



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 12:33 AM UTC

PDB ID : 8SNB / pdb_00008snb
EMDB ID : EMD-40619
Title : atomic model of sea urchin sperm doublet microtubule (48-nm periodicity)
Authors : Zeng, J.; Zhang, R.
Deposited on : 2023-04-26
Resolution : 3.30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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 : **FAILED**
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 3.30 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 [i](#)

There are 58 unique types of molecules in this entry. The entry contains 1270897 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 CFAP96(C4orf47).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	42	Total	C	N	O	S	0	0
			324	205	55	61	3		
1	1B	267	Total	C	N	O	S	0	0
			2033	1284	371	373	5		

- Molecule 2 is a protein called Coiled-coil domain-containing protein 105.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1E	419	Total	C	N	O	S	0	0
			3281	2005	647	619	10		
2	1F	170	Total	C	N	O	S	0	0
			1281	781	237	257	6		
2	1G	294	Total	C	N	O	S	0	0
			2355	1440	478	432	5		
2	1H	420	Total	C	N	O	S	0	0
			3294	2012	649	623	10		

- Molecule 3 is a protein called Coiled-coil domain-containing protein 81.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1K	175	Total	C	N	O	S	0	0
			1406	897	246	257	6		
3	1L	175	Total	C	N	O	S	0	0
			1406	897	246	257	6		
3	1M	175	Total	C	N	O	S	0	0
			1393	889	244	254	6		
3	1v	207	Total	C	N	O	S	0	0
			1719	1051	329	333	6		
3	1w	87	Total	C	N	O	S	0	0
			727	441	145	138	3		
3	1x	250	Total	C	N	O	S	0	0
			2088	1276	406	401	5		
3	1y	198	Total	C	N	O	S	0	0
			1639	999	315	319	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	1z	87	Total	C	N	O	S	0	0
			727	441	145	138	3		
3	2a	54	Total	C	N	O	S	0	0
			452	276	83	90	3		

- Molecule 4 is a protein called FAM166C.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1P	203	Total	C	N	O	S	0	0
			1628	993	310	317	8		
4	1Q	138	Total	C	N	O	S	0	0
			1130	686	223	217	4		

- Molecule 5 is a protein called Protein FAM166B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1T	228	Total	C	N	O	S	0	0
			1845	1171	328	337	9		
5	1U	111	Total	C	N	O	S	0	0
			898	575	158	161	4		
5	1V	229	Total	C	N	O	S	0	0
			1857	1180	329	339	9		
5	1W	107	Total	C	N	O	S	0	0
			871	549	156	162	4		

- Molecule 6 is a protein called CFAP144(FAM183A).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1Y	119	Total	C	N	O	S	0	0
			1009	638	176	191	4		

- Molecule 7 is a protein called Outer dense fiber protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1a	134	Total	C	N	O	S	0	0
			1030	647	184	193	6		
7	1b	122	Total	C	N	O	S	0	0
			922	578	169	171	4		
7	5E	154	Total	C	N	O	S	0	0
			1158	727	211	215	5		
7	5F	112	Total	C	N	O	S	0	0
			861	542	153	160	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	5G	142	Total	C	N	O	S	0	0
			1074	675	194	201	4		
7	5H	117	Total	C	N	O	S	0	0
			896	563	160	167	6		
7	5I	27	Total	C	N	O	S	0	0
			198	126	35	36	1		
7	5J	233	Total	C	N	O	S	0	0
			1776	1115	321	330	10		
7	5K	134	Total	C	N	O	S	0	0
			1011	635	184	188	4		
7	5L	125	Total	C	N	O	S	0	0
			958	603	170	179	6		
7	5M	14	Total	C	N	O		0	0
			112	71	18	23			
7	5N	244	Total	C	N	O	S	0	0
			1856	1166	335	345	10		
7	5O	15	Total	C	N	O		0	0
			117	78	20	19			

- Molecule 8 is a protein called Tex33.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1d	101	Total	C	N	O	S	0	0
			808	521	136	148	3		

- Molecule 9 is a protein called C20Orf85.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1f	36	Total	C	N	O		0	0
			339	216	70	53			
9	1g	51	Total	C	N	O	S	0	0
			473	300	91	81	1		

- Molecule 10 is a protein called ATP6V1FNB.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1i	34	Total	C	N	O		0	0
			304	197	52	55			
10	1j	31	Total	C	N	O		0	0
			275	177	48	50			
10	9M	84	Total	C	N	O	S	0	0
			705	453	125	124	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	9N	84	Total	C	N	O	S	0	0
			705	453	125	124	3		
10	9O	41	Total	C	N	O		0	0
			344	222	62	60			

- Molecule 11 is a protein called Tex26(LOC100888047).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1l	39	Total	C	N	O	S	0	0
			300	193	50	55	2		
11	1m	39	Total	C	N	O	S	0	0
			300	193	50	55	2		

- Molecule 12 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1o	29	Total	C	N	O	S	0	0
			252	155	51	44	2		
12	1p	30	Total	C	N	O	S	0	0
			261	160	52	47	2		
12	1q	46	Total	C	N	O	S	0	0
			382	240	69	72	1		
12	1r	27	Total	C	N	O	S	0	0
			235	146	49	38	2		

- Molecule 13 is a protein called Enkurin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2A	250	Total	C	N	O	S	0	0
			2045	1285	363	388	9		
13	2B	251	Total	C	N	O	S	0	0
			2051	1289	366	387	9		
13	2C	251	Total	C	N	O	S	0	0
			2054	1290	365	390	9		
13	2D	79	Total	C	N	O	S	0	0
			637	402	110	123	2		

- Molecule 14 is a protein called CFAP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2G	227	Total	C	N	O	S	0	0
			1874	1159	364	346	5		

- Molecule 15 is a protein called Cilia- and flagella-associated protein 126.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2J	107	Total	C	N	O	S	0	0
			862	534	161	164	3		
15	2K	107	Total	C	N	O	S	0	0
			862	534	161	164	3		
15	2L	107	Total	C	N	O	S	0	0
			862	534	161	164	3		

- Molecule 16 is a protein called Flagellar FliJ protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2O	119	Total	C	N	O	S	0	0
			978	611	184	182	1		

- Molecule 17 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2R	120	Total	C	N	O	S	0	0
			1035	628	200	202	5		
17	2S	376	Total	C	N	O	S	0	0
			3254	1957	631	647	19		

- Molecule 18 is a protein called Cilia- and flagella-associated protein 161.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2V	284	Total	C	N	O	S	0	0
			2215	1382	392	427	14		
18	2W	284	Total	C	N	O	S	0	0
			2215	1382	392	427	14		

- Molecule 19 is a protein called CFA20 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3A	187	Total	C	N	O	S	0	0
			1550	996	273	274	7		
19	3B	187	Total	C	N	O	S	0	0
			1550	996	273	274	7		
19	3C	180	Total	C	N	O	S	0	0
			1496	963	265	261	7		
19	3D	176	Total	C	N	O	S	0	0
			1463	942	259	255	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	3E	186	Total	C	N	O	S	0	0
			1542	990	272	273	7		
19	3F	187	Total	C	N	O	S	0	0
			1550	996	273	274	7		
19	3G	186	Total	C	N	O	S	0	0
			1542	990	272	273	7		

- Molecule 20 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3J	495	Total	C	N	O	S	0	0
			3933	2460	699	763	11		
20	3K	70	Total	C	N	O	S	0	0
			550	340	103	103	4		

- Molecule 21 is a protein called Trichohyalin-plectin-homology domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3N	258	Total	C	N	O	S	0	0
			2126	1306	406	405	9		
21	3O	278	Total	C	N	O	S	0	0
			2329	1429	444	450	6		

- Molecule 22 is a protein called CFAP276.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3R	165	Total	C	N	O	S	0	0
			1317	820	242	252	3		
22	3S	127	Total	C	N	O	S	0	0
			1006	625	191	188	2		
22	3T	165	Total	C	N	O	S	0	0
			1317	820	242	252	3		

- Molecule 23 is a protein called Cilia- and flagella-associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3W	384	Total	C	N	O	S	0	0
			3224	1971	601	640	12		
23	3X	315	Total	C	N	O	S	0	0
			2661	1623	506	523	9		
23	3Y	104	Total	C	N	O	S	0	0
			862	523	168	168	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
23	3Z	172	Total	C	N	O	S	0	0
			1415	865	259	284	7		

- Molecule 24 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4A	617	Total	C	N	O	S	0	0
			4804	3030	841	902	31		
24	4B	615	Total	C	N	O	S	0	0
			4792	3022	839	901	30		
24	4C	617	Total	C	N	O	S	0	0
			4804	3030	841	902	31		

- Molecule 25 is a protein called Trichohyalin-plectin-homology domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4F	313	Total	C	N	O	S	0	0
			2613	1593	502	502	16		
25	4G	206	Total	C	N	O	S	0	0
			1753	1065	343	333	12		

- Molecule 26 is a protein called Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4J	378	Total	C	N	O	S	0	0
			2987	1875	520	569	23		
26	4K	376	Total	C	N	O	S	0	0
			2976	1869	518	566	23		

- Molecule 27 is a protein called Cilia- and flagella-associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4N	151	Total	C	N	O	S	0	0
			1237	772	235	224	6		
27	4O	108	Total	C	N	O	S	0	0
			878	553	162	159	4		
27	4P	150	Total	C	N	O	S	0	0
			1220	761	230	223	6		
27	4Q	93	Total	C	N	O	S	0	0
			744	462	146	133	3		

- Molecule 28 is a protein called Cilia- and flagella-associated protein 97.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4T	143	Total	C	N	O	S	0	0
			1221	767	234	211	9		
28	4U	143	Total	C	N	O	S	0	0
			1221	767	234	211	9		
28	4V	14	Total	C	N	O	S	0	0
			116	77	19	19	1		

- Molecule 29 is a protein called HeLo_like_N(LOC577943).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4Y	300	Total	C	N	O	S	0	0
			2422	1513	448	453	8		

- Molecule 30 is a protein called Outer dense fiber protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5A	35	Total	C	N	O	S	0	0
			265	168	50	46	1		
30	5B	213	Total	C	N	O	S	0	0
			1650	1038	306	299	7		
30	9Y	140	Total	C	N	O	S	0	0
			1083	677	208	193	5		
30	9Z	101	Total	C	N	O	S	0	0
			783	495	145	140	3		

- Molecule 31 is a protein called PACRG.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6A	225	Total	C	N	O	S	0	0
			1792	1151	310	323	8		
31	6B	219	Total	C	N	O	S	0	0
			1737	1116	299	314	8		
31	6C	223	Total	C	N	O	S	0	0
			1769	1139	304	318	8		
31	6D	224	Total	C	N	O	S	0	0
			1784	1147	308	321	8		
31	6E	224	Total	C	N	O	S	0	0
			1784	1147	308	321	8		
31	6F	224	Total	C	N	O	S	0	0
			1784	1147	308	321	8		

- Molecule 32 is a protein called Pierce1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6I	78	Total	C	N	O	S	0	0
			632	397	112	119	4		
32	6J	53	Total	C	N	O	S	0	0
			410	258	69	78	5		

- Molecule 33 is a protein called Protein phosphatase 1 regulatory subunit 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6M	391	Total	C	N	O	S	0	0
			3107	1936	567	593	11		
33	6N	80	Total	C	N	O	S	0	0
			648	406	121	119	2		

- Molecule 34 is a protein called RIB35.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	6Q	201	Total	C	N	O	S	0	0
			1634	1028	292	306	8		
34	6R	72	Total	C	N	O	S	0	0
			598	384	107	104	3		

- Molecule 35 is a protein called RIB43A-like with coiled-coils protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	6U	149	Total	C	N	O	S	0	0
			1242	750	239	249	4		
35	6V	274	Total	C	N	O	S	0	0
			2273	1370	435	458	10		
35	6W	243	Total	C	N	O	S	0	0
			2035	1227	391	408	9		
35	6X	121	Total	C	N	O	S	0	0
			1030	627	200	200	3		

- Molecule 36 is a protein called EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	7A	725	Total	C	N	O	S	0	0
			5901	3763	1025	1093	20		
36	7B	455	Total	C	N	O	S	0	0
			3734	2386	641	694	13		
36	7C	543	Total	C	N	O	S	0	0
			4414	2816	773	810	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
36	7D	724	Total	C	N	O	S	0	0
			5894	3758	1024	1092	20		

- Molecule 37 is a protein called Flagellar protofilament ribbon protein rib74.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	7G	529	Total	C	N	O	S	0	0
			4301	2746	733	805	17		
37	7H	529	Total	C	N	O	S	0	0
			4301	2746	733	805	17		
37	7I	616	Total	C	N	O	S	0	0
			4996	3177	856	942	21		

- Molecule 38 is a protein called SAXO3(LOC115918676).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	7M	263	Total	C	N	O	S	0	0
			2153	1350	401	391	11		
38	7N	68	Total	C	N	O	S	0	0
			527	339	82	101	5		

- Molecule 39 is a protein called TEPP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	7Q	145	Total	C	N	O	S	0	0
			1199	760	220	215	4		
39	7R	142	Total	C	N	O	S	0	0
			1140	713	213	210	4		

- Molecule 40 is a protein called SPATA48.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	7U	93	Total	C	N	O	S	0	0
			755	476	136	134	9		
40	7V	53	Total	C	N	O		0	0
			456	289	89	78			

- Molecule 41 is a protein called Sperm-associated antigen 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	7Y	200	Total	C	N	O	S	0	0
			1593	991	270	327	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	7Z	64	Total	C	N	O	S	0	0
			491	297	89	103	2		

- Molecule 42 is a protein called Testicular haploid expressed gene protein-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	8A	243	Total	C	N	O	S	0	0
			1931	1213	359	354	5		

- Molecule 43 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	8D	397	Total	C	N	O	S	0	0
			3244	1990	594	640	20		
43	8E	178	Total	C	N	O	S	0	0
			1476	906	268	295	7		
43	8F	265	Total	C	N	O	S	0	0
			2142	1309	397	421	15		
43	8G	397	Total	C	N	O	S	0	0
			3244	1990	594	640	20		

- Molecule 44 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	8J	403	Total	C	N	O	S	0	0
			3272	1986	606	668	12		
44	8K	322	Total	C	N	O	S	0	0
			2623	1594	485	534	10		
44	8L	403	Total	C	N	O	S	0	0
			3272	1986	606	668	12		
44	8M	128	Total	C	N	O	S	0	0
			1041	632	190	216	3		
44	8N	17	Total	C	N	O	S	0	0
			144	84	30	29	1		

- Molecule 45 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	8Q	21	Total	C	N	O		0	0
			176	112	34	30			
45	8R	400	Total	C	N	O	S	0	0
			3241	1979	597	650	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	8S	304	Total	C	N	O	S	0	0
			2476	1513	453	499	11		
45	8T	400	Total	C	N	O	S	0	0
			3241	1979	597	650	15		
45	8U	120	Total	C	N	O	S	0	0
			958	584	180	189	5		

- Molecule 46 is a protein called Tex43.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	8X	104	Total	C	N	O	S	0	0
			879	553	164	157	5		
46	8Y	104	Total	C	N	O	S	0	0
			879	553	164	157	5		
46	8Z	104	Total	C	N	O	S	0	0
			879	553	164	157	5		

- Molecule 47 is a protein called Tex36(CFAP95, C9orf135).

Mol	Chain	Residues	Atoms					AltConf	Trace
47	9A	207	Total	C	N	O	S	0	0
			1704	1053	314	334	3		

- Molecule 48 is a protein called CFAP90(C5orf49).

Mol	Chain	Residues	Atoms					AltConf	Trace
48	9D	96	Total	C	N	O	S	0	0
			808	504	157	145	2		

- Molecule 49 is a protein called Tex49.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	9G	150	Total	C	N	O	S	0	0
			1229	787	216	221	5		

- Molecule 50 is a protein called Tex49_homologue(LOC580808).

Mol	Chain	Residues	Atoms					AltConf	Trace
50	9J	101	Total	C	N	O	S	0	0
			822	513	157	147	5		

- Molecule 51 is a protein called CFAP68(UPF0686, C11orf1).

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9R	142	Total	C	N	O	S	0	0
			1166	736	208	220	2		

- Molecule 52 is a protein called SPATA45.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	9T	75	Total	C	N	O	S	0	0
			629	388	119	117	5		

- Molecule 53 is a protein called C4orf45.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	9V	24	Total	C	N	O		0	0
			190	117	39	34			
53	9W	70	Total	C	N	O		0	0
			602	391	107	104			

- Molecule 54 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	AB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	AE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	AG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	AI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	AK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	AM	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	BA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	BB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	BE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	BG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	BI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	BK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	BM	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CM	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DM	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	EA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	EC	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	EE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	EG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	EI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	EK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	HA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	HB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	HE	432	Total	C	N	O	S	0	0
			3382	2144	575	641	22		
54	HG	435	Total	C	N	O	S	0	0
			3406	2160	579	645	22		
54	HI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	HK	435	Total	C	N	O	S	0	0
			3406	2160	579	645	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	IA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	IB	434	Total	C	N	O	S	0	0
			3398	2154	578	644	22		
54	IE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	IG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	II	435	Total	C	N	O	S	0	0
			3402	2156	579	645	22		
54	IK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	IM	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	JA	432	Total	C	N	O	S	0	0
			3387	2148	576	641	22		
54	JB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	JE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	JG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	JI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	JK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	KA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	KB	434	Total	C	N	O	S	0	0
			3398	2154	578	644	22		
54	KE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	KG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	KI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	KK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	LA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	LB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	LE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	LG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	LI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	LK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	MA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	MB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	ME	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	MG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	MI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	MK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	ML	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	NA	435	Total	C	N	O	S	0	0
			3406	2160	579	645	22		
54	NB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	NE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	NG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	NI	434	Total	C	N	O	S	0	0
			3398	2154	578	644	22		
54	NL	433	Total	C	N	O	S	0	0
			3391	2150	577	642	22		
54	OA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	OB	434	Total	C	N	O	S	0	0
			3398	2154	578	644	22		
54	OE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	OG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	OI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	OK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	OL	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	PA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	PB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	PE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	PG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	PI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	PK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	PL	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	QA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	QB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	QE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	QG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	QI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	QK	433	Total	C	N	O	S	0	0
			3391	2150	577	642	22		
54	QL	436	Total	C	N	O	S	0	0
			3410	2162	580	646	22		
54	RA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	RB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	RE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	RG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	RI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	RK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	RL	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SA	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SB	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	TA	436	Total 3410	C 2162	N 580	O 646	S 22	0	0
54	TB	436	Total 3410	C 2162	N 580	O 646	S 22	0	0
54	TE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	TG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	TI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	TK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	UA	436	Total 3410	C 2162	N 580	O 646	S 22	0	0
54	UB	434	Total 3395	C 2152	N 578	O 643	S 22	0	0
54	UE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	UG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	UI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	UK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	VA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	VB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	VE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	VG	435	Total	C	N	O	S	0	0
			3406	2160	579	645	22		
54	VI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	VK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	WA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	WB	436	Total	C	N	O	S	0	0
			3410	2162	580	646	22		
54	WE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	WG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	WI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	WK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		

- Molecule 55 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AC	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	AD	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	AF	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	AH	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	AJ	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	AL	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	BC	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
55	BD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	BF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	BH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	BJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	BL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	EB	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	ED	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	EF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	EH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
55	EJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	EL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	EM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
55	HJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	IC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	ID	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	IF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	IH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	IJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	IL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
55	KL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	NC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	ND	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	NF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	NH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	NJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	NK	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
55	NM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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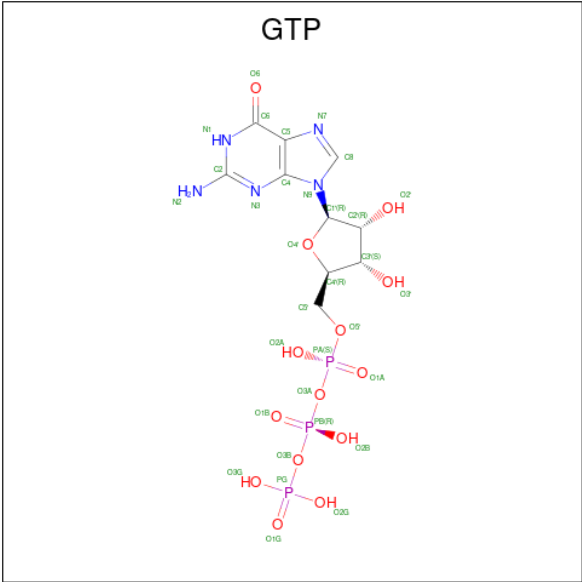
Mol	Chain	Residues	Atoms					AltConf	Trace
55	RF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	UC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	UD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	UF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
55	UH	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	UJ	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	UL	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	UM	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VC	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VD	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VF	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VH	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VJ	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VL	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VM	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WC	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WD	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WF	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WH	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WJ	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WL	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		

- Molecule 56 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
56	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AB	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AI	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AK	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AM	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BA	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BB	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BI	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BK	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BM	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
56	CA	1	Total 32	C 10	N 5	O 14	P 3	0
56	CB	1	Total 32	C 10	N 5	O 14	P 3	0
56	CE	1	Total 32	C 10	N 5	O 14	P 3	0
56	CG	1	Total 32	C 10	N 5	O 14	P 3	0
56	CI	1	Total 32	C 10	N 5	O 14	P 3	0
56	CK	1	Total 32	C 10	N 5	O 14	P 3	0
56	CM	1	Total 32	C 10	N 5	O 14	P 3	0
56	DA	1	Total 32	C 10	N 5	O 14	P 3	0
56	DB	1	Total 32	C 10	N 5	O 14	P 3	0
56	DE	1	Total 32	C 10	N 5	O 14	P 3	0
56	DG	1	Total 32	C 10	N 5	O 14	P 3	0
56	DI	1	Total 32	C 10	N 5	O 14	P 3	0
56	DK	1	Total 32	C 10	N 5	O 14	P 3	0
56	DM	1	Total 32	C 10	N 5	O 14	P 3	0
56	EA	1	Total 32	C 10	N 5	O 14	P 3	0
56	EC	1	Total 32	C 10	N 5	O 14	P 3	0
56	EE	1	Total 32	C 10	N 5	O 14	P 3	0
56	EG	1	Total 32	C 10	N 5	O 14	P 3	0
56	EI	1	Total 32	C 10	N 5	O 14	P 3	0
56	EK	1	Total 32	C 10	N 5	O 14	P 3	0
56	FA	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
56	FB	1	Total 32	C 10	N 5	O 14	P 3	0
56	FE	1	Total 32	C 10	N 5	O 14	P 3	0
56	FG	1	Total 32	C 10	N 5	O 14	P 3	0
56	FI	1	Total 32	C 10	N 5	O 14	P 3	0
56	FK	1	Total 32	C 10	N 5	O 14	P 3	0
56	GA	1	Total 32	C 10	N 5	O 14	P 3	0
56	GB	1	Total 32	C 10	N 5	O 14	P 3	0
56	GE	1	Total 32	C 10	N 5	O 14	P 3	0
56	GG	1	Total 32	C 10	N 5	O 14	P 3	0
56	GI	1	Total 32	C 10	N 5	O 14	P 3	0
56	GK	1	Total 32	C 10	N 5	O 14	P 3	0
56	HA	1	Total 32	C 10	N 5	O 14	P 3	0
56	HB	1	Total 32	C 10	N 5	O 14	P 3	0
56	HE	1	Total 32	C 10	N 5	O 14	P 3	0
56	HG	1	Total 32	C 10	N 5	O 14	P 3	0
56	HI	1	Total 32	C 10	N 5	O 14	P 3	0
56	HK	1	Total 32	C 10	N 5	O 14	P 3	0
56	IA	1	Total 32	C 10	N 5	O 14	P 3	0
56	IB	1	Total 32	C 10	N 5	O 14	P 3	0
56	IE	1	Total 32	C 10	N 5	O 14	P 3	0
56	IG	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
56	II	1	Total 32	C 10	N 5	O 14	P 3	0
56	IK	1	Total 32	C 10	N 5	O 14	P 3	0
56	IM	1	Total 32	C 10	N 5	O 14	P 3	0
56	JA	1	Total 32	C 10	N 5	O 14	P 3	0
56	JB	1	Total 32	C 10	N 5	O 14	P 3	0
56	JE	1	Total 32	C 10	N 5	O 14	P 3	0
56	JG	1	Total 32	C 10	N 5	O 14	P 3	0
56	JI	1	Total 32	C 10	N 5	O 14	P 3	0
56	JK	1	Total 32	C 10	N 5	O 14	P 3	0
56	KA	1	Total 32	C 10	N 5	O 14	P 3	0
56	KB	1	Total 32	C 10	N 5	O 14	P 3	0
56	KE	1	Total 32	C 10	N 5	O 14	P 3	0
56	KG	1	Total 32	C 10	N 5	O 14	P 3	0
56	KI	1	Total 32	C 10	N 5	O 14	P 3	0
56	KK	1	Total 32	C 10	N 5	O 14	P 3	0
56	LA	1	Total 32	C 10	N 5	O 14	P 3	0
56	LB	1	Total 32	C 10	N 5	O 14	P 3	0
56	LE	1	Total 32	C 10	N 5	O 14	P 3	0
56	LG	1	Total 32	C 10	N 5	O 14	P 3	0
56	LI	1	Total 32	C 10	N 5	O 14	P 3	0
56	LK	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
56	MA	1	Total 32	C 10	N 5	O 14	P 3	0
56	MB	1	Total 32	C 10	N 5	O 14	P 3	0
56	ME	1	Total 32	C 10	N 5	O 14	P 3	0
56	MG	1	Total 32	C 10	N 5	O 14	P 3	0
56	MI	1	Total 32	C 10	N 5	O 14	P 3	0
56	MK	1	Total 32	C 10	N 5	O 14	P 3	0
56	ML	1	Total 32	C 10	N 5	O 14	P 3	0
56	NA	1	Total 32	C 10	N 5	O 14	P 3	0
56	NB	1	Total 32	C 10	N 5	O 14	P 3	0
56	NE	1	Total 32	C 10	N 5	O 14	P 3	0
56	NG	1	Total 32	C 10	N 5	O 14	P 3	0
56	NI	1	Total 32	C 10	N 5	O 14	P 3	0
56	NL	1	Total 32	C 10	N 5	O 14	P 3	0
56	OA	1	Total 32	C 10	N 5	O 14	P 3	0
56	OB	1	Total 32	C 10	N 5	O 14	P 3	0
56	OE	1	Total 32	C 10	N 5	O 14	P 3	0
56	OG	1	Total 32	C 10	N 5	O 14	P 3	0
56	OI	1	Total 32	C 10	N 5	O 14	P 3	0
56	OK	1	Total 32	C 10	N 5	O 14	P 3	0
56	OL	1	Total 32	C 10	N 5	O 14	P 3	0
56	PA	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
56	PB	1	Total 32	C 10	N 5	O 14	P 3	0
56	PE	1	Total 32	C 10	N 5	O 14	P 3	0
56	PG	1	Total 32	C 10	N 5	O 14	P 3	0
56	PI	1	Total 32	C 10	N 5	O 14	P 3	0
56	PK	1	Total 32	C 10	N 5	O 14	P 3	0
56	PL	1	Total 32	C 10	N 5	O 14	P 3	0
56	QA	1	Total 32	C 10	N 5	O 14	P 3	0
56	QB	1	Total 32	C 10	N 5	O 14	P 3	0
56	QE	1	Total 32	C 10	N 5	O 14	P 3	0
56	QG	1	Total 32	C 10	N 5	O 14	P 3	0
56	QI	1	Total 32	C 10	N 5	O 14	P 3	0
56	QK	1	Total 32	C 10	N 5	O 14	P 3	0
56	QL	1	Total 32	C 10	N 5	O 14	P 3	0
56	RA	1	Total 32	C 10	N 5	O 14	P 3	0
56	RB	1	Total 32	C 10	N 5	O 14	P 3	0
56	RE	1	Total 32	C 10	N 5	O 14	P 3	0
56	RG	1	Total 32	C 10	N 5	O 14	P 3	0
56	RI	1	Total 32	C 10	N 5	O 14	P 3	0
56	RK	1	Total 32	C 10	N 5	O 14	P 3	0
56	RL	1	Total 32	C 10	N 5	O 14	P 3	0
56	SA	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
56	SB	1	Total 32	C 10	N 5	O 14	P 3	0
56	SE	1	Total 32	C 10	N 5	O 14	P 3	0
56	SG	1	Total 32	C 10	N 5	O 14	P 3	0
56	SI	1	Total 32	C 10	N 5	O 14	P 3	0
56	SK	1	Total 32	C 10	N 5	O 14	P 3	0
56	TA	1	Total 32	C 10	N 5	O 14	P 3	0
56	TB	1	Total 32	C 10	N 5	O 14	P 3	0
56	TE	1	Total 32	C 10	N 5	O 14	P 3	0
56	TG	1	Total 32	C 10	N 5	O 14	P 3	0
56	TI	1	Total 32	C 10	N 5	O 14	P 3	0
56	TK	1	Total 32	C 10	N 5	O 14	P 3	0
56	UA	1	Total 32	C 10	N 5	O 14	P 3	0
56	UB	1	Total 32	C 10	N 5	O 14	P 3	0
56	UE	1	Total 32	C 10	N 5	O 14	P 3	0
56	UG	1	Total 32	C 10	N 5	O 14	P 3	0
56	UI	1	Total 32	C 10	N 5	O 14	P 3	0
56	UK	1	Total 32	C 10	N 5	O 14	P 3	0
56	VA	1	Total 32	C 10	N 5	O 14	P 3	0
56	VB	1	Total 32	C 10	N 5	O 14	P 3	0
56	VE	1	Total 32	C 10	N 5	O 14	P 3	0
56	VG	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
56	VI	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	VK	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	WA	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	WB	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	WE	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	WG	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	WI	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	WK	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
57	AA	1	Total	Mg	0
			1	1	
57	AB	1	Total	Mg	0
			1	1	
57	AE	1	Total	Mg	0
			1	1	
57	AG	1	Total	Mg	0
			1	1	
57	AI	1	Total	Mg	0
			1	1	
57	AK	1	Total	Mg	0
			1	1	
57	AM	1	Total	Mg	0
			1	1	
57	BA	1	Total	Mg	0
			1	1	
57	BB	1	Total	Mg	0
			1	1	
57	BE	1	Total	Mg	0
			1	1	
57	BG	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	BI	1	1	1	0
57	BK	1	1	1	0
57	BM	1	1	1	0
57	CA	1	1	1	0
57	CB	1	1	1	0
57	CE	1	1	1	0
57	CG	1	1	1	0
57	CI	1	1	1	0
57	CK	1	1	1	0
57	CM	1	1	1	0
57	DA	1	1	1	0
57	DB	1	1	1	0
57	DE	1	1	1	0
57	DG	1	1	1	0
57	DI	1	1	1	0
57	DK	1	1	1	0
57	DM	1	1	1	0
57	EA	1	1	1	0
57	EC	1	1	1	0
57	EE	1	1	1	0
57	EG	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
57	EI	1	Total 1	Mg 1	0
57	EK	1	Total 1	Mg 1	0
57	FA	1	Total 1	Mg 1	0
57	FB	1	Total 1	Mg 1	0
57	FE	1	Total 1	Mg 1	0
57	FG	1	Total 1	Mg 1	0
57	FI	1	Total 1	Mg 1	0
57	FK	1	Total 1	Mg 1	0
57	GA	1	Total 1	Mg 1	0
57	GB	1	Total 1	Mg 1	0
57	GE	1	Total 1	Mg 1	0
57	GG	1	Total 1	Mg 1	0
57	GI	1	Total 1	Mg 1	0
57	GK	1	Total 1	Mg 1	0
57	HA	1	Total 1	Mg 1	0
57	HB	1	Total 1	Mg 1	0
57	HE	1	Total 1	Mg 1	0
57	HG	1	Total 1	Mg 1	0
57	HI	1	Total 1	Mg 1	0
57	HK	1	Total 1	Mg 1	0
57	IA	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
57	IB	1	Total 1	Mg 1	0
57	IE	1	Total 1	Mg 1	0
57	IG	1	Total 1	Mg 1	0
57	II	1	Total 1	Mg 1	0
57	IK	1	Total 1	Mg 1	0
57	IM	1	Total 1	Mg 1	0
57	JA	1	Total 1	Mg 1	0
57	JB	1	Total 1	Mg 1	0
57	JE	1	Total 1	Mg 1	0
57	JG	1	Total 1	Mg 1	0
57	JI	1	Total 1	Mg 1	0
57	JK	1	Total 1	Mg 1	0
57	KA	1	Total 1	Mg 1	0
57	KB	1	Total 1	Mg 1	0
57	KE	1	Total 1	Mg 1	0
57	KG	1	Total 1	Mg 1	0
57	KI	1	Total 1	Mg 1	0
57	KK	1	Total 1	Mg 1	0
57	LA	1	Total 1	Mg 1	0
57	LB	1	Total 1	Mg 1	0
57	LE	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
57	LG	1	Total 1	Mg 1	0
57	LI	1	Total 1	Mg 1	0
57	LK	1	Total 1	Mg 1	0
57	MA	1	Total 1	Mg 1	0
57	MB	1	Total 1	Mg 1	0
57	ME	1	Total 1	Mg 1	0
57	MG	1	Total 1	Mg 1	0
57	MI	1	Total 1	Mg 1	0
57	MK	1	Total 1	Mg 1	0
57	ML	1	Total 1	Mg 1	0
57	NA	1	Total 1	Mg 1	0
57	NB	1	Total 1	Mg 1	0
57	NE	1	Total 1	Mg 1	0
57	NG	1	Total 1	Mg 1	0
57	NI	1	Total 1	Mg 1	0
57	NL	1	Total 1	Mg 1	0
57	OA	1	Total 1	Mg 1	0
57	OB	1	Total 1	Mg 1	0
57	OE	1	Total 1	Mg 1	0
57	OG	1	Total 1	Mg 1	0
57	OI	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
57	OK	1	Total 1	Mg 1	0
57	OL	1	Total 1	Mg 1	0
57	PA	1	Total 1	Mg 1	0
57	PB	1	Total 1	Mg 1	0
57	PE	1	Total 1	Mg 1	0
57	PG	1	Total 1	Mg 1	0
57	PI	1	Total 1	Mg 1	0
57	PK	1	Total 1	Mg 1	0
57	PL	1	Total 1	Mg 1	0
57	QA	1	Total 1	Mg 1	0
57	QB	1	Total 1	Mg 1	0
57	QE	1	Total 1	Mg 1	0
57	QG	1	Total 1	Mg 1	0
57	QI	1	Total 1	Mg 1	0
57	QK	1	Total 1	Mg 1	0
57	QL	1	Total 1	Mg 1	0
57	RA	1	Total 1	Mg 1	0
57	RB	1	Total 1	Mg 1	0
57	RE	1	Total 1	Mg 1	0
57	RG	1	Total 1	Mg 1	0
57	RI	1	Total 1	Mg 1	0

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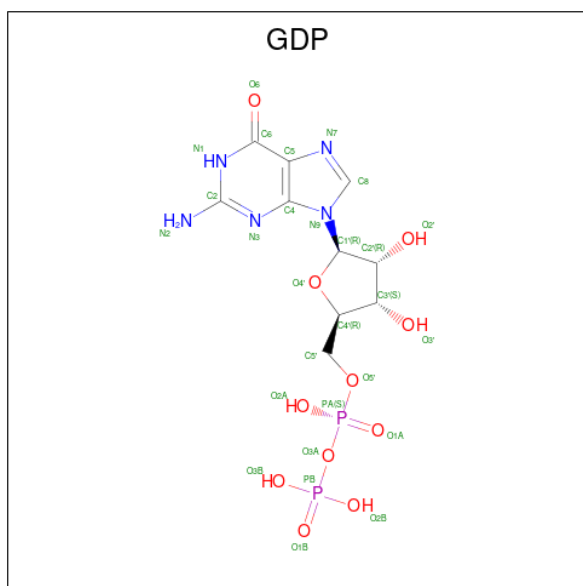
Mol	Chain	Residues	Atoms		AltConf
57	RK	1	Total 1	Mg 1	0
57	RL	1	Total 1	Mg 1	0
57	SA	1	Total 1	Mg 1	0
57	SB	1	Total 1	Mg 1	0
57	SE	1	Total 1	Mg 1	0
57	SG	1	Total 1	Mg 1	0
57	SI	1	Total 1	Mg 1	0
57	SK	1	Total 1	Mg 1	0
57	TA	1	Total 1	Mg 1	0
57	TB	1	Total 1	Mg 1	0
57	TE	1	Total 1	Mg 1	0
57	TG	1	Total 1	Mg 1	0
57	TI	1	Total 1	Mg 1	0
57	TK	1	Total 1	Mg 1	0
57	UA	1	Total 1	Mg 1	0
57	UB	1	Total 1	Mg 1	0
57	UE	1	Total 1	Mg 1	0
57	UG	1	Total 1	Mg 1	0
57	UI	1	Total 1	Mg 1	0
57	UK	1	Total 1	Mg 1	0
57	VA	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
57	VB	1	Total	Mg	0
			1	1	
57	VE	1	Total	Mg	0
			1	1	
57	VG	1	Total	Mg	0
			1	1	
57	VI	1	Total	Mg	0
			1	1	
57	VK	1	Total	Mg	0
			1	1	
57	WA	1	Total	Mg	0
			1	1	
57	WB	1	Total	Mg	0
			1	1	
57	WE	1	Total	Mg	0
			1	1	
57	WG	1	Total	Mg	0
			1	1	
57	WI	1	Total	Mg	0
			1	1	
57	WK	1	Total	Mg	0
			1	1	

- Molecule 58 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
58	AC	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	AD	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	AF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	AH	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	AJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	AL	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BC	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BD	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BH	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	BL	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CC	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CH	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	CL	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	DC	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	DD	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	DF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	DH	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
58	DJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	DL	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	EB	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	ED	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	EF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	EH	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	EJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	EL	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	EM	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	FC	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	FD	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	FF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	FH	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	FJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	FL	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	FM	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	GC	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	GD	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	GF	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	GH	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	GJ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
58	GL	1	Total 28	C 10	N 5	O 11	P 2	0
58	GM	1	Total 28	C 10	N 5	O 11	P 2	0
58	HC	1	Total 28	C 10	N 5	O 11	P 2	0
58	HD	1	Total 28	C 10	N 5	O 11	P 2	0
58	HF	1	Total 28	C 10	N 5	O 11	P 2	0
58	HH	1	Total 28	C 10	N 5	O 11	P 2	0
58	HJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	HL	1	Total 28	C 10	N 5	O 11	P 2	0
58	HM	1	Total 28	C 10	N 5	O 11	P 2	0
58	IC	1	Total 28	C 10	N 5	O 11	P 2	0
58	ID	1	Total 28	C 10	N 5	O 11	P 2	0
58	IF	1	Total 28	C 10	N 5	O 11	P 2	0
58	IH	1	Total 28	C 10	N 5	O 11	P 2	0
58	IJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	IL	1	Total 28	C 10	N 5	O 11	P 2	0
58	JC	1	Total 28	C 10	N 5	O 11	P 2	0
58	JD	1	Total 28	C 10	N 5	O 11	P 2	0
58	JF	1	Total 28	C 10	N 5	O 11	P 2	0
58	JH	1	Total 28	C 10	N 5	O 11	P 2	0
58	JJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	JL	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
58	JM	1	Total 28	C 10	N 5	O 11	P 2	0
58	KC	1	Total 28	C 10	N 5	O 11	P 2	0
58	KD	1	Total 28	C 10	N 5	O 11	P 2	0
58	KF	1	Total 28	C 10	N 5	O 11	P 2	0
58	KH	1	Total 28	C 10	N 5	O 11	P 2	0
58	KJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	KL	1	Total 28	C 10	N 5	O 11	P 2	0
58	KM	1	Total 28	C 10	N 5	O 11	P 2	0
58	LC	1	Total 28	C 10	N 5	O 11	P 2	0
58	LD	1	Total 28	C 10	N 5	O 11	P 2	0
58	LF	1	Total 28	C 10	N 5	O 11	P 2	0
58	LH	1	Total 28	C 10	N 5	O 11	P 2	0
58	LJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	LL	1	Total 28	C 10	N 5	O 11	P 2	0
58	LM	1	Total 28	C 10	N 5	O 11	P 2	0
58	MC	1	Total 28	C 10	N 5	O 11	P 2	0
58	MD	1	Total 28	C 10	N 5	O 11	P 2	0
58	MF	1	Total 28	C 10	N 5	O 11	P 2	0
58	MH	1	Total 28	C 10	N 5	O 11	P 2	0
58	MJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	MM	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
58	NC	1	Total 28	C 10	N 5	O 11	P 2	0
58	ND	1	Total 28	C 10	N 5	O 11	P 2	0
58	NF	1	Total 28	C 10	N 5	O 11	P 2	0
58	NH	1	Total 28	C 10	N 5	O 11	P 2	0
58	NJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	NK	1	Total 28	C 10	N 5	O 11	P 2	0
58	NM	1	Total 28	C 10	N 5	O 11	P 2	0
58	OC	1	Total 28	C 10	N 5	O 11	P 2	0
58	OD	1	Total 28	C 10	N 5	O 11	P 2	0
58	OF	1	Total 28	C 10	N 5	O 11	P 2	0
58	OH	1	Total 28	C 10	N 5	O 11	P 2	0
58	OJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	OM	1	Total 28	C 10	N 5	O 11	P 2	0
58	PC	1	Total 28	C 10	N 5	O 11	P 2	0
58	PD	1	Total 28	C 10	N 5	O 11	P 2	0
58	PF	1	Total 28	C 10	N 5	O 11	P 2	0
58	PH	1	Total 28	C 10	N 5	O 11	P 2	0
58	PJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	PM	1	Total 28	C 10	N 5	O 11	P 2	0
58	QC	1	Total 28	C 10	N 5	O 11	P 2	0
58	QD	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
58	QF	1	Total 28	C 10	N 5	O 11	P 2	0
58	QH	1	Total 28	C 10	N 5	O 11	P 2	0
58	QJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	QM	1	Total 28	C 10	N 5	O 11	P 2	0
58	RC	1	Total 28	C 10	N 5	O 11	P 2	0
58	RD	1	Total 28	C 10	N 5	O 11	P 2	0
58	RF	1	Total 28	C 10	N 5	O 11	P 2	0
58	RH	1	Total 28	C 10	N 5	O 11	P 2	0
58	RJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	RM	1	Total 28	C 10	N 5	O 11	P 2	0
58	SC	1	Total 28	C 10	N 5	O 11	P 2	0
58	SD	1	Total 28	C 10	N 5	O 11	P 2	0
58	SF	1	Total 28	C 10	N 5	O 11	P 2	0
58	SH	1	Total 28	C 10	N 5	O 11	P 2	0
58	SJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	SL	1	Total 28	C 10	N 5	O 11	P 2	0
58	SM	1	Total 28	C 10	N 5	O 11	P 2	0
58	TC	1	Total 28	C 10	N 5	O 11	P 2	0
58	TD	1	Total 28	C 10	N 5	O 11	P 2	0
58	TF	1	Total 28	C 10	N 5	O 11	P 2	0
58	TH	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
58	TJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	TL	1	Total 28	C 10	N 5	O 11	P 2	0
58	TM	1	Total 28	C 10	N 5	O 11	P 2	0
58	UC	1	Total 28	C 10	N 5	O 11	P 2	0
58	UD	1	Total 28	C 10	N 5	O 11	P 2	0
58	UF	1	Total 28	C 10	N 5	O 11	P 2	0
58	UH	1	Total 28	C 10	N 5	O 11	P 2	0
58	UJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	UL	1	Total 28	C 10	N 5	O 11	P 2	0
58	UM	1	Total 28	C 10	N 5	O 11	P 2	0
58	VC	1	Total 28	C 10	N 5	O 11	P 2	0
58	VD	1	Total 28	C 10	N 5	O 11	P 2	0
58	VF	1	Total 28	C 10	N 5	O 11	P 2	0
58	VH	1	Total 28	C 10	N 5	O 11	P 2	0
58	VJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	VL	1	Total 28	C 10	N 5	O 11	P 2	0
58	VM	1	Total 28	C 10	N 5	O 11	P 2	0
58	WC	1	Total 28	C 10	N 5	O 11	P 2	0
58	WD	1	Total 28	C 10	N 5	O 11	P 2	0
58	WF	1	Total 28	C 10	N 5	O 11	P 2	0
58	WH	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
58	WJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
58	WL	1	Total	C	N	O	P	0
			28	10	5	11	2	

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, Not provided	
Number of particles used	127673	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	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 446 ligands modelled in this entry, 148 are monoatomic - leaving 298 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
56	GTP	UE	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
56	GTP	HE	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)
56	GTP	PE	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
58	GDP	FD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	DE	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.57	8 (16%)
58	GDP	KD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	QH	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.71	8 (17%)
58	GDP	QM	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
58	GDP	TF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
58	GDP	PH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	HH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	PC	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	PF	501	-	29,30,30	1.10	2 (6%)	45,47,47	2.06	9 (20%)
58	GDP	SJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	HG	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	8 (16%)
56	GTP	BG	501	57	33,34,34	1.00	2 (6%)	50,54,54	1.61	10 (20%)
56	GTP	UK	501	57	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	KA	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
58	GDP	CF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	GD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
58	GDP	MJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	KL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	NF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	6 (13%)
58	GDP	OC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
58	GDP	TL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	VM	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	EM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	5 (11%)
56	GTP	CG	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.55	8 (16%)
56	GTP	SG	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
58	GDP	VL	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.65	4 (8%)
56	GTP	ML	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	QK	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	GTP	QI	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
56	GTP	TA	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.61	9 (18%)
56	GTP	VI	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	HL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
56	GTP	OB	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	VA	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
58	GDP	WF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	CA	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
58	GDP	VH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	7 (15%)
58	GDP	FC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
56	GTP	FA	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
58	GDP	AL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	BD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	CB	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
58	GDP	BF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
58	GDP	MD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	FI	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.61	9 (18%)
58	GDP	KC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	NI	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	CK	501	-	33,34,34	1.00	3 (9%)	50,54,54	1.59	10 (20%)
56	GTP	OI	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	VG	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
58	GDP	AF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
58	GDP	PJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
58	GDP	UF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
58	GDP	TH	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
56	GTP	EE	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
56	GTP	UB	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	8 (16%)
58	GDP	CD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	BH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	DB	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	IG	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	IB	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
58	GDP	JM	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
58	GDP	NC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	GDP	KH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	TI	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.55	9 (18%)
56	GTP	RE	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.56	8 (16%)
58	GDP	FF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	7 (15%)
56	GTP	OE	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.59	8 (16%)
58	GDP	RF	501	-	29,30,30	1.13	4 (13%)	45,47,47	1.66	6 (13%)
56	GTP	PI	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
56	GTP	DI	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
58	GDP	EL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	6 (13%)
56	GTP	OG	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	GJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	IF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	II	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
58	GDP	OM	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	8 (17%)
56	GTP	LI	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	SE	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.60	8 (16%)
58	GDP	MM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
56	GTP	EC	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
58	GDP	RM	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.80	8 (17%)
56	GTP	WE	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
58	GDP	OH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	OL	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
58	GDP	SL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
58	GDP	DF	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.65	6 (13%)
56	GTP	KI	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
58	GDP	FJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
56	GTP	SK	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.59	8 (16%)
58	GDP	WL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
56	GTP	PB	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.61	9 (18%)
58	GDP	CL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	QA	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)
58	GDP	NK	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	BI	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	PG	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	RA	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.56	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	GDP	BJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	SI	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.57	8 (16%)
56	GTP	JK	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)
56	GTP	GE	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.56	9 (18%)
58	GDP	BC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
58	GDP	EB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
58	GDP	HF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	HB	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	MA	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	SB	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.56	9 (18%)
56	GTP	VE	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
58	GDP	IC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.81	7 (15%)
58	GDP	ID	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	6 (13%)
58	GDP	IL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	RJ	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.79	6 (13%)
56	GTP	CM	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	TJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
56	GTP	FK	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
56	GTP	CE	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	8 (16%)
58	GDP	QJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
58	GDP	RD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
58	GDP	JJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	TB	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	BB	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
56	GTP	TK	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
58	GDP	HM	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.78	7 (15%)
58	GDP	MH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	PM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	DD	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.70	6 (13%)
56	GTP	TE	501	57	33,34,34	0.88	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	FG	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
58	GDP	SF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	7 (15%)
58	GDP	VJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
58	GDP	LM	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
56	GTP	AK	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	GTP	MI	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
56	GTP	AB	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	VK	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	WA	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	DJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.82	7 (15%)
58	GDP	DL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
56	GTP	OK	501	57	33,34,34	0.89	1 (3%)	50,54,54	1.56	9 (18%)
58	GDP	PD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
58	GDP	SD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
56	GTP	NE	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	IK	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
58	GDP	WD	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	7 (15%)
58	GDP	MF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	MB	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	NB	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	LG	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	DC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	SM	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
58	GDP	WC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	JG	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
58	GDP	LL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	6 (13%)
58	GDP	QD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
58	GDP	KF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
58	GDP	JC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
58	GDP	MC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	EJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	RG	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	TM	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.78	7 (15%)
58	GDP	NM	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
56	GTP	JB	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	PK	501	57	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	IE	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)
58	GDP	EH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	DM	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
58	GDP	FL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	GTP	EK	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
58	GDP	GH	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	7 (15%)
56	GTP	WI	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	OF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	VC	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	DG	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
58	GDP	UM	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	BM	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.59	10 (20%)
56	GTP	DK	501	57	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	JE	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
58	GDP	GC	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
56	GTP	AG	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
58	GDP	IH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	NG	501	57	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	LE	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
58	GDP	AJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
58	GDP	IJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	BA	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	RK	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	CJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
56	GTP	GI	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
56	GTP	BK	501	57	33,34,34	0.99	2 (6%)	50,54,54	1.60	10 (20%)
56	GTP	UI	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
58	GDP	GM	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
58	GDP	KM	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	FM	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
58	GDP	NJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
58	GDP	ND	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	QF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
58	GDP	RC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
58	GDP	CC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	PA	501	57	33,34,34	0.96	2 (6%)	50,54,54	1.56	9 (18%)
56	GTP	NA	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	LF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	NH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	GDP	UD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	7 (15%)
58	GDP	GL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	6 (13%)
58	GDP	RH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	AI	501	57	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	JI	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.56	8 (16%)
58	GDP	LD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	HI	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	QE	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
56	GTP	WB	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
58	GDP	HC	501	-	29,30,30	1.21	4 (13%)	45,47,47	1.65	7 (15%)
56	GTP	DA	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.55	8 (16%)
56	GTP	EA	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
58	GDP	WH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	IM	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.59	8 (16%)
56	GTP	KB	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
56	GTP	LK	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
56	GTP	QL	501	57	33,34,34	0.99	4 (12%)	50,54,54	1.64	9 (18%)
56	GTP	WG	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
58	GDP	UH	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	6 (13%)
58	GDP	JD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	WJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
56	GTP	LB	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	NL	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
58	GDP	JH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	5 (11%)
58	GDP	GF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	TG	501	57	33,34,34	0.95	2 (6%)	50,54,54	1.63	8 (16%)
58	GDP	AD	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.73	7 (15%)
58	GDP	HD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	UC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	ME	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.58	8 (16%)
58	GDP	VF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	LC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	HK	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
58	GDP	OJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	OD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	GTP	EG	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	8 (16%)
56	GTP	AA	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	HA	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	KE	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	QB	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
56	GTP	CI	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	GK	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	UG	501	57	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
56	GTP	VB	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	MK	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	ED	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	7 (15%)
58	GDP	TD	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	LH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
56	GTP	GA	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.60	9 (18%)
56	GTP	KK	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.57	8 (16%)
58	GDP	UL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
56	GTP	WK	501	57	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	FE	501	57	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	JA	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	UJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	VD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	8 (17%)
56	GTP	IA	501	57	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	JF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
56	GTP	BE	501	57	33,34,34	0.88	1 (3%)	50,54,54	1.64	9 (18%)
58	GDP	CH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
58	GDP	SH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
56	GTP	RB	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
56	GTP	RL	501	57	33,34,34	1.01	2 (6%)	50,54,54	1.59	9 (18%)
58	GDP	SC	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	BL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	AM	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
58	GDP	QC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	HJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
56	GTP	GB	501	57	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	MG	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	GTP	LA	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.58	8 (16%)
56	GTP	OA	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	SA	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
56	GTP	UA	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
58	GDP	EF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	7 (15%)
58	GDP	JL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.65	5 (11%)
56	GTP	GG	501	57	33,34,34	0.90	1 (3%)	50,54,54	1.57	9 (18%)
56	GTP	QG	501	57	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
58	GDP	TC	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
58	GDP	DH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
58	GDP	FH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
56	GTP	FB	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
56	GTP	PL	501	57	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
58	GDP	AC	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
58	GDP	KJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
56	GTP	EI	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
58	GDP	AH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	RI	501	57	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
58	GDP	LJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
56	GTP	KG	501	57	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
56	GTP	AE	501	57	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)

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
56	GTP	UE	501	57	-	4/22/38/38	0/3/3/3
56	GTP	HE	501	57	-	6/22/38/38	0/3/3/3
56	GTP	PE	501	57	-	3/22/38/38	0/3/3/3
58	GDP	FD	501	-	-	1/16/32/32	0/3/3/3
56	GTP	DE	501	57	-	3/22/38/38	0/3/3/3
58	GDP	KD	501	-	-	2/16/32/32	0/3/3/3
58	GDP	QH	501	-	-	5/16/32/32	0/3/3/3
58	GDP	QM	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	TF	501	-	-	1/16/32/32	0/3/3/3
58	GDP	PH	501	-	-	2/16/32/32	0/3/3/3
58	GDP	HH	501	-	-	1/16/32/32	0/3/3/3
58	GDP	PC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	PF	501	-	-	1/16/32/32	0/3/3/3
58	GDP	SJ	501	-	-	2/16/32/32	0/3/3/3
56	GTP	HG	501	57	-	3/22/38/38	0/3/3/3
56	GTP	BG	501	57	-	8/22/38/38	0/3/3/3
56	GTP	UK	501	57	-	9/22/38/38	0/3/3/3
56	GTP	KA	501	57	-	2/22/38/38	0/3/3/3
58	GDP	CF	501	-	-	2/16/32/32	0/3/3/3
58	GDP	GD	501	-	-	1/16/32/32	0/3/3/3
58	GDP	MJ	501	-	-	3/16/32/32	0/3/3/3
58	GDP	KL	501	-	-	2/16/32/32	0/3/3/3
58	GDP	NF	501	-	-	2/16/32/32	0/3/3/3
58	GDP	OC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	TL	501	-	-	2/16/32/32	0/3/3/3
58	GDP	VM	501	-	-	2/16/32/32	0/3/3/3
58	GDP	EM	501	-	-	2/16/32/32	0/3/3/3
56	GTP	CG	501	57	-	4/22/38/38	0/3/3/3
56	GTP	SG	501	57	-	7/22/38/38	0/3/3/3
58	GDP	VL	501	-	-	5/16/32/32	0/3/3/3
56	GTP	ML	501	57	-	3/22/38/38	0/3/3/3
56	GTP	QK	501	57	-	3/22/38/38	0/3/3/3
56	GTP	QI	501	57	-	2/22/38/38	0/3/3/3
56	GTP	TA	501	57	-	8/22/38/38	0/3/3/3
56	GTP	VI	501	57	-	3/22/38/38	0/3/3/3
58	GDP	HL	501	-	-	3/16/32/32	0/3/3/3
56	GTP	OB	501	57	-	3/22/38/38	0/3/3/3
56	GTP	VA	501	57	-	3/22/38/38	0/3/3/3
58	GDP	WF	501	-	-	2/16/32/32	0/3/3/3
56	GTP	CA	501	57	-	3/22/38/38	0/3/3/3
58	GDP	VH	501	-	-	3/16/32/32	0/3/3/3
58	GDP	FC	501	-	-	2/16/32/32	0/3/3/3
56	GTP	FA	501	57	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	AL	501	-	-	2/16/32/32	0/3/3/3
58	GDP	BD	501	-	-	3/16/32/32	0/3/3/3
56	GTP	CB	501	57	-	2/22/38/38	0/3/3/3
58	GDP	BF	501	-	-	1/16/32/32	0/3/3/3
58	GDP	MD	501	-	-	1/16/32/32	0/3/3/3
56	GTP	FI	501	57	-	3/22/38/38	0/3/3/3
58	GDP	KC	501	-	-	2/16/32/32	0/3/3/3
56	GTP	NI	501	57	-	6/22/38/38	0/3/3/3
56	GTP	CK	501	-	-	7/22/38/38	0/3/3/3
56	GTP	OI	501	57	-	4/22/38/38	0/3/3/3
56	GTP	VG	501	57	-	4/22/38/38	0/3/3/3
58	GDP	AF	501	-	-	2/16/32/32	0/3/3/3
58	GDP	PJ	501	-	-	2/16/32/32	0/3/3/3
58	GDP	UF	501	-	-	2/16/32/32	0/3/3/3
58	GDP	TH	501	-	-	2/16/32/32	0/3/3/3
56	GTP	EE	501	57	-	1/22/38/38	0/3/3/3
56	GTP	UB	501	57	-	3/22/38/38	0/3/3/3
58	GDP	CD	501	-	-	3/16/32/32	0/3/3/3
58	GDP	BH	501	-	-	1/16/32/32	0/3/3/3
56	GTP	DB	501	57	-	1/22/38/38	0/3/3/3
56	GTP	IG	501	57	-	6/22/38/38	0/3/3/3
56	GTP	IB	501	57	-	5/22/38/38	0/3/3/3
58	GDP	JM	501	-	-	1/16/32/32	0/3/3/3
58	GDP	NC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	KH	501	-	-	2/16/32/32	0/3/3/3
56	GTP	TI	501	57	-	7/22/38/38	0/3/3/3
56	GTP	RE	501	57	-	3/22/38/38	0/3/3/3
58	GDP	FF	501	-	-	2/16/32/32	0/3/3/3
56	GTP	OE	501	57	-	7/22/38/38	0/3/3/3
58	GDP	RF	501	-	-	5/16/32/32	0/3/3/3
56	GTP	PI	501	57	-	3/22/38/38	0/3/3/3
56	GTP	DI	501	57	-	2/22/38/38	0/3/3/3
58	GDP	EL	501	-	-	1/16/32/32	0/3/3/3
56	GTP	OG	501	57	-	3/22/38/38	0/3/3/3
58	GDP	GJ	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	IF	501	-	-	2/16/32/32	0/3/3/3
56	GTP	II	501	57	-	8/22/38/38	0/3/3/3
58	GDP	OM	501	-	-	2/16/32/32	0/3/3/3
56	GTP	LI	501	57	-	2/22/38/38	0/3/3/3
56	GTP	SE	501	57	-	6/22/38/38	0/3/3/3
58	GDP	MM	501	-	-	2/16/32/32	0/3/3/3
56	GTP	EC	501	57	-	3/22/38/38	0/3/3/3
58	GDP	RM	501	-	-	2/16/32/32	0/3/3/3
56	GTP	WE	501	57	-	4/22/38/38	0/3/3/3
58	GDP	OH	501	-	-	2/16/32/32	0/3/3/3
56	GTP	OL	501	57	-	7/22/38/38	0/3/3/3
58	GDP	SL	501	-	-	2/16/32/32	0/3/3/3
58	GDP	DF	501	-	-	1/16/32/32	0/3/3/3
56	GTP	KI	501	57	-	1/22/38/38	0/3/3/3
58	GDP	FJ	501	-	-	2/16/32/32	0/3/3/3
56	GTP	SK	501	57	-	3/22/38/38	0/3/3/3
58	GDP	WL	501	-	-	1/16/32/32	0/3/3/3
56	GTP	PB	501	57	-	3/22/38/38	0/3/3/3
58	GDP	CL	501	-	-	2/16/32/32	0/3/3/3
56	GTP	QA	501	57	-	6/22/38/38	0/3/3/3
58	GDP	NK	501	-	-	1/16/32/32	0/3/3/3
56	GTP	BI	501	57	-	7/22/38/38	0/3/3/3
56	GTP	PG	501	57	-	7/22/38/38	0/3/3/3
56	GTP	RA	501	57	-	3/22/38/38	0/3/3/3
58	GDP	BJ	501	-	-	2/16/32/32	0/3/3/3
56	GTP	SI	501	57	-	2/22/38/38	0/3/3/3
56	GTP	JK	501	57	-	8/22/38/38	0/3/3/3
56	GTP	GE	501	57	-	2/22/38/38	0/3/3/3
58	GDP	BC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	EB	501	-	-	1/16/32/32	0/3/3/3
58	GDP	HF	501	-	-	2/16/32/32	0/3/3/3
56	GTP	HB	501	57	-	3/22/38/38	0/3/3/3
56	GTP	MA	501	57	-	3/22/38/38	0/3/3/3
56	GTP	SB	501	57	-	1/22/38/38	0/3/3/3
56	GTP	VE	501	57	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	IC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	ID	501	-	-	2/16/32/32	0/3/3/3
58	GDP	IL	501	-	-	2/16/32/32	0/3/3/3
58	GDP	RJ	501	-	-	1/16/32/32	0/3/3/3
56	GTP	CM	501	57	-	4/22/38/38	0/3/3/3
58	GDP	TJ	501	-	-	1/16/32/32	0/3/3/3
56	GTP	FK	501	57	-	7/22/38/38	0/3/3/3
56	GTP	CE	501	57	-	3/22/38/38	0/3/3/3
58	GDP	QJ	501	-	-	1/16/32/32	0/3/3/3
58	GDP	RD	501	-	-	2/16/32/32	0/3/3/3
58	GDP	JJ	501	-	-	3/16/32/32	0/3/3/3
56	GTP	TB	501	57	-	8/22/38/38	0/3/3/3
56	GTP	BB	501	57	-	4/22/38/38	0/3/3/3
56	GTP	TK	501	57	-	4/22/38/38	0/3/3/3
58	GDP	HM	501	-	-	1/16/32/32	0/3/3/3
58	GDP	MH	501	-	-	2/16/32/32	0/3/3/3
58	GDP	PM	501	-	-	2/16/32/32	0/3/3/3
58	GDP	DD	501	-	-	3/16/32/32	0/3/3/3
56	GTP	TE	501	57	-	4/22/38/38	0/3/3/3
56	GTP	FG	501	57	-	5/22/38/38	0/3/3/3
58	GDP	SF	501	-	-	3/16/32/32	0/3/3/3
58	GDP	VJ	501	-	-	1/16/32/32	0/3/3/3
58	GDP	LM	501	-	-	1/16/32/32	0/3/3/3
56	GTP	AK	501	57	-	5/22/38/38	0/3/3/3
56	GTP	MI	501	57	-	3/22/38/38	0/3/3/3
56	GTP	AB	501	57	-	3/22/38/38	0/3/3/3
56	GTP	VK	501	57	-	7/22/38/38	0/3/3/3
56	GTP	WA	501	57	-	1/22/38/38	0/3/3/3
58	GDP	DJ	501	-	-	4/16/32/32	0/3/3/3
58	GDP	DL	501	-	-	1/16/32/32	0/3/3/3
56	GTP	OK	501	57	-	6/22/38/38	0/3/3/3
58	GDP	PD	501	-	-	1/16/32/32	0/3/3/3
58	GDP	SD	501	-	-	4/16/32/32	0/3/3/3
56	GTP	NE	501	57	-	3/22/38/38	0/3/3/3
56	GTP	IK	501	57	-	4/22/38/38	0/3/3/3
58	GDP	WD	501	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	MF	501	-	-	2/16/32/32	0/3/3/3
56	GTP	MB	501	57	-	5/22/38/38	0/3/3/3
56	GTP	NB	501	57	-	10/22/38/38	0/3/3/3
56	GTP	LG	501	57	-	3/22/38/38	0/3/3/3
58	GDP	DC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	SM	501	-	-	1/16/32/32	0/3/3/3
58	GDP	WC	501	-	-	1/16/32/32	0/3/3/3
56	GTP	JG	501	57	-	3/22/38/38	0/3/3/3
58	GDP	LL	501	-	-	1/16/32/32	0/3/3/3
58	GDP	QD	501	-	-	1/16/32/32	0/3/3/3
58	GDP	KF	501	-	-	2/16/32/32	0/3/3/3
58	GDP	JC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	MC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	EJ	501	-	-	1/16/32/32	0/3/3/3
56	GTP	RG	501	57	-	2/22/38/38	0/3/3/3
58	GDP	TM	501	-	-	1/16/32/32	0/3/3/3
58	GDP	NM	501	-	-	2/16/32/32	0/3/3/3
56	GTP	JB	501	57	-	3/22/38/38	0/3/3/3
56	GTP	PK	501	57	-	1/22/38/38	0/3/3/3
56	GTP	IE	501	57	-	6/22/38/38	0/3/3/3
58	GDP	EH	501	-	-	2/16/32/32	0/3/3/3
56	GTP	DM	501	57	-	3/22/38/38	0/3/3/3
58	GDP	FL	501	-	-	2/16/32/32	0/3/3/3
56	GTP	EK	501	57	-	2/22/38/38	0/3/3/3
58	GDP	GH	501	-	-	1/16/32/32	0/3/3/3
56	GTP	WI	501	57	-	6/22/38/38	0/3/3/3
58	GDP	OF	501	-	-	2/16/32/32	0/3/3/3
58	GDP	VC	501	-	-	1/16/32/32	0/3/3/3
56	GTP	DG	501	57	-	5/22/38/38	0/3/3/3
58	GDP	UM	501	-	-	2/16/32/32	0/3/3/3
56	GTP	BM	501	57	-	9/22/38/38	0/3/3/3
56	GTP	DK	501	57	-	5/22/38/38	0/3/3/3
56	GTP	JE	501	57	-	3/22/38/38	0/3/3/3
58	GDP	GC	501	-	-	2/16/32/32	0/3/3/3
56	GTP	AG	501	57	-	4/22/38/38	0/3/3/3
58	GDP	IH	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	NG	501	57	-	7/22/38/38	0/3/3/3
56	GTP	LE	501	57	-	3/22/38/38	0/3/3/3
58	GDP	AJ	501	-	-	2/16/32/32	0/3/3/3
58	GDP	IJ	501	-	-	1/16/32/32	0/3/3/3
56	GTP	BA	501	57	-	3/22/38/38	0/3/3/3
56	GTP	RK	501	57	-	3/22/38/38	0/3/3/3
58	GDP	CJ	501	-	-	2/16/32/32	0/3/3/3
56	GTP	GI	501	57	-	3/22/38/38	0/3/3/3
56	GTP	BK	501	57	-	5/22/38/38	0/3/3/3
56	GTP	UI	501	57	-	3/22/38/38	0/3/3/3
58	GDP	GM	501	-	-	2/16/32/32	0/3/3/3
58	GDP	KM	501	-	-	1/16/32/32	0/3/3/3
58	GDP	FM	501	-	-	1/16/32/32	0/3/3/3
58	GDP	NJ	501	-	-	2/16/32/32	0/3/3/3
58	GDP	ND	501	-	-	1/16/32/32	0/3/3/3
58	GDP	QF	501	-	-	4/16/32/32	0/3/3/3
58	GDP	RC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	CC	501	-	-	2/16/32/32	0/3/3/3
56	GTP	PA	501	57	-	3/22/38/38	0/3/3/3
56	GTP	NA	501	57	-	3/22/38/38	0/3/3/3
58	GDP	LF	501	-	-	3/16/32/32	0/3/3/3
58	GDP	NH	501	-	-	2/16/32/32	0/3/3/3
58	GDP	UD	501	-	-	3/16/32/32	0/3/3/3
58	GDP	GL	501	-	-	1/16/32/32	0/3/3/3
58	GDP	RH	501	-	-	1/16/32/32	0/3/3/3
56	GTP	AI	501	57	-	3/22/38/38	0/3/3/3
56	GTP	JI	501	57	-	2/22/38/38	0/3/3/3
58	GDP	LD	501	-	-	2/16/32/32	0/3/3/3
56	GTP	HI	501	57	-	6/22/38/38	0/3/3/3
56	GTP	QE	501	57	-	2/22/38/38	0/3/3/3
56	GTP	WB	501	57	-	7/22/38/38	0/3/3/3
58	GDP	HC	501	-	-	5/16/32/32	0/3/3/3
56	GTP	DA	501	57	-	3/22/38/38	0/3/3/3
56	GTP	EA	501	57	-	2/22/38/38	0/3/3/3
58	GDP	WH	501	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	IM	501	57	-	7/22/38/38	0/3/3/3
56	GTP	KB	501	57	-	2/22/38/38	0/3/3/3
56	GTP	LK	501	57	-	8/22/38/38	0/3/3/3
56	GTP	QL	501	57	-	9/22/38/38	0/3/3/3
56	GTP	WG	501	57	-	2/22/38/38	0/3/3/3
58	GDP	UH	501	-	-	2/16/32/32	0/3/3/3
58	GDP	JD	501	-	-	2/16/32/32	0/3/3/3
58	GDP	WJ	501	-	-	2/16/32/32	0/3/3/3
56	GTP	LB	501	57	-	3/22/38/38	0/3/3/3
56	GTP	NL	501	57	-	4/22/38/38	0/3/3/3
58	GDP	JH	501	-	-	1/16/32/32	0/3/3/3
58	GDP	GF	501	-	-	2/16/32/32	0/3/3/3
56	GTP	TG	501	57	-	6/22/38/38	0/3/3/3
58	GDP	AD	501	-	-	5/16/32/32	0/3/3/3
58	GDP	HD	501	-	-	2/16/32/32	0/3/3/3
58	GDP	UC	501	-	-	2/16/32/32	0/3/3/3
56	GTP	ME	501	57	-	6/22/38/38	0/3/3/3
58	GDP	VF	501	-	-	1/16/32/32	0/3/3/3
58	GDP	LC	501	-	-	2/16/32/32	0/3/3/3
56	GTP	HK	501	57	-	10/22/38/38	0/3/3/3
58	GDP	OJ	501	-	-	1/16/32/32	0/3/3/3
58	GDP	OD	501	-	-	4/16/32/32	0/3/3/3
56	GTP	EG	501	57	-	3/22/38/38	0/3/3/3
56	GTP	AA	501	57	-	7/22/38/38	0/3/3/3
56	GTP	HA	501	57	-	3/22/38/38	0/3/3/3
56	GTP	KE	501	57	-	2/22/38/38	0/3/3/3
56	GTP	QB	501	57	-	3/22/38/38	0/3/3/3
56	GTP	CI	501	57	-	2/22/38/38	0/3/3/3
56	GTP	GK	501	57	-	4/22/38/38	0/3/3/3
56	GTP	UG	501	57	-	6/22/38/38	0/3/3/3
56	GTP	VB	501	57	-	6/22/38/38	0/3/3/3
56	GTP	MK	501	57	-	6/22/38/38	0/3/3/3
58	GDP	ED	501	-	-	2/16/32/32	0/3/3/3
58	GDP	TD	501	-	-	3/16/32/32	0/3/3/3
58	GDP	LH	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	GA	501	57	-	6/22/38/38	0/3/3/3
56	GTP	KK	501	57	-	4/22/38/38	0/3/3/3
58	GDP	UL	501	-	-	3/16/32/32	0/3/3/3
56	GTP	WK	501	57	-	6/22/38/38	0/3/3/3
56	GTP	FE	501	57	-	8/22/38/38	0/3/3/3
56	GTP	JA	501	57	-	3/22/38/38	0/3/3/3
58	GDP	UJ	501	-	-	2/16/32/32	0/3/3/3
58	GDP	VD	501	-	-	1/16/32/32	0/3/3/3
56	GTP	IA	501	57	-	2/22/38/38	0/3/3/3
58	GDP	JF	501	-	-	2/16/32/32	0/3/3/3
56	GTP	BE	501	57	-	3/22/38/38	0/3/3/3
58	GDP	CH	501	-	-	2/16/32/32	0/3/3/3
58	GDP	SH	501	-	-	2/16/32/32	0/3/3/3
56	GTP	RB	501	57	-	6/22/38/38	0/3/3/3
56	GTP	RL	501	57	-	8/22/38/38	0/3/3/3
58	GDP	SC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	BL	501	-	-	2/16/32/32	0/3/3/3
56	GTP	AM	501	57	-	6/22/38/38	0/3/3/3
58	GDP	QC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	HJ	501	-	-	2/16/32/32	0/3/3/3
56	GTP	GB	501	57	-	3/22/38/38	0/3/3/3
56	GTP	MG	501	57	-	3/22/38/38	0/3/3/3
56	GTP	LA	501	57	-	7/22/38/38	0/3/3/3
56	GTP	OA	501	57	-	3/22/38/38	0/3/3/3
56	GTP	SA	501	57	-	4/22/38/38	0/3/3/3
56	GTP	UA	501	57	-	8/22/38/38	0/3/3/3
58	GDP	EF	501	-	-	2/16/32/32	0/3/3/3
58	GDP	JL	501	-	-	3/16/32/32	0/3/3/3
56	GTP	GG	501	57	-	3/22/38/38	0/3/3/3
56	GTP	QG	501	57	-	6/22/38/38	0/3/3/3
58	GDP	TC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	DH	501	-	-	1/16/32/32	0/3/3/3
58	GDP	FH	501	-	-	3/16/32/32	0/3/3/3
56	GTP	FB	501	57	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	PL	501	57	-	3/22/38/38	0/3/3/3
58	GDP	AC	501	-	-	2/16/32/32	0/3/3/3
58	GDP	KJ	501	-	-	2/16/32/32	0/3/3/3
56	GTP	EI	501	57	-	2/22/38/38	0/3/3/3
58	GDP	AH	501	-	-	3/16/32/32	0/3/3/3
56	GTP	RI	501	57	-	5/22/38/38	0/3/3/3
58	GDP	LJ	501	-	-	4/16/32/32	0/3/3/3
56	GTP	KG	501	57	-	3/22/38/38	0/3/3/3
56	GTP	AE	501	57	-	6/22/38/38	0/3/3/3

The worst 5 of 610 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	NK	501	GDP	C5-C4	3.20	1.47	1.38
58	GH	501	GDP	C5-C4	3.19	1.47	1.38
58	VM	501	GDP	C5-C4	3.19	1.47	1.38
58	GM	501	GDP	C5-C4	3.18	1.47	1.38
58	LM	501	GDP	C5-C4	3.18	1.47	1.38

The worst 5 of 2311 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	PF	501	GDP	C5-C4-N3	-7.16	116.99	128.39
58	EL	501	GDP	C5-C4-N3	-6.37	118.25	128.39
58	FF	501	GDP	C5-C4-N3	-6.37	118.25	128.39
58	DJ	501	GDP	C5-C4-N3	-6.33	118.32	128.39
58	RJ	501	GDP	C5-C4-N3	-6.33	118.32	128.39

There are no chirality outliers.

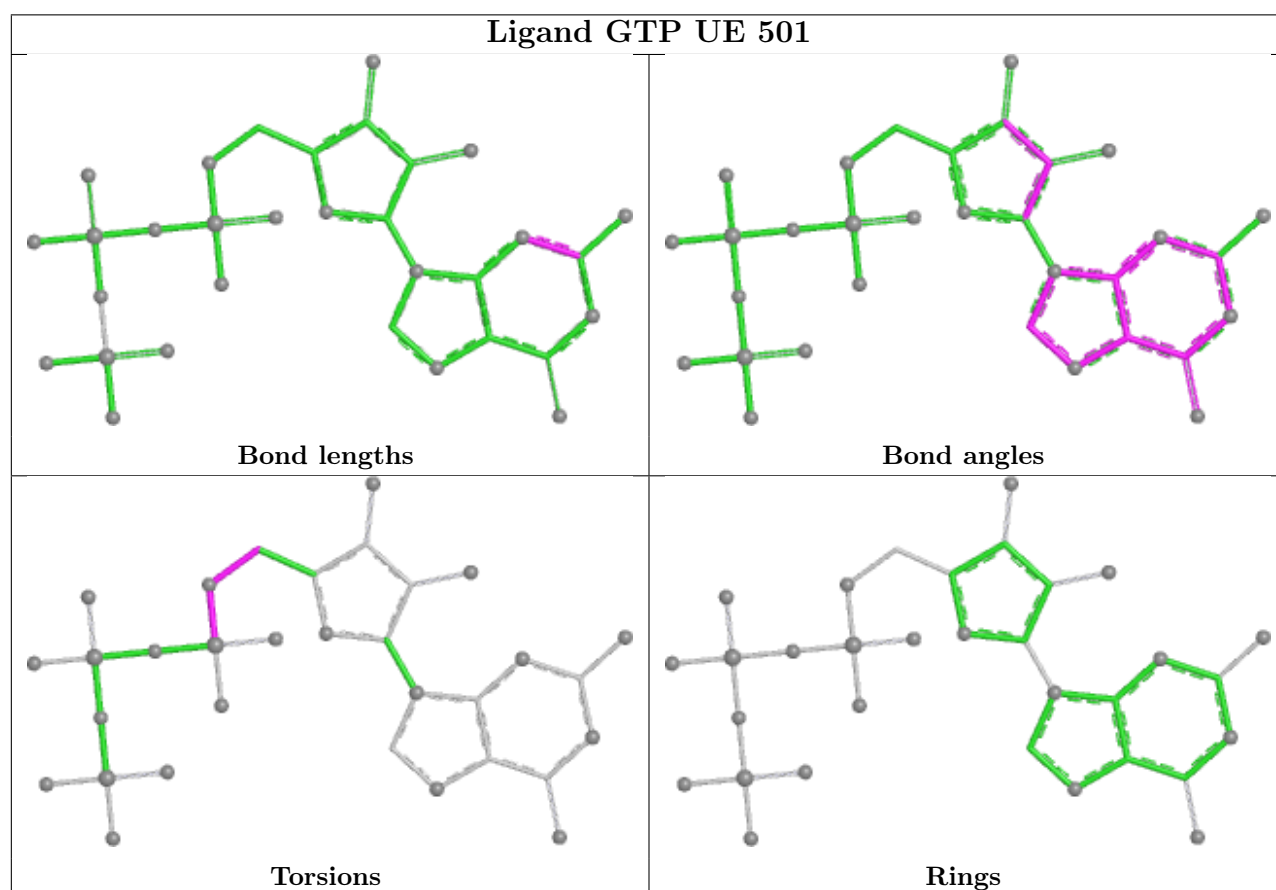
5 of 937 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	AA	501	GTP	C5'-O5'-PA-O3A
56	AA	501	GTP	C5'-O5'-PA-O1A
56	AA	501	GTP	C5'-O5'-PA-O2A
56	AB	501	GTP	C5'-O5'-PA-O3A
56	AE	501	GTP	C5'-O5'-PA-O3A

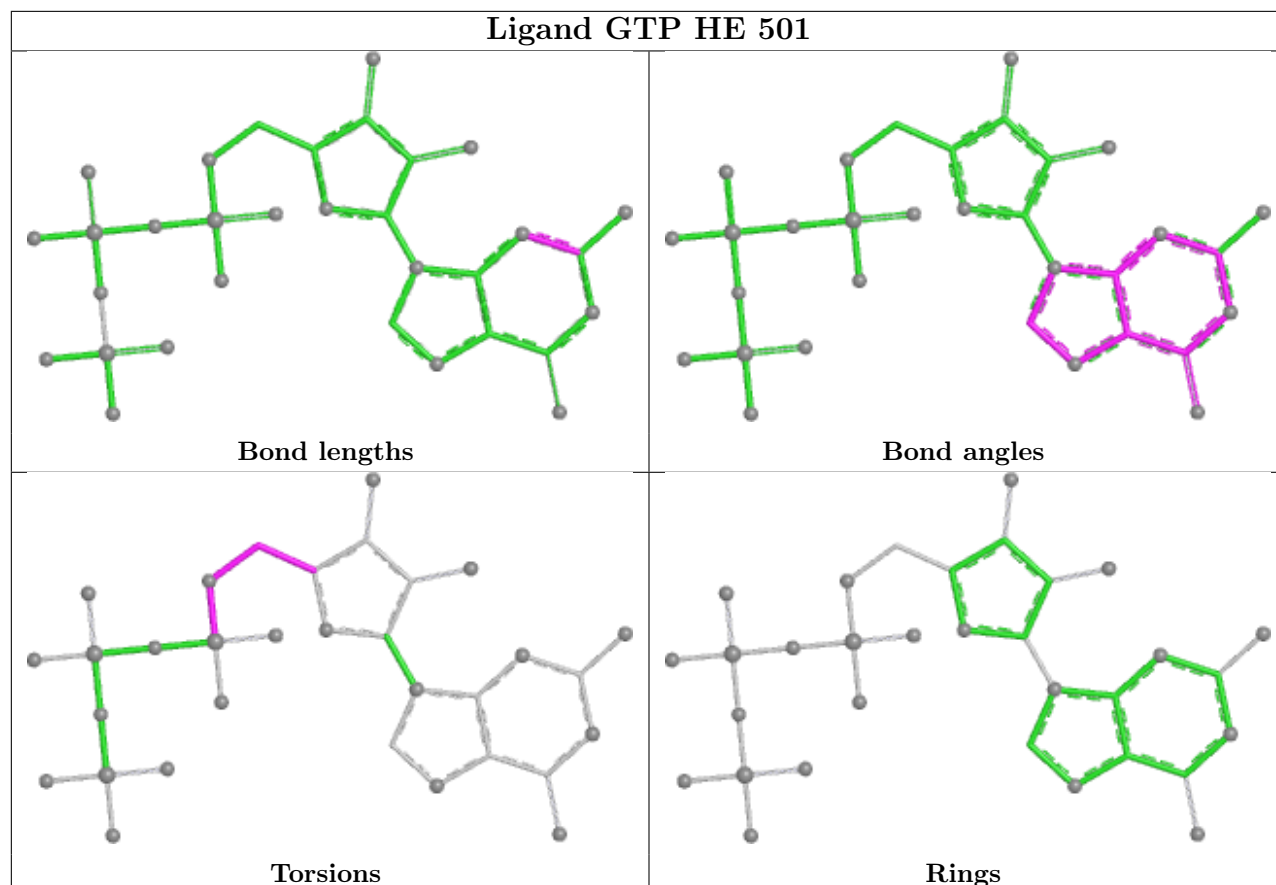
There are no ring outliers.

No monomer is involved in short contacts.

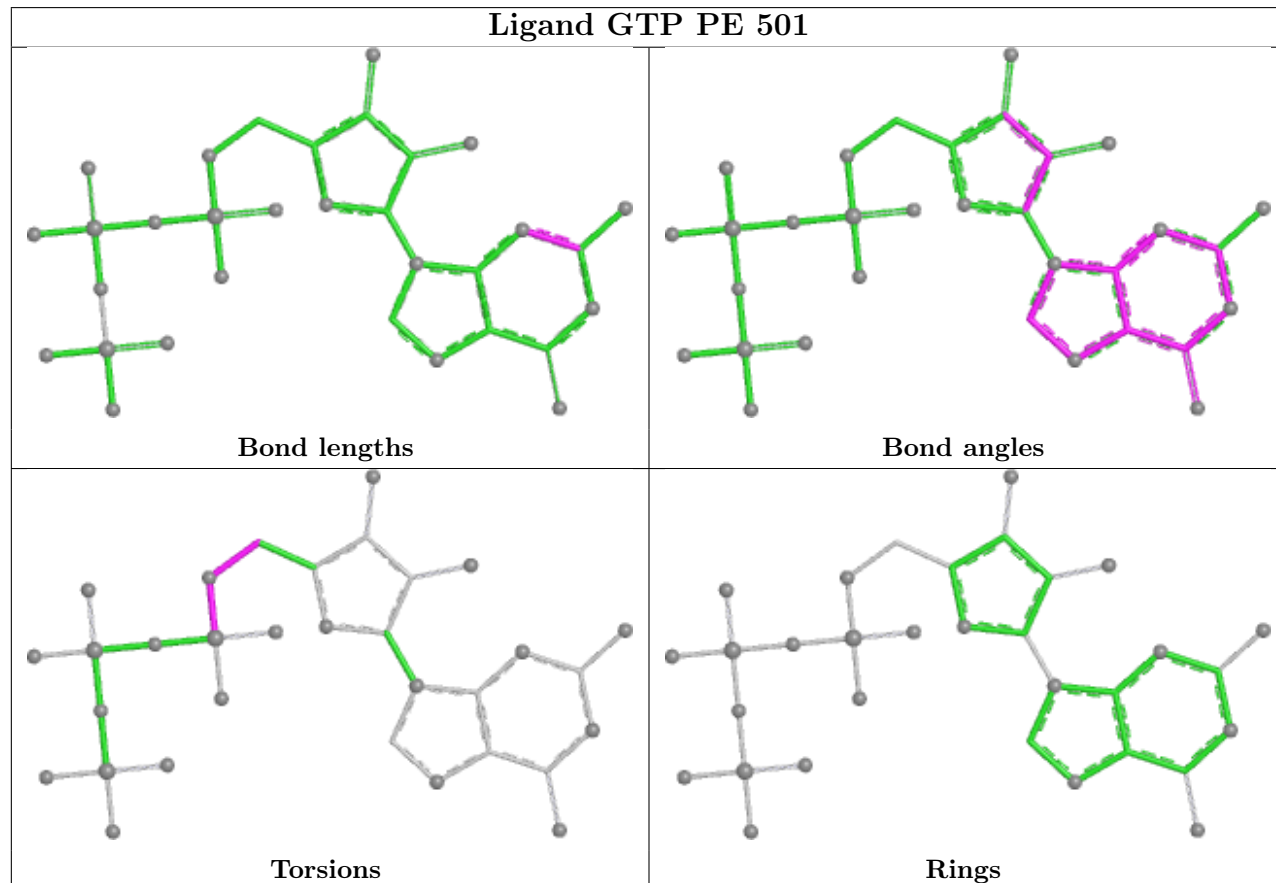
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

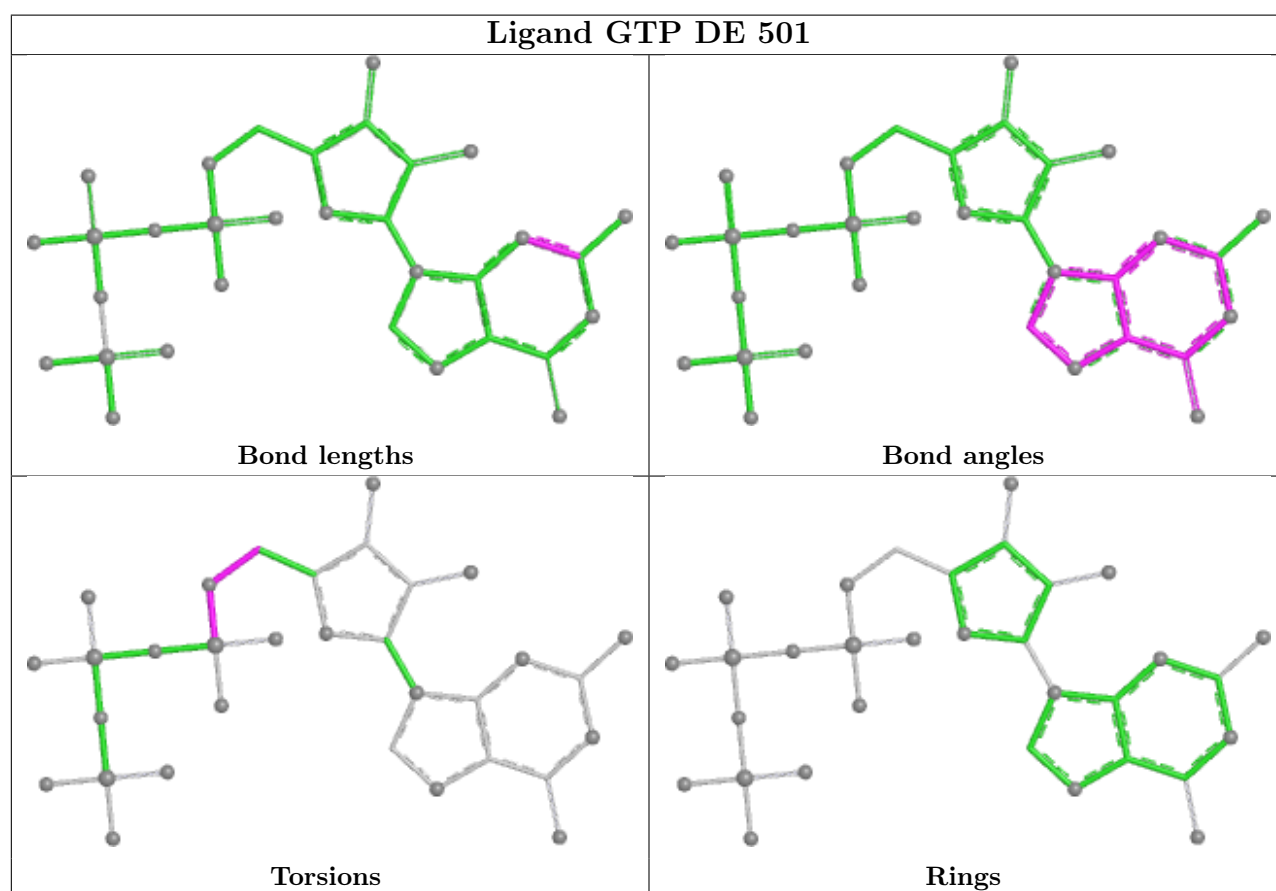
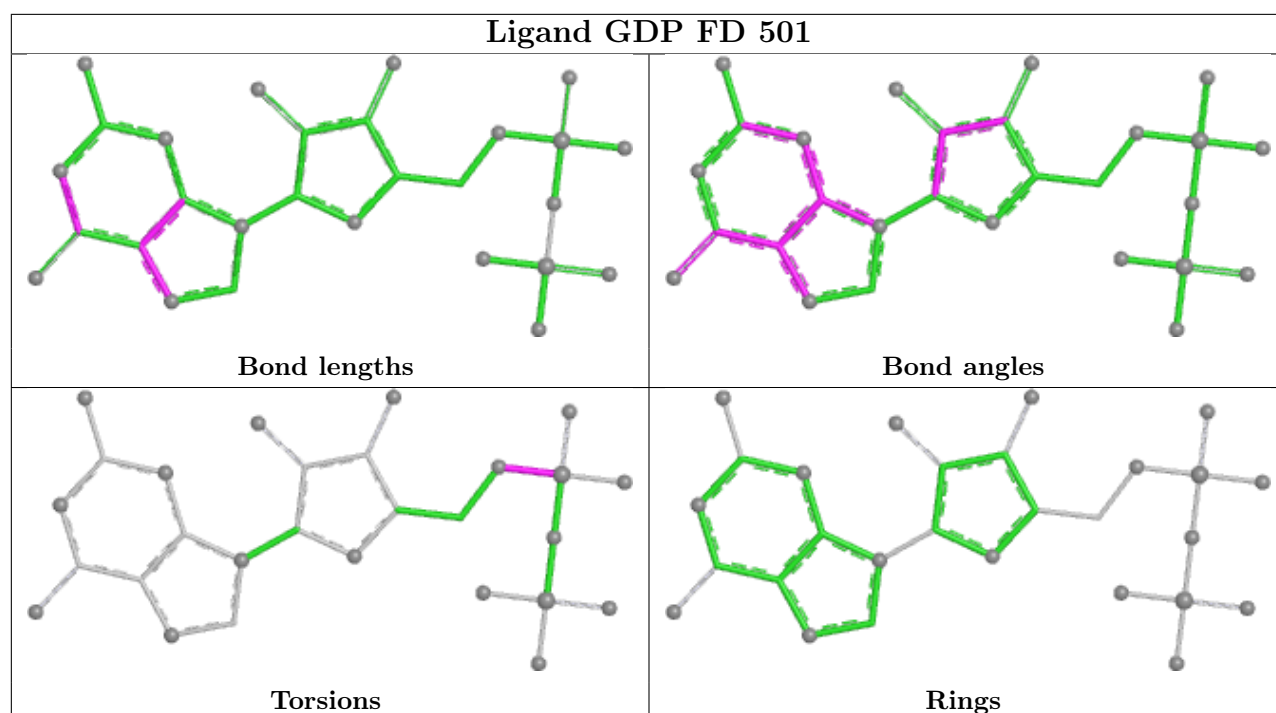


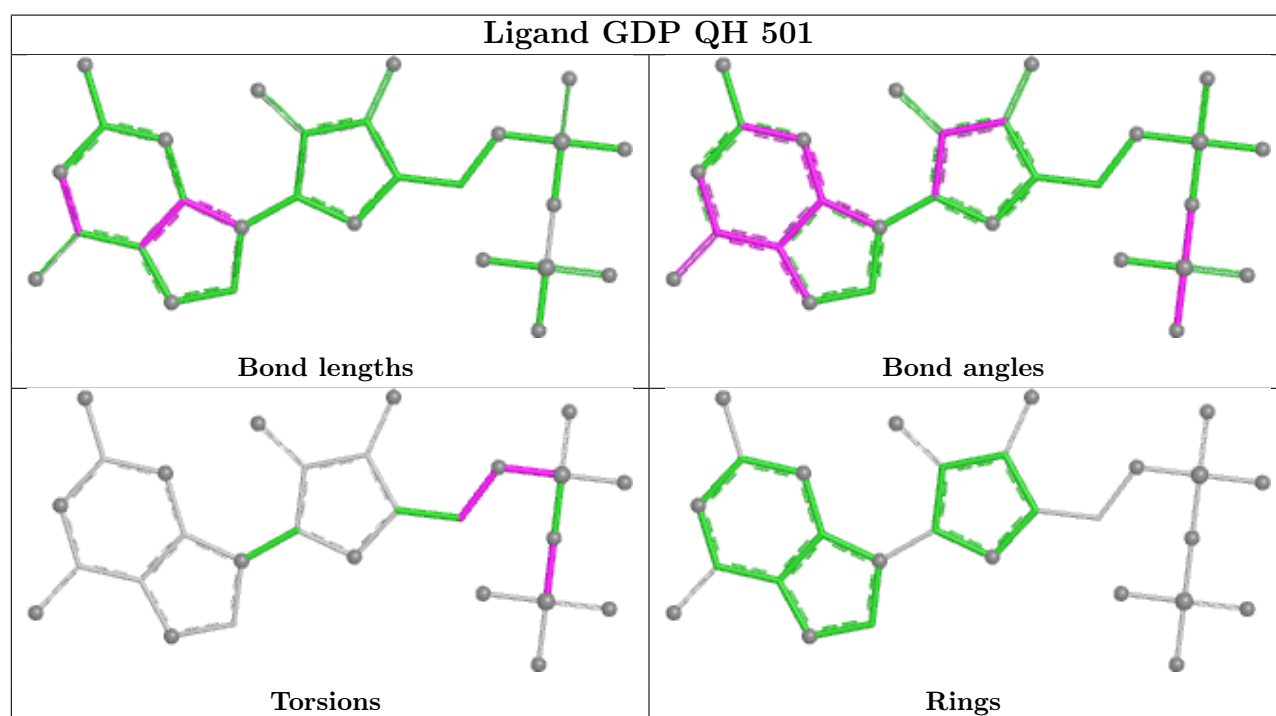
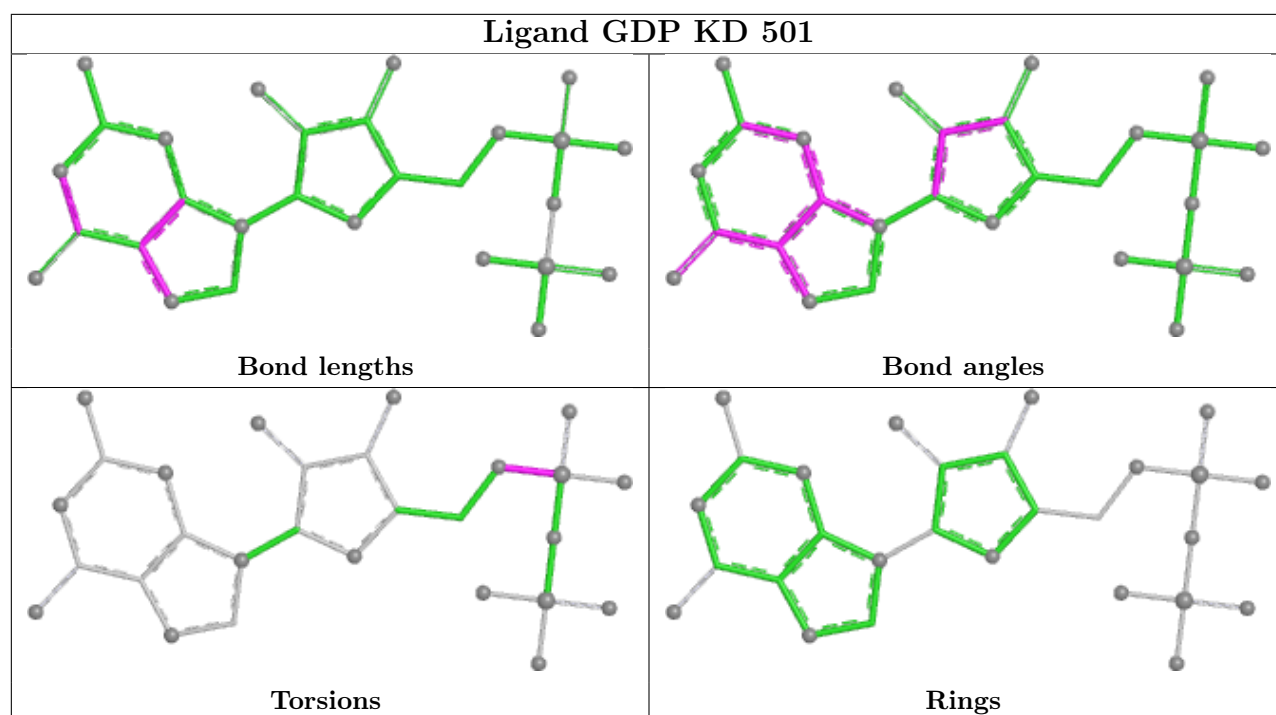
Ligand GTP HE 501

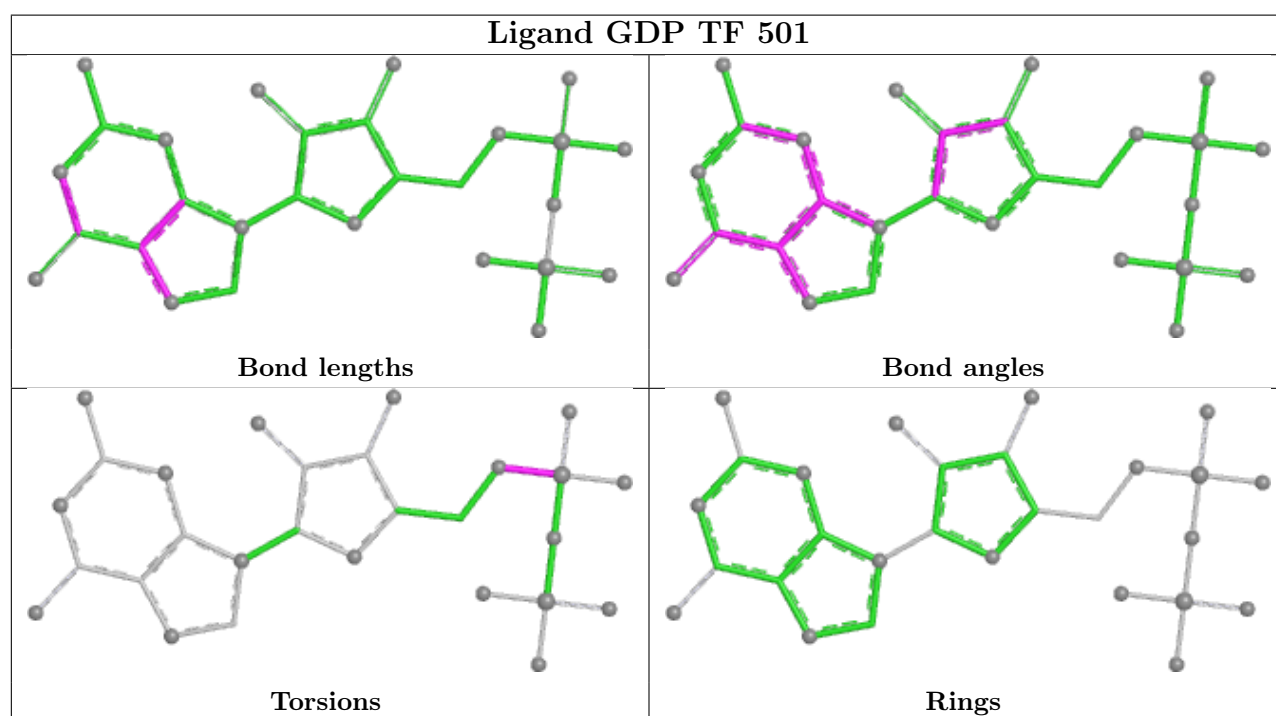
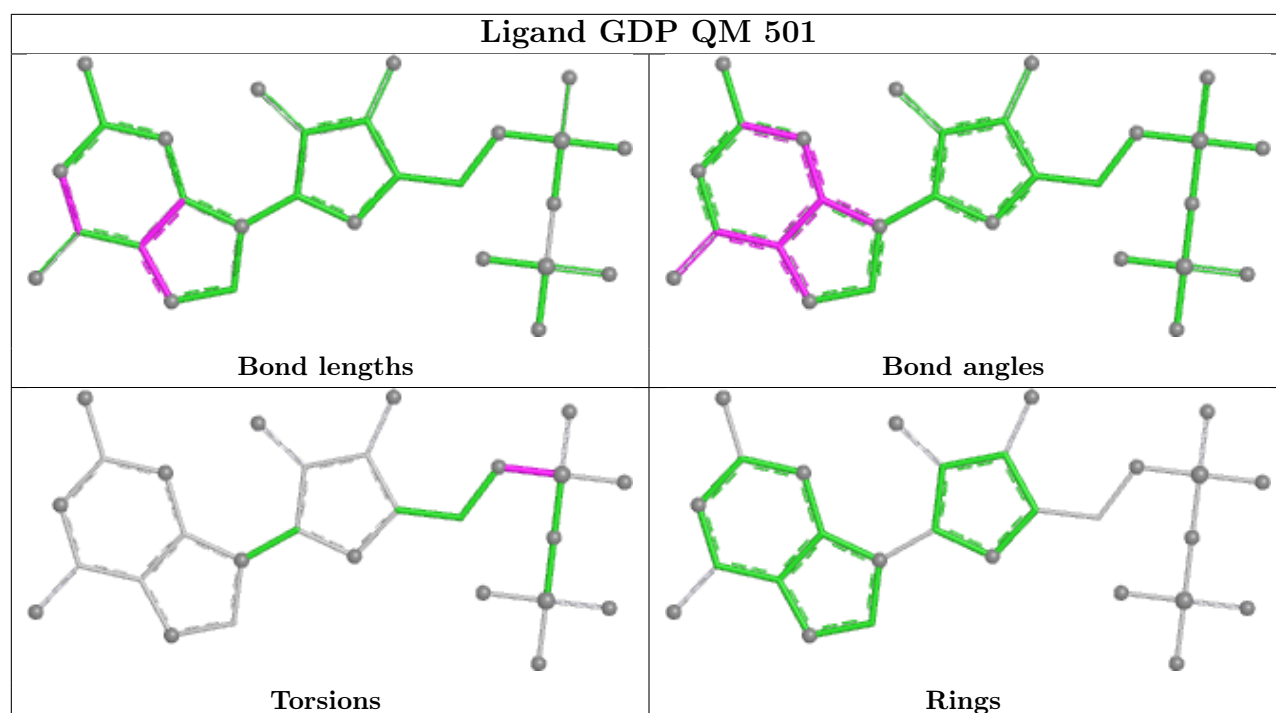


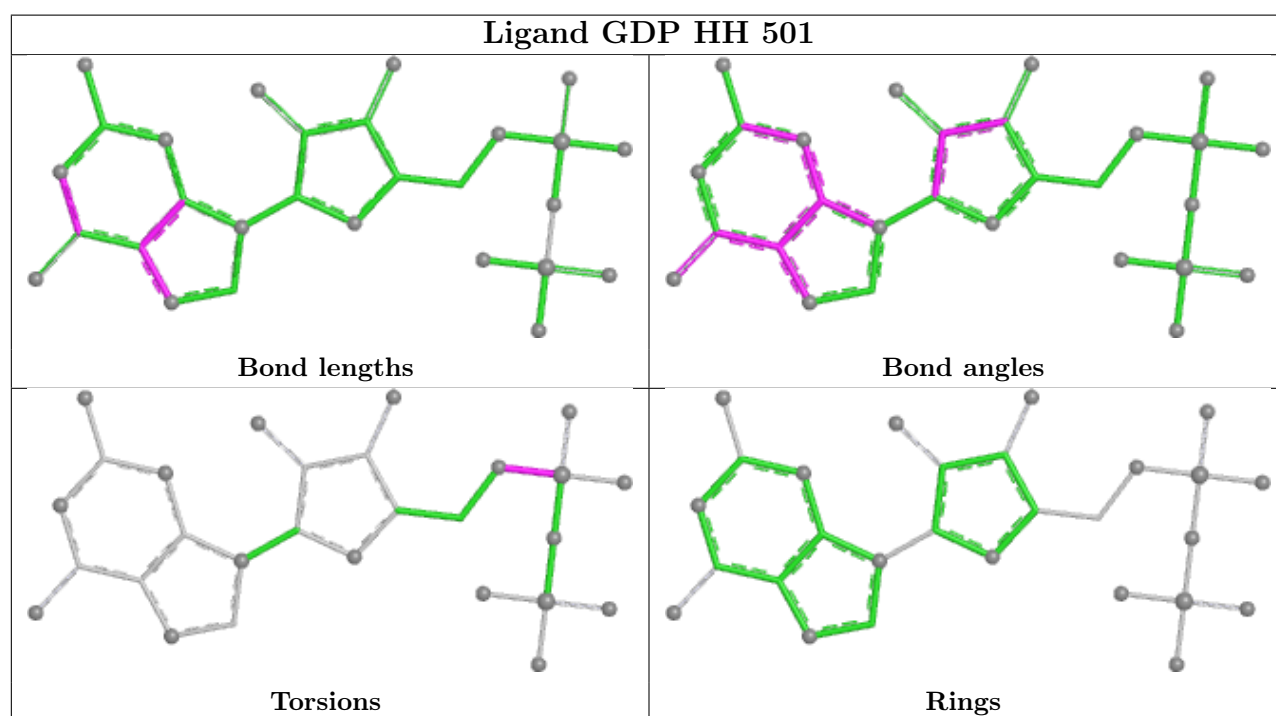
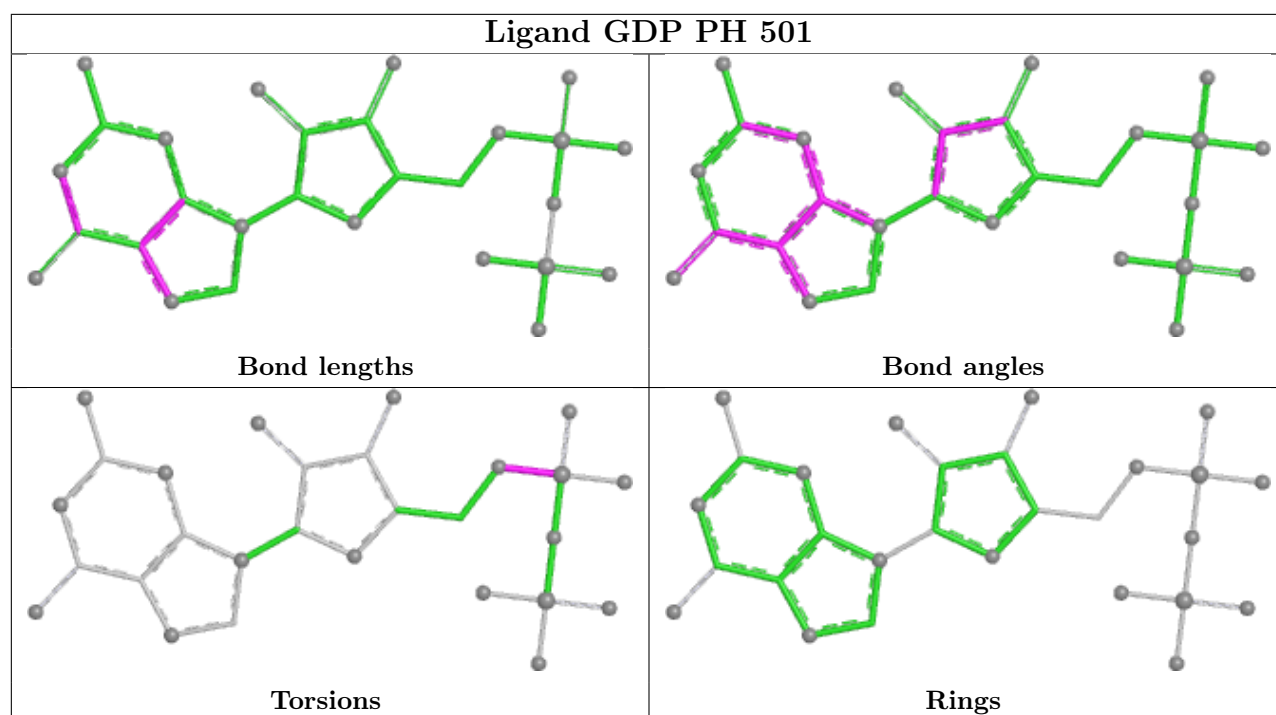
Ligand GTP PE 501

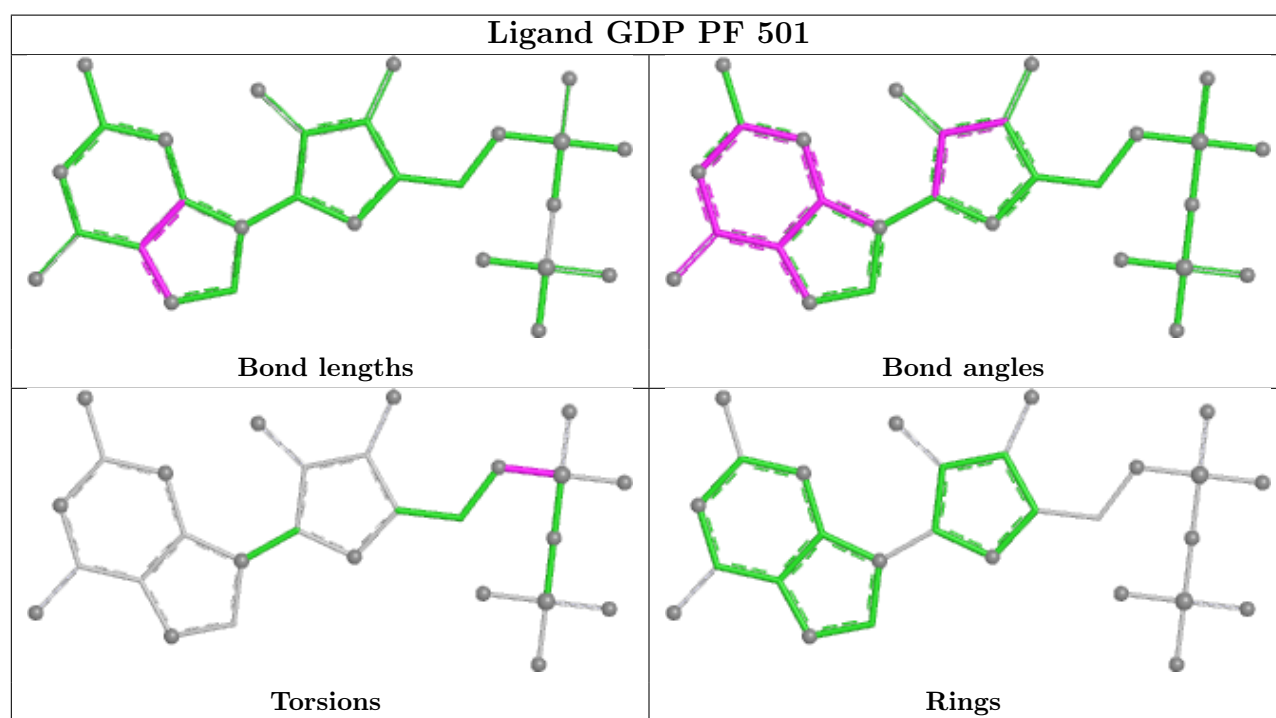
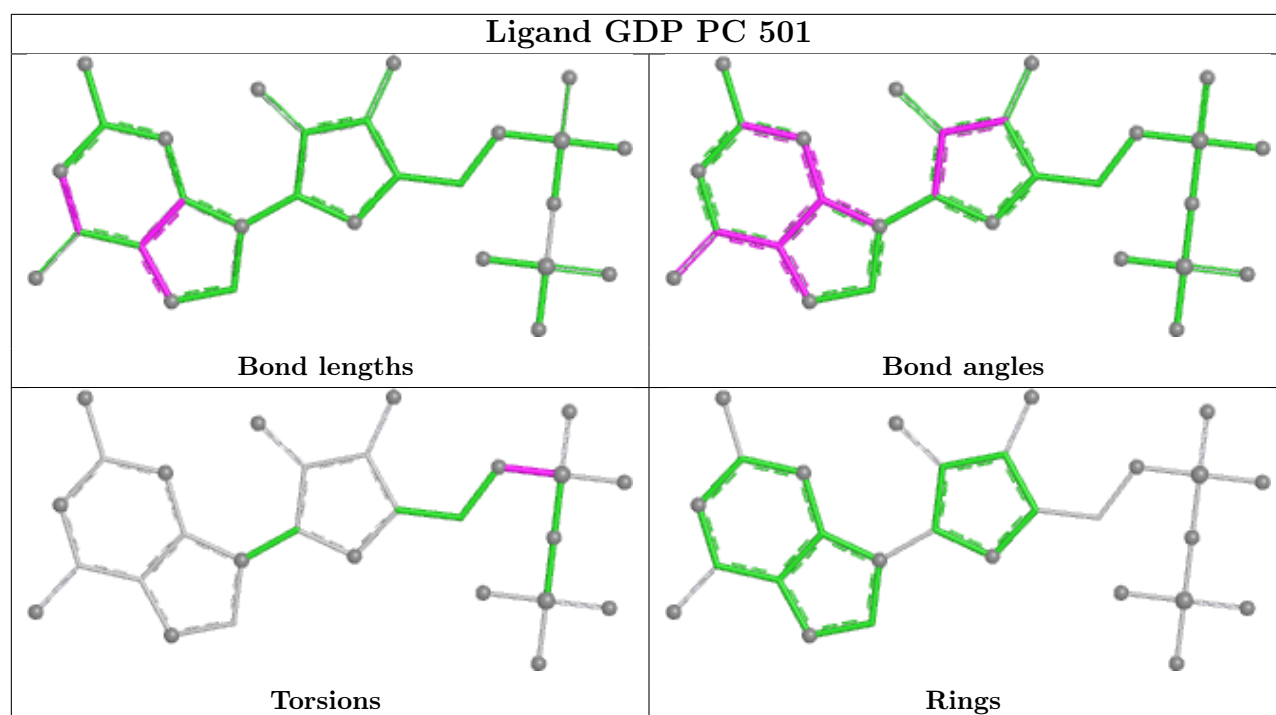


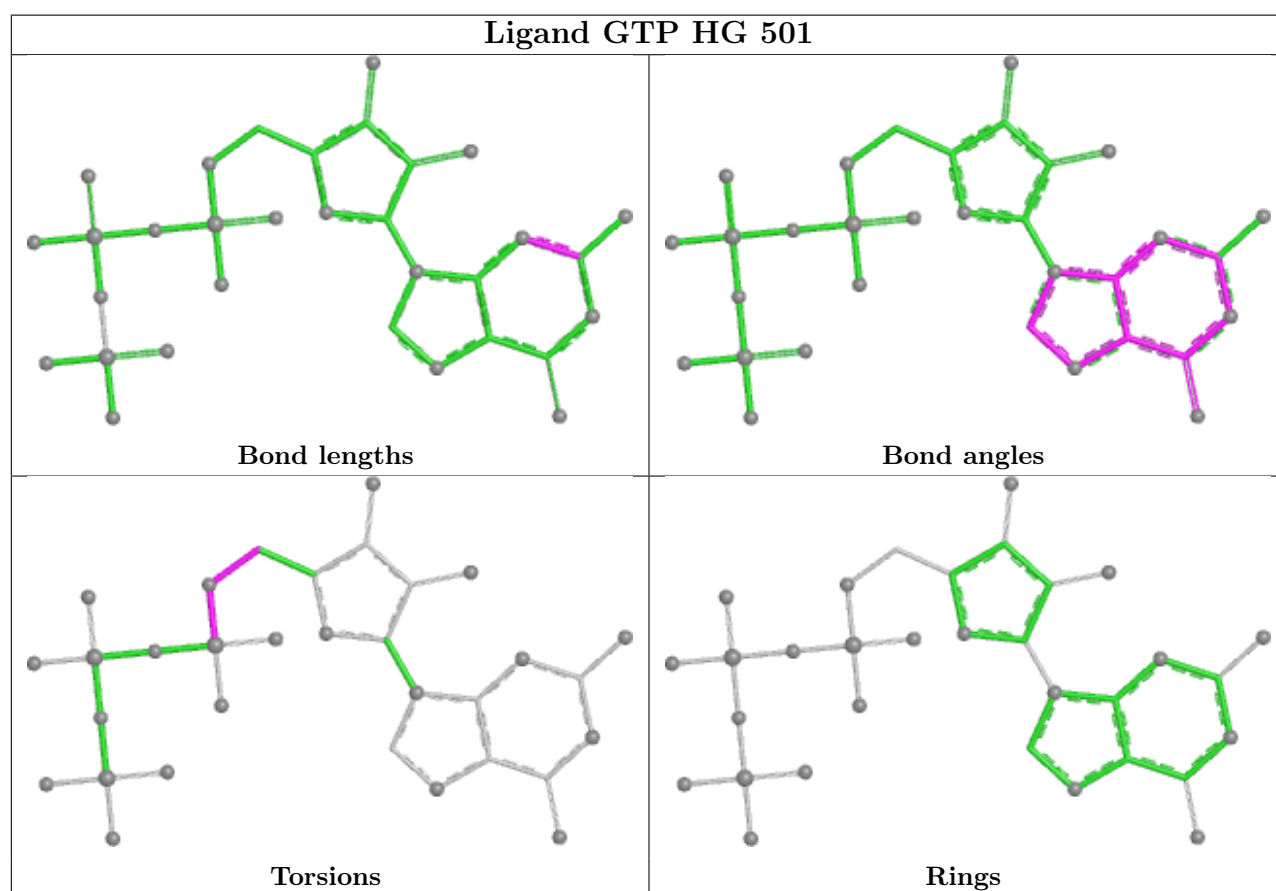
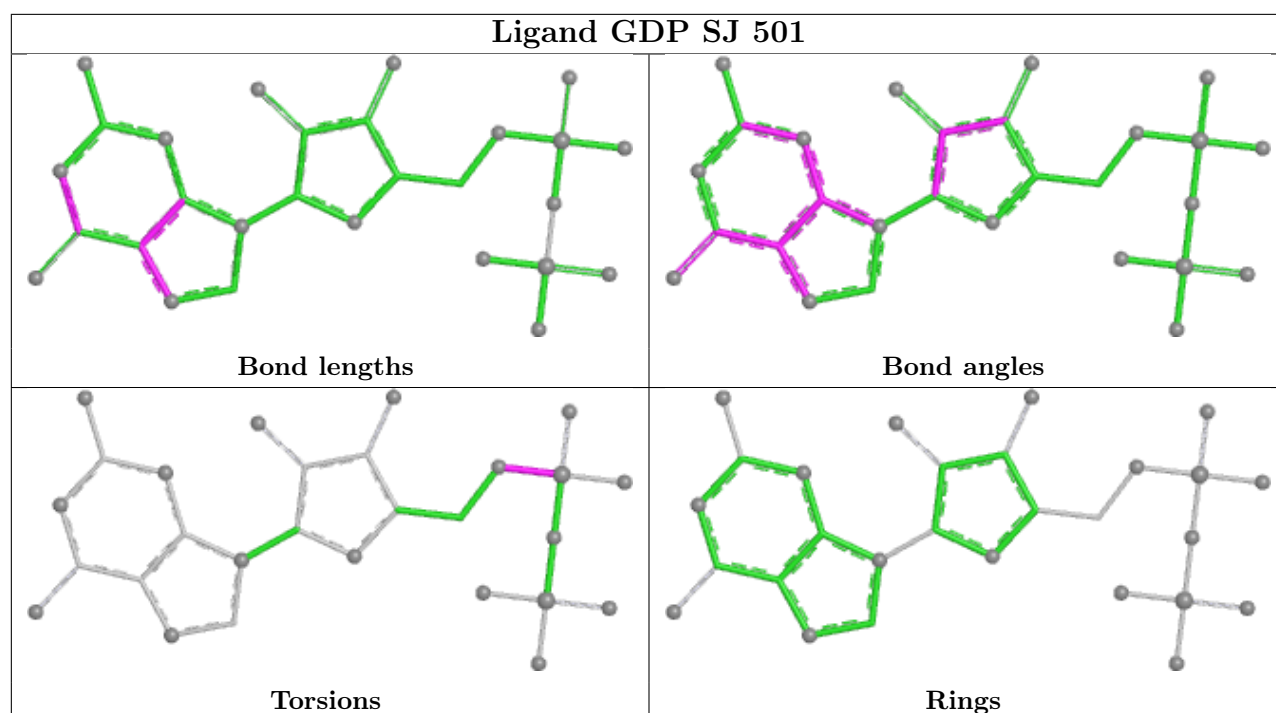




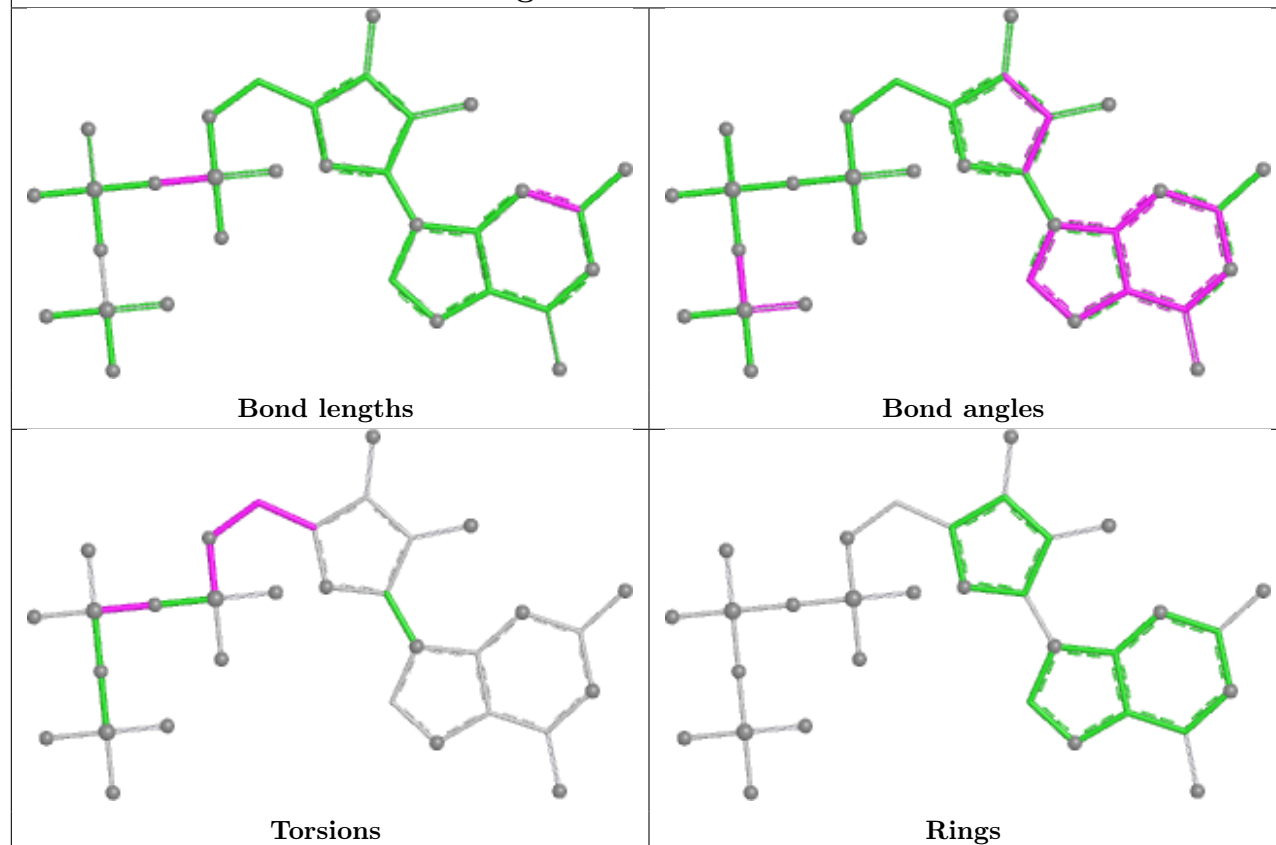




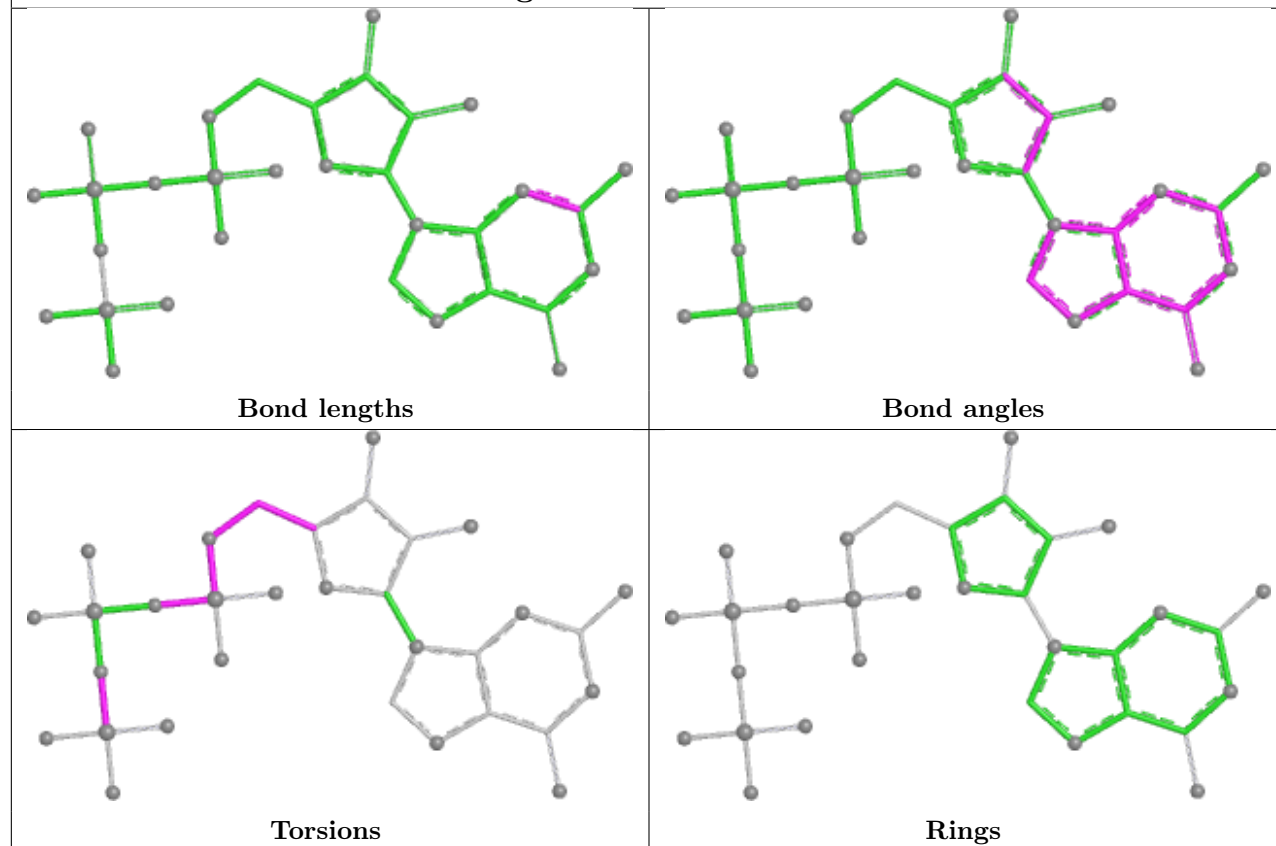


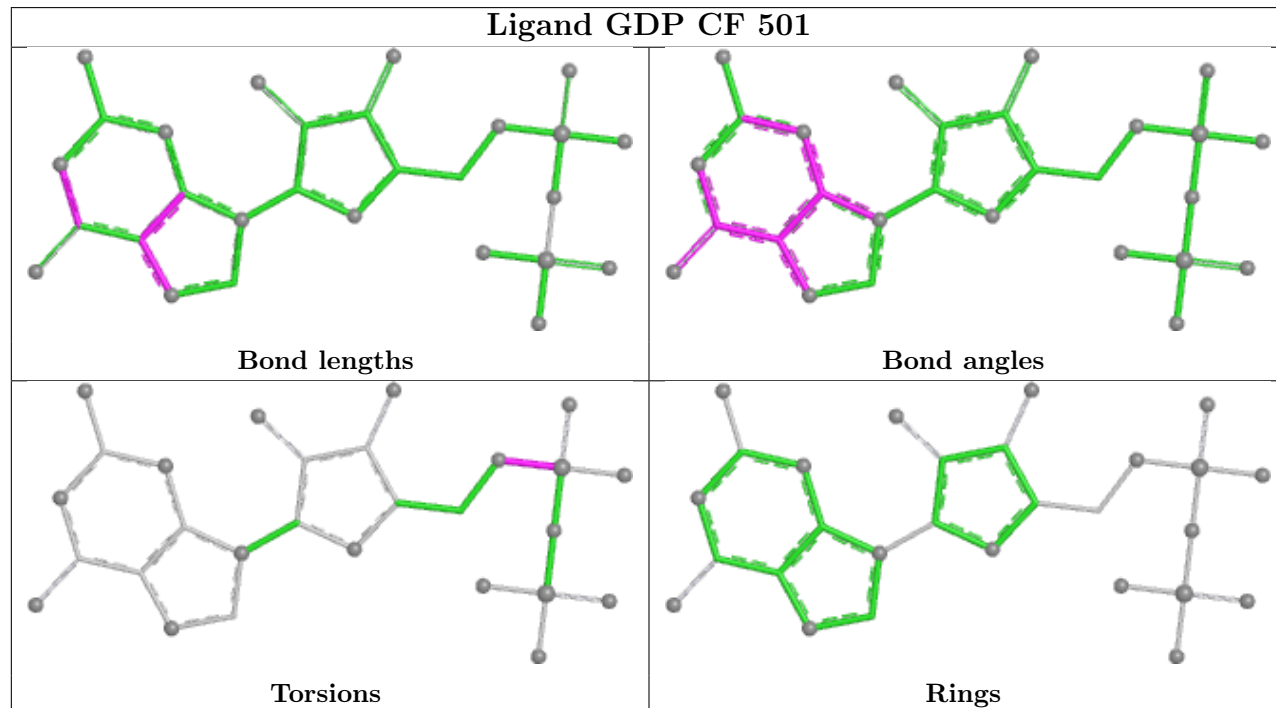
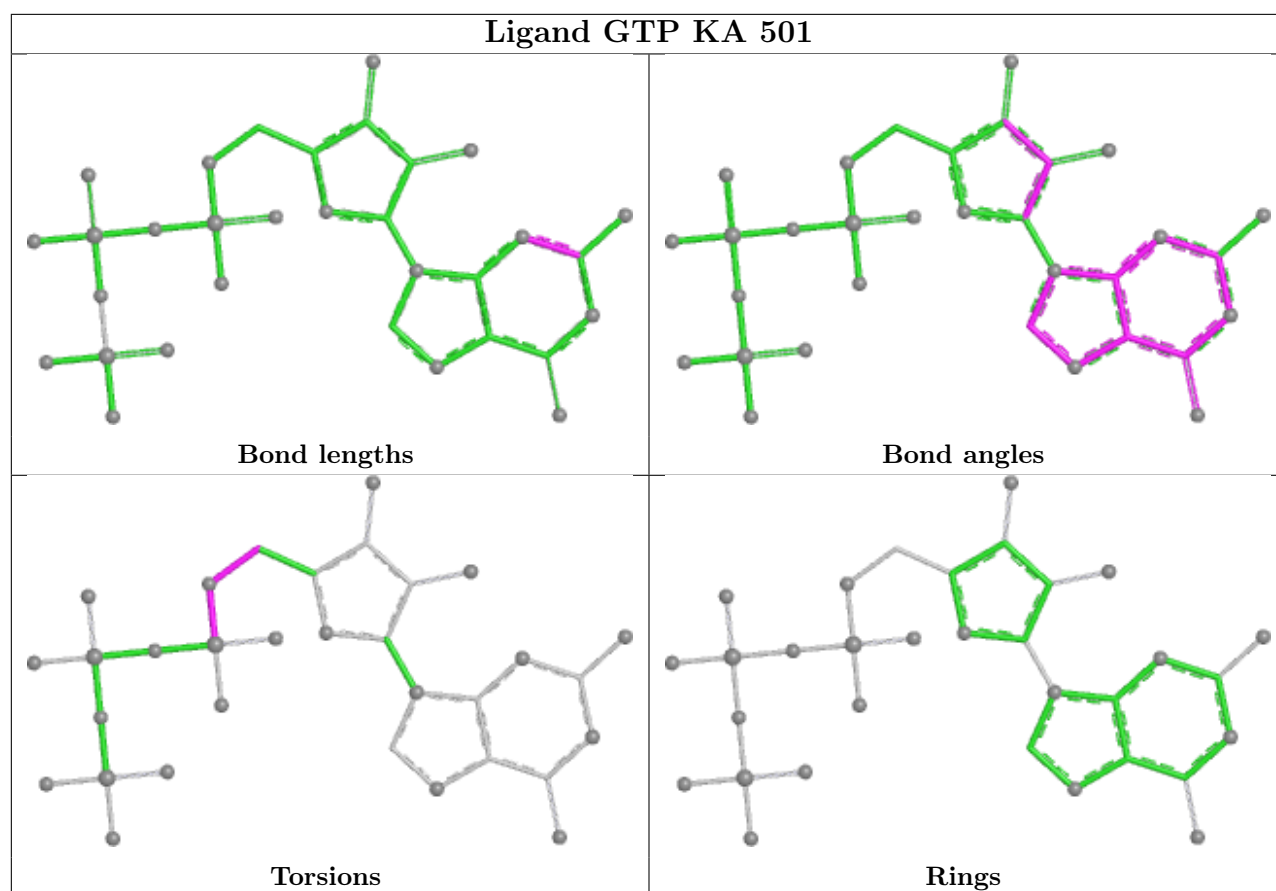


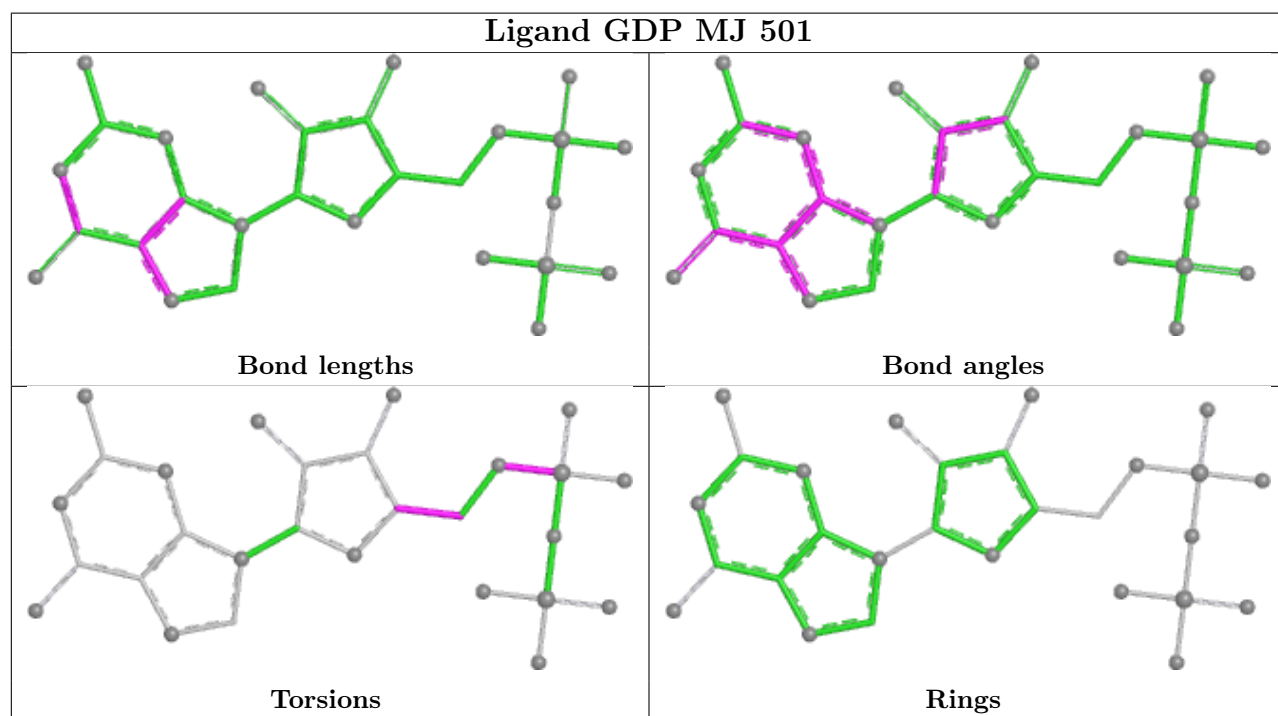
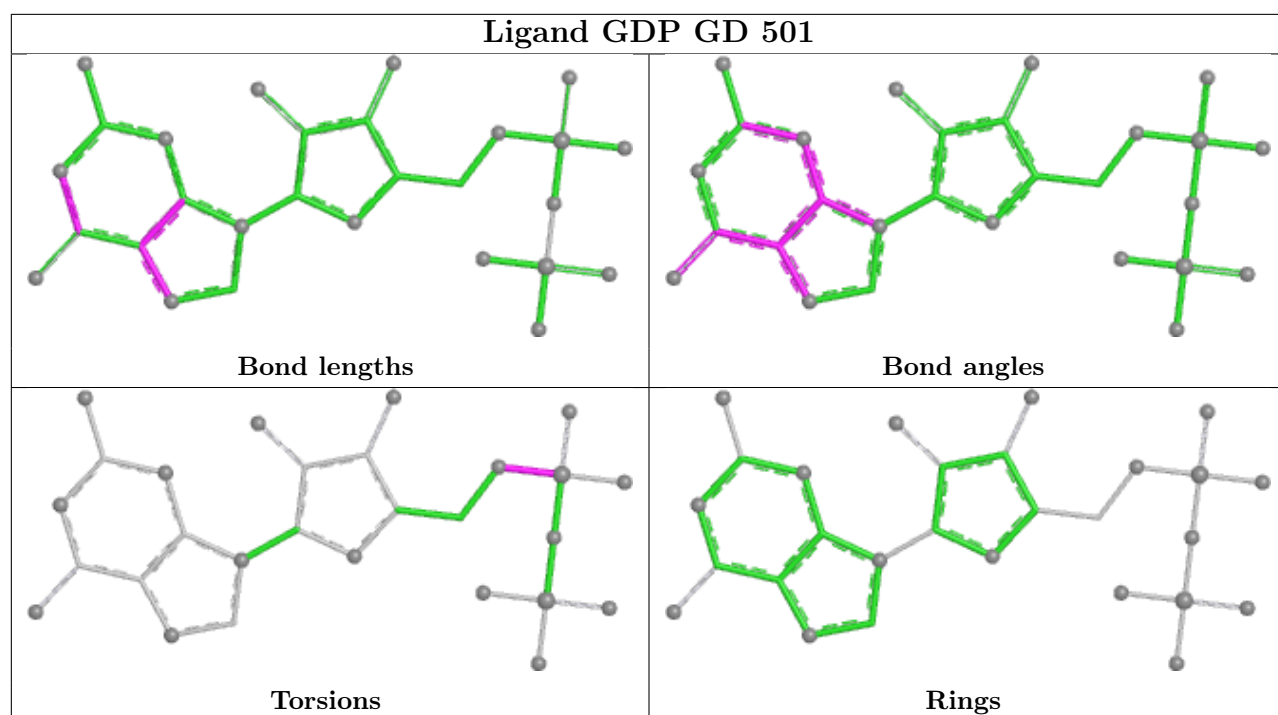
Ligand GTP BG 501

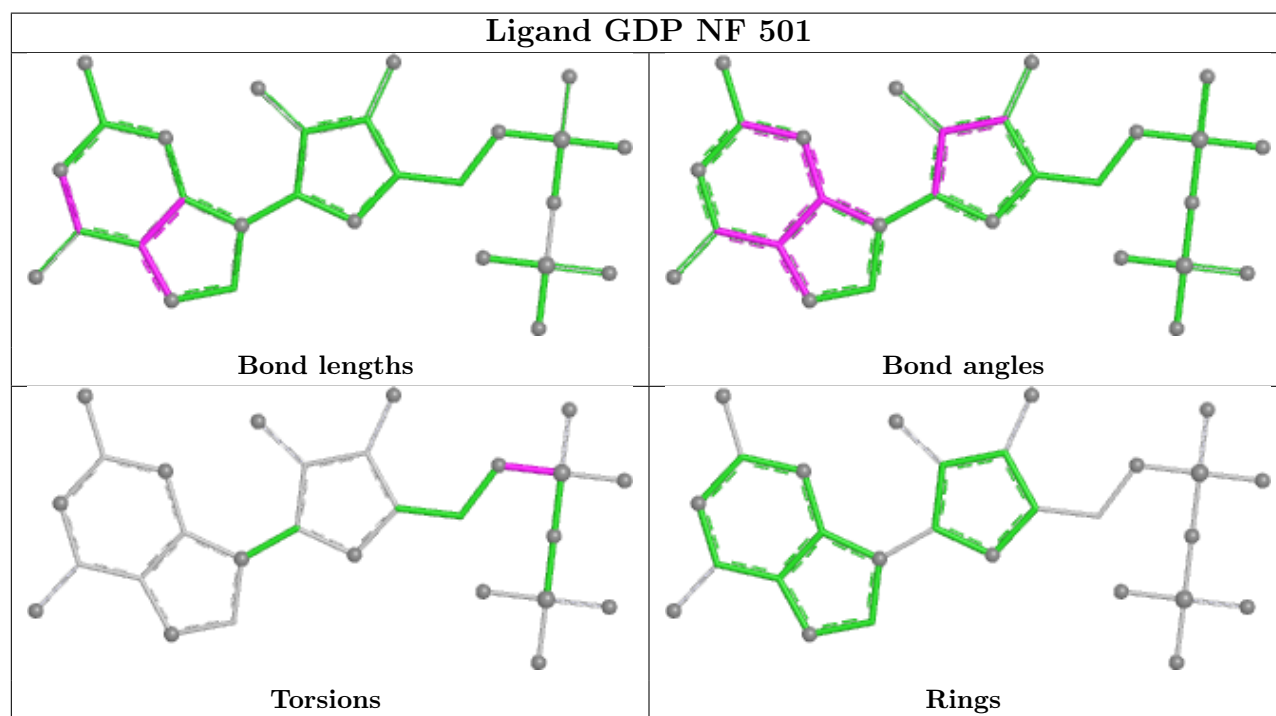
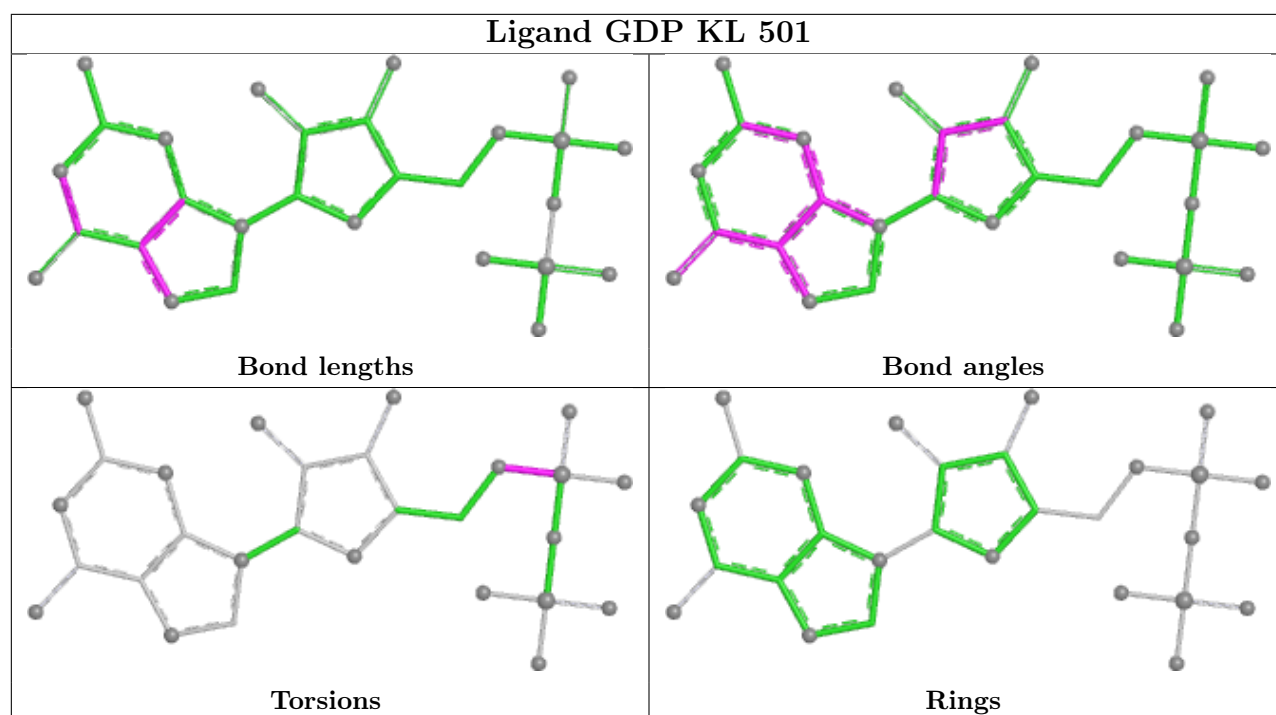


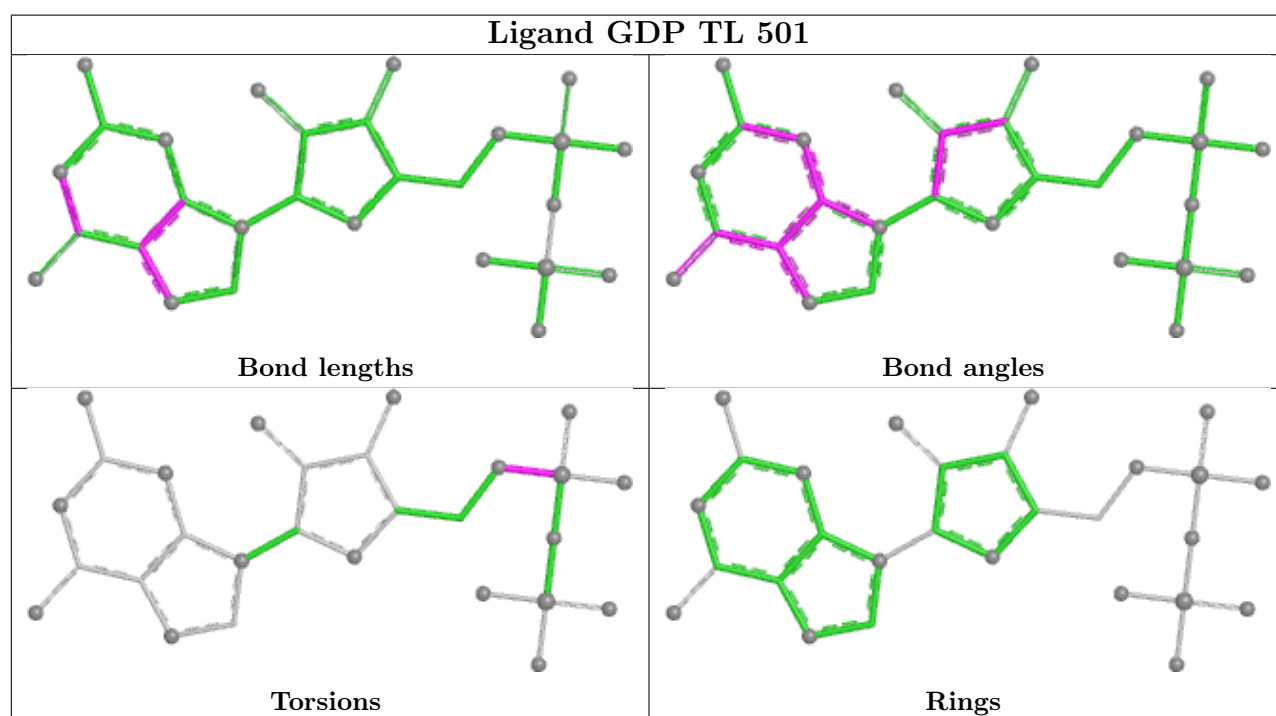
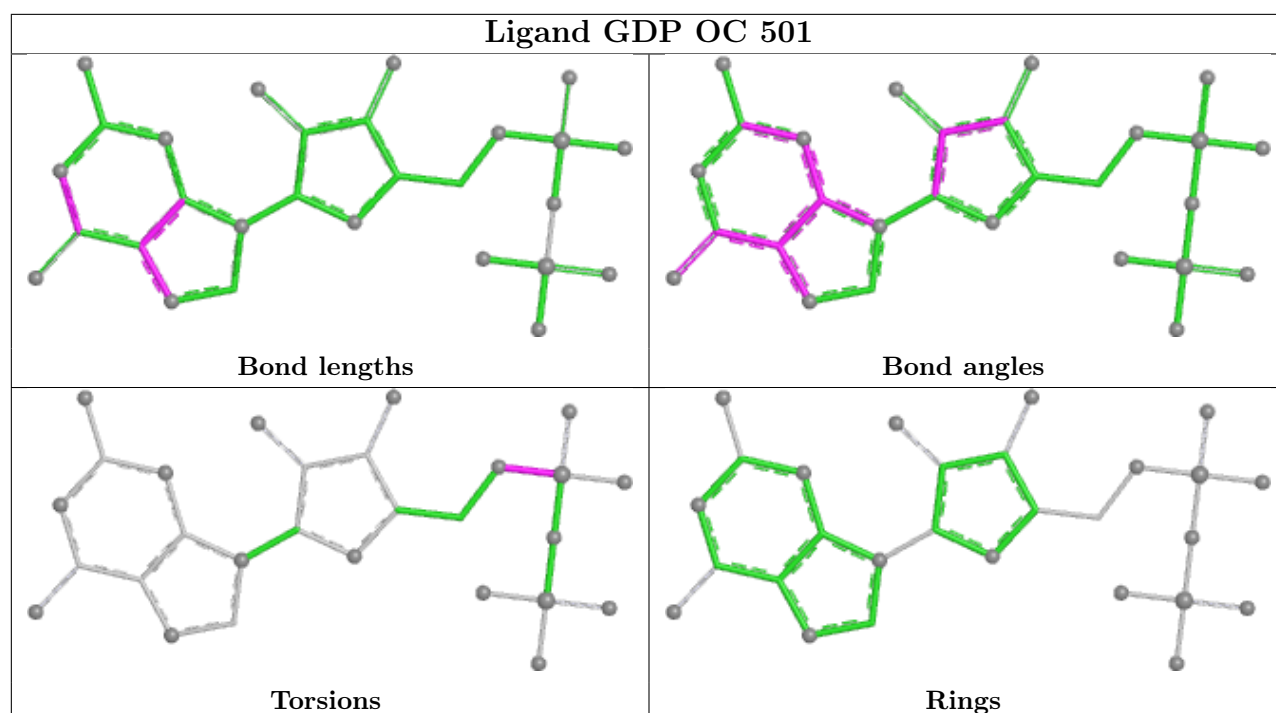
Ligand GTP UK 501

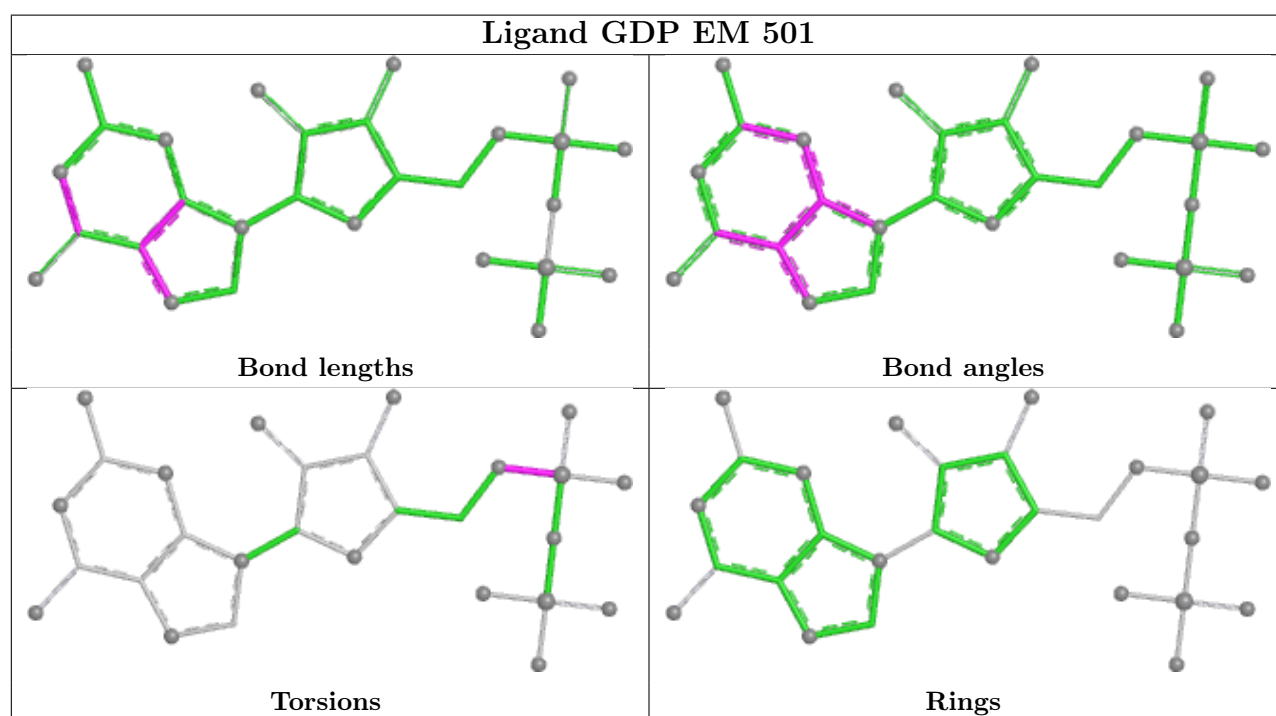
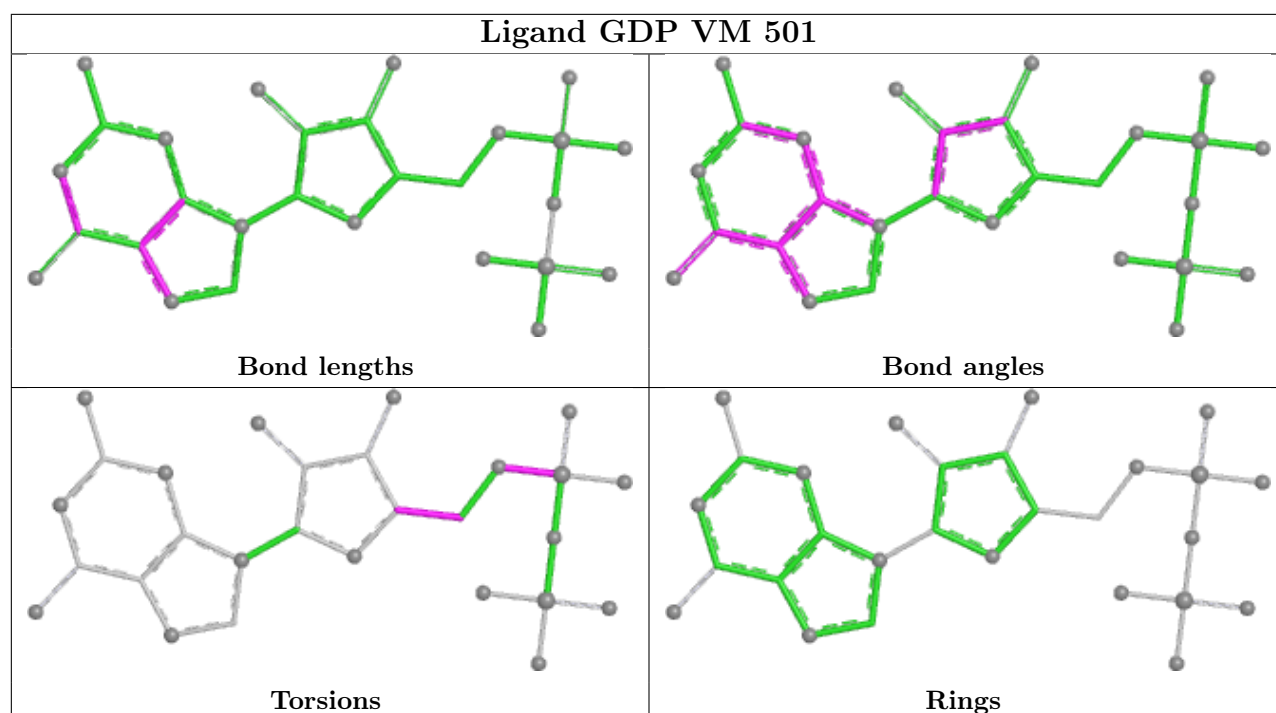




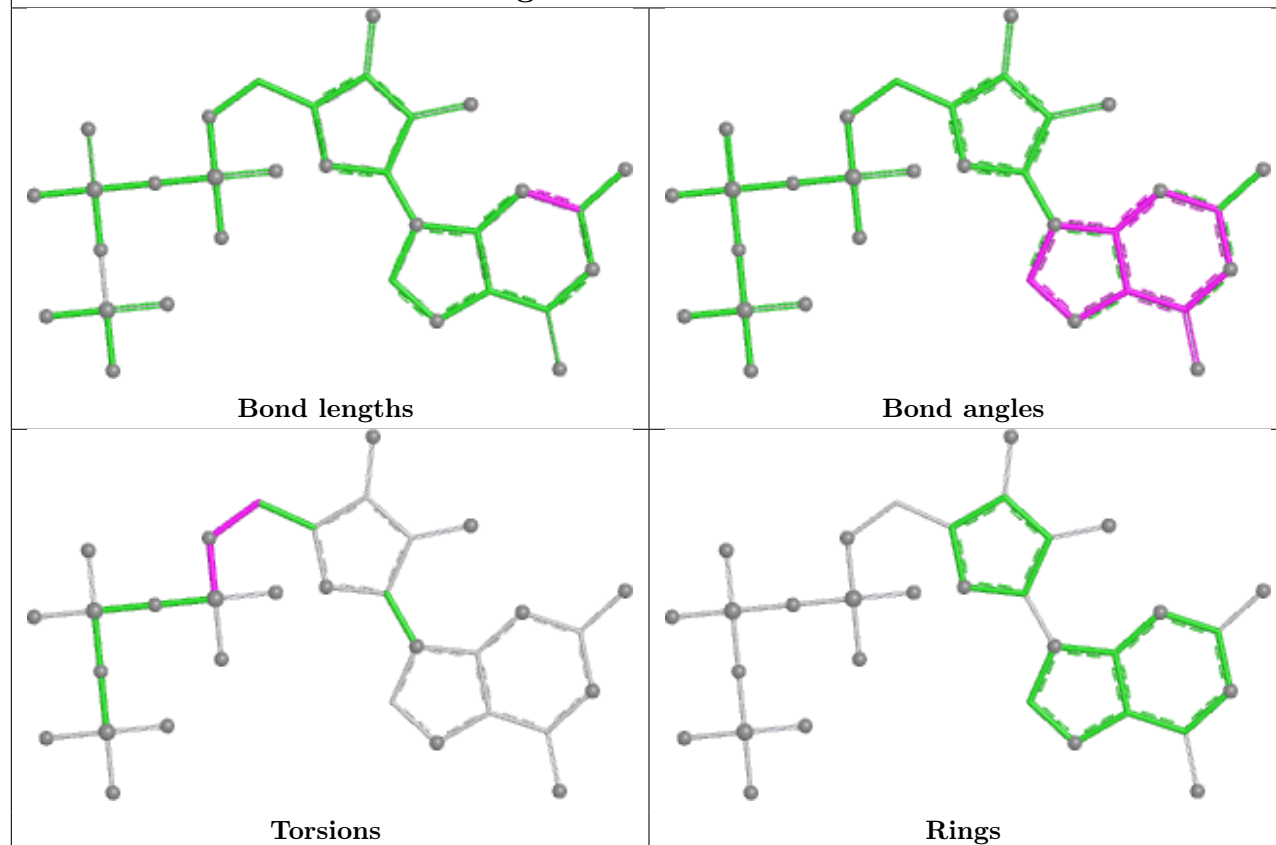




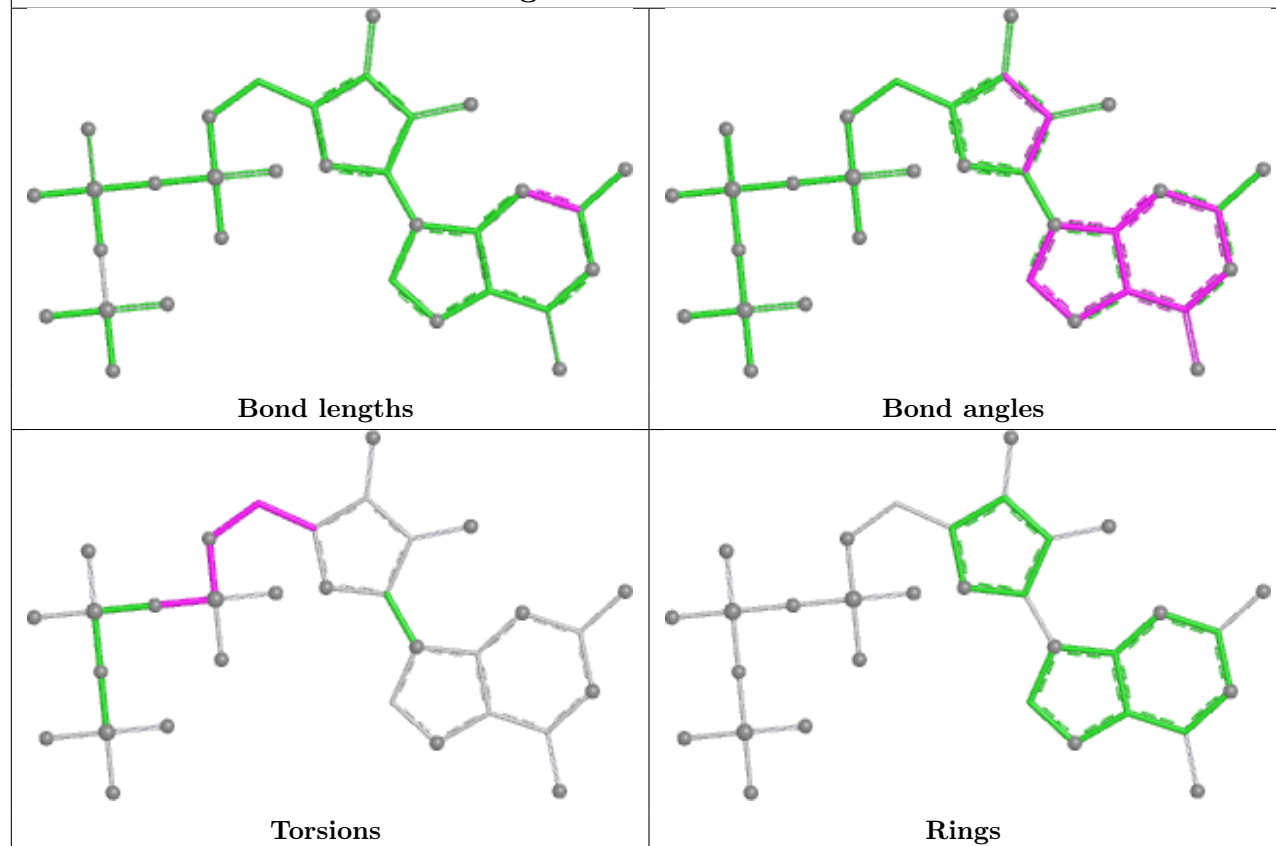


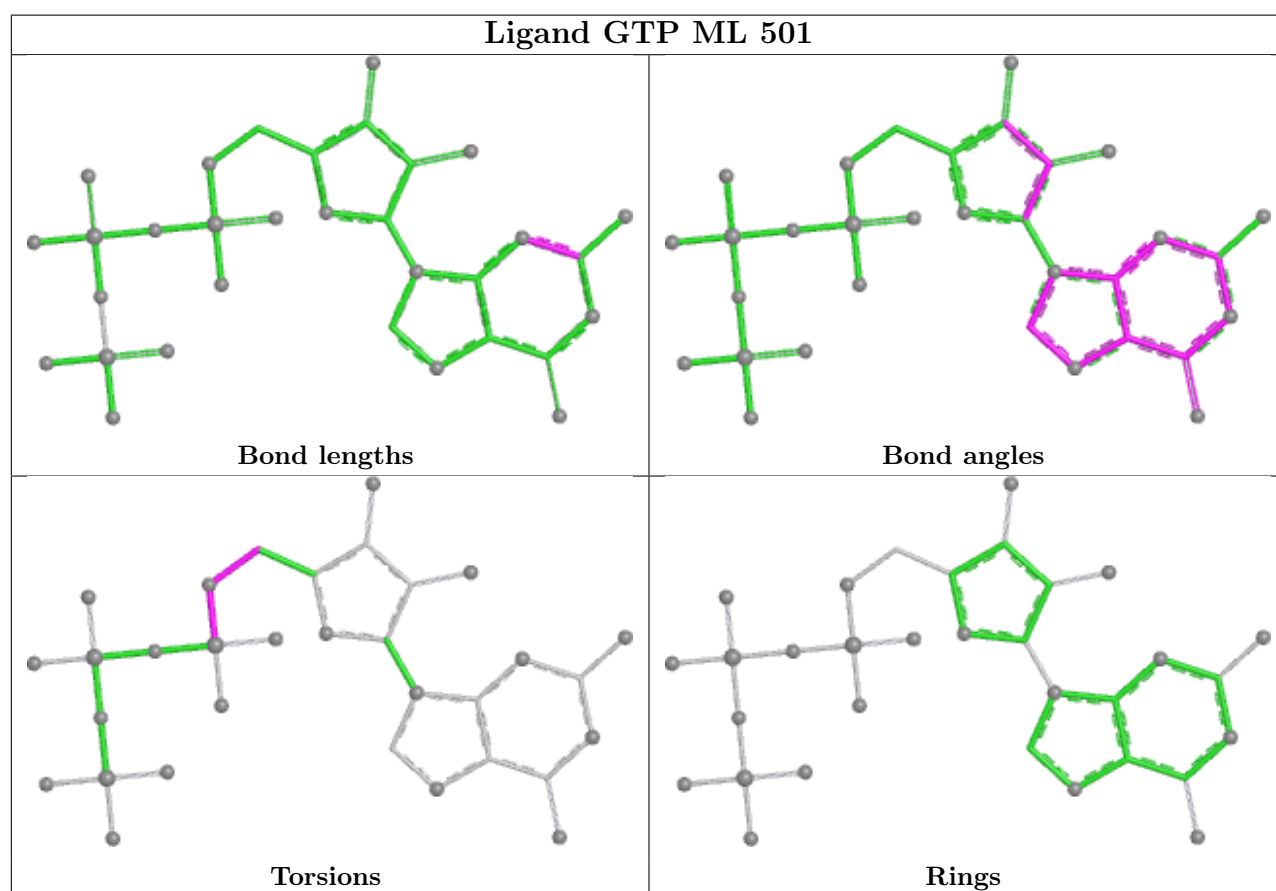
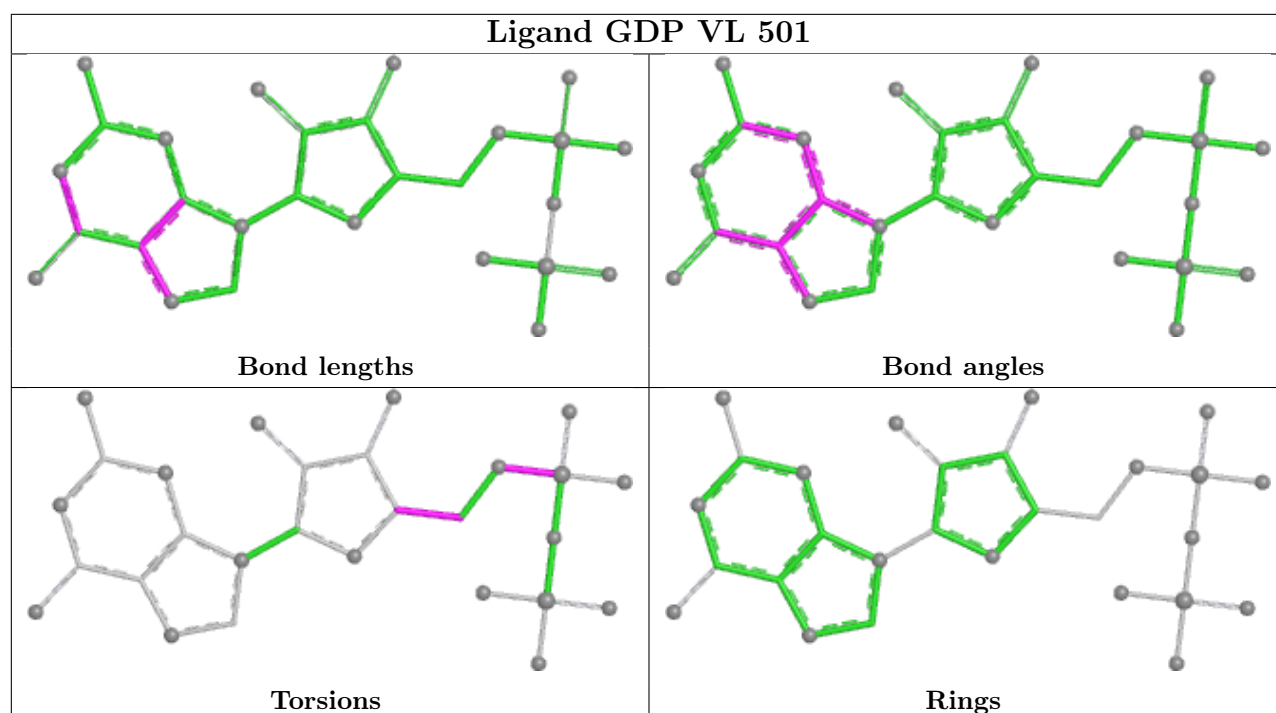


Ligand GTP CG 501

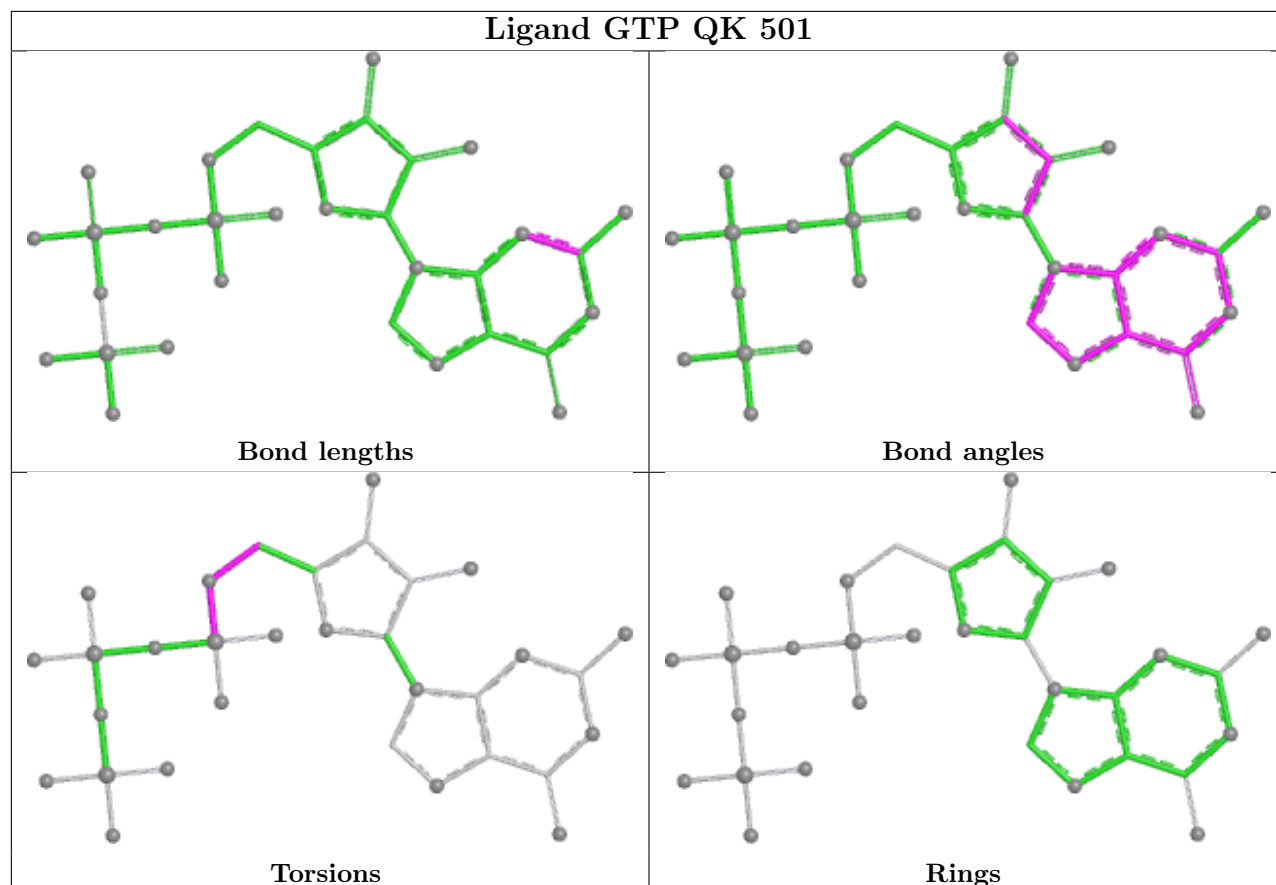


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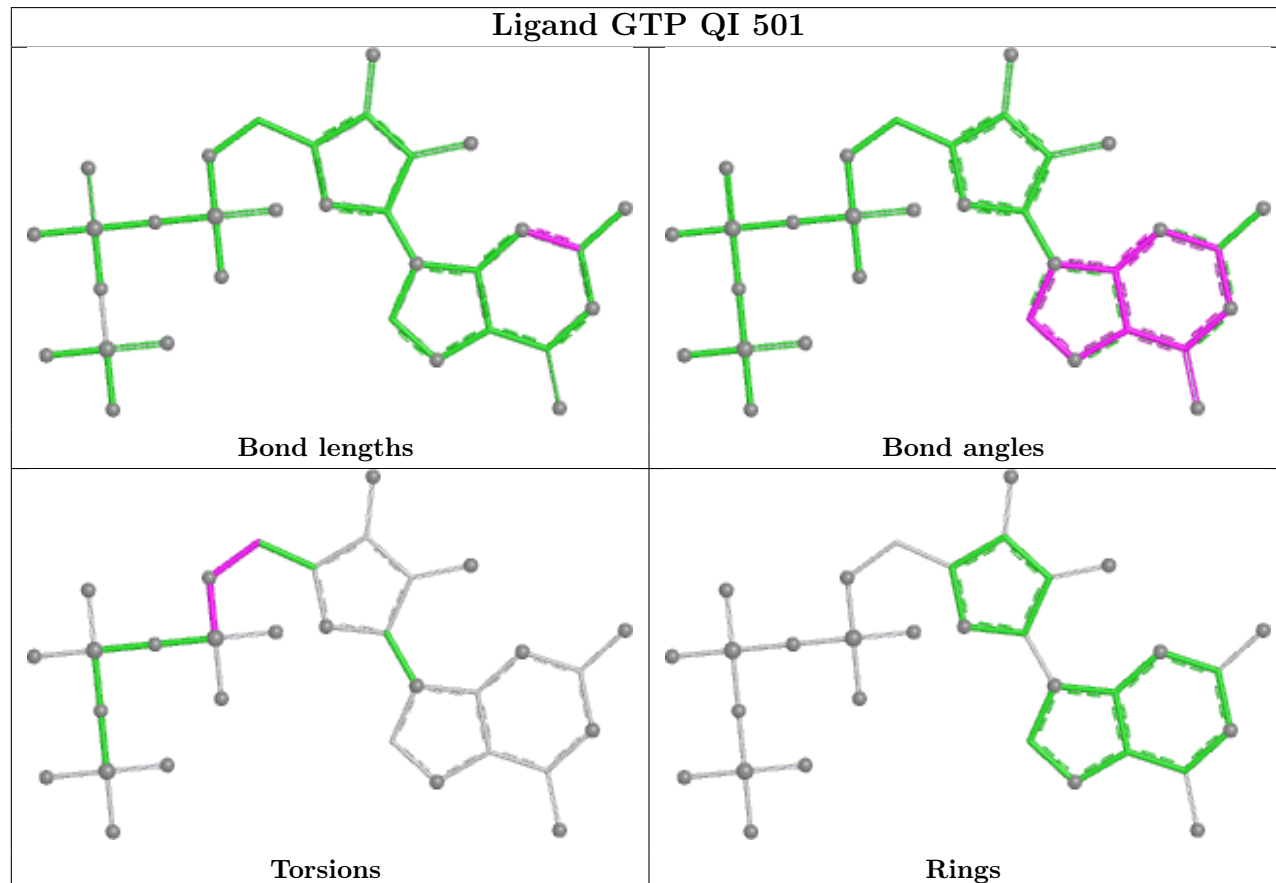




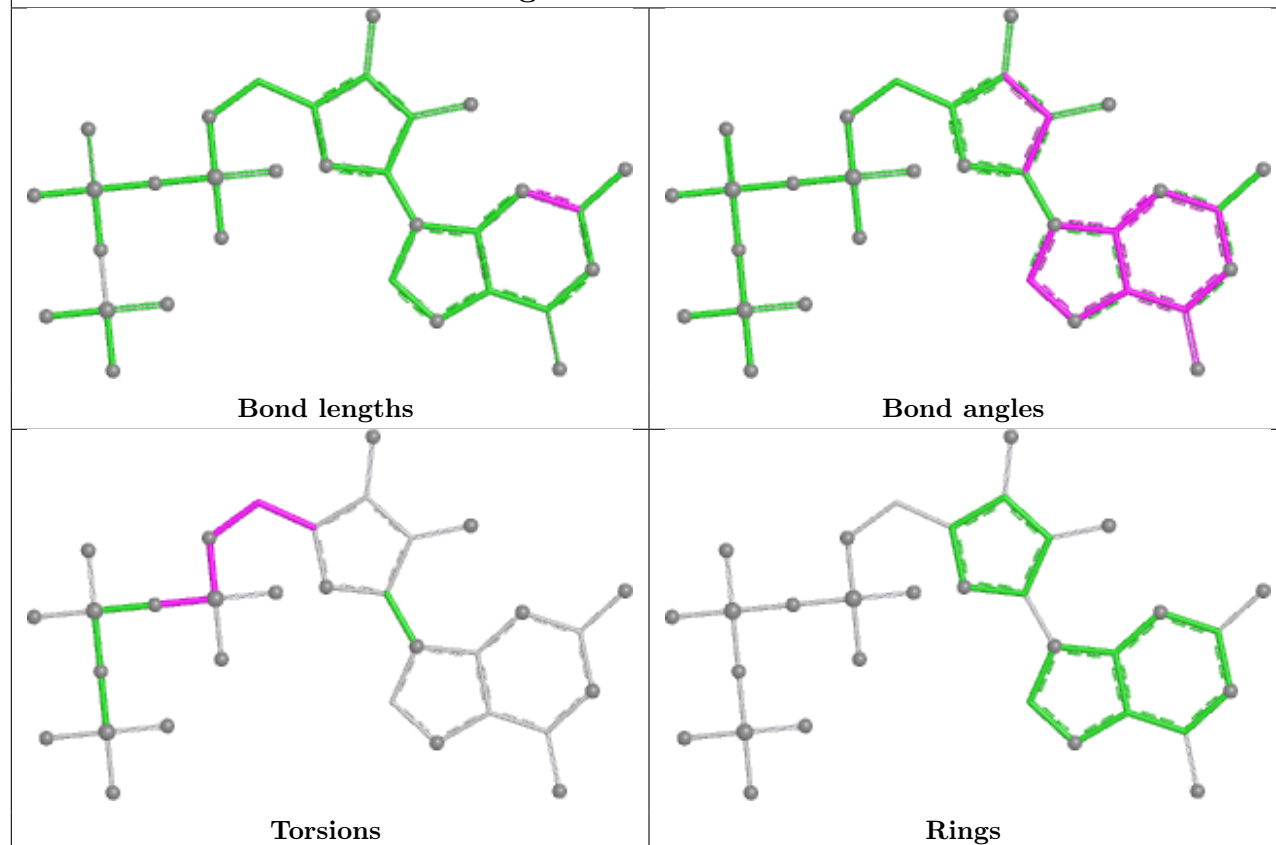
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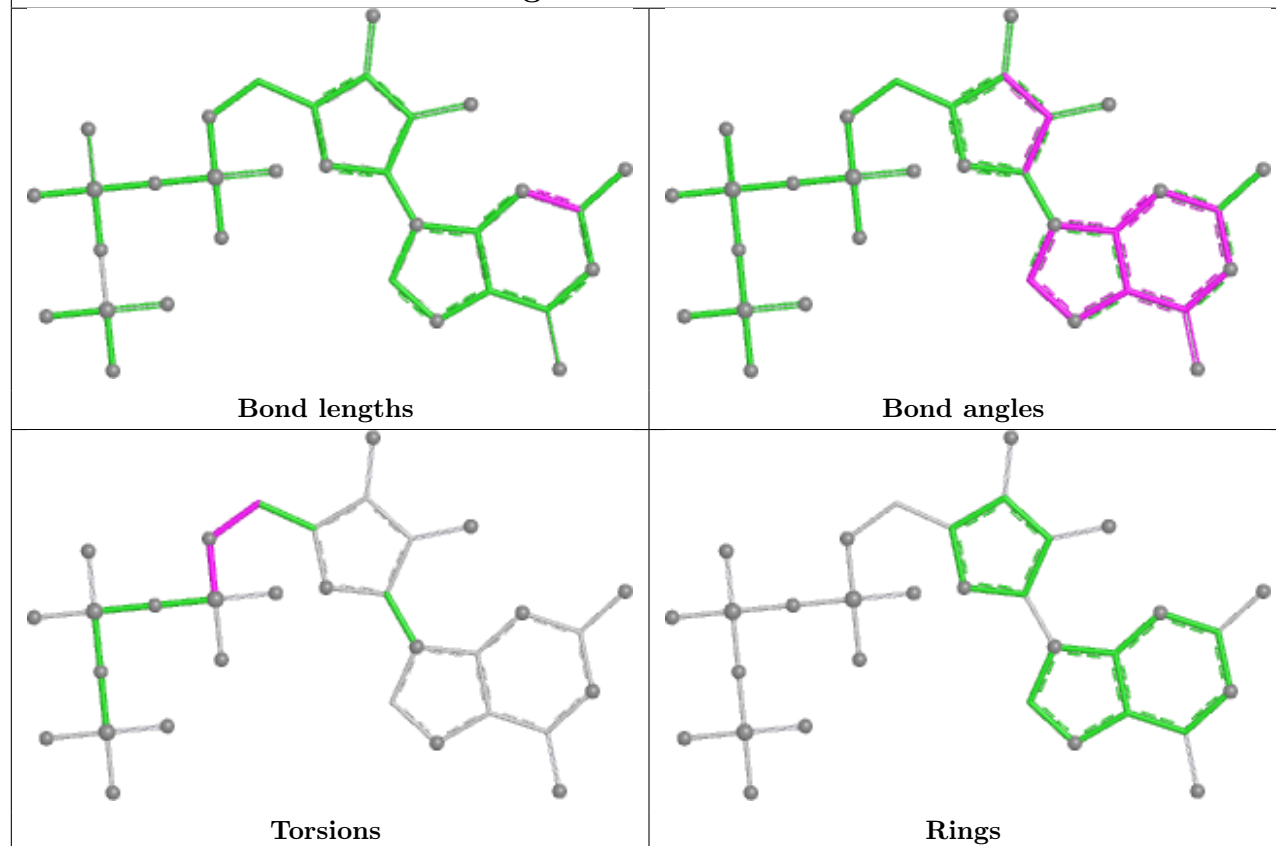
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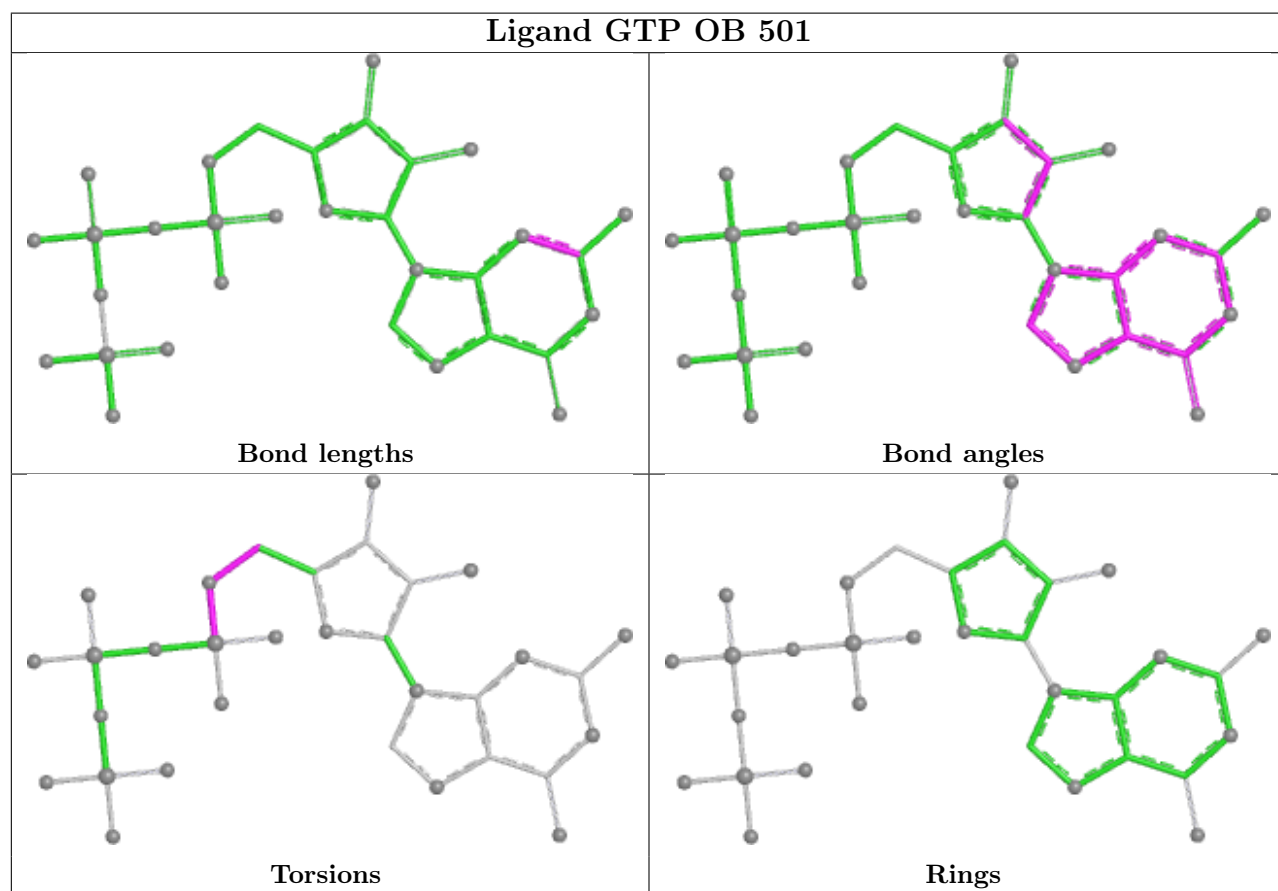
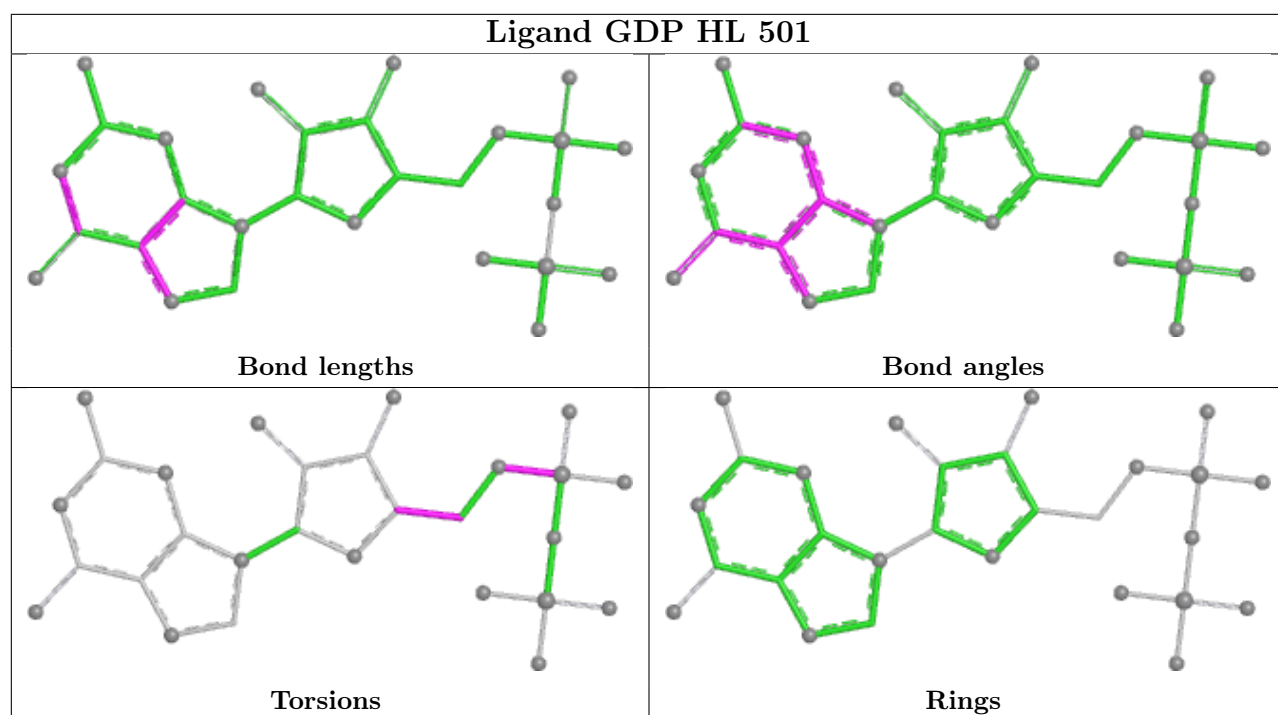


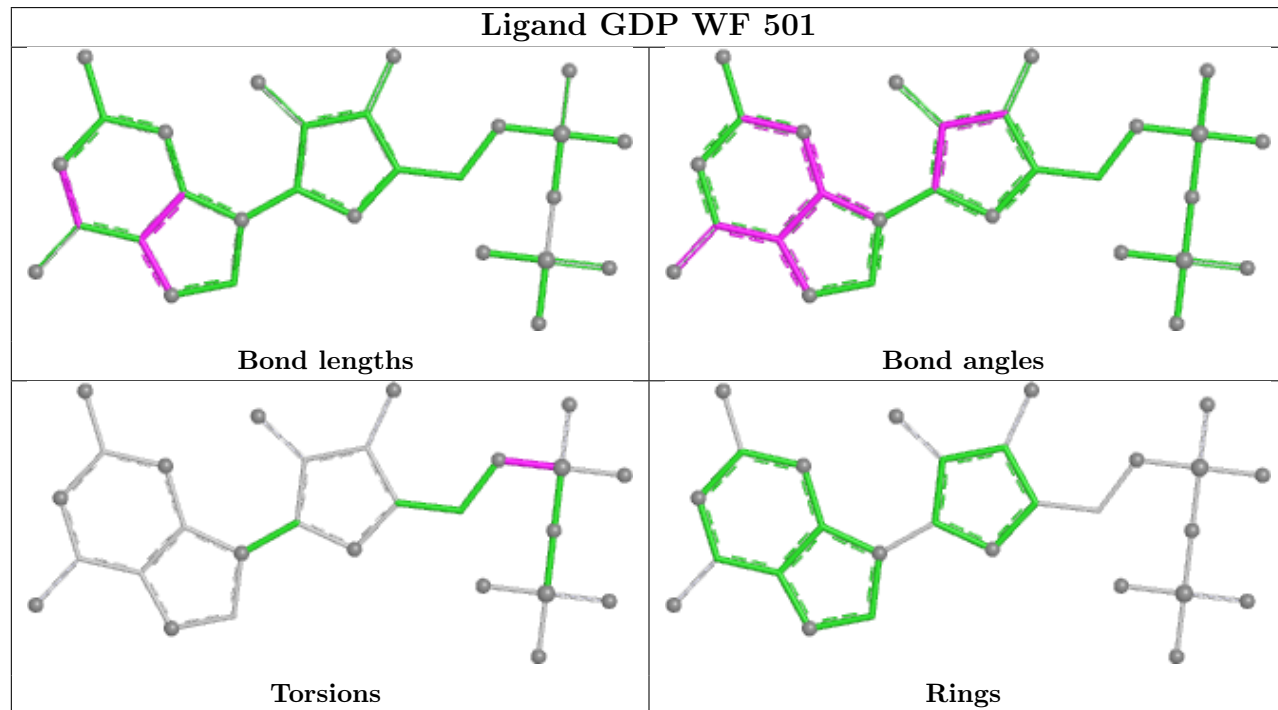
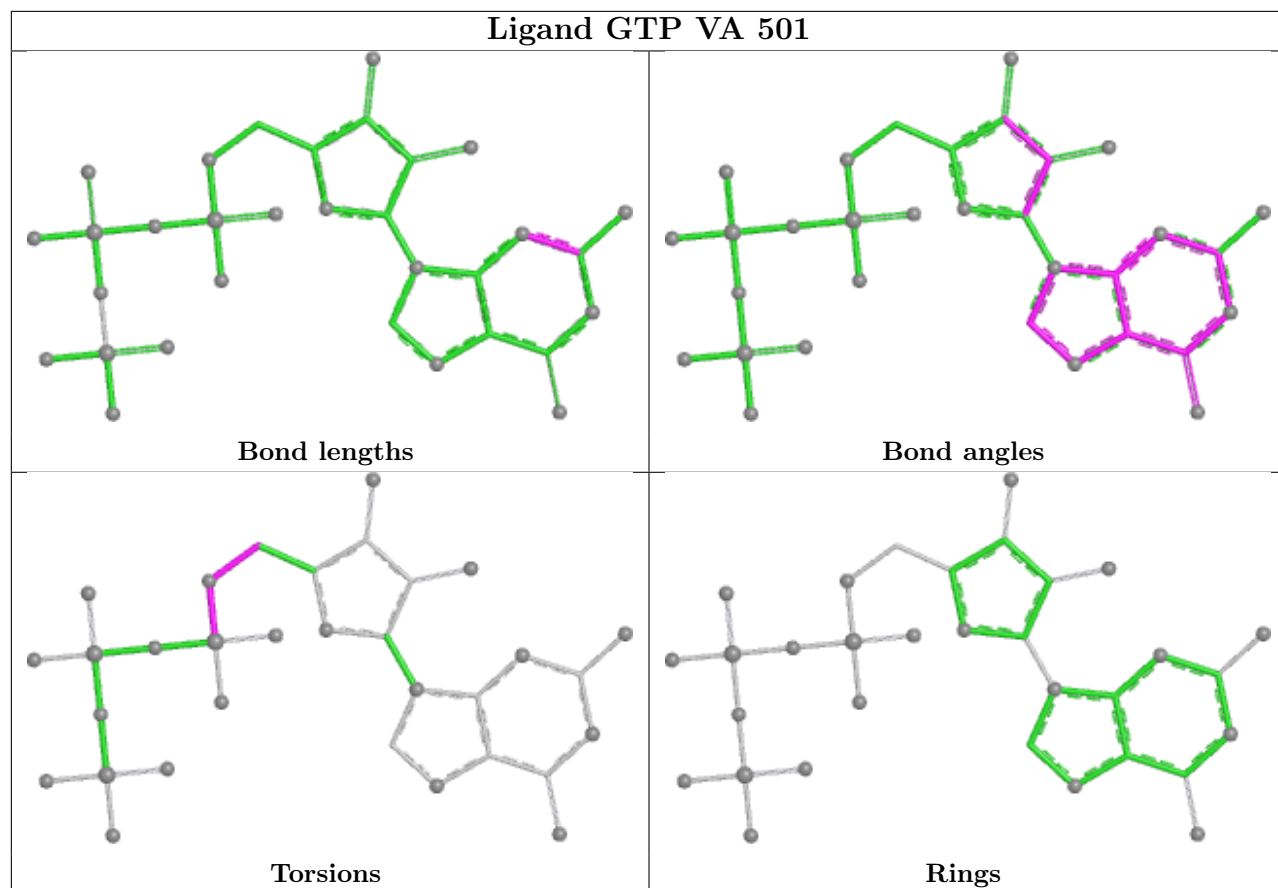
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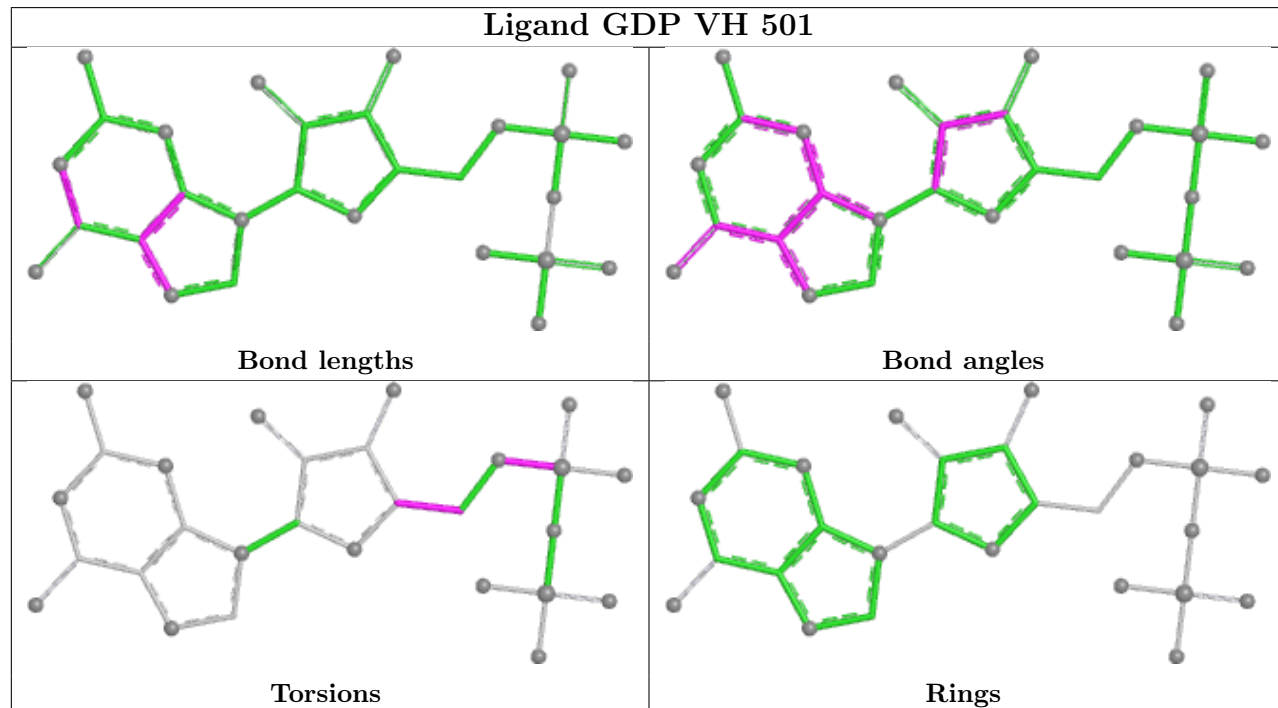
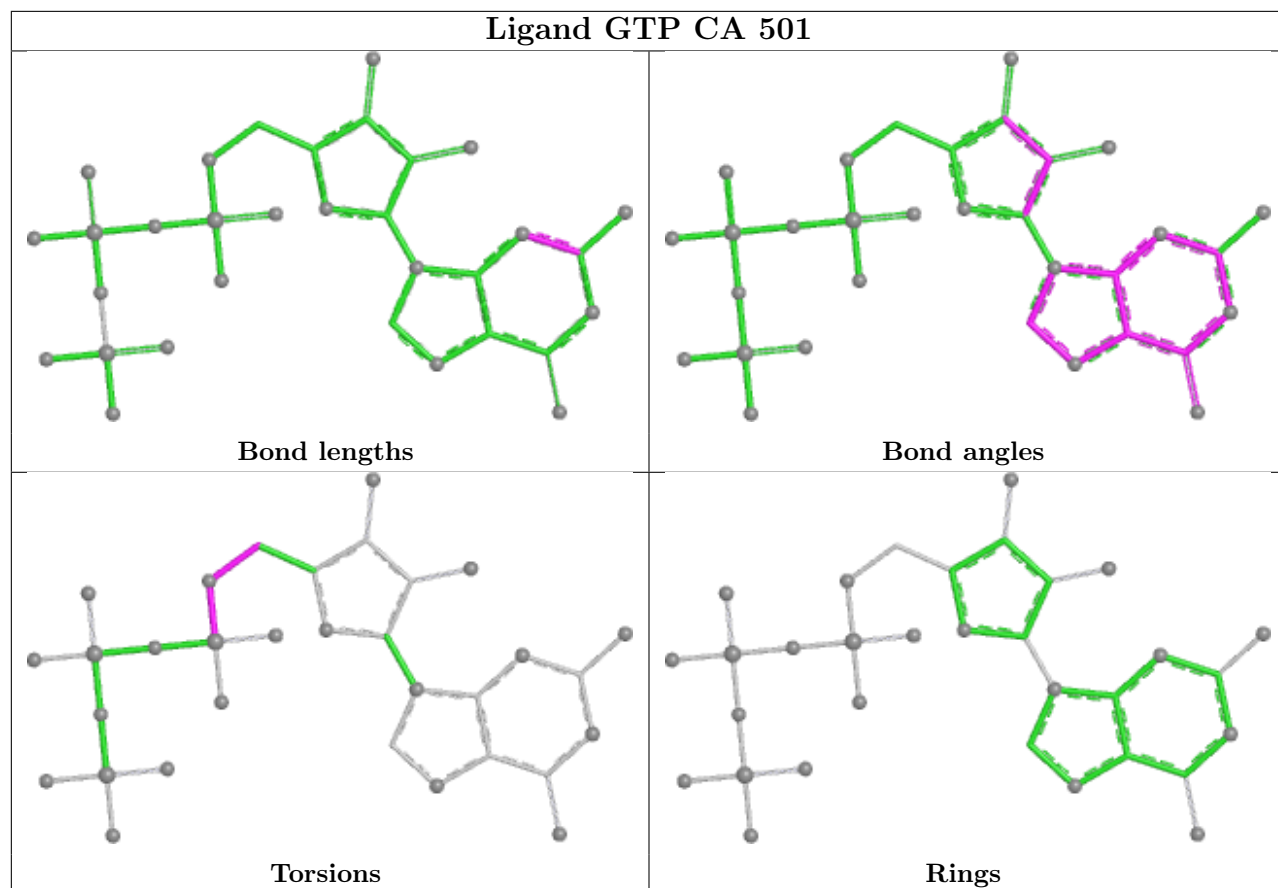


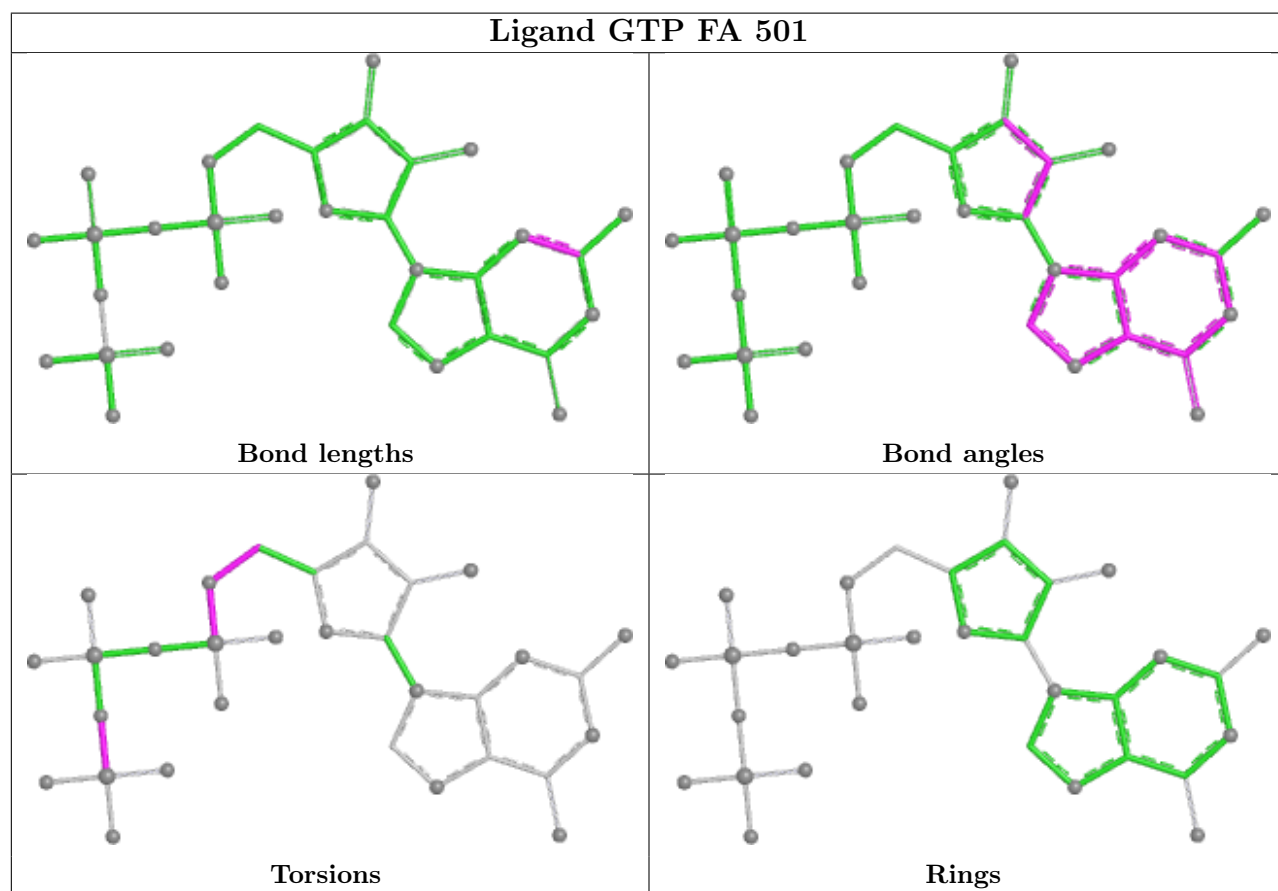
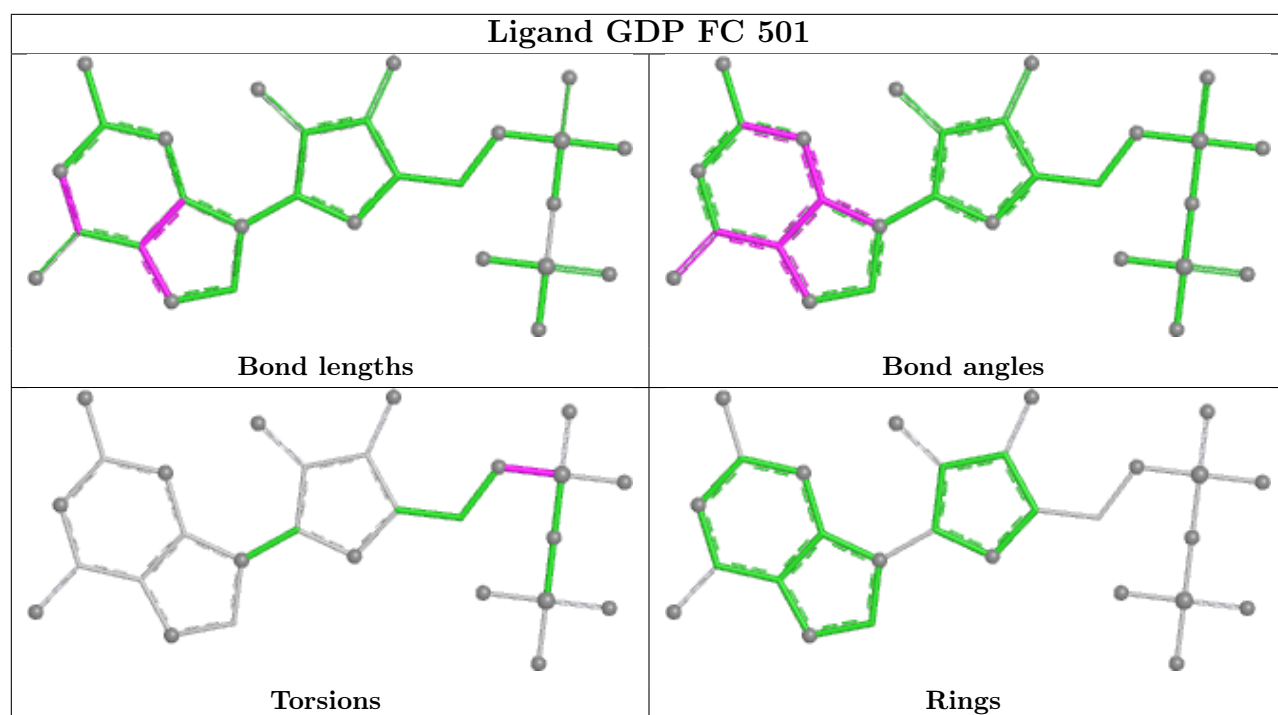
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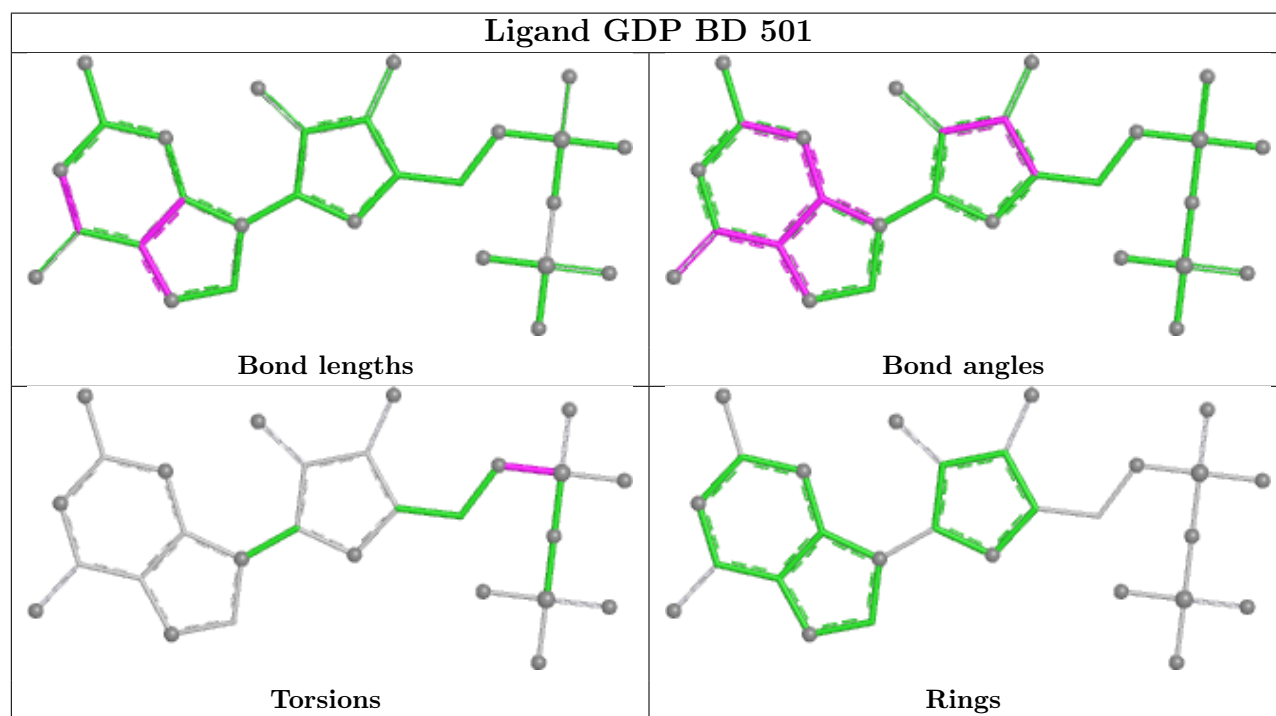
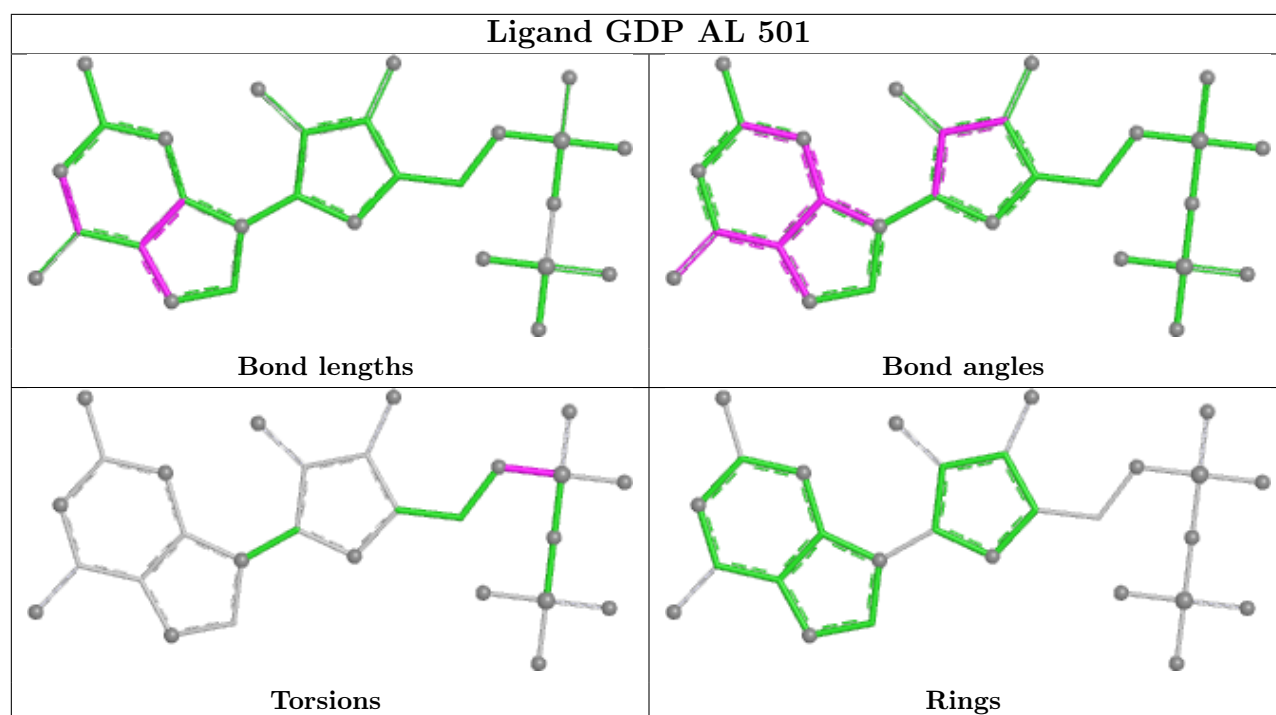


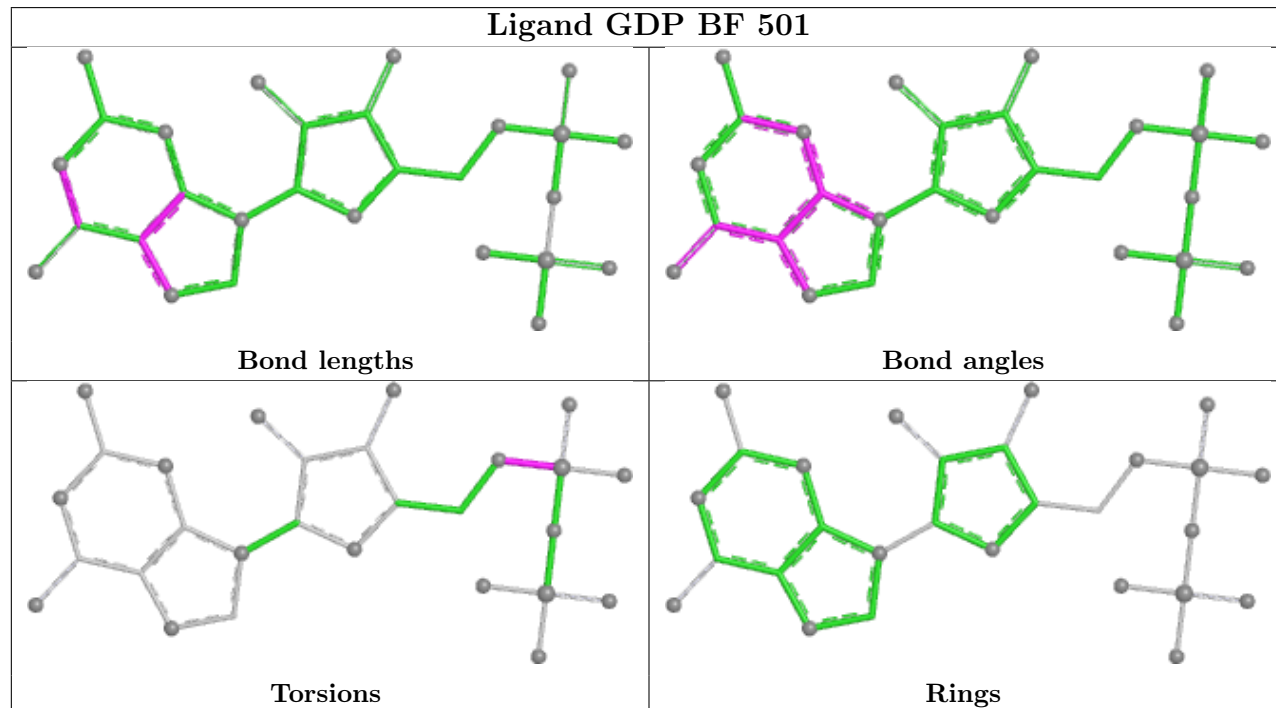
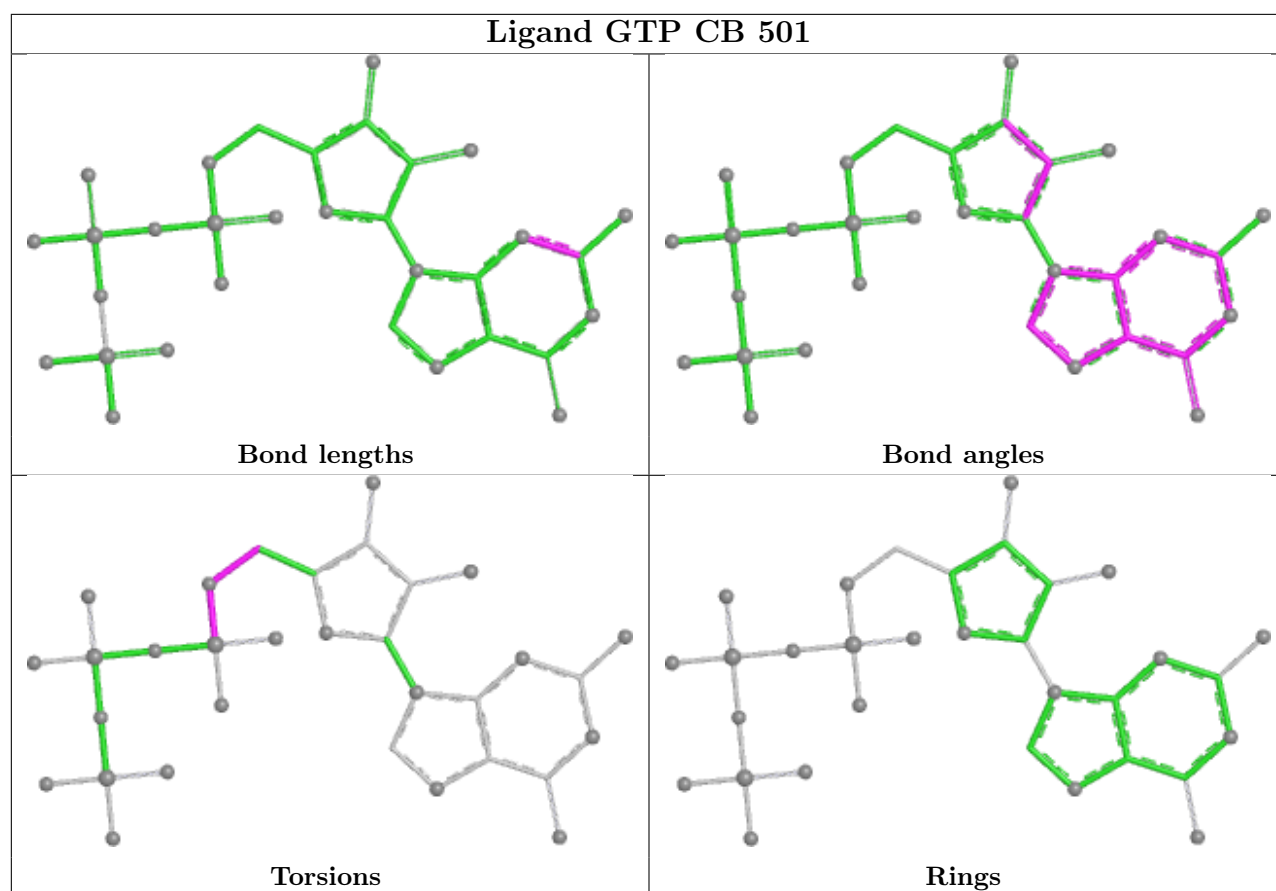


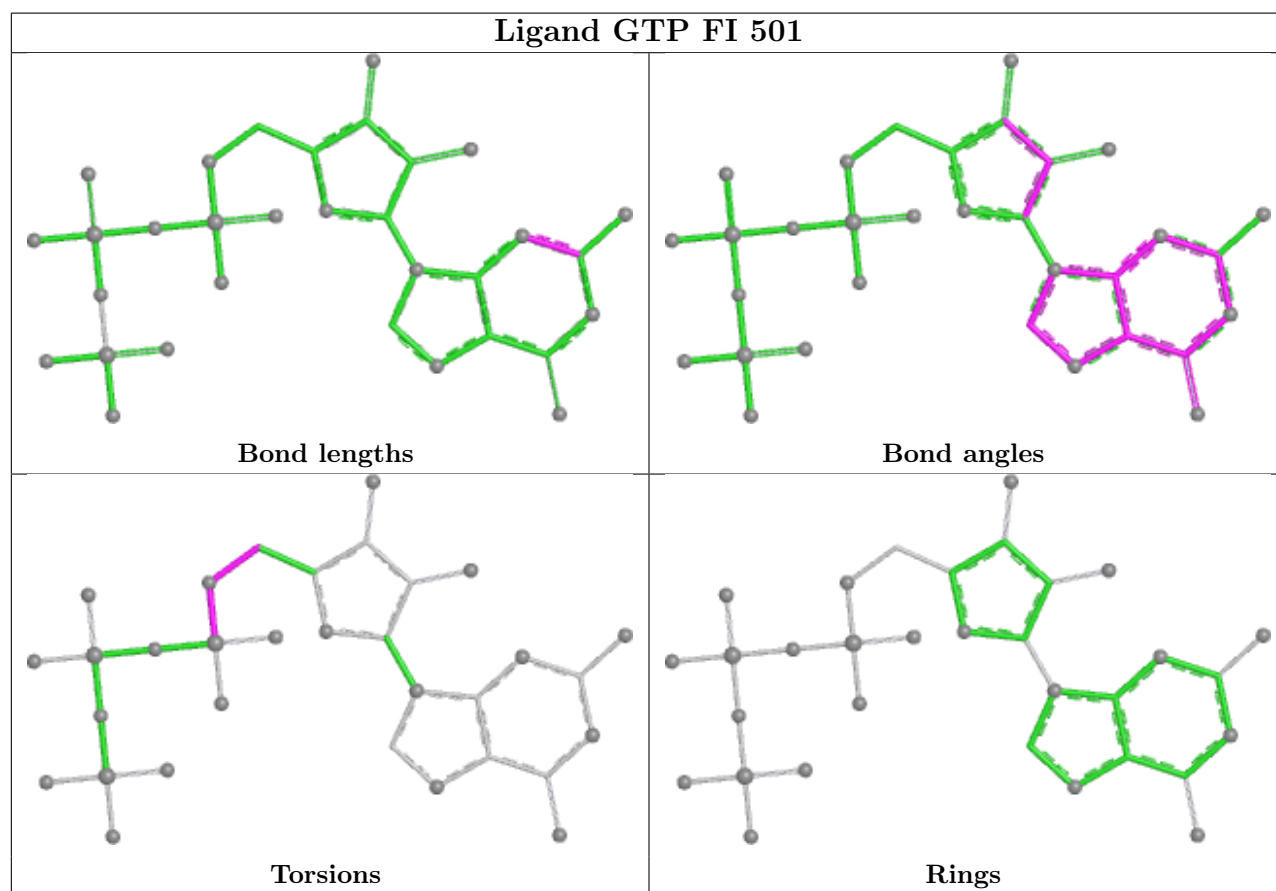
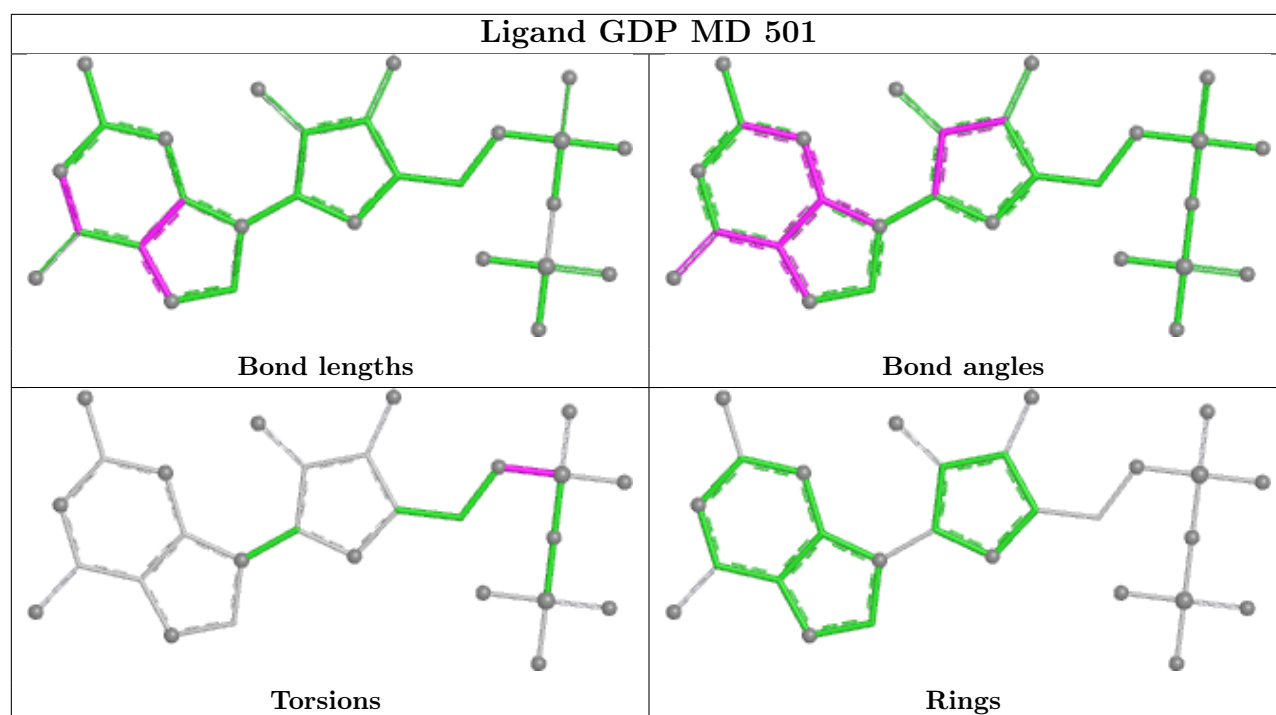


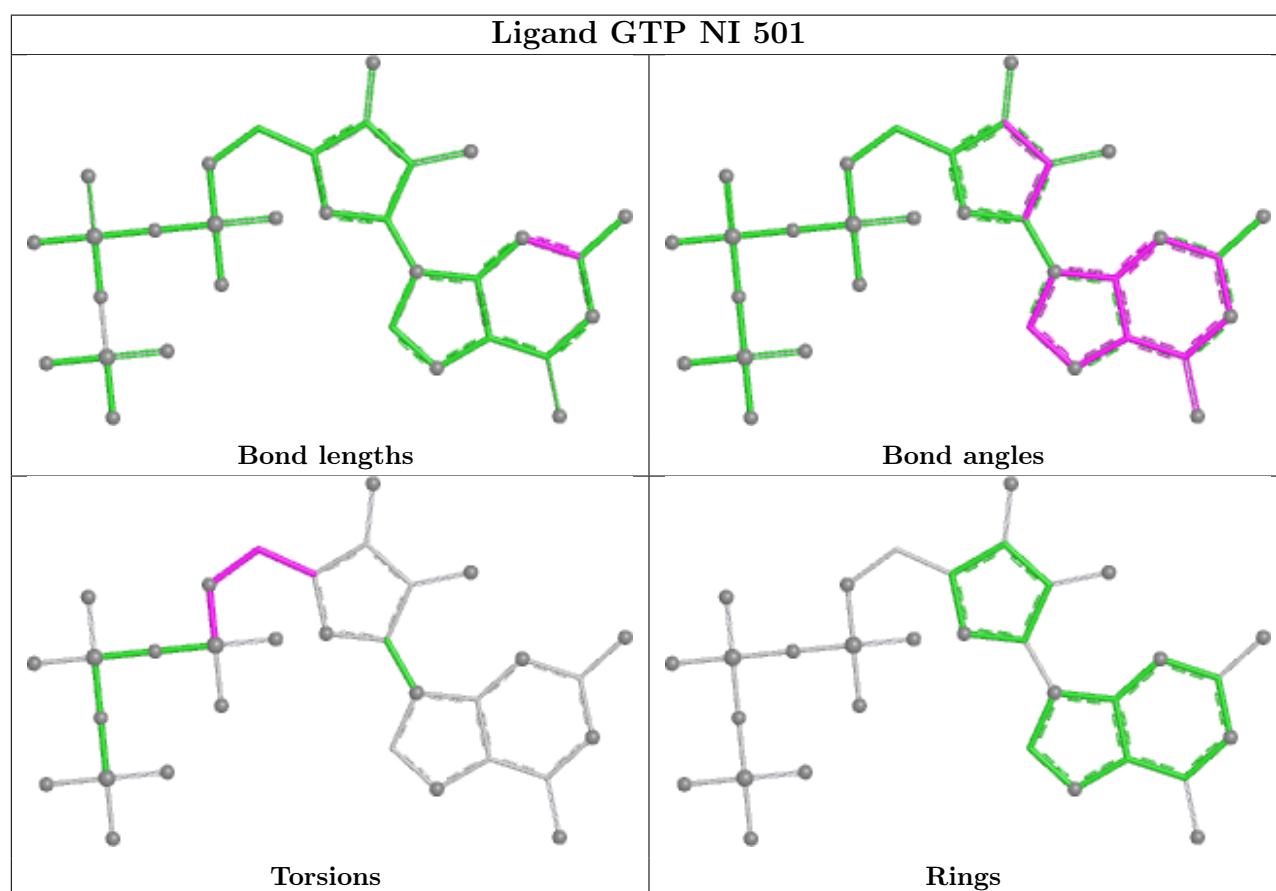
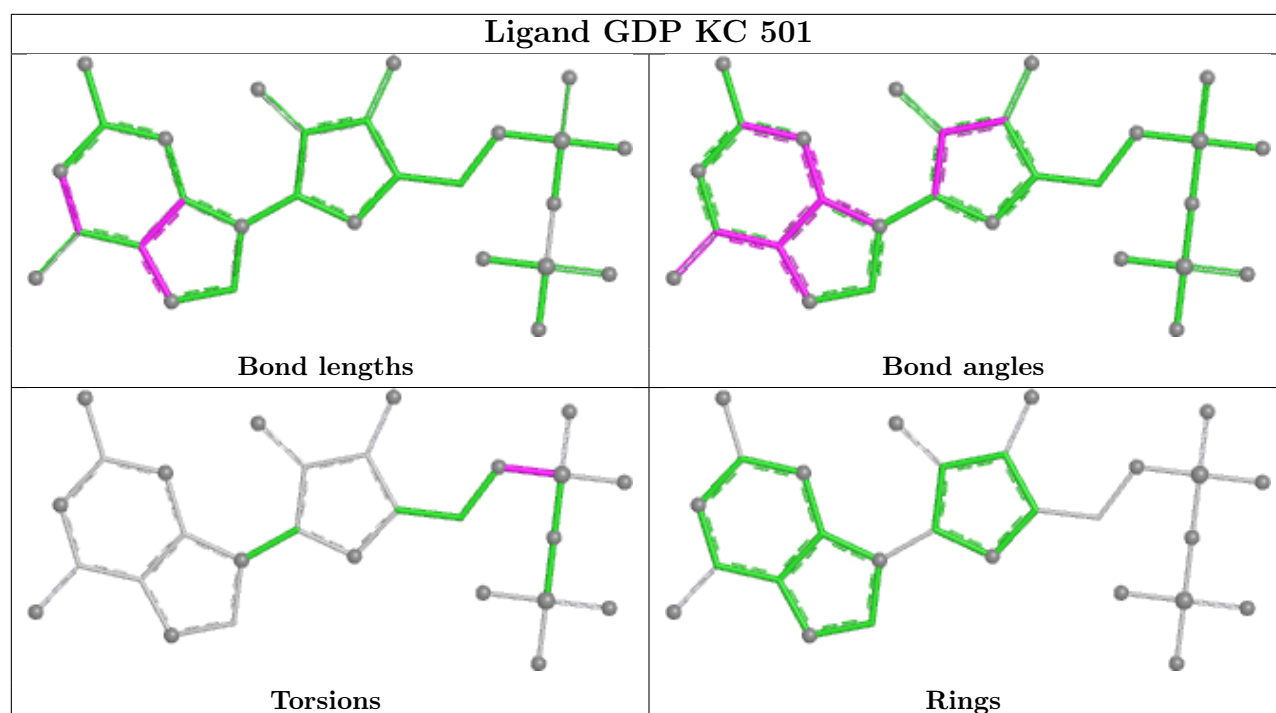




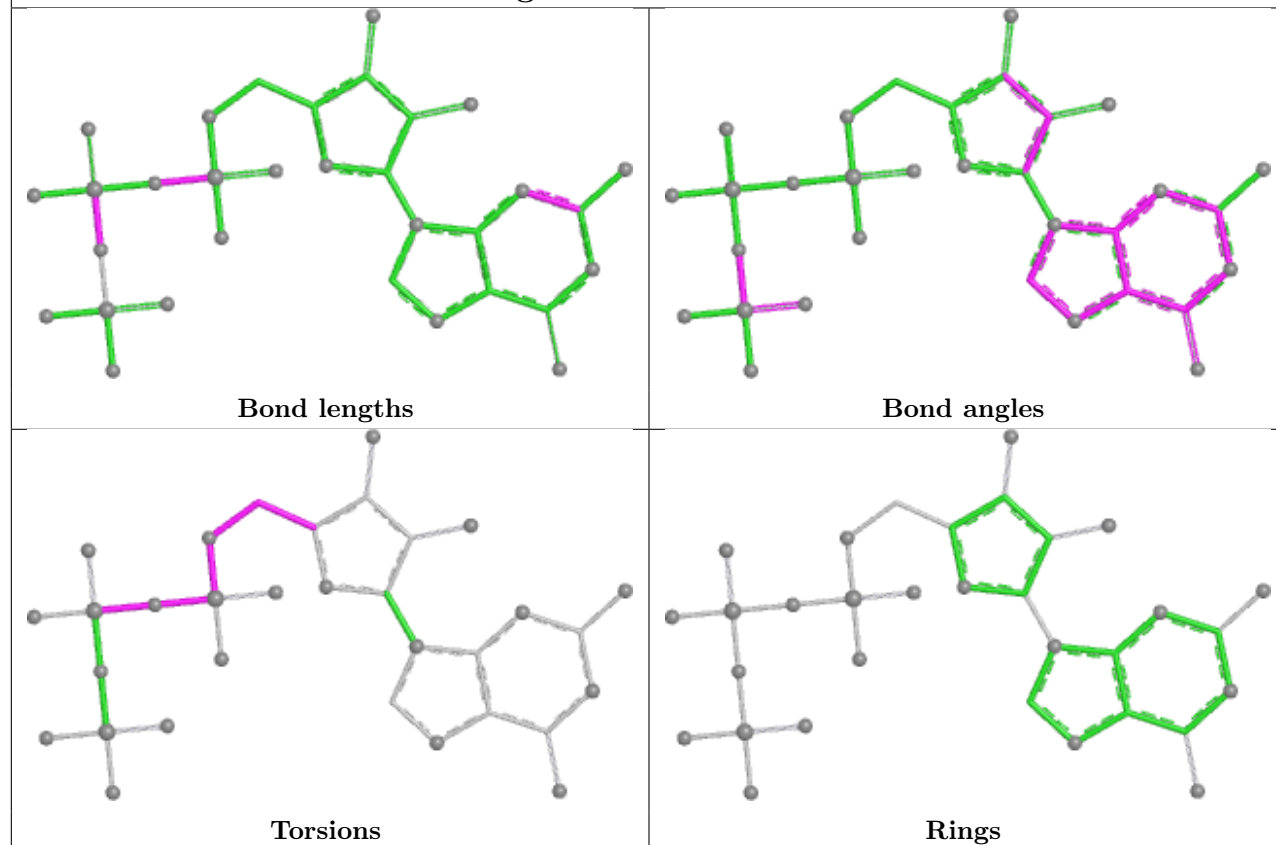




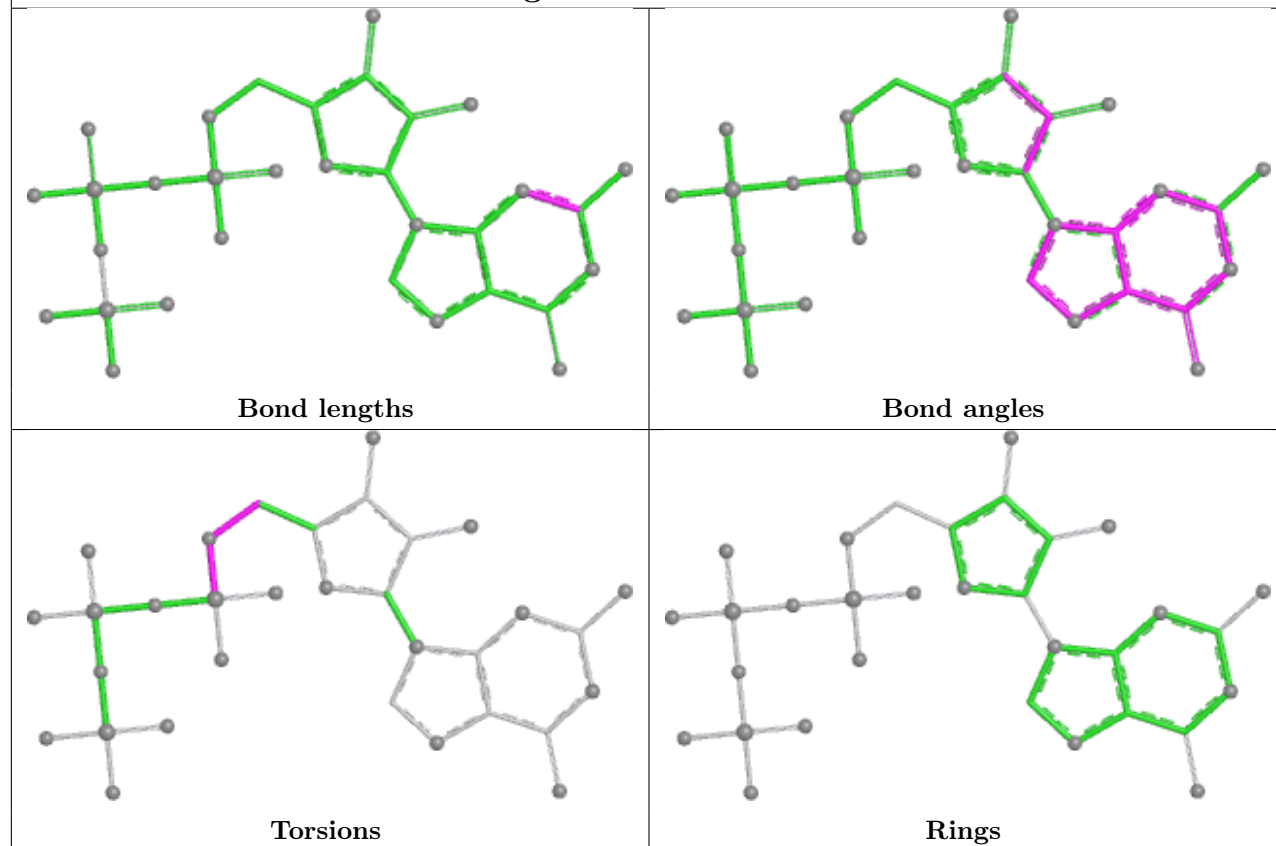




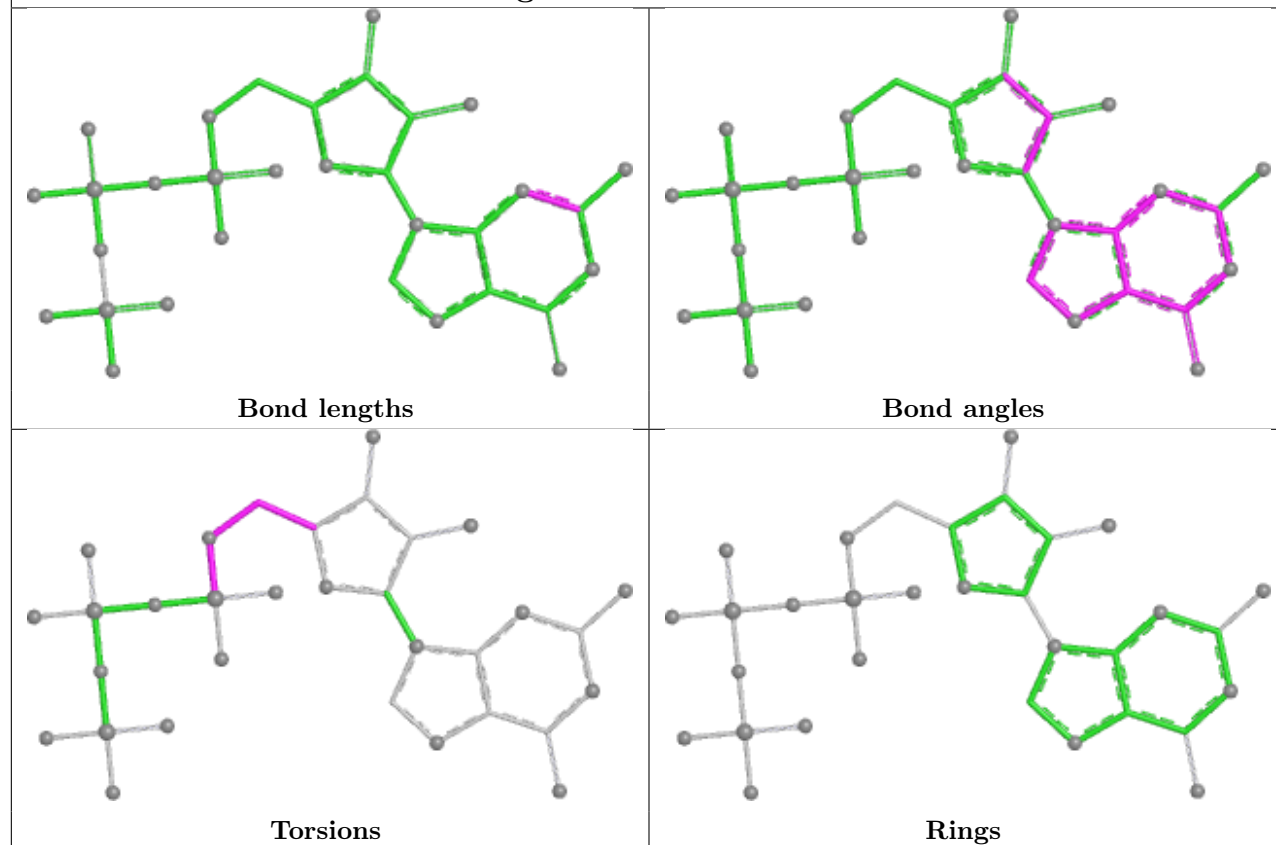
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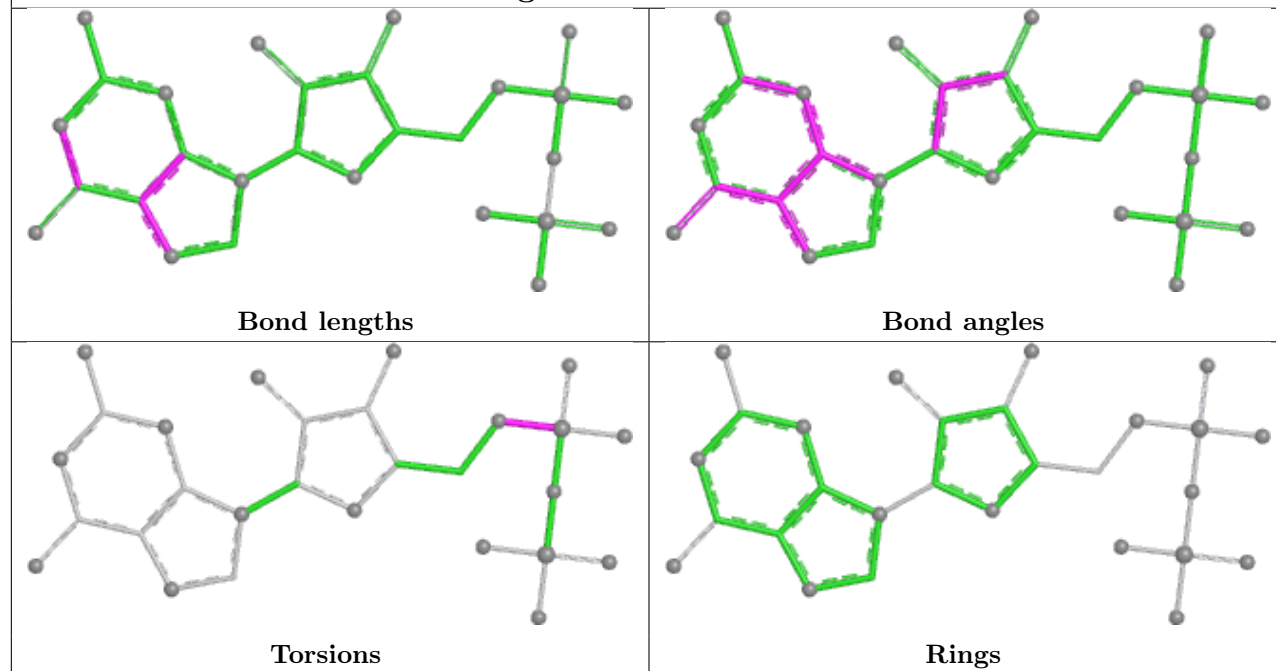
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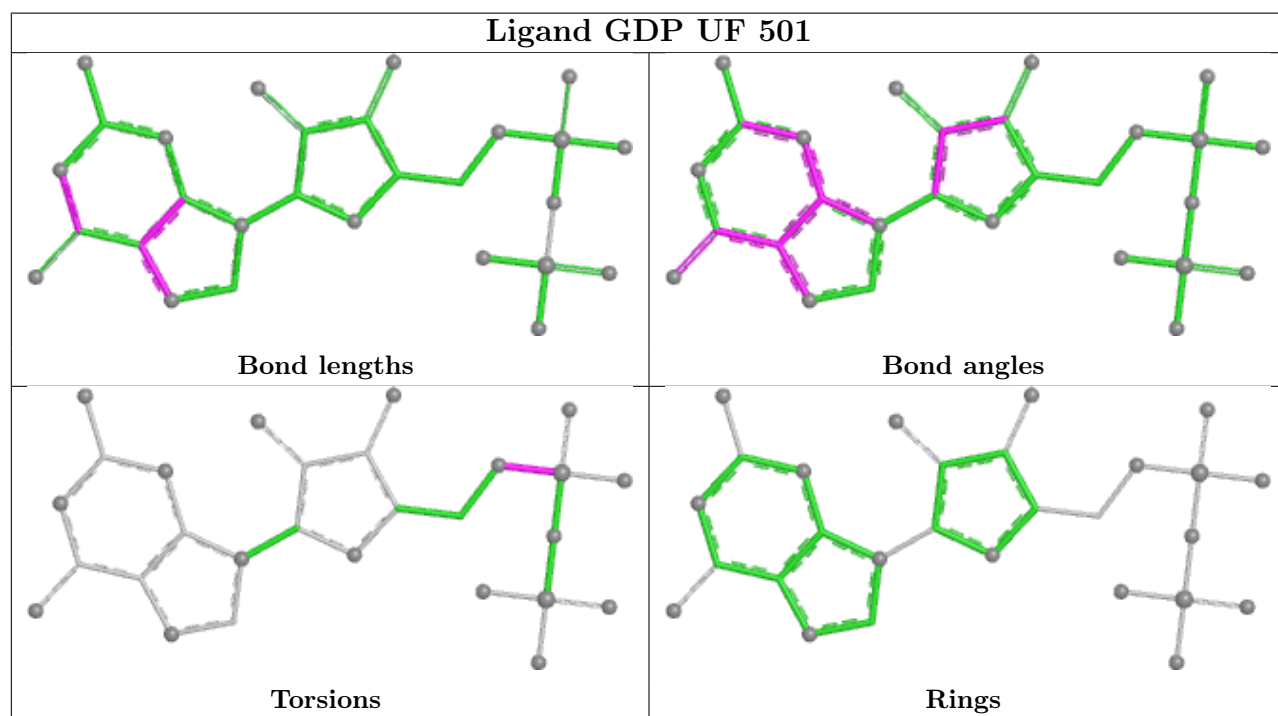
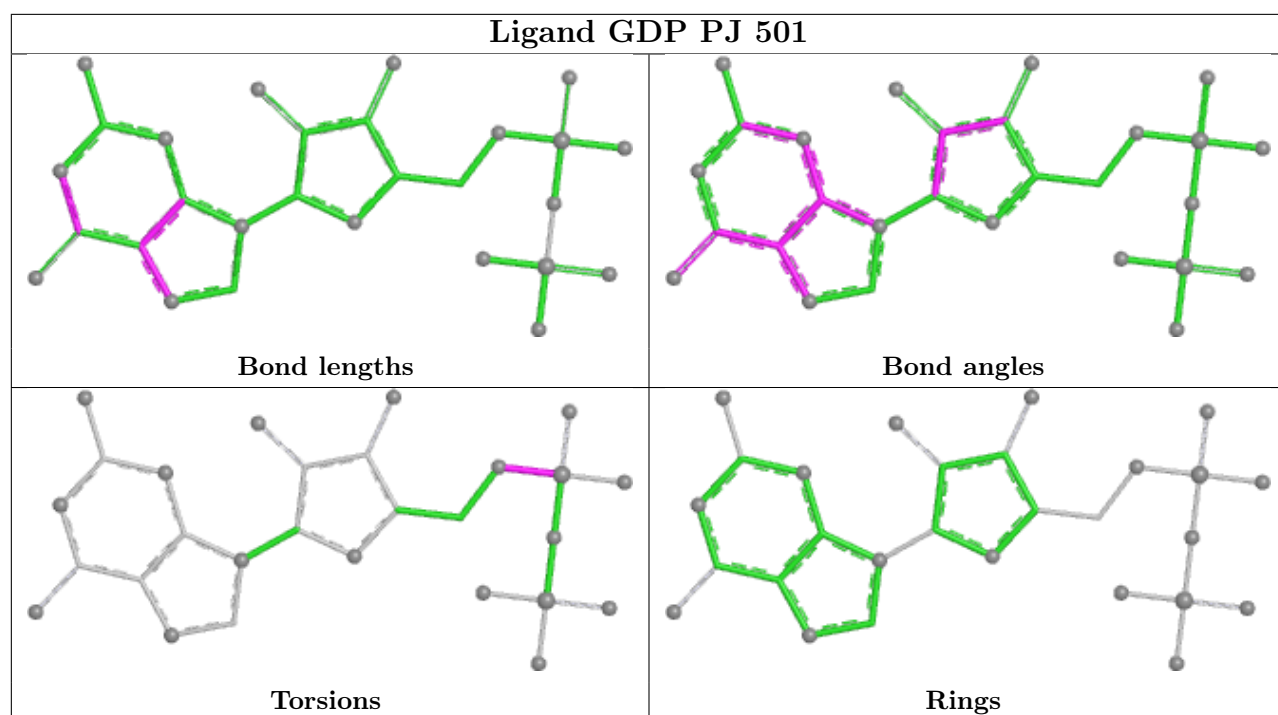


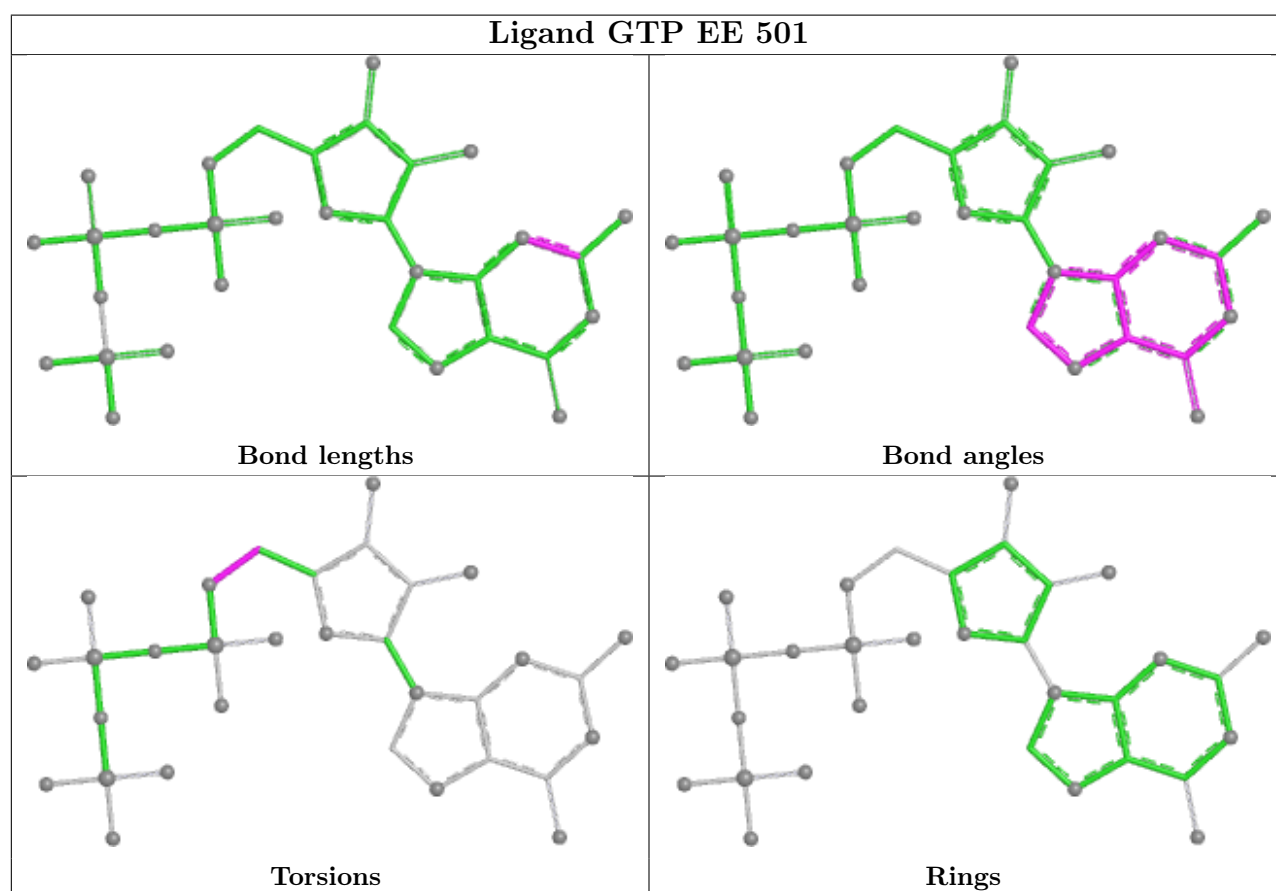
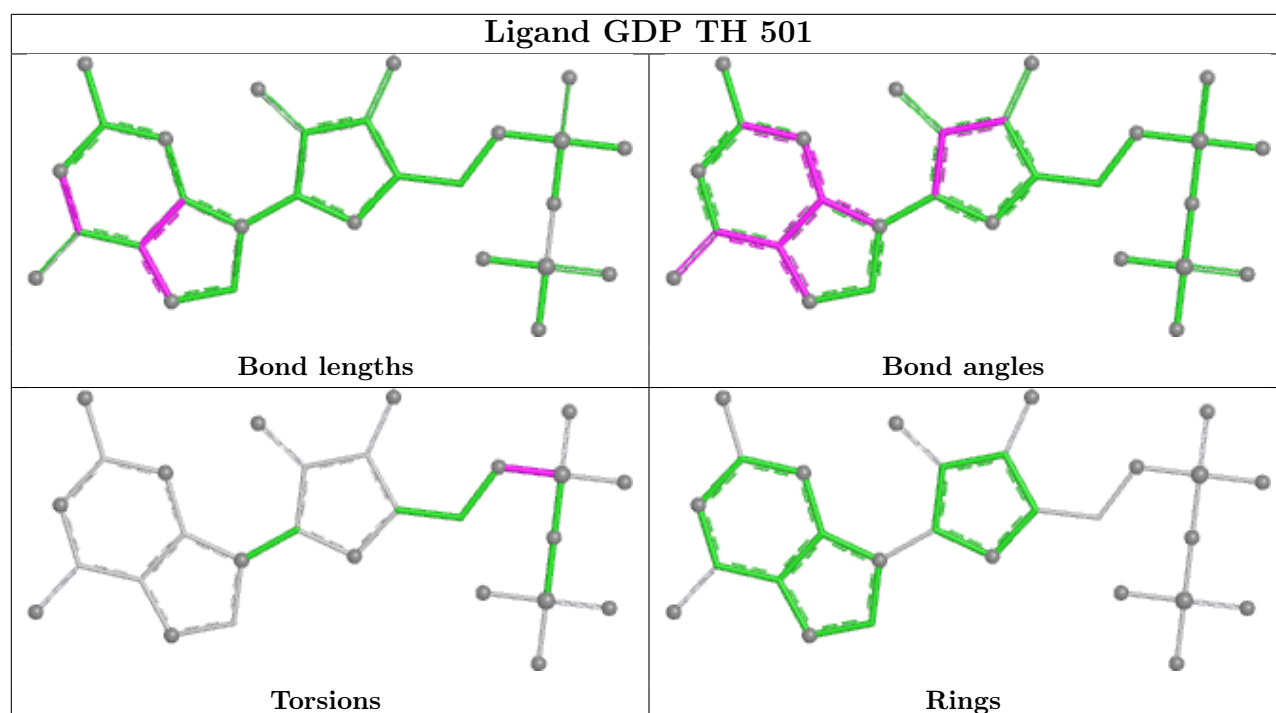
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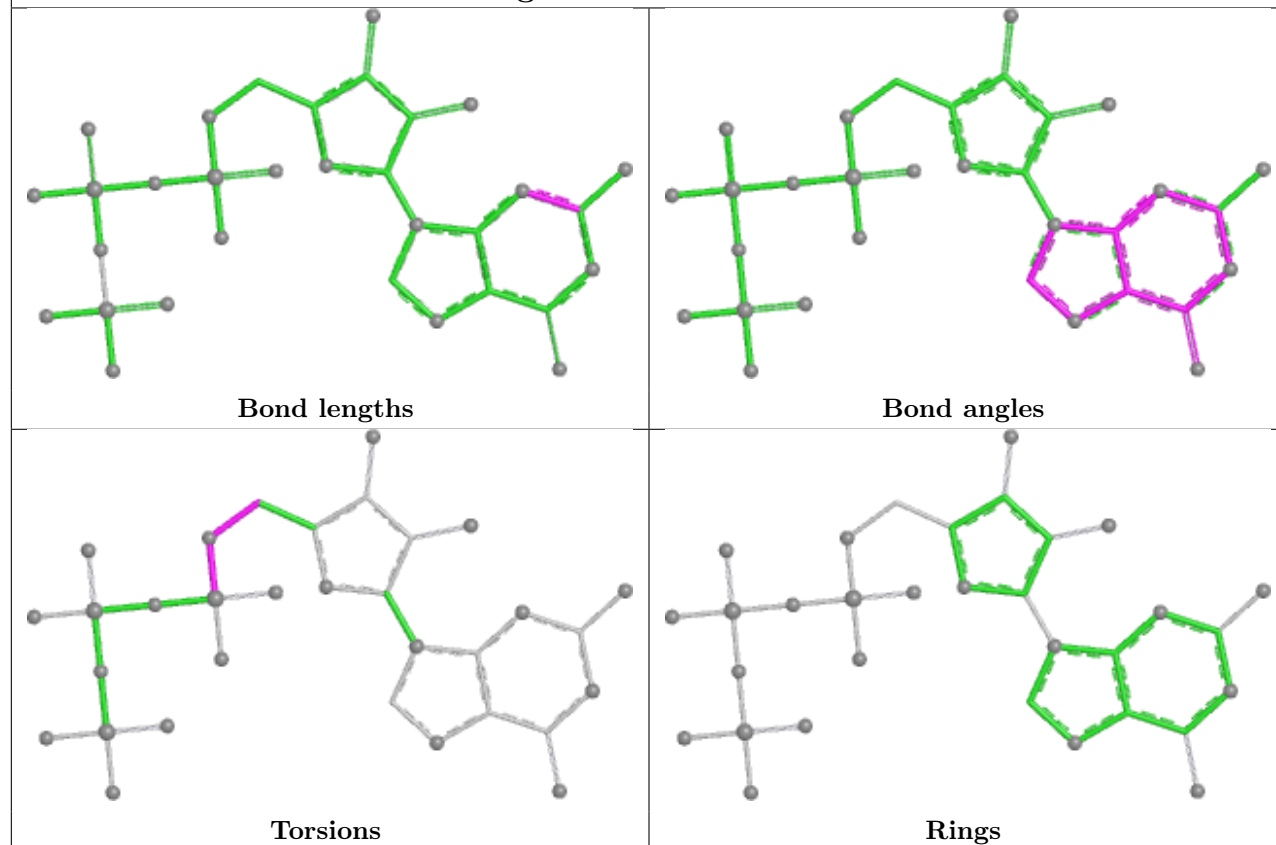
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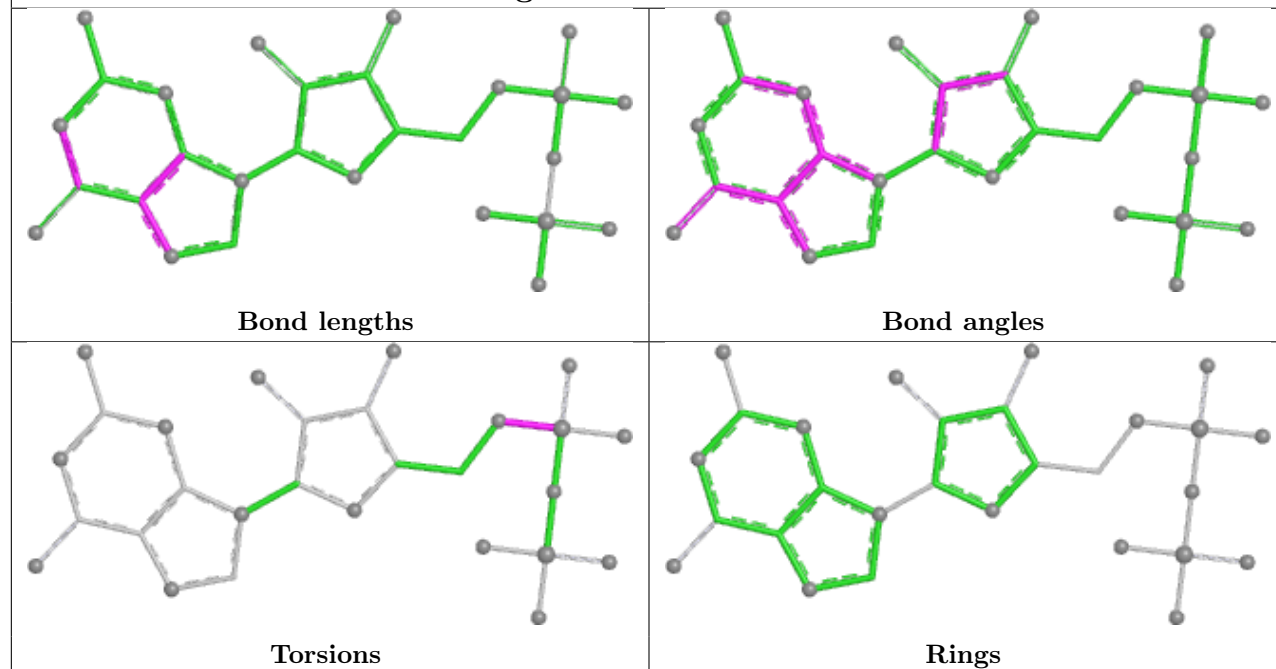


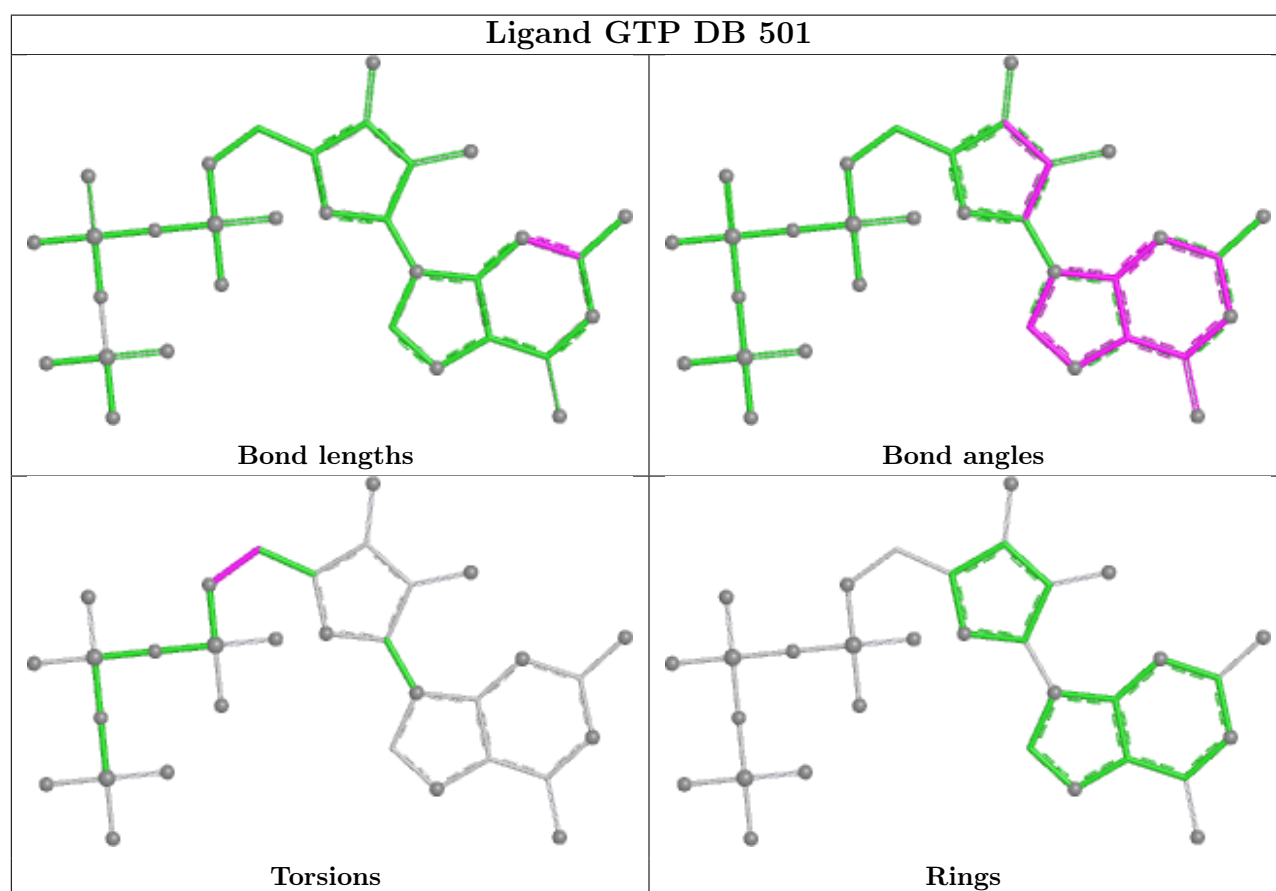
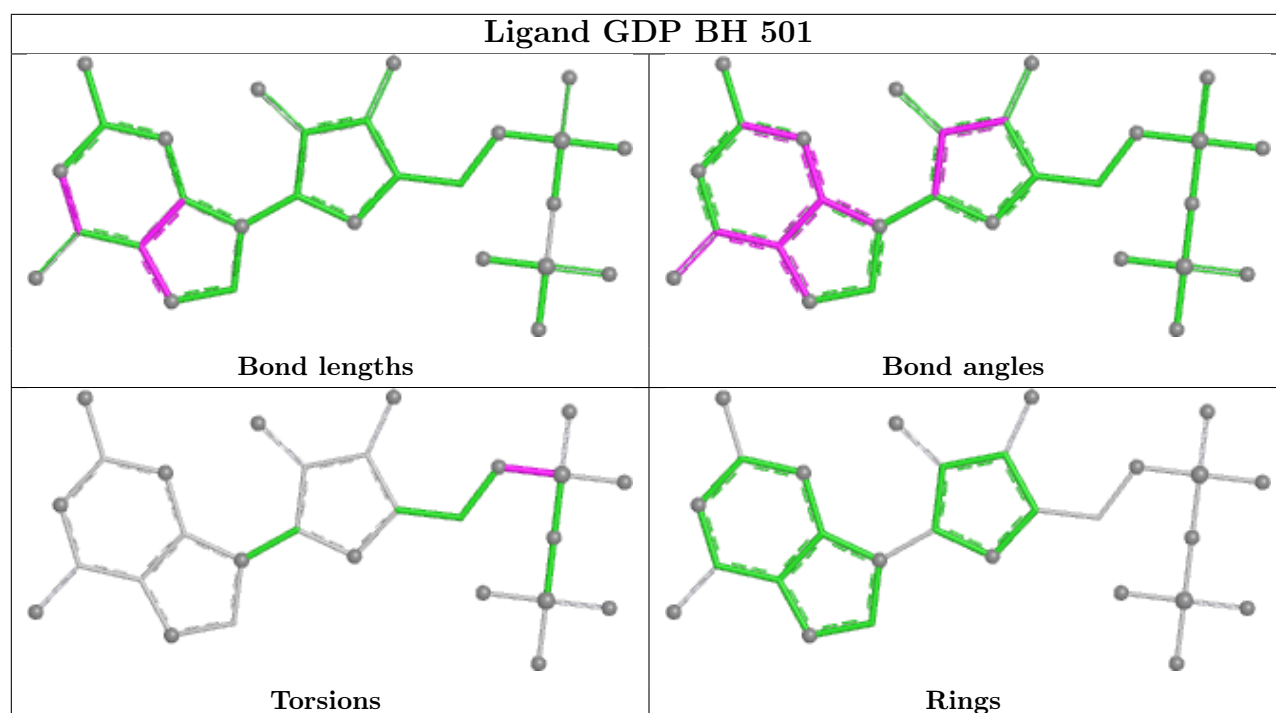


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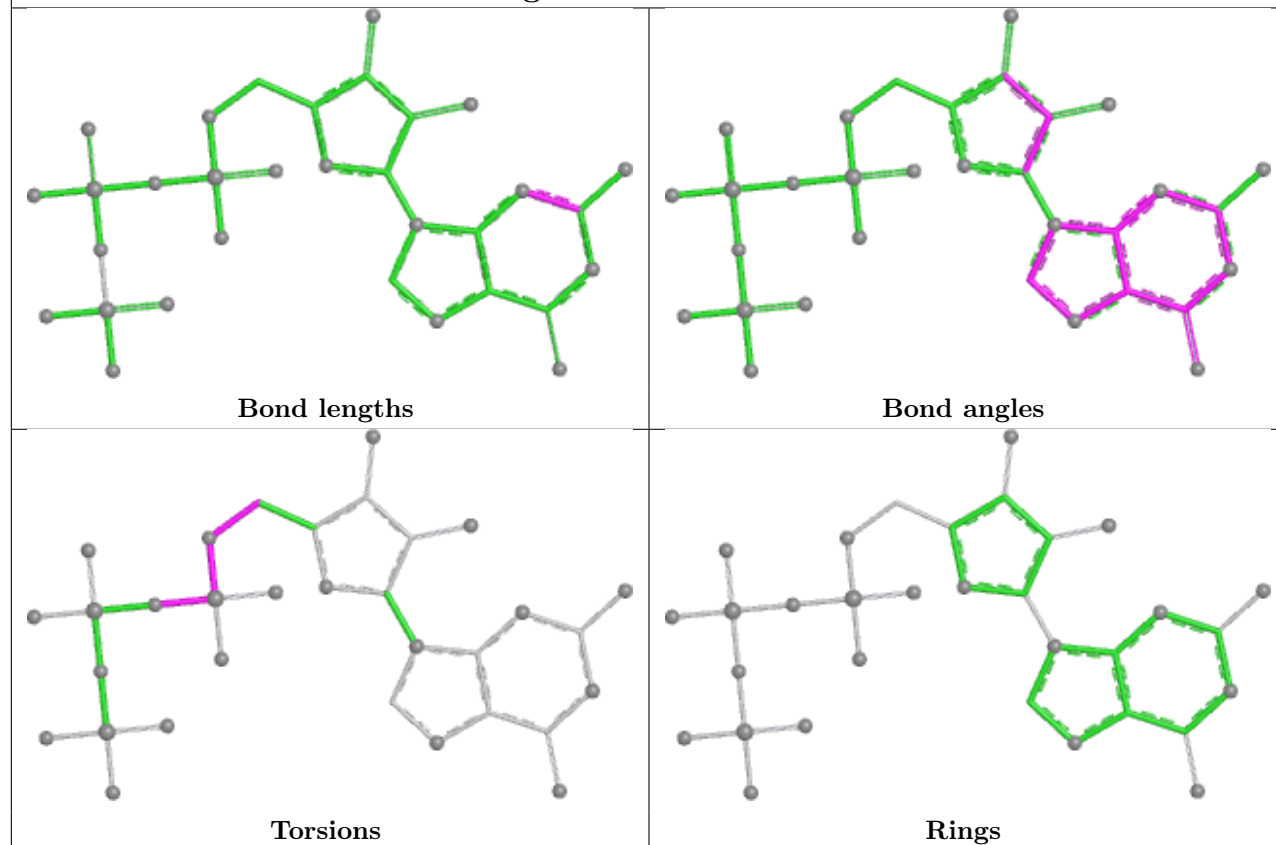


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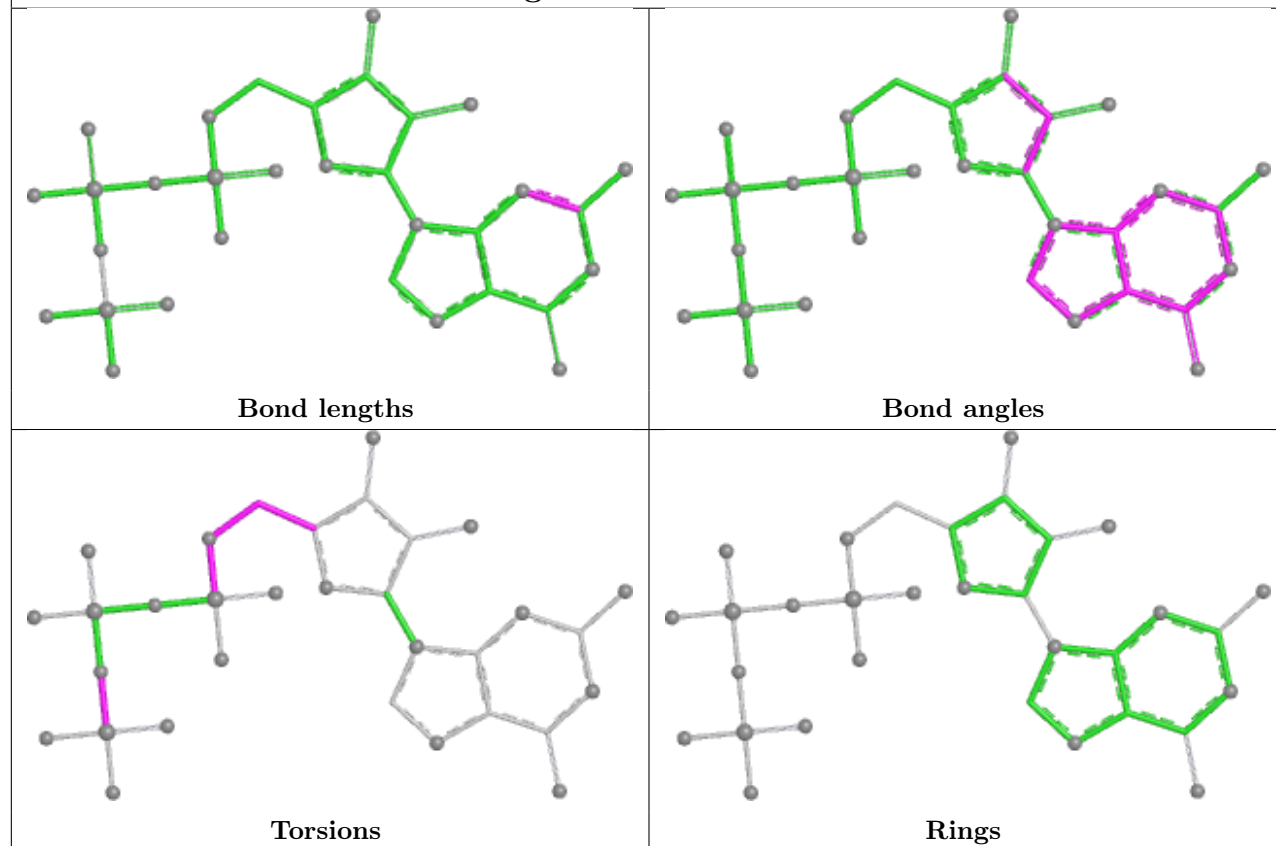


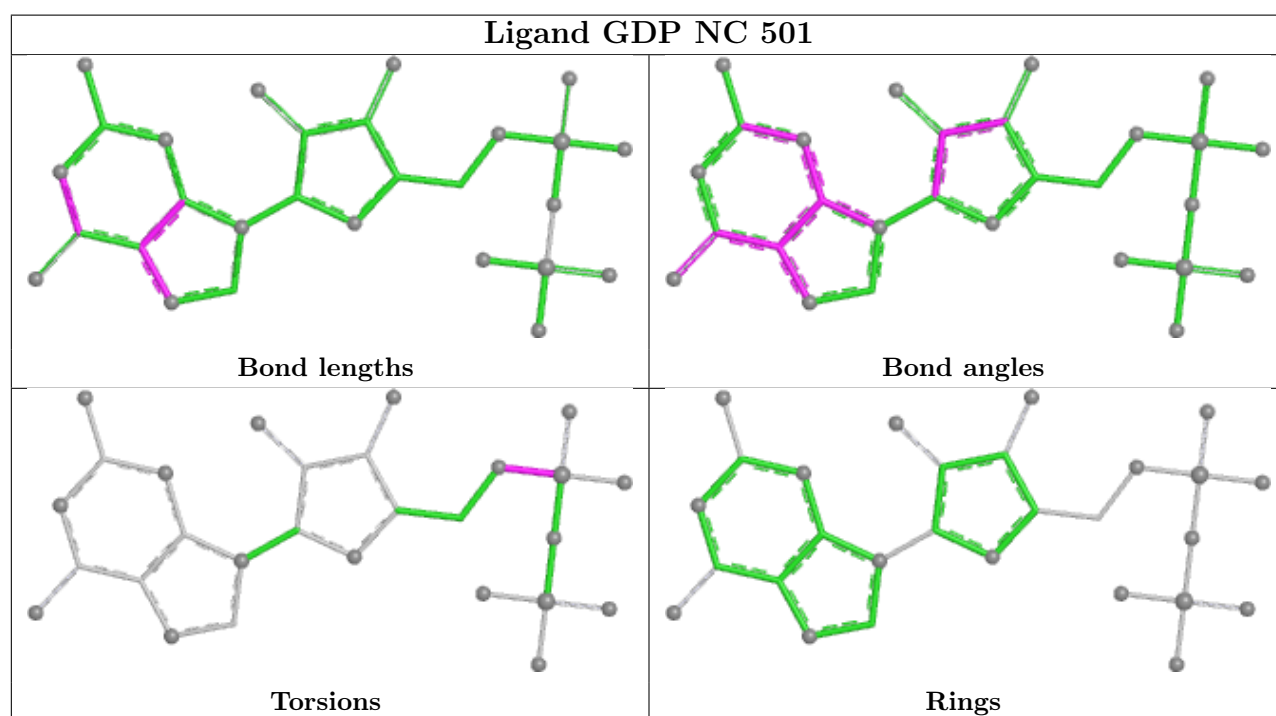
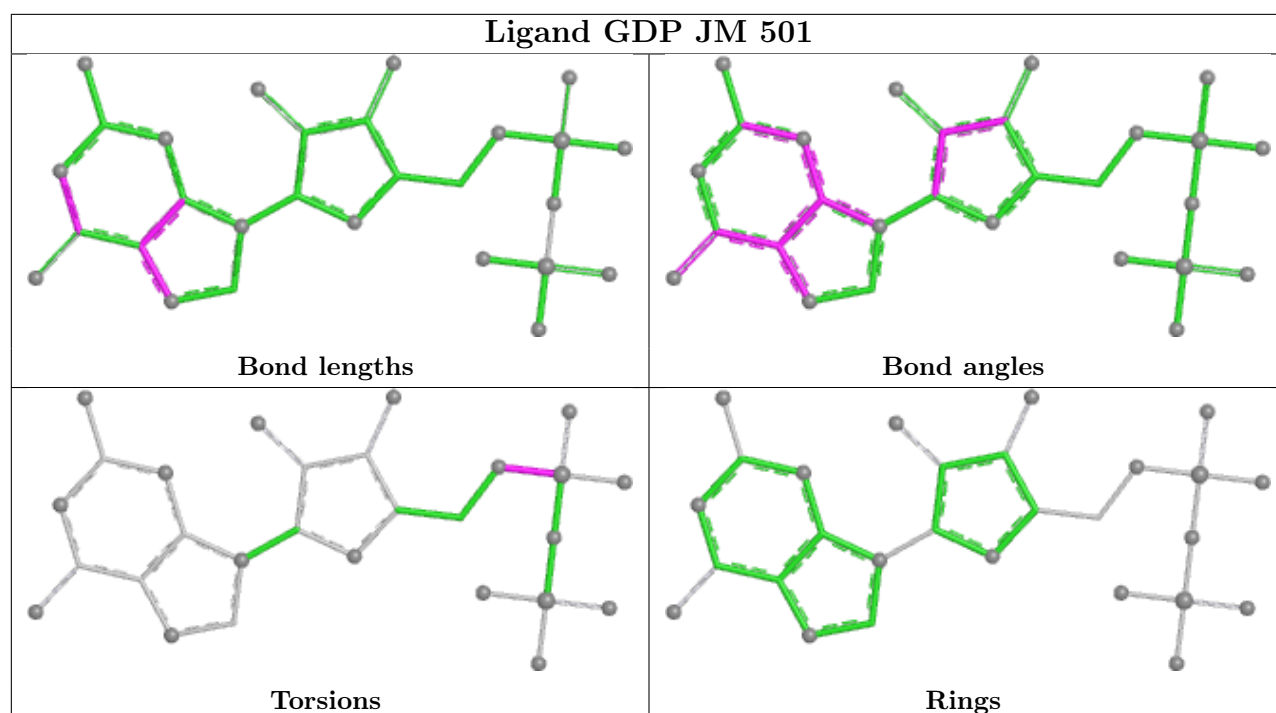


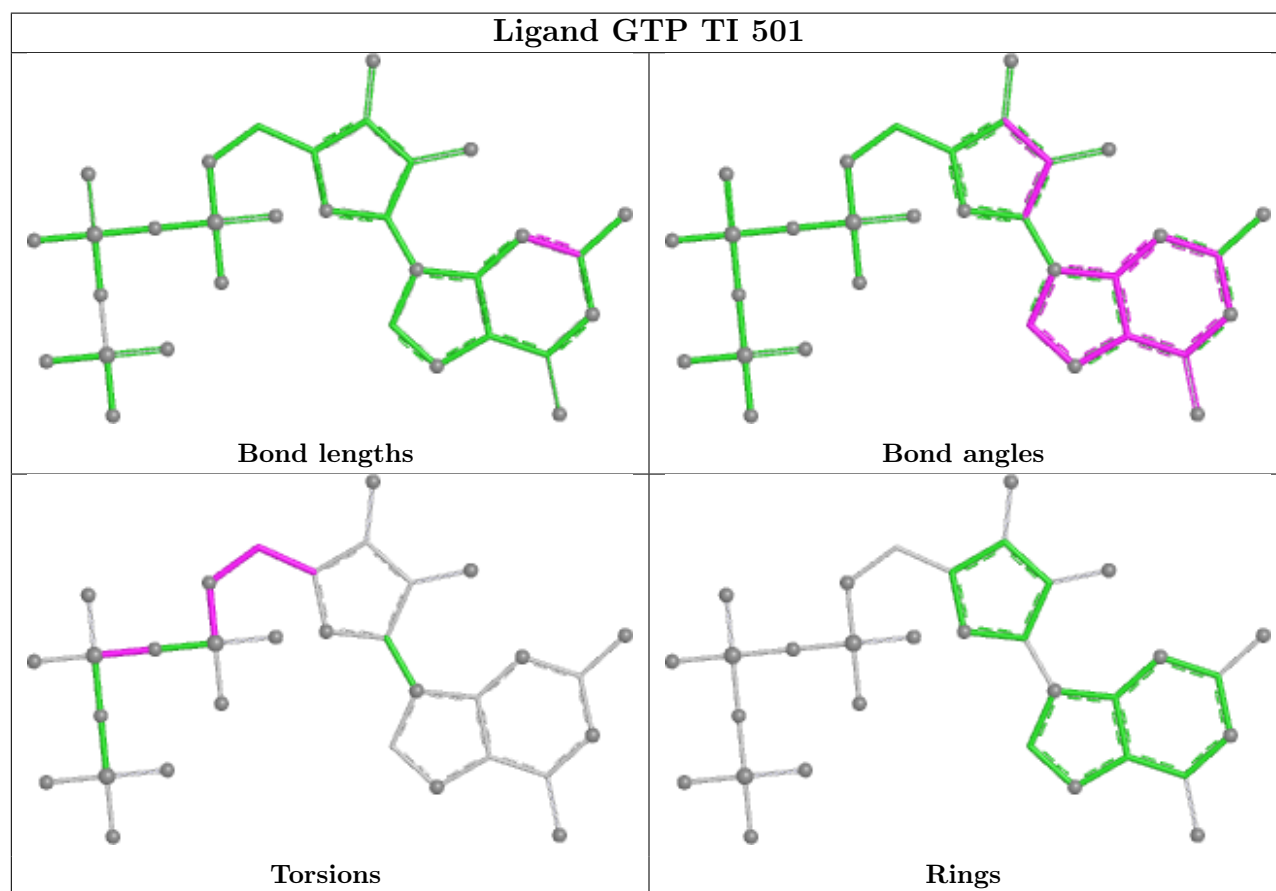
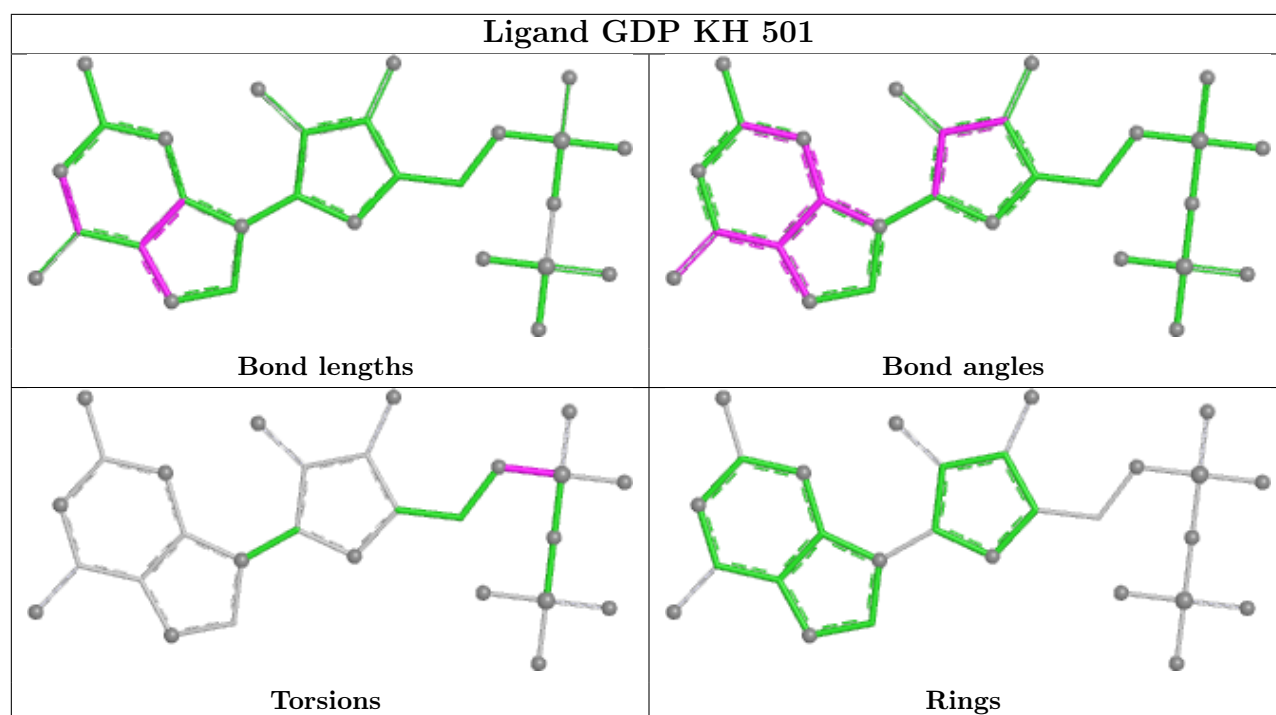
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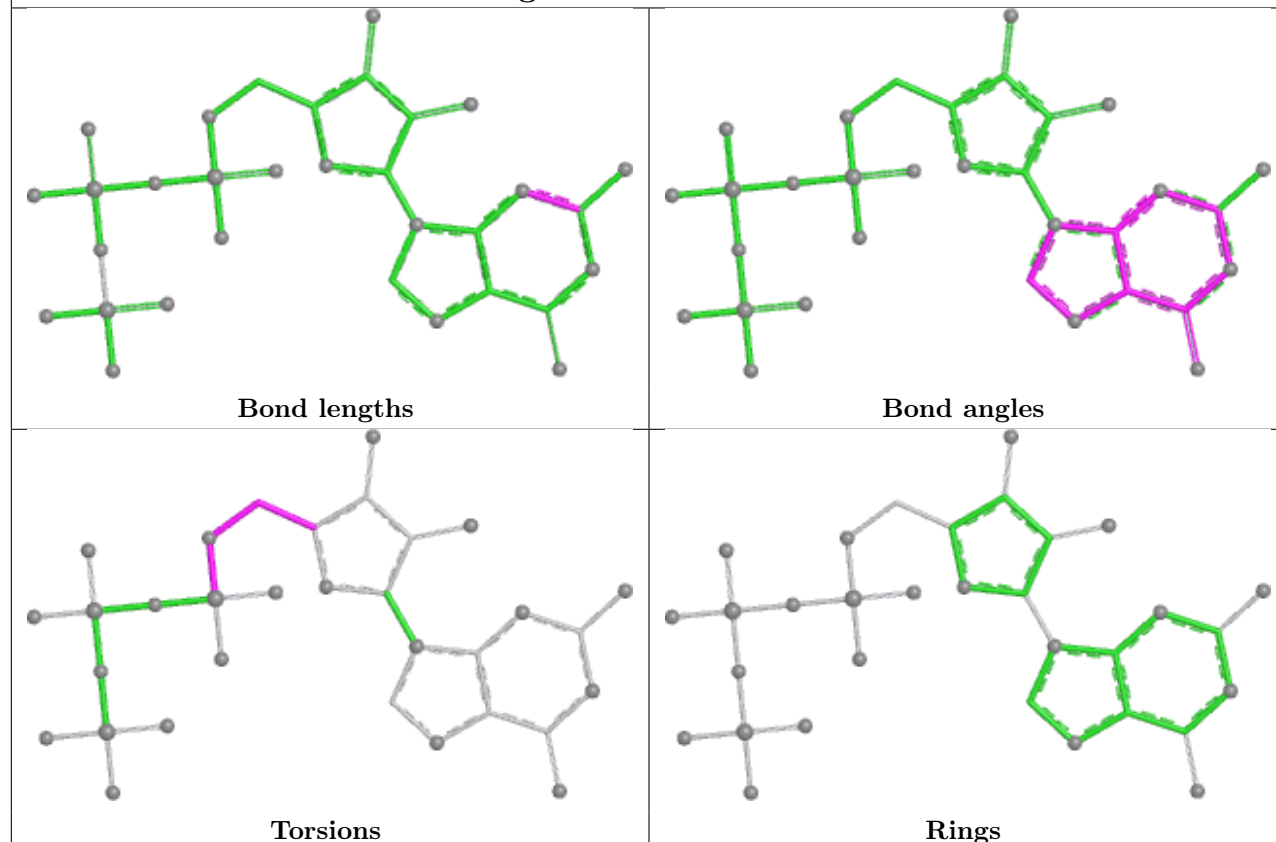
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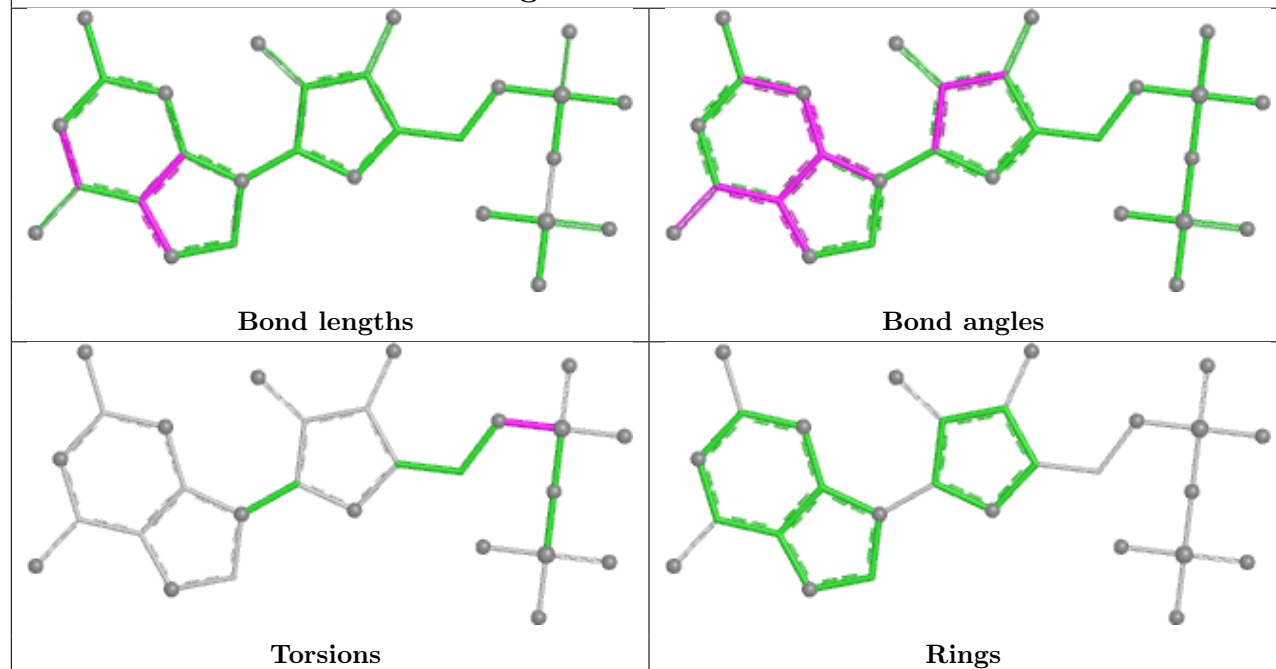


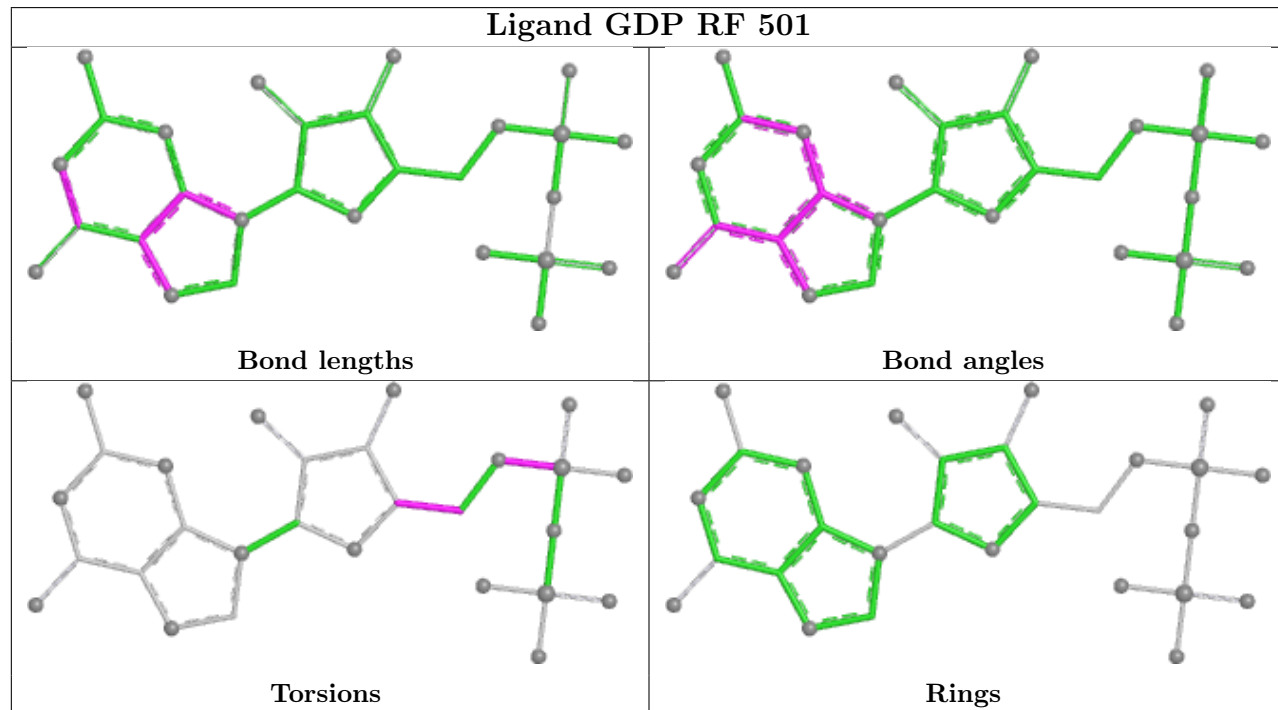
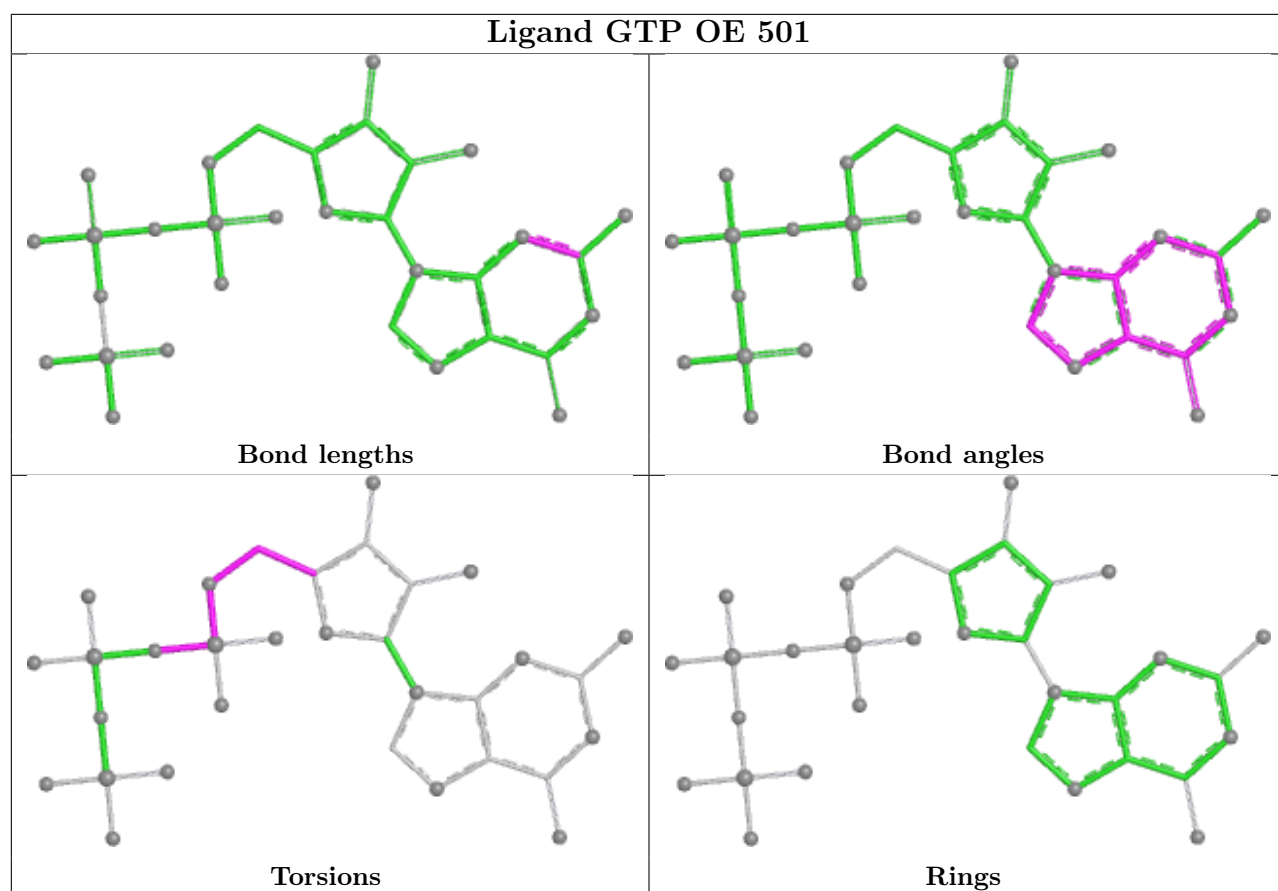


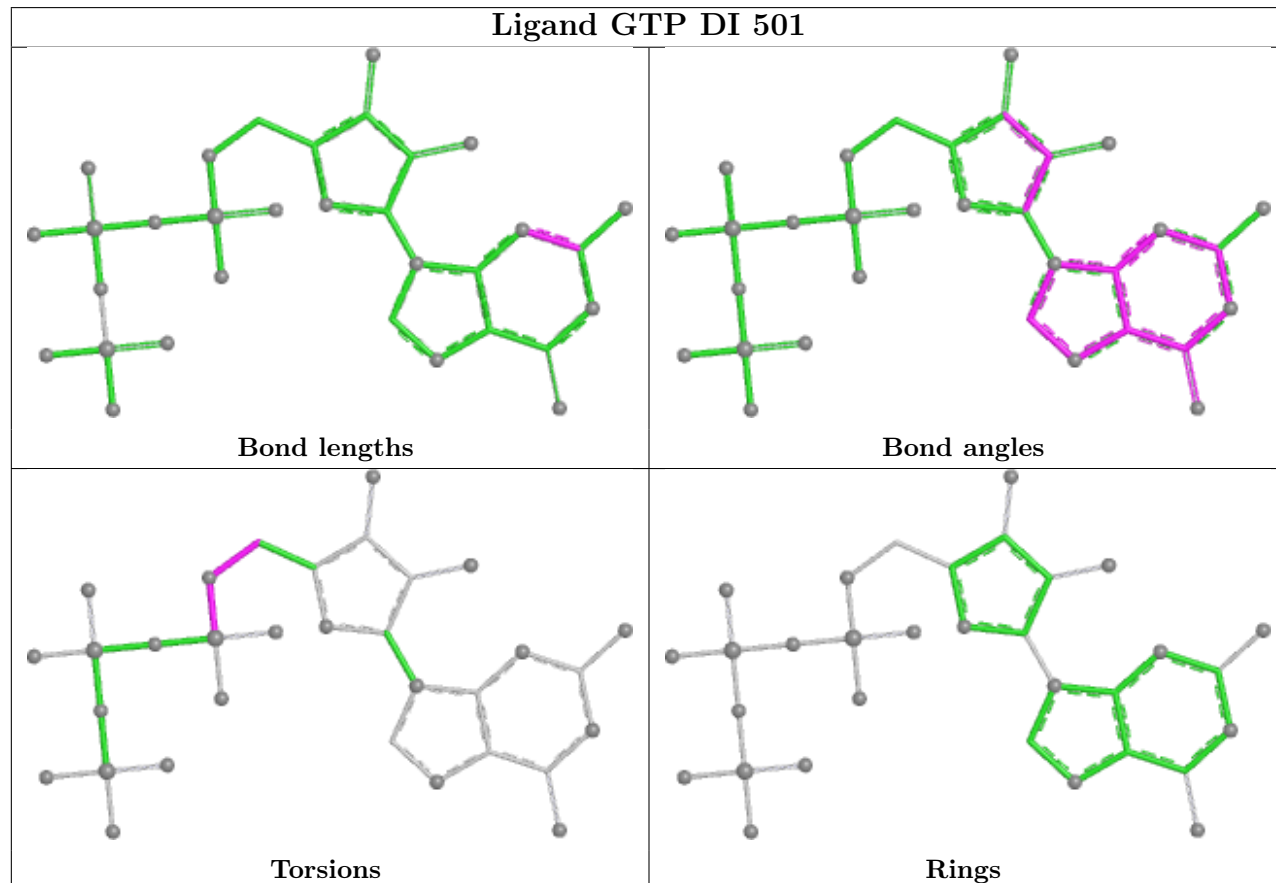
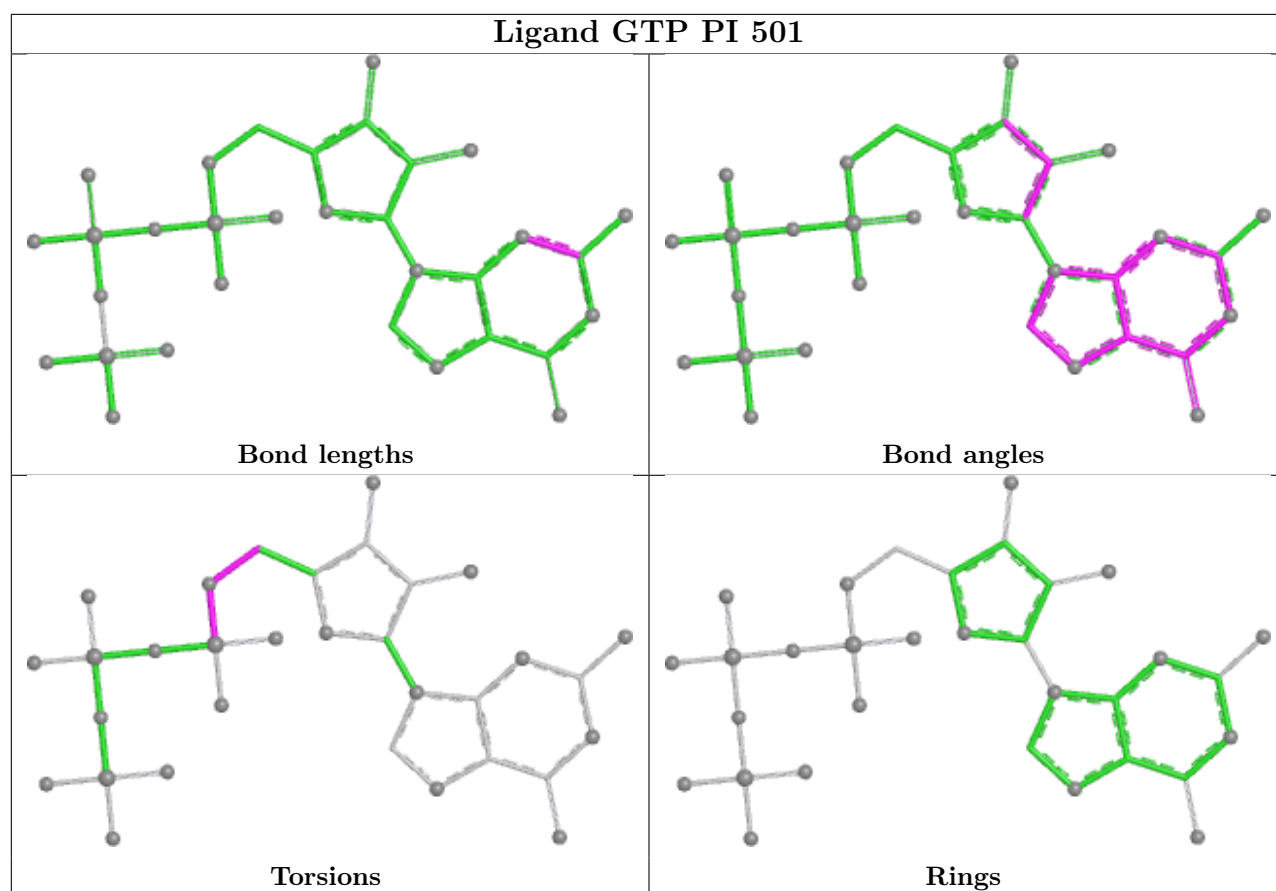
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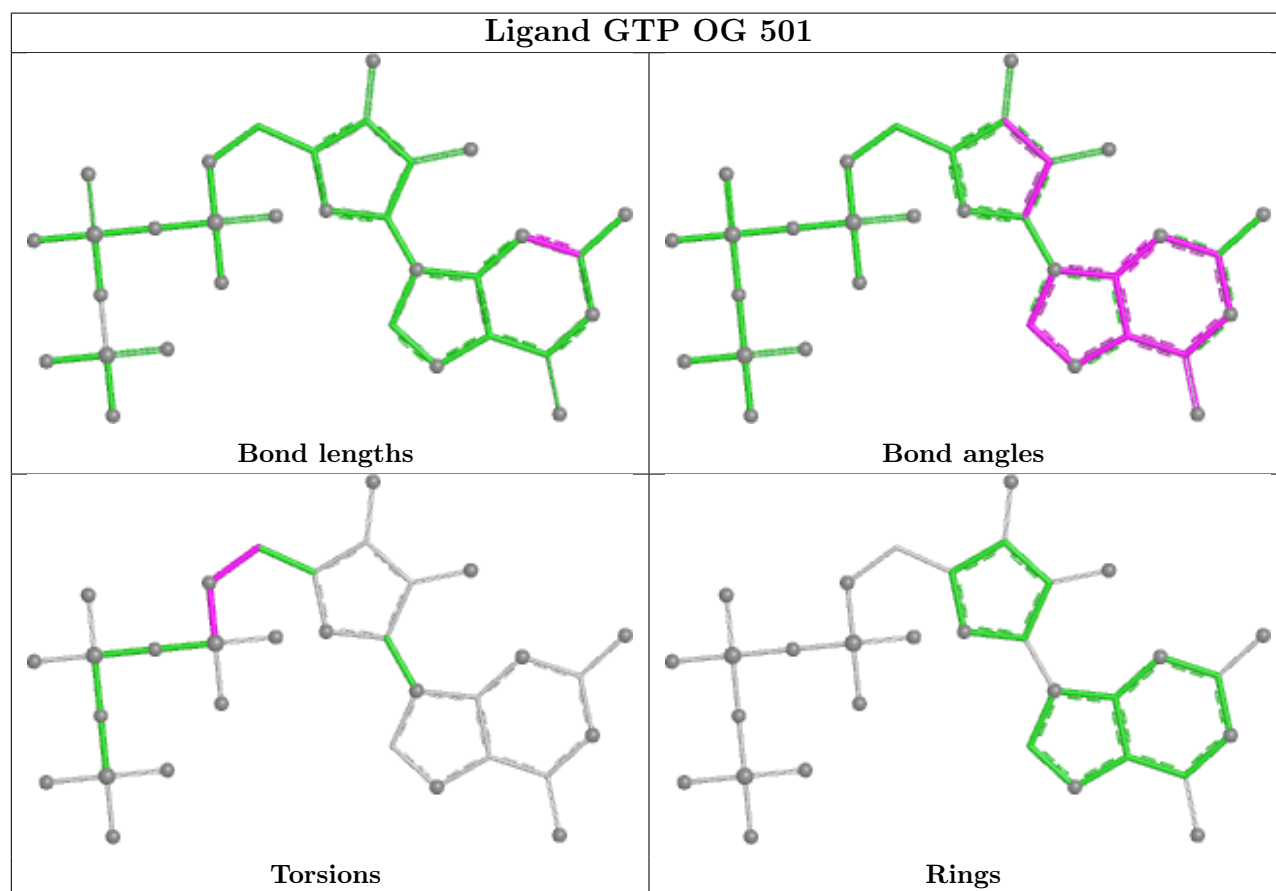
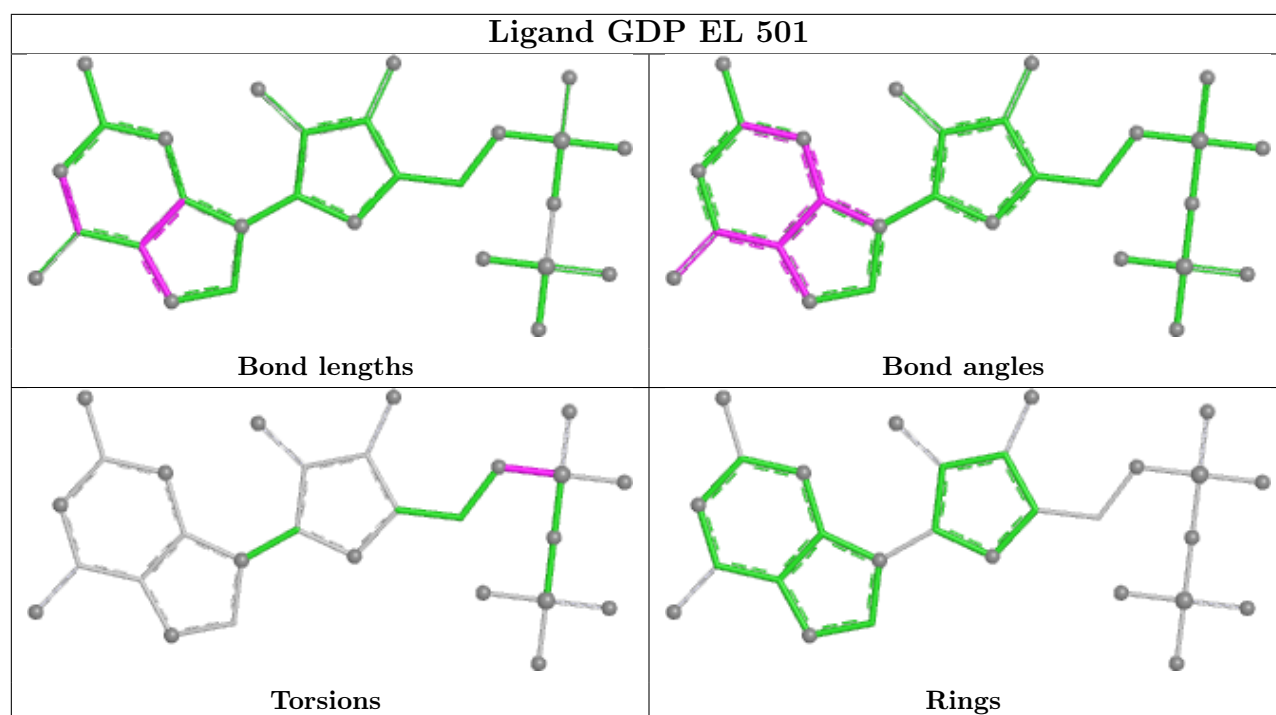


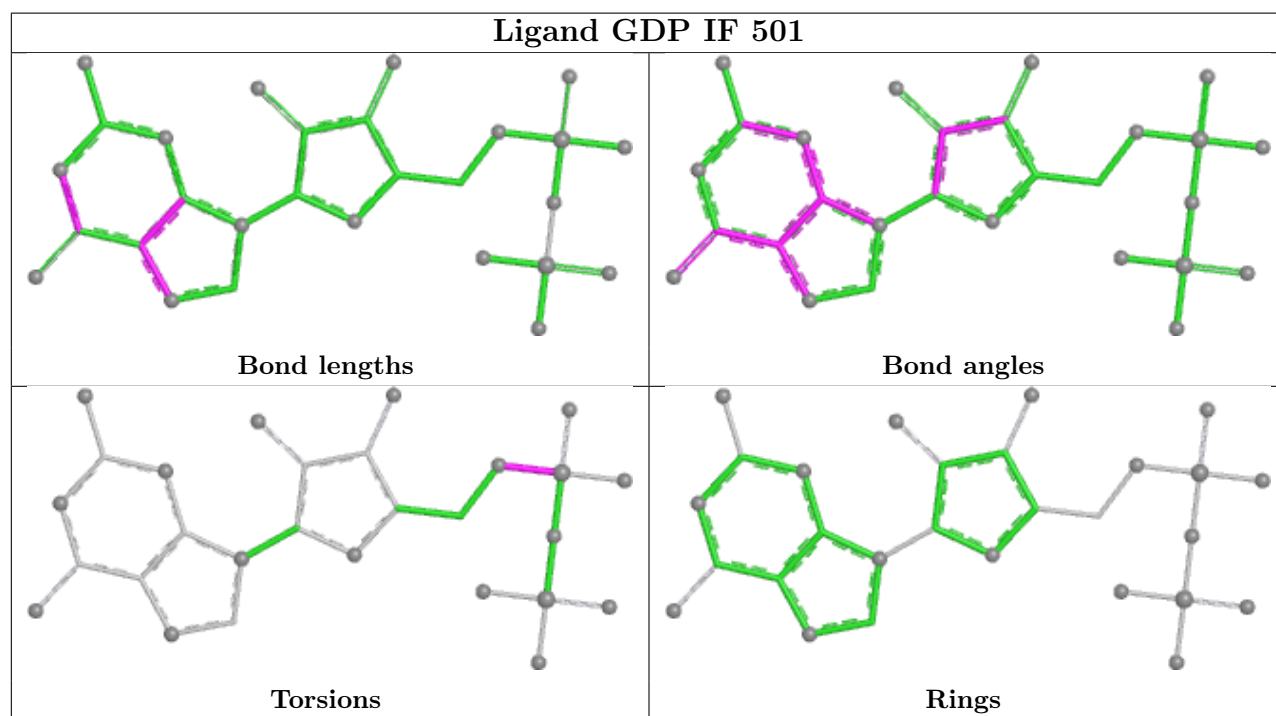
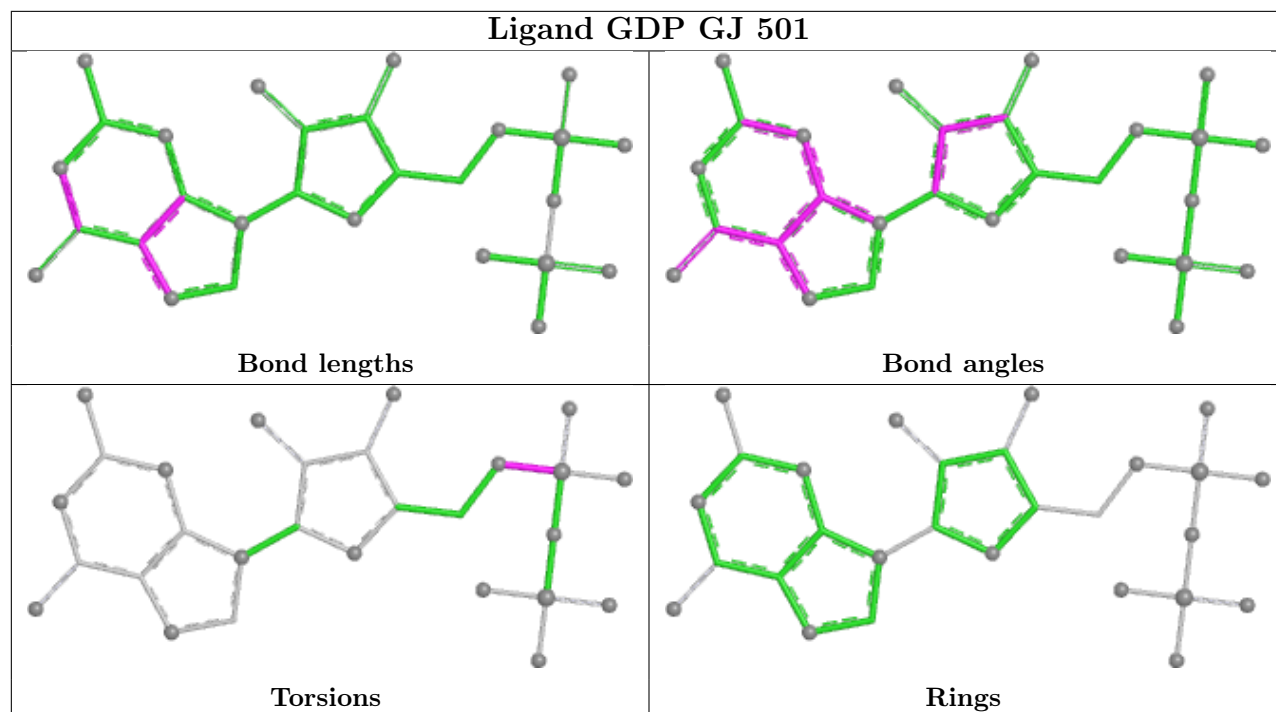
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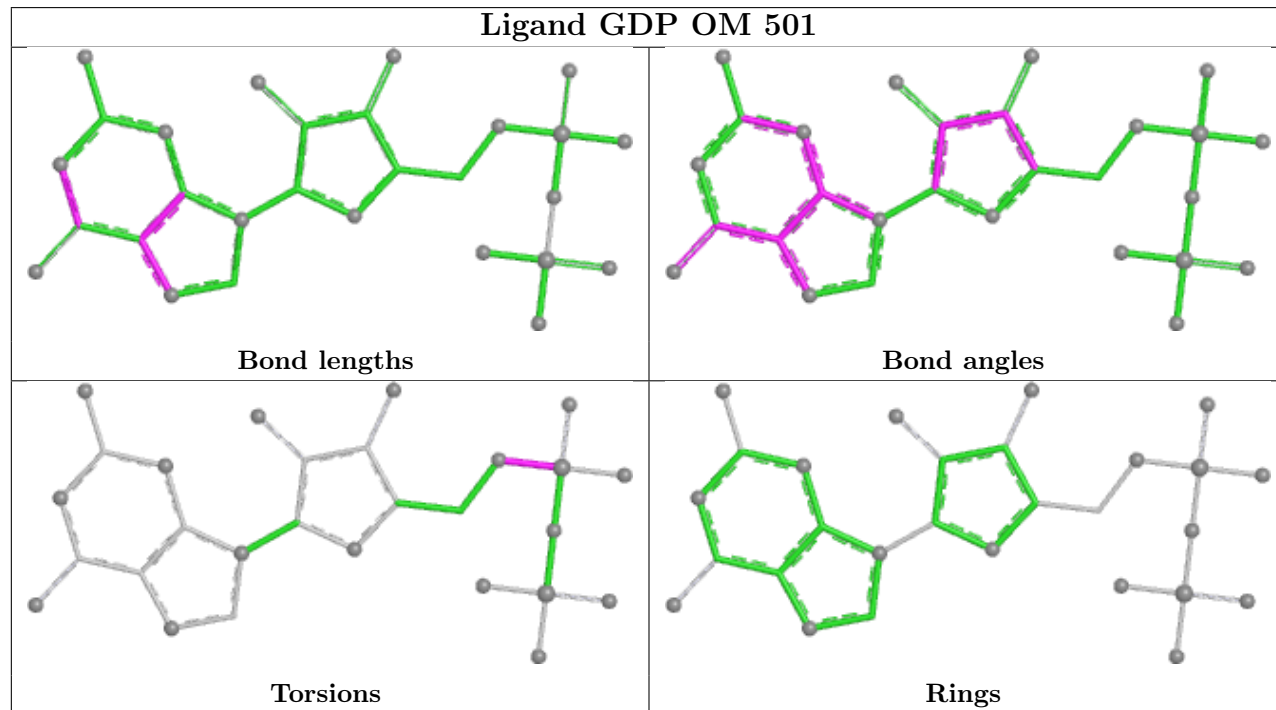
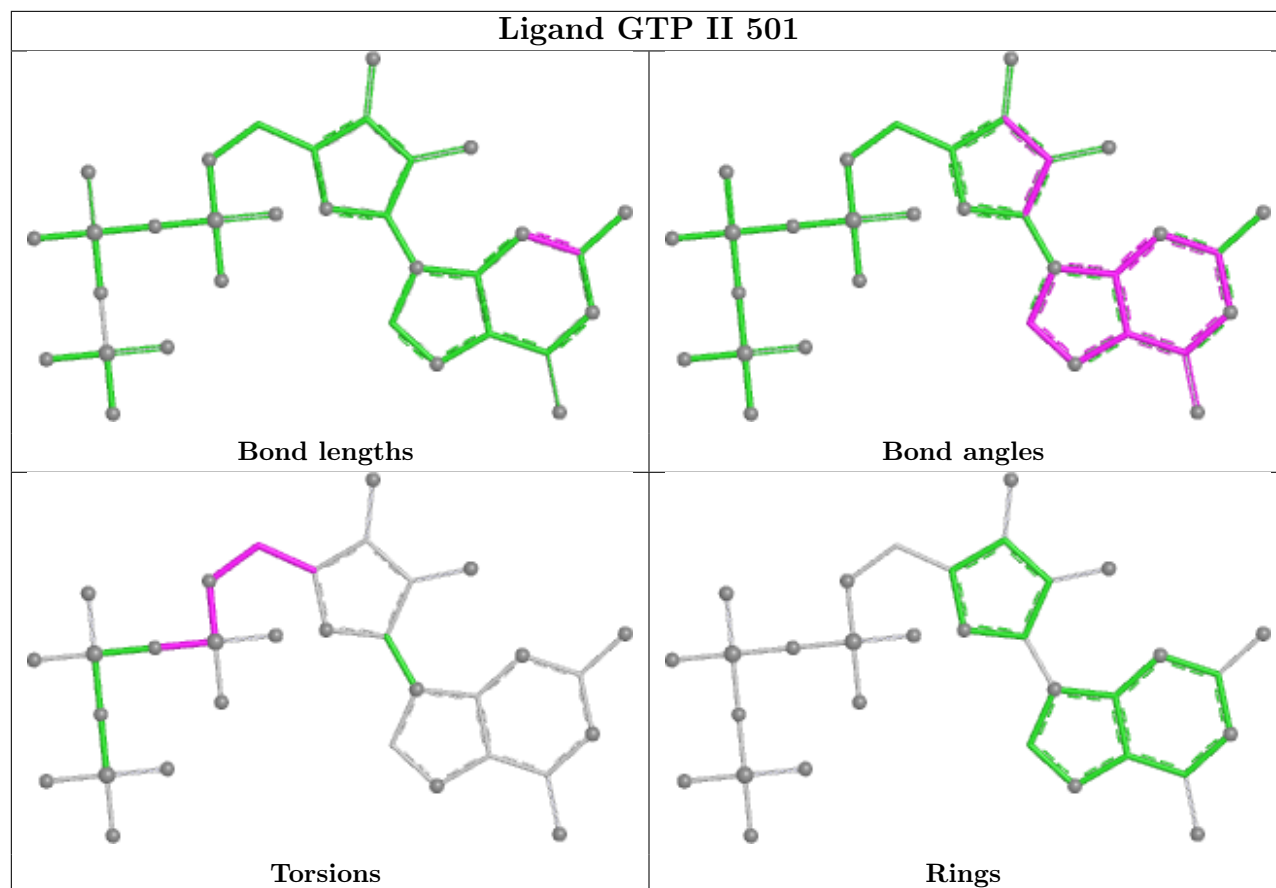


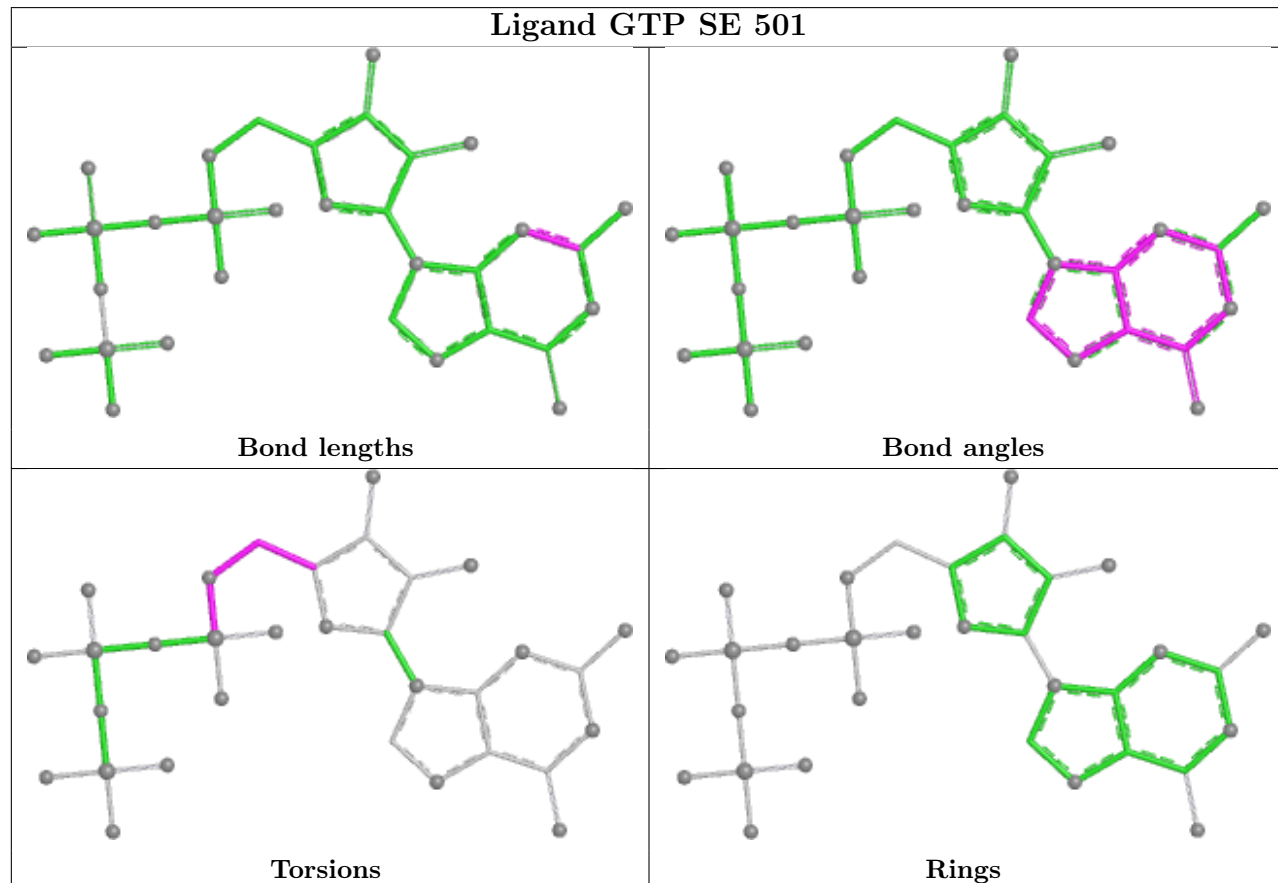
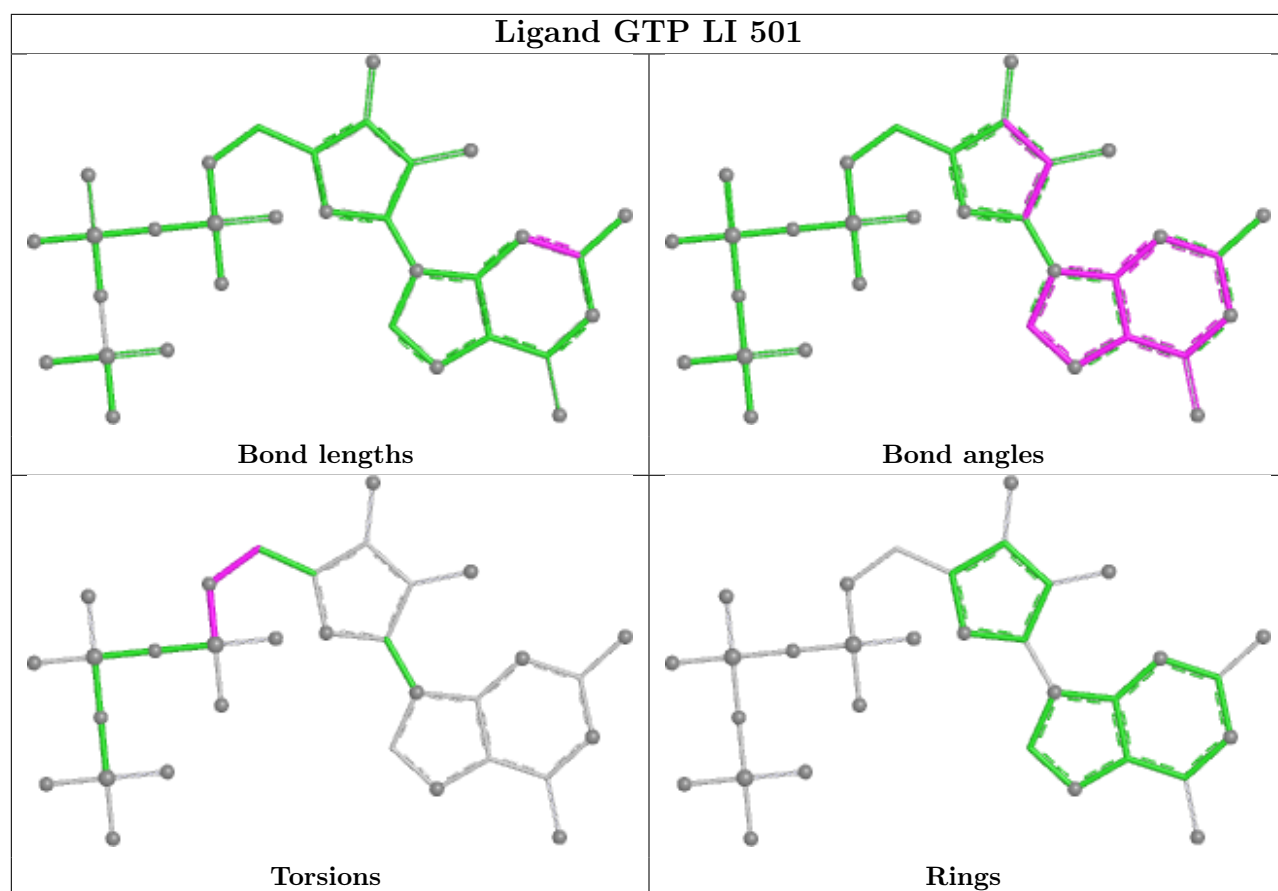


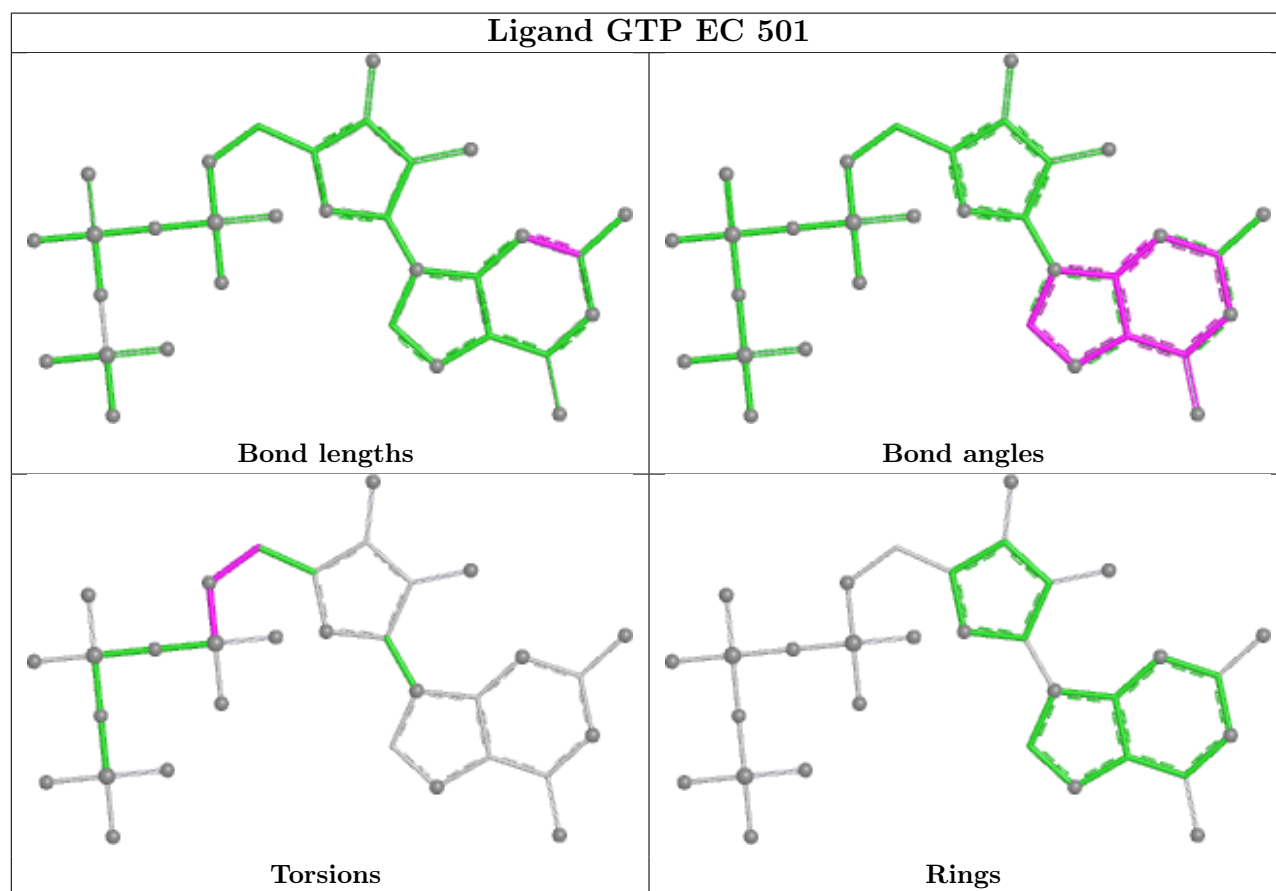
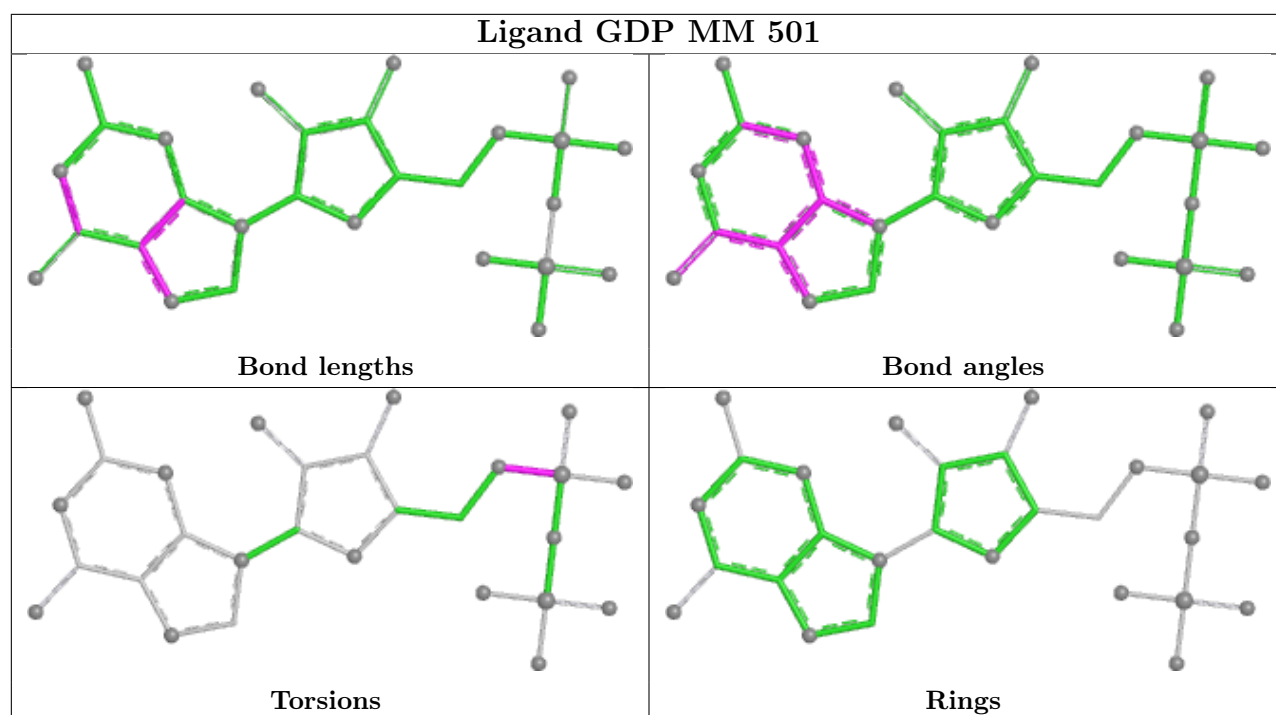




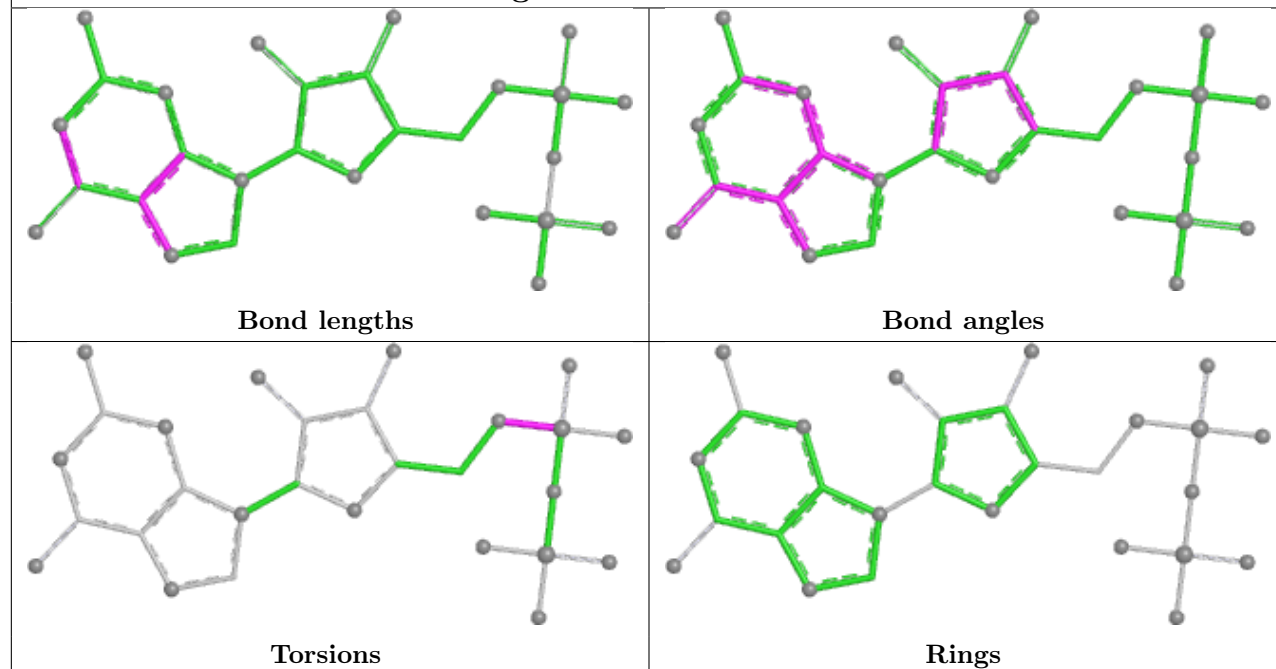




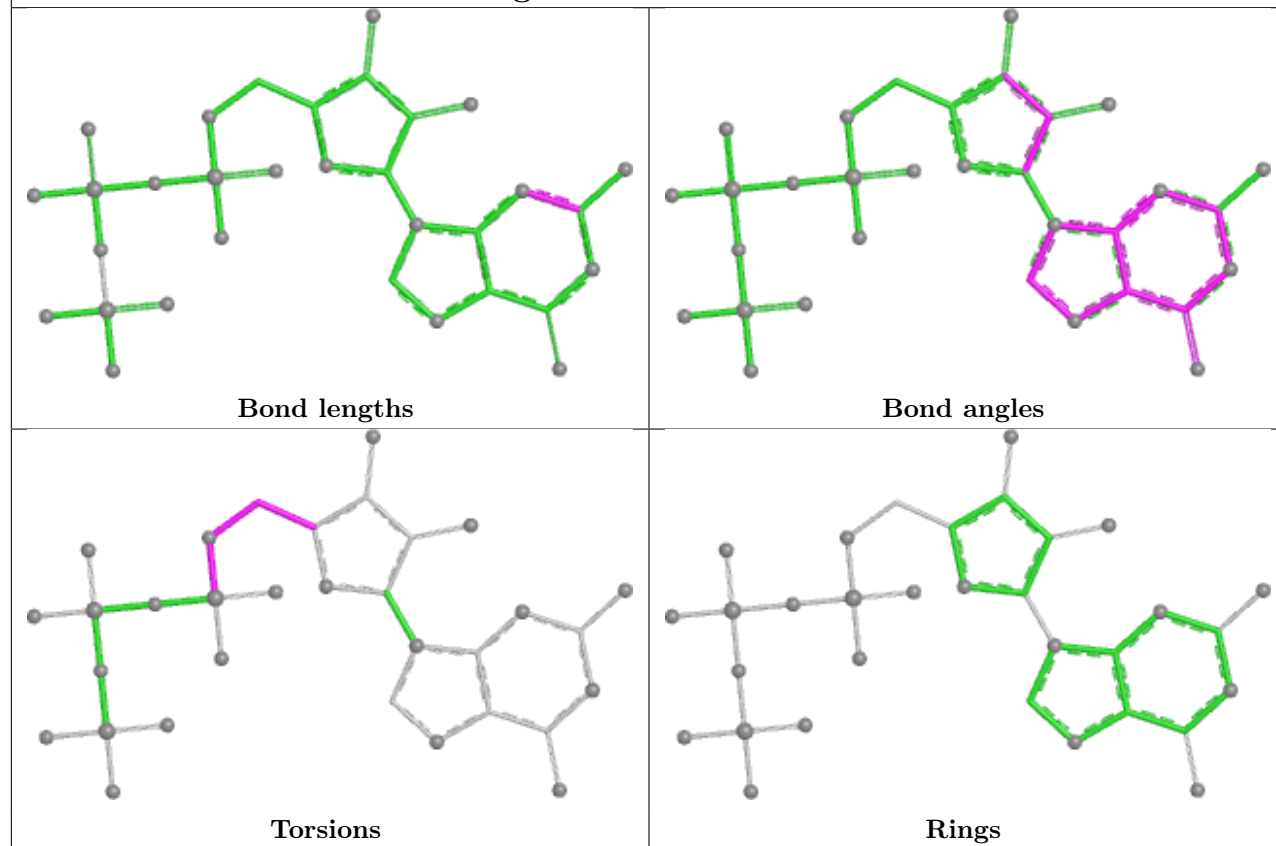


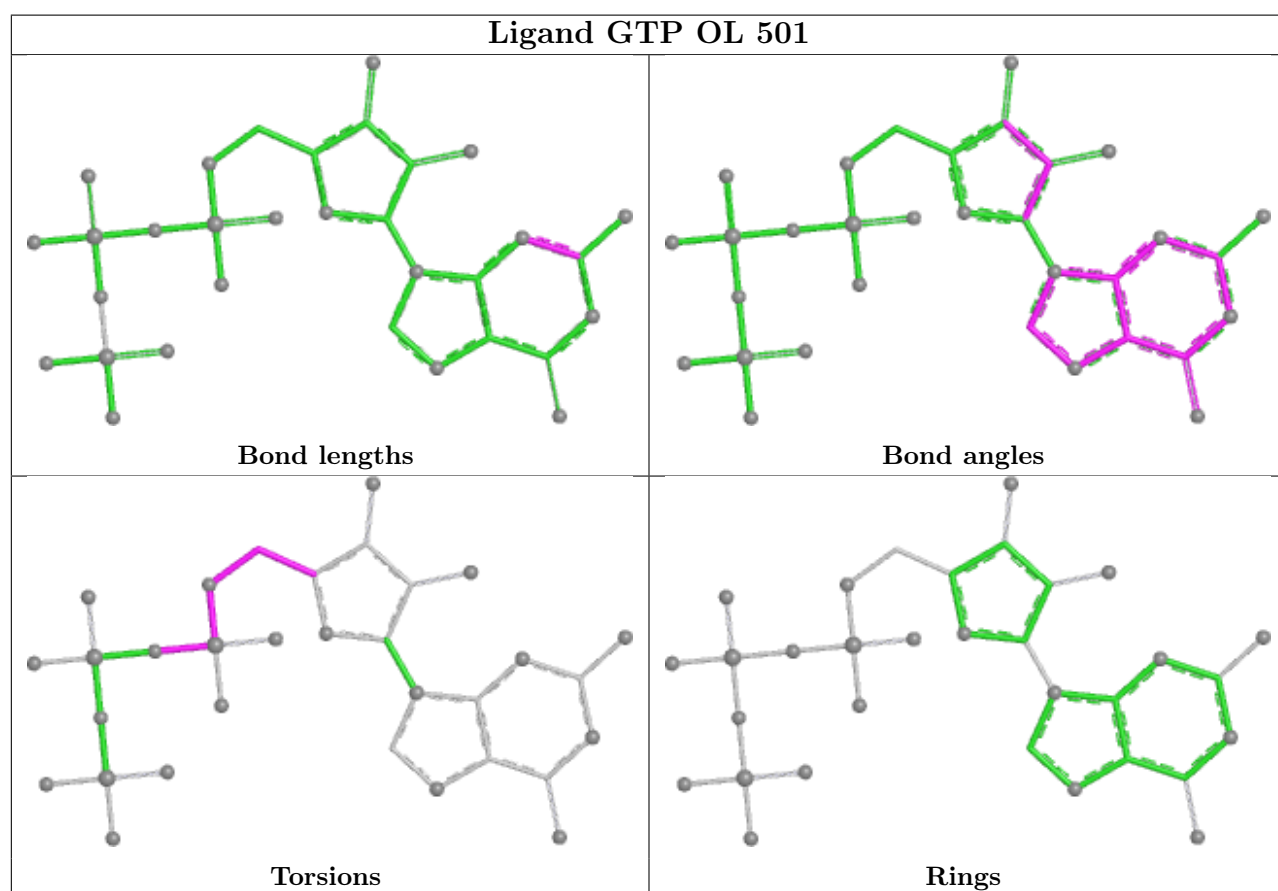
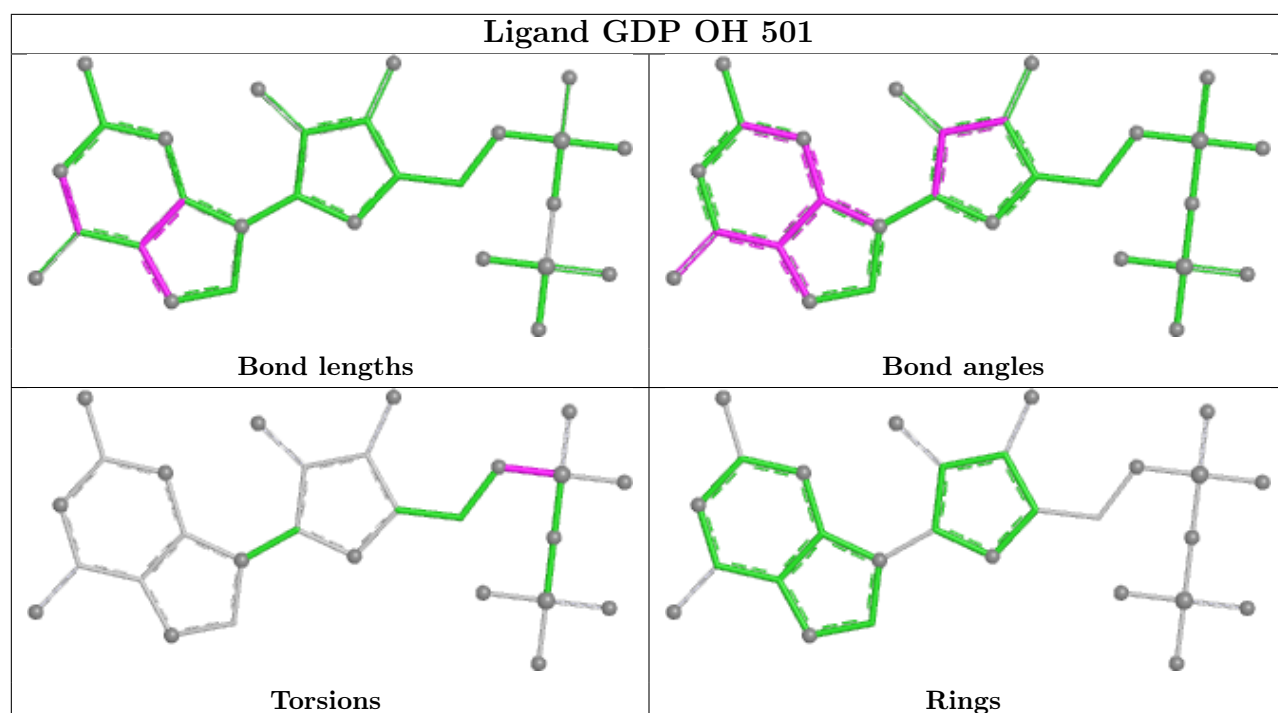


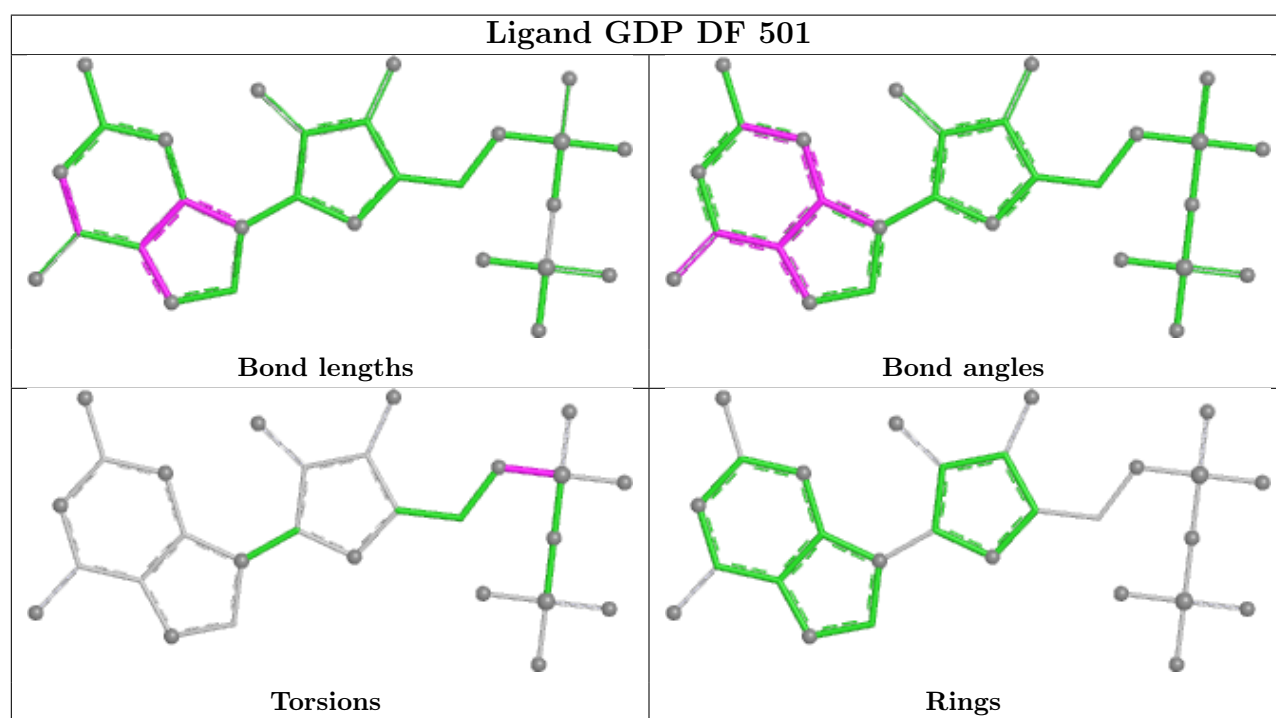
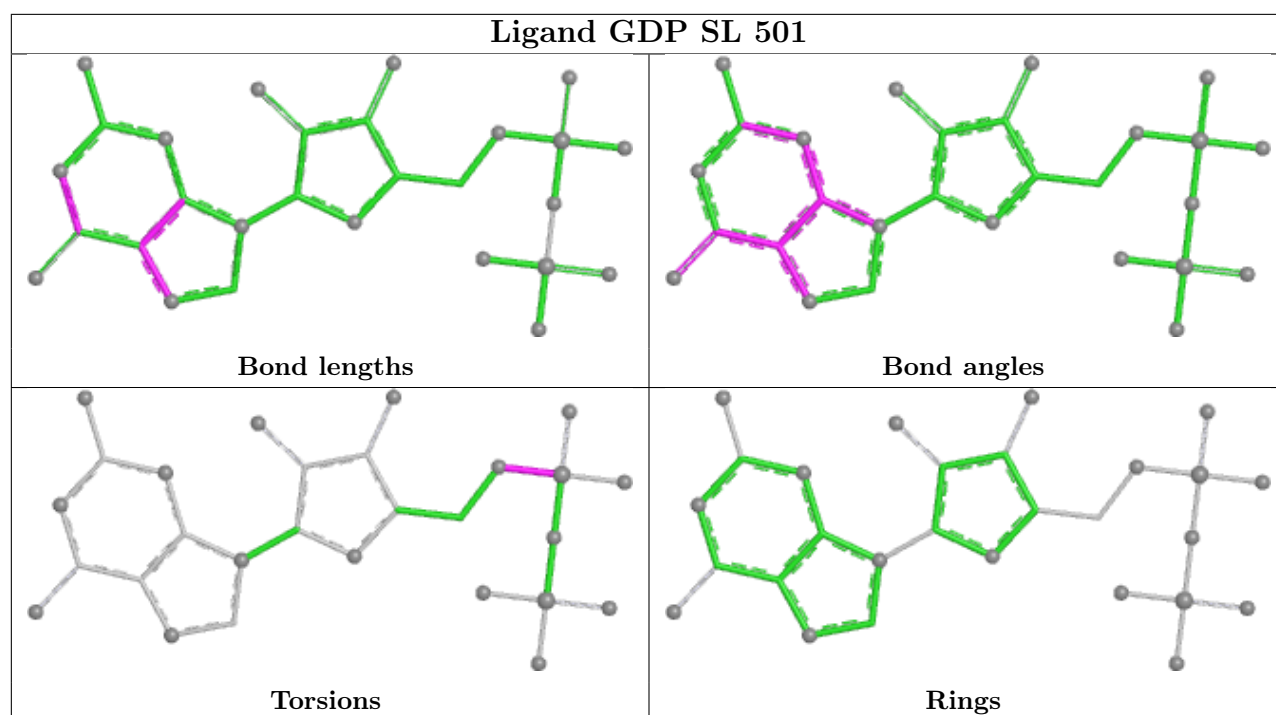
Ligand GDP RM 501

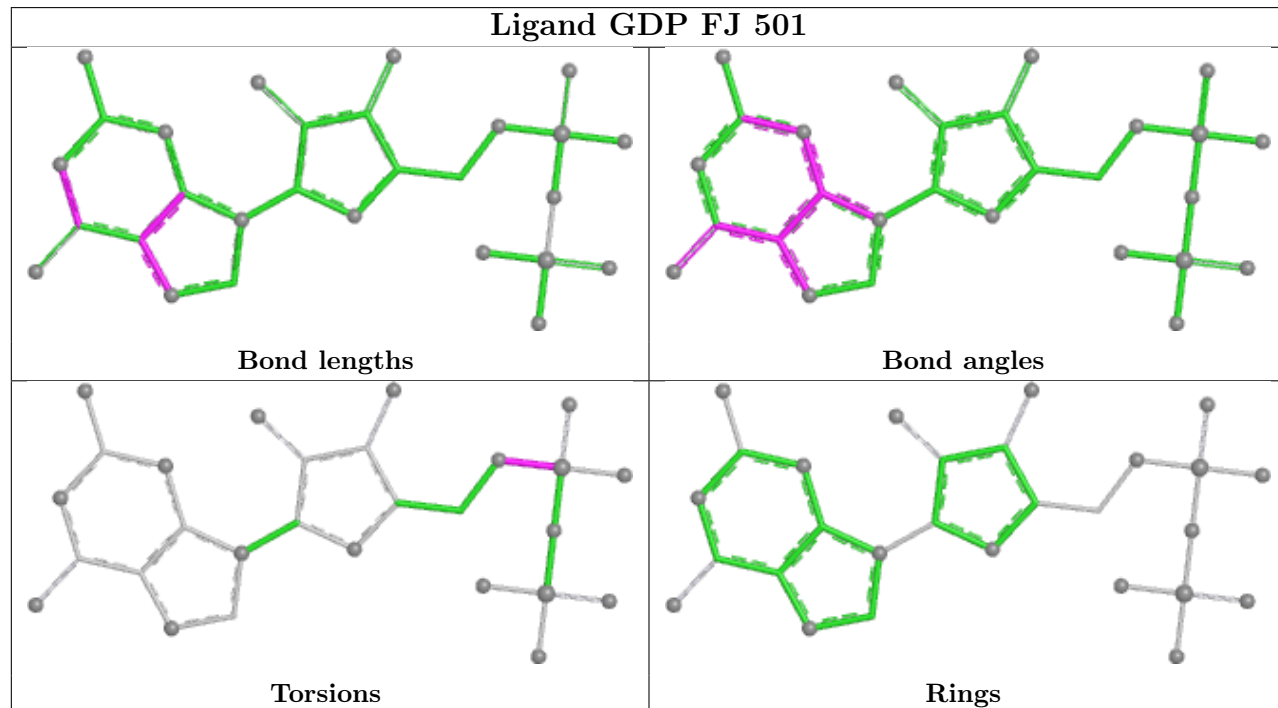
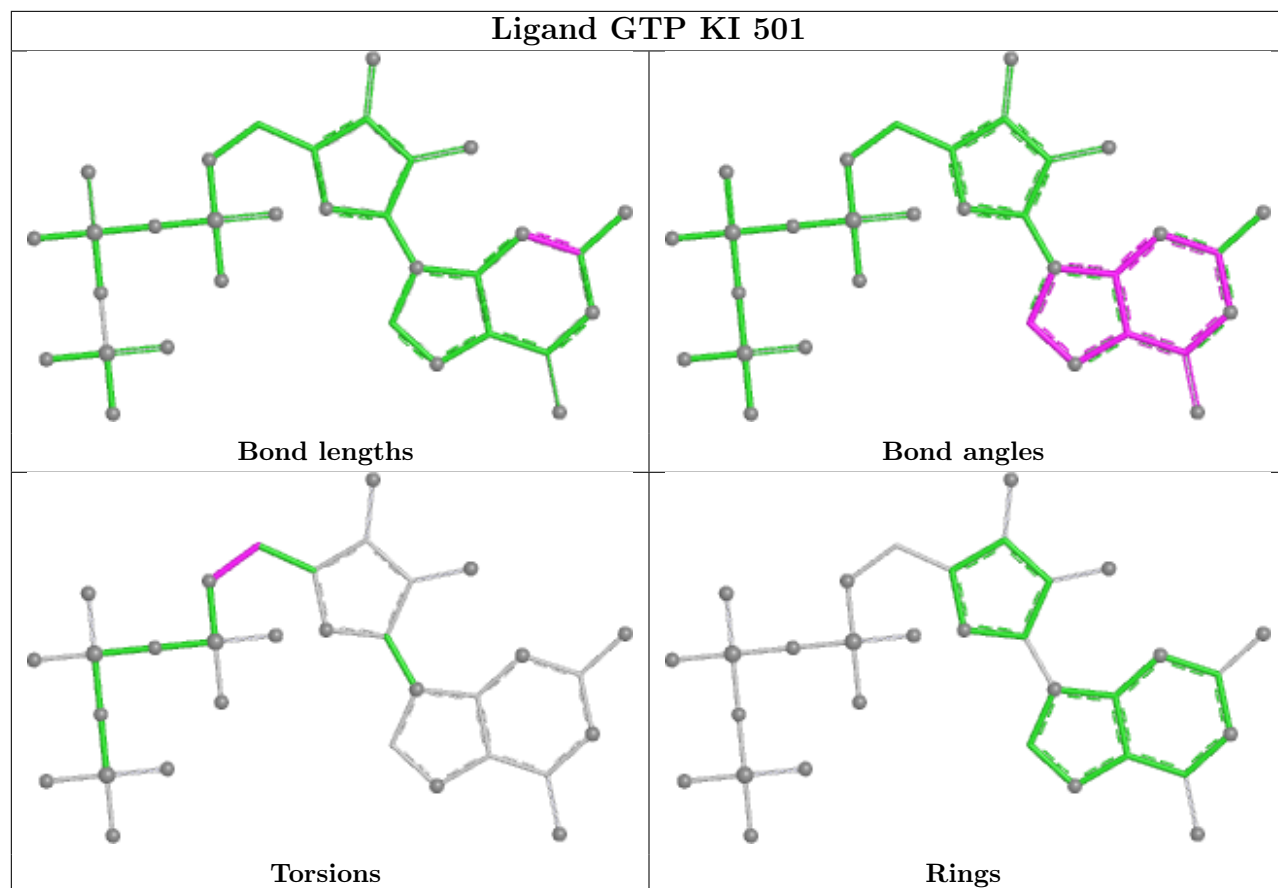


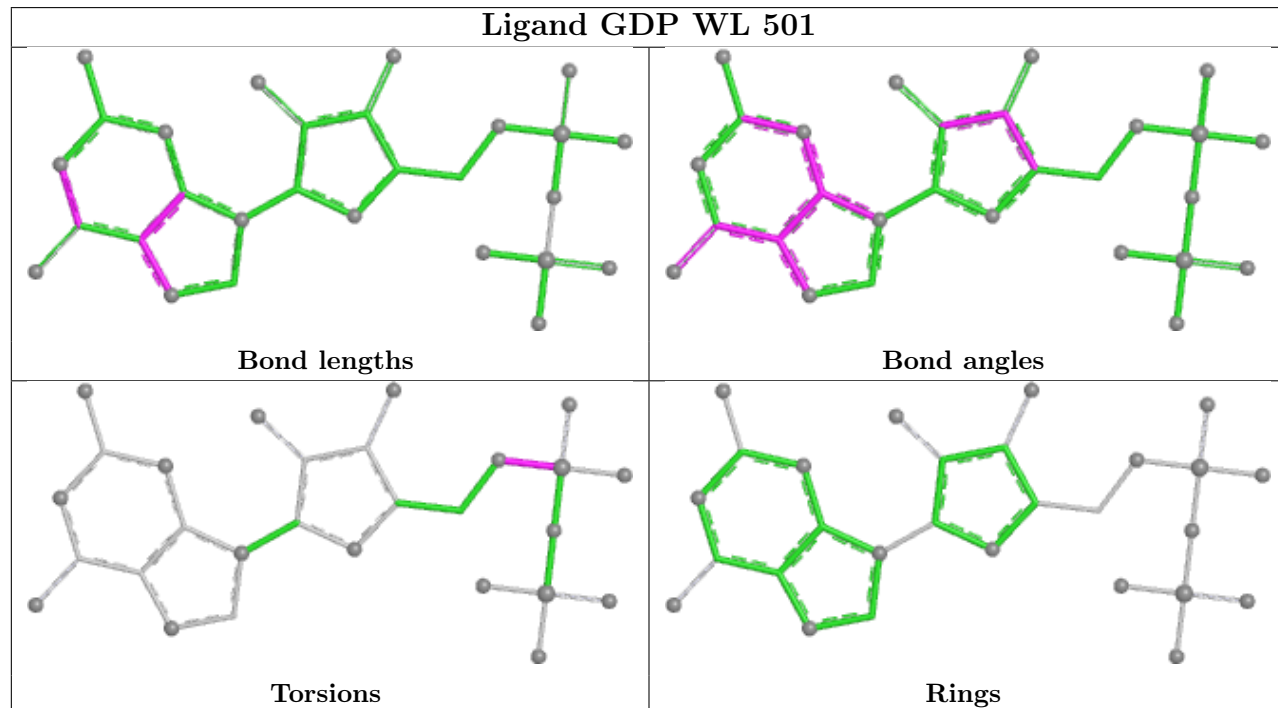
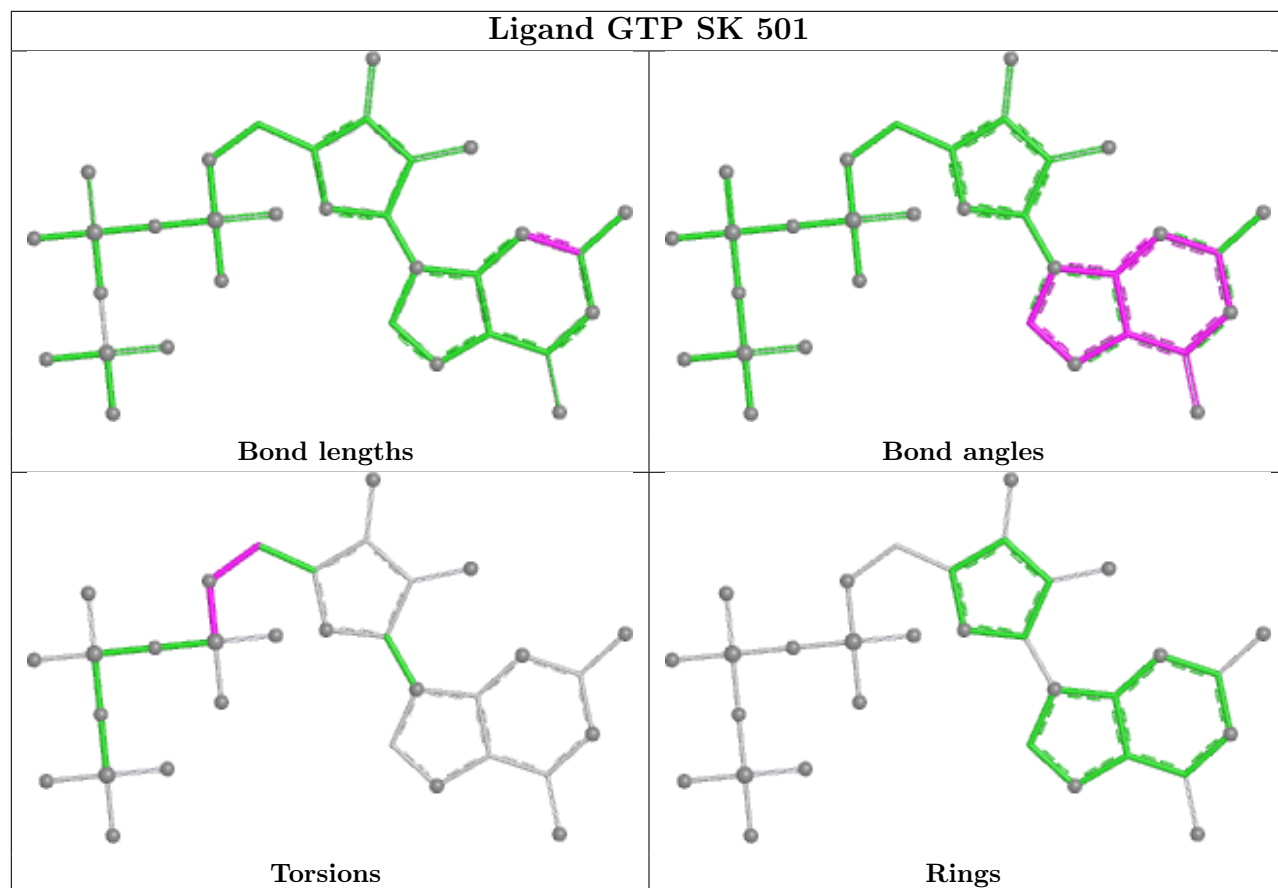
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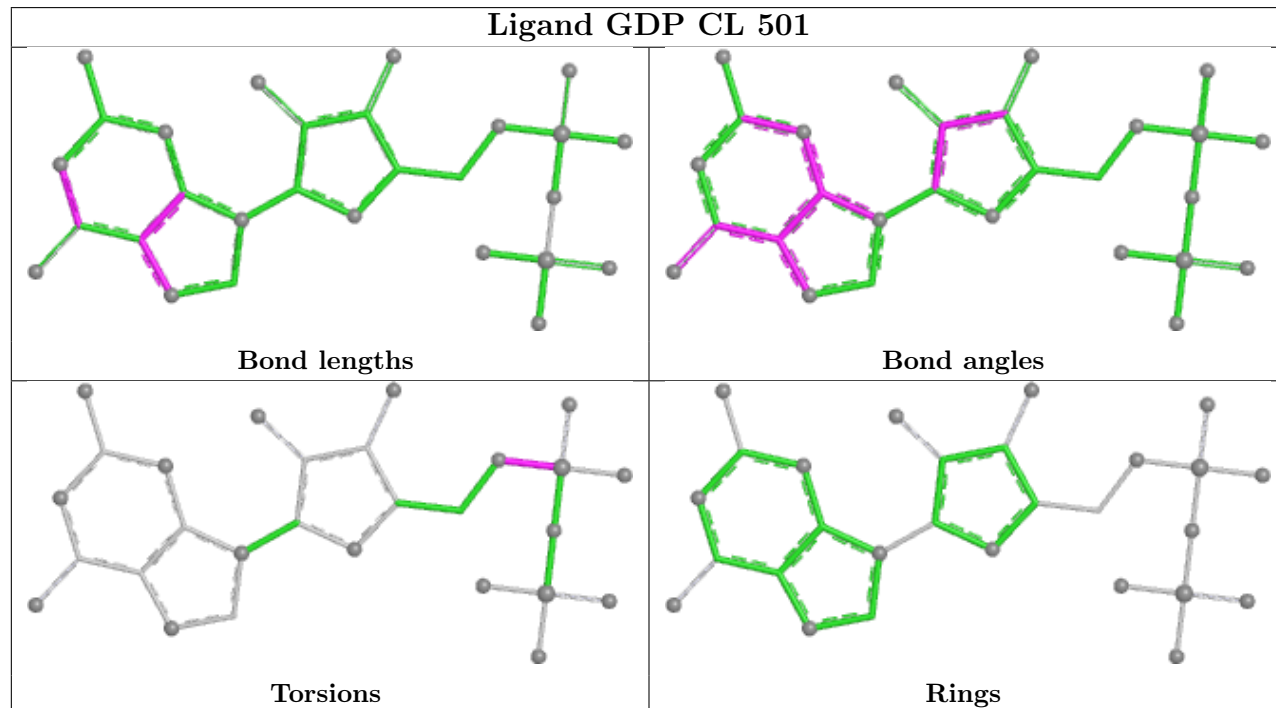
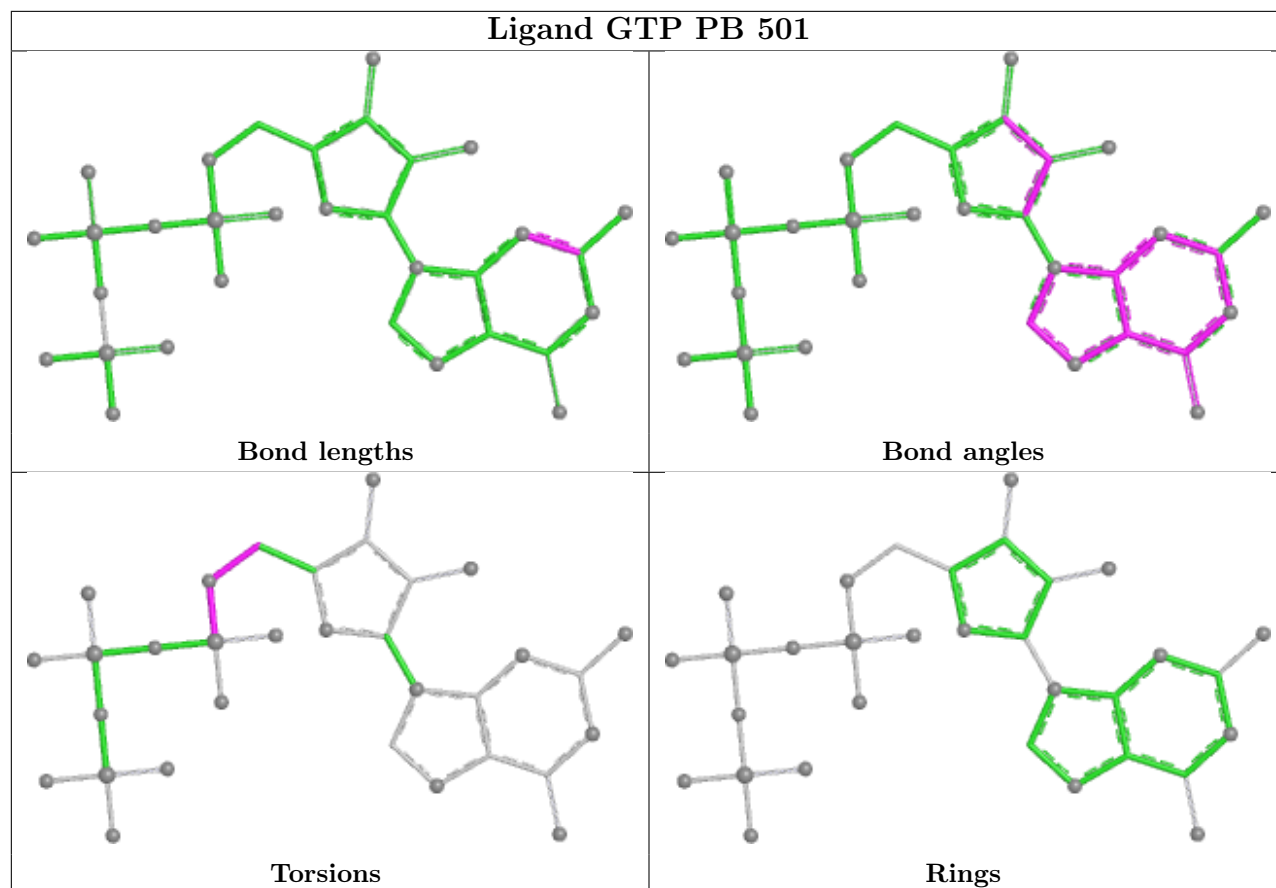




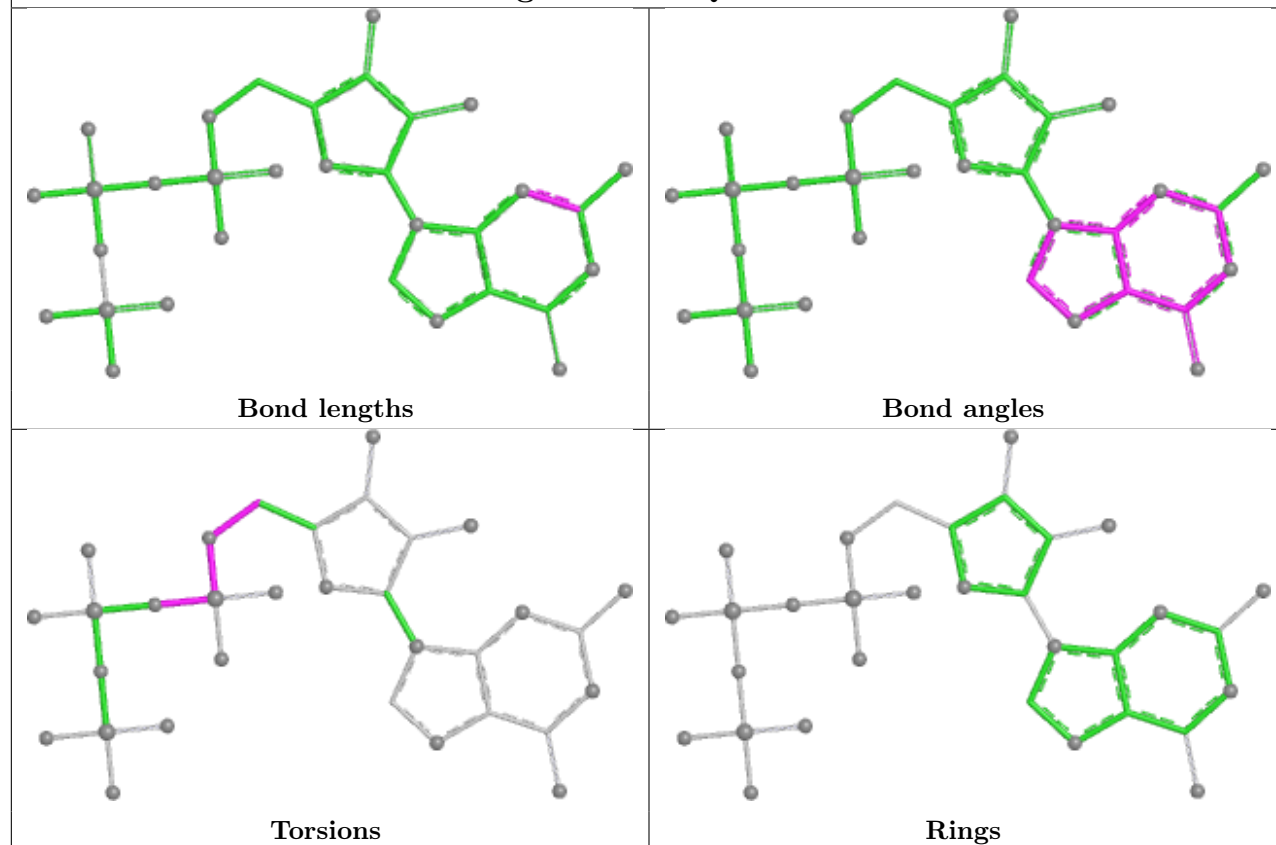




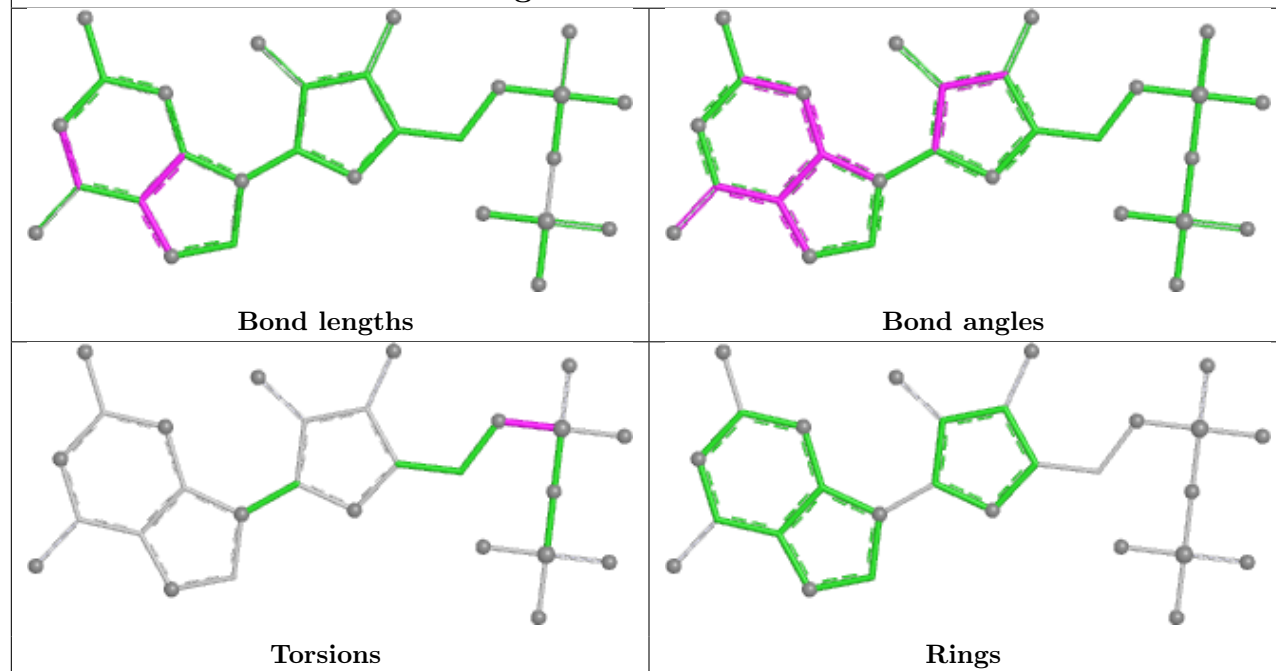


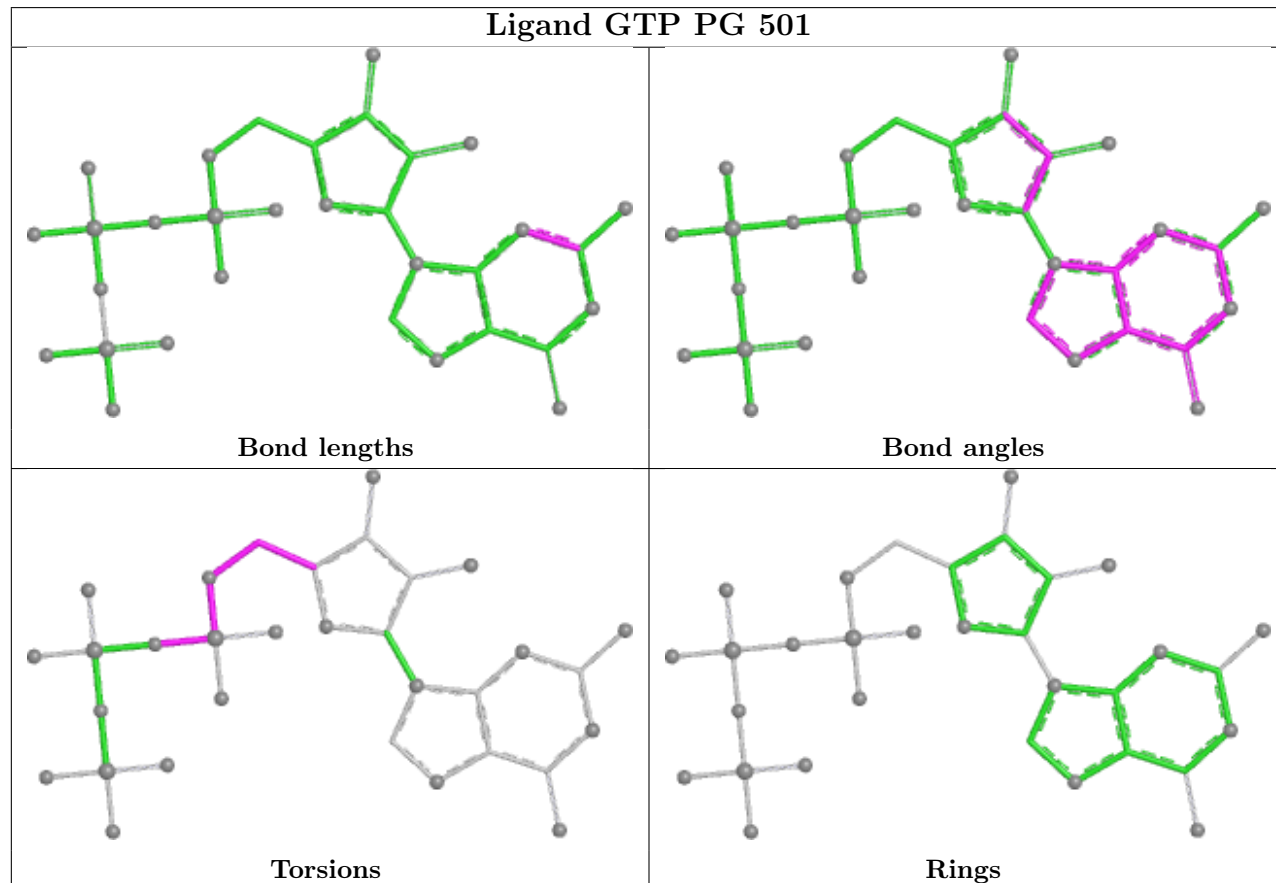
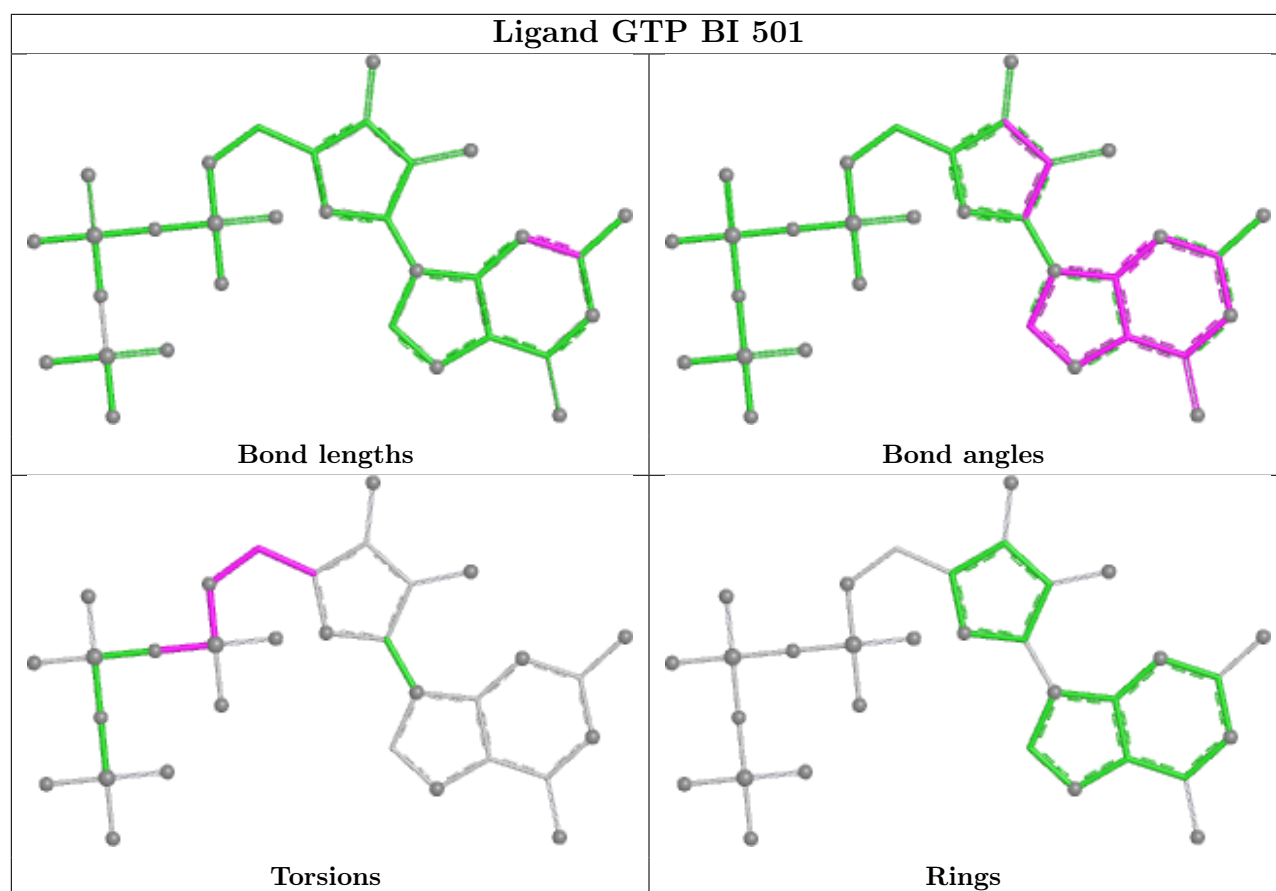


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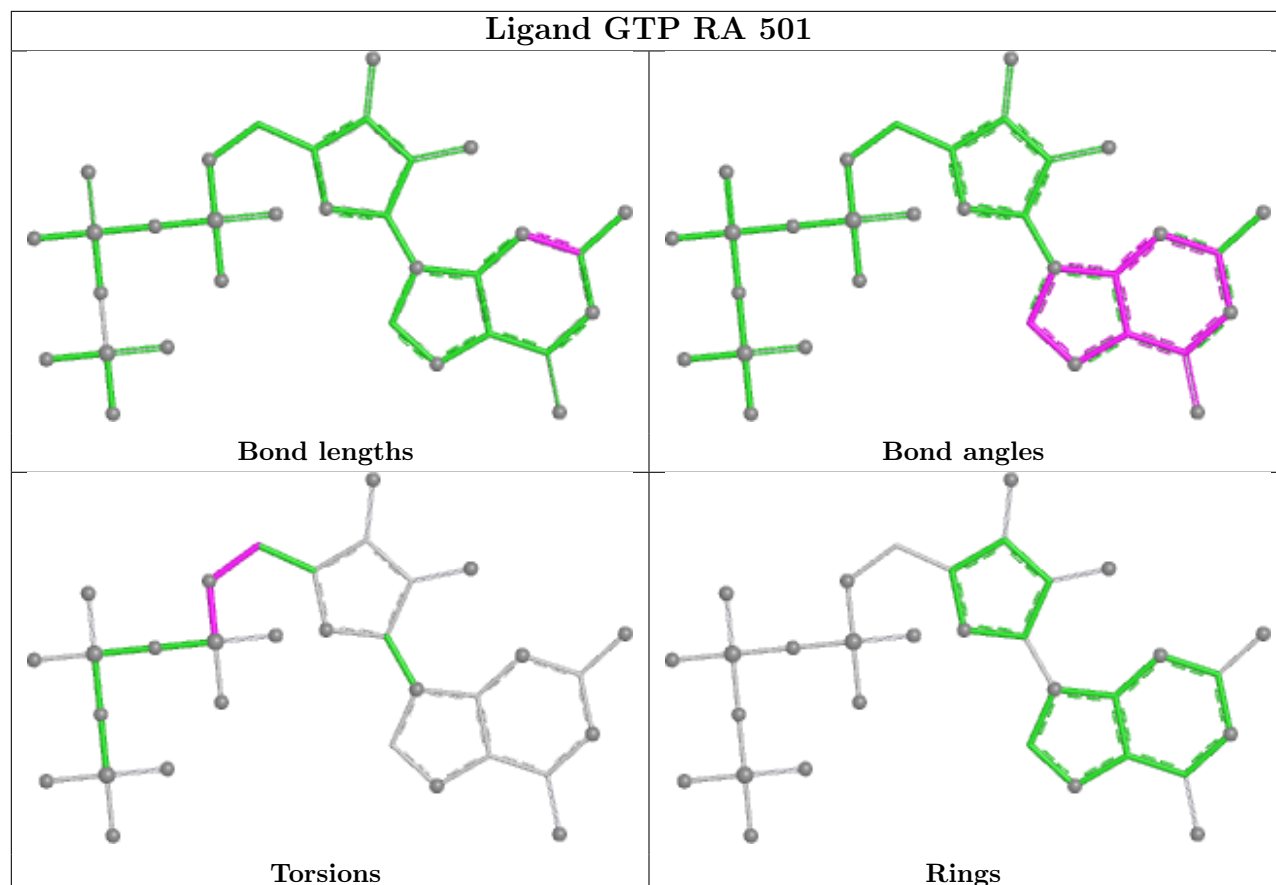


Ligand GDP NK 501

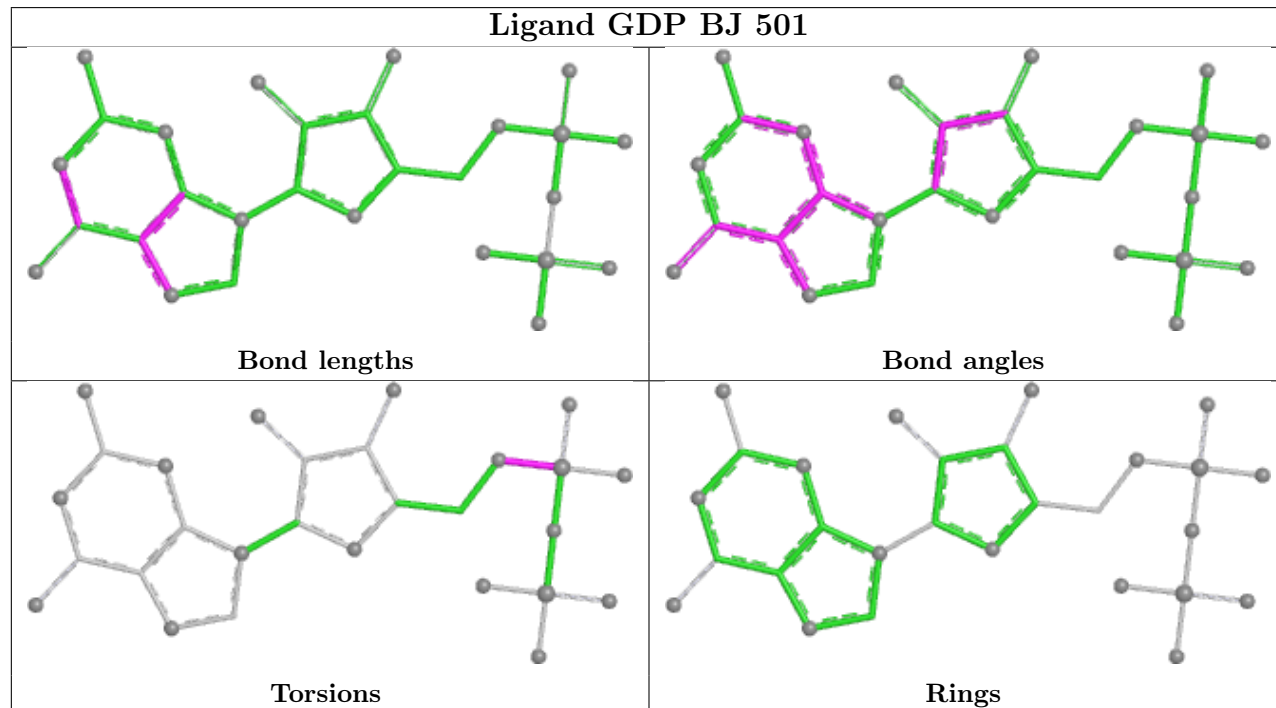


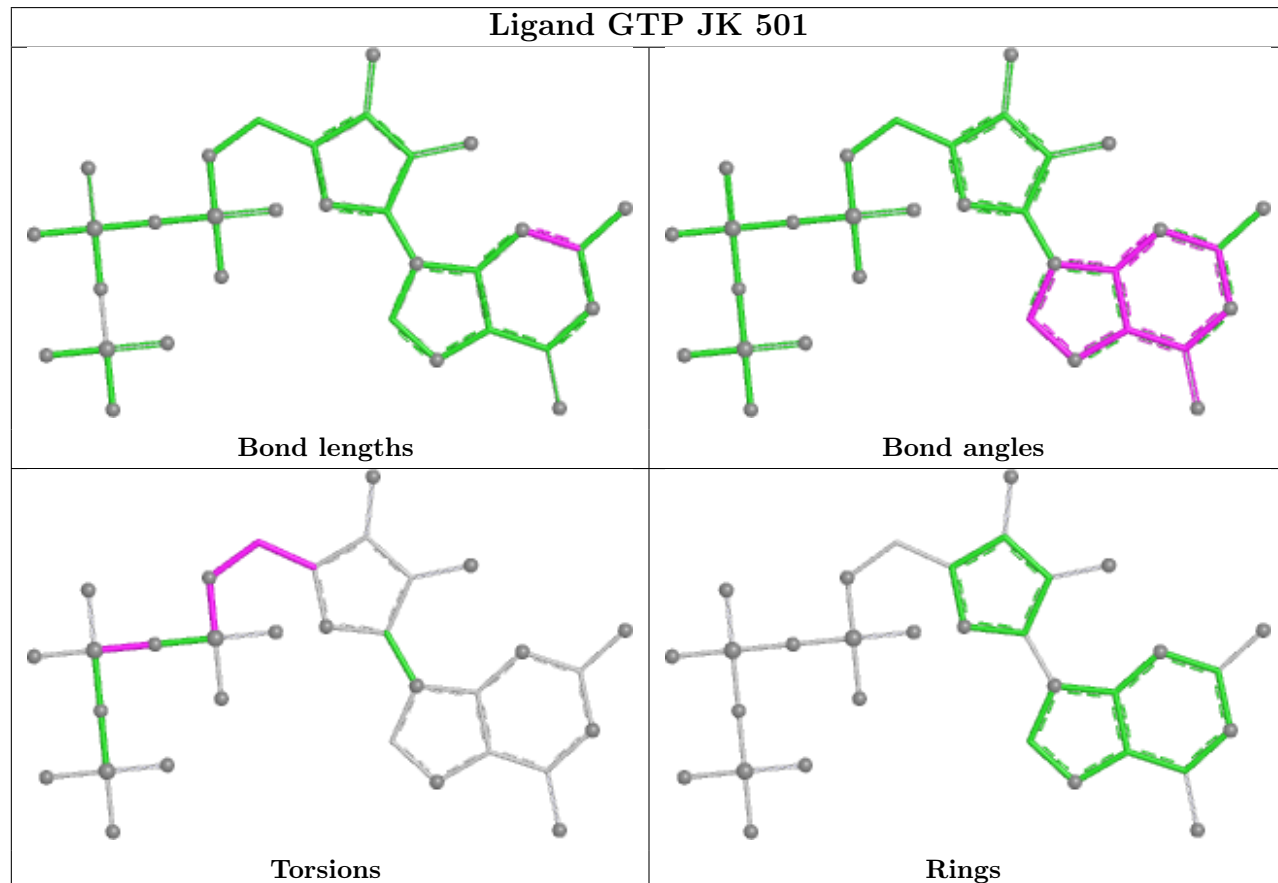
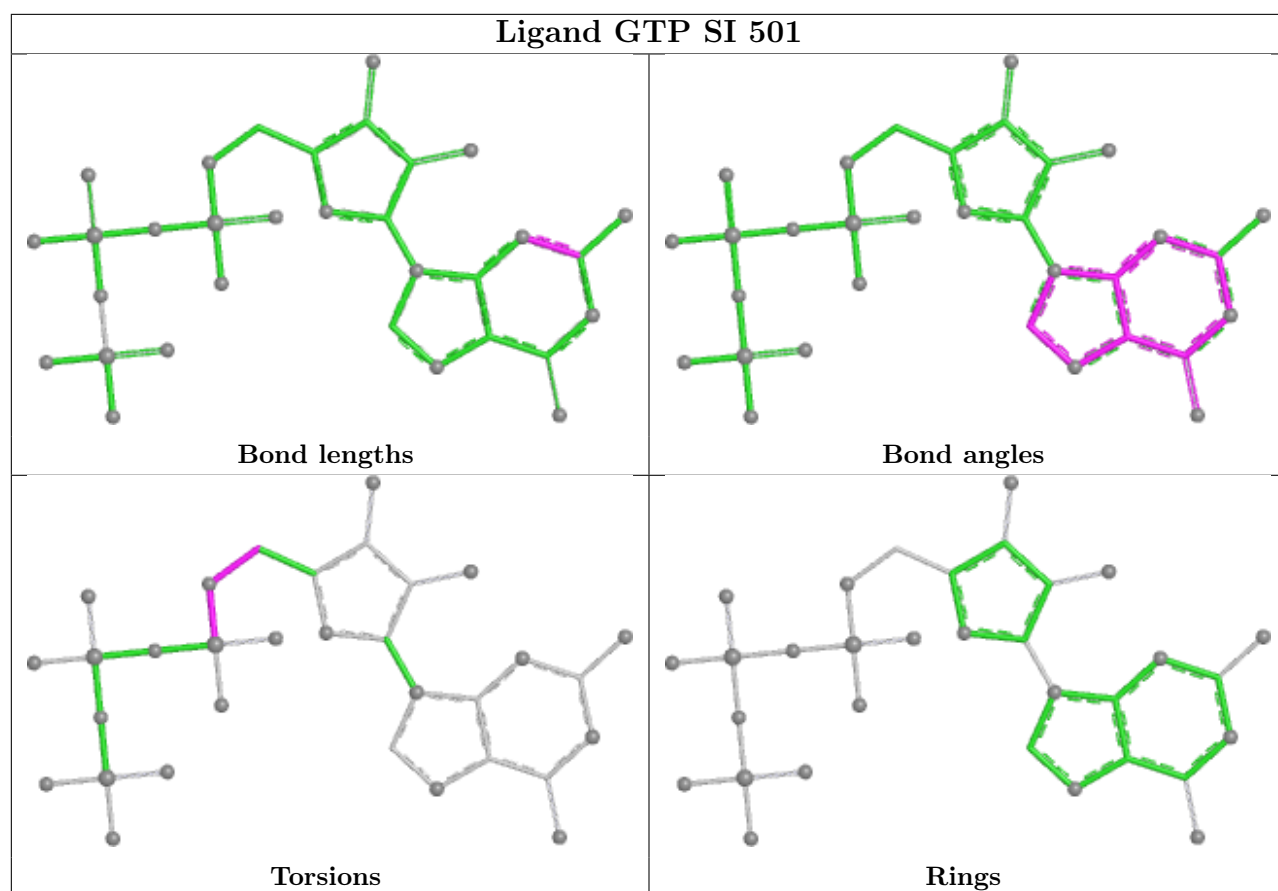


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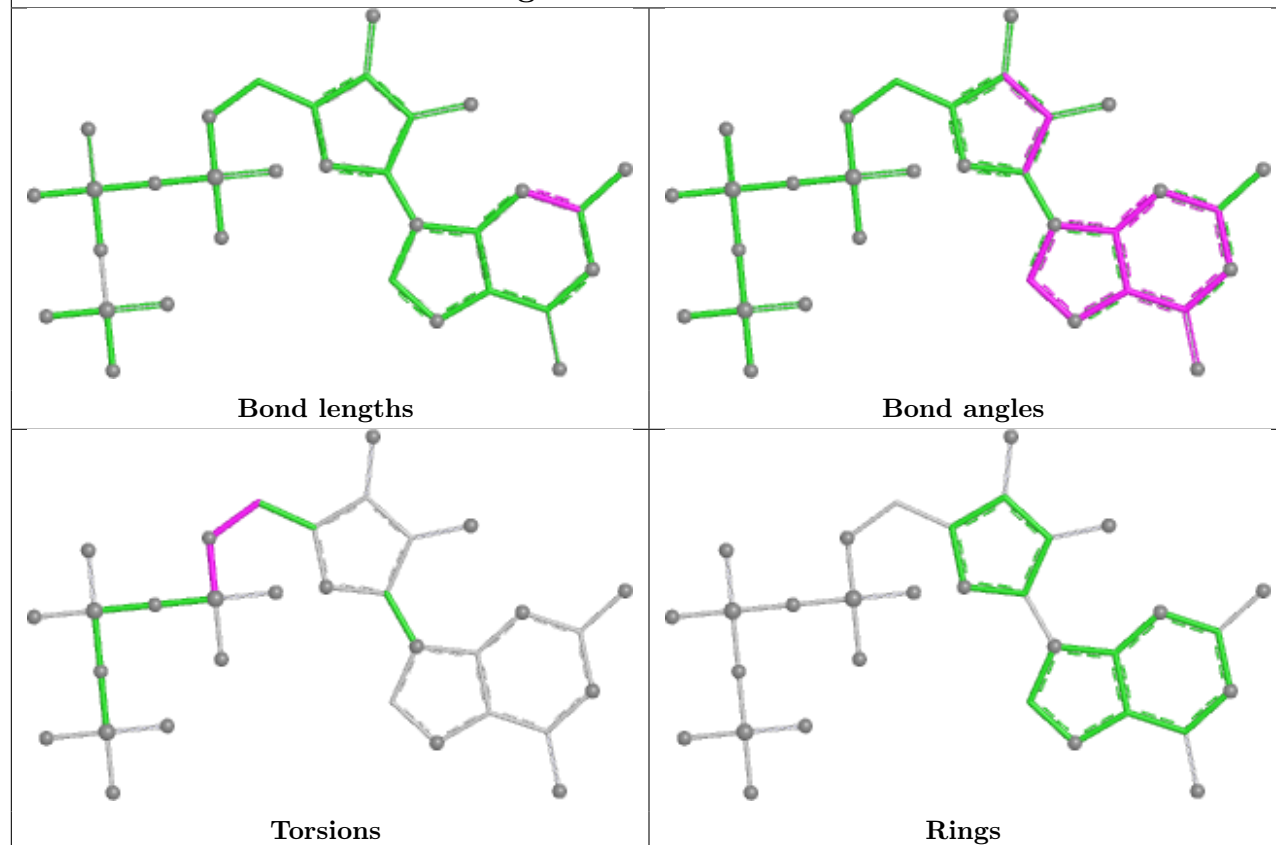


Ligand GDP BJ 501

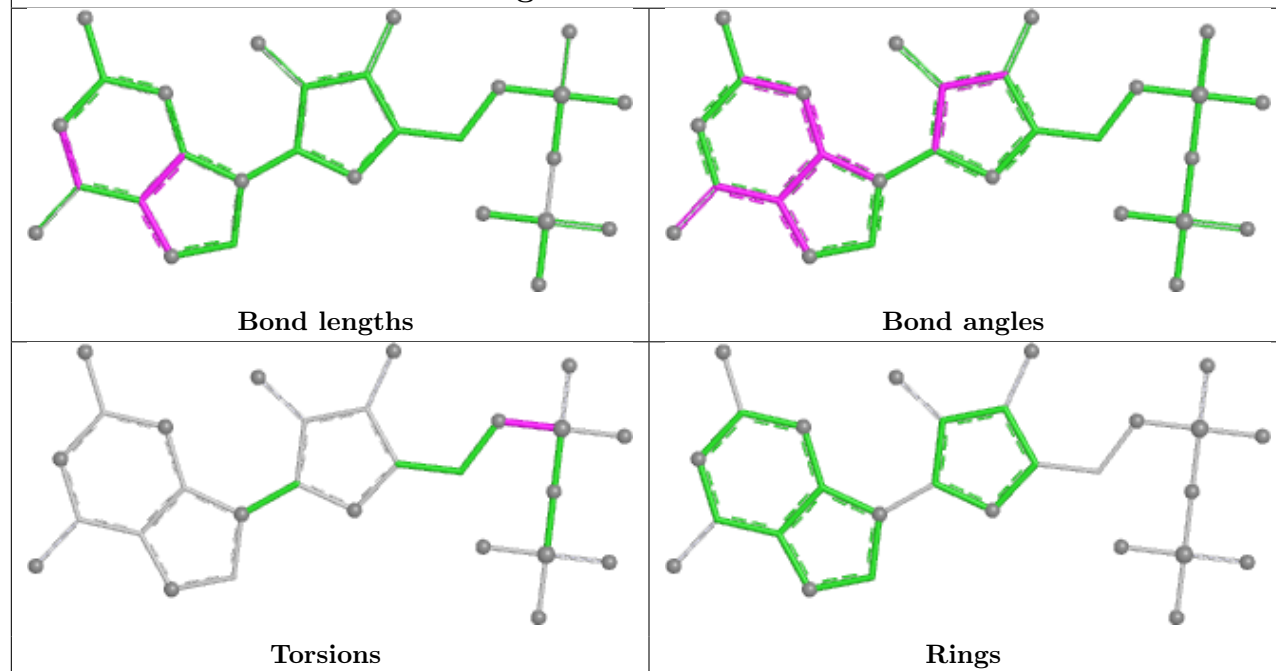


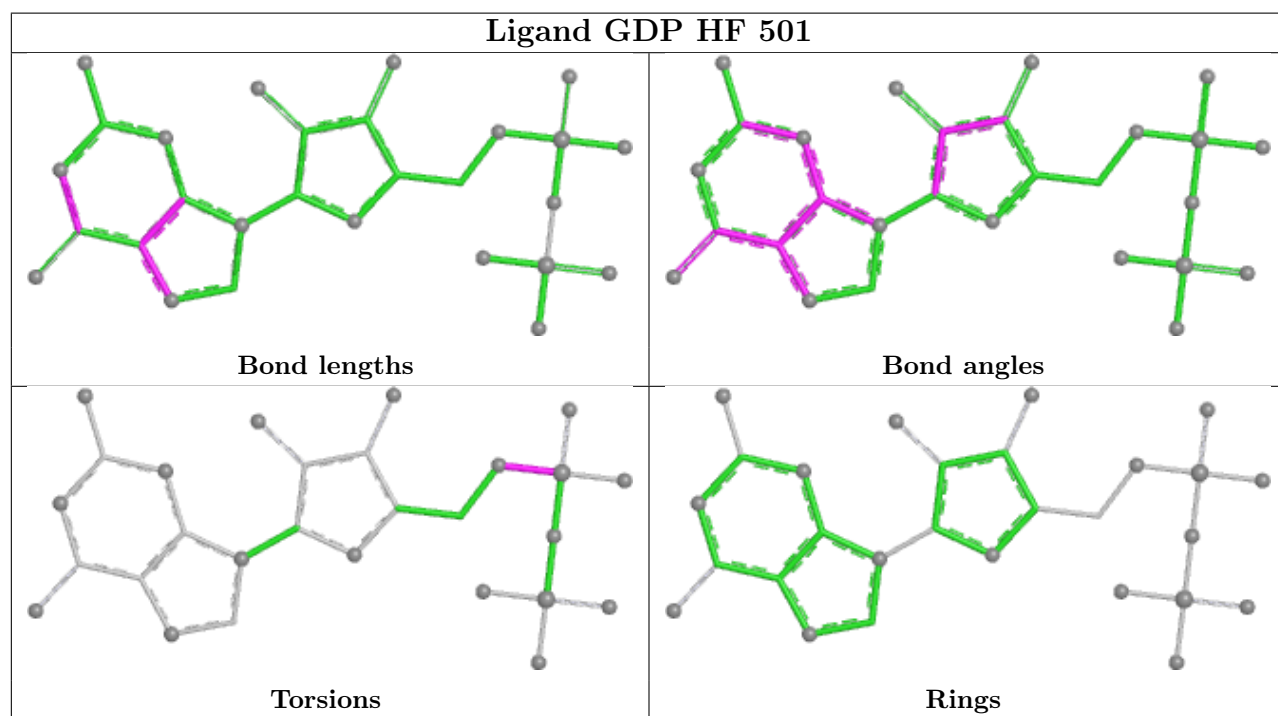
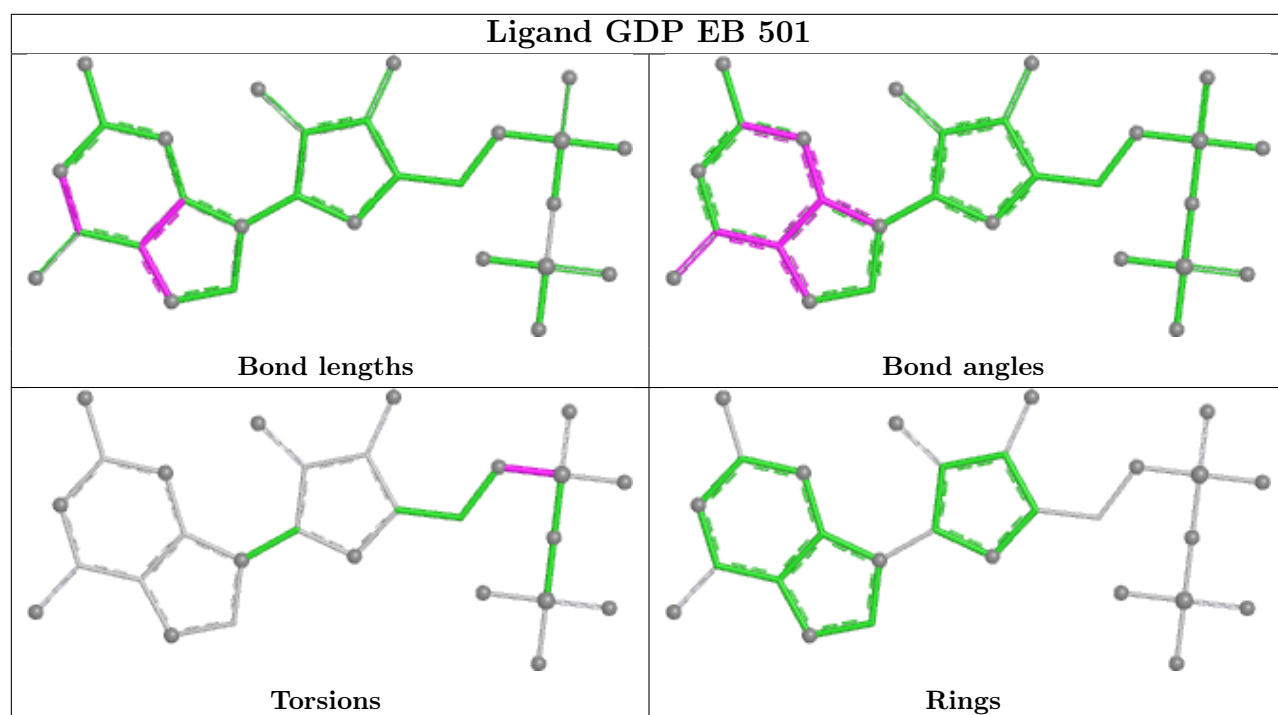


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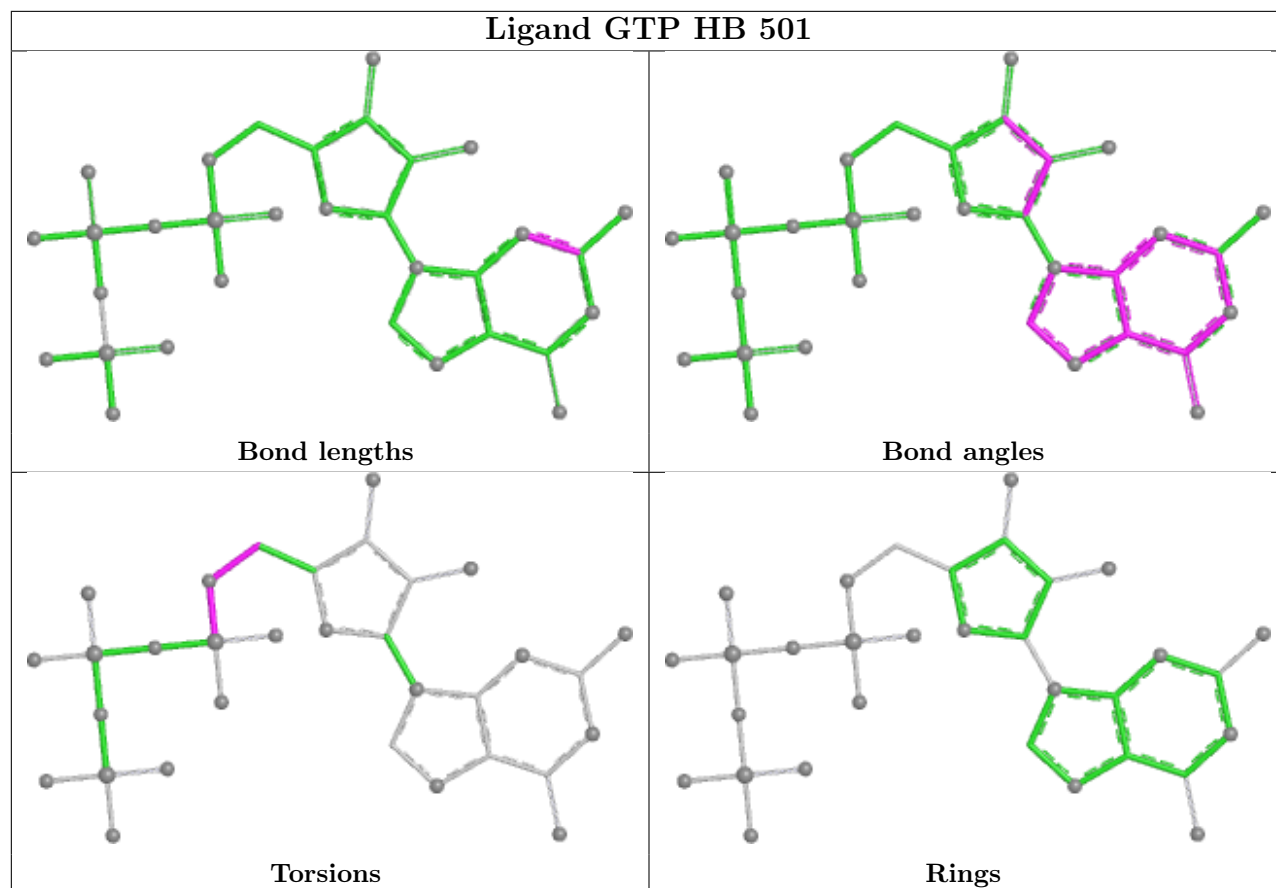


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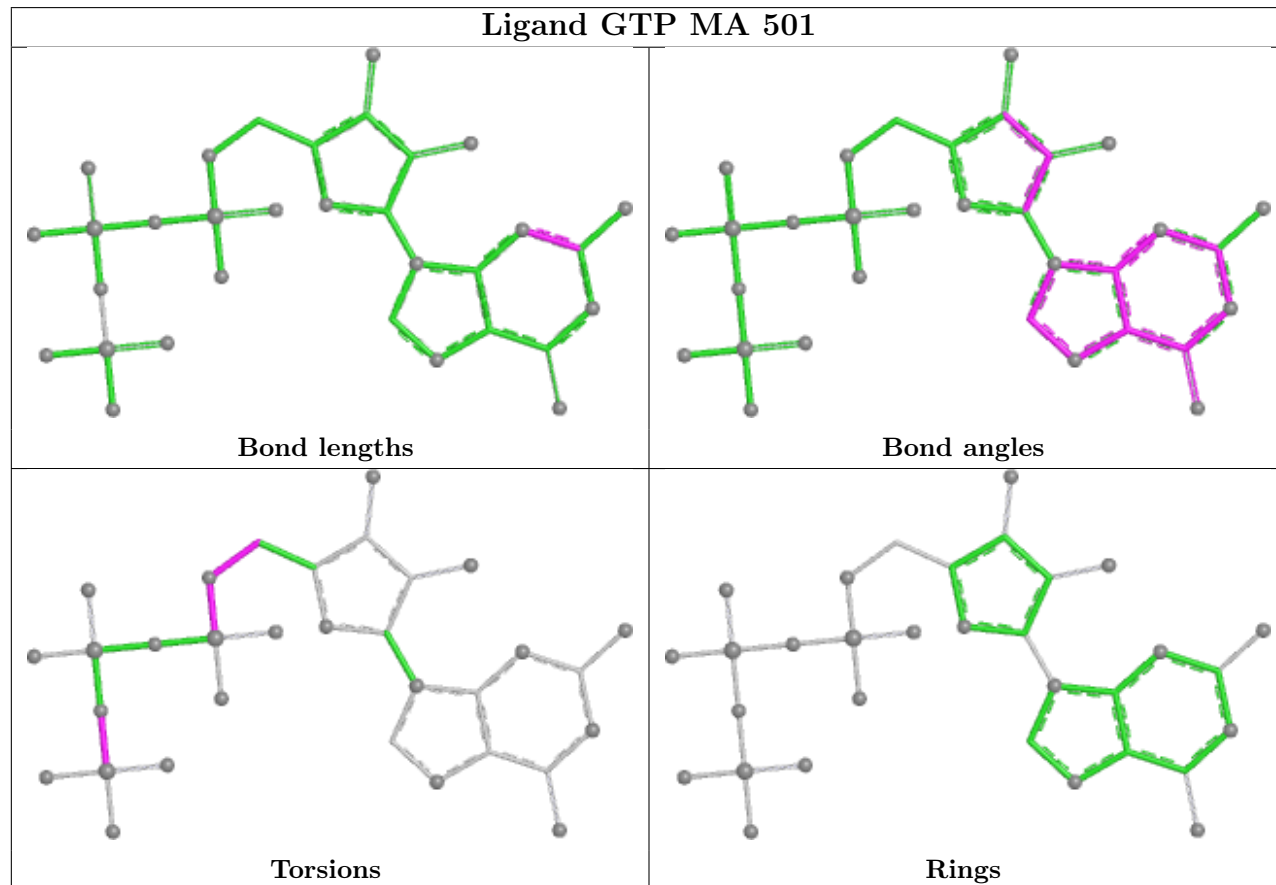




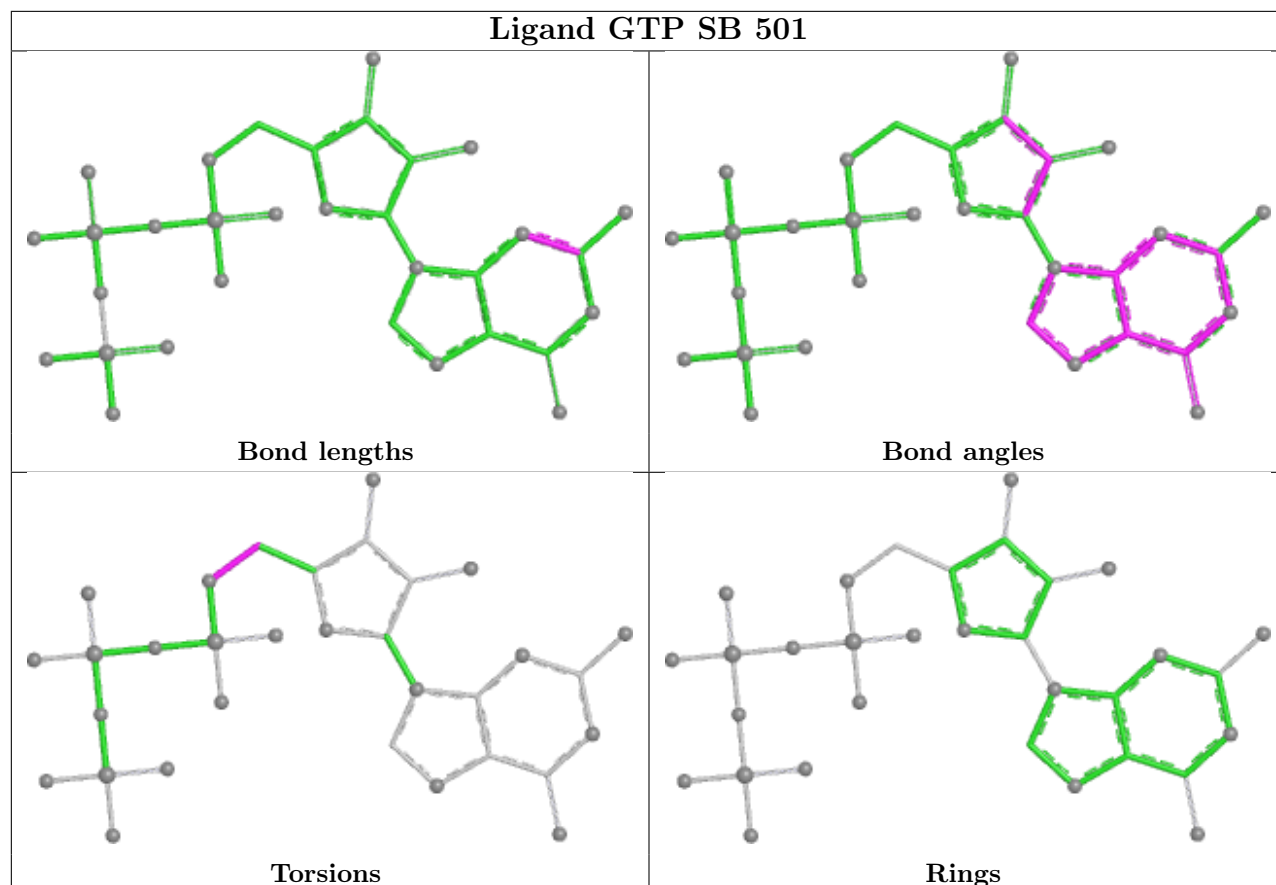
Ligand GTP HB 501



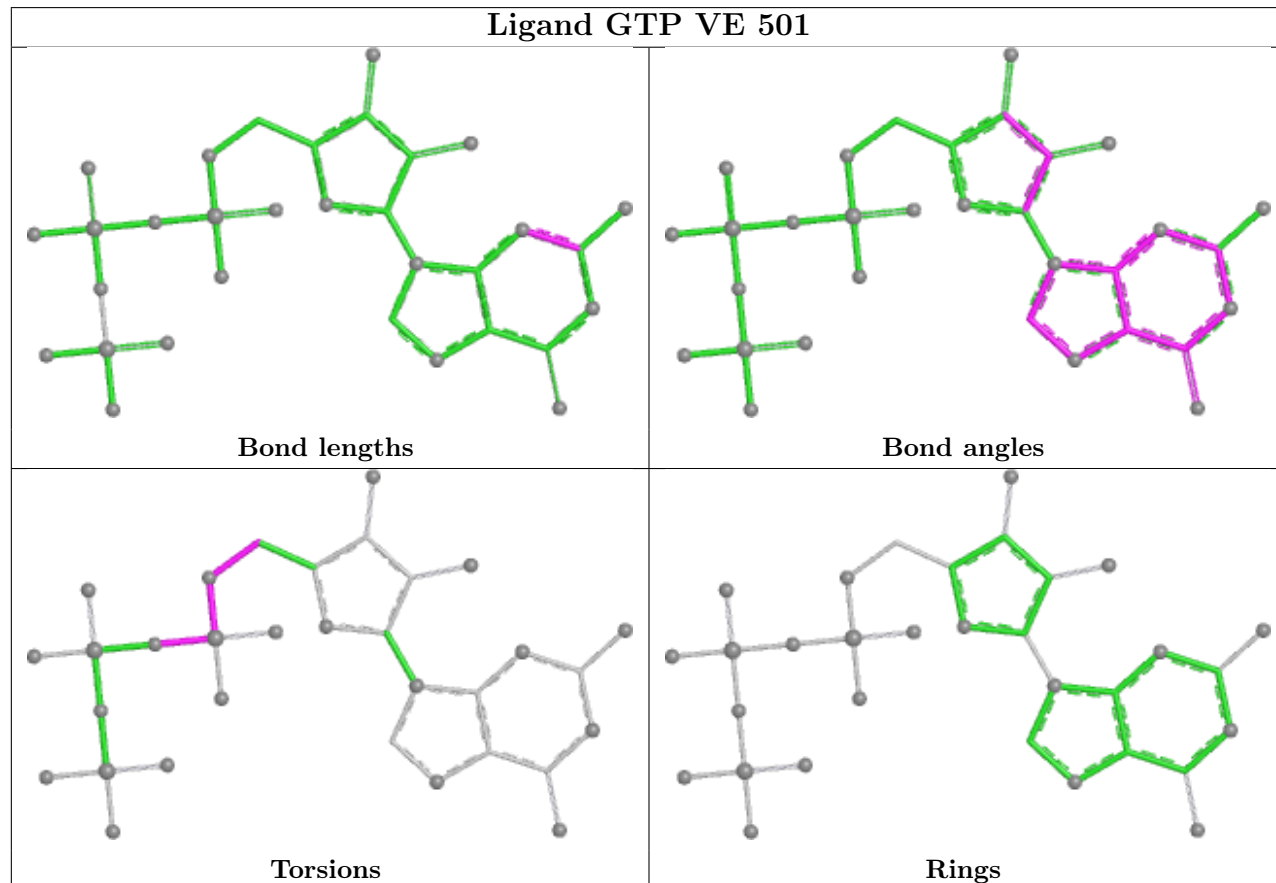
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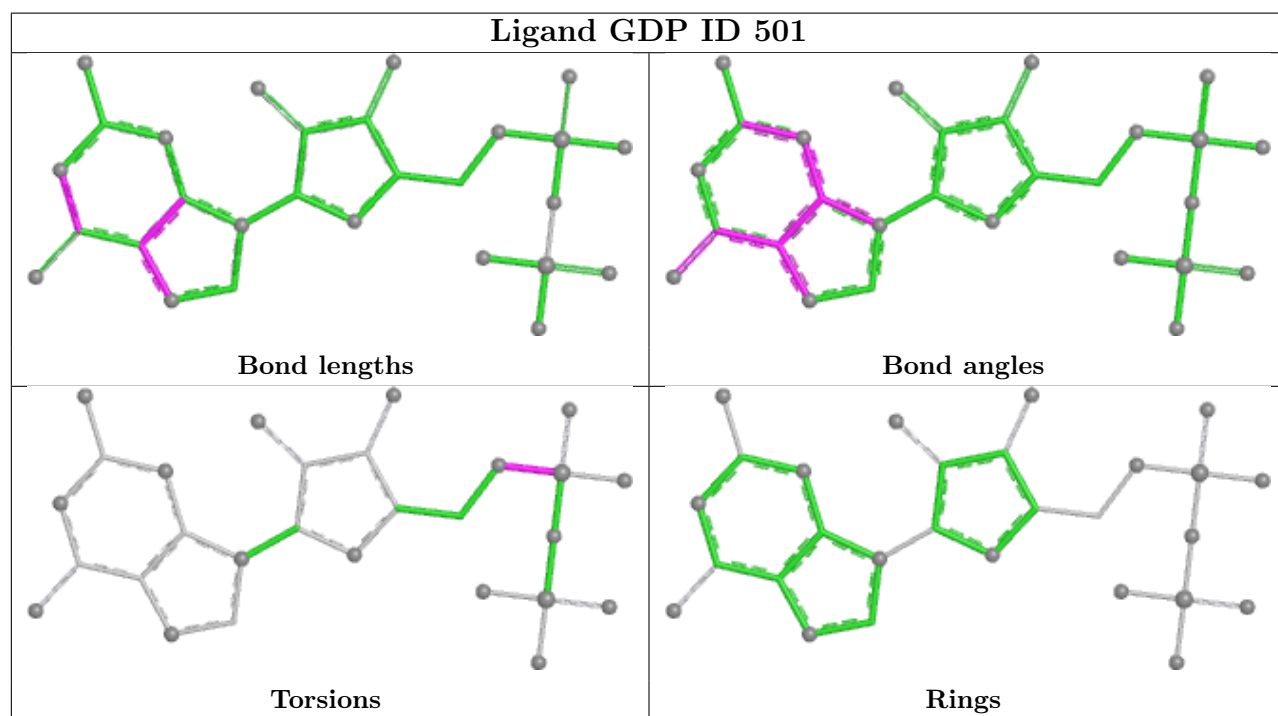
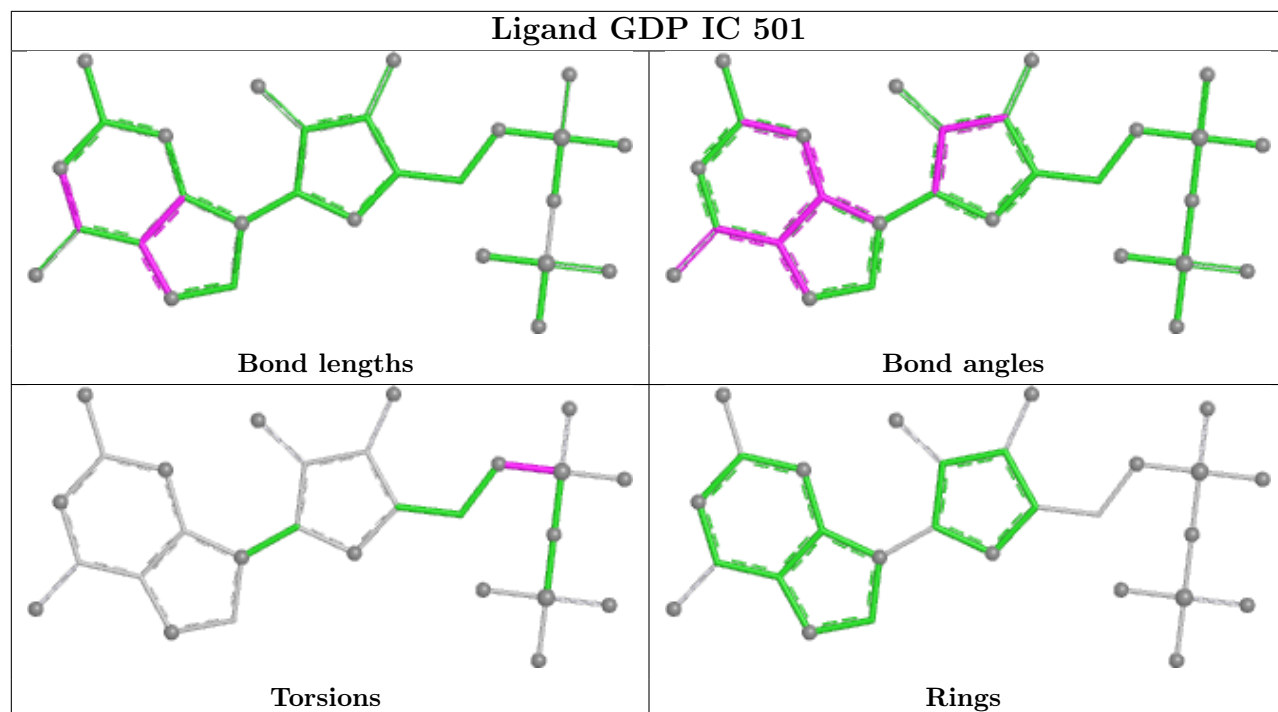


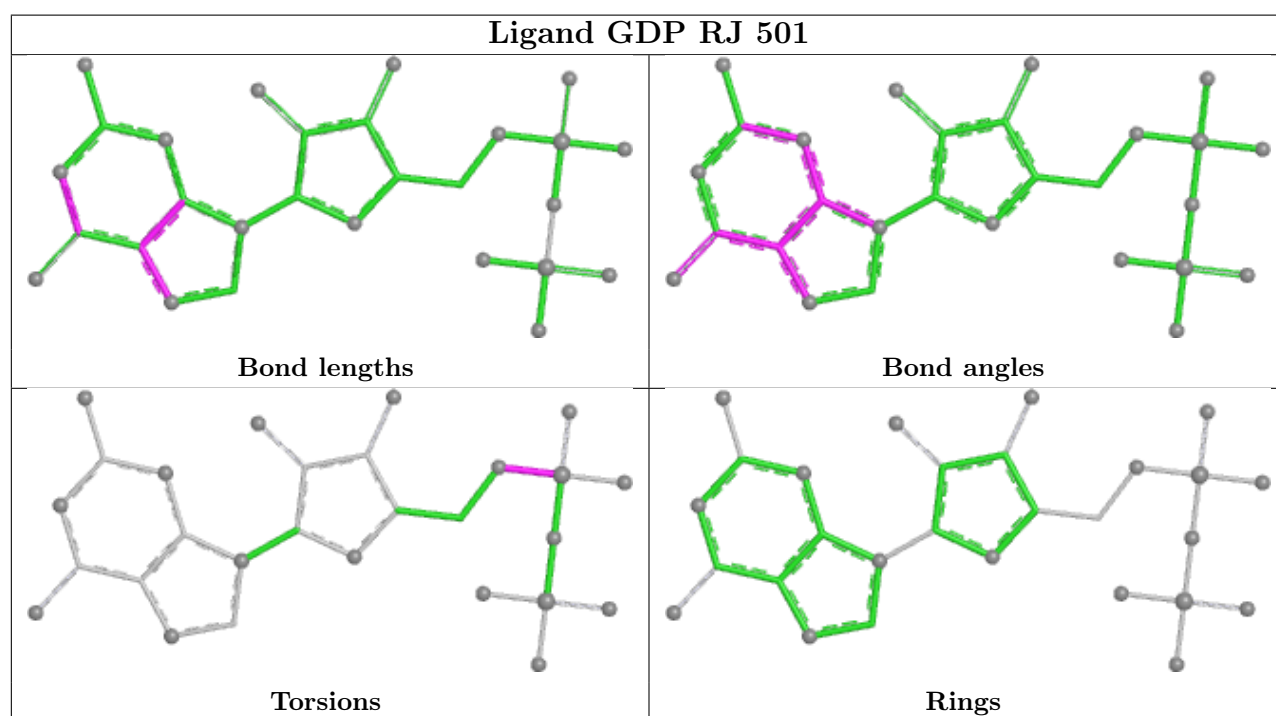
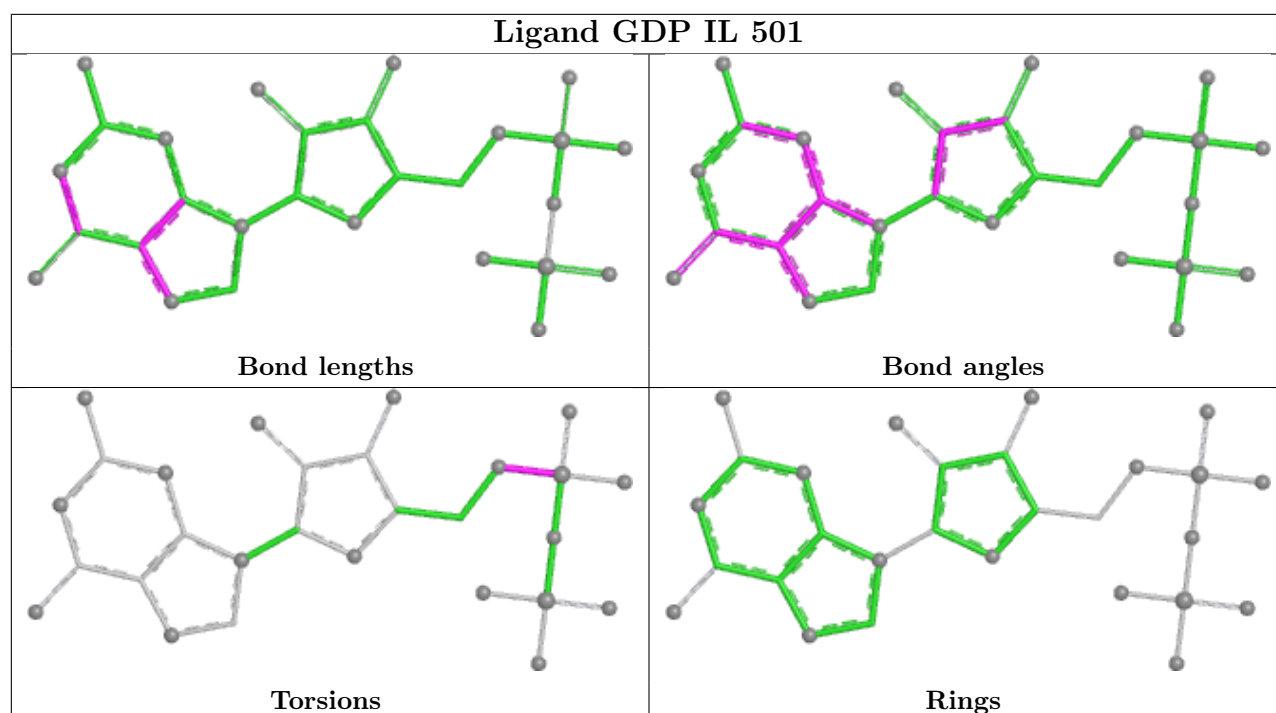
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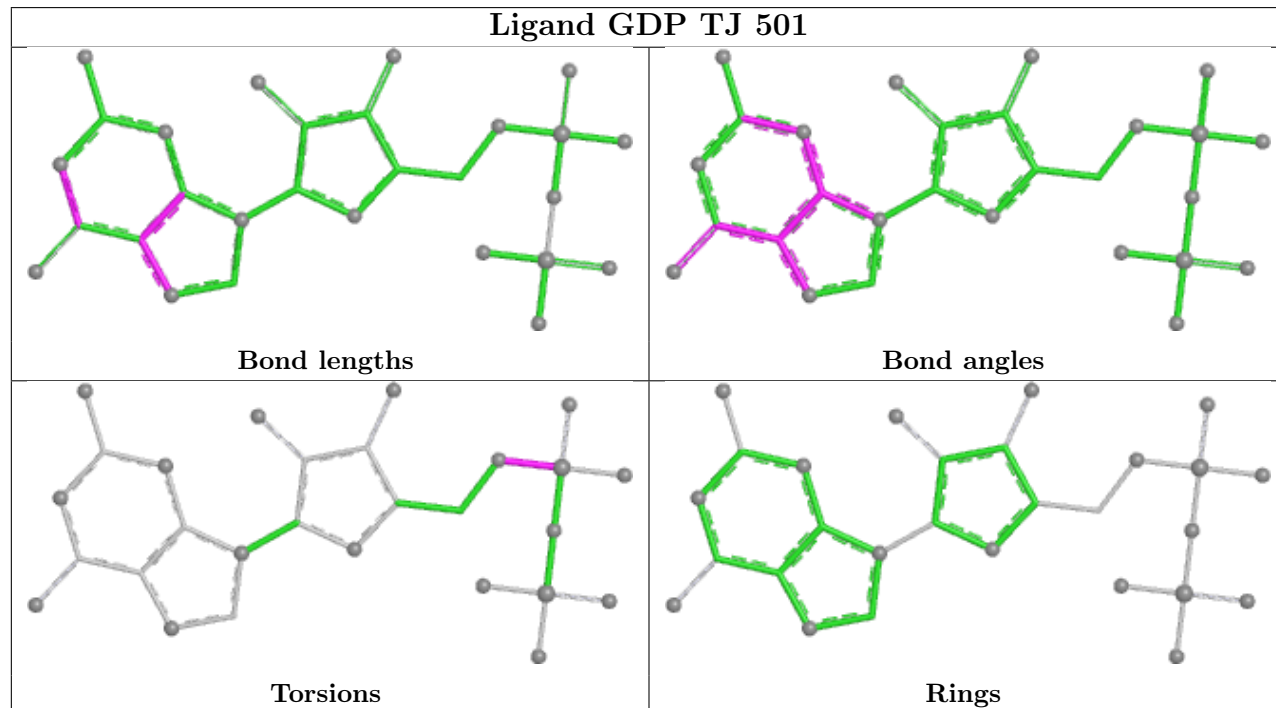
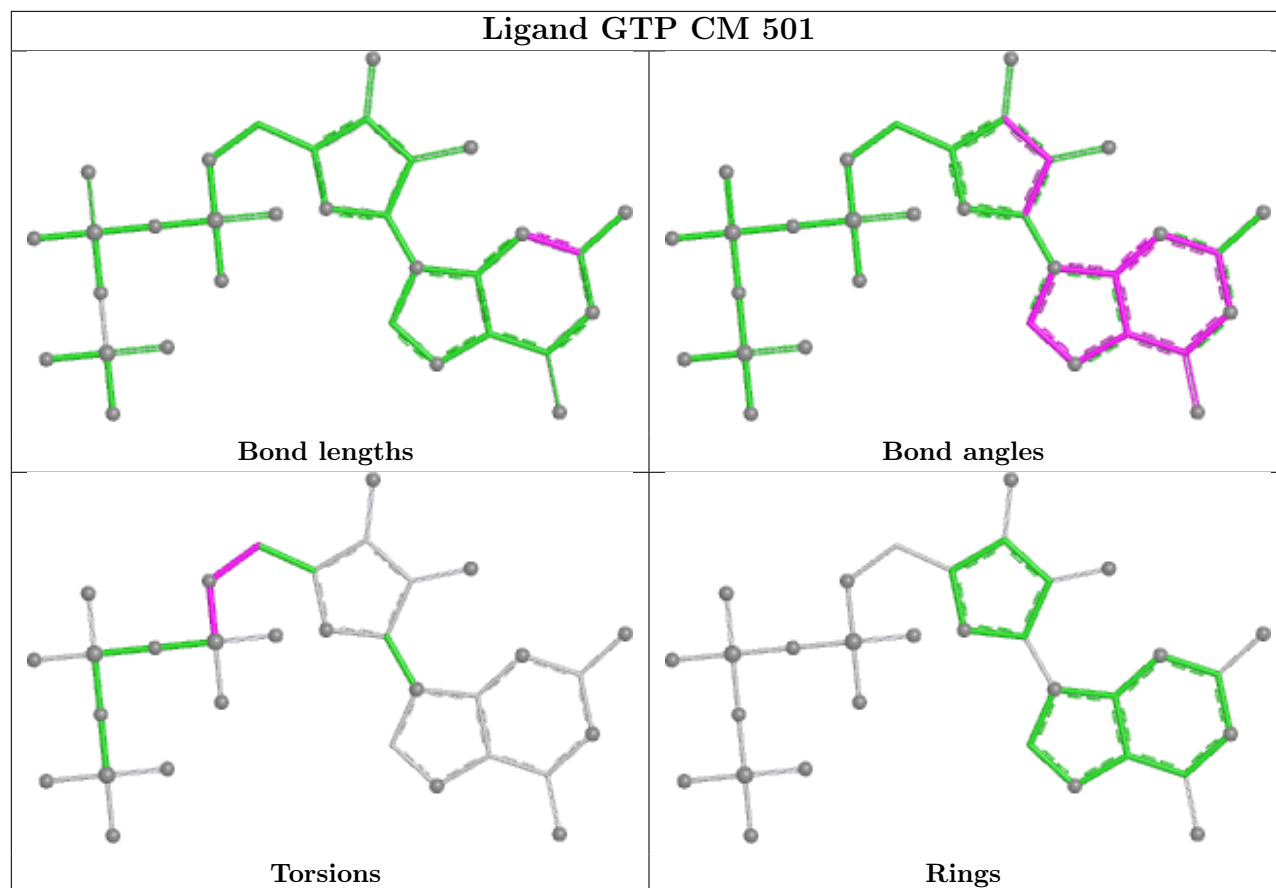


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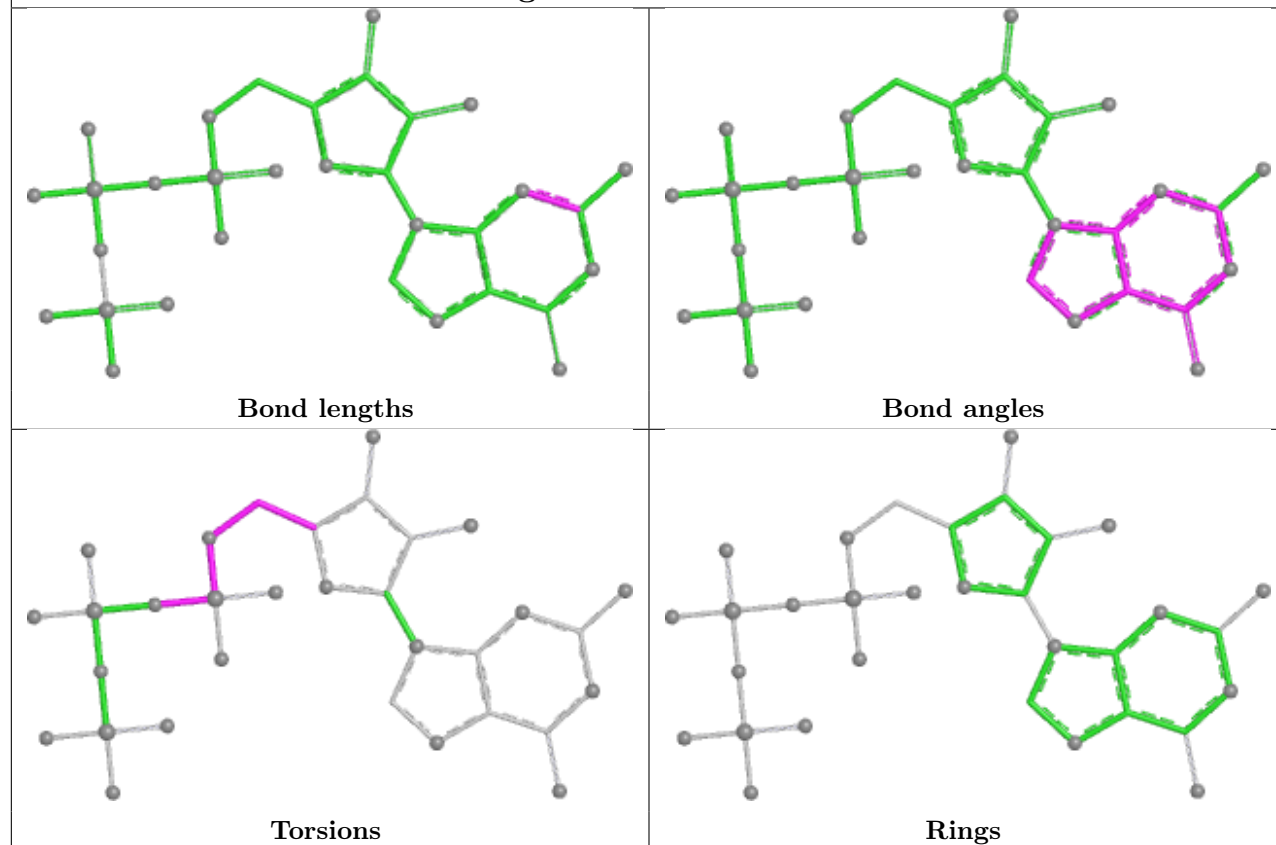




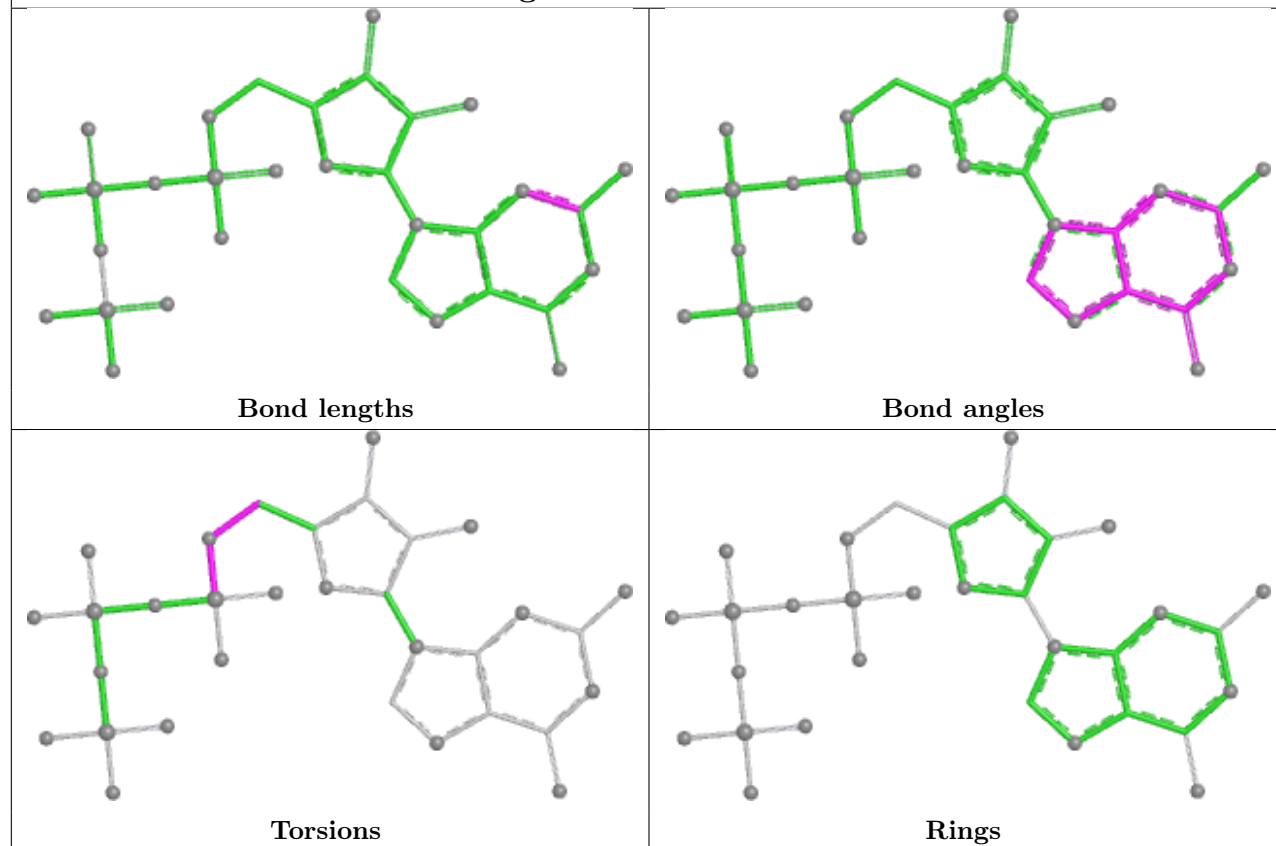


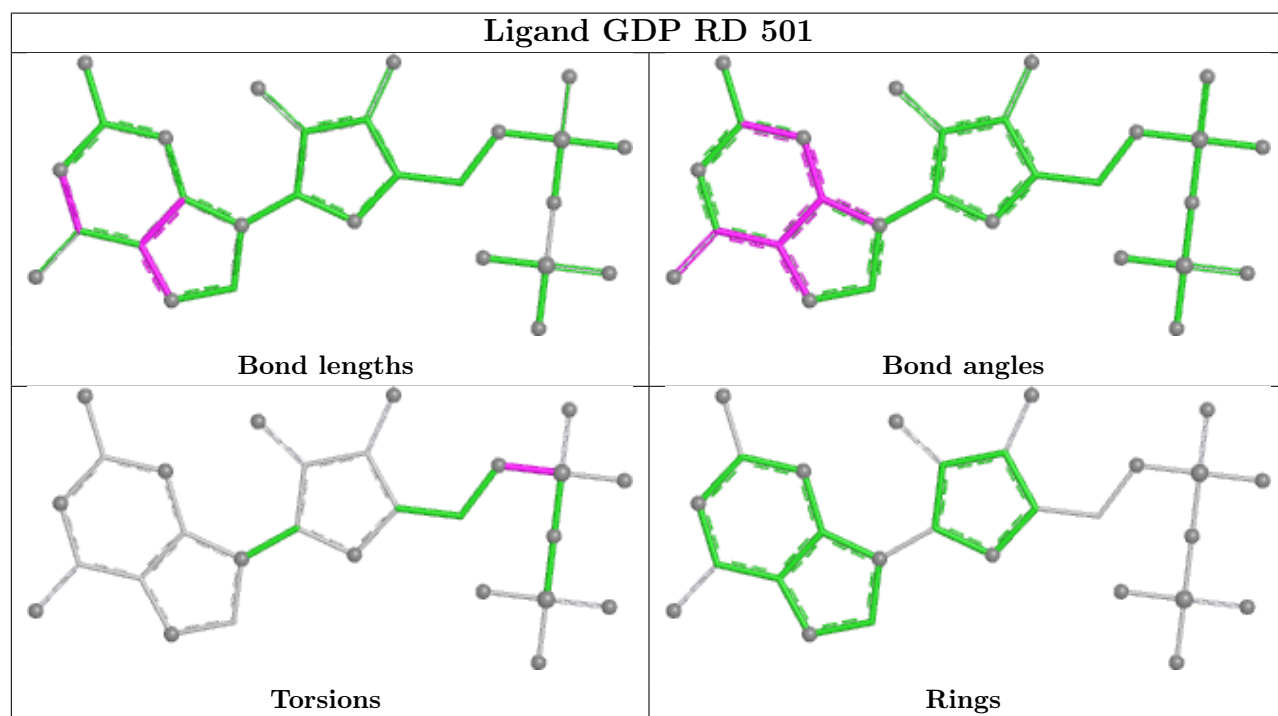
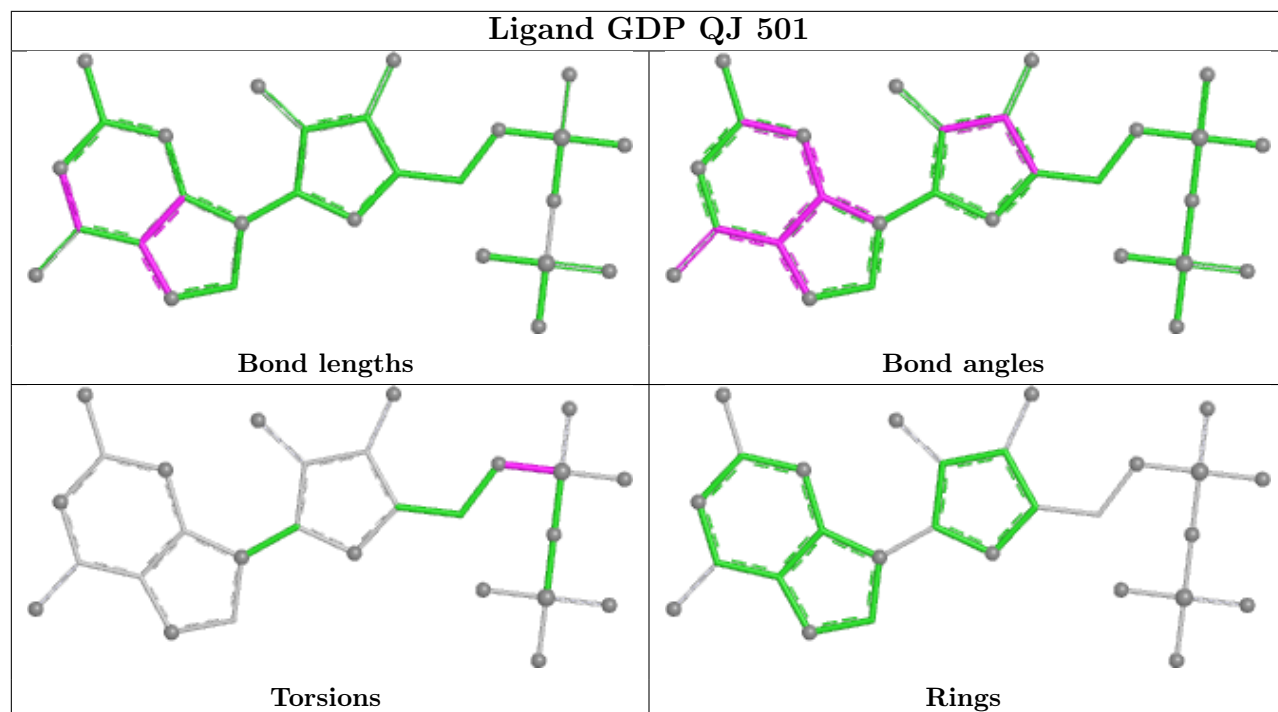


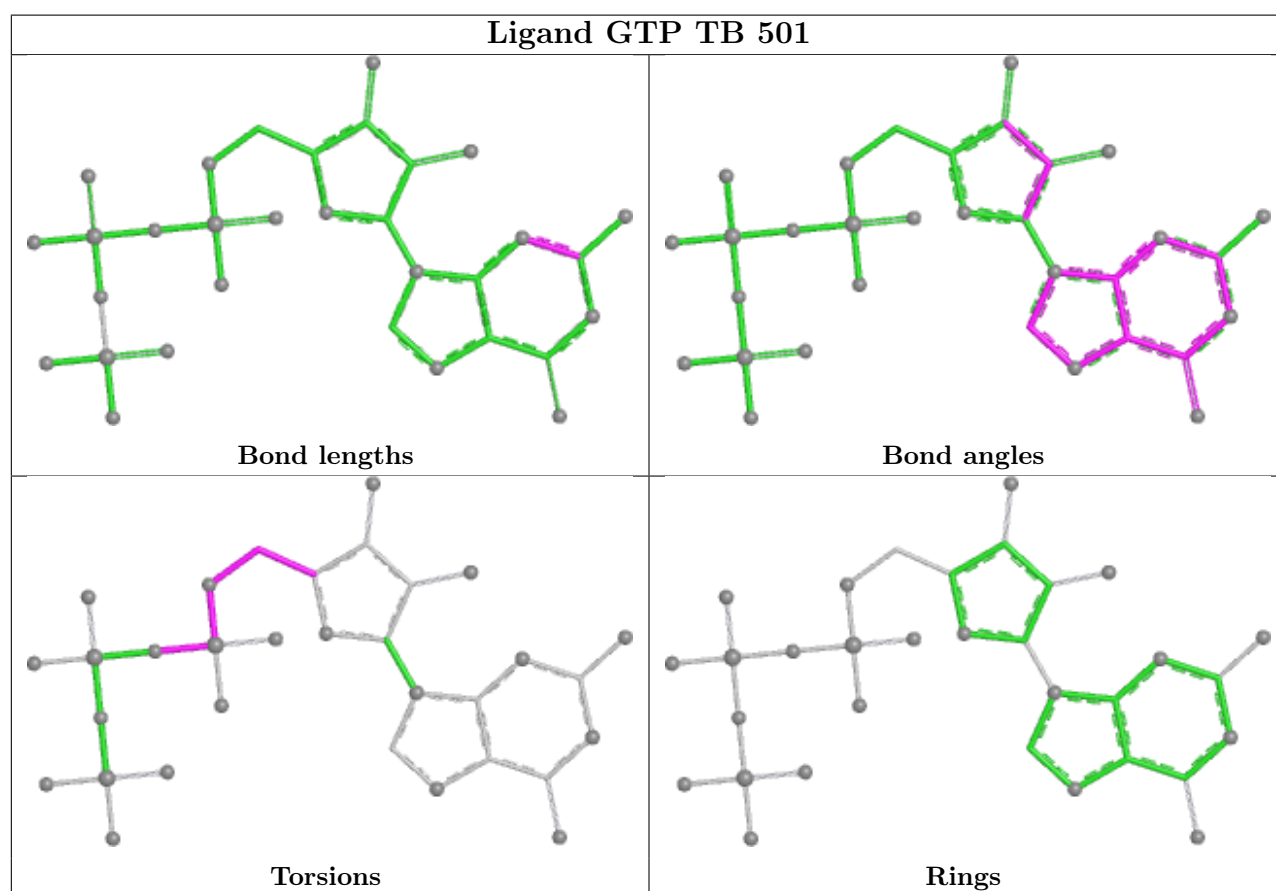
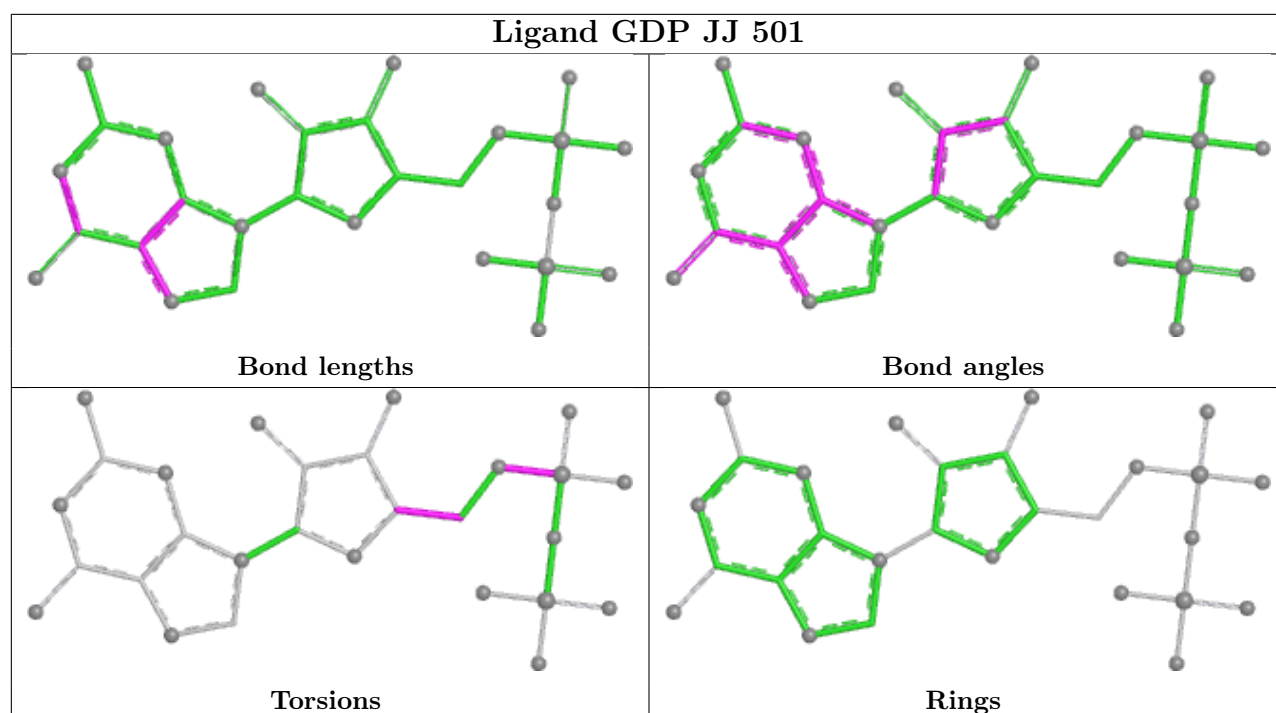
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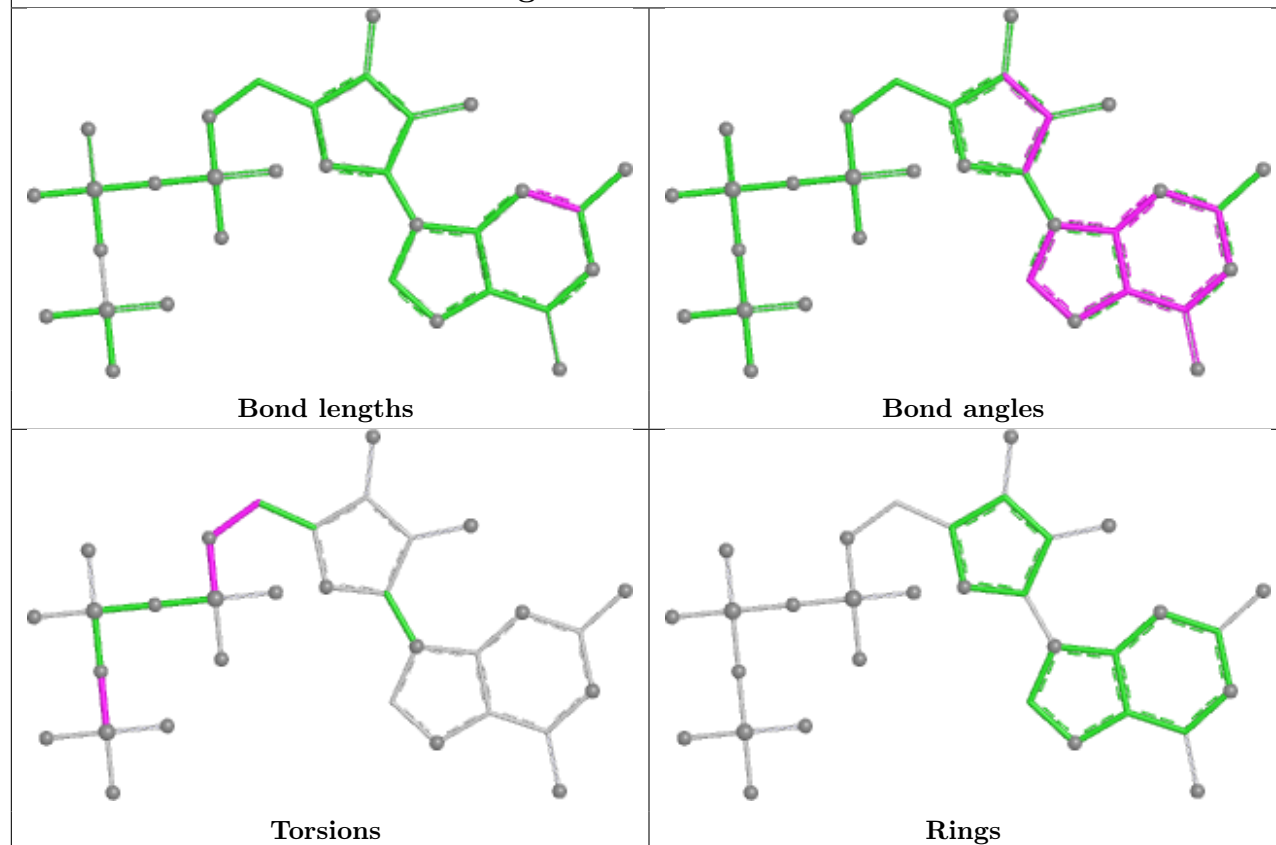
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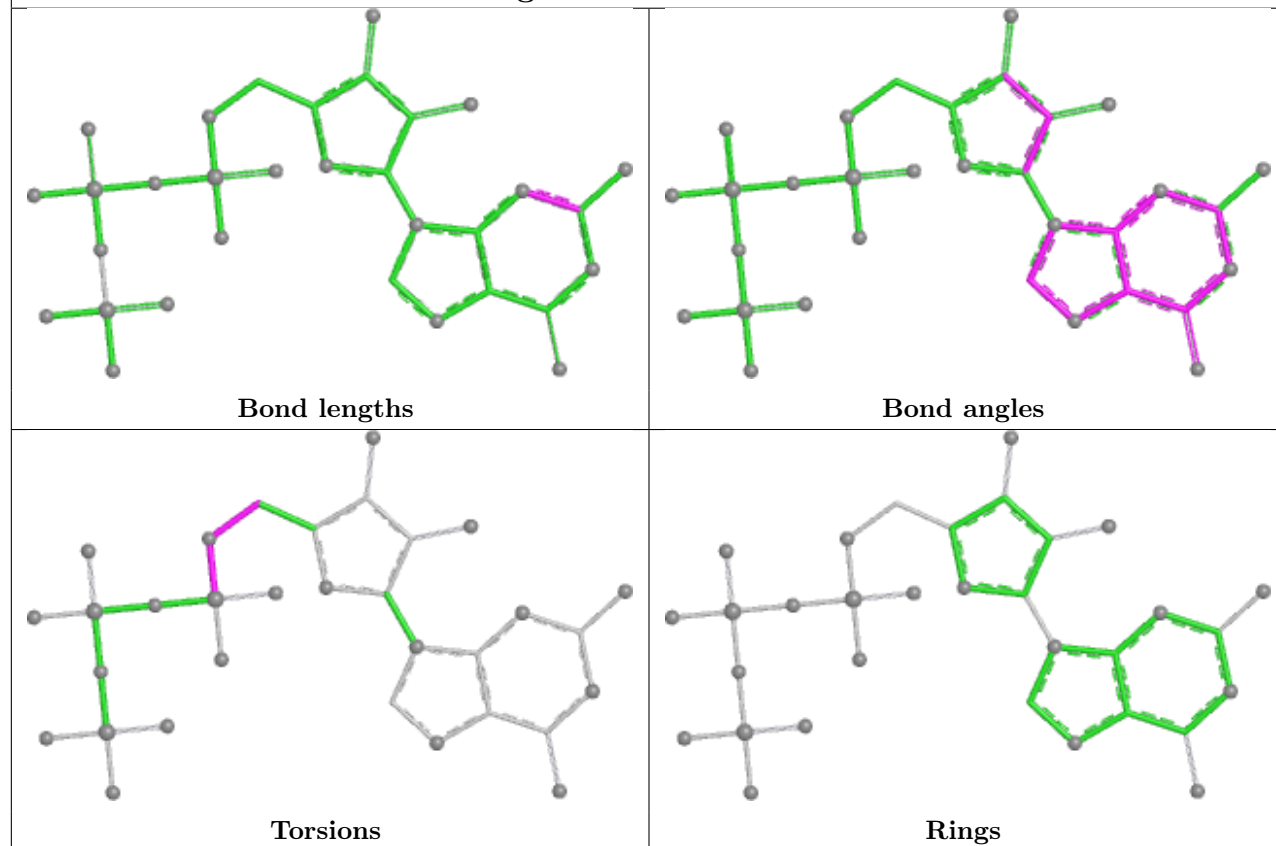


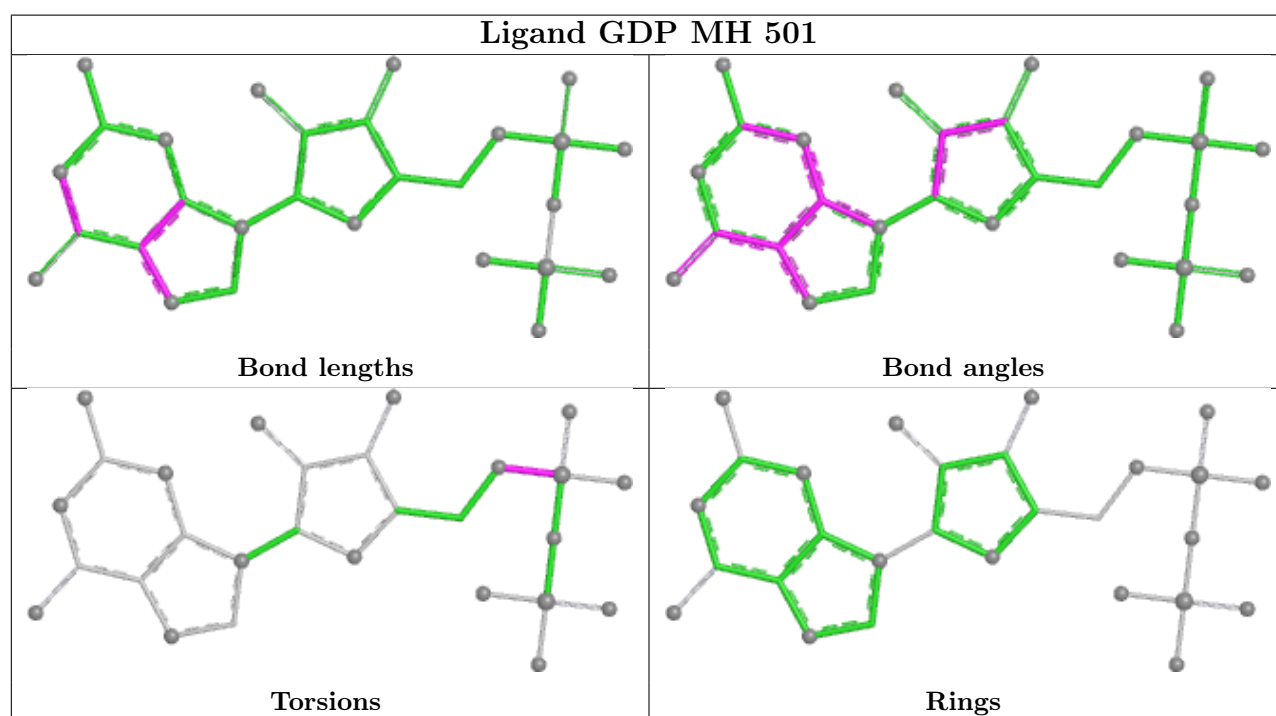
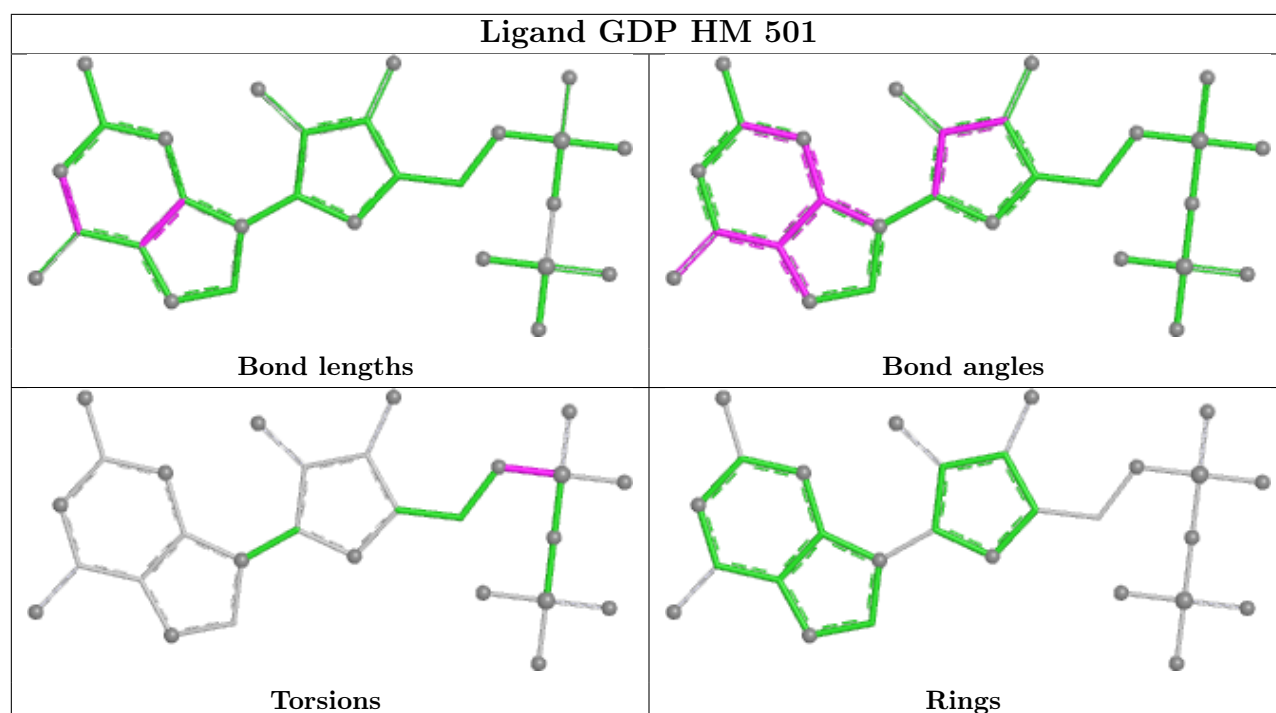


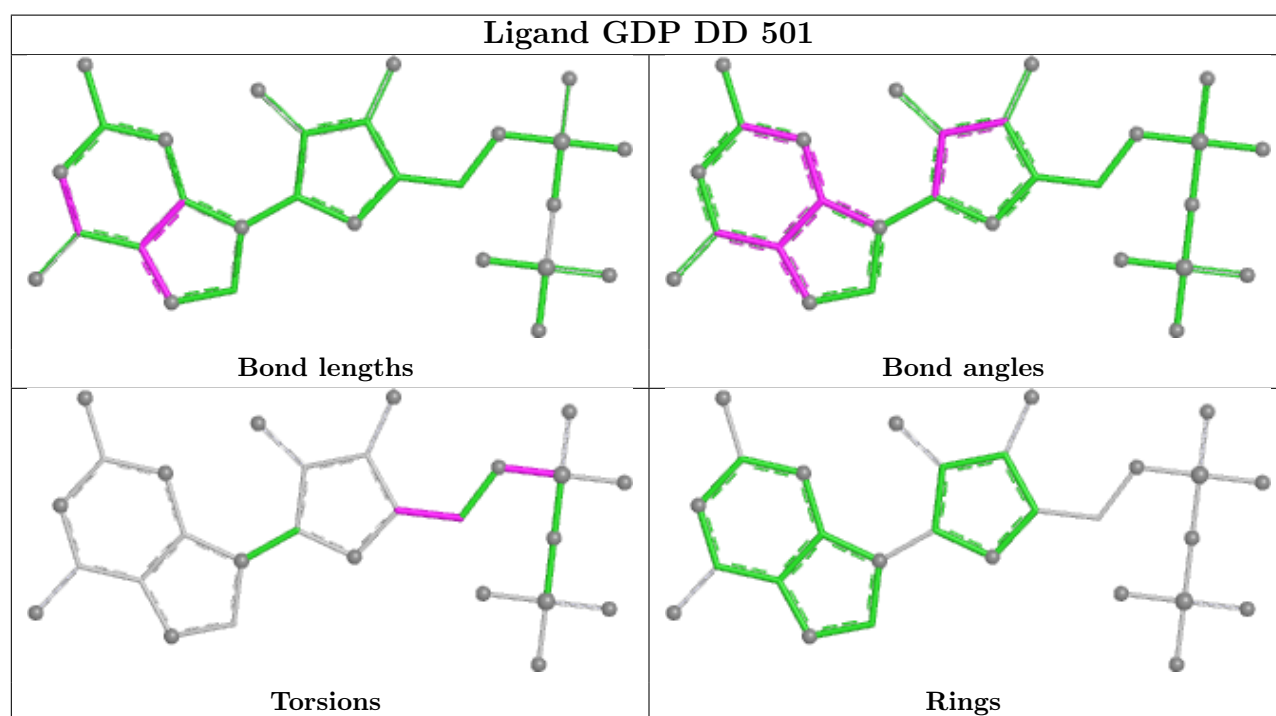
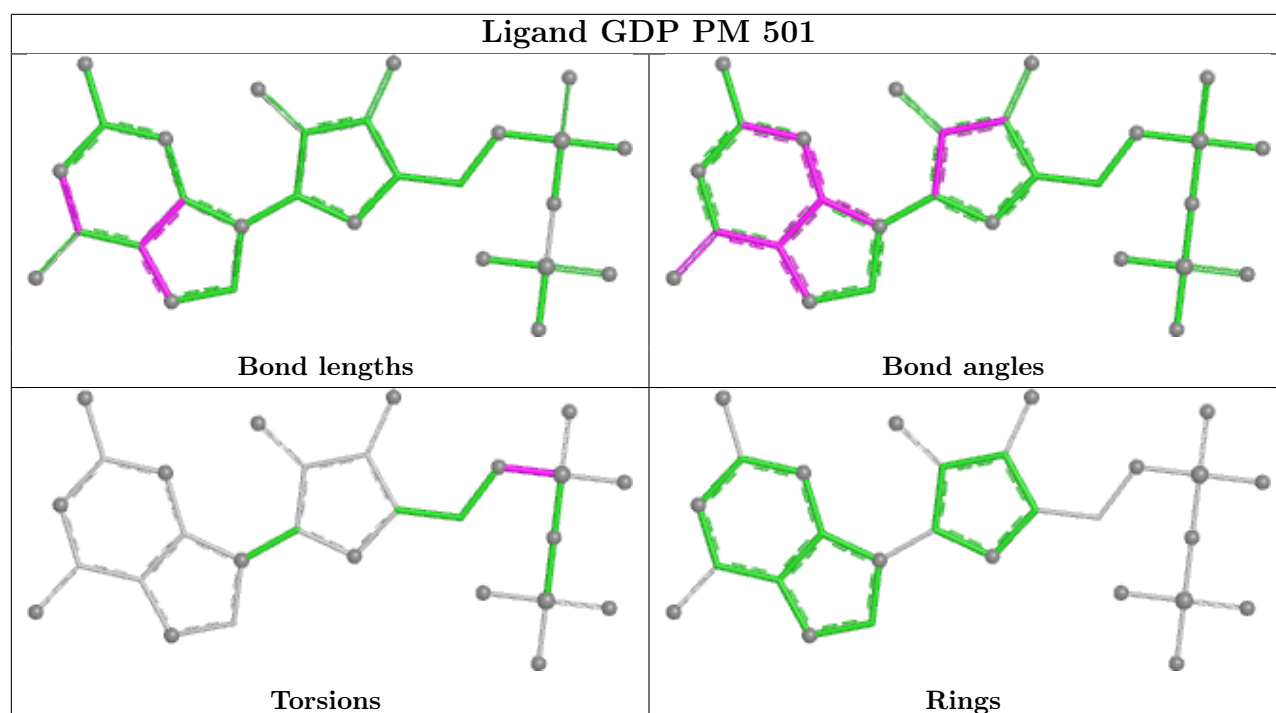
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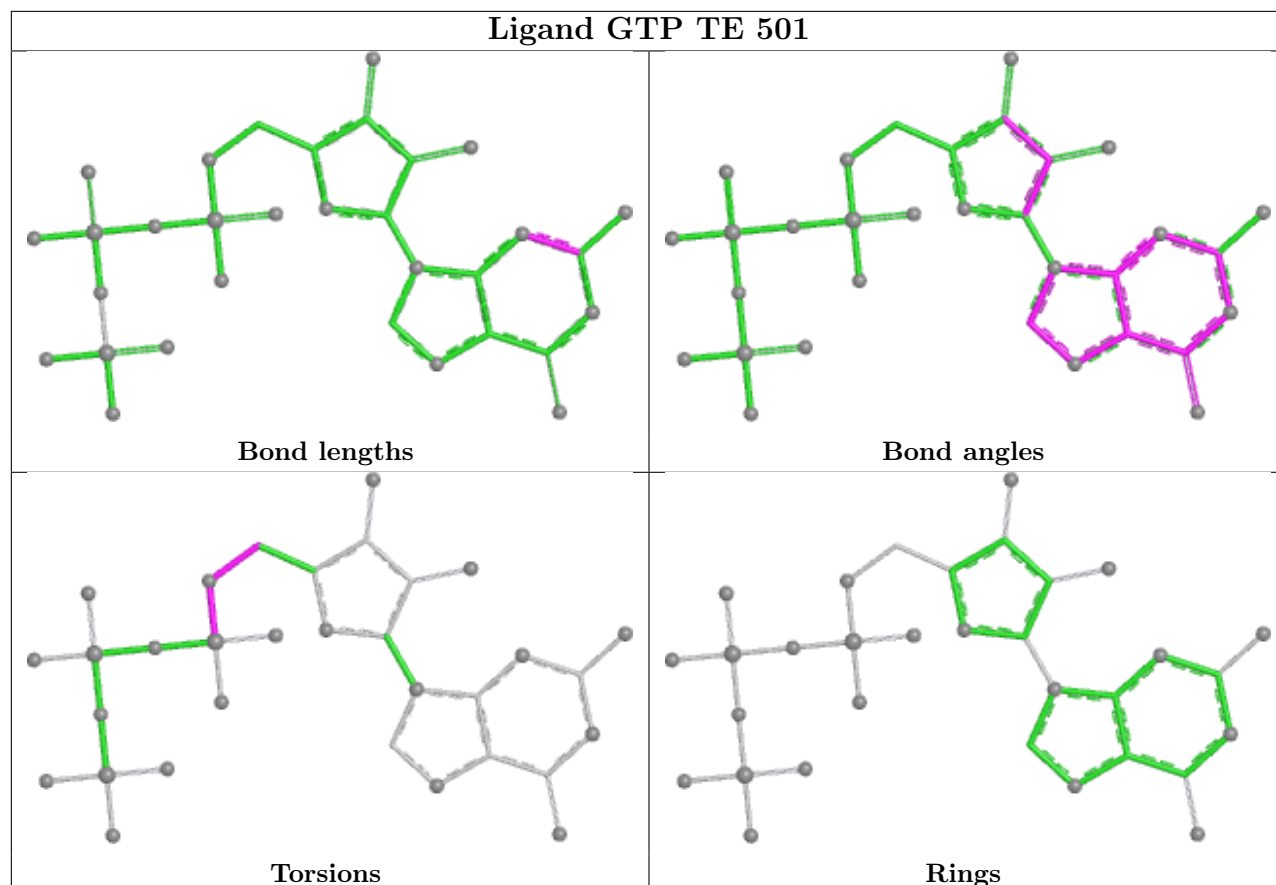
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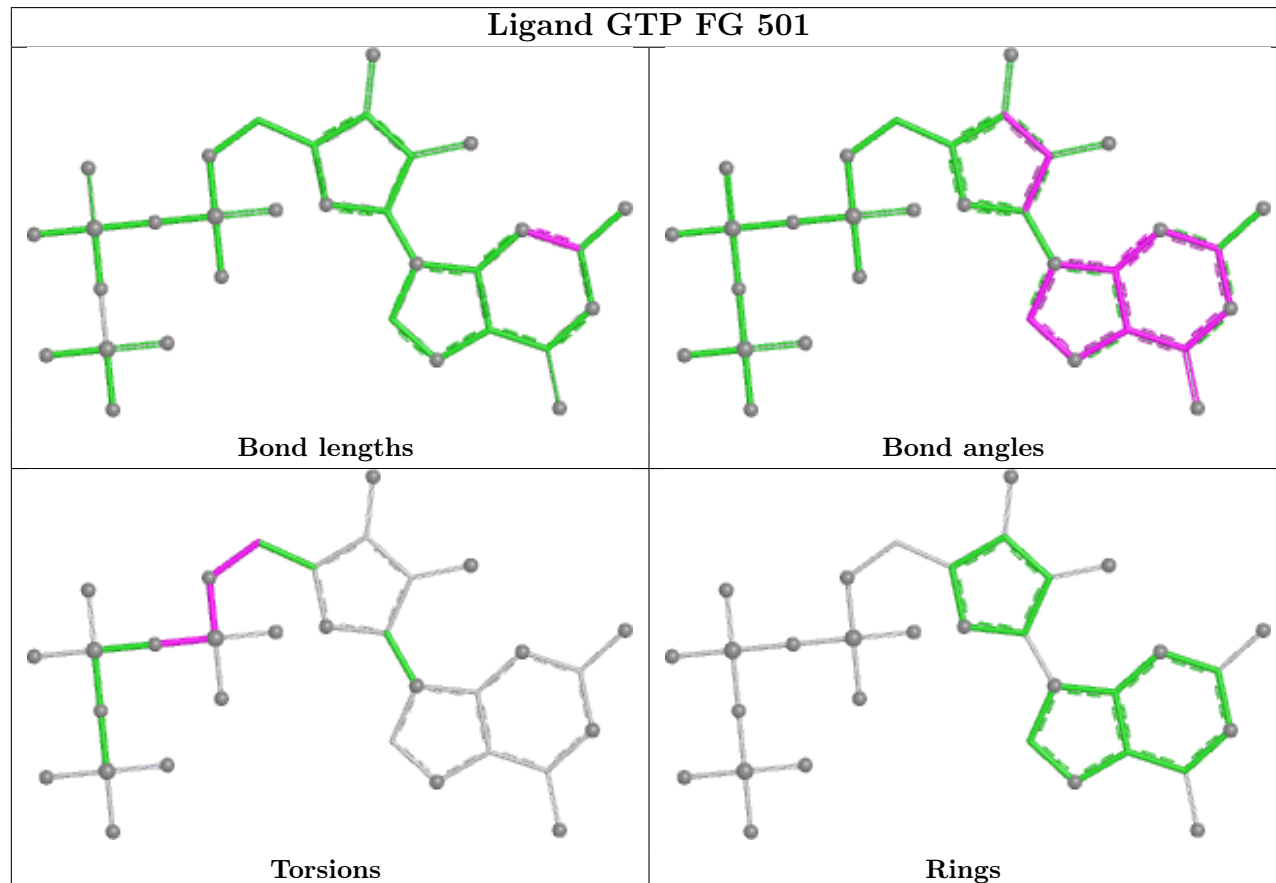


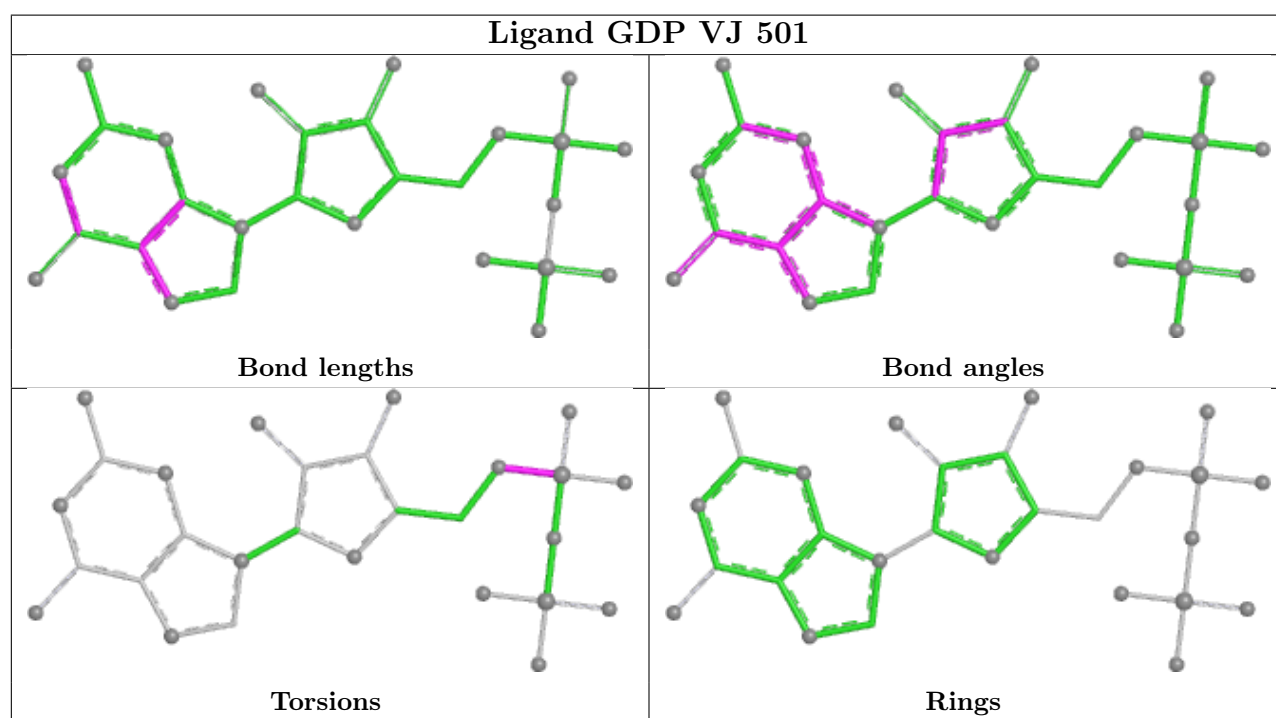
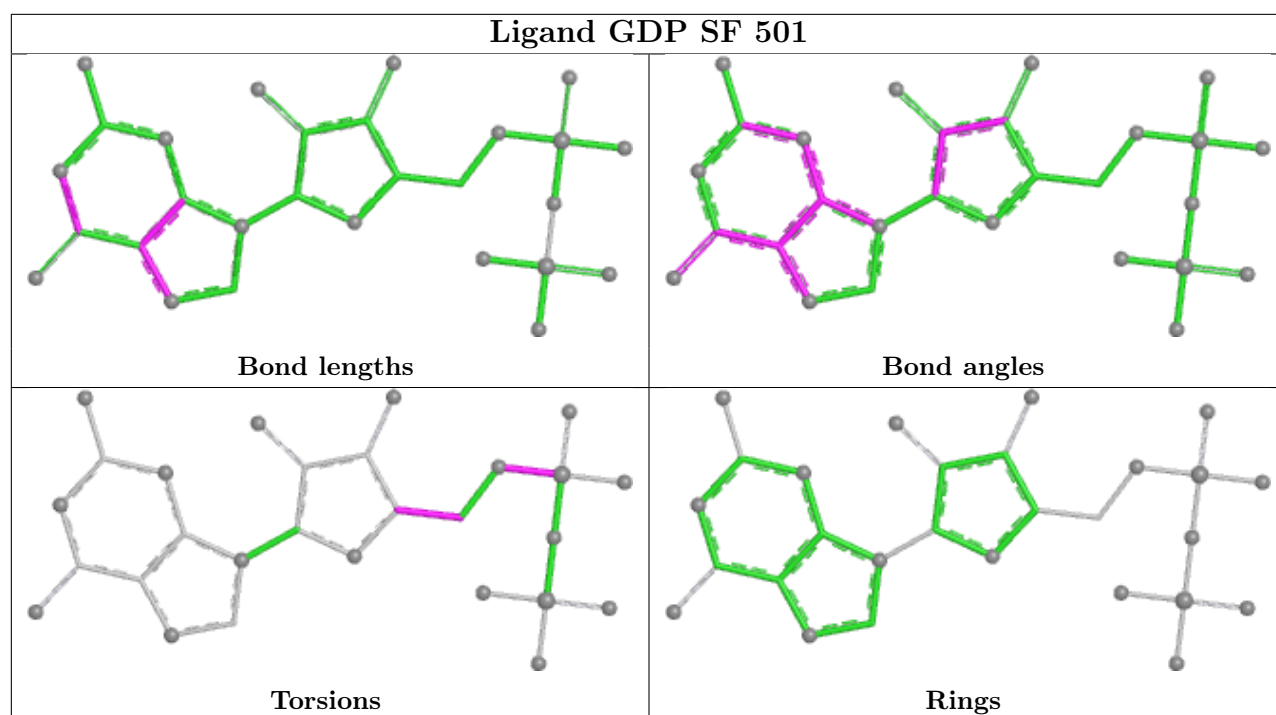


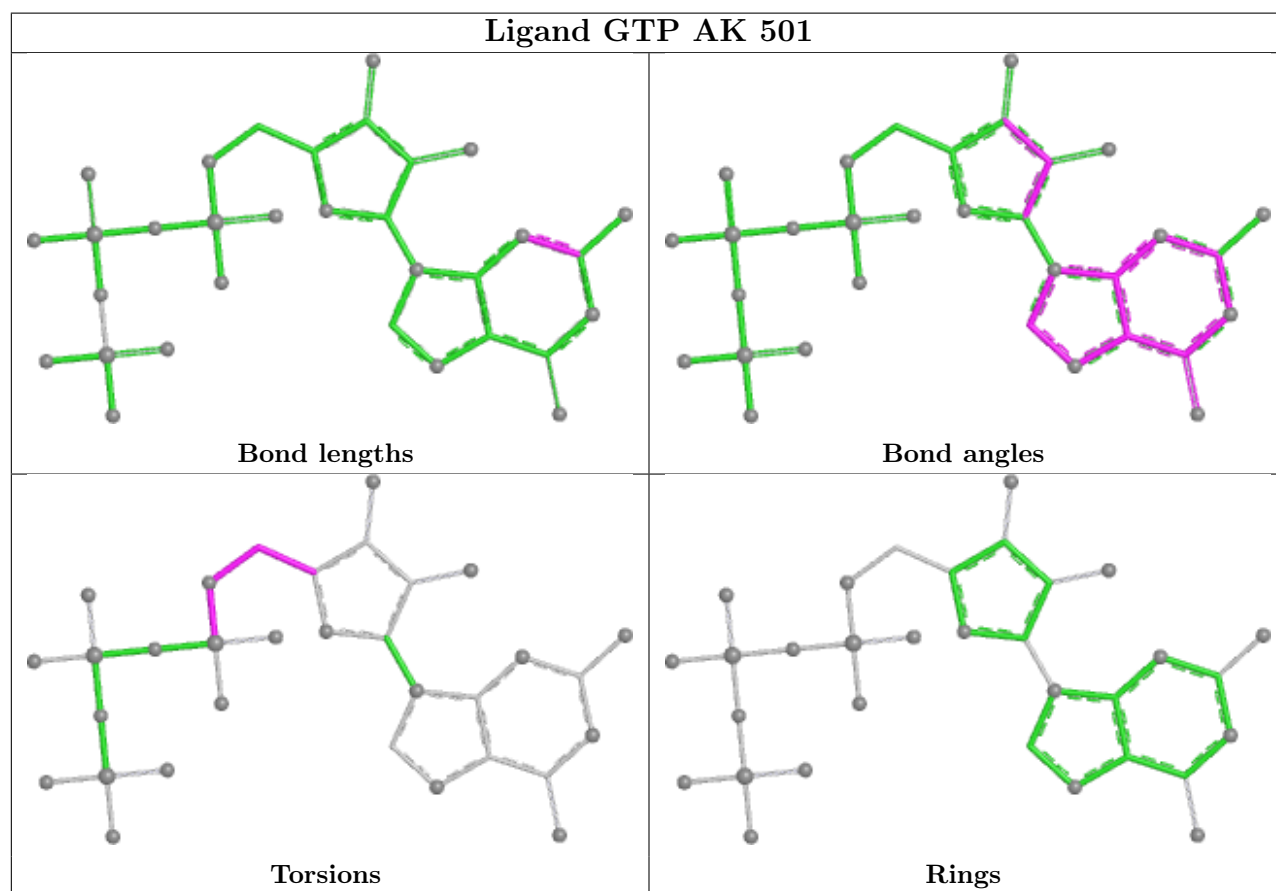
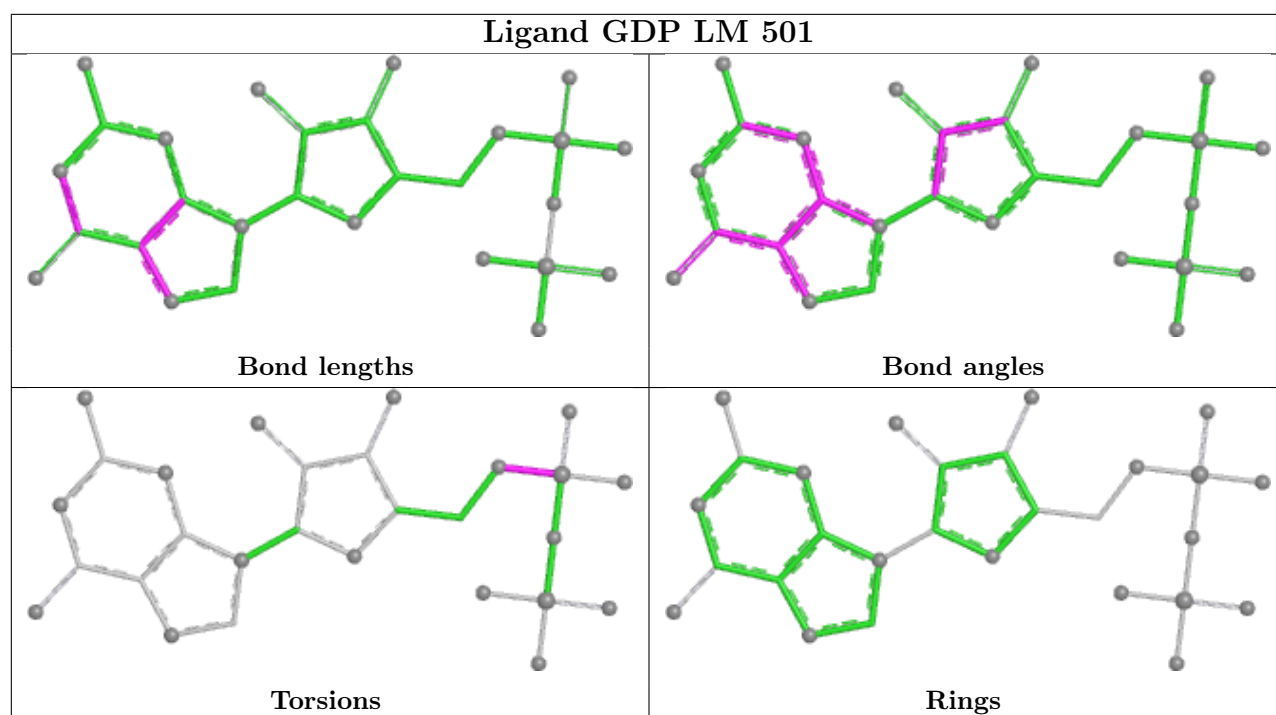
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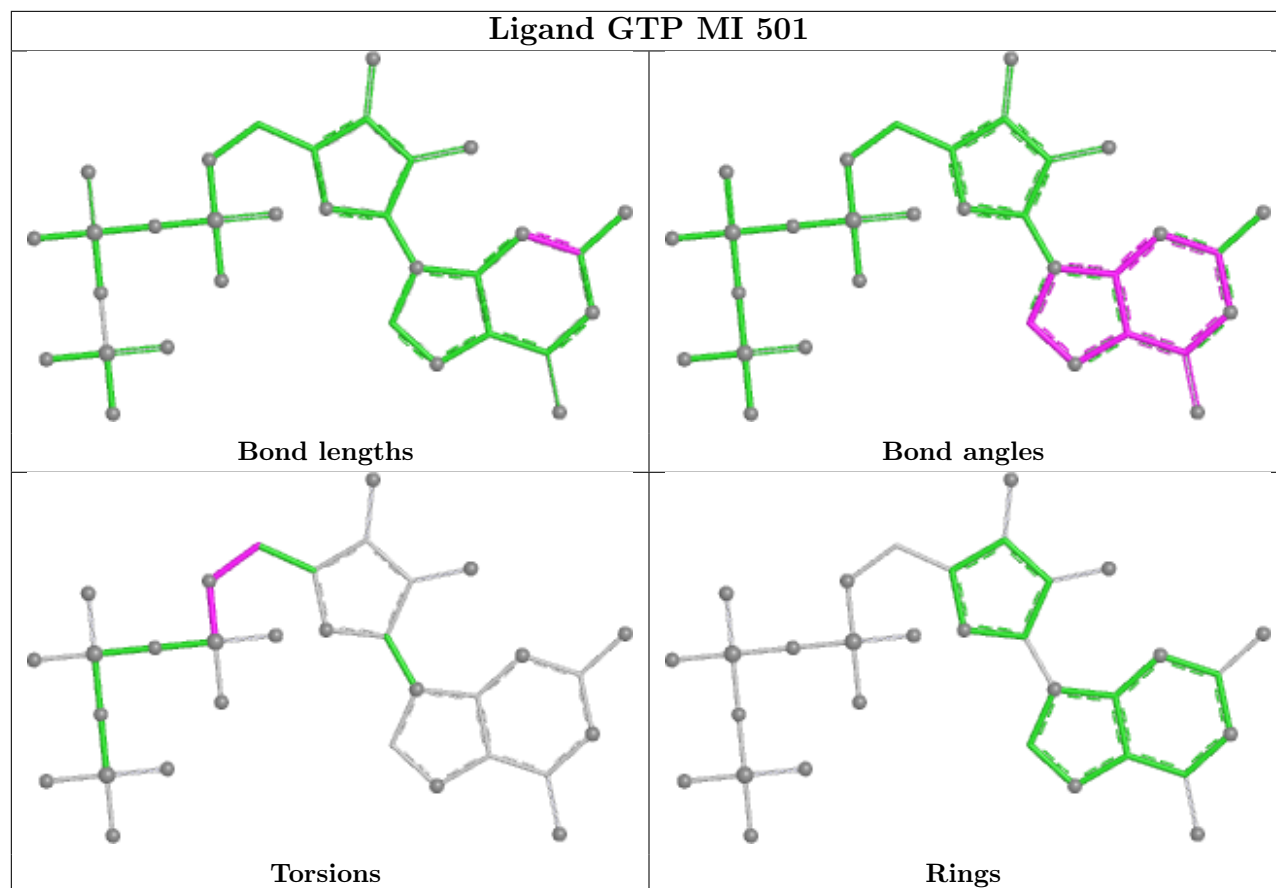
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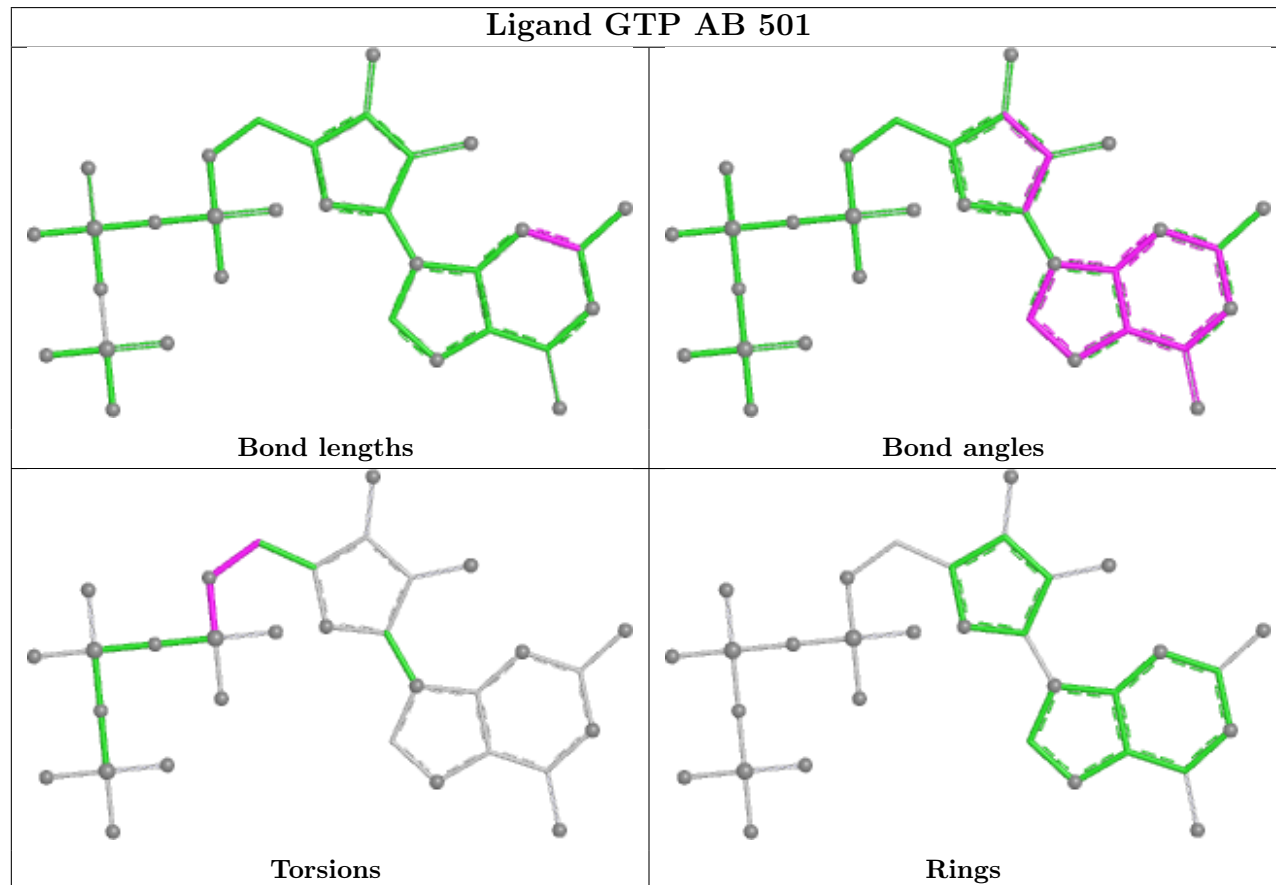




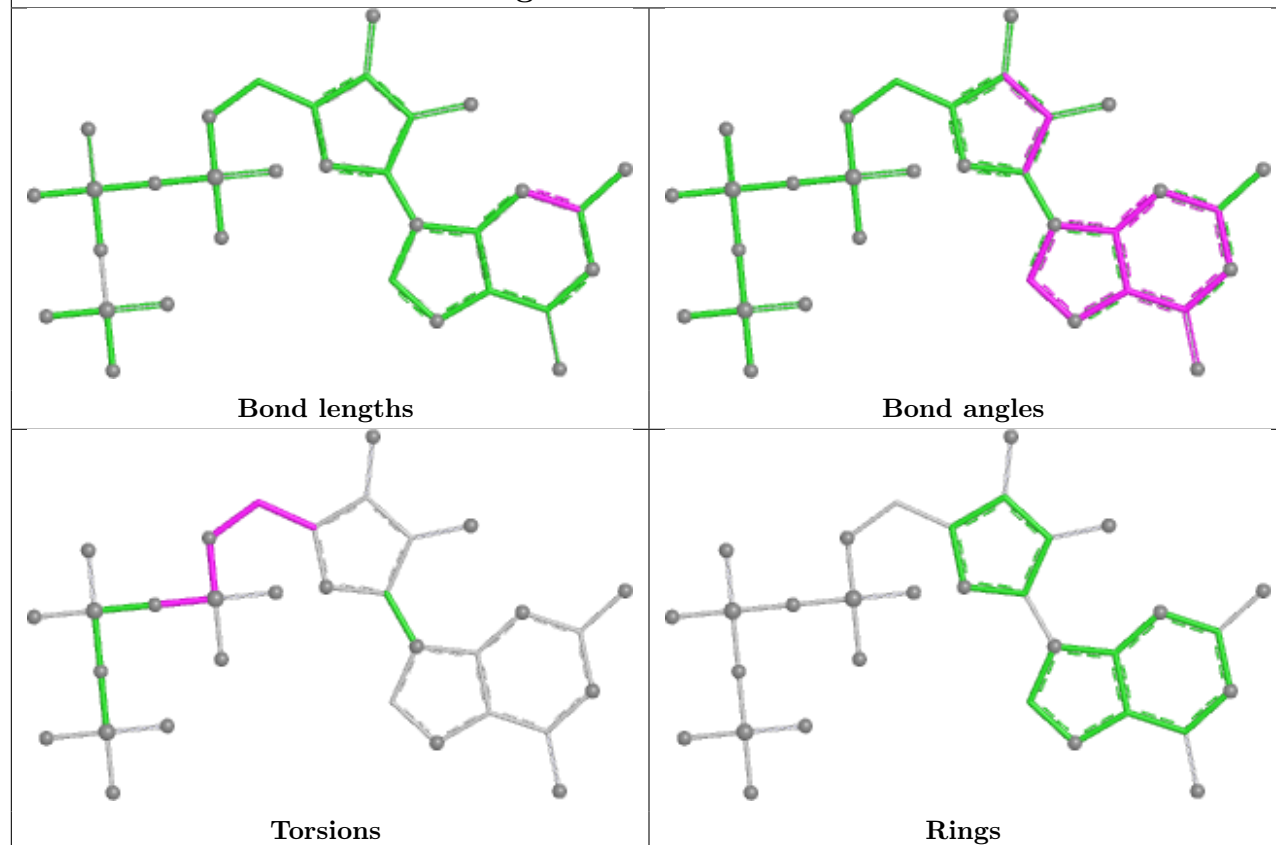
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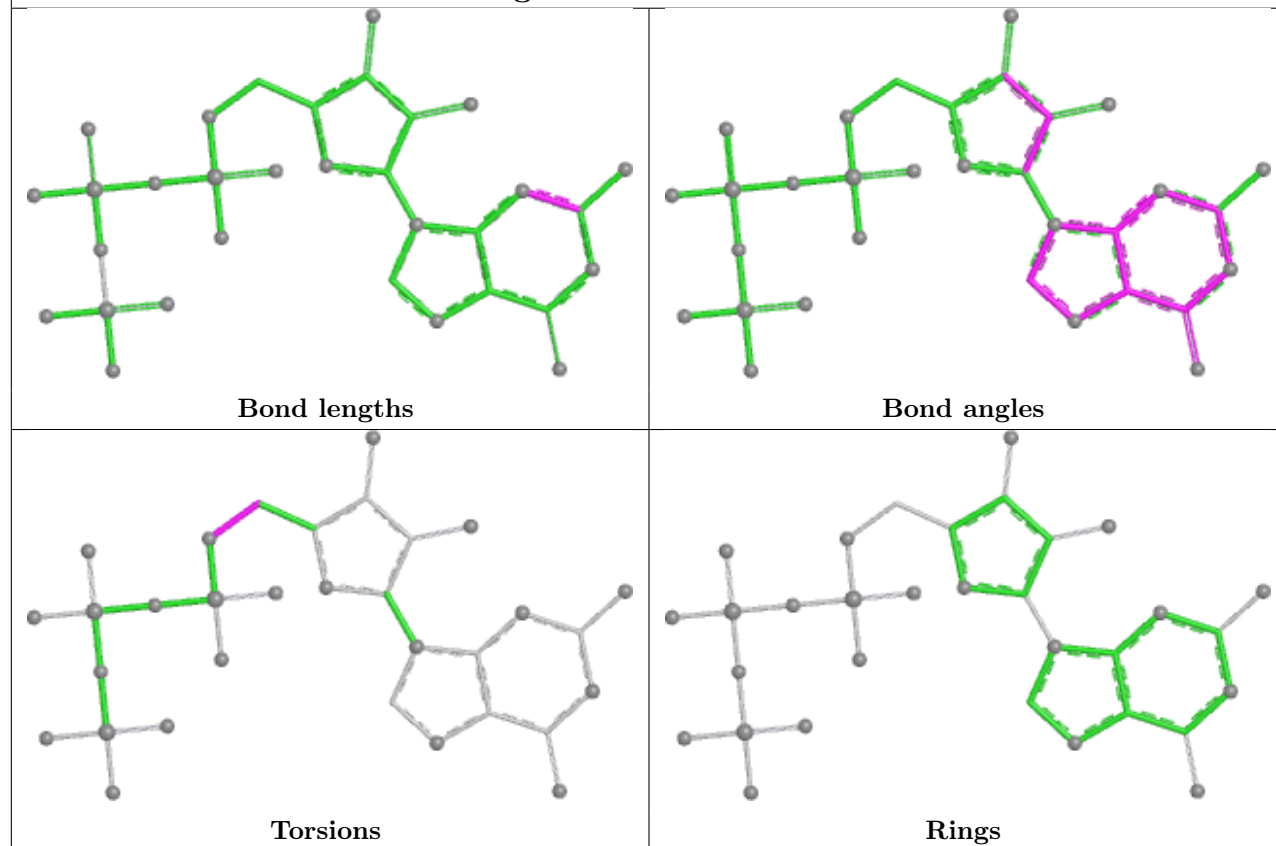
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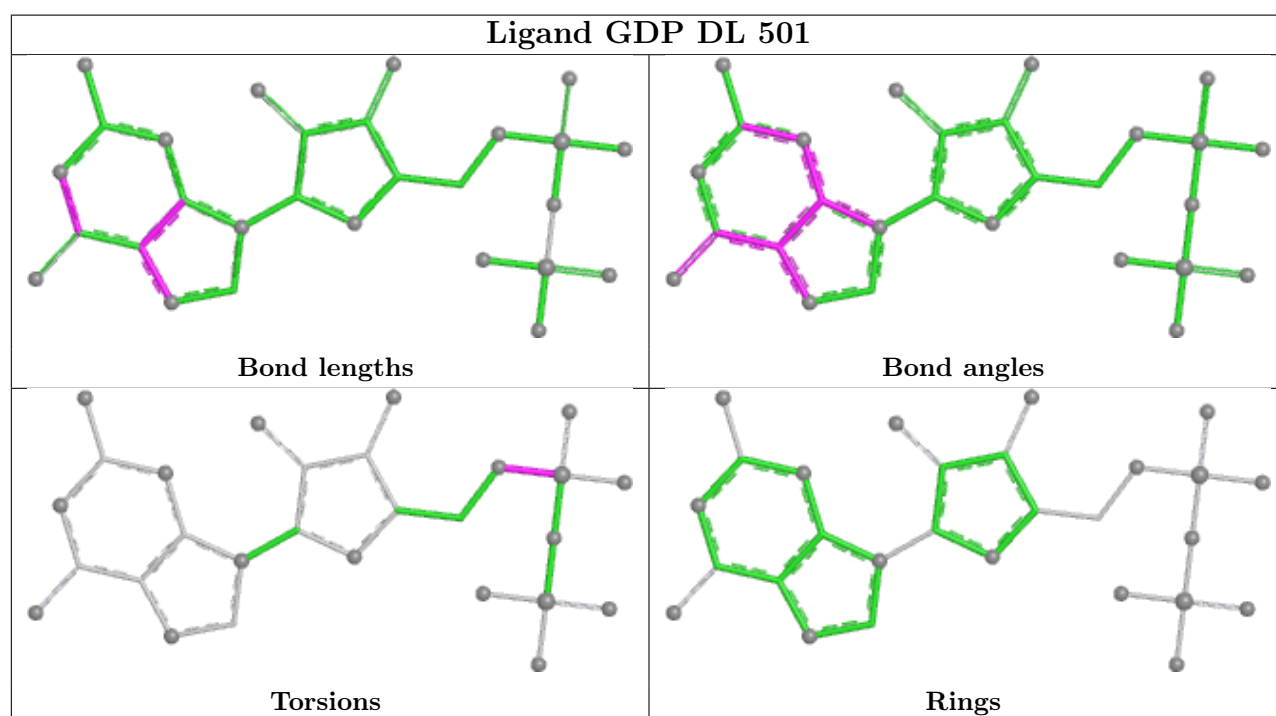
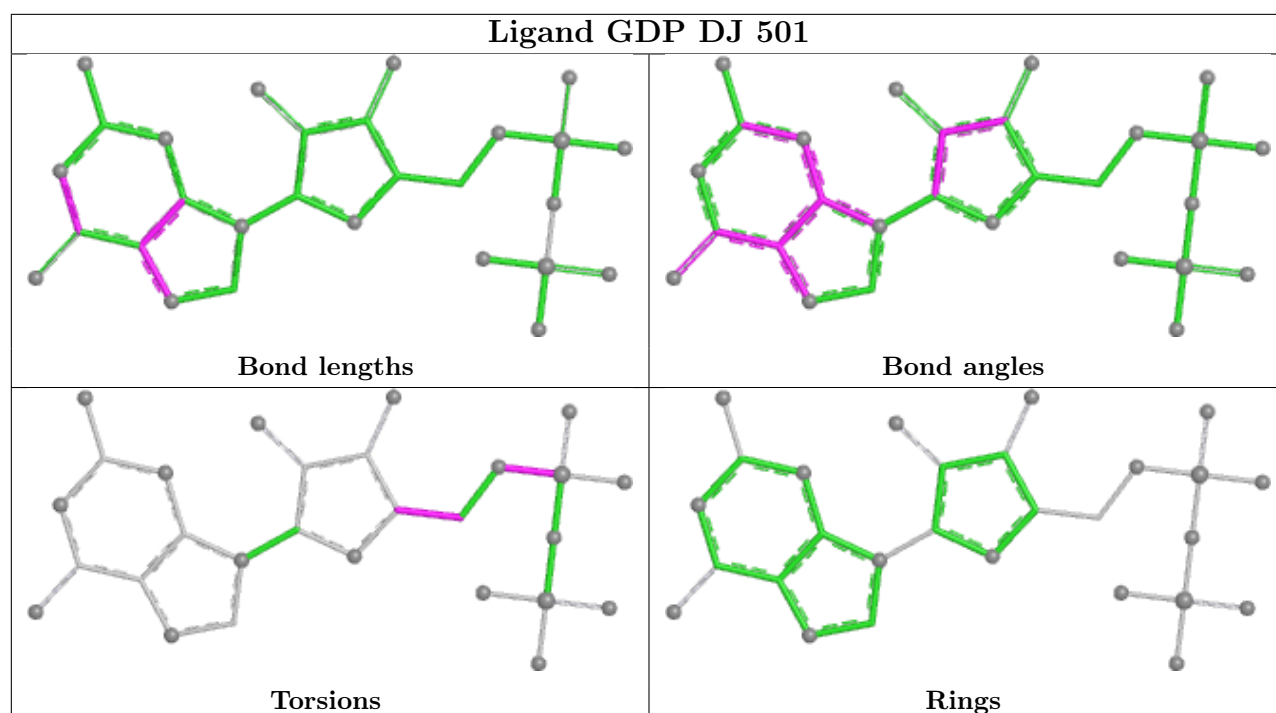


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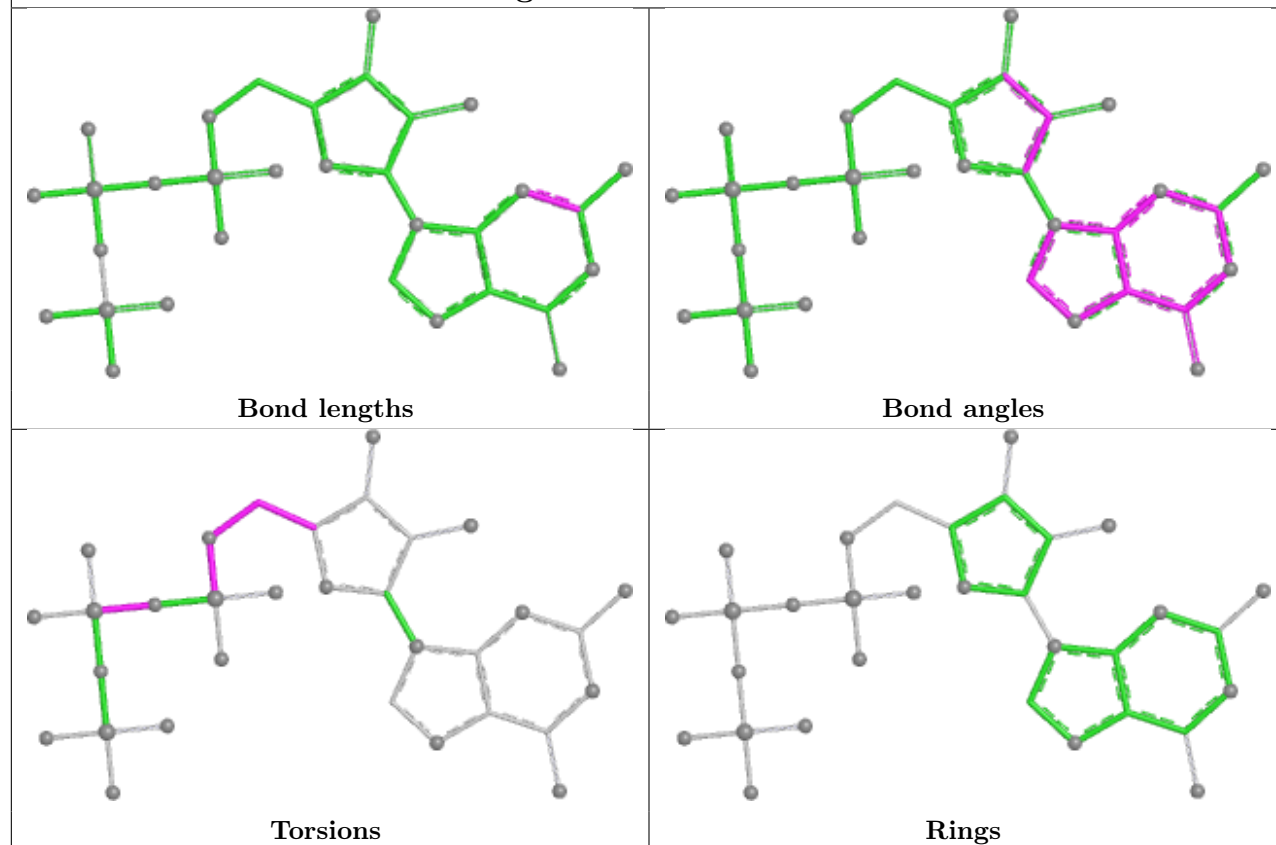


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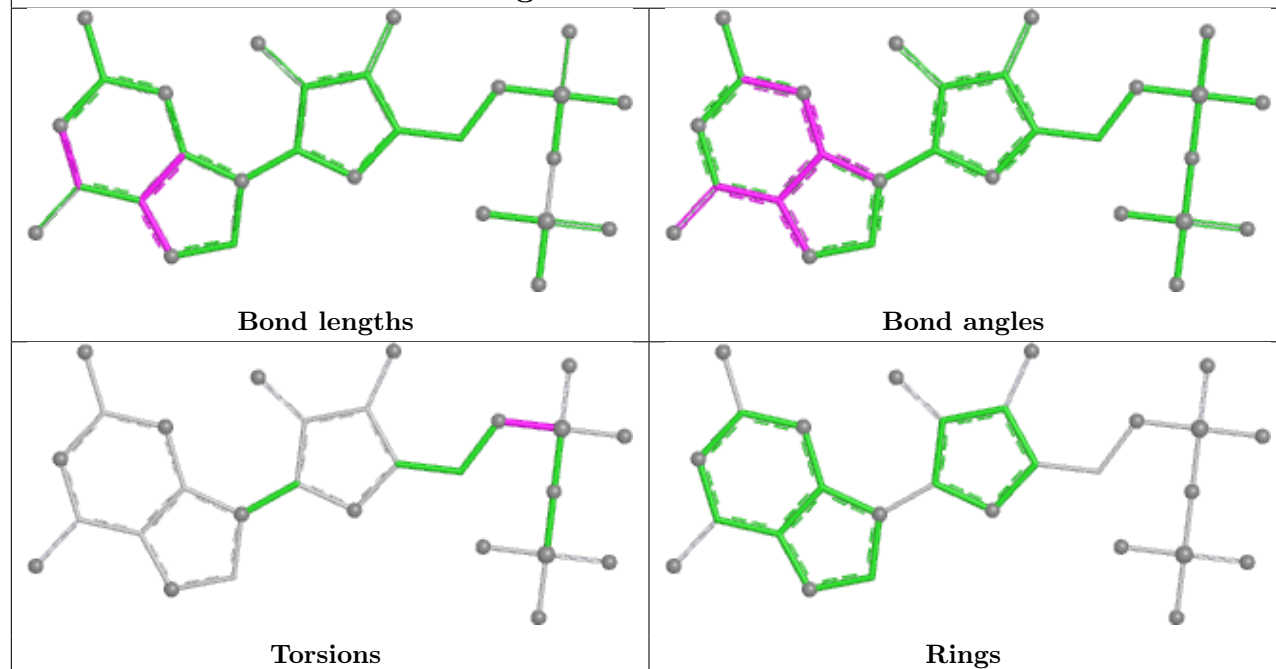


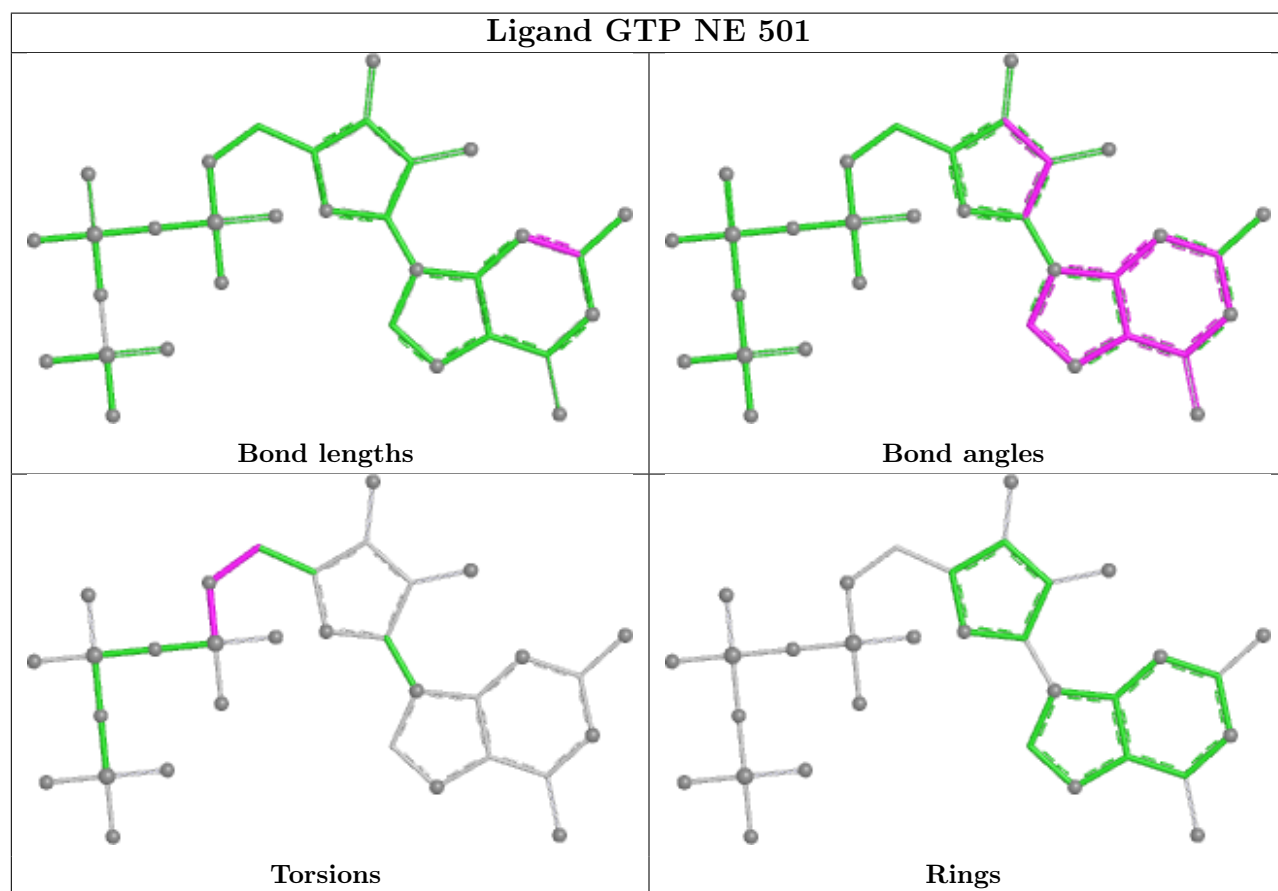
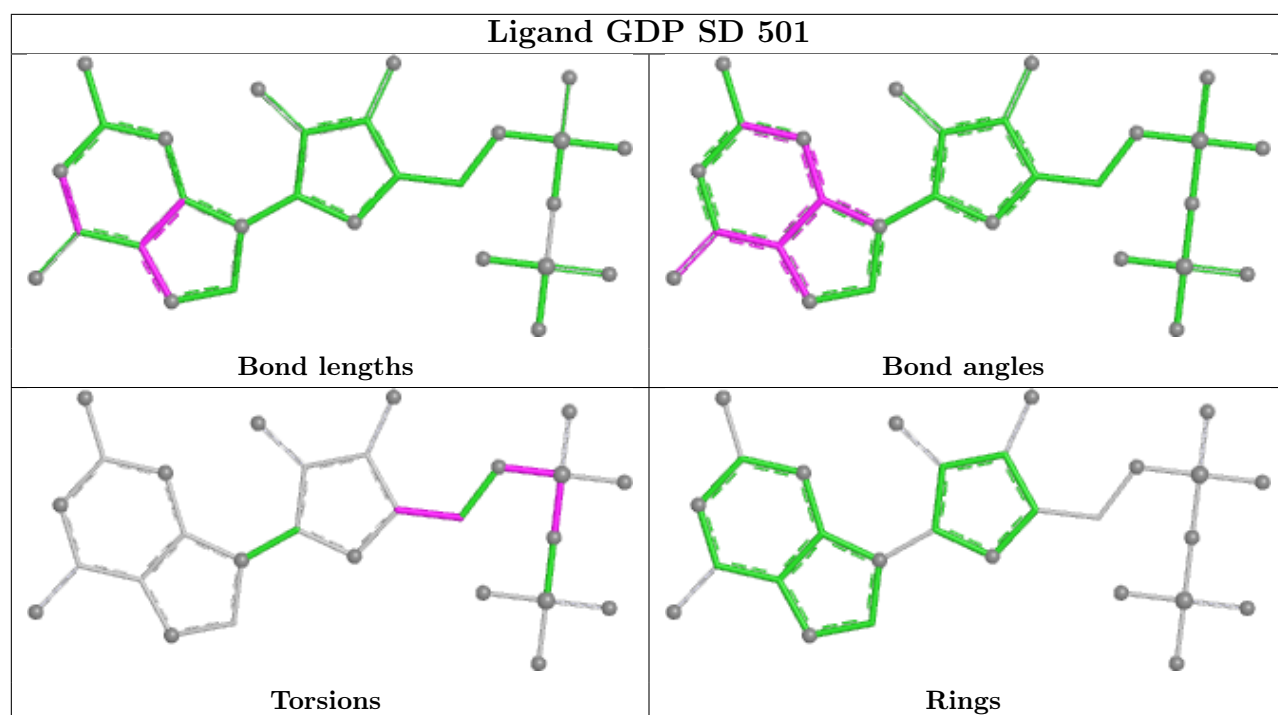


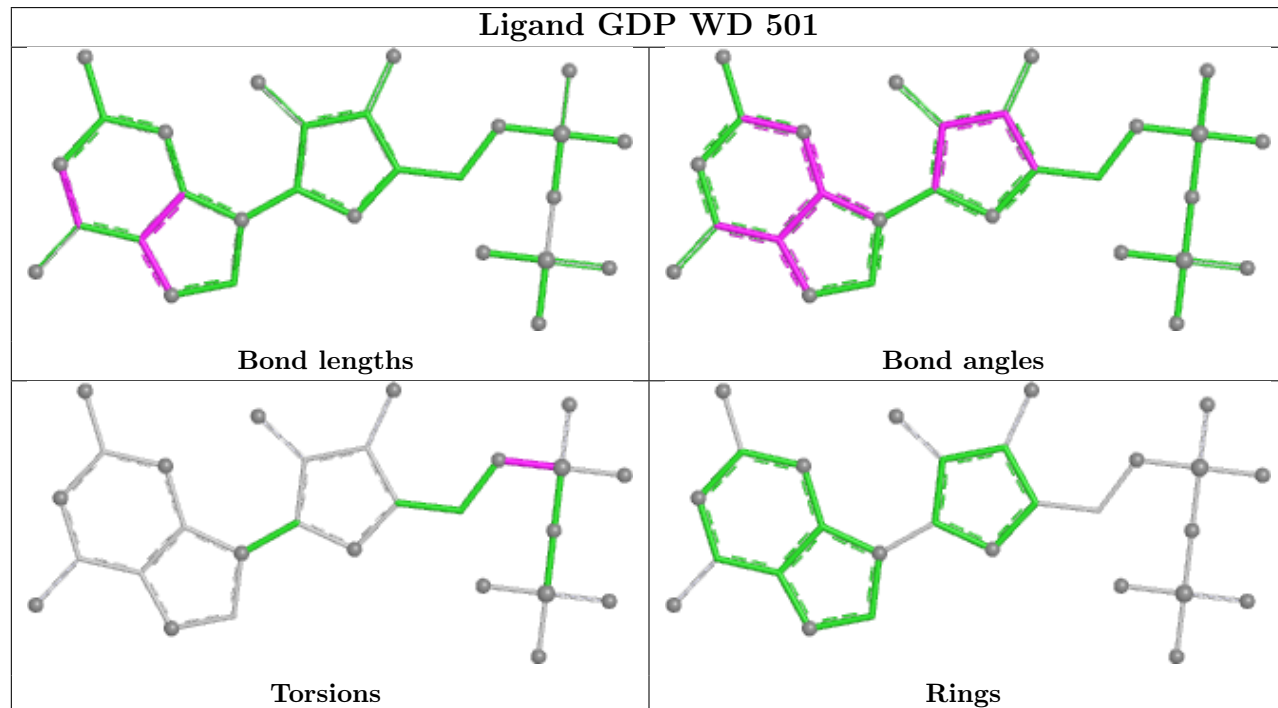
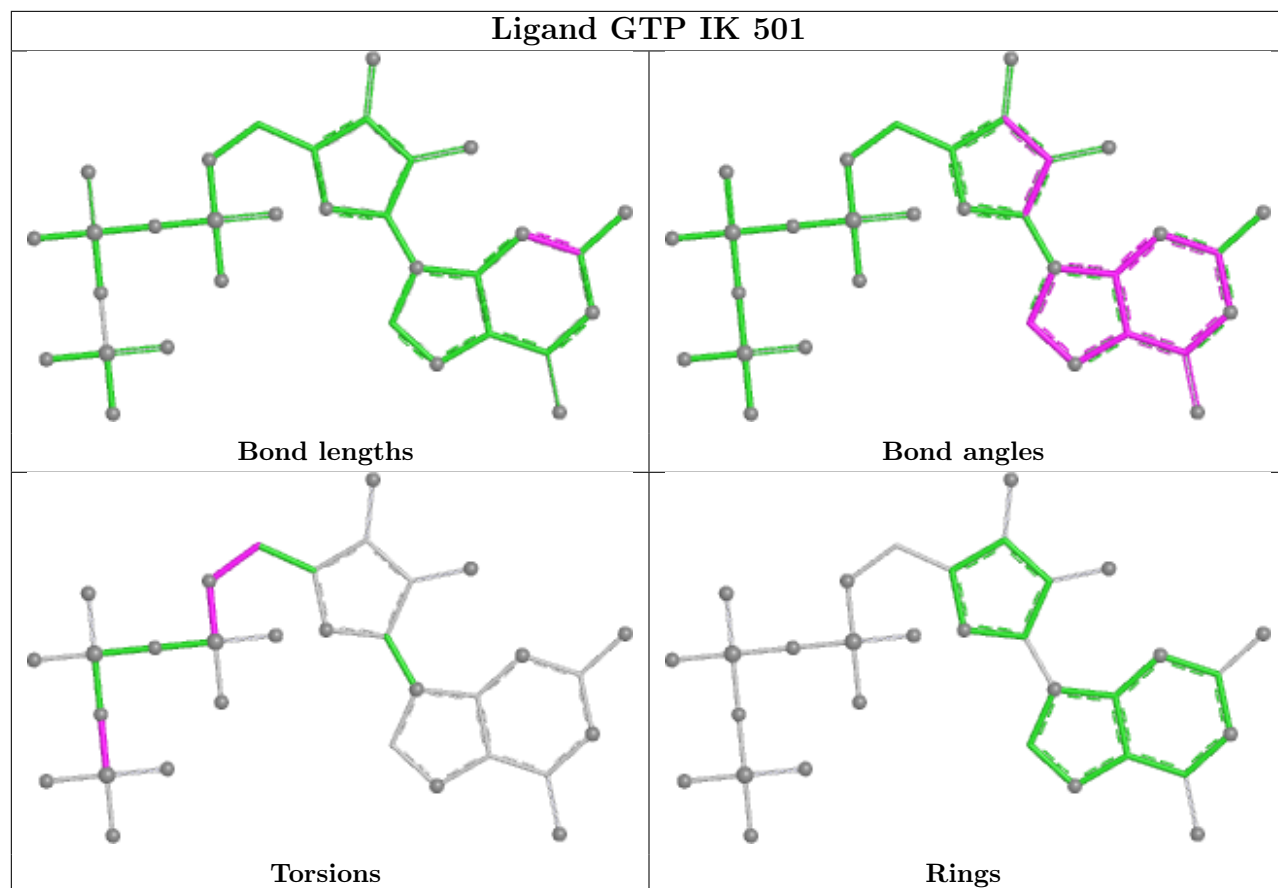
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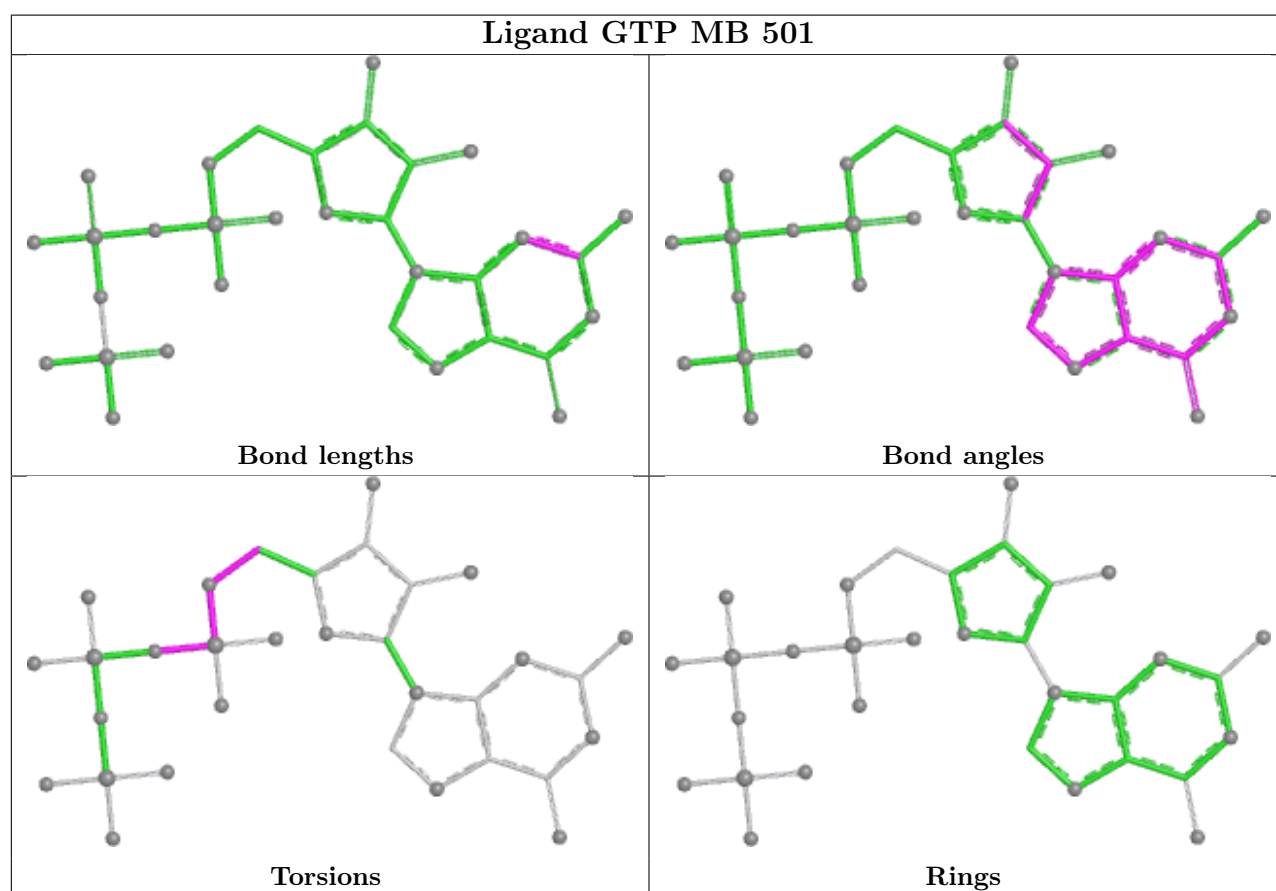
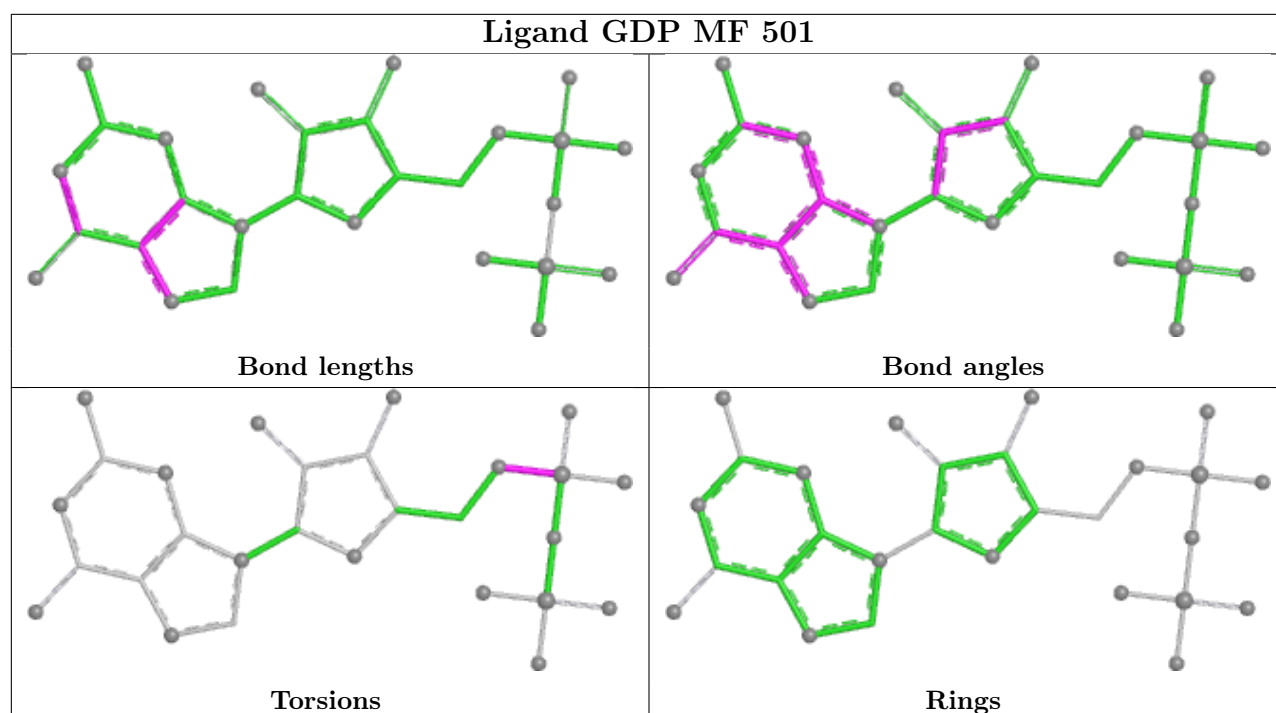


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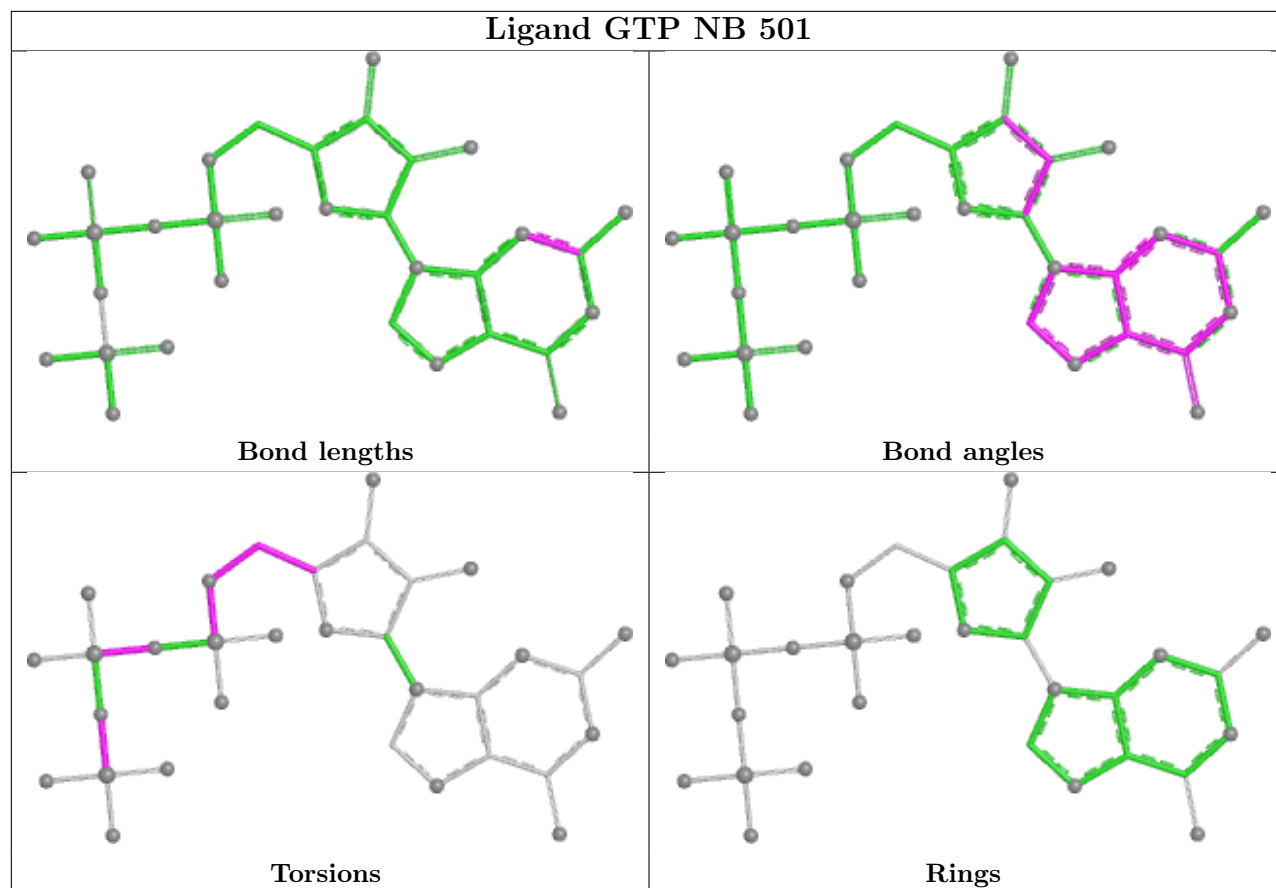




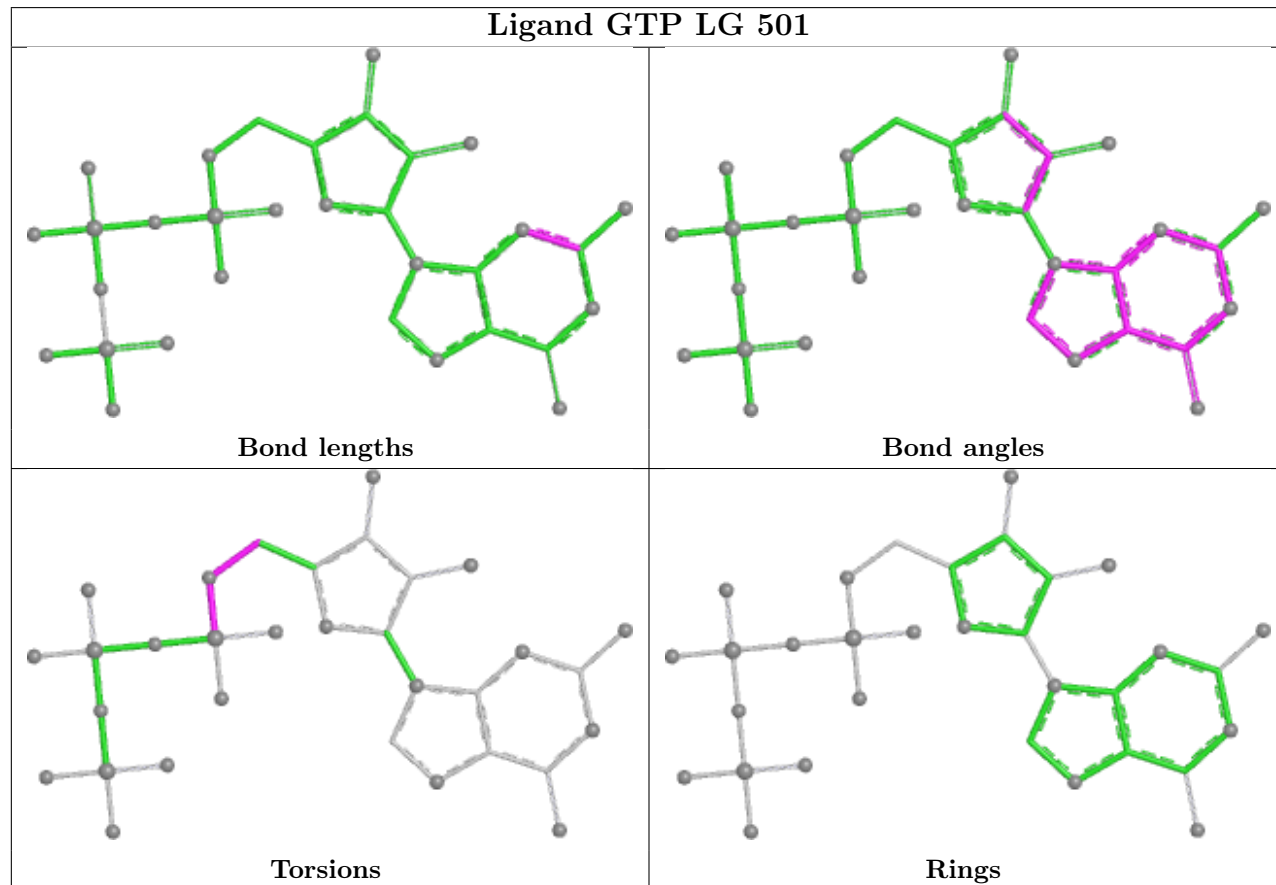


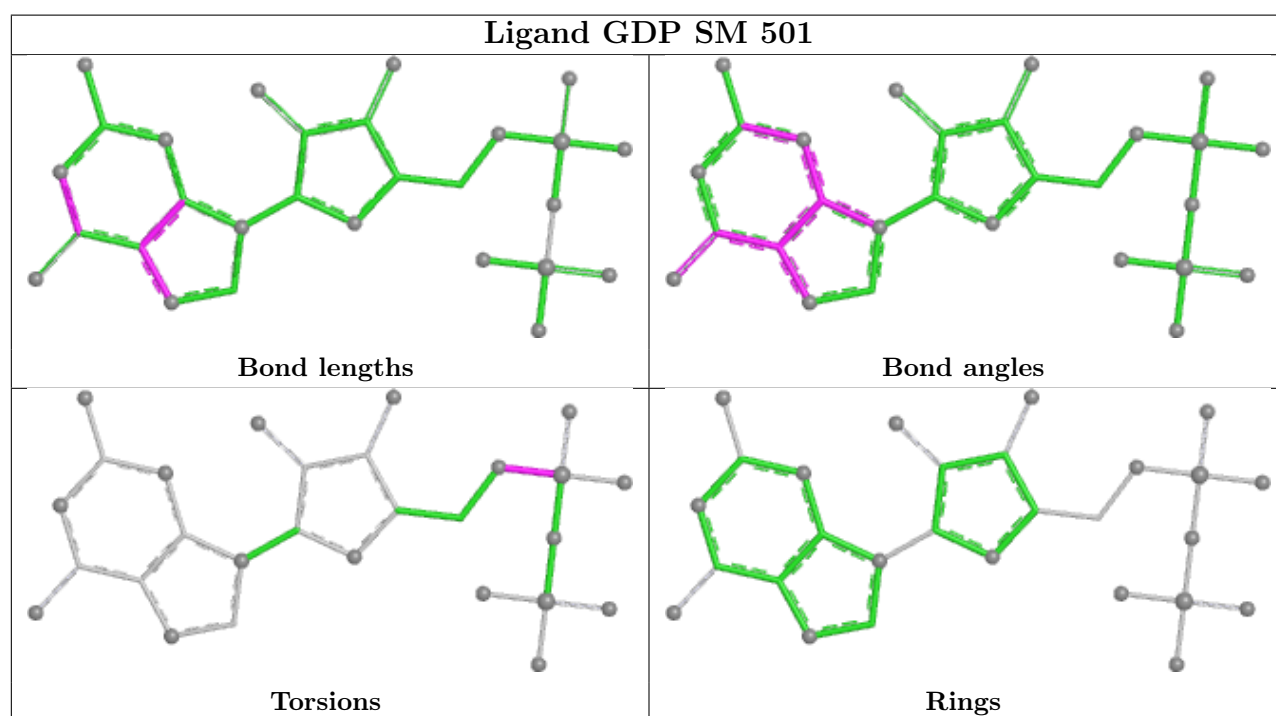
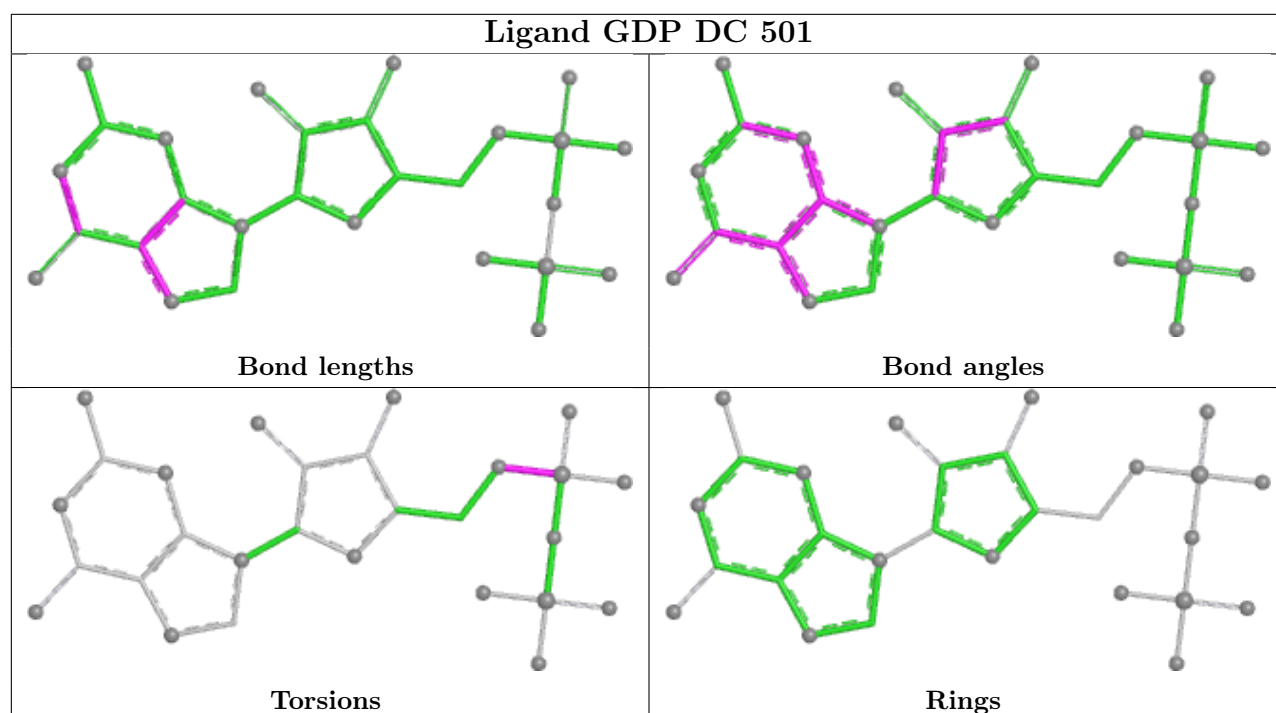


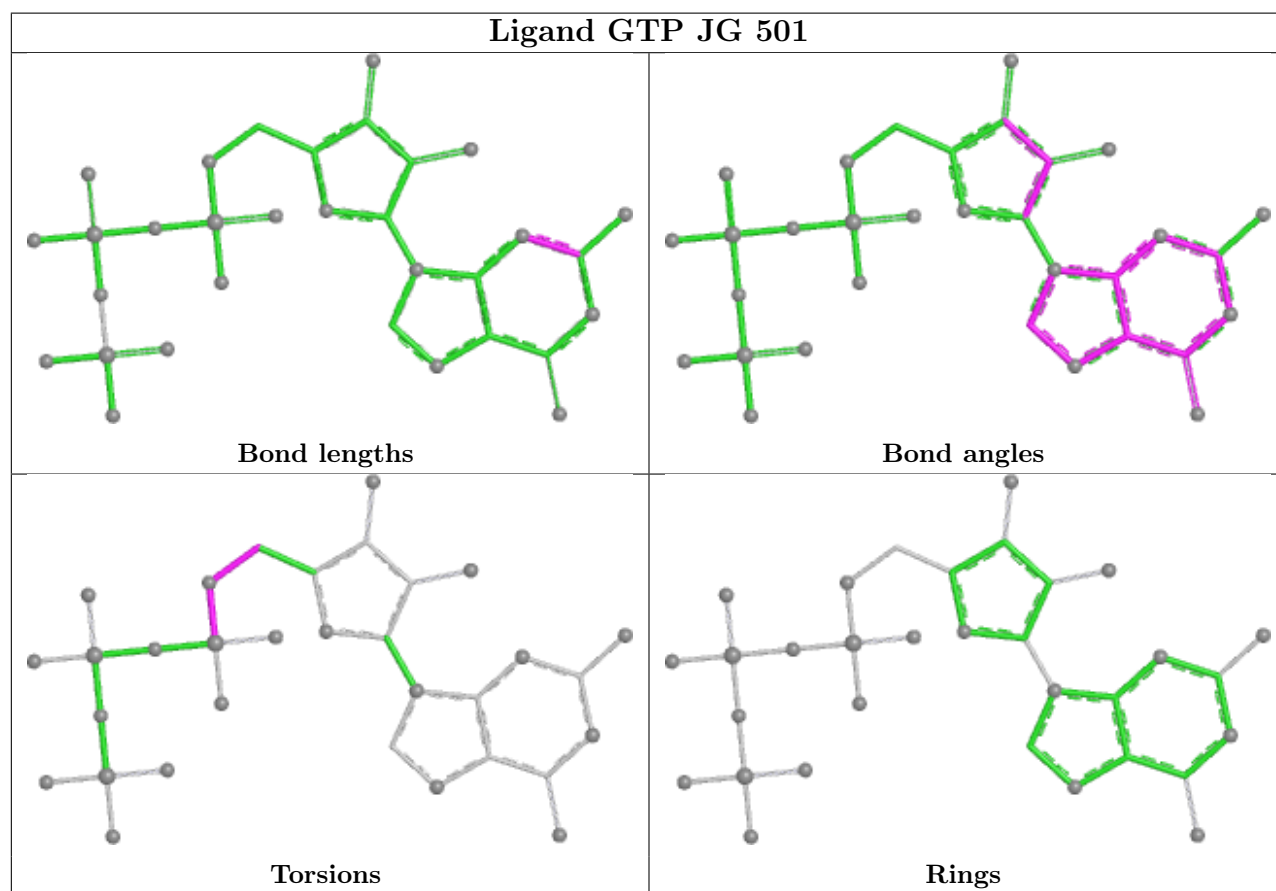
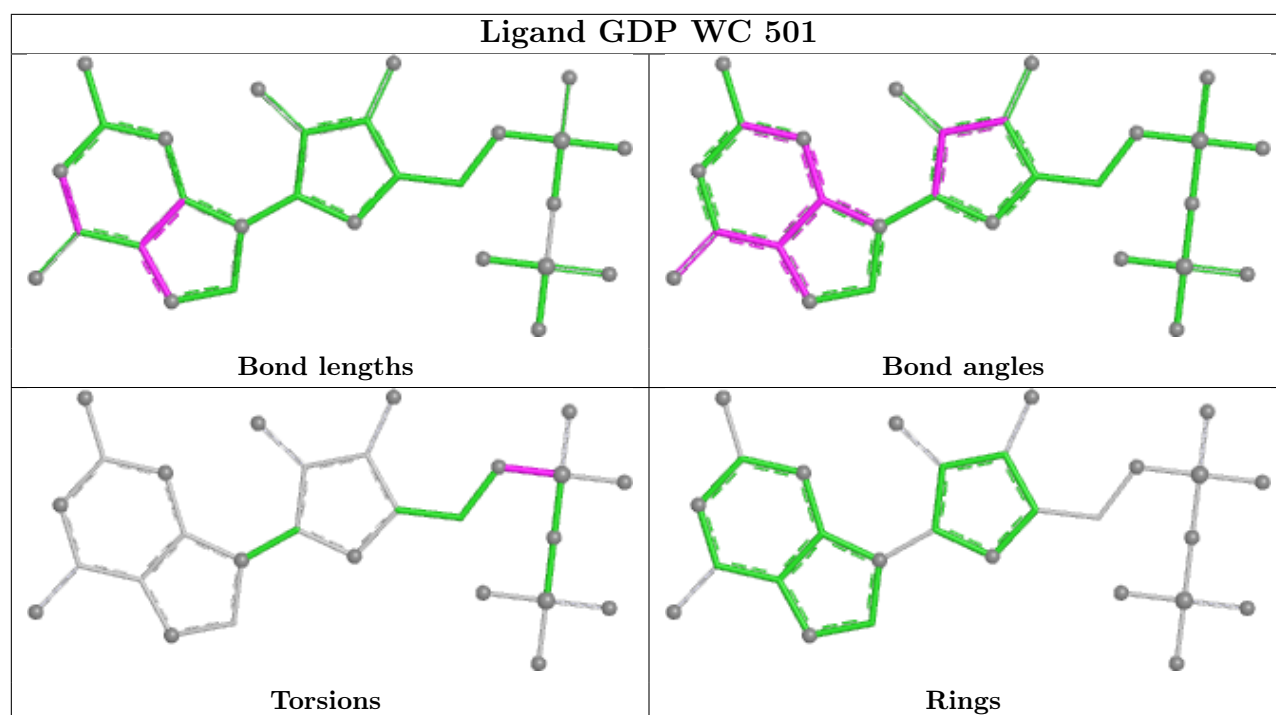
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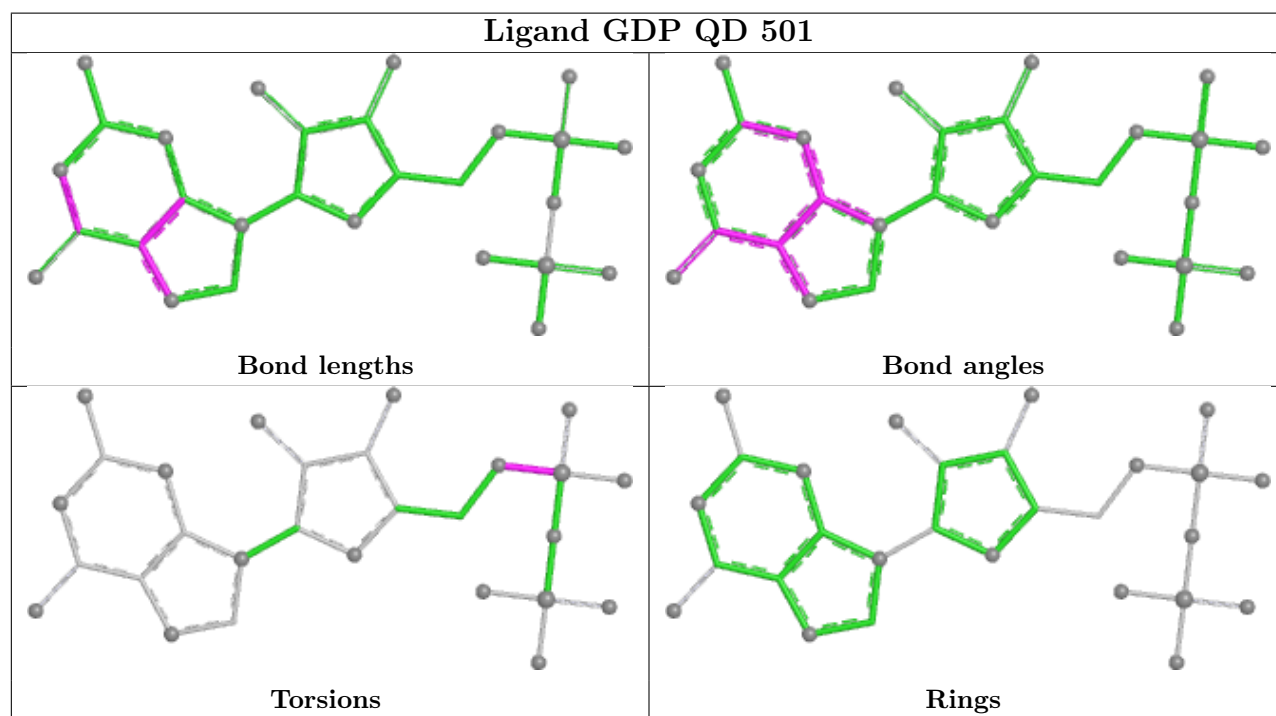
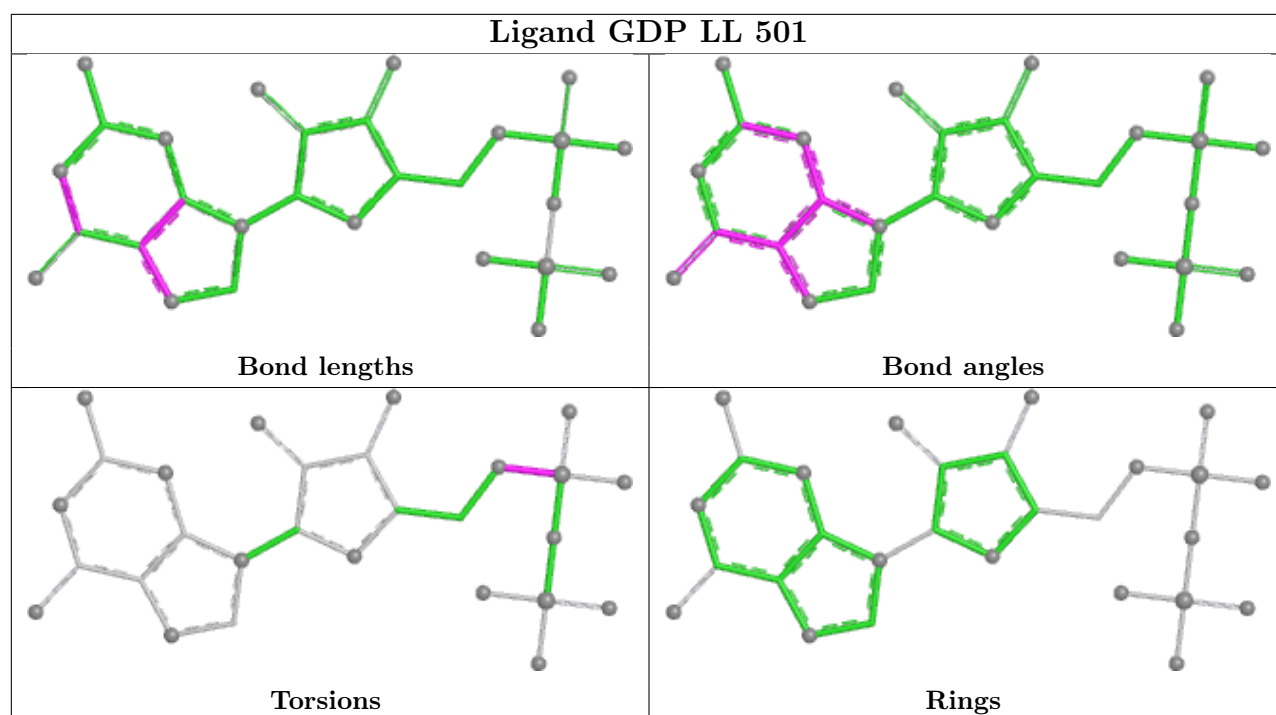


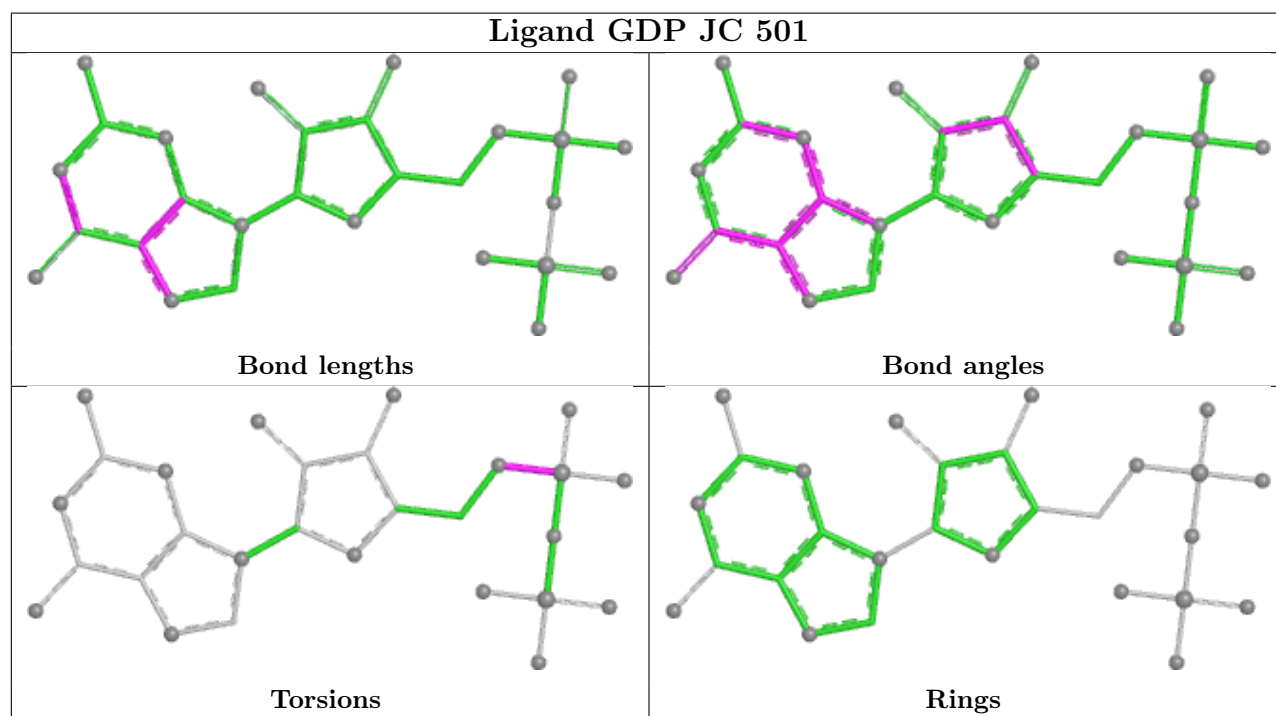
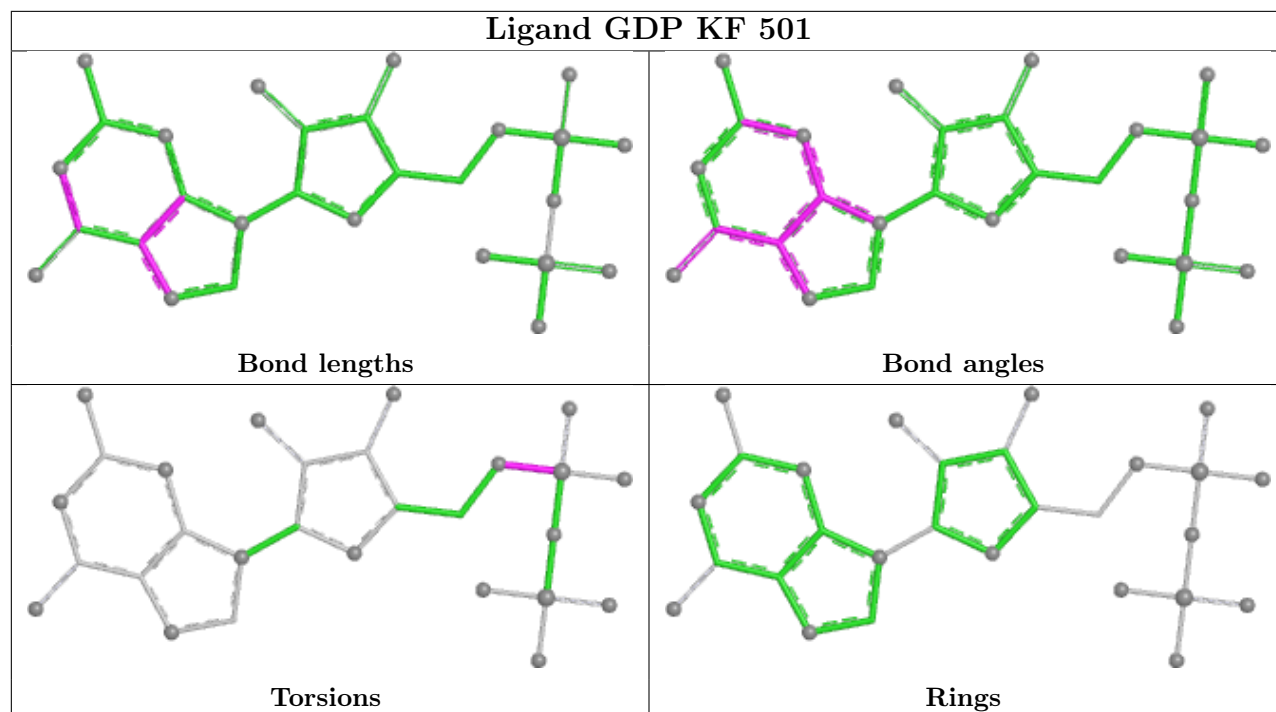
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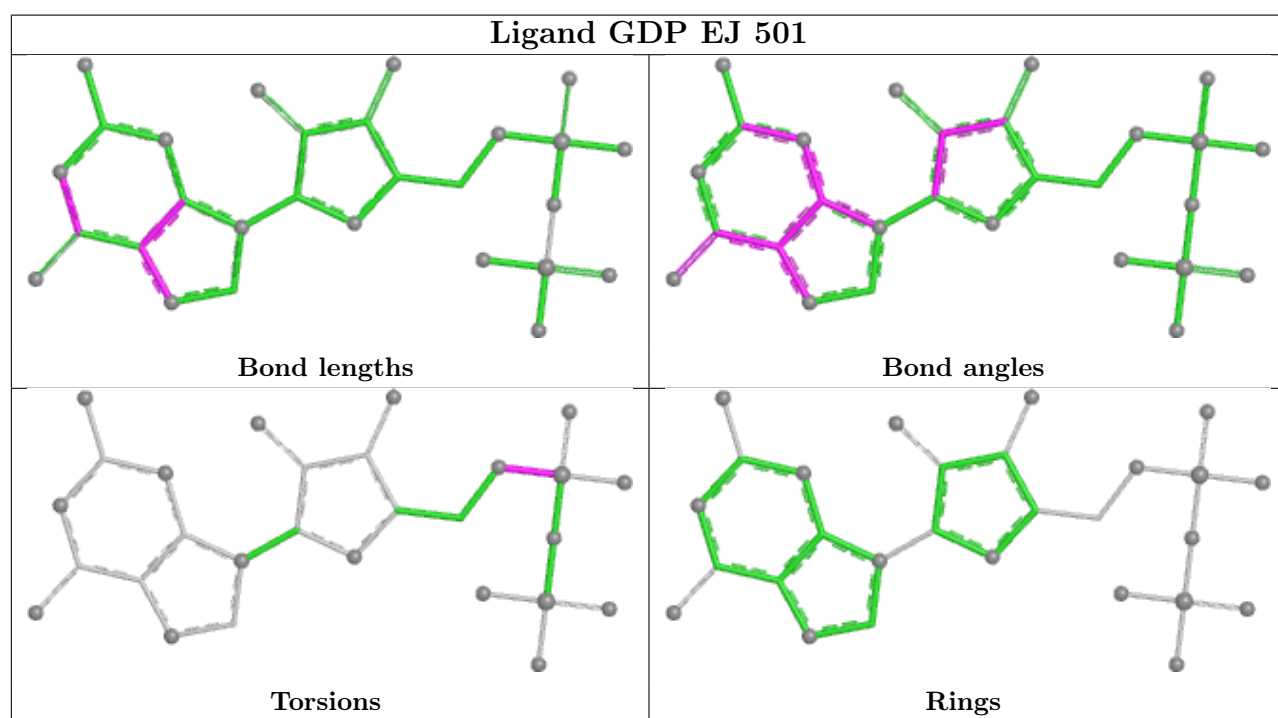
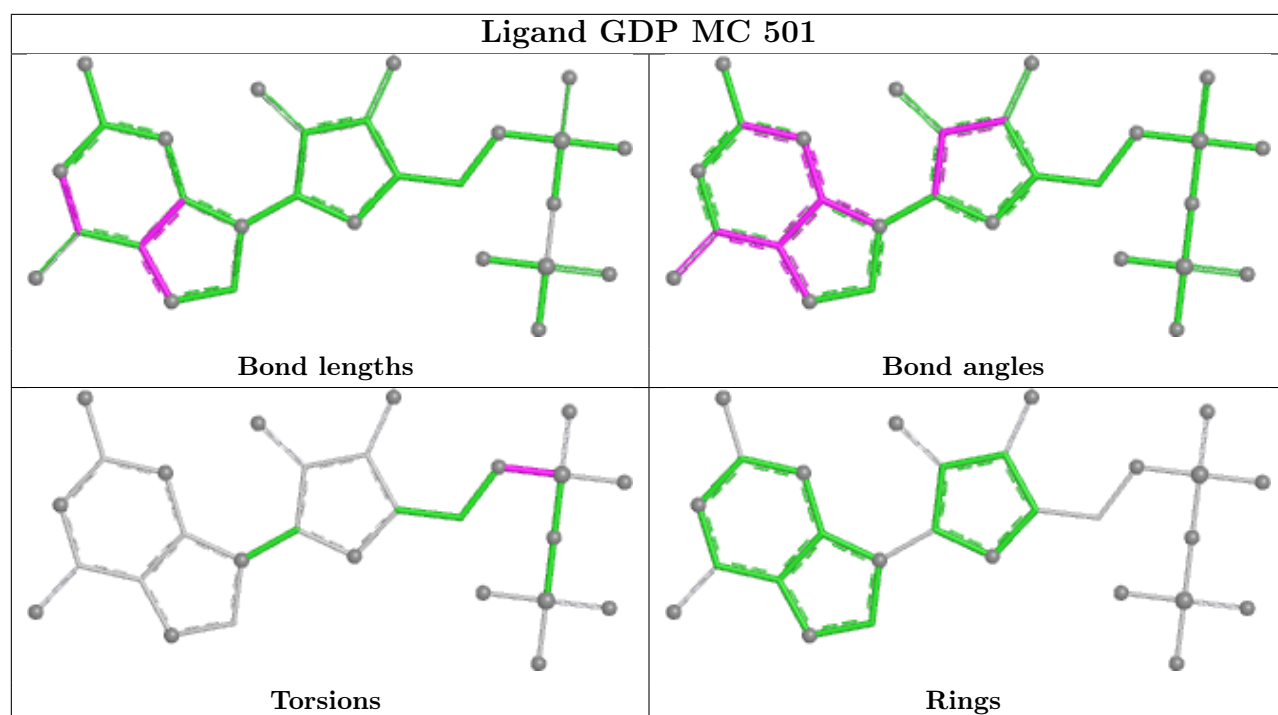




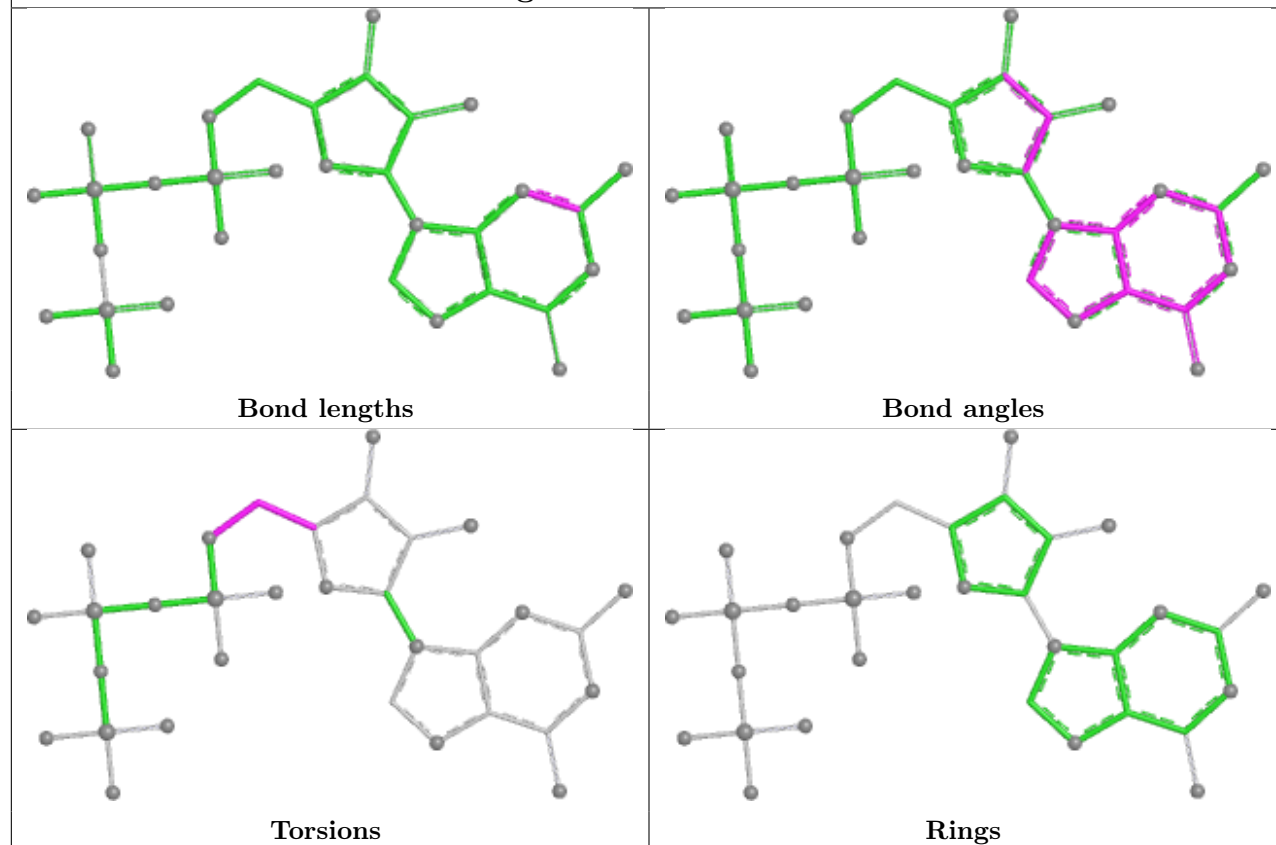




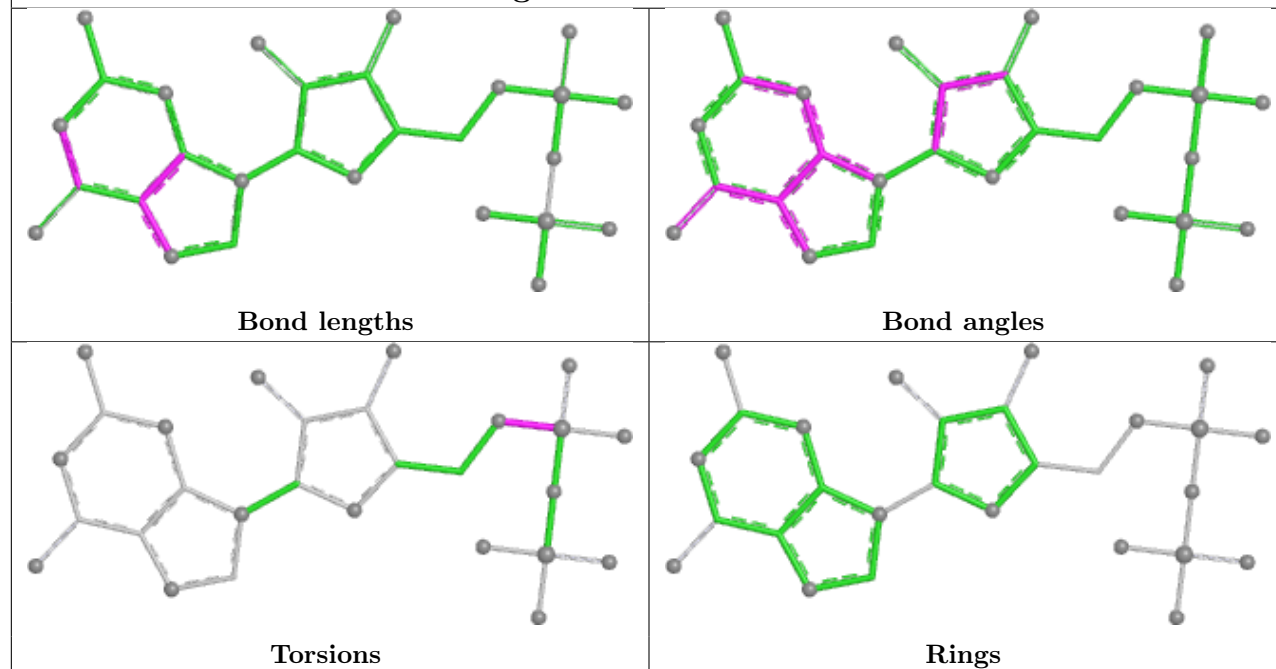


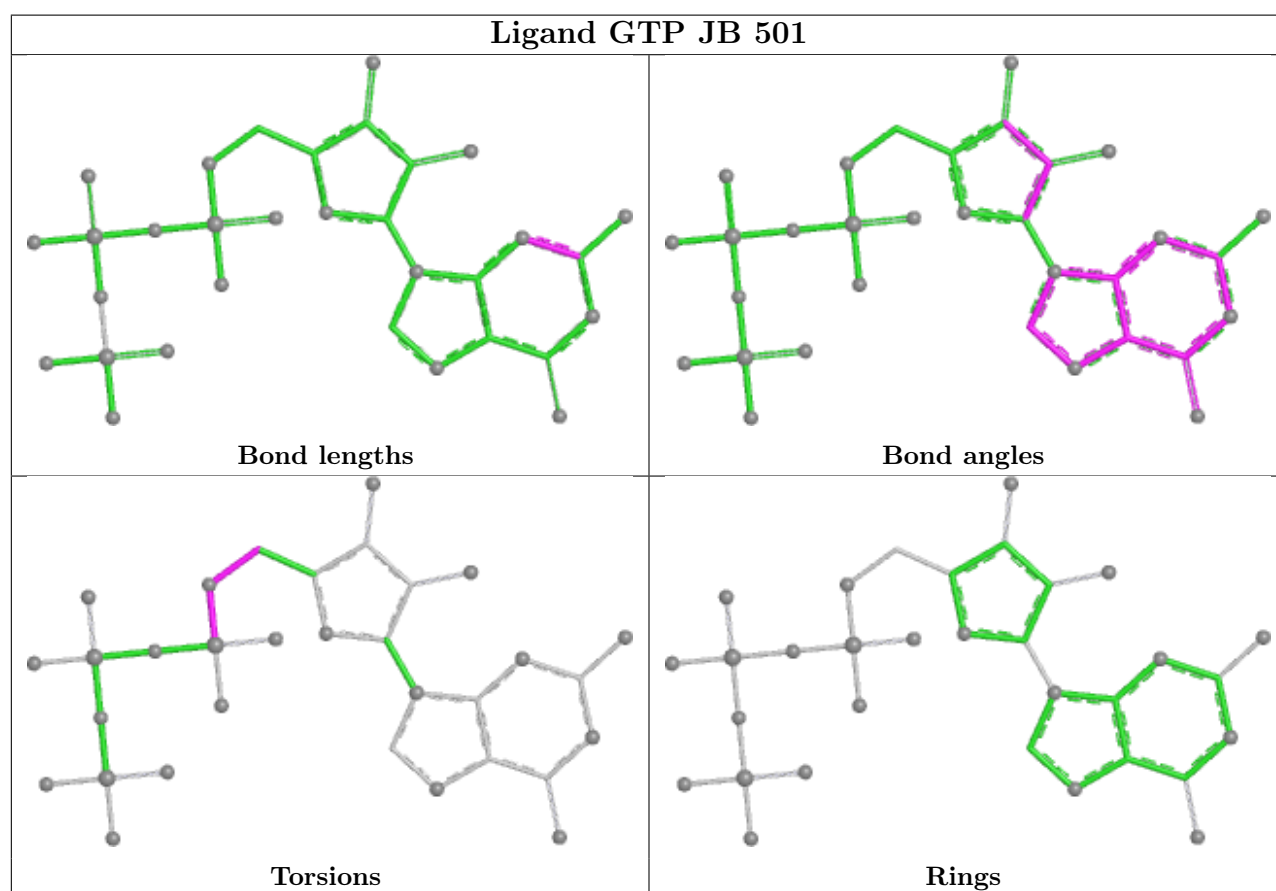
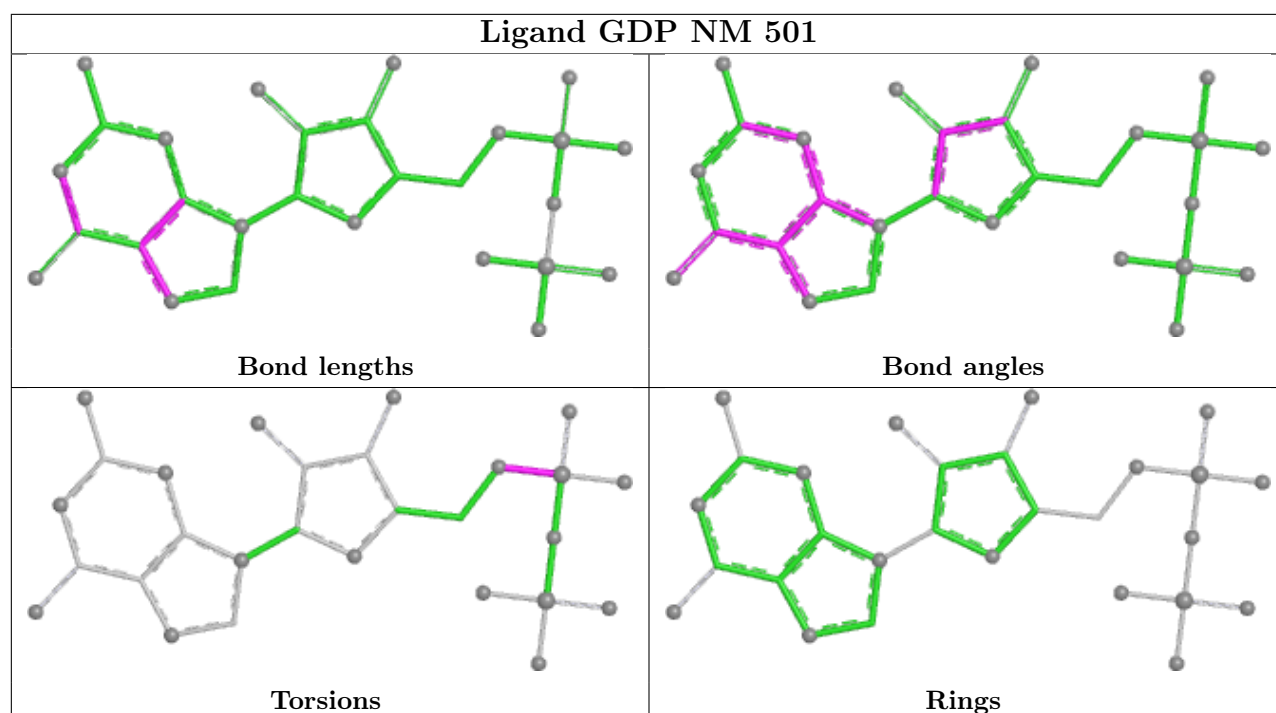


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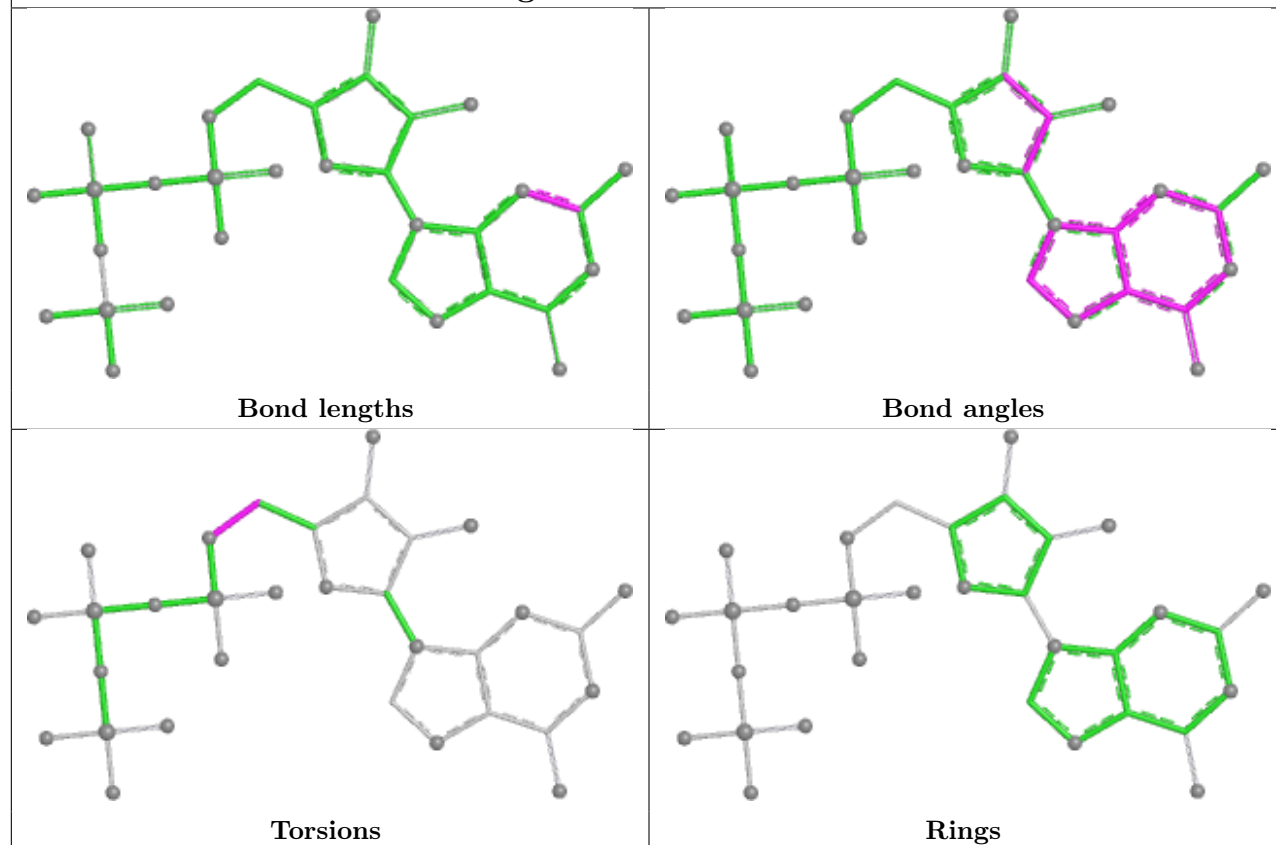


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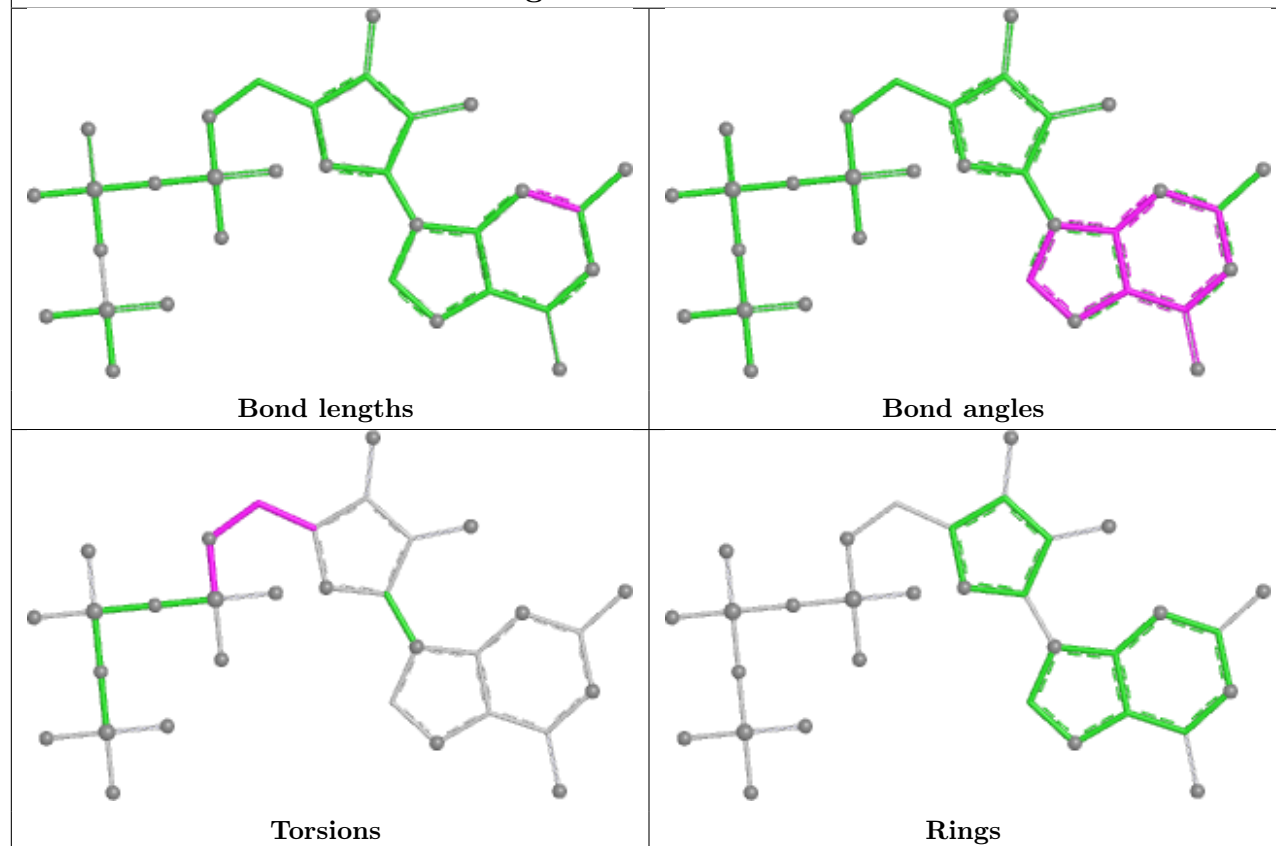


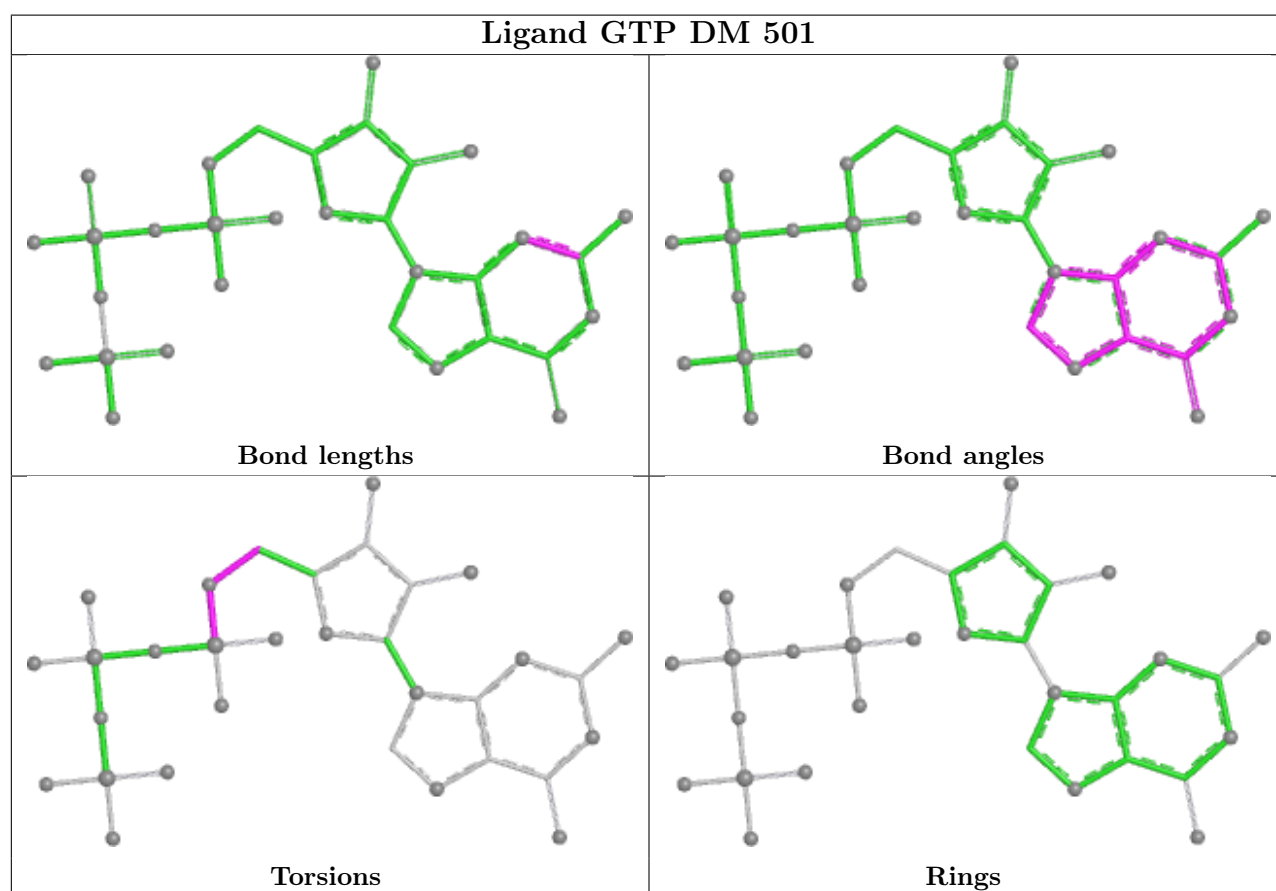
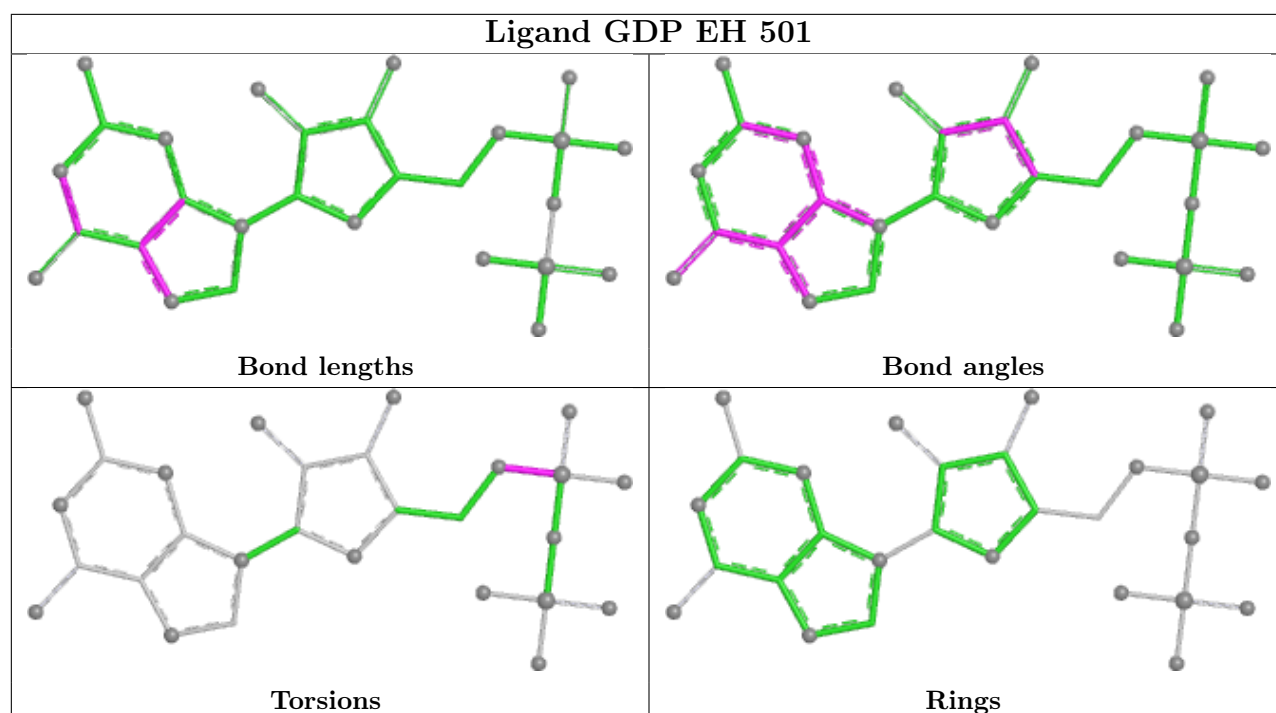


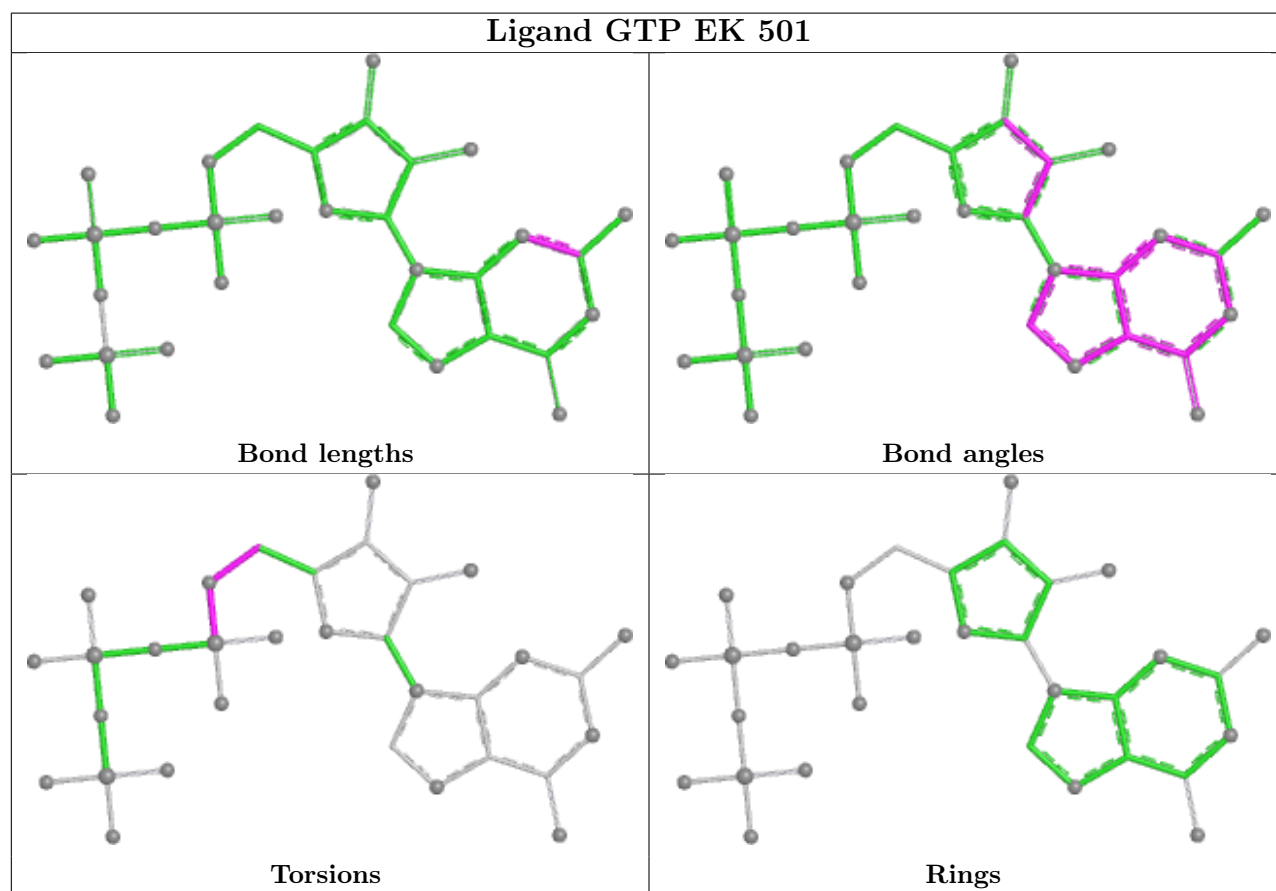
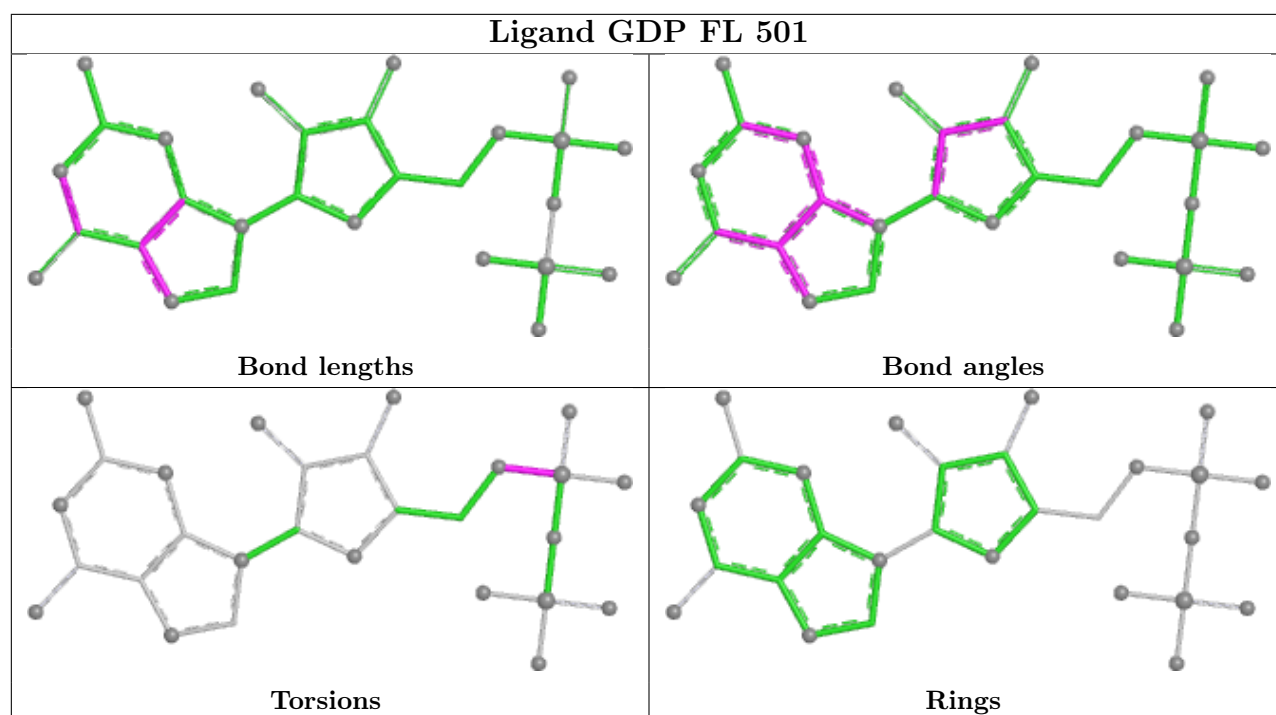
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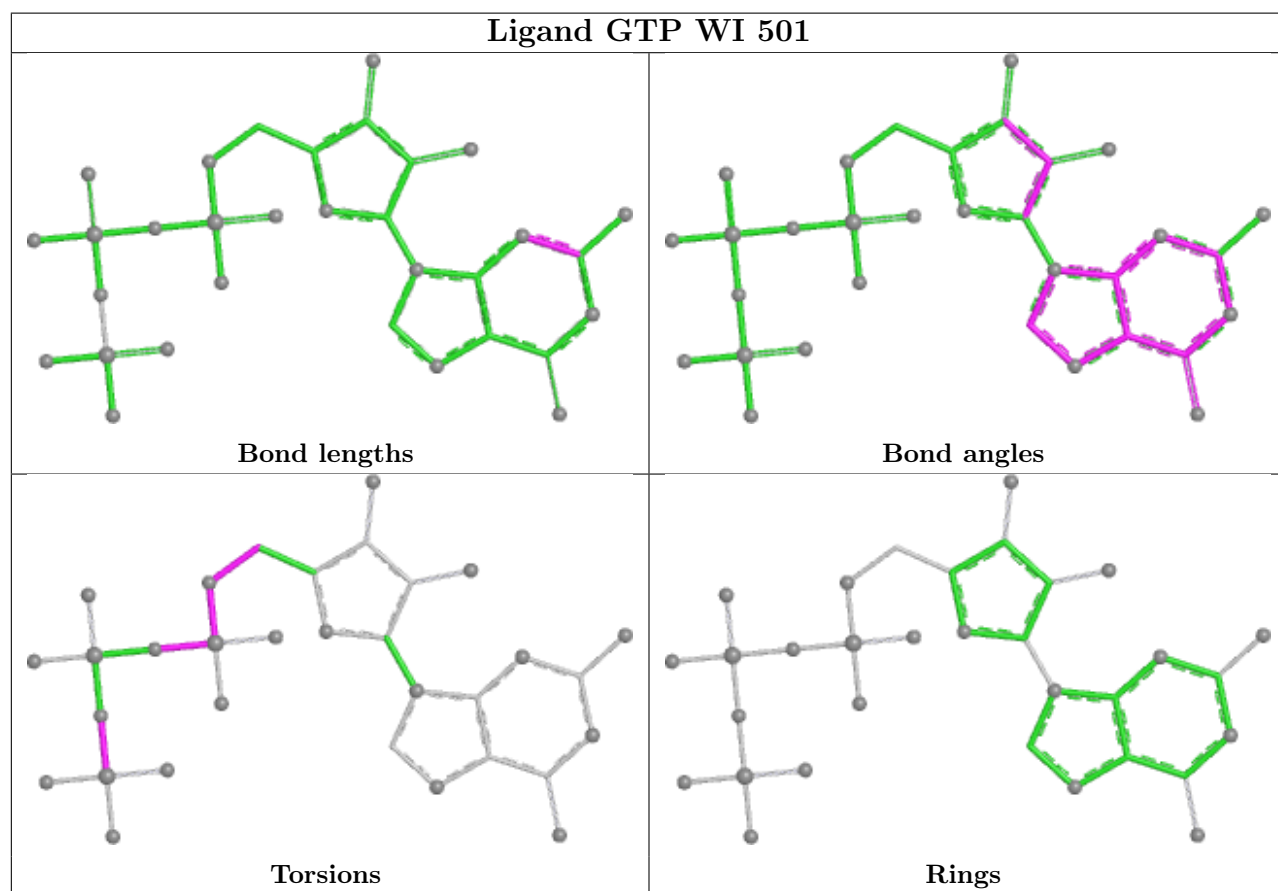
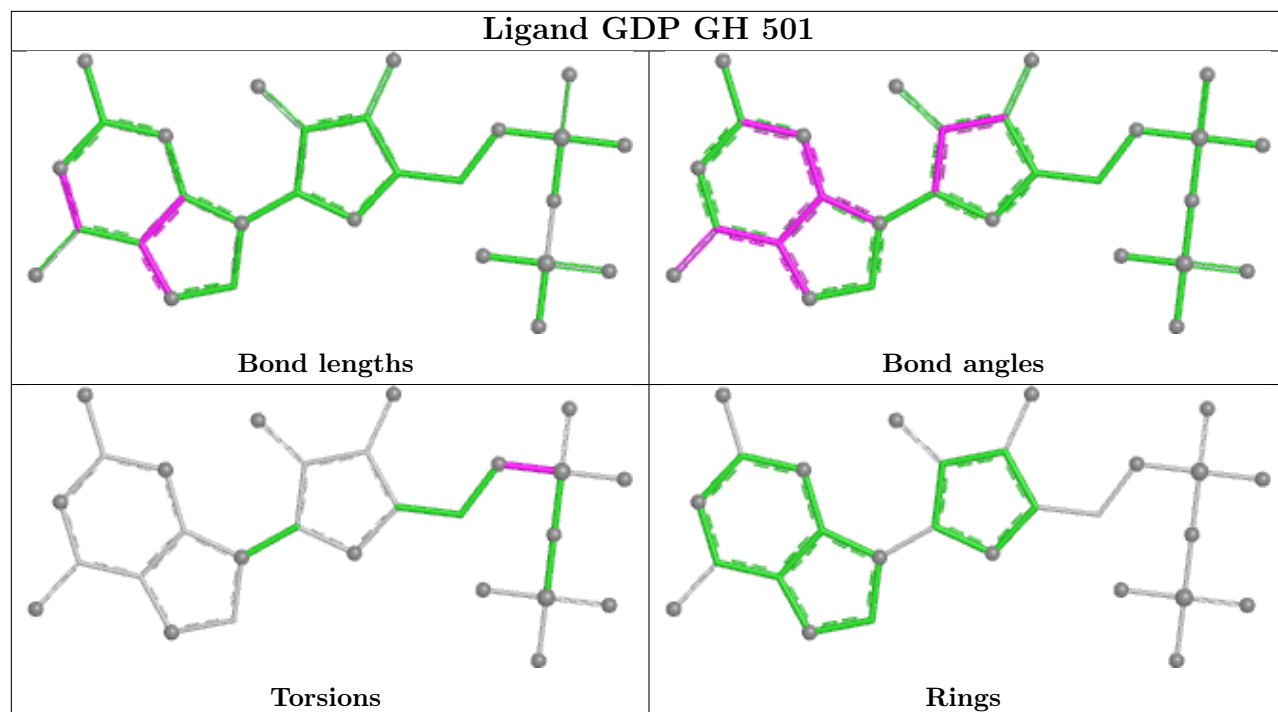


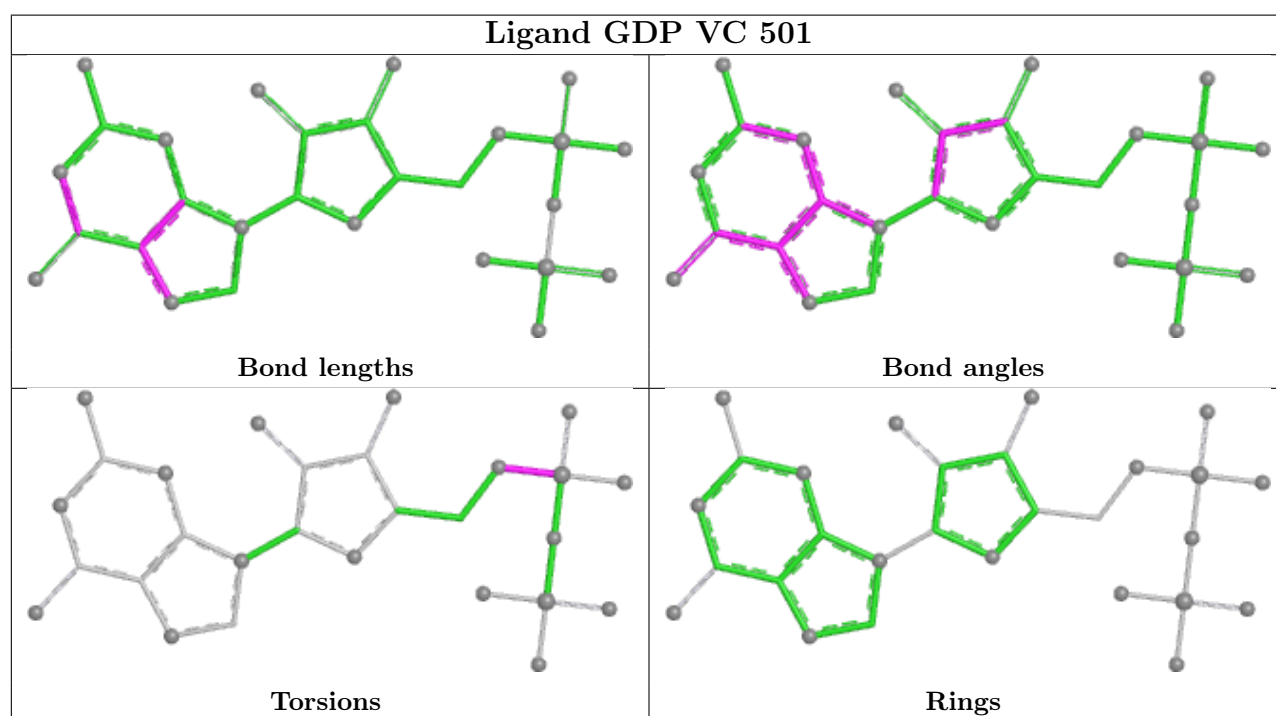
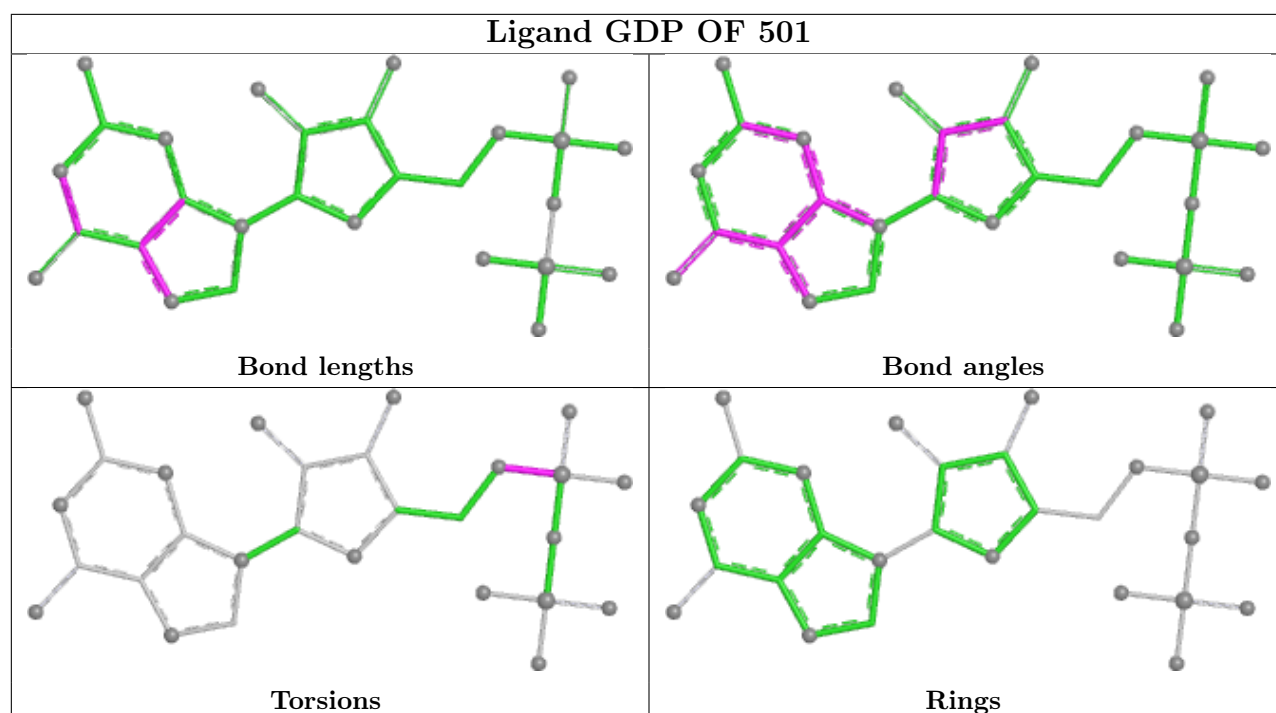
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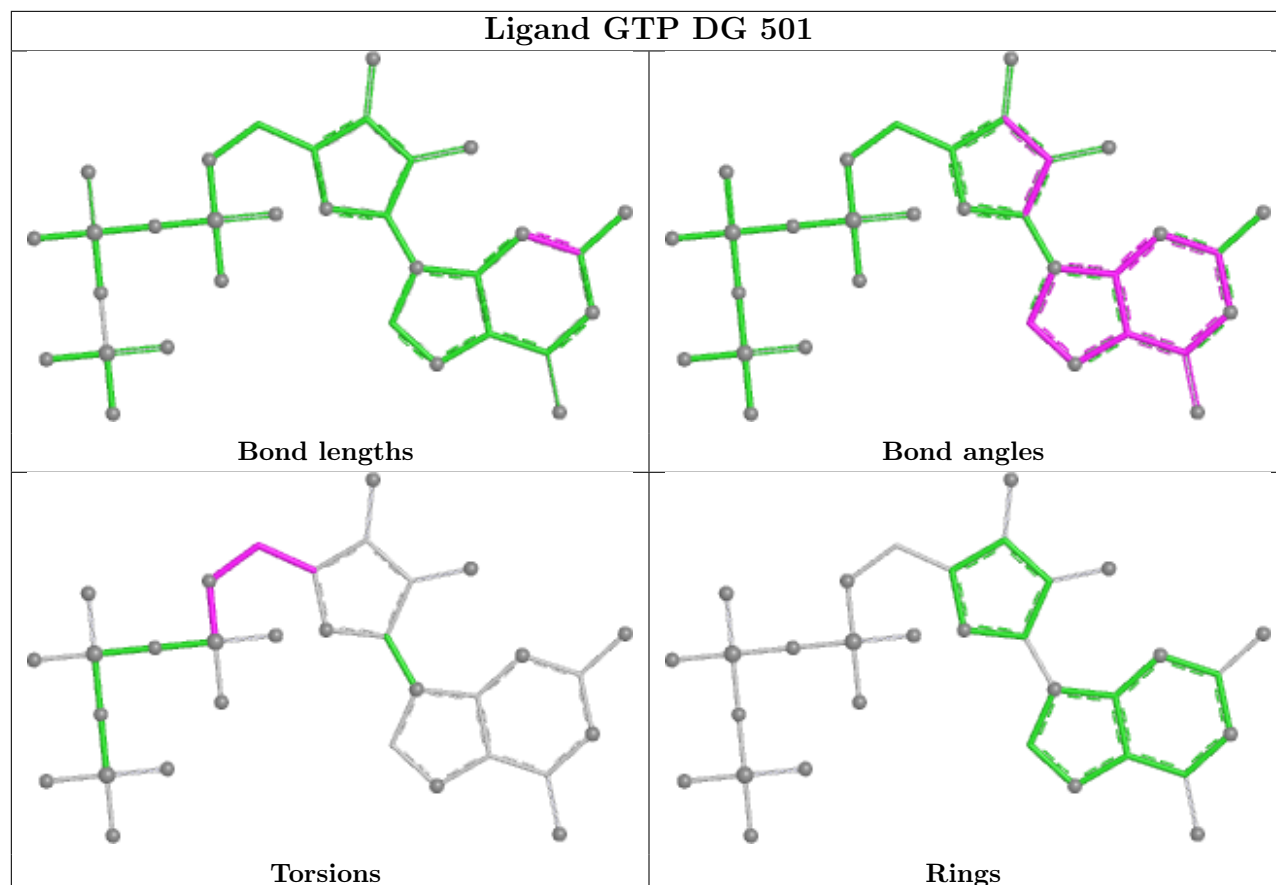




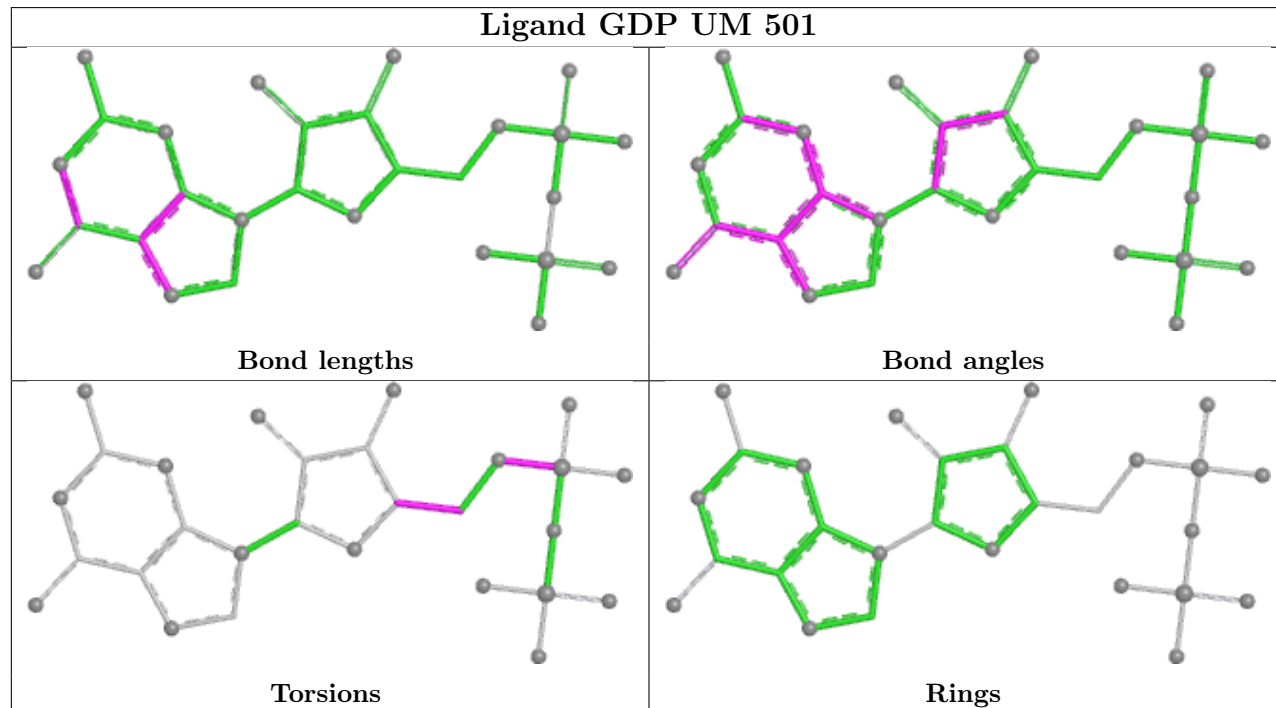




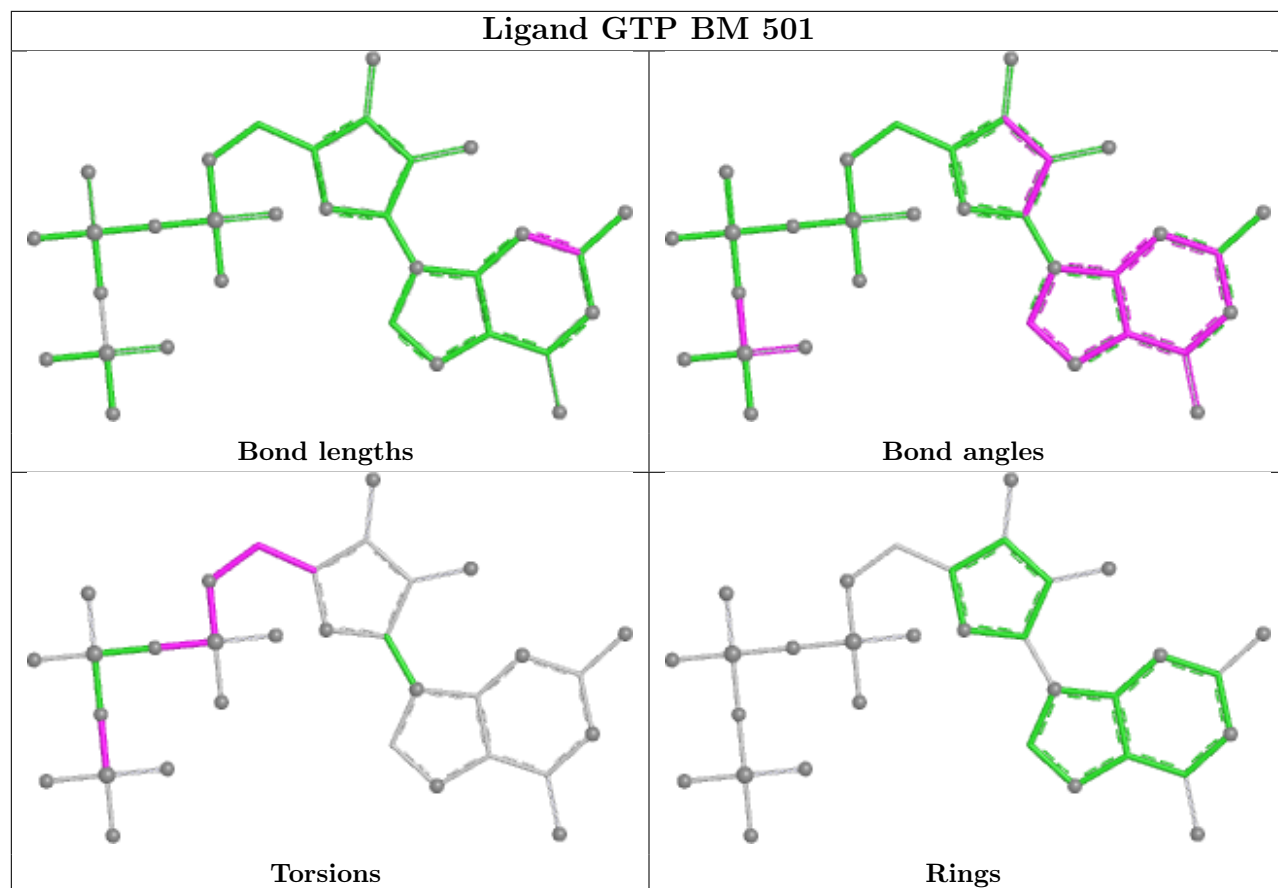
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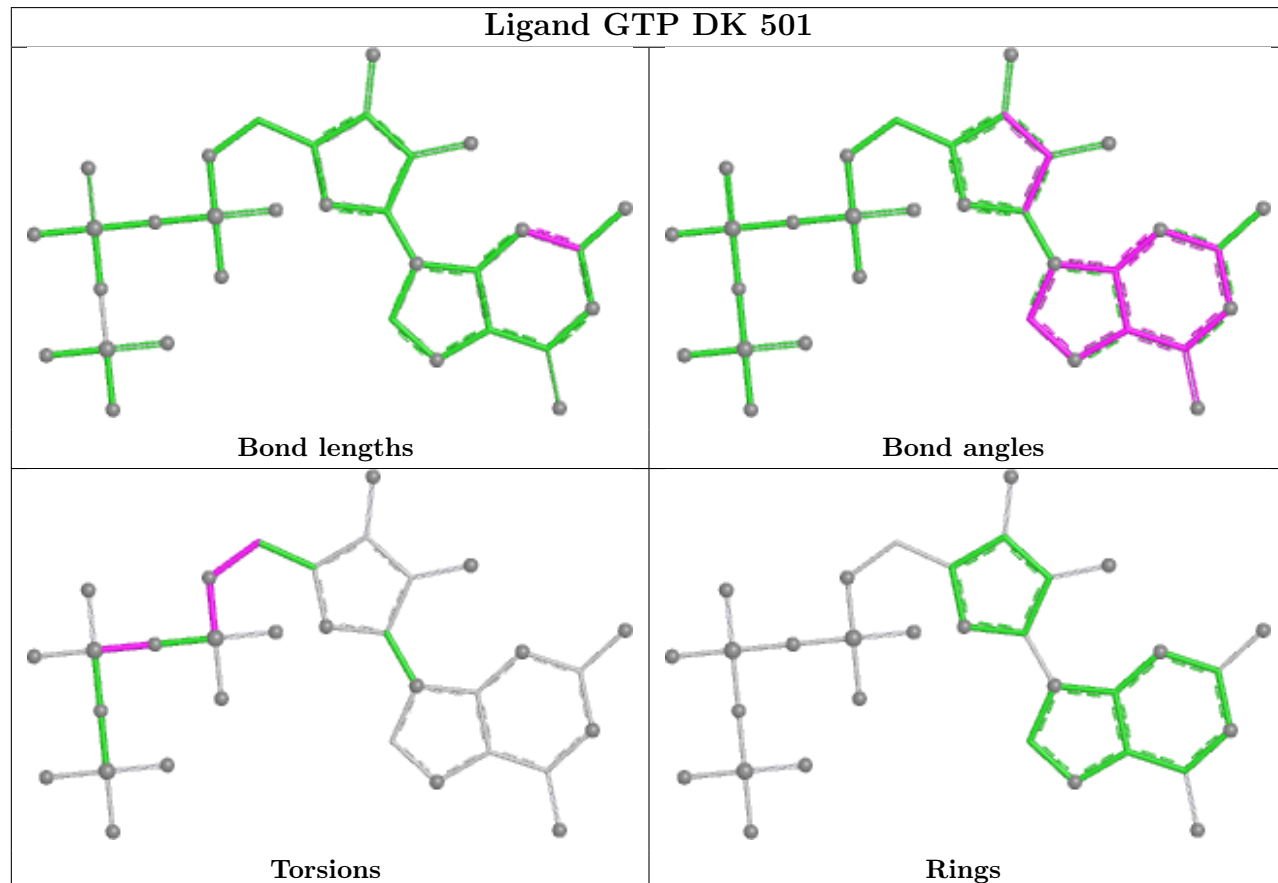
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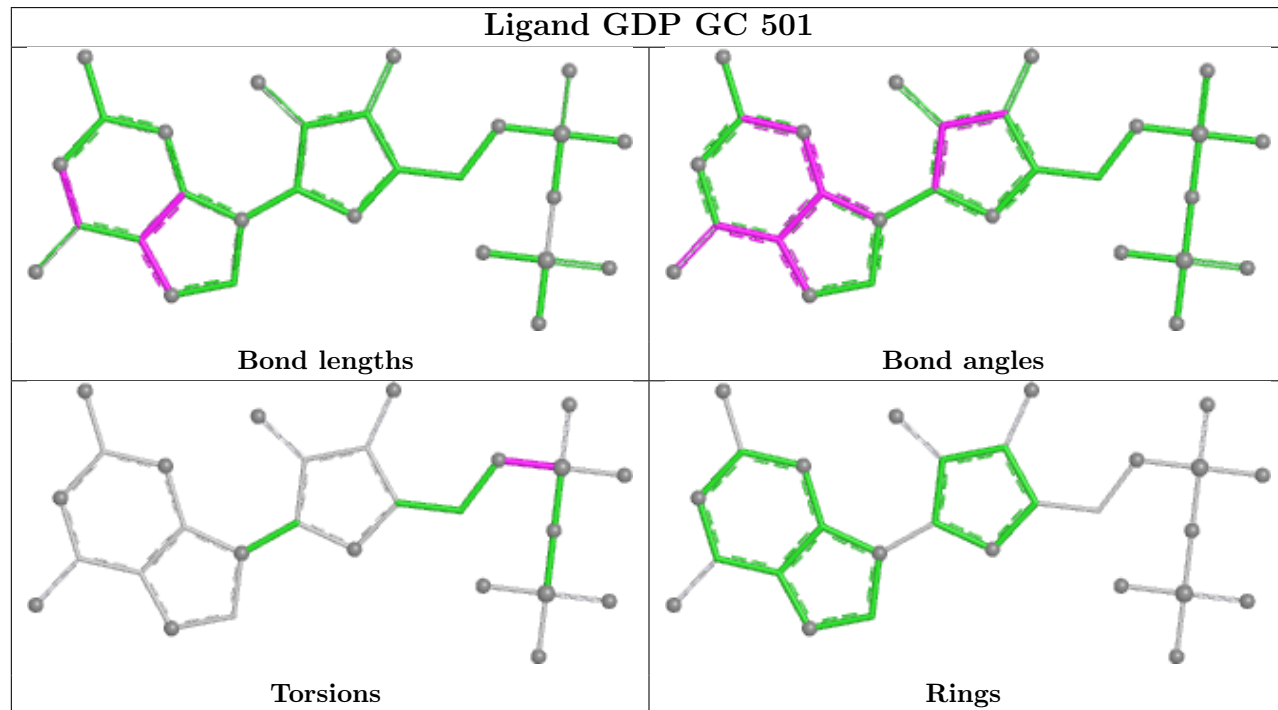
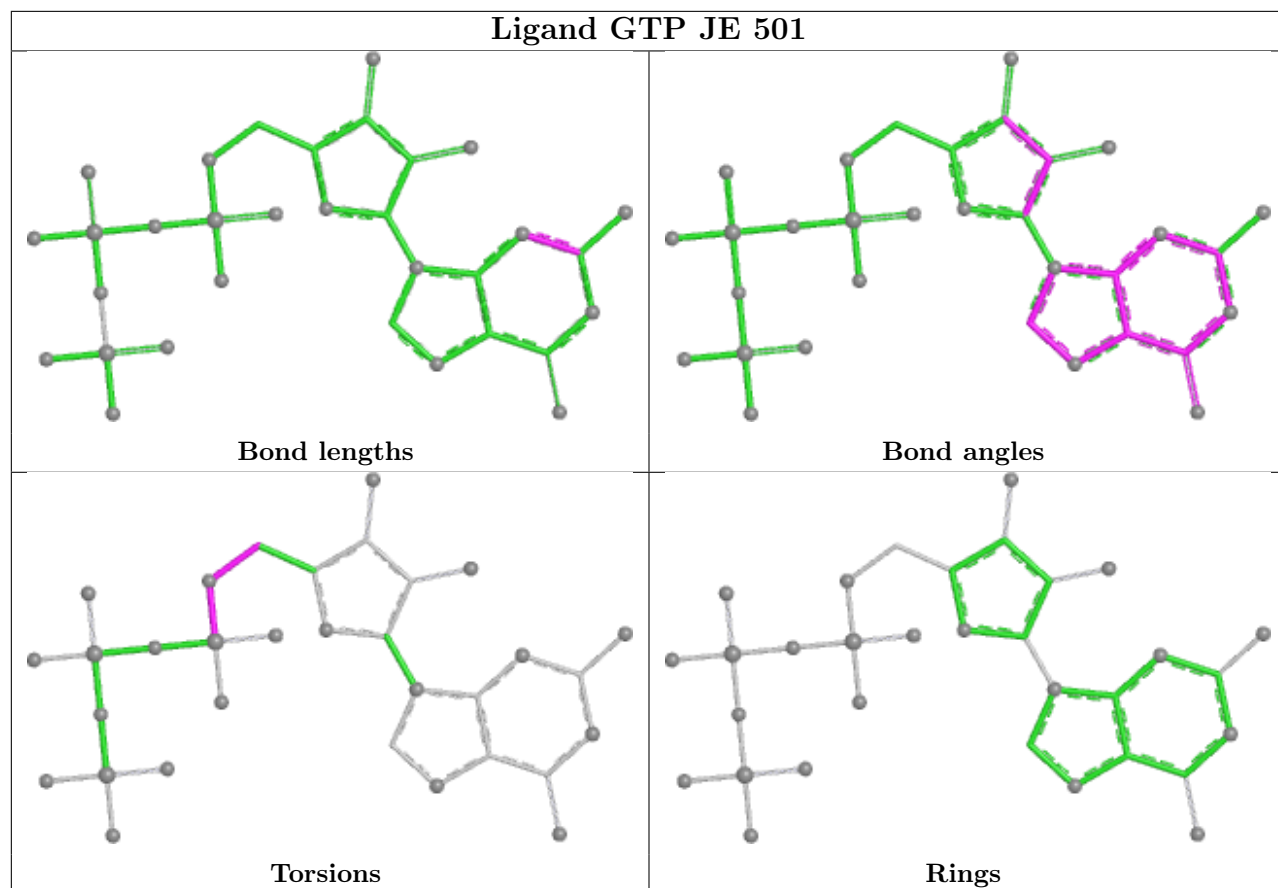


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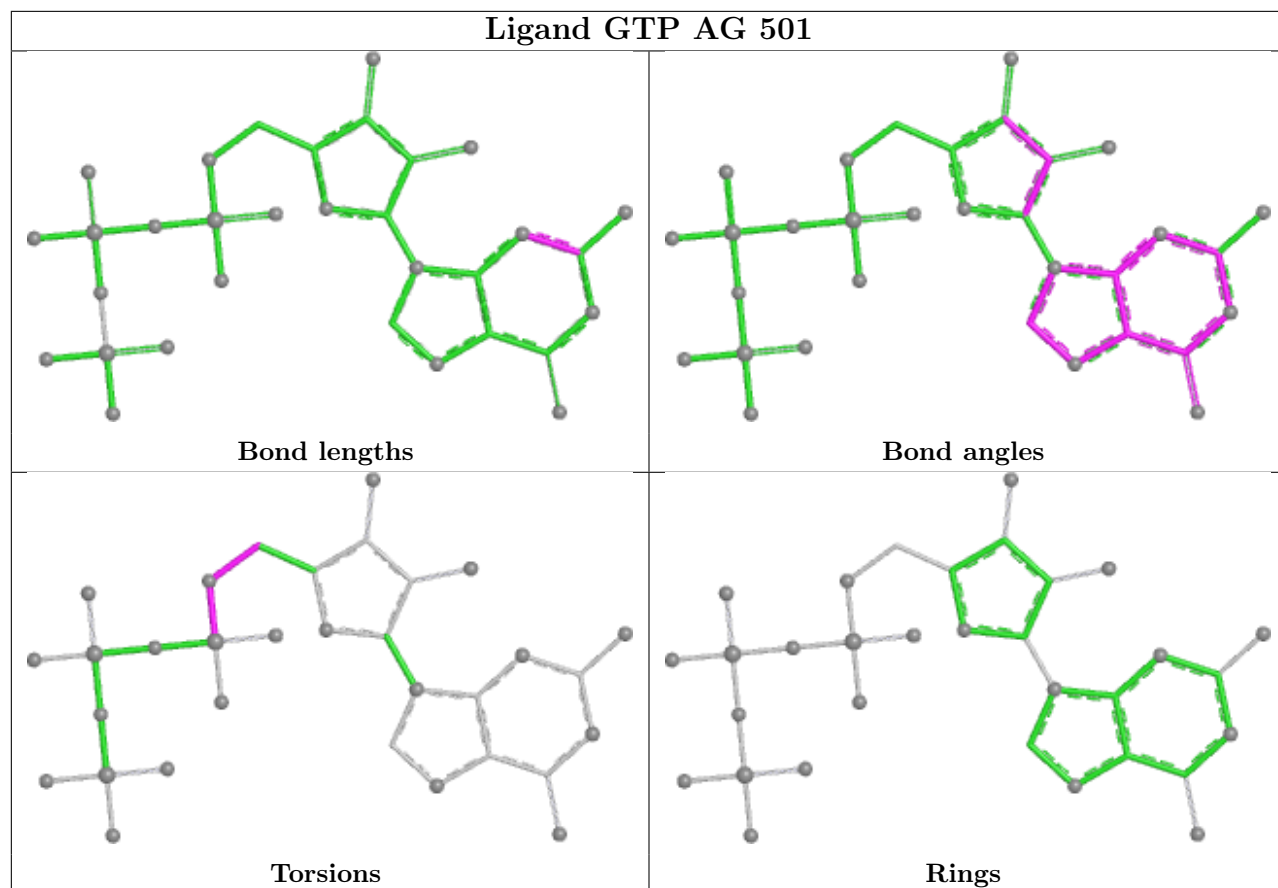


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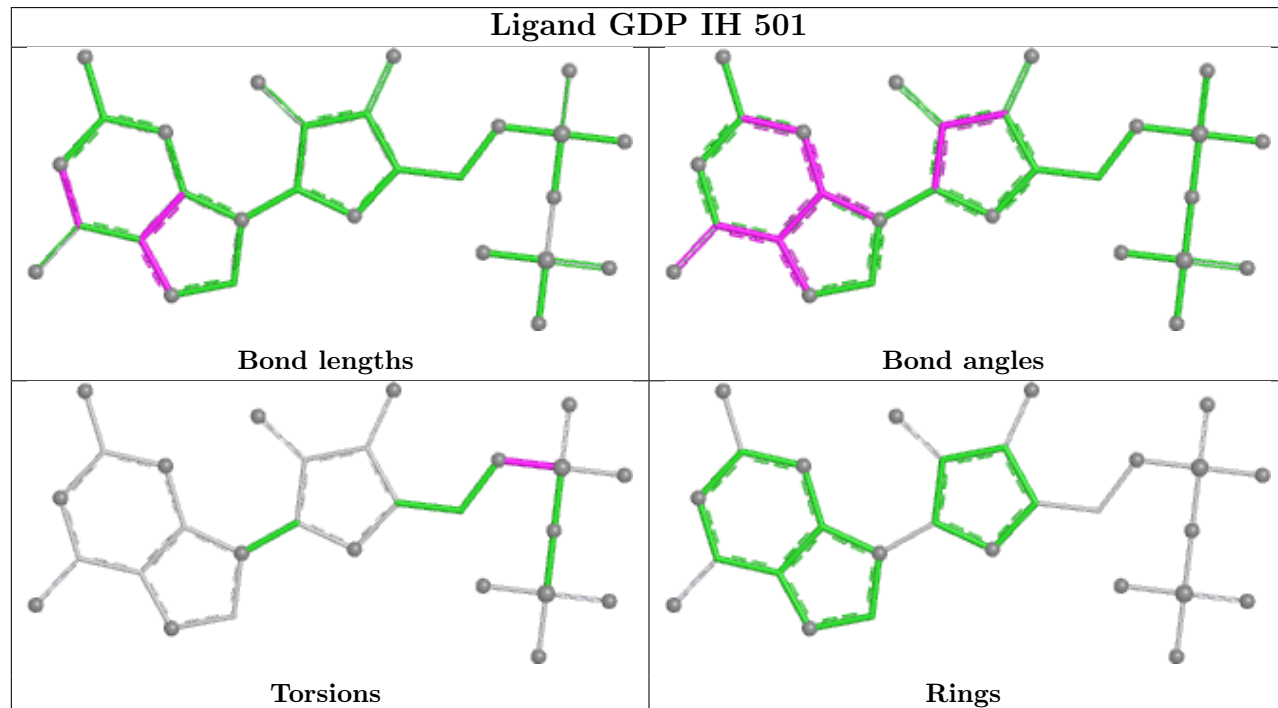




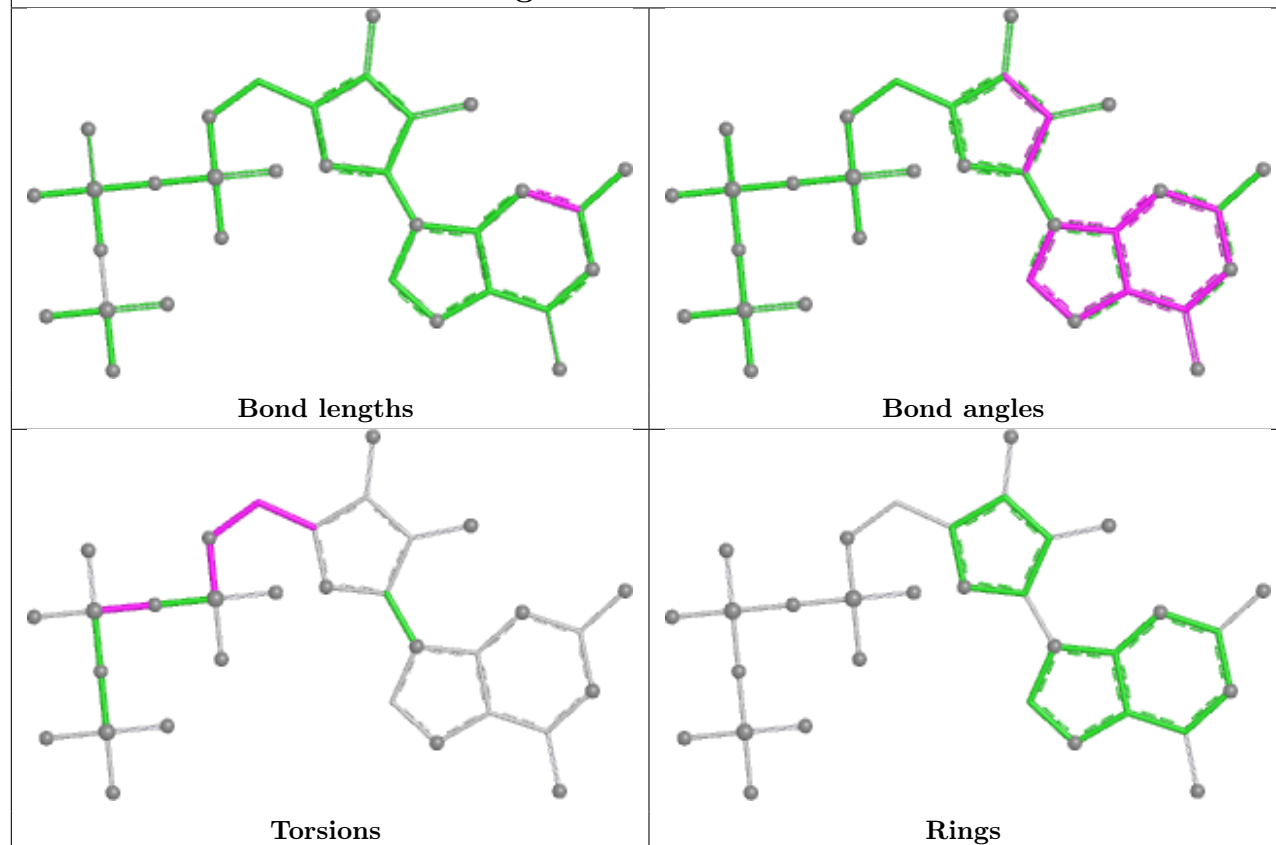
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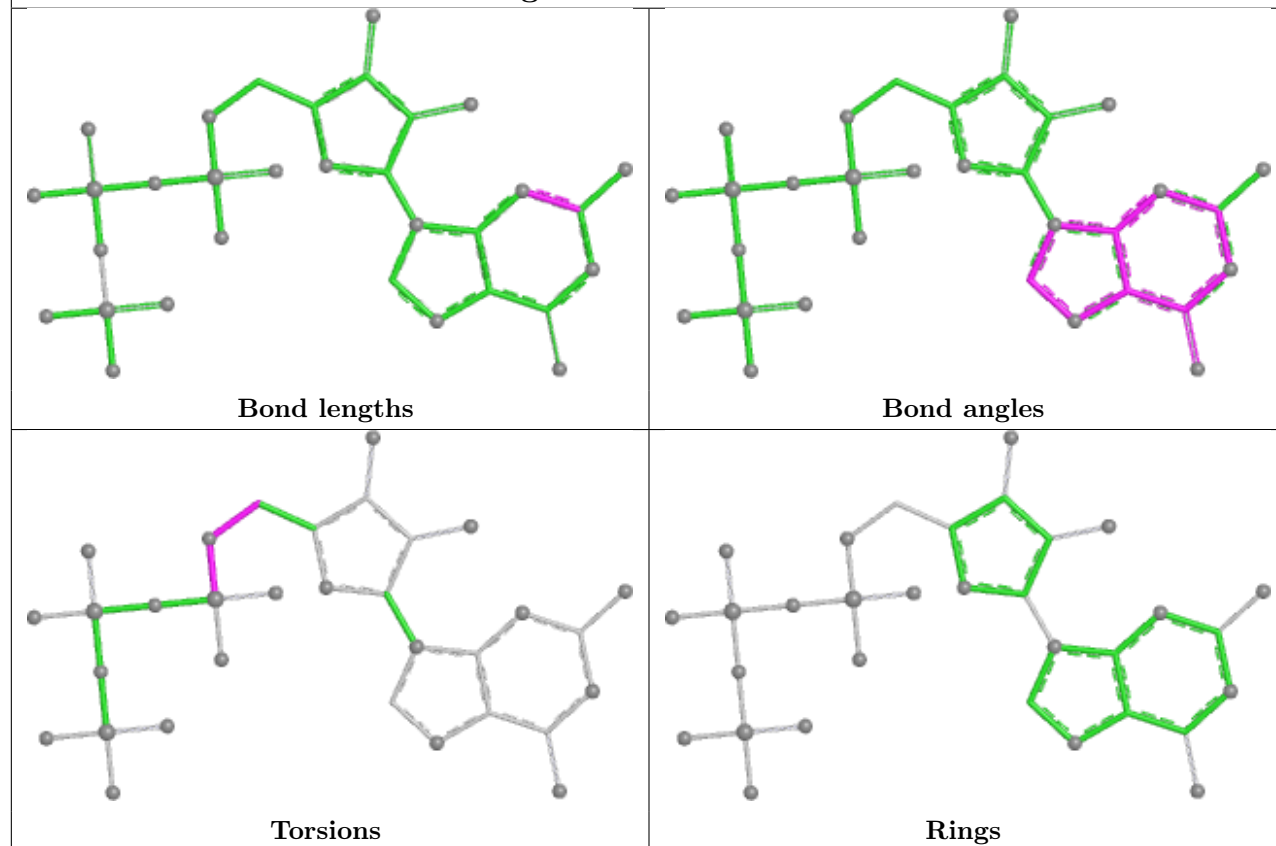
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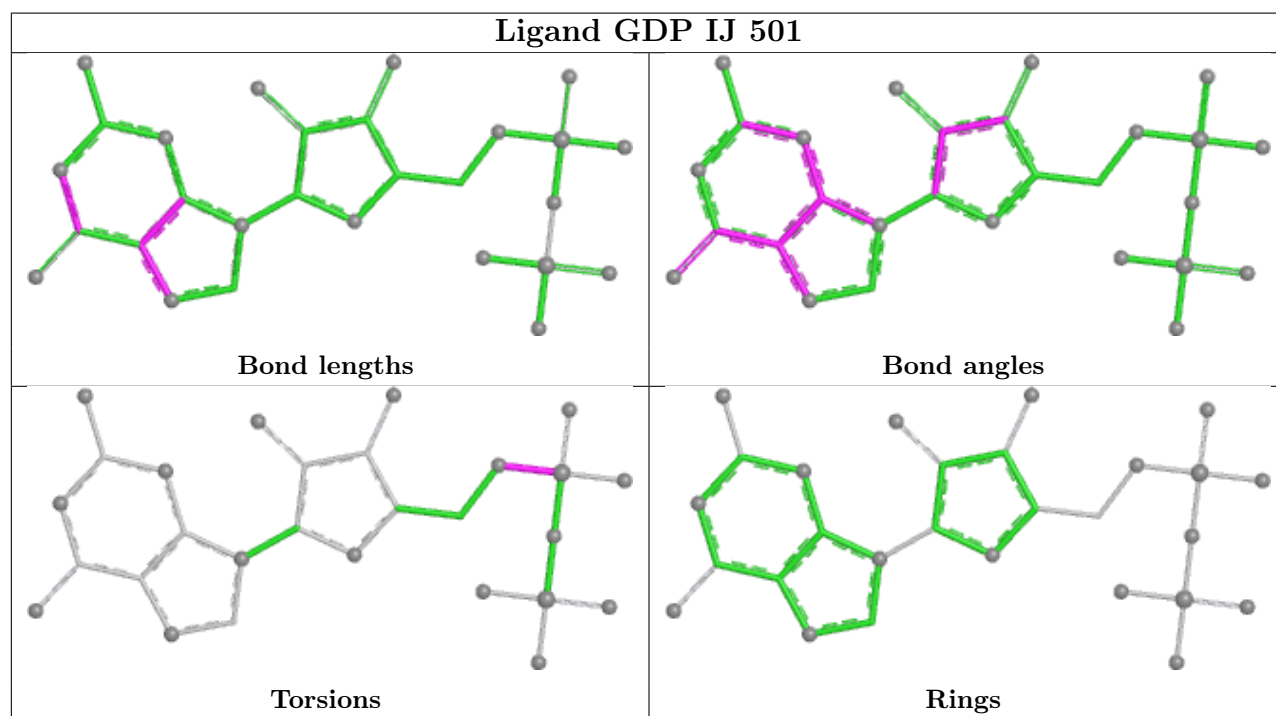
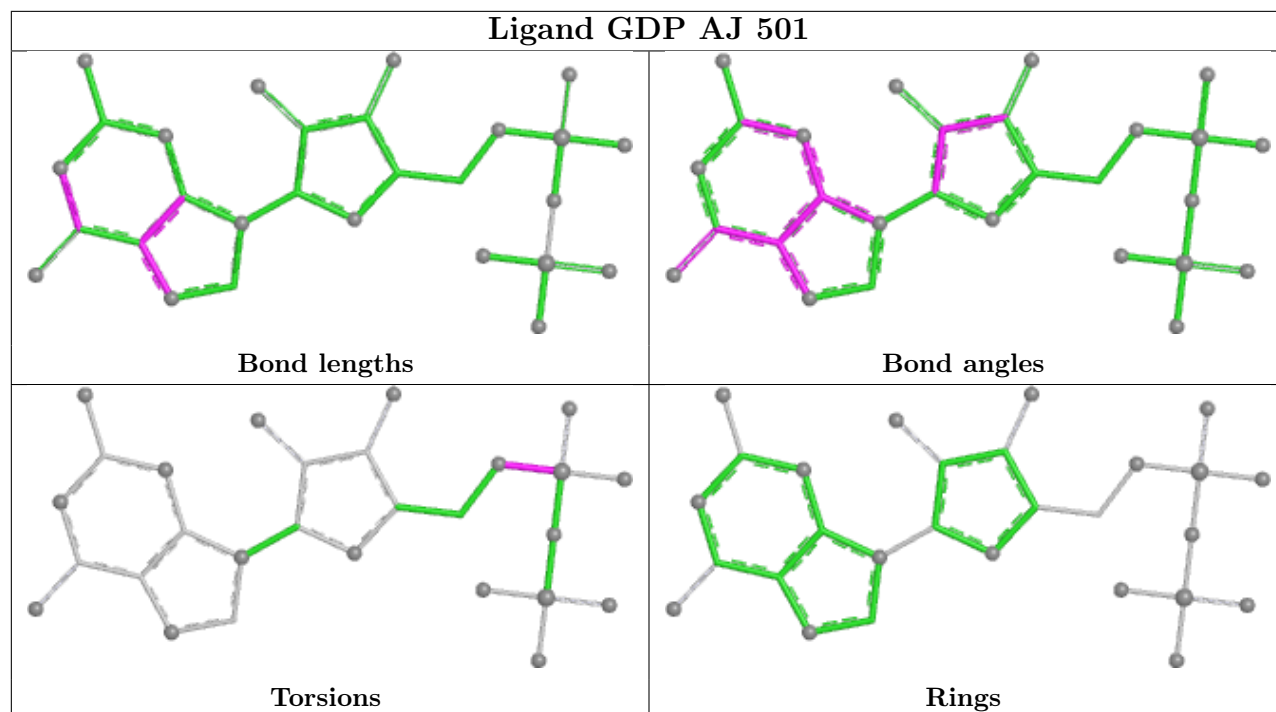


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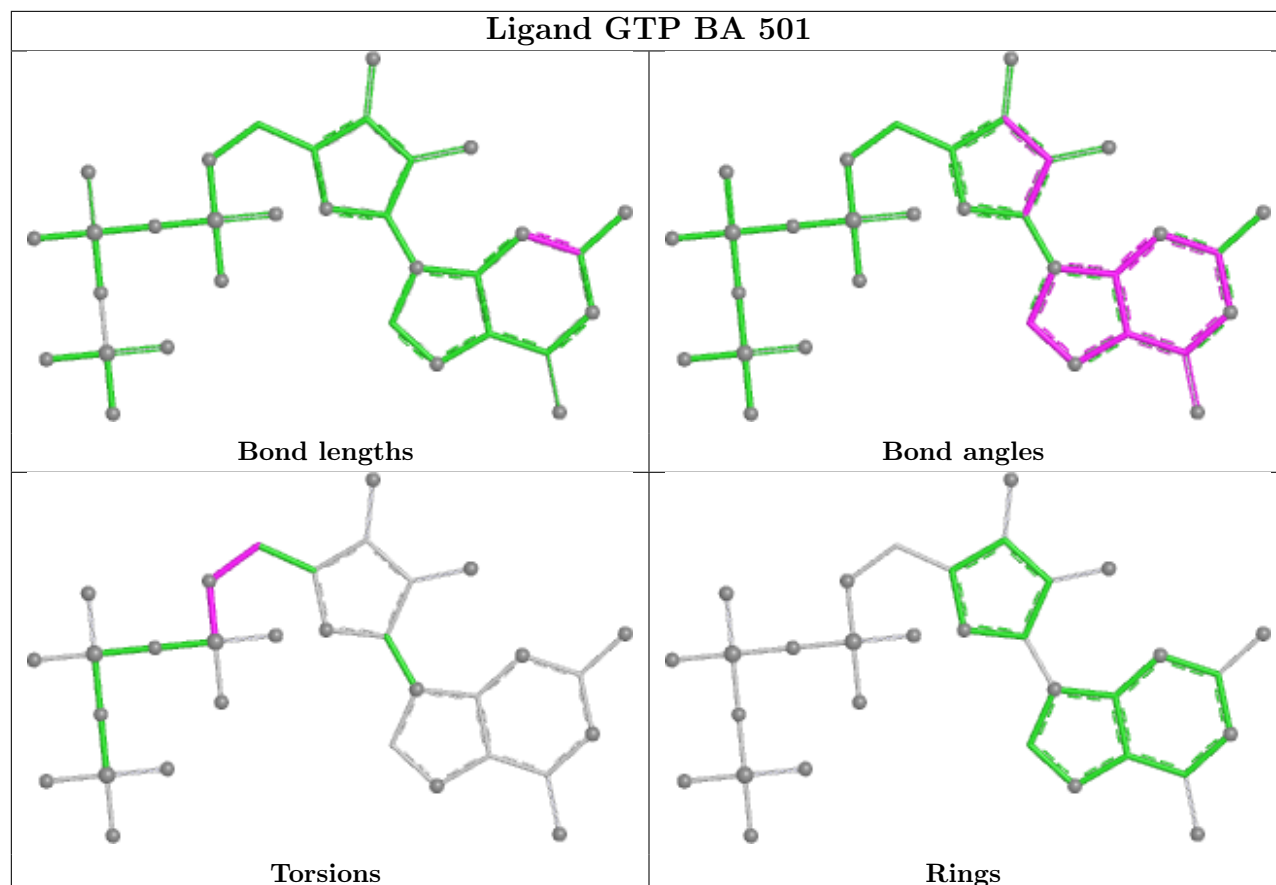


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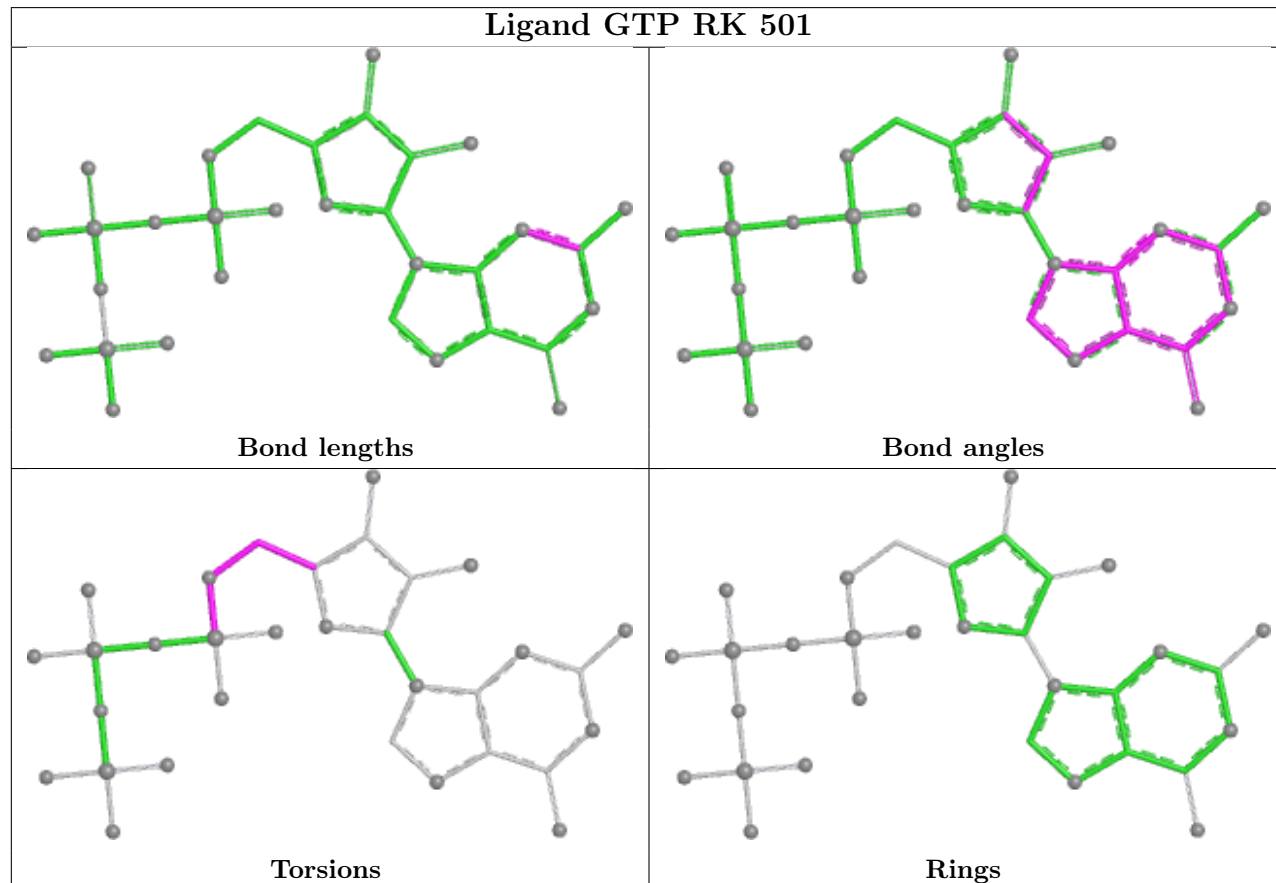


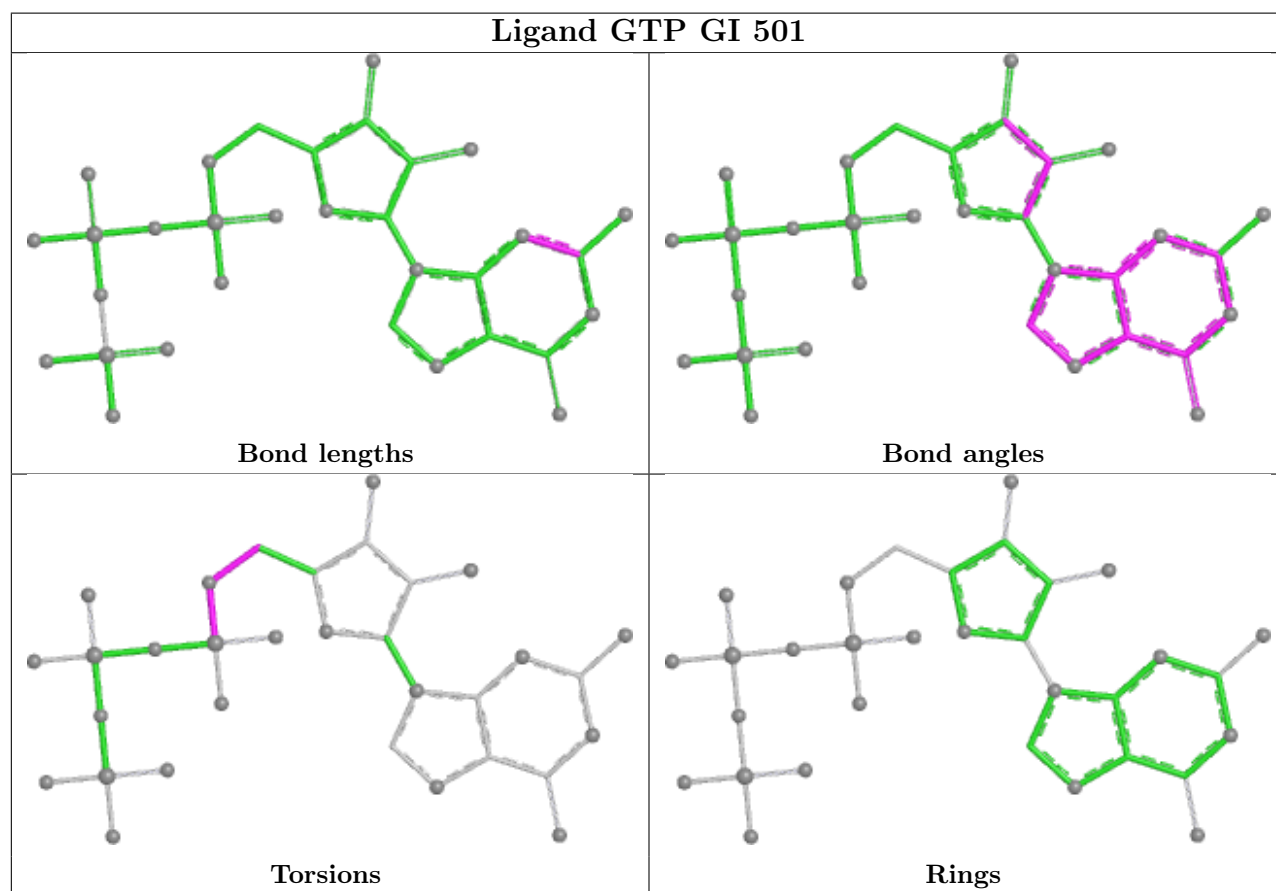
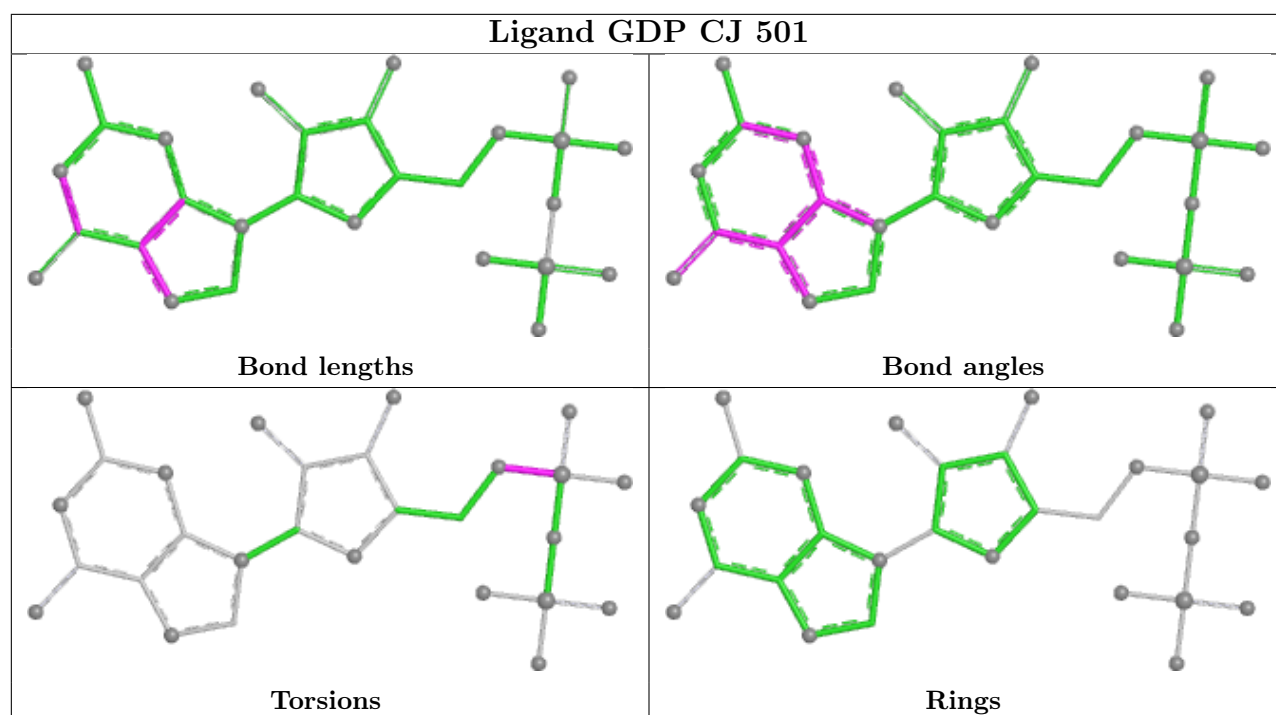


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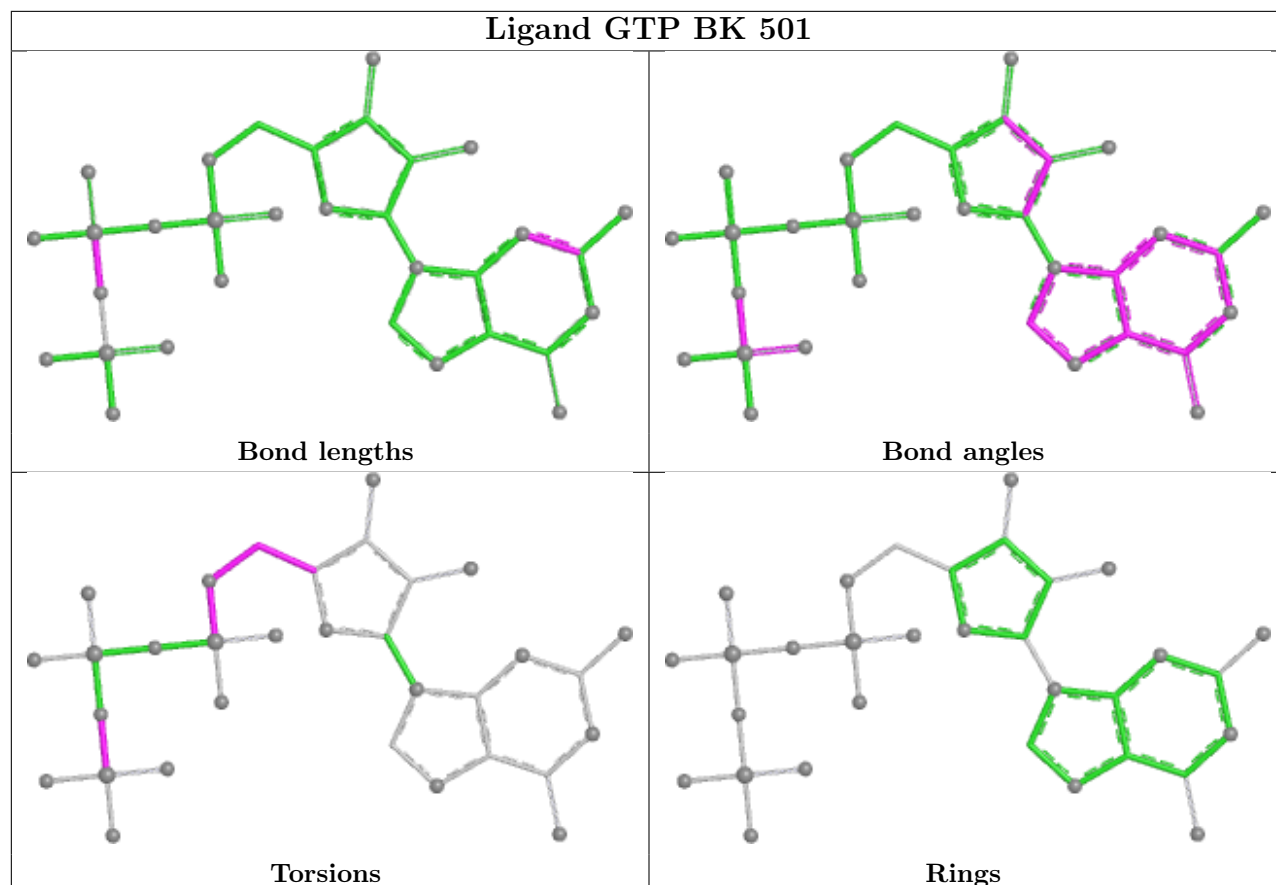


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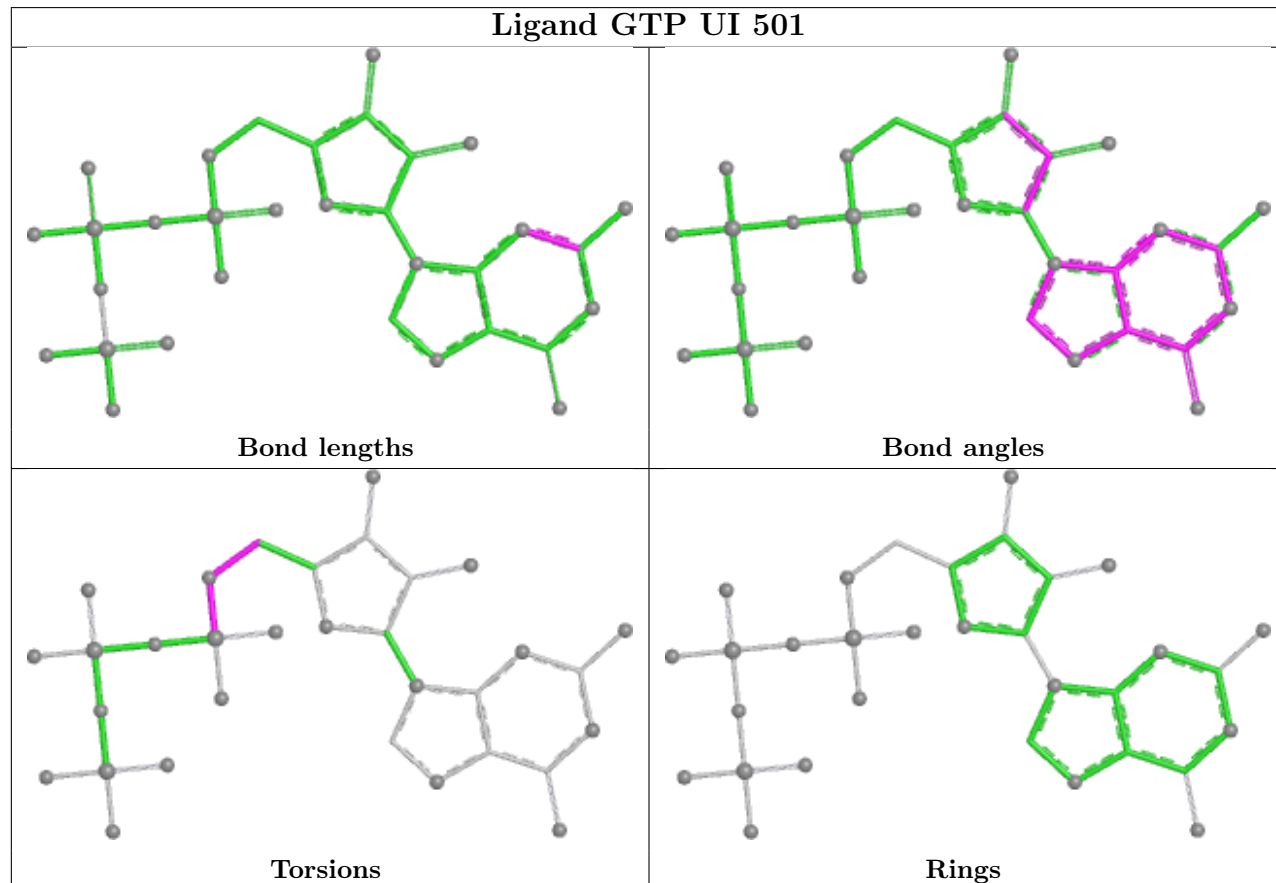


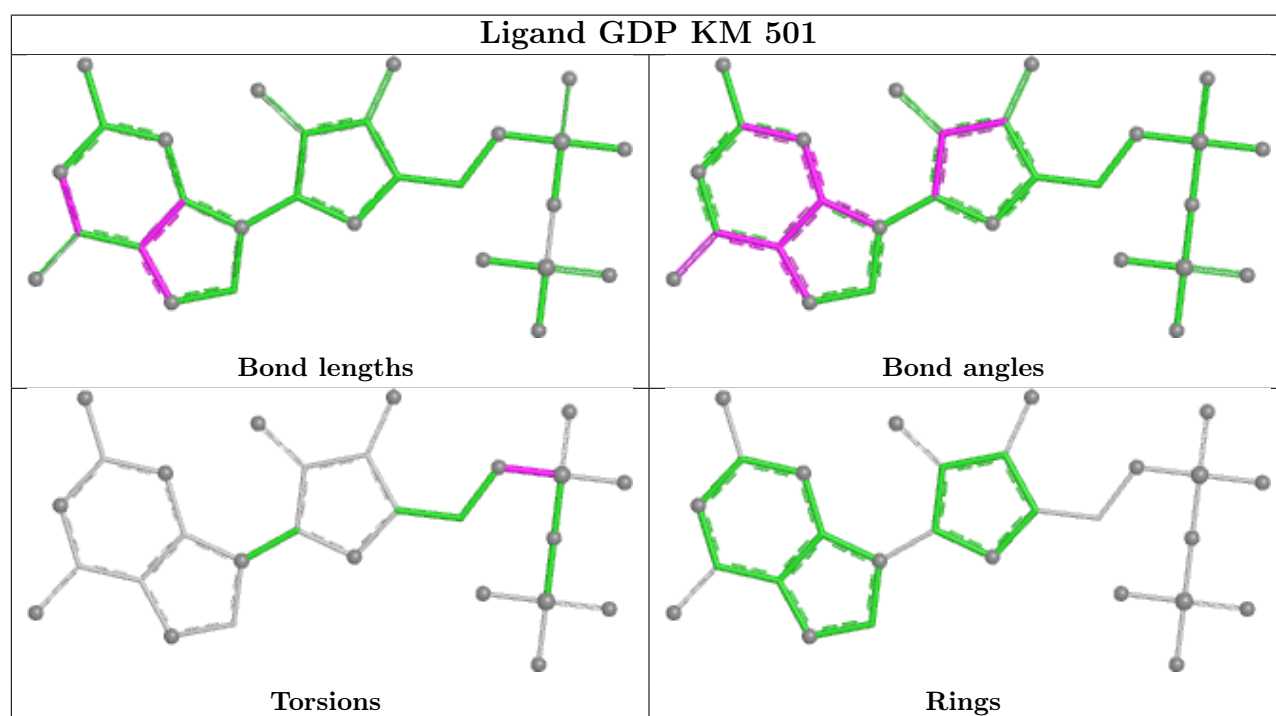
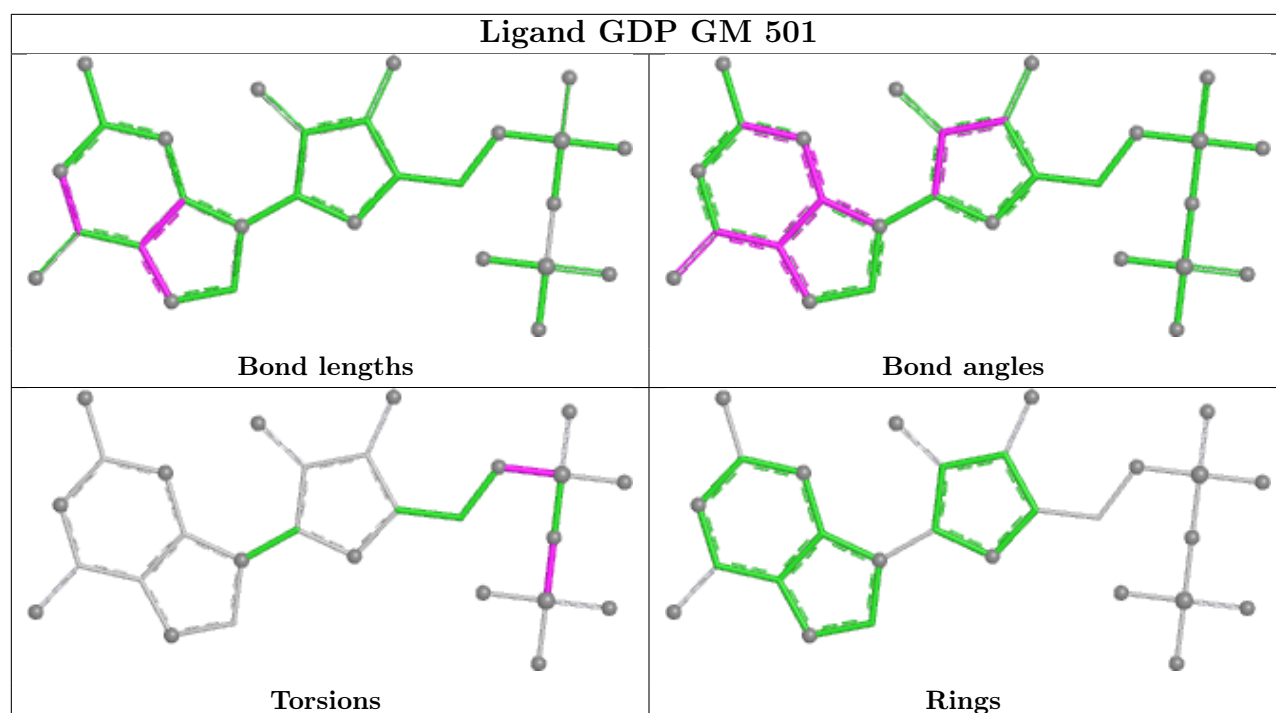


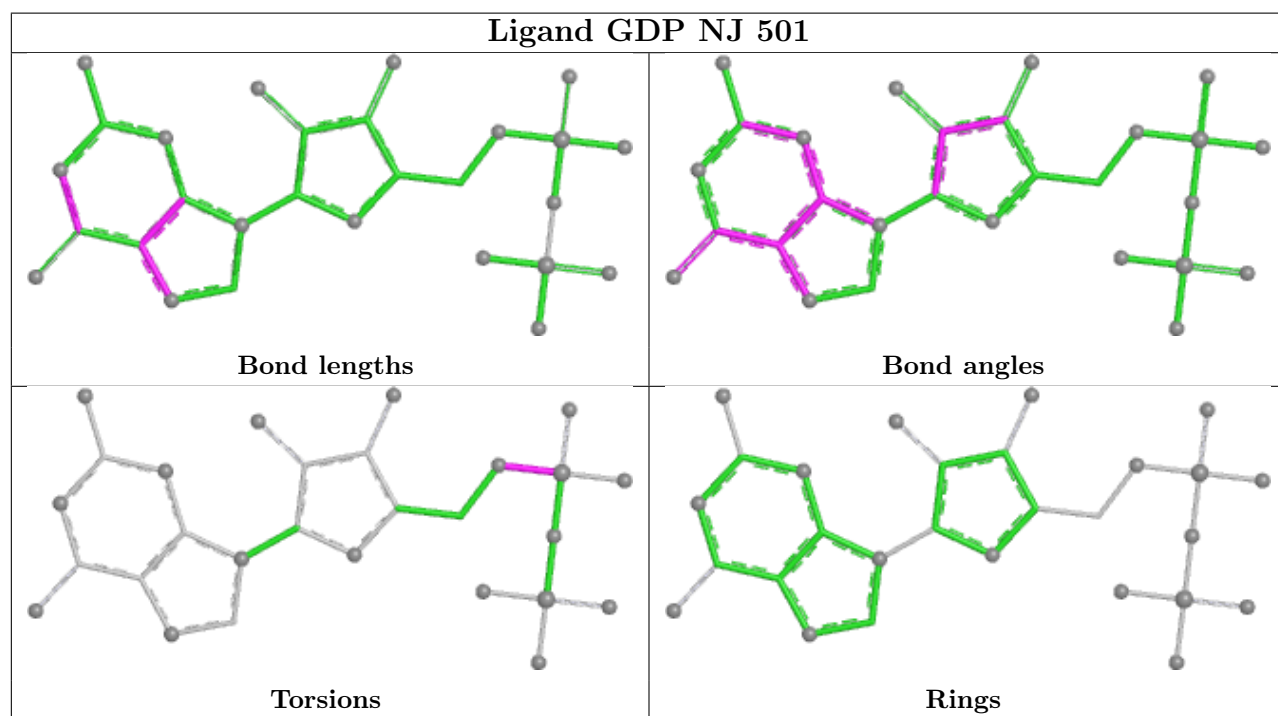
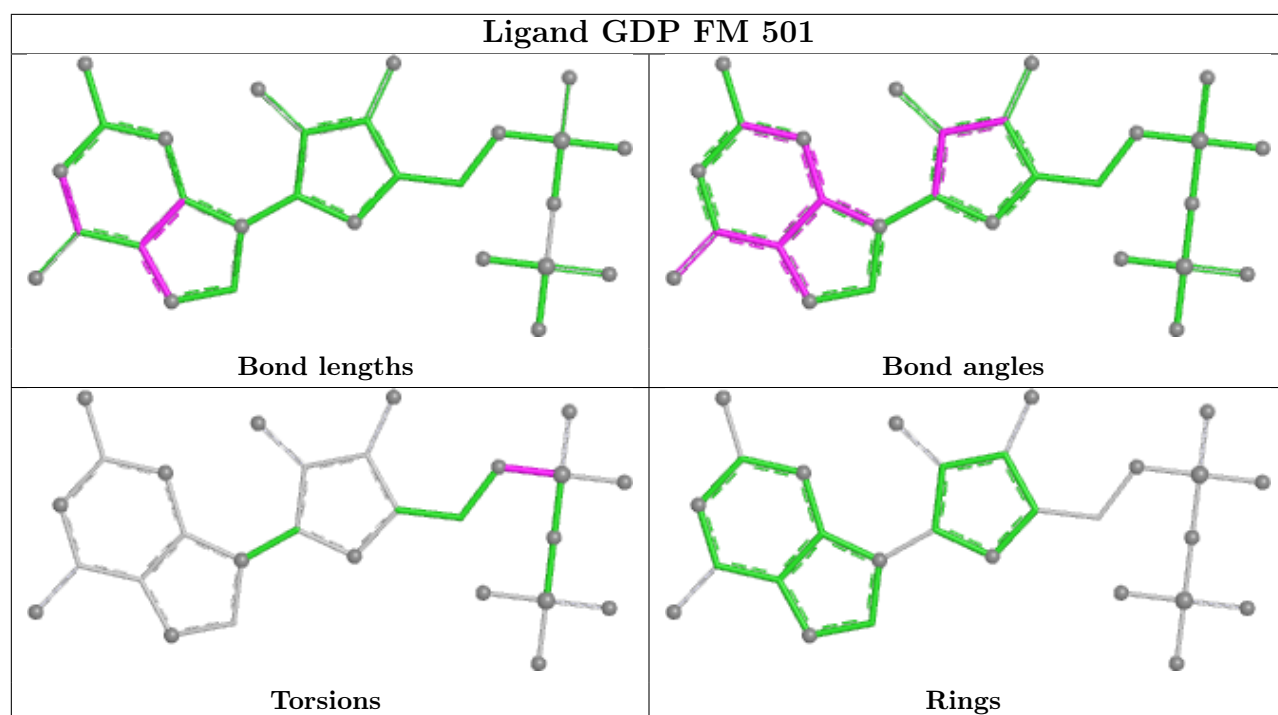
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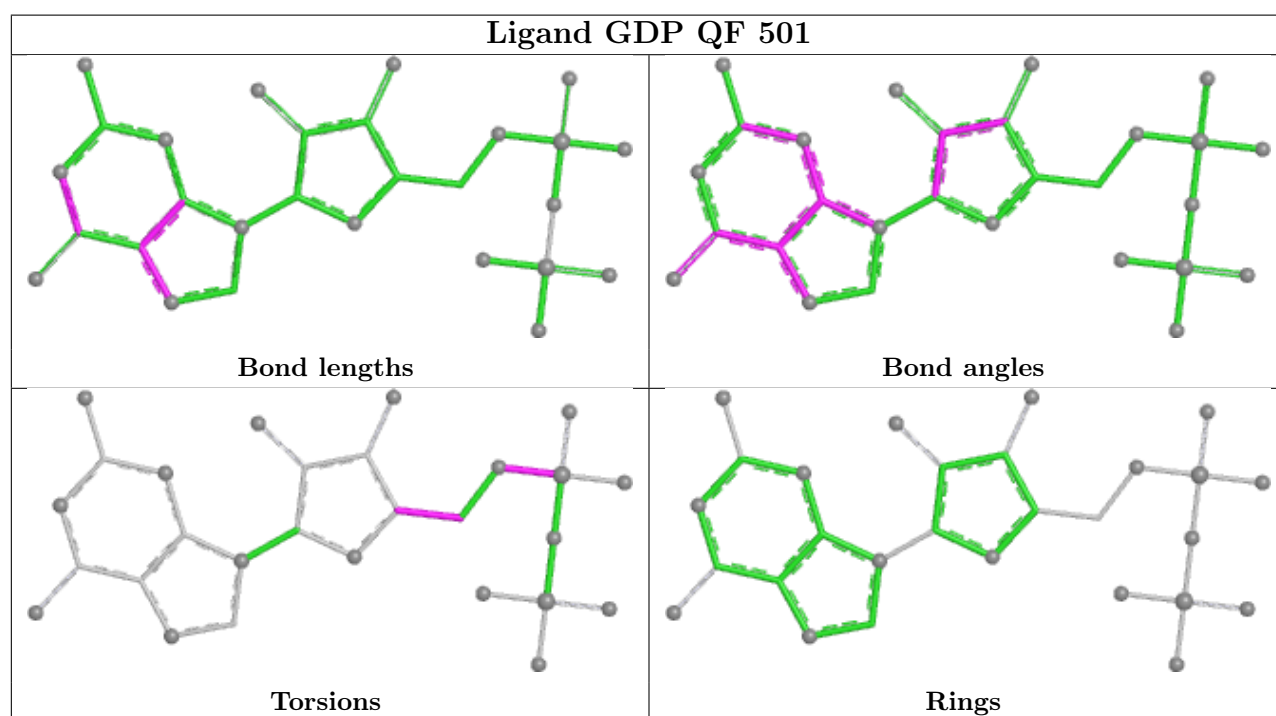
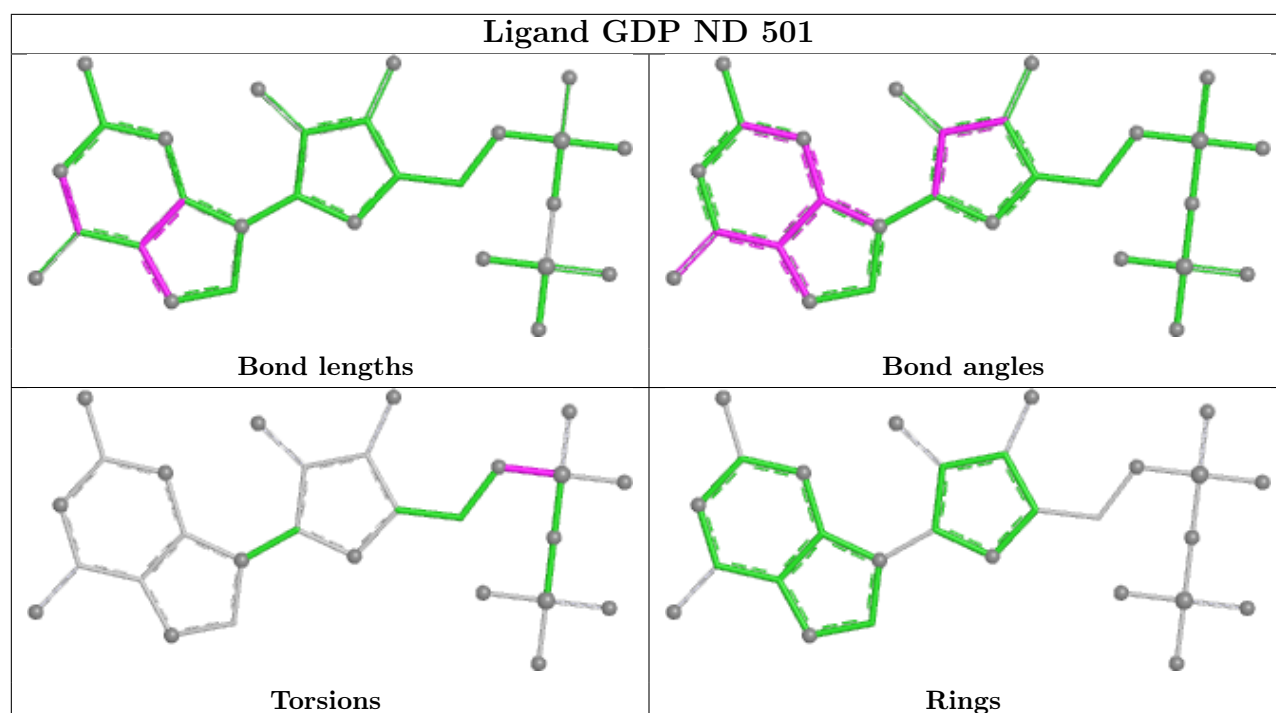


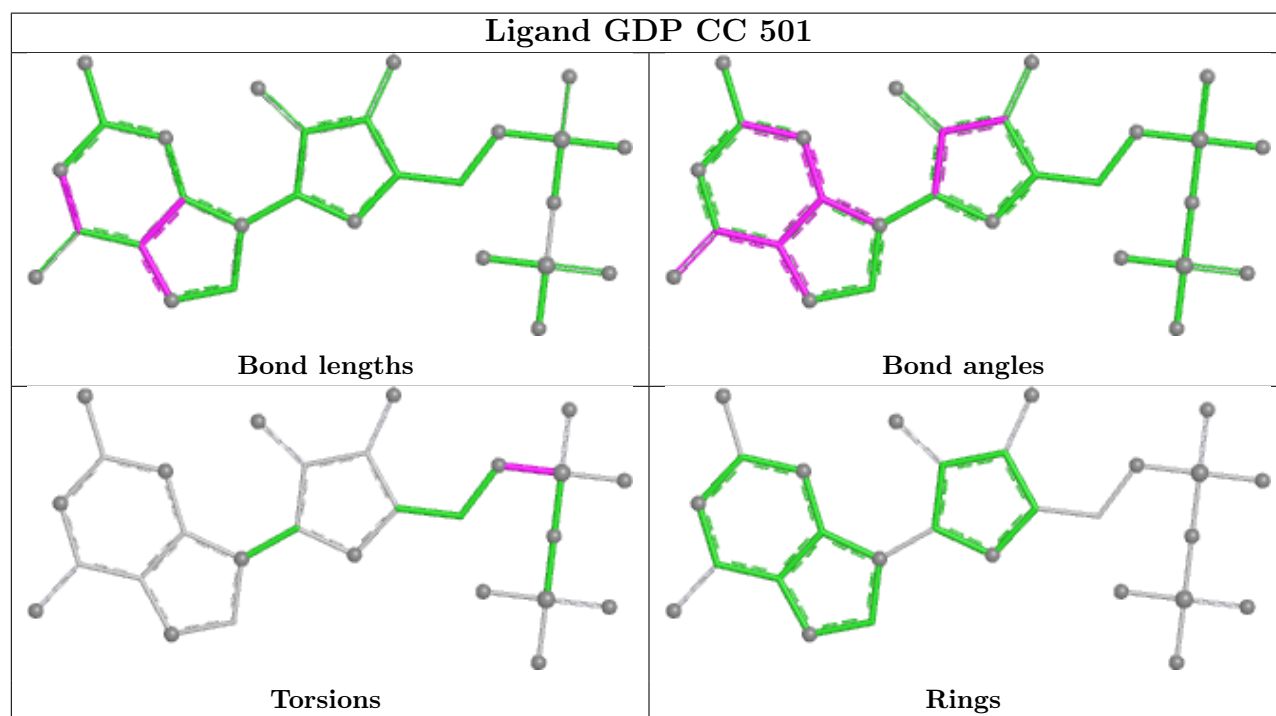
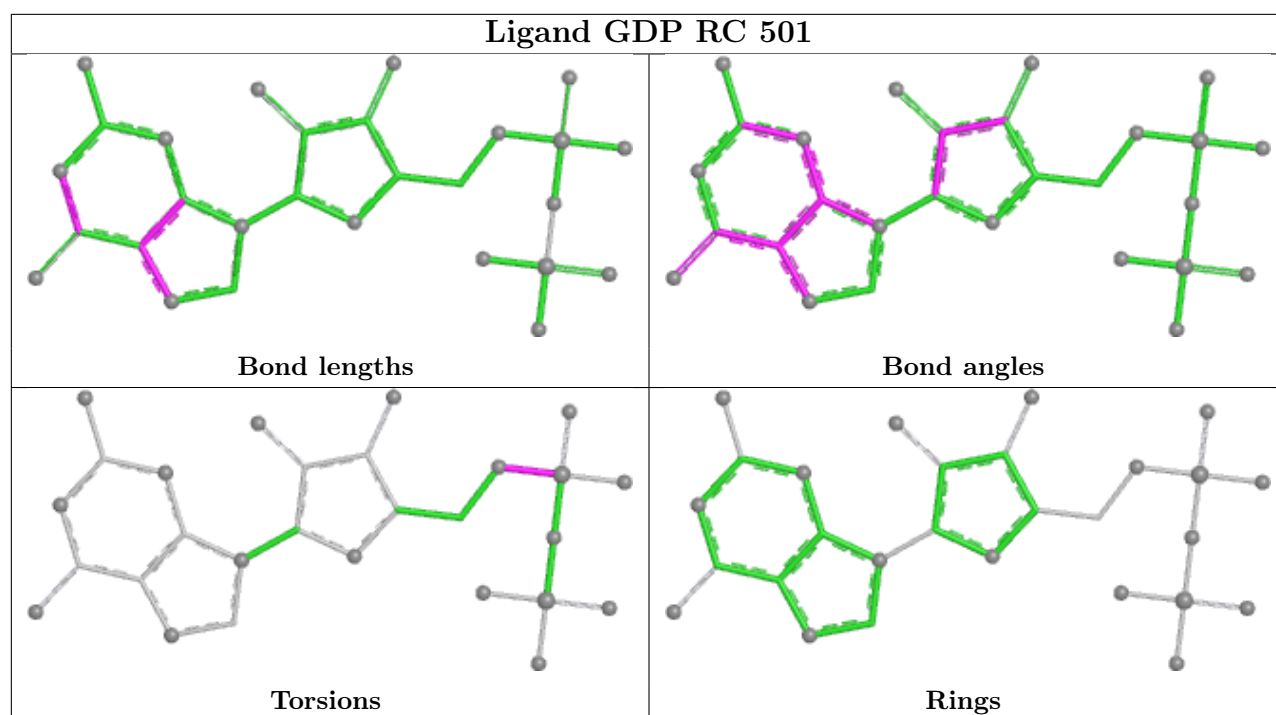
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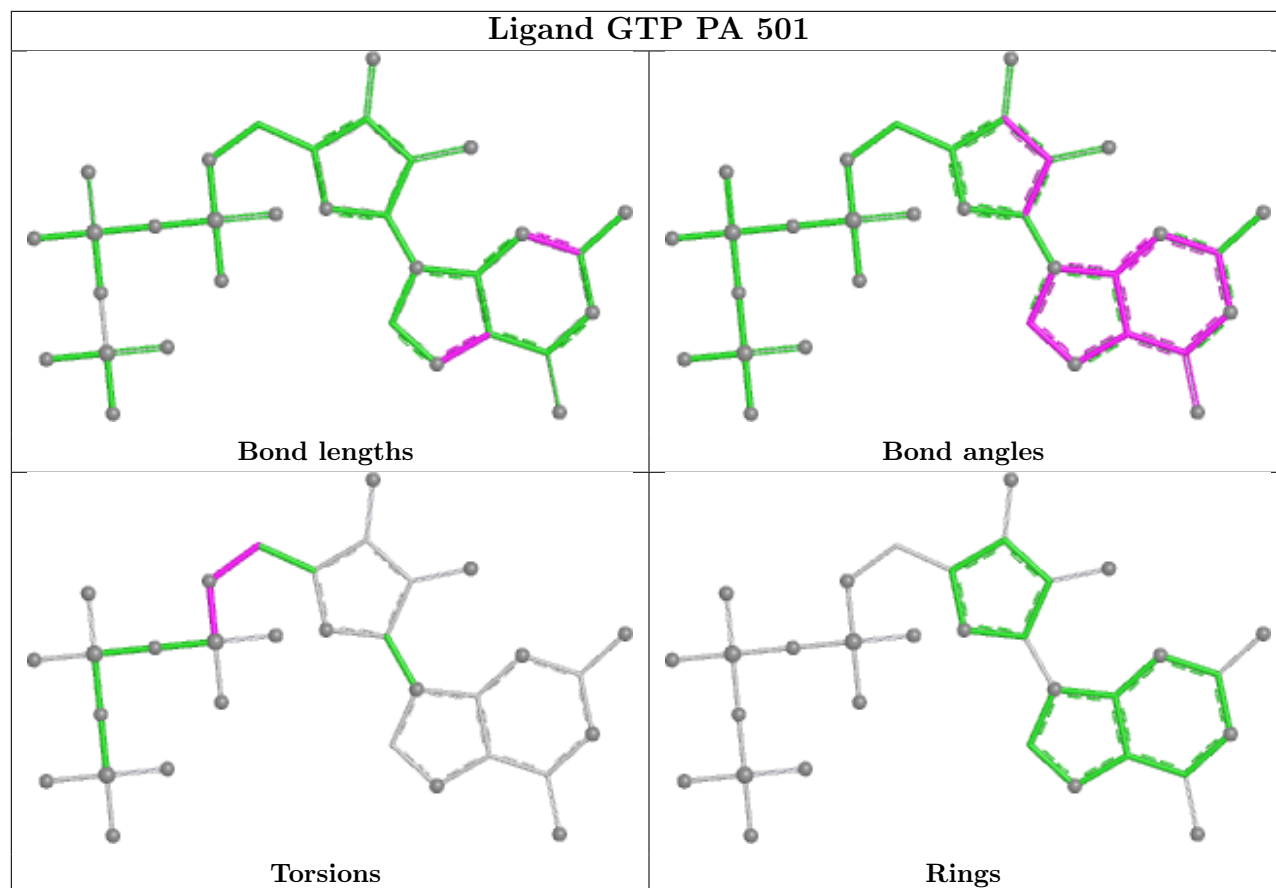




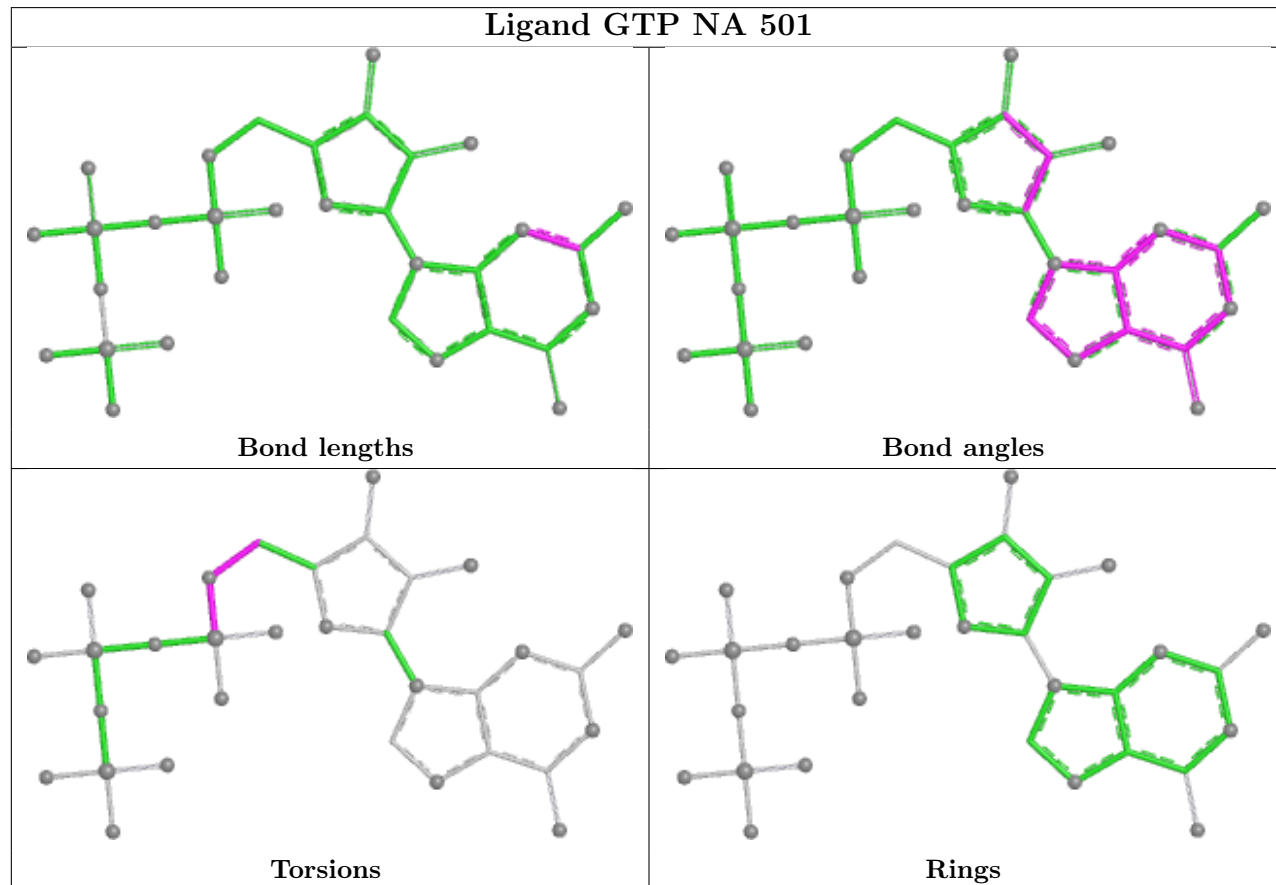


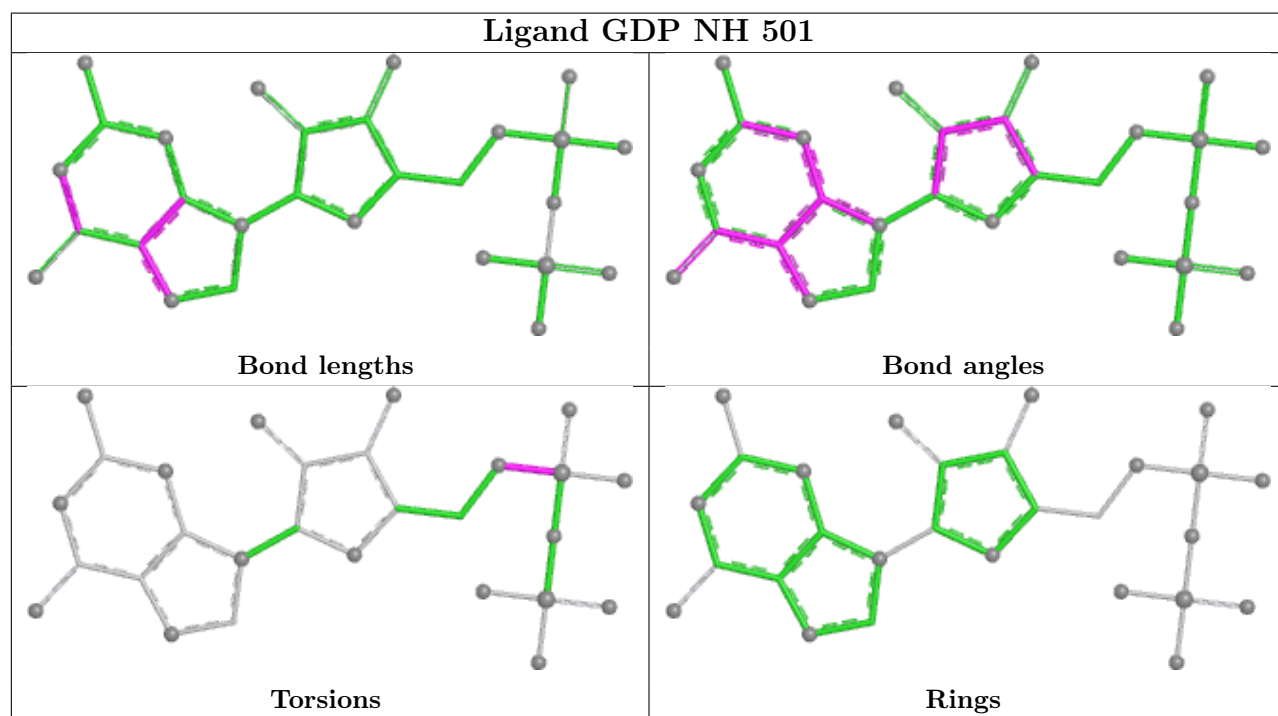
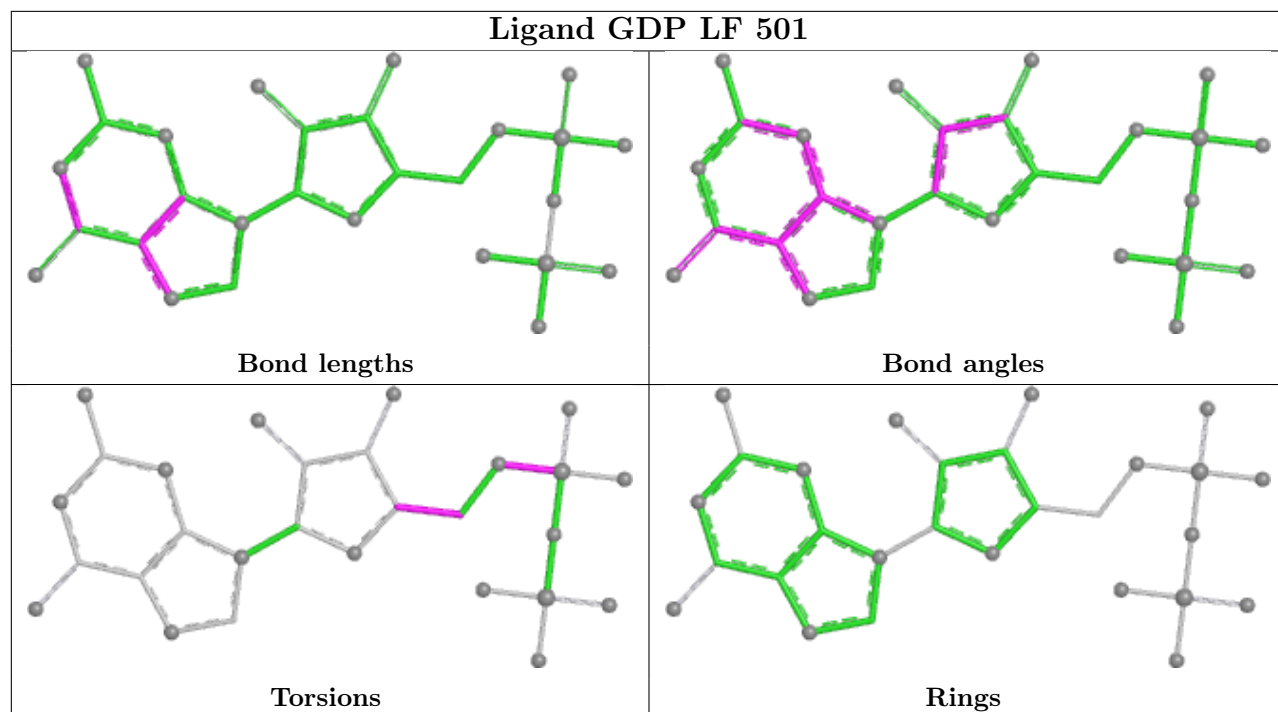


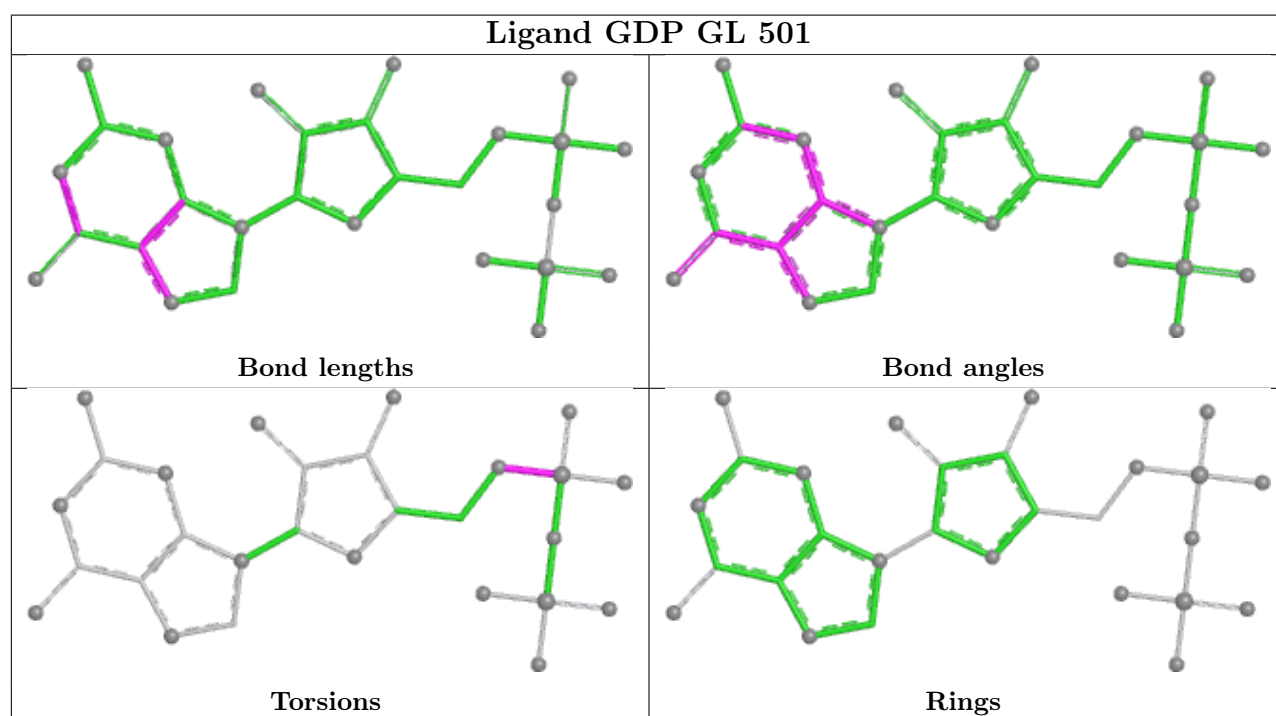
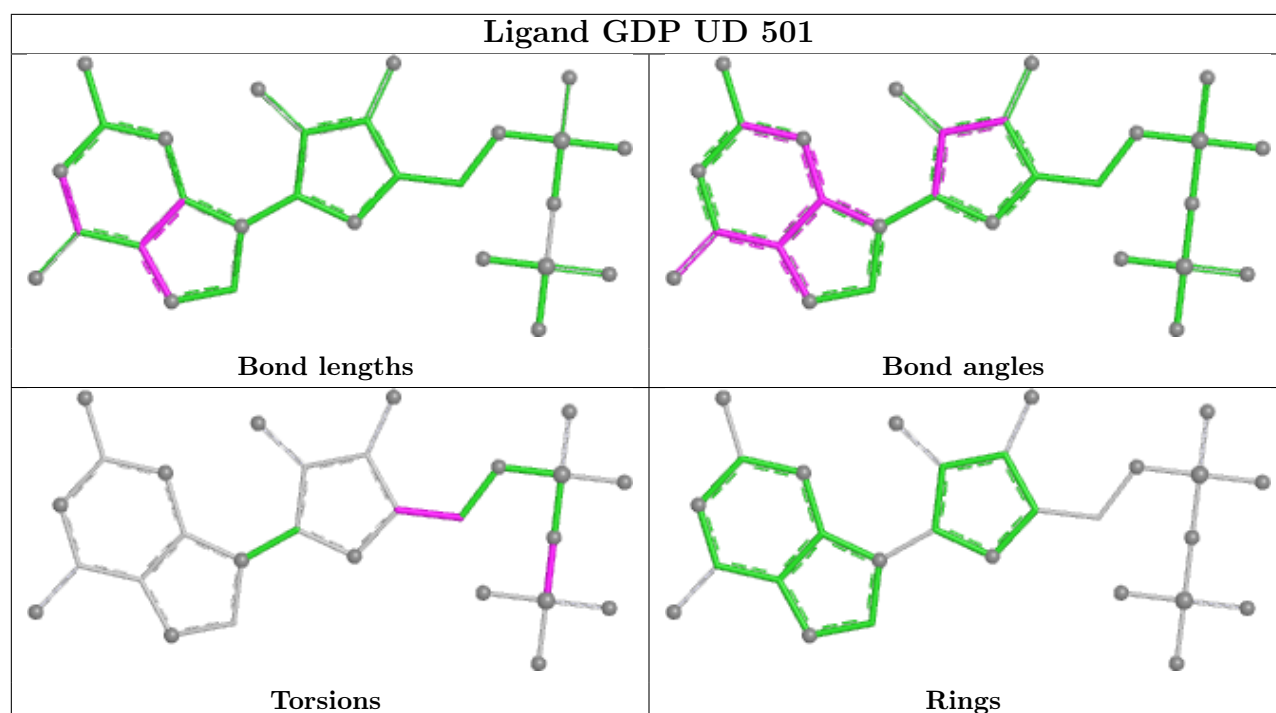
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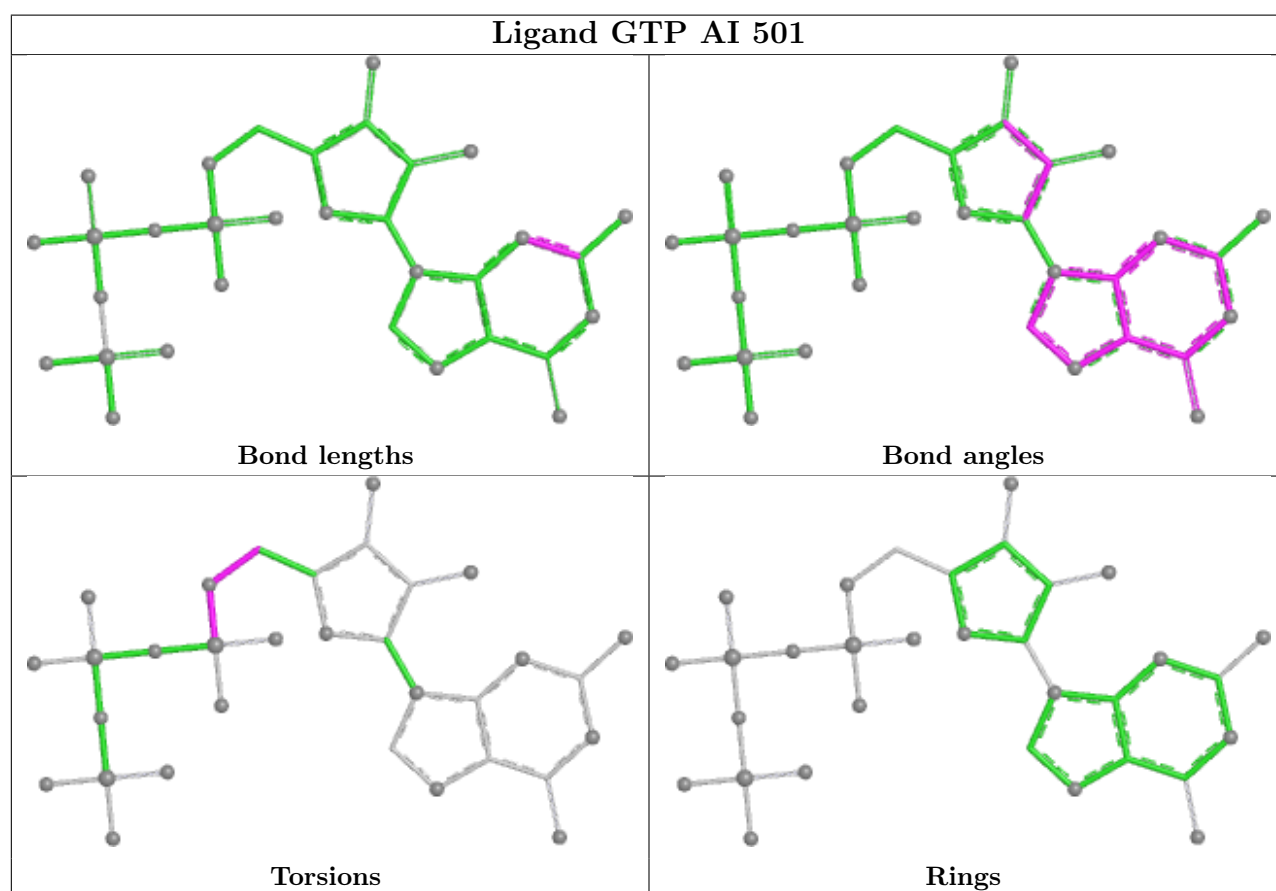
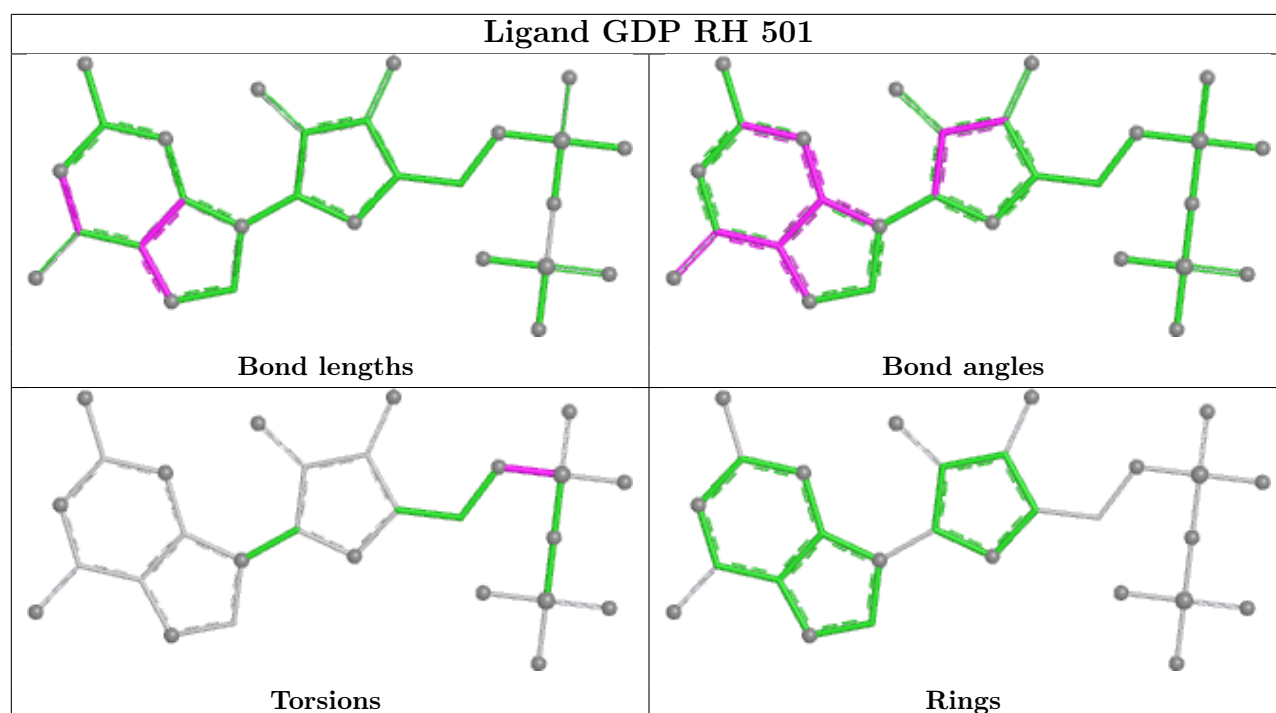


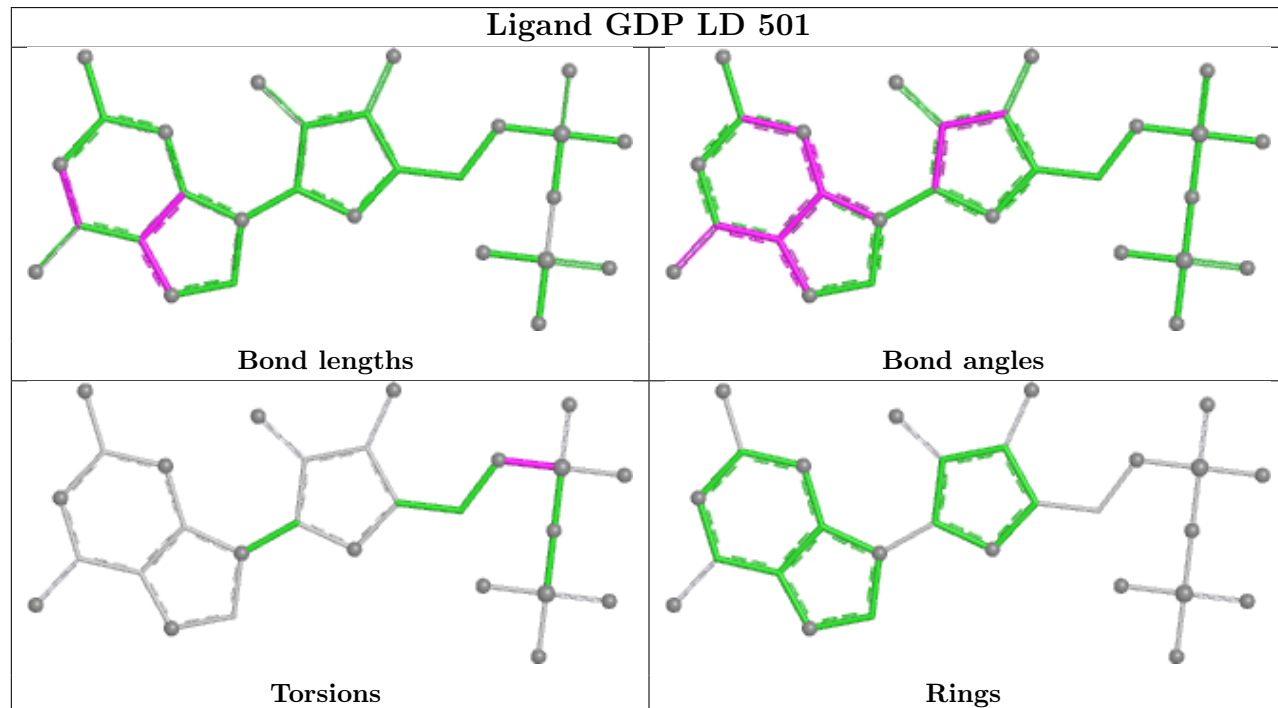
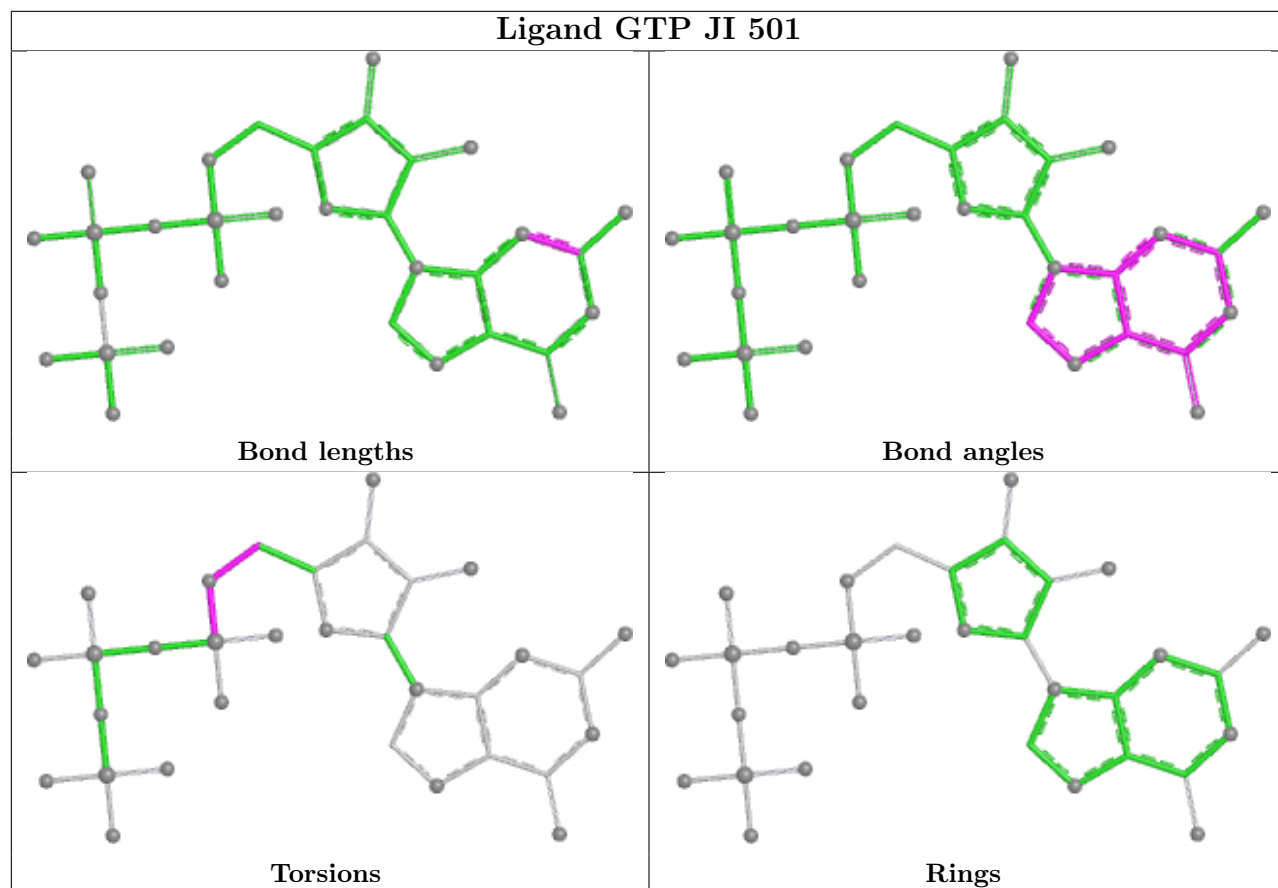
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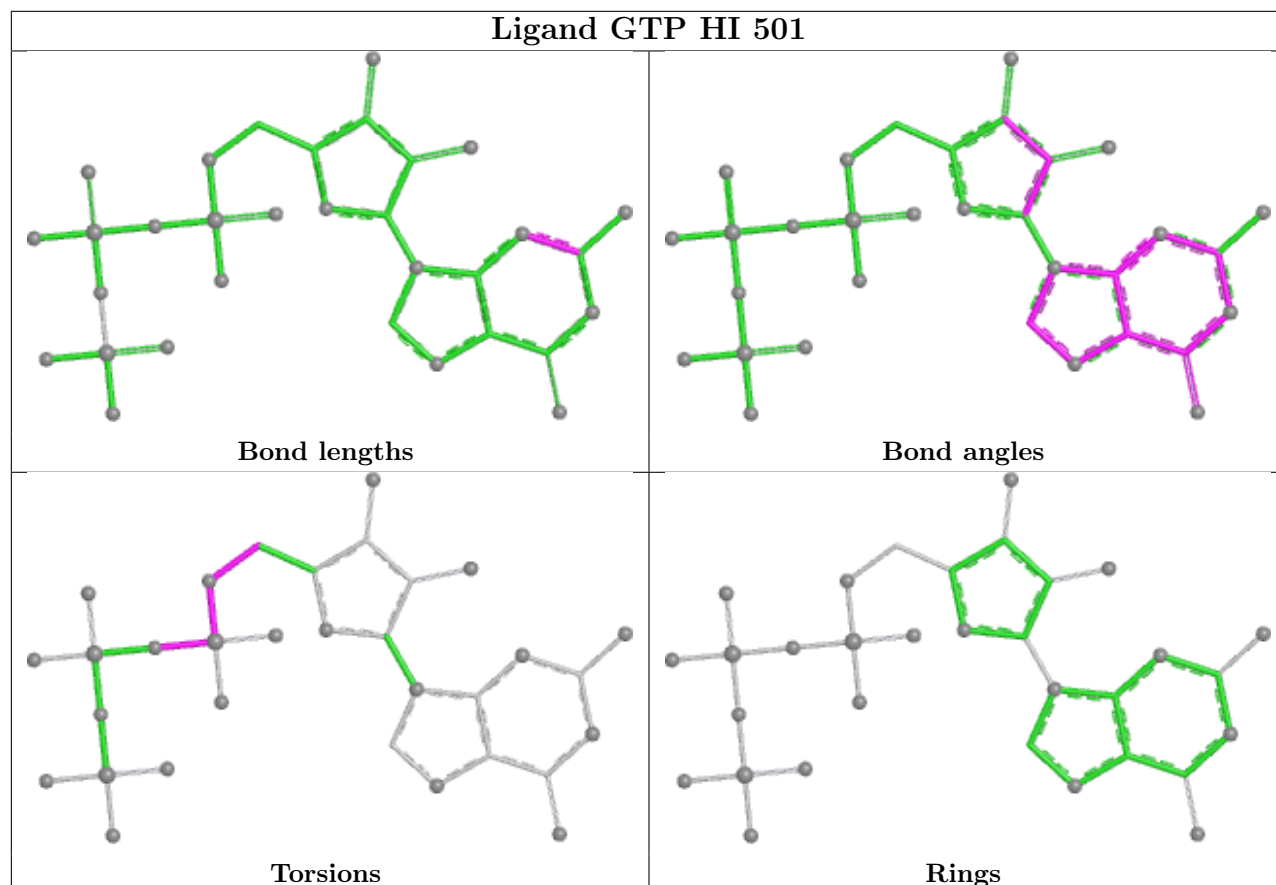




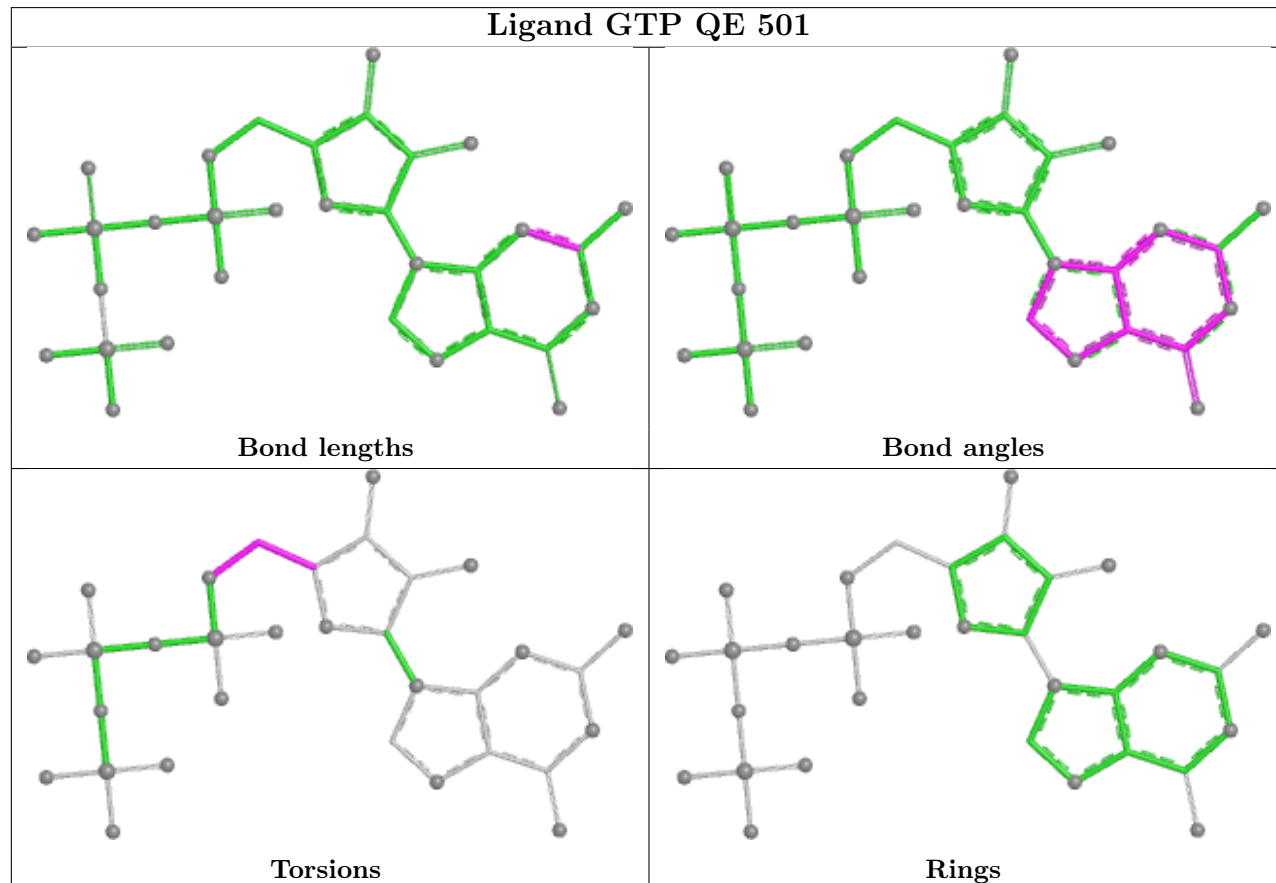




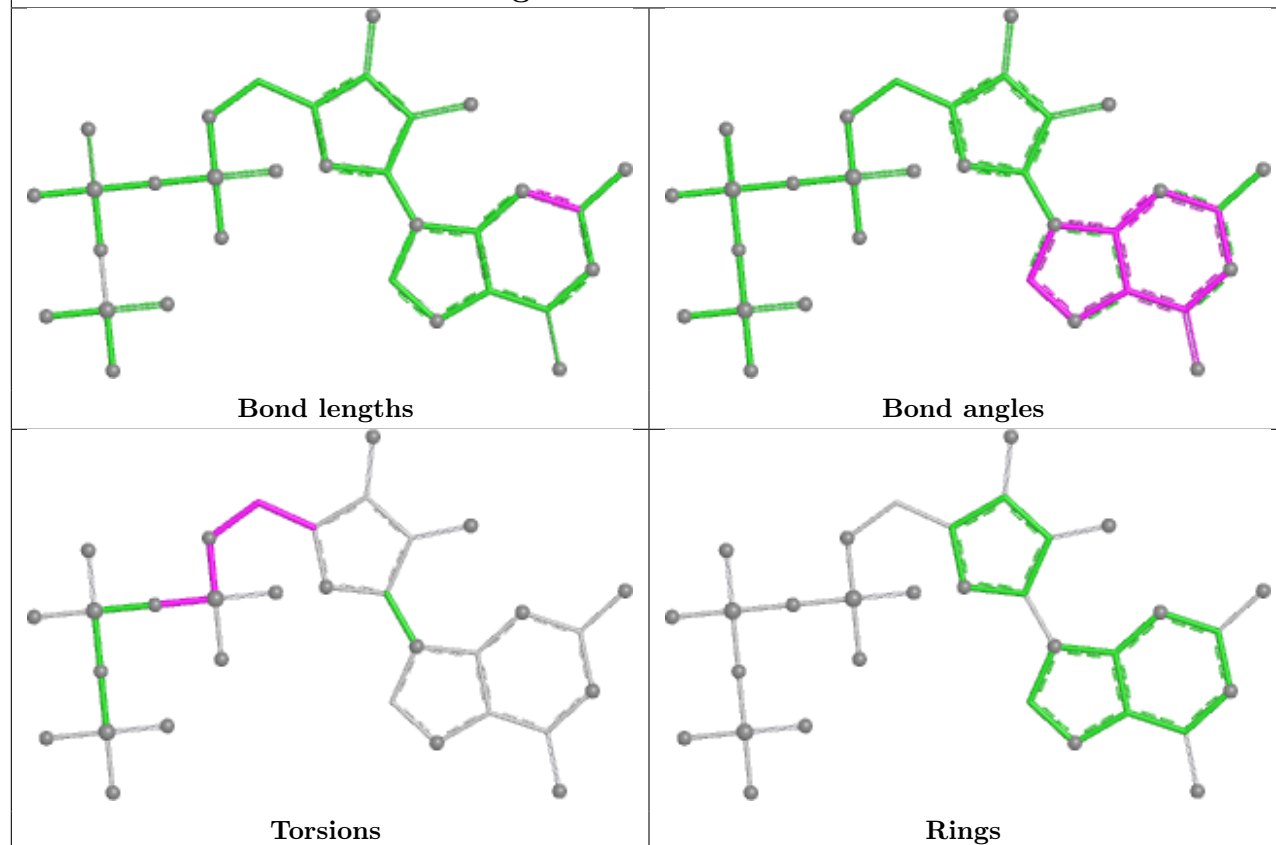
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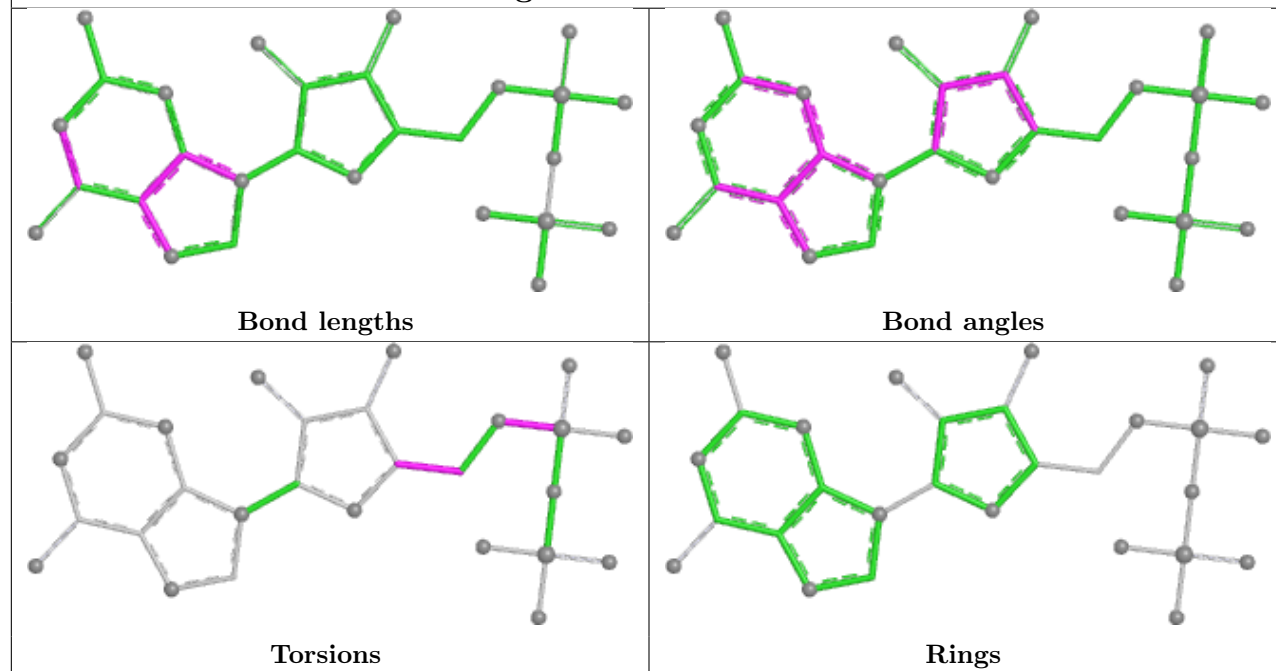
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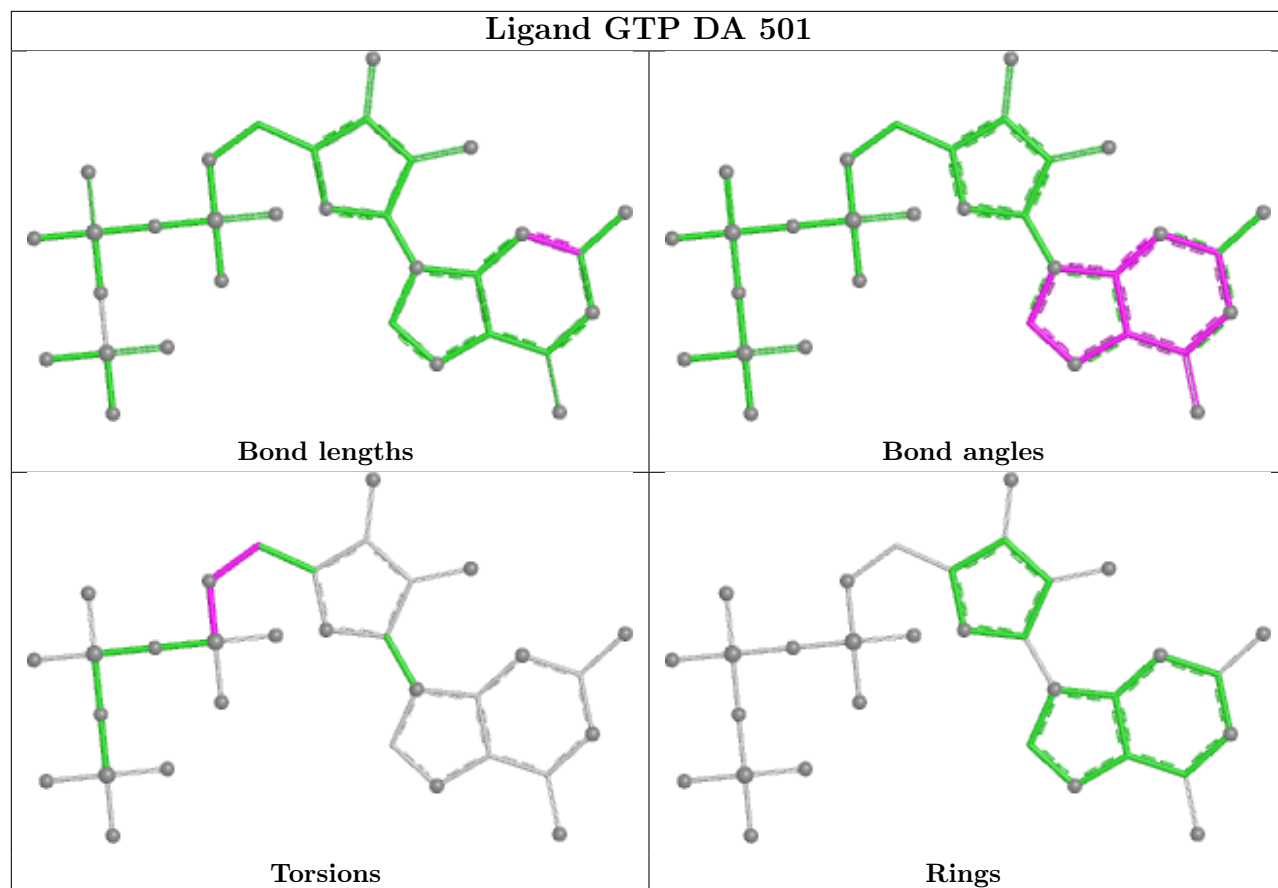
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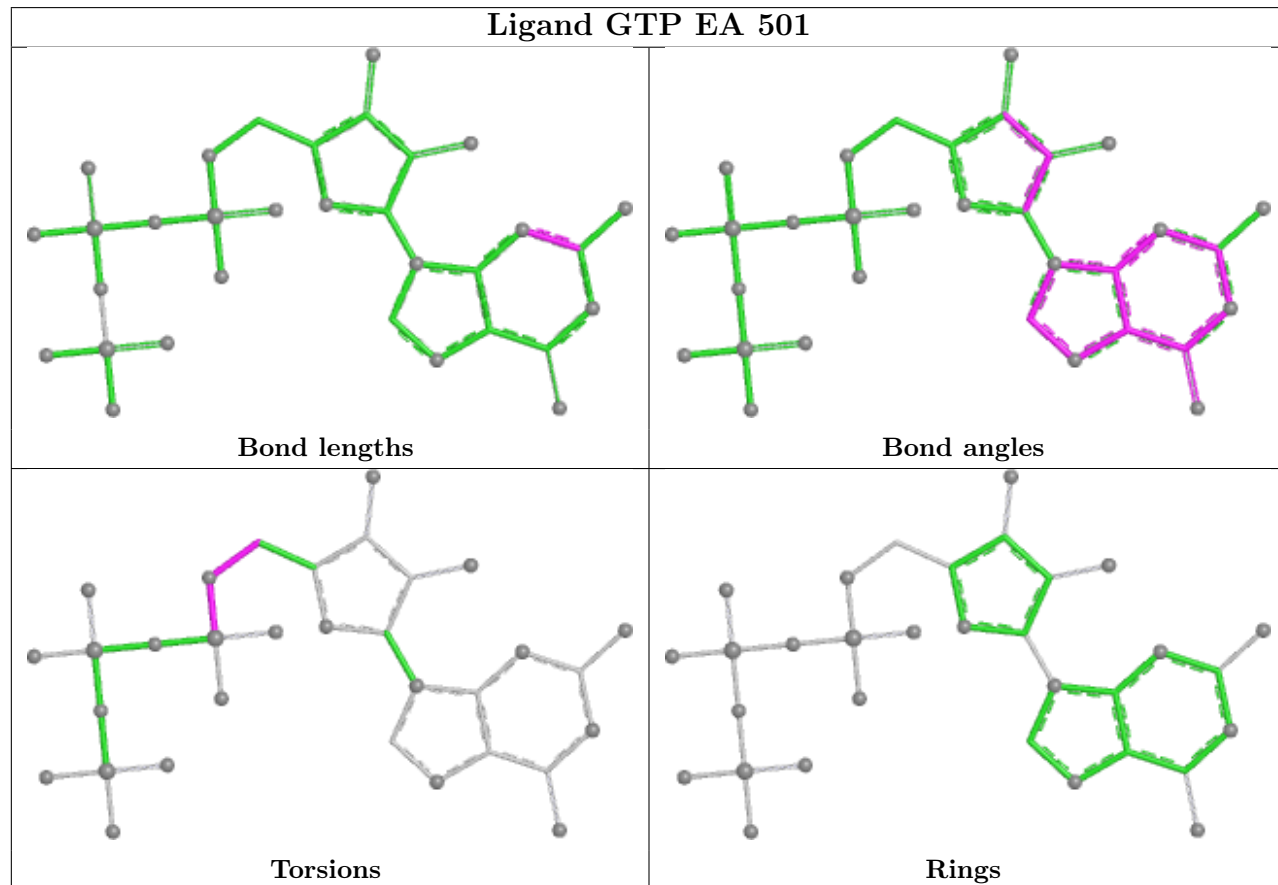
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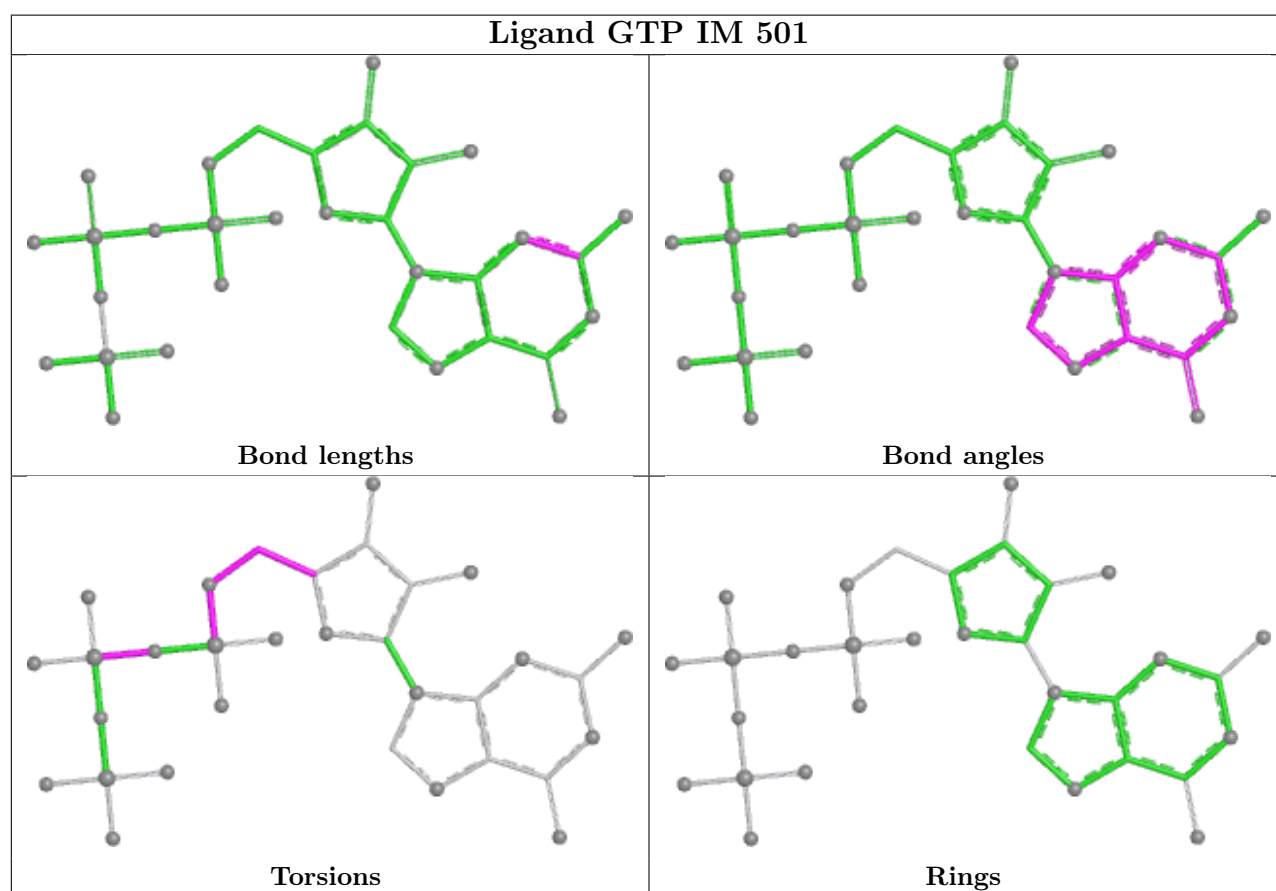
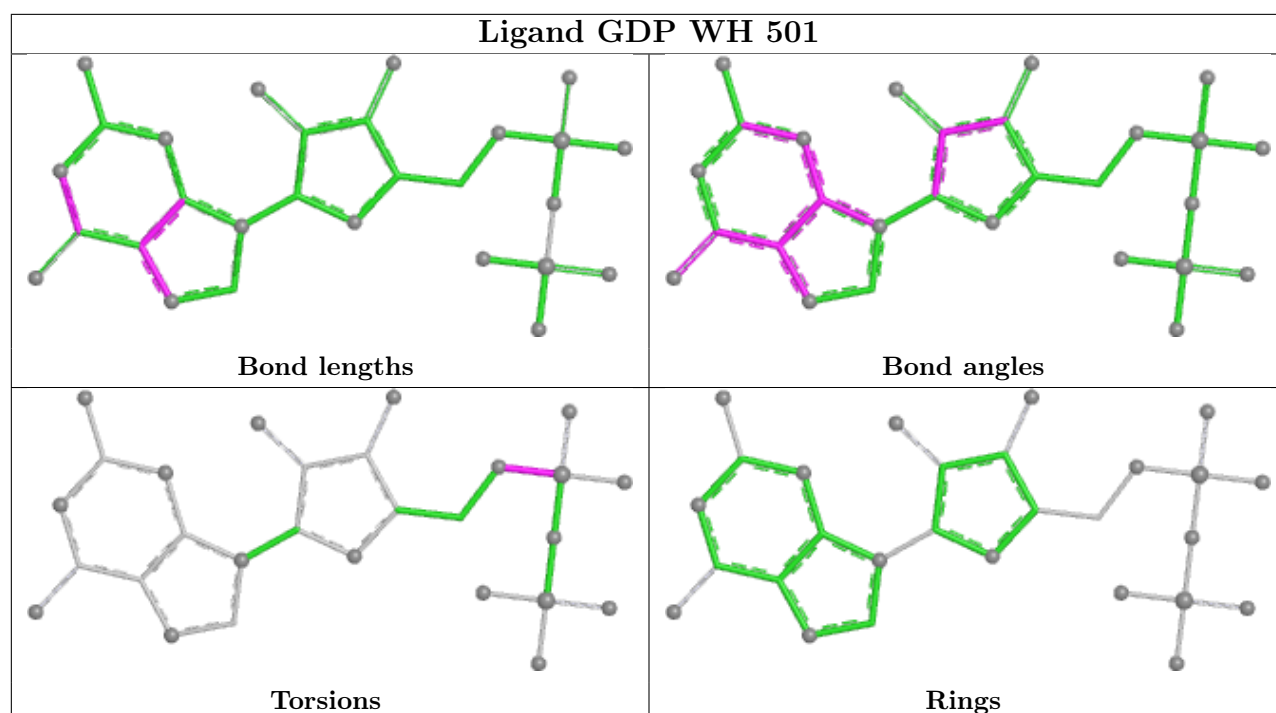


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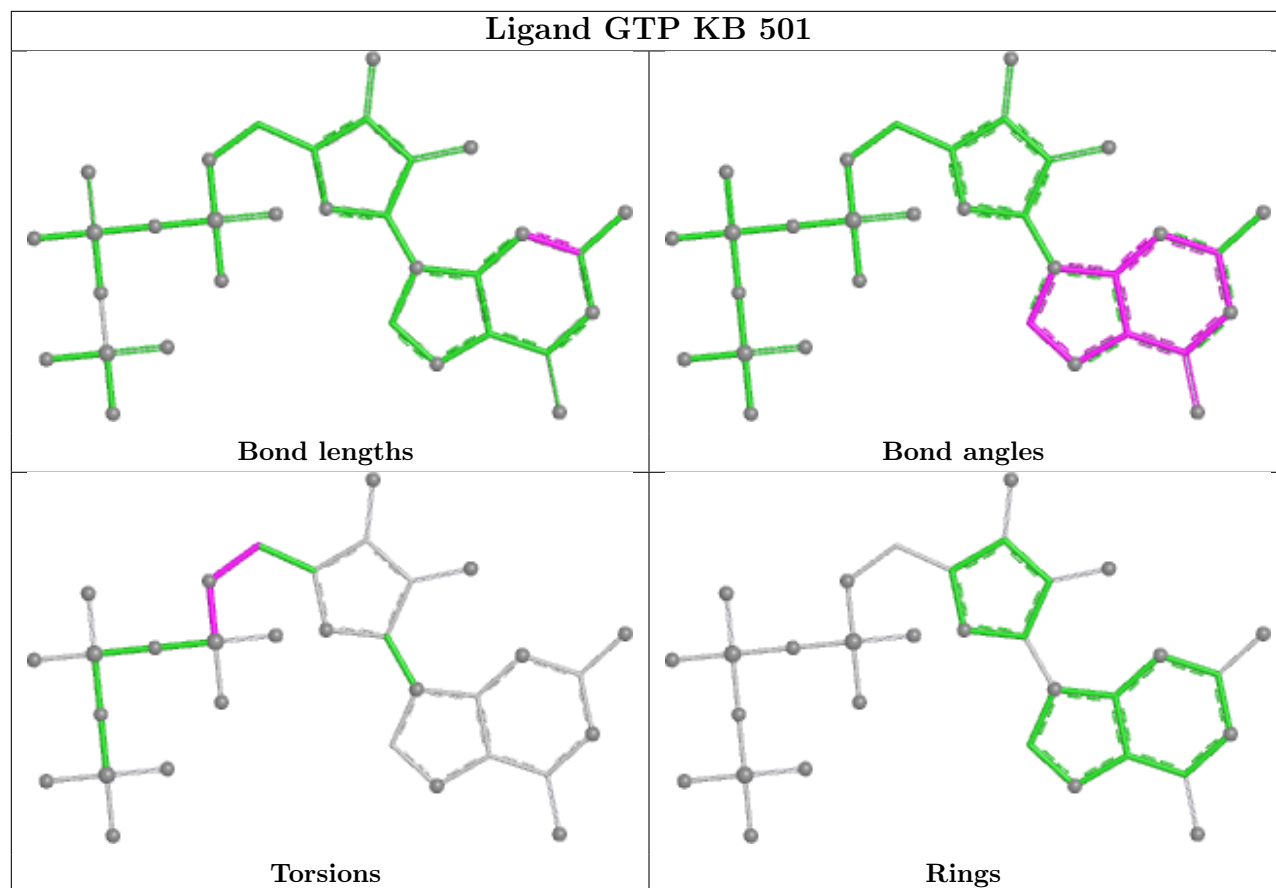


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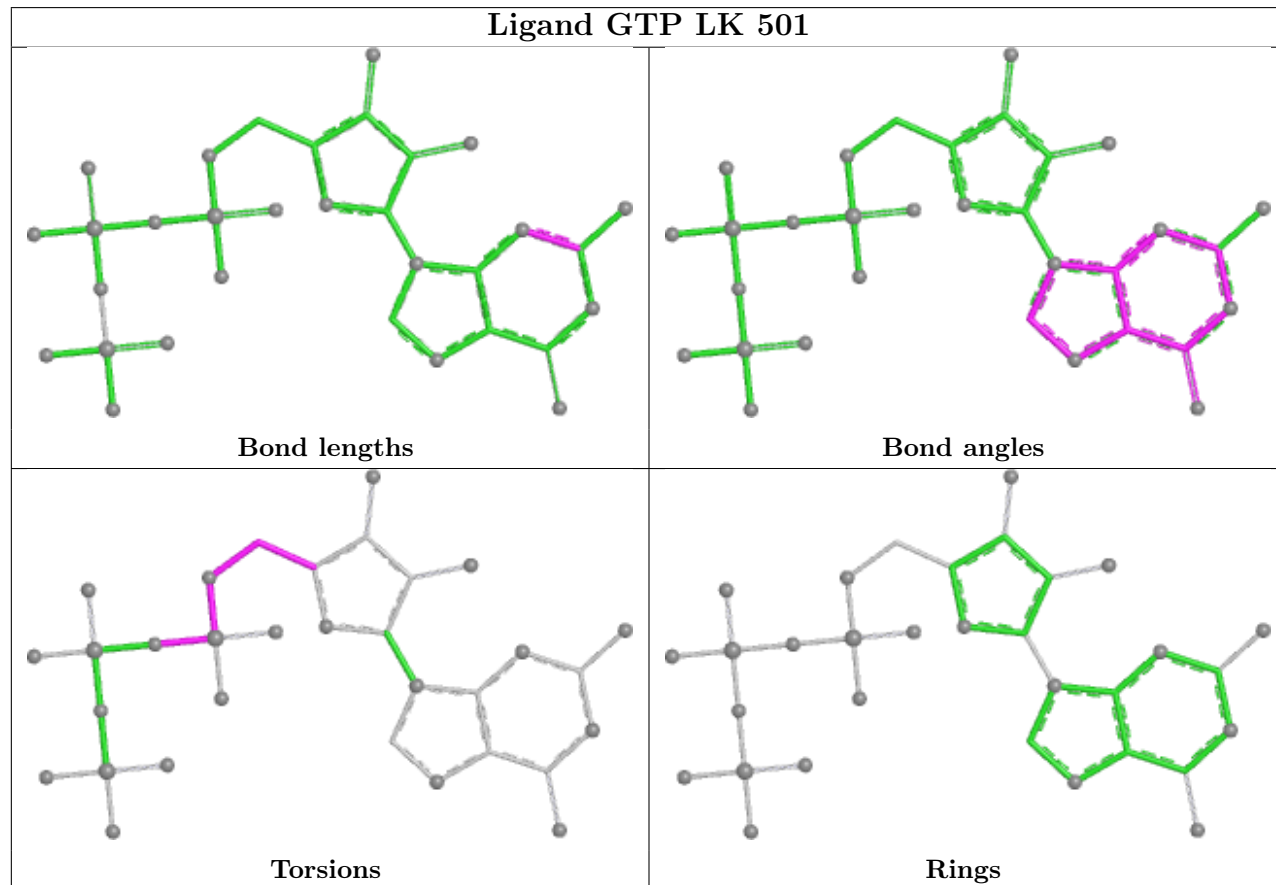




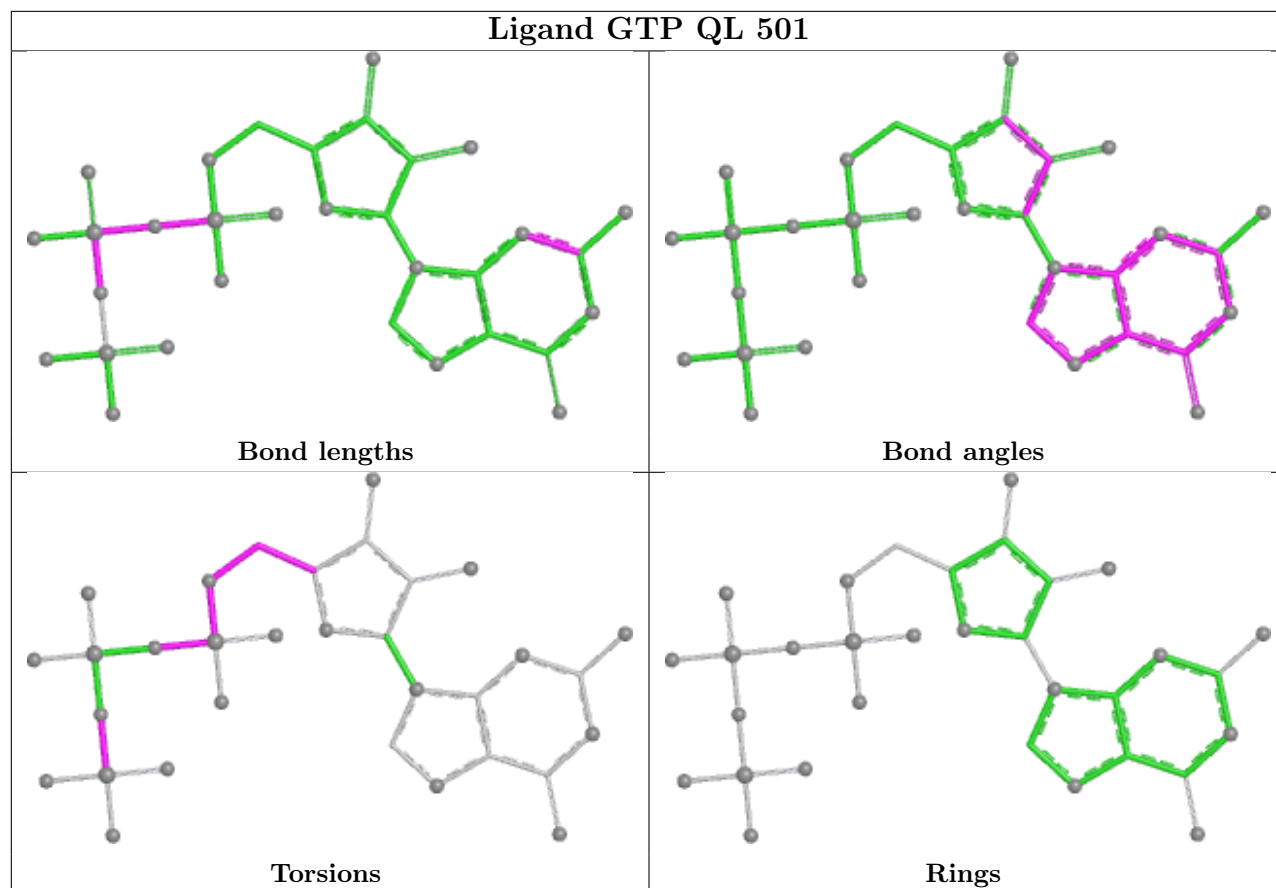
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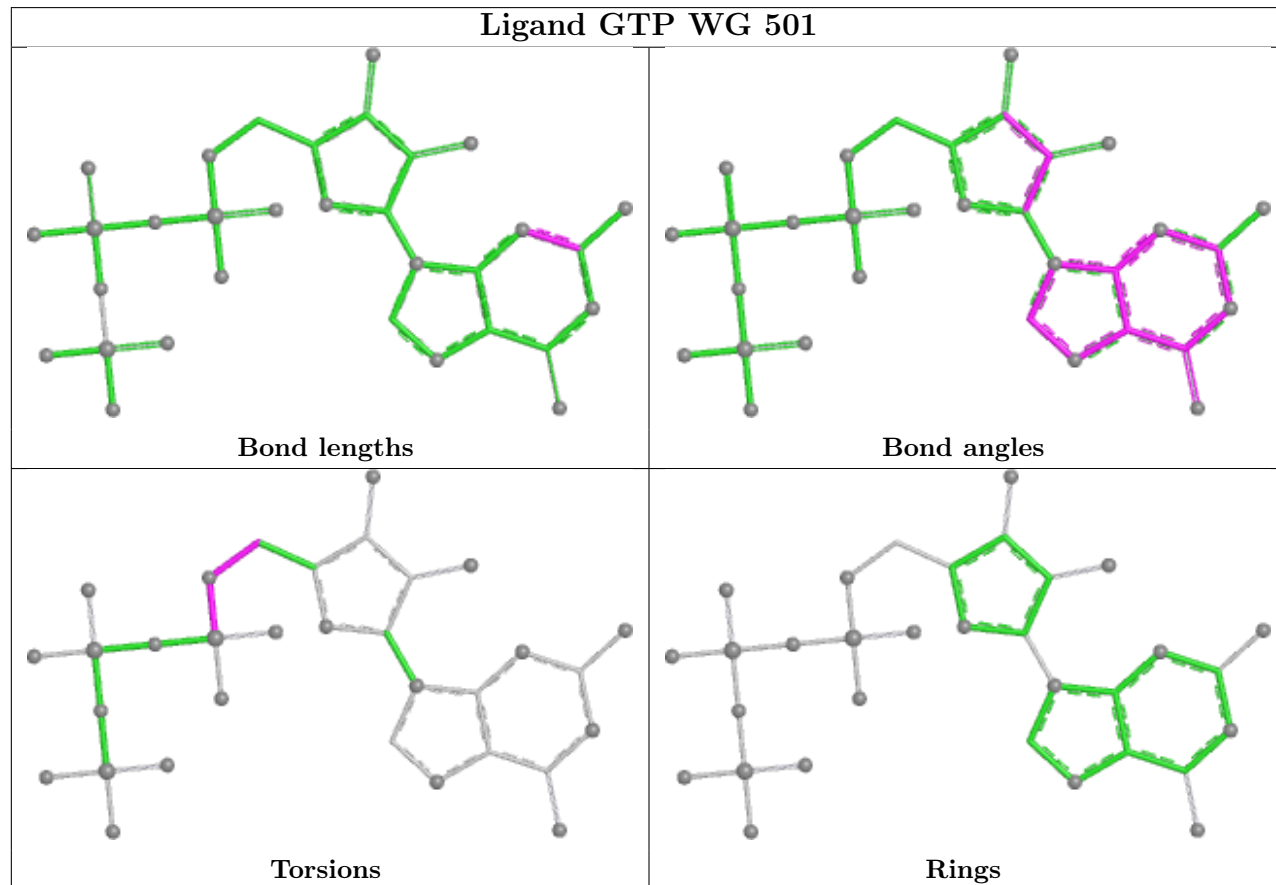
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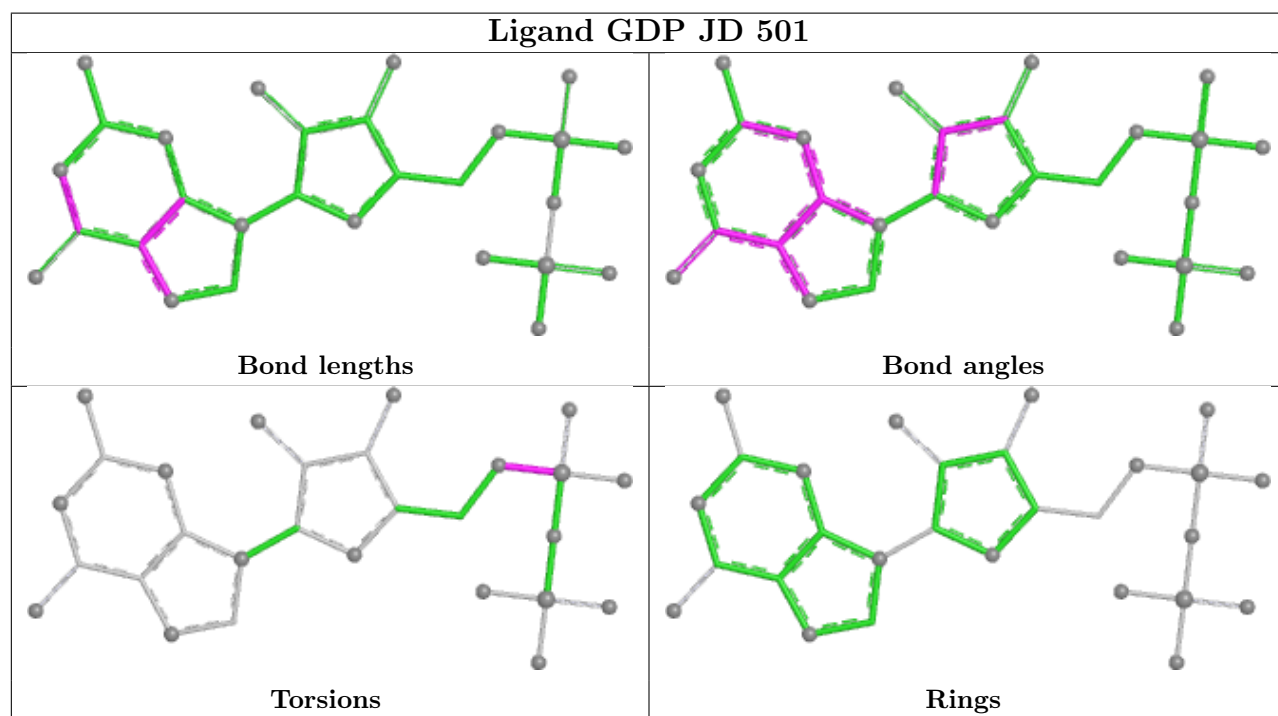
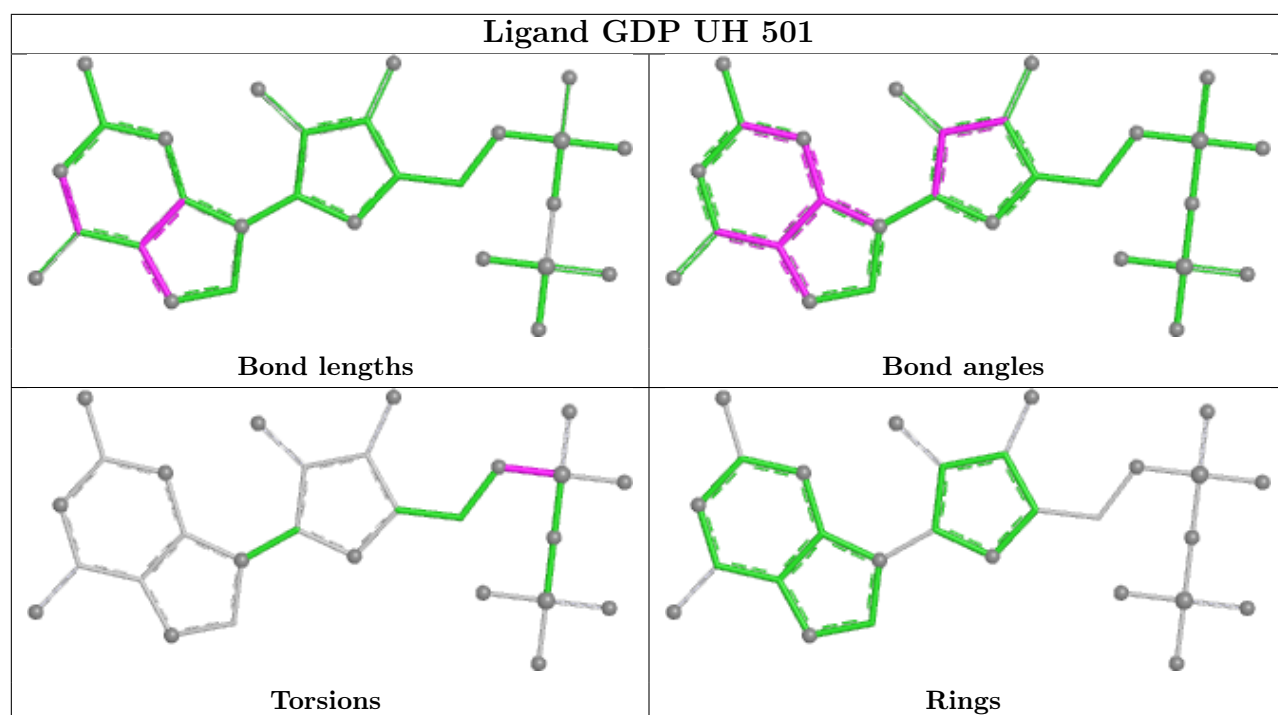


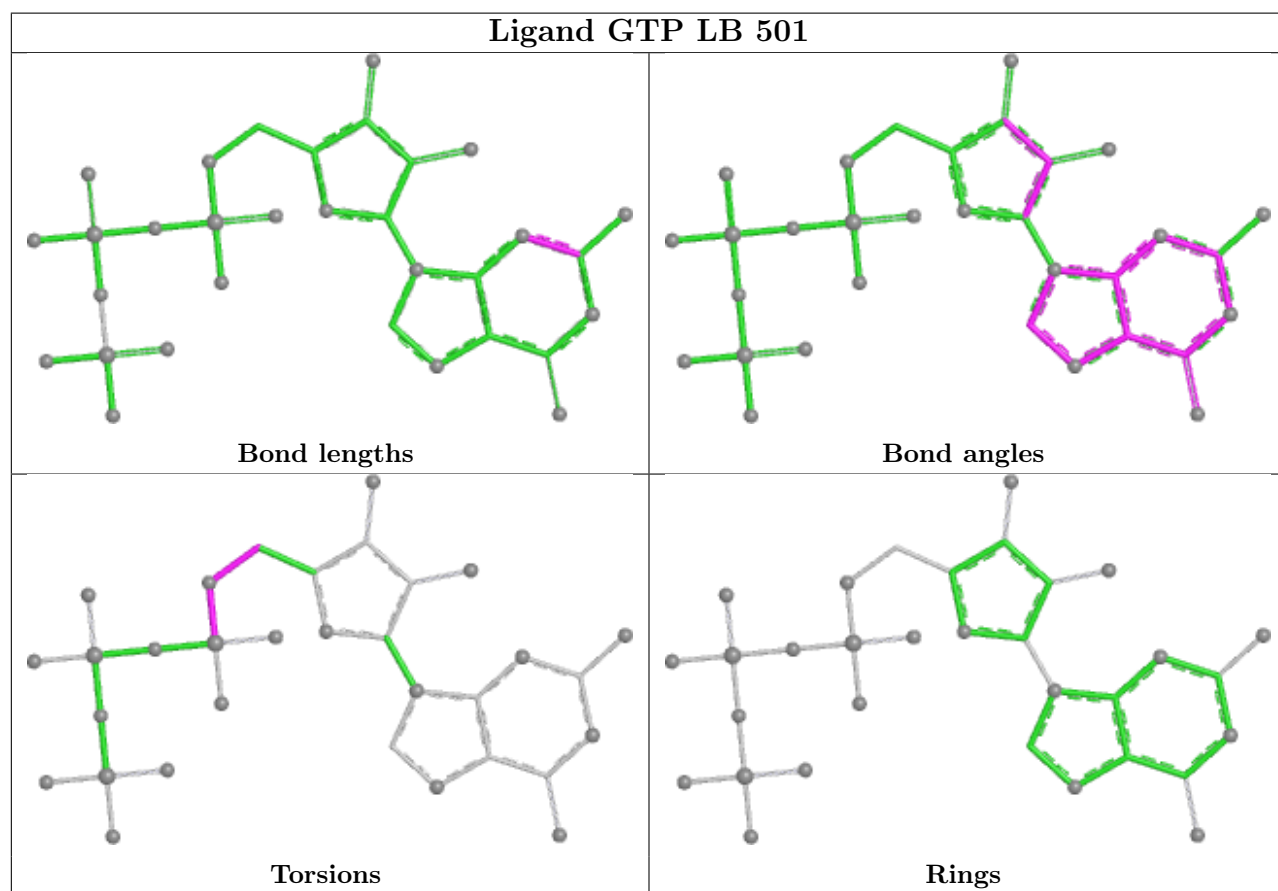
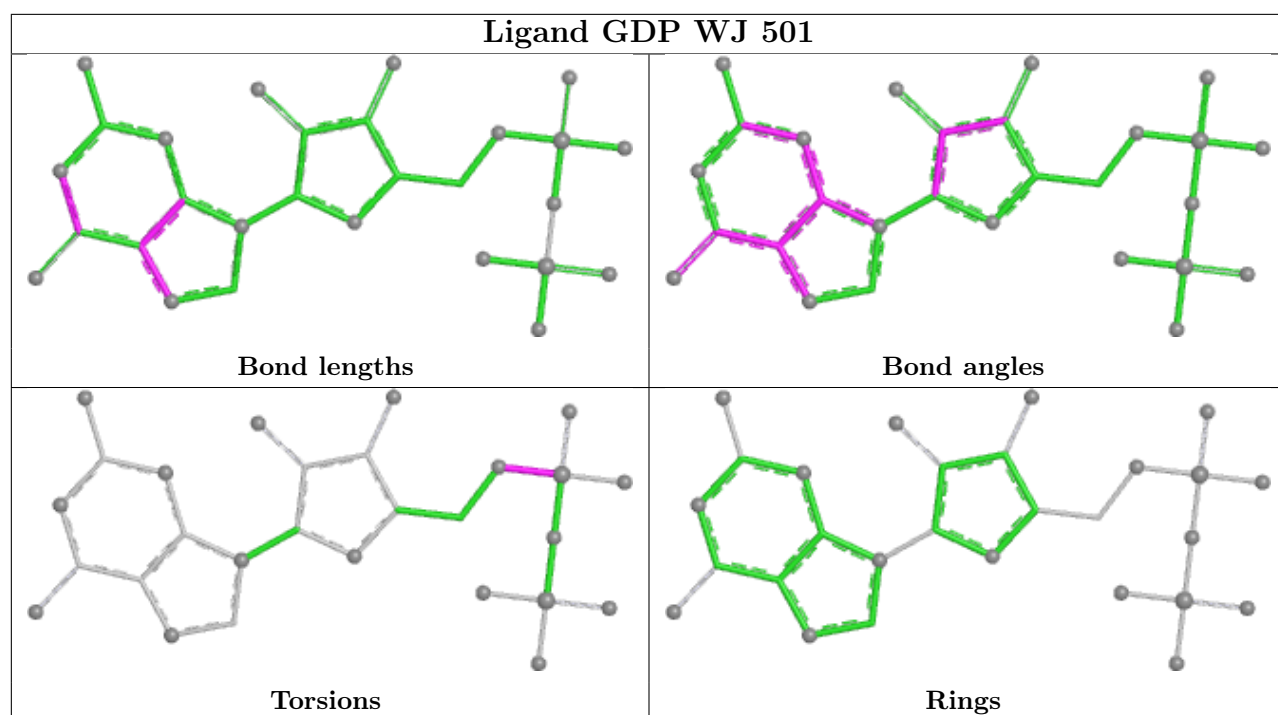
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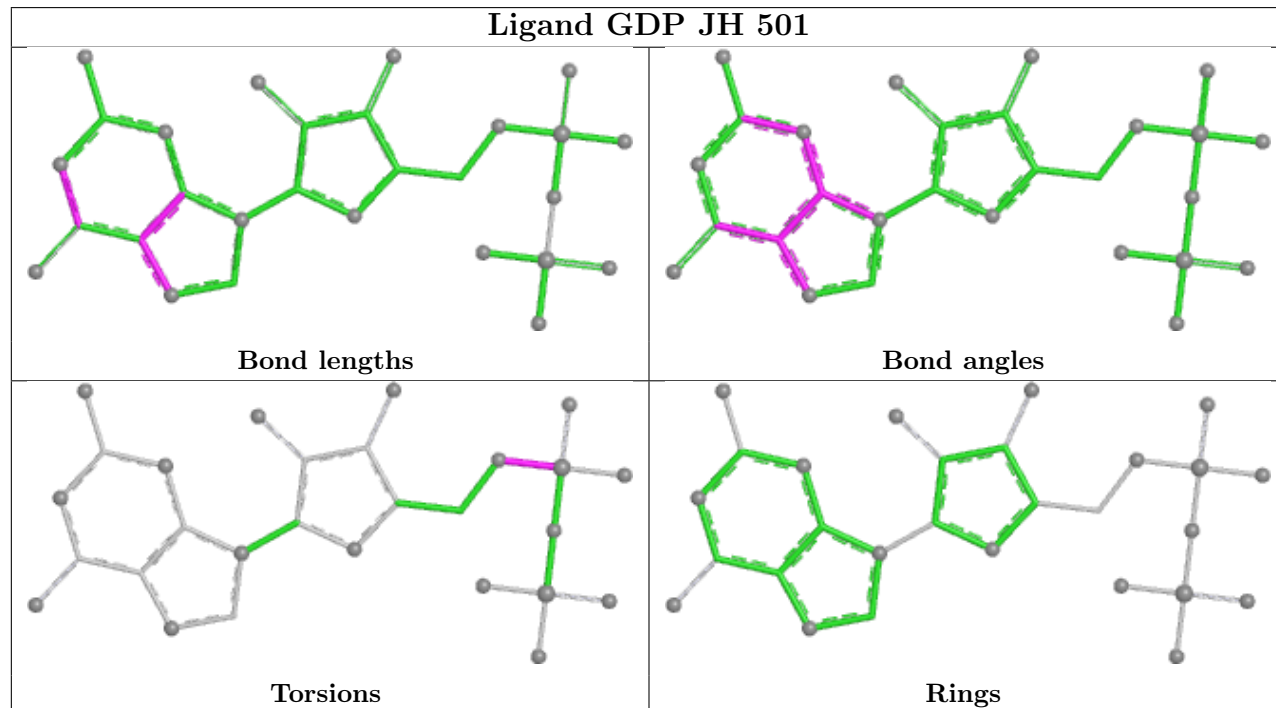
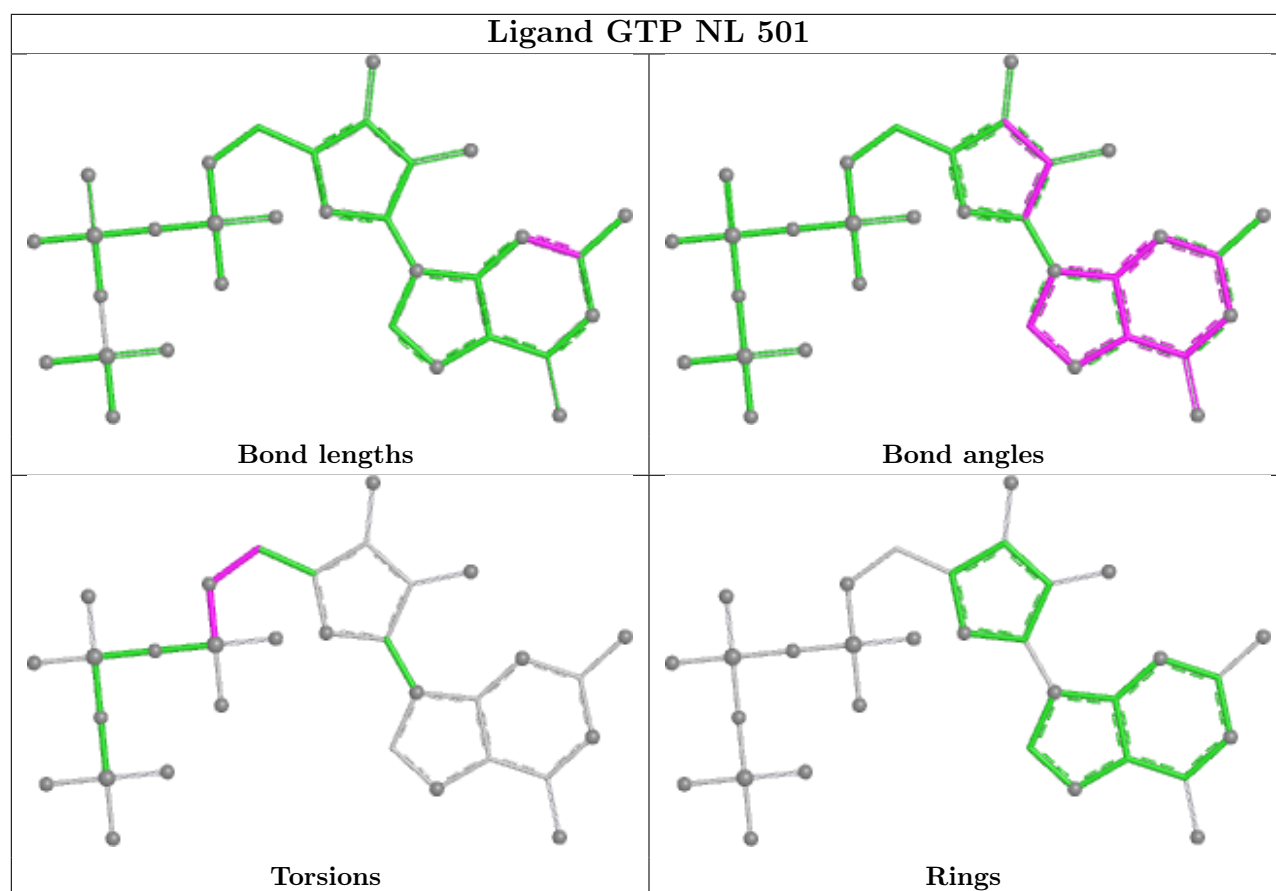


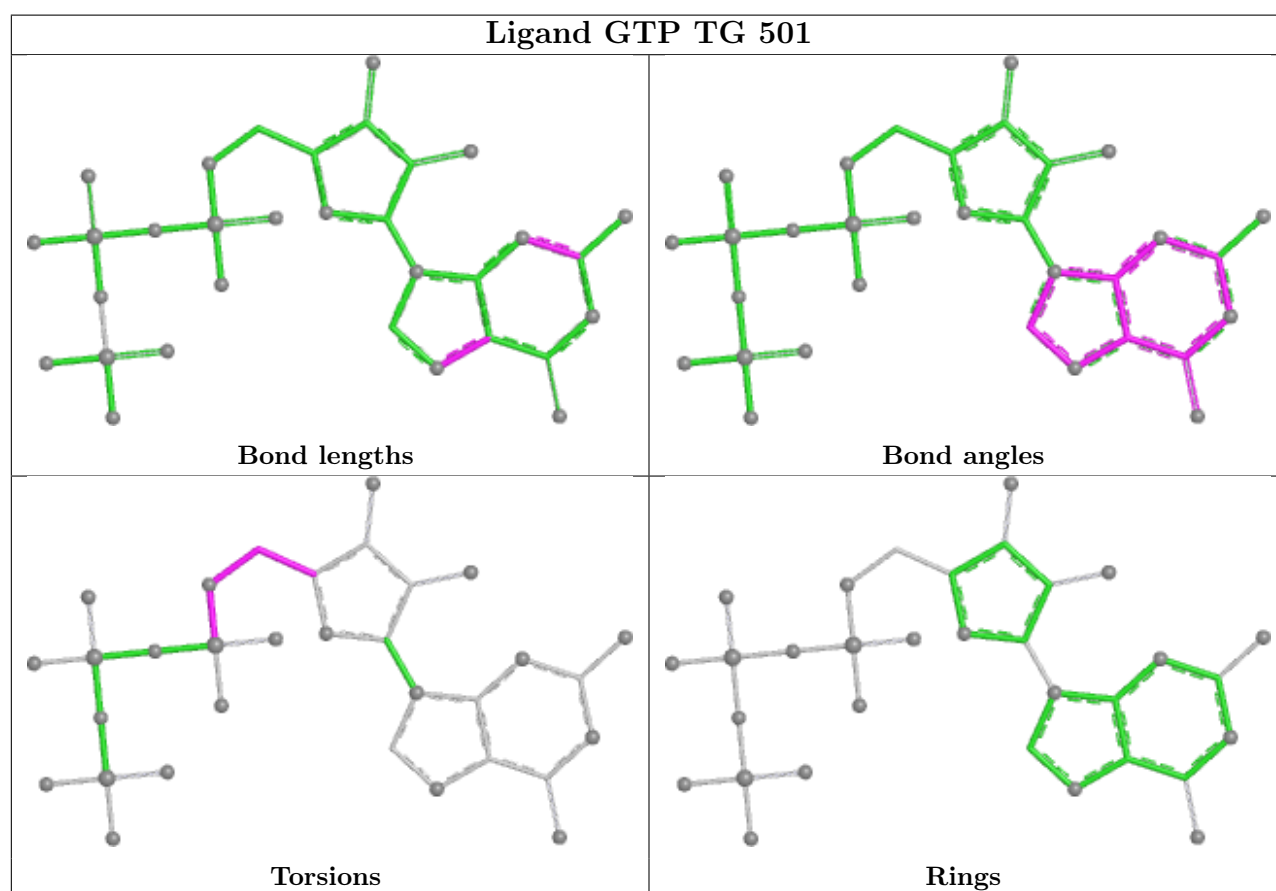
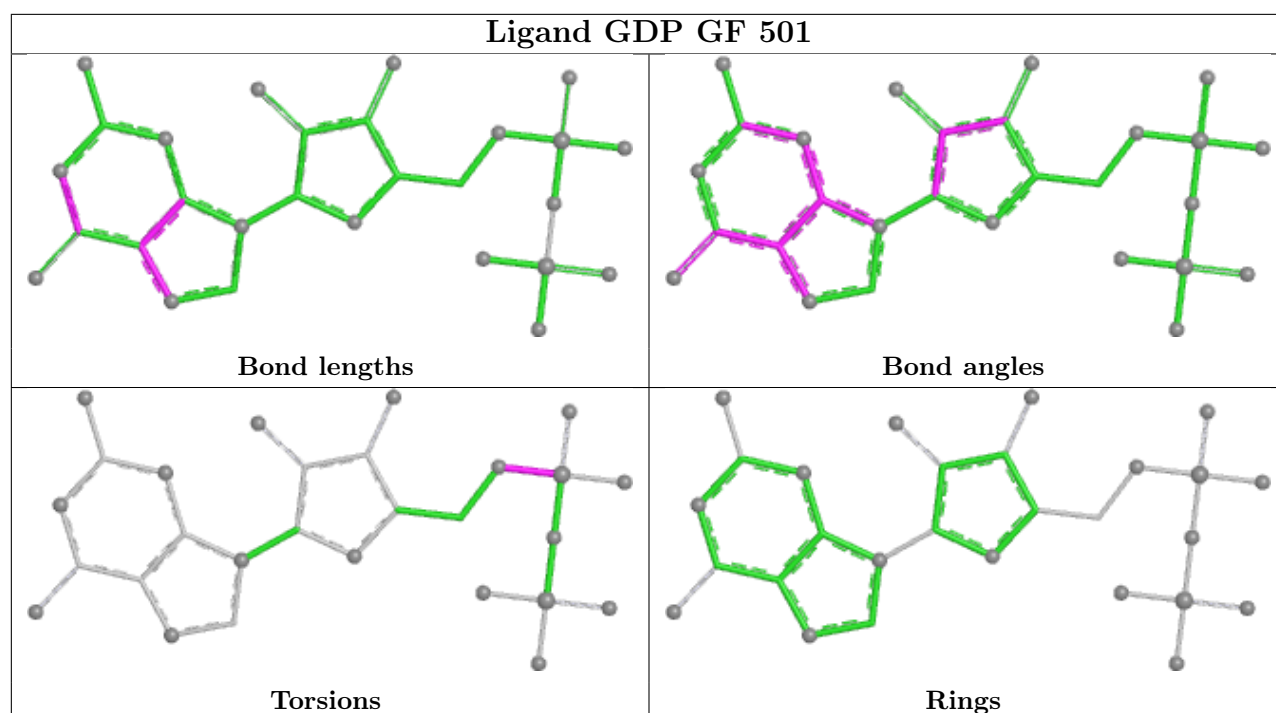
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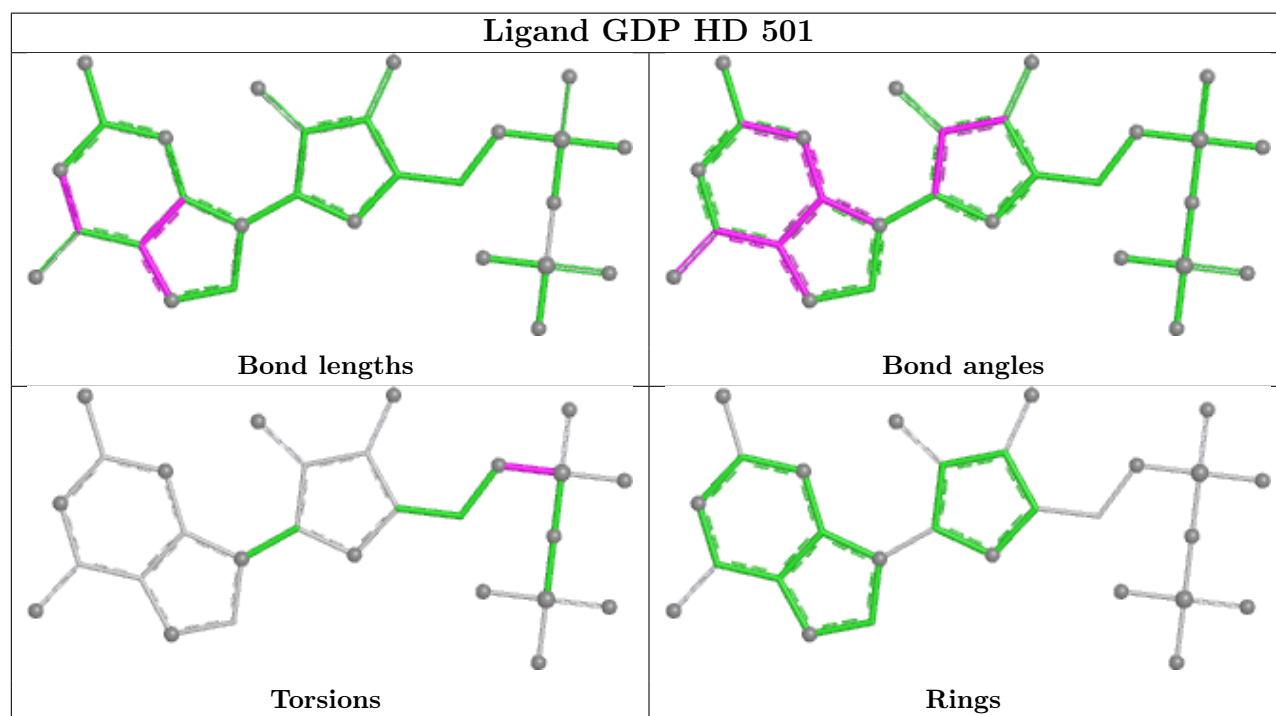
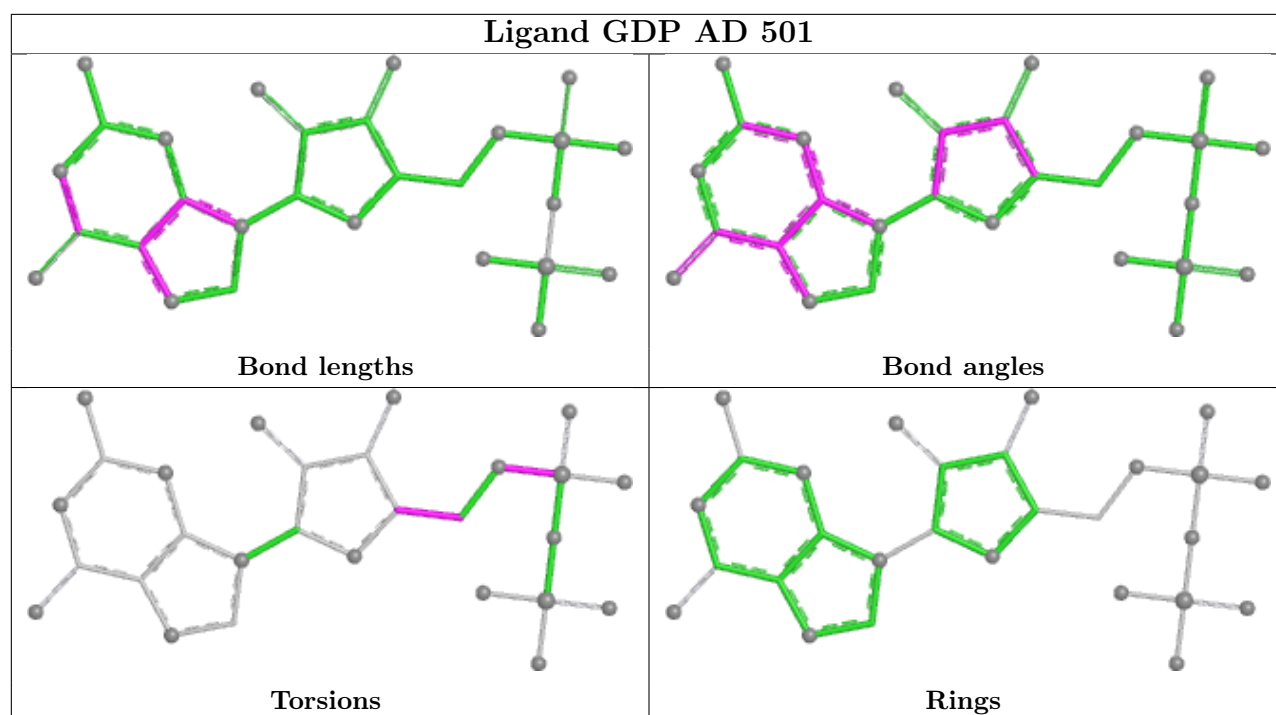


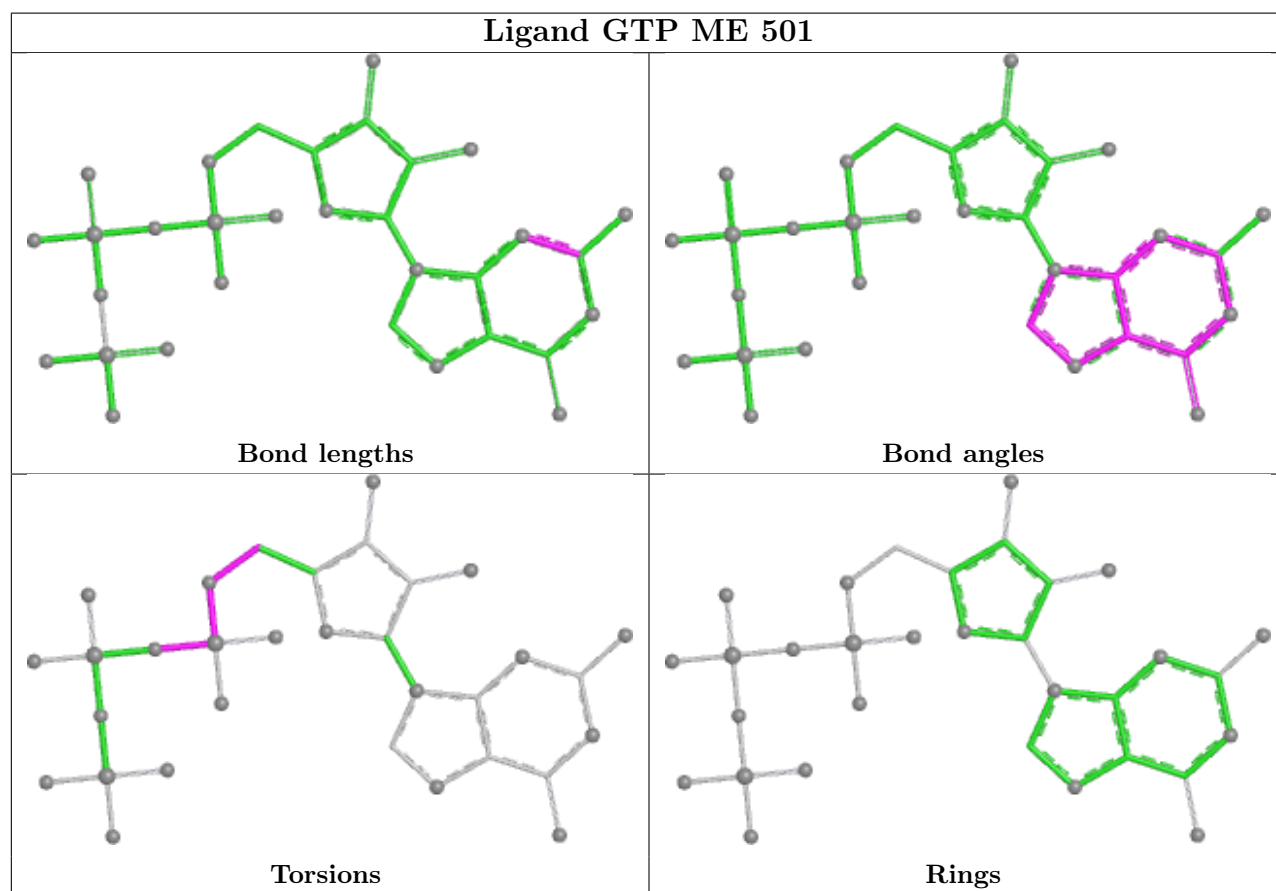
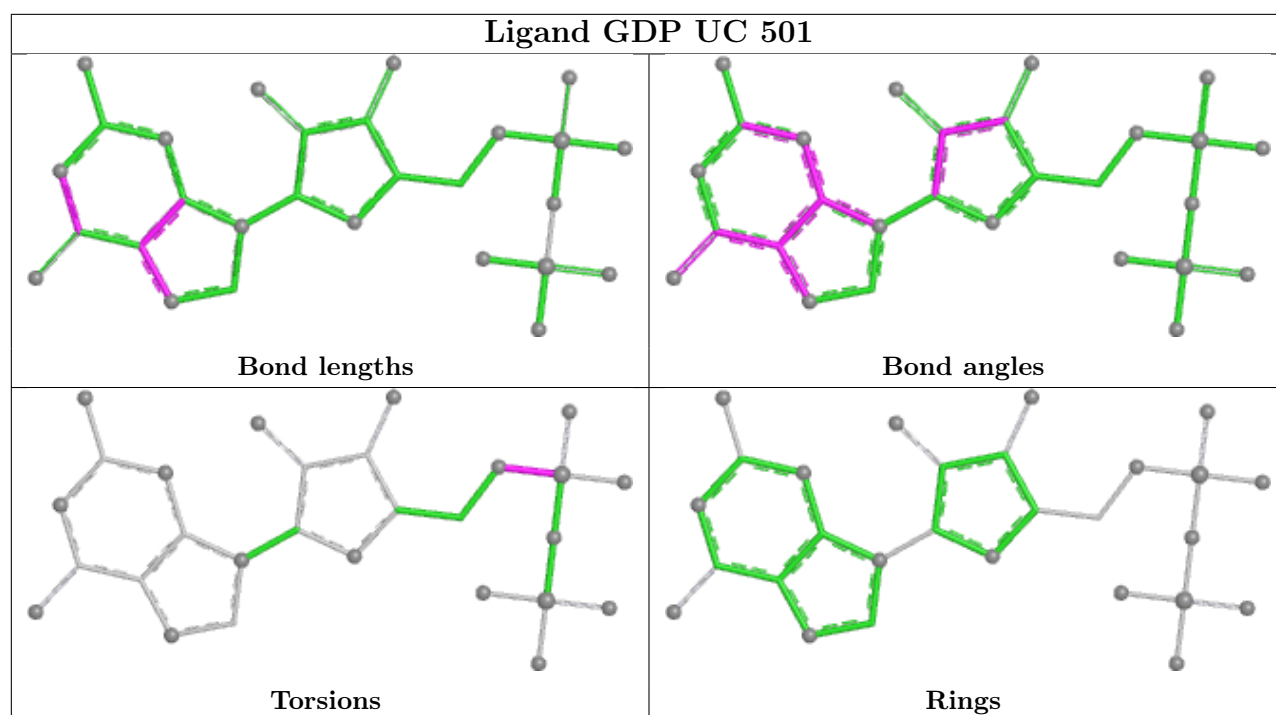


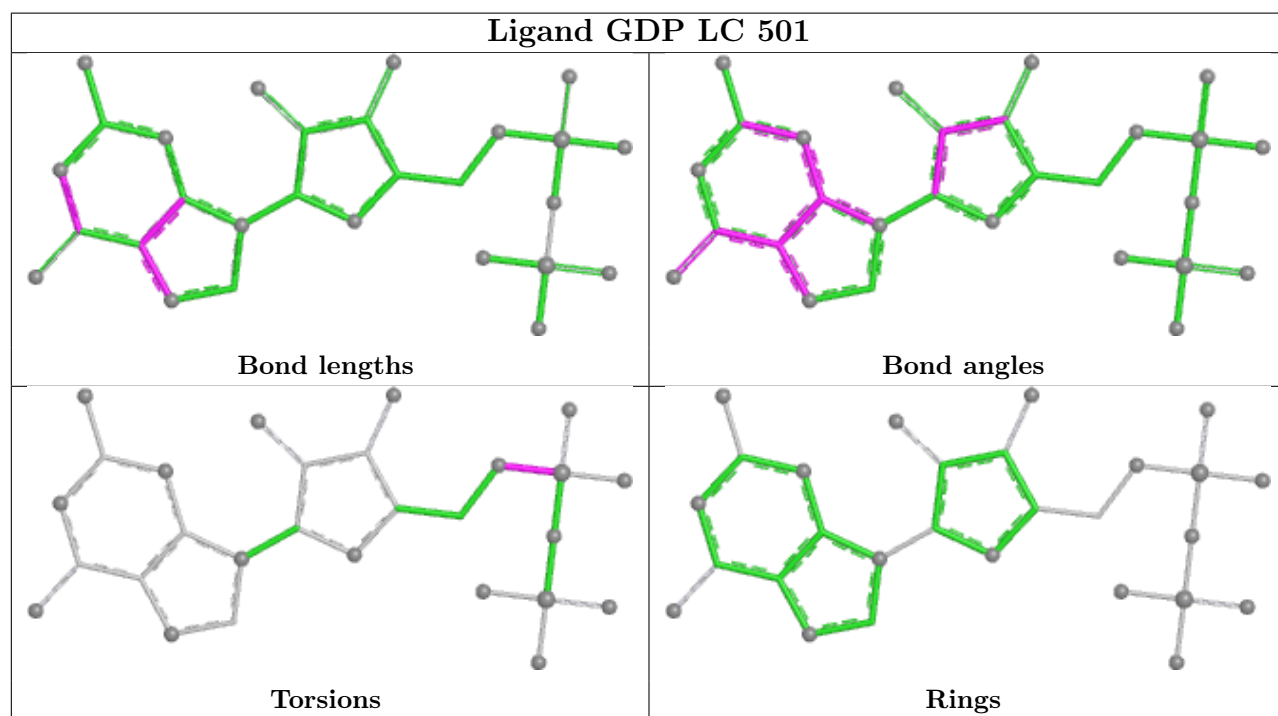
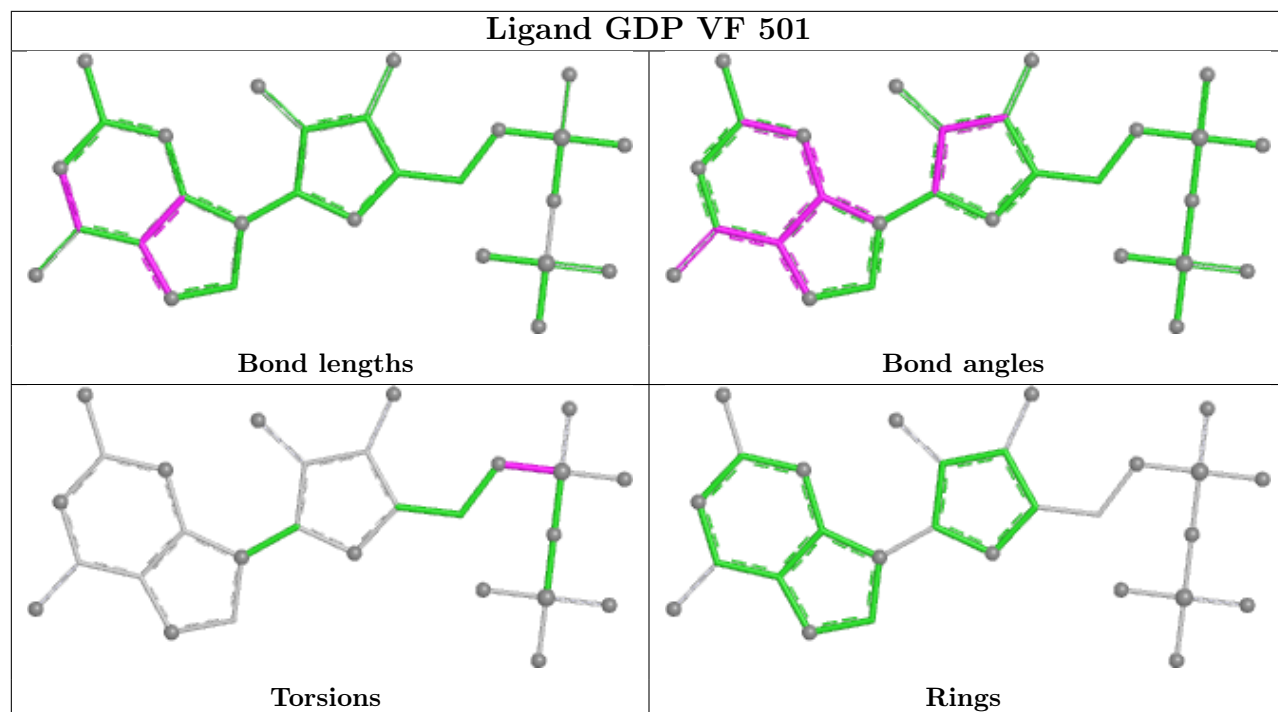




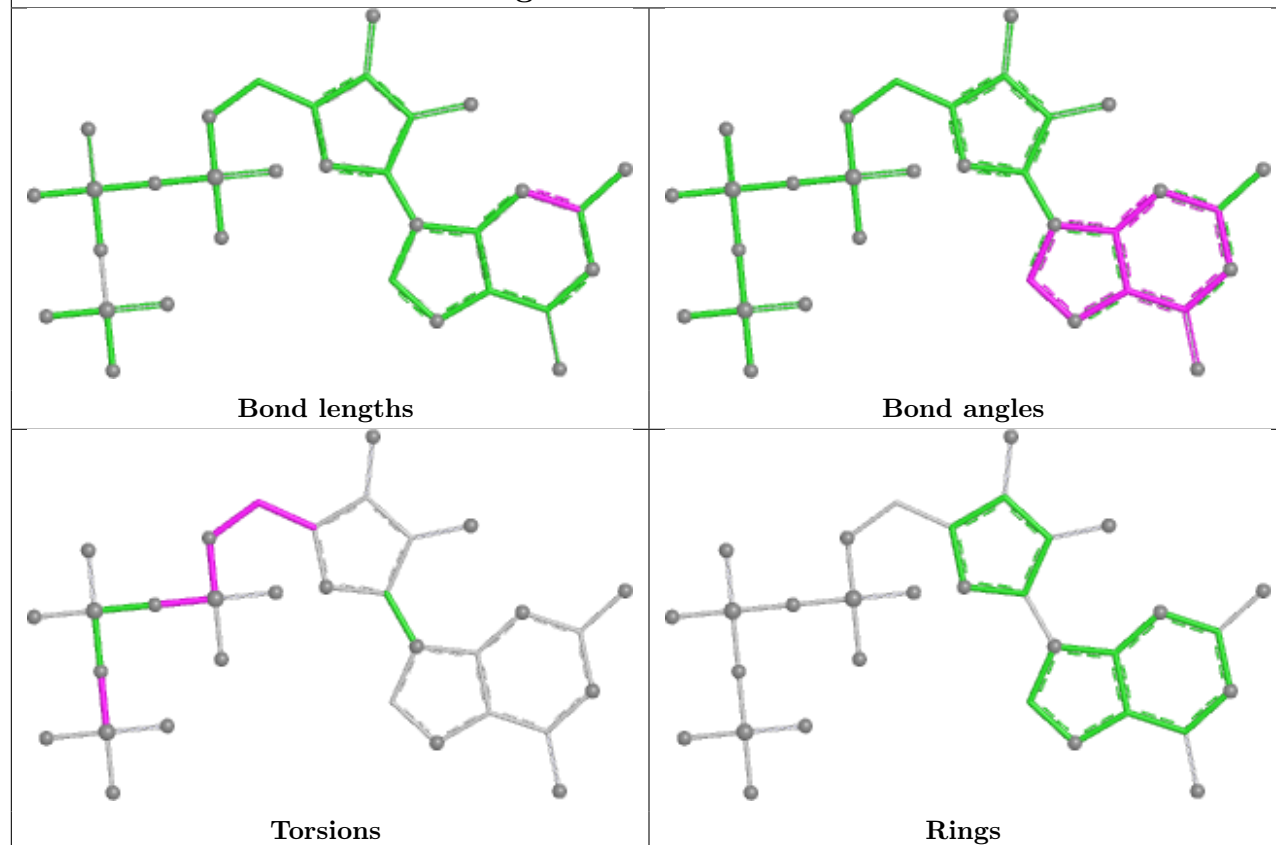




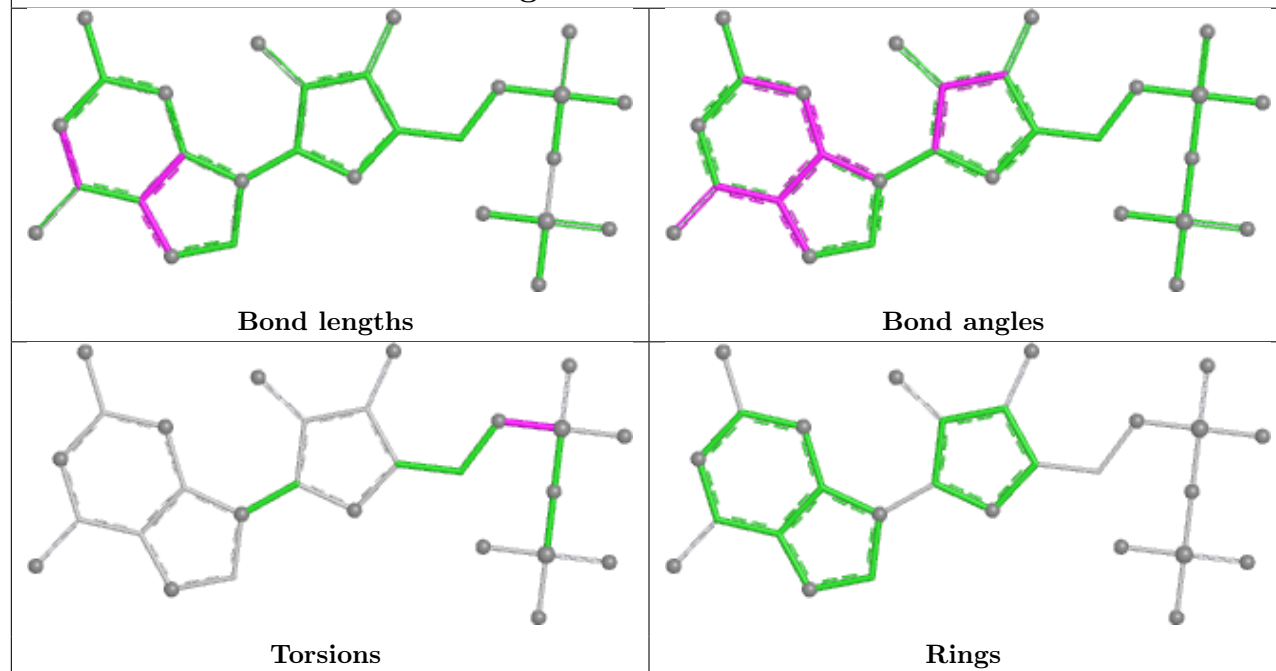


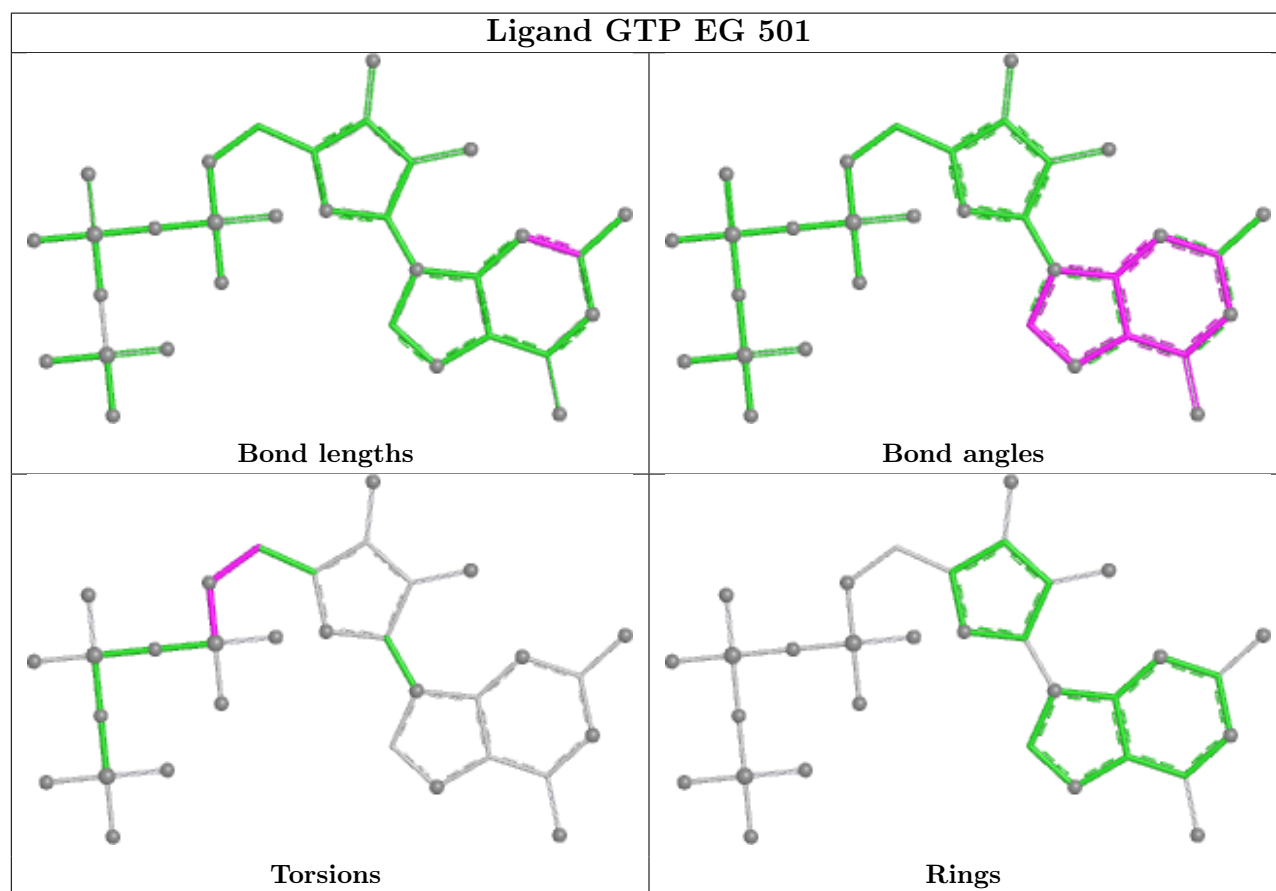
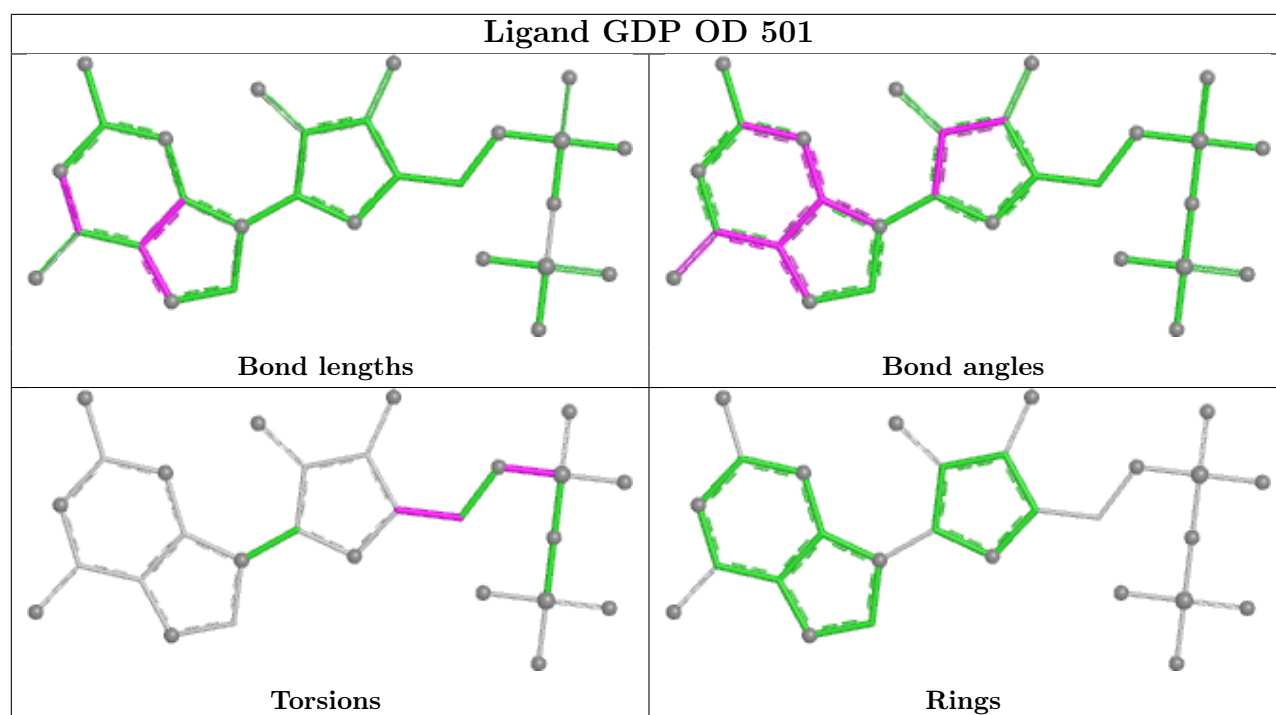


Ligand GTP HK 501

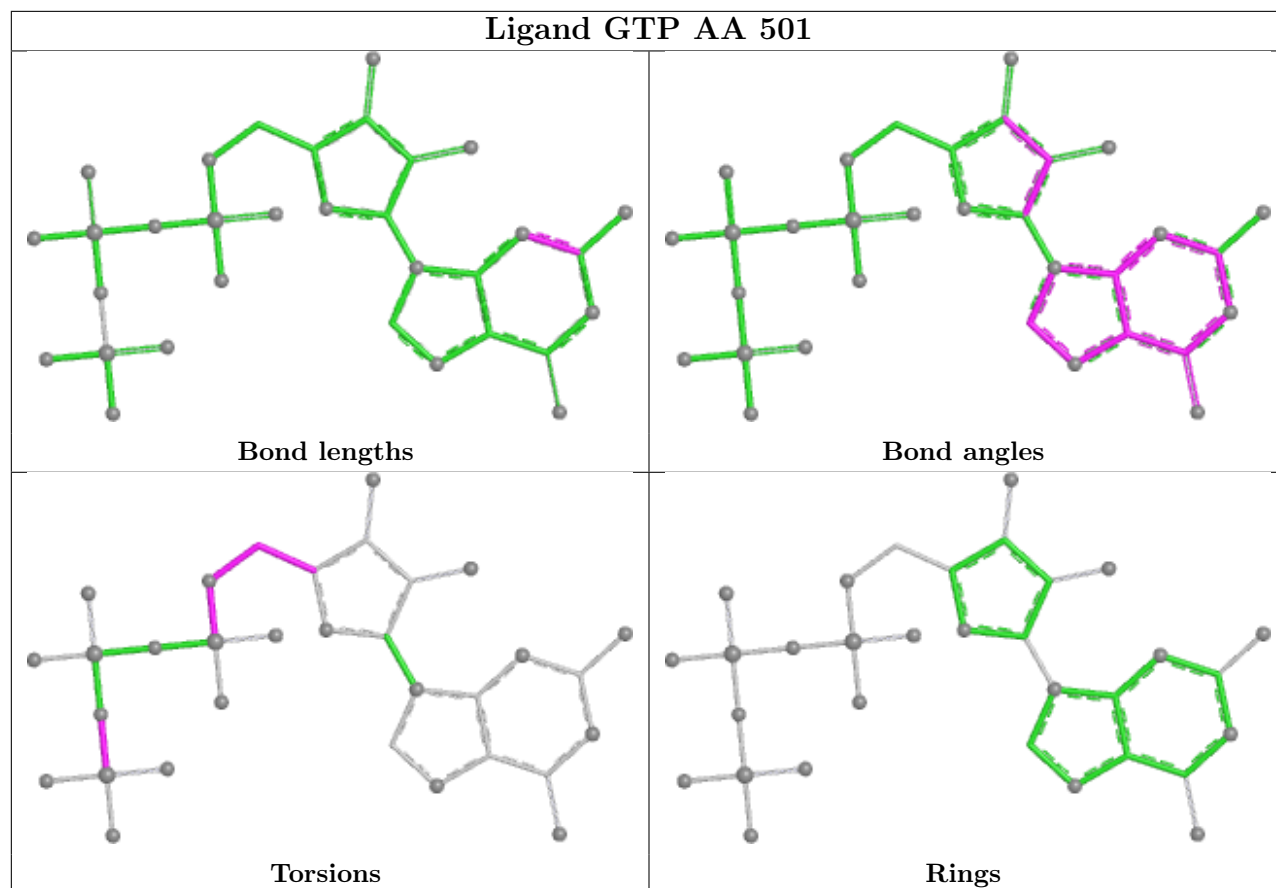


Ligand GDP OJ 501

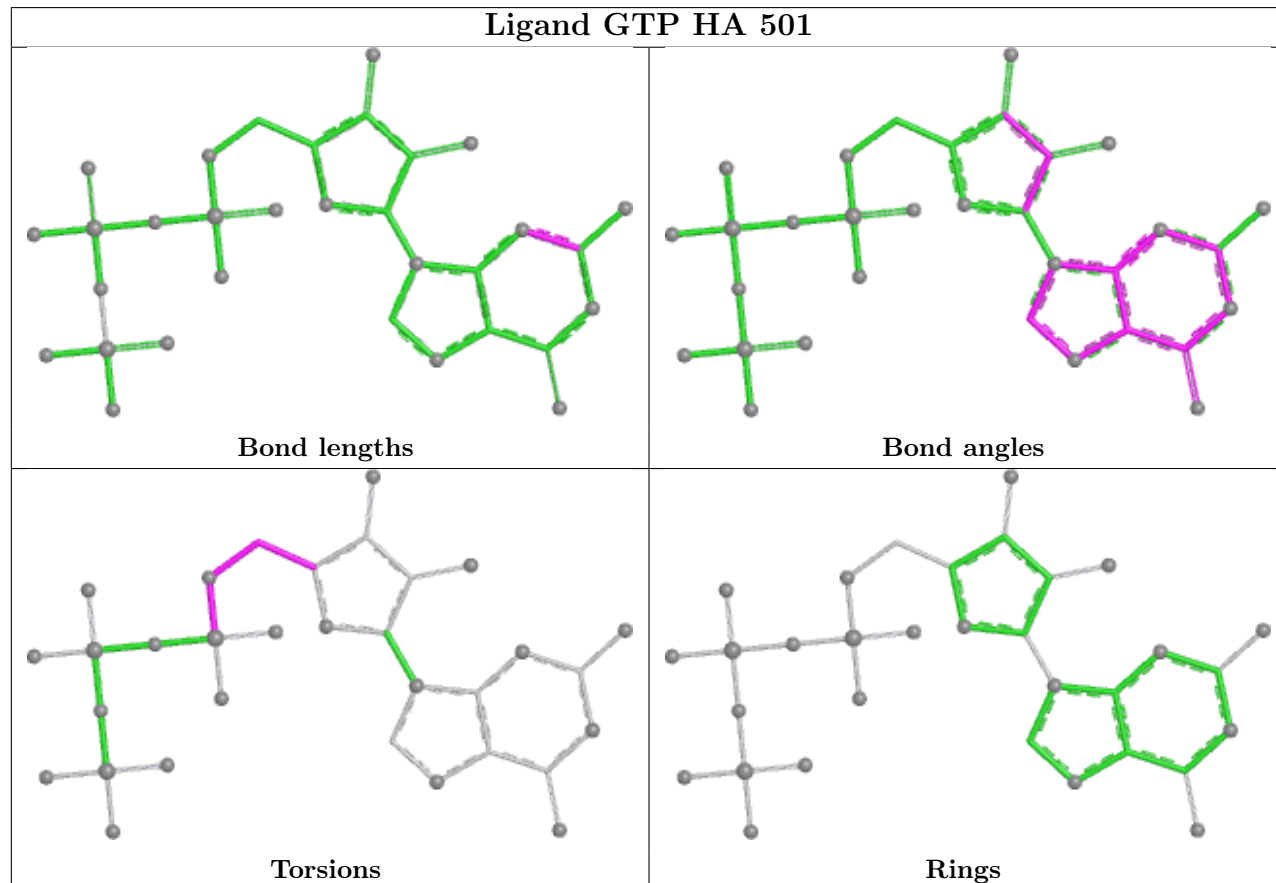




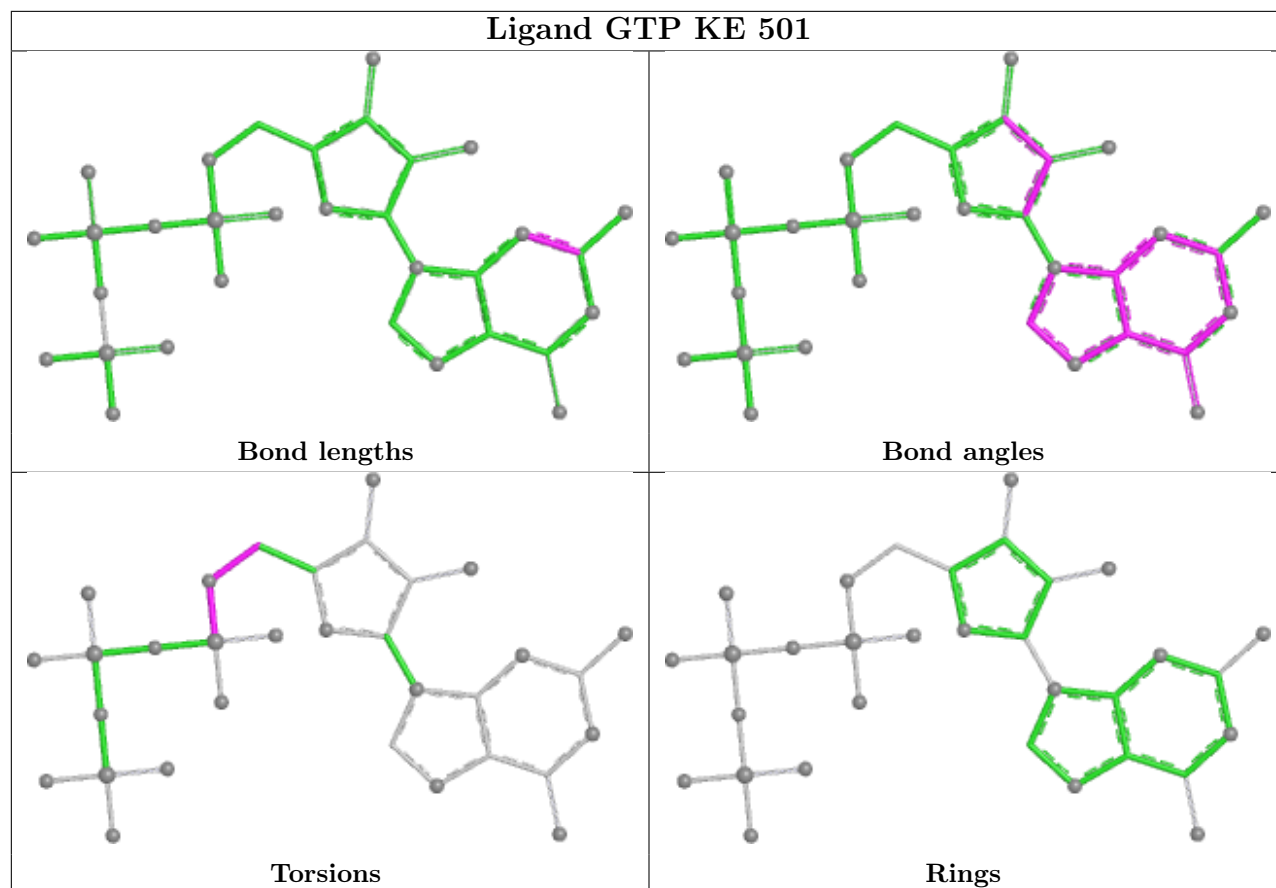
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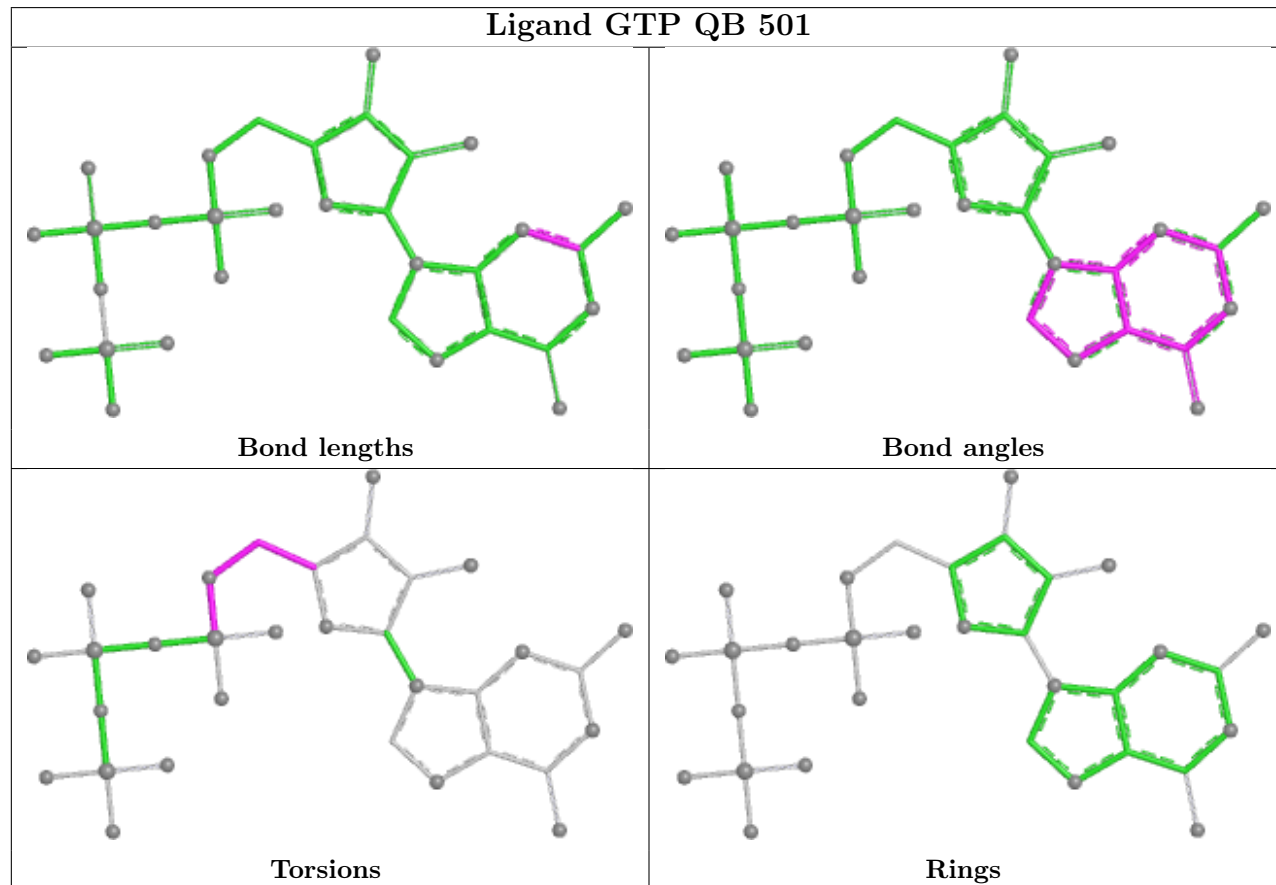
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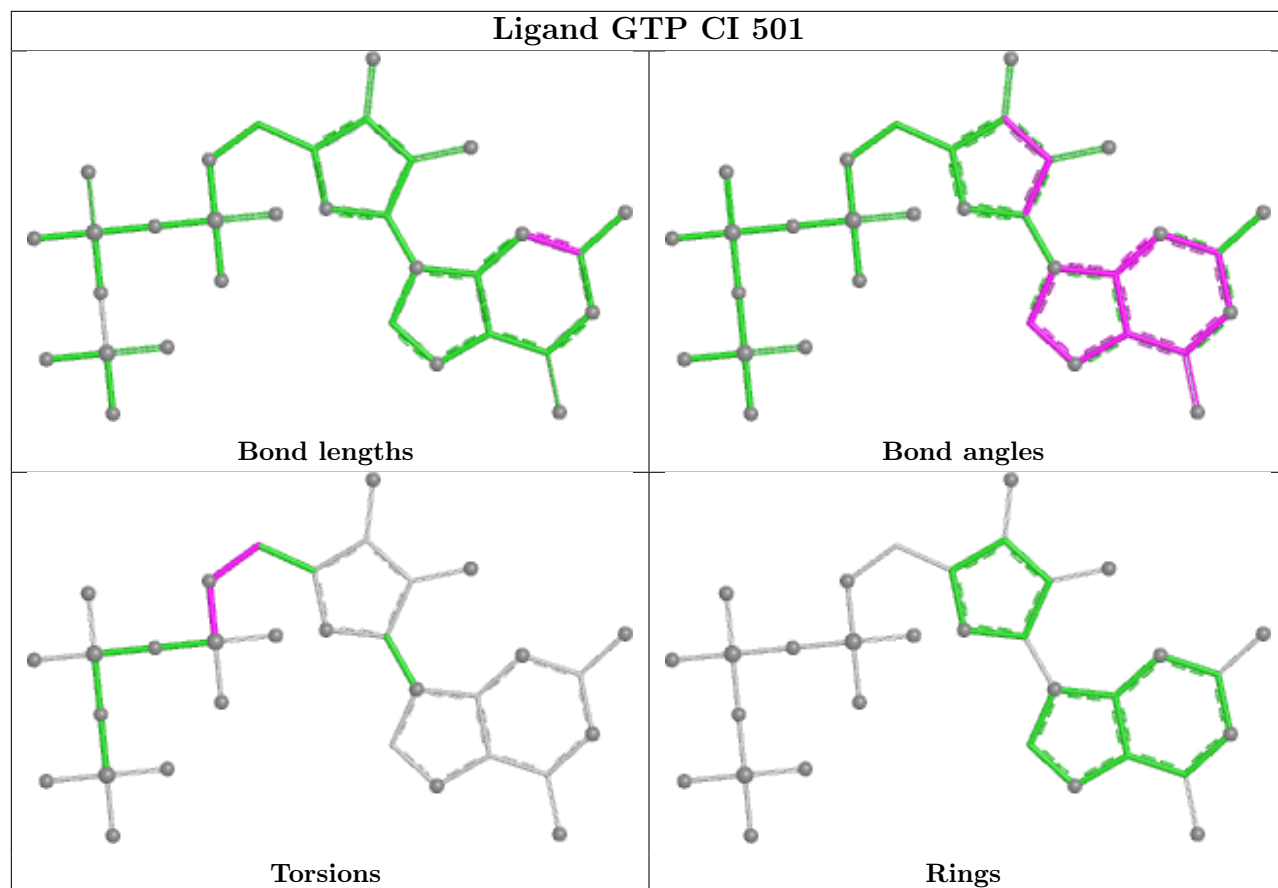
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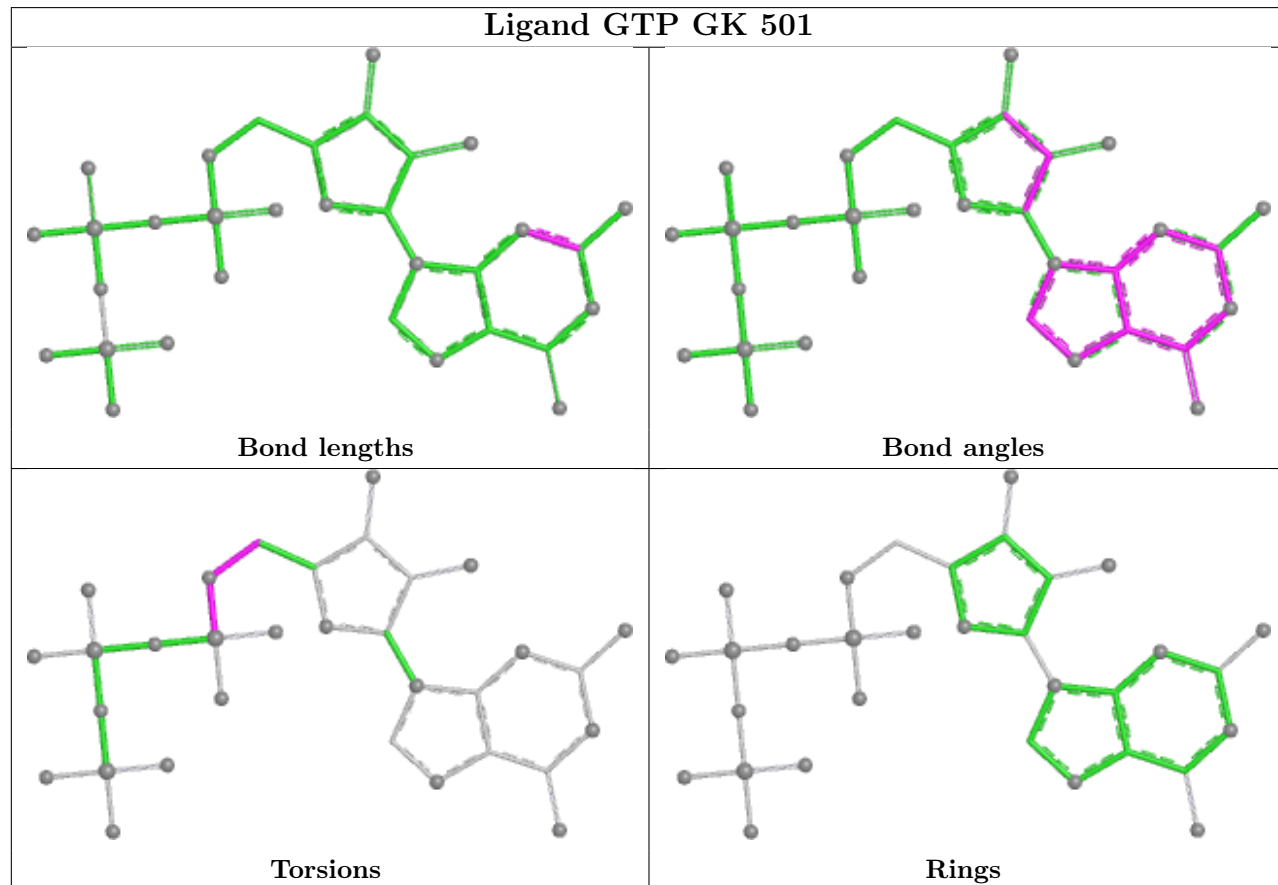
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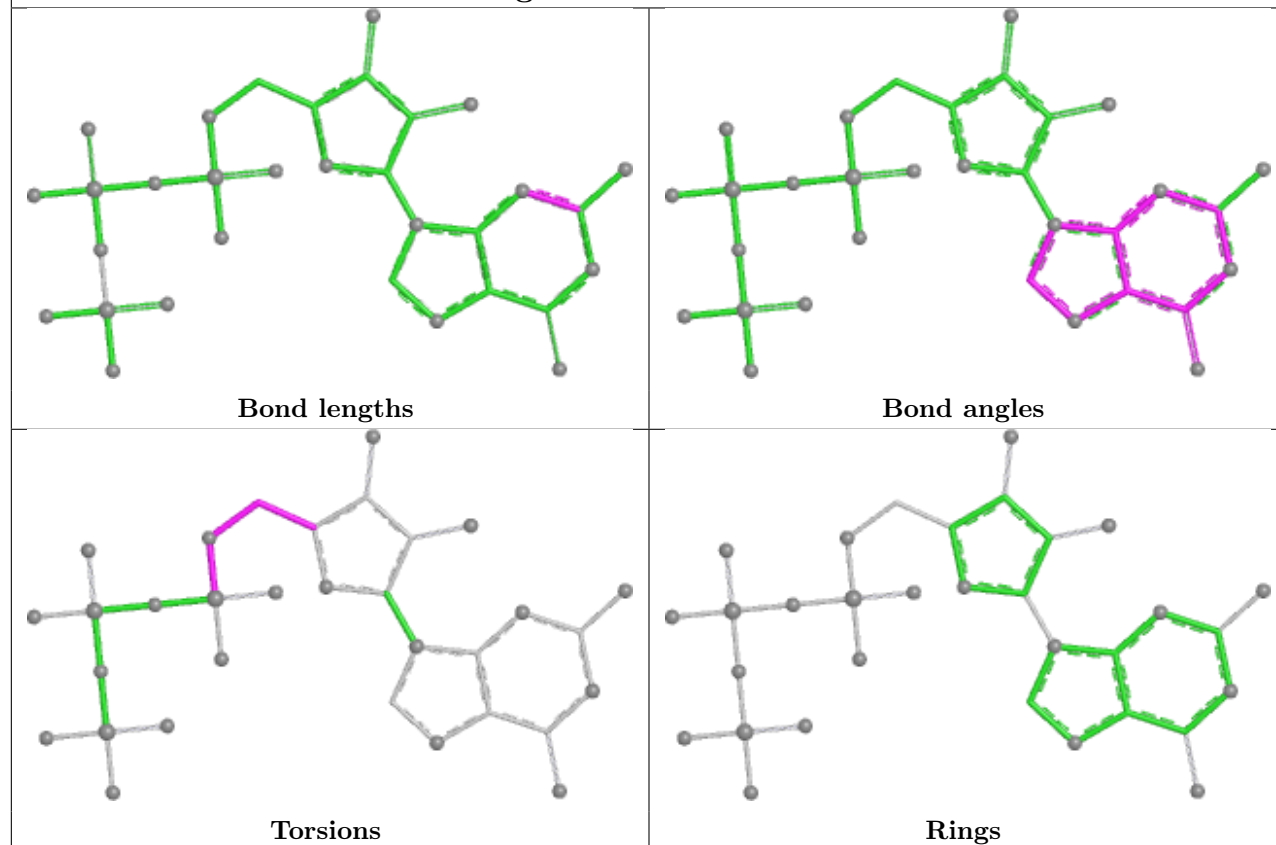
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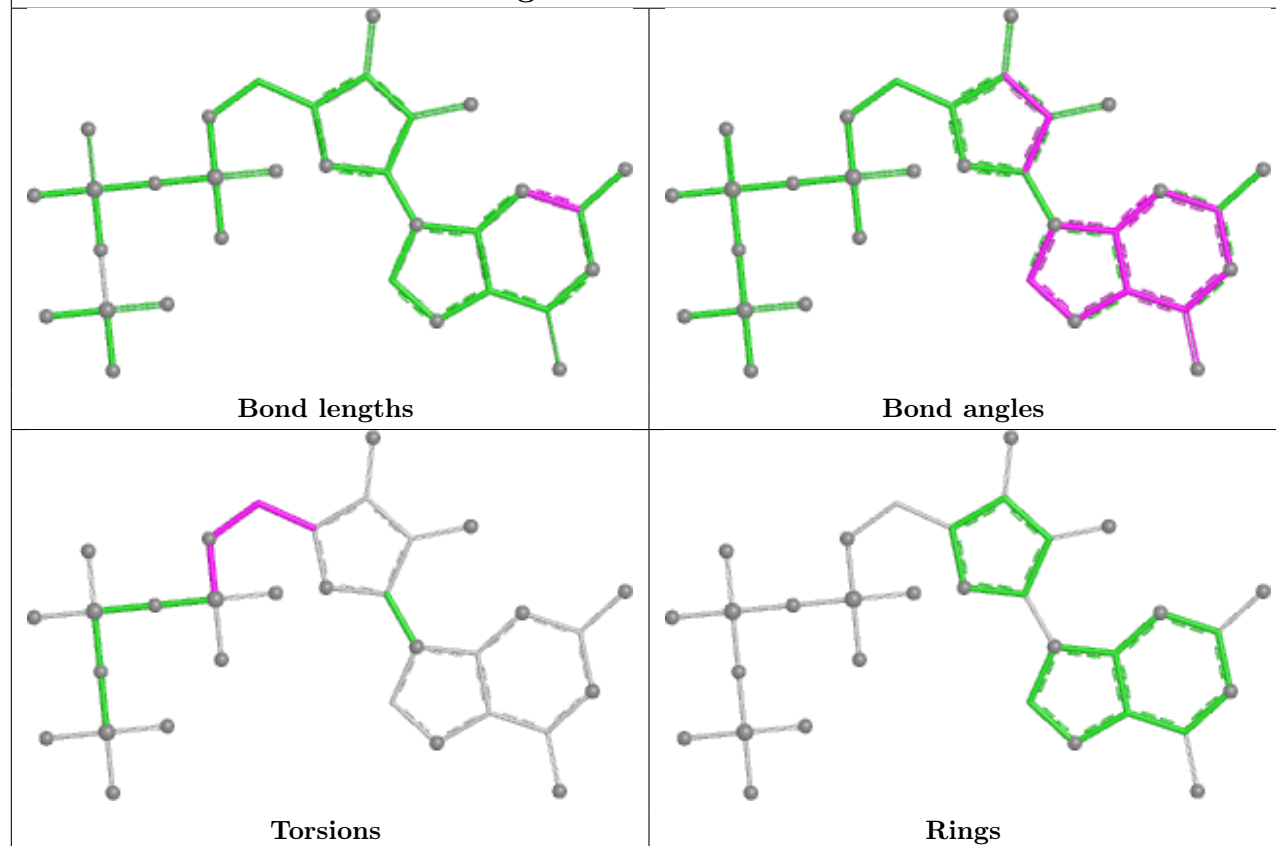
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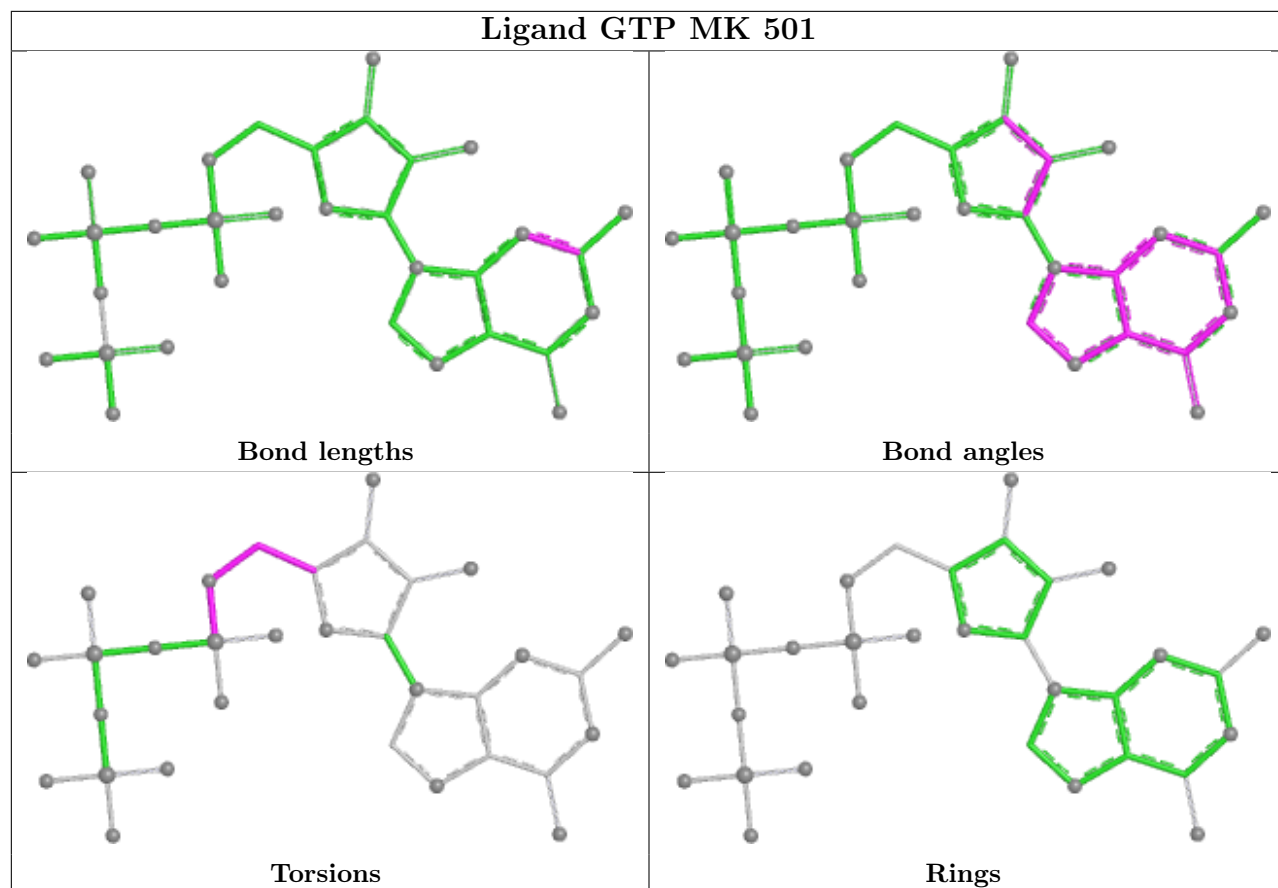
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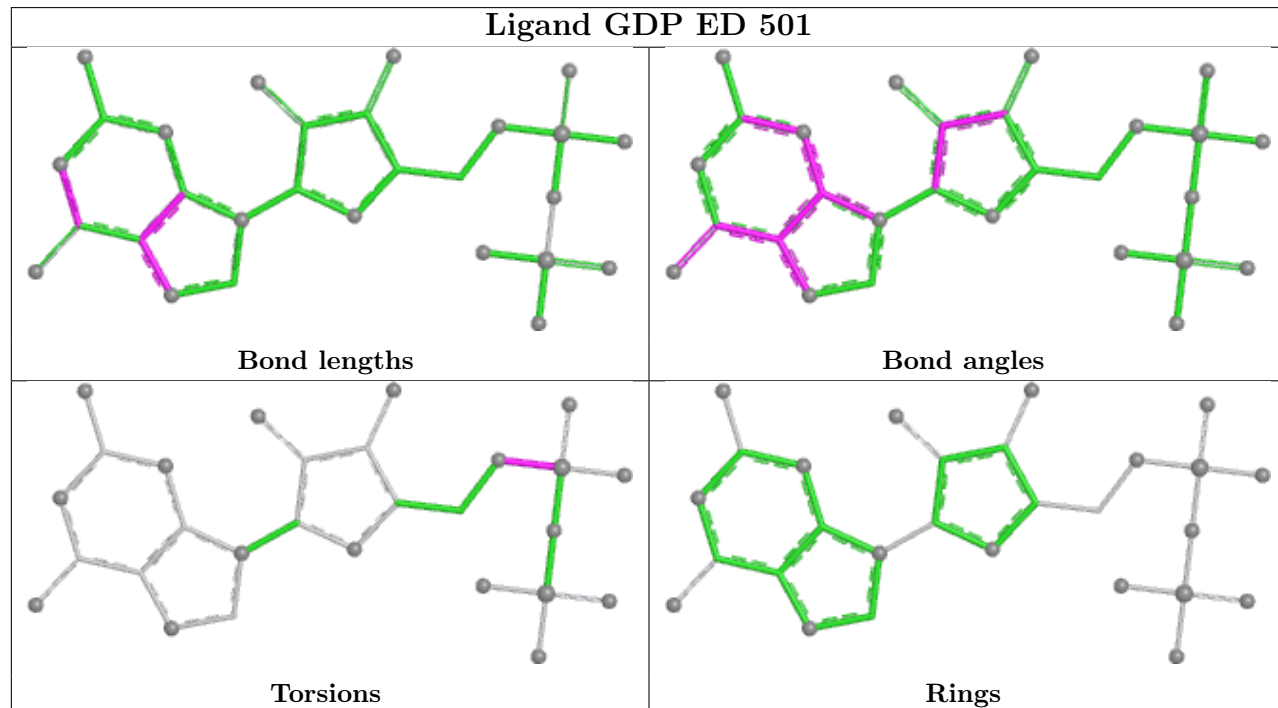
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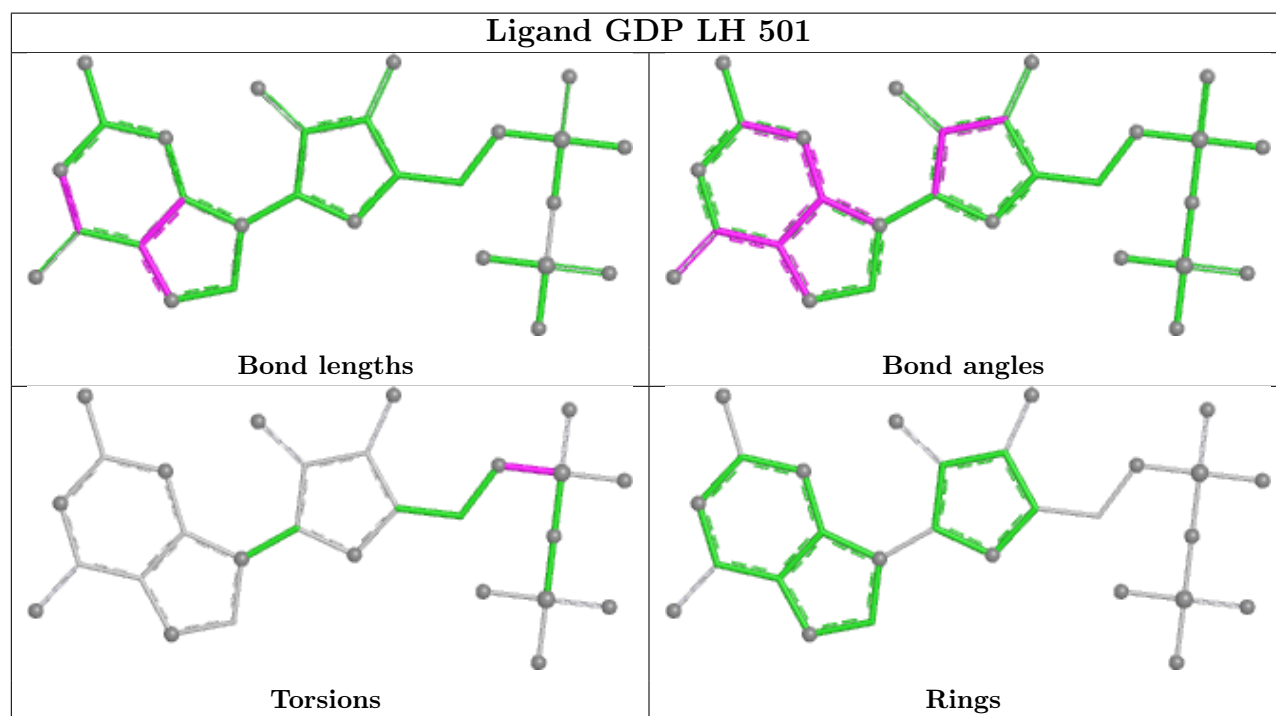
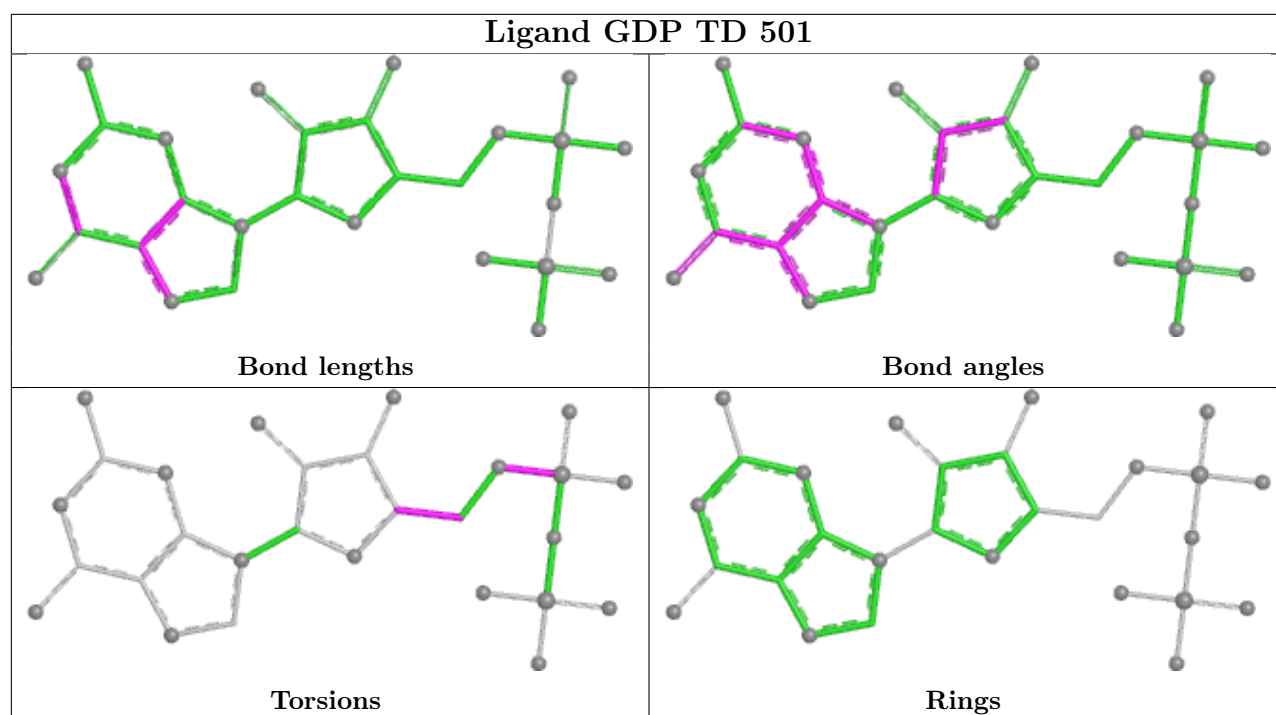


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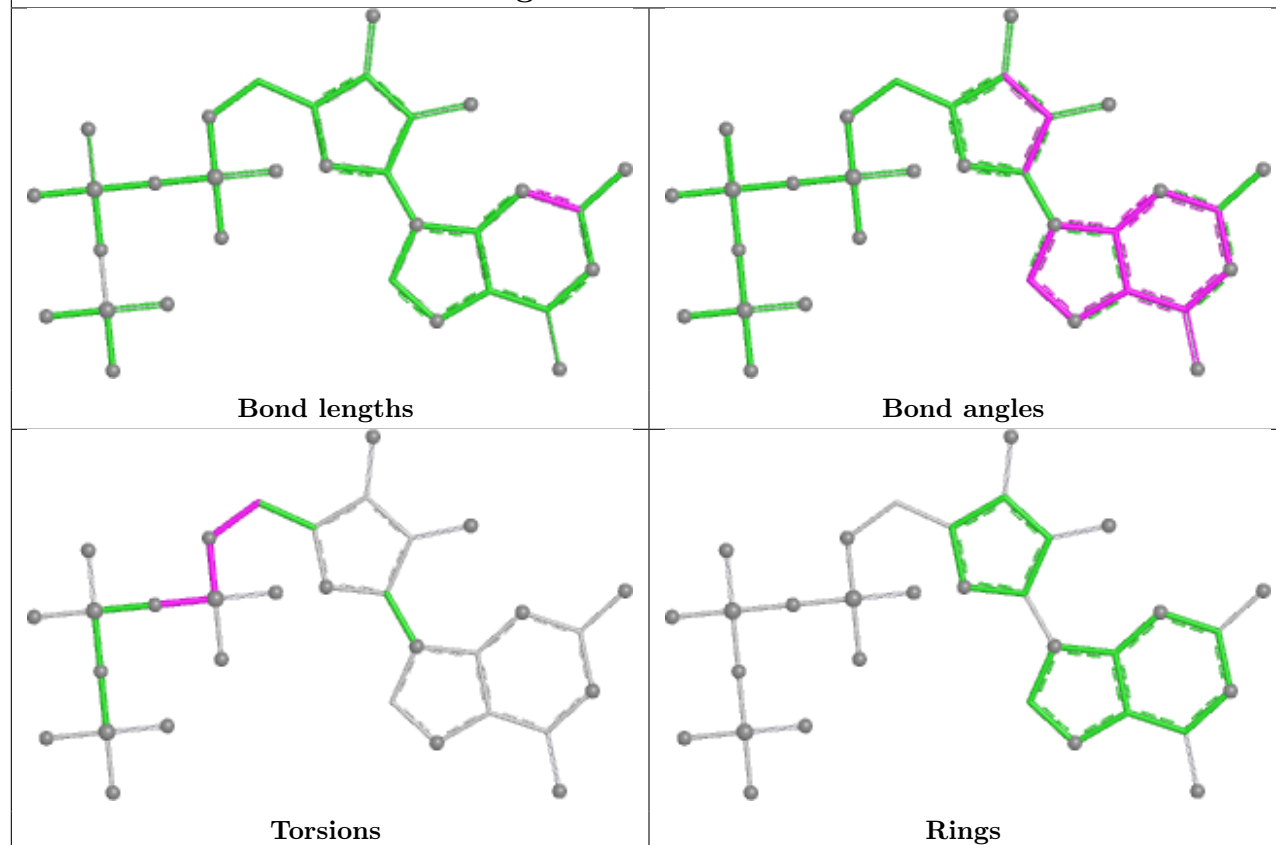


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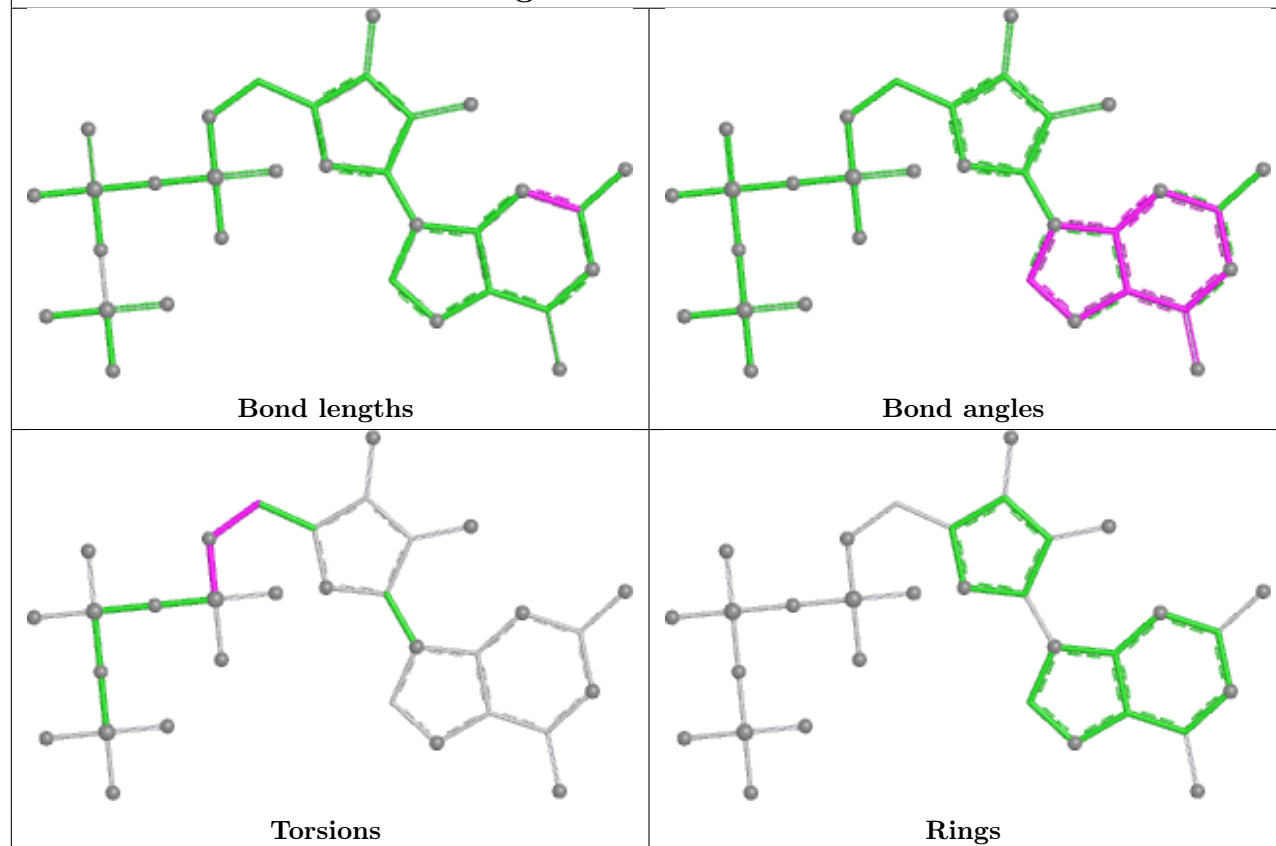


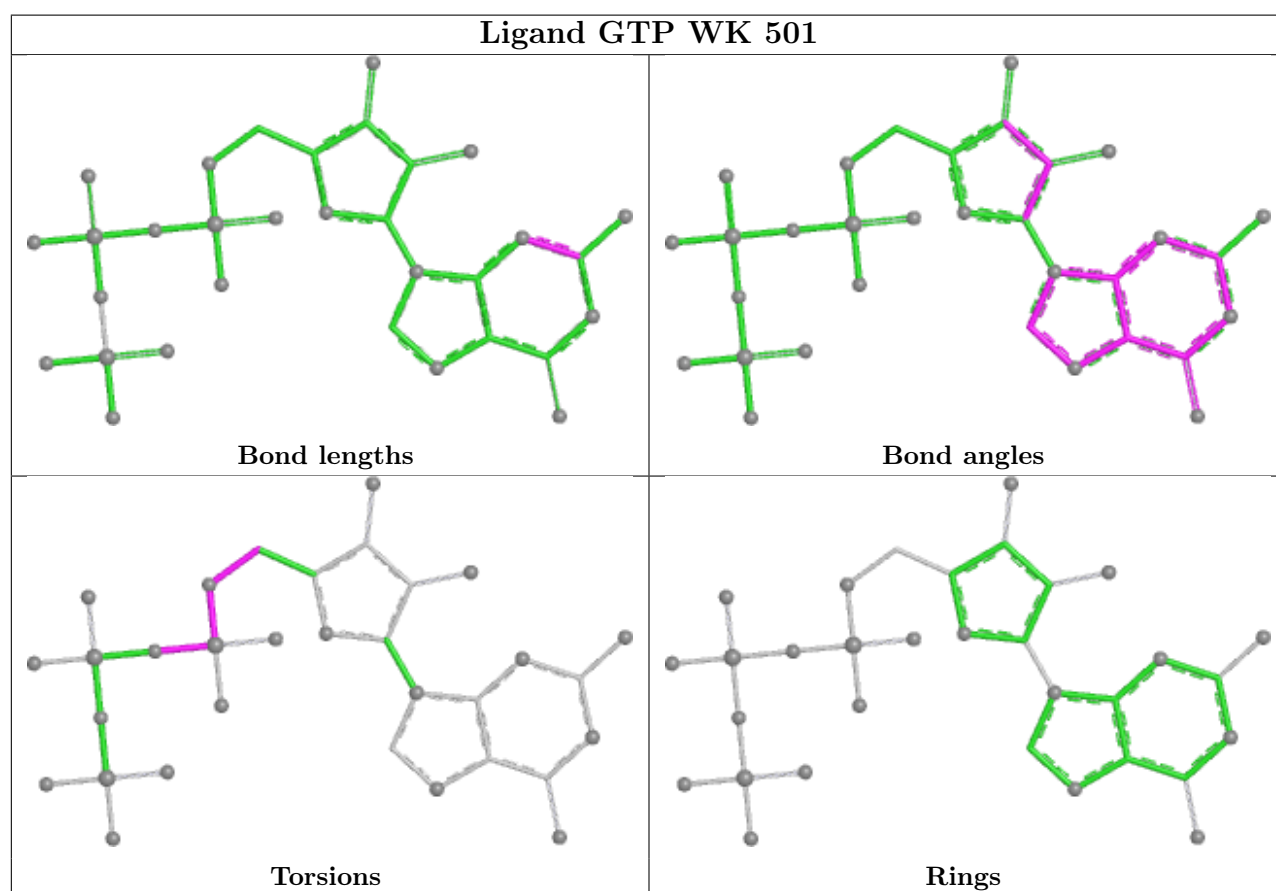
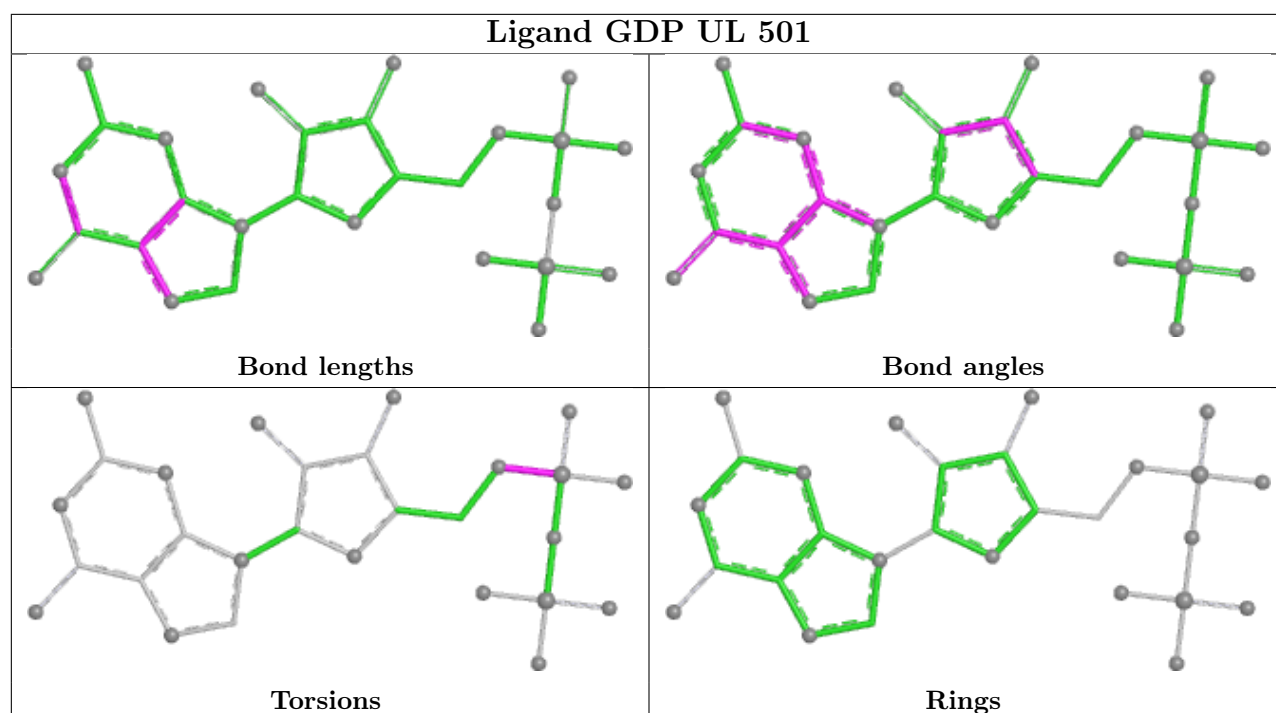


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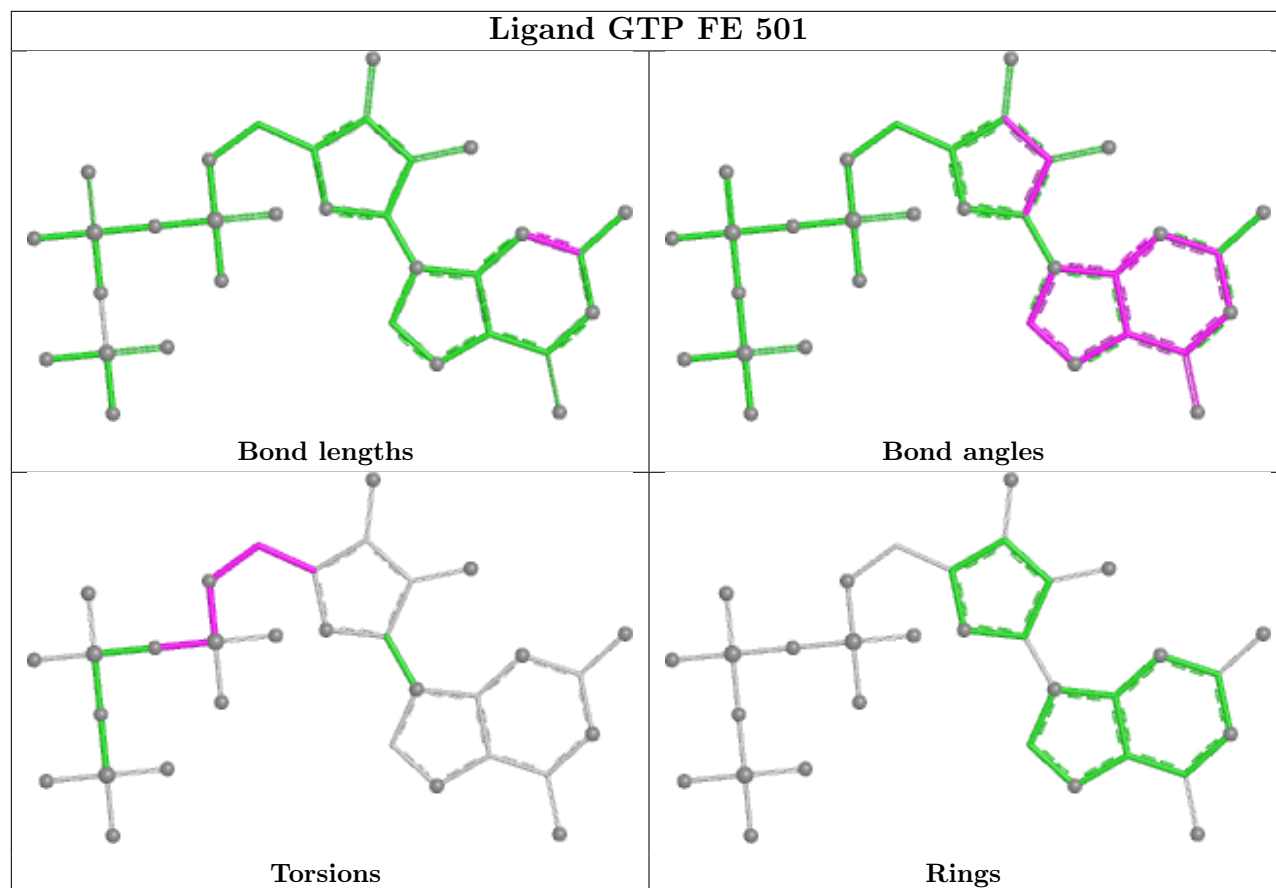


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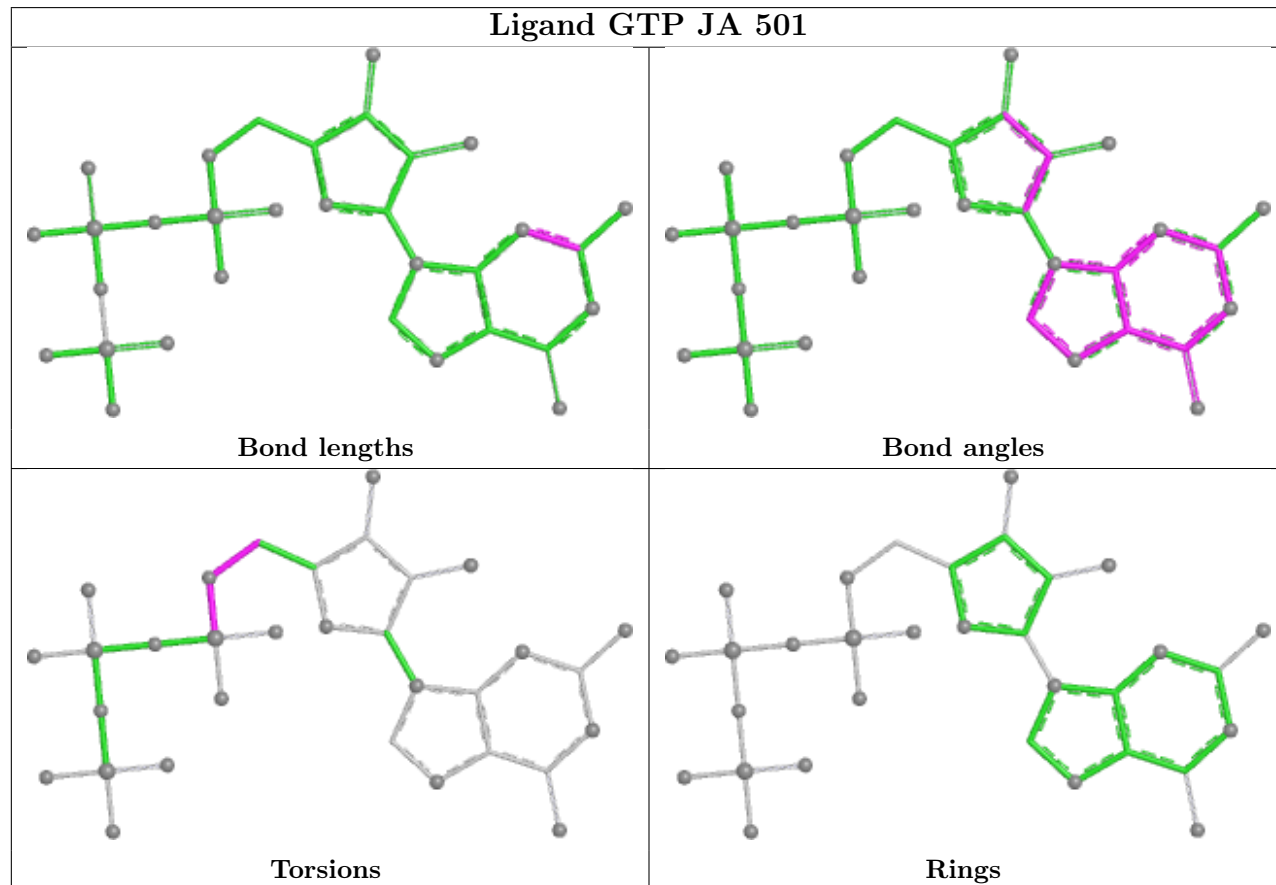


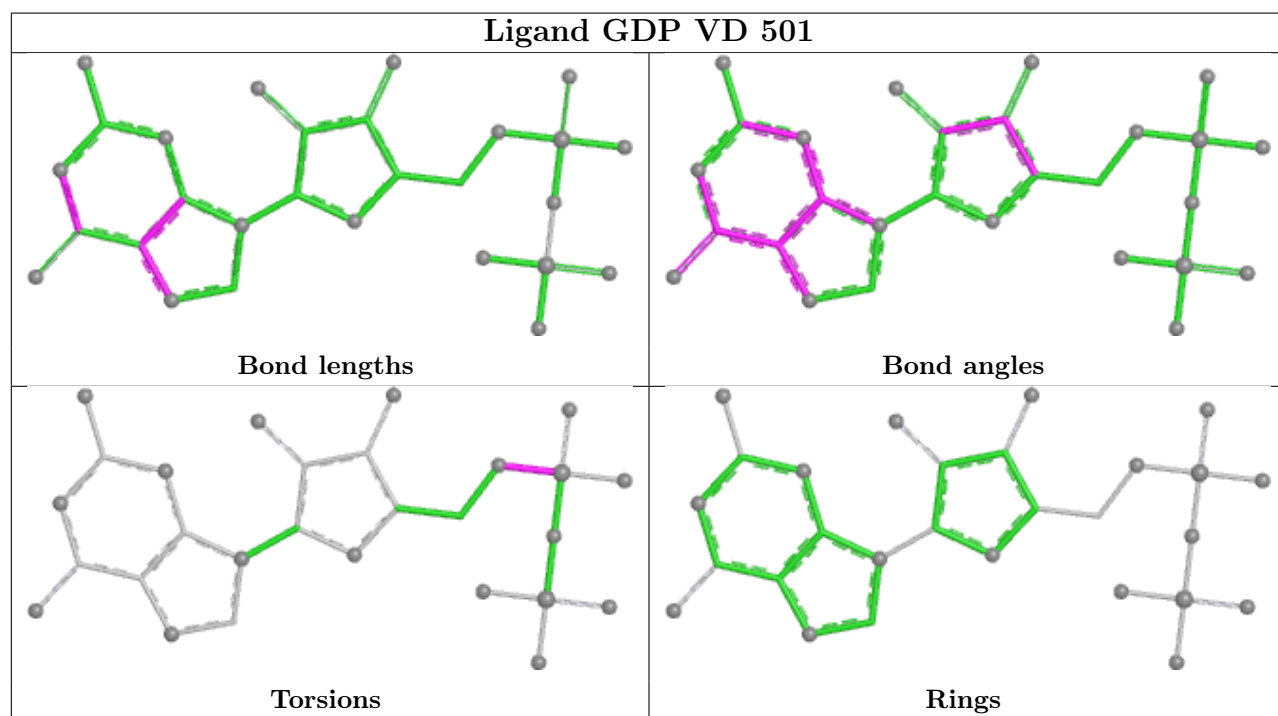
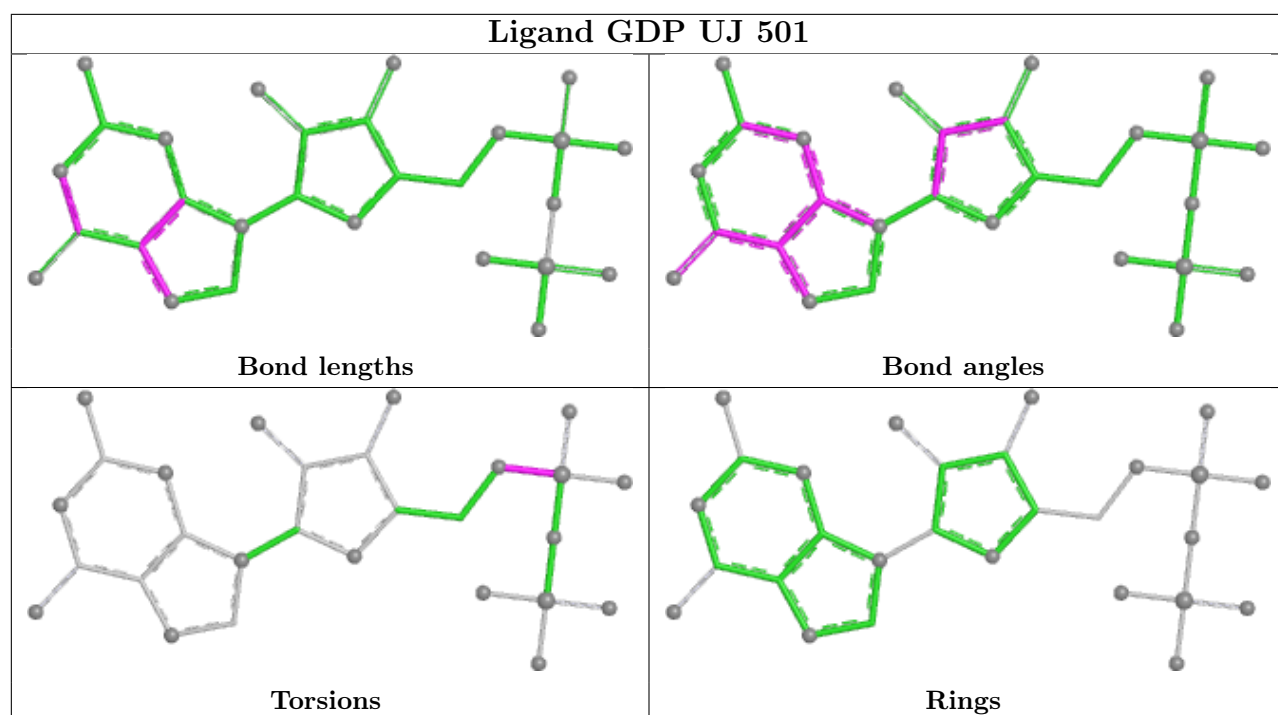


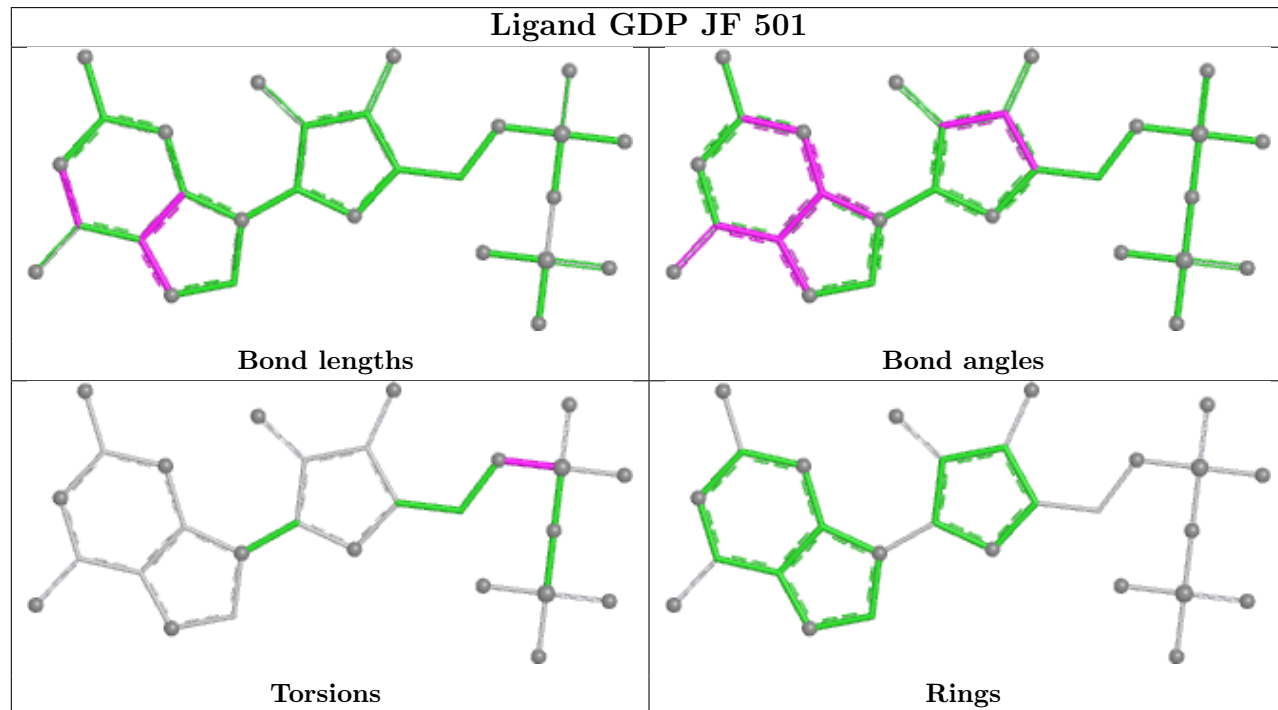
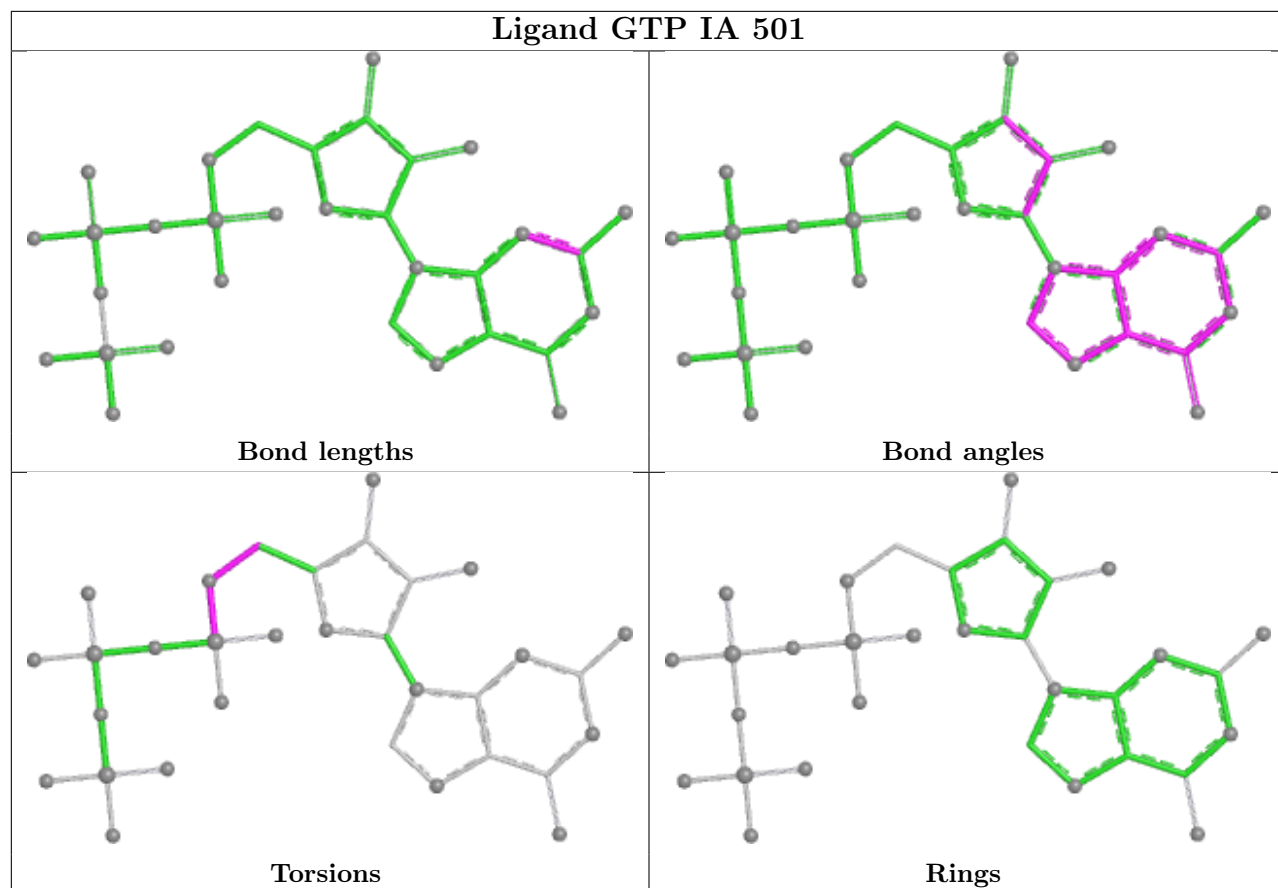
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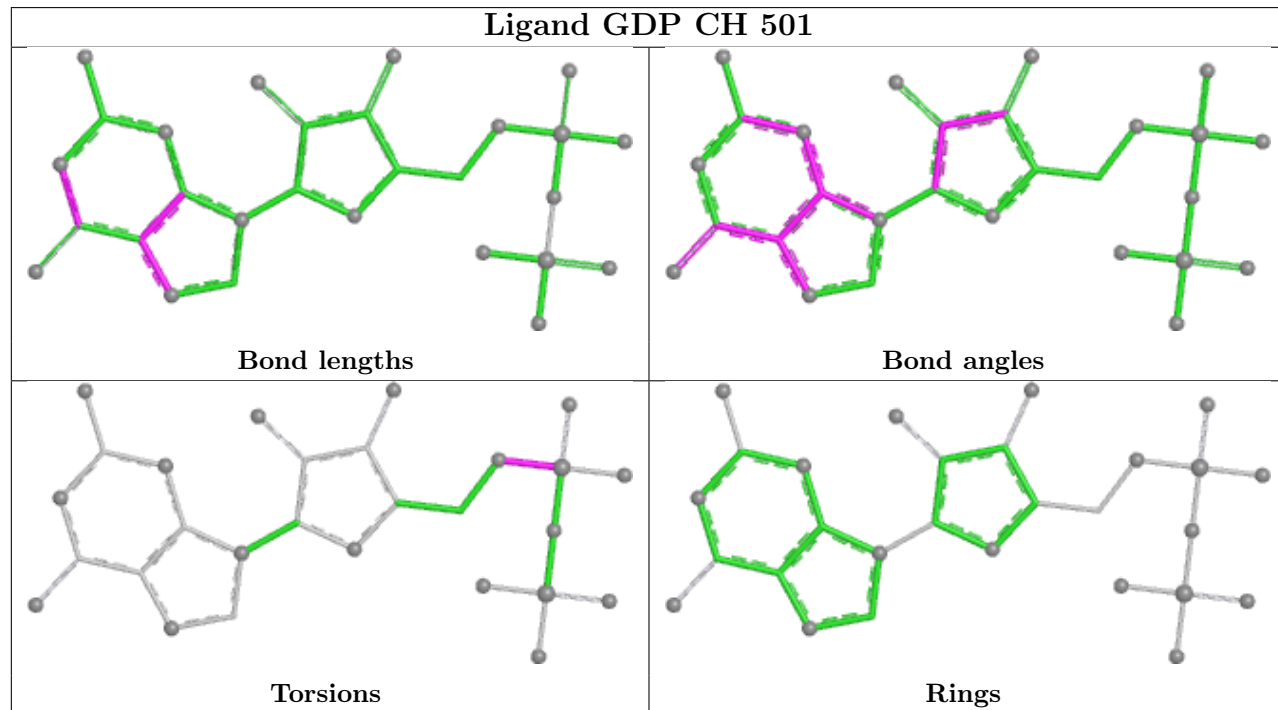
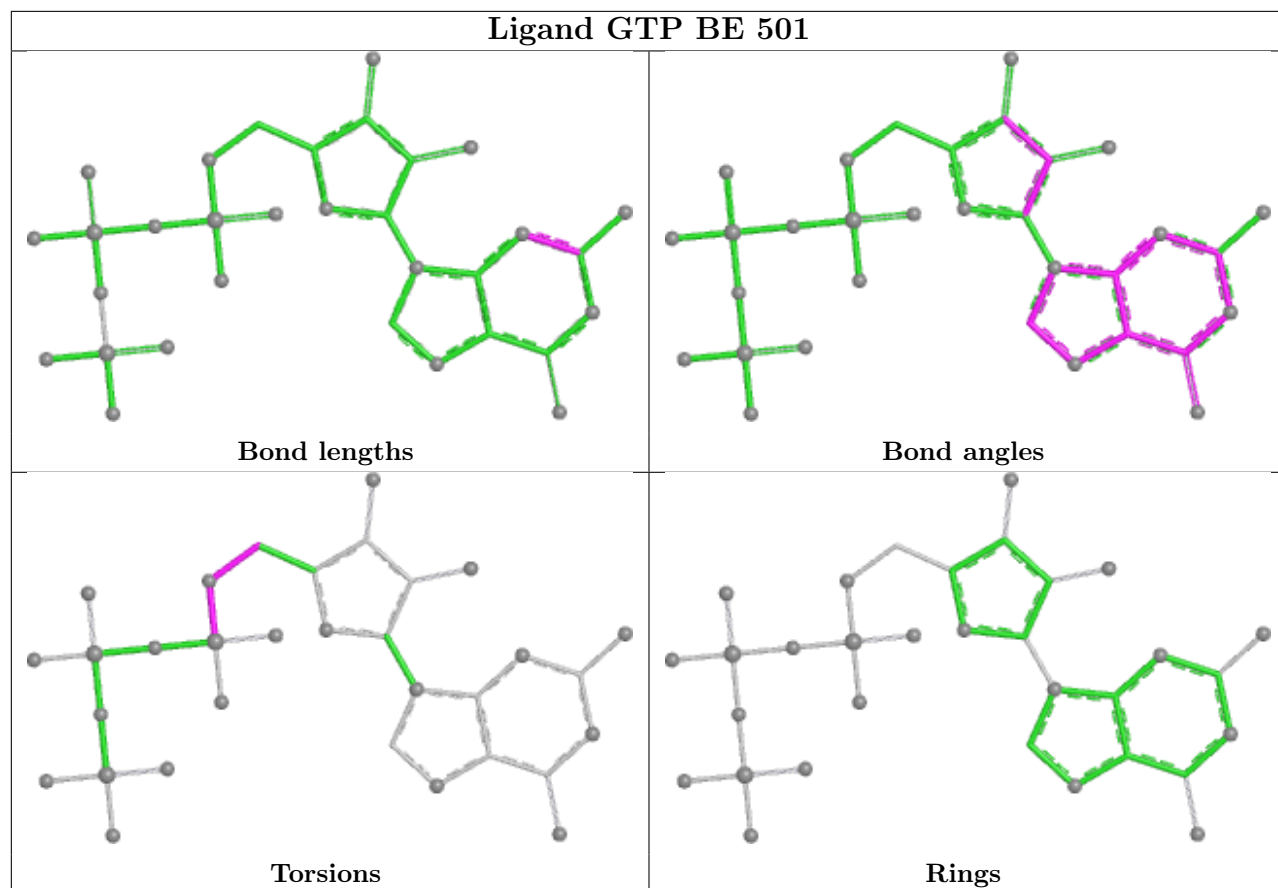


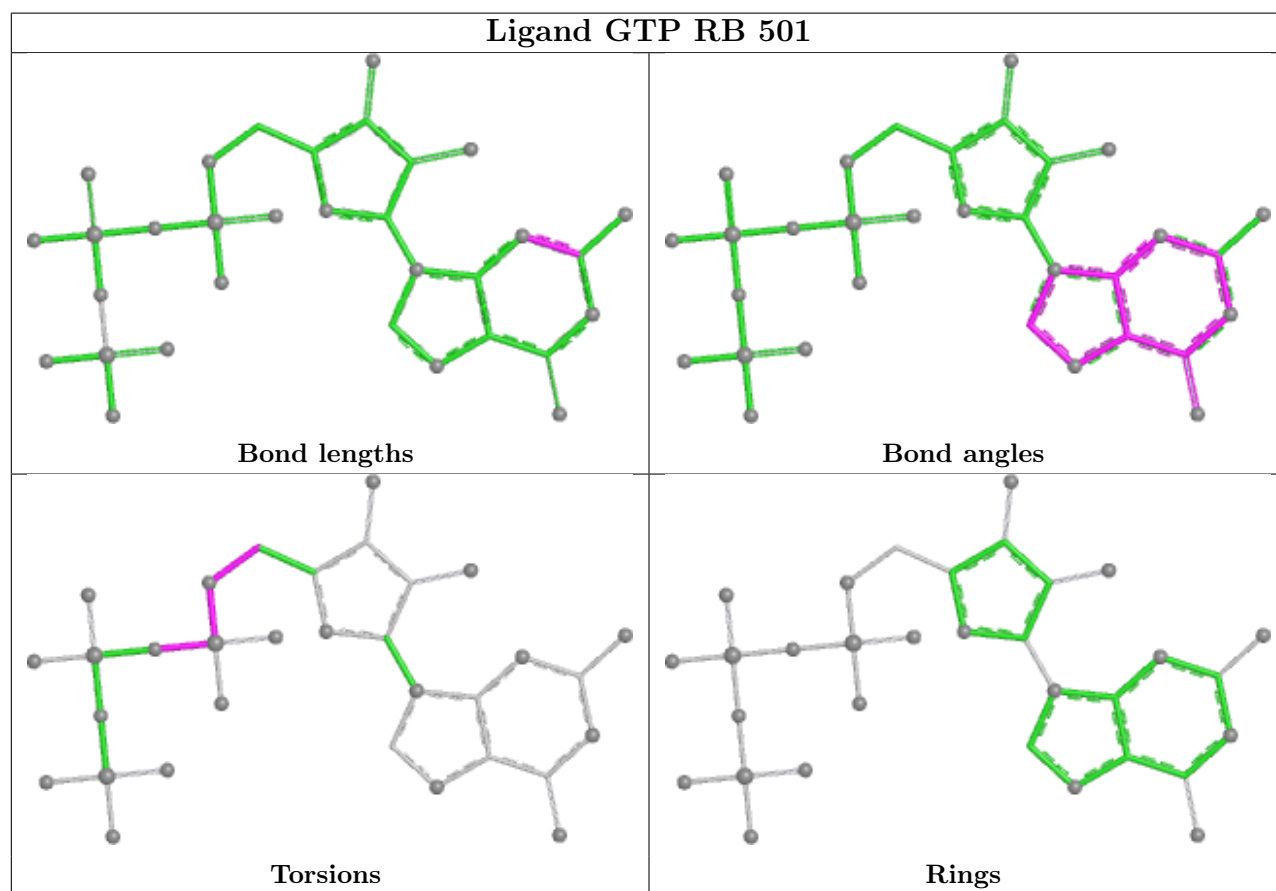
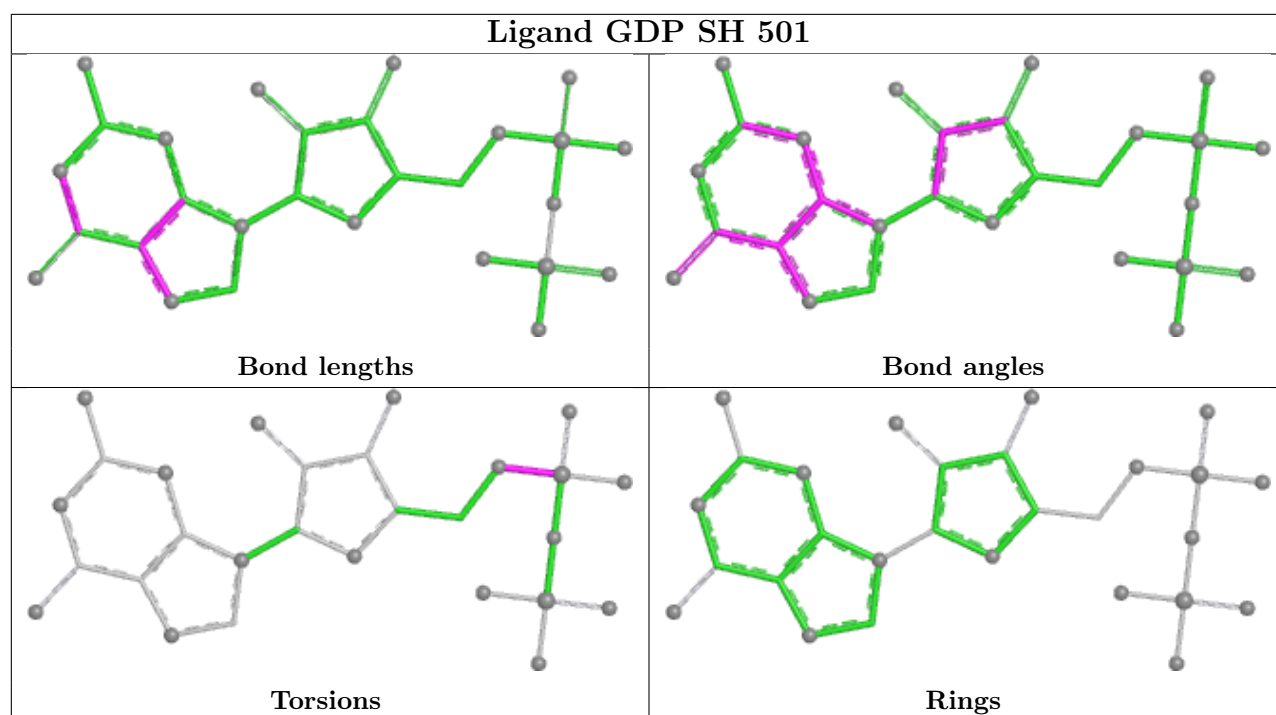
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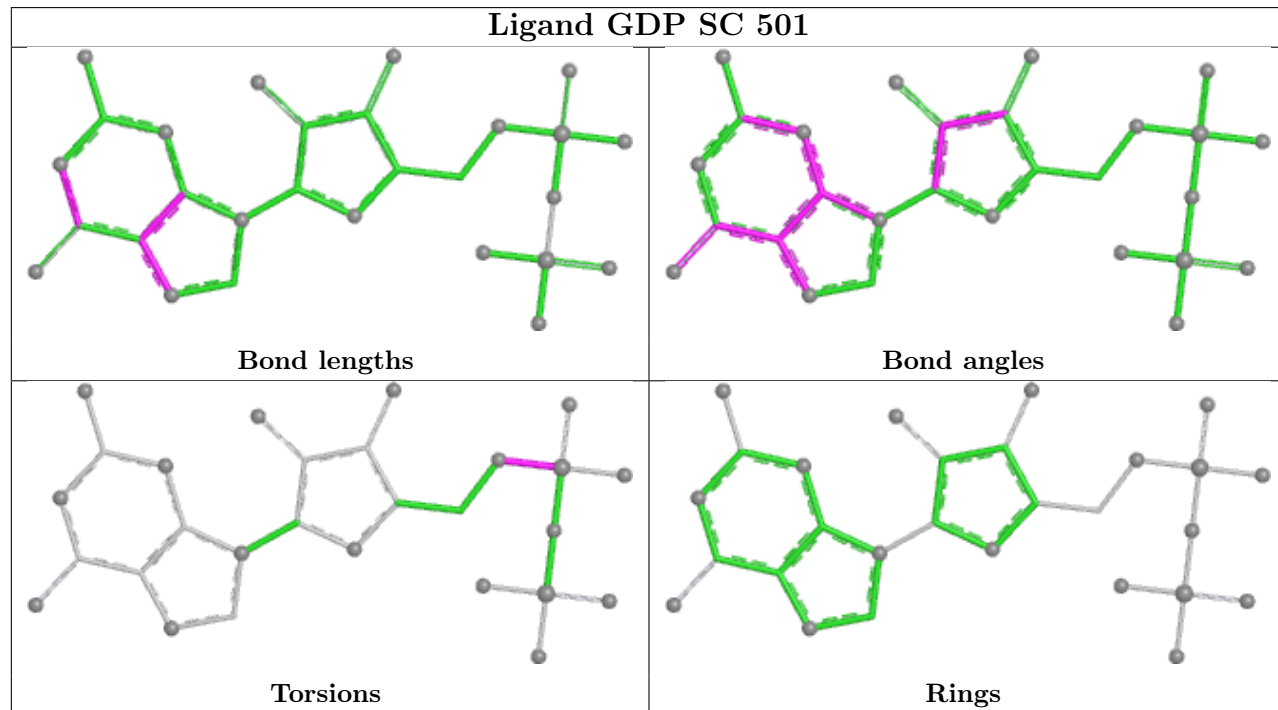
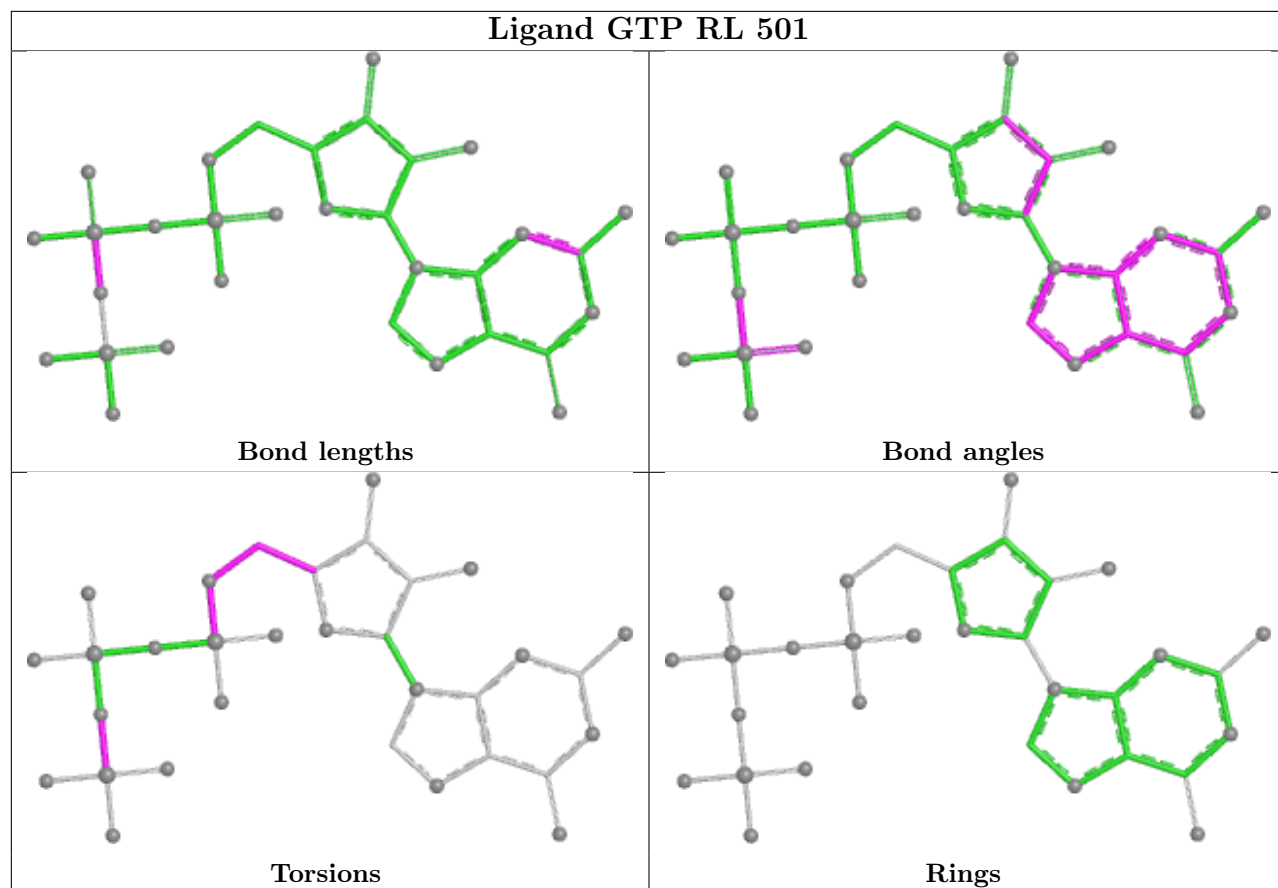


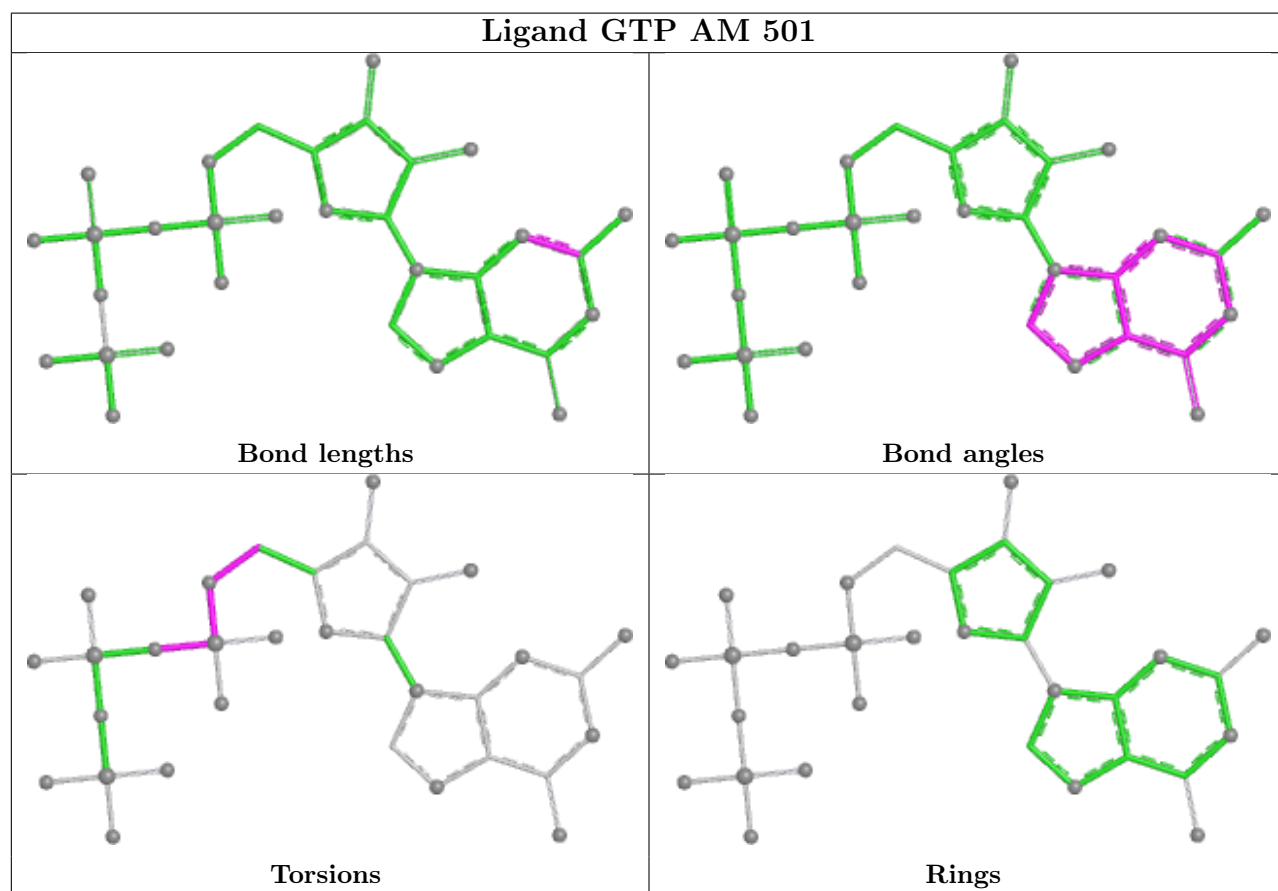
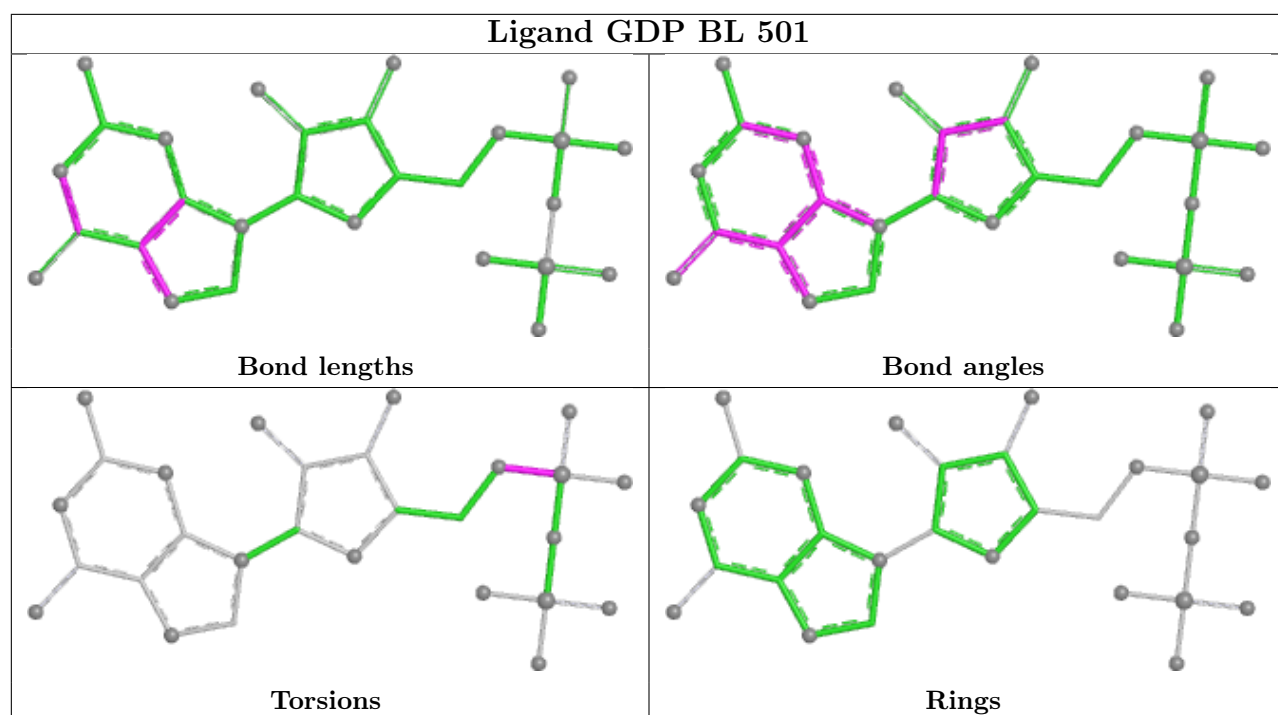


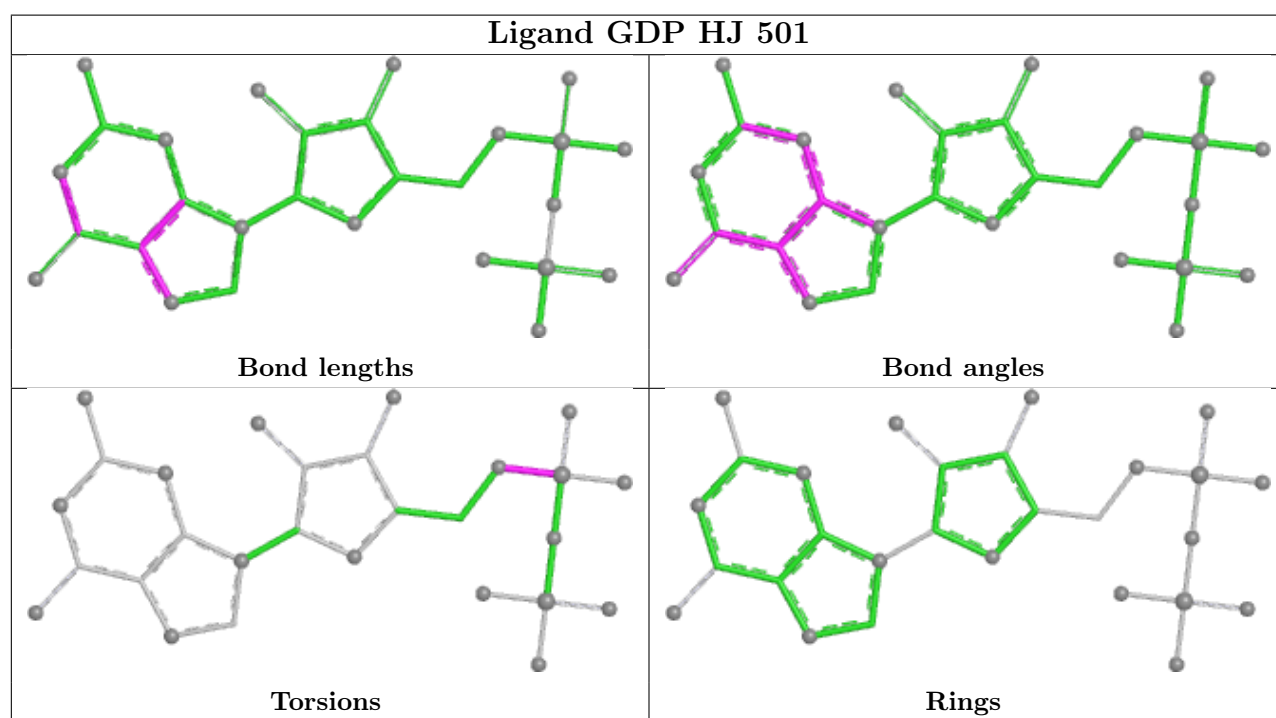
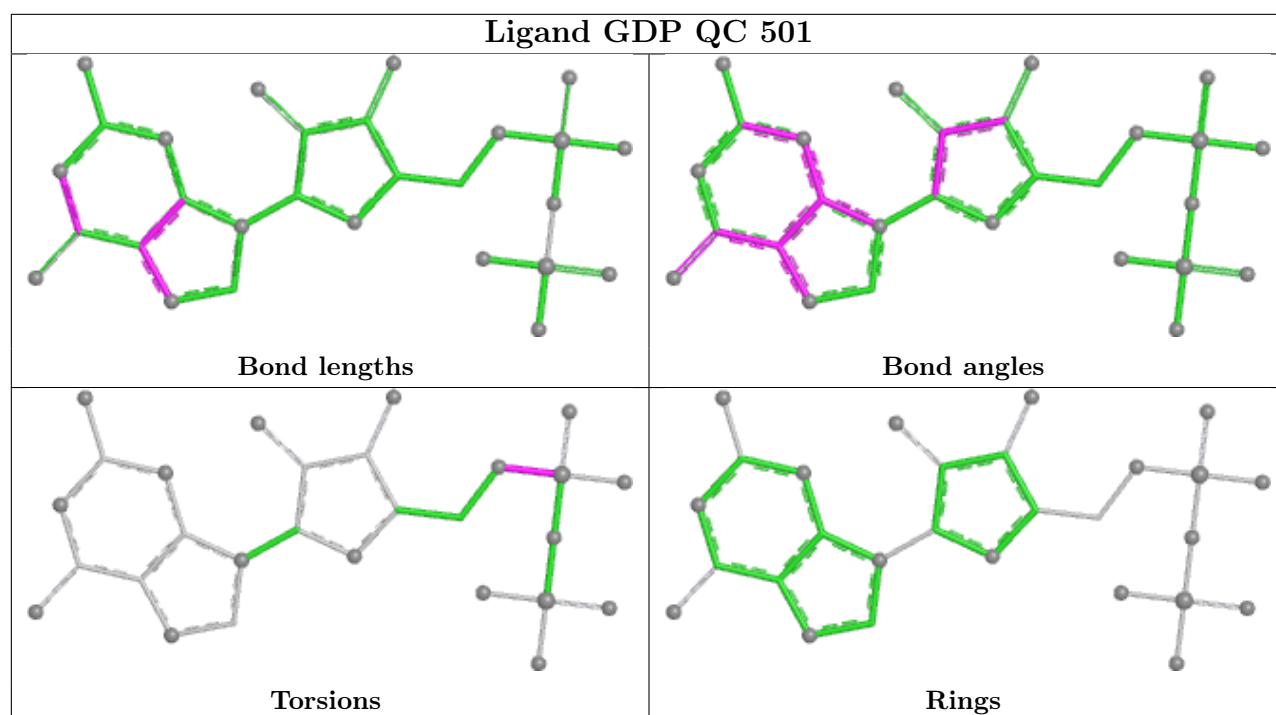




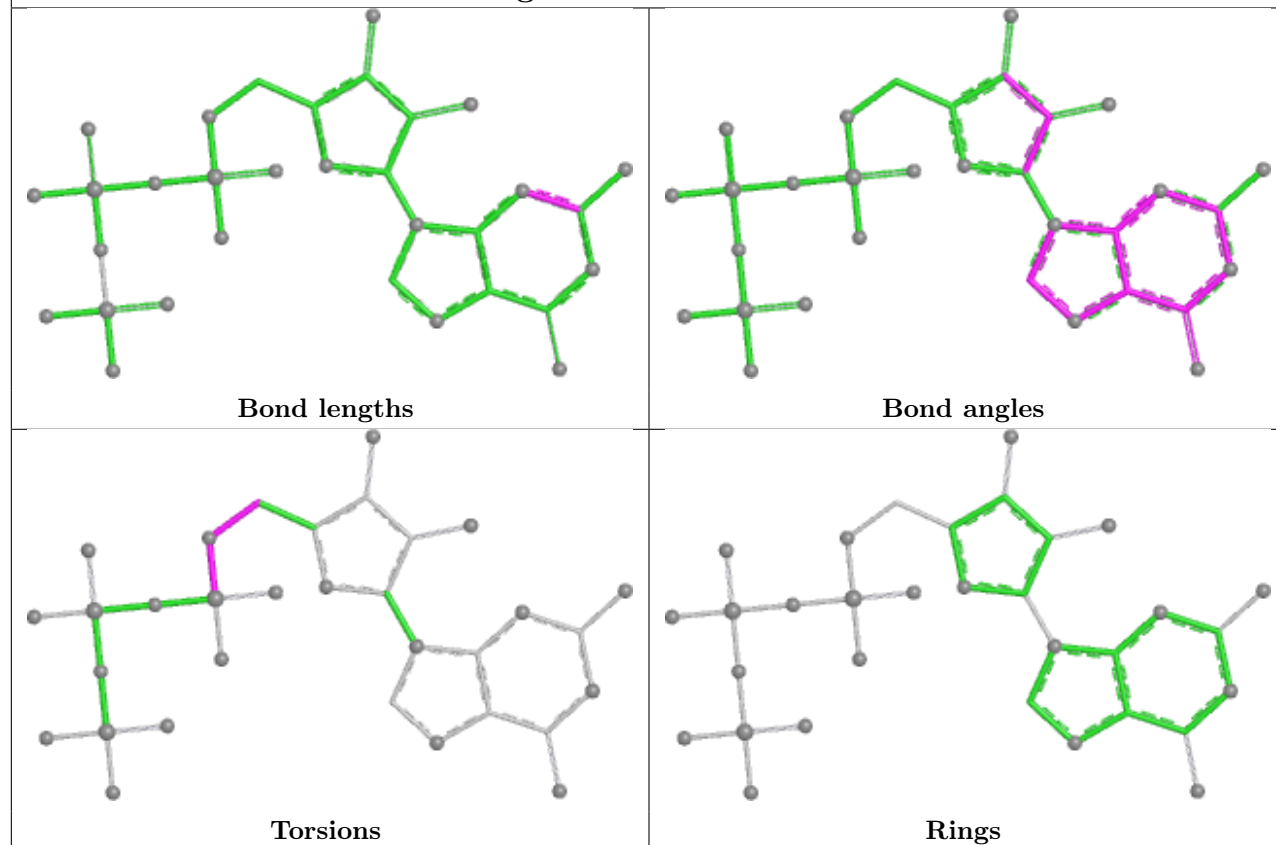




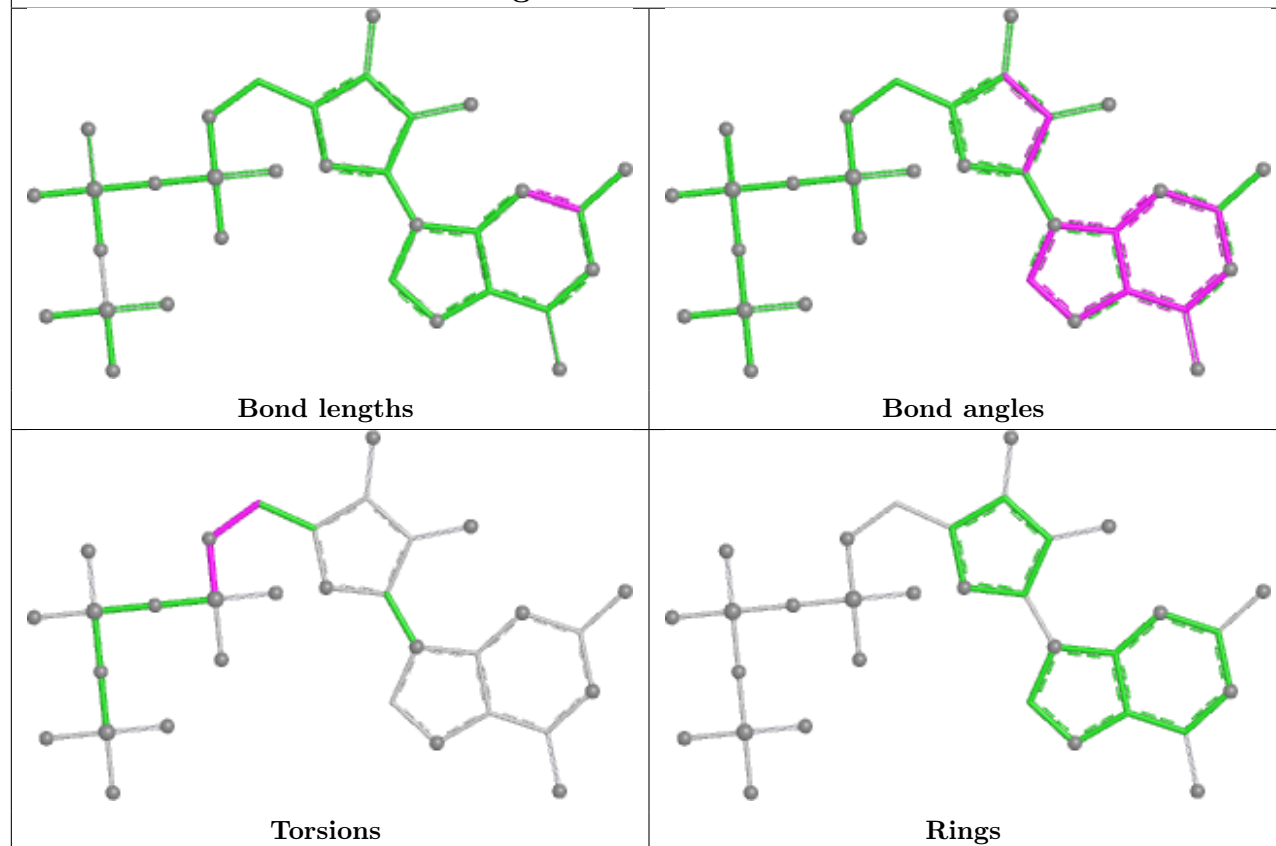




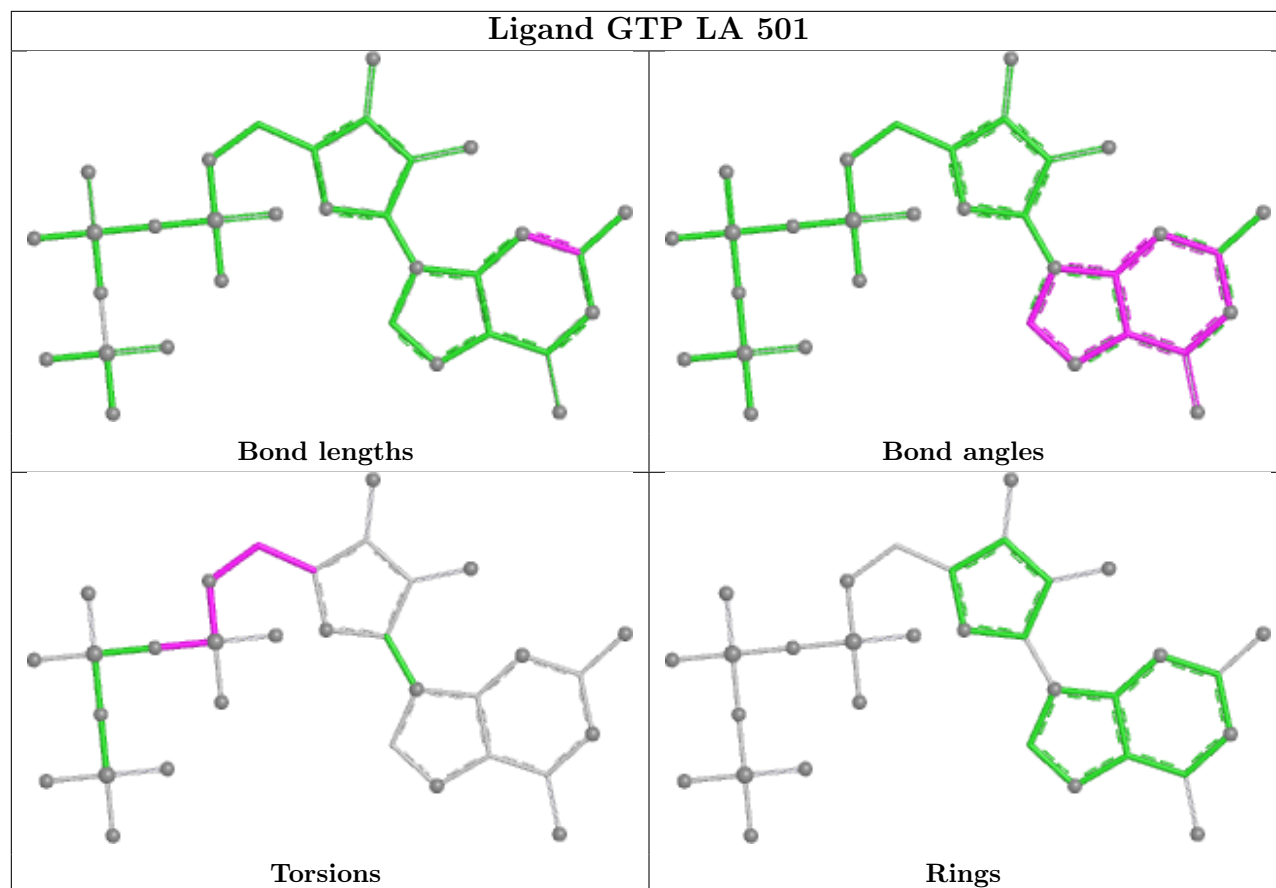
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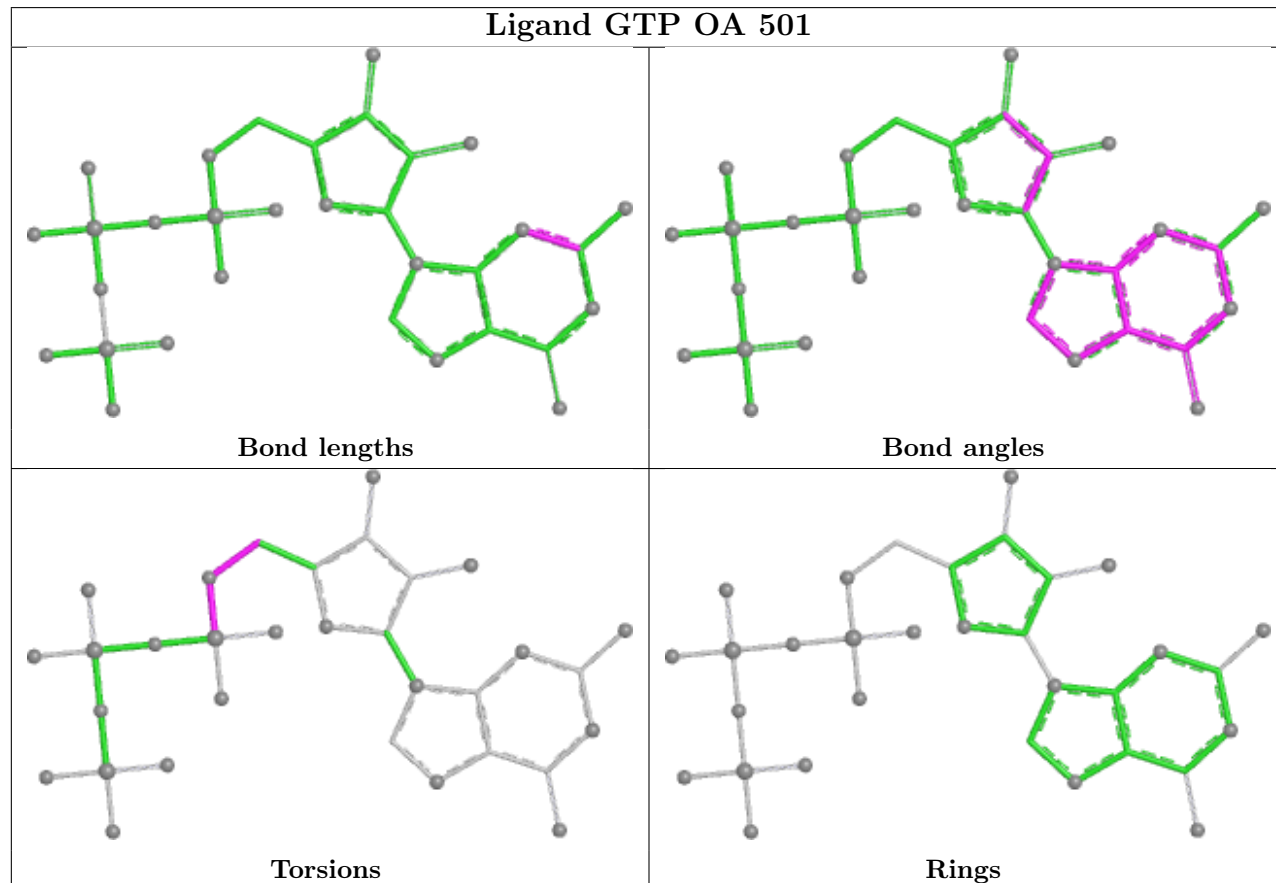
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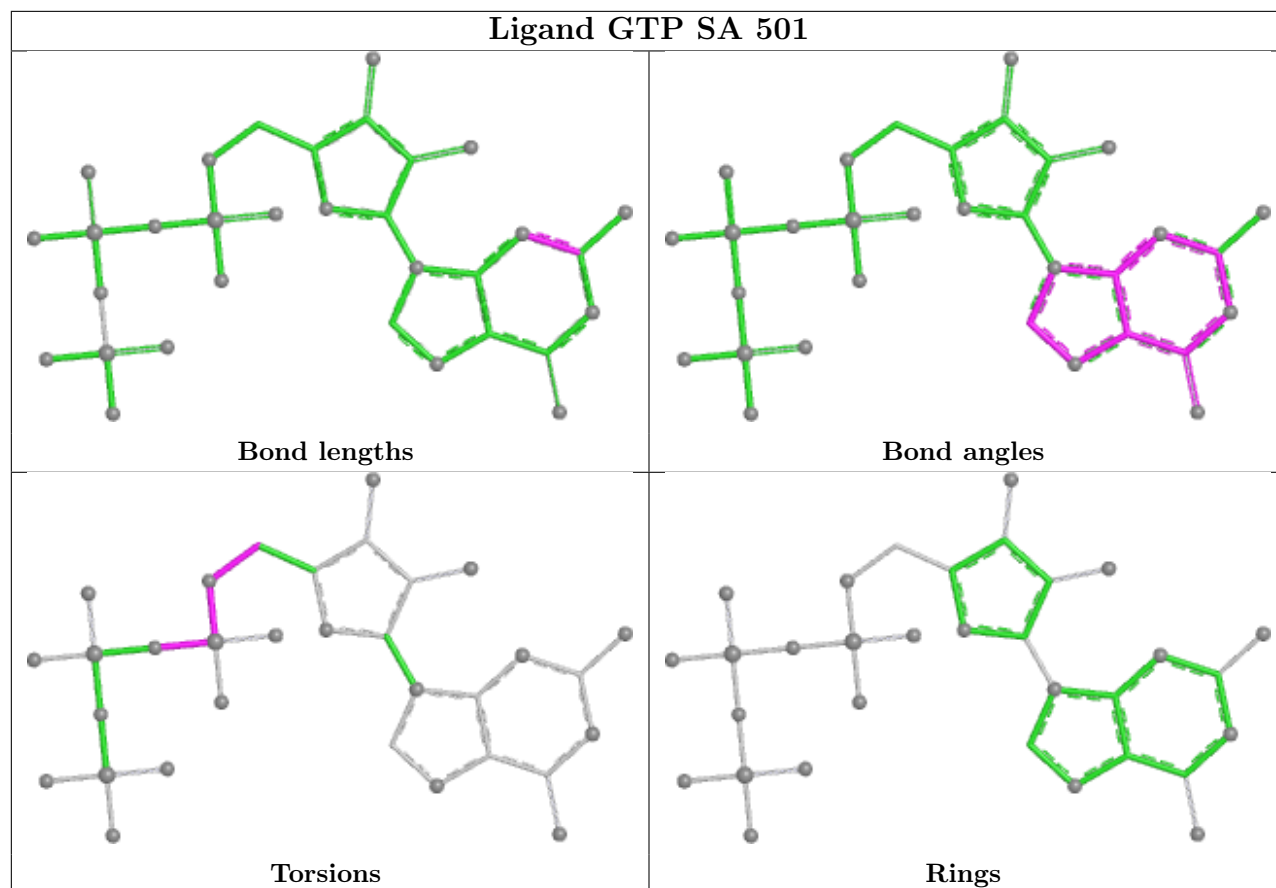
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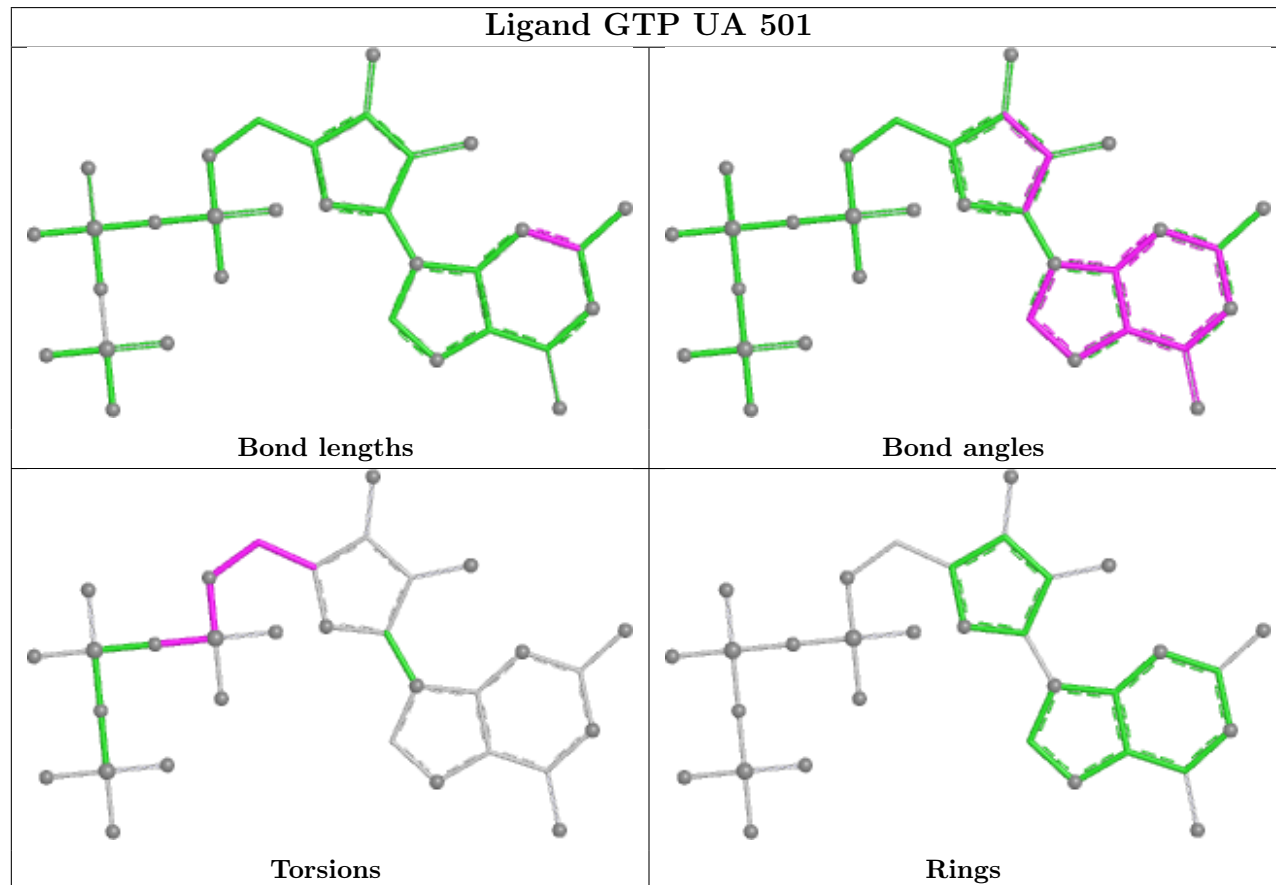
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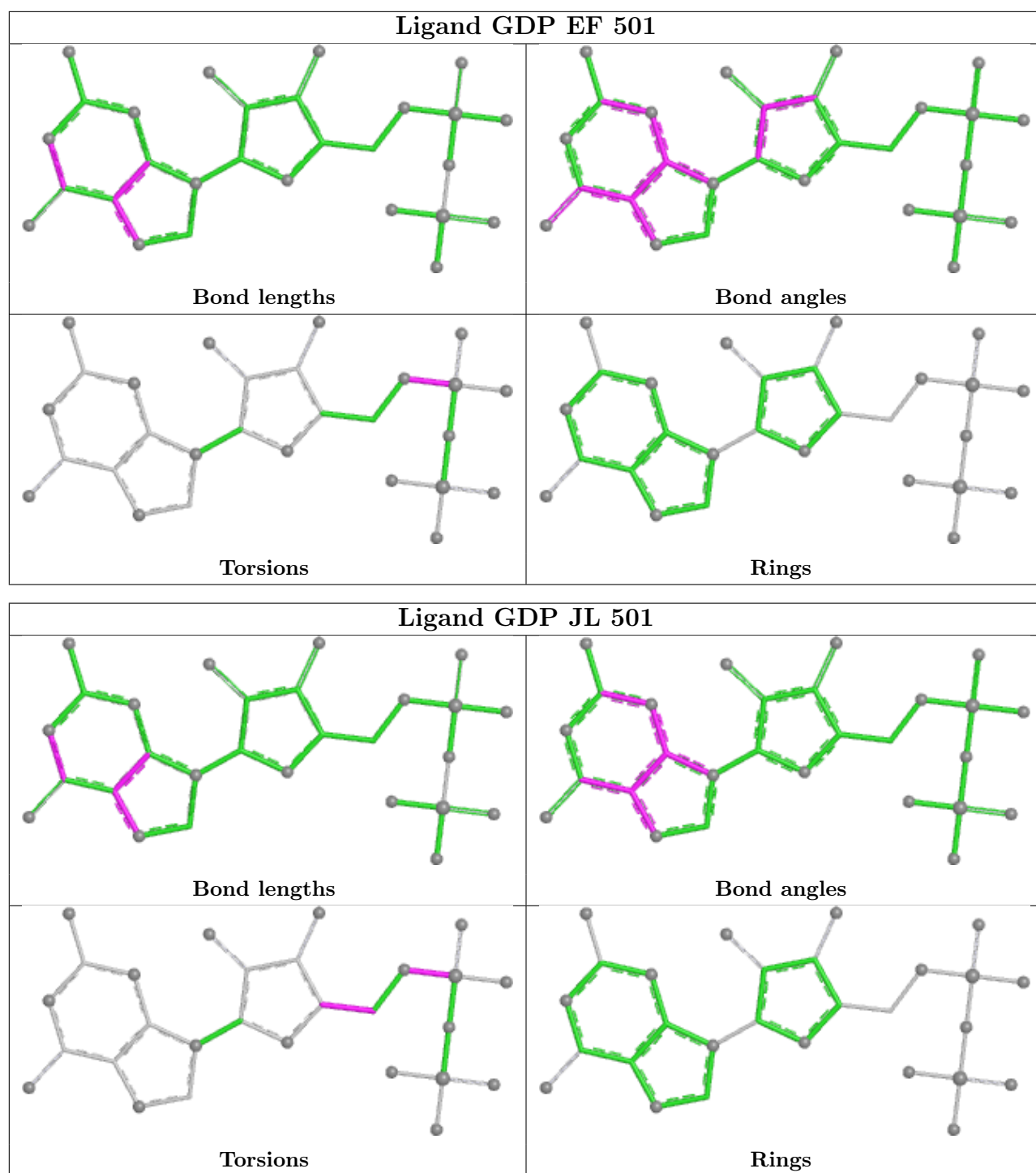


Ligand GTP SA 501

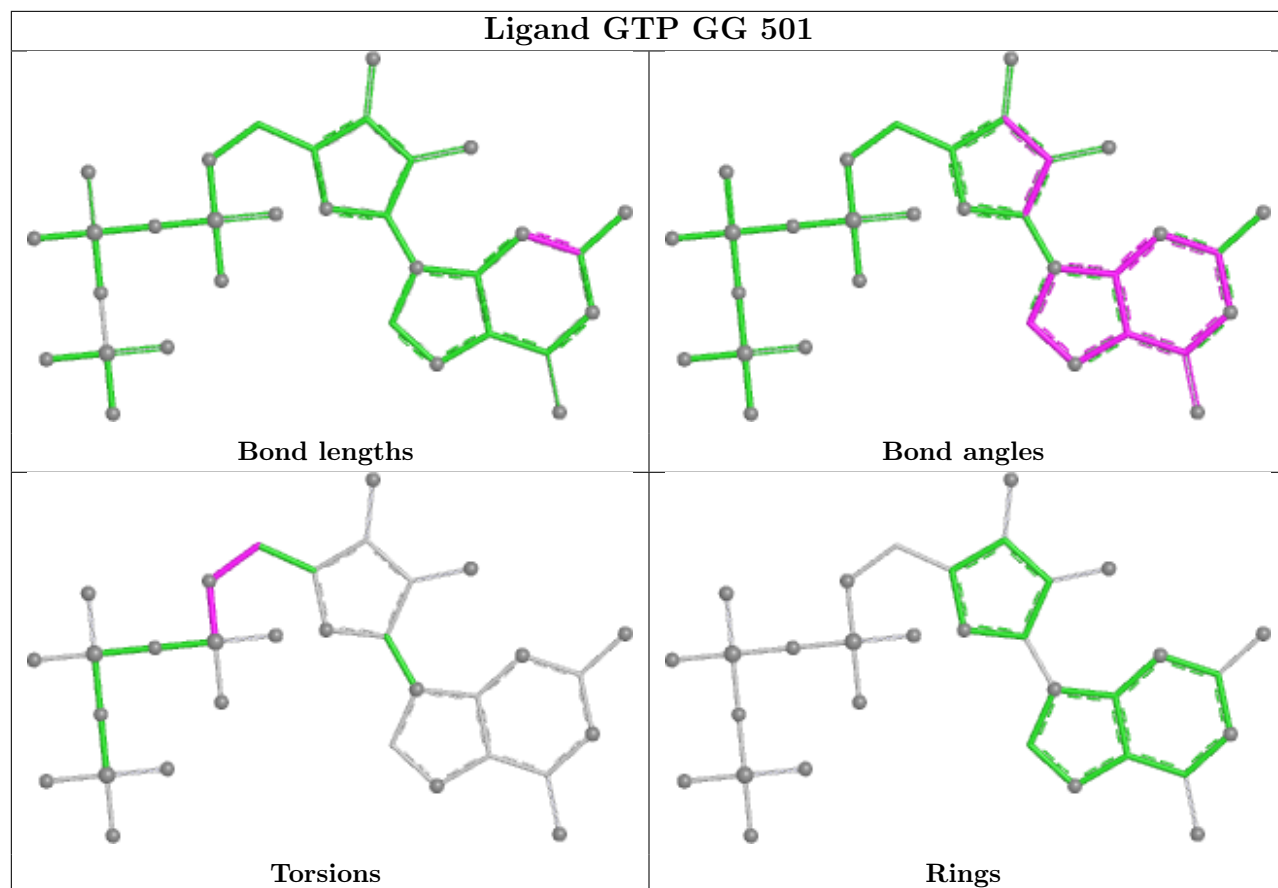


Ligand GTP UA 501

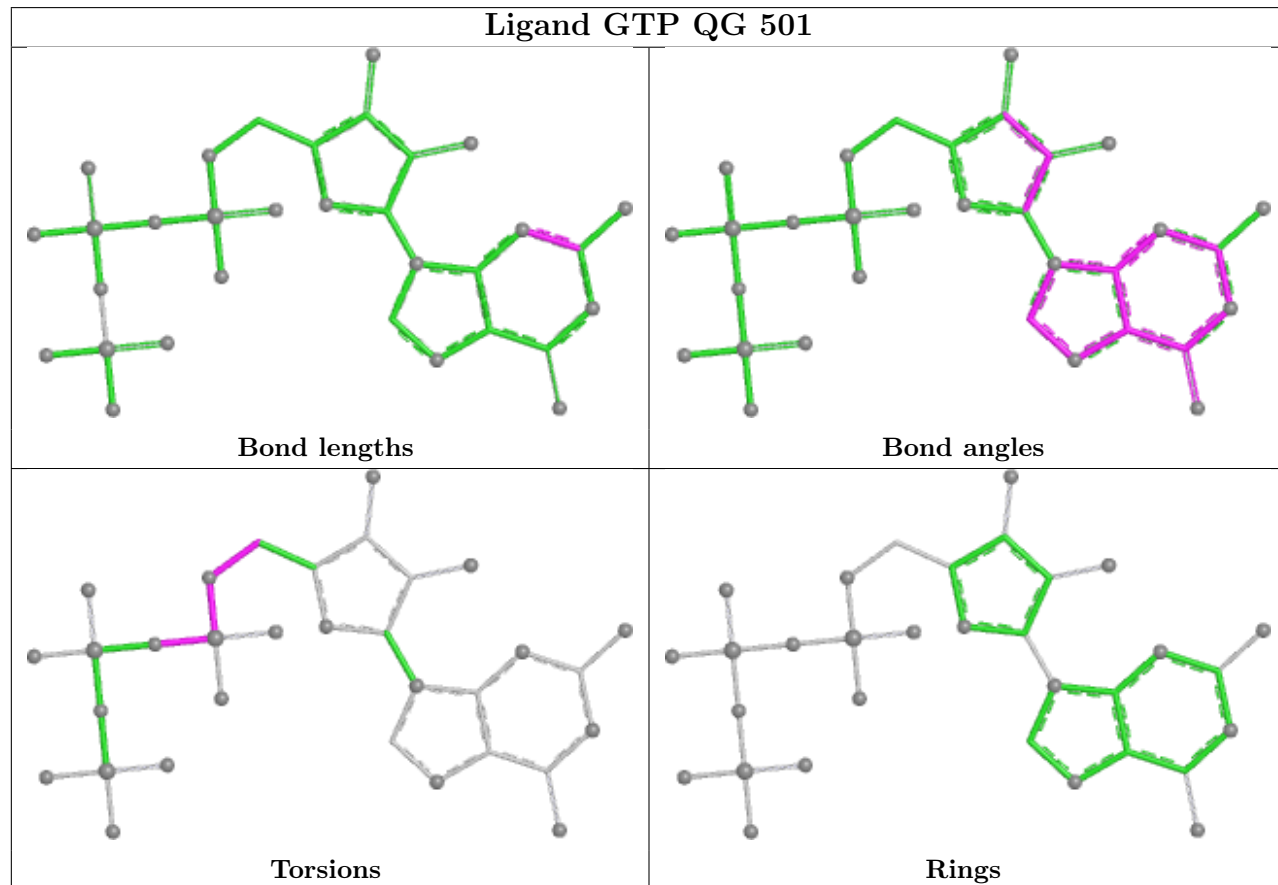


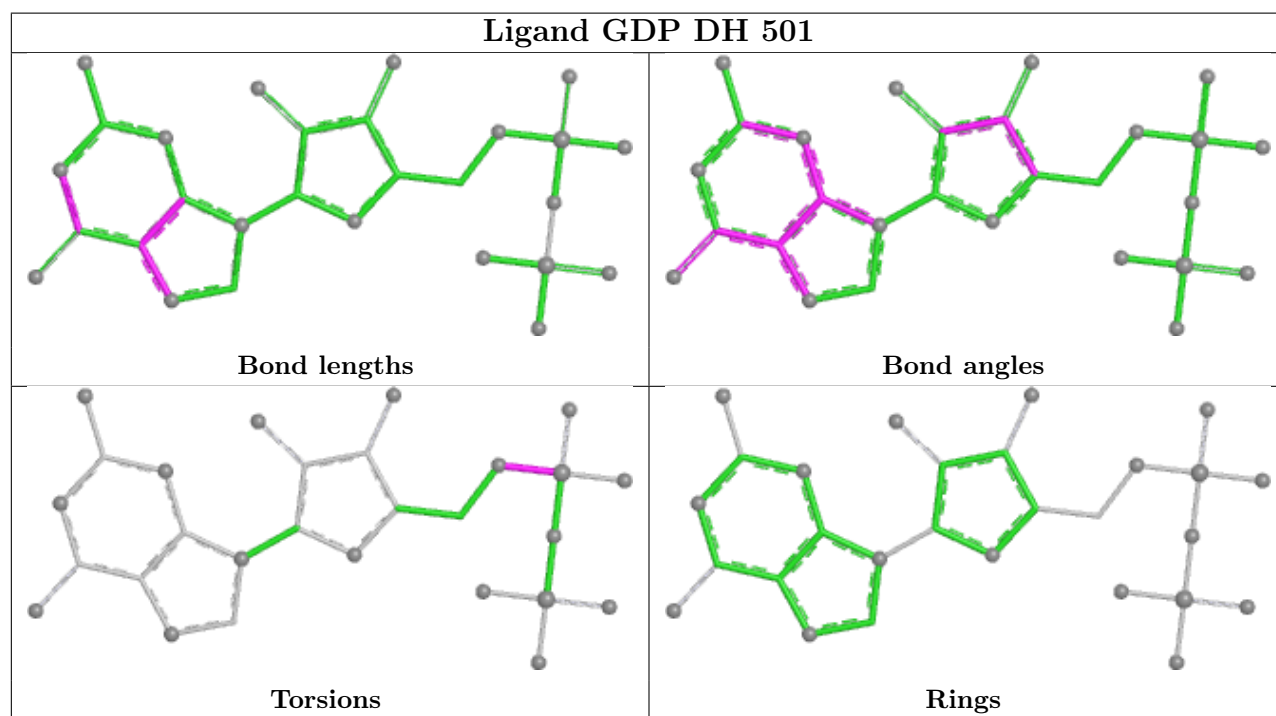
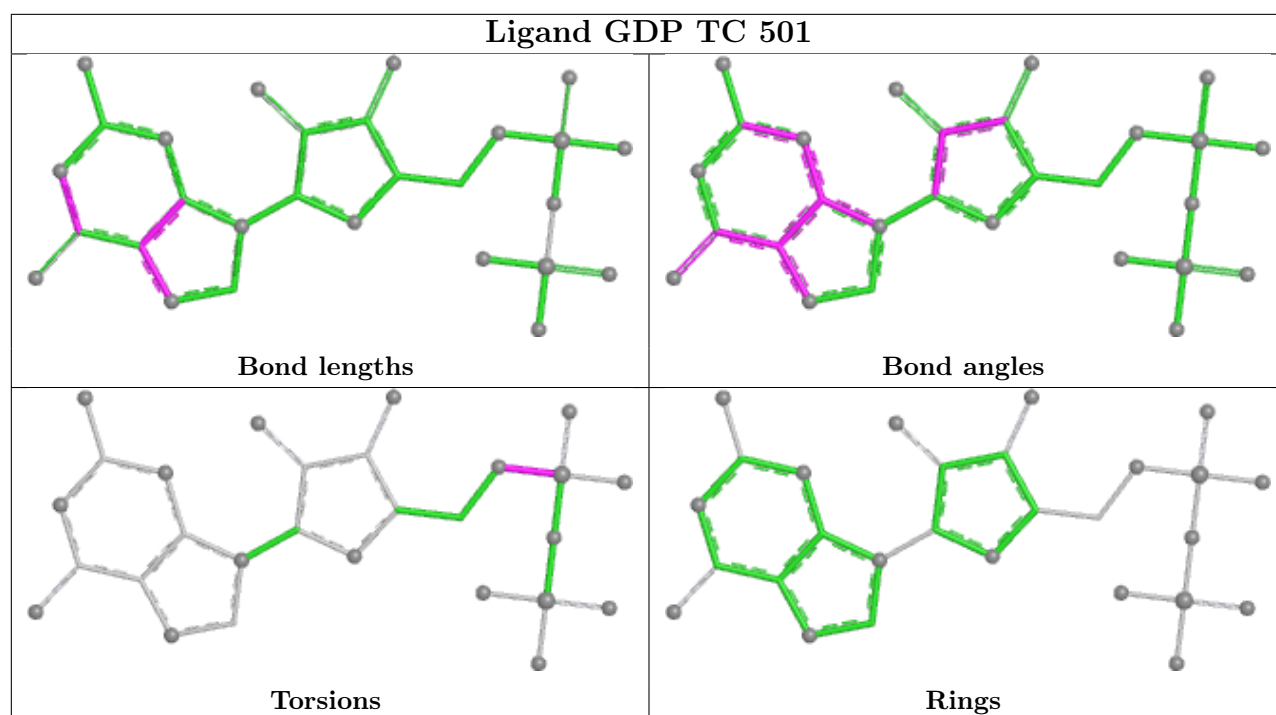


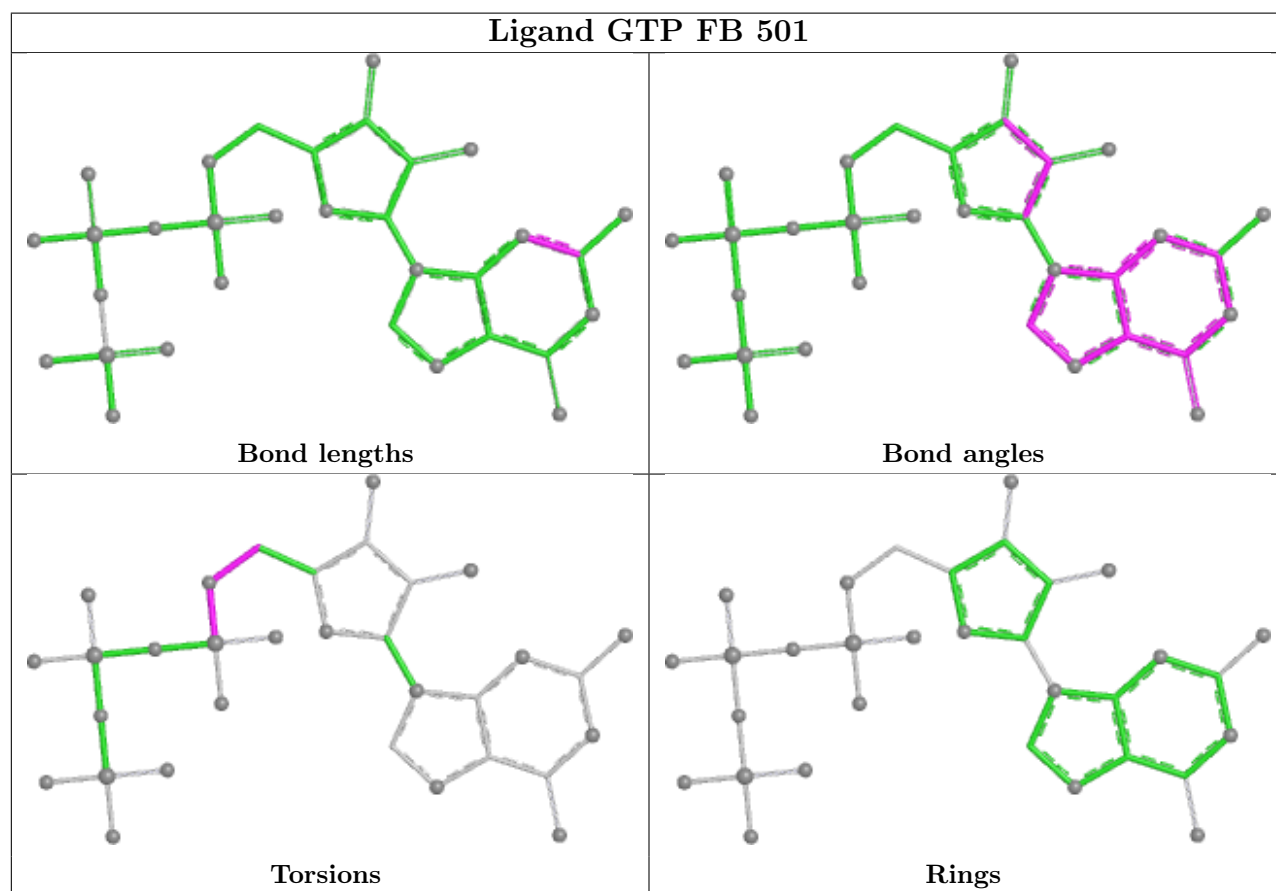
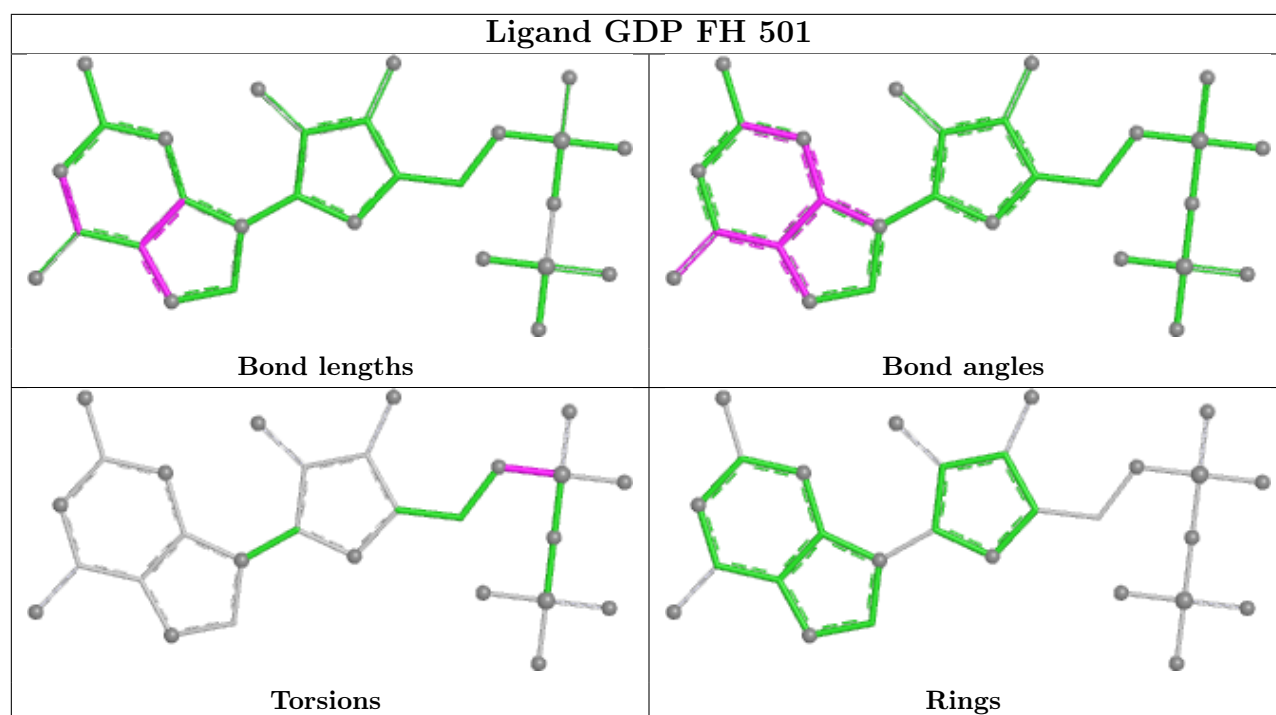
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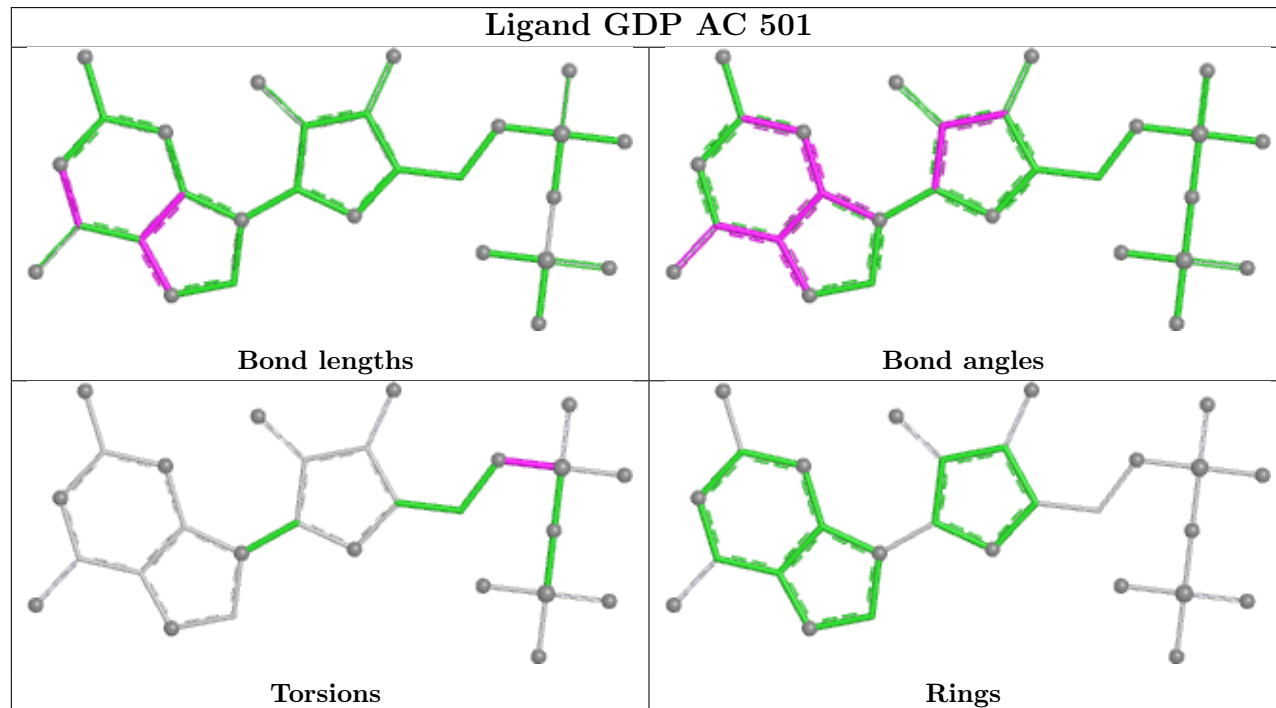
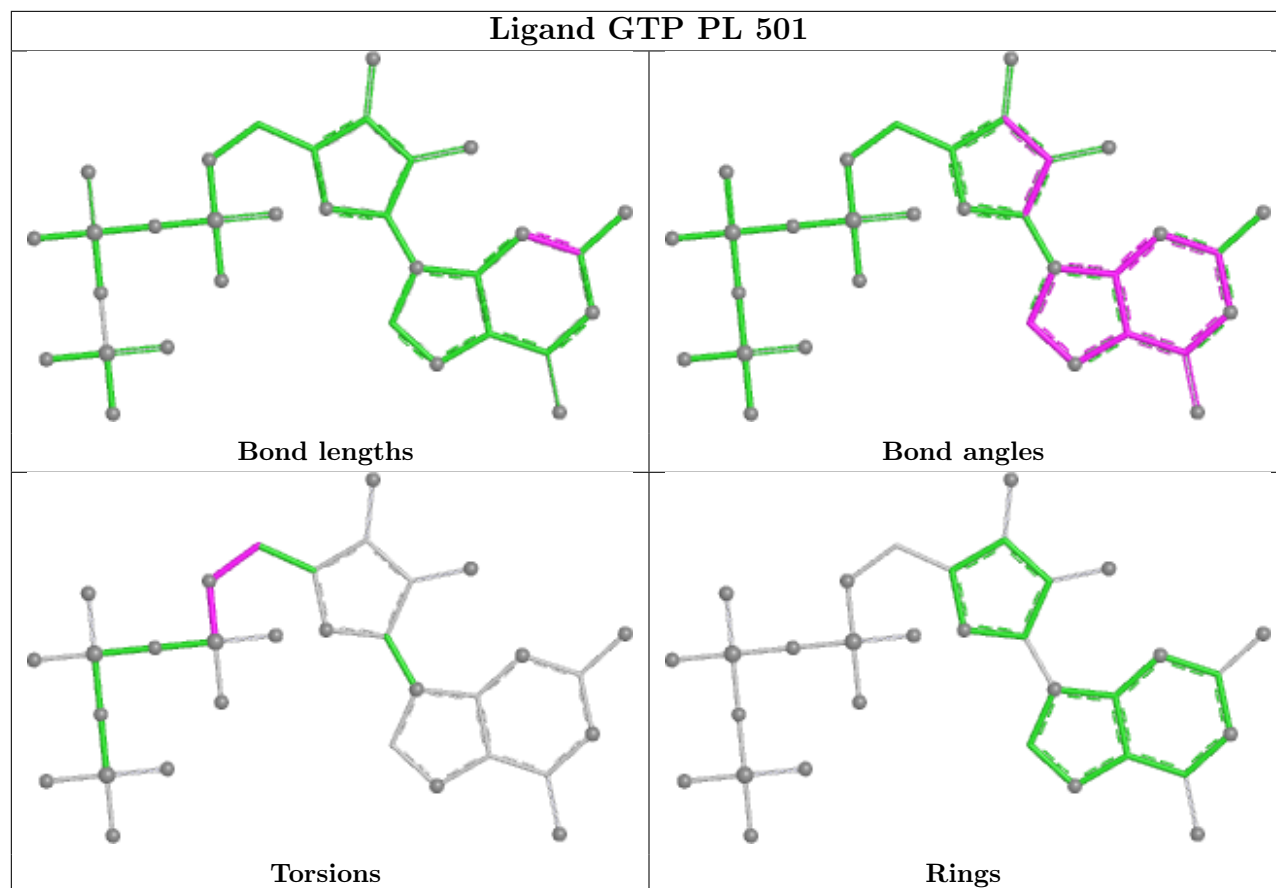


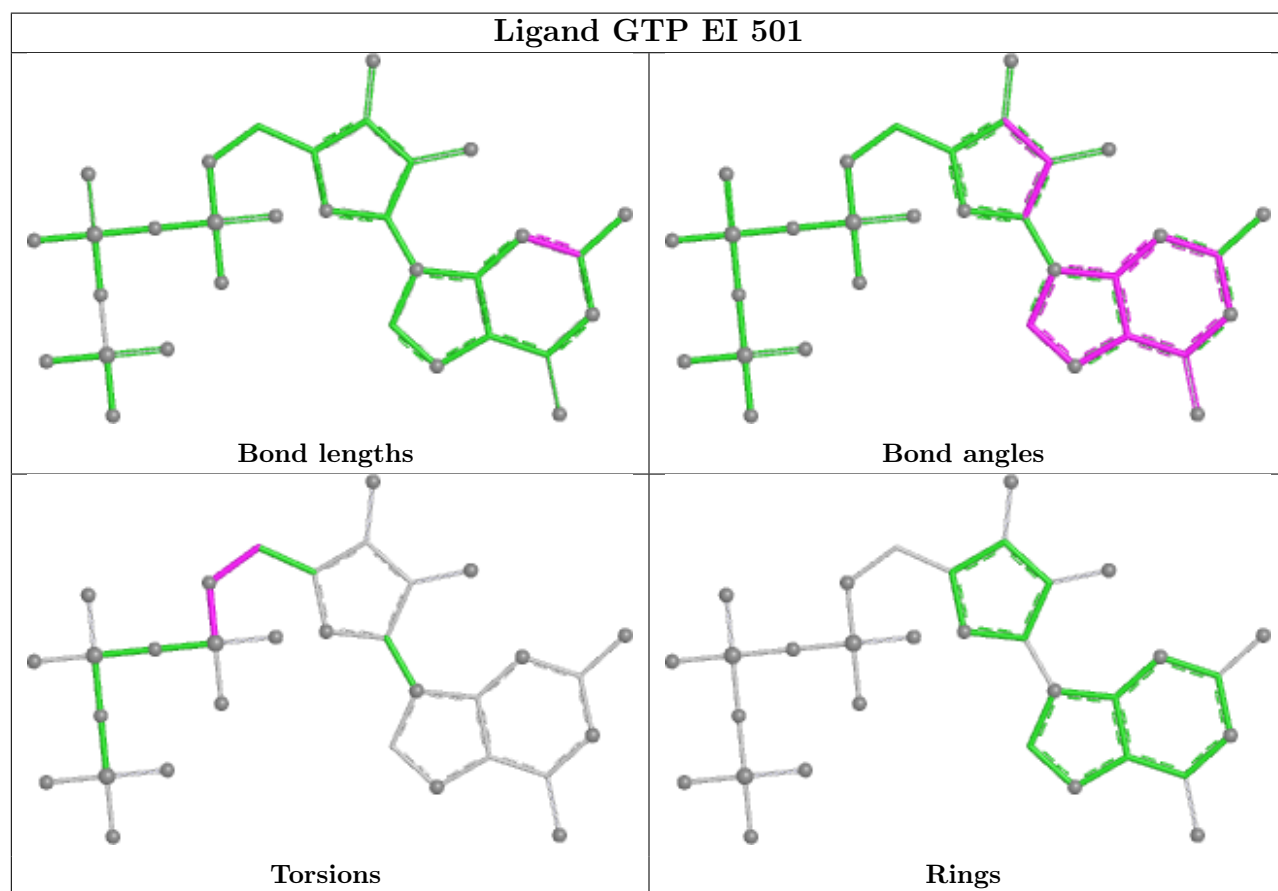
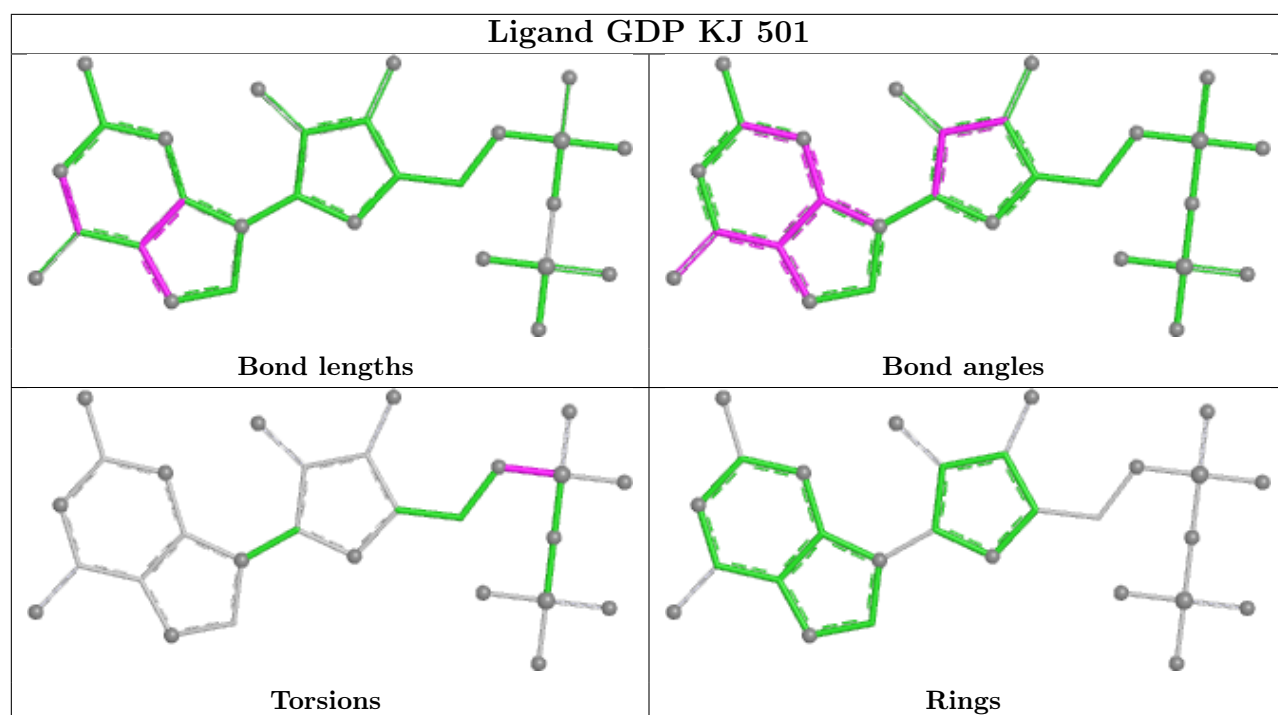
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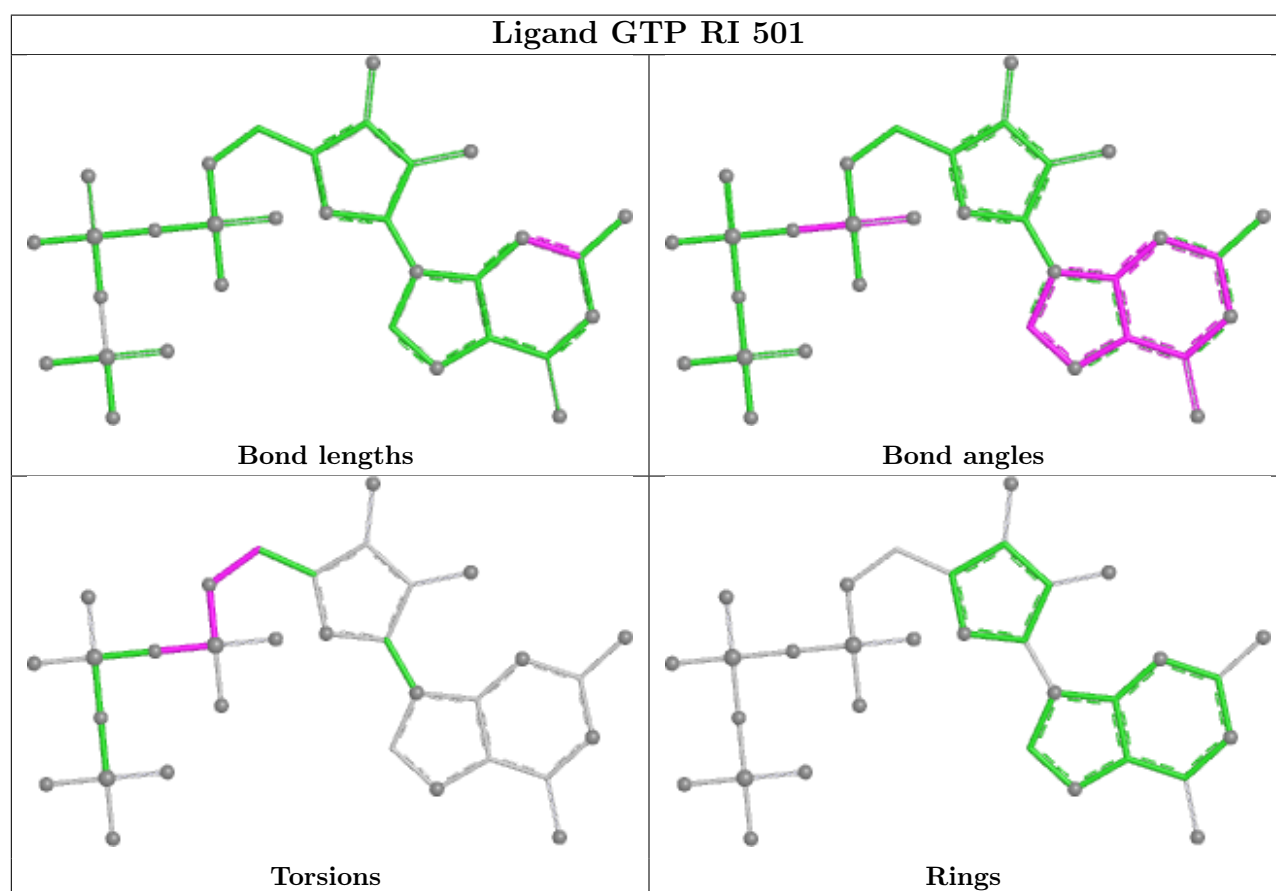
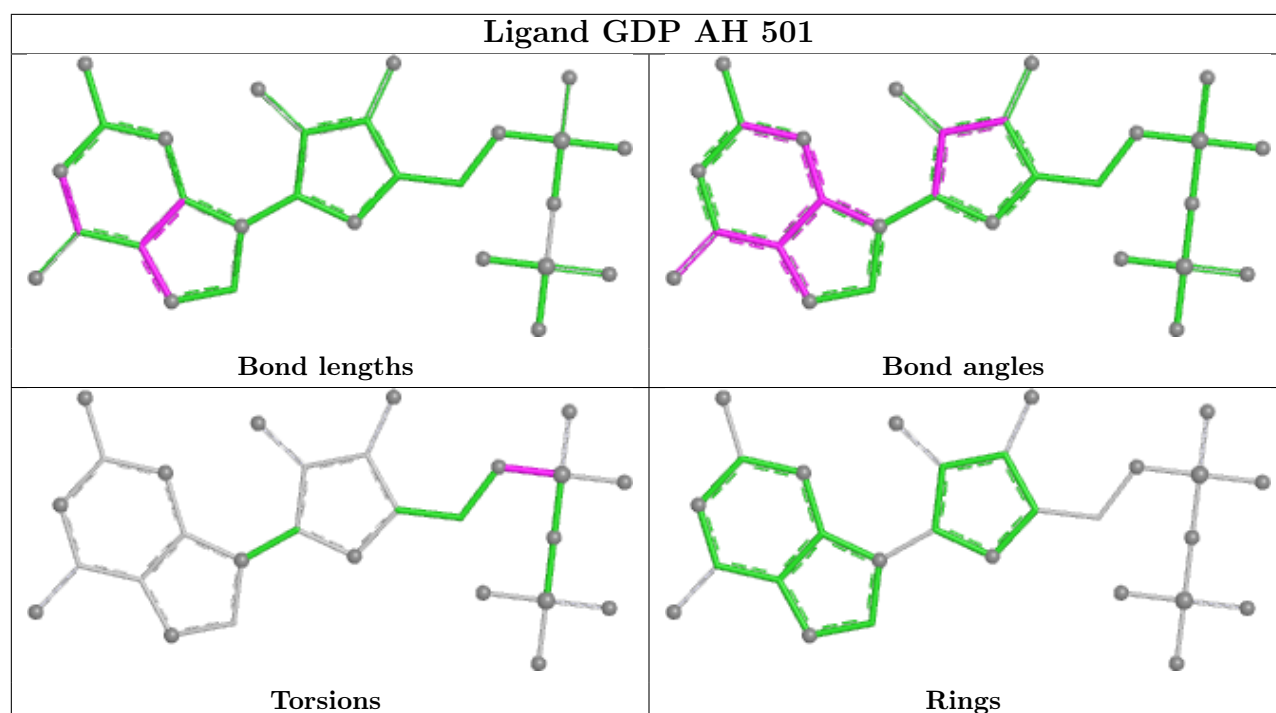


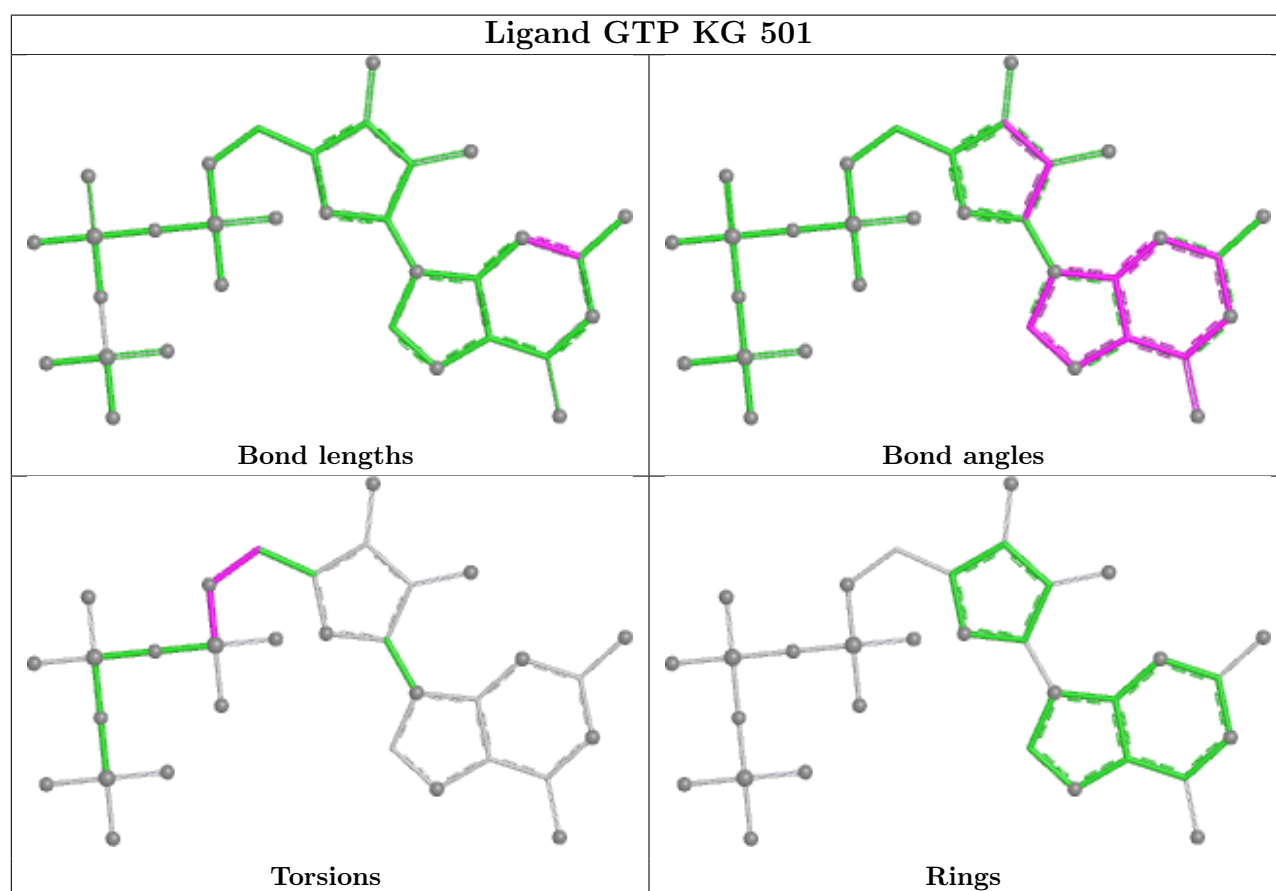
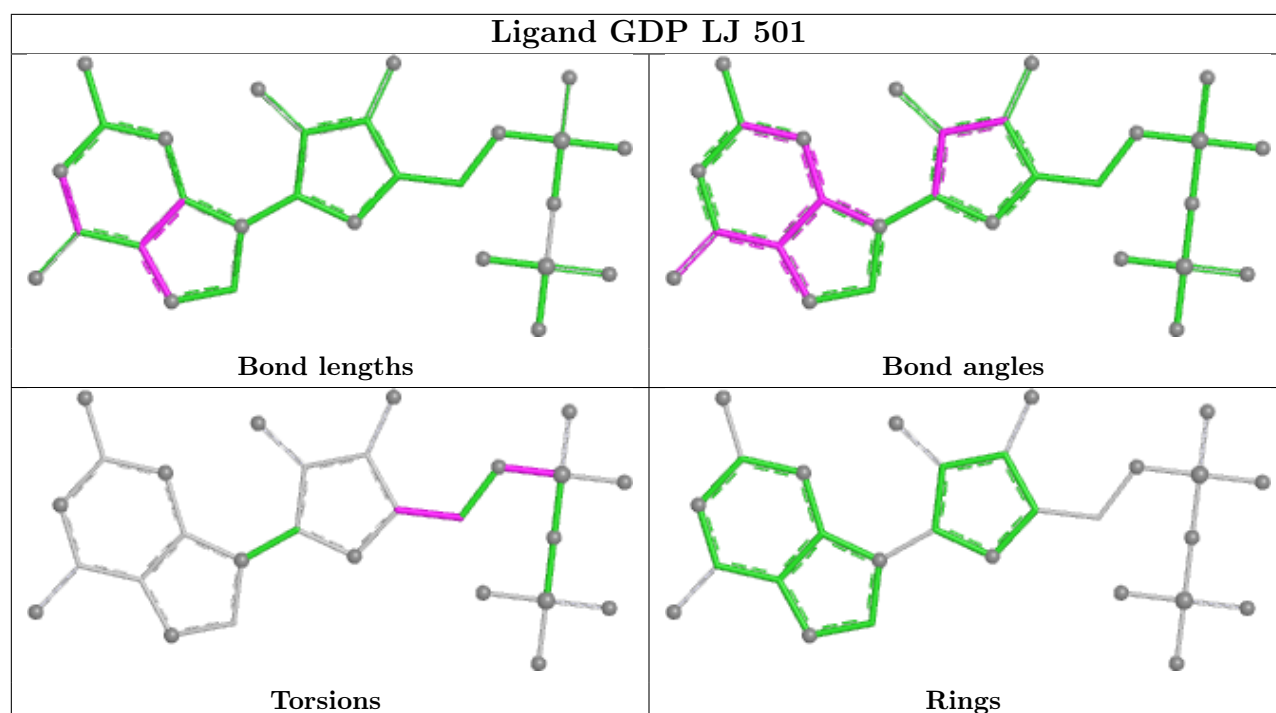


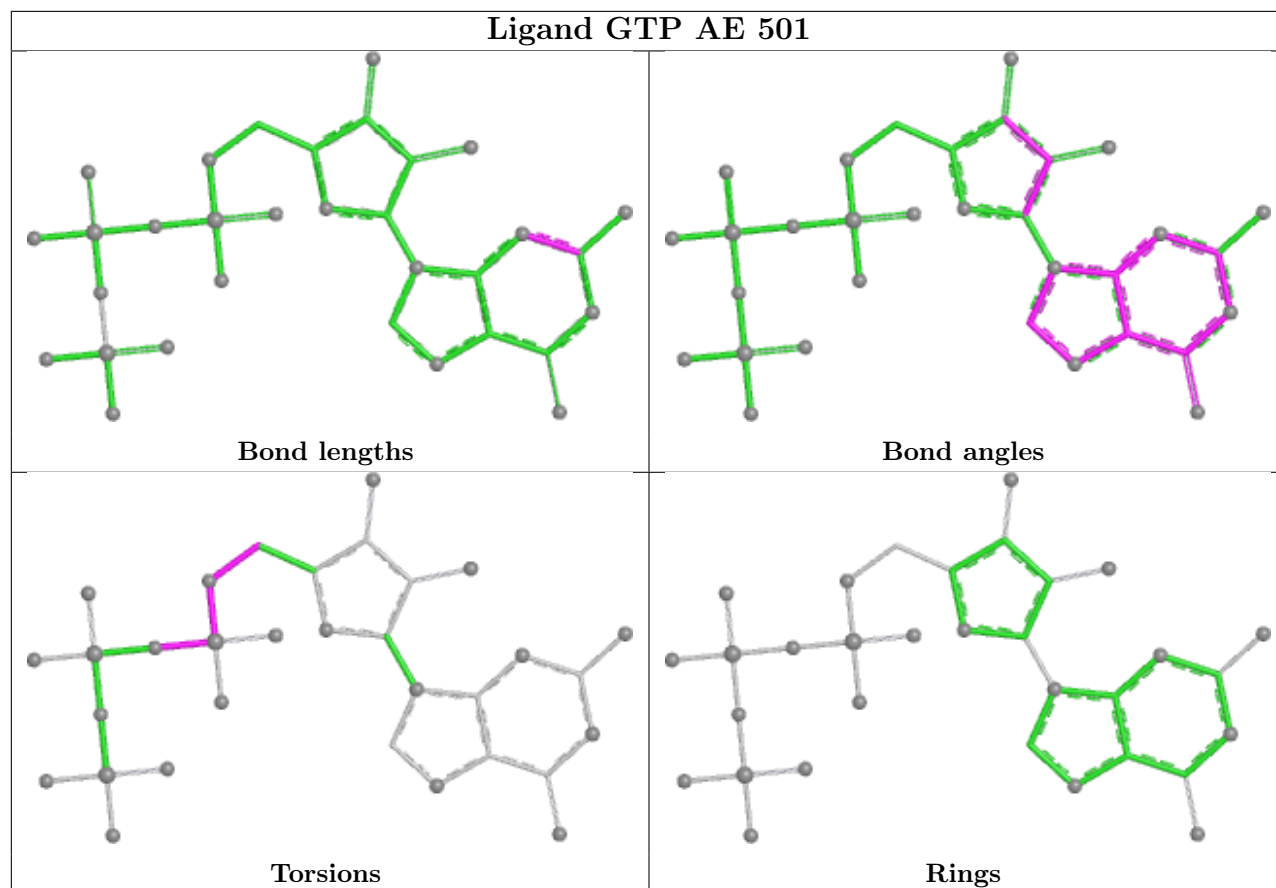












4.7 Other polymers [i](#)

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

This section contains visualisations of the EMDB entry EMD-40619. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

5.1 Orthogonal projections

This section was not generated.

5.2 Central slices

This section was not generated.

5.3 Largest variance slices

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

5.5 Orthogonal surface views

This section was not generated.

5.6 Mask visualisation

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

6 Map analysis ⓘ

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

6.1 Map-value distribution ⓘ

This section was not generated.

6.2 Volume estimate versus contour level ⓘ

This section was not generated.

6.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation ⓘ

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

8 Map-model fit

This section was not generated.