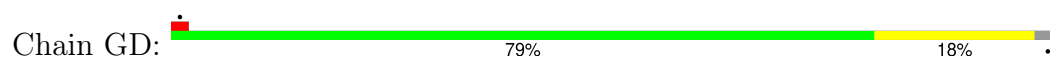




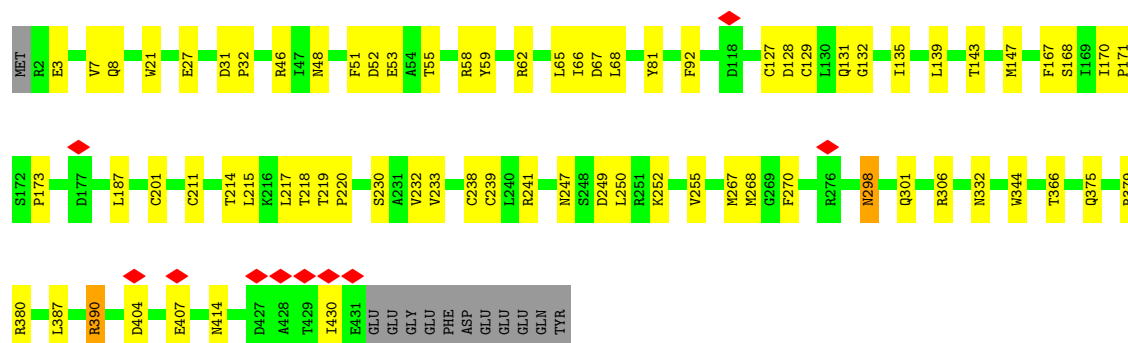
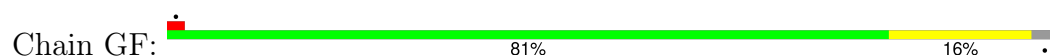
• Molecule 60: Tubulin beta chain



• Molecule 60: Tubulin beta chain

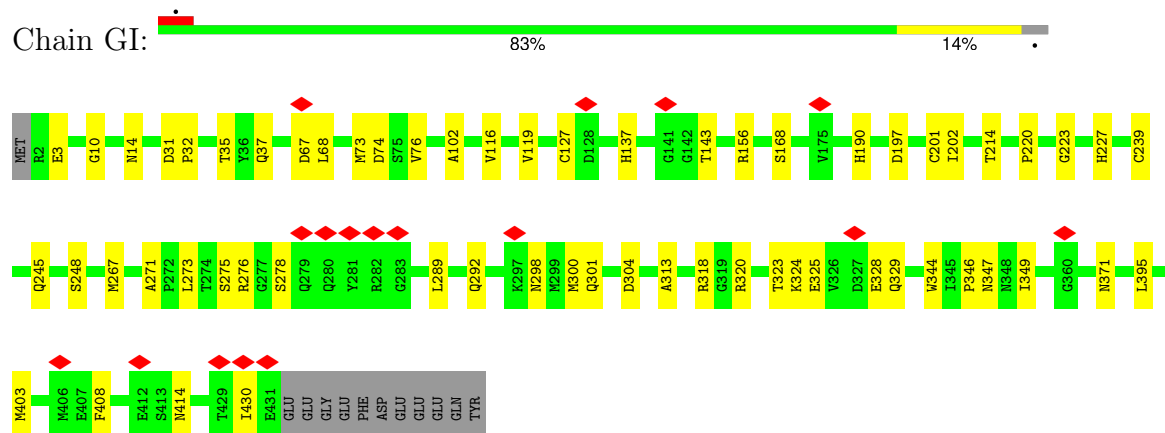


• Molecule 60: Tubulin beta chain



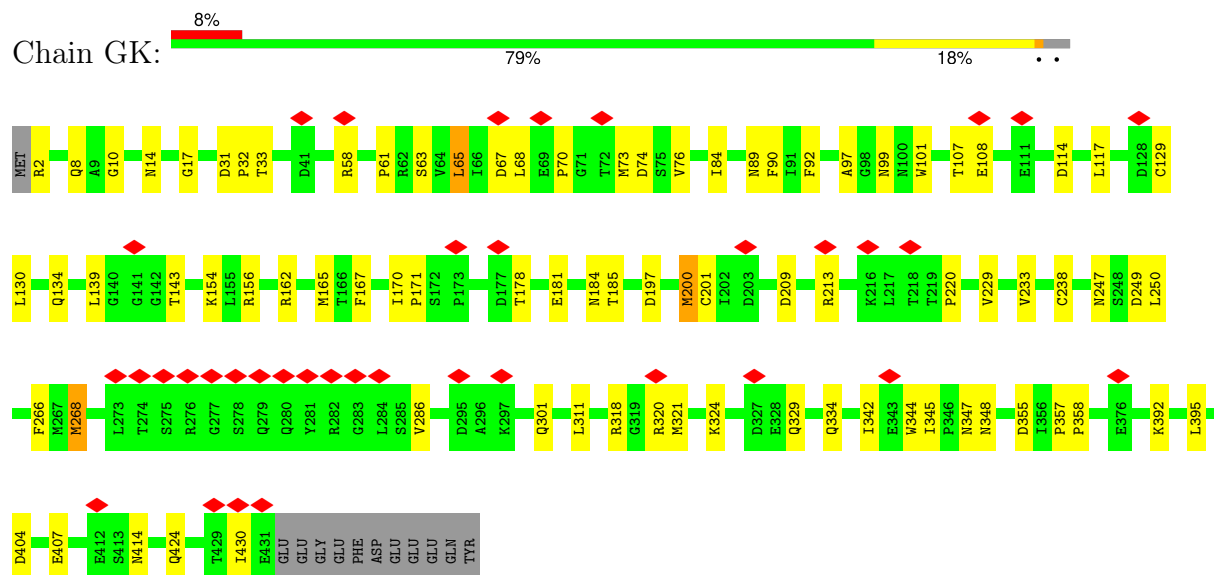
- Molecule 60: Tubulin beta chain

Chain GI:



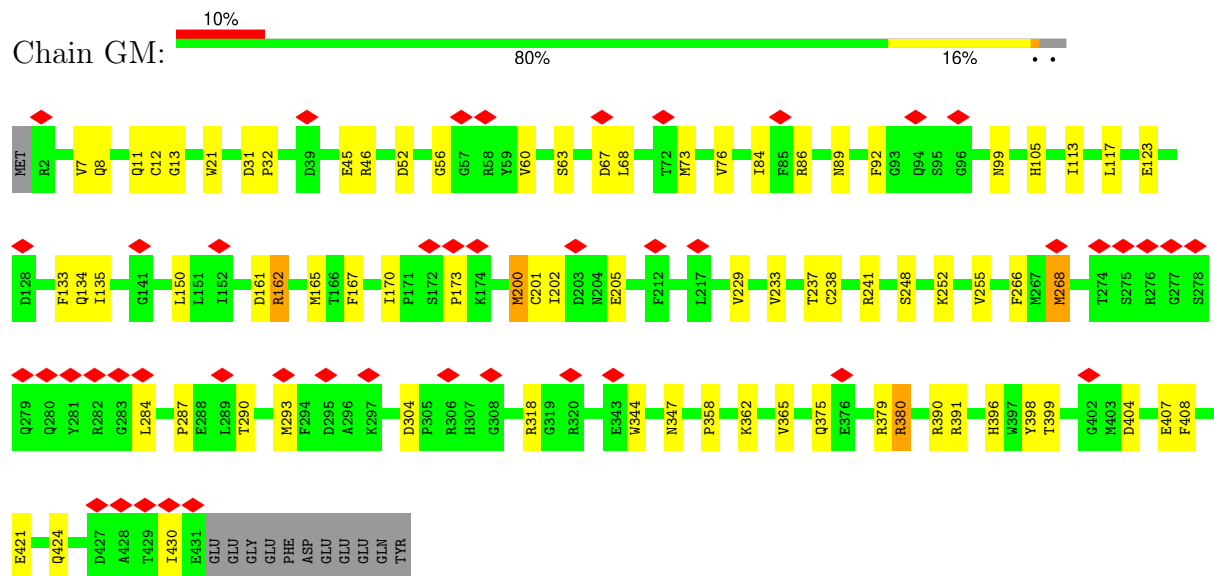
- Molecule 60: Tubulin beta chain

Chain GK:

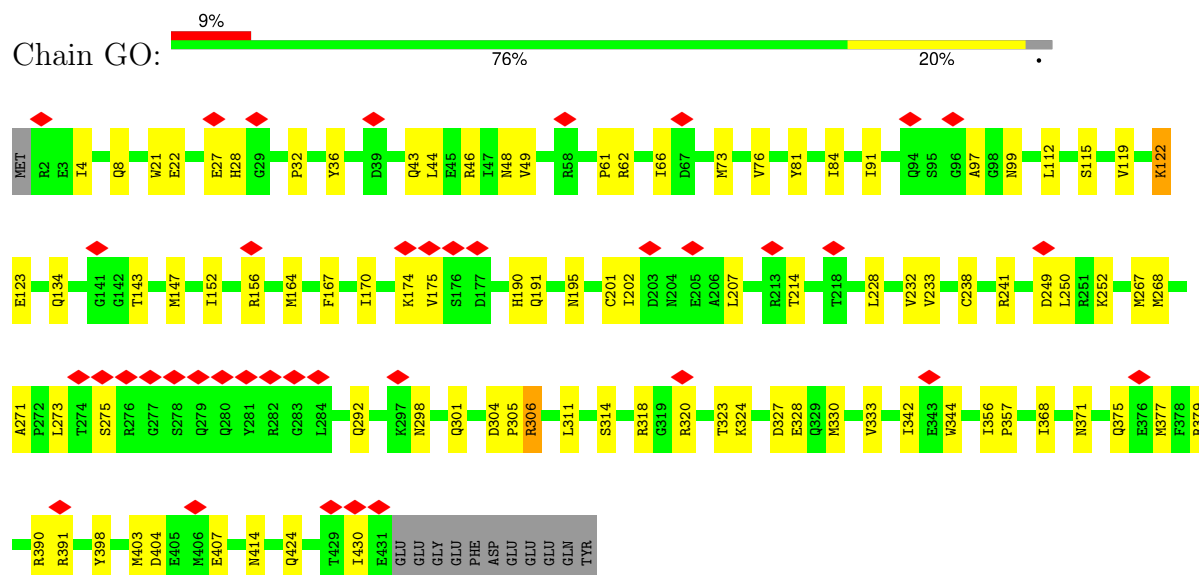


- Molecule 60: Tubulin beta chain

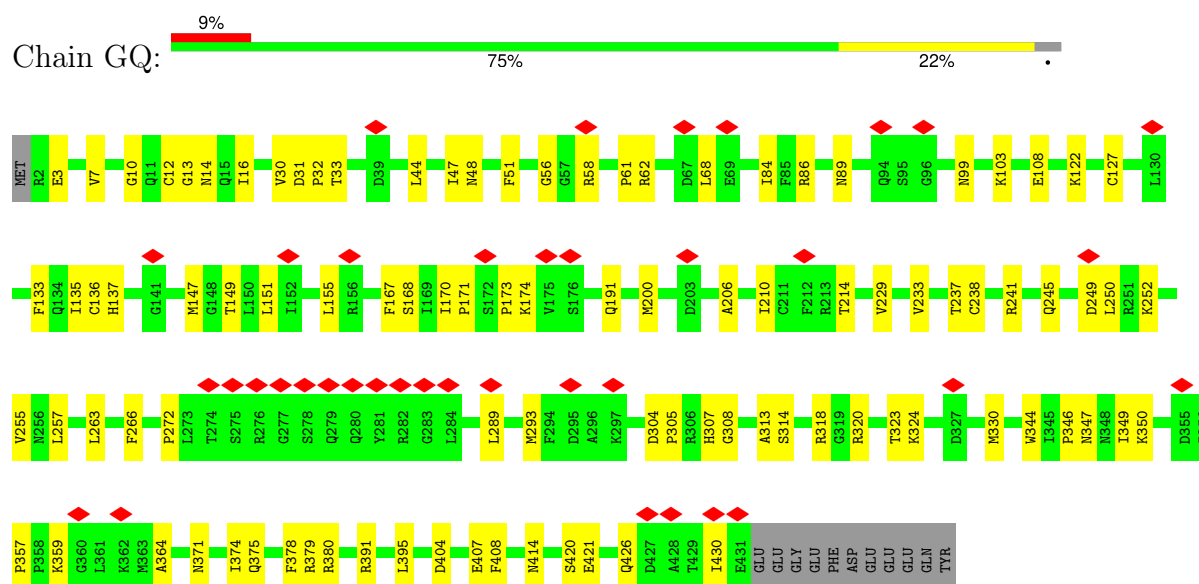
Chain GM:



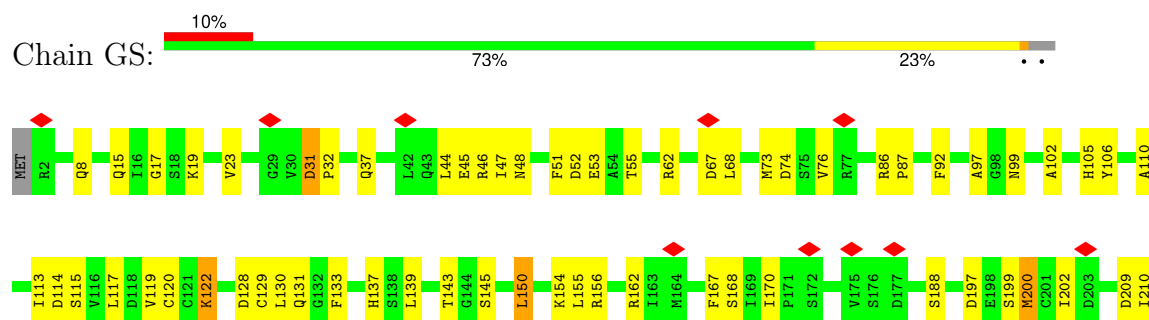
- Molecule 60: Tubulin beta chain



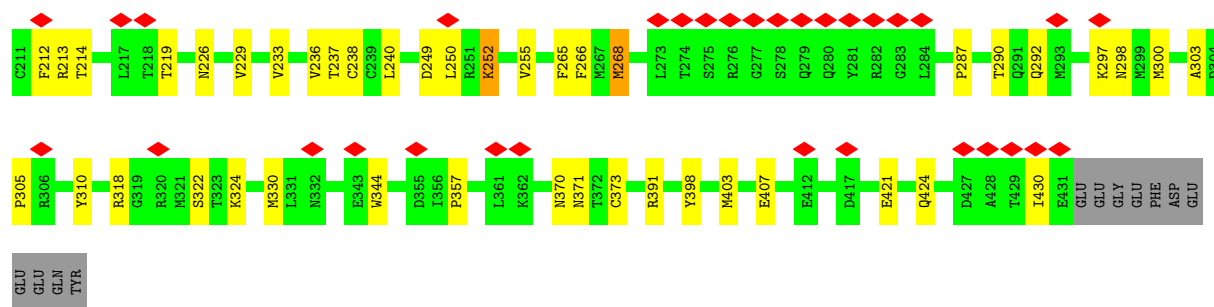
- Molecule 60: Tubulin beta chain



- Molecule 60: Tubulin beta chain

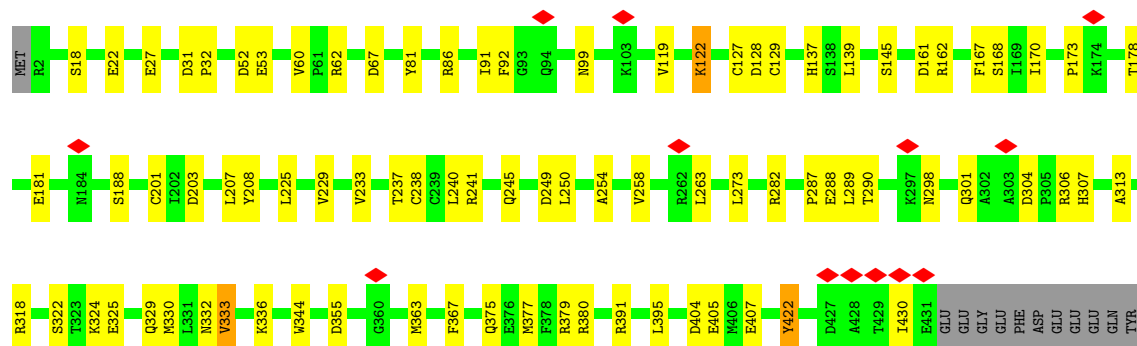






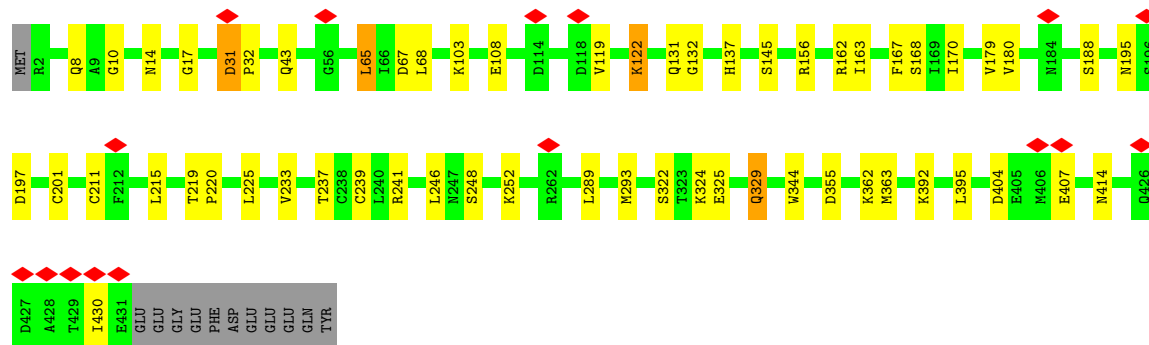
• Molecule 60: Tubulin beta chain

Chain GV: 78% 19%



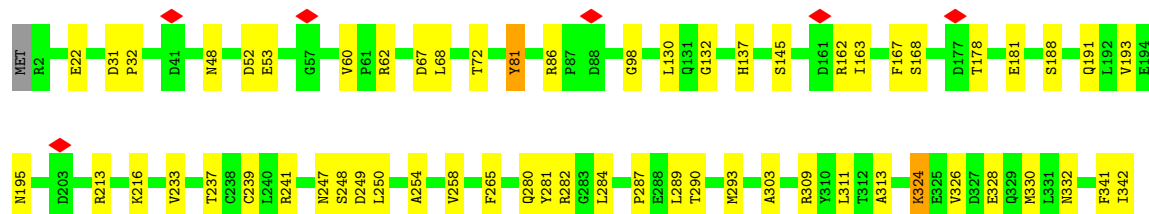
• Molecule 60: Tubulin beta chain

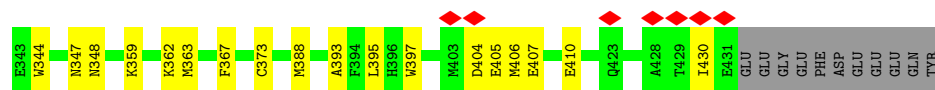
Chain GX: 84% 12%



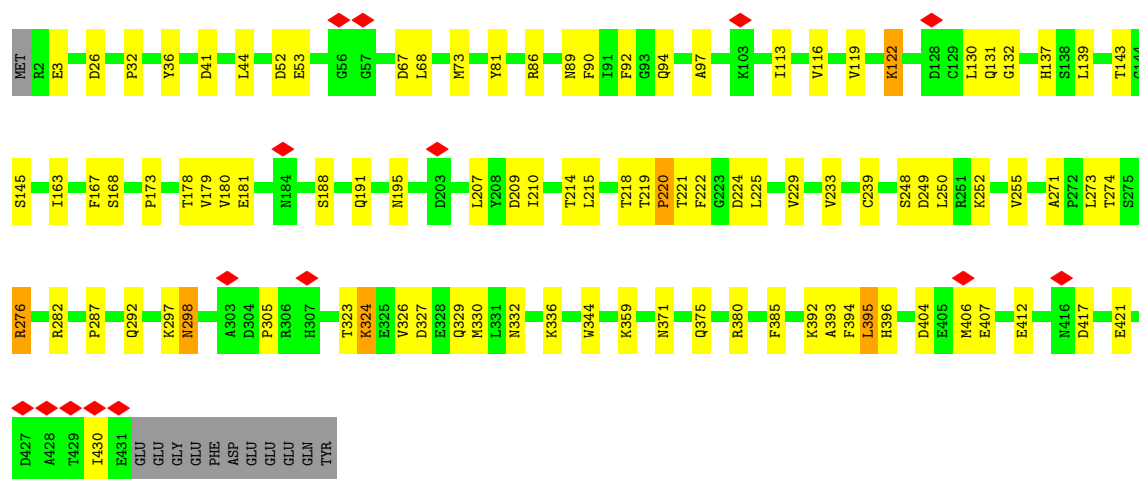
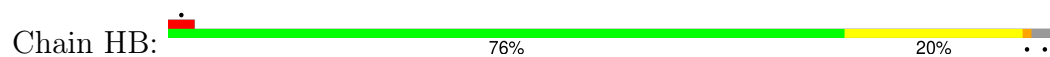
• Molecule 60: Tubulin beta chain

Chain GZ: 80% 17%

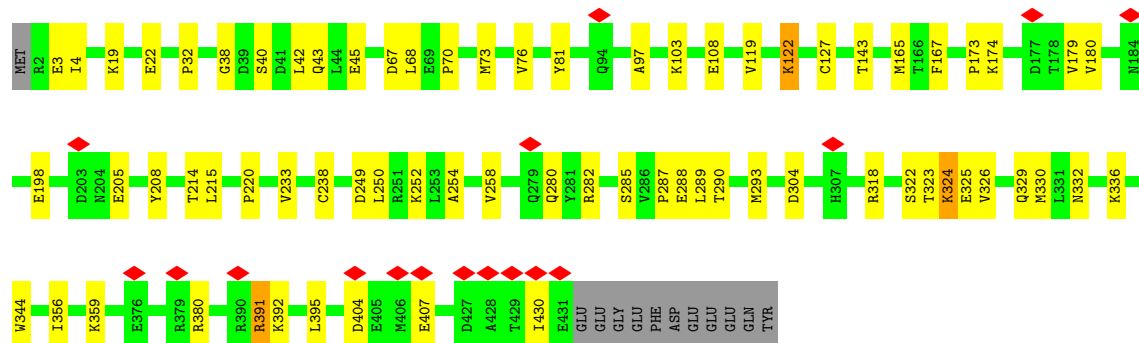
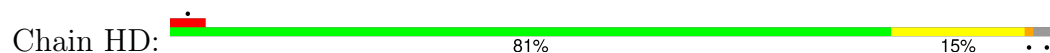




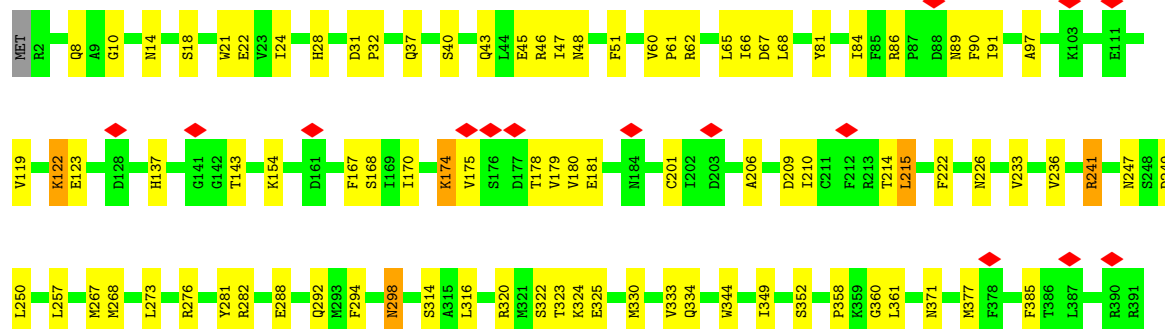
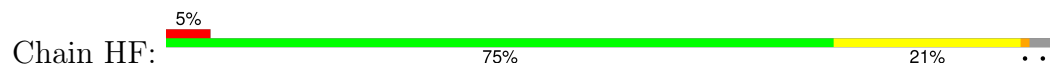
• Molecule 60: Tubulin beta chain

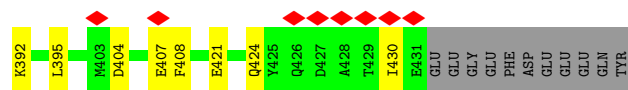


• Molecule 60: Tubulin beta chain



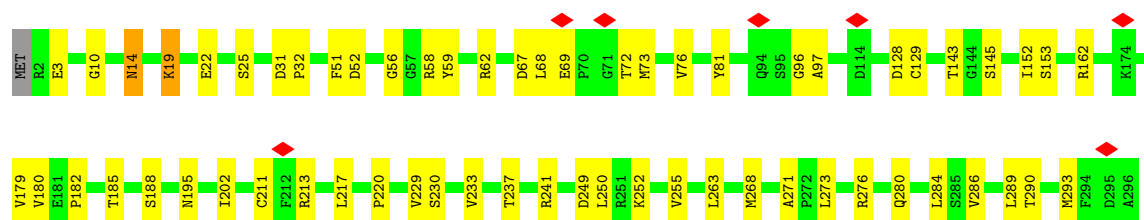
• Molecule 60: Tubulin beta chain





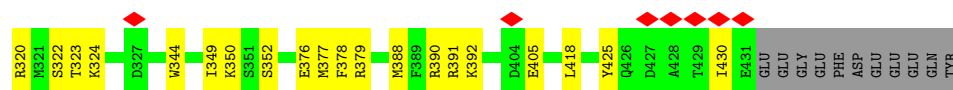
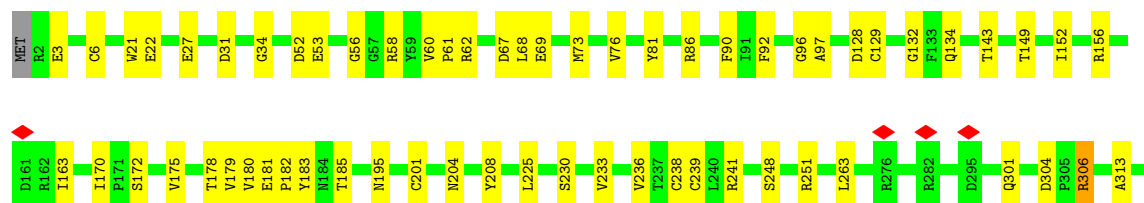
- Molecule 60: Tubulin beta chain

Chain HH: 78% 19%



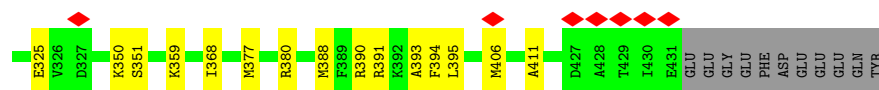
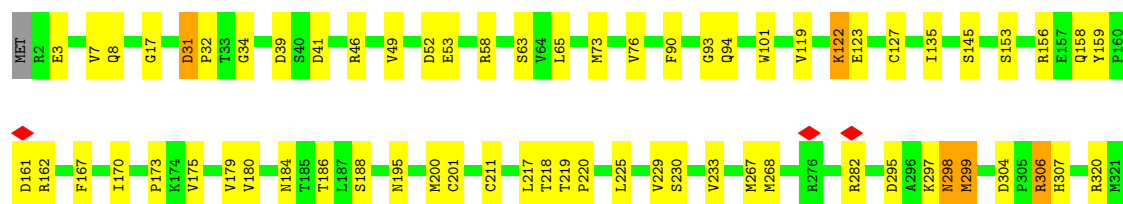
- Molecule 60: Tubulin beta chain

Chain HJ: 79% 18%



- Molecule 60: Tubulin beta chain

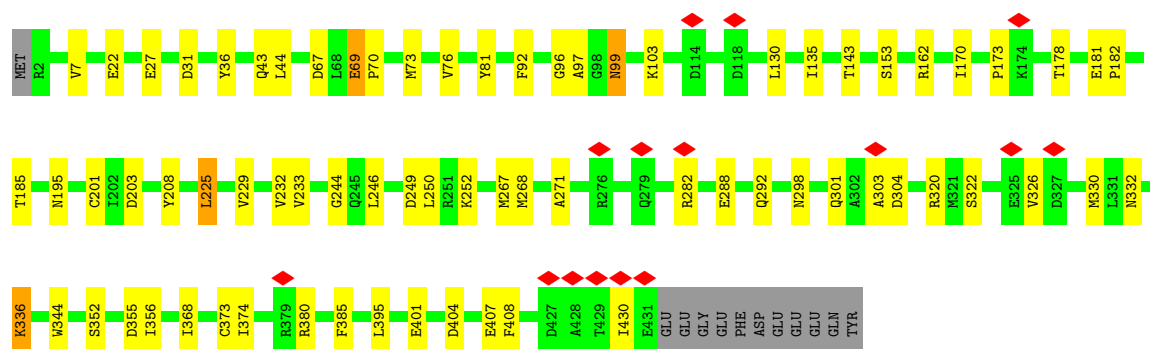
Chain HL: 79% 17%



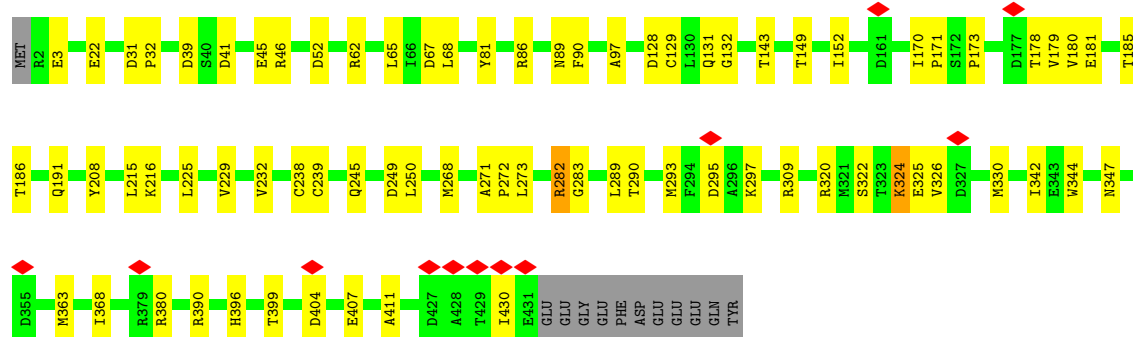
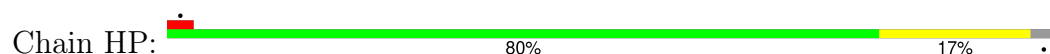
- Molecule 60: Tubulin beta chain

Chain HN: 81% 16%

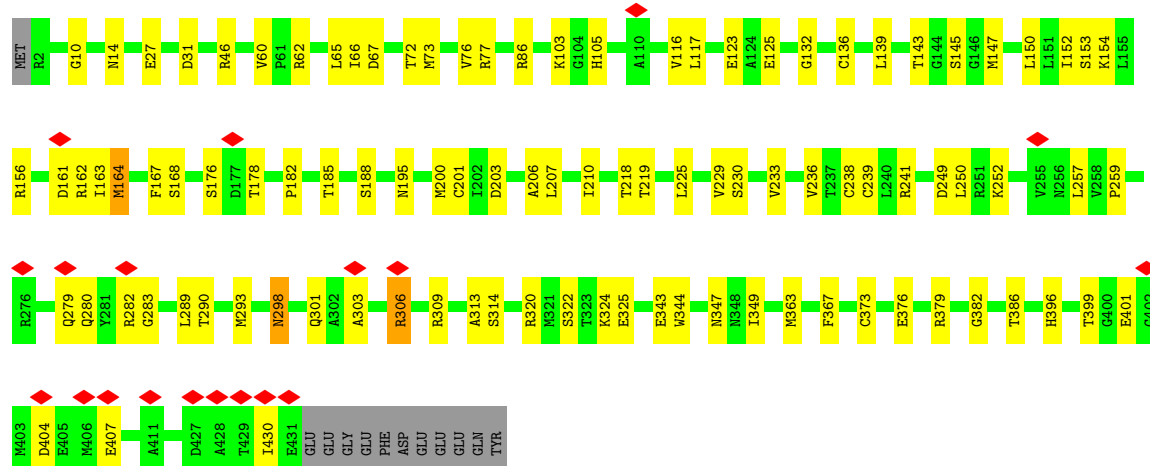
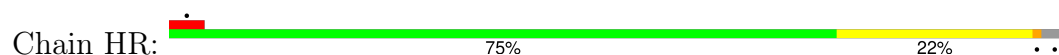




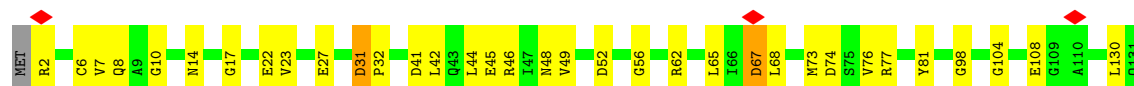
• Molecule 60: Tubulin beta chain

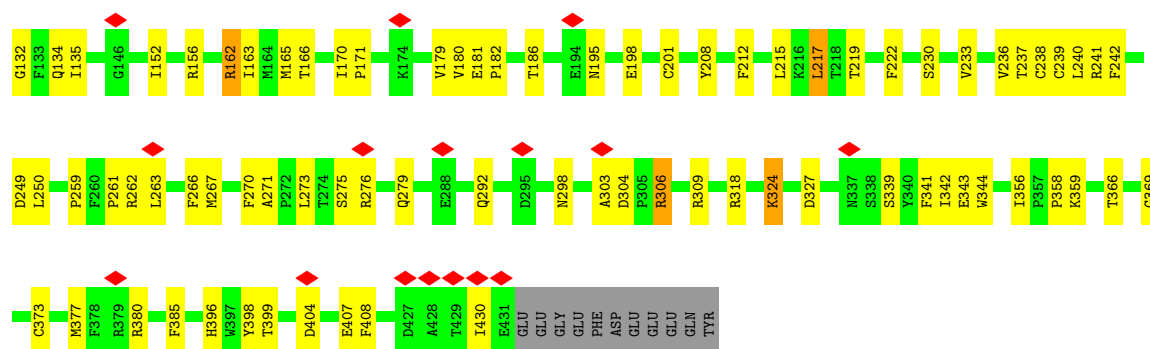


• Molecule 60: Tubulin beta chain

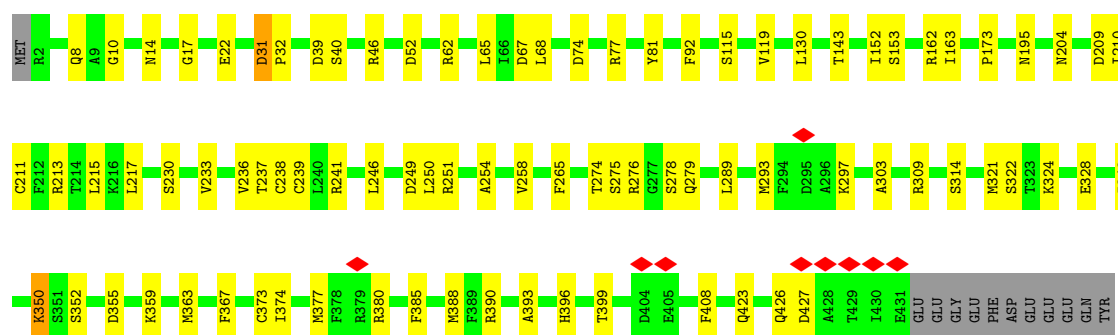
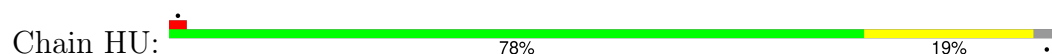


• Molecule 60: Tubulin beta chain

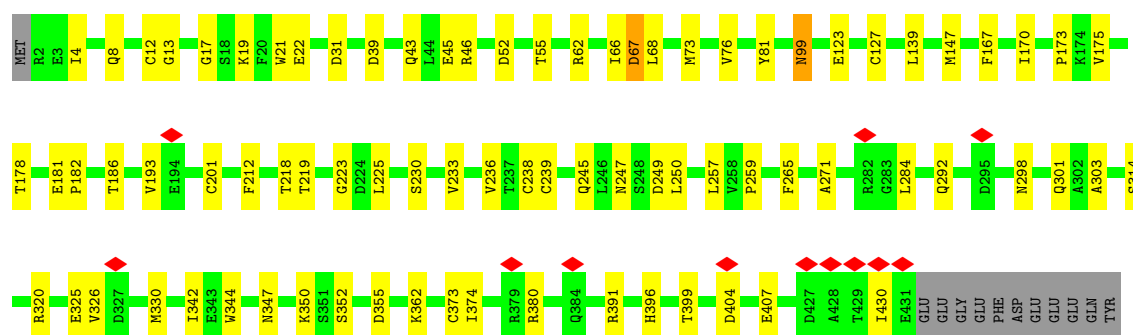
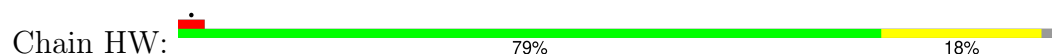




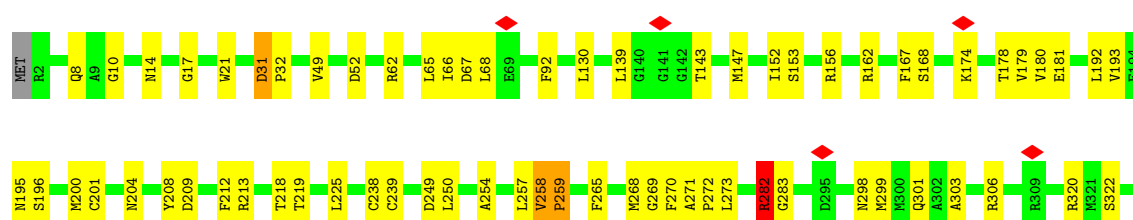
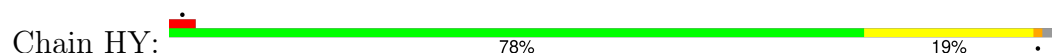
• Molecule 60: Tubulin beta chain

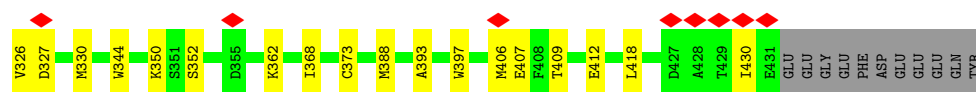


• Molecule 60: Tubulin beta chain

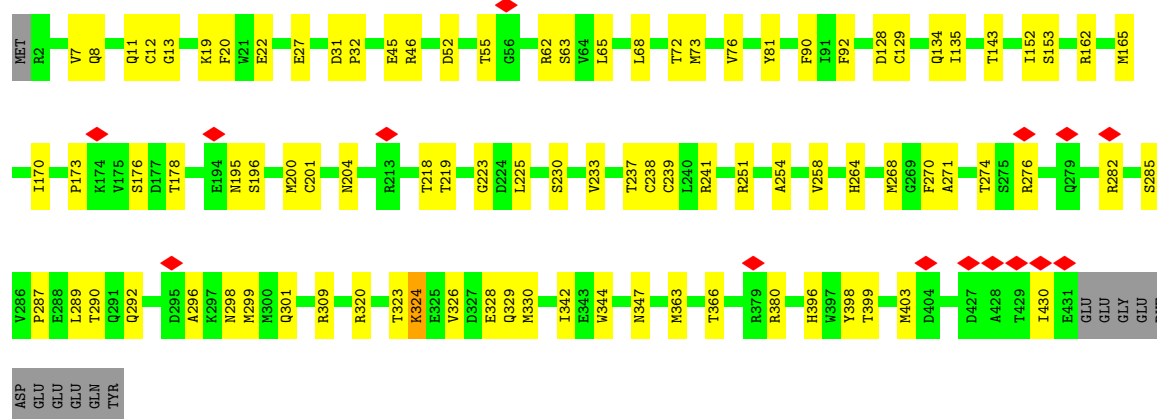
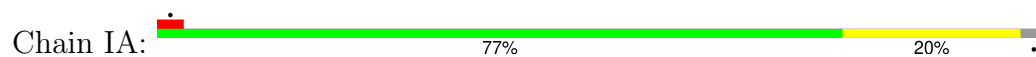


• Molecule 60: Tubulin beta chain

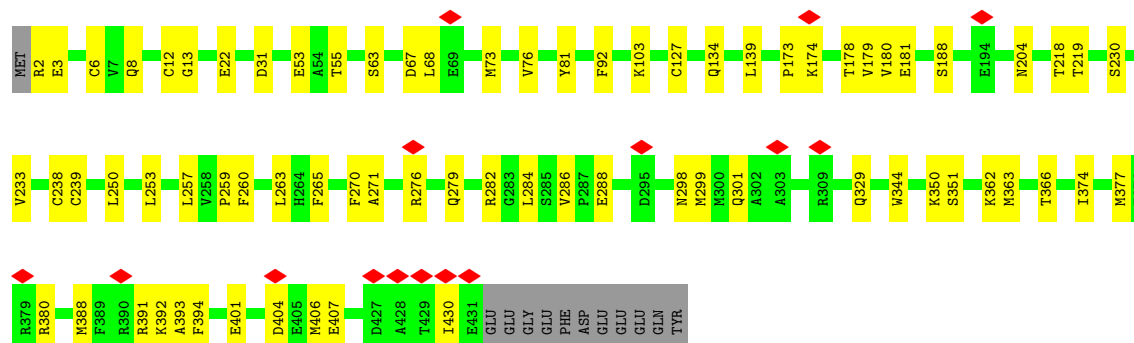
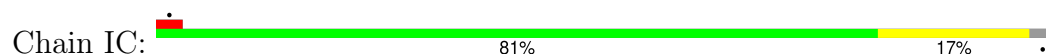




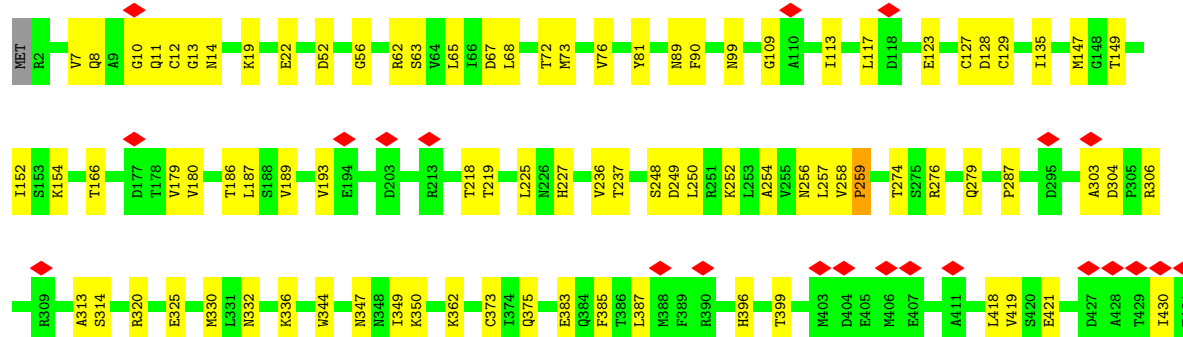
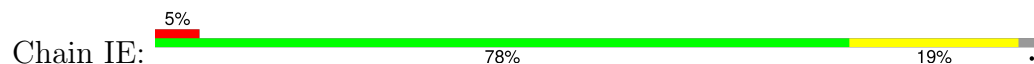
• Molecule 60: Tubulin beta chain



• Molecule 60: Tubulin beta chain




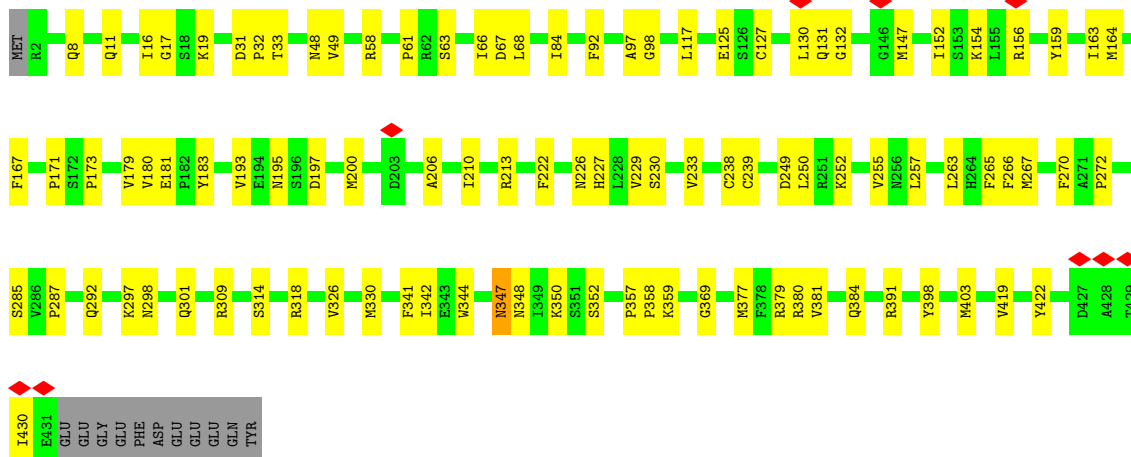
• Molecule 60: Tubulin beta chain




GLU  
GLU  
GLY  
GLU  
PHE  
ASP  
GLU  
GLU  
GLN  
TYR

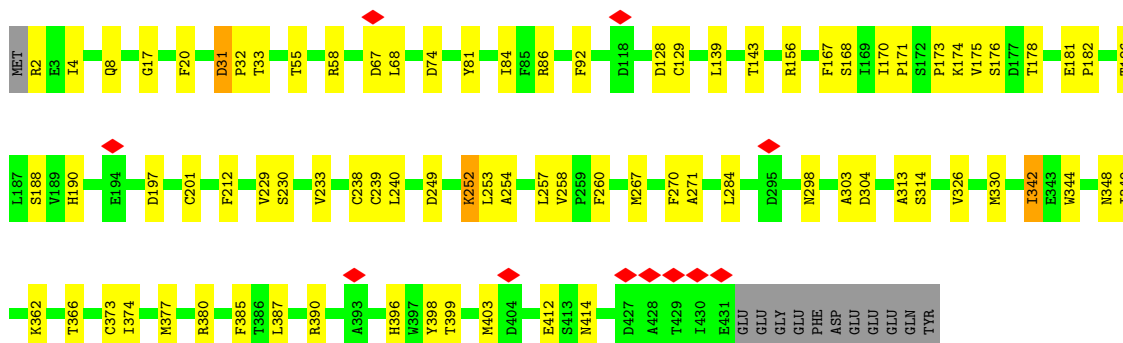
• Molecule 60: Tubulin beta chain

Chain IF:  75% 22%




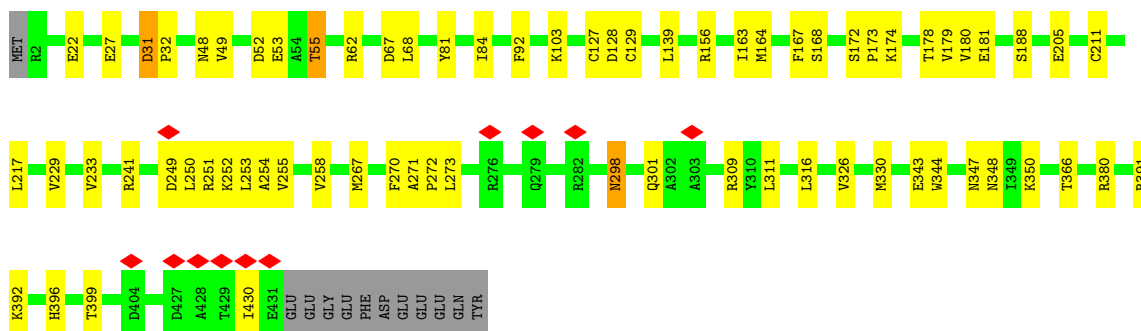
• Molecule 60: Tubulin beta chain

Chain IH:  79% 18%




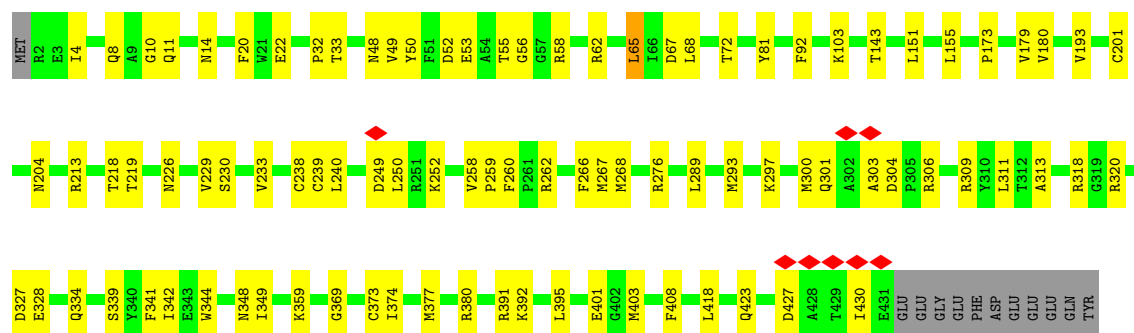
• Molecule 60: Tubulin beta chain

Chain IJ:  81% 15%




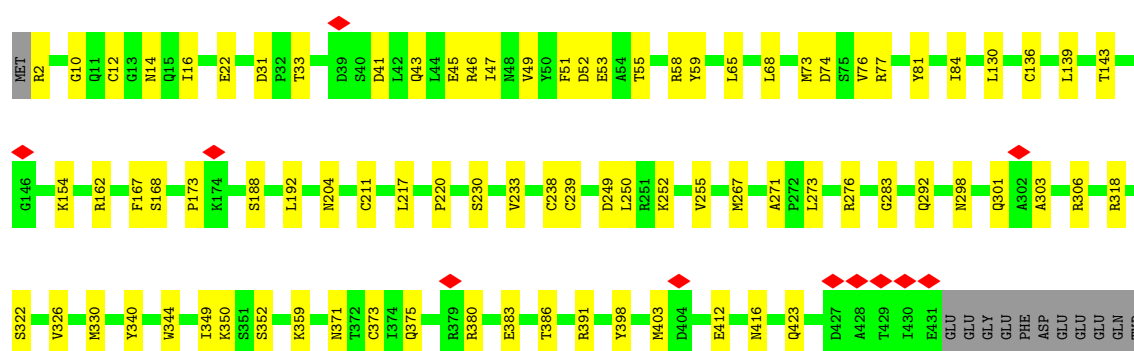
• Molecule 60: Tubulin beta chain

Chain IL:  76% 21%



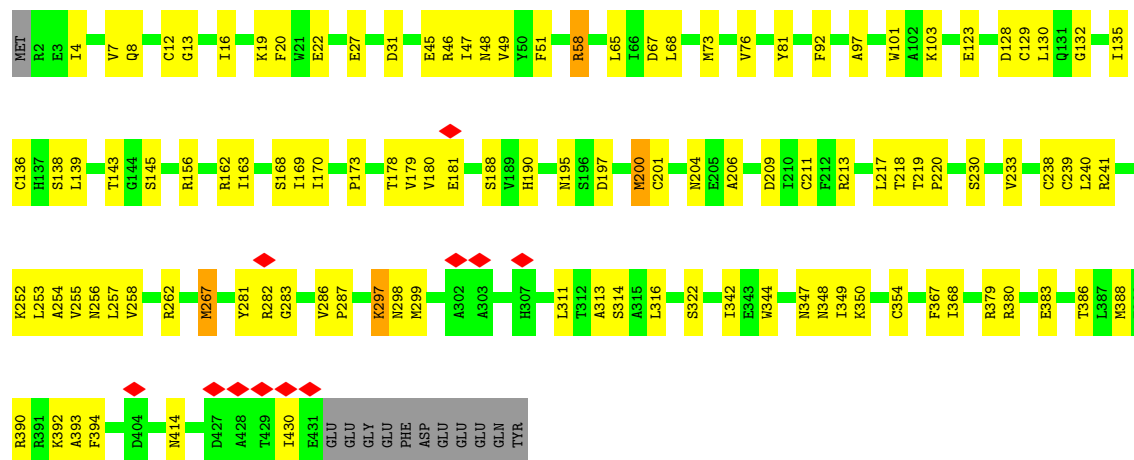
• Molecule 60: Tubulin beta chain

Chain IN:  79% 19%




• Molecule 60: Tubulin beta chain

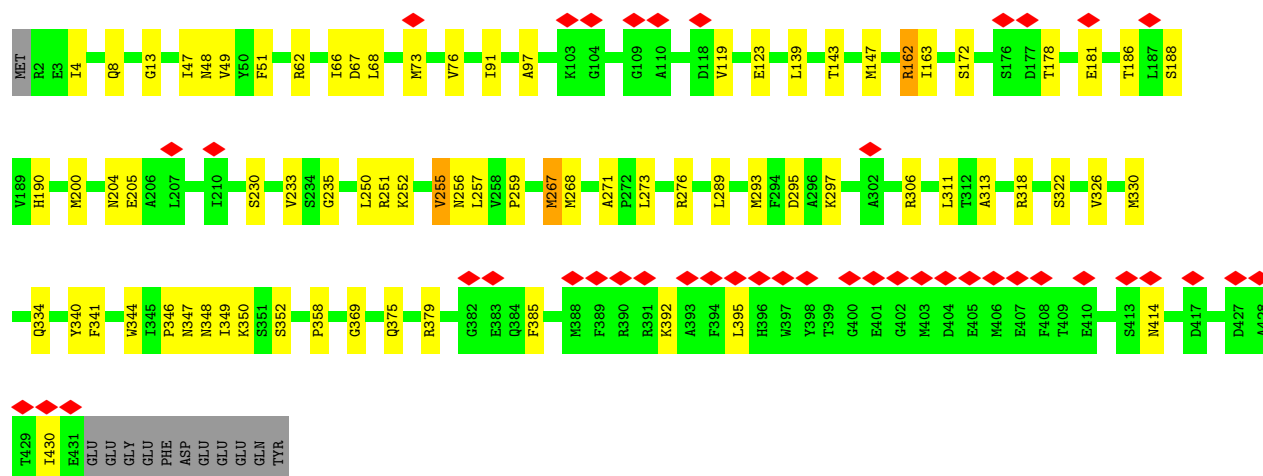
Chain IP:  72% 25%



• Molecule 60: Tubulin beta chain

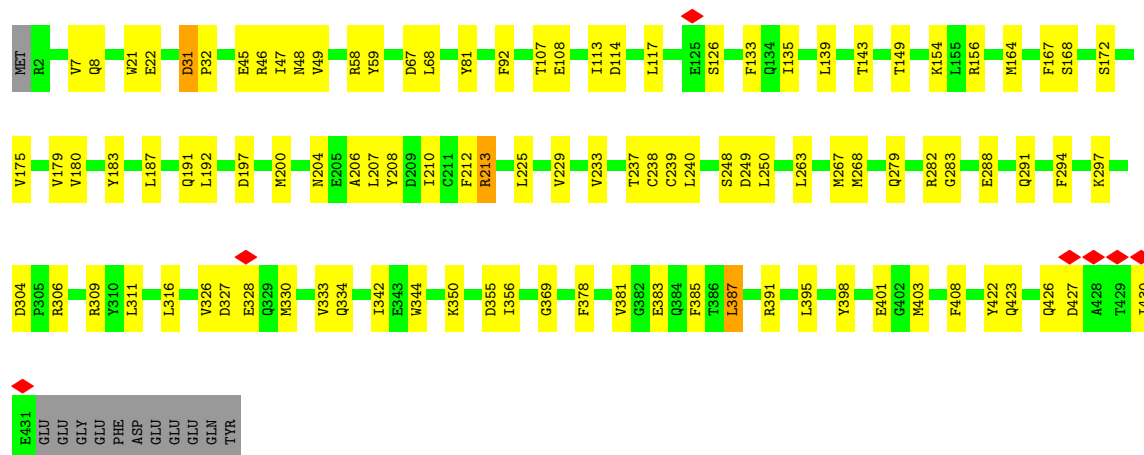
Chain IR:  10% 80% 17%





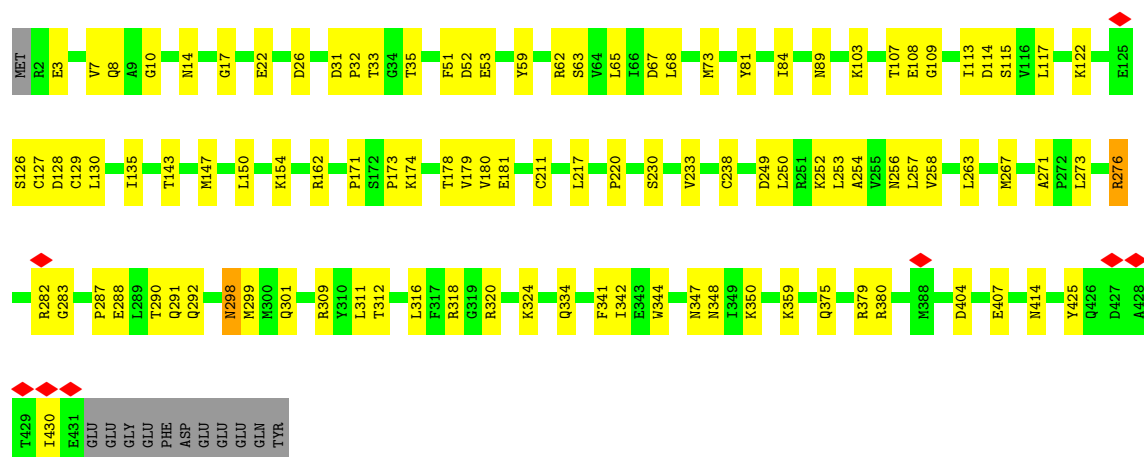
• Molecule 60: Tubulin beta chain

Chain IS: 74% 23%

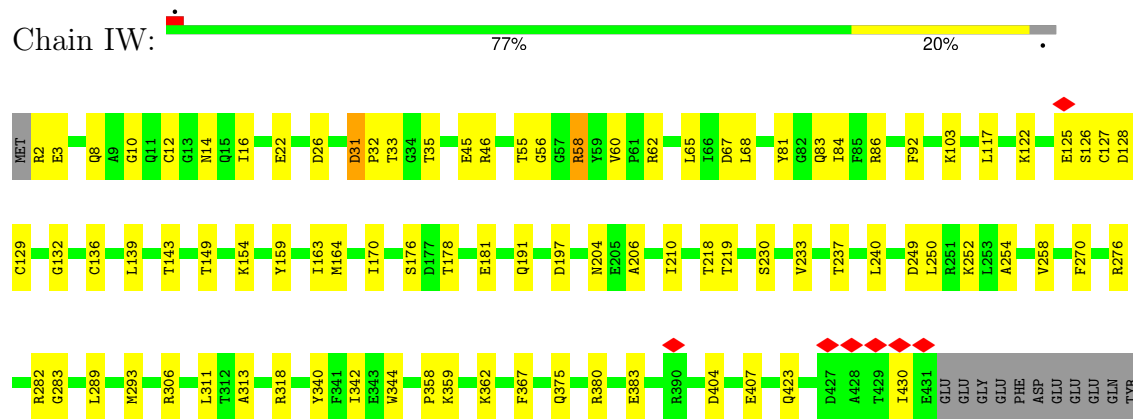


• Molecule 60: Tubulin beta chain

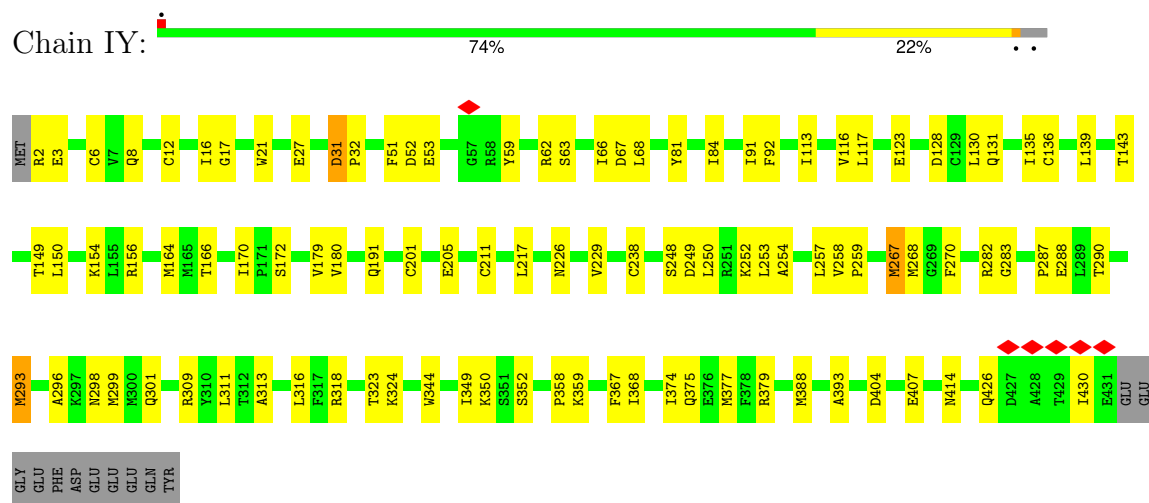
Chain IU: 74% 23%



## ● Molecule 60: Tubulin beta chain



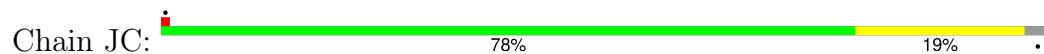
## ● Molecule 60: Tubulin beta chain

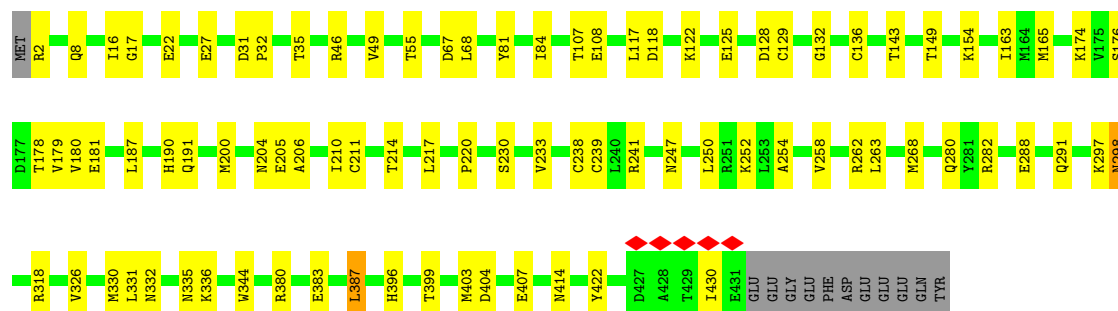


## ● Molecule 60: Tubulin beta chain



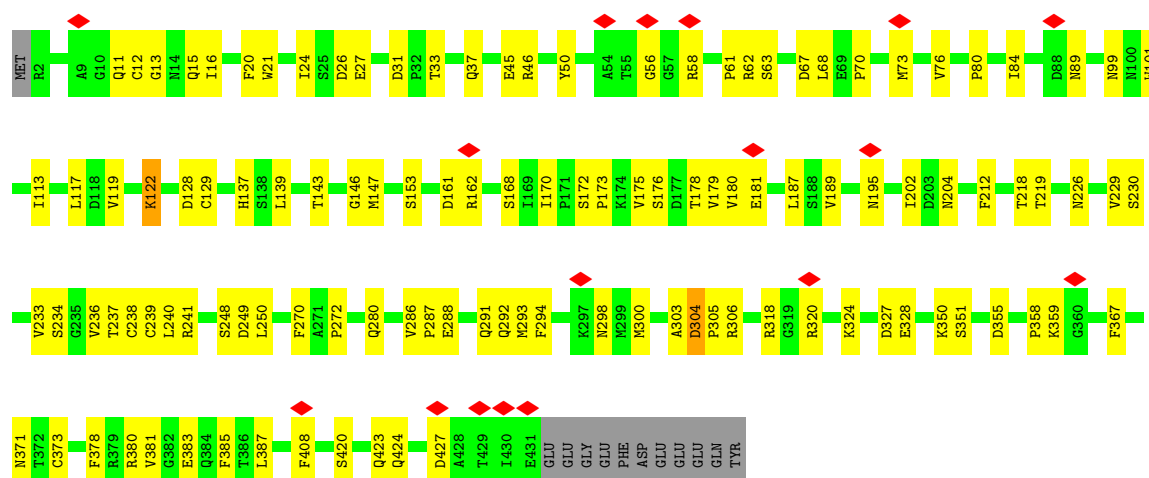
## ● Molecule 60: Tubulin beta chain





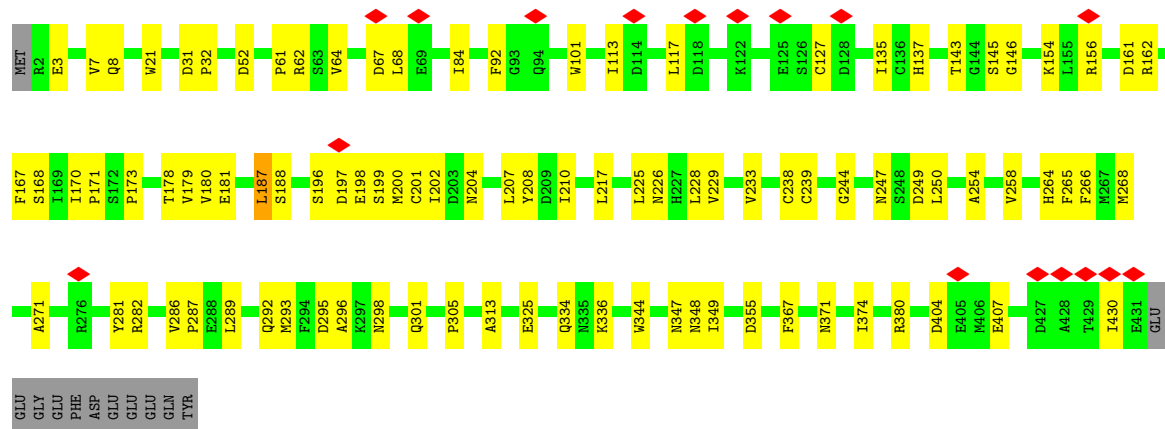
• Molecule 60: Tubulin beta chain

Chain JE: 71% 26%



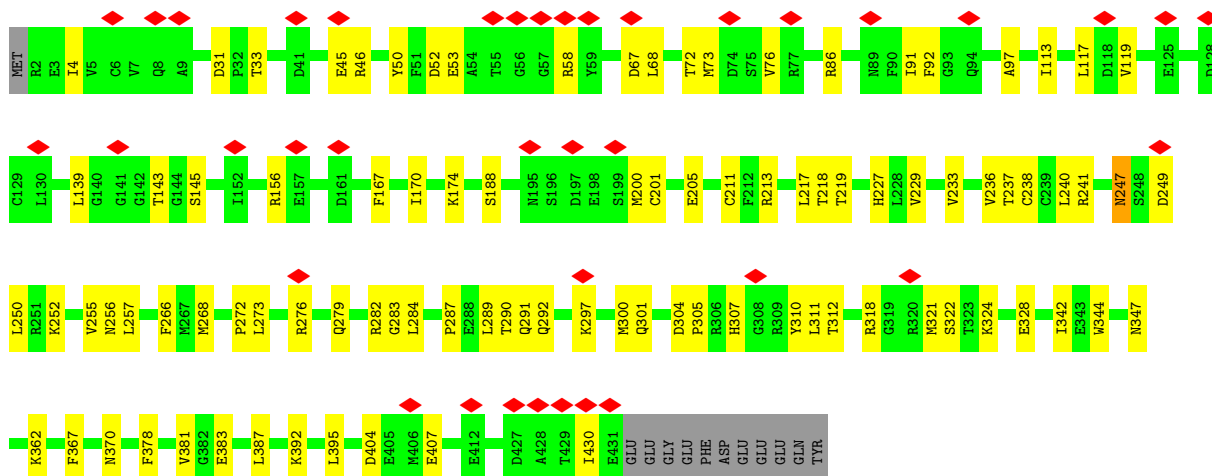
• Molecule 60: Tubulin beta chain

Chain JG: 76% 21%

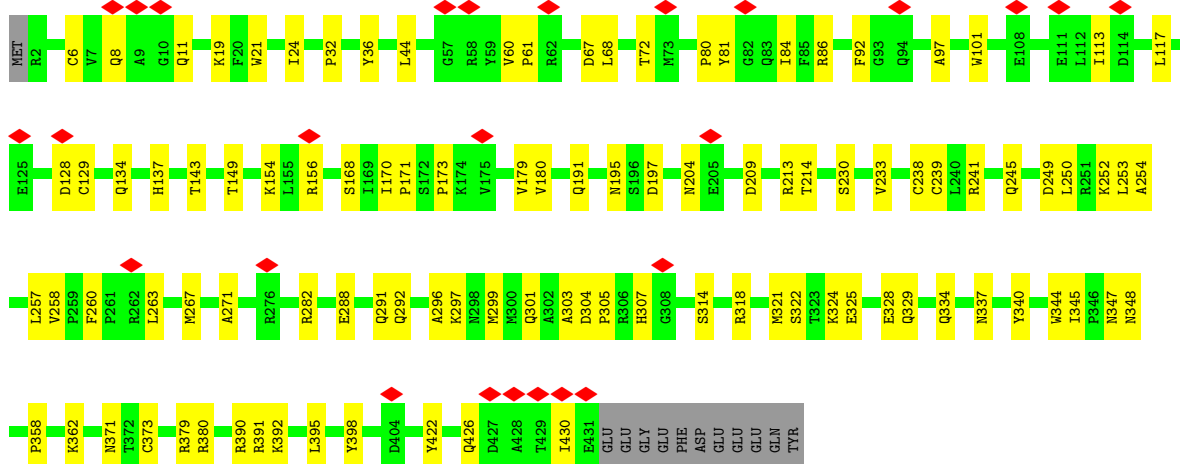
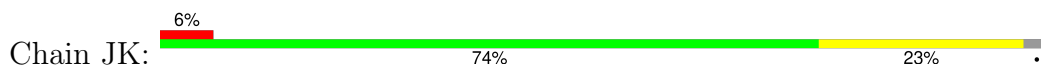


• Molecule 60: Tubulin beta chain

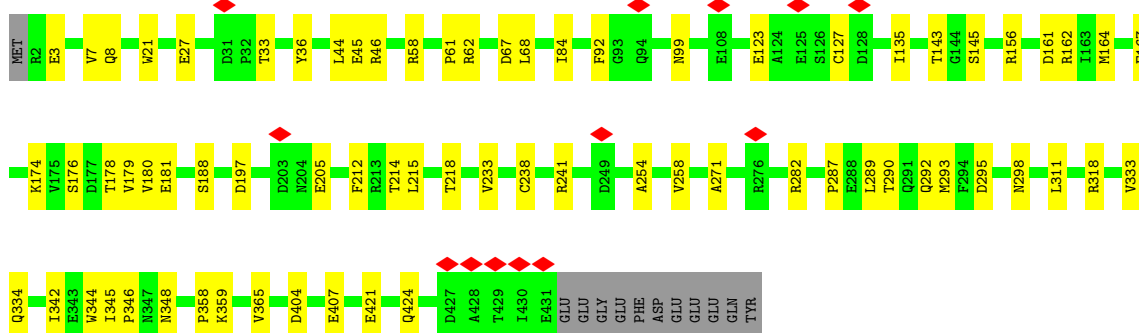
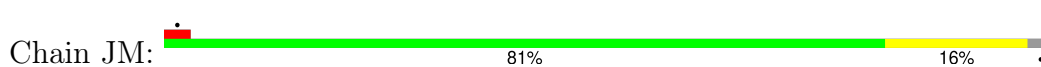
Chain JI: 9% 76% 21%



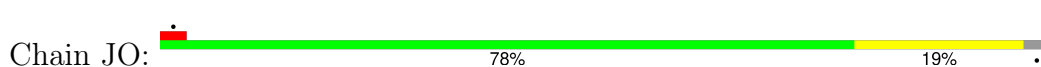
• Molecule 60: Tubulin beta chain

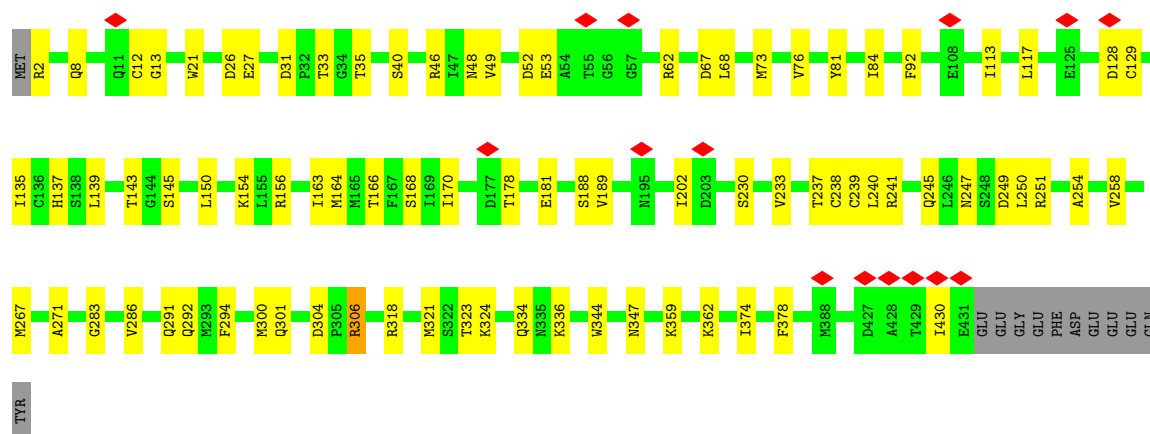


• Molecule 60: Tubulin beta chain

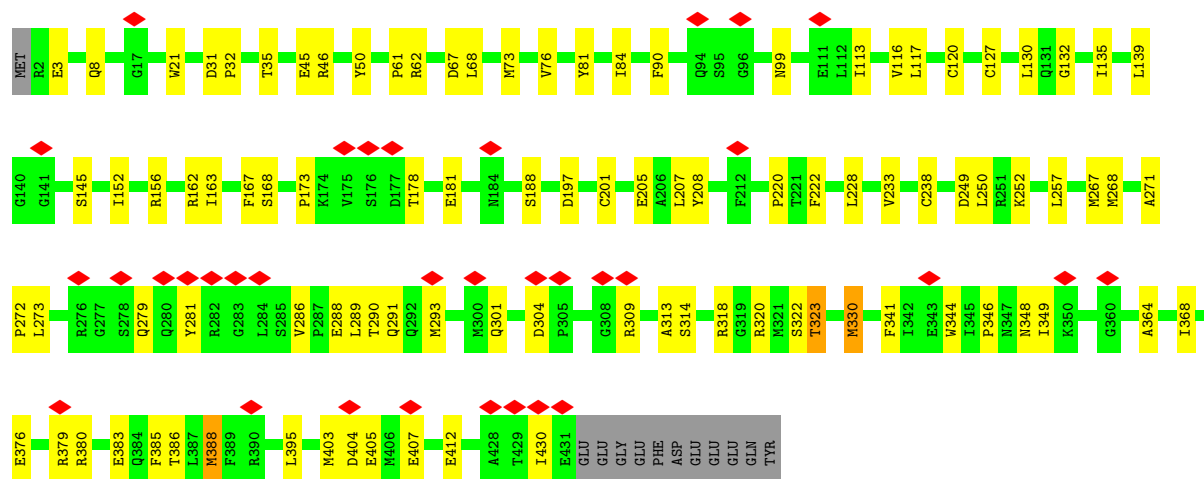
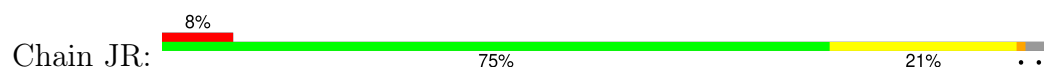


• Molecule 60: Tubulin beta chain

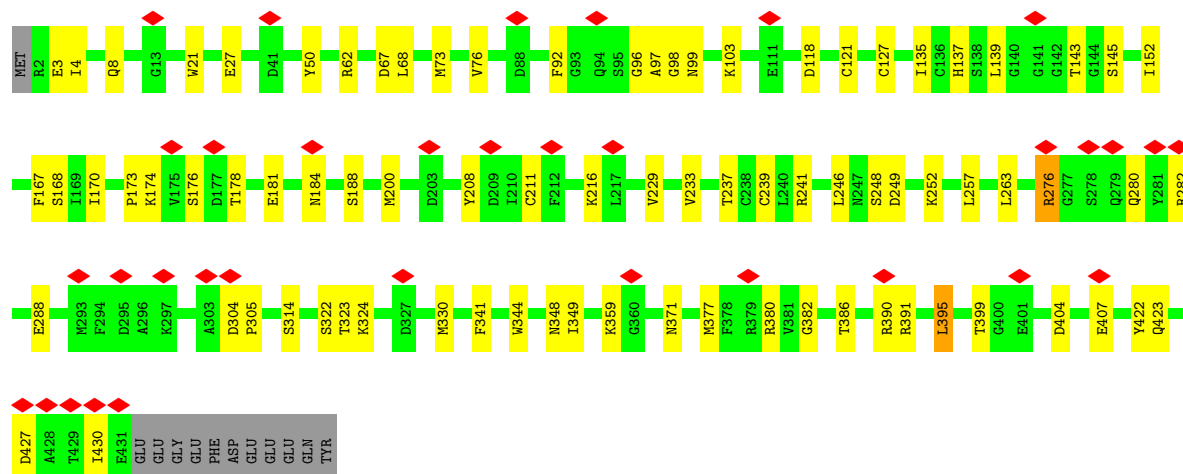
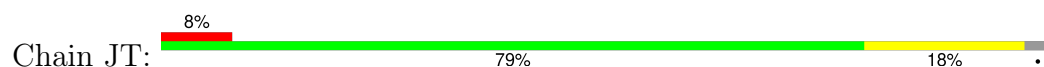




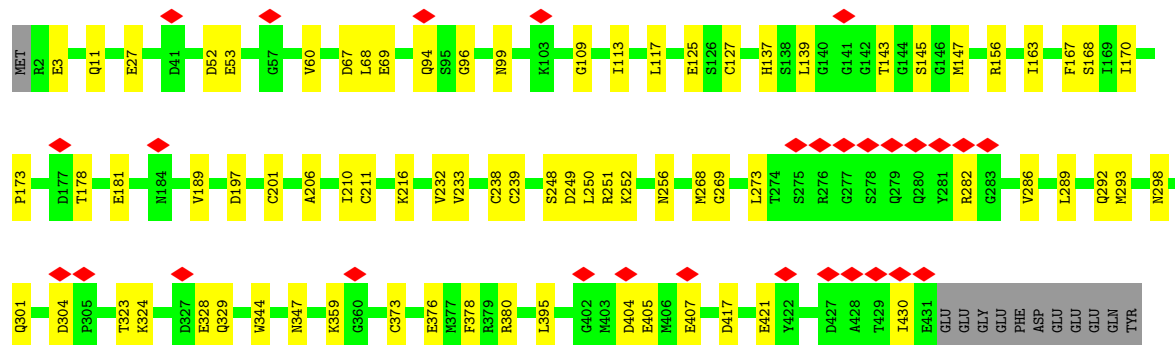

• Molecule 60: Tubulin beta chain



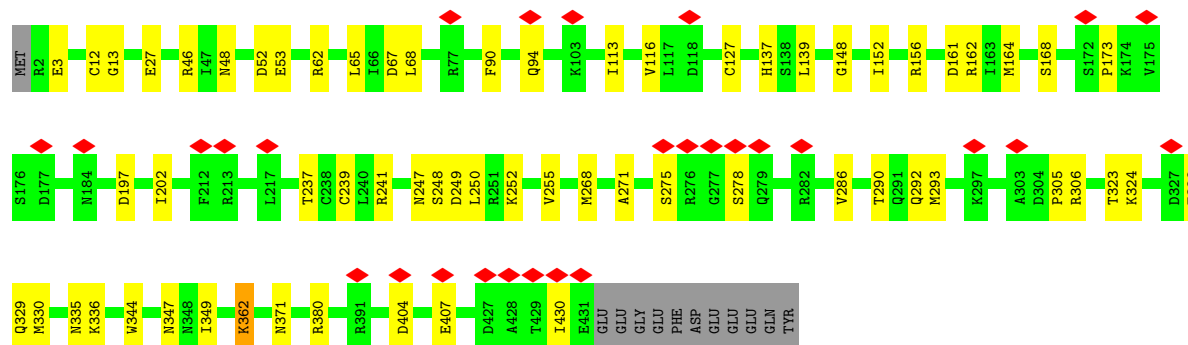

• Molecule 60: Tubulin beta chain



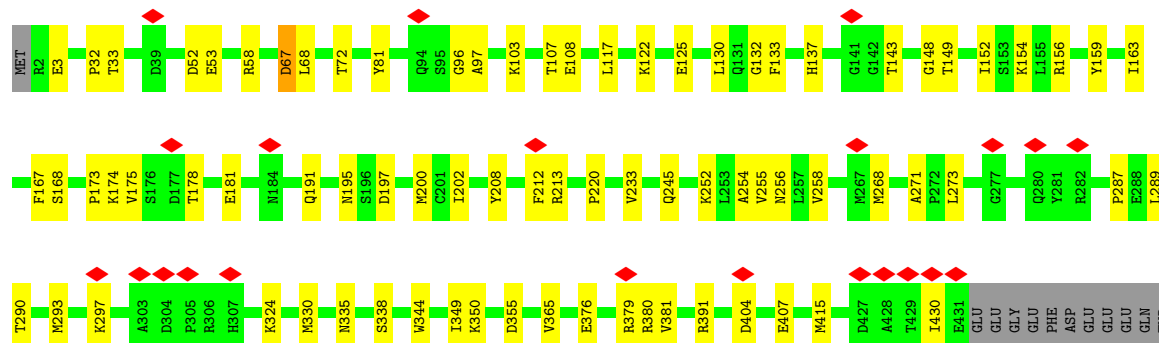

## • Molecule 60: Tubulin beta chain

Chain JV: 

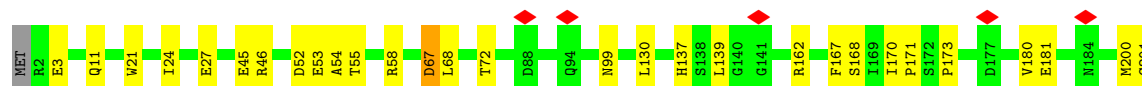

## • Molecule 60: Tubulin beta chain

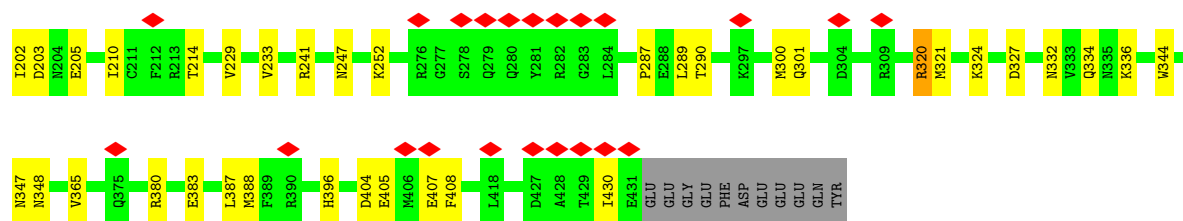
Chain JX: 

## • Molecule 60: Tubulin beta chain

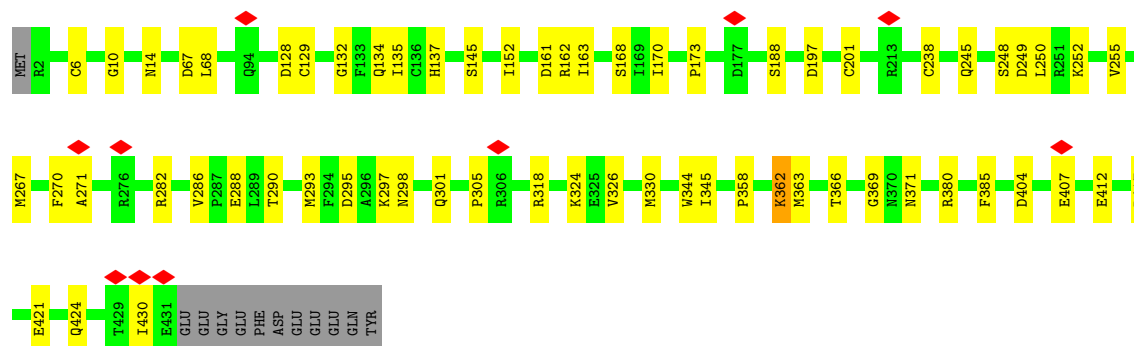
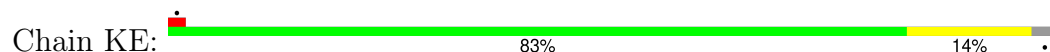
Chain JZ: 

## • Molecule 60: Tubulin beta chain

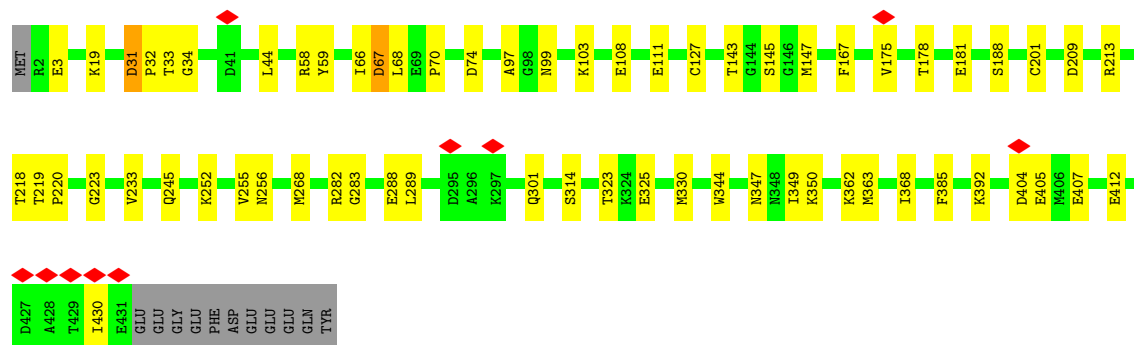
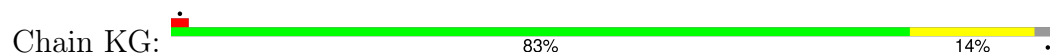
Chain KB: 



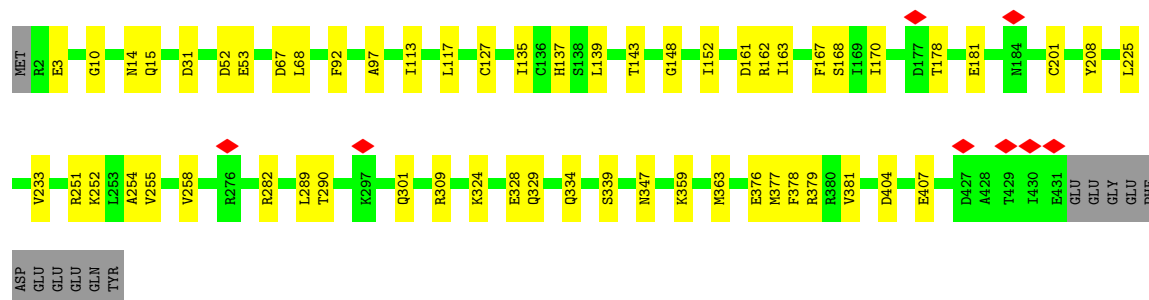
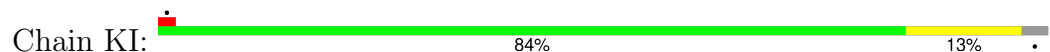
• Molecule 60: Tubulin beta chain



• Molecule 60: Tubulin beta chain

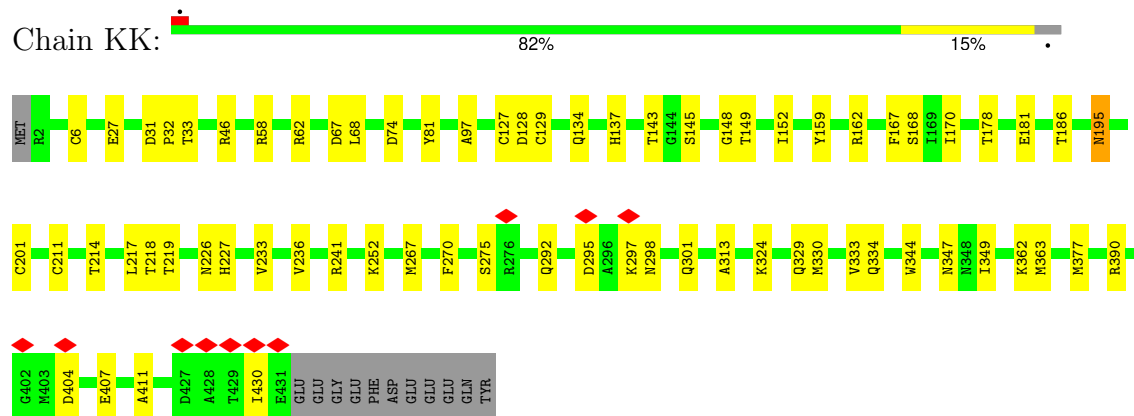


• Molecule 60: Tubulin beta chain



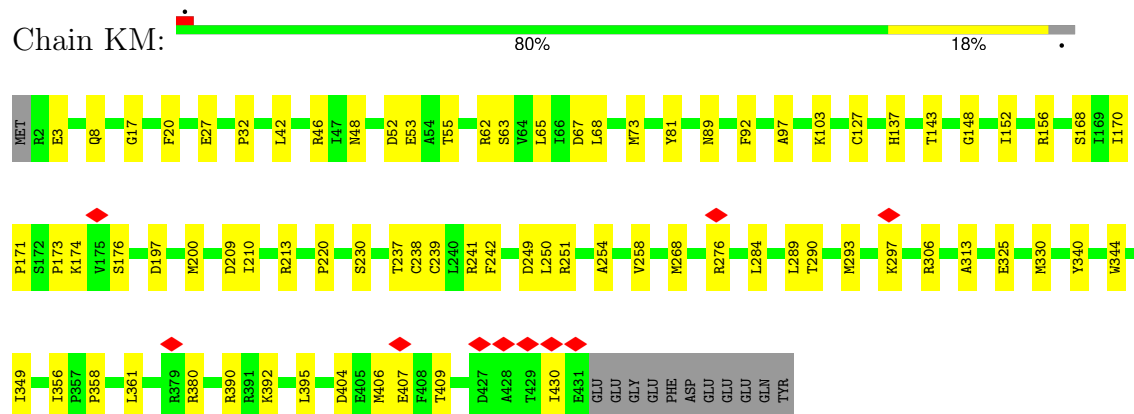
## • Molecule 60: Tubulin beta chain

Chain KK:



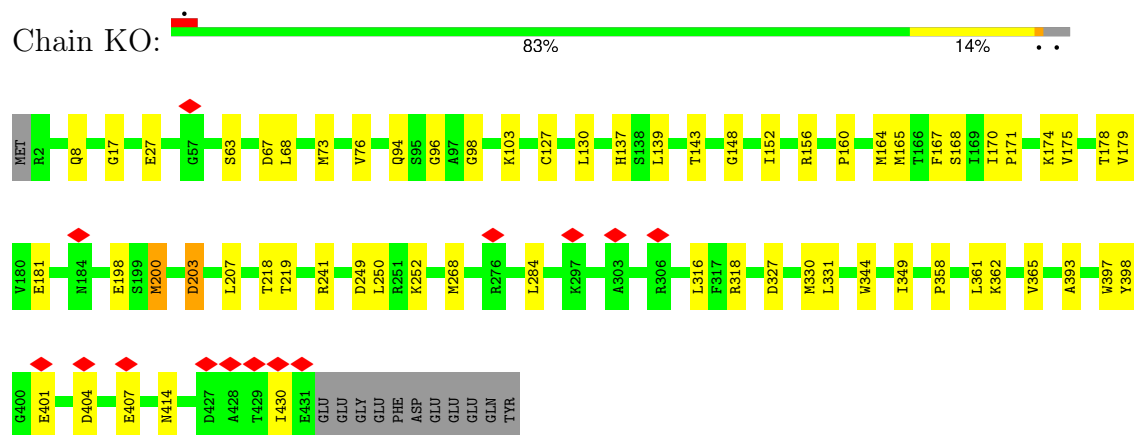
## • Molecule 60: Tubulin beta chain

Chain KM:



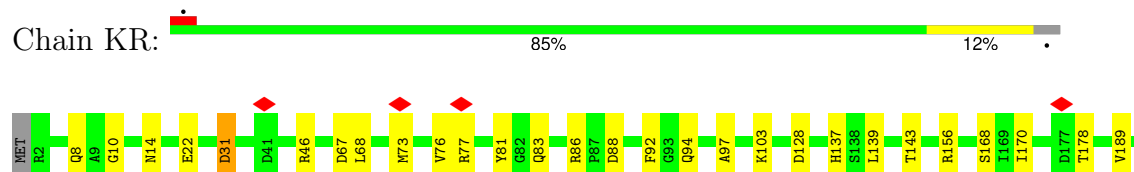
## • Molecule 60: Tubulin beta chain

Chain KO:

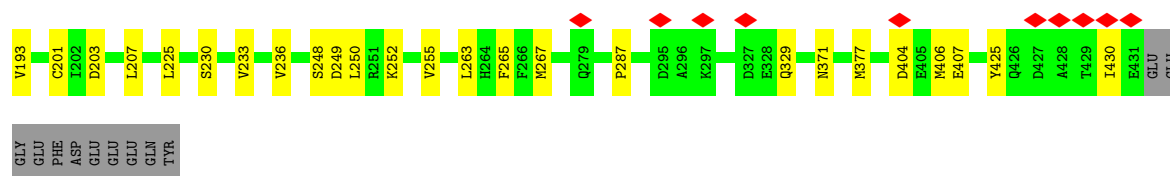


## • Molecule 60: Tubulin beta chain

Chain KR:

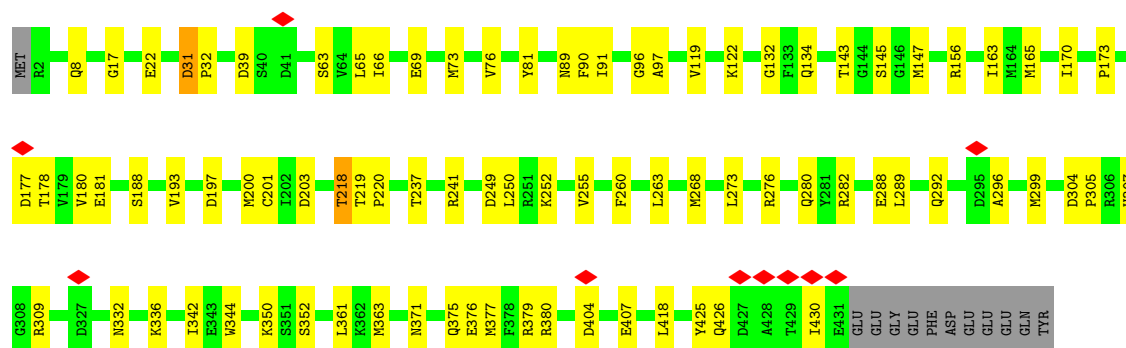






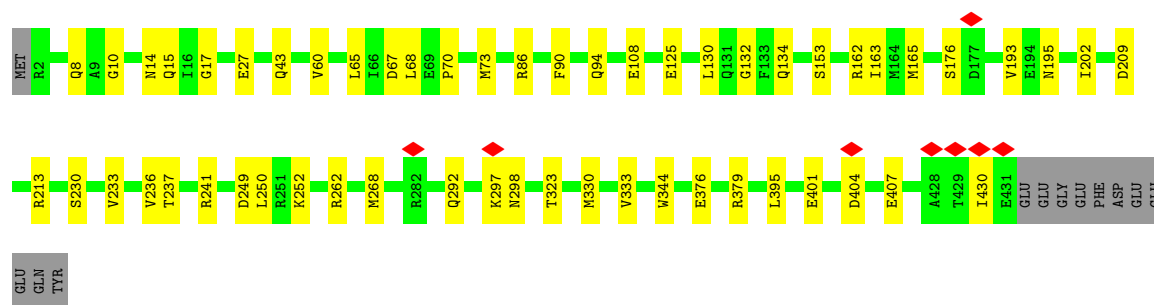
- Molecule 60: Tubulin beta chain

Chain KT: 78% 19%



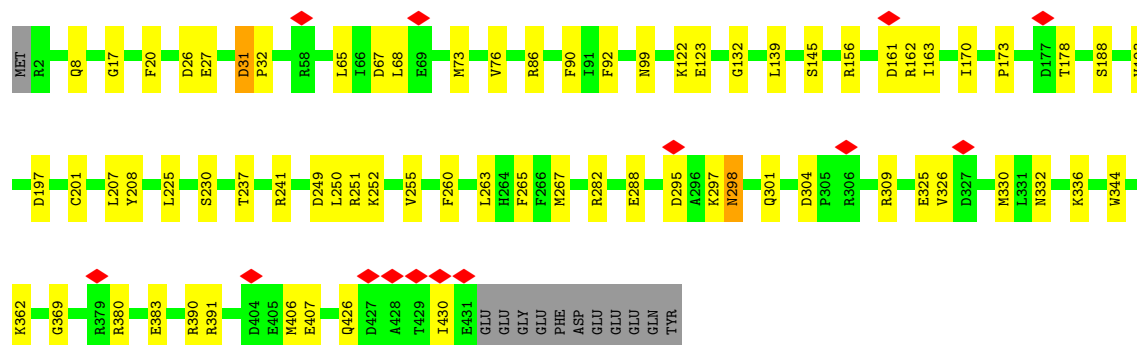
- Molecule 60: Tubulin beta chain

Chain KV: 85% 12%

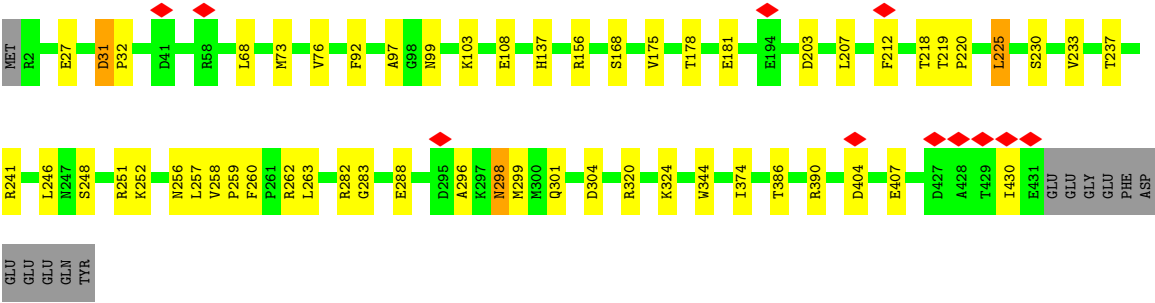
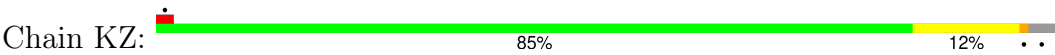


- Molecule 60: Tubulin beta chain

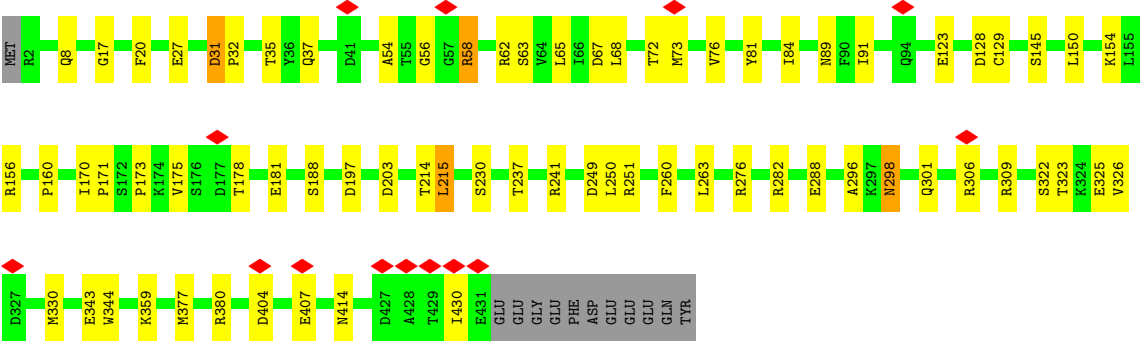
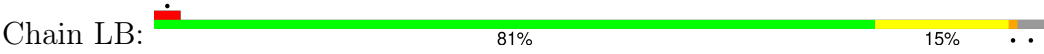
Chain KX: 81% 16%



- Molecule 60: Tubulin beta chain



• Molecule 60: Tubulin beta chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	455012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.875	Depositor
Minimum map value	0.000	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.17	Depositor
Map size ( $\text{\AA}$ )	499.40002, 358.6, 641.3	wwPDB
Map dimensions	454, 326, 583	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0A	0.29	0/5506	0.56	1/7437 (0.0%)
1	0B	0.28	0/6058	0.54	0/8179
1	0C	0.28	0/6100	0.56	1/8236 (0.0%)
1	0D	0.28	0/1091	0.51	0/1482
2	0E	0.28	0/6005	0.54	1/8131 (0.0%)
3	0F	0.29	0/5505	0.55	0/7432
4	0G	0.27	0/6276	0.56	2/8472 (0.0%)
5	0H	0.33	0/2303	0.58	1/3061 (0.0%)
5	0I	0.33	0/1065	0.56	0/1412
5	0J	0.25	0/378	0.58	0/496
5	0K	0.33	0/3170	0.56	0/4220
6	0M	0.32	0/2593	0.60	0/3444
6	0N	0.33	0/1464	0.62	0/1948
7	0O	0.31	0/1296	0.65	0/1720
7	0P	0.34	0/2600	0.68	0/3451
8	0Q	0.30	0/2642	0.53	1/3581 (0.0%)
9	0R	0.28	0/2741	0.55	1/3718 (0.0%)
10	0S	0.29	0/3398	0.52	0/4607
11	0T	0.29	0/3352	0.53	0/4527
12	0U	0.29	0/2503	0.54	0/3389
13	0V	0.27	0/1285	0.53	0/1751
14	0W	0.29	0/845	0.61	0/1129
15	0X	0.29	0/1489	0.54	0/2011
16	0Y	0.28	0/2164	0.53	0/2952
17	0Z	0.28	0/3791	0.52	0/5129
18	1A	0.29	0/2993	0.54	1/4043 (0.0%)
19	1B	0.29	0/2307	0.56	0/3114
20	1C	0.28	0/1956	0.56	0/2647
21	1D	0.29	0/2432	0.57	0/3302
22	1E	0.28	0/1923	0.52	0/2598
23	1F	0.28	0/1898	0.56	0/2574
24	1G	0.29	0/1316	0.56	1/1786 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
25	1H	0.26	0/2045	0.55	0/2779
26	1I	0.27	0/2596	0.54	0/3530
26	1J	0.27	0/726	0.52	0/982
27	1K	0.29	0/2168	0.56	0/2923
27	1L	0.27	0/1124	0.58	0/1511
28	1M	0.26	0/1813	0.54	1/2455 (0.0%)
28	1N	0.28	0/833	0.53	0/1127
29	1O	0.31	0/983	0.52	0/1343
29	1P	0.33	0/437	0.54	0/597
29	4X	0.27	0/361	0.48	0/494
30	1Q	0.29	0/2279	0.58	1/3083 (0.0%)
30	1R	0.29	0/2279	0.54	0/3083
30	1S	0.30	0/2279	0.56	0/3083
31	1T	0.28	0/1862	0.51	0/2526
31	1U	0.28	0/1862	0.51	0/2526
32	1V	0.29	0/1572	0.56	0/2124
32	1W	0.28	0/1572	0.55	0/2124
32	1X	0.29	0/1572	0.55	0/2124
32	1Y	0.30	0/1572	0.54	0/2124
32	1Z	0.29	0/1572	0.55	0/2124
32	2A	0.31	0/1572	0.55	0/2124
33	2B	0.28	0/4752	0.58	1/6445 (0.0%)
33	2C	0.28	0/4809	0.58	2/6522 (0.0%)
33	2D	0.27	0/4809	0.59	2/6522 (0.0%)
34	2E	0.29	0/1903	0.58	1/2566 (0.0%)
34	2F	0.29	0/1903	0.54	0/2566
35	2G	0.27	0/1488	0.57	0/1995
35	2H	0.28	0/1266	0.60	0/1688
36	2I	0.29	0/2276	0.56	1/3084 (0.0%)
36	2J	0.29	0/2243	0.57	1/3038 (0.0%)
36	2K	0.27	0/2243	0.55	0/3038
37	2L	0.27	0/1944	0.54	0/2631
37	2M	0.28	0/1944	0.52	0/2631
38	2N	0.30	0/1951	0.54	0/2639
39	2O	0.32	0/1607	0.59	0/2137
39	2P	0.38	0/2602	0.63	0/3452
39	2Q	0.33	0/2692	0.61	0/3587
39	2R	0.36	0/1619	0.69	0/2144
40	2S	0.27	0/654	0.68	0/875
40	2T	0.31	0/3705	0.62	1/4926 (0.0%)
40	2U	0.30	0/571	0.57	0/763
41	2V	0.28	0/1077	0.55	0/1443
41	2W	0.32	0/1998	0.62	0/2655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
41	2X	0.28	0/449	0.63	0/603
41	2Y	0.31	0/2842	0.58	0/3790
41	2Z	0.31	0/2287	0.62	2/3054 (0.1%)
41	3A	0.31	0/967	0.63	0/1288
41	3B	0.32	0/1443	0.61	0/1938
41	3C	0.31	0/1814	0.63	0/2410
41	3D	0.35	0/2167	0.65	0/2881
42	3E	0.27	0/534	0.50	0/730
42	3F	0.29	0/1527	0.52	0/2073
42	3G	0.28	0/1435	0.55	0/1954
42	3H	0.28	0/654	0.60	1/883 (0.1%)
42	3I	0.28	0/918	0.54	0/1249
42	3J	0.27	0/1218	0.53	0/1650
42	3K	0.27	0/415	0.53	0/567
42	3L	0.32	0/1538	0.59	0/2084
42	3M	0.28	0/1574	0.57	1/2141 (0.0%)
42	3N	0.36	0/508	0.56	0/687
42	3O	0.31	0/1008	0.59	2/1370 (0.1%)
42	3P	0.27	0/995	0.56	0/1347
43	3Q	0.26	0/1329	0.53	0/1791
44	3R	0.32	0/1370	0.57	0/1856
45	3S	0.29	0/1304	0.54	0/1756
46	3T	0.28	0/1443	0.53	0/1957
46	3U	0.28	0/1160	0.52	0/1568
47	3V	0.29	0/1961	0.55	0/2639
47	3W	0.28	0/1947	0.59	1/2622 (0.0%)
47	3X	0.31	0/1883	0.61	0/2536
48	3Y	0.31	0/2061	0.59	0/2778
48	3Z	0.29	0/1004	0.64	0/1344
48	4A	0.29	0/1977	0.59	0/2662
49	4B	0.25	0/868	0.54	0/1157
49	4C	0.25	0/899	0.53	0/1199
49	4D	0.27	0/839	0.52	0/1119
50	4E	0.26	0/328	0.64	0/437
50	4F	0.26	0/1071	0.50	0/1439
50	4G	0.26	0/328	0.68	0/437
51	4H	0.31	0/1686	0.54	0/2272
52	4I	0.29	0/1042	0.51	0/1404
52	4J	0.40	0/229	0.54	0/310
53	4K	0.32	0/1707	0.57	0/2317
53	4L	0.31	0/907	0.56	0/1223
54	4M	0.27	0/1396	0.63	1/1865 (0.1%)
54	4N	0.25	0/1396	0.57	0/1865

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
54	4O	0.25	0/1389	0.55	0/1855
55	4P	0.27	0/1205	0.59	1/1602 (0.1%)
56	4Q	0.26	0/590	0.56	0/788
57	4R	0.31	0/1132	0.66	0/1514
57	4S	0.27	0/1172	0.62	0/1568
57	4Y	0.25	0/333	0.59	0/447
58	4T	0.28	0/655	0.67	0/877
58	4U	0.28	0/655	0.62	0/877
58	4V	0.28	0/655	0.60	0/877
58	4W	0.29	0/655	0.62	0/877
59	AA	0.34	0/3494	0.62	0/4744
59	AC	0.33	0/3494	0.62	0/4744
59	AE	0.34	0/3494	0.63	0/4744
59	AG	0.34	0/3494	0.61	0/4744
59	AI	0.32	0/3494	0.61	0/4744
59	AK	0.32	0/3494	0.61	0/4744
59	AM	0.33	0/3494	0.65	0/4744
59	AO	0.34	0/3494	0.65	0/4744
59	AQ	0.34	0/3494	0.63	0/4744
59	AS	0.34	0/3494	0.66	1/4744 (0.0%)
59	AU	0.33	0/3494	0.66	2/4744 (0.0%)
59	AW	0.33	0/3494	0.61	0/4744
59	AY	0.32	0/3494	0.63	1/4744 (0.0%)
59	BA	0.30	0/3494	0.61	0/4744
59	BC	0.33	0/3494	0.66	3/4744 (0.1%)
59	BE	0.33	0/3494	0.62	0/4744
59	BG	0.34	0/3494	0.62	0/4744
59	BI	0.34	0/3494	0.66	2/4744 (0.0%)
59	BK	0.32	0/3494	0.63	0/4744
59	BM	0.32	0/3494	0.63	1/4744 (0.0%)
59	BO	0.33	0/3494	0.60	0/4744
59	BQ	0.34	0/3494	0.62	1/4744 (0.0%)
59	BS	0.35	0/3494	0.63	1/4744 (0.0%)
59	BU	0.37	0/3494	0.64	1/4744 (0.0%)
59	BW	0.35	0/3494	0.63	0/4744
59	BX	0.32	0/3494	0.64	1/4744 (0.0%)
59	BZ	0.32	0/3494	0.63	1/4744 (0.0%)
59	CB	0.31	0/3494	0.62	0/4744
59	CD	0.33	0/3494	0.64	1/4744 (0.0%)
59	CF	0.32	0/3494	0.63	1/4744 (0.0%)
59	CH	0.33	0/3494	0.63	1/4744 (0.0%)
59	CJ	0.33	0/3494	0.67	2/4744 (0.0%)
59	CM	0.33	0/3494	0.62	0/4744

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
59	CO	0.31	0/3494	0.62	0/4744
59	CQ	0.32	0/3494	0.62	0/4744
59	CS	0.31	0/3494	0.64	0/4744
59	CU	0.33	0/3494	0.64	1/4744 (0.0%)
59	CW	0.31	0/3494	0.62	0/4744
59	CY	0.33	0/3494	0.58	0/4744
59	DA	0.32	0/3494	0.61	0/4744
59	DC	0.31	0/3494	0.59	0/4744
59	DE	0.34	0/3494	0.65	3/4744 (0.1%)
59	DG	0.35	0/3494	0.62	1/4744 (0.0%)
59	DI	0.32	0/3494	0.64	2/4744 (0.0%)
59	DK	0.33	0/3494	0.62	0/4744
59	DM	0.33	0/3494	0.63	0/4744
59	DO	0.34	0/3494	0.66	3/4744 (0.1%)
59	DQ	0.32	0/3494	0.61	1/4744 (0.0%)
59	DS	0.33	0/3494	0.64	2/4744 (0.0%)
59	DU	0.33	0/3494	0.60	0/4744
59	DX	0.32	0/3494	0.62	1/4744 (0.0%)
59	DZ	0.33	0/3494	0.59	0/4744
59	EB	0.32	0/3494	0.60	0/4744
59	ED	0.33	0/3494	0.60	1/4744 (0.0%)
59	EF	0.32	0/3494	0.60	0/4744
59	EH	0.31	0/3494	0.58	0/4744
59	EJ	0.31	0/3494	0.60	0/4744
59	EL	0.33	0/3494	0.62	0/4744
59	EN	0.31	0/3494	0.61	0/4744
59	EP	0.31	0/3494	0.61	0/4744
59	ER	0.32	0/3494	0.63	2/4744 (0.0%)
59	ET	0.32	0/3494	0.62	1/4744 (0.0%)
59	EV	0.31	0/3494	0.60	0/4744
59	EX	0.32	0/3494	0.60	0/4744
59	EZ	0.33	0/3494	0.61	1/4744 (0.0%)
59	FB	0.32	0/3494	0.60	3/4744 (0.1%)
59	FD	0.33	0/3494	0.63	0/4744
59	FF	0.33	0/3494	0.57	0/4744
59	FH	0.33	0/3494	0.63	1/4744 (0.0%)
59	FJ	0.31	0/3494	0.60	1/4744 (0.0%)
59	FL	0.32	0/3494	0.60	0/4744
59	FN	0.32	0/3494	0.62	1/4744 (0.0%)
59	FP	0.35	0/3494	0.60	0/4744
59	FR	0.31	0/3494	0.59	0/4744
59	FT	0.32	0/3494	0.60	1/4744 (0.0%)
59	FU	0.32	0/3494	0.63	1/4744 (0.0%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
59	FW	0.31	0/3494	0.59	1/4744 (0.0%)
59	FY	0.35	0/3494	0.61	0/4744
59	GA	0.32	0/3494	0.61	0/4744
59	GC	0.34	0/3494	0.60	0/4744
59	GE	0.31	0/3494	0.60	0/4744
59	GG	0.36	0/3494	0.63	0/4744
59	GH	0.35	0/3494	0.64	1/4744 (0.0%)
59	GJ	0.31	0/3494	0.61	1/4744 (0.0%)
59	GL	0.33	0/3494	0.64	0/4744
59	GN	0.33	0/3494	0.64	0/4744
59	GP	0.33	0/3494	0.67	0/4744
59	GR	0.32	0/3494	0.64	3/4744 (0.1%)
59	GT	0.34	0/3494	0.68	2/4744 (0.0%)
59	GU	0.33	0/3494	0.63	2/4744 (0.0%)
59	GW	0.34	0/3494	0.63	0/4744
59	GY	0.34	0/3494	0.67	2/4744 (0.0%)
59	HA	0.34	0/3494	0.64	1/4744 (0.0%)
59	HC	0.35	0/3494	0.64	0/4744
59	HE	0.34	0/3494	0.67	1/4744 (0.0%)
59	HG	0.33	0/3494	0.64	1/4744 (0.0%)
59	HI	0.33	0/3494	0.65	0/4744
59	HK	0.32	0/3494	0.64	1/4744 (0.0%)
59	HM	0.34	0/3494	0.67	3/4744 (0.1%)
59	HO	0.33	0/3494	0.62	0/4744
59	HQ	0.35	0/3494	0.68	1/4744 (0.0%)
59	HT	0.33	0/3494	0.66	4/4744 (0.1%)
59	HV	0.30	0/3494	0.62	1/4744 (0.0%)
59	HX	0.34	0/3494	0.63	1/4744 (0.0%)
59	HZ	0.34	0/3494	0.65	1/4744 (0.0%)
59	IB	0.34	0/3494	0.65	1/4744 (0.0%)
59	ID	0.32	0/3494	0.65	1/4744 (0.0%)
59	IG	0.35	0/3494	0.65	2/4744 (0.0%)
59	II	0.34	0/3494	0.64	1/4744 (0.0%)
59	IK	0.33	0/3494	0.65	0/4744
59	IM	0.34	0/3494	0.65	1/4744 (0.0%)
59	IO	0.31	0/3494	0.63	0/4744
59	IQ	0.32	0/3494	0.65	1/4744 (0.0%)
59	IT	0.34	0/3494	0.63	0/4744
59	IV	0.35	0/3494	0.63	1/4744 (0.0%)
59	IX	0.34	0/3494	0.66	1/4744 (0.0%)
59	IZ	0.35	0/3494	0.66	0/4744
59	JB	0.32	0/3494	0.60	0/4744
59	JD	0.36	0/3494	0.66	1/4744 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
59	JF	0.32	0/3494	0.62	1/4744 (0.0%)
59	JH	0.33	0/3494	0.64	0/4744
59	JJ	0.35	0/3494	0.66	1/4744 (0.0%)
59	JL	0.33	0/3494	0.65	1/4744 (0.0%)
59	JN	0.34	0/3494	0.63	0/4744
59	JP	0.34	0/3494	0.63	2/4744 (0.0%)
59	JQ	0.33	0/3494	0.67	1/4744 (0.0%)
59	JS	0.37	0/3494	0.67	0/4744
59	JU	0.32	0/3494	0.65	0/4744
59	JW	0.33	0/3494	0.66	1/4744 (0.0%)
59	JY	0.34	0/3494	0.65	0/4744
59	KA	0.33	0/3494	0.68	1/4744 (0.0%)
59	KC	0.33	0/3494	0.65	0/4744
59	KD	0.33	0/3494	0.65	0/4744
59	KF	0.32	0/3494	0.60	0/4744
59	KH	0.32	0/3494	0.61	1/4744 (0.0%)
59	KJ	0.33	0/3494	0.65	2/4744 (0.0%)
59	KL	0.31	0/3494	0.61	0/4744
59	KN	0.34	0/3494	0.62	0/4744
59	KP	0.38	0/3494	0.70	1/4744 (0.0%)
59	KQ	0.31	0/3494	0.62	1/4744 (0.0%)
59	KS	0.31	0/3494	0.61	1/4744 (0.0%)
59	KU	0.32	0/3494	0.61	0/4744
59	KW	0.32	0/3494	0.65	1/4744 (0.0%)
59	KY	0.32	0/3494	0.62	0/4744
59	LA	0.32	0/3494	0.62	1/4744 (0.0%)
60	AB	0.35	0/3443	0.61	1/4657 (0.0%)
60	AD	0.32	0/3443	0.63	1/4657 (0.0%)
60	AF	0.34	0/3443	0.67	3/4657 (0.1%)
60	AH	0.30	0/3443	0.60	1/4657 (0.0%)
60	AJ	0.31	0/3443	0.62	2/4657 (0.0%)
60	AL	0.31	0/3443	0.62	1/4657 (0.0%)
60	AN	0.35	0/3443	0.64	2/4657 (0.0%)
60	AP	0.33	0/3443	0.66	3/4657 (0.1%)
60	AR	0.35	0/3443	0.65	1/4657 (0.0%)
60	AT	0.32	0/3443	0.64	1/4657 (0.0%)
60	AV	0.33	0/3443	0.64	1/4657 (0.0%)
60	AX	0.33	0/3443	0.68	2/4657 (0.0%)
60	AZ	0.32	0/3443	0.66	2/4657 (0.0%)
60	BB	0.31	0/3443	0.62	4/4657 (0.1%)
60	BD	0.34	0/3443	0.68	2/4657 (0.0%)
60	BF	0.33	0/3443	0.66	4/4657 (0.1%)
60	BH	0.34	0/3443	0.62	1/4657 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	BJ	0.36	0/3443	0.66	2/4657 (0.0%)
60	BL	0.32	0/3443	0.67	1/4657 (0.0%)
60	BN	0.30	0/3443	0.62	3/4657 (0.1%)
60	BP	0.34	0/3443	0.66	2/4657 (0.0%)
60	BR	0.34	0/3443	0.66	1/4657 (0.0%)
60	BT	0.33	0/3443	0.63	2/4657 (0.0%)
60	BV	0.33	0/3443	0.65	2/4657 (0.0%)
60	BY	0.34	0/3443	0.64	2/4657 (0.0%)
60	CA	0.33	0/3443	0.63	1/4657 (0.0%)
60	CC	0.34	0/3443	0.68	2/4657 (0.0%)
60	CE	0.33	0/3443	0.65	1/4657 (0.0%)
60	CG	0.33	0/3443	0.67	3/4657 (0.1%)
60	CI	0.34	0/3443	0.70	2/4657 (0.0%)
60	CL	0.31	0/3443	0.62	1/4657 (0.0%)
60	CN	0.31	0/3443	0.64	1/4657 (0.0%)
60	CP	0.32	0/3443	0.65	3/4657 (0.1%)
60	CR	0.35	0/3443	0.66	1/4657 (0.0%)
60	CT	0.32	0/3443	0.66	5/4657 (0.1%)
60	CV	0.32	0/3443	0.67	3/4657 (0.1%)
60	CX	0.34	0/3443	0.63	1/4657 (0.0%)
60	CZ	0.33	0/3443	0.63	0/4657
60	DB	0.34	0/3443	0.61	1/4657 (0.0%)
60	DD	0.31	0/3443	0.64	1/4657 (0.0%)
60	DF	0.32	0/3443	0.62	0/4657
60	DH	0.32	0/3443	0.63	1/4657 (0.0%)
60	DJ	0.31	0/3443	0.62	1/4657 (0.0%)
60	DL	0.33	0/3443	0.63	2/4657 (0.0%)
60	DN	0.32	0/3443	0.65	1/4657 (0.0%)
60	DP	0.34	0/3443	0.65	3/4657 (0.1%)
60	DR	0.32	0/3443	0.66	2/4657 (0.0%)
60	DT	0.32	0/3443	0.62	2/4657 (0.0%)
60	DV	0.33	0/3443	0.62	1/4657 (0.0%)
60	DW	0.32	0/3443	0.63	1/4657 (0.0%)
60	DY	0.32	0/3443	0.62	1/4657 (0.0%)
60	EA	0.32	0/3443	0.66	2/4657 (0.0%)
60	EC	0.32	0/3443	0.63	2/4657 (0.0%)
60	EE	0.34	0/3443	0.63	1/4657 (0.0%)
60	EG	0.32	0/3443	0.60	0/4657
60	EI	0.32	0/3443	0.61	0/4657
60	EK	0.32	0/3443	0.60	1/4657 (0.0%)
60	EM	0.32	0/3443	0.64	2/4657 (0.0%)
60	EO	0.32	0/3443	0.60	0/4657
60	EQ	0.32	0/3443	0.64	2/4657 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	ES	0.31	0/3443	0.62	1/4657 (0.0%)
60	EU	0.33	0/3443	0.65	2/4657 (0.0%)
60	EW	0.31	0/3443	0.61	2/4657 (0.0%)
60	EY	0.30	0/3443	0.61	0/4657
60	FA	0.30	0/3443	0.58	1/4657 (0.0%)
60	FC	0.32	0/3443	0.60	0/4657
60	FE	0.31	0/3443	0.57	0/4657
60	FG	0.31	0/3443	0.62	2/4657 (0.0%)
60	FI	0.37	0/3443	0.63	1/4657 (0.0%)
60	FK	0.31	0/3443	0.60	0/4657
60	FM	0.30	0/3443	0.59	1/4657 (0.0%)
60	FO	0.31	0/3443	0.63	0/4657
60	FQ	0.35	0/3443	0.64	1/4657 (0.0%)
60	FS	0.30	0/3443	0.62	2/4657 (0.0%)
60	FV	0.31	0/3443	0.61	0/4657
60	FX	0.31	0/3443	0.60	1/4657 (0.0%)
60	FZ	0.32	0/3443	0.64	0/4657
60	GB	0.31	0/3443	0.62	1/4657 (0.0%)
60	GD	0.33	0/3443	0.64	1/4657 (0.0%)
60	GF	0.32	0/3443	0.65	2/4657 (0.0%)
60	GI	0.31	0/3443	0.61	2/4657 (0.0%)
60	GK	0.31	0/3443	0.67	5/4657 (0.1%)
60	GM	0.32	0/3443	0.68	6/4657 (0.1%)
60	GO	0.31	0/3443	0.64	1/4657 (0.0%)
60	GQ	0.32	0/3443	0.67	1/4657 (0.0%)
60	GS	0.32	0/3443	0.73	9/4657 (0.2%)
60	GV	0.35	0/3443	0.66	0/4657
60	GX	0.32	0/3443	0.64	3/4657 (0.1%)
60	GZ	0.34	0/3443	0.66	2/4657 (0.0%)
60	HB	0.34	0/3443	0.65	2/4657 (0.0%)
60	HD	0.34	0/3443	0.66	2/4657 (0.0%)
60	HF	0.35	0/3443	0.68	3/4657 (0.1%)
60	HH	0.34	0/3443	0.65	3/4657 (0.1%)
60	HJ	0.33	0/3443	0.65	2/4657 (0.0%)
60	HL	0.32	0/3443	0.68	6/4657 (0.1%)
60	HN	0.33	0/3443	0.66	5/4657 (0.1%)
60	HP	0.34	0/3443	0.63	1/4657 (0.0%)
60	HR	0.32	0/3443	0.68	3/4657 (0.1%)
60	HS	0.36	0/3443	0.68	3/4657 (0.1%)
60	HU	0.32	0/3443	0.63	1/4657 (0.0%)
60	HW	0.32	0/3443	0.63	4/4657 (0.1%)
60	HY	0.32	0/3443	0.70	4/4657 (0.1%)
60	IA	0.31	0/3443	0.63	2/4657 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	IC	0.34	0/3443	0.65	3/4657 (0.1%)
60	IE	0.31	0/3443	0.68	2/4657 (0.0%)
60	IF	0.33	0/3443	0.66	0/4657
60	IH	0.32	0/3443	0.69	4/4657 (0.1%)
60	IJ	0.31	0/3443	0.62	2/4657 (0.0%)
60	IL	0.31	0/3443	0.64	1/4657 (0.0%)
60	IN	0.32	0/3443	0.65	1/4657 (0.0%)
60	IP	0.37	0/3443	0.70	4/4657 (0.1%)
60	IR	0.34	0/3443	0.65	1/4657 (0.0%)
60	IS	0.33	0/3443	0.69	6/4657 (0.1%)
60	IU	0.32	0/3443	0.65	1/4657 (0.0%)
60	IW	0.32	0/3443	0.65	1/4657 (0.0%)
60	IY	0.36	0/3443	0.69	1/4657 (0.0%)
60	JA	0.33	0/3443	0.63	2/4657 (0.0%)
60	JC	0.35	0/3443	0.69	3/4657 (0.1%)
60	JE	0.35	0/3443	0.70	1/4657 (0.0%)
60	JG	0.31	0/3443	0.66	2/4657 (0.0%)
60	JI	0.31	0/3443	0.65	0/4657
60	JK	0.32	0/3443	0.66	1/4657 (0.0%)
60	JM	0.31	0/3443	0.64	0/4657
60	JO	0.32	0/3443	0.62	0/4657
60	JR	0.34	0/3443	0.64	3/4657 (0.1%)
60	JT	0.34	0/3443	0.64	1/4657 (0.0%)
60	JV	0.31	0/3443	0.64	1/4657 (0.0%)
60	JX	0.32	0/3443	0.64	1/4657 (0.0%)
60	JZ	0.32	0/3443	0.64	1/4657 (0.0%)
60	KB	0.34	0/3443	0.67	2/4657 (0.0%)
60	KE	0.30	0/3443	0.62	1/4657 (0.0%)
60	KG	0.31	0/3443	0.63	2/4657 (0.0%)
60	KI	0.30	0/3443	0.63	1/4657 (0.0%)
60	KK	0.32	0/3443	0.60	0/4657
60	KM	0.33	0/3443	0.63	0/4657
60	KO	0.36	0/3443	0.66	0/4657
60	KR	0.32	0/3443	0.64	2/4657 (0.0%)
60	KT	0.33	0/3443	0.63	1/4657 (0.0%)
60	KV	0.31	0/3443	0.62	2/4657 (0.0%)
60	KX	0.32	0/3443	0.65	2/4657 (0.0%)
60	KZ	0.33	0/3443	0.65	2/4657 (0.0%)
60	LB	0.32	0/3443	0.65	2/4657 (0.0%)
All	All	0.32	0/1231985	0.62	376/1667820 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
23	1F	0	1
29	1O	0	1
36	2J	0	1
41	3D	0	1
42	3O	0	1
48	4A	0	1
53	4L	0	1
59	AW	0	1
59	BC	0	1
59	BW	0	1
59	CB	0	1
59	CD	0	1
59	DM	0	1
59	DU	0	3
59	FP	0	2
59	GT	0	1
59	GU	0	1
59	GY	0	2
59	HA	0	1
59	HT	0	3
59	JH	0	1
59	JQ	0	1
59	JY	0	2
59	KN	0	1
60	AN	0	1
60	BD	0	1
60	BF	0	1
60	BJ	0	1
60	BP	0	1
60	CA	0	1
60	DB	0	1
60	DL	0	2
60	FA	0	1
60	FI	0	1
60	GF	0	1
60	HD	0	1
60	HF	0	1
60	HS	0	1
60	HY	0	1
60	IR	0	2
60	IW	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
60	KB	0	1
60	KO	0	1
60	KZ	0	2
All	All	0	54

There are no bond length outliers.

The worst 5 of 376 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	DR	31	ASP	CB-CG-OD1	8.18	125.66	118.30
60	BF	31	ASP	CB-CG-OD1	8.15	125.63	118.30
60	EC	130	LEU	CA-CB-CG	8.07	133.87	115.30
60	HW	31	ASP	CB-CG-OD1	7.99	125.49	118.30
60	KZ	31	ASP	CB-CG-OD1	7.98	125.48	118.30

There are no chirality outliers.

5 of 54 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	1F	95	ARG	Sidechain
29	1O	68	ARG	Sidechain
36	2J	287	ARG	Sidechain
41	3D	121	ARG	Sidechain
42	3O	234	ARG	Sidechain

## 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	0A	5390	0	5328	47	0
1	0B	5933	0	5864	50	0
1	0C	5972	0	5894	43	0
1	0D	1064	0	1037	7	0
2	0E	5862	0	5700	70	0
3	0F	5389	0	5312	74	0
4	0G	6157	0	6132	70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	0H	2274	0	2235	35	0
5	0I	1052	0	1023	13	0
5	0J	376	0	399	1	0
5	0K	3130	0	3087	33	0
6	0M	2576	0	2600	27	0
6	0N	1449	0	1484	15	0
7	0O	1288	0	1299	31	0
7	0P	2584	0	2623	39	0
8	0Q	2587	0	2547	11	0
9	0R	2685	0	2682	21	0
10	0S	3331	0	3274	17	0
11	0T	3295	0	3282	21	0
12	0U	2446	0	2448	27	0
13	0V	1262	0	1280	13	0
14	0W	836	0	819	6	0
15	0X	1457	0	1453	20	0
16	0Y	2100	0	2006	21	0
17	0Z	3717	0	3694	47	0
18	1A	2920	0	2749	29	0
19	1B	2252	0	2204	26	0
20	1C	1908	0	1818	17	0
21	1D	2371	0	2347	19	0
22	1E	1880	0	1835	22	0
23	1F	1861	0	1811	28	0
24	1G	1287	0	1283	14	0
25	1H	2005	0	2025	23	0
26	1I	2535	0	2459	25	0
26	1J	707	0	693	7	0
27	1K	2119	0	2082	37	0
27	1L	1103	0	1056	15	0
28	1M	1778	0	1791	19	0
28	1N	814	0	777	6	0
29	1O	953	0	909	9	0
29	1P	423	0	404	2	0
29	4X	348	0	329	3	0
30	1Q	2223	0	2243	13	0
30	1R	2223	0	2243	23	0
30	1S	2223	0	2243	21	0
31	1T	1819	0	1830	18	0
31	1U	1819	0	1830	14	0
32	1V	1537	0	1552	16	0
32	1W	1537	0	1552	19	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	1X	1537	0	1552	15	0
32	1Y	1537	0	1552	21	0
32	1Z	1537	0	1552	18	0
32	2A	1537	0	1552	15	0
33	2B	4671	0	4640	55	0
33	2C	4727	0	4691	56	0
33	2D	4727	0	4691	66	0
34	2E	1867	0	1871	21	0
34	2F	1867	0	1871	28	0
35	2G	1456	0	1465	16	0
35	2H	1248	0	1281	20	0
36	2I	2217	0	2172	24	0
36	2J	2186	0	2149	24	0
36	2K	2186	0	2149	30	0
37	2L	1900	0	1873	20	0
37	2M	1900	0	1873	13	0
38	2N	1911	0	1903	15	0
39	2O	1599	0	1604	28	0
39	2P	2590	0	2644	37	0
39	2Q	2678	0	2711	35	0
39	2R	1613	0	1637	34	0
40	2S	647	0	634	14	0
40	2T	3667	0	3654	50	0
40	2U	564	0	551	2	0
41	2V	1062	0	1074	11	0
41	2W	1977	0	1952	30	0
41	2X	441	0	453	8	0
41	2Y	2808	0	2818	41	0
41	2Z	2259	0	2282	30	0
41	3A	954	0	924	22	0
41	3B	1421	0	1446	13	0
41	3C	1797	0	1776	27	0
41	3D	2146	0	2141	38	0
42	3E	517	0	507	3	0
42	3F	1483	0	1458	15	0
42	3G	1388	0	1363	21	0
42	3H	638	0	625	12	0
42	3I	890	0	880	9	0
42	3J	1184	0	1160	20	0
42	3K	401	0	395	10	0
42	3L	1496	0	1461	33	0
42	3M	1526	0	1501	27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	3N	497	0	487	20	0
42	3O	977	0	957	16	0
42	3P	967	0	951	19	0
43	3Q	1293	0	1241	24	0
44	3R	1338	0	1333	24	0
45	3S	1281	0	1266	23	0
46	3T	1398	0	1393	10	0
46	3U	1120	0	1049	15	0
47	3V	1919	0	1893	39	0
47	3W	1905	0	1880	31	0
47	3X	1843	0	1813	39	0
48	3Y	2017	0	1970	42	0
48	3Z	990	0	963	22	0
48	4A	1937	0	1886	34	0
49	4B	858	0	877	3	0
49	4C	889	0	910	7	0
49	4D	831	0	855	8	0
50	4E	327	0	326	6	0
50	4F	1054	0	997	5	0
50	4G	327	0	326	3	0
51	4H	1642	0	1602	15	0
52	4I	1013	0	978	23	0
52	4J	222	0	220	6	0
53	4K	1650	0	1620	35	0
53	4L	882	0	864	17	0
54	4M	1380	0	1384	18	0
54	4N	1380	0	1384	31	0
54	4O	1373	0	1377	24	0
55	4P	1193	0	1203	25	0
56	4Q	583	0	599	9	0
57	4R	1116	0	1116	25	0
57	4S	1155	0	1161	16	0
57	4Y	327	0	330	9	0
58	4T	643	0	632	9	0
58	4U	643	0	632	9	0
58	4V	643	0	632	8	0
58	4W	643	0	632	6	0
59	AA	3421	0	3336	34	0
59	AC	3421	0	3336	36	0
59	AE	3421	0	3336	27	0
59	AG	3421	0	3336	33	0
59	AI	3421	0	3336	35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AK	3421	0	3336	30	0
59	AM	3421	0	3336	38	0
59	AO	3421	0	3336	36	0
59	AQ	3421	0	3336	34	0
59	AS	3421	0	3336	40	0
59	AU	3421	0	3336	34	0
59	AW	3421	0	3336	29	0
59	AY	3421	0	3336	49	0
59	BA	3421	0	3336	37	0
59	BC	3421	0	3336	39	0
59	BE	3421	0	3336	57	0
59	BG	3421	0	3336	48	0
59	BI	3421	0	3336	54	0
59	BK	3421	0	3336	35	0
59	BM	3421	0	3336	39	0
59	BO	3421	0	3336	32	0
59	BQ	3421	0	3336	42	0
59	BS	3421	0	3336	41	0
59	BU	3421	0	3336	49	0
59	BW	3421	0	3336	42	0
59	BX	3421	0	3336	48	0
59	BZ	3421	0	3336	41	0
59	CB	3421	0	3336	30	0
59	CD	3421	0	3336	44	0
59	CF	3421	0	3336	46	0
59	CH	3421	0	3336	45	0
59	CJ	3421	0	3336	38	0
59	CM	3421	0	3336	42	0
59	CO	3421	0	3336	41	0
59	CQ	3421	0	3336	40	0
59	CS	3421	0	3336	40	0
59	CU	3421	0	3336	47	0
59	CW	3421	0	3336	37	0
59	CY	3421	0	3336	28	0
59	DA	3421	0	3336	29	0
59	DC	3421	0	3336	39	0
59	DE	3421	0	3336	36	0
59	DG	3421	0	3336	35	0
59	DI	3421	0	3336	38	0
59	DK	3421	0	3336	43	0
59	DM	3421	0	3336	44	0
59	DO	3421	0	3336	36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	DQ	3421	0	3336	28	0
59	DS	3421	0	3336	36	0
59	DU	3421	0	3336	25	0
59	DX	3421	0	3336	33	0
59	DZ	3421	0	3336	31	0
59	EB	3421	0	3336	34	0
59	ED	3421	0	3336	32	0
59	EF	3421	0	3336	28	0
59	EH	3421	0	3336	29	0
59	EJ	3421	0	3336	29	0
59	EL	3421	0	3336	33	0
59	EN	3421	0	3336	35	0
59	EP	3421	0	3336	48	0
59	ER	3421	0	3336	52	0
59	ET	3421	0	3336	35	0
59	EV	3421	0	3336	32	0
59	EX	3421	0	3336	37	0
59	EZ	3421	0	3336	36	0
59	FB	3421	0	3336	33	0
59	FD	3421	0	3336	30	0
59	FF	3421	0	3336	24	0
59	FH	3421	0	3336	33	0
59	FJ	3421	0	3336	30	0
59	FL	3421	0	3336	21	0
59	FN	3421	0	3336	24	0
59	FP	3421	0	3336	30	0
59	FR	3421	0	3336	26	0
59	FT	3421	0	3336	29	0
59	FU	3421	0	3336	47	0
59	FW	3421	0	3336	34	0
59	FY	3421	0	3336	27	0
59	GA	3421	0	3336	30	0
59	GC	3421	0	3336	39	0
59	GE	3421	0	3336	51	0
59	GG	3421	0	3336	37	0
59	GH	3421	0	3336	56	0
59	GJ	3421	0	3336	34	0
59	GL	3421	0	3336	51	0
59	GN	3421	0	3336	52	0
59	GP	3421	0	3336	62	0
59	GR	3421	0	3336	59	0
59	GT	3421	0	3336	48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	GU	3421	0	3336	45	0
59	GW	3421	0	3336	46	0
59	GY	3421	0	3336	62	0
59	HA	3421	0	3336	54	0
59	HC	3421	0	3336	57	0
59	HE	3421	0	3336	63	0
59	HG	3421	0	3336	43	0
59	HI	3421	0	3336	54	0
59	HK	3421	0	3336	49	0
59	HM	3421	0	3336	53	0
59	HO	3421	0	3336	40	0
59	HQ	3421	0	3336	55	0
59	HT	3421	0	3336	49	0
59	HV	3421	0	3336	47	0
59	HX	3421	0	3336	62	0
59	HZ	3421	0	3336	68	0
59	IB	3421	0	3336	52	0
59	ID	3421	0	3336	48	0
59	IG	3421	0	3336	57	0
59	II	3421	0	3336	49	0
59	IK	3421	0	3336	52	0
59	IM	3421	0	3336	55	0
59	IO	3421	0	3336	40	0
59	IQ	3421	0	3336	62	0
59	IT	3421	0	3336	57	0
59	IV	3421	0	3336	44	0
59	IX	3421	0	3336	62	0
59	IZ	3421	0	3336	69	0
59	JB	3421	0	3336	45	0
59	JD	3421	0	3336	61	0
59	JF	3421	0	3336	43	0
59	JH	3421	0	3336	44	0
59	JJ	3421	0	3336	68	0
59	JL	3421	0	3336	49	0
59	JN	3421	0	3336	49	0
59	JP	3421	0	3336	43	0
59	JQ	3421	0	3336	54	0
59	JS	3421	0	3336	59	0
59	JU	3421	0	3336	63	0
59	JW	3421	0	3336	69	0
59	JY	3421	0	3336	49	0
59	KA	3421	0	3336	50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	KC	3421	0	3336	47	0
59	KD	3421	0	3336	49	0
59	KF	3421	0	3336	35	0
59	KH	3421	0	3336	50	0
59	KJ	3421	0	3336	41	0
59	KL	3421	0	3336	41	0
59	KN	3421	0	3336	48	0
59	KP	3421	0	3336	63	0
59	KQ	3421	0	3336	49	0
59	KS	3421	0	3336	38	0
59	KU	3421	0	3336	31	0
59	KW	3421	0	3336	39	0
59	KY	3421	0	3336	38	0
59	LA	3421	0	3336	42	0
60	AB	3372	0	3255	45	0
60	AD	3372	0	3255	41	0
60	AF	3372	0	3255	43	0
60	AH	3372	0	3255	33	0
60	AJ	3372	0	3255	42	0
60	AL	3372	0	3255	35	0
60	AN	3372	0	3255	42	0
60	AP	3372	0	3255	32	0
60	AR	3372	0	3255	47	0
60	AT	3372	0	3255	48	0
60	AV	3372	0	3255	44	0
60	AX	3372	0	3255	57	0
60	AZ	3372	0	3255	61	0
60	BB	3372	0	3255	37	0
60	BD	3372	0	3255	50	0
60	BF	3372	0	3255	47	0
60	BH	3372	0	3255	46	0
60	BJ	3372	0	3255	52	0
60	BL	3372	0	3255	52	0
60	BN	3372	0	3255	41	0
60	BP	3372	0	3255	49	0
60	BR	3372	0	3255	55	0
60	BT	3372	0	3255	48	0
60	BV	3372	0	3255	51	0
60	BY	3372	0	3255	46	0
60	CA	3372	0	3255	55	0
60	CC	3372	0	3255	64	0
60	CE	3372	0	3255	45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	CG	3372	0	3255	65	0
60	CI	3372	0	3255	62	0
60	CL	3372	0	3255	42	0
60	CN	3372	0	3255	45	0
60	CP	3372	0	3255	58	0
60	CR	3372	0	3255	66	0
60	CT	3372	0	3255	54	0
60	CV	3372	0	3255	61	0
60	CX	3372	0	3255	38	0
60	CZ	3372	0	3255	40	0
60	DB	3372	0	3255	46	0
60	DD	3372	0	3255	51	0
60	DF	3372	0	3255	45	0
60	DH	3372	0	3255	34	0
60	DJ	3372	0	3255	43	0
60	DL	3372	0	3255	44	0
60	DN	3372	0	3255	55	0
60	DP	3372	0	3255	46	0
60	DR	3372	0	3255	52	0
60	DT	3372	0	3255	32	0
60	DV	3372	0	3255	36	0
60	DW	3372	0	3255	49	0
60	DY	3372	0	3255	41	0
60	EA	3372	0	3255	46	0
60	EC	3372	0	3255	45	0
60	EE	3372	0	3255	39	0
60	EG	3372	0	3255	34	0
60	EI	3372	0	3255	36	0
60	EK	3372	0	3255	58	0
60	EM	3372	0	3255	47	0
60	EO	3372	0	3255	53	0
60	EQ	3372	0	3255	72	0
60	ES	3372	0	3255	49	0
60	EU	3372	0	3255	46	0
60	EW	3372	0	3255	37	0
60	EY	3372	0	3255	45	0
60	FA	3372	0	3255	29	0
60	FC	3372	0	3255	52	0
60	FE	3372	0	3255	32	0
60	FG	3372	0	3255	37	0
60	FI	3372	0	3255	52	0
60	FK	3372	0	3255	36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	FM	3372	0	3255	37	0
60	FO	3372	0	3255	46	0
60	FQ	3372	0	3255	51	0
60	FS	3372	0	3255	51	0
60	FV	3372	0	3255	46	0
60	FX	3372	0	3255	39	0
60	FZ	3372	0	3255	34	0
60	GB	3372	0	3255	42	0
60	GD	3372	0	3255	56	0
60	GF	3372	0	3255	46	0
60	GI	3372	0	3255	37	0
60	GK	3372	0	3255	53	0
60	GM	3372	0	3255	56	0
60	GO	3372	0	3255	63	0
60	GQ	3372	0	3255	70	0
60	GS	3372	0	3255	77	0
60	GV	3372	0	3255	57	0
60	GX	3372	0	3255	38	0
60	GZ	3372	0	3255	51	0
60	HB	3372	0	3255	62	0
60	HD	3372	0	3255	54	0
60	HF	3372	0	3255	68	0
60	HH	3372	0	3255	57	0
60	HJ	3372	0	3255	54	0
60	HL	3372	0	3255	51	0
60	HN	3372	0	3255	51	0
60	HP	3372	0	3255	48	0
60	HR	3372	0	3255	69	0
60	HS	3372	0	3255	74	0
60	HU	3372	0	3255	56	0
60	HW	3372	0	3255	55	0
60	HY	3372	0	3255	56	0
60	IA	3372	0	3255	59	0
60	IC	3372	0	3255	48	0
60	IE	3372	0	3255	62	0
60	IF	3372	0	3255	67	0
60	IH	3372	0	3255	55	0
60	IJ	3372	0	3255	48	0
60	IL	3372	0	3255	67	0
60	IN	3372	0	3255	61	0
60	IP	3372	0	3255	79	0
60	IR	3372	0	3255	49	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	IS	3372	0	3255	71	0
60	IU	3372	0	3255	76	0
60	IW	3372	0	3255	67	0
60	IY	3372	0	3255	68	0
60	JA	3372	0	3255	62	0
60	JC	3372	0	3255	61	0
60	JE	3372	0	3255	88	0
60	JG	3372	0	3255	71	0
60	JI	3372	0	3255	62	0
60	JK	3372	0	3255	83	0
60	JM	3372	0	3255	51	0
60	JO	3372	0	3255	57	0
60	JR	3372	0	3255	65	0
60	JT	3372	0	3255	57	0
60	JV	3372	0	3255	58	0
60	JX	3372	0	3255	47	0
60	JZ	3372	0	3255	55	0
60	KB	3372	0	3255	46	0
60	KE	3372	0	3255	44	0
60	KG	3372	0	3255	51	0
60	KI	3372	0	3255	34	0
60	KK	3372	0	3255	51	0
60	KM	3372	0	3255	52	0
60	KO	3372	0	3255	40	0
60	KR	3372	0	3255	38	0
60	KT	3372	0	3255	57	0
60	KV	3372	0	3255	40	0
60	KX	3372	0	3255	50	0
60	KZ	3372	0	3255	39	0
60	LB	3372	0	3255	47	0
61	2I	2	0	0	0	0
61	2K	1	0	0	0	0
61	2N	1	0	0	0	0
61	3V	2	0	0	0	0
61	3W	2	0	0	0	0
61	3X	3	0	0	0	0
61	3Y	2	0	0	0	0
61	4A	1	0	0	0	0
61	4B	1	0	0	0	0
61	4C	1	0	0	0	0
61	4D	1	0	0	0	0
61	4F	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	FB	1	0	0	0	0
61	FN	1	0	0	0	0
61	FP	1	0	0	0	0
61	FR	1	0	0	0	0
62	AA	32	0	12	1	0
62	AC	32	0	12	1	0
62	AE	32	0	12	0	0
62	AG	32	0	12	1	0
62	AI	32	0	12	0	0
62	AK	32	0	12	0	0
62	AM	32	0	12	0	0
62	AO	32	0	12	0	0
62	AQ	32	0	12	1	0
62	AS	32	0	12	2	0
62	AU	32	0	12	0	0
62	AW	32	0	12	0	0
62	AY	32	0	12	1	0
62	BA	32	0	12	1	0
62	BC	32	0	12	1	0
62	BE	32	0	12	1	0
62	BG	32	0	12	1	0
62	BI	32	0	12	1	0
62	BK	32	0	12	0	0
62	BM	32	0	12	1	0
62	BO	32	0	12	0	0
62	BQ	32	0	12	1	0
62	BS	32	0	12	0	0
62	BU	32	0	12	0	0
62	BW	32	0	12	1	0
62	BX	32	0	12	0	0
62	BZ	32	0	12	0	0
62	CB	32	0	12	0	0
62	CD	32	0	12	0	0
62	CF	32	0	12	0	0
62	CH	32	0	12	0	0
62	CJ	32	0	12	1	0
62	CM	32	0	12	1	0
62	CO	32	0	12	2	0
62	CQ	32	0	12	2	0
62	CS	32	0	12	1	0
62	CU	32	0	12	1	0
62	CW	32	0	12	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	CY	32	0	12	1	0
62	DA	32	0	12	0	0
62	DC	32	0	12	0	0
62	DE	32	0	12	0	0
62	DG	32	0	12	0	0
62	DI	32	0	12	1	0
62	DK	32	0	12	0	0
62	DM	32	0	12	0	0
62	DO	32	0	12	0	0
62	DQ	32	0	12	0	0
62	DS	32	0	12	0	0
62	DU	32	0	12	0	0
62	DX	32	0	12	0	0
62	DZ	32	0	12	0	0
62	EB	32	0	12	1	0
62	ED	32	0	12	0	0
62	EF	32	0	12	0	0
62	EH	32	0	12	1	0
62	EJ	32	0	12	1	0
62	EL	32	0	12	0	0
62	EN	32	0	12	0	0
62	EP	32	0	12	0	0
62	ER	32	0	12	0	0
62	ET	32	0	12	0	0
62	EV	32	0	12	0	0
62	EX	32	0	12	0	0
62	EZ	32	0	12	1	0
62	FB	32	0	12	0	0
62	FD	32	0	12	0	0
62	FF	32	0	12	0	0
62	FH	32	0	12	1	0
62	FJ	32	0	12	0	0
62	FL	32	0	12	0	0
62	FN	32	0	12	0	0
62	FP	32	0	12	0	0
62	FR	32	0	12	0	0
62	FT	32	0	12	0	0
62	FU	32	0	12	1	0
62	FW	32	0	12	0	0
62	FY	32	0	12	0	0
62	GA	32	0	12	0	0
62	GC	32	0	12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	GE	32	0	12	0	0
62	GG	32	0	12	0	0
62	GH	32	0	12	0	0
62	GJ	32	0	12	0	0
62	GL	32	0	12	0	0
62	GN	32	0	12	1	0
62	GP	32	0	12	1	0
62	GR	32	0	12	0	0
62	GT	32	0	12	0	0
62	GU	32	0	12	1	0
62	GW	32	0	12	0	0
62	GY	32	0	12	0	0
62	HA	32	0	12	1	0
62	HC	32	0	12	3	0
62	HE	32	0	12	0	0
62	HG	32	0	12	1	0
62	HI	32	0	12	0	0
62	HK	32	0	12	1	0
62	HM	32	0	12	1	0
62	HO	32	0	12	1	0
62	HQ	32	0	12	2	0
62	HT	32	0	12	1	0
62	HV	32	0	12	0	0
62	HX	32	0	12	0	0
62	HZ	32	0	12	1	0
62	IB	32	0	12	1	0
62	ID	32	0	12	1	0
62	IG	32	0	12	0	0
62	II	32	0	12	0	0
62	IK	32	0	12	1	0
62	IM	32	0	12	0	0
62	IO	32	0	12	0	0
62	IQ	32	0	12	1	0
62	IT	32	0	12	0	0
62	IV	32	0	12	0	0
62	IX	32	0	12	1	0
62	IZ	32	0	12	1	0
62	JB	32	0	12	1	0
62	JD	32	0	12	0	0
62	JF	32	0	12	2	0
62	JH	32	0	12	0	0
62	JJ	32	0	12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	JL	32	0	12	0	0
62	JN	32	0	12	1	0
62	JP	32	0	12	0	0
62	JQ	32	0	12	0	0
62	JS	32	0	12	0	0
62	JU	32	0	12	0	0
62	JW	32	0	12	1	0
62	JY	32	0	12	0	0
62	KA	32	0	12	0	0
62	KC	32	0	12	0	0
62	KD	32	0	12	1	0
62	KF	32	0	12	1	0
62	KH	32	0	12	1	0
62	KJ	32	0	12	0	0
62	KL	32	0	12	1	0
62	KN	32	0	12	0	0
62	KP	32	0	12	1	0
62	KQ	32	0	12	0	0
62	KS	32	0	12	0	0
62	KU	32	0	12	0	0
62	KW	32	0	12	1	0
62	KY	32	0	12	1	0
62	LA	32	0	12	0	0
63	AA	1	0	0	0	0
63	AC	1	0	0	0	0
63	AE	1	0	0	0	0
63	AG	1	0	0	0	0
63	AI	1	0	0	0	0
63	AK	1	0	0	0	0
63	AM	1	0	0	0	0
63	AO	1	0	0	0	0
63	AQ	1	0	0	0	0
63	AS	1	0	0	0	0
63	AU	1	0	0	0	0
63	AW	1	0	0	0	0
63	AY	1	0	0	0	0
63	BA	1	0	0	0	0
63	BC	1	0	0	0	0
63	BE	1	0	0	0	0
63	BG	1	0	0	0	0
63	BI	1	0	0	0	0
63	BK	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	BM	1	0	0	0	0
63	BO	1	0	0	0	0
63	BQ	1	0	0	0	0
63	BS	1	0	0	0	0
63	BU	1	0	0	0	0
63	BW	1	0	0	0	0
63	BX	1	0	0	0	0
63	CA	1	0	0	0	0
63	CB	1	0	0	0	0
63	CD	1	0	0	0	0
63	CF	1	0	0	0	0
63	CH	1	0	0	0	0
63	CJ	1	0	0	0	0
63	CM	1	0	0	0	0
63	CO	1	0	0	0	0
63	CQ	1	0	0	0	0
63	CS	1	0	0	0	0
63	CU	1	0	0	0	0
63	CW	1	0	0	0	0
63	CY	1	0	0	0	0
63	DA	1	0	0	0	0
63	DC	1	0	0	0	0
63	DE	1	0	0	0	0
63	DG	1	0	0	0	0
63	DI	1	0	0	0	0
63	DK	1	0	0	0	0
63	DM	1	0	0	0	0
63	DO	1	0	0	0	0
63	DQ	1	0	0	0	0
63	DS	1	0	0	0	0
63	DU	1	0	0	0	0
63	DX	1	0	0	0	0
63	DZ	1	0	0	0	0
63	EB	1	0	0	0	0
63	ED	1	0	0	0	0
63	EF	1	0	0	0	0
63	EH	1	0	0	0	0
63	EJ	1	0	0	0	0
63	EL	1	0	0	0	0
63	EN	1	0	0	0	0
63	EP	1	0	0	0	0
63	ER	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	ET	1	0	0	0	0
63	EV	1	0	0	0	0
63	EX	1	0	0	0	0
63	EZ	1	0	0	0	0
63	FB	1	0	0	0	0
63	FD	1	0	0	0	0
63	FF	1	0	0	0	0
63	FH	1	0	0	0	0
63	FJ	1	0	0	0	0
63	FL	1	0	0	0	0
63	FN	1	0	0	0	0
63	FP	1	0	0	0	0
63	FR	1	0	0	0	0
63	FT	1	0	0	0	0
63	FU	1	0	0	0	0
63	FW	1	0	0	0	0
63	FY	1	0	0	0	0
63	GA	1	0	0	0	0
63	GC	1	0	0	0	0
63	GE	1	0	0	0	0
63	GG	1	0	0	0	0
63	GH	1	0	0	0	0
63	GJ	1	0	0	0	0
63	GL	1	0	0	0	0
63	GN	1	0	0	0	0
63	GP	1	0	0	0	0
63	GR	1	0	0	0	0
63	GT	1	0	0	0	0
63	GU	1	0	0	0	0
63	GW	1	0	0	0	0
63	GY	1	0	0	0	0
63	HA	1	0	0	0	0
63	HC	1	0	0	0	0
63	HE	1	0	0	0	0
63	HG	1	0	0	0	0
63	HI	1	0	0	0	0
63	HK	1	0	0	0	0
63	HM	1	0	0	0	0
63	HO	1	0	0	0	0
63	HQ	1	0	0	0	0
63	HT	1	0	0	0	0
63	HV	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	HX	1	0	0	0	0
63	HZ	1	0	0	0	0
63	IB	1	0	0	0	0
63	ID	1	0	0	0	0
63	IG	1	0	0	0	0
63	II	1	0	0	0	0
63	IK	1	0	0	0	0
63	IM	1	0	0	0	0
63	IO	1	0	0	0	0
63	IQ	1	0	0	0	0
63	IT	1	0	0	0	0
63	IV	1	0	0	0	0
63	IX	1	0	0	0	0
63	IZ	1	0	0	0	0
63	JB	1	0	0	0	0
63	JD	1	0	0	0	0
63	JF	1	0	0	0	0
63	JH	1	0	0	0	0
63	JJ	1	0	0	0	0
63	JL	1	0	0	0	0
63	JN	1	0	0	0	0
63	JP	1	0	0	0	0
63	JQ	1	0	0	0	0
63	JS	1	0	0	0	0
63	JU	1	0	0	0	0
63	JW	1	0	0	0	0
63	JY	1	0	0	0	0
63	KA	1	0	0	0	0
63	KC	1	0	0	0	0
63	KD	1	0	0	0	0
63	KF	1	0	0	0	0
63	KH	1	0	0	0	0
63	KJ	1	0	0	0	0
63	KL	1	0	0	0	0
63	KN	1	0	0	0	0
63	KP	1	0	0	0	0
63	KQ	1	0	0	0	0
63	KS	1	0	0	0	0
63	KU	1	0	0	0	0
63	KW	1	0	0	0	0
63	KY	1	0	0	0	0
63	LA	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	AB	28	0	12	0	0
64	AD	28	0	12	1	0
64	AF	28	0	12	0	0
64	AH	28	0	12	0	0
64	AJ	28	0	12	0	0
64	AL	28	0	12	0	0
64	AN	28	0	12	0	0
64	AP	28	0	12	0	0
64	AR	28	0	12	0	0
64	AT	28	0	12	1	0
64	AV	28	0	12	1	0
64	AX	28	0	12	0	0
64	AZ	28	0	12	0	0
64	BB	28	0	12	0	0
64	BD	28	0	12	0	0
64	BF	28	0	12	0	0
64	BH	28	0	12	0	0
64	BJ	28	0	12	0	0
64	BL	28	0	12	0	0
64	BN	28	0	12	1	0
64	BP	28	0	12	0	0
64	BR	28	0	12	1	0
64	BT	28	0	12	1	0
64	BV	28	0	12	1	0
64	BY	28	0	12	0	0
64	CA	28	0	12	0	0
64	CC	28	0	12	0	0
64	CE	28	0	12	1	0
64	CG	28	0	12	1	0
64	CI	28	0	12	1	0
64	CL	28	0	12	1	0
64	CN	28	0	12	1	0
64	CP	28	0	12	2	0
64	CR	28	0	12	0	0
64	CT	28	0	12	0	0
64	CV	28	0	12	1	0
64	CX	28	0	12	0	0
64	CZ	28	0	12	1	0
64	DB	28	0	12	0	0
64	DD	28	0	12	0	0
64	DF	28	0	12	0	0
64	DH	28	0	12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	DJ	28	0	12	0	0
64	DL	28	0	12	0	0
64	DN	28	0	12	1	0
64	DP	28	0	12	0	0
64	DR	28	0	12	0	0
64	DT	28	0	12	0	0
64	DV	28	0	12	0	0
64	DW	28	0	12	0	0
64	DY	28	0	12	0	0
64	EA	28	0	12	0	0
64	EC	28	0	12	0	0
64	EE	28	0	12	0	0
64	EG	28	0	12	0	0
64	EI	28	0	12	0	0
64	EK	28	0	12	1	0
64	EM	28	0	12	1	0
64	EO	28	0	12	0	0
64	EQ	28	0	12	1	0
64	ES	28	0	12	1	0
64	EU	28	0	12	1	0
64	EW	28	0	12	0	0
64	EY	28	0	12	1	0
64	FA	28	0	12	1	0
64	FC	28	0	12	1	0
64	FE	28	0	12	0	0
64	FG	28	0	12	0	0
64	FI	28	0	12	0	0
64	FK	28	0	12	0	0
64	FM	28	0	12	0	0
64	FO	28	0	12	0	0
64	FQ	28	0	12	0	0
64	FS	28	0	12	1	0
64	FV	28	0	12	0	0
64	FX	28	0	12	0	0
64	FZ	28	0	12	0	0
64	GB	28	0	12	1	0
64	GD	28	0	12	1	0
64	GF	28	0	12	0	0
64	GI	28	0	12	0	0
64	GK	28	0	12	0	0
64	GM	28	0	12	0	0
64	GO	28	0	12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	GQ	28	0	12	0	0
64	GS	28	0	12	0	0
64	GV	28	0	12	0	0
64	GX	28	0	12	0	0
64	GZ	28	0	12	0	0
64	HB	28	0	12	0	0
64	HD	28	0	12	0	0
64	HF	28	0	12	0	0
64	HH	28	0	12	0	0
64	HJ	28	0	12	1	0
64	HL	28	0	12	0	0
64	HN	28	0	12	0	0
64	HP	28	0	12	0	0
64	HR	28	0	12	0	0
64	HS	28	0	12	0	0
64	HU	28	0	12	1	0
64	HW	28	0	12	0	0
64	HY	28	0	12	1	0
64	IA	28	0	12	1	0
64	IC	28	0	12	1	0
64	IE	28	0	12	1	0
64	IF	28	0	12	1	0
64	IH	28	0	12	0	0
64	IJ	28	0	12	1	0
64	IL	28	0	12	3	0
64	IN	28	0	12	1	0
64	IP	28	0	12	2	0
64	IR	28	0	12	1	0
64	IS	28	0	12	1	0
64	IU	28	0	12	0	0
64	IW	28	0	12	1	0
64	IY	28	0	12	0	0
64	JA	28	0	12	1	0
64	JC	28	0	12	1	0
64	JE	28	0	12	1	0
64	JG	28	0	12	1	0
64	JI	28	0	12	0	0
64	JK	28	0	12	2	0
64	JM	28	0	12	0	0
64	JO	28	0	12	0	0
64	JR	28	0	12	0	0
64	JT	28	0	12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	JV	28	0	12	0	0
64	JX	28	0	12	0	0
64	JZ	28	0	12	0	0
64	KB	28	0	12	0	0
64	KE	28	0	12	0	0
64	KG	28	0	12	0	0
64	KI	28	0	12	1	0
64	KK	28	0	12	1	0
64	KM	28	0	12	0	0
64	KO	28	0	12	1	0
64	KR	28	0	12	0	0
64	KT	28	0	12	0	0
64	KV	28	0	12	1	0
64	KX	28	0	12	0	0
64	KZ	28	0	12	0	0
64	LB	28	0	12	0	0
All	All	1215524	0	1179168	14500	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 6.

The worst 5 of 14500 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)
48:3Y:50:CYS:SG	48:3Y:90:HIS:HB2	1.43	1.55
48:3Y:50:CYS:SG	48:3Y:90:HIS:CB	2.16	1.30
48:3Y:50:CYS:SG	48:3Y:90:HIS:CA	2.35	1.13
47:3W:36:HIS:CD2	47:3W:40:TYR:O	2.15	1.00
48:3Y:50:CYS:SG	48:3Y:90:HIS:N	2.34	1.00

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	0A	660/752 (88%)	636 (96%)	23 (4%)	1 (0%)	44	73
1	0B	726/752 (96%)	705 (97%)	20 (3%)	1 (0%)	48	77
1	0C	730/752 (97%)	706 (97%)	24 (3%)	0	100	100
1	0D	129/752 (17%)	126 (98%)	3 (2%)	0	100	100
2	0E	722/779 (93%)	703 (97%)	19 (3%)	0	100	100
3	0F	659/724 (91%)	629 (95%)	30 (5%)	0	100	100
4	0G	754/779 (97%)	713 (95%)	41 (5%)	0	100	100
5	0H	259/385 (67%)	254 (98%)	5 (2%)	0	100	100
5	0I	115/385 (30%)	111 (96%)	4 (4%)	0	100	100
5	0J	42/385 (11%)	40 (95%)	2 (5%)	0	100	100
5	0K	361/385 (94%)	353 (98%)	8 (2%)	0	100	100
6	0M	302/483 (62%)	300 (99%)	2 (1%)	0	100	100
6	0N	165/483 (34%)	160 (97%)	5 (3%)	0	100	100
7	0O	152/436 (35%)	152 (100%)	0	0	100	100
7	0P	301/436 (69%)	301 (100%)	0	0	100	100
8	0Q	330/334 (99%)	323 (98%)	7 (2%)	0	100	100
9	0R	341/349 (98%)	327 (96%)	14 (4%)	0	100	100
10	0S	417/422 (99%)	406 (97%)	11 (3%)	0	100	100
11	0T	410/422 (97%)	388 (95%)	22 (5%)	0	100	100
12	0U	302/331 (91%)	289 (96%)	13 (4%)	0	100	100
13	0V	166/219 (76%)	158 (95%)	8 (5%)	0	100	100
14	0W	103/130 (79%)	100 (97%)	3 (3%)	0	100	100
15	0X	177/270 (66%)	172 (97%)	5 (3%)	0	100	100
16	0Y	267/301 (89%)	260 (97%)	7 (3%)	0	100	100
17	0Z	468/552 (85%)	456 (97%)	12 (3%)	0	100	100
18	1A	355/359 (99%)	346 (98%)	9 (2%)	0	100	100
19	1B	270/297 (91%)	264 (98%)	6 (2%)	0	100	100
20	1C	245/282 (87%)	230 (94%)	15 (6%)	0	100	100
21	1D	296/320 (92%)	281 (95%)	15 (5%)	0	100	100
22	1E	235/249 (94%)	224 (95%)	11 (5%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	1F	230/254 (91%)	220 (96%)	10 (4%)	0	100	100
24	1G	163/182 (90%)	155 (95%)	8 (5%)	0	100	100
25	1H	254/386 (66%)	249 (98%)	5 (2%)	0	100	100
26	1I	316/417 (76%)	305 (96%)	11 (4%)	0	100	100
26	1J	87/417 (21%)	84 (97%)	3 (3%)	0	100	100
27	1K	265/415 (64%)	250 (94%)	15 (6%)	0	100	100
27	1L	134/415 (32%)	128 (96%)	6 (4%)	0	100	100
28	1M	219/415 (53%)	203 (93%)	16 (7%)	0	100	100
28	1N	99/415 (24%)	92 (93%)	7 (7%)	0	100	100
29	1O	116/247 (47%)	112 (97%)	4 (3%)	0	100	100
29	1P	54/247 (22%)	53 (98%)	1 (2%)	0	100	100
29	4X	40/247 (16%)	38 (95%)	2 (5%)	0	100	100
30	1Q	273/300 (91%)	262 (96%)	11 (4%)	0	100	100
30	1R	273/300 (91%)	261 (96%)	12 (4%)	0	100	100
30	1S	273/300 (91%)	265 (97%)	8 (3%)	0	100	100
31	1T	222/312 (71%)	218 (98%)	4 (2%)	0	100	100
31	1U	222/312 (71%)	217 (98%)	5 (2%)	0	100	100
32	1V	183/294 (62%)	174 (95%)	9 (5%)	0	100	100
32	1W	183/294 (62%)	175 (96%)	8 (4%)	0	100	100
32	1X	183/294 (62%)	176 (96%)	7 (4%)	0	100	100
32	1Y	183/294 (62%)	175 (96%)	8 (4%)	0	100	100
32	1Z	183/294 (62%)	173 (94%)	10 (6%)	0	100	100
32	2A	183/294 (62%)	174 (95%)	9 (5%)	0	100	100
33	2B	618/629 (98%)	571 (92%)	47 (8%)	0	100	100
33	2C	625/629 (99%)	574 (92%)	51 (8%)	0	100	100
33	2D	625/629 (99%)	570 (91%)	55 (9%)	0	100	100
34	2E	238/274 (87%)	228 (96%)	10 (4%)	0	100	100
34	2F	238/274 (87%)	229 (96%)	9 (4%)	0	100	100
35	2G	171/374 (46%)	162 (95%)	9 (5%)	0	100	100
35	2H	146/374 (39%)	141 (97%)	5 (3%)	0	100	100
36	2I	277/369 (75%)	260 (94%)	17 (6%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	2J	273/369 (74%)	260 (95%)	13 (5%)	0	100	100
36	2K	273/369 (74%)	263 (96%)	10 (4%)	0	100	100
37	2L	234/272 (86%)	224 (96%)	10 (4%)	0	100	100
37	2M	234/272 (86%)	224 (96%)	10 (4%)	0	100	100
38	2N	237/262 (90%)	231 (98%)	6 (2%)	0	100	100
39	2O	185/483 (38%)	183 (99%)	2 (1%)	0	100	100
39	2P	301/483 (62%)	299 (99%)	2 (1%)	0	100	100
39	2Q	317/483 (66%)	313 (99%)	4 (1%)	0	100	100
39	2R	187/483 (39%)	186 (100%)	1 (0%)	0	100	100
40	2S	77/515 (15%)	74 (96%)	3 (4%)	0	100	100
40	2T	433/515 (84%)	427 (99%)	6 (1%)	0	100	100
40	2U	64/515 (12%)	63 (98%)	1 (2%)	0	100	100
41	2V	122/348 (35%)	122 (100%)	0	0	100	100
41	2W	231/348 (66%)	226 (98%)	5 (2%)	0	100	100
41	2X	50/348 (14%)	50 (100%)	0	0	100	100
41	2Y	331/348 (95%)	329 (99%)	2 (1%)	0	100	100
41	2Z	270/348 (78%)	269 (100%)	1 (0%)	0	100	100
41	3A	108/348 (31%)	107 (99%)	1 (1%)	0	100	100
41	3B	171/348 (49%)	171 (100%)	0	0	100	100
41	3C	211/348 (61%)	206 (98%)	5 (2%)	0	100	100
41	3D	251/348 (72%)	248 (99%)	3 (1%)	0	100	100
42	3E	62/266 (23%)	61 (98%)	1 (2%)	0	100	100
42	3F	180/266 (68%)	172 (96%)	8 (4%)	0	100	100
42	3G	166/266 (62%)	158 (95%)	8 (5%)	0	100	100
42	3H	76/266 (29%)	72 (95%)	4 (5%)	0	100	100
42	3I	106/266 (40%)	103 (97%)	3 (3%)	0	100	100
42	3J	143/266 (54%)	137 (96%)	6 (4%)	0	100	100
42	3K	49/266 (18%)	48 (98%)	1 (2%)	0	100	100
42	3L	178/266 (67%)	164 (92%)	14 (8%)	0	100	100
42	3M	181/266 (68%)	174 (96%)	7 (4%)	0	100	100
42	3N	59/266 (22%)	59 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	3O	115/266 (43%)	112 (97%)	3 (3%)	0	100	100
42	3P	115/266 (43%)	110 (96%)	5 (4%)	0	100	100
43	3Q	152/270 (56%)	146 (96%)	6 (4%)	0	100	100
44	3R	159/325 (49%)	155 (98%)	4 (2%)	0	100	100
45	3S	157/191 (82%)	150 (96%)	7 (4%)	0	100	100
46	3T	170/320 (53%)	162 (95%)	8 (5%)	0	100	100
46	3U	135/320 (42%)	129 (96%)	6 (4%)	0	100	100
47	3V	235/278 (84%)	220 (94%)	15 (6%)	0	100	100
47	3W	234/278 (84%)	223 (95%)	11 (5%)	0	100	100
47	3X	225/278 (81%)	210 (93%)	15 (7%)	0	100	100
48	3Y	247/269 (92%)	232 (94%)	15 (6%)	0	100	100
48	3Z	118/269 (44%)	112 (95%)	6 (5%)	0	100	100
48	4A	235/269 (87%)	221 (94%)	14 (6%)	0	100	100
49	4B	100/420 (24%)	97 (97%)	3 (3%)	0	100	100
49	4C	104/420 (25%)	100 (96%)	4 (4%)	0	100	100
49	4D	95/420 (23%)	93 (98%)	2 (2%)	0	100	100
50	4E	38/337 (11%)	38 (100%)	0	0	100	100
50	4F	127/337 (38%)	125 (98%)	2 (2%)	0	100	100
50	4G	38/337 (11%)	37 (97%)	1 (3%)	0	100	100
51	4H	201/329 (61%)	197 (98%)	4 (2%)	0	100	100
52	4I	128/350 (37%)	125 (98%)	3 (2%)	0	100	100
52	4J	26/350 (7%)	23 (88%)	3 (12%)	0	100	100
53	4K	198/286 (69%)	186 (94%)	12 (6%)	0	100	100
53	4L	105/286 (37%)	99 (94%)	6 (6%)	0	100	100
54	4M	156/193 (81%)	155 (99%)	1 (1%)	0	100	100
54	4N	156/193 (81%)	155 (99%)	1 (1%)	0	100	100
54	4O	155/193 (80%)	154 (99%)	1 (1%)	0	100	100
55	4P	138/191 (72%)	134 (97%)	4 (3%)	0	100	100
56	4Q	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
57	4R	125/161 (78%)	124 (99%)	1 (1%)	0	100	100
57	4S	130/161 (81%)	128 (98%)	2 (2%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	4Y	36/161 (22%)	32 (89%)	4 (11%)	0	100	100
58	4T	70/867 (8%)	70 (100%)	0	0	100	100
58	4U	70/867 (8%)	70 (100%)	0	0	100	100
58	4V	70/867 (8%)	70 (100%)	0	0	100	100
58	4W	70/867 (8%)	70 (100%)	0	0	100	100
59	AA	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	AC	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	AE	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	AG	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	AI	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	AK	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	AM	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	AO	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	AQ	440/451 (98%)	420 (96%)	20 (4%)	0	100	100
59	AS	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	AU	440/451 (98%)	428 (97%)	12 (3%)	0	100	100
59	AW	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	AY	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	BA	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	BC	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	BE	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	BG	440/451 (98%)	422 (96%)	18 (4%)	0	100	100
59	BI	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	BK	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	BM	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	BO	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	BQ	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	BS	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	BU	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	BW	440/451 (98%)	424 (96%)	15 (3%)	1 (0%)	44	73
59	BX	440/451 (98%)	420 (96%)	20 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	BZ	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	CB	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	CD	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	CF	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	CH	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	CJ	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	CM	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	CO	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	CQ	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	CS	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	CU	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	CW	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	CY	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	DA	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	DC	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	DE	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	DG	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	DI	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	DK	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	DM	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	DO	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	DQ	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	DS	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	DU	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	DX	440/451 (98%)	423 (96%)	16 (4%)	1 (0%)	44	73
59	DZ	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	EB	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	ED	440/451 (98%)	428 (97%)	12 (3%)	0	100	100
59	EF	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	EH	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	EJ	440/451 (98%)	426 (97%)	14 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	EL	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	EN	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	EP	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	ER	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	ET	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	EV	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	EX	440/451 (98%)	428 (97%)	12 (3%)	0	100	100
59	EZ	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	FB	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	FD	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	FF	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	FH	440/451 (98%)	425 (97%)	14 (3%)	1 (0%)	44	73
59	FJ	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	FL	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	FN	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	FP	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	FR	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	FT	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	FU	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	FW	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	FY	440/451 (98%)	421 (96%)	19 (4%)	0	100	100
59	GA	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	GC	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	GE	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	GG	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	GH	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	GJ	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	GL	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	GN	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	GP	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	GR	440/451 (98%)	427 (97%)	13 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	GT	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	GU	440/451 (98%)	421 (96%)	18 (4%)	1 (0%)	44	73
59	GW	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	GY	440/451 (98%)	427 (97%)	11 (2%)	2 (0%)	25	56
59	HA	440/451 (98%)	421 (96%)	18 (4%)	1 (0%)	44	73
59	HC	440/451 (98%)	425 (97%)	14 (3%)	1 (0%)	44	73
59	HE	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	HG	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	HI	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	HK	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	HM	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	HO	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	HQ	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	HT	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	HV	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	HX	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	HZ	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	IB	440/451 (98%)	428 (97%)	12 (3%)	0	100	100
59	ID	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	IG	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	II	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	IK	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	IM	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	IO	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	IQ	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	IT	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	IV	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	IX	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	IZ	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	JB	440/451 (98%)	428 (97%)	12 (3%)	0	100	100
59	JD	440/451 (98%)	424 (96%)	16 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	JF	440/451 (98%)	428 (97%)	12 (3%)	0	100	100
59	JH	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	JJ	440/451 (98%)	422 (96%)	18 (4%)	0	100	100
59	JL	440/451 (98%)	428 (97%)	12 (3%)	0	100	100
59	JN	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	JP	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	JQ	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	JS	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	JU	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	JW	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	JY	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	KA	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	KC	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	KD	440/451 (98%)	422 (96%)	18 (4%)	0	100	100
59	KF	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	KH	440/451 (98%)	427 (97%)	13 (3%)	0	100	100
59	KJ	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
59	KL	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	KN	440/451 (98%)	422 (96%)	18 (4%)	0	100	100
59	KP	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	KQ	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	KS	440/451 (98%)	423 (96%)	17 (4%)	0	100	100
59	KU	440/451 (98%)	424 (96%)	16 (4%)	0	100	100
59	KW	440/451 (98%)	425 (97%)	15 (3%)	0	100	100
59	KY	440/451 (98%)	423 (96%)	16 (4%)	1 (0%)	44	73
59	LA	440/451 (98%)	426 (97%)	14 (3%)	0	100	100
60	AB	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	AD	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	AF	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	AH	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	AJ	428/442 (97%)	419 (98%)	9 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	AL	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	AN	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	AP	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	AR	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	AT	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	AV	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	AX	428/442 (97%)	416 (97%)	12 (3%)	0	100	100
60	AZ	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	BB	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	BD	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	BF	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	BH	428/442 (97%)	415 (97%)	12 (3%)	1 (0%)	44	73
60	BJ	428/442 (97%)	416 (97%)	11 (3%)	1 (0%)	44	73
60	BL	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	BN	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	BP	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	BR	428/442 (97%)	415 (97%)	12 (3%)	1 (0%)	44	73
60	BT	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	BV	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	BY	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	CA	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	CC	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	CE	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	CG	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	CI	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	CL	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	CN	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	CP	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	CR	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	CT	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	CV	428/442 (97%)	420 (98%)	8 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	CX	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	CZ	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	DB	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	DD	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	DF	428/442 (97%)	416 (97%)	12 (3%)	0	100	100
60	DH	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	DJ	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	DL	428/442 (97%)	419 (98%)	8 (2%)	1 (0%)	44	73
60	DN	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	DP	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	DR	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	DT	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	DV	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	DW	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	DY	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	EA	428/442 (97%)	413 (96%)	15 (4%)	0	100	100
60	EC	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	EE	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	EG	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	EI	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	EK	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	EM	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	EO	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	EQ	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	ES	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	EU	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	EW	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	EY	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	FA	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	FC	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	FE	428/442 (97%)	420 (98%)	8 (2%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	FG	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	FI	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	FK	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	FM	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	FO	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	FQ	428/442 (97%)	419 (98%)	8 (2%)	1 (0%)	44	73
60	FS	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	FV	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	FX	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	FZ	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	GB	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	GD	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	GF	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	GI	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	GK	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	GM	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	GO	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	GQ	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	GS	428/442 (97%)	416 (97%)	12 (3%)	0	100	100
60	GV	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	GX	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	GZ	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	HB	428/442 (97%)	418 (98%)	9 (2%)	1 (0%)	44	73
60	HD	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	HF	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	HH	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	HJ	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	HL	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	HN	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	HP	428/442 (97%)	416 (97%)	12 (3%)	0	100	100
60	HR	428/442 (97%)	419 (98%)	9 (2%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	HS	428/442 (97%)	415 (97%)	13 (3%)	0	100	100
60	HU	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	HW	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	HY	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	IA	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	IC	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	IE	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	IF	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	IH	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	IJ	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	IL	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	IN	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	IP	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	IR	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	IS	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	IU	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	IW	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	IY	428/442 (97%)	414 (97%)	14 (3%)	0	100	100
60	JA	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	JC	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	JE	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	JG	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	JI	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	JK	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
60	JM	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	JO	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	JR	428/442 (97%)	416 (97%)	12 (3%)	0	100	100
60	JT	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	JV	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	JX	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	JZ	428/442 (97%)	419 (98%)	9 (2%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	KB	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	KE	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	KG	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
60	KI	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	KK	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	KM	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	KO	428/442 (97%)	415 (97%)	11 (3%)	2 (0%)	25	56
60	KR	428/442 (97%)	418 (98%)	10 (2%)	0	100	100
60	KT	428/442 (97%)	417 (97%)	11 (3%)	0	100	100
60	KV	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	KX	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	KZ	428/442 (97%)	419 (98%)	9 (2%)	0	100	100
60	LB	428/442 (97%)	420 (98%)	8 (2%)	0	100	100
All	All	152773/175732 (87%)	148265 (97%)	4489 (3%)	19 (0%)	100	100

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
60	DL	393	ALA
59	GU	439	SER
59	HC	261	PRO
60	KO	393	ALA
59	KY	403	ALA

### 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	0A	587/669 (88%)	580 (99%)	7 (1%)	67	89
1	0B	649/669 (97%)	646 (100%)	3 (0%)	86	95
1	0C	653/669 (98%)	650 (100%)	3 (0%)	86	95

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0D	117/669 (18%)	117 (100%)	0	100	100
2	0E	632/674 (94%)	631 (100%)	1 (0%)	92	97
3	0F	590/640 (92%)	588 (100%)	2 (0%)	91	97
4	0G	686/707 (97%)	684 (100%)	2 (0%)	91	97
5	0H	235/344 (68%)	233 (99%)	2 (1%)	75	92
5	0I	109/344 (32%)	109 (100%)	0	100	100
5	0J	39/344 (11%)	39 (100%)	0	100	100
5	0K	325/344 (94%)	325 (100%)	0	100	100
6	0M	261/421 (62%)	260 (100%)	1 (0%)	89	96
6	0N	150/421 (36%)	149 (99%)	1 (1%)	81	94
7	0O	129/376 (34%)	128 (99%)	1 (1%)	79	93
7	0P	263/376 (70%)	258 (98%)	5 (2%)	52	82
8	0Q	284/286 (99%)	282 (99%)	2 (1%)	81	94
9	0R	290/296 (98%)	289 (100%)	1 (0%)	91	97
10	0S	363/366 (99%)	362 (100%)	1 (0%)	91	97
11	0T	364/371 (98%)	363 (100%)	1 (0%)	91	97
12	0U	270/292 (92%)	270 (100%)	0	100	100
13	0V	139/180 (77%)	138 (99%)	1 (1%)	81	94
14	0W	86/105 (82%)	86 (100%)	0	100	100
15	0X	160/235 (68%)	160 (100%)	0	100	100
16	0Y	227/253 (90%)	227 (100%)	0	100	100
17	0Z	409/479 (85%)	405 (99%)	4 (1%)	73	91
18	1A	315/317 (99%)	313 (99%)	2 (1%)	84	95
19	1B	242/259 (93%)	240 (99%)	2 (1%)	79	93
20	1C	207/234 (88%)	207 (100%)	0	100	100
21	1D	251/269 (93%)	250 (100%)	1 (0%)	89	96
22	1E	205/215 (95%)	204 (100%)	1 (0%)	86	95
23	1F	207/226 (92%)	206 (100%)	1 (0%)	86	95
24	1G	144/156 (92%)	143 (99%)	1 (1%)	81	94
25	1H	227/332 (68%)	226 (100%)	1 (0%)	89	96
26	1I	270/349 (77%)	270 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	1J	77/349 (22%)	77 (100%)	0	100	100
27	1K	225/348 (65%)	223 (99%)	2 (1%)	75	92
27	1L	118/348 (34%)	118 (100%)	0	100	100
28	1M	192/347 (55%)	191 (100%)	1 (0%)	86	95
28	1N	85/347 (24%)	84 (99%)	1 (1%)	67	89
29	1O	105/196 (54%)	105 (100%)	0	100	100
29	1P	46/196 (24%)	46 (100%)	0	100	100
29	4X	39/196 (20%)	39 (100%)	0	100	100
30	1Q	234/253 (92%)	233 (100%)	1 (0%)	89	96
30	1R	234/253 (92%)	234 (100%)	0	100	100
30	1S	234/253 (92%)	234 (100%)	0	100	100
31	1T	200/274 (73%)	200 (100%)	0	100	100
31	1U	200/274 (73%)	199 (100%)	1 (0%)	86	95
32	1V	173/270 (64%)	173 (100%)	0	100	100
32	1W	173/270 (64%)	173 (100%)	0	100	100
32	1X	173/270 (64%)	173 (100%)	0	100	100
32	1Y	173/270 (64%)	171 (99%)	2 (1%)	67	89
32	1Z	173/270 (64%)	173 (100%)	0	100	100
32	2A	173/270 (64%)	172 (99%)	1 (1%)	84	95
33	2B	512/519 (99%)	510 (100%)	2 (0%)	89	96
33	2C	517/519 (100%)	515 (100%)	2 (0%)	89	96
33	2D	517/519 (100%)	516 (100%)	1 (0%)	92	97
34	2E	200/230 (87%)	200 (100%)	0	100	100
34	2F	200/230 (87%)	199 (100%)	1 (0%)	86	95
35	2G	160/321 (50%)	160 (100%)	0	100	100
35	2H	137/321 (43%)	135 (98%)	2 (2%)	60	86
36	2I	245/311 (79%)	244 (100%)	1 (0%)	89	96
36	2J	241/311 (78%)	239 (99%)	2 (1%)	79	93
36	2K	241/311 (78%)	241 (100%)	0	100	100
37	2L	209/236 (89%)	209 (100%)	0	100	100
37	2M	209/236 (89%)	209 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	2N	211/234 (90%)	211 (100%)	0	100	100
39	2O	172/426 (40%)	169 (98%)	3 (2%)	56	84
39	2P	269/426 (63%)	266 (99%)	3 (1%)	70	90
39	2Q	284/426 (67%)	279 (98%)	5 (2%)	54	83
39	2R	166/426 (39%)	166 (100%)	0	100	100
40	2S	68/448 (15%)	67 (98%)	1 (2%)	60	86
40	2T	382/448 (85%)	380 (100%)	2 (0%)	86	95
40	2U	59/448 (13%)	59 (100%)	0	100	100
41	2V	111/303 (37%)	110 (99%)	1 (1%)	75	92
41	2W	201/303 (66%)	200 (100%)	1 (0%)	86	95
41	2X	49/303 (16%)	49 (100%)	0	100	100
41	2Y	290/303 (96%)	288 (99%)	2 (1%)	81	94
41	2Z	233/303 (77%)	232 (100%)	1 (0%)	89	96
41	3A	97/303 (32%)	96 (99%)	1 (1%)	73	91
41	3B	149/303 (49%)	146 (98%)	3 (2%)	50	81
41	3C	184/303 (61%)	184 (100%)	0	100	100
41	3D	218/303 (72%)	214 (98%)	4 (2%)	54	83
42	3E	58/235 (25%)	57 (98%)	1 (2%)	56	84
42	3F	164/235 (70%)	161 (98%)	3 (2%)	54	83
42	3G	153/235 (65%)	152 (99%)	1 (1%)	81	94
42	3H	72/235 (31%)	71 (99%)	1 (1%)	62	87
42	3I	100/235 (43%)	100 (100%)	0	100	100
42	3J	132/235 (56%)	132 (100%)	0	100	100
42	3K	46/235 (20%)	45 (98%)	1 (2%)	47	79
42	3L	166/235 (71%)	163 (98%)	3 (2%)	54	83
42	3M	170/235 (72%)	169 (99%)	1 (1%)	84	95
42	3N	58/235 (25%)	56 (97%)	2 (3%)	32	66
42	3O	109/235 (46%)	108 (99%)	1 (1%)	75	92
42	3P	108/235 (46%)	107 (99%)	1 (1%)	75	92
43	3Q	143/242 (59%)	142 (99%)	1 (1%)	81	94
44	3R	151/289 (52%)	149 (99%)	2 (1%)	65	88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	3S	136/159 (86%)	135 (99%)	1 (1%)	81	94
46	3T	147/267 (55%)	146 (99%)	1 (1%)	81	94
46	3U	119/267 (45%)	119 (100%)	0	100	100
47	3V	206/237 (87%)	206 (100%)	0	100	100
47	3W	205/237 (86%)	204 (100%)	1 (0%)	86	95
47	3X	198/237 (84%)	196 (99%)	2 (1%)	73	91
48	3Y	212/229 (93%)	210 (99%)	2 (1%)	75	92
48	3Z	102/229 (44%)	101 (99%)	1 (1%)	73	91
48	4A	204/229 (89%)	204 (100%)	0	100	100
49	4B	96/350 (27%)	95 (99%)	1 (1%)	73	91
49	4C	100/350 (29%)	99 (99%)	1 (1%)	73	91
49	4D	94/350 (27%)	92 (98%)	2 (2%)	48	80
50	4E	35/283 (12%)	35 (100%)	0	100	100
50	4F	118/283 (42%)	118 (100%)	0	100	100
50	4G	35/283 (12%)	34 (97%)	1 (3%)	37	71
51	4H	164/273 (60%)	163 (99%)	1 (1%)	84	95
52	4I	112/301 (37%)	111 (99%)	1 (1%)	75	92
52	4J	25/301 (8%)	24 (96%)	1 (4%)	27	60
53	4K	177/255 (69%)	176 (99%)	1 (1%)	84	95
53	4L	95/255 (37%)	94 (99%)	1 (1%)	70	90
54	4M	153/182 (84%)	153 (100%)	0	100	100
54	4N	153/182 (84%)	153 (100%)	0	100	100
54	4O	152/182 (84%)	151 (99%)	1 (1%)	81	94
55	4P	132/177 (75%)	131 (99%)	1 (1%)	79	93
56	4Q	63/149 (42%)	63 (100%)	0	100	100
57	4R	120/148 (81%)	117 (98%)	3 (2%)	42	75
57	4S	124/148 (84%)	124 (100%)	0	100	100
57	4Y	35/148 (24%)	35 (100%)	0	100	100
58	4T	67/763 (9%)	66 (98%)	1 (2%)	60	86
58	4U	67/763 (9%)	66 (98%)	1 (2%)	60	86
58	4V	67/763 (9%)	67 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	4W	67/763 (9%)	66 (98%)	1 (2%)	60	86
59	AA	368/376 (98%)	368 (100%)	0	100	100
59	AC	368/376 (98%)	368 (100%)	0	100	100
59	AE	368/376 (98%)	368 (100%)	0	100	100
59	AG	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	AI	368/376 (98%)	368 (100%)	0	100	100
59	AK	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	AM	368/376 (98%)	368 (100%)	0	100	100
59	AO	368/376 (98%)	368 (100%)	0	100	100
59	AQ	368/376 (98%)	368 (100%)	0	100	100
59	AS	368/376 (98%)	368 (100%)	0	100	100
59	AU	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	AW	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	AY	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	BA	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	BC	368/376 (98%)	368 (100%)	0	100	100
59	BE	368/376 (98%)	368 (100%)	0	100	100
59	BG	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	BI	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	BK	368/376 (98%)	368 (100%)	0	100	100
59	BM	368/376 (98%)	368 (100%)	0	100	100
59	BO	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	BQ	368/376 (98%)	368 (100%)	0	100	100
59	BS	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	BU	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	BW	368/376 (98%)	368 (100%)	0	100	100
59	BX	368/376 (98%)	368 (100%)	0	100	100
59	BZ	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	CB	368/376 (98%)	368 (100%)	0	100	100
59	CD	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	CF	368/376 (98%)	368 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	CH	368/376 (98%)	368 (100%)	0	100	100
59	CJ	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	CM	368/376 (98%)	368 (100%)	0	100	100
59	CO	368/376 (98%)	368 (100%)	0	100	100
59	CQ	368/376 (98%)	368 (100%)	0	100	100
59	CS	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	CU	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	CW	368/376 (98%)	368 (100%)	0	100	100
59	CY	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	DA	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	DC	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	DE	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	DG	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	DI	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	DK	368/376 (98%)	368 (100%)	0	100	100
59	DM	368/376 (98%)	368 (100%)	0	100	100
59	DO	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	DQ	368/376 (98%)	368 (100%)	0	100	100
59	DS	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	DU	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	DX	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	DZ	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	EB	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	ED	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	EF	368/376 (98%)	368 (100%)	0	100	100
59	EH	368/376 (98%)	368 (100%)	0	100	100
59	EJ	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	EL	368/376 (98%)	368 (100%)	0	100	100
59	EN	368/376 (98%)	368 (100%)	0	100	100
59	EP	368/376 (98%)	368 (100%)	0	100	100
59	ER	368/376 (98%)	368 (100%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	ET	368/376 (98%)	368 (100%)	0	100	100
59	EV	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	EX	368/376 (98%)	368 (100%)	0	100	100
59	EZ	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	FB	368/376 (98%)	368 (100%)	0	100	100
59	FD	368/376 (98%)	368 (100%)	0	100	100
59	FF	368/376 (98%)	368 (100%)	0	100	100
59	FH	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	FJ	368/376 (98%)	368 (100%)	0	100	100
59	FL	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	FN	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	FP	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	FR	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	FT	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	FU	368/376 (98%)	368 (100%)	0	100	100
59	FW	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	FY	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	GA	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	GC	368/376 (98%)	368 (100%)	0	100	100
59	GE	368/376 (98%)	368 (100%)	0	100	100
59	GG	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	GH	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	GJ	368/376 (98%)	368 (100%)	0	100	100
59	GL	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	GN	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	GP	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	GR	368/376 (98%)	368 (100%)	0	100	100
59	GT	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	GU	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	GW	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	GY	368/376 (98%)	366 (100%)	2 (0%)	86	95

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	HA	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	HC	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	HE	368/376 (98%)	368 (100%)	0	100	100
59	HG	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	HI	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	HK	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	HM	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	HO	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	HQ	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	HT	368/376 (98%)	364 (99%)	4 (1%)	70	90
59	HV	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	HX	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	HZ	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	IB	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	ID	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	IG	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	II	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	IK	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	IM	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	IO	368/376 (98%)	368 (100%)	0	100	100
59	IQ	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	IT	368/376 (98%)	368 (100%)	0	100	100
59	IV	368/376 (98%)	365 (99%)	3 (1%)	79	93
59	IX	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	IZ	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	JB	368/376 (98%)	368 (100%)	0	100	100
59	JD	368/376 (98%)	364 (99%)	4 (1%)	70	90
59	JF	368/376 (98%)	368 (100%)	0	100	100
59	JH	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	JJ	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	JL	368/376 (98%)	368 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	JN	368/376 (98%)	368 (100%)	0	100	100
59	JP	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	JQ	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	JS	368/376 (98%)	364 (99%)	4 (1%)	70	90
59	JU	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	JW	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	JY	368/376 (98%)	368 (100%)	0	100	100
59	KA	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	KC	368/376 (98%)	364 (99%)	4 (1%)	70	90
59	KD	368/376 (98%)	368 (100%)	0	100	100
59	KF	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	KH	368/376 (98%)	368 (100%)	0	100	100
59	KJ	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	KL	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	KN	368/376 (98%)	367 (100%)	1 (0%)	91	97
59	KP	368/376 (98%)	366 (100%)	2 (0%)	86	95
59	KQ	368/376 (98%)	368 (100%)	0	100	100
59	KS	368/376 (98%)	368 (100%)	0	100	100
59	KU	368/376 (98%)	368 (100%)	0	100	100
59	KW	368/376 (98%)	368 (100%)	0	100	100
59	KY	368/376 (98%)	368 (100%)	0	100	100
59	LA	368/376 (98%)	368 (100%)	0	100	100
60	AB	374/385 (97%)	374 (100%)	0	100	100
60	AD	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	AF	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	AH	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	AJ	374/385 (97%)	374 (100%)	0	100	100
60	AL	374/385 (97%)	374 (100%)	0	100	100
60	AN	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	AP	374/385 (97%)	370 (99%)	4 (1%)	70	90
60	AR	374/385 (97%)	372 (100%)	2 (0%)	86	95

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	AT	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	AV	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	AX	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	AZ	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	BB	374/385 (97%)	374 (100%)	0	100	100
60	BD	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	BF	374/385 (97%)	374 (100%)	0	100	100
60	BH	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	BJ	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	BL	374/385 (97%)	374 (100%)	0	100	100
60	BN	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	BP	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	BR	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	BT	374/385 (97%)	374 (100%)	0	100	100
60	BV	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	BY	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	CA	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	CC	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	CE	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	CG	374/385 (97%)	374 (100%)	0	100	100
60	CI	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	CL	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	CN	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	CP	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	CR	374/385 (97%)	369 (99%)	5 (1%)	65	88
60	CT	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	CV	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	CX	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	CZ	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	DB	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	DD	374/385 (97%)	374 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	DF	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	DH	374/385 (97%)	374 (100%)	0	100	100
60	DJ	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	DL	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	DN	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	DP	374/385 (97%)	374 (100%)	0	100	100
60	DR	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	DT	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	DV	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	DW	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	DY	374/385 (97%)	374 (100%)	0	100	100
60	EA	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	EC	374/385 (97%)	374 (100%)	0	100	100
60	EE	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	EG	374/385 (97%)	374 (100%)	0	100	100
60	EI	374/385 (97%)	374 (100%)	0	100	100
60	EK	374/385 (97%)	374 (100%)	0	100	100
60	EM	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	EO	374/385 (97%)	374 (100%)	0	100	100
60	EQ	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	ES	374/385 (97%)	374 (100%)	0	100	100
60	EU	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	EW	374/385 (97%)	374 (100%)	0	100	100
60	EY	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	FA	374/385 (97%)	374 (100%)	0	100	100
60	FC	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	FE	374/385 (97%)	374 (100%)	0	100	100
60	FG	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	FI	374/385 (97%)	368 (98%)	6 (2%)	58	85
60	FK	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	FM	374/385 (97%)	373 (100%)	1 (0%)	91	97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	FO	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	FQ	374/385 (97%)	370 (99%)	4 (1%)	70	90
60	FS	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	FV	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	FX	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	FZ	374/385 (97%)	374 (100%)	0	100	100
60	GB	374/385 (97%)	374 (100%)	0	100	100
60	GD	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	GF	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	GI	374/385 (97%)	374 (100%)	0	100	100
60	GK	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	GM	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	GO	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	GQ	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	GS	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	GV	374/385 (97%)	370 (99%)	4 (1%)	70	90
60	GX	374/385 (97%)	370 (99%)	4 (1%)	70	90
60	GZ	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	HB	374/385 (97%)	366 (98%)	8 (2%)	48	80
60	HD	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	HF	374/385 (97%)	368 (98%)	6 (2%)	58	85
60	HH	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	HJ	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	HL	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	HN	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	HP	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	HR	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	HS	374/385 (97%)	368 (98%)	6 (2%)	58	85
60	HU	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	HW	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	HY	374/385 (97%)	372 (100%)	2 (0%)	86	95

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	IA	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	IC	374/385 (97%)	374 (100%)	0	100	100
60	IE	374/385 (97%)	374 (100%)	0	100	100
60	IF	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	IH	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	IJ	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	IL	374/385 (97%)	374 (100%)	0	100	100
60	IN	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	IP	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	IR	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	IS	374/385 (97%)	374 (100%)	0	100	100
60	IU	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	IW	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	IY	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	JA	374/385 (97%)	374 (100%)	0	100	100
60	JC	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	JE	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	JG	374/385 (97%)	374 (100%)	0	100	100
60	JI	374/385 (97%)	370 (99%)	4 (1%)	70	90
60	JK	374/385 (97%)	374 (100%)	0	100	100
60	JM	374/385 (97%)	374 (100%)	0	100	100
60	JO	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	JR	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	JT	374/385 (97%)	372 (100%)	2 (0%)	86	95
60	JV	374/385 (97%)	374 (100%)	0	100	100
60	JX	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	JZ	374/385 (97%)	374 (100%)	0	100	100
60	KB	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	KE	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	KG	374/385 (97%)	374 (100%)	0	100	100
60	KI	374/385 (97%)	373 (100%)	1 (0%)	91	97

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	KK	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	KM	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	KO	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	KR	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	KT	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	KV	374/385 (97%)	374 (100%)	0	100	100
60	KX	374/385 (97%)	373 (100%)	1 (0%)	91	97
60	KZ	374/385 (97%)	371 (99%)	3 (1%)	79	93
60	LB	374/385 (97%)	369 (99%)	5 (1%)	65	88
All	All	131521/150498 (87%)	131008 (100%)	513 (0%)	88	96

5 of 513 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
60	JI	227	HIS
59	JS	223	THR
60	JI	58	ARG
60	BY	99	ASN
59	BU	339	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 371 such sidechains are listed below:

Mol	Chain	Res	Type
60	GX	414	ASN
60	IR	347	ASN
60	HF	43	GLN
59	HV	128	ASN
59	IZ	91	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 456 ligands modelled in this entry, 169 are monoatomic - leaving 287 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
62	GTP	JN	501	63	29,34,34	1.24	1 (3%)	35,54,54	1.32	5 (14%)
62	GTP	IB	602	63	29,34,34	1.20	1 (3%)	35,54,54	1.33	4 (11%)
64	GDP	EK	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.14	3 (10%)
64	GDP	FI	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	3 (10%)
64	GDP	FM	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.11	3 (10%)
62	GTP	CY	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.36	5 (14%)
62	GTP	KP	501	63	29,34,34	1.23	3 (10%)	35,54,54	1.37	5 (14%)
64	GDP	IU	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	3 (10%)
64	GDP	EW	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.04	3 (10%)
64	GDP	EE	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	3 (10%)
62	GTP	BI	501	63	29,34,34	1.22	2 (6%)	35,54,54	1.38	5 (14%)
62	GTP	EL	602	63	29,34,34	1.21	1 (3%)	35,54,54	1.32	4 (11%)
62	GTP	KU	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.33	4 (11%)
62	GTP	ER	602	63	29,34,34	1.21	1 (3%)	35,54,54	1.33	5 (14%)
64	GDP	GQ	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.09	3 (10%)
62	GTP	GT	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.33	5 (14%)
64	GDP	IH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	3 (10%)
62	GTP	DA	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.35	4 (11%)
64	GDP	CT	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.12	3 (10%)
62	GTP	DZ	602	63	29,34,34	1.21	1 (3%)	35,54,54	1.34	5 (14%)
64	GDP	HL	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.12	3 (10%)
64	GDP	HY	501	-	25,30,30	1.03	2 (8%)	30,47,47	1.12	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	GDP	EG	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.12	3 (10%)
62	GTP	CF	602	63	29,34,34	1.20	1 (3%)	35,54,54	1.31	5 (14%)
64	GDP	AL	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.14	3 (10%)
62	GTP	DI	602	63	29,34,34	1.20	2 (6%)	35,54,54	1.35	5 (14%)
64	GDP	JV	501	-	25,30,30	1.02	2 (8%)	30,47,47	1.15	3 (10%)
62	GTP	KJ	602	63	29,34,34	1.22	2 (6%)	35,54,54	1.41	5 (14%)
64	GDP	AZ	501	-	25,30,30	0.97	2 (8%)	30,47,47	1.09	3 (10%)
64	GDP	BD	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.14	3 (10%)
62	GTP	CQ	602	63	29,34,34	1.20	2 (6%)	35,54,54	1.35	5 (14%)
62	GTP	DG	602	63	29,34,34	1.20	2 (6%)	35,54,54	1.39	4 (11%)
64	GDP	DY	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.12	3 (10%)
62	GTP	II	501	63	29,34,34	1.24	1 (3%)	35,54,54	1.35	5 (14%)
64	GDP	DT	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.12	3 (10%)
64	GDP	EC	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.10	3 (10%)
64	GDP	KI	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.15	3 (10%)
64	GDP	CR	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.17	3 (10%)
64	GDP	DD	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.15	3 (10%)
64	GDP	KV	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.18	3 (10%)
64	GDP	AH	501	-	25,30,30	0.97	2 (8%)	30,47,47	1.11	3 (10%)
62	GTP	GP	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.36	5 (14%)
62	GTP	IK	602	63	29,34,34	1.23	2 (6%)	35,54,54	1.41	5 (14%)
62	GTP	IO	501	63	29,34,34	1.24	1 (3%)	35,54,54	1.34	5 (14%)
64	GDP	IJ	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.13	3 (10%)
64	GDP	HW	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.14	3 (10%)
64	GDP	JC	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	3 (10%)
64	GDP	KG	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.11	3 (10%)
62	GTP	AG	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.37	5 (14%)
62	GTP	DE	501	63	29,34,34	1.18	2 (6%)	35,54,54	1.41	4 (11%)
62	GTP	FY	602	63	29,34,34	1.22	2 (6%)	35,54,54	1.39	5 (14%)
62	GTP	CU	602	63	29,34,34	1.19	1 (3%)	35,54,54	1.36	4 (11%)
64	GDP	JG	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	3 (10%)
62	GTP	GN	602	63	29,34,34	1.22	1 (3%)	35,54,54	1.39	5 (14%)
62	GTP	HE	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.38	6 (17%)
64	GDP	HB	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.16	3 (10%)
64	GDP	CE	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	GTP	JF	501	63	29,34,34	1.22	1 (3%)	35,54,54	1.33	5 (14%)
62	GTP	AY	602	63	29,34,34	1.21	2 (6%)	35,54,54	1.34	5 (14%)
62	GTP	BE	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.35	5 (14%)
62	GTP	IM	602	63	29,34,34	1.23	1 (3%)	35,54,54	1.36	5 (14%)
64	GDP	KB	501	-	25,30,30	1.04	2 (8%)	30,47,47	1.15	3 (10%)
62	GTP	FN	502	63	29,34,34	1.20	1 (3%)	35,54,54	1.33	5 (14%)
64	GDP	HP	501	-	25,30,30	1.02	2 (8%)	30,47,47	1.23	3 (10%)
62	GTP	DO	602	63	29,34,34	1.23	2 (6%)	35,54,54	1.38	5 (14%)
62	GTP	HO	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.44	4 (11%)
64	GDP	GF	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.17	3 (10%)
62	GTP	BA	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.35	5 (14%)
62	GTP	CH	602	63	29,34,34	1.23	2 (6%)	35,54,54	1.34	4 (11%)
62	GTP	EX	602	63	29,34,34	1.19	1 (3%)	35,54,54	1.35	5 (14%)
64	GDP	JZ	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.08	3 (10%)
64	GDP	DR	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.11	3 (10%)
64	GDP	JA	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	3 (10%)
64	GDP	IR	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.09	3 (10%)
62	GTP	JS	602	63	29,34,34	1.00	2 (6%)	35,54,54	0.78	0
64	GDP	HU	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.10	3 (10%)
64	GDP	FS	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.12	3 (10%)
62	GTP	KQ	602	63	29,34,34	1.19	2 (6%)	35,54,54	1.39	5 (14%)
62	GTP	EB	501	63	29,34,34	1.21	1 (3%)	35,54,54	1.32	5 (14%)
64	GDP	FG	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.15	3 (10%)
62	GTP	JY	602	63	29,34,34	1.21	2 (6%)	35,54,54	1.36	5 (14%)
64	GDP	GX	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.13	3 (10%)
64	GDP	DN	501	-	25,30,30	0.97	2 (8%)	30,47,47	1.12	3 (10%)
64	GDP	DP	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.15	3 (10%)
62	GTP	AC	501	63	29,34,34	1.18	1 (3%)	35,54,54	1.35	5 (14%)
62	GTP	AU	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.35	5 (14%)
62	GTP	EF	602	63	29,34,34	1.19	1 (3%)	35,54,54	1.30	5 (14%)
64	GDP	EI	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	3 (10%)
64	GDP	FA	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.05	2 (6%)
64	GDP	GO	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.14	3 (10%)
62	GTP	DX	501	63	29,34,34	1.21	1 (3%)	35,54,54	1.33	5 (14%)
64	GDP	HF	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.14	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	GDP	HN	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.16	3 (10%)
62	GTP	FU	602	63	29,34,34	1.21	3 (10%)	35,54,54	1.36	5 (14%)
64	GDP	DL	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.10	3 (10%)
64	GDP	EO	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	3 (10%)
62	GTP	KF	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.37	5 (14%)
64	GDP	IE	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.09	3 (10%)
62	GTP	DU	602	63	29,34,34	1.22	2 (6%)	35,54,54	1.36	5 (14%)
64	GDP	FE	501	-	25,30,30	0.97	2 (8%)	30,47,47	1.10	3 (10%)
64	GDP	BP	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.13	3 (10%)
64	GDP	JT	501	-	25,30,30	1.03	2 (8%)	30,47,47	1.23	3 (10%)
62	GTP	JD	501	63	29,34,34	1.21	1 (3%)	35,54,54	1.36	5 (14%)
62	GTP	IV	602	63	29,34,34	1.22	2 (6%)	35,54,54	1.34	5 (14%)
64	GDP	HH	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.20	3 (10%)
62	GTP	GA	501	63	29,34,34	1.21	1 (3%)	35,54,54	1.40	4 (11%)
62	GTP	DM	602	63	29,34,34	1.21	2 (6%)	35,54,54	1.35	5 (14%)
62	GTP	KC	602	63	29,34,34	1.27	3 (10%)	35,54,54	1.43	5 (14%)
64	GDP	AB	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.14	3 (10%)
62	GTP	BW	501	63	29,34,34	1.23	2 (6%)	35,54,54	1.37	5 (14%)
64	GDP	KT	501	-	25,30,30	1.02	2 (8%)	30,47,47	1.19	3 (10%)
62	GTP	FL	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.32	5 (14%)
64	GDP	IP	501	-	25,30,30	1.03	2 (8%)	30,47,47	1.11	3 (10%)
62	GTP	KN	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.36	4 (11%)
64	GDP	FQ	501	-	25,30,30	0.97	2 (8%)	30,47,47	1.14	3 (10%)
64	GDP	KK	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.18	3 (10%)
64	GDP	HR	501	-	25,30,30	1.04	2 (8%)	30,47,47	1.20	3 (10%)
62	GTP	GL	501	63	29,34,34	1.18	2 (6%)	35,54,54	1.31	5 (14%)
62	GTP	KS	602	63	29,34,34	1.19	2 (6%)	35,54,54	1.32	5 (14%)
62	GTP	BM	501	63	29,34,34	1.20	1 (3%)	35,54,54	1.32	5 (14%)
64	GDP	GD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	3 (10%)
64	GDP	GS	501	-	25,30,30	0.97	2 (8%)	30,47,47	1.09	3 (10%)
62	GTP	GC	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.38	5 (14%)
62	GTP	KL	602	63	29,34,34	1.20	1 (3%)	35,54,54	1.37	4 (11%)
64	GDP	AV	501	-	25,30,30	1.02	2 (8%)	30,47,47	1.18	3 (10%)
64	GDP	CN	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.13	3 (10%)
64	GDP	DV	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.16	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	GDP	DF	501	-	25,30,30	1.03	3 (12%)	30,47,47	0.78	0
64	GDP	FC	501	-	25,30,30	0.97	2 (8%)	30,47,47	1.06	3 (10%)
64	GDP	JX	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.13	3 (10%)
62	GTP	ED	602	63	29,34,34	1.20	1 (3%)	35,54,54	1.31	5 (14%)
62	GTP	DC	602	63	29,34,34	1.20	2 (6%)	35,54,54	1.35	5 (14%)
64	GDP	JE	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.10	3 (10%)
64	GDP	IS	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.14	3 (10%)
62	GTP	GE	501	63	29,34,34	1.21	1 (3%)	35,54,54	1.36	4 (11%)
64	GDP	EQ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.20	3 (10%)
64	GDP	GV	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.12	3 (10%)
64	GDP	DW	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.10	3 (10%)
64	GDP	KO	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.10	3 (10%)
64	GDP	JI	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	3 (10%)
62	GTP	CS	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.36	5 (14%)
62	GTP	EV	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.34	5 (14%)
62	GTP	FH	501	63	29,34,34	1.19	1 (3%)	35,54,54	1.33	5 (14%)
62	GTP	BU	501	63	29,34,34	1.21	1 (3%)	35,54,54	1.35	4 (11%)
62	GTP	BZ	501	63	29,34,34	1.18	1 (3%)	35,54,54	1.34	5 (14%)
62	GTP	ID	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.40	5 (14%)
62	GTP	HA	501	63	29,34,34	1.22	2 (6%)	35,54,54	1.35	5 (14%)
62	GTP	IG	501	63	29,34,34	1.24	1 (3%)	35,54,54	1.36	5 (14%)
62	GTP	HT	501	63	29,34,34	1.20	1 (3%)	35,54,54	1.34	4 (11%)
62	GTP	JU	602	63	29,34,34	1.20	2 (6%)	35,54,54	1.38	5 (14%)
62	GTP	AE	602	63	29,34,34	1.19	2 (6%)	35,54,54	1.38	5 (14%)
62	GTP	BK	602	63	29,34,34	1.21	1 (3%)	35,54,54	1.32	4 (11%)
62	GTP	HX	501	63	29,34,34	1.21	1 (3%)	35,54,54	1.37	5 (14%)
64	GDP	AD	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.12	3 (10%)
62	GTP	KH	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.36	5 (14%)
62	GTP	ET	602	63	29,34,34	1.21	2 (6%)	35,54,54	1.36	5 (14%)
64	GDP	ES	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	3 (10%)
64	GDP	FO	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.17	3 (10%)
62	GTP	AK	602	63	29,34,34	1.20	2 (6%)	35,54,54	1.34	5 (14%)
64	GDP	KZ	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.09	3 (10%)
64	GDP	HS	501	-	25,30,30	1.02	2 (8%)	30,47,47	1.13	3 (10%)
64	GDP	JM	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.13	3 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	GTP	JJ	501	63	29,34,34	1.22	1 (3%)	35,54,54	1.35	5 (14%)
62	GTP	IZ	602	63	29,34,34	1.24	1 (3%)	35,54,54	1.36	5 (14%)
64	GDP	HD	501	-	25,30,30	1.03	2 (8%)	30,47,47	1.23	3 (10%)
62	GTP	HK	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.35	4 (11%)
62	GTP	JL	602	63	29,34,34	1.19	1 (3%)	35,54,54	1.30	4 (11%)
62	GTP	FF	501	63	29,34,34	1.19	1 (3%)	35,54,54	1.34	5 (14%)
62	GTP	GJ	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.35	5 (14%)
62	GTP	JH	501	63	29,34,34	1.19	1 (3%)	35,54,54	1.38	5 (14%)
62	GTP	DK	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.38	5 (14%)
62	GTP	CM	602	63	29,34,34	1.20	2 (6%)	35,54,54	1.34	4 (11%)
62	GTP	HG	602	63	29,34,34	1.21	2 (6%)	35,54,54	1.39	4 (11%)
64	GDP	BR	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
62	GTP	AM	602	63	29,34,34	1.19	2 (6%)	35,54,54	1.39	5 (14%)
62	GTP	BX	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.38	5 (14%)
64	GDP	CV	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.14	3 (10%)
62	GTP	KD	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.41	5 (14%)
62	GTP	JP	501	63	29,34,34	1.20	1 (3%)	35,54,54	1.33	5 (14%)
64	GDP	GB	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.18	3 (10%)
64	GDP	LB	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.17	3 (10%)
64	GDP	EU	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.14	3 (10%)
64	GDP	BV	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	3 (10%)
62	GTP	GW	501	63	29,34,34	1.18	2 (6%)	35,54,54	1.34	5 (14%)
62	GTP	CB	501	63	29,34,34	1.20	1 (3%)	35,54,54	1.30	4 (11%)
62	GTP	KY	602	63	29,34,34	1.18	2 (6%)	35,54,54	1.35	5 (14%)
62	GTP	BG	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.33	5 (14%)
64	GDP	BY	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.15	3 (10%)
62	GTP	EH	501	63	29,34,34	1.18	1 (3%)	35,54,54	1.33	5 (14%)
62	GTP	HC	602	63	29,34,34	1.19	2 (6%)	35,54,54	1.35	5 (14%)
64	GDP	AN	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.17	3 (10%)
64	GDP	CG	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	3 (10%)
64	GDP	BT	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	3 (10%)
64	GDP	BL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	3 (10%)
64	GDP	JR	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.12	3 (10%)
64	GDP	DJ	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.12	3 (10%)
62	GTP	BC	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.33	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	GTP	JW	602	63	29,34,34	1.20	2 (6%)	35,54,54	1.37	5 (14%)
64	GDP	CP	501	-	25,30,30	1.03	2 (8%)	30,47,47	1.20	3 (10%)
64	GDP	FX	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.16	3 (10%)
62	GTP	HM	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.34	4 (11%)
64	GDP	CL	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.13	3 (10%)
64	GDP	AJ	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.11	3 (10%)
64	GDP	EA	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.12	3 (10%)
62	GTP	HZ	501	63	29,34,34	1.21	1 (3%)	35,54,54	1.35	4 (11%)
64	GDP	HJ	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.13	3 (10%)
64	GDP	CZ	501	-	25,30,30	1.03	2 (8%)	30,47,47	1.17	3 (10%)
64	GDP	IW	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	3 (10%)
64	GDP	AF	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.19	3 (10%)
62	GTP	IT	602	63	29,34,34	1.22	1 (3%)	35,54,54	1.32	5 (14%)
62	GTP	HI	602	63	29,34,34	1.21	2 (6%)	35,54,54	1.36	5 (14%)
62	GTP	HQ	501	63	29,34,34	1.18	2 (6%)	35,54,54	1.36	5 (14%)
62	GTP	AQ	501	63	29,34,34	1.20	1 (3%)	35,54,54	1.43	5 (14%)
64	GDP	KR	501	-	25,30,30	1.02	2 (8%)	30,47,47	1.15	3 (10%)
64	GDP	JO	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.17	3 (10%)
62	GTP	FR	502	63	29,34,34	1.19	1 (3%)	35,54,54	1.35	5 (14%)
62	GTP	DQ	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.38	5 (14%)
64	GDP	KX	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.13	3 (10%)
64	GDP	KM	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.13	3 (10%)
62	GTP	EZ	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.34	5 (14%)
62	GTP	AS	602	63	29,34,34	1.17	1 (3%)	35,54,54	1.37	5 (14%)
62	GTP	GU	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.38	5 (14%)
62	GTP	EP	602	63	29,34,34	1.23	1 (3%)	35,54,54	1.34	5 (14%)
64	GDP	AP	501	-	25,30,30	1.02	2 (8%)	30,47,47	1.21	3 (10%)
64	GDP	BF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.10	3 (10%)
64	GDP	DH	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.21	3 (10%)
62	GTP	FD	602	63	29,34,34	1.19	1 (3%)	35,54,54	1.32	5 (14%)
64	GDP	IC	501	-	25,30,30	1.02	2 (8%)	30,47,47	1.21	3 (10%)
64	GDP	FK	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.10	3 (10%)
62	GTP	BS	501	63	29,34,34	1.20	1 (3%)	35,54,54	1.33	4 (11%)
64	GDP	JK	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.17	3 (10%)
62	GTP	HV	501	63	29,34,34	1.22	1 (3%)	35,54,54	1.36	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	GTP	AO	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.38	5 (14%)
64	GDP	BH	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	3 (10%)
64	GDP	GZ	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.15	3 (10%)
62	GTP	CW	602	63	29,34,34	1.21	2 (6%)	35,54,54	1.35	4 (11%)
64	GDP	IN	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	3 (10%)
62	GTP	EN	602	63	29,34,34	1.20	1 (3%)	35,54,54	1.33	4 (11%)
62	GTP	KA	602	63	29,34,34	1.19	2 (6%)	35,54,54	1.37	5 (14%)
62	GTP	EJ	602	63	29,34,34	1.19	1 (3%)	35,54,54	1.32	5 (14%)
62	GTP	FJ	602	63	29,34,34	1.20	1 (3%)	35,54,54	1.36	5 (14%)
62	GTP	GY	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.36	5 (14%)
62	GTP	FB	502	63	29,34,34	1.21	1 (3%)	35,54,54	1.36	5 (14%)
64	GDP	CI	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	3 (10%)
64	GDP	FV	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.13	3 (10%)
64	GDP	BN	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	3 (10%)
62	GTP	IX	501	63	29,34,34	1.21	1 (3%)	35,54,54	1.37	5 (14%)
64	GDP	BB	501	-	25,30,30	0.97	2 (8%)	30,47,47	1.10	3 (10%)
64	GDP	FZ	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.16	3 (10%)
64	GDP	GK	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.08	3 (10%)
64	GDP	GM	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.16	3 (10%)
62	GTP	CJ	501	63	29,34,34	1.23	2 (6%)	35,54,54	1.38	5 (14%)
62	GTP	FT	602	63	29,34,34	1.19	2 (6%)	35,54,54	1.35	5 (14%)
64	GDP	CX	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.14	3 (10%)
64	GDP	IA	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	3 (10%)
64	GDP	IY	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	3 (10%)
64	GDP	CC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	3 (10%)
62	GTP	GG	501	63	29,34,34	1.19	1 (3%)	35,54,54	1.39	5 (14%)
62	GTP	JQ	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.39	5 (14%)
64	GDP	KE	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.11	3 (10%)
62	GTP	DS	501	63	29,34,34	1.21	1 (3%)	35,54,54	1.36	5 (14%)
64	GDP	IF	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.16	3 (10%)
64	GDP	IL	501	-	25,30,30	1.04	2 (8%)	30,47,47	1.21	3 (10%)
62	GTP	JB	501	63	29,34,34	1.23	1 (3%)	35,54,54	1.35	5 (14%)
62	GTP	FP	502	63	29,34,34	1.19	2 (6%)	35,54,54	1.33	5 (14%)
62	GTP	AA	501	63	29,34,34	1.20	2 (6%)	35,54,54	1.37	4 (11%)
62	GTP	AI	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.33	4 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	GTP	AW	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.34	5 (14%)
62	GTP	GR	501	63	29,34,34	1.21	2 (6%)	35,54,54	1.34	5 (14%)
62	GTP	IQ	501	63	29,34,34	1.25	2 (6%)	35,54,54	1.39	5 (14%)
62	GTP	CO	501	63	29,34,34	1.17	1 (3%)	35,54,54	1.34	4 (11%)
62	GTP	LA	501	63	29,34,34	1.19	2 (6%)	35,54,54	1.35	5 (14%)
64	GDP	AT	501	-	25,30,30	1.02	2 (8%)	30,47,47	1.15	3 (10%)
64	GDP	CA	602	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	3 (10%)
64	GDP	AR	501	-	25,30,30	0.97	2 (8%)	30,47,47	1.12	3 (10%)
62	GTP	CD	501	63	29,34,34	1.24	1 (3%)	35,54,54	1.31	3 (8%)
64	GDP	EM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.13	3 (10%)
62	GTP	FW	501	63	29,34,34	1.22	1 (3%)	35,54,54	1.37	4 (11%)
64	GDP	DB	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.13	3 (10%)
64	GDP	GI	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.14	3 (10%)
62	GTP	KW	602	63	29,34,34	1.18	2 (6%)	35,54,54	1.36	5 (14%)
62	GTP	BO	501	63	29,34,34	1.19	1 (3%)	35,54,54	1.32	5 (14%)
64	GDP	BJ	501	-	25,30,30	0.99	2 (8%)	30,47,47	1.12	3 (10%)
64	GDP	AX	501	-	25,30,30	0.98	2 (8%)	30,47,47	1.08	3 (10%)
64	GDP	EY	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	3 (10%)
62	GTP	GH	602	63	29,34,34	1.22	2 (6%)	35,54,54	1.34	4 (11%)
62	GTP	BQ	602	63	29,34,34	1.20	1 (3%)	35,54,54	1.32	5 (14%)

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
62	GTP	JN	501	63	-	5/18/38/38	0/3/3/3
62	GTP	IB	602	63	-	5/18/38/38	0/3/3/3
64	GDP	EK	501	-	-	2/12/32/32	0/3/3/3
64	GDP	FI	501	-	-	2/12/32/32	0/3/3/3
64	GDP	FM	501	-	-	2/12/32/32	0/3/3/3
62	GTP	CY	501	63	-	5/18/38/38	0/3/3/3
62	GTP	KP	501	63	-	5/18/38/38	0/3/3/3
64	GDP	IU	501	-	-	2/12/32/32	0/3/3/3
64	GDP	EW	501	-	-	2/12/32/32	0/3/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	GDP	EE	501	-	-	2/12/32/32	0/3/3/3
62	GTP	BI	501	63	-	5/18/38/38	0/3/3/3
62	GTP	EL	602	63	-	5/18/38/38	0/3/3/3
62	GTP	KU	501	63	-	5/18/38/38	0/3/3/3
62	GTP	ER	602	63	-	5/18/38/38	0/3/3/3
64	GDP	GQ	501	-	-	2/12/32/32	0/3/3/3
62	GTP	GT	501	63	-	5/18/38/38	0/3/3/3
64	GDP	IH	501	-	-	2/12/32/32	0/3/3/3
62	GTP	DA	501	63	-	5/18/38/38	0/3/3/3
64	GDP	CT	501	-	-	2/12/32/32	0/3/3/3
62	GTP	DZ	602	63	-	5/18/38/38	0/3/3/3
64	GDP	HL	501	-	-	2/12/32/32	0/3/3/3
64	GDP	HY	501	-	-	2/12/32/32	0/3/3/3
64	GDP	EG	501	-	-	2/12/32/32	0/3/3/3
62	GTP	CF	602	63	-	5/18/38/38	0/3/3/3
64	GDP	AL	501	-	-	2/12/32/32	0/3/3/3
62	GTP	DI	602	63	-	5/18/38/38	0/3/3/3
64	GDP	JV	501	-	-	2/12/32/32	0/3/3/3
62	GTP	KJ	602	63	-	5/18/38/38	0/3/3/3
64	GDP	AZ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	BD	501	-	-	2/12/32/32	0/3/3/3
62	GTP	CQ	602	63	-	5/18/38/38	0/3/3/3
62	GTP	DG	602	63	-	5/18/38/38	0/3/3/3
64	GDP	DY	501	-	-	2/12/32/32	0/3/3/3
62	GTP	II	501	63	-	5/18/38/38	0/3/3/3
64	GDP	DT	501	-	-	2/12/32/32	0/3/3/3
64	GDP	EC	501	-	-	2/12/32/32	0/3/3/3
64	GDP	KI	501	-	-	2/12/32/32	0/3/3/3
64	GDP	CR	501	-	-	2/12/32/32	0/3/3/3
64	GDP	DD	501	-	-	2/12/32/32	0/3/3/3
64	GDP	KV	501	-	-	2/12/32/32	0/3/3/3
64	GDP	AH	501	-	-	2/12/32/32	0/3/3/3
62	GTP	GP	501	63	-	5/18/38/38	0/3/3/3
62	GTP	IK	602	63	-	5/18/38/38	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GTP	IO	501	63	-	5/18/38/38	0/3/3/3
64	GDP	IJ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	HW	501	-	-	2/12/32/32	0/3/3/3
64	GDP	JC	501	-	-	2/12/32/32	0/3/3/3
64	GDP	KG	501	-	-	2/12/32/32	0/3/3/3
62	GTP	AG	501	63	-	5/18/38/38	0/3/3/3
62	GTP	DE	501	63	-	5/18/38/38	0/3/3/3
62	GTP	FY	602	63	-	5/18/38/38	0/3/3/3
62	GTP	CU	602	63	-	5/18/38/38	0/3/3/3
64	GDP	JG	501	-	-	2/12/32/32	0/3/3/3
62	GTP	GN	602	63	-	5/18/38/38	0/3/3/3
62	GTP	HE	501	63	-	5/18/38/38	0/3/3/3
64	GDP	HB	501	-	-	2/12/32/32	0/3/3/3
64	GDP	CE	501	-	-	2/12/32/32	0/3/3/3
62	GTP	JF	501	63	-	5/18/38/38	0/3/3/3
62	GTP	AY	602	63	-	5/18/38/38	0/3/3/3
62	GTP	BE	501	63	-	5/18/38/38	0/3/3/3
62	GTP	IM	602	63	-	5/18/38/38	0/3/3/3
64	GDP	KB	501	-	-	2/12/32/32	0/3/3/3
62	GTP	FN	502	63	-	5/18/38/38	0/3/3/3
64	GDP	HP	501	-	-	2/12/32/32	0/3/3/3
62	GTP	DO	602	63	-	5/18/38/38	0/3/3/3
62	GTP	HO	501	63	-	5/18/38/38	0/3/3/3
64	GDP	GF	501	-	-	2/12/32/32	0/3/3/3
62	GTP	BA	501	63	-	5/18/38/38	0/3/3/3
62	GTP	CH	602	63	-	5/18/38/38	0/3/3/3
62	GTP	EX	602	63	-	5/18/38/38	0/3/3/3
64	GDP	JZ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	DR	501	-	-	2/12/32/32	0/3/3/3
64	GDP	JA	501	-	-	2/12/32/32	0/3/3/3
64	GDP	IR	501	-	-	2/12/32/32	0/3/3/3
62	GTP	JS	602	63	-	5/18/38/38	0/3/3/3
64	GDP	HU	501	-	-	2/12/32/32	0/3/3/3
64	GDP	FS	501	-	-	2/12/32/32	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GTP	KQ	602	63	-	5/18/38/38	0/3/3/3
62	GTP	EB	501	63	-	5/18/38/38	0/3/3/3
64	GDP	FG	501	-	-	2/12/32/32	0/3/3/3
62	GTP	JY	602	63	-	5/18/38/38	0/3/3/3
64	GDP	GX	501	-	-	2/12/32/32	0/3/3/3
64	GDP	DN	501	-	-	2/12/32/32	0/3/3/3
64	GDP	DP	501	-	-	2/12/32/32	0/3/3/3
62	GTP	AC	501	63	-	5/18/38/38	0/3/3/3
62	GTP	AU	501	63	-	5/18/38/38	0/3/3/3
62	GTP	EF	602	63	-	5/18/38/38	0/3/3/3
64	GDP	EI	501	-	-	2/12/32/32	0/3/3/3
64	GDP	FA	501	-	-	2/12/32/32	0/3/3/3
64	GDP	GO	501	-	-	2/12/32/32	0/3/3/3
62	GTP	DX	501	63	-	5/18/38/38	0/3/3/3
64	GDP	HF	501	-	-	2/12/32/32	0/3/3/3
64	GDP	HN	501	-	-	2/12/32/32	0/3/3/3
62	GTP	FU	602	63	-	5/18/38/38	0/3/3/3
64	GDP	DL	501	-	-	2/12/32/32	0/3/3/3
64	GDP	EO	501	-	-	2/12/32/32	0/3/3/3
62	GTP	KF	501	63	-	5/18/38/38	0/3/3/3
64	GDP	IE	501	-	-	2/12/32/32	0/3/3/3
62	GTP	DU	602	63	-	5/18/38/38	0/3/3/3
64	GDP	FE	501	-	-	2/12/32/32	0/3/3/3
64	GDP	BP	501	-	-	2/12/32/32	0/3/3/3
64	GDP	JT	501	-	-	2/12/32/32	0/3/3/3
62	GTP	JD	501	63	-	5/18/38/38	0/3/3/3
62	GTP	IV	602	63	-	5/18/38/38	0/3/3/3
64	GDP	HH	501	-	-	2/12/32/32	0/3/3/3
62	GTP	GA	501	63	-	5/18/38/38	0/3/3/3
62	GTP	DM	602	63	-	5/18/38/38	0/3/3/3
62	GTP	KC	602	63	-	5/18/38/38	0/3/3/3
64	GDP	AB	501	-	-	2/12/32/32	0/3/3/3
62	GTP	BW	501	63	-	5/18/38/38	0/3/3/3
64	GDP	KT	501	-	-	2/12/32/32	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GTP	FL	501	63	-	5/18/38/38	0/3/3/3
64	GDP	IP	501	-	-	2/12/32/32	0/3/3/3
62	GTP	KN	501	63	-	5/18/38/38	0/3/3/3
64	GDP	FQ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	KK	501	-	-	2/12/32/32	0/3/3/3
64	GDP	HR	501	-	-	2/12/32/32	0/3/3/3
62	GTP	GL	501	63	-	5/18/38/38	0/3/3/3
62	GTP	KS	602	63	-	5/18/38/38	0/3/3/3
62	GTP	BM	501	63	-	5/18/38/38	0/3/3/3
64	GDP	GD	501	-	-	2/12/32/32	0/3/3/3
64	GDP	GS	501	-	-	2/12/32/32	0/3/3/3
62	GTP	GC	501	63	-	5/18/38/38	0/3/3/3
62	GTP	KL	602	63	-	5/18/38/38	0/3/3/3
64	GDP	AV	501	-	-	2/12/32/32	0/3/3/3
64	GDP	CN	501	-	-	2/12/32/32	0/3/3/3
64	GDP	DV	501	-	-	2/12/32/32	0/3/3/3
64	GDP	DF	501	-	-	3/12/32/32	0/3/3/3
64	GDP	FC	501	-	-	2/12/32/32	0/3/3/3
64	GDP	JX	501	-	-	2/12/32/32	0/3/3/3
62	GTP	ED	602	63	-	5/18/38/38	0/3/3/3
62	GTP	DC	602	63	-	5/18/38/38	0/3/3/3
64	GDP	JE	501	-	-	2/12/32/32	0/3/3/3
64	GDP	IS	501	-	-	2/12/32/32	0/3/3/3
62	GTP	GE	501	63	-	5/18/38/38	0/3/3/3
64	GDP	EQ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	GV	501	-	-	2/12/32/32	0/3/3/3
64	GDP	DW	501	-	-	2/12/32/32	0/3/3/3
64	GDP	KO	501	-	-	2/12/32/32	0/3/3/3
64	GDP	JI	501	-	-	2/12/32/32	0/3/3/3
62	GTP	CS	501	63	-	5/18/38/38	0/3/3/3
62	GTP	EV	501	63	-	5/18/38/38	0/3/3/3
62	GTP	FH	501	63	-	5/18/38/38	0/3/3/3
62	GTP	BU	501	63	-	5/18/38/38	0/3/3/3
62	GTP	BZ	501	63	-	5/18/38/38	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GTP	ID	501	63	-	5/18/38/38	0/3/3/3
62	GTP	HA	501	63	-	5/18/38/38	0/3/3/3
62	GTP	IG	501	63	-	5/18/38/38	0/3/3/3
62	GTP	HT	501	63	-	5/18/38/38	0/3/3/3
62	GTP	JU	602	63	-	5/18/38/38	0/3/3/3
62	GTP	AE	602	63	-	5/18/38/38	0/3/3/3
62	GTP	BK	602	63	-	5/18/38/38	0/3/3/3
62	GTP	HX	501	63	-	5/18/38/38	0/3/3/3
64	GDP	AD	501	-	-	2/12/32/32	0/3/3/3
62	GTP	KH	501	63	-	5/18/38/38	0/3/3/3
62	GTP	ET	602	63	-	5/18/38/38	0/3/3/3
64	GDP	ES	501	-	-	2/12/32/32	0/3/3/3
64	GDP	FO	501	-	-	2/12/32/32	0/3/3/3
62	GTP	AK	602	63	-	5/18/38/38	0/3/3/3
64	GDP	KZ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	HS	501	-	-	2/12/32/32	0/3/3/3
64	GDP	JM	501	-	-	2/12/32/32	0/3/3/3
62	GTP	JJ	501	63	-	5/18/38/38	0/3/3/3
62	GTP	IZ	602	63	-	5/18/38/38	0/3/3/3
64	GDP	HD	501	-	-	2/12/32/32	0/3/3/3
62	GTP	HK	501	63	-	5/18/38/38	0/3/3/3
62	GTP	JL	602	63	-	5/18/38/38	0/3/3/3
62	GTP	FF	501	63	-	5/18/38/38	0/3/3/3
62	GTP	GJ	501	63	-	5/18/38/38	0/3/3/3
62	GTP	JH	501	63	-	5/18/38/38	0/3/3/3
62	GTP	DK	501	63	-	5/18/38/38	0/3/3/3
62	GTP	CM	602	63	-	5/18/38/38	0/3/3/3
62	GTP	HG	602	63	-	5/18/38/38	0/3/3/3
64	GDP	BR	501	-	-	2/12/32/32	0/3/3/3
62	GTP	AM	602	63	-	5/18/38/38	0/3/3/3
62	GTP	BX	501	63	-	5/18/38/38	0/3/3/3
64	GDP	CV	501	-	-	2/12/32/32	0/3/3/3
62	GTP	KD	501	63	-	5/18/38/38	0/3/3/3
62	GTP	JP	501	63	-	5/18/38/38	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	GDP	GB	501	-	-	2/12/32/32	0/3/3/3
64	GDP	LB	501	-	-	2/12/32/32	0/3/3/3
64	GDP	EU	501	-	-	2/12/32/32	0/3/3/3
64	GDP	BV	501	-	-	2/12/32/32	0/3/3/3
62	GTP	GW	501	63	-	5/18/38/38	0/3/3/3
62	GTP	CB	501	63	-	5/18/38/38	0/3/3/3
62	GTP	KY	602	63	-	5/18/38/38	0/3/3/3
62	GTP	BG	501	63	-	5/18/38/38	0/3/3/3
64	GDP	BY	501	-	-	2/12/32/32	0/3/3/3
62	GTP	EH	501	63	-	5/18/38/38	0/3/3/3
62	GTP	HC	602	63	-	5/18/38/38	0/3/3/3
64	GDP	AN	501	-	-	2/12/32/32	0/3/3/3
64	GDP	CG	501	-	-	2/12/32/32	0/3/3/3
64	GDP	BT	501	-	-	2/12/32/32	0/3/3/3
64	GDP	BL	501	-	-	2/12/32/32	0/3/3/3
64	GDP	JR	501	-	-	2/12/32/32	0/3/3/3
64	GDP	DJ	501	-	-	2/12/32/32	0/3/3/3
62	GTP	BC	501	63	-	5/18/38/38	0/3/3/3
62	GTP	JW	602	63	-	5/18/38/38	0/3/3/3
64	GDP	CP	501	-	-	2/12/32/32	0/3/3/3
64	GDP	FX	501	-	-	2/12/32/32	0/3/3/3
62	GTP	HM	501	63	-	5/18/38/38	0/3/3/3
64	GDP	CL	501	-	-	2/12/32/32	0/3/3/3
64	GDP	AJ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	EA	501	-	-	2/12/32/32	0/3/3/3
62	GTP	HZ	501	63	-	5/18/38/38	0/3/3/3
64	GDP	HJ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	CZ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	IW	501	-	-	2/12/32/32	0/3/3/3
64	GDP	AF	501	-	-	2/12/32/32	0/3/3/3
62	GTP	IT	602	63	-	5/18/38/38	0/3/3/3
62	GTP	HI	602	63	-	5/18/38/38	0/3/3/3
62	GTP	HQ	501	63	-	5/18/38/38	0/3/3/3
62	GTP	AQ	501	63	-	5/18/38/38	0/3/3/3

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	GDP	KR	501	-	-	2/12/32/32	0/3/3/3
64	GDP	JO	501	-	-	2/12/32/32	0/3/3/3
62	GTP	FR	502	63	-	5/18/38/38	0/3/3/3
62	GTP	DQ	501	63	-	5/18/38/38	0/3/3/3
64	GDP	KX	501	-	-	2/12/32/32	0/3/3/3
64	GDP	KM	501	-	-	2/12/32/32	0/3/3/3
62	GTP	EZ	501	63	-	5/18/38/38	0/3/3/3
62	GTP	AS	602	63	-	5/18/38/38	0/3/3/3
62	GTP	GU	501	63	-	5/18/38/38	0/3/3/3
62	GTP	EP	602	63	-	5/18/38/38	0/3/3/3
64	GDP	AP	501	-	-	2/12/32/32	0/3/3/3
64	GDP	BF	501	-	-	2/12/32/32	0/3/3/3
64	GDP	DH	501	-	-	2/12/32/32	0/3/3/3
62	GTP	FD	602	63	-	5/18/38/38	0/3/3/3
64	GDP	IC	501	-	-	2/12/32/32	0/3/3/3
64	GDP	FK	501	-	-	2/12/32/32	0/3/3/3
62	GTP	BS	501	63	-	5/18/38/38	0/3/3/3
64	GDP	JK	501	-	-	2/12/32/32	0/3/3/3
62	GTP	HV	501	63	-	5/18/38/38	0/3/3/3
62	GTP	AO	501	63	-	5/18/38/38	0/3/3/3
64	GDP	BH	501	-	-	2/12/32/32	0/3/3/3
64	GDP	GZ	501	-	-	2/12/32/32	0/3/3/3
62	GTP	CW	602	63	-	5/18/38/38	0/3/3/3
64	GDP	IN	501	-	-	2/12/32/32	0/3/3/3
62	GTP	EN	602	63	-	5/18/38/38	0/3/3/3
62	GTP	KA	602	63	-	5/18/38/38	0/3/3/3
62	GTP	EJ	602	63	-	5/18/38/38	0/3/3/3
62	GTP	FJ	602	63	-	5/18/38/38	0/3/3/3
62	GTP	GY	501	63	-	5/18/38/38	0/3/3/3
62	GTP	FB	502	63	-	5/18/38/38	0/3/3/3
64	GDP	CI	501	-	-	2/12/32/32	0/3/3/3
64	GDP	FV	501	-	-	2/12/32/32	0/3/3/3
64	GDP	BN	501	-	-	2/12/32/32	0/3/3/3
62	GTP	IX	501	63	-	5/18/38/38	0/3/3/3

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	GDP	BB	501	-	-	2/12/32/32	0/3/3/3
64	GDP	FZ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	GK	501	-	-	2/12/32/32	0/3/3/3
64	GDP	GM	501	-	-	2/12/32/32	0/3/3/3
62	GTP	CJ	501	63	-	5/18/38/38	0/3/3/3
62	GTP	FT	602	63	-	5/18/38/38	0/3/3/3
64	GDP	CX	501	-	-	2/12/32/32	0/3/3/3
64	GDP	IA	501	-	-	2/12/32/32	0/3/3/3
64	GDP	IY	501	-	-	2/12/32/32	0/3/3/3
64	GDP	CC	501	-	-	2/12/32/32	0/3/3/3
62	GTP	GG	501	63	-	5/18/38/38	0/3/3/3
62	GTP	JQ	501	63	-	5/18/38/38	0/3/3/3
64	GDP	KE	501	-	-	2/12/32/32	0/3/3/3
62	GTP	DS	501	63	-	5/18/38/38	0/3/3/3
64	GDP	IF	501	-	-	2/12/32/32	0/3/3/3
64	GDP	IL	501	-	-	2/12/32/32	0/3/3/3
62	GTP	JB	501	63	-	5/18/38/38	0/3/3/3
62	GTP	FP	502	63	-	5/18/38/38	0/3/3/3
62	GTP	AA	501	63	-	5/18/38/38	0/3/3/3
62	GTP	AI	501	63	-	5/18/38/38	0/3/3/3
62	GTP	AW	501	63	-	5/18/38/38	0/3/3/3
62	GTP	GR	501	63	-	5/18/38/38	0/3/3/3
62	GTP	IQ	501	63	-	5/18/38/38	0/3/3/3
62	GTP	CO	501	63	-	5/18/38/38	0/3/3/3
62	GTP	LA	501	63	-	5/18/38/38	0/3/3/3
64	GDP	AT	501	-	-	2/12/32/32	0/3/3/3
64	GDP	CA	602	-	-	2/12/32/32	0/3/3/3
64	GDP	AR	501	-	-	2/12/32/32	0/3/3/3
62	GTP	CD	501	63	-	5/18/38/38	0/3/3/3
64	GDP	EM	501	-	-	2/12/32/32	0/3/3/3
62	GTP	FW	501	63	-	5/18/38/38	0/3/3/3
64	GDP	DB	501	-	-	2/12/32/32	0/3/3/3
64	GDP	GI	501	-	-	2/12/32/32	0/3/3/3
62	GTP	KW	602	63	-	5/18/38/38	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GTP	BO	501	63	-	5/18/38/38	0/3/3/3
64	GDP	BJ	501	-	-	2/12/32/32	0/3/3/3
64	GDP	AX	501	-	-	2/12/32/32	0/3/3/3
64	GDP	EY	501	-	-	2/12/32/32	0/3/3/3
62	GTP	GH	602	63	-	5/18/38/38	0/3/3/3
62	GTP	BQ	602	63	-	5/18/38/38	0/3/3/3

The worst 5 of 478 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	JF	501	GTP	C5-C6	-4.56	1.38	1.47
62	BU	501	GTP	C5-C6	-4.56	1.38	1.47
62	CD	501	GTP	C5-C6	-4.54	1.38	1.47
62	DZ	602	GTP	C5-C6	-4.53	1.38	1.47
62	JJ	501	GTP	C5-C6	-4.53	1.38	1.47

The worst 5 of 1109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	HM	501	GTP	C8-N7-C5	3.85	109.10	102.55
62	HG	602	GTP	C8-N7-C5	3.82	109.06	102.55
62	IK	602	GTP	C8-N7-C5	3.82	109.05	102.55
62	BX	501	GTP	C8-N7-C5	3.80	109.02	102.55
62	DA	501	GTP	C8-N7-C5	3.80	109.01	102.55

There are no chirality outliers.

5 of 1010 torsion outliers are listed below:

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

There are no ring outliers.

108 monomers are involved in 121 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	JN	501	GTP	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	IB	602	GTP	1	0
64	EK	501	GDP	1	0
62	CY	501	GTP	1	0
62	KP	501	GTP	1	0
62	BI	501	GTP	1	0
64	HY	501	GDP	1	0
62	DI	602	GTP	1	0
62	CQ	602	GTP	2	0
64	KI	501	GDP	1	0
64	KV	501	GDP	1	0
62	GP	501	GTP	1	0
62	IK	602	GTP	1	0
64	IJ	501	GDP	1	0
64	JC	501	GDP	1	0
62	AG	501	GTP	1	0
62	CU	602	GTP	1	0
64	JG	501	GDP	1	0
62	GN	602	GTP	1	0
64	CE	501	GDP	1	0
62	JF	501	GTP	2	0
62	AY	602	GTP	1	0
62	BE	501	GTP	1	0
62	HO	501	GTP	1	0
62	BA	501	GTP	1	0
64	JA	501	GDP	1	0
64	IR	501	GDP	1	0
64	HU	501	GDP	1	0
64	FS	501	GDP	1	0
62	EB	501	GTP	1	0
64	DN	501	GDP	1	0
62	AC	501	GTP	1	0
64	FA	501	GDP	1	0
62	FU	602	GTP	1	0
62	KF	501	GTP	1	0
64	IE	501	GDP	1	0
62	BW	501	GTP	1	0
64	IP	501	GDP	2	0
64	KK	501	GDP	1	0
62	BM	501	GTP	1	0
64	GD	501	GDP	1	0
62	KL	602	GTP	1	0
64	AV	501	GDP	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	CN	501	GDP	1	0
64	FC	501	GDP	1	0
64	JE	501	GDP	1	0
64	IS	501	GDP	1	0
64	EQ	501	GDP	1	0
64	KO	501	GDP	1	0
62	CS	501	GTP	1	0
62	FH	501	GTP	1	0
62	ID	501	GTP	1	0
62	HA	501	GTP	1	0
62	HT	501	GTP	1	0
64	AD	501	GDP	1	0
62	KH	501	GTP	1	0
64	ES	501	GDP	1	0
62	IZ	602	GTP	1	0
62	HK	501	GTP	1	0
62	CM	602	GTP	1	0
62	HG	602	GTP	1	0
64	BR	501	GDP	1	0
64	CV	501	GDP	1	0
62	KD	501	GTP	1	0
64	GB	501	GDP	1	0
64	EU	501	GDP	1	0
64	BV	501	GDP	1	0
62	KY	602	GTP	1	0
62	BG	501	GTP	1	0
62	EH	501	GTP	1	0
62	HC	602	GTP	3	0
64	CG	501	GDP	1	0
64	BT	501	GDP	1	0
62	BC	501	GTP	1	0
62	JW	602	GTP	1	0
64	CP	501	GDP	2	0
62	HM	501	GTP	1	0
64	CL	501	GDP	1	0
62	HZ	501	GTP	1	0
64	HJ	501	GDP	1	0
64	CZ	501	GDP	1	0
64	IW	501	GDP	1	0
62	HQ	501	GTP	2	0
62	AQ	501	GTP	1	0
62	EZ	501	GTP	1	0

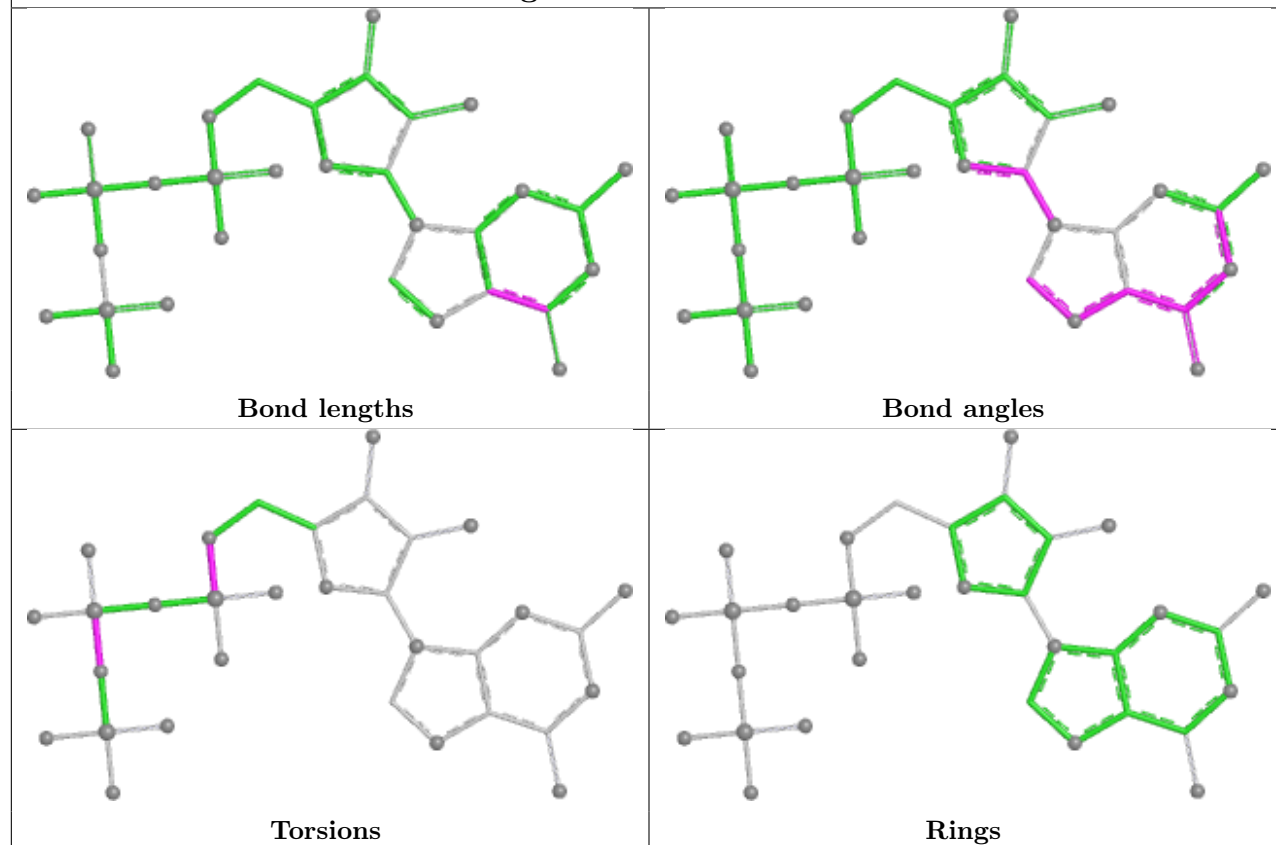
*Continued on next page...*

*Continued from previous page...*

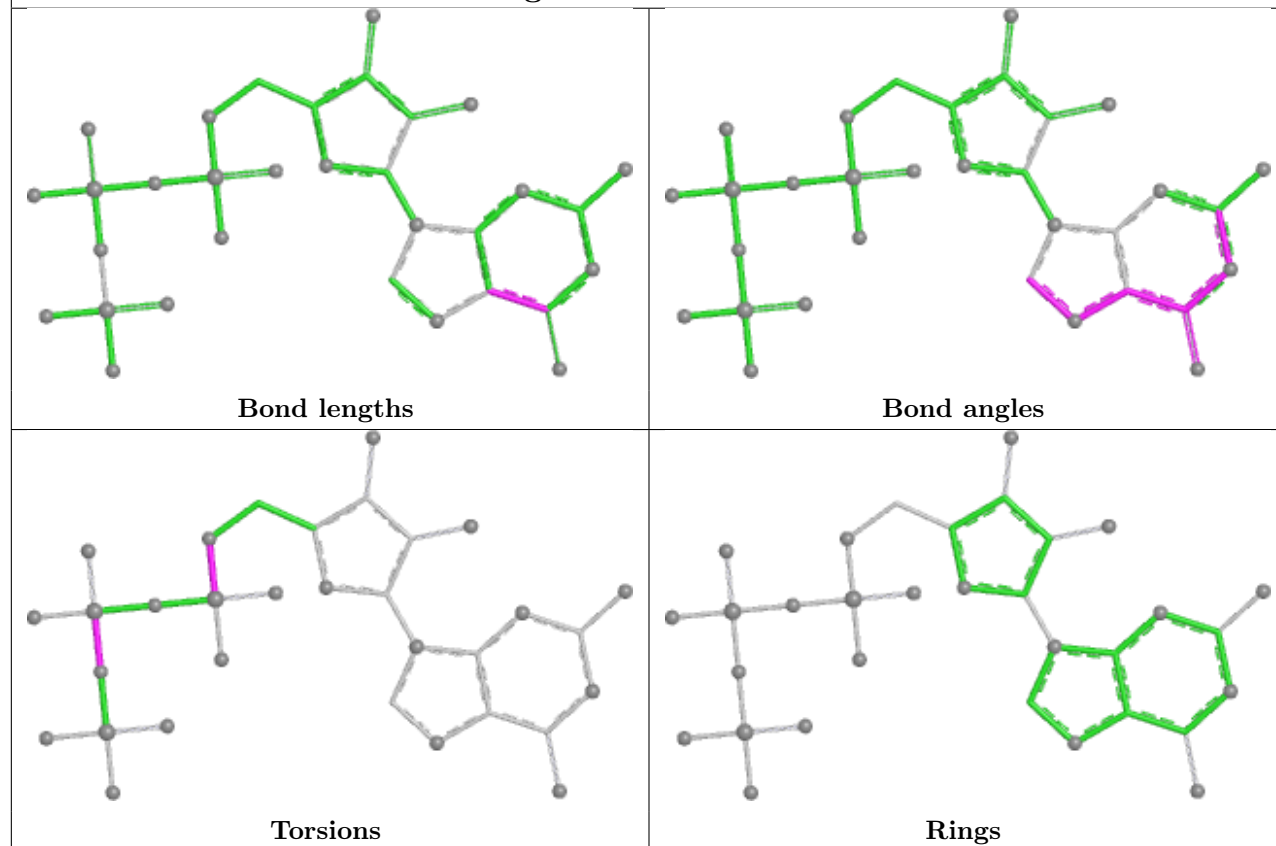
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	AS	602	GTP	2	0
62	GU	501	GTP	1	0
64	IC	501	GDP	1	0
64	JK	501	GDP	2	0
62	CW	602	GTP	2	0
64	IN	501	GDP	1	0
62	EJ	602	GTP	1	0
64	CI	501	GDP	1	0
64	BN	501	GDP	1	0
62	IX	501	GTP	1	0
62	CJ	501	GTP	1	0
64	IA	501	GDP	1	0
64	IF	501	GDP	1	0
64	IL	501	GDP	3	0
62	JB	501	GTP	1	0
62	AA	501	GTP	1	0
62	IQ	501	GTP	1	0
62	CO	501	GTP	2	0
64	AT	501	GDP	1	0
64	EM	501	GDP	1	0
62	KW	602	GTP	1	0
64	EY	501	GDP	1	0
62	BQ	602	GTP	1	0

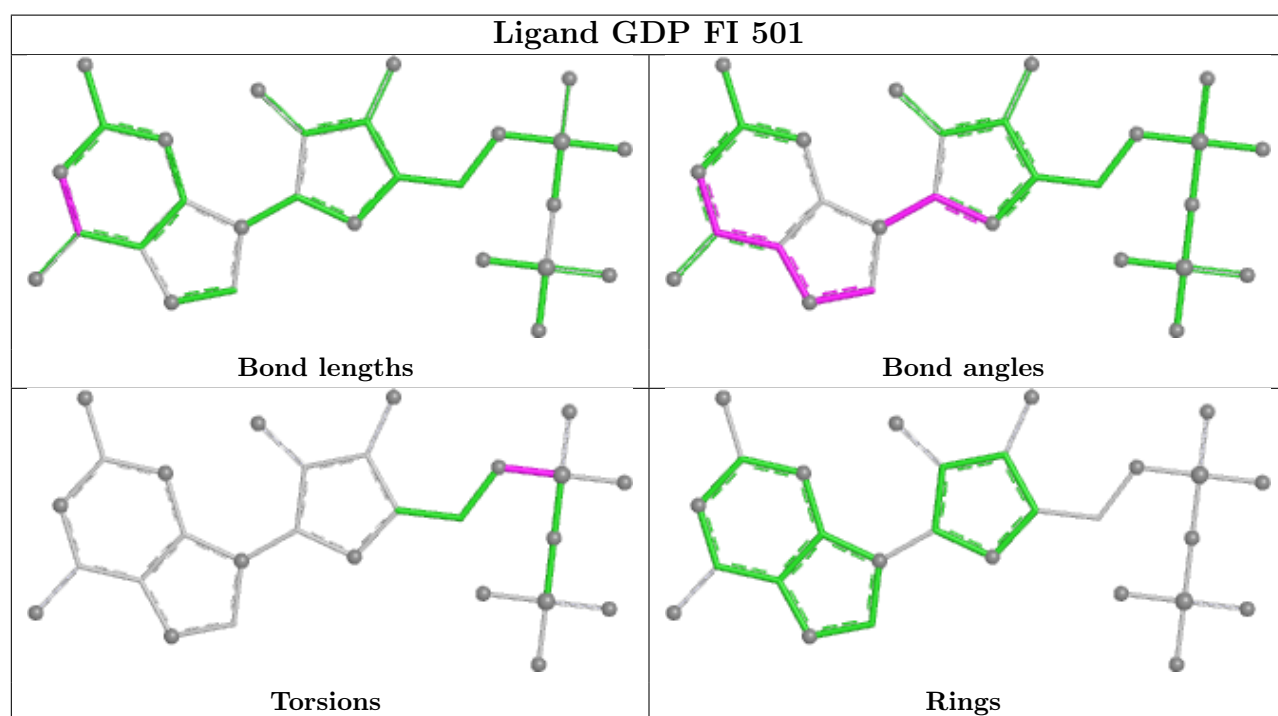
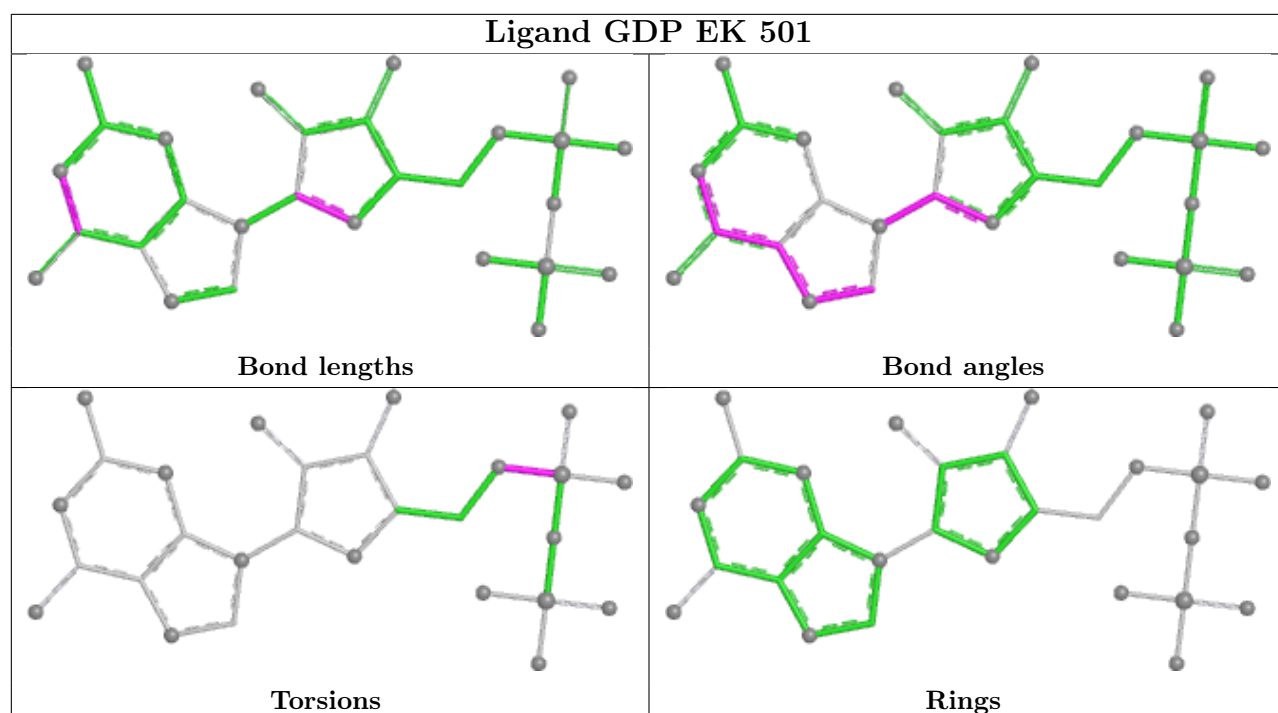
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

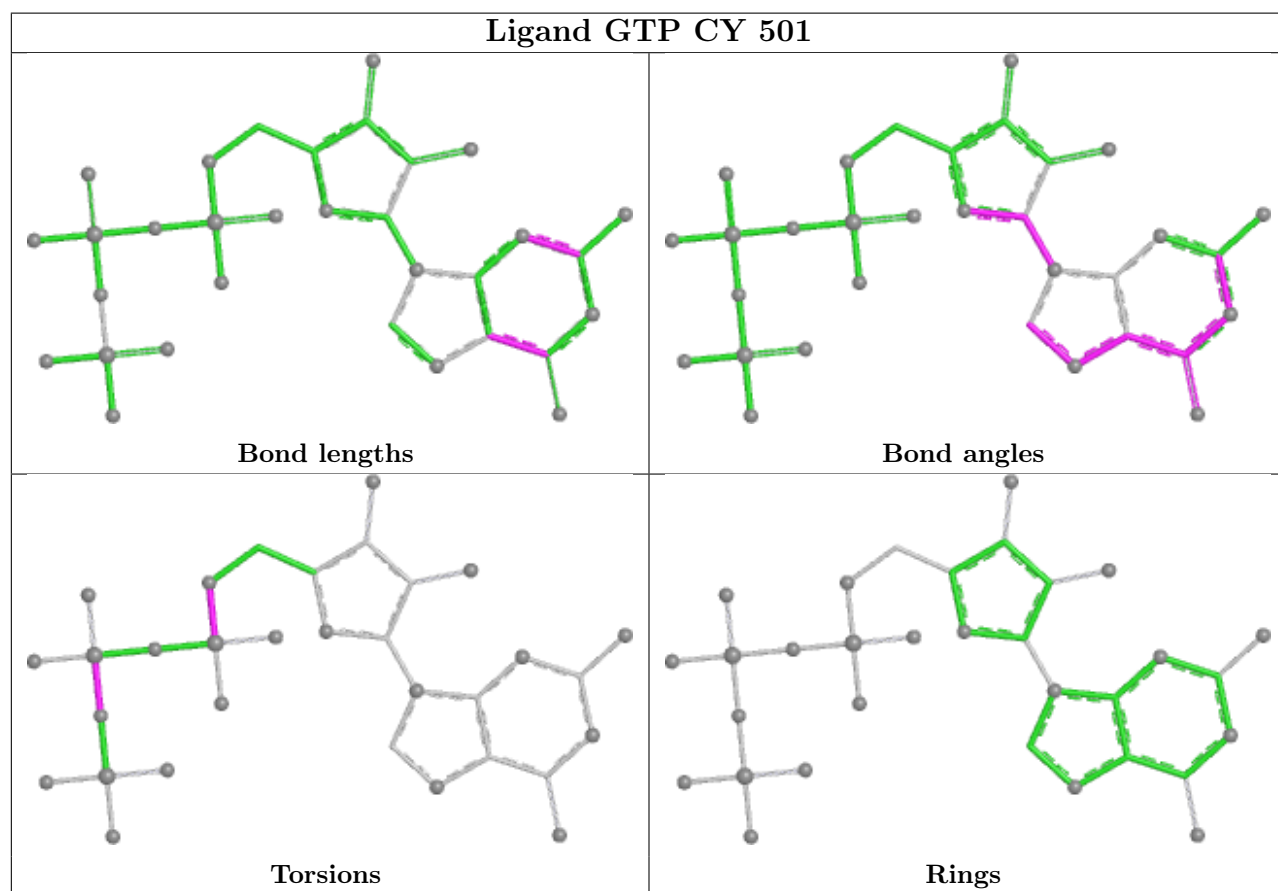
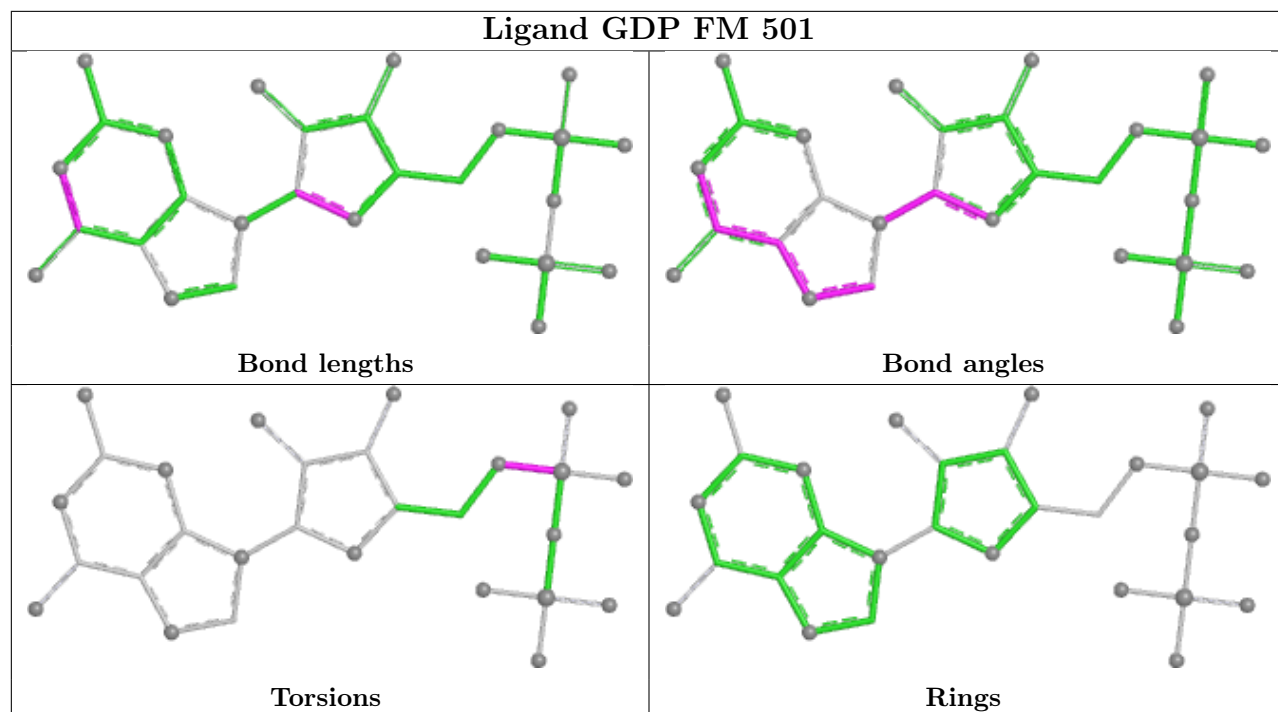
## Ligand GTP JN 501



## Ligand GTP IB 602

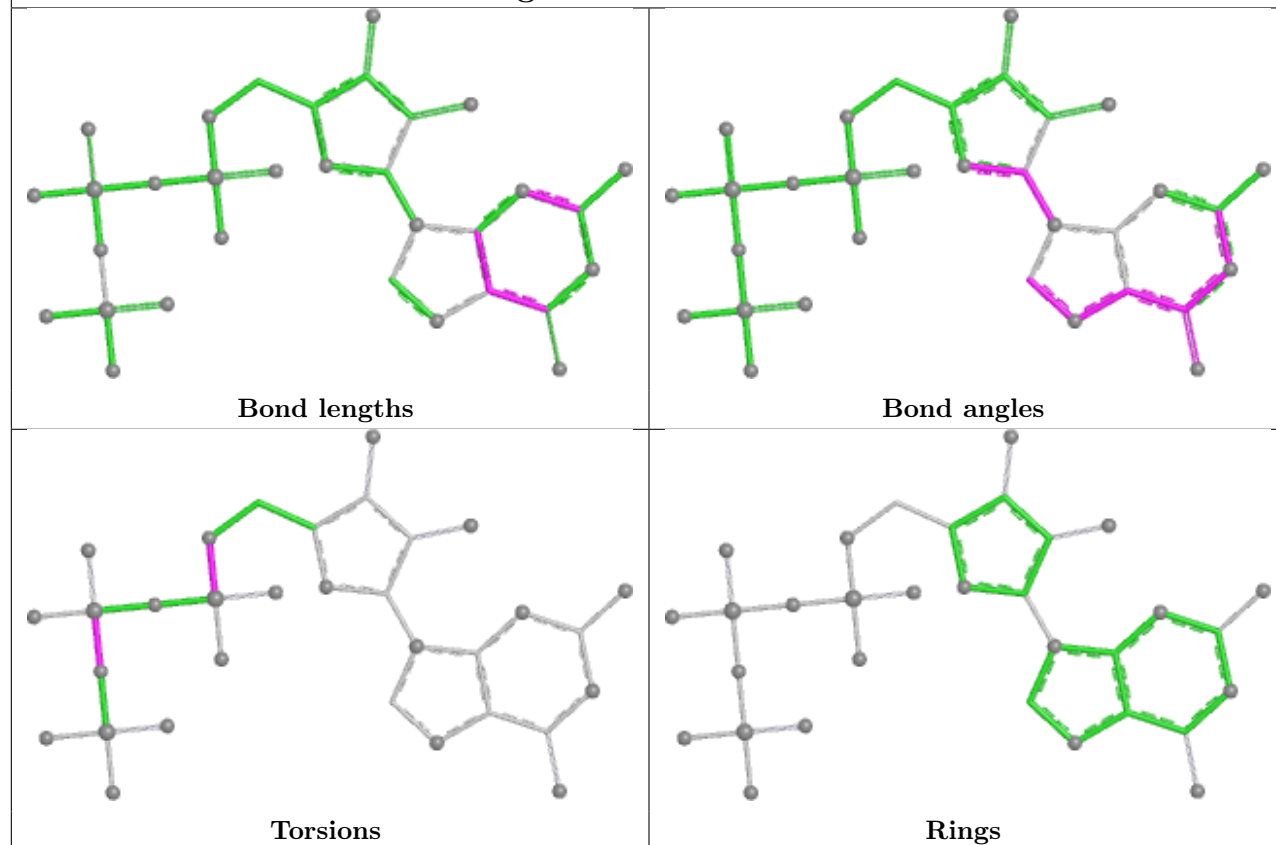




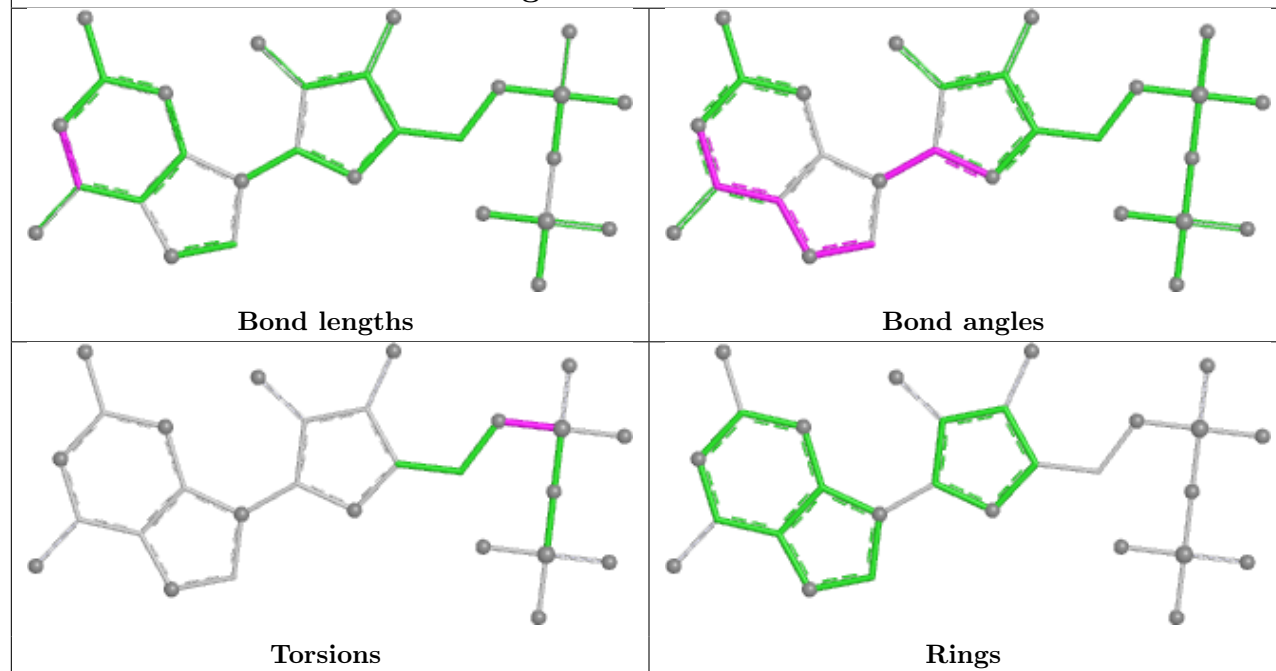


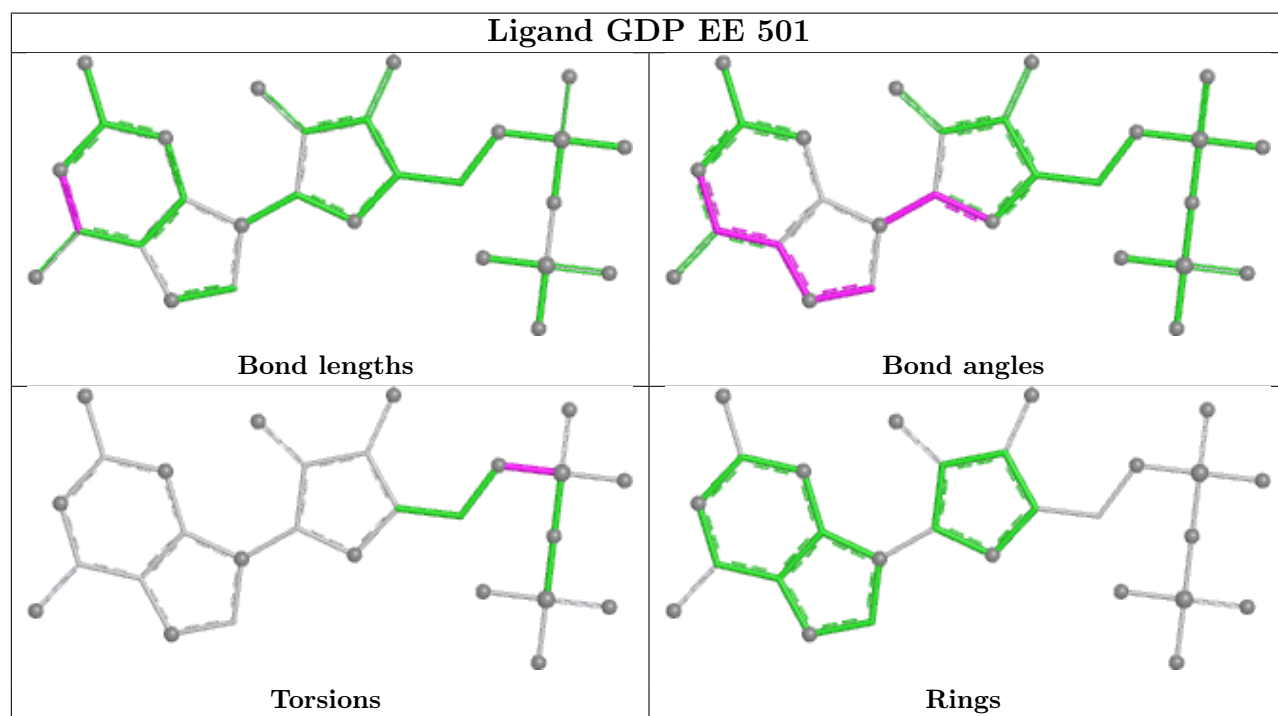
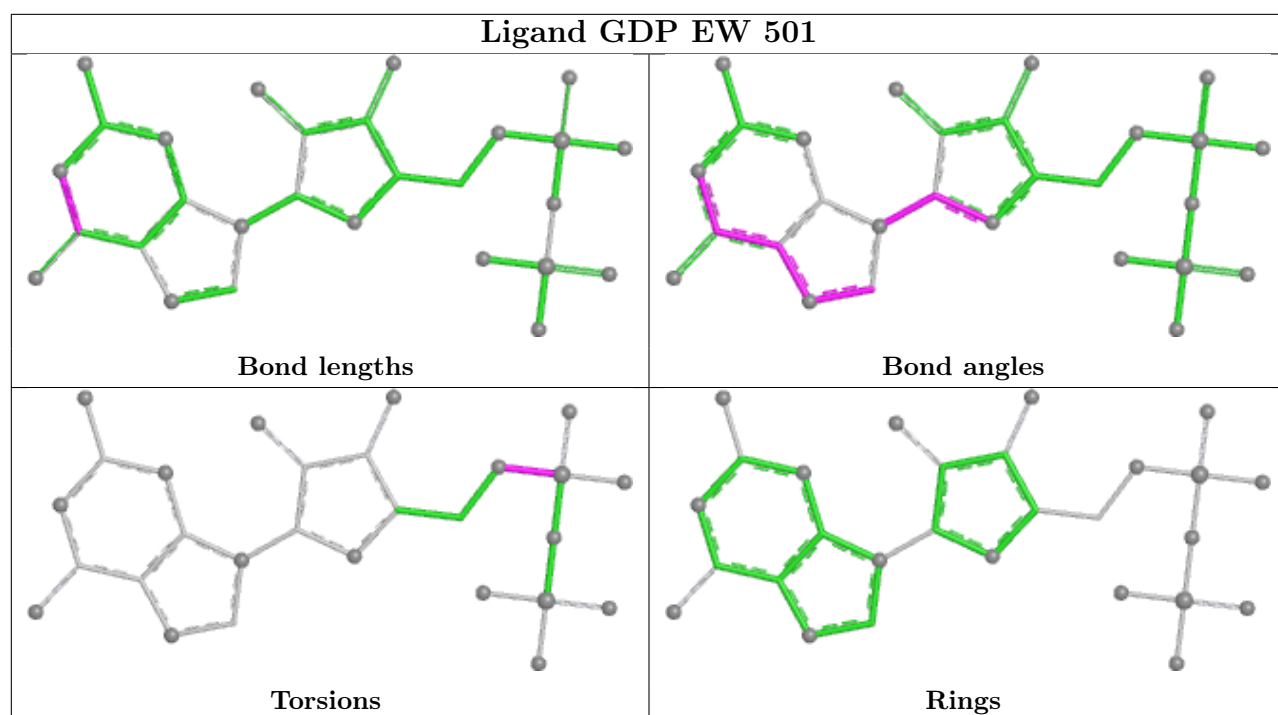


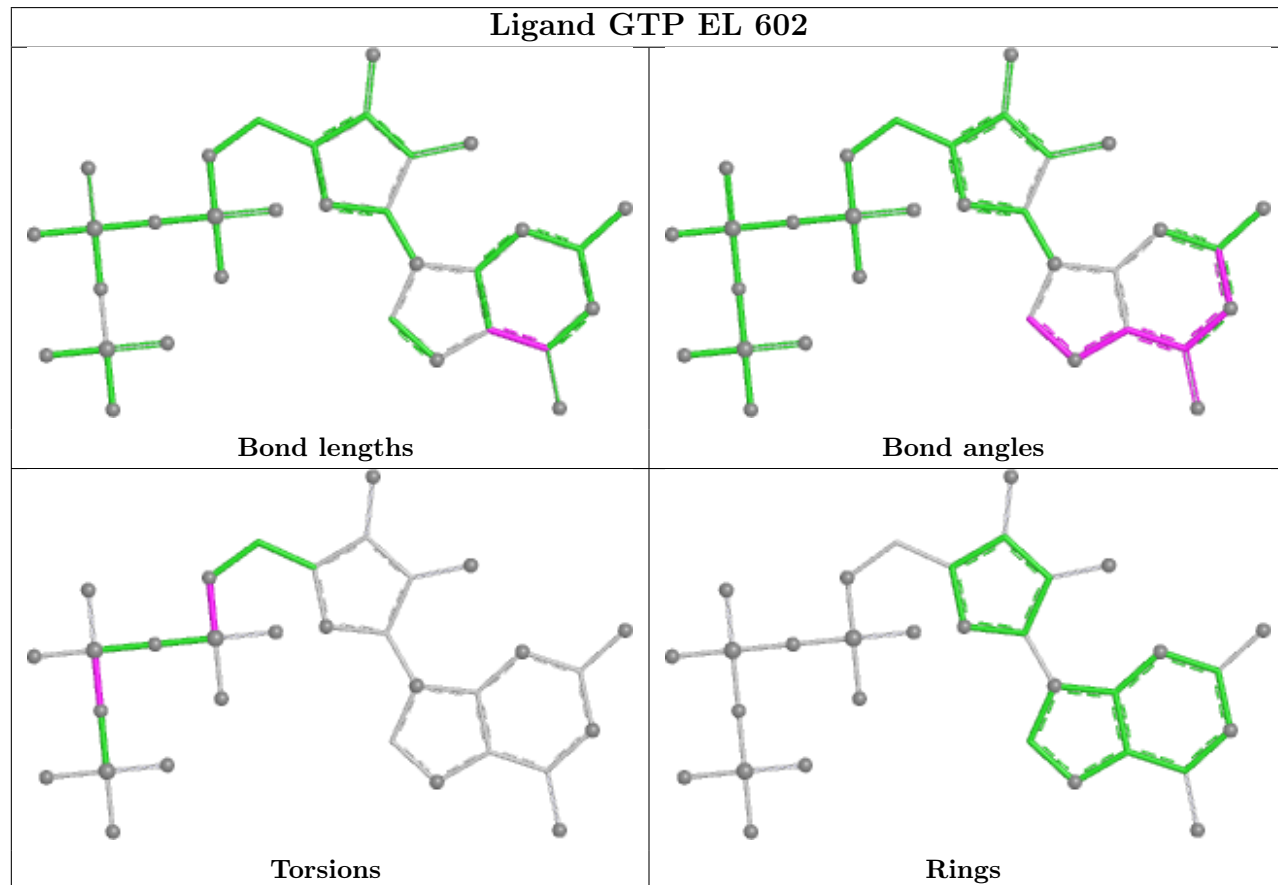
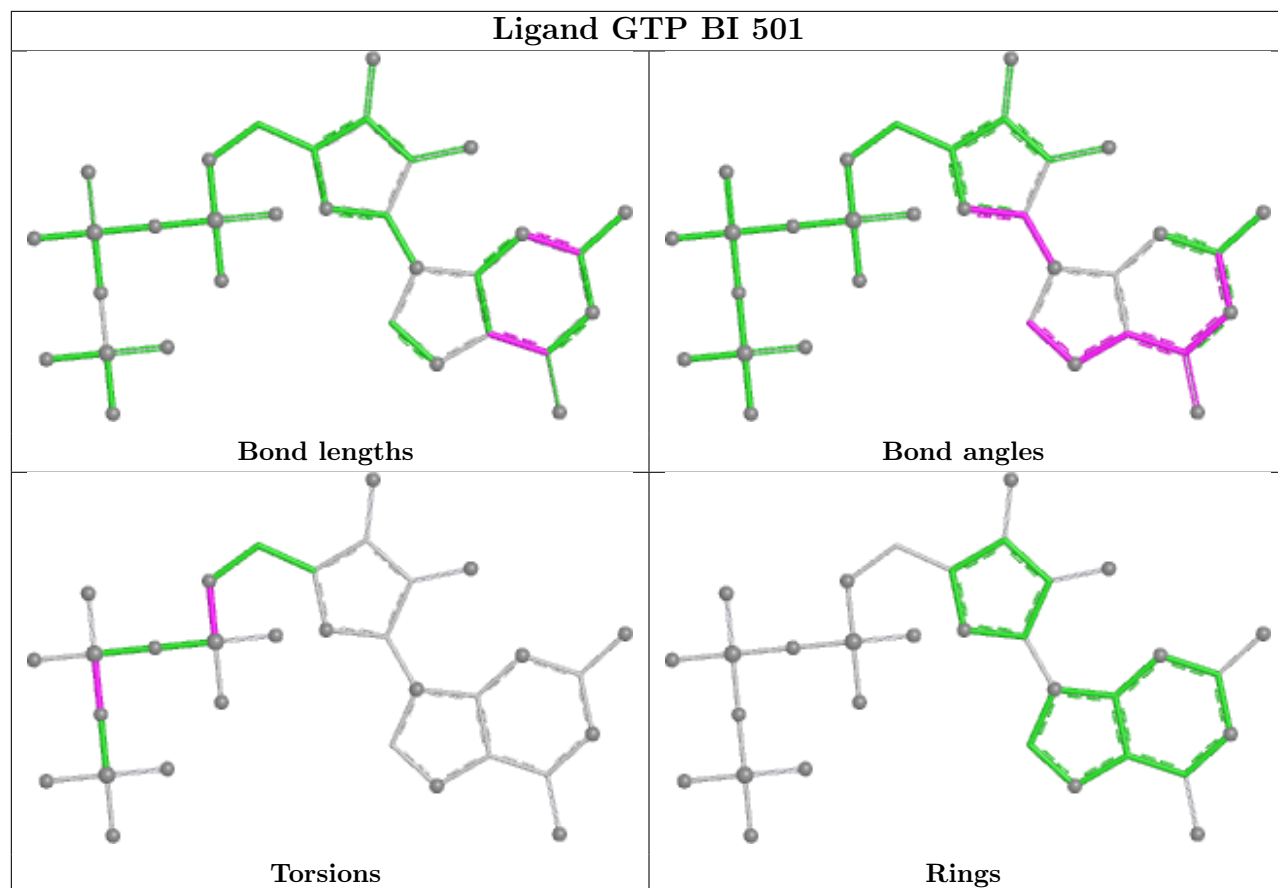
## Ligand GTP KP 501



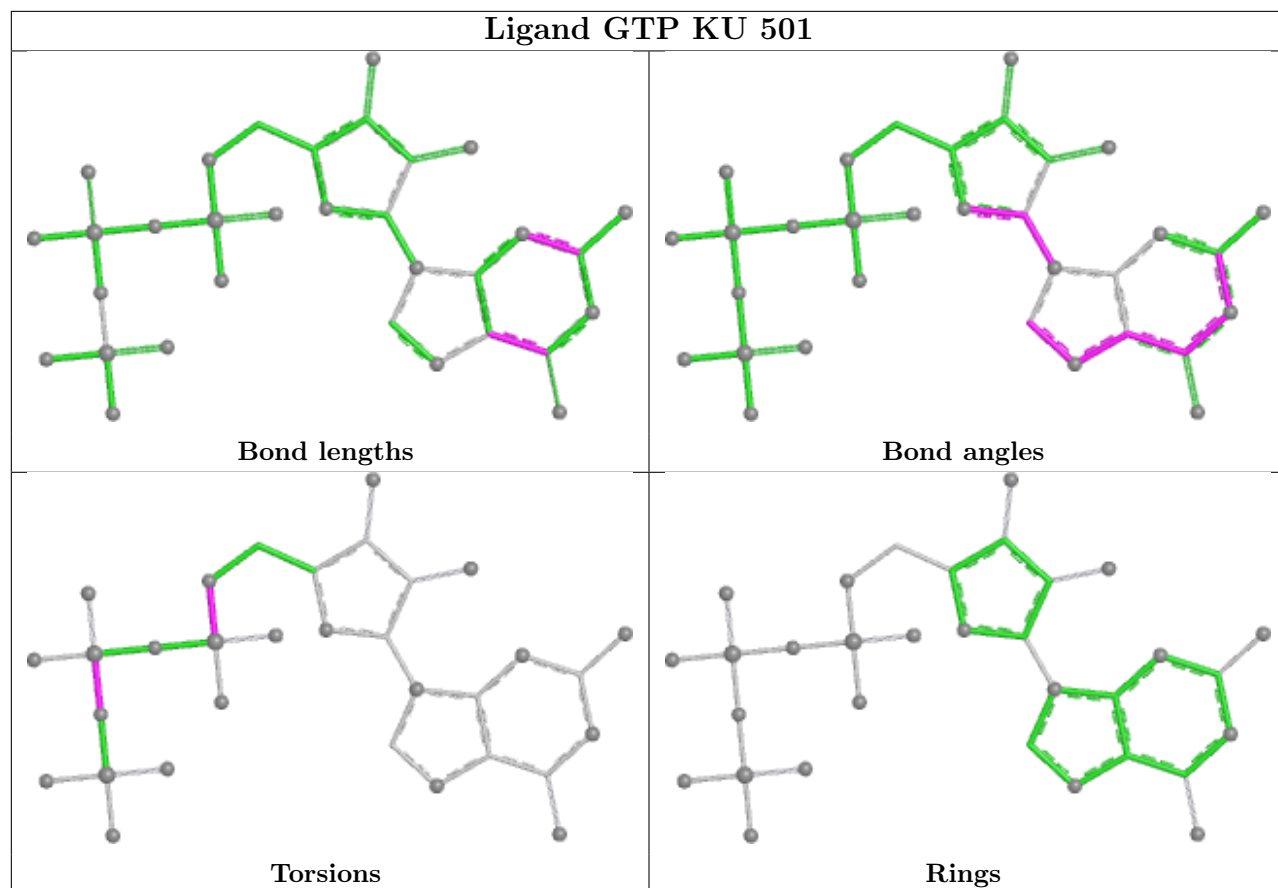
## Ligand GDP IU 501



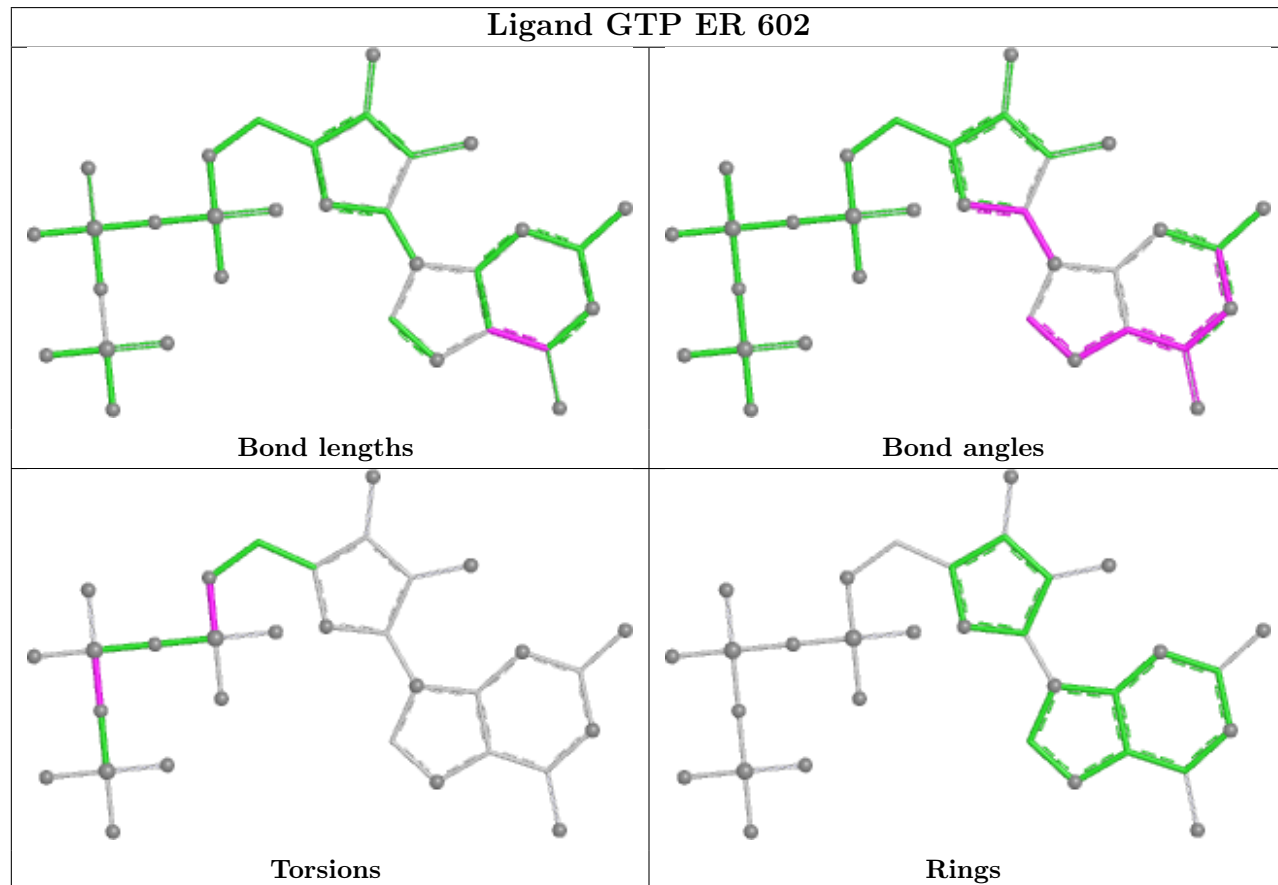


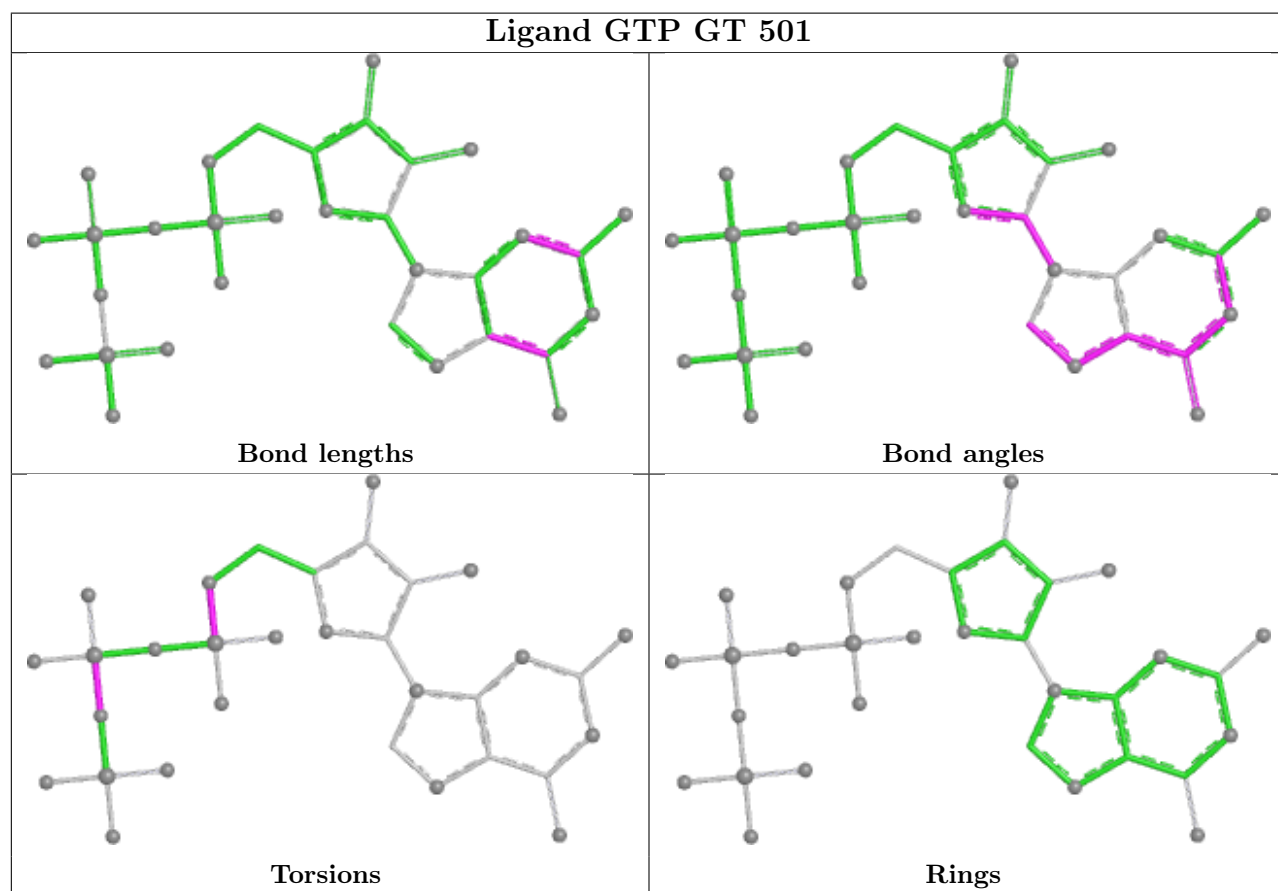
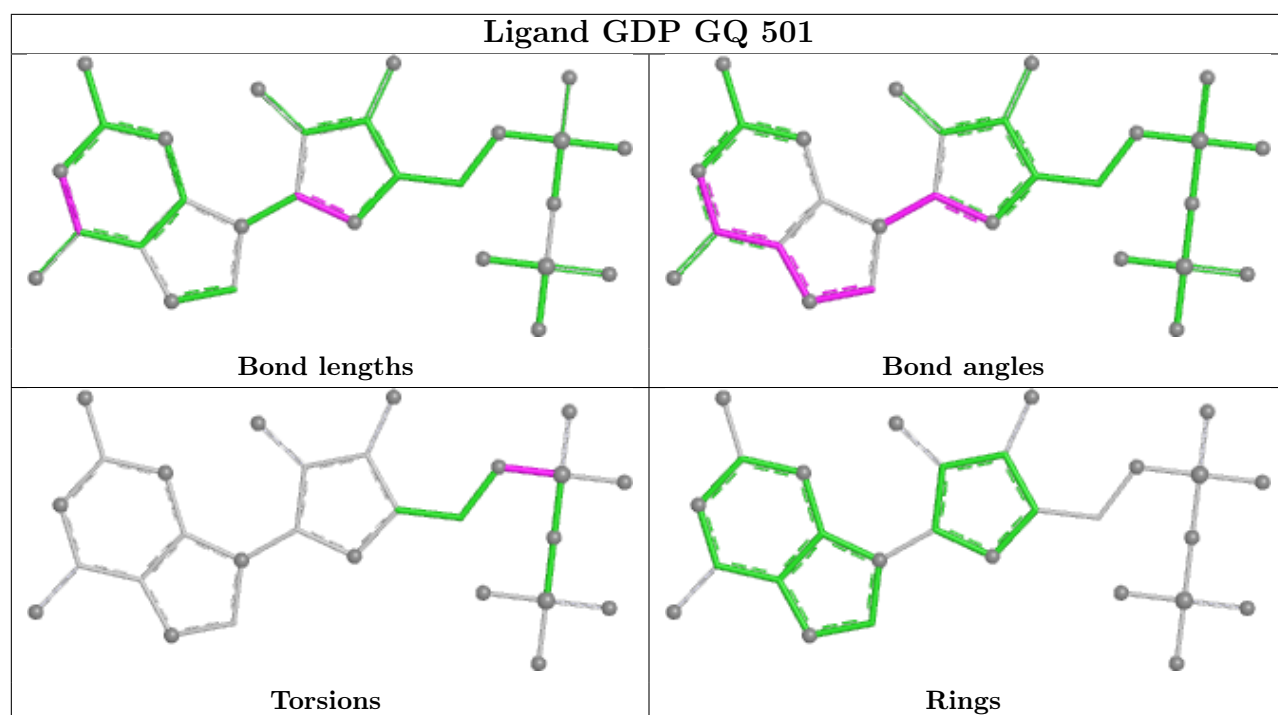


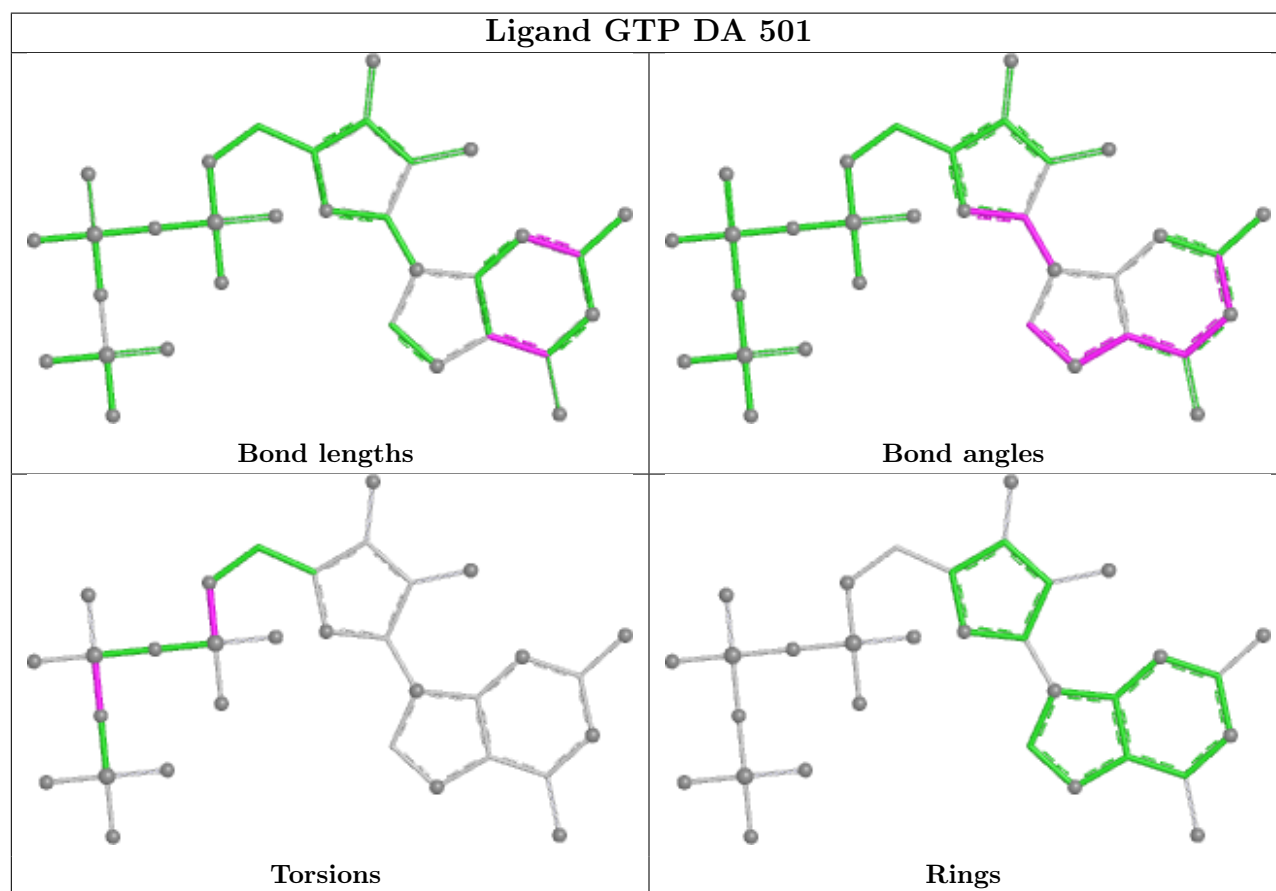
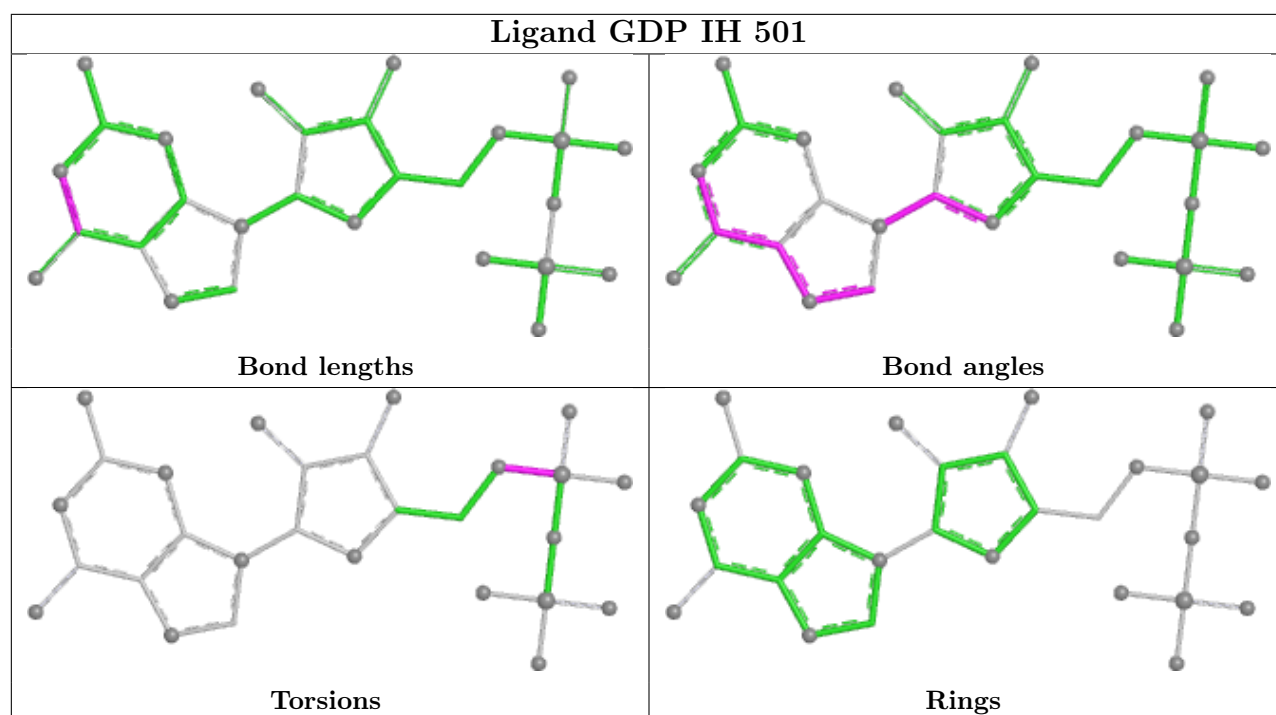
## Ligand GTP KU 501

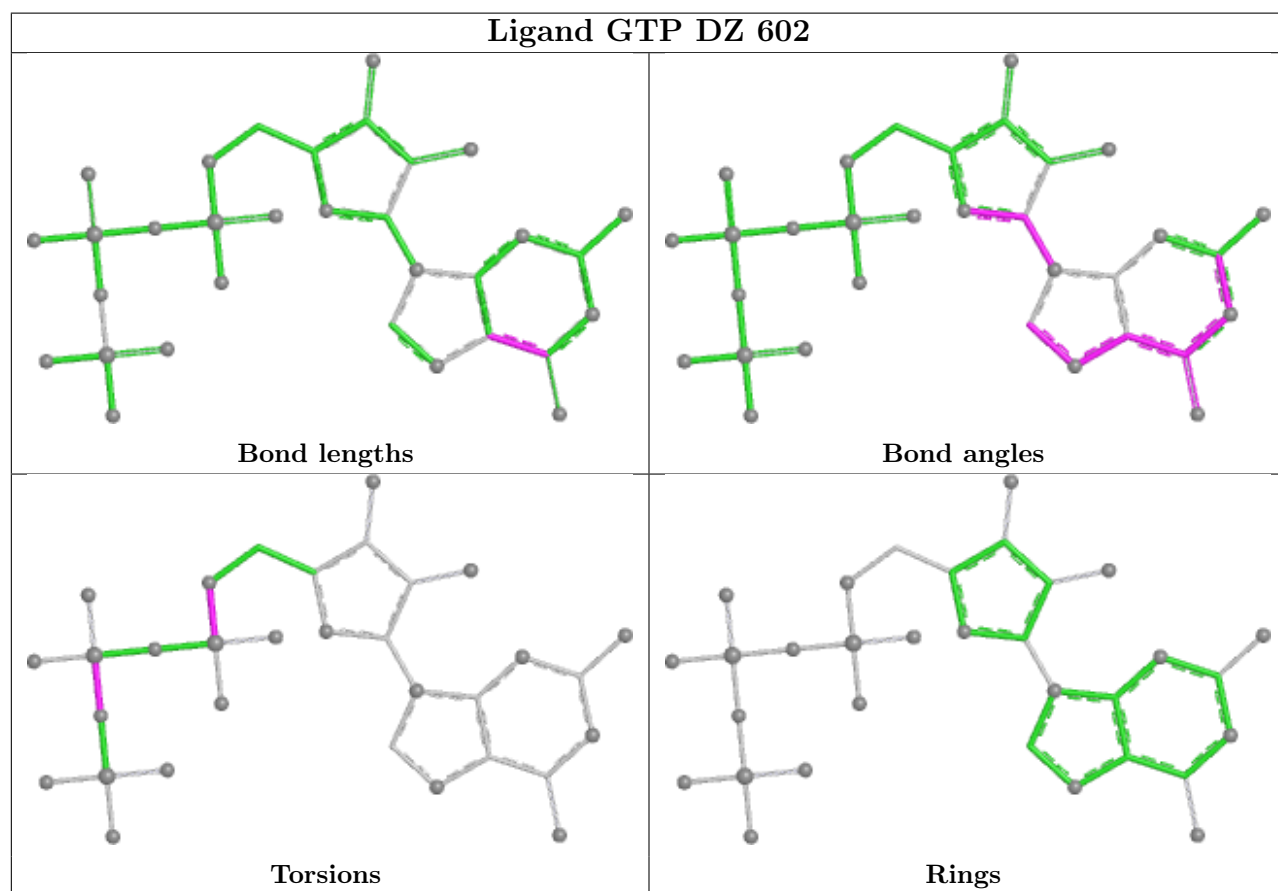
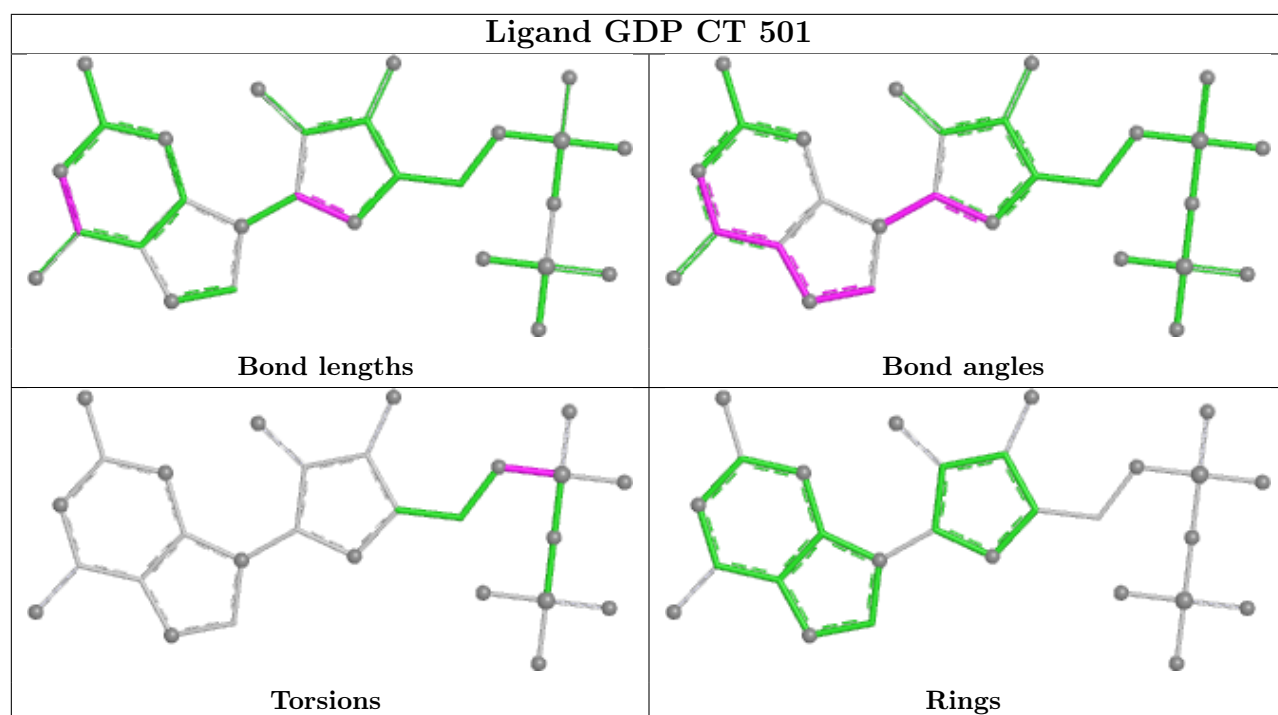


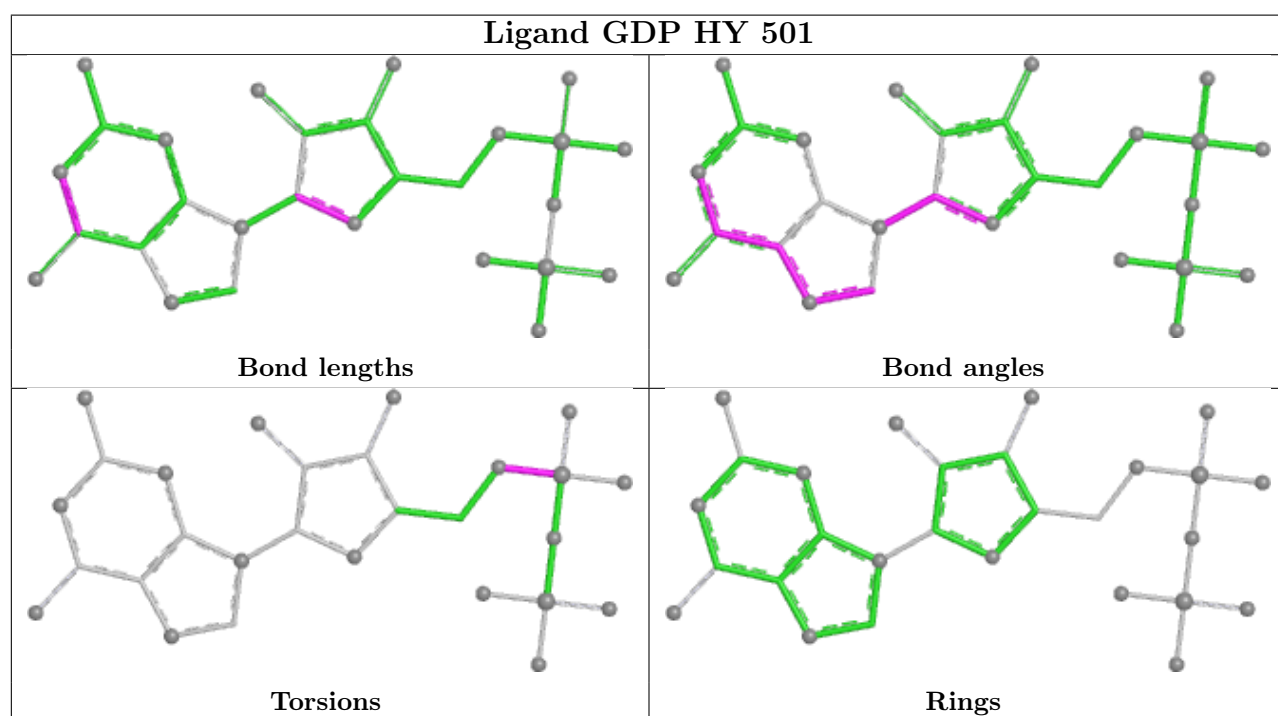
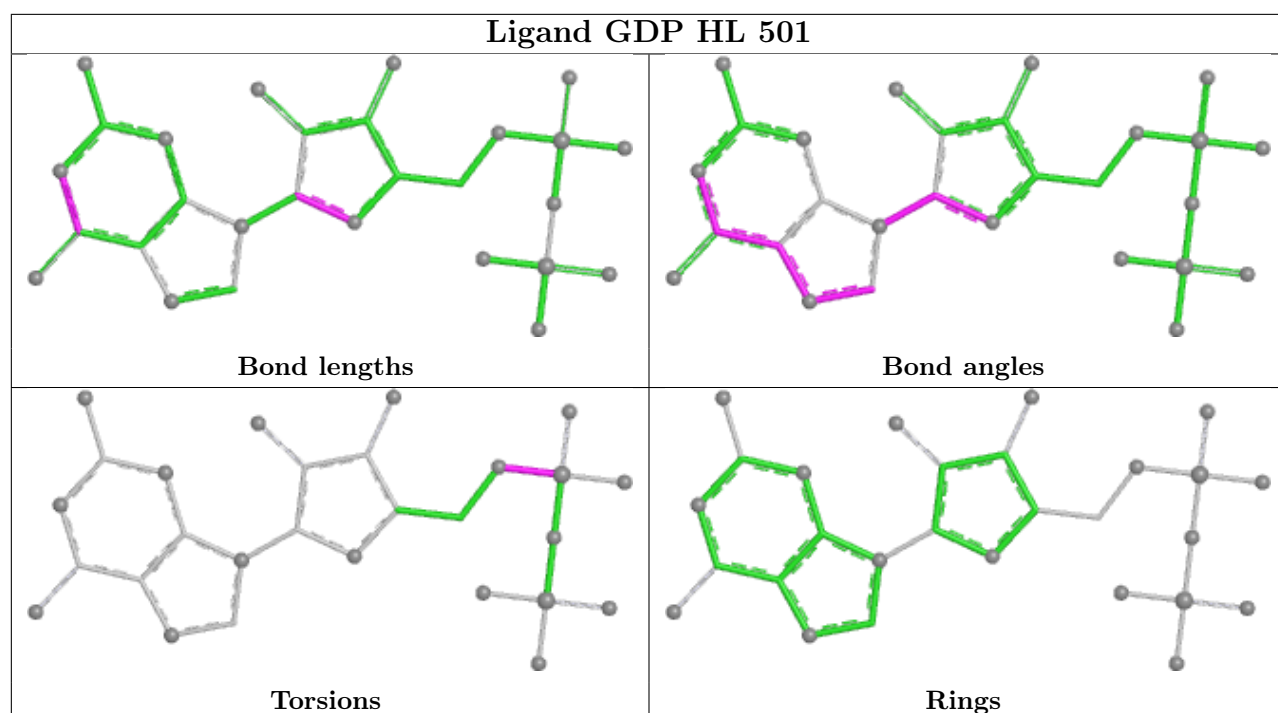
## Ligand GTP ER 602



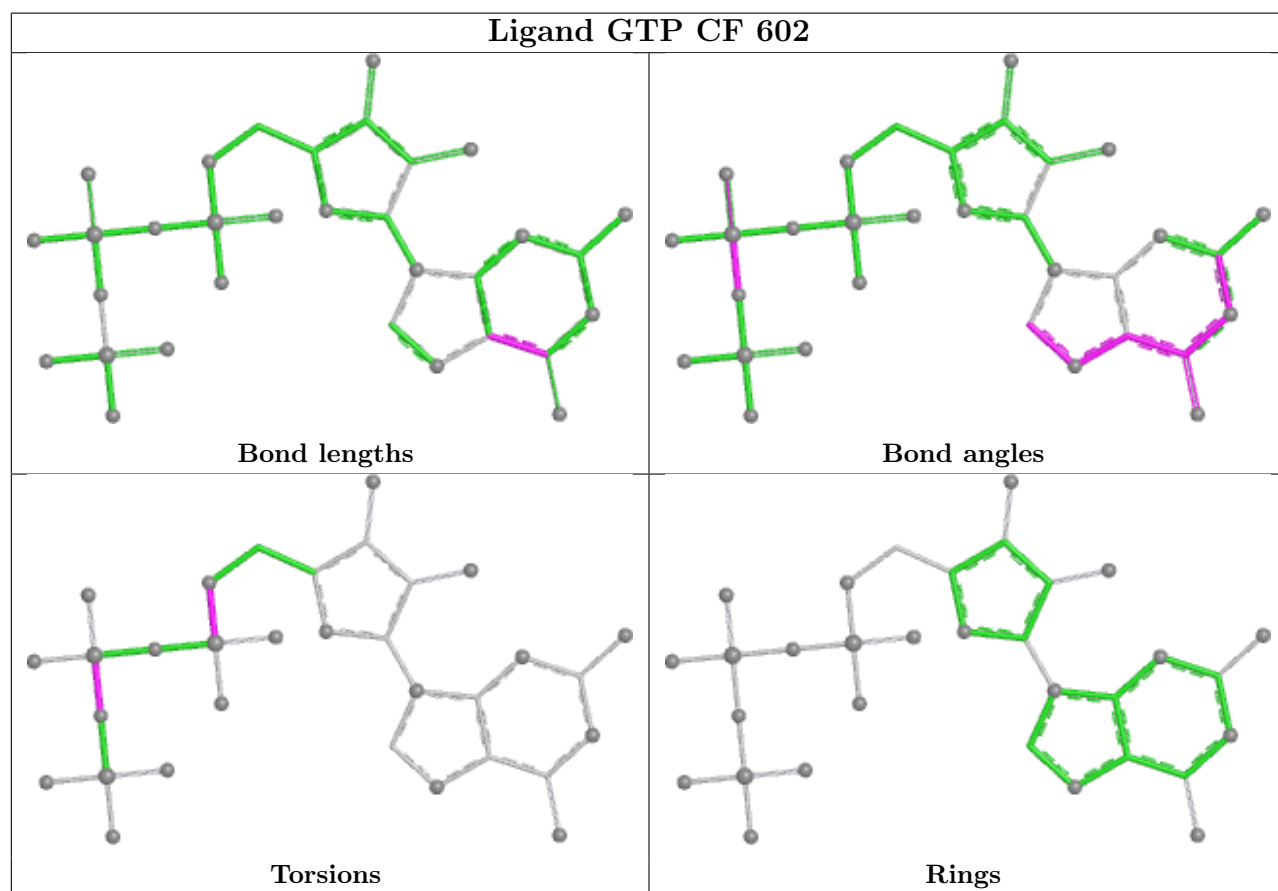
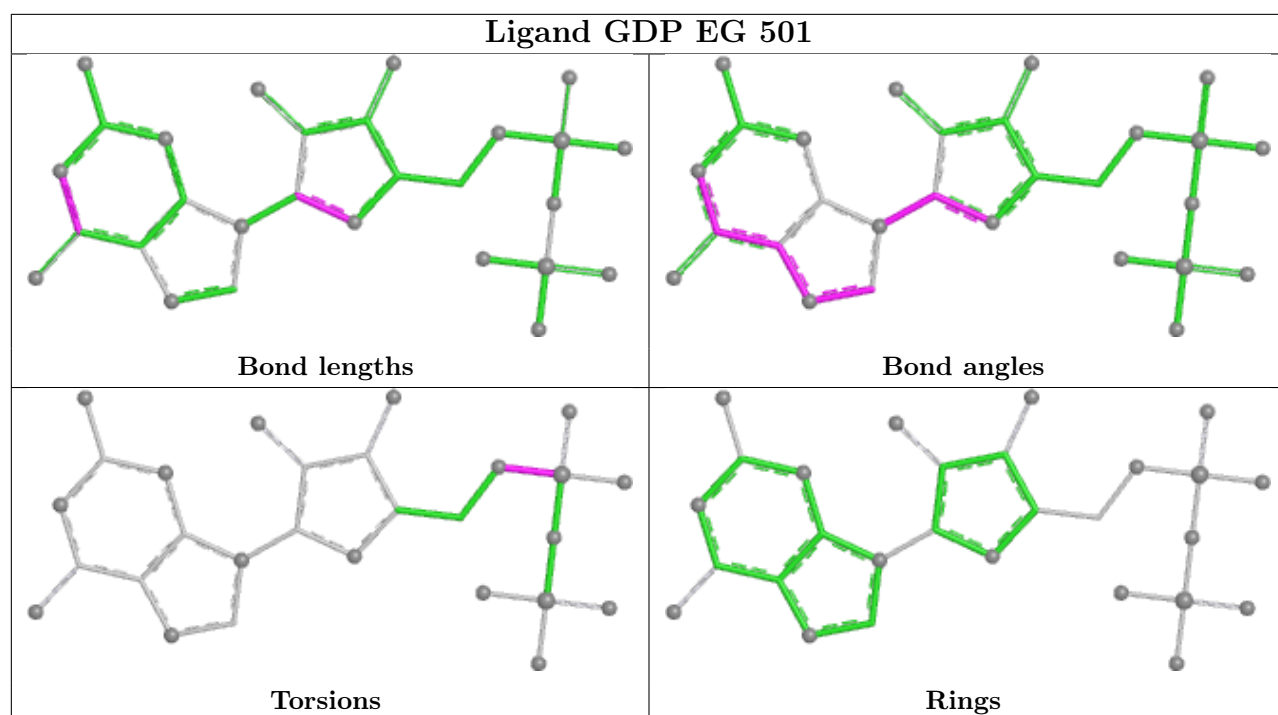


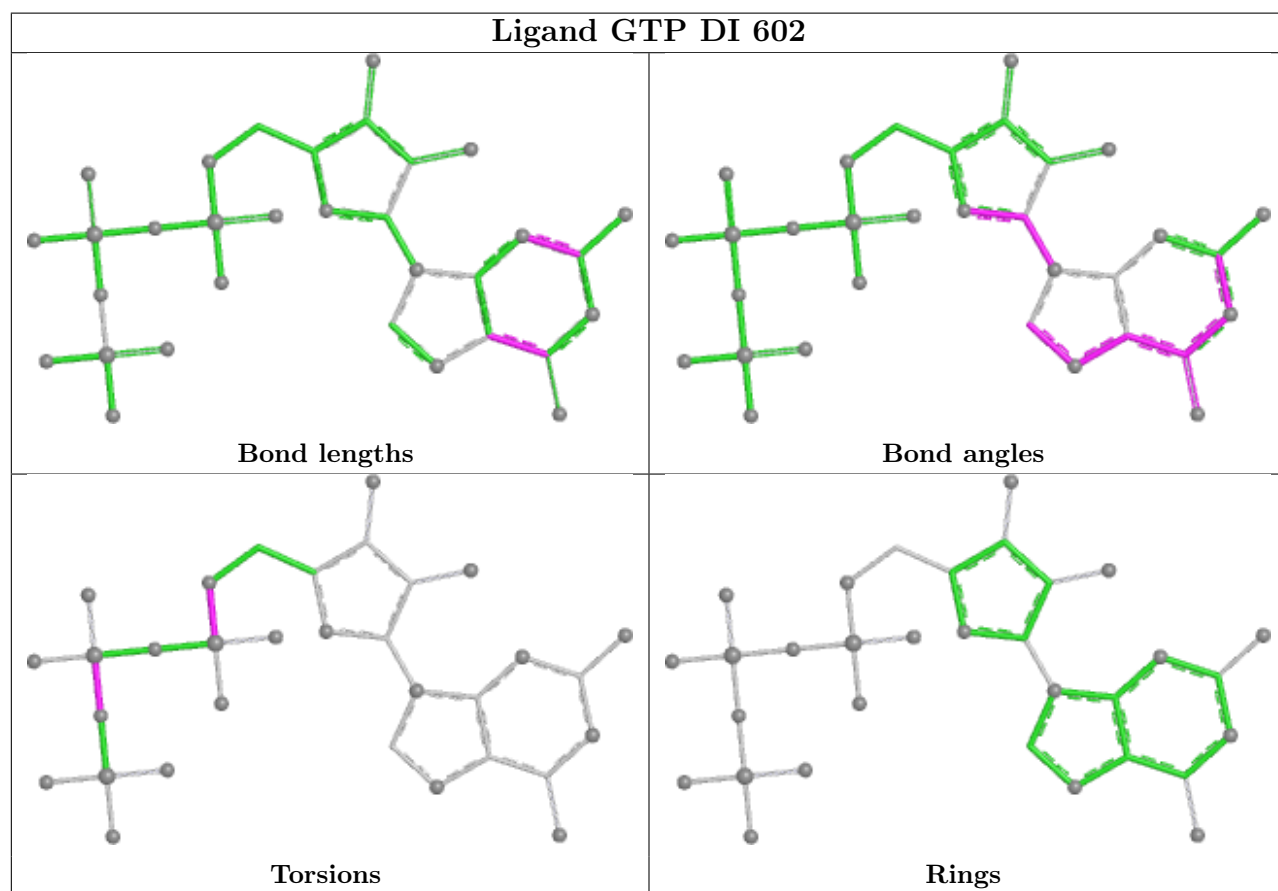
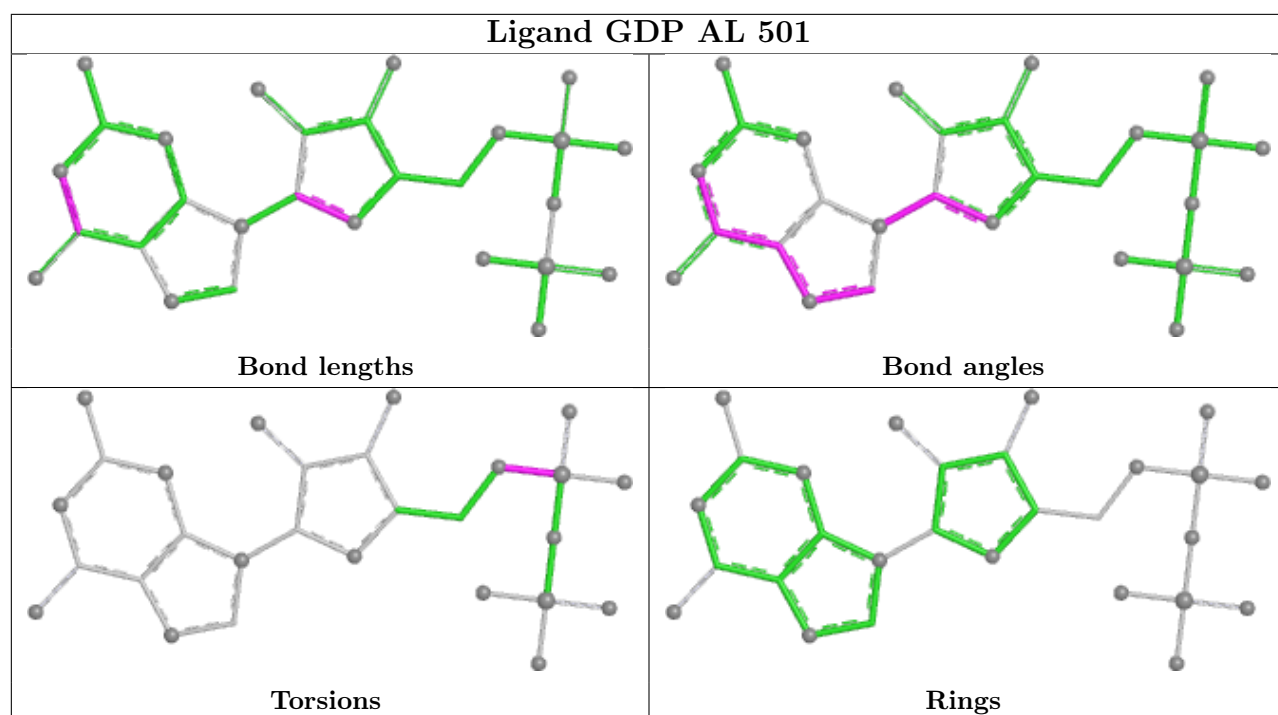


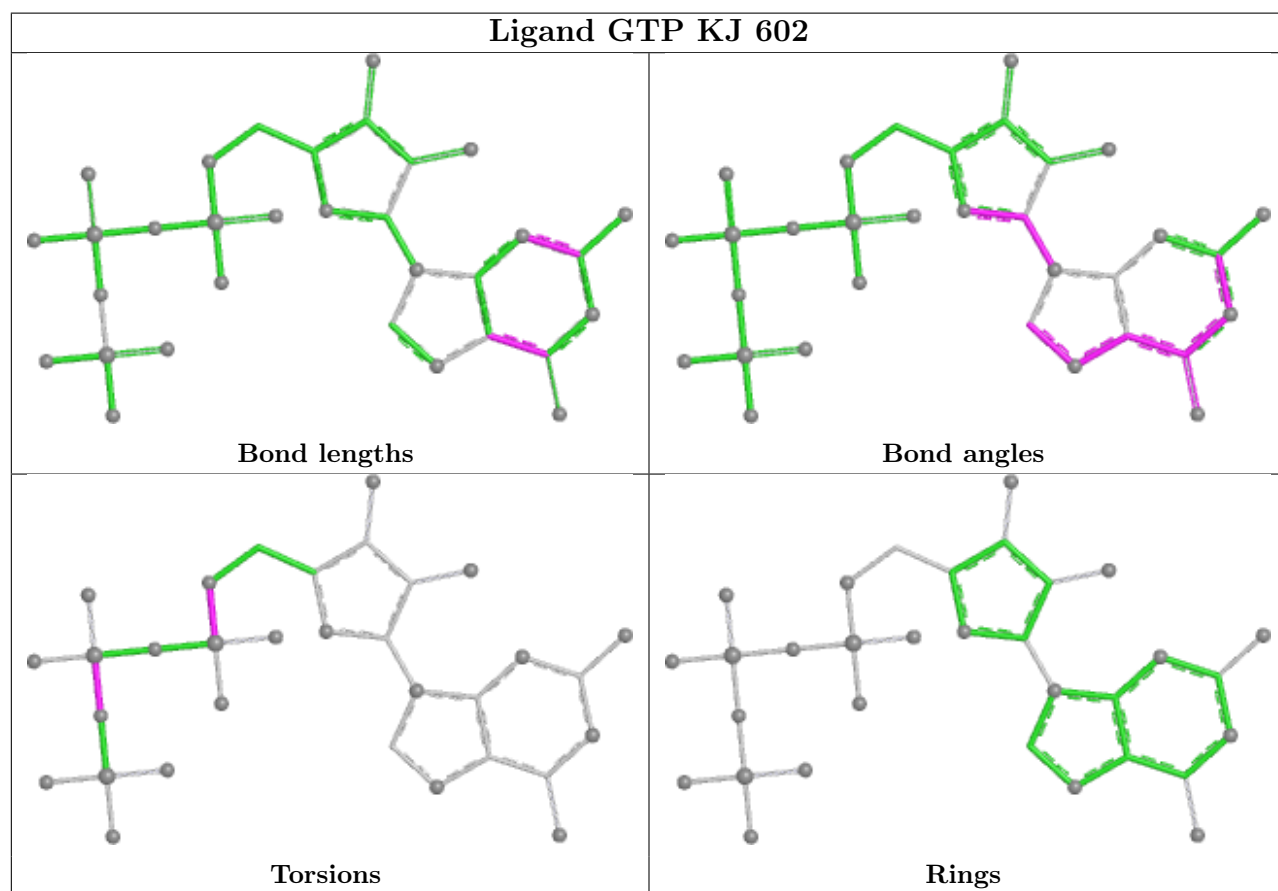
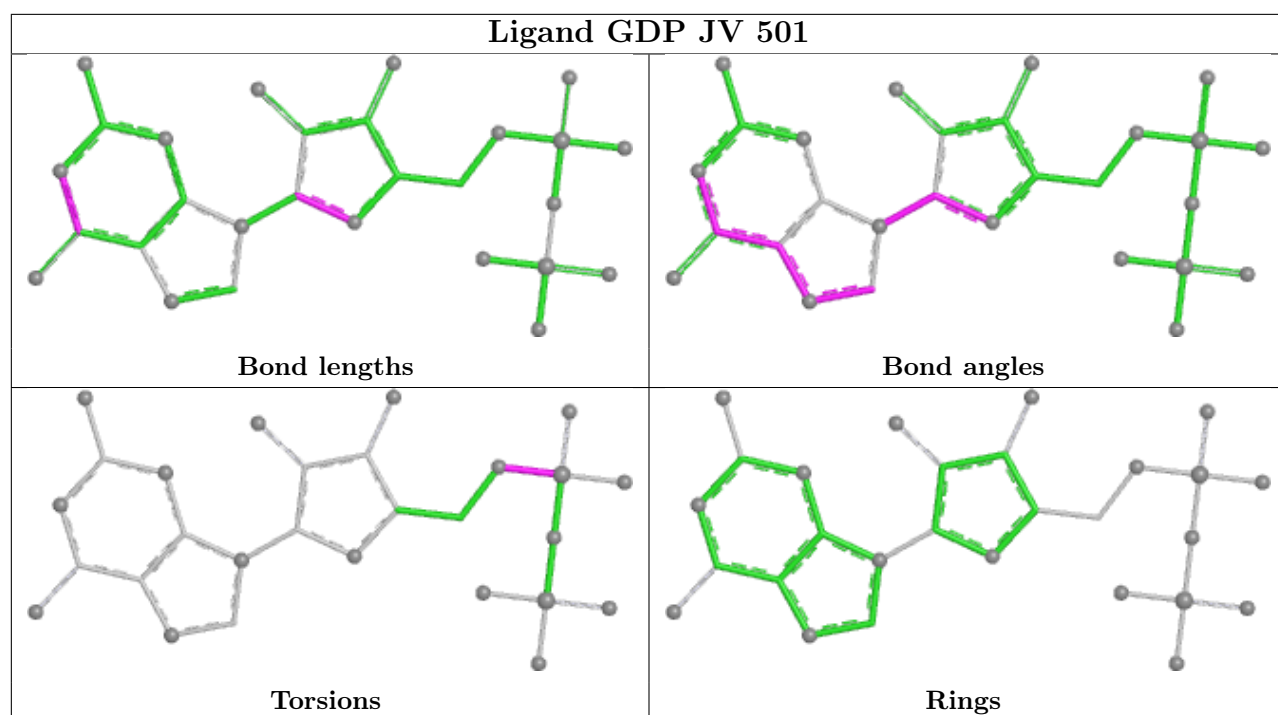


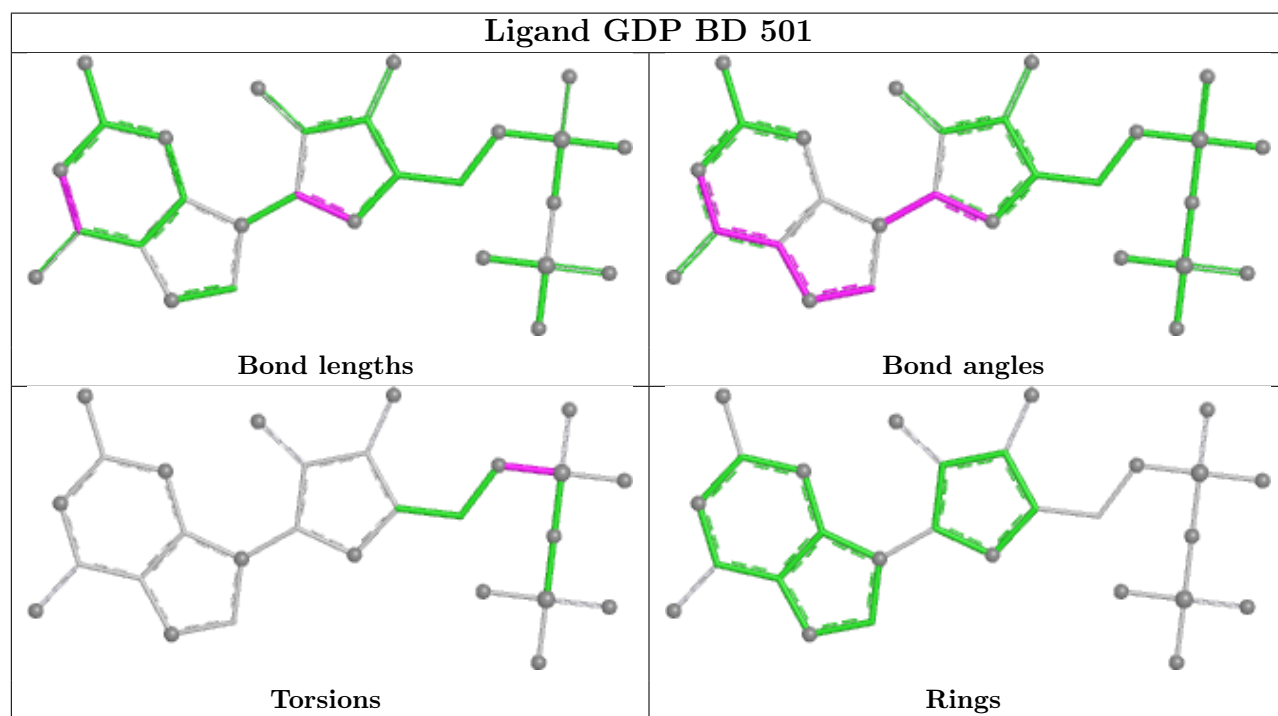
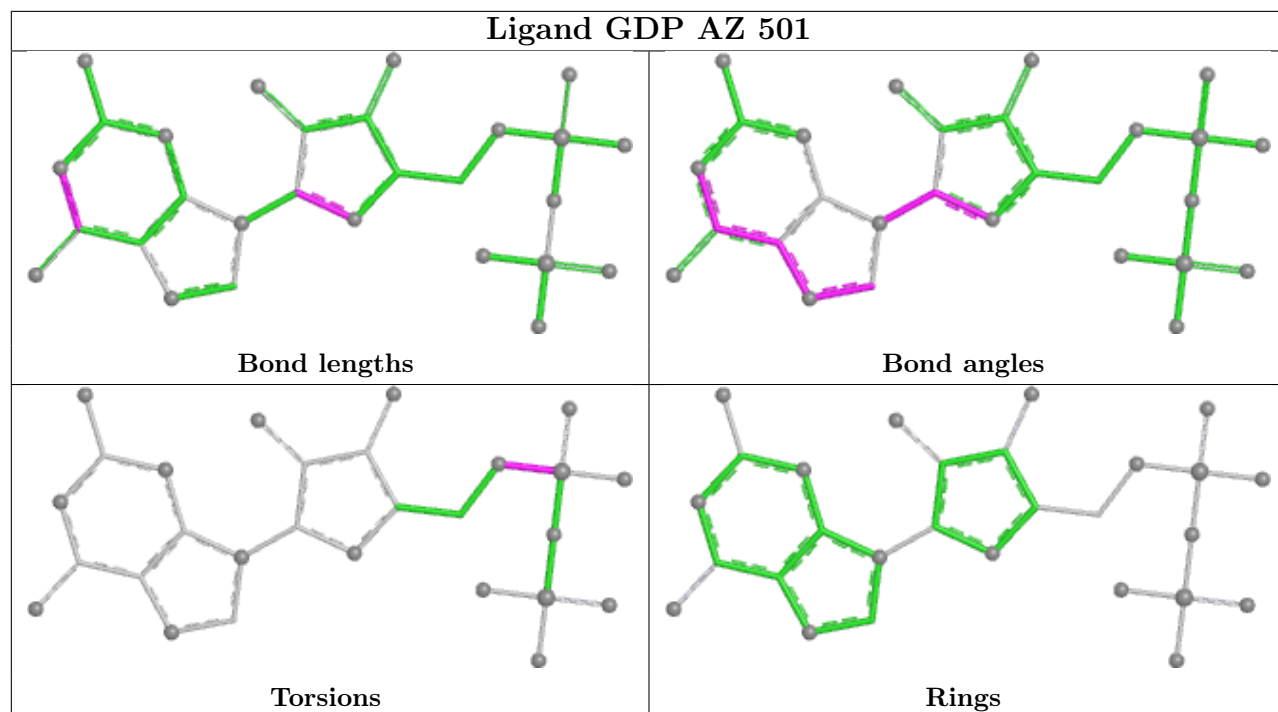




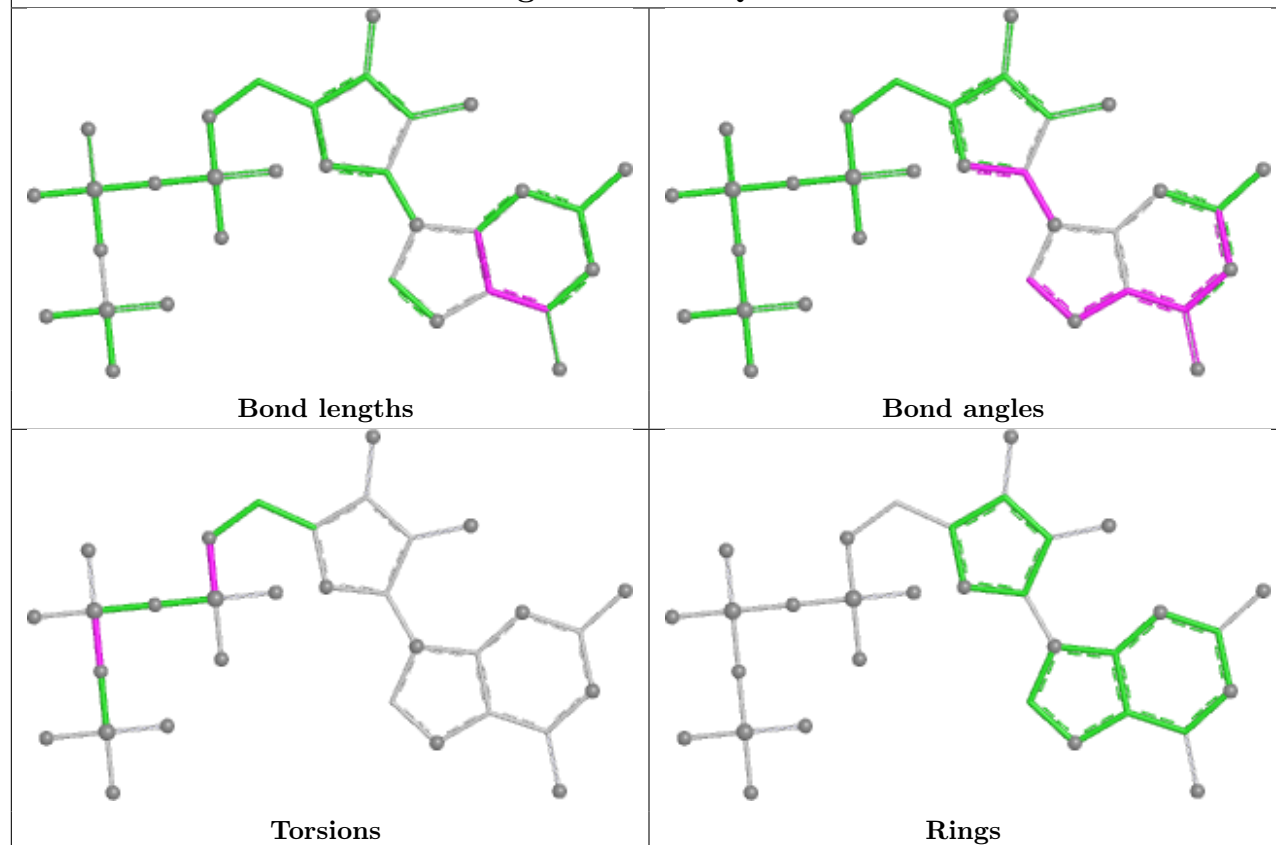




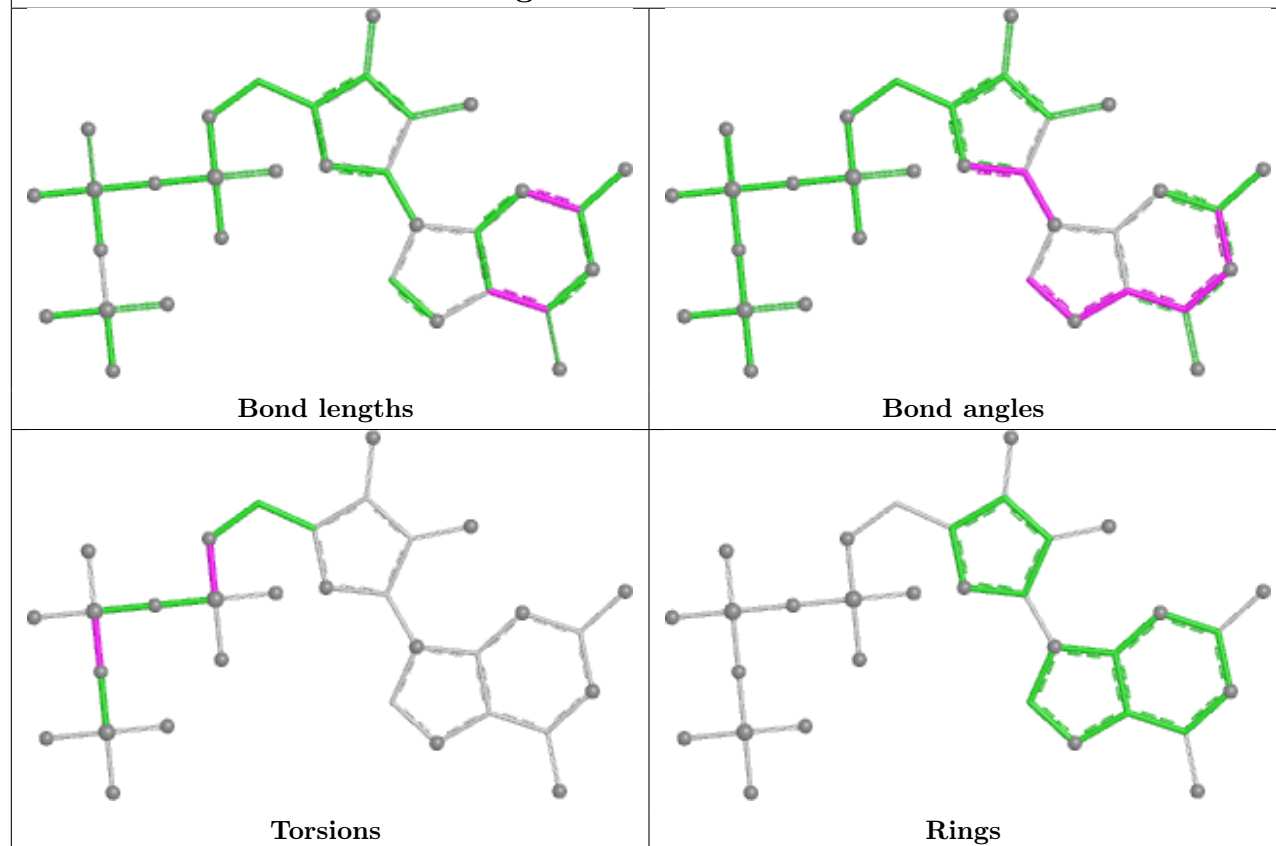


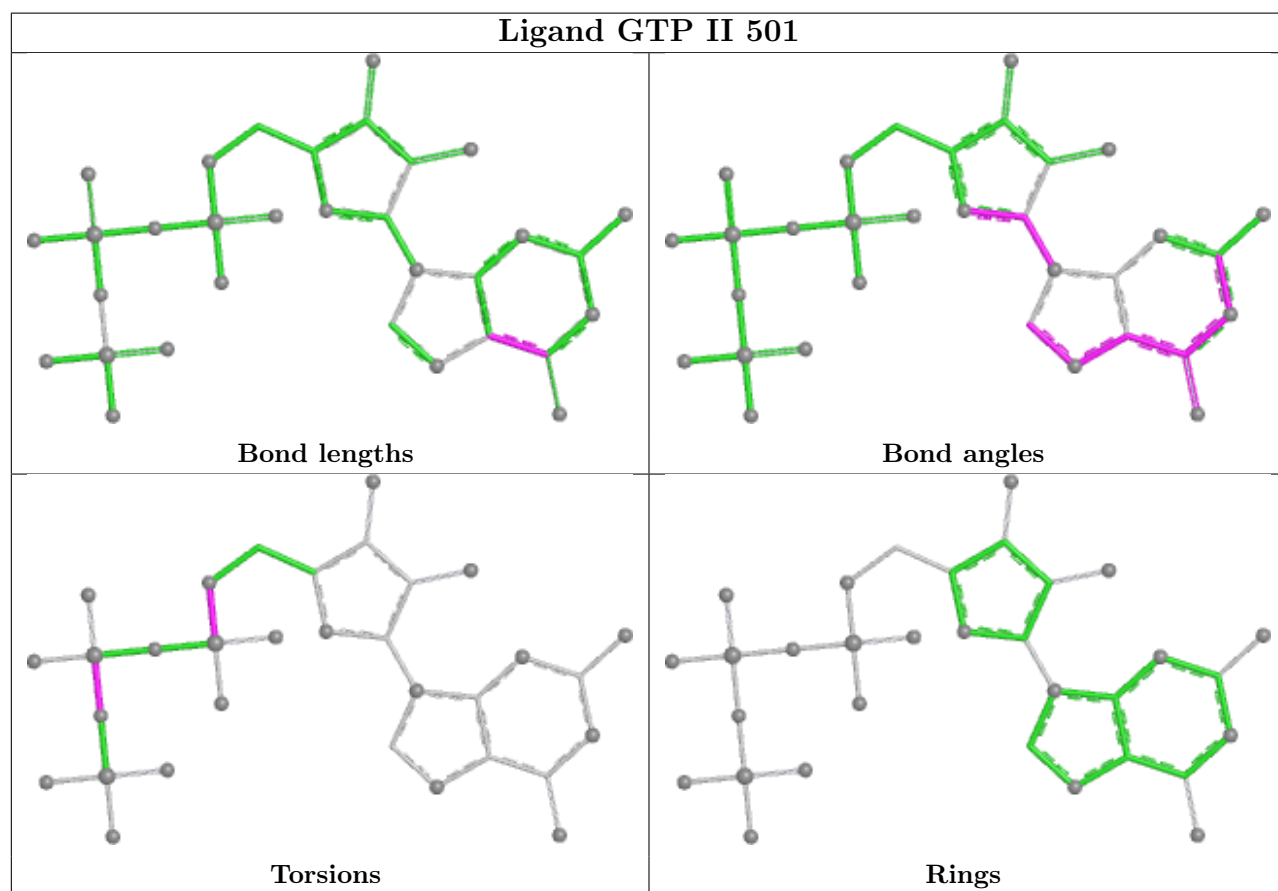
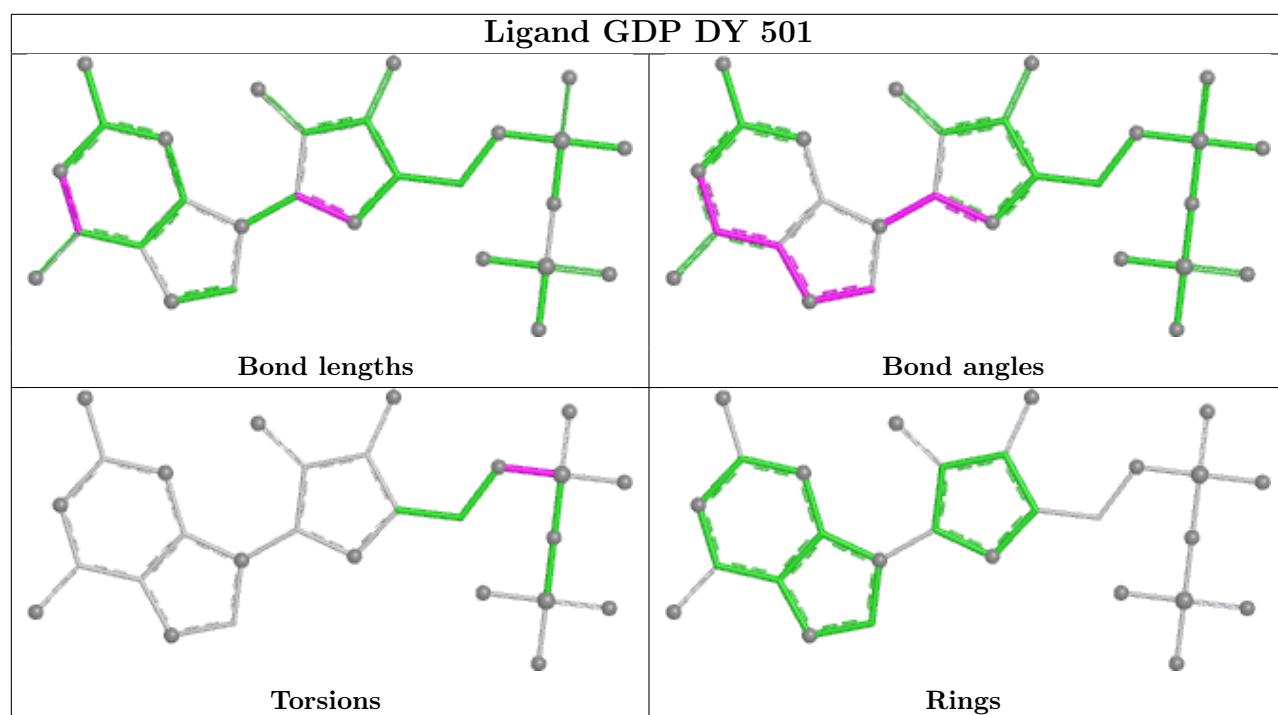


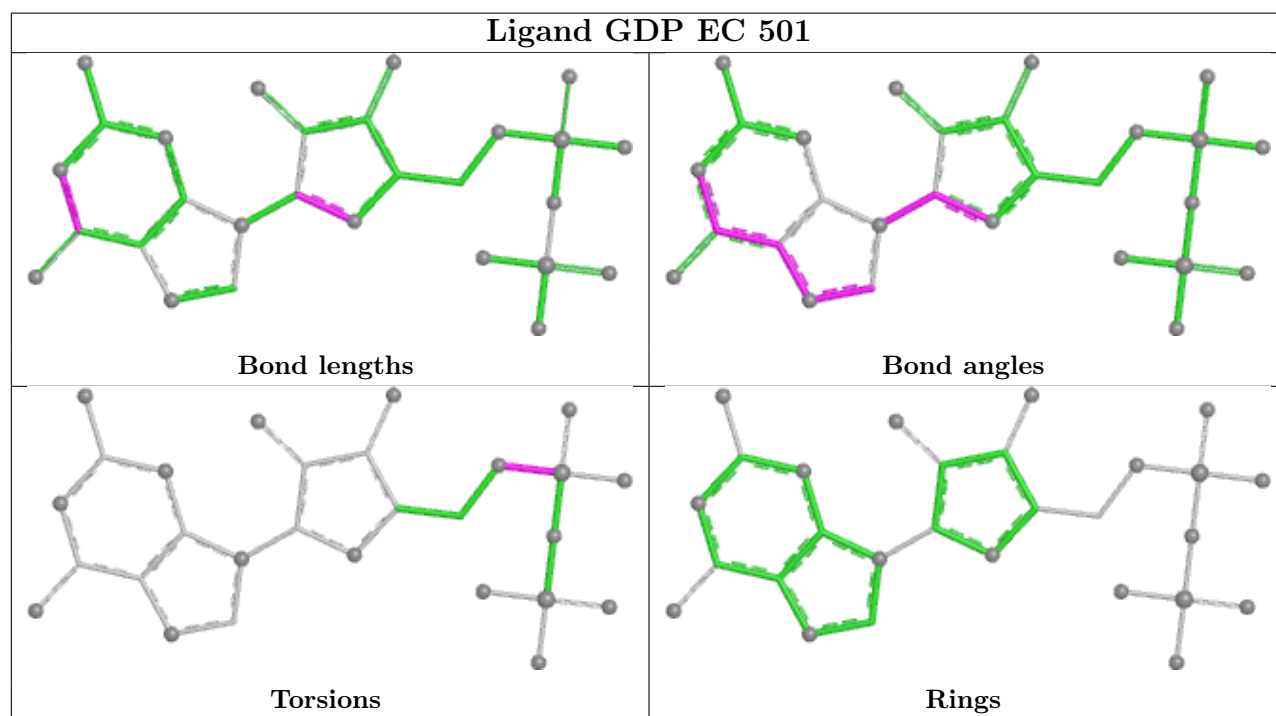
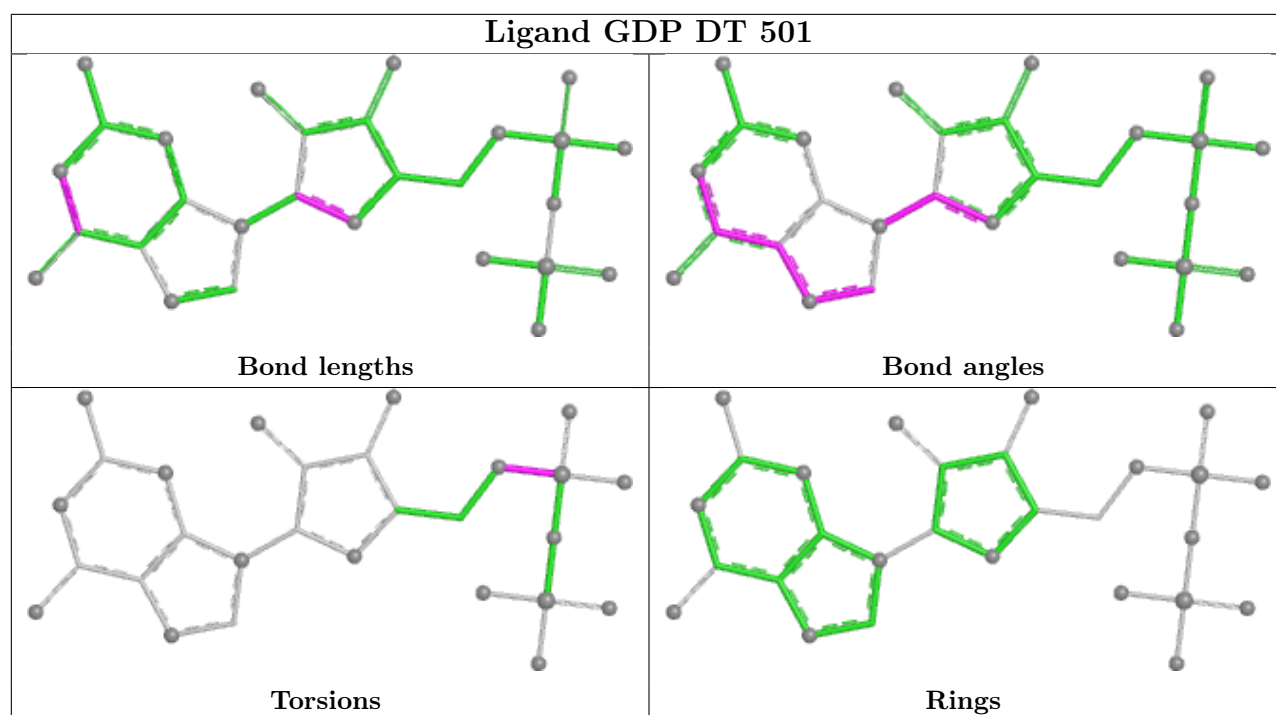
## Ligand GTP CQ 602

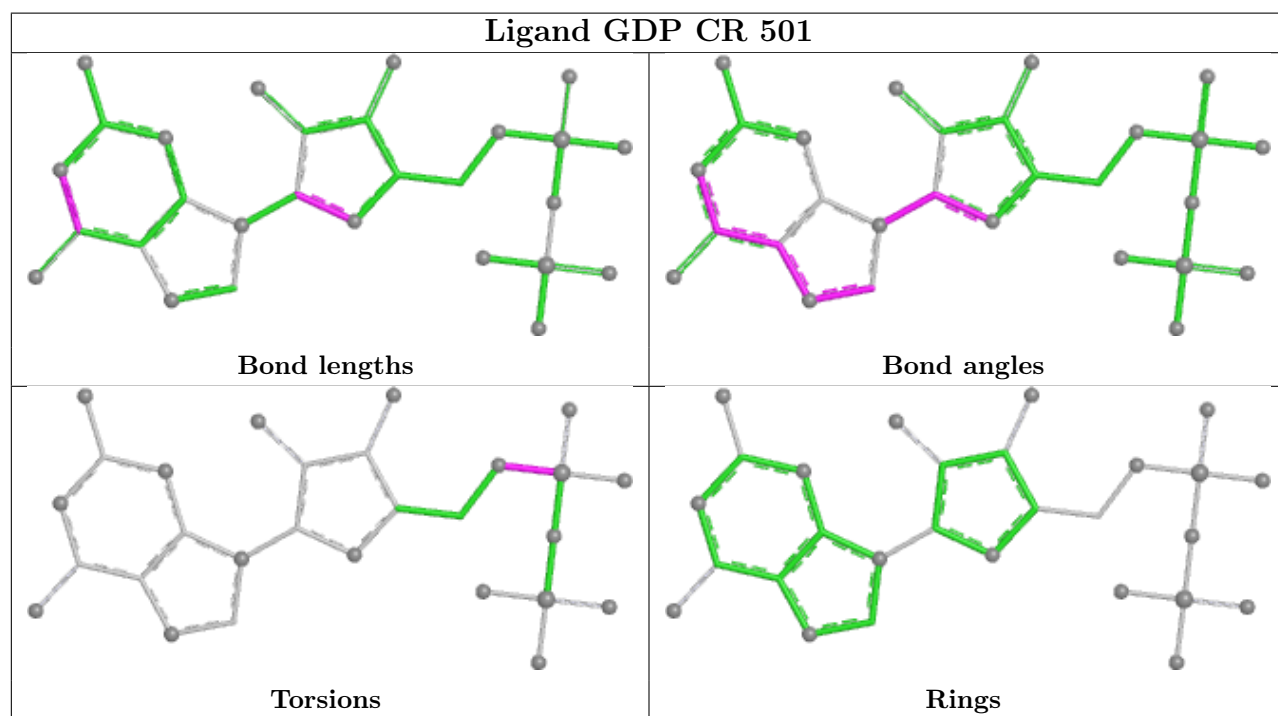
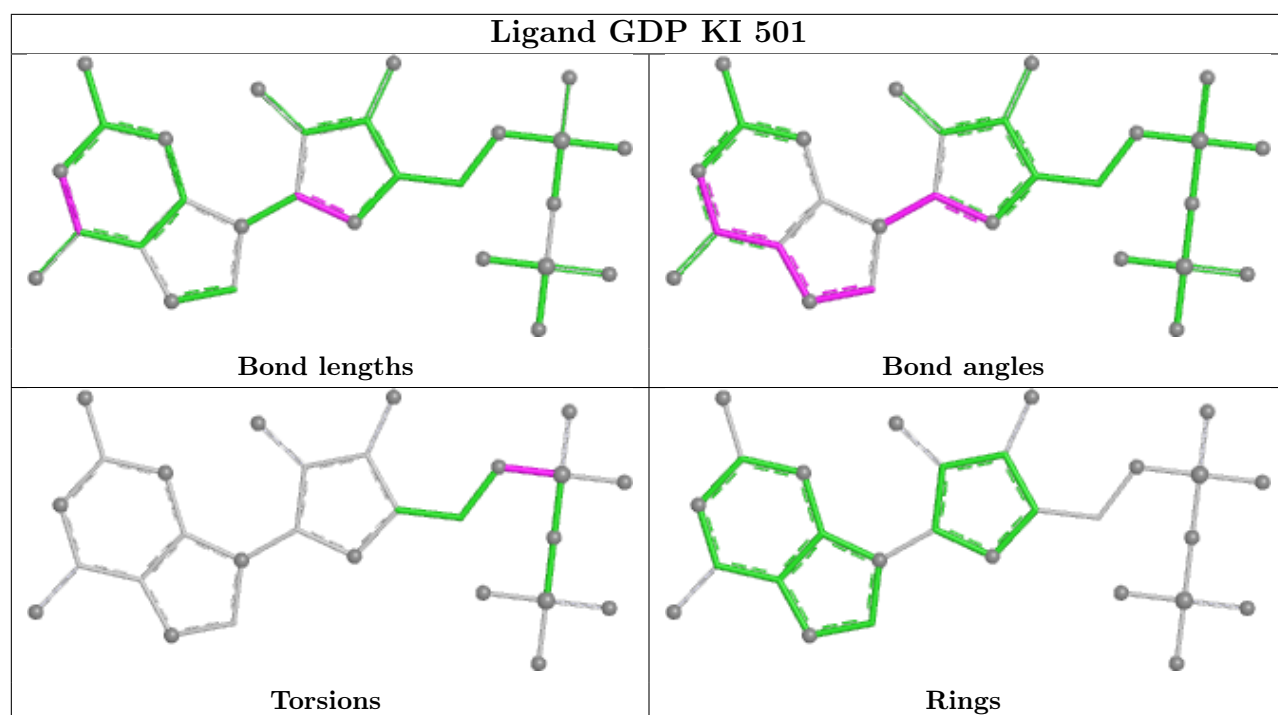


## Ligand GTP DG 602

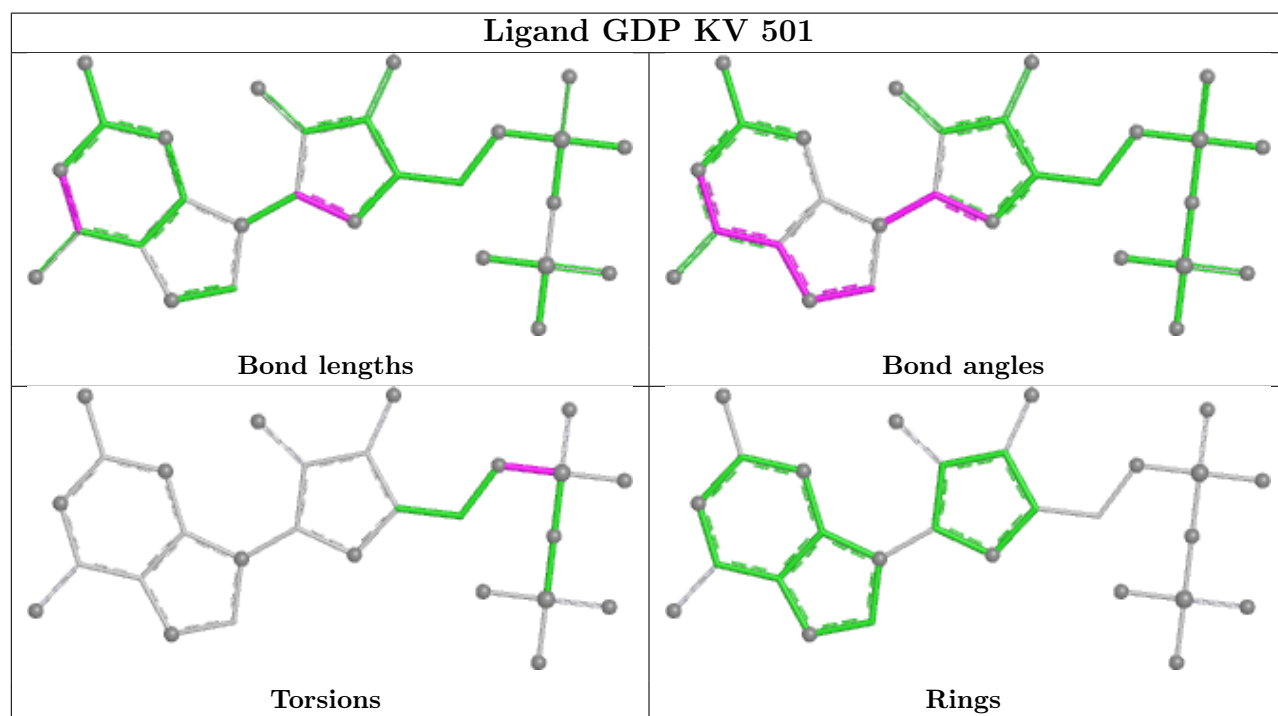
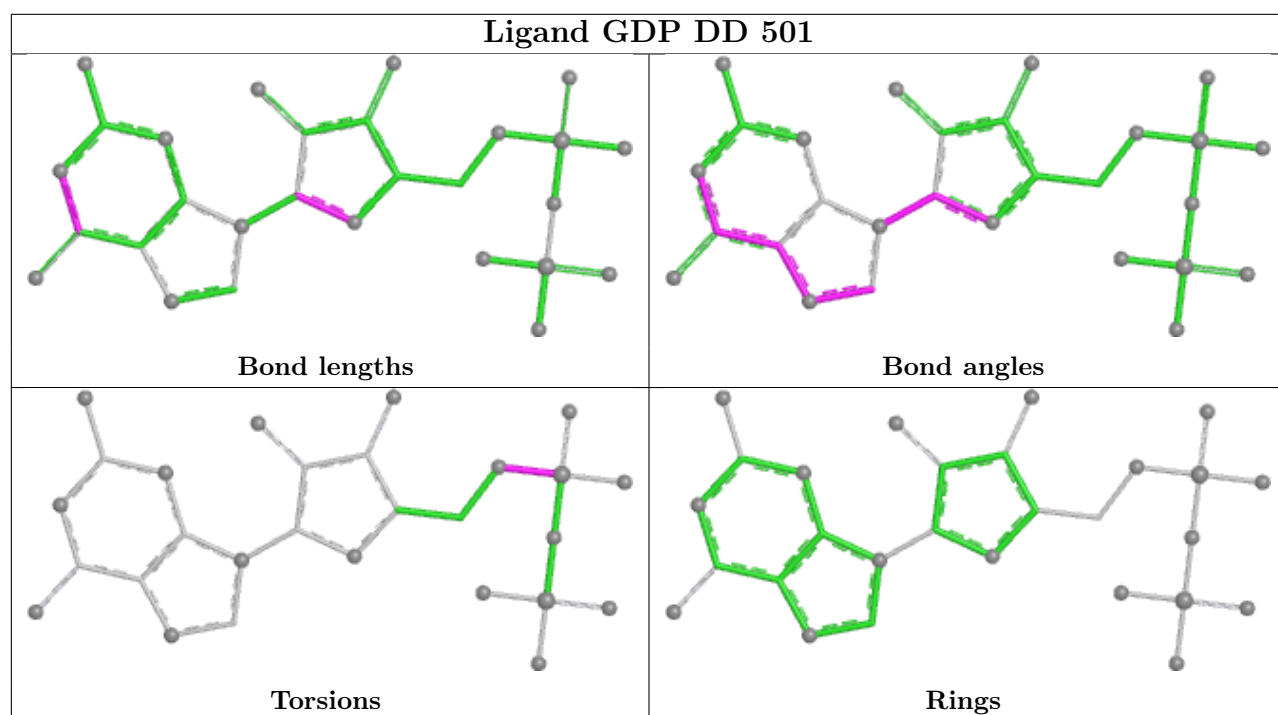


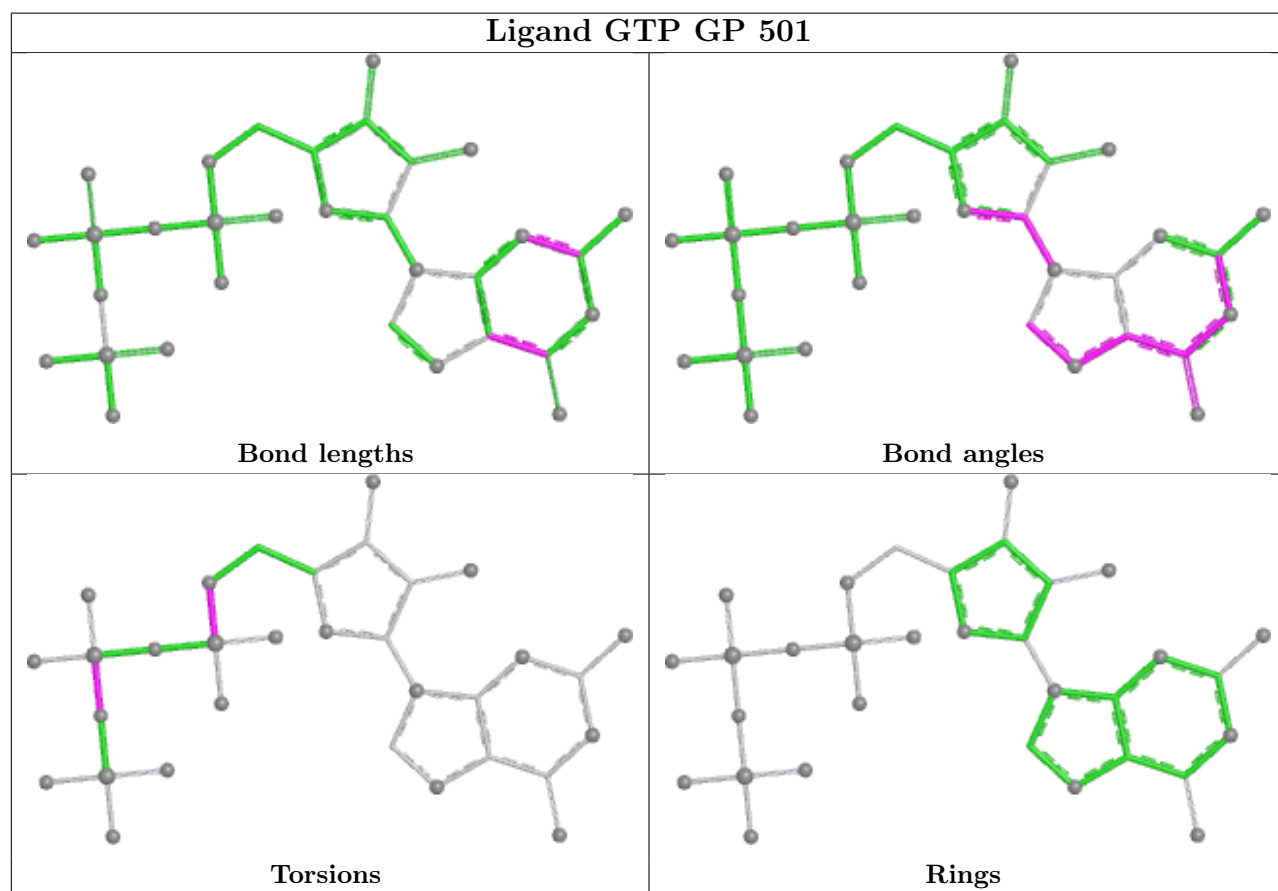
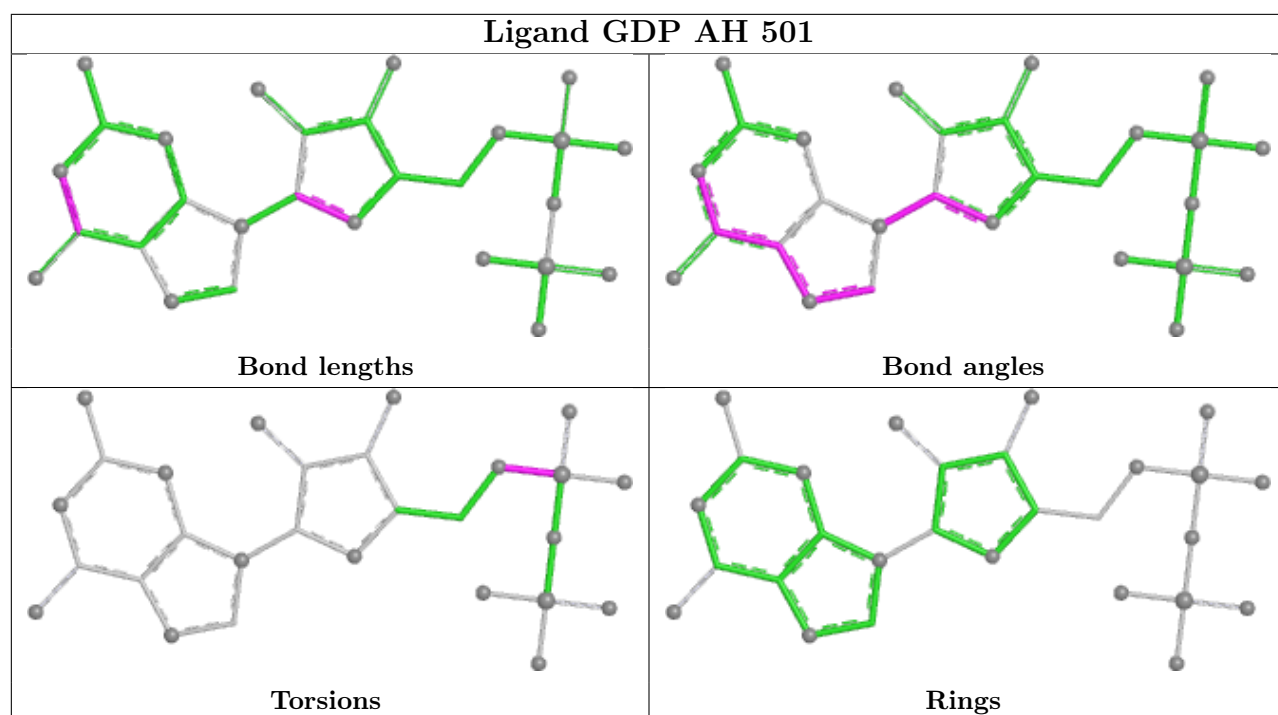




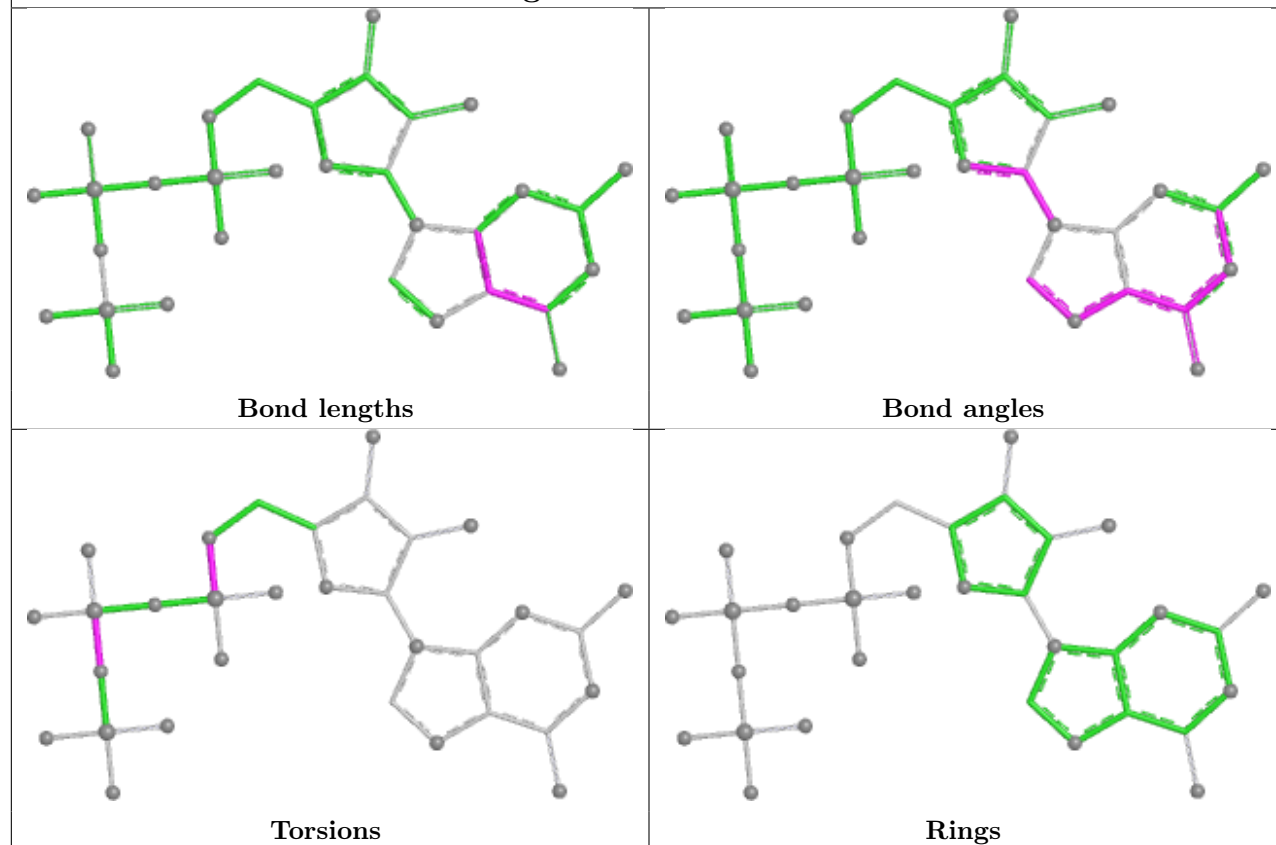




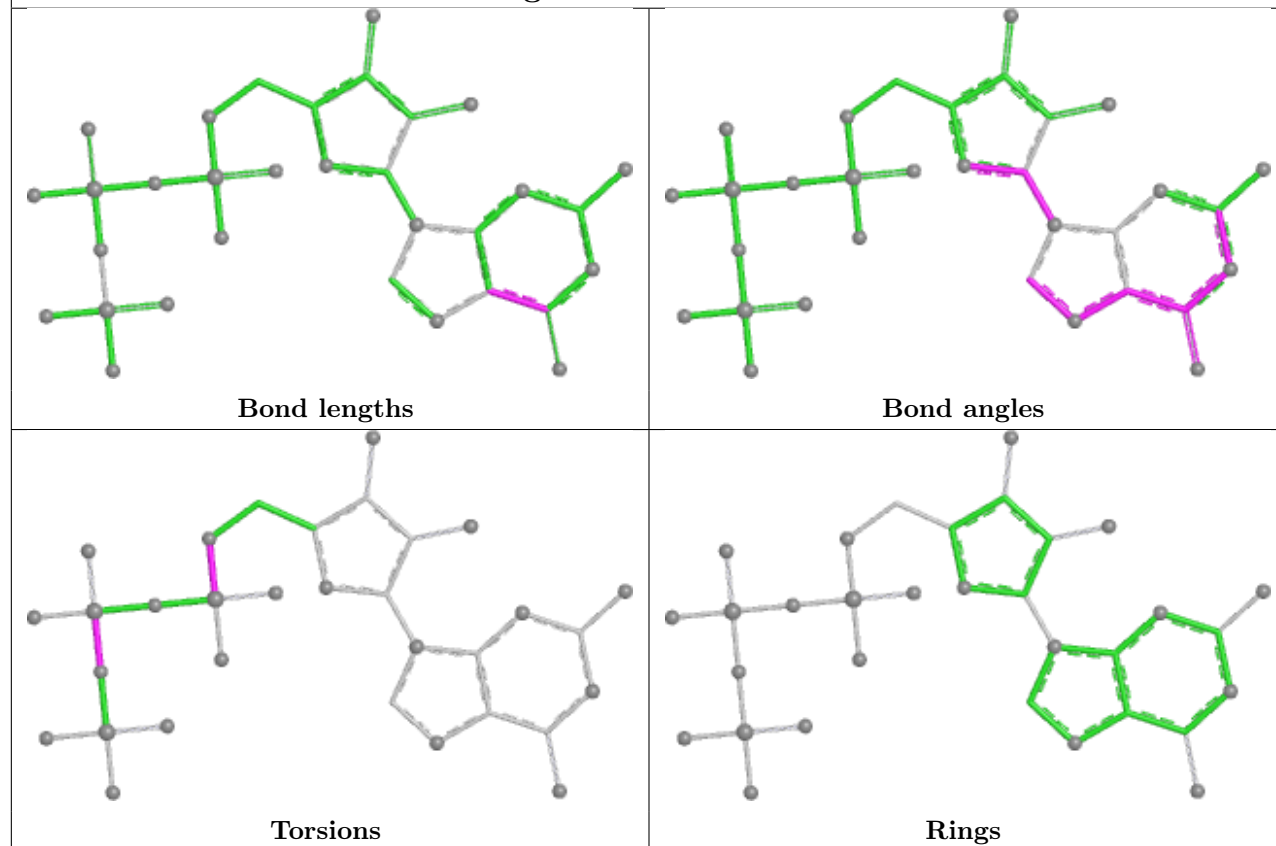


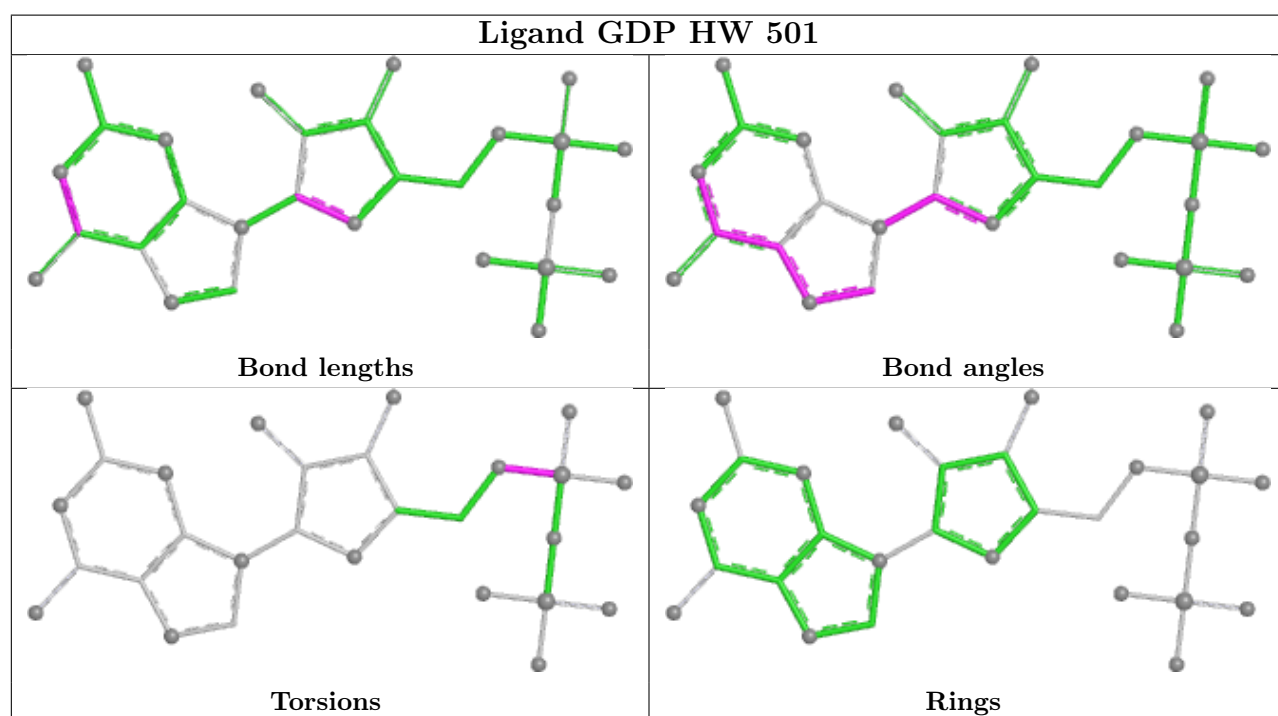
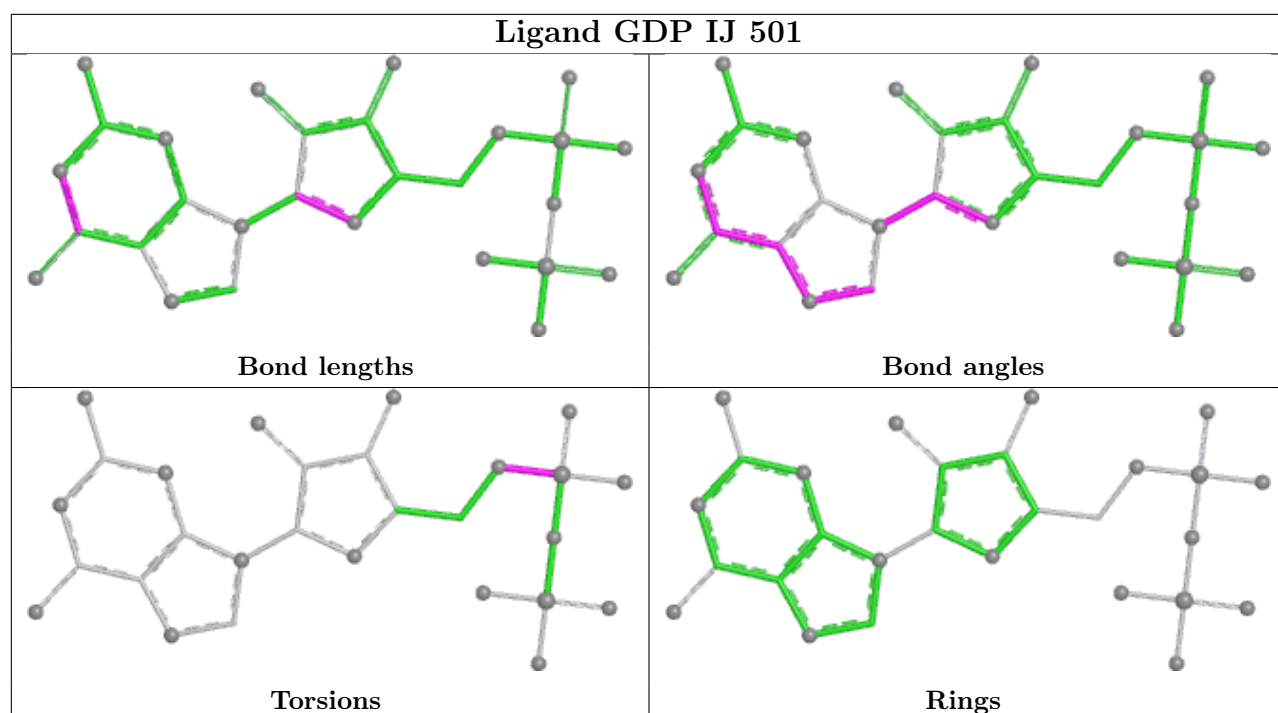


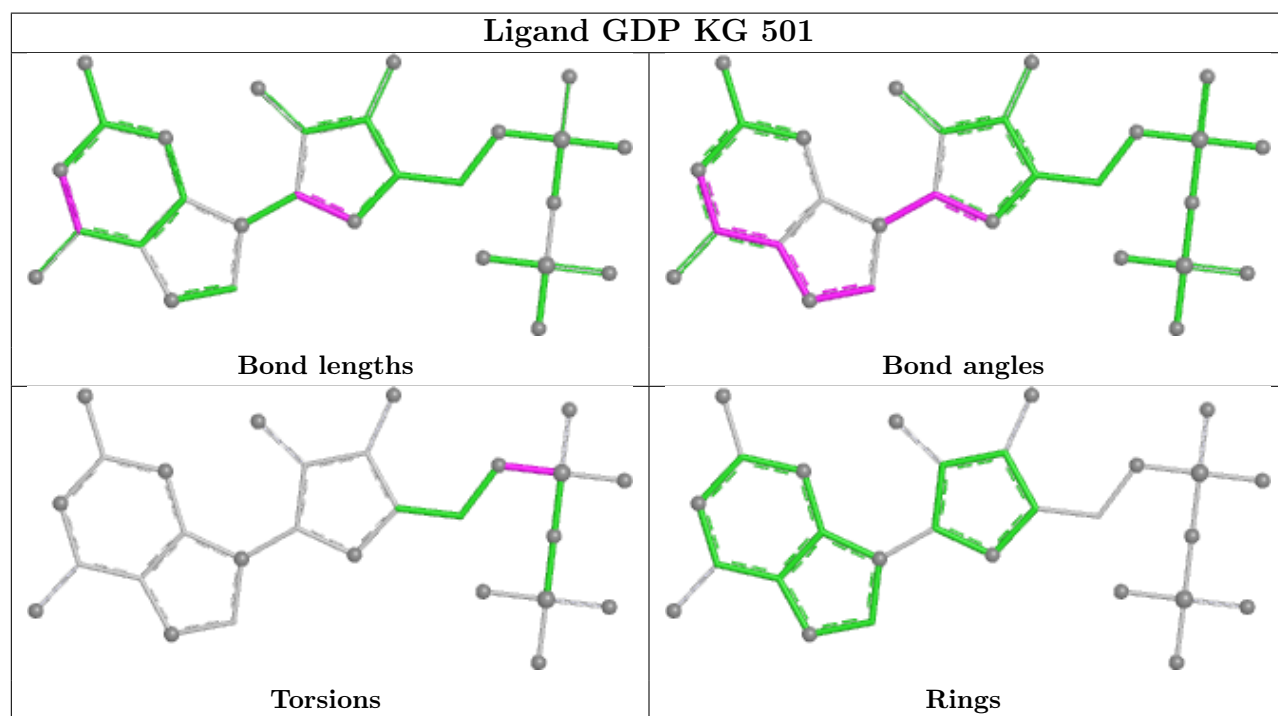
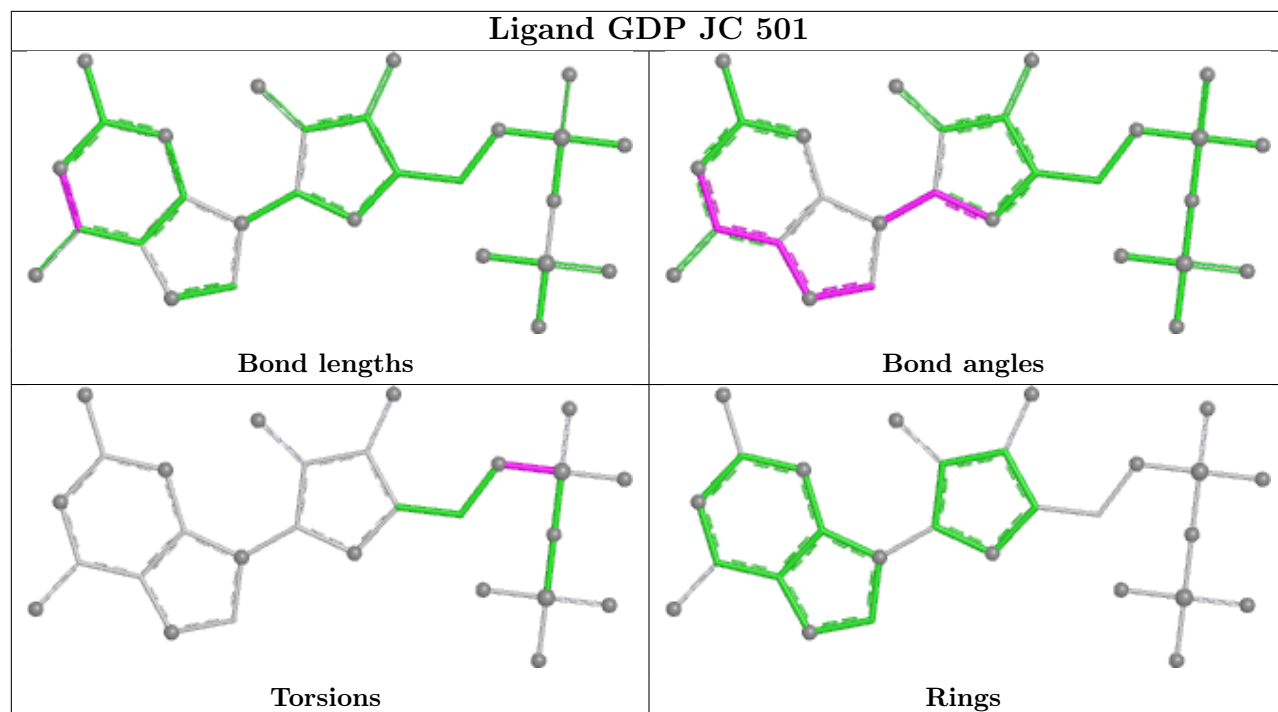
## Ligand GTP IK 602



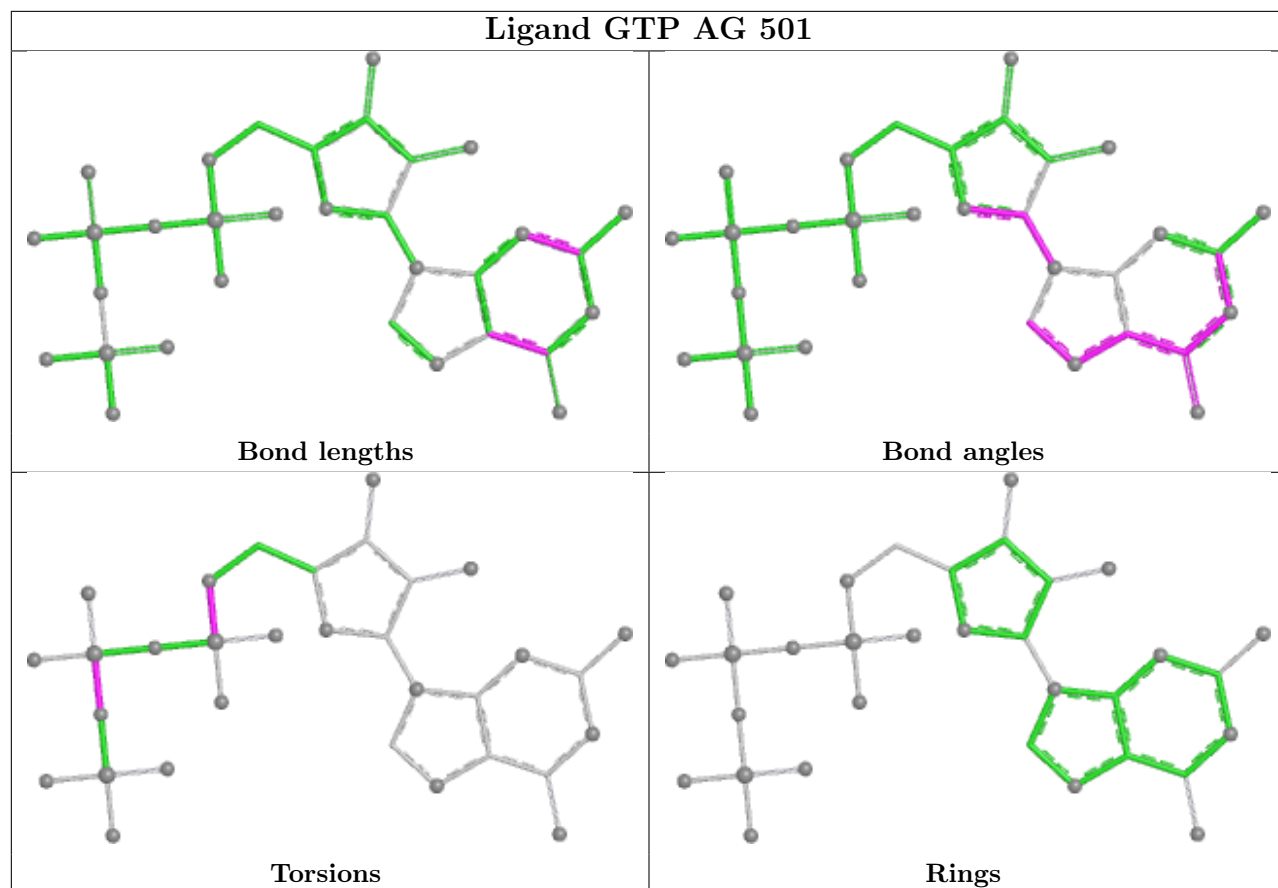
## Ligand GTP IO 501



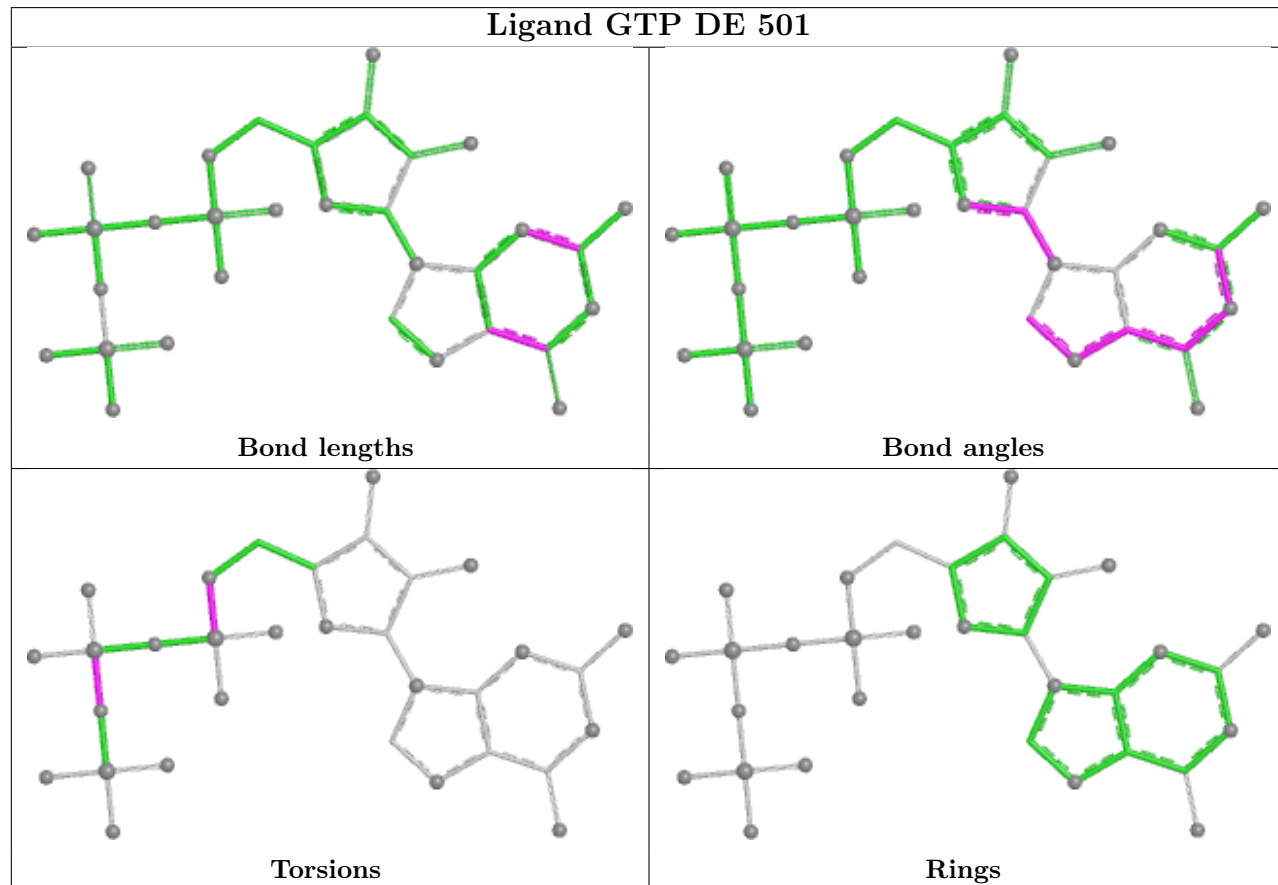




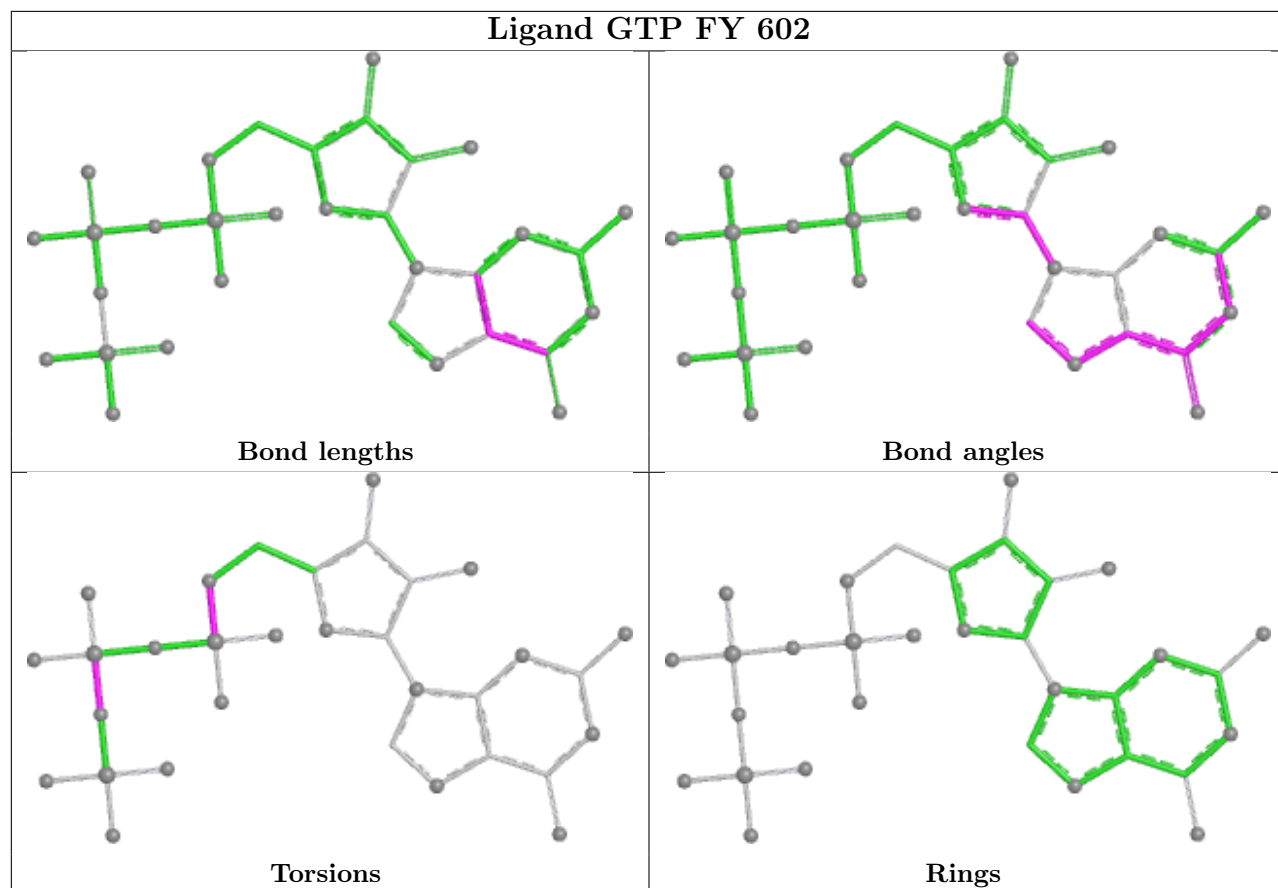
## Ligand GTP AG 501



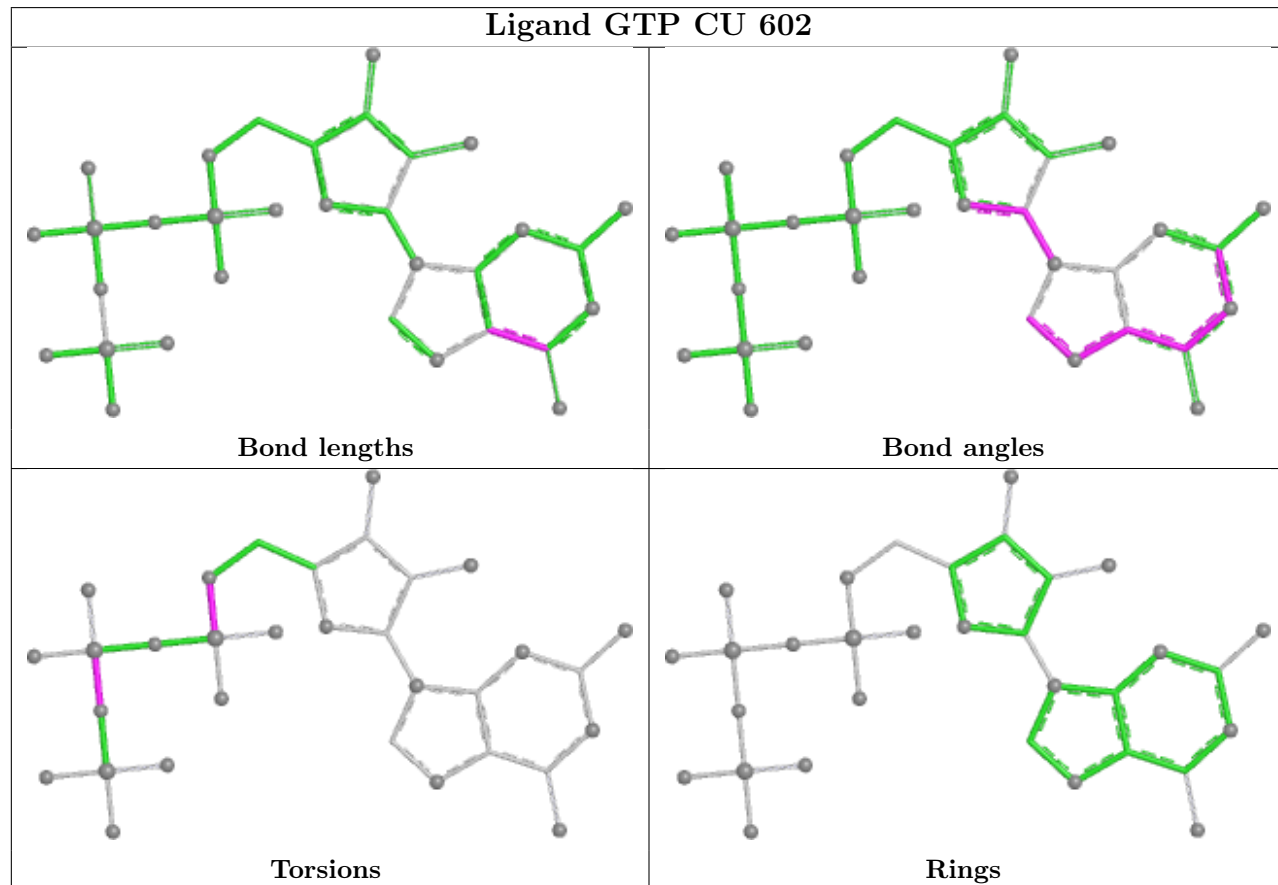
## Ligand GTP DE 501

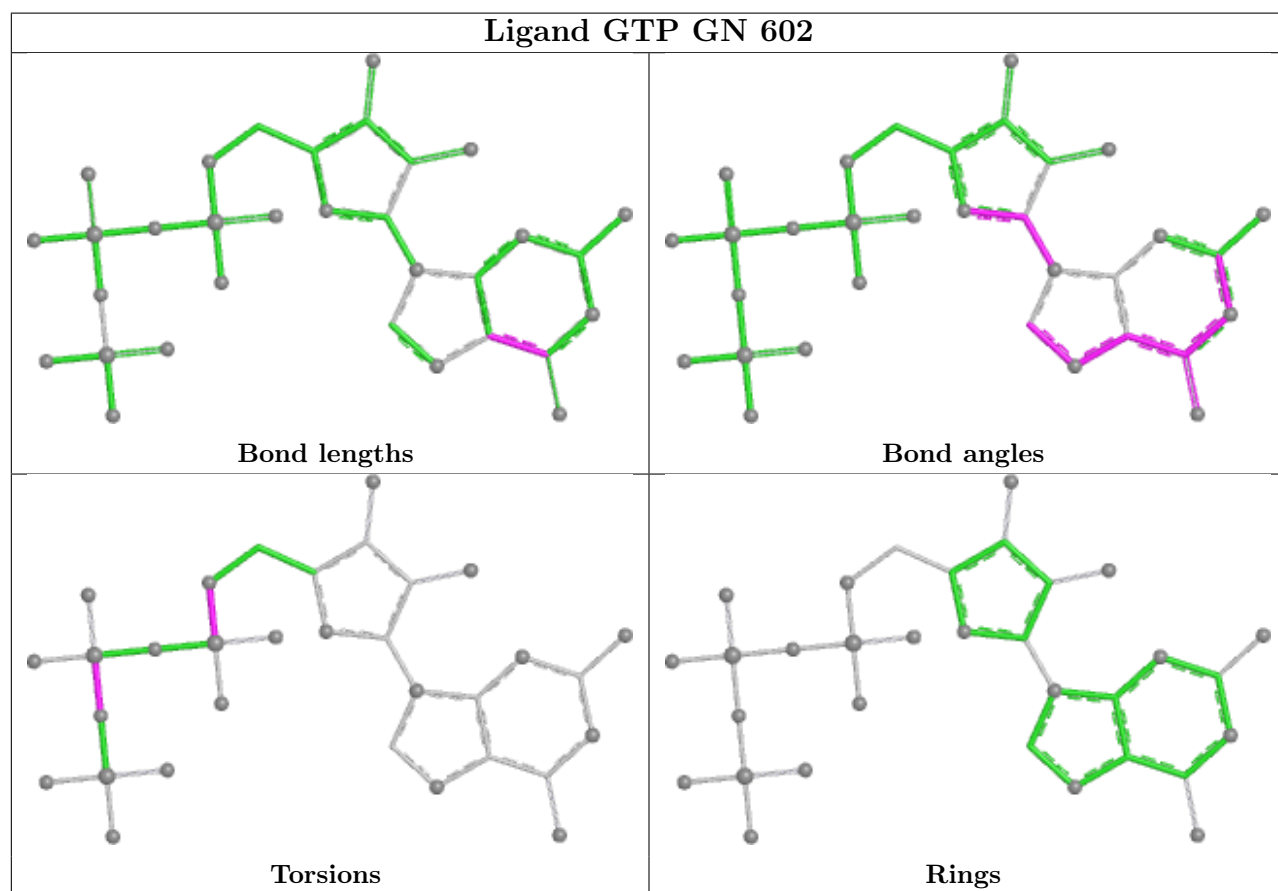
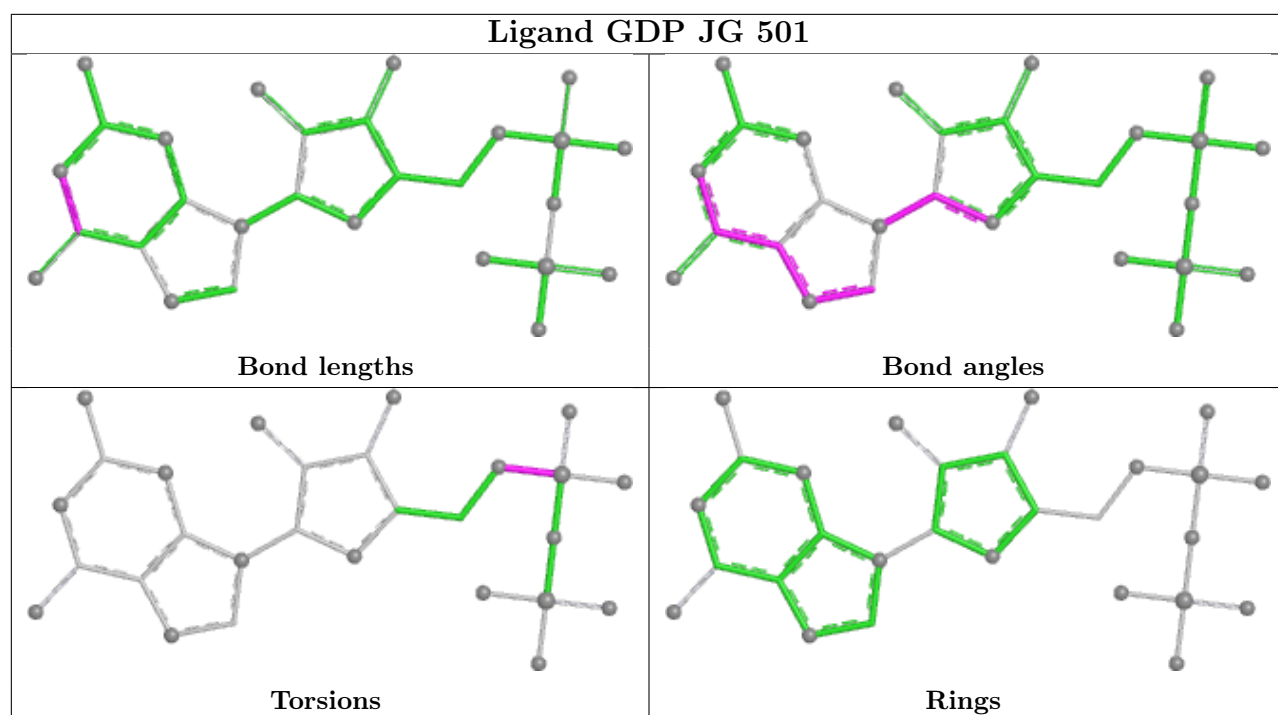


## Ligand GTP FY 602



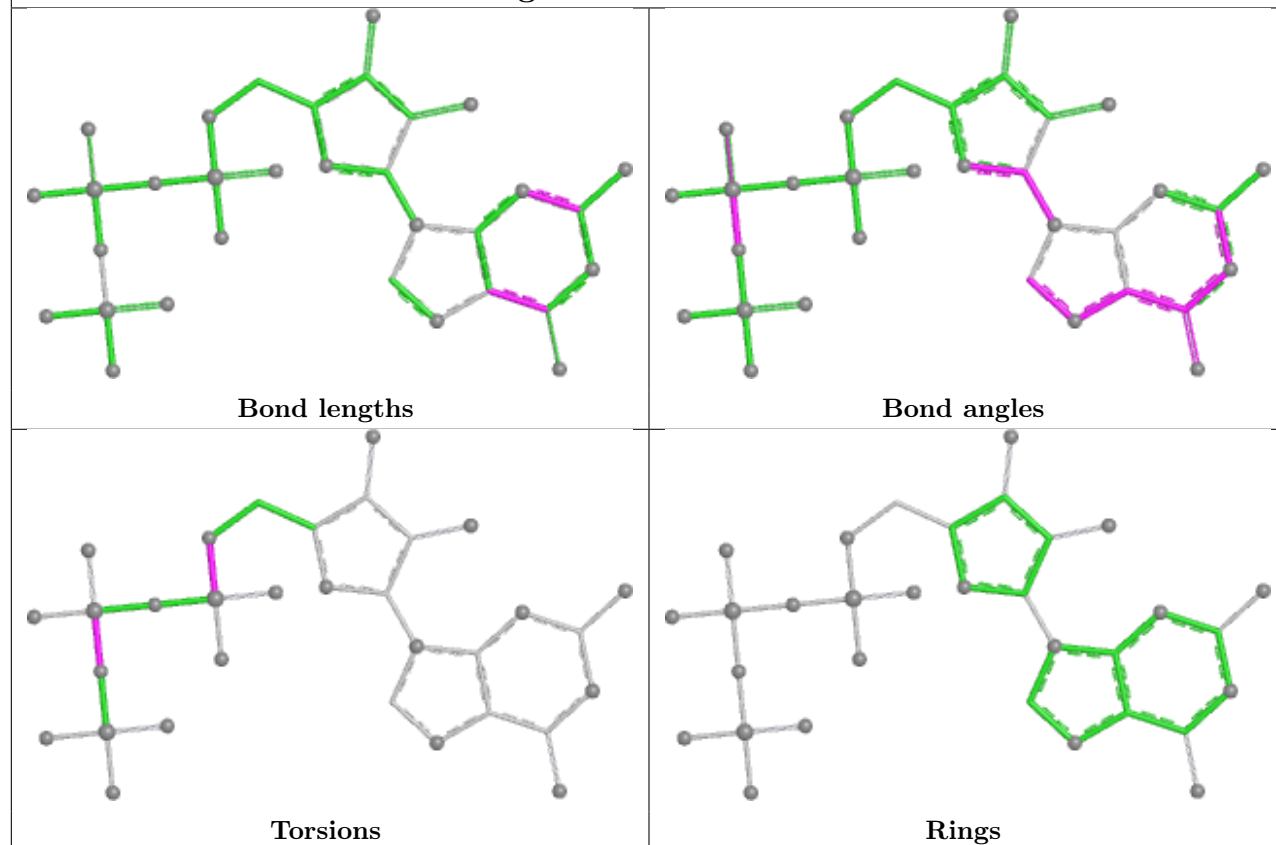
## Ligand GTP CU 602



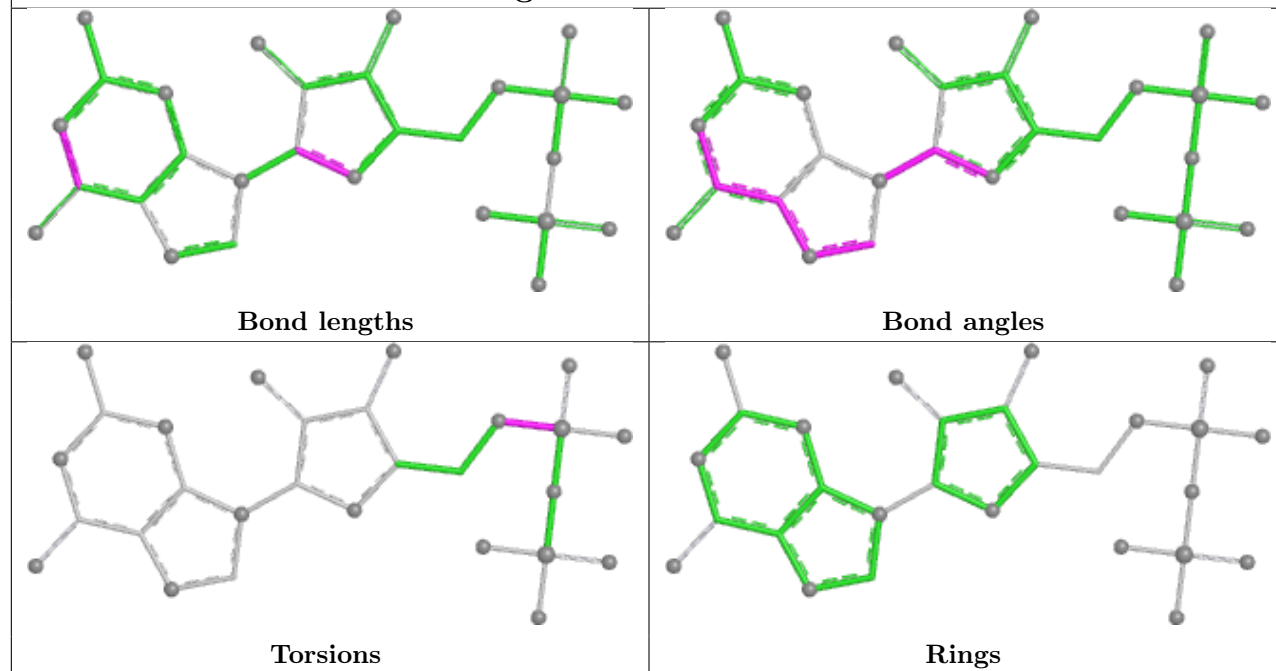


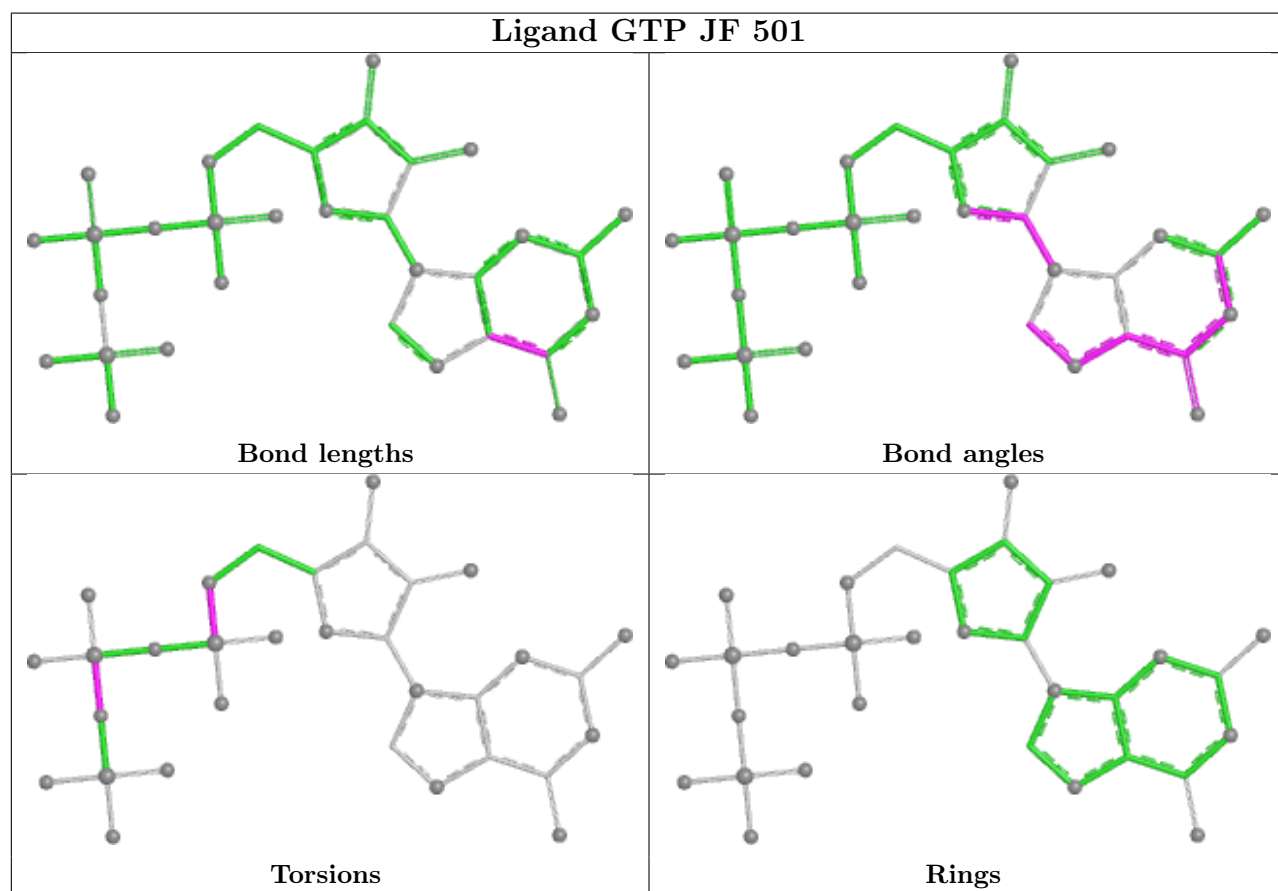
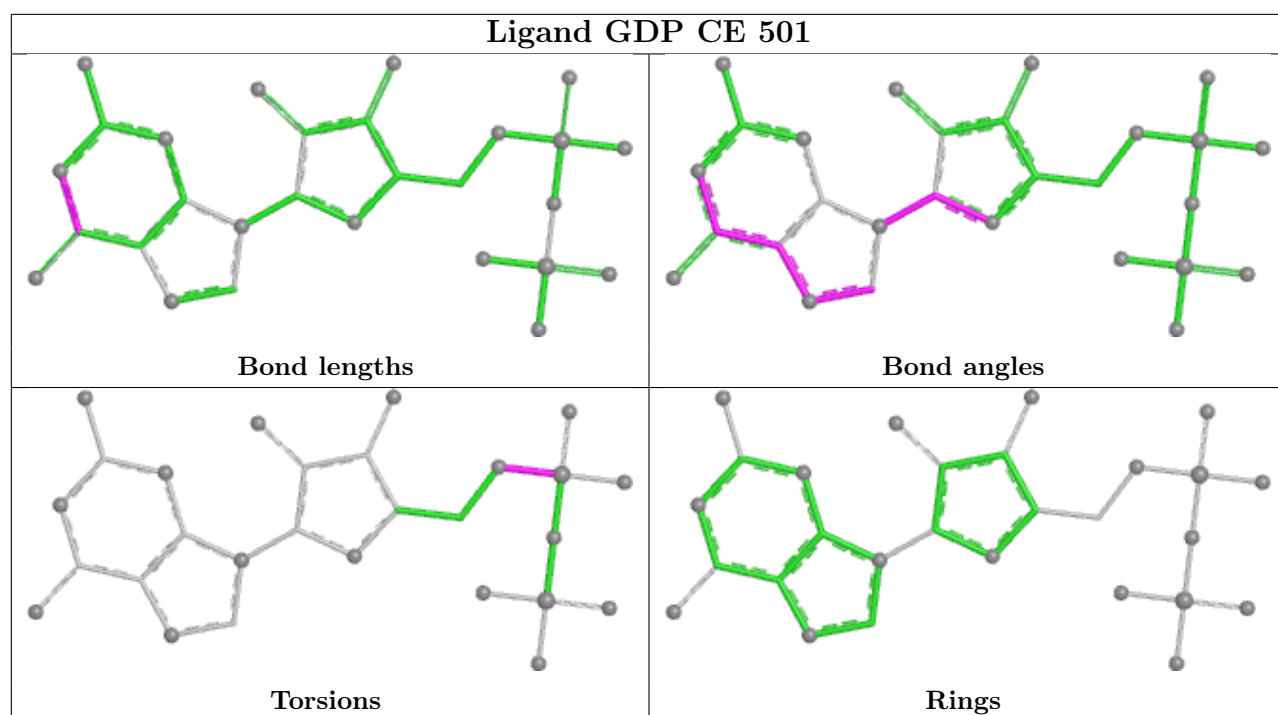


## Ligand GTP HE 501

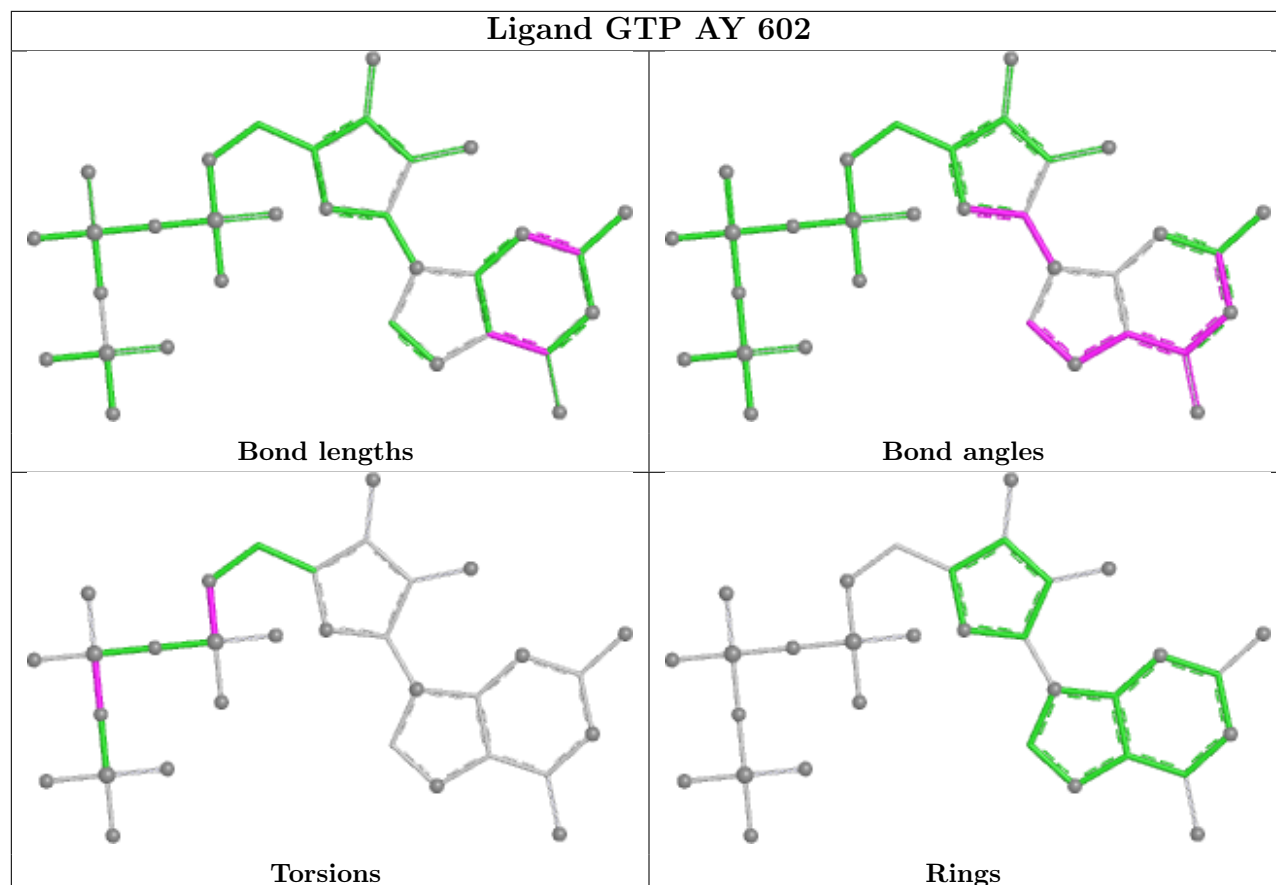


## Ligand GDP HB 501

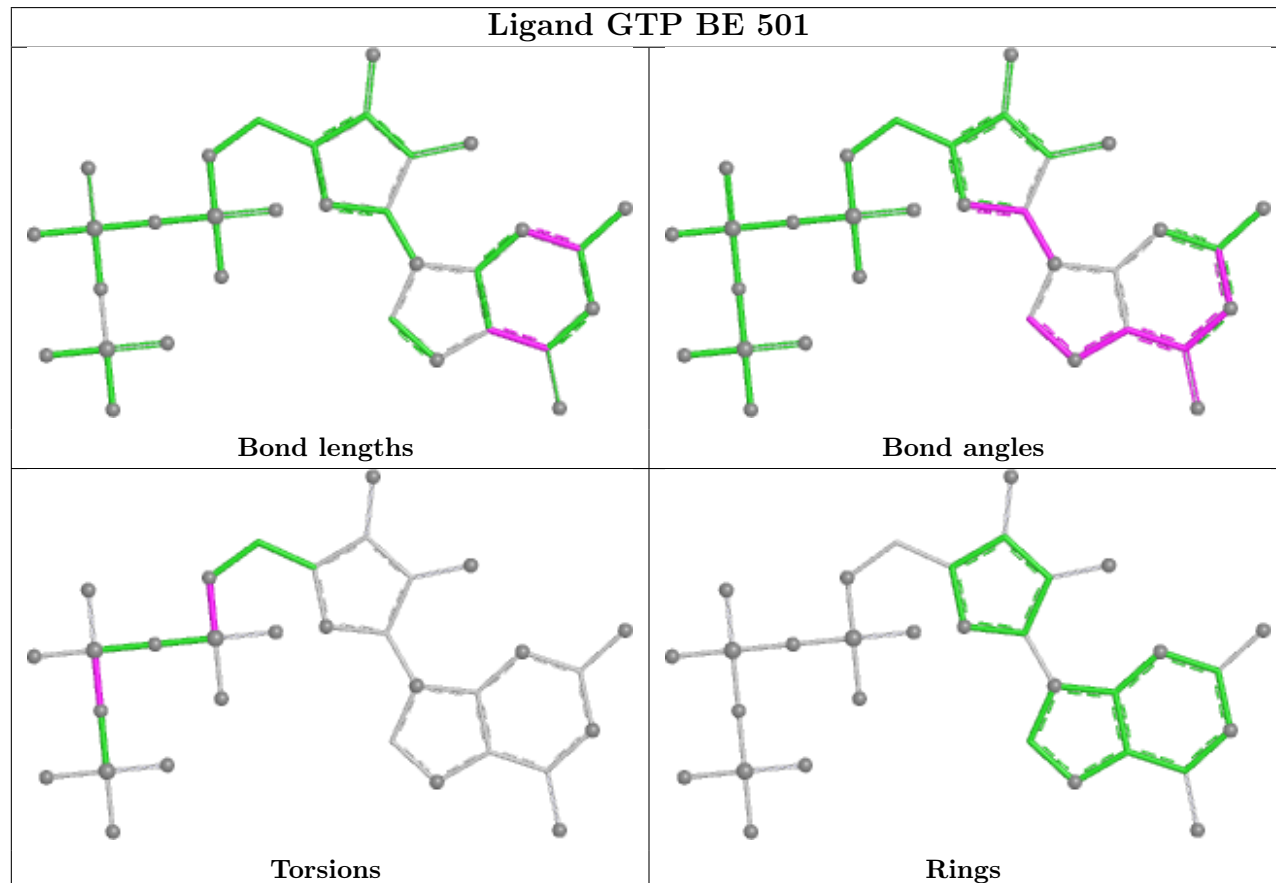


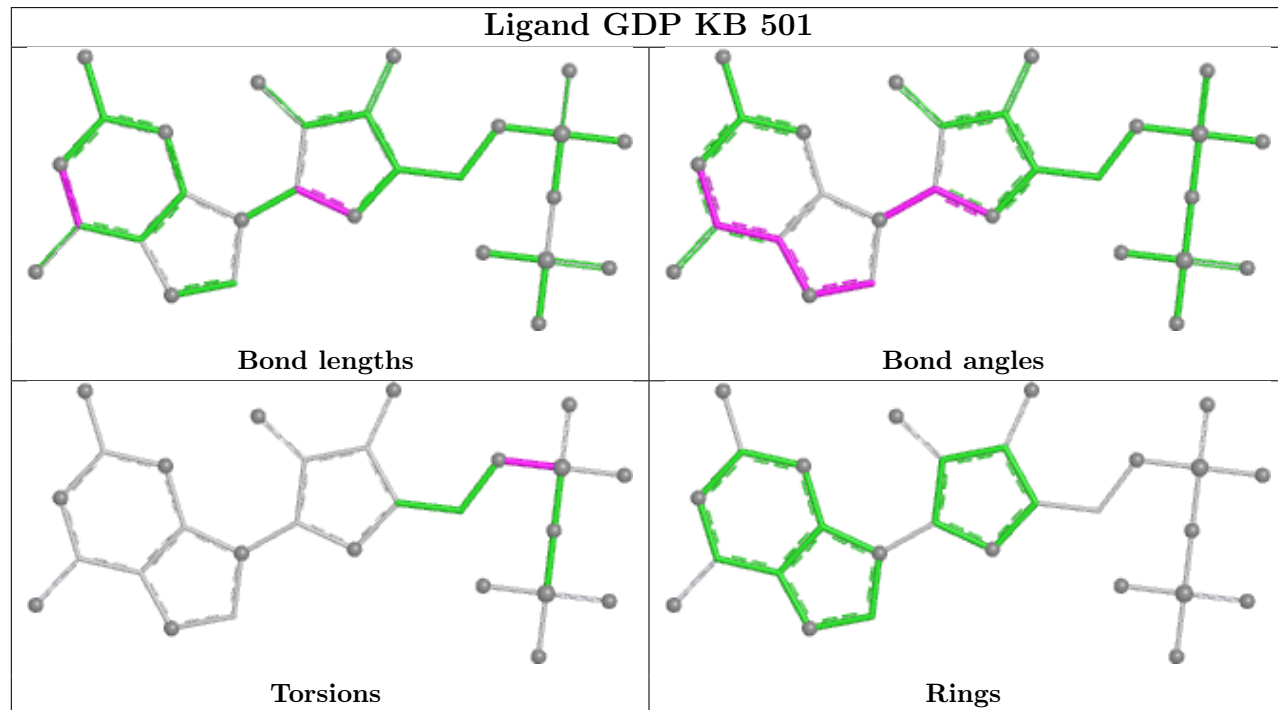
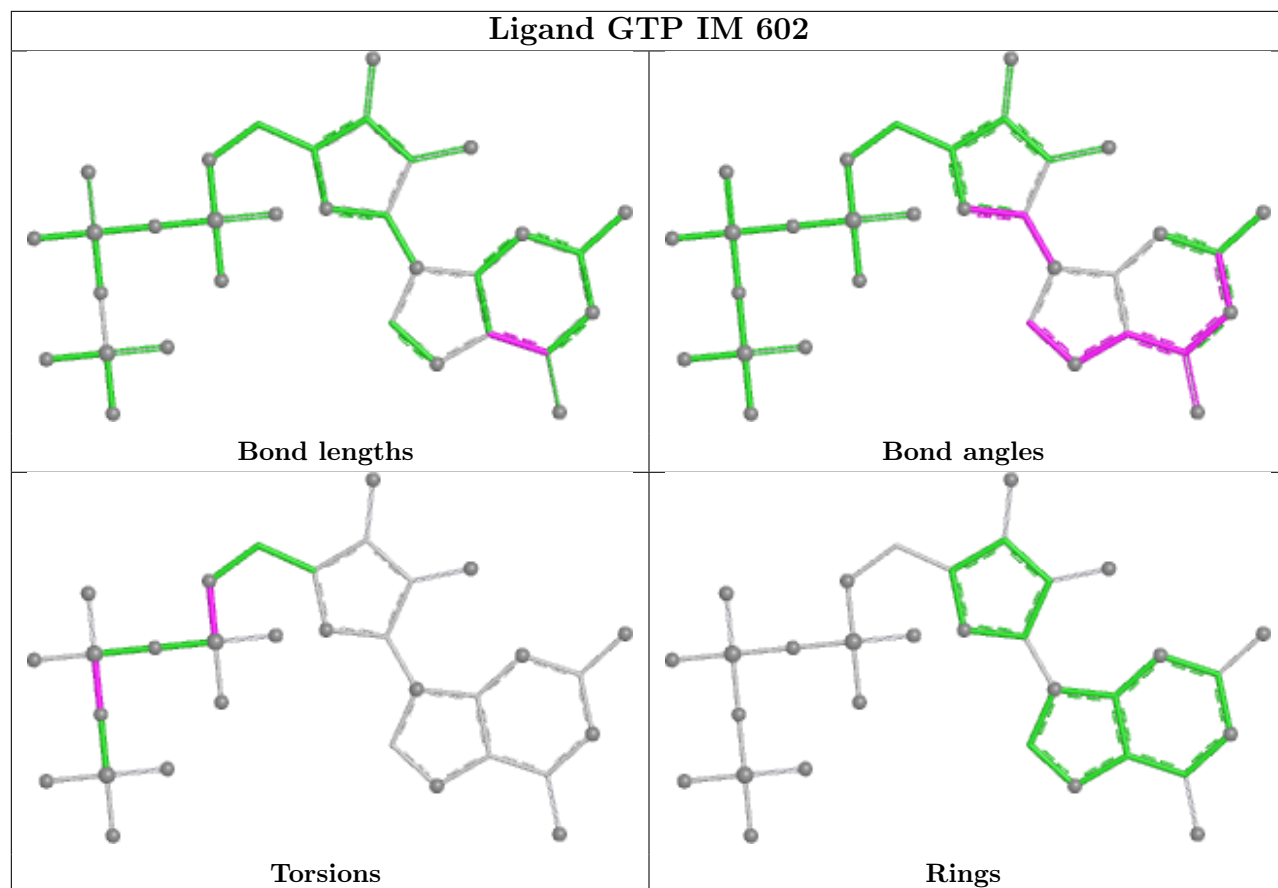


## Ligand GTP AY 602

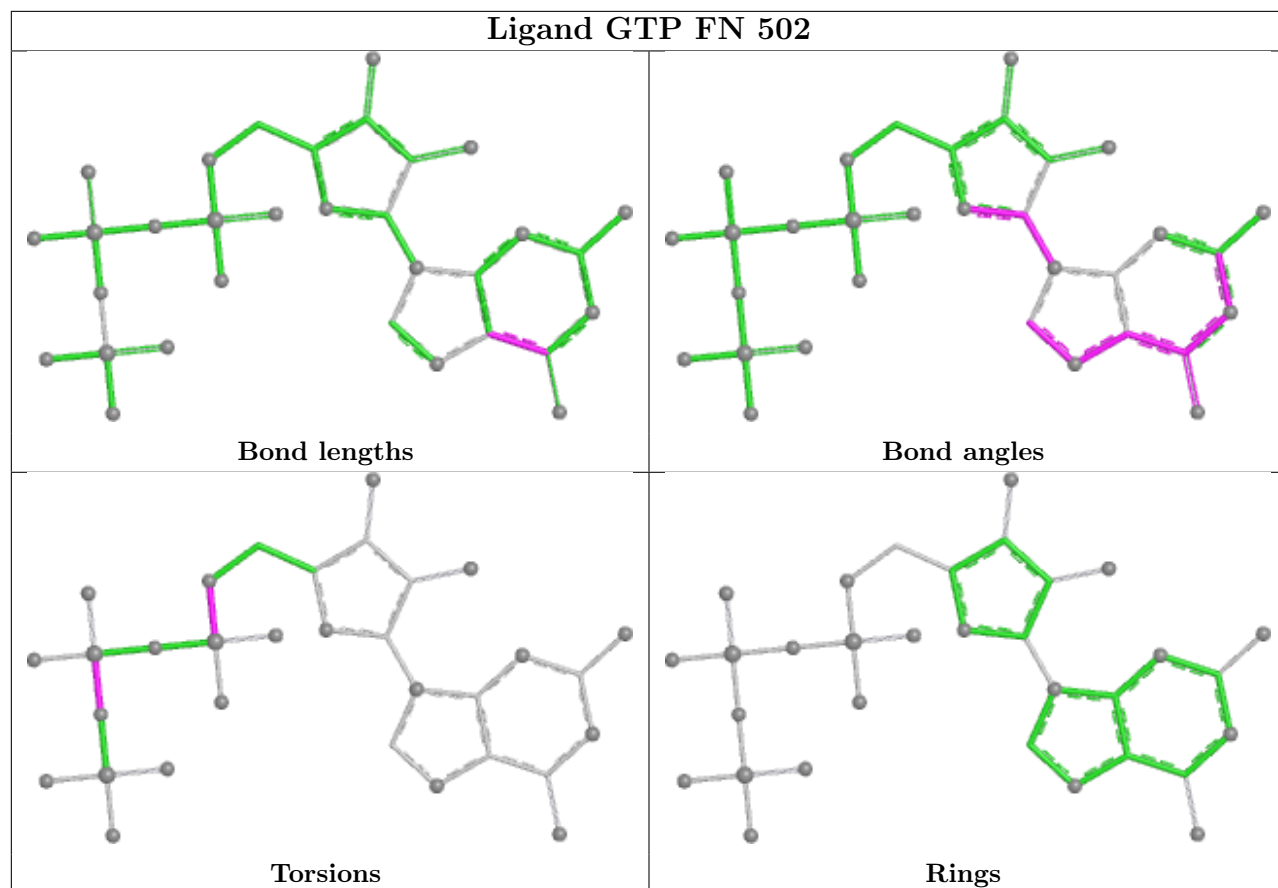


## Ligand GTP BE 501

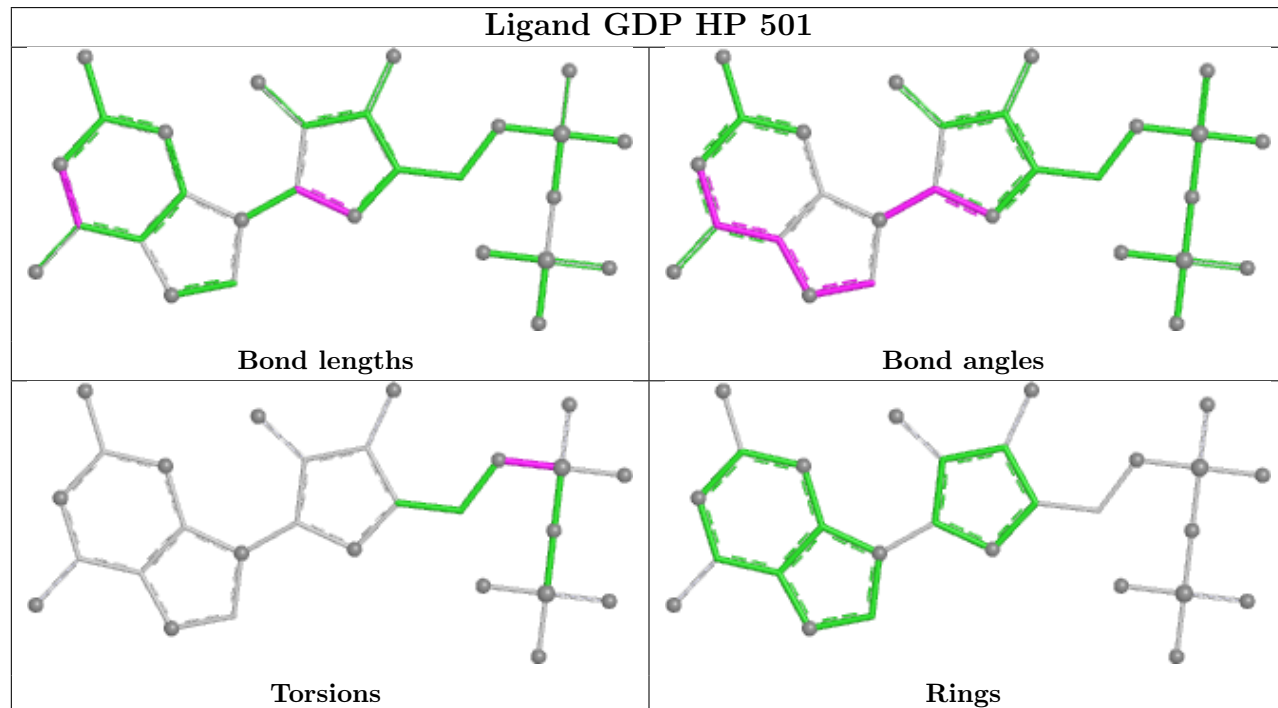




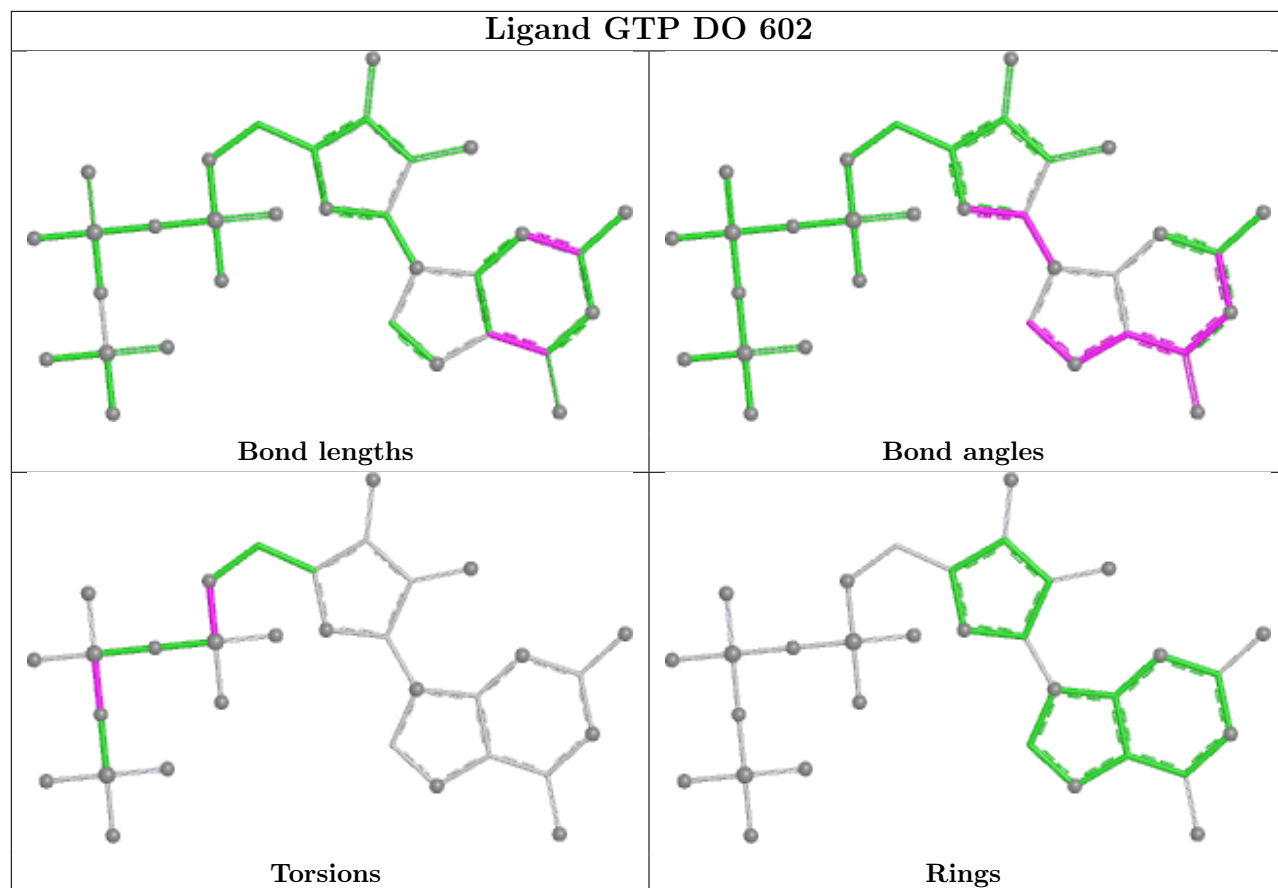
## Ligand GTP FN 502



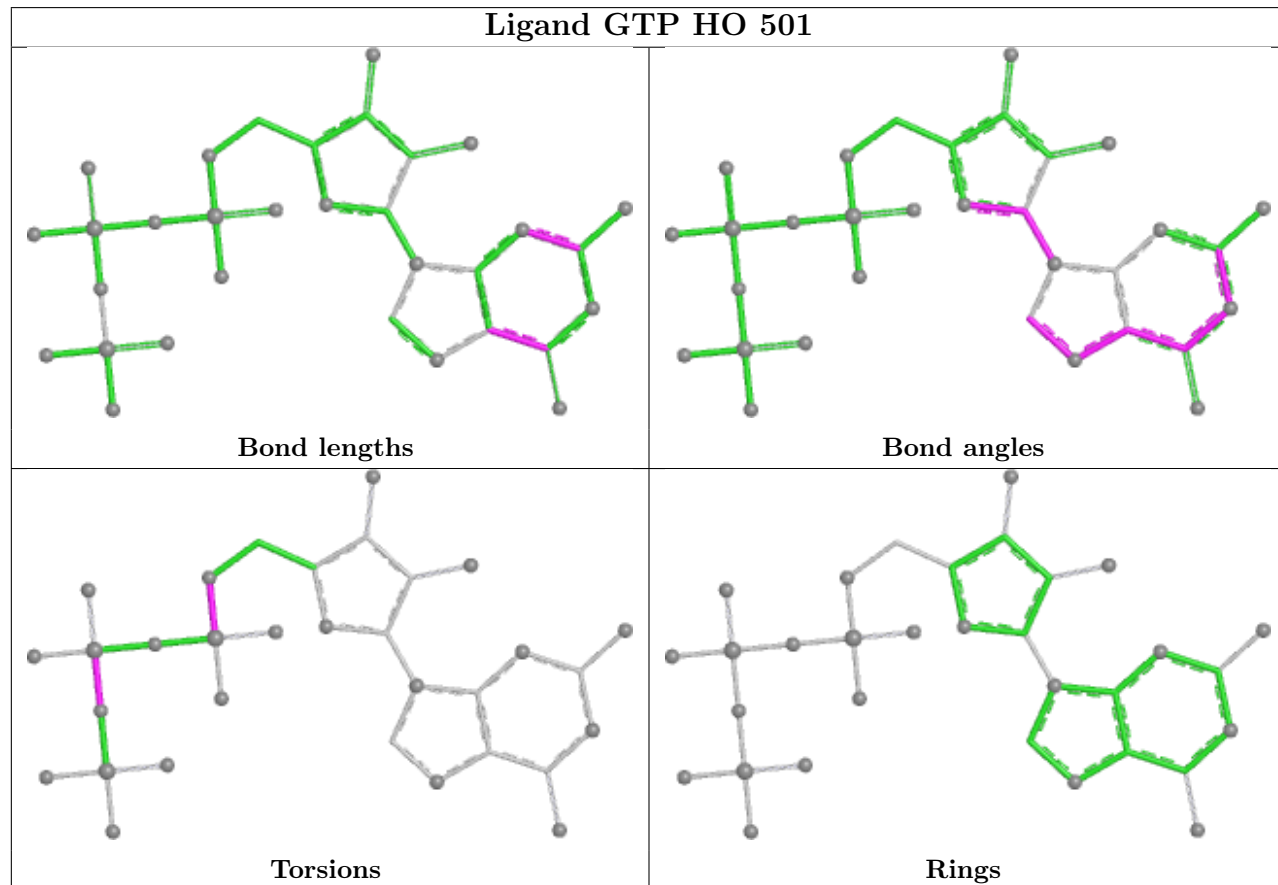
## Ligand GDP HP 501

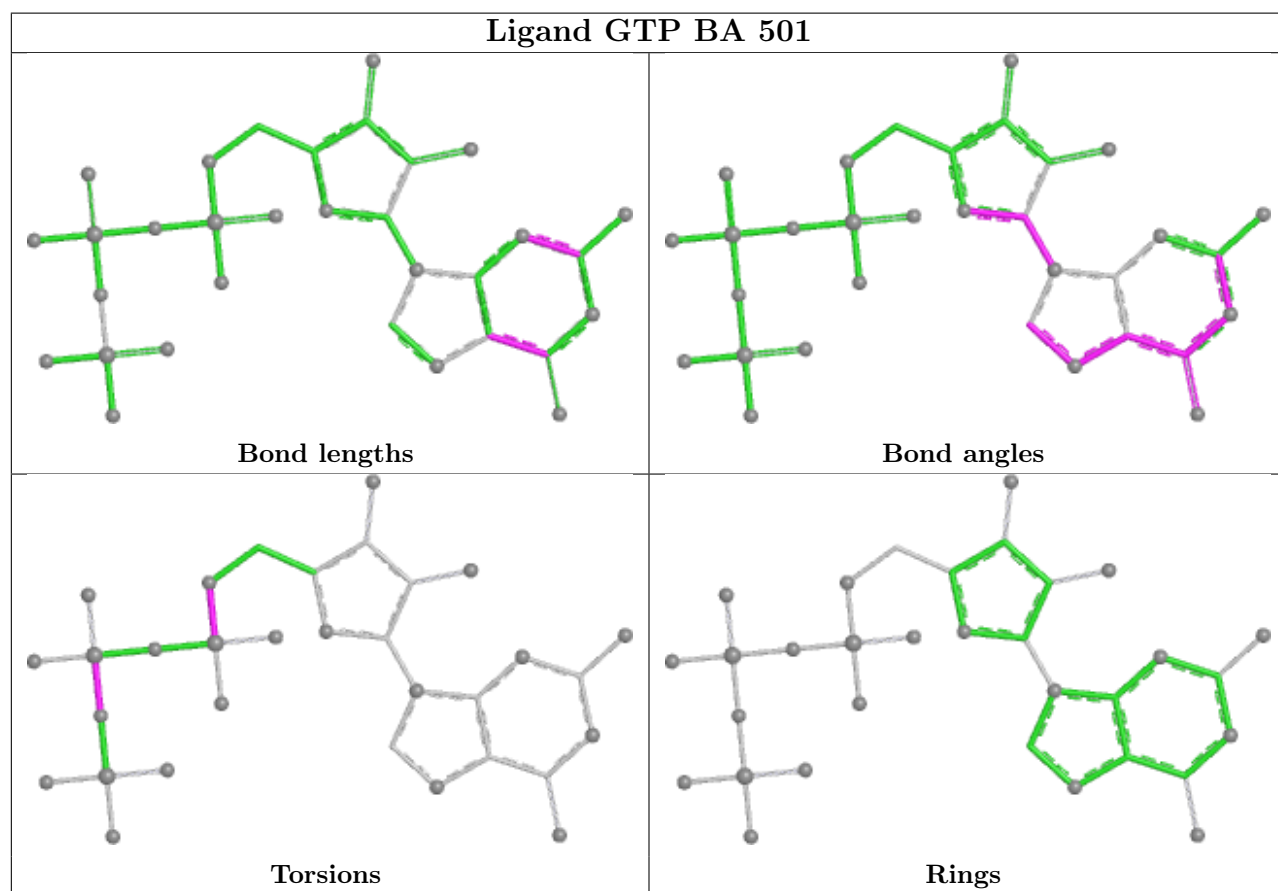
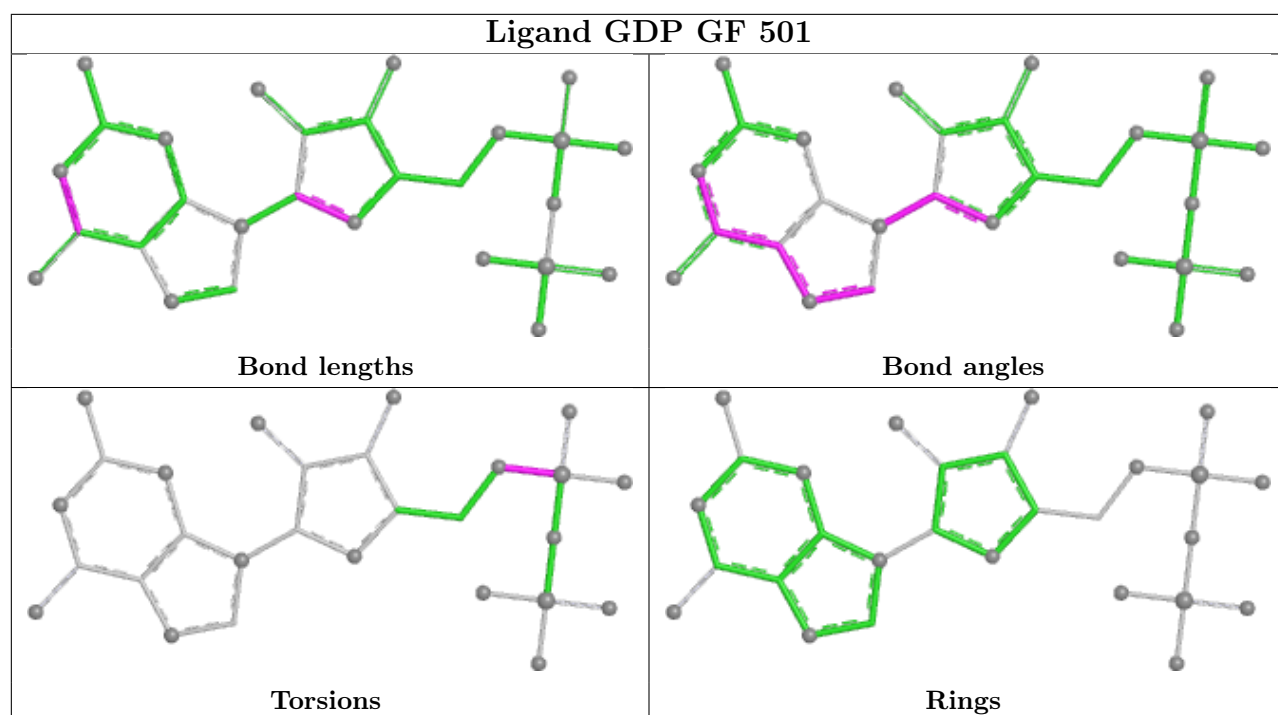


## Ligand GTP DO 602

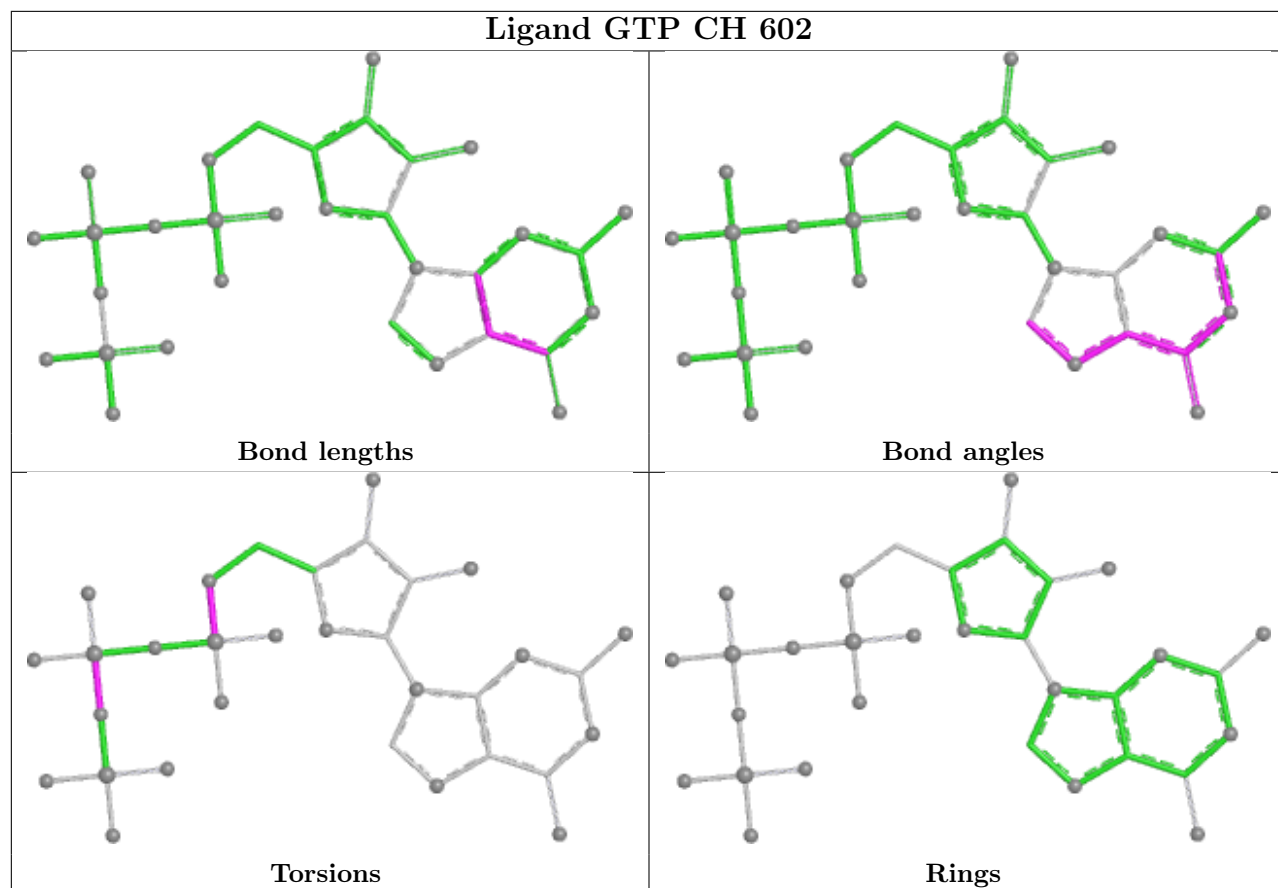


## Ligand GTP HO 501

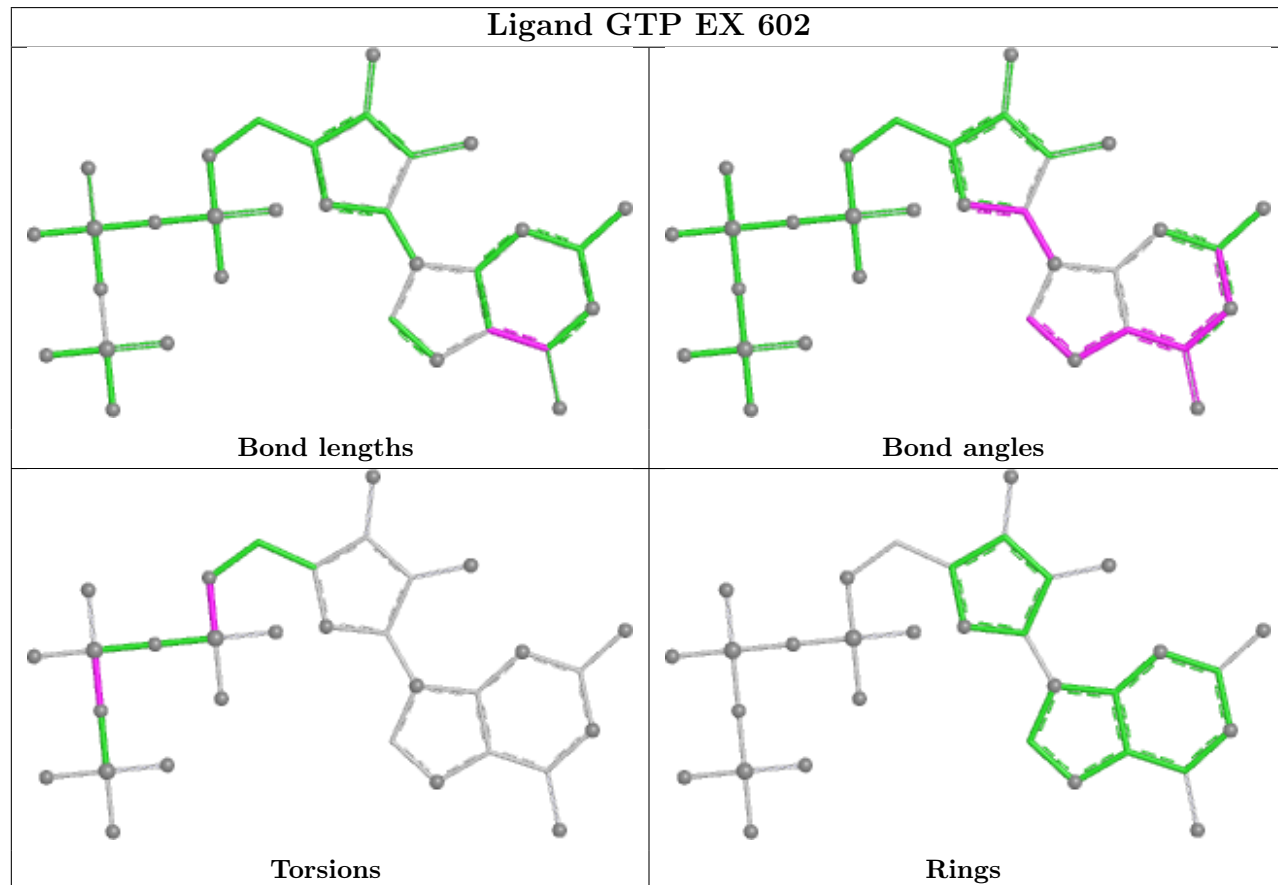




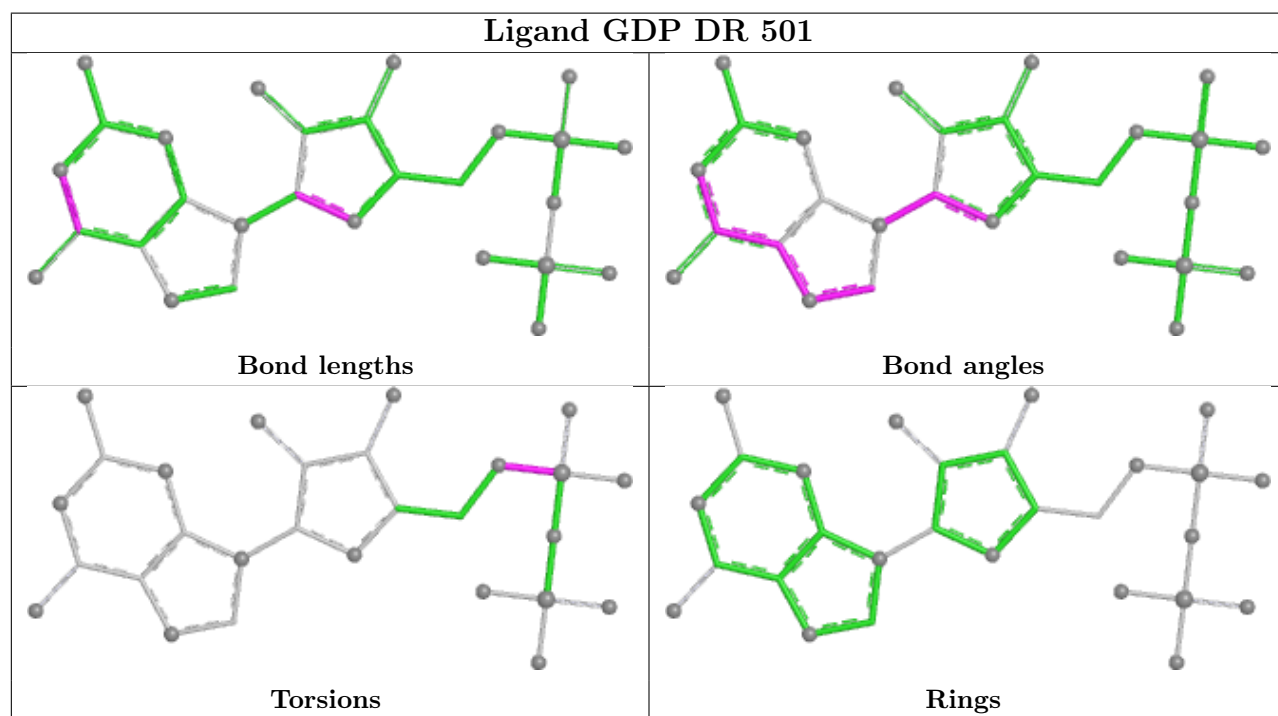
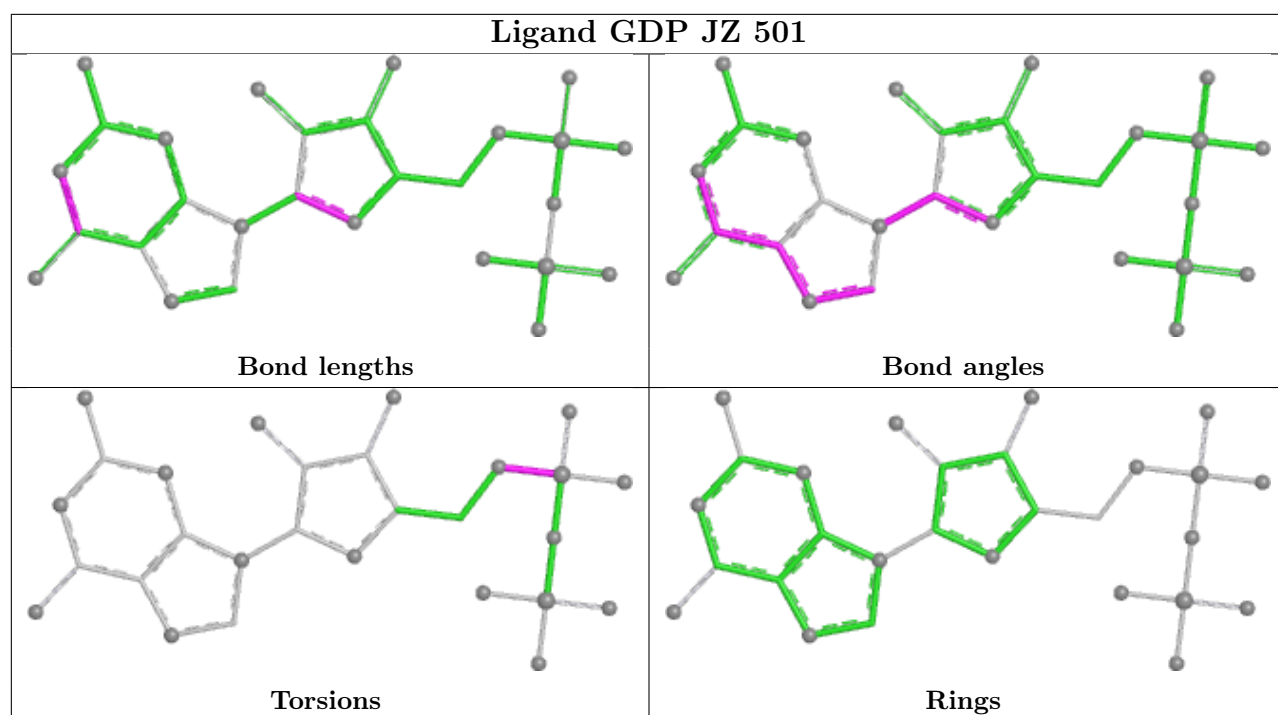
## Ligand GTP CH 602

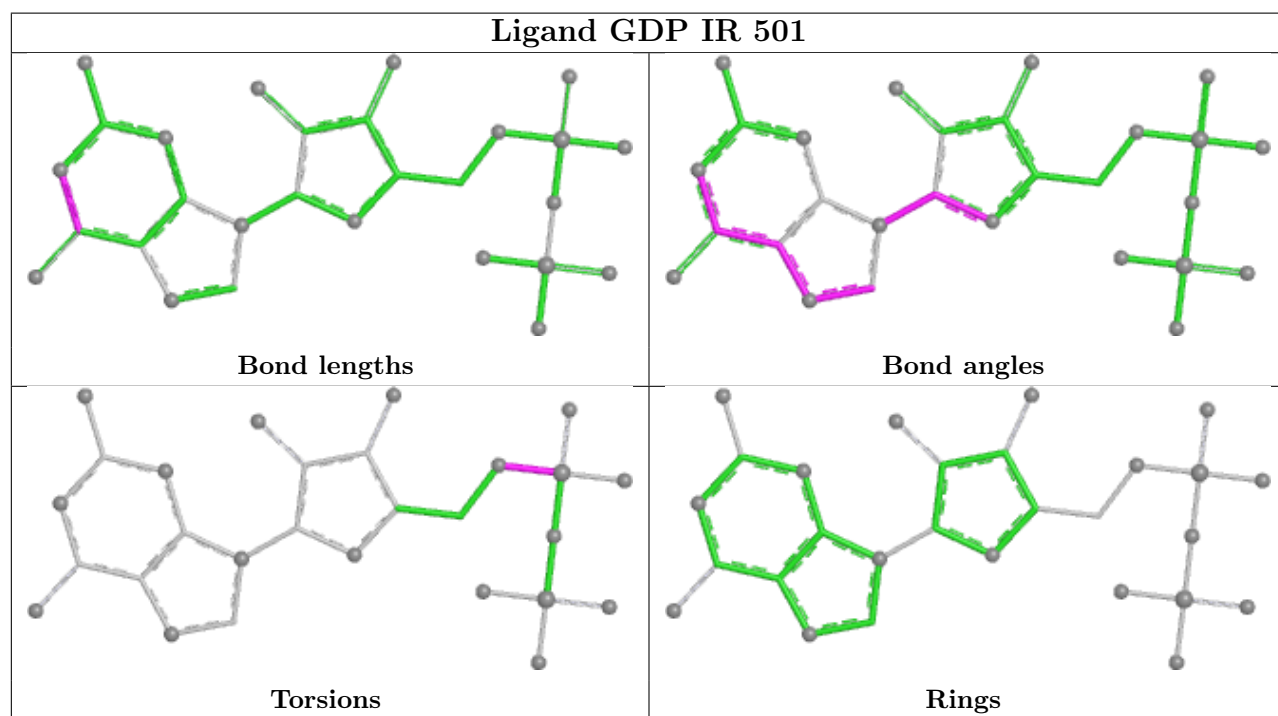
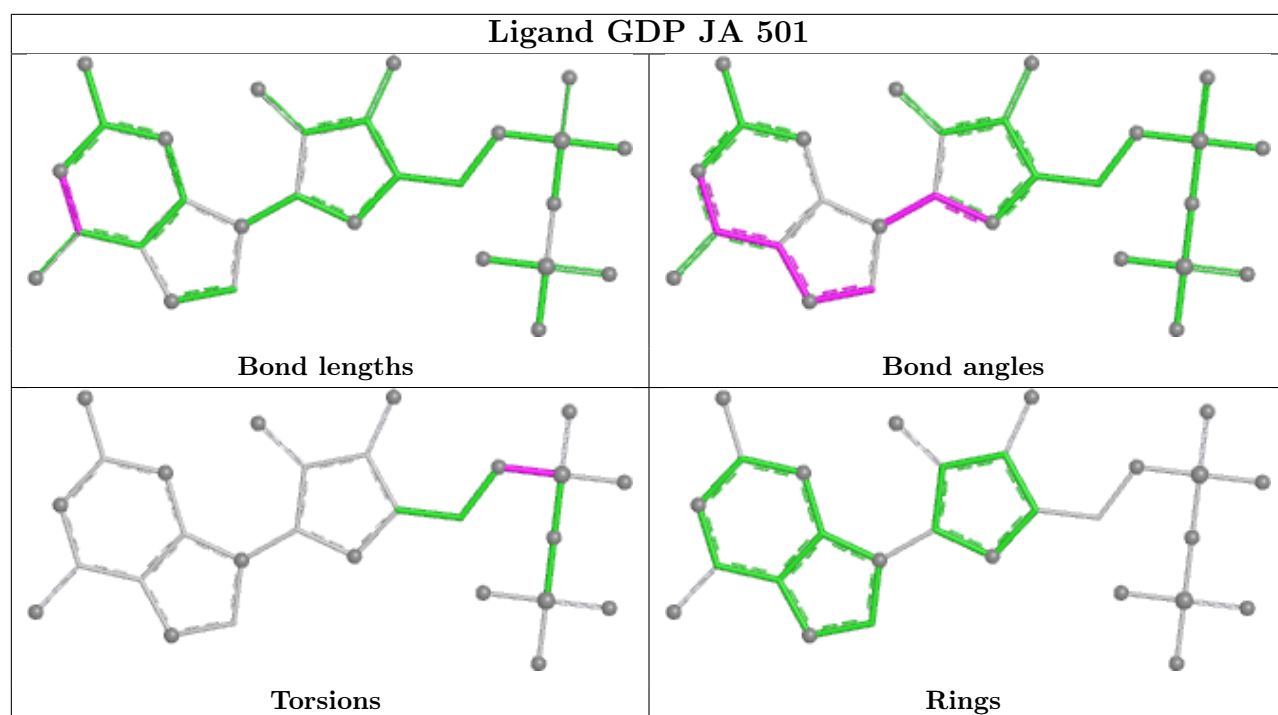


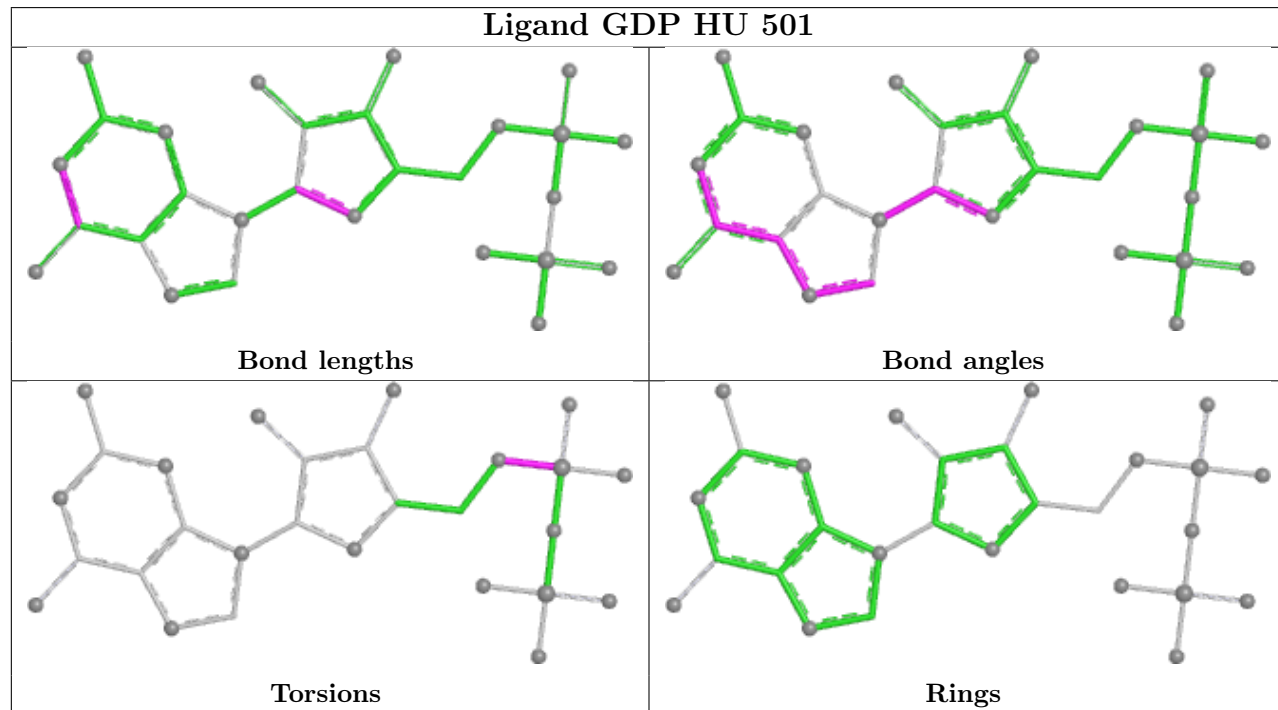
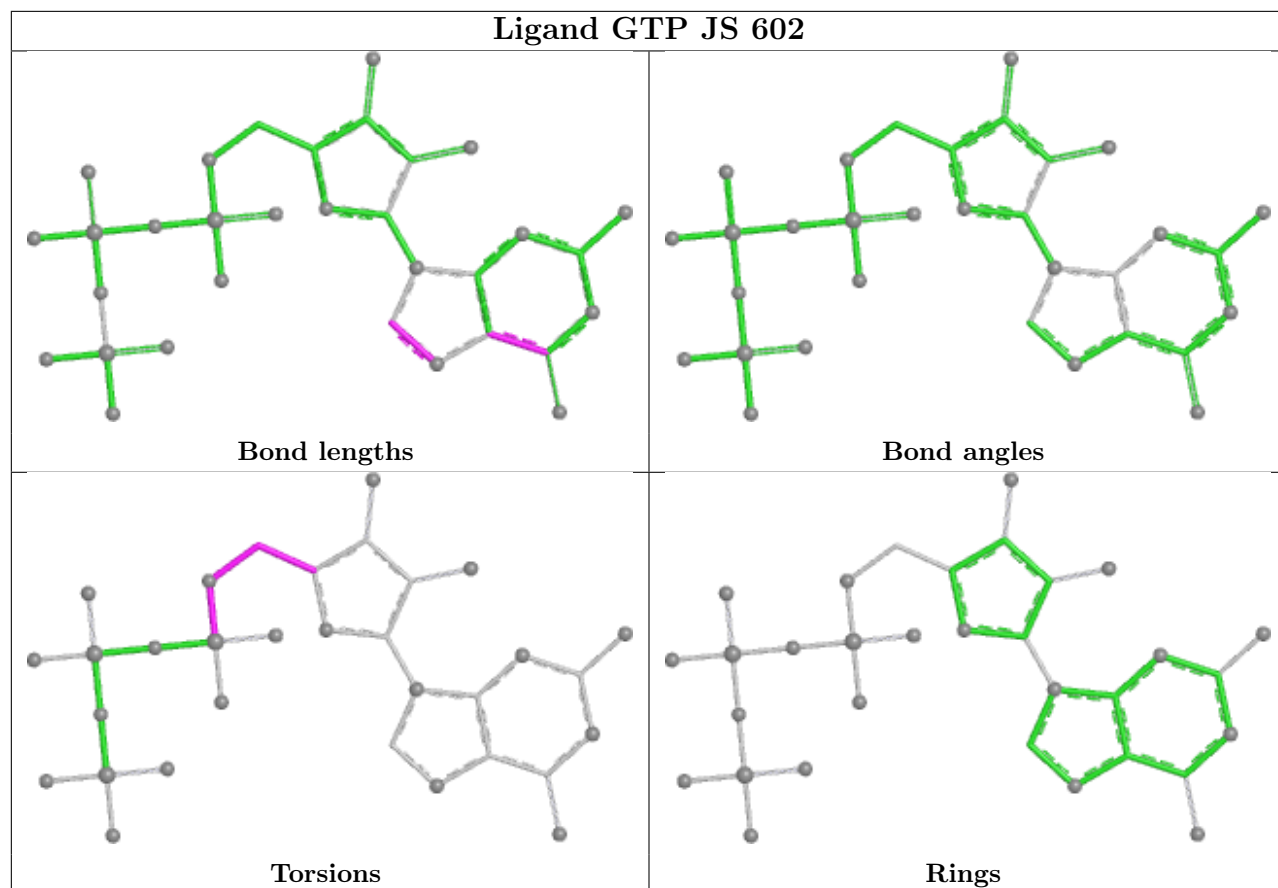
## Ligand GTP EX 602

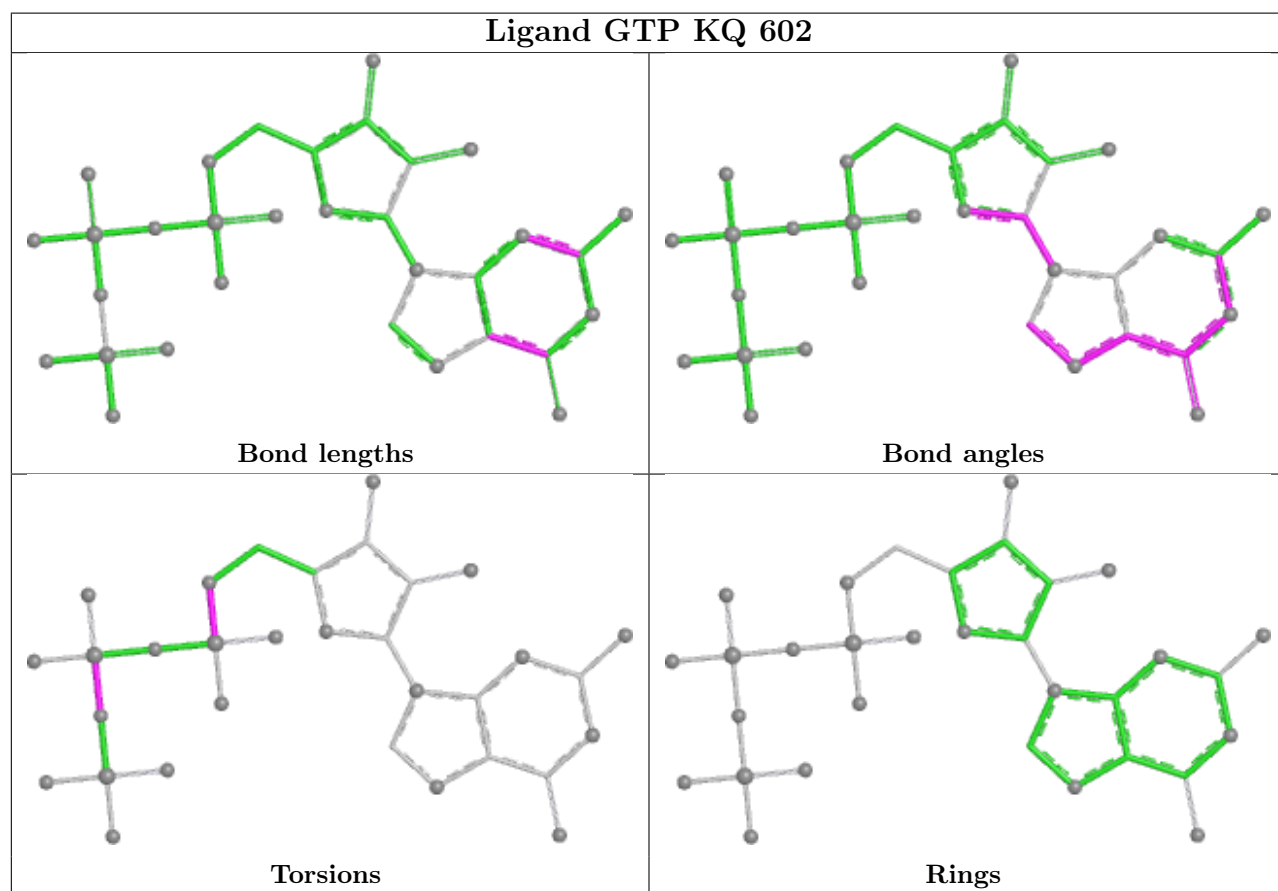
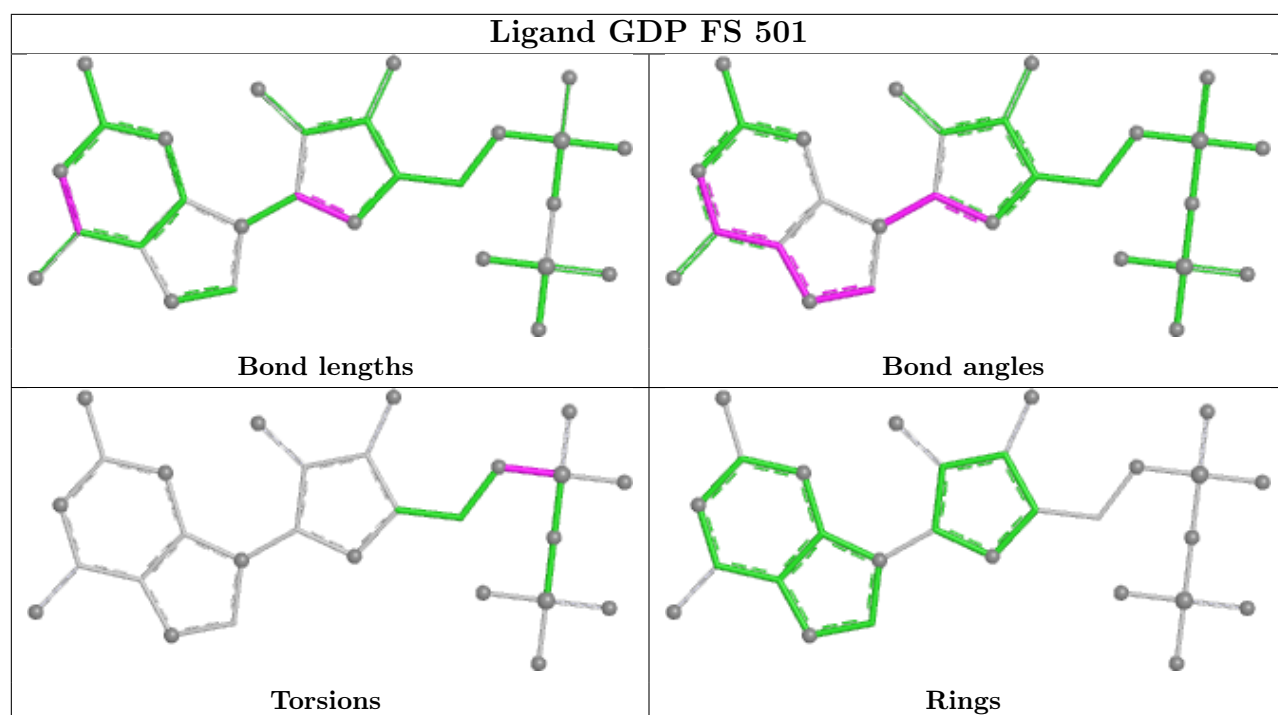




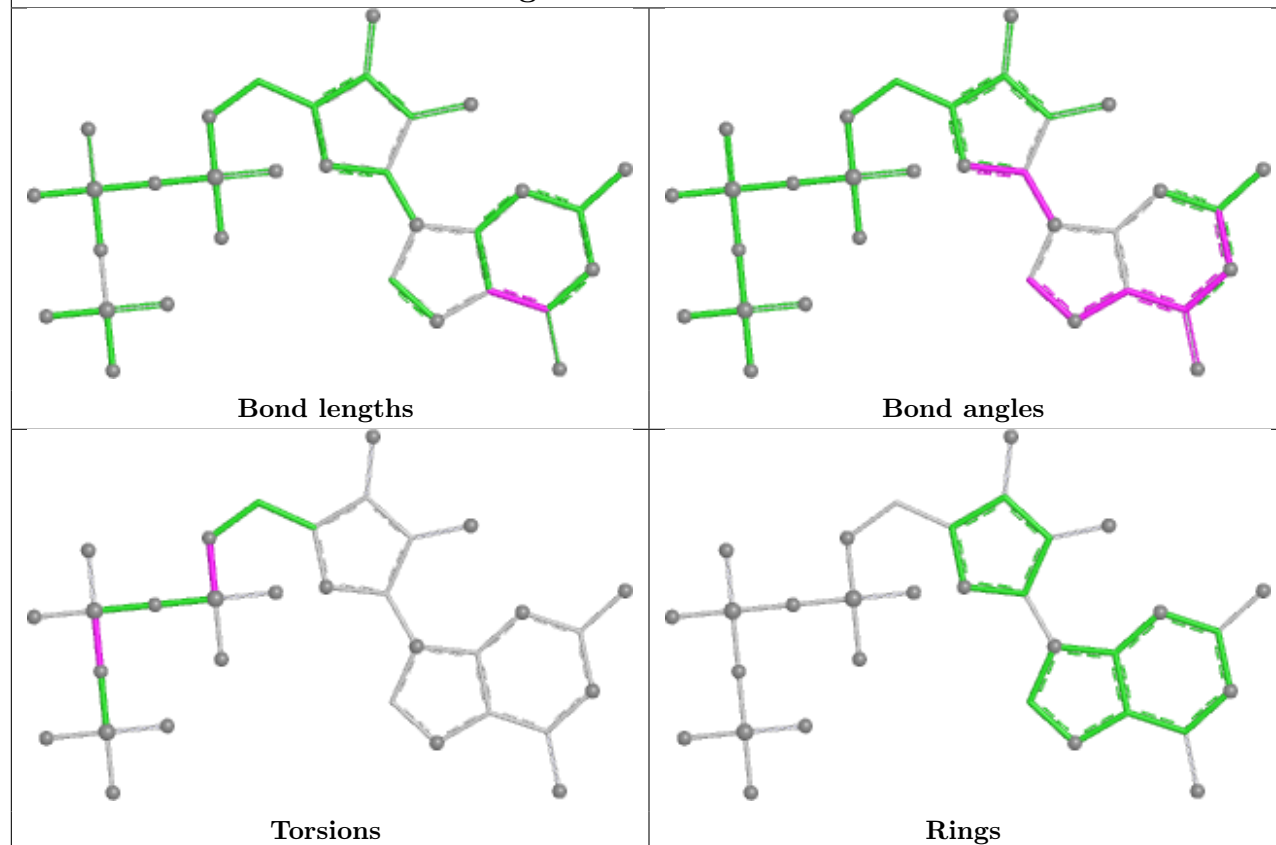




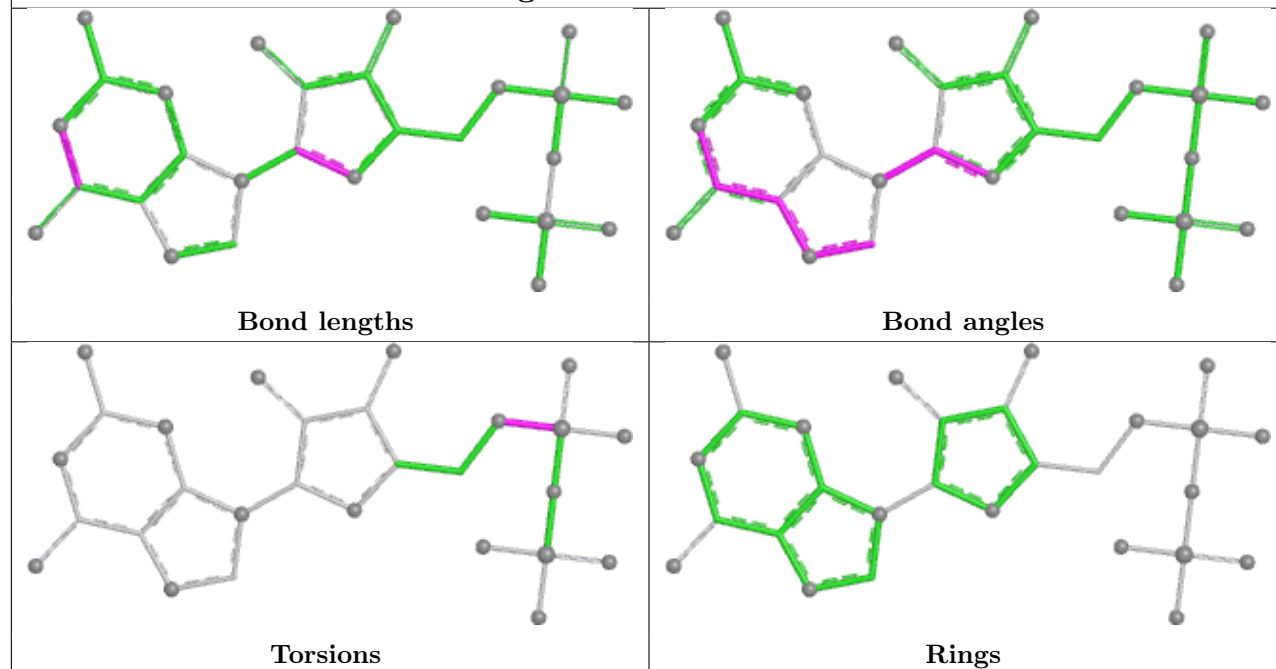




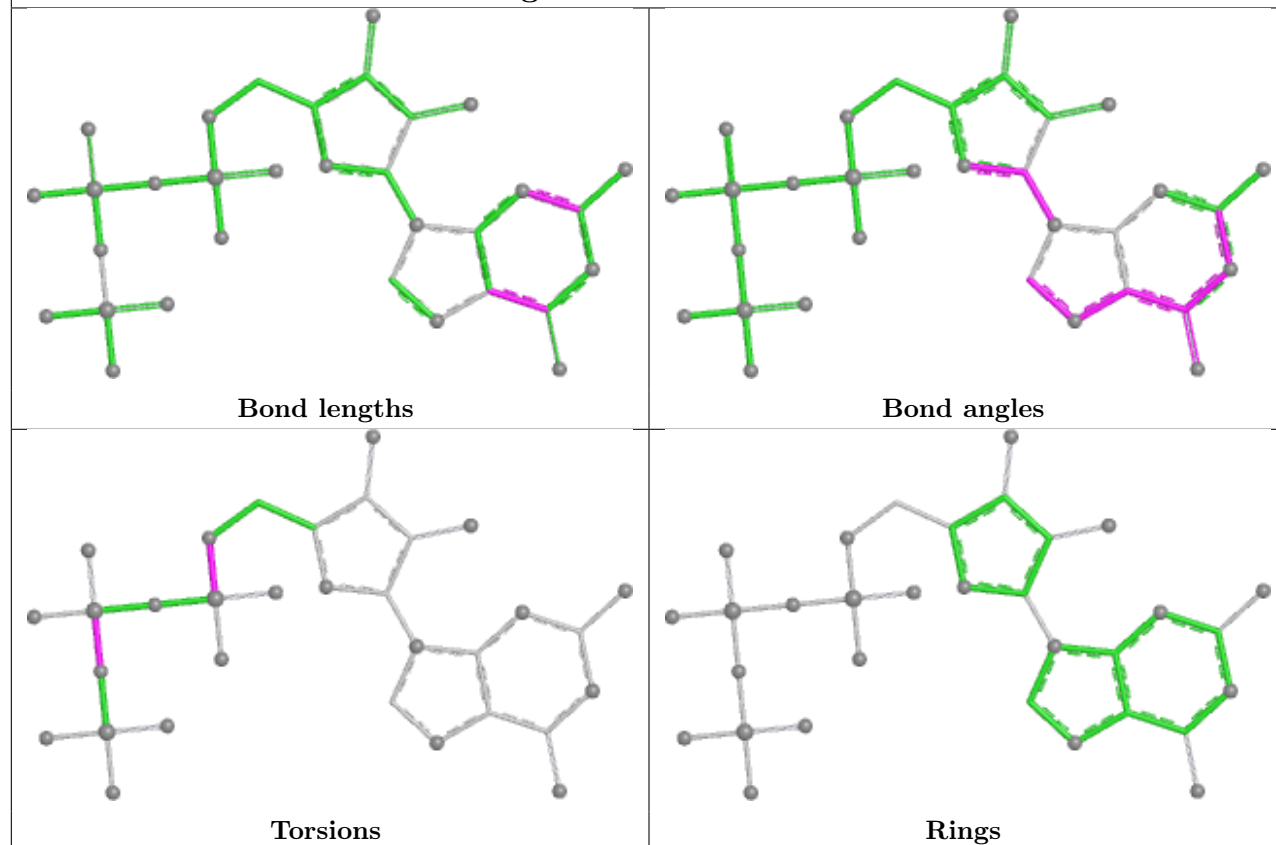
## Ligand GTP EB 501



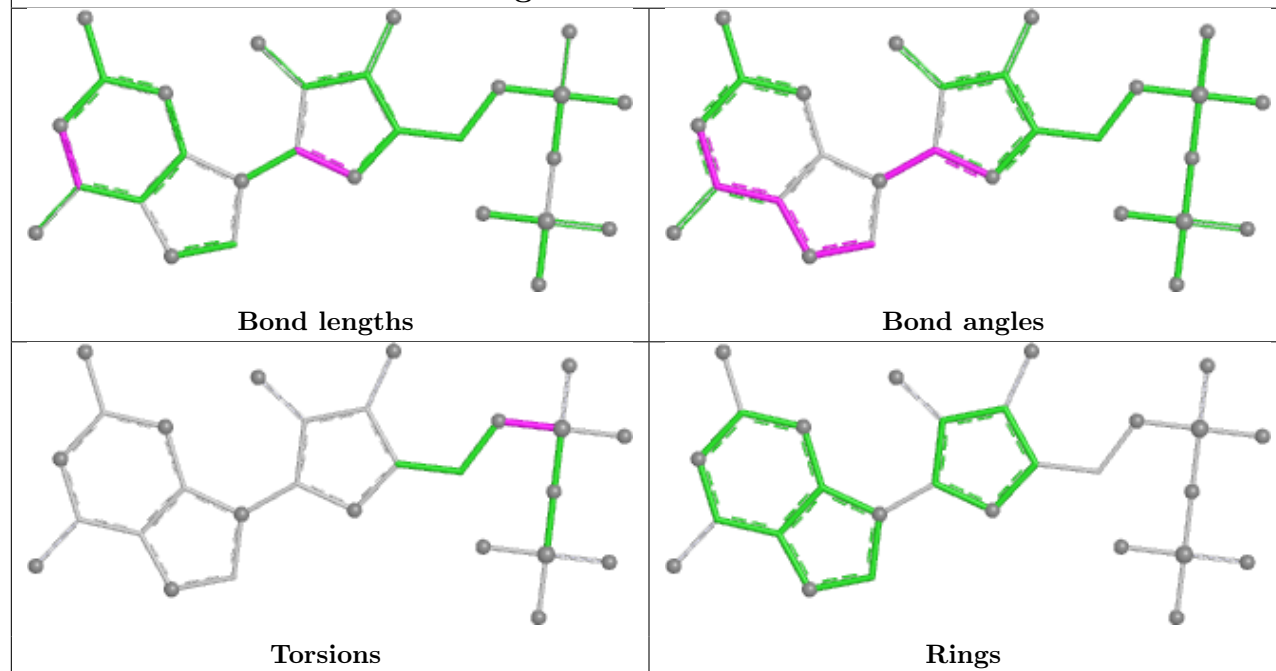
## Ligand GDP FG 501

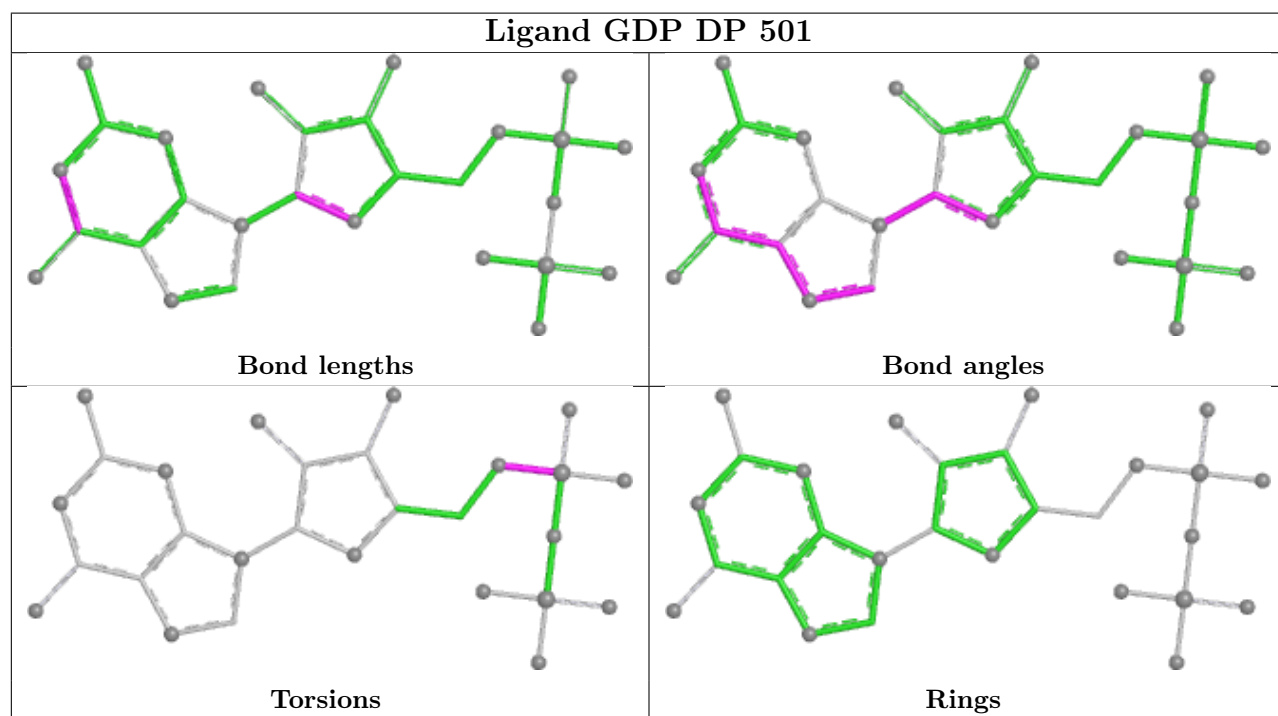
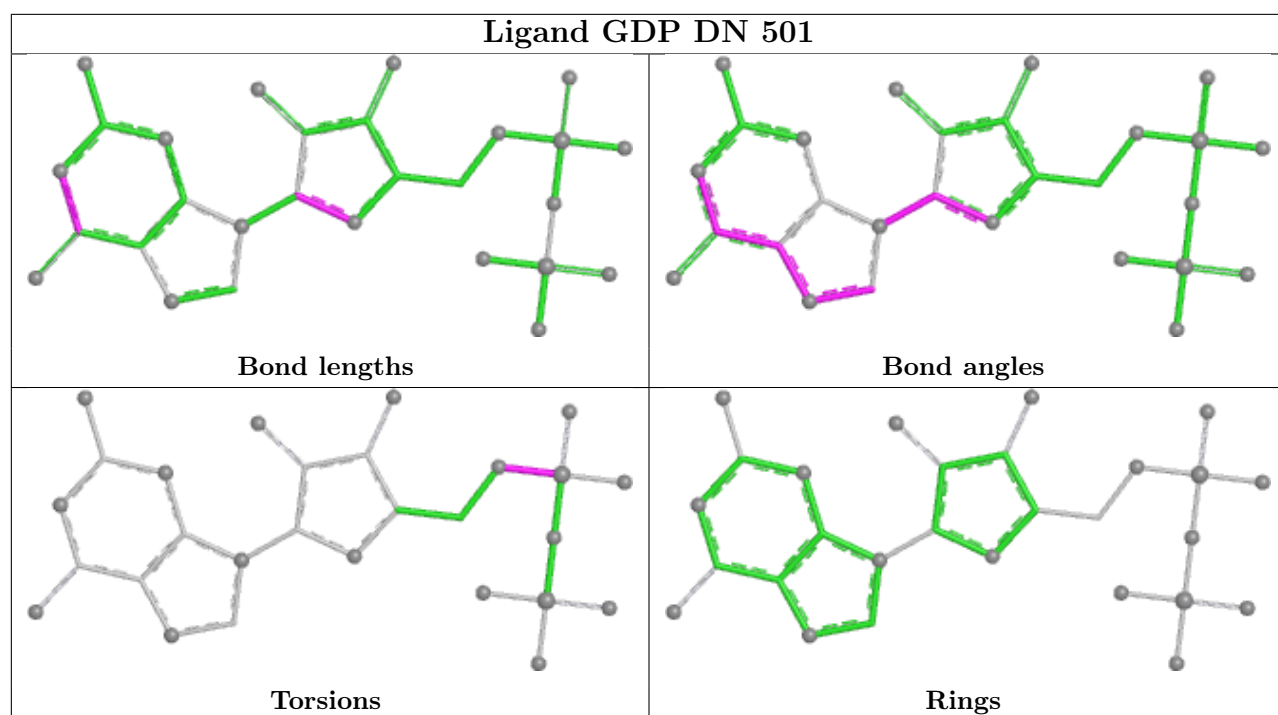


## Ligand GTP JY 602

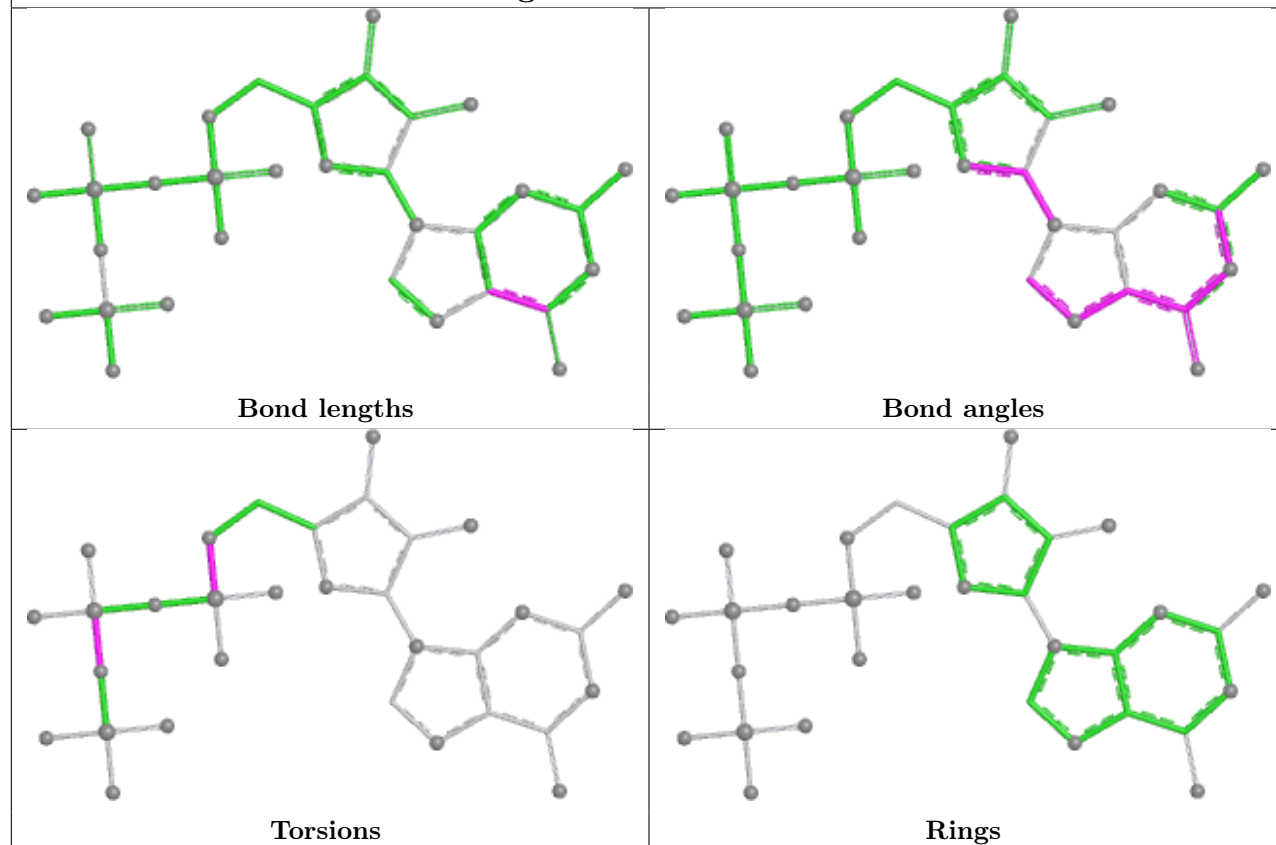


## Ligand GDP GX 501

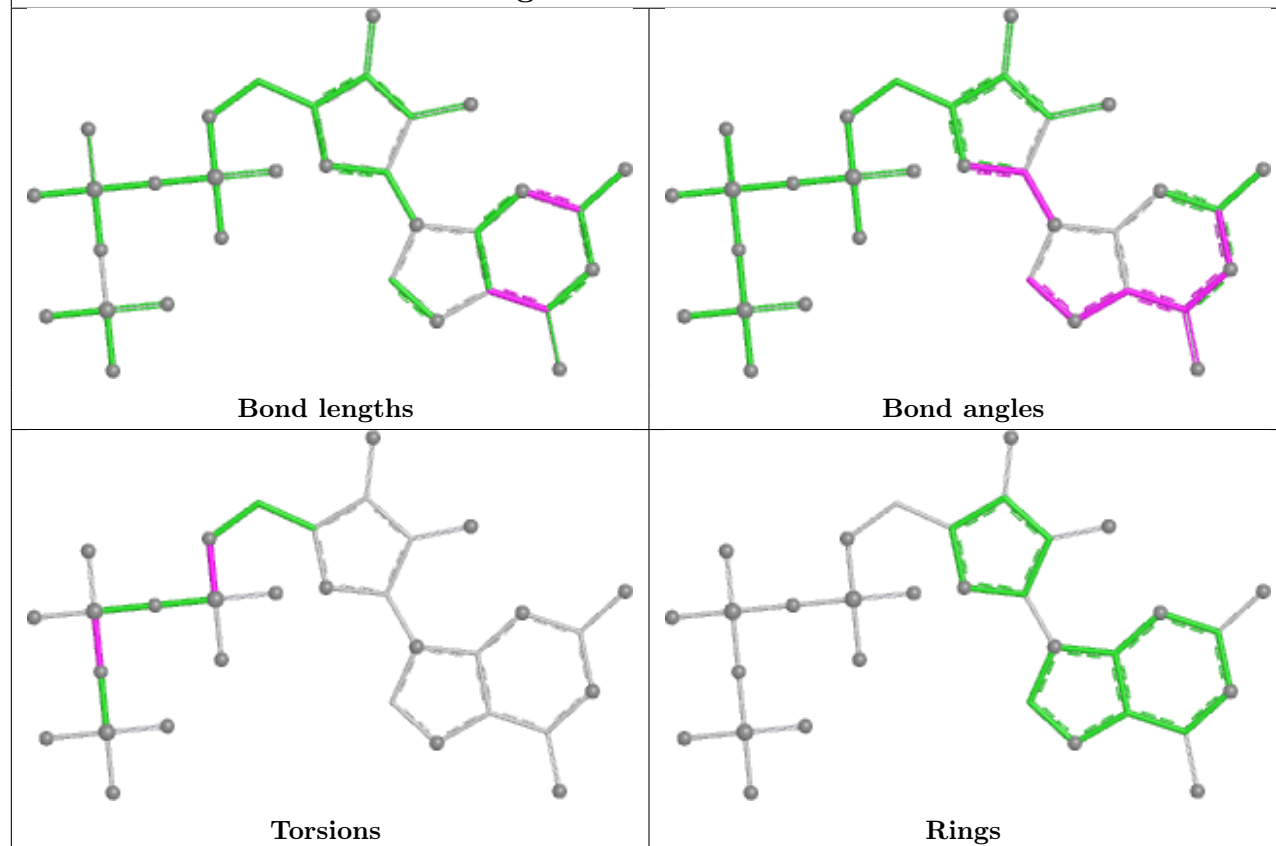




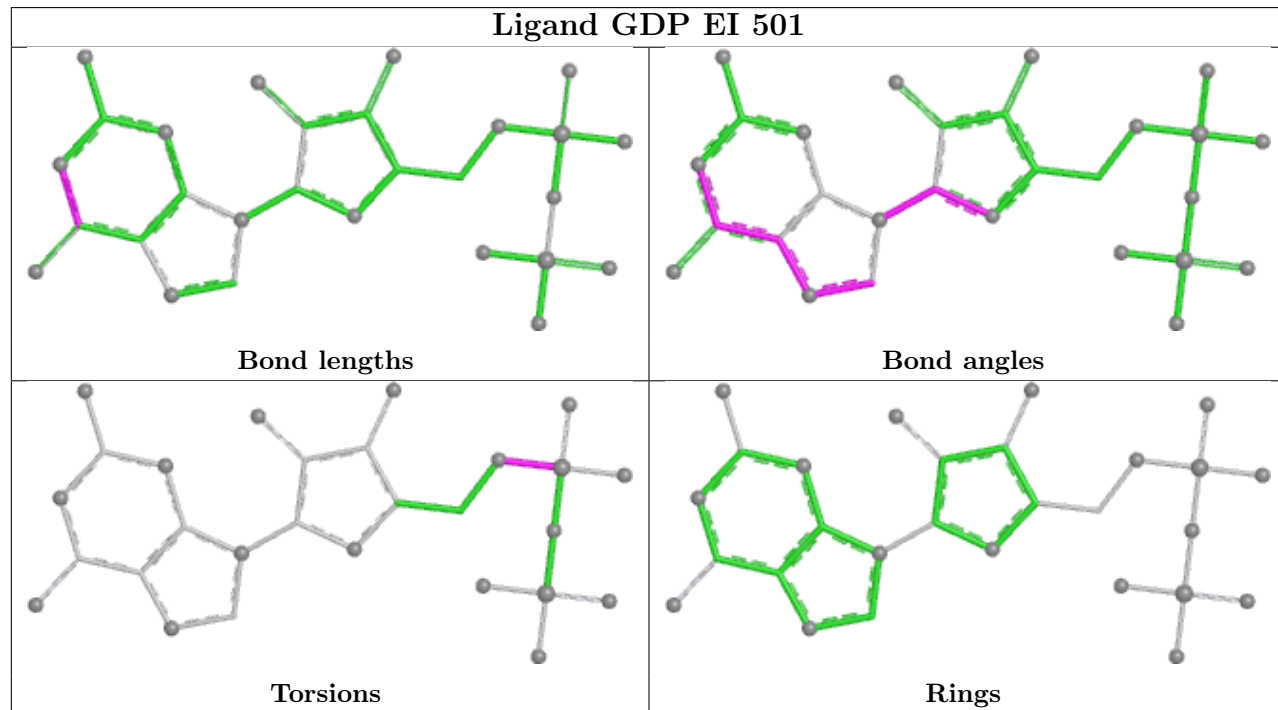
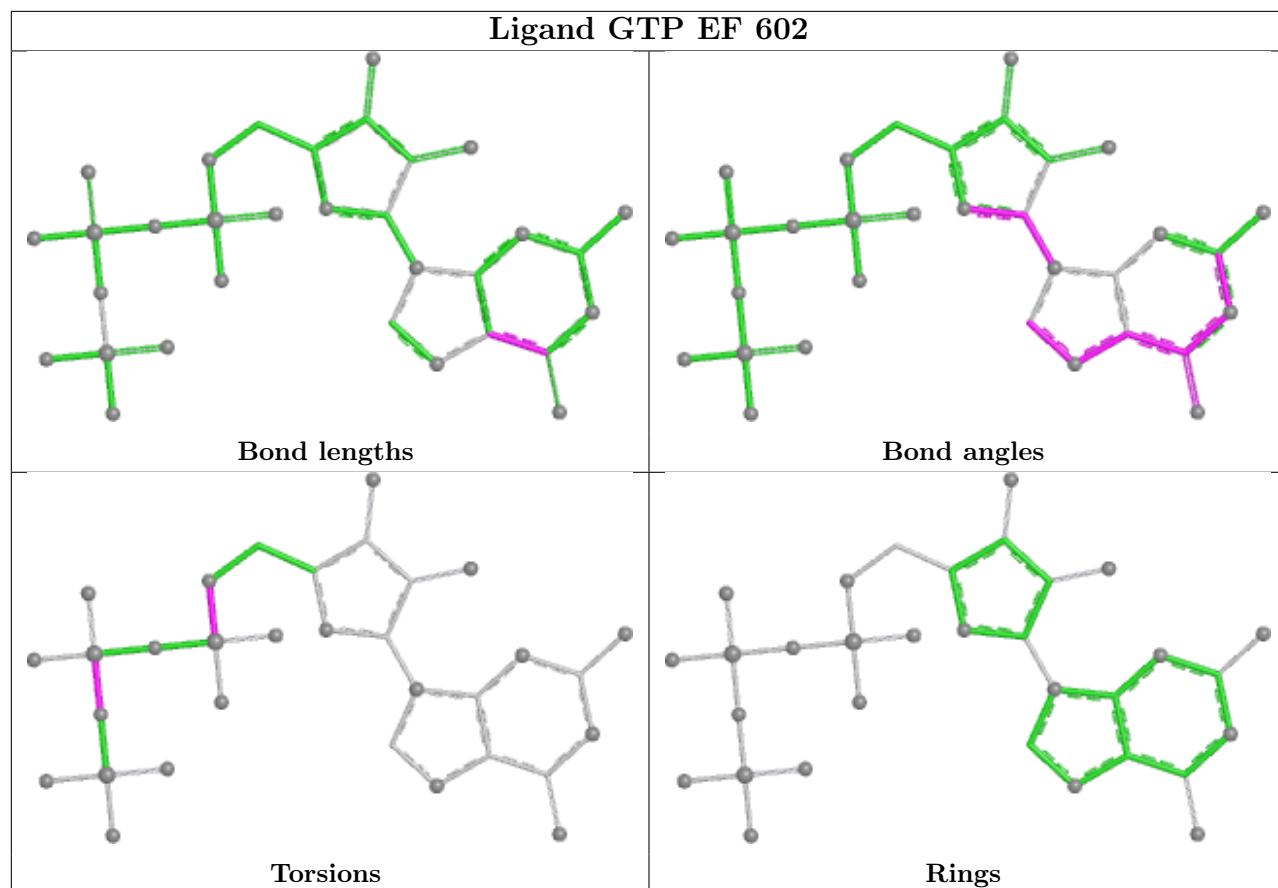
## Ligand GTP AC 501

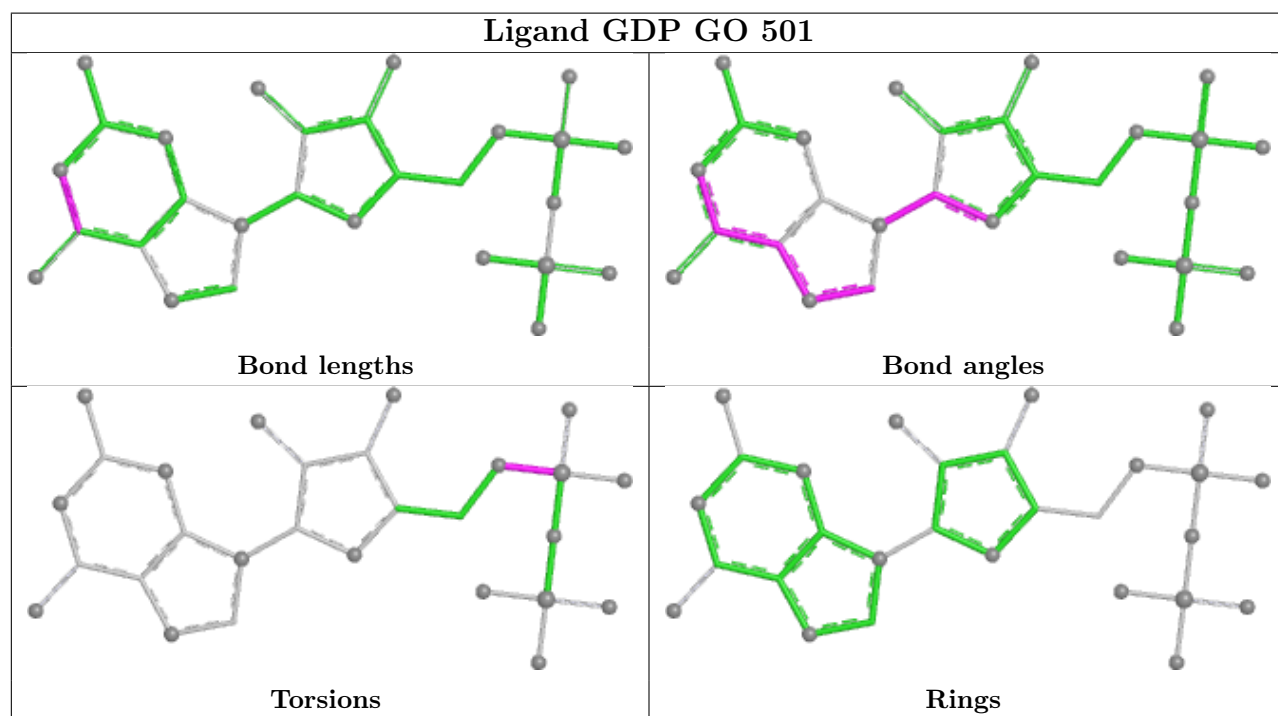
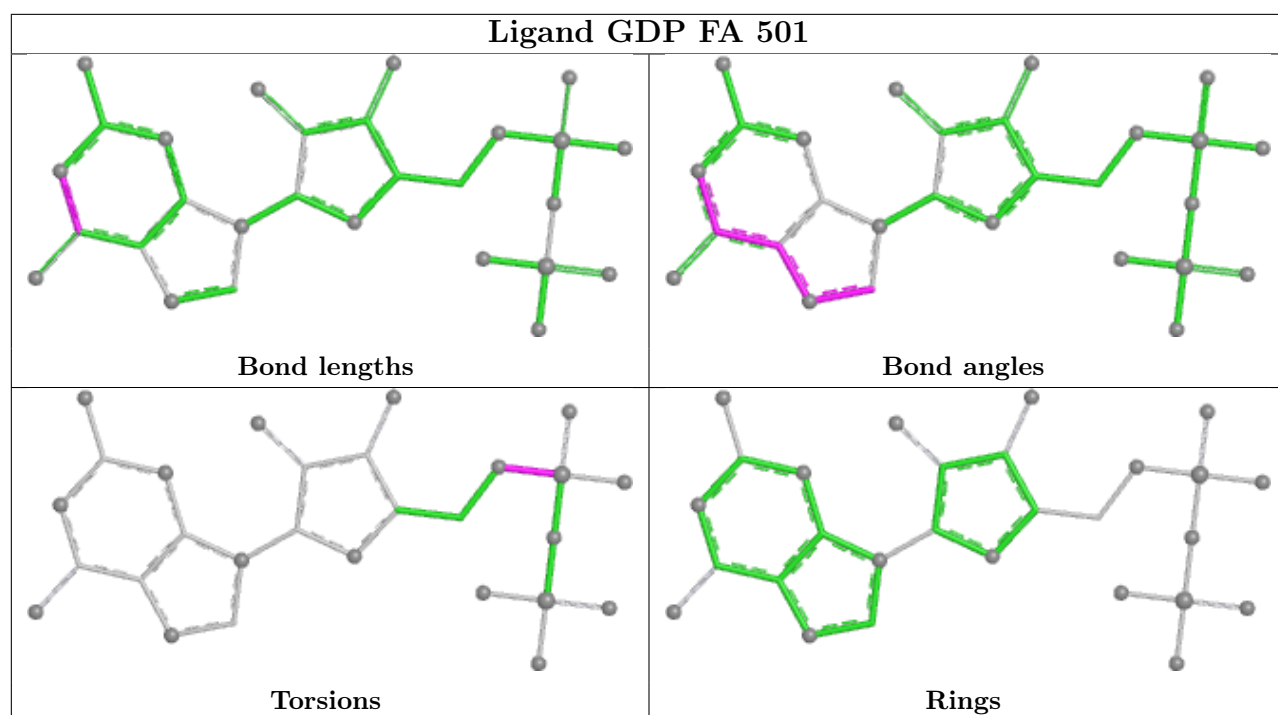


## Ligand GTP AU 501

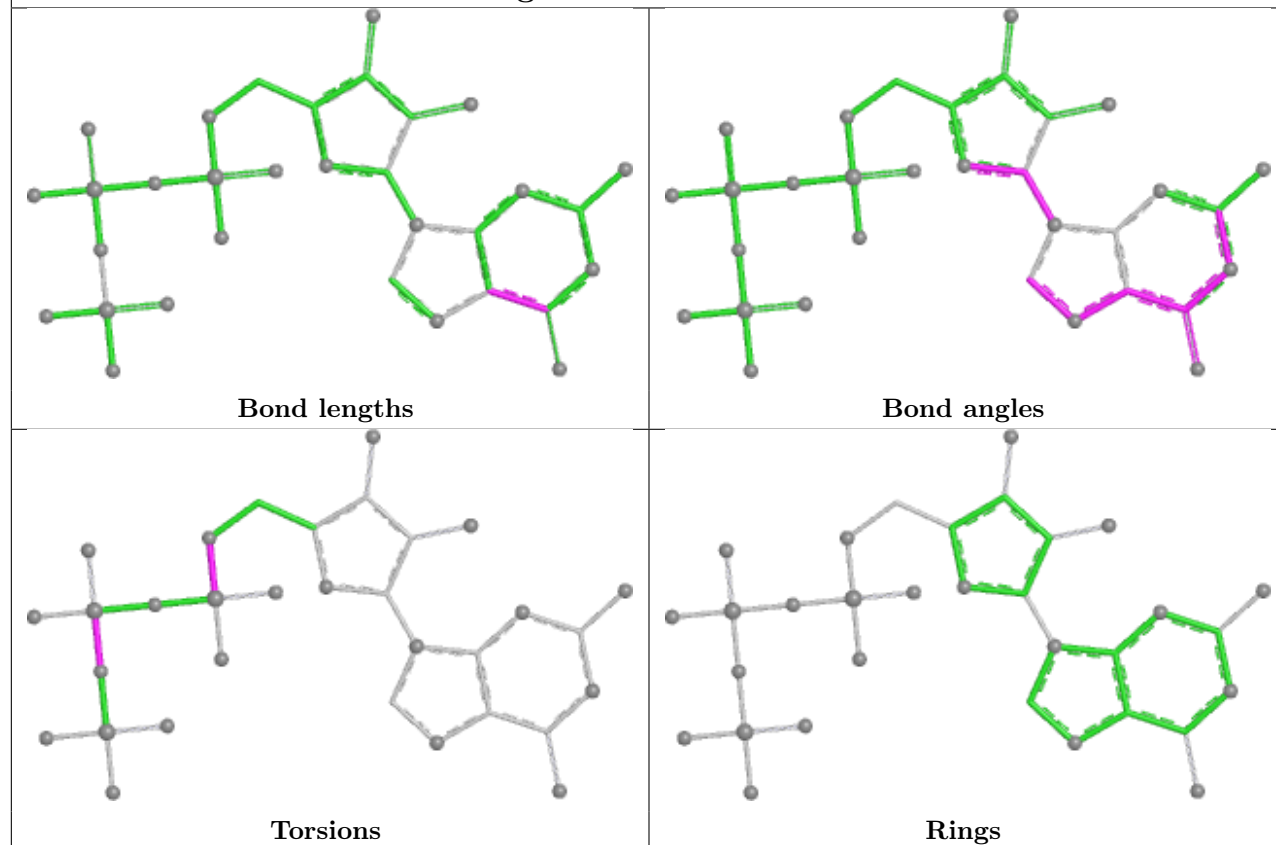




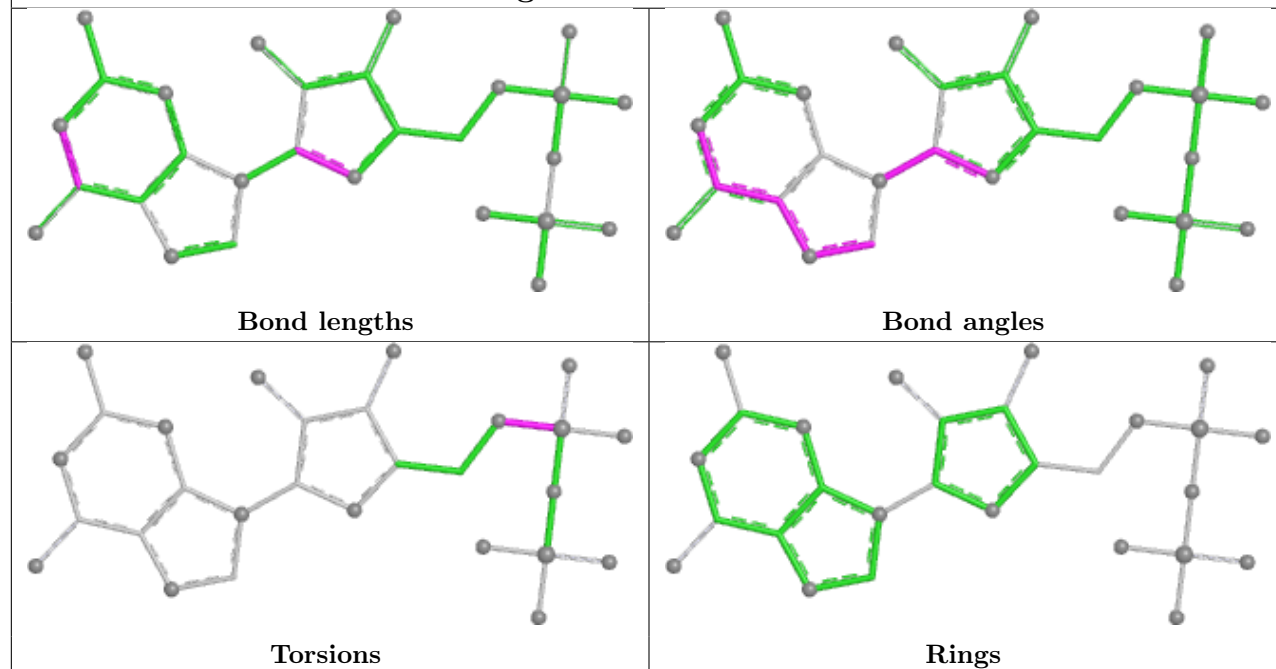




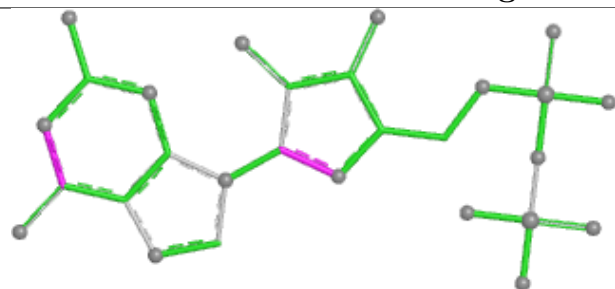
## Ligand GTP DX 501



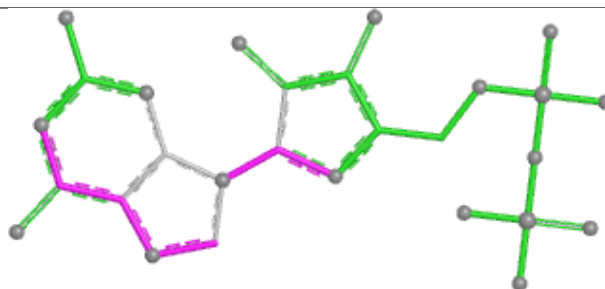
## Ligand GDP HF 501



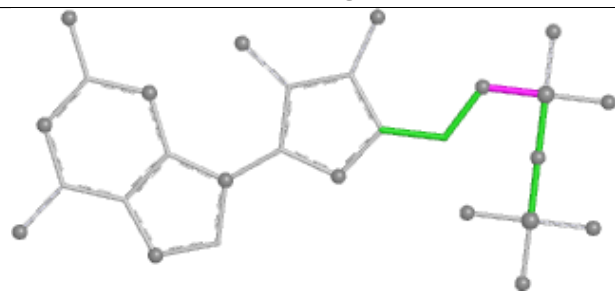
## Ligand GDP HN 501



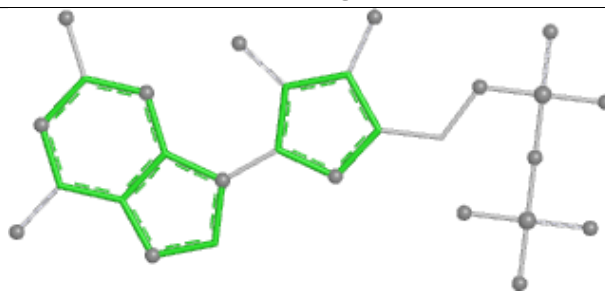
Bond lengths



Bond angles

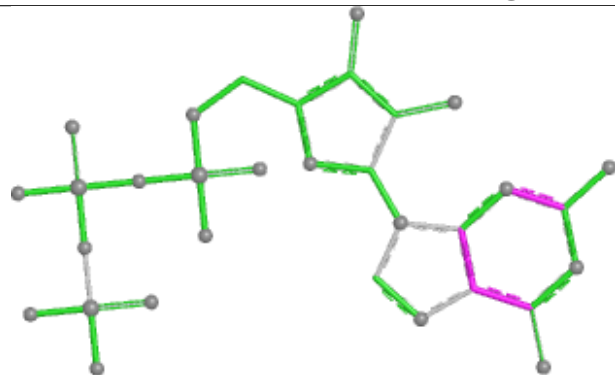


Torsions

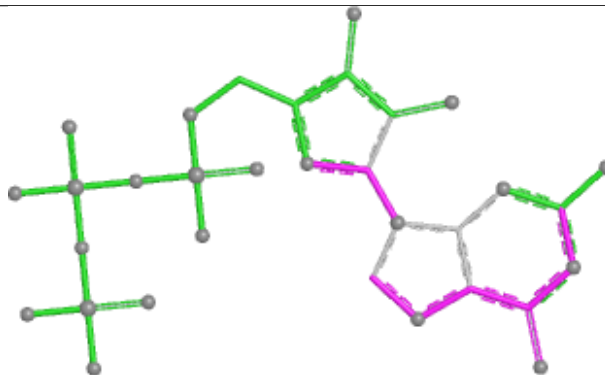


Rings

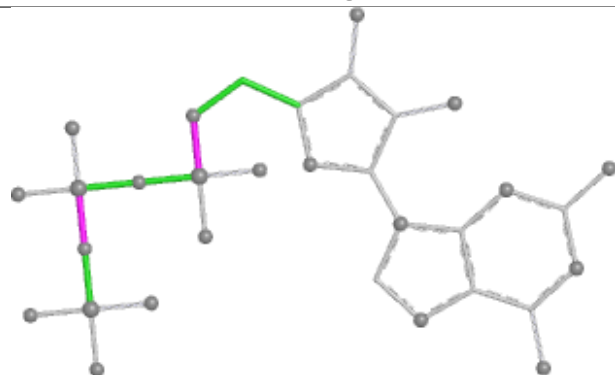
## Ligand GTP FU 602



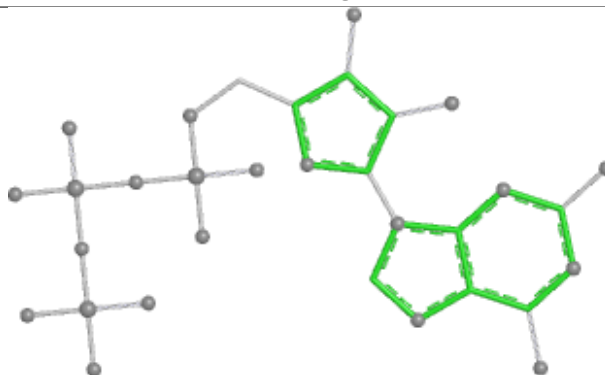
Bond lengths



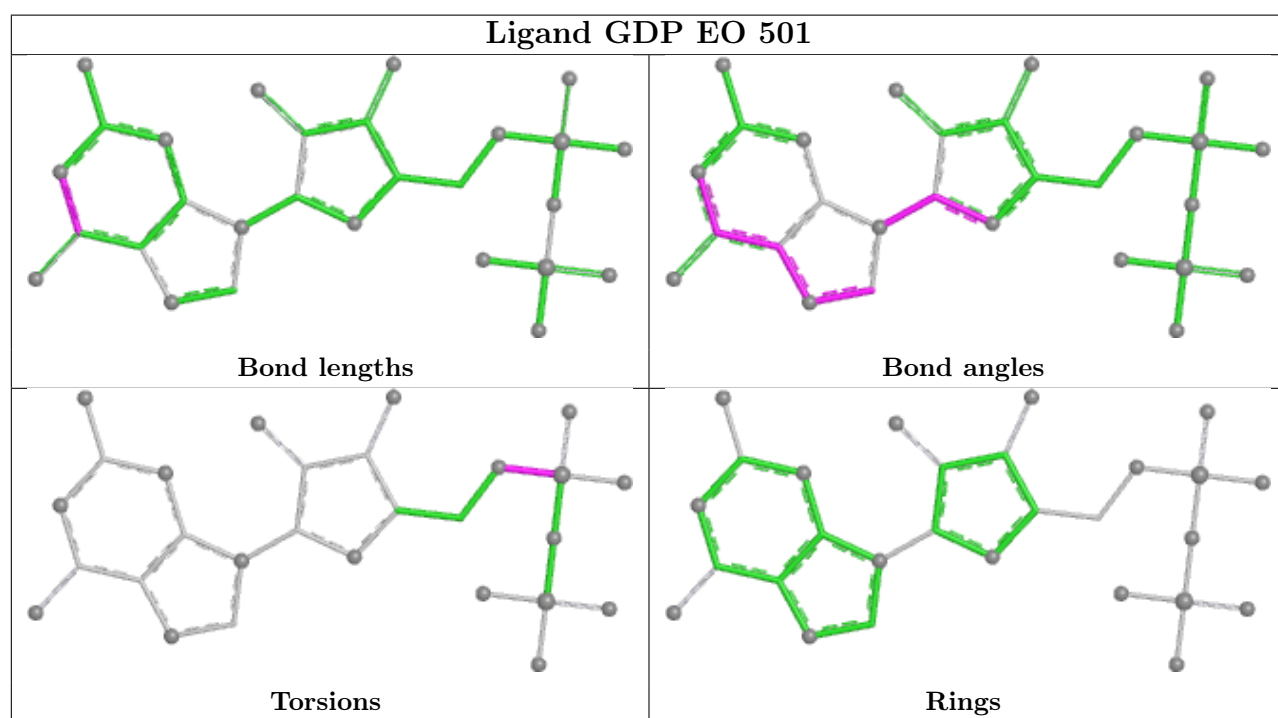
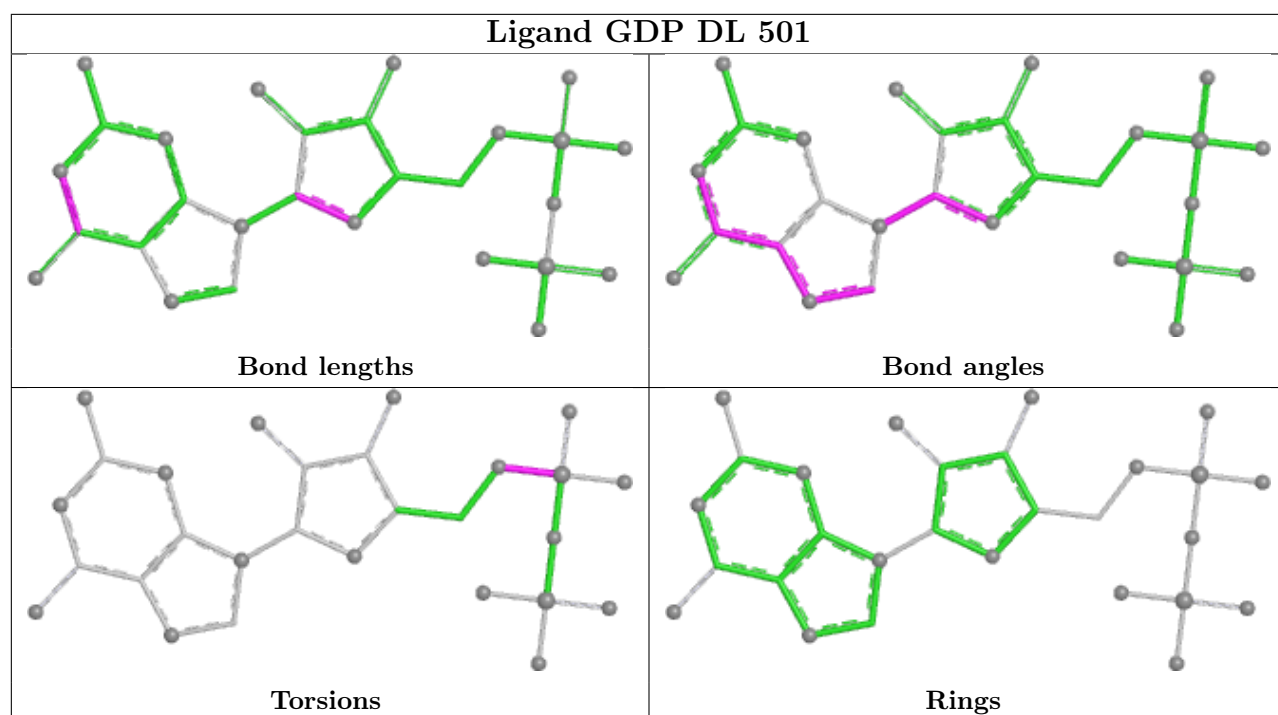
Bond angles

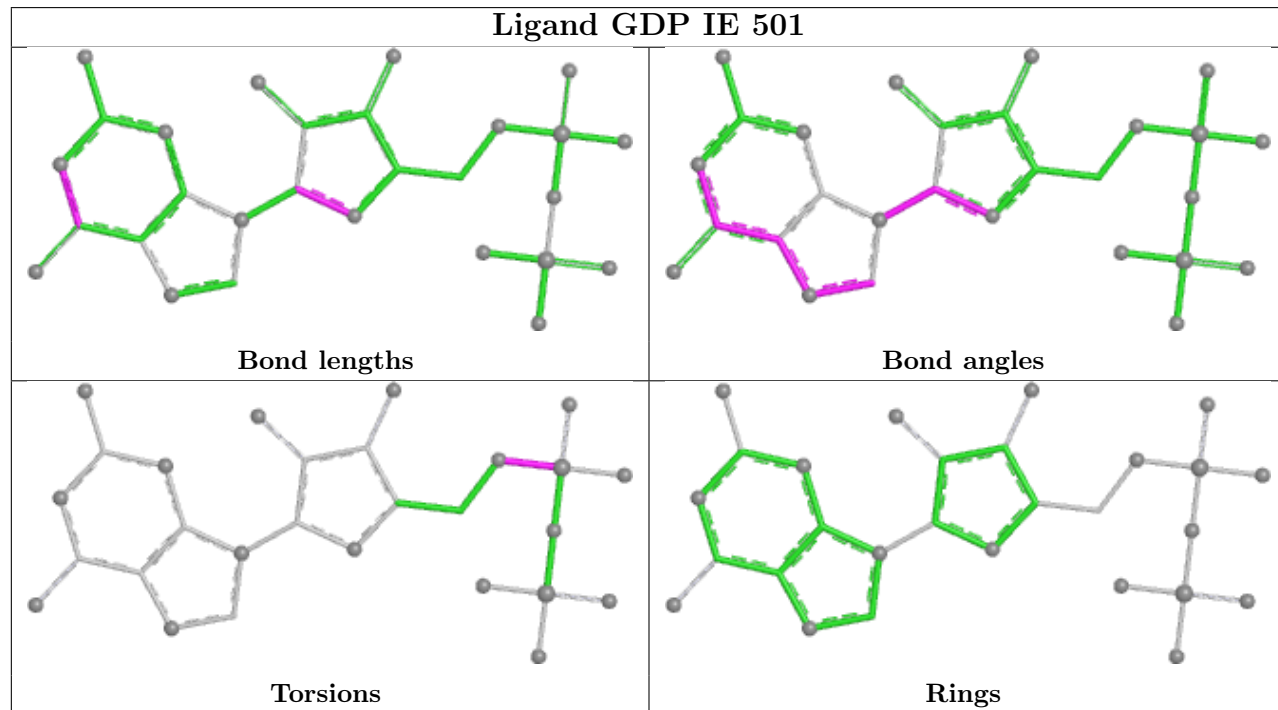
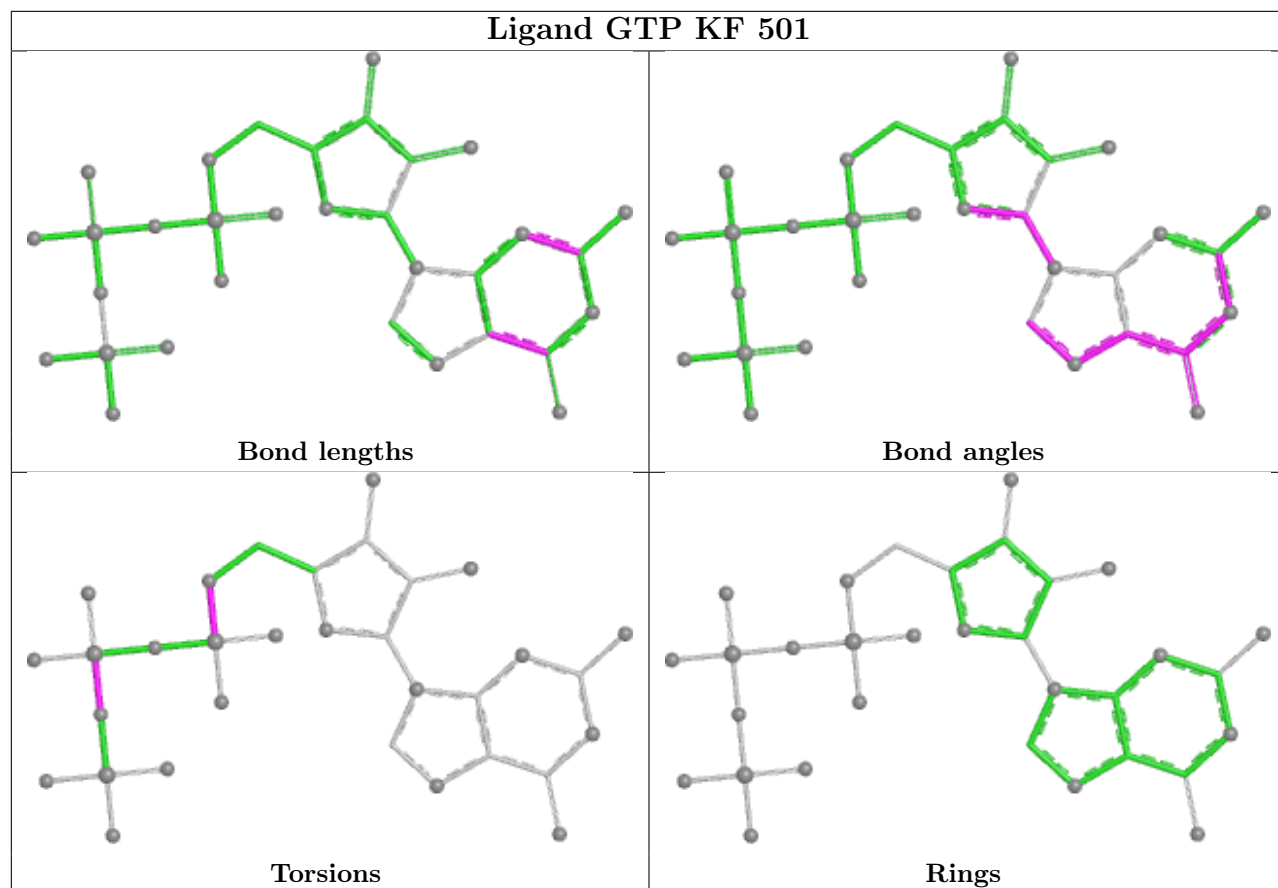


Torsions

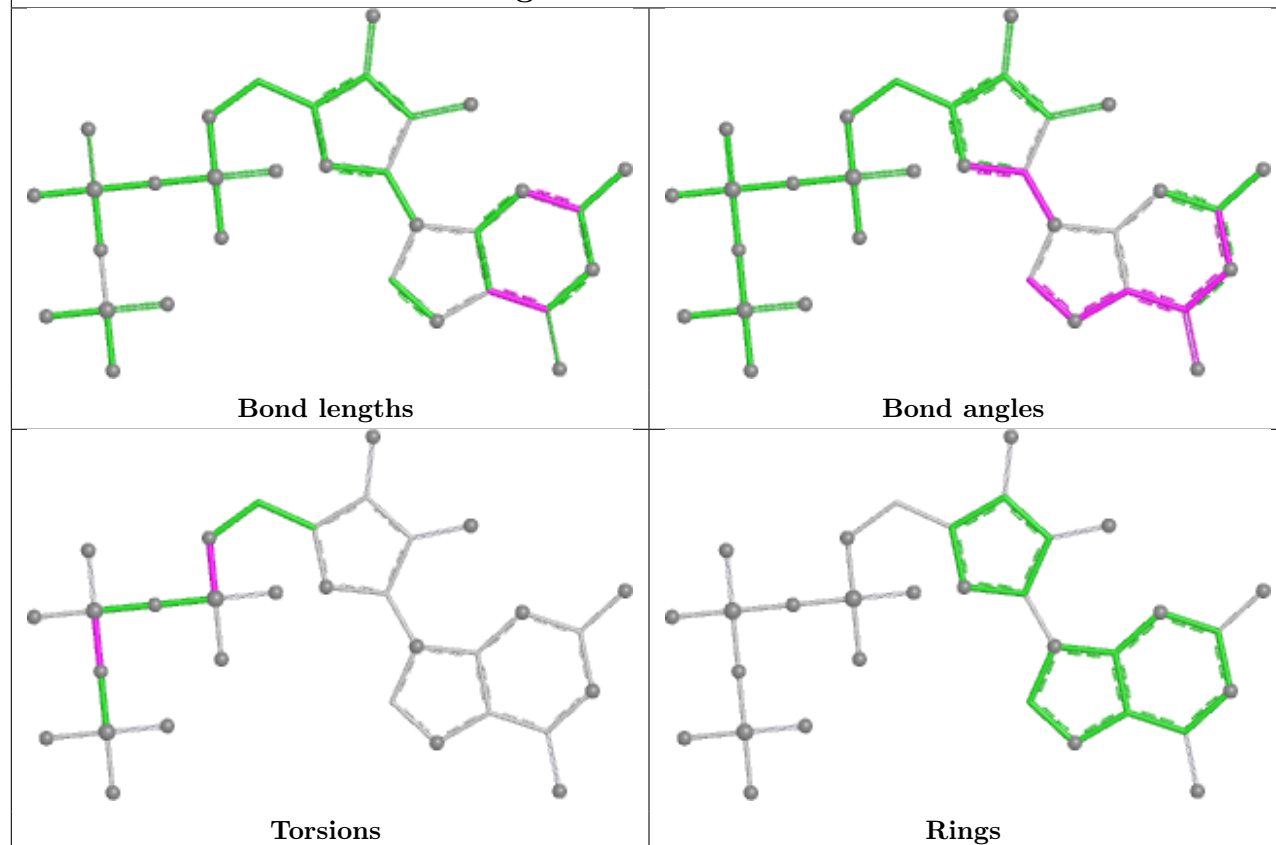


Rings

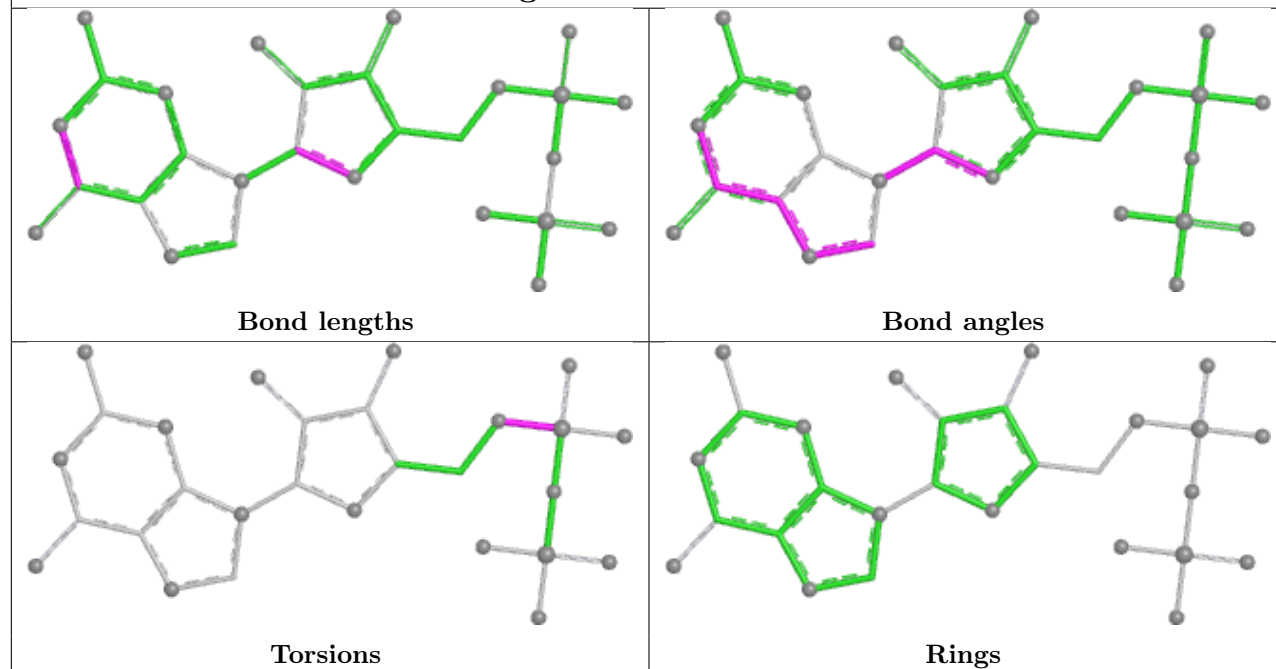


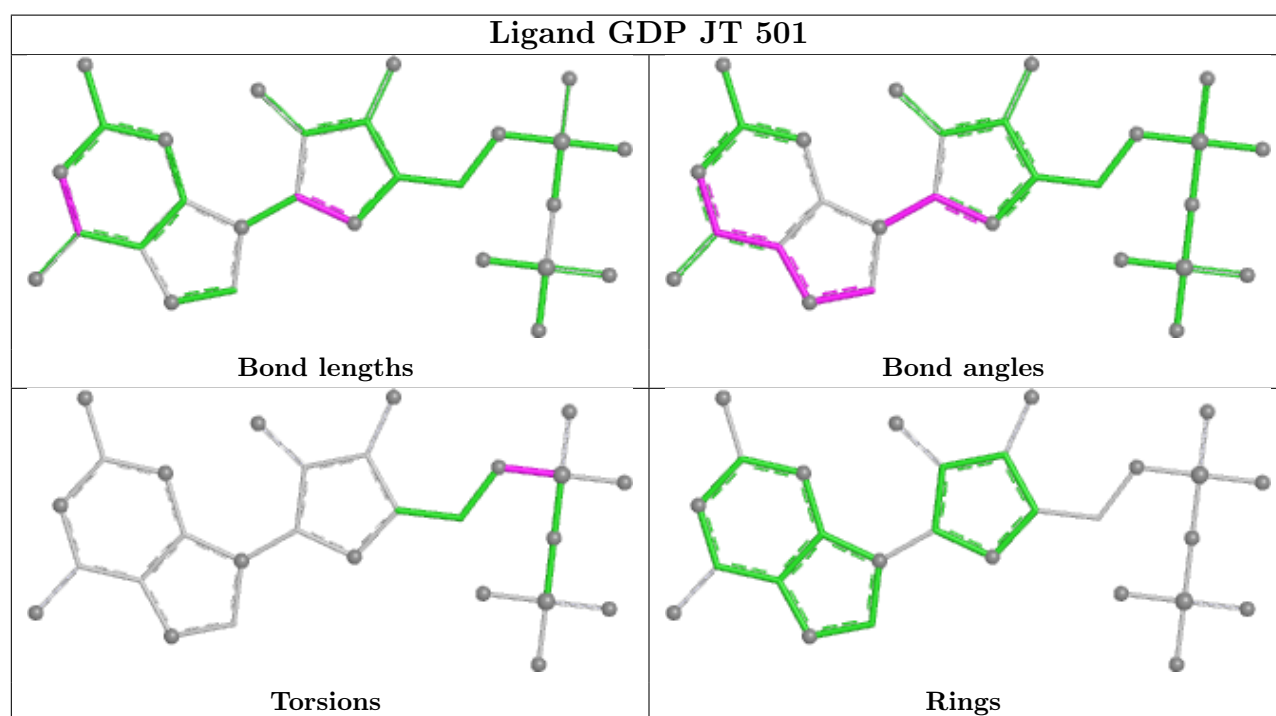
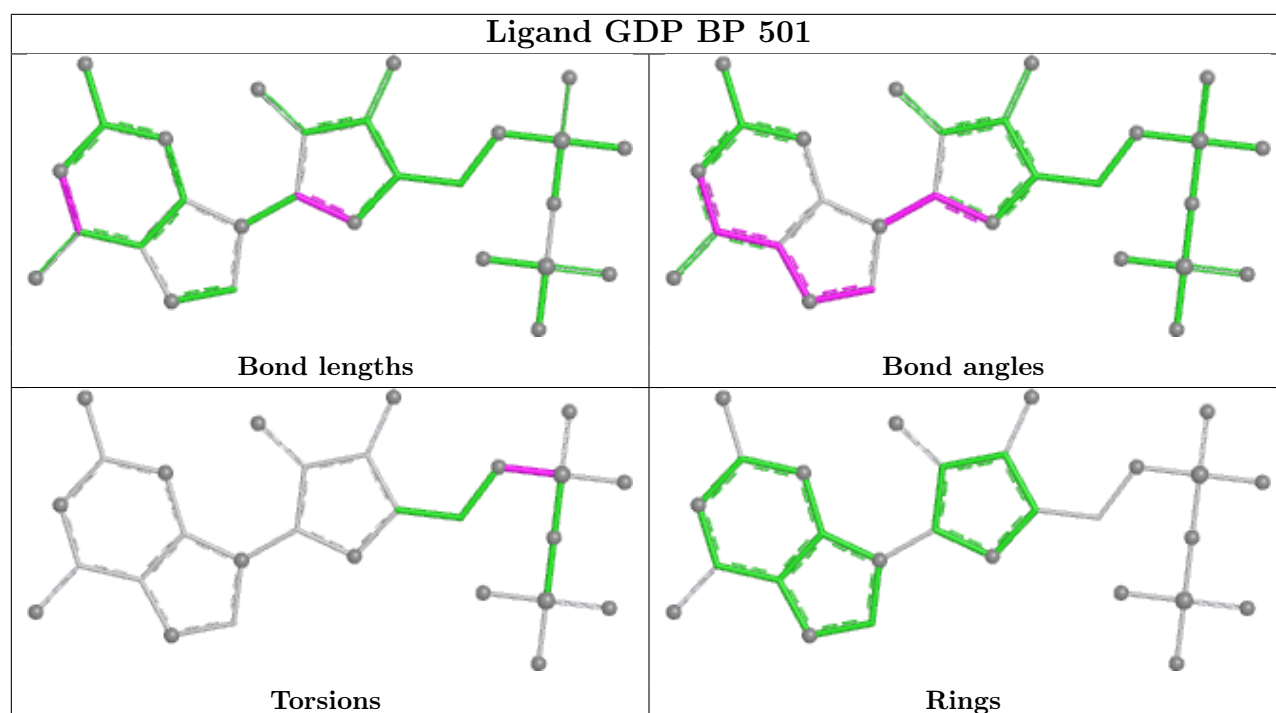


## Ligand GTP DU 602



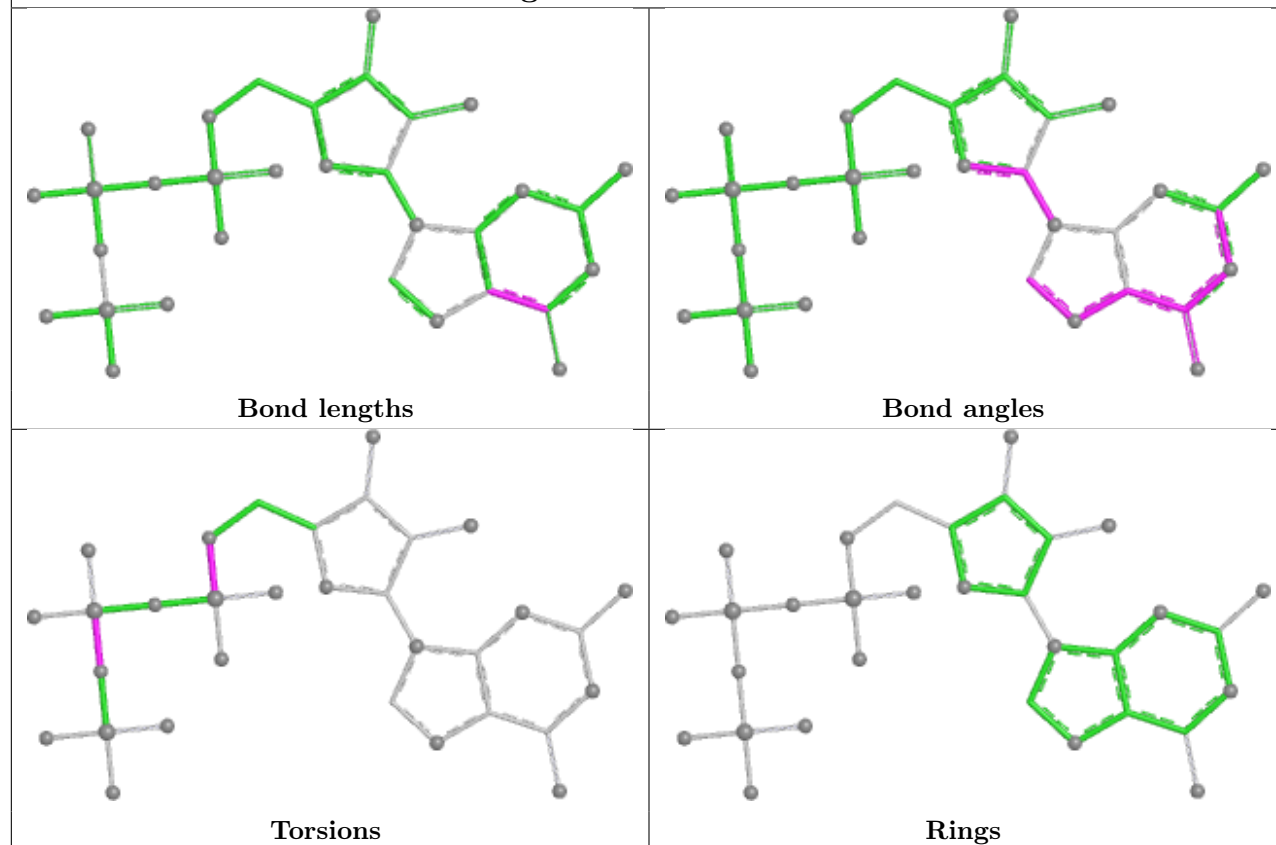
## Ligand GDP FE 501



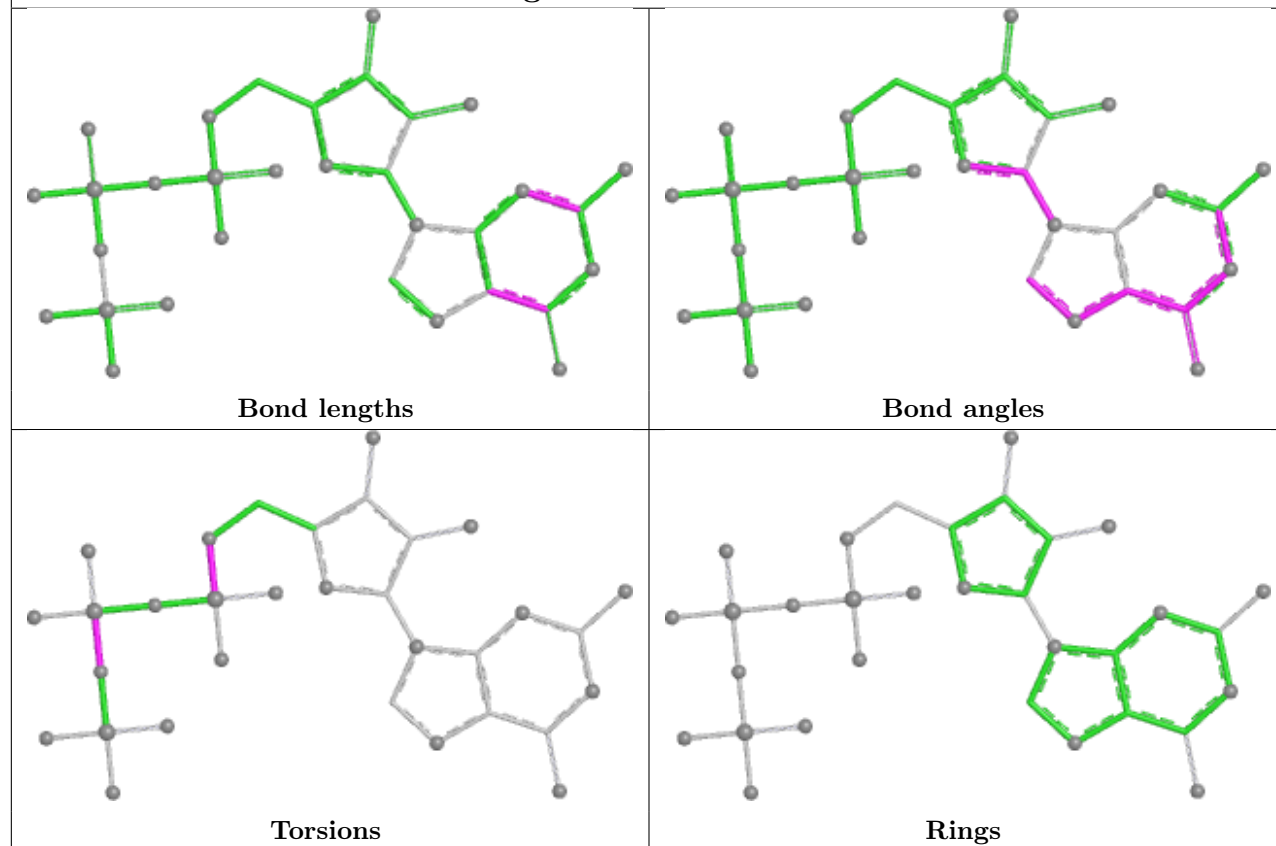


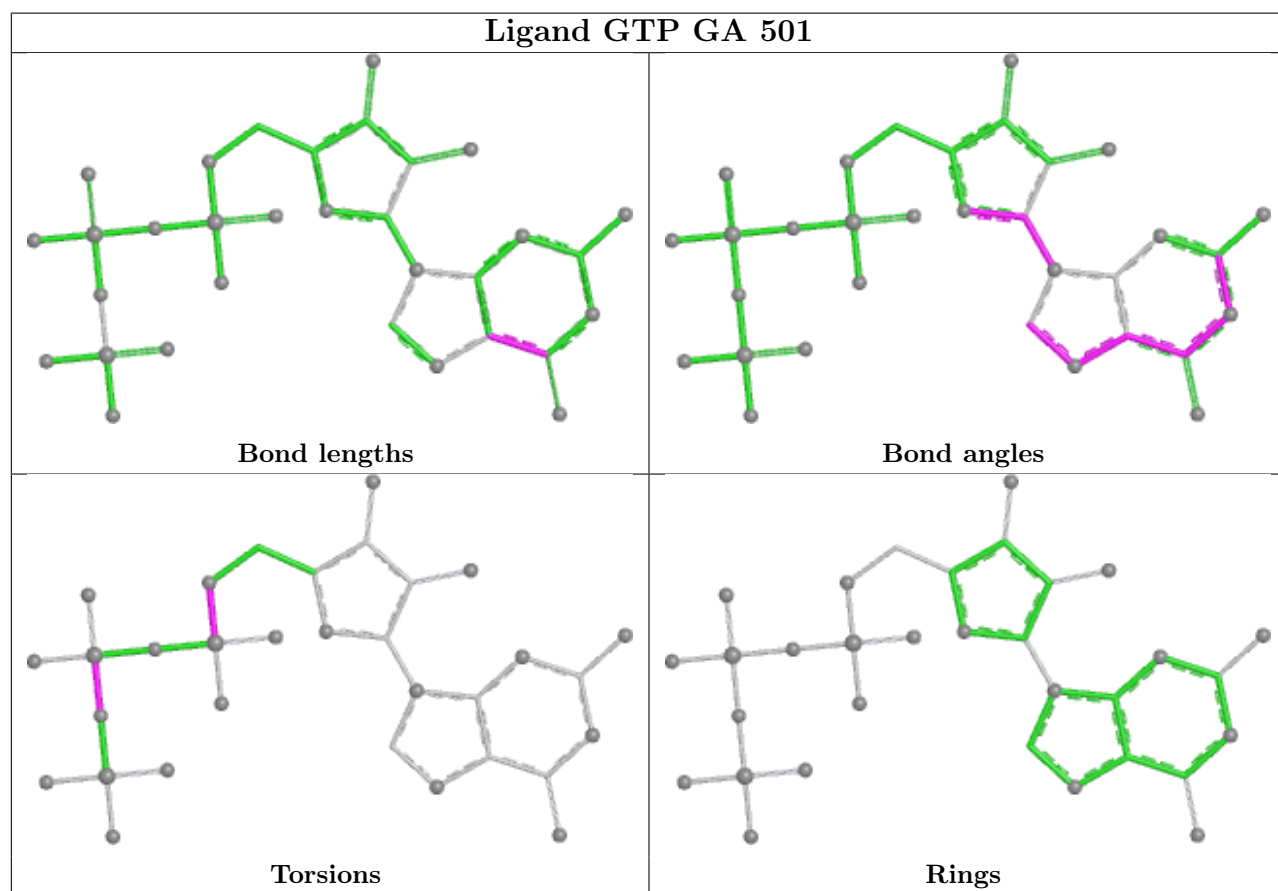
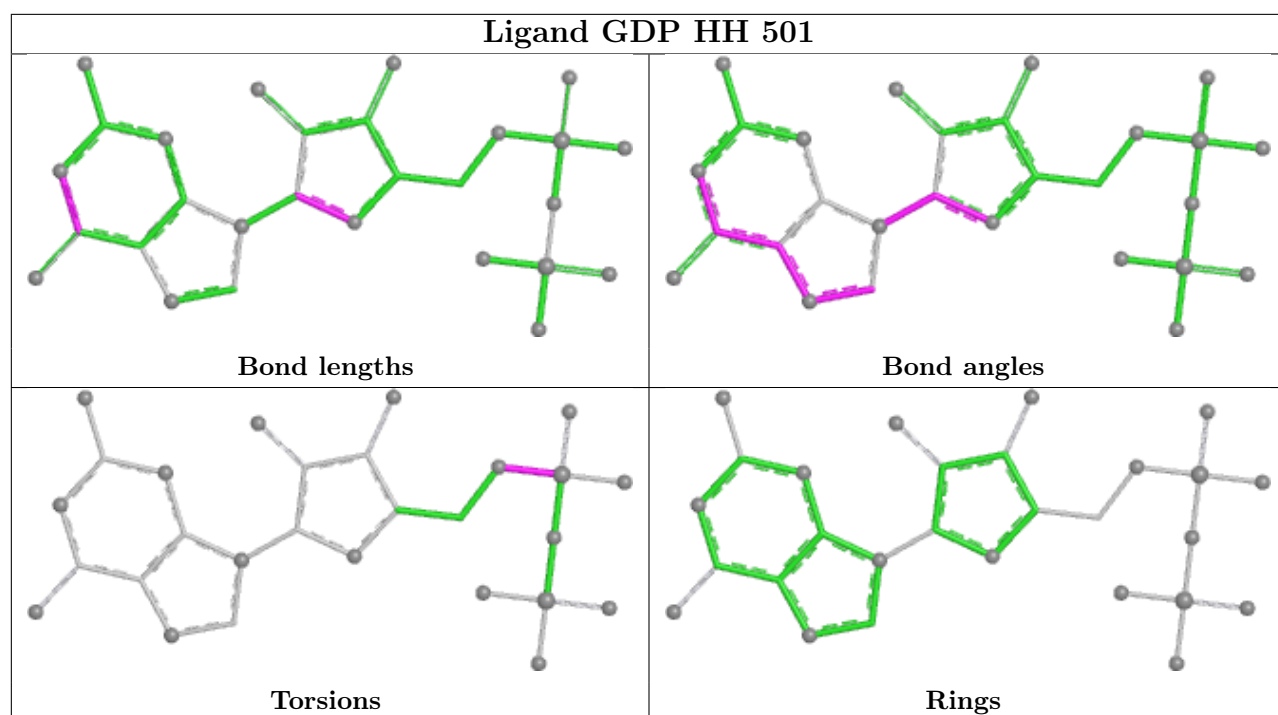


## Ligand GTP JD 501

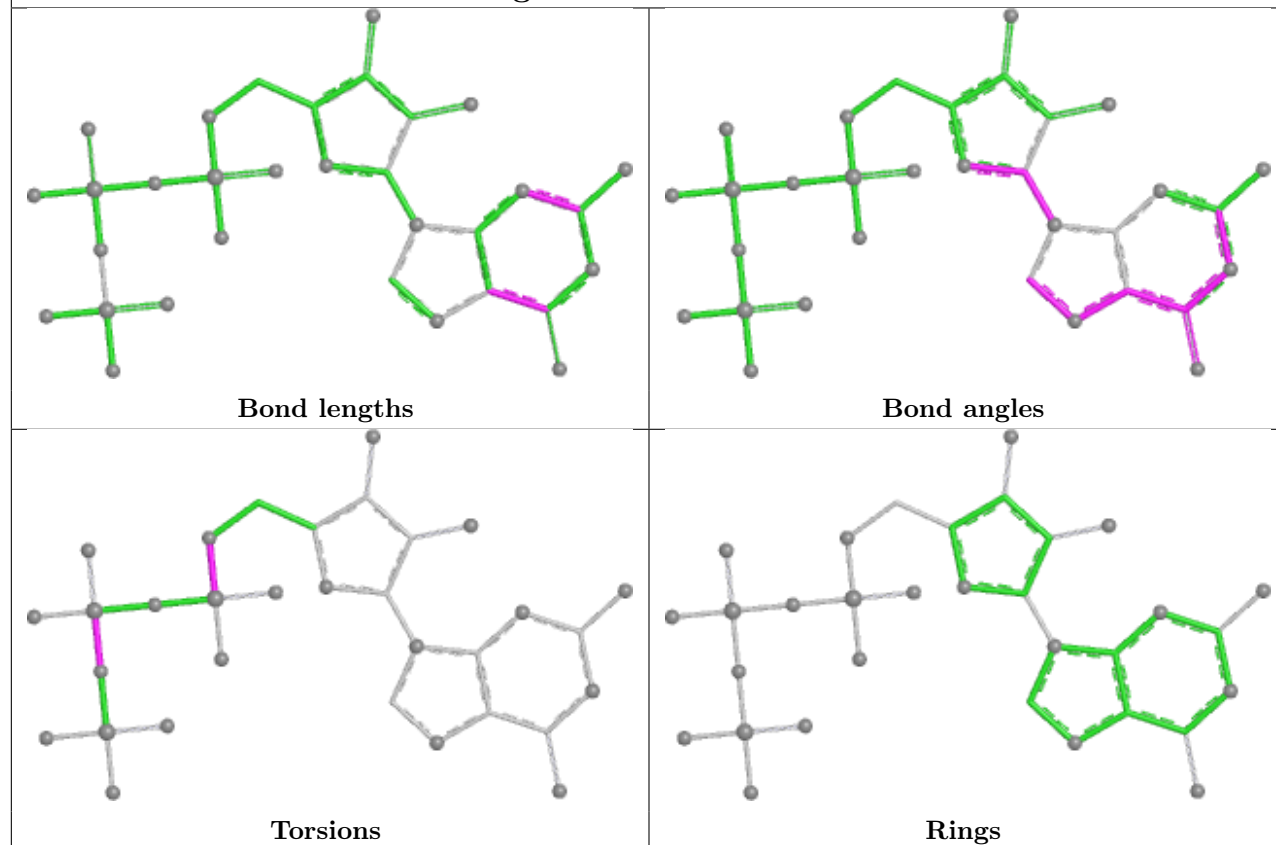


## Ligand GTP IV 602

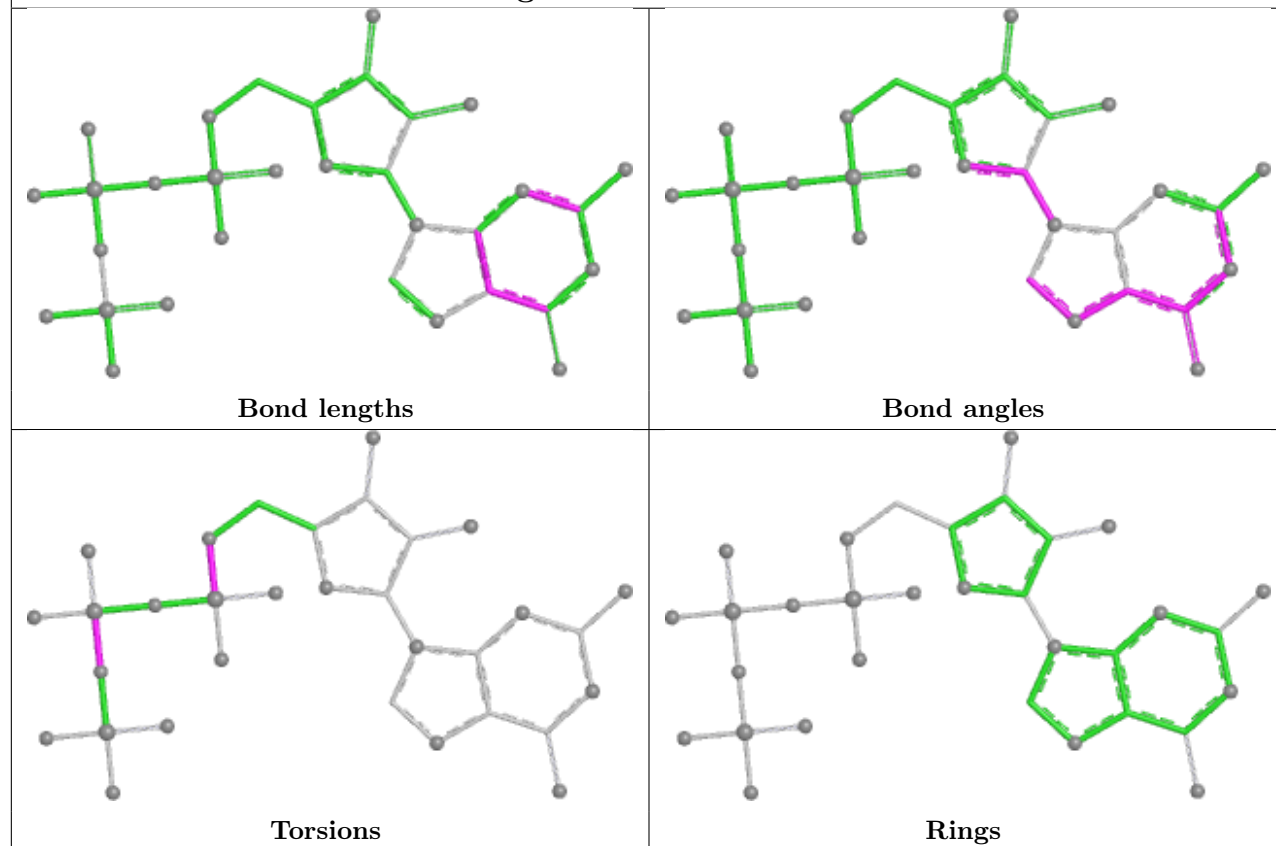


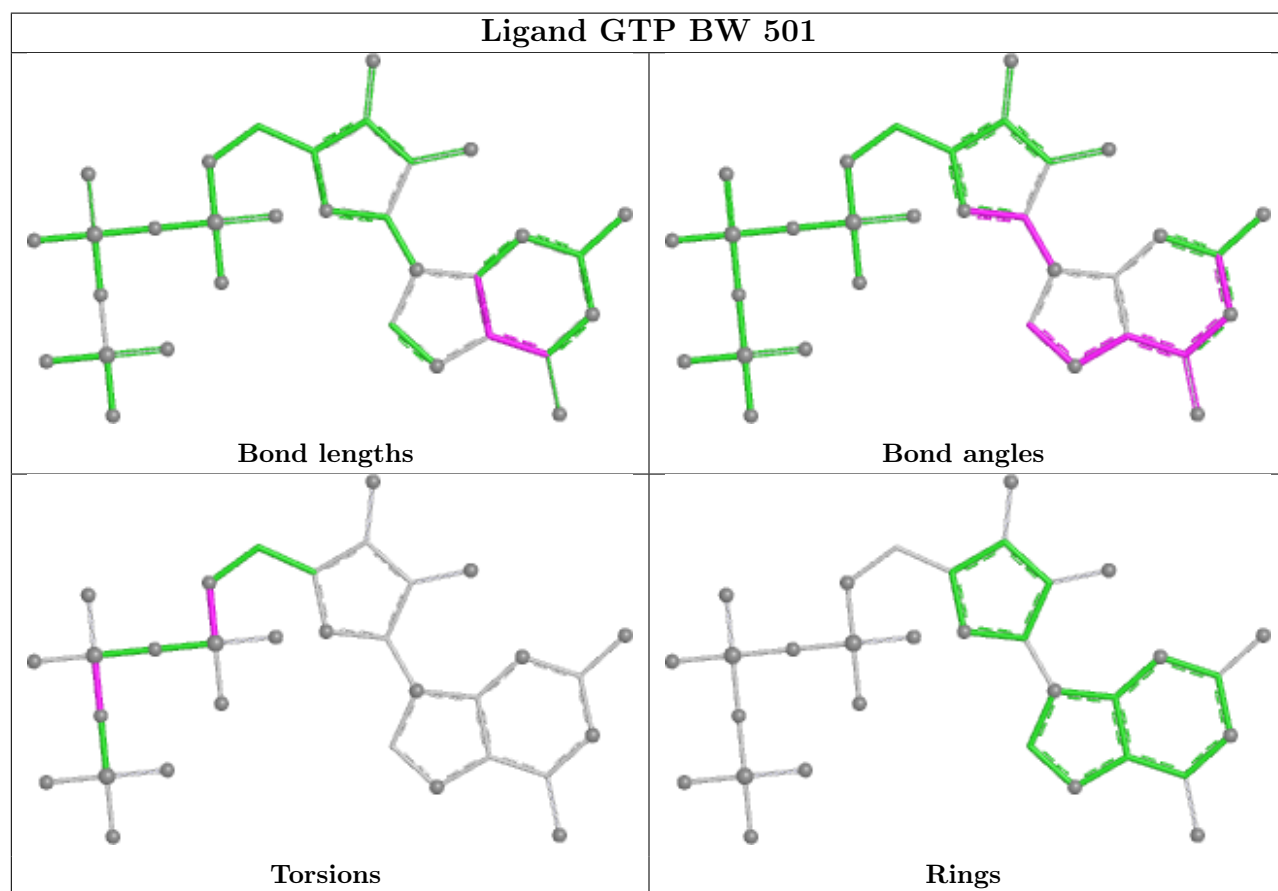
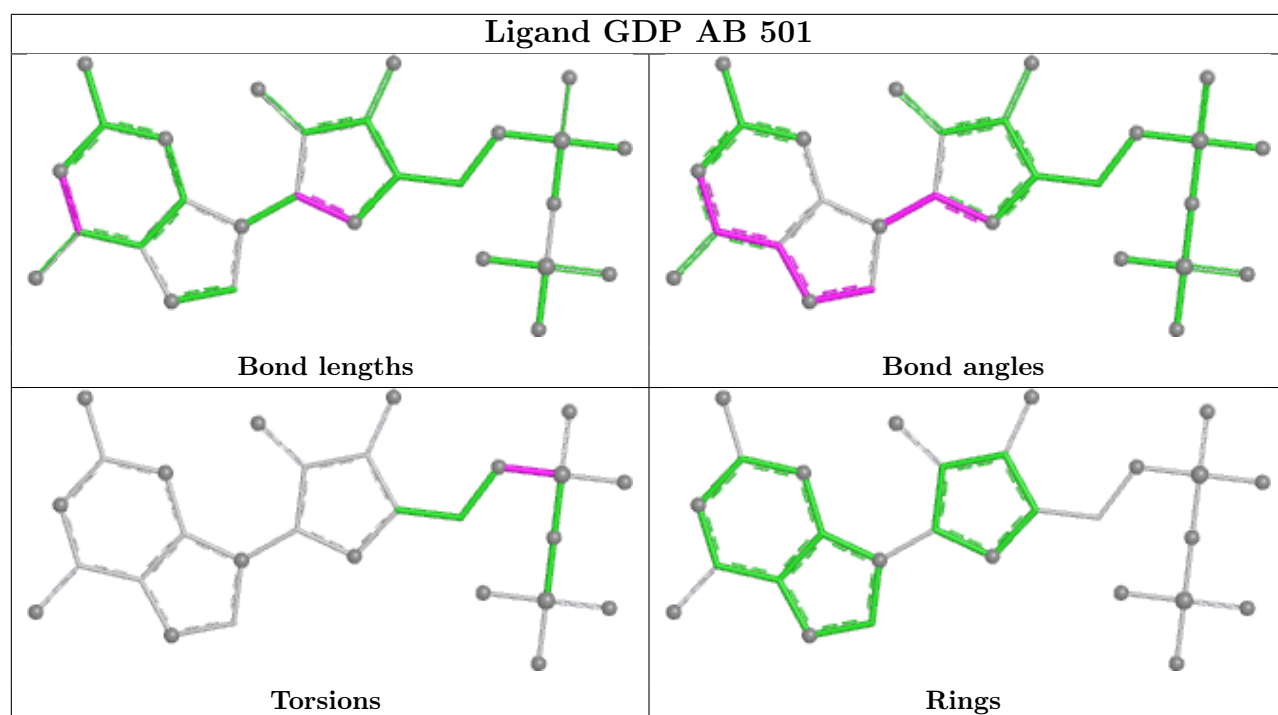


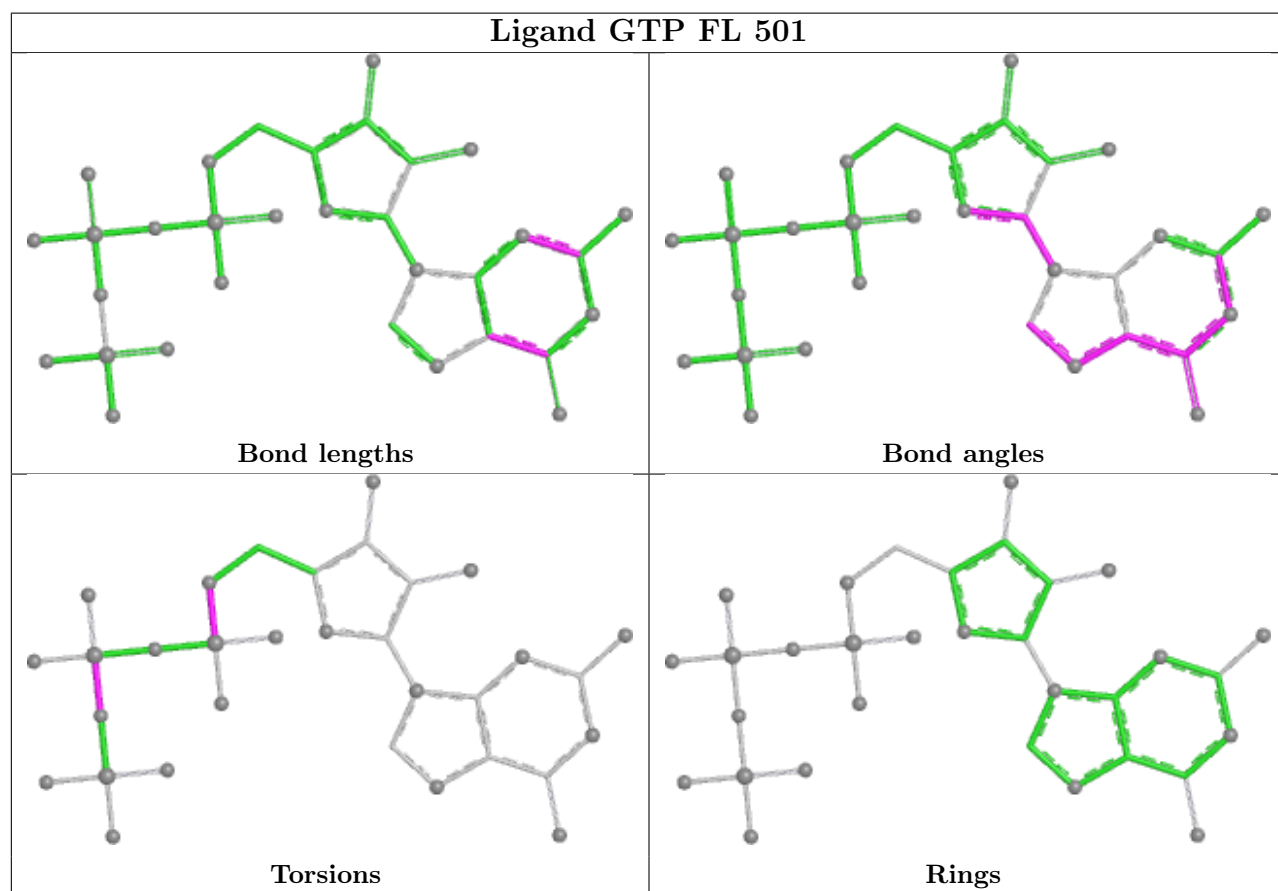
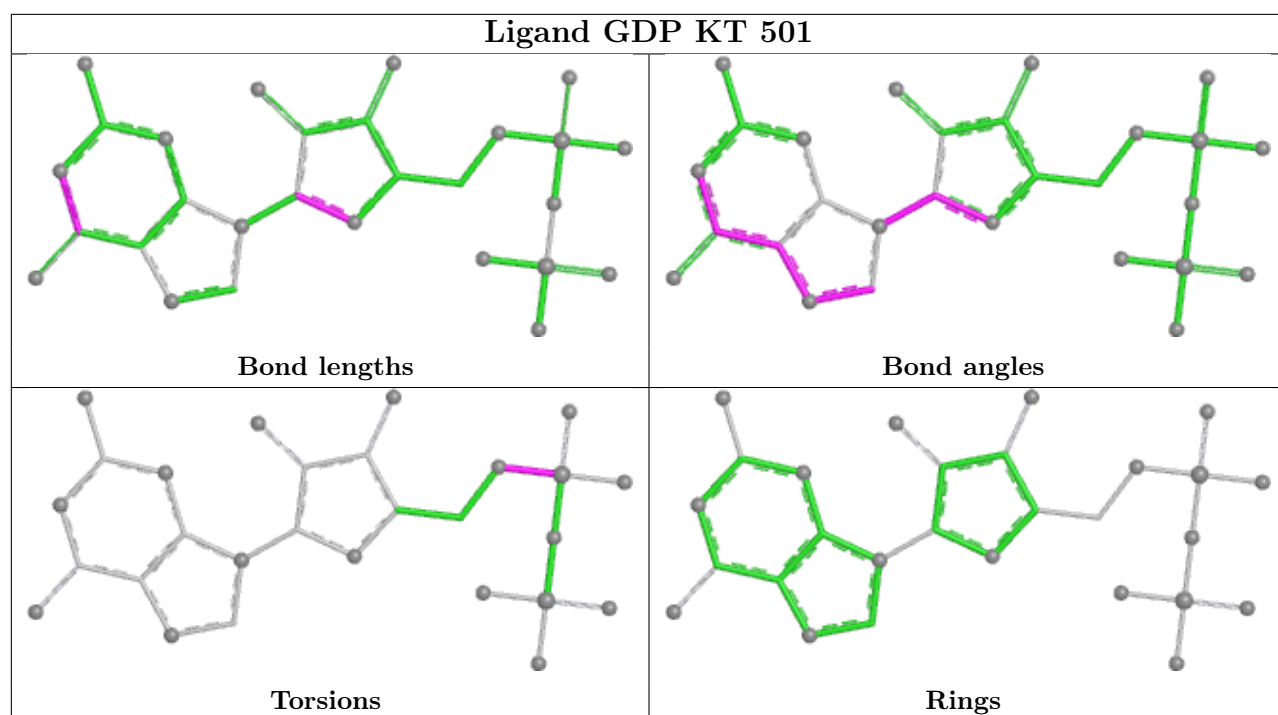
## Ligand GTP DM 602

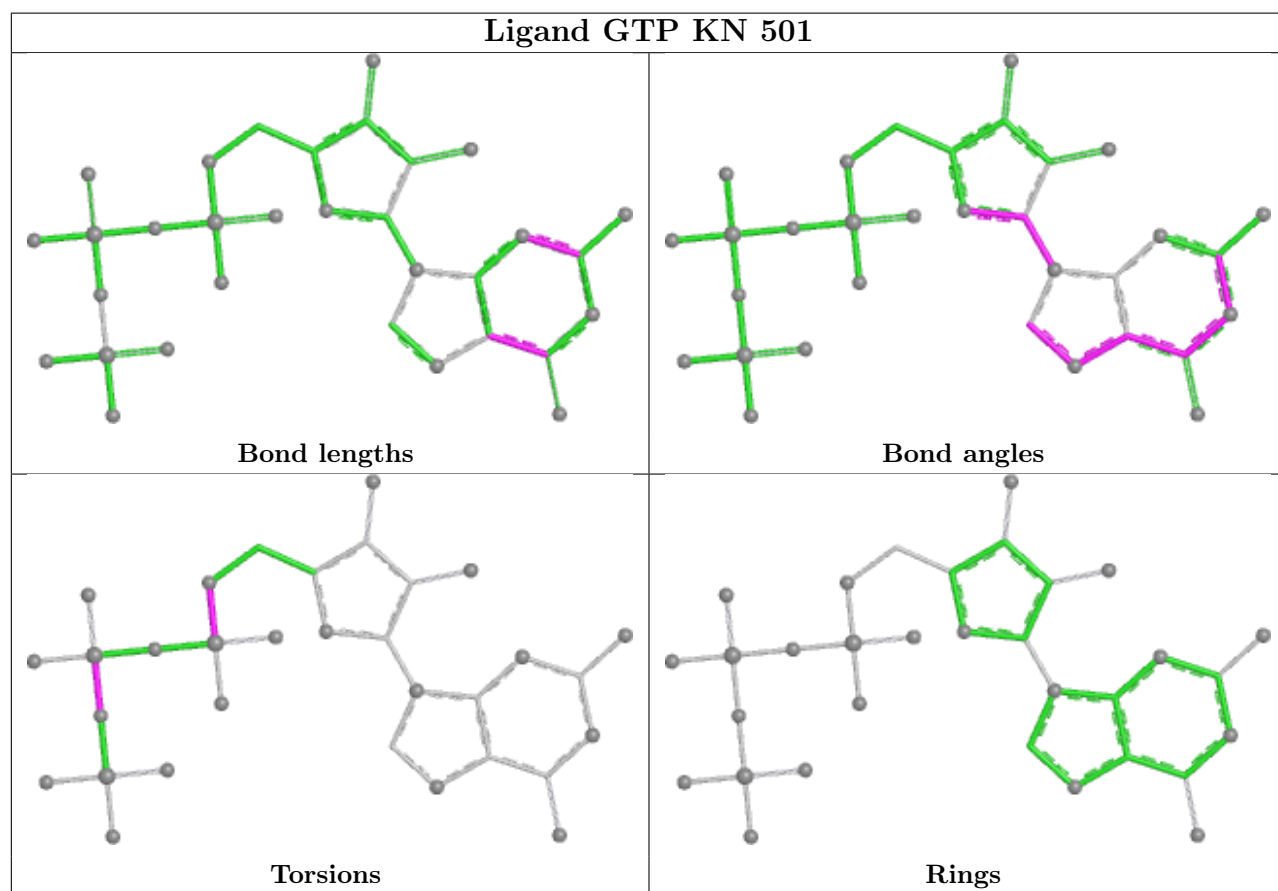
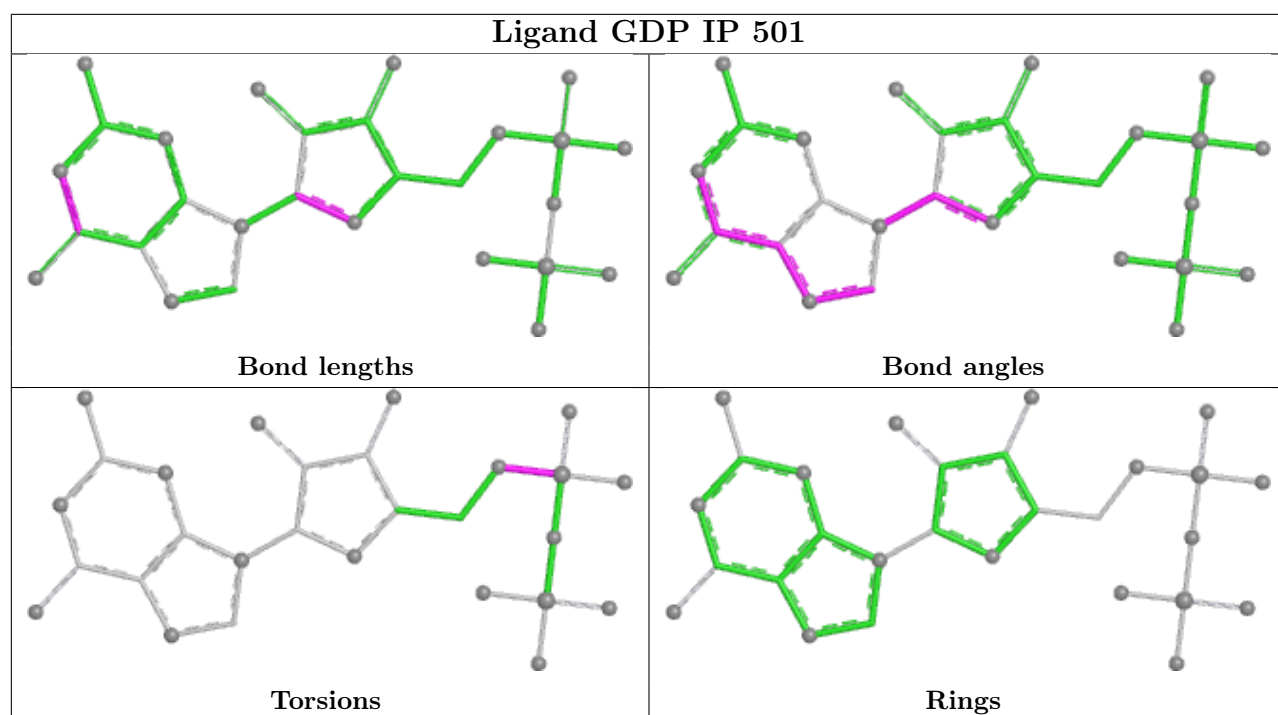


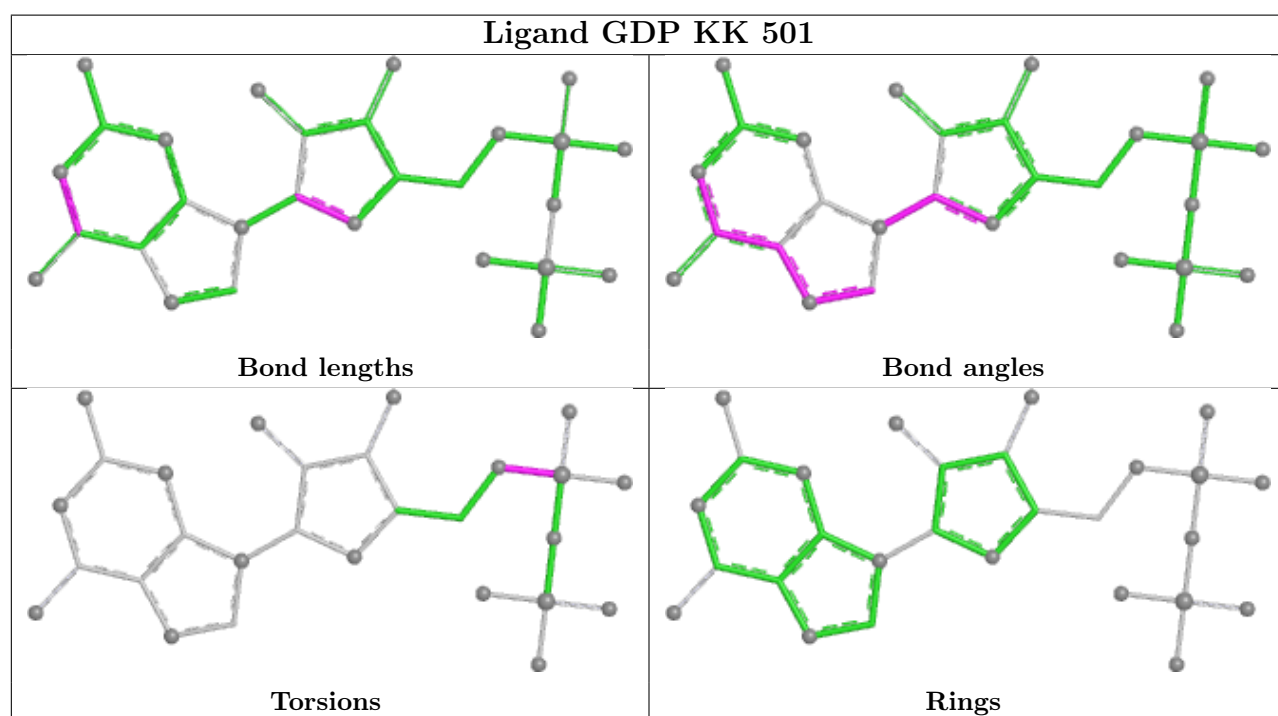
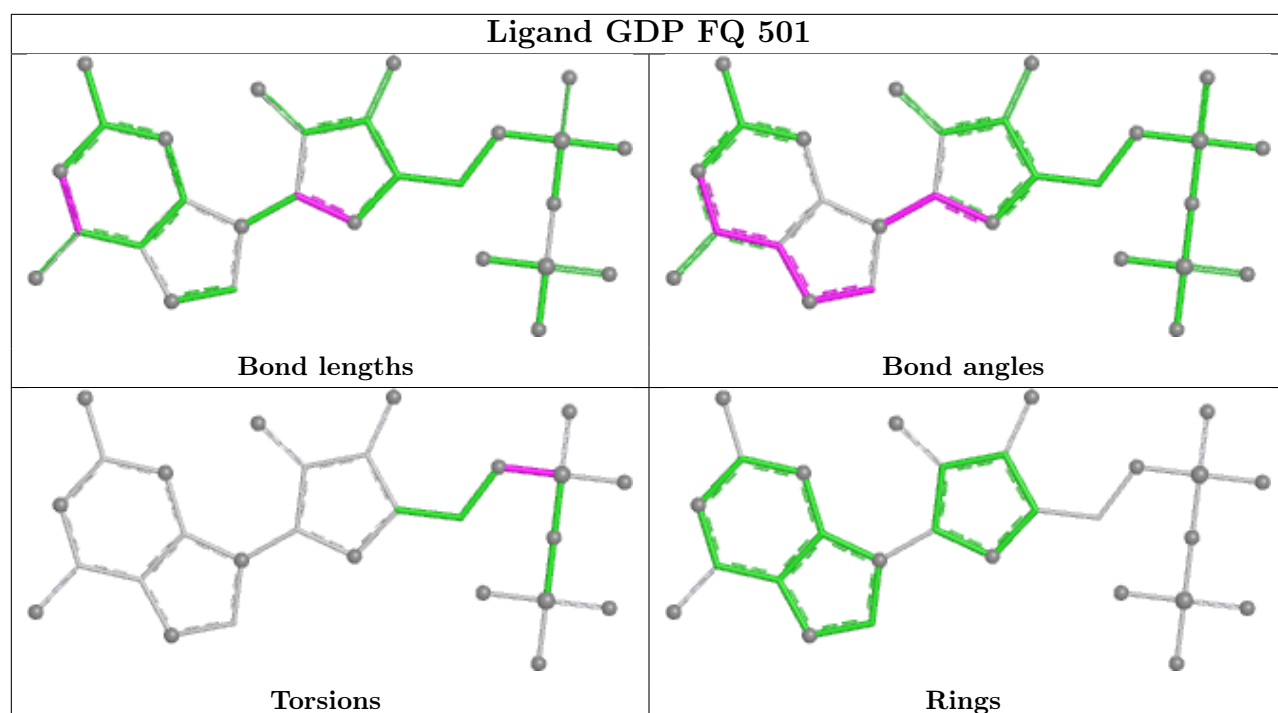
## Ligand GTP KC 602

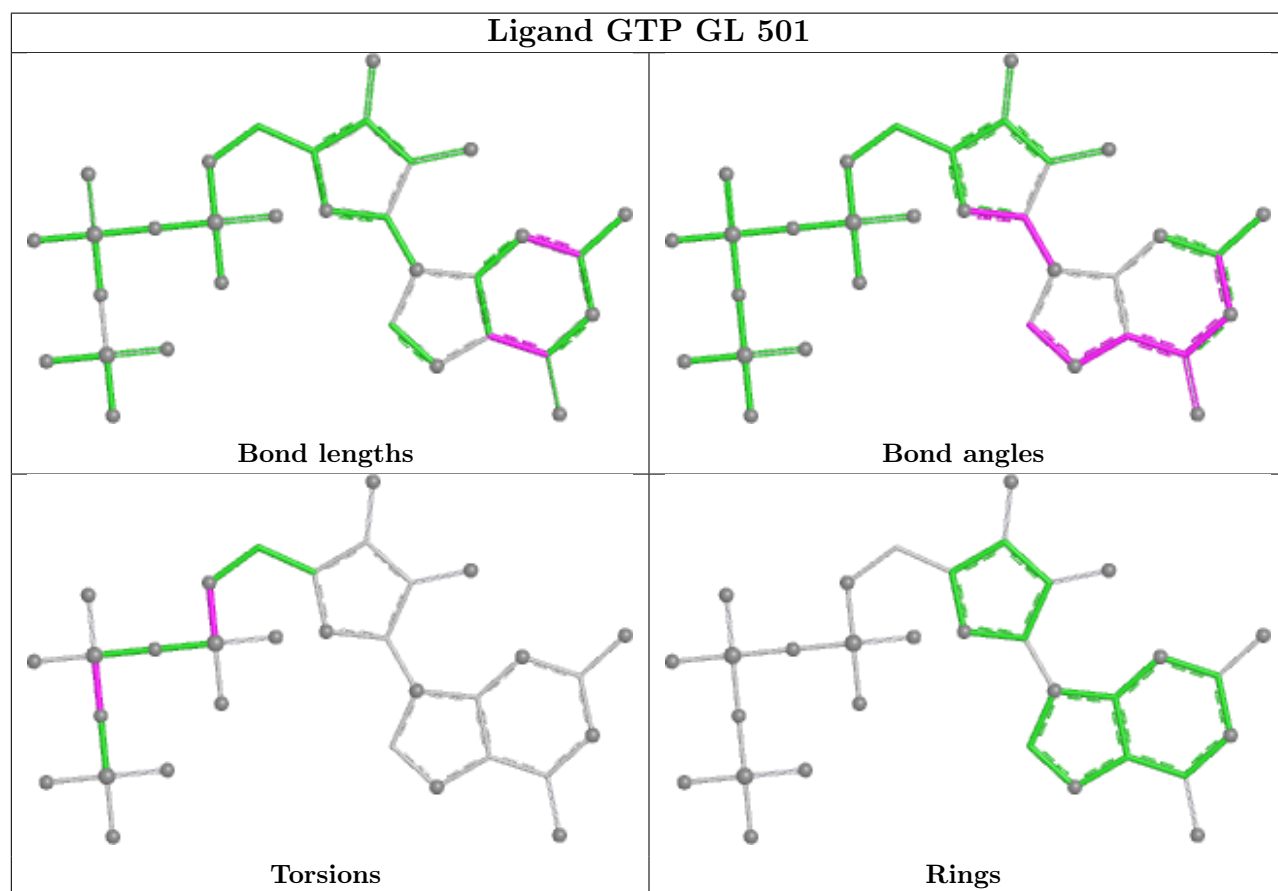
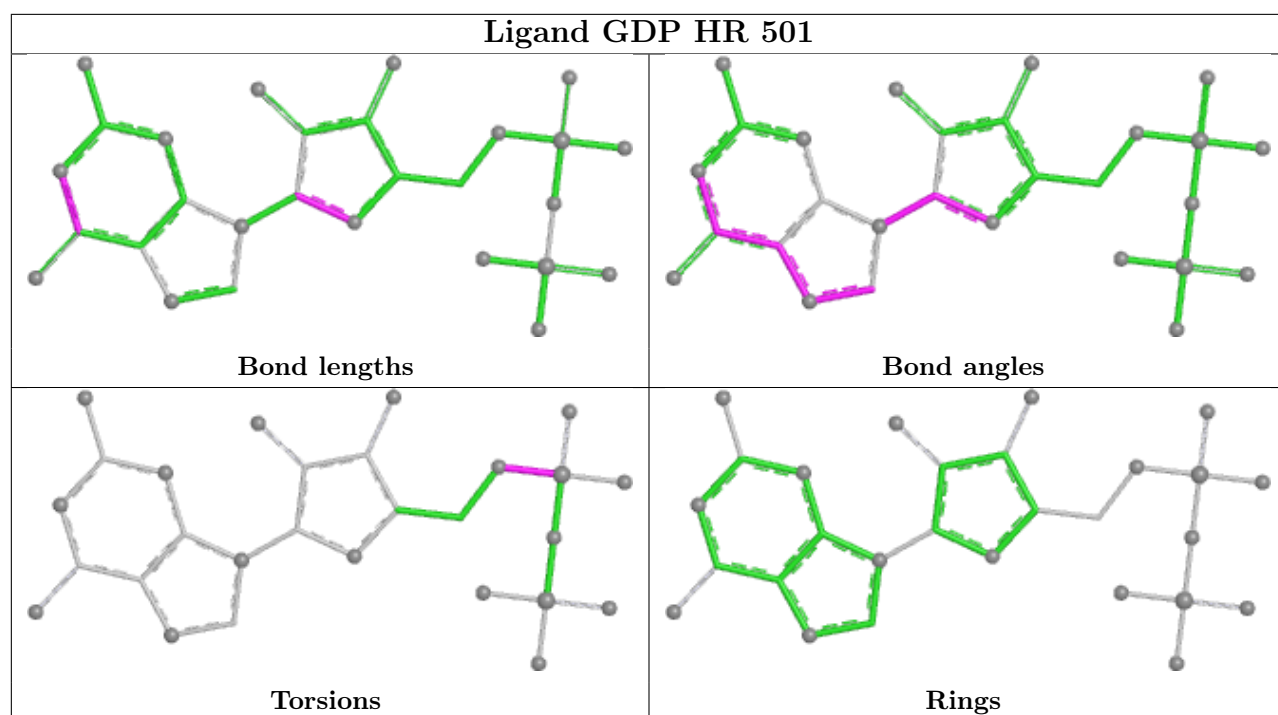






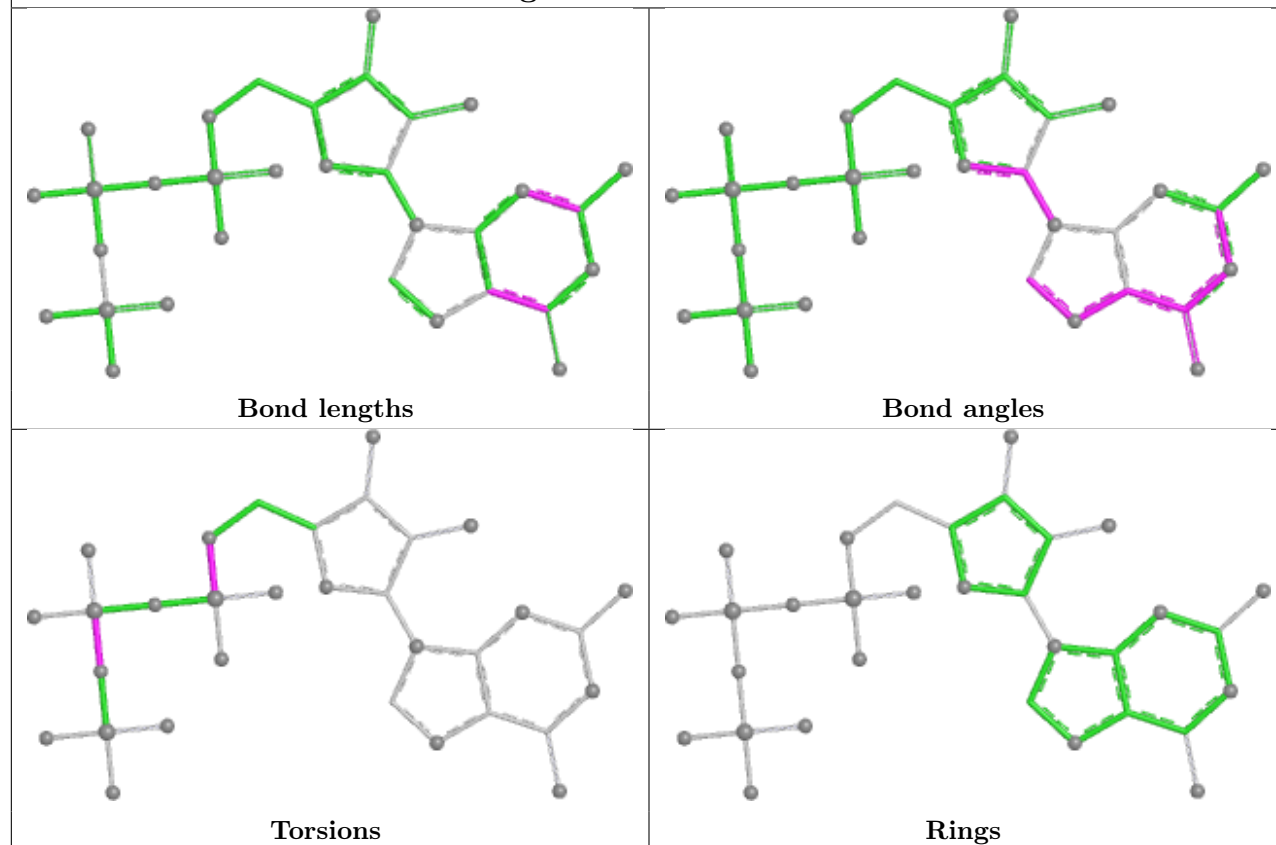




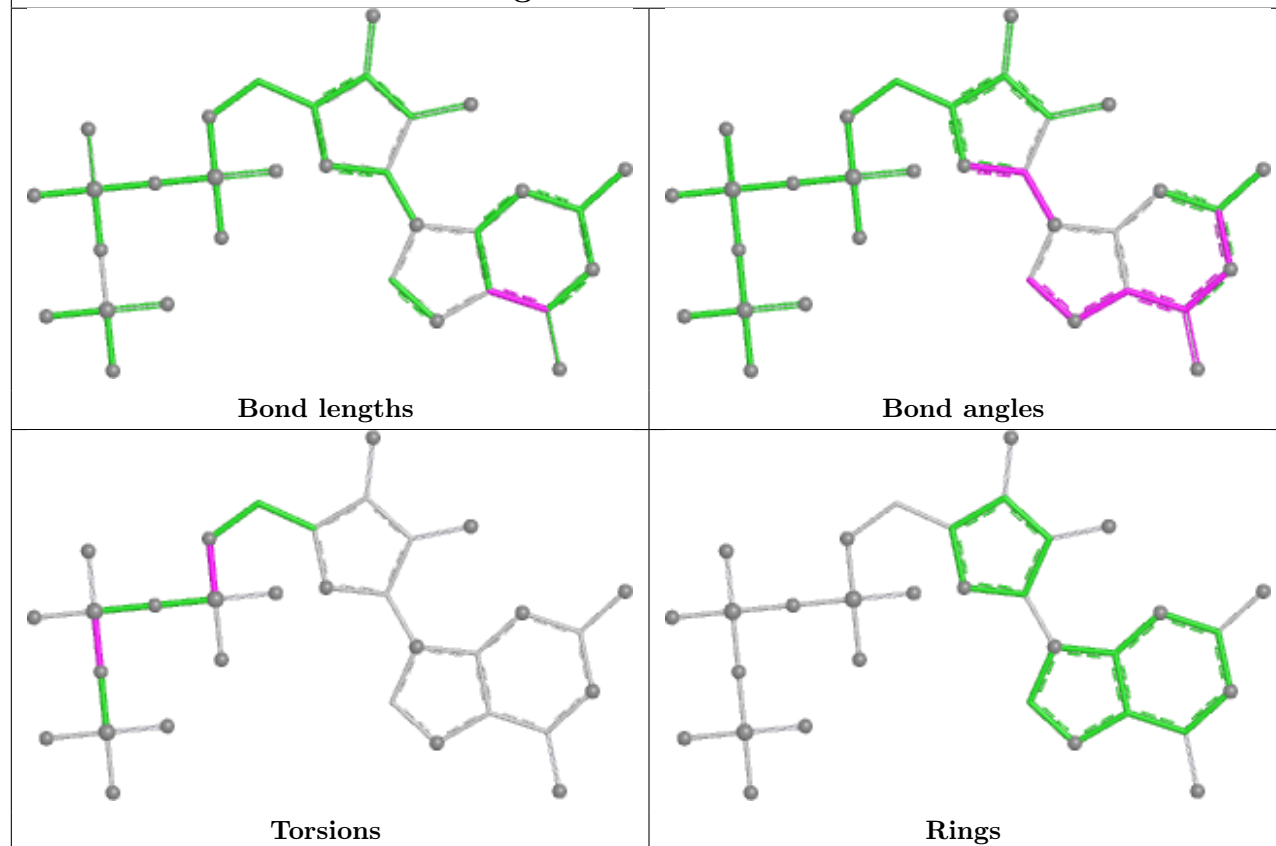


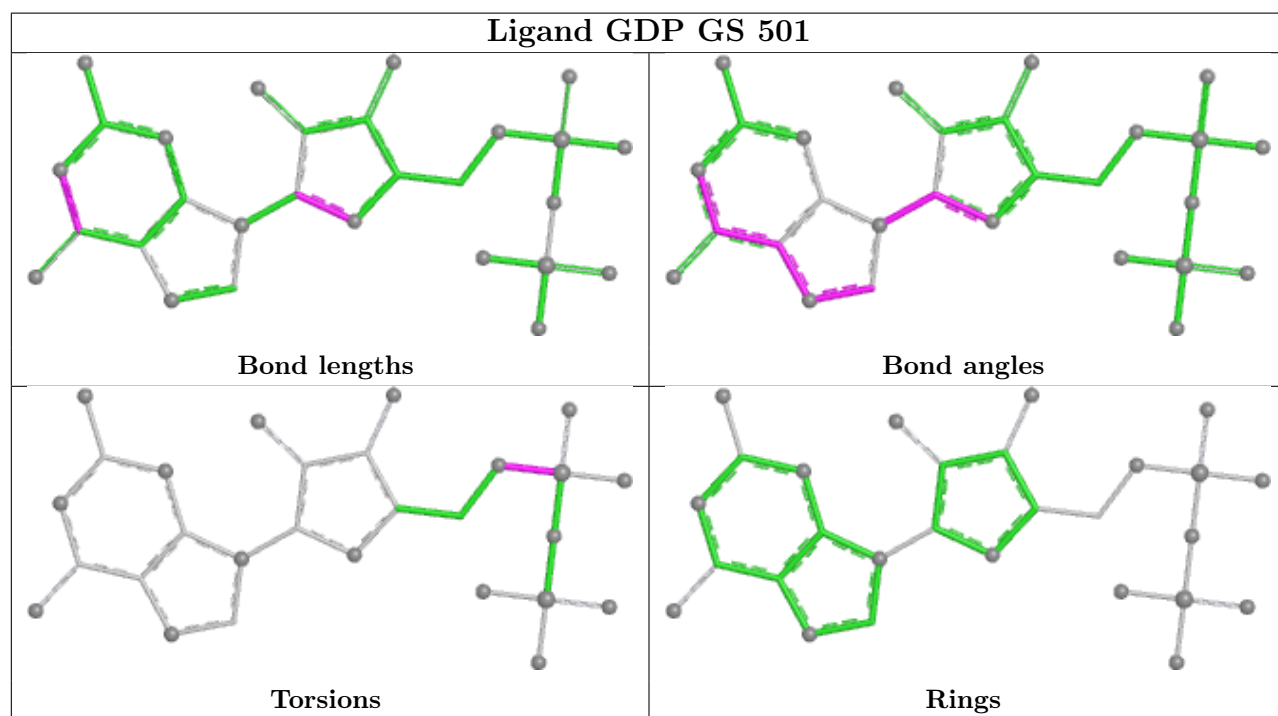
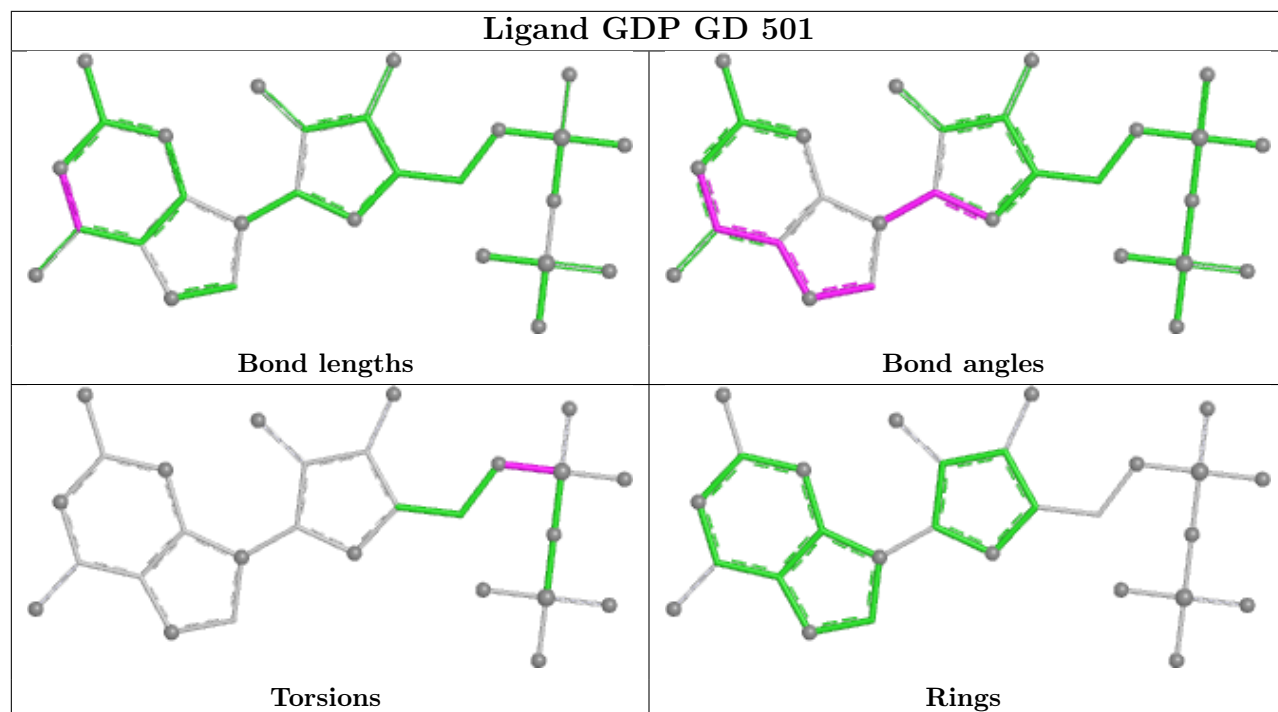


## Ligand GTP KS 602

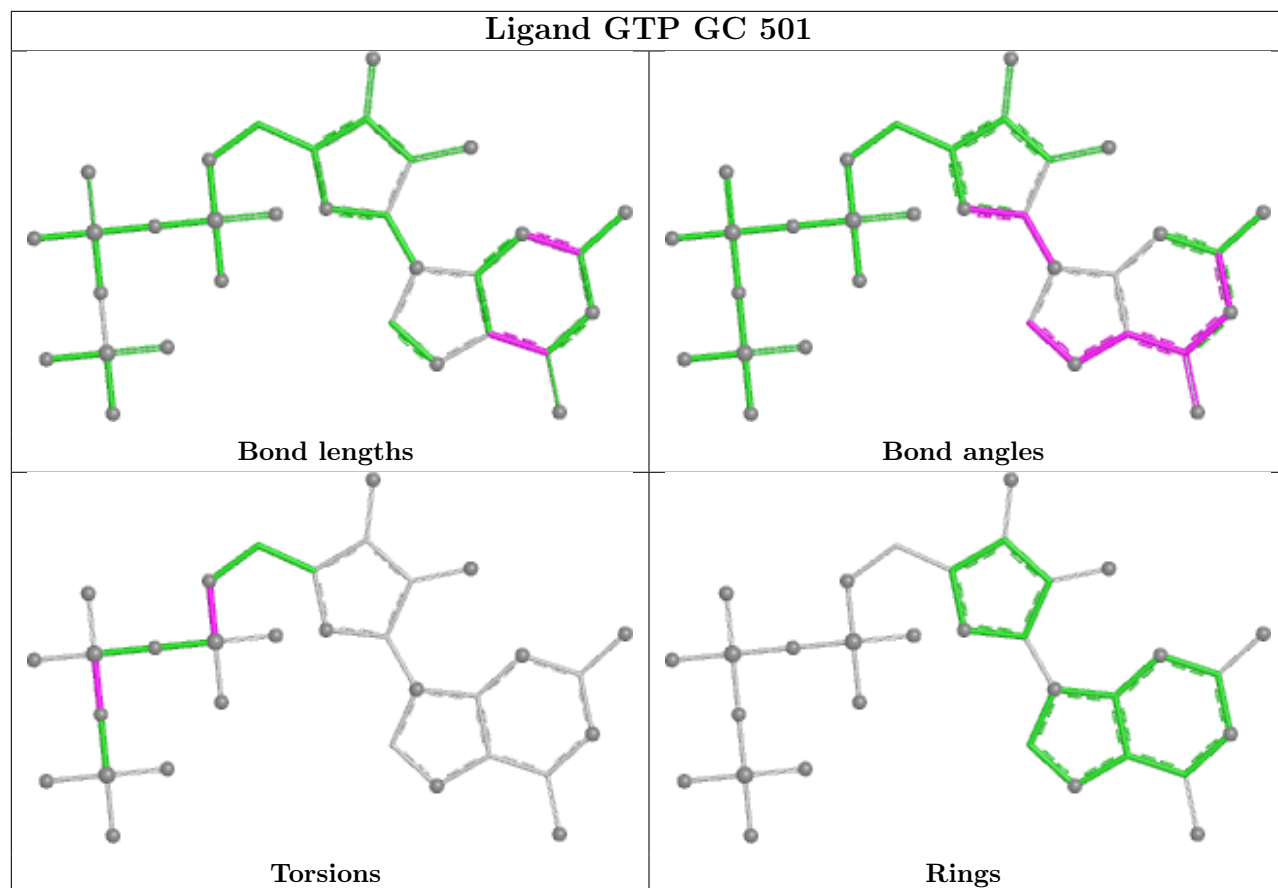


## Ligand GTP BM 501

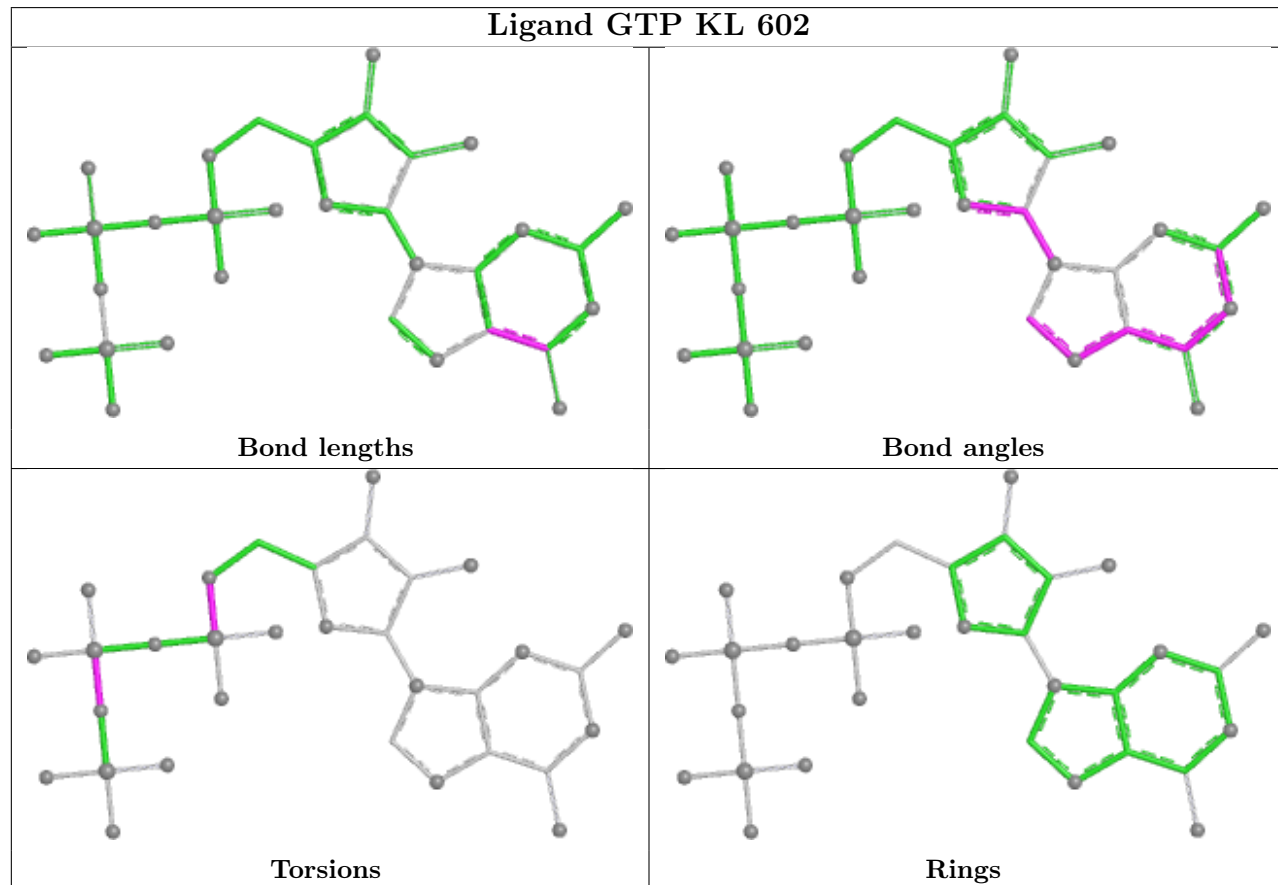


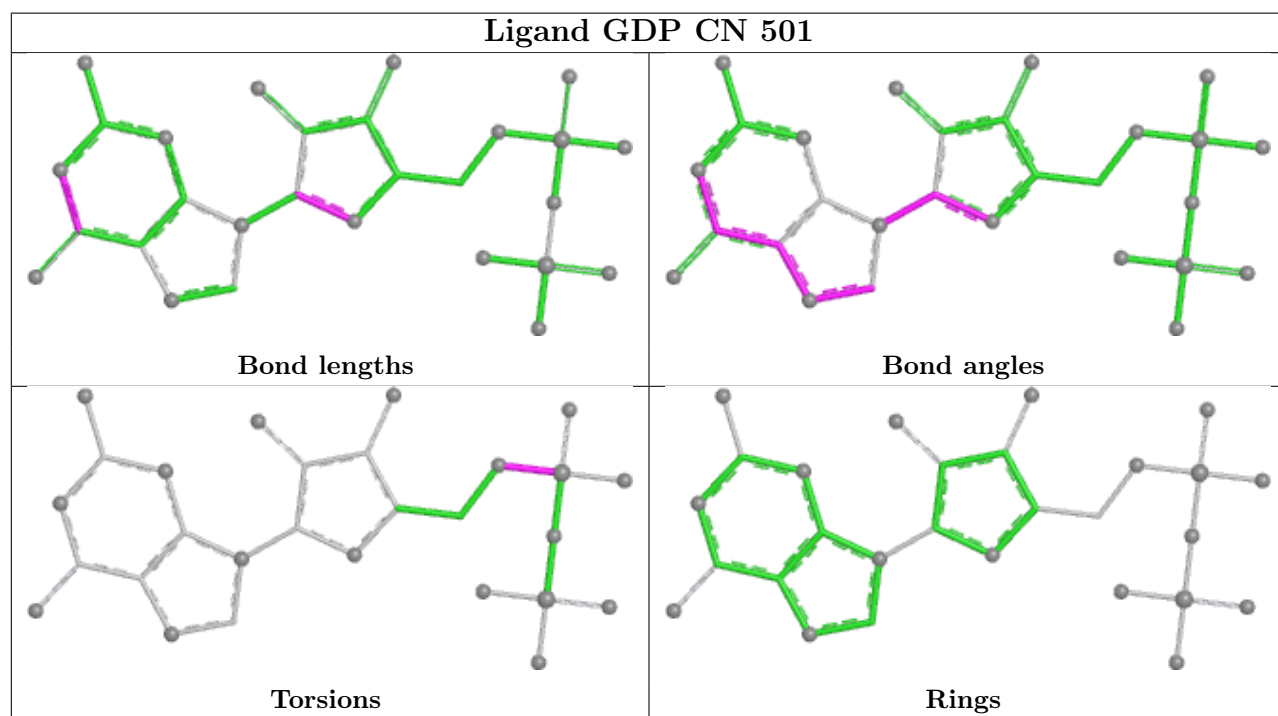
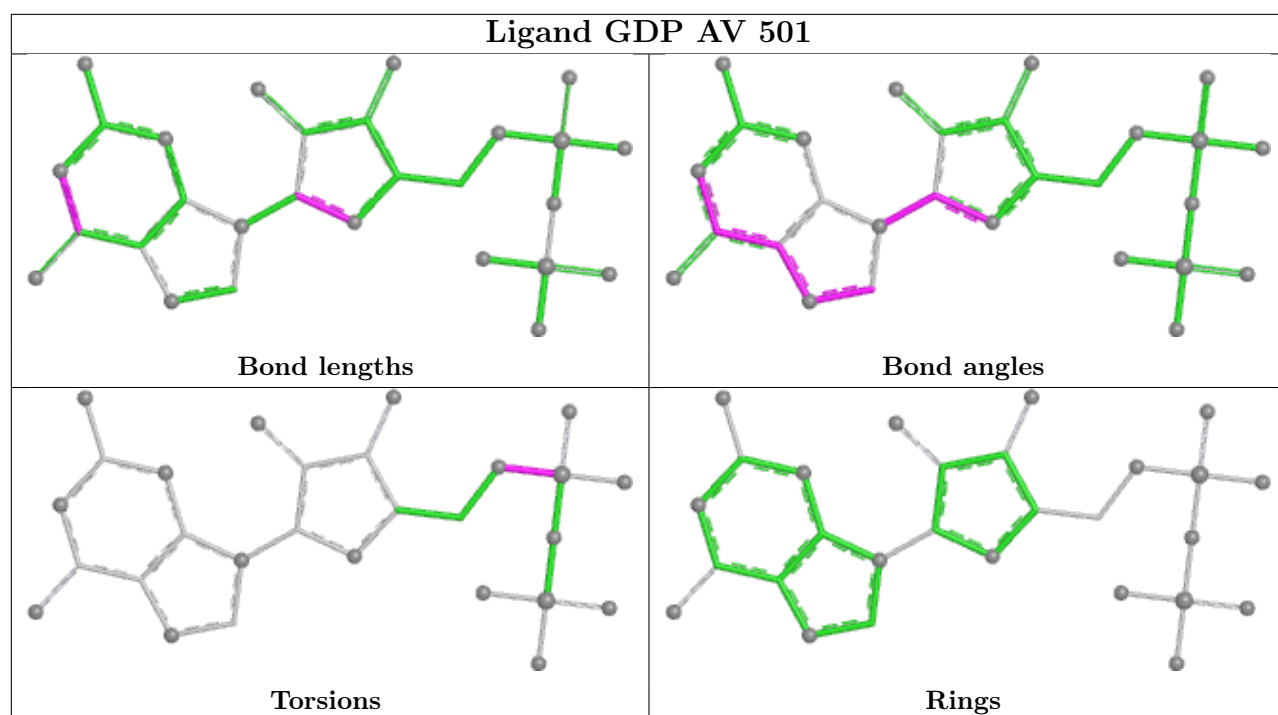


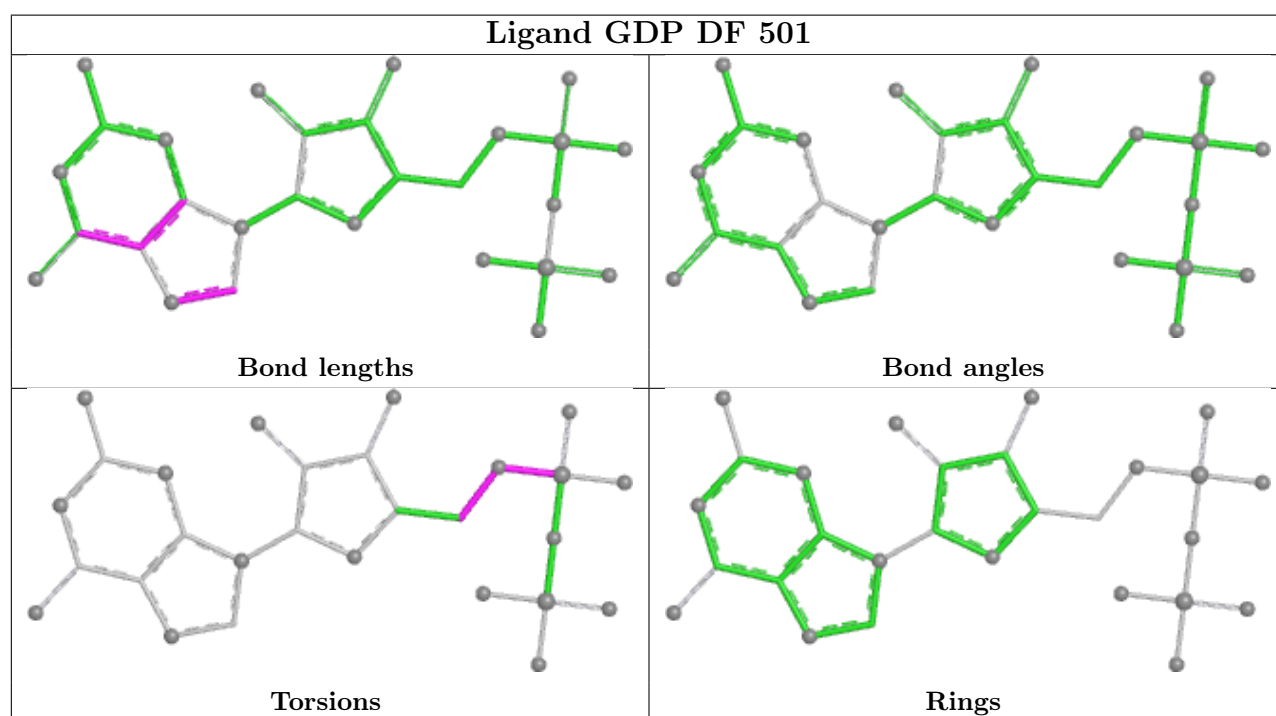
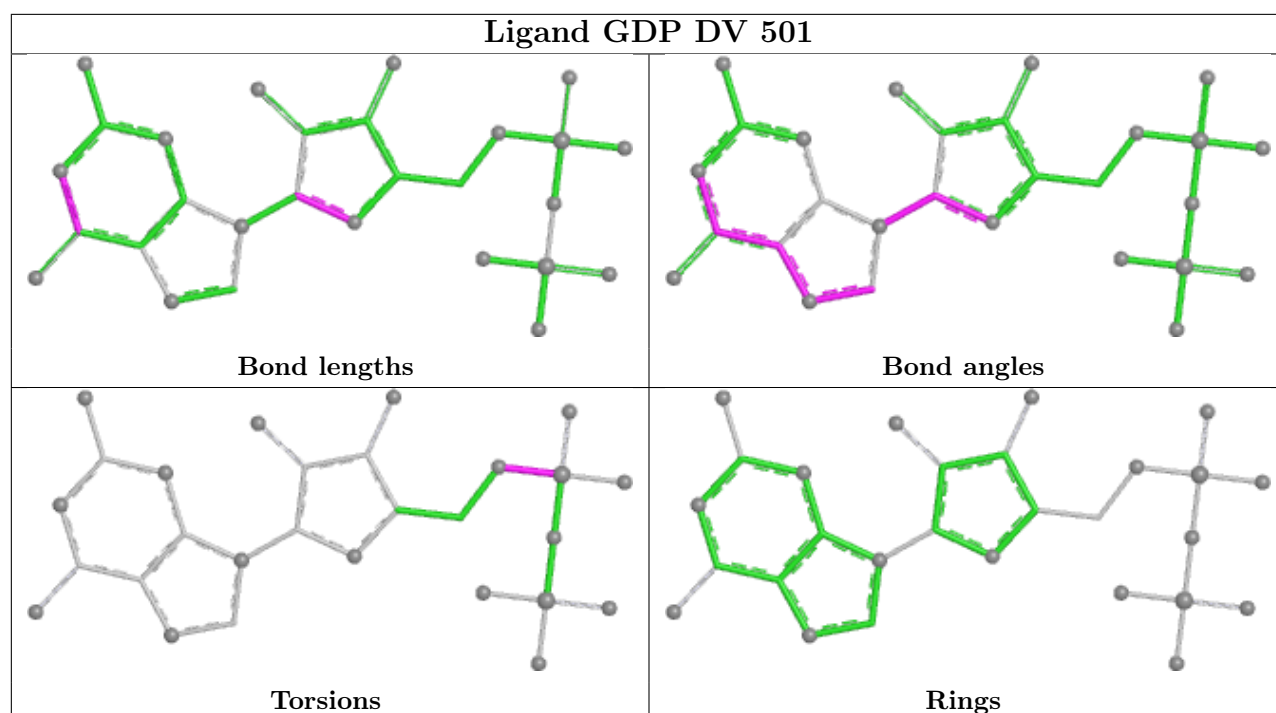
## Ligand GTP GC 501

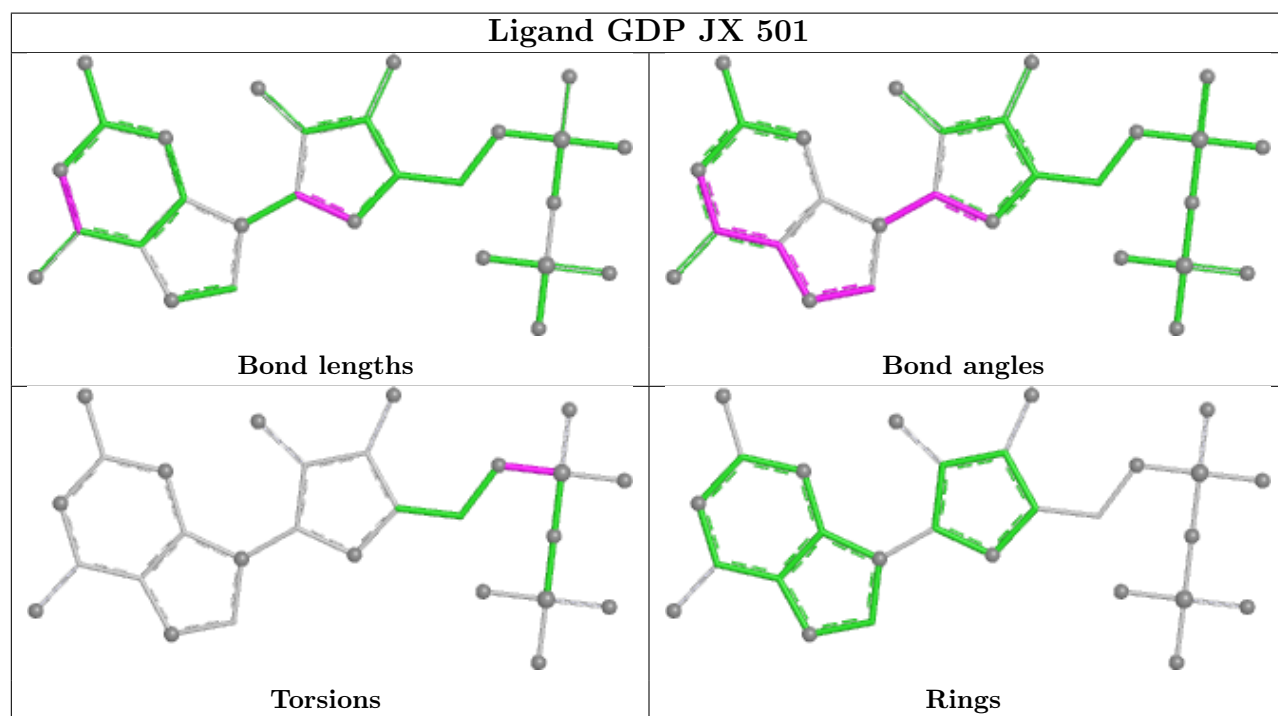
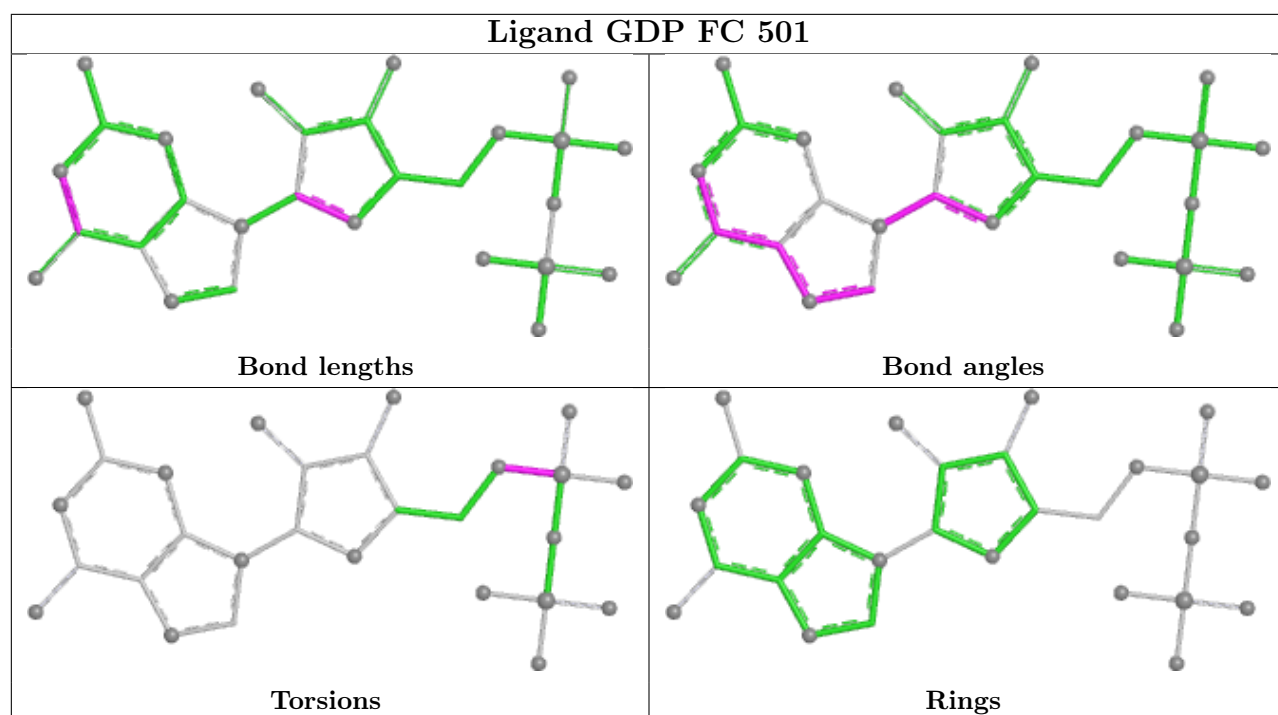


## Ligand GTP KL 602

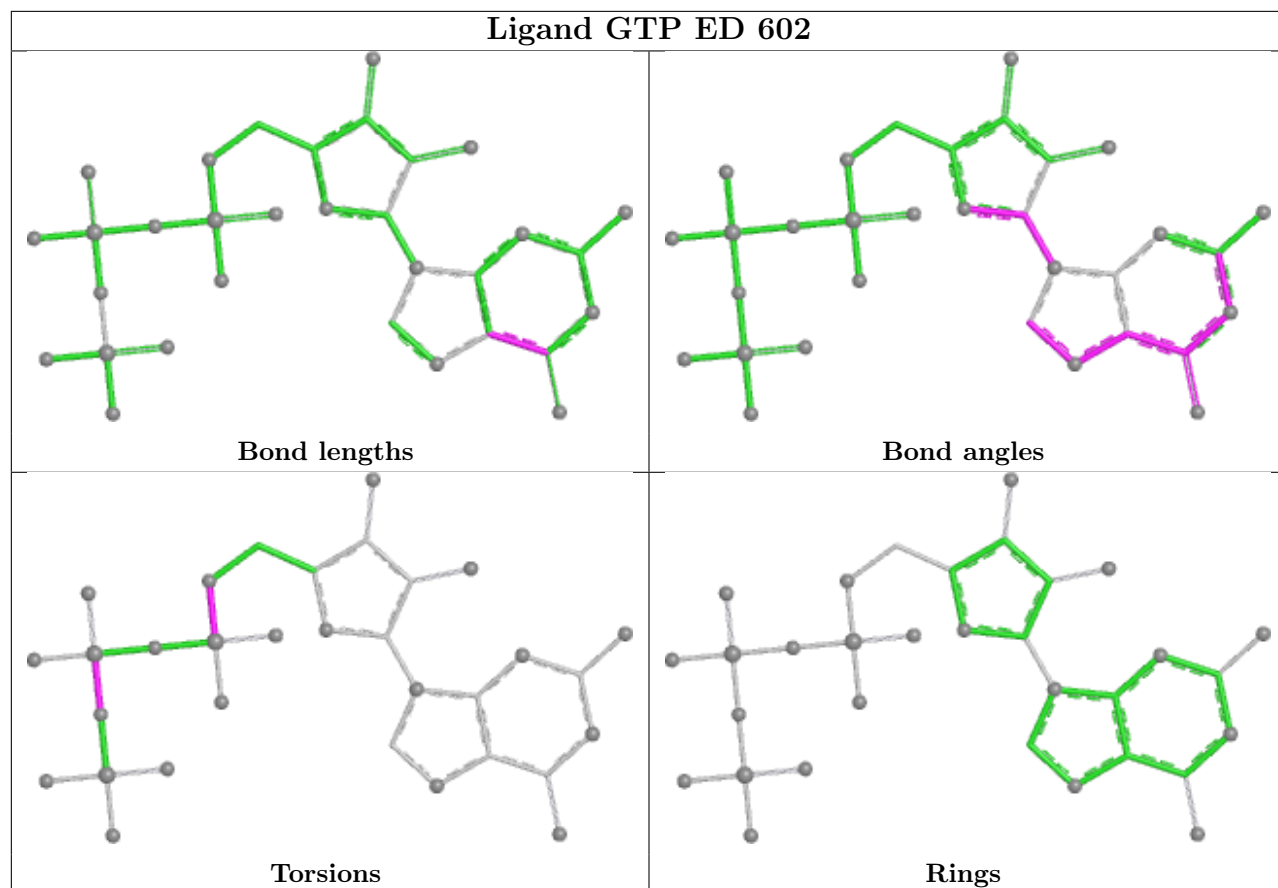




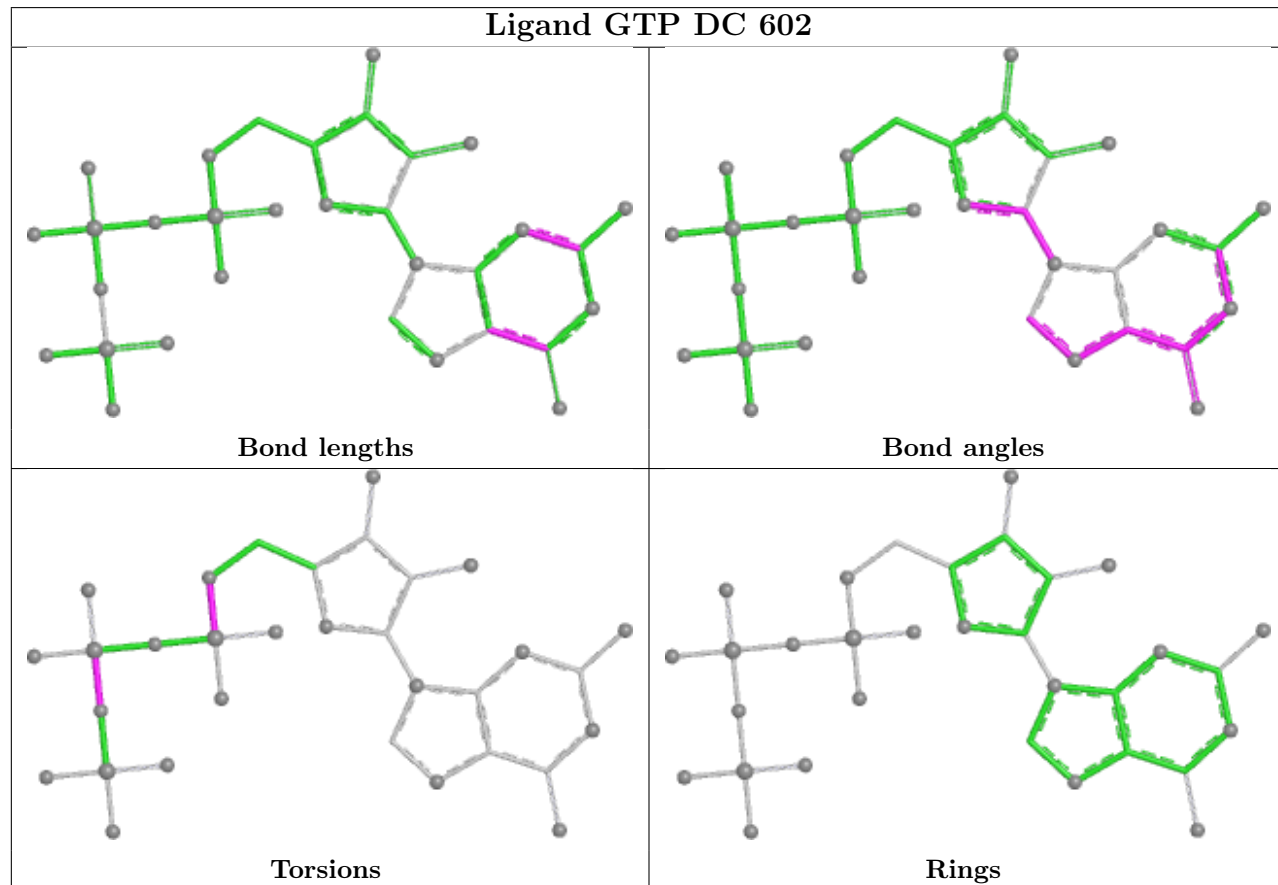


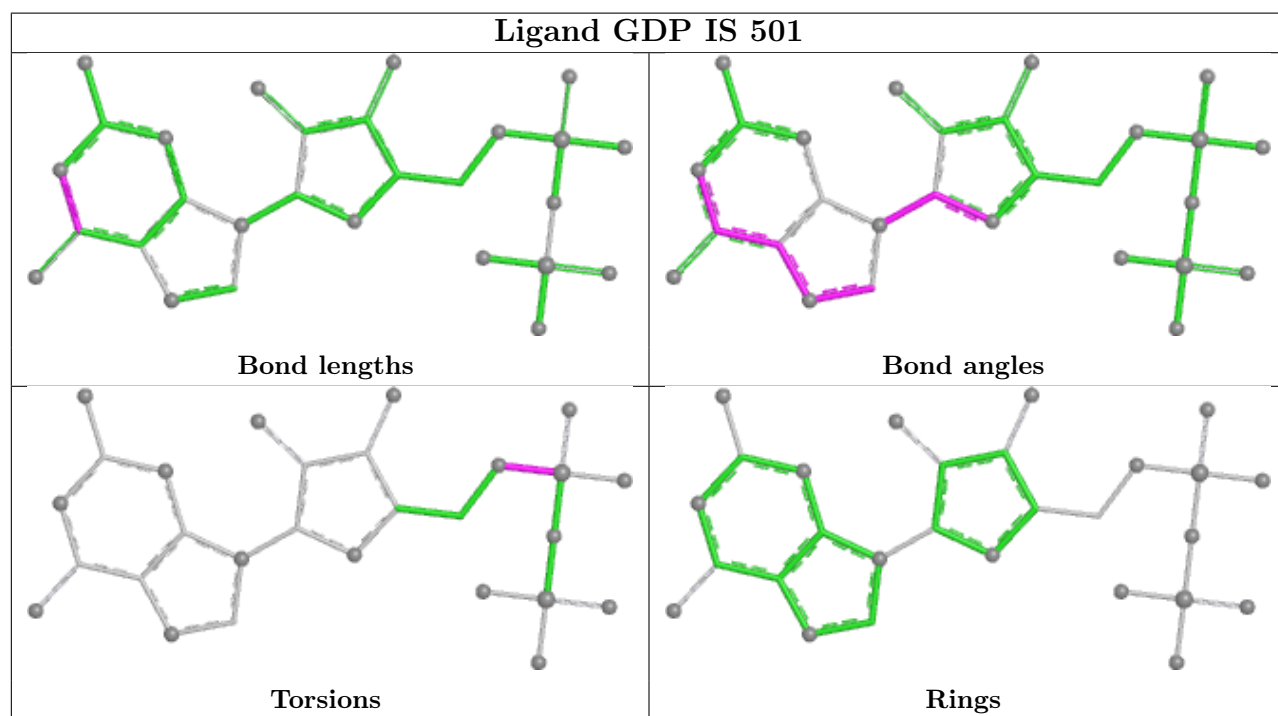
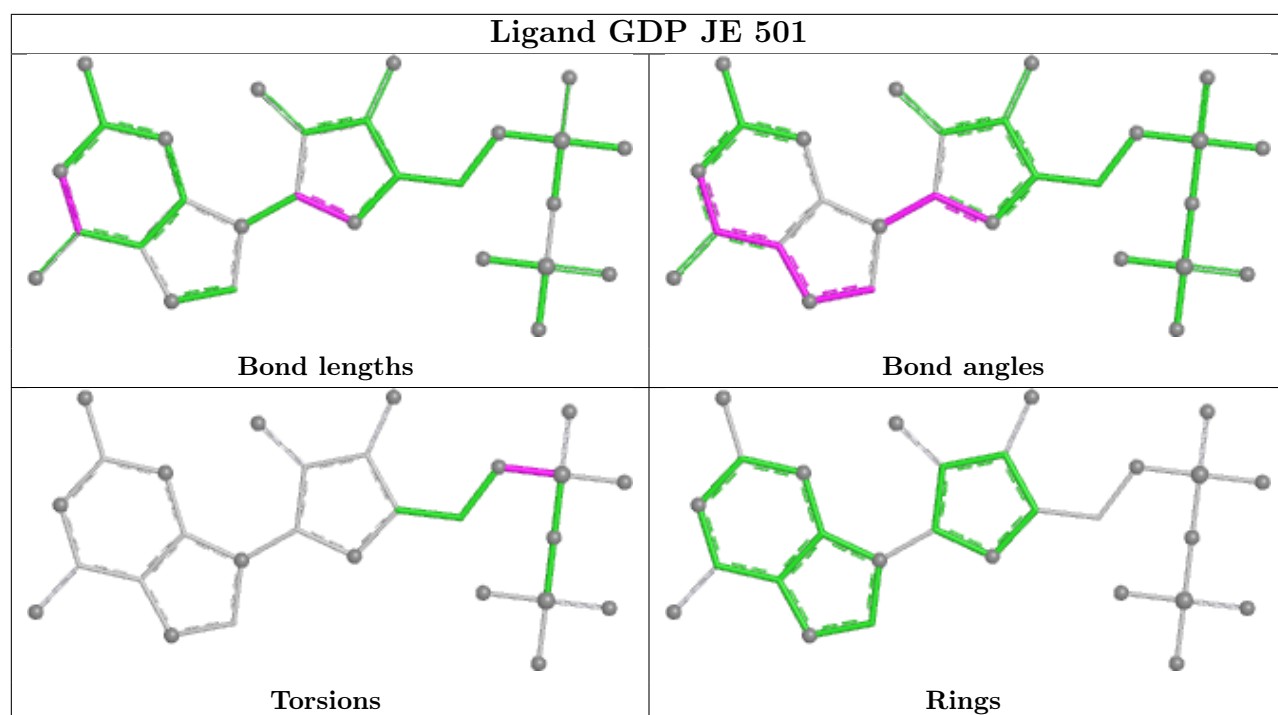


## Ligand GTP ED 602

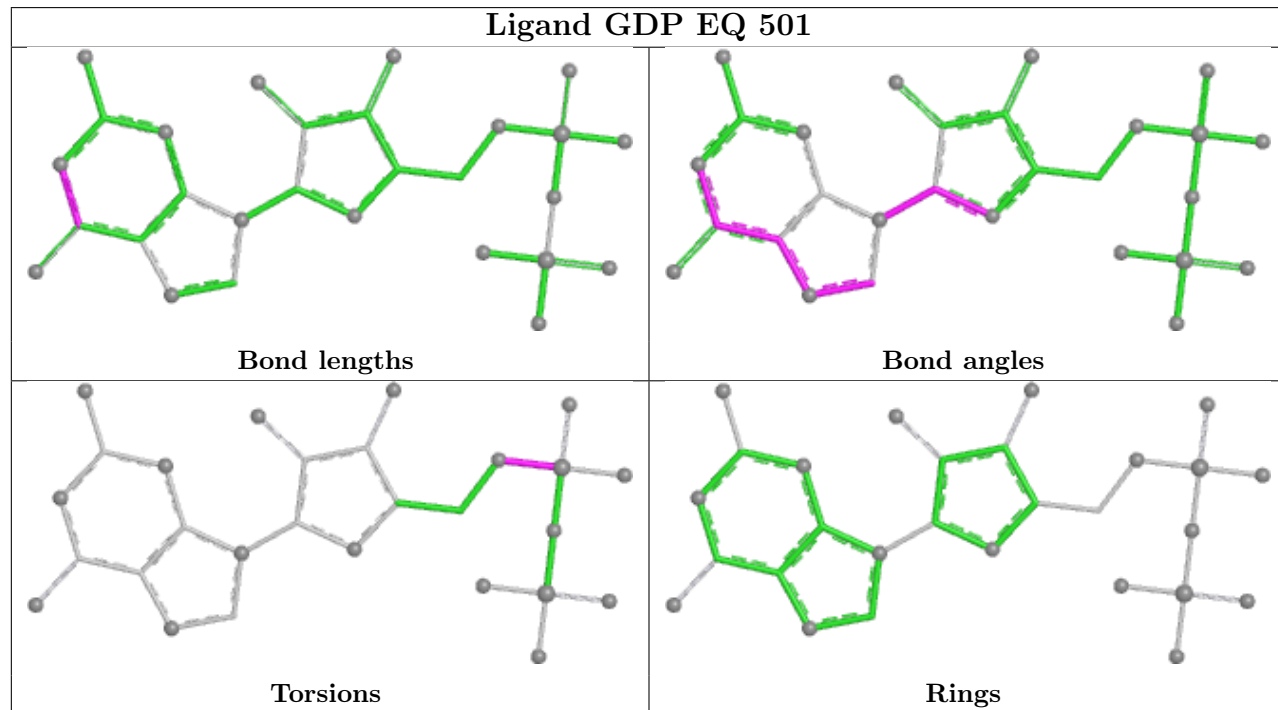
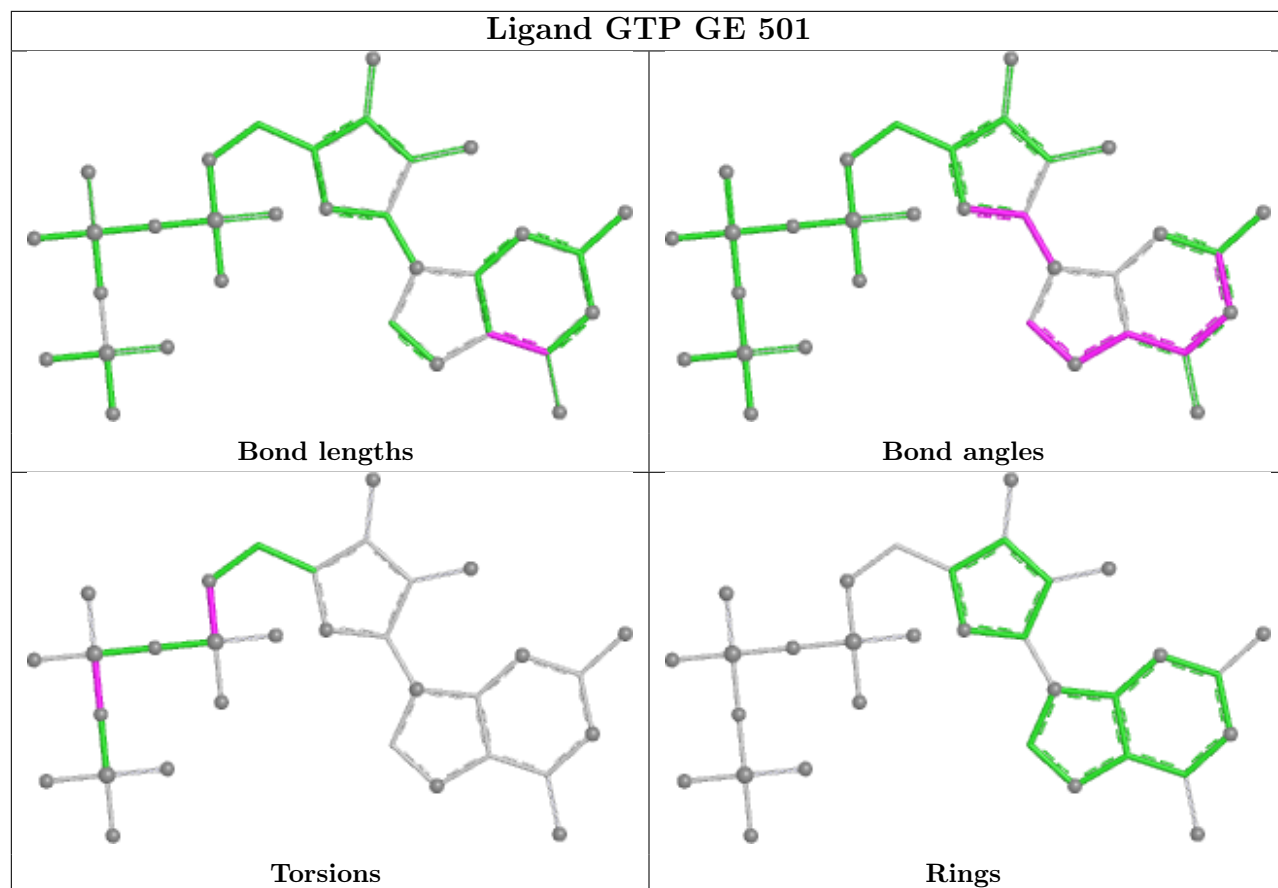


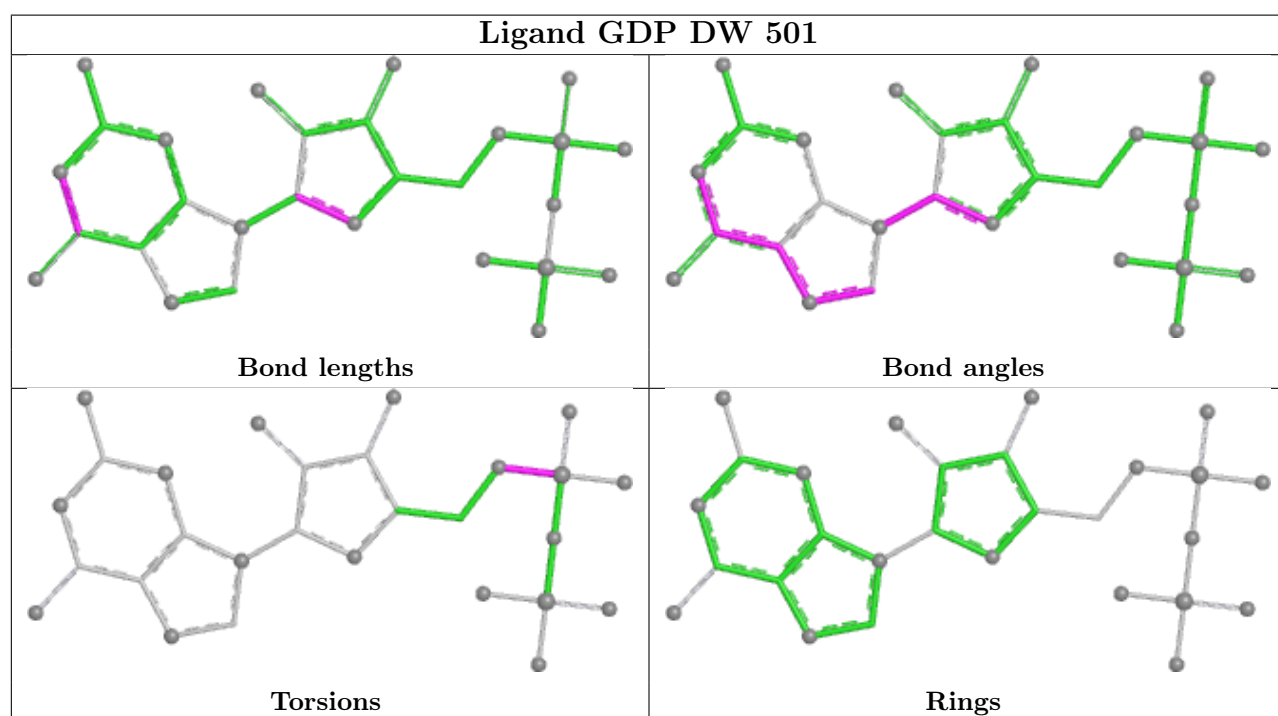
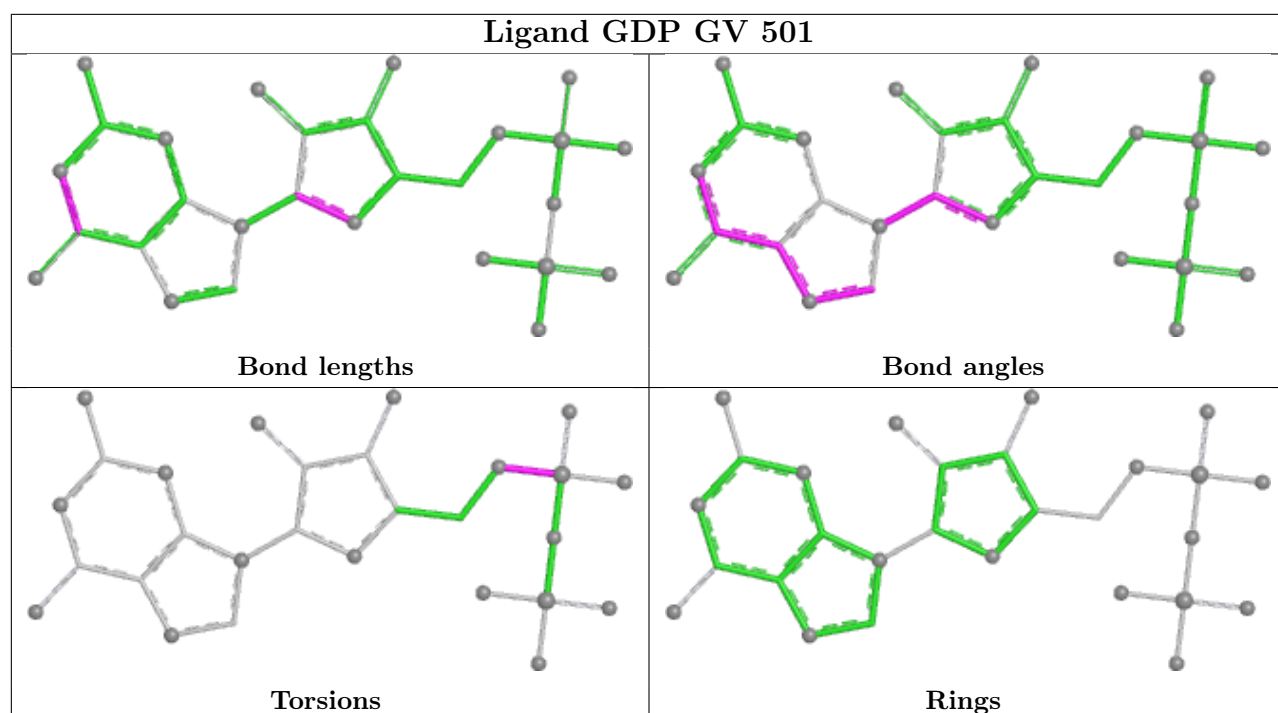
## Ligand GTP DC 602

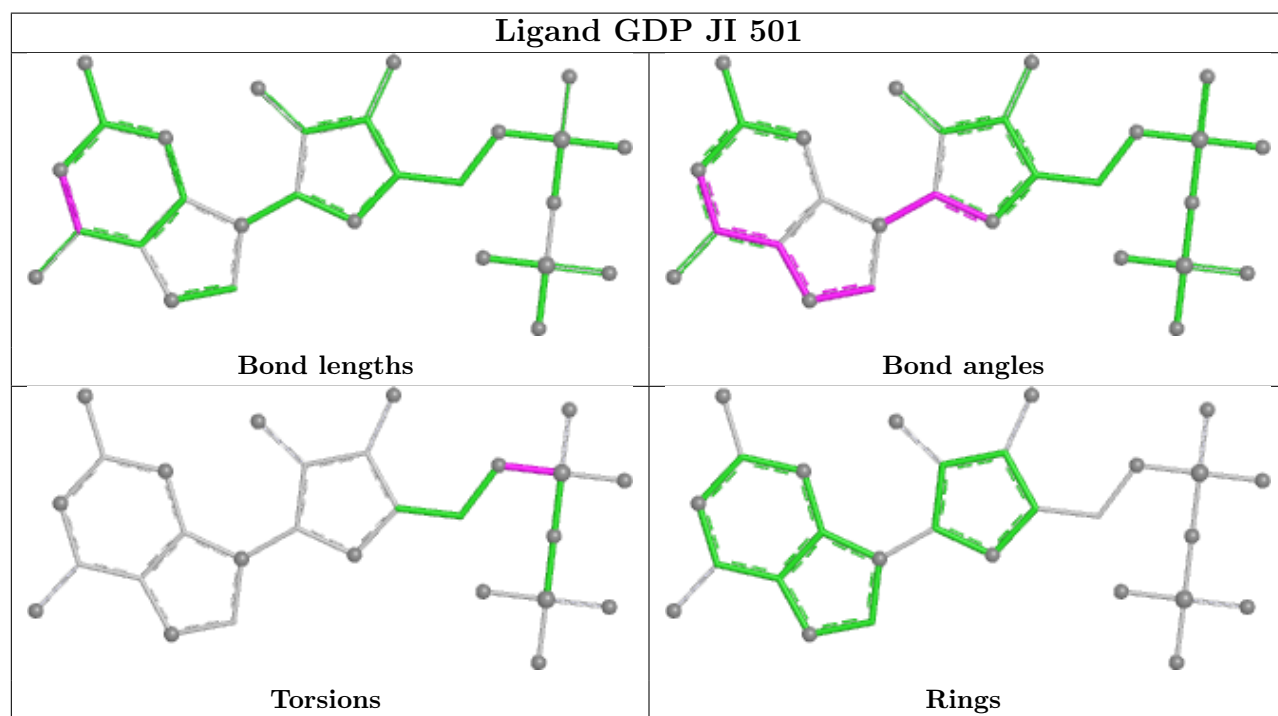
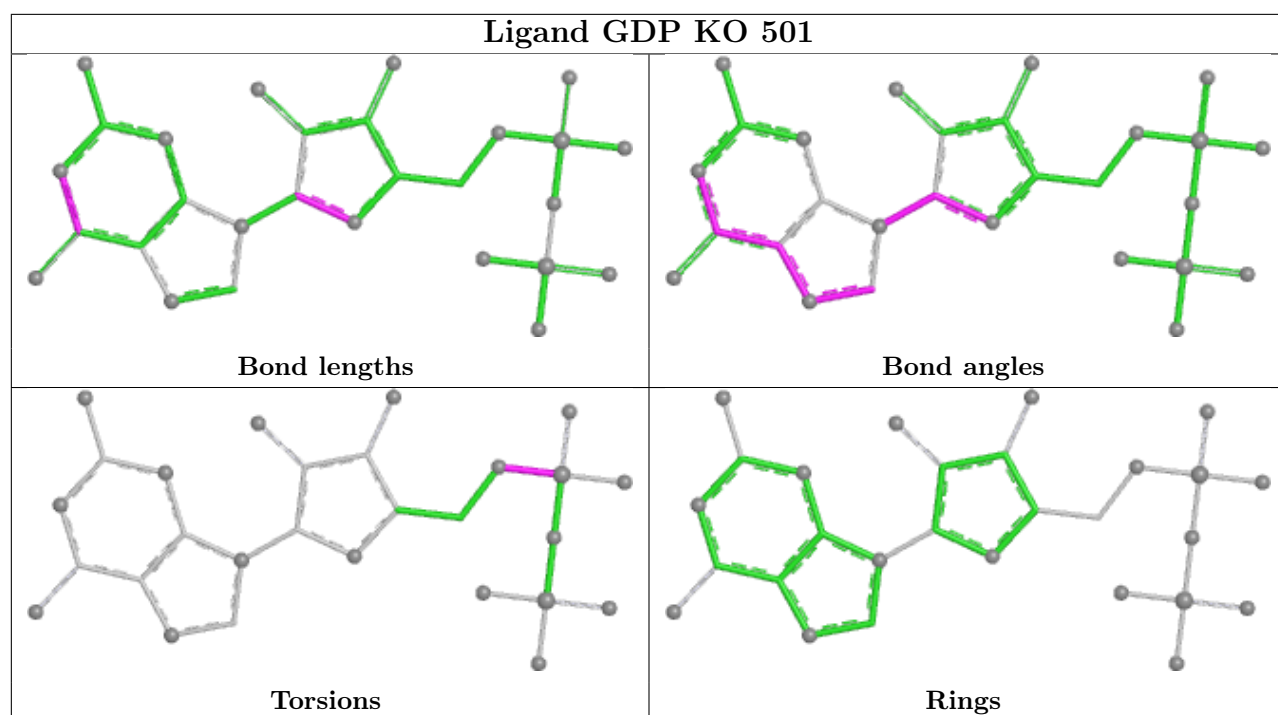




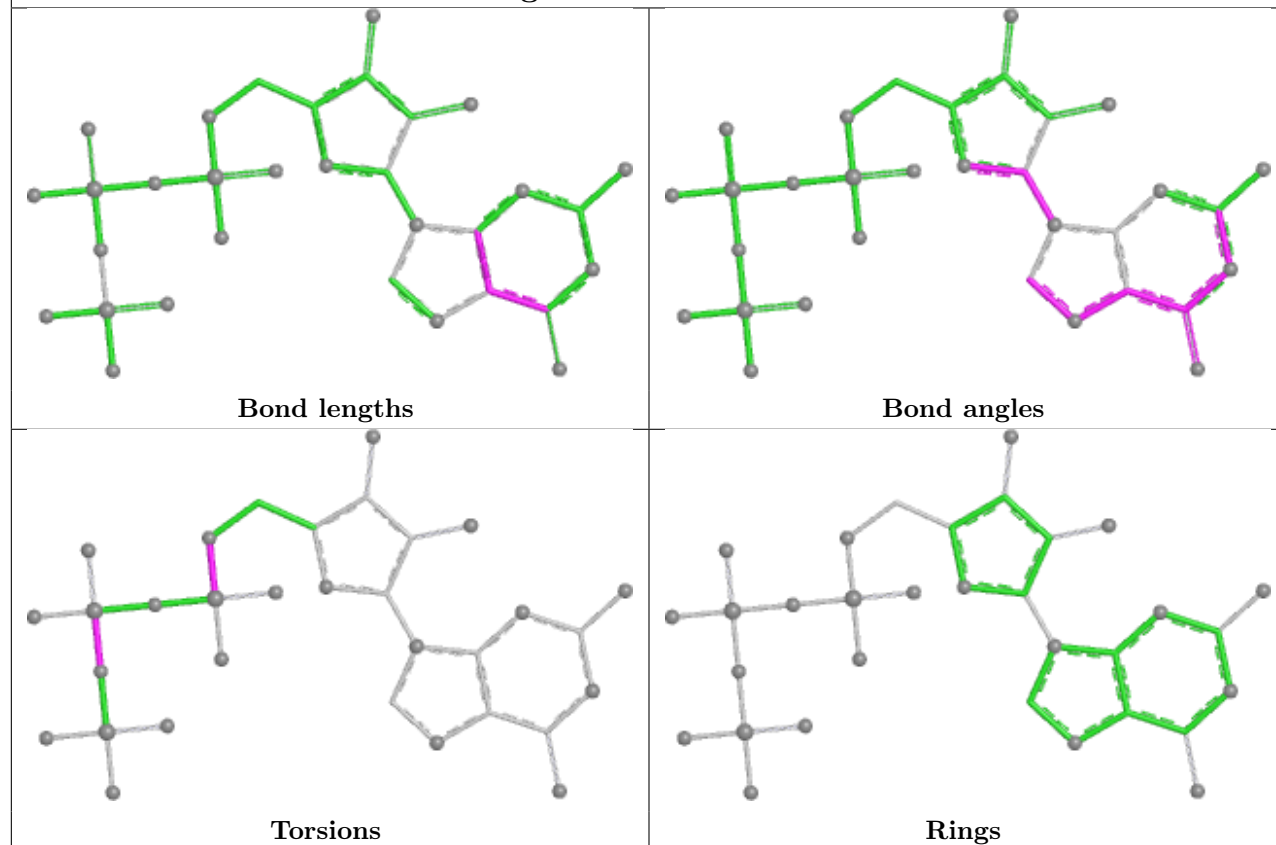




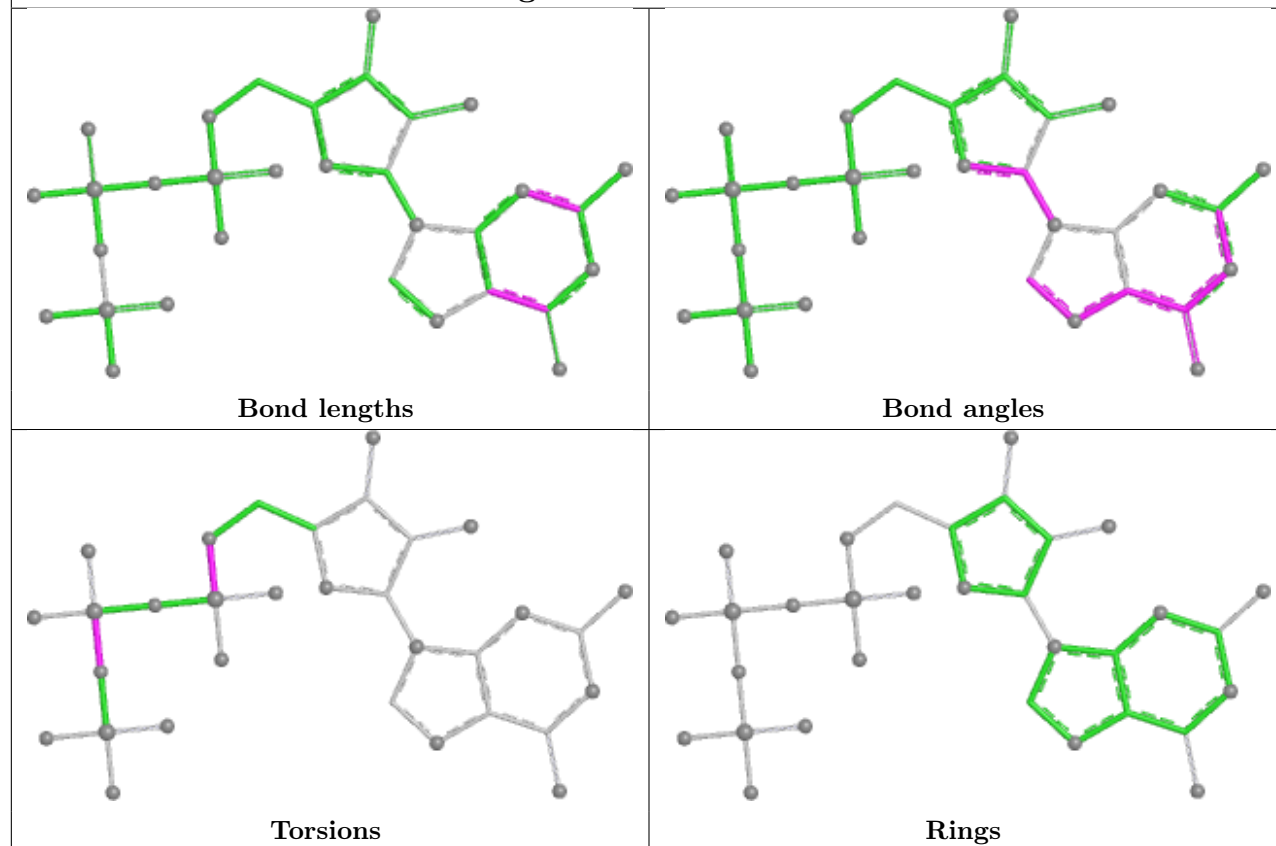




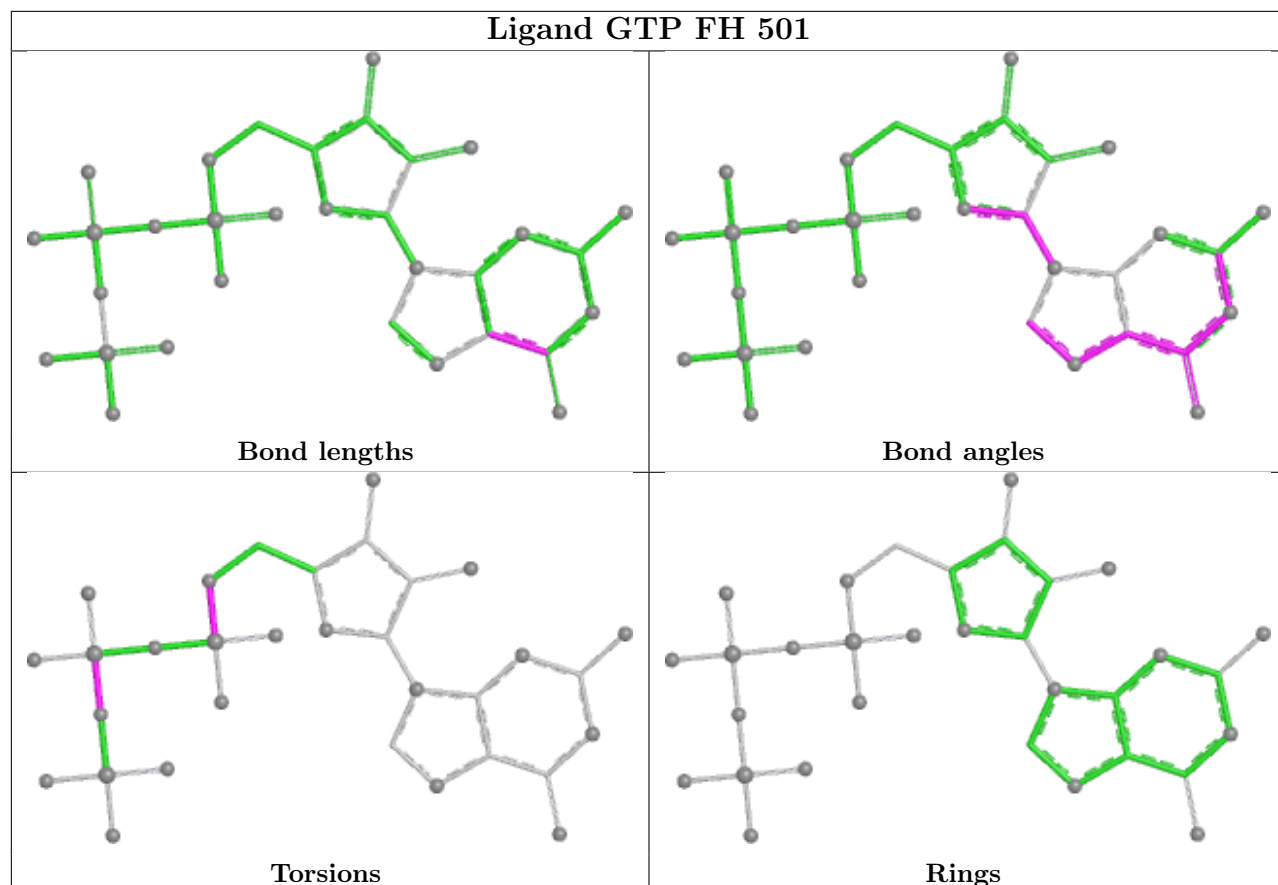
## Ligand GTP CS 501



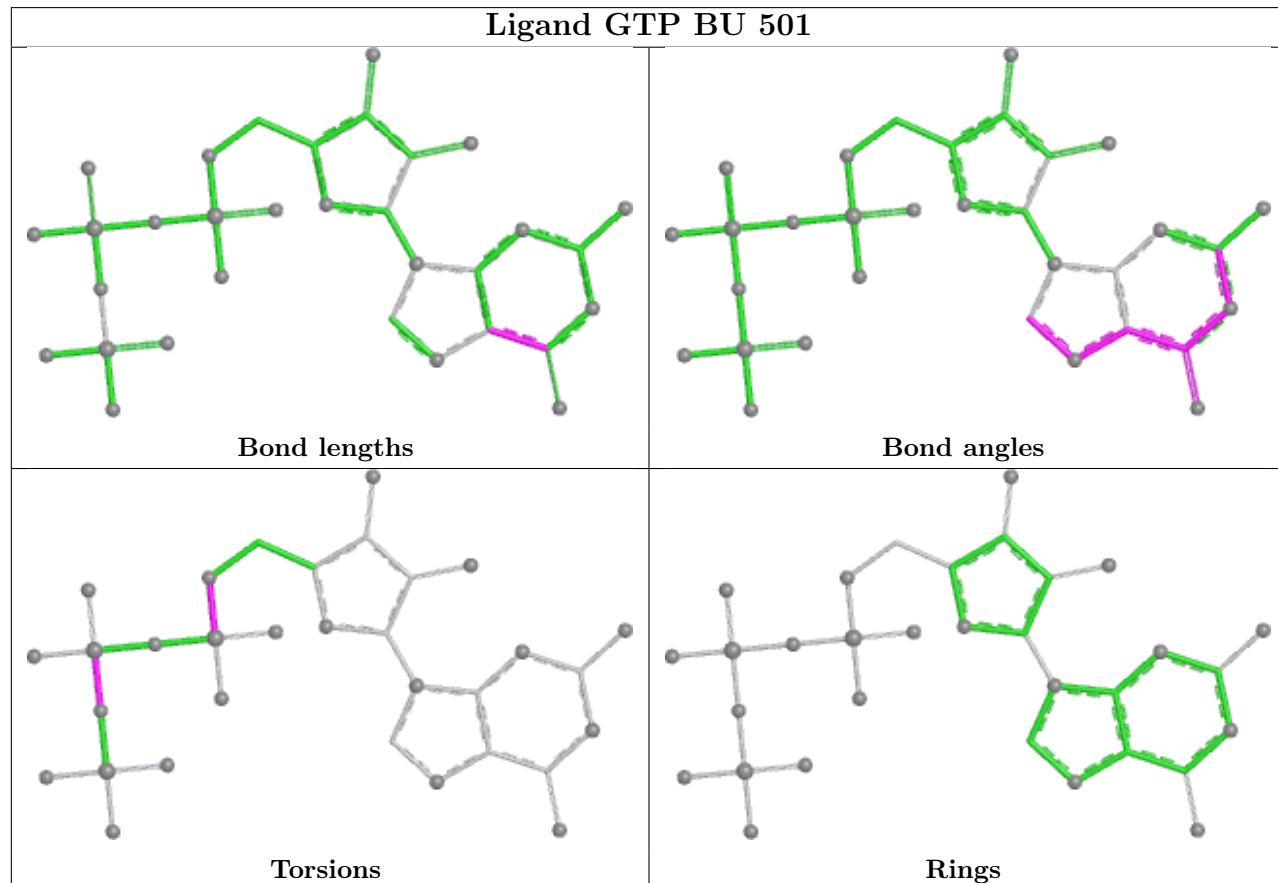
## Ligand GTP EV 501



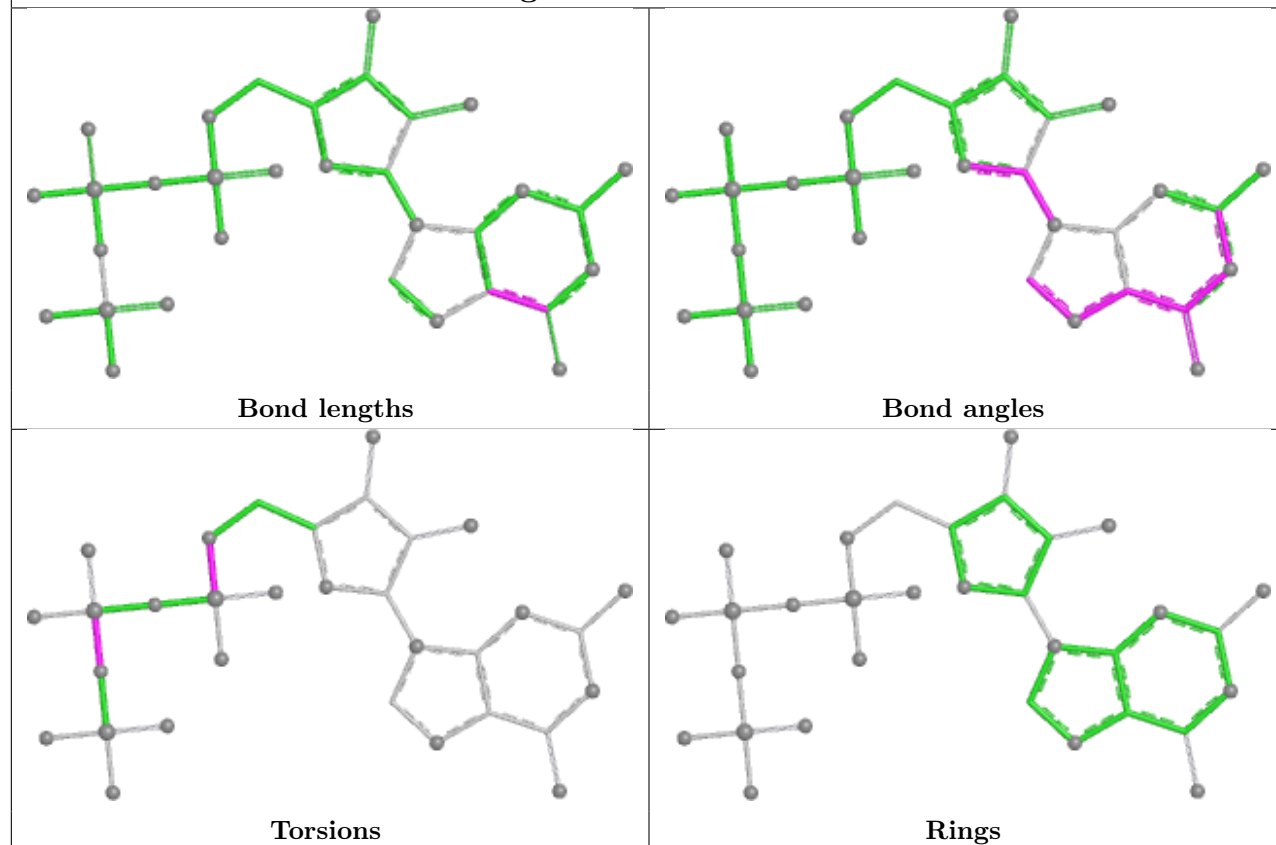
## Ligand GTP FH 501



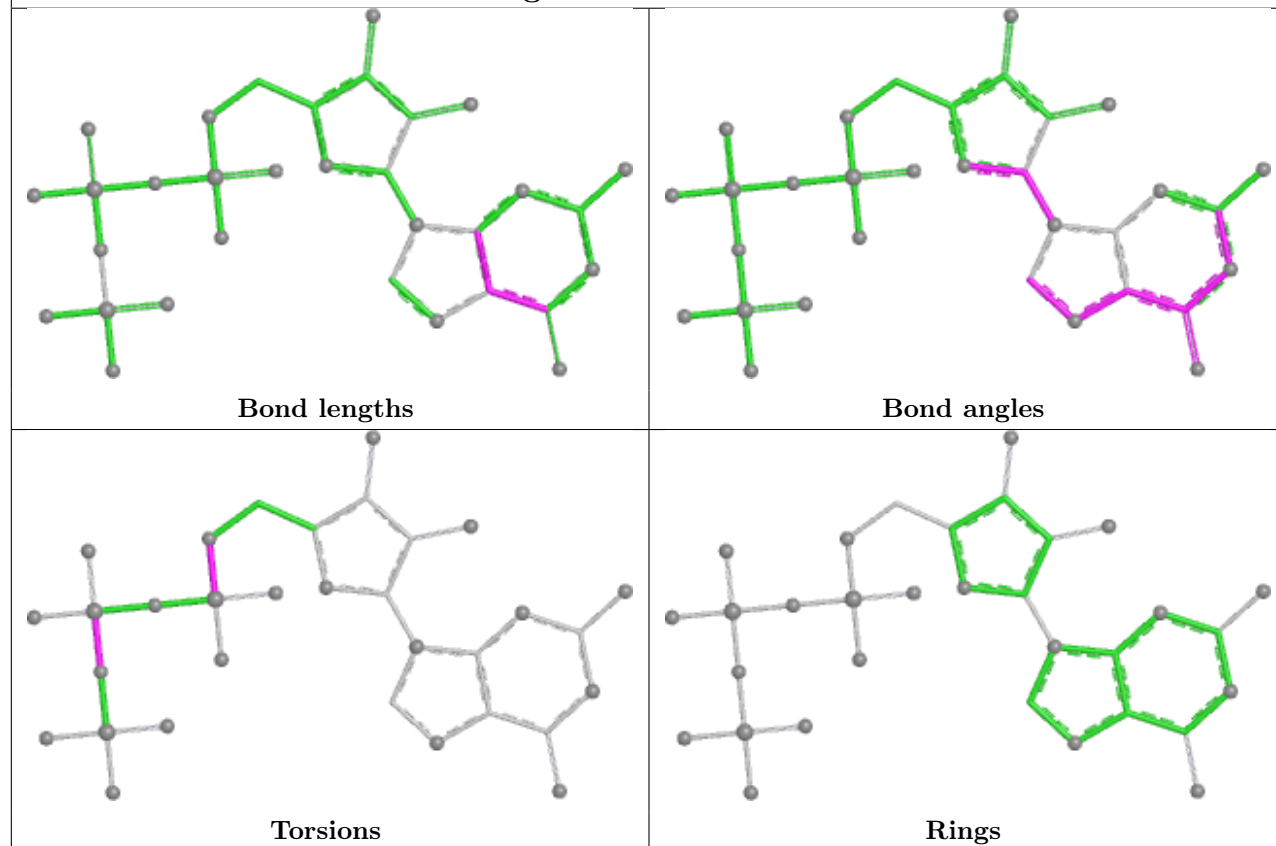
## Ligand GTP BU 501



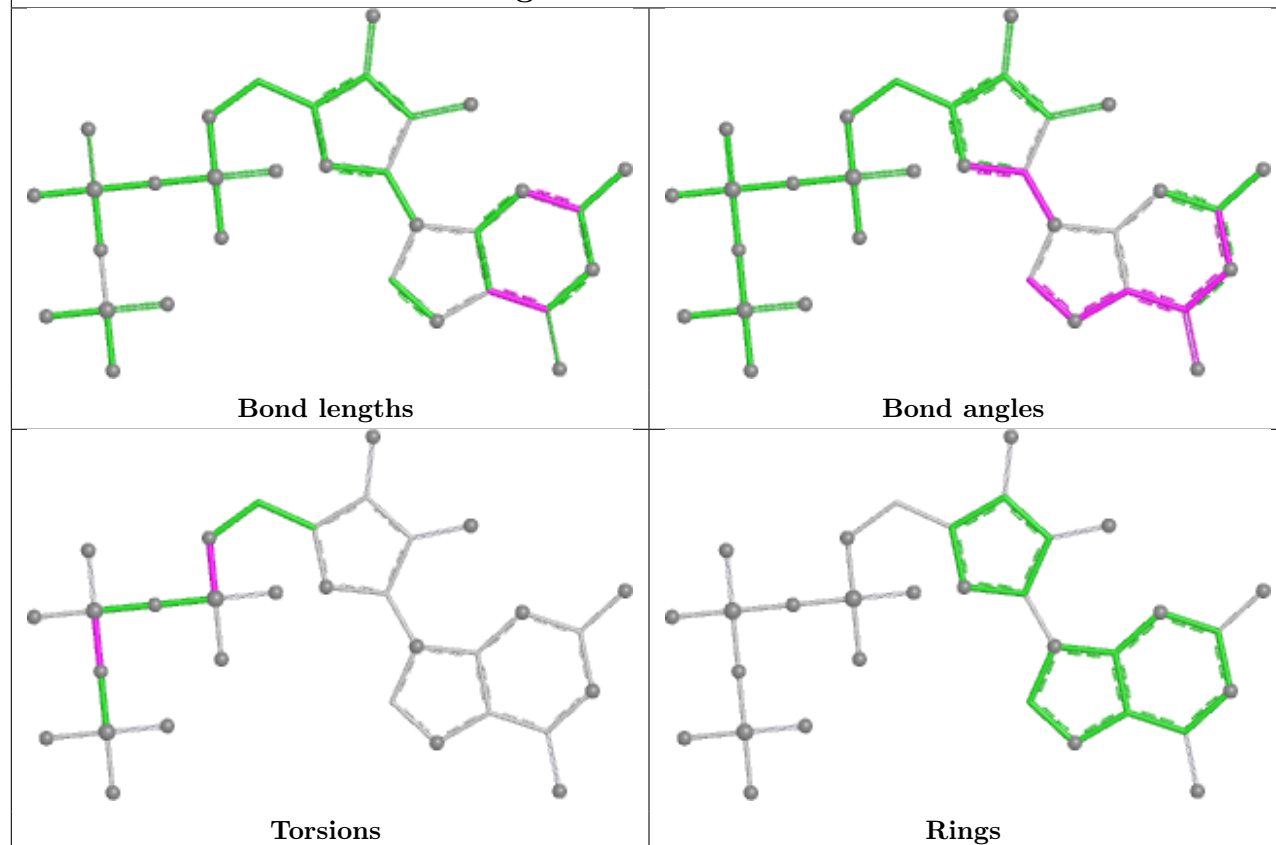
## Ligand GTP BZ 501



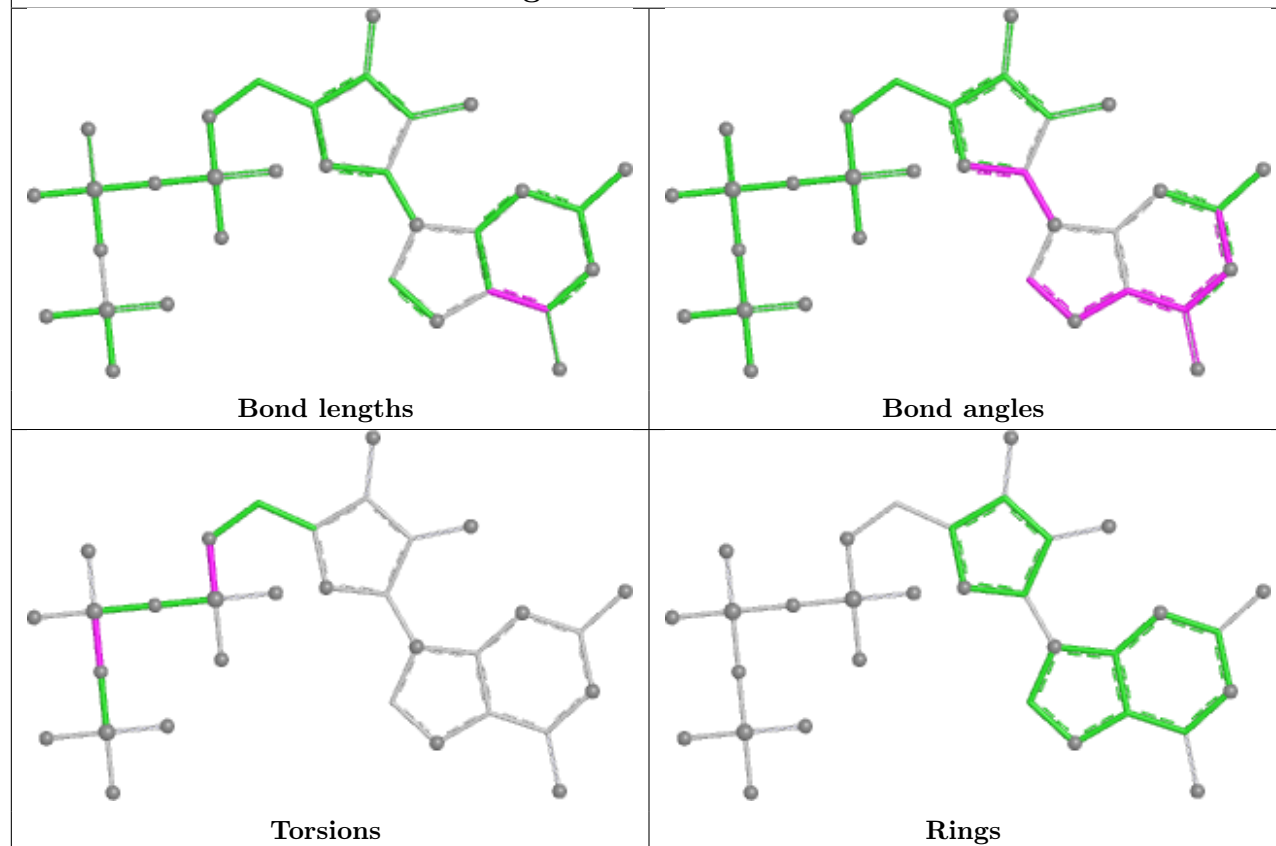
## Ligand GTP ID 501



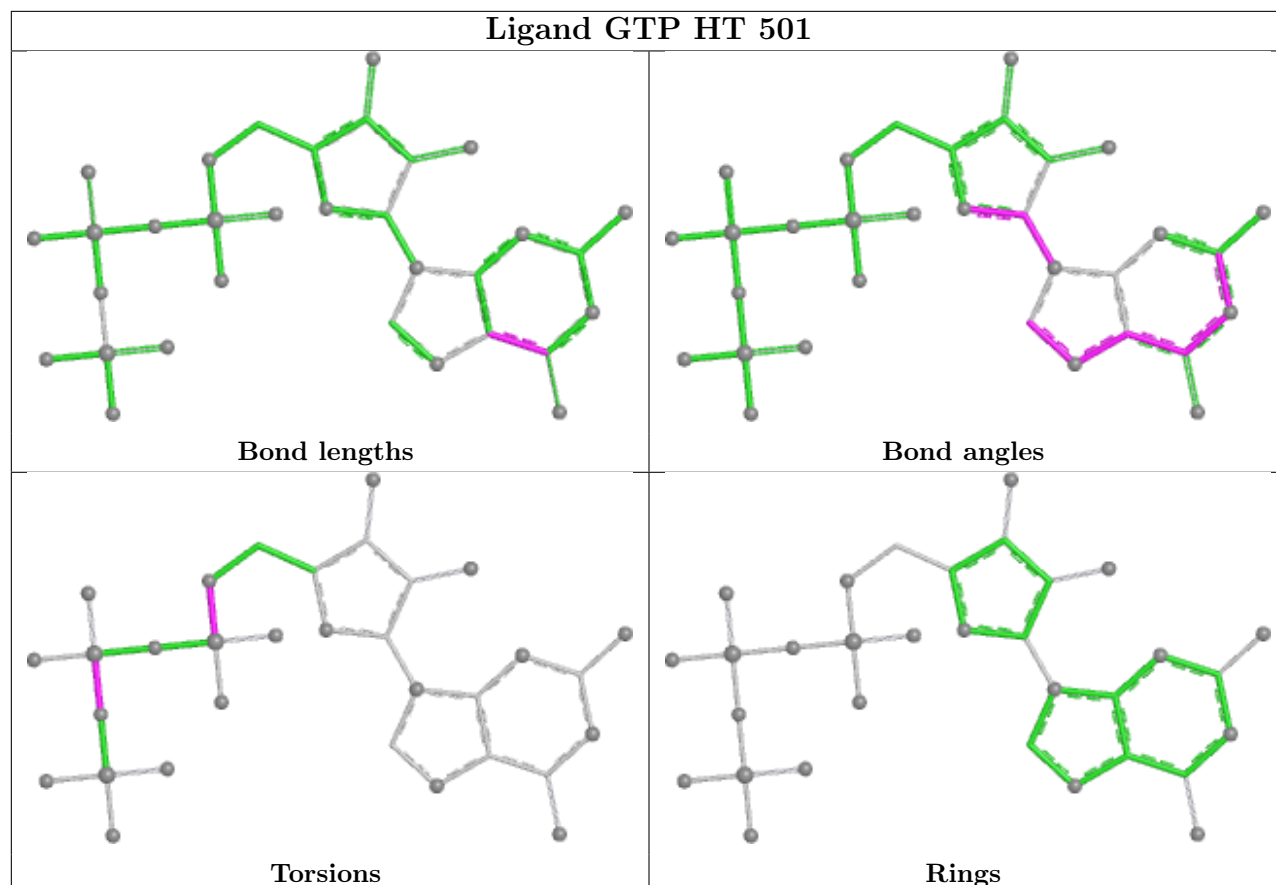
## Ligand GTP HA 501



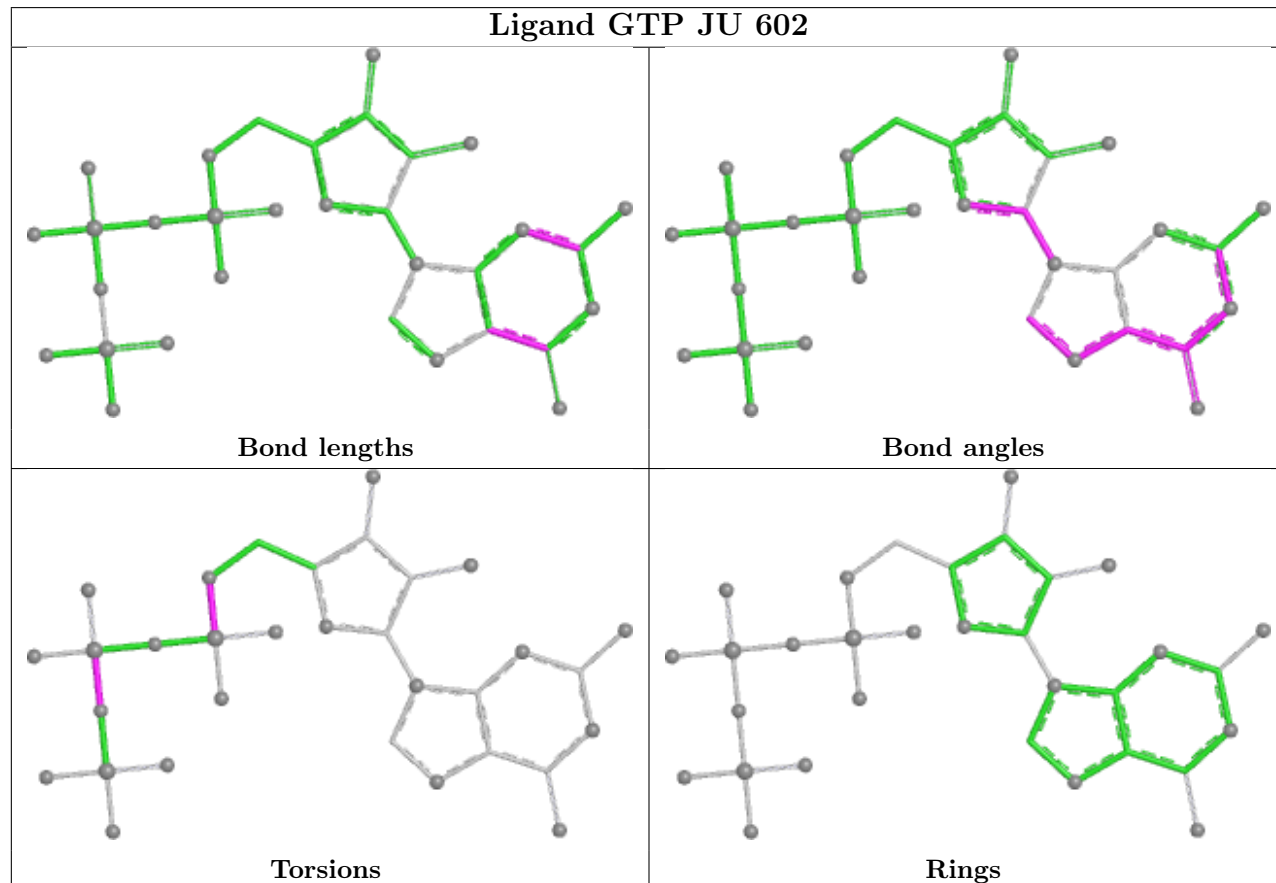
## Ligand GTP IG 501



## Ligand GTP HT 501

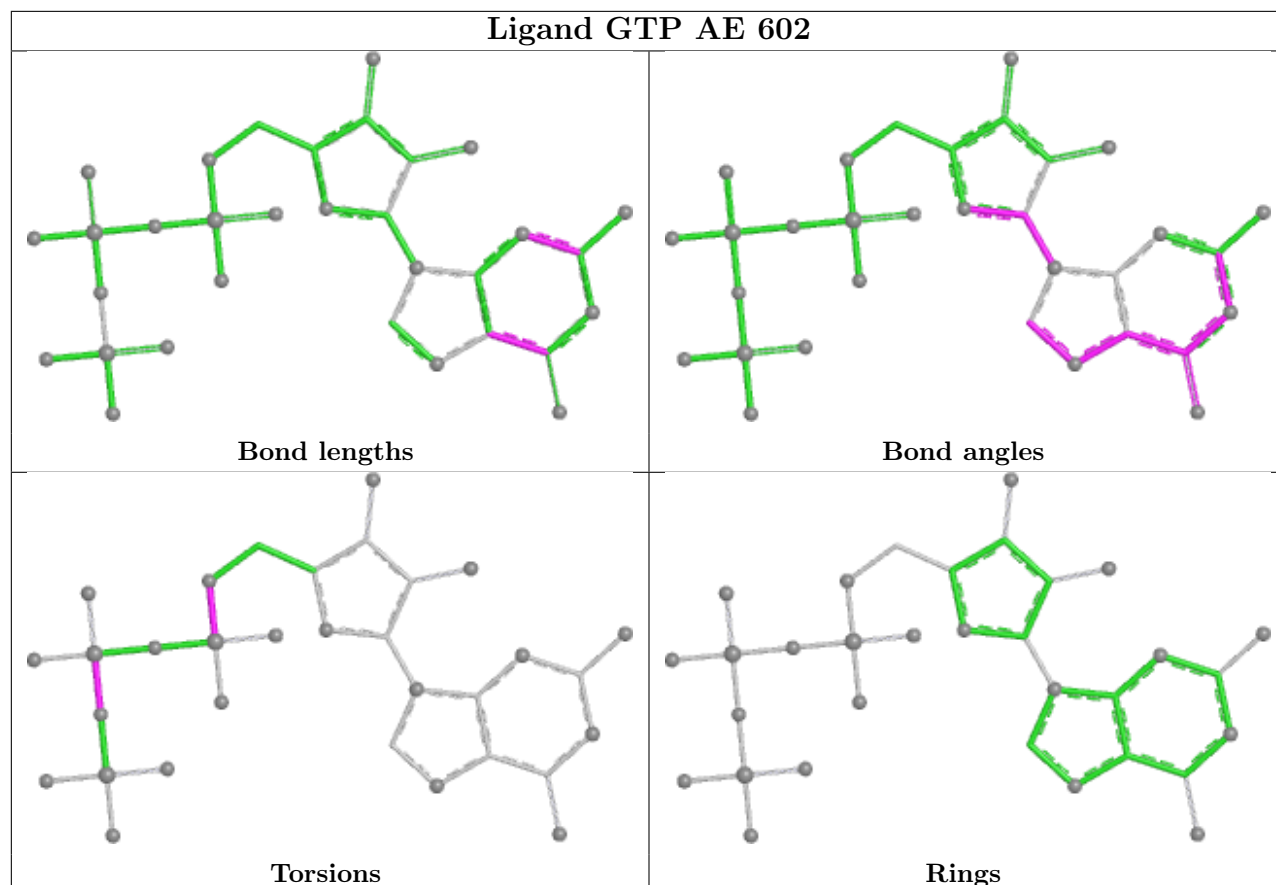


## Ligand GTP JU 602

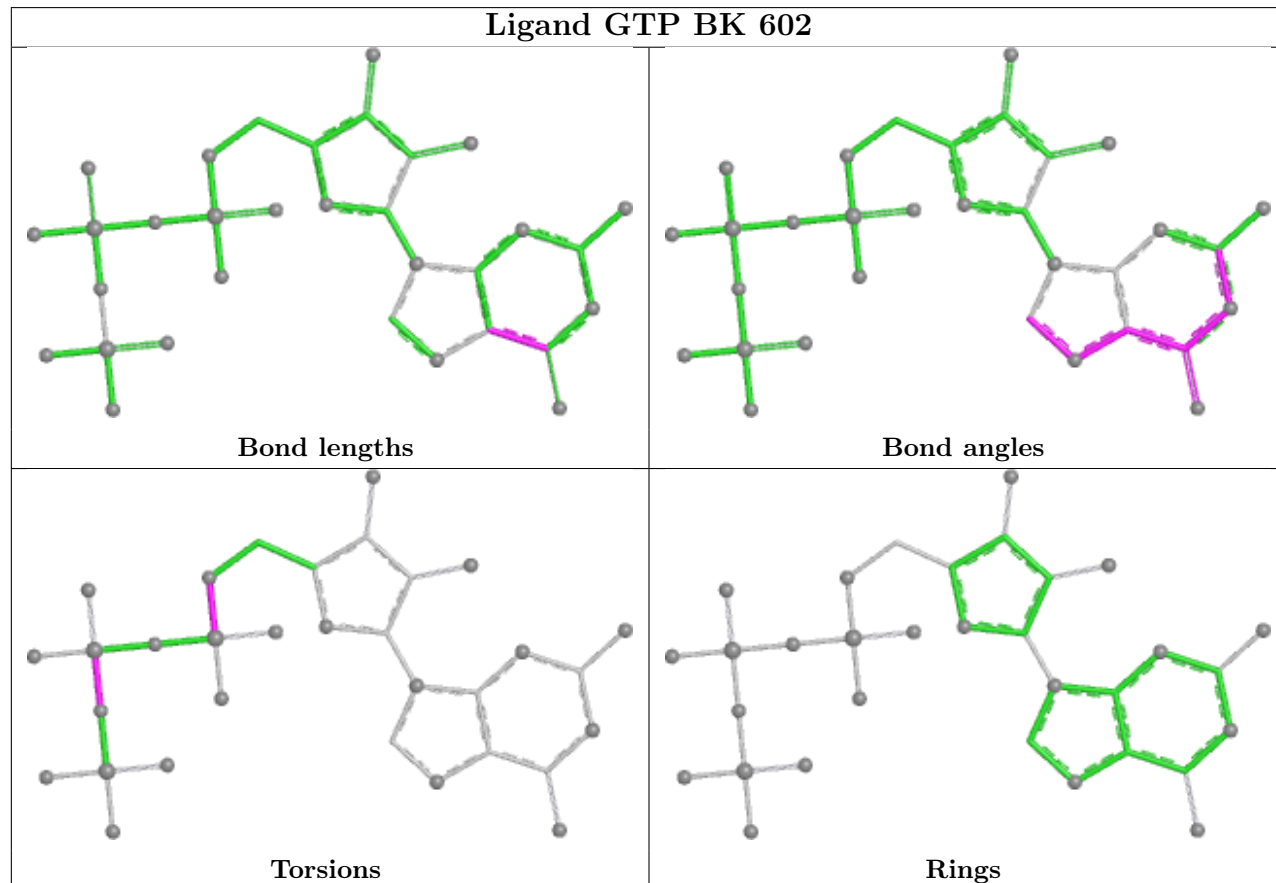




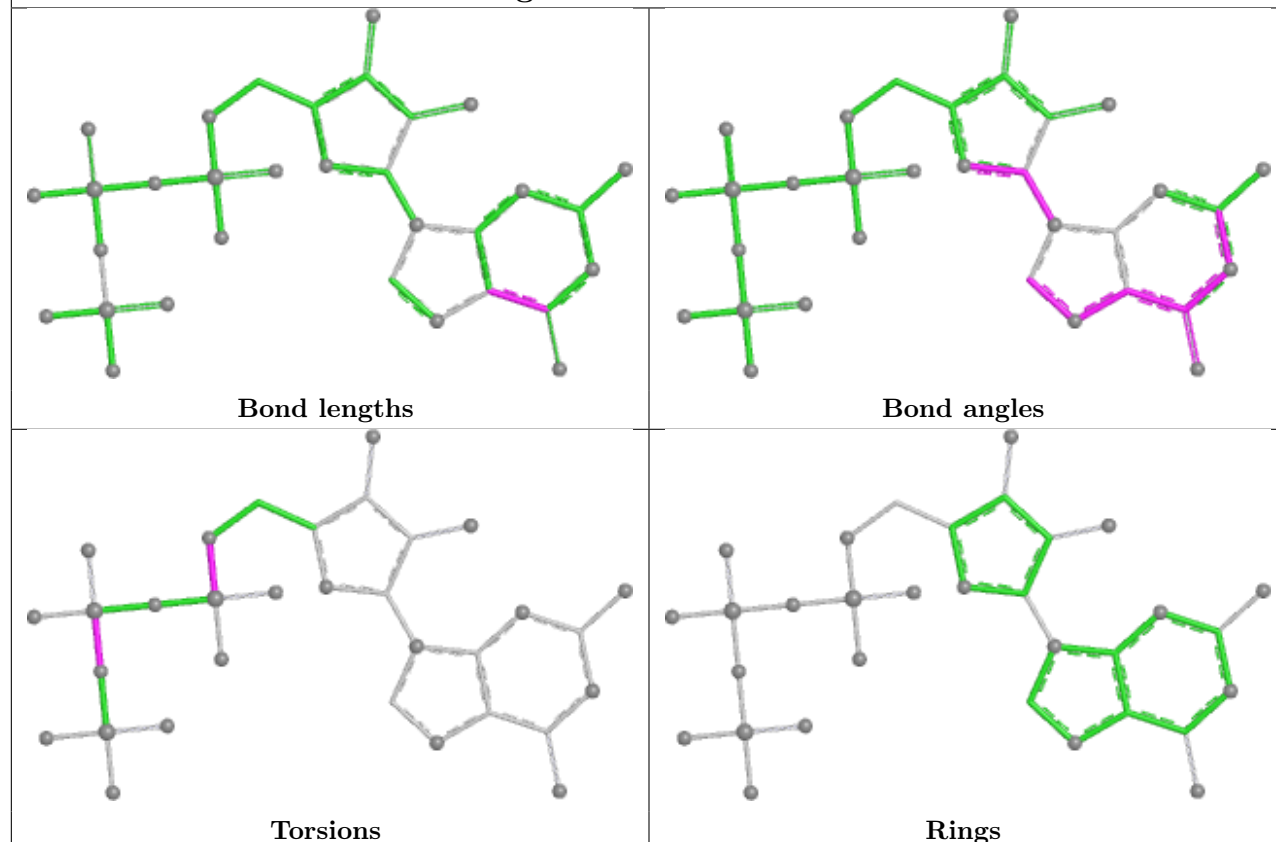
## Ligand GTP AE 602



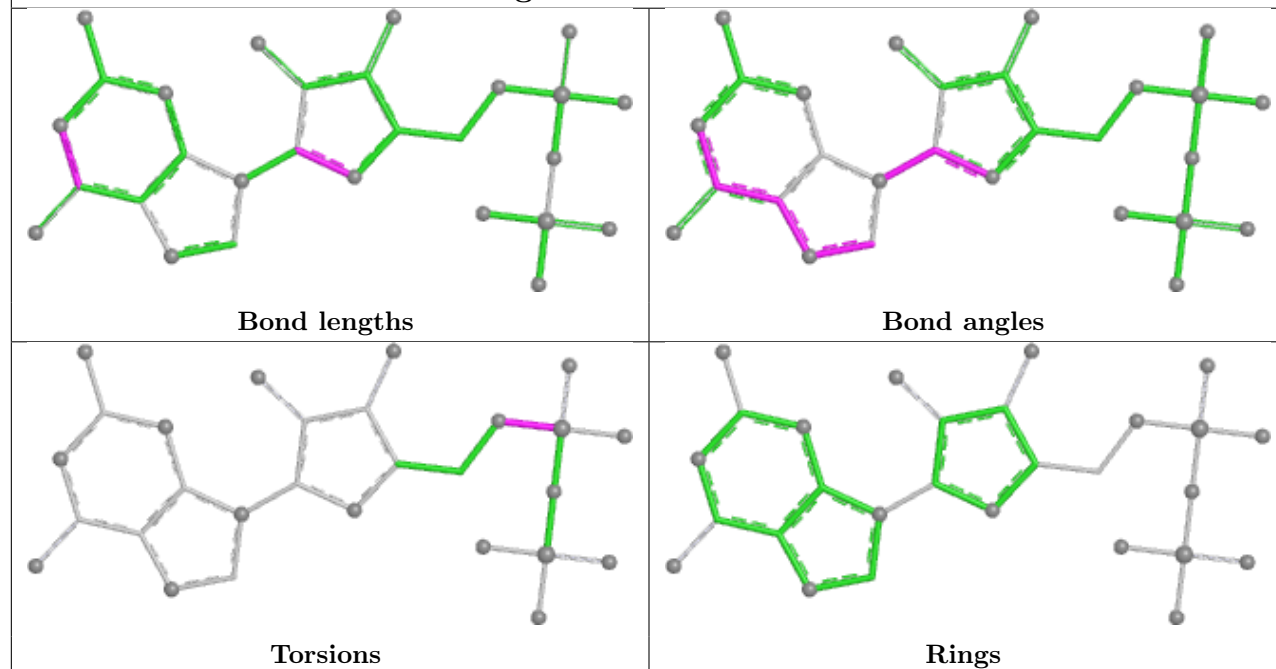
## Ligand GTP BK 602



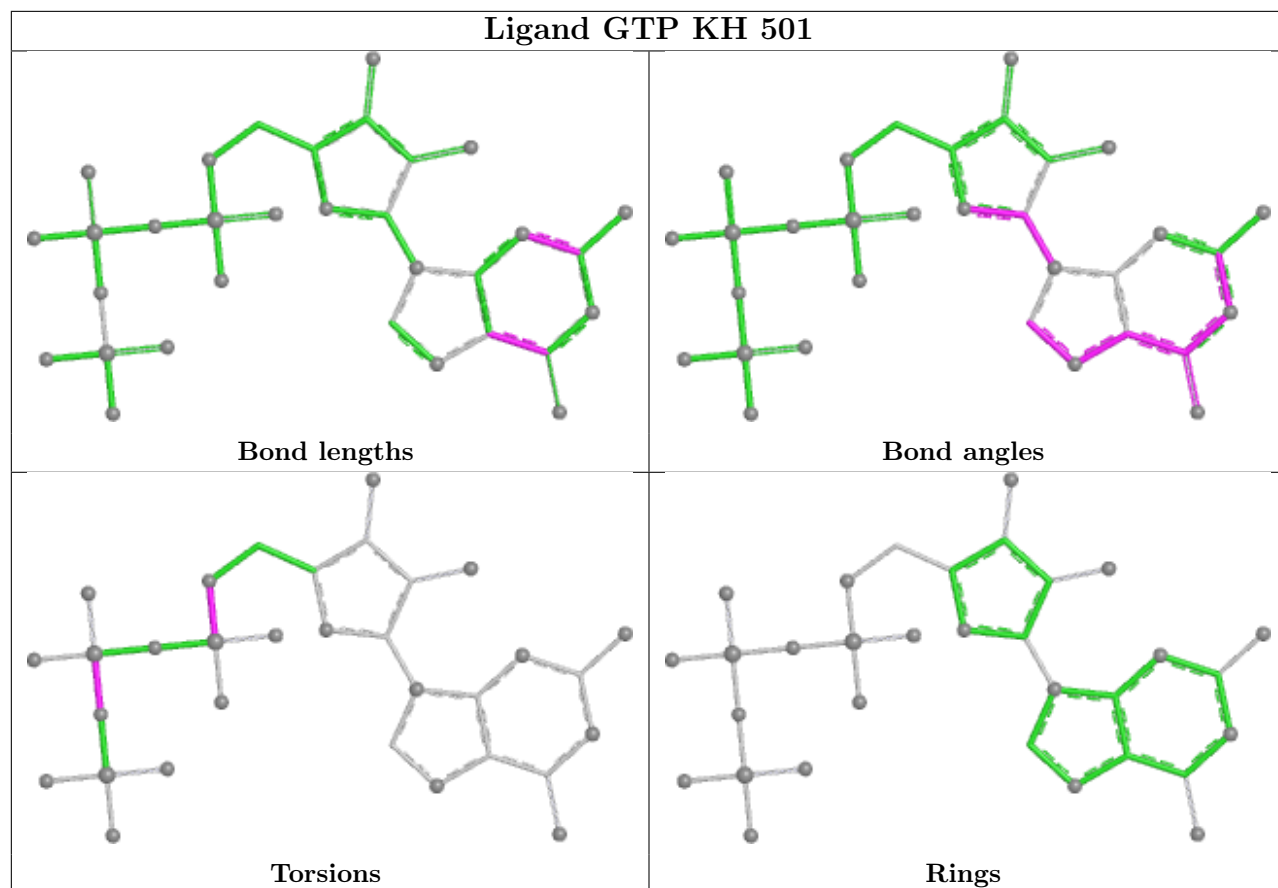
## Ligand GTP HX 501



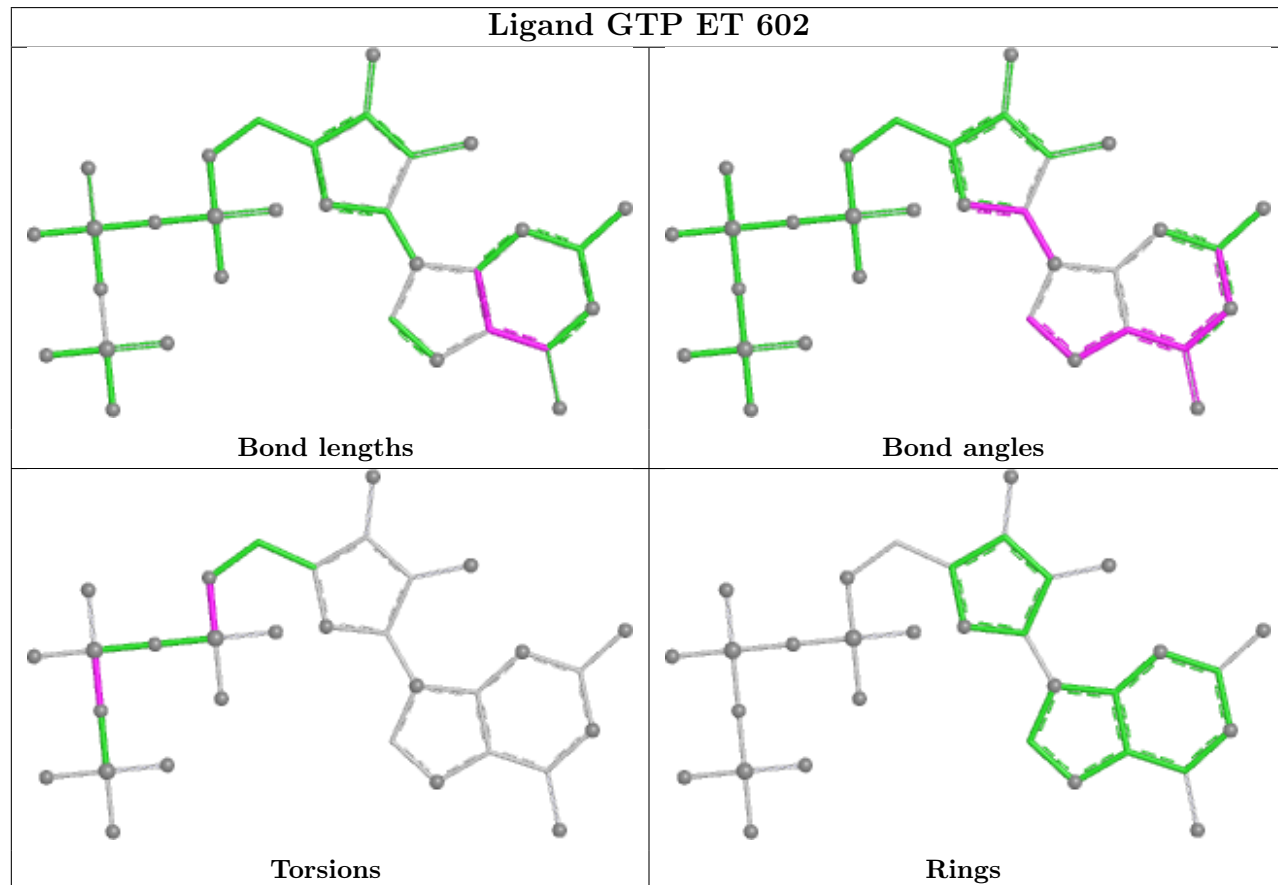
## Ligand GDP AD 501

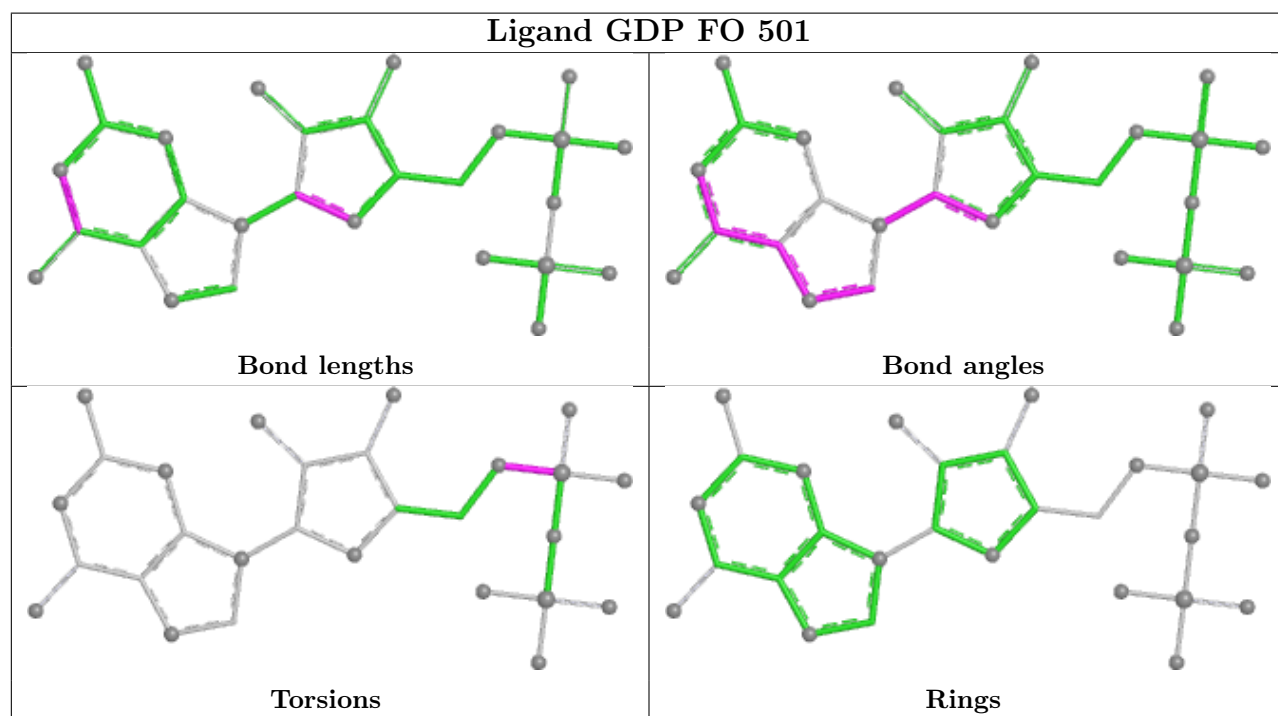
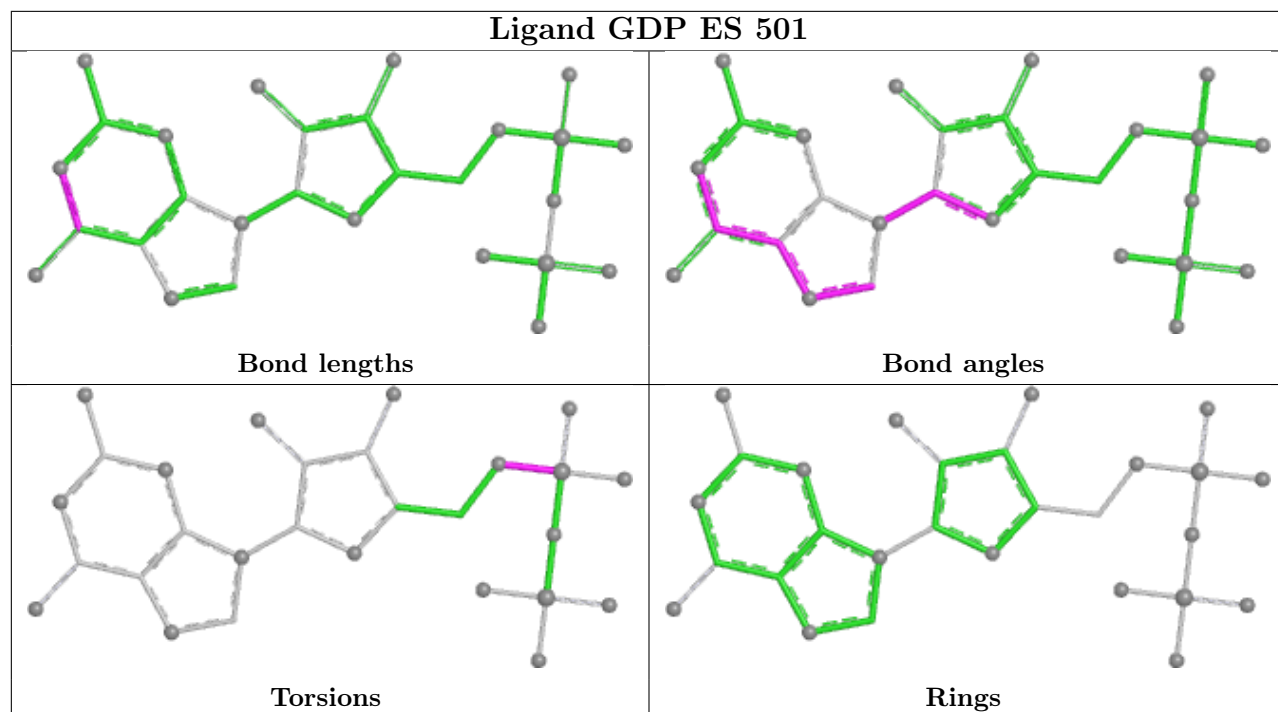


## Ligand GTP KH 501

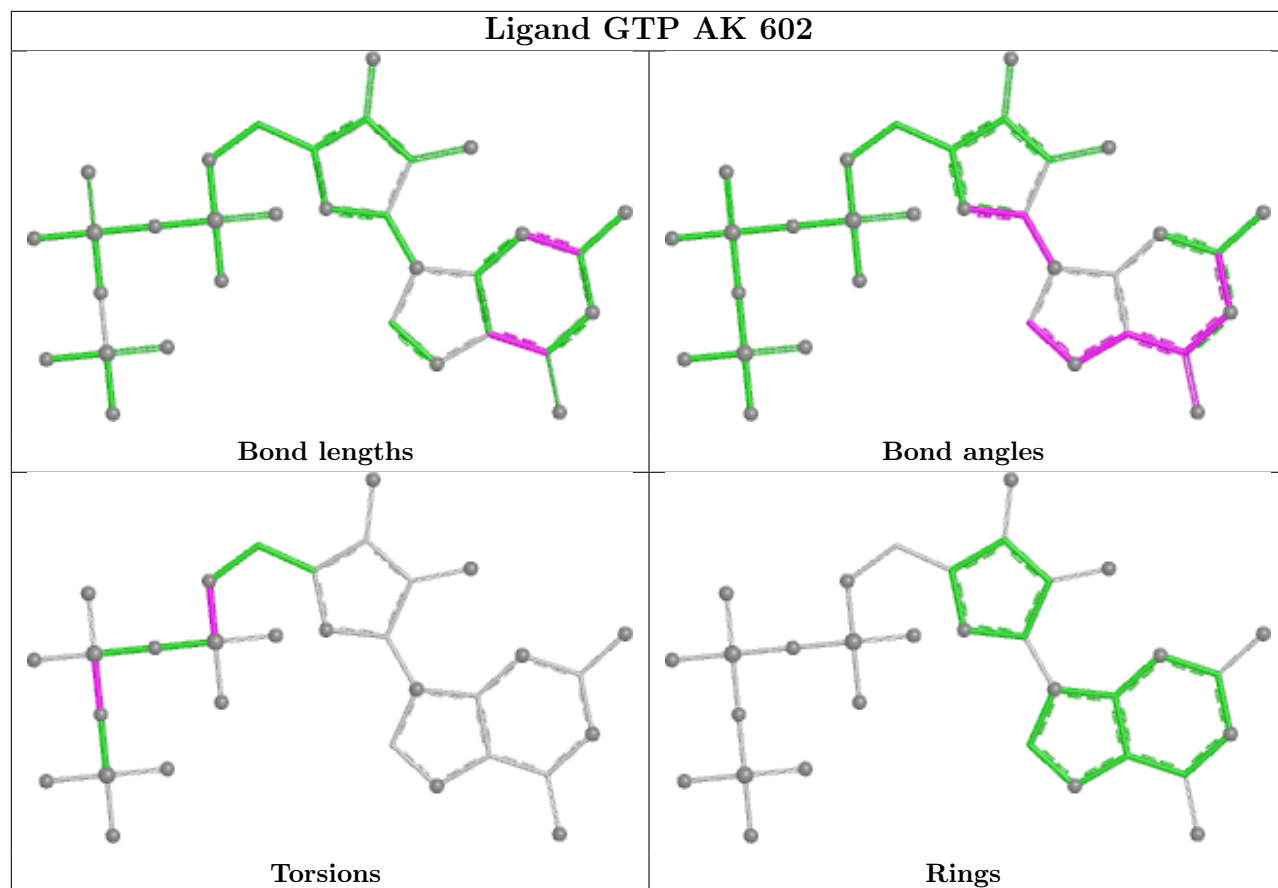


## Ligand GTP ET 602

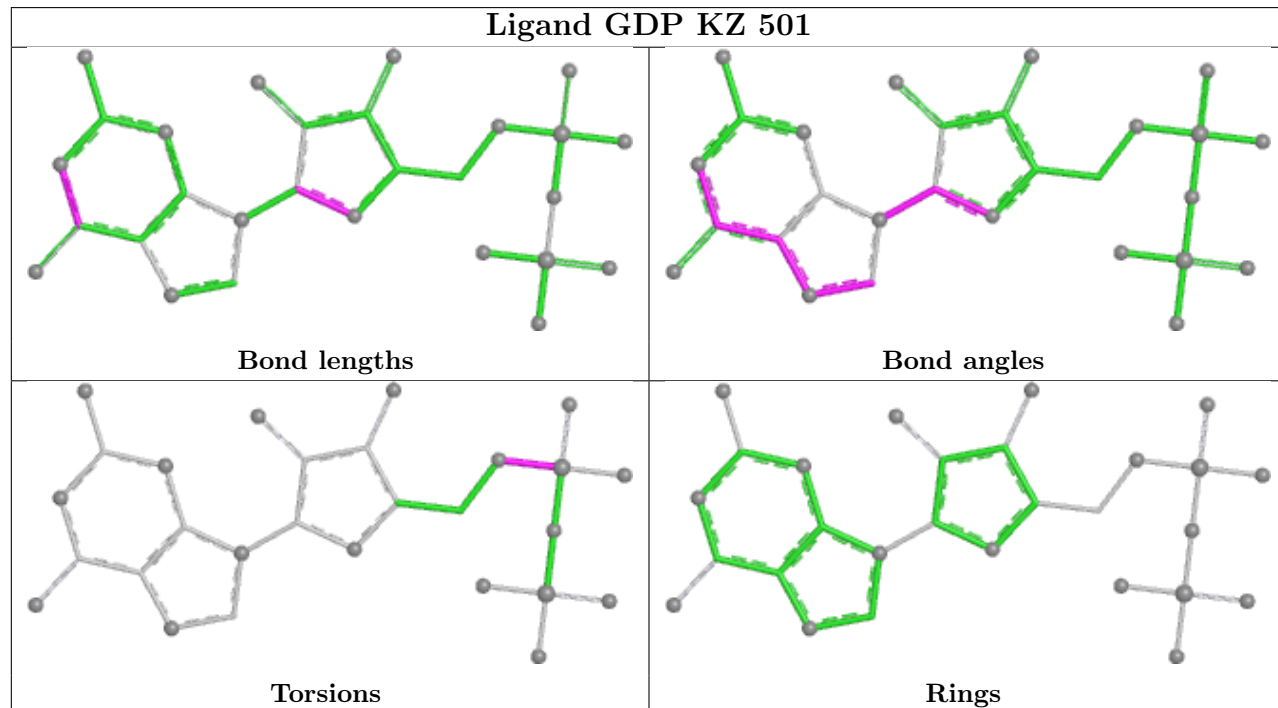


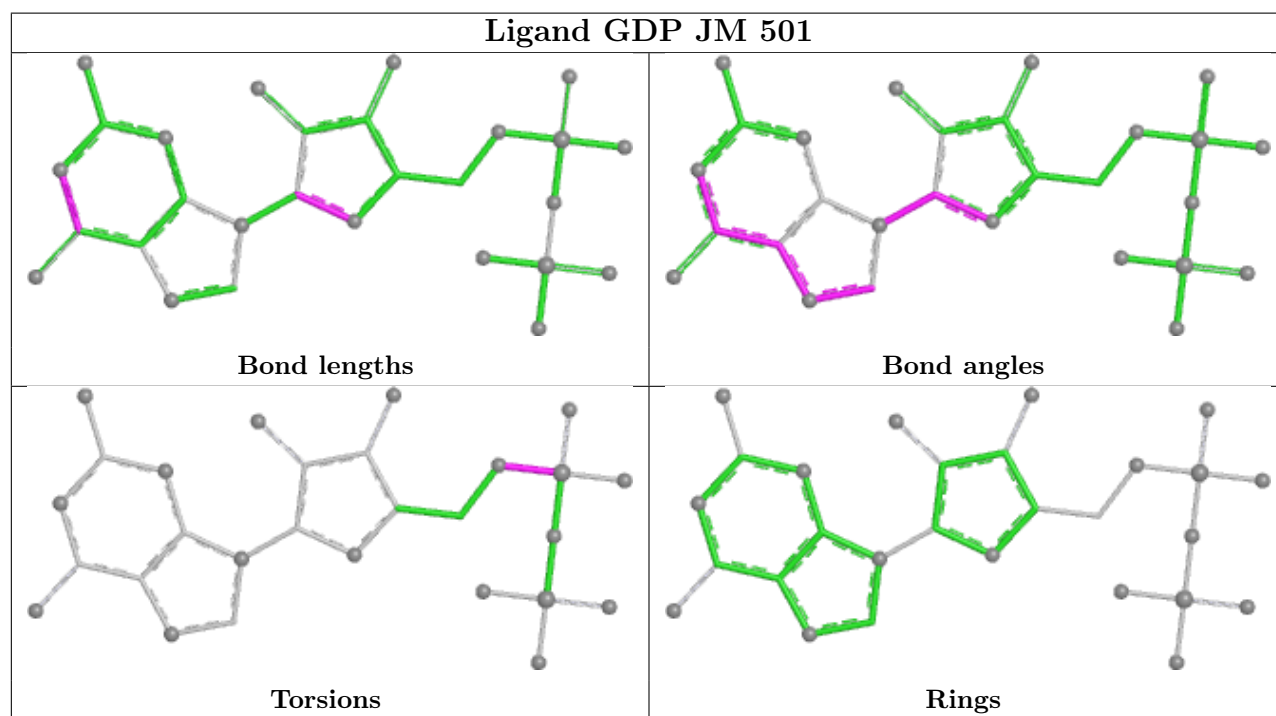
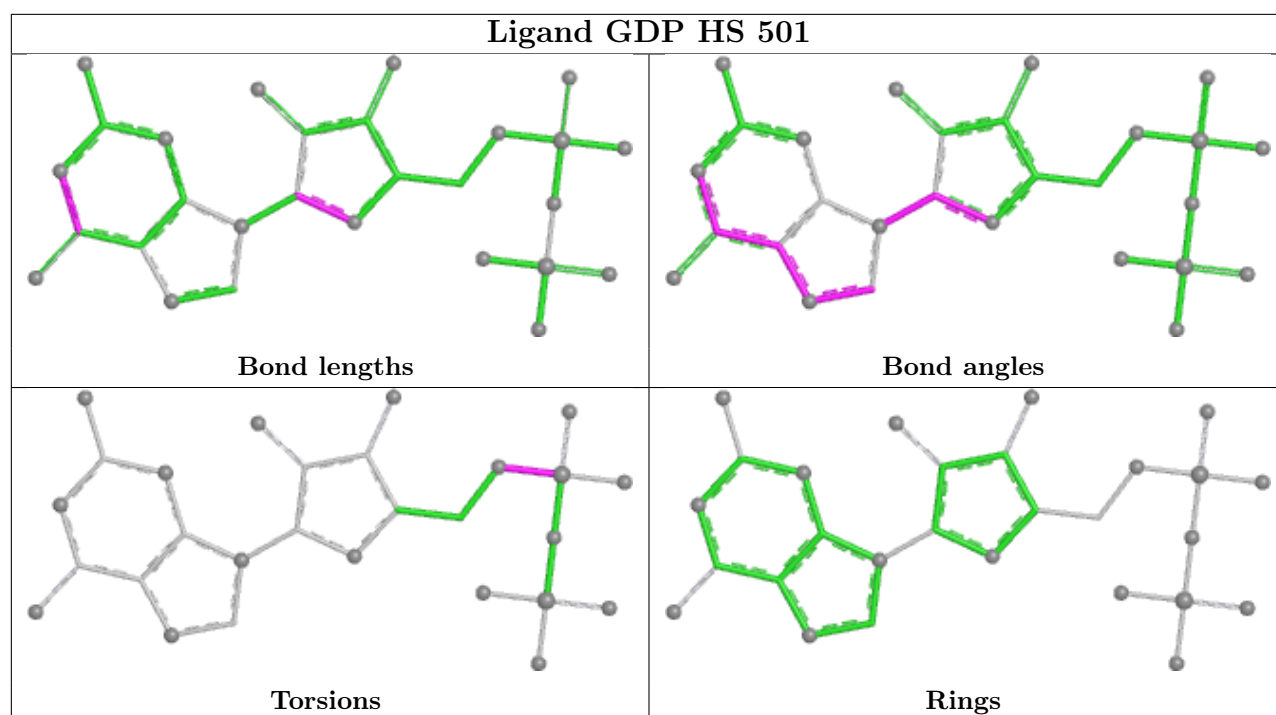


## Ligand GTP AK 602

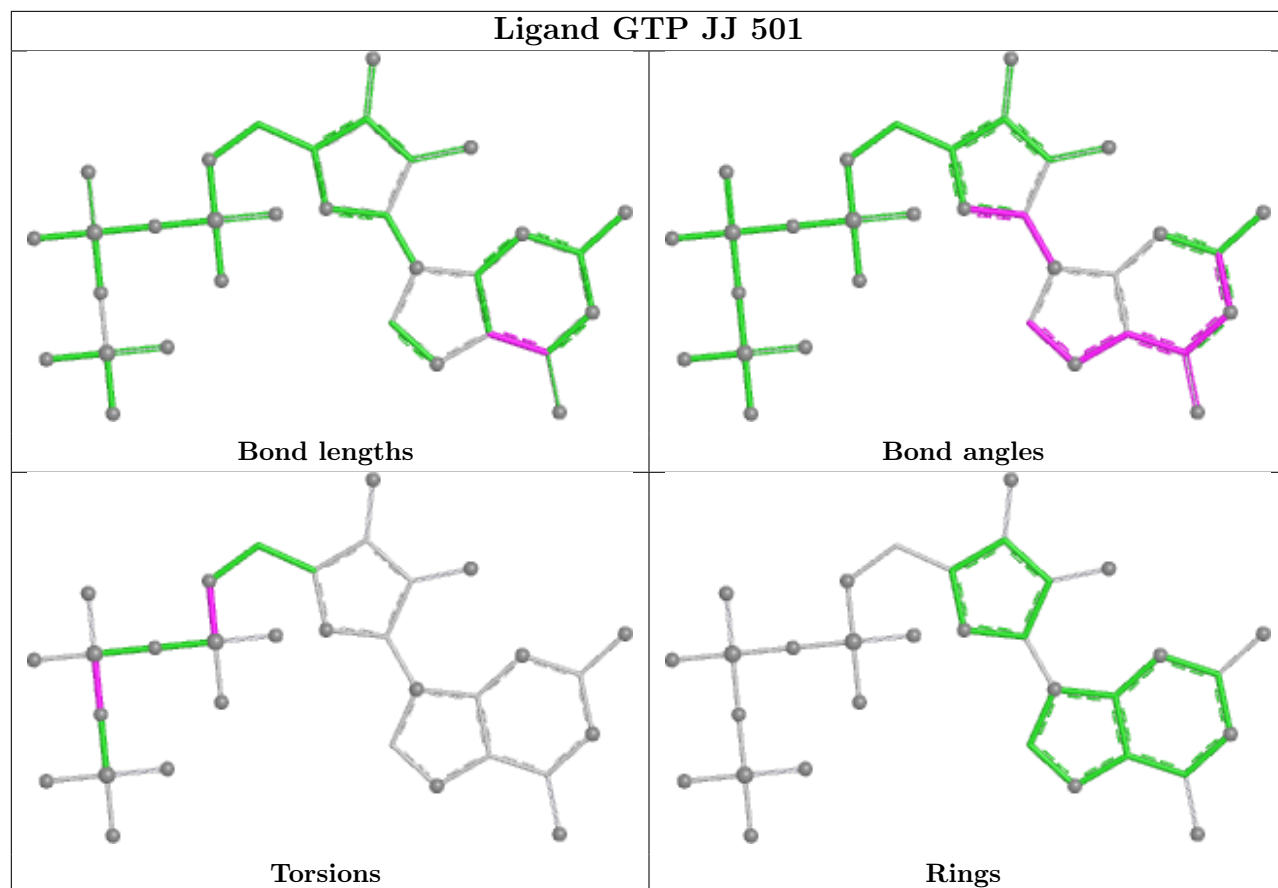


## Ligand GDP KZ 501

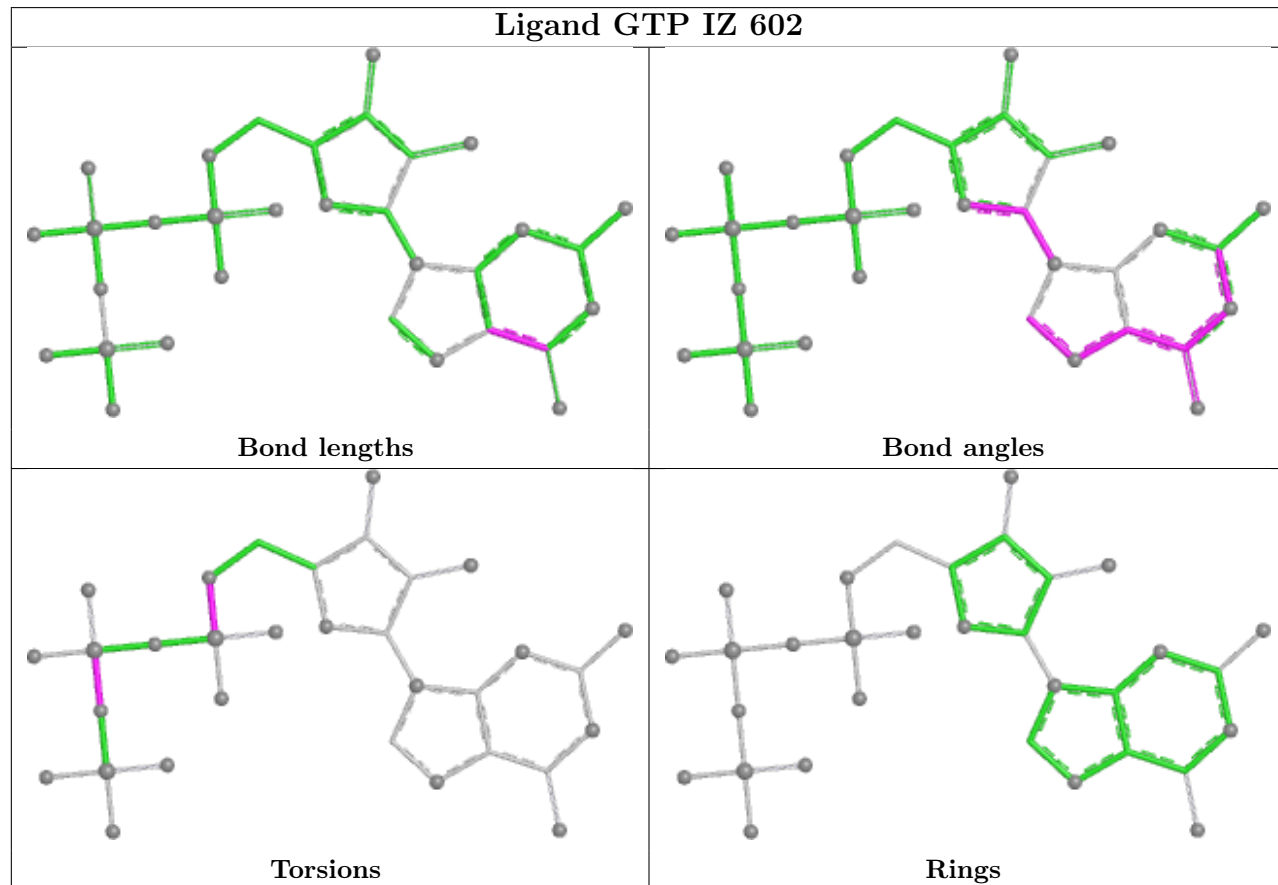


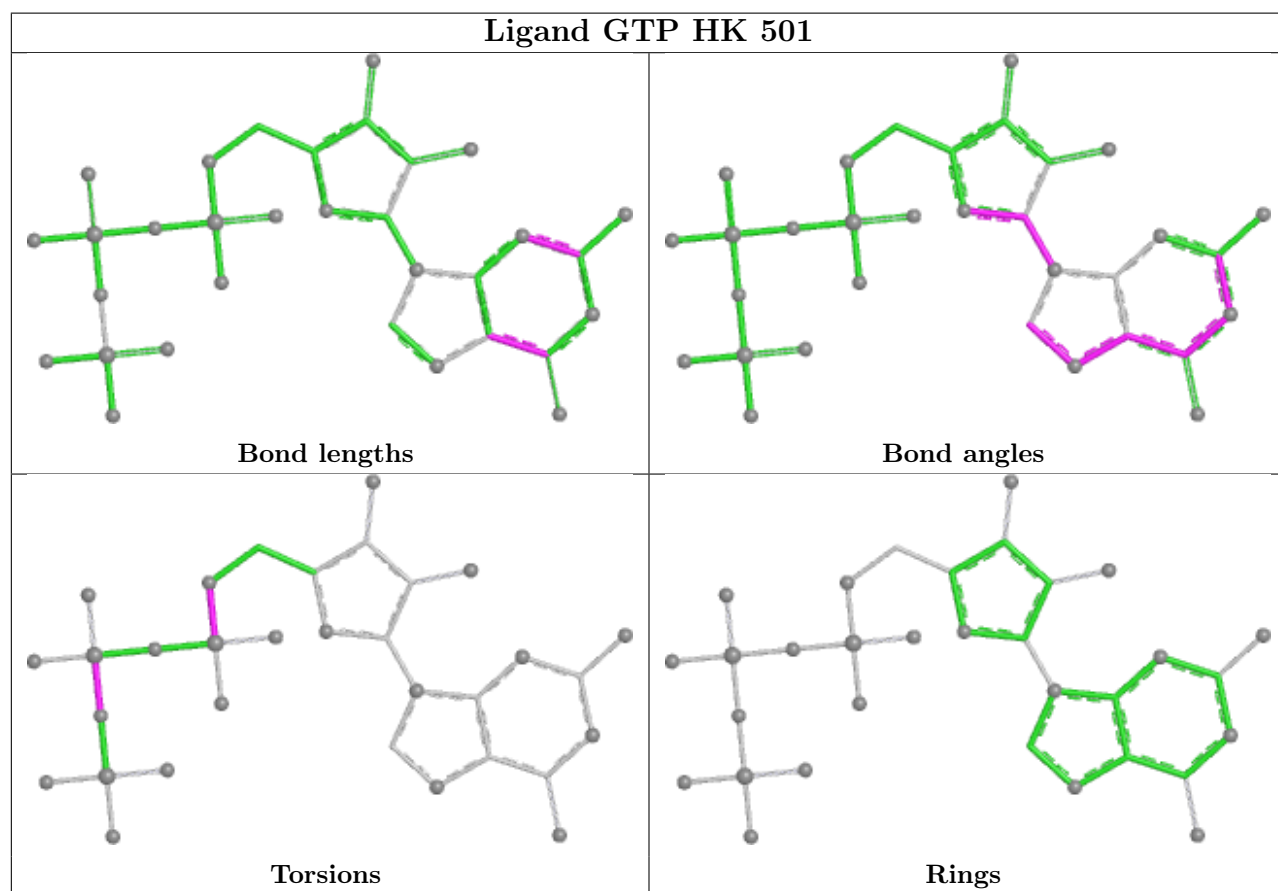
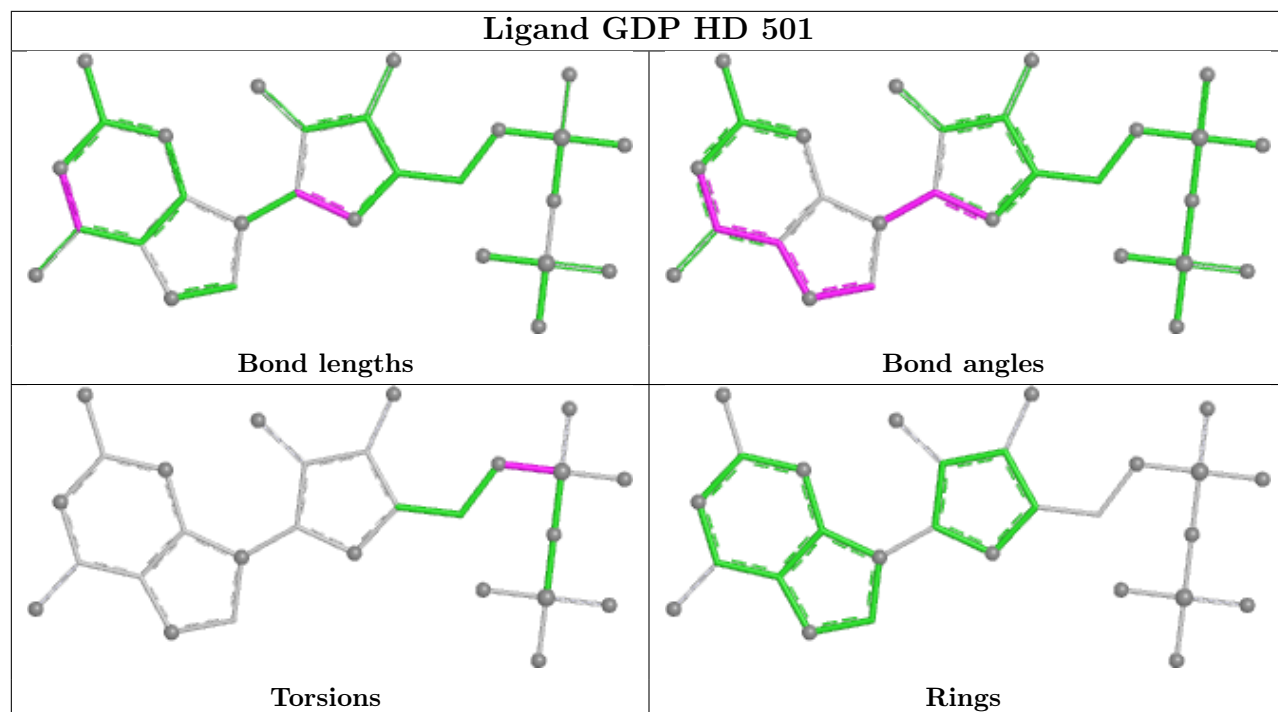


## Ligand GTP JJ 501



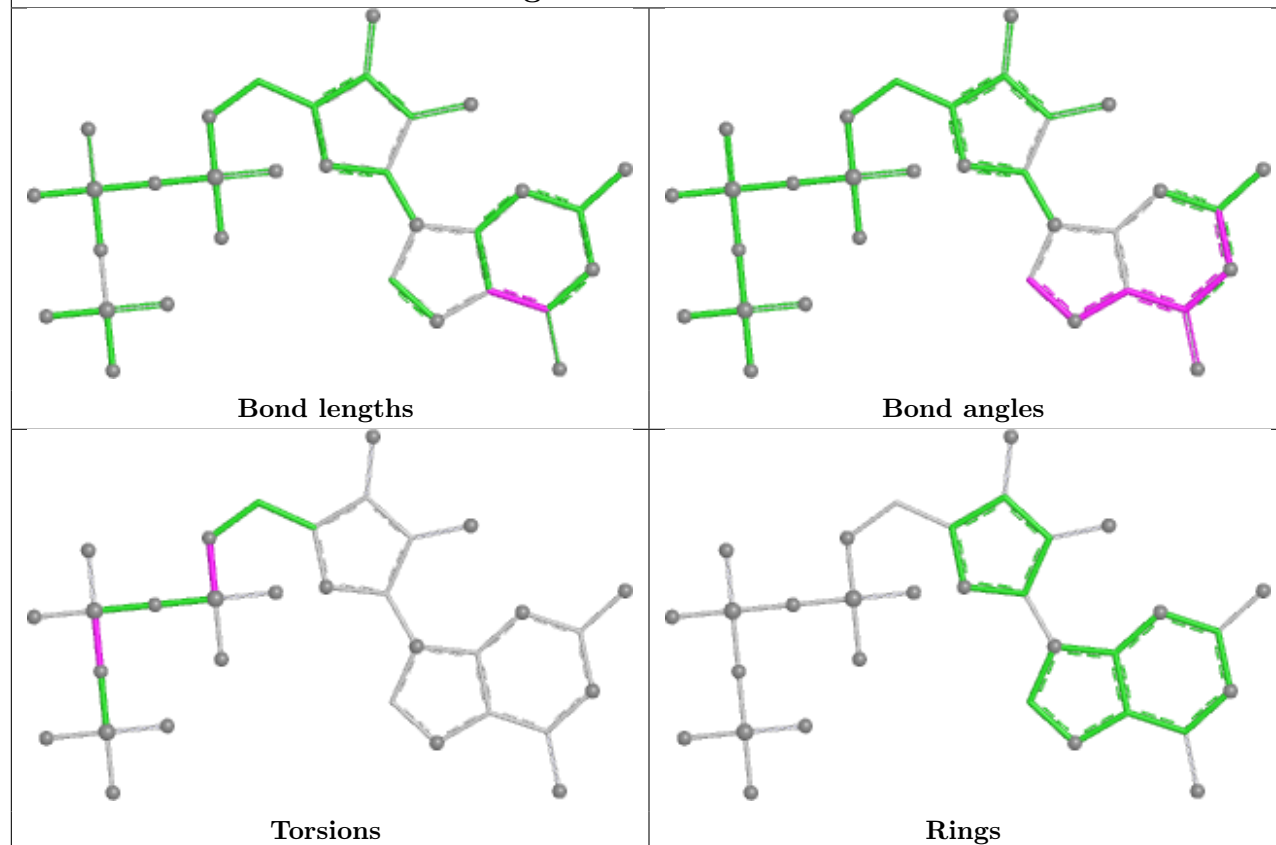
## Ligand GTP IZ 602



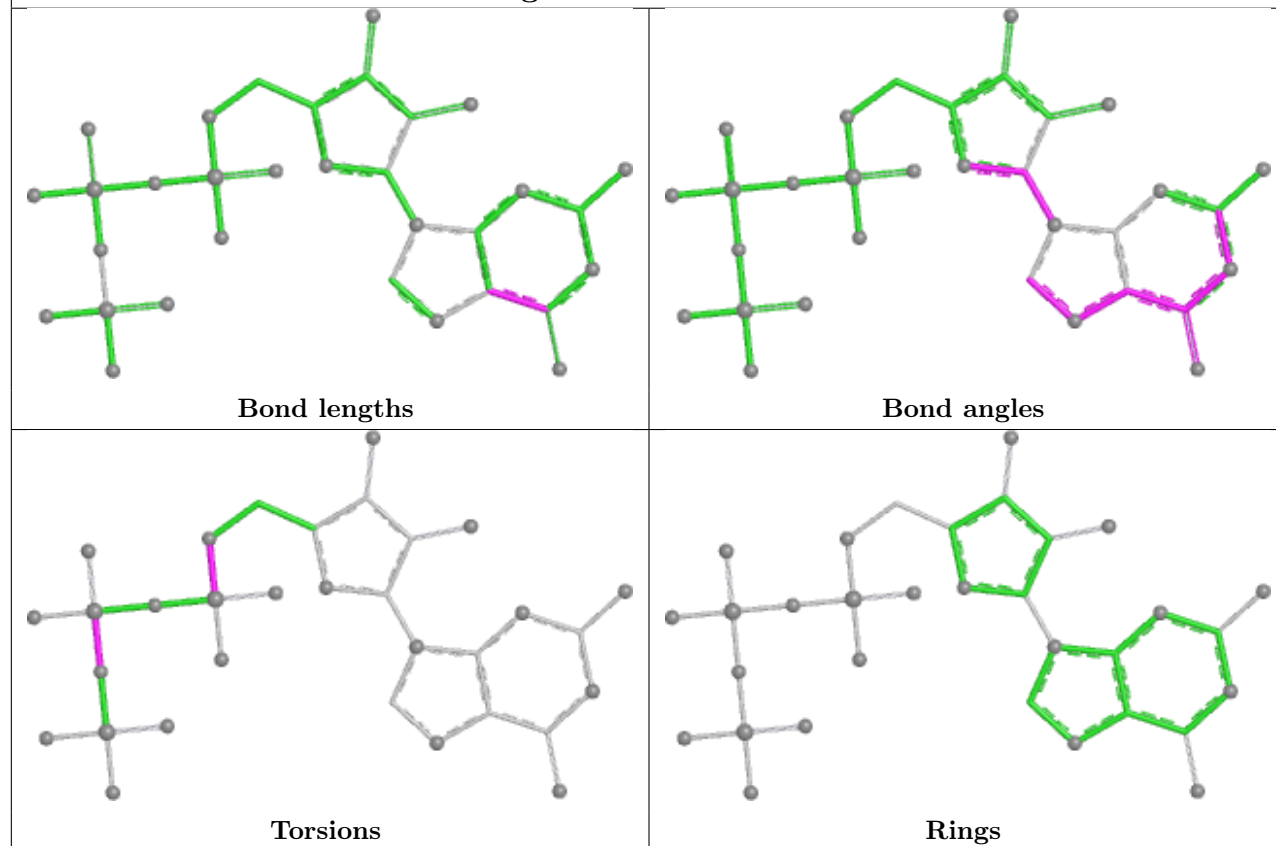




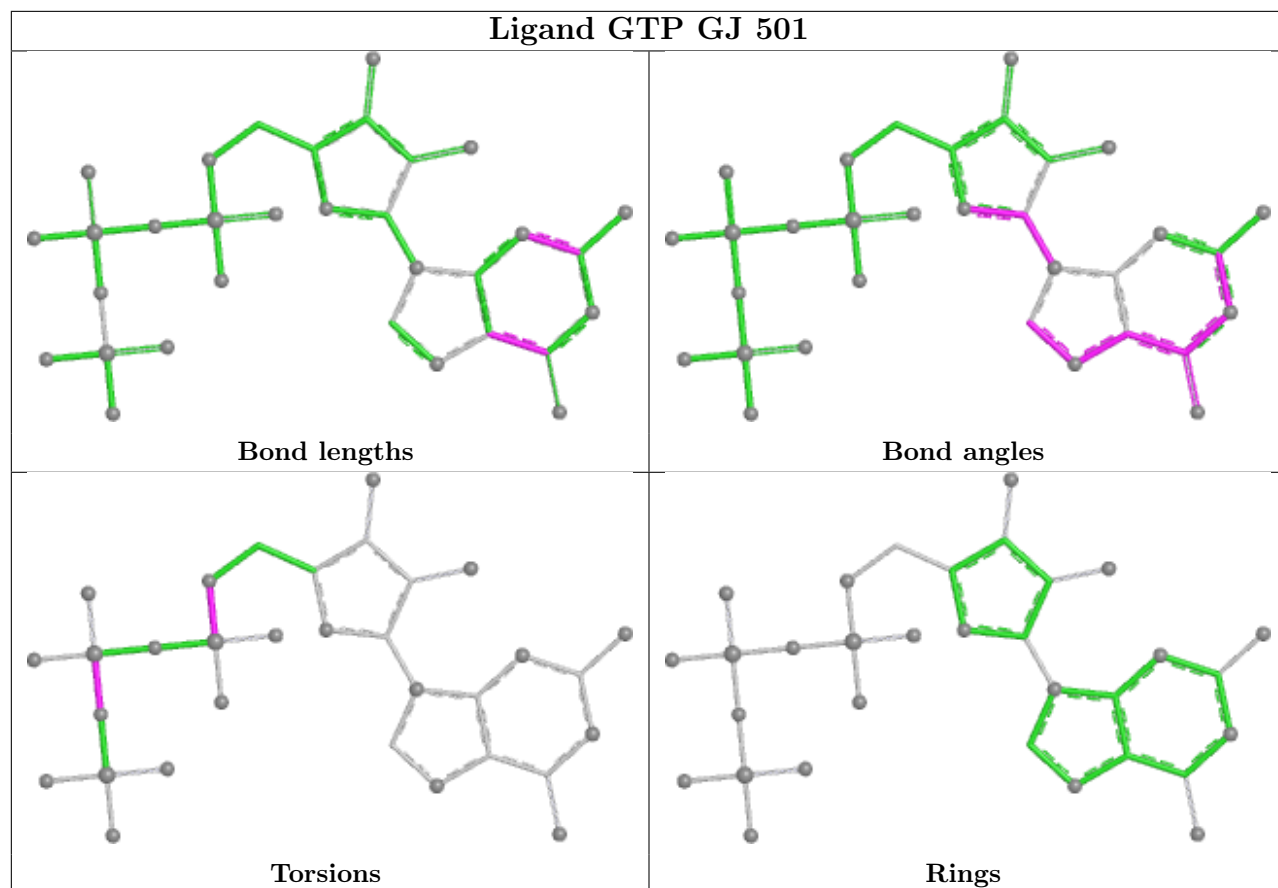
## Ligand GTP JL 602



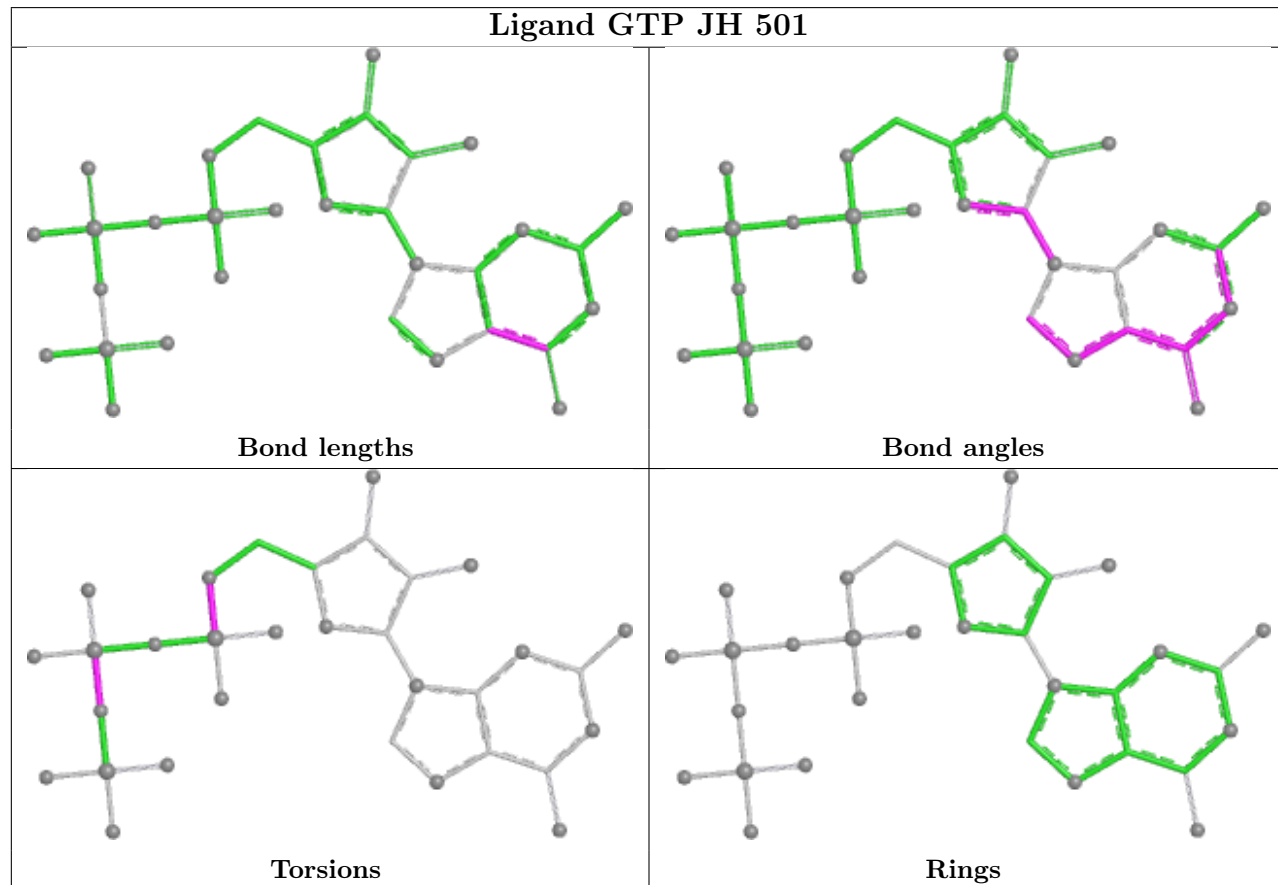
## Ligand GTP FF 501



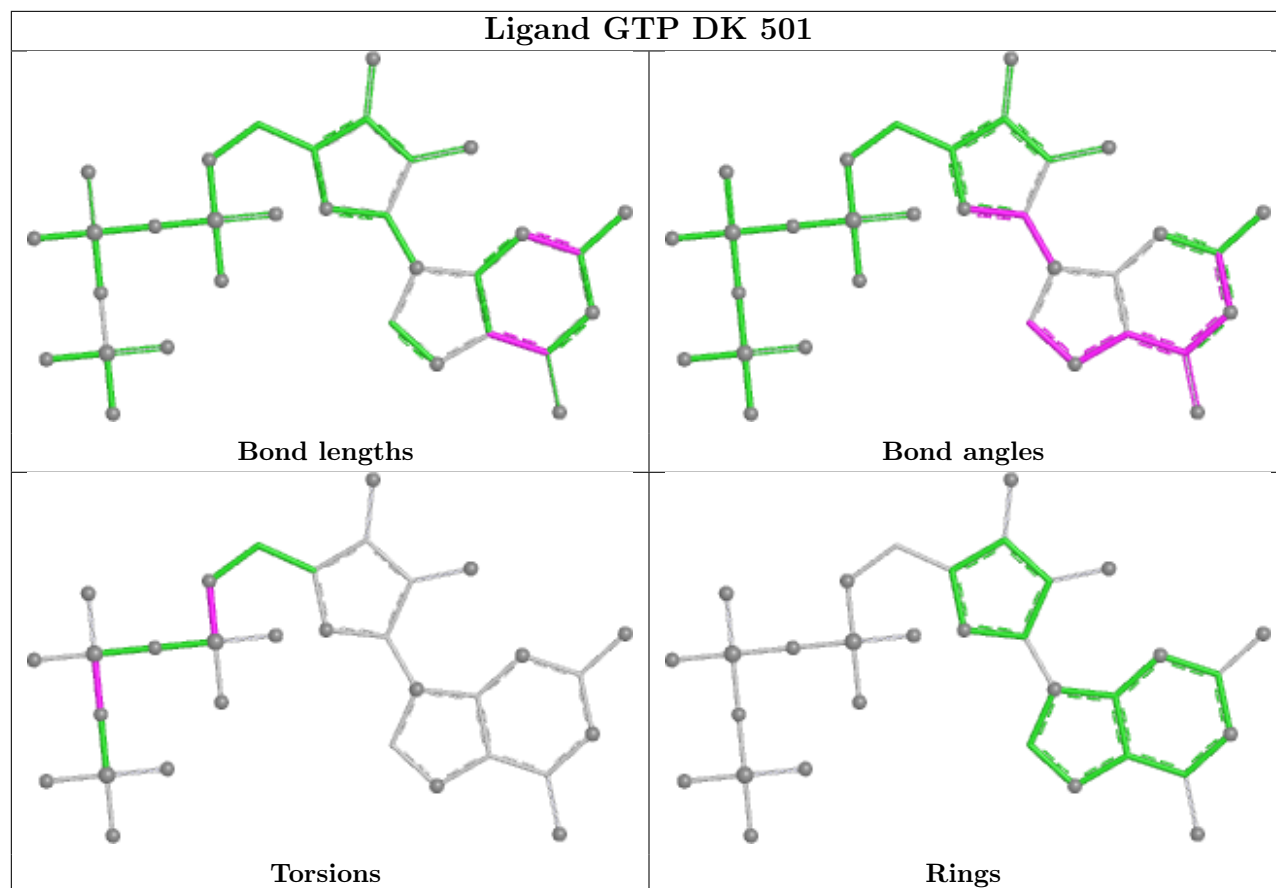
## Ligand GTP GJ 501



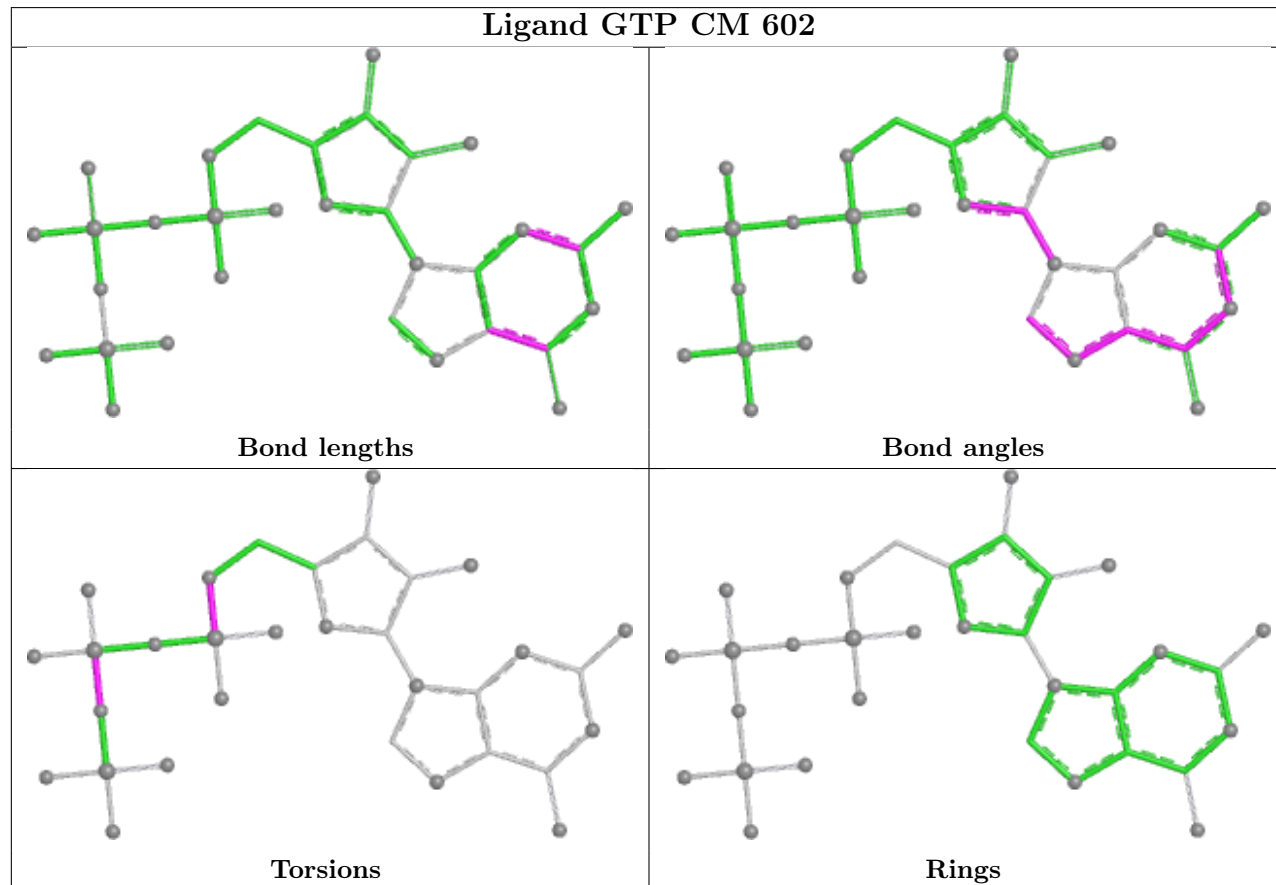
## Ligand GTP JH 501



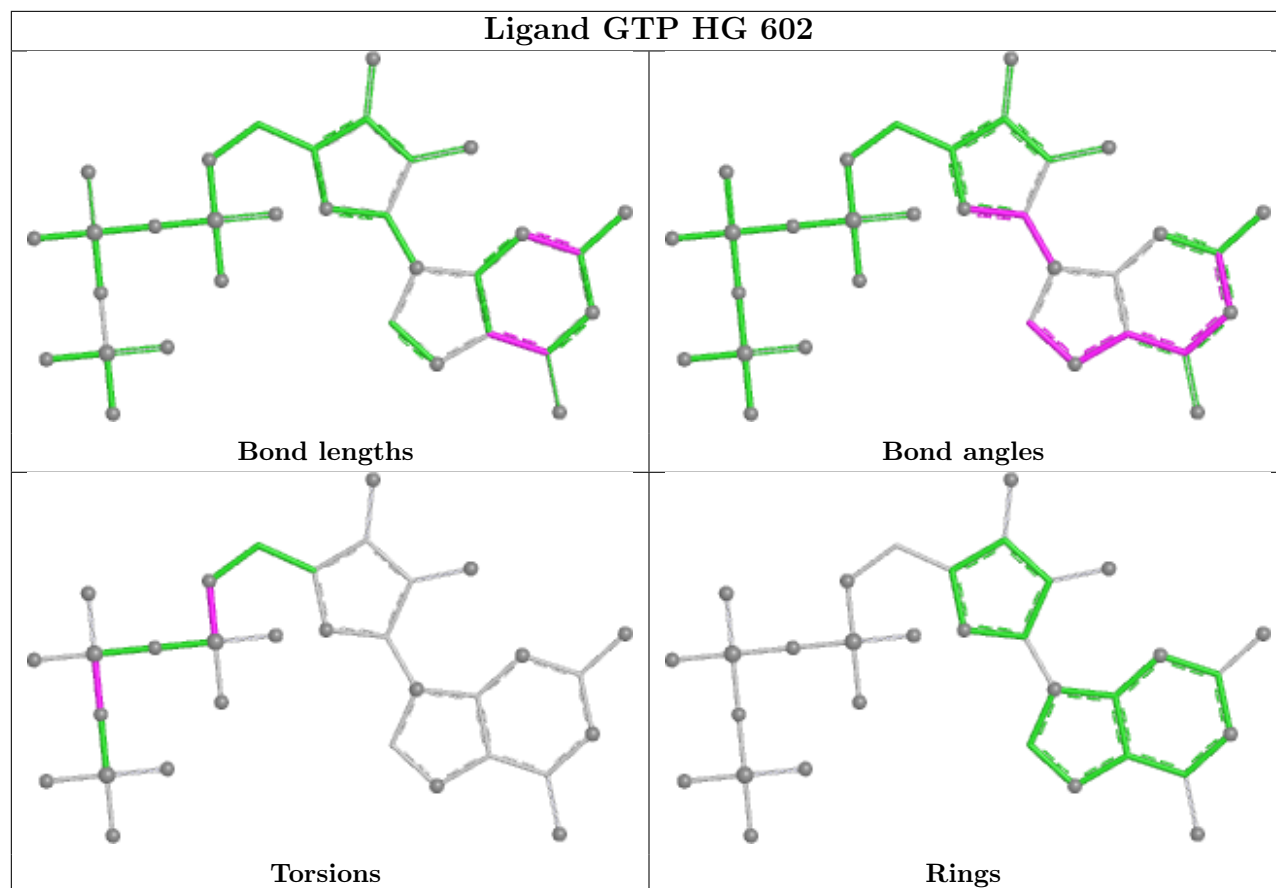
## Ligand GTP DK 501



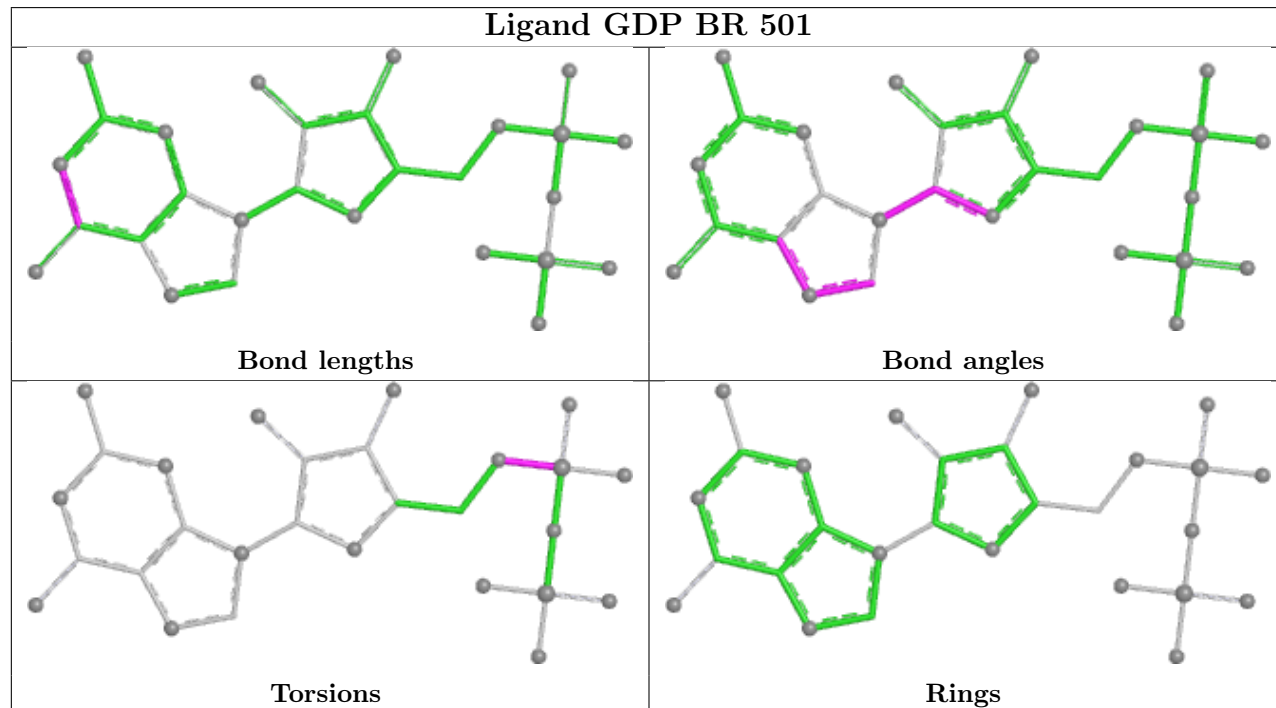
## Ligand GTP CM 602



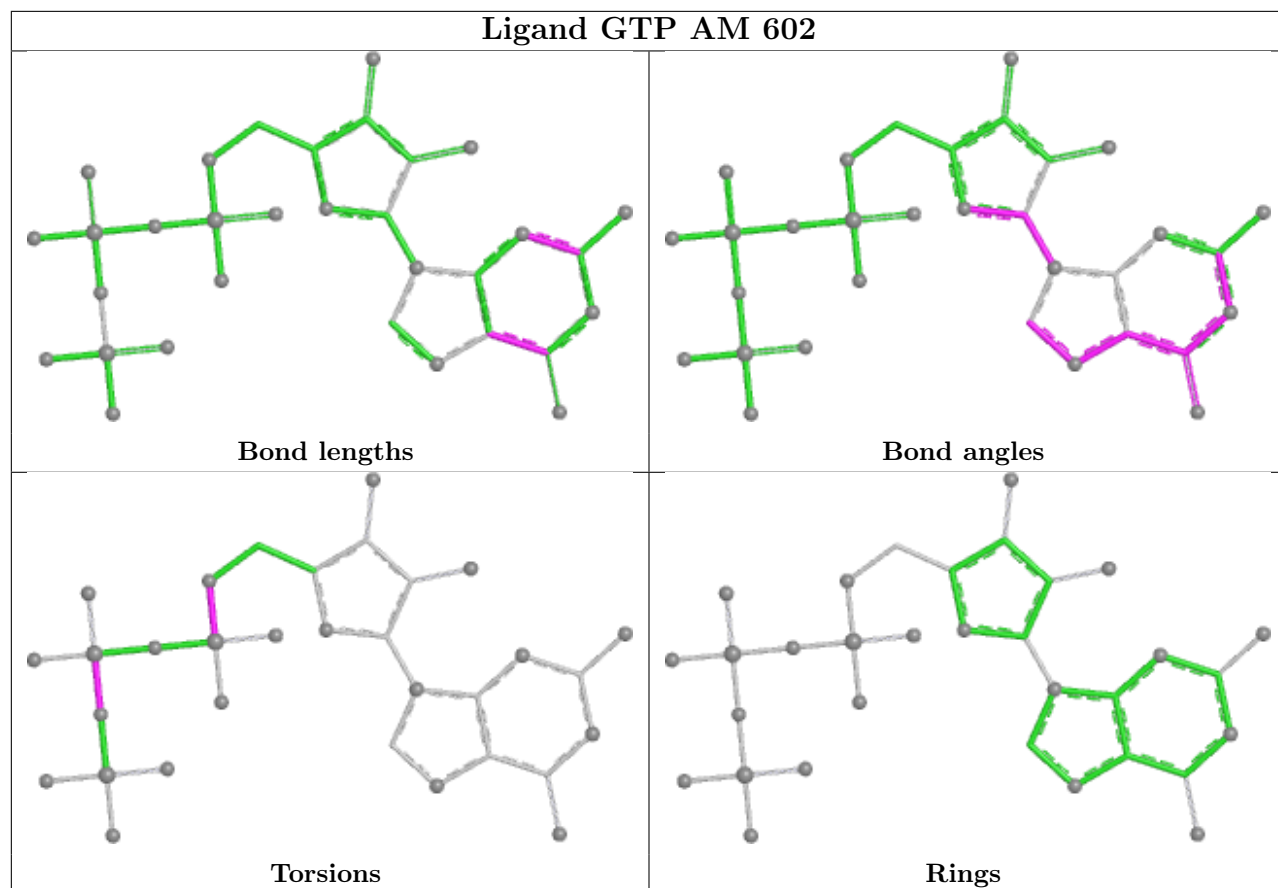
## Ligand GTP HG 602



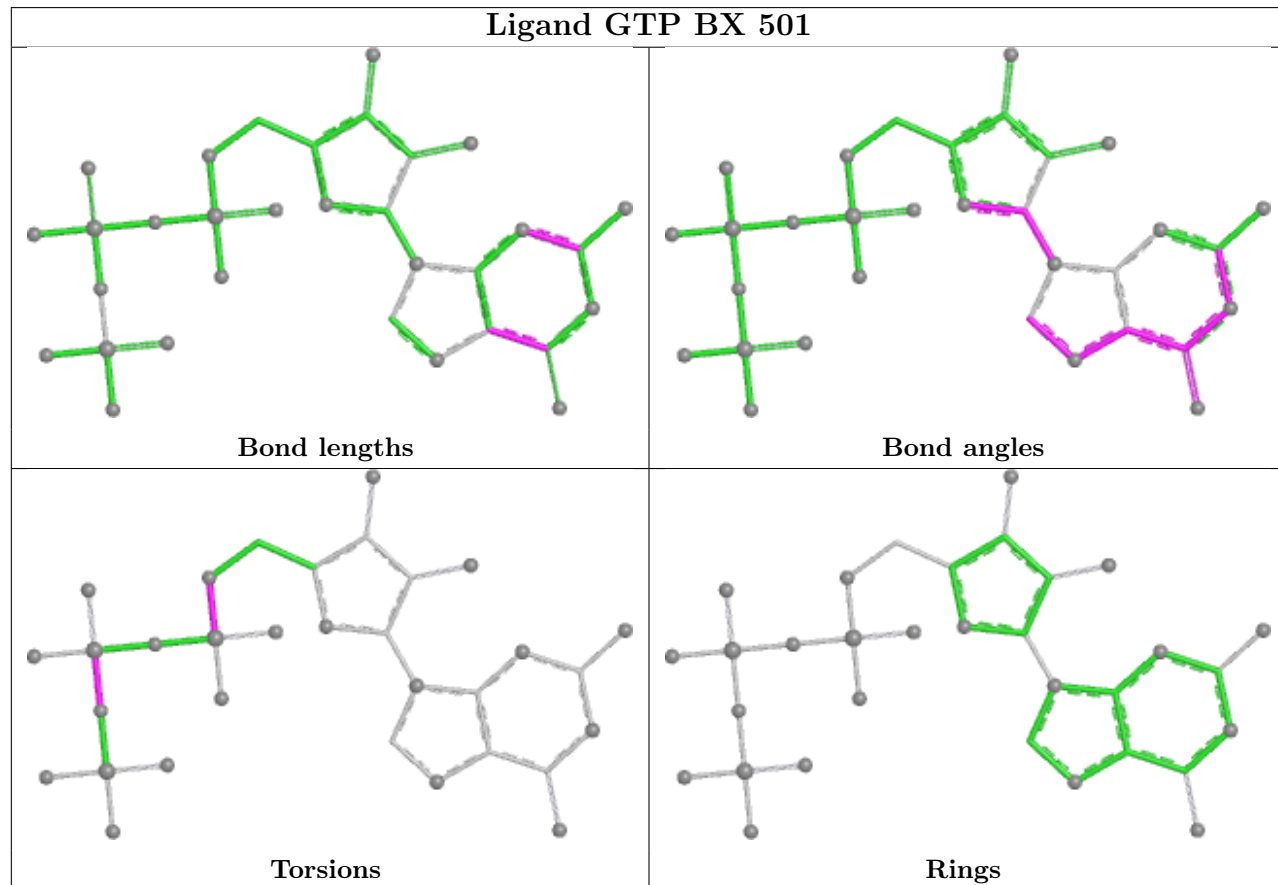
## Ligand GDP BR 501



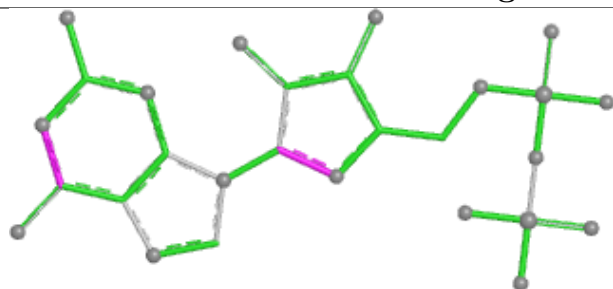
## Ligand GTP AM 602



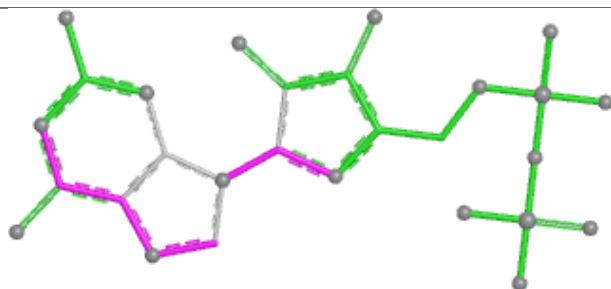
## Ligand GTP BX 501



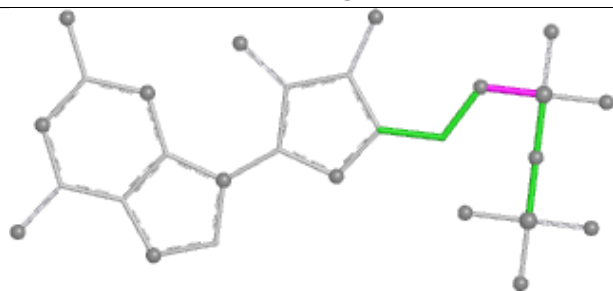
## Ligand GDP CV 501



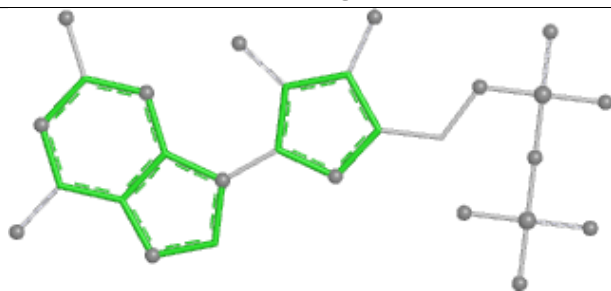
Bond lengths



Bond angles

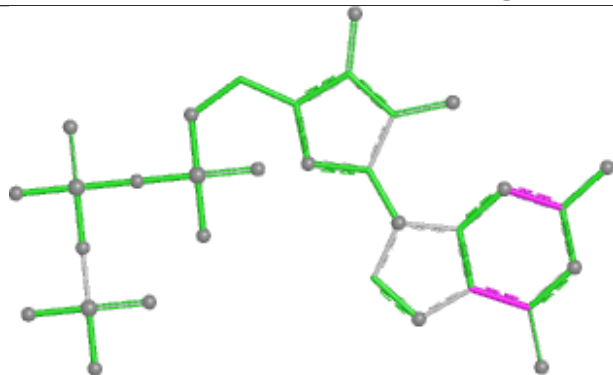


Torsions

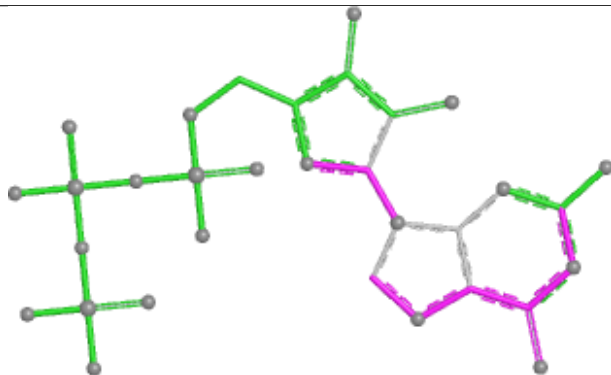


Rings

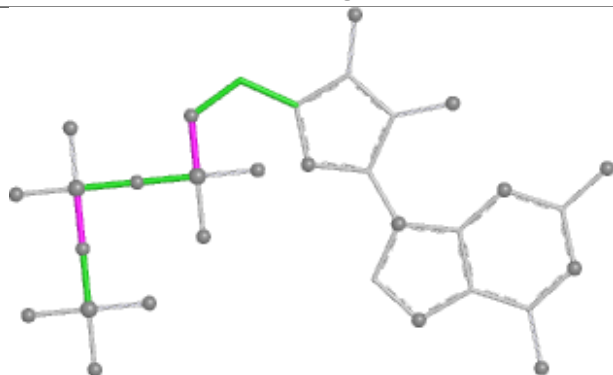
## Ligand GTP KD 501



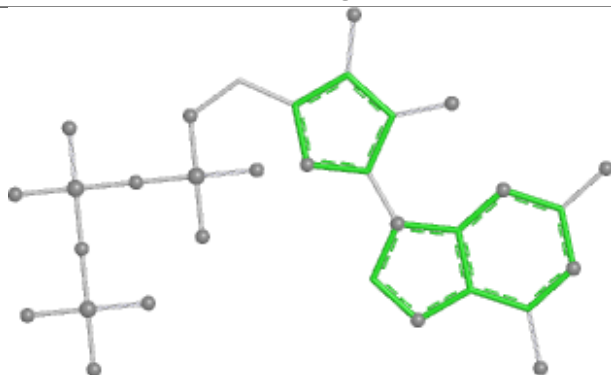
Bond lengths



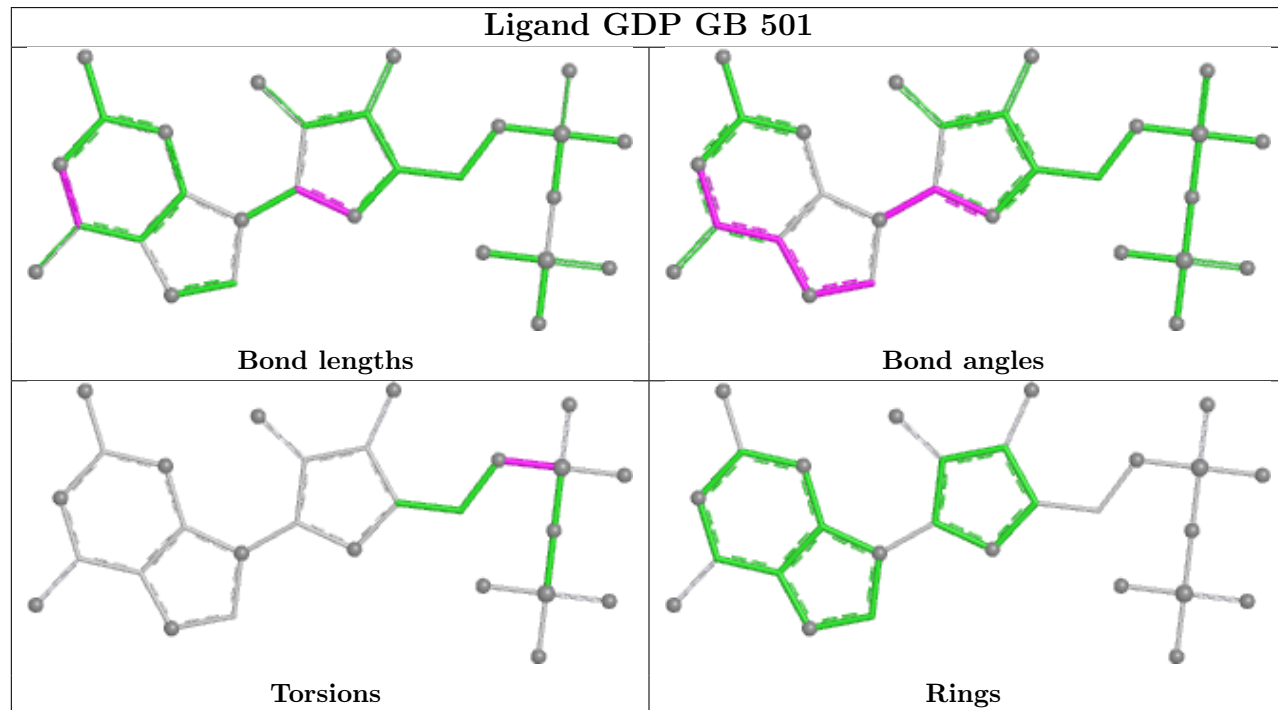
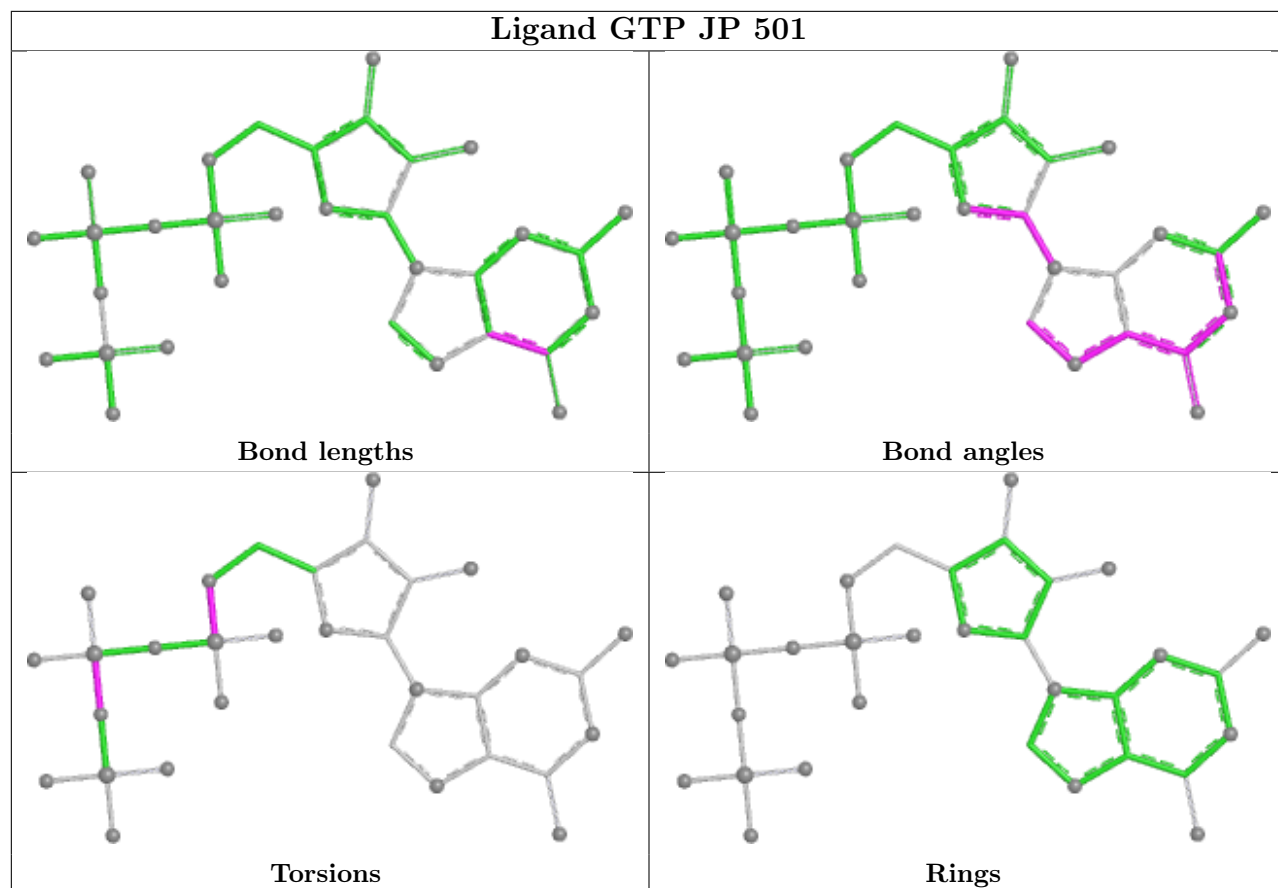
Bond angles

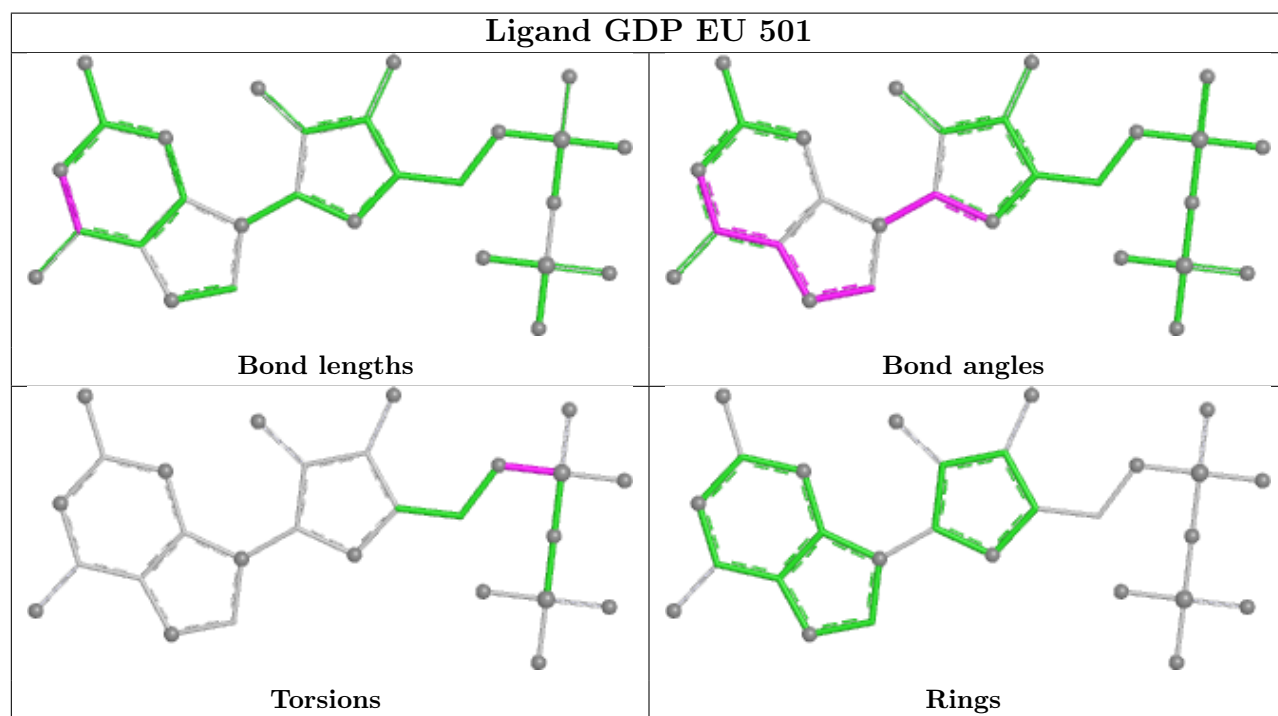
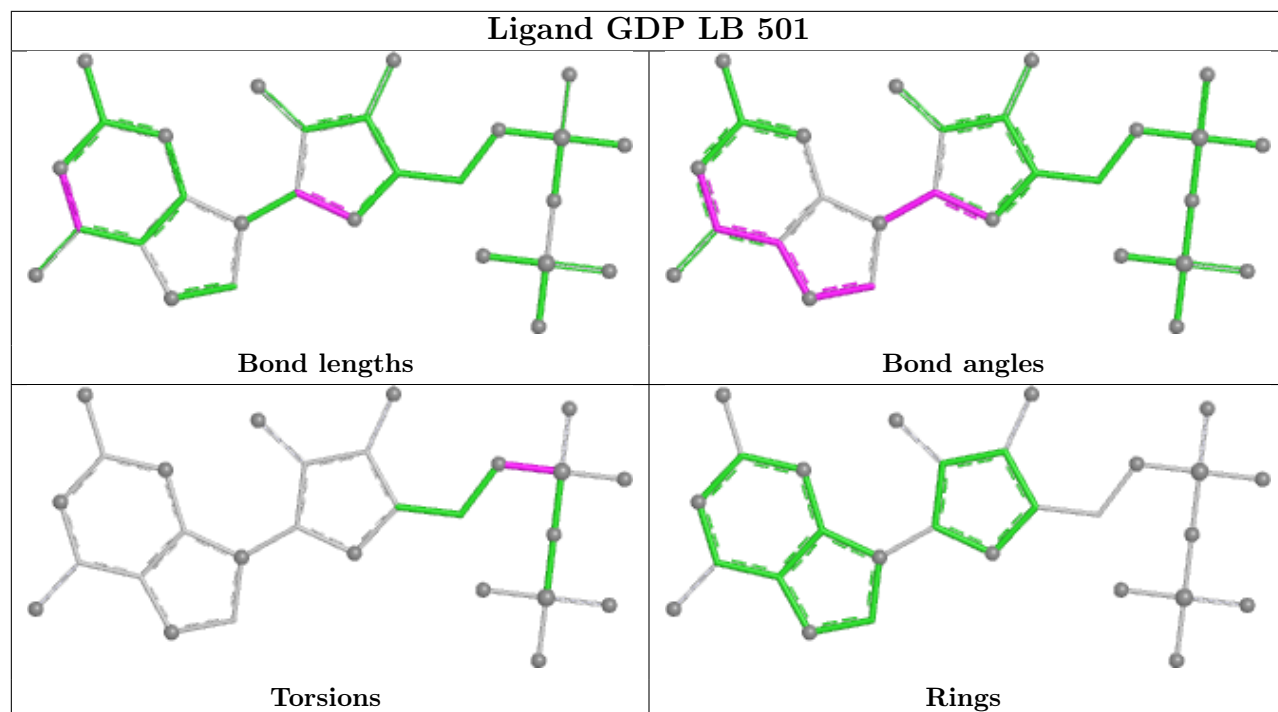


Torsions

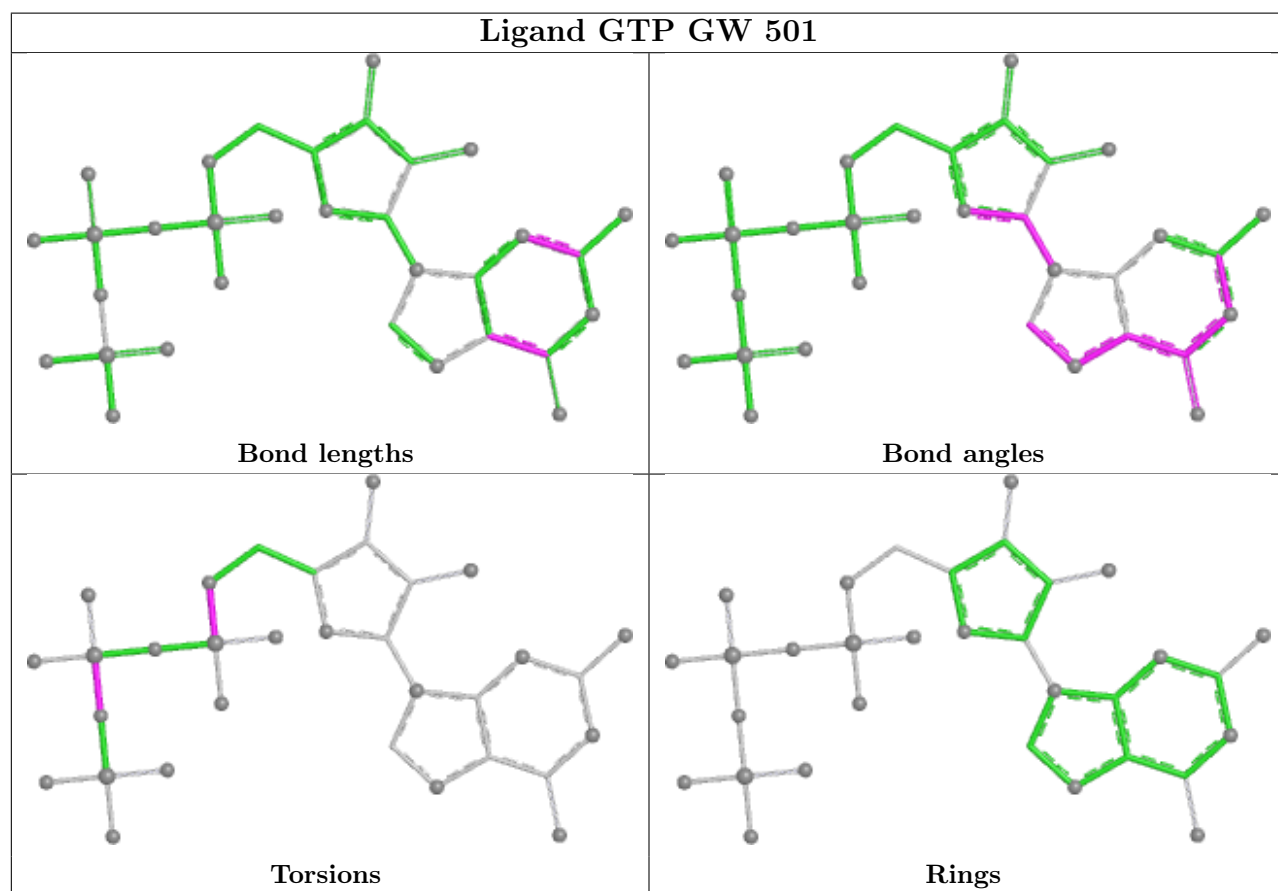
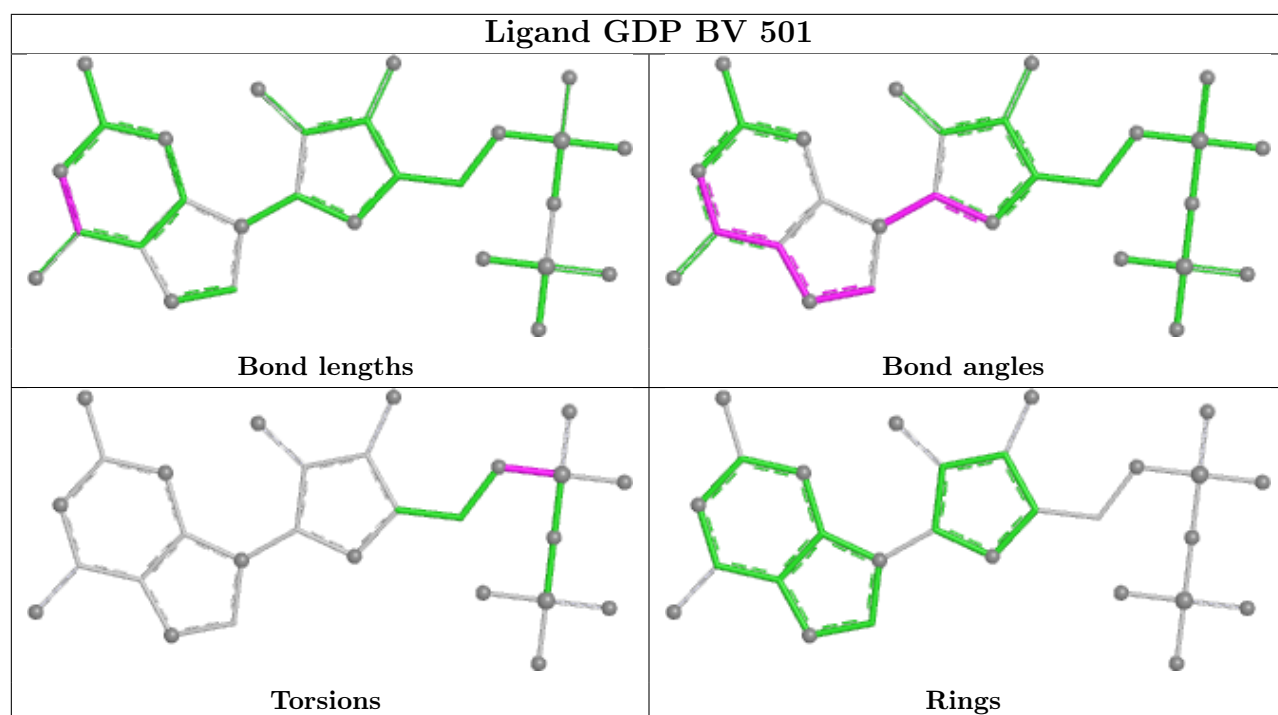


Rings

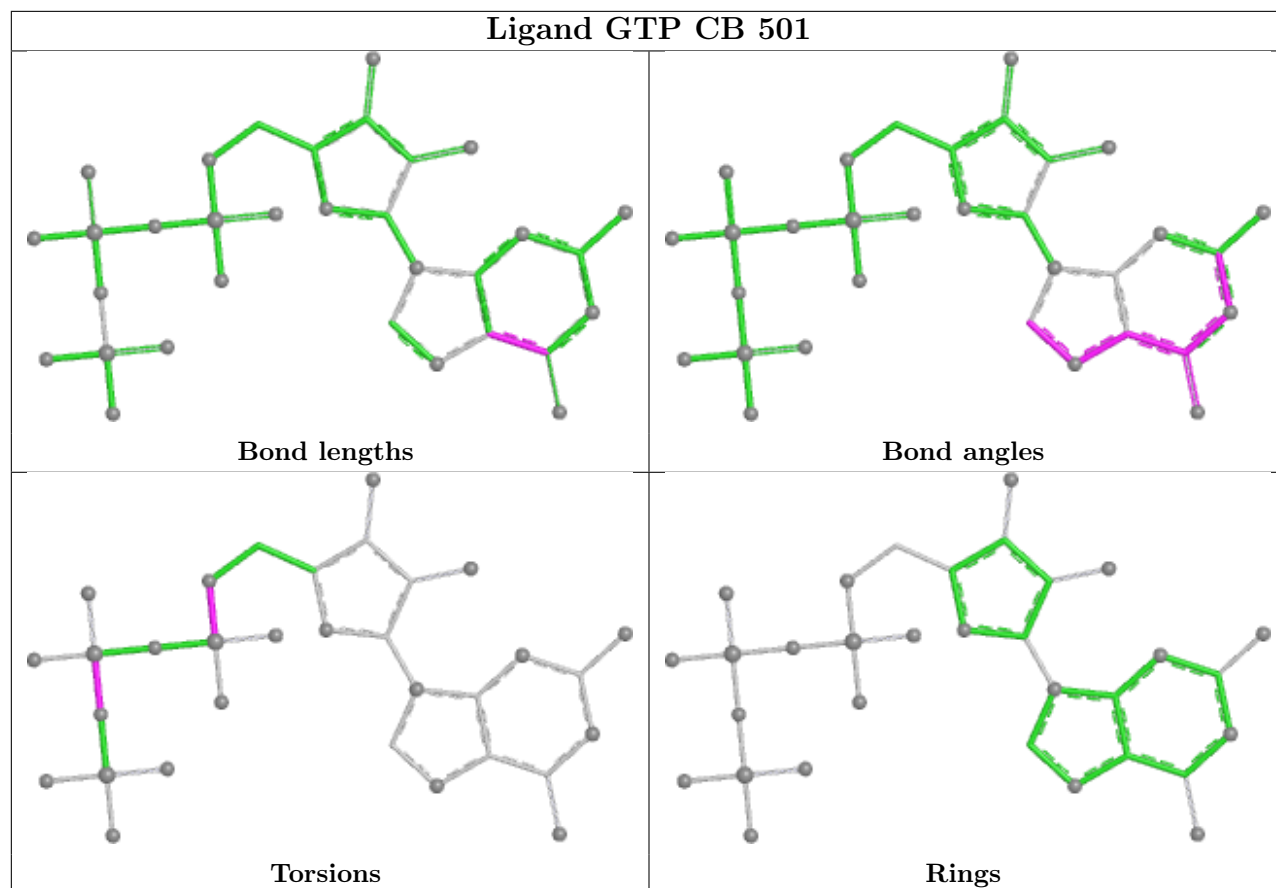




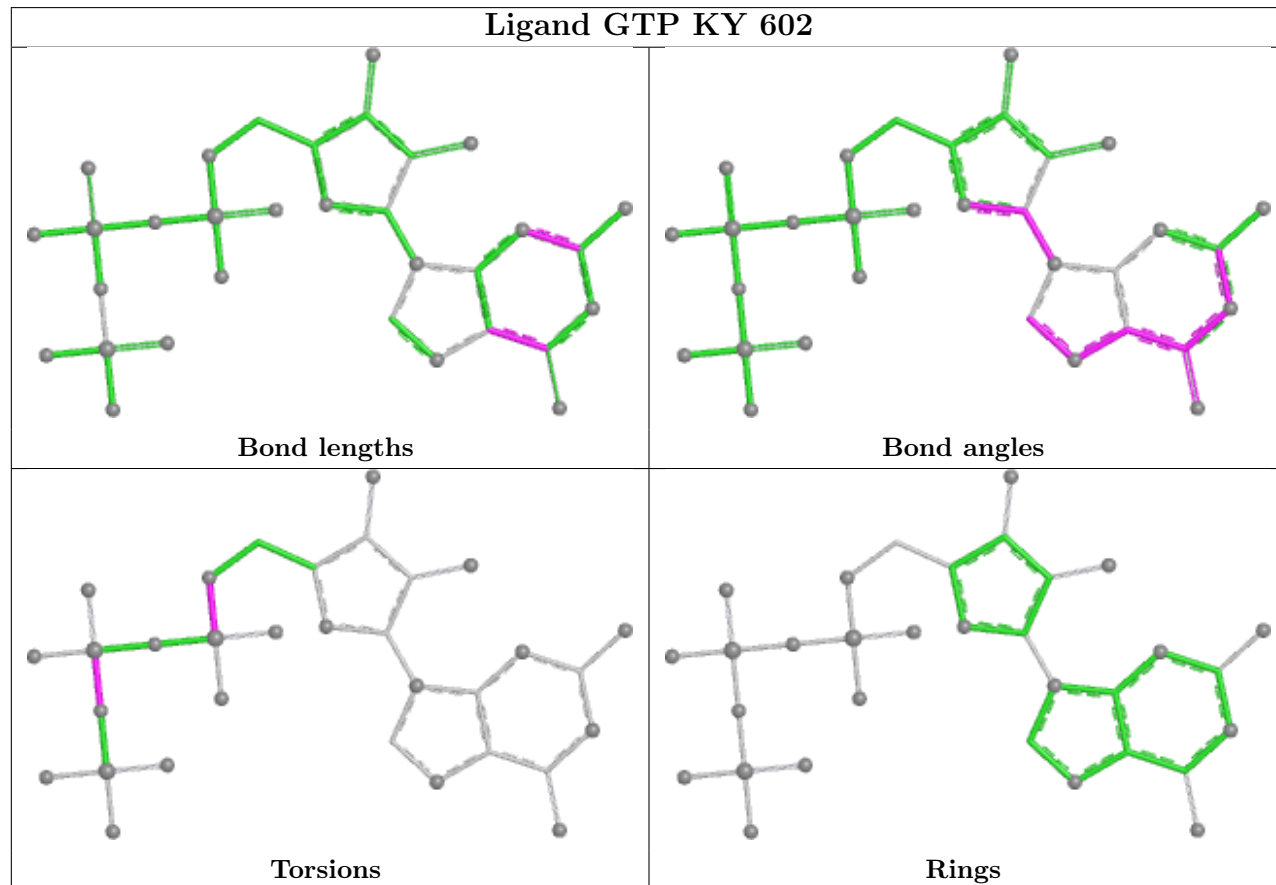




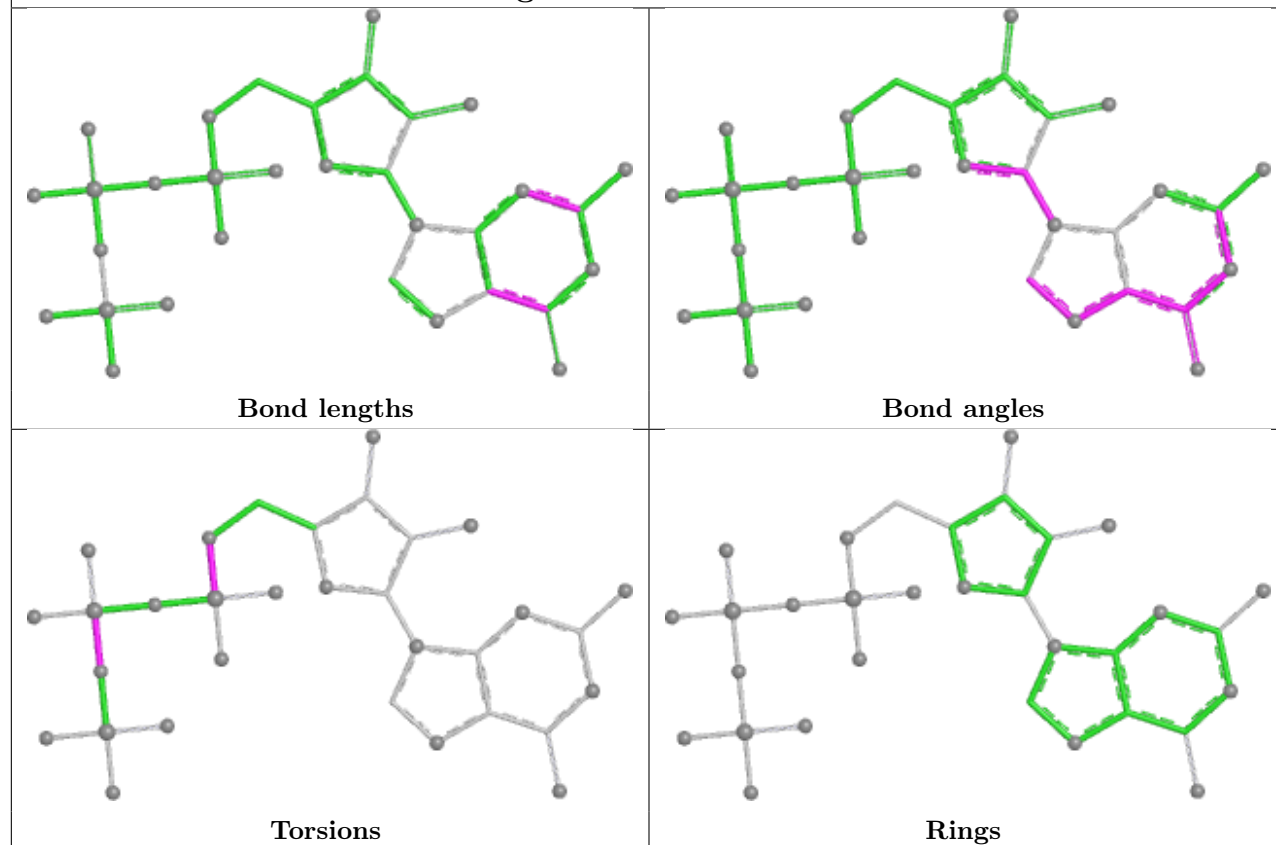
## Ligand GTP CB 501



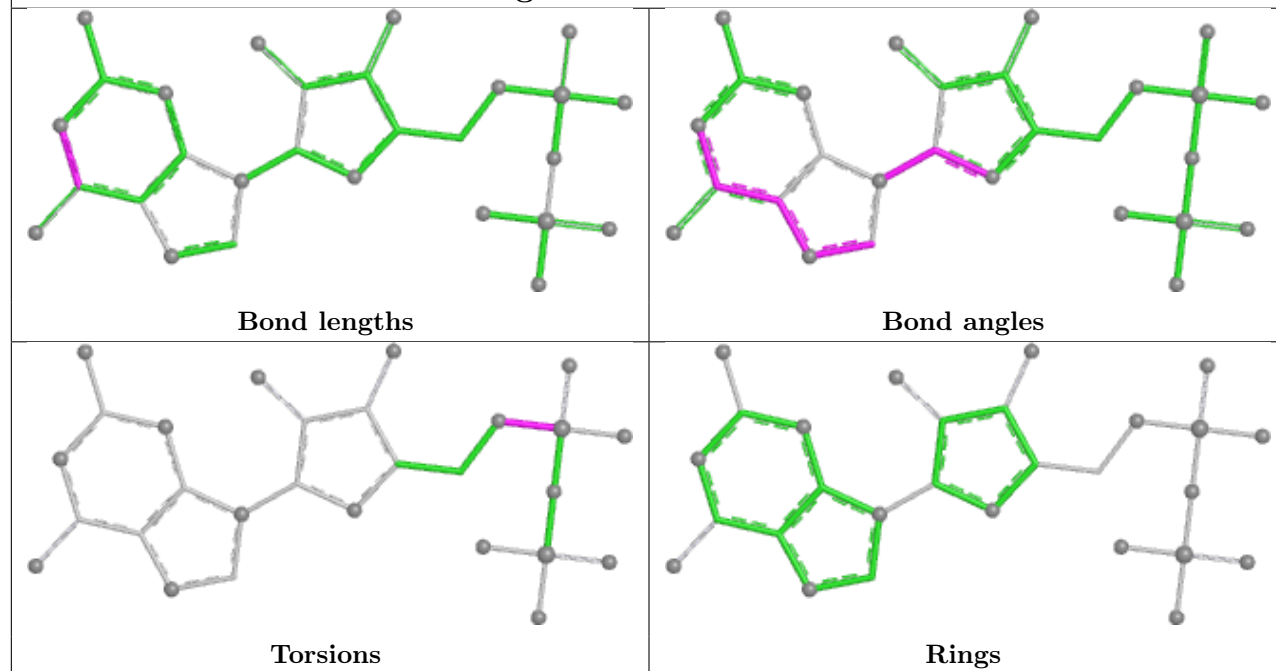
## Ligand GTP KY 602



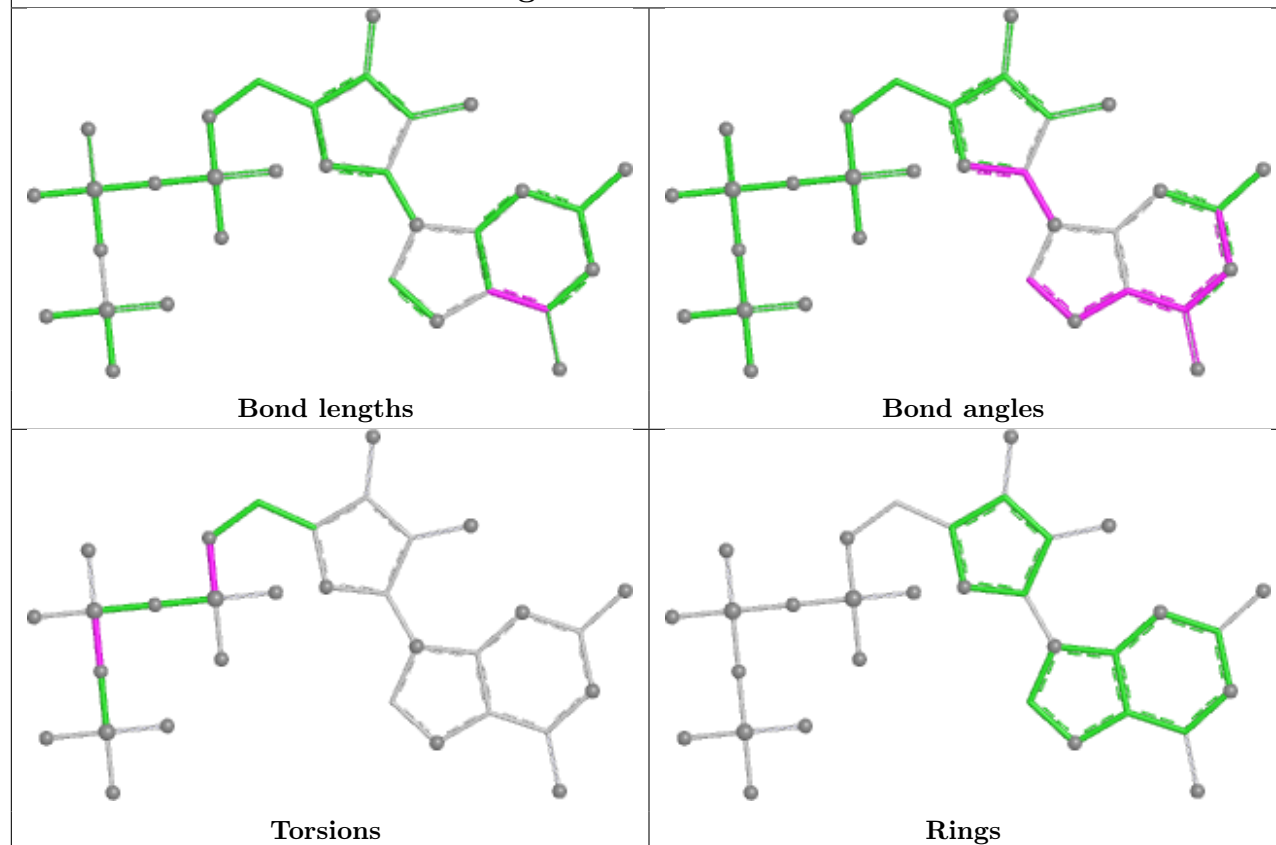
## Ligand GTP BG 501



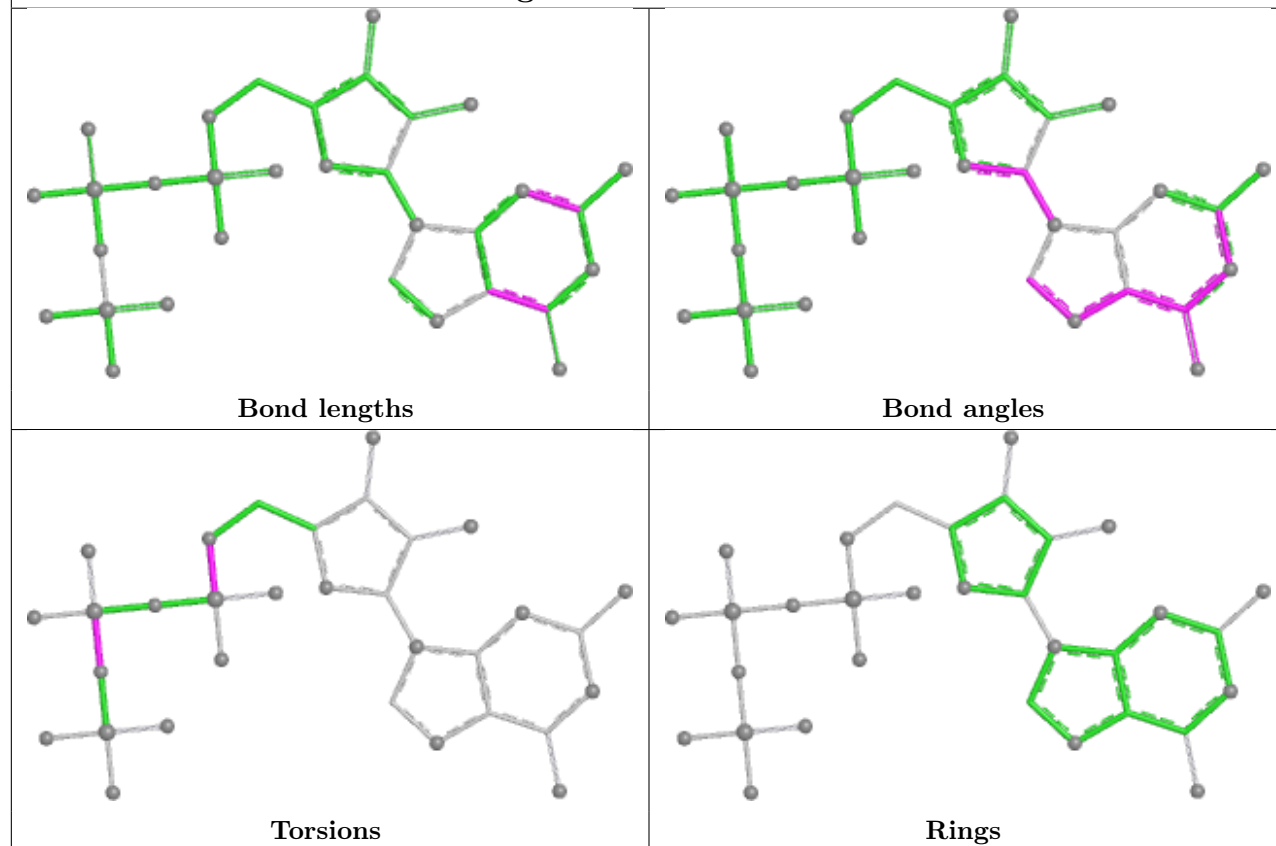
## Ligand GDP BY 501

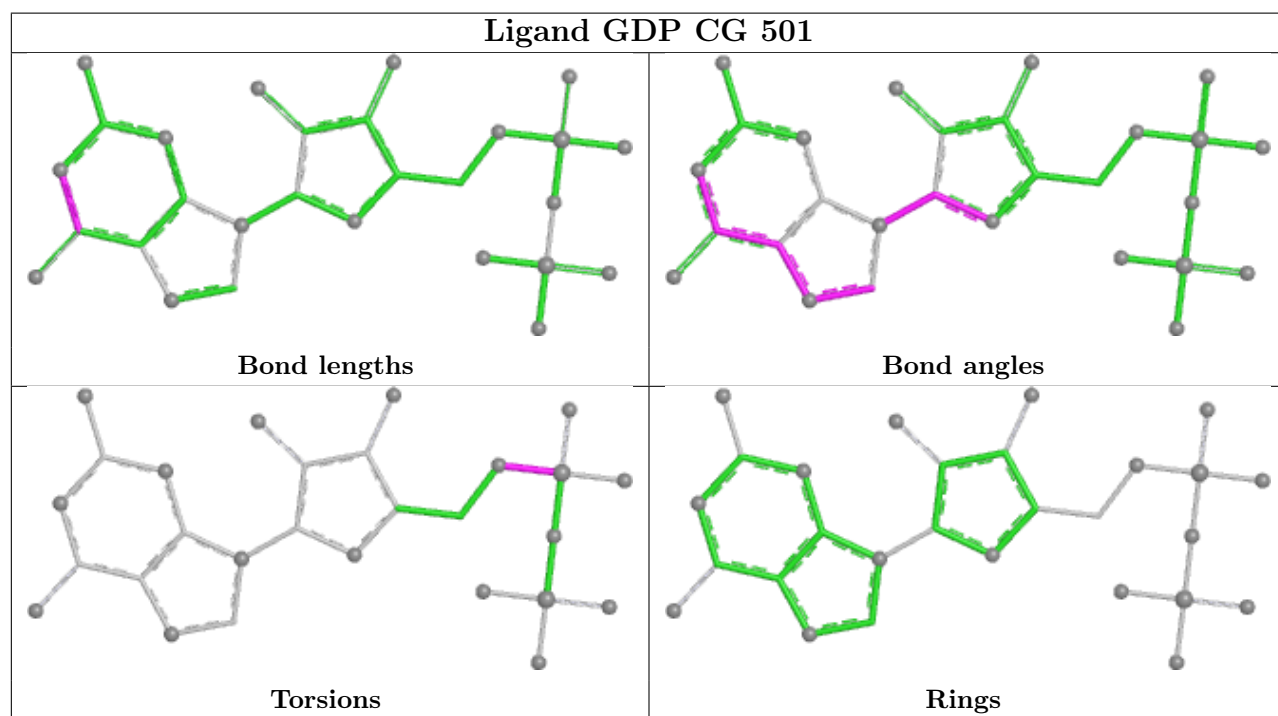
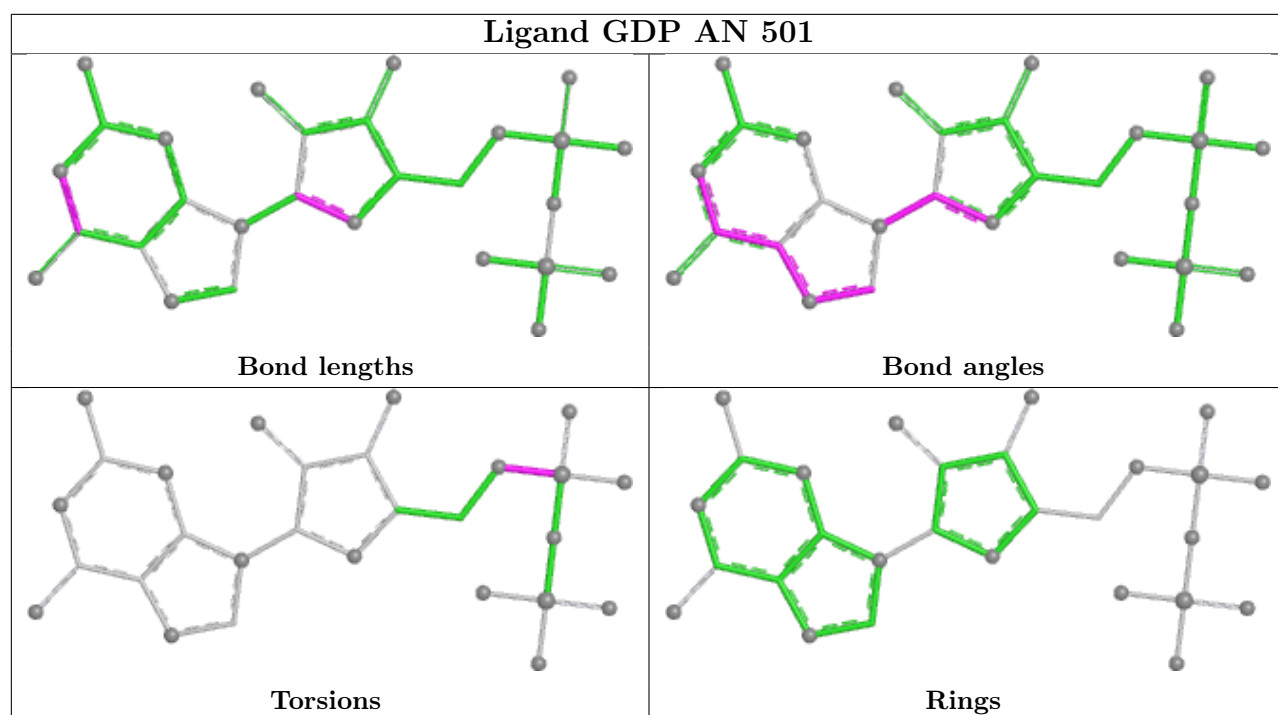


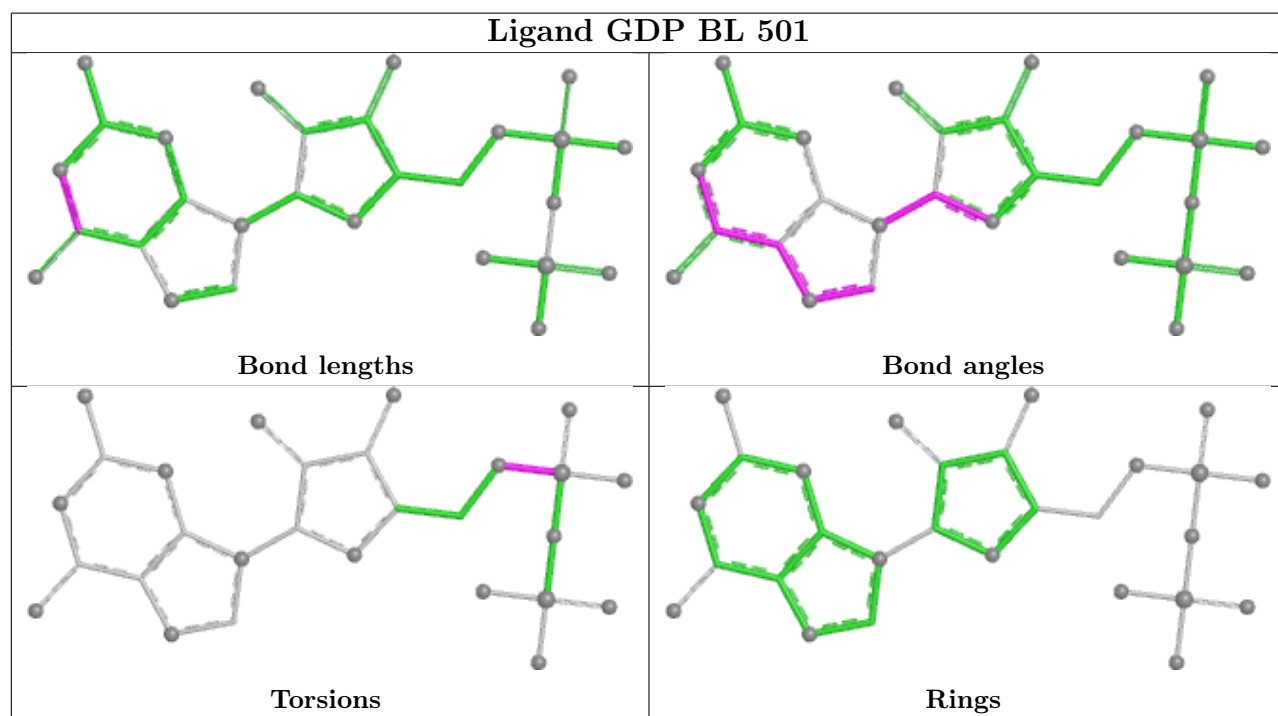
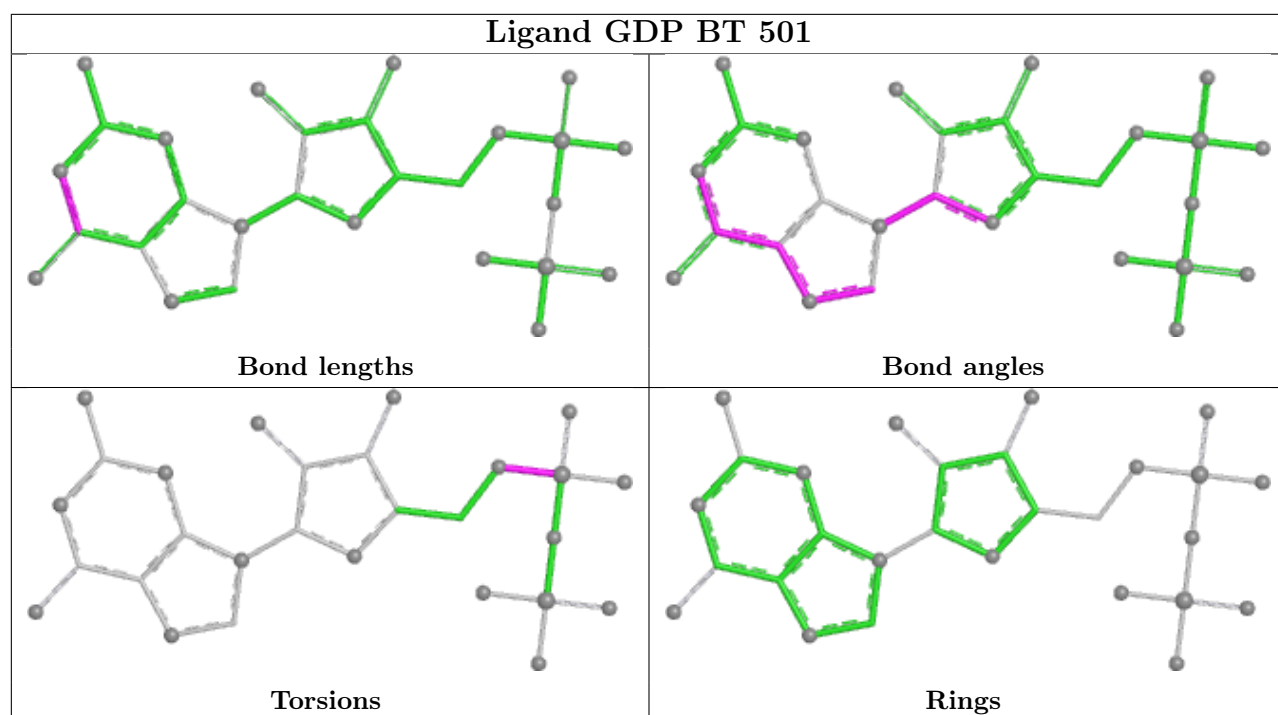
## Ligand GTP EH 501

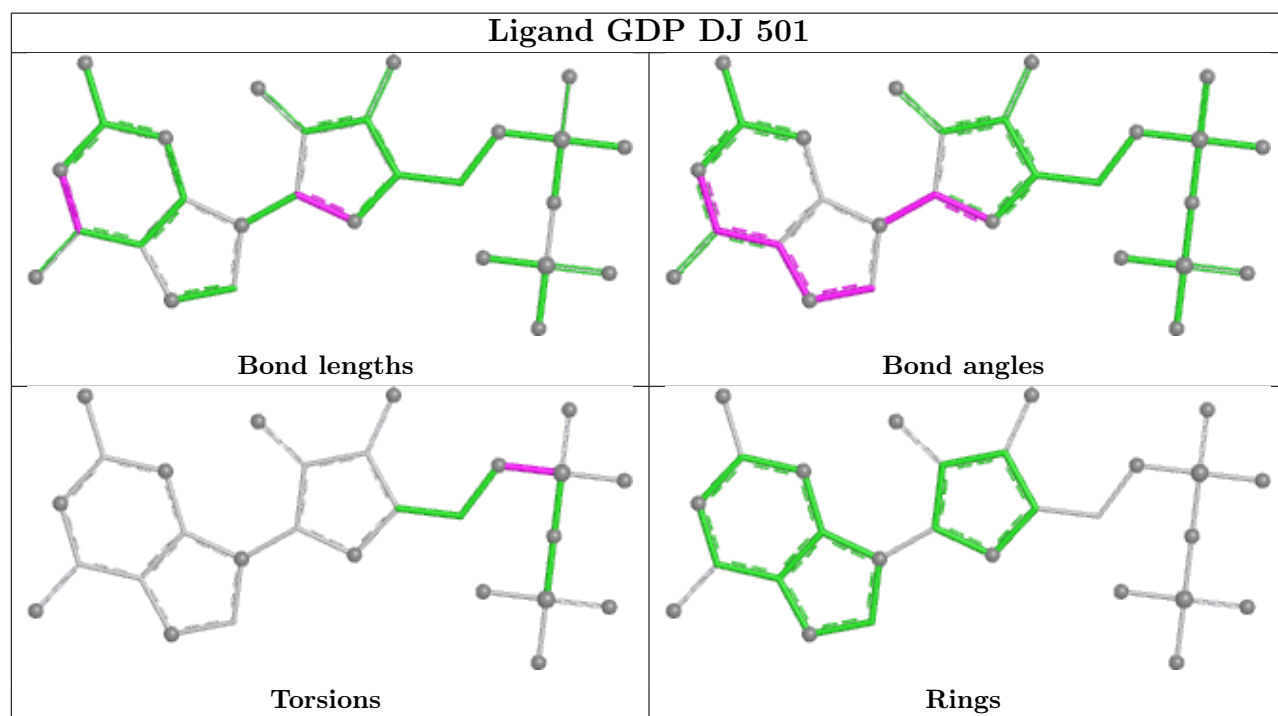
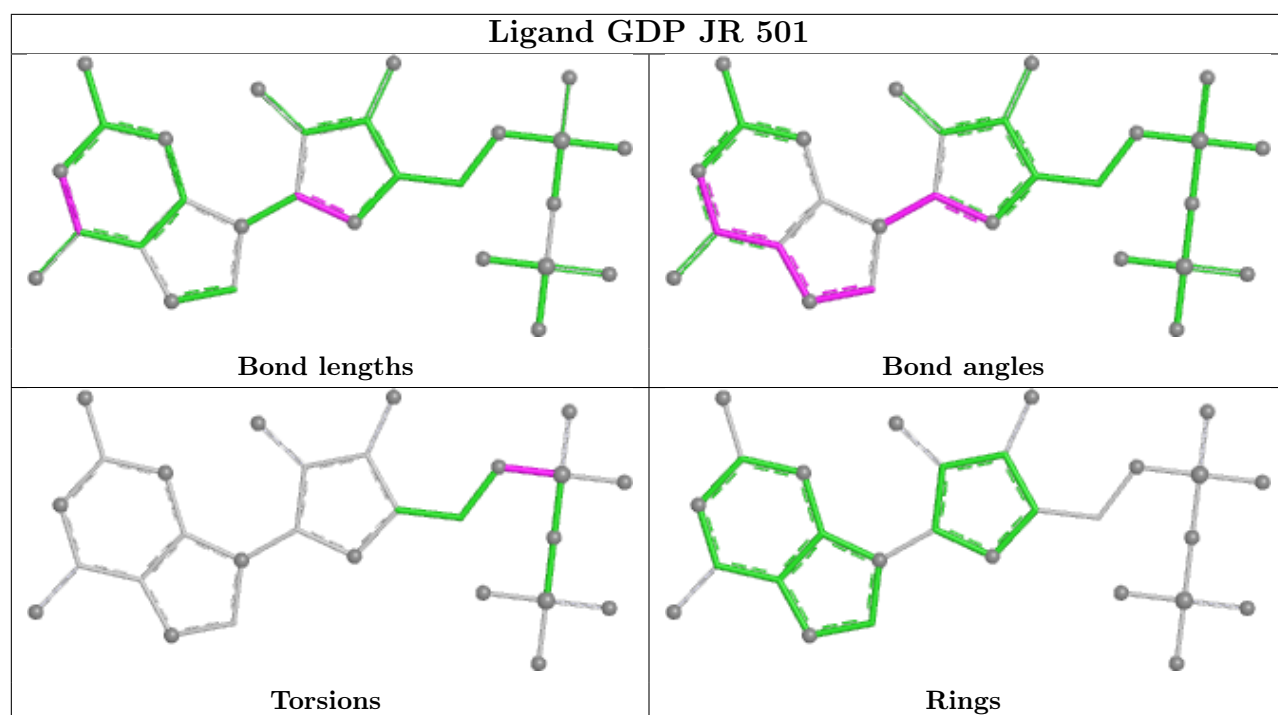


## Ligand GTP HC 602

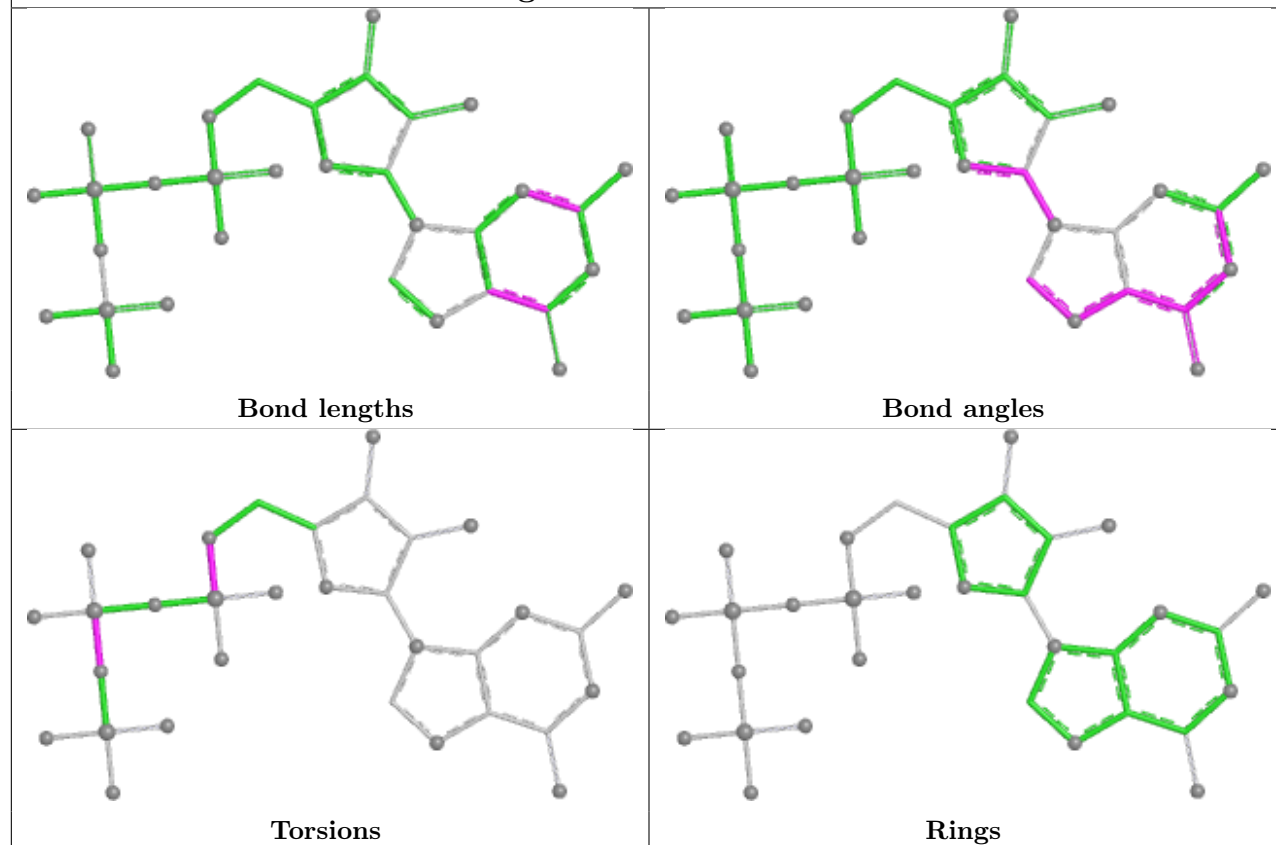




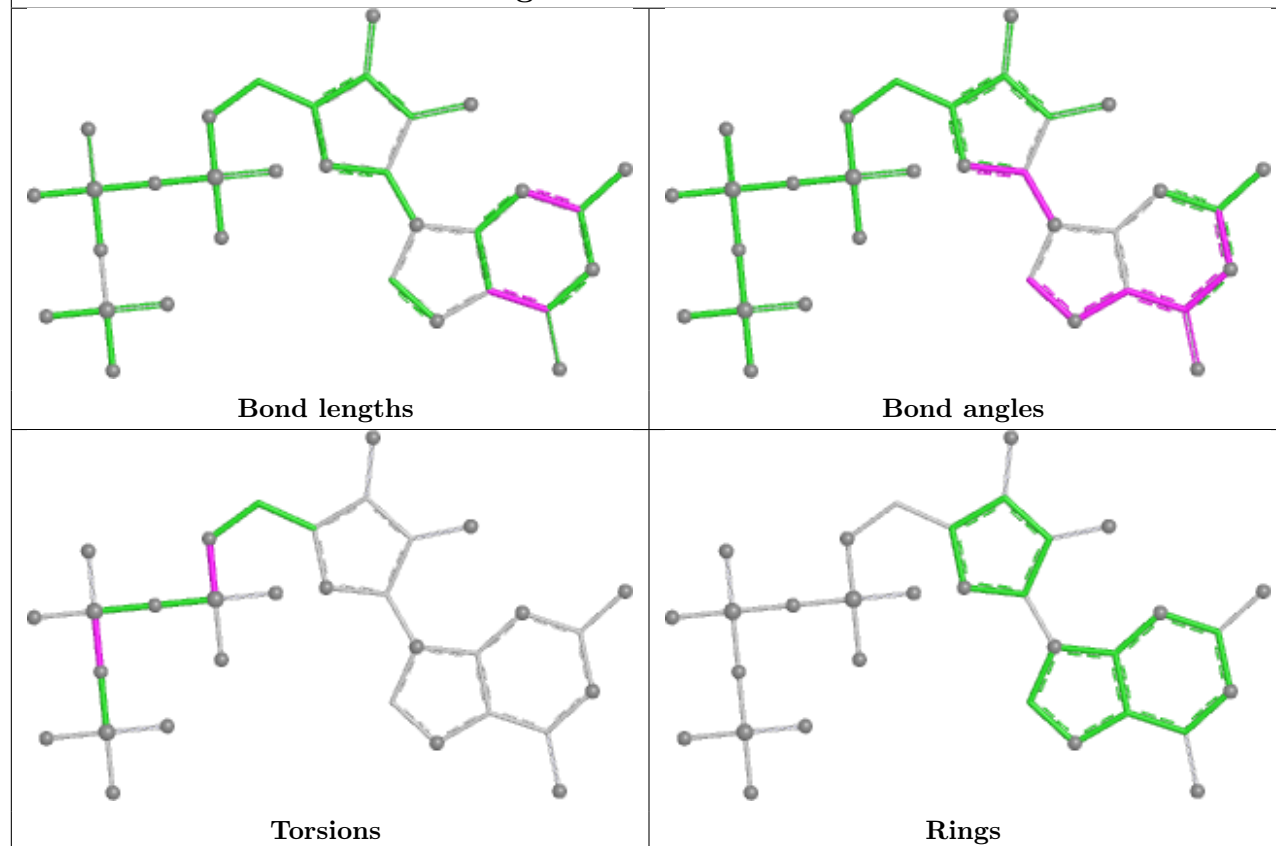




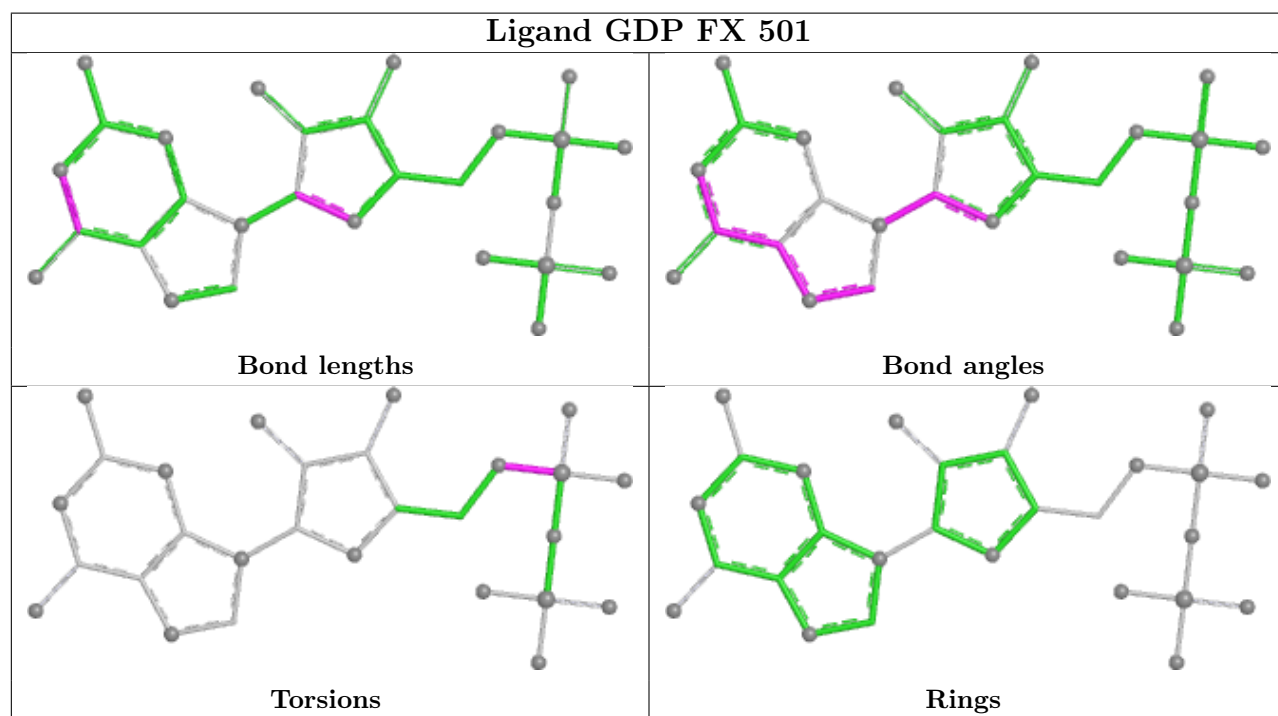
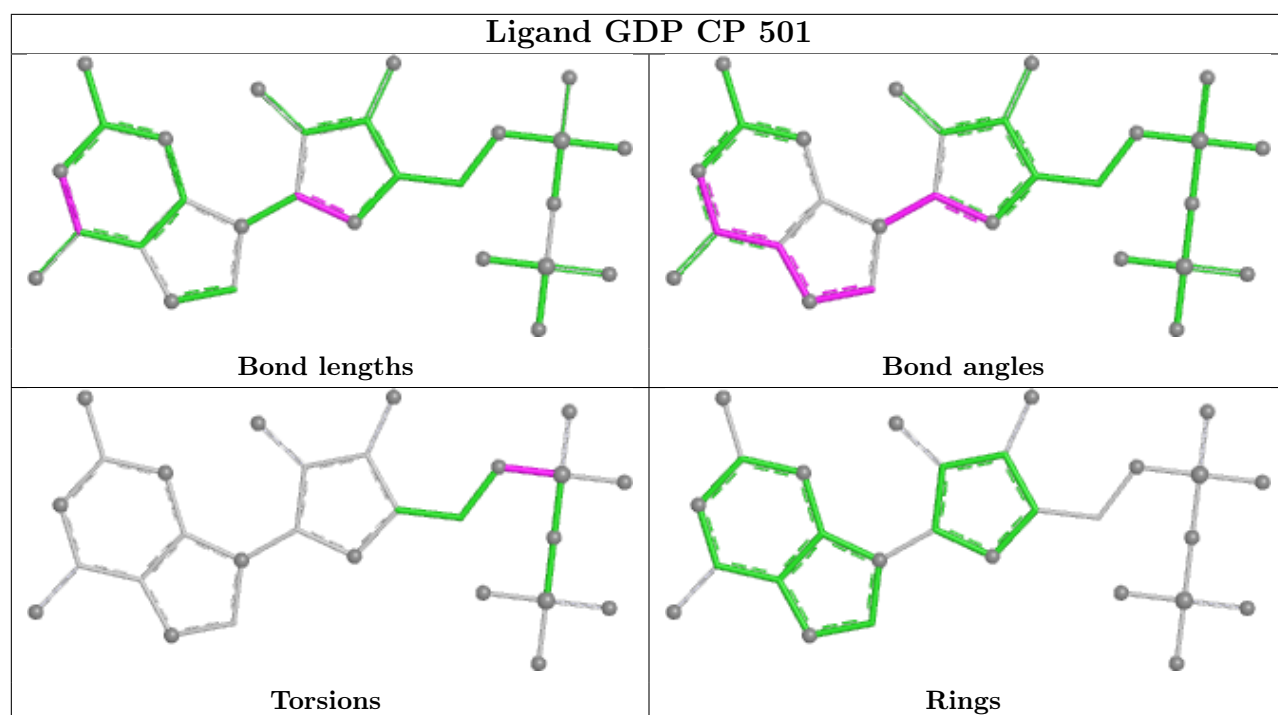
## Ligand GTP BC 501



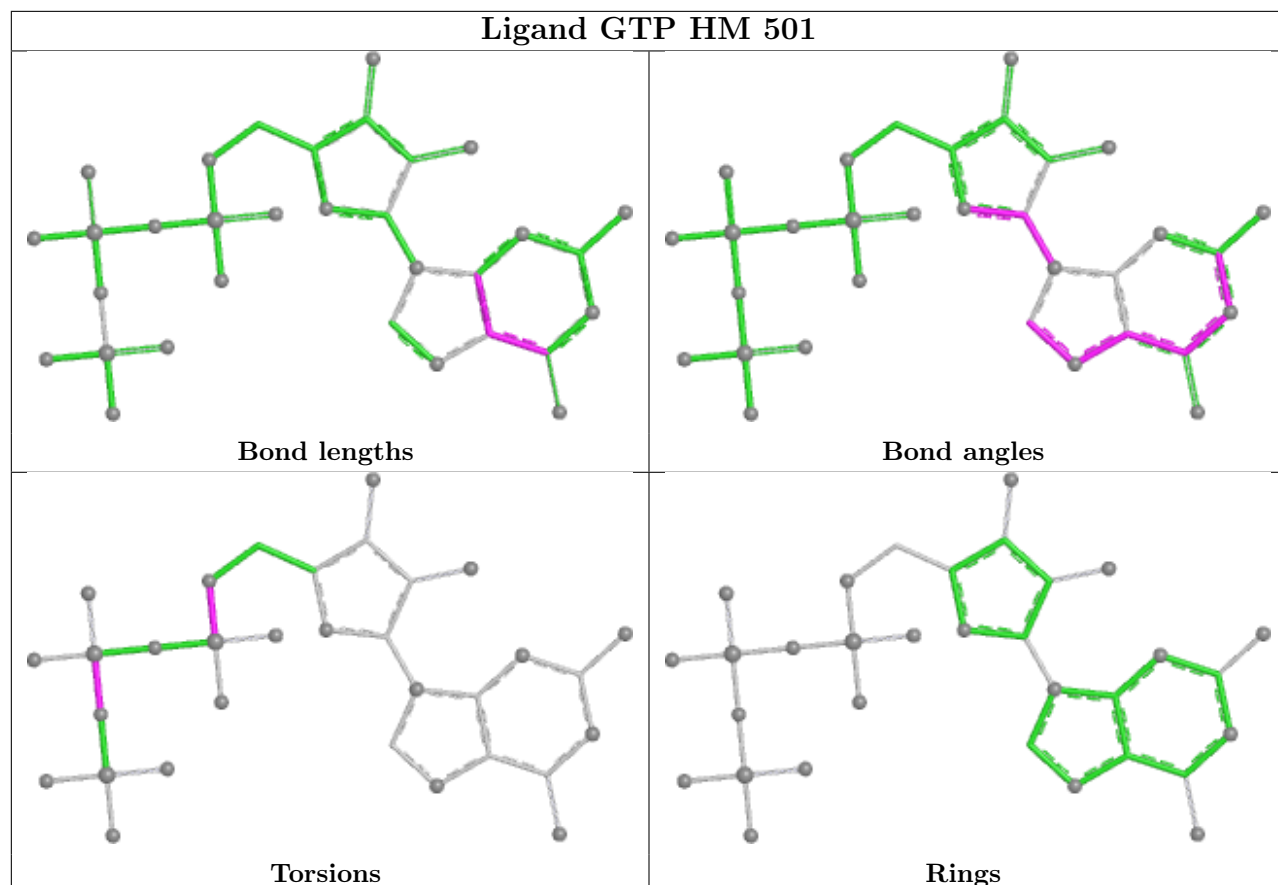
## Ligand GTP JW 602



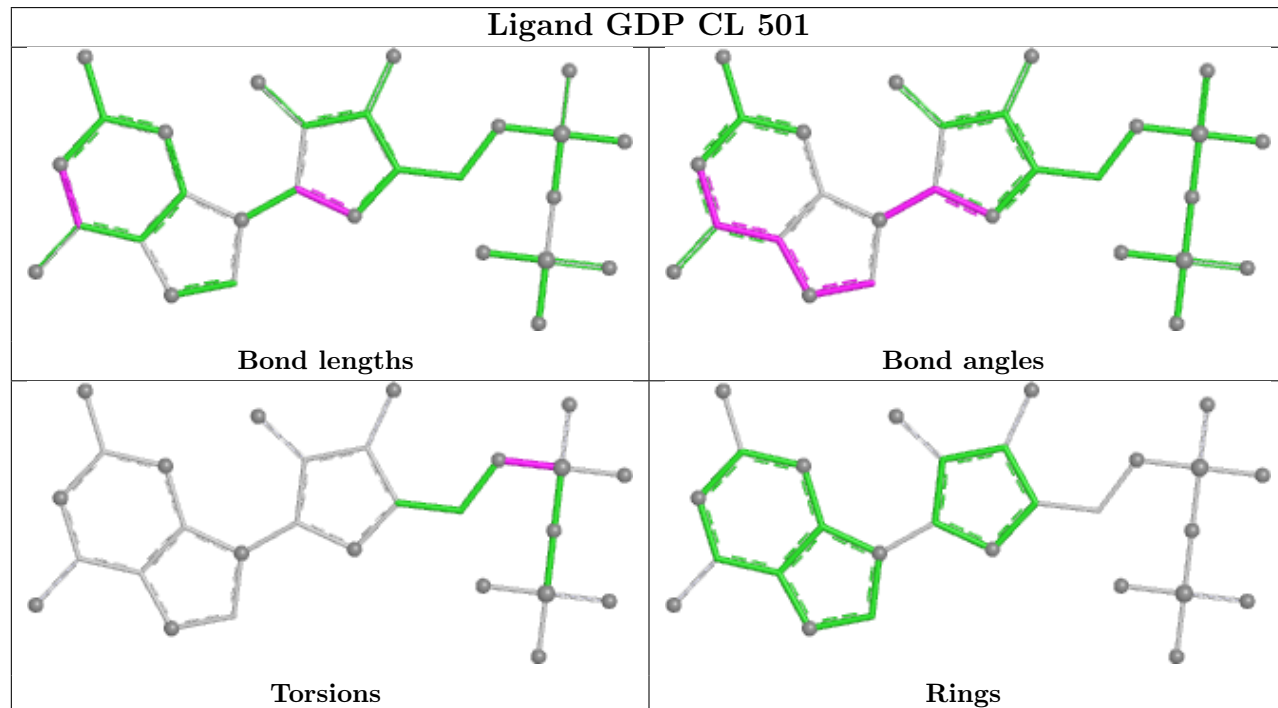


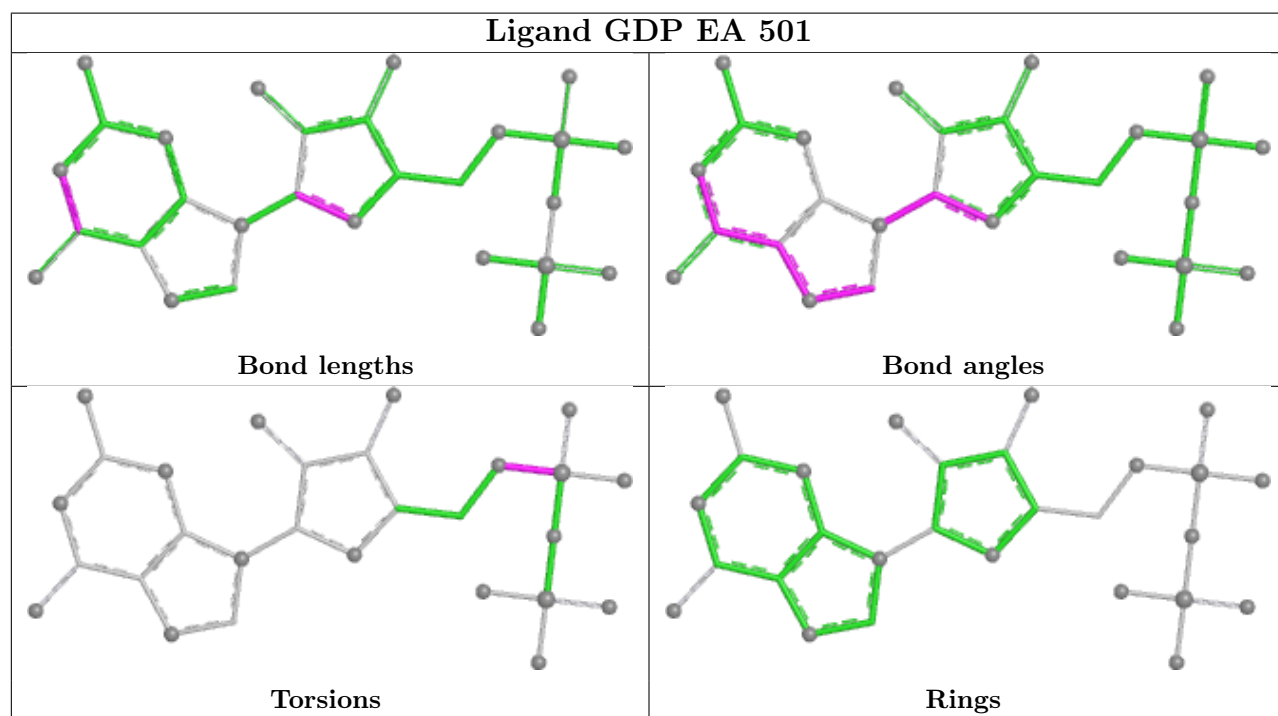
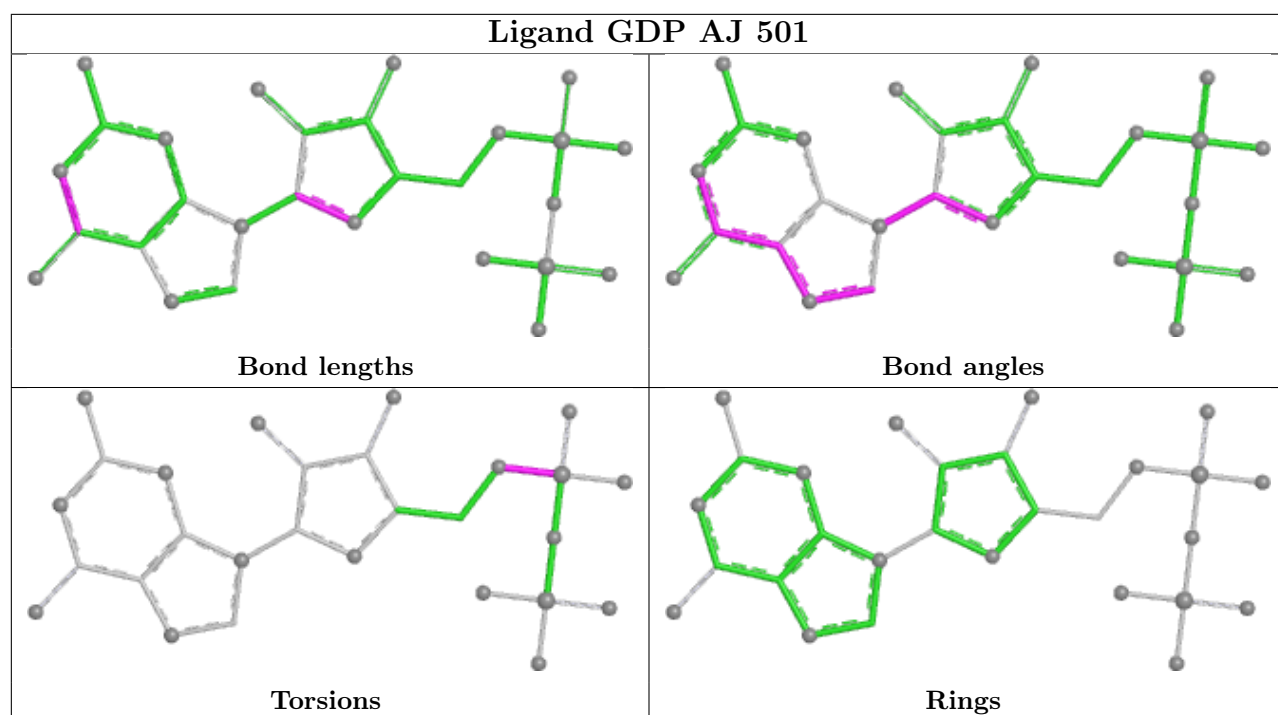


## Ligand GTP HM 501

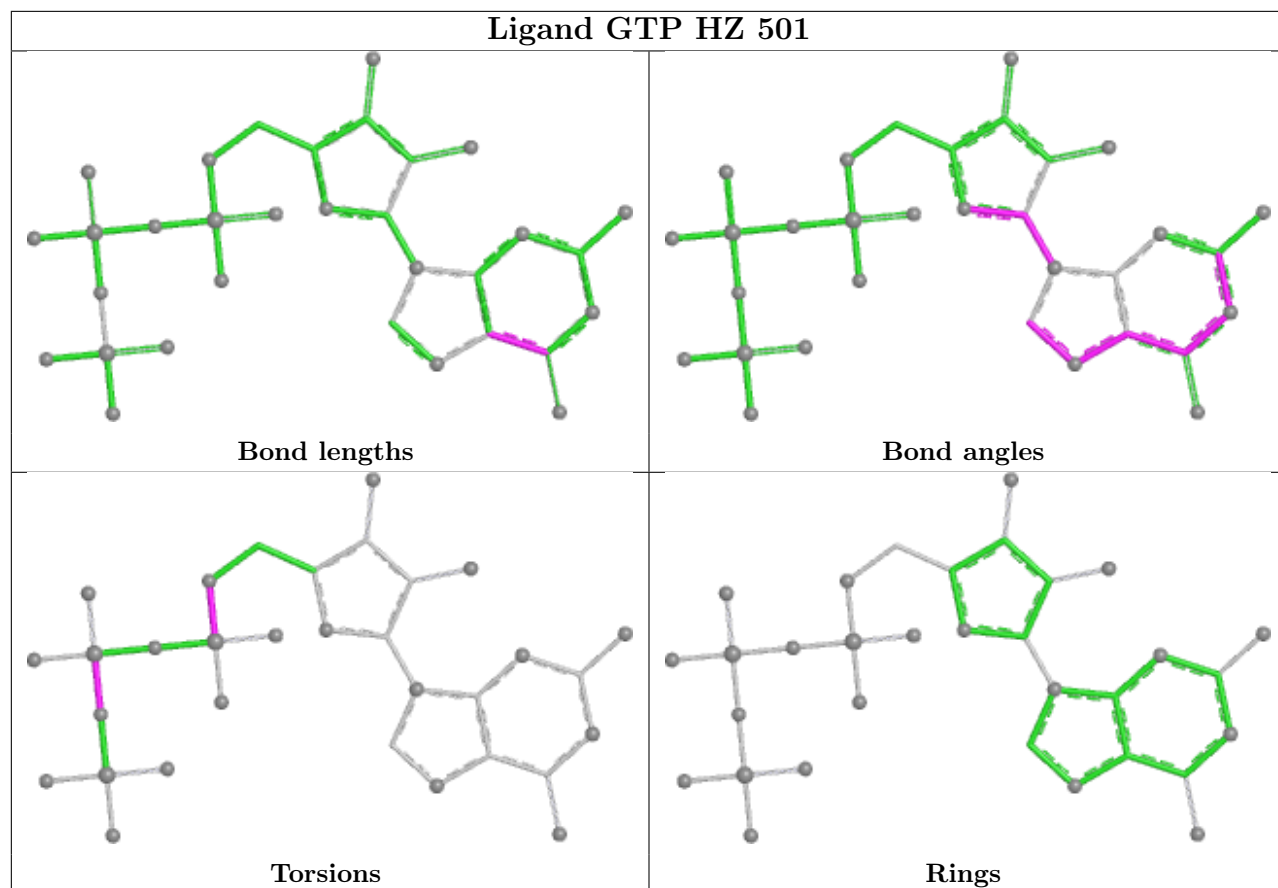


## Ligand GDP CL 501

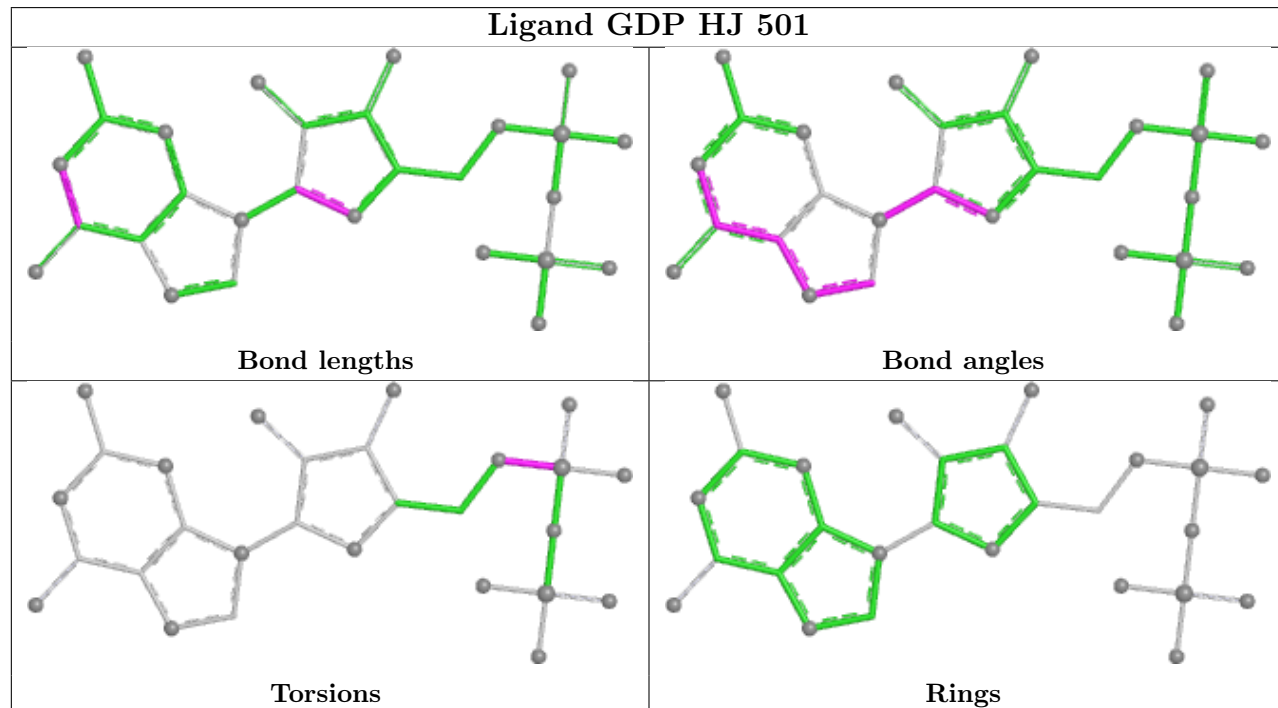


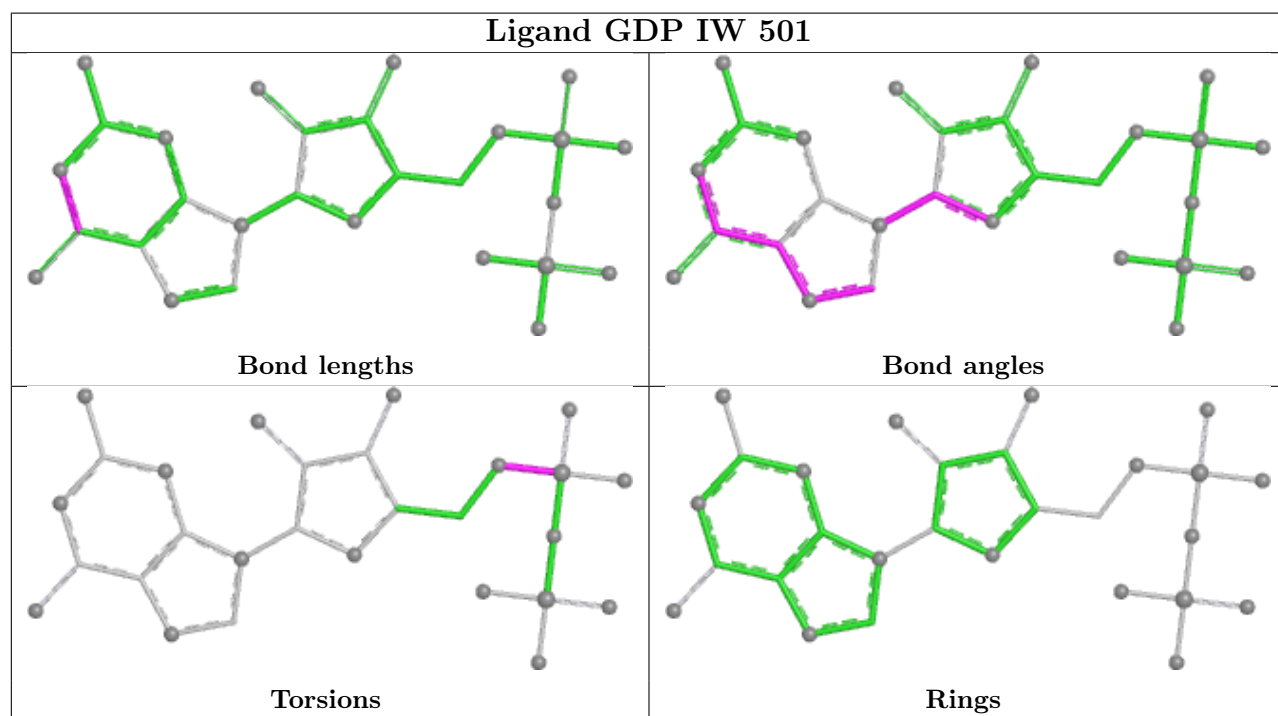
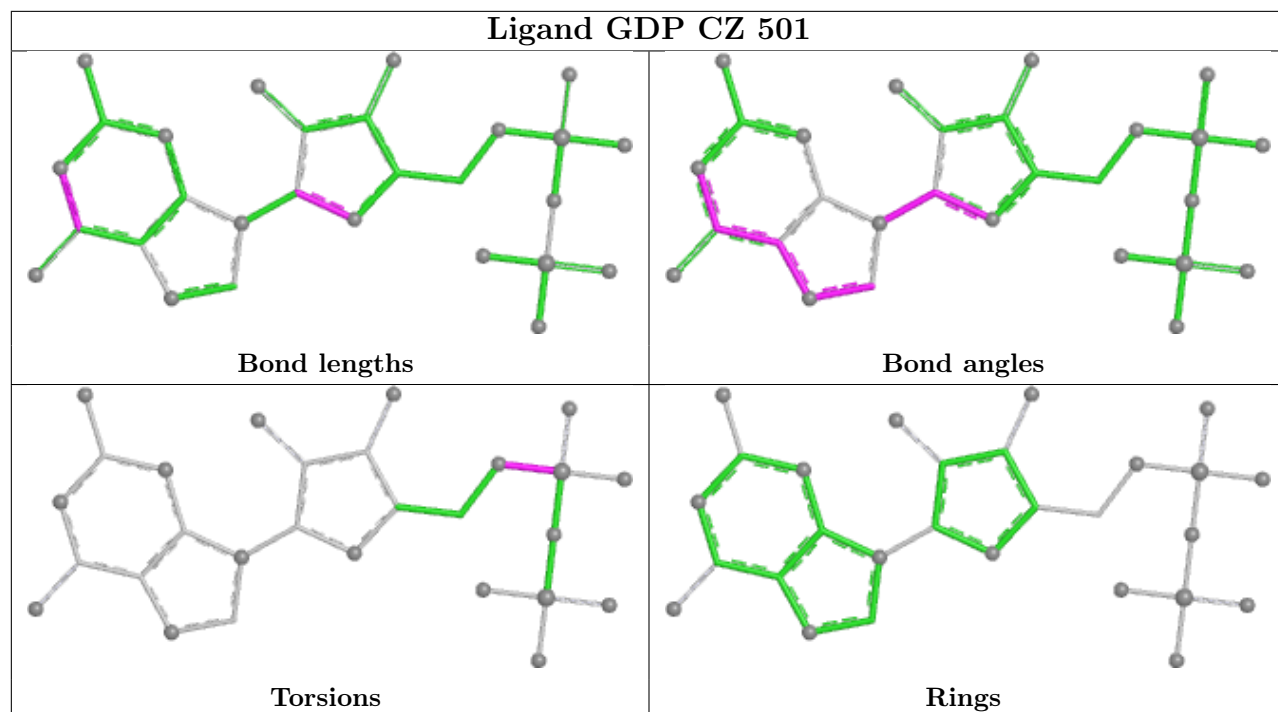


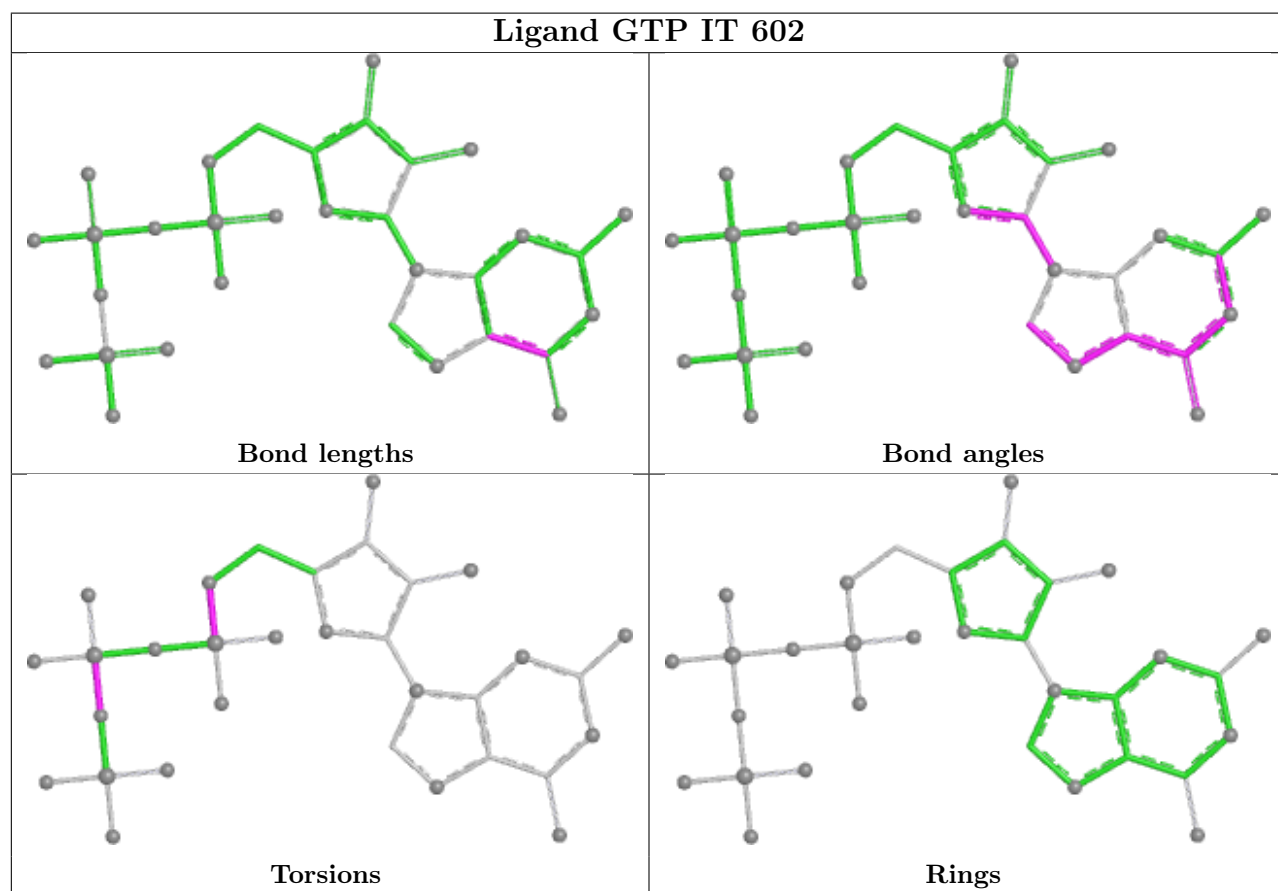
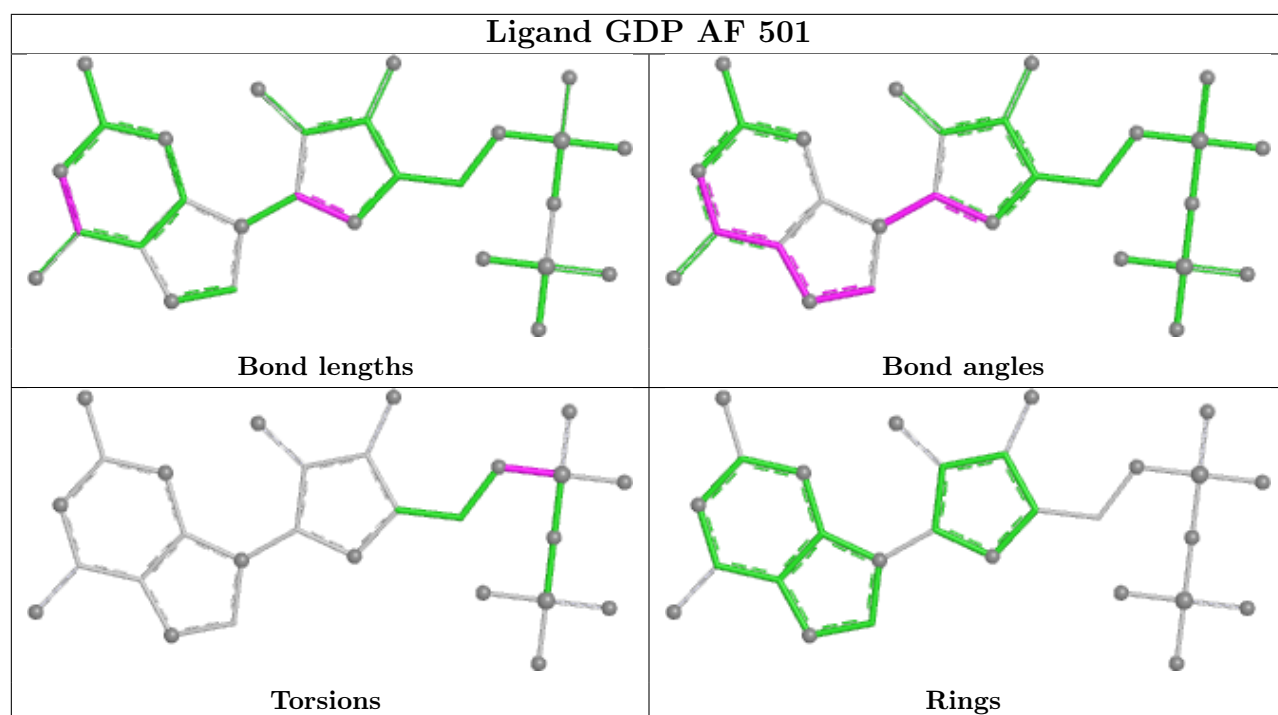
## Ligand GTP HZ 501



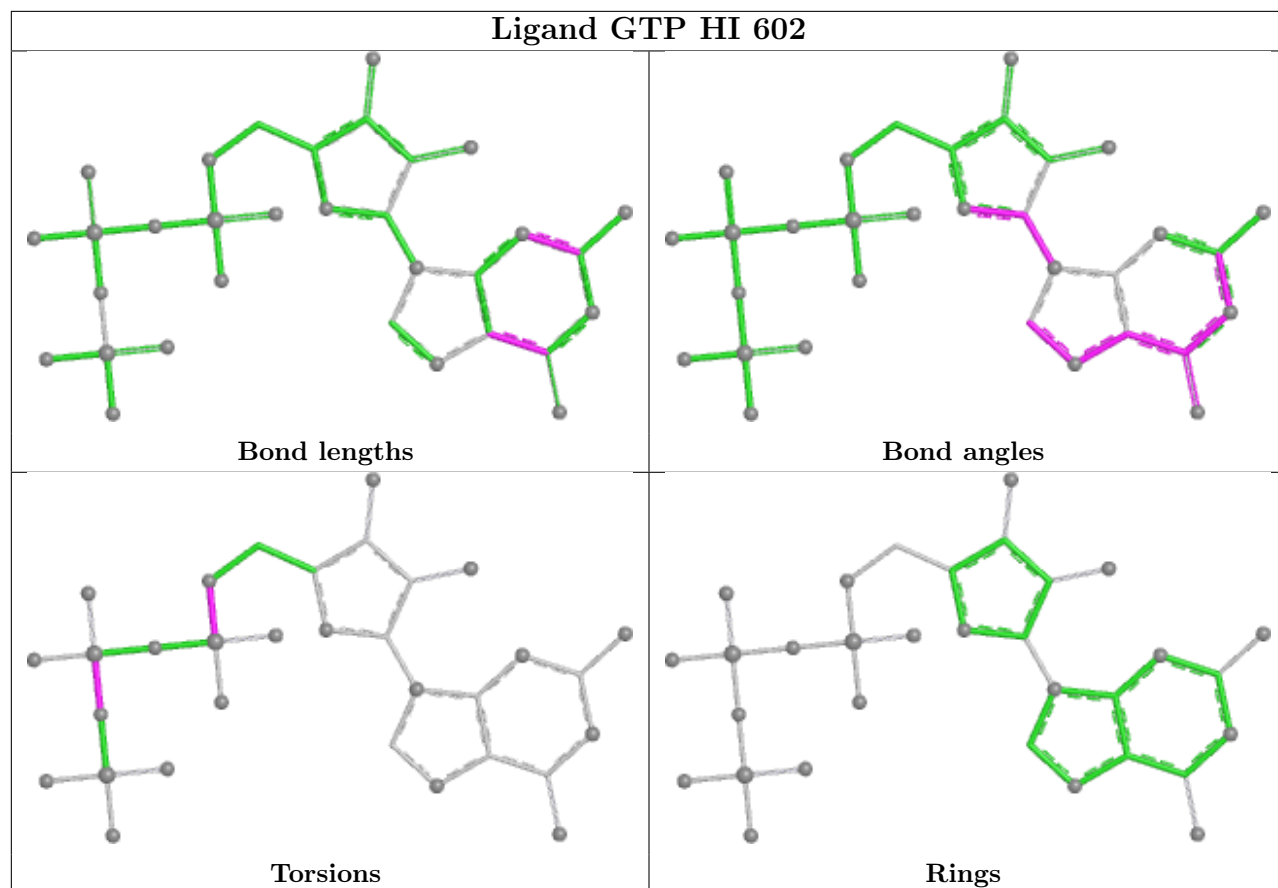
## Ligand GDP HJ 501



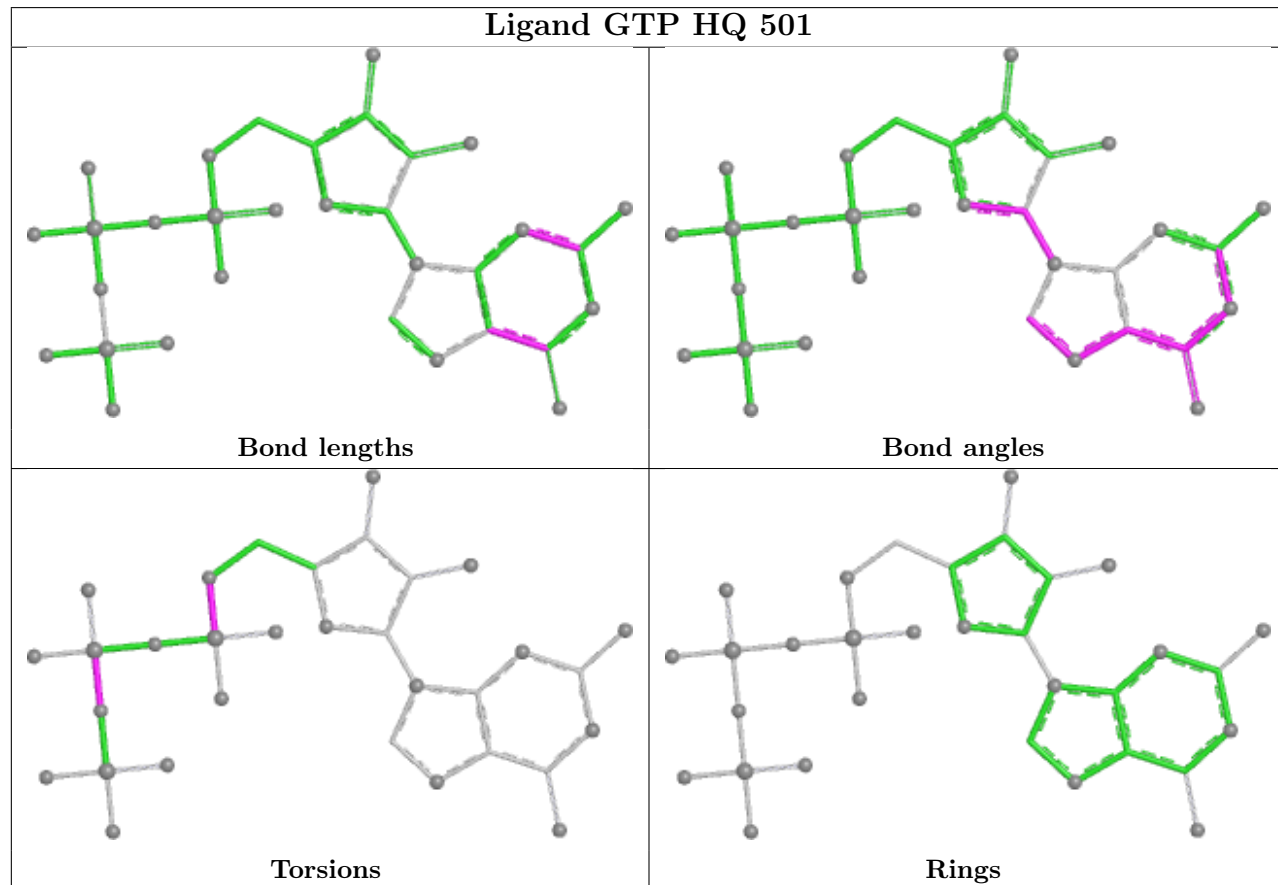


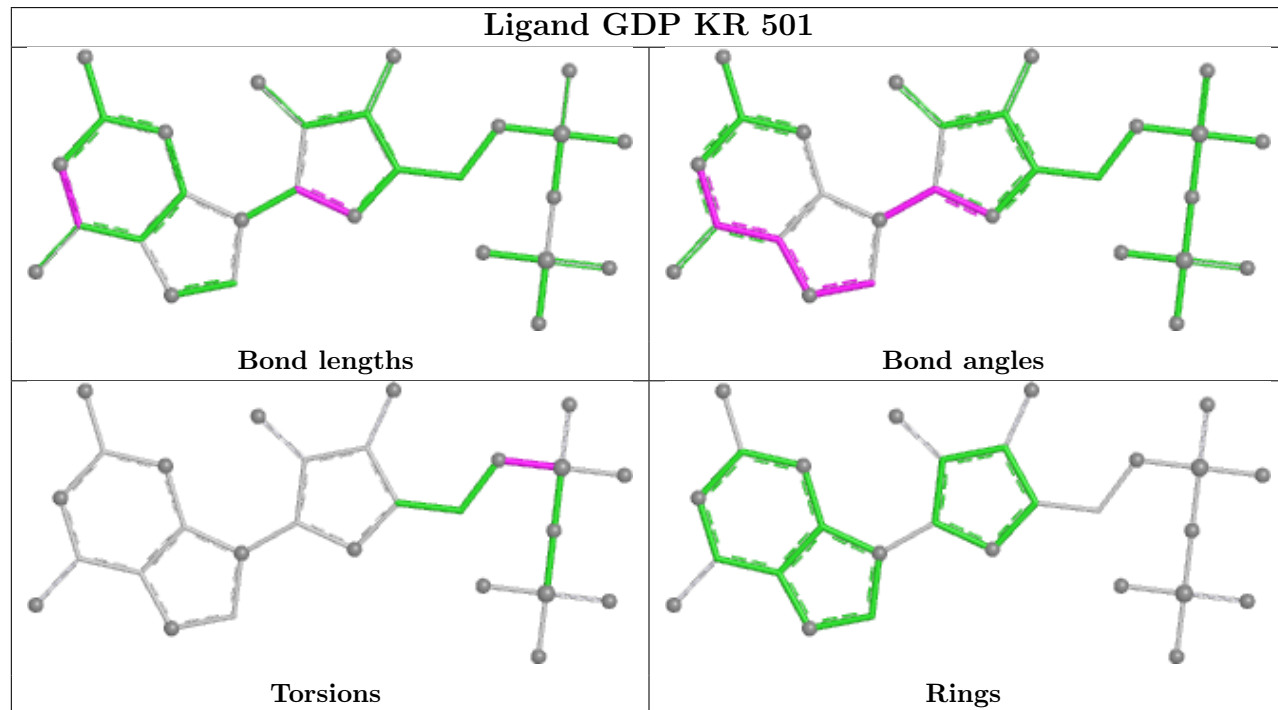
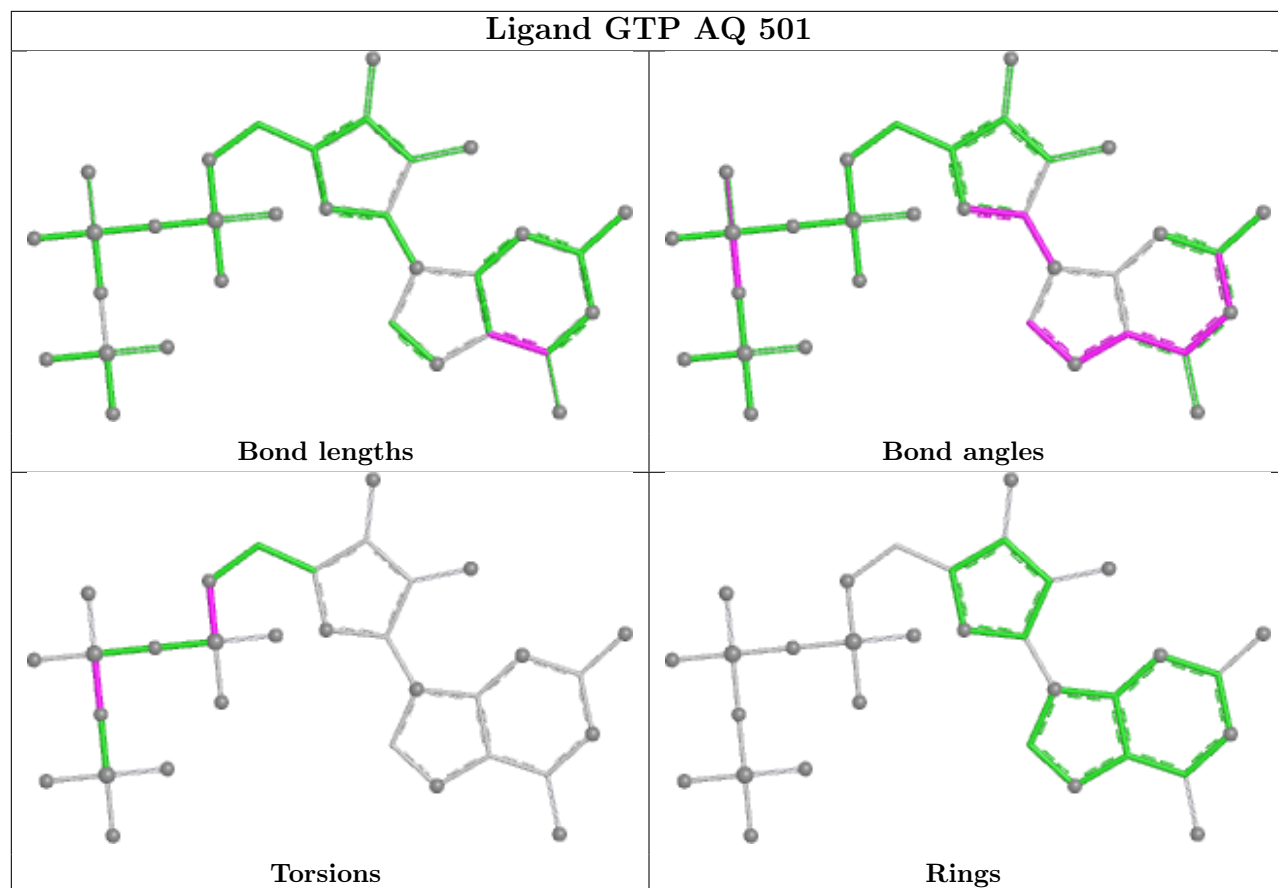


## Ligand GTP HI 602

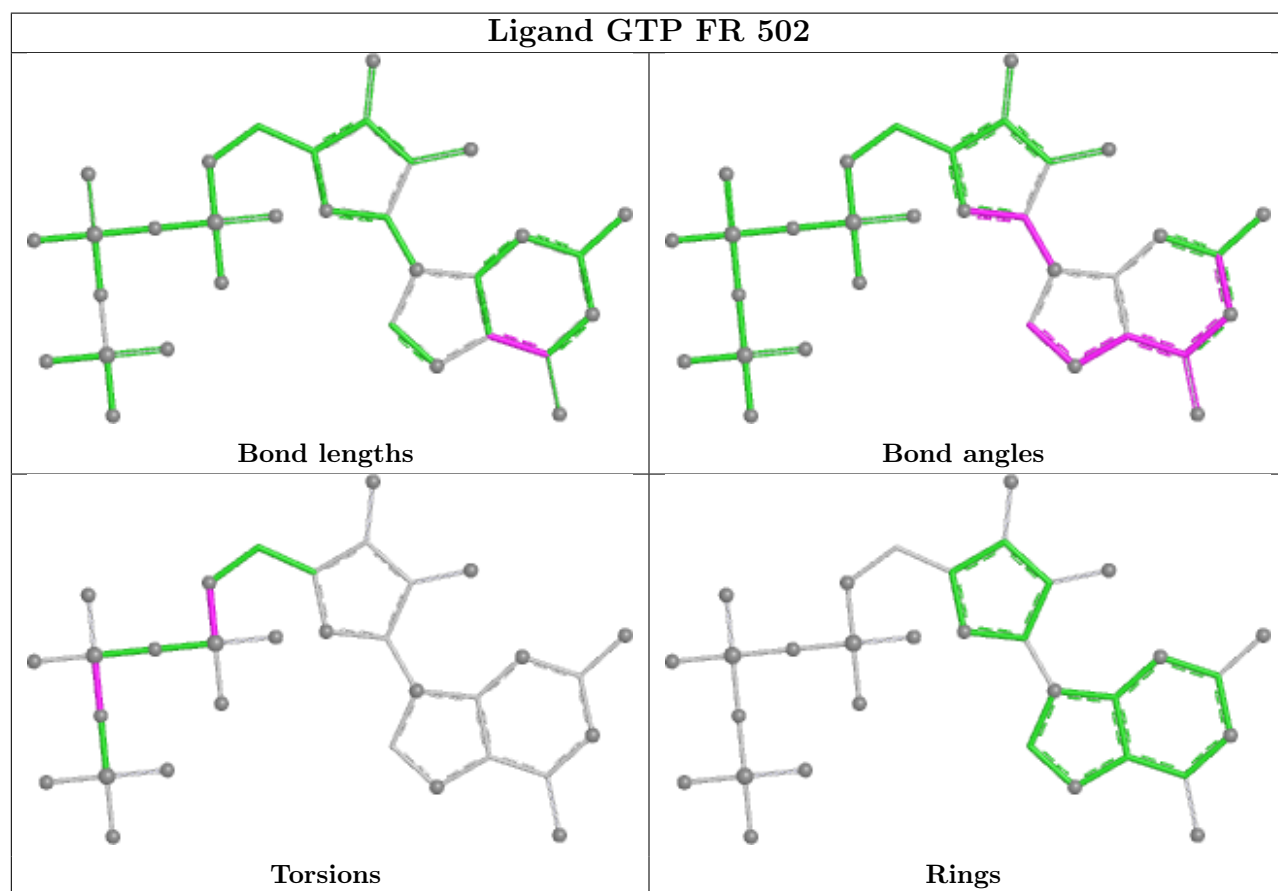
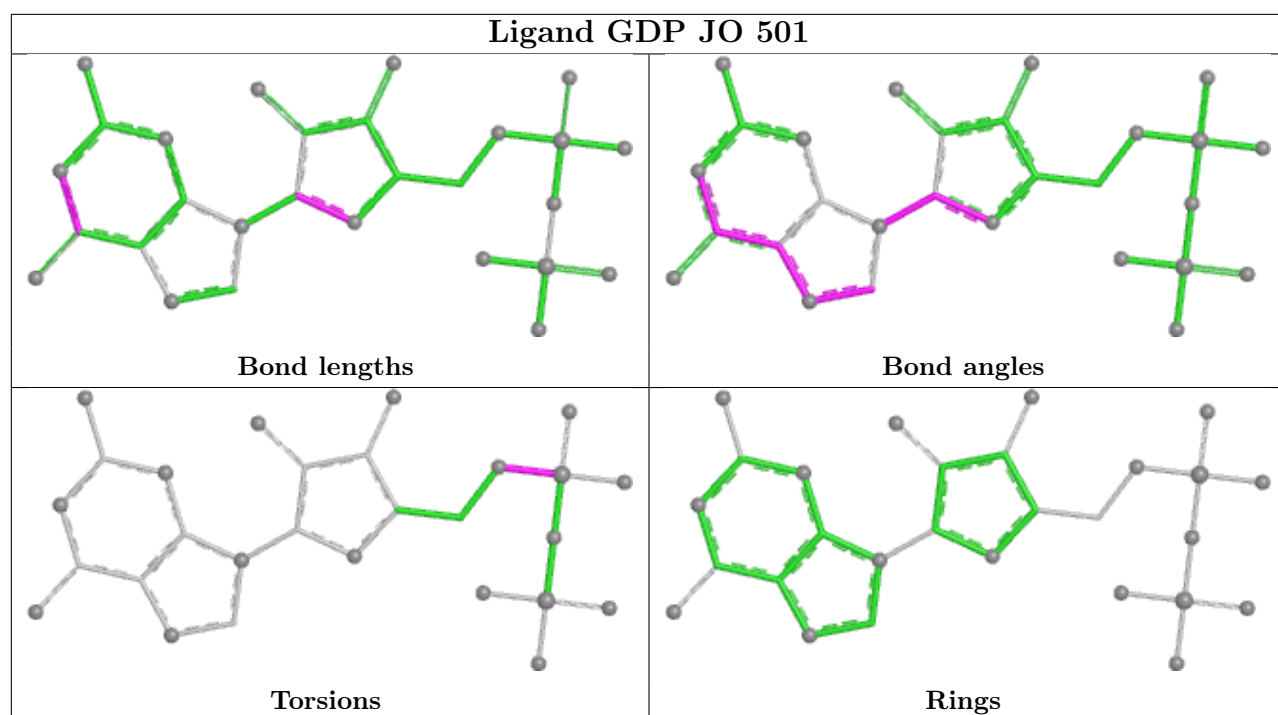


## Ligand GTP HQ 501

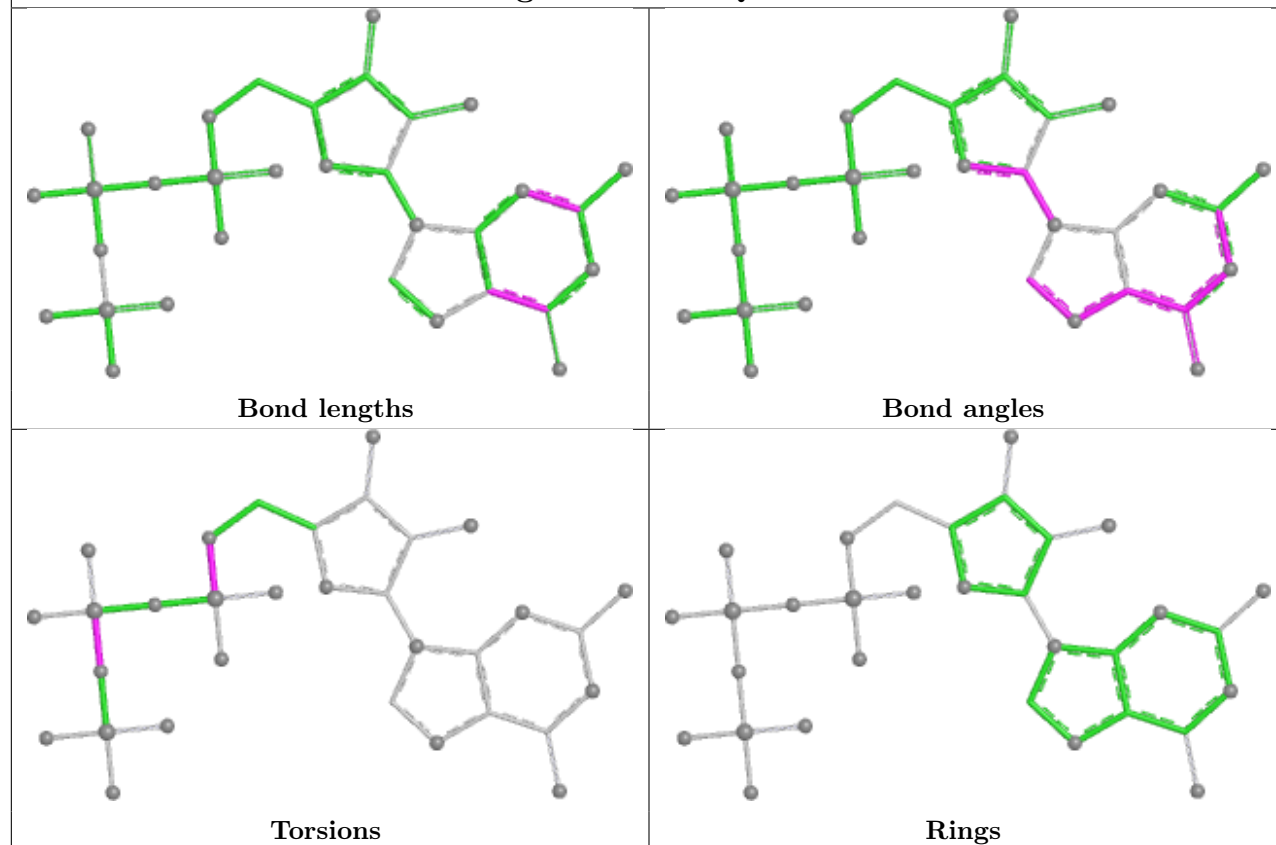




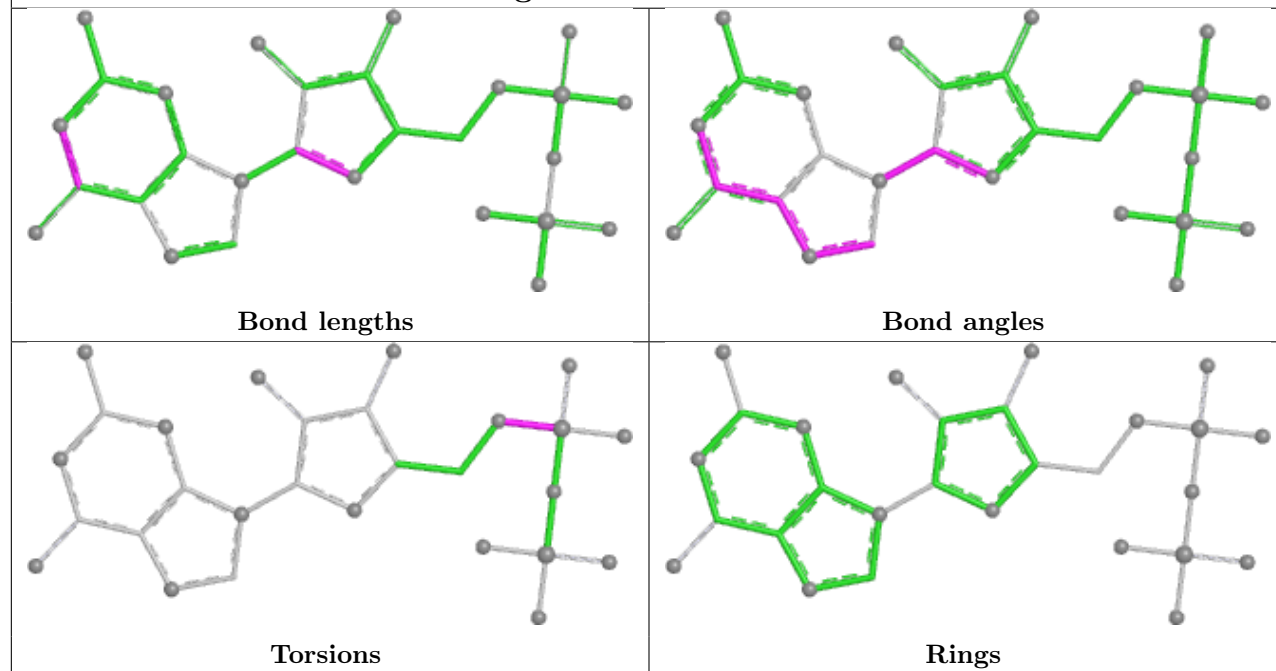


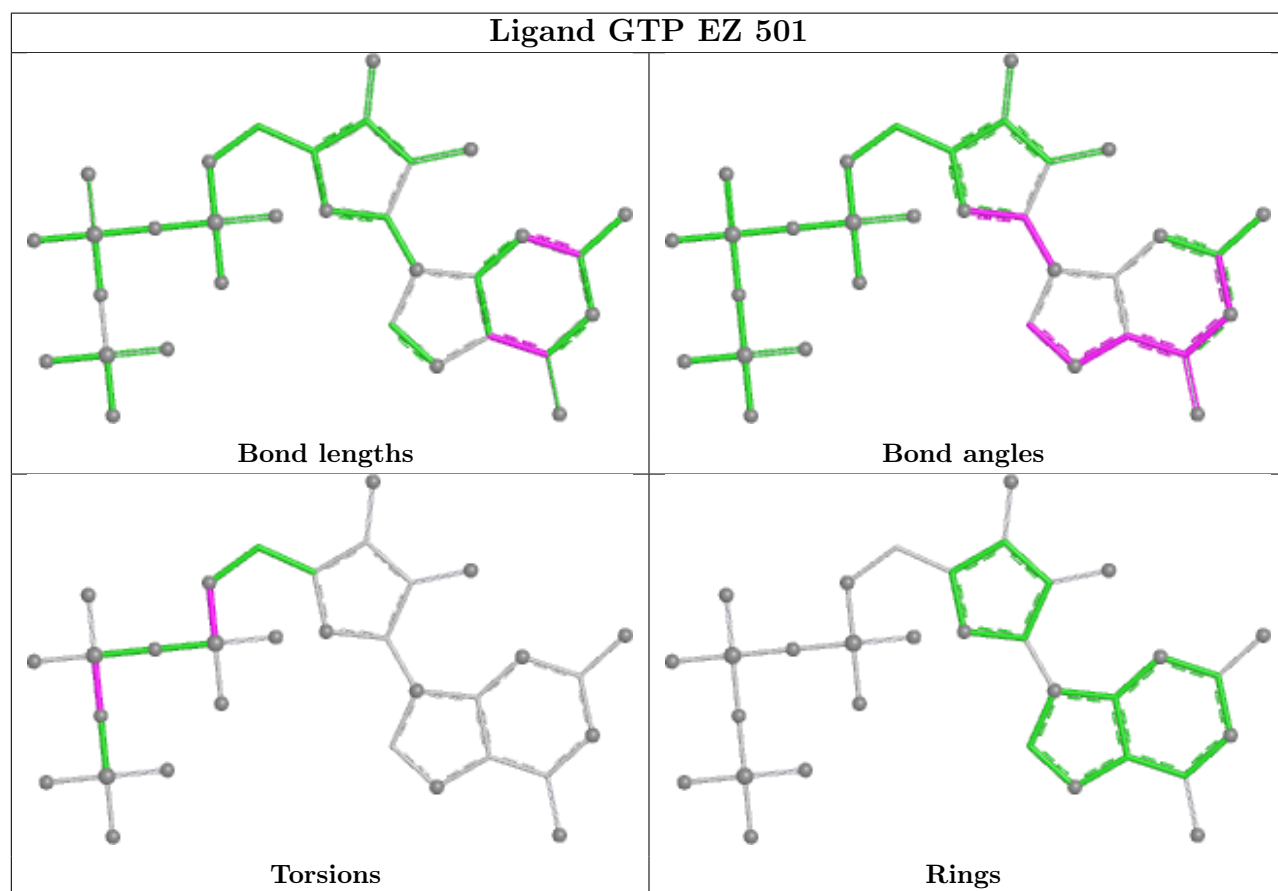
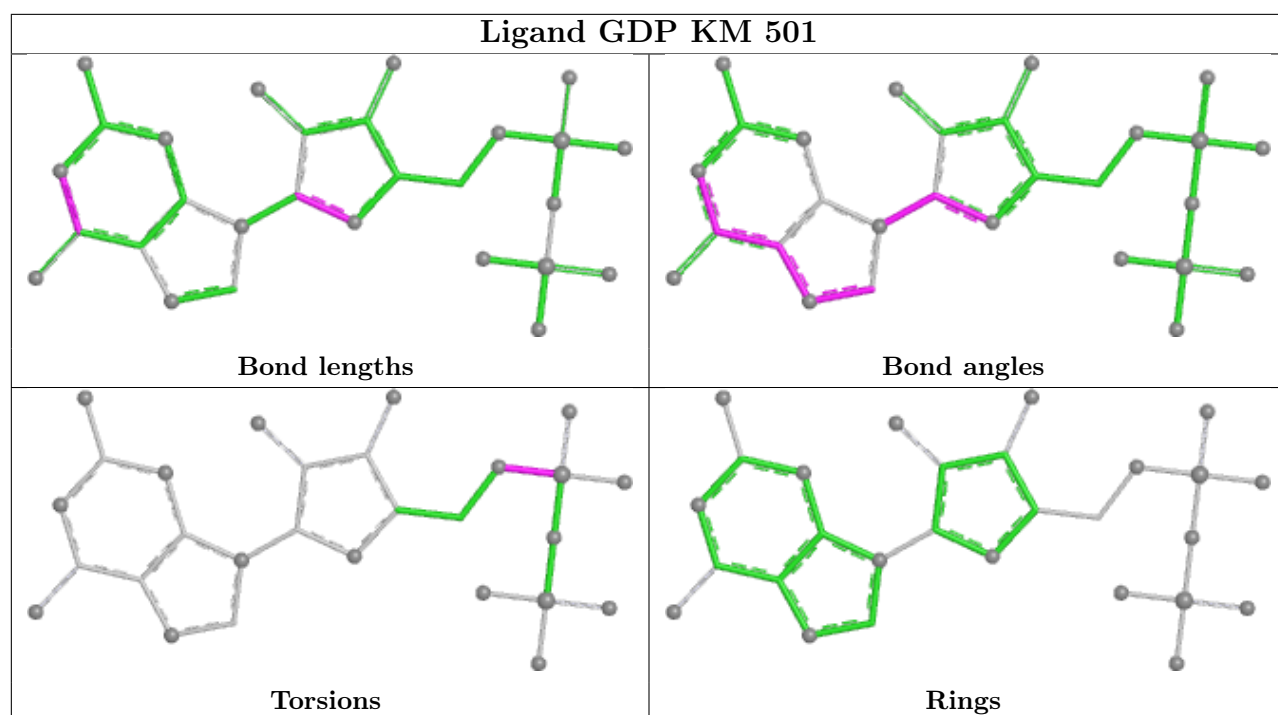


## Ligand GTP DQ 501

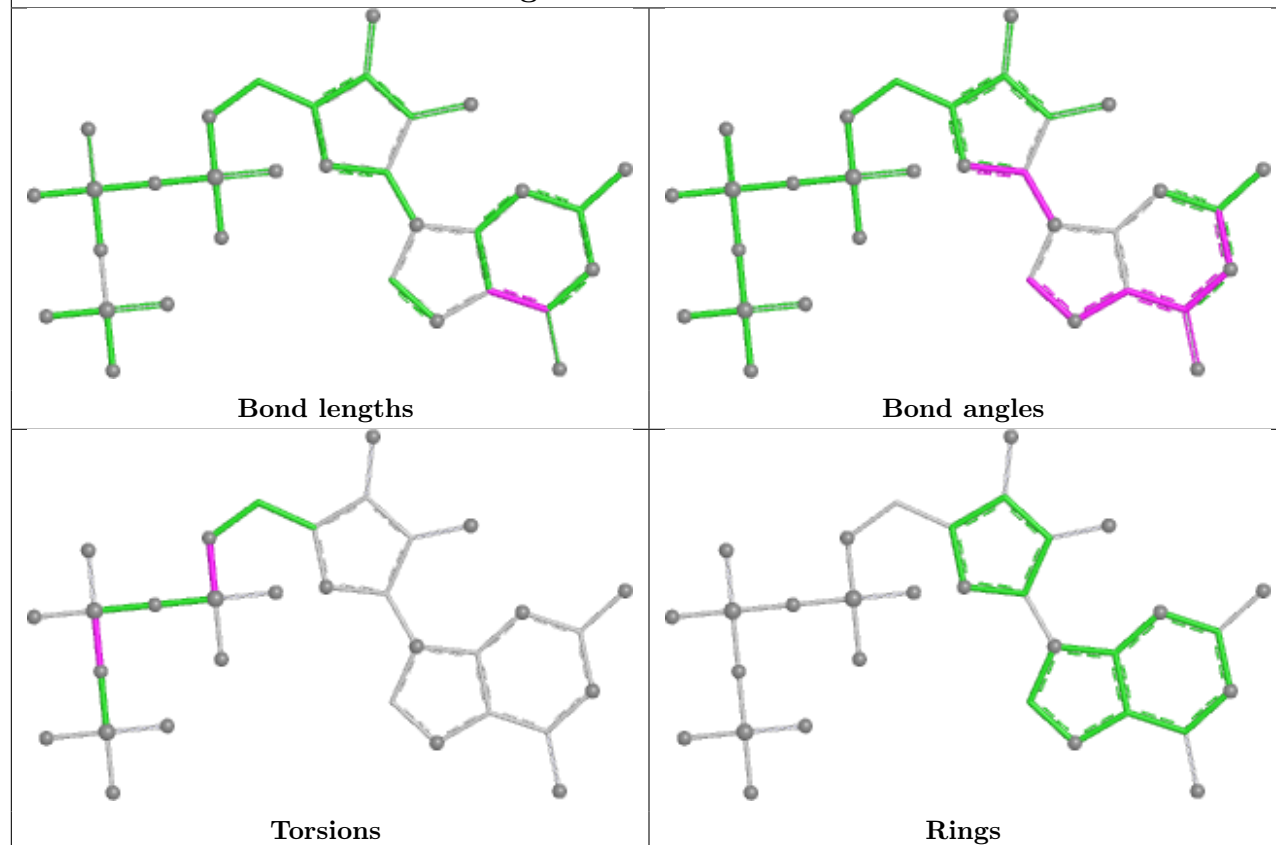


## Ligand GDP KX 501

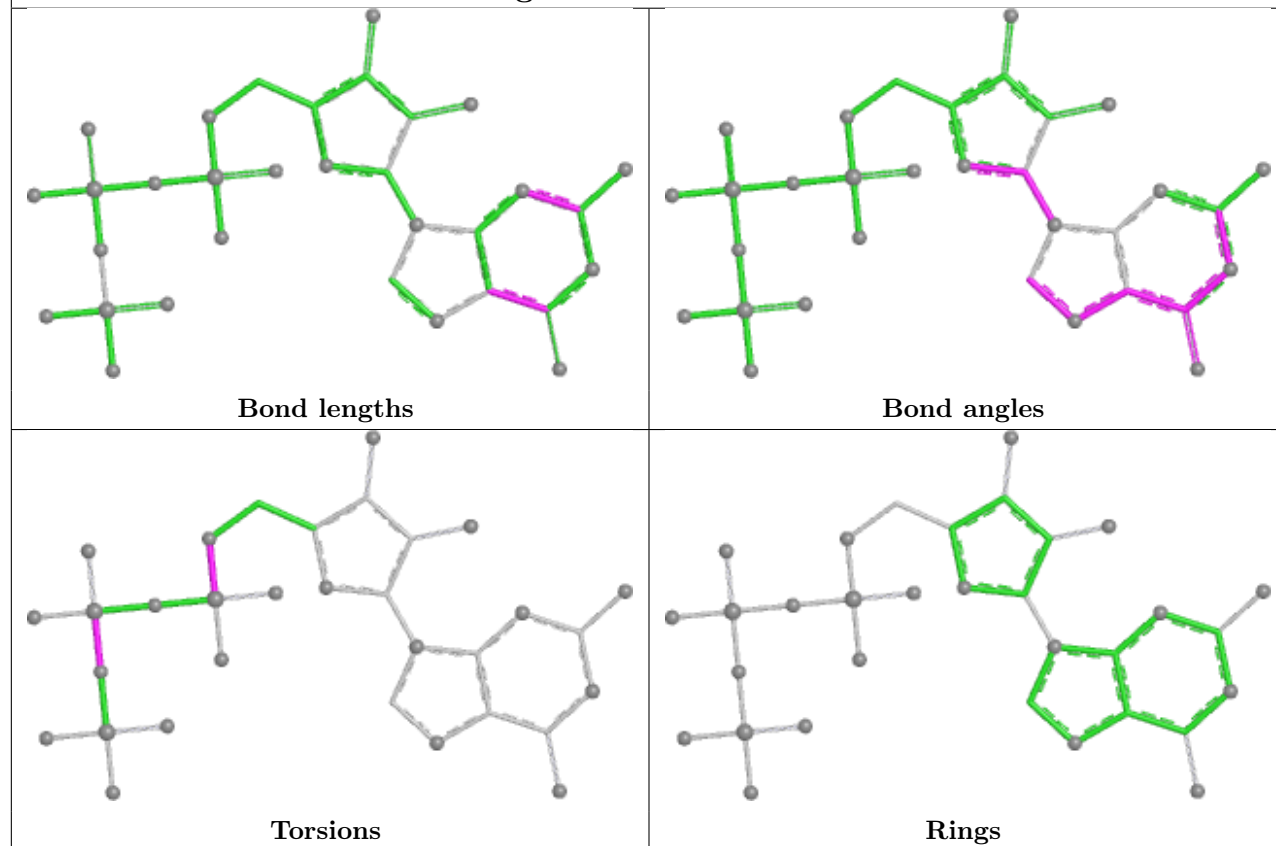




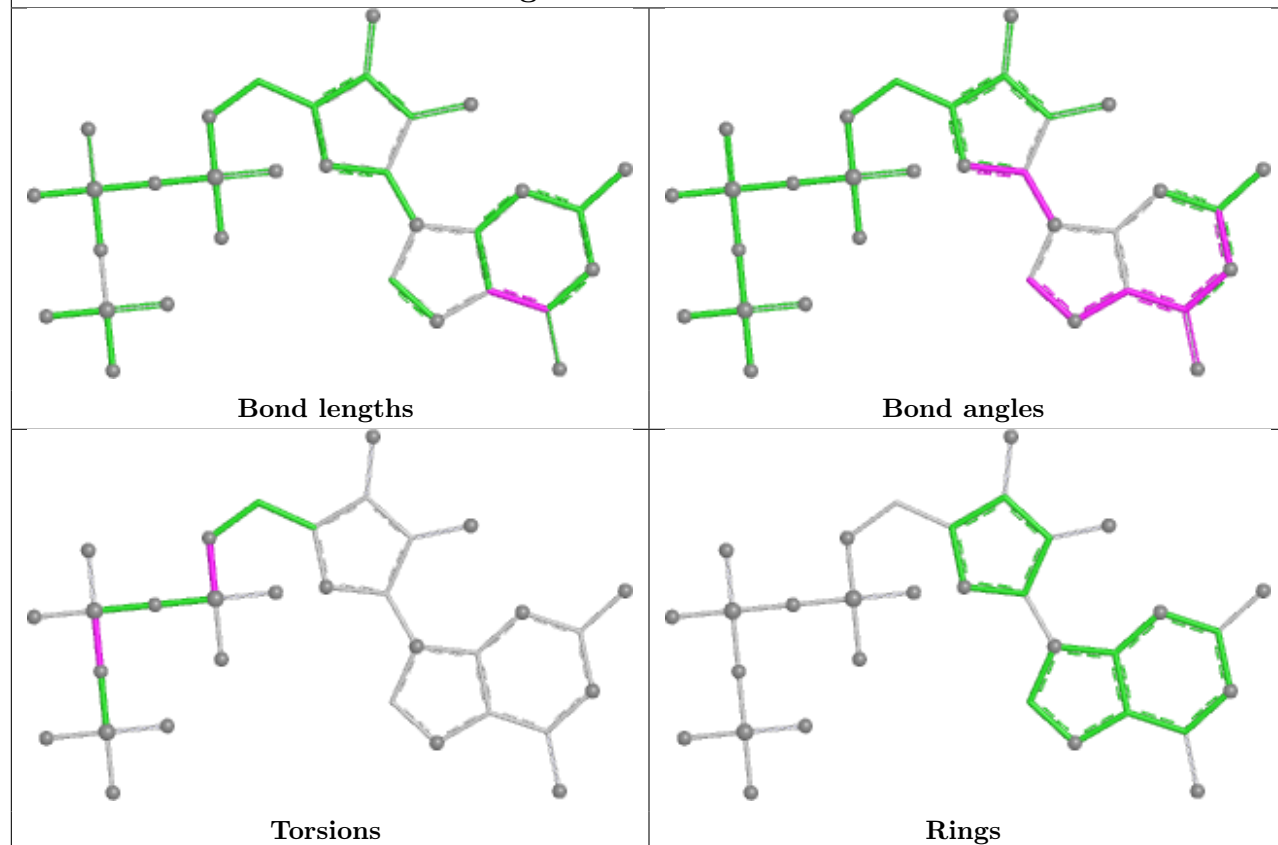
## Ligand GTP AS 602



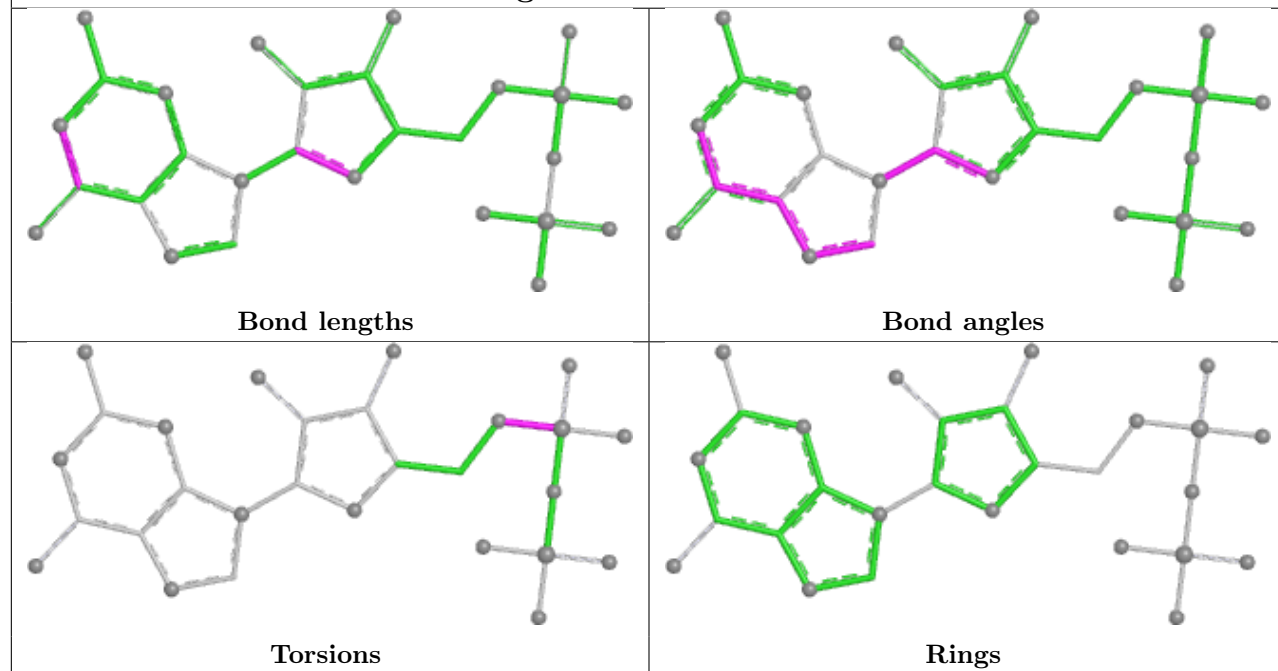
## Ligand GTP GU 501

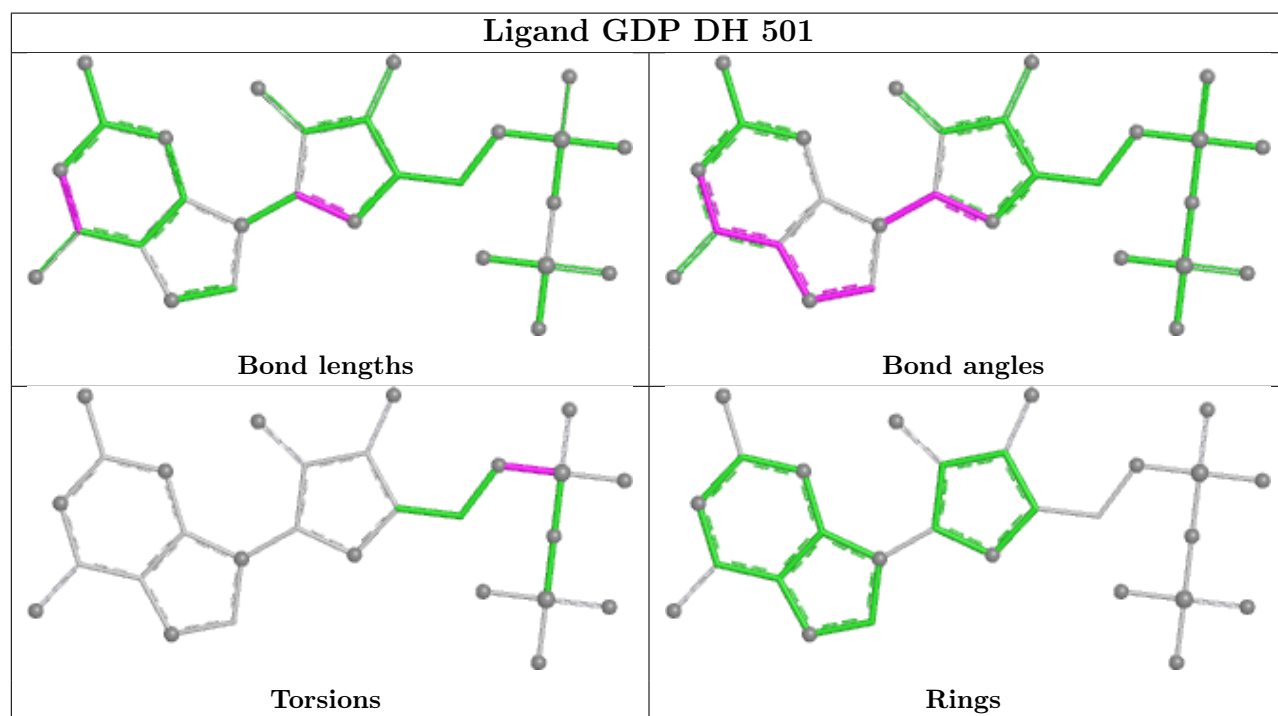
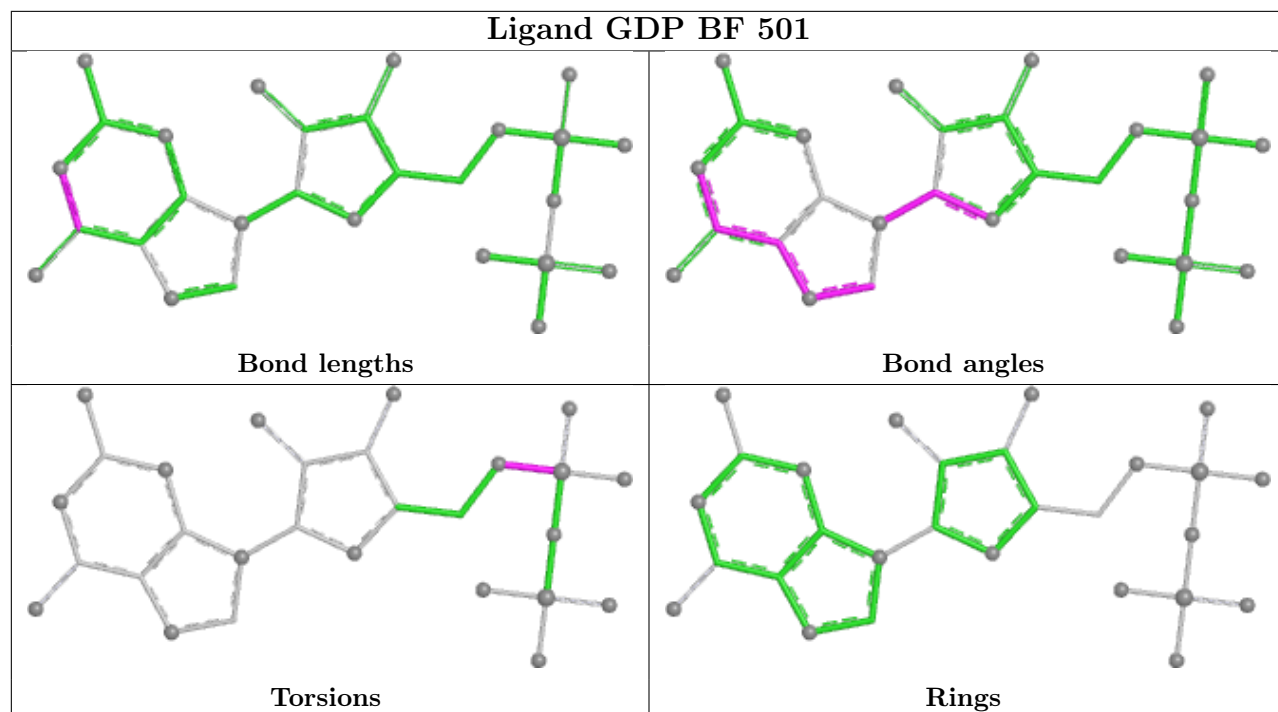


## Ligand GTP EP 602

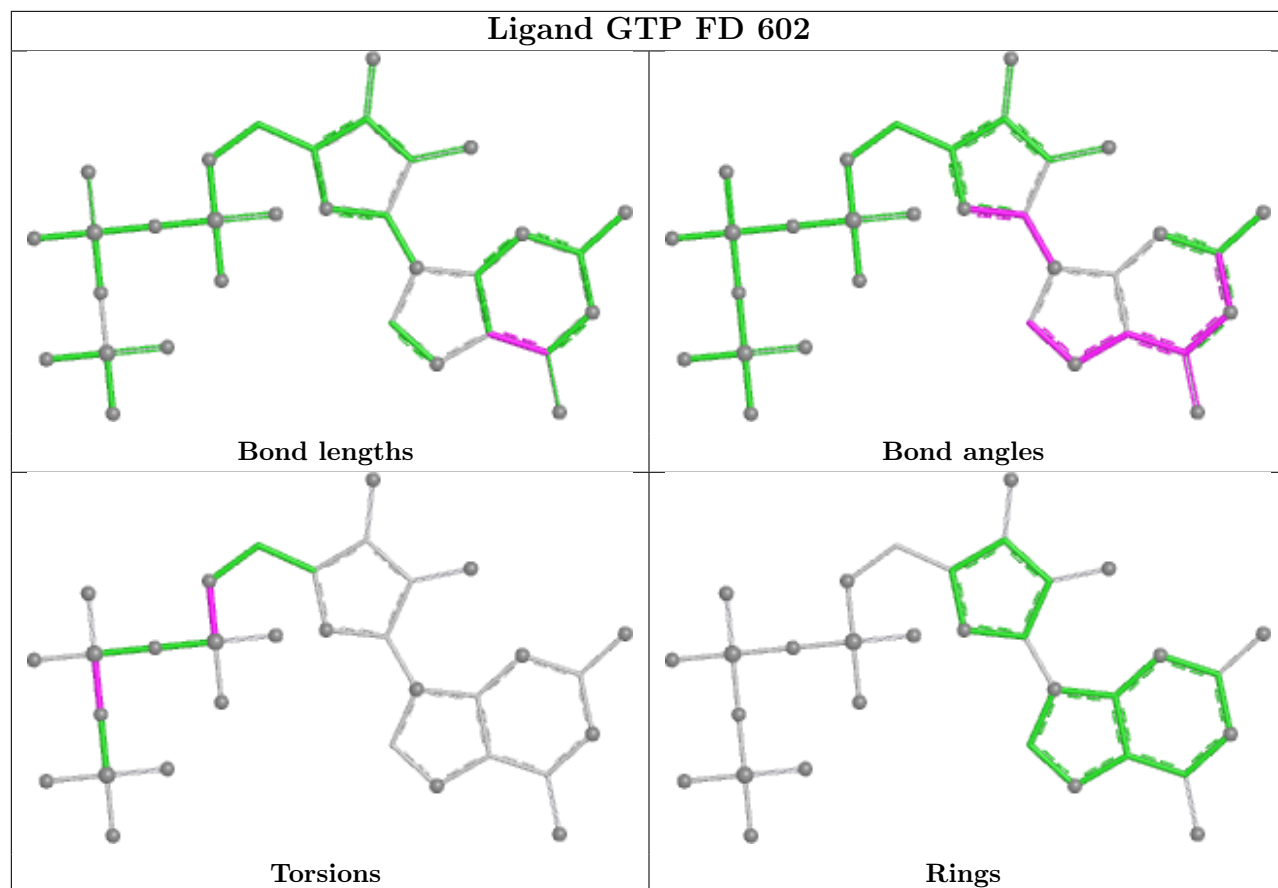


## Ligand GDP AP 501

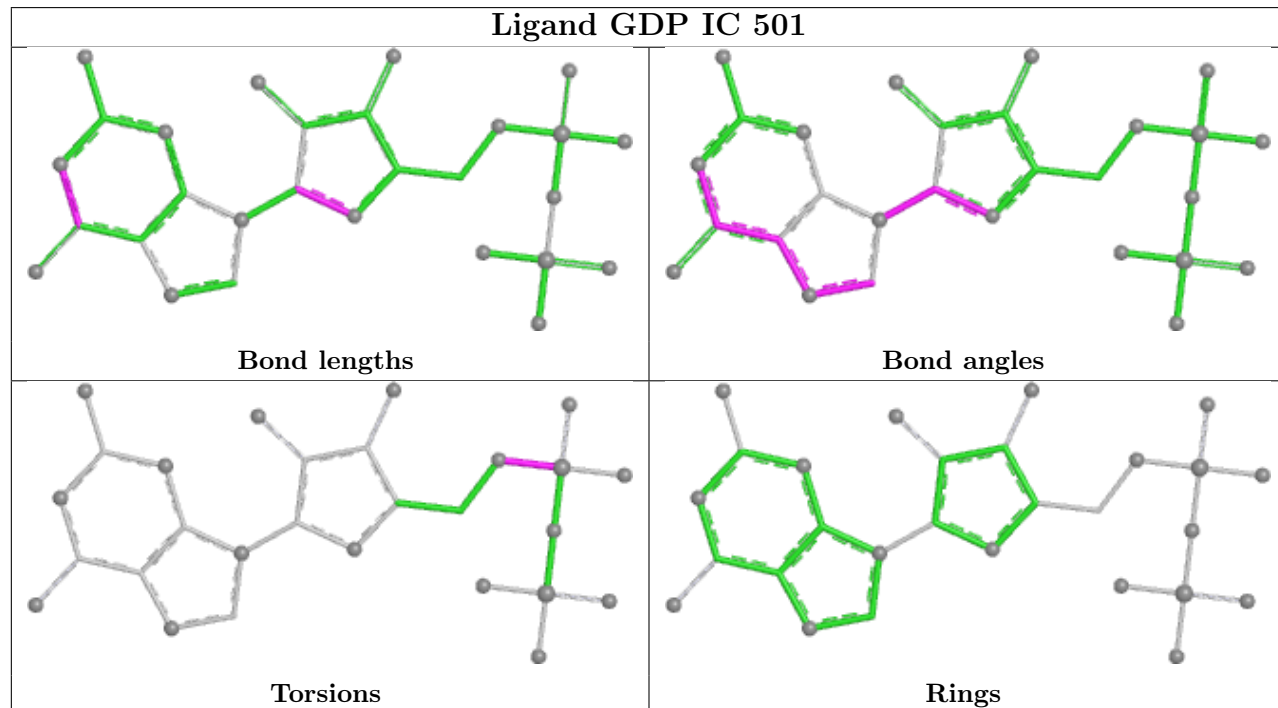


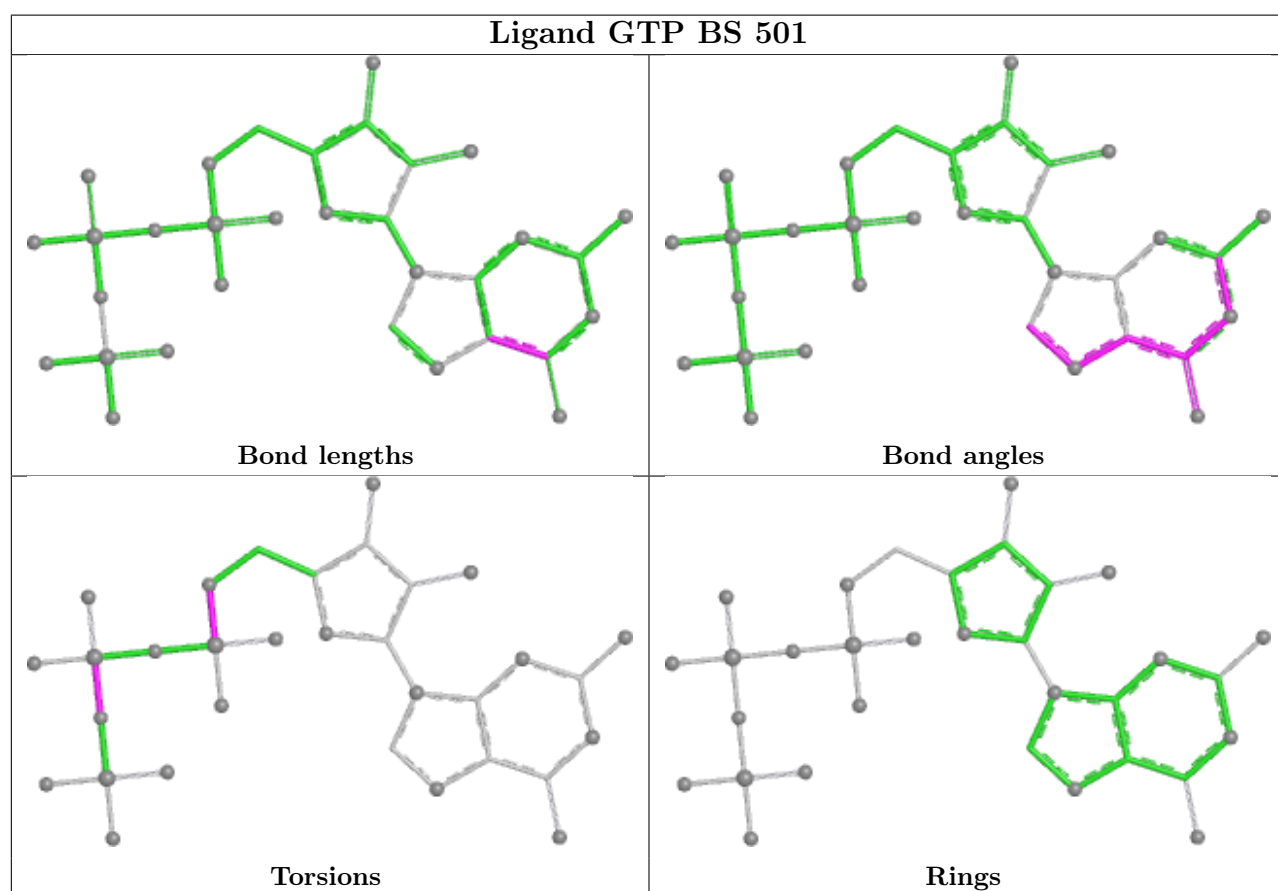
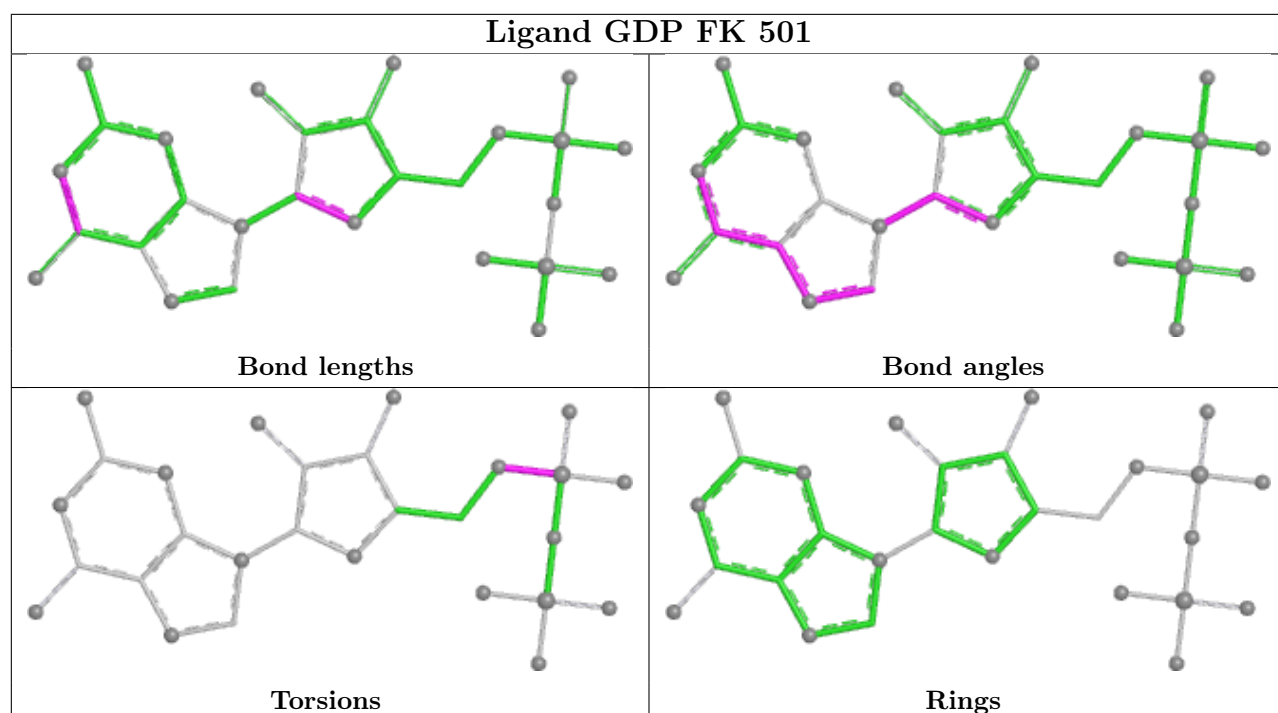


## Ligand GTP FD 602



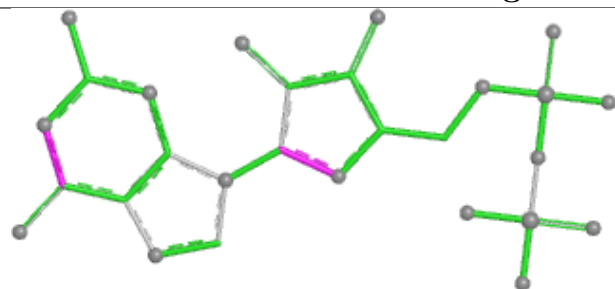
## Ligand GDP IC 501



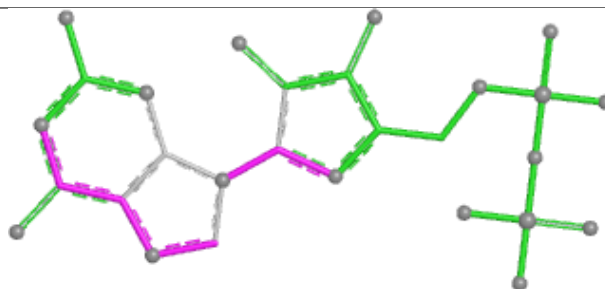




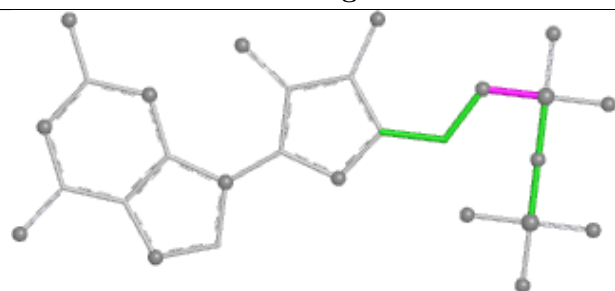
## Ligand GDP JK 501



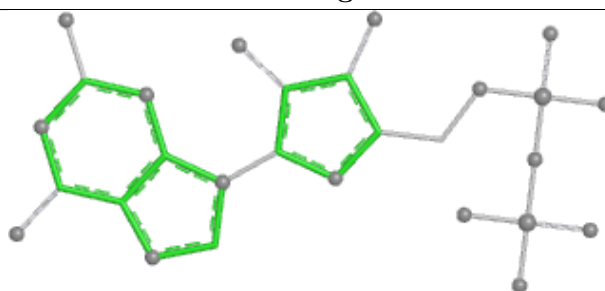
Bond lengths



Bond angles

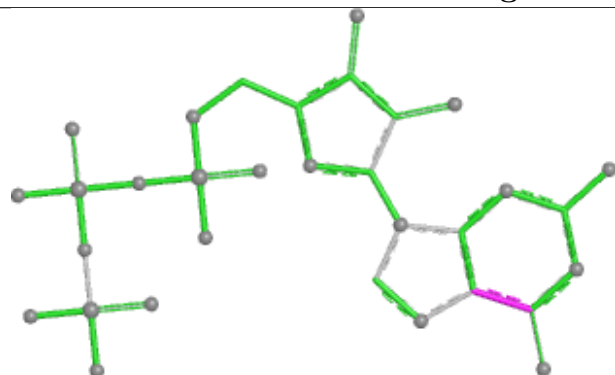


Torsions

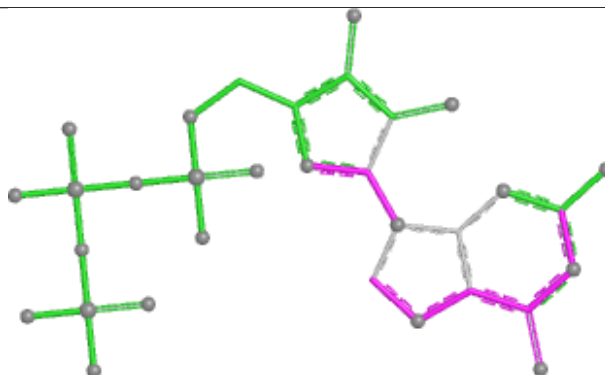


Rings

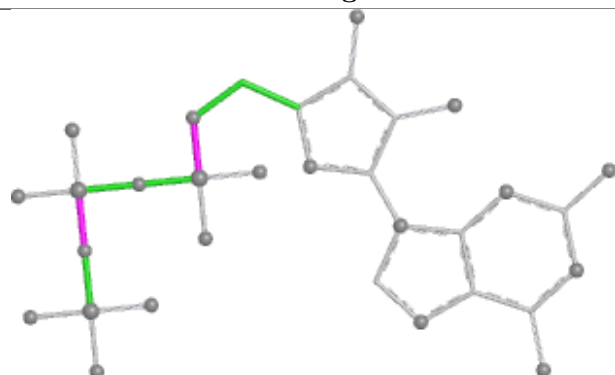
## Ligand GTP HV 501



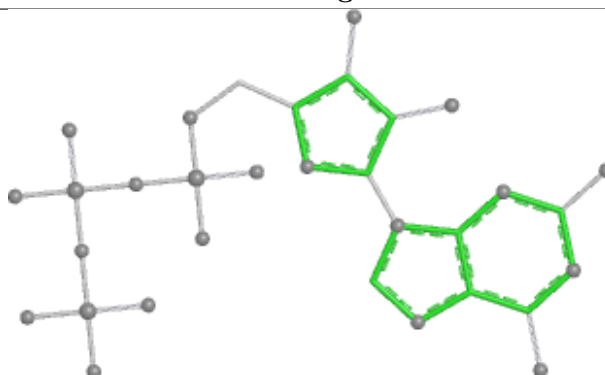
Bond lengths



Bond angles

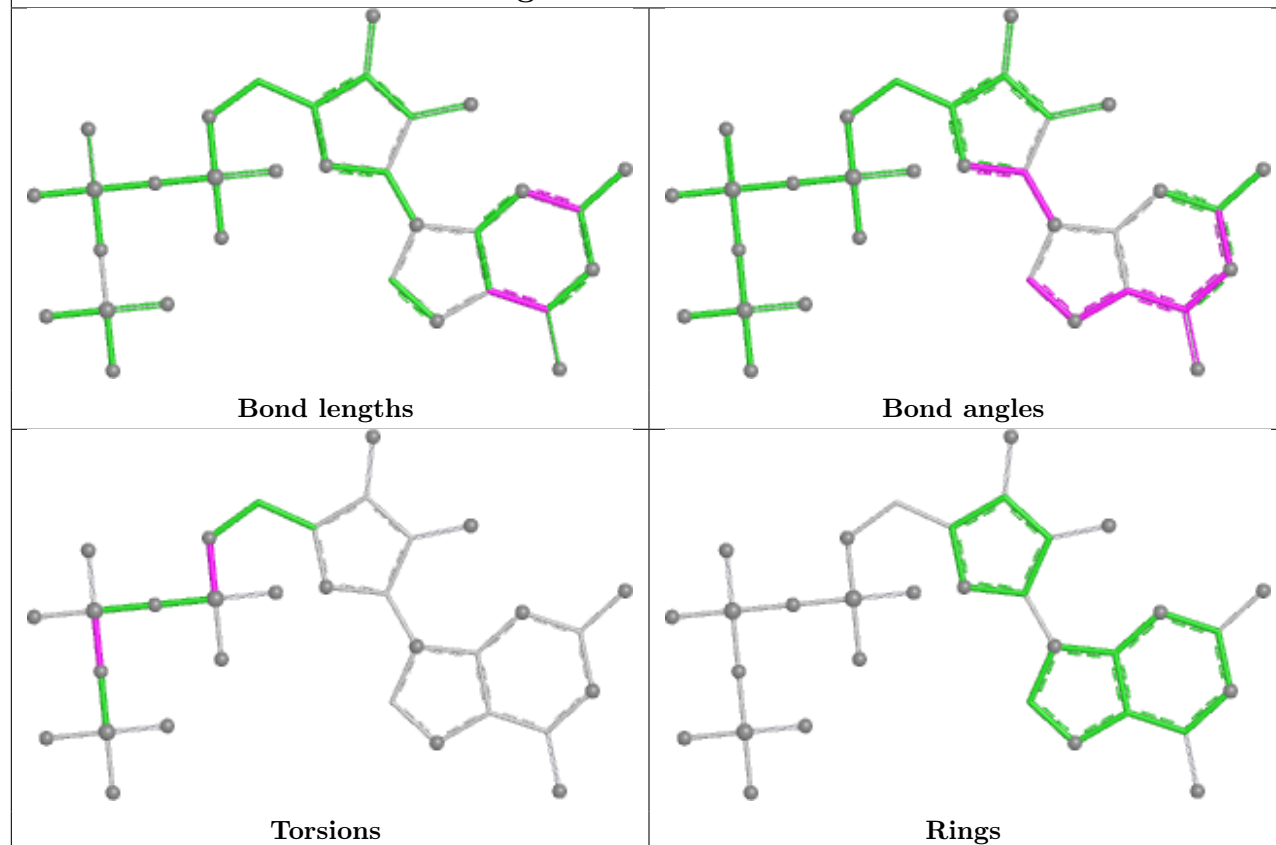


Torsions

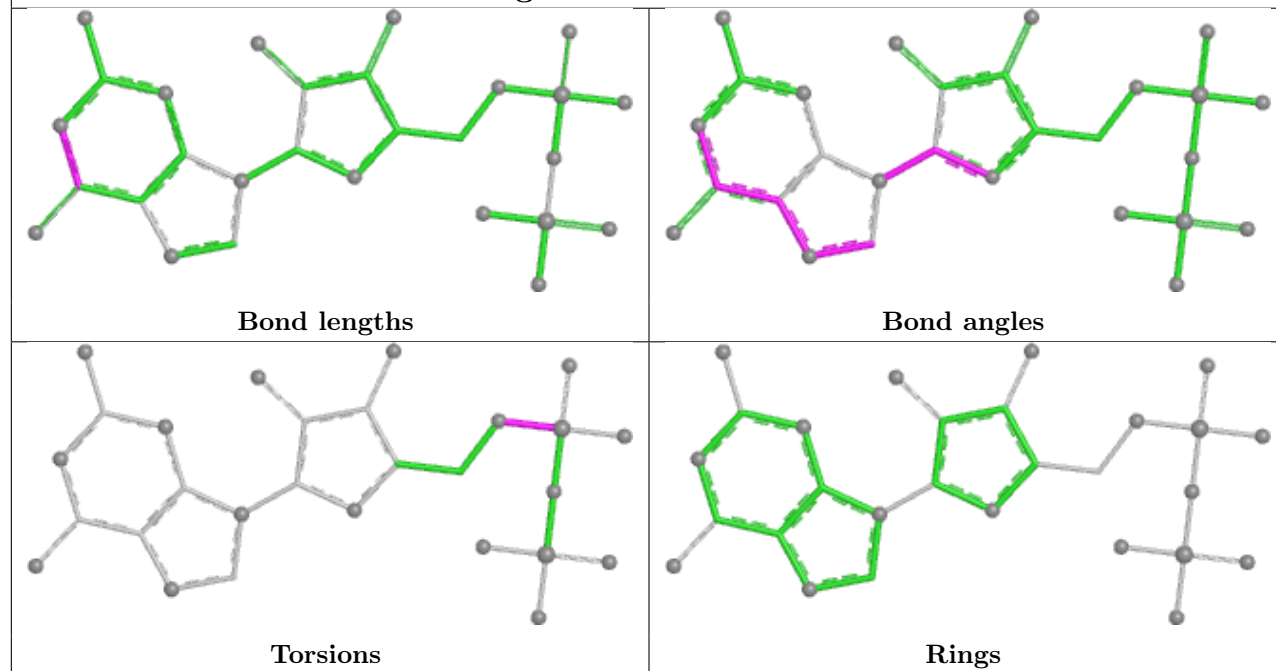


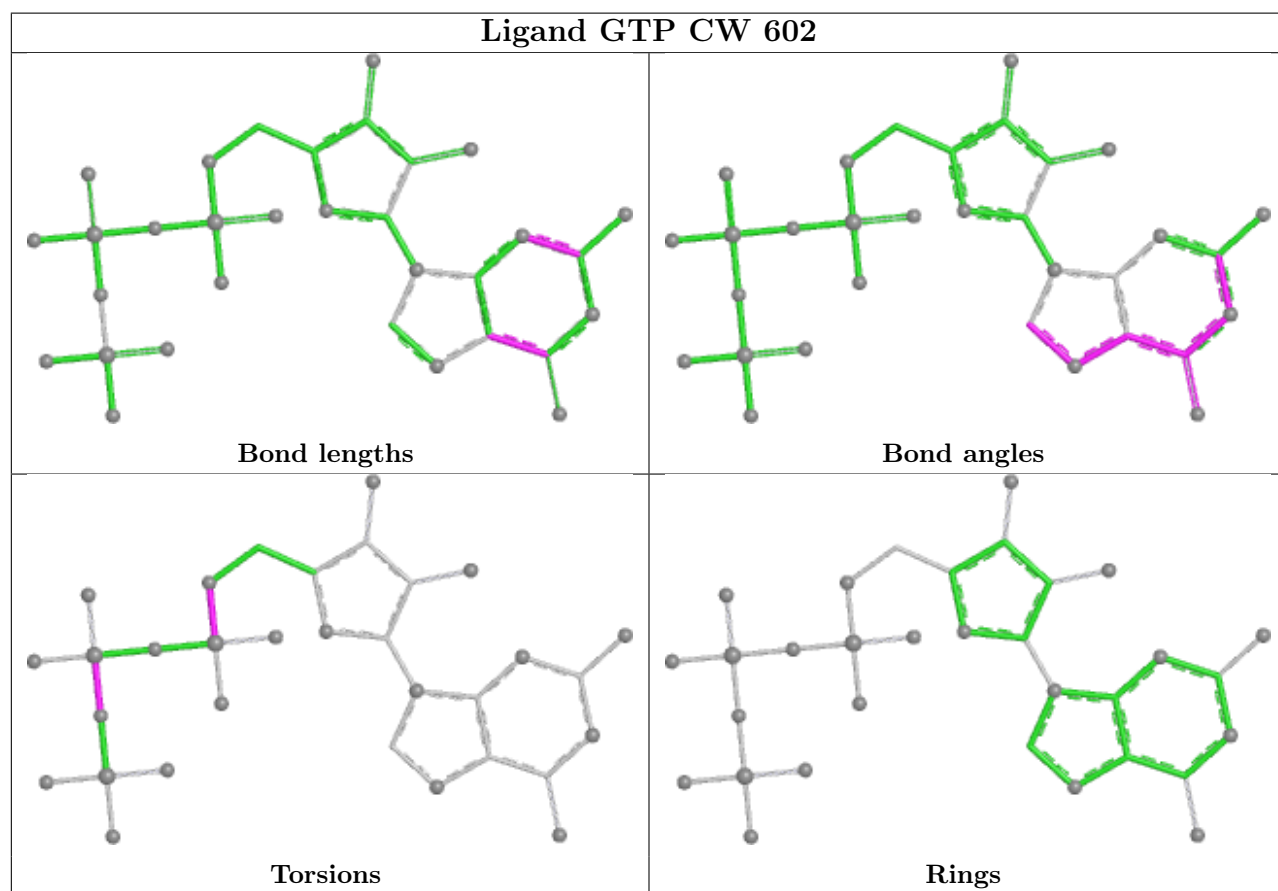
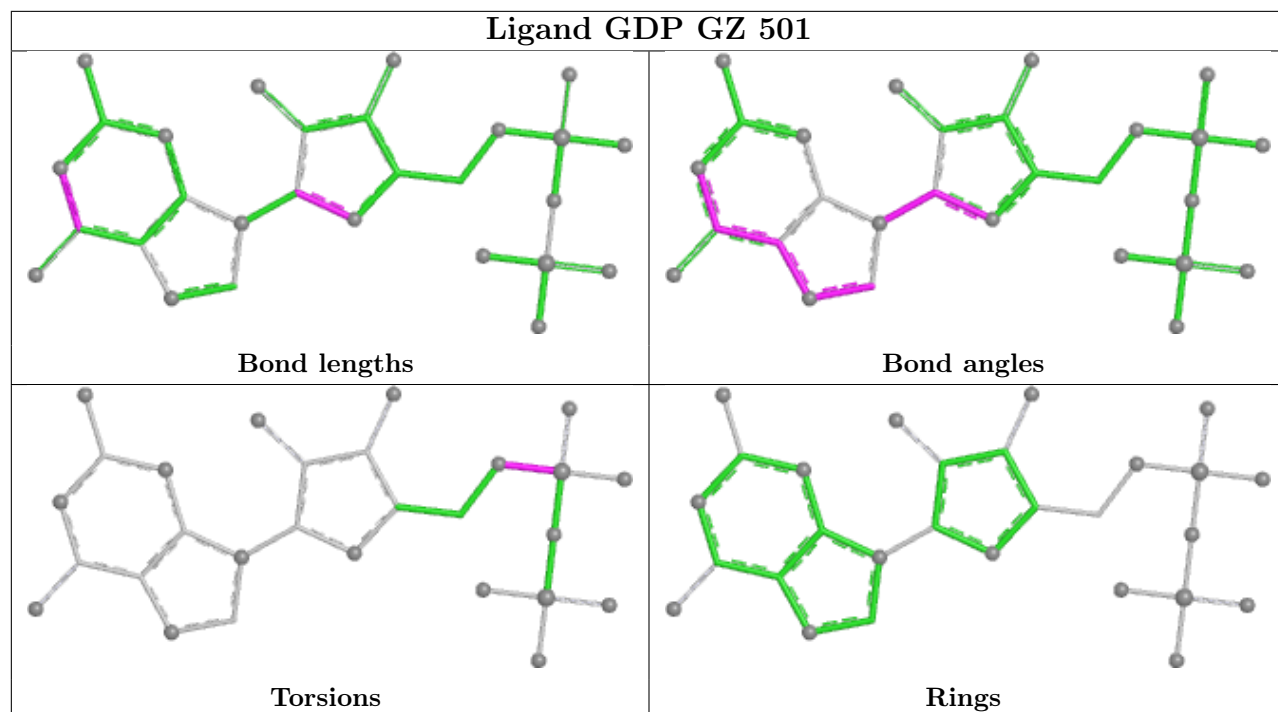
Rings

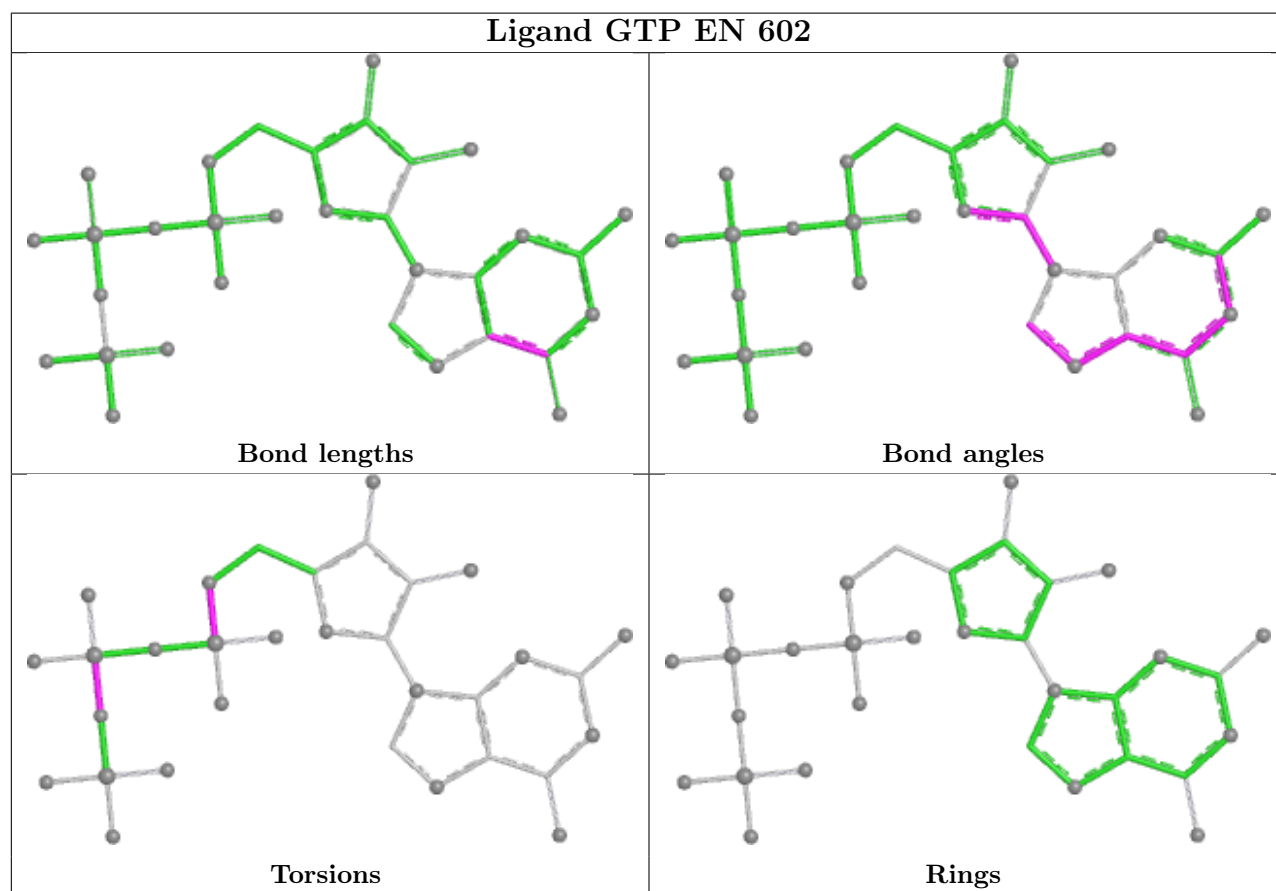
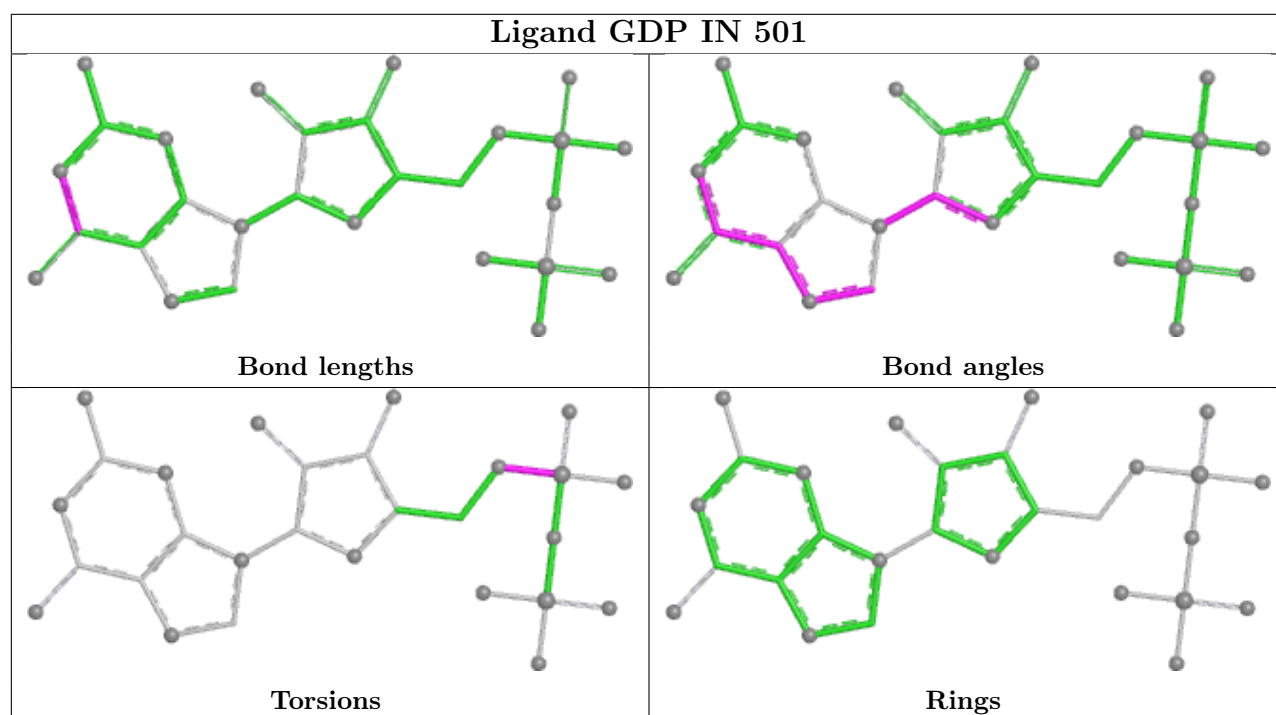
## Ligand GTP AO 501



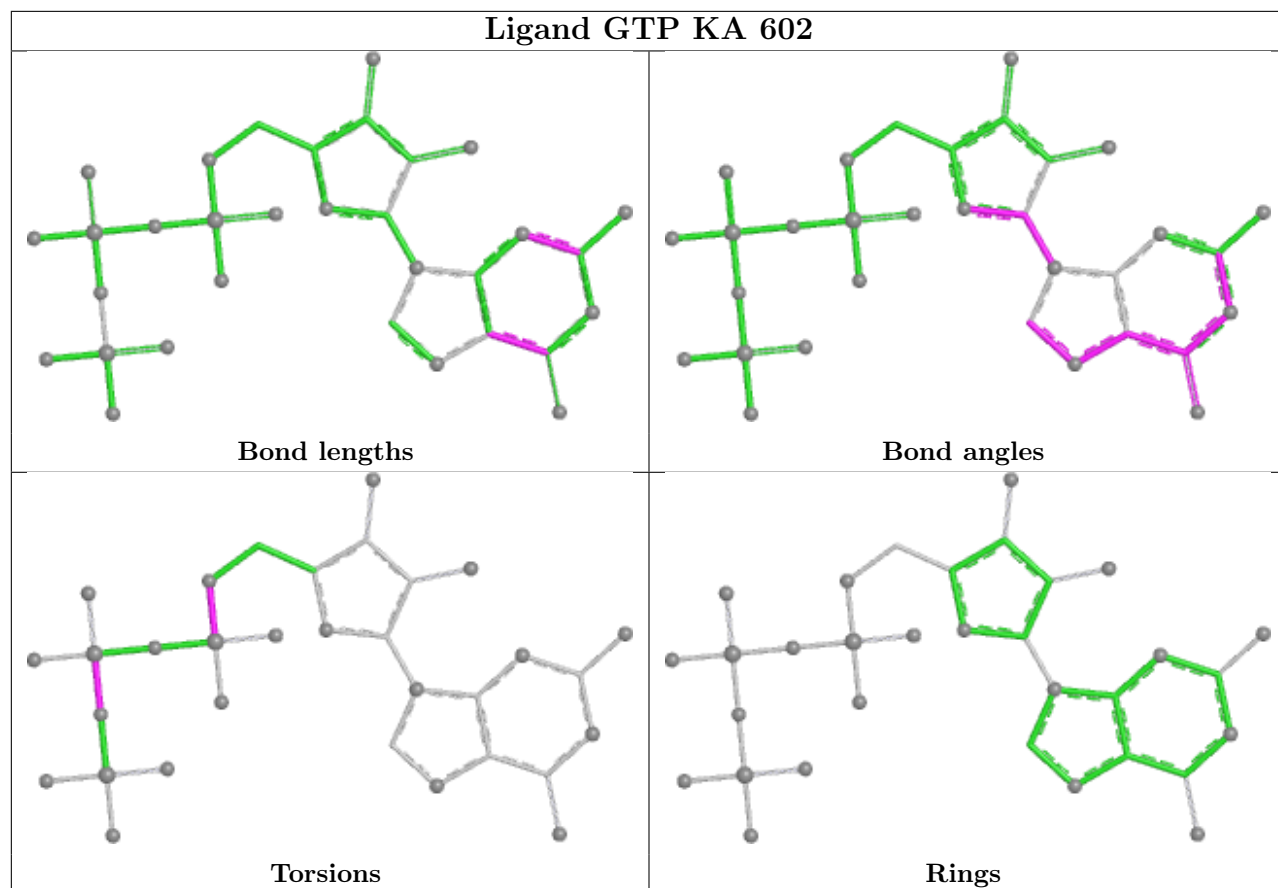
## Ligand GDP BH 501



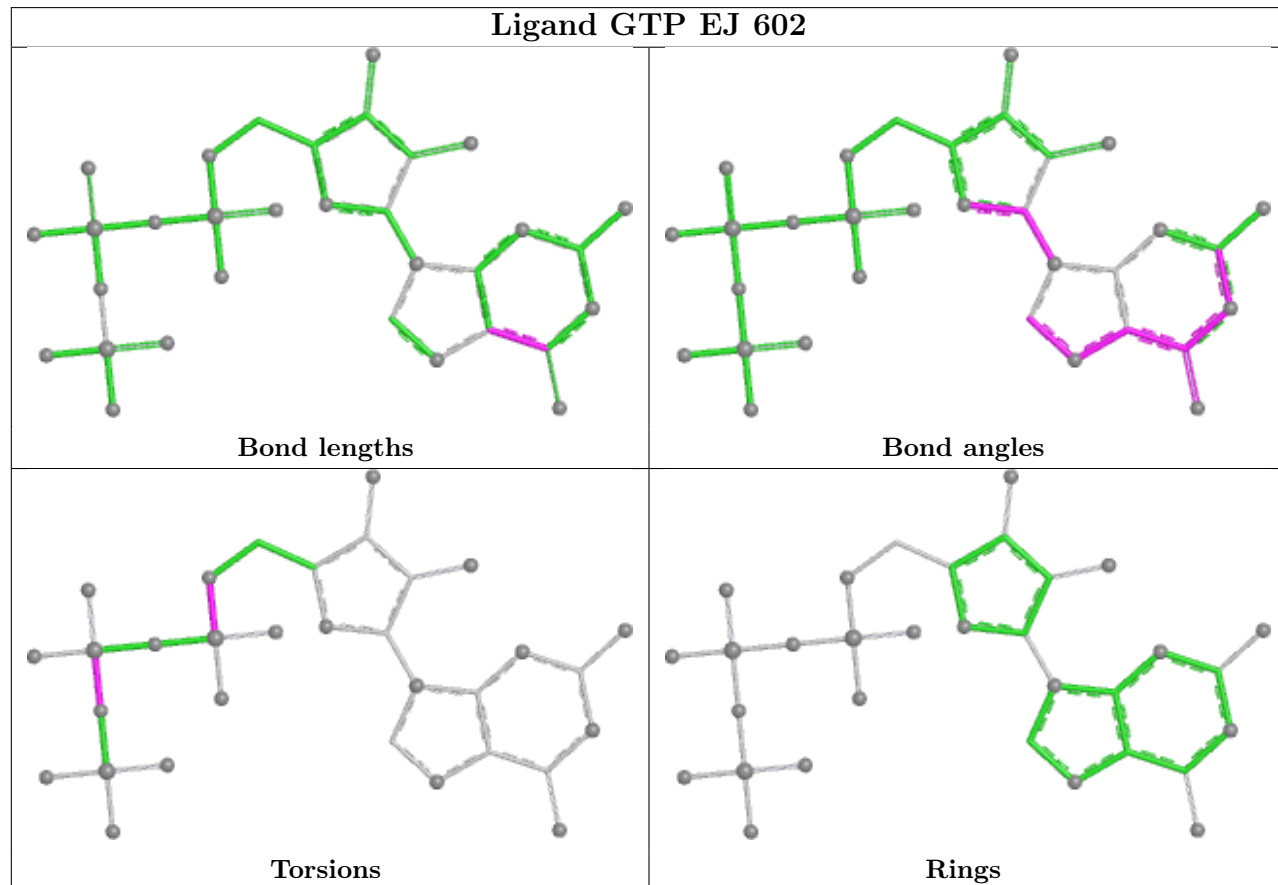




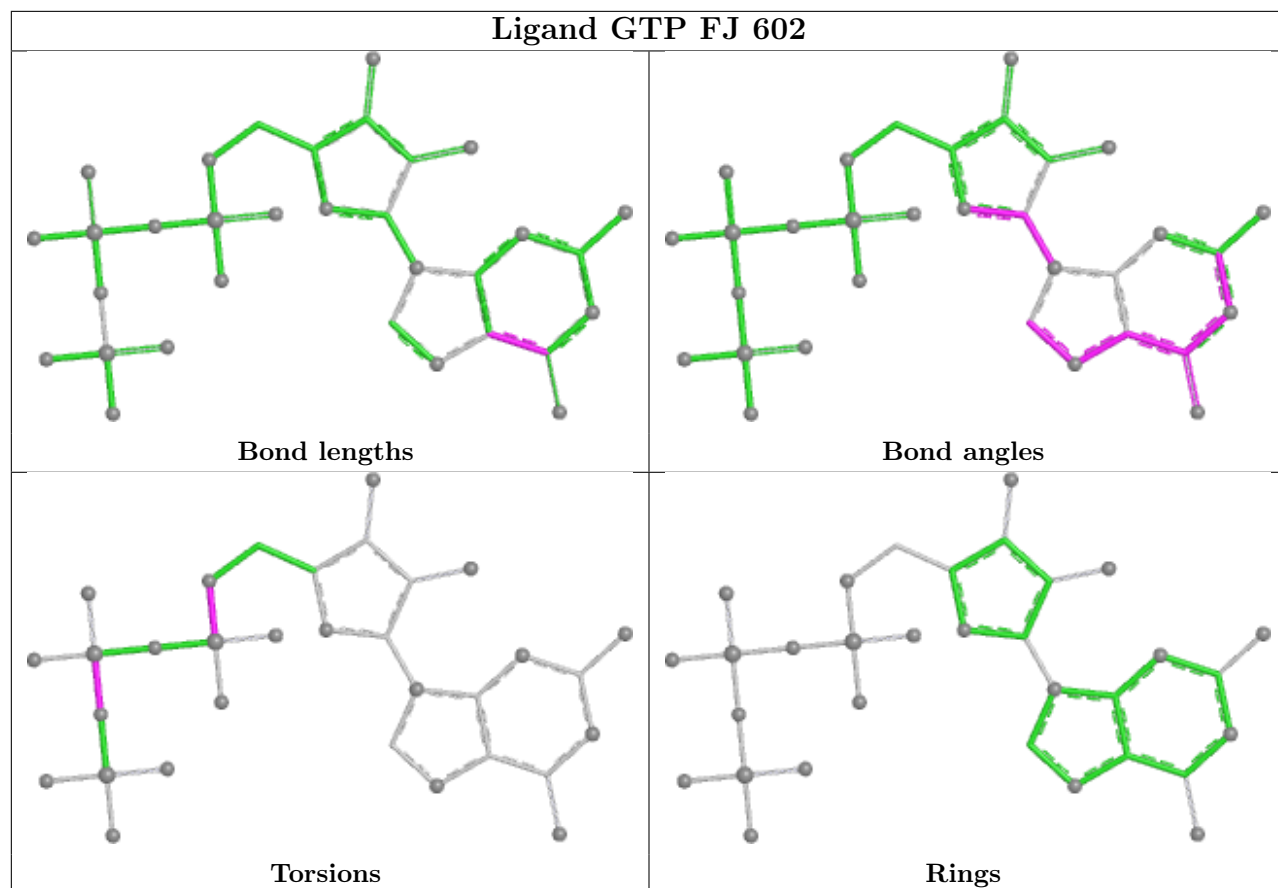
## Ligand GTP KA 602



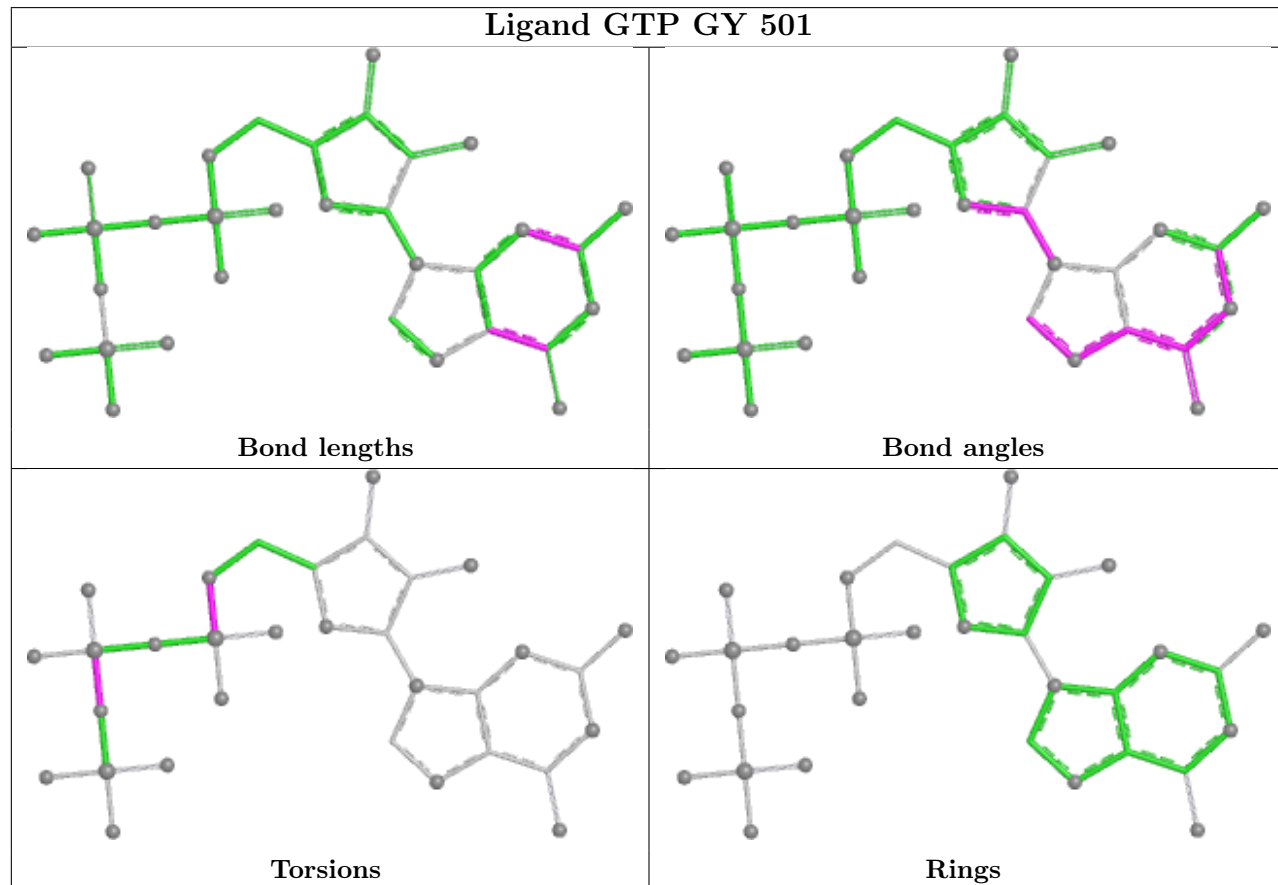
## Ligand GTP EJ 602

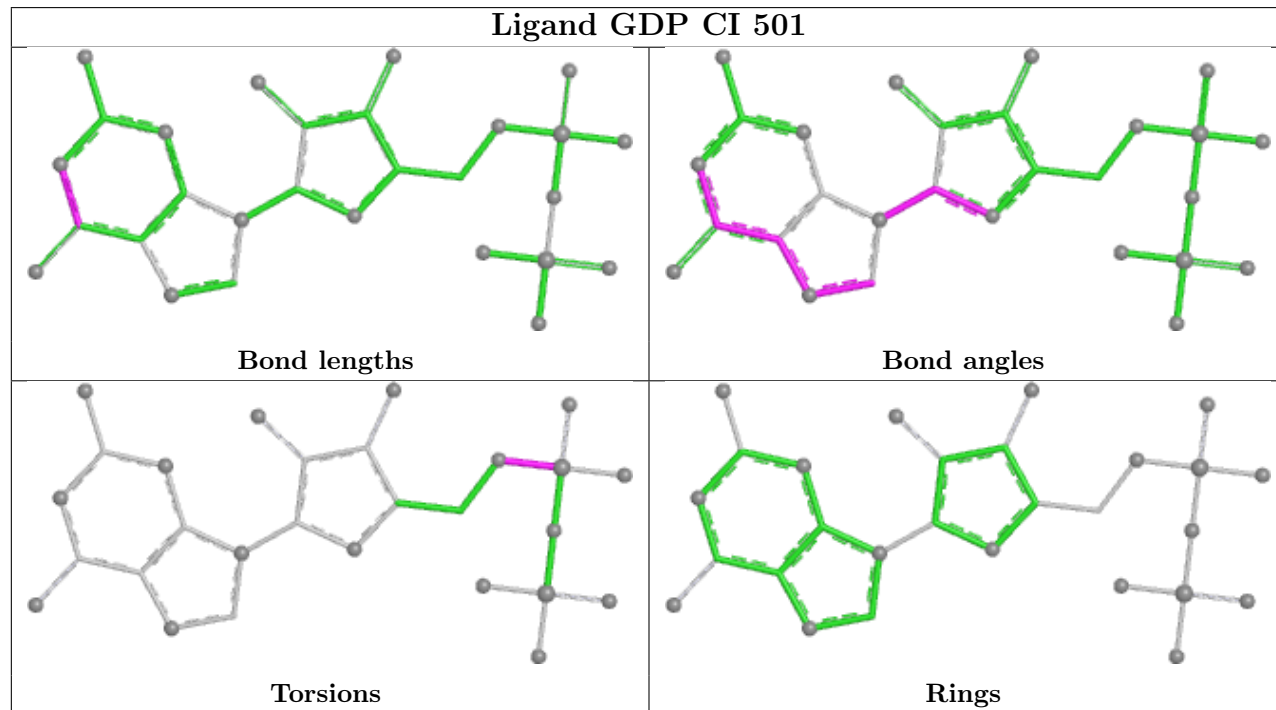
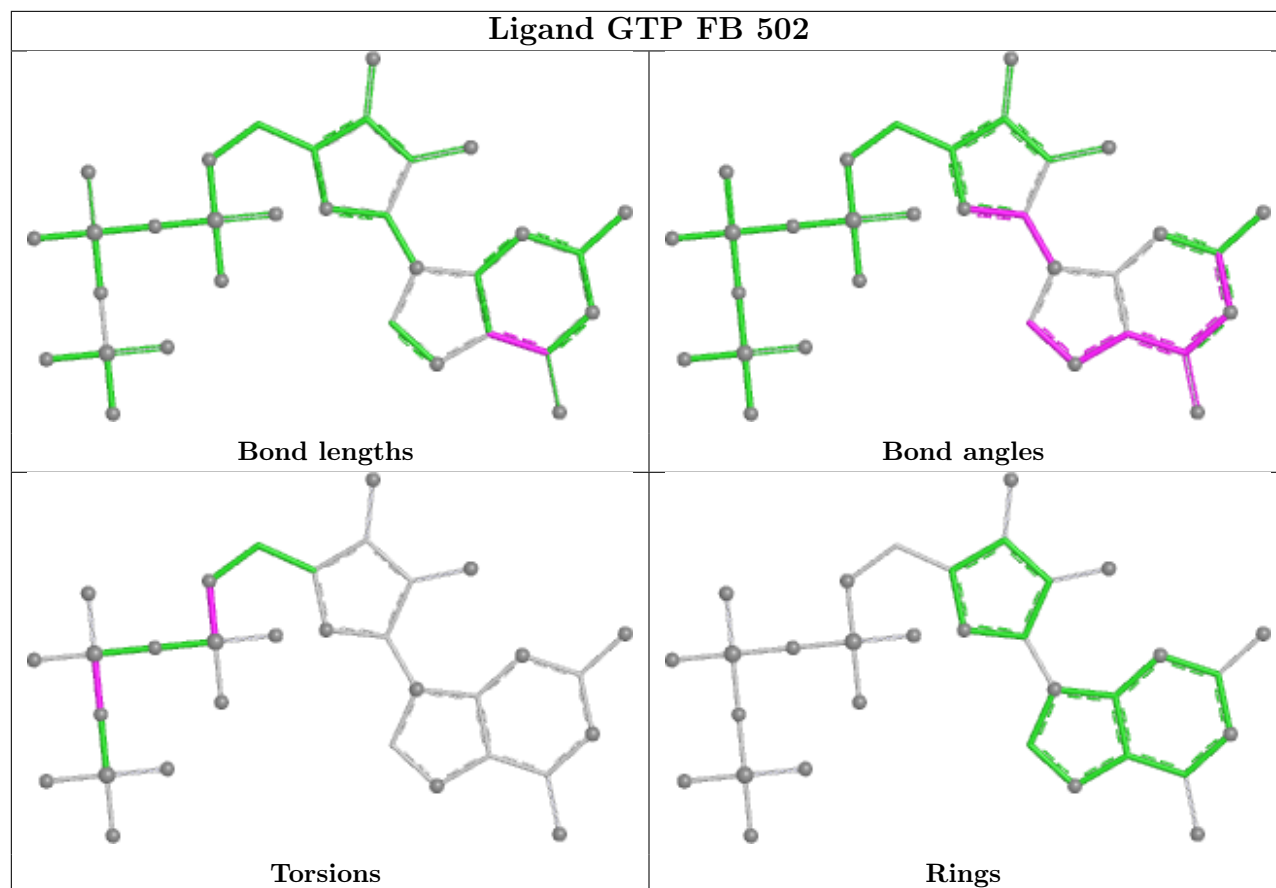


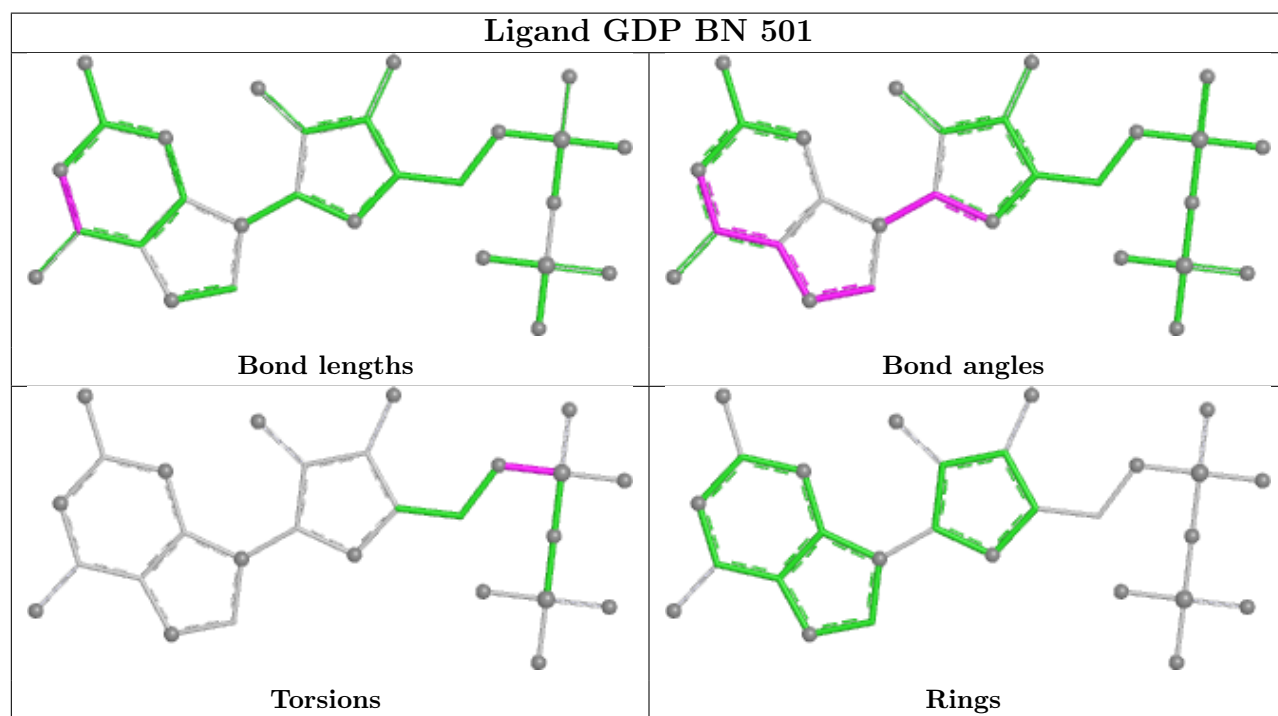
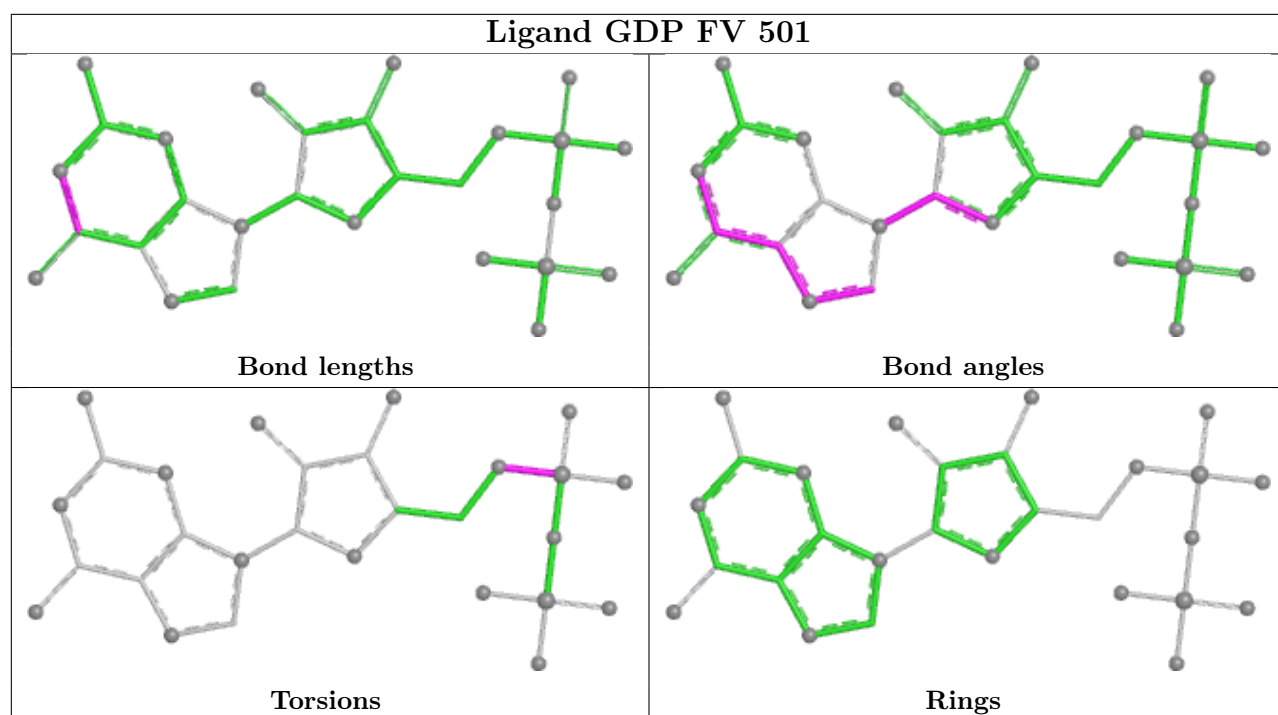
## Ligand GTP FJ 602



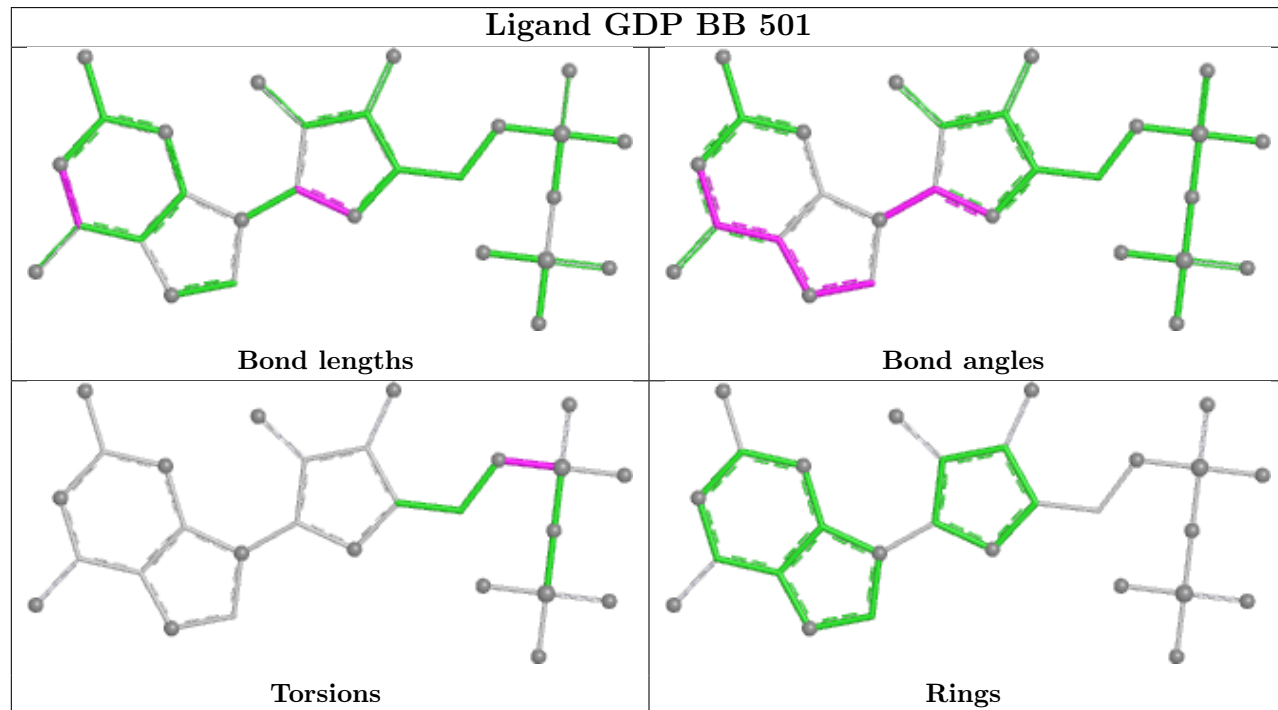
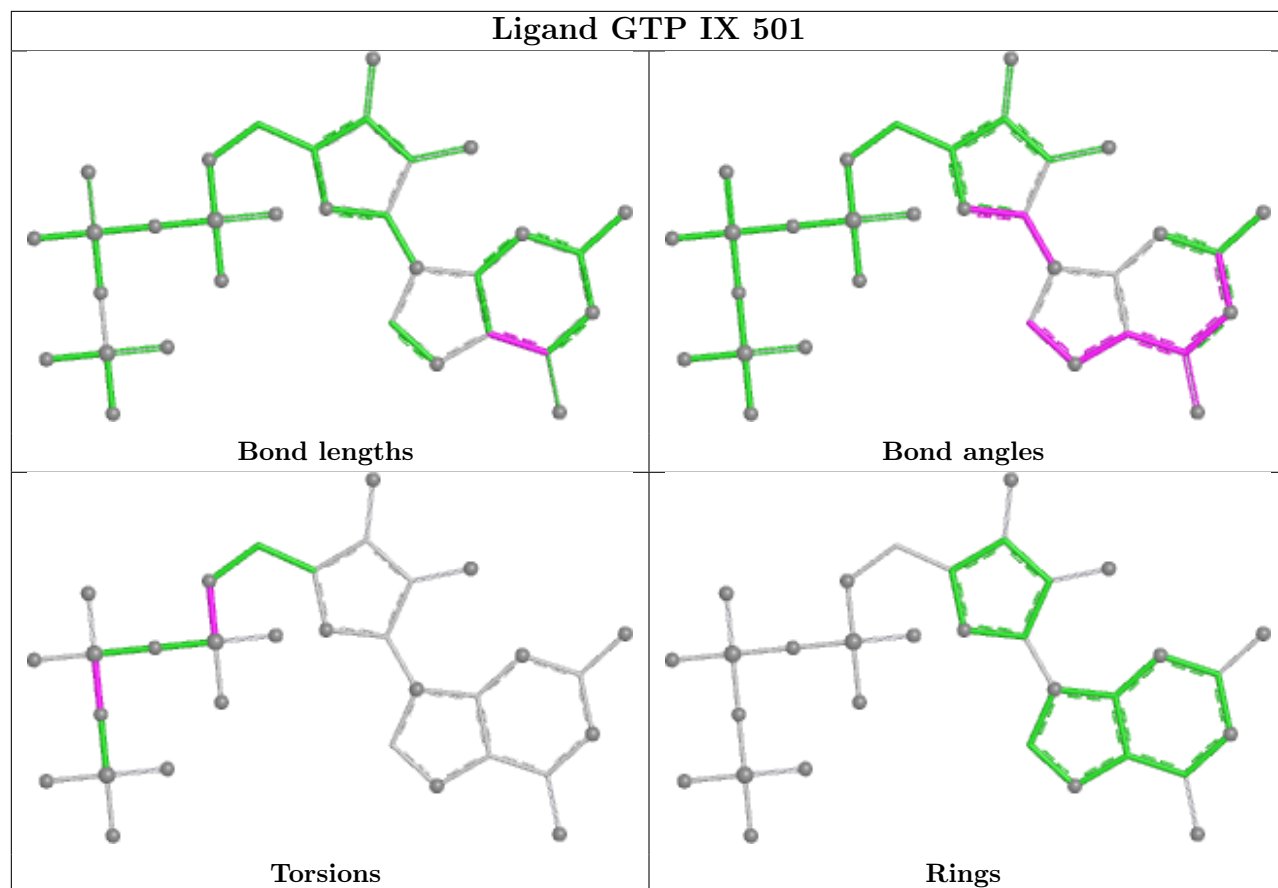
## Ligand GTP GY 501

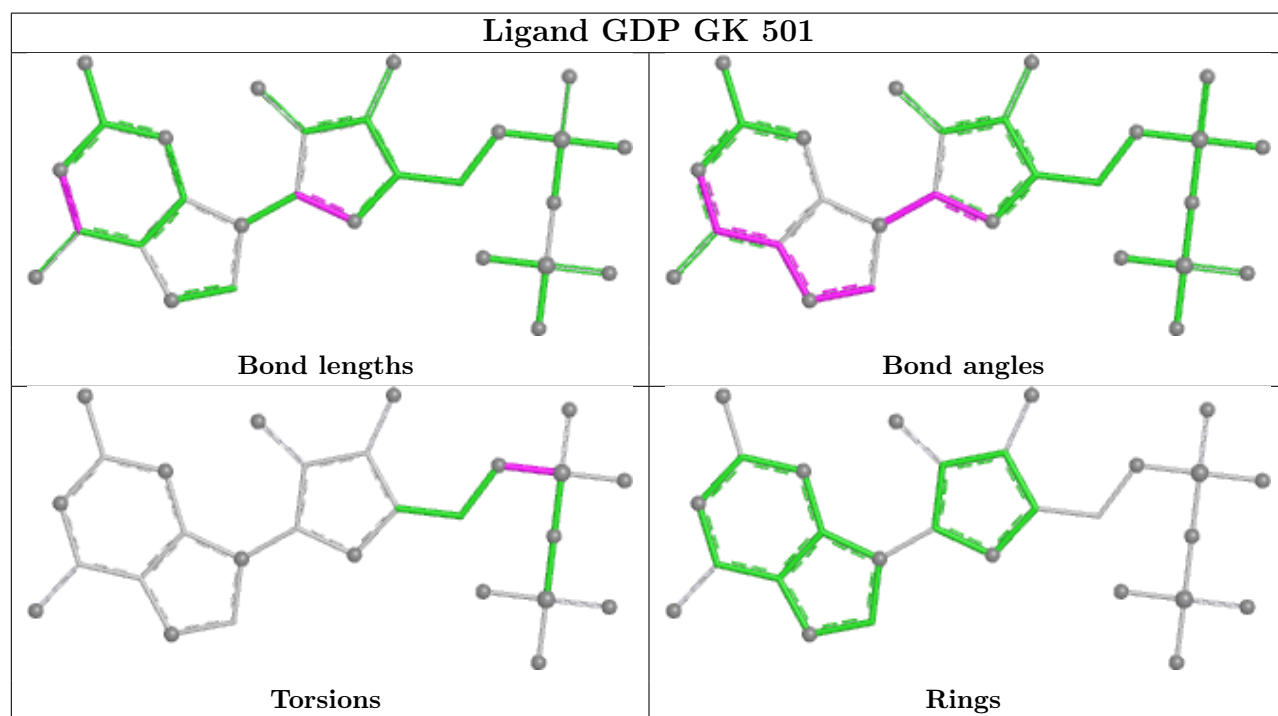
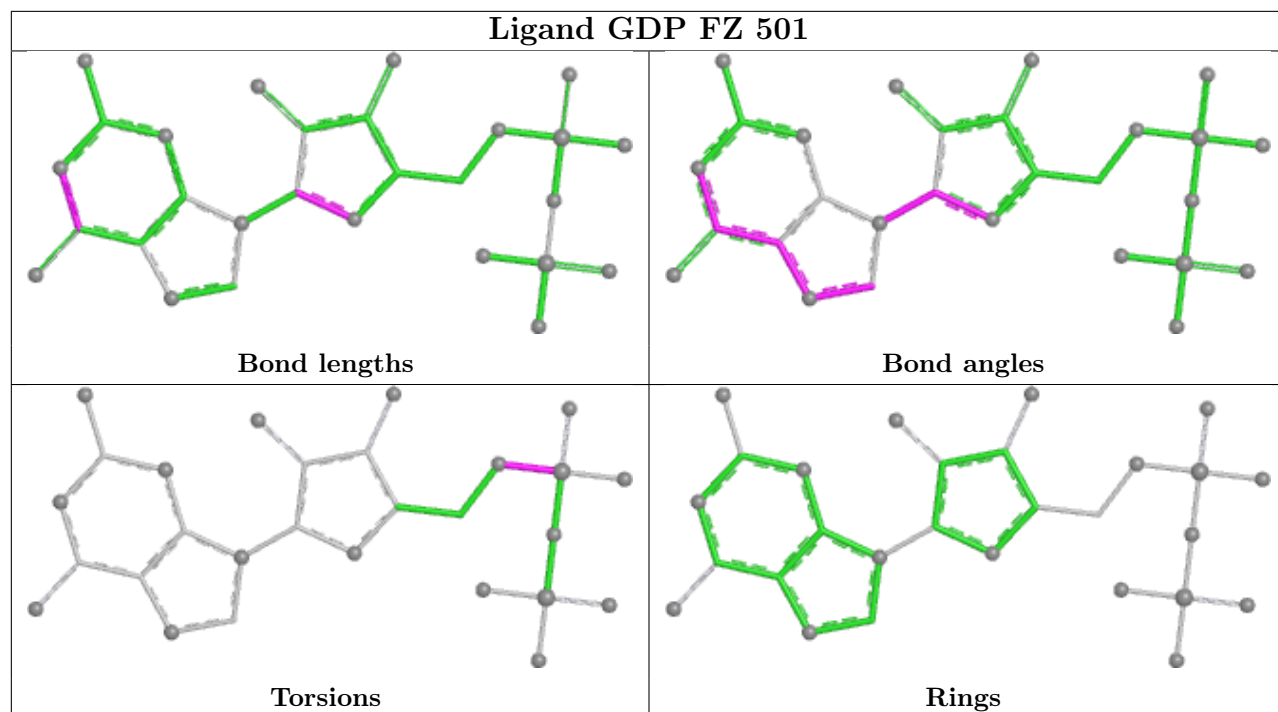


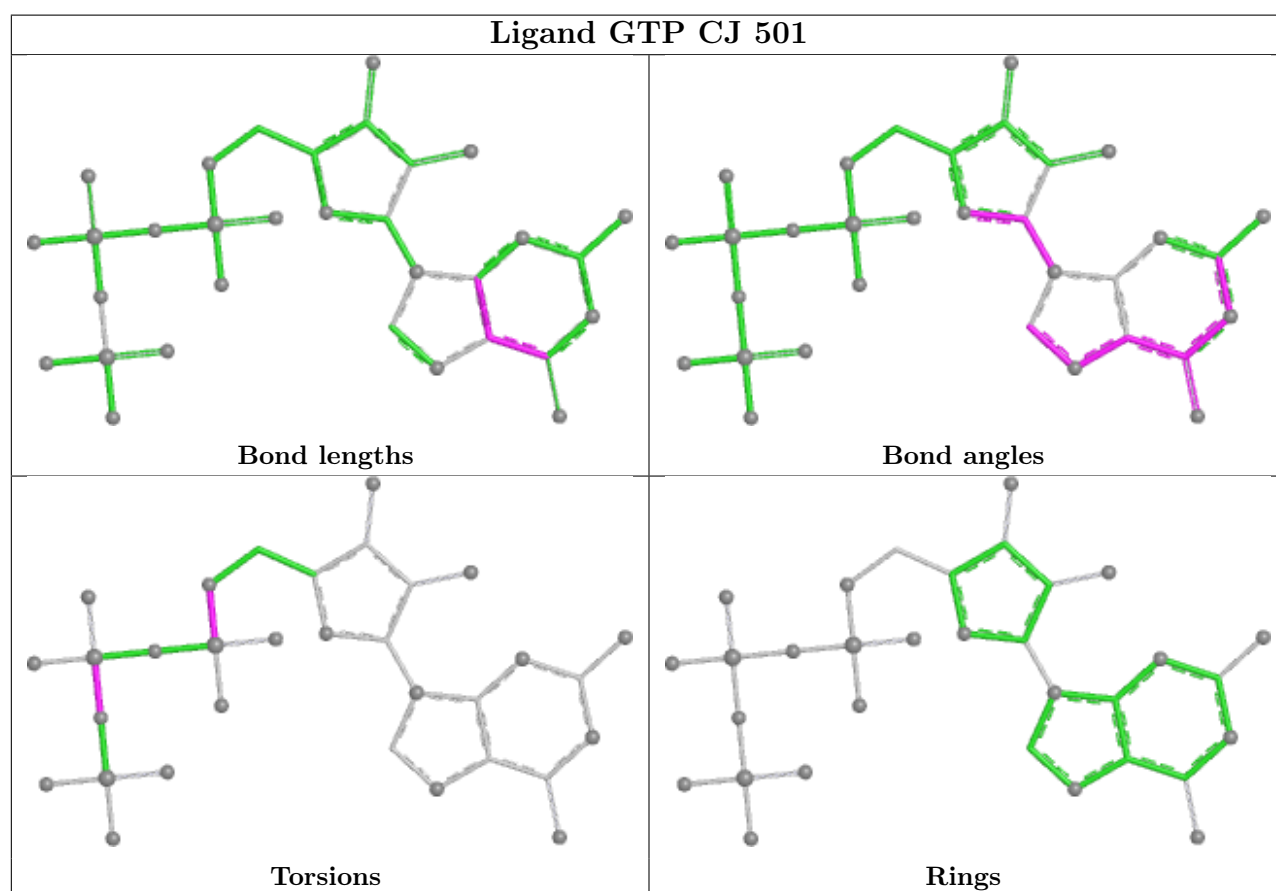
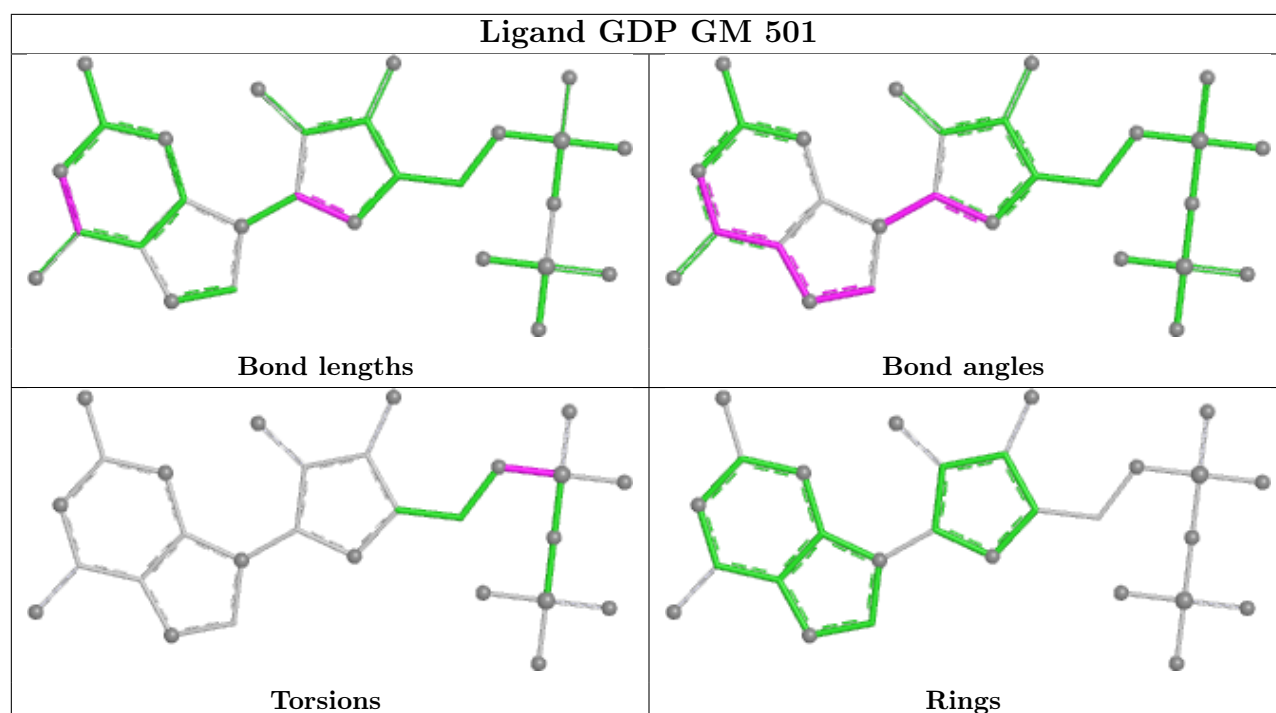


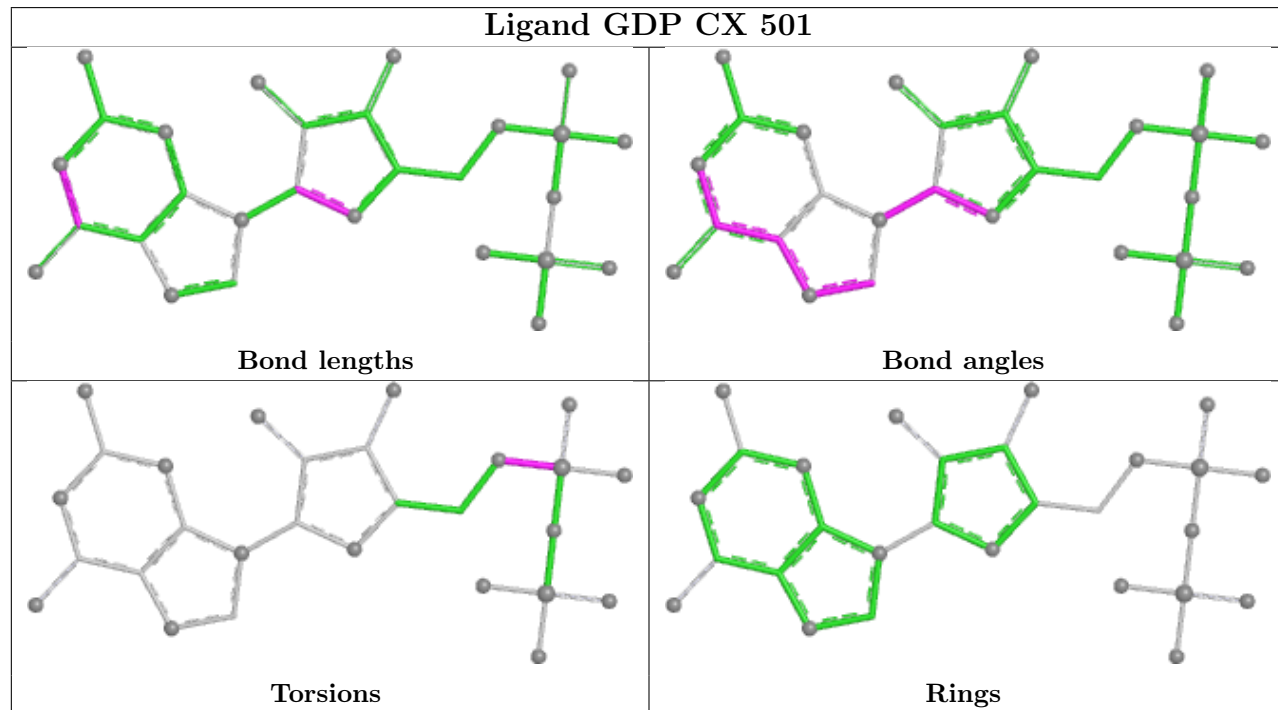
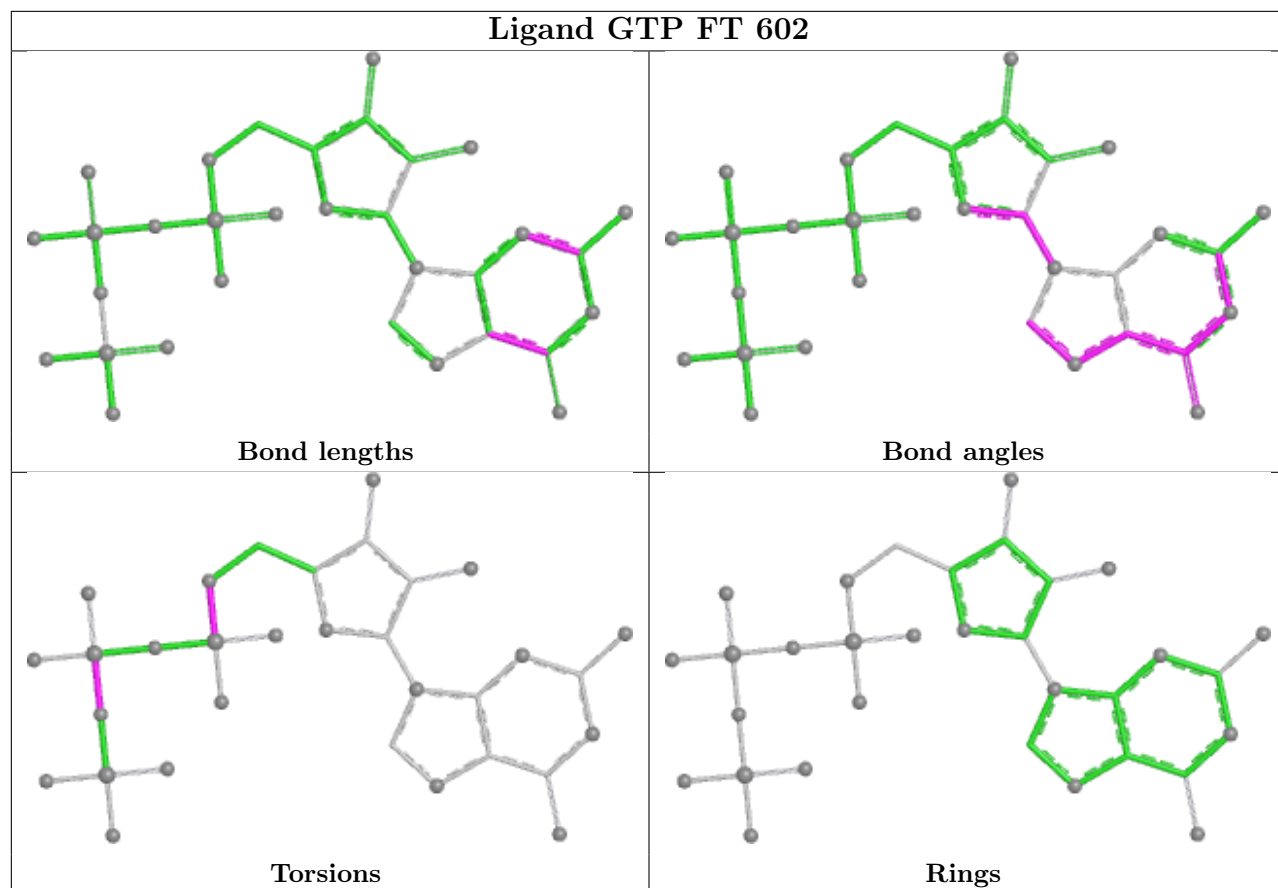


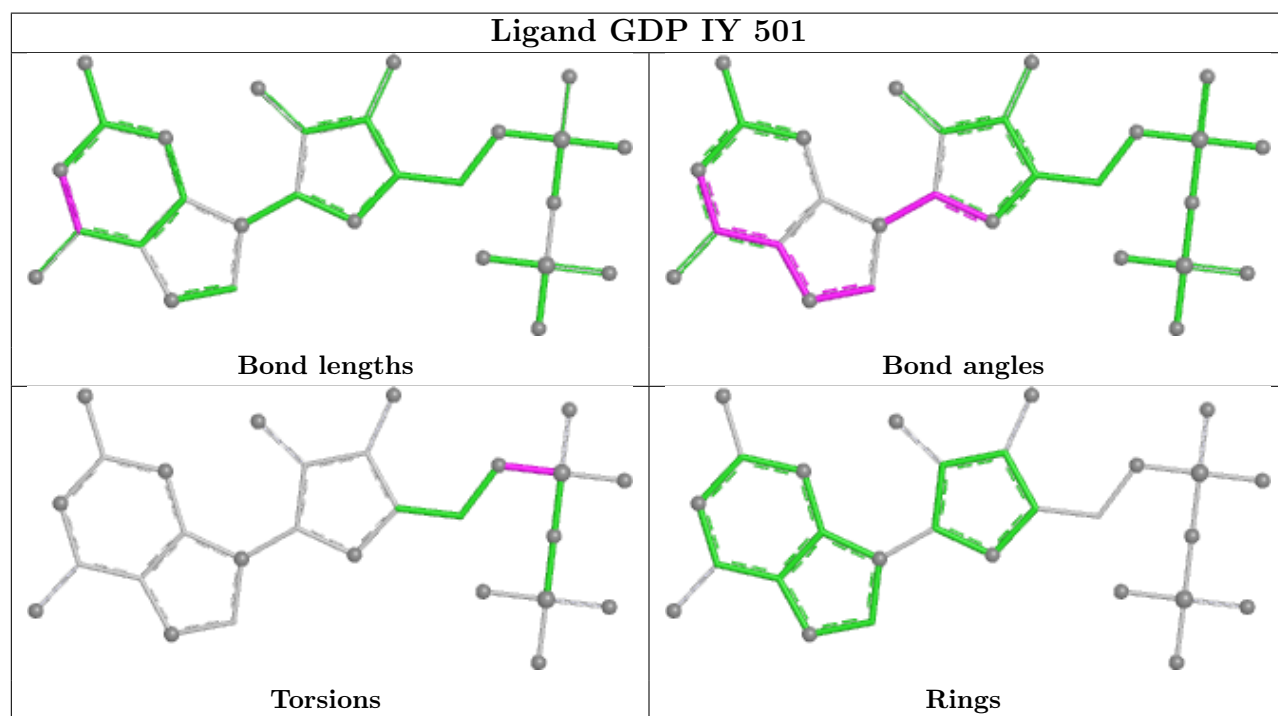
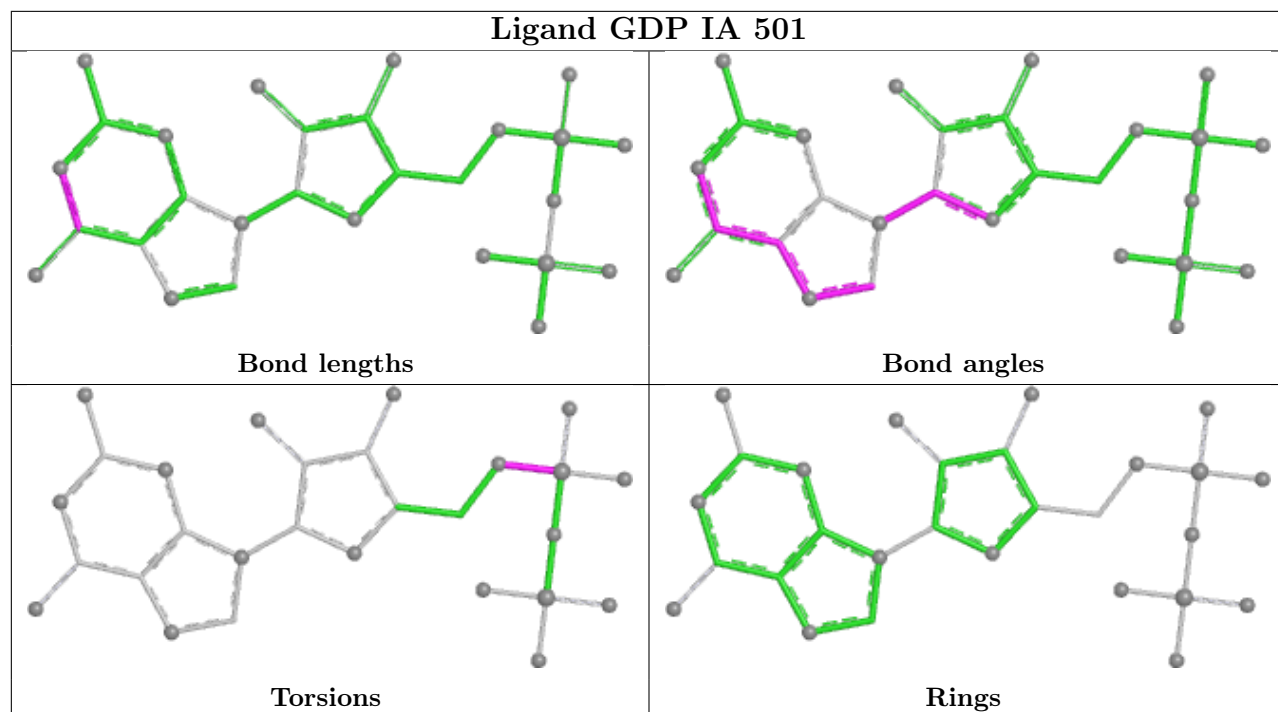


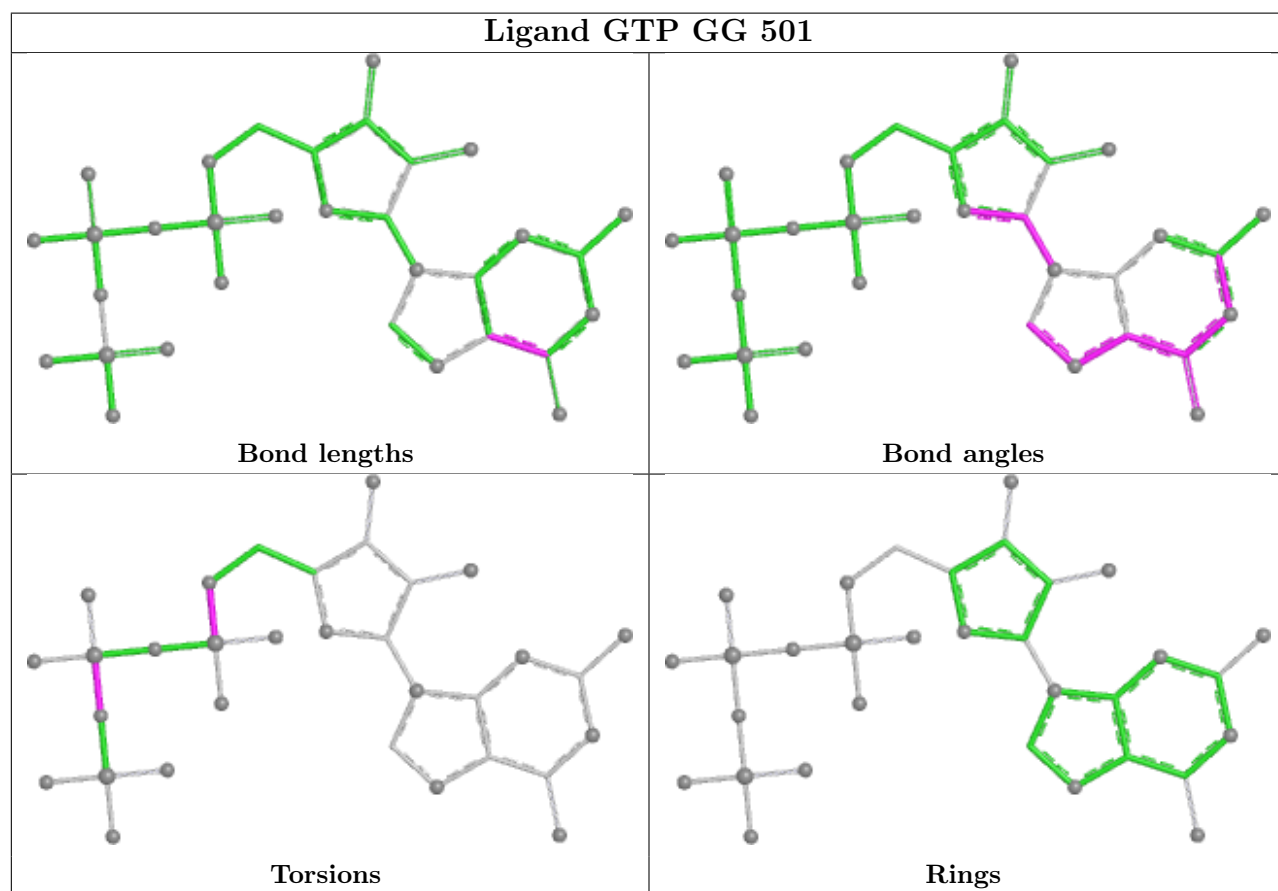
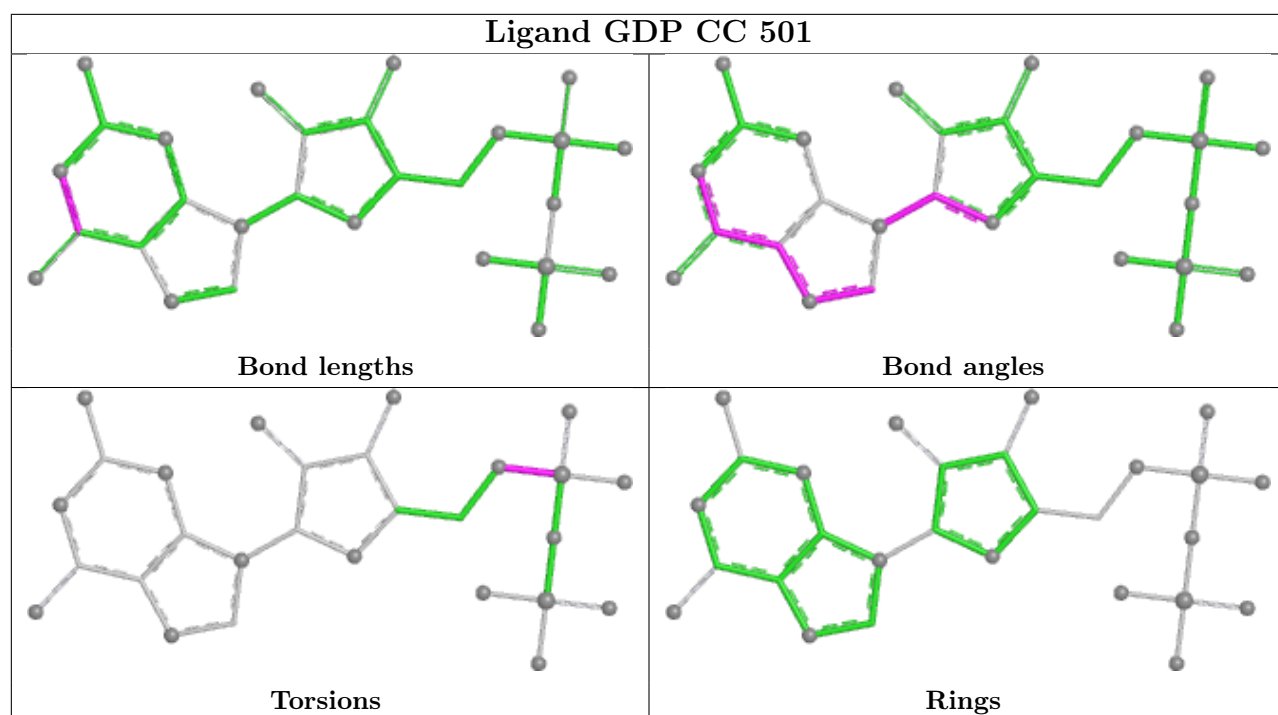


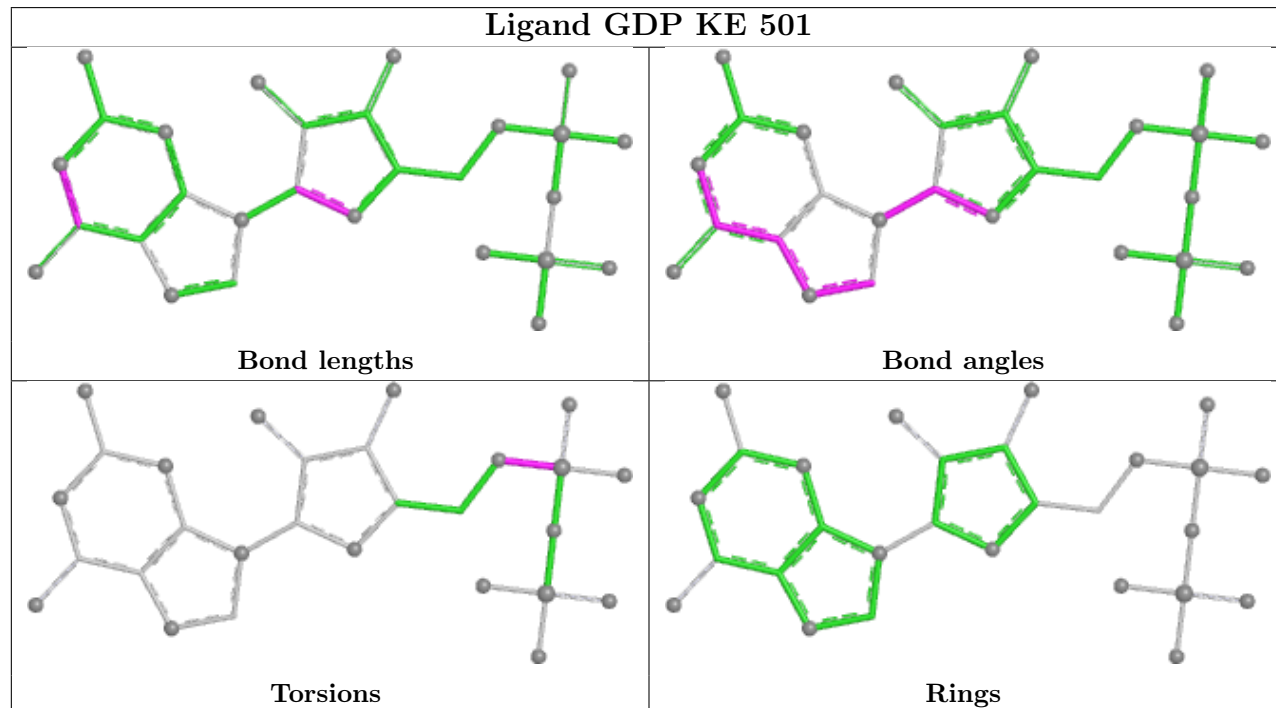
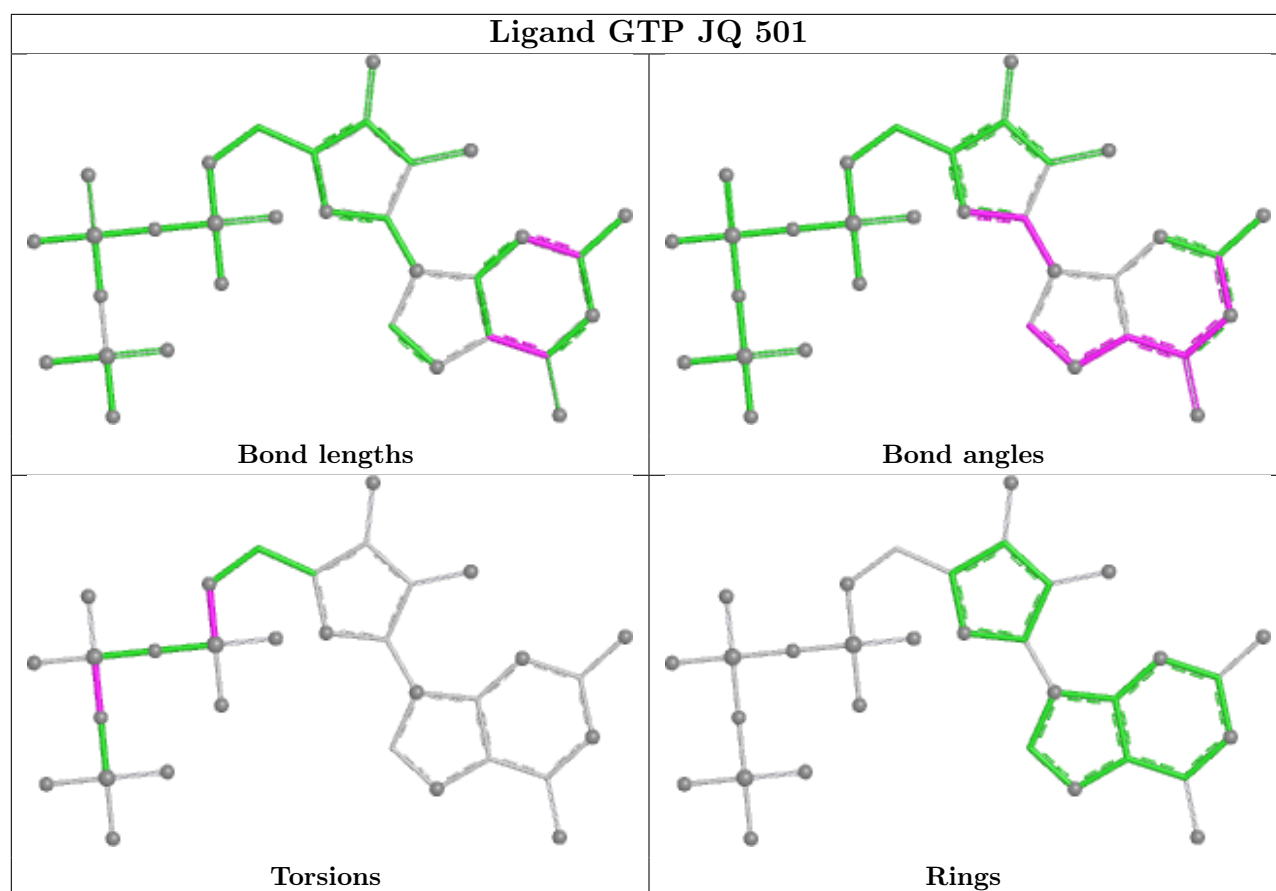


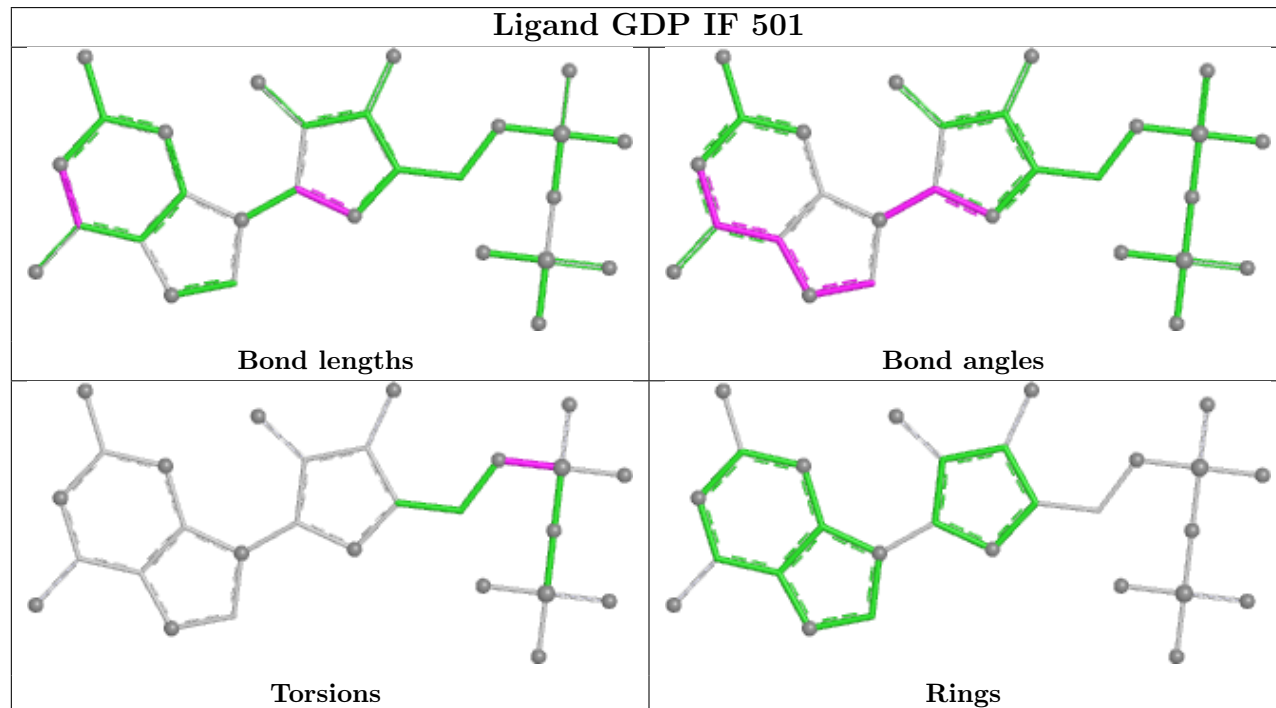
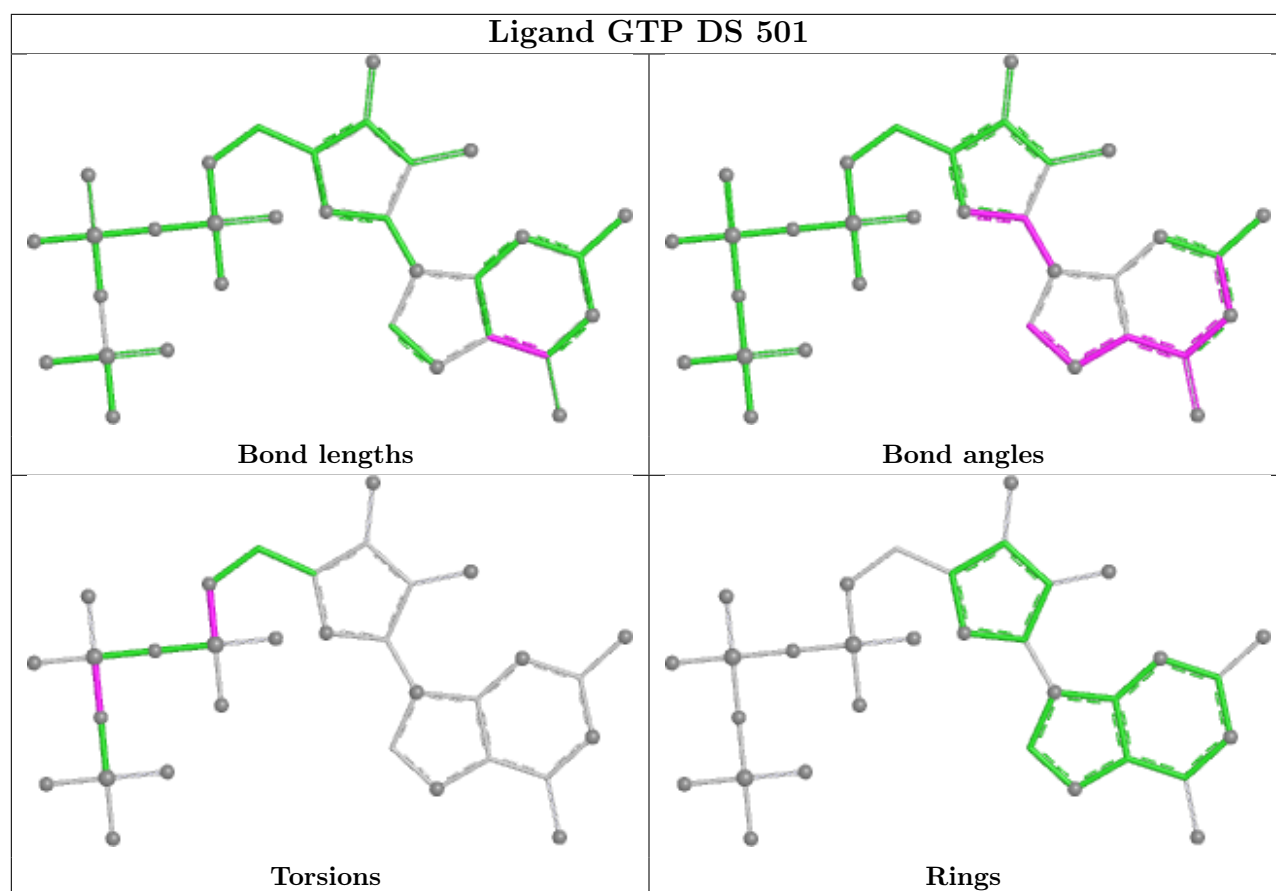




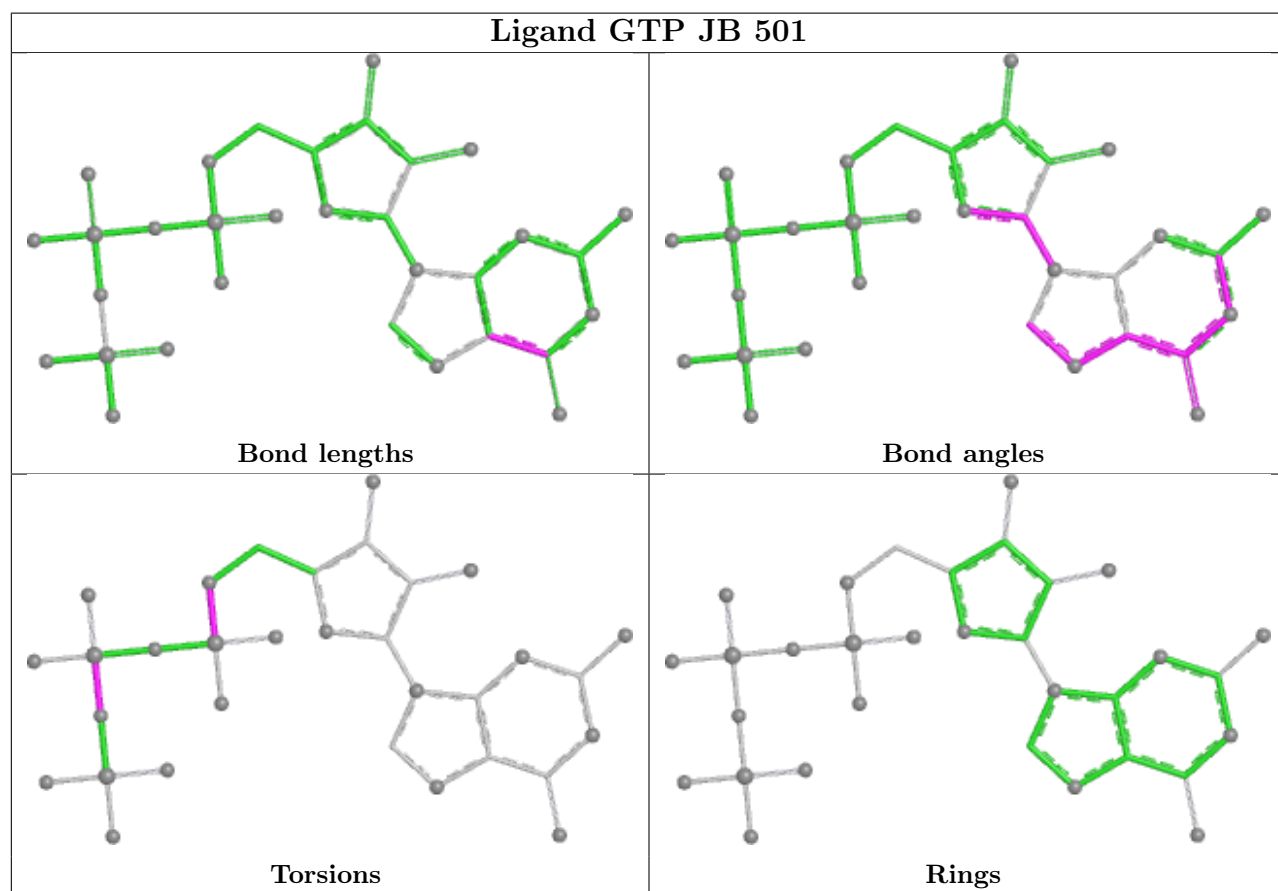
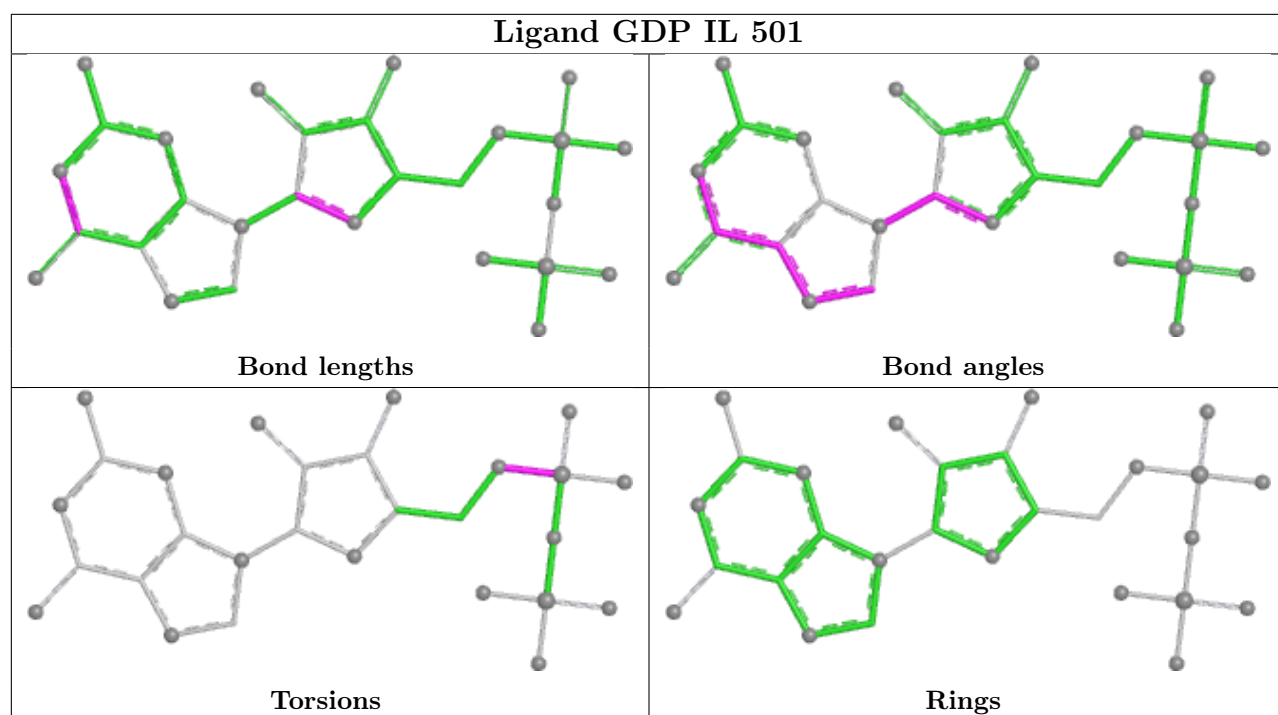




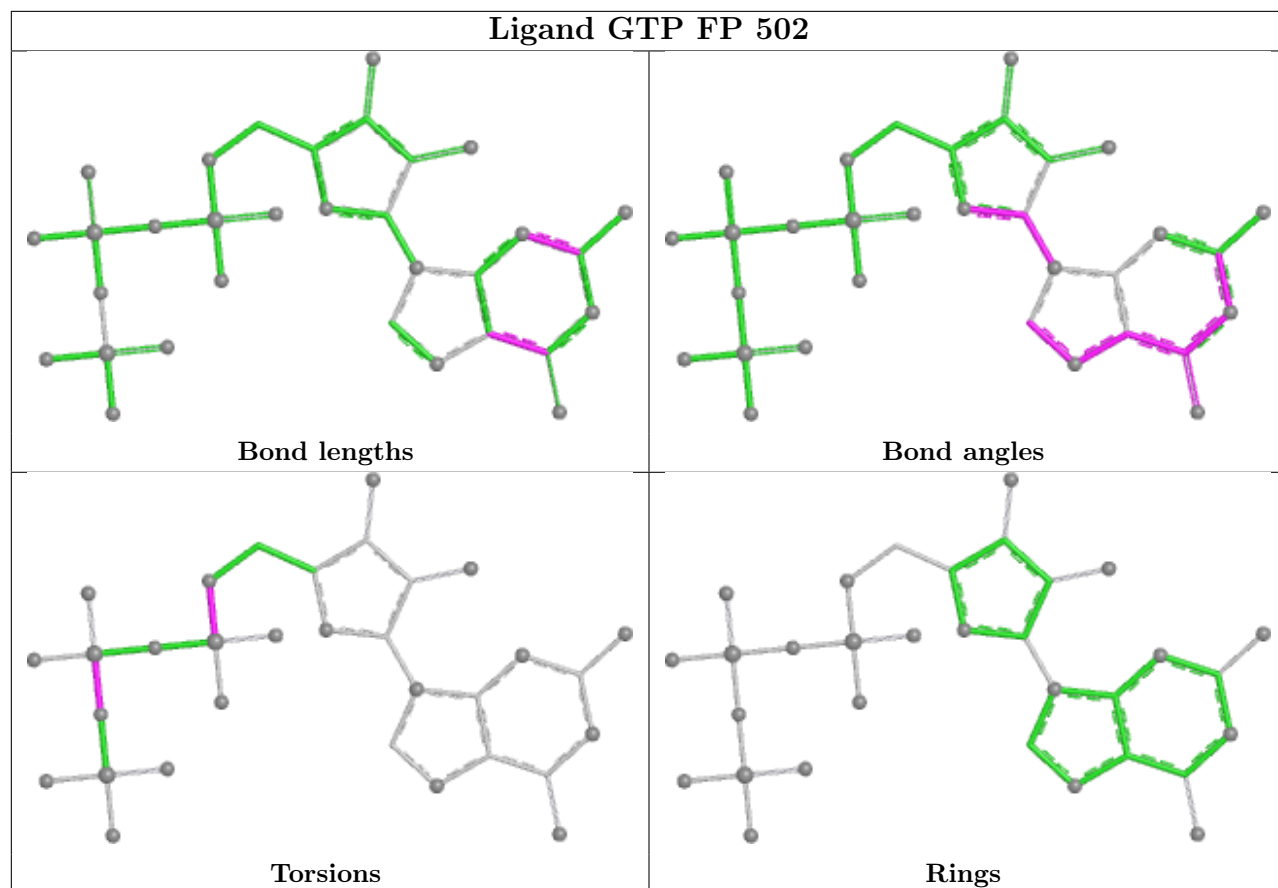




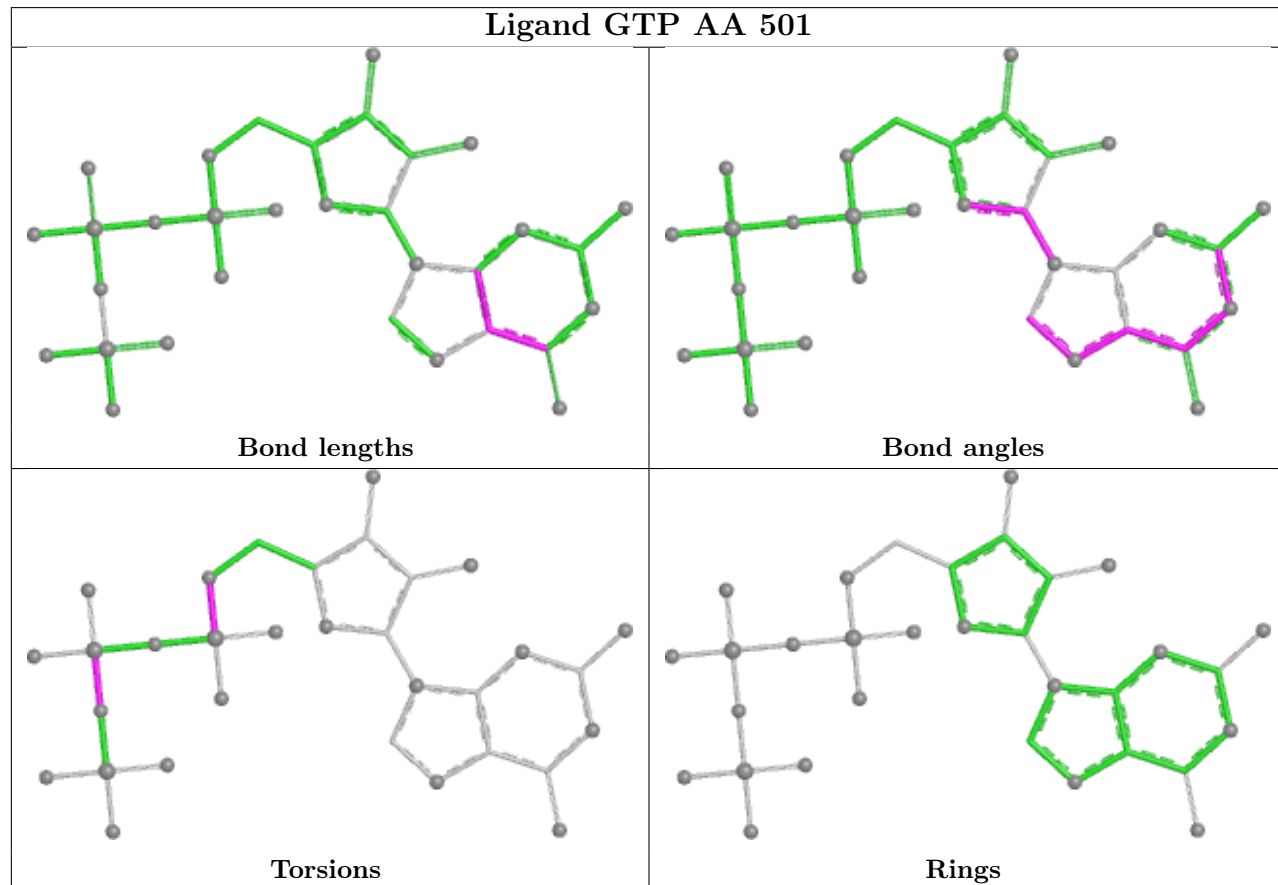




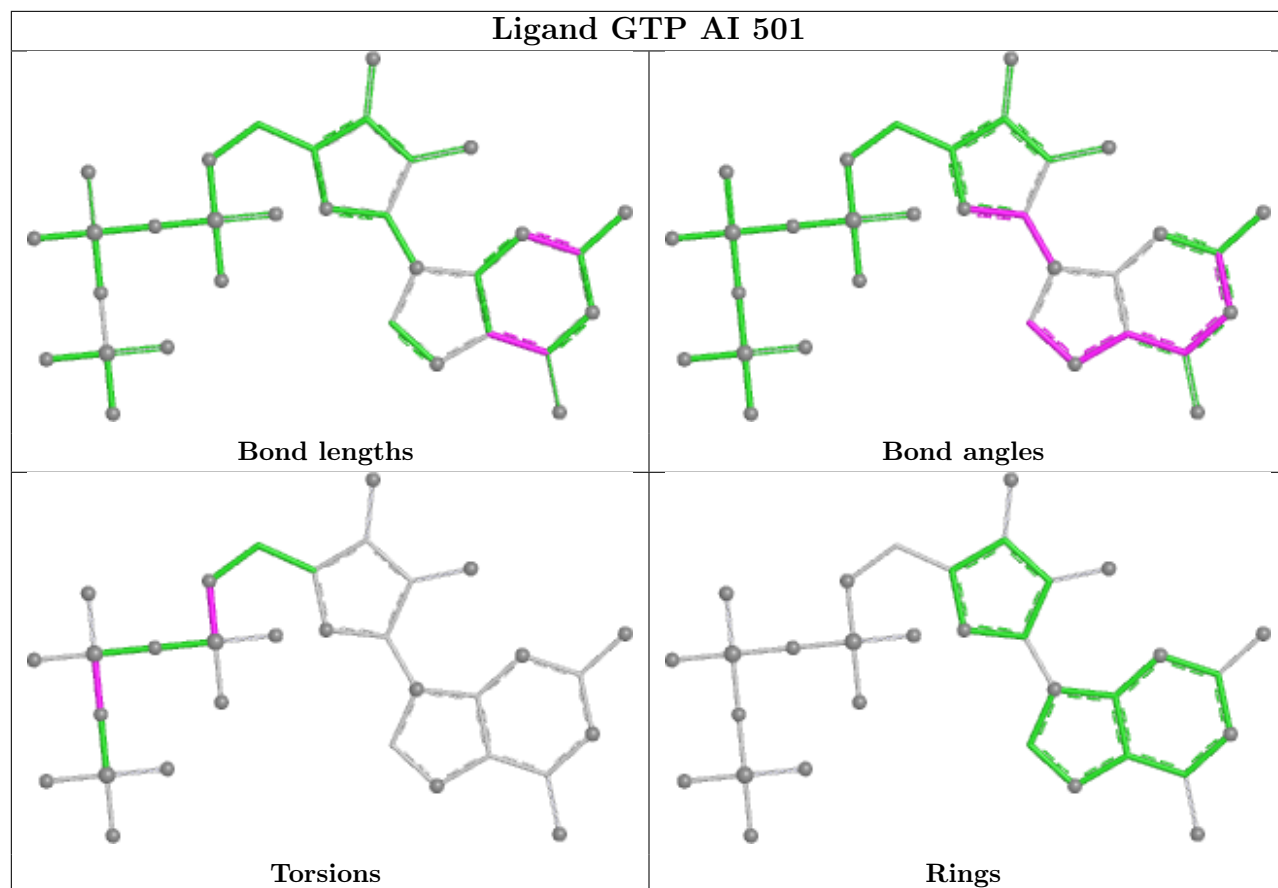
## Ligand GTP FP 502



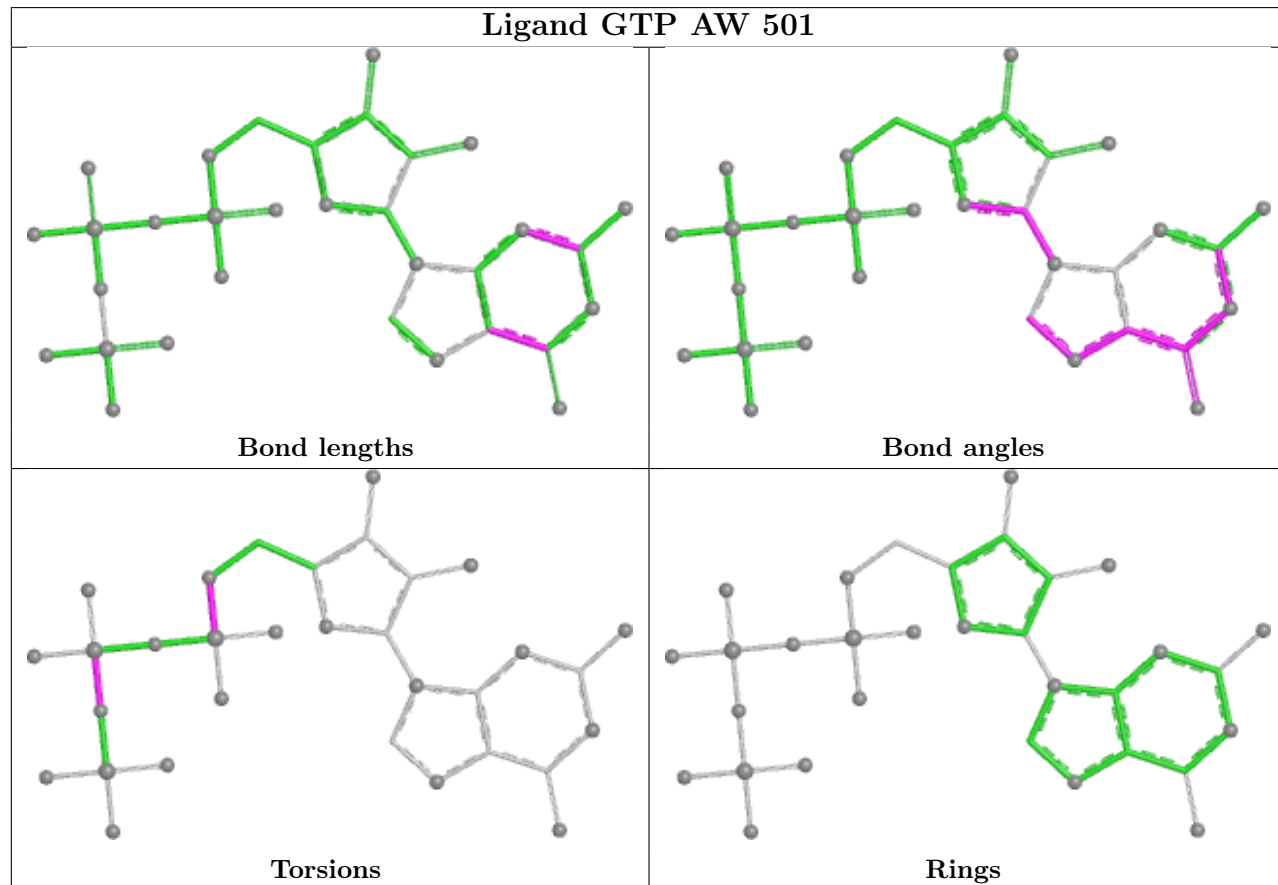
## Ligand GTP AA 501



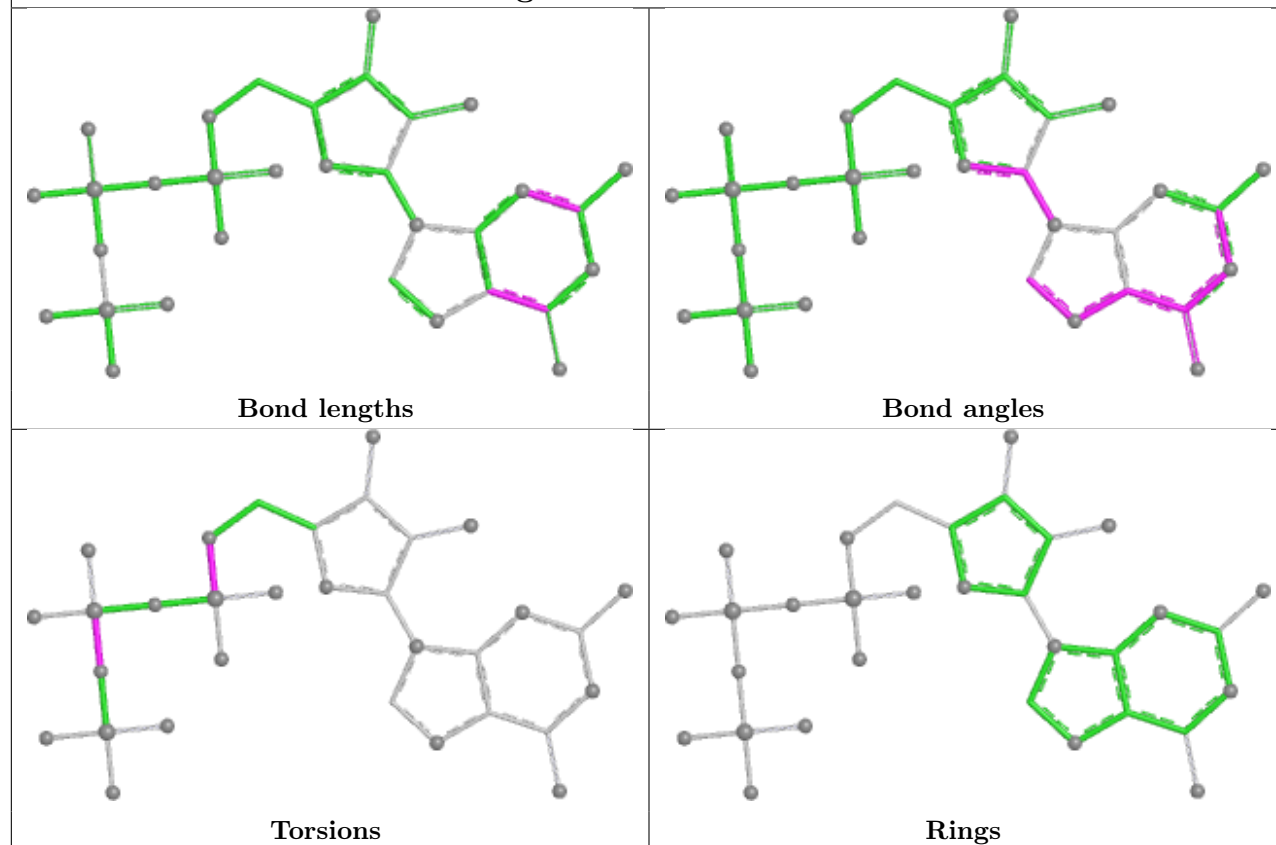
## Ligand GTP AI 501



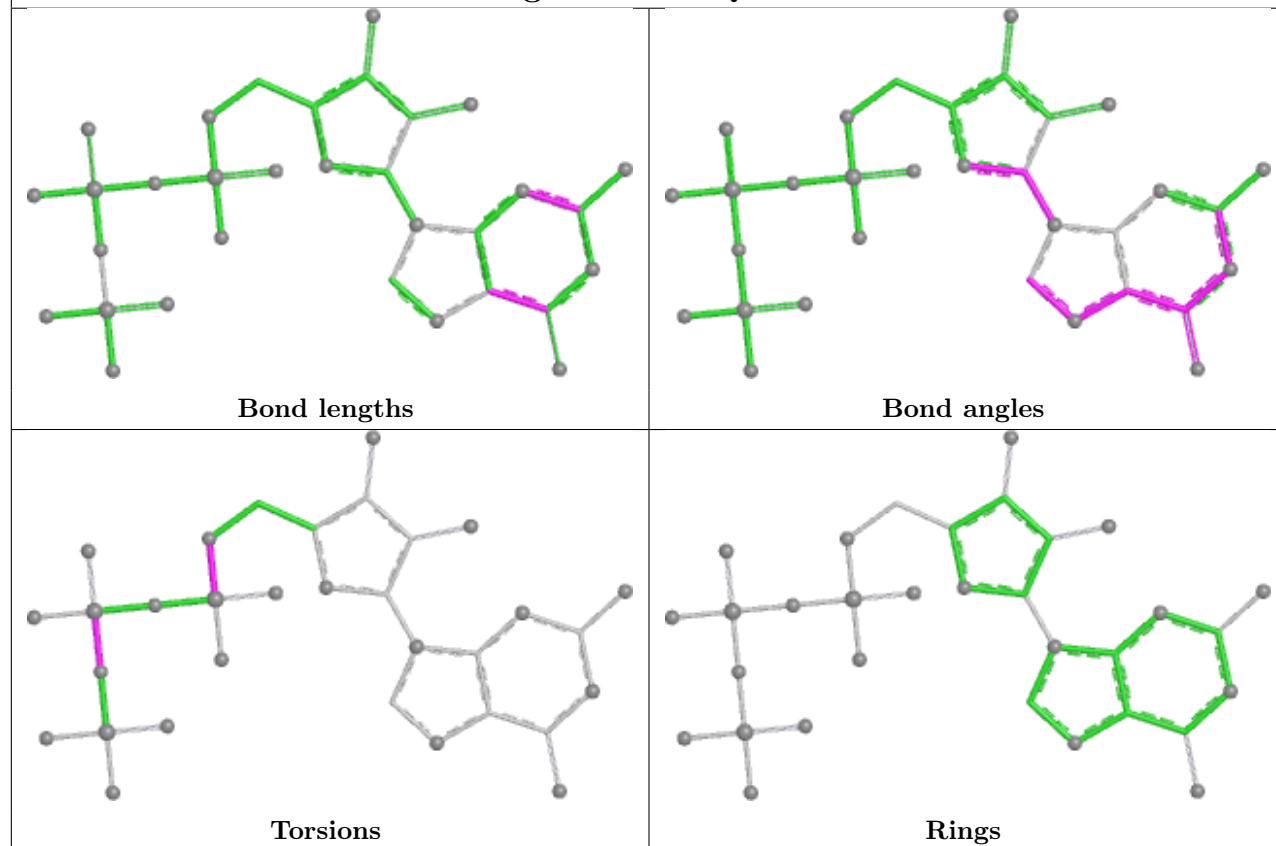
## Ligand GTP AW 501



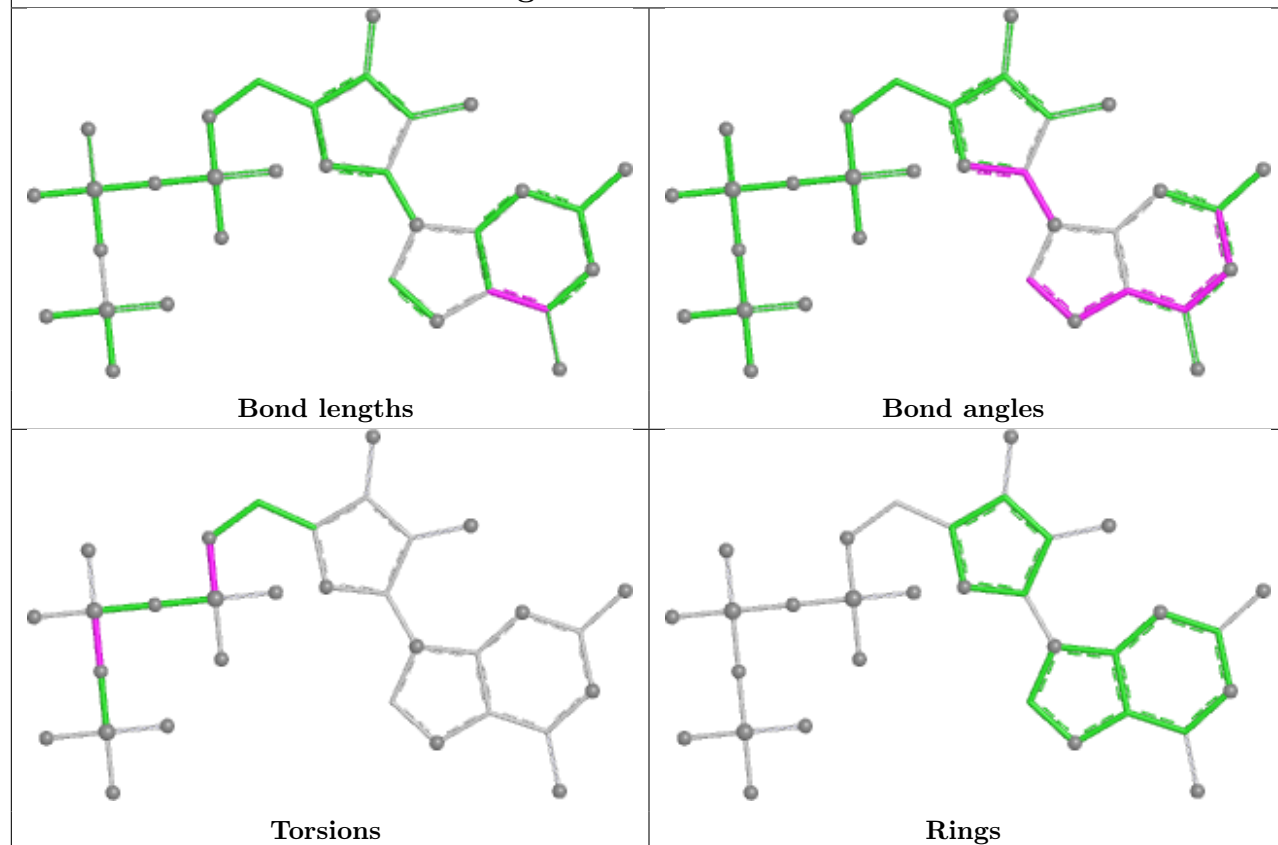
## Ligand GTP GR 501



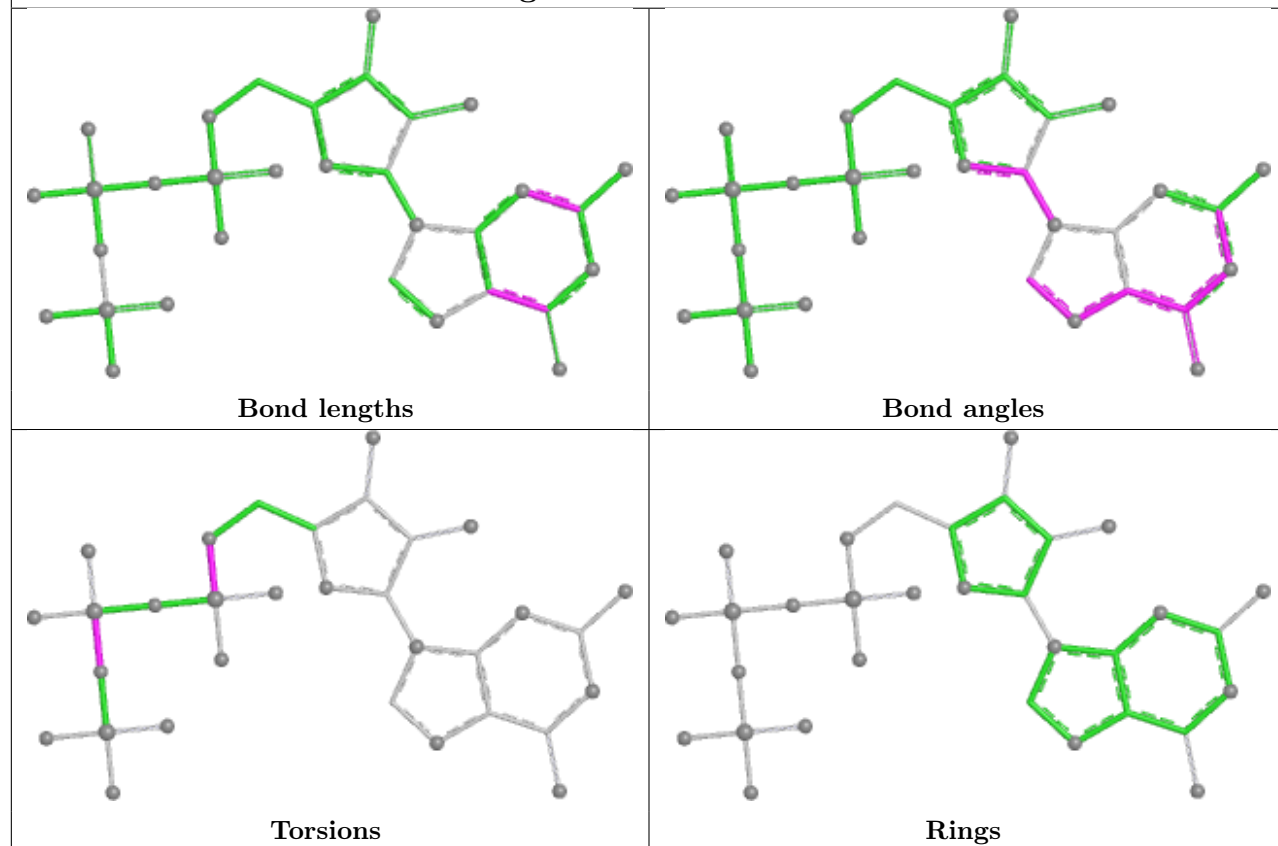
## Ligand GTP IQ 501

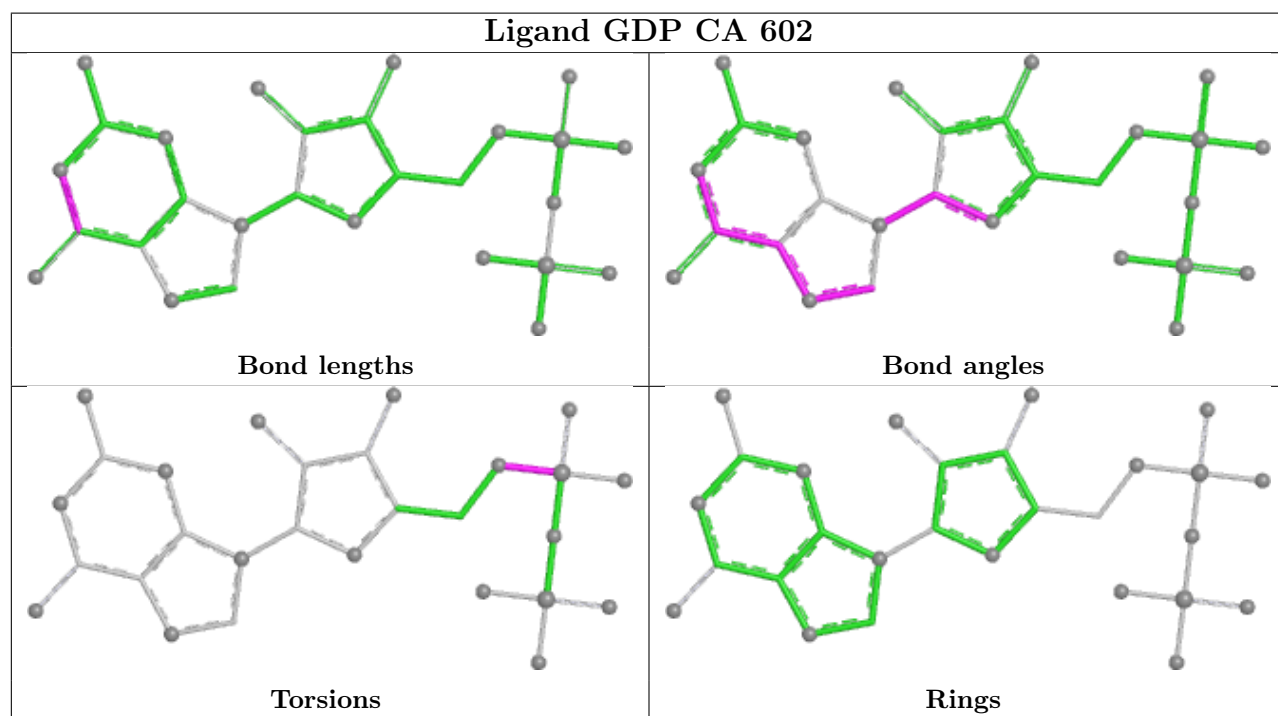
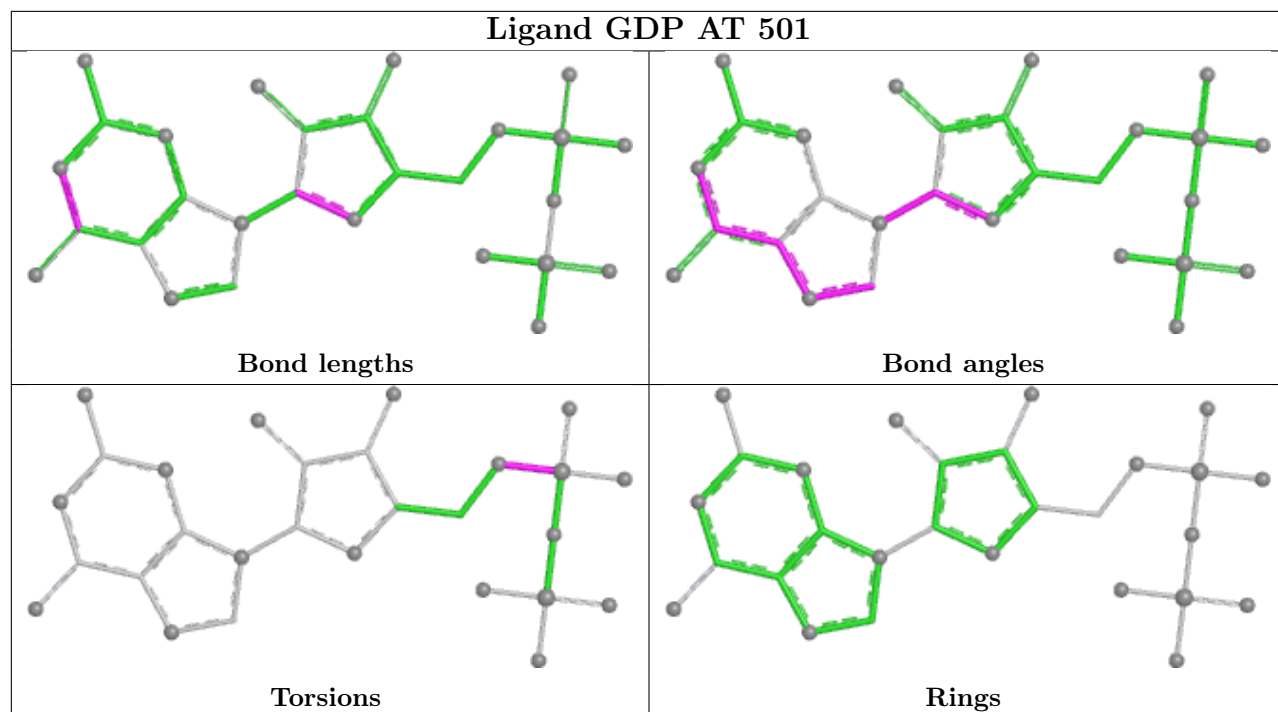


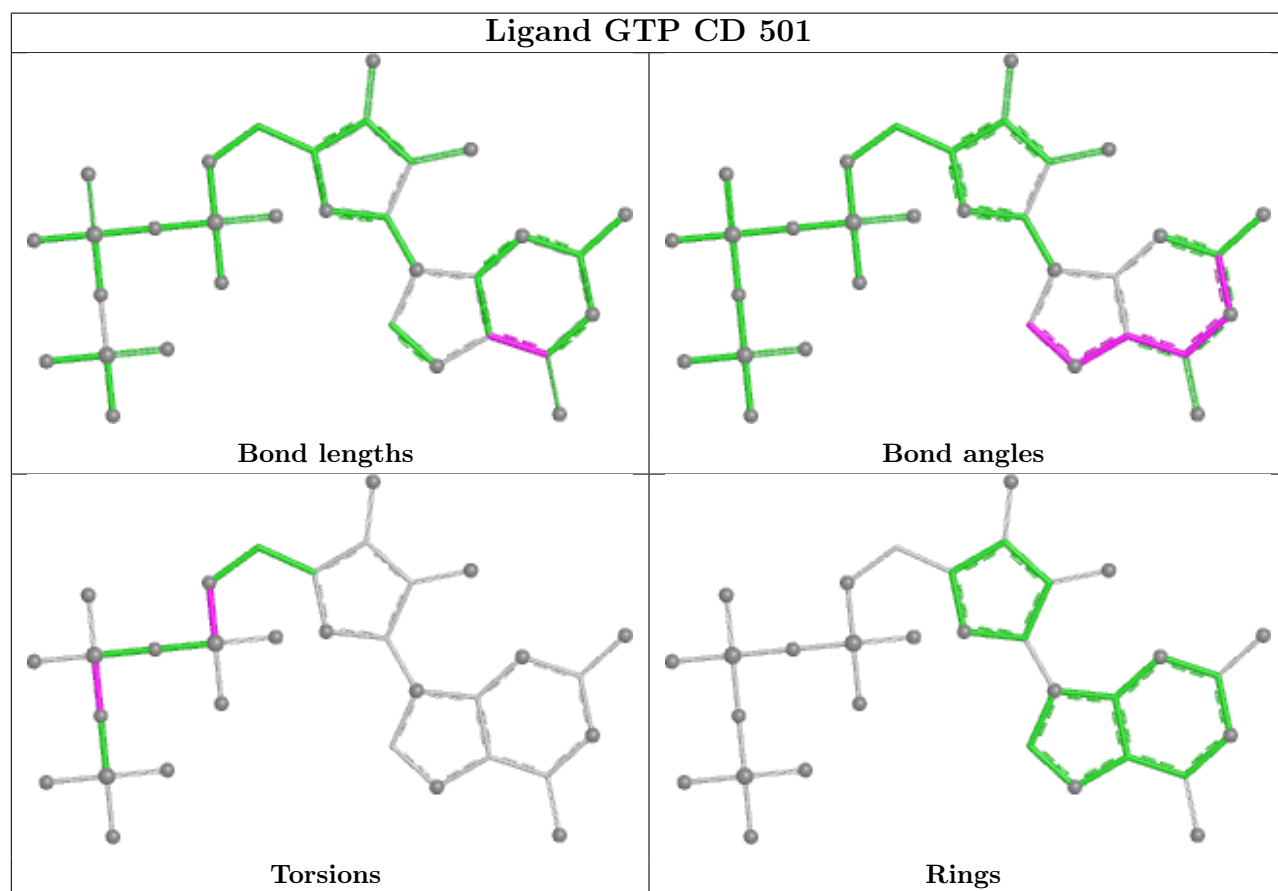
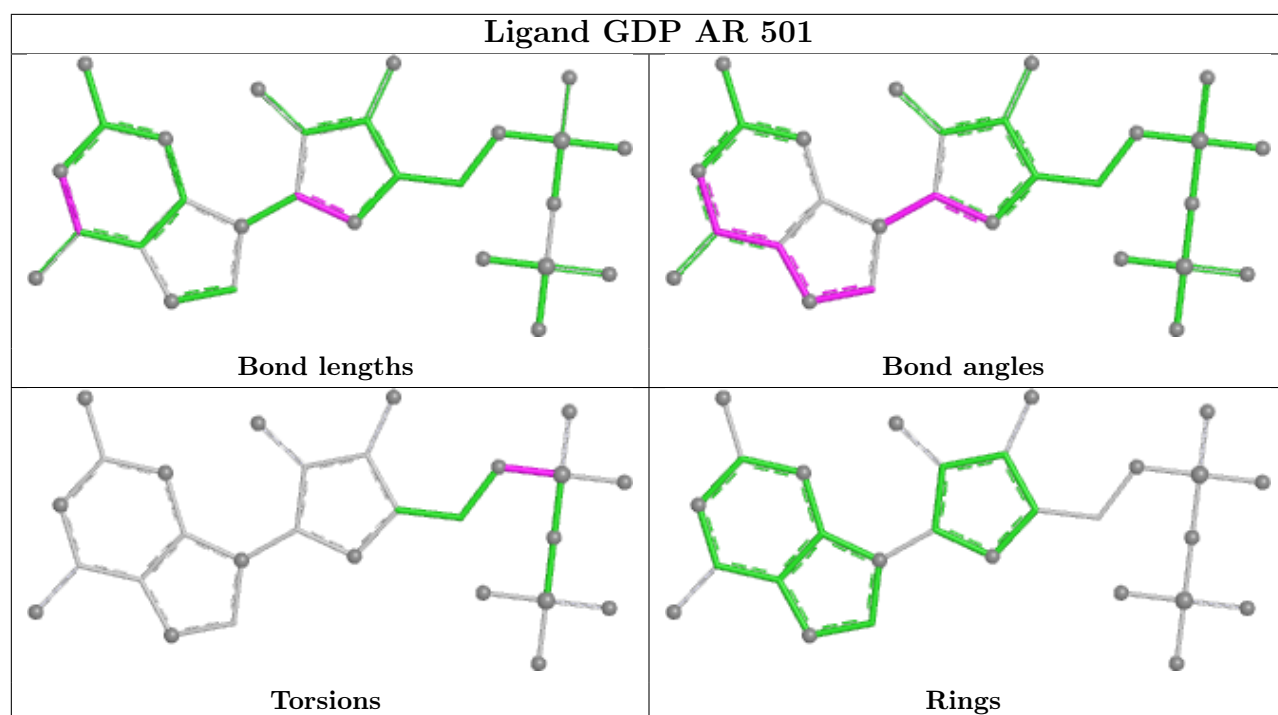
## Ligand GTP CO 501

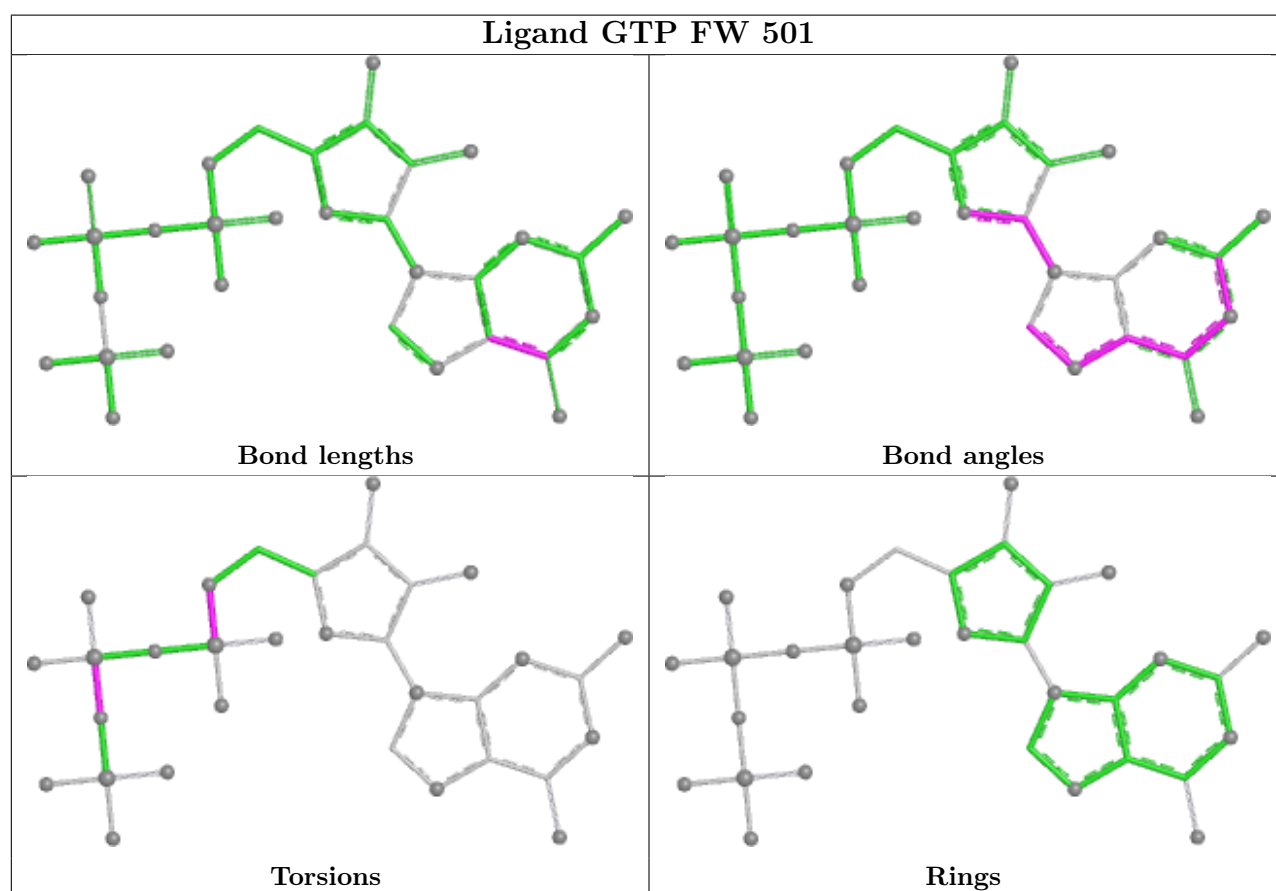
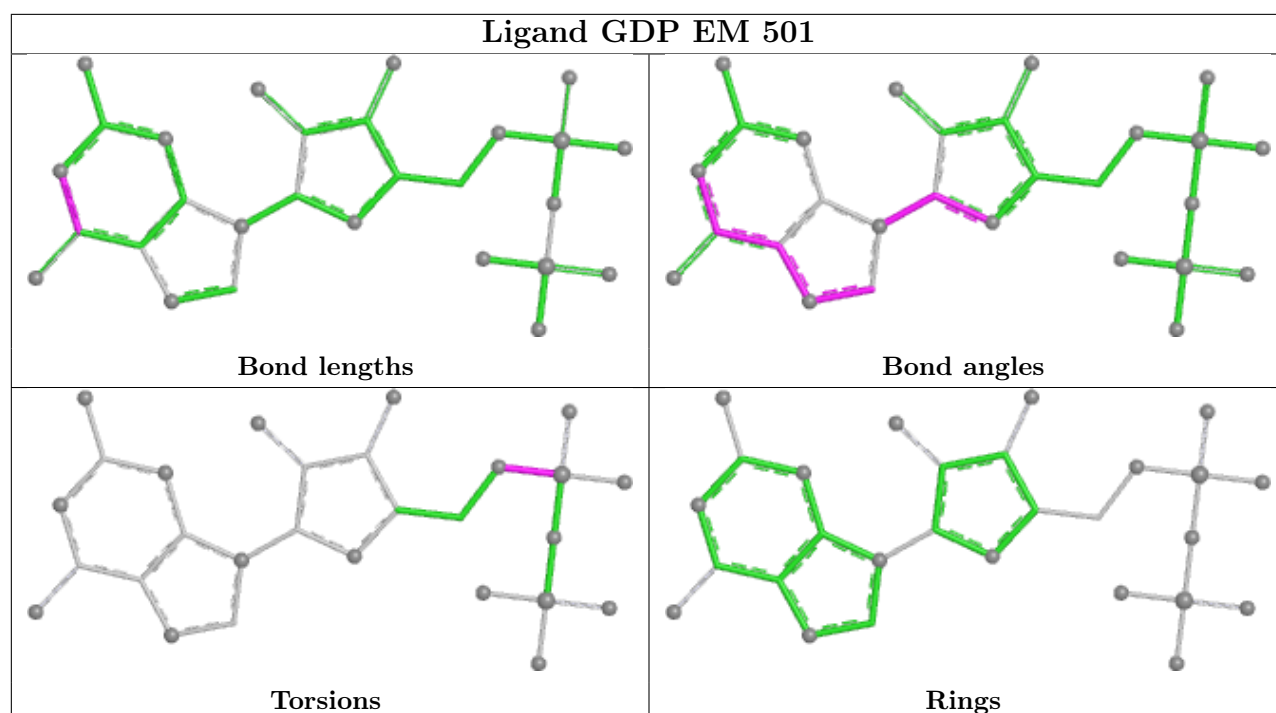


## Ligand GTP LA 501

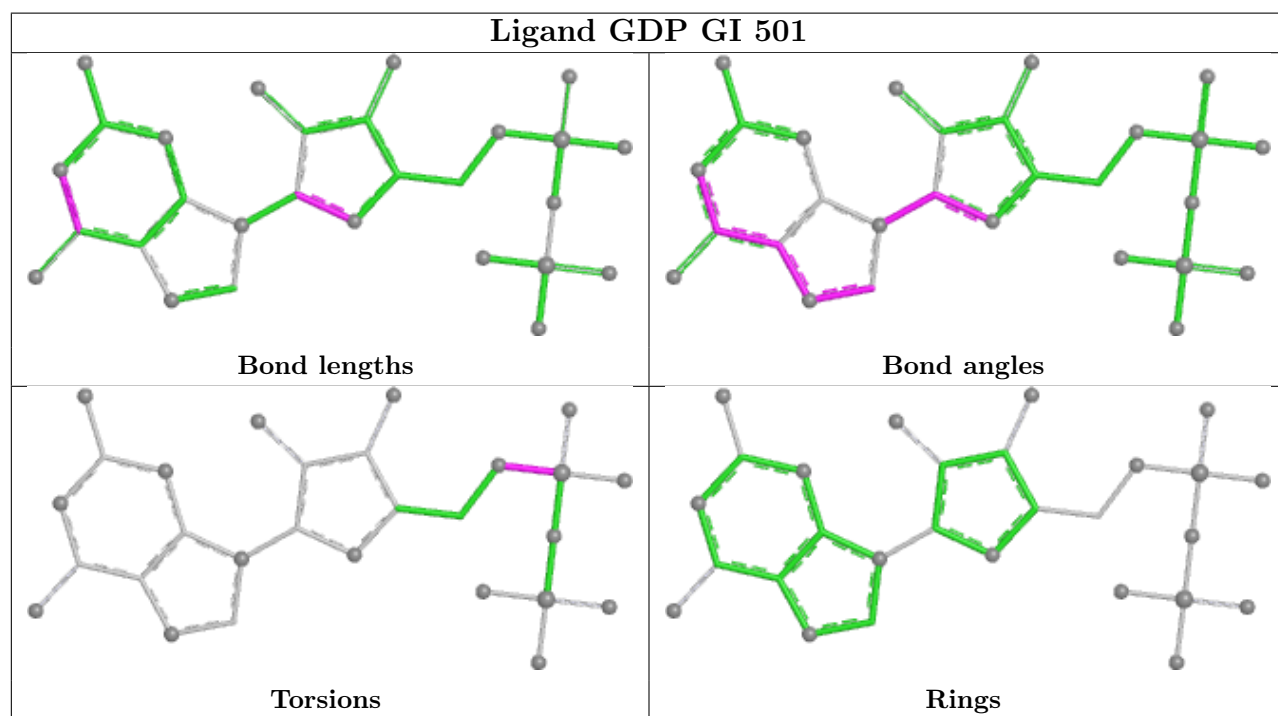
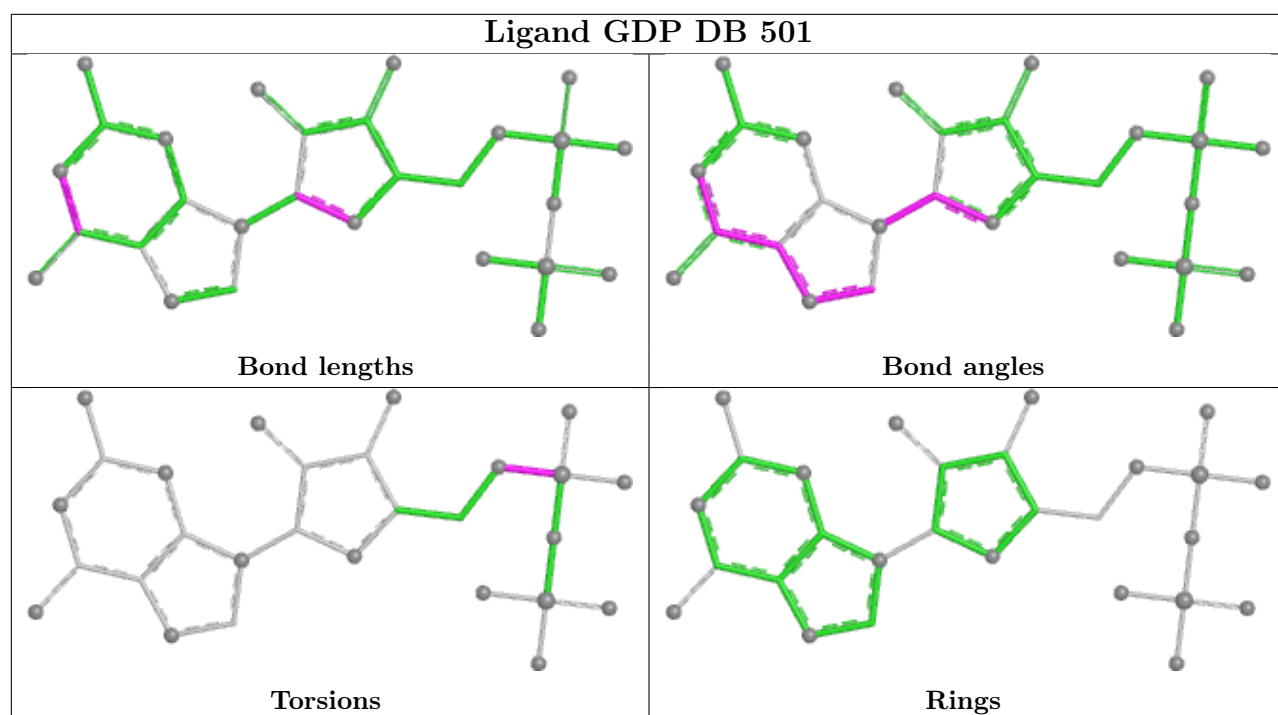




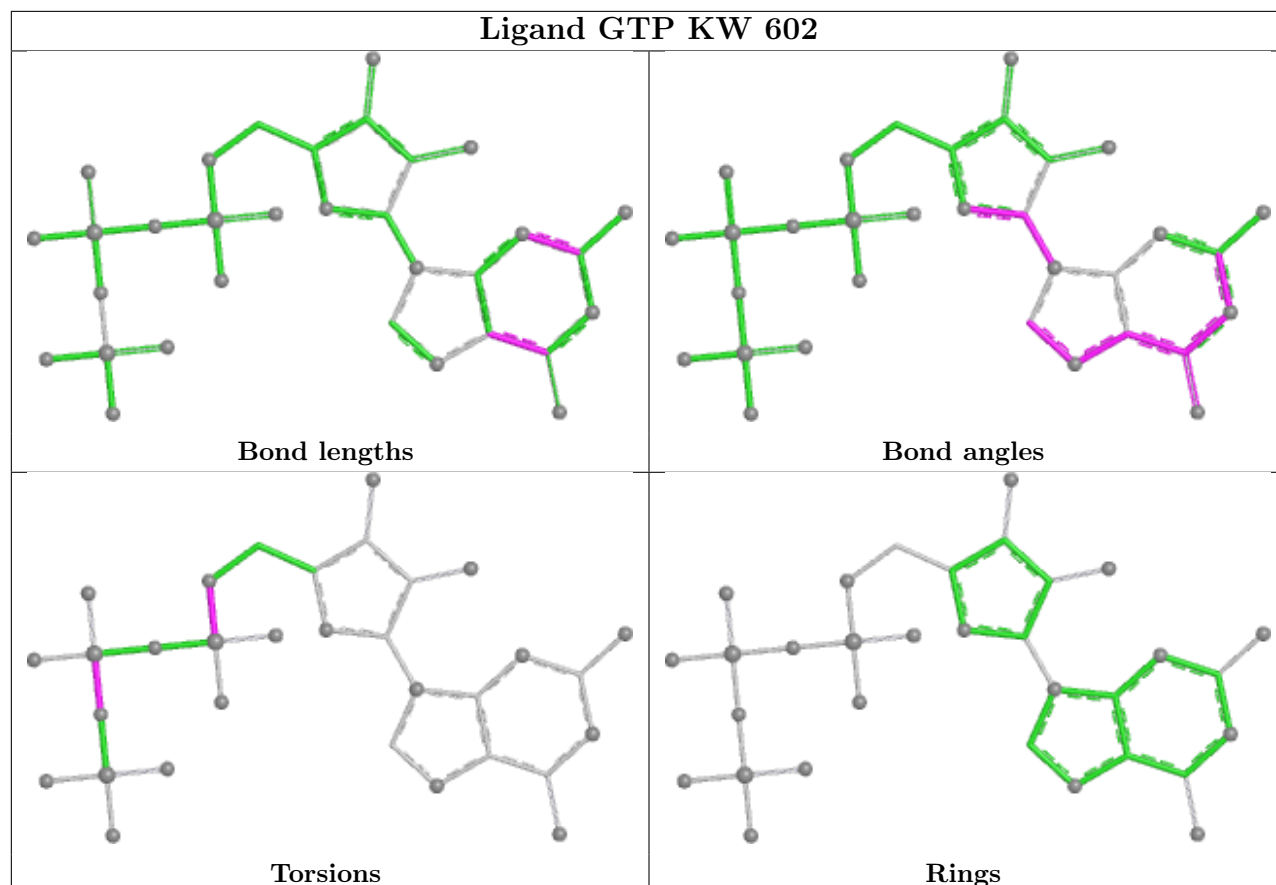




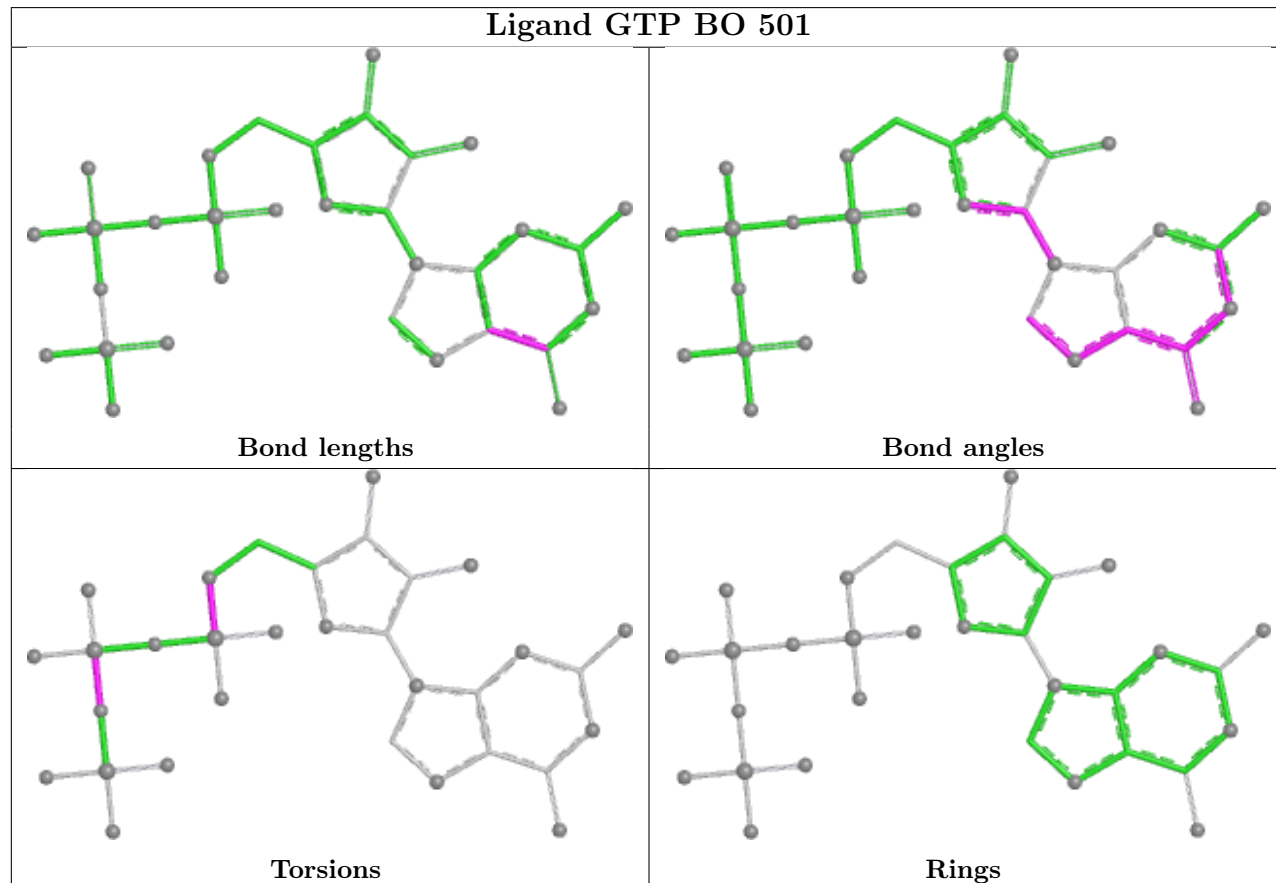


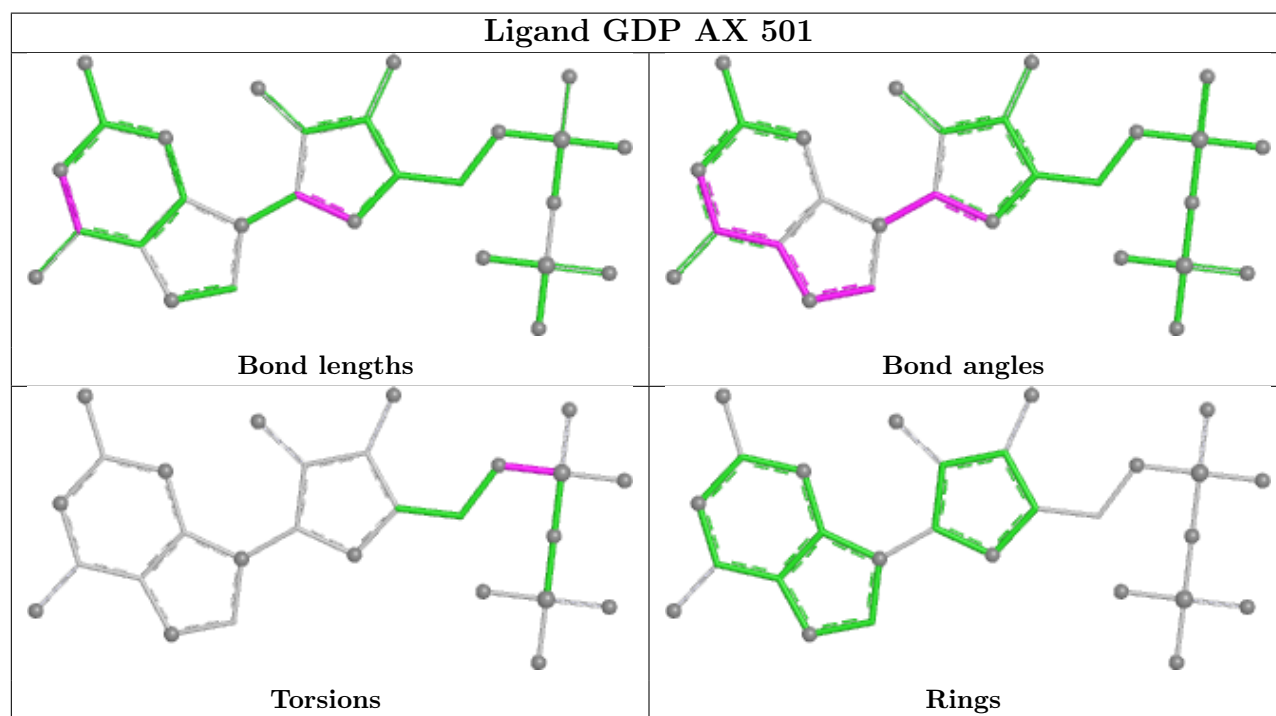
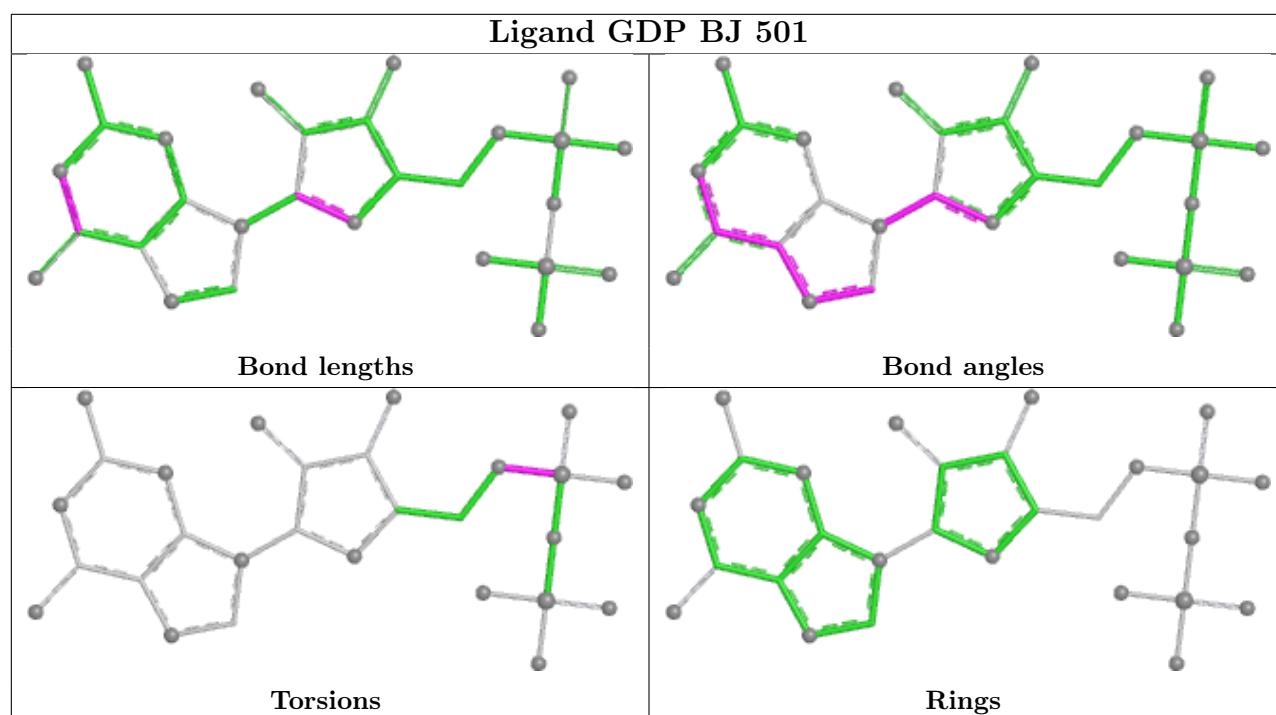


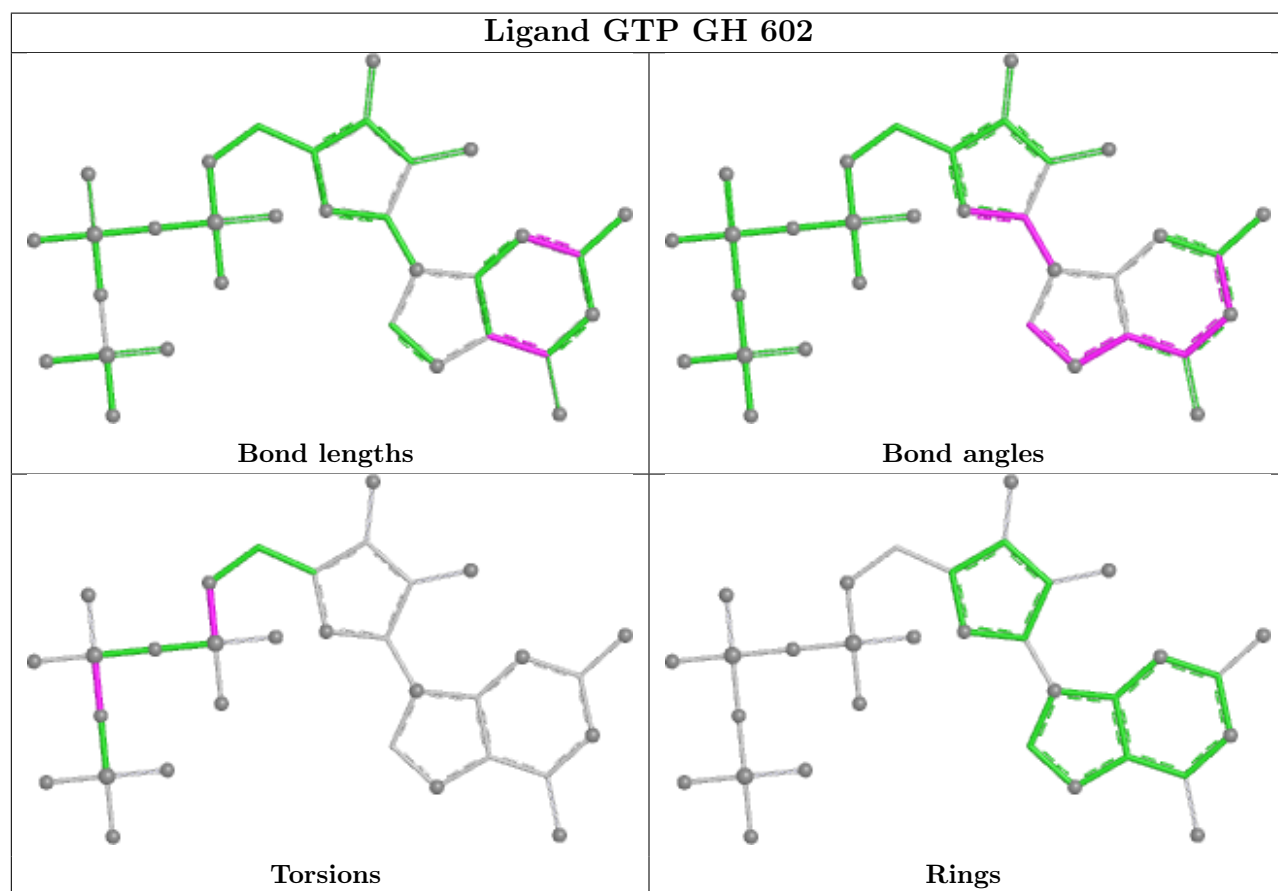
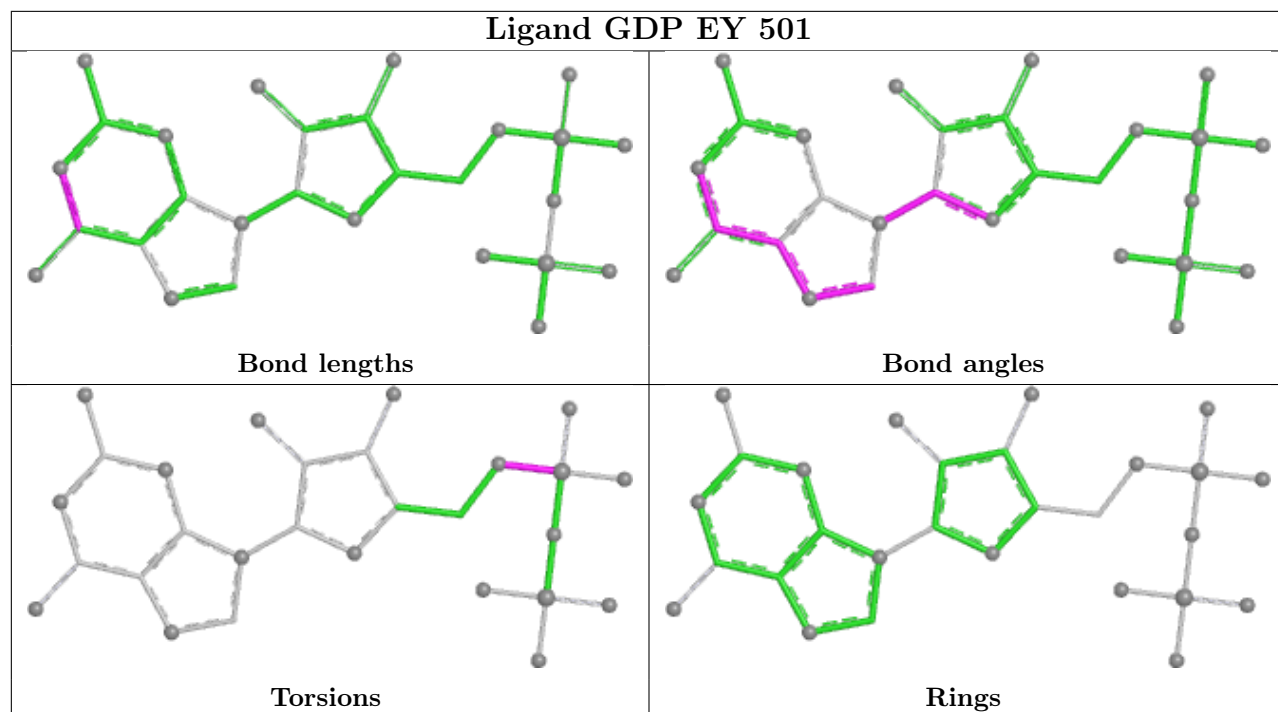
## Ligand GTP KW 602

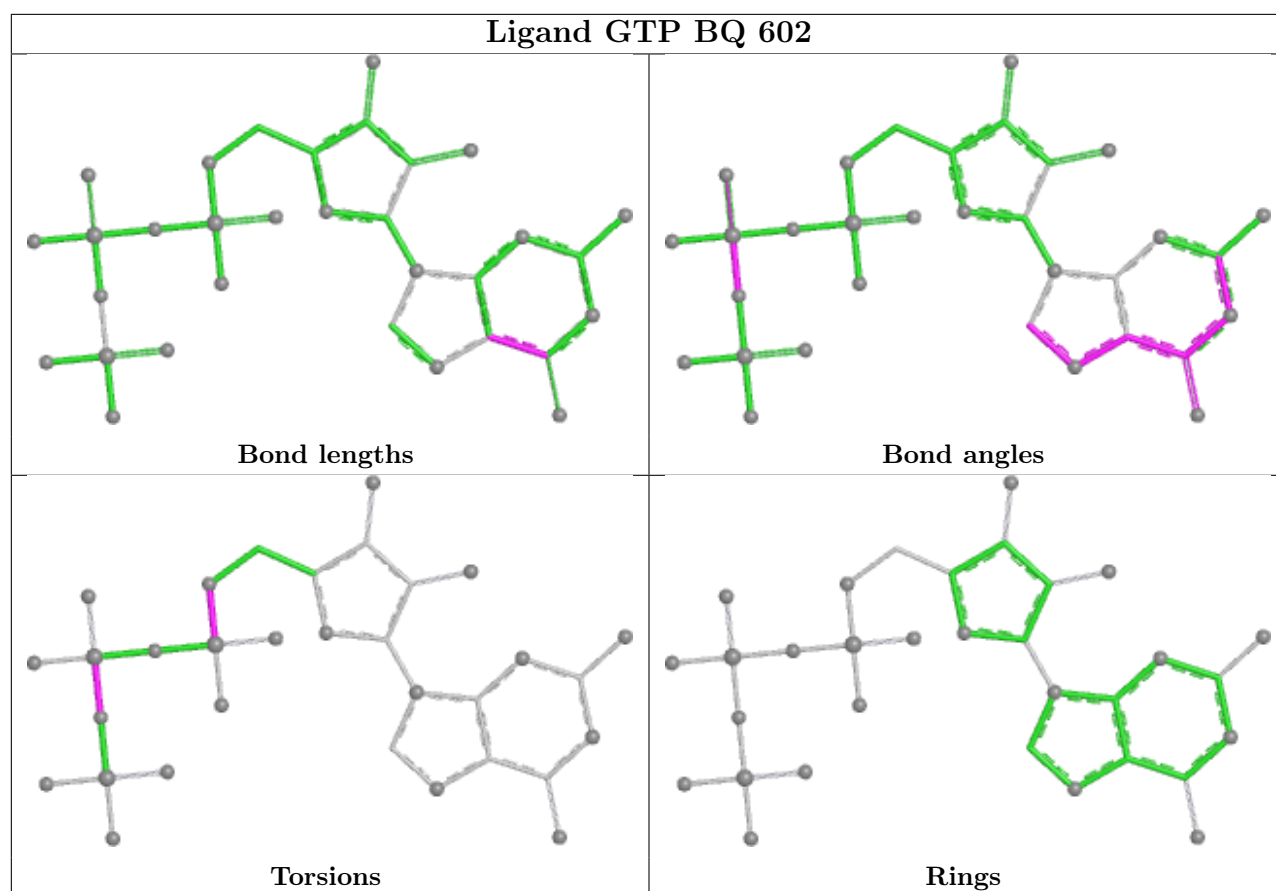


## Ligand GTP BO 501









## 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.

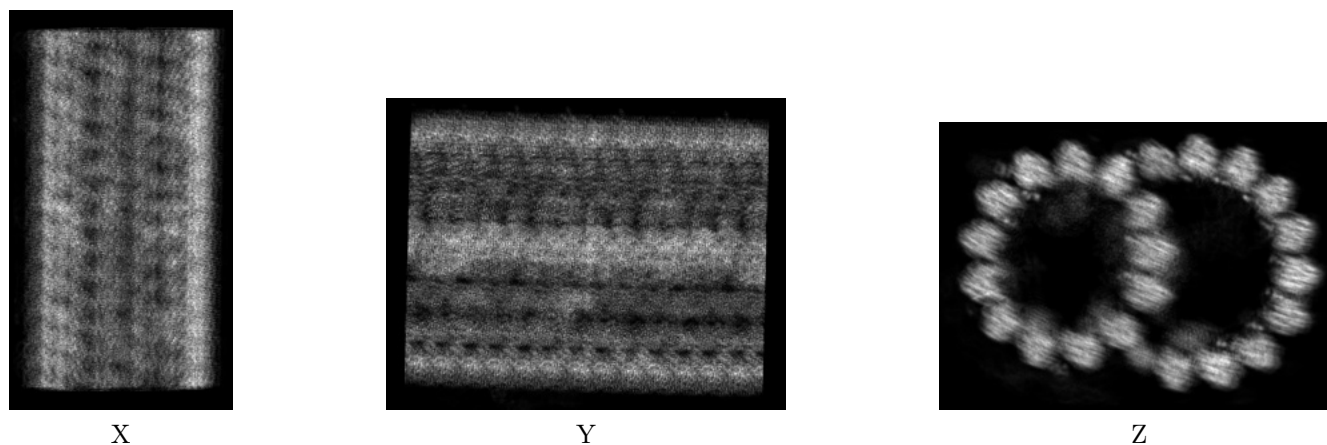
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47451. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

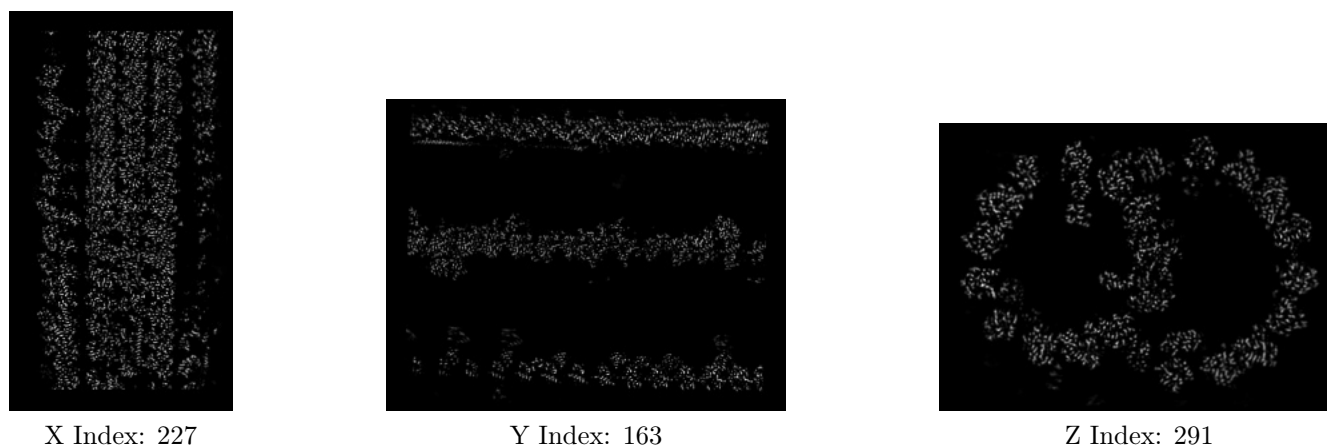
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

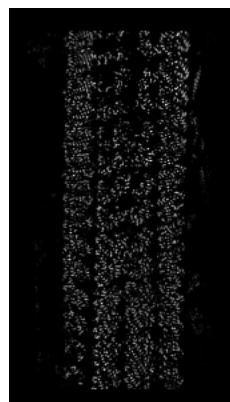
#### 6.2.1 Primary map



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: 62



Y Index: 273

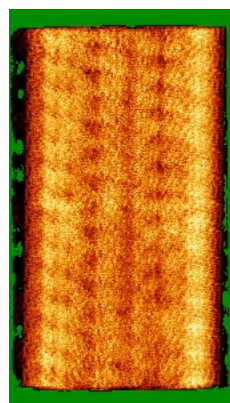


Z Index: 295

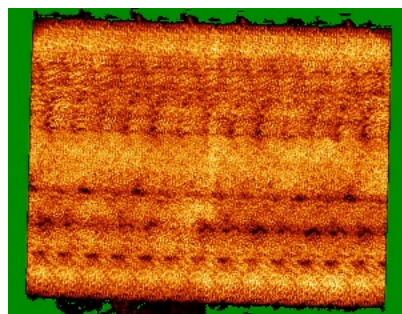
The images above show the largest variance slices of the map in three orthogonal directions.

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

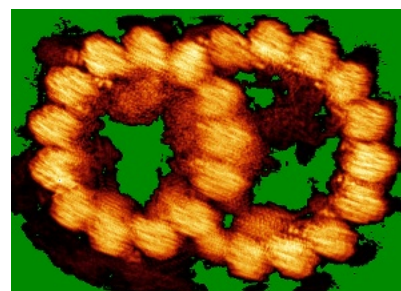
### 6.4.1 Primary map



X



Y



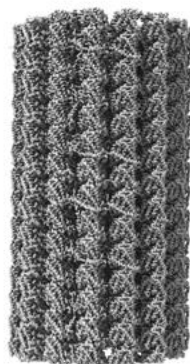
Z

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

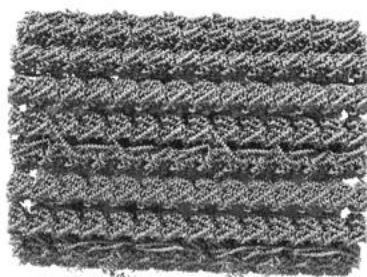


## 6.5 Orthogonal surface views [i](#)

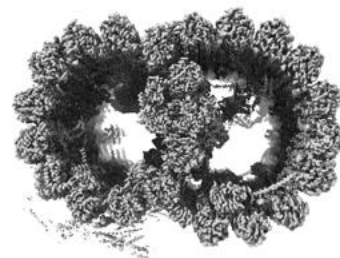
### 6.5.1 Primary map



X



Y



Z

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

## 6.6 Mask visualisation [i](#)

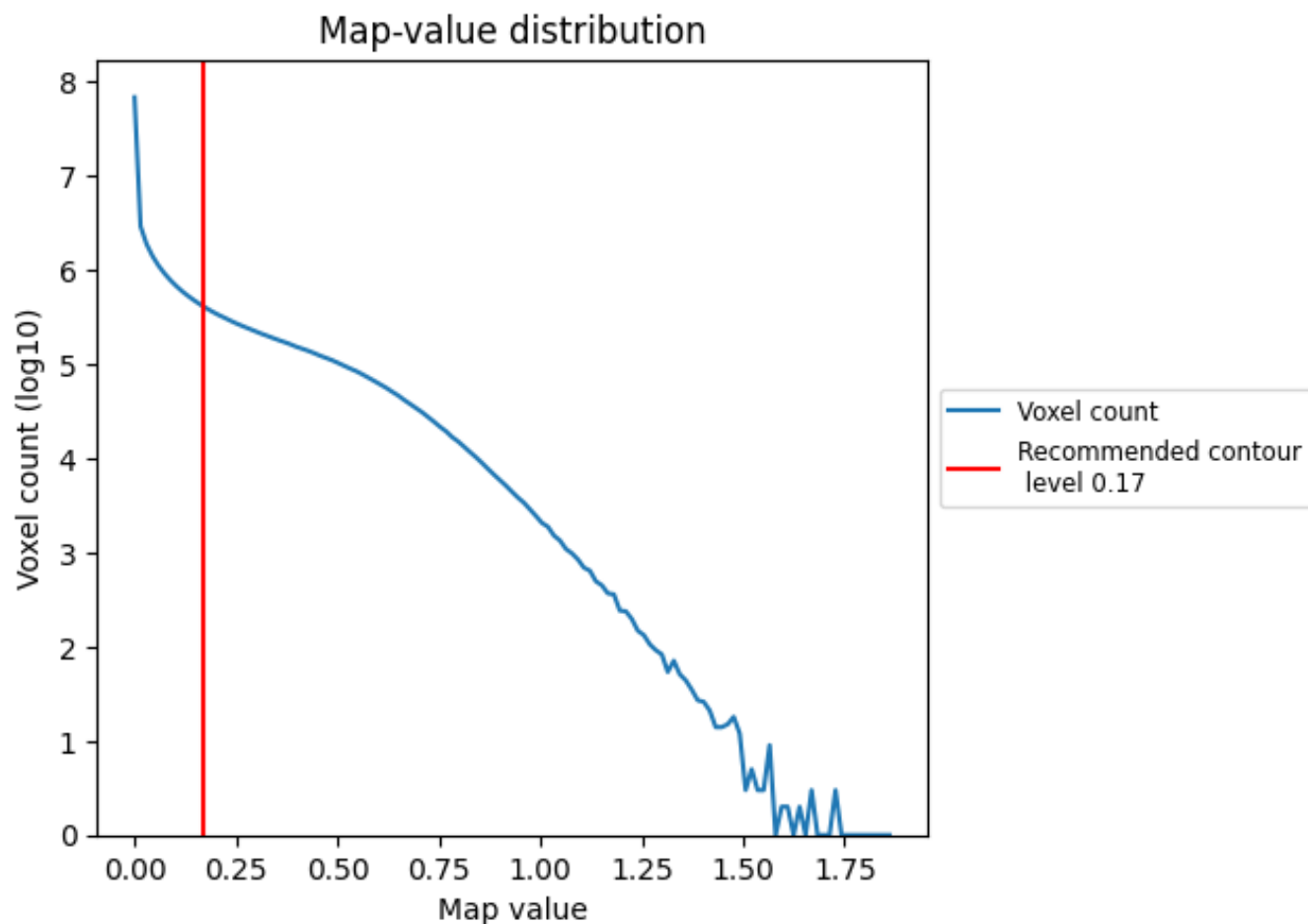
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis ⓘ

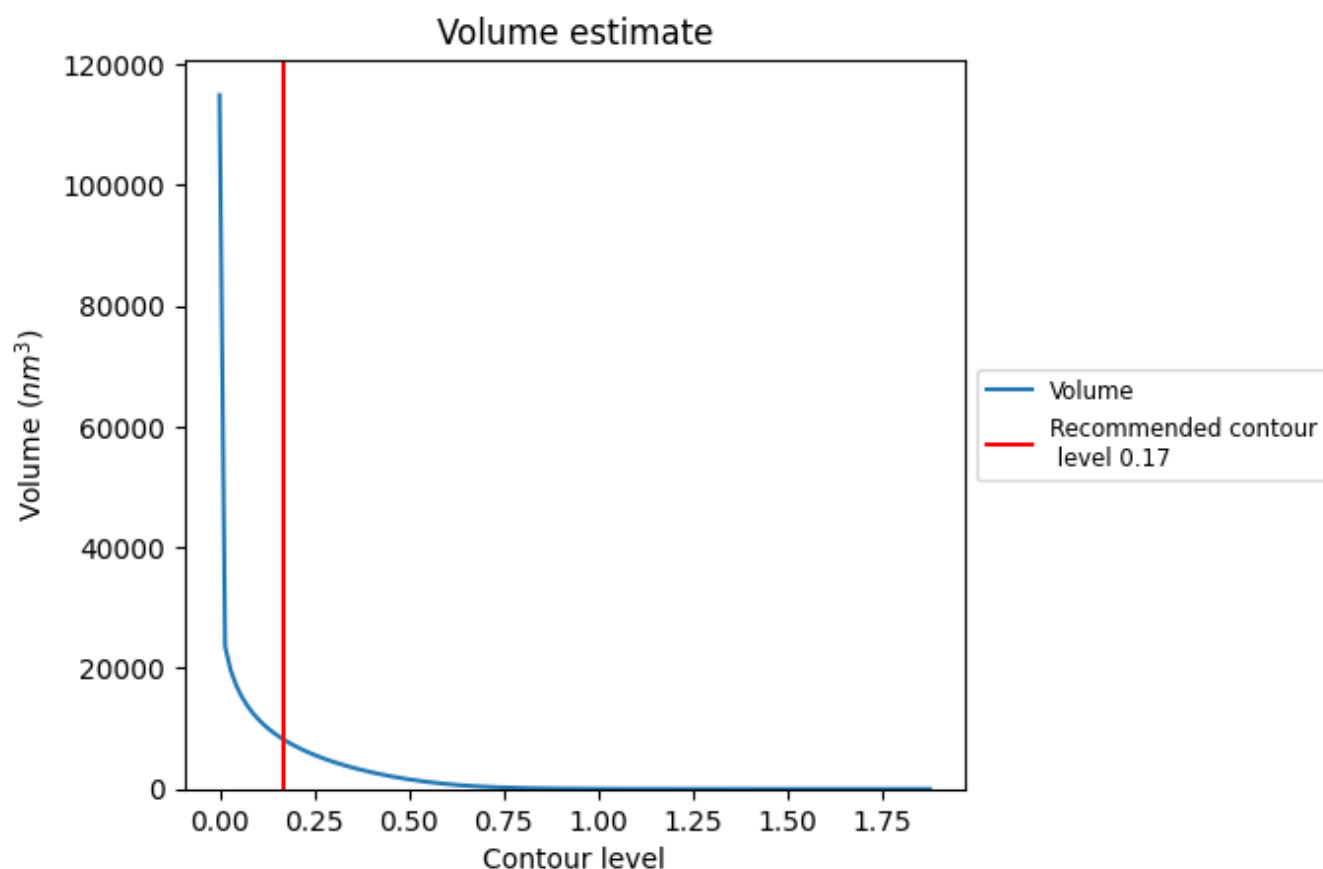
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution ⓘ



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 8147 nm<sup>3</sup>; this corresponds to an approximate mass of 7360 kDa.

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

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

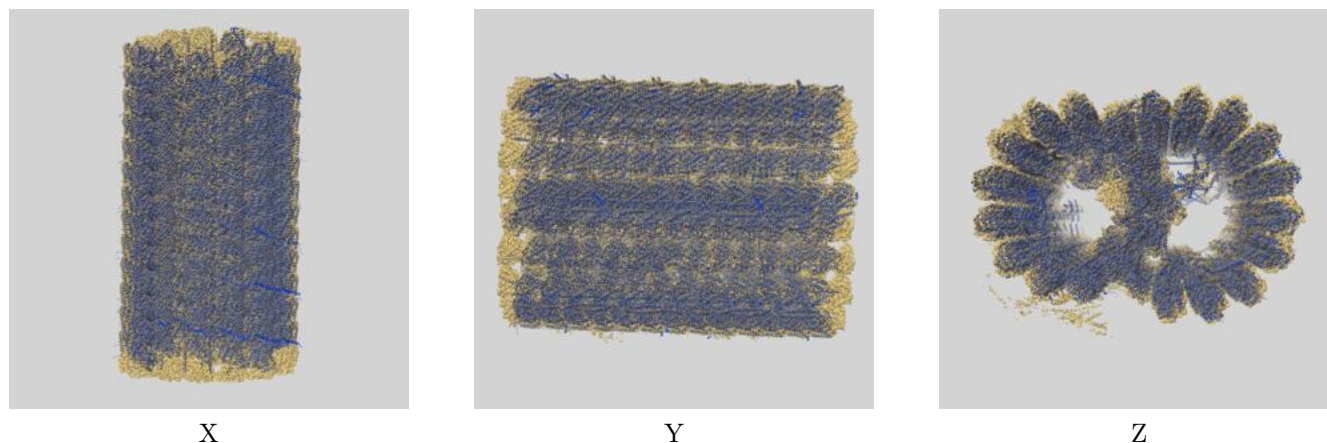
## 8 Fourier-Shell correlation

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

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

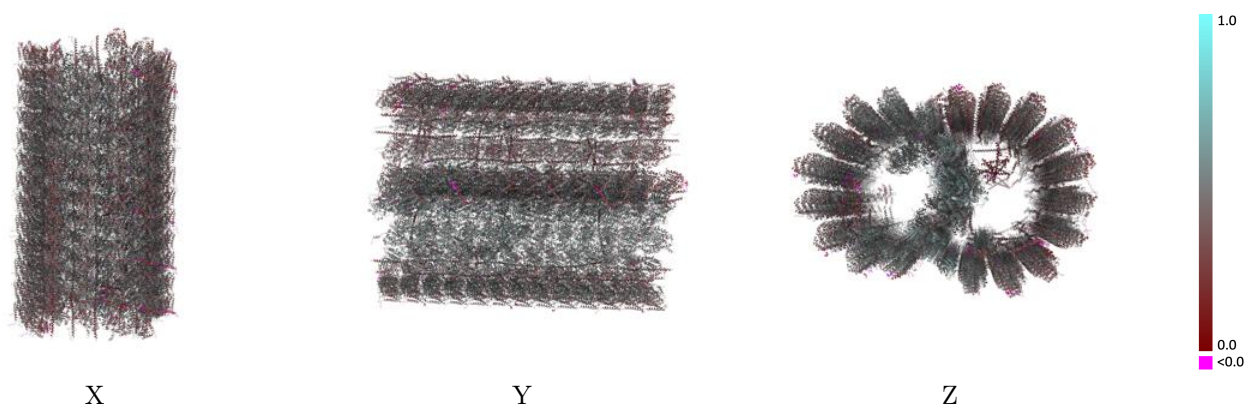
This section contains information regarding the fit between EMDB map EMD-47451 and PDB model 9E2G. Per-residue inclusion information can be found in section [3](#) on page [69](#).

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



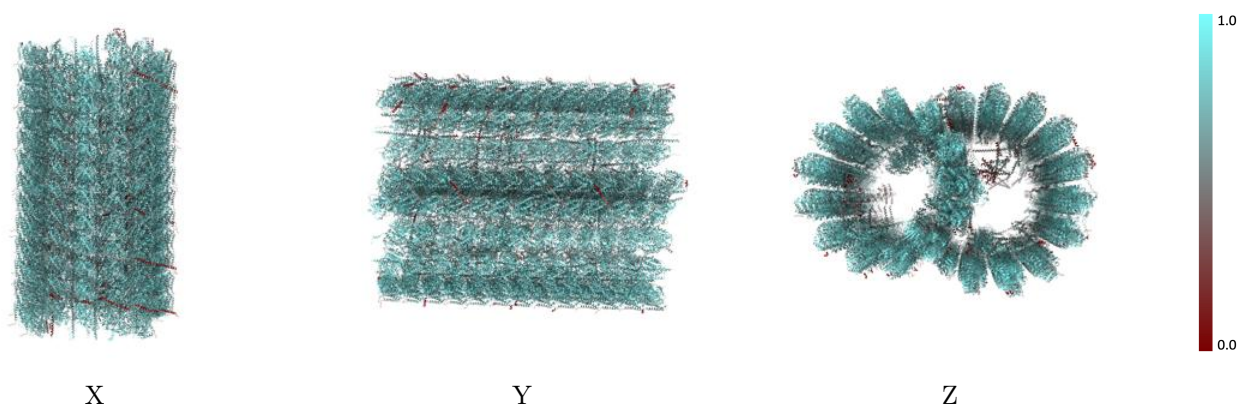
The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



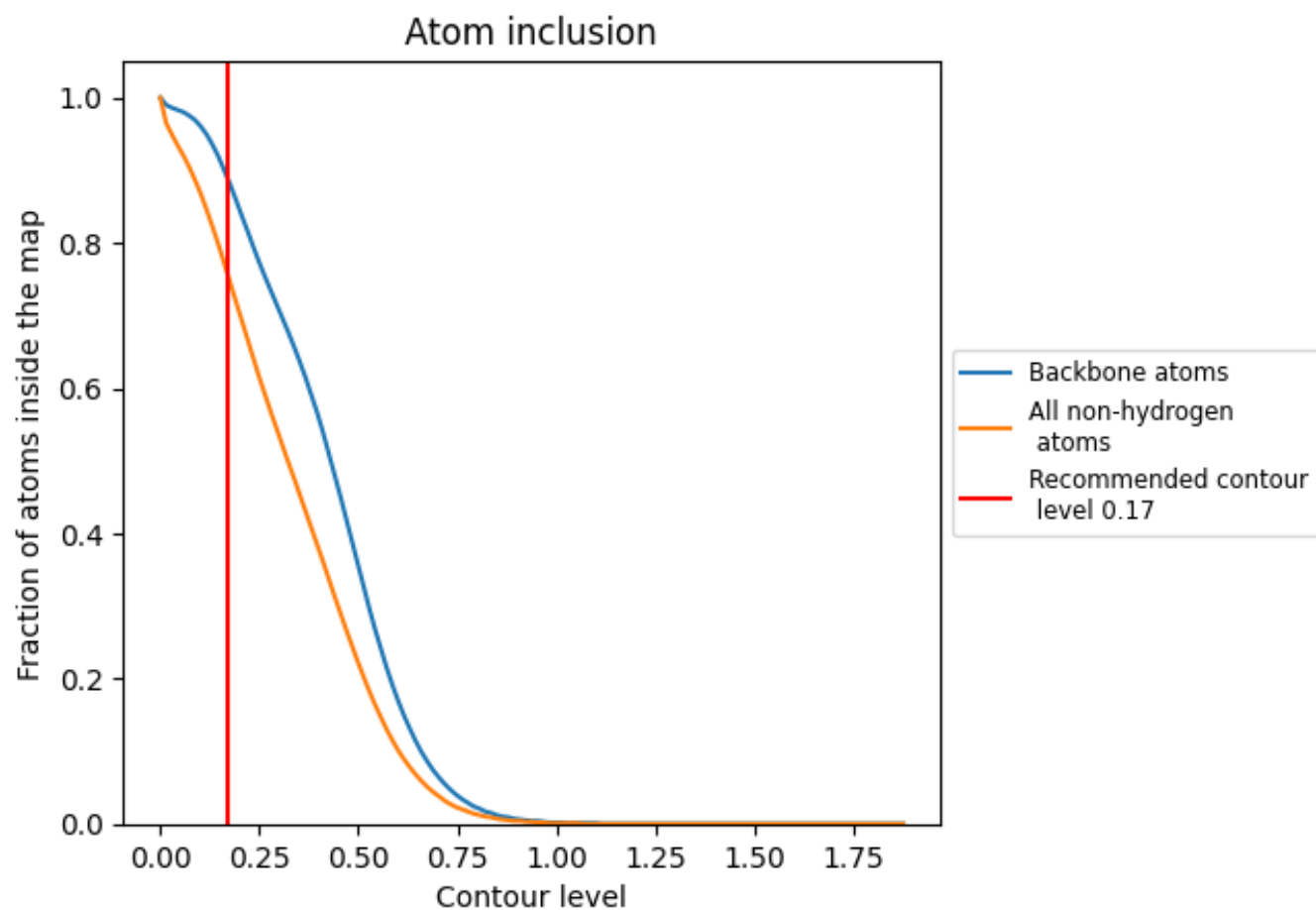
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 89% of all backbone atoms, 76% 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	 0.7570	 0.4460
0A	 0.6420	 0.4160
0B	 0.6060	 0.4160
0C	 0.6360	 0.4210
0D	 0.7970	 0.4920
0E	 0.6630	 0.4650
0F	 0.7100	 0.4550
0G	 0.6220	 0.4320
0H	 0.7830	 0.4950
0I	 0.7850	 0.4930
0J	 0.8180	 0.5320
0K	 0.8120	 0.5220
0M	 0.6620	 0.3940
0N	 0.6230	 0.3500
0O	 0.6650	 0.3370
0P	 0.6310	 0.3240
0Q	 0.8620	 0.5220
0R	 0.7440	 0.4880
0S	 0.8490	 0.5080
0T	 0.7440	 0.4860
0U	 0.6900	 0.4450
0V	 0.4830	 0.3260
0W	 0.6390	 0.4210
0X	 0.7500	 0.4310
0Y	 0.7850	 0.5150
0Z	 0.7210	 0.4880
1A	 0.8140	 0.5240
1B	 0.7790	 0.4830
1C	 0.7630	 0.4940
1D	 0.7700	 0.4620
1E	 0.7370	 0.4860
1F	 0.7030	 0.4830
1G	 0.6620	 0.4670
1H	 0.7300	 0.4790
1I	 0.7800	 0.5040



*Continued on next page...*





















































































*Continued from previous page...*

Chain	Atom inclusion	Q-score
1J	 0.6810	 0.5000
1K	 0.6800	 0.4750
1L	 0.6740	 0.4440
1M	 0.6560	 0.4570
1N	 0.6520	 0.4610
1O	 0.7970	 0.5310
1P	 0.7640	 0.5120
1Q	 0.7380	 0.4780
1R	 0.7670	 0.4900
1S	 0.7270	 0.4750
1T	 0.7080	 0.4910
1U	 0.7260	 0.4950
1V	 0.7670	 0.4980
1W	 0.7750	 0.5080
1X	 0.8040	 0.5110
1Y	 0.7750	 0.5050
1Z	 0.7860	 0.5220
2A	 0.7500	 0.4950
2B	 0.7490	 0.4780
2C	 0.7840	 0.4890
2D	 0.7340	 0.4500
2E	 0.7290	 0.4420
2F	 0.6990	 0.4520
2G	 0.5850	 0.3580
2H	 0.5320	 0.3120
2I	 0.7660	 0.4880
2J	 0.7490	 0.4930
2K	 0.7460	 0.4960
2L	 0.7190	 0.4910
2M	 0.7010	 0.4990
2N	 0.8260	 0.5140
2O	 0.5650	 0.3390
2P	 0.6100	 0.3420
2Q	 0.5110	 0.3250
2R	 0.4520	 0.2680
2S	 0.5990	 0.3030
2T	 0.6420	 0.3660
2U	 0.7190	 0.3640
2V	 0.5770	 0.3560
2W	 0.5460	 0.3080
2X	 0.7140	 0.3800
2Y	 0.5770	 0.3480

*Continued on next page...*























































































*Continued from previous page...*

Chain	Atom inclusion	Q-score
2Z	 0.5350	 0.3150
3A	 0.6440	 0.3570
3B	 0.6340	 0.3570
3C	 0.5910	 0.3190
3D	 0.5500	 0.3070
3E	 0.4160	 0.2830
3F	 0.5310	 0.3650
3G	 0.6460	 0.4010
3H	 0.5480	 0.3660
3I	 0.5690	 0.3940
3J	 0.6110	 0.3890
3K	 0.6060	 0.3690
3L	 0.6670	 0.4010
3M	 0.6910	 0.4110
3N	 0.6180	 0.3740
3O	 0.6150	 0.3750
3P	 0.5670	 0.3730
3Q	 0.5590	 0.3490
3R	 0.6760	 0.4370
3S	 0.7590	 0.4570
3T	 0.7900	 0.5230
3U	 0.8190	 0.5370
3V	 0.6530	 0.3930
3W	 0.5690	 0.3960
3X	 0.5590	 0.3440
3Y	 0.6150	 0.3750
3Z	 0.4020	 0.2880
4A	 0.3890	 0.3010
4B	 0.4660	 0.3430
4C	 0.5120	 0.3860
4D	 0.4730	 0.3400
4E	 0.1720	 0.1420
4F	 0.4990	 0.3640
4G	 0.2410	 0.1250
4H	 0.4700	 0.3550
4I	 0.6920	 0.4370
4J	 0.7640	 0.4900
4K	 0.7200	 0.4430
4L	 0.6370	 0.3830
4M	 0.3290	 0.2340
4N	 0.2980	 0.2290
4O	 0.0670	 0.1310





















































































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
4P	 0.4330	 0.2620
4Q	 0.5880	 0.3530
4R	 0.6430	 0.3570
4S	 0.6390	 0.4010
4T	 0.3660	 0.2730
4U	 0.5120	 0.3430
4V	 0.3810	 0.2610
4W	 0.5780	 0.3530
4X	 0.7830	 0.5370
4Y	 0.5520	 0.3820
AA	 0.7880	 0.4830
AB	 0.7980	 0.4980
AC	 0.8020	 0.5010
AD	 0.8140	 0.4980
AE	 0.8160	 0.5090
AF	 0.8310	 0.5010
AG	 0.7880	 0.4860
AH	 0.7910	 0.4890
AI	 0.7870	 0.4890
AJ	 0.7940	 0.4750
AK	 0.7700	 0.4700
AL	 0.7870	 0.4700
AM	 0.7980	 0.4440
AN	 0.8140	 0.4620
AO	 0.8030	 0.4590
AP	 0.8240	 0.4700
AQ	 0.8120	 0.4700
AR	 0.8290	 0.4690
AS	 0.7940	 0.4410
AT	 0.7960	 0.4520
AU	 0.7810	 0.4550
AV	 0.7880	 0.4440
AW	 0.7760	 0.4400
AX	 0.7880	 0.4310
AY	 0.7630	 0.4260
AZ	 0.7860	 0.4430
BA	 0.7690	 0.4420
BB	 0.7930	 0.4570
BC	 0.7620	 0.4350
BD	 0.7760	 0.4270
BE	 0.8070	 0.4490
BF	 0.8100	 0.4590





















































































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
BG	 0.7930	 0.4490
BH	 0.8040	 0.4520
BI	 0.7650	 0.4230
BJ	 0.7930	 0.4260
BK	 0.7430	 0.4240
BL	 0.7690	 0.4420
BM	 0.7600	 0.4560
BN	 0.7780	 0.4570
BO	 0.7600	 0.4550
BP	 0.7690	 0.4490
BQ	 0.7790	 0.4500
BR	 0.7650	 0.4510
BS	 0.7800	 0.4610
BT	 0.7690	 0.4500
BU	 0.7640	 0.4450
BV	 0.7830	 0.4460
BW	 0.7450	 0.4270
BX	 0.7390	 0.4050
BY	 0.7900	 0.4410
BZ	 0.7820	 0.4470
CA	 0.8080	 0.4570
CB	 0.7810	 0.4590
CC	 0.7940	 0.4520
CD	 0.7820	 0.4420
CE	 0.7740	 0.4360
CF	 0.7710	 0.4380
CG	 0.7750	 0.4300
CH	 0.7750	 0.4410
CI	 0.7780	 0.4350
CJ	 0.7500	 0.4240
CL	 0.7750	 0.4420
CM	 0.7590	 0.4480
CN	 0.7810	 0.4490
CO	 0.7520	 0.4450
CP	 0.7810	 0.4540
CQ	 0.7690	 0.4450
CR	 0.7800	 0.4240
CS	 0.7530	 0.4290
CT	 0.7780	 0.4390
CU	 0.7600	 0.4380
CV	 0.7920	 0.4450
CW	 0.7540	 0.4210





















































































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
CX	 0.7940	 0.4670
CY	 0.8010	 0.4930
CZ	 0.7880	 0.4810
DA	 0.7840	 0.4880
DB	 0.7920	 0.4790
DC	 0.7820	 0.4800
DD	 0.7860	 0.4530
DE	 0.7810	 0.4780
DF	 0.7890	 0.4720
DG	 0.7890	 0.4810
DH	 0.7910	 0.4660
DI	 0.7880	 0.4730
DJ	 0.8060	 0.4590
DK	 0.7850	 0.4610
DL	 0.8010	 0.4720
DM	 0.7830	 0.4640
DN	 0.8030	 0.4660
DO	 0.7940	 0.4710
DP	 0.8130	 0.4690
DQ	 0.7870	 0.4670
DR	 0.8090	 0.4780
DS	 0.7810	 0.4730
DT	 0.7970	 0.4770
DU	 0.7700	 0.4670
DV	 0.7880	 0.4570
DW	 0.8000	 0.4790
DX	 0.8010	 0.4960
DY	 0.8070	 0.4950
DZ	 0.8090	 0.5040
EA	 0.7910	 0.4890
EB	 0.8020	 0.5030
EC	 0.8240	 0.5000
ED	 0.8100	 0.4910
EE	 0.7850	 0.4880
EF	 0.7900	 0.5000
EG	 0.8020	 0.4960
EH	 0.7930	 0.4920
EI	 0.7960	 0.4870
EJ	 0.7970	 0.4890
EK	 0.8130	 0.5030
EL	 0.8180	 0.5080
EM	 0.8150	 0.5020





















































































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
EN	 0.8030	 0.4920
EO	 0.8120	 0.4900
EP	 0.8070	 0.4820
EQ	 0.7910	 0.4790
ER	 0.7840	 0.4740
ES	 0.7940	 0.4860
ET	 0.7950	 0.4880
EU	 0.7960	 0.4840
EV	 0.8300	 0.5180
EW	 0.8590	 0.5340
EX	 0.8390	 0.5290
EY	 0.8350	 0.5210
EZ	 0.8300	 0.5210
FA	 0.8520	 0.5410
FB	 0.8700	 0.5460
FC	 0.8350	 0.5260
FD	 0.8350	 0.5120
FE	 0.8770	 0.5280
FF	 0.8660	 0.5240
FG	 0.8320	 0.5150
FH	 0.7960	 0.4960
FI	 0.8120	 0.5050
FJ	 0.8110	 0.5160
FK	 0.8040	 0.5140
FL	 0.7980	 0.5010
FM	 0.8040	 0.5030
FN	 0.8170	 0.5010
FO	 0.7990	 0.5030
FP	 0.7970	 0.4960
FQ	 0.8110	 0.4980
FR	 0.8040	 0.4870
FS	 0.7790	 0.4840
FT	 0.7880	 0.4830
FU	 0.8160	 0.4630
FV	 0.8280	 0.4810
FW	 0.8310	 0.4970
FX	 0.8390	 0.4980
FY	 0.8160	 0.4900
FZ	 0.8420	 0.4960
GA	 0.8350	 0.4880
GB	 0.8290	 0.4830
GC	 0.8200	 0.4860





















































































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
GD	 0.8330	 0.4910
GE	 0.8220	 0.4780
GF	 0.8160	 0.4670
GG	 0.7930	 0.4560
GH	 0.6930	 0.4200
GI	 0.7320	 0.4460
GJ	 0.7190	 0.4470
GK	 0.6990	 0.4270
GL	 0.6330	 0.3960
GM	 0.6450	 0.3740
GN	 0.6740	 0.3840
GO	 0.6750	 0.3970
GP	 0.6510	 0.3990
GQ	 0.6670	 0.4010
GR	 0.6310	 0.3840
GS	 0.6480	 0.3600
GT	 0.6190	 0.3440
GU	 0.7560	 0.4160
GV	 0.7680	 0.4340
GW	 0.7560	 0.4340
GX	 0.7630	 0.4340
GY	 0.7430	 0.4120
GZ	 0.7580	 0.4080
HA	 0.7720	 0.4100
HB	 0.7630	 0.4170
HC	 0.7630	 0.4180
HD	 0.7770	 0.4120
HE	 0.7530	 0.3960
HF	 0.7480	 0.3800
HG	 0.7450	 0.4190
HH	 0.7770	 0.4270
HI	 0.7660	 0.4340
HJ	 0.7720	 0.4370
HK	 0.7600	 0.4310
HL	 0.7680	 0.4120
HM	 0.7630	 0.4420
HN	 0.7730	 0.4490
HO	 0.7780	 0.4340
HP	 0.8020	 0.4310
HQ	 0.7570	 0.4060
HR	 0.7430	 0.3970
HS	 0.7360	 0.3900





















































































*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
HT	 0.7430	 0.4160
HU	 0.7830	 0.4290
HV	 0.7510	 0.4380
HW	 0.7810	 0.4520
HX	 0.7500	 0.4240
HY	 0.7770	 0.4140
HZ	 0.7450	 0.4180
IA	 0.7580	 0.4390
IB	 0.7450	 0.4260
IC	 0.8020	 0.4280
ID	 0.7630	 0.4150
IE	 0.7440	 0.4010
IF	 0.7510	 0.4040
IG	 0.7510	 0.4270
IH	 0.7700	 0.4370
II	 0.7570	 0.4350
IJ	 0.7700	 0.4410
IK	 0.7470	 0.4200
IL	 0.7750	 0.4070
IM	 0.7530	 0.4170
IN	 0.7670	 0.4350
IO	 0.7450	 0.4310
IP	 0.7610	 0.4280
IQ	 0.7510	 0.4180
IR	 0.7040	 0.3930
IS	 0.7800	 0.3990
IT	 0.7910	 0.4240
IU	 0.7870	 0.4230
IV	 0.7970	 0.4410
IW	 0.8090	 0.4360
IX	 0.7940	 0.4100
IY	 0.8220	 0.4100
IZ	 0.8150	 0.4340
JA	 0.8220	 0.4500
JB	 0.8120	 0.4400
JC	 0.8270	 0.4400
JD	 0.7980	 0.4130
JE	 0.7180	 0.3660
JF	 0.7180	 0.3890
JG	 0.7150	 0.3940
JH	 0.7060	 0.3880
JI	 0.7030	 0.3840

*Continued on next page...*







*Continued from previous page...*

Chain	Atom inclusion	Q-score
JJ	 0.7210	 0.3830
JK	 0.7180	 0.3900
JL	 0.7430	 0.4310
JM	 0.7640	 0.4480
JN	 0.7560	 0.4480
JO	 0.7620	 0.4430
JP	 0.7510	 0.4150
JQ	 0.6940	 0.3570
JR	 0.6960	 0.3780
JS	 0.7320	 0.4090
JT	 0.7230	 0.4070
JU	 0.7390	 0.4210
JV	 0.7390	 0.4100
JW	 0.7590	 0.4140
JX	 0.7450	 0.4210
JY	 0.7440	 0.4350
JZ	 0.7420	 0.4270
KA	 0.7410	 0.4260
KB	 0.7370	 0.4020
KC	 0.6720	 0.3340
KD	 0.7850	 0.4130
KE	 0.7990	 0.4330
KF	 0.7970	 0.4510
KG	 0.8120	 0.4600
KH	 0.8020	 0.4520
KI	 0.8050	 0.4510
KJ	 0.8120	 0.4410
KK	 0.8160	 0.4570
KL	 0.7950	 0.4540
KM	 0.8110	 0.4540
KN	 0.7970	 0.4480
KO	 0.7910	 0.4280
KP	 0.7700	 0.3890
KQ	 0.7500	 0.4390
KR	 0.7570	 0.4540
KS	 0.7860	 0.4770
KT	 0.7820	 0.4790
KU	 0.7770	 0.4720
KV	 0.7700	 0.4750
KW	 0.7910	 0.4770
KX	 0.7730	 0.4690
KY	 0.7710	 0.4650

*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
KZ	 0.7870	 0.4810
LA	 0.7850	 0.4830
LB	 0.7690	 0.4540