



## wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 05:14 PM UTC

PDB ID : 9E2G / pdb\_00009e2g  
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>.

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : **FAILED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

## 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.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

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

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

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

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

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

- Molecule 4 is a protein called CMF34/CARP4.

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

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

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

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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
			Total	C	N	O	S		
11	0T	414	3295	2050	603	624	18	0	0

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

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

- Molecule 13 is a protein called TbMIP23.

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

- Molecule 14 is a protein called FAP141.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a protein called FAP107/MC11.

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

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

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

- Molecule 24 is a protein called FAP95/MC6.

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

- Molecule 25 is a protein called FAP129.

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

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

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

- Molecule 27 is a protein called FAP21.

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

- Molecule 28 is a protein called Flagellar associated protein.

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

- Molecule 29 is a protein called TbRib26b.

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

- Molecule 30 is a protein called PACRGA.

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

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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		

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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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
50	4E	40	Total	C	N	O	S	0	0
			327	199	60	67	1		

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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
			Total	C	N	O	S		
56	4Q	71	583	368	100	113	2	0	0

- Molecule 57 is a protein called KIAA1430 homologue.

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

- Molecule 58 is a protein called Starmaker.

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

- Molecule 59 is a protein called Tubulin alpha chain.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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

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

- Molecule 60 is a protein called Tubulin beta chain.

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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

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

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

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

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

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

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

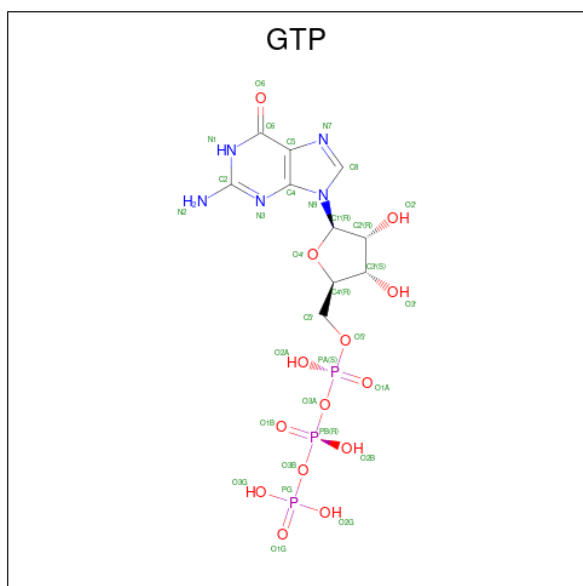
Mol	Chain	Residues	Atoms		AltConf
61	2I	2	Total 2	Zn 2	0
61	2K	1	Total 1	Zn 1	0
61	2N	1	Total 1	Zn 1	0
61	3V	2	Total 2	Zn 2	0
61	3W	2	Total 2	Zn 2	0
61	3X	3	Total 3	Zn 3	0
61	3Y	2	Total 2	Zn 2	0
61	4A	1	Total 1	Zn 1	0
61	4B	1	Total 1	Zn 1	0
61	4C	1	Total 1	Zn 1	0

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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 (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
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	

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
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

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
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

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

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

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

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

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

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

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

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

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

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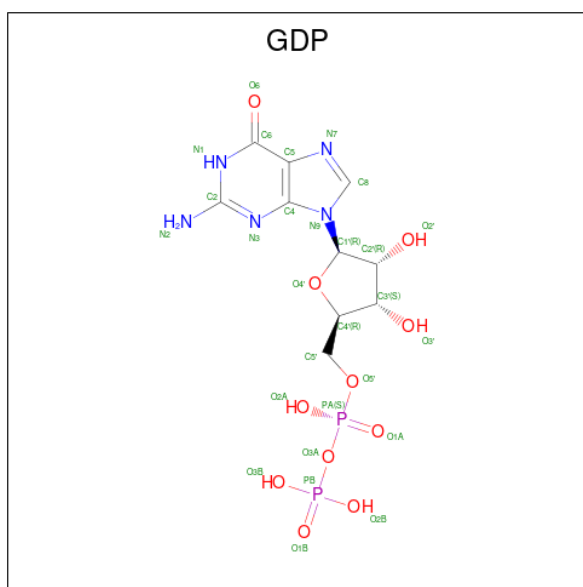
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
63	IM	1	1	1	0
63	IO	1	1	1	0
63	IQ	1	1	1	0
63	IT	1	1	1	0
63	IV	1	1	1	0
63	IX	1	1	1	0
63	IZ	1	1	1	0
63	JB	1	1	1	0
63	JD	1	1	1	0
63	JF	1	1	1	0
63	JH	1	1	1	0
63	JJ	1	1	1	0
63	JL	1	1	1	0
63	JN	1	1	1	0
63	JP	1	1	1	0
63	JQ	1	1	1	0
63	JS	1	1	1	0
63	JU	1	1	1	0
63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

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

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
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	

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

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

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

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

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

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

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

MolProbity failed to run properly - this section is therefore empty.

### 3 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

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 4.6 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
64	GDP	GV	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
64	GDP	IE	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
62	GTP	ID	501	63	33,34,34	0.88	0	50,54,54	1.62	8 (16%)
62	GTP	JU	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	FC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
64	GDP	JC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.70	6 (13%)
64	GDP	BR	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.70	6 (13%)
64	GDP	GI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
62	GTP	CF	602	63	33,34,34	0.88	0	50,54,54	1.55	9 (18%)
64	GDP	GS	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	AS	602	63	33,34,34	0.84	0	50,54,54	1.58	8 (16%)
62	GTP	GE	501	63	33,34,34	0.89	0	50,54,54	1.59	8 (16%)
64	GDP	EW	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	6 (13%)
64	GDP	IR	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	JD	501	63	33,34,34	0.87	0	50,54,54	1.58	8 (16%)
62	GTP	CU	602	63	33,34,34	0.87	0	50,54,54	1.59	8 (16%)
62	GTP	IM	602	63	33,34,34	0.91	0	50,54,54	1.60	8 (16%)
62	GTP	CH	602	63	33,34,34	0.90	1 (3%)	50,54,54	1.58	8 (16%)
62	GTP	IG	501	63	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	GB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
64	GDP	IS	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	KP	501	63	33,34,34	0.89	2 (6%)	50,54,54	1.59	8 (16%)
64	GDP	AN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
62	GTP	BG	501	63	33,34,34	0.86	1 (3%)	50,54,54	1.56	8 (16%)
64	GDP	KT	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	5 (11%)
64	GDP	DV	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	KO	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	EZ	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.58	8 (16%)
62	GTP	HI	602	63	33,34,34	0.90	1 (3%)	50,54,54	1.60	8 (16%)
62	GTP	HT	501	63	33,34,34	0.89	0	50,54,54	1.58	8 (16%)
64	GDP	FA	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	KS	602	63	33,34,34	0.88	2 (6%)	50,54,54	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	GDP	HN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	5 (11%)
62	GTP	DA	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	IA	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
64	GDP	BN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
64	GDP	BY	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.76	7 (15%)
64	GDP	DF	501	-	29,30,30	0.50	0	45,47,47	0.49	0
62	GTP	HE	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.60	9 (18%)
62	GTP	GG	501	63	33,34,34	0.86	0	50,54,54	1.62	8 (16%)
64	GDP	JX	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	BB	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	6 (13%)
64	GDP	KV	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
64	GDP	HL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
62	GTP	BU	501	63	33,34,34	0.89	1 (3%)	50,54,54	1.58	8 (16%)
62	GTP	HG	602	63	33,34,34	0.89	1 (3%)	50,54,54	1.62	8 (16%)
62	GTP	FL	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.57	8 (16%)
62	GTP	AG	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.60	8 (16%)
62	GTP	BM	501	63	33,34,34	0.88	0	50,54,54	1.56	8 (16%)
62	GTP	JN	501	63	33,34,34	0.91	0	50,54,54	1.53	8 (16%)
62	GTP	EP	602	63	33,34,34	0.90	0	50,54,54	1.57	8 (16%)
62	GTP	KQ	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.61	8 (16%)
64	GDP	HH	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	6 (13%)
64	GDP	CE	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.69	6 (13%)
62	GTP	FU	602	63	33,34,34	0.89	2 (6%)	50,54,54	1.59	8 (16%)
64	GDP	BL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.69	6 (13%)
64	GDP	KM	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	LA	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.60	8 (16%)
62	GTP	FP	502	63	33,34,34	0.88	1 (3%)	50,54,54	1.56	8 (16%)
64	GDP	AR	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	BW	501	63	33,34,34	0.89	0	50,54,54	1.58	8 (16%)
62	GTP	GY	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	IU	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	GN	602	63	33,34,34	0.89	0	50,54,54	1.57	8 (16%)
64	GDP	EU	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
64	GDP	JR	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	FQ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	GDP	JK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	6 (13%)
62	GTP	EB	501	63	33,34,34	0.87	0	50,54,54	1.56	8 (16%)
62	GTP	IX	501	63	33,34,34	0.87	0	50,54,54	1.59	8 (16%)
62	GTP	HC	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	EQ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
62	GTP	KY	602	63	33,34,34	0.85	1 (3%)	50,54,54	1.60	8 (16%)
62	GTP	FT	602	63	33,34,34	0.87	1 (3%)	50,54,54	1.59	8 (16%)
62	GTP	IK	602	63	33,34,34	0.88	0	50,54,54	1.63	8 (16%)
62	GTP	KL	602	63	33,34,34	0.87	0	50,54,54	1.58	8 (16%)
64	GDP	IP	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	DE	501	63	33,34,34	0.87	2 (6%)	50,54,54	1.64	8 (16%)
62	GTP	GA	501	63	33,34,34	0.89	0	50,54,54	1.62	8 (16%)
64	GDP	DD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
62	GTP	AI	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
64	GDP	HY	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.74	5 (11%)
62	GTP	HX	501	63	33,34,34	0.89	1 (3%)	50,54,54	1.60	8 (16%)
62	GTP	BI	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.58	8 (16%)
64	GDP	EA	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.70	6 (13%)
64	GDP	KX	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	KK	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
64	GDP	DB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	5 (11%)
64	GDP	FE	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	KA	602	63	33,34,34	0.87	2 (6%)	50,54,54	1.59	8 (16%)
62	GTP	HO	501	63	33,34,34	0.91	2 (6%)	50,54,54	1.64	10 (20%)
62	GTP	ET	602	63	33,34,34	0.89	0	50,54,54	1.58	8 (16%)
64	GDP	DT	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	KW	602	63	33,34,34	0.87	1 (3%)	50,54,54	1.60	8 (16%)
64	GDP	DR	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	DI	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.60	8 (16%)
62	GTP	JH	501	63	33,34,34	0.87	0	50,54,54	1.58	8 (16%)
64	GDP	BP	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	DK	501	63	33,34,34	0.89	1 (3%)	50,54,54	1.60	8 (16%)
62	GTP	JF	501	63	33,34,34	0.87	0	50,54,54	1.53	8 (16%)
64	GDP	IF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	CD	501	63	33,34,34	0.92	1 (3%)	50,54,54	1.57	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	GDP	AF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
64	GDP	FO	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	AB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	5 (11%)
62	GTP	DU	602	63	33,34,34	0.89	2 (6%)	50,54,54	1.59	8 (16%)
64	GDP	KI	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
64	GDP	FG	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
62	GTP	HK	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
62	GTP	FF	501	63	33,34,34	0.87	0	50,54,54	1.57	8 (16%)
64	GDP	JO	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	FY	602	63	33,34,34	0.89	1 (3%)	50,54,54	1.61	8 (16%)
64	GDP	CZ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
64	GDP	IN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	GT	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.54	8 (16%)
62	GTP	JY	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	HJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	5 (11%)
62	GTP	AC	501	63	33,34,34	0.87	0	50,54,54	1.59	8 (16%)
62	GTP	BE	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.57	8 (16%)
62	GTP	JW	602	63	33,34,34	0.87	2 (6%)	50,54,54	1.60	8 (16%)
64	GDP	CL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)
62	GTP	CQ	602	63	33,34,34	0.88	2 (6%)	50,54,54	1.61	8 (16%)
64	GDP	EI	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
64	GDP	IC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
62	GTP	GP	501	63	33,34,34	0.89	1 (3%)	50,54,54	1.57	8 (16%)
62	GTP	IB	602	63	33,34,34	0.88	0	50,54,54	1.57	8 (16%)
62	GTP	CM	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.57	8 (16%)
64	GDP	AX	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
64	GDP	FX	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	KE	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
64	GDP	BV	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	KH	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	CX	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
62	GTP	IV	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.55	8 (16%)
64	GDP	GZ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
64	GDP	AP	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
64	GDP	BH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	GDP	JE	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	6 (13%)
64	GDP	IW	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	GC	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
62	GTP	GJ	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.56	8 (16%)
62	GTP	AU	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
64	GDP	BF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
64	GDP	BJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
64	GDP	CG	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	FD	602	63	33,34,34	0.88	0	50,54,54	1.55	8 (16%)
62	GTP	DS	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.57	8 (16%)
62	GTP	HZ	501	63	33,34,34	0.89	0	50,54,54	1.59	8 (16%)
64	GDP	CV	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)
64	GDP	EY	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
64	GDP	HF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	HU	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	JQ	501	63	33,34,34	0.88	2 (6%)	50,54,54	1.61	8 (16%)
64	GDP	CC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	FB	502	63	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	LB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	6 (13%)
62	GTP	JL	602	63	33,34,34	0.86	0	50,54,54	1.53	8 (16%)
64	GDP	HW	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	CR	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	6 (13%)
64	GDP	CN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	5 (11%)
62	GTP	GR	501	63	33,34,34	0.89	1 (3%)	50,54,54	1.56	8 (16%)
64	GDP	CA	602	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
64	GDP	IY	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	6 (13%)
62	GTP	DC	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
64	GDP	EM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
64	GDP	ES	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.70	6 (13%)
64	GDP	DL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	DM	602	63	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	KZ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	JZ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	AE	602	63	33,34,34	0.89	2 (6%)	50,54,54	1.61	8 (16%)
62	GTP	DZ	602	63	33,34,34	0.87	0	50,54,54	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	GTP	KD	501	63	33,34,34	0.86	2 (6%)	50,54,54	1.60	9 (18%)
64	GDP	DN	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	6 (13%)
64	GDP	CI	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.77	6 (13%)
64	GDP	HR	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	7 (15%)
62	GTP	AQ	501	63	33,34,34	0.86	1 (3%)	50,54,54	1.60	10 (20%)
64	GDP	EG	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	EX	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
62	GTP	GU	501	63	33,34,34	0.88	2 (6%)	50,54,54	1.61	8 (16%)
62	GTP	IQ	501	63	33,34,34	0.91	1 (3%)	50,54,54	1.63	8 (16%)
62	GTP	JP	501	63	33,34,34	0.86	1 (3%)	50,54,54	1.56	8 (16%)
64	GDP	IH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	6 (13%)
64	GDP	JI	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.70	6 (13%)
64	GDP	CP	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	5 (11%)
62	GTP	DO	602	63	33,34,34	0.89	1 (3%)	50,54,54	1.59	8 (16%)
62	GTP	FR	502	63	33,34,34	0.87	1 (3%)	50,54,54	1.57	8 (16%)
62	GTP	GW	501	63	33,34,34	0.86	1 (3%)	50,54,54	1.58	8 (16%)
62	GTP	EJ	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.57	8 (16%)
64	GDP	FI	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
62	GTP	AA	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.61	8 (16%)
64	GDP	JG	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
64	GDP	HS	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	5 (11%)
62	GTP	CS	501	63	33,34,34	0.89	0	50,54,54	1.59	8 (16%)
62	GTP	IO	501	63	33,34,34	0.91	0	50,54,54	1.59	8 (16%)
62	GTP	DQ	501	63	33,34,34	0.87	2 (6%)	50,54,54	1.59	8 (16%)
64	GDP	GO	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	CY	501	63	33,34,34	0.86	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	GX	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
64	GDP	AH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	EL	602	63	33,34,34	0.88	0	50,54,54	1.56	8 (16%)
64	GDP	KR	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
62	GTP	KJ	602	63	33,34,34	0.89	2 (6%)	50,54,54	1.61	8 (16%)
64	GDP	AL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	AM	602	63	33,34,34	0.85	2 (6%)	50,54,54	1.60	8 (16%)
64	GDP	AJ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	BK	602	63	33,34,34	0.89	0	50,54,54	1.55	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	GDP	EO	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	6 (13%)
62	GTP	BQ	602	63	33,34,34	0.86	0	50,54,54	1.55	9 (18%)
62	GTP	BA	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.57	8 (16%)
62	GTP	FN	502	63	33,34,34	0.88	1 (3%)	50,54,54	1.56	8 (16%)
64	GDP	DJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	HM	501	63	33,34,34	0.87	0	50,54,54	1.59	8 (16%)
64	GDP	HD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
64	GDP	EK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	AY	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.55	8 (16%)
64	GDP	JM	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.71	6 (13%)
64	GDP	EC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.71	6 (13%)
64	GDP	DW	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.71	6 (13%)
64	GDP	FM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	IT	602	63	33,34,34	0.88	0	50,54,54	1.54	8 (16%)
62	GTP	JJ	501	63	33,34,34	0.89	1 (3%)	50,54,54	1.55	8 (16%)
64	GDP	DH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
64	GDP	FK	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	EV	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.57	8 (16%)
62	GTP	FJ	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
62	GTP	ED	602	63	33,34,34	0.86	0	50,54,54	1.55	8 (16%)
64	GDP	EE	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.71	6 (13%)
64	GDP	GM	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	7 (15%)
64	GDP	DP	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	FS	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	FW	501	63	33,34,34	0.90	0	50,54,54	1.59	8 (16%)
62	GTP	KC	602	63	33,34,34	0.92	2 (6%)	50,54,54	1.62	8 (16%)
62	GTP	EH	501	63	33,34,34	0.86	0	50,54,54	1.56	8 (16%)
64	GDP	BT	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.70	6 (13%)
64	GDP	FZ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
62	GTP	BZ	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.59	8 (16%)
64	GDP	GK	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	AW	501	63	33,34,34	0.87	2 (6%)	50,54,54	1.56	8 (16%)
62	GTP	EF	602	63	33,34,34	0.86	0	50,54,54	1.54	8 (16%)
62	GTP	II	501	63	33,34,34	0.90	0	50,54,54	1.58	8 (16%)
62	GTP	JB	501	63	33,34,34	0.89	0	50,54,54	1.57	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	GDP	DY	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	HQ	501	63	33,34,34	0.86	1 (3%)	50,54,54	1.61	8 (16%)
64	GDP	KG	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	FH	501	63	33,34,34	0.86	0	50,54,54	1.57	8 (16%)
62	GTP	CO	501	63	33,34,34	0.86	0	50,54,54	1.58	8 (16%)
64	GDP	JT	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
64	GDP	HB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
62	GTP	CJ	501	63	33,34,34	0.89	0	50,54,54	1.62	8 (16%)
62	GTP	KN	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
64	GDP	AT	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
64	GDP	AZ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.70	6 (13%)
64	GDP	KB	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	KF	501	63	33,34,34	0.86	1 (3%)	50,54,54	1.59	8 (16%)
62	GTP	BC	501	63	33,34,34	0.87	1 (3%)	50,54,54	1.57	8 (16%)
62	GTP	CB	501	63	33,34,34	0.87	0	50,54,54	1.57	8 (16%)
62	GTP	DG	602	63	33,34,34	0.89	1 (3%)	50,54,54	1.62	9 (18%)
64	GDP	HP	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.80	8 (17%)
64	GDP	IL	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.77	7 (15%)
62	GTP	AO	501	63	33,34,34	0.88	2 (6%)	50,54,54	1.59	8 (16%)
64	GDP	IJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	AK	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
62	GTP	BS	501	63	33,34,34	0.87	0	50,54,54	1.56	8 (16%)
64	GDP	BD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	AD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
64	GDP	AV	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
62	GTP	IZ	602	63	33,34,34	0.89	0	50,54,54	1.56	8 (16%)
62	GTP	ER	602	63	33,34,34	0.89	1 (3%)	50,54,54	1.57	8 (16%)
62	GTP	HV	501	63	33,34,34	0.90	0	50,54,54	1.58	8 (16%)
62	GTP	CW	602	63	33,34,34	0.89	1 (3%)	50,54,54	1.58	8 (16%)
64	GDP	FV	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.73	6 (13%)
62	GTP	KU	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
62	GTP	EN	602	63	33,34,34	0.88	0	50,54,54	1.55	8 (16%)
64	GDP	GF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
64	GDP	GQ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	HA	501	63	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
64	GDP	JA	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
62	GTP	DX	501	63	33,34,34	0.86	0	50,54,54	1.56	8 (16%)
64	GDP	JV	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
62	GTP	BO	501	63	33,34,34	0.87	0	50,54,54	1.55	8 (16%)
64	GDP	GD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
64	GDP	CT	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	5 (11%)
62	GTP	JS	602	63	33,34,34	0.53	0	50,54,54	0.56	0
62	GTP	GL	501	63	33,34,34	0.86	1 (3%)	50,54,54	1.55	8 (16%)
62	GTP	BX	501	63	33,34,34	0.88	1 (3%)	50,54,54	1.61	8 (16%)
62	GTP	GH	602	63	33,34,34	0.88	1 (3%)	50,54,54	1.56	8 (16%)

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
64	GDP	GV	501	-	-	2/16/32/32	0/3/3/3
64	GDP	IE	501	-	-	2/16/32/32	0/3/3/3
62	GTP	ID	501	63	-	5/22/38/38	0/3/3/3
62	GTP	JU	602	63	-	5/22/38/38	0/3/3/3
64	GDP	FC	501	-	-	2/16/32/32	0/3/3/3
64	GDP	JC	501	-	-	2/16/32/32	0/3/3/3
64	GDP	BR	501	-	-	2/16/32/32	0/3/3/3
64	GDP	GI	501	-	-	2/16/32/32	0/3/3/3
62	GTP	CF	602	63	-	5/22/38/38	0/3/3/3
64	GDP	GS	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AS	602	63	-	5/22/38/38	0/3/3/3
62	GTP	GE	501	63	-	5/22/38/38	0/3/3/3
64	GDP	EW	501	-	-	2/16/32/32	0/3/3/3
64	GDP	IR	501	-	-	2/16/32/32	0/3/3/3
62	GTP	JD	501	63	-	5/22/38/38	0/3/3/3
62	GTP	CU	602	63	-	5/22/38/38	0/3/3/3
62	GTP	IM	602	63	-	5/22/38/38	0/3/3/3
62	GTP	CH	602	63	-	5/22/38/38	0/3/3/3
62	GTP	IG	501	63	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	GDP	GB	501	-	-	2/16/32/32	0/3/3/3
64	GDP	IS	501	-	-	2/16/32/32	0/3/3/3
62	GTP	KP	501	63	-	5/22/38/38	0/3/3/3
64	GDP	AN	501	-	-	2/16/32/32	0/3/3/3
62	GTP	BG	501	63	-	5/22/38/38	0/3/3/3
64	GDP	KT	501	-	-	2/16/32/32	0/3/3/3
64	GDP	DV	501	-	-	2/16/32/32	0/3/3/3
64	GDP	KO	501	-	-	2/16/32/32	0/3/3/3
62	GTP	EZ	501	63	-	5/22/38/38	0/3/3/3
62	GTP	HI	602	63	-	5/22/38/38	0/3/3/3
62	GTP	HT	501	63	-	5/22/38/38	0/3/3/3
64	GDP	FA	501	-	-	2/16/32/32	0/3/3/3
62	GTP	KS	602	63	-	5/22/38/38	0/3/3/3
64	GDP	HN	501	-	-	2/16/32/32	0/3/3/3
62	GTP	DA	501	63	-	5/22/38/38	0/3/3/3
64	GDP	IA	501	-	-	2/16/32/32	0/3/3/3
64	GDP	BN	501	-	-	2/16/32/32	0/3/3/3
64	GDP	BY	501	-	-	2/16/32/32	0/3/3/3
64	GDP	DF	501	-	-	3/16/32/32	0/3/3/3
62	GTP	HE	501	63	-	5/22/38/38	0/3/3/3
62	GTP	GG	501	63	-	5/22/38/38	0/3/3/3
64	GDP	JX	501	-	-	2/16/32/32	0/3/3/3
64	GDP	BB	501	-	-	2/16/32/32	0/3/3/3
64	GDP	KV	501	-	-	2/16/32/32	0/3/3/3
64	GDP	HL	501	-	-	2/16/32/32	0/3/3/3
62	GTP	BU	501	63	-	5/22/38/38	0/3/3/3
62	GTP	HG	602	63	-	5/22/38/38	0/3/3/3
62	GTP	FL	501	63	-	5/22/38/38	0/3/3/3
62	GTP	AG	501	63	-	5/22/38/38	0/3/3/3
62	GTP	BM	501	63	-	5/22/38/38	0/3/3/3
62	GTP	JN	501	63	-	5/22/38/38	0/3/3/3
62	GTP	EP	602	63	-	5/22/38/38	0/3/3/3
62	GTP	KQ	602	63	-	5/22/38/38	0/3/3/3
64	GDP	HH	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	GDP	CE	501	-	-	2/16/32/32	0/3/3/3
62	GTP	FU	602	63	-	5/22/38/38	0/3/3/3
64	GDP	BL	501	-	-	2/16/32/32	0/3/3/3
64	GDP	KM	501	-	-	2/16/32/32	0/3/3/3
62	GTP	LA	501	63	-	5/22/38/38	0/3/3/3
62	GTP	FP	502	63	-	5/22/38/38	0/3/3/3
64	GDP	AR	501	-	-	2/16/32/32	0/3/3/3
62	GTP	BW	501	63	-	5/22/38/38	0/3/3/3
62	GTP	GY	501	63	-	5/22/38/38	0/3/3/3
64	GDP	IU	501	-	-	2/16/32/32	0/3/3/3
62	GTP	GN	602	63	-	5/22/38/38	0/3/3/3
64	GDP	EU	501	-	-	2/16/32/32	0/3/3/3
64	GDP	JR	501	-	-	2/16/32/32	0/3/3/3
64	GDP	FQ	501	-	-	2/16/32/32	0/3/3/3
64	GDP	JK	501	-	-	2/16/32/32	0/3/3/3
62	GTP	EB	501	63	-	5/22/38/38	0/3/3/3
62	GTP	IX	501	63	-	5/22/38/38	0/3/3/3
62	GTP	HC	602	63	-	5/22/38/38	0/3/3/3
64	GDP	EQ	501	-	-	2/16/32/32	0/3/3/3
62	GTP	KY	602	63	-	5/22/38/38	0/3/3/3
62	GTP	FT	602	63	-	5/22/38/38	0/3/3/3
62	GTP	IK	602	63	-	5/22/38/38	0/3/3/3
62	GTP	KL	602	63	-	5/22/38/38	0/3/3/3
64	GDP	IP	501	-	-	2/16/32/32	0/3/3/3
62	GTP	DE	501	63	-	5/22/38/38	0/3/3/3
62	GTP	GA	501	63	-	5/22/38/38	0/3/3/3
64	GDP	DD	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AI	501	63	-	5/22/38/38	0/3/3/3
64	GDP	HY	501	-	-	2/16/32/32	0/3/3/3
62	GTP	HX	501	63	-	5/22/38/38	0/3/3/3
62	GTP	BI	501	63	-	5/22/38/38	0/3/3/3
64	GDP	EA	501	-	-	2/16/32/32	0/3/3/3
64	GDP	KX	501	-	-	2/16/32/32	0/3/3/3
64	GDP	KK	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	GDP	DB	501	-	-	2/16/32/32	0/3/3/3
64	GDP	FE	501	-	-	2/16/32/32	0/3/3/3
62	GTP	KA	602	63	-	5/22/38/38	0/3/3/3
62	GTP	HO	501	63	-	5/22/38/38	0/3/3/3
62	GTP	ET	602	63	-	5/22/38/38	0/3/3/3
64	GDP	DT	501	-	-	2/16/32/32	0/3/3/3
62	GTP	KW	602	63	-	5/22/38/38	0/3/3/3
64	GDP	DR	501	-	-	2/16/32/32	0/3/3/3
62	GTP	DI	602	63	-	5/22/38/38	0/3/3/3
62	GTP	JH	501	63	-	5/22/38/38	0/3/3/3
64	GDP	BP	501	-	-	2/16/32/32	0/3/3/3
62	GTP	DK	501	63	-	5/22/38/38	0/3/3/3
62	GTP	JF	501	63	-	5/22/38/38	0/3/3/3
64	GDP	IF	501	-	-	2/16/32/32	0/3/3/3
62	GTP	CD	501	63	-	5/22/38/38	0/3/3/3
64	GDP	AF	501	-	-	2/16/32/32	0/3/3/3
64	GDP	FO	501	-	-	2/16/32/32	0/3/3/3
64	GDP	AB	501	-	-	2/16/32/32	0/3/3/3
62	GTP	DU	602	63	-	5/22/38/38	0/3/3/3
64	GDP	KI	501	-	-	2/16/32/32	0/3/3/3
64	GDP	FG	501	-	-	2/16/32/32	0/3/3/3
62	GTP	HK	501	63	-	5/22/38/38	0/3/3/3
62	GTP	FF	501	63	-	5/22/38/38	0/3/3/3
64	GDP	JO	501	-	-	2/16/32/32	0/3/3/3
62	GTP	FY	602	63	-	5/22/38/38	0/3/3/3
64	GDP	CZ	501	-	-	2/16/32/32	0/3/3/3
64	GDP	IN	501	-	-	2/16/32/32	0/3/3/3
62	GTP	GT	501	63	-	5/22/38/38	0/3/3/3
62	GTP	JY	602	63	-	5/22/38/38	0/3/3/3
64	GDP	HJ	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AC	501	63	-	5/22/38/38	0/3/3/3
62	GTP	BE	501	63	-	5/22/38/38	0/3/3/3
62	GTP	JW	602	63	-	5/22/38/38	0/3/3/3
64	GDP	CL	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GTP	CQ	602	63	-	5/22/38/38	0/3/3/3
64	GDP	EI	501	-	-	2/16/32/32	0/3/3/3
64	GDP	IC	501	-	-	2/16/32/32	0/3/3/3
62	GTP	GP	501	63	-	5/22/38/38	0/3/3/3
62	GTP	IB	602	63	-	5/22/38/38	0/3/3/3
62	GTP	CM	602	63	-	5/22/38/38	0/3/3/3
64	GDP	AX	501	-	-	2/16/32/32	0/3/3/3
64	GDP	FX	501	-	-	2/16/32/32	0/3/3/3
64	GDP	KE	501	-	-	2/16/32/32	0/3/3/3
64	GDP	BV	501	-	-	2/16/32/32	0/3/3/3
62	GTP	KH	501	63	-	5/22/38/38	0/3/3/3
64	GDP	CX	501	-	-	2/16/32/32	0/3/3/3
62	GTP	IV	602	63	-	5/22/38/38	0/3/3/3
64	GDP	GZ	501	-	-	2/16/32/32	0/3/3/3
64	GDP	AP	501	-	-	2/16/32/32	0/3/3/3
64	GDP	BH	501	-	-	2/16/32/32	0/3/3/3
64	GDP	JE	501	-	-	2/16/32/32	0/3/3/3
64	GDP	IW	501	-	-	2/16/32/32	0/3/3/3
62	GTP	GC	501	63	-	5/22/38/38	0/3/3/3
62	GTP	GJ	501	63	-	5/22/38/38	0/3/3/3
62	GTP	AU	501	63	-	5/22/38/38	0/3/3/3
64	GDP	BF	501	-	-	2/16/32/32	0/3/3/3
64	GDP	BJ	501	-	-	2/16/32/32	0/3/3/3
64	GDP	CG	501	-	-	2/16/32/32	0/3/3/3
62	GTP	FD	602	63	-	5/22/38/38	0/3/3/3
62	GTP	DS	501	63	-	5/22/38/38	0/3/3/3
62	GTP	HZ	501	63	-	5/22/38/38	0/3/3/3
64	GDP	CV	501	-	-	2/16/32/32	0/3/3/3
64	GDP	EY	501	-	-	2/16/32/32	0/3/3/3
64	GDP	HF	501	-	-	2/16/32/32	0/3/3/3
64	GDP	HU	501	-	-	2/16/32/32	0/3/3/3
62	GTP	JQ	501	63	-	5/22/38/38	0/3/3/3
64	GDP	CC	501	-	-	2/16/32/32	0/3/3/3
62	GTP	FB	502	63	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	GDP	LB	501	-	-	2/16/32/32	0/3/3/3
62	GTP	JL	602	63	-	5/22/38/38	0/3/3/3
64	GDP	HW	501	-	-	2/16/32/32	0/3/3/3
64	GDP	CR	501	-	-	2/16/32/32	0/3/3/3
64	GDP	CN	501	-	-	2/16/32/32	0/3/3/3
62	GTP	GR	501	63	-	5/22/38/38	0/3/3/3
64	GDP	CA	602	-	-	2/16/32/32	0/3/3/3
64	GDP	IY	501	-	-	2/16/32/32	0/3/3/3
62	GTP	DC	602	63	-	5/22/38/38	0/3/3/3
64	GDP	EM	501	-	-	2/16/32/32	0/3/3/3
64	GDP	ES	501	-	-	2/16/32/32	0/3/3/3
64	GDP	DL	501	-	-	2/16/32/32	0/3/3/3
62	GTP	DM	602	63	-	5/22/38/38	0/3/3/3
64	GDP	KZ	501	-	-	2/16/32/32	0/3/3/3
64	GDP	JZ	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AE	602	63	-	5/22/38/38	0/3/3/3
62	GTP	DZ	602	63	-	5/22/38/38	0/3/3/3
62	GTP	KD	501	63	-	5/22/38/38	0/3/3/3
64	GDP	DN	501	-	-	2/16/32/32	0/3/3/3
64	GDP	CI	501	-	-	2/16/32/32	0/3/3/3
64	GDP	HR	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AQ	501	63	-	5/22/38/38	0/3/3/3
64	GDP	EG	501	-	-	2/16/32/32	0/3/3/3
62	GTP	EX	602	63	-	5/22/38/38	0/3/3/3
62	GTP	GU	501	63	-	5/22/38/38	0/3/3/3
62	GTP	IQ	501	63	-	5/22/38/38	0/3/3/3
62	GTP	JP	501	63	-	5/22/38/38	0/3/3/3
64	GDP	IH	501	-	-	2/16/32/32	0/3/3/3
64	GDP	JI	501	-	-	2/16/32/32	0/3/3/3
64	GDP	CP	501	-	-	2/16/32/32	0/3/3/3
62	GTP	DO	602	63	-	5/22/38/38	0/3/3/3
62	GTP	FR	502	63	-	5/22/38/38	0/3/3/3
62	GTP	GW	501	63	-	5/22/38/38	0/3/3/3
62	GTP	EJ	602	63	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	GDP	FI	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AA	501	63	-	5/22/38/38	0/3/3/3
64	GDP	JG	501	-	-	2/16/32/32	0/3/3/3
64	GDP	HS	501	-	-	2/16/32/32	0/3/3/3
62	GTP	CS	501	63	-	5/22/38/38	0/3/3/3
62	GTP	IO	501	63	-	5/22/38/38	0/3/3/3
62	GTP	DQ	501	63	-	5/22/38/38	0/3/3/3
64	GDP	GO	501	-	-	2/16/32/32	0/3/3/3
62	GTP	CY	501	63	-	5/22/38/38	0/3/3/3
64	GDP	GX	501	-	-	2/16/32/32	0/3/3/3
64	GDP	AH	501	-	-	2/16/32/32	0/3/3/3
62	GTP	EL	602	63	-	5/22/38/38	0/3/3/3
64	GDP	KR	501	-	-	2/16/32/32	0/3/3/3
62	GTP	KJ	602	63	-	5/22/38/38	0/3/3/3
64	GDP	AL	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AM	602	63	-	5/22/38/38	0/3/3/3
64	GDP	AJ	501	-	-	2/16/32/32	0/3/3/3
62	GTP	BK	602	63	-	5/22/38/38	0/3/3/3
64	GDP	EO	501	-	-	2/16/32/32	0/3/3/3
62	GTP	BQ	602	63	-	5/22/38/38	0/3/3/3
62	GTP	BA	501	63	-	5/22/38/38	0/3/3/3
62	GTP	FN	502	63	-	5/22/38/38	0/3/3/3
64	GDP	DJ	501	-	-	2/16/32/32	0/3/3/3
62	GTP	HM	501	63	-	5/22/38/38	0/3/3/3
64	GDP	HD	501	-	-	2/16/32/32	0/3/3/3
64	GDP	EK	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AY	602	63	-	5/22/38/38	0/3/3/3
64	GDP	JM	501	-	-	2/16/32/32	0/3/3/3
64	GDP	EC	501	-	-	2/16/32/32	0/3/3/3
64	GDP	DW	501	-	-	2/16/32/32	0/3/3/3
64	GDP	FM	501	-	-	2/16/32/32	0/3/3/3
62	GTP	IT	602	63	-	5/22/38/38	0/3/3/3
62	GTP	JJ	501	63	-	5/22/38/38	0/3/3/3
64	GDP	DH	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	GDP	FK	501	-	-	2/16/32/32	0/3/3/3
62	GTP	EV	501	63	-	5/22/38/38	0/3/3/3
62	GTP	FJ	602	63	-	5/22/38/38	0/3/3/3
62	GTP	ED	602	63	-	5/22/38/38	0/3/3/3
64	GDP	EE	501	-	-	2/16/32/32	0/3/3/3
64	GDP	GM	501	-	-	2/16/32/32	0/3/3/3
64	GDP	DP	501	-	-	2/16/32/32	0/3/3/3
64	GDP	FS	501	-	-	2/16/32/32	0/3/3/3
62	GTP	FW	501	63	-	5/22/38/38	0/3/3/3
62	GTP	KC	602	63	-	5/22/38/38	0/3/3/3
62	GTP	EH	501	63	-	5/22/38/38	0/3/3/3
64	GDP	BT	501	-	-	2/16/32/32	0/3/3/3
64	GDP	FZ	501	-	-	2/16/32/32	0/3/3/3
62	GTP	BZ	501	63	-	5/22/38/38	0/3/3/3
64	GDP	GK	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AW	501	63	-	5/22/38/38	0/3/3/3
62	GTP	EF	602	63	-	5/22/38/38	0/3/3/3
62	GTP	II	501	63	-	5/22/38/38	0/3/3/3
62	GTP	JB	501	63	-	5/22/38/38	0/3/3/3
64	GDP	DY	501	-	-	2/16/32/32	0/3/3/3
62	GTP	HQ	501	63	-	5/22/38/38	0/3/3/3
64	GDP	KG	501	-	-	2/16/32/32	0/3/3/3
62	GTP	FH	501	63	-	5/22/38/38	0/3/3/3
62	GTP	CO	501	63	-	5/22/38/38	0/3/3/3
64	GDP	JT	501	-	-	2/16/32/32	0/3/3/3
64	GDP	HB	501	-	-	2/16/32/32	0/3/3/3
62	GTP	CJ	501	63	-	5/22/38/38	0/3/3/3
62	GTP	KN	501	63	-	5/22/38/38	0/3/3/3
64	GDP	AT	501	-	-	2/16/32/32	0/3/3/3
64	GDP	AZ	501	-	-	2/16/32/32	0/3/3/3
64	GDP	KB	501	-	-	2/16/32/32	0/3/3/3
62	GTP	KF	501	63	-	5/22/38/38	0/3/3/3
62	GTP	BC	501	63	-	5/22/38/38	0/3/3/3
62	GTP	CB	501	63	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	GTP	DG	602	63	-	5/22/38/38	0/3/3/3
64	GDP	HP	501	-	-	2/16/32/32	0/3/3/3
64	GDP	IL	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AO	501	63	-	5/22/38/38	0/3/3/3
64	GDP	IJ	501	-	-	2/16/32/32	0/3/3/3
62	GTP	AK	602	63	-	5/22/38/38	0/3/3/3
62	GTP	BS	501	63	-	5/22/38/38	0/3/3/3
64	GDP	BD	501	-	-	2/16/32/32	0/3/3/3
64	GDP	AD	501	-	-	2/16/32/32	0/3/3/3
64	GDP	AV	501	-	-	2/16/32/32	0/3/3/3
62	GTP	IZ	602	63	-	5/22/38/38	0/3/3/3
62	GTP	ER	602	63	-	5/22/38/38	0/3/3/3
62	GTP	HV	501	63	-	5/22/38/38	0/3/3/3
62	GTP	CW	602	63	-	5/22/38/38	0/3/3/3
64	GDP	FV	501	-	-	2/16/32/32	0/3/3/3
62	GTP	KU	501	63	-	5/22/38/38	0/3/3/3
62	GTP	EN	602	63	-	5/22/38/38	0/3/3/3
64	GDP	GF	501	-	-	2/16/32/32	0/3/3/3
64	GDP	GQ	501	-	-	2/16/32/32	0/3/3/3
62	GTP	HA	501	63	-	5/22/38/38	0/3/3/3
64	GDP	JA	501	-	-	2/16/32/32	0/3/3/3
62	GTP	DX	501	63	-	5/22/38/38	0/3/3/3
64	GDP	JV	501	-	-	2/16/32/32	0/3/3/3
62	GTP	BO	501	63	-	5/22/38/38	0/3/3/3
64	GDP	GD	501	-	-	2/16/32/32	0/3/3/3
64	GDP	CT	501	-	-	2/16/32/32	0/3/3/3
62	GTP	JS	602	63	-	5/22/38/38	0/3/3/3
62	GTP	GL	501	63	-	5/22/38/38	0/3/3/3
62	GTP	BX	501	63	-	5/22/38/38	0/3/3/3
62	GTP	GH	602	63	-	5/22/38/38	0/3/3/3

The worst 5 of 534 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	DL	501	GDP	C5-C4	3.03	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	GK	501	GDP	C5-C4	3.03	1.47	1.38
64	AV	501	GDP	C5-C4	3.02	1.47	1.38
64	HP	501	GDP	C5-C4	3.00	1.47	1.38
64	IL	501	GDP	C5-C4	2.99	1.47	1.38

The worst 5 of 2014 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	CI	501	GDP	C5-C4-N3	-6.53	118.00	128.39
64	HP	501	GDP	C5-C4-N3	-6.43	118.15	128.39
64	IL	501	GDP	C5-C4-N3	-6.41	118.19	128.39
64	BY	501	GDP	C5-C4-N3	-6.38	118.23	128.39
64	IP	501	GDP	C5-C4-N3	-6.37	118.25	128.39

There are no chirality outliers.

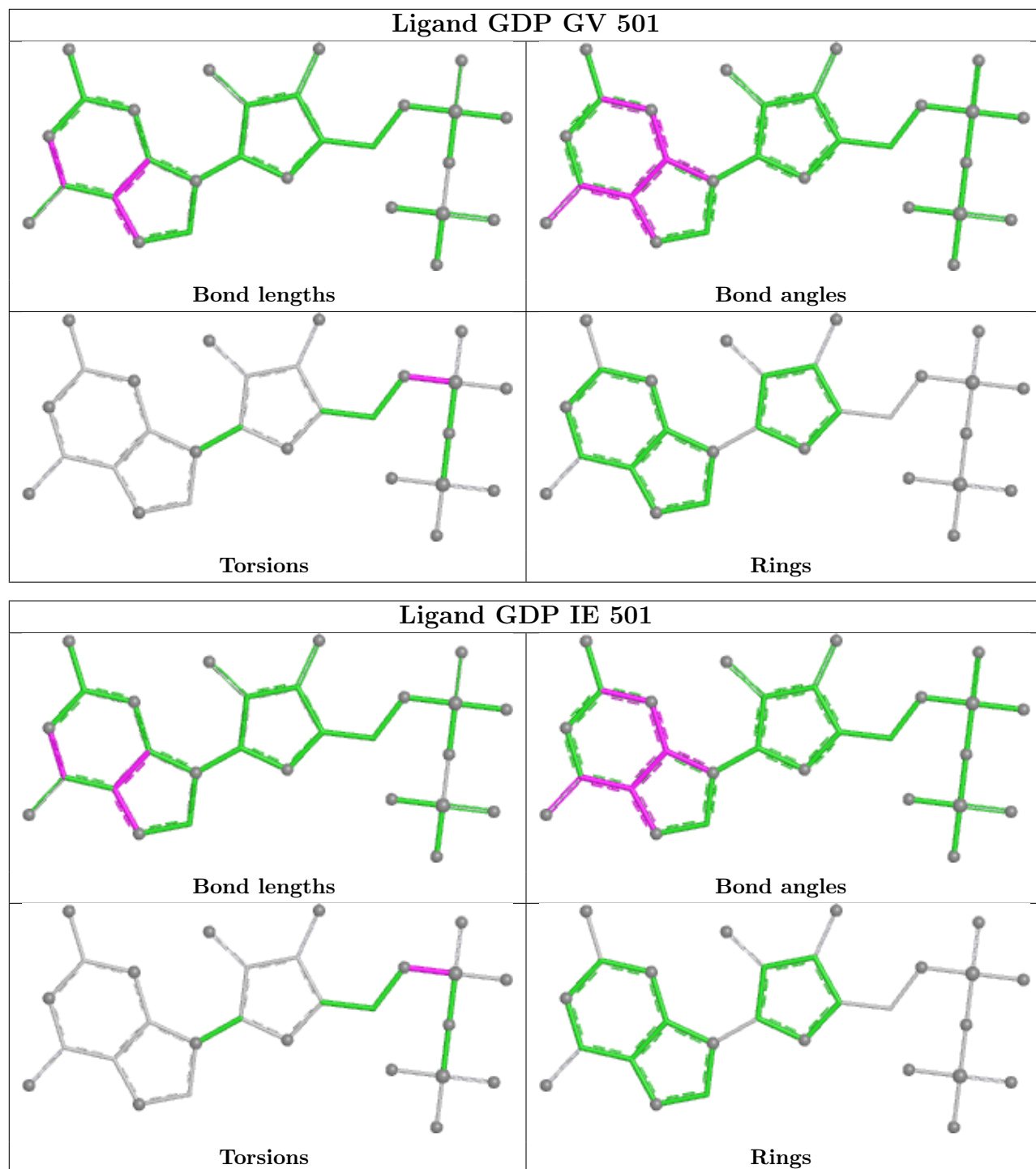
5 of 1010 torsion outliers are listed below:

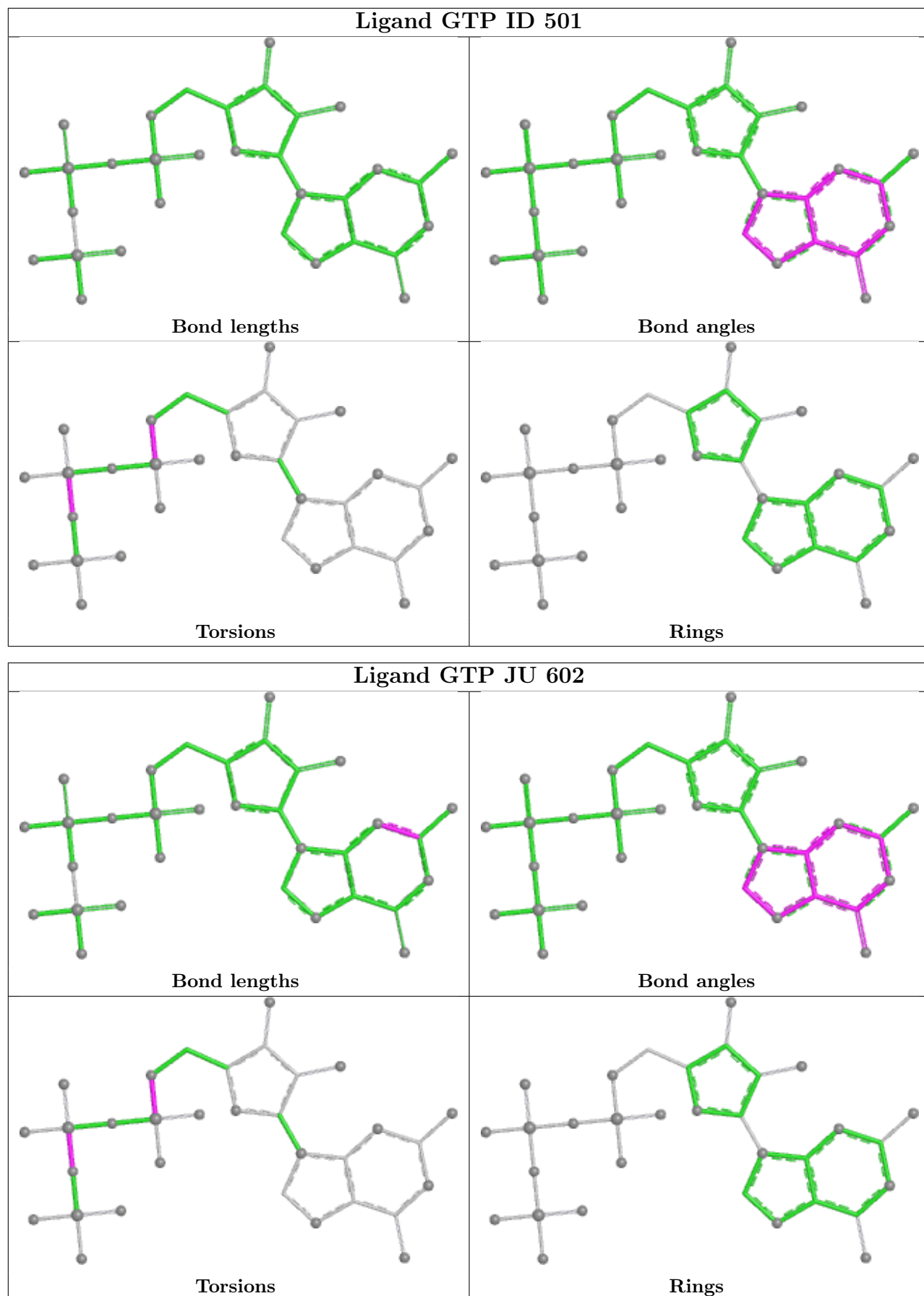
Mol	Chain	Res	Type	Atoms
62	AA	501	GTP	C5'-O5'-PA-O3A
62	AA	501	GTP	C5'-O5'-PA-O1A
62	AA	501	GTP	C5'-O5'-PA-O2A
62	AC	501	GTP	C5'-O5'-PA-O3A
62	AC	501	GTP	C5'-O5'-PA-O1A

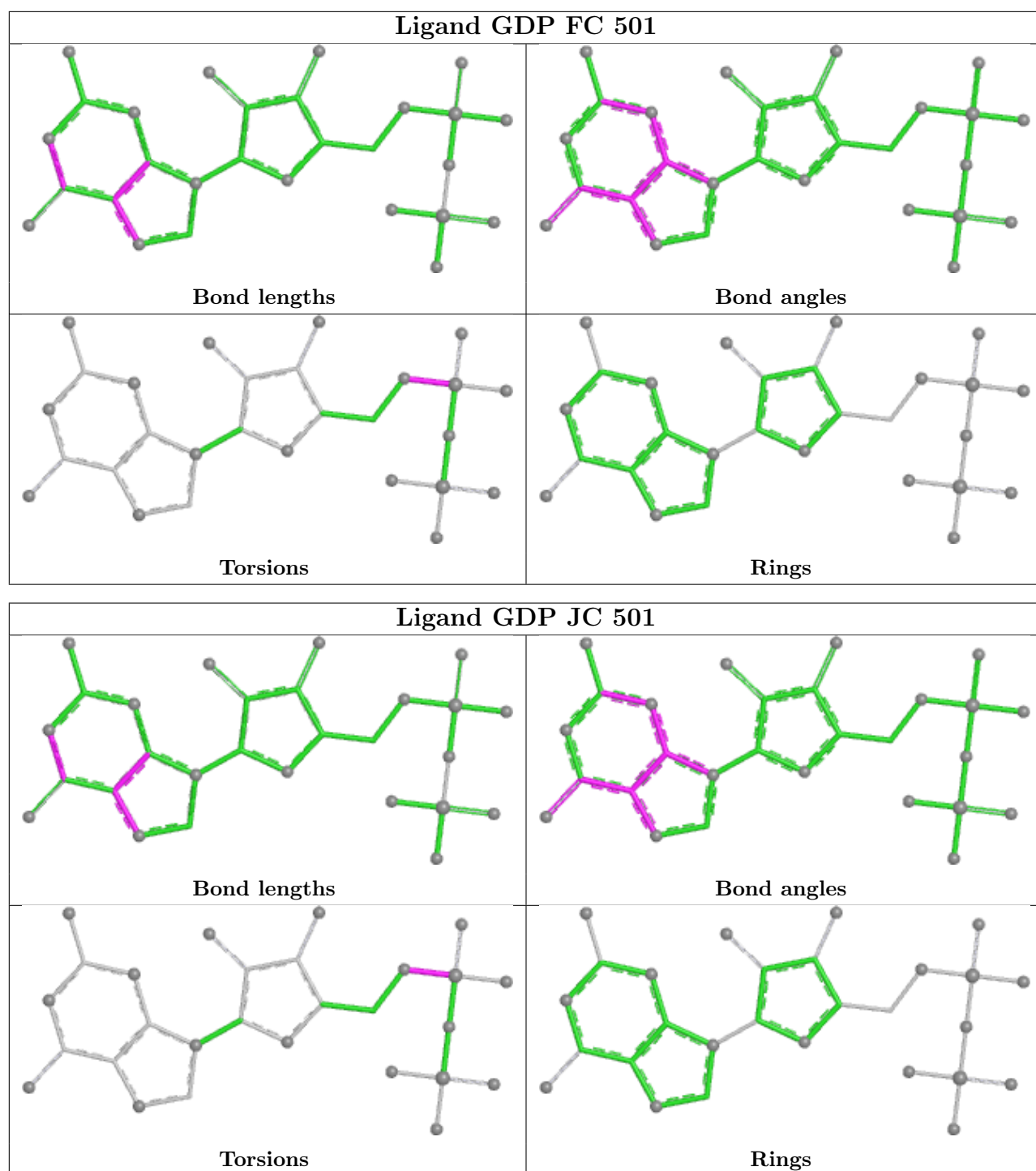
There are no ring outliers.

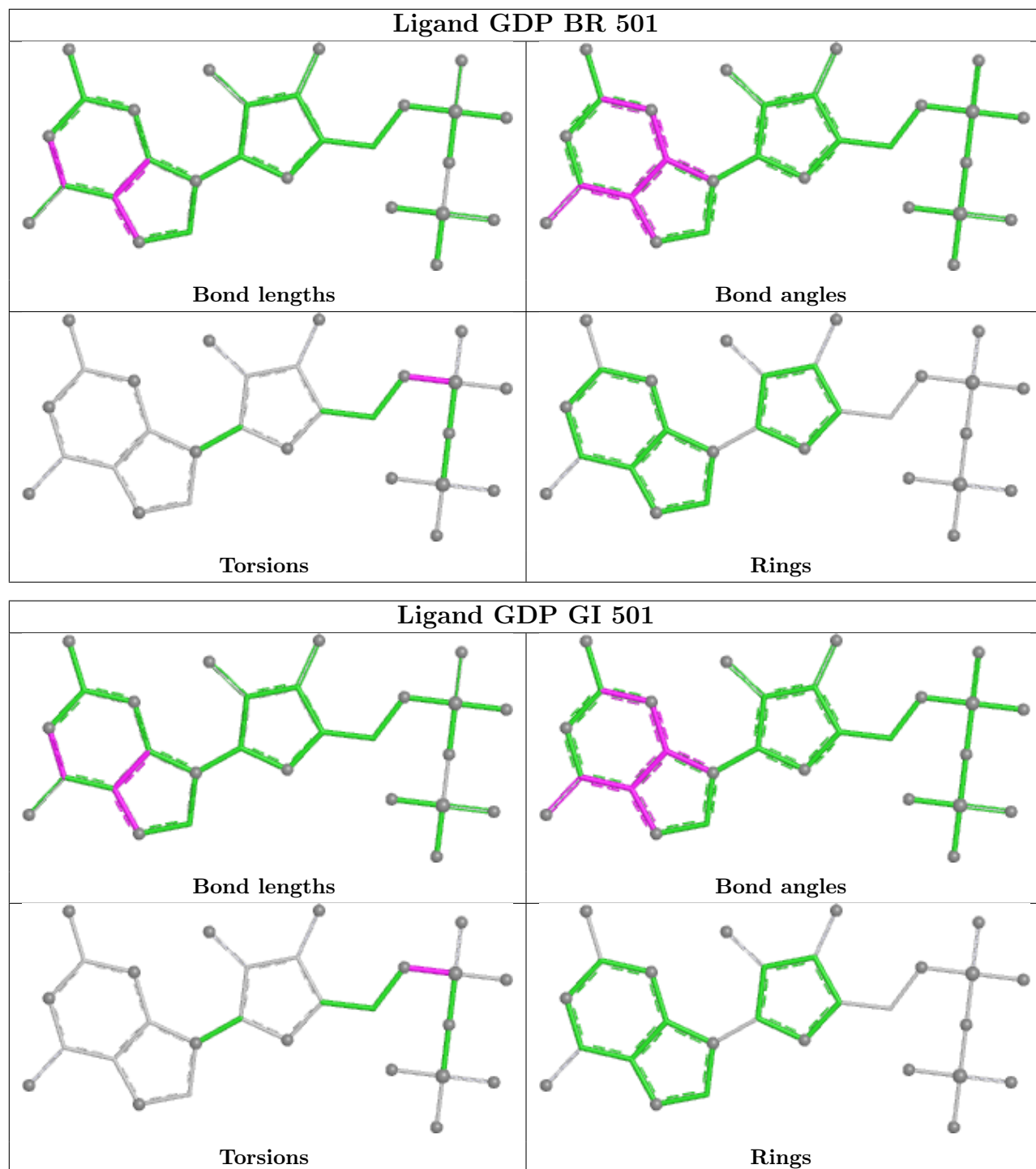
No monomer is involved in short contacts.

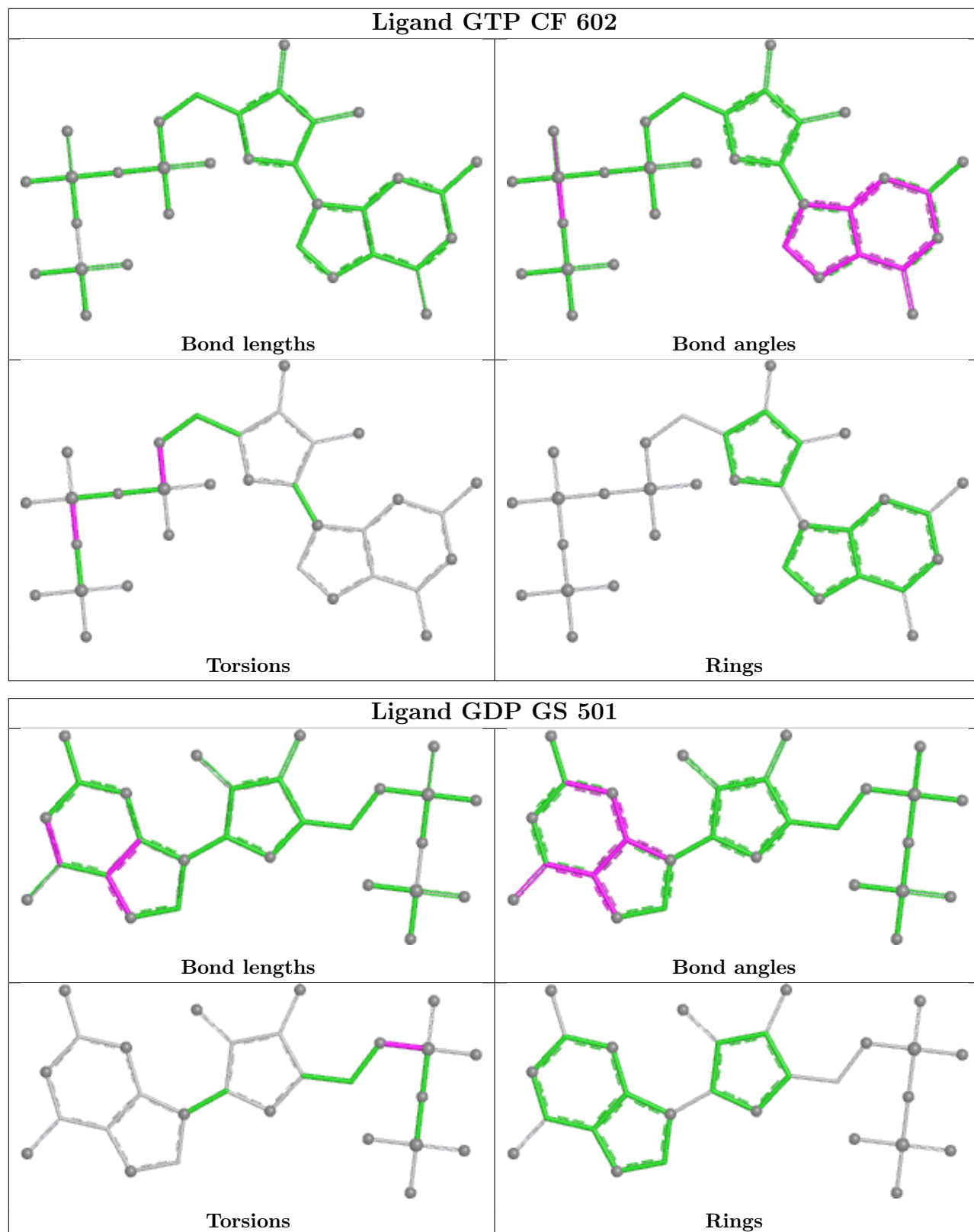
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

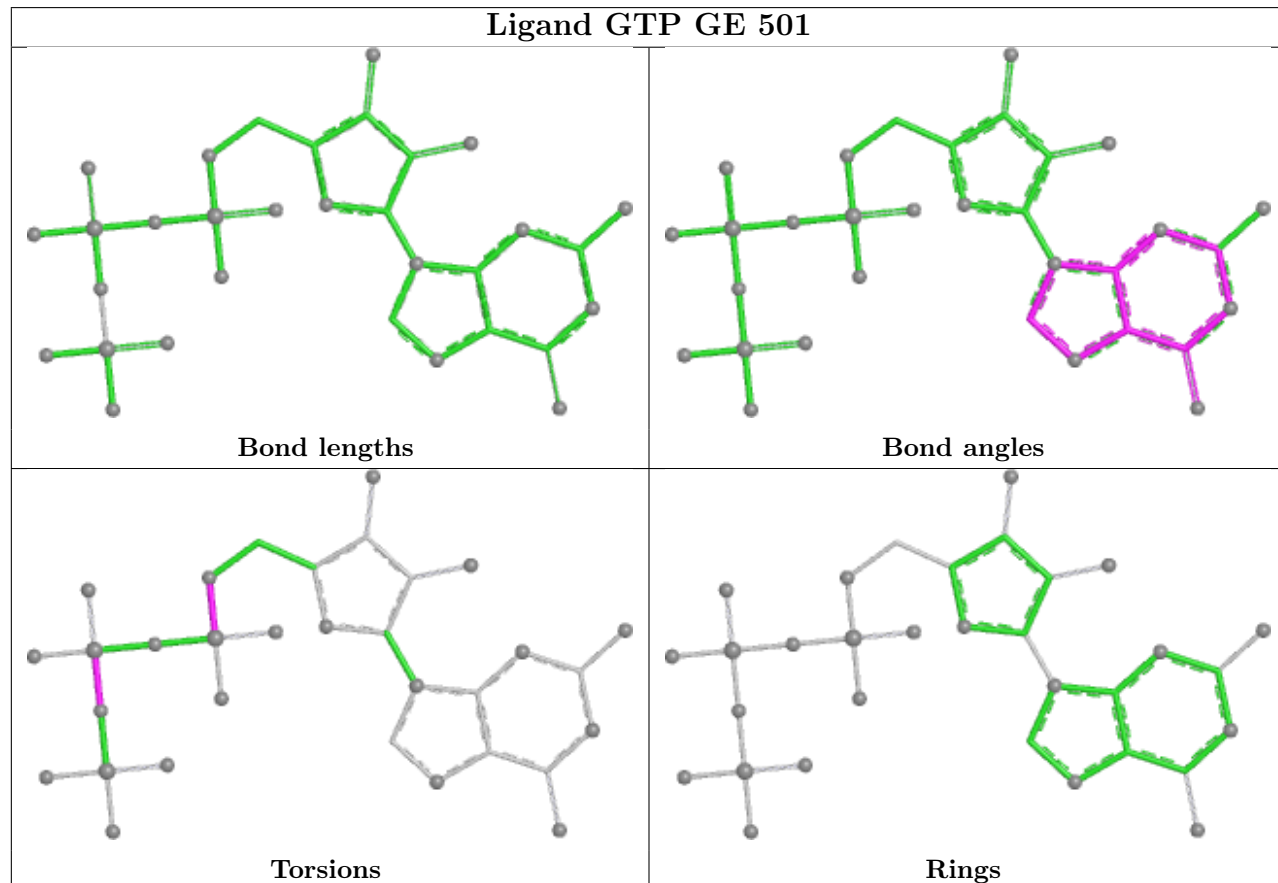
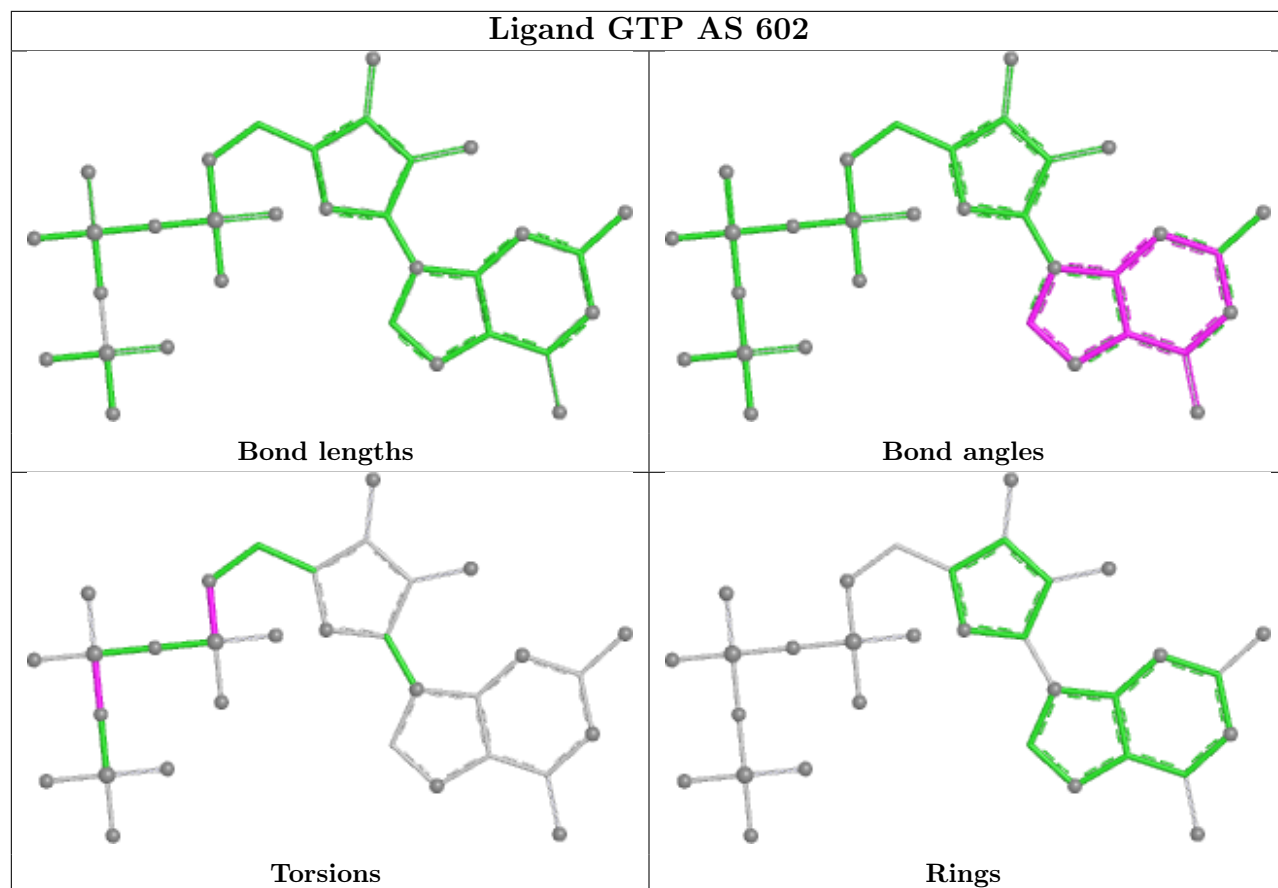


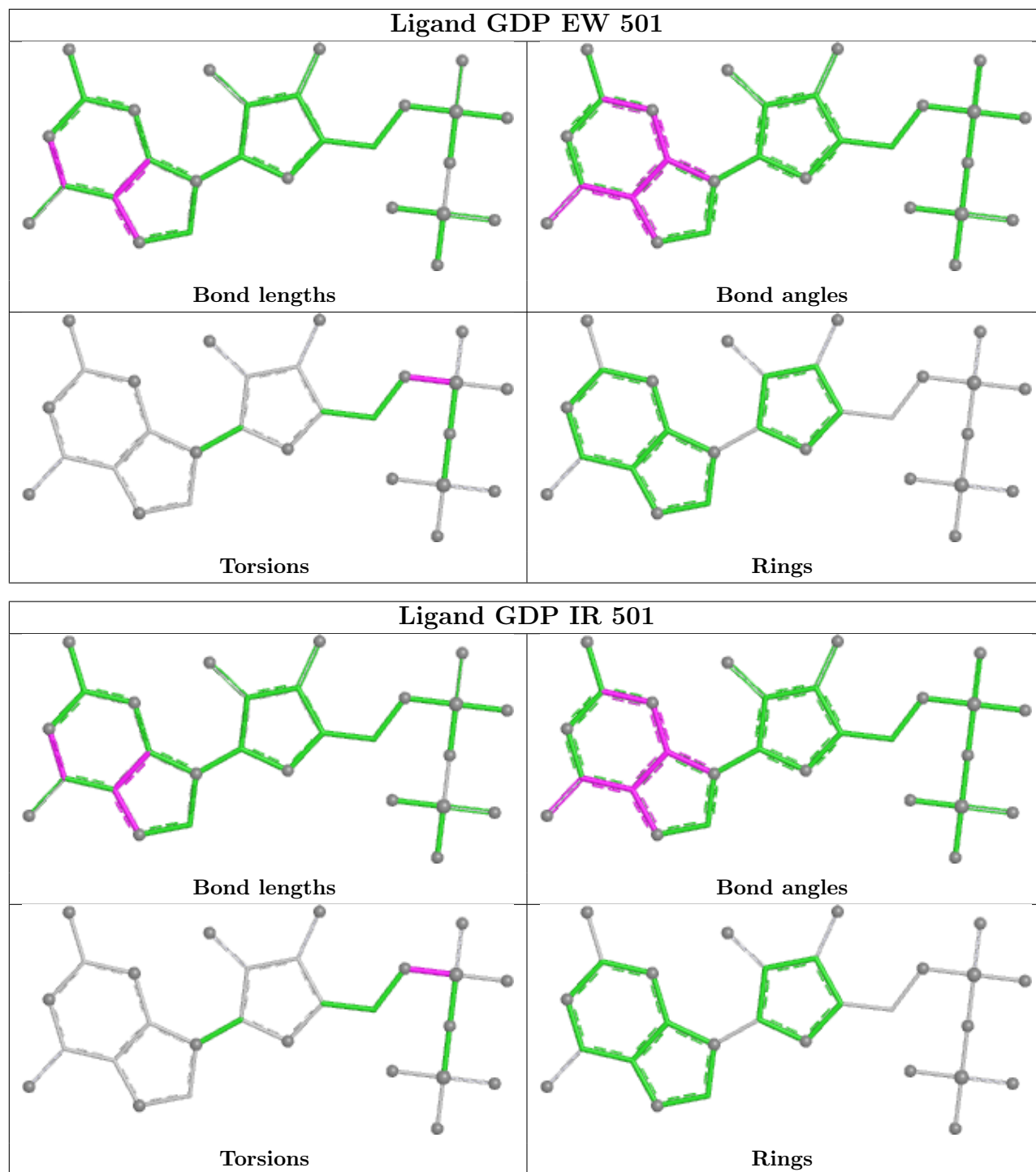


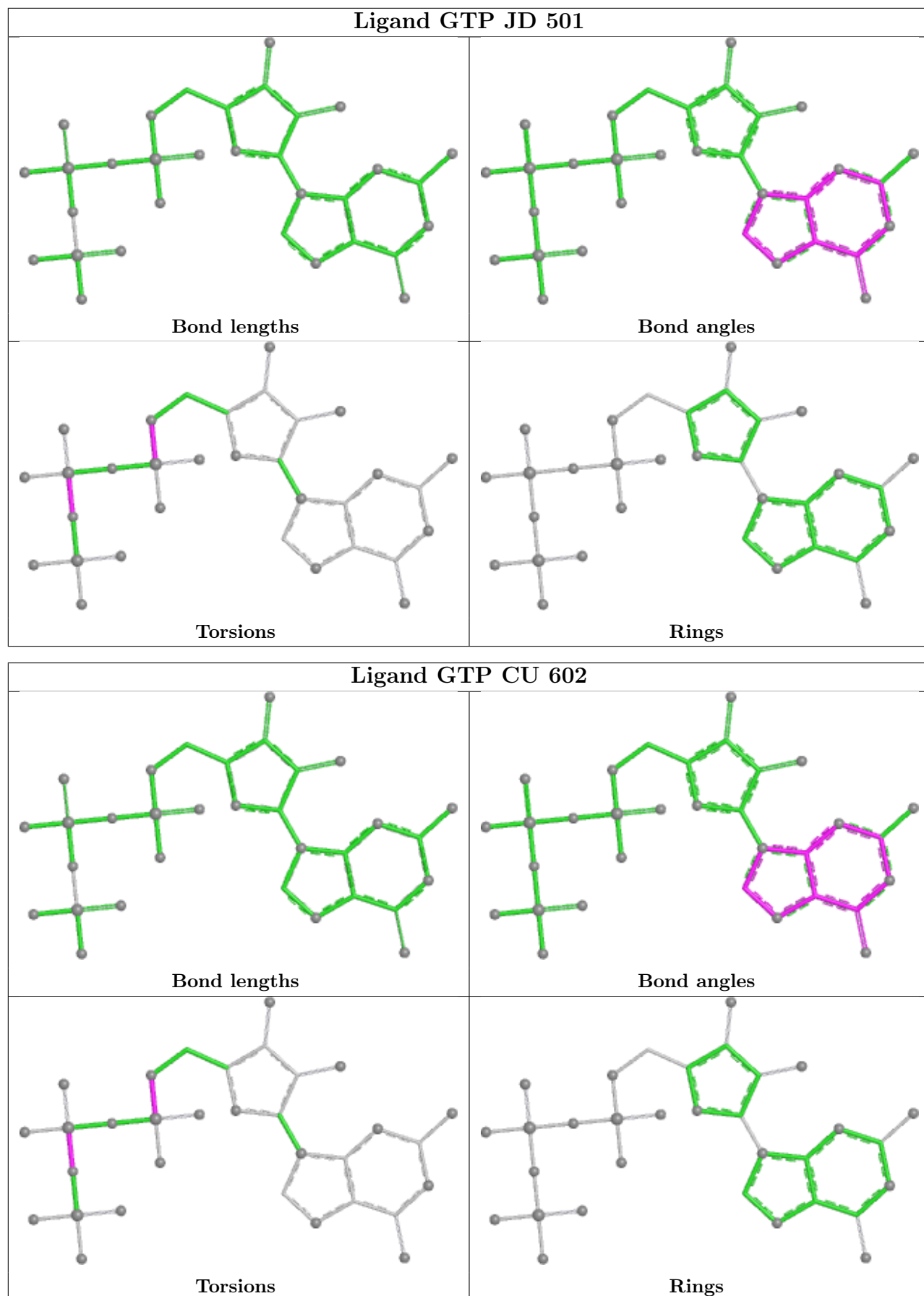


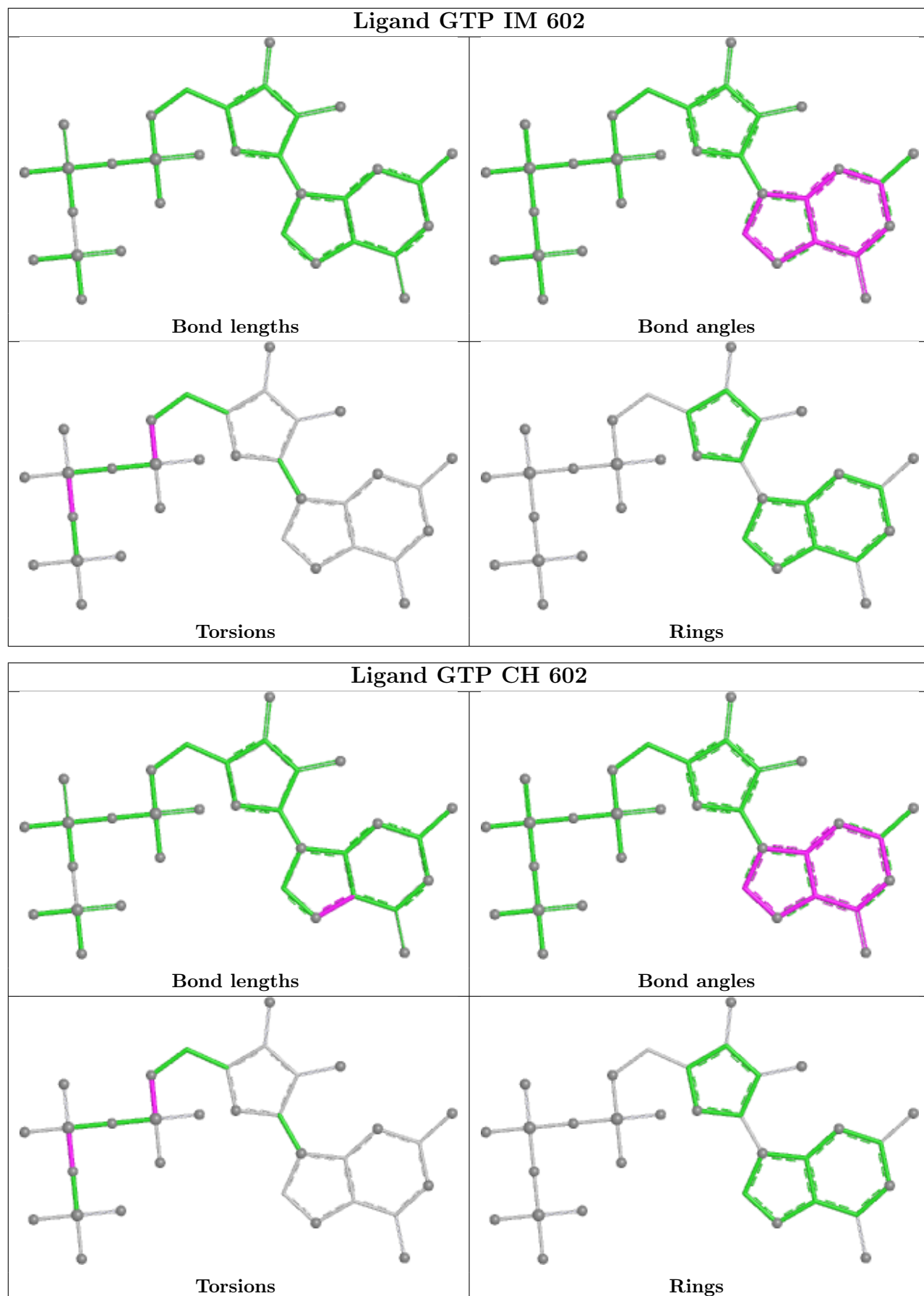


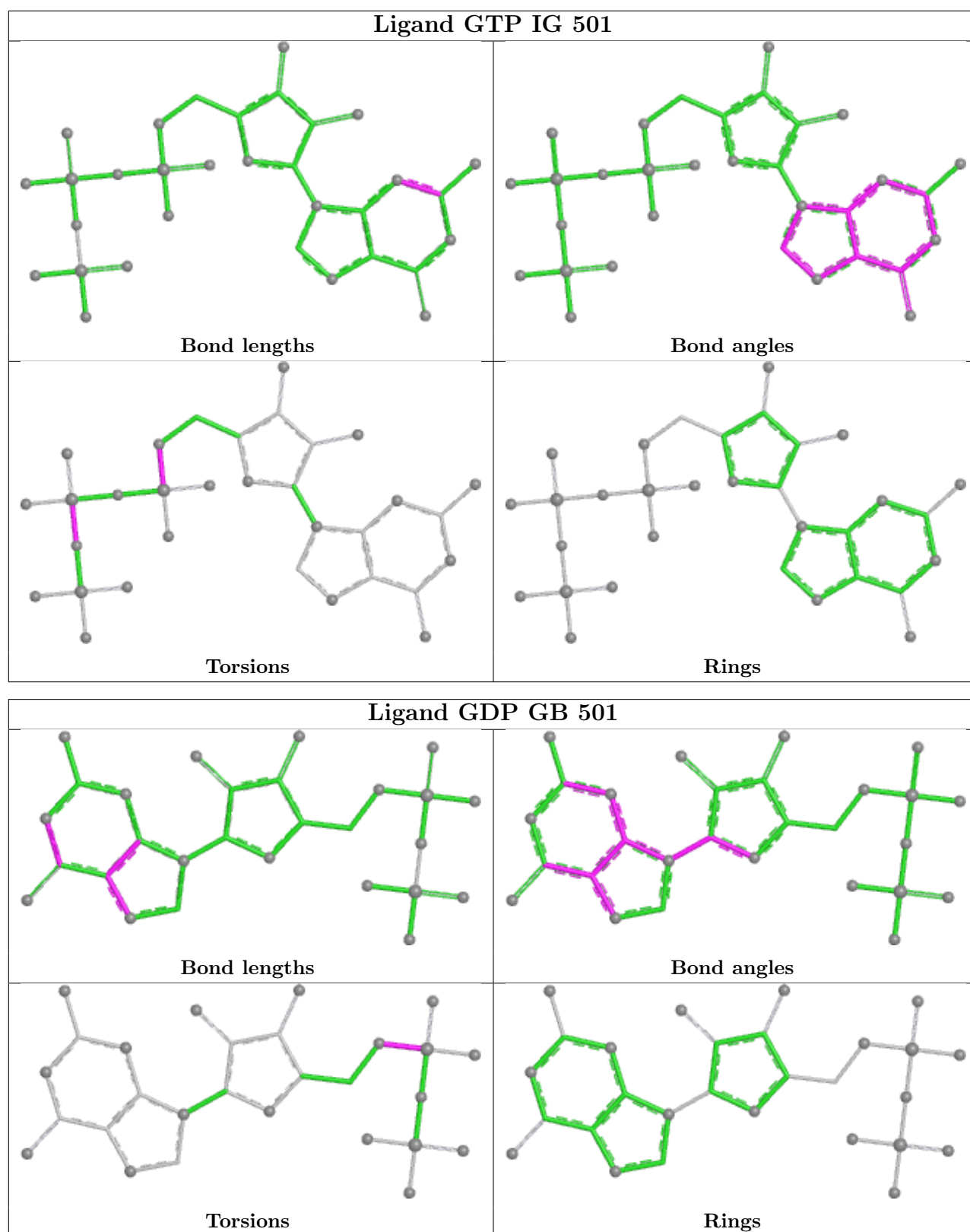


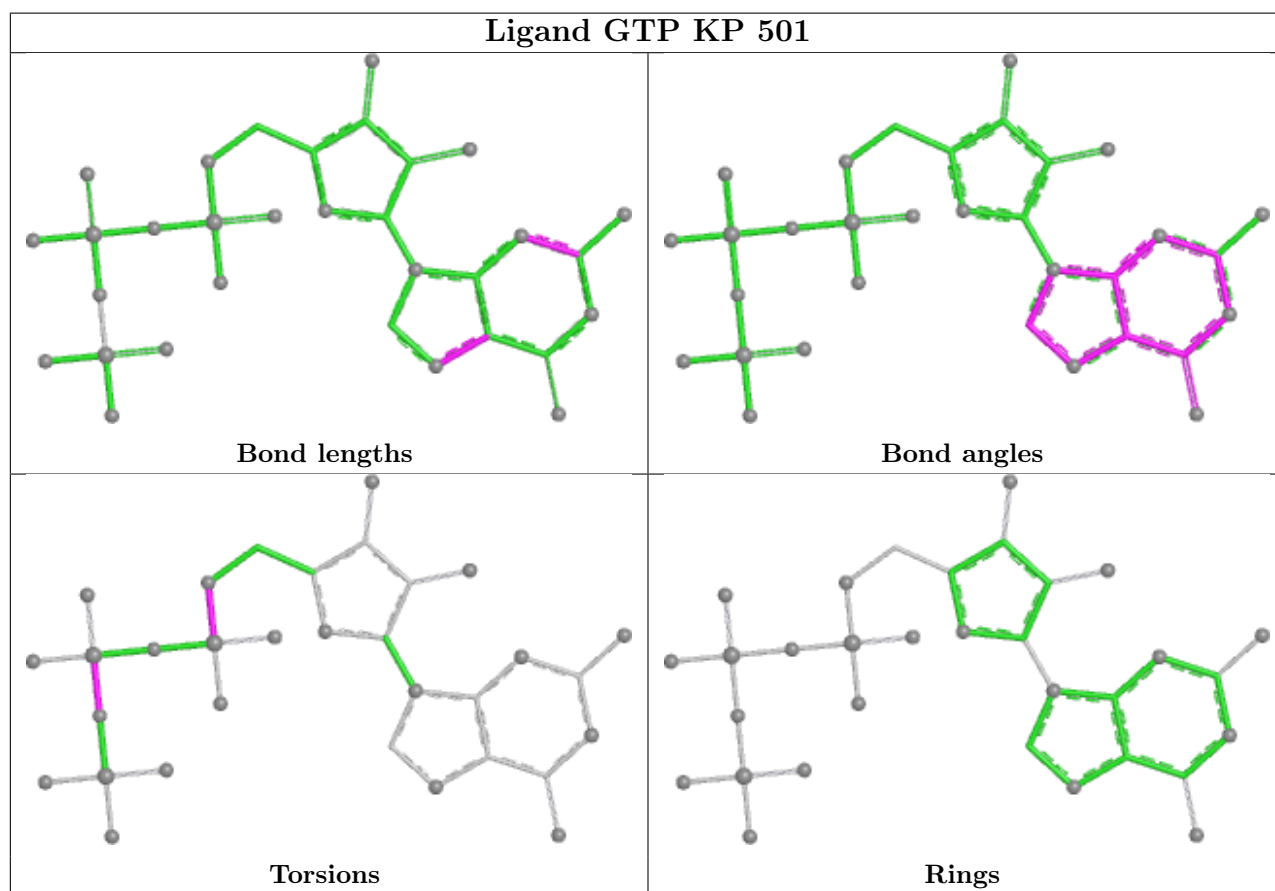
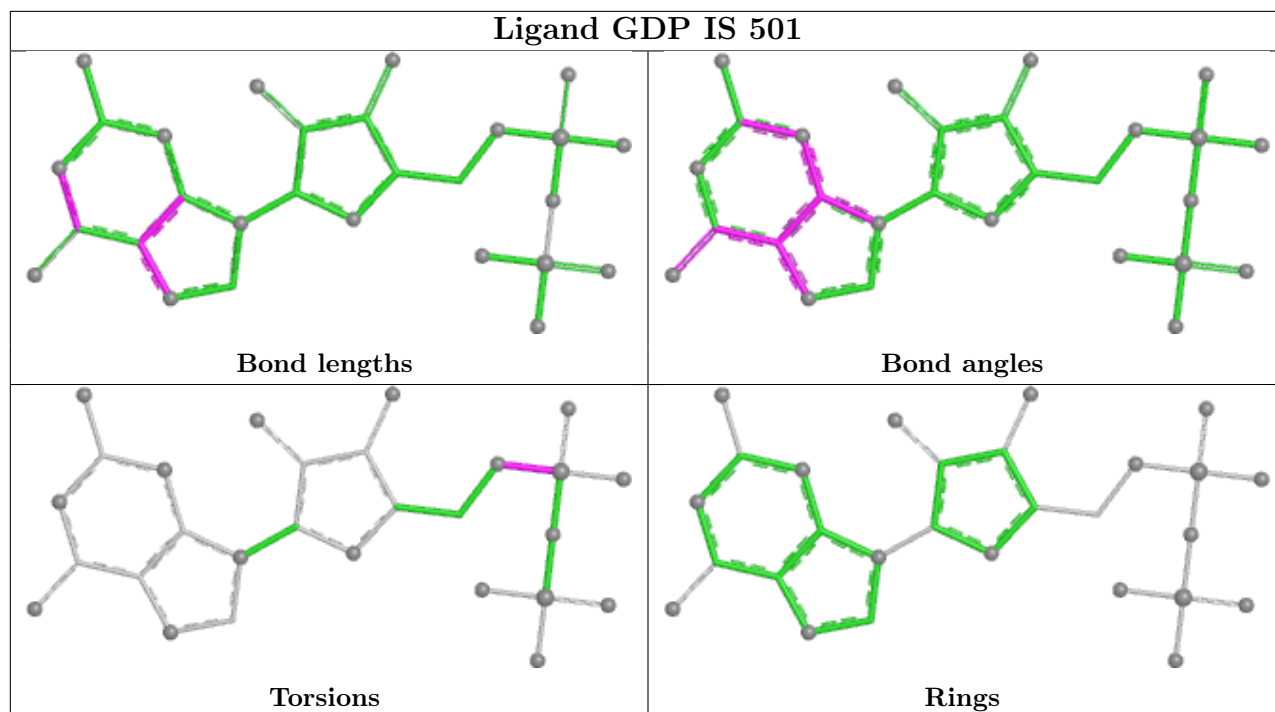


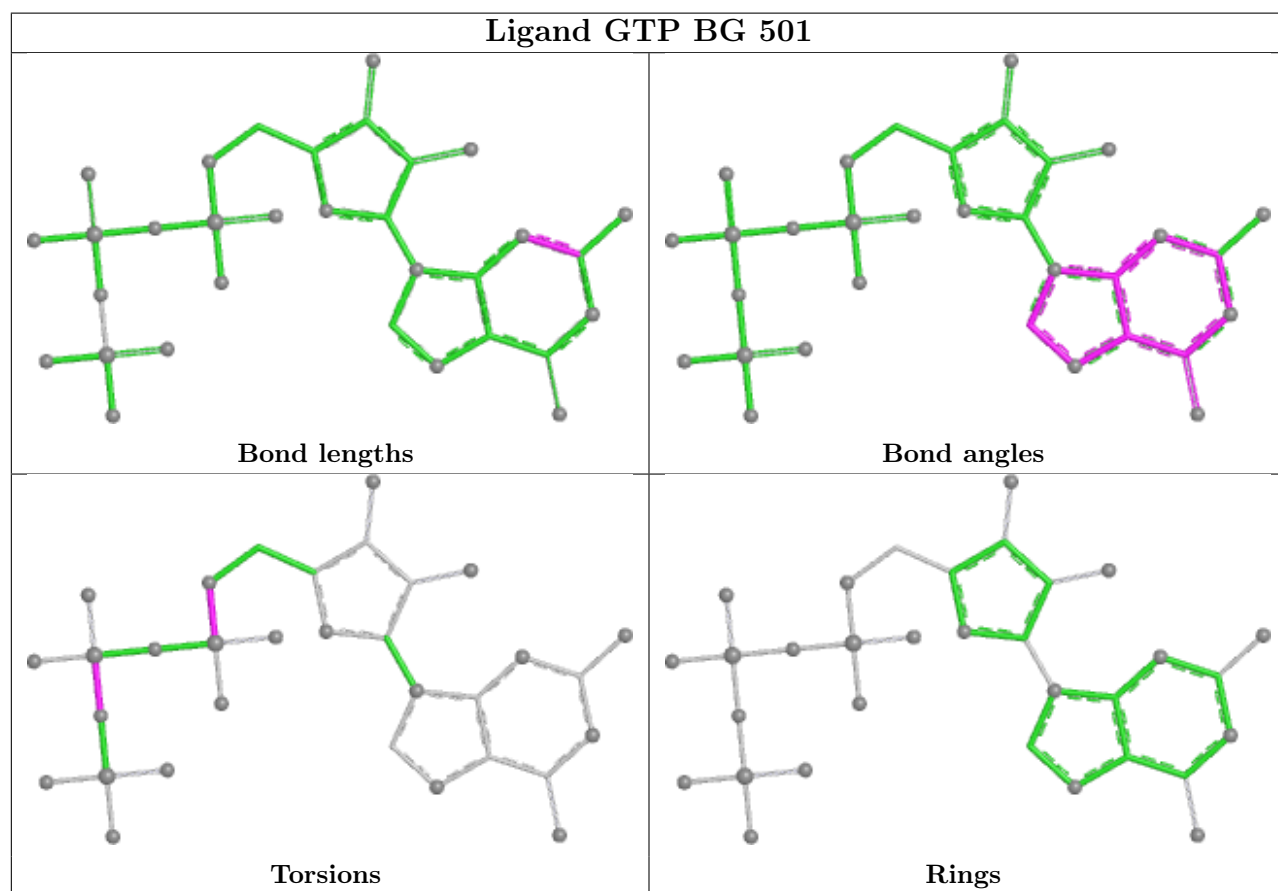
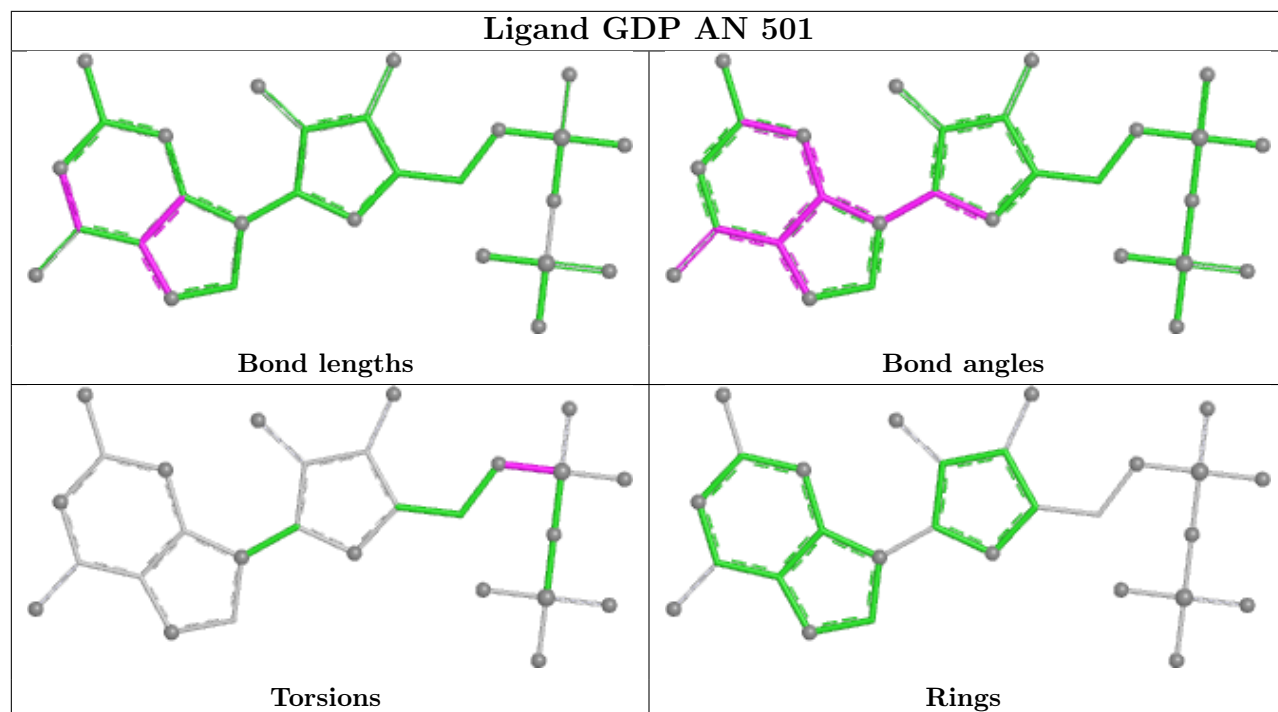


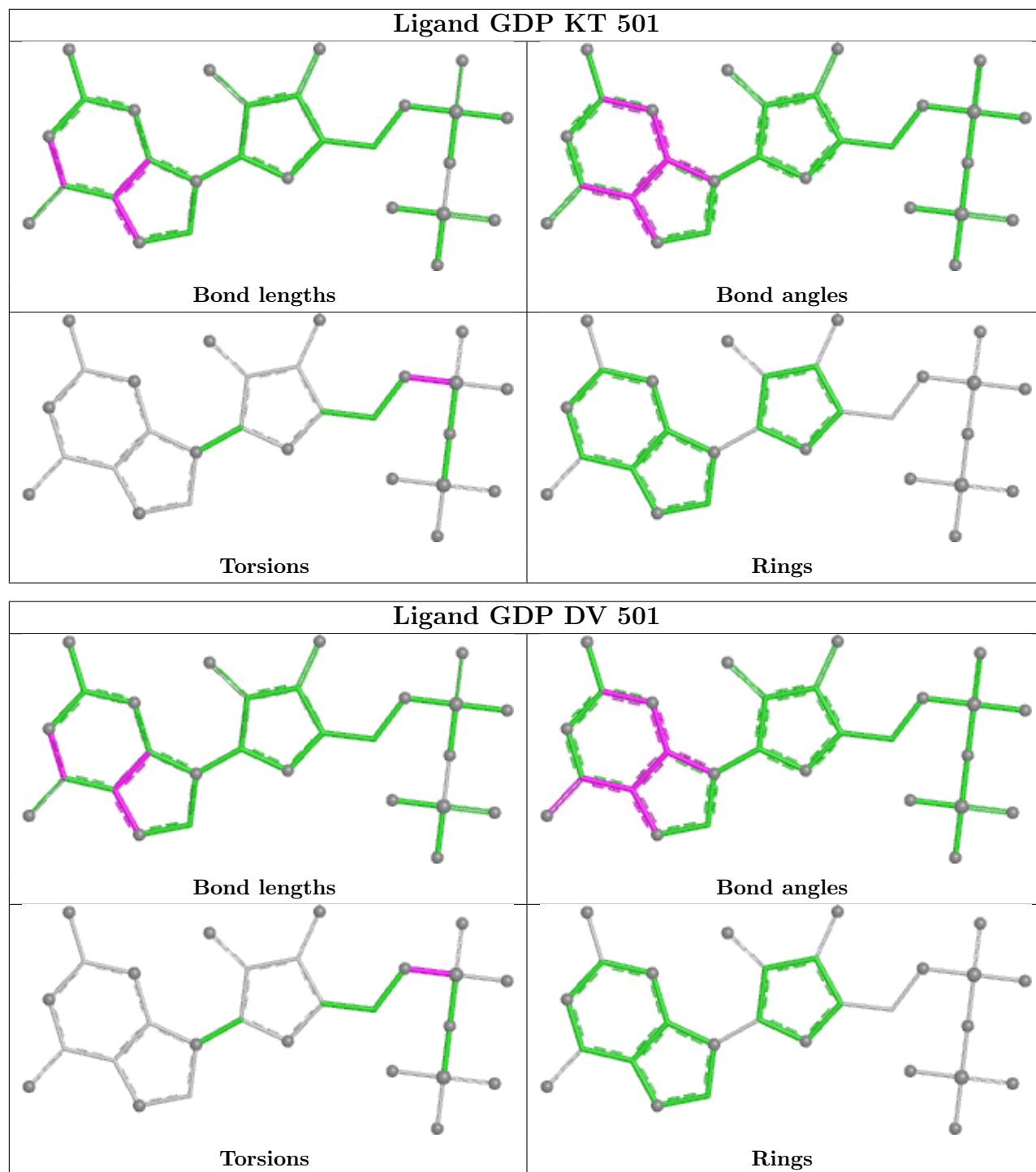


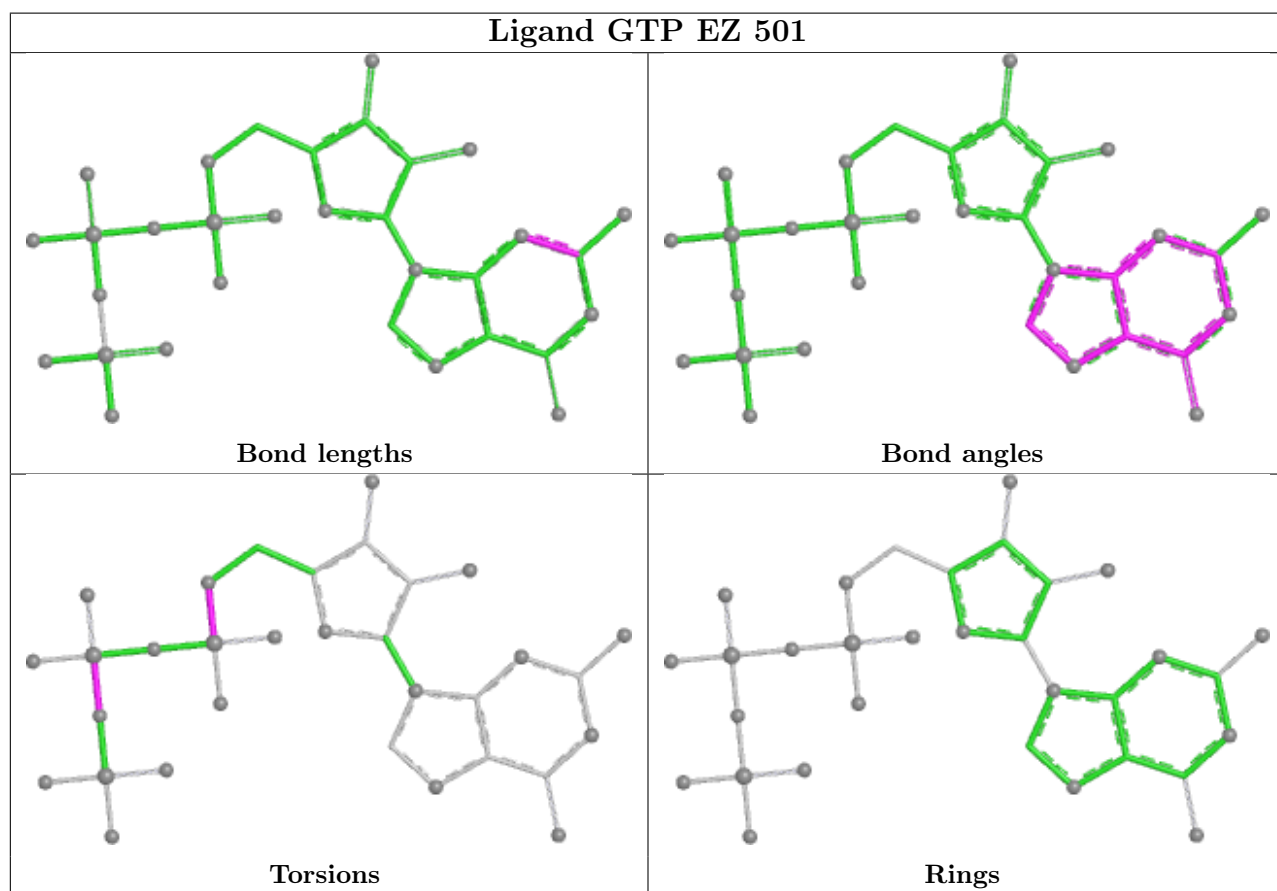
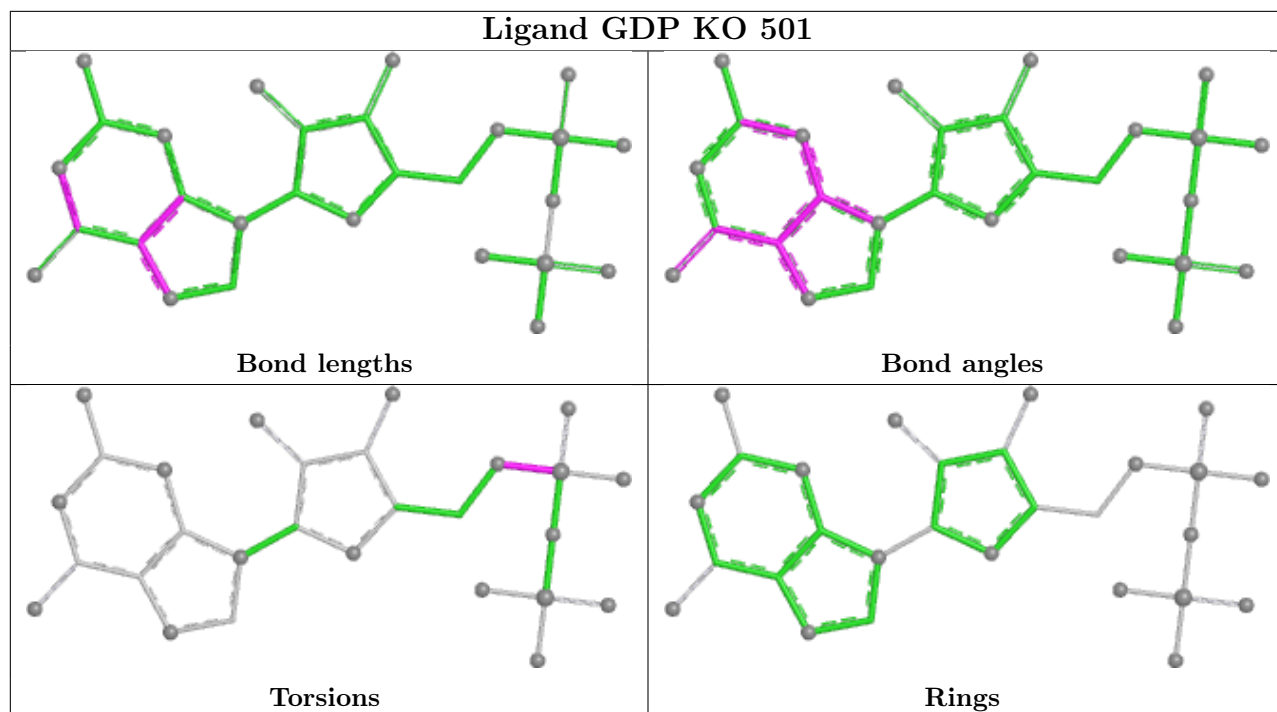


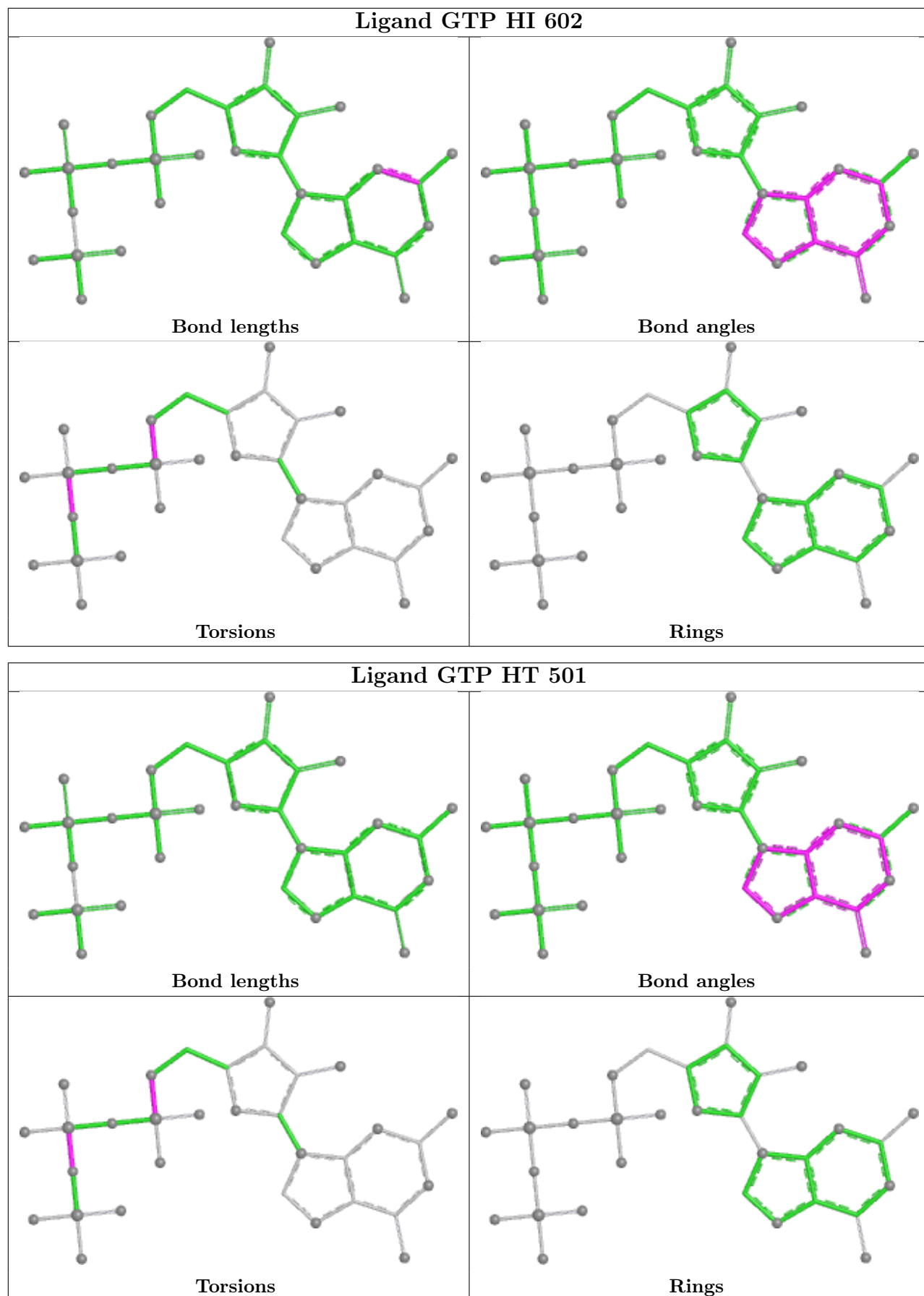


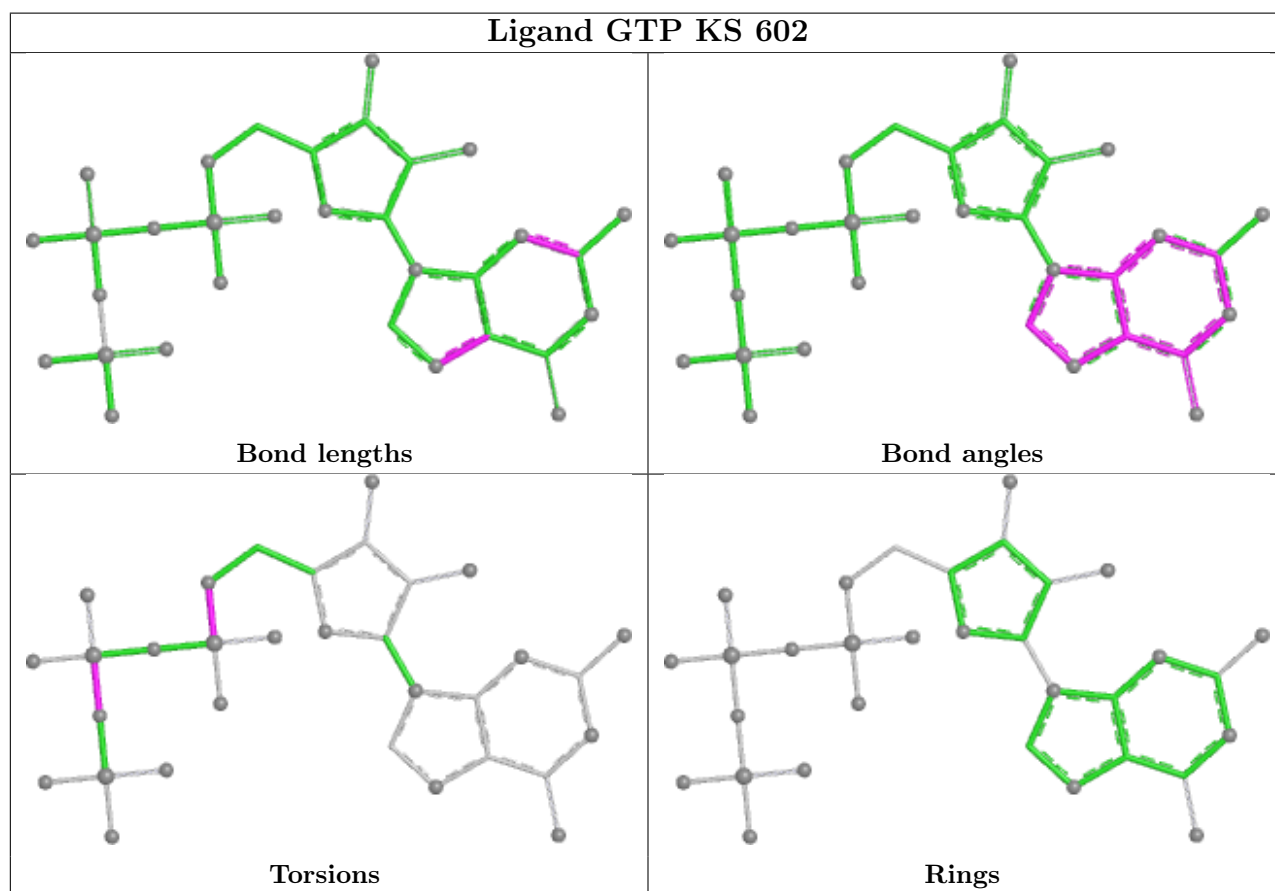
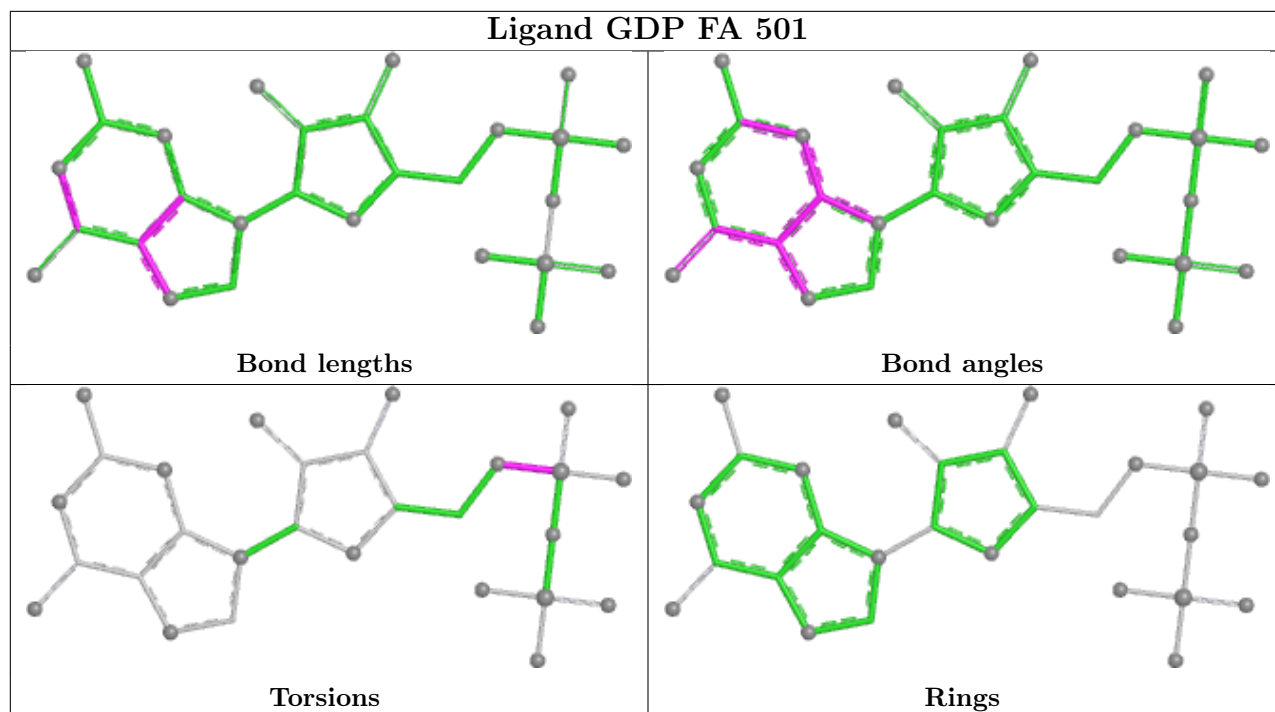


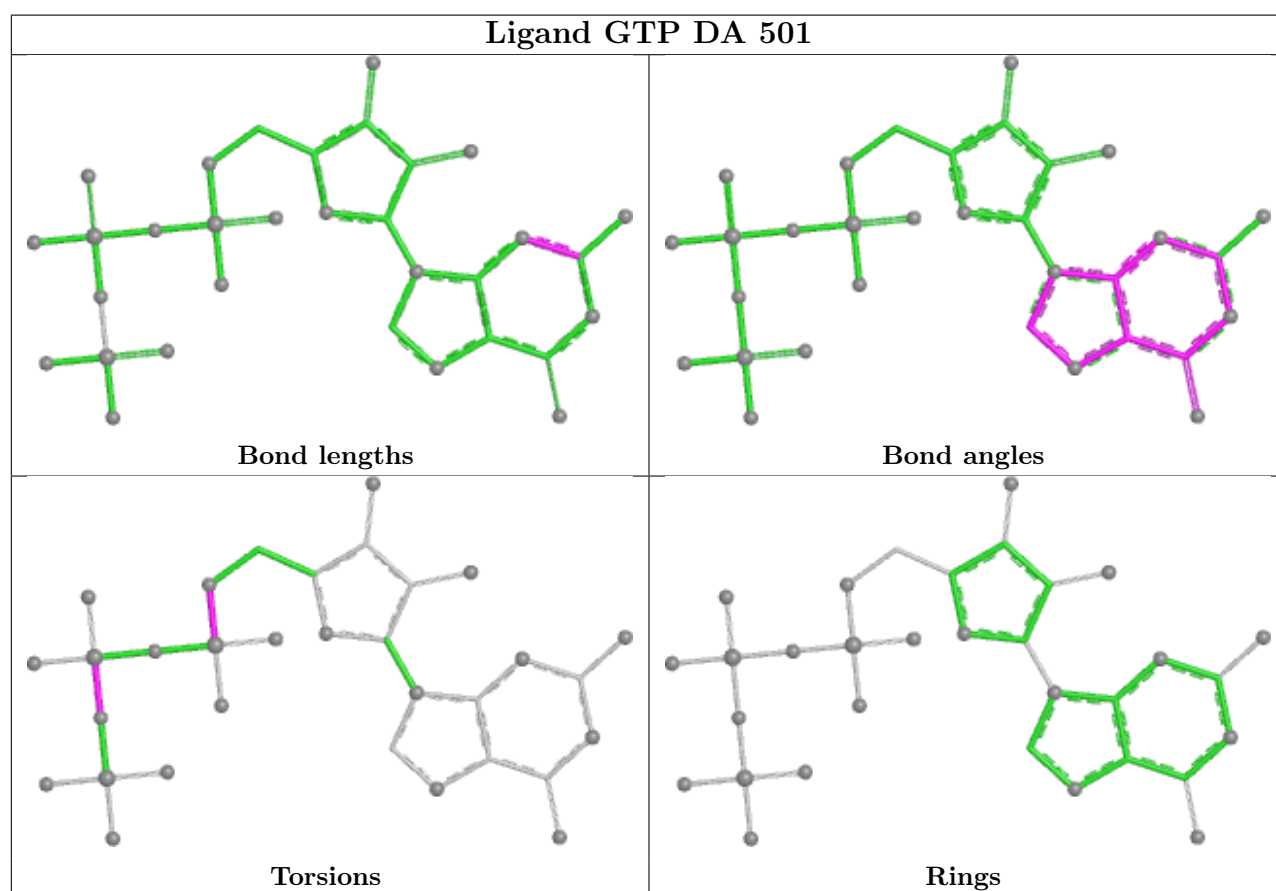
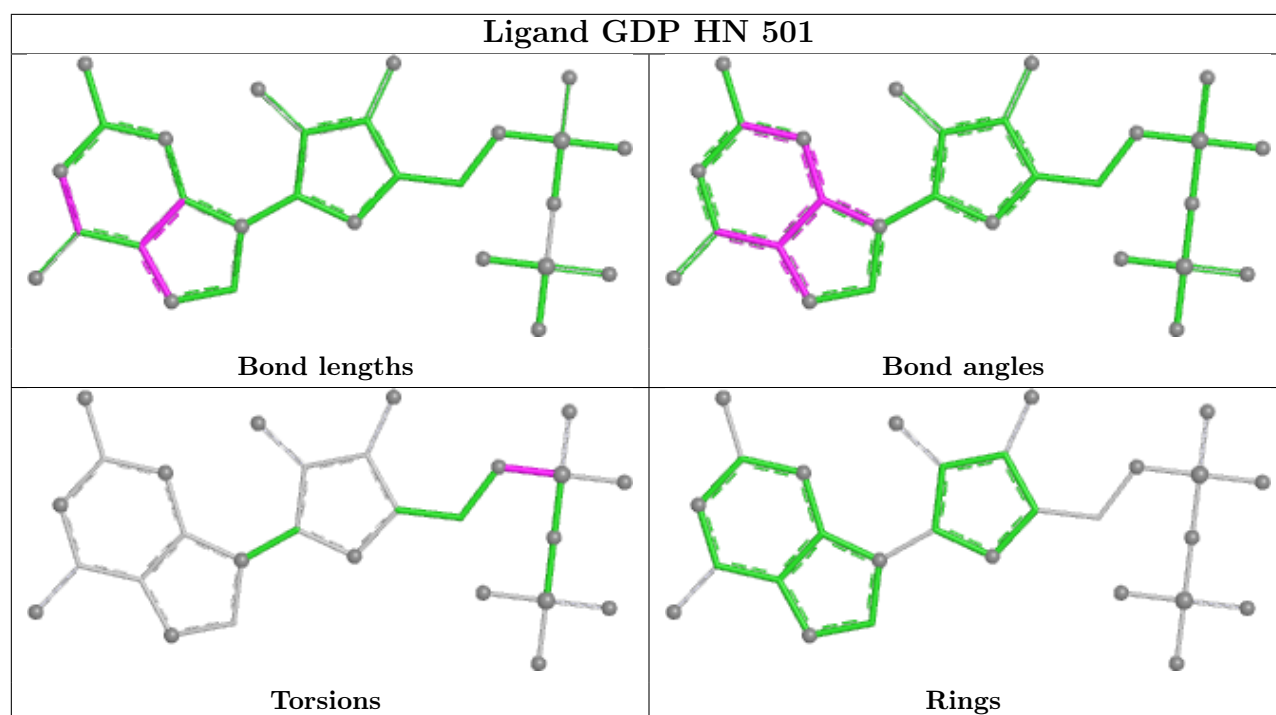


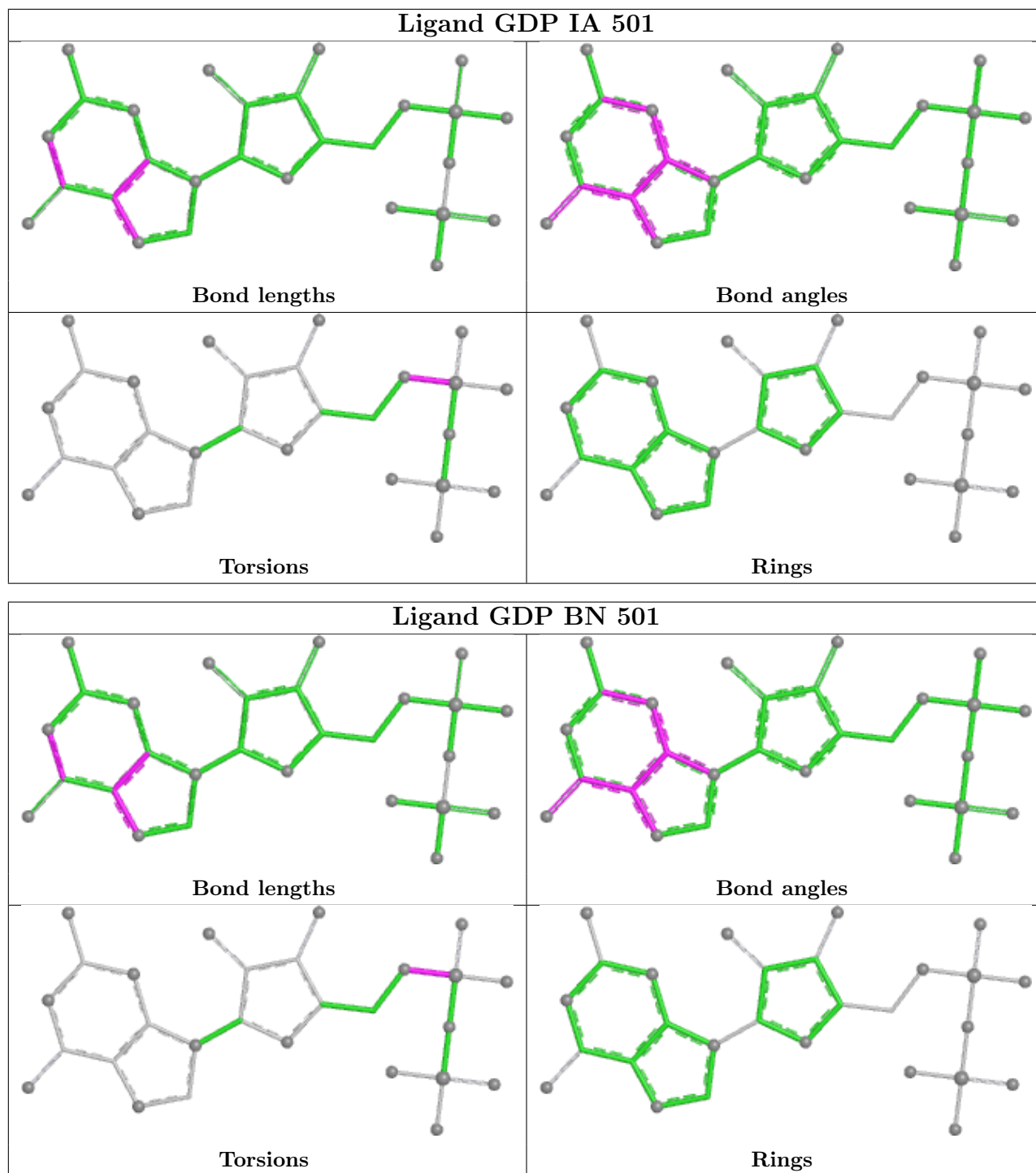


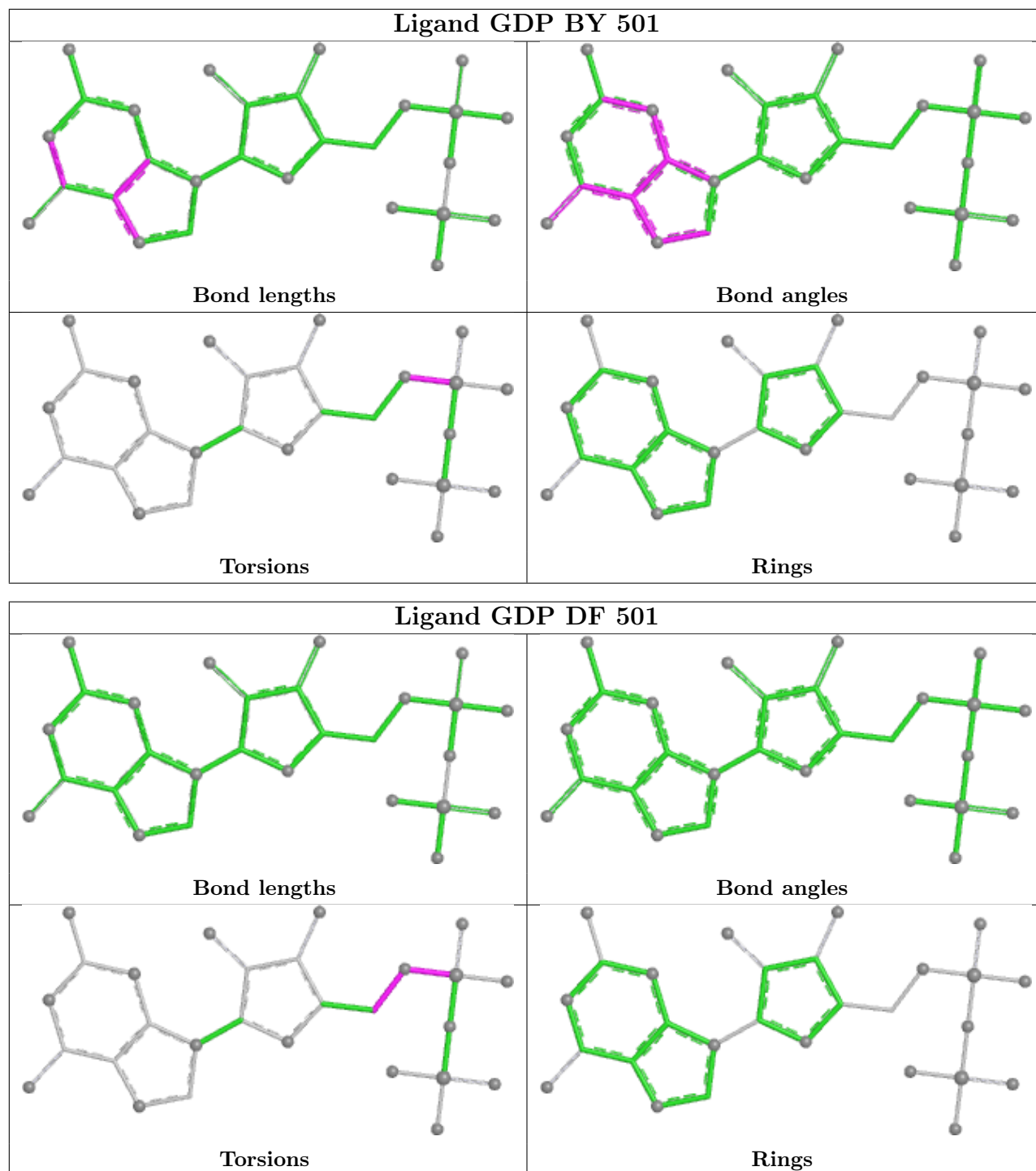


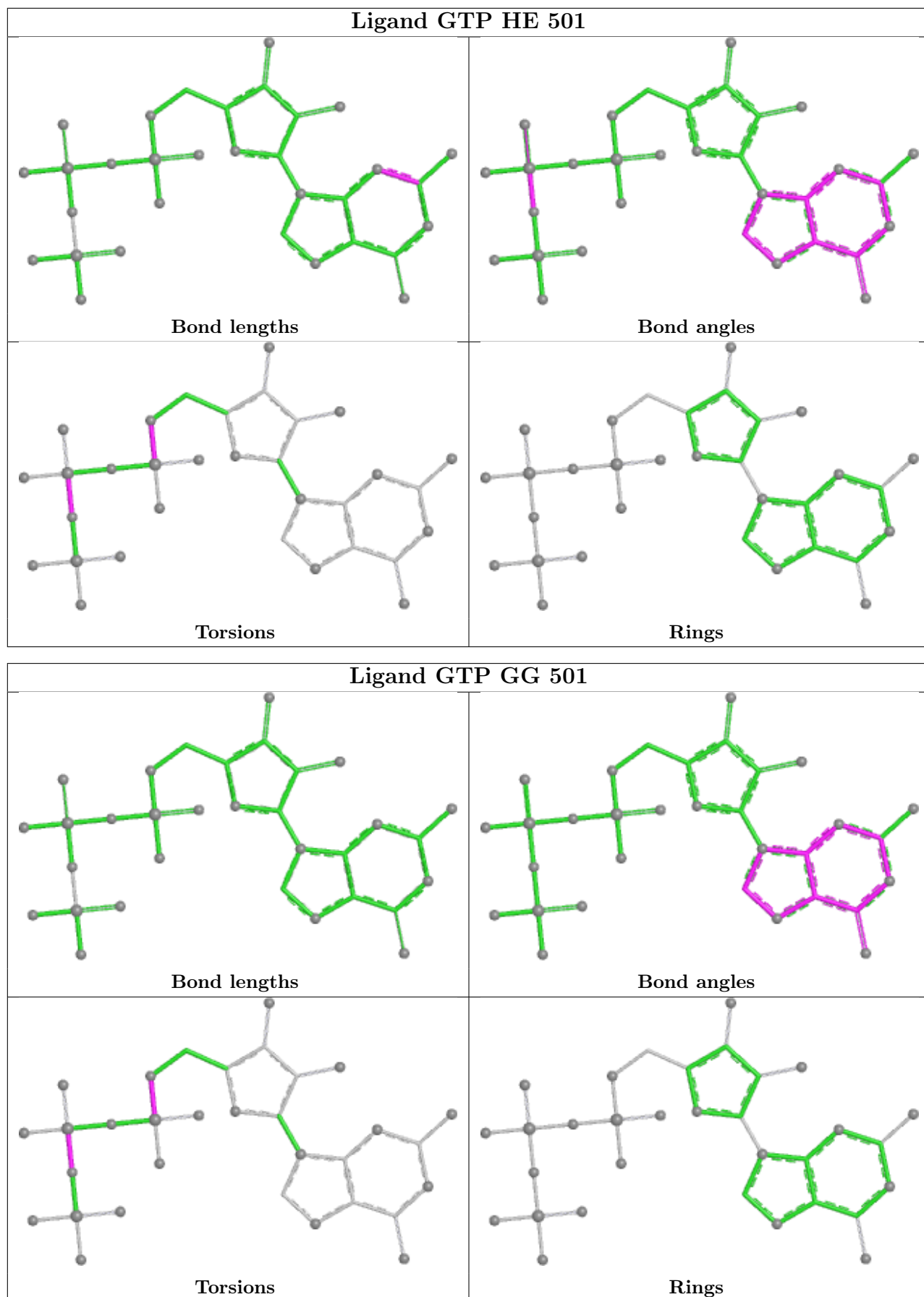


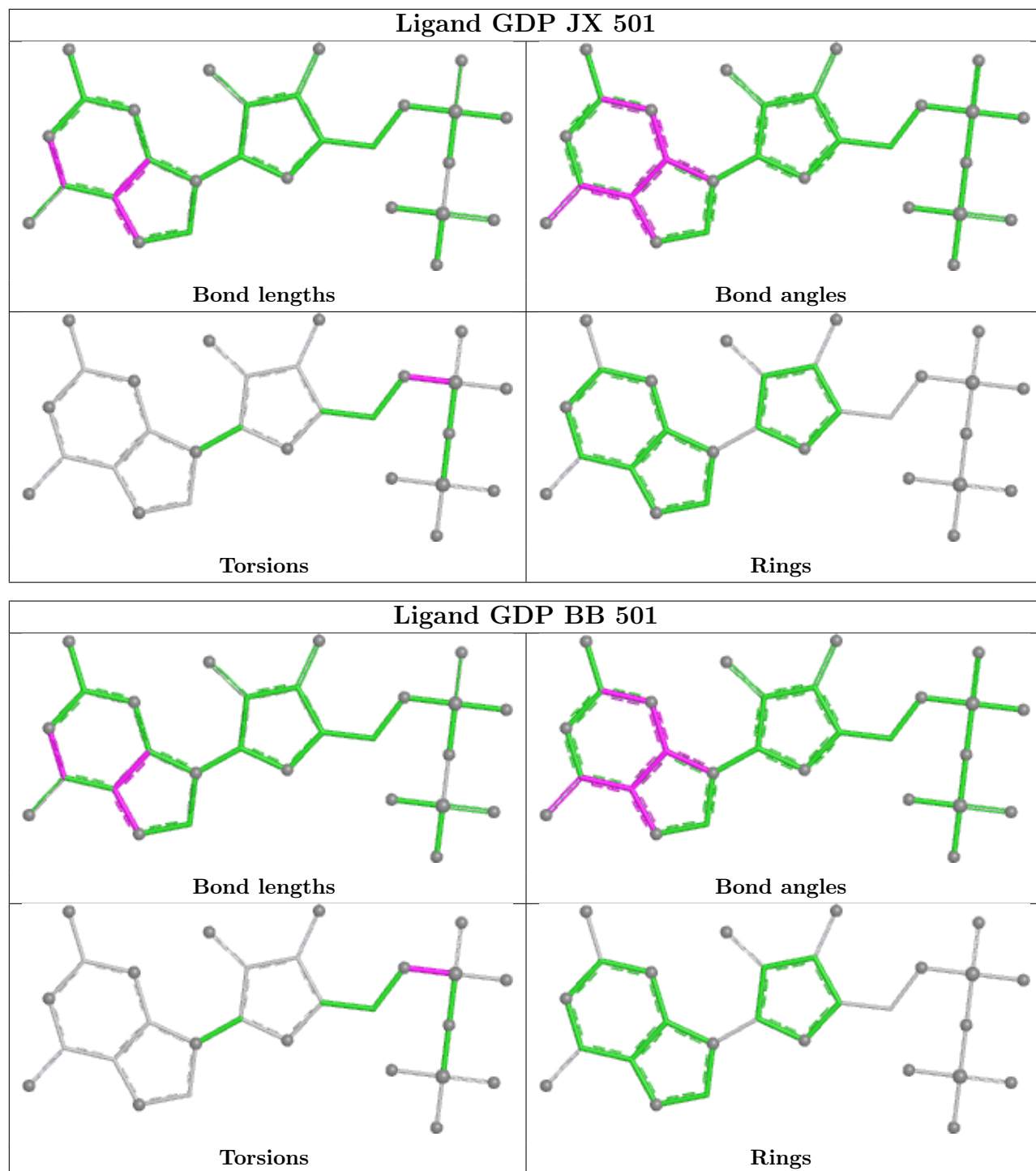


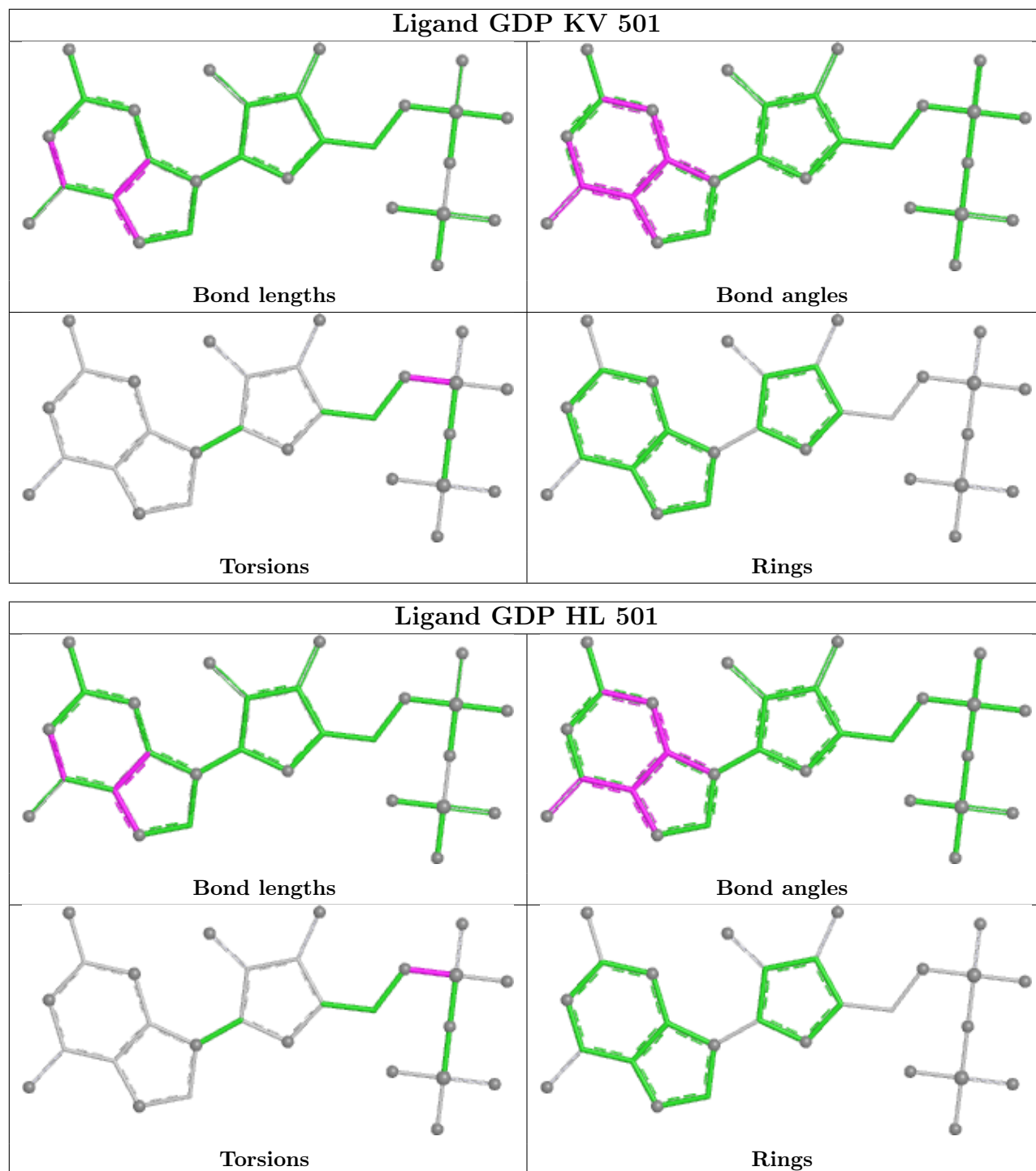


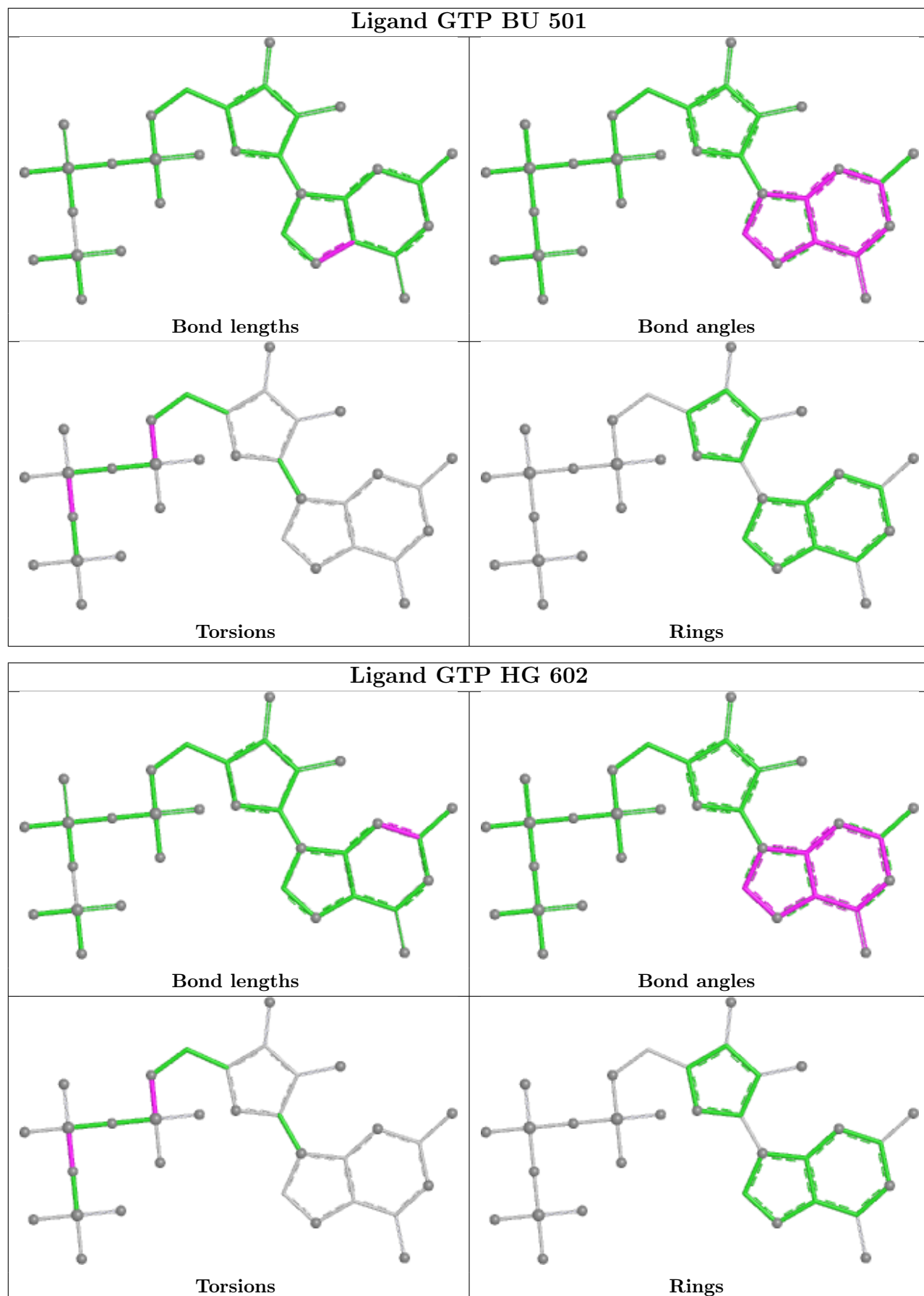


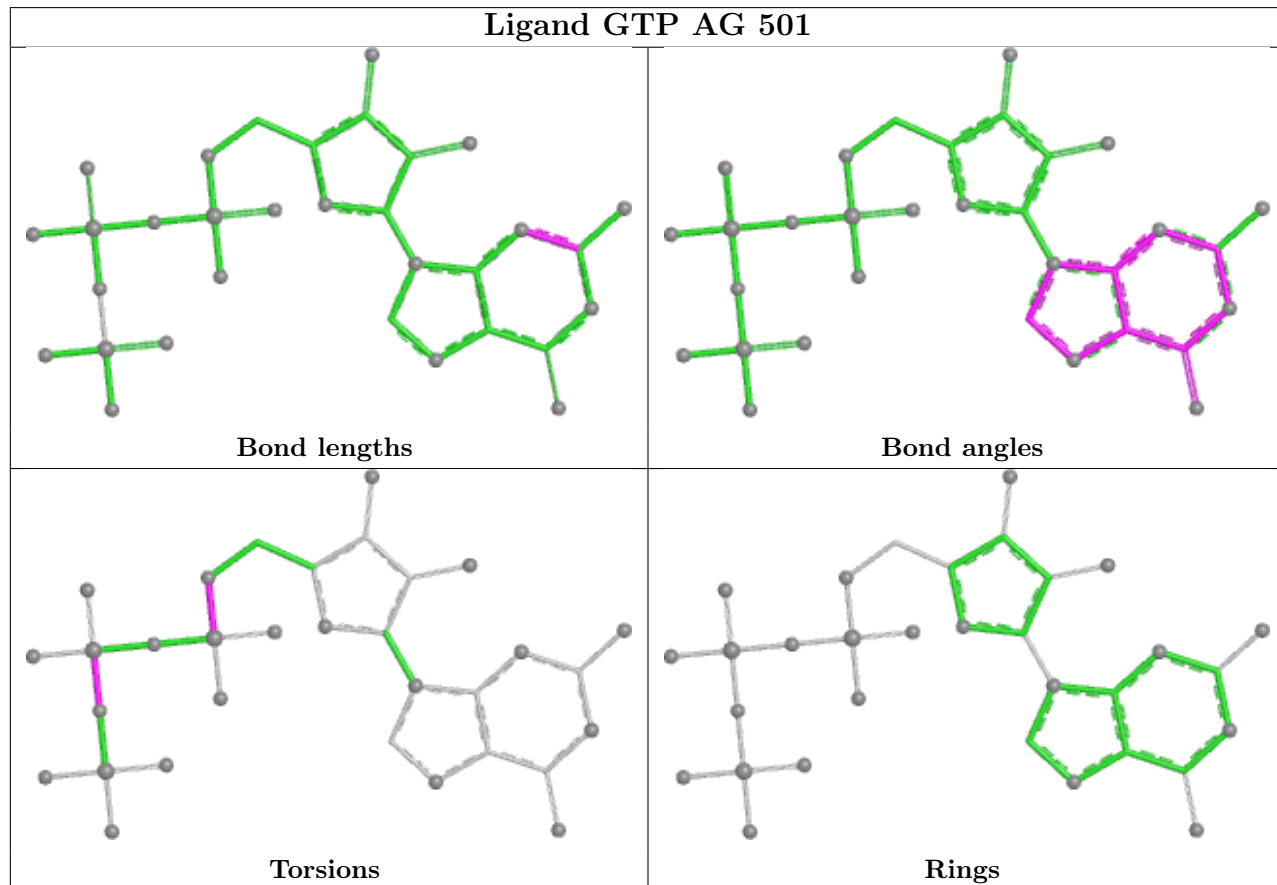
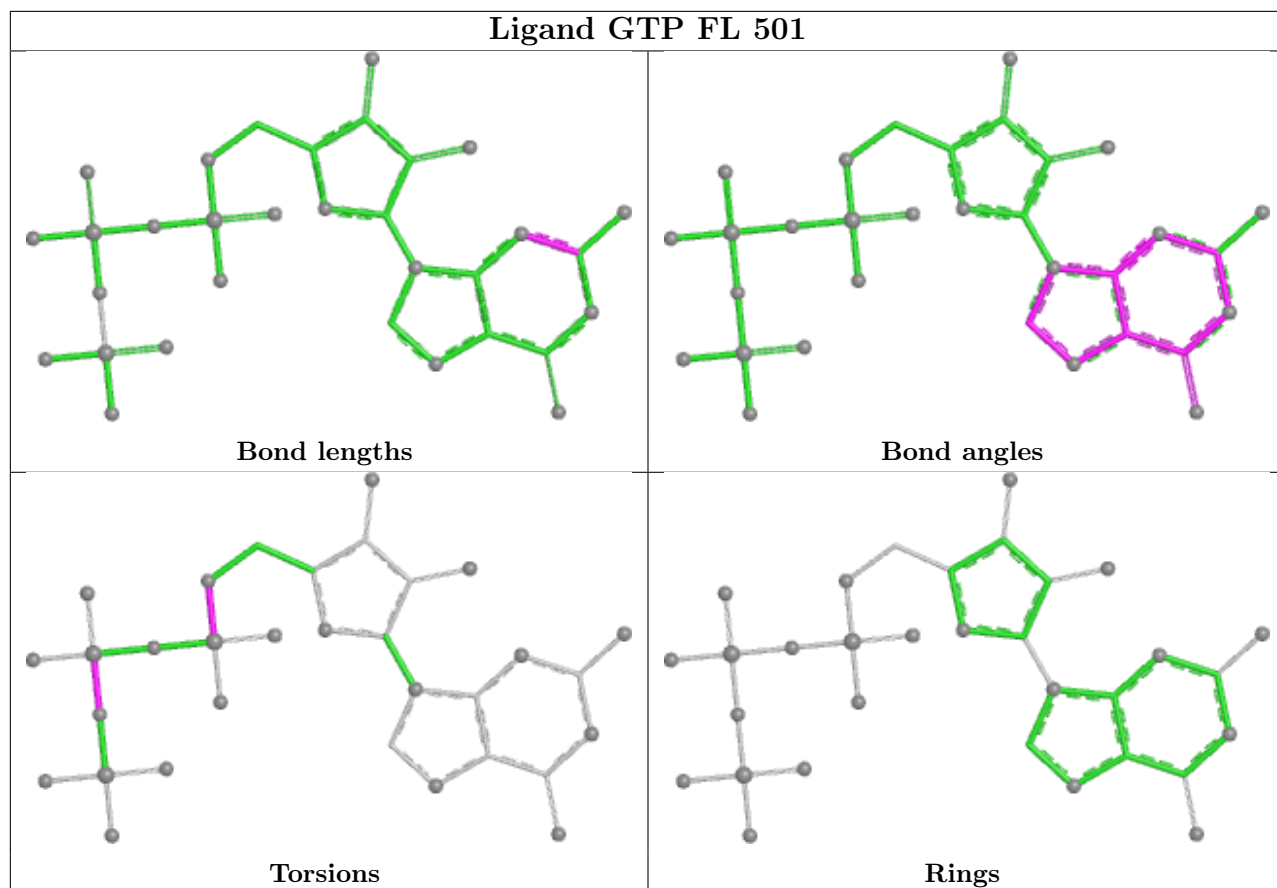


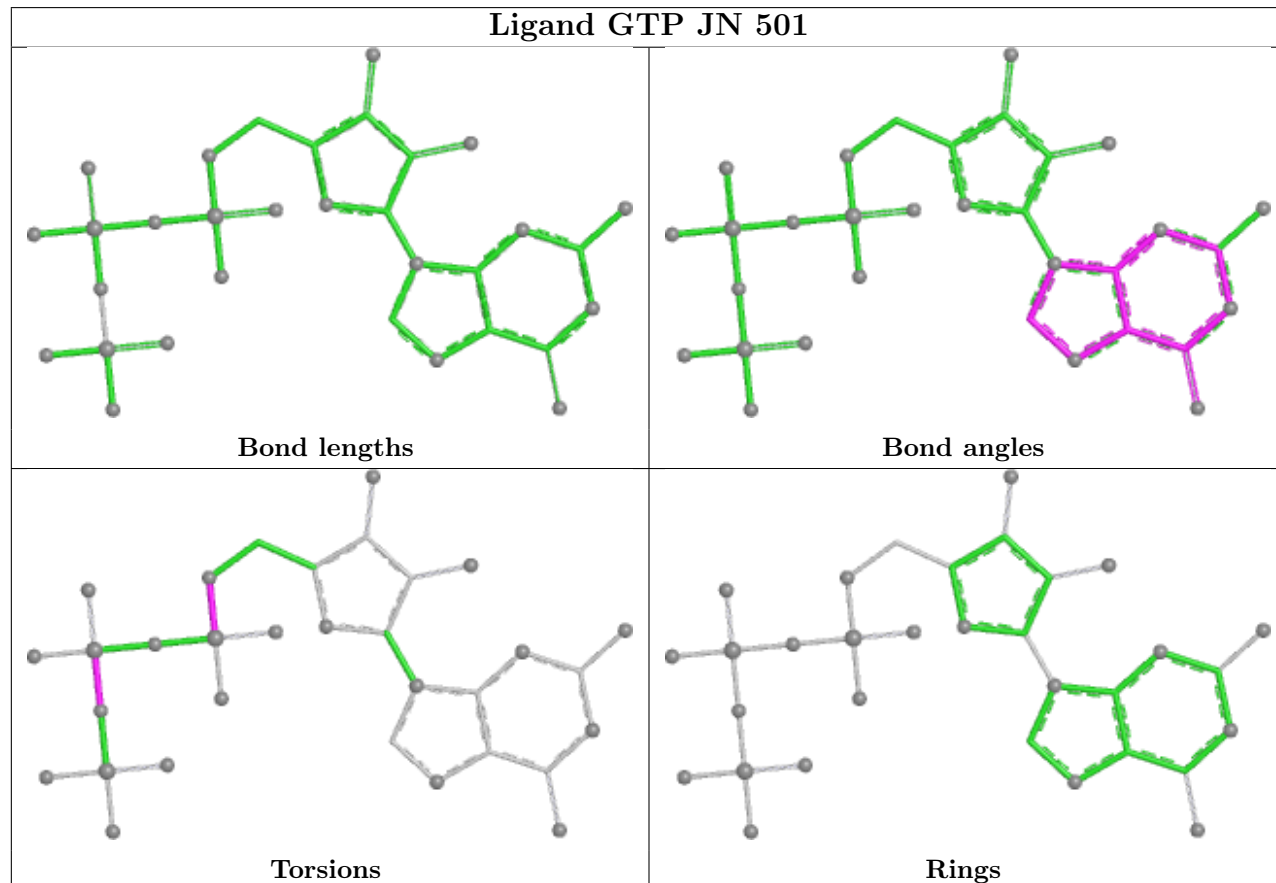
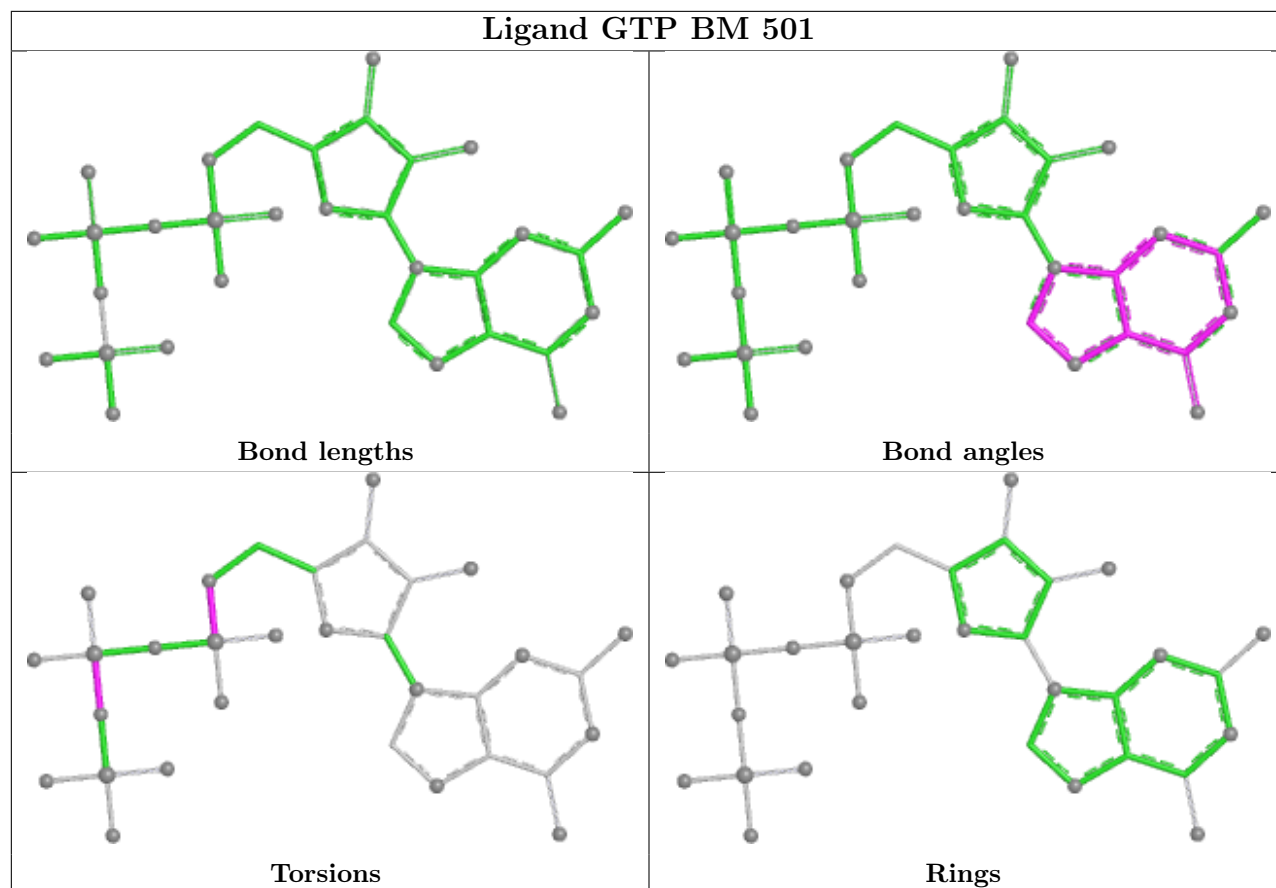


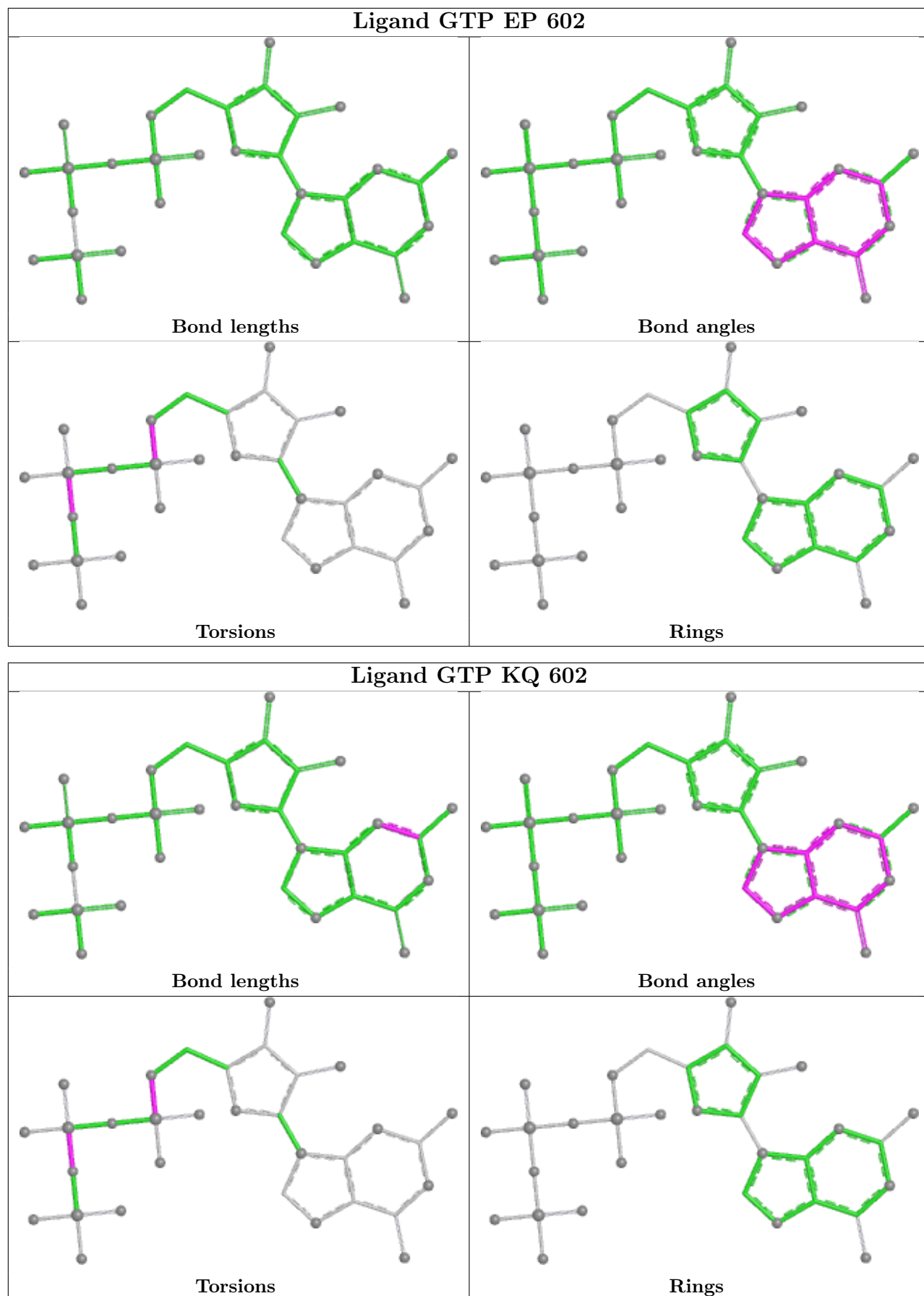


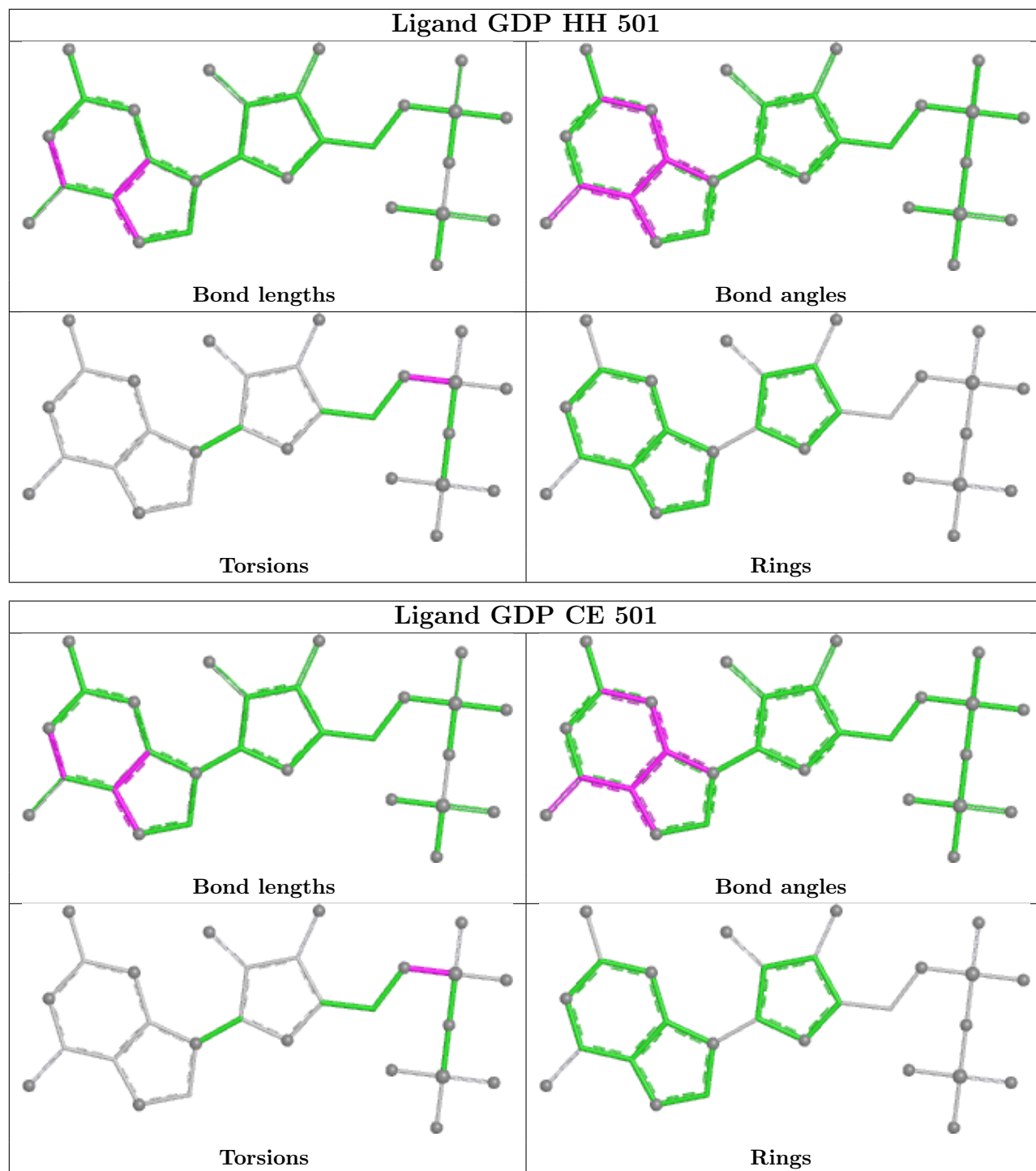


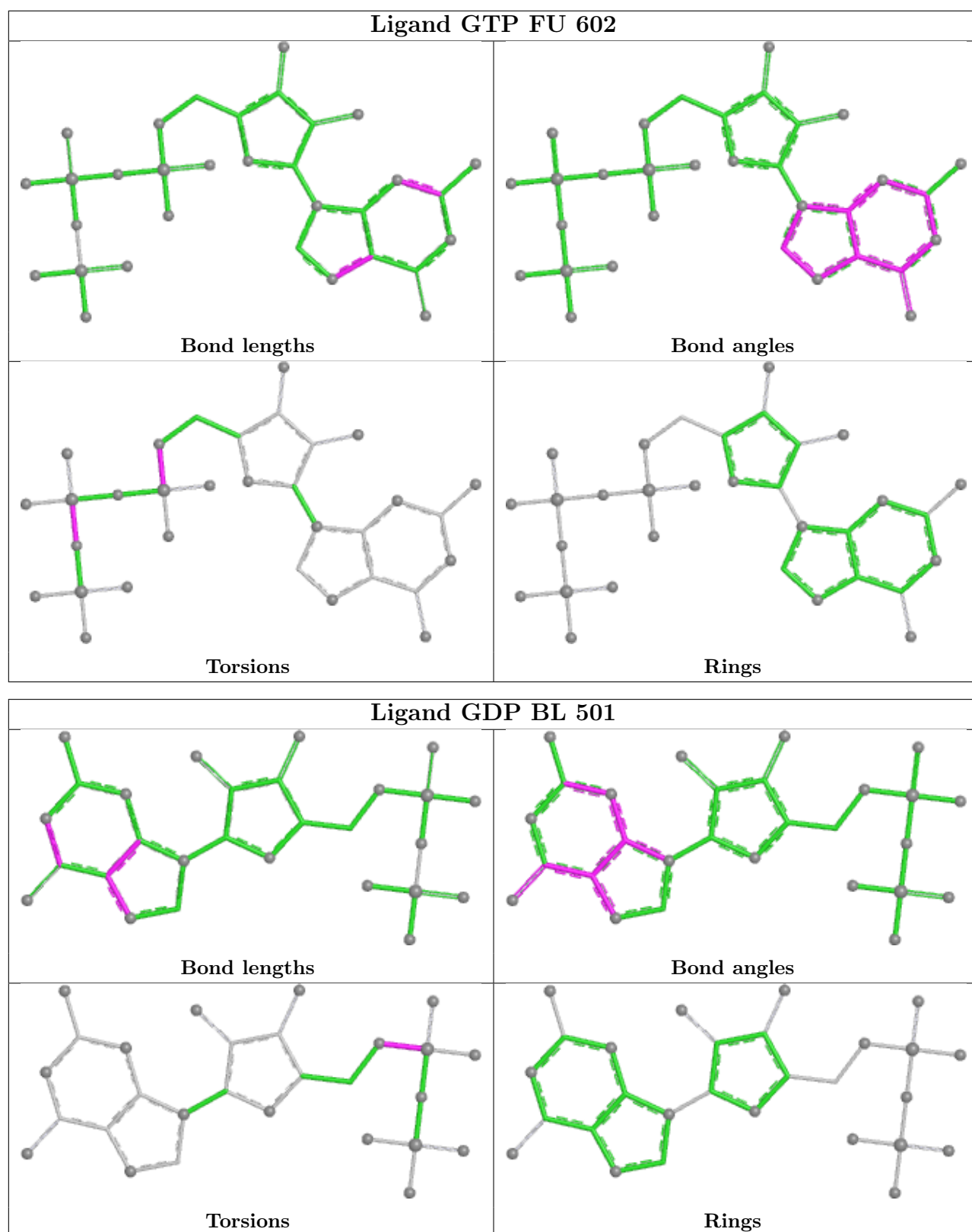


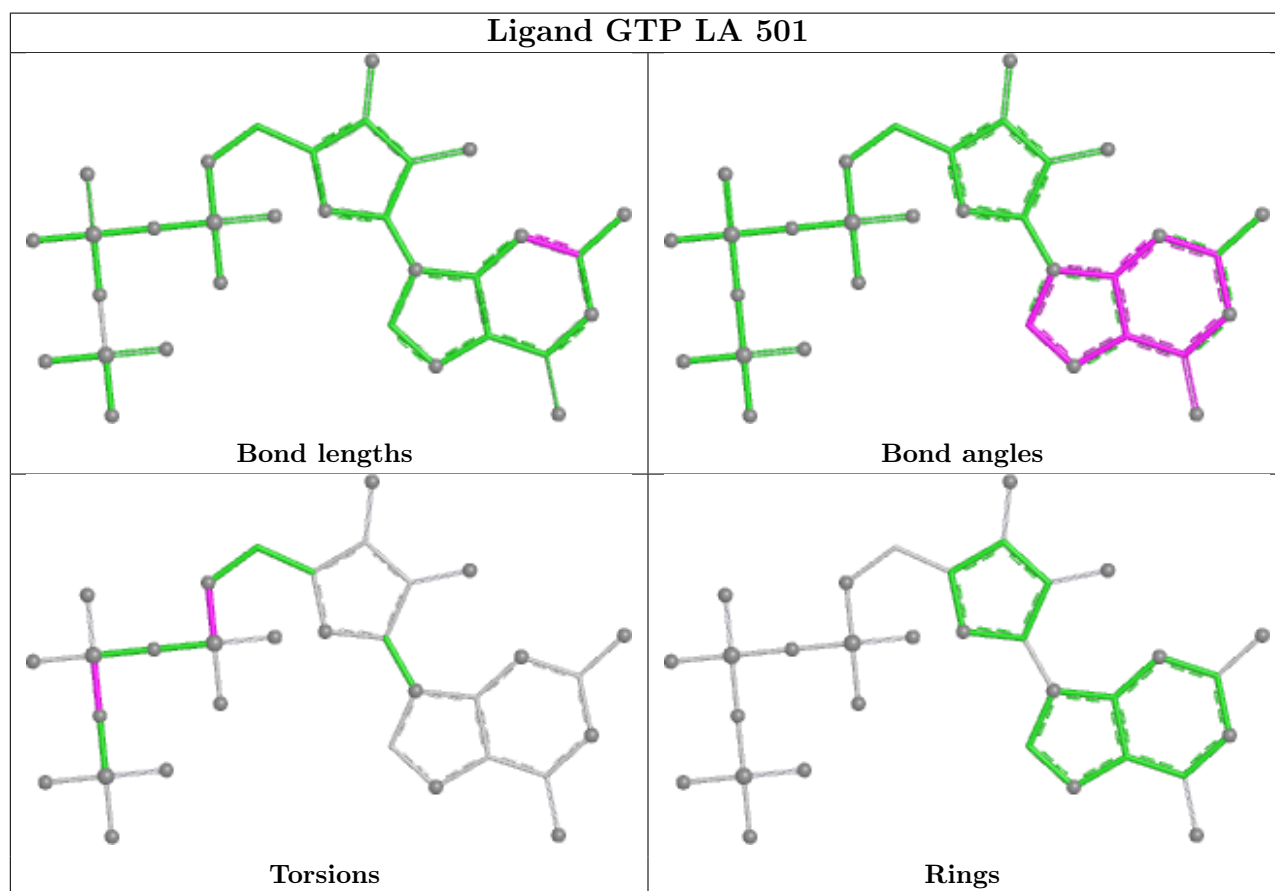
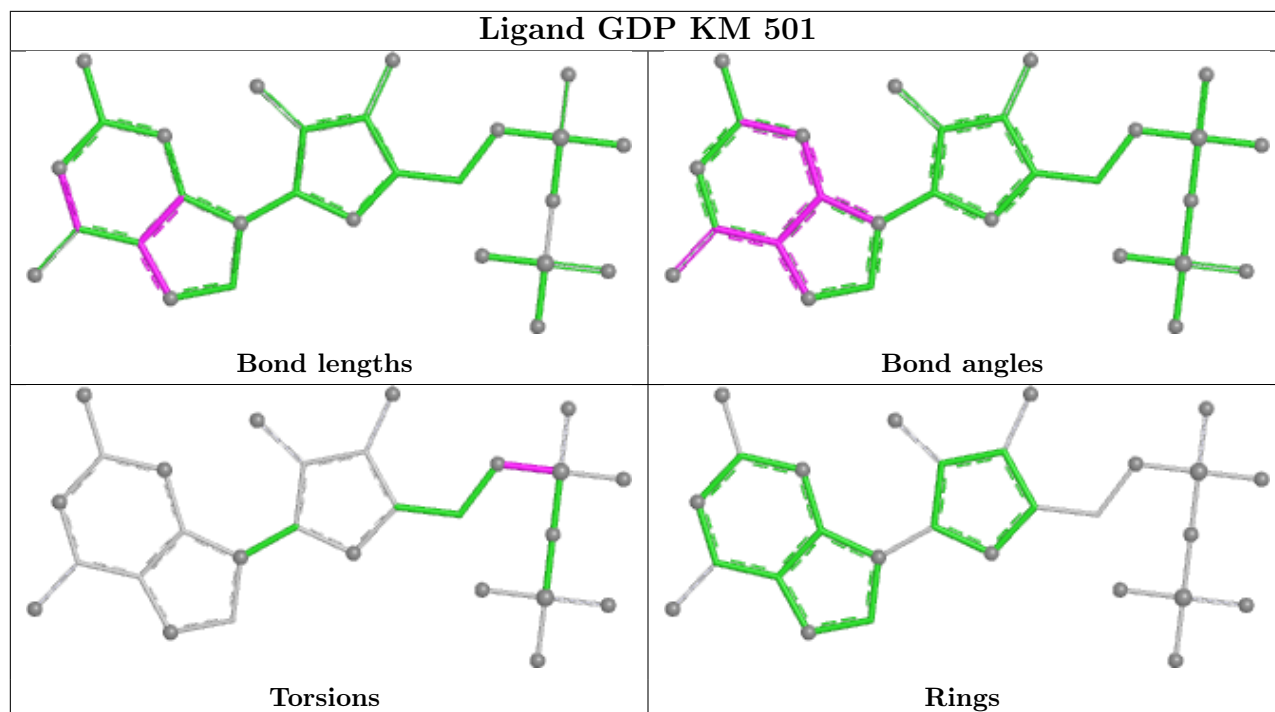


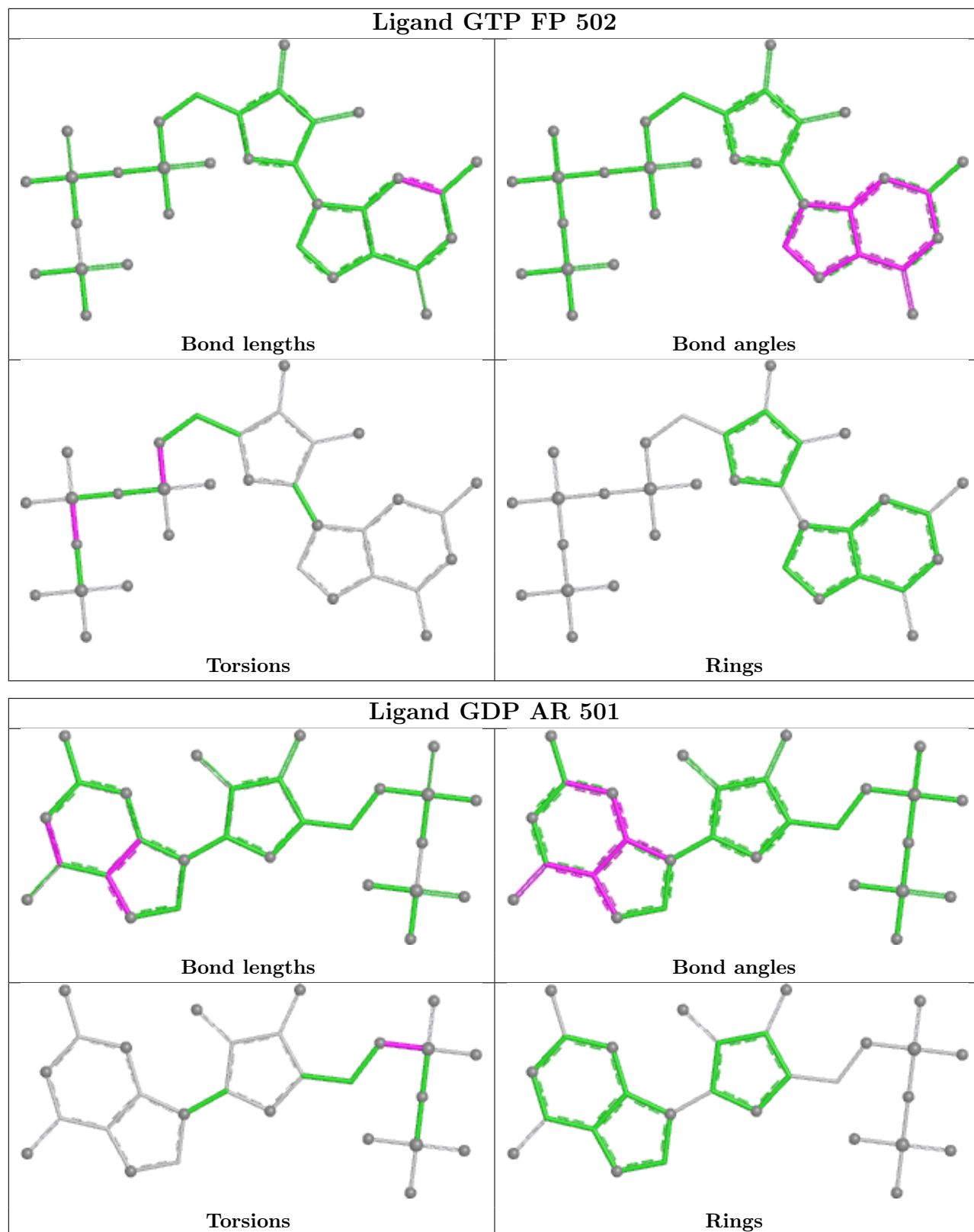


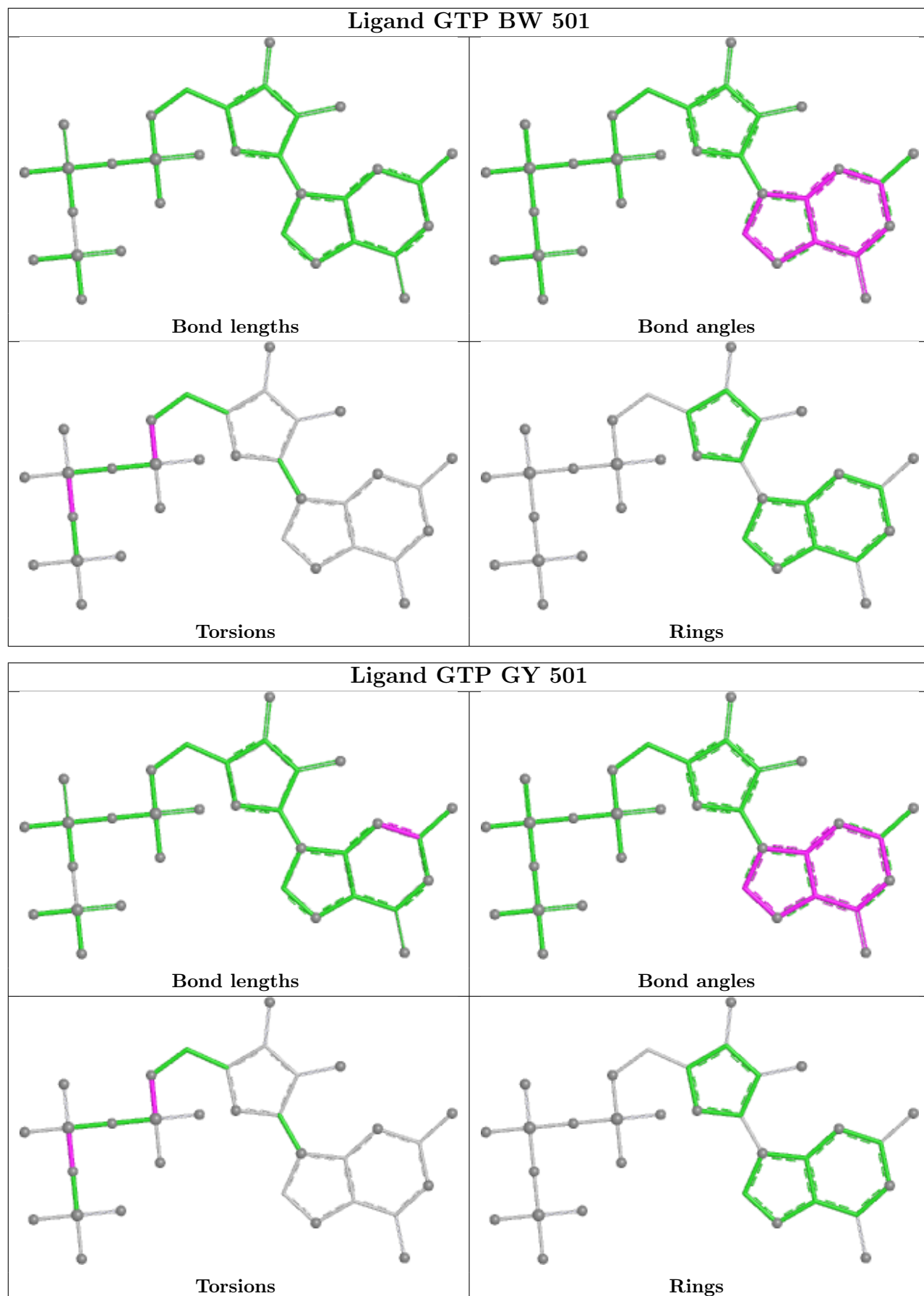


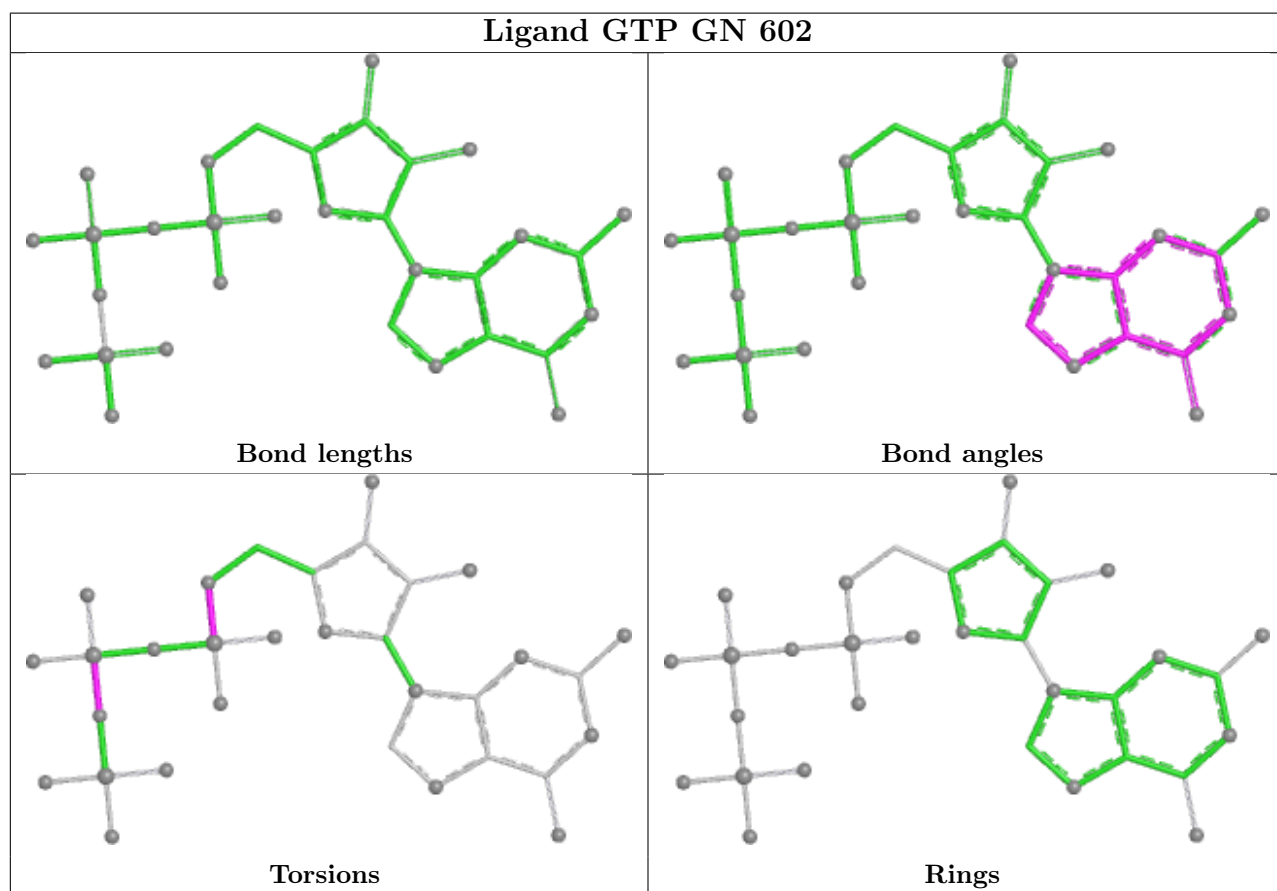
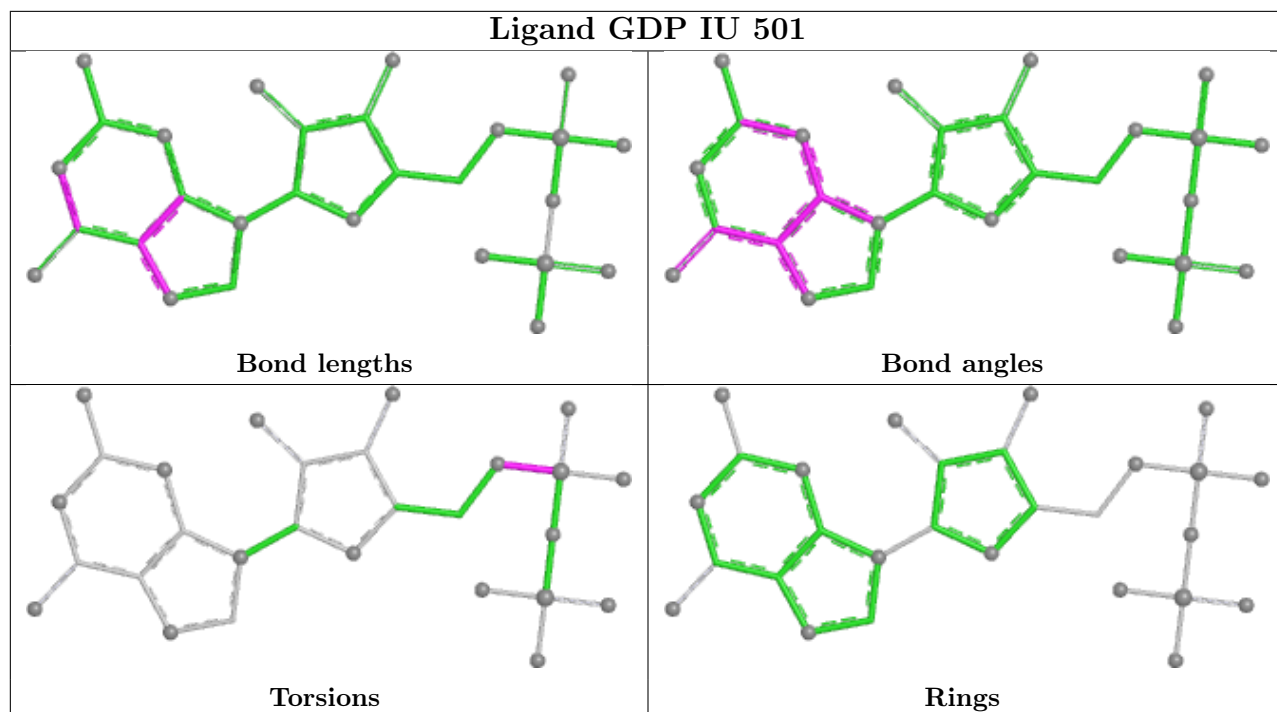


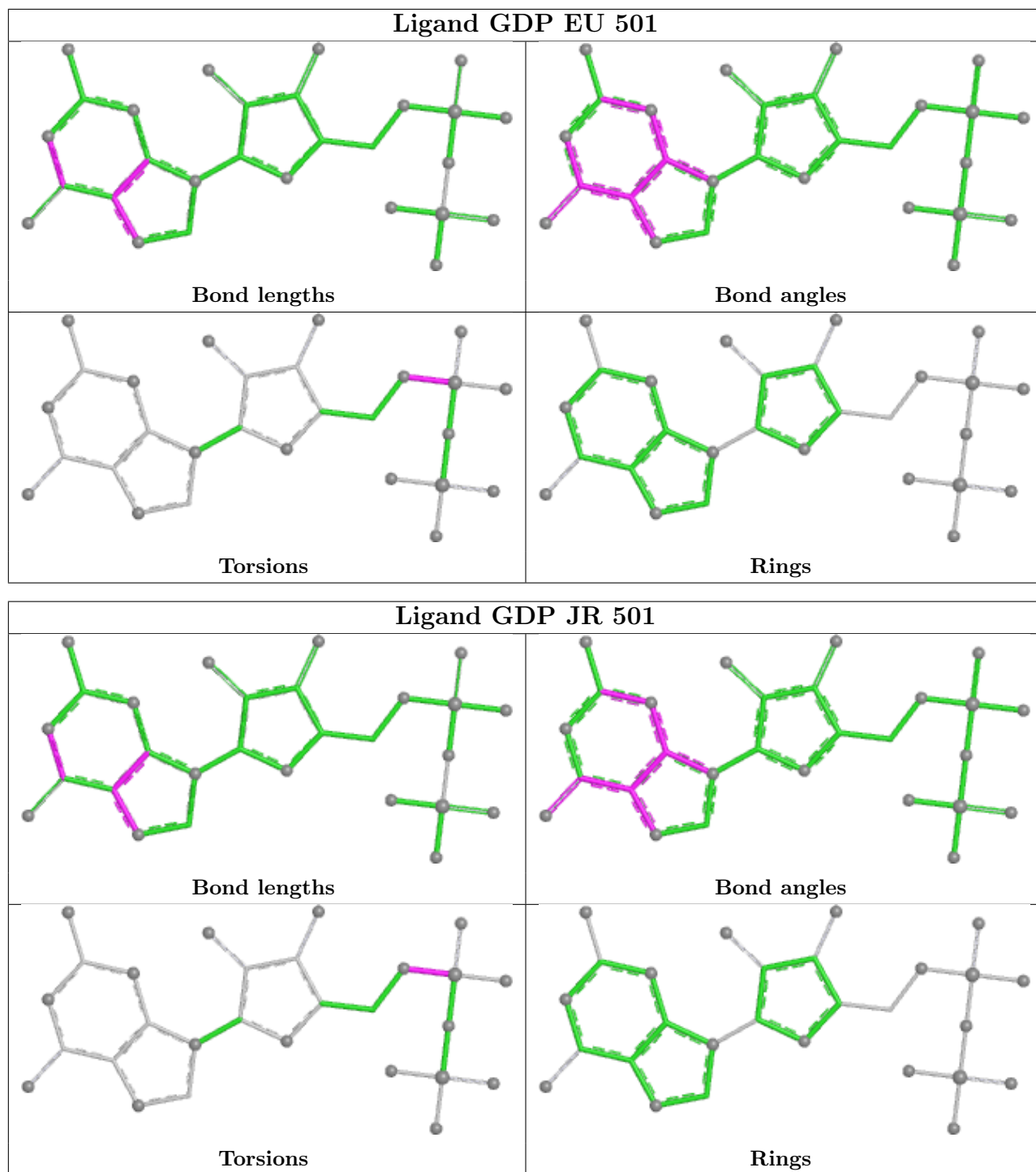


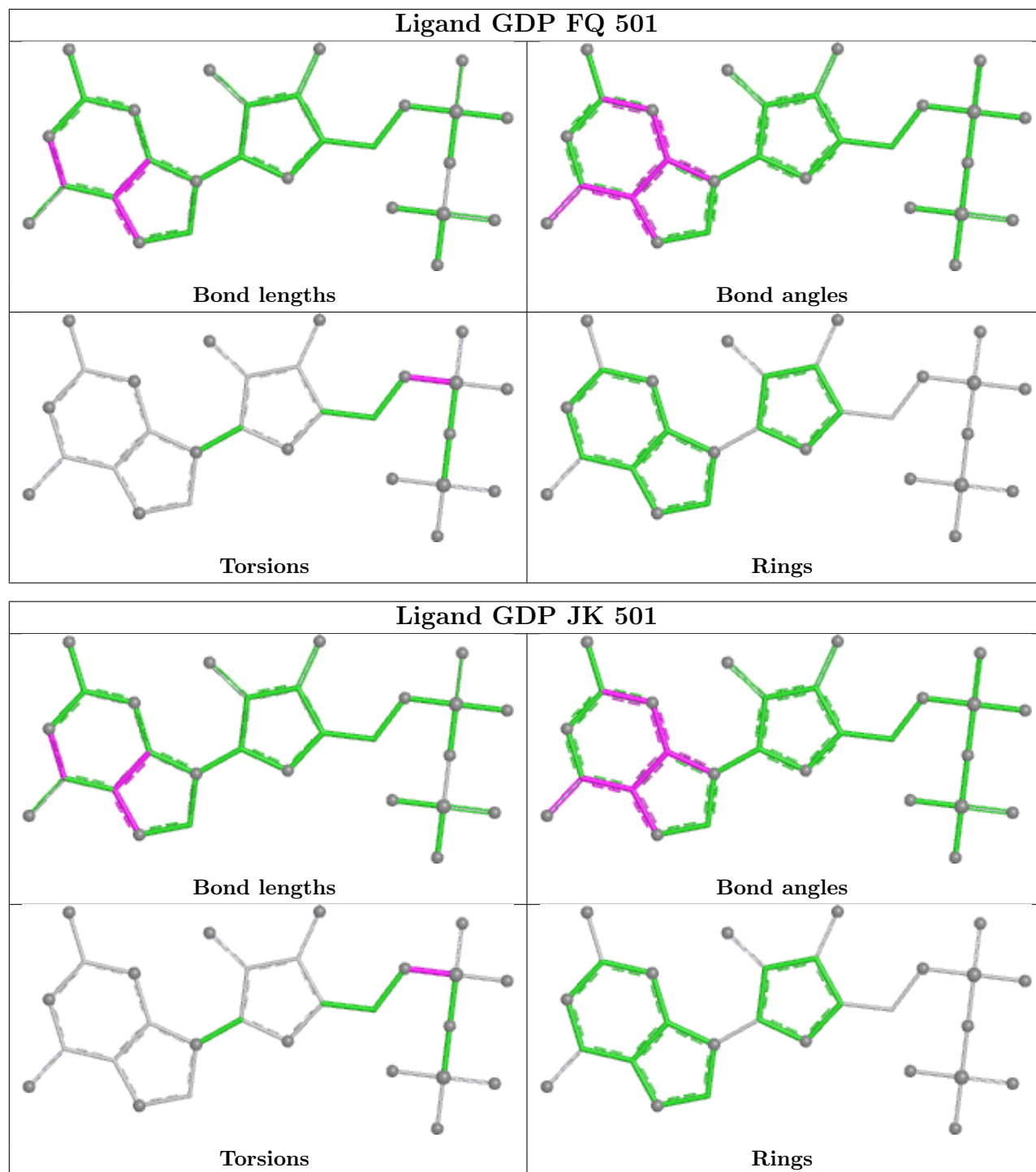


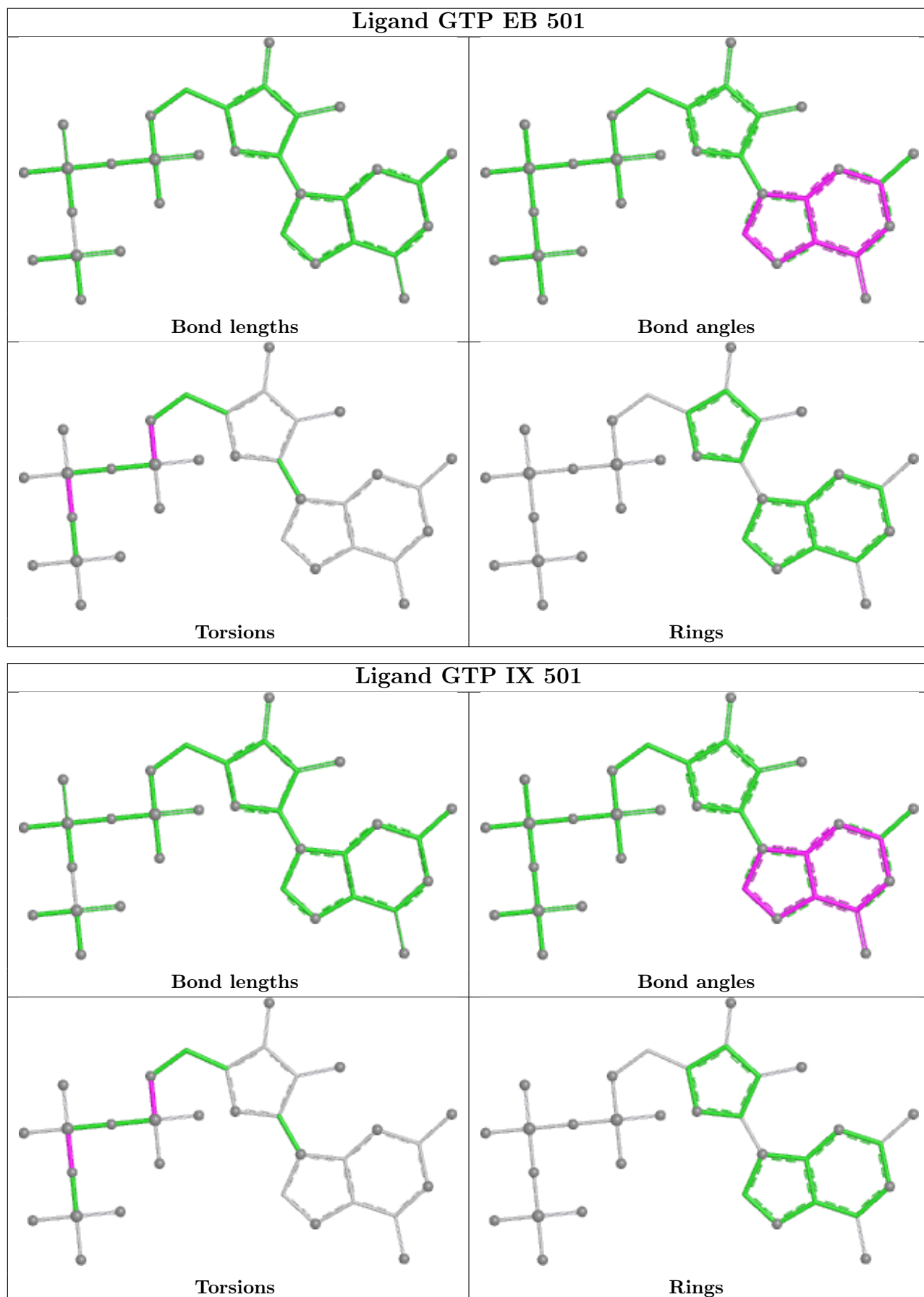


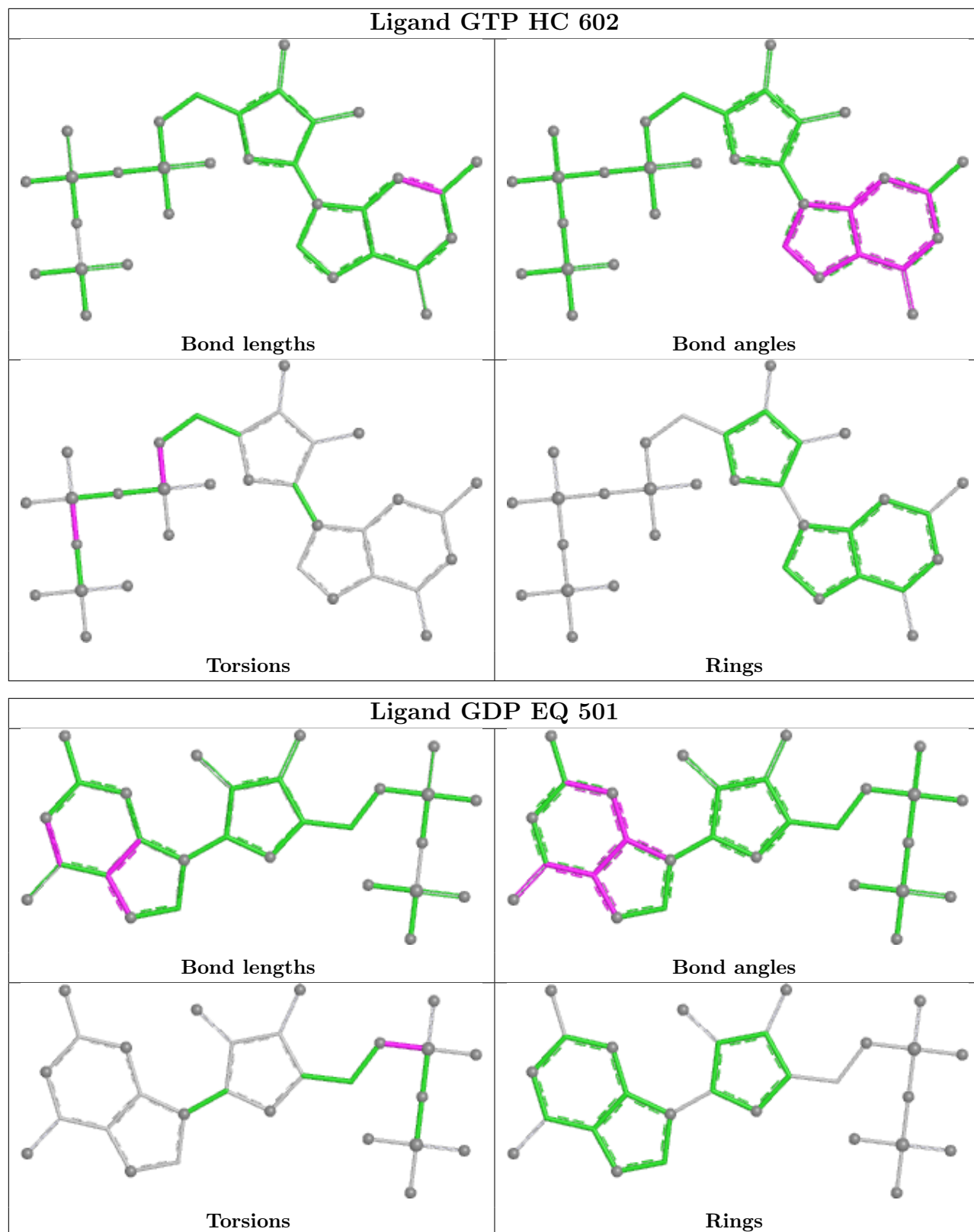


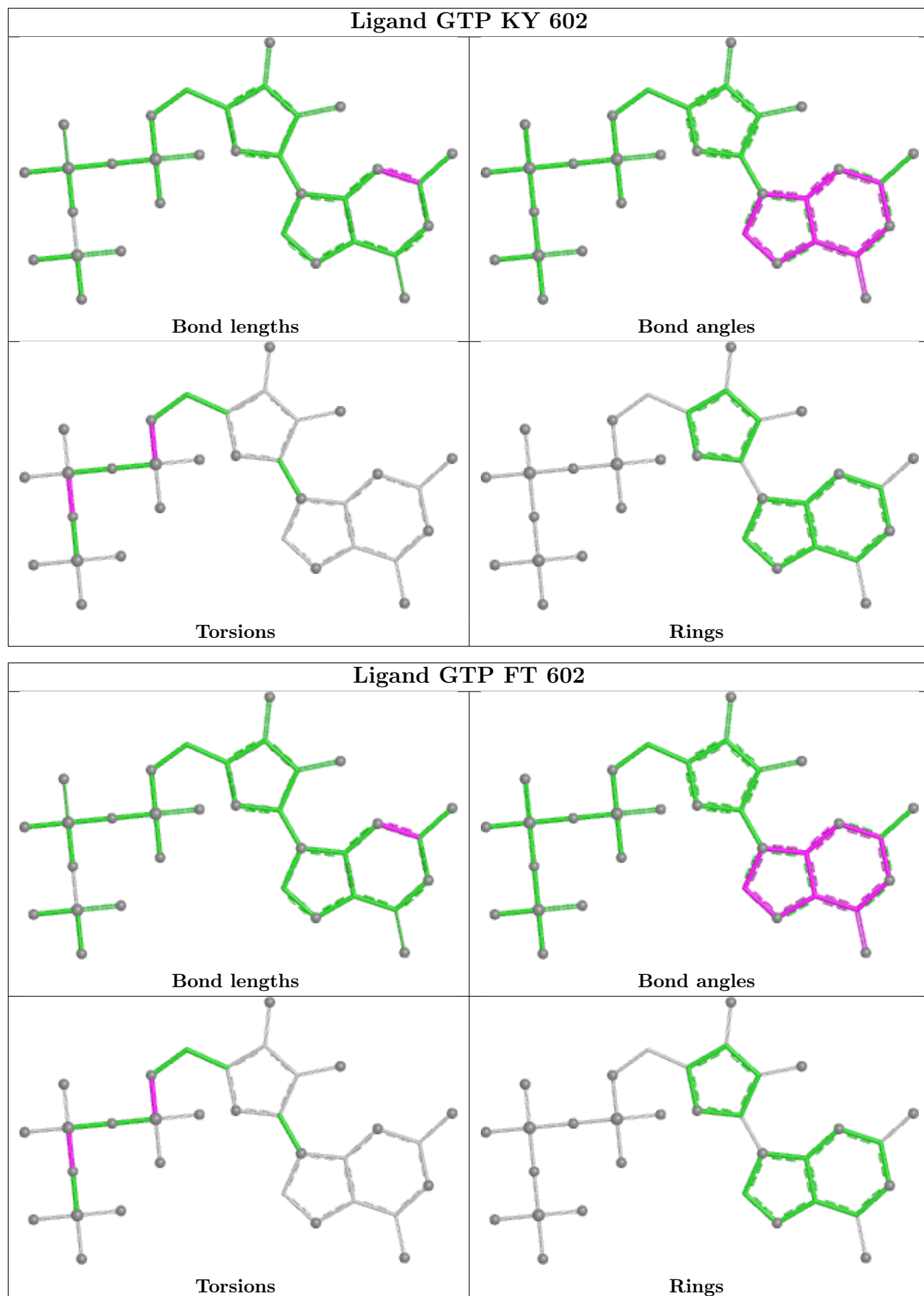


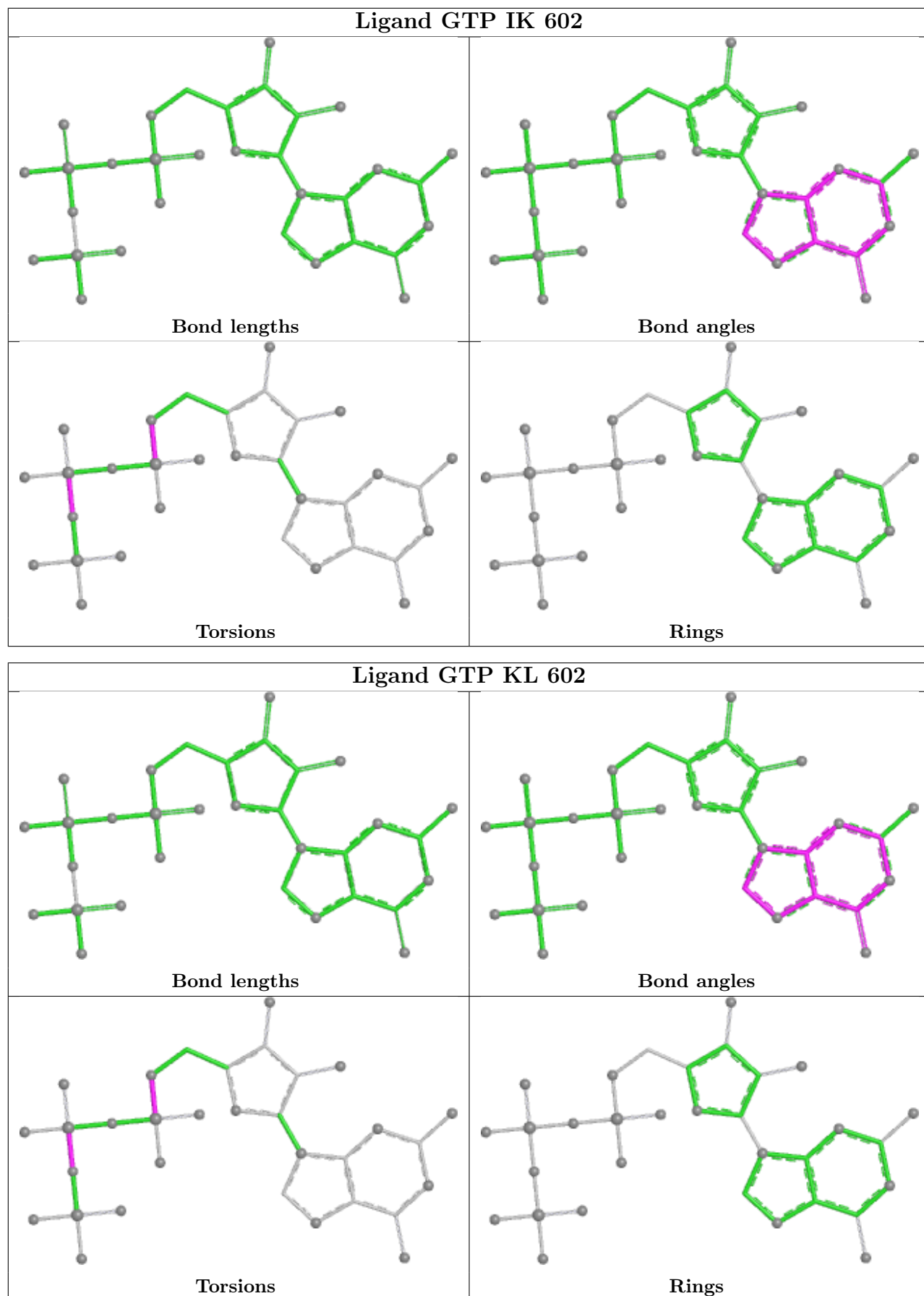


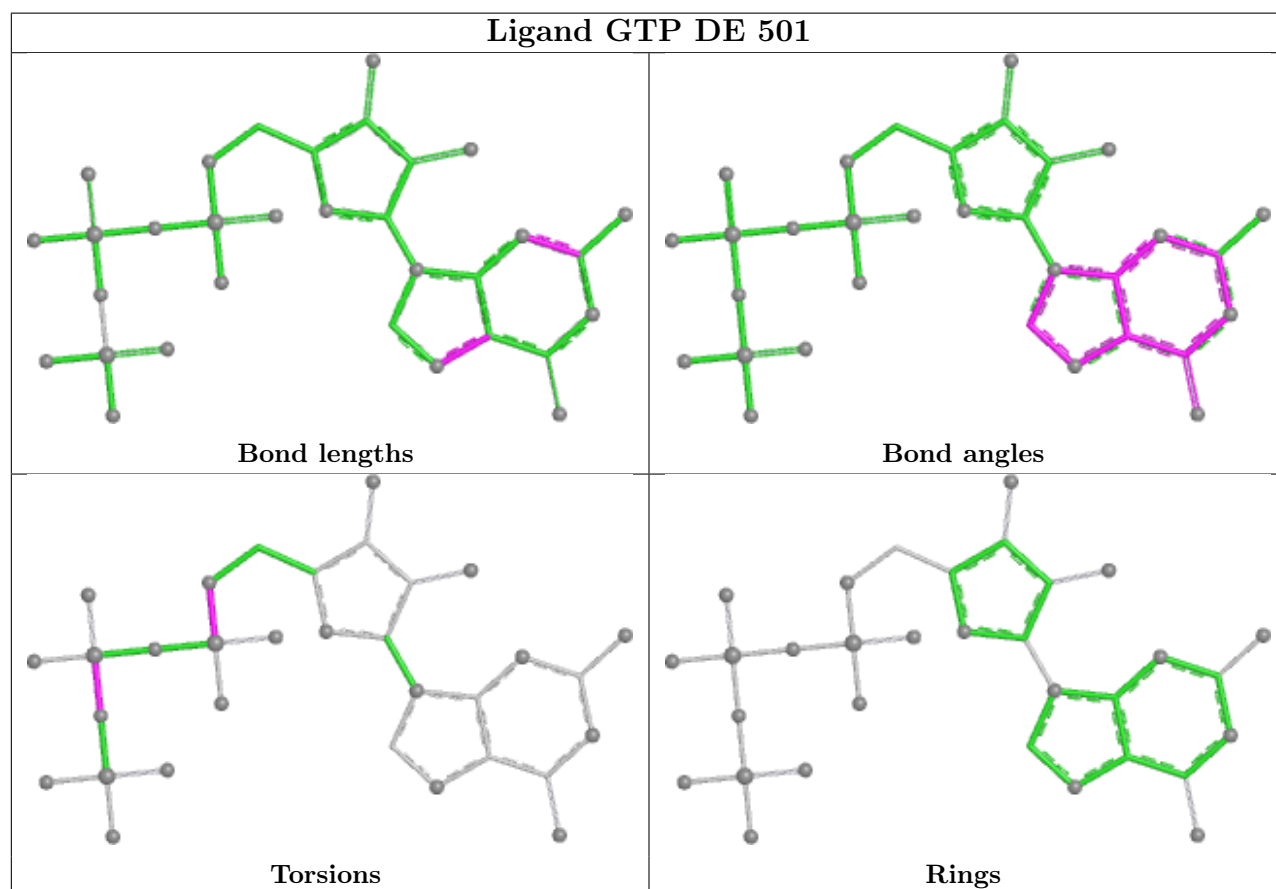
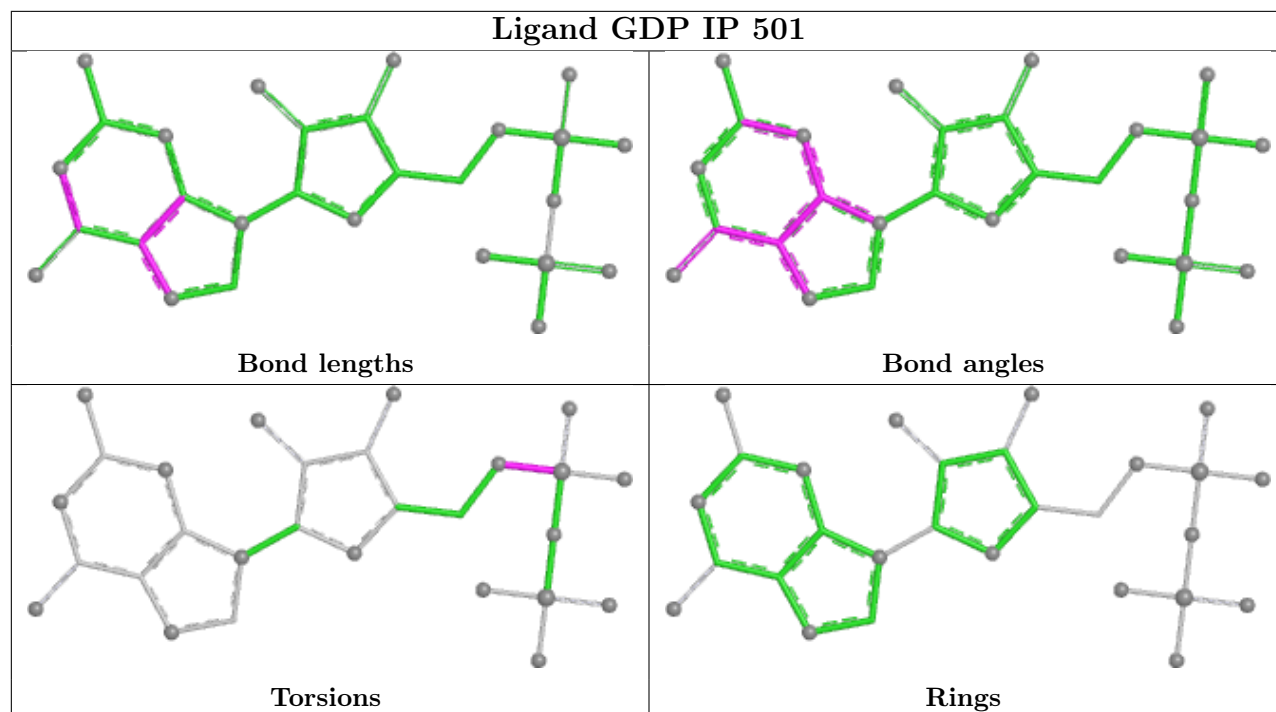


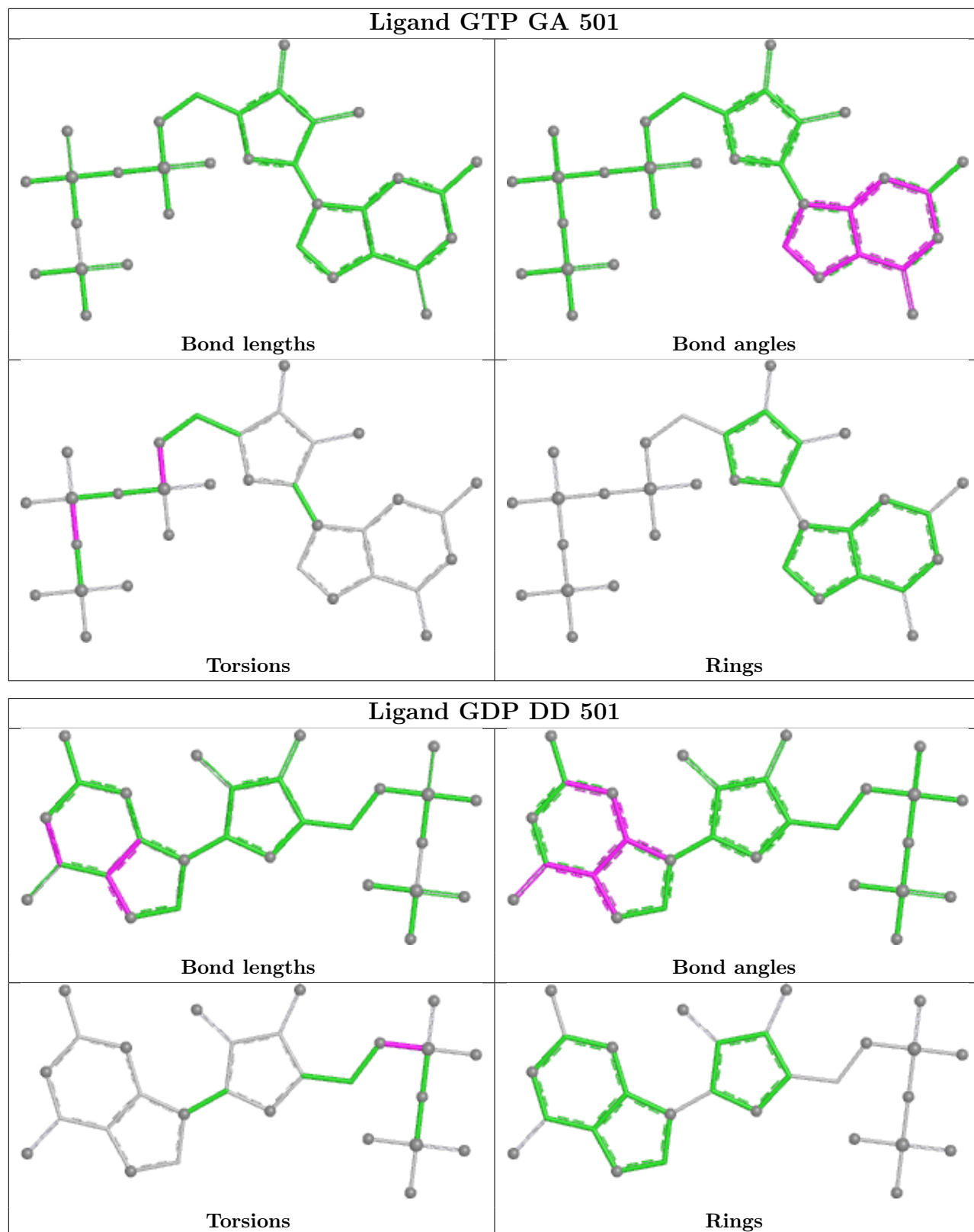


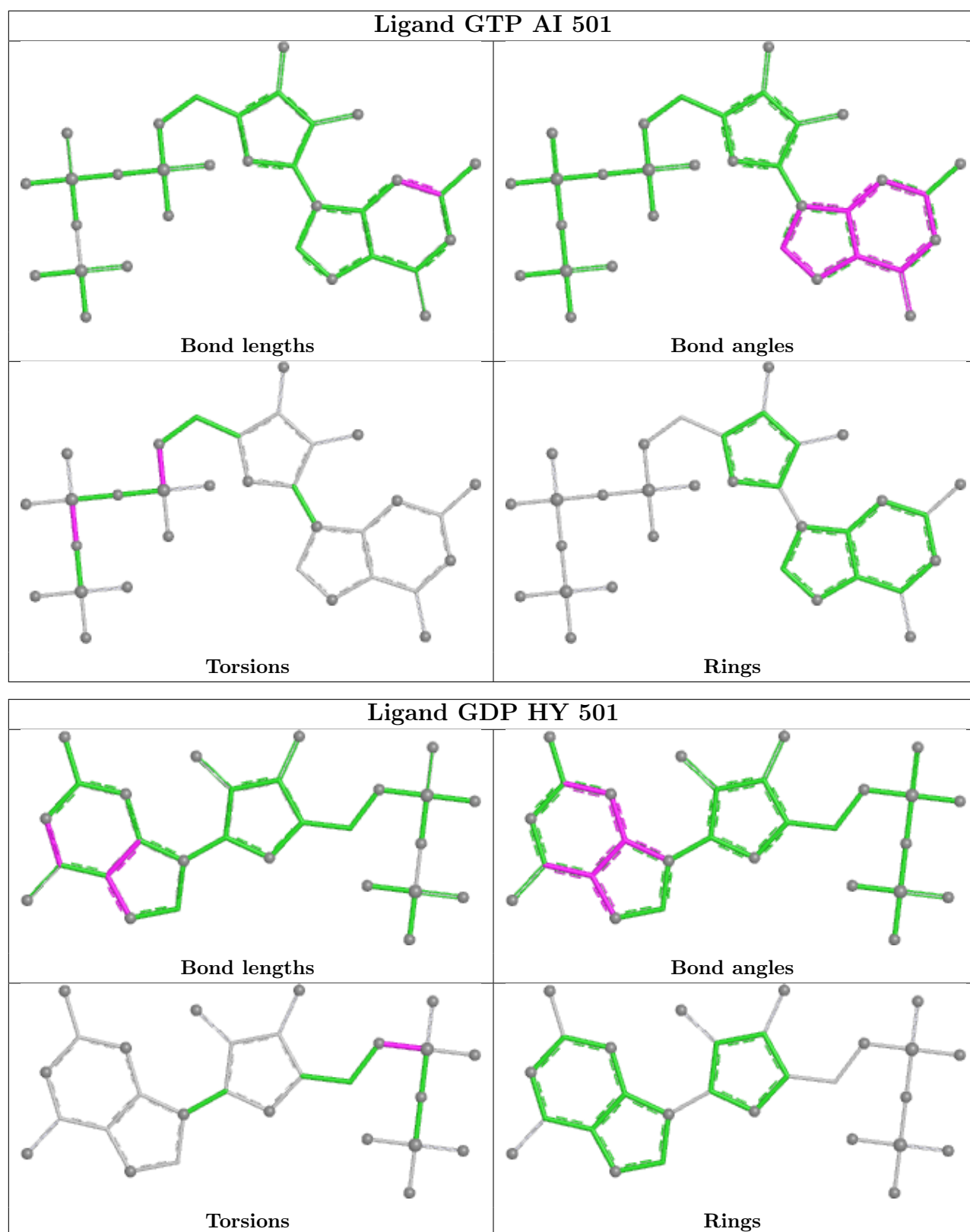


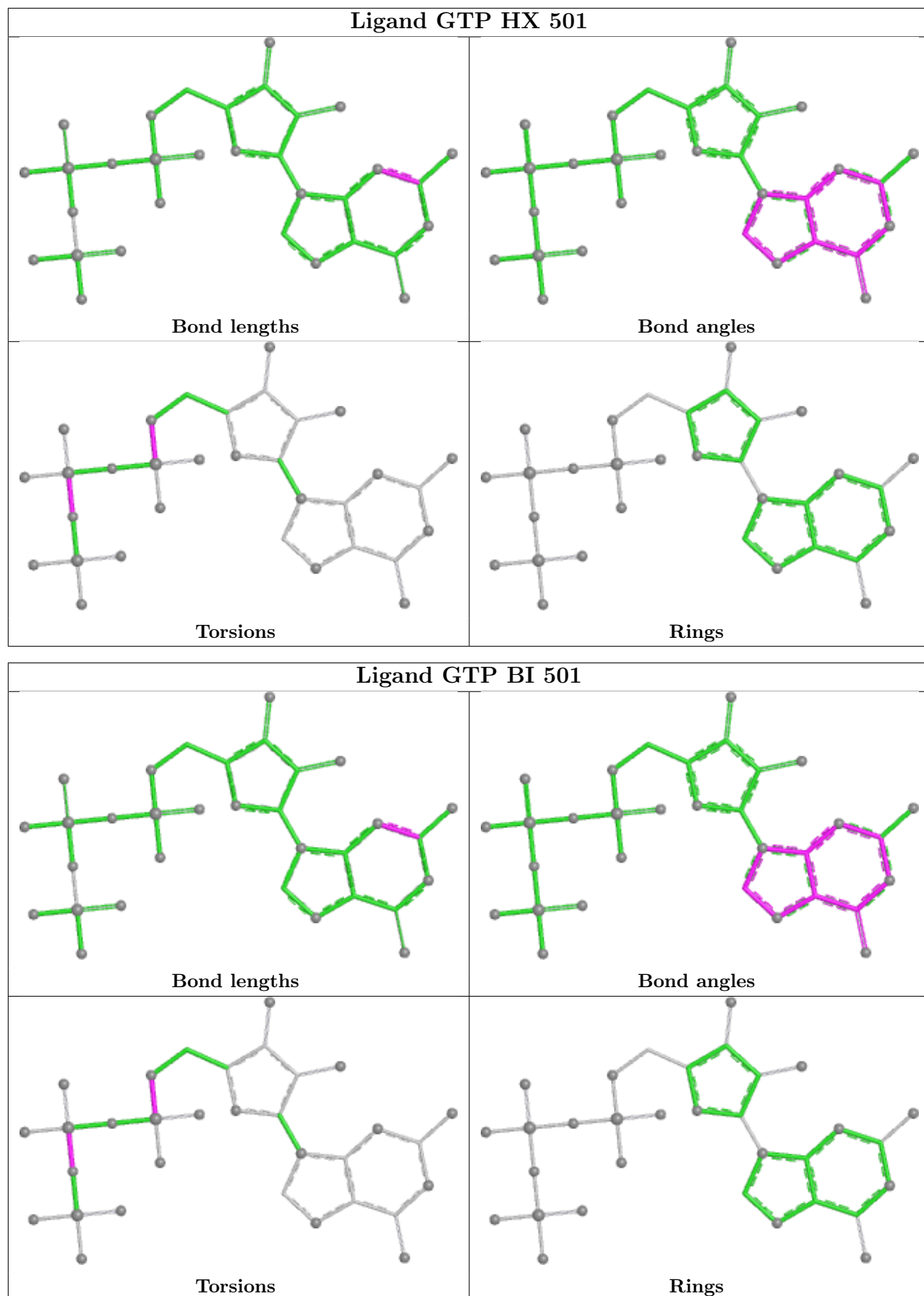


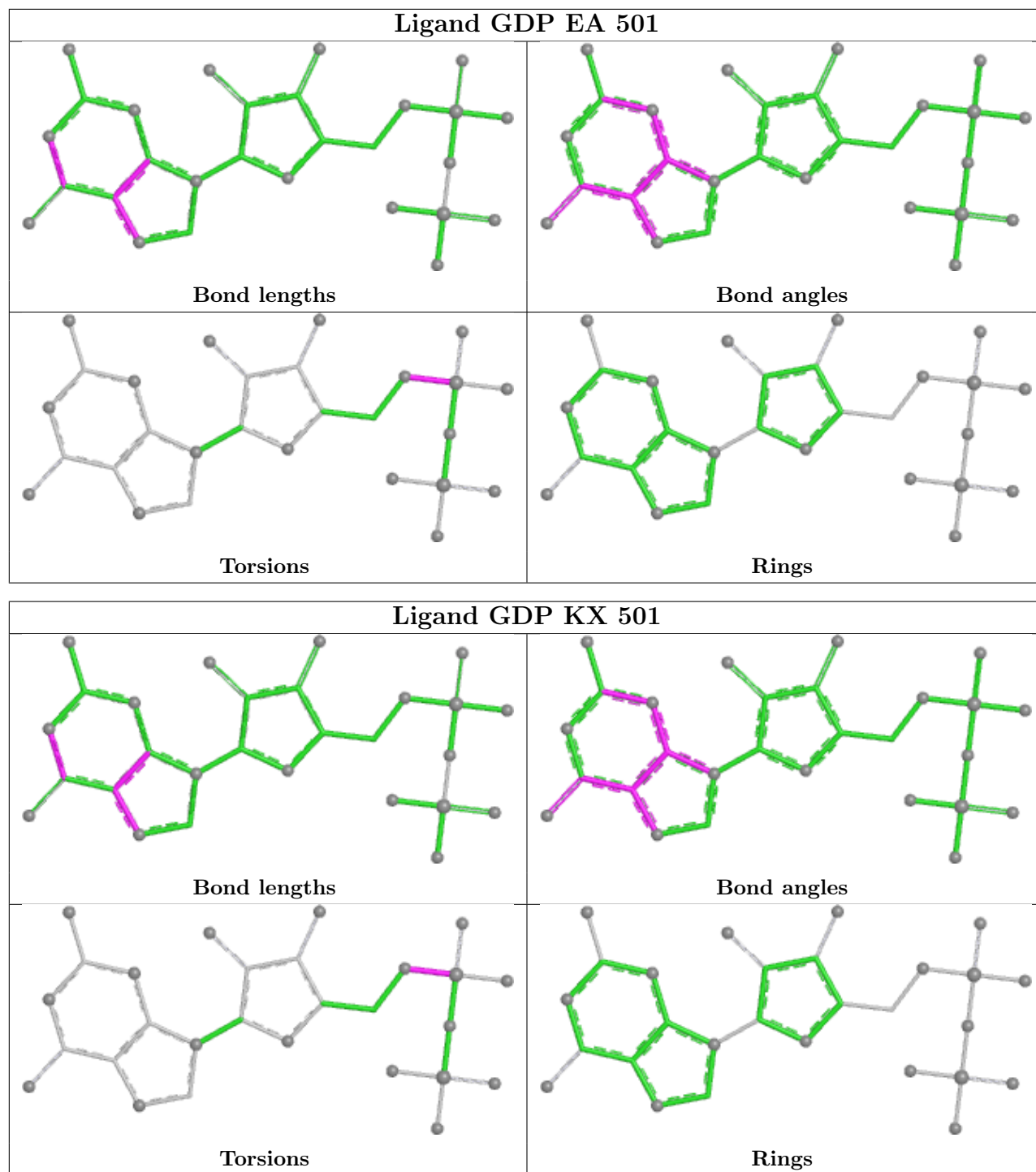


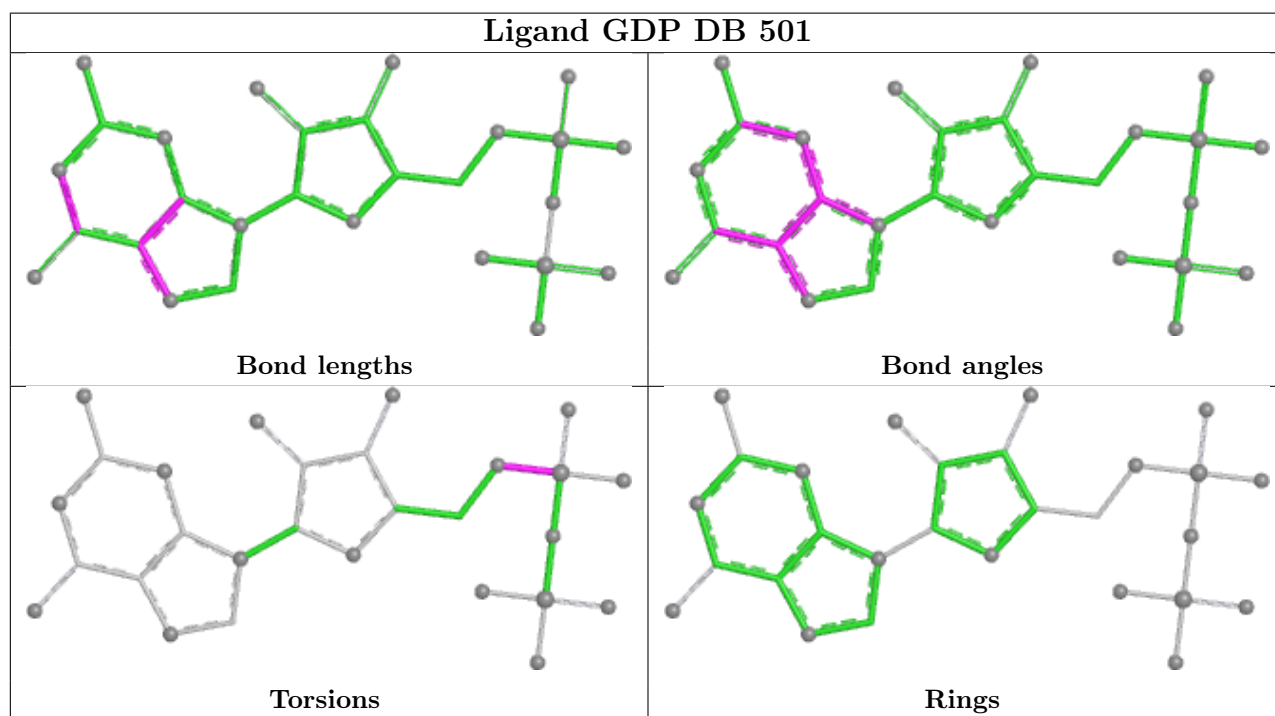
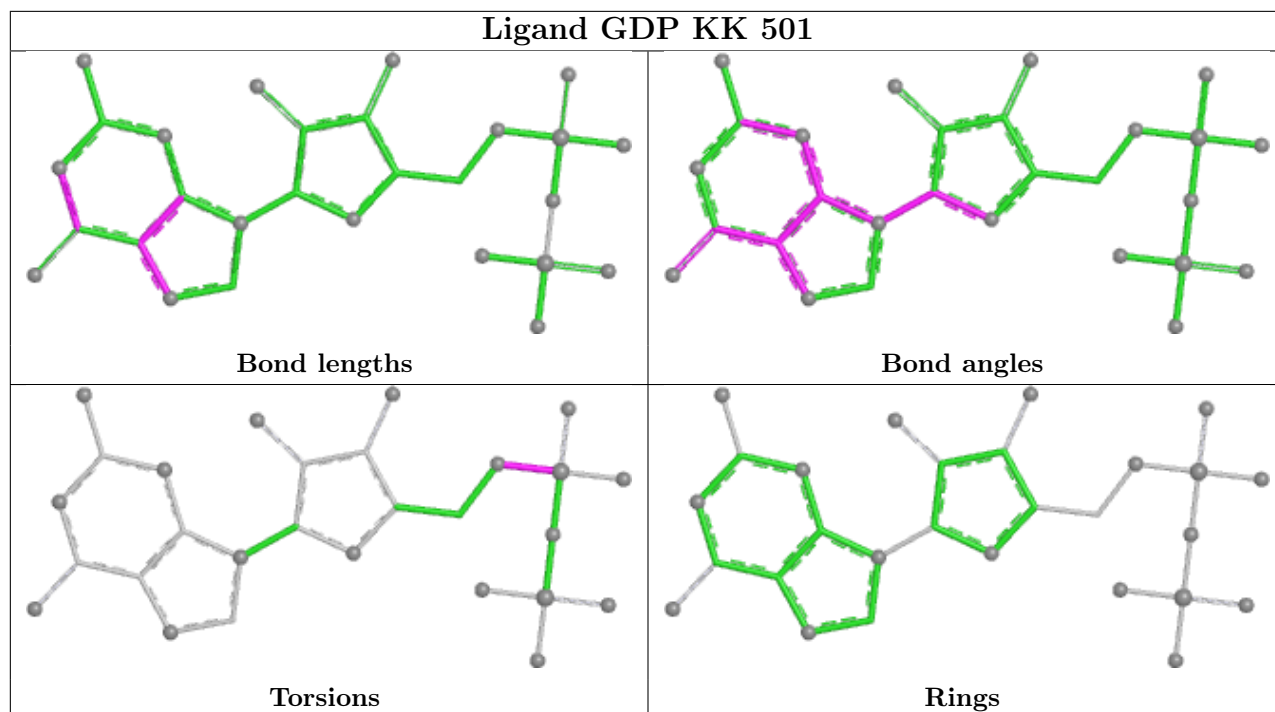


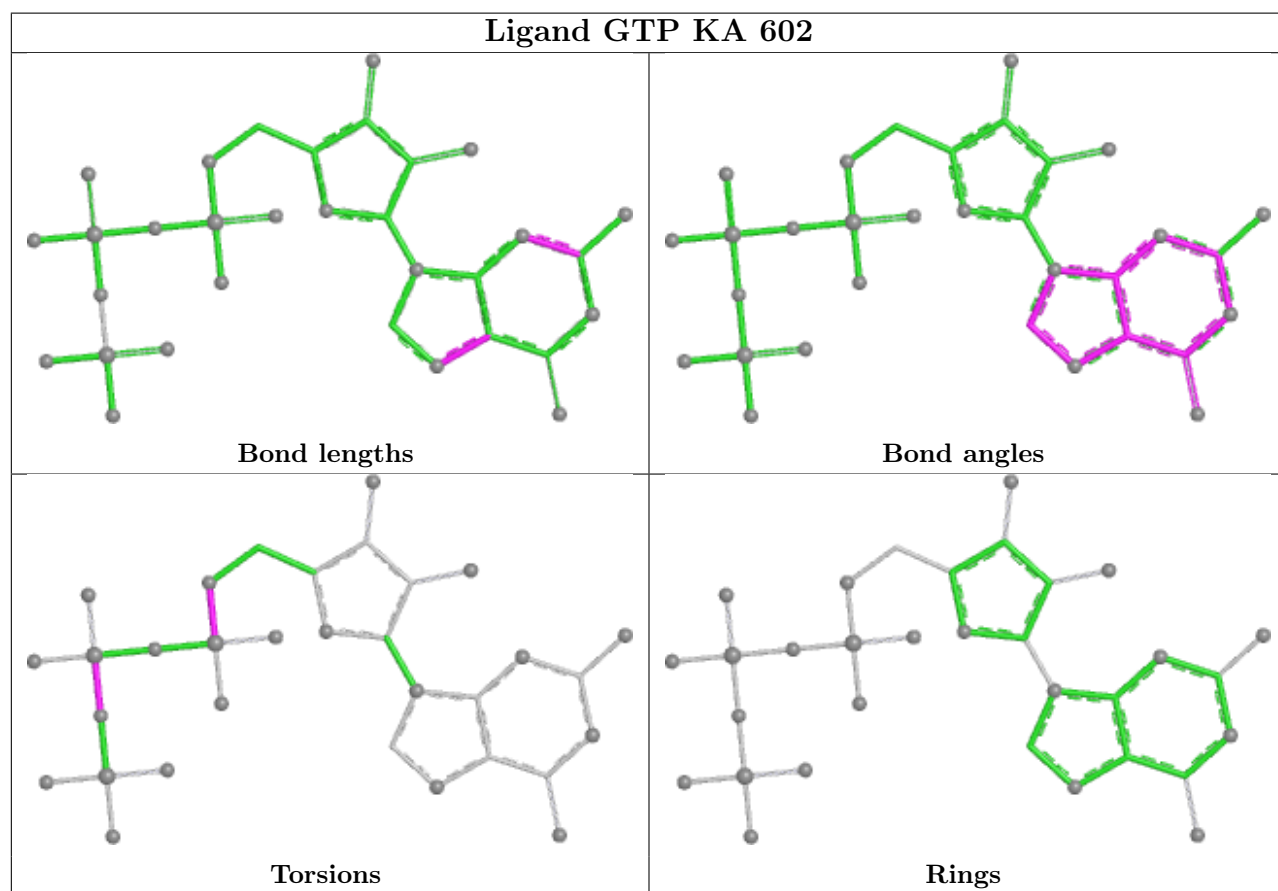
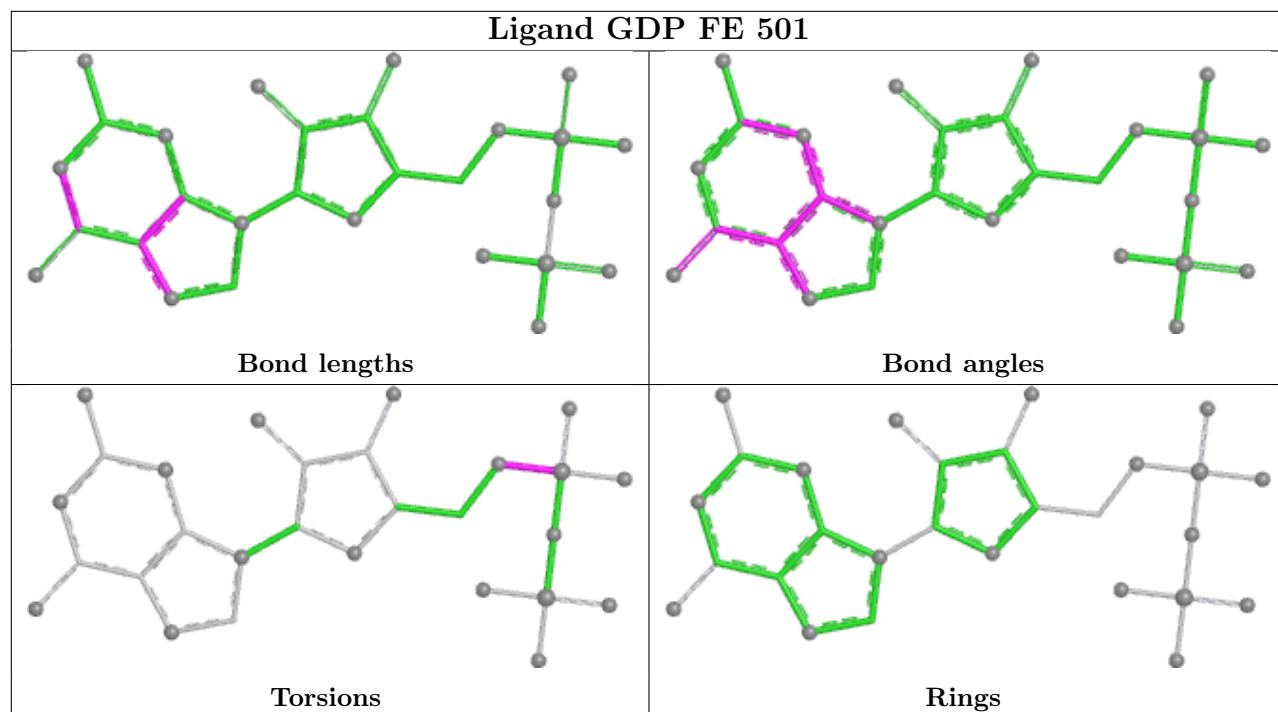


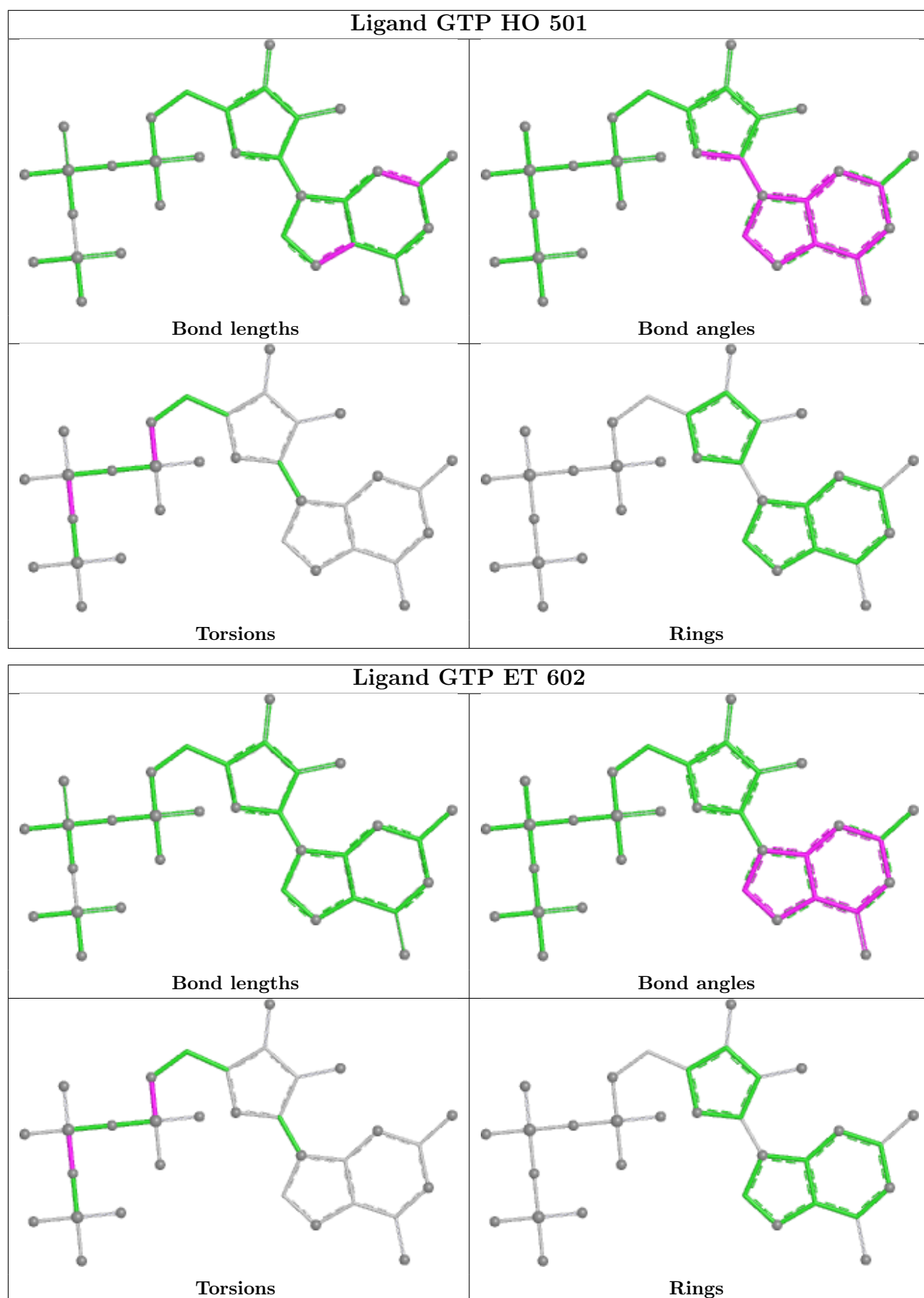


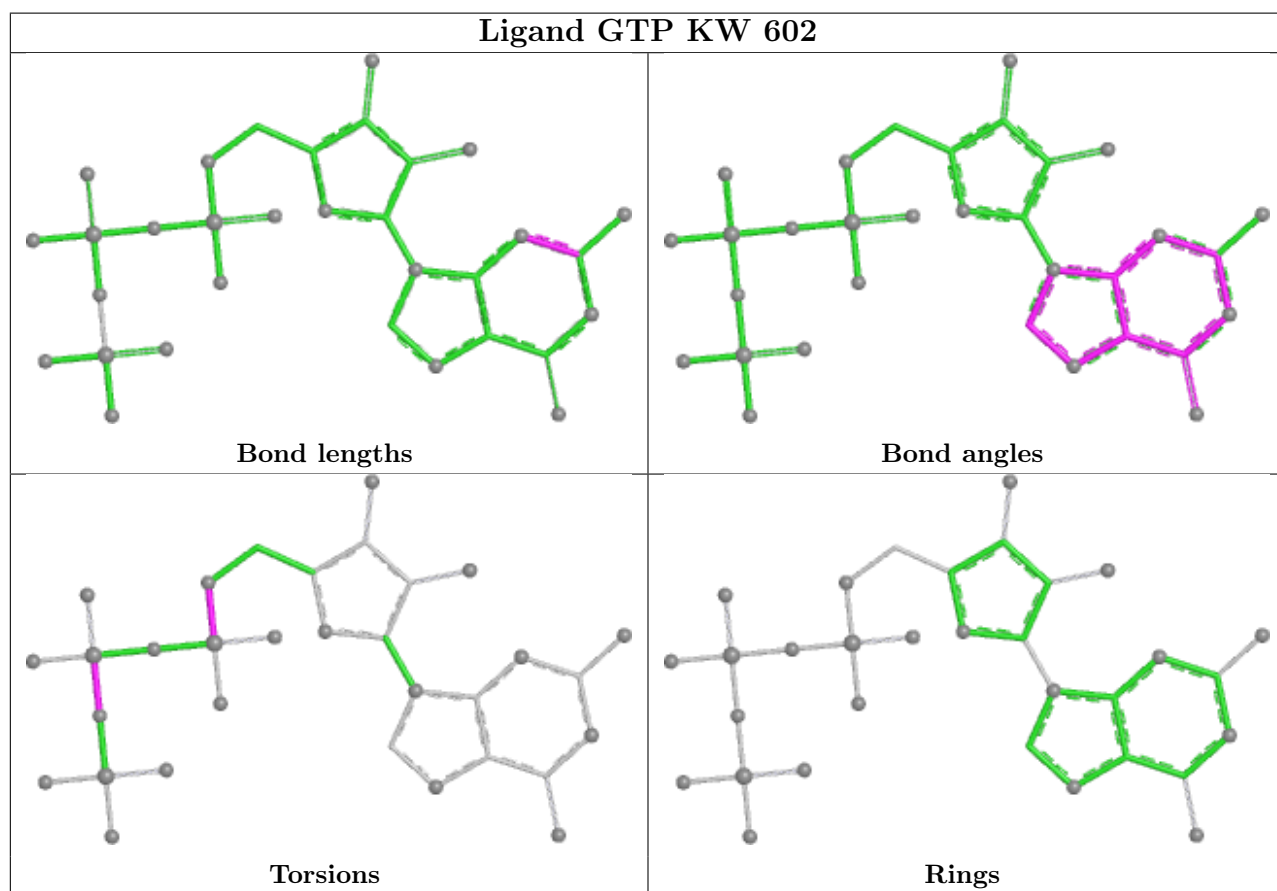
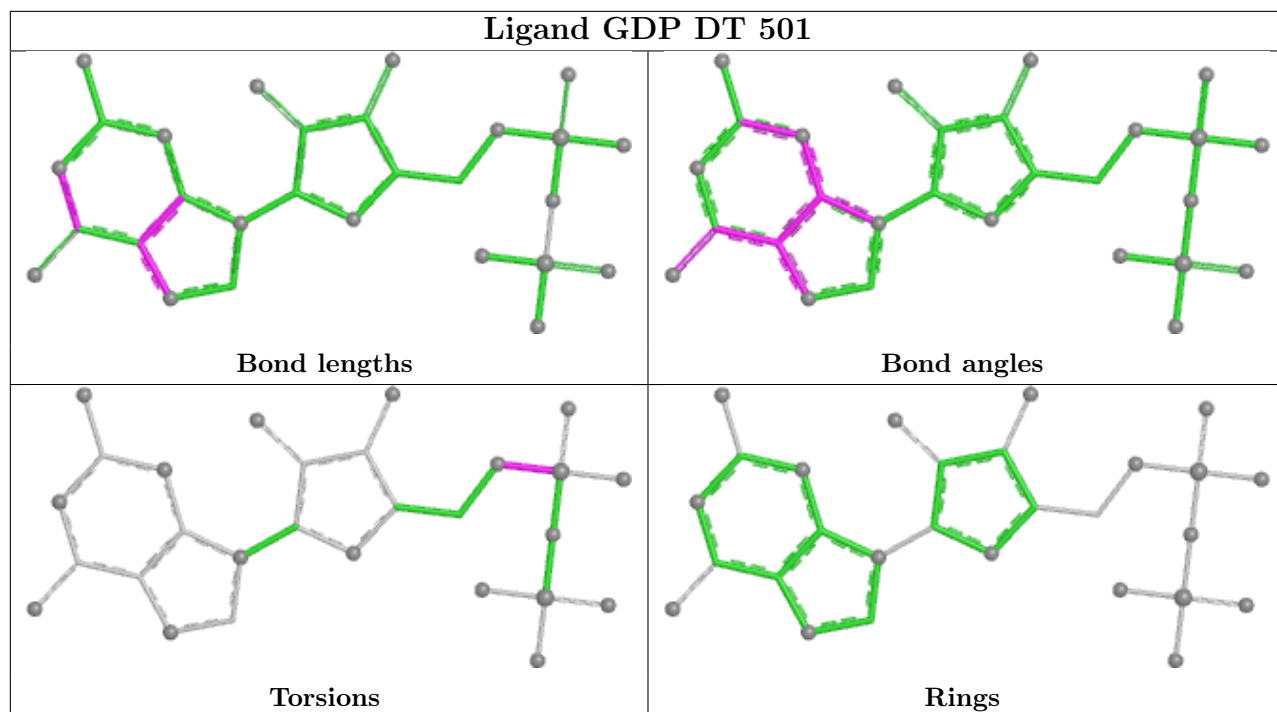


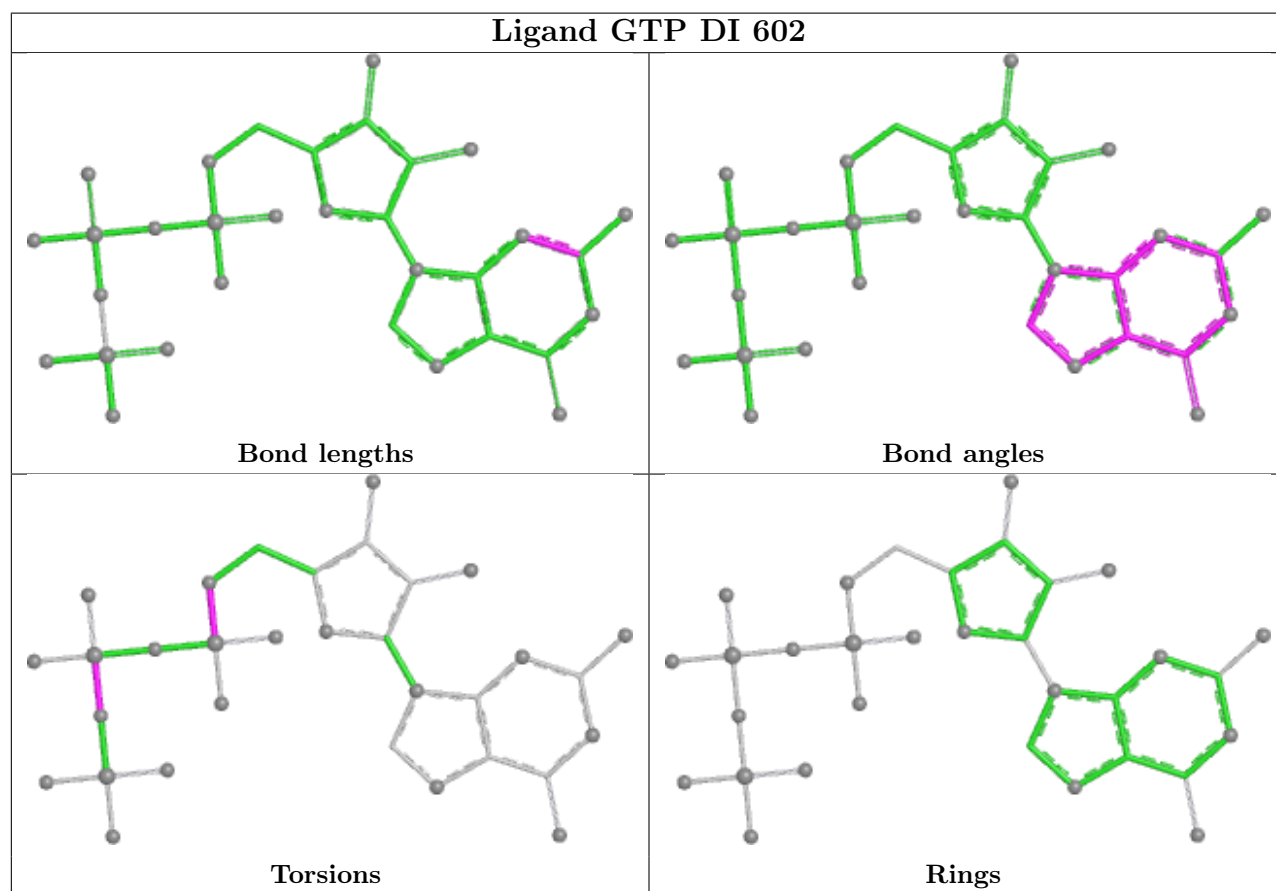
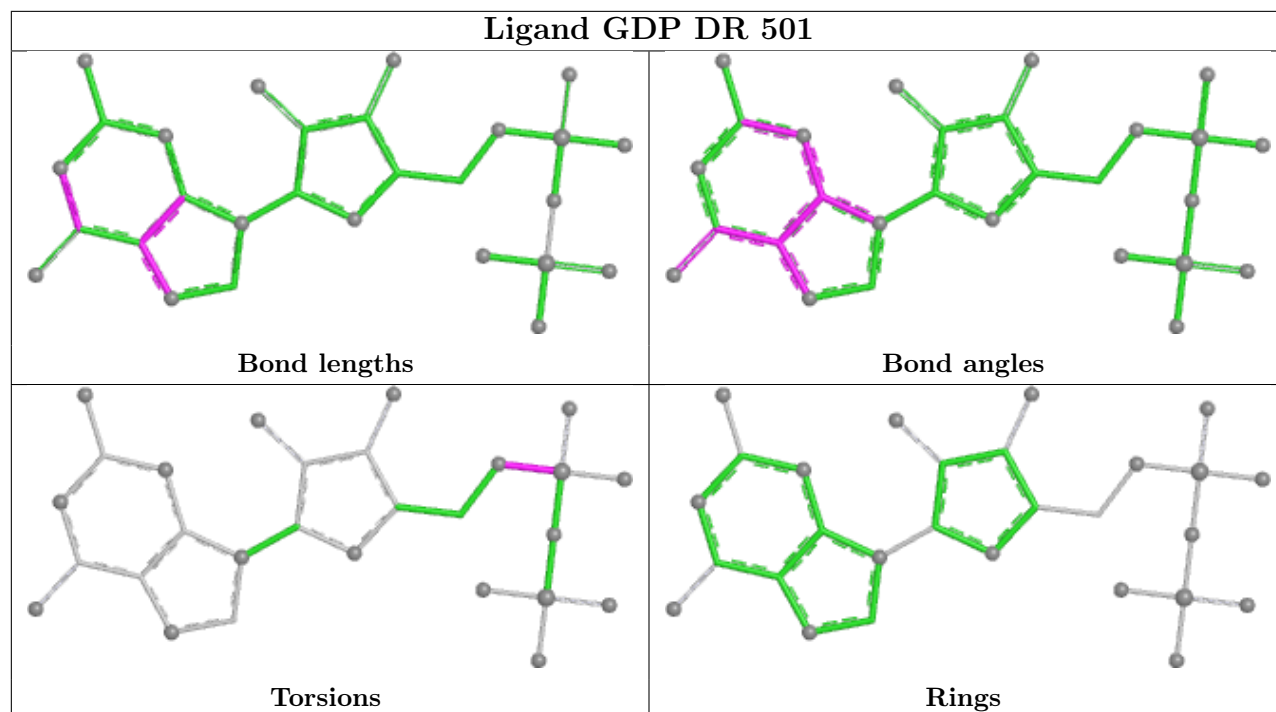


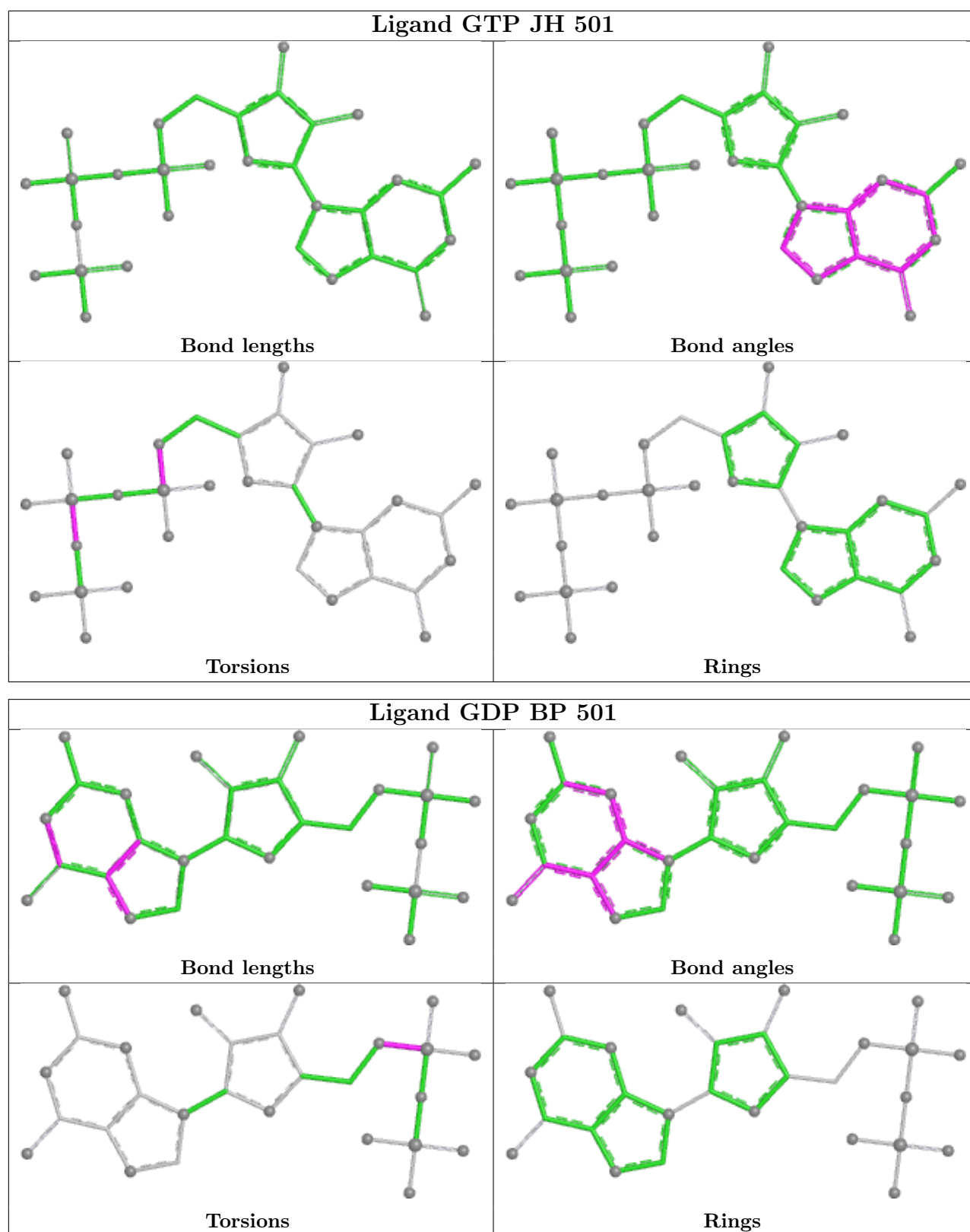


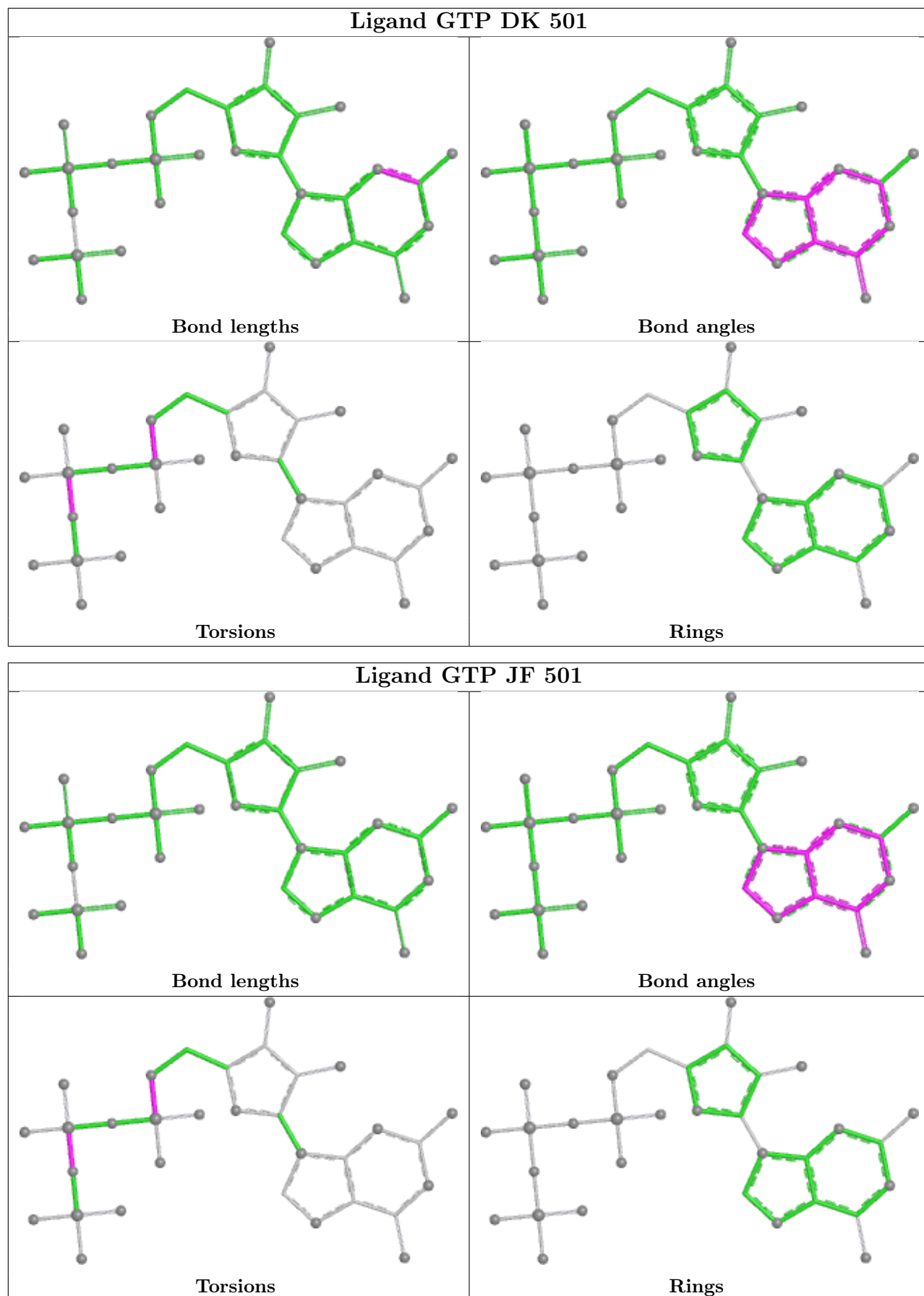


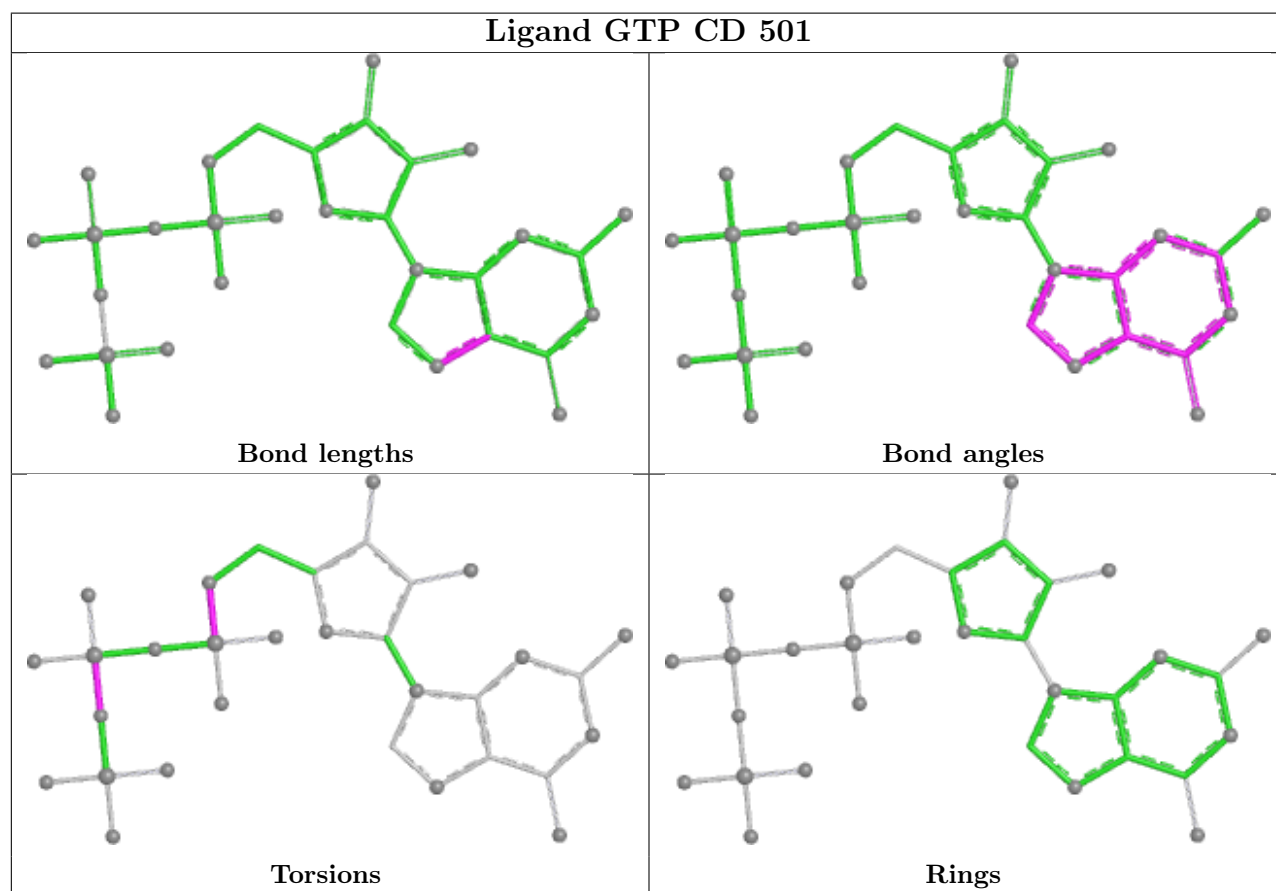
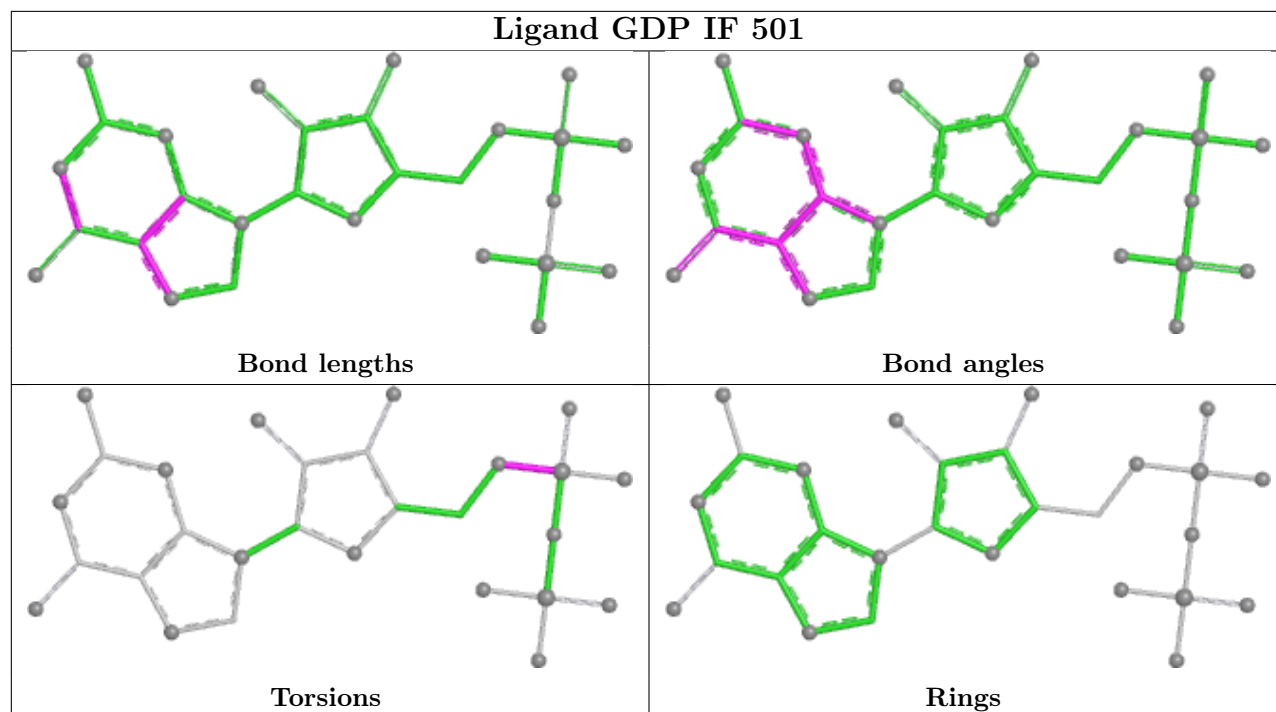


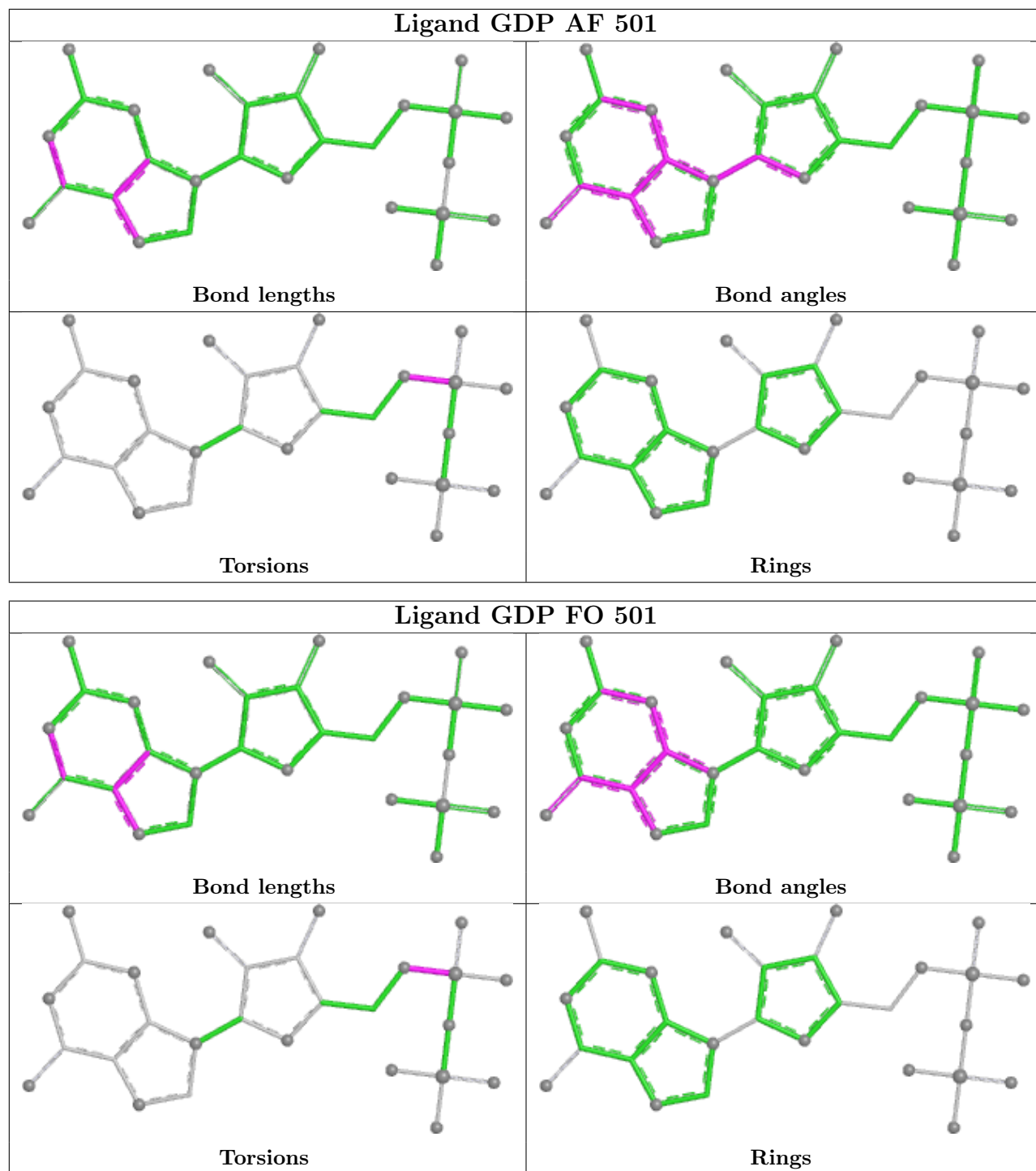


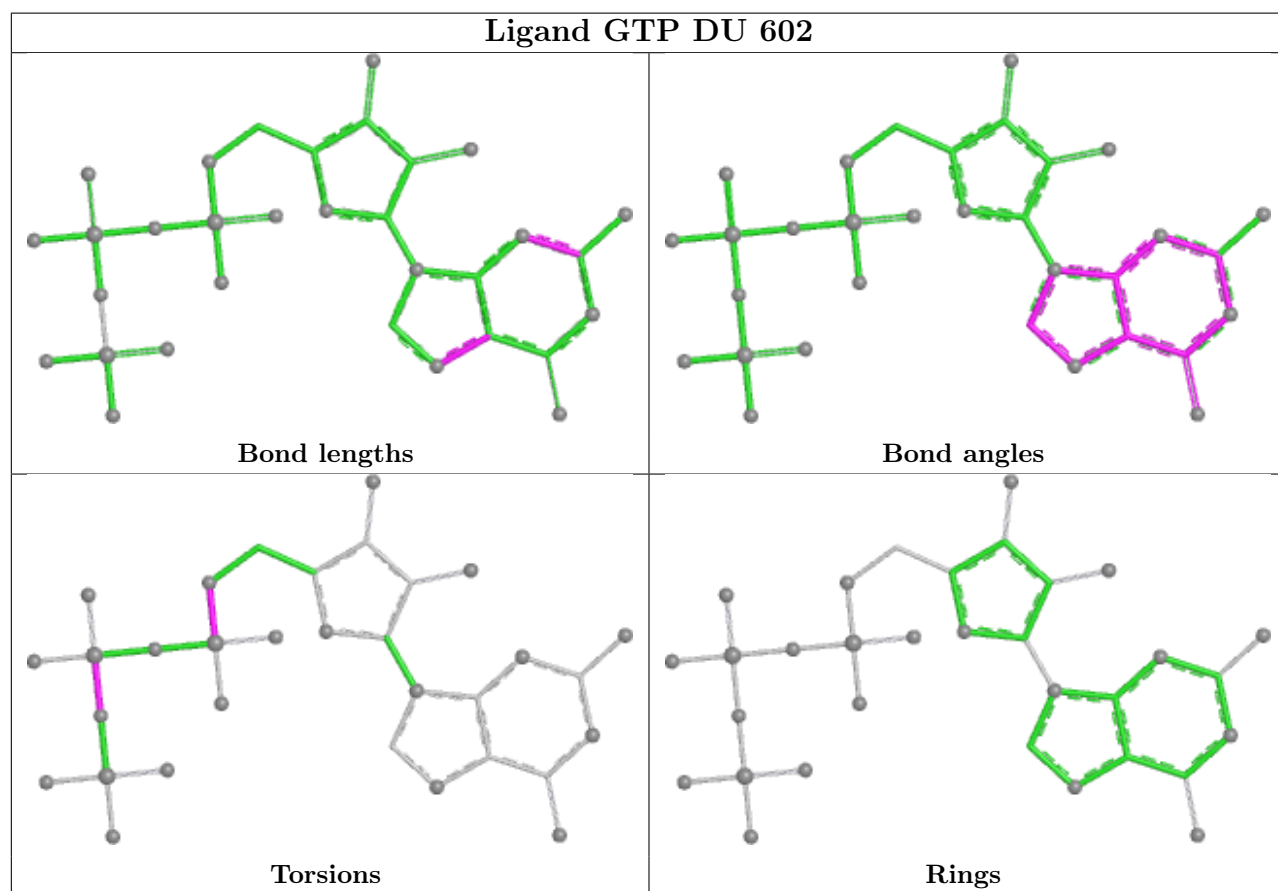
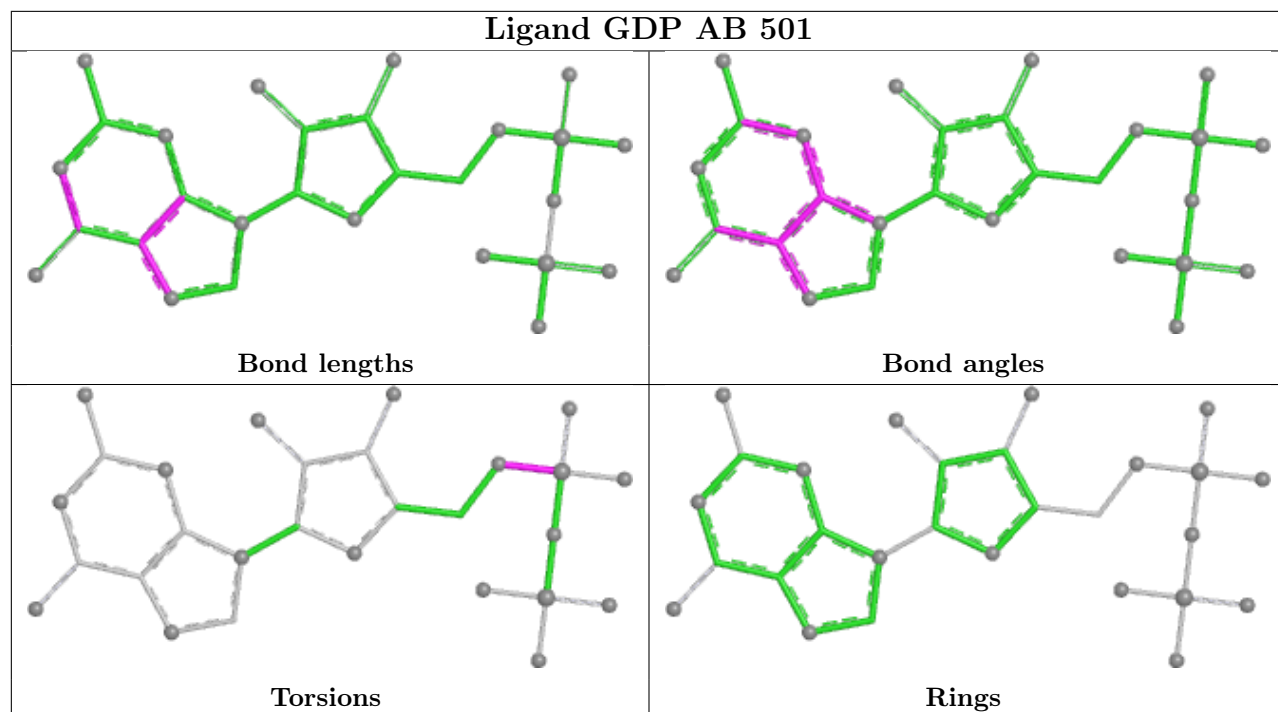


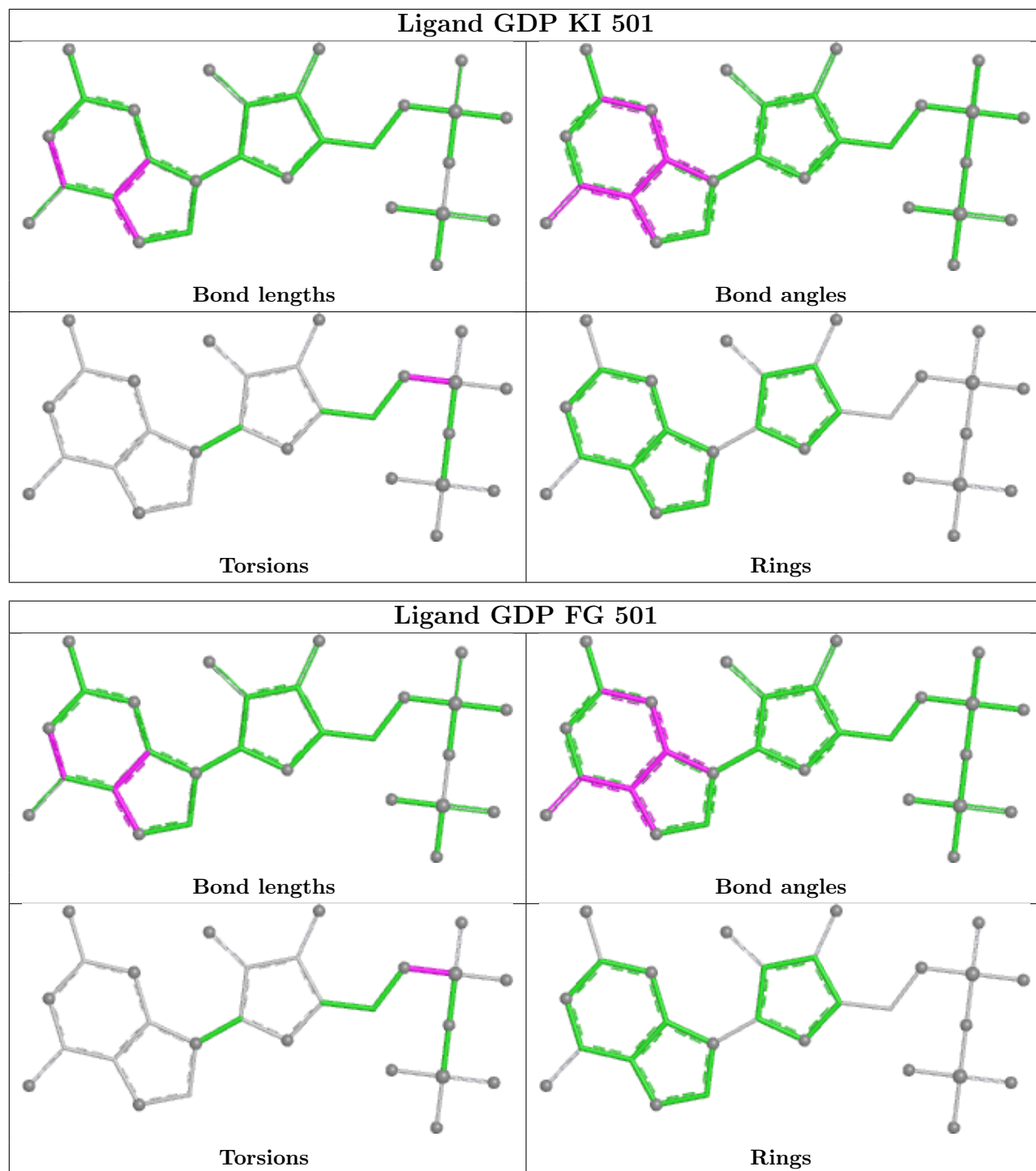


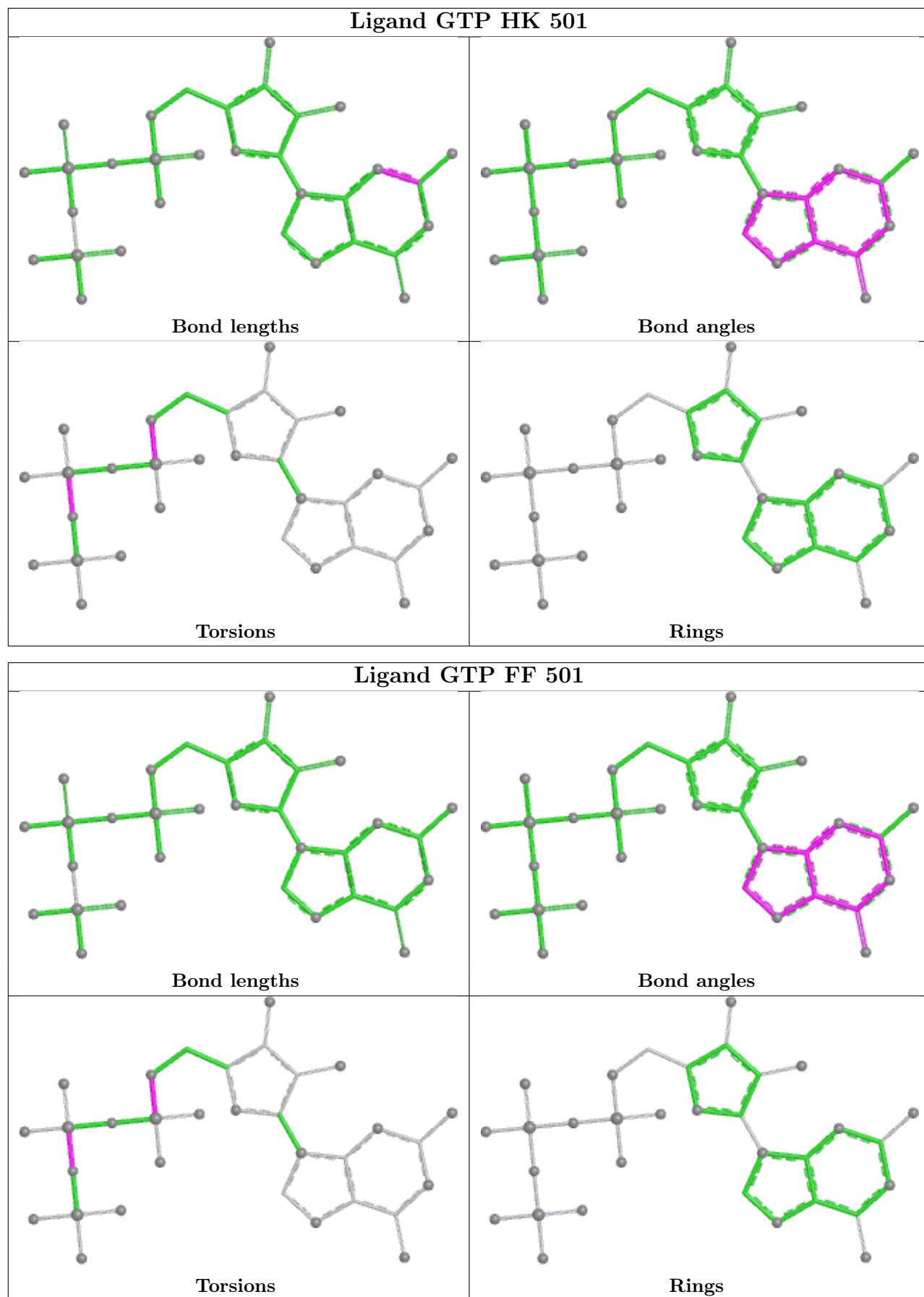


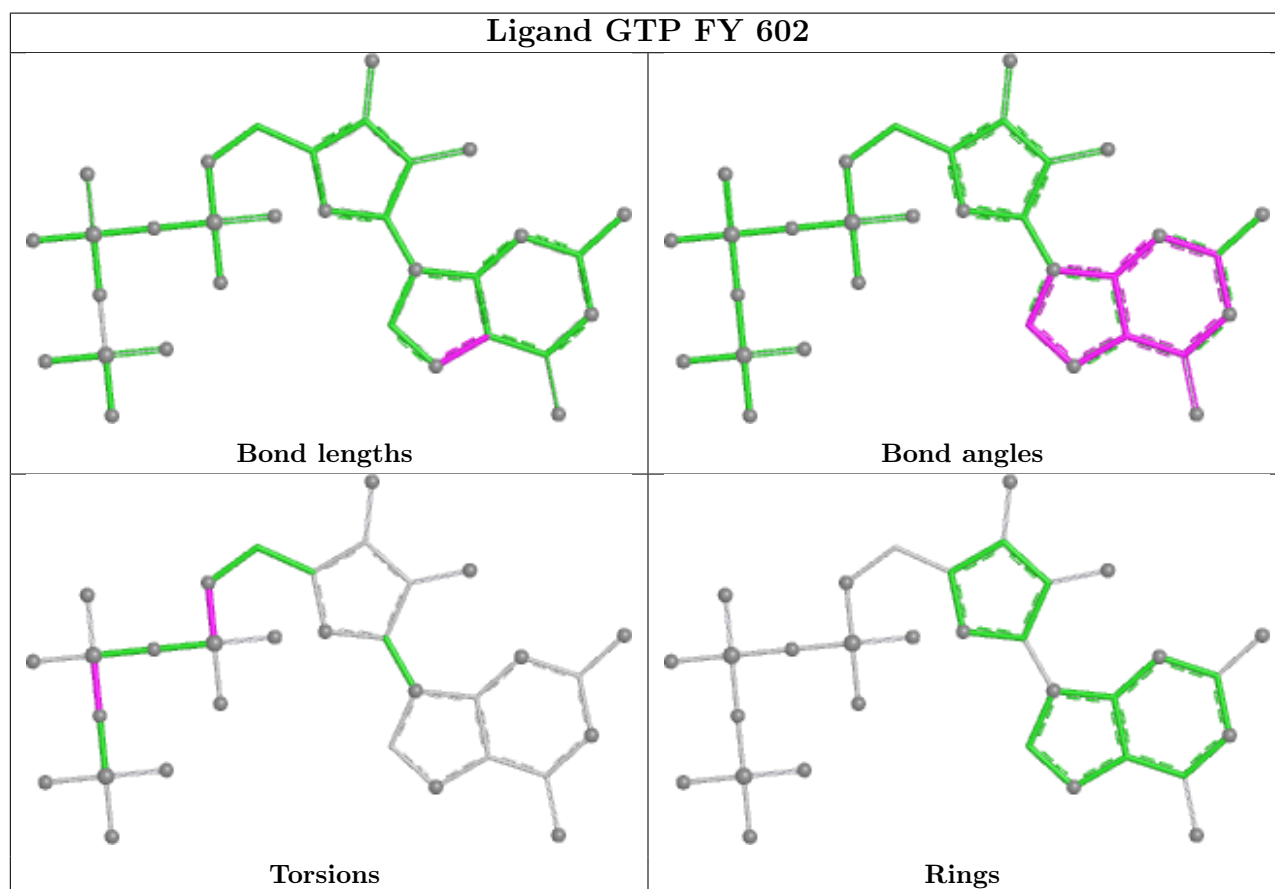
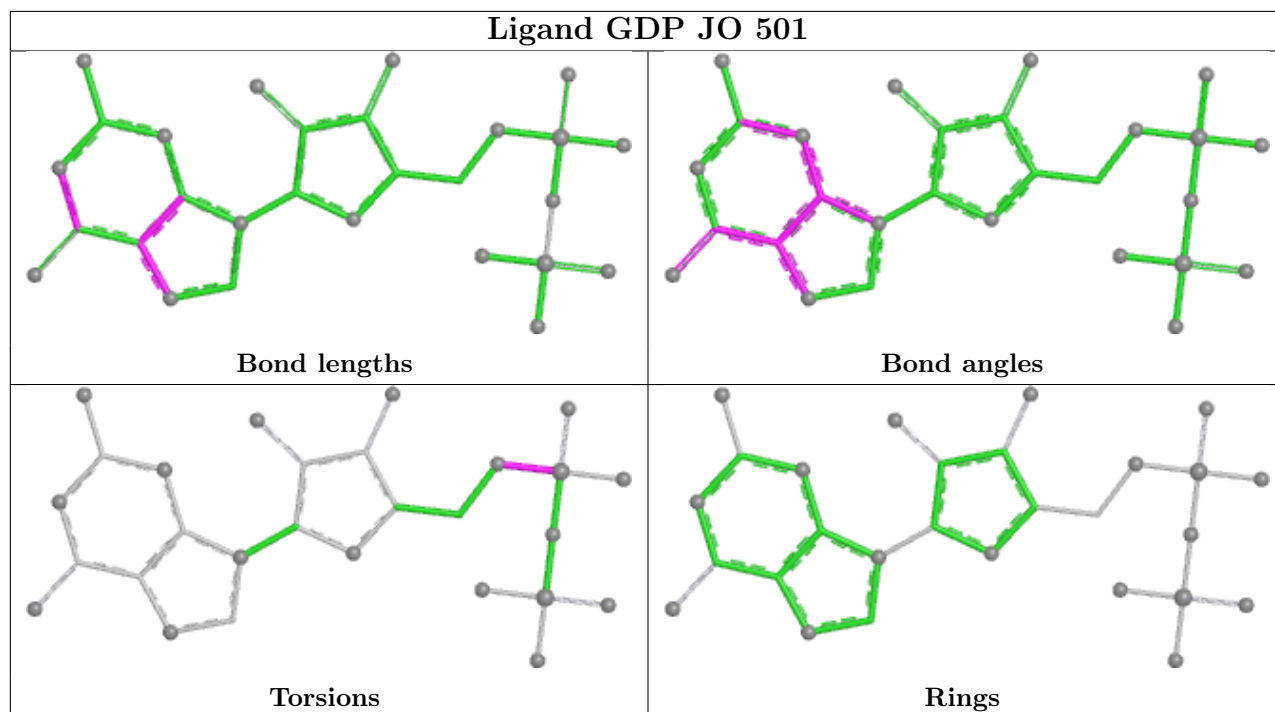


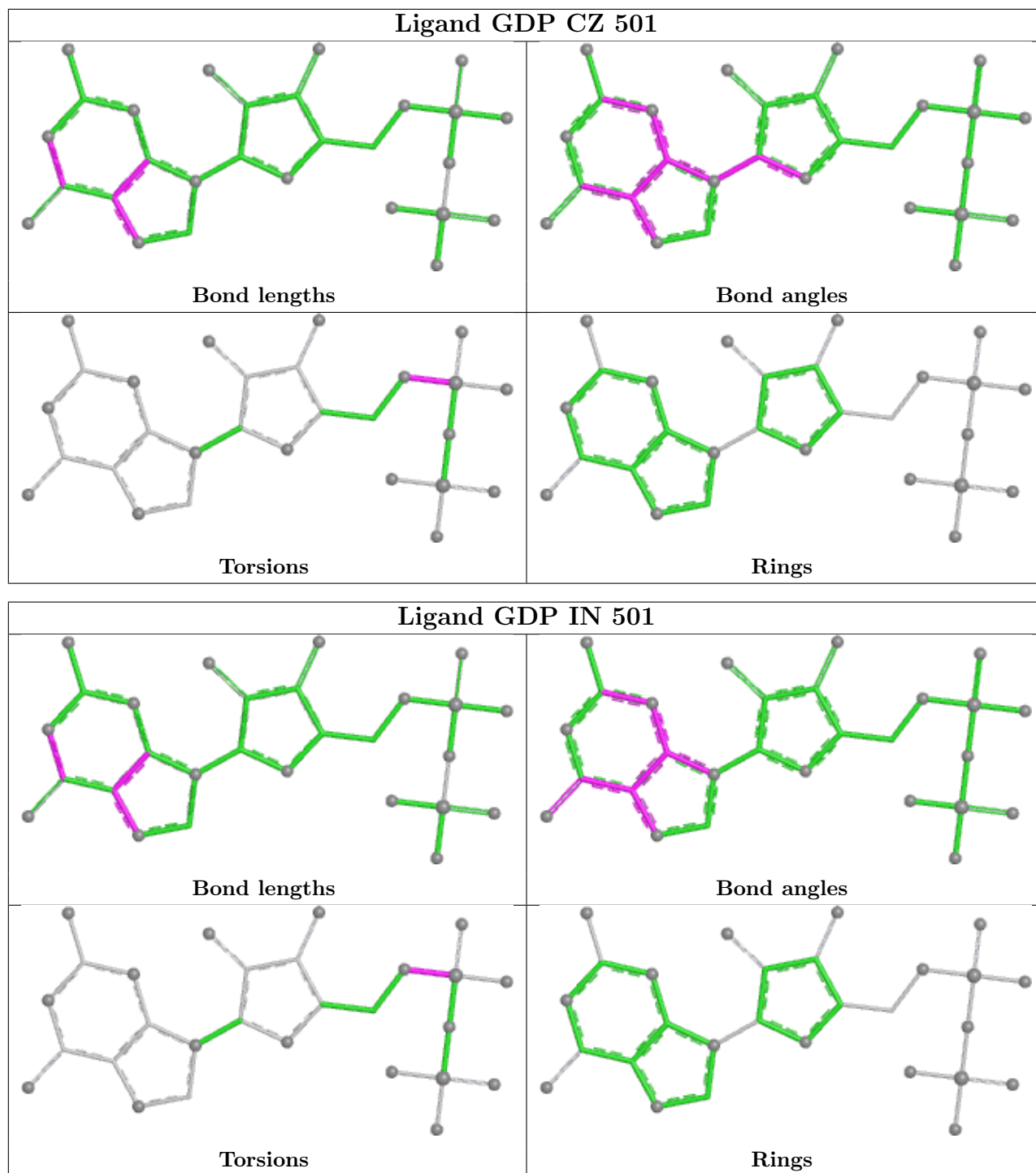


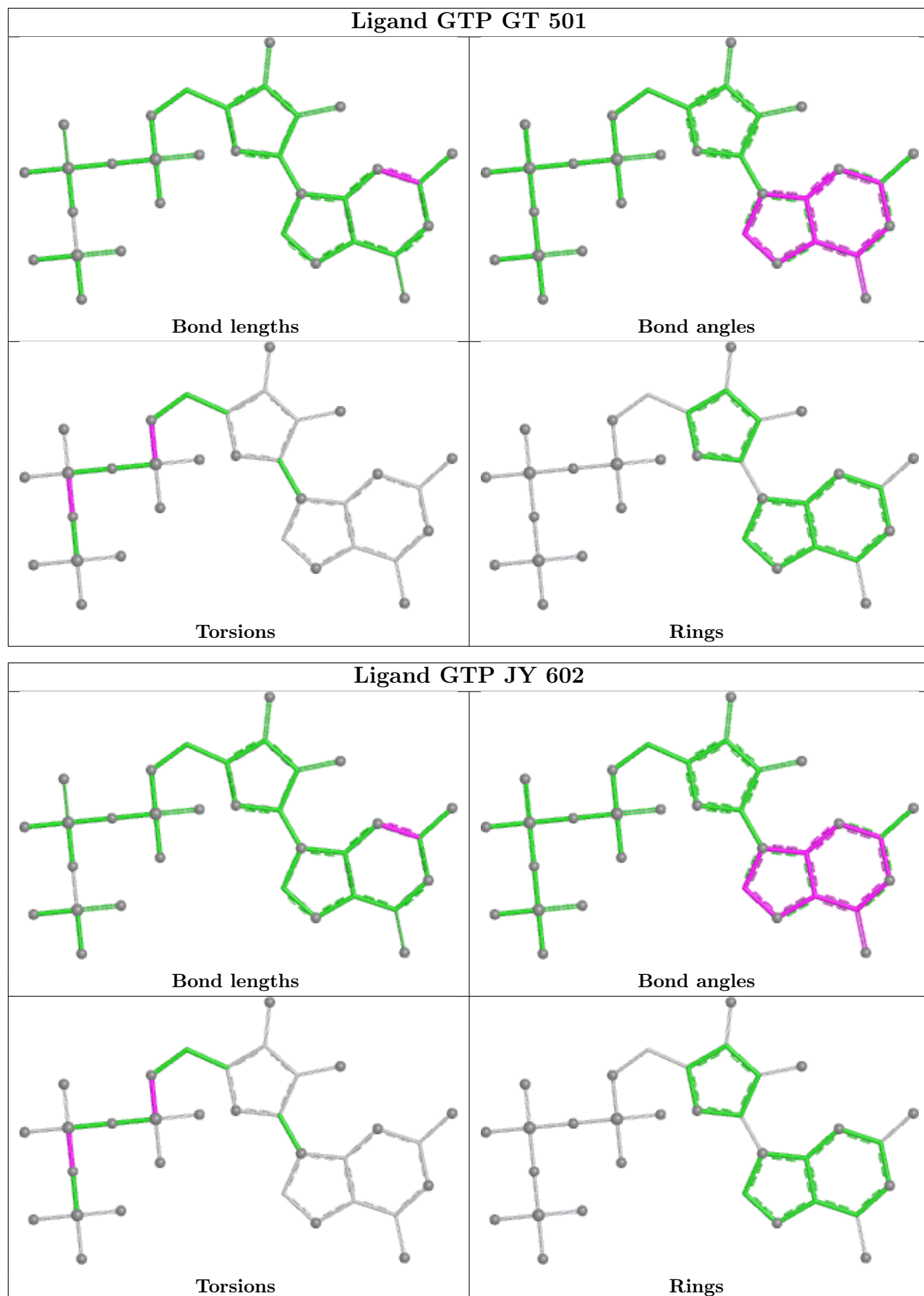


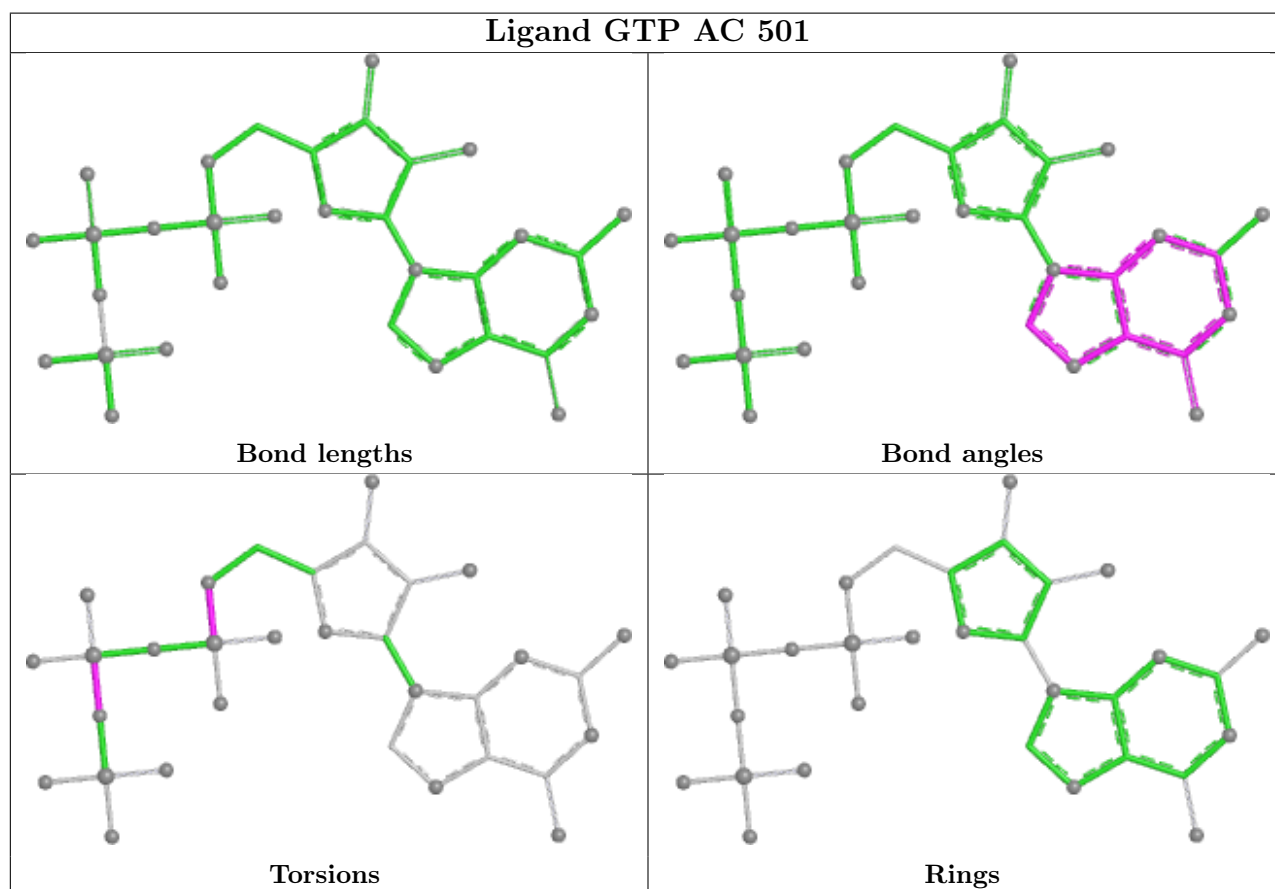
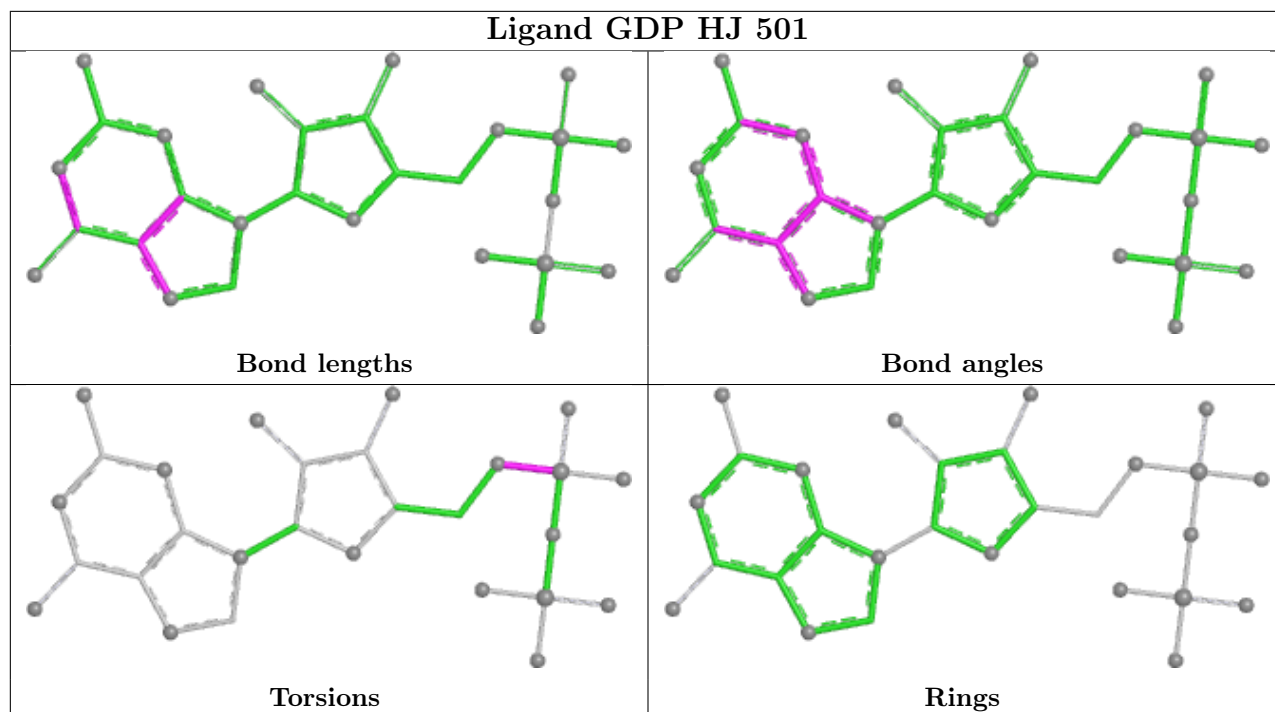


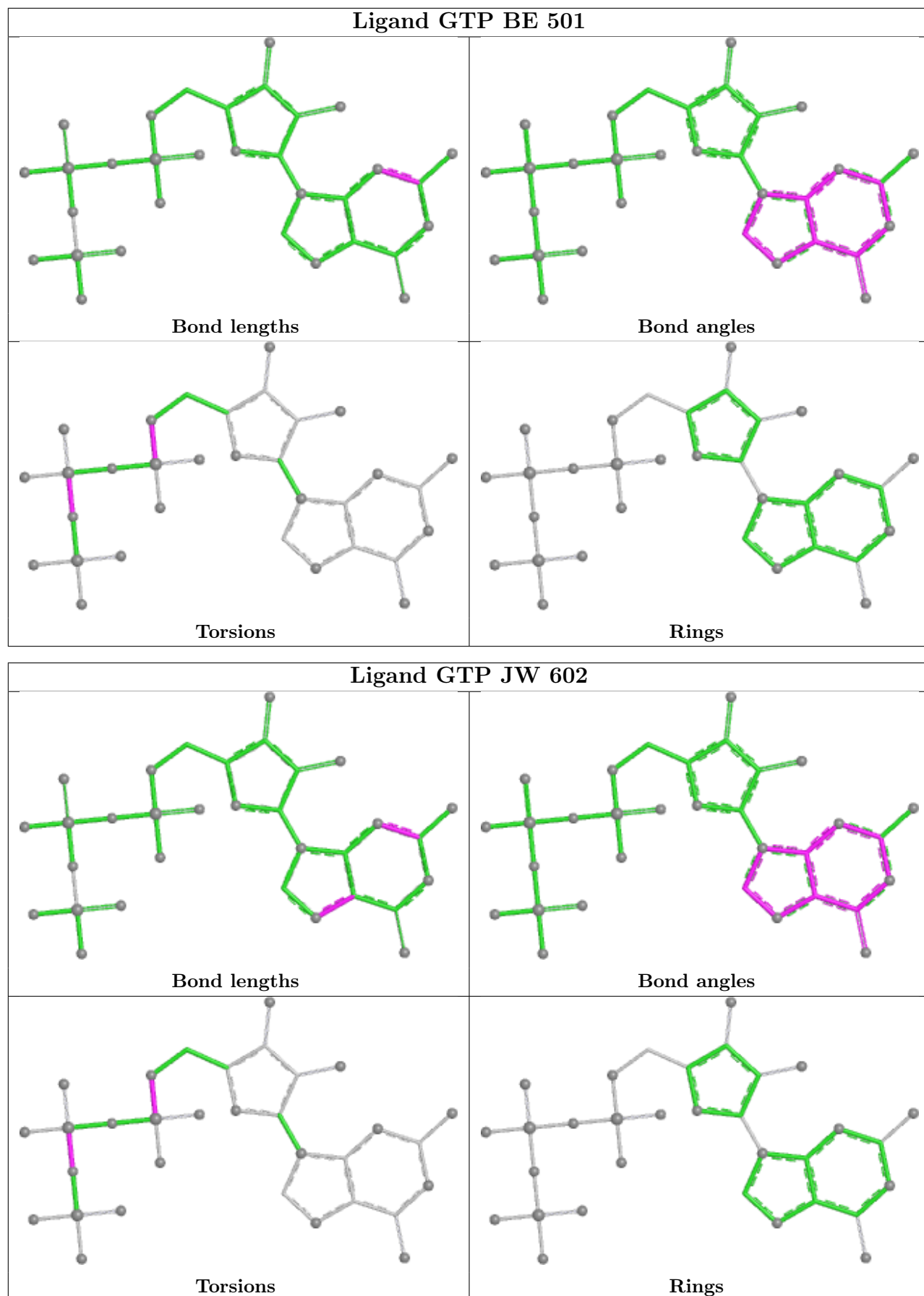


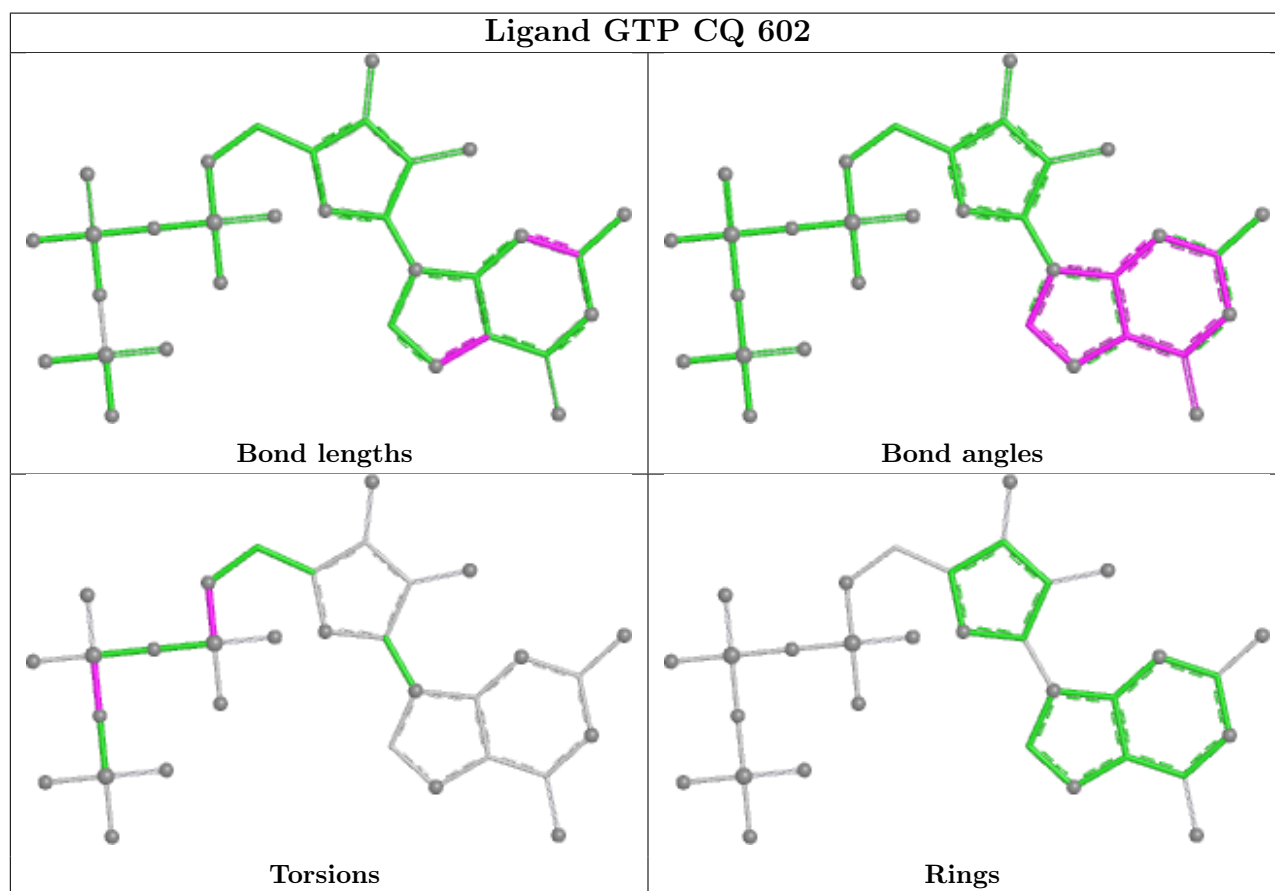
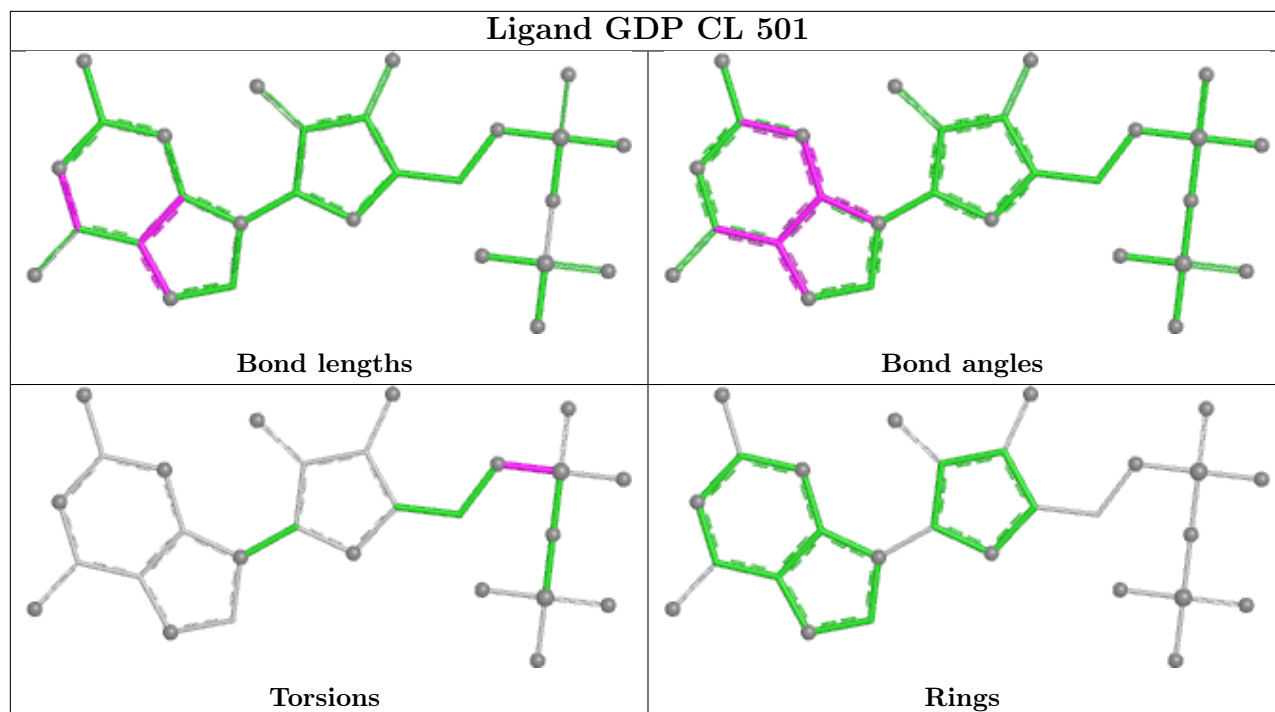


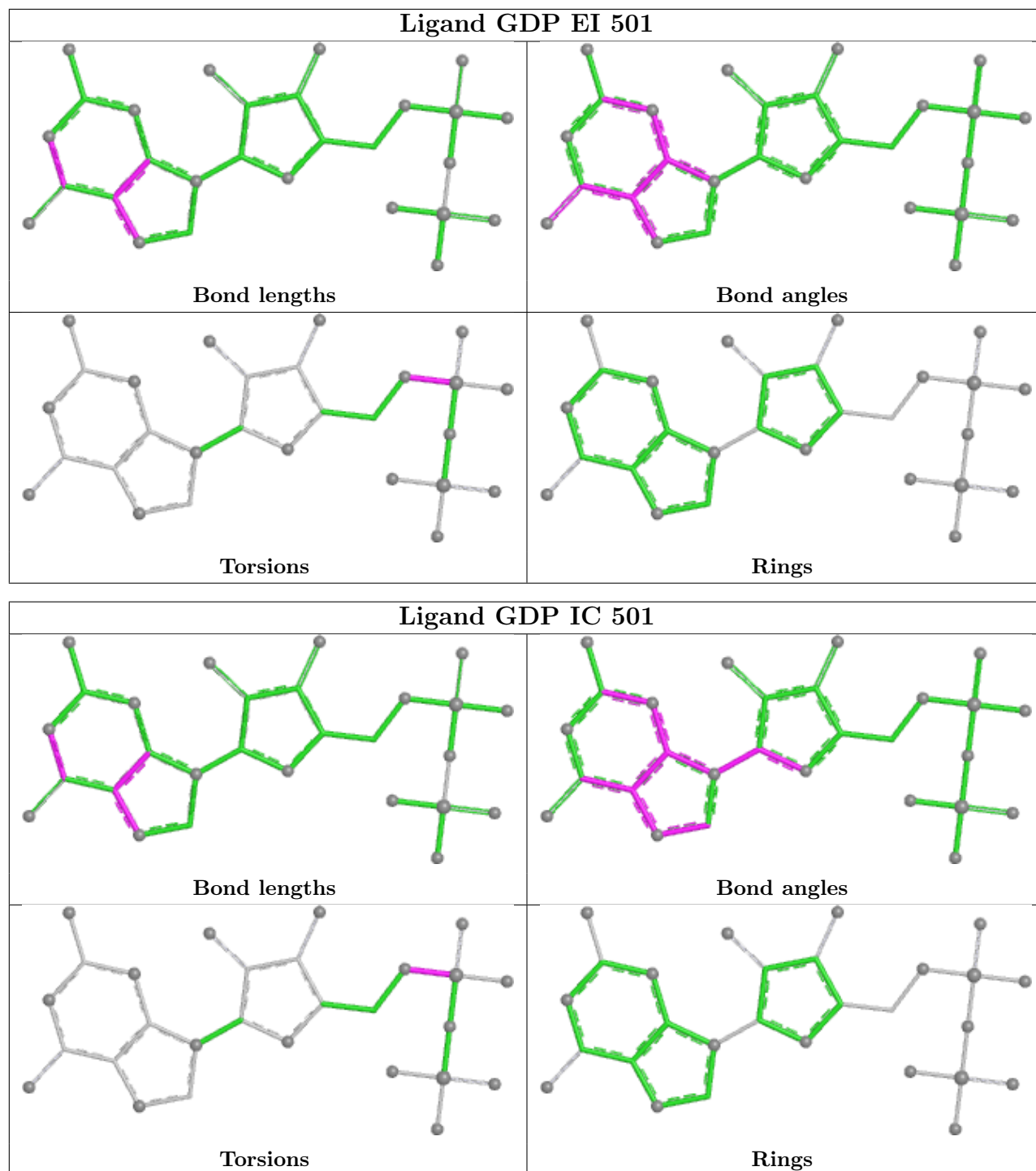


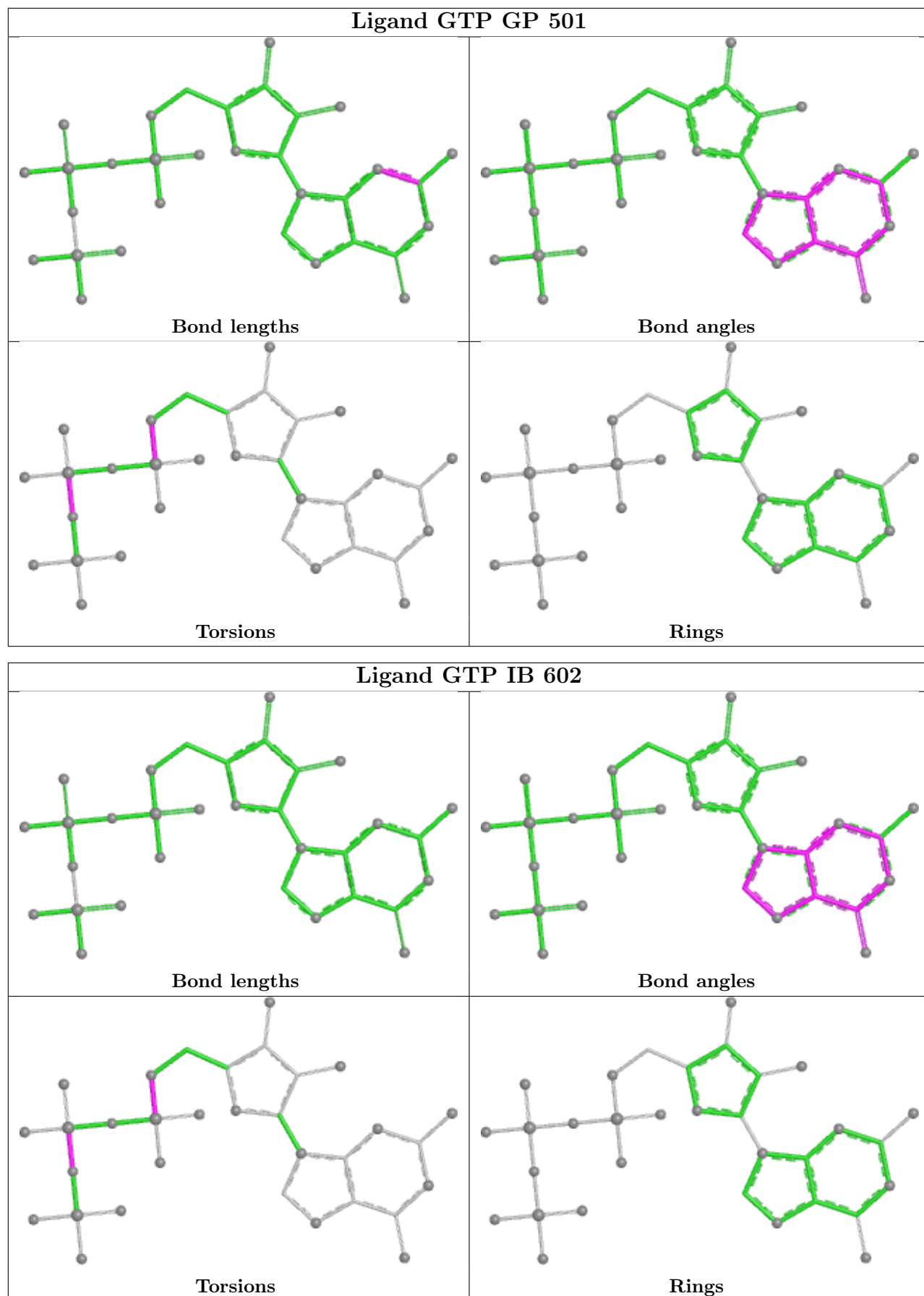


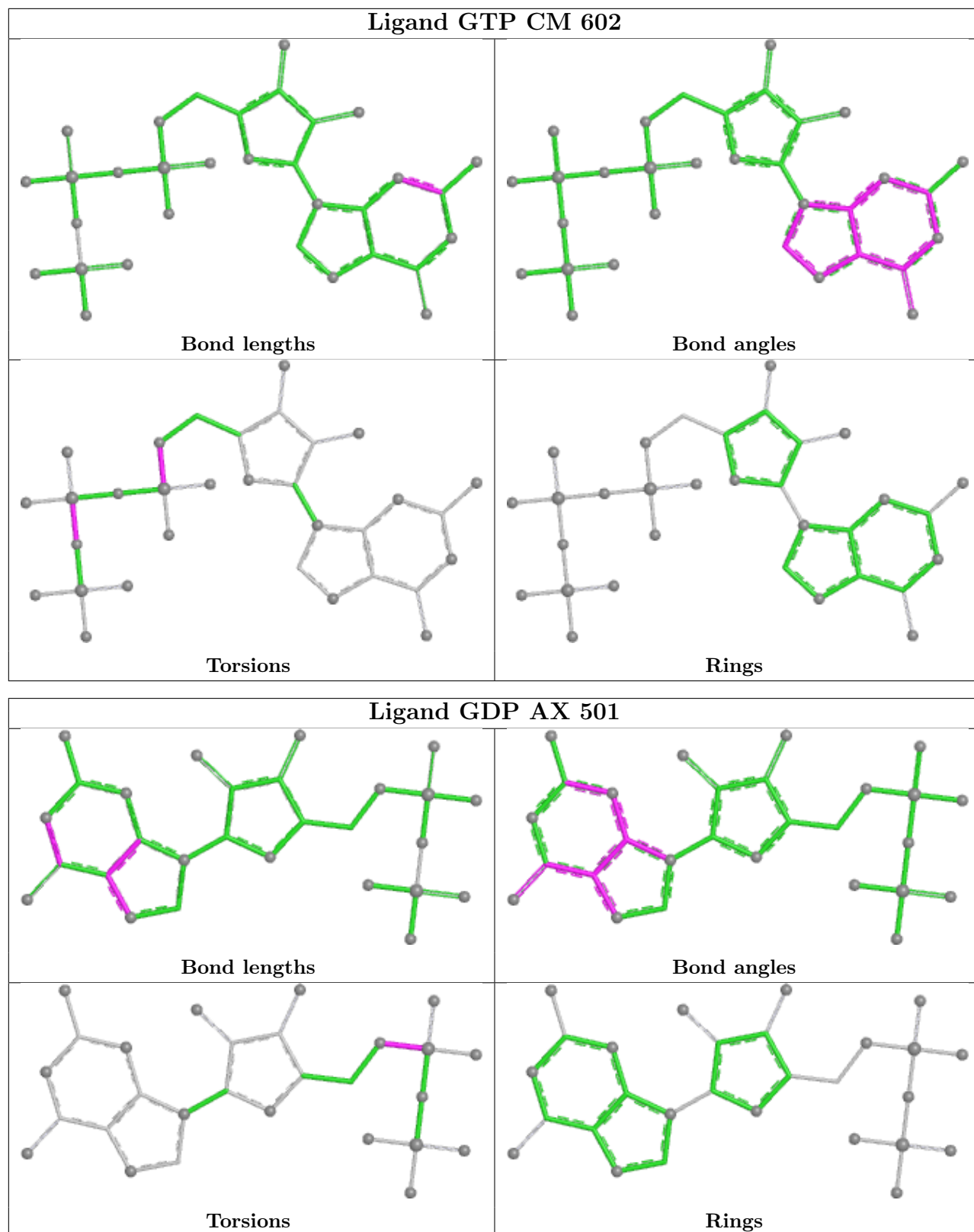


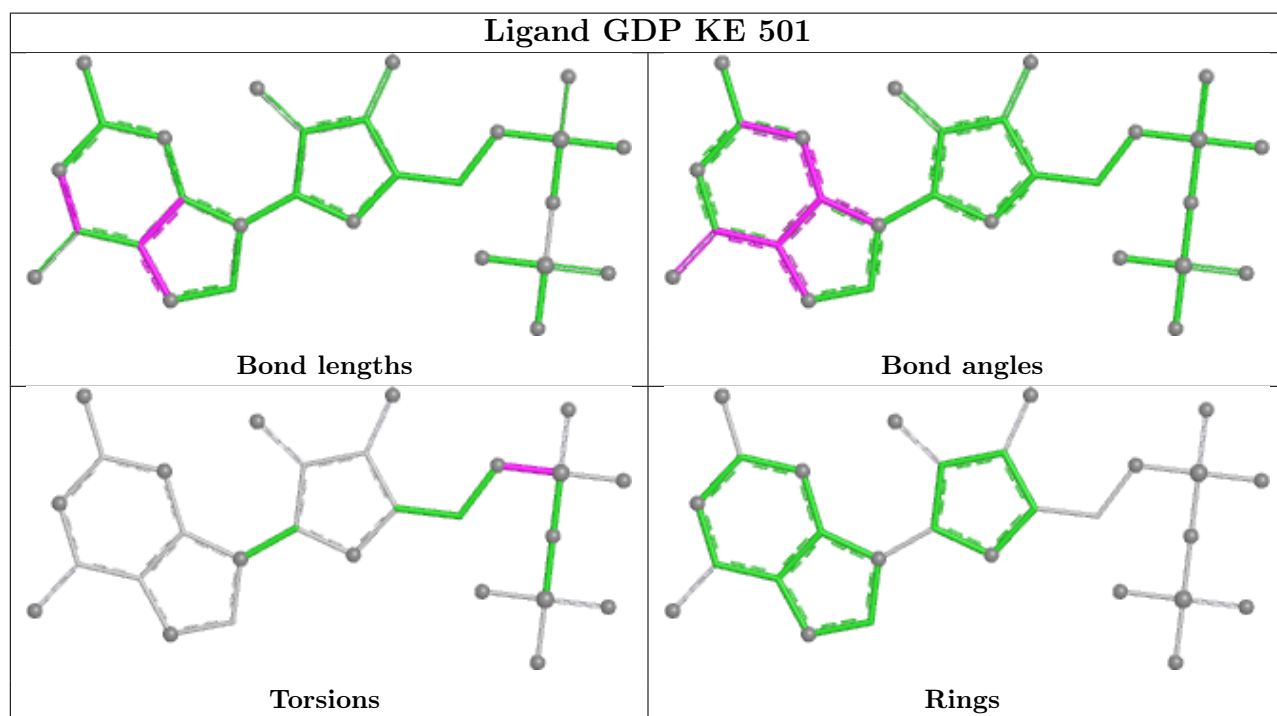
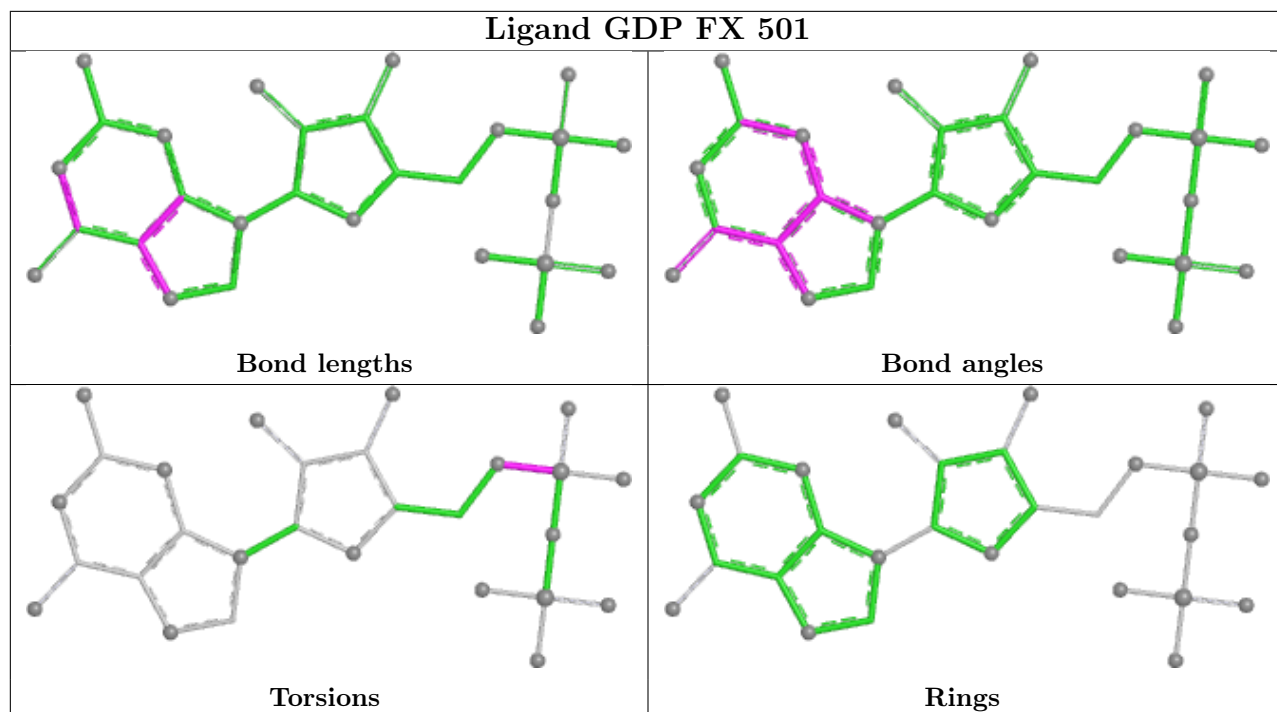


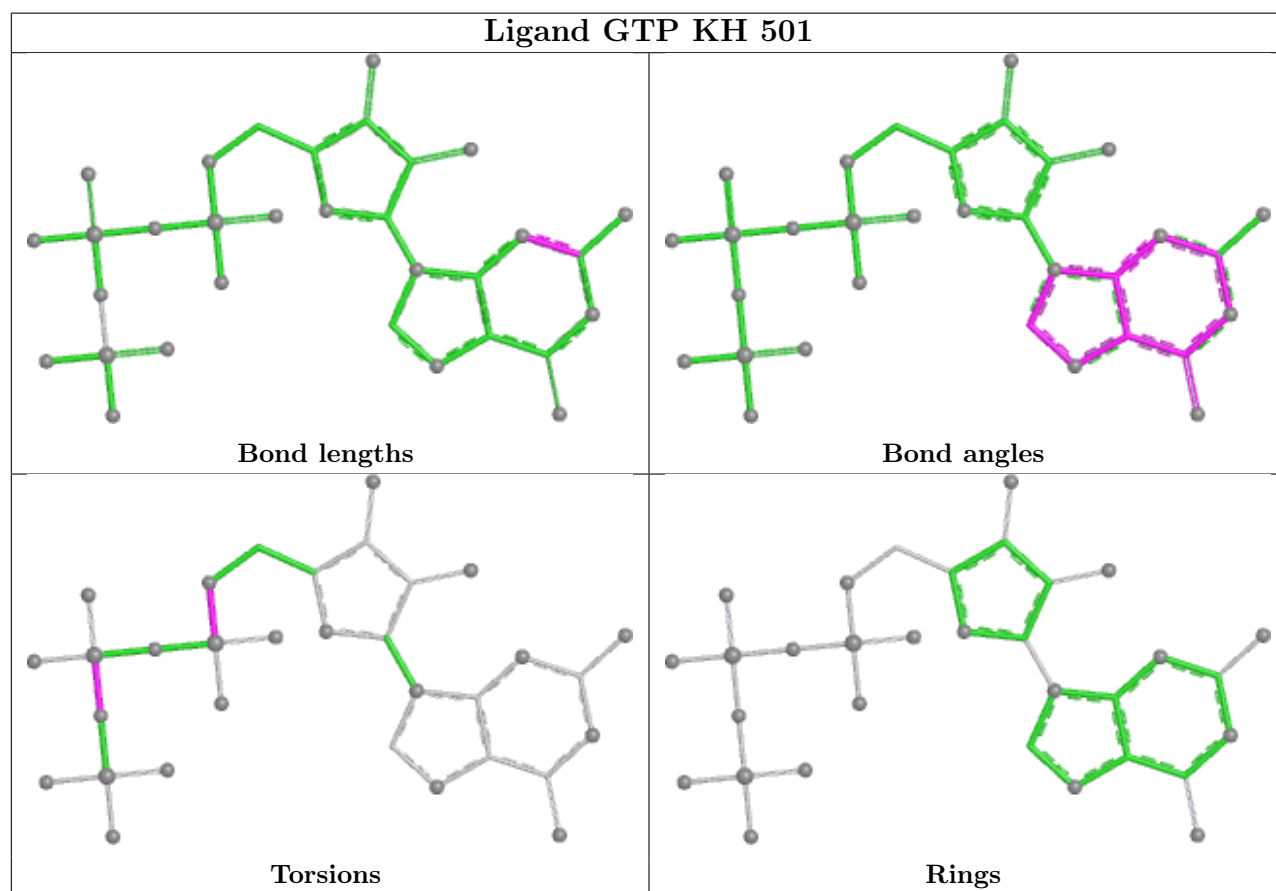
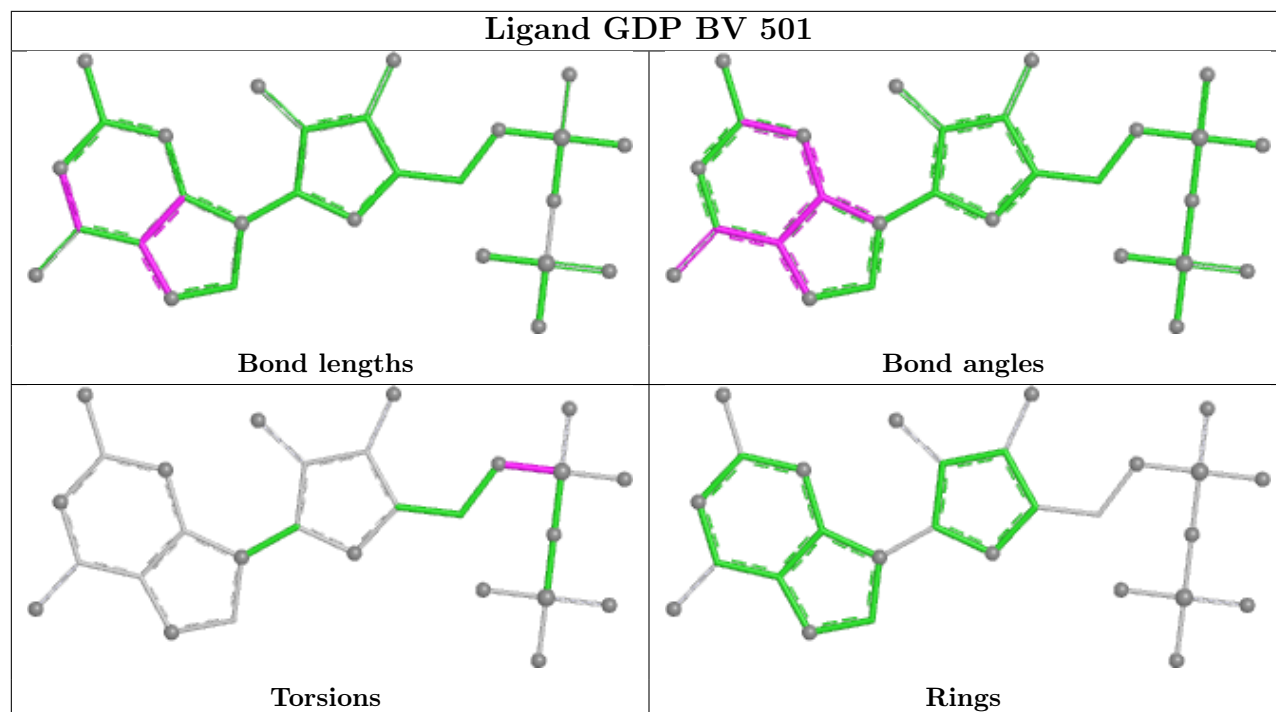


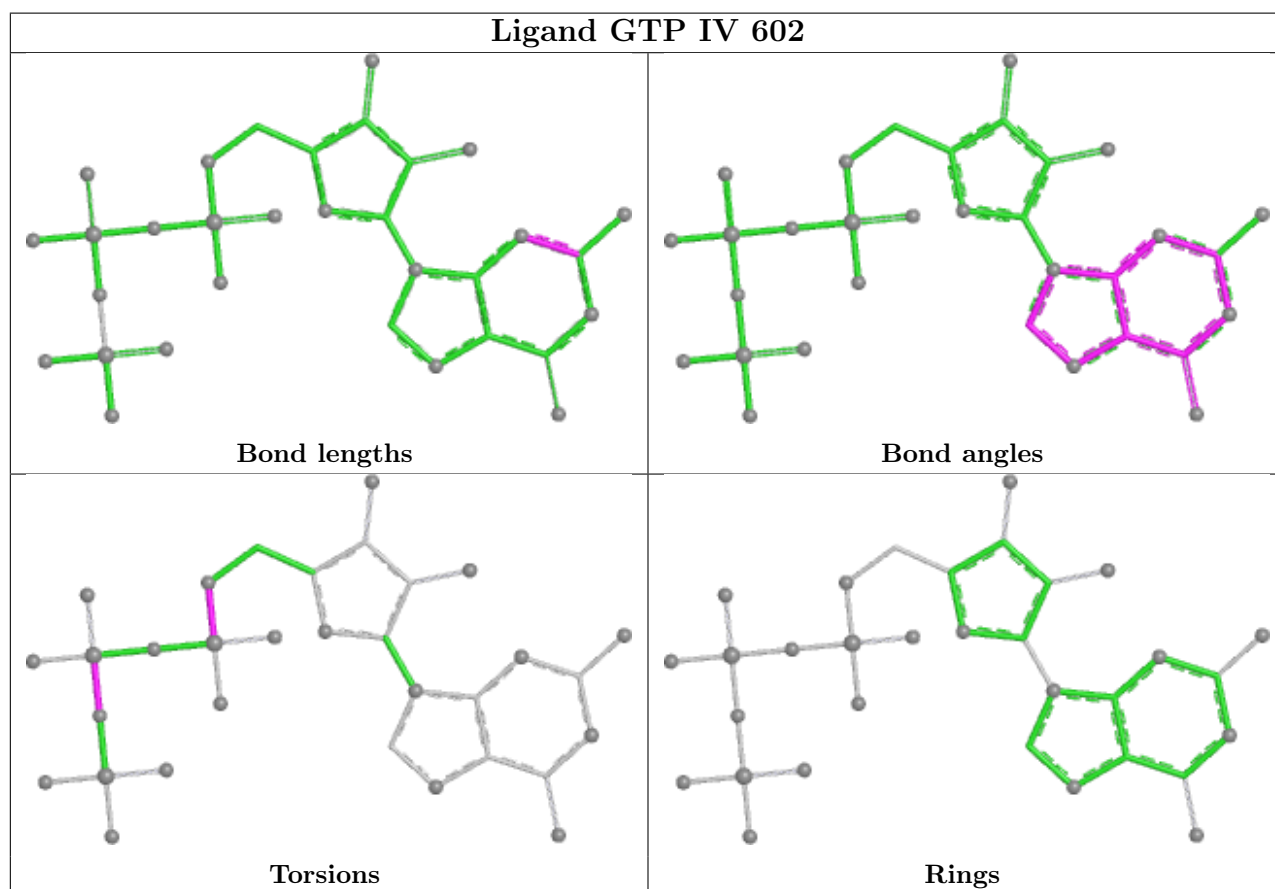
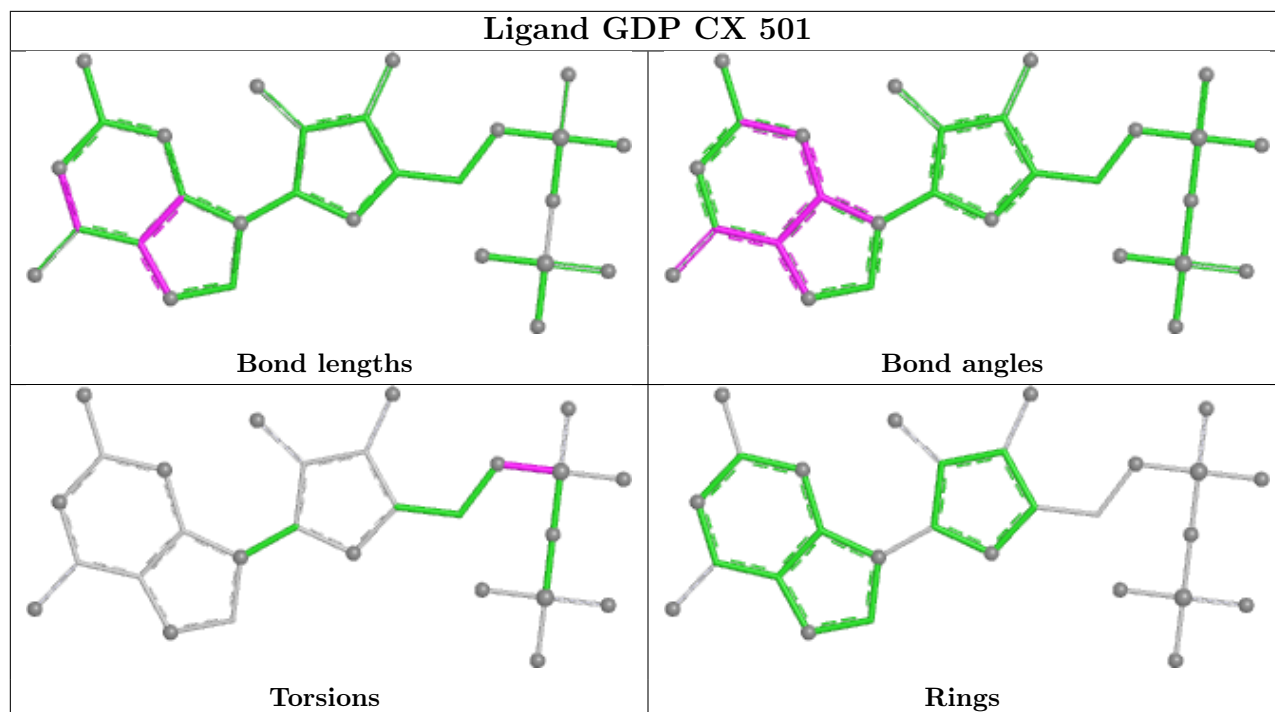


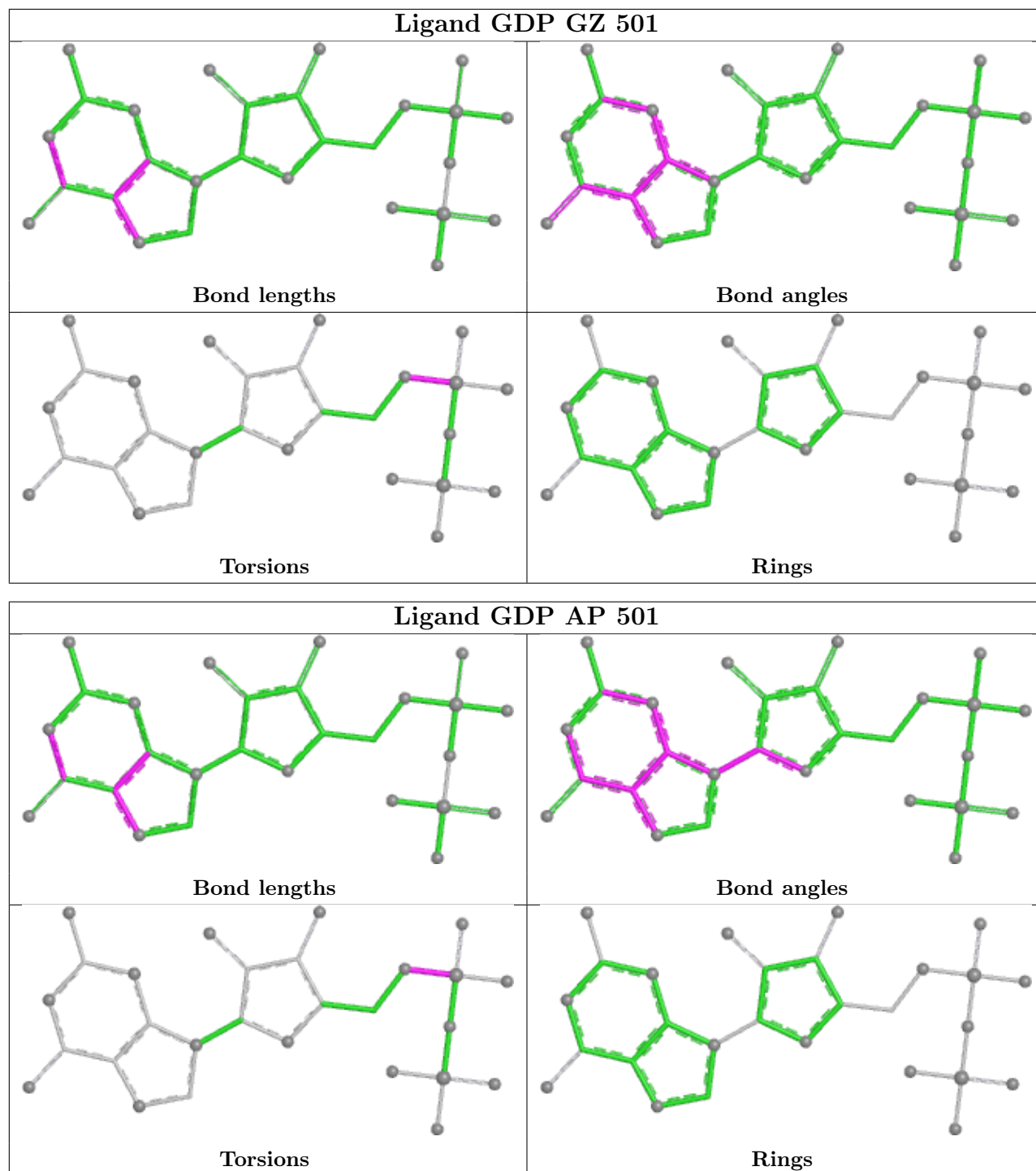


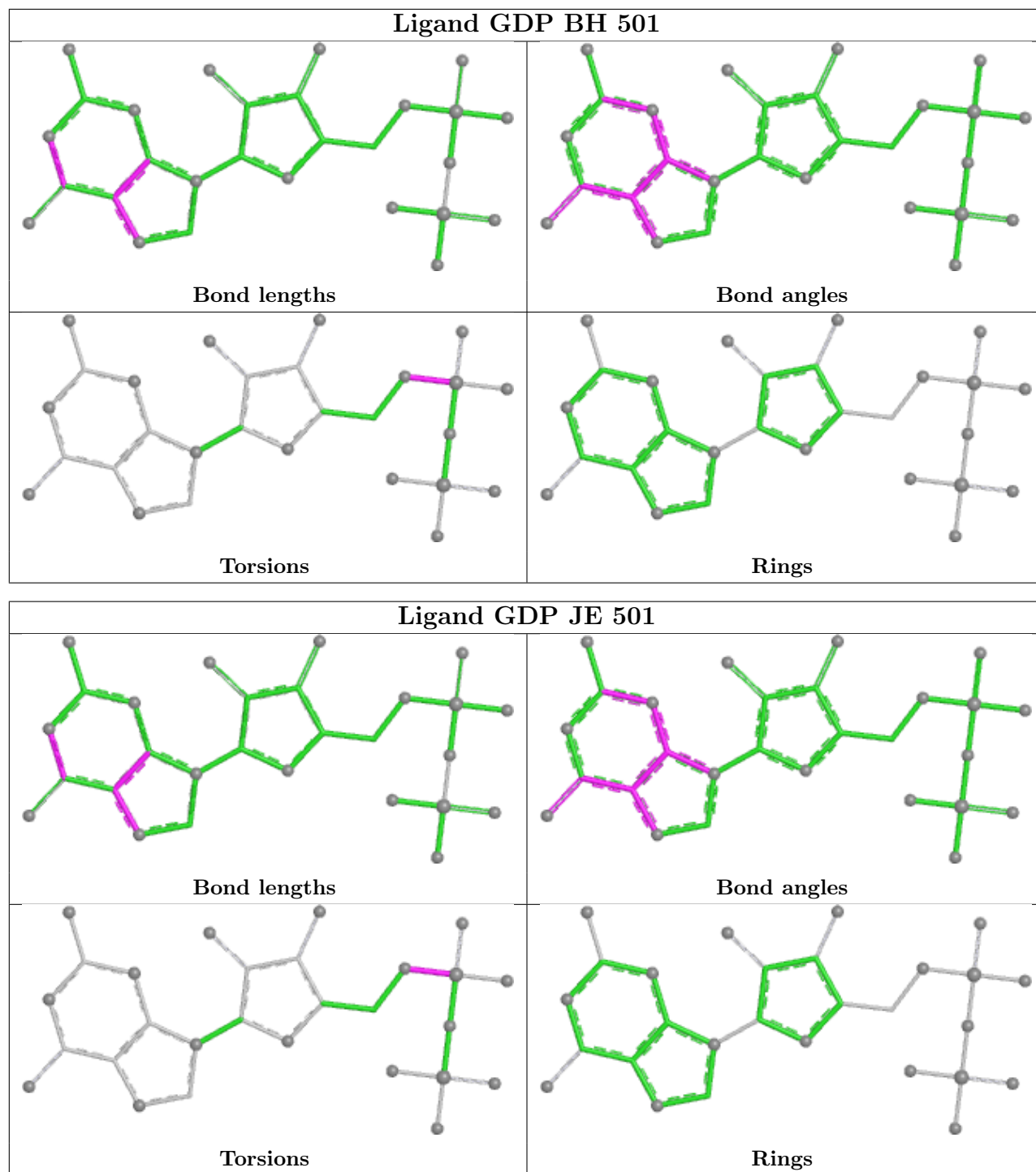


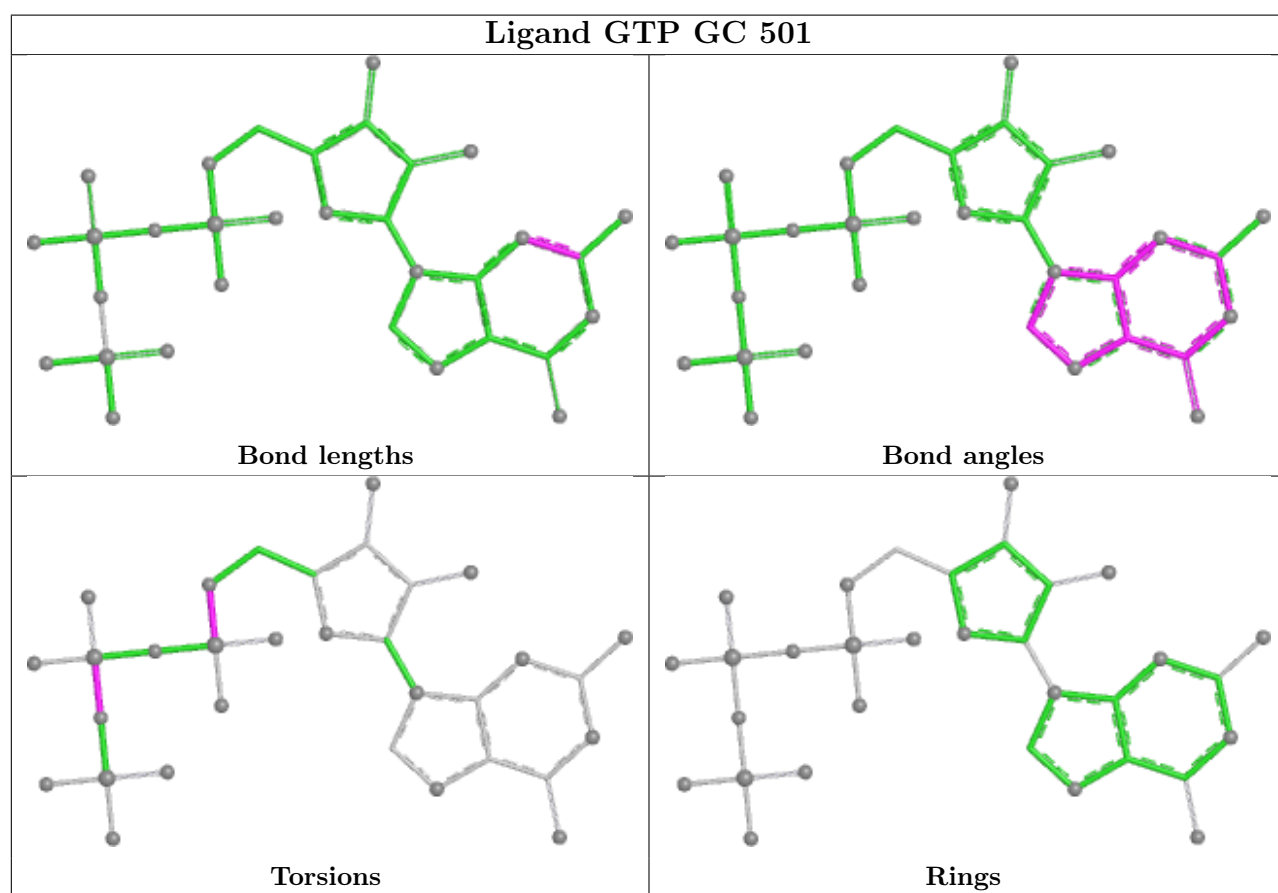
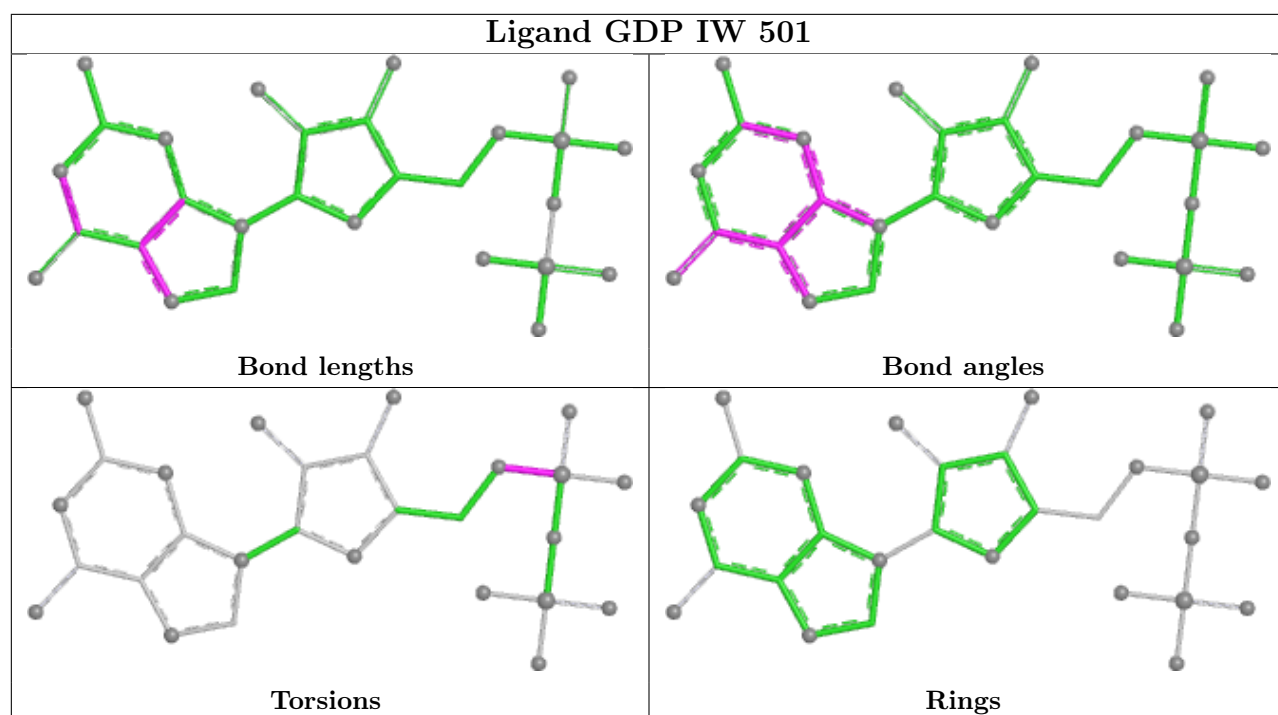


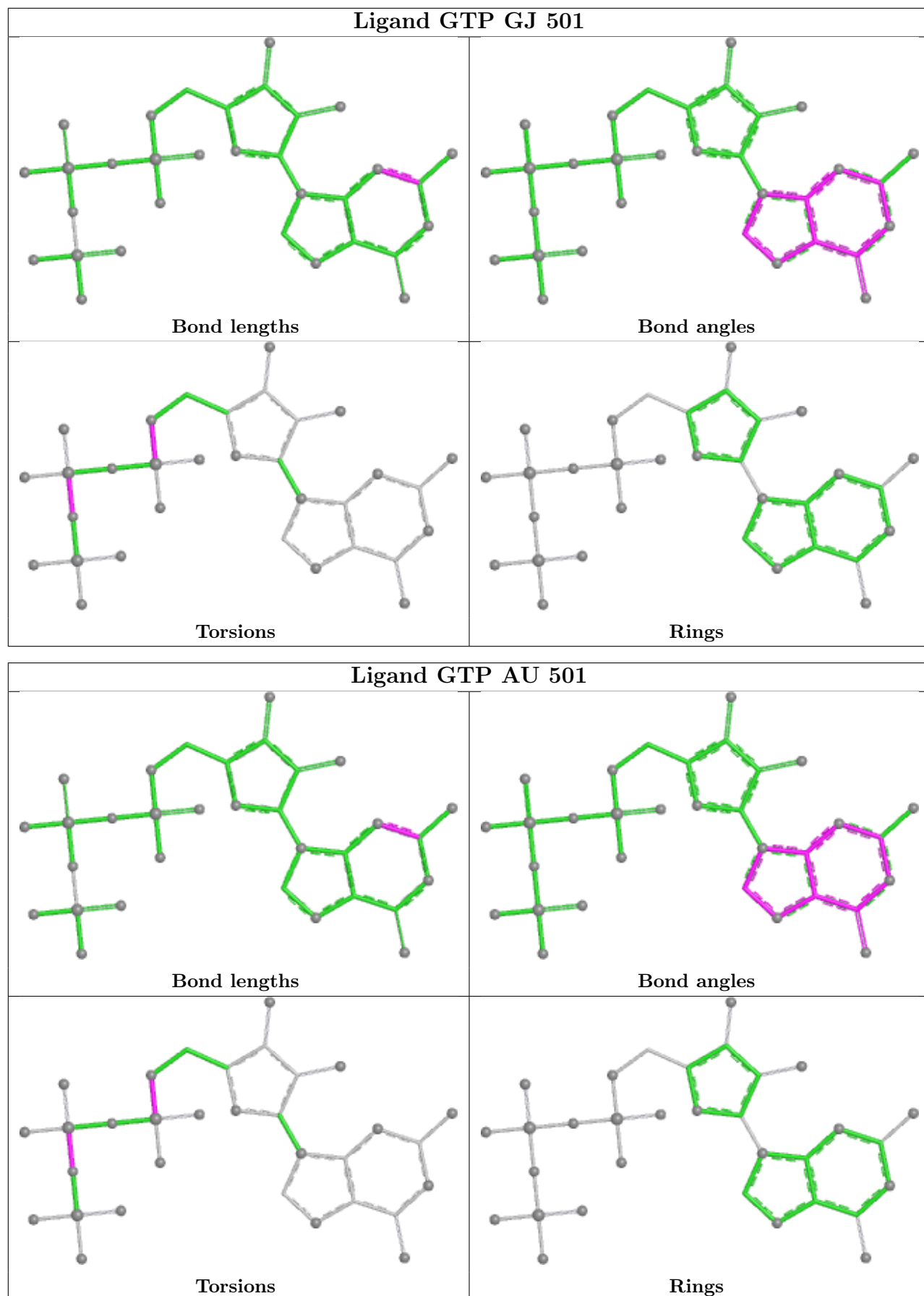


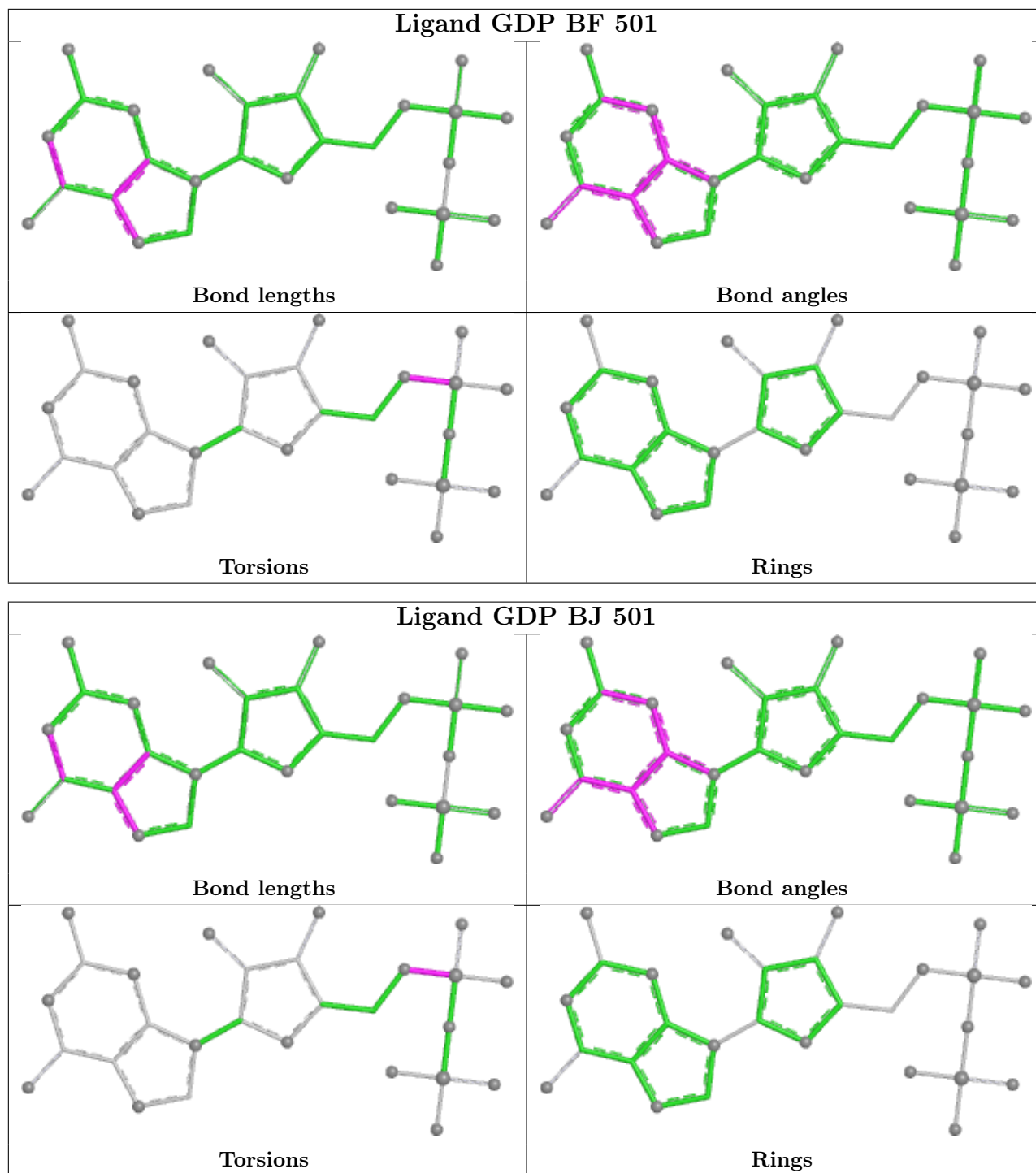


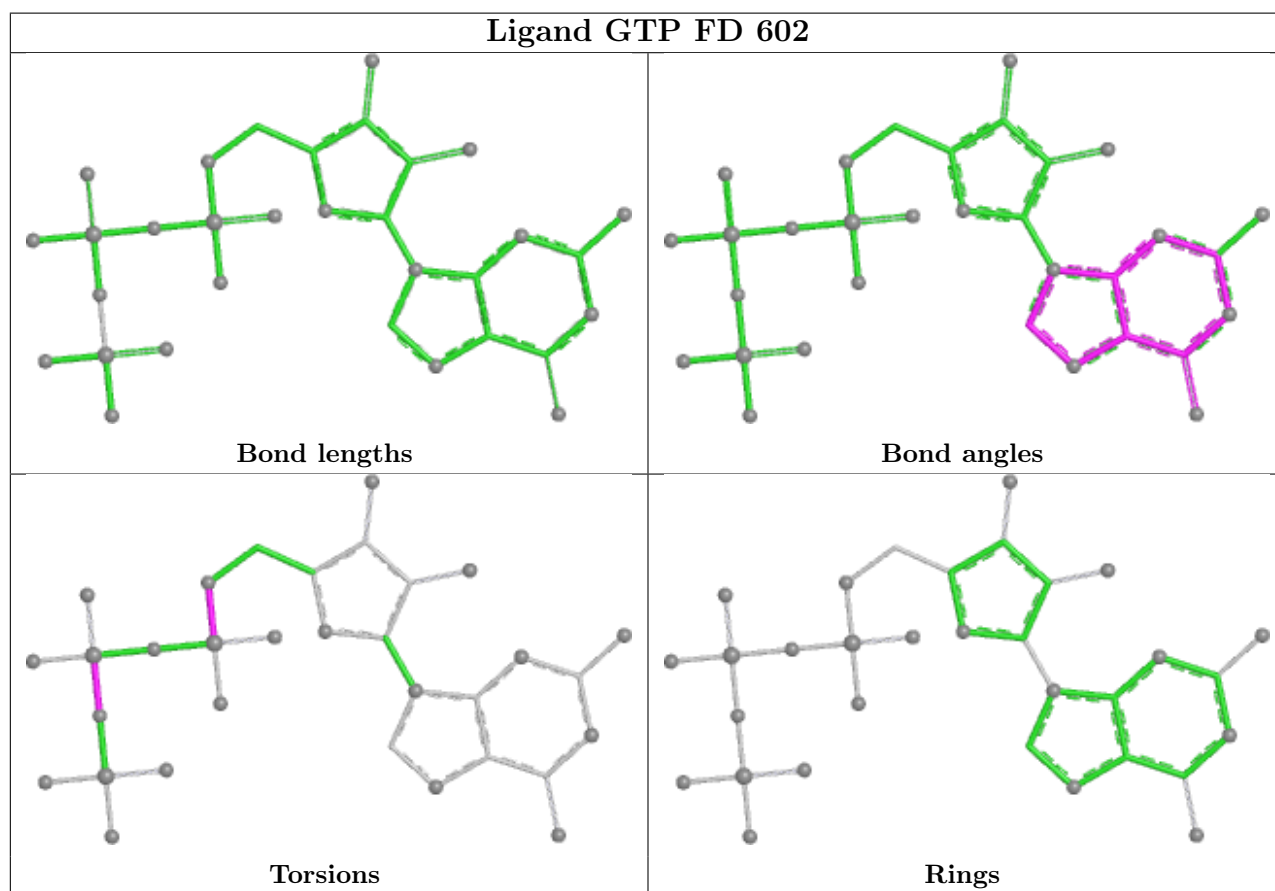
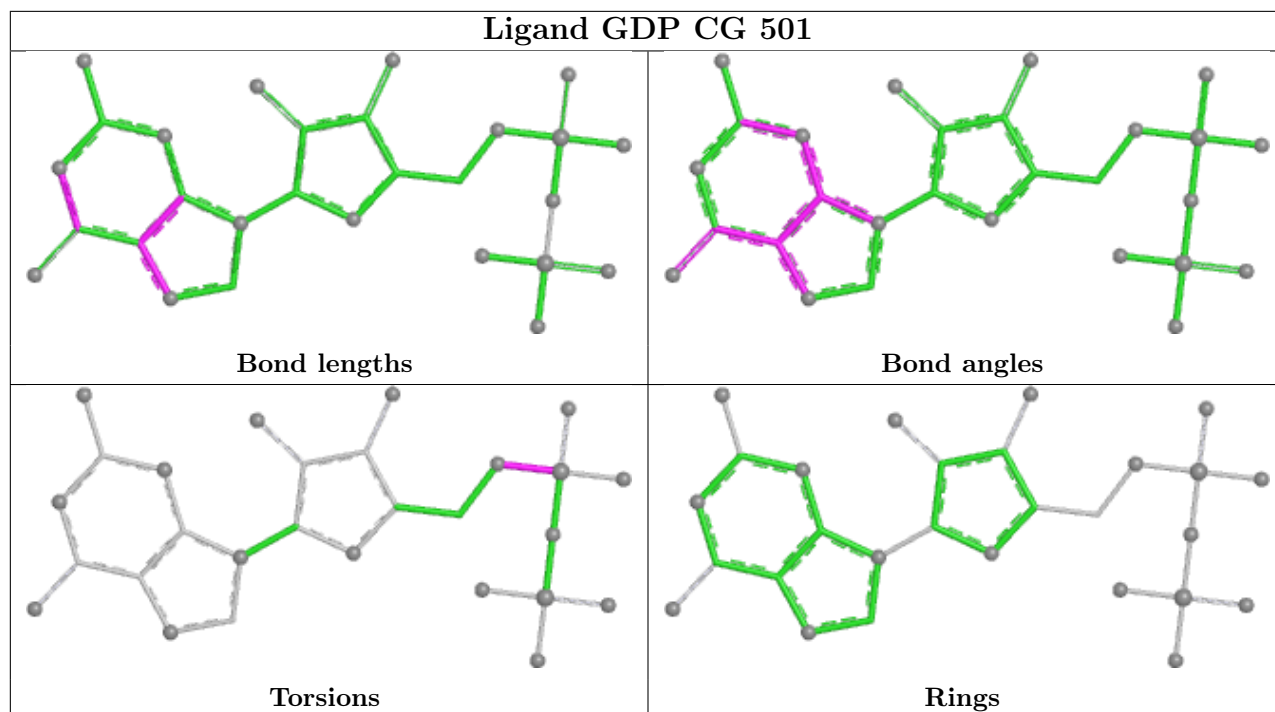


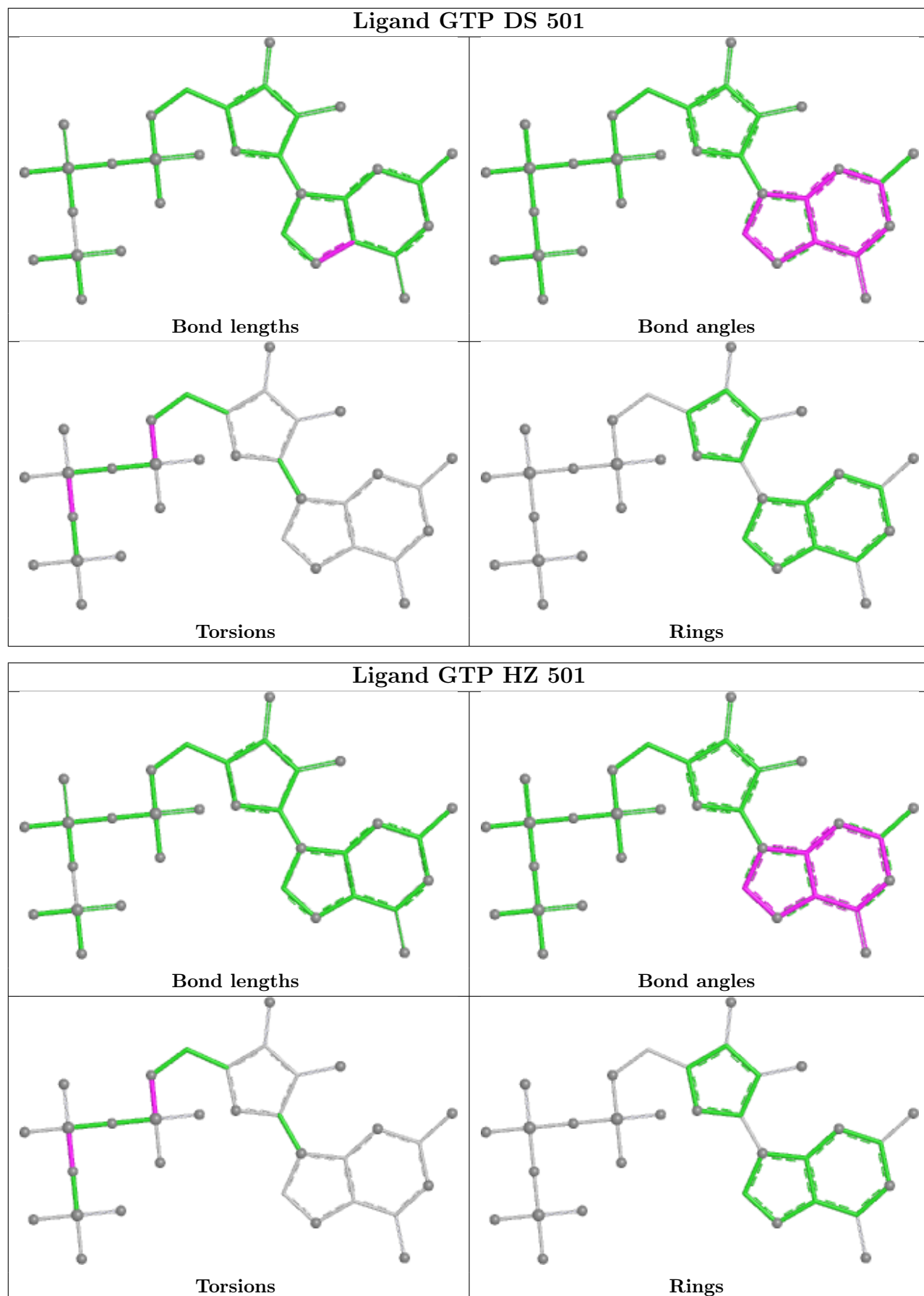


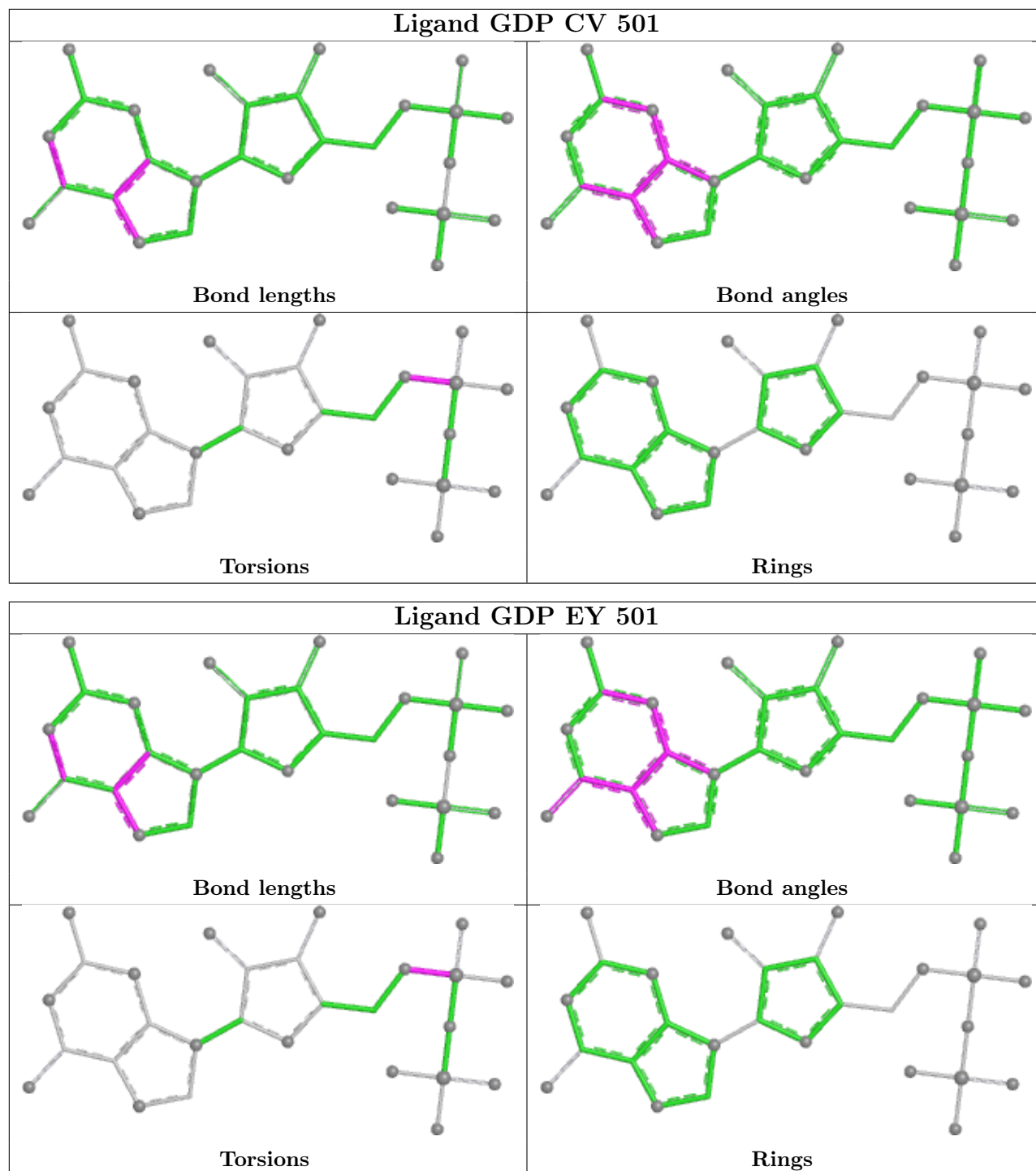


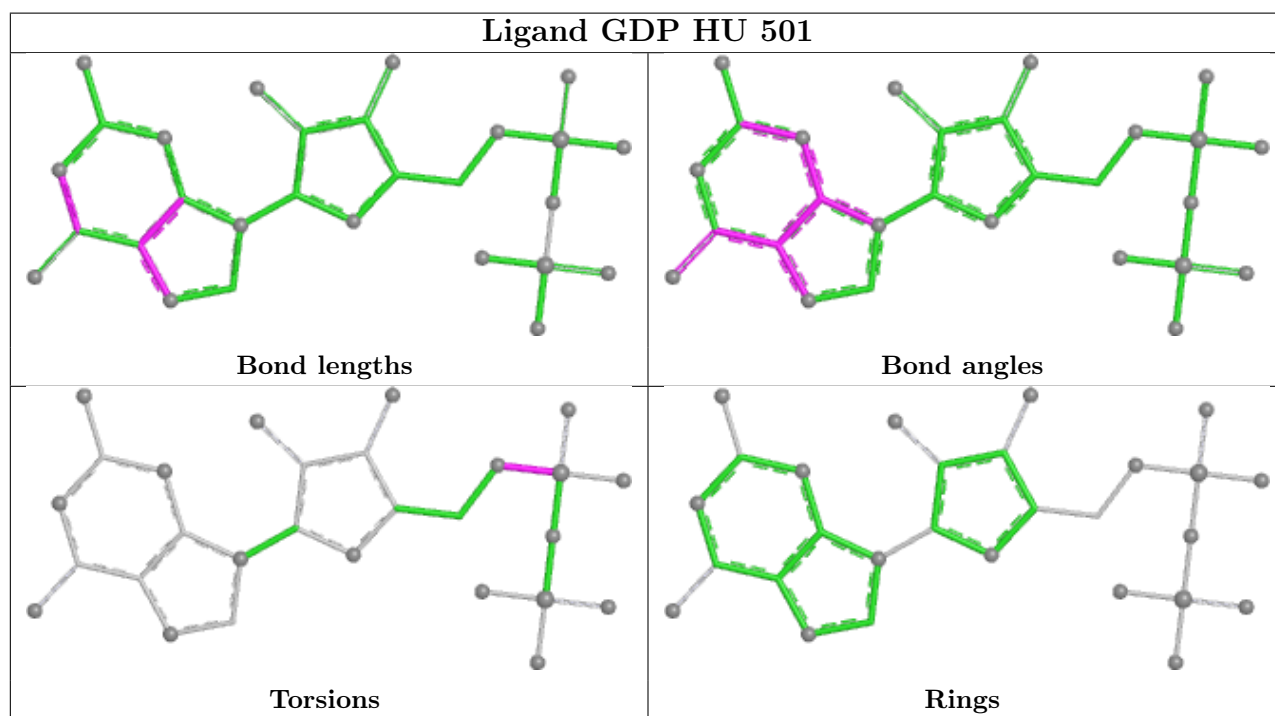
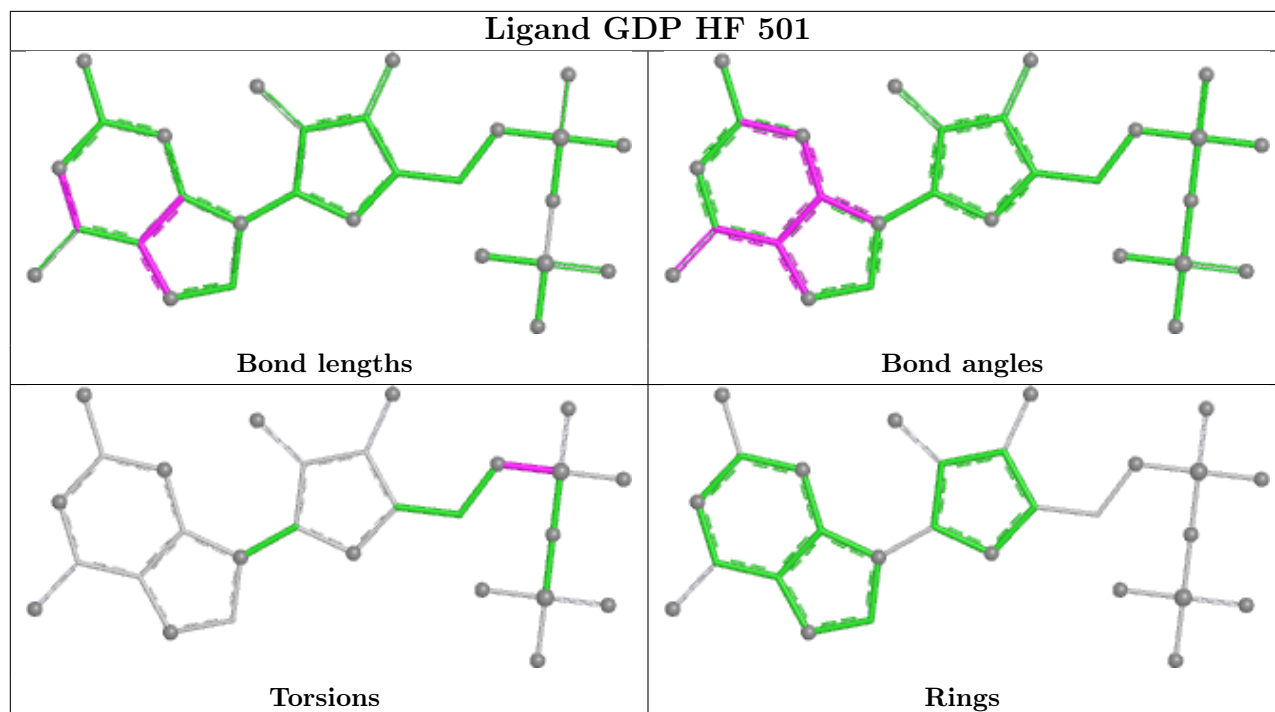


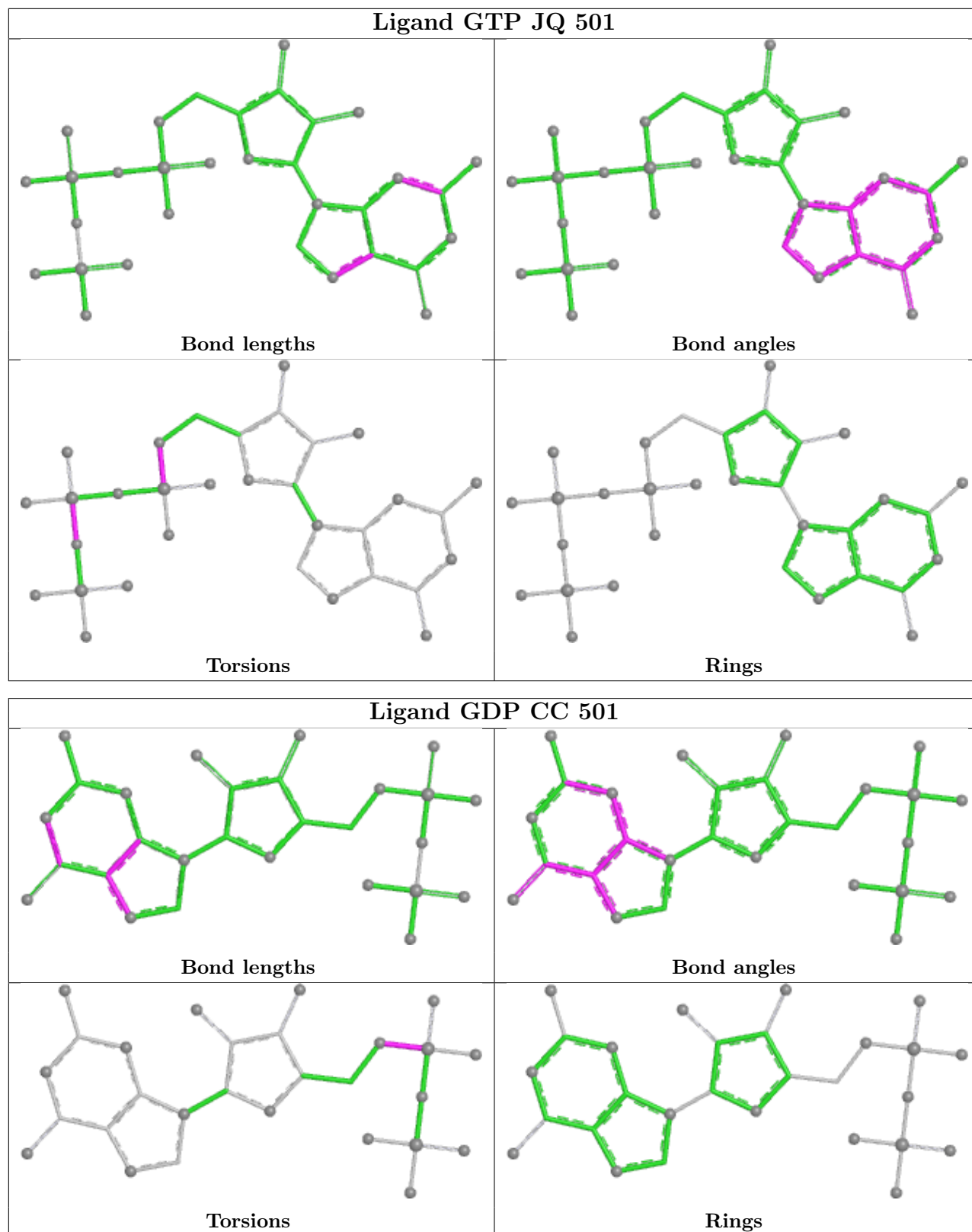


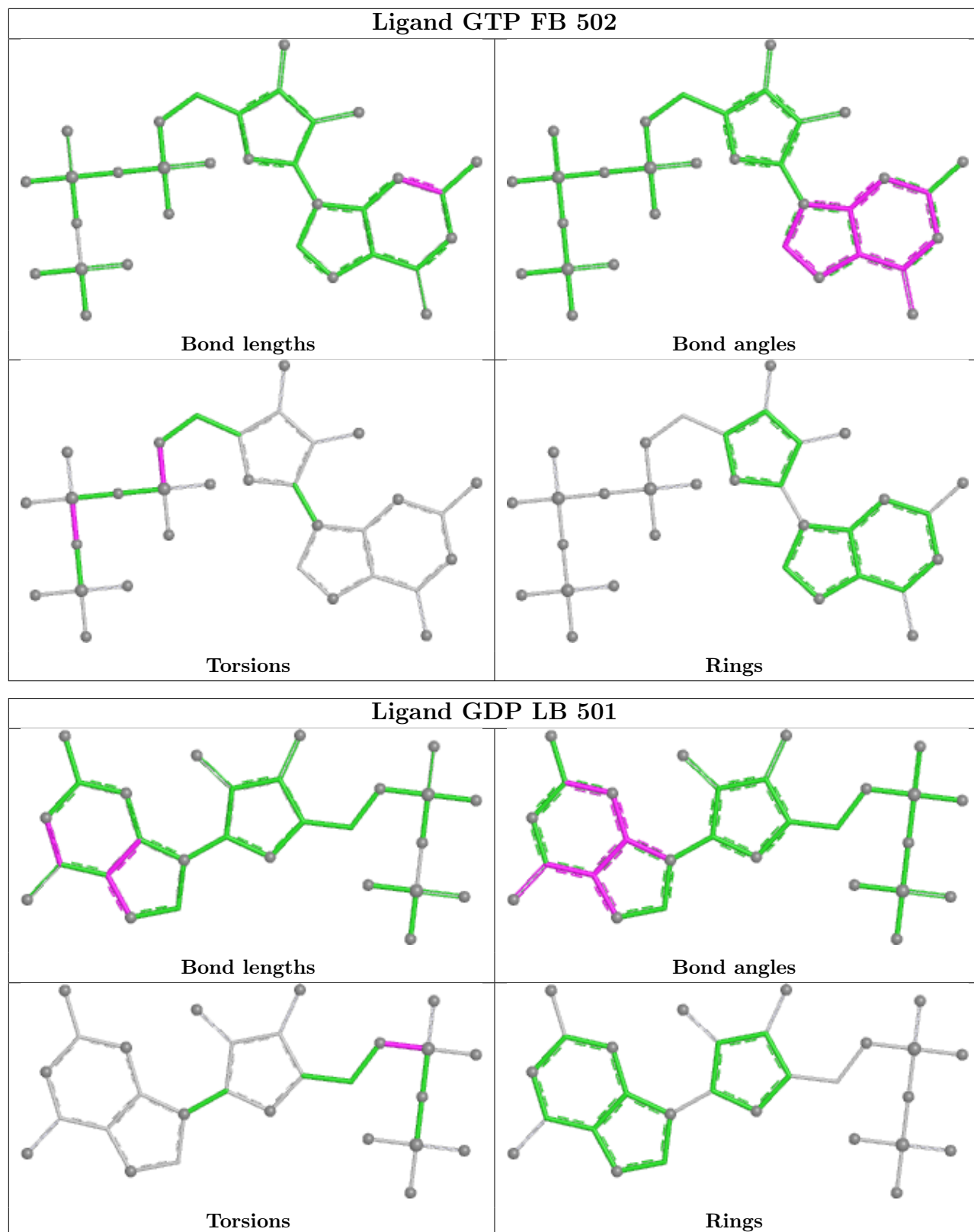


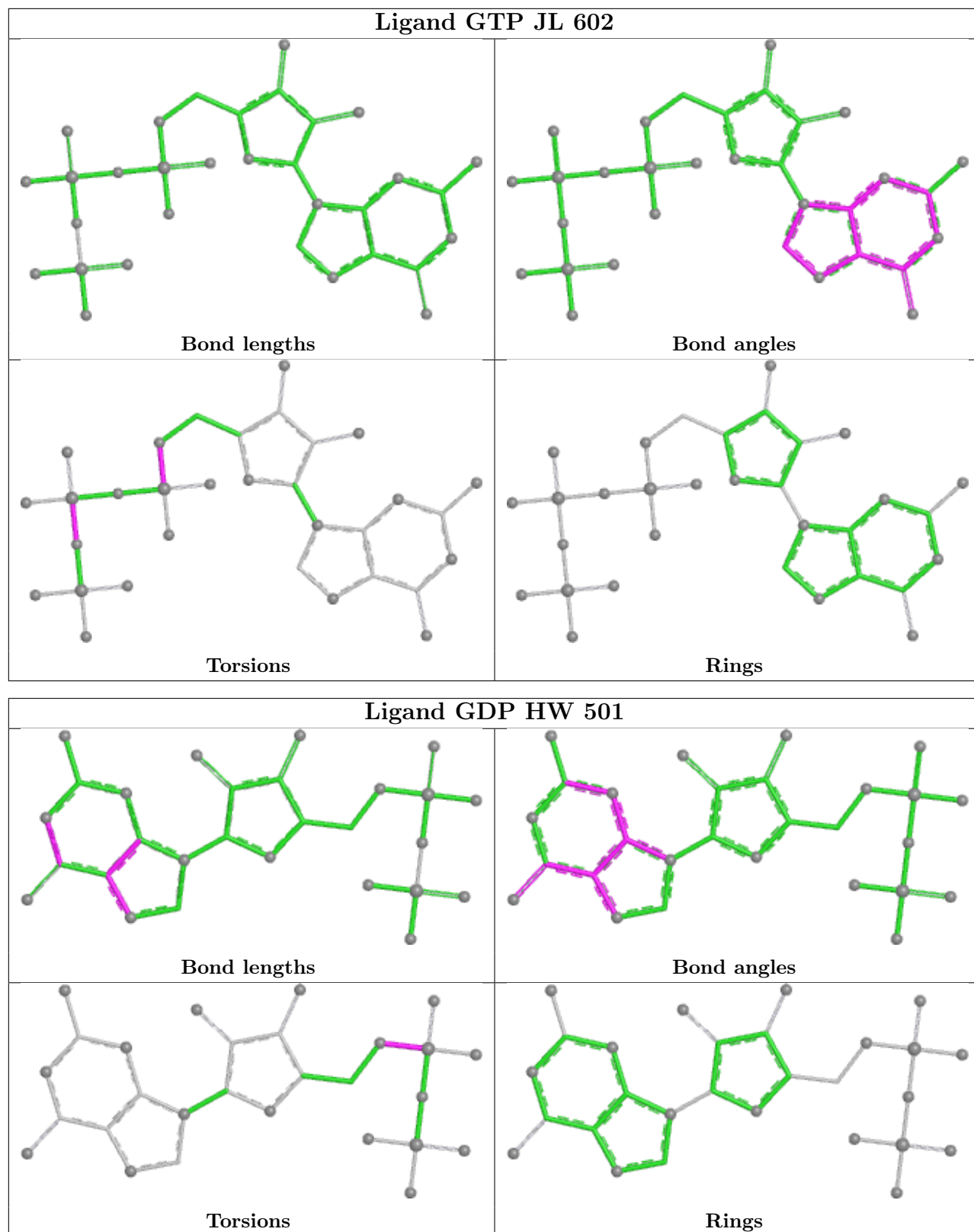


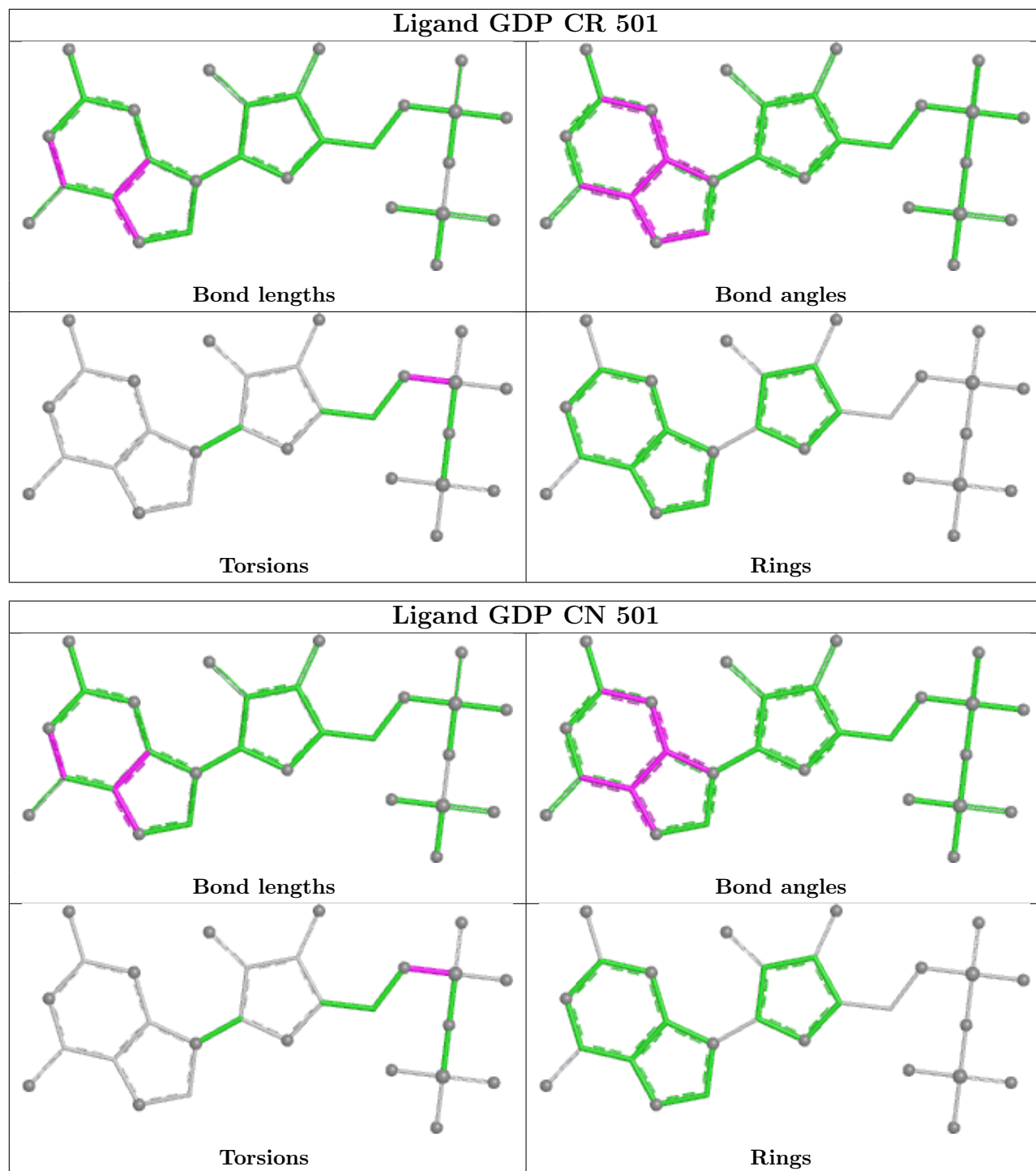


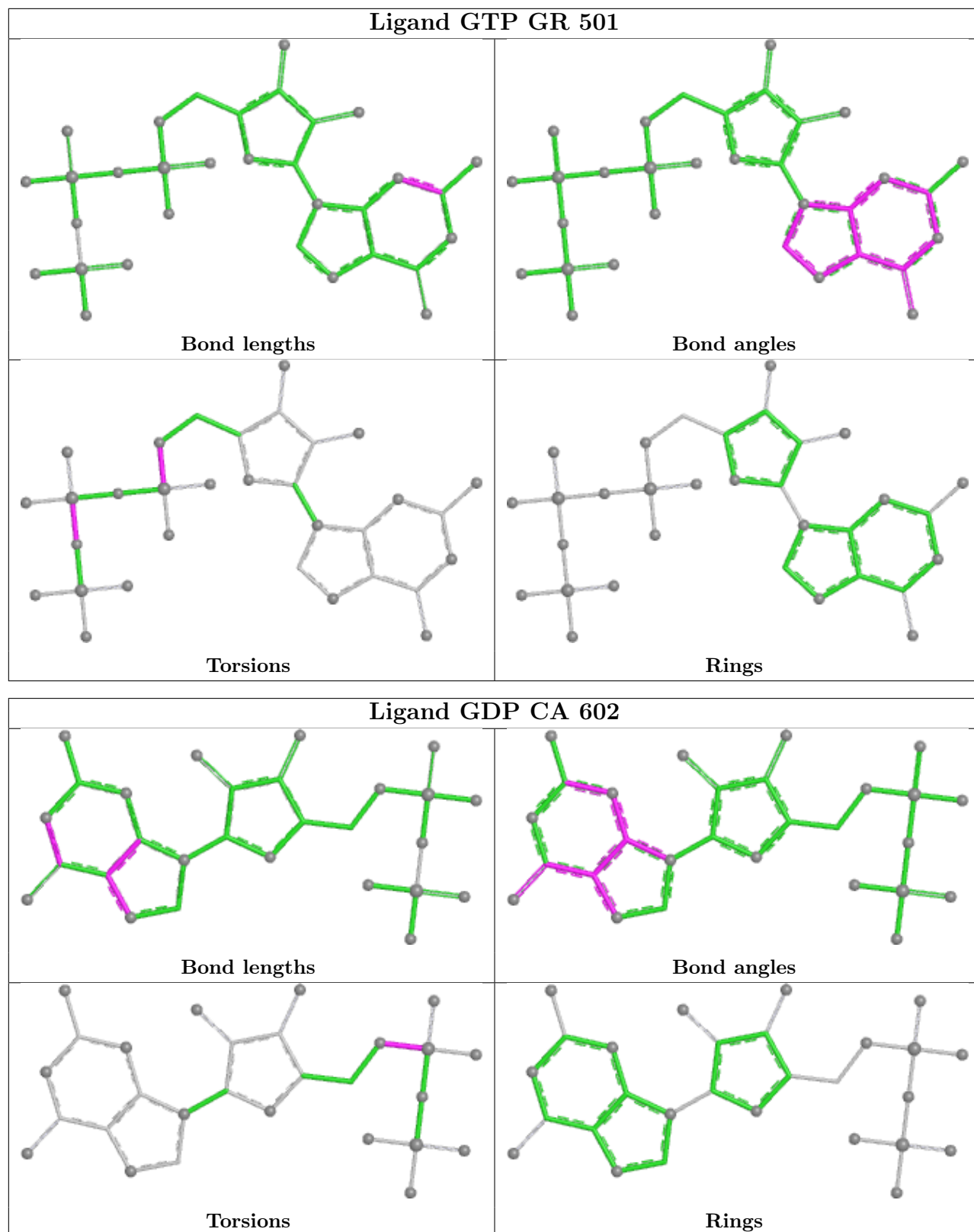


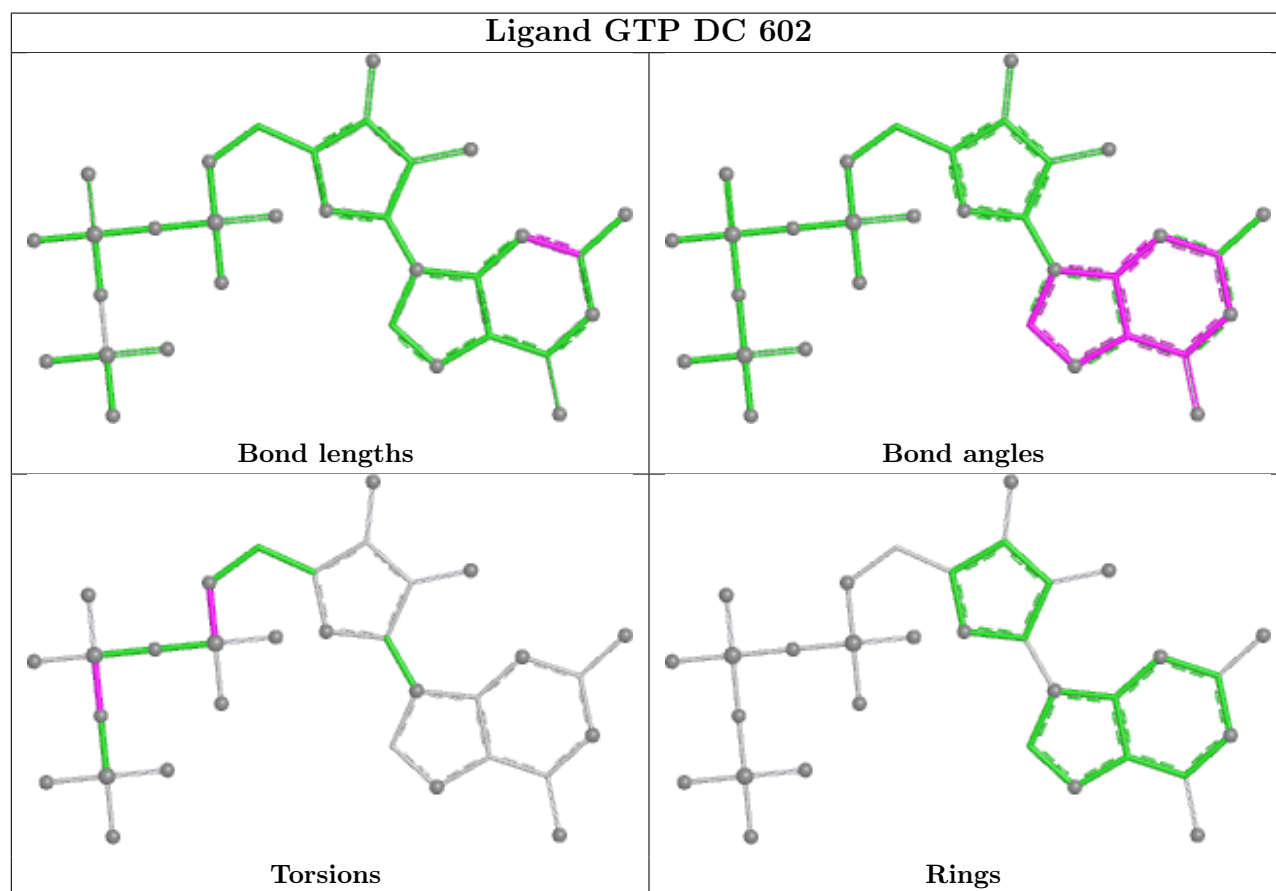
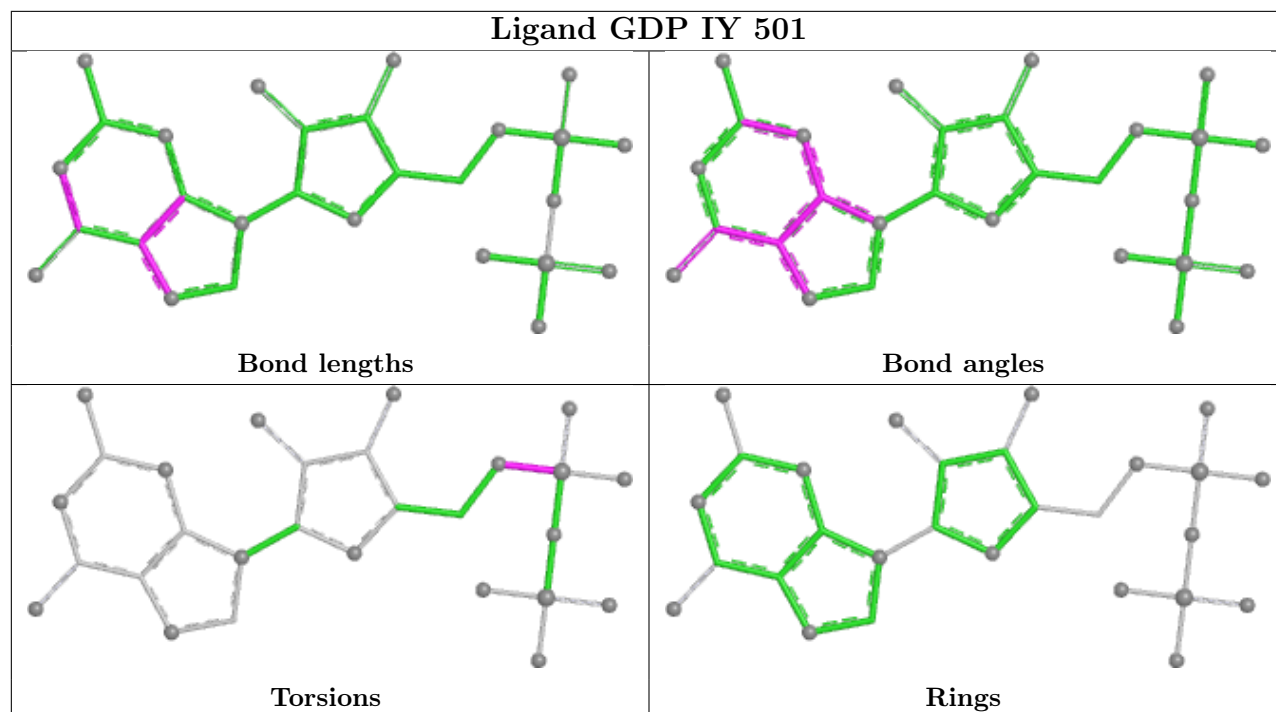


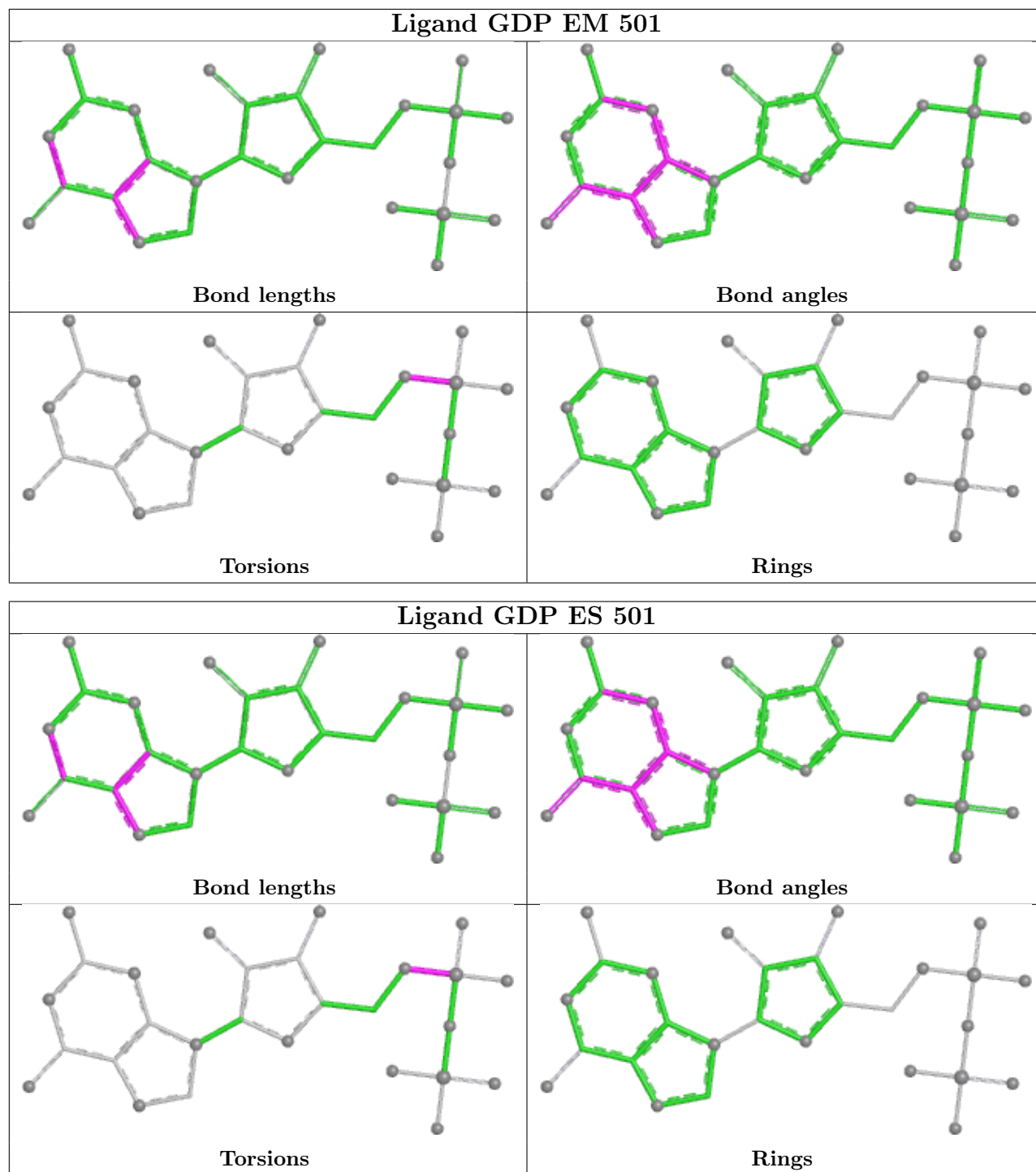


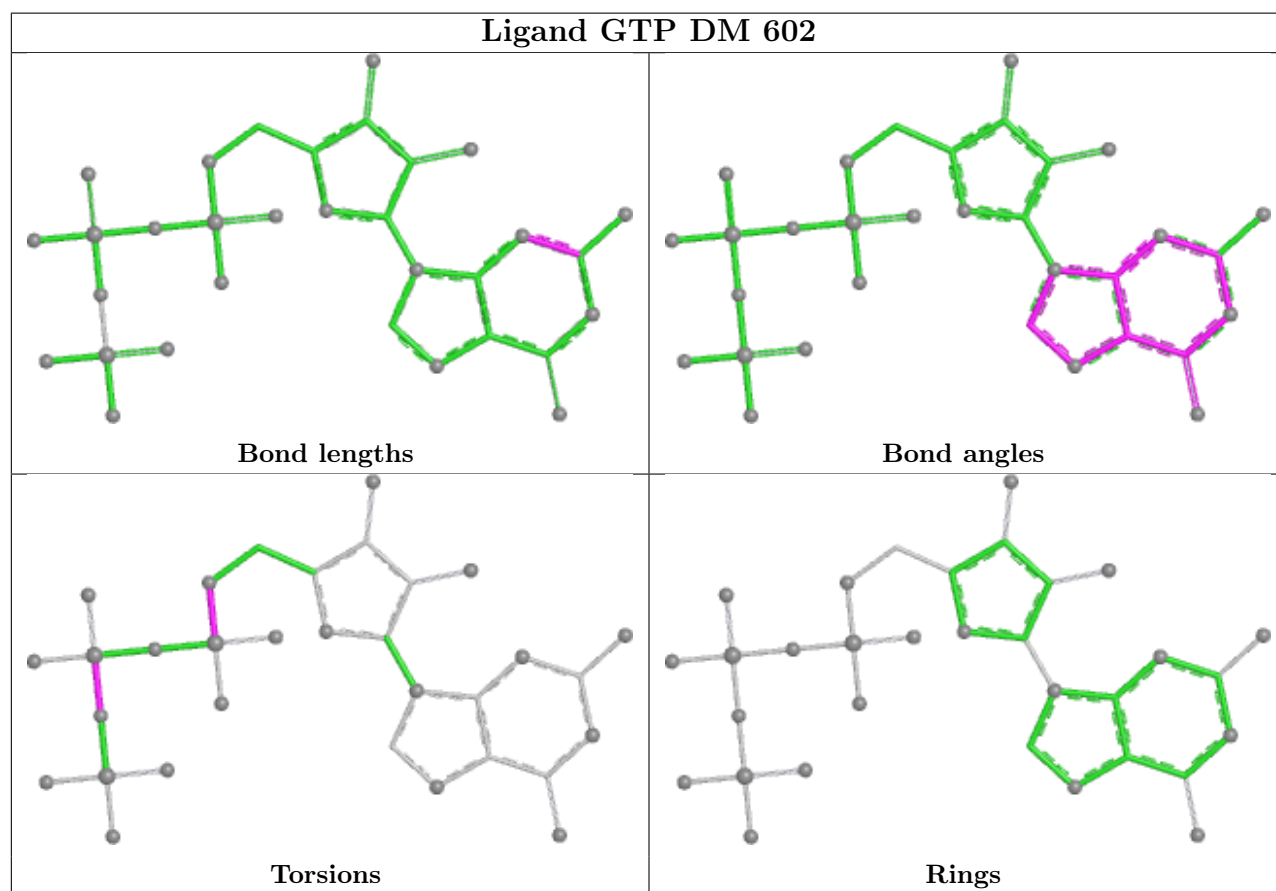
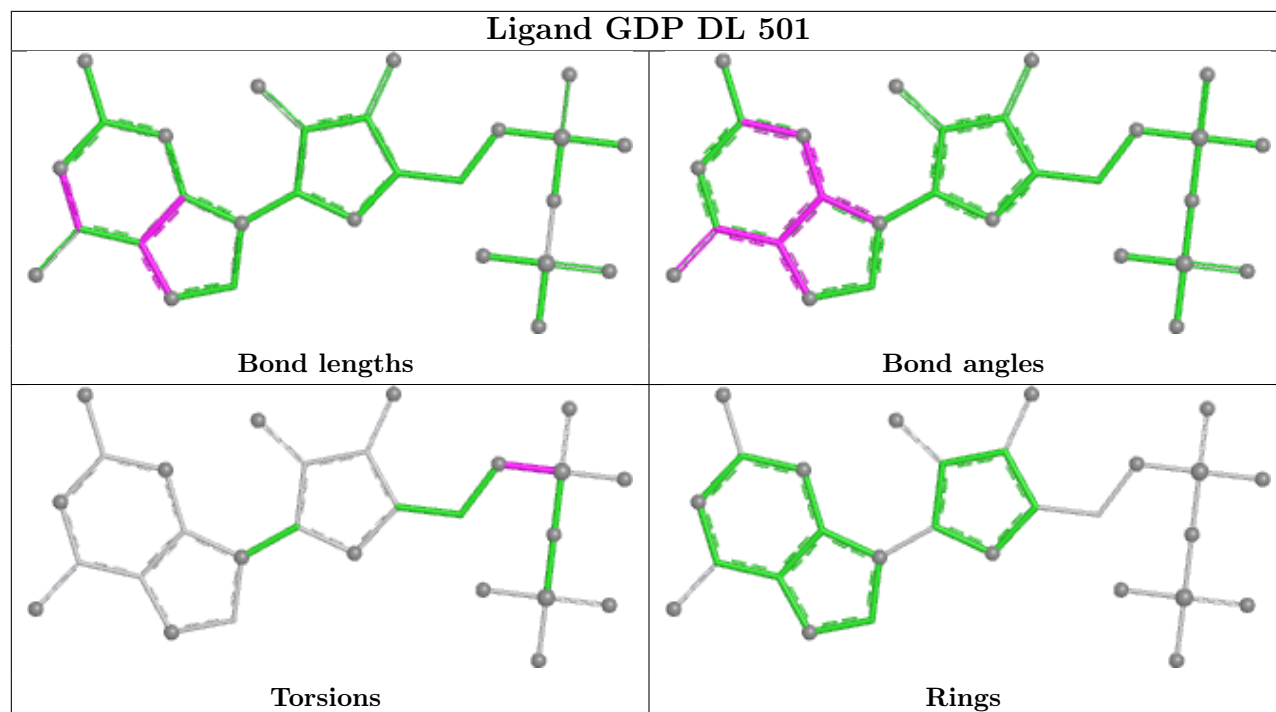


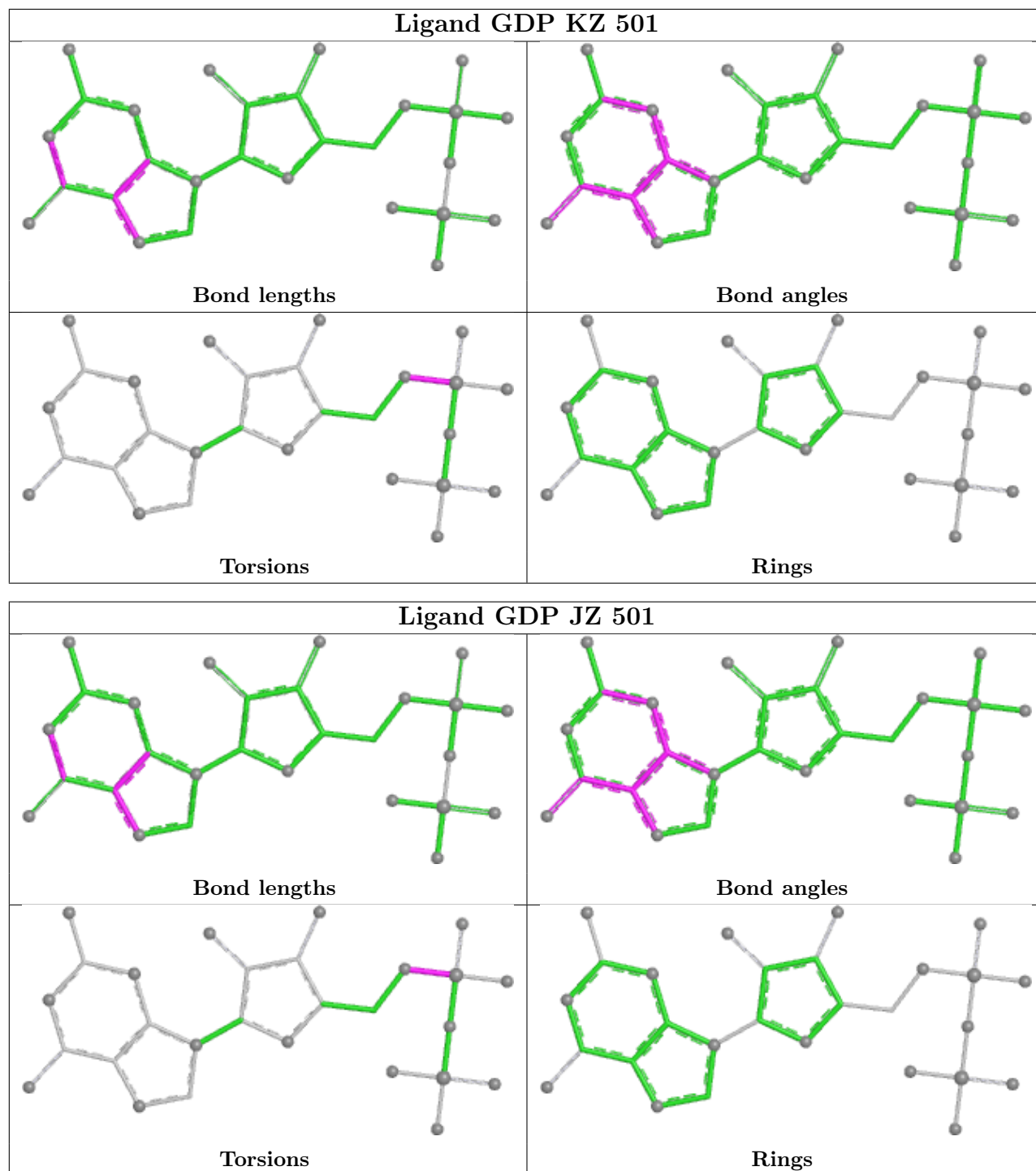


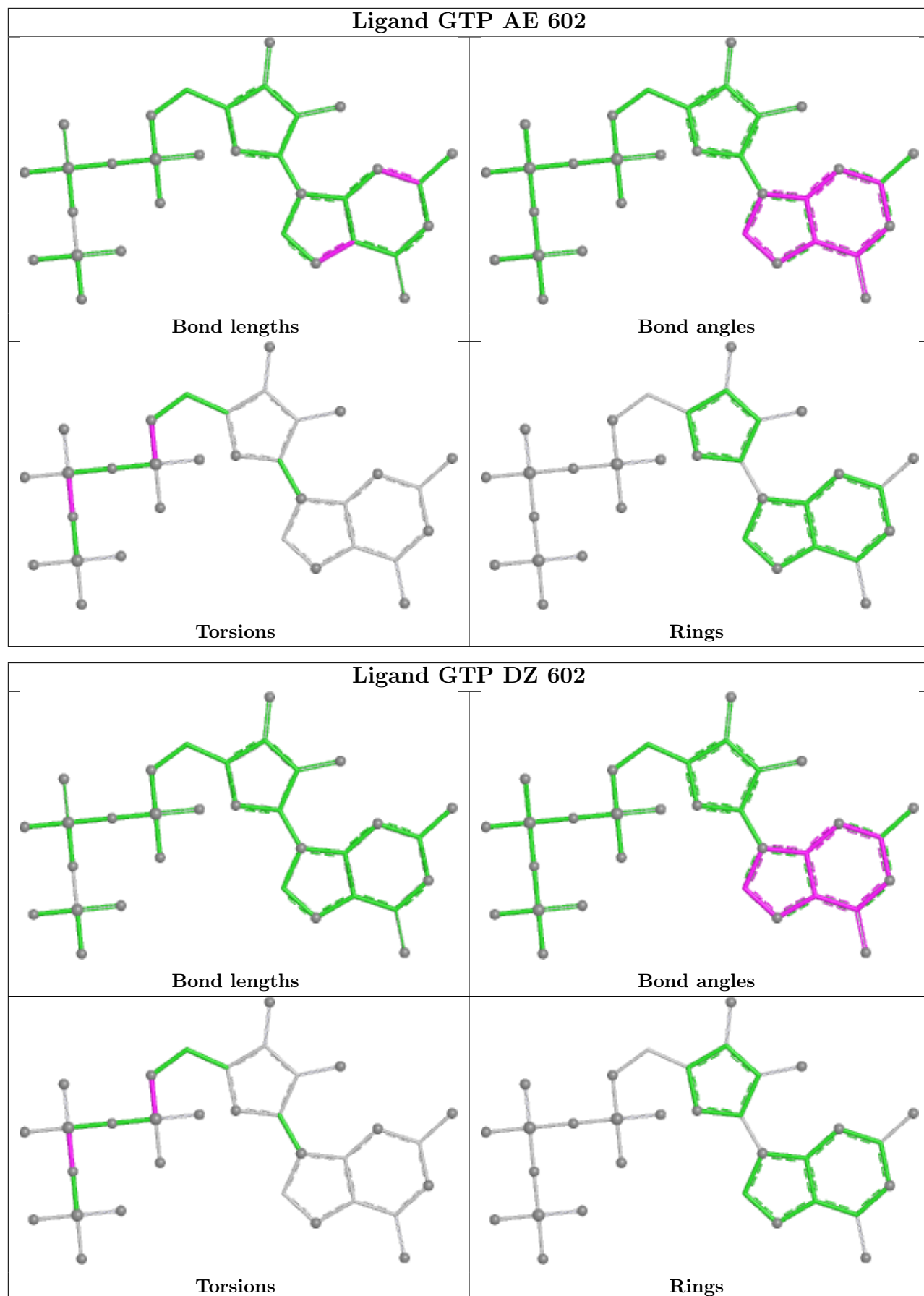


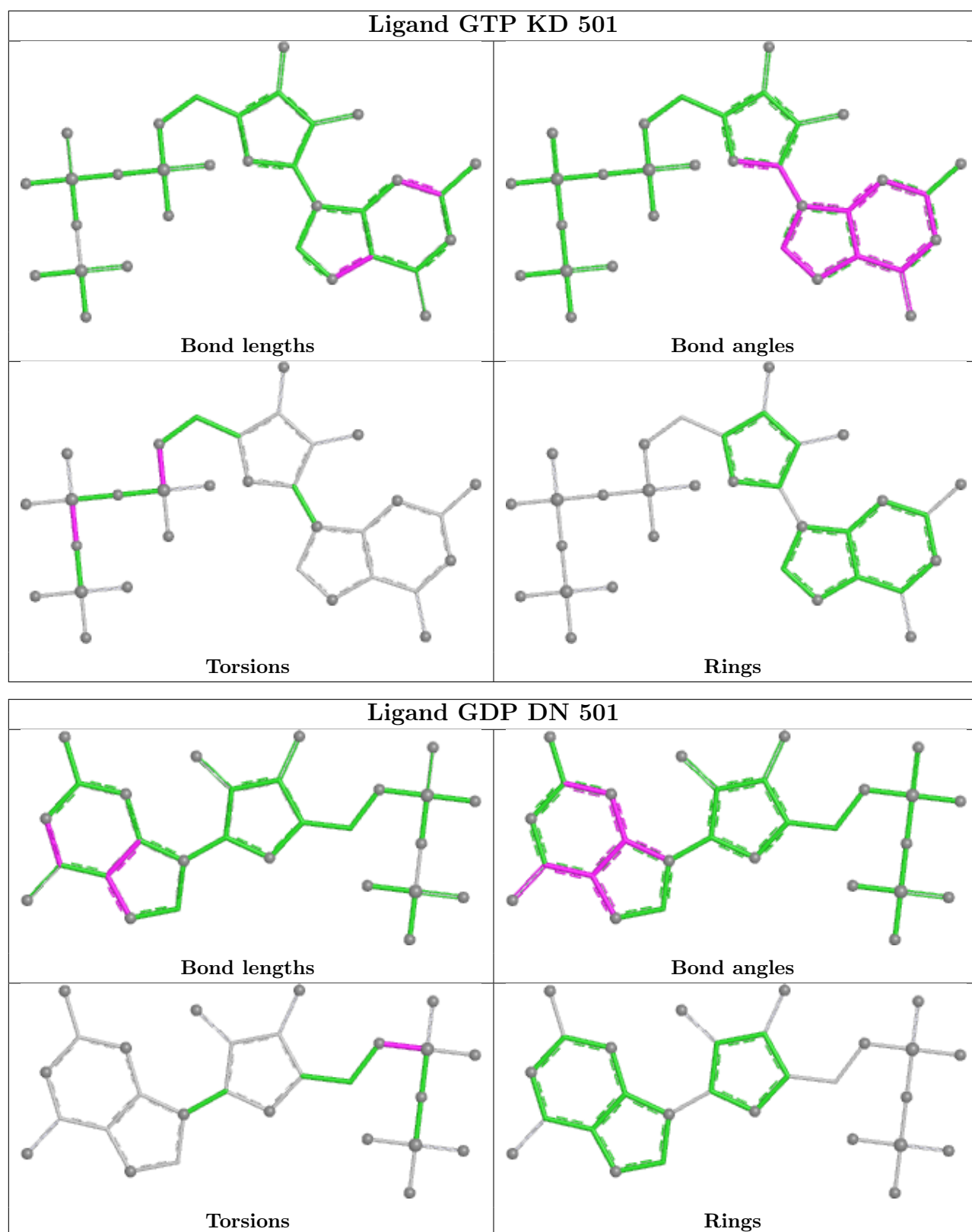


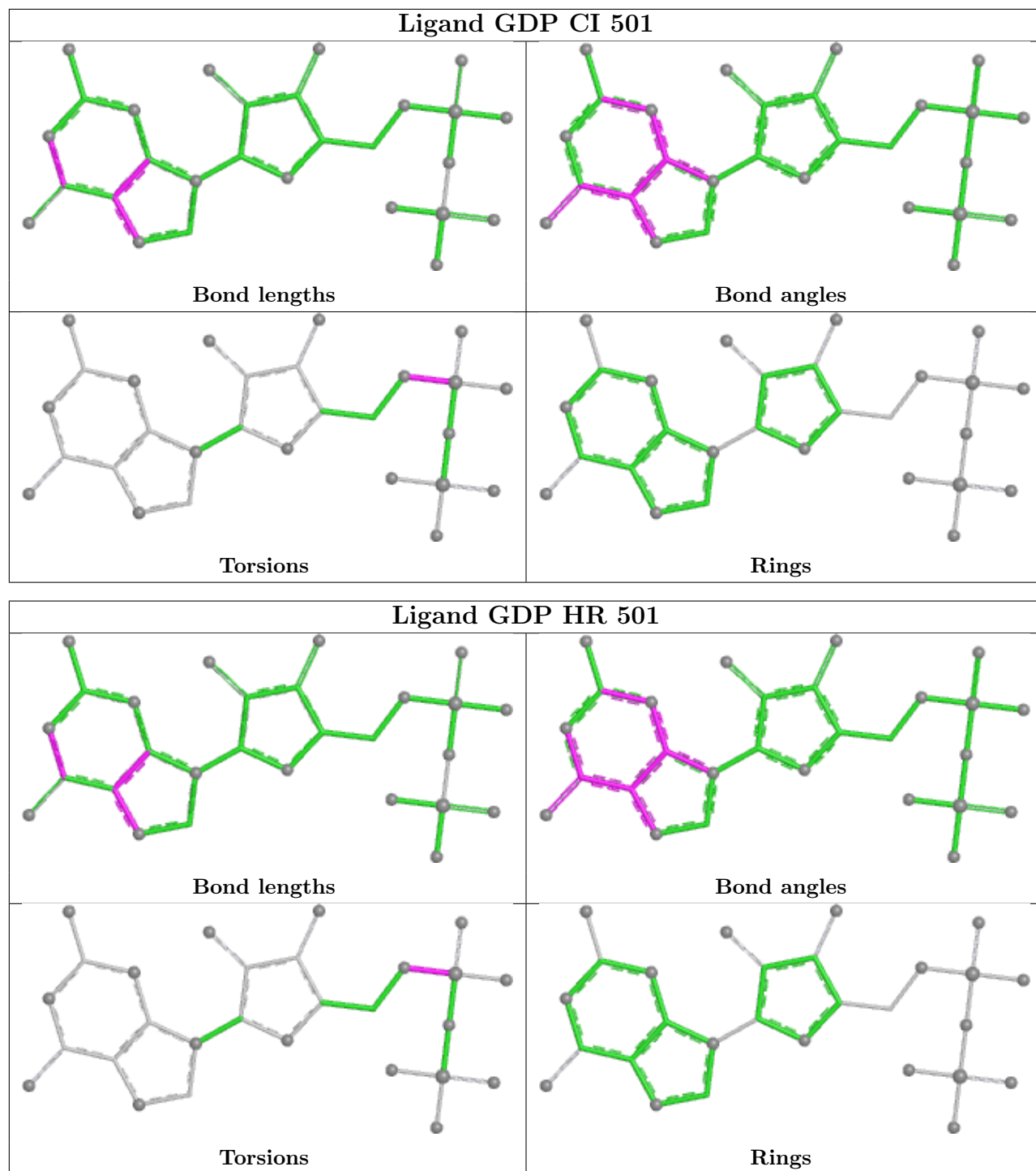


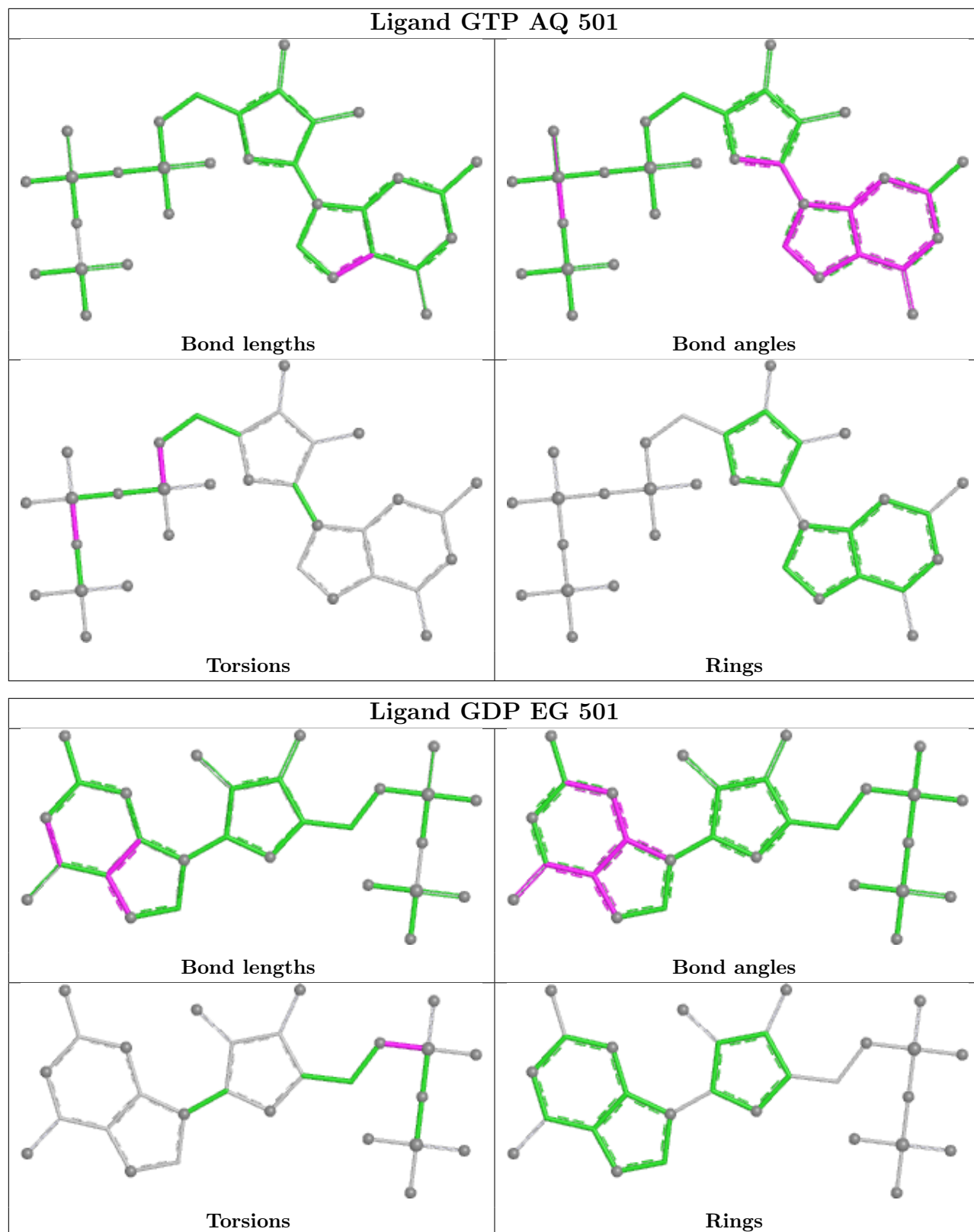


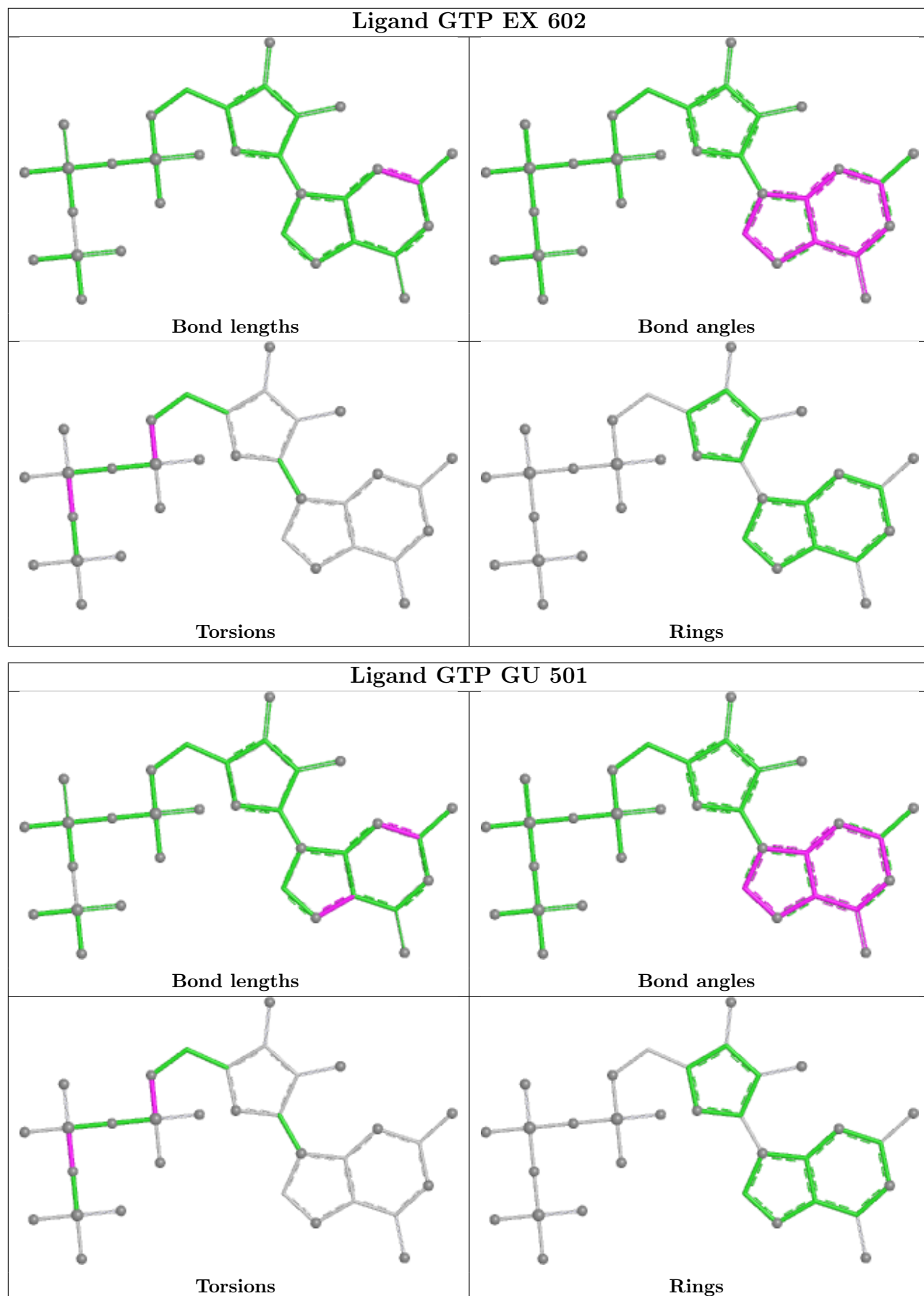


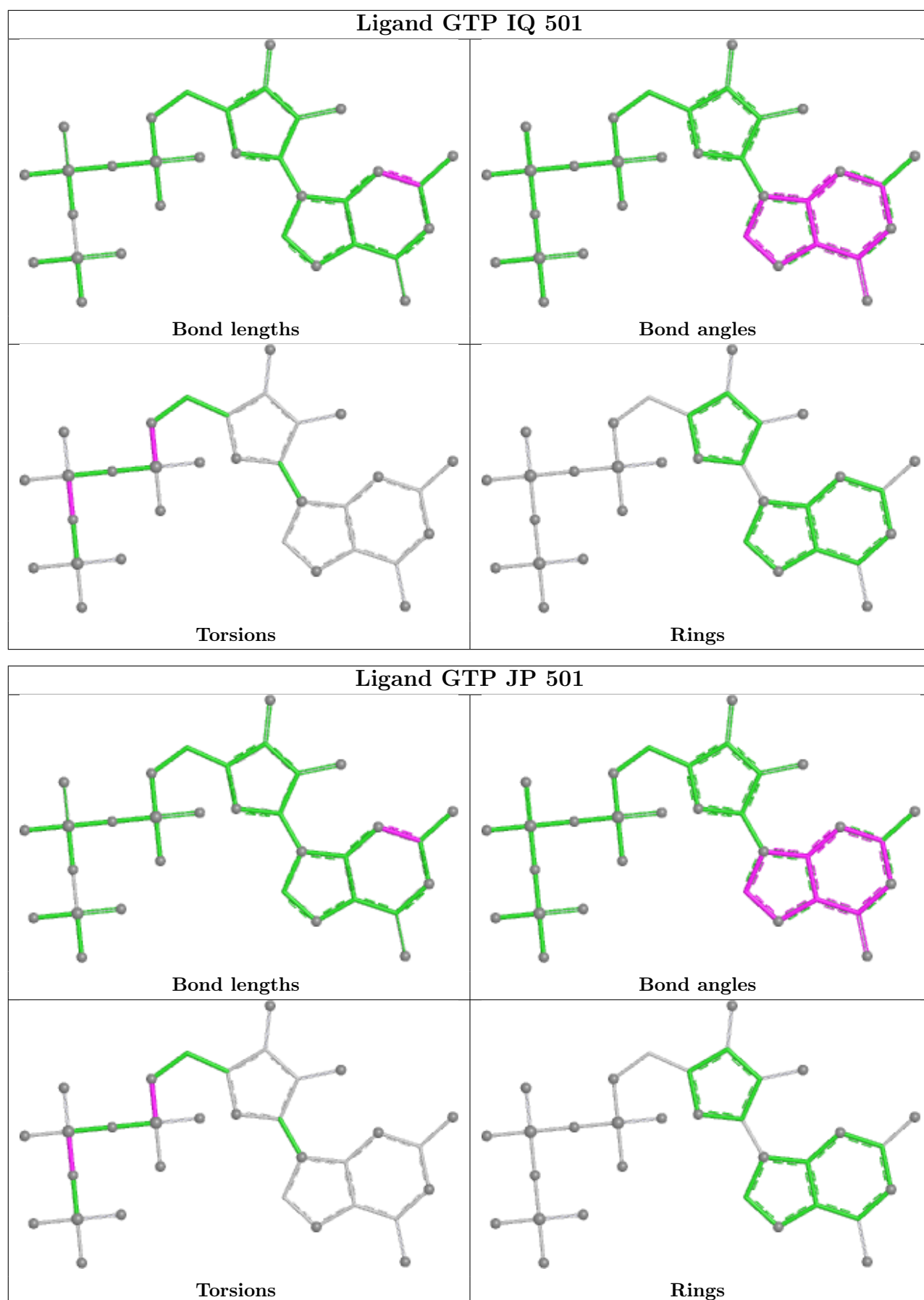


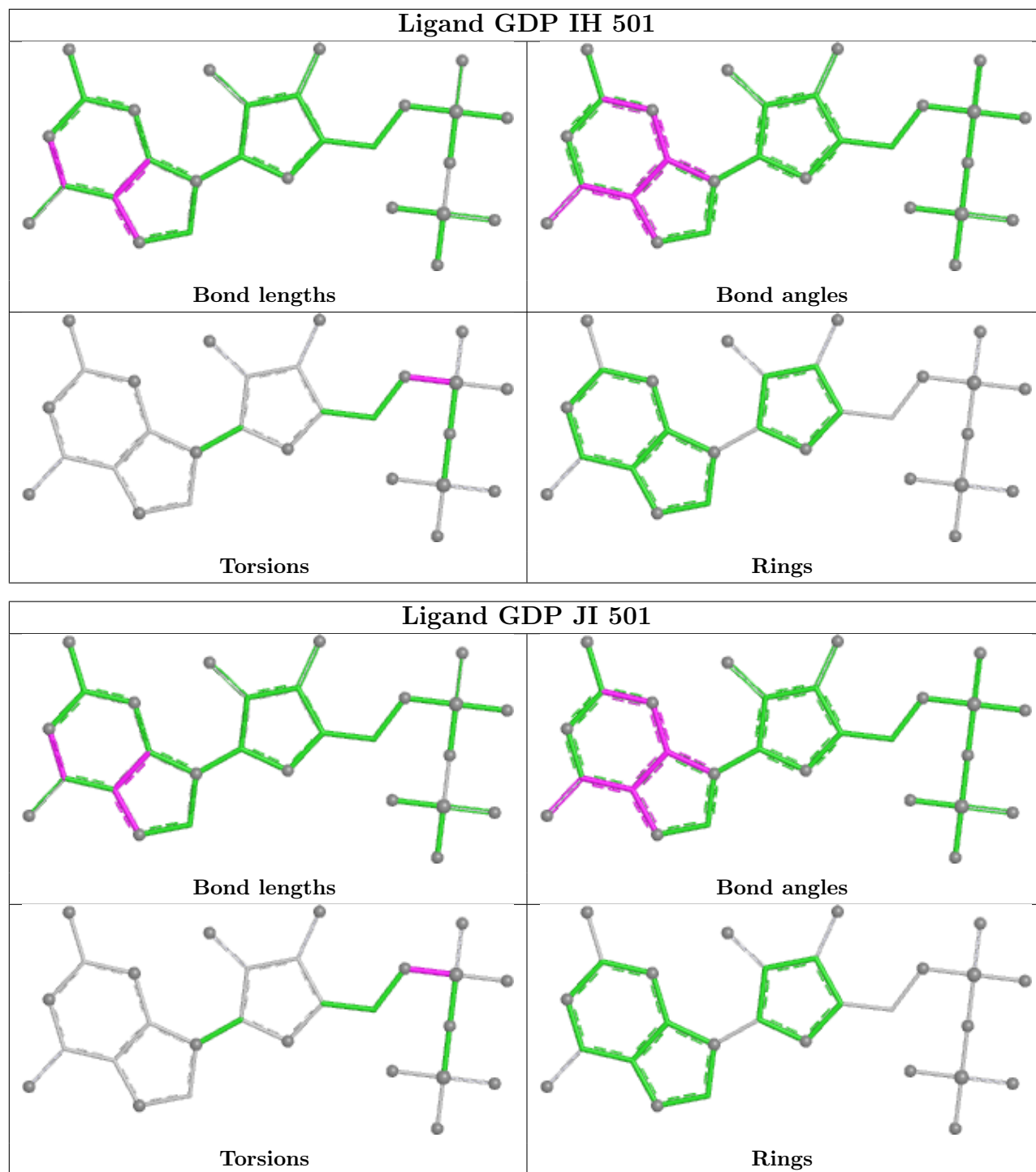


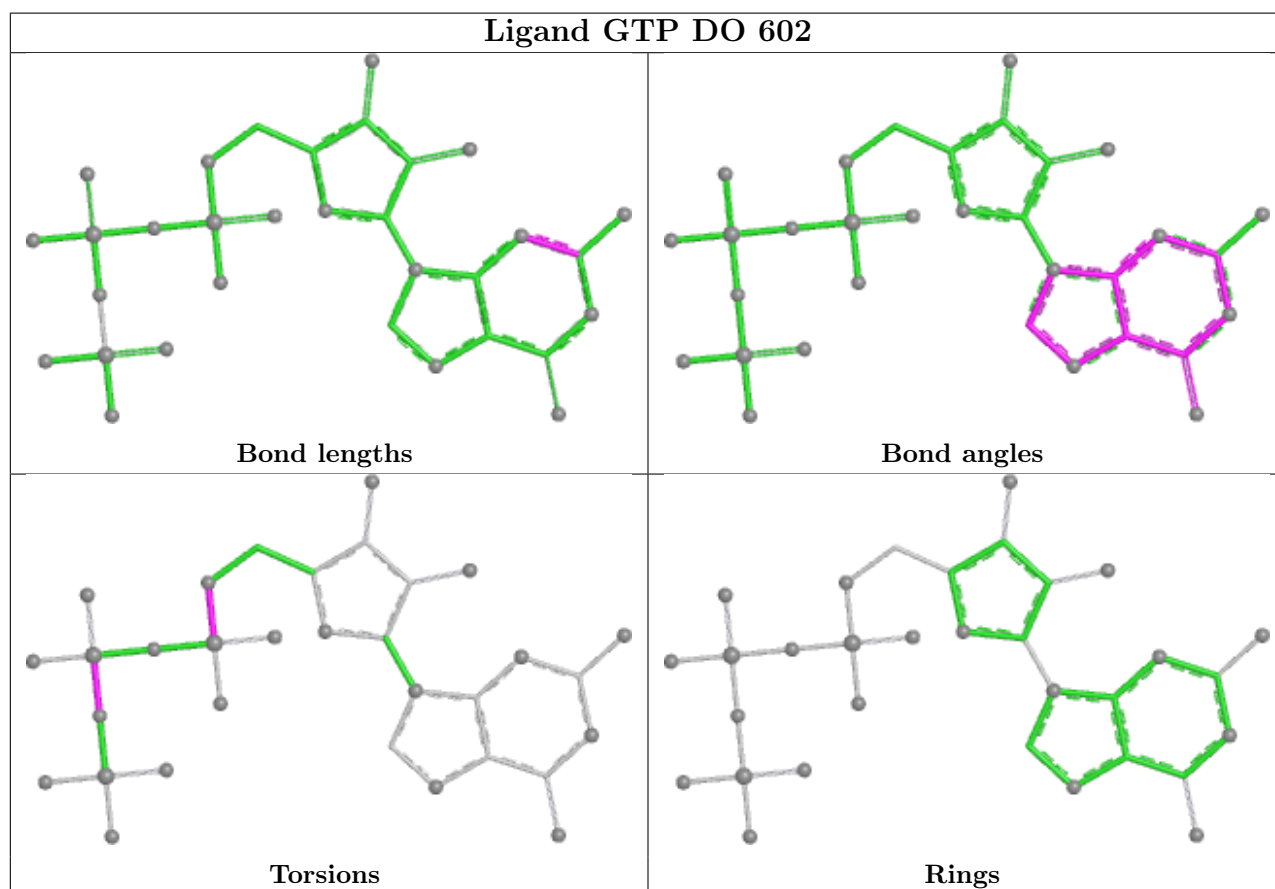
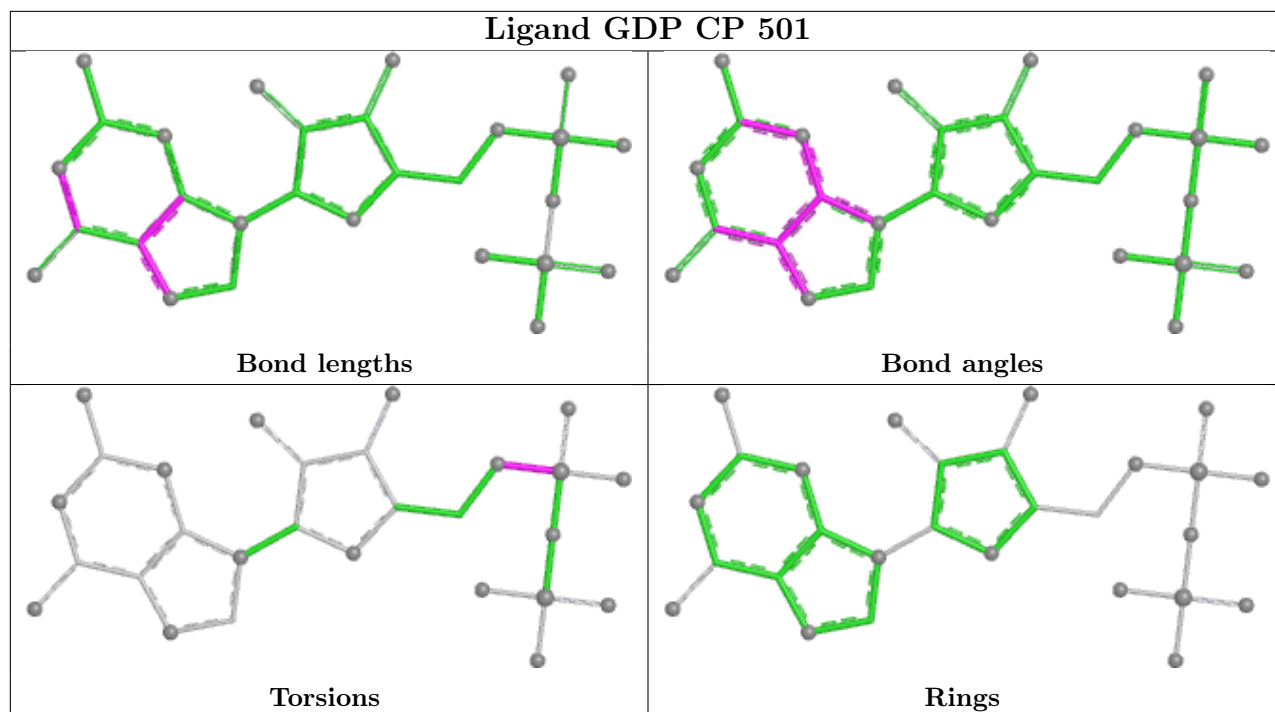


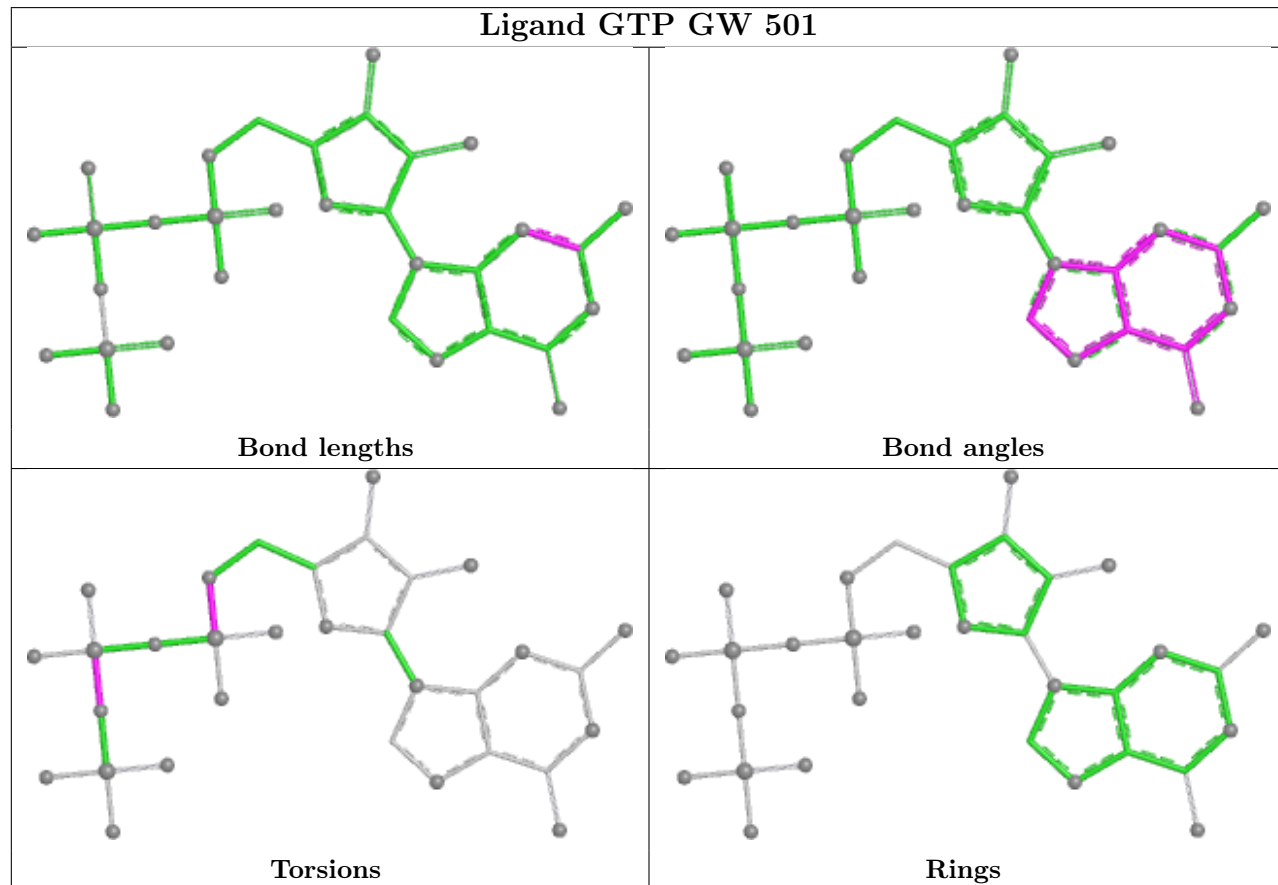
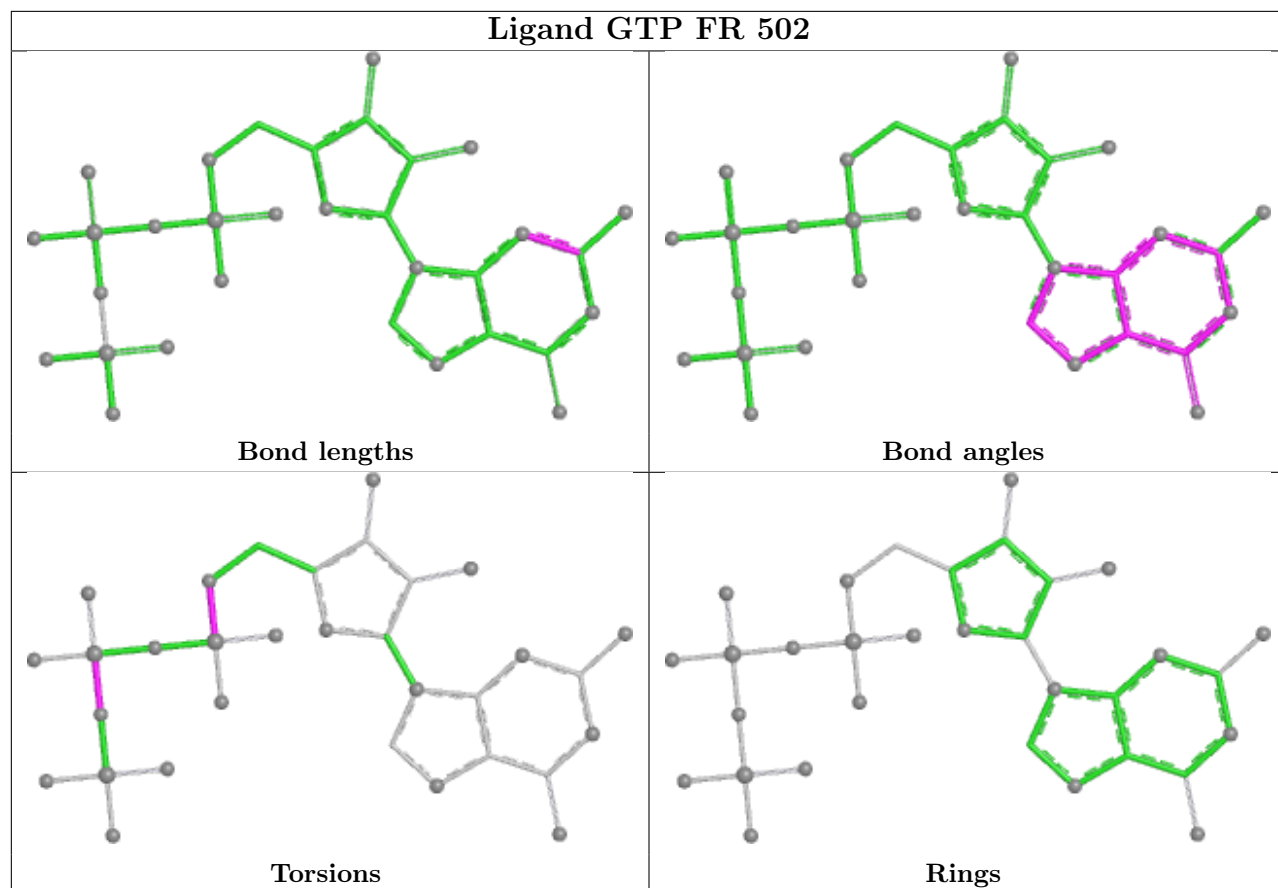


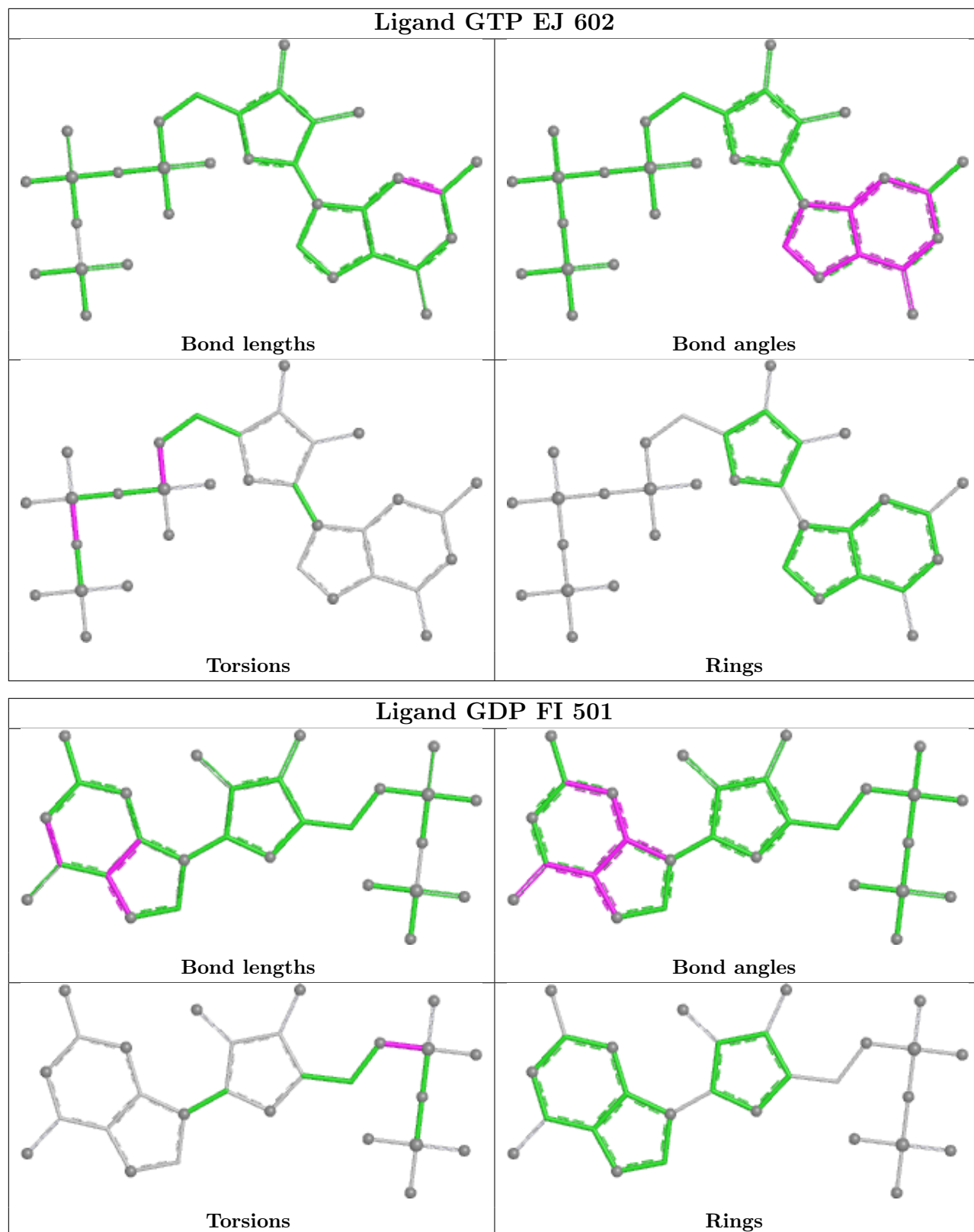


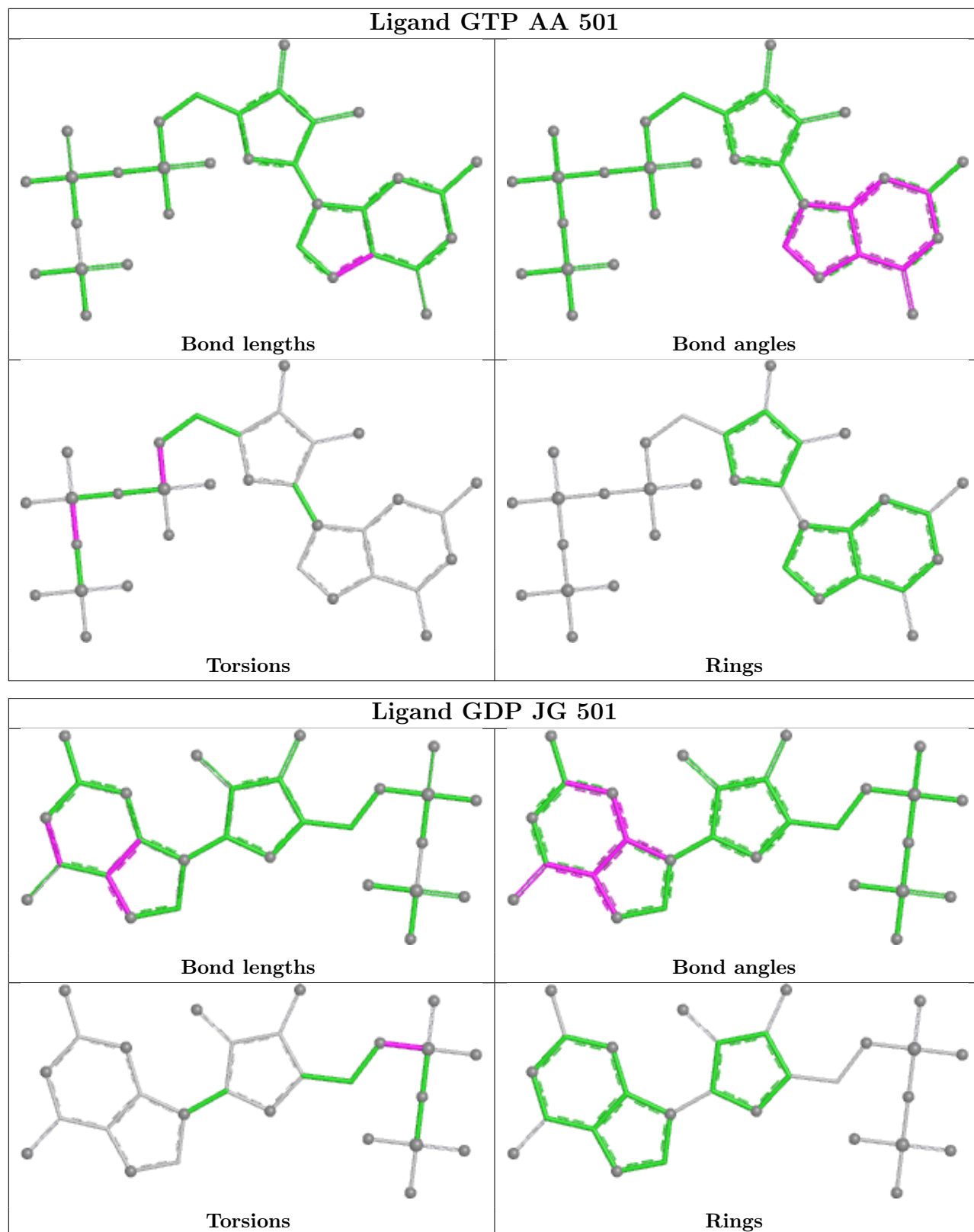


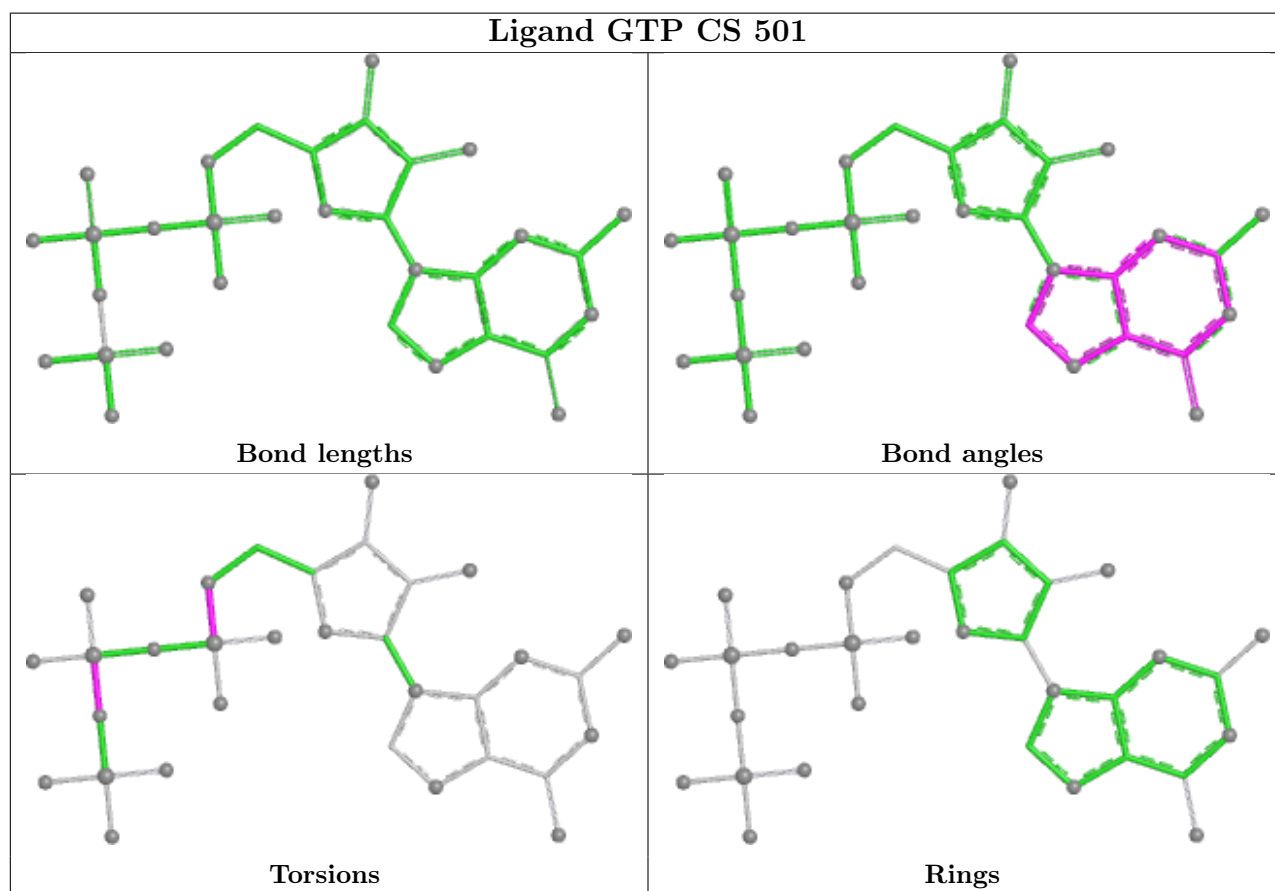
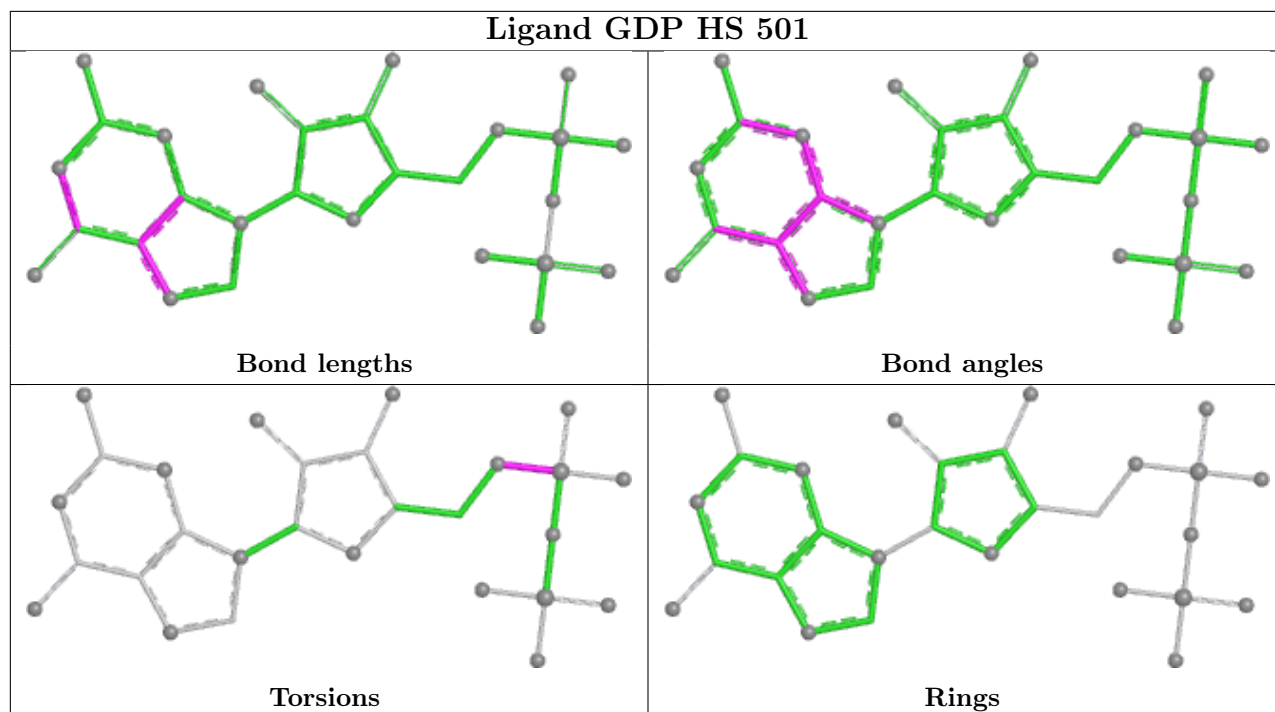


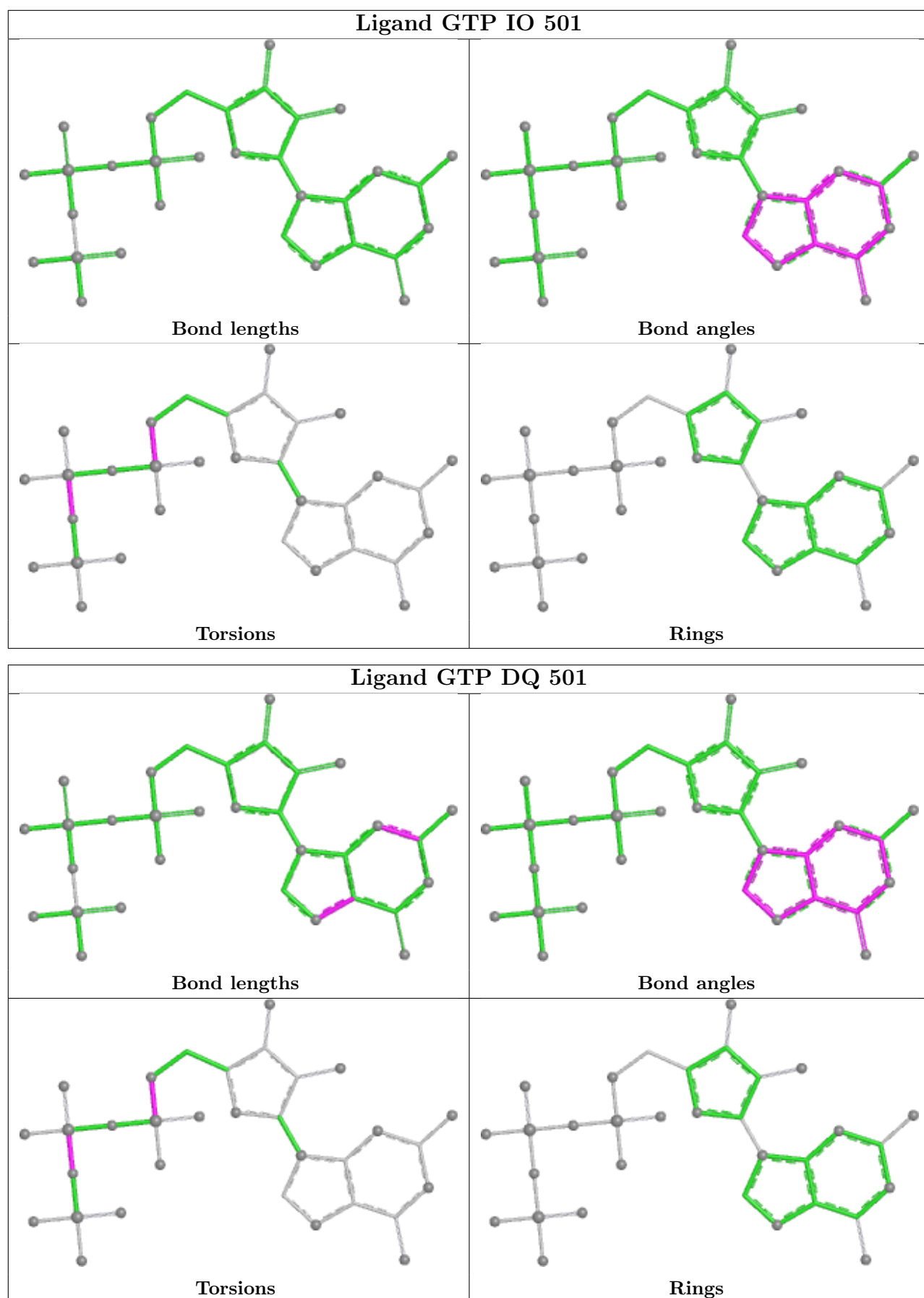


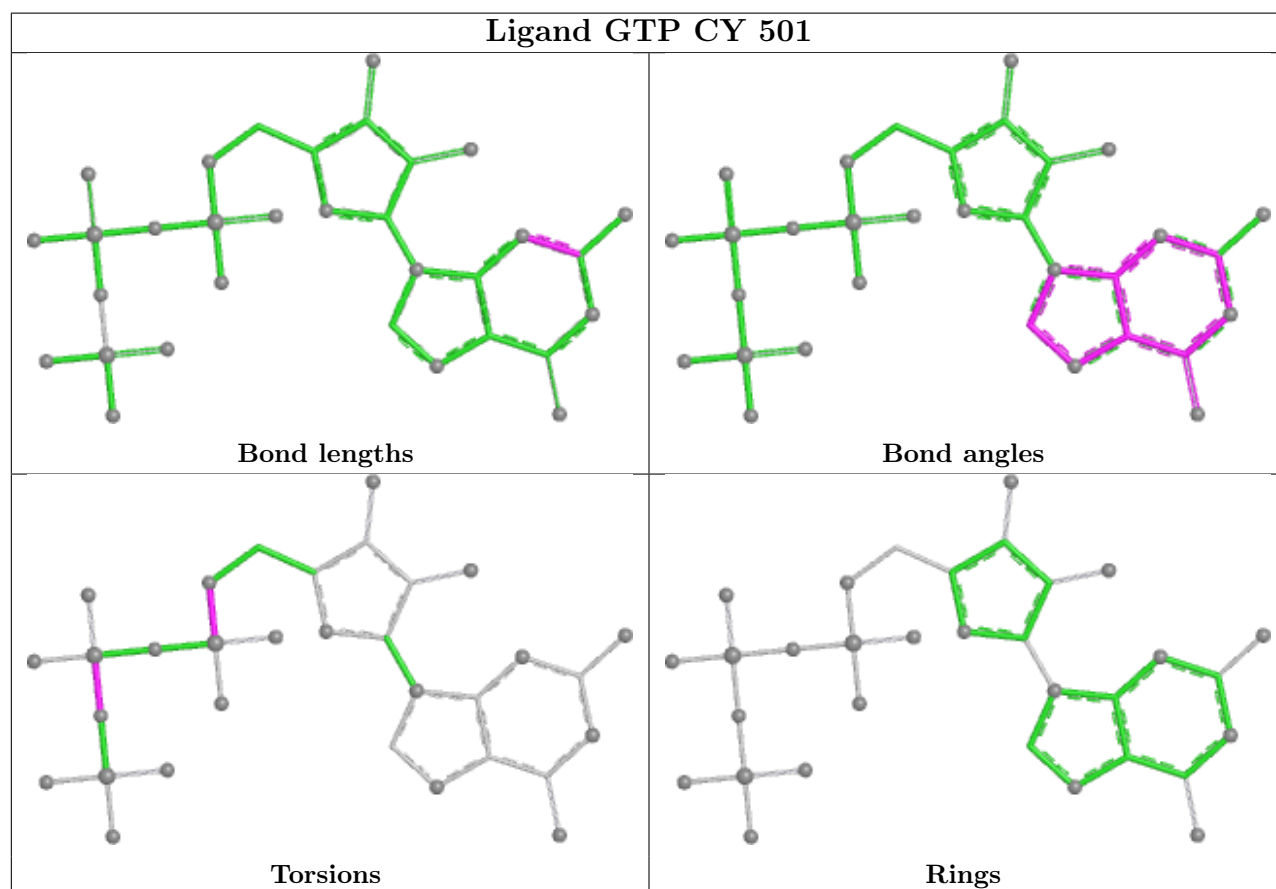
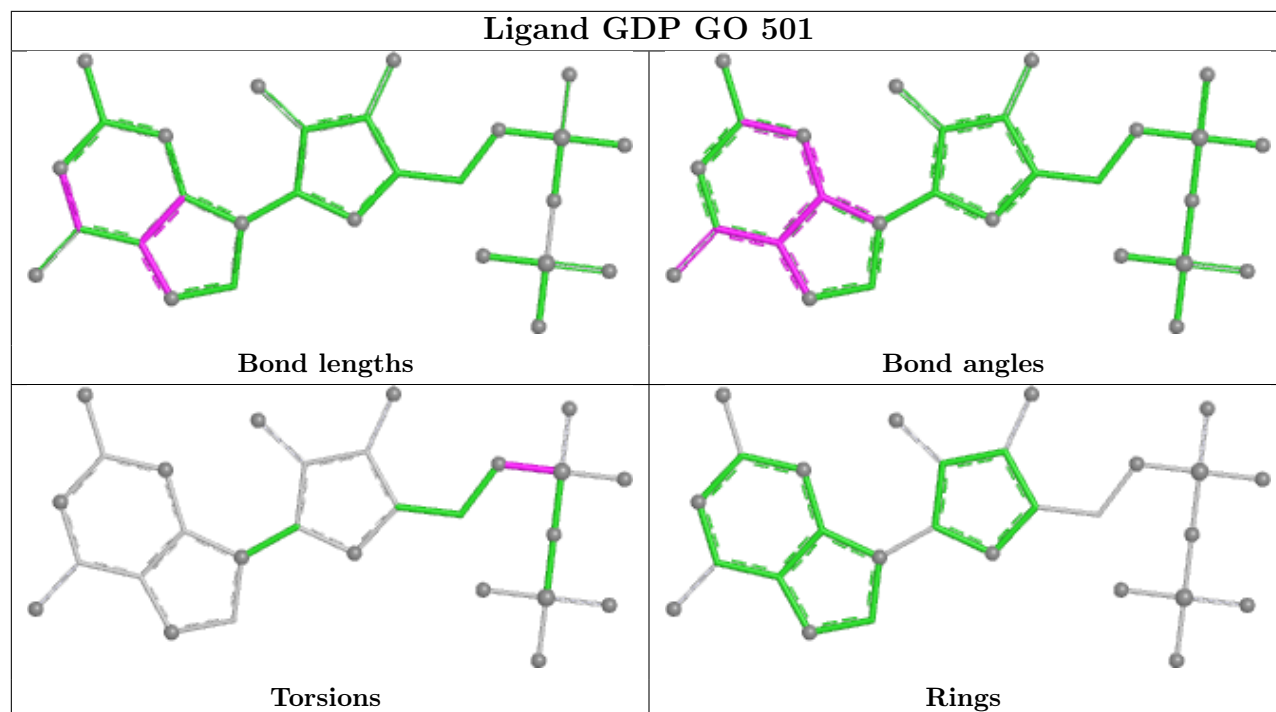


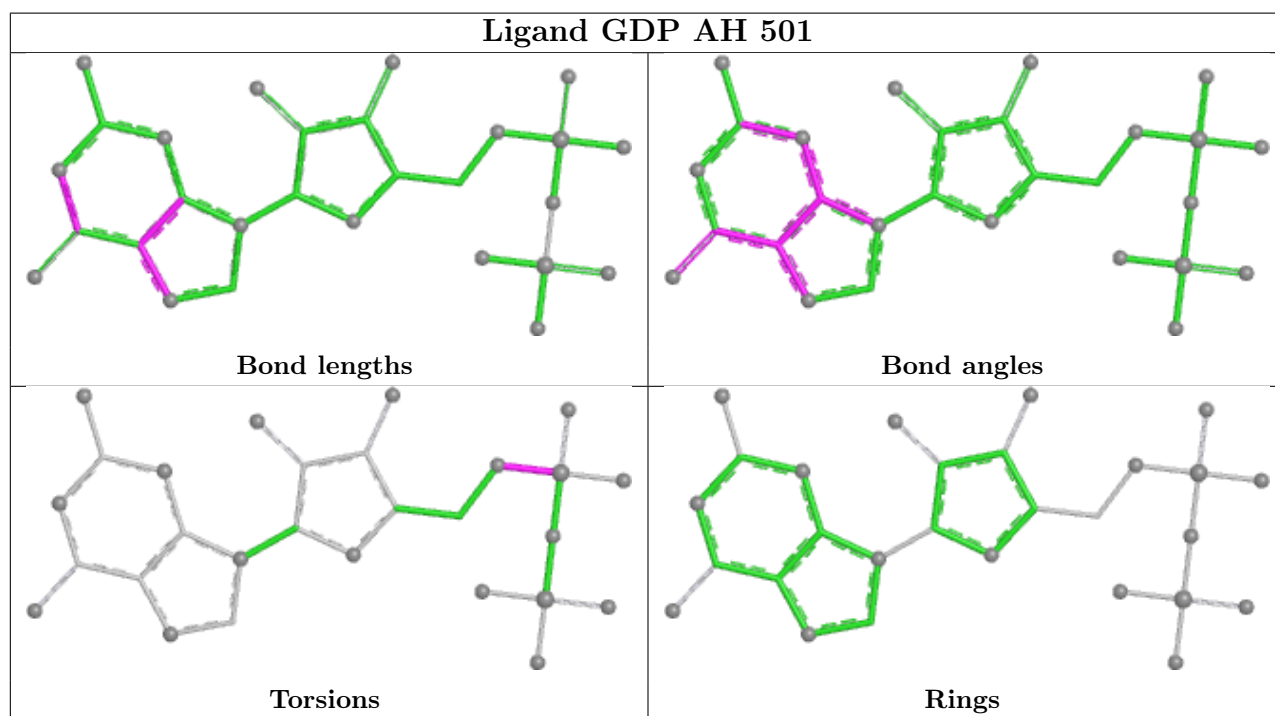
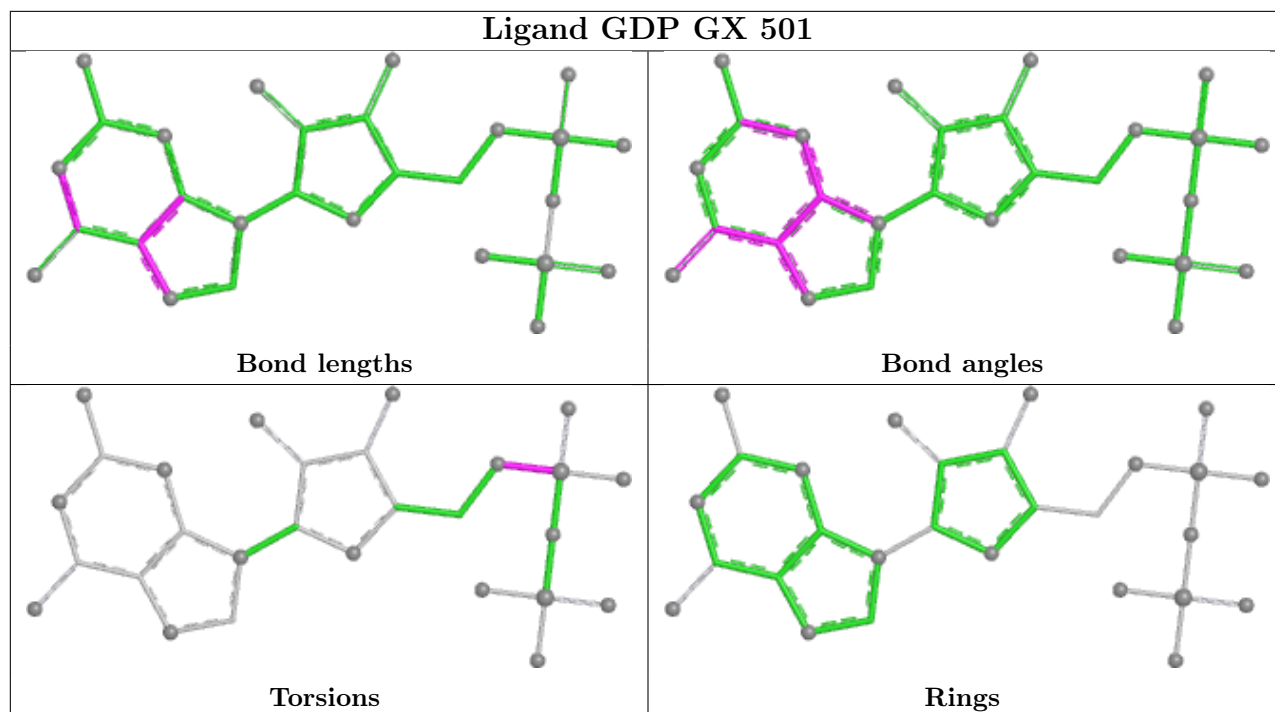


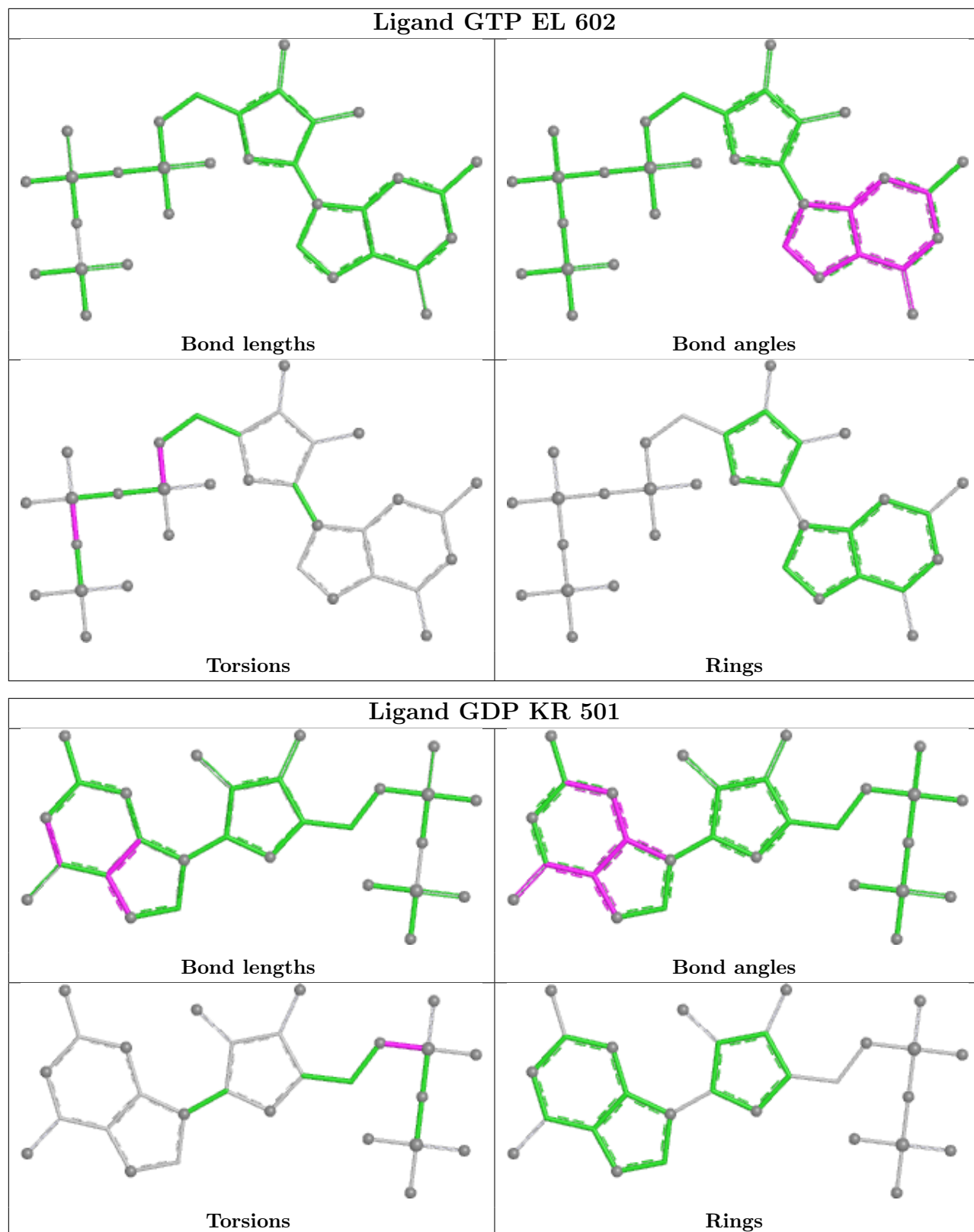


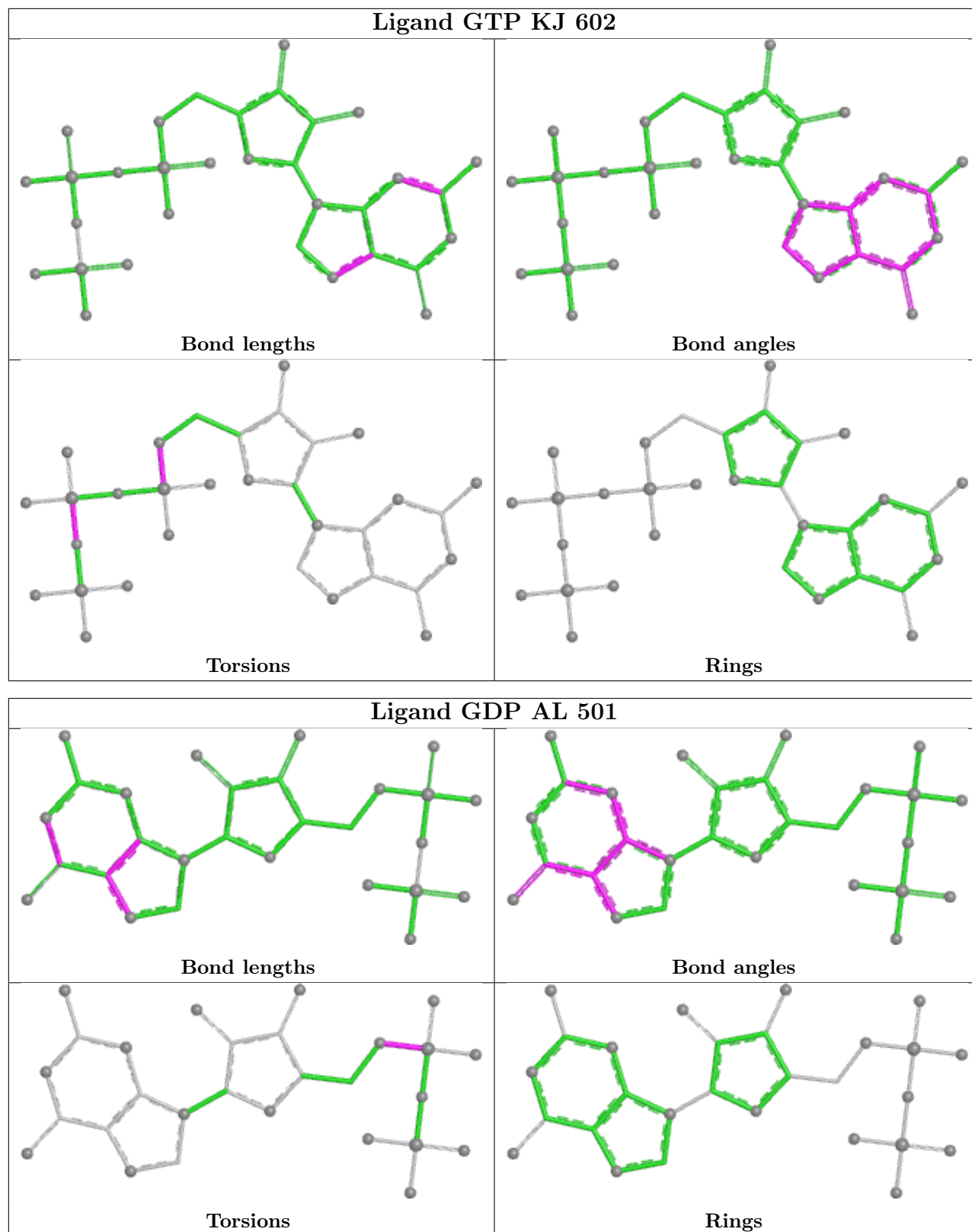


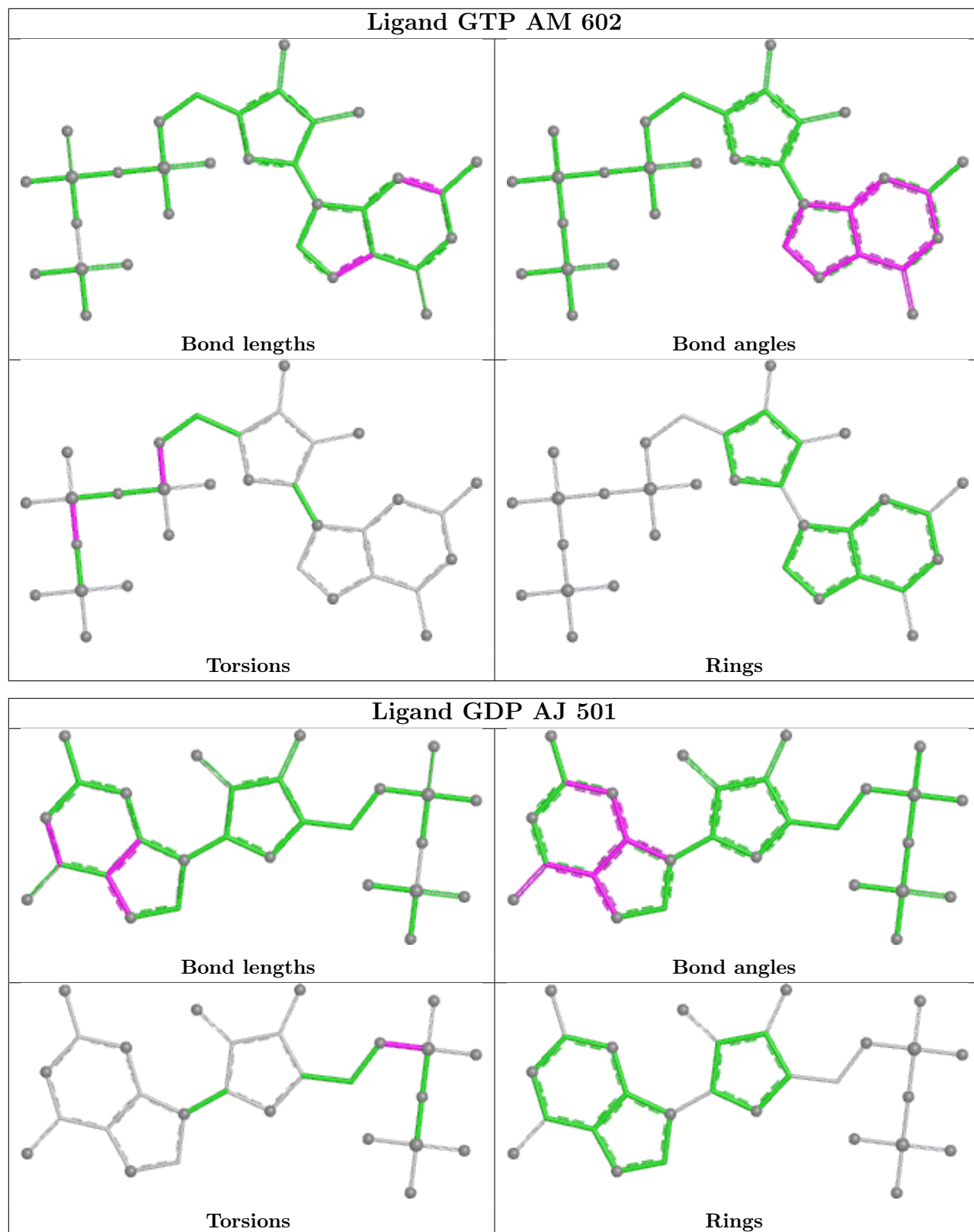


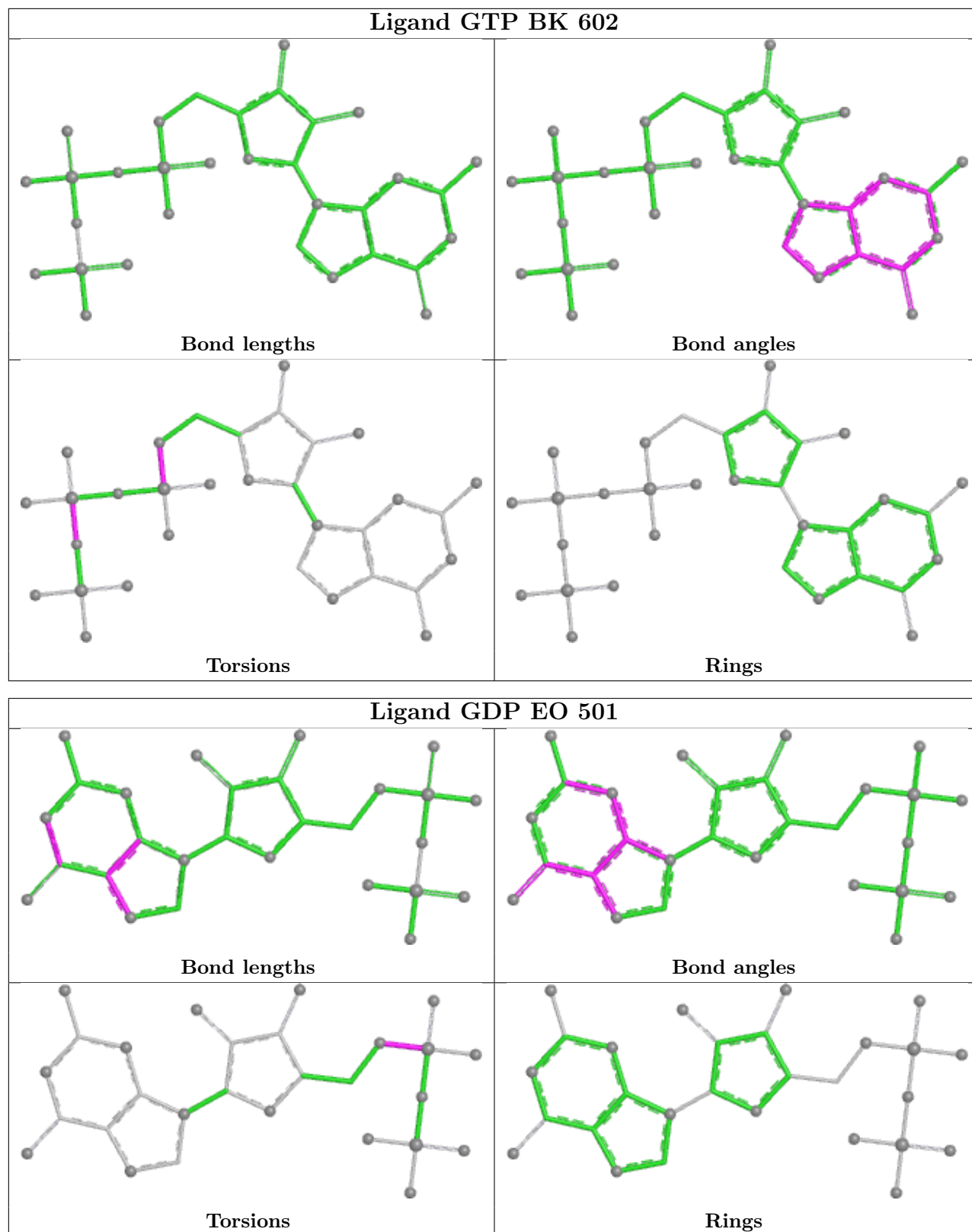


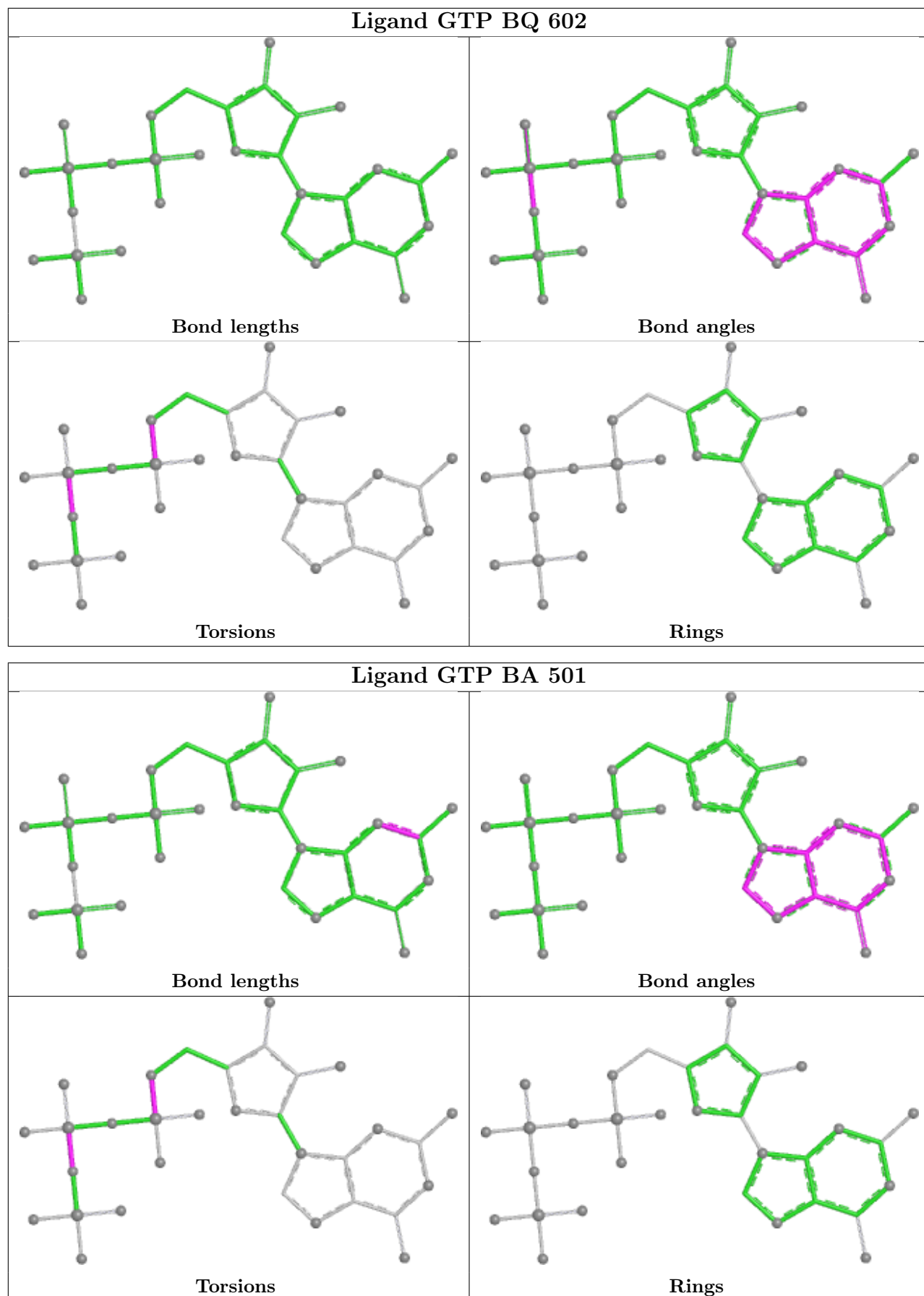


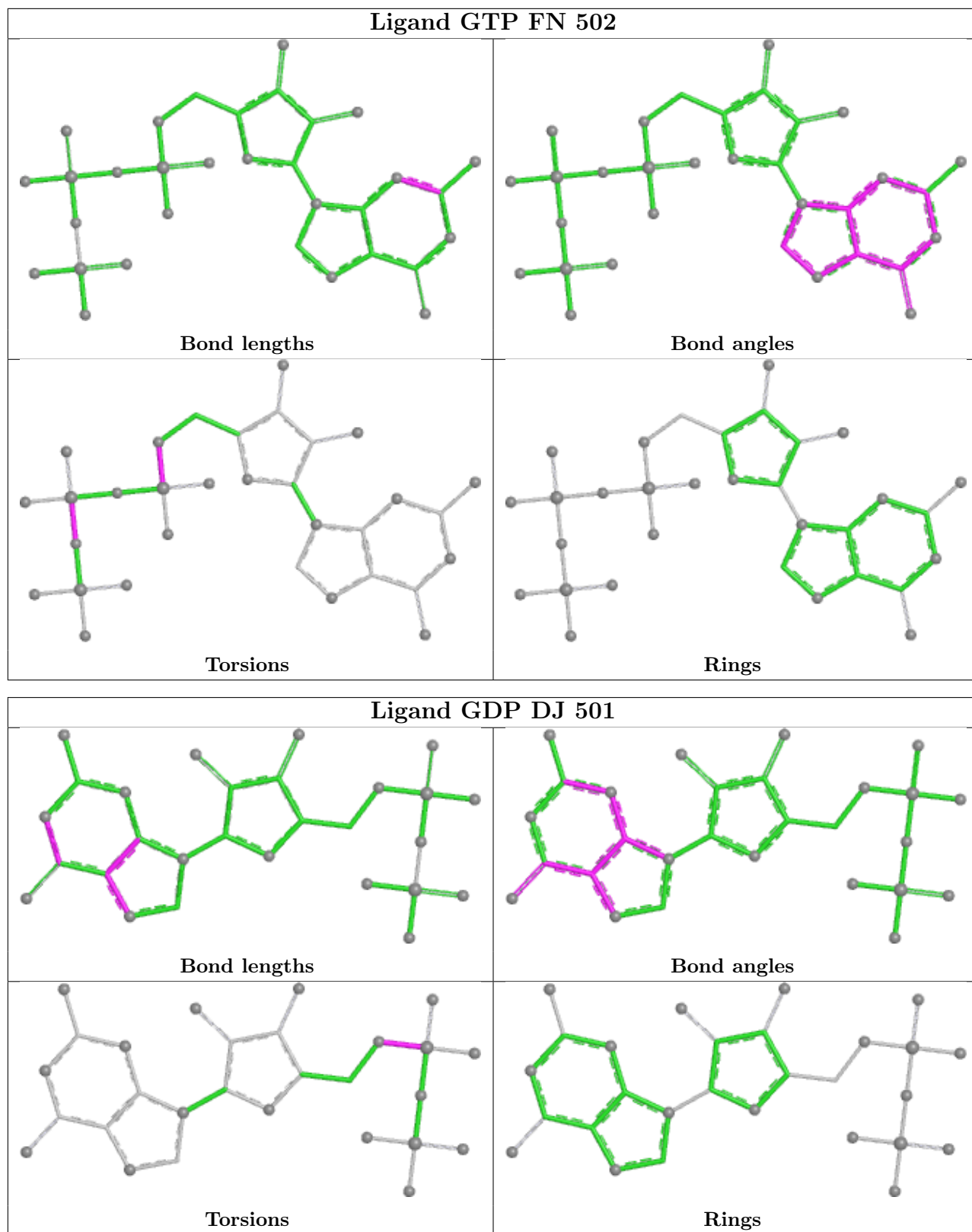


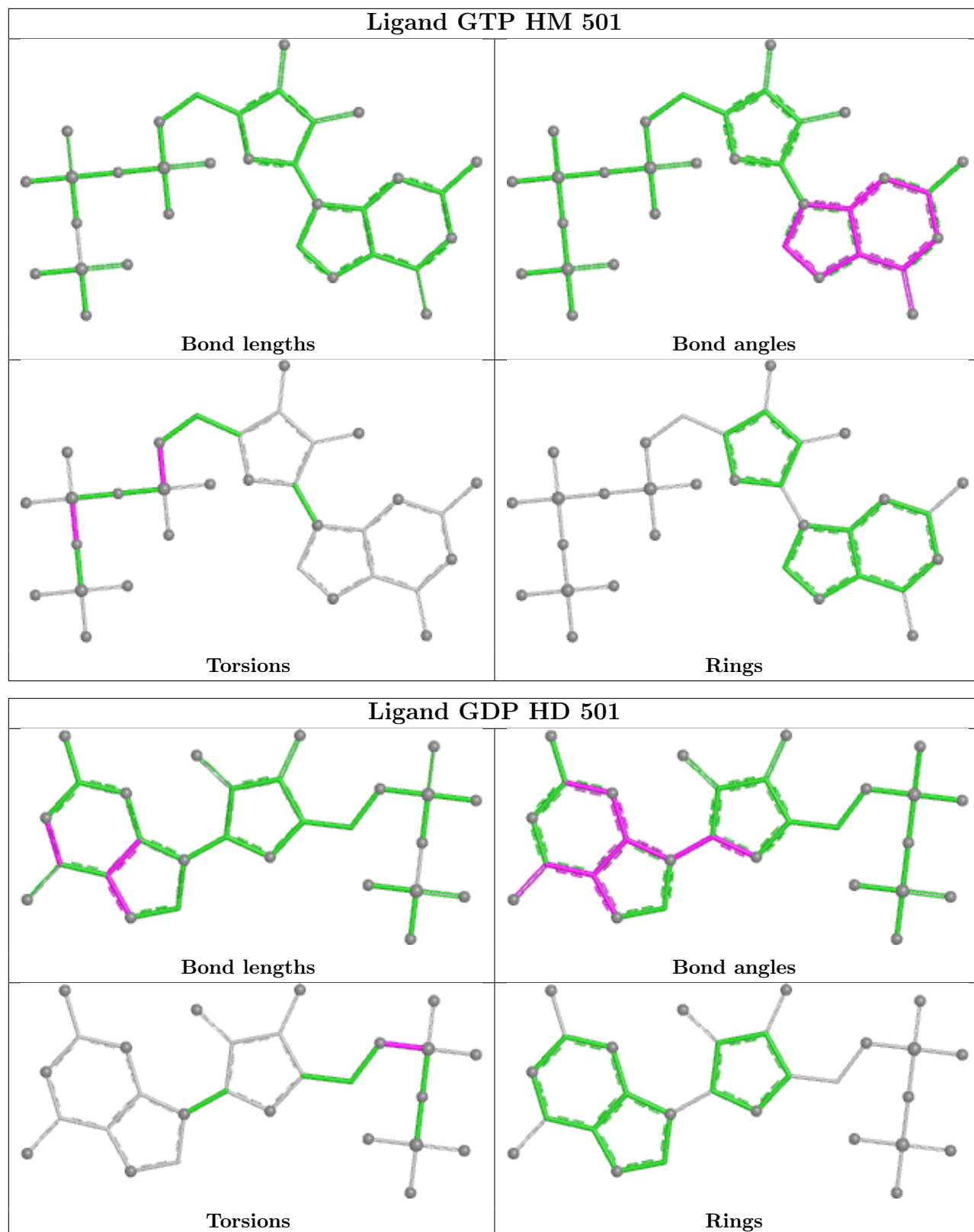


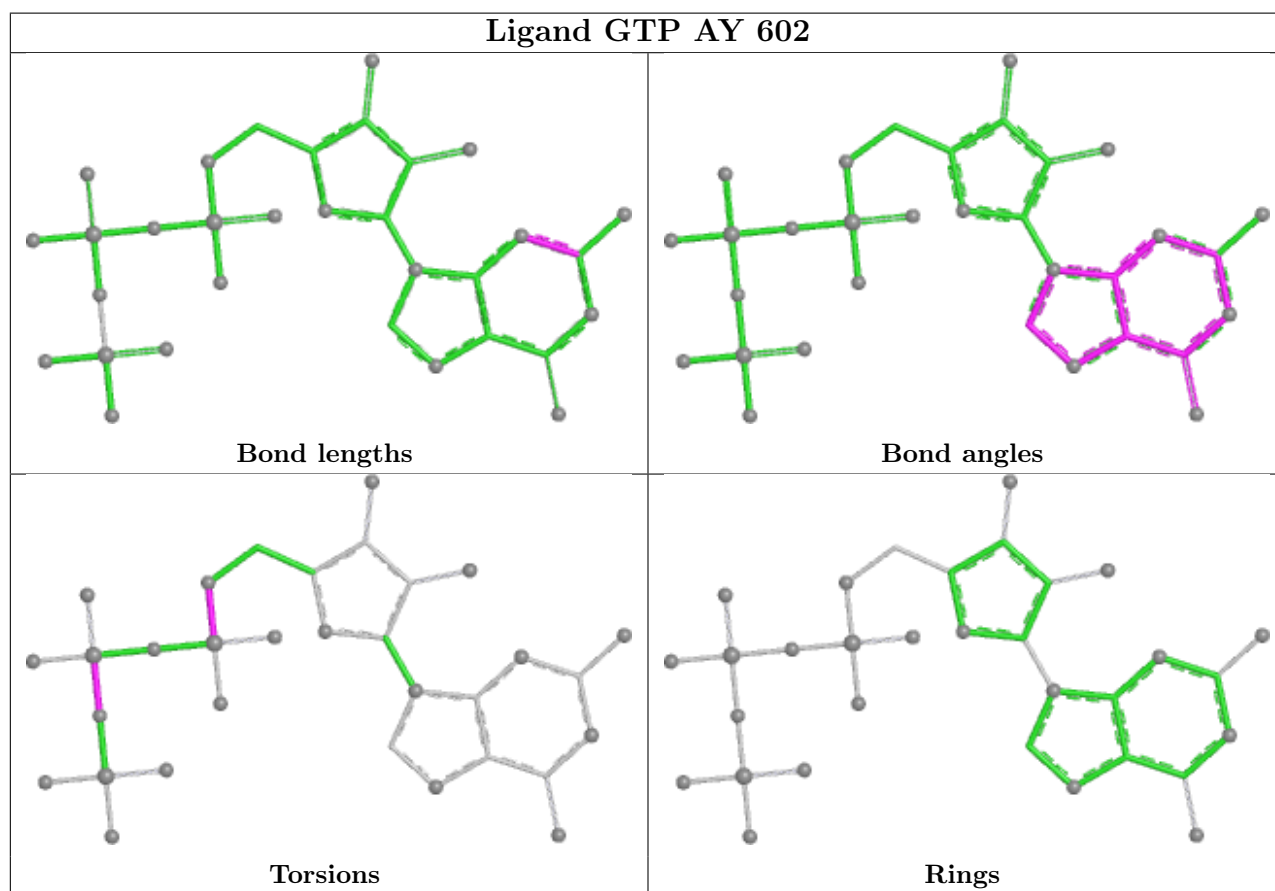
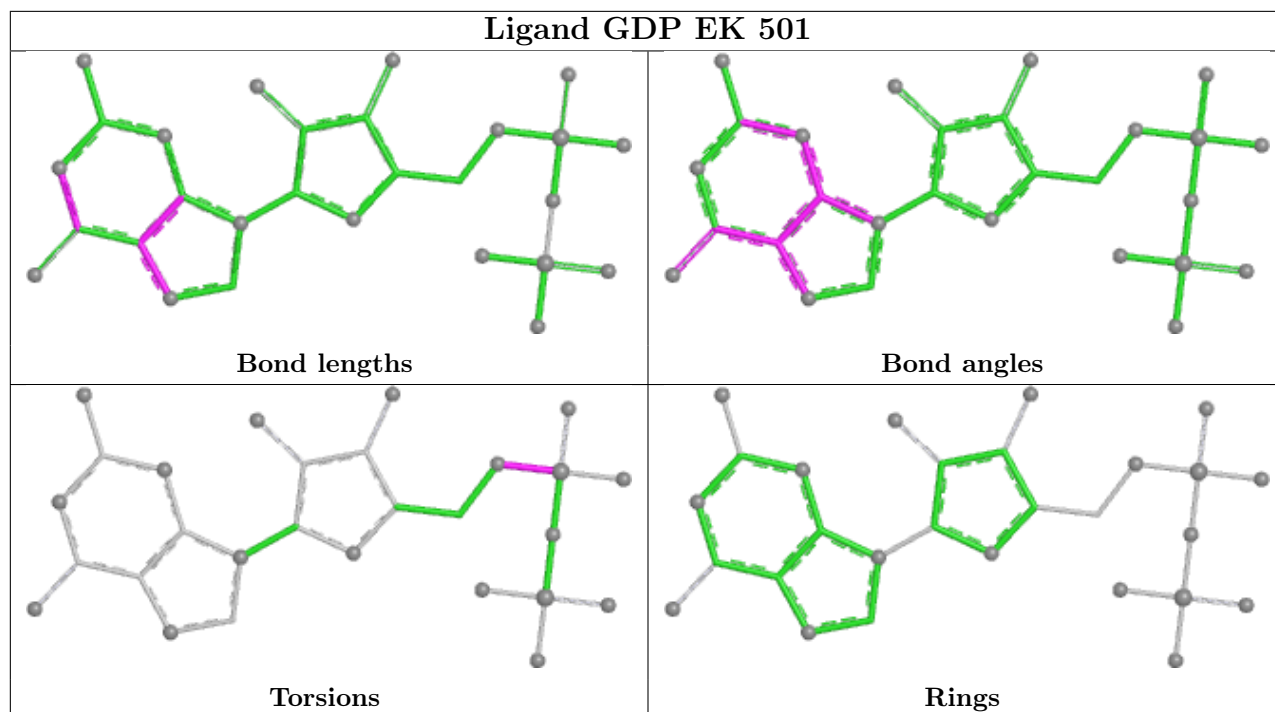


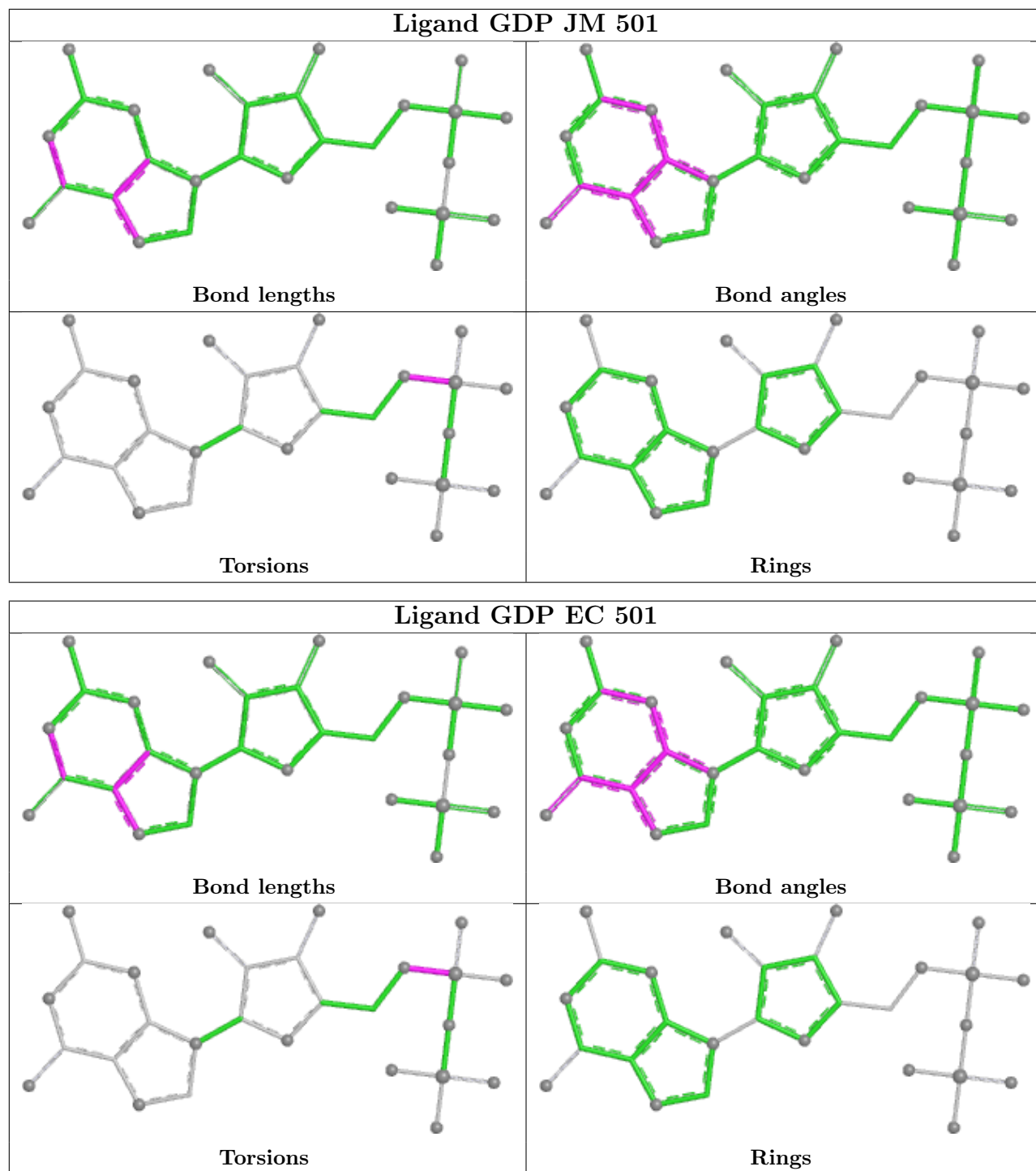


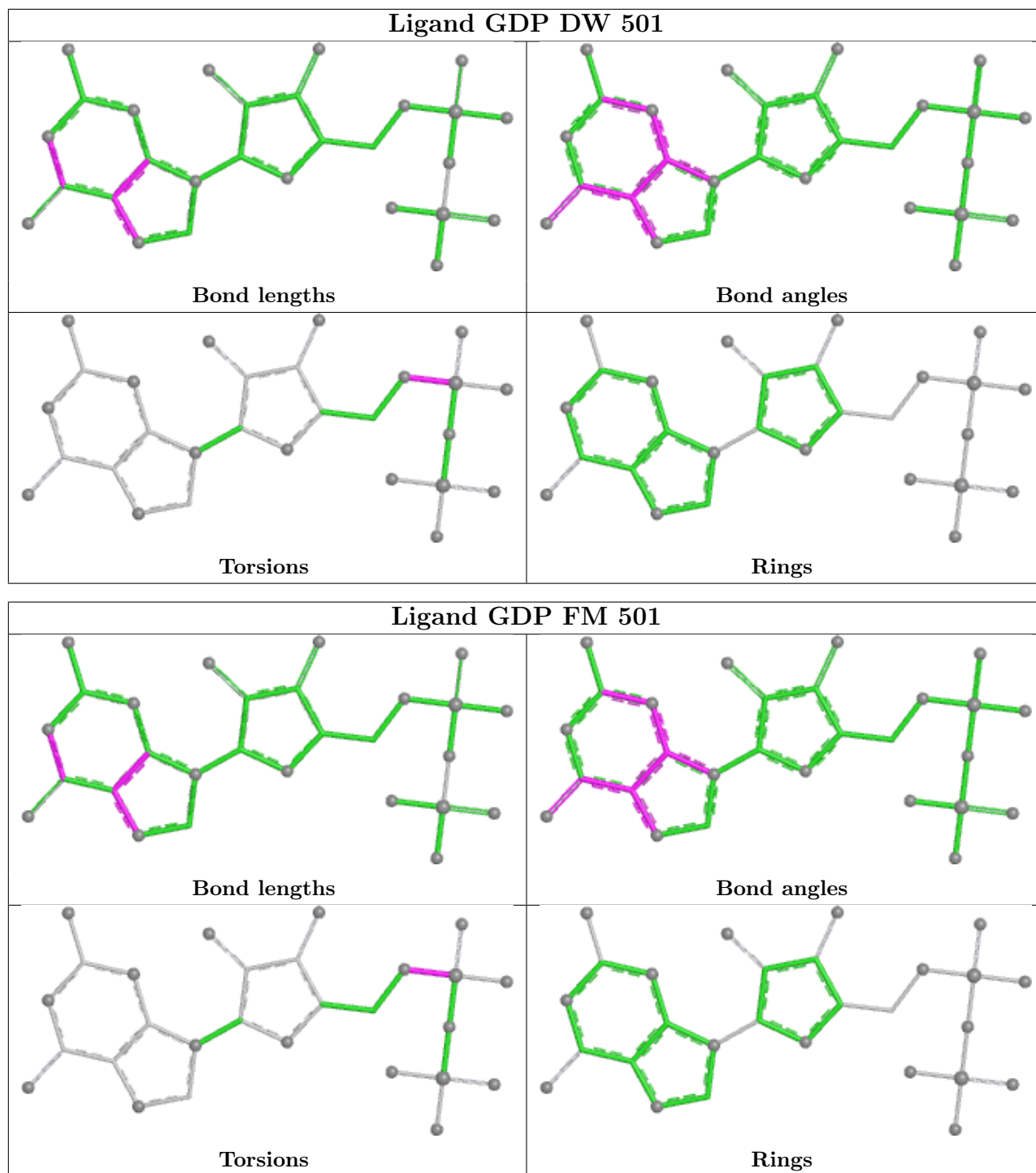


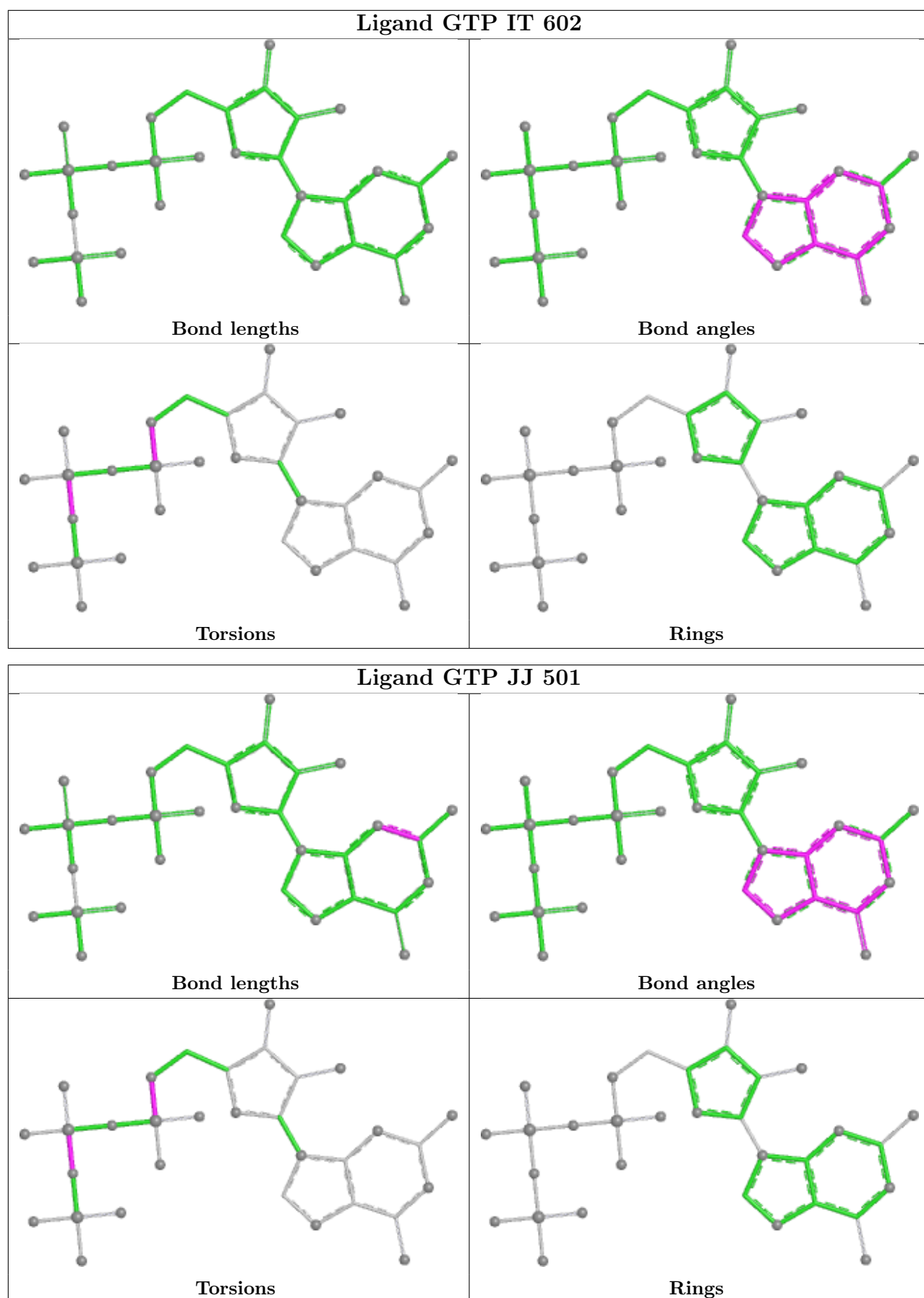


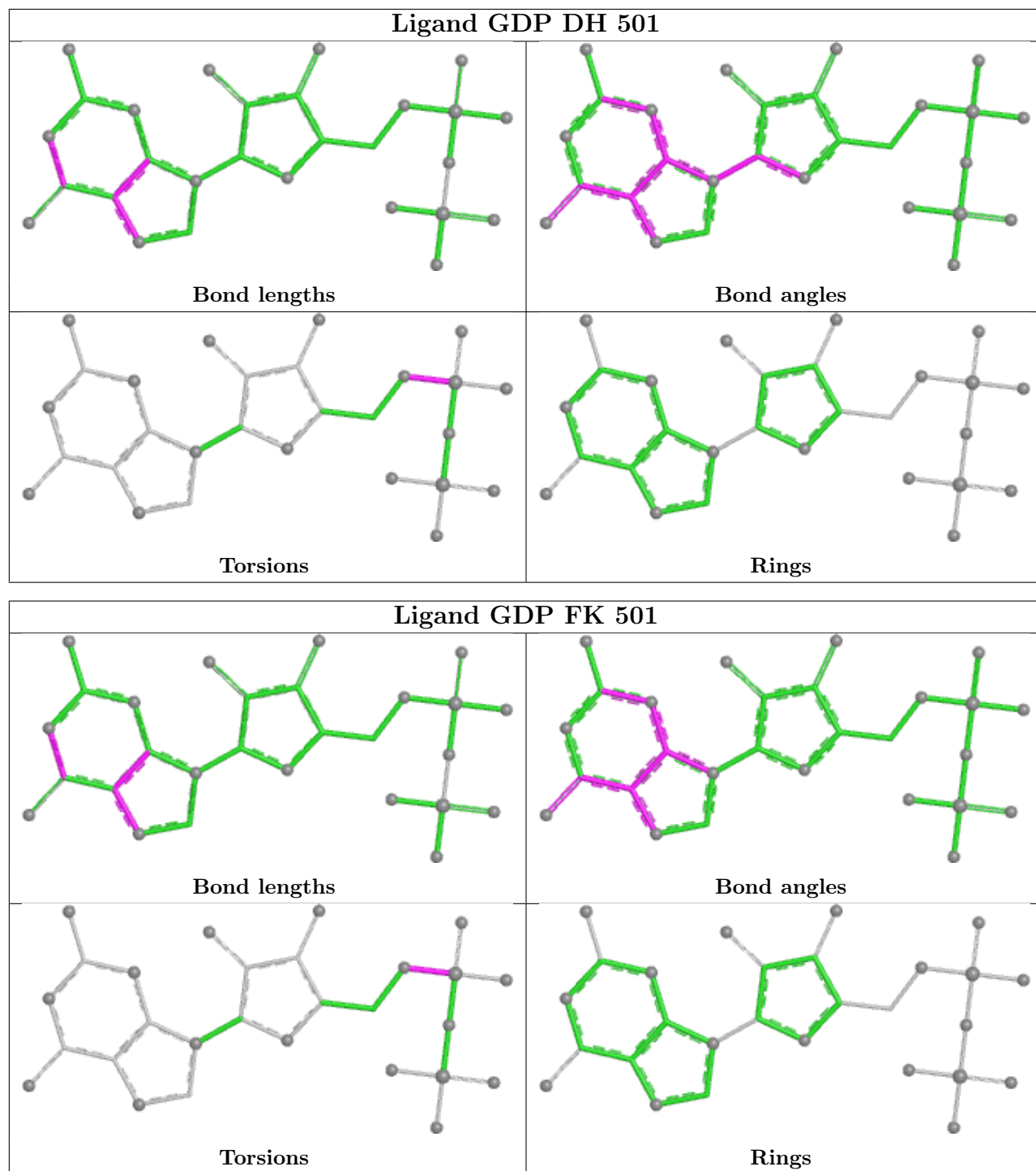


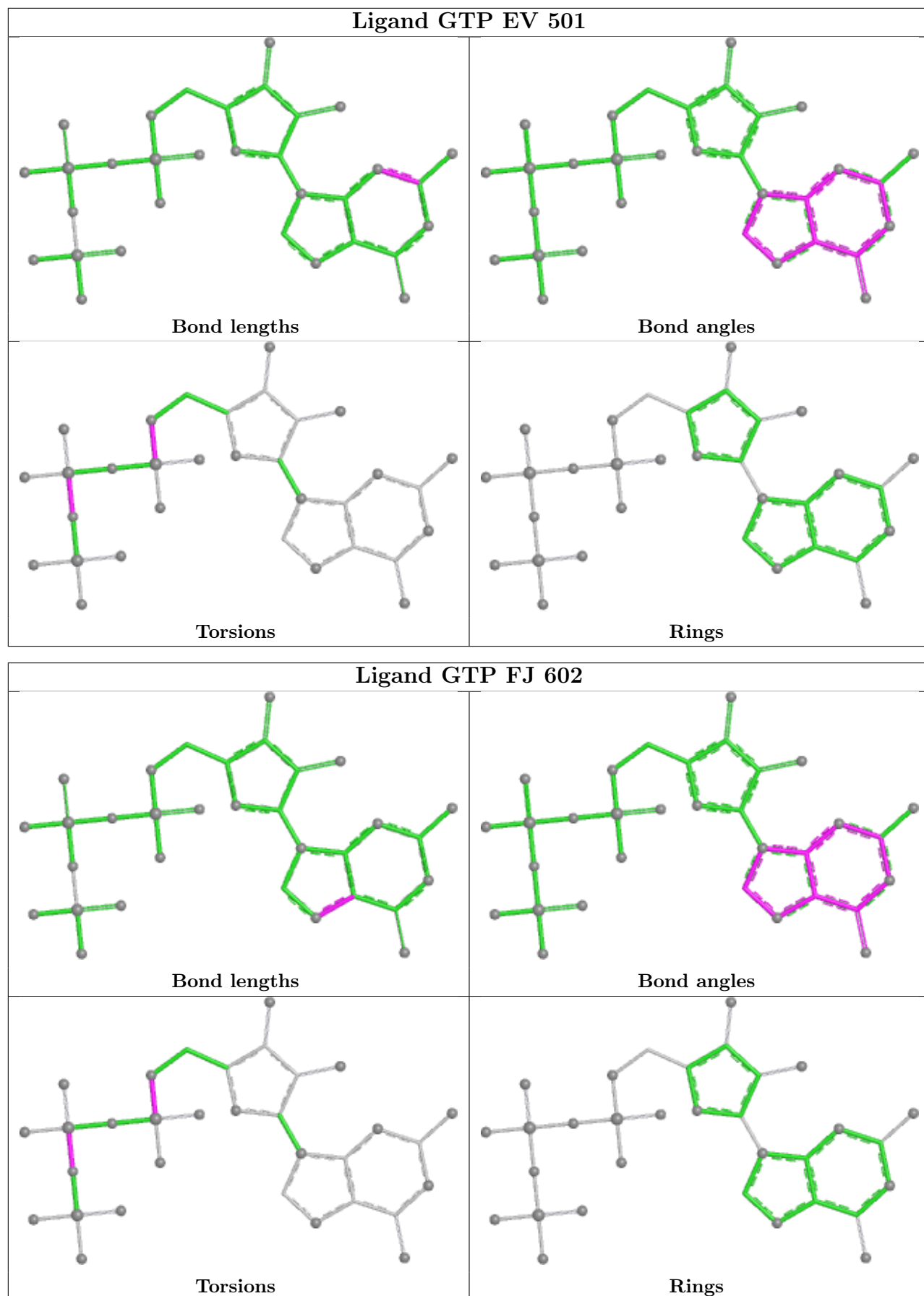


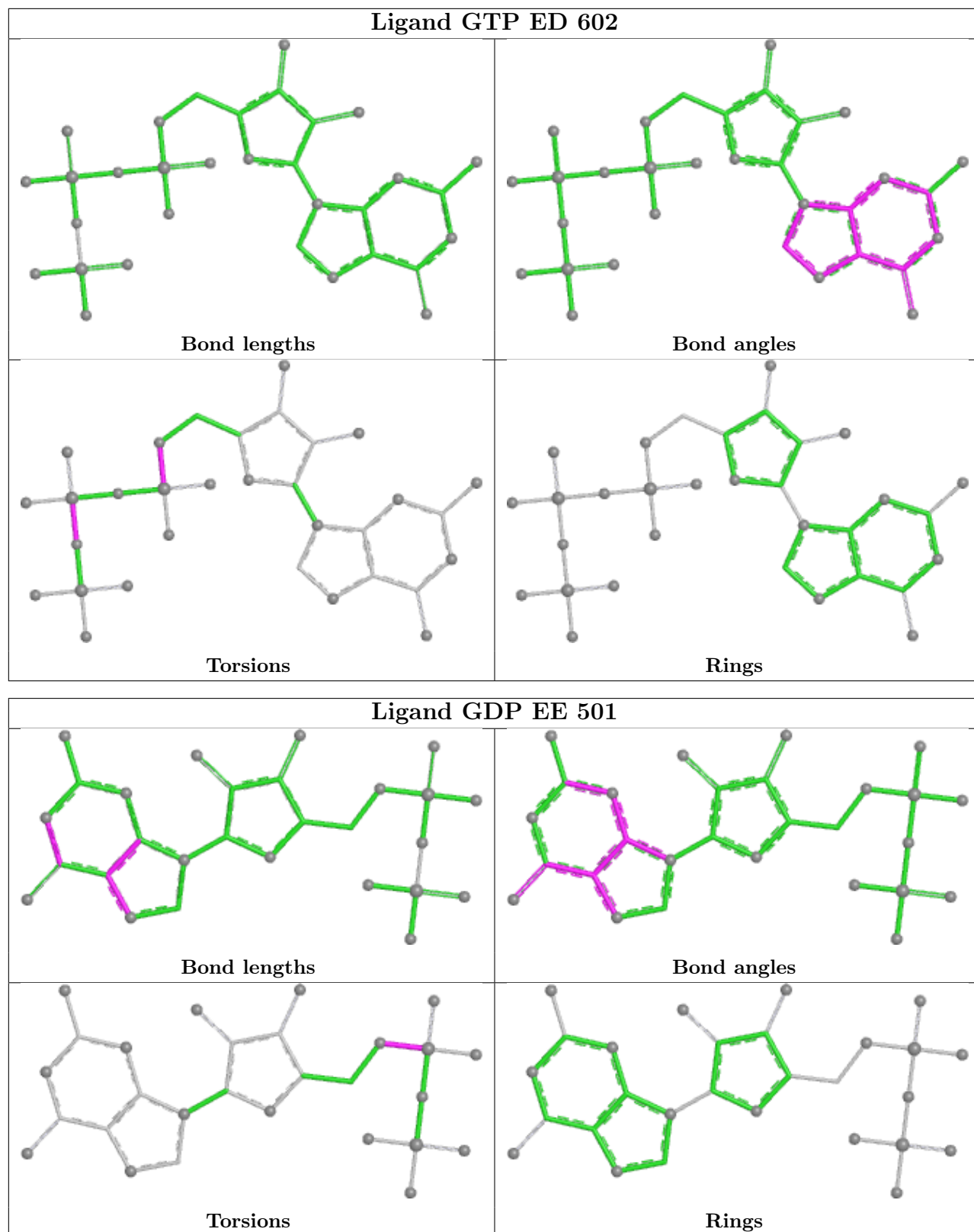


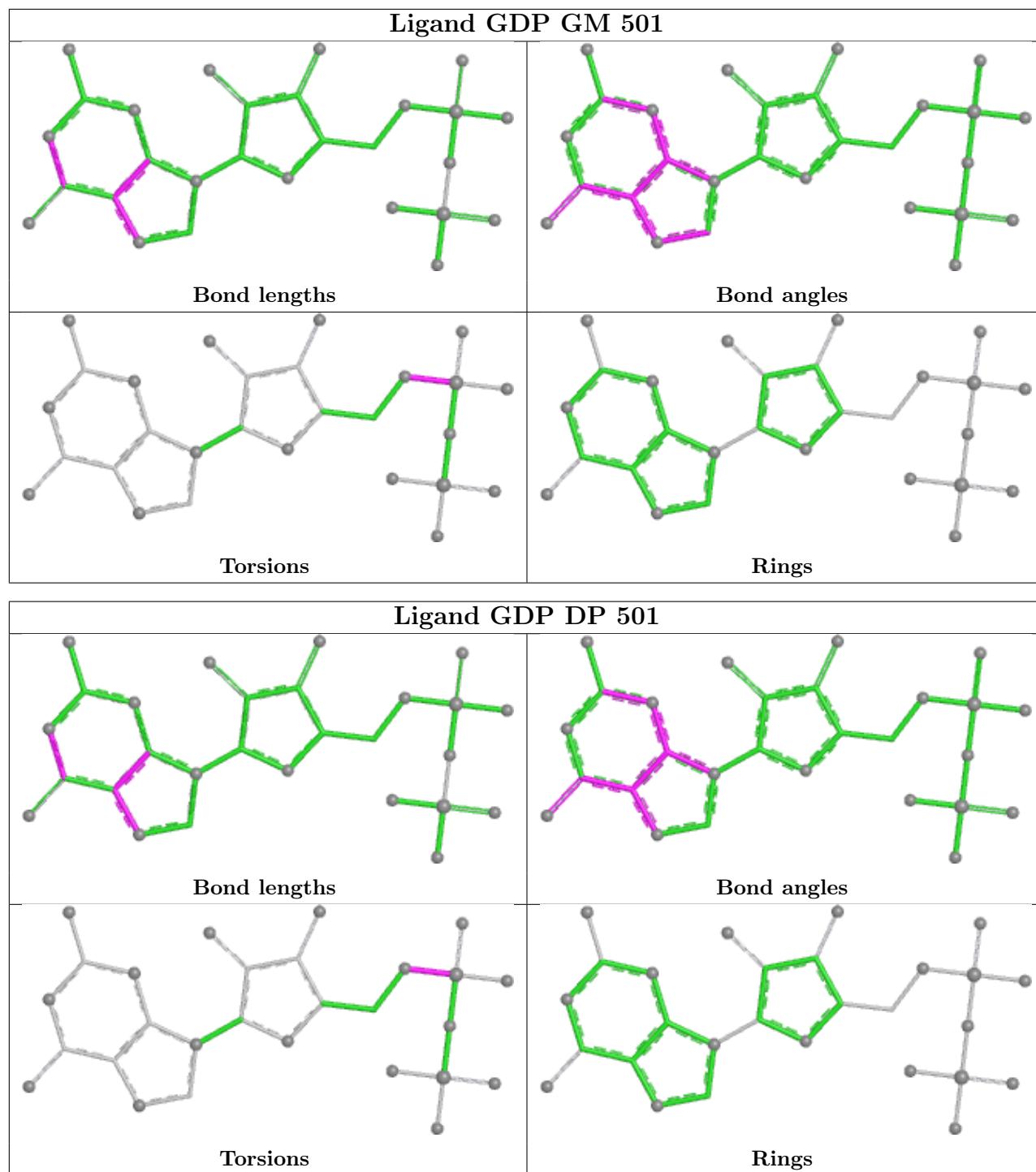


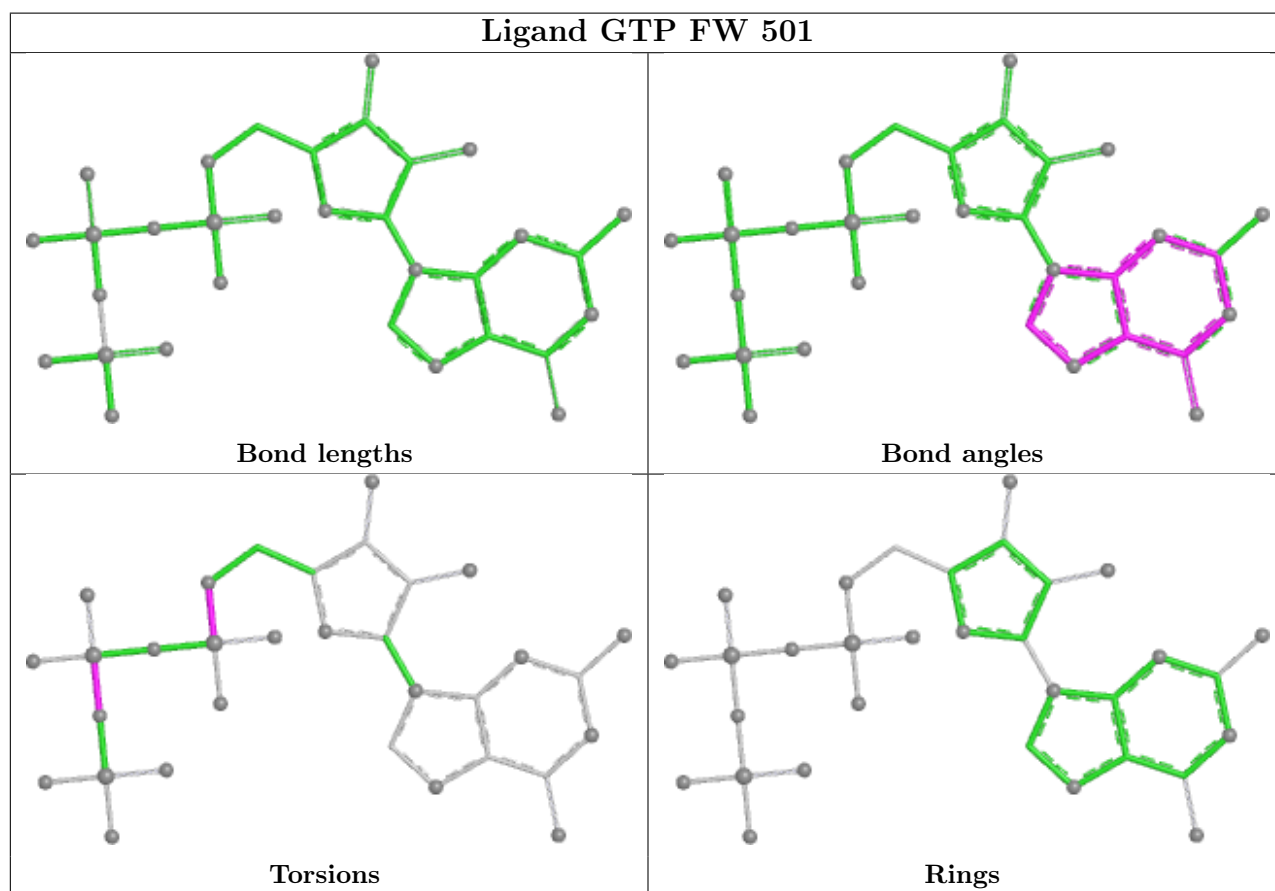
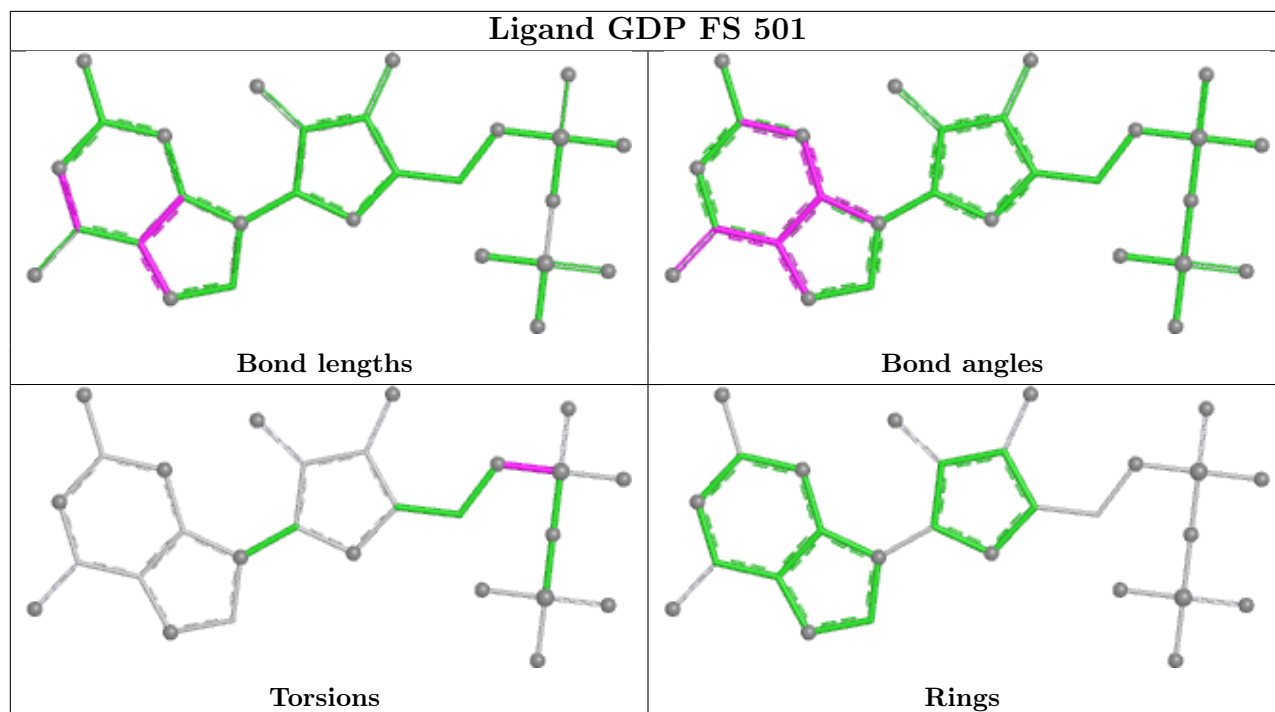


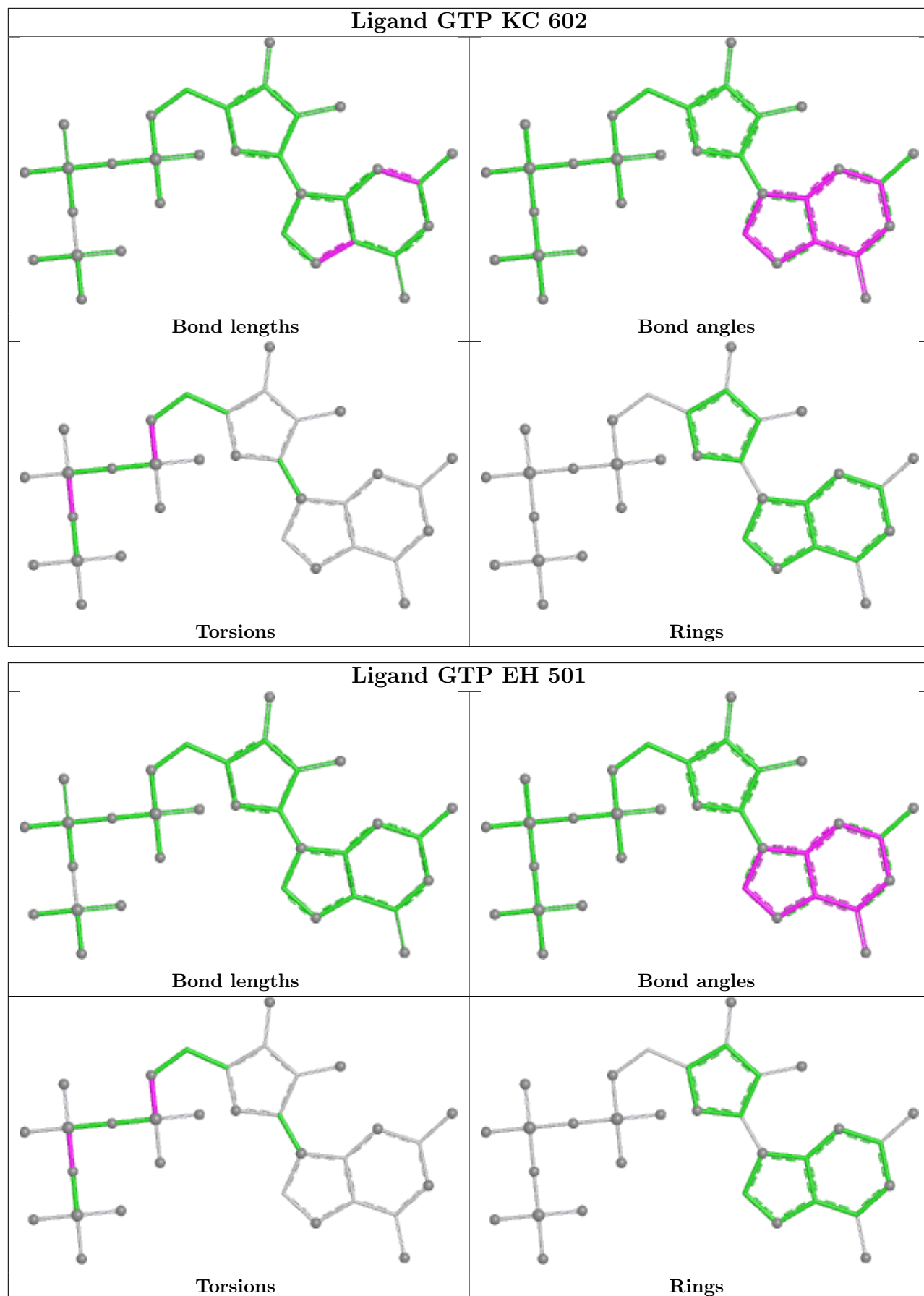


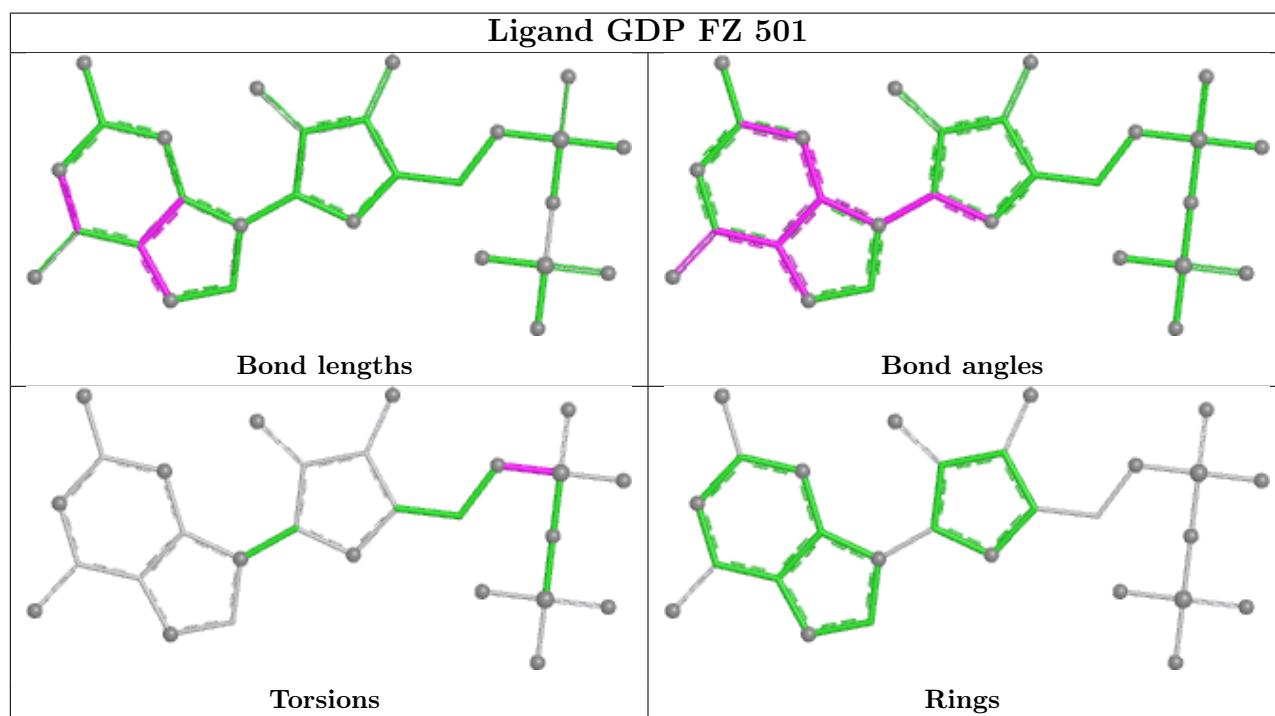
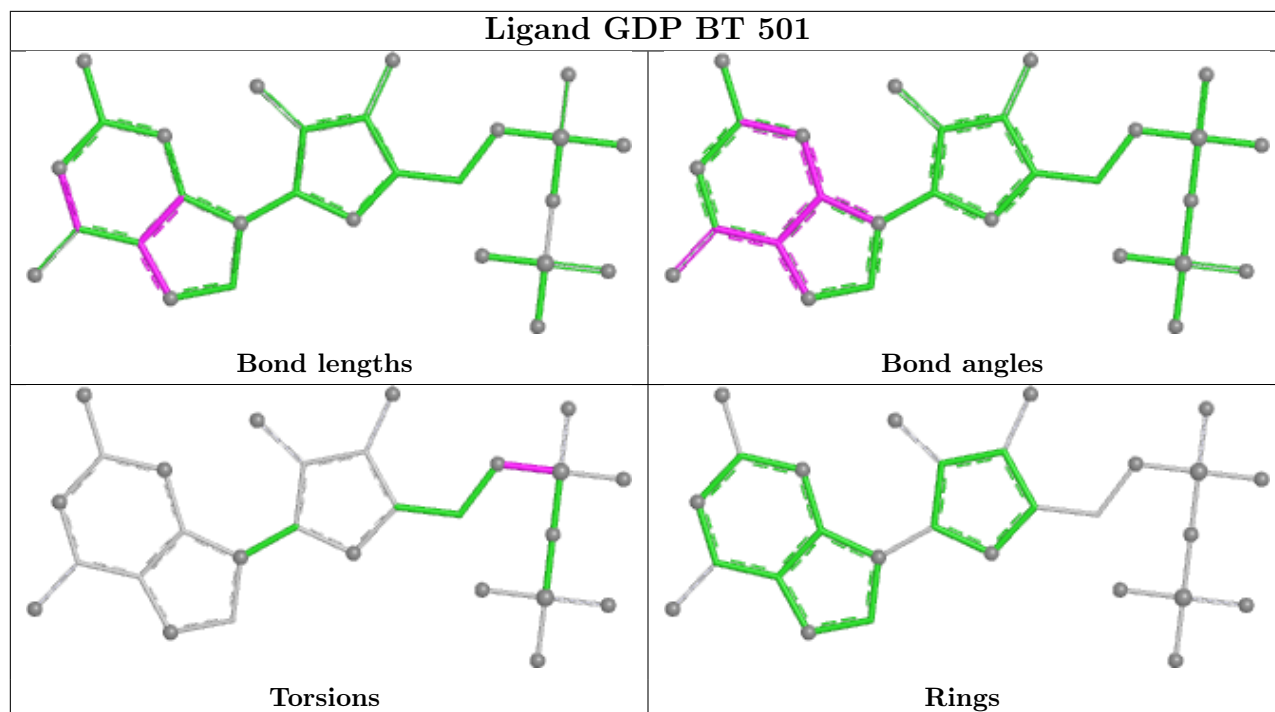


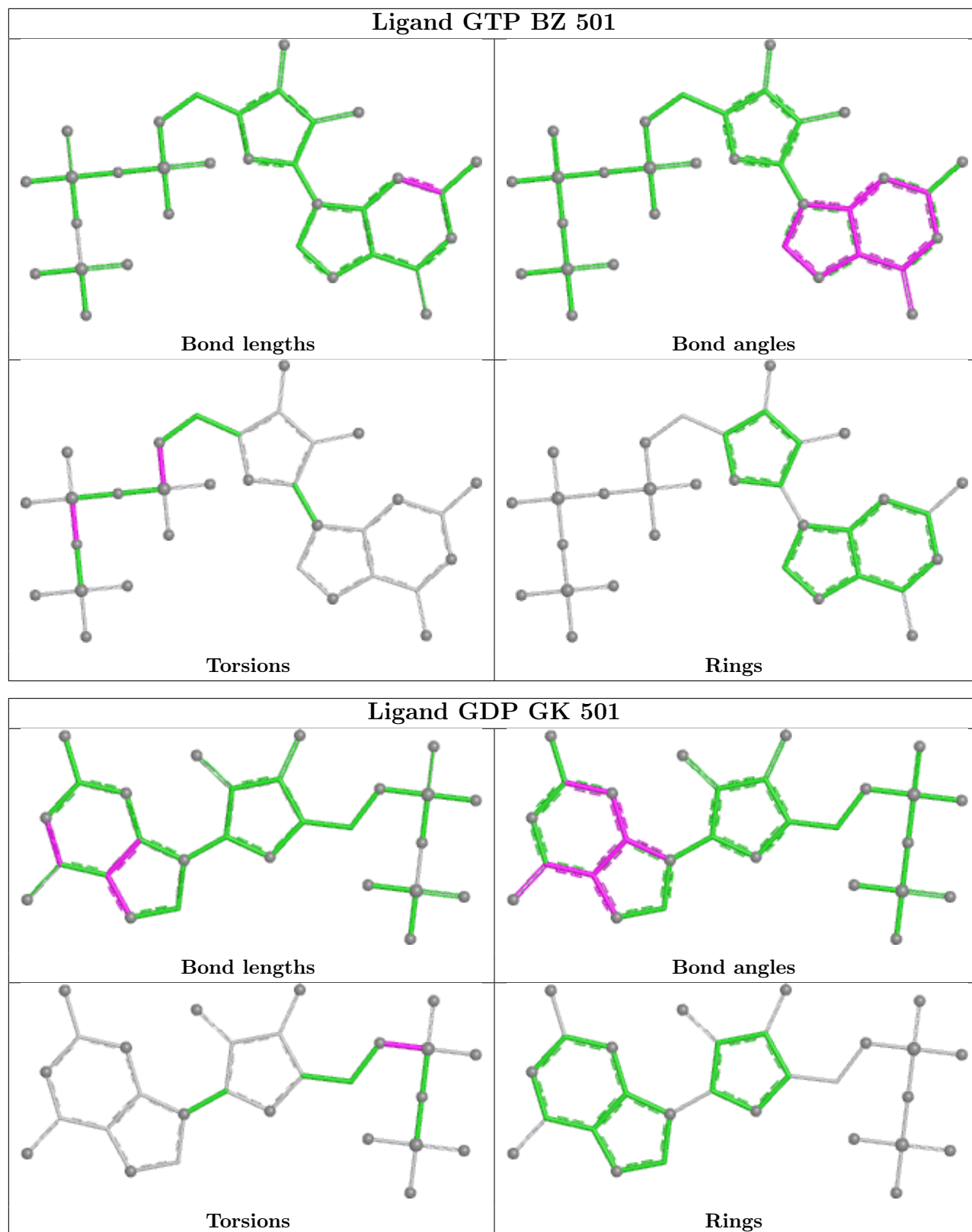


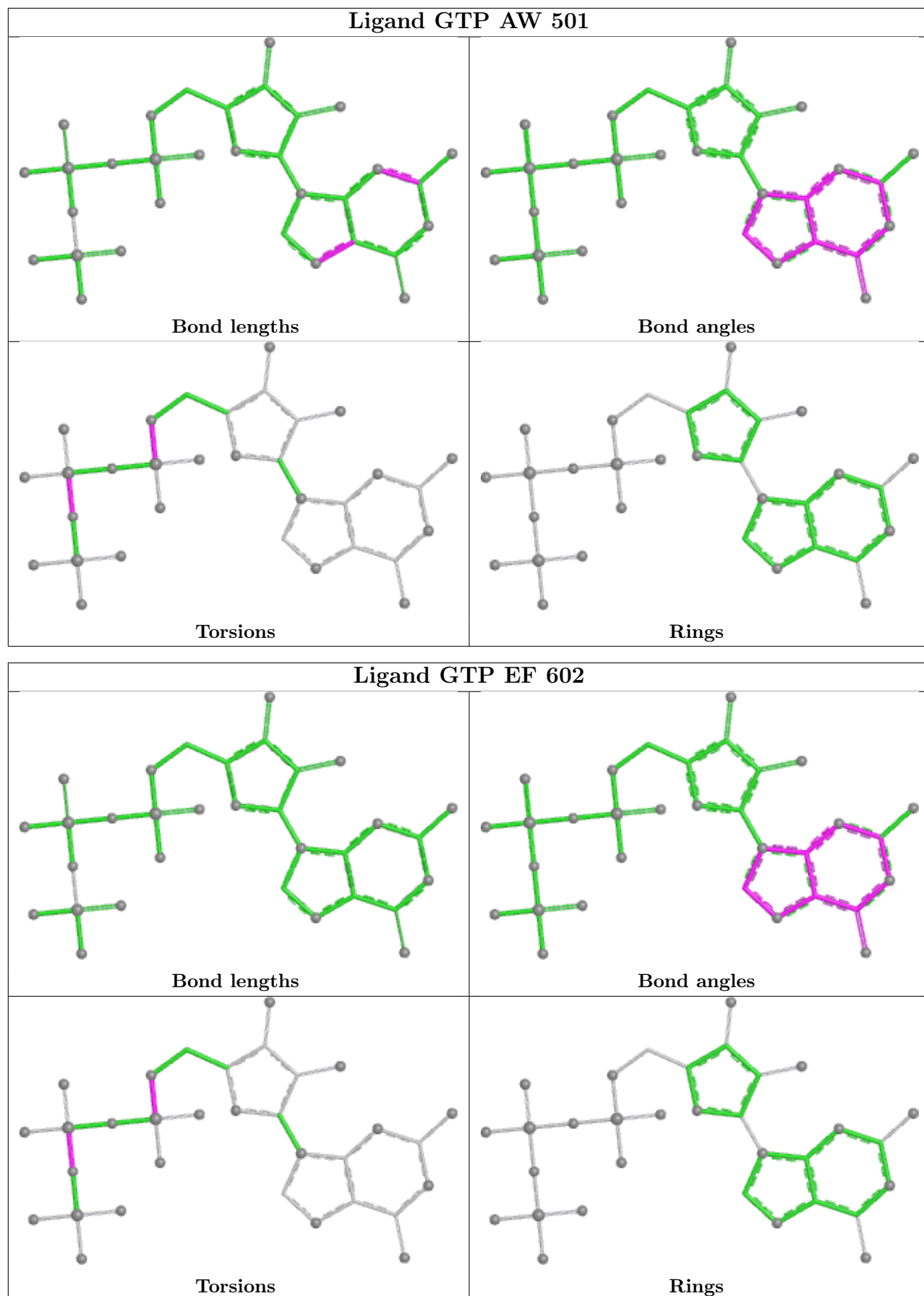


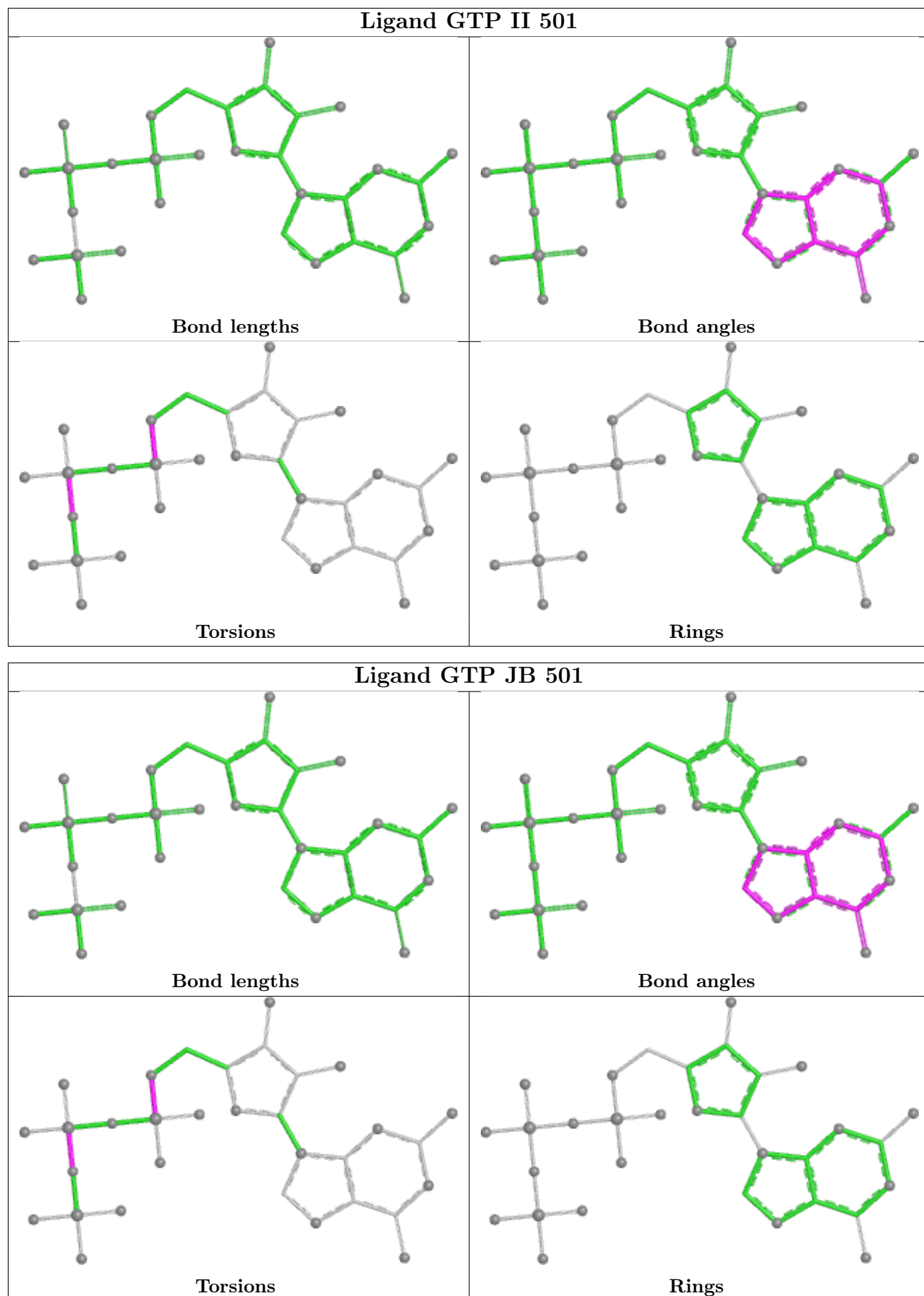


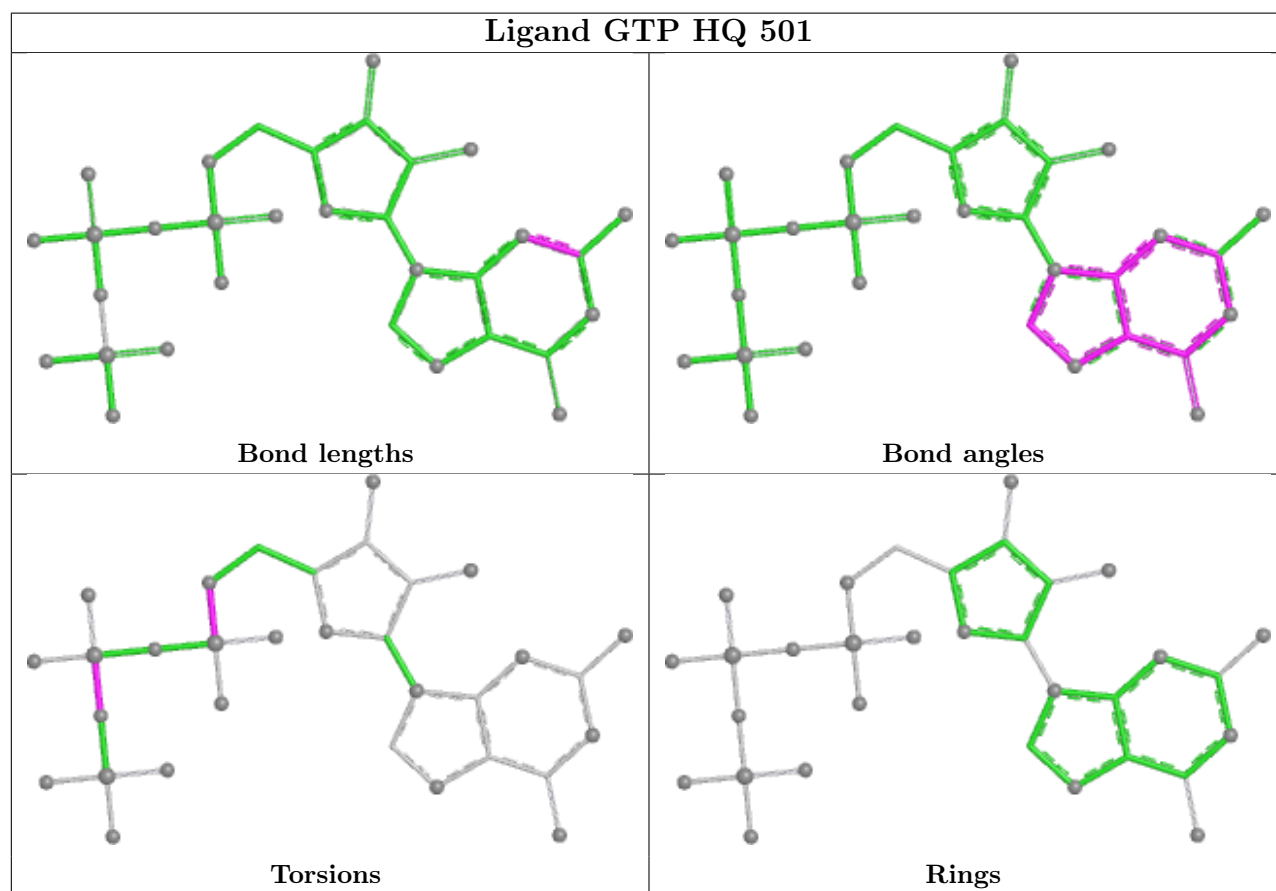
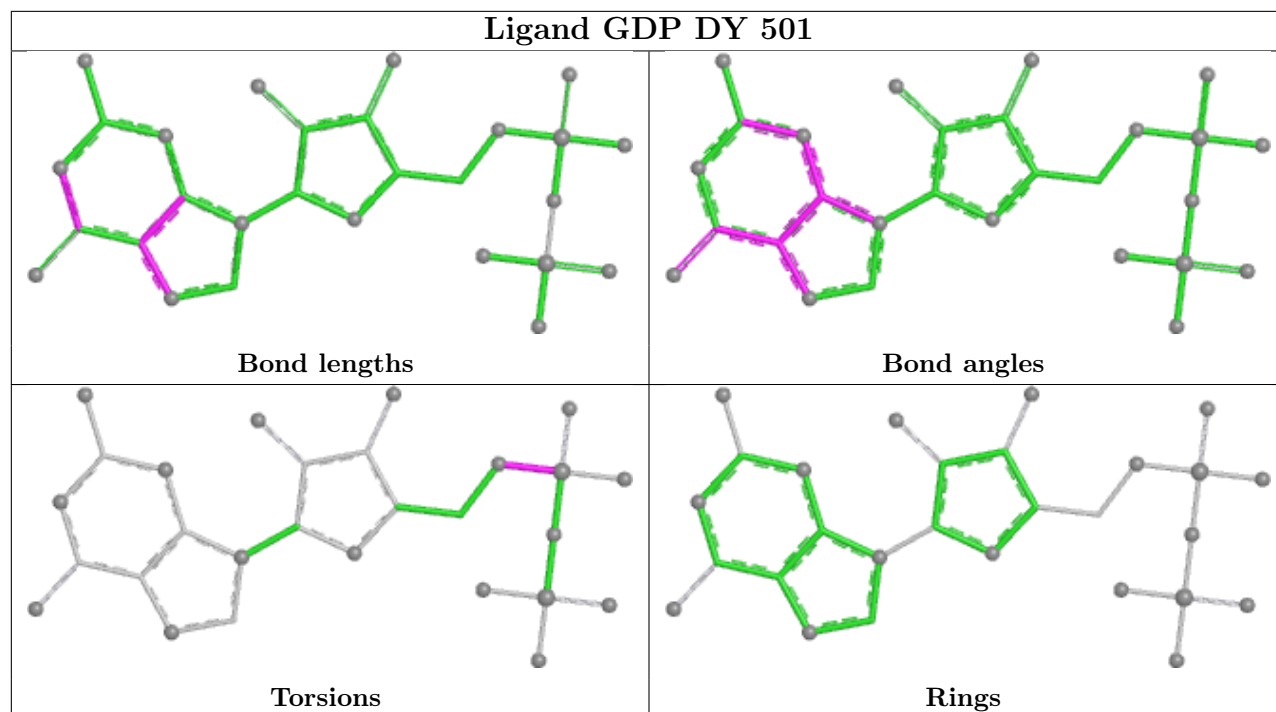


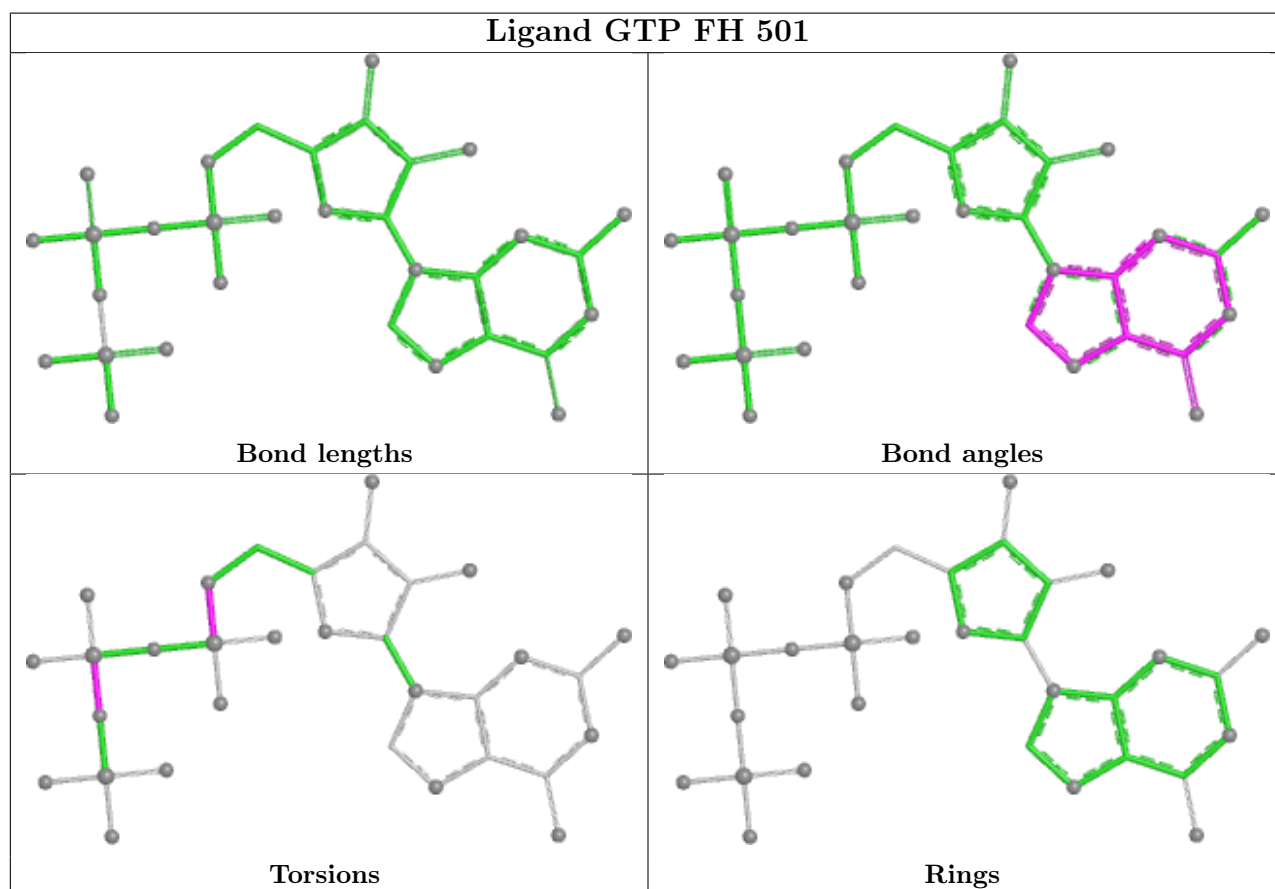
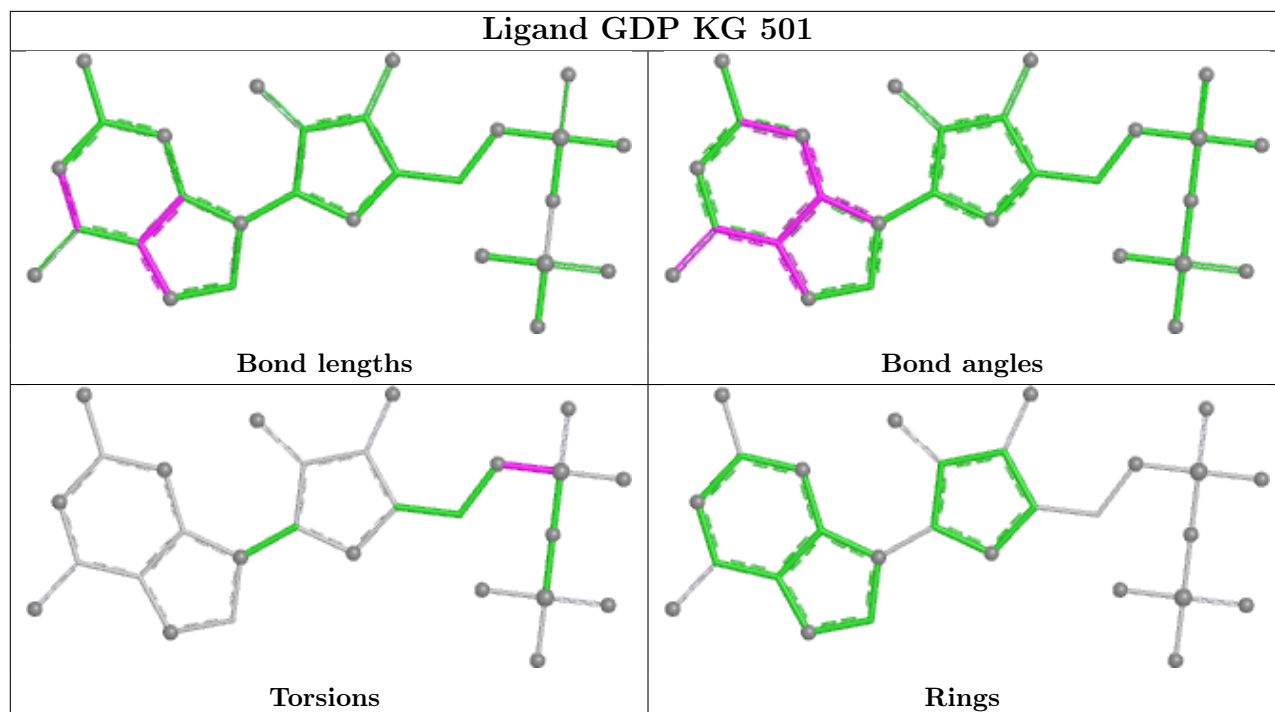


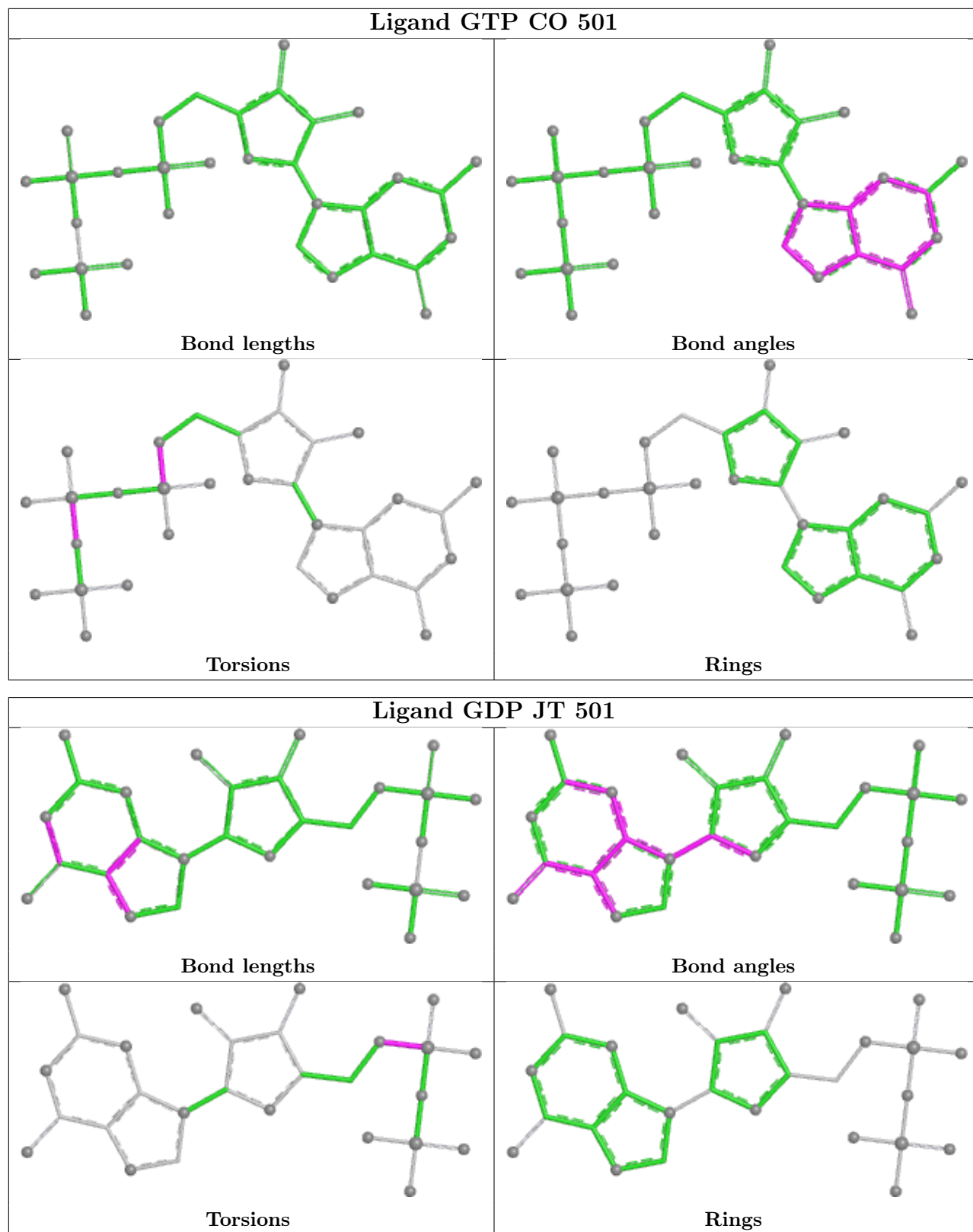


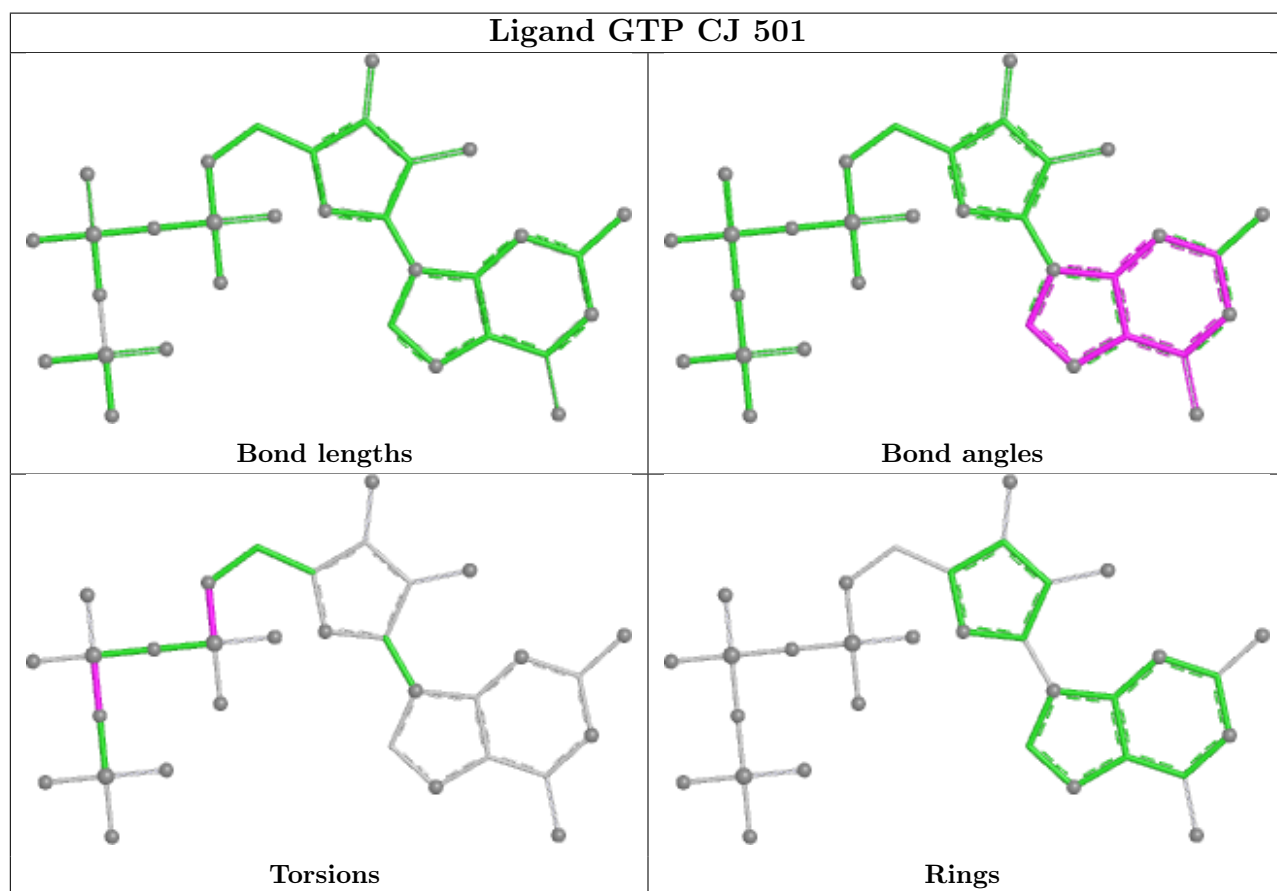
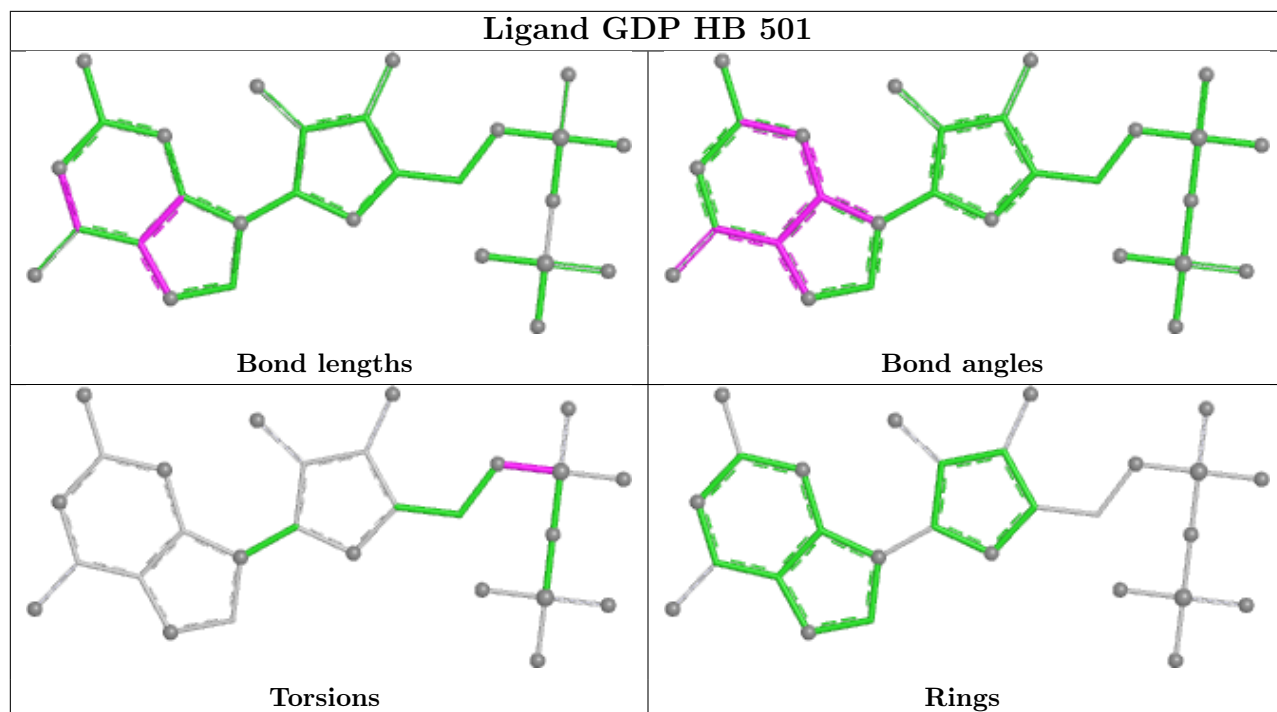


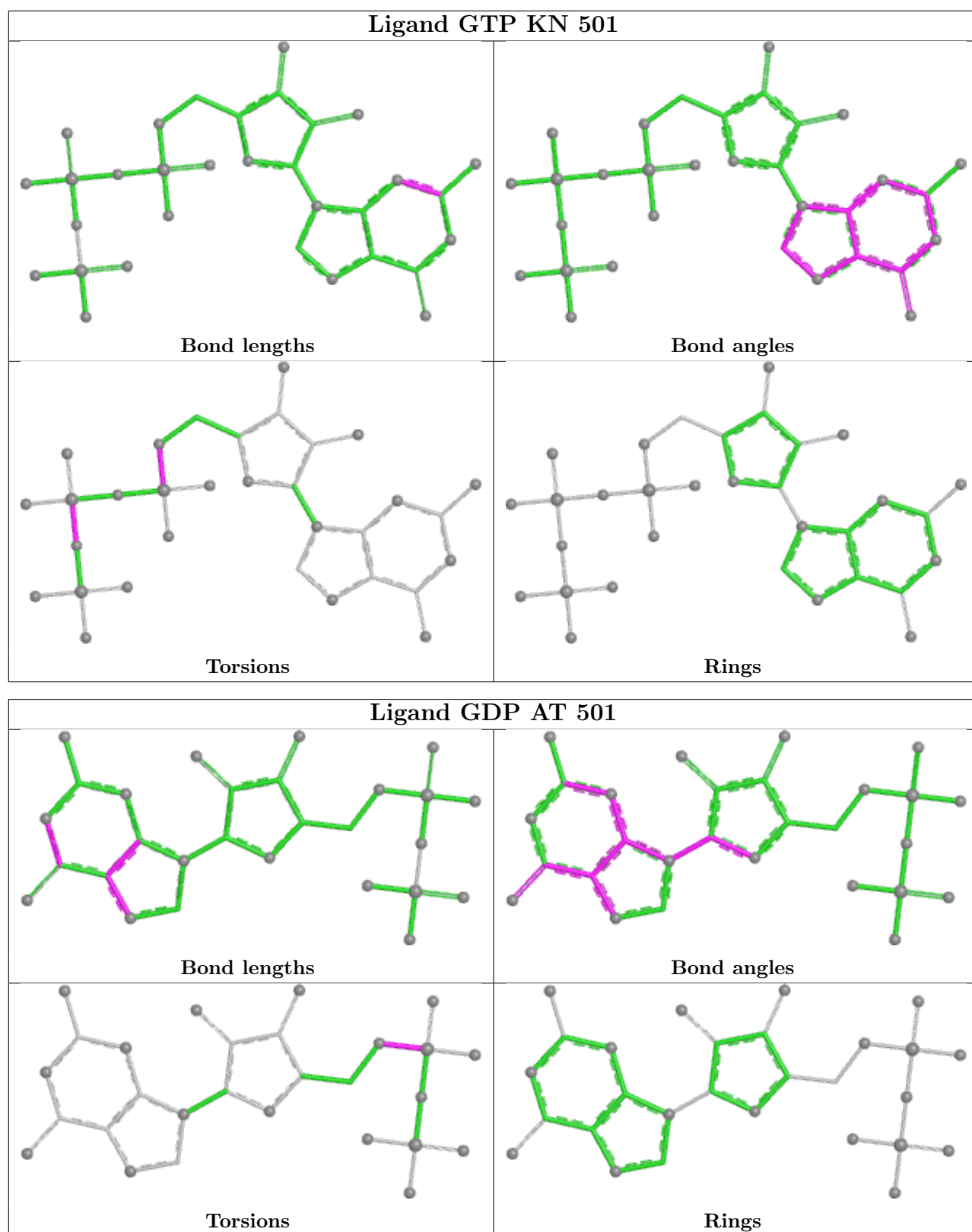


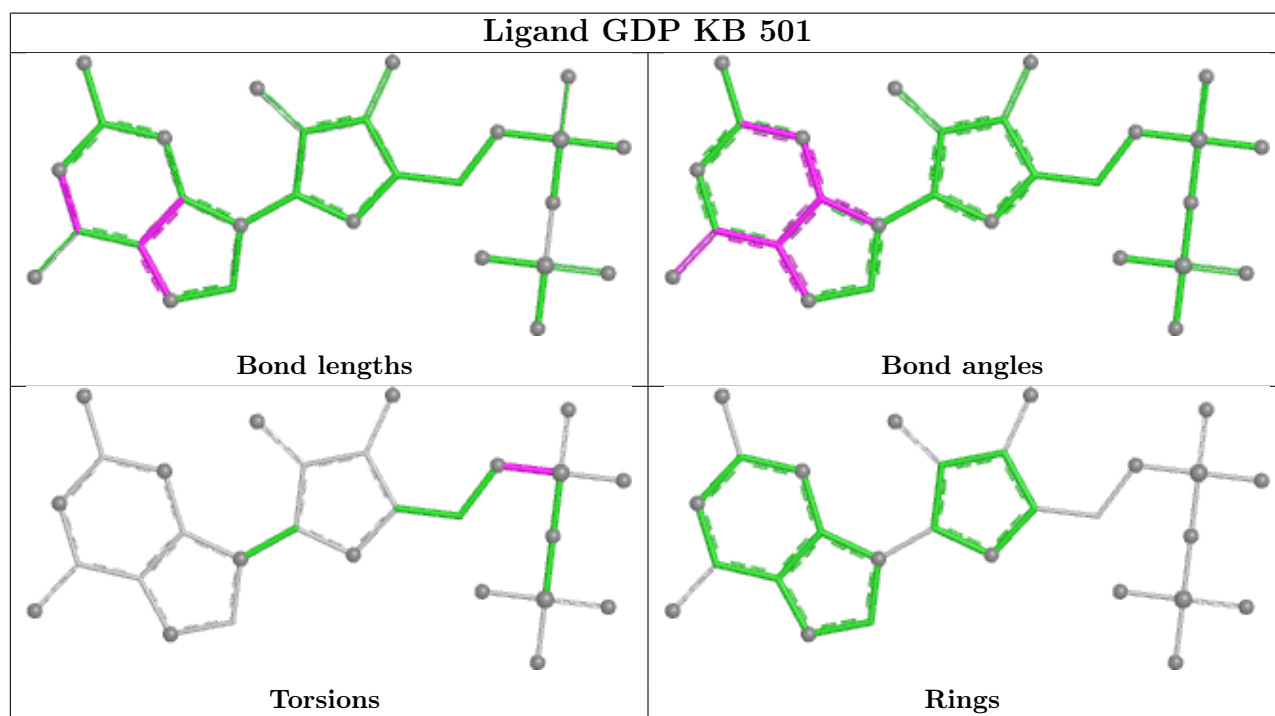
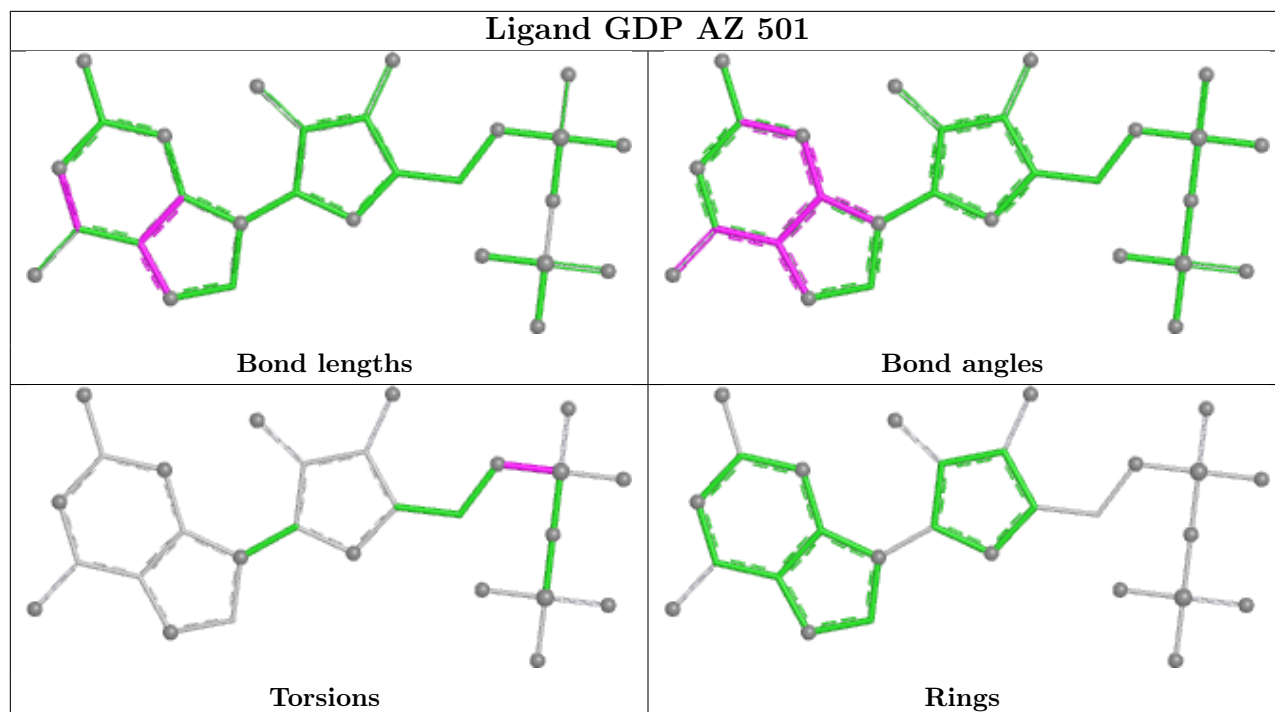


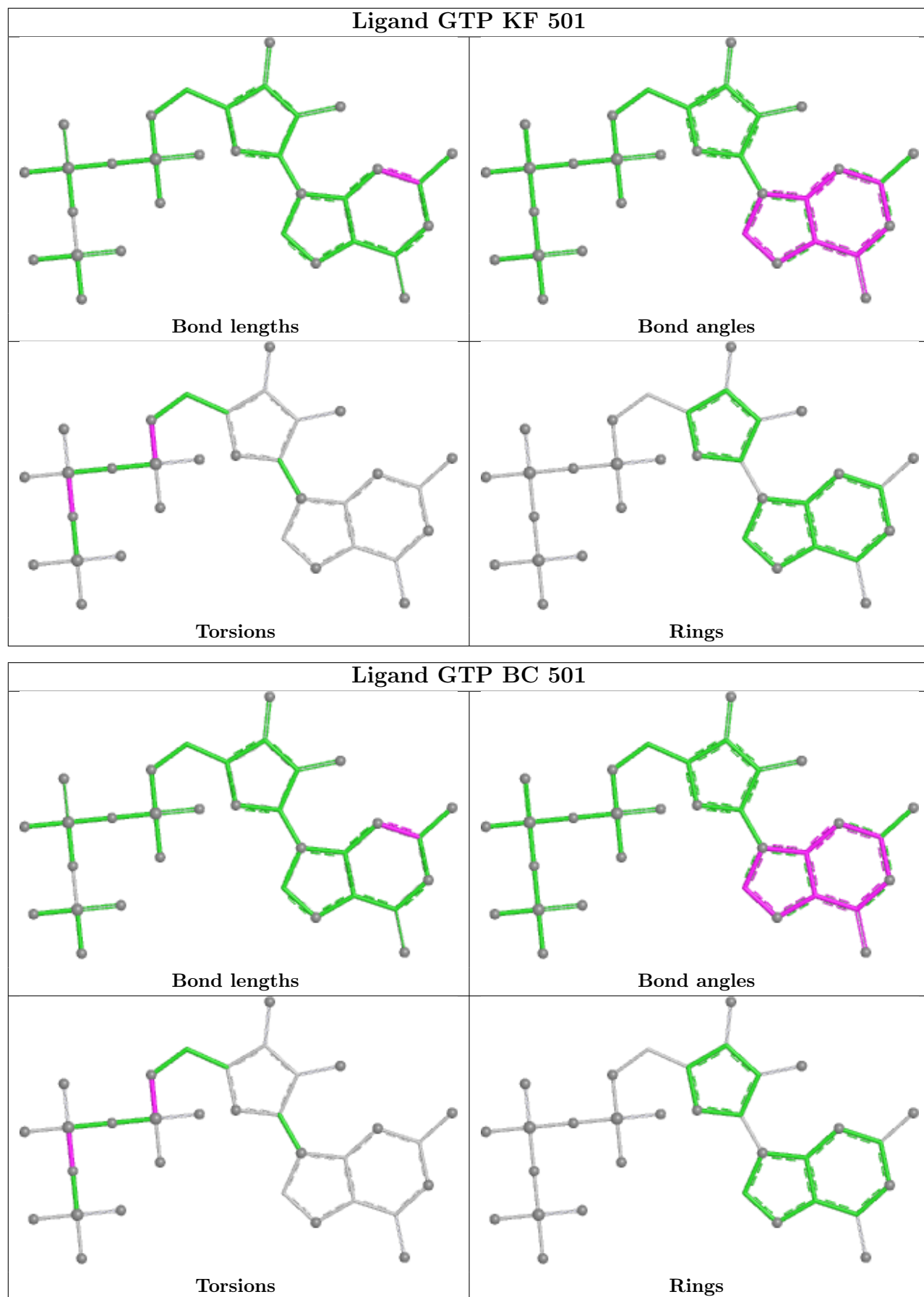


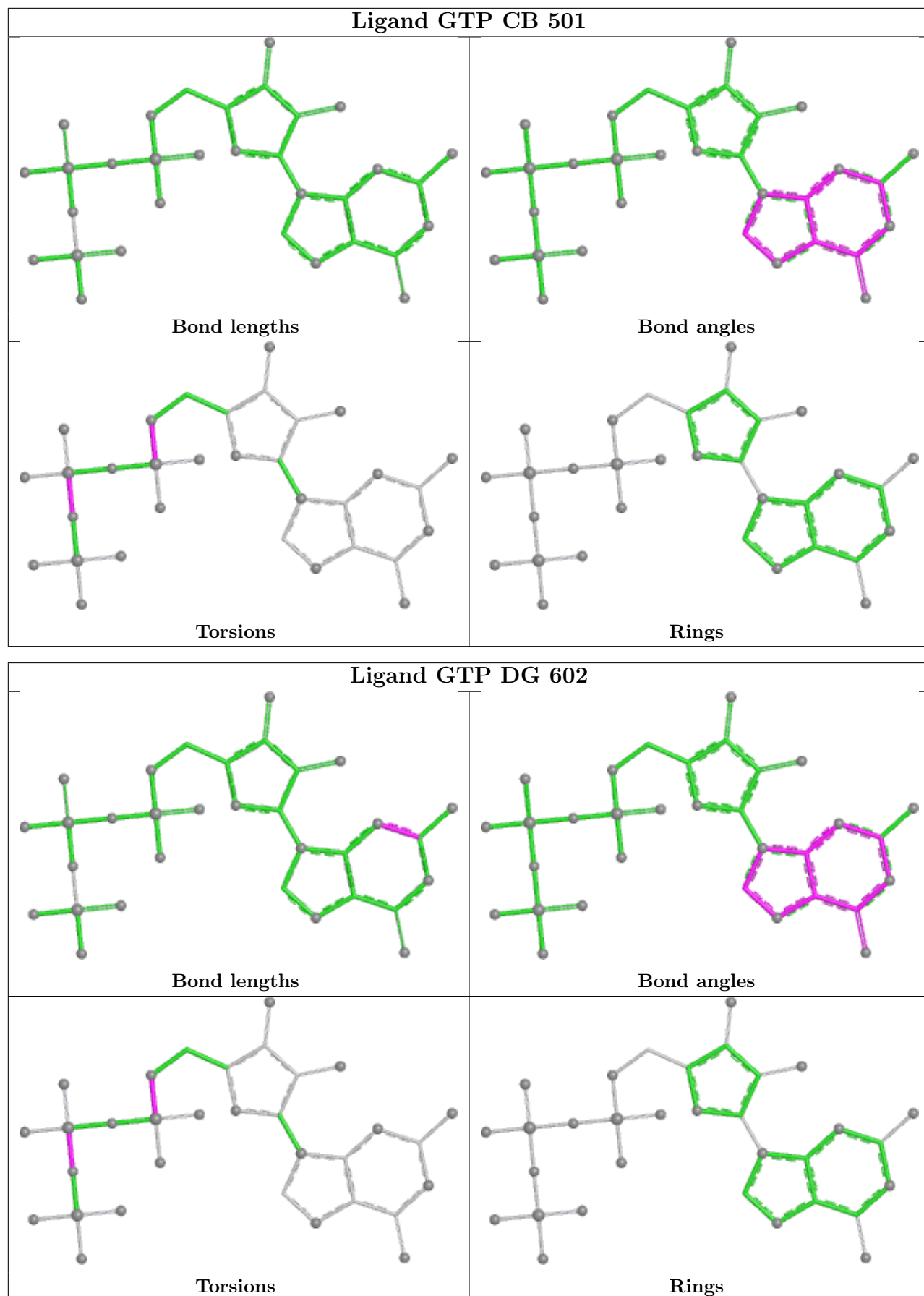


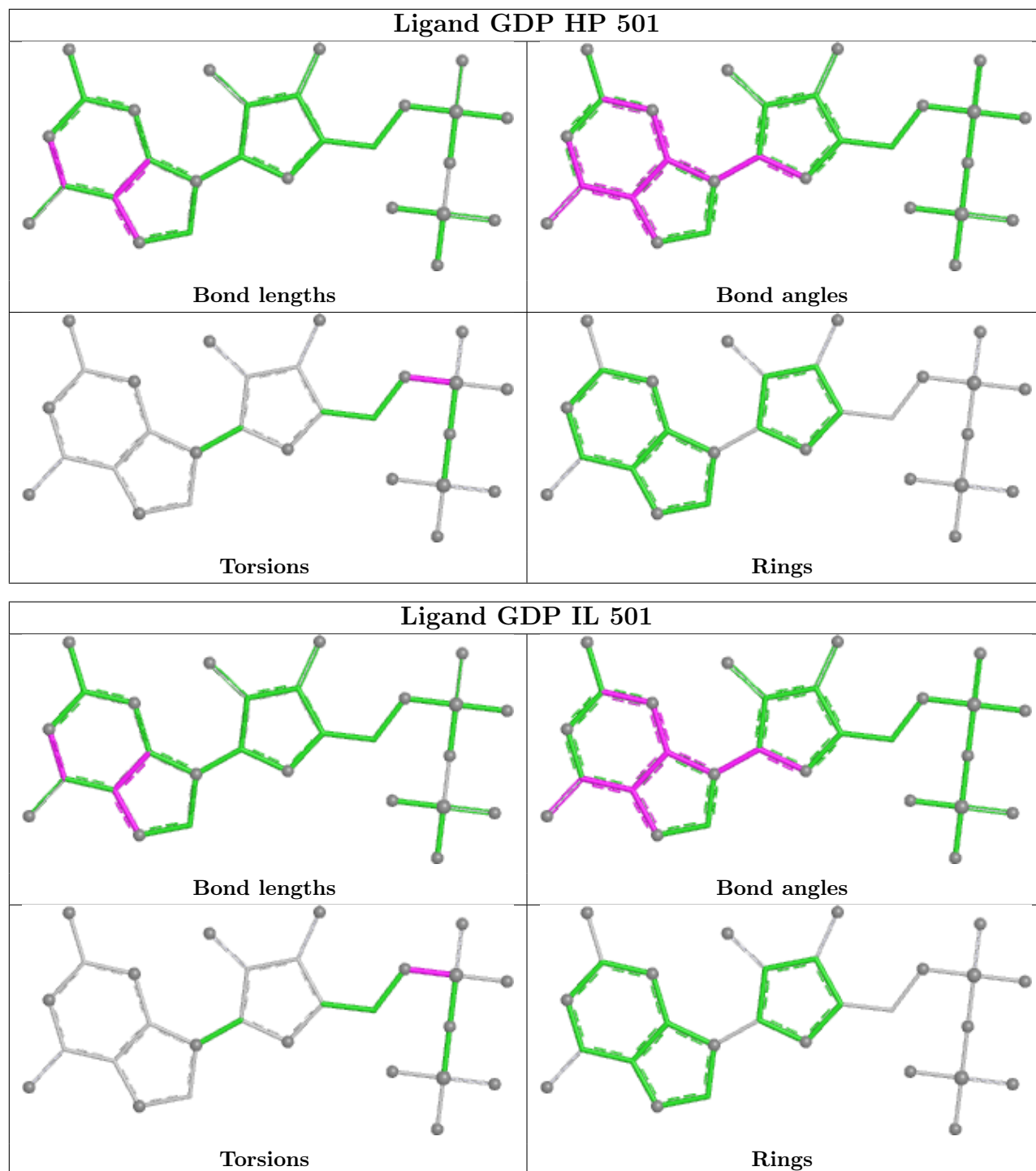


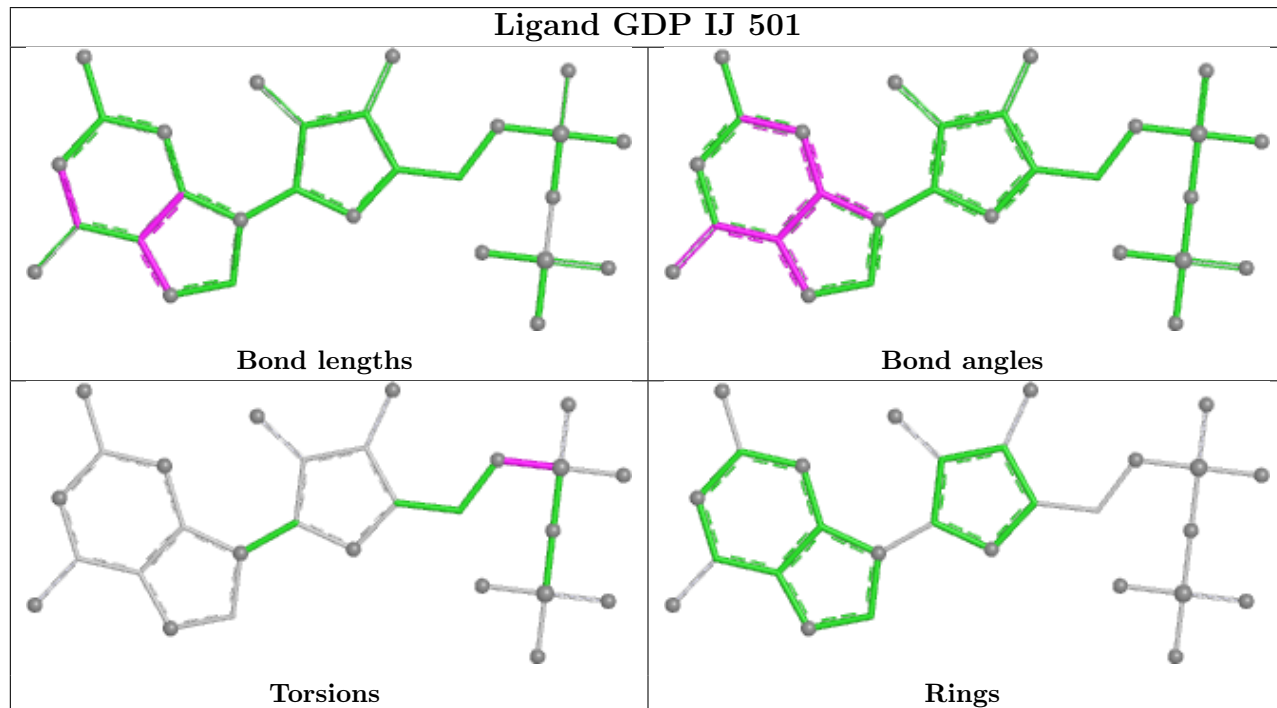
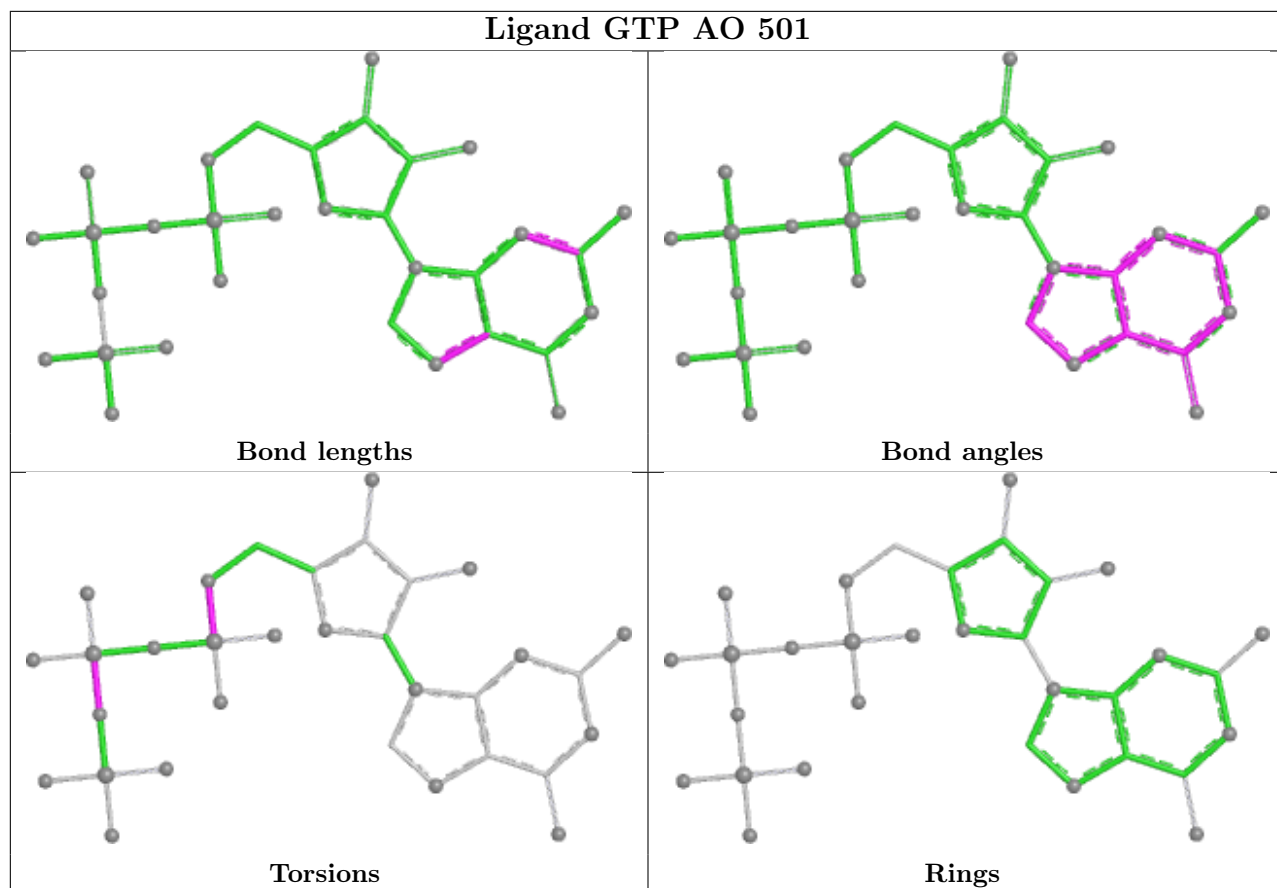


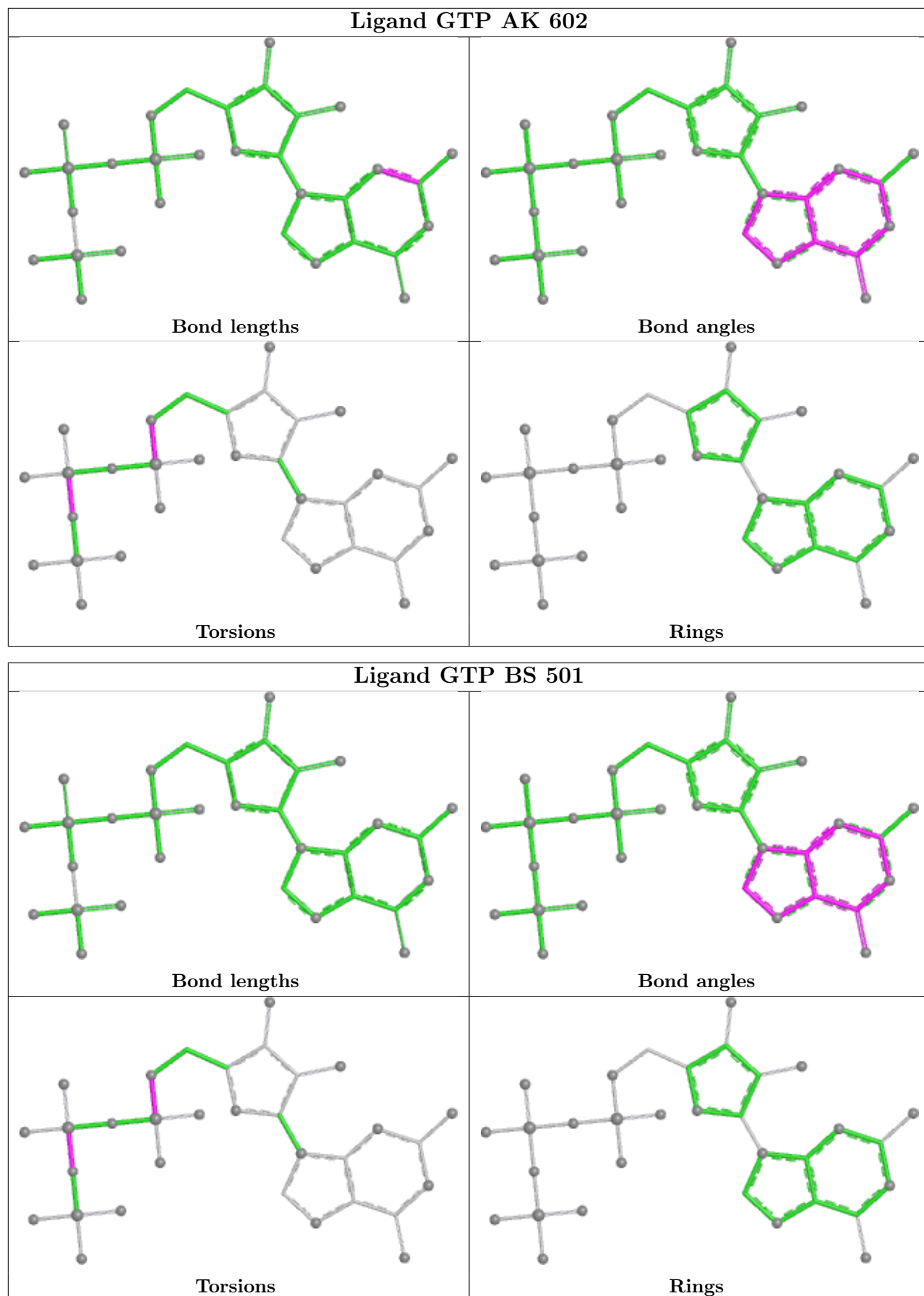


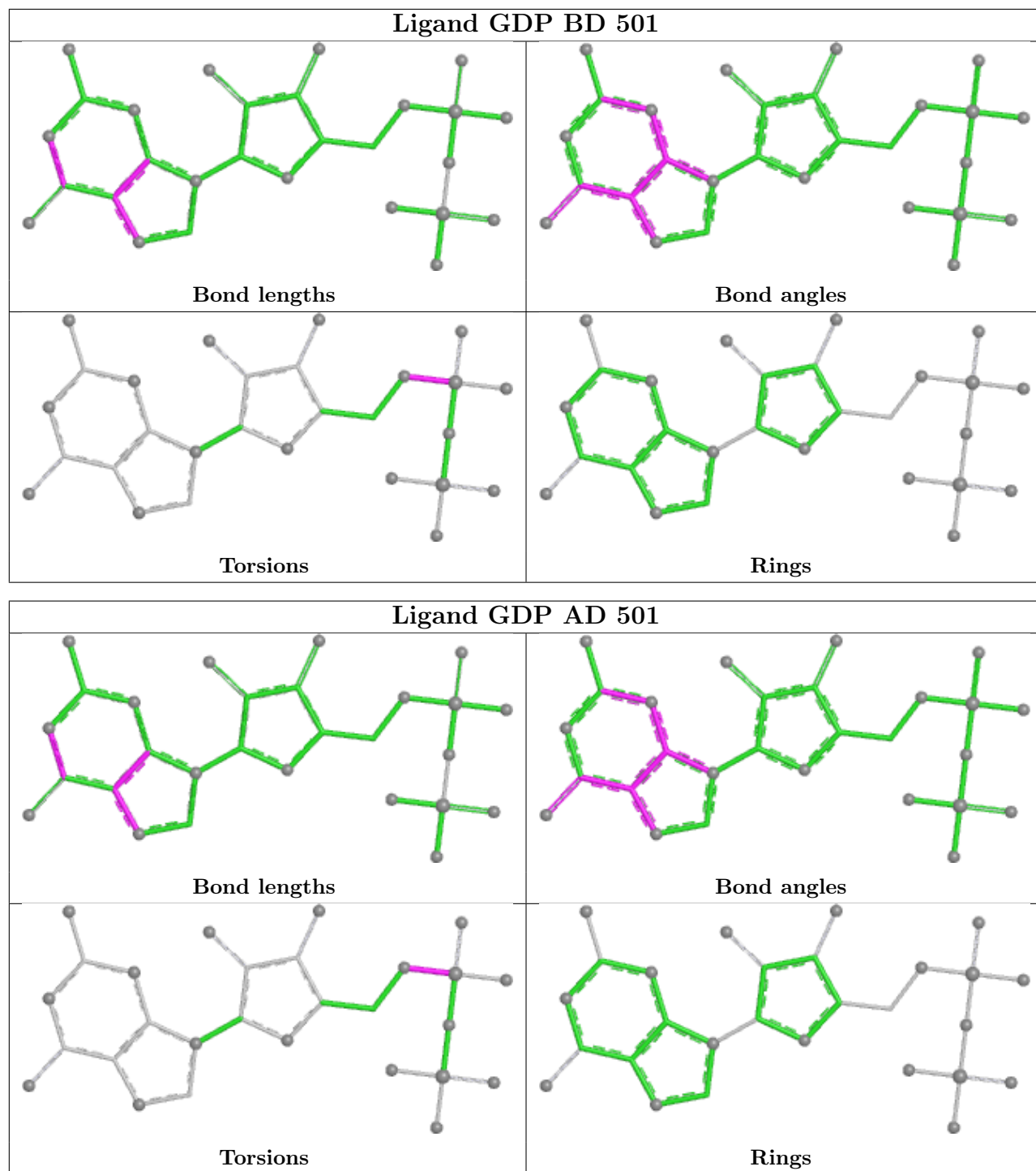


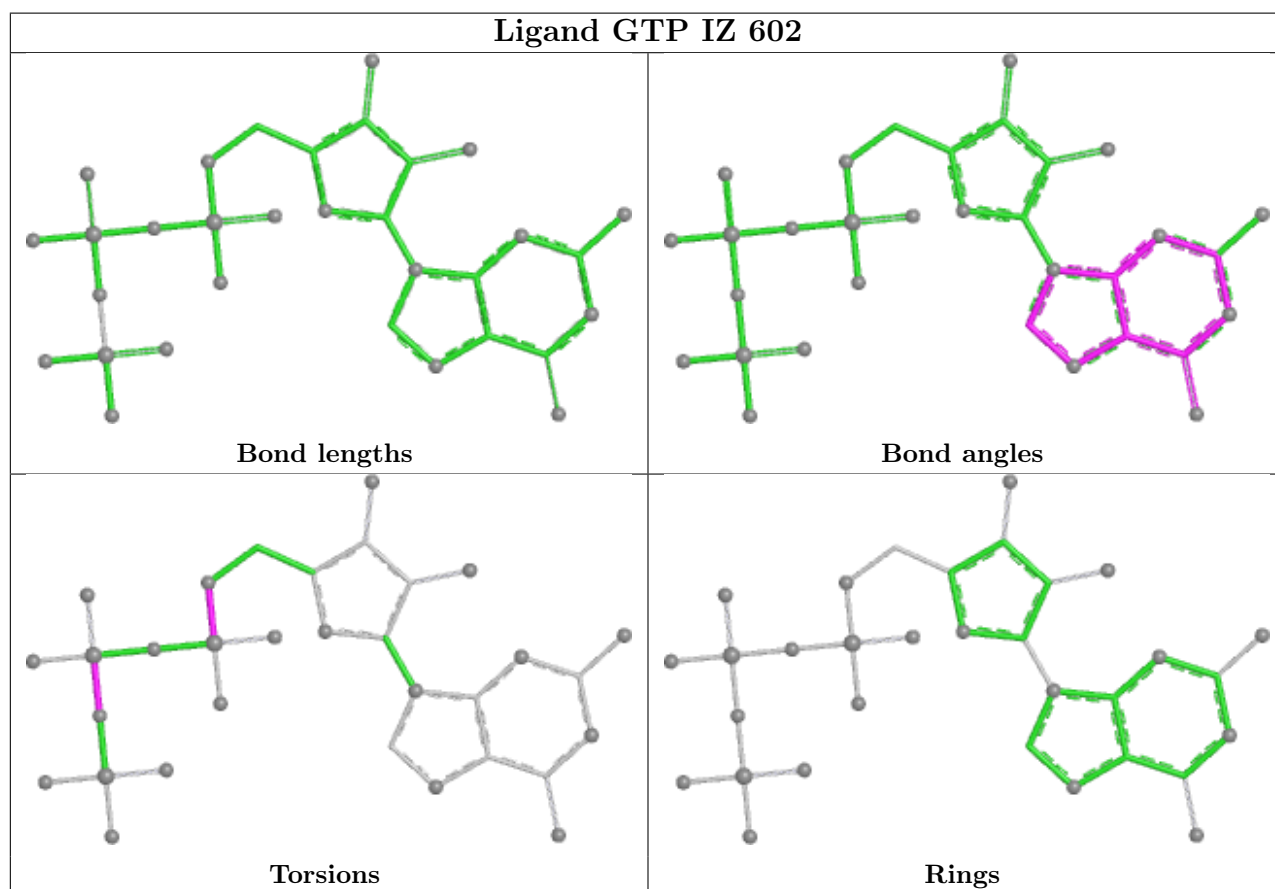
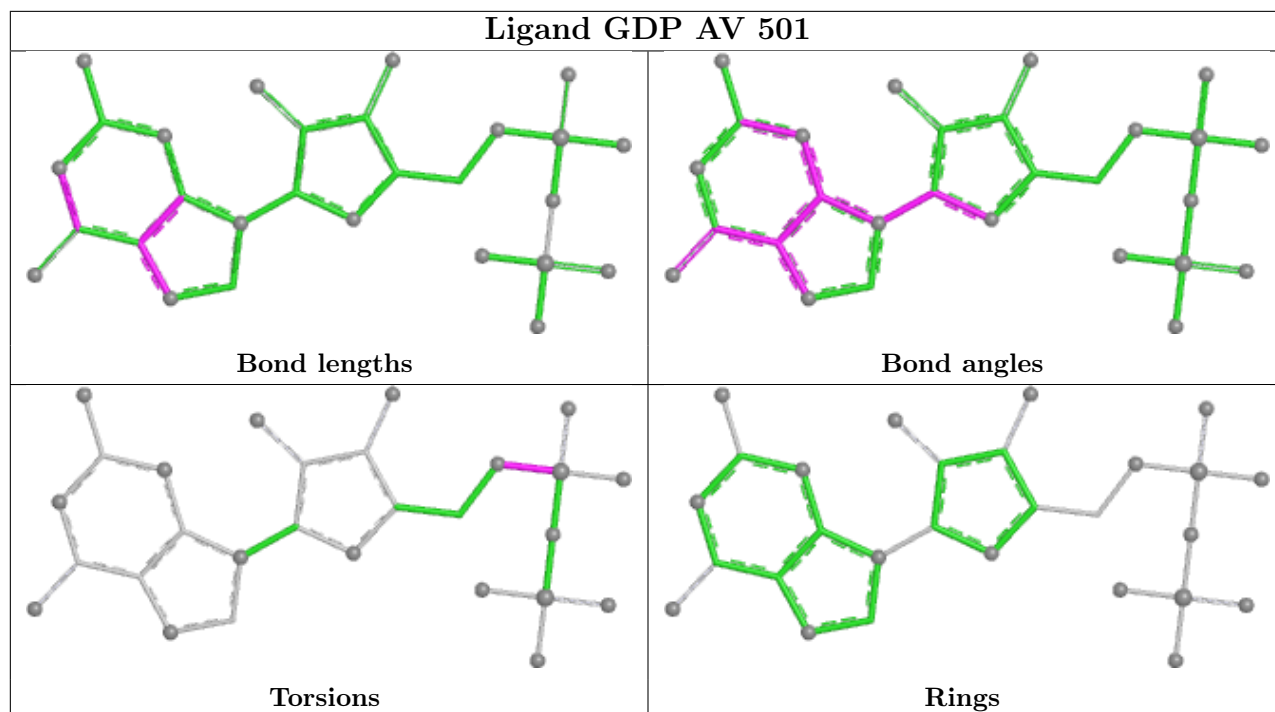


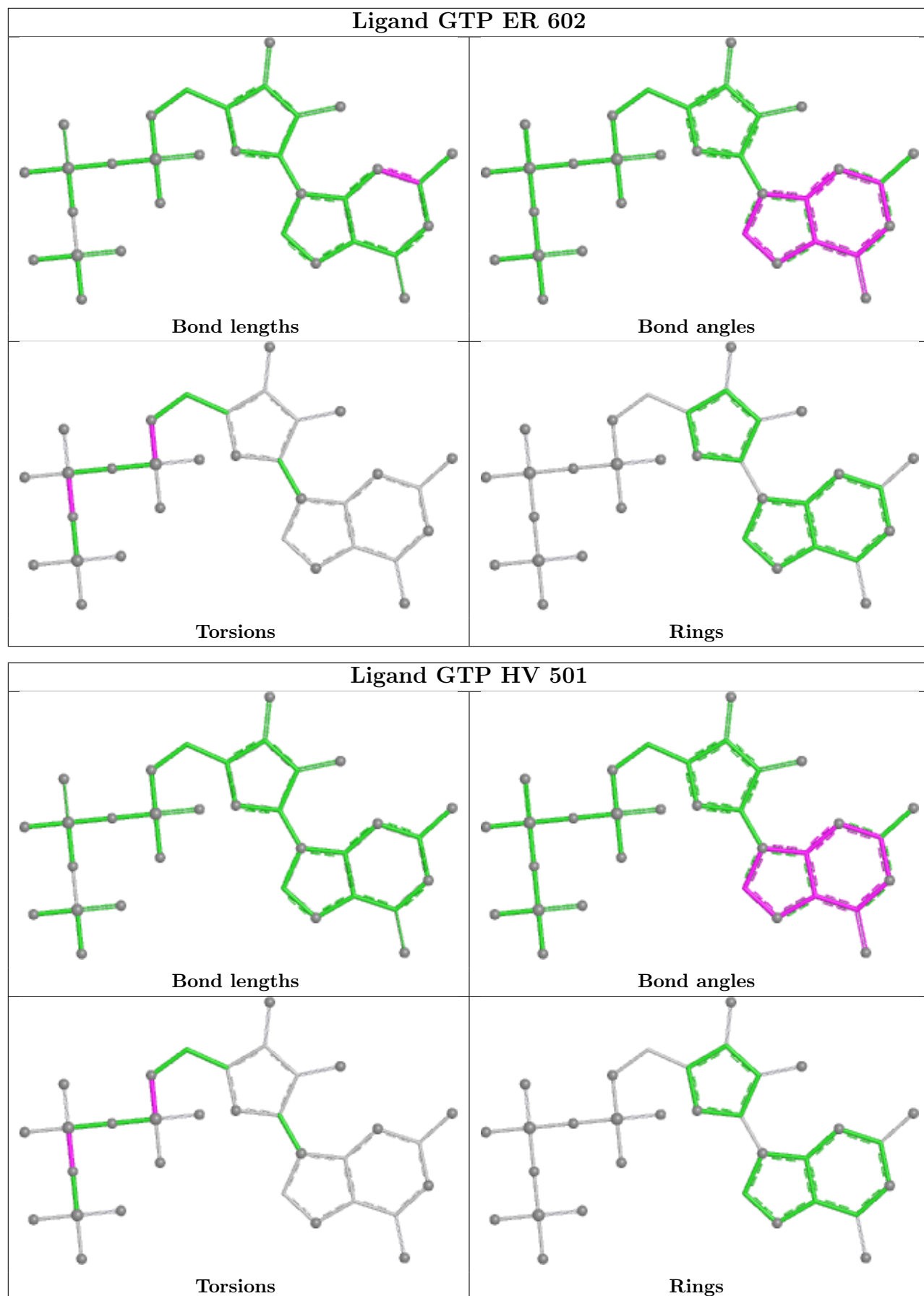


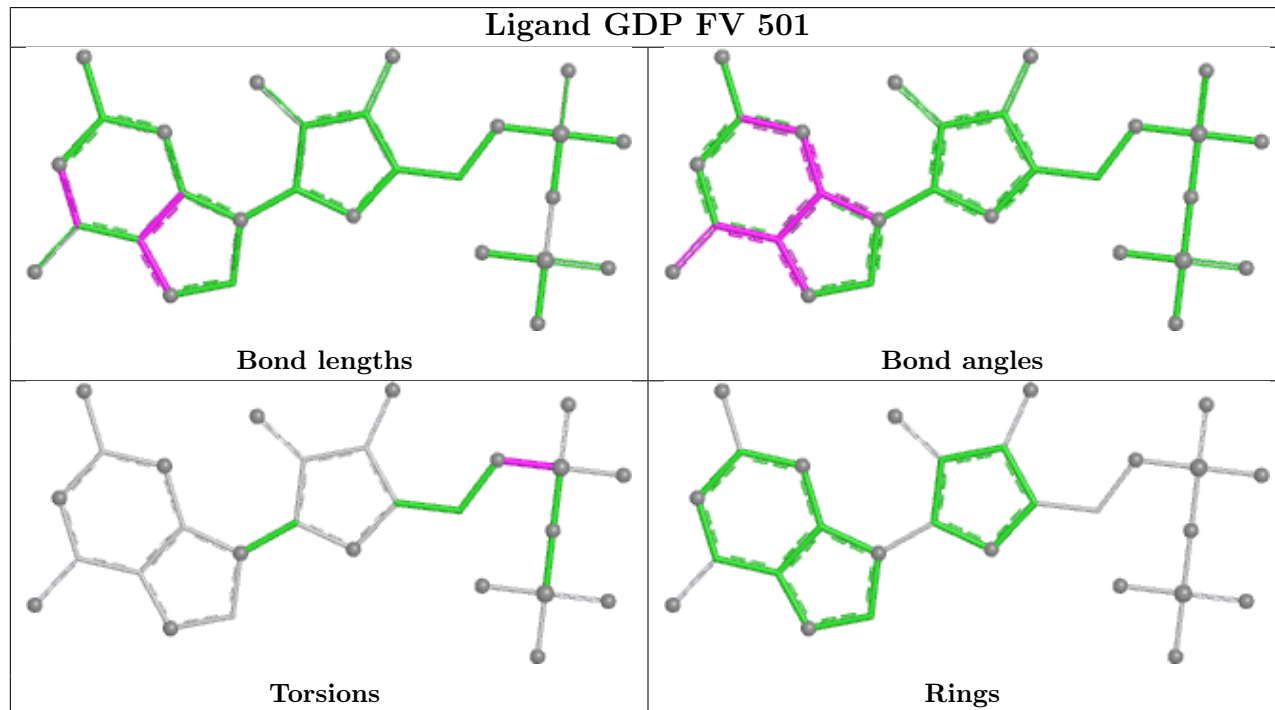
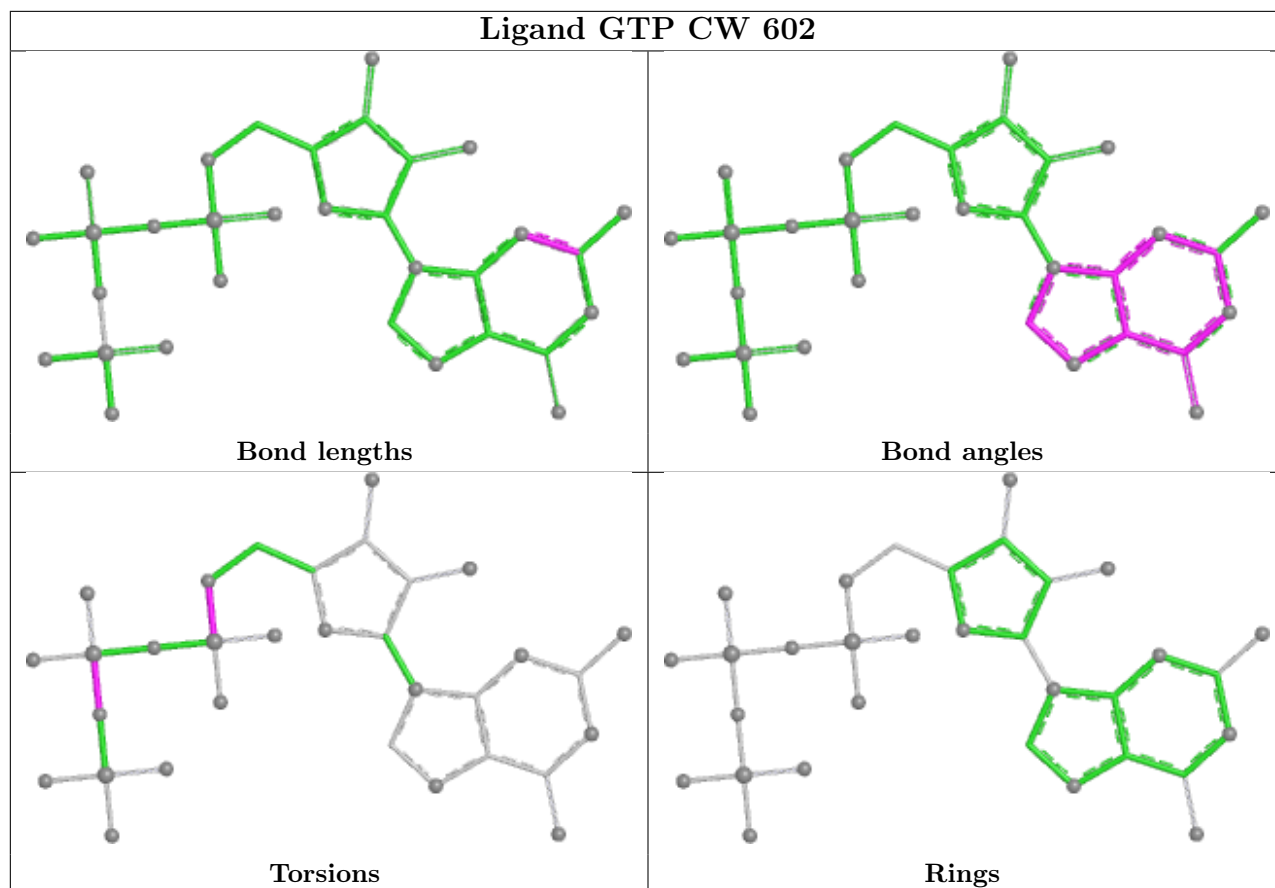


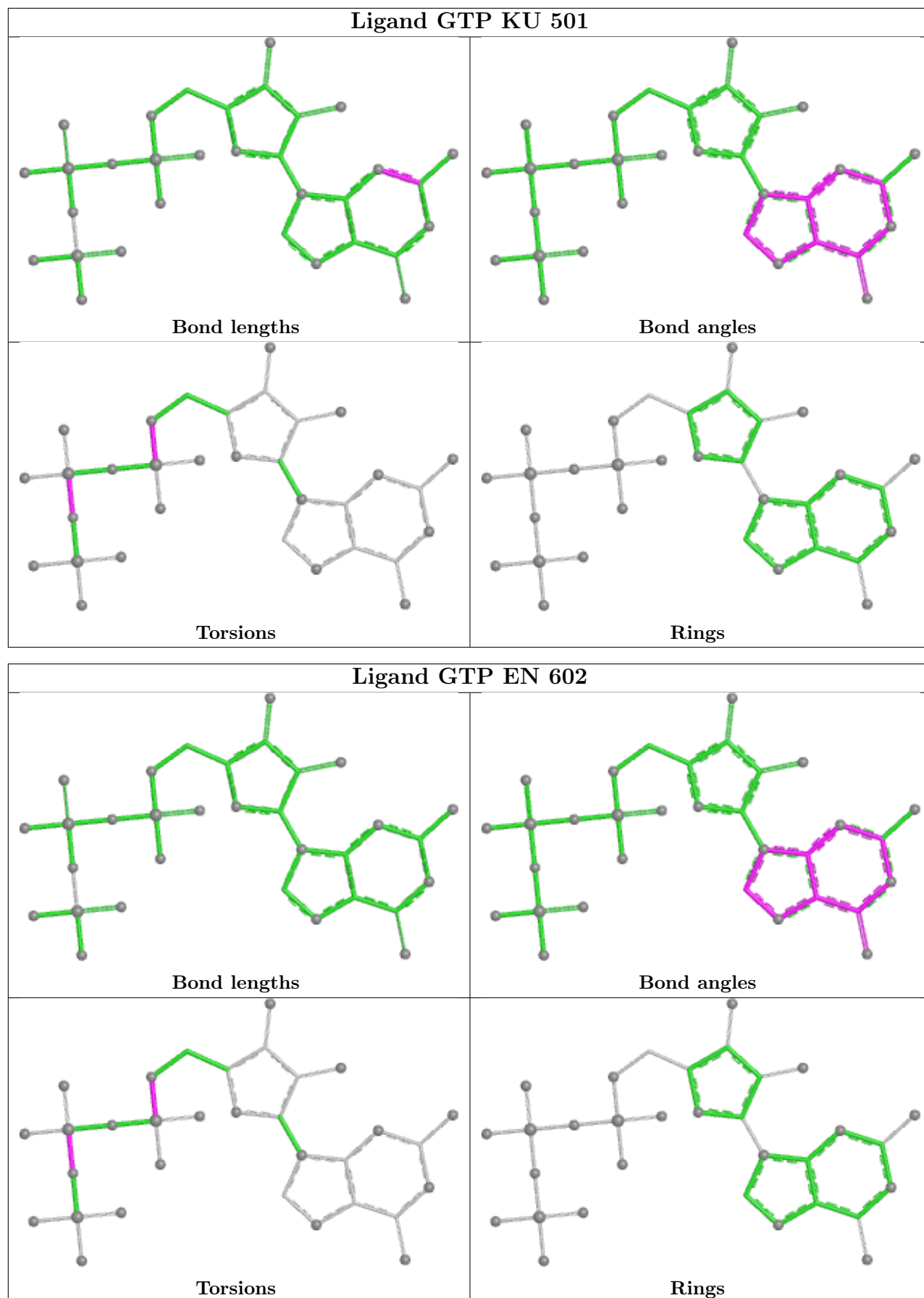


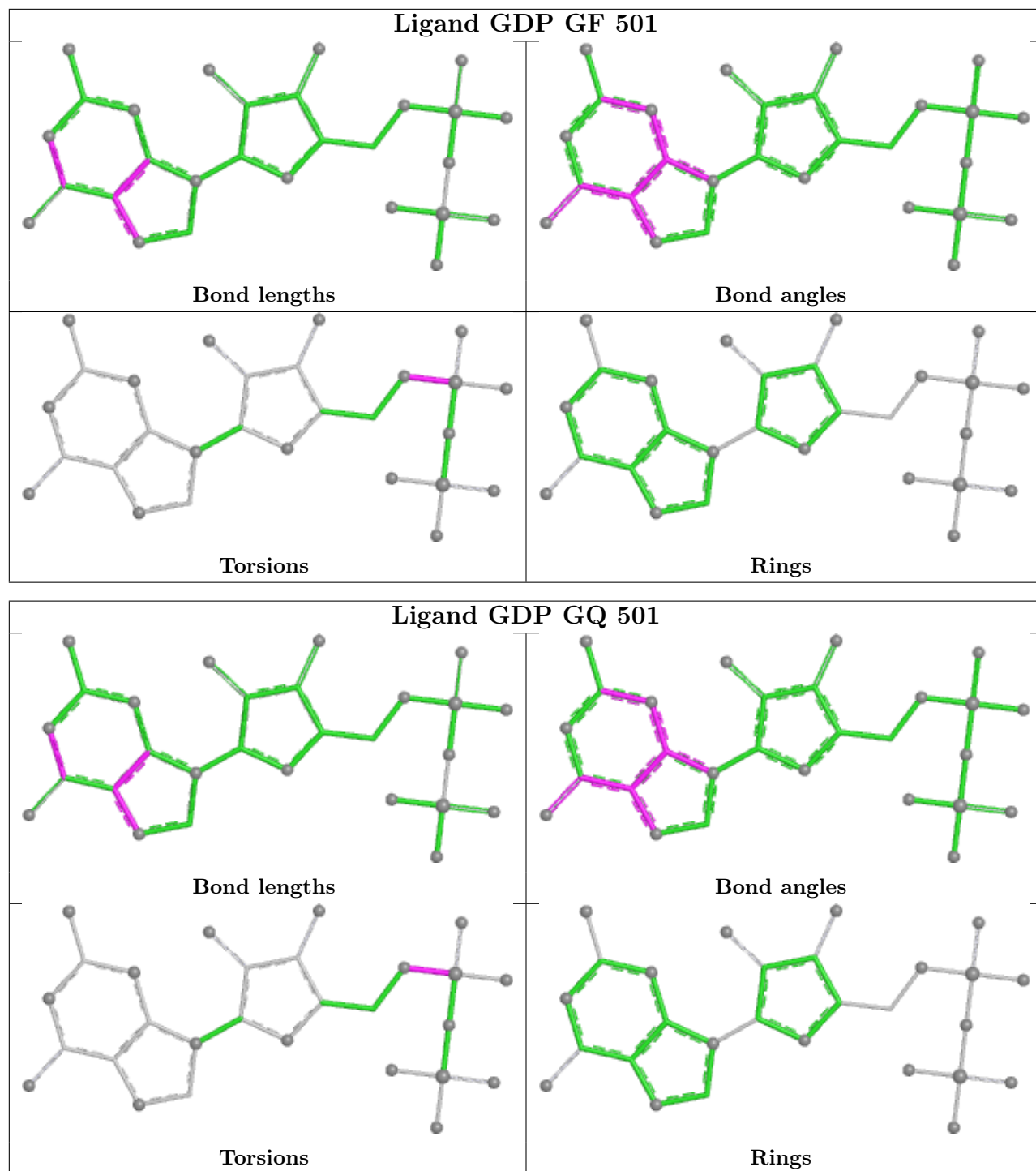


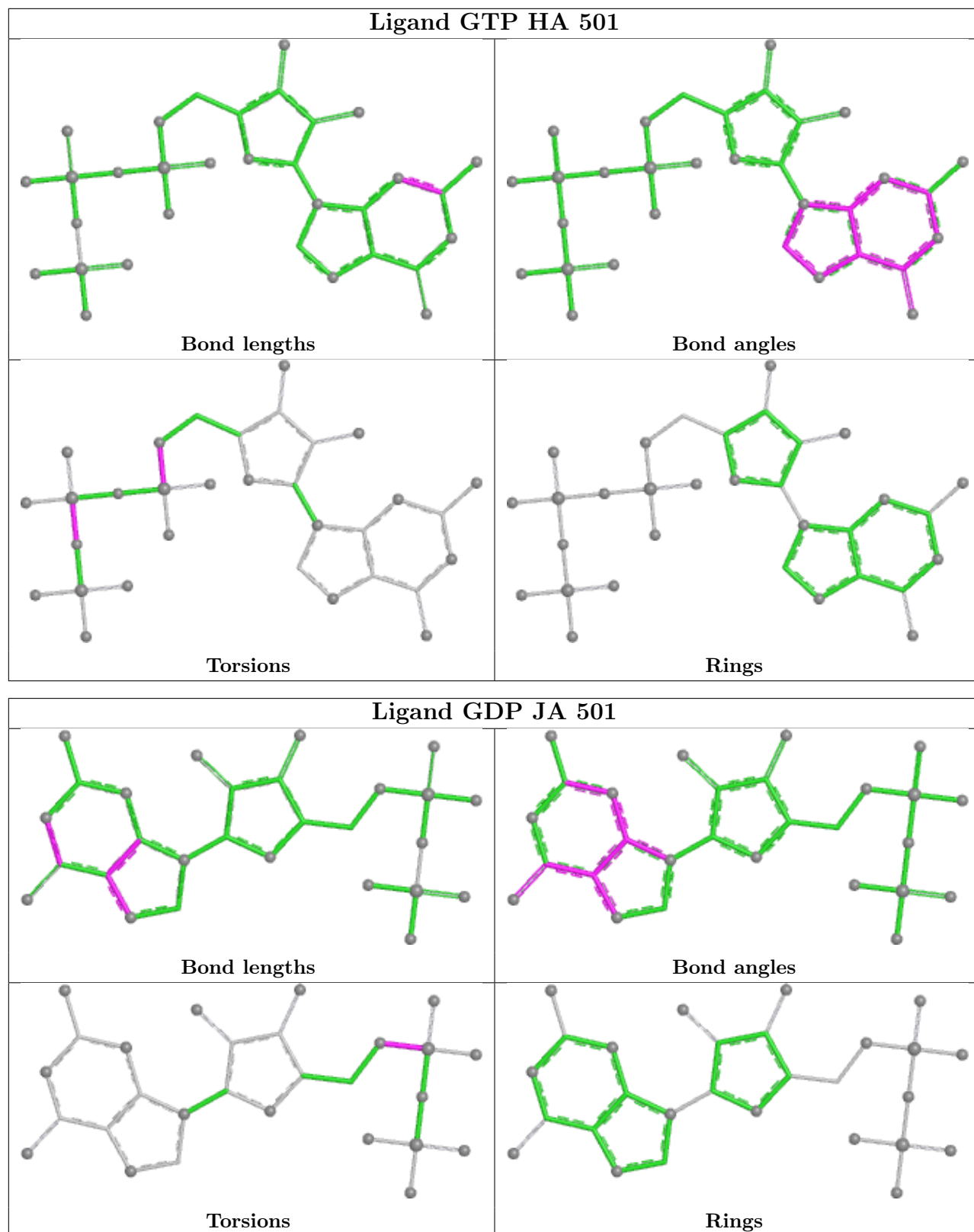


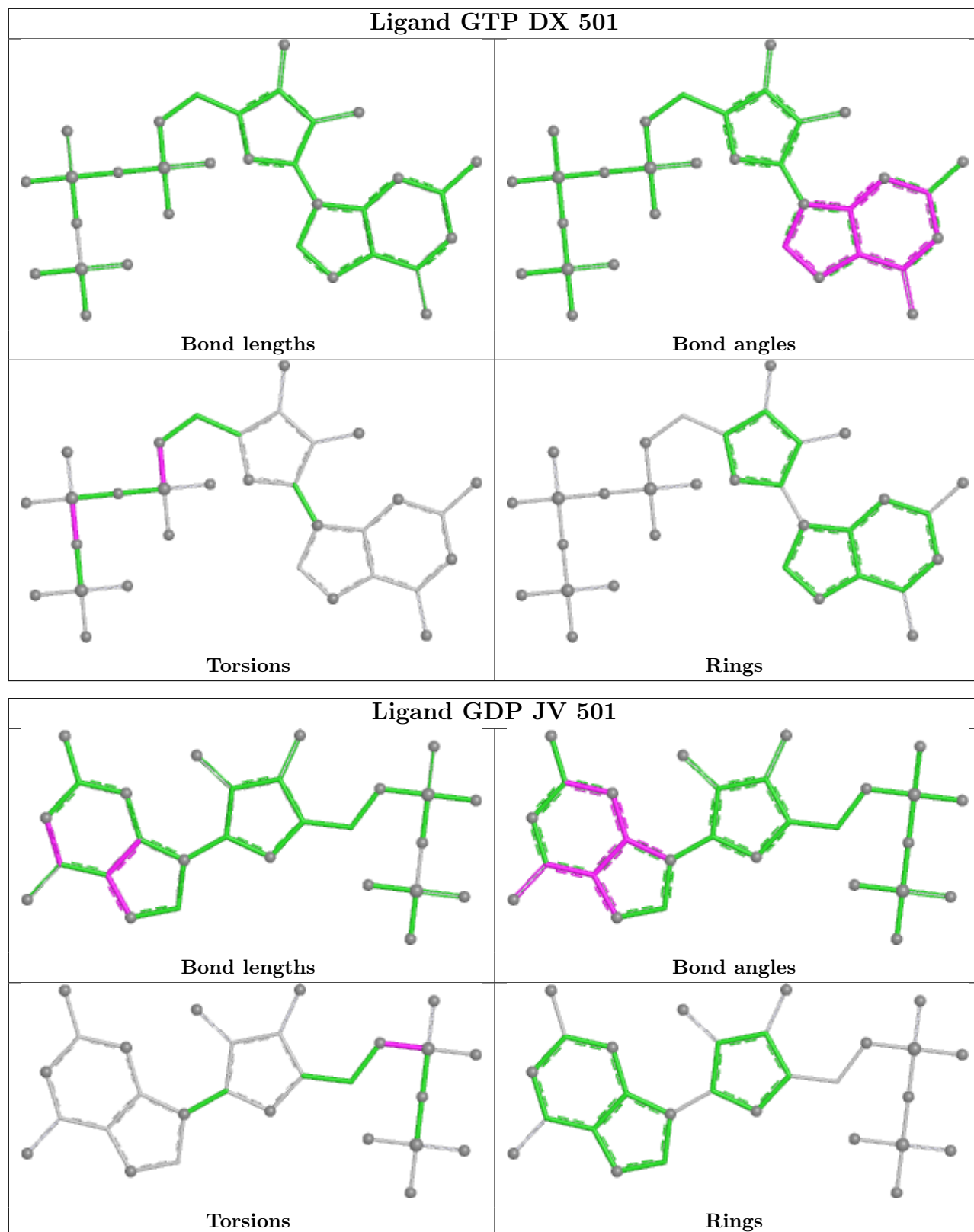


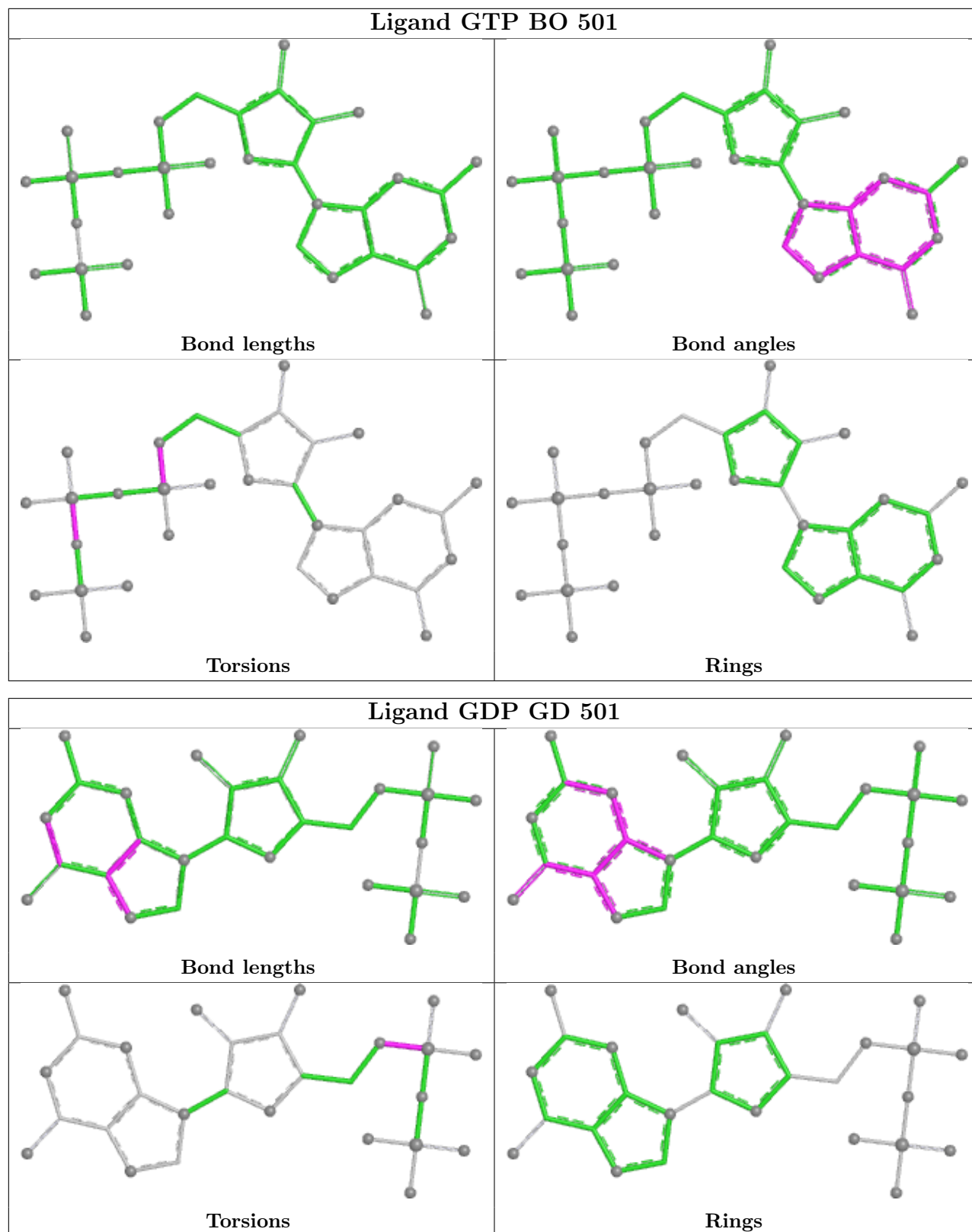


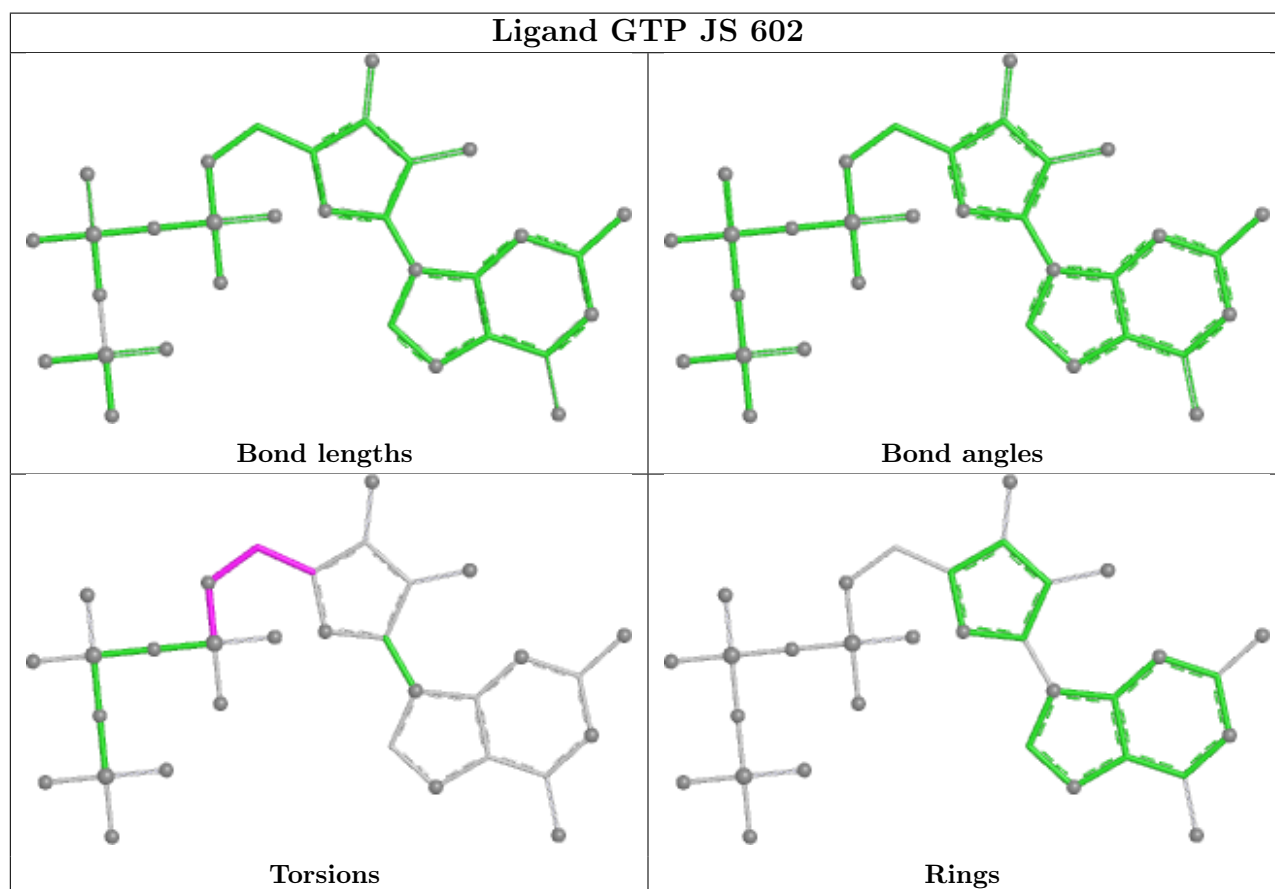
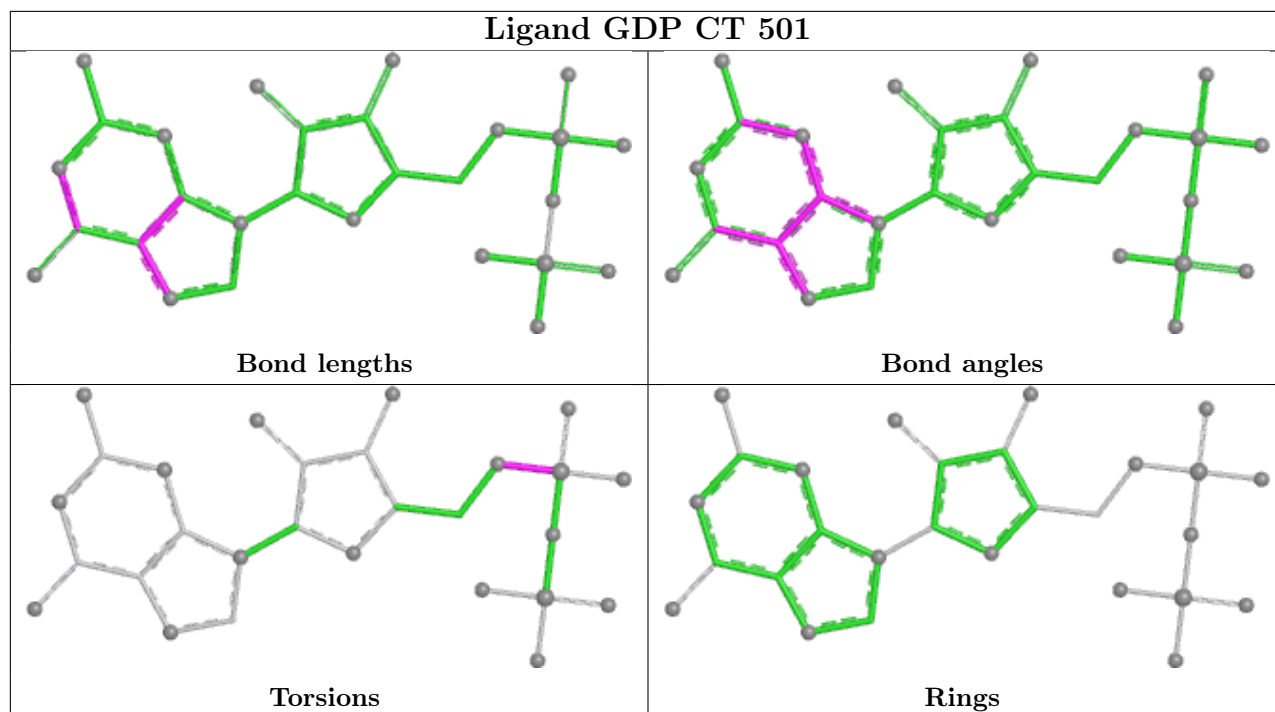


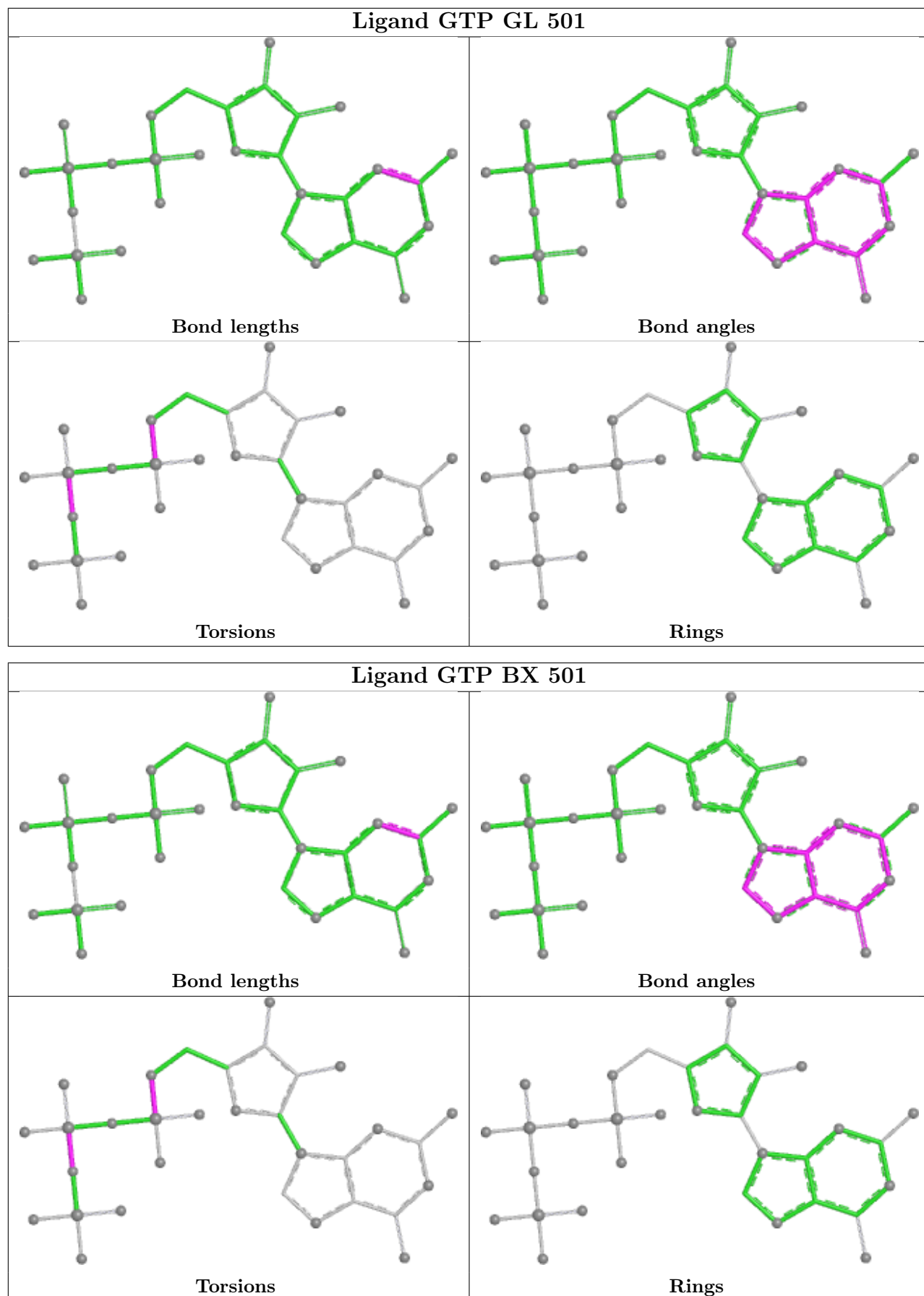


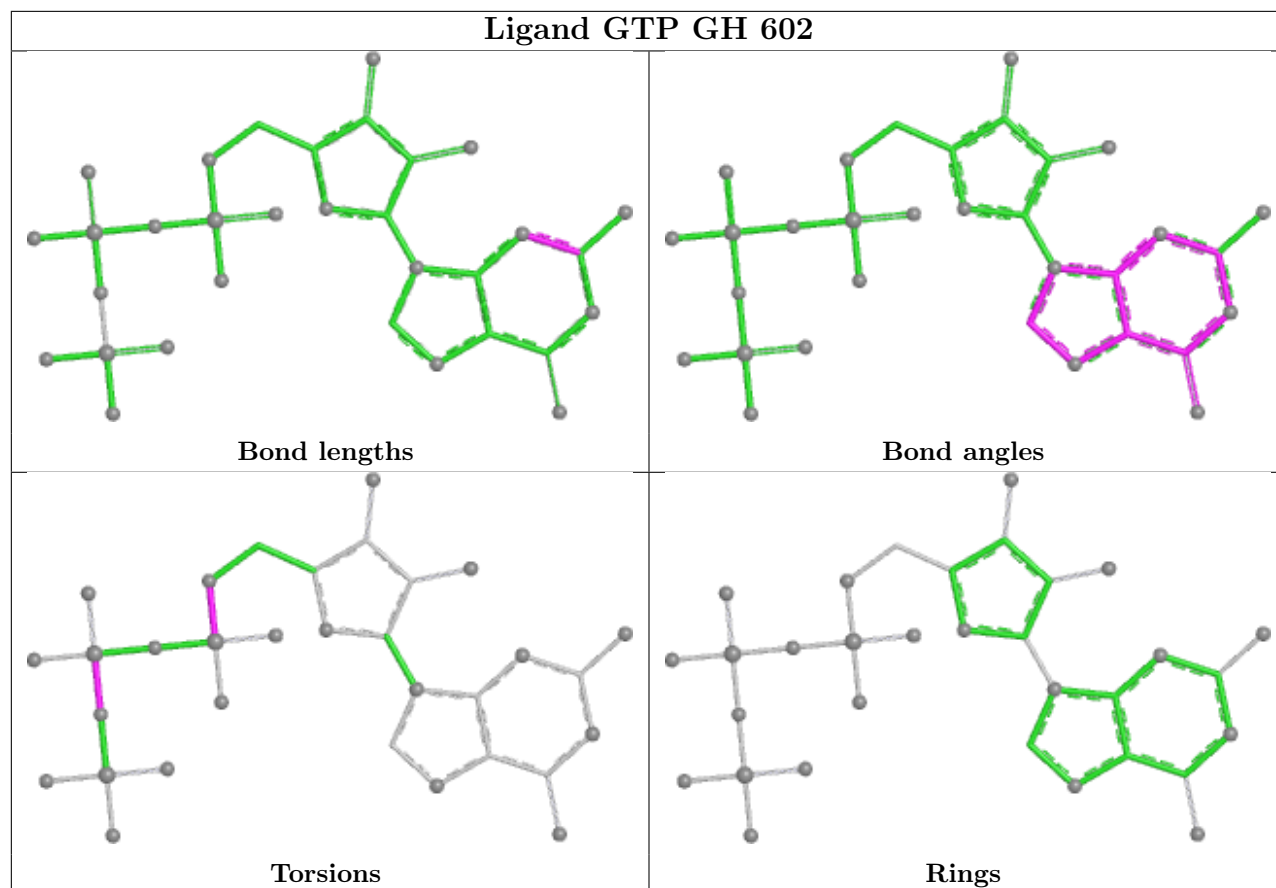












#### 4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

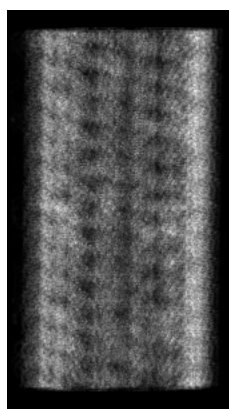
## 5 Map visualisation [i](#)

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.

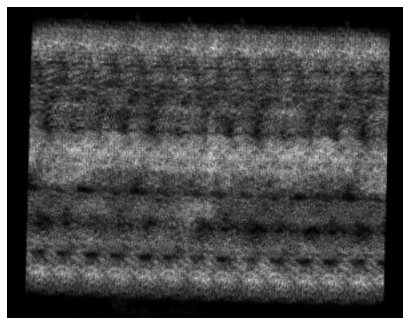
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

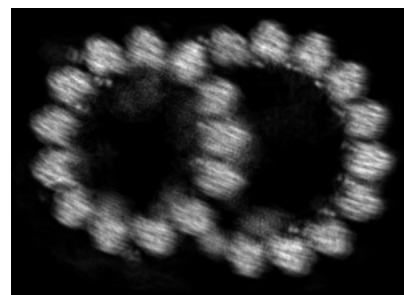
#### 5.1.1 Primary map



X



Y

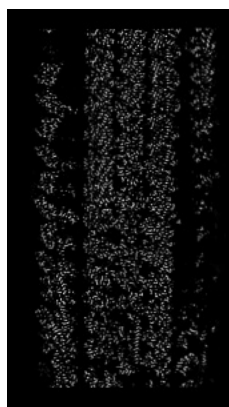


Z

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

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

#### 5.2.1 Primary map



X Index: 227



Y Index: 163

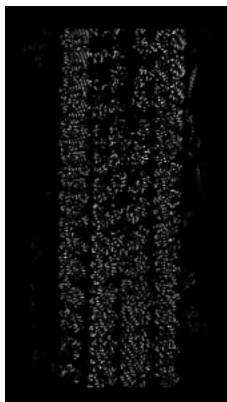


Z Index: 291

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

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

#### 5.3.1 Primary map



X Index: 62



Y Index: 273

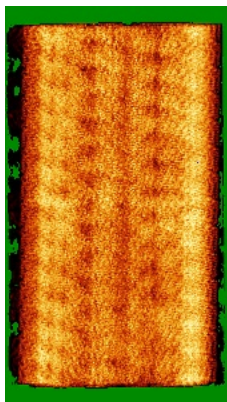


Z Index: 295

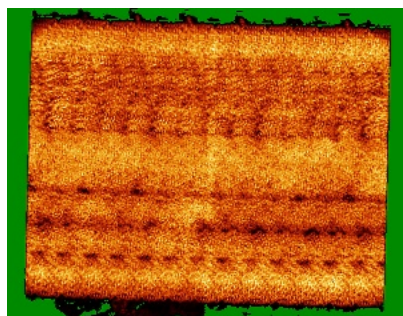
The images above show the largest variance slices of the map in three orthogonal directions.

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

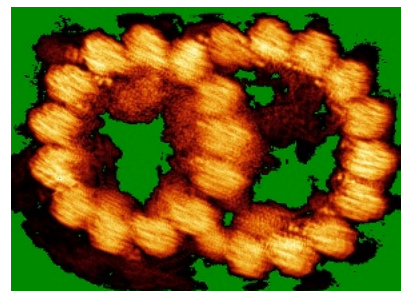
#### 5.4.1 Primary map



X



Y

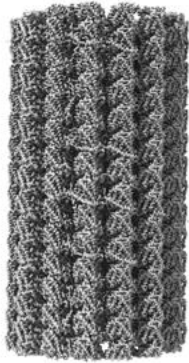


Z

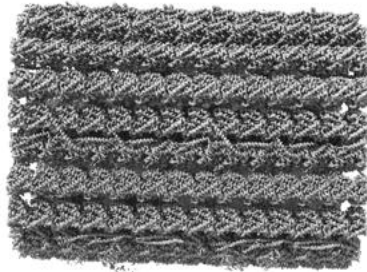
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

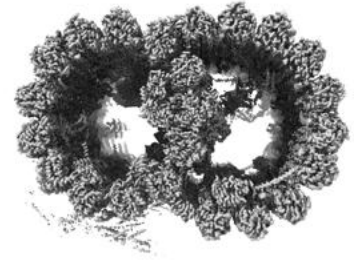
### 5.5.1 Primary map



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.

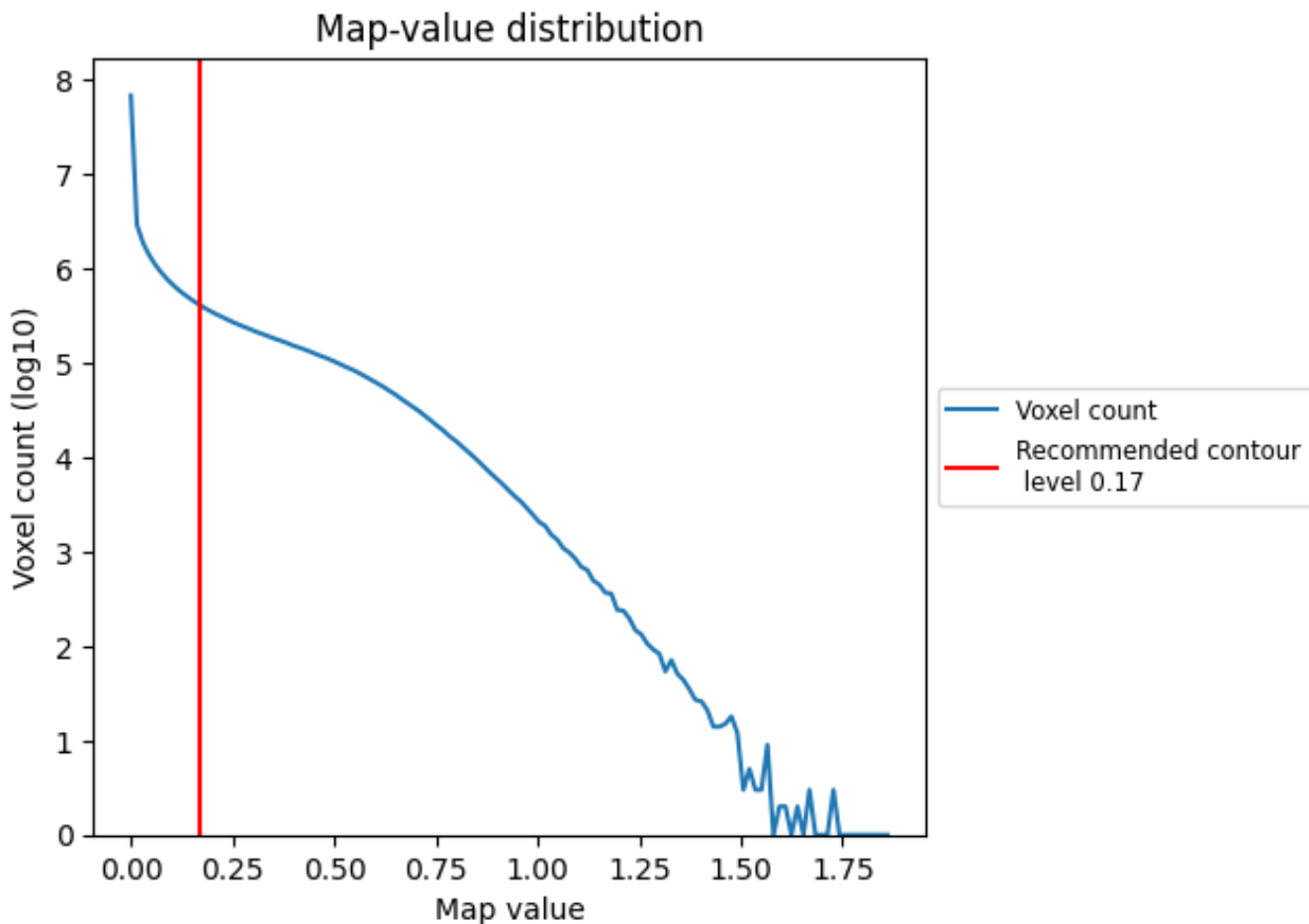
## 5.6 Mask visualisation [i](#)

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

## 6 Map analysis [i](#)

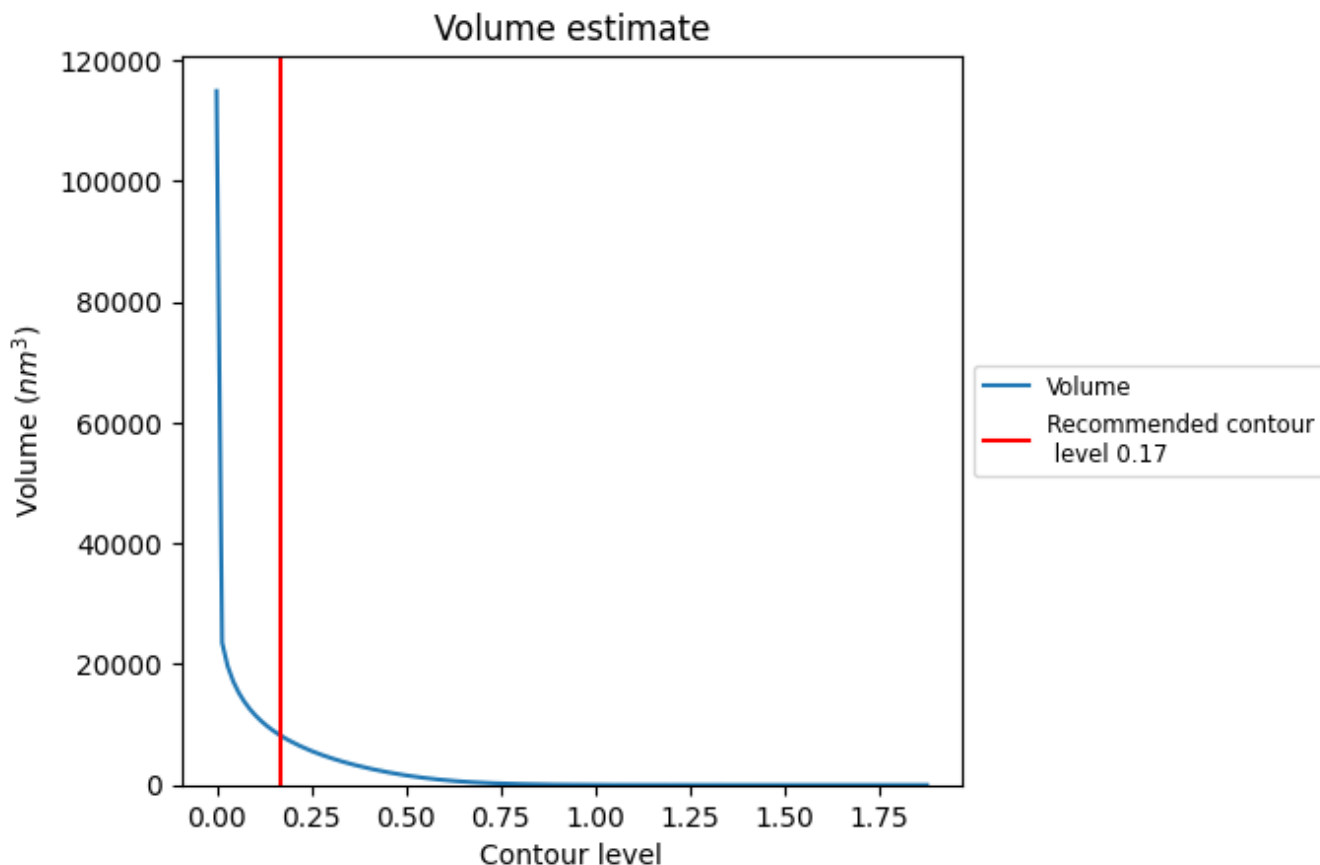
This section contains the results of statistical analysis of the map.

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



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

## 6.2 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.

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

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

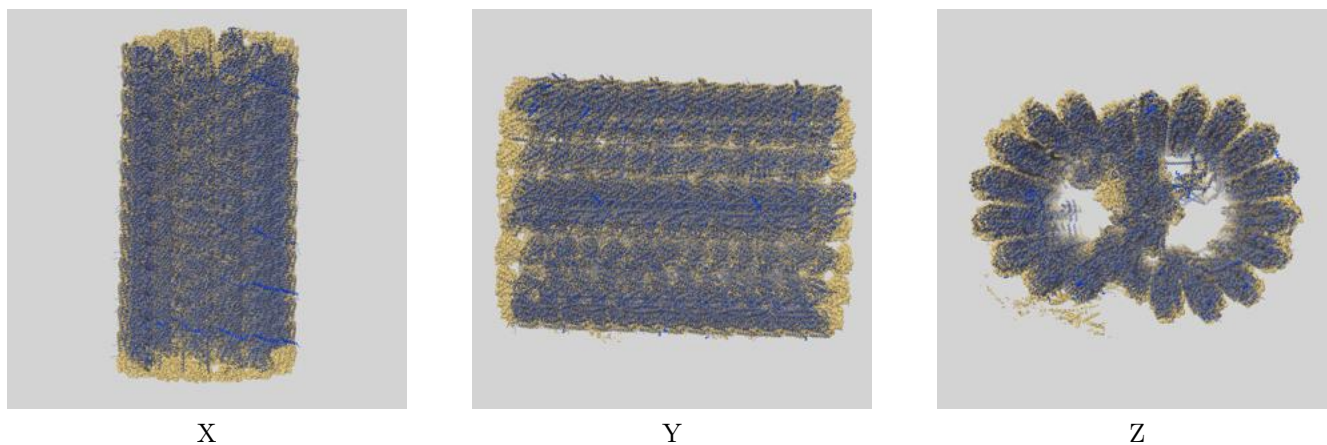
## 7 Fourier-Shell correlation

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

## 8 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 ?? on page ??.

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

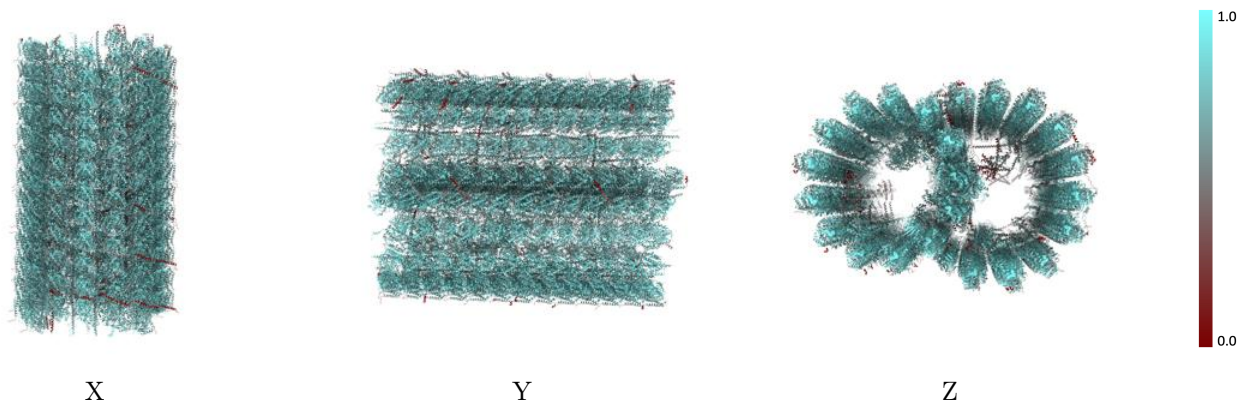


The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

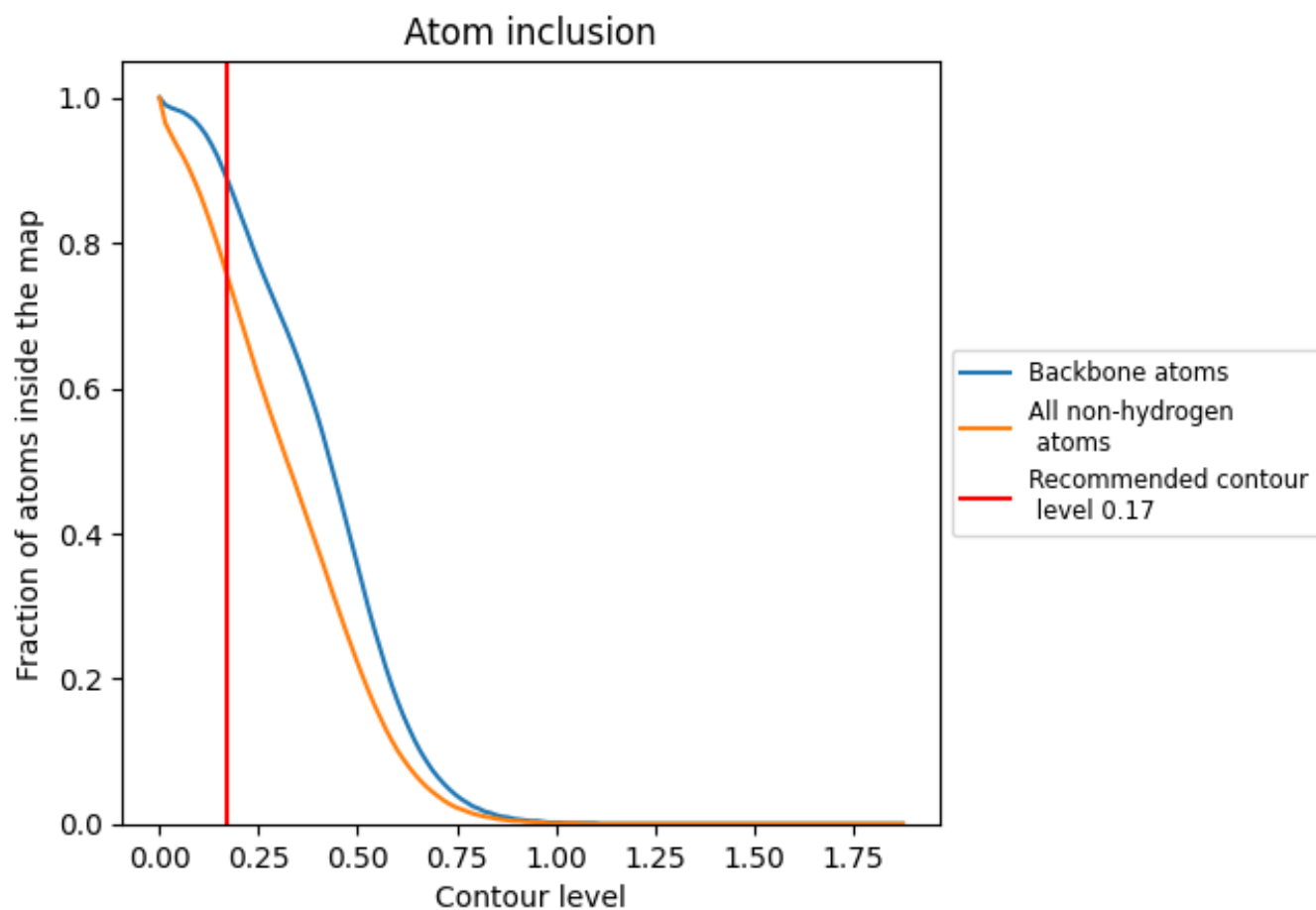
This section was not generated.

## 8.3 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).

## 8.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 8.5 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
All	0.7570
0A	0.6420
0B	0.6060
0C	0.6360
0D	0.7970
0E	0.6630
0F	0.7100
0G	0.6220
0H	0.7830
0I	0.7850
0J	0.8180
0K	0.8120
0M	0.6620
0N	0.6230
0O	0.6650
0P	0.6310
0Q	0.8620
0R	0.7440
0S	0.8490
0T	0.7440
0U	0.6900
0V	0.4830
0W	0.6390
0X	0.7500
0Y	0.7850
0Z	0.7210
1A	0.8140
1B	0.7790
1C	0.7630
1D	0.7700
1E	0.7370
1F	0.7030
1G	0.6620
1H	0.7300
1I	0.7800



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Chain	Atom inclusion
1J	0.6810
1K	0.6800
1L	0.6740
1M	0.6560
1N	0.6520
1O	0.7970
1P	0.7640
1Q	0.7380
1R	0.7670
1S	0.7270
1T	0.7080
1U	0.7260
1V	0.7670
1W	0.7750
1X	0.8040
1Y	0.7750
1Z	0.7860
2A	0.7500
2B	0.7490
2C	0.7840
2D	0.7340
2E	0.7290
2F	0.6990
2G	0.5850
2H	0.5320
2I	0.7660
2J	0.7490
2K	0.7460
2L	0.7190
2M	0.7010
2N	0.8260
2O	0.5650
2P	0.6100
2Q	0.5110
2R	0.4520
2S	0.5990
2T	0.6420
2U	0.7190
2V	0.5770
2W	0.5460
2X	0.7140
2Y	0.5770











































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Chain	Atom inclusion
2Z	0.5350
3A	0.6440
3B	0.6340
3C	0.5910
3D	0.5500
3E	0.4160
3F	0.5310
3G	0.6460
3H	0.5480
3I	0.5690
3J	0.6110
3K	0.6060
3L	0.6670
3M	0.6910
3N	0.6180
3O	0.6150
3P	0.5670
3Q	0.5590
3R	0.6760
3S	0.7590
3T	0.7900
3U	0.8190
3V	0.6530
3W	0.5690
3X	0.5590
3Y	0.6150
3Z	0.4020
4A	0.3890
4B	0.4660
4C	0.5120
4D	0.4730
4E	0.1720
4F	0.4990
4G	0.2410
4H	0.4700
4I	0.6920
4J	0.7640
4K	0.7200
4L	0.6370
4M	0.3290
4N	0.2980
4O	0.0670











































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Chain	Atom inclusion
4P	 0.4330
4Q	 0.5880
4R	 0.6430
4S	 0.6390
4T	 0.3660
4U	 0.5120
4V	 0.3810
4W	 0.5780
4X	 0.7830
4Y	 0.5520
AA	 0.7880
AB	 0.7980
AC	 0.8020
AD	 0.8140
AE	 0.8160
AF	 0.8310
AG	 0.7880
AH	 0.7910
AI	 0.7870
AJ	 0.7940
AK	 0.7700
AL	 0.7870
AM	 0.7980
AN	 0.8140
AO	 0.8030
AP	 0.8240
AQ	 0.8120
AR	 0.8290
AS	 0.7940
AT	 0.7960
AU	 0.7810
AV	 0.7880
AW	 0.7760
AX	 0.7880
AY	 0.7630
AZ	 0.7860
BA	 0.7690
BB	 0.7930
BC	 0.7620
BD	 0.7760
BE	 0.8070
BF	 0.8100











































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Chain	Atom inclusion
BG	 0.7930
BH	 0.8040
BI	 0.7650
BJ	 0.7930
BK	 0.7430
BL	 0.7690
BM	 0.7600
BN	 0.7780
BO	 0.7600
BP	 0.7690
BQ	 0.7790
BR	 0.7650
BS	 0.7800
BT	 0.7690
BU	 0.7640
BV	 0.7830
BW	 0.7450
BX	 0.7390
BY	 0.7900
BZ	 0.7820
CA	 0.8080
CB	 0.7810
CC	 0.7940
CD	 0.7820
CE	 0.7740
CF	 0.7710
CG	 0.7750
CH	 0.7750
CI	 0.7780
CJ	 0.7500
CL	 0.7750
CM	 0.7590
CN	 0.7810
CO	 0.7520
CP	 0.7810
CQ	 0.7690
CR	 0.7800
CS	 0.7530
CT	 0.7780
CU	 0.7600
CV	 0.7920
CW	 0.7540











































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<b>Chain</b>	<b>Atom inclusion</b>
CX	 0.7940
CY	 0.8010
CZ	 0.7880
DA	 0.7840
DB	 0.7920
DC	 0.7820
DD	 0.7860
DE	 0.7810
DF	 0.7890
DG	 0.7890
DH	 0.7910
DI	 0.7880
DJ	 0.8060
DK	 0.7850
DL	 0.8010
DM	 0.7830
DN	 0.8030
DO	 0.7940
DP	 0.8130
DQ	 0.7870
DR	 0.8090
DS	 0.7810
DT	 0.7970
DU	 0.7700
DV	 0.7880
DW	 0.8000
DX	 0.8010
DY	 0.8070
DZ	 0.8090
EA	 0.7910
EB	 0.8020
EC	 0.8240
ED	 0.8100
EE	 0.7850
EF	 0.7900
EG	 0.8020
EH	 0.7930
EI	 0.7960
EJ	 0.7970
EK	 0.8130
EL	 0.8180
EM	 0.8150











































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<b>Chain</b>	<b>Atom inclusion</b>
EN	 0.8030
EO	 0.8120
EP	 0.8070
EQ	 0.7910
ER	 0.7840
ES	 0.7940
ET	 0.7950
EU	 0.7960
EV	 0.8300
EW	 0.8590
EX	 0.8390
EY	 0.8350
EZ	 0.8300
FA	 0.8520
FB	 0.8700
FC	 0.8350
FD	 0.8350
FE	 0.8770
FF	 0.8660
FG	 0.8320
FH	 0.7960
FI	 0.8120
FJ	 0.8110
FK	 0.8040
FL	 0.7980
FM	 0.8040
FN	 0.8170
FO	 0.7990
FP	 0.7970
FQ	 0.8110
FR	 0.8040
FS	 0.7790
FT	 0.7880
FU	 0.8160
FV	 0.8280
FW	 0.8310
FX	 0.8390
FY	 0.8160
FZ	 0.8420
GA	 0.8350
GB	 0.8290
GC	 0.8200

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Chain	Atom inclusion
GD	 0.8330
GE	 0.8220
GF	 0.8160
GG	 0.7930
GH	 0.6930
GI	 0.7320
GJ	 0.7190
GK	 0.6990
GL	 0.6330
GM	 0.6450
GN	 0.6740
GO	 0.6750
GP	 0.6510
GQ	 0.6670
GR	 0.6310
GS	 0.6480
GT	 0.6190
GU	 0.7560
GV	 0.7680
GW	 0.7560
GX	 0.7630
GY	 0.7430
GZ	 0.7580
HA	 0.7720
HB	 0.7630
HC	 0.7630
HD	 0.7770
HE	 0.7530
HF	 0.7480
HG	 0.7450
HH	 0.7770
HI	 0.7660
HJ	 0.7720
HK	 0.7600
HL	 0.7680
HM	 0.7630
HN	 0.7730
HO	 0.7780
HP	 0.8020
HQ	 0.7570
HR	 0.7430
HS	 0.7360











































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Chain	Atom inclusion
HT	0.7430
HU	0.7830
HV	0.7510
HW	0.7810
HX	0.7500
HY	0.7770
HZ	0.7450
IA	0.7580
IB	0.7450
IC	0.8020
ID	0.7630
IE	0.7440
IF	0.7510
IG	0.7510
IH	0.7700
II	0.7570
IJ	0.7700
IK	0.7470
IL	0.7750
IM	0.7530
IN	0.7670
IO	0.7450
IP	0.7610
IQ	0.7510
IR	0.7040
IS	0.7800
IT	0.7910
IU	0.7870
IV	0.7970
IW	0.8090
IX	0.7940
IY	0.8220
IZ	0.8150
JA	0.8220
JB	0.8120
JC	0.8270
JD	0.7980
JE	0.7180
JF	0.7180
JG	0.7150
JH	0.7060
JI	0.7030




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<b>Chain</b>	<b>Atom inclusion</b>
JJ	 0.7210
JK	 0.7180
JL	 0.7430
JM	 0.7640
JN	 0.7560
JO	 0.7620
JP	 0.7510
JQ	 0.6940
JR	 0.6960
JS	 0.7320
JT	 0.7230
JU	 0.7390
JV	 0.7390
JW	 0.7590
JX	 0.7450
JY	 0.7440
JZ	 0.7420
KA	 0.7410
KB	 0.7370
KC	 0.6720
KD	 0.7850
KE	 0.7990
KF	 0.7970
KG	 0.8120
KH	 0.8020
KI	 0.8050
KJ	 0.8120
KK	 0.8160
KL	 0.7950
KM	 0.8110
KN	 0.7970
KO	 0.7910
KP	 0.7700
KQ	 0.7500
KR	 0.7570
KS	 0.7860
KT	 0.7820
KU	 0.7770
KV	 0.7700
KW	 0.7910
KX	 0.7730
KY	 0.7710

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Chain	Atom inclusion
KZ	 0.7870
LA	 0.7850
LB	 0.7690