



## wwPDB EM Validation Summary Report ⓘ

Apr 1, 2026 – 04:04 AM UTC

PDB ID : 9CPB / pdb\_00009cpb  
EMDB ID : EMD-45801  
Title : Atomic model of bovine Fallopian tube cilia doublet microtubule (48-nm periodicity)  
Authors : Sun, C.; Zeng, J.; Zhang, R.  
Deposited on : 2024-07-18  
Resolution : 3.52 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : **FAILED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

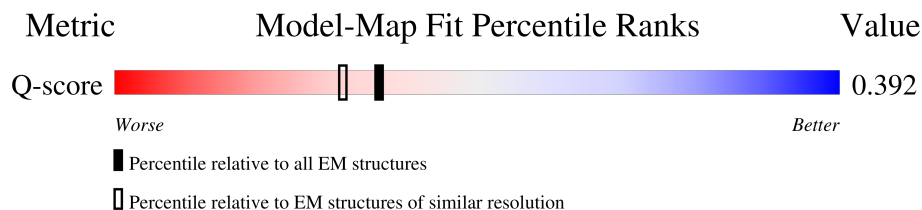
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.52 Å.

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



Metric	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	13017 ( 3.02 - 4.02 )

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

## 2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 1132145 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 Armadillo repeat containing 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1A	493	Total	C	N	O	0	0
			2437	1451	493	493		

- Molecule 2 is a protein called Coiled-coil domain containing 114.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1D	134	Total	C	N	O	S	0	0
			1109	675	215	216	3		
2	1E	187	Total	C	N	O	S	0	0
			1569	955	314	294	6		
2	1F	83	Total	C	N	O	S	0	0
			698	424	145	125	4		

- Molecule 3 is a protein called Coiled-coil domain containing 173.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1H	83	Total	C	N	O	S	0	0
			685	426	121	136	2		
3	1I	377	Total	C	N	O	S	0	0
			3234	2007	605	612	10		

- Molecule 4 is a protein called Uncharacterized protein C1orf158 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1K	159	Total	C	N	O	S	0	0
			1348	877	241	229	1		
4	1L	32	Total	C	N	O		0	0
			269	170	48	51			

- Molecule 5 is a protein called Protein Flattop.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1N	114	Total	C	N	O	S	0	0
			894	569	162	161	2		
5	1O	116	Total	C	N	O	S	0	0
			910	580	165	163	2		
5	1P	118	Total	C	N	O	S	0	0
			928	590	169	167	2		

- Molecule 6 is a protein called CFAP141.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1R	91	Total	C	N	O	S	0	0
			785	495	151	133	6		

- Molecule 7 is a protein called Cilia and flagella associated protein 161.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1T	255	Total	C	N	O	S	0	0
			2055	1302	369	373	11		
7	1U	255	Total	C	N	O	S	0	0
			2055	1302	369	373	11		

- Molecule 8 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1W	136	Total	C	N	O	S	0	0
			1143	741	196	200	6		
8	1X	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		
8	1Y	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		
8	1Z	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		
8	2A	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		
8	2B	184	Total	C	N	O	S	0	0
			1532	984	268	273	7		

- Molecule 9 is a protein called EF-hand domain family member B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2D	451	Total	C	N	O	S	0	0
			3649	2326	650	660	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	2E	101	Total	C	N	O	S	0	0
			816	513	145	156	2		

- Molecule 10 is a protein called CFAP276.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2F	79	Total	C	N	O		0	0
			631	395	116	120			
10	2G	79	Total	C	N	O		0	0
			631	395	116	120			
10	2H	79	Total	C	N	O		0	0
			631	395	116	120			

- Molecule 11 is a protein called Cilia and flagella associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2J	162	Total	C	N	O	S	0	0
			1349	837	245	258	9		
11	2K	296	Total	C	N	O	S	0	0
			2554	1543	517	485	9		
11	2L	275	Total	C	N	O	S	0	0
			2330	1426	438	450	16		
11	2M	186	Total	C	N	O	S	0	0
			1589	961	327	299	2		

- Molecule 12 is a protein called Cilia and flagella associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2O	609	Total	C	N	O	S	0	0
			4713	2985	822	874	32		
12	2P	609	Total	C	N	O	S	0	0
			4713	2985	822	874	32		
12	2Q	609	Total	C	N	O	S	0	0
			4713	2985	822	874	32		

- Molecule 13 is a protein called Methyl-CpG binding domain protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2S	281	Total	C	N	O	S	0	0
			2081	1267	402	403	9		
13	2T	199	Total	C	N	O	S	0	0
			1694	1032	321	329	12		

- Molecule 14 is a protein called Cilia and flagella associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2V	34	Total	C	N	O	S	0	0
			287	183	56	46	2		
14	2W	215	Total	C	N	O	S	0	0
			1756	1109	335	303	9		
14	2X	210	Total	C	N	O	S	0	0
			1711	1080	326	296	9		
14	2Y	165	Total	C	N	O	S	0	0
			1327	838	250	232	7		

- Molecule 15 is a protein called CFAP95.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3A	183	Total	C	N	O	S	0	0
			1487	932	258	288	9		

- Molecule 16 is a protein called Cilia-and flagella-associated protein 96.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3C	211	Total	C	N	O	S	0	0
			1693	1077	291	318	7		
16	3D	71	Total	C	N	O	S	0	0
			531	339	94	95	3		

- Molecule 17 is a protein called EF-hand calcium-binding domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3F	105	Total	C	N	O		0	0
			520	310	105	105			

- Molecule 18 is a protein called EF-hand calcium binding domain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3H	97	Total	C	N	O		0	0
			481	287	97	97			

- Molecule 19 is a protein called EF-hand domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3J	431	Total	C	N	O	S	0	0
			3563	2303	597	649	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	3K	443	Total	C	N	O	S	0	0
			3652	2361	613	664	14		
19	3L	452	Total	C	N	O	S	0	0
			3726	2406	627	678	15		

- Molecule 20 is a protein called EFHC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3N	286	Total	C	N	O	S	0	0
			2388	1534	406	438	10		
20	3O	579	Total	C	N	O	S	0	0
			4781	3067	810	878	26		
20	3P	581	Total	C	N	O	S	0	0
			4787	3070	808	884	25		
20	3Q	290	Total	C	N	O	S	0	0
			2409	1545	404	445	15		

- Molecule 21 is a protein called Enkurin, TRPC channel interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3S	70	Total	C	N	O	S	0	0
			563	356	95	110	2		
21	3T	235	Total	C	N	O	S	0	0
			1939	1242	336	354	7		
21	3U	235	Total	C	N	O	S	0	0
			1939	1242	336	354	7		
21	3V	205	Total	C	N	O	S	0	0
			1696	1087	295	307	7		

- Molecule 22 is a protein called Protein FAM166B.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3X	129	Total	C	N	O	S	0	0
			1014	662	172	174	6		
22	3Y	142	Total	C	N	O	S	0	0
			1116	732	189	189	6		
22	3Z	135	Total	C	N	O	S	0	0
			1059	690	181	182	6		
22	4A	107	Total	C	N	O	S	0	0
			840	548	142	144	6		
22	4B	105	Total	C	N	O	S	0	0
			830	538	143	143	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
22	4C	85	Total	C	N	O	S	0	0
			667	433	111	118	5		

- Molecule 23 is a protein called Cilia- and flagella-associated protein 144.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4D	116	Total	C	N	O	S	0	0
			992	627	186	177	2		

- Molecule 24 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4F	151	Total	C	N	O	S	0	0
			1261	772	241	244	4		
24	4G	335	Total	C	N	O	S	0	0
			2883	1786	528	553	16		

- Molecule 25 is a protein called Nucleoside diphosphate kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4I	372	Total	C	N	O	S	0	0
			2533	1589	451	481	12		
25	4J	372	Total	C	N	O	S	0	0
			2947	1880	499	546	22		

- Molecule 26 is a protein called Outer dynein arm-docking complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4K	132	Total	C	N	O	S	0	0
			1102	683	204	212	3		
26	4L	228	Total	C	N	O	S	0	0
			1911	1190	353	364	4		
26	4M	104	Total	C	N	O	S	0	0
			876	549	164	162	1		

- Molecule 27 is a protein called PACRG protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4O	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		
27	4P	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	4Q	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		
27	4R	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		
27	4S	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		
27	4T	219	Total	C	N	O	S	0	0
			1767	1144	298	316	9		

- Molecule 28 is a protein called Pierce1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4V	37	Total	C	N	O	S	0	0
			304	191	52	58	3		
28	4W	79	Total	C	N	O	S	0	0
			654	415	118	119	2		

- Molecule 29 is a protein called Pierce2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4Y	96	Total	C	N	O	S	0	0
			775	496	130	142	7		

- Molecule 30 is a protein called RIB43A-like with coiled-coils protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5A	350	Total	C	N	O	S	0	0
			2915	1775	574	553	13		
30	5B	16	Total	C	N	O		0	0
			133	81	24	28			

- Molecule 31 is a protein called Sperm acrosome associated 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5D	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		
31	5E	157	Total	C	N	O	S	0	0
			1254	784	222	237	11		
31	5F	159	Total	C	N	O	S	0	0
			1277	799	228	239	11		
31	5G	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	5H	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		
31	5I	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		
31	5J	157	Total	C	N	O	S	0	0
			1260	787	225	237	11		

- Molecule 32 is a protein called Tektin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5L	116	Total	C	N	O	S	0	0
			943	585	176	180	2		
32	5M	392	Total	C	N	O	S	0	0
			3231	2011	588	623	9		
32	5N	392	Total	C	N	O	S	0	0
			3231	2011	588	623	9		
32	5O	291	Total	C	N	O	S	0	0
			2414	1505	434	468	7		

- Molecule 33 is a protein called Tektin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5Q	109	Total	C	N	O	S	0	0
			901	548	176	175	2		
33	5R	399	Total	C	N	O	S	0	0
			3250	2002	602	632	14		
33	5S	399	Total	C	N	O	S	0	0
			3250	2002	602	632	14		
33	5T	306	Total	C	N	O	S	0	0
			2498	1546	453	486	13		
33	5V	308	Total	C	N	O	S	0	0
			2513	1560	453	487	13		
33	5W	408	Total	C	N	O	S	0	0
			3336	2055	618	649	14		
33	5X	408	Total	C	N	O	S	0	0
			3336	2055	618	649	14		
33	5Y	107	Total	C	N	O	S	0	0
			877	533	170	172	2		

- Molecule 34 is a protein called Tektin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	6A	273	Total	C	N	O	S	0	0
			2240	1377	412	440	11		
34	6B	392	Total	C	N	O	S	0	0
			3189	1962	583	629	15		
34	6C	393	Total	C	N	O	S	0	0
			3200	1968	587	630	15		
34	6D	123	Total	C	N	O	S	0	0
			992	612	180	197	3		
34	6E	59	Total	C	N	O	S	0	0
			487	301	91	93	2		
34	6F	358	Total	C	N	O	S	0	0
			2896	1786	526	569	15		
34	6G	416	Total	C	N	O	S	0	0
			3386	2084	618	667	17		
34	6H	368	Total	C	N	O	S	0	0
			2989	1840	545	589	15		
34	6I	63	Total	C	N	O	S	0	0
			531	324	101	104	2		
34	6J	65	Total	C	N	O	S	0	0
			553	347	100	105	1		
34	6K	371	Total	C	N	O	S	0	0
			3022	1869	546	593	14		
34	6L	418	Total	C	N	O	S	0	0
			3411	2107	621	667	16		
34	6M	361	Total	C	N	O	S	0	0
			2923	1804	532	572	15		
34	6N	54	Total	C	N	O	S	0	0
			445	275	83	85	2		

- Molecule 35 is a protein called Tektin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	6P	180	Total	C	N	O	S	0	0
			1491	915	272	298	6		
35	6Q	410	Total	C	N	O	S	0	0
			3364	2070	628	651	15		
35	6R	410	Total	C	N	O	S	0	0
			3364	2070	628	651	15		
35	6S	254	Total	C	N	O	S	0	0
			2057	1269	390	389	9		
35	6T	236	Total	C	N	O	S	0	0
			1917	1184	365	359	9		
35	6U	419	Total	C	N	O	S	0	0
			3413	2097	638	663	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
35	6V	437	Total	C	N	O	S	0	0
			3571	2201	666	688	16		
35	6W	215	Total	C	N	O	S	0	0
			1766	1088	324	347	7		

- Molecule 36 is a protein called TTC25 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	6Y	192	Total	C	N	O	S	0	0
			1300	812	232	249	7		
36	6Z	192	Total	C	N	O	S	0	0
			1300	812	232	249	7		

- Molecule 37 is a protein called Ciliary microtubule associated protein 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	7C	119	Total	C	N	O	S	0	0
			898	571	159	163	5		
37	7D	80	Total	C	N	O	S	0	0
			618	404	113	99	2		
37	7E	85	Total	C	N	O	S	0	0
			625	398	111	113	3		
37	7F	67	Total	C	N	O	S	0	0
			519	338	89	91	1		

- Molecule 38 is a protein called Ciliary microtubule associated protein 1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	7H	85	Total	C	N	O	S	0	0
			637	409	108	114	6		
38	7I	34	Total	C	N	O	S	0	0
			238	151	43	42	2		

- Molecule 39 is a protein called Cilia and flagella associated protein 90.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	7K	107	Total	C	N	O	S	0	0
			878	543	174	160	1		
39	7L	46	Total	C	N	O	S	0	0
			382	249	65	67	1		

- Molecule 40 is a protein called Sperm associated antigen 8.



Mol	Chain	Residues	Atoms					AltConf	Trace
40	7N	64	Total	C	N	O	S	0	0
			524	324	93	104	3		

- Molecule 41 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AB	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
41	AD	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
41	AF	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
41	AH	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
41	AJ	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
41	AL	436	Total	C	N	O	S	0	0
			3424	2150	584	664	26		
41	BB	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	BD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	BF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
41	BH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	BJ	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	BL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
41	CB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	CD	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	CF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
41	CH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	CJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
41	CL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
41	DB	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	DD	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	DF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	DH	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	DJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	DL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
41	ED	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	EF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	EH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	EJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	EL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
41	FD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	FF	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	FH	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	FJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	FL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
41	GD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	GF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	GH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	GJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	GL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
41	HB	426	Total 3348	C 2105	N 574	O 643	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	HD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	HF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
41	HH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	HJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
41	HL	425	Total	C	N	O	S	0	0
			3340	2100	573	642	25		
41	ID	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	IF	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
41	IH	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	IJ	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
41	IL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	IN	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
41	JD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	JF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	JH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	JJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	JL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	KD	428	Total	C	N	O	S	0	0
			3361	2112	576	647	26		
41	KF	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	KH	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		
41	KJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	KL	429	Total	C	N	O	S	0	0
			3368	2116	577	649	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	KN	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	LD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	LF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	LH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	LJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	LL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	LN	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	MD	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	MF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	MH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	MJ	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	ML	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	MN	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	NB	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	ND	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	NF	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	NH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	NJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	NL	396	Total 3118	C 1966	N 533	O 597	S 22	0	0
41	OB	425	Total 3339	C 2100	N 572	O 641	S 26	0	0
41	OD	424	Total 3327	C 2091	N 571	O 639	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	OF	425	Total 3339	C 2100	N 572	O 641	S 26	0	0
41	OH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	OJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	OL	424	Total 3327	C 2091	N 571	O 639	S 26	0	0
41	PB	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	PD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	PF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	PH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	PJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	PL	425	Total 3340	C 2100	N 573	O 642	S 25	0	0
41	QB	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	QD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	QF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	QH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	QJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	QL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	RB	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	RD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	RF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	RH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	RJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	RL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	SD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	SF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	SH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	SJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	SL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	TD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	TF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	TH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	TJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	TL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	UD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	UF	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	UH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	UJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	UL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0
41	VD	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	VF	427	Total 3356	C 2109	N 575	O 646	S 26	0	0
41	VH	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	VJ	428	Total 3361	C 2112	N 576	O 647	S 26	0	0
41	VL	426	Total 3348	C 2105	N 574	O 643	S 26	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	WD	427	Total	C	N	O	S	0	0
			3356	2109	575	646	26		
41	WF	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	WH	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	WJ	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	WL	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		
41	WN	426	Total	C	N	O	S	0	0
			3348	2105	574	643	26		

- Molecule 42 is a protein called Tubulin alpha-1D chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AC	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	AE	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	AG	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	AI	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	AK	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	BC	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	BE	433	Total	C	N	O	S	0	0
			3396	2151	576	646	23		
42	BG	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	BI	430	Total	C	N	O	S	0	0
			3374	2138	573	640	23		
42	BK	439	Total	C	N	O	S	0	0
			3430	2170	583	654	23		
42	CC	438	Total	C	N	O	S	0	0
			3424	2167	582	652	23		
42	CE	438	Total	C	N	O	S	0	0
			3424	2167	582	652	23		
42	CG	439	Total	C	N	O	S	0	0
			3430	2170	583	654	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	CI	439	Total	C	N	O	S	0	0
			3430	2170	583	654	23		
42	CK	439	Total	C	N	O	S	0	0
			3430	2170	583	654	23		
42	CM	439	Total	C	N	O	S	0	0
			3430	2170	583	654	23		
42	DC	429	Total	C	N	O	S	0	0
			3366	2134	572	637	23		
42	DE	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	DG	431	Total	C	N	O	S	0	0
			3379	2142	574	640	23		
42	DI	429	Total	C	N	O	S	0	0
			3364	2133	572	636	23		
42	DK	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	DM	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	EC	439	Total	C	N	O	S	0	0
			3430	2170	583	654	23		
42	EE	441	Total	C	N	O	S	0	0
			3446	2180	585	658	23		
42	EG	434	Total	C	N	O	S	0	0
			3404	2157	578	646	23		
42	EI	436	Total	C	N	O	S	0	0
			3408	2158	580	648	22		
42	EK	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	EM	428	Total	C	N	O	S	0	0
			3358	2130	571	634	23		
42	FC	431	Total	C	N	O	S	0	0
			3379	2142	574	640	23		
42	FE	425	Total	C	N	O	S	0	0
			3339	2118	568	631	22		
42	FG	426	Total	C	N	O	S	0	0
			3346	2123	569	632	22		
42	FI	427	Total	C	N	O	S	0	0
			3347	2121	570	633	23		
42	FK	424	Total	C	N	O	S	0	0
			3326	2109	566	629	22		
42	FM	429	Total	C	N	O	S	0	0
			3365	2132	572	638	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	GC	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	GE	430	Total	C	N	O	S	0	0
			3371	2138	573	637	23		
42	GG	433	Total	C	N	O	S	0	0
			3393	2149	576	645	23		
42	GI	429	Total	C	N	O	S	0	0
			3365	2135	572	635	23		
42	GK	429	Total	C	N	O	S	0	0
			3364	2133	572	636	23		
42	GM	439	Total	C	N	O	S	0	0
			3430	2170	583	654	23		
42	HC	427	Total	C	N	O	S	0	0
			3350	2126	570	631	23		
42	HE	430	Total	C	N	O	S	0	0
			3374	2138	573	640	23		
42	HG	430	Total	C	N	O	S	0	0
			3371	2138	573	637	23		
42	HI	430	Total	C	N	O	S	0	0
			3371	2138	573	637	23		
42	HK	431	Total	C	N	O	S	0	0
			3379	2142	574	640	23		
42	HM	429	Total	C	N	O	S	0	0
			3365	2132	572	638	23		
42	IC	429	Total	C	N	O	S	0	0
			3365	2135	572	635	23		
42	IE	432	Total	C	N	O	S	0	0
			3388	2147	575	643	23		
42	IG	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	II	432	Total	C	N	O	S	0	0
			3387	2146	575	643	23		
42	IK	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	IM	431	Total	C	N	O	S	0	0
			3378	2140	574	641	23		
42	JC	432	Total	C	N	O	S	0	0
			3384	2143	575	643	23		
42	JE	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	JG	428	Total	C	N	O	S	0	0
			3358	2130	571	634	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	JI	429	Total	C	N	O	S	0	0
			3366	2134	572	637	23		
42	JK	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	JM	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	KC	432	Total	C	N	O	S	0	0
			3384	2143	575	643	23		
42	KE	431	Total	C	N	O	S	0	0
			3380	2141	574	642	23		
42	KG	430	Total	C	N	O	S	0	0
			3370	2136	573	638	23		
42	KI	428	Total	C	N	O	S	0	0
			3358	2130	571	634	23		
42	KK	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	KM	432	Total	C	N	O	S	0	0
			3376	2138	575	641	22		
42	LC	433	Total	C	N	O	S	0	0
			3393	2149	576	645	23		
42	LE	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	LG	433	Total	C	N	O	S	0	0
			3393	2149	576	645	23		
42	LI	434	Total	C	N	O	S	0	0
			3397	2151	577	646	23		
42	LK	435	Total	C	N	O	S	0	0
			3401	2153	578	647	23		
42	LM	431	Total	C	N	O	S	0	0
			3378	2140	574	641	23		
42	MC	439	Total	C	N	O	S	0	0
			3430	2170	583	654	23		
42	ME	429	Total	C	N	O	S	0	0
			3366	2134	572	637	23		
42	MG	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	MI	431	Total	C	N	O	S	0	0
			3379	2142	574	640	23		
42	MK	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	MM	431	Total	C	N	O	S	0	0
			3376	2138	574	642	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	NA	430	Total	C	N	O	S	0	0
			3372	2136	573	641	22		
42	NC	429	Total	C	N	O	S	0	0
			3365	2135	572	635	23		
42	NE	430	Total	C	N	O	S	0	0
			3374	2140	573	638	23		
42	NG	432	Total	C	N	O	S	0	0
			3387	2146	575	643	23		
42	NI	432	Total	C	N	O	S	0	0
			3387	2146	575	643	23		
42	NK	430	Total	C	N	O	S	0	0
			3374	2138	573	640	23		
42	OA	428	Total	C	N	O	S	0	0
			3358	2129	571	636	22		
42	OC	429	Total	C	N	O	S	0	0
			3366	2134	572	637	23		
42	OE	433	Total	C	N	O	S	0	0
			3396	2151	576	646	23		
42	OG	433	Total	C	N	O	S	0	0
			3391	2148	576	644	23		
42	OI	432	Total	C	N	O	S	0	0
			3387	2146	575	643	23		
42	OK	431	Total	C	N	O	S	0	0
			3380	2141	574	642	23		
42	PA	368	Total	C	N	O	S	0	0
			2872	1820	487	545	20		
42	PC	432	Total	C	N	O	S	0	0
			3386	2144	575	644	23		
42	PE	431	Total	C	N	O	S	0	0
			3380	2143	574	640	23		
42	PG	430	Total	C	N	O	S	0	0
			3371	2138	573	637	23		
42	PI	427	Total	C	N	O	S	0	0
			3349	2123	570	634	22		
42	PK	430	Total	C	N	O	S	0	0
			3371	2138	573	637	23		
42	QC	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	QE	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	QG	431	Total	C	N	O	S	0	0
			3380	2141	574	642	23		

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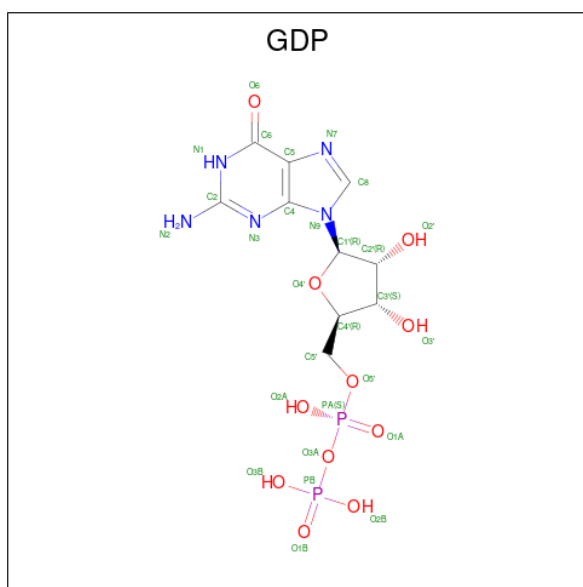
Mol	Chain	Residues	Atoms					AltConf	Trace
42	QI	429	Total	C	N	O	S	0	0
			3366	2134	572	637	23		
42	QK	431	Total	C	N	O	S	0	0
			3380	2141	574	642	23		
42	RC	432	Total	C	N	O	S	0	0
			3387	2146	575	643	23		
42	RE	428	Total	C	N	O	S	0	0
			3358	2130	571	634	23		
42	RG	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	RI	431	Total	C	N	O	S	0	0
			3379	2142	574	640	23		
42	RK	431	Total	C	N	O	S	0	0
			3379	2142	574	640	23		
42	SC	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	SE	431	Total	C	N	O	S	0	0
			3381	2142	574	642	23		
42	SG	431	Total	C	N	O	S	0	0
			3379	2142	574	640	23		
42	SI	427	Total	C	N	O	S	0	0
			3358	2129	569	637	23		
42	SK	432	Total	C	N	O	S	0	0
			3387	2146	575	643	23		
42	SM	431	Total	C	N	O	S	0	0
			3378	2140	574	641	23		
42	TC	430	Total	C	N	O	S	0	0
			3371	2138	573	637	23		
42	TE	432	Total	C	N	O	S	0	0
			3388	2147	575	643	23		
42	TG	430	Total	C	N	O	S	0	0
			3371	2138	573	637	23		
42	TI	430	Total	C	N	O	S	0	0
			3371	2138	573	637	23		
42	TK	432	Total	C	N	O	S	0	0
			3387	2146	575	643	23		
42	TM	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	UC	433	Total	C	N	O	S	0	0
			3393	2149	576	645	23		
42	UE	432	Total	C	N	O	S	0	0
			3388	2147	575	643	23		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	UG	433	Total	C	N	O	S	0	0
			3393	2149	576	645	23		
42	UI	433	Total	C	N	O	S	0	0
			3393	2149	576	645	23		
42	UK	433	Total	C	N	O	S	0	0
			3391	2148	576	644	23		
42	UM	431	Total	C	N	O	S	0	0
			3378	2140	574	641	23		
42	VC	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	VE	433	Total	C	N	O	S	0	0
			3396	2151	576	646	23		
42	VG	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	VI	433	Total	C	N	O	S	0	0
			3393	2149	576	645	23		
42	VK	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	VM	430	Total	C	N	O	S	0	0
			3372	2137	573	639	23		
42	WC	440	Total	C	N	O	S	0	0
			3437	2175	584	655	23		
42	WE	431	Total	C	N	O	S	0	0
			3380	2141	574	642	23		
42	WG	439	Total	C	N	O	S	0	0
			3430	2170	583	654	23		
42	WI	431	Total	C	N	O	S	0	0
			3380	2141	574	642	23		
42	WK	438	Total	C	N	O	S	0	0
			3424	2167	582	652	23		
42	WM	431	Total	C	N	O	S	0	0
			3378	2140	574	641	23		

- Molecule 43 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
43	AB	1	Total 28	C 10	N 5	O 11	P 2	0
43	AD	1	Total 28	C 10	N 5	O 11	P 2	0
43	AF	1	Total 28	C 10	N 5	O 11	P 2	0
43	AH	1	Total 28	C 10	N 5	O 11	P 2	0
43	AJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	AL	1	Total 28	C 10	N 5	O 11	P 2	0
43	BB	1	Total 28	C 10	N 5	O 11	P 2	0
43	BD	1	Total 28	C 10	N 5	O 11	P 2	0
43	BF	1	Total 28	C 10	N 5	O 11	P 2	0
43	BH	1	Total 28	C 10	N 5	O 11	P 2	0
43	BJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	BL	1	Total 28	C 10	N 5	O 11	P 2	0
43	CB	1	Total 28	C 10	N 5	O 11	P 2	0
43	CD	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
43	CF	1	Total 28	C 10	N 5	O 11	P 2	0
43	CH	1	Total 28	C 10	N 5	O 11	P 2	0
43	CJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	CL	1	Total 28	C 10	N 5	O 11	P 2	0
43	DB	1	Total 28	C 10	N 5	O 11	P 2	0
43	DD	1	Total 28	C 10	N 5	O 11	P 2	0
43	DF	1	Total 28	C 10	N 5	O 11	P 2	0
43	DH	1	Total 28	C 10	N 5	O 11	P 2	0
43	DJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	DL	1	Total 28	C 10	N 5	O 11	P 2	0
43	ED	1	Total 28	C 10	N 5	O 11	P 2	0
43	EF	1	Total 28	C 10	N 5	O 11	P 2	0
43	EH	1	Total 28	C 10	N 5	O 11	P 2	0
43	EJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	EL	1	Total 28	C 10	N 5	O 11	P 2	0
43	FD	1	Total 28	C 10	N 5	O 11	P 2	0
43	FF	1	Total 28	C 10	N 5	O 11	P 2	0
43	FH	1	Total 28	C 10	N 5	O 11	P 2	0
43	FJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	FL	1	Total 28	C 10	N 5	O 11	P 2	0
43	GD	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
43	GF	1	Total 28	C 10	N 5	O 11	P 2	0
43	GH	1	Total 28	C 10	N 5	O 11	P 2	0
43	GJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	GL	1	Total 28	C 10	N 5	O 11	P 2	0
43	HB	1	Total 28	C 10	N 5	O 11	P 2	0
43	HD	1	Total 28	C 10	N 5	O 11	P 2	0
43	HF	1	Total 28	C 10	N 5	O 11	P 2	0
43	HH	1	Total 28	C 10	N 5	O 11	P 2	0
43	HJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	HL	1	Total 28	C 10	N 5	O 11	P 2	0
43	ID	1	Total 28	C 10	N 5	O 11	P 2	0
43	IF	1	Total 28	C 10	N 5	O 11	P 2	0
43	IH	1	Total 28	C 10	N 5	O 11	P 2	0
43	IJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	IL	1	Total 28	C 10	N 5	O 11	P 2	0
43	IN	1	Total 28	C 10	N 5	O 11	P 2	0
43	JD	1	Total 28	C 10	N 5	O 11	P 2	0
43	JF	1	Total 28	C 10	N 5	O 11	P 2	0
43	JH	1	Total 28	C 10	N 5	O 11	P 2	0
43	JJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	JL	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
43	KD	1	Total 28	C 10	N 5	O 11	P 2	0
43	KF	1	Total 28	C 10	N 5	O 11	P 2	0
43	KG	1	Total 28	C 10	N 5	O 11	P 2	0
43	KJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	KL	1	Total 28	C 10	N 5	O 11	P 2	0
43	KN	1	Total 28	C 10	N 5	O 11	P 2	0
43	LD	1	Total 28	C 10	N 5	O 11	P 2	0
43	LF	1	Total 28	C 10	N 5	O 11	P 2	0
43	LH	1	Total 28	C 10	N 5	O 11	P 2	0
43	LJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	LL	1	Total 28	C 10	N 5	O 11	P 2	0
43	LN	1	Total 28	C 10	N 5	O 11	P 2	0
43	MD	1	Total 28	C 10	N 5	O 11	P 2	0
43	MF	1	Total 28	C 10	N 5	O 11	P 2	0
43	MH	1	Total 28	C 10	N 5	O 11	P 2	0
43	MJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	ML	1	Total 28	C 10	N 5	O 11	P 2	0
43	MN	1	Total 28	C 10	N 5	O 11	P 2	0
43	NB	1	Total 28	C 10	N 5	O 11	P 2	0
43	ND	1	Total 28	C 10	N 5	O 11	P 2	0
43	NF	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
43	NH	1	Total 28	C 10	N 5	O 11	P 2	0
43	NJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	NL	1	Total 28	C 10	N 5	O 11	P 2	0
43	OB	1	Total 28	C 10	N 5	O 11	P 2	0
43	OD	1	Total 28	C 10	N 5	O 11	P 2	0
43	OF	1	Total 28	C 10	N 5	O 11	P 2	0
43	OH	1	Total 28	C 10	N 5	O 11	P 2	0
43	OJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	OL	1	Total 28	C 10	N 5	O 11	P 2	0
43	PB	1	Total 28	C 10	N 5	O 11	P 2	0
43	PD	1	Total 28	C 10	N 5	O 11	P 2	0
43	PF	1	Total 28	C 10	N 5	O 11	P 2	0
43	PH	1	Total 28	C 10	N 5	O 11	P 2	0
43	PJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	PL	1	Total 28	C 10	N 5	O 11	P 2	0
43	QB	1	Total 28	C 10	N 5	O 11	P 2	0
43	QD	1	Total 28	C 10	N 5	O 11	P 2	0
43	QF	1	Total 28	C 10	N 5	O 11	P 2	0
43	QH	1	Total 28	C 10	N 5	O 11	P 2	0
43	QJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	QL	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
43	RB	1	Total 28	C 10	N 5	O 11	P 2	0
43	RD	1	Total 28	C 10	N 5	O 11	P 2	0
43	RF	1	Total 28	C 10	N 5	O 11	P 2	0
43	RH	1	Total 28	C 10	N 5	O 11	P 2	0
43	RJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	RL	1	Total 28	C 10	N 5	O 11	P 2	0
43	SD	1	Total 28	C 10	N 5	O 11	P 2	0
43	SF	1	Total 28	C 10	N 5	O 11	P 2	0
43	SH	1	Total 28	C 10	N 5	O 11	P 2	0
43	SJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	SL	1	Total 28	C 10	N 5	O 11	P 2	0
43	TD	1	Total 28	C 10	N 5	O 11	P 2	0
43	TF	1	Total 28	C 10	N 5	O 11	P 2	0
43	TH	1	Total 28	C 10	N 5	O 11	P 2	0
43	TJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	TL	1	Total 28	C 10	N 5	O 11	P 2	0
43	UD	1	Total 28	C 10	N 5	O 11	P 2	0
43	UF	1	Total 28	C 10	N 5	O 11	P 2	0
43	UH	1	Total 28	C 10	N 5	O 11	P 2	0
43	UJ	1	Total 28	C 10	N 5	O 11	P 2	0
43	UL	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
43	VD	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	VF	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	VH	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	VJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	VL	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	WD	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	WF	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	WH	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	WJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	WL	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	WN	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 44 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
44	AB	1	Total	Mg	0
			1	1	
44	AE	1	Total	Mg	0
			1	1	
44	AG	1	Total	Mg	0
			1	1	
44	AI	1	Total	Mg	0
			1	1	
44	AK	1	Total	Mg	0
			1	1	
44	BC	1	Total	Mg	0
			1	1	
44	BE	1	Total	Mg	0
			1	1	
44	BG	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
44	BI	1	Total 1	Mg 1	0
44	BK	1	Total 1	Mg 1	0
44	CC	1	Total 1	Mg 1	0
44	CE	1	Total 1	Mg 1	0
44	CI	1	Total 1	Mg 1	0
44	CK	1	Total 1	Mg 1	0
44	CM	1	Total 1	Mg 1	0
44	DM	1	Total 1	Mg 1	0
44	EK	1	Total 1	Mg 1	0
44	FC	1	Total 1	Mg 1	0
44	FD	1	Total 1	Mg 1	0
44	FG	1	Total 1	Mg 1	0
44	FI	1	Total 1	Mg 1	0
44	FK	1	Total 1	Mg 1	0
44	FL	1	Total 1	Mg 1	0
44	GC	1	Total 1	Mg 1	0
44	GE	1	Total 1	Mg 1	0
44	GG	1	Total 1	Mg 1	0
44	GI	1	Total 1	Mg 1	0
44	GK	1	Total 1	Mg 1	0
44	GM	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
44	HC	1	Total 1	Mg 1	0
44	HE	1	Total 1	Mg 1	0
44	HG	1	Total 1	Mg 1	0
44	HI	1	Total 1	Mg 1	0
44	HK	1	Total 1	Mg 1	0
44	HM	1	Total 1	Mg 1	0
44	IC	1	Total 1	Mg 1	0
44	IE	1	Total 1	Mg 1	0
44	IG	1	Total 1	Mg 1	0
44	IK	1	Total 1	Mg 1	0
44	IL	1	Total 1	Mg 1	0
44	JC	1	Total 1	Mg 1	0
44	JE	1	Total 1	Mg 1	0
44	JG	1	Total 1	Mg 1	0
44	JI	1	Total 1	Mg 1	0
44	JK	1	Total 1	Mg 1	0
44	JM	1	Total 1	Mg 1	0
44	KC	1	Total 1	Mg 1	0
44	KE	1	Total 1	Mg 1	0
44	KG	1	Total 1	Mg 1	0
44	KI	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
44	KK	1	Total 1	Mg 1	0
44	KM	1	Total 1	Mg 1	0
44	LC	1	Total 1	Mg 1	0
44	LD	1	Total 1	Mg 1	0
44	LG	1	Total 1	Mg 1	0
44	LI	1	Total 1	Mg 1	0
44	LK	1	Total 1	Mg 1	0
44	LM	1	Total 1	Mg 1	0
44	MC	1	Total 1	Mg 1	0
44	ME	1	Total 1	Mg 1	0
44	MH	1	Total 1	Mg 1	0
44	MK	1	Total 1	Mg 1	0
44	MM	1	Total 1	Mg 1	0
44	NA	1	Total 1	Mg 1	0
44	NB	1	Total 1	Mg 1	0
44	NE	1	Total 1	Mg 1	0
44	NG	1	Total 1	Mg 1	0
44	NI	1	Total 1	Mg 1	0
44	NK	1	Total 1	Mg 1	0
44	OA	1	Total 1	Mg 1	0
44	OC	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
44	OE	1	Total 1	Mg 1	0
44	OI	1	Total 1	Mg 1	0
44	OK	1	Total 1	Mg 1	0
44	PC	1	Total 1	Mg 1	0
44	PE	1	Total 1	Mg 1	0
44	PG	1	Total 1	Mg 1	0
44	PI	1	Total 1	Mg 1	0
44	SC	1	Total 1	Mg 1	0
44	SD	1	Total 1	Mg 1	0
44	SF	1	Total 1	Mg 1	0
44	SH	1	Total 1	Mg 1	0
44	SJ	1	Total 1	Mg 1	0
44	TC	1	Total 1	Mg 1	0
44	TD	1	Total 1	Mg 1	0
44	TF	1	Total 1	Mg 1	0
44	TI	1	Total 1	Mg 1	0
44	TK	1	Total 1	Mg 1	0
44	TL	1	Total 1	Mg 1	0
44	UE	1	Total 1	Mg 1	0
44	UG	1	Total 1	Mg 1	0
44	UI	1	Total 1	Mg 1	0

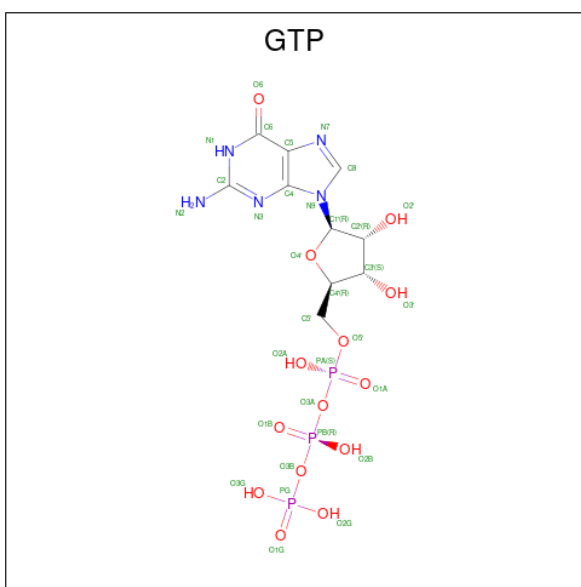
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Mol	Chain	Residues	Atoms		AltConf
44	UK	1	Total 1	Mg 1	0
44	UM	1	Total 1	Mg 1	0
44	VC	1	Total 1	Mg 1	0
44	VE	1	Total 1	Mg 1	0
44	VG	1	Total 1	Mg 1	0
44	VI	1	Total 1	Mg 1	0
44	VJ	1	Total 1	Mg 1	0
44	VM	1	Total 1	Mg 1	0
44	WC	1	Total 1	Mg 1	0
44	WD	1	Total 1	Mg 1	0
44	WG	1	Total 1	Mg 1	0
44	WI	1	Total 1	Mg 1	0
44	WK	1	Total 1	Mg 1	0
44	WM	1	Total 1	Mg 1	0

- Molecule 45 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
45	AC	1	Total 32	C 10	N 5	O 14	P 3	0
45	AE	1	Total 32	C 10	N 5	O 14	P 3	0
45	AF	1	Total 32	C 10	N 5	O 14	P 3	0
45	AI	1	Total 32	C 10	N 5	O 14	P 3	0
45	AK	1	Total 32	C 10	N 5	O 14	P 3	0
45	BC	1	Total 32	C 10	N 5	O 14	P 3	0
45	BE	1	Total 32	C 10	N 5	O 14	P 3	0
45	BG	1	Total 32	C 10	N 5	O 14	P 3	0
45	BI	1	Total 32	C 10	N 5	O 14	P 3	0
45	BK	1	Total 32	C 10	N 5	O 14	P 3	0
45	CC	1	Total 32	C 10	N 5	O 14	P 3	0
45	CE	1	Total 32	C 10	N 5	O 14	P 3	0
45	CG	1	Total 32	C 10	N 5	O 14	P 3	0
45	CI	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
45	CK	1	Total 32	C 10	N 5	O 14	P 3	0
45	CM	1	Total 32	C 10	N 5	O 14	P 3	0
45	DC	1	Total 32	C 10	N 5	O 14	P 3	0
45	DE	1	Total 32	C 10	N 5	O 14	P 3	0
45	DG	1	Total 32	C 10	N 5	O 14	P 3	0
45	DI	1	Total 32	C 10	N 5	O 14	P 3	0
45	DK	1	Total 32	C 10	N 5	O 14	P 3	0
45	DM	1	Total 32	C 10	N 5	O 14	P 3	0
45	EC	1	Total 32	C 10	N 5	O 14	P 3	0
45	EE	1	Total 32	C 10	N 5	O 14	P 3	0
45	EG	1	Total 32	C 10	N 5	O 14	P 3	0
45	EI	1	Total 32	C 10	N 5	O 14	P 3	0
45	EK	1	Total 32	C 10	N 5	O 14	P 3	0
45	EM	1	Total 32	C 10	N 5	O 14	P 3	0
45	FC	1	Total 32	C 10	N 5	O 14	P 3	0
45	FE	1	Total 32	C 10	N 5	O 14	P 3	0
45	FF	1	Total 32	C 10	N 5	O 14	P 3	0
45	FI	1	Total 32	C 10	N 5	O 14	P 3	0
45	FK	1	Total 32	C 10	N 5	O 14	P 3	0
45	FM	1	Total 32	C 10	N 5	O 14	P 3	0
45	GC	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
45	GE	1	Total 32	C 10	N 5	O 14	P 3	0
45	GF	1	Total 32	C 10	N 5	O 14	P 3	0
45	GI	1	Total 32	C 10	N 5	O 14	P 3	0
45	GK	1	Total 32	C 10	N 5	O 14	P 3	0
45	GM	1	Total 32	C 10	N 5	O 14	P 3	0
45	HC	1	Total 32	C 10	N 5	O 14	P 3	0
45	HE	1	Total 32	C 10	N 5	O 14	P 3	0
45	HG	1	Total 32	C 10	N 5	O 14	P 3	0
45	HI	1	Total 32	C 10	N 5	O 14	P 3	0
45	HK	1	Total 32	C 10	N 5	O 14	P 3	0
45	HM	1	Total 32	C 10	N 5	O 14	P 3	0
45	IC	1	Total 32	C 10	N 5	O 14	P 3	0
45	IE	1	Total 32	C 10	N 5	O 14	P 3	0
45	IG	1	Total 32	C 10	N 5	O 14	P 3	0
45	II	1	Total 32	C 10	N 5	O 14	P 3	0
45	IK	1	Total 32	C 10	N 5	O 14	P 3	0
45	IM	1	Total 32	C 10	N 5	O 14	P 3	0
45	JC	1	Total 32	C 10	N 5	O 14	P 3	0
45	JE	1	Total 32	C 10	N 5	O 14	P 3	0
45	JG	1	Total 32	C 10	N 5	O 14	P 3	0
45	JI	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
45	JK	1	Total 32	C 10	N 5	O 14	P 3	0
45	JM	1	Total 32	C 10	N 5	O 14	P 3	0
45	KC	1	Total 32	C 10	N 5	O 14	P 3	0
45	KE	1	Total 32	C 10	N 5	O 14	P 3	0
45	KG	1	Total 32	C 10	N 5	O 14	P 3	0
45	KI	1	Total 32	C 10	N 5	O 14	P 3	0
45	KK	1	Total 32	C 10	N 5	O 14	P 3	0
45	KM	1	Total 32	C 10	N 5	O 14	P 3	0
45	LC	1	Total 32	C 10	N 5	O 14	P 3	0
45	LE	1	Total 32	C 10	N 5	O 14	P 3	0
45	LF	1	Total 32	C 10	N 5	O 14	P 3	0
45	LI	1	Total 32	C 10	N 5	O 14	P 3	0
45	LK	1	Total 32	C 10	N 5	O 14	P 3	0
45	LM	1	Total 32	C 10	N 5	O 14	P 3	0
45	MC	1	Total 32	C 10	N 5	O 14	P 3	0
45	ME	1	Total 32	C 10	N 5	O 14	P 3	0
45	MG	1	Total 32	C 10	N 5	O 14	P 3	0
45	MI	1	Total 32	C 10	N 5	O 14	P 3	0
45	MK	1	Total 32	C 10	N 5	O 14	P 3	0
45	MM	1	Total 32	C 10	N 5	O 14	P 3	0
45	NA	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
45	NC	1	Total 32	C 10	N 5	O 14	P 3	0
45	NE	1	Total 32	C 10	N 5	O 14	P 3	0
45	NG	1	Total 32	C 10	N 5	O 14	P 3	0
45	NI	1	Total 32	C 10	N 5	O 14	P 3	0
45	NK	1	Total 32	C 10	N 5	O 14	P 3	0
45	OA	1	Total 32	C 10	N 5	O 14	P 3	0
45	OC	1	Total 32	C 10	N 5	O 14	P 3	0
45	OE	1	Total 32	C 10	N 5	O 14	P 3	0
45	OG	1	Total 32	C 10	N 5	O 14	P 3	0
45	OI	1	Total 32	C 10	N 5	O 14	P 3	0
45	OK	1	Total 32	C 10	N 5	O 14	P 3	0
45	PA	1	Total 32	C 10	N 5	O 14	P 3	0
45	PC	1	Total 32	C 10	N 5	O 14	P 3	0
45	PE	1	Total 32	C 10	N 5	O 14	P 3	0
45	PG	1	Total 32	C 10	N 5	O 14	P 3	0
45	PI	1	Total 32	C 10	N 5	O 14	P 3	0
45	PK	1	Total 32	C 10	N 5	O 14	P 3	0
45	QC	1	Total 32	C 10	N 5	O 14	P 3	0
45	QE	1	Total 32	C 10	N 5	O 14	P 3	0
45	QG	1	Total 32	C 10	N 5	O 14	P 3	0
45	QI	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
45	QK	1	Total 32	C 10	N 5	O 14	P 3	0
45	RC	1	Total 32	C 10	N 5	O 14	P 3	0
45	RE	1	Total 32	C 10	N 5	O 14	P 3	0
45	RG	1	Total 32	C 10	N 5	O 14	P 3	0
45	RI	1	Total 32	C 10	N 5	O 14	P 3	0
45	RK	1	Total 32	C 10	N 5	O 14	P 3	0
45	SC	1	Total 32	C 10	N 5	O 14	P 3	0
45	SE	1	Total 32	C 10	N 5	O 14	P 3	0
45	SG	1	Total 32	C 10	N 5	O 14	P 3	0
45	SI	1	Total 32	C 10	N 5	O 14	P 3	0
45	SK	1	Total 32	C 10	N 5	O 14	P 3	0
45	SM	1	Total 32	C 10	N 5	O 14	P 3	0
45	TC	1	Total 32	C 10	N 5	O 14	P 3	0
45	TE	1	Total 32	C 10	N 5	O 14	P 3	0
45	TG	1	Total 32	C 10	N 5	O 14	P 3	0
45	TI	1	Total 32	C 10	N 5	O 14	P 3	0
45	TK	1	Total 32	C 10	N 5	O 14	P 3	0
45	TM	1	Total 32	C 10	N 5	O 14	P 3	0
45	UC	1	Total 32	C 10	N 5	O 14	P 3	0
45	UE	1	Total 32	C 10	N 5	O 14	P 3	0
45	UG	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
45	UI	1	Total 32	C 10	N 5	O 14	P 3	0
45	UK	1	Total 32	C 10	N 5	O 14	P 3	0
45	UM	1	Total 32	C 10	N 5	O 14	P 3	0
45	VC	1	Total 32	C 10	N 5	O 14	P 3	0
45	VE	1	Total 32	C 10	N 5	O 14	P 3	0
45	VG	1	Total 32	C 10	N 5	O 14	P 3	0
45	VI	1	Total 32	C 10	N 5	O 14	P 3	0
45	VK	1	Total 32	C 10	N 5	O 14	P 3	0
45	VM	1	Total 32	C 10	N 5	O 14	P 3	0
45	WC	1	Total 32	C 10	N 5	O 14	P 3	0
45	WE	1	Total 32	C 10	N 5	O 14	P 3	0
45	WG	1	Total 32	C 10	N 5	O 14	P 3	0
45	WI	1	Total 32	C 10	N 5	O 14	P 3	0
45	WK	1	Total 32	C 10	N 5	O 14	P 3	0
45	WM	1	Total 32	C 10	N 5	O 14	P 3	0

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



### 3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	153589	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.542	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	686.08, 686.08, 686.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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 370 ligands modelled in this entry, 106 are monoatomic - leaving 264 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
43	GDP	AL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	7 (15%)
45	GTP	RG	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.68	12 (24%)
43	GDP	KJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	7 (15%)
45	GTP	DK	501	-	33,34,34	0.99	3 (9%)	50,54,54	1.69	10 (20%)
45	GTP	QG	501	-	33,34,34	0.90	2 (6%)	50,54,54	1.69	9 (18%)
43	GDP	KG	503	-	29,30,30	1.15	3 (10%)	45,47,47	1.85	8 (17%)
43	GDP	GL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
43	GDP	CH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
43	GDP	OD	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.78	6 (13%)
45	GTP	CG	501	-	33,34,34	0.90	0	50,54,54	1.54	10 (20%)
43	GDP	CL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
45	GTP	OE	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.61	9 (18%)
45	GTP	BG	501	44	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
45	GTP	EM	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
45	GTP	FC	501	44	33,34,34	1.03	3 (9%)	50,54,54	1.64	9 (18%)
45	GTP	WK	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.64	9 (18%)
43	GDP	VD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
43	GDP	BD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	7 (15%)
45	GTP	LF	502	44	33,34,34	0.95	2 (6%)	50,54,54	1.64	9 (18%)
43	GDP	FJ	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.75	8 (17%)
43	GDP	NH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
45	GTP	MC	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.62	10 (20%)
45	GTP	BK	501	44	33,34,34	0.91	2 (6%)	50,54,54	1.70	10 (20%)
45	GTP	PK	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
43	GDP	DJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
43	GDP	GF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
45	GTP	HE	501	44	33,34,34	0.97	1 (3%)	50,54,54	1.60	9 (18%)
43	GDP	BL	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.79	7 (15%)
45	GTP	LK	501	44	33,34,34	1.00	3 (9%)	50,54,54	1.61	11 (22%)
45	GTP	VG	501	44	33,34,34	0.97	2 (6%)	50,54,54	1.59	9 (18%)
45	GTP	KK	501	44	33,34,34	0.97	0	50,54,54	1.59	10 (20%)
45	GTP	JG	501	44	33,34,34	1.01	2 (6%)	50,54,54	1.60	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
43	GDP	CB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
45	GTP	QK	501	-	33,34,34	0.98	3 (9%)	50,54,54	1.70	10 (20%)
45	GTP	WG	501	44	33,34,34	0.93	1 (3%)	50,54,54	1.63	9 (18%)
43	GDP	LH	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	8 (17%)
43	GDP	NF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
43	GDP	QF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	6 (13%)
43	GDP	SF	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.70	9 (20%)
45	GTP	DE	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.78	10 (20%)
45	GTP	TC	501	44	33,34,34	0.94	1 (3%)	50,54,54	1.61	8 (16%)
45	GTP	UM	501	44	33,34,34	0.87	0	50,54,54	1.58	10 (20%)
43	GDP	SJ	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.72	6 (13%)
45	GTP	BI	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.64	9 (18%)
43	GDP	GD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
45	GTP	VE	501	44	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
43	GDP	IH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.84	7 (15%)
43	GDP	QD	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	6 (13%)
43	GDP	OF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
45	GTP	RI	501	-	33,34,34	0.92	2 (6%)	50,54,54	2.05	12 (24%)
45	GTP	JM	501	44	33,34,34	0.89	1 (3%)	50,54,54	1.57	9 (18%)
45	GTP	BC	501	44	33,34,34	1.01	2 (6%)	50,54,54	1.55	10 (20%)
43	GDP	KF	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	7 (15%)
43	GDP	IL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.83	8 (17%)
43	GDP	RD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.80	7 (15%)
45	GTP	CK	501	44	33,34,34	0.96	1 (3%)	50,54,54	1.66	10 (20%)
45	GTP	JK	501	44	33,34,34	0.94	1 (3%)	50,54,54	1.60	8 (16%)
43	GDP	LN	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	7 (15%)
45	GTP	KG	501	44	33,34,34	0.99	2 (6%)	50,54,54	1.58	8 (16%)
45	GTP	NK	501	44	33,34,34	1.03	3 (9%)	50,54,54	1.57	9 (18%)
45	GTP	OK	501	44	33,34,34	1.05	3 (9%)	50,54,54	1.60	9 (18%)
43	GDP	NJ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.80	7 (15%)
43	GDP	BF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	7 (15%)
43	GDP	DL	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.81	6 (13%)
43	GDP	TL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.80	7 (15%)
45	GTP	DM	501	44	33,34,34	0.95	2 (6%)	50,54,54	1.63	10 (20%)
45	GTP	PC	501	44	33,34,34	1.00	1 (3%)	50,54,54	1.59	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	GTP	FK	501	44	33,34,34	1.05	3 (9%)	50,54,54	1.61	10 (20%)
43	GDP	FL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	5 (11%)
45	GTP	JI	501	44	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
45	GTP	TM	501	44	33,34,34	0.88	1 (3%)	50,54,54	1.69	11 (22%)
45	GTP	UK	501	44	33,34,34	1.00	2 (6%)	50,54,54	1.65	8 (16%)
45	GTP	LM	501	44	33,34,34	0.97	1 (3%)	50,54,54	1.62	10 (20%)
45	GTP	OG	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
45	GTP	ME	501	44	33,34,34	0.93	1 (3%)	50,54,54	1.60	8 (16%)
45	GTP	EC	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.64	9 (18%)
45	GTP	KI	501	44	33,34,34	0.92	1 (3%)	50,54,54	1.60	10 (20%)
45	GTP	QC	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.48	8 (16%)
45	GTP	SC	501	44	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
45	GTP	FM	501	44	33,34,34	0.97	1 (3%)	50,54,54	1.59	9 (18%)
43	GDP	AD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
43	GDP	MN	501	-	29,30,30	1.13	4 (13%)	45,47,47	1.77	6 (13%)
45	GTP	RK	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
43	GDP	AF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
45	GTP	PI	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
45	GTP	SE	501	44	33,34,34	0.95	2 (6%)	50,54,54	1.71	9 (18%)
43	GDP	ND	501	-	29,30,30	1.21	3 (10%)	45,47,47	1.80	7 (15%)
45	GTP	WE	501	44	33,34,34	0.96	1 (3%)	50,54,54	1.55	8 (16%)
43	GDP	QH	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.84	8 (17%)
45	GTP	GF	502	44	33,34,34	0.94	2 (6%)	50,54,54	1.53	8 (16%)
45	GTP	KE	501	44	33,34,34	0.96	1 (3%)	50,54,54	1.60	9 (18%)
45	GTP	LI	501	44	33,34,34	0.93	1 (3%)	50,54,54	1.61	8 (16%)
45	GTP	VC	501	44	33,34,34	0.97	1 (3%)	50,54,54	1.61	10 (20%)
45	GTP	EG	501	-	33,34,34	1.02	2 (6%)	50,54,54	1.68	8 (16%)
43	GDP	UF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
43	GDP	WD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
43	GDP	LJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
43	GDP	PD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
45	GTP	HI	501	44	33,34,34	1.00	2 (6%)	50,54,54	1.57	9 (18%)
43	GDP	JD	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.74	6 (13%)
43	GDP	JJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
45	GTP	MI	501	44	33,34,34	0.92	0	50,54,54	1.53	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	GTP	UI	501	44	33,34,34	0.87	0	50,54,54	1.50	7 (14%)
45	GTP	WC	501	44	33,34,34	0.90	1 (3%)	50,54,54	1.58	8 (16%)
45	GTP	SM	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.62	10 (20%)
45	GTP	VM	501	44	33,34,34	0.91	0	50,54,54	1.61	11 (22%)
43	GDP	WL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	6 (13%)
45	GTP	HM	501	44	33,34,34	1.00	3 (9%)	50,54,54	1.65	11 (22%)
45	GTP	QI	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.61	9 (18%)
43	GDP	HH	501	-	29,30,30	1.18	4 (13%)	45,47,47	2.25	13 (28%)
45	GTP	FE	501	44	33,34,34	0.94	1 (3%)	50,54,54	1.60	8 (16%)
43	GDP	ID	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	8 (17%)
45	GTP	CI	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.85	10 (20%)
43	GDP	WJ	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.80	5 (11%)
43	GDP	VJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
45	GTP	CE	501	44	33,34,34	0.96	0	50,54,54	1.46	8 (16%)
43	GDP	MD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
45	GTP	JC	501	44	33,34,34	0.90	0	50,54,54	1.59	9 (18%)
43	GDP	LF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
43	GDP	SH	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	8 (17%)
45	GTP	AC	501	44	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
43	GDP	CD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	5 (11%)
43	GDP	KN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
43	GDP	WF	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	7 (15%)
45	GTP	GM	501	44	33,34,34	0.88	1 (3%)	50,54,54	1.58	9 (18%)
45	GTP	AE	501	44	33,34,34	0.89	1 (3%)	50,54,54	1.64	9 (18%)
45	GTP	VI	501	44	33,34,34	0.96	1 (3%)	50,54,54	1.57	10 (20%)
43	GDP	KL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
43	GDP	DD	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.77	6 (13%)
43	GDP	EH	501	-	29,30,30	1.23	4 (13%)	45,47,47	2.07	8 (17%)
43	GDP	EF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
45	GTP	GK	501	44	33,34,34	0.90	1 (3%)	50,54,54	1.61	9 (18%)
45	GTP	PG	501	44	33,34,34	0.92	0	50,54,54	1.55	9 (18%)
43	GDP	AB	501	-	29,30,30	1.09	3 (10%)	45,47,47	1.76	10 (22%)
45	GTP	EI	501	-	33,34,34	0.92	0	50,54,54	1.46	7 (14%)
43	GDP	BJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
45	GTP	AF	502	44	33,34,34	0.94	1 (3%)	50,54,54	1.63	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	GTP	TK	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.67	12 (24%)
43	GDP	CF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	5 (11%)
43	GDP	GH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	6 (13%)
43	GDP	KD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
45	GTP	TE	501	44	33,34,34	0.98	1 (3%)	50,54,54	1.70	12 (24%)
45	GTP	SG	501	44	33,34,34	0.98	1 (3%)	50,54,54	1.62	7 (14%)
45	GTP	BE	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
45	GTP	FF	502	44	33,34,34	0.93	1 (3%)	50,54,54	1.64	8 (16%)
43	GDP	JF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
43	GDP	TJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	8 (17%)
43	GDP	QB	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.80	7 (15%)
45	GTP	LE	501	44	33,34,34	0.92	1 (3%)	50,54,54	1.61	9 (18%)
43	GDP	IJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
43	GDP	BB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.85	9 (20%)
43	GDP	FF	501	-	29,30,30	1.39	4 (13%)	45,47,47	2.18	9 (20%)
43	GDP	JL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.82	9 (20%)
43	GDP	LL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
45	GTP	NE	501	44	33,34,34	0.83	1 (3%)	50,54,54	1.65	10 (20%)
43	GDP	RL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
43	GDP	DH	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.83	6 (13%)
45	GTP	RE	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.61	10 (20%)
43	GDP	DF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
43	GDP	VL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
43	GDP	VH	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.67	6 (13%)
45	GTP	GC	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.87	8 (16%)
45	GTP	HK	501	44	33,34,34	0.99	1 (3%)	50,54,54	1.61	9 (18%)
43	GDP	NL	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.92	8 (17%)
45	GTP	SI	501	44	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
45	GTP	TG	501	44	33,34,34	0.89	1 (3%)	50,54,54	1.55	8 (16%)
43	GDP	ED	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
43	GDP	HJ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
43	GDP	RJ	501	-	29,30,30	1.11	3 (10%)	45,47,47	1.81	7 (15%)
45	GTP	FI	501	44	33,34,34	0.89	1 (3%)	50,54,54	1.56	9 (18%)
45	GTP	HG	501	44	33,34,34	0.93	1 (3%)	50,54,54	1.51	9 (18%)
43	GDP	WH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	GTP	IC	501	44	33,34,34	0.95	0	50,54,54	1.48	10 (20%)
45	GTP	II	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
43	GDP	FH	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
45	GTP	DC	501	-	33,34,34	0.86	0	50,54,54	1.64	10 (20%)
43	GDP	MH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	6 (13%)
43	GDP	TF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
45	GTP	AK	501	44	33,34,34	0.94	1 (3%)	50,54,54	1.64	9 (18%)
45	GTP	DI	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.59	10 (20%)
45	GTP	TI	501	44	33,34,34	0.99	2 (6%)	50,54,54	1.57	8 (16%)
43	GDP	CJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
43	GDP	UD	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.76	6 (13%)
43	GDP	IN	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.91	9 (20%)
43	GDP	QL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.80	7 (15%)
45	GTP	IM	501	44	33,34,34	0.94	0	50,54,54	1.59	8 (16%)
43	GDP	AH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
43	GDP	HB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
43	GDP	PJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
43	GDP	UJ	501	-	29,30,30	1.51	5 (17%)	45,47,47	1.99	9 (20%)
43	GDP	TH	501	-	29,30,30	1.20	3 (10%)	45,47,47	1.85	7 (15%)
43	GDP	EL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
45	GTP	WI	501	44	33,34,34	0.92	1 (3%)	50,54,54	1.83	11 (22%)
45	GTP	OA	501	44	33,34,34	1.06	4 (12%)	50,54,54	1.62	10 (20%)
43	GDP	EJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.82	7 (15%)
43	GDP	ML	501	-	29,30,30	1.14	4 (13%)	45,47,47	1.78	7 (15%)
45	GTP	DG	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.63	9 (18%)
43	GDP	MJ	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.82	7 (15%)
43	GDP	RB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
43	GDP	IF	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	7 (15%)
43	GDP	JH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	7 (15%)
43	GDP	RF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
43	GDP	FD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
43	GDP	LD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
43	GDP	QJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	8 (17%)
43	GDP	HD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
43	GDP	PF	501	-	29,30,30	1.15	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
45	GTP	MK	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.64	9 (18%)
43	GDP	VF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
43	GDP	GJ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
45	GTP	NG	501	44	33,34,34	0.86	0	50,54,54	1.60	9 (18%)
43	GDP	SD	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	7 (15%)
43	GDP	HF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	8 (17%)
43	GDP	OL	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	6 (13%)
43	GDP	DB	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.77	6 (13%)
43	GDP	OJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	6 (13%)
45	GTP	IG	501	44	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
43	GDP	PB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	5 (11%)
45	GTP	MM	501	44	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
45	GTP	HC	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.63	9 (18%)
45	GTP	MG	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.56	8 (16%)
45	GTP	PE	501	44	33,34,34	0.96	2 (6%)	50,54,54	1.65	10 (20%)
45	GTP	WM	501	44	33,34,34	0.91	1 (3%)	50,54,54	1.59	10 (20%)
43	GDP	AJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.79	7 (15%)
45	GTP	JE	501	44	33,34,34	1.18	3 (9%)	50,54,54	1.68	8 (16%)
45	GTP	LC	501	44	33,34,34	0.94	1 (3%)	50,54,54	1.60	9 (18%)
45	GTP	GI	501	44	33,34,34	0.99	2 (6%)	50,54,54	1.70	9 (18%)
43	GDP	MF	501	-	29,30,30	1.30	4 (13%)	45,47,47	1.81	6 (13%)
45	GTP	AI	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.61	8 (16%)
45	GTP	QE	501	-	33,34,34	0.89	2 (6%)	50,54,54	1.79	12 (24%)
45	GTP	UC	501	-	33,34,34	1.08	2 (6%)	50,54,54	1.62	11 (22%)
43	GDP	OH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.69	6 (13%)
45	GTP	NI	501	44	33,34,34	0.92	0	50,54,54	1.65	10 (20%)
43	GDP	TD	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.83	8 (17%)
45	GTP	UG	501	44	33,34,34	0.88	1 (3%)	50,54,54	1.58	8 (16%)
45	GTP	GE	501	44	33,34,34	0.93	1 (3%)	50,54,54	1.63	9 (18%)
45	GTP	OC	501	44	33,34,34	0.89	1 (3%)	50,54,54	1.59	10 (20%)
45	GTP	RC	501	-	33,34,34	0.92	1 (3%)	50,54,54	1.55	8 (16%)
45	GTP	OI	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
43	GDP	HL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
43	GDP	PH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
45	GTP	VK	501	44	33,34,34	0.97	1 (3%)	50,54,54	1.64	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	GTP	CC	501	44	33,34,34	0.97	2 (6%)	50,54,54	1.59	9 (18%)
45	GTP	IE	501	44	33,34,34	0.95	1 (3%)	50,54,54	1.61	11 (22%)
43	GDP	UL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.80	7 (15%)
45	GTP	UE	501	44	33,34,34	0.94	1 (3%)	50,54,54	1.62	9 (18%)
45	GTP	PA	501	-	33,34,34	0.95	0	50,54,54	1.64	9 (18%)
45	GTP	IK	501	44	33,34,34	1.05	3 (9%)	50,54,54	1.90	10 (20%)
43	GDP	PL	501	-	29,30,30	1.28	5 (17%)	45,47,47	1.82	8 (17%)
45	GTP	KC	501	44	33,34,34	0.90	1 (3%)	50,54,54	1.59	9 (18%)
45	GTP	KM	501	44	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)
45	GTP	EK	501	44	33,34,34	0.96	2 (6%)	50,54,54	1.64	10 (20%)
45	GTP	NA	501	44	33,34,34	0.90	1 (3%)	50,54,54	1.66	11 (22%)
43	GDP	OB	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.78	8 (17%)
43	GDP	UH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
43	GDP	RH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
45	GTP	NC	501	44	33,34,34	0.90	1 (3%)	50,54,54	1.61	8 (16%)
43	GDP	SL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.85	7 (15%)
45	GTP	SK	501	44	33,34,34	0.93	0	50,54,54	1.62	8 (16%)
45	GTP	EE	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
43	GDP	WN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.71	6 (13%)
45	GTP	CM	501	44	33,34,34	0.88	0	50,54,54	1.58	11 (22%)
43	GDP	BH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
43	GDP	NB	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.75	7 (15%)

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
43	GDP	AL	501	-	-	2/16/32/32	0/3/3/3
45	GTP	RG	501	-	-	6/22/38/38	0/3/3/3
43	GDP	KJ	501	-	-	1/16/32/32	0/3/3/3
45	GTP	DK	501	-	-	5/22/38/38	0/3/3/3
45	GTP	QG	501	-	-	4/22/38/38	0/3/3/3
43	GDP	KG	503	-	-	0/16/32/32	0/3/3/3
43	GDP	GL	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	GDP	CH	501	-	-	3/16/32/32	0/3/3/3
43	GDP	OD	501	-	-	2/16/32/32	0/3/3/3
45	GTP	CG	501	-	-	5/22/38/38	0/3/3/3
43	GDP	CL	501	-	-	2/16/32/32	0/3/3/3
45	GTP	OE	501	44	-	7/22/38/38	0/3/3/3
45	GTP	BG	501	44	-	6/22/38/38	0/3/3/3
45	GTP	EM	501	-	-	6/22/38/38	0/3/3/3
45	GTP	FC	501	44	-	7/22/38/38	0/3/3/3
45	GTP	WK	501	44	-	7/22/38/38	0/3/3/3
43	GDP	VD	501	-	-	5/16/32/32	0/3/3/3
43	GDP	BD	501	-	-	1/16/32/32	0/3/3/3
45	GTP	LF	502	44	-	9/22/38/38	0/3/3/3
43	GDP	FJ	501	-	-	4/16/32/32	0/3/3/3
43	GDP	NH	501	-	-	1/16/32/32	0/3/3/3
45	GTP	MC	501	44	-	6/22/38/38	0/3/3/3
45	GTP	BK	501	44	-	8/22/38/38	0/3/3/3
45	GTP	PK	501	-	-	3/22/38/38	0/3/3/3
43	GDP	DJ	501	-	-	1/16/32/32	0/3/3/3
43	GDP	GF	501	-	-	5/16/32/32	0/3/3/3
45	GTP	HE	501	44	-	4/22/38/38	0/3/3/3
43	GDP	BL	501	-	-	1/16/32/32	0/3/3/3
45	GTP	LK	501	44	-	9/22/38/38	0/3/3/3
45	GTP	VG	501	44	-	3/22/38/38	0/3/3/3
45	GTP	KK	501	44	-	7/22/38/38	0/3/3/3
45	GTP	JG	501	44	-	3/22/38/38	0/3/3/3
43	GDP	CB	501	-	-	4/16/32/32	0/3/3/3
45	GTP	QK	501	-	-	6/22/38/38	0/3/3/3
45	GTP	WG	501	44	-	5/22/38/38	0/3/3/3
43	GDP	LH	501	-	-	3/16/32/32	0/3/3/3
43	GDP	NF	501	-	-	3/16/32/32	0/3/3/3
43	GDP	QF	501	-	-	2/16/32/32	0/3/3/3
43	GDP	SF	501	-	-	1/16/32/32	0/3/3/3
45	GTP	DE	501	-	-	5/22/38/38	0/3/3/3
45	GTP	TC	501	44	-	3/22/38/38	0/3/3/3
45	GTP	UM	501	44	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	GDP	SJ	501	-	-	3/16/32/32	0/3/3/3
45	GTP	BI	501	44	-	6/22/38/38	0/3/3/3
43	GDP	GD	501	-	-	3/16/32/32	0/3/3/3
45	GTP	VE	501	44	-	4/22/38/38	0/3/3/3
43	GDP	IH	501	-	-	3/16/32/32	0/3/3/3
43	GDP	QD	501	-	-	1/16/32/32	0/3/3/3
43	GDP	OF	501	-	-	3/16/32/32	0/3/3/3
45	GTP	RI	501	-	-	5/22/38/38	0/3/3/3
45	GTP	JM	501	44	-	3/22/38/38	0/3/3/3
45	GTP	BC	501	44	-	4/22/38/38	0/3/3/3
43	GDP	KF	501	-	-	3/16/32/32	0/3/3/3
43	GDP	IL	501	-	-	6/16/32/32	0/3/3/3
43	GDP	RD	501	-	-	1/16/32/32	0/3/3/3
45	GTP	CK	501	44	-	5/22/38/38	0/3/3/3
45	GTP	JK	501	44	-	9/22/38/38	0/3/3/3
43	GDP	LN	501	-	-	3/16/32/32	0/3/3/3
45	GTP	KG	501	44	-	5/22/38/38	0/3/3/3
45	GTP	NK	501	44	-	6/22/38/38	0/3/3/3
45	GTP	OK	501	44	-	6/22/38/38	0/3/3/3
43	GDP	NJ	501	-	-	2/16/32/32	0/3/3/3
43	GDP	BF	501	-	-	2/16/32/32	0/3/3/3
43	GDP	DL	501	-	-	5/16/32/32	0/3/3/3
43	GDP	TL	501	-	-	2/16/32/32	0/3/3/3
45	GTP	DM	501	44	-	2/22/38/38	0/3/3/3
45	GTP	PC	501	44	-	8/22/38/38	0/3/3/3
45	GTP	FK	501	44	-	7/22/38/38	0/3/3/3
43	GDP	FL	501	-	-	3/16/32/32	0/3/3/3
45	GTP	JI	501	44	-	1/22/38/38	0/3/3/3
45	GTP	TM	501	44	-	4/22/38/38	0/3/3/3
45	GTP	UK	501	44	-	6/22/38/38	0/3/3/3
45	GTP	LM	501	44	-	6/22/38/38	0/3/3/3
45	GTP	OG	501	-	-	1/22/38/38	0/3/3/3
45	GTP	ME	501	44	-	5/22/38/38	0/3/3/3
45	GTP	EC	501	-	-	7/22/38/38	0/3/3/3
45	GTP	KI	501	44	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	QC	501	-	-	8/22/38/38	0/3/3/3
45	GTP	SC	501	44	-	4/22/38/38	0/3/3/3
45	GTP	FM	501	44	-	3/22/38/38	0/3/3/3
43	GDP	AD	501	-	-	4/16/32/32	0/3/3/3
43	GDP	MN	501	-	-	4/16/32/32	0/3/3/3
45	GTP	RK	501	-	-	3/22/38/38	0/3/3/3
43	GDP	AF	501	-	-	3/16/32/32	0/3/3/3
45	GTP	PI	501	44	-	1/22/38/38	0/3/3/3
45	GTP	SE	501	44	-	6/22/38/38	0/3/3/3
43	GDP	ND	501	-	-	1/16/32/32	0/3/3/3
45	GTP	WE	501	44	-	5/22/38/38	0/3/3/3
43	GDP	QH	501	-	-	2/16/32/32	0/3/3/3
45	GTP	GF	502	44	-	6/22/38/38	0/3/3/3
45	GTP	KE	501	44	-	6/22/38/38	0/3/3/3
45	GTP	LI	501	44	-	4/22/38/38	0/3/3/3
45	GTP	VC	501	44	-	4/22/38/38	0/3/3/3
45	GTP	EG	501	-	-	4/22/38/38	0/3/3/3
43	GDP	UF	501	-	-	0/16/32/32	0/3/3/3
43	GDP	WD	501	-	-	1/16/32/32	0/3/3/3
43	GDP	LJ	501	-	-	6/16/32/32	0/3/3/3
43	GDP	PD	501	-	-	3/16/32/32	0/3/3/3
45	GTP	HI	501	44	-	4/22/38/38	0/3/3/3
43	GDP	JD	501	-	-	0/16/32/32	0/3/3/3
43	GDP	JJ	501	-	-	1/16/32/32	0/3/3/3
45	GTP	MI	501	44	-	7/22/38/38	0/3/3/3
45	GTP	UI	501	44	-	7/22/38/38	0/3/3/3
45	GTP	WC	501	44	-	0/22/38/38	0/3/3/3
45	GTP	SM	501	-	-	5/22/38/38	0/3/3/3
45	GTP	VM	501	44	-	5/22/38/38	0/3/3/3
43	GDP	WL	501	-	-	2/16/32/32	0/3/3/3
45	GTP	HM	501	44	-	8/22/38/38	0/3/3/3
45	GTP	QI	501	-	-	6/22/38/38	0/3/3/3
43	GDP	HH	501	-	-	6/16/32/32	0/3/3/3
45	GTP	FE	501	44	-	4/22/38/38	0/3/3/3
43	GDP	ID	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	CI	501	44	-	5/22/38/38	0/3/3/3
43	GDP	WJ	501	-	-	3/16/32/32	0/3/3/3
43	GDP	VJ	501	-	-	1/16/32/32	0/3/3/3
45	GTP	CE	501	44	-	3/22/38/38	0/3/3/3
43	GDP	MD	501	-	-	1/16/32/32	0/3/3/3
45	GTP	JC	501	44	-	1/22/38/38	0/3/3/3
43	GDP	LF	501	-	-	1/16/32/32	0/3/3/3
43	GDP	SH	501	-	-	0/16/32/32	0/3/3/3
45	GTP	AC	501	44	-	6/22/38/38	0/3/3/3
43	GDP	CD	501	-	-	2/16/32/32	0/3/3/3
43	GDP	KN	501	-	-	2/16/32/32	0/3/3/3
43	GDP	WF	501	-	-	1/16/32/32	0/3/3/3
45	GTP	GM	501	44	-	5/22/38/38	0/3/3/3
45	GTP	AE	501	44	-	4/22/38/38	0/3/3/3
45	GTP	VI	501	44	-	6/22/38/38	0/3/3/3
43	GDP	KL	501	-	-	0/16/32/32	0/3/3/3
43	GDP	DD	501	-	-	1/16/32/32	0/3/3/3
43	GDP	EH	501	-	-	1/16/32/32	0/3/3/3
43	GDP	EF	501	-	-	3/16/32/32	0/3/3/3
45	GTP	GK	501	44	-	6/22/38/38	0/3/3/3
45	GTP	PG	501	44	-	8/22/38/38	0/3/3/3
43	GDP	AB	501	-	-	3/16/32/32	0/3/3/3
45	GTP	EI	501	-	-	3/22/38/38	0/3/3/3
43	GDP	BJ	501	-	-	2/16/32/32	0/3/3/3
45	GTP	AF	502	44	-	7/22/38/38	0/3/3/3
45	GTP	TK	501	44	-	3/22/38/38	0/3/3/3
43	GDP	CF	501	-	-	3/16/32/32	0/3/3/3
43	GDP	GH	501	-	-	2/16/32/32	0/3/3/3
43	GDP	KD	501	-	-	3/16/32/32	0/3/3/3
45	GTP	TE	501	44	-	6/22/38/38	0/3/3/3
45	GTP	SG	501	44	-	4/22/38/38	0/3/3/3
45	GTP	BE	501	44	-	5/22/38/38	0/3/3/3
45	GTP	FF	502	44	-	6/22/38/38	0/3/3/3
43	GDP	JF	501	-	-	0/16/32/32	0/3/3/3
43	GDP	TJ	501	-	-	0/16/32/32	0/3/3/3
43	GDP	QB	501	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	LE	501	44	-	6/22/38/38	0/3/3/3
43	GDP	IJ	501	-	-	1/16/32/32	0/3/3/3
43	GDP	BB	501	-	-	3/16/32/32	0/3/3/3
43	GDP	FF	501	-	-	3/16/32/32	0/3/3/3
43	GDP	JL	501	-	-	0/16/32/32	0/3/3/3
43	GDP	LL	501	-	-	2/16/32/32	0/3/3/3
45	GTP	NE	501	44	-	4/22/38/38	0/3/3/3
43	GDP	RL	501	-	-	1/16/32/32	0/3/3/3
43	GDP	DH	501	-	-	1/16/32/32	0/3/3/3
45	GTP	RE	501	-	-	7/22/38/38	0/3/3/3
43	GDP	DF	501	-	-	2/16/32/32	0/3/3/3
43	GDP	VL	501	-	-	2/16/32/32	0/3/3/3
43	GDP	VH	501	-	-	1/16/32/32	0/3/3/3
45	GTP	GC	501	44	-	5/22/38/38	0/3/3/3
45	GTP	HK	501	44	-	7/22/38/38	0/3/3/3
43	GDP	NL	501	-	-	3/16/32/32	0/3/3/3
45	GTP	SI	501	44	-	6/22/38/38	0/3/3/3
45	GTP	TG	501	44	-	2/22/38/38	0/3/3/3
43	GDP	ED	501	-	-	1/16/32/32	0/3/3/3
43	GDP	HJ	501	-	-	3/16/32/32	0/3/3/3
43	GDP	RJ	501	-	-	2/16/32/32	0/3/3/3
45	GTP	FI	501	44	-	4/22/38/38	0/3/3/3
45	GTP	HG	501	44	-	2/22/38/38	0/3/3/3
43	GDP	WH	501	-	-	5/16/32/32	0/3/3/3
45	GTP	IC	501	44	-	4/22/38/38	0/3/3/3
45	GTP	II	501	-	-	3/22/38/38	0/3/3/3
43	GDP	FH	501	-	-	1/16/32/32	0/3/3/3
45	GTP	DC	501	-	-	11/22/38/38	0/3/3/3
43	GDP	MH	501	-	-	2/16/32/32	0/3/3/3
43	GDP	TF	501	-	-	1/16/32/32	0/3/3/3
45	GTP	AK	501	44	-	7/22/38/38	0/3/3/3
45	GTP	DI	501	-	-	4/22/38/38	0/3/3/3
45	GTP	TI	501	44	-	6/22/38/38	0/3/3/3
43	GDP	CJ	501	-	-	2/16/32/32	0/3/3/3
43	GDP	UD	501	-	-	4/16/32/32	0/3/3/3
43	GDP	IN	501	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	GDP	QL	501	-	-	3/16/32/32	0/3/3/3
45	GTP	IM	501	44	-	6/22/38/38	0/3/3/3
43	GDP	AH	501	-	-	5/16/32/32	0/3/3/3
43	GDP	HB	501	-	-	4/16/32/32	0/3/3/3
43	GDP	PJ	501	-	-	2/16/32/32	0/3/3/3
43	GDP	UJ	501	-	-	4/16/32/32	0/3/3/3
43	GDP	TH	501	-	-	2/16/32/32	0/3/3/3
43	GDP	EL	501	-	-	2/16/32/32	0/3/3/3
45	GTP	WI	501	44	-	2/22/38/38	0/3/3/3
45	GTP	OA	501	44	-	7/22/38/38	0/3/3/3
43	GDP	EJ	501	-	-	4/16/32/32	0/3/3/3
43	GDP	ML	501	-	-	0/16/32/32	0/3/3/3
45	GTP	DG	501	-	-	7/22/38/38	0/3/3/3
43	GDP	MJ	501	-	-	4/16/32/32	0/3/3/3
43	GDP	RB	501	-	-	1/16/32/32	0/3/3/3
43	GDP	IF	501	-	-	1/16/32/32	0/3/3/3
43	GDP	JH	501	-	-	1/16/32/32	0/3/3/3
43	GDP	RF	501	-	-	0/16/32/32	0/3/3/3
43	GDP	FD	501	-	-	4/16/32/32	0/3/3/3
43	GDP	LD	501	-	-	4/16/32/32	0/3/3/3
43	GDP	QJ	501	-	-	1/16/32/32	0/3/3/3
43	GDP	HD	501	-	-	5/16/32/32	0/3/3/3
43	GDP	PF	501	-	-	2/16/32/32	0/3/3/3
45	GTP	MK	501	44	-	7/22/38/38	0/3/3/3
43	GDP	VF	501	-	-	2/16/32/32	0/3/3/3
43	GDP	GJ	501	-	-	0/16/32/32	0/3/3/3
45	GTP	NG	501	44	-	7/22/38/38	0/3/3/3
43	GDP	SD	501	-	-	1/16/32/32	0/3/3/3
43	GDP	HF	501	-	-	2/16/32/32	0/3/3/3
43	GDP	OL	501	-	-	2/16/32/32	0/3/3/3
43	GDP	DB	501	-	-	6/16/32/32	0/3/3/3
43	GDP	OJ	501	-	-	2/16/32/32	0/3/3/3
45	GTP	IG	501	44	-	6/22/38/38	0/3/3/3
43	GDP	PB	501	-	-	2/16/32/32	0/3/3/3
45	GTP	MM	501	44	-	6/22/38/38	0/3/3/3
45	GTP	HC	501	44	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	GTP	MG	501	-	-	4/22/38/38	0/3/3/3
45	GTP	PE	501	44	-	5/22/38/38	0/3/3/3
45	GTP	WM	501	44	-	6/22/38/38	0/3/3/3
43	GDP	AJ	501	-	-	2/16/32/32	0/3/3/3
45	GTP	JE	501	44	-	9/22/38/38	0/3/3/3
45	GTP	LC	501	44	-	4/22/38/38	0/3/3/3
45	GTP	GI	501	44	-	2/22/38/38	0/3/3/3
43	GDP	MF	501	-	-	2/16/32/32	0/3/3/3
45	GTP	AI	501	44	-	7/22/38/38	0/3/3/3
45	GTP	QE	501	-	-	6/22/38/38	0/3/3/3
45	GTP	UC	501	-	-	6/22/38/38	0/3/3/3
43	GDP	OH	501	-	-	0/16/32/32	0/3/3/3
45	GTP	NI	501	44	-	7/22/38/38	0/3/3/3
43	GDP	TD	501	-	-	1/16/32/32	0/3/3/3
45	GTP	UG	501	44	-	4/22/38/38	0/3/3/3
45	GTP	GE	501	44	-	4/22/38/38	0/3/3/3
45	GTP	OC	501	44	-	8/22/38/38	0/3/3/3
45	GTP	RC	501	-	-	7/22/38/38	0/3/3/3
45	GTP	OI	501	44	-	6/22/38/38	0/3/3/3
43	GDP	HL	501	-	-	2/16/32/32	0/3/3/3
43	GDP	PH	501	-	-	2/16/32/32	0/3/3/3
45	GTP	VK	501	44	-	5/22/38/38	0/3/3/3
45	GTP	CC	501	44	-	7/22/38/38	0/3/3/3
45	GTP	IE	501	44	-	5/22/38/38	0/3/3/3
43	GDP	UL	501	-	-	1/16/32/32	0/3/3/3
45	GTP	UE	501	44	-	4/22/38/38	0/3/3/3
45	GTP	PA	501	-	-	5/22/38/38	0/3/3/3
45	GTP	IK	501	44	-	4/22/38/38	0/3/3/3
43	GDP	PL	501	-	-	1/16/32/32	0/3/3/3
45	GTP	KC	501	44	-	5/22/38/38	0/3/3/3
45	GTP	KM	501	44	-	2/22/38/38	0/3/3/3
45	GTP	EK	501	44	-	3/22/38/38	0/3/3/3
45	GTP	NA	501	44	-	5/22/38/38	0/3/3/3
43	GDP	OB	501	-	-	3/16/32/32	0/3/3/3
43	GDP	UH	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	GDP	RH	501	-	-	0/16/32/32	0/3/3/3
45	GTP	NC	501	44	-	7/22/38/38	0/3/3/3
43	GDP	SL	501	-	-	1/16/32/32	0/3/3/3
45	GTP	SK	501	44	-	6/22/38/38	0/3/3/3
45	GTP	EE	501	-	-	4/22/38/38	0/3/3/3
43	GDP	WN	501	-	-	0/16/32/32	0/3/3/3
45	GTP	CM	501	44	-	4/22/38/38	0/3/3/3
43	GDP	BH	501	-	-	4/16/32/32	0/3/3/3
43	GDP	NB	501	-	-	4/16/32/32	0/3/3/3

The worst 5 of 565 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	UJ	501	GDP	C2-N2	4.08	1.43	1.34
43	FF	501	GDP	C6-N1	-3.50	1.32	1.38
43	MF	501	GDP	PA-O3A	3.44	1.63	1.59
43	FF	501	GDP	C5-C4	3.31	1.47	1.38
43	UJ	501	GDP	C5-C4	3.29	1.47	1.38

The worst 5 of 2137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	FF	501	GDP	C5-C4-N3	-7.10	117.08	128.39
43	IN	501	GDP	C5-C4-N3	-6.86	117.47	128.39
43	NL	501	GDP	C5-C4-N3	-6.79	117.58	128.39
43	PL	501	GDP	C5-C4-N3	-6.58	117.92	128.39
43	ND	501	GDP	C5-C4-N3	-6.49	118.06	128.39

There are no chirality outliers.

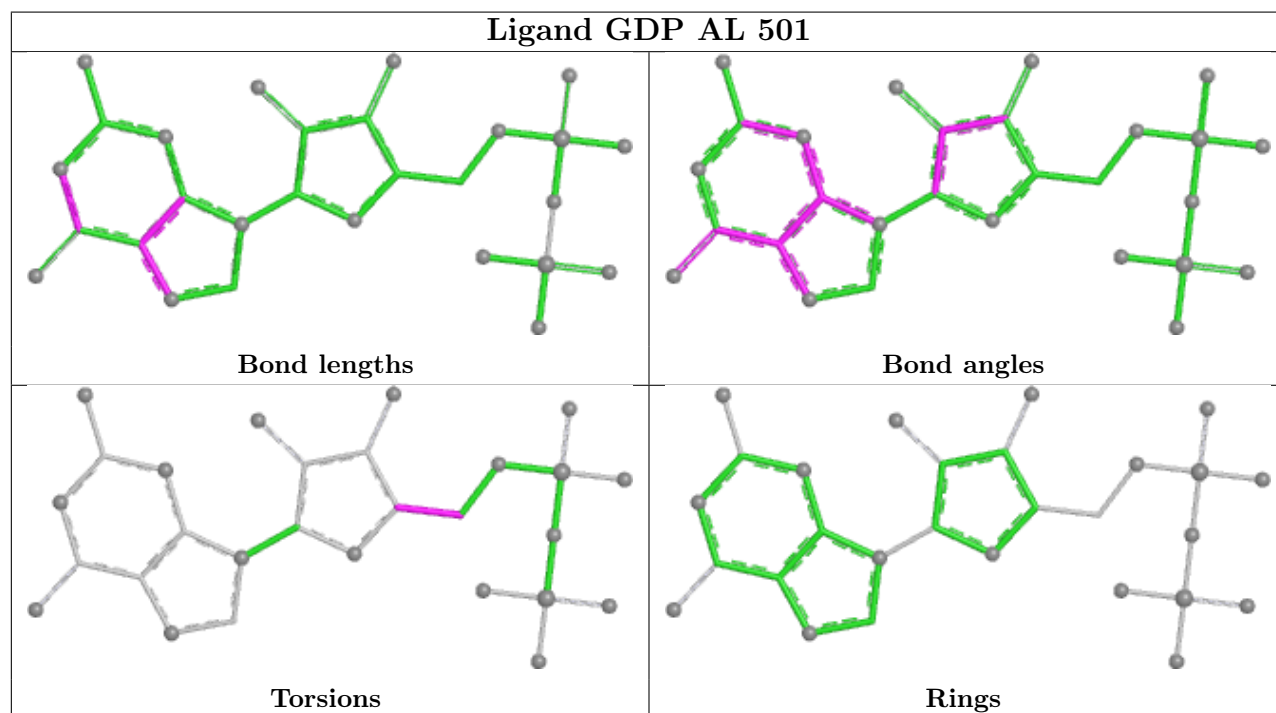
5 of 974 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	AB	501	GDP	C5'-O5'-PA-O1A
43	AB	501	GDP	O4'-C4'-C5'-O5'
43	AB	501	GDP	C3'-C4'-C5'-O5'
43	AF	501	GDP	O4'-C4'-C5'-O5'
43	AF	501	GDP	C3'-C4'-C5'-O5'

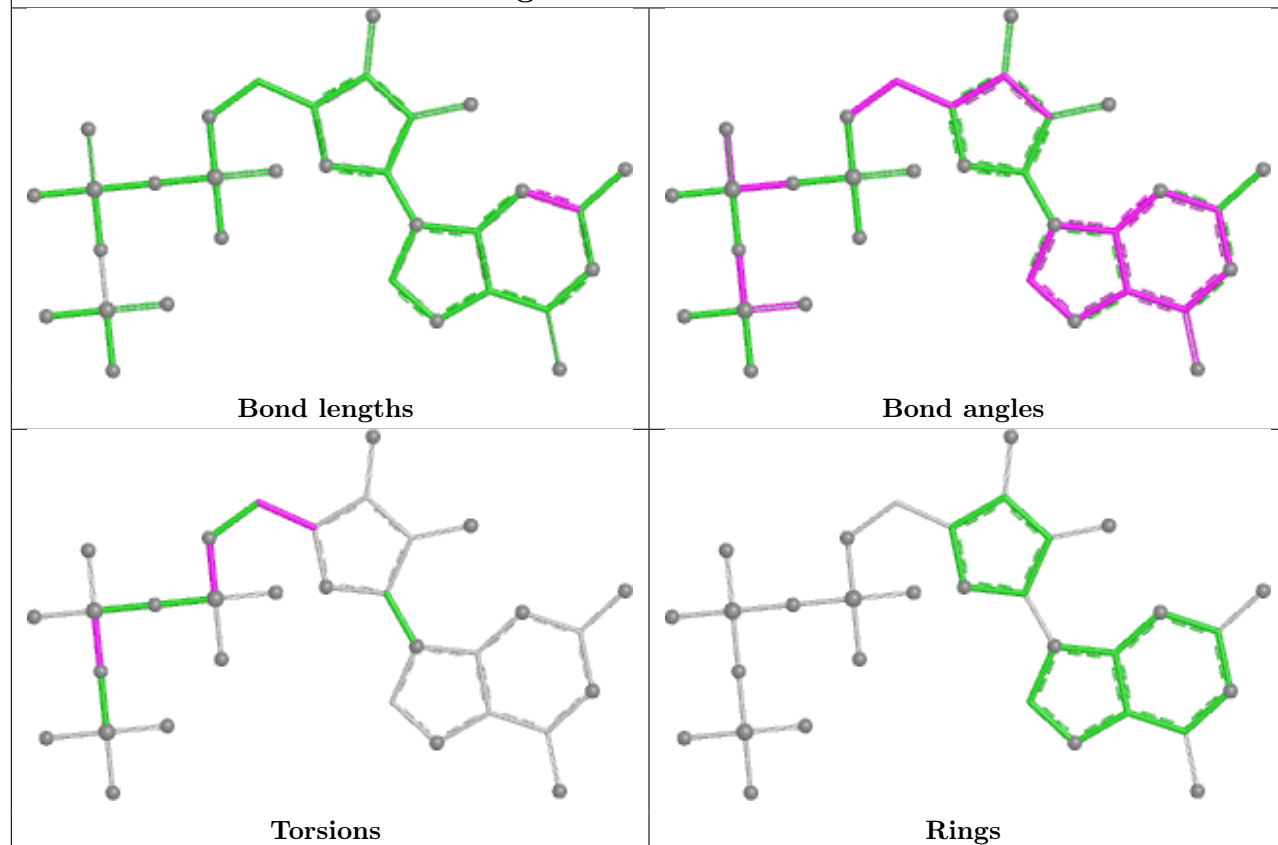
There are no ring outliers.

No monomer is involved in short contacts.

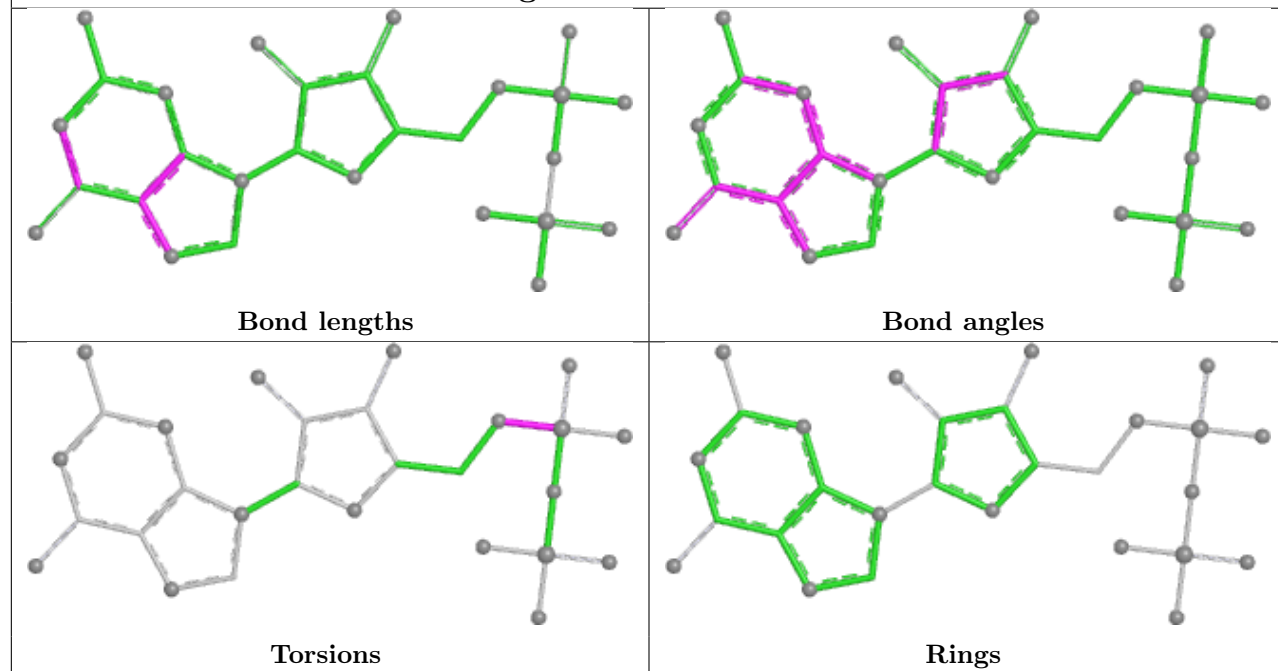
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



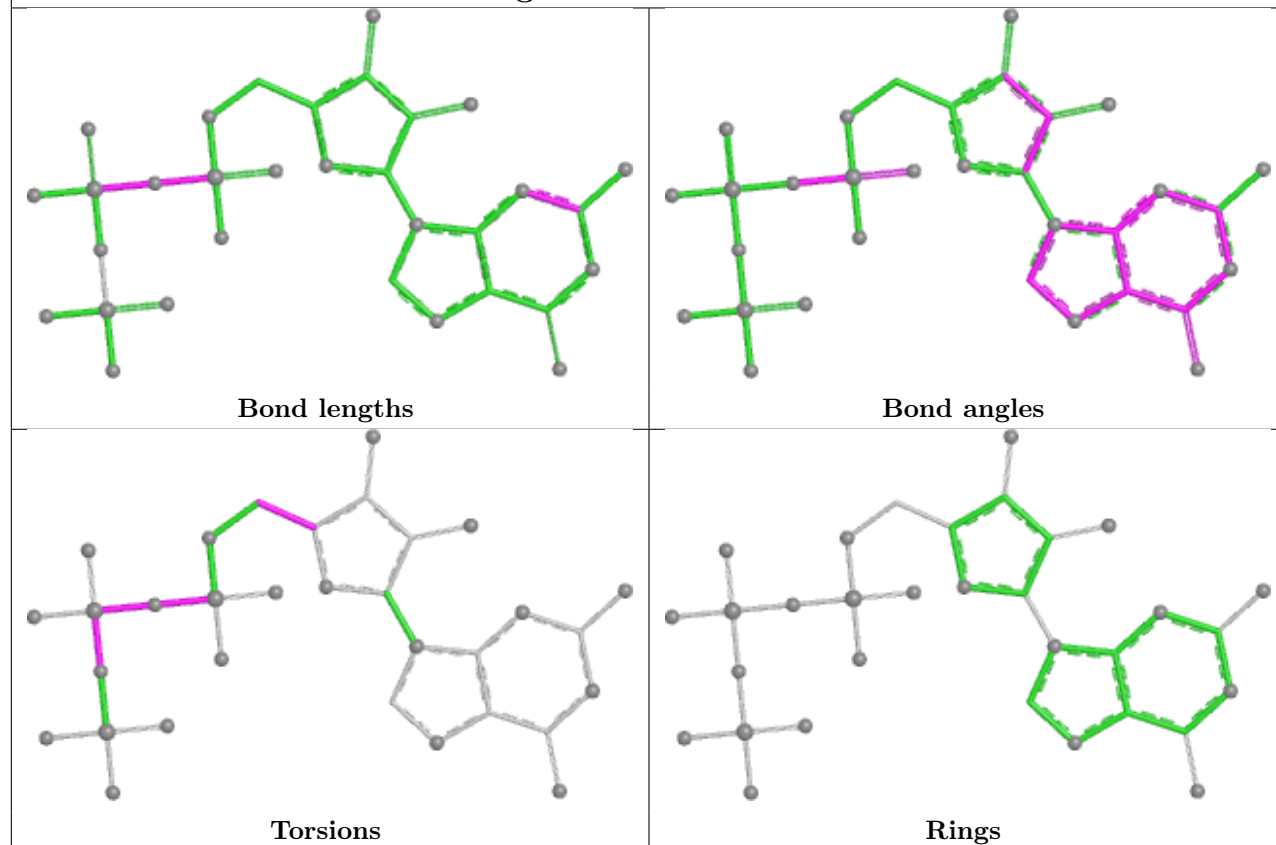
## Ligand GTP RG 501



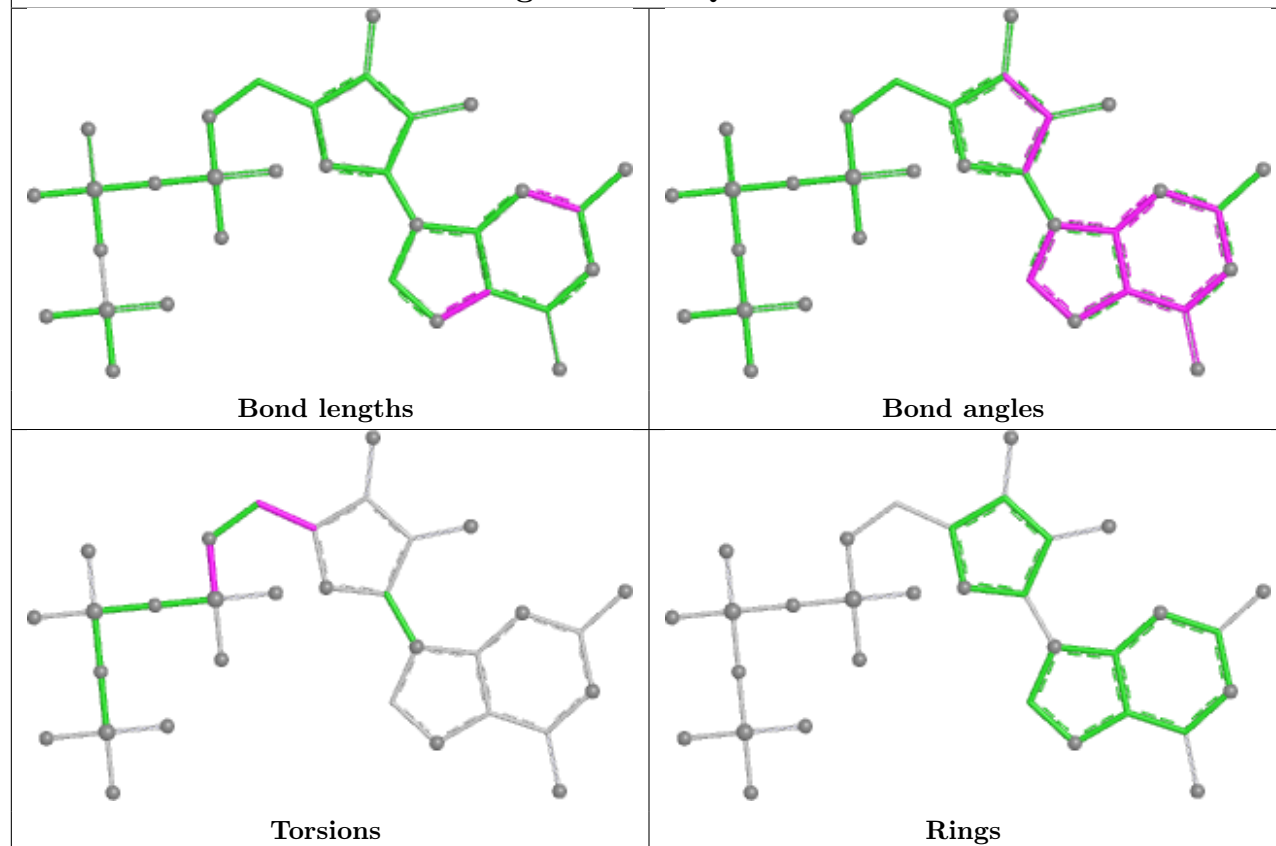
## Ligand GDP KJ 501

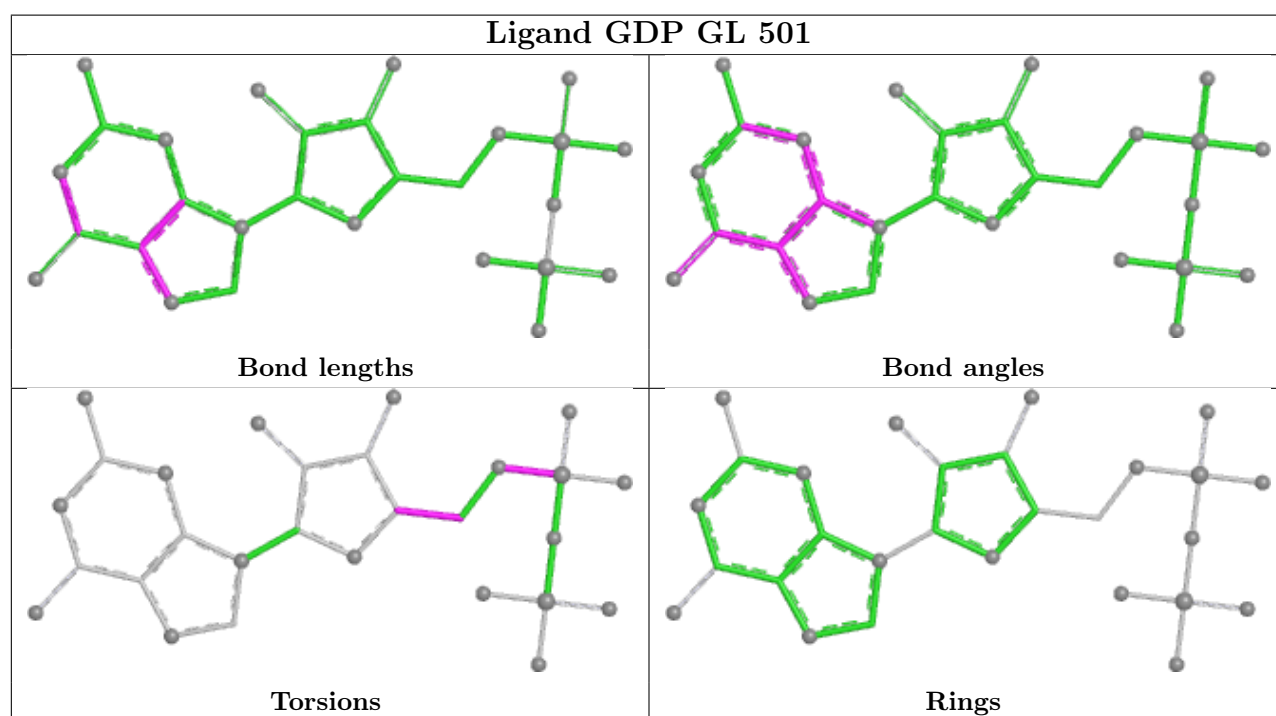
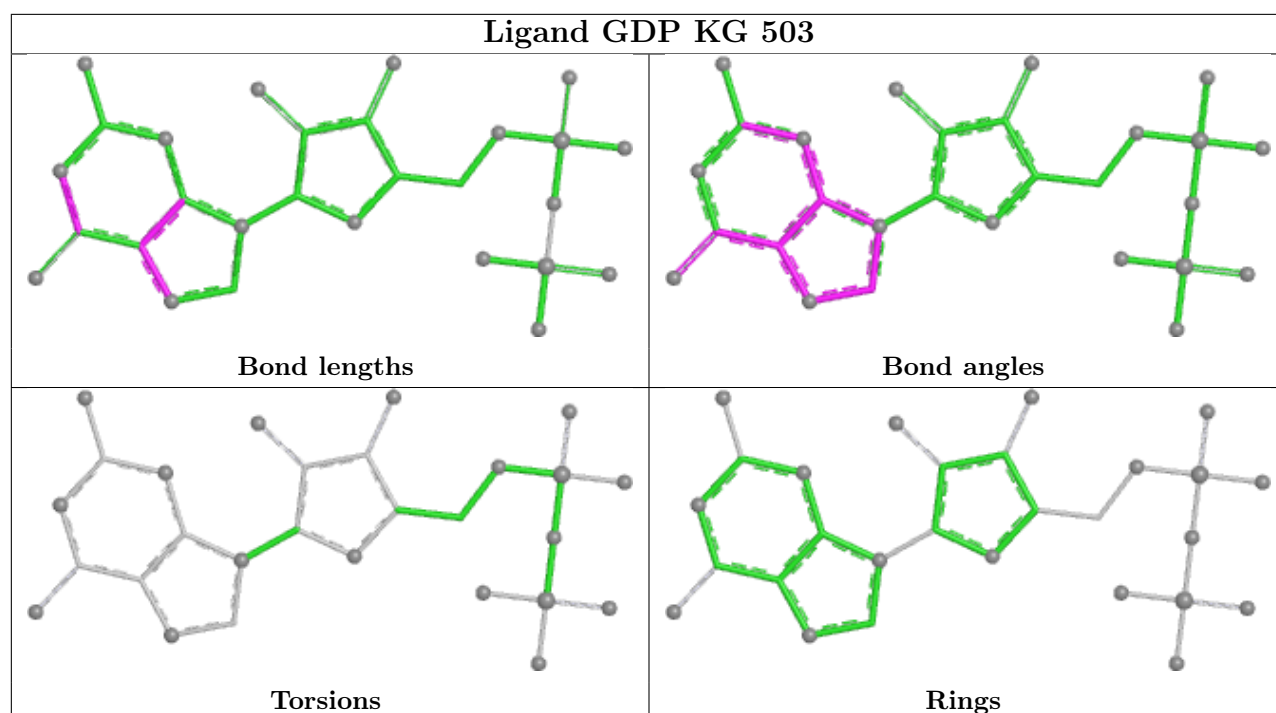


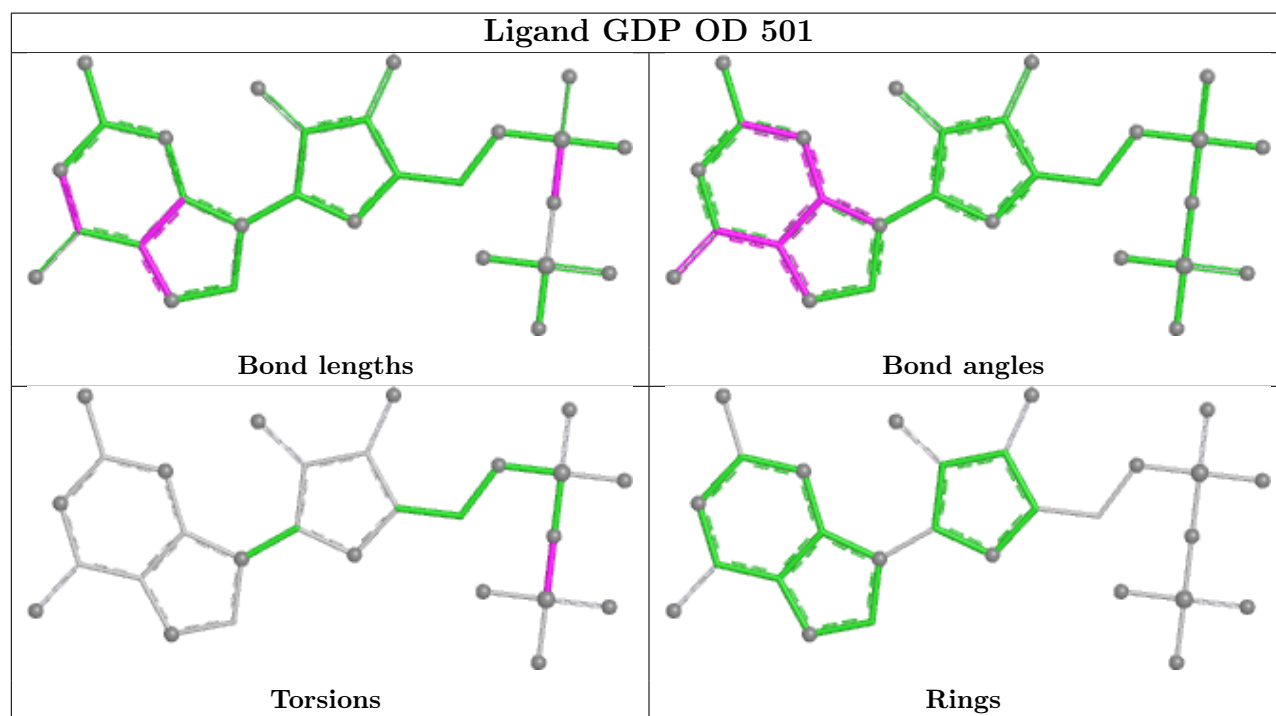
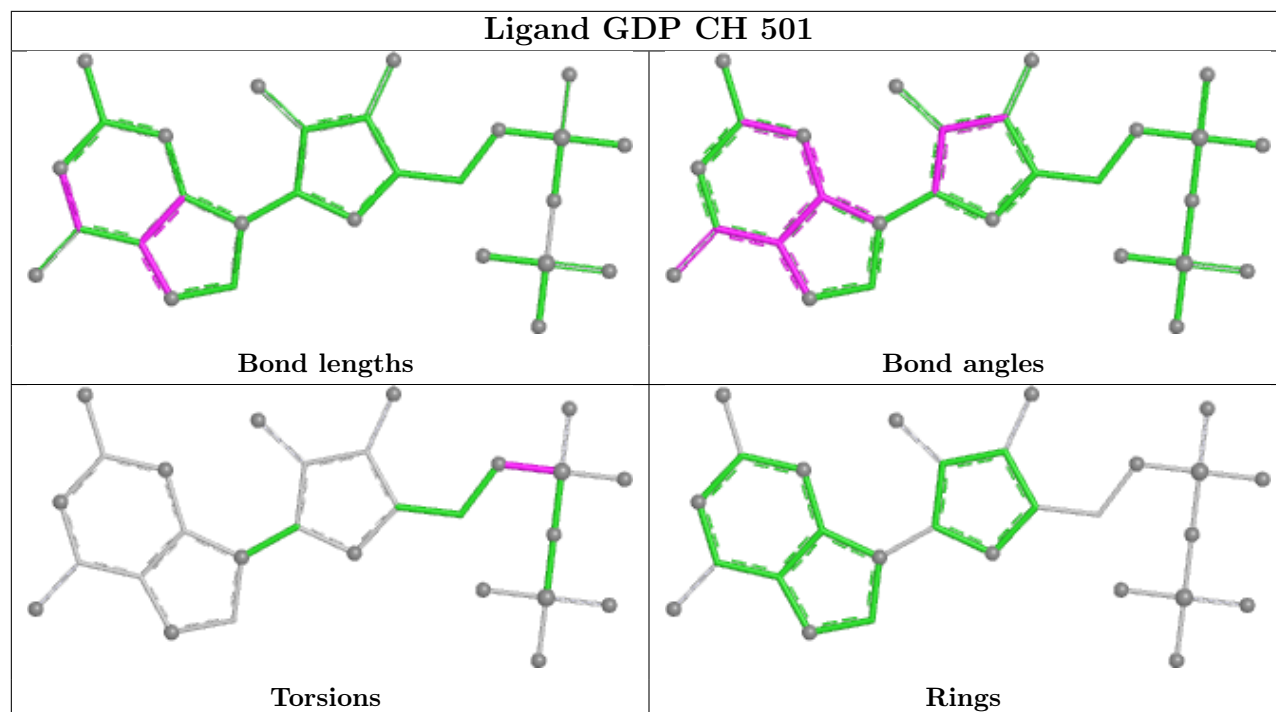
## Ligand GTP DK 501

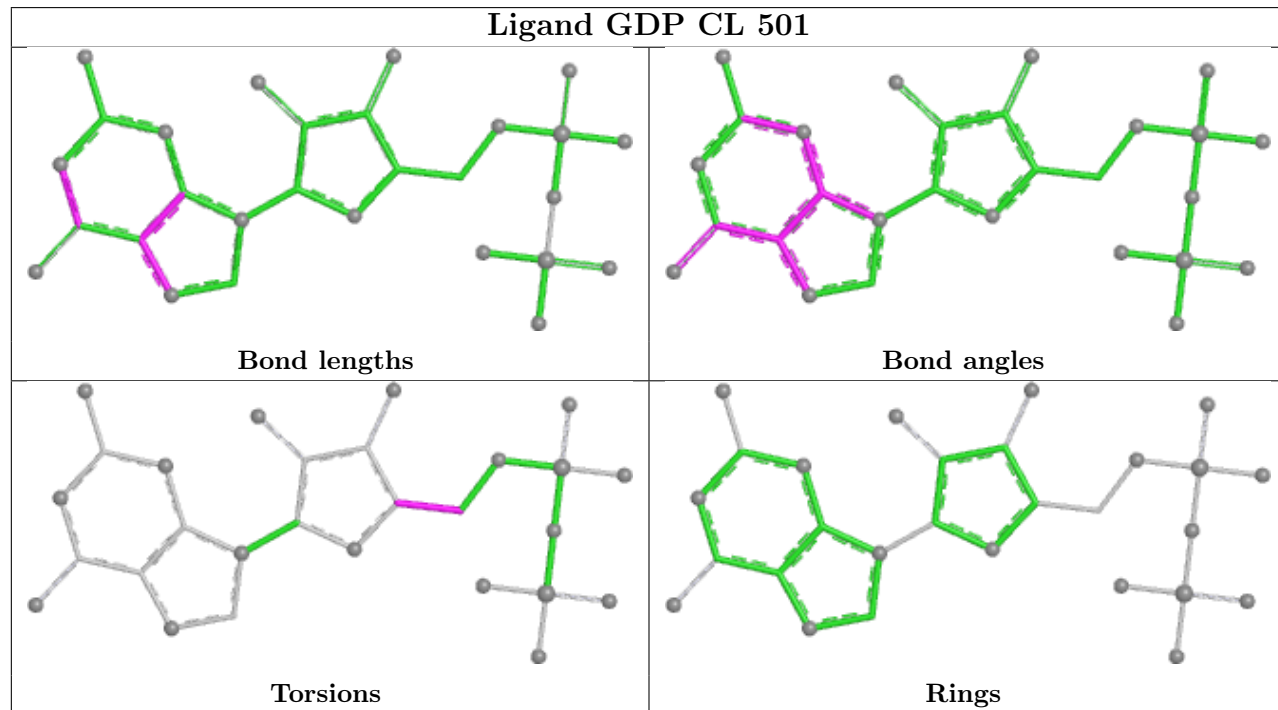
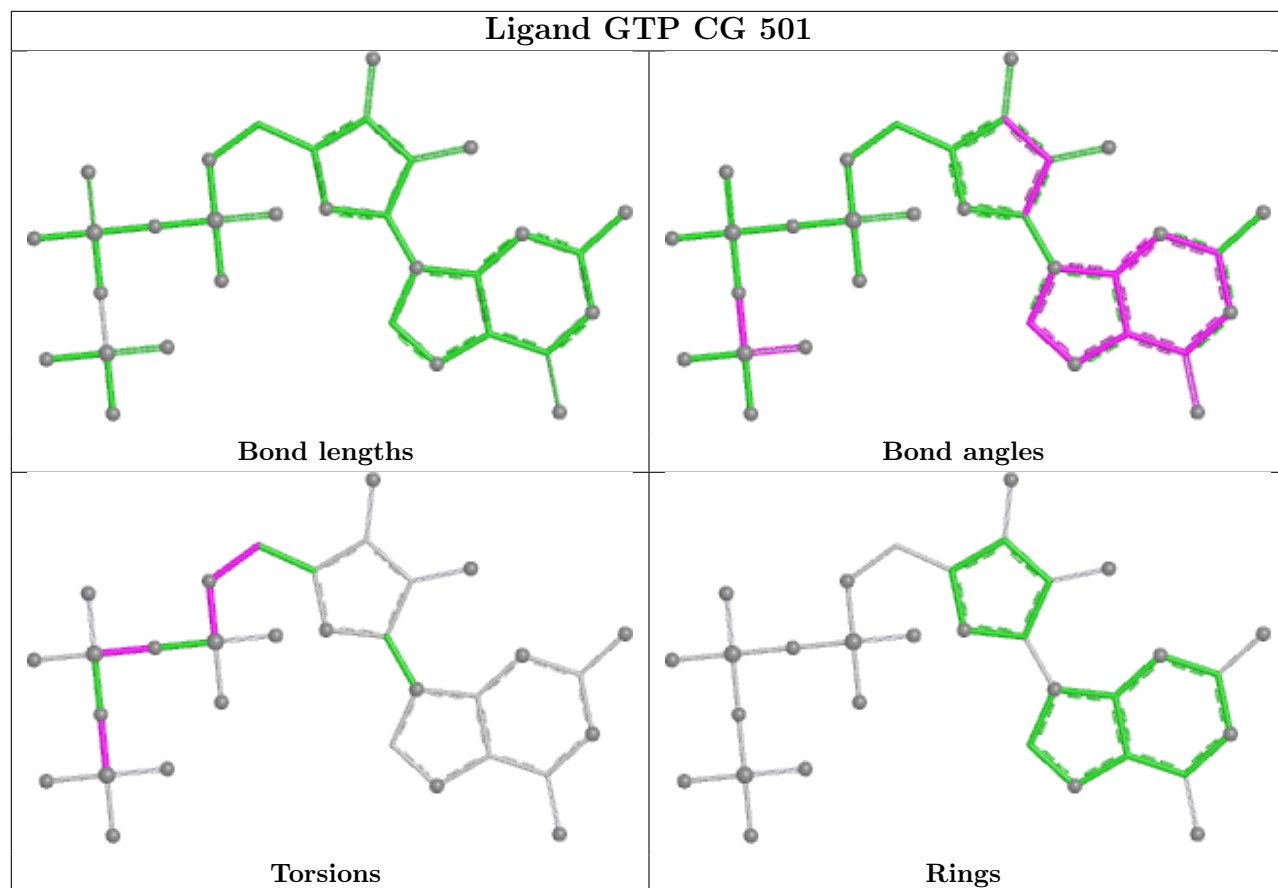


## Ligand GTP QG 501



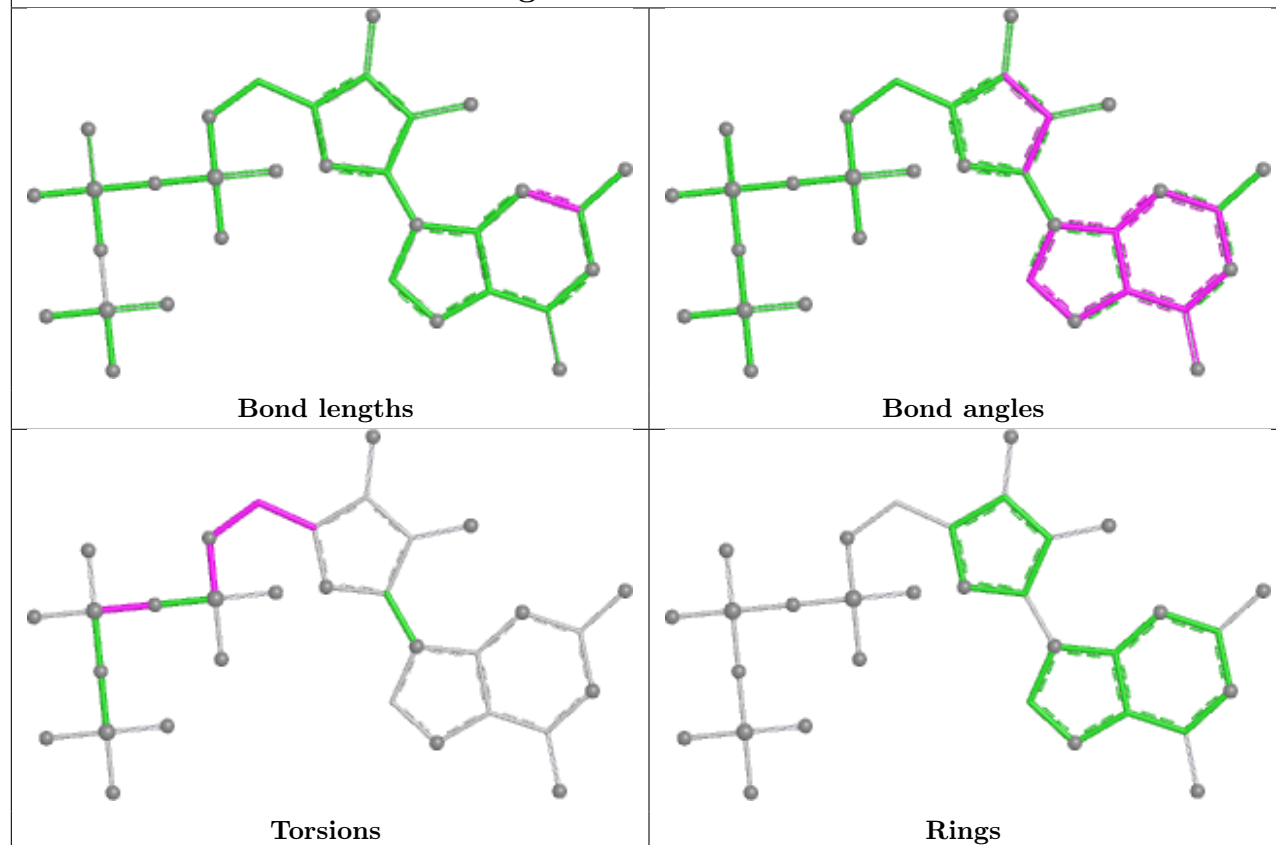




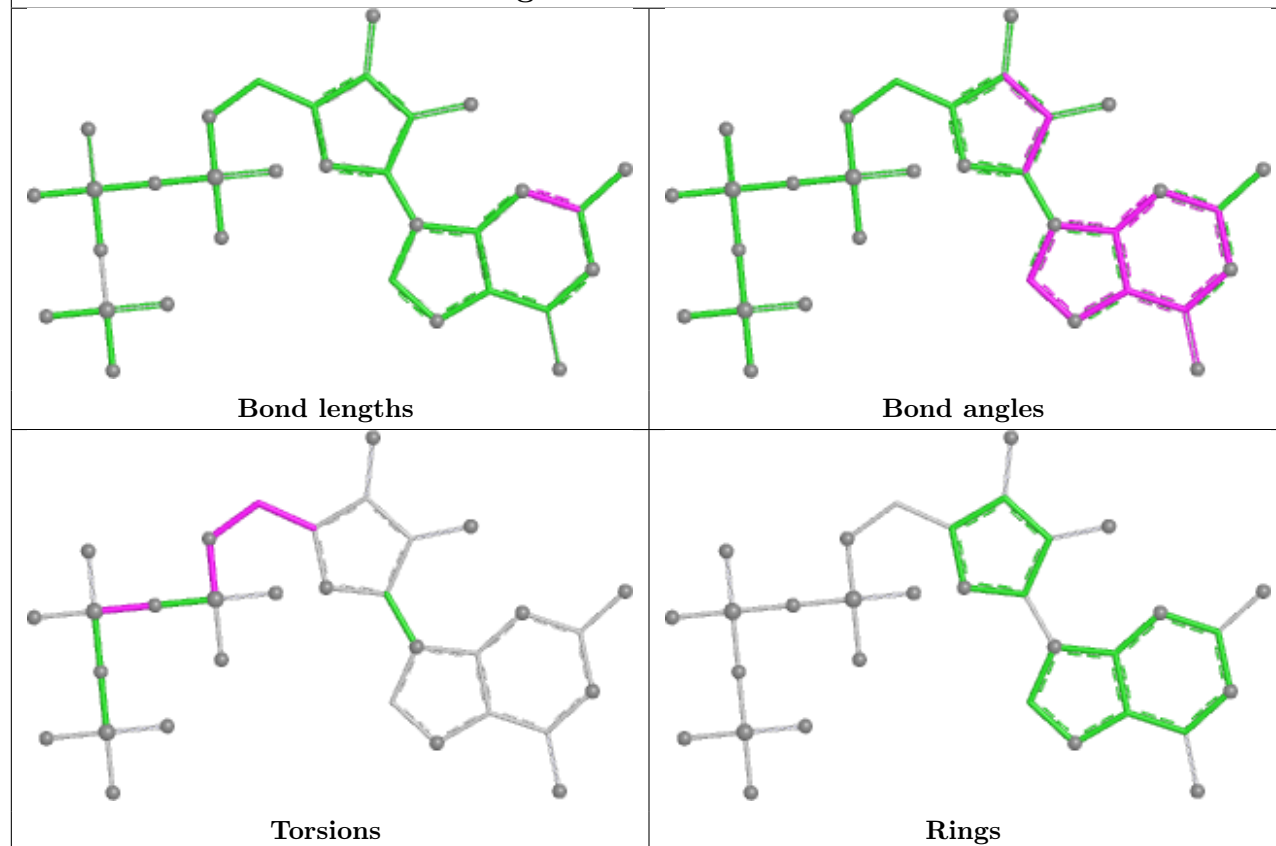




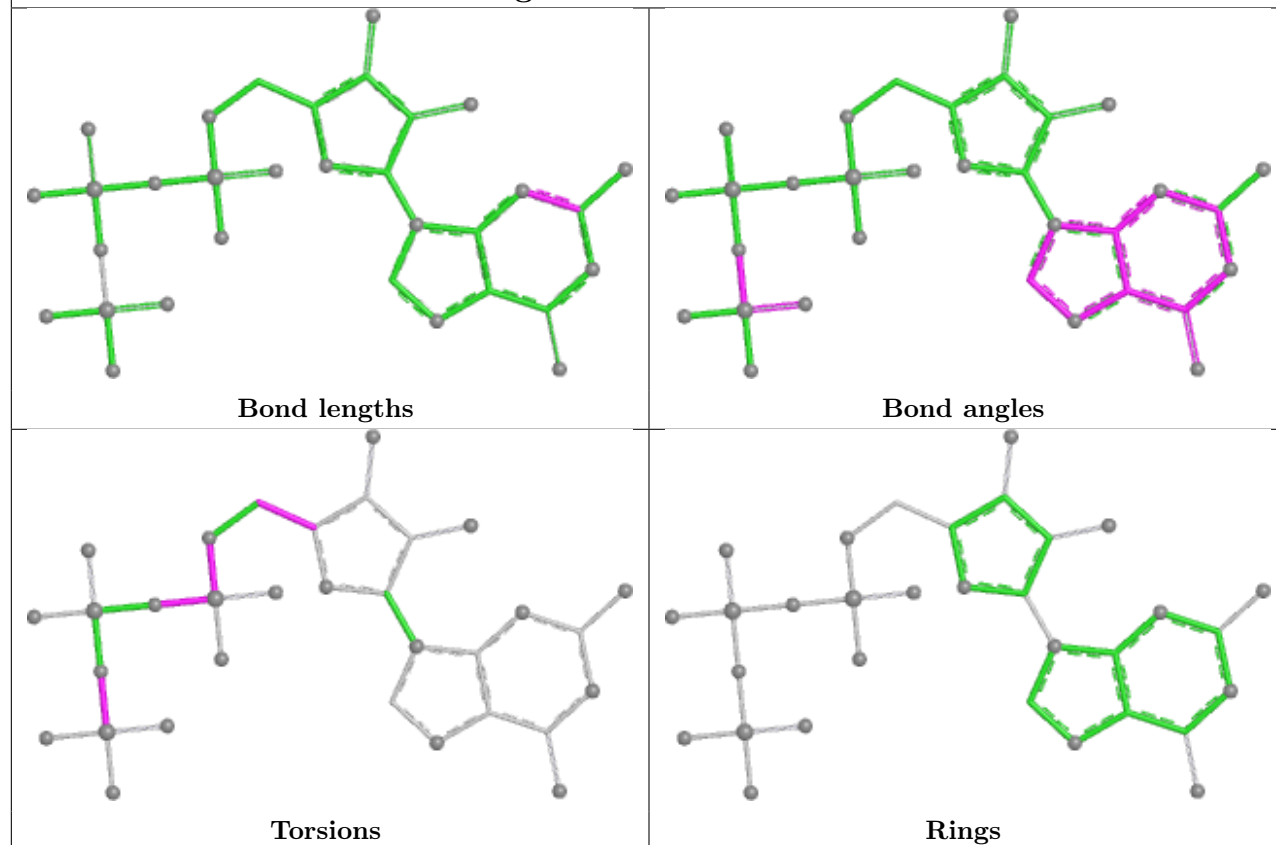
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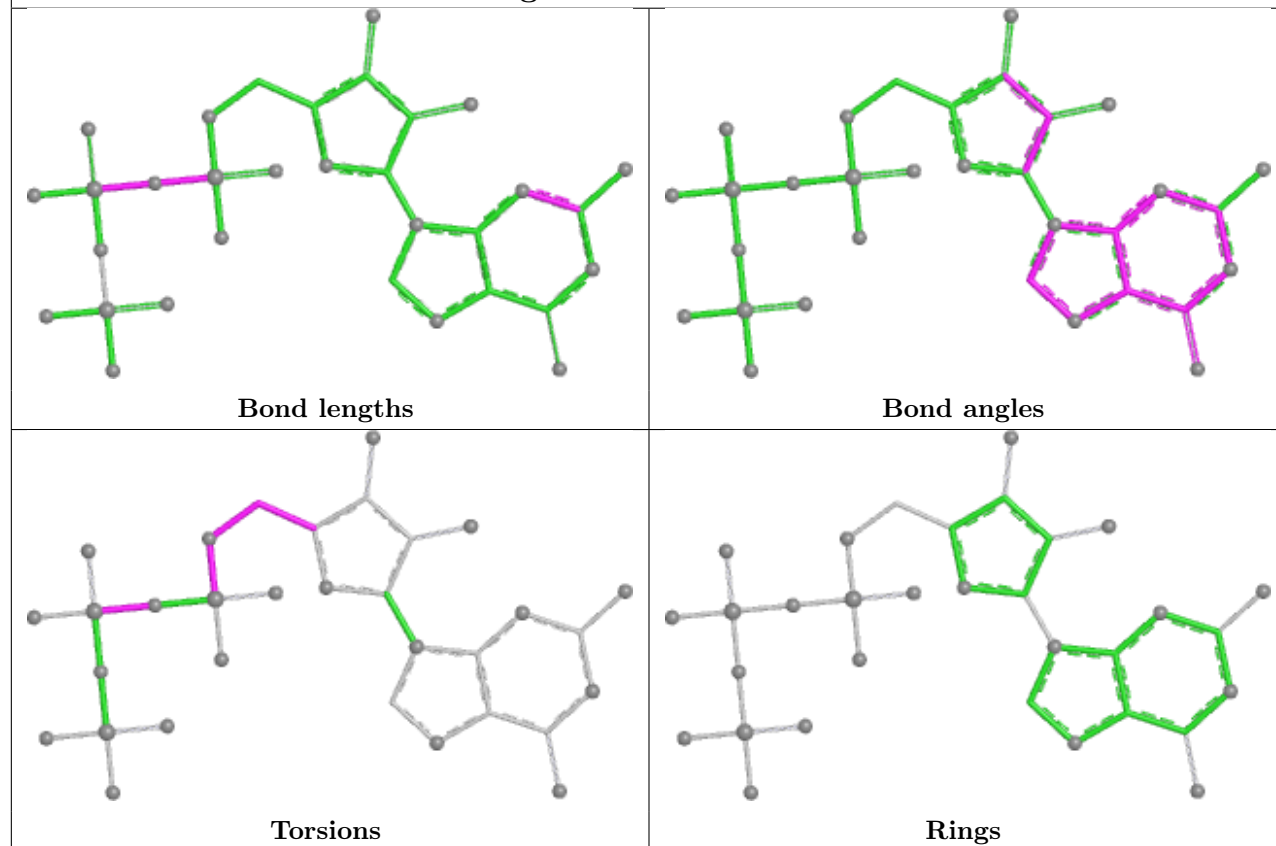
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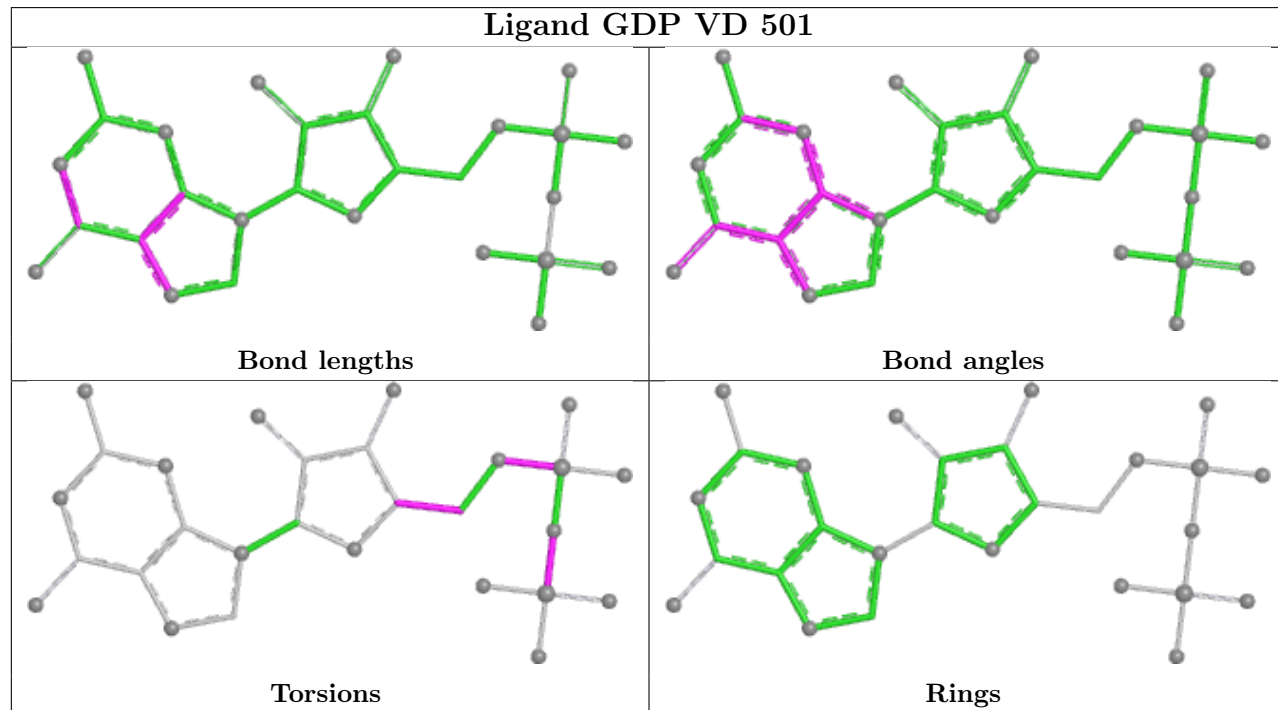
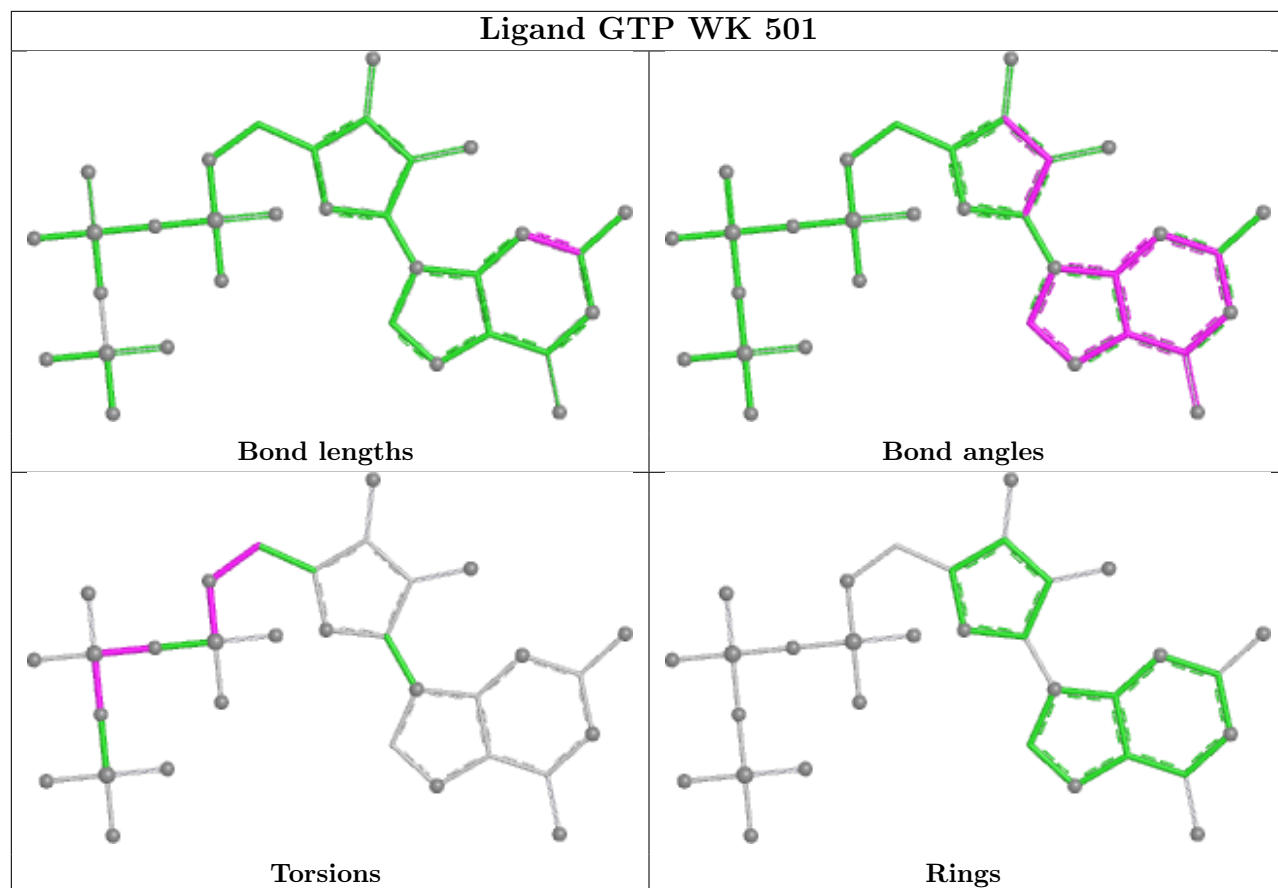


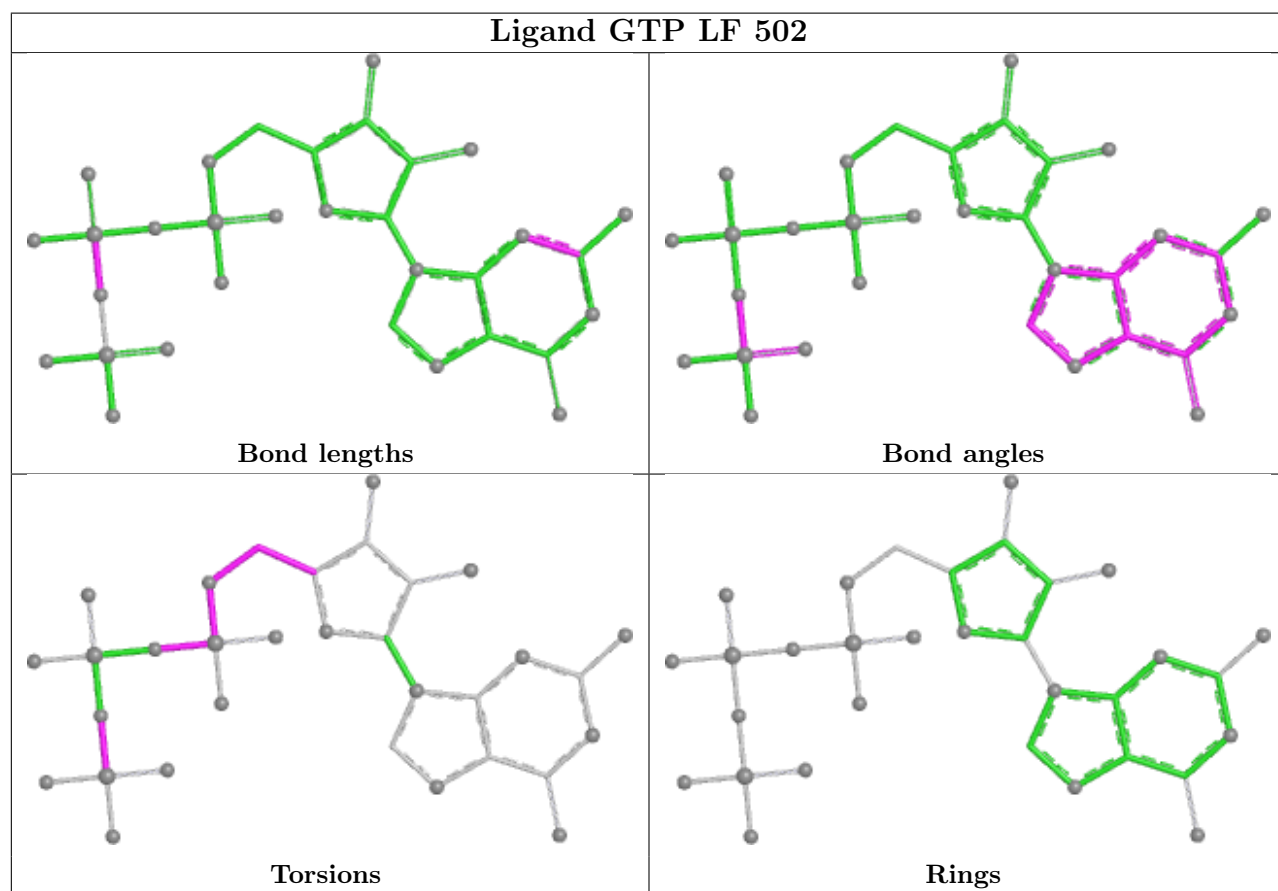
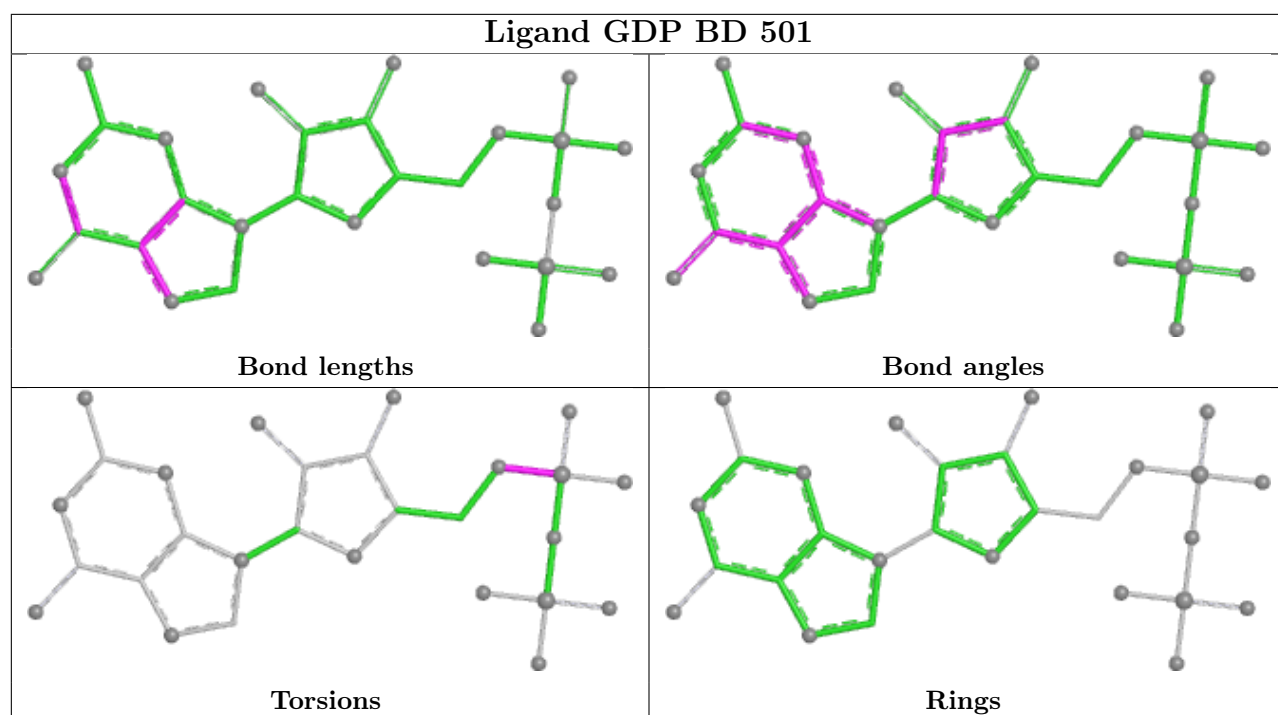
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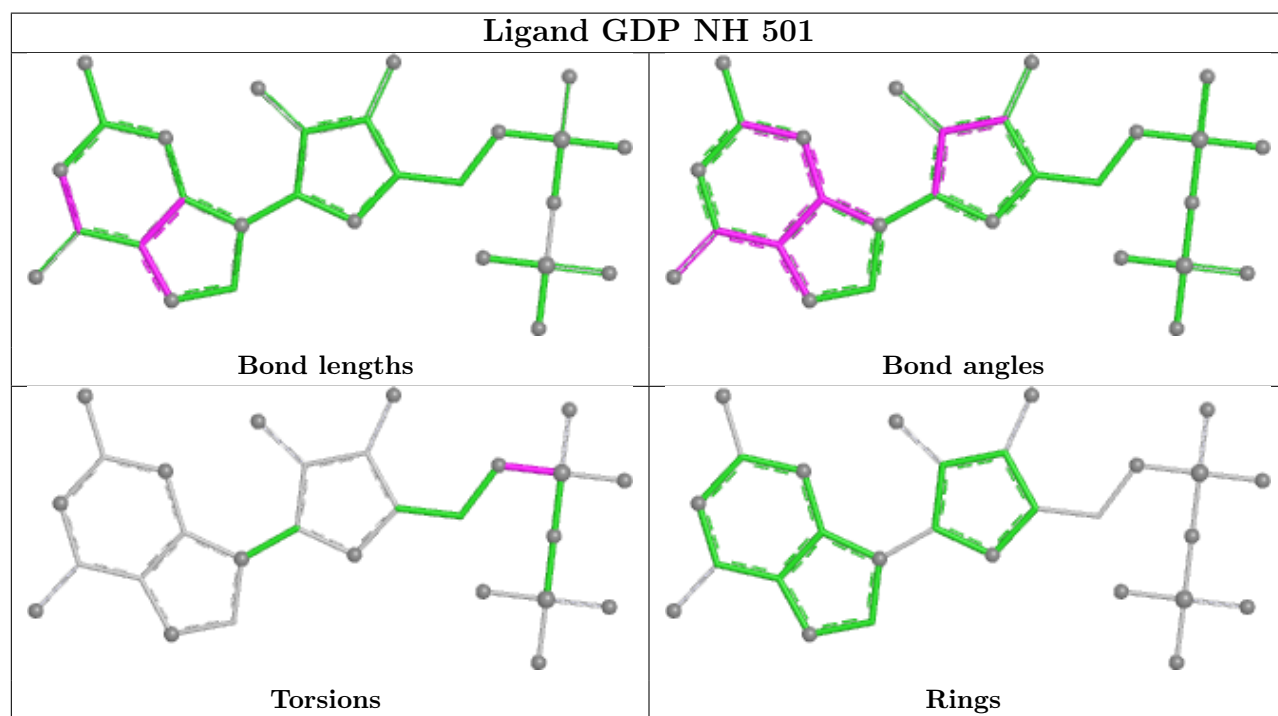
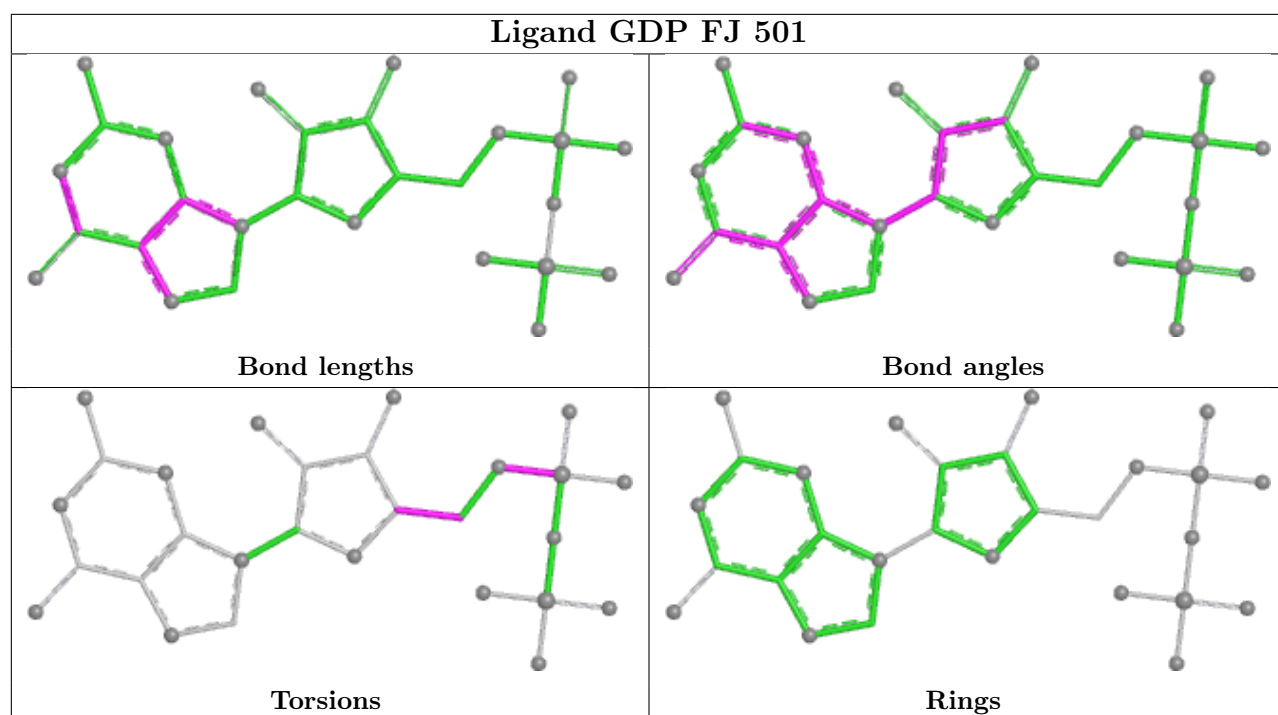


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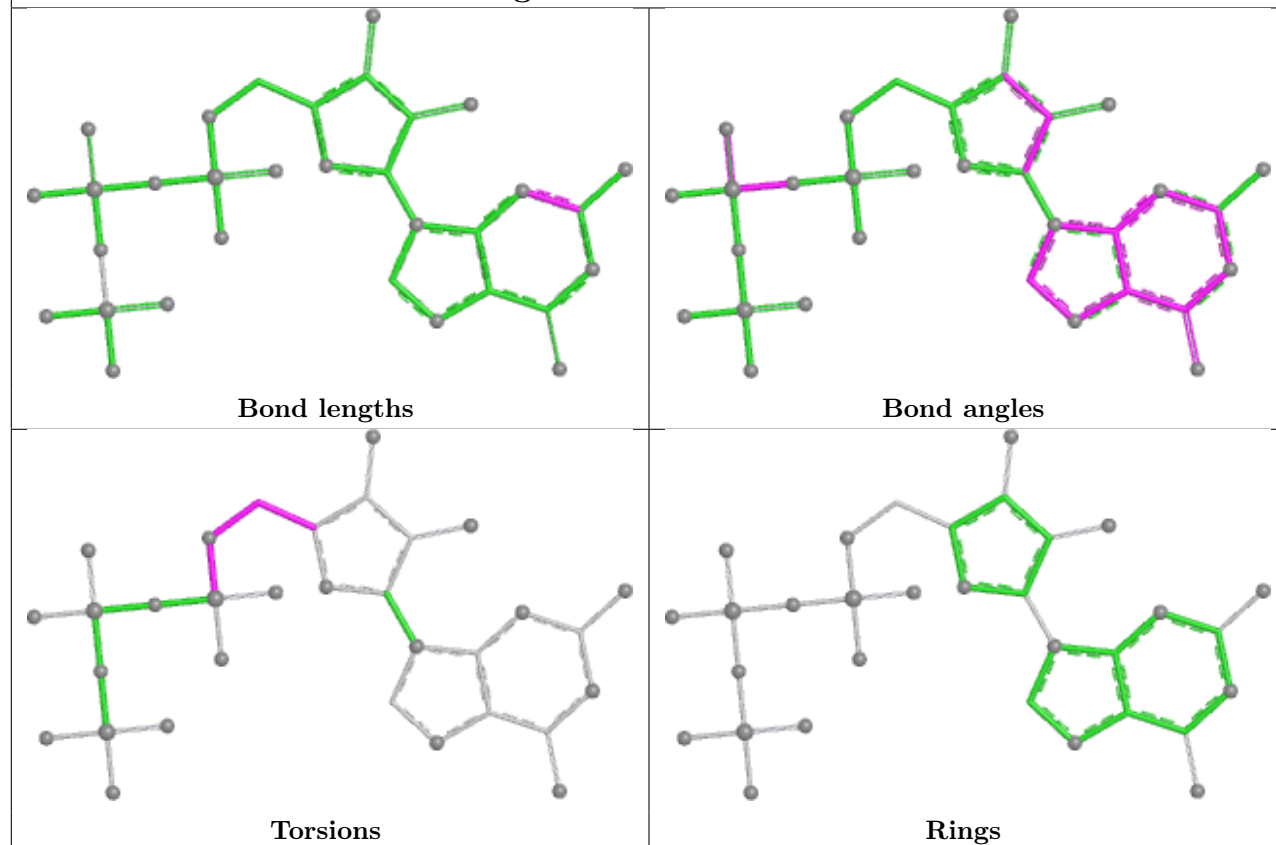




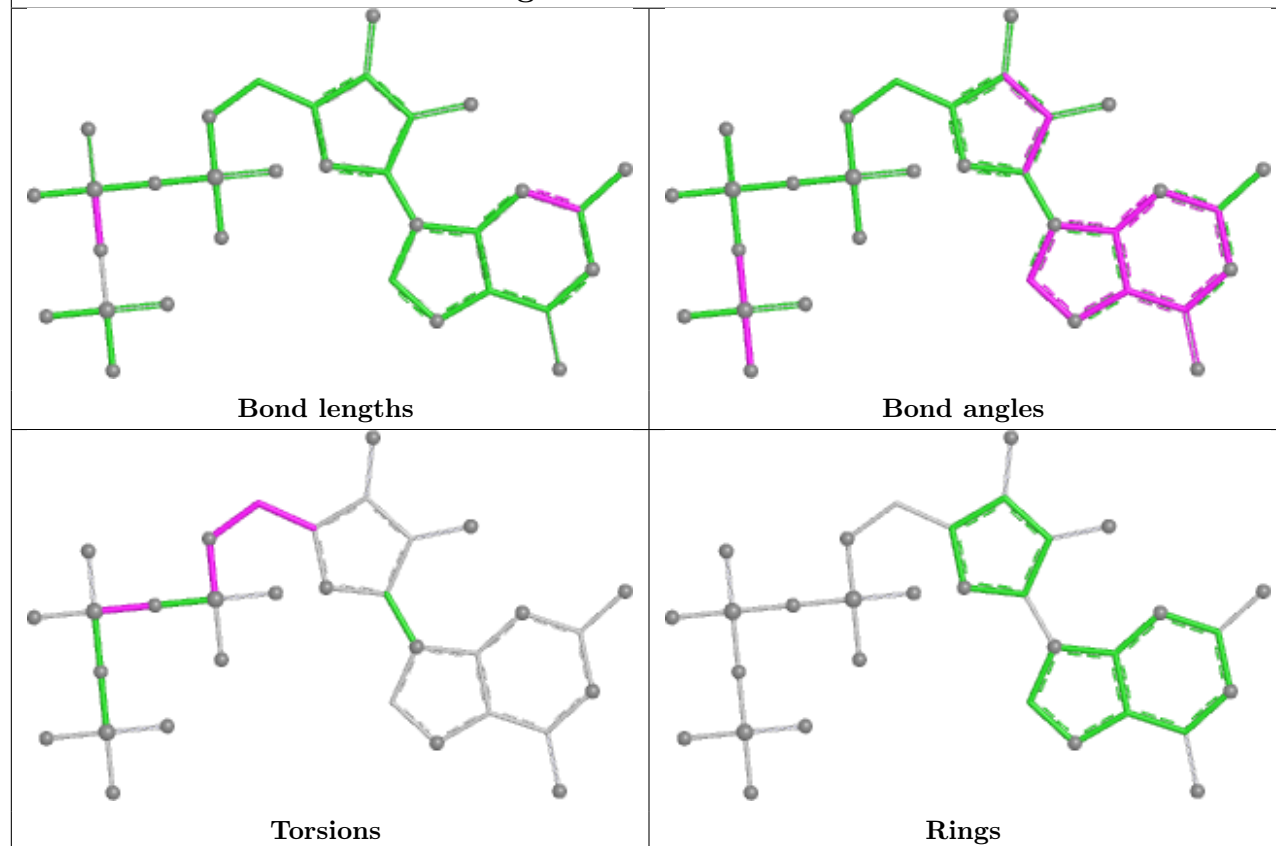


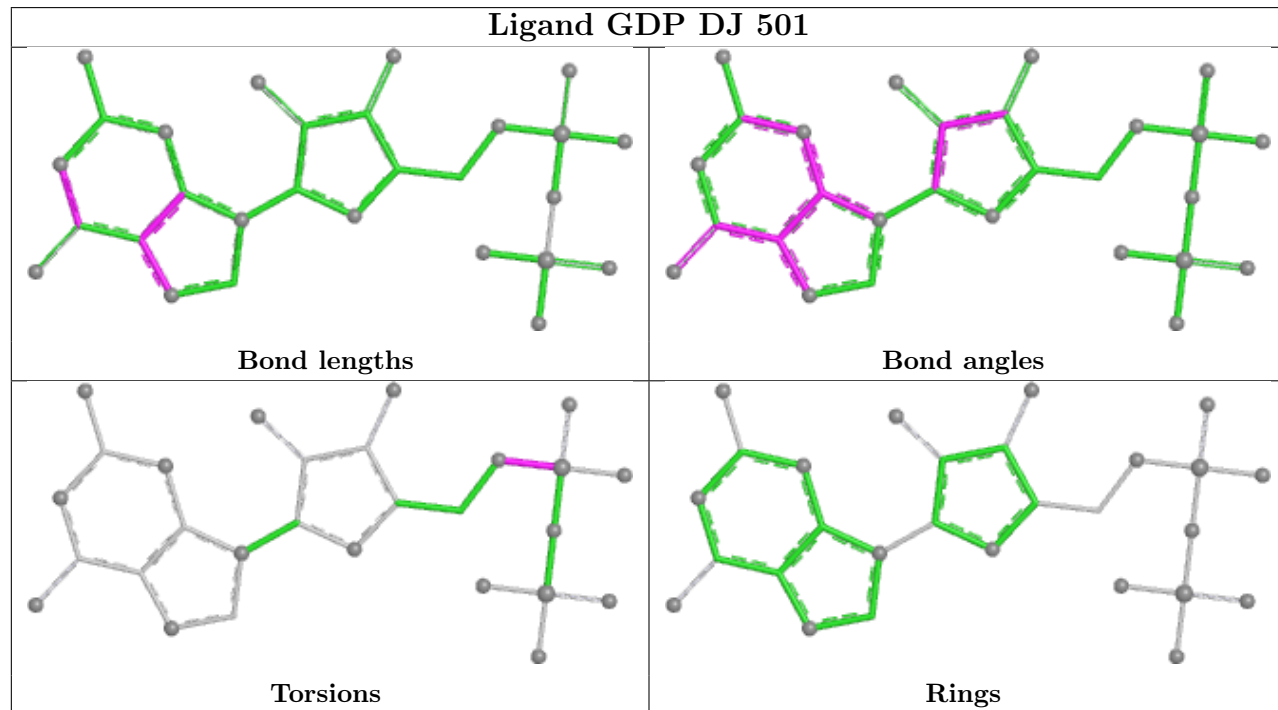
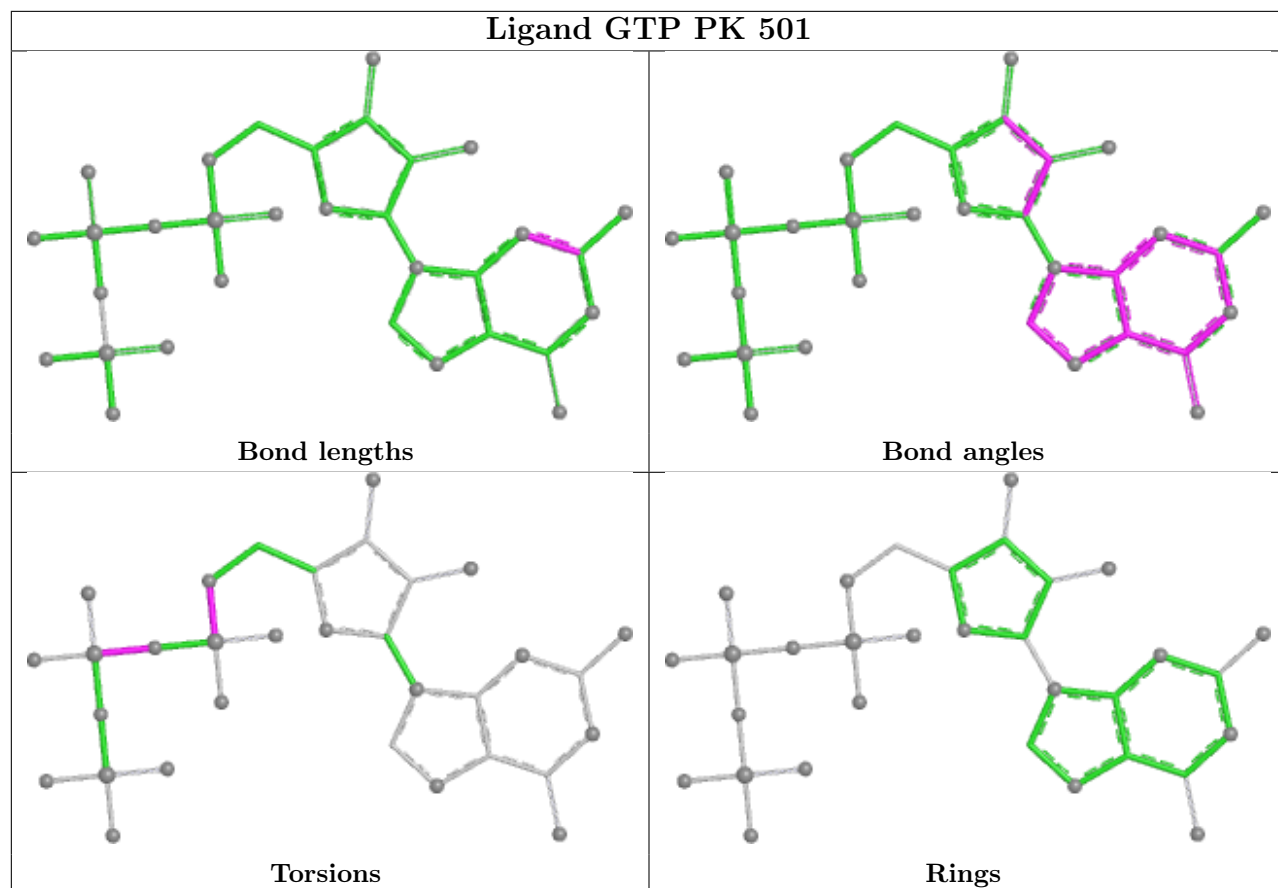


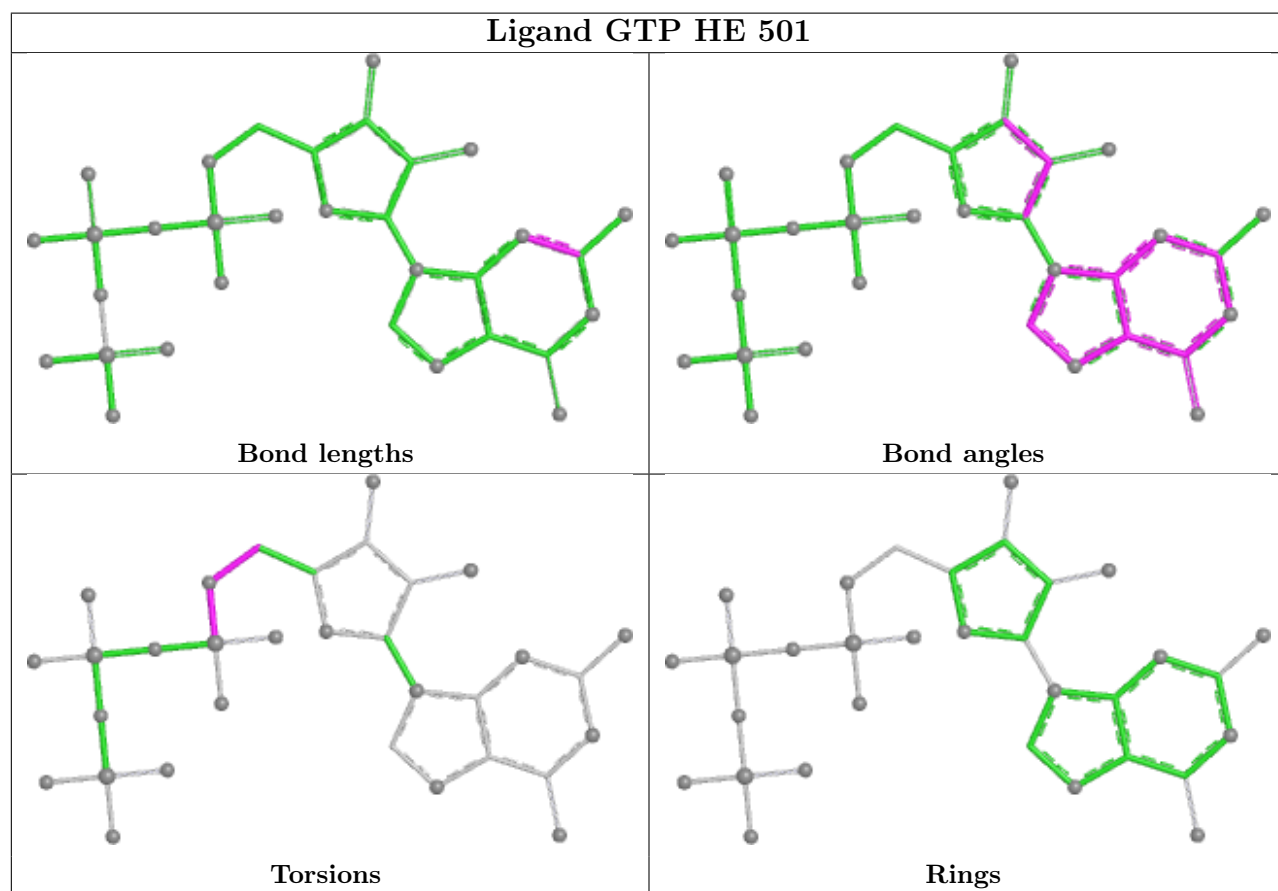
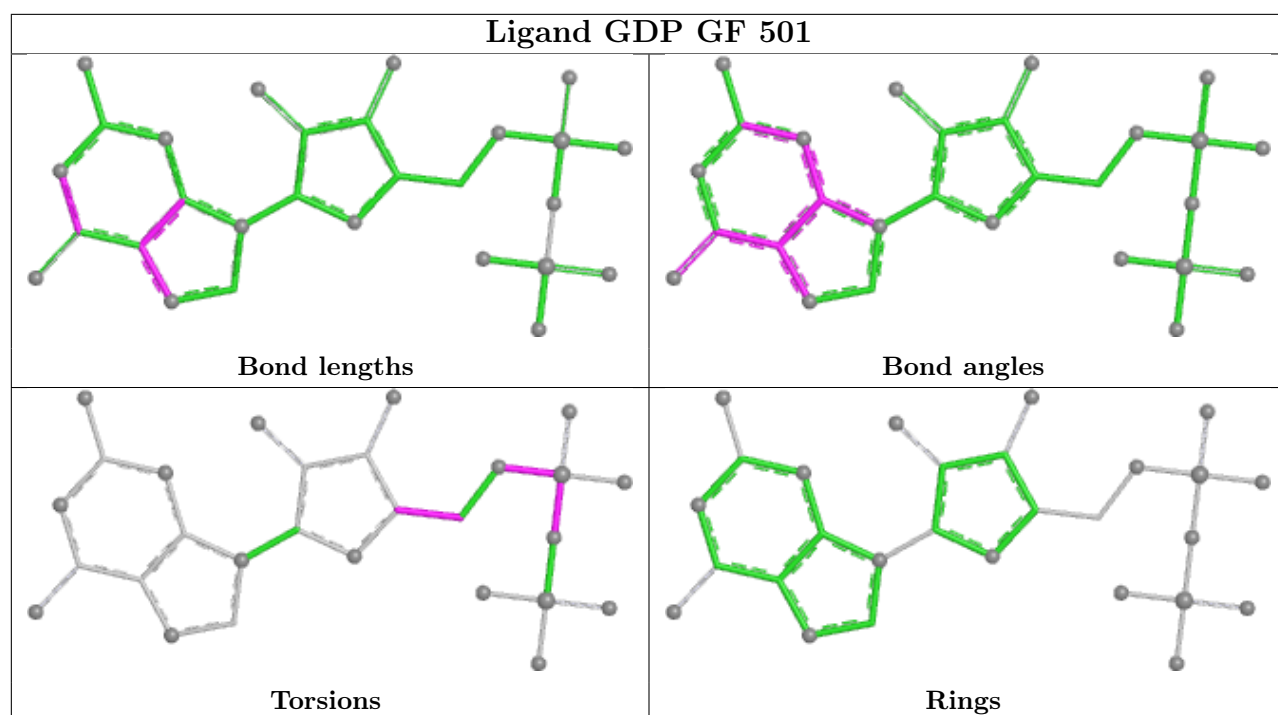
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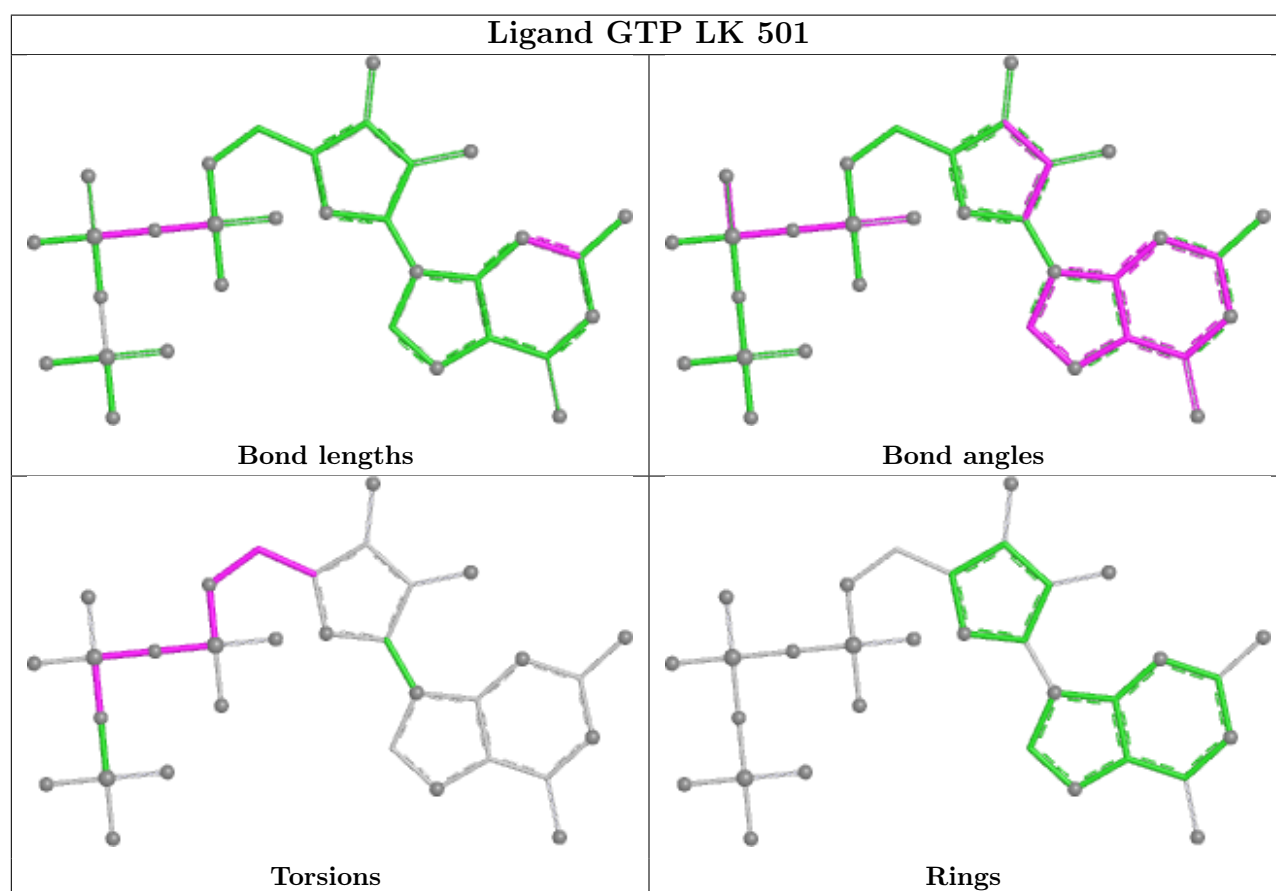
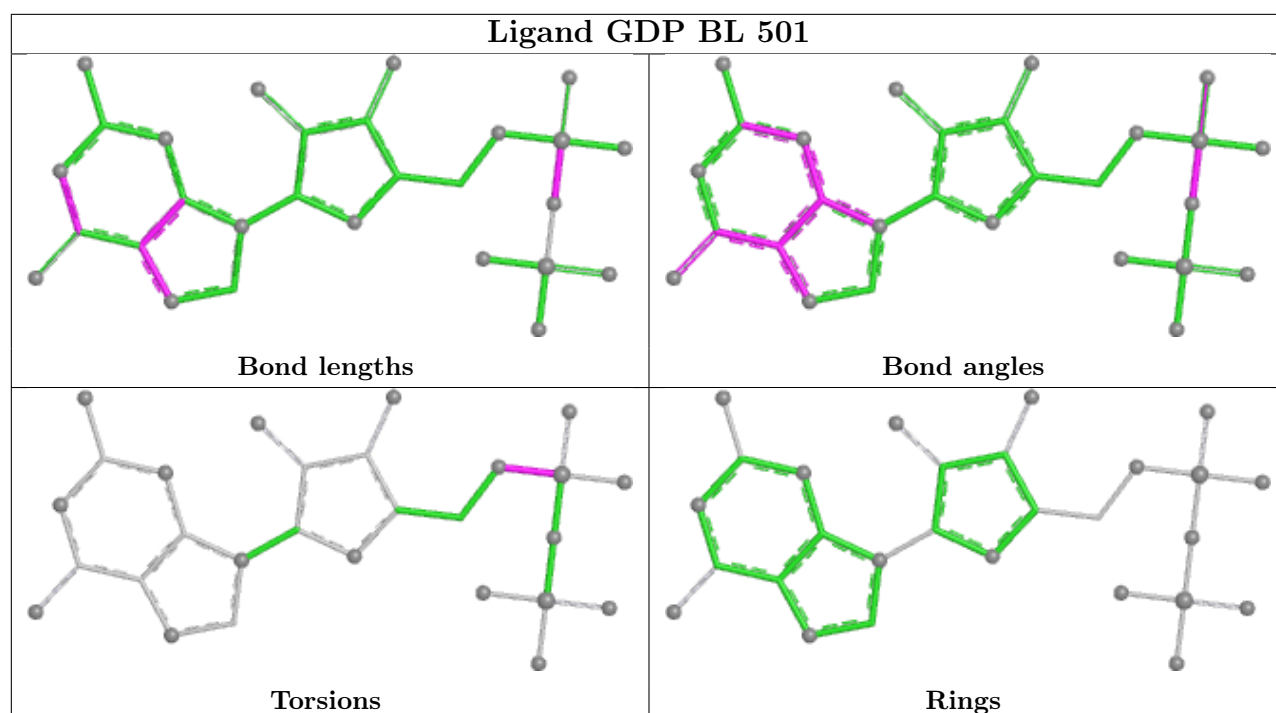
## Ligand GTP BK 501



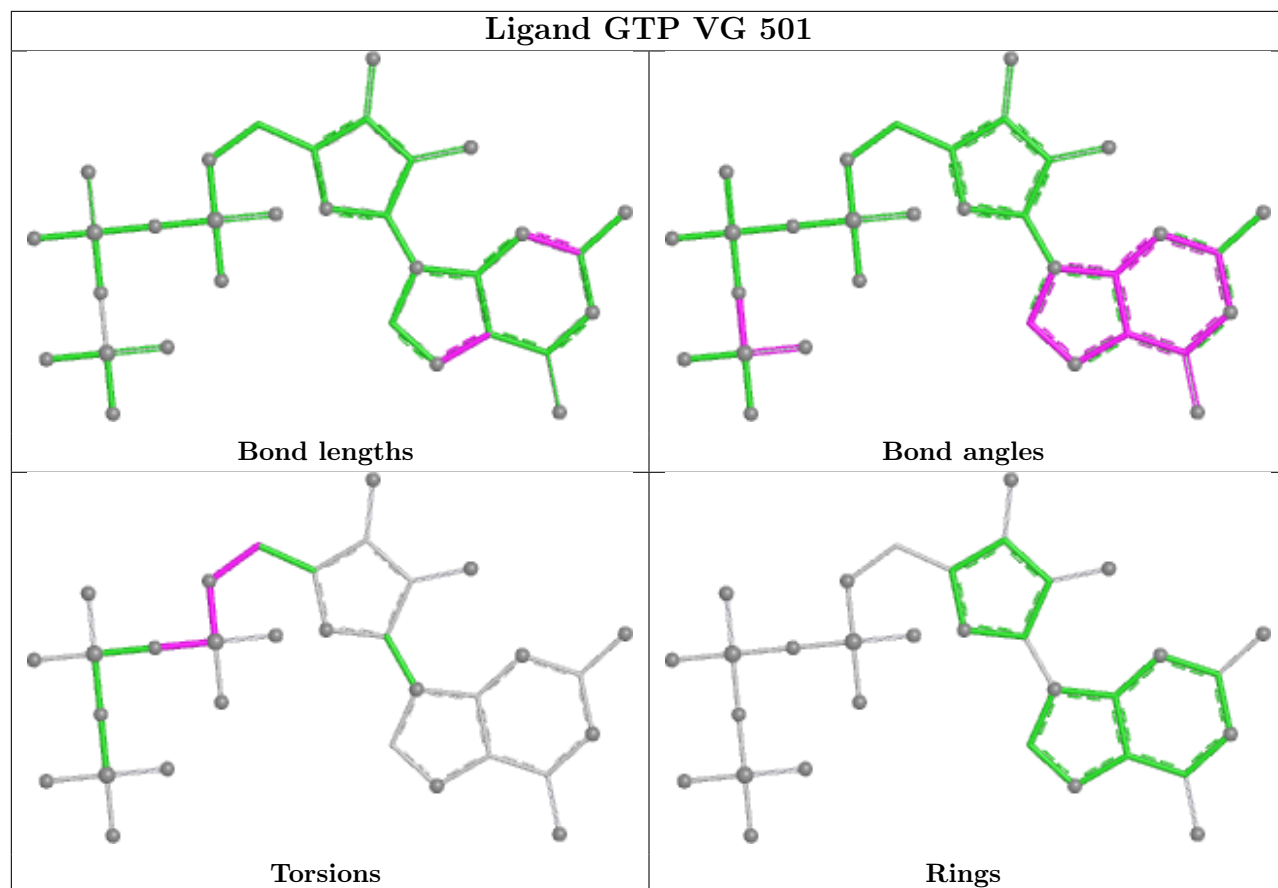




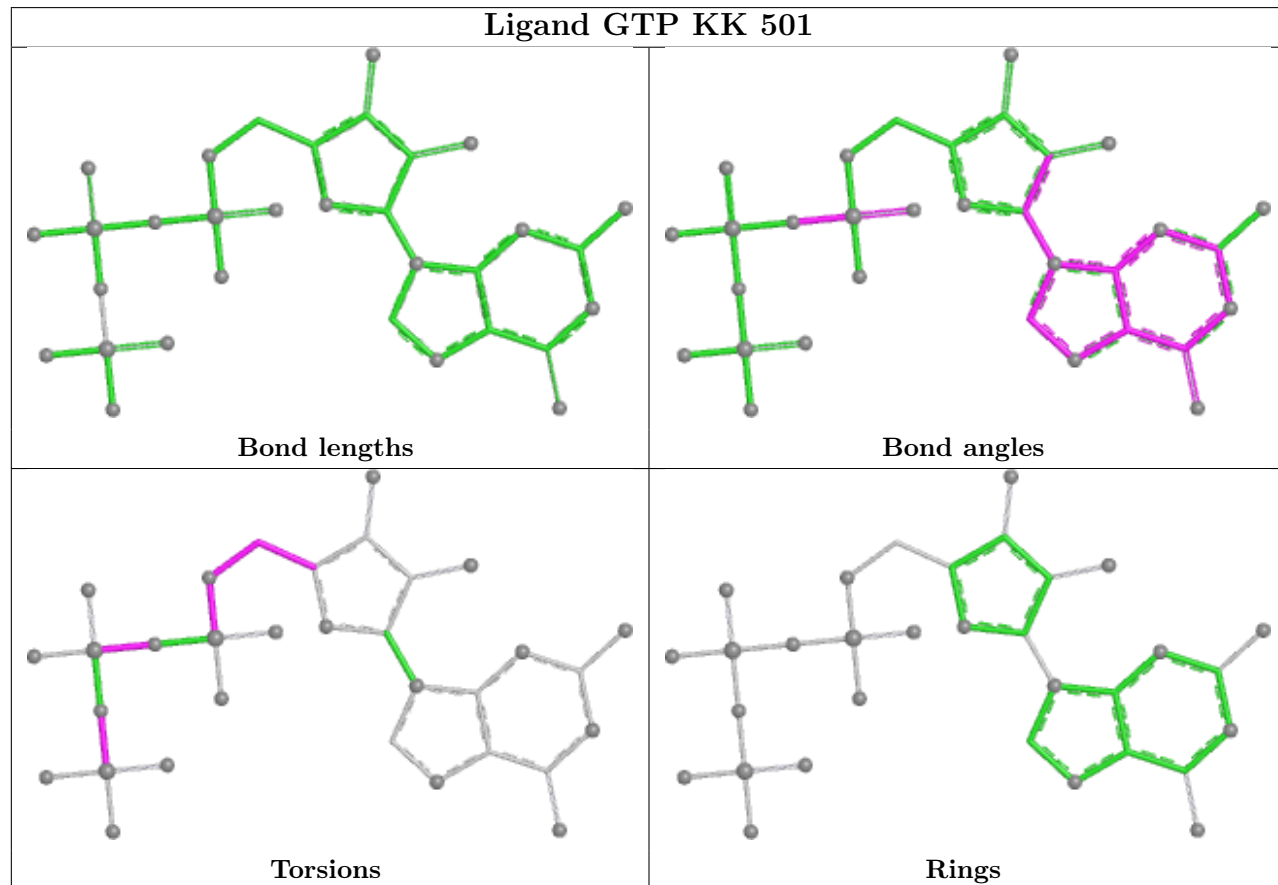


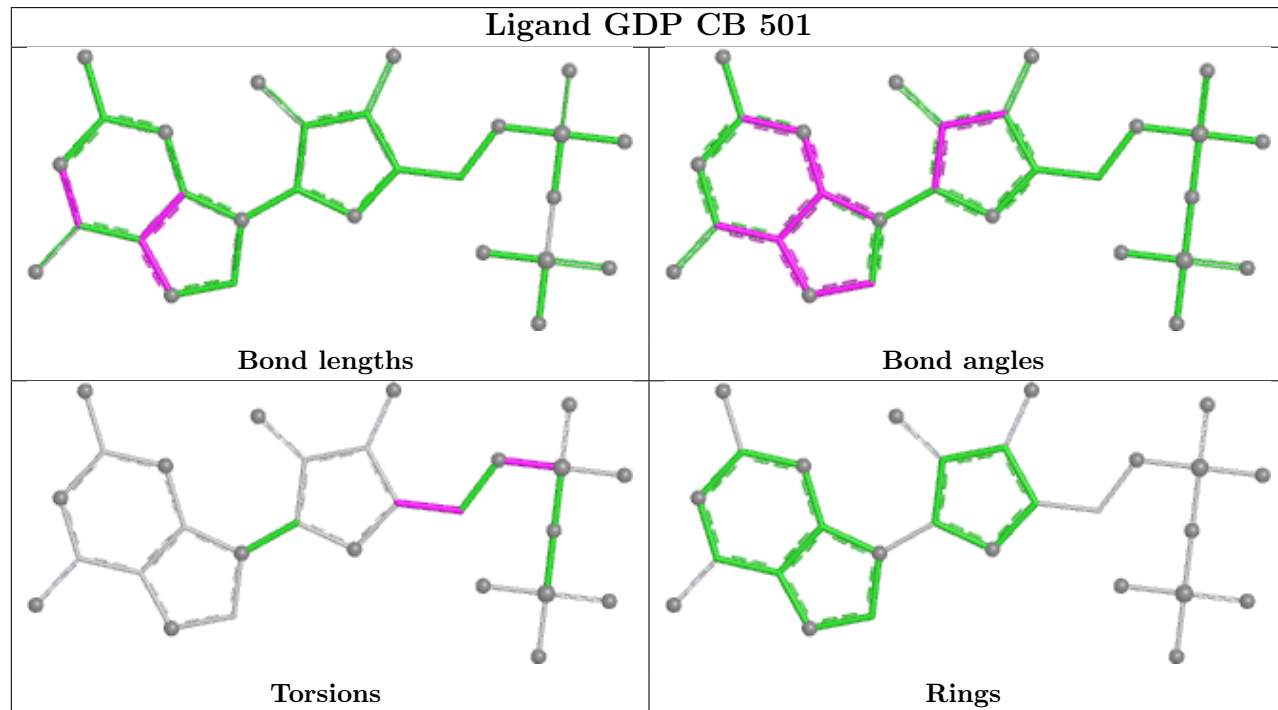
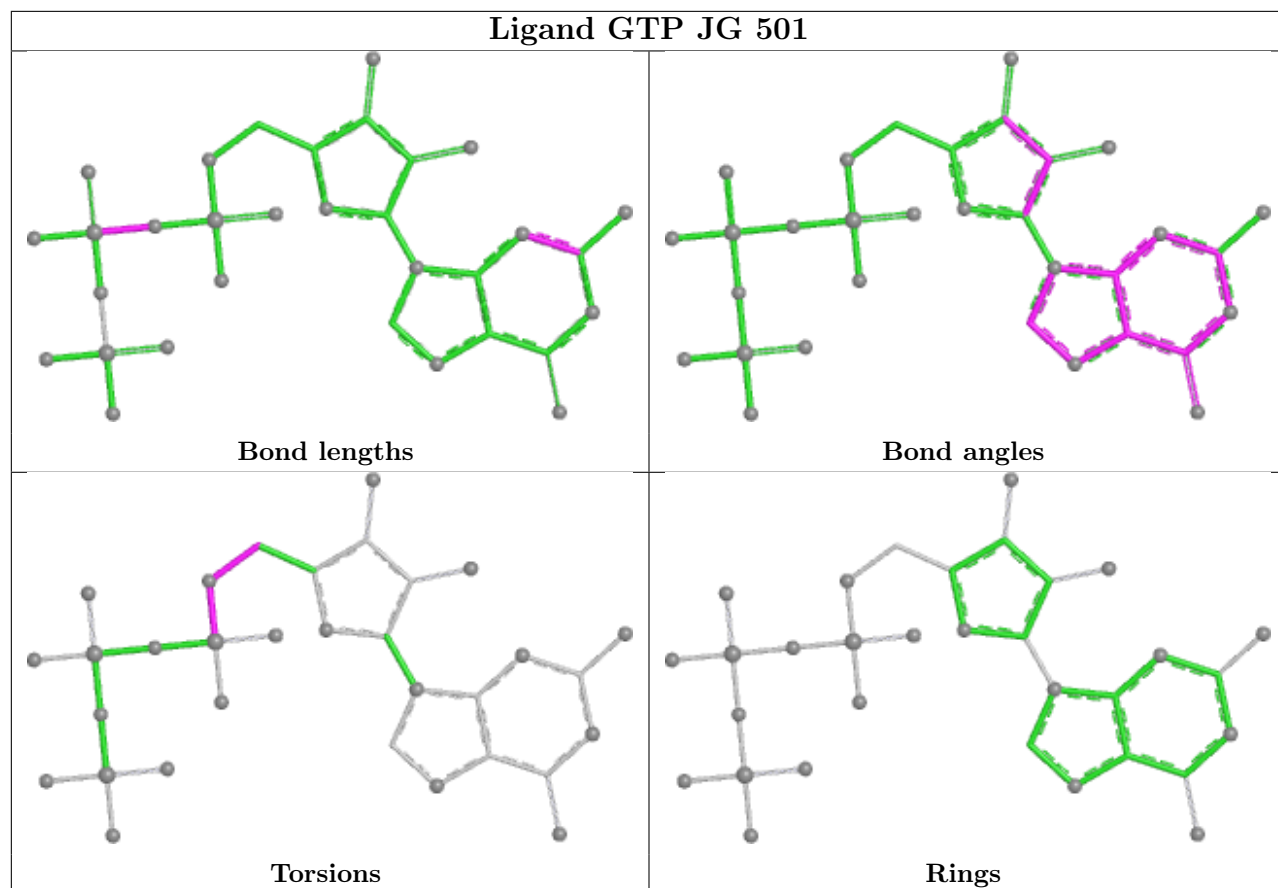


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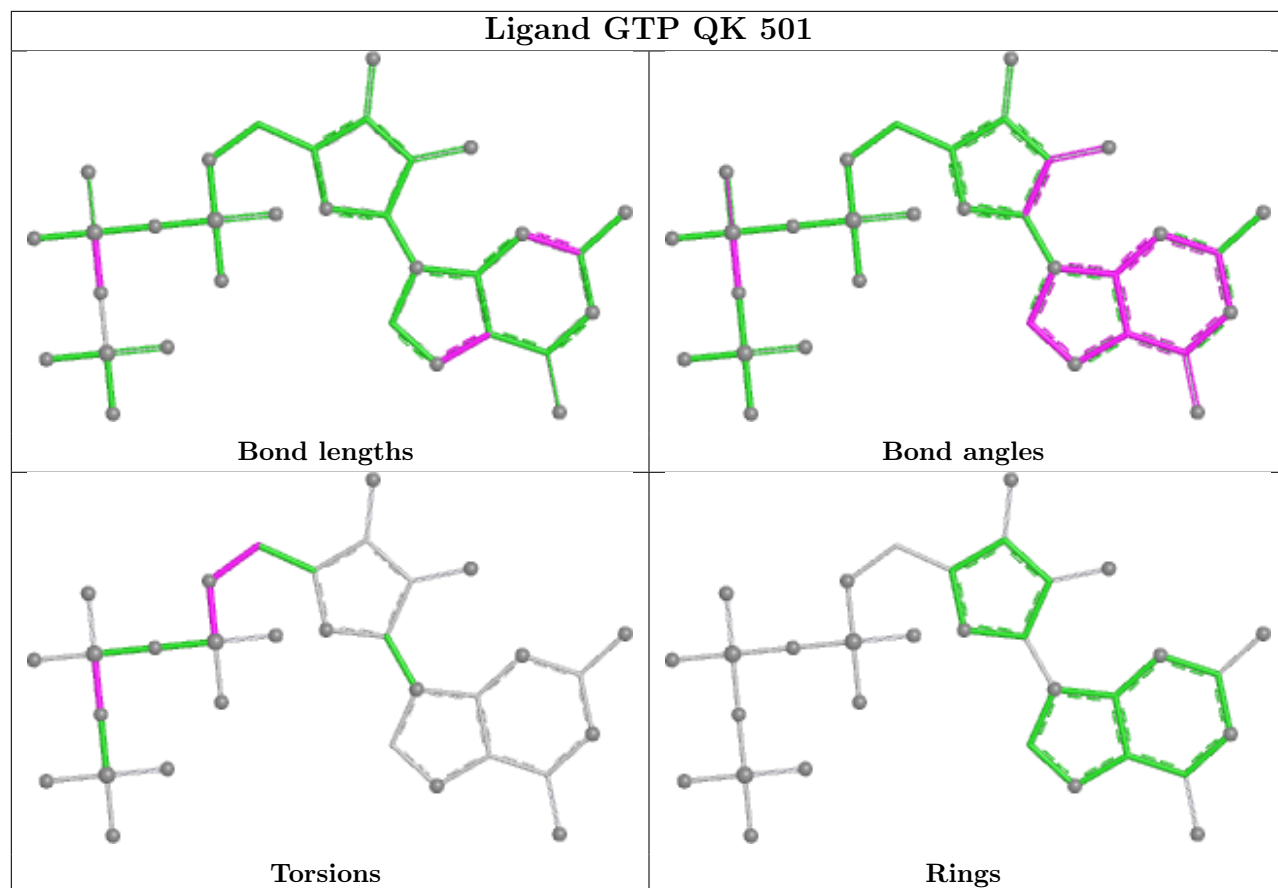


## Ligand GTP KK 501

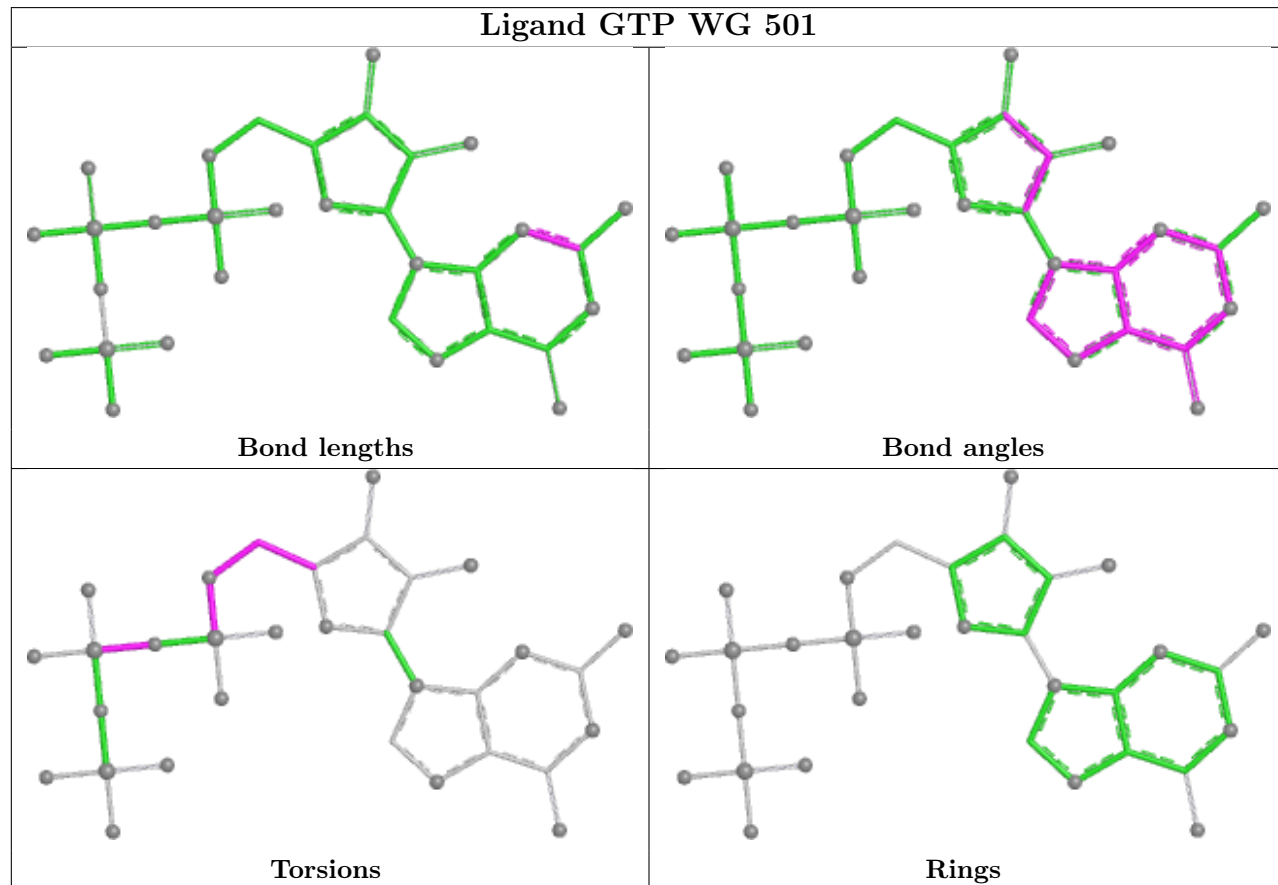


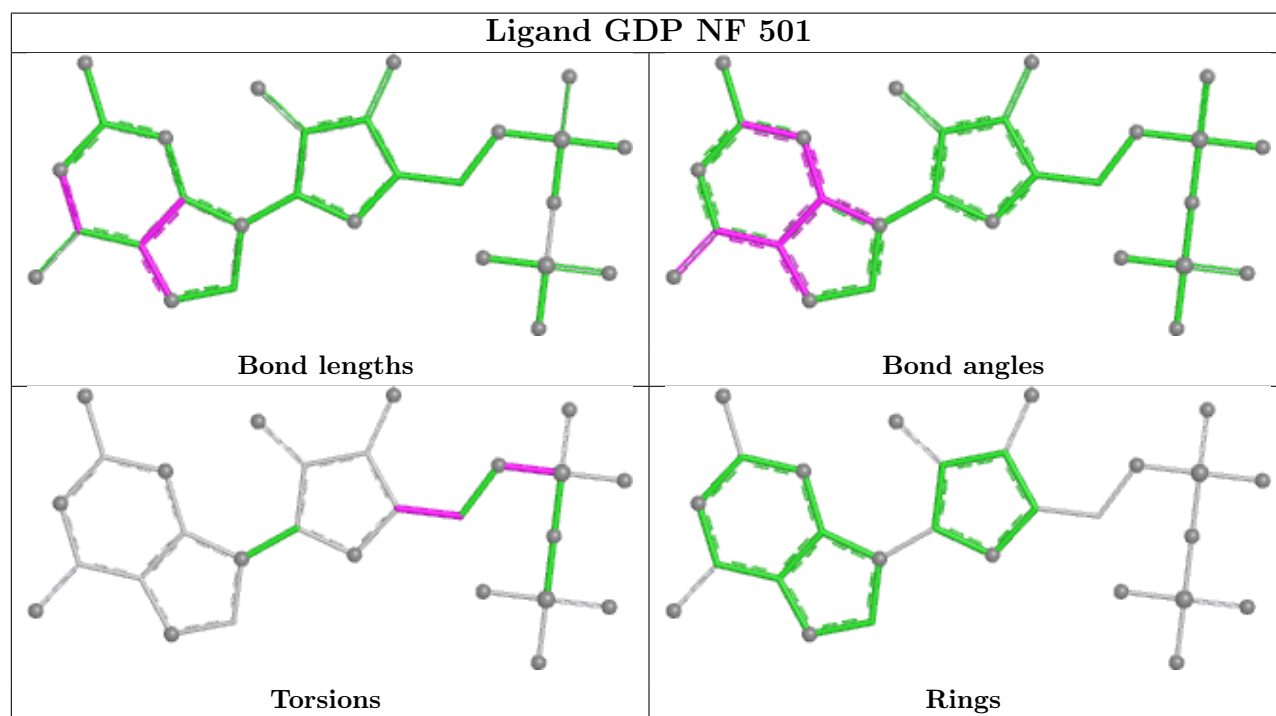
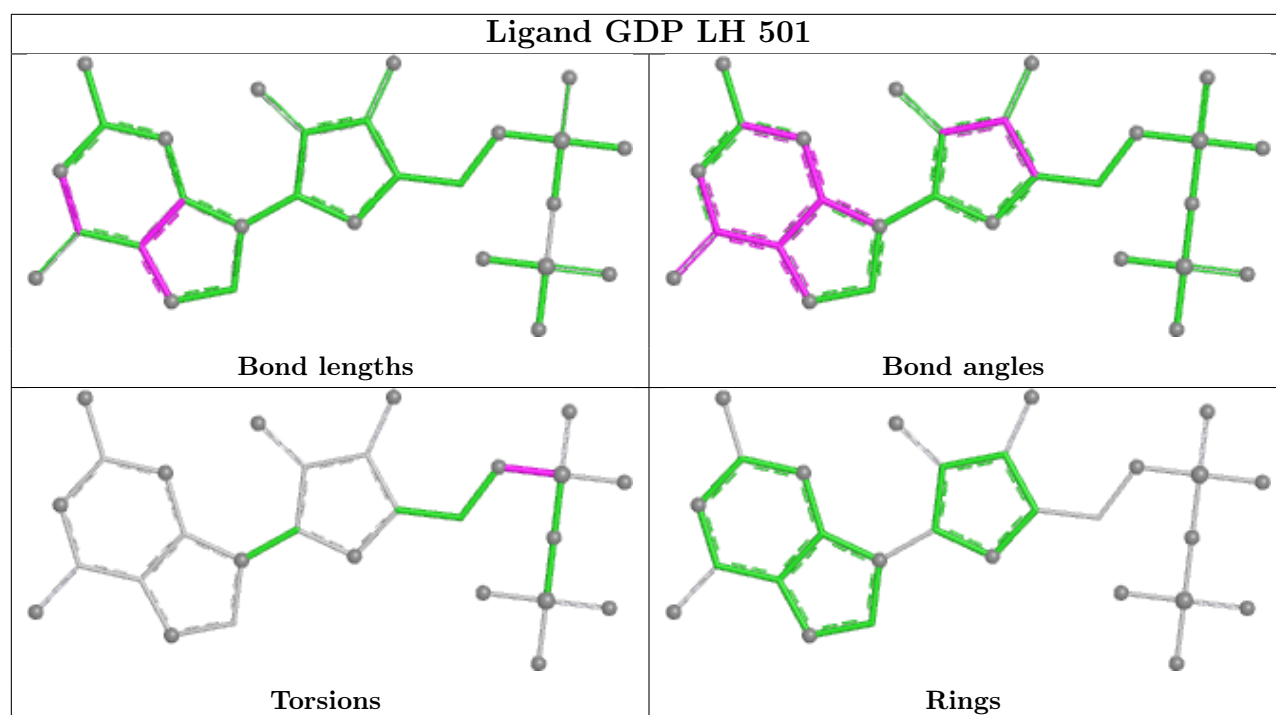


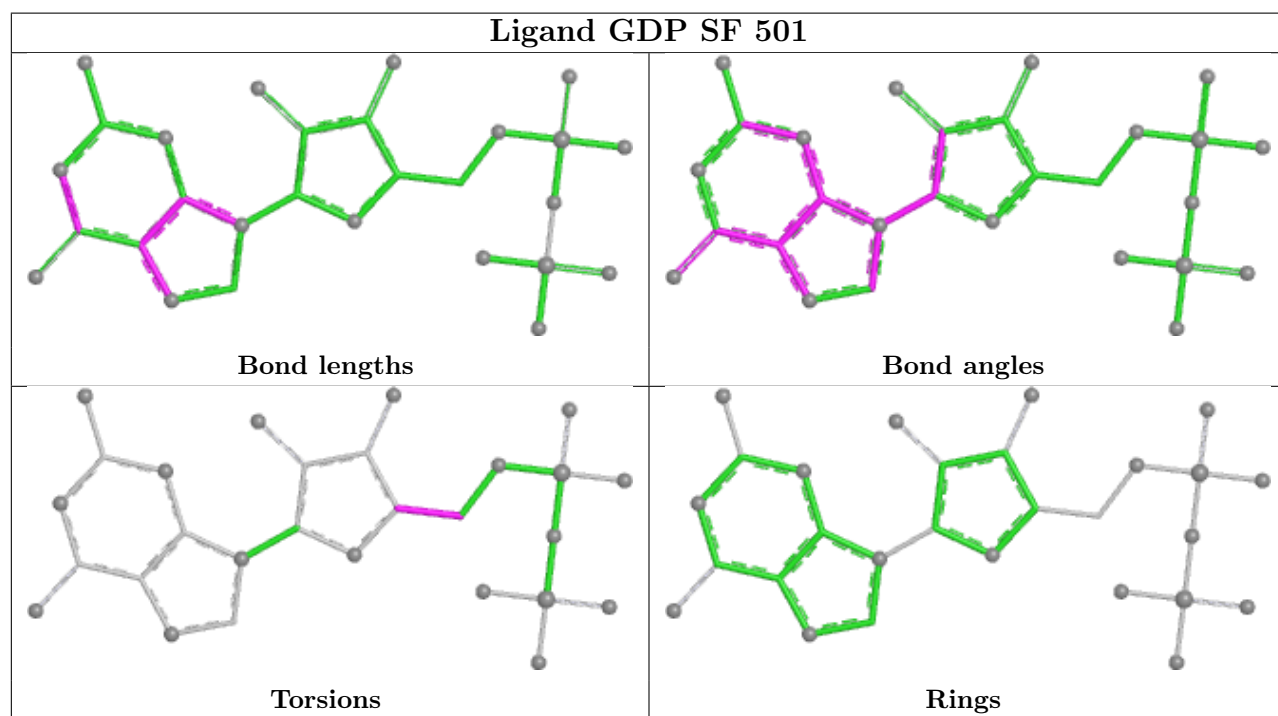
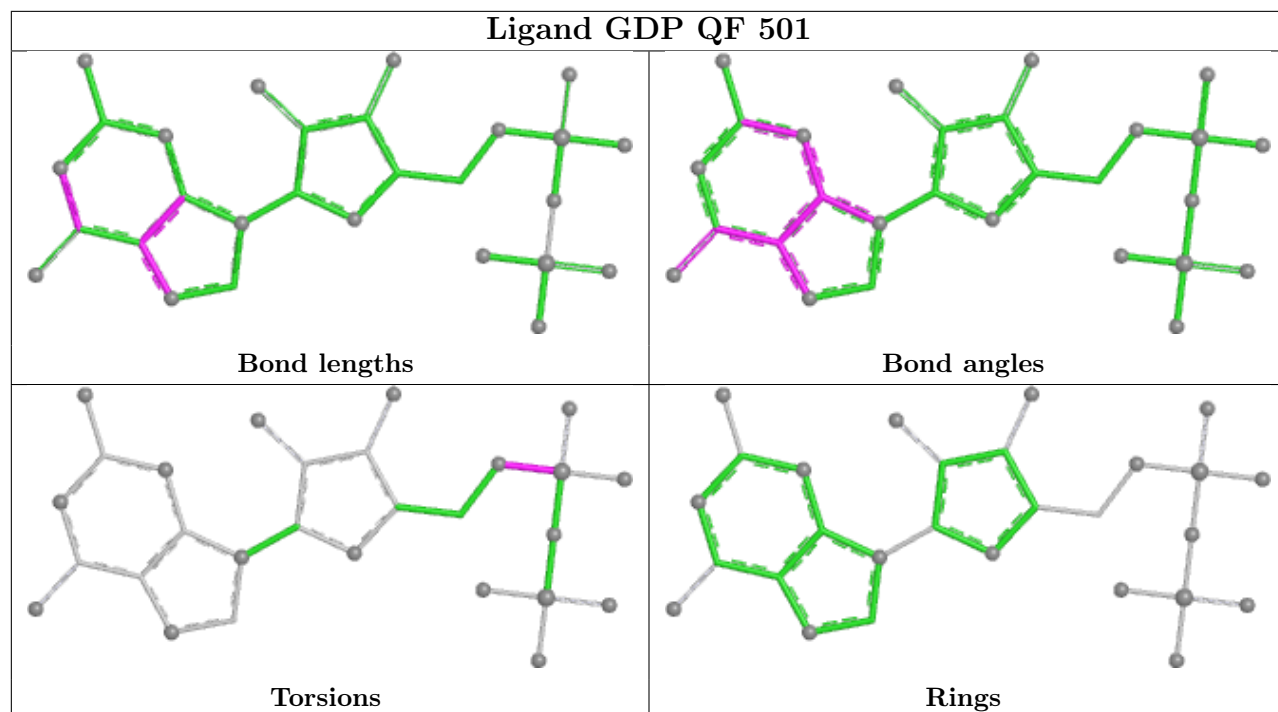
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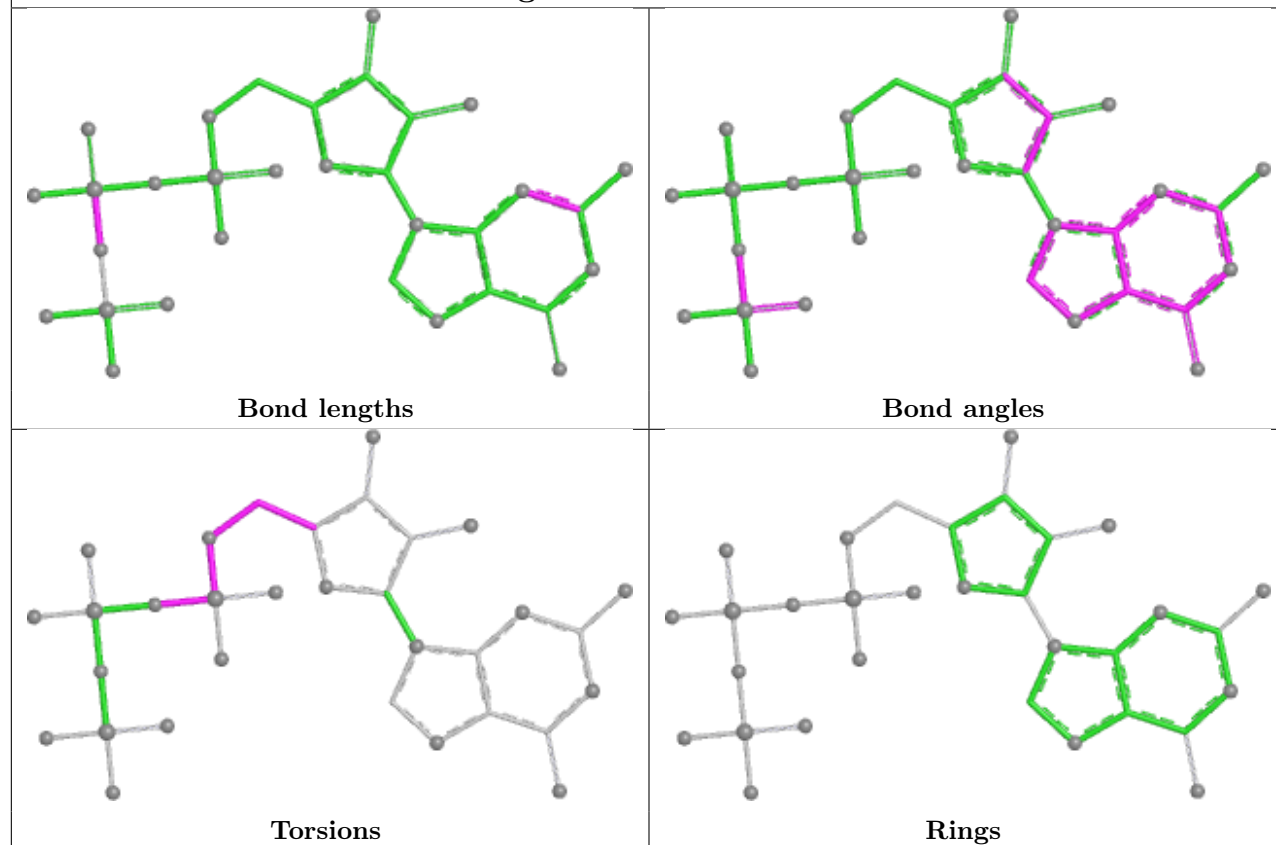
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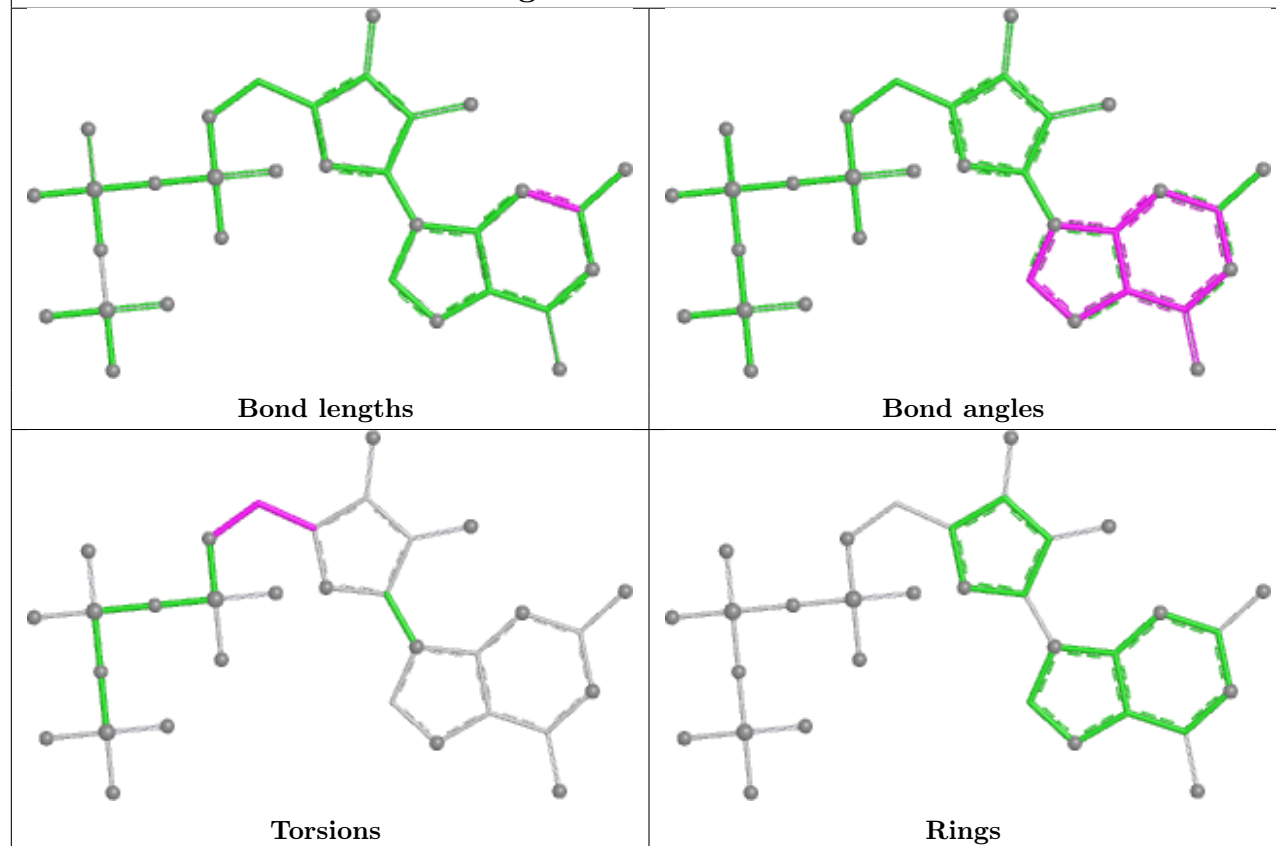




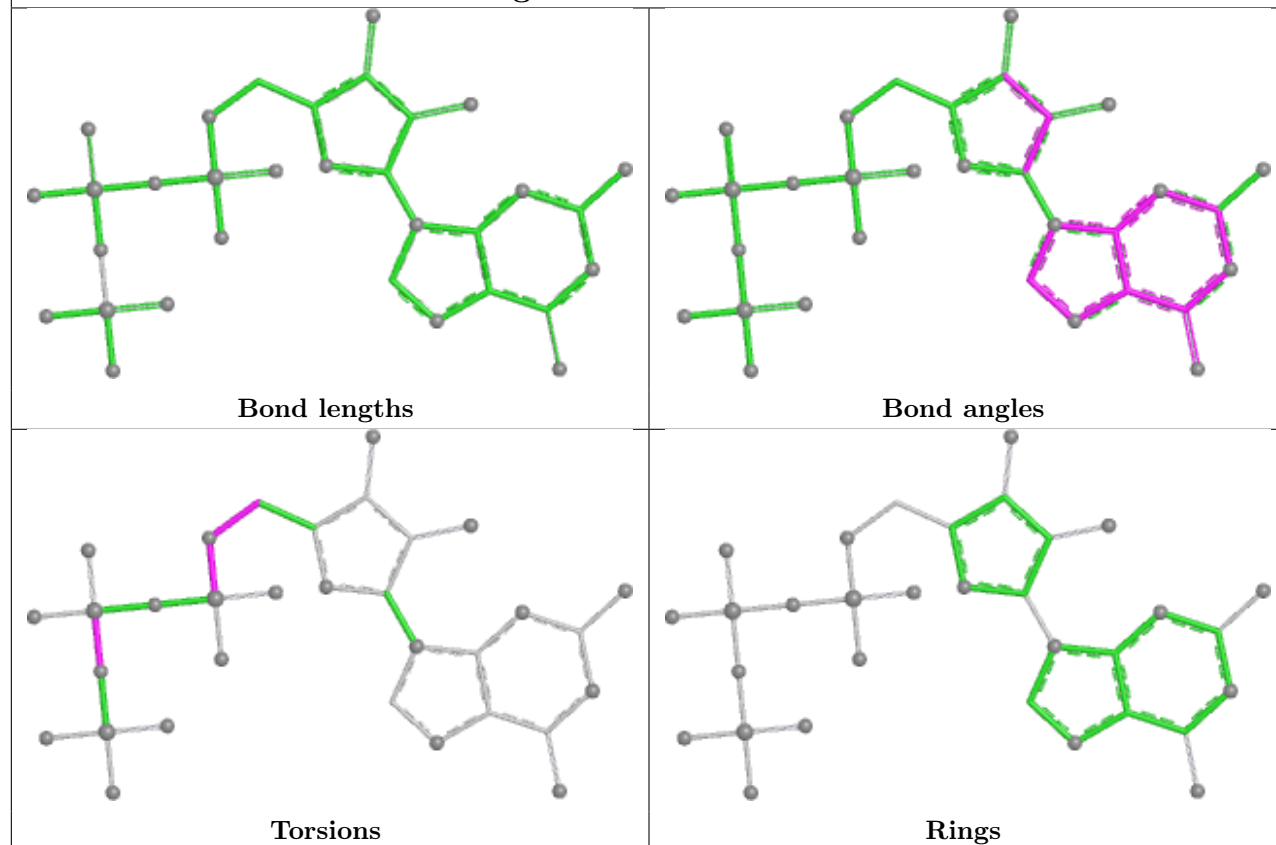
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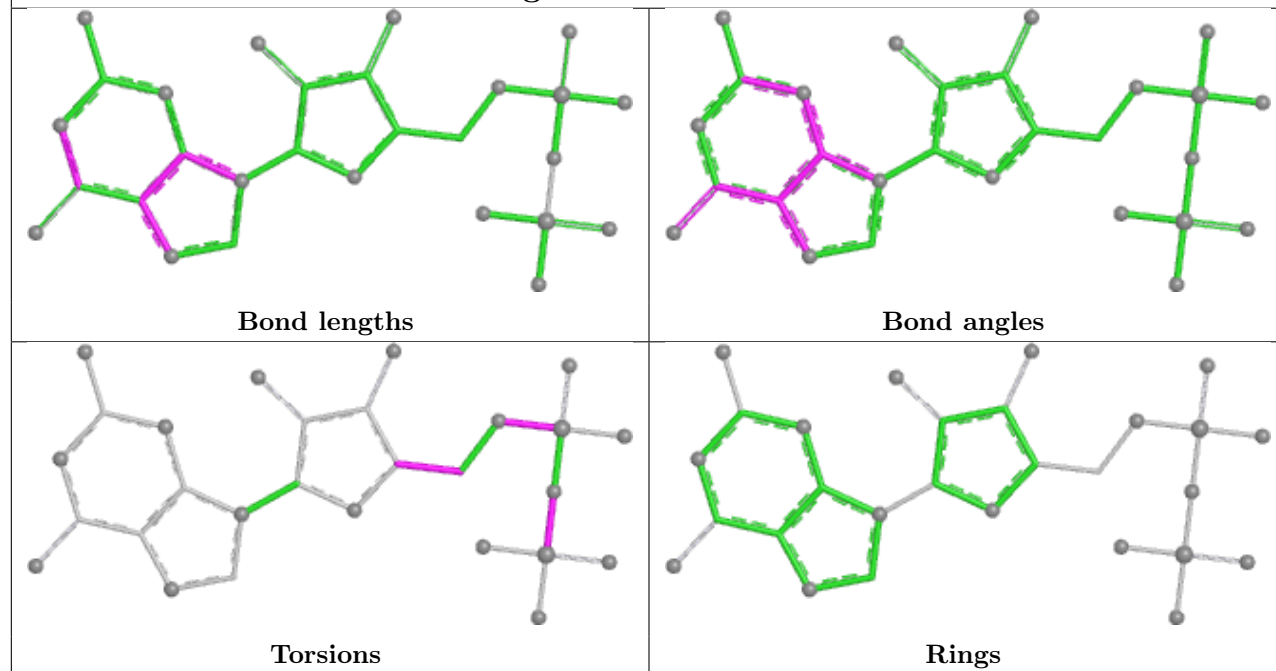
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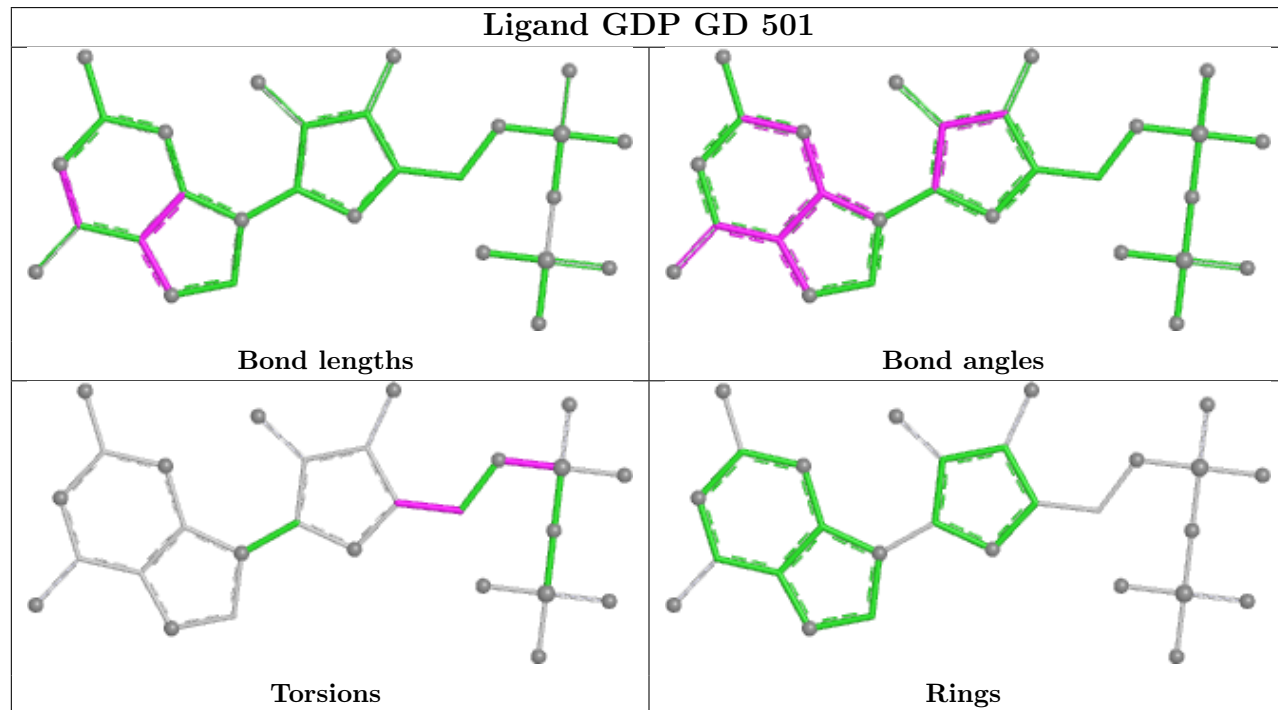
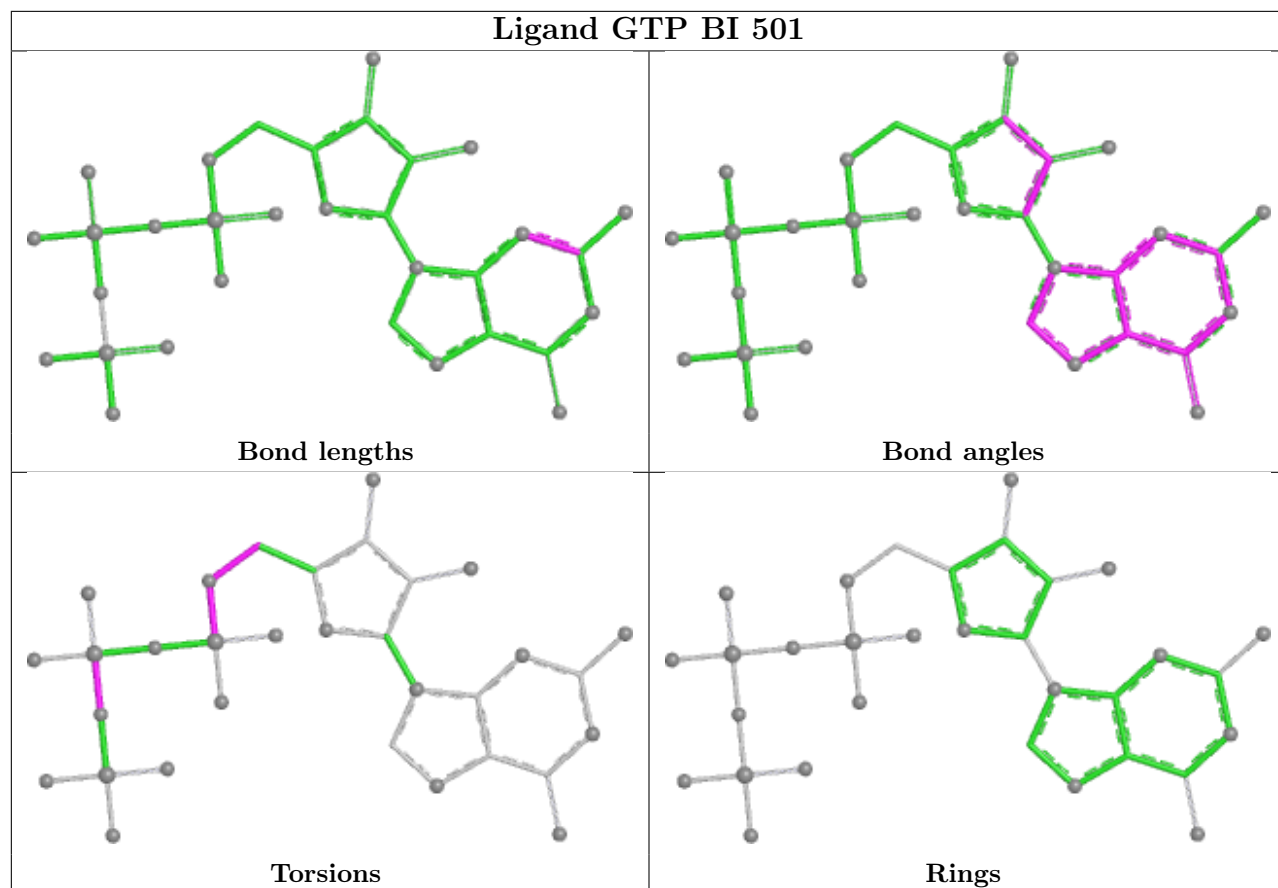
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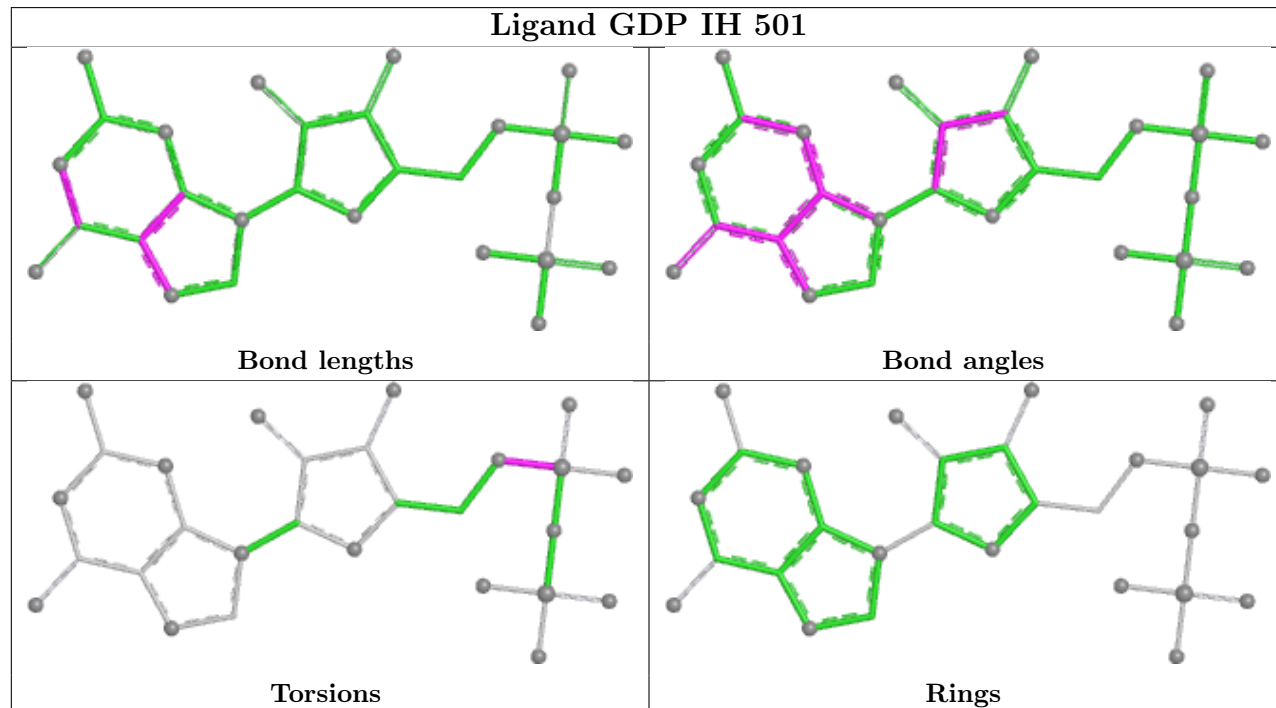
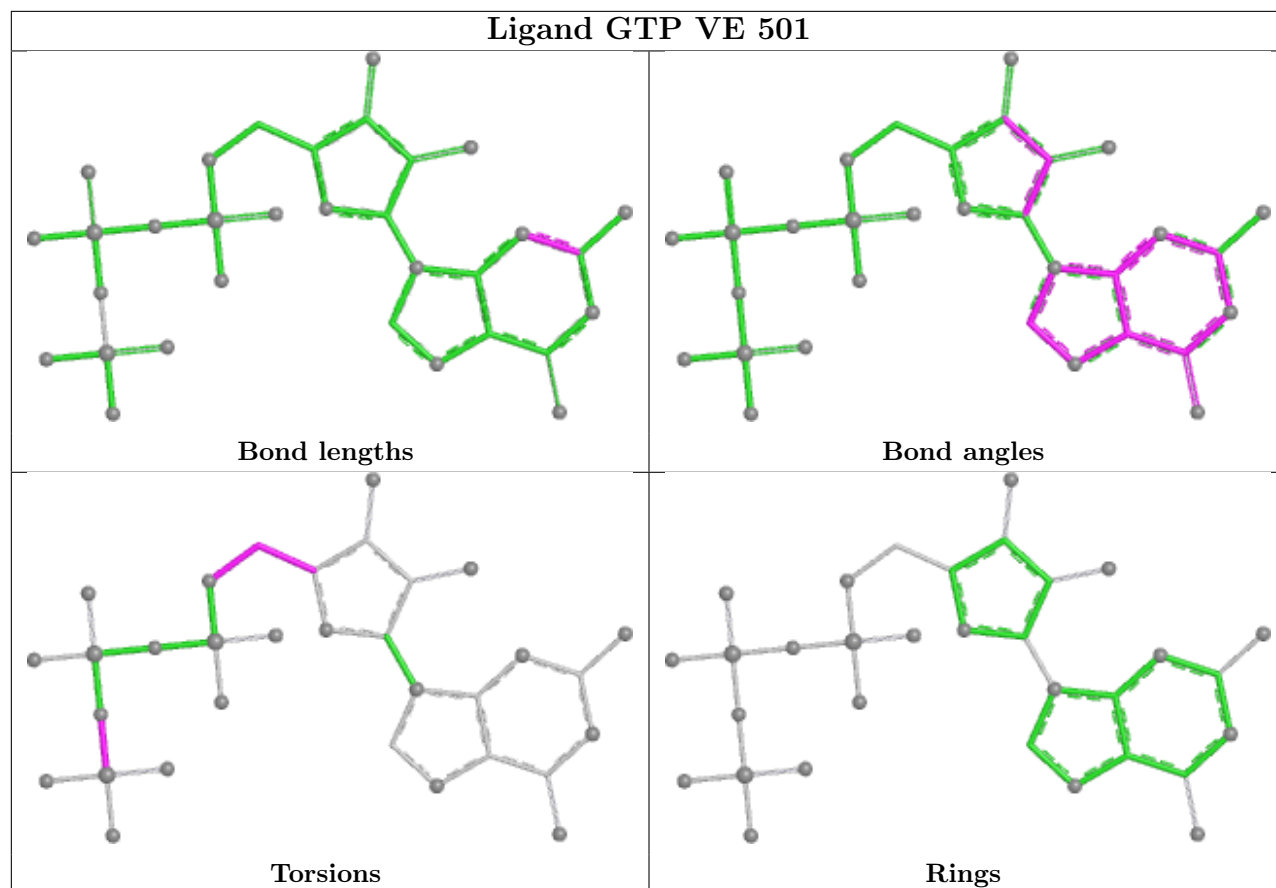


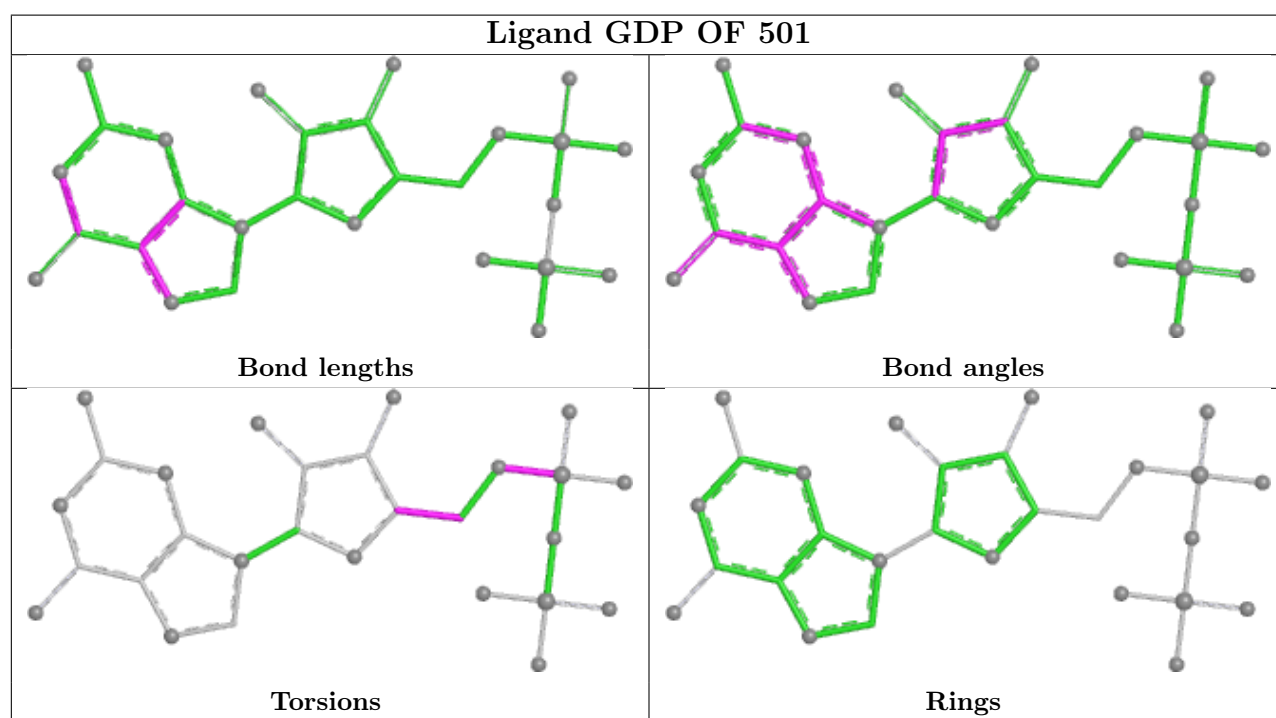
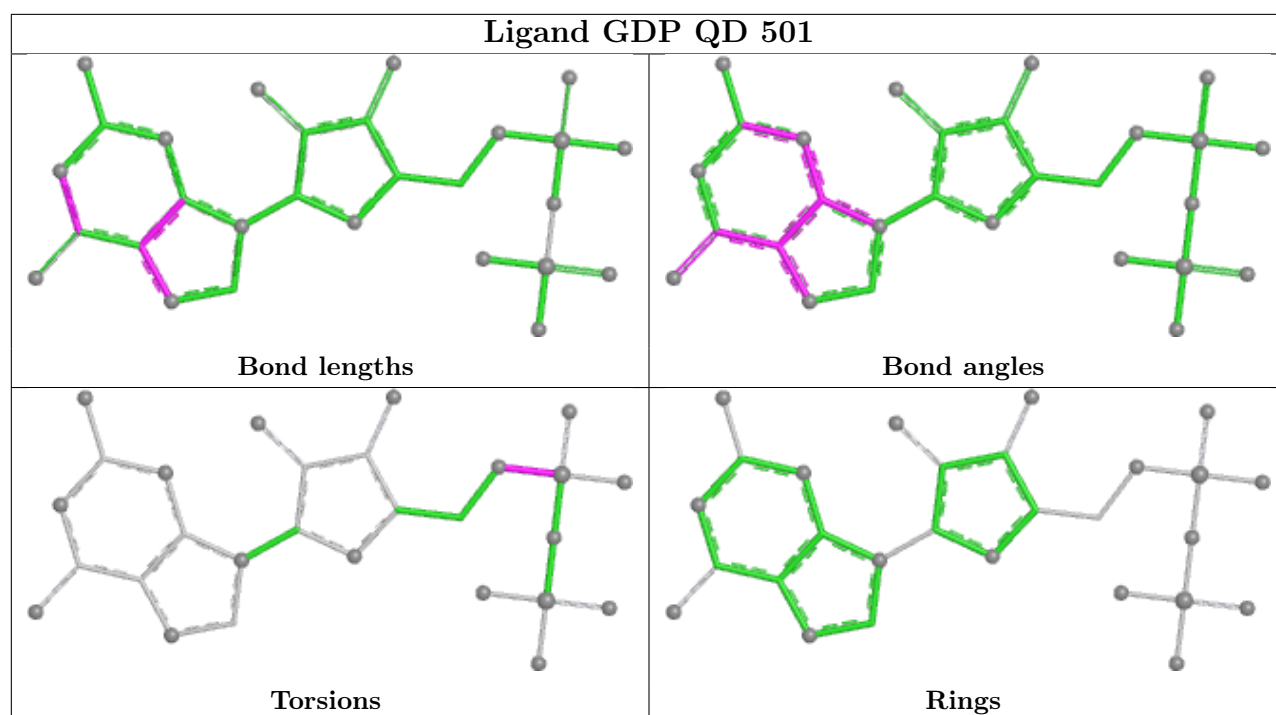
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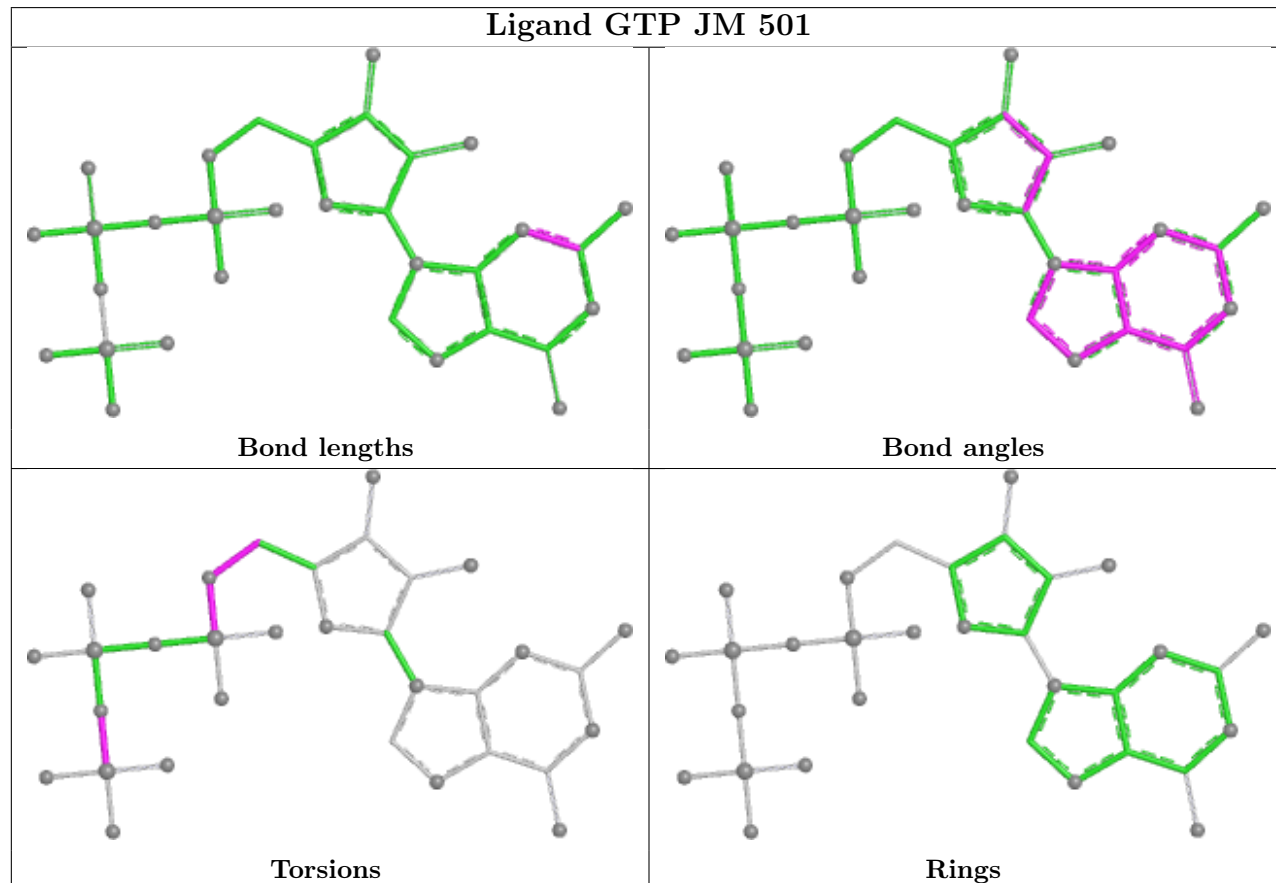
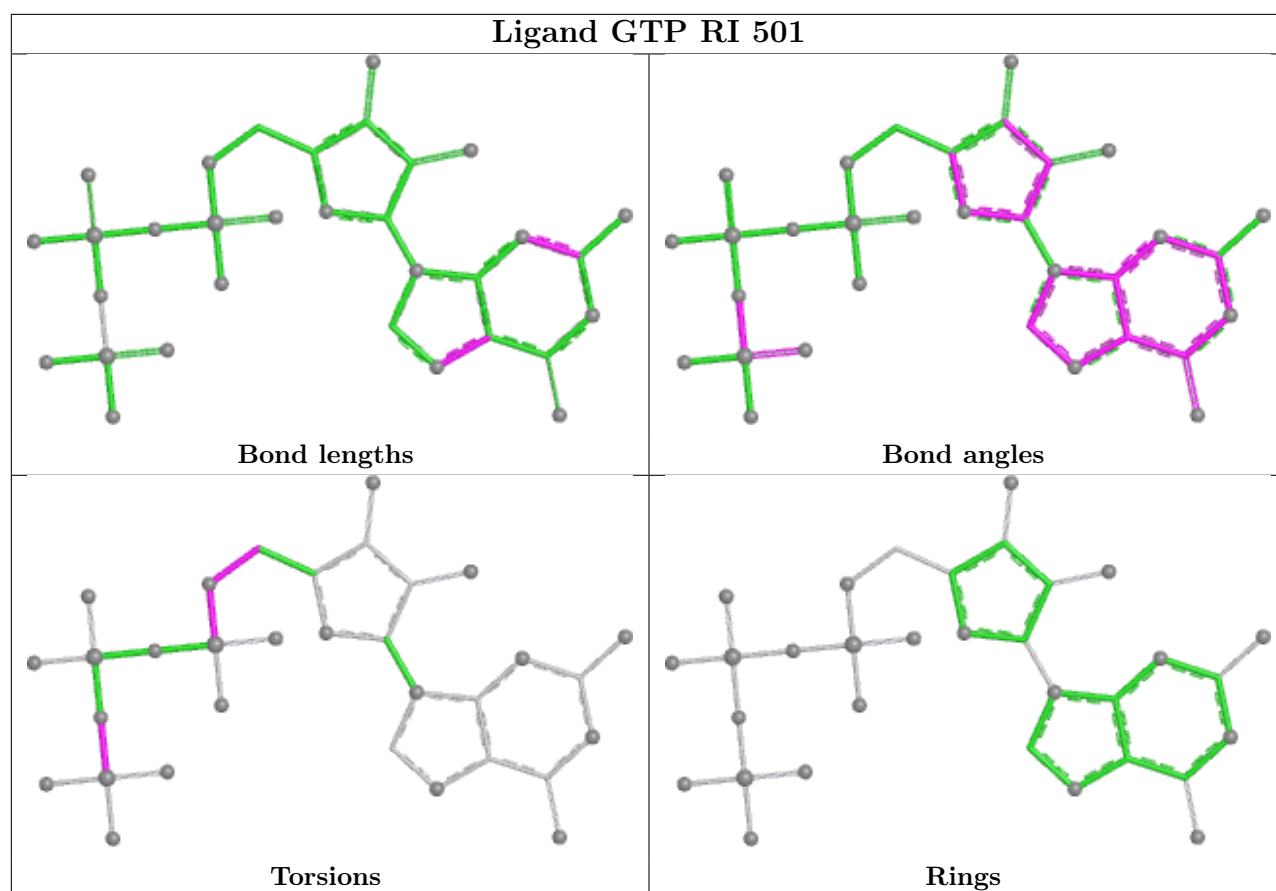


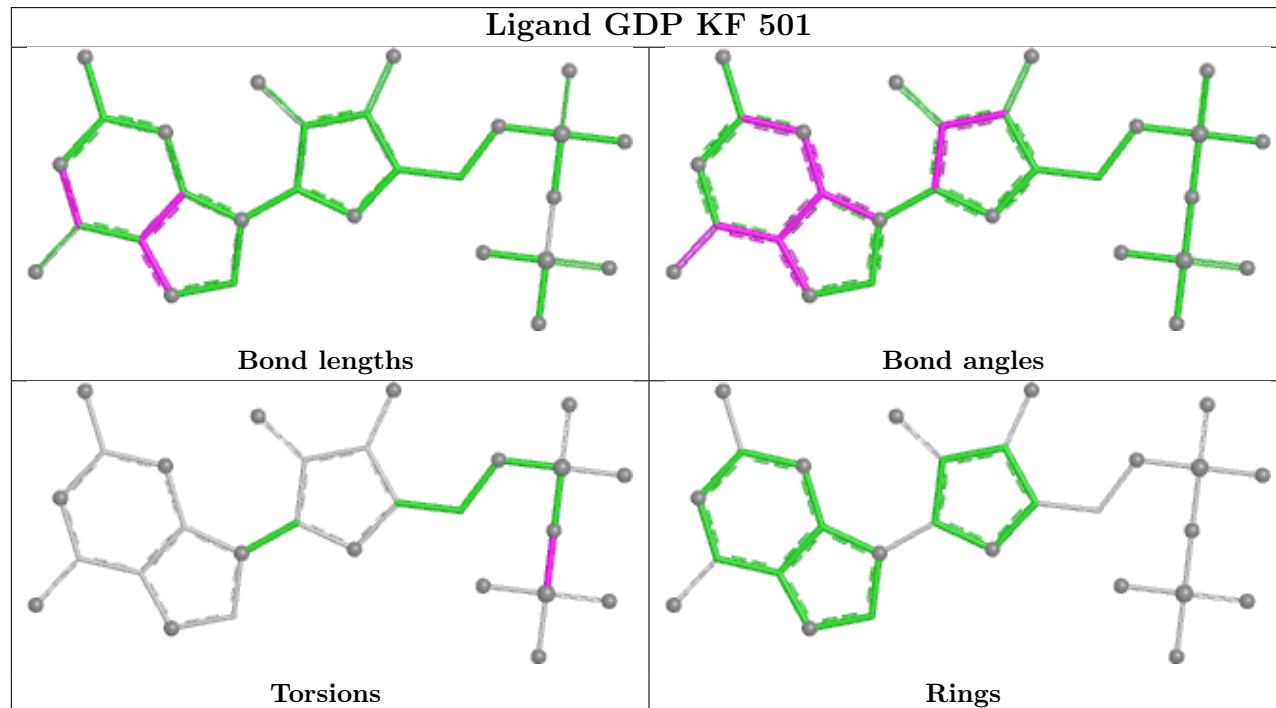
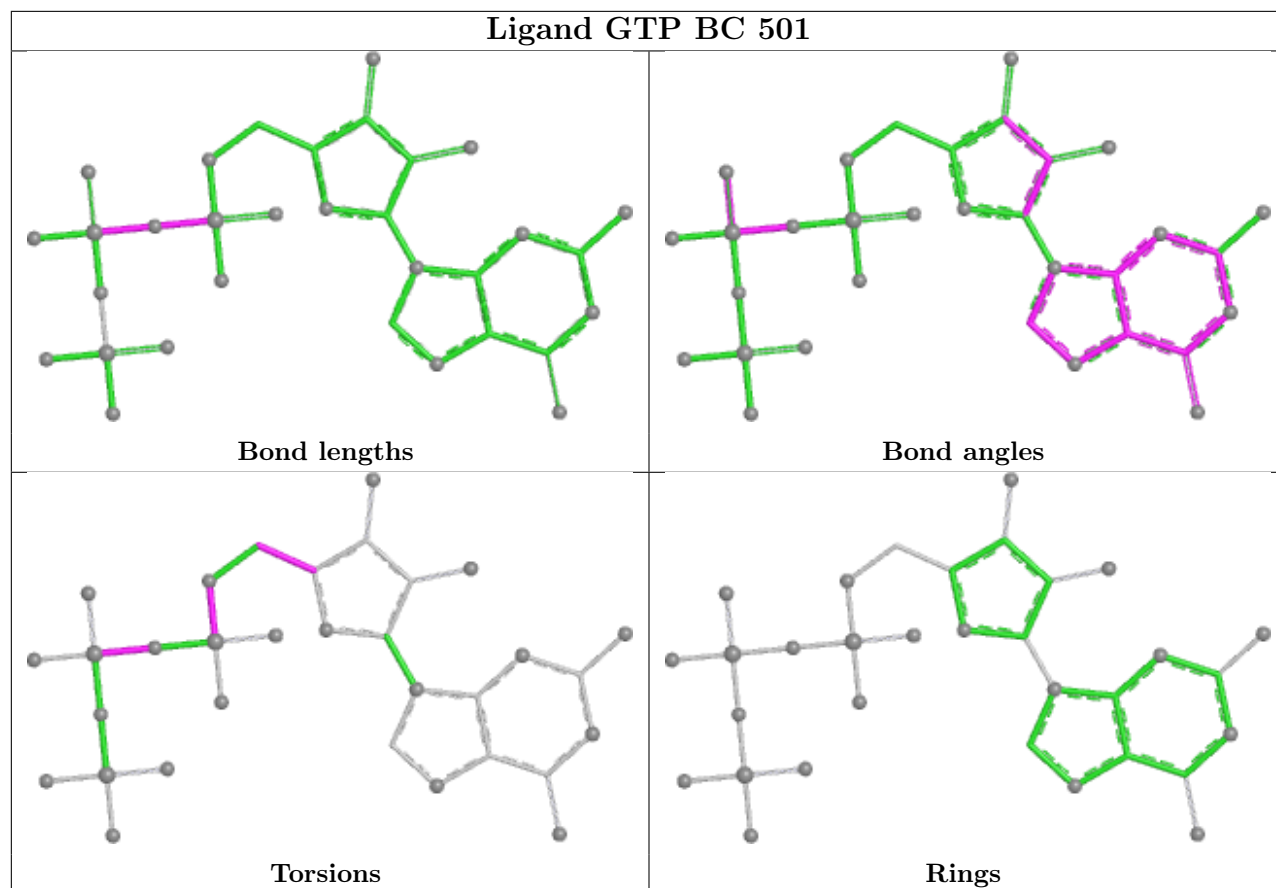


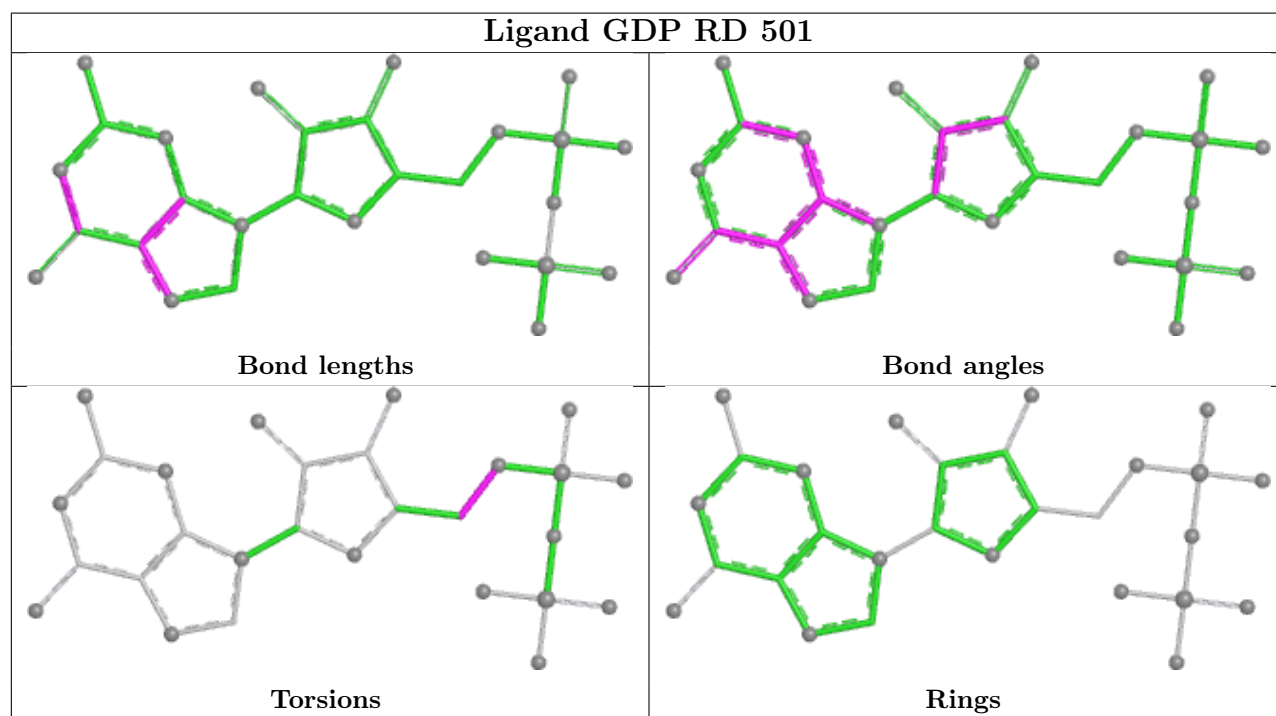
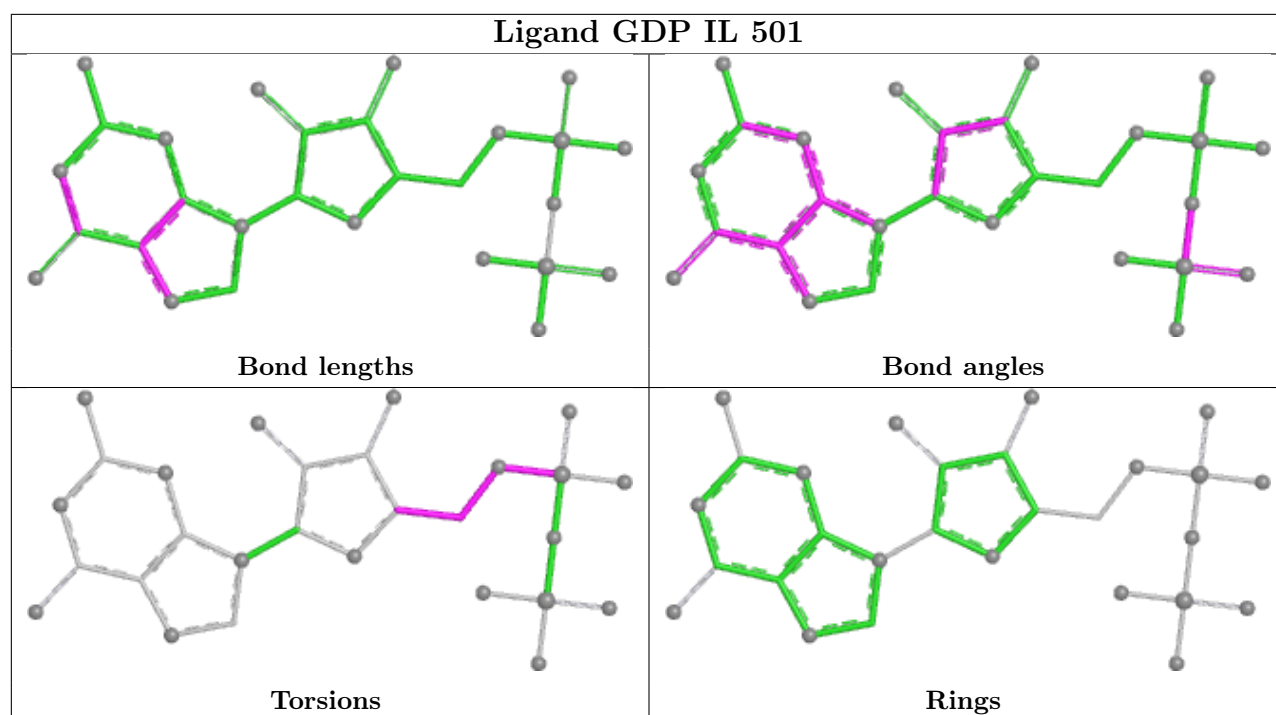




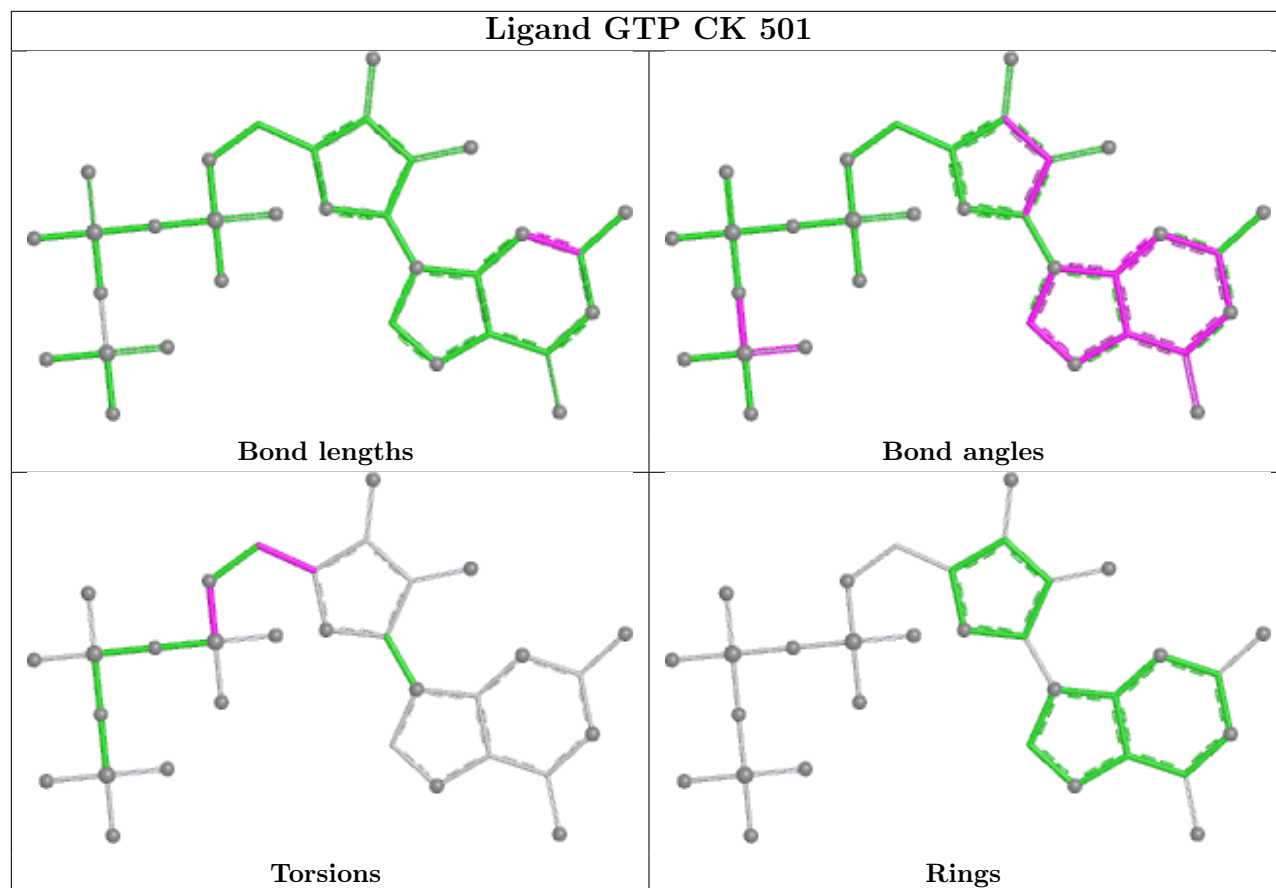




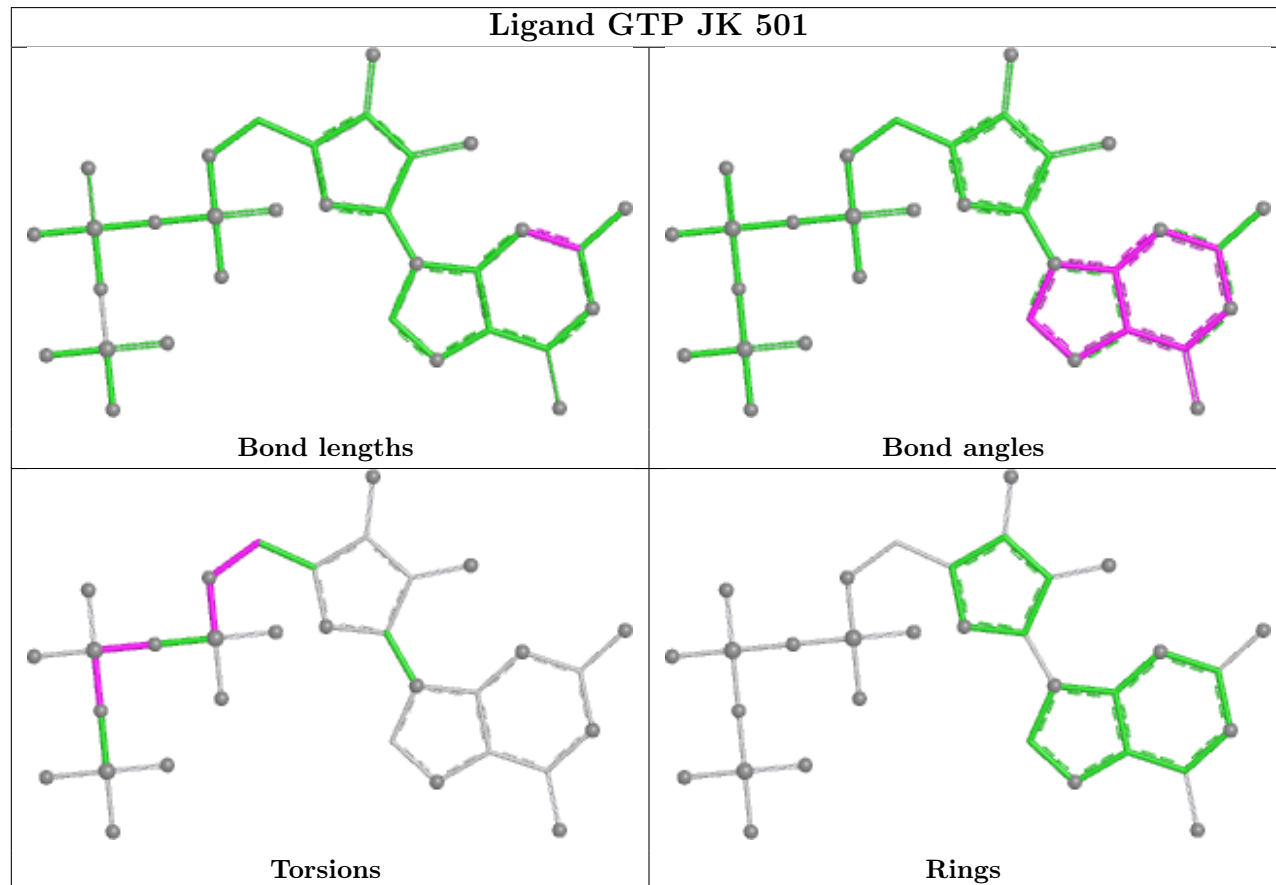


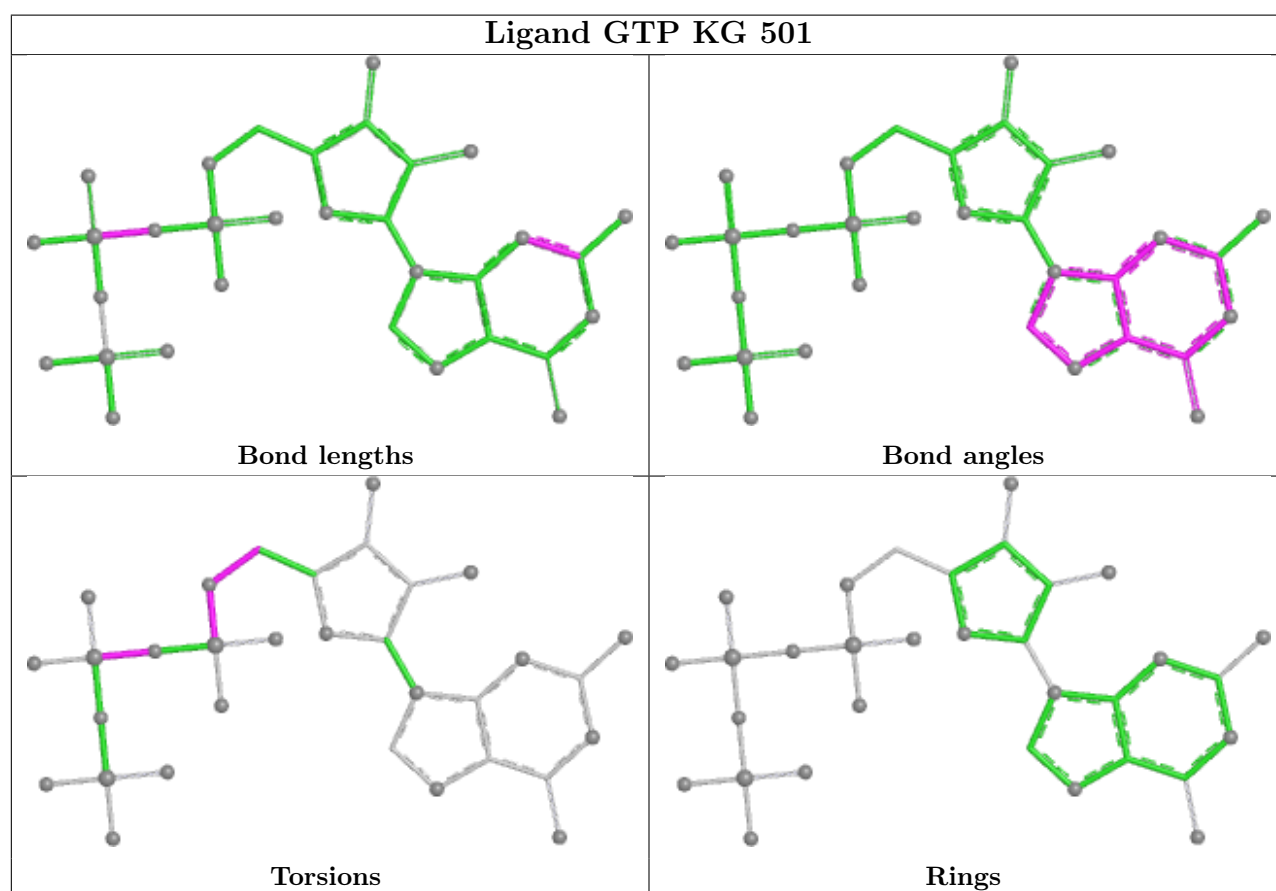
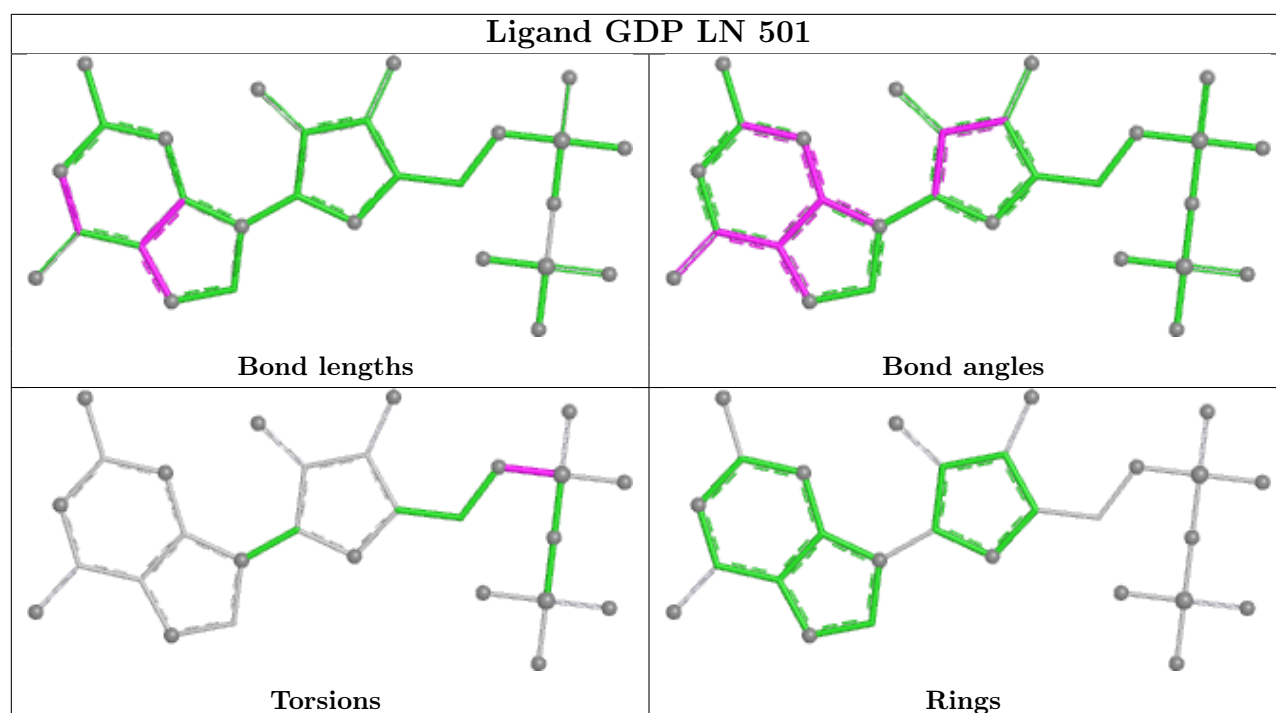


## Ligand GTP CK 501



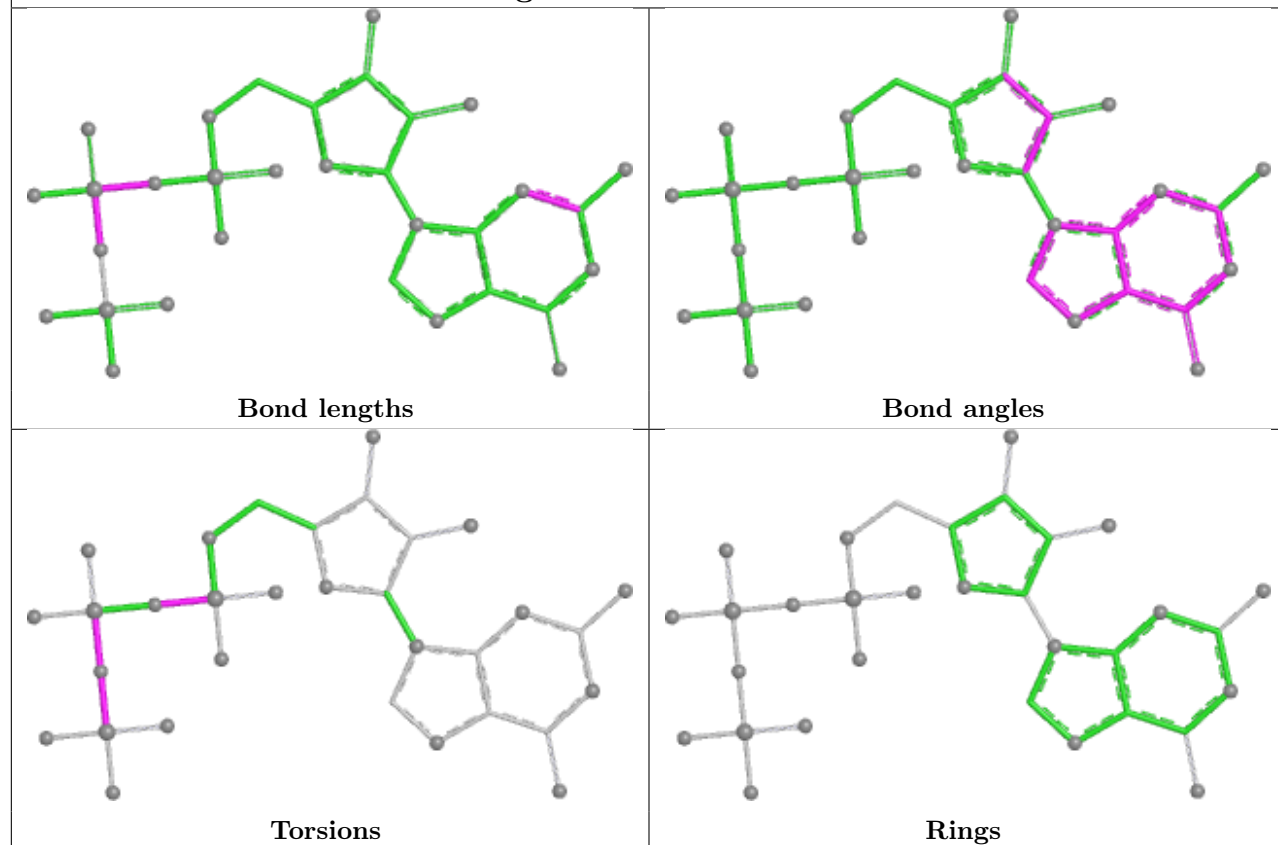
## Ligand GTP JK 501



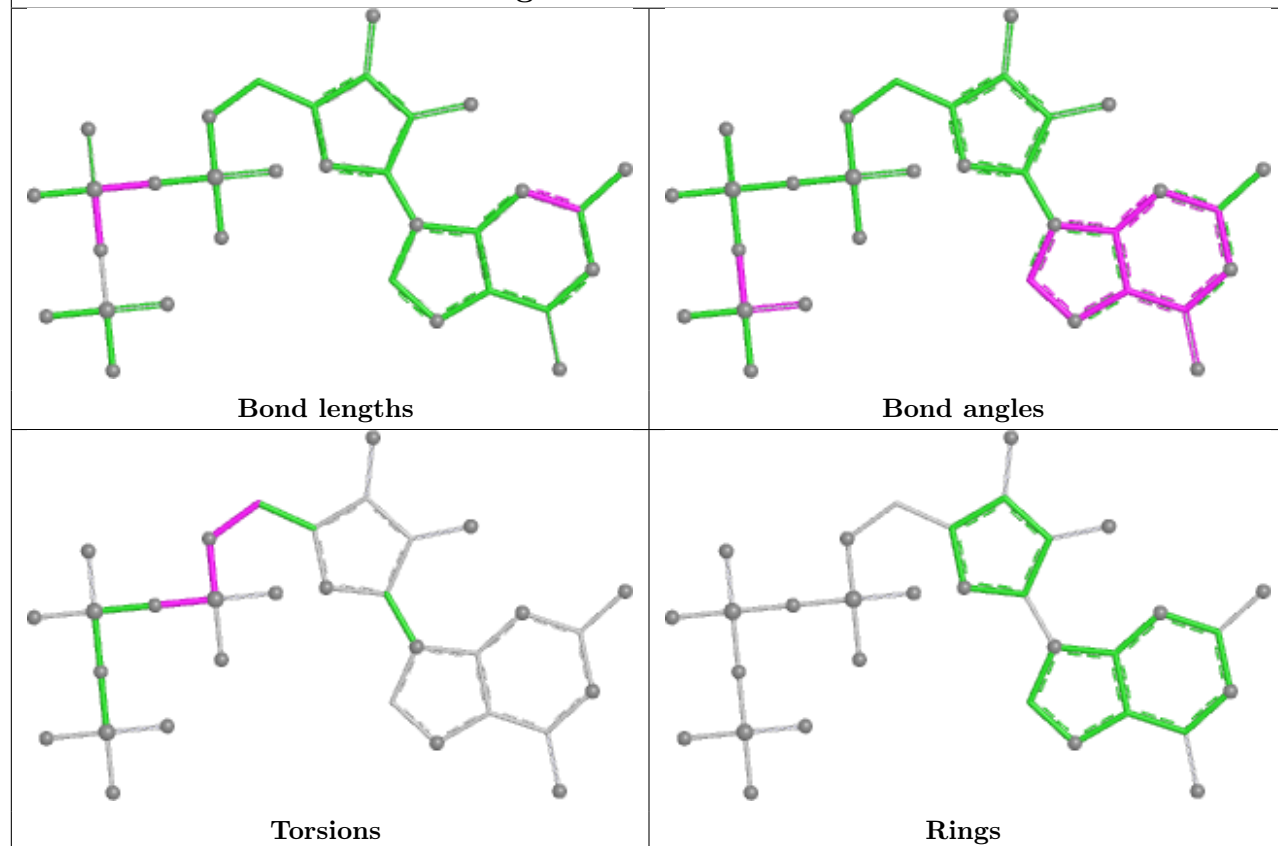


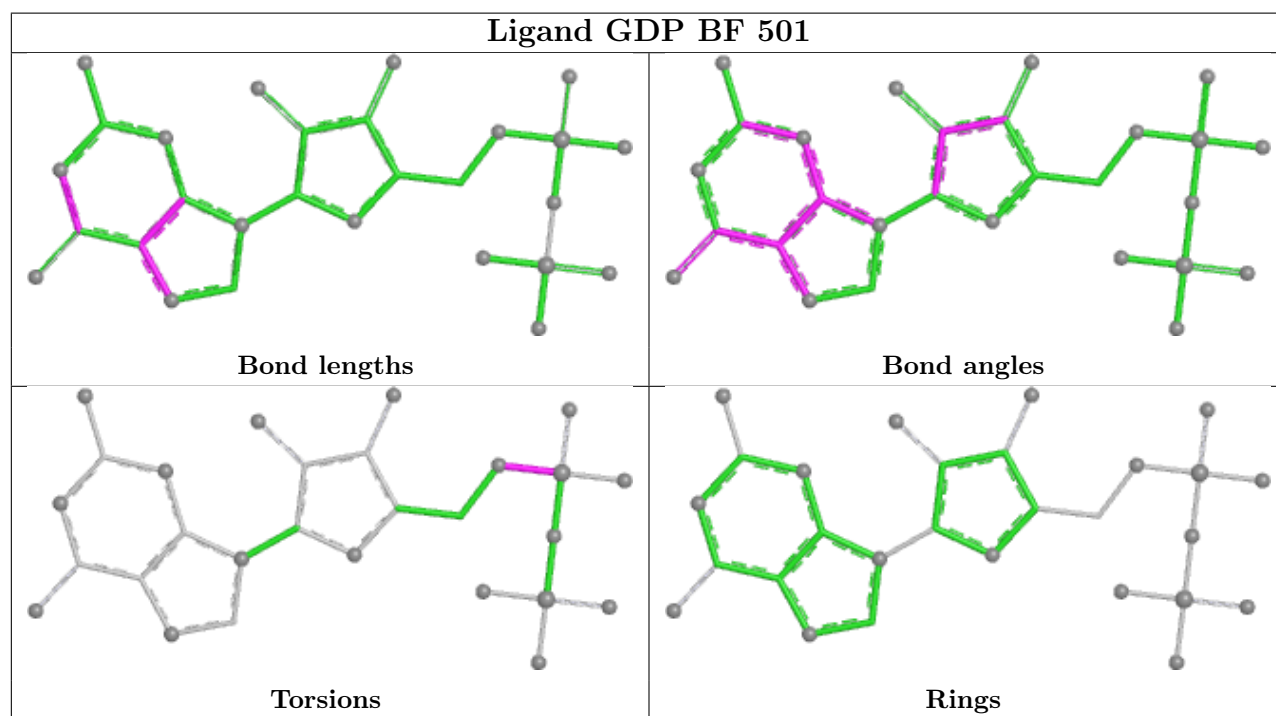
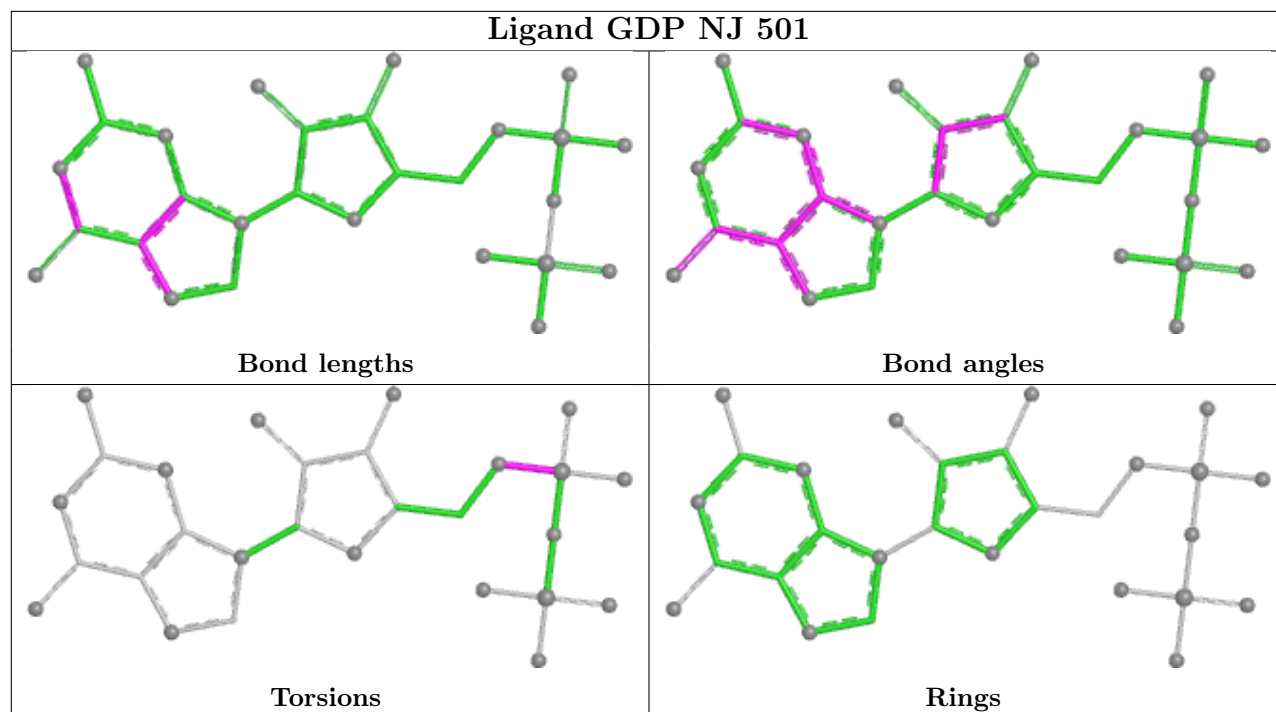


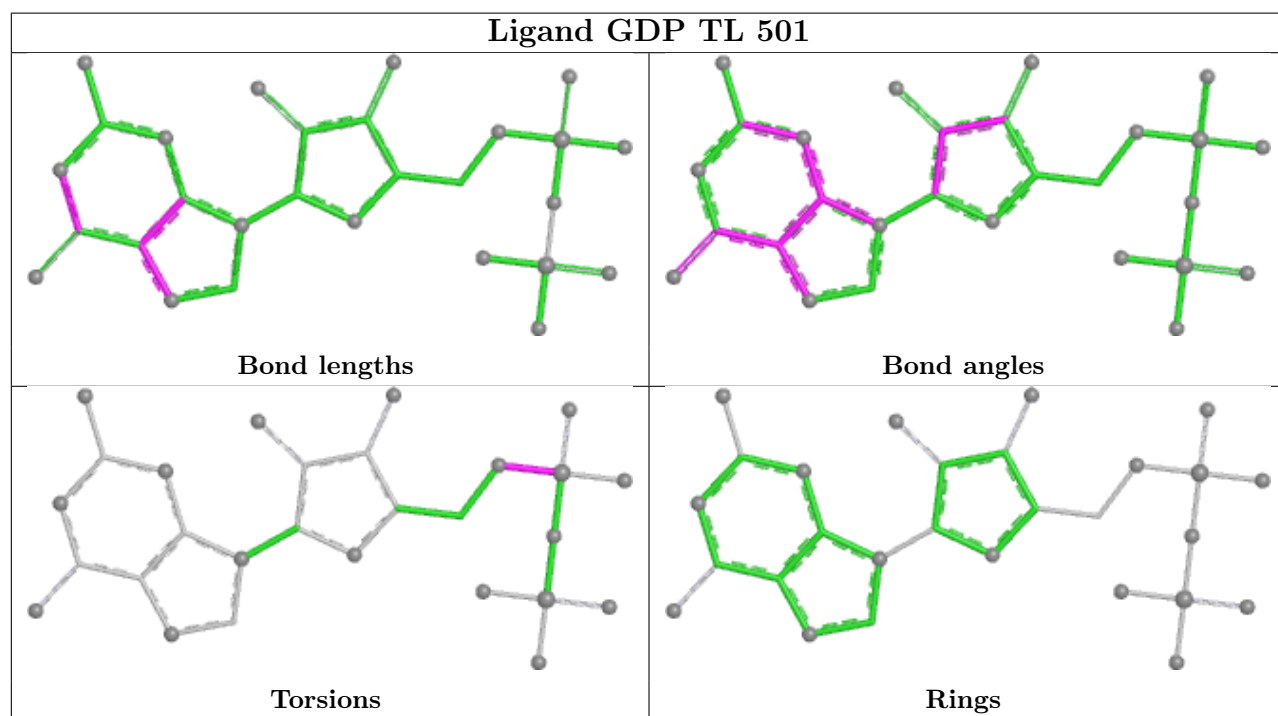
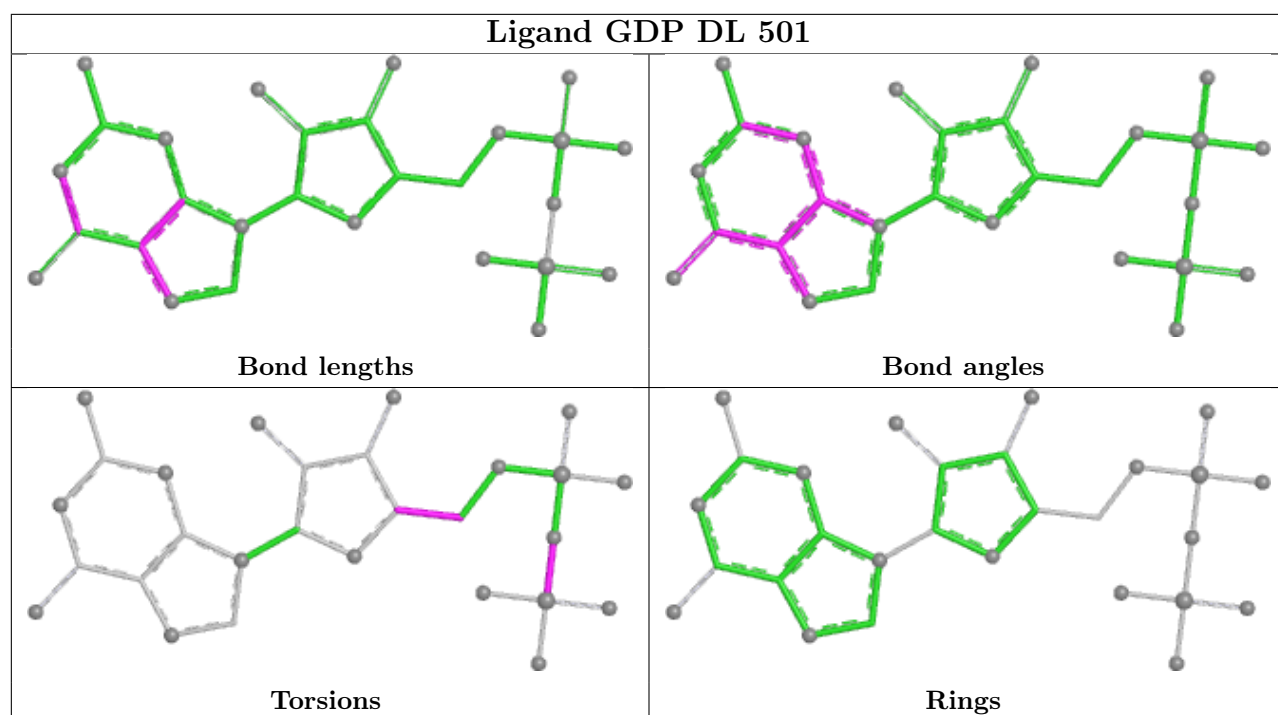
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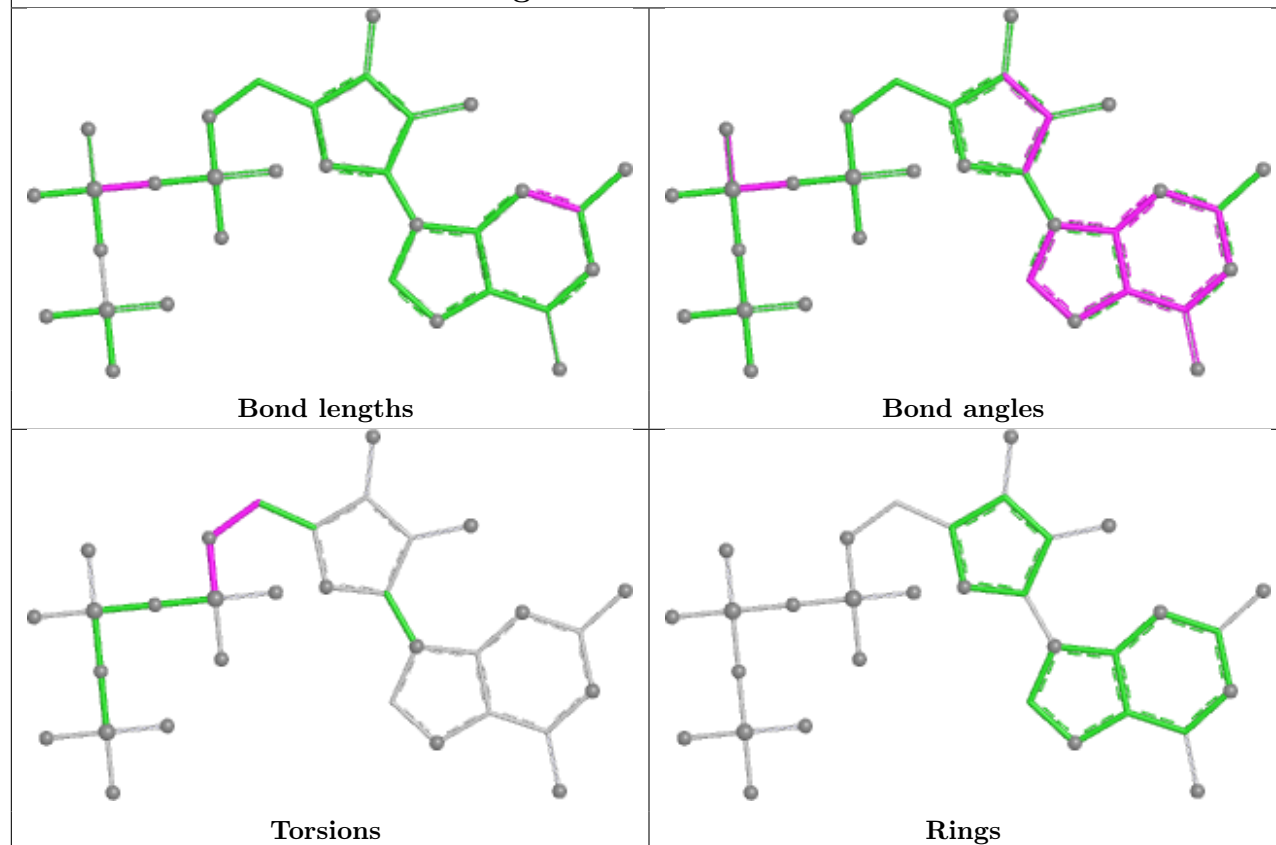
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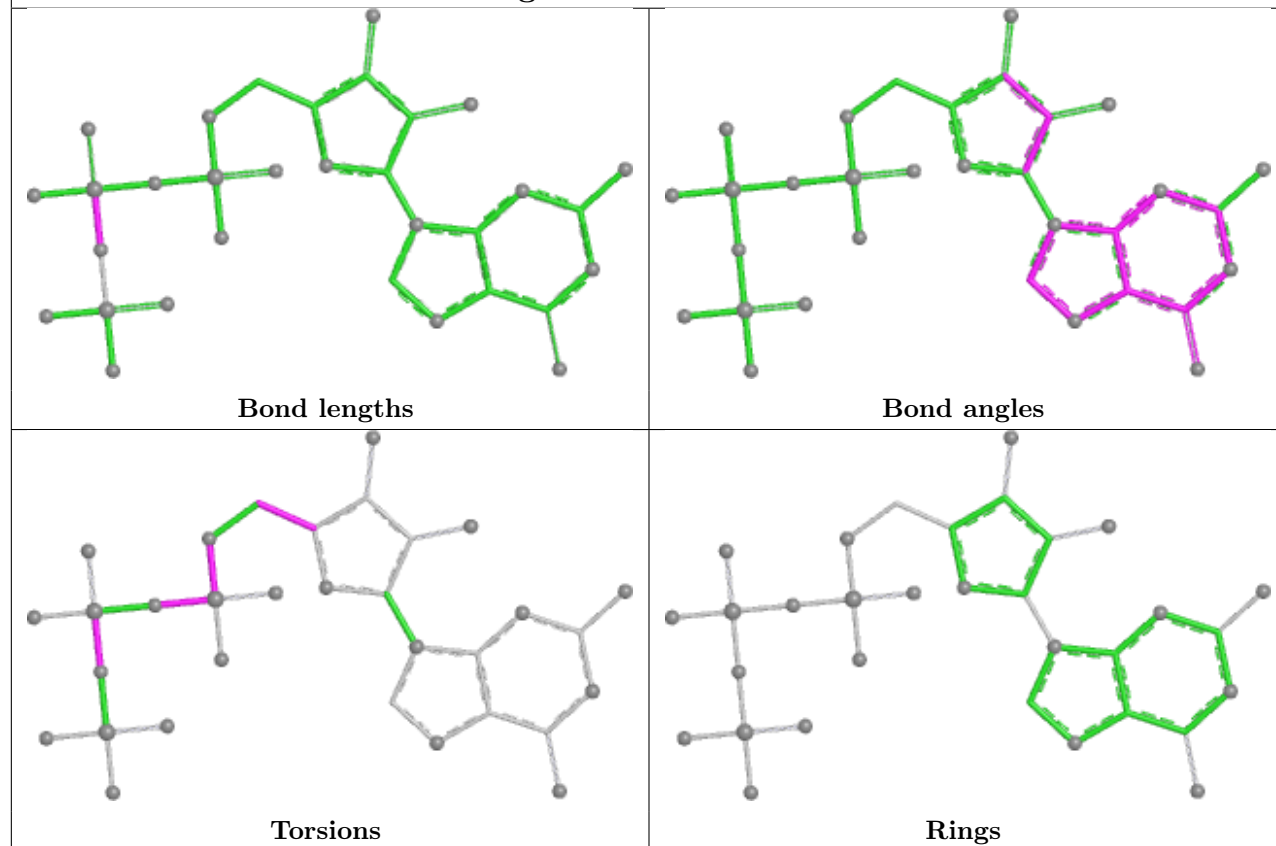


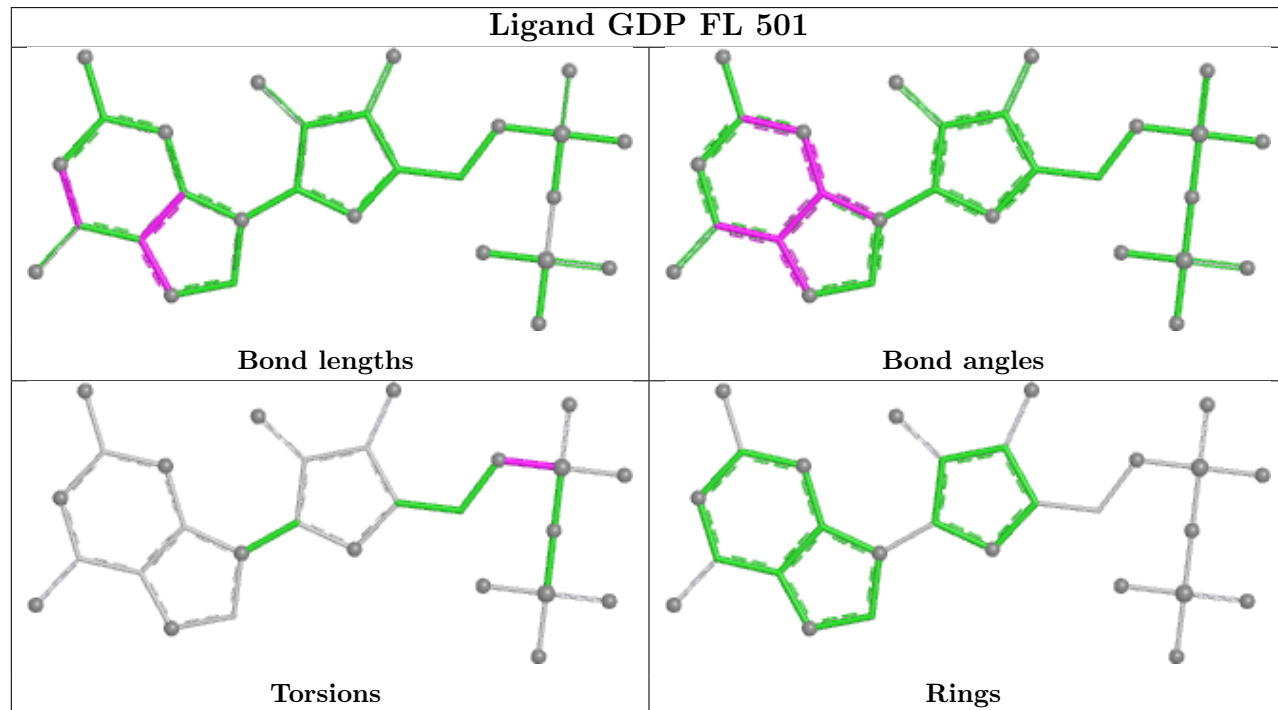
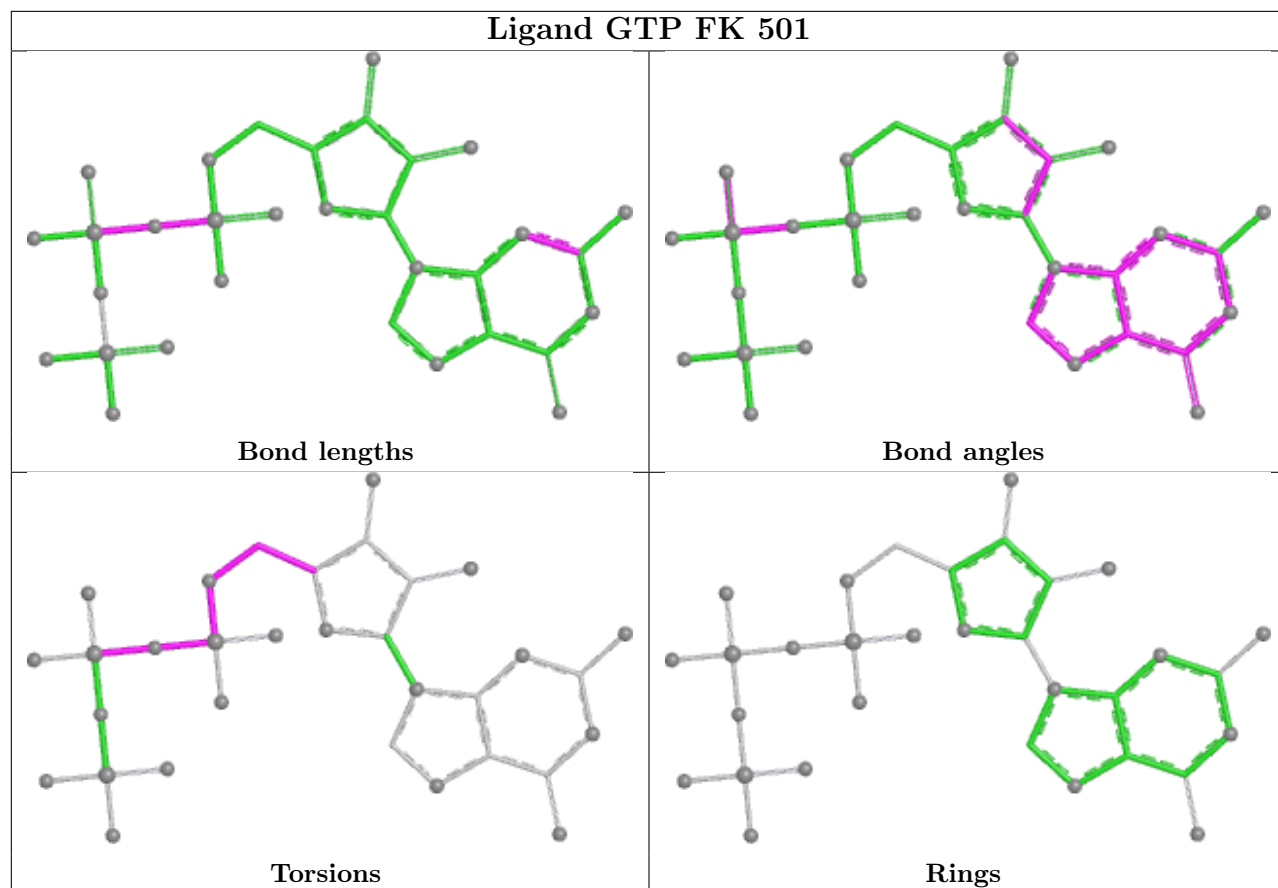


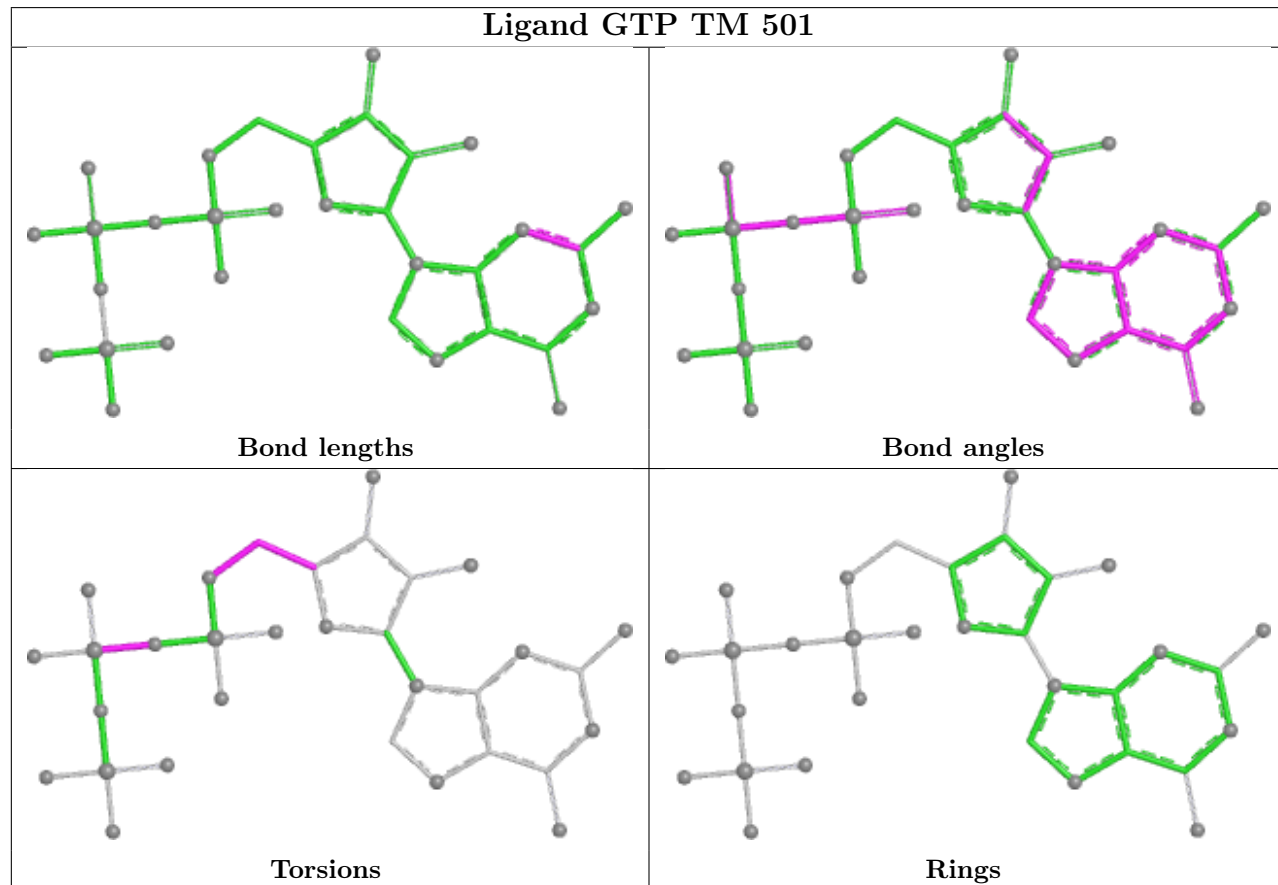
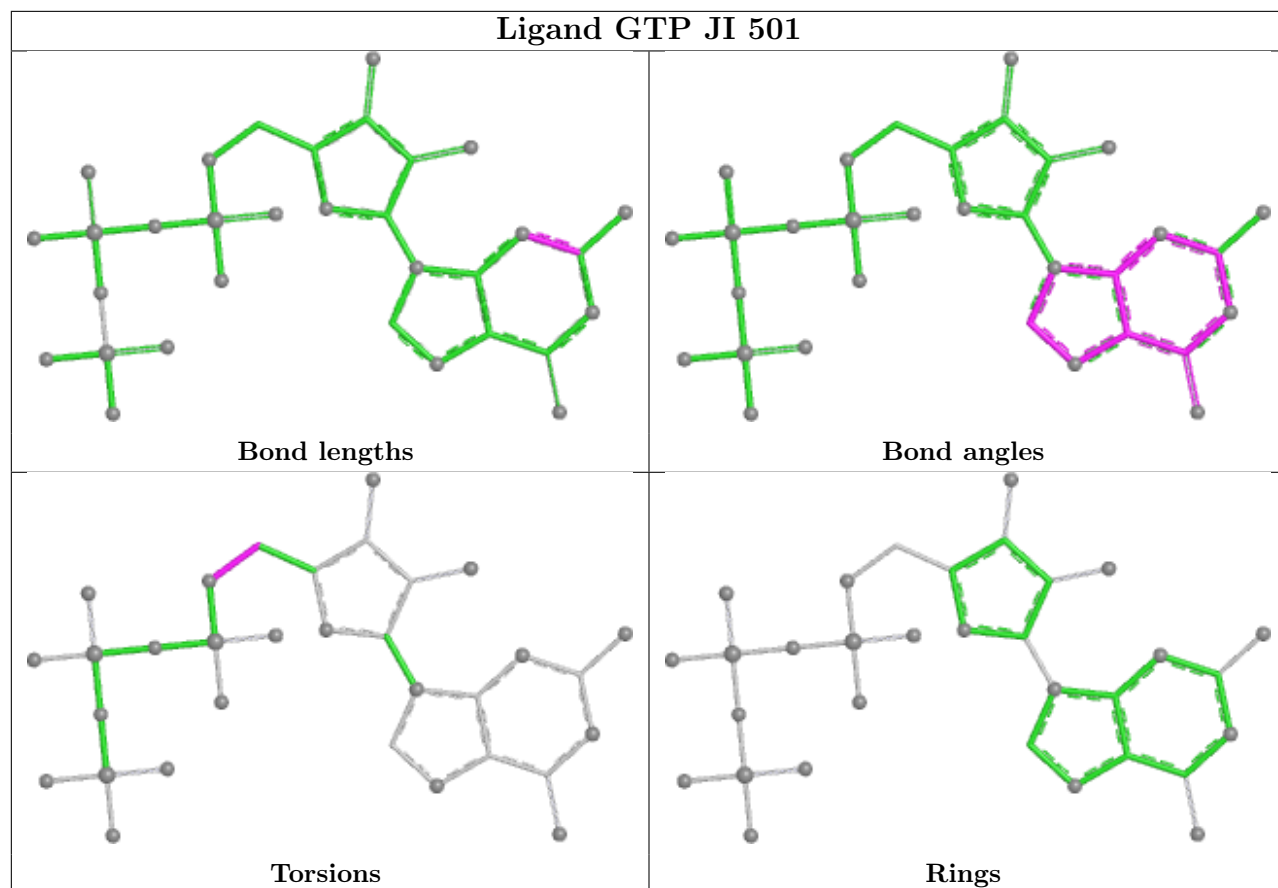
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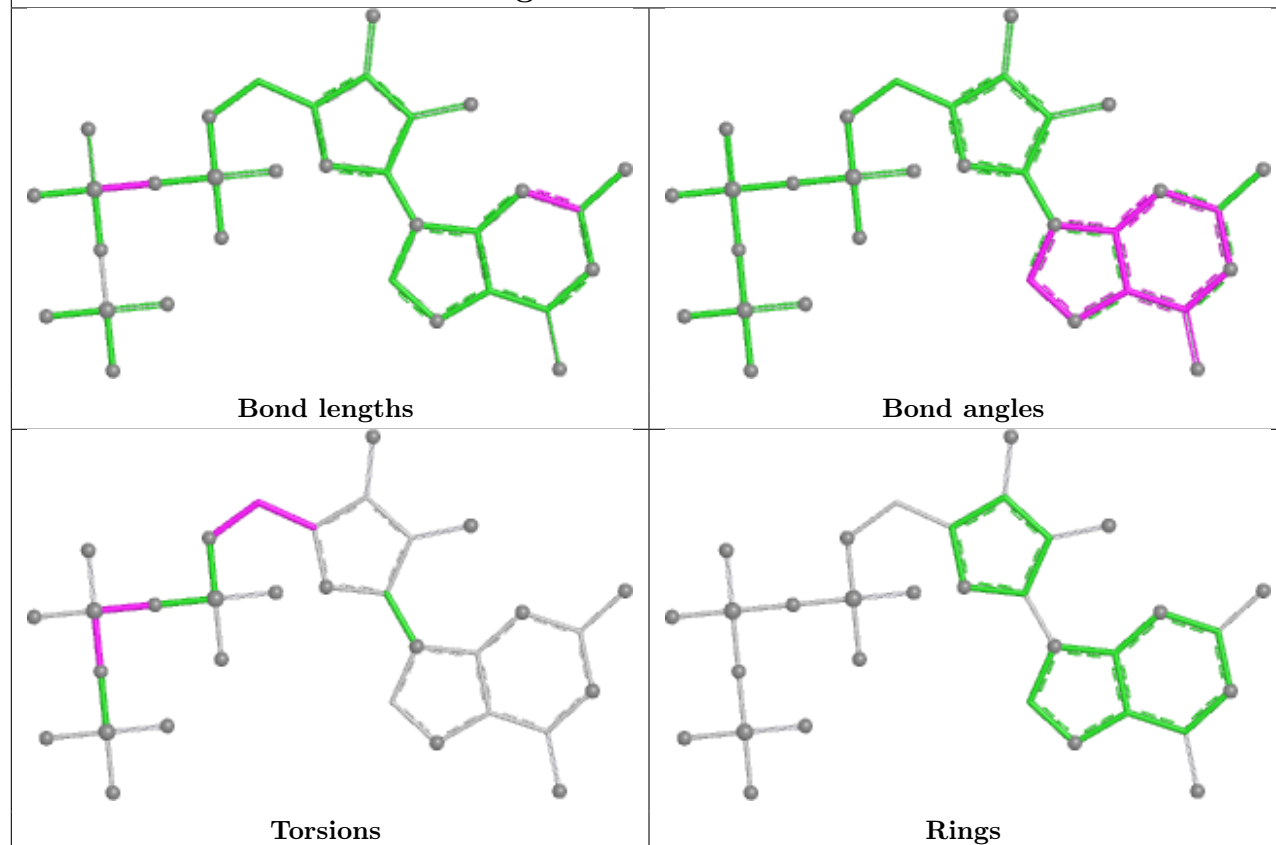
## Ligand GTP PC 501



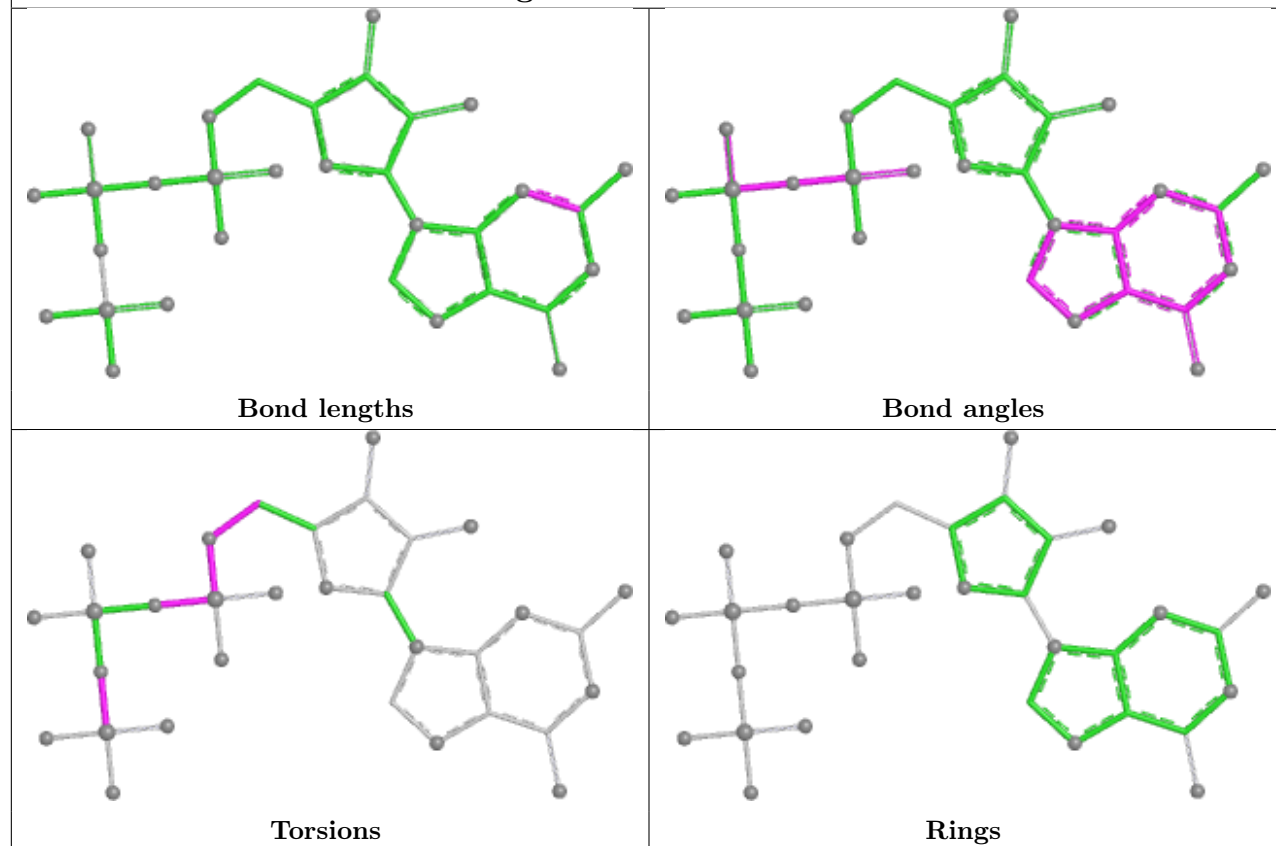




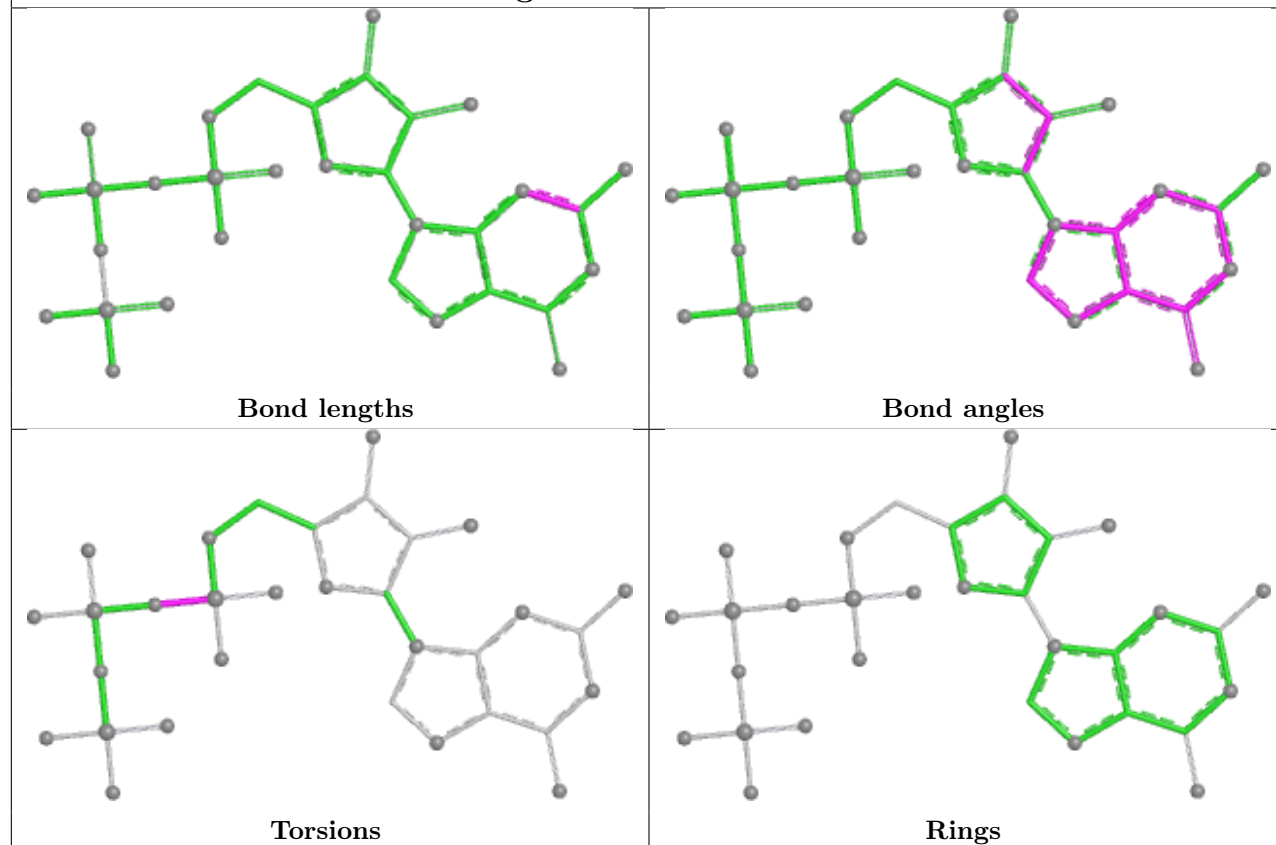
## Ligand GTP UK 501



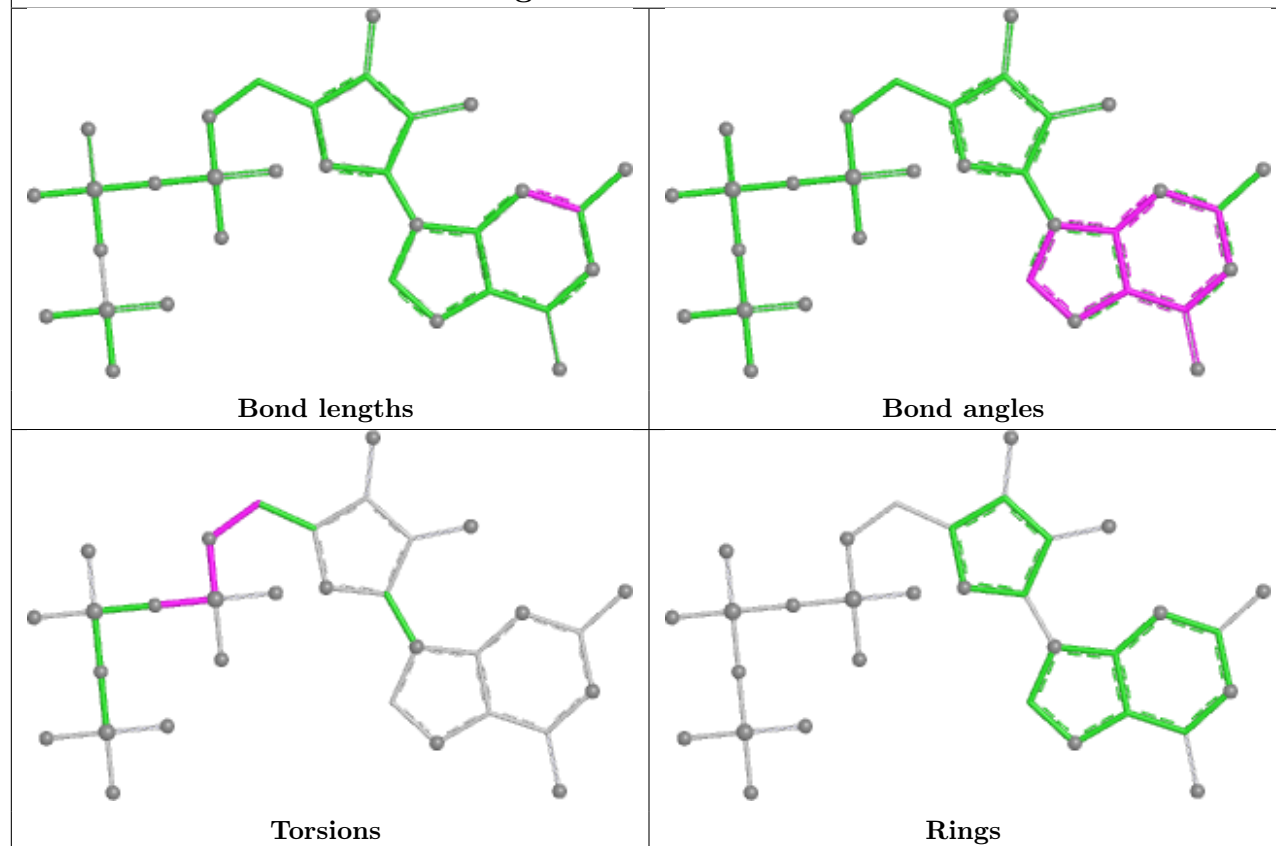
## Ligand GTP LM 501



## Ligand GTP OG 501

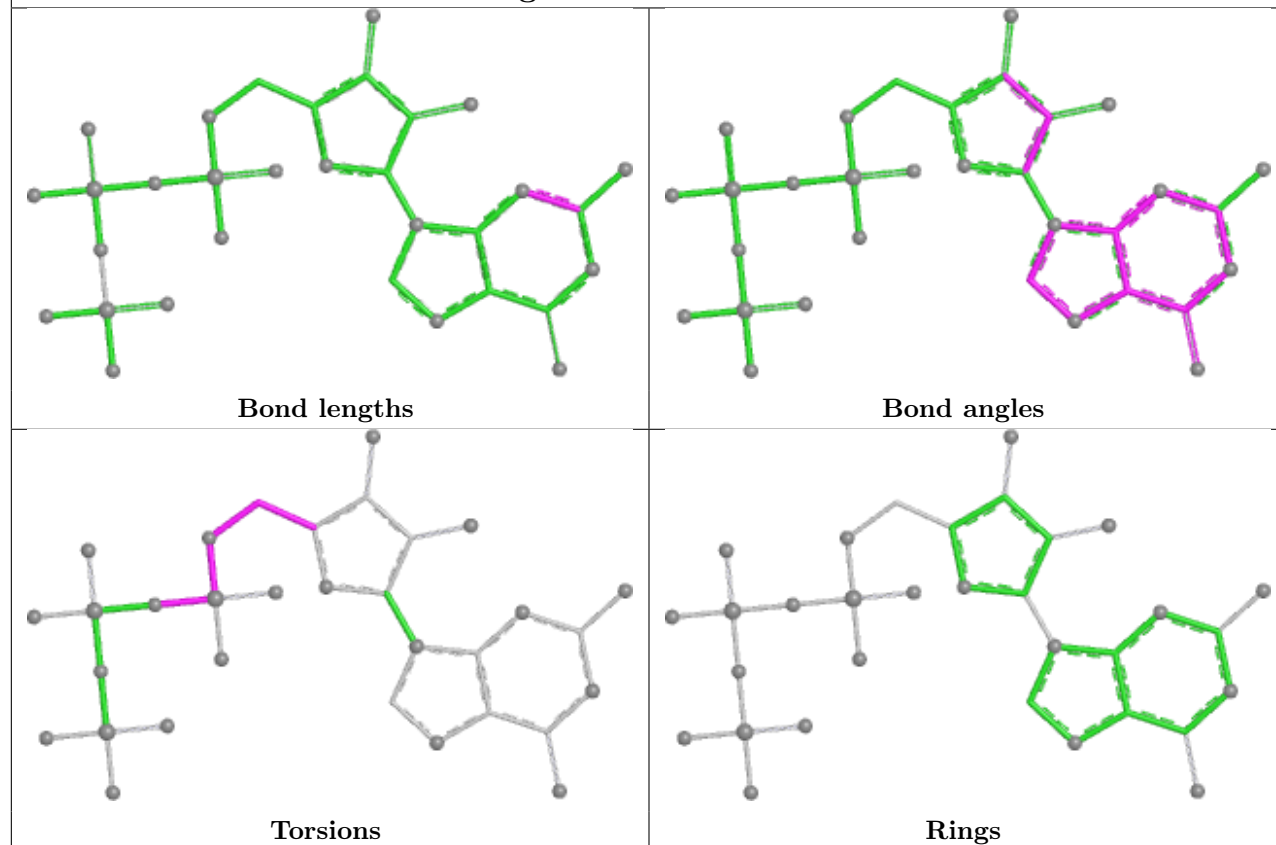


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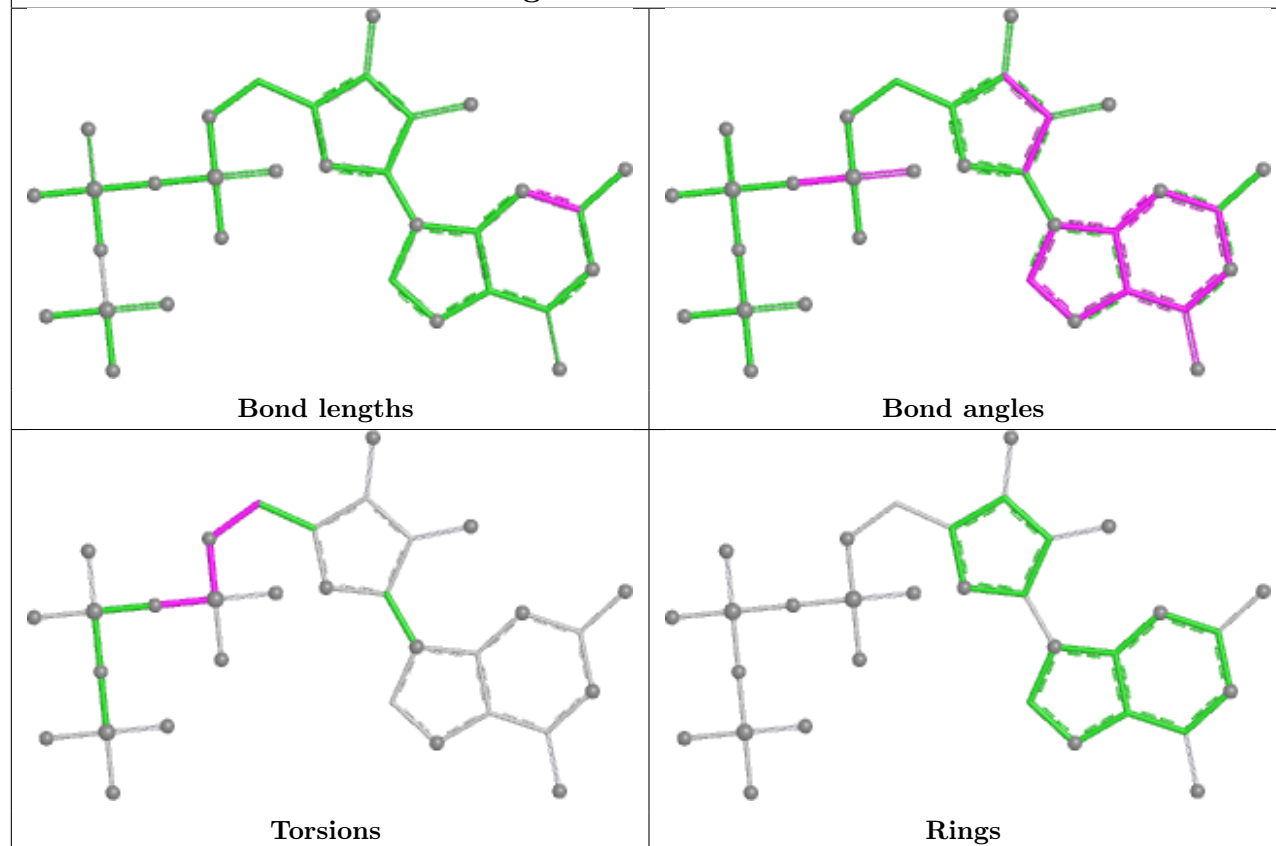




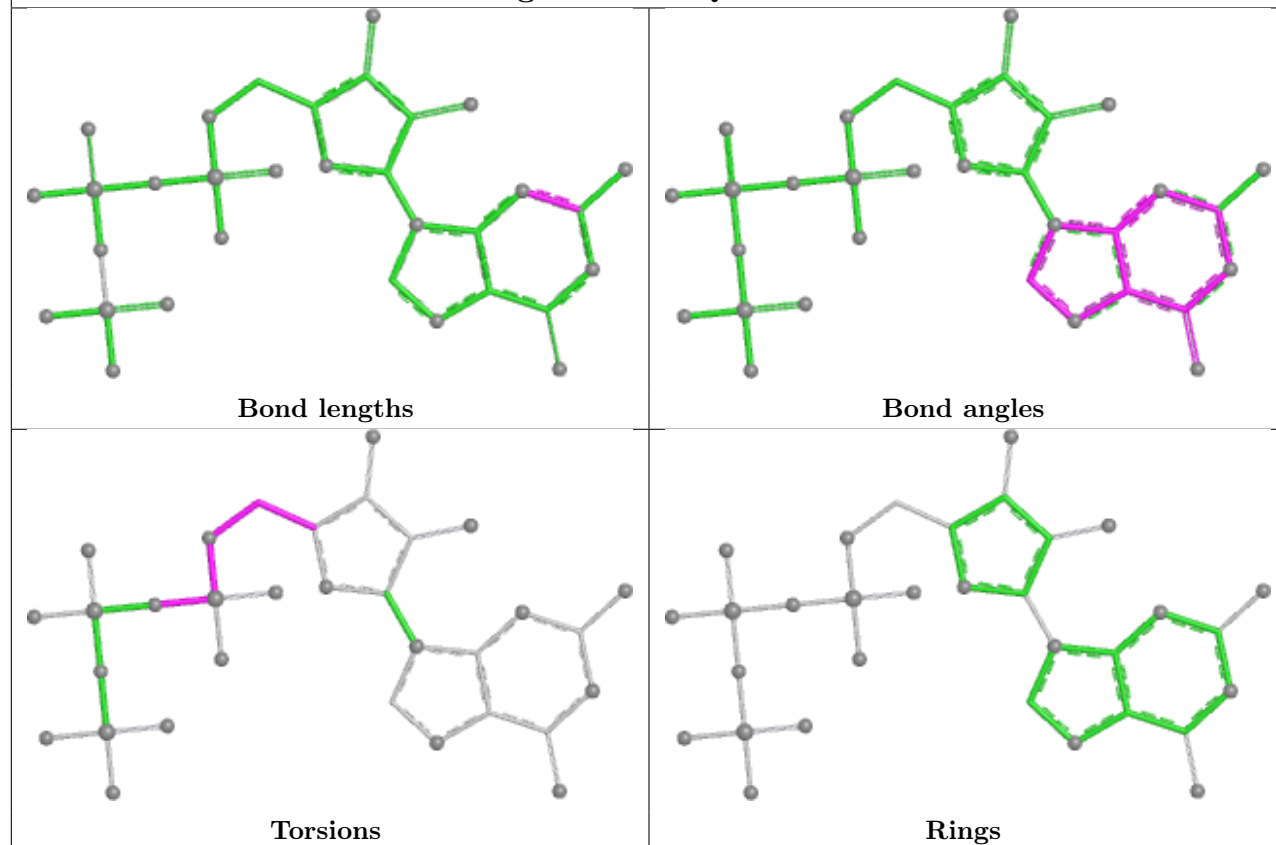
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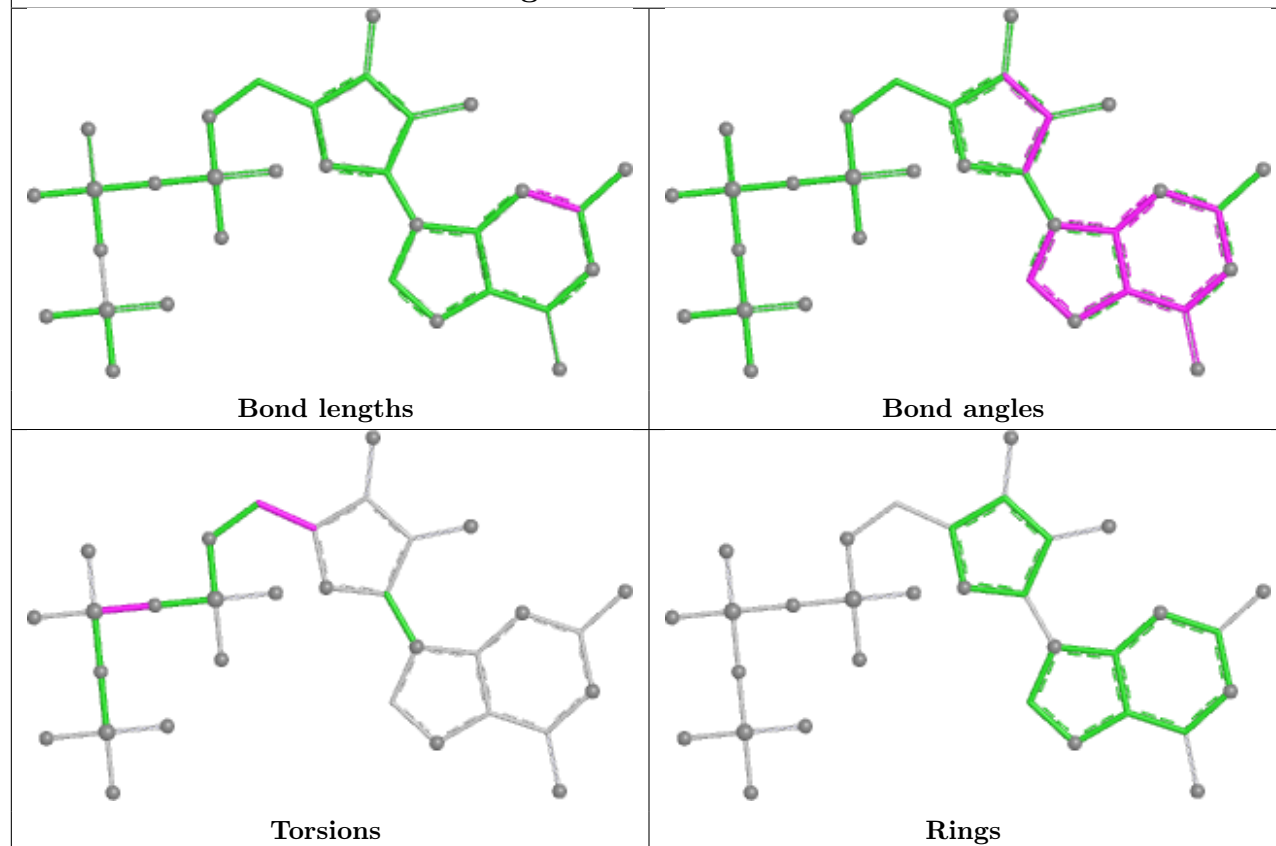
## Ligand GTP KI 501

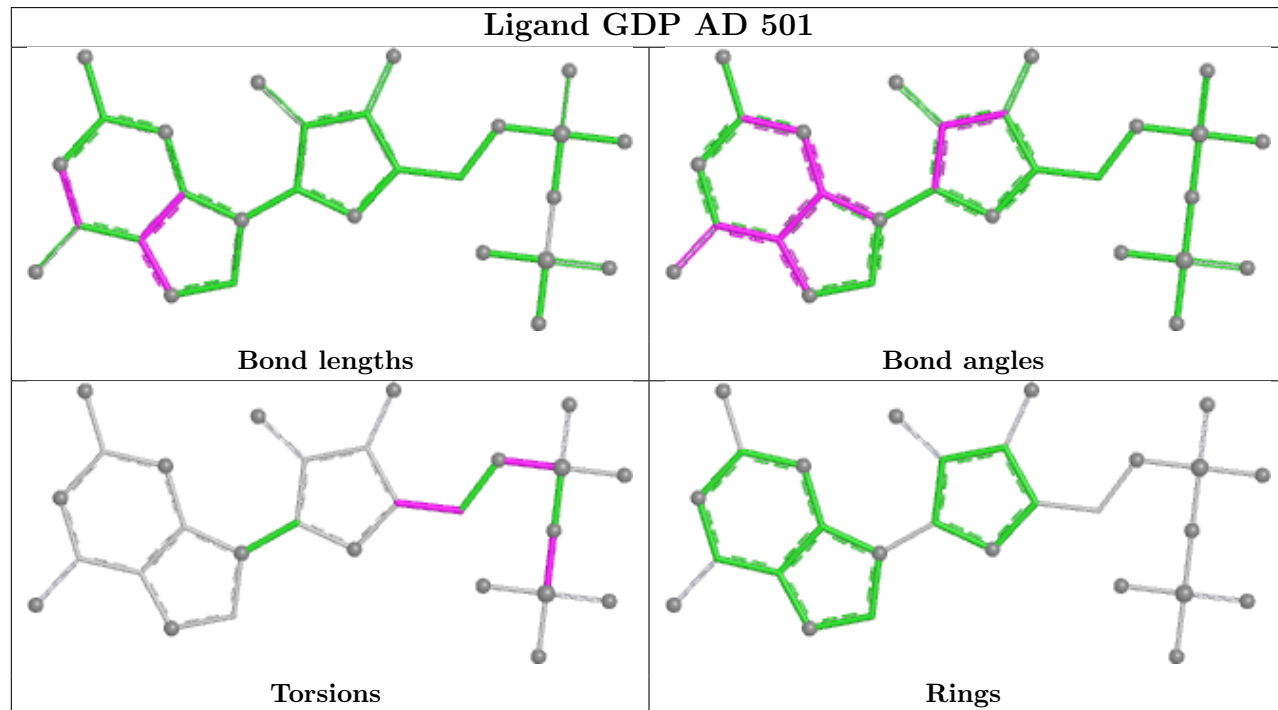
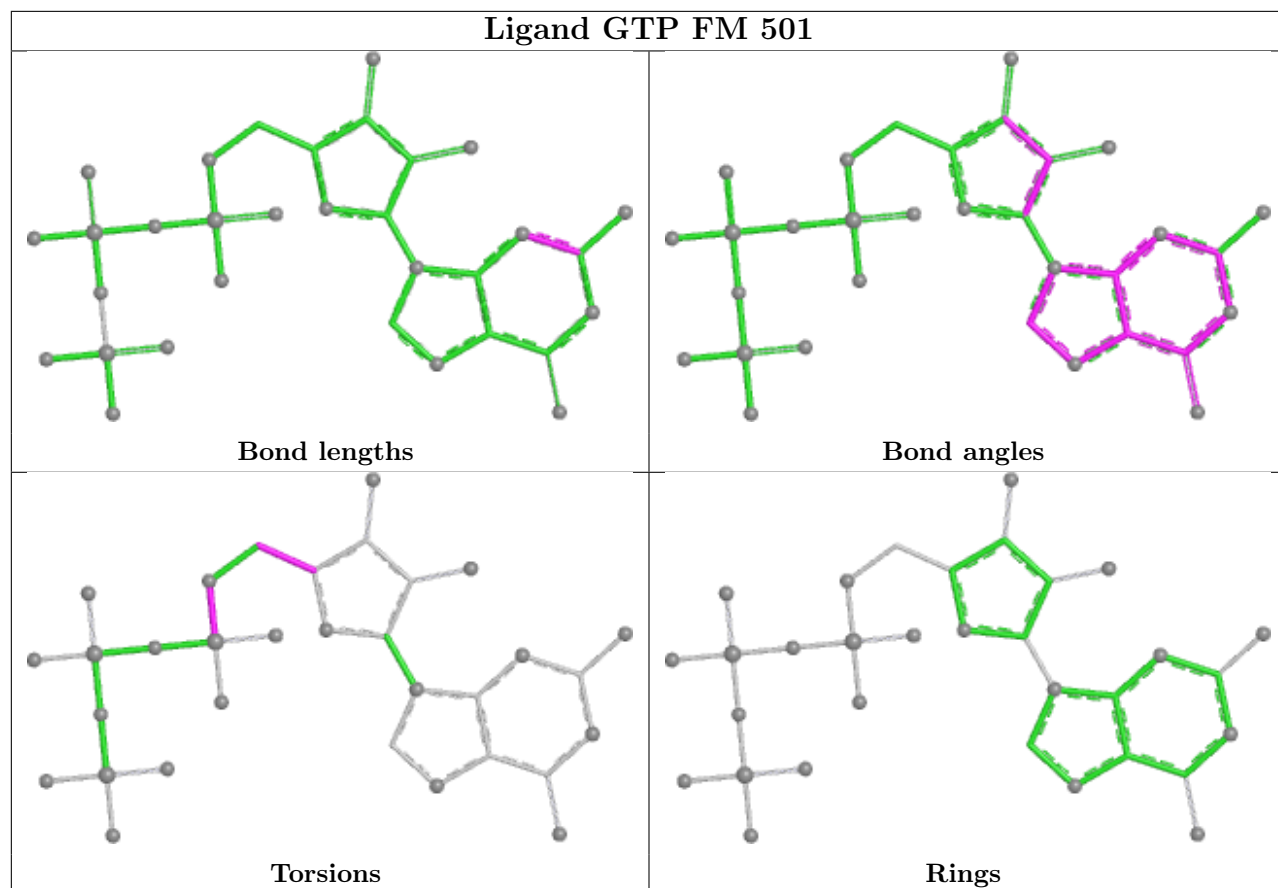


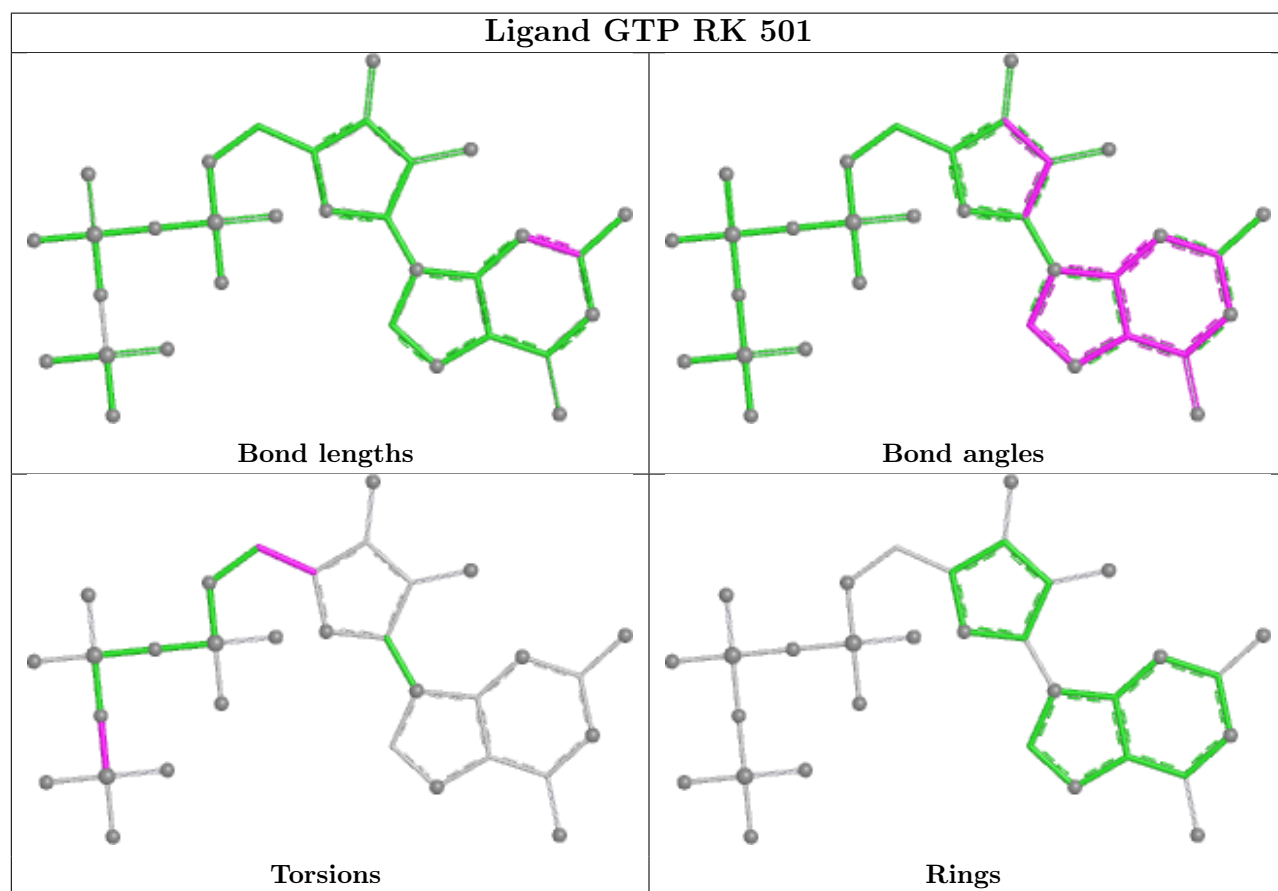
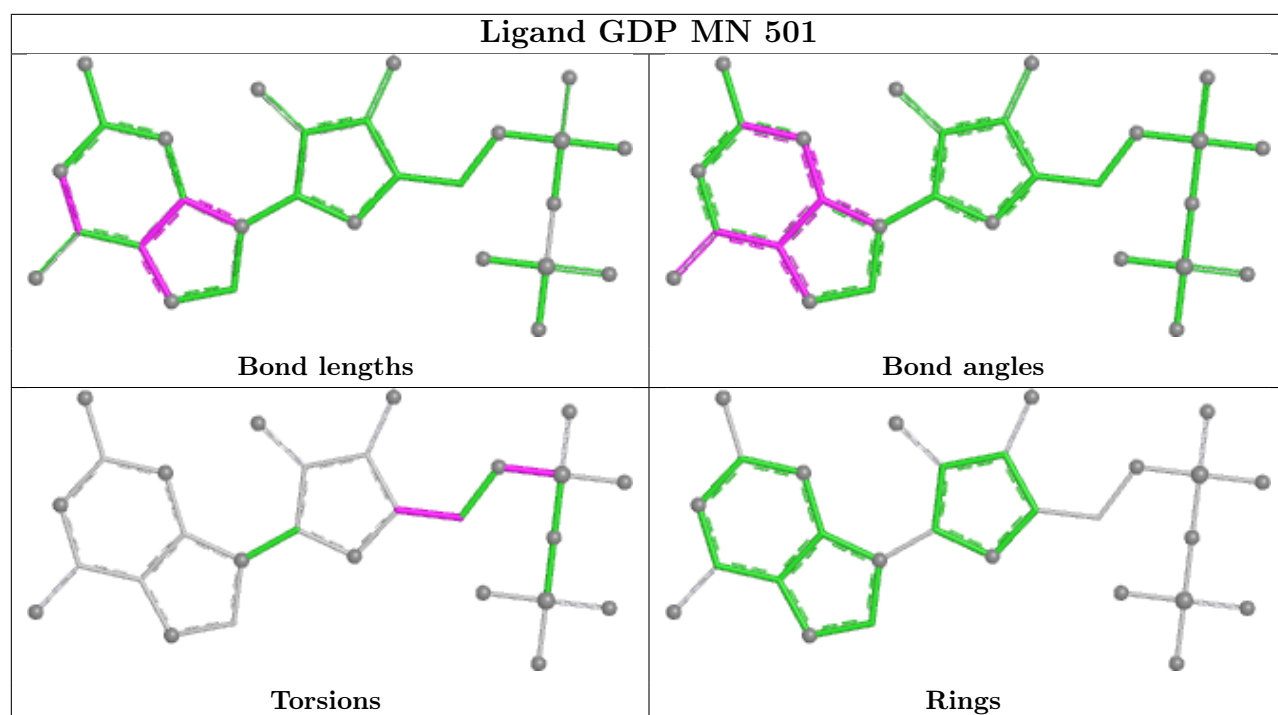
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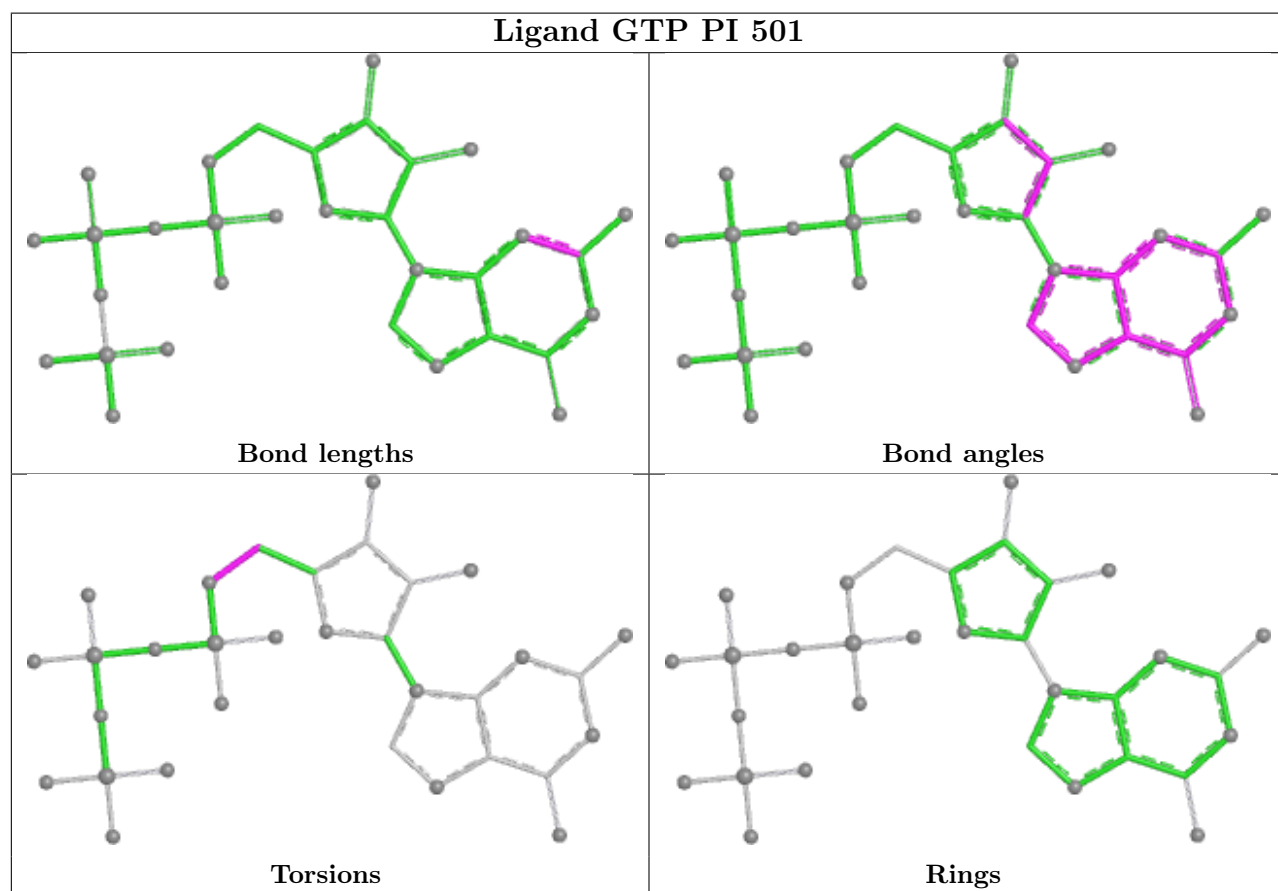
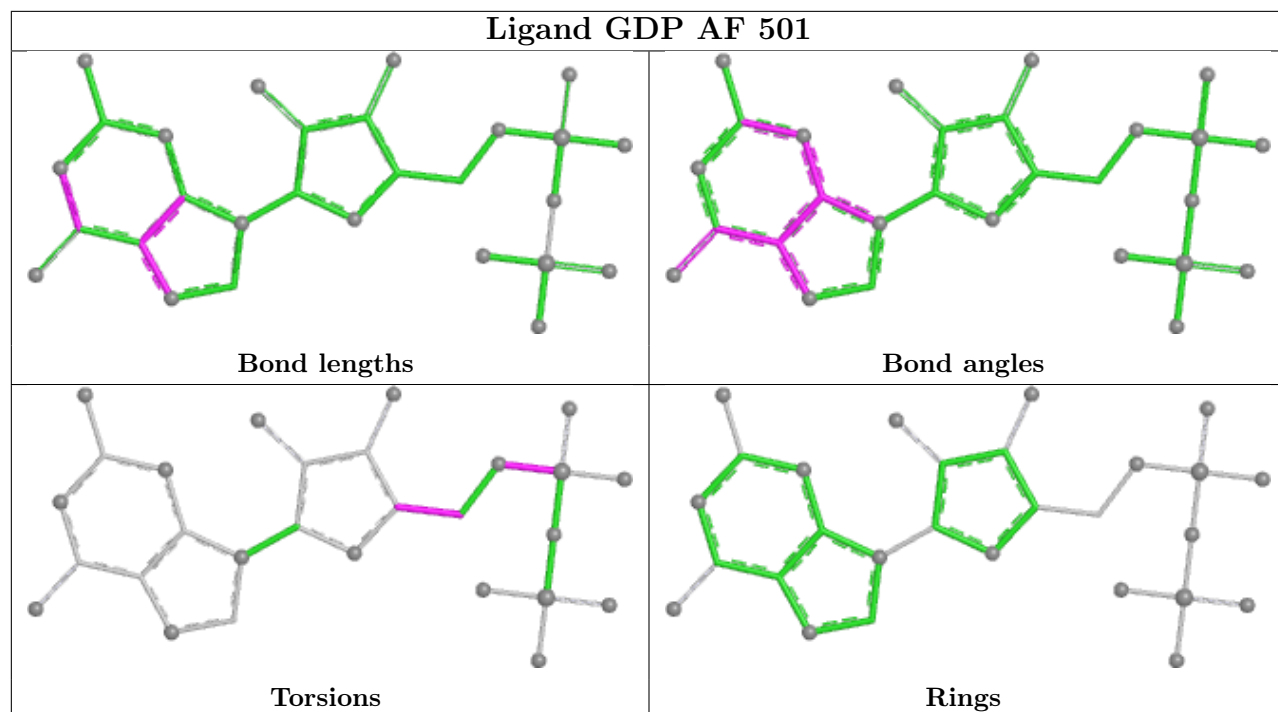


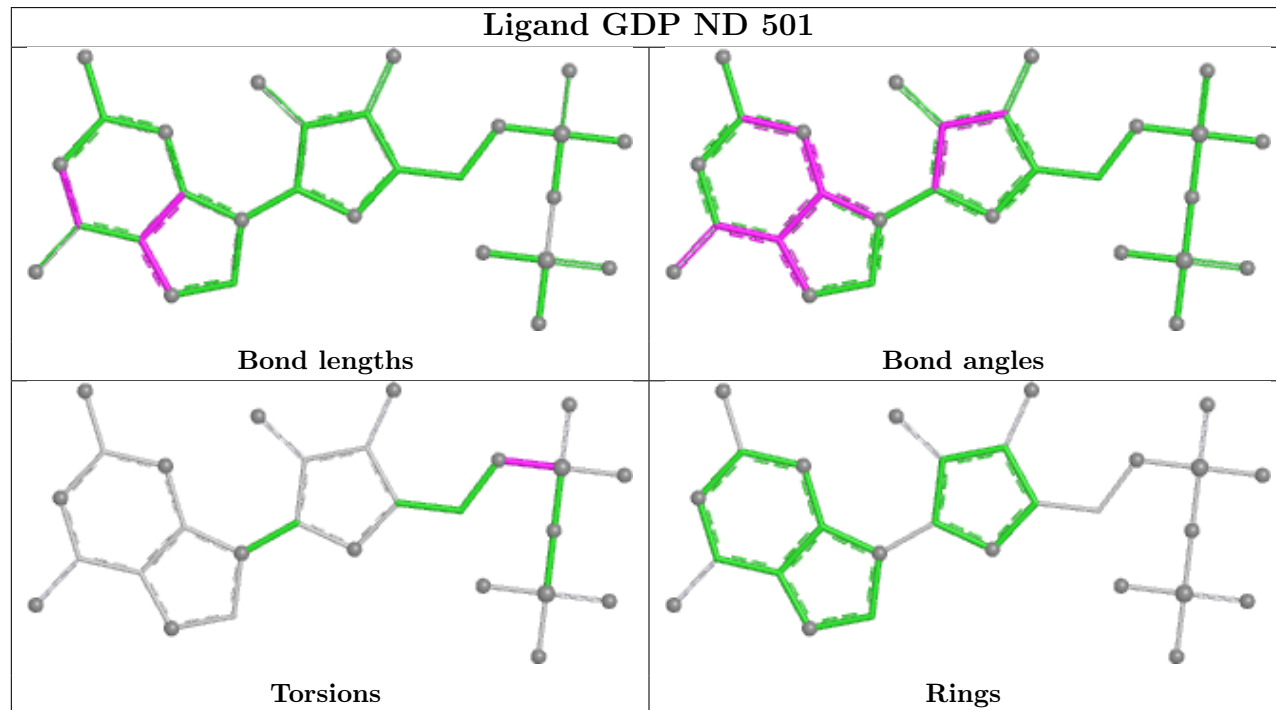
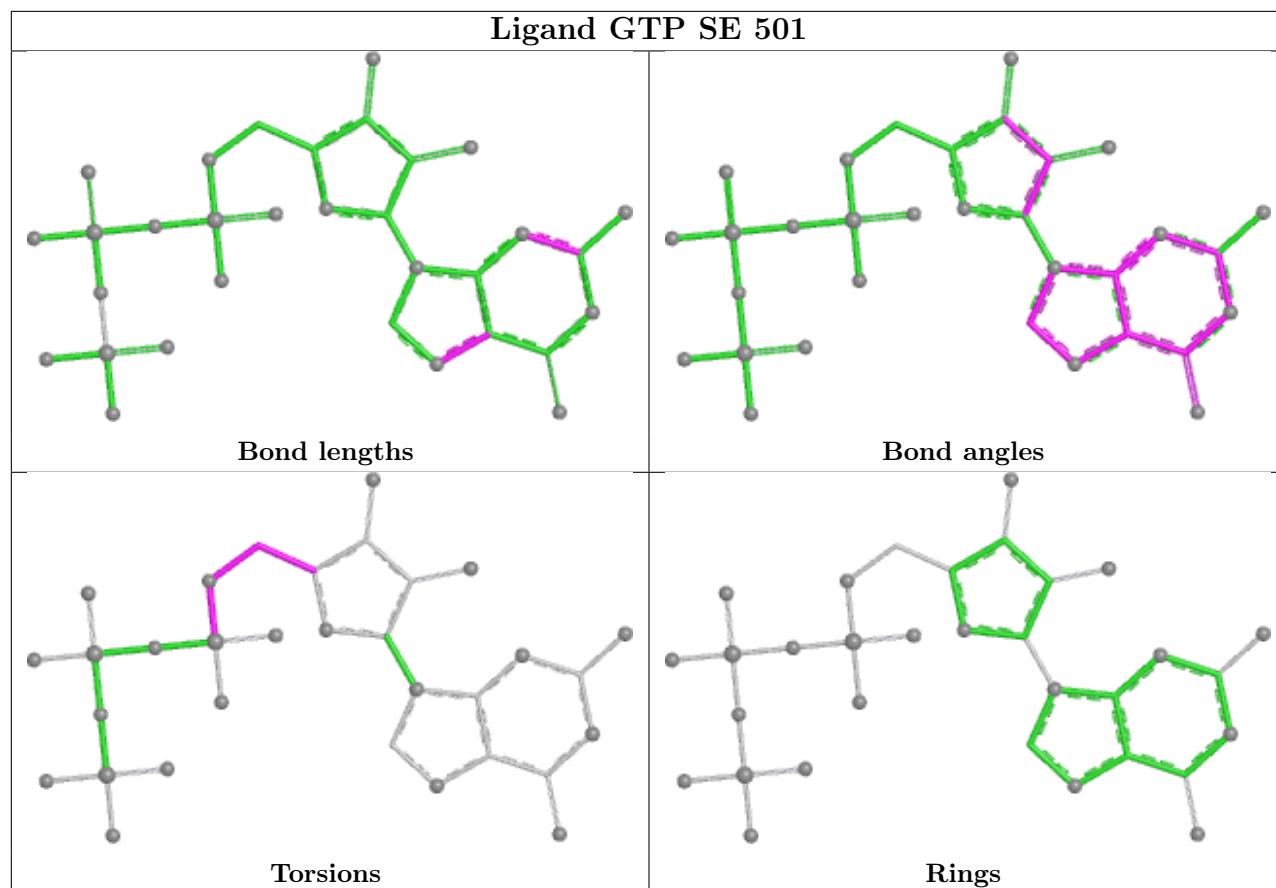
## Ligand GTP SC 501



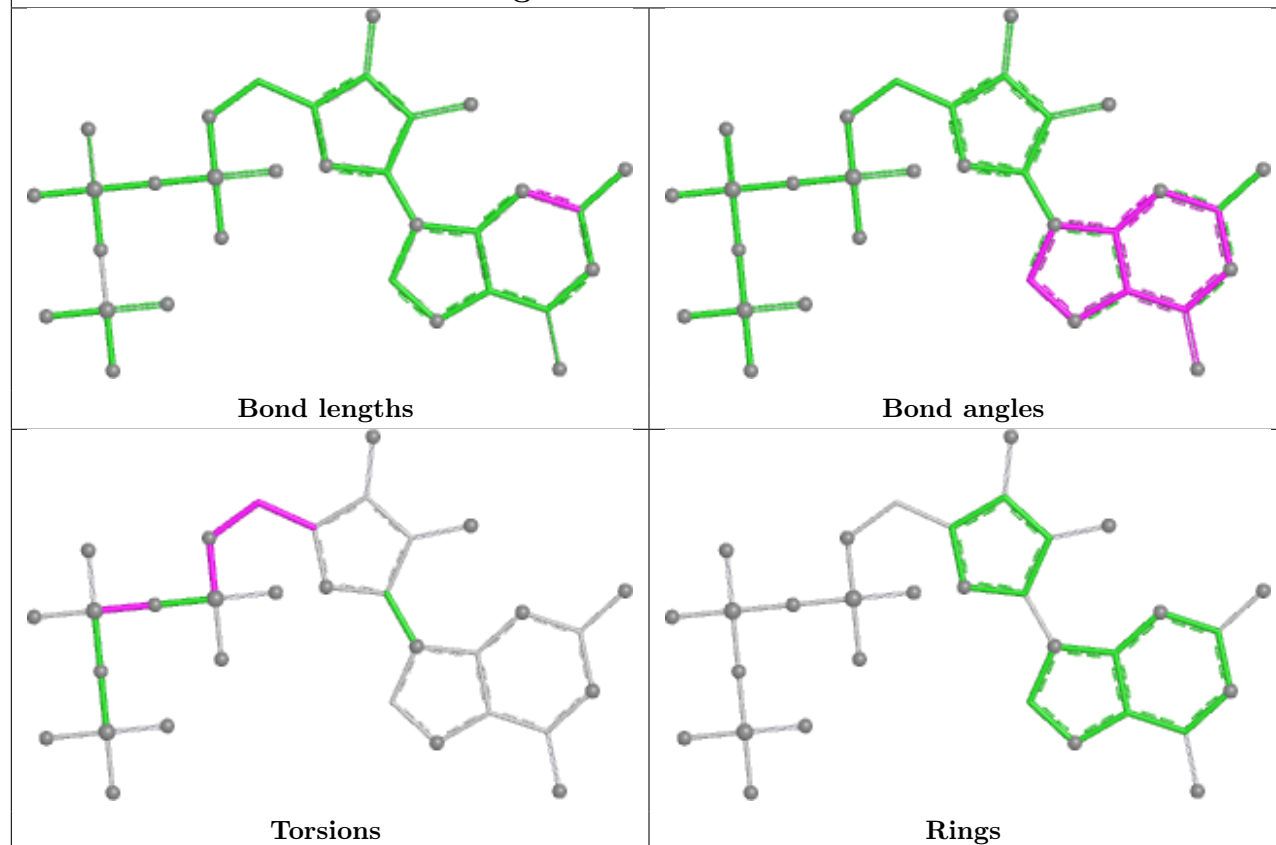




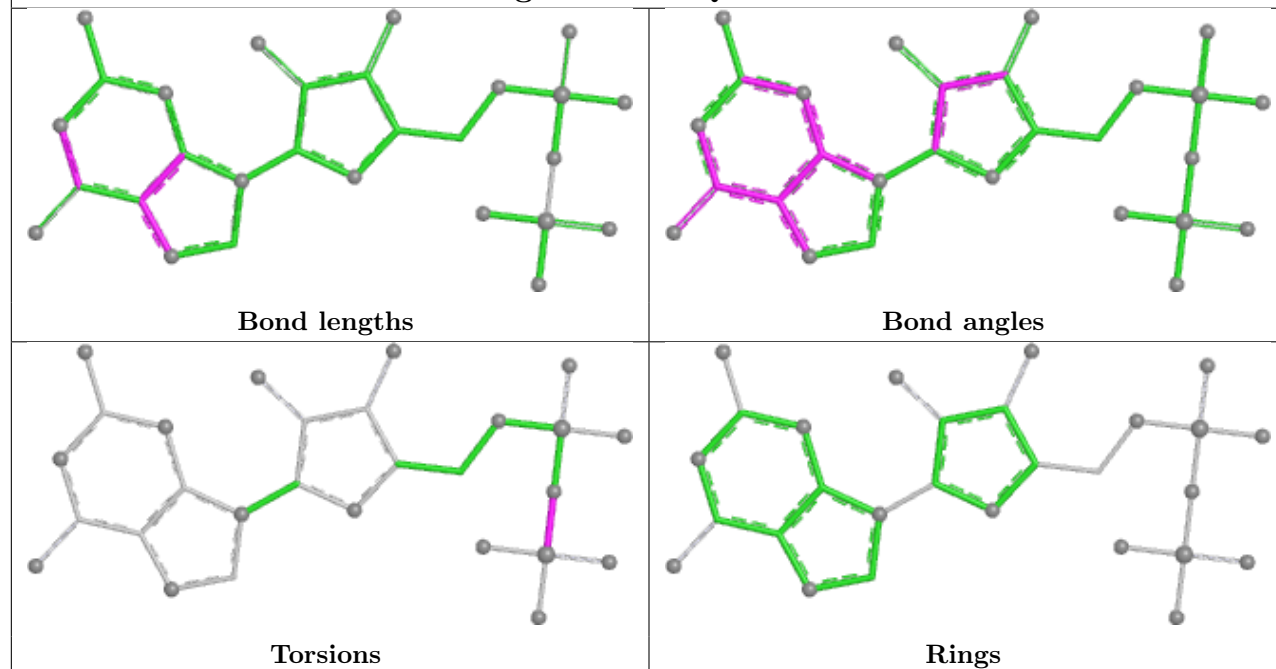




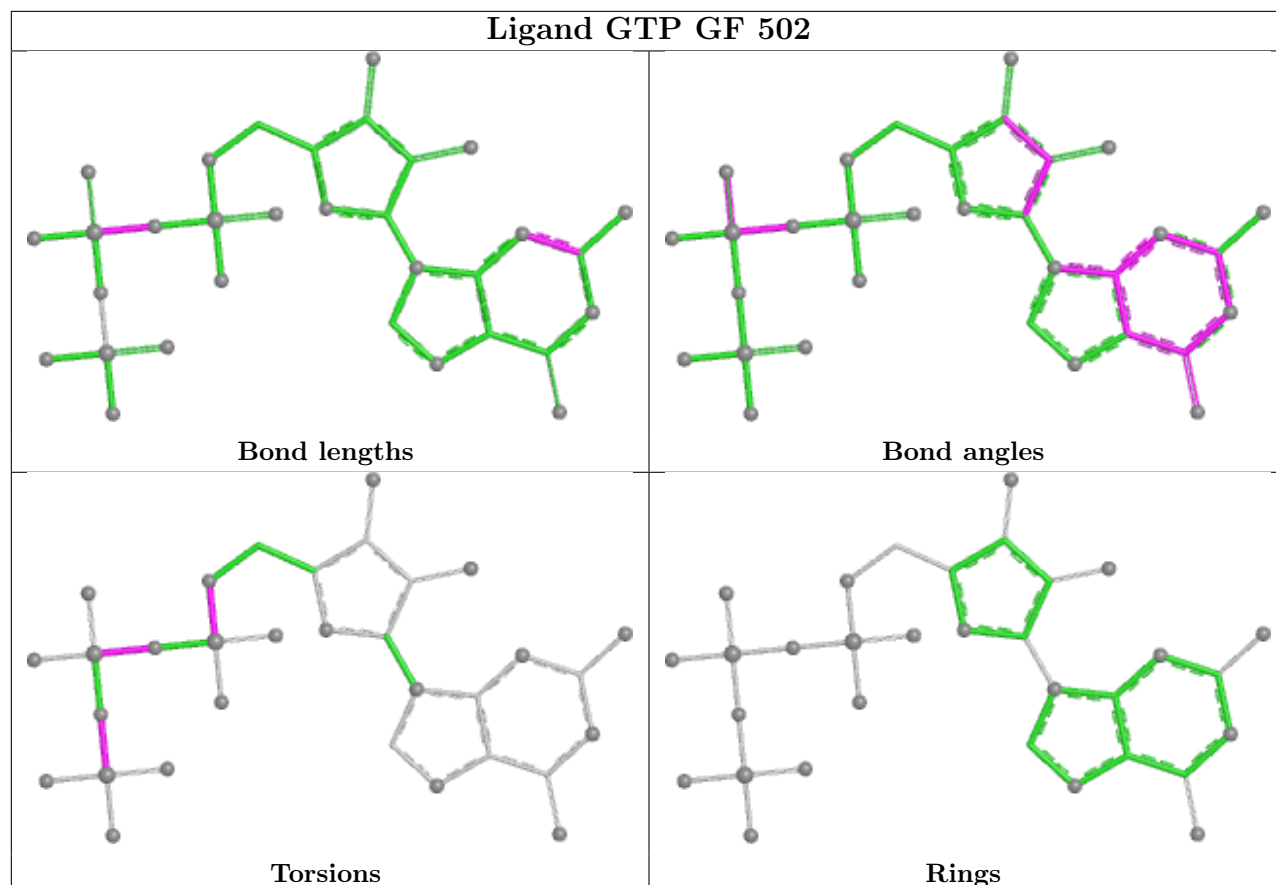
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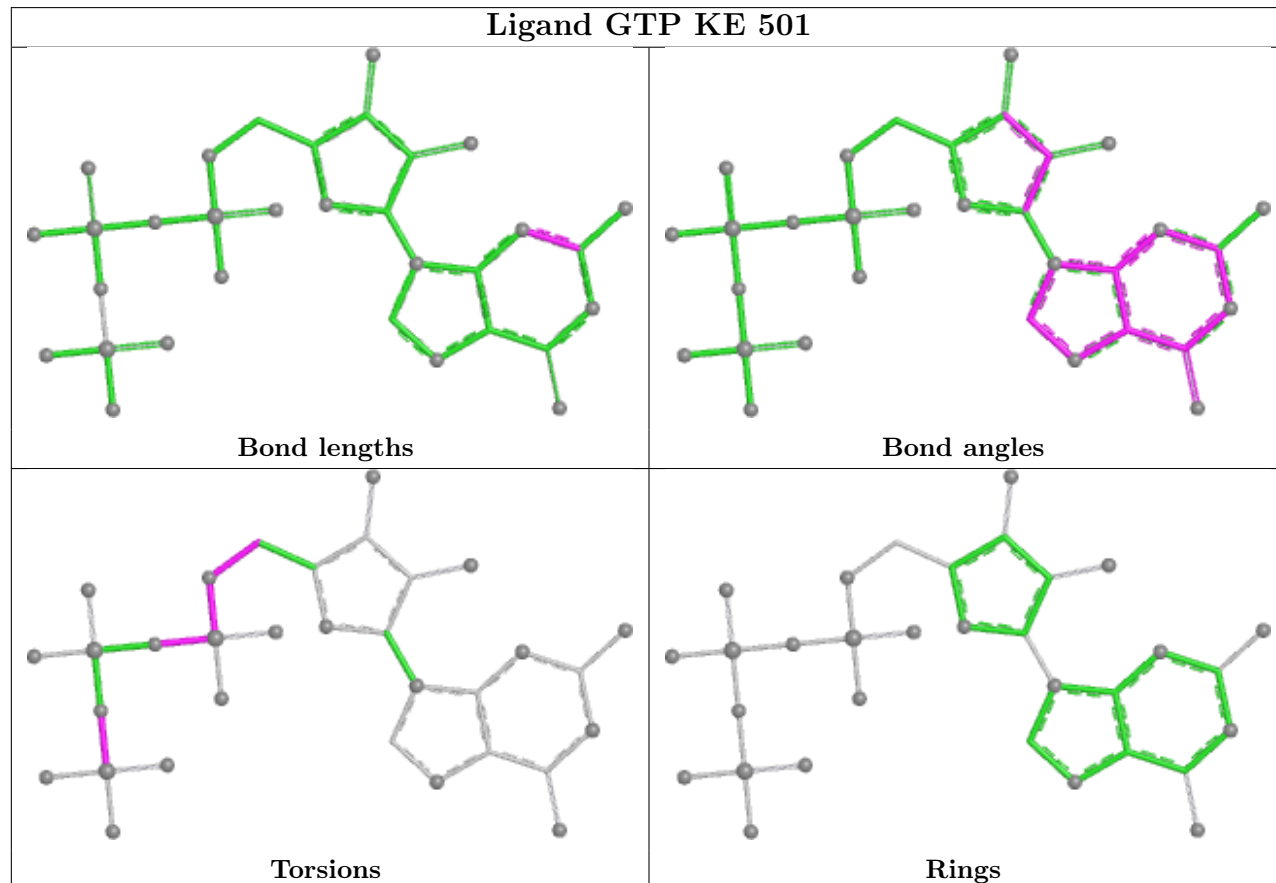
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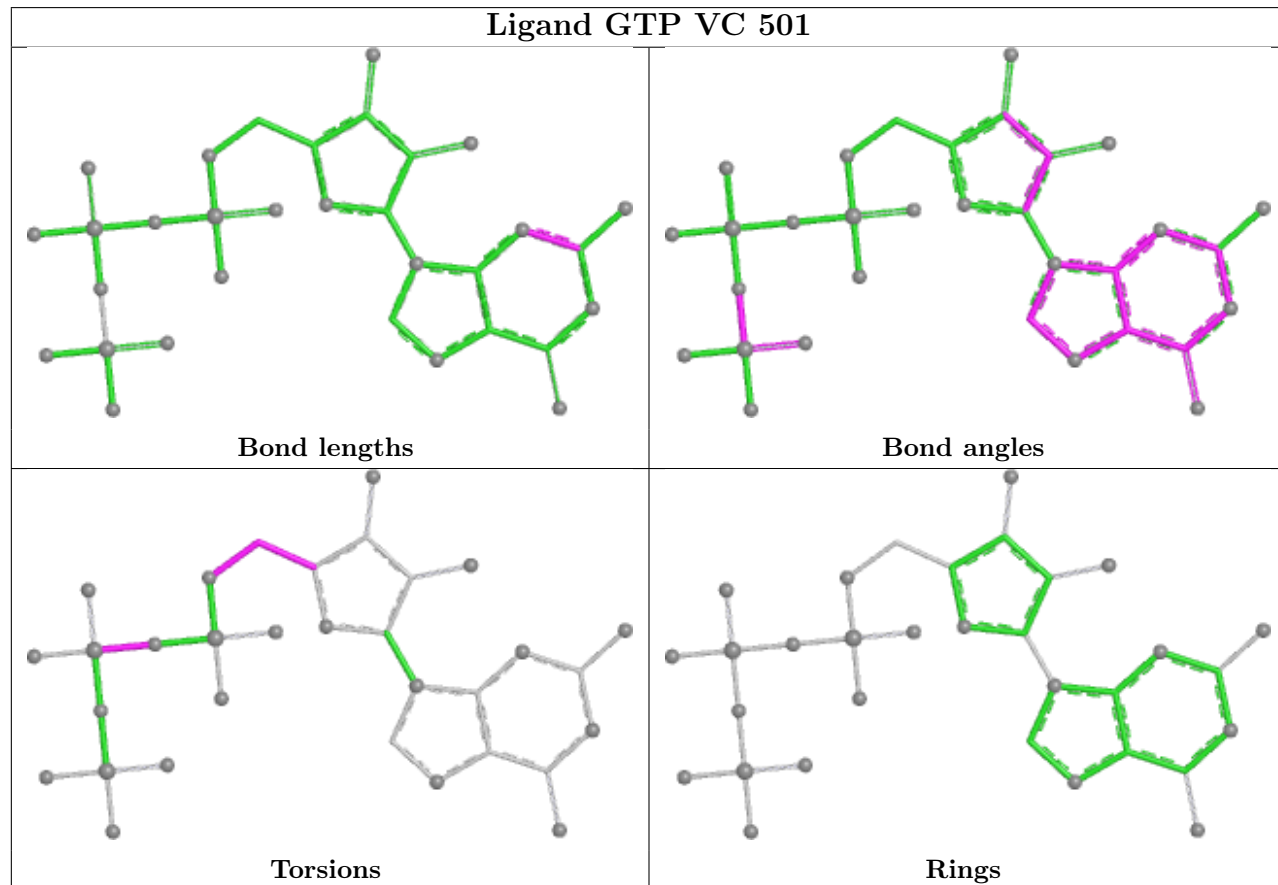
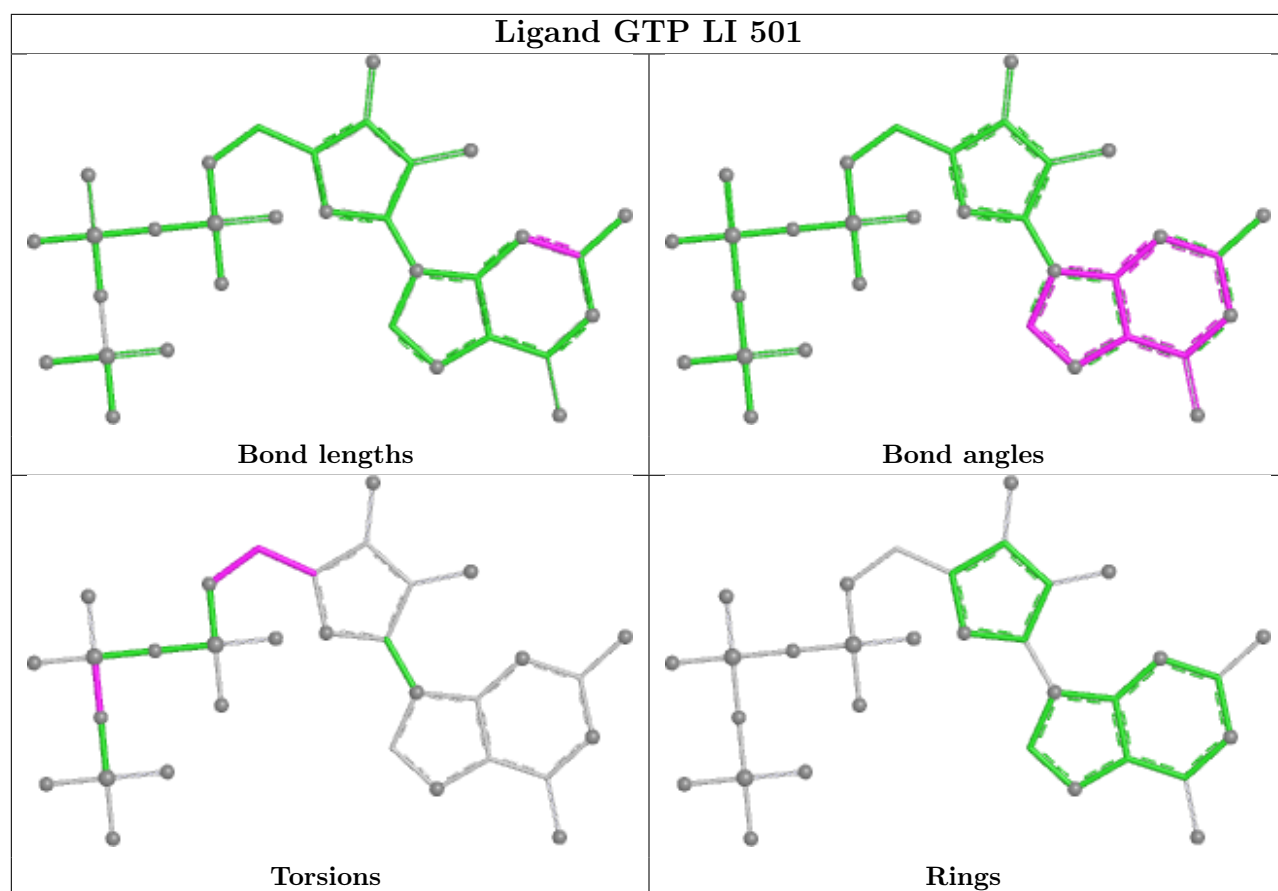
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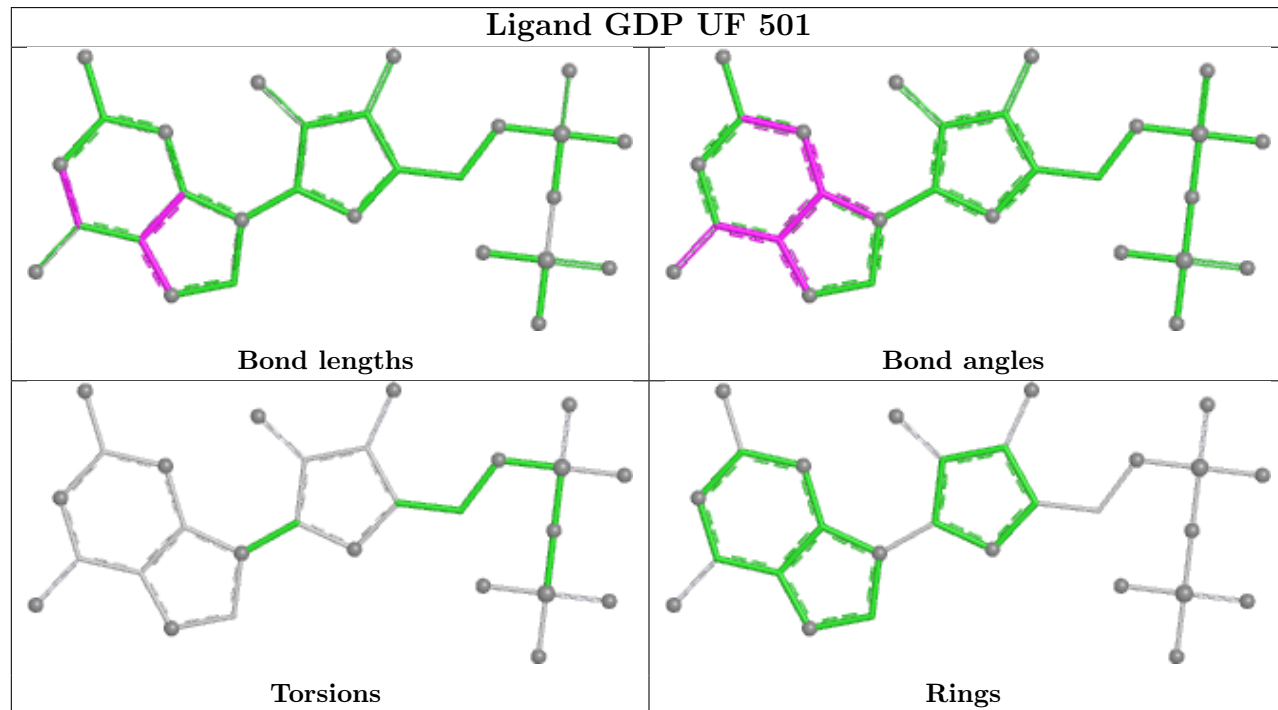
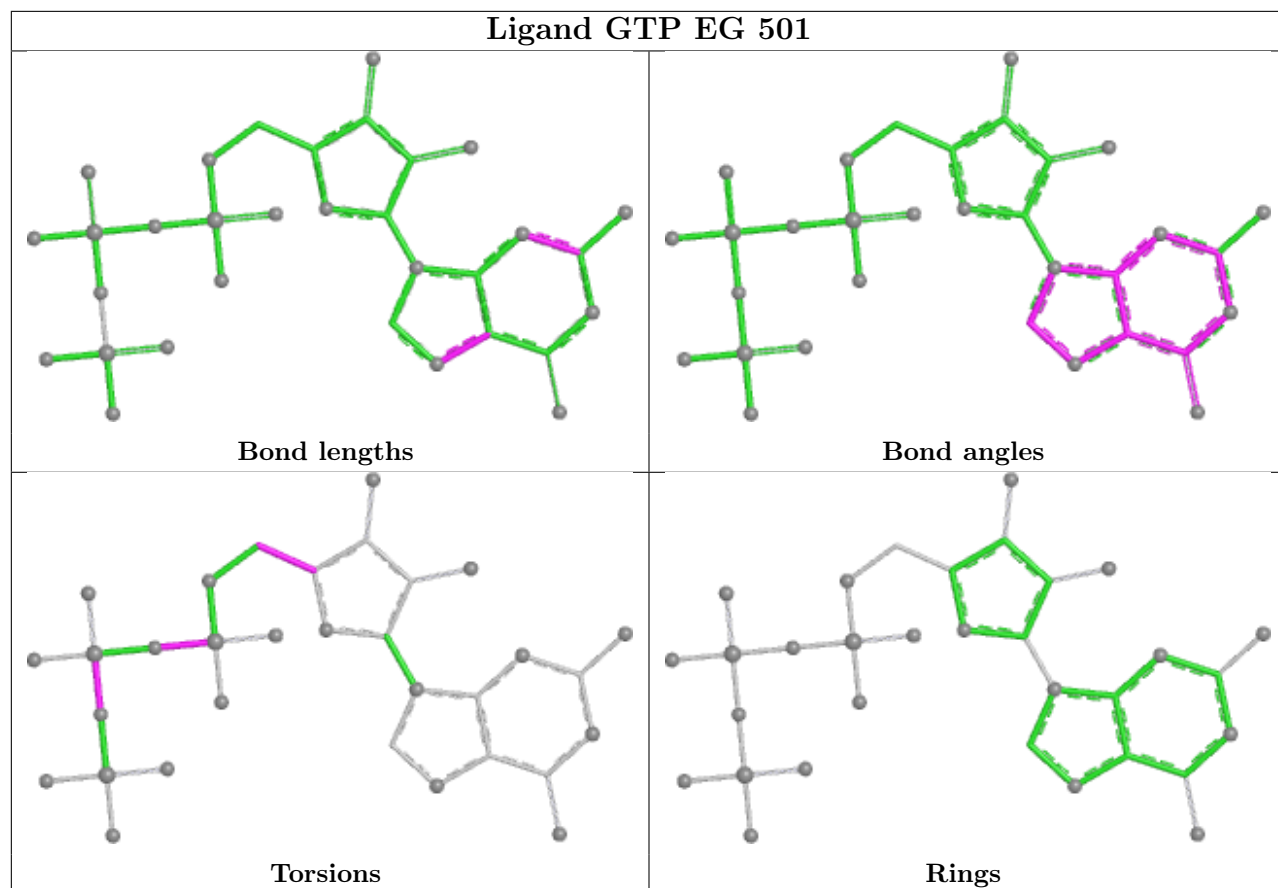


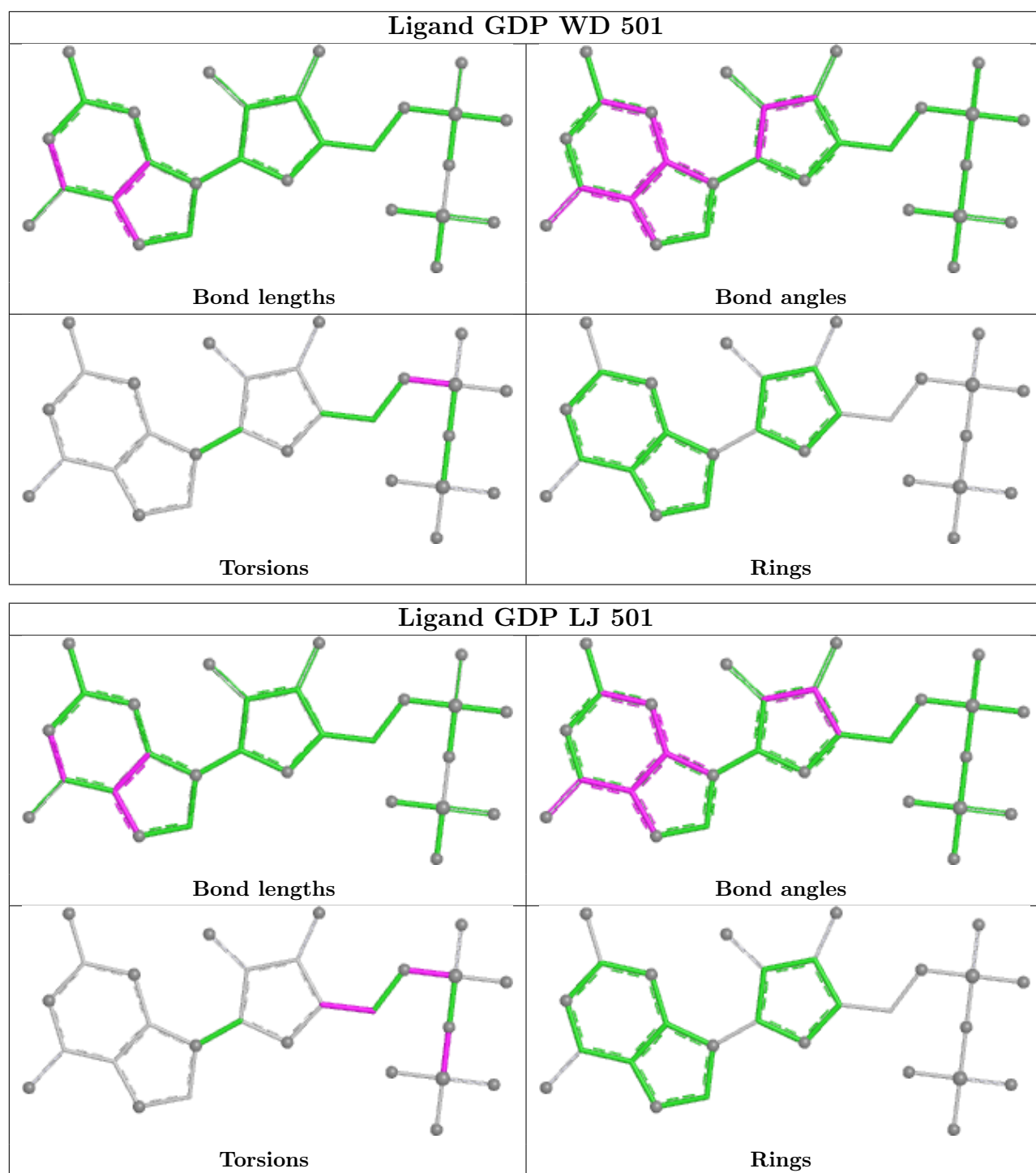
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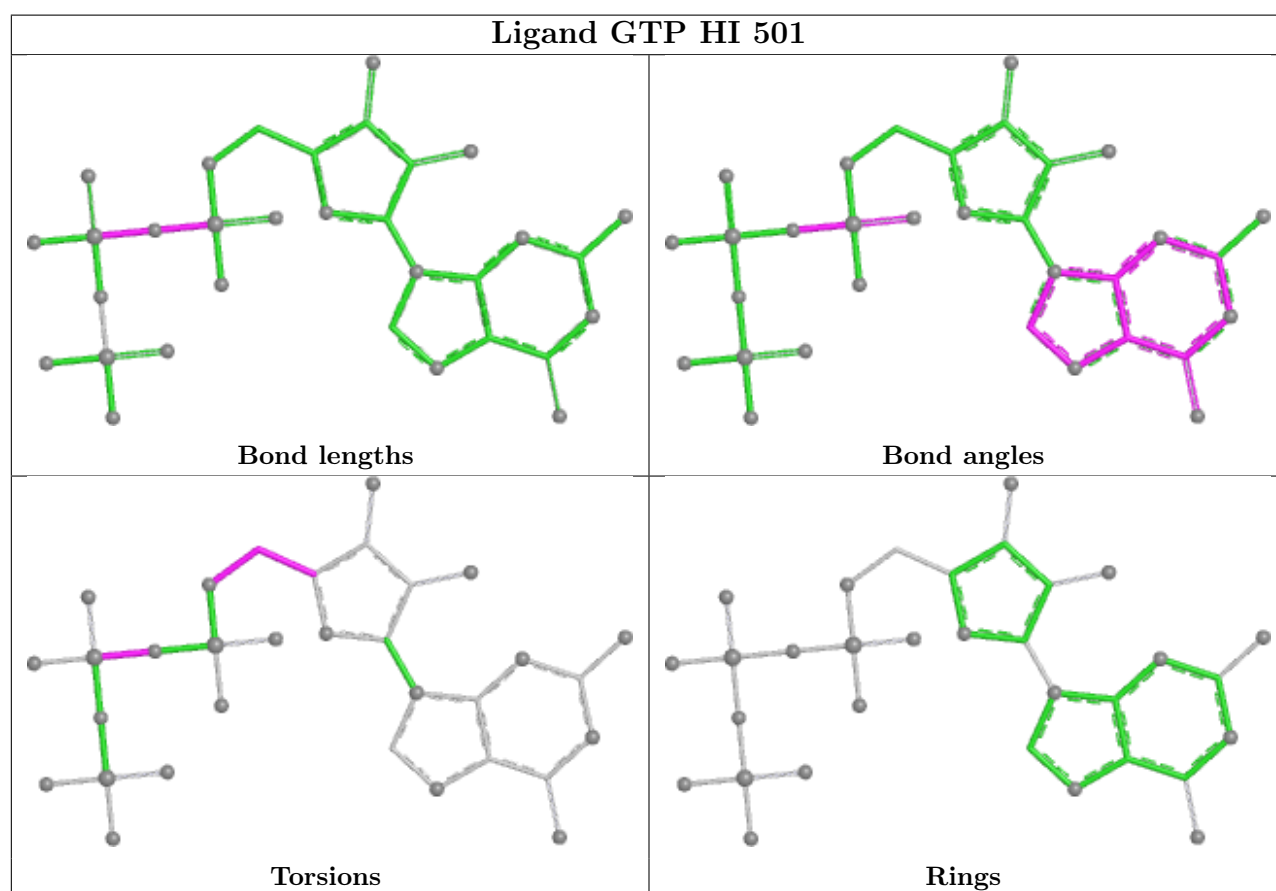
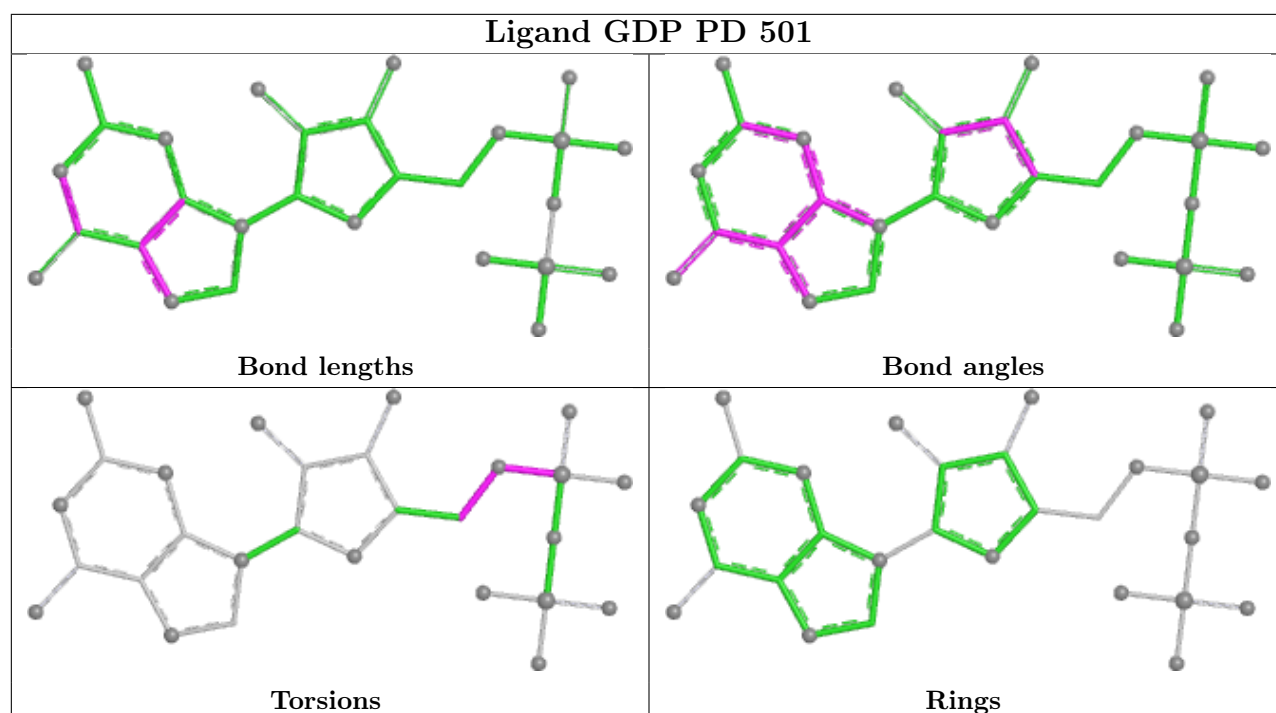


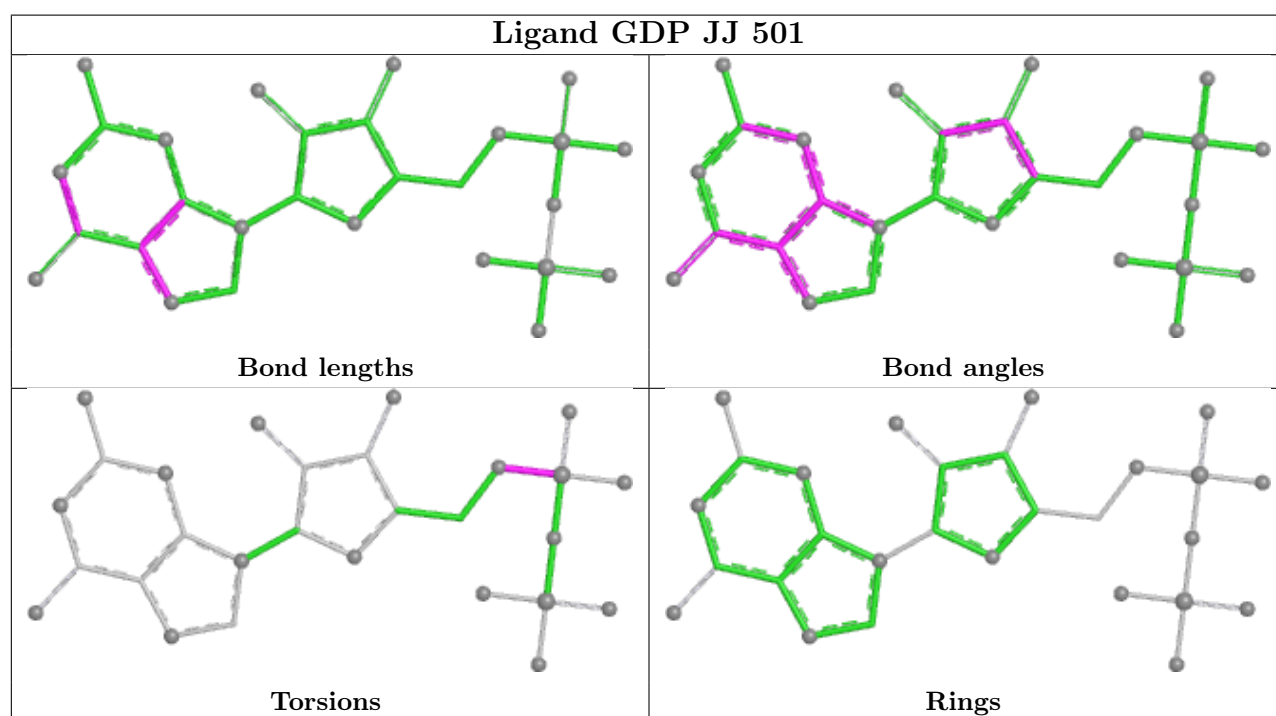
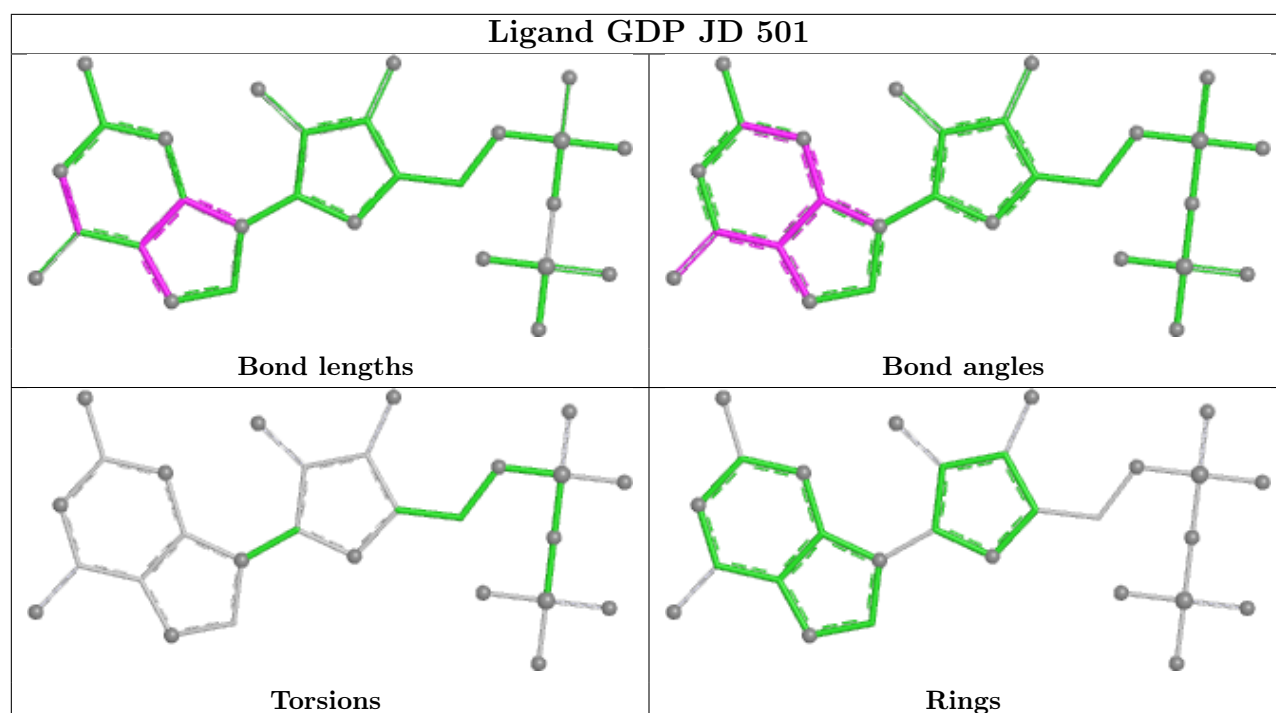




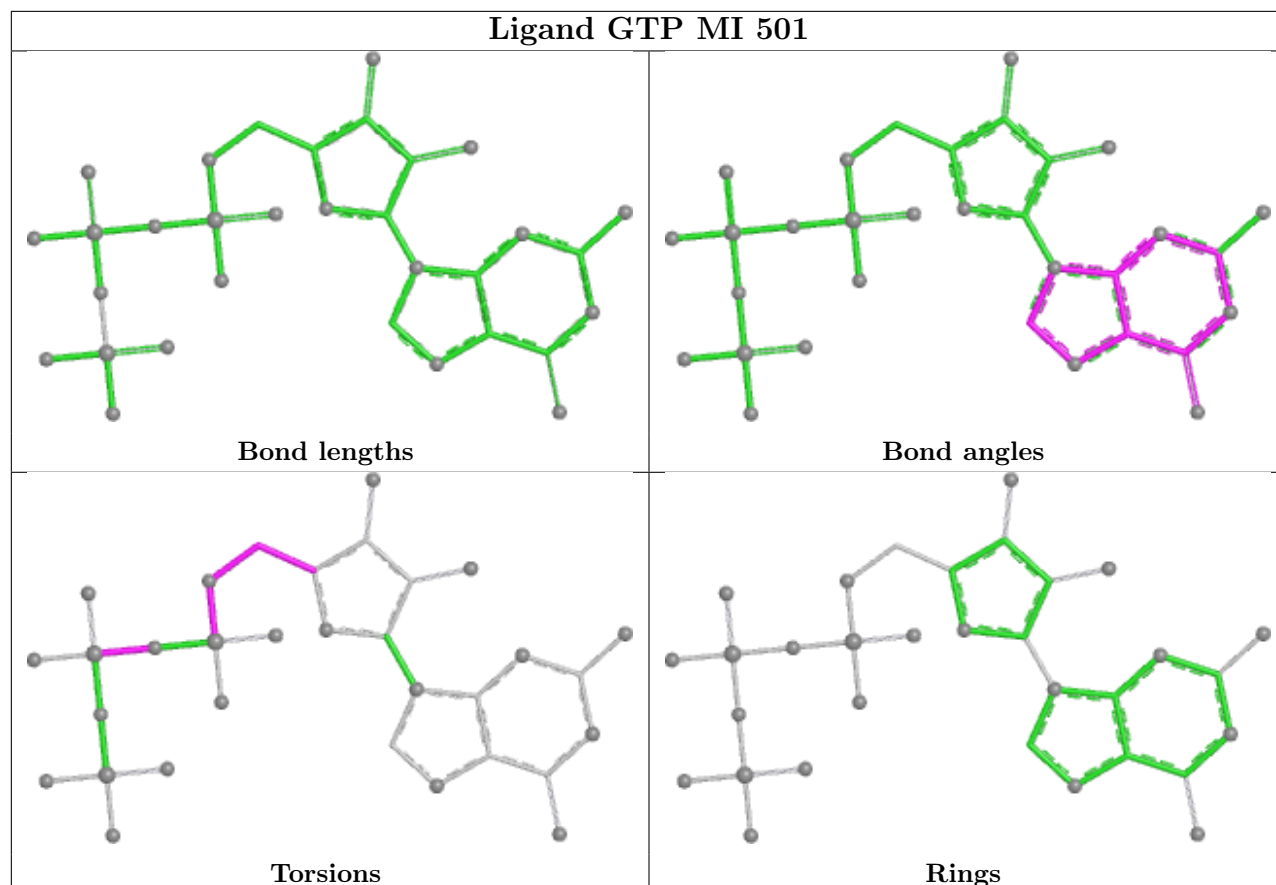




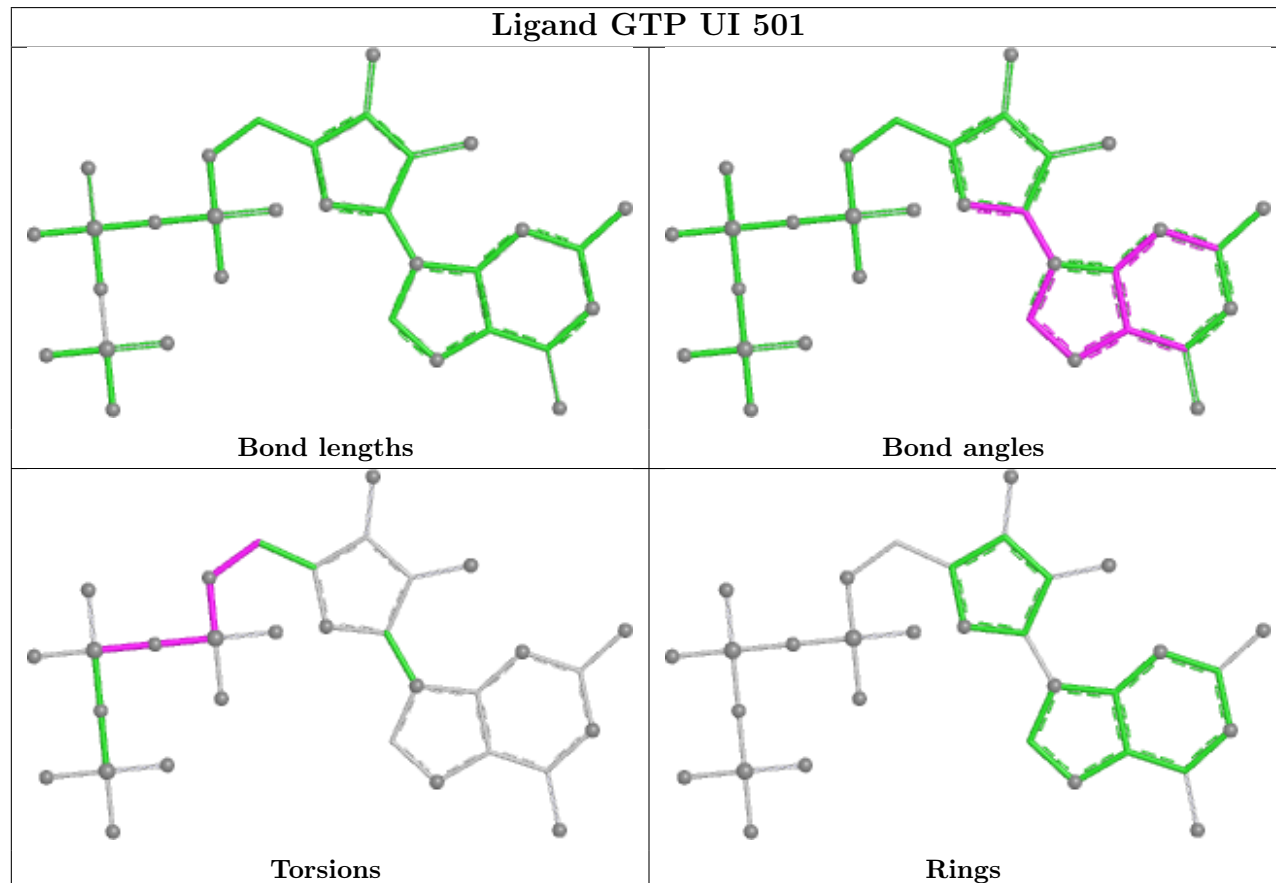




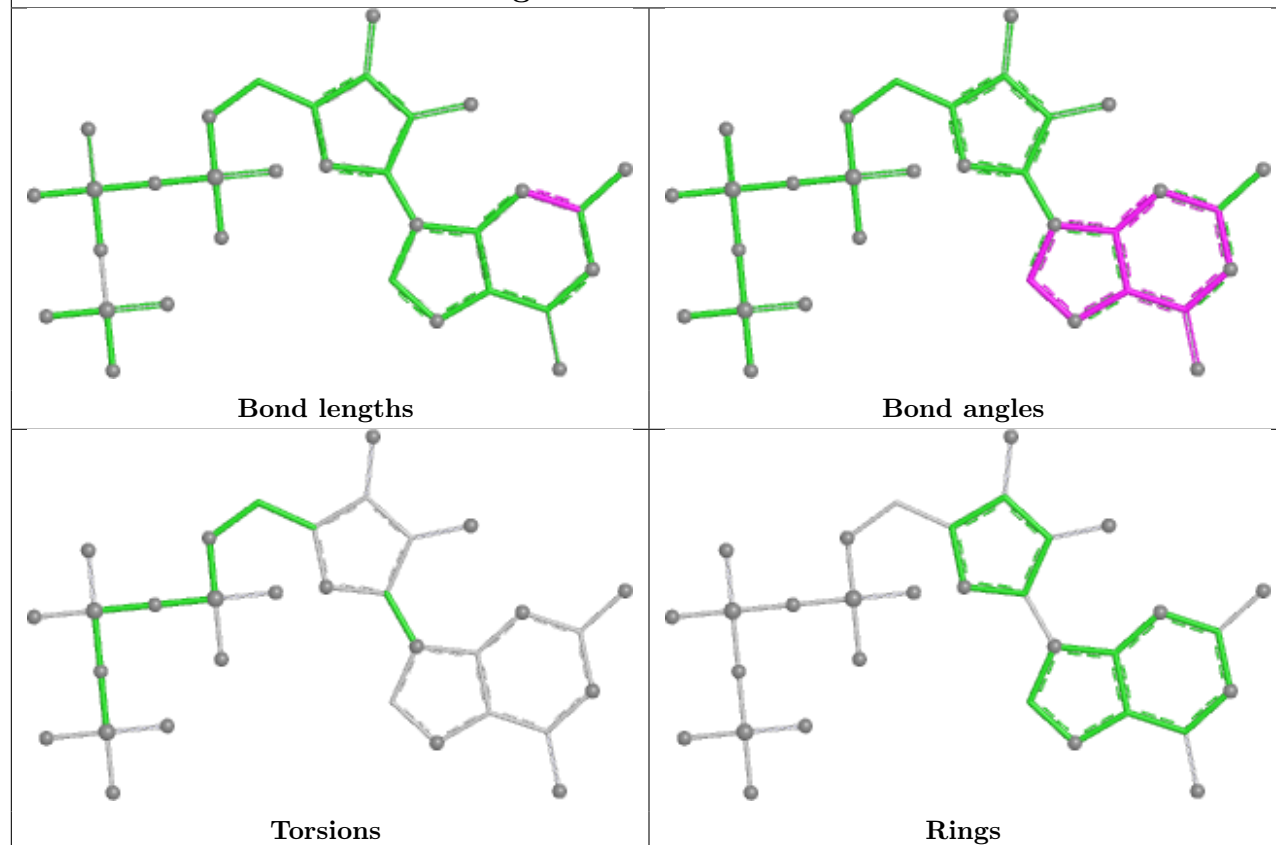
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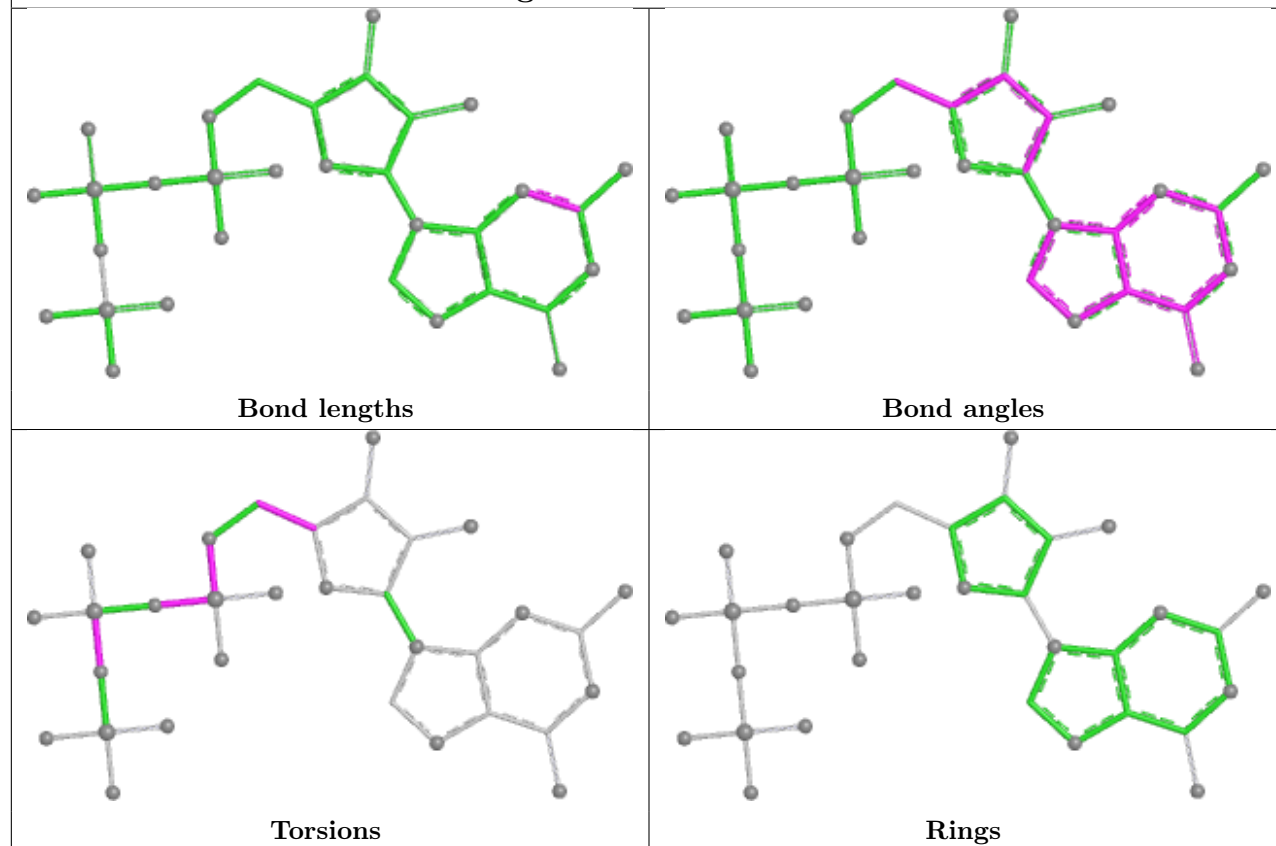
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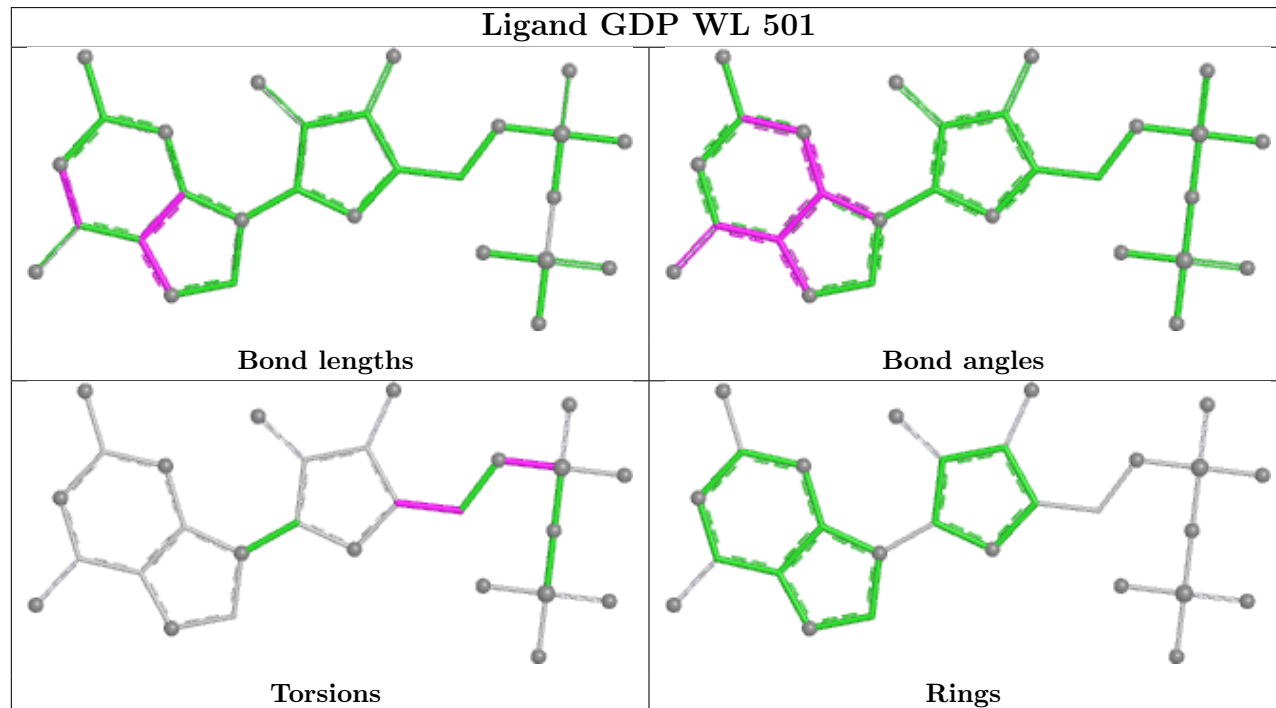
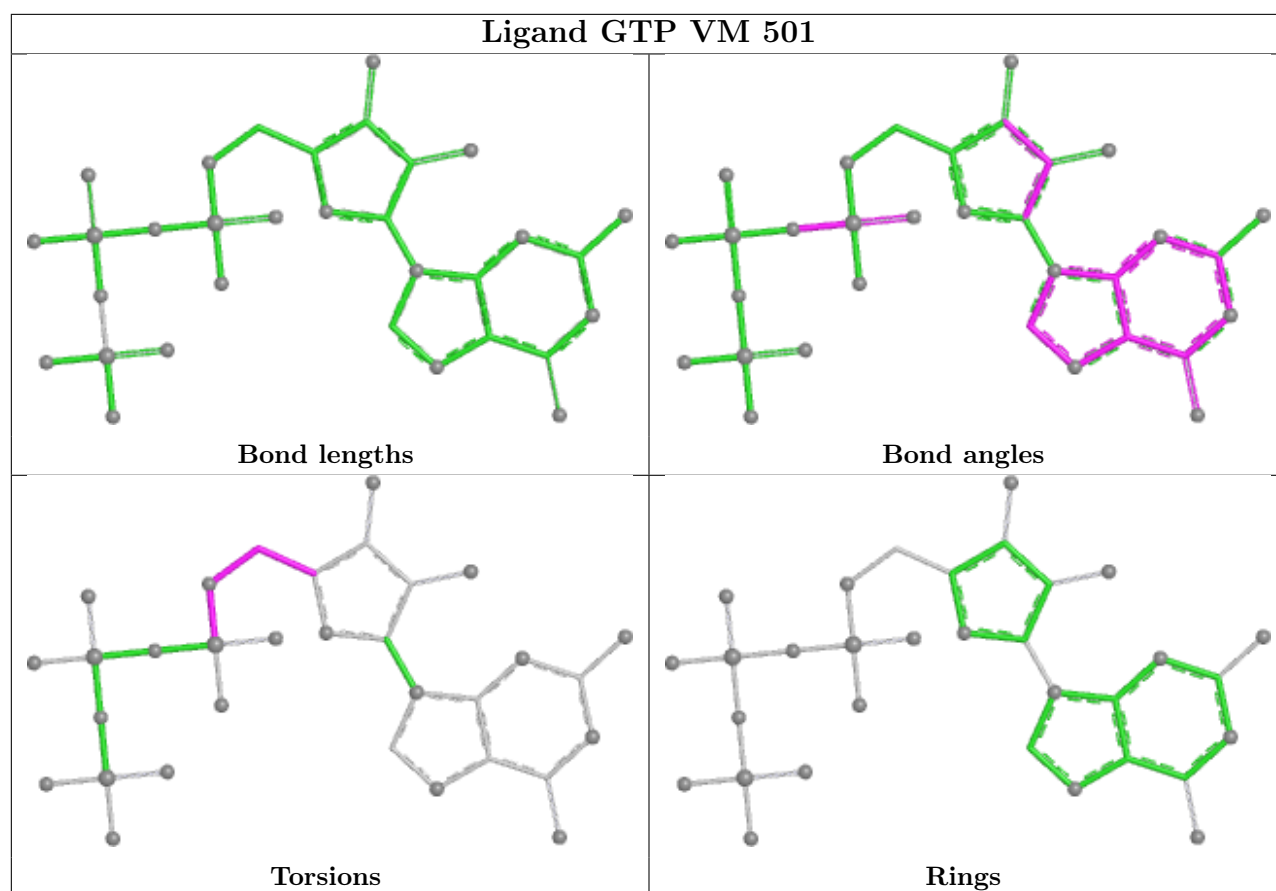


## Ligand GTP WC 501



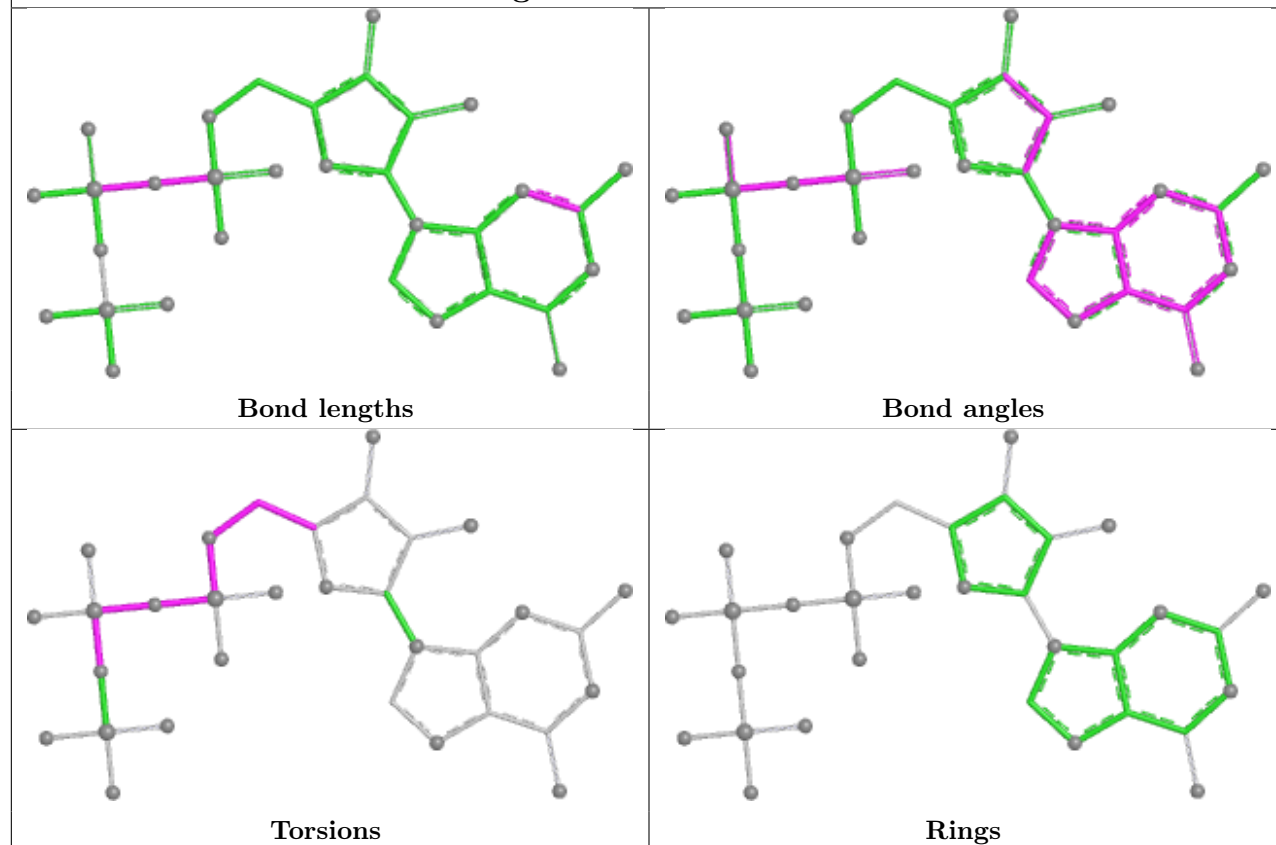
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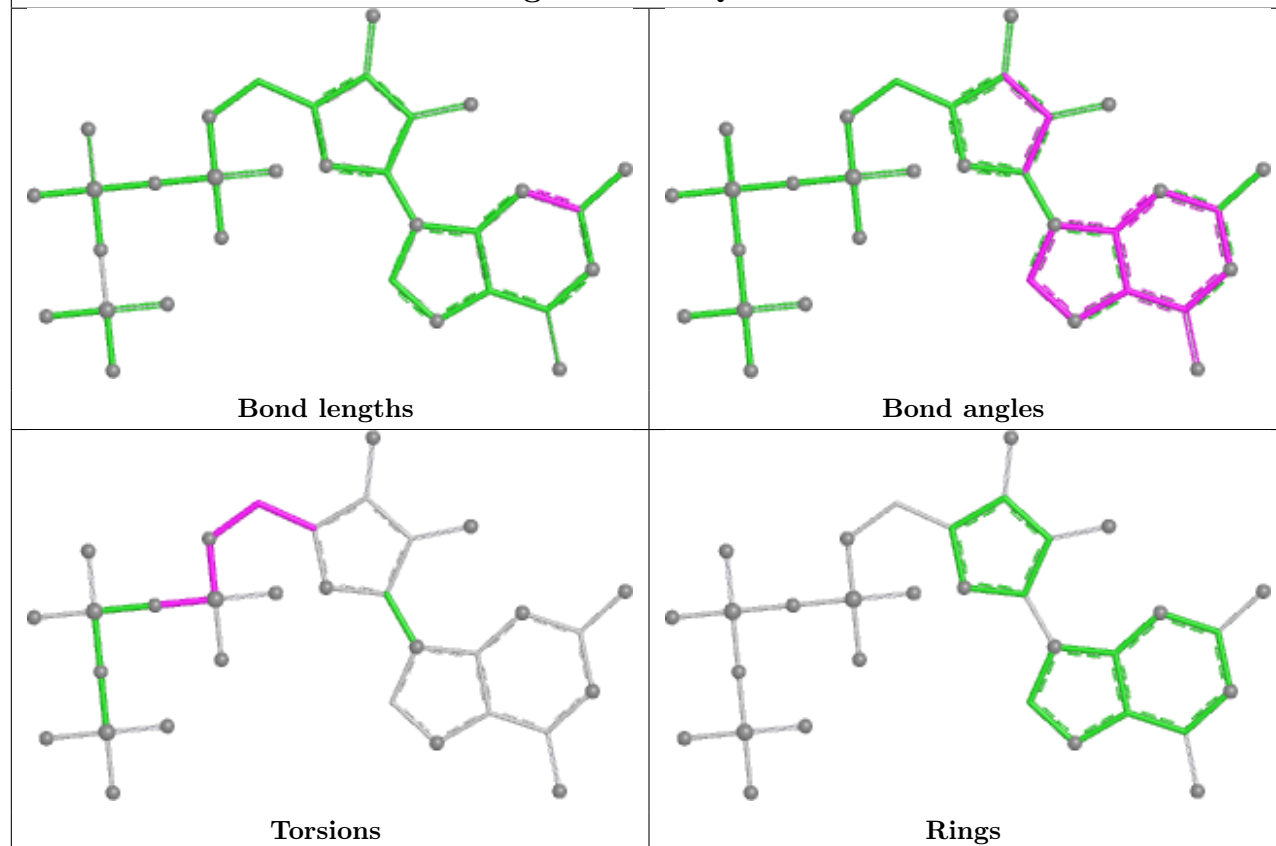


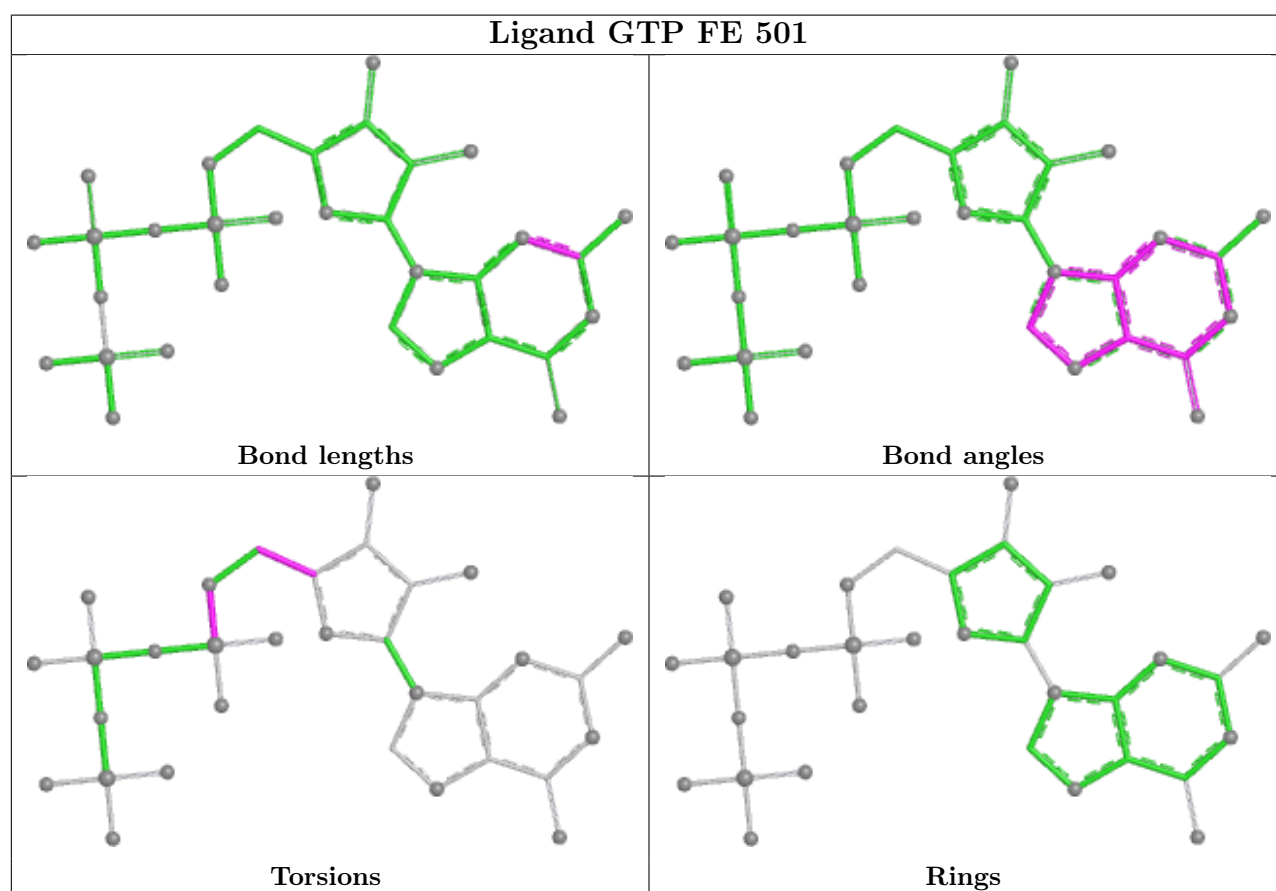
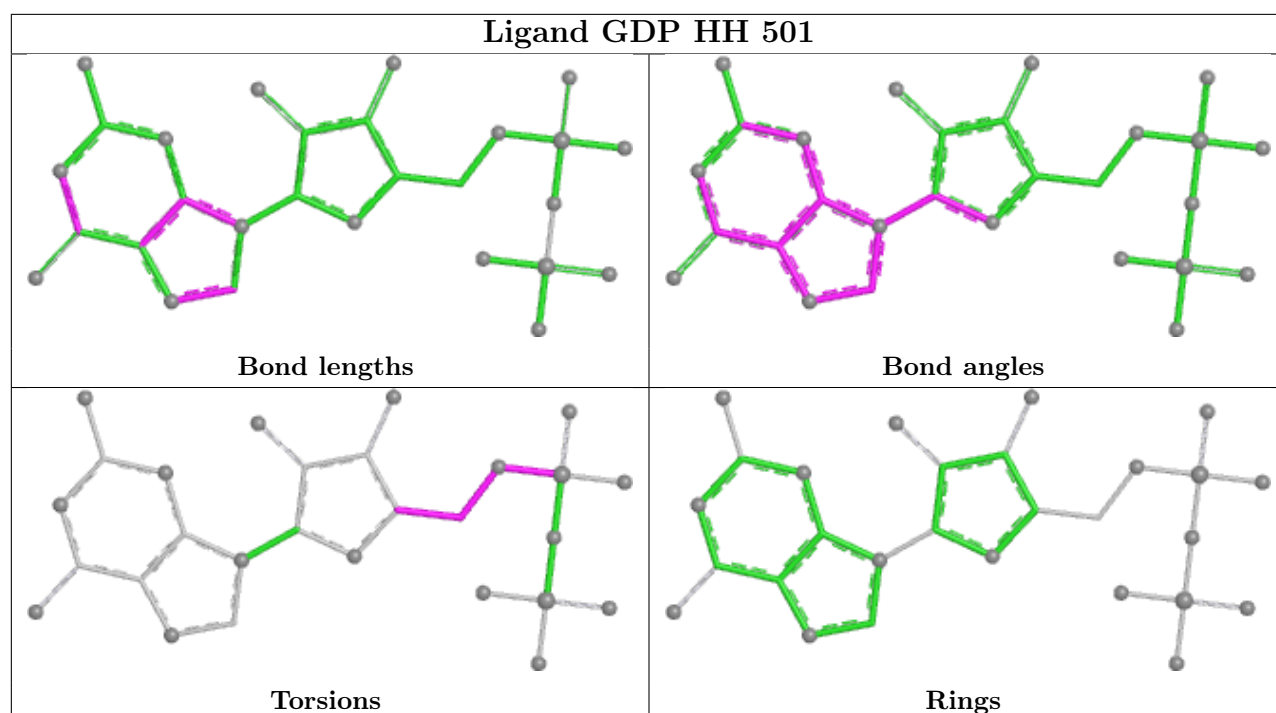


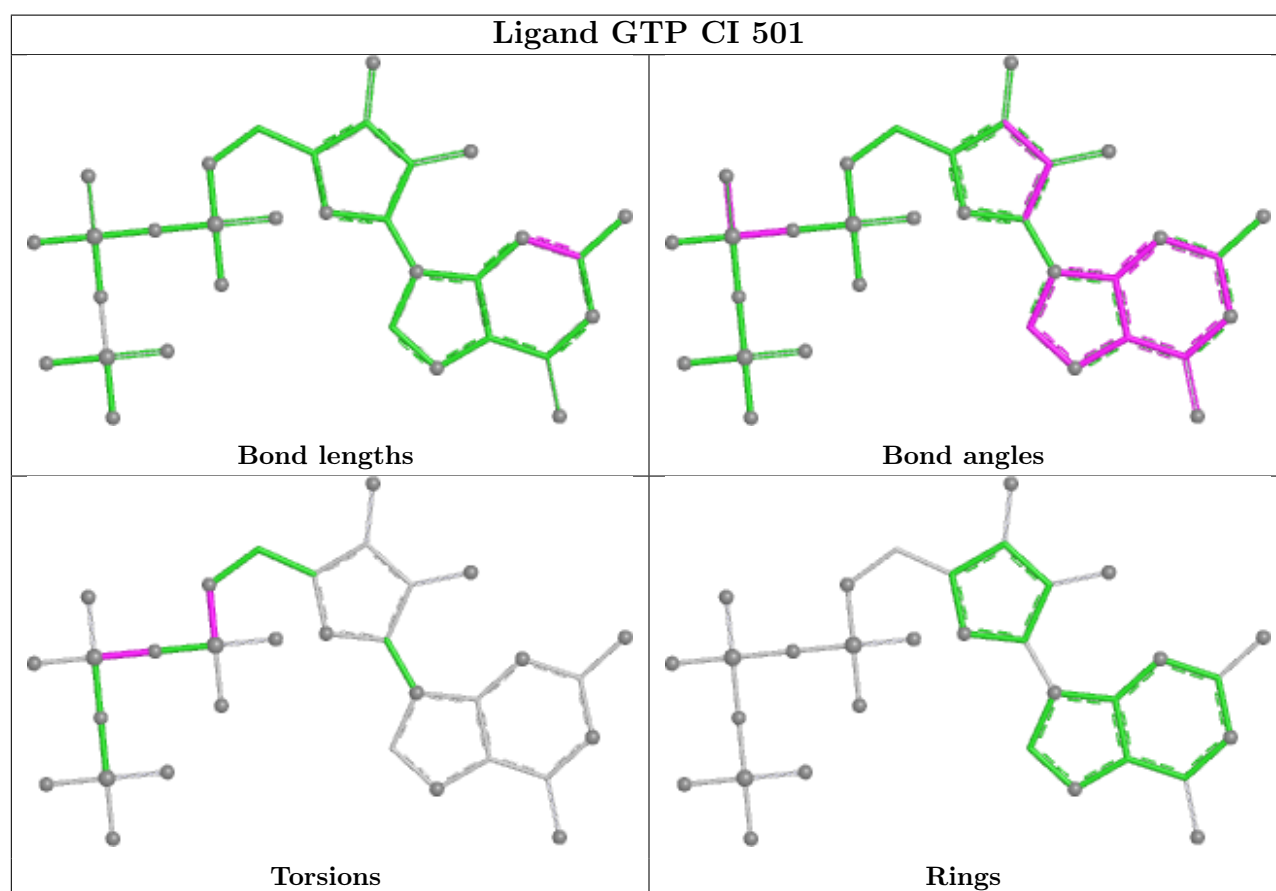
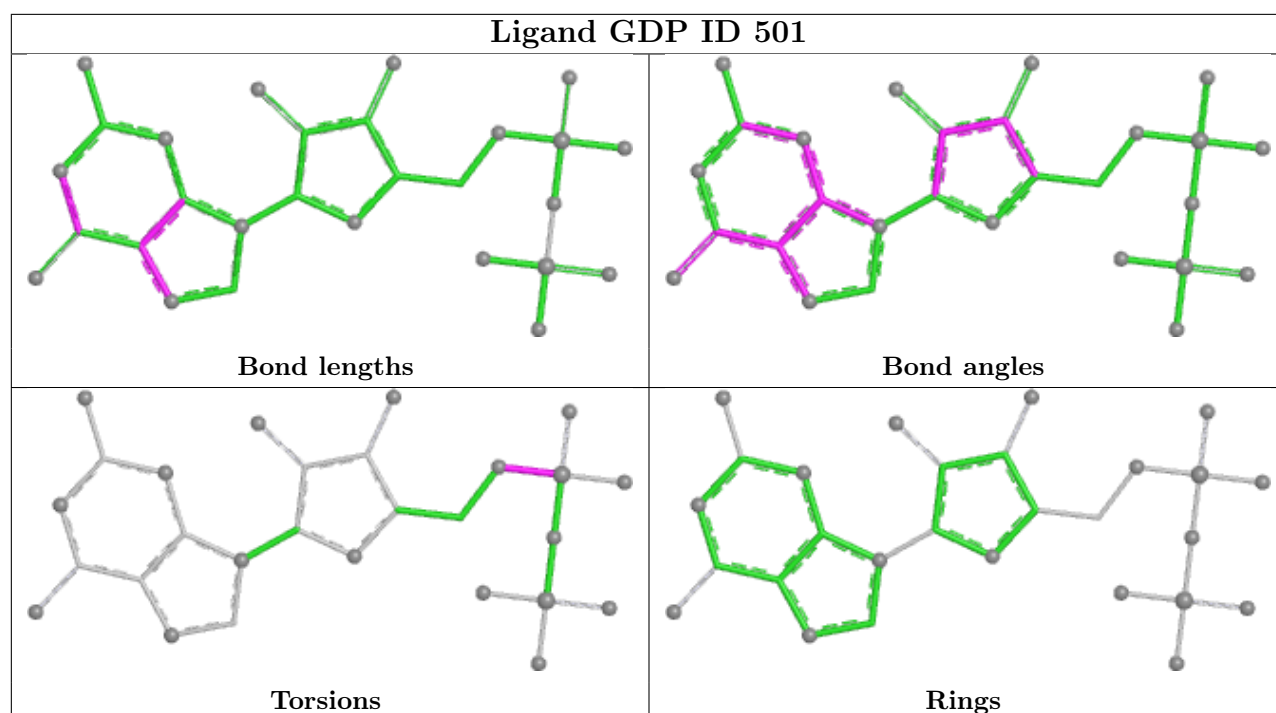
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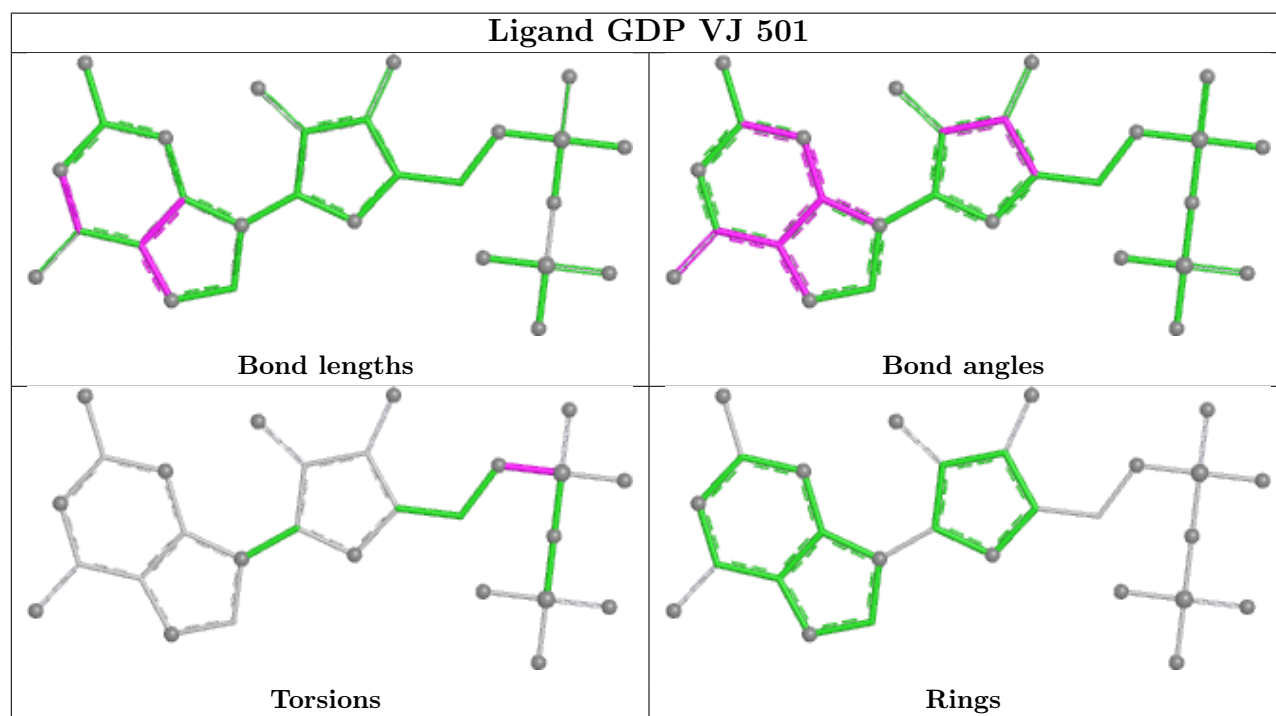
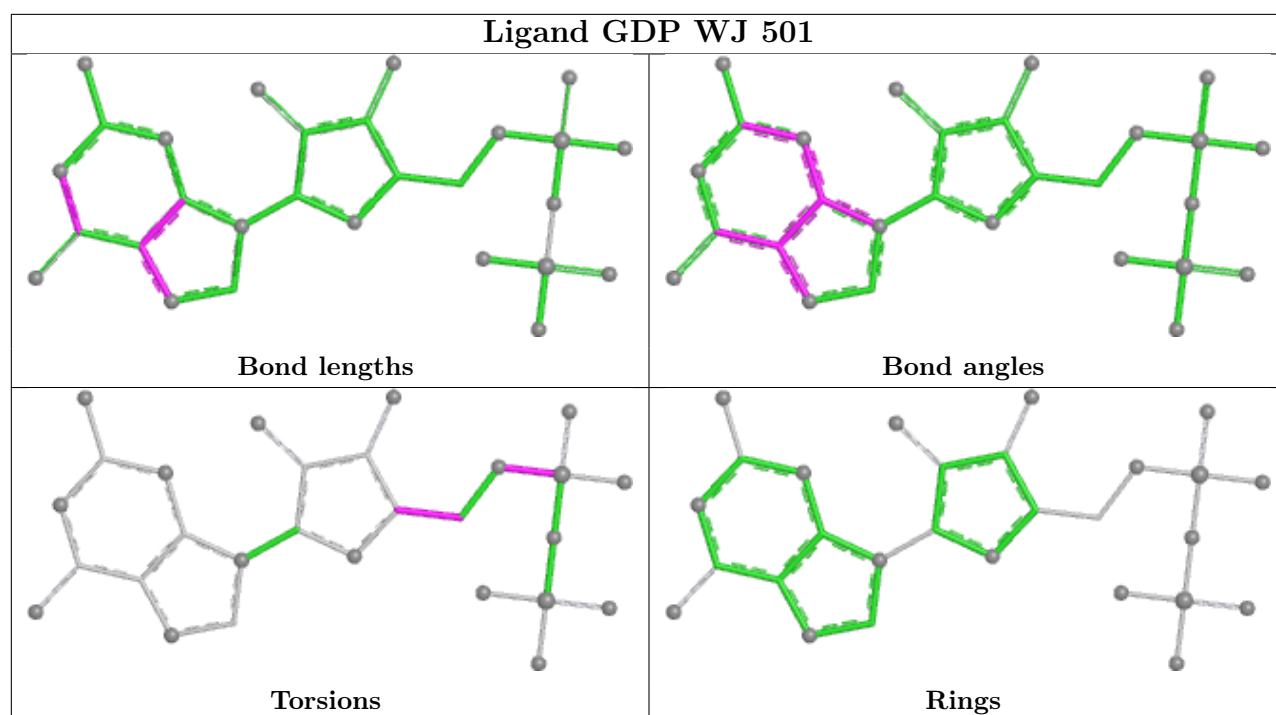


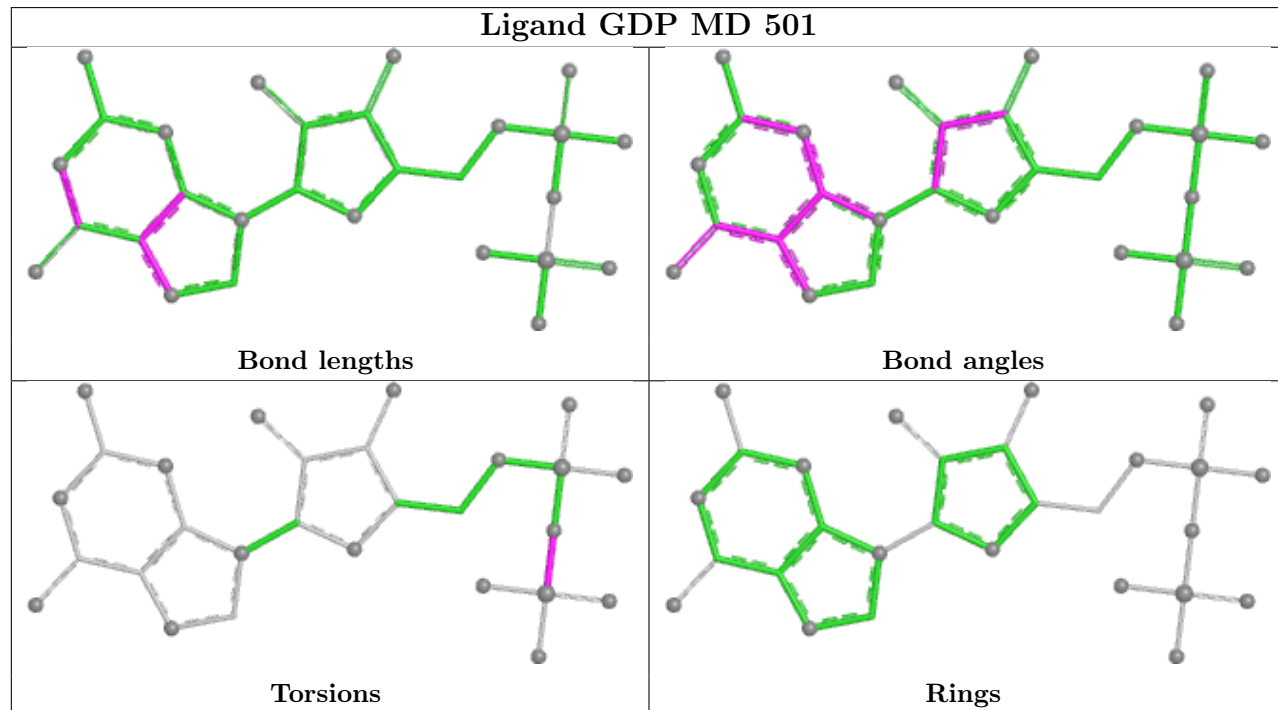
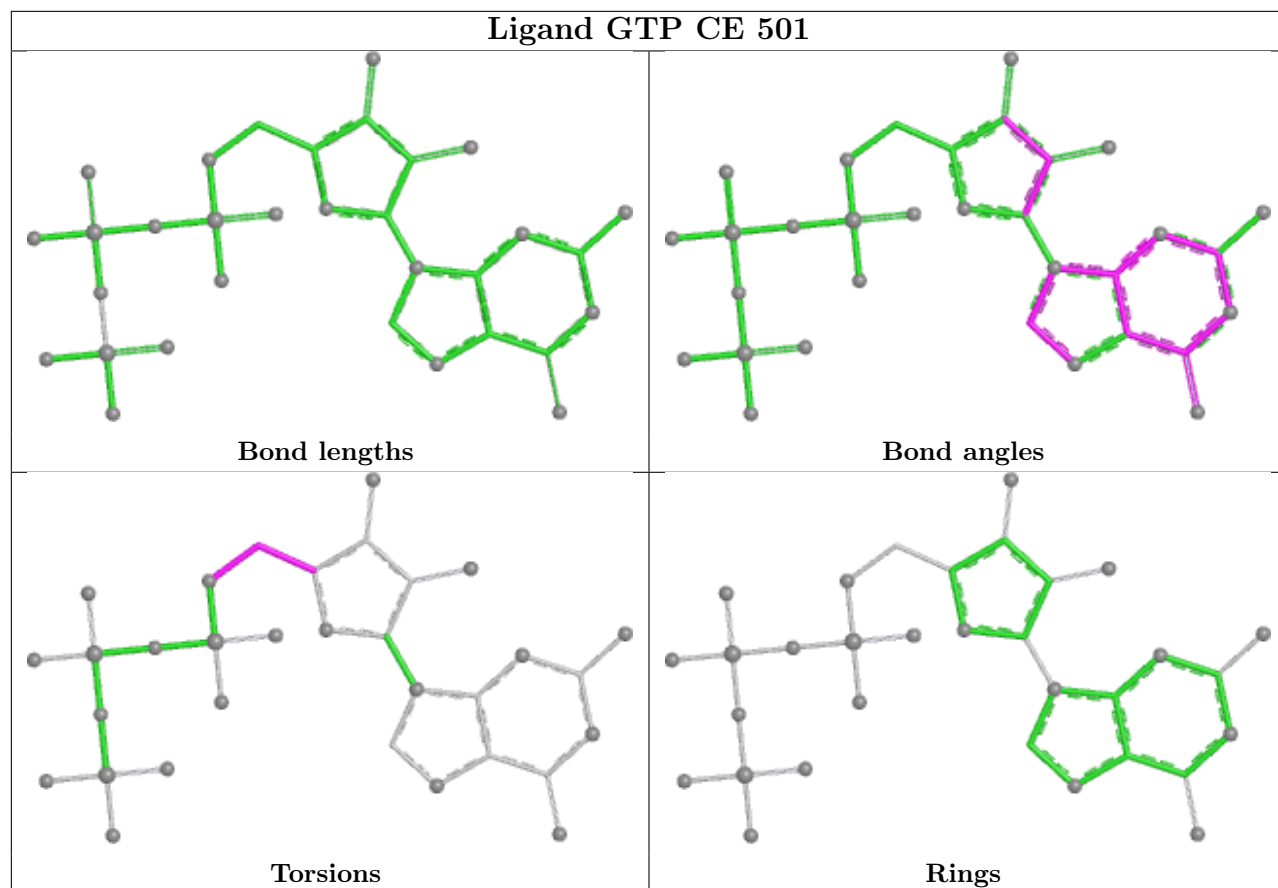
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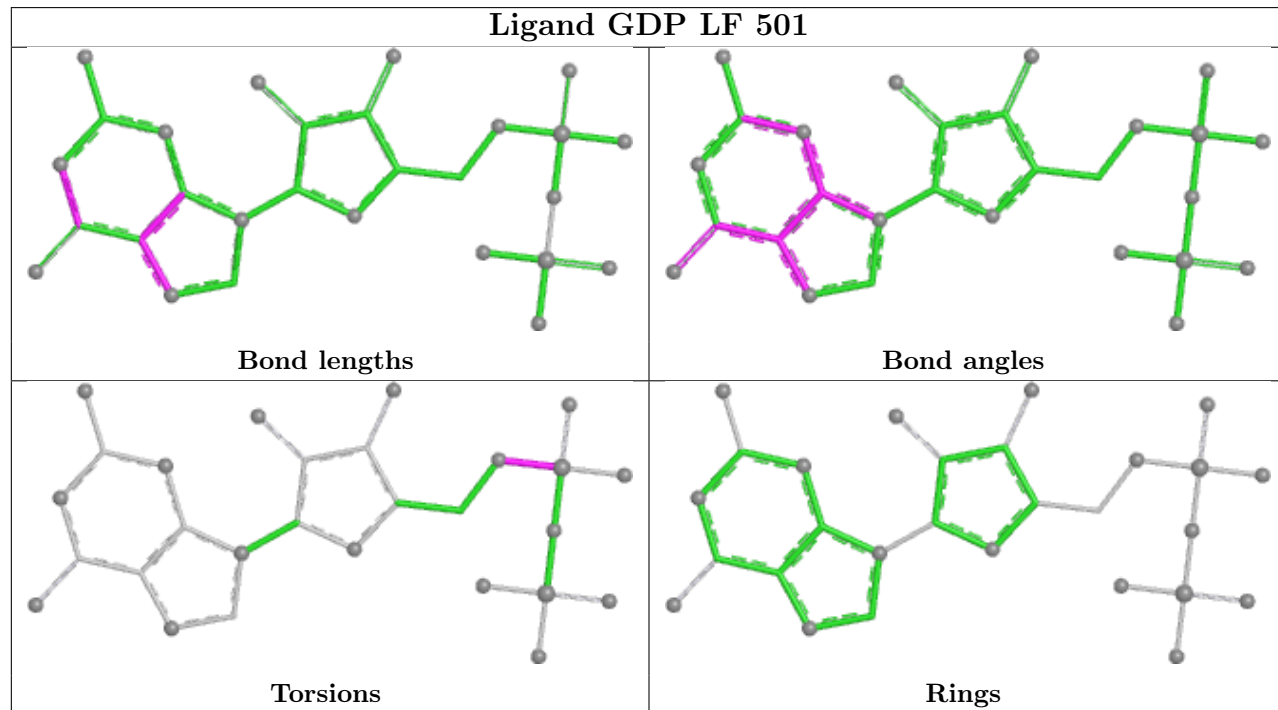
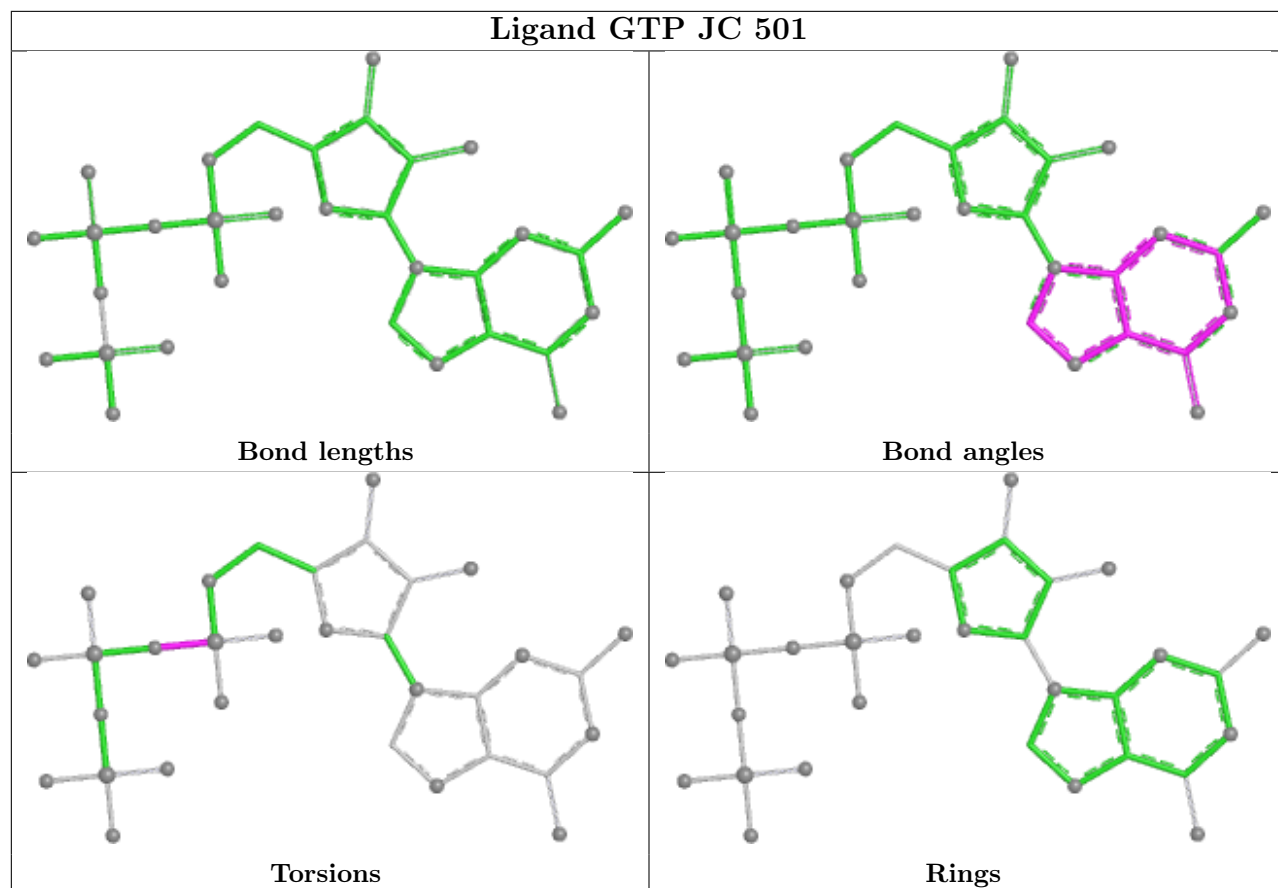


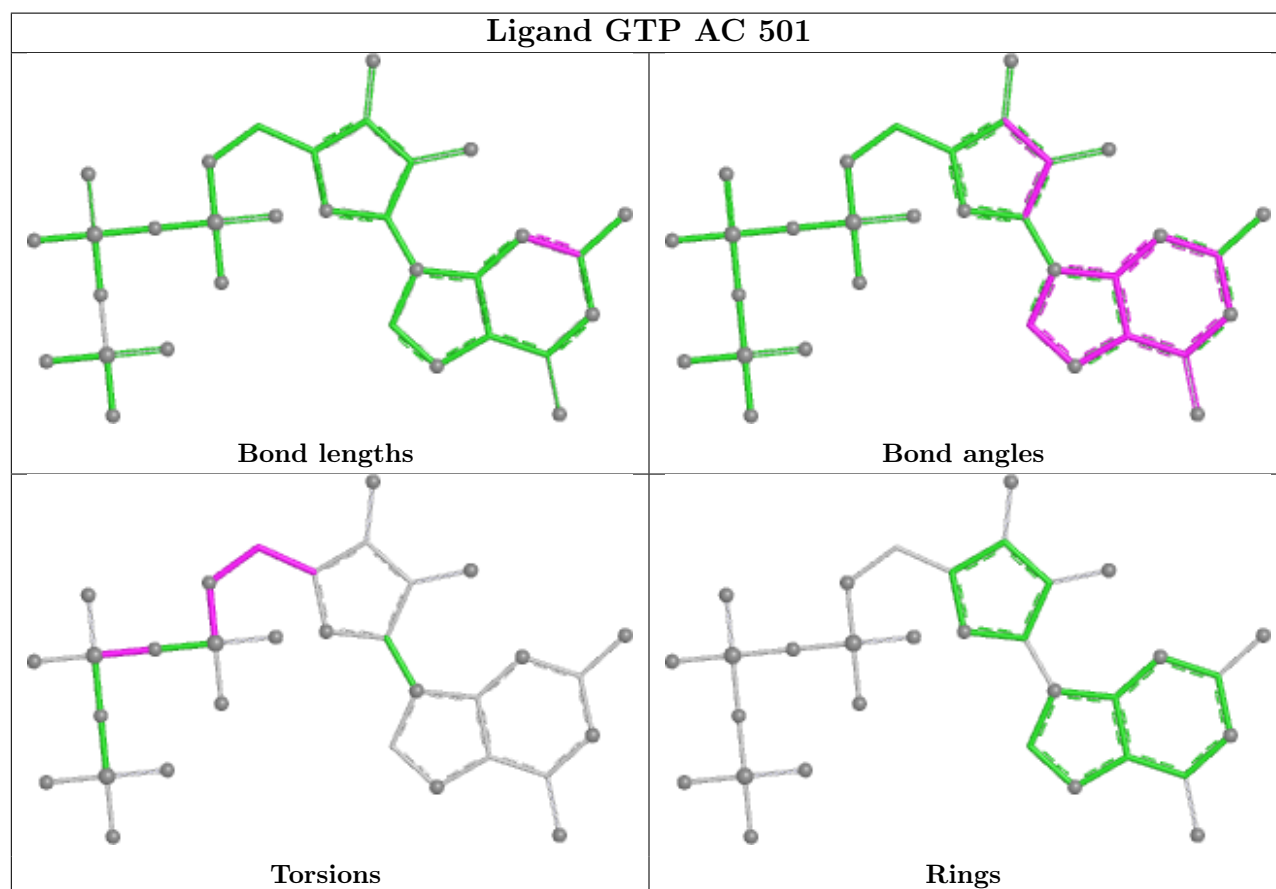
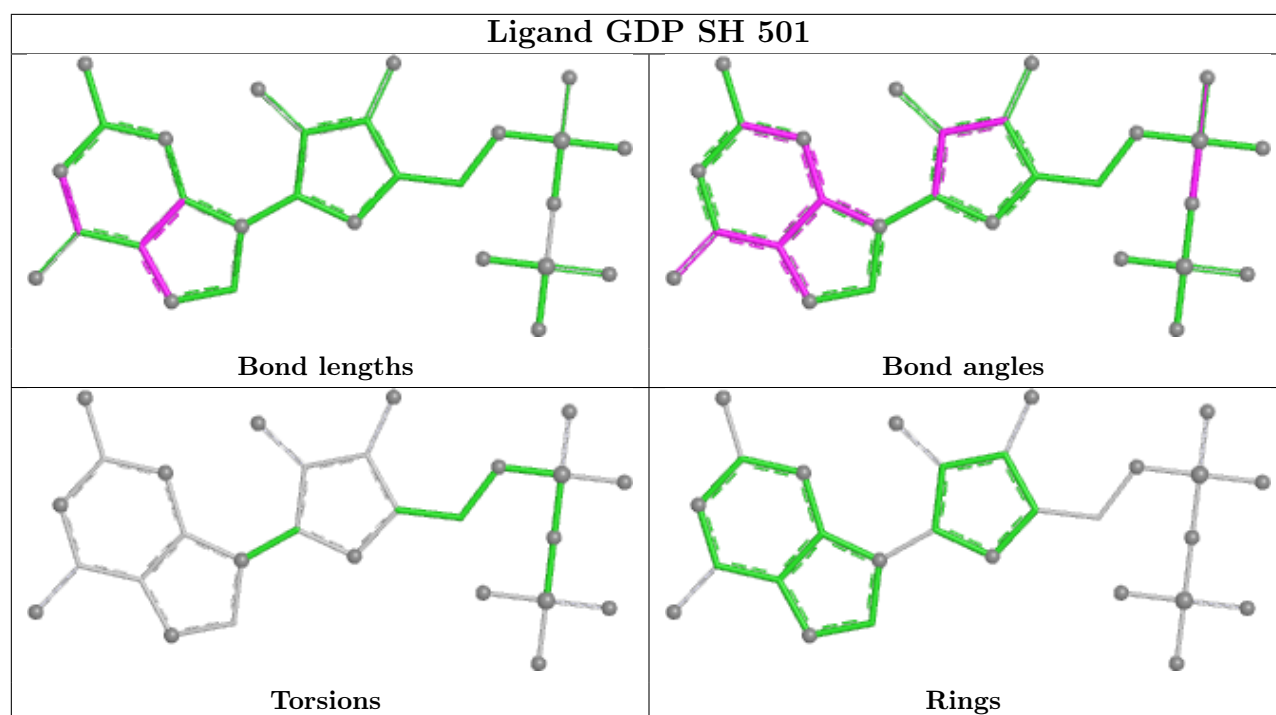


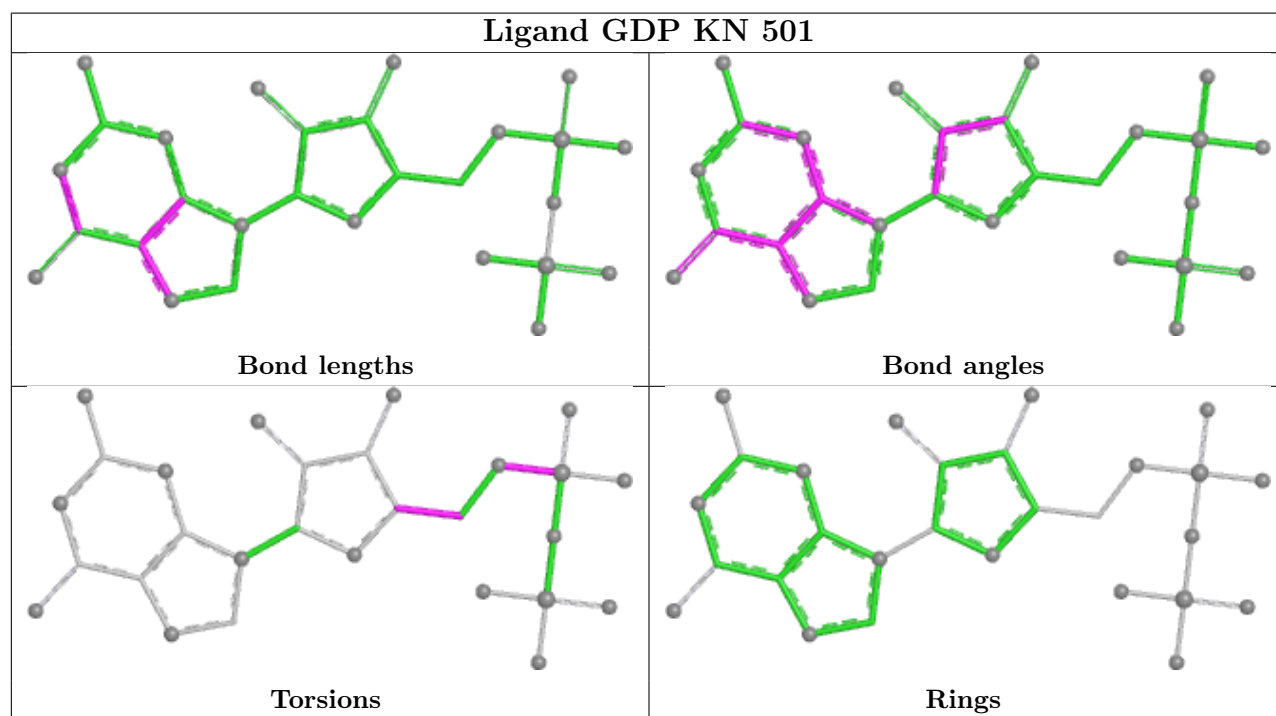
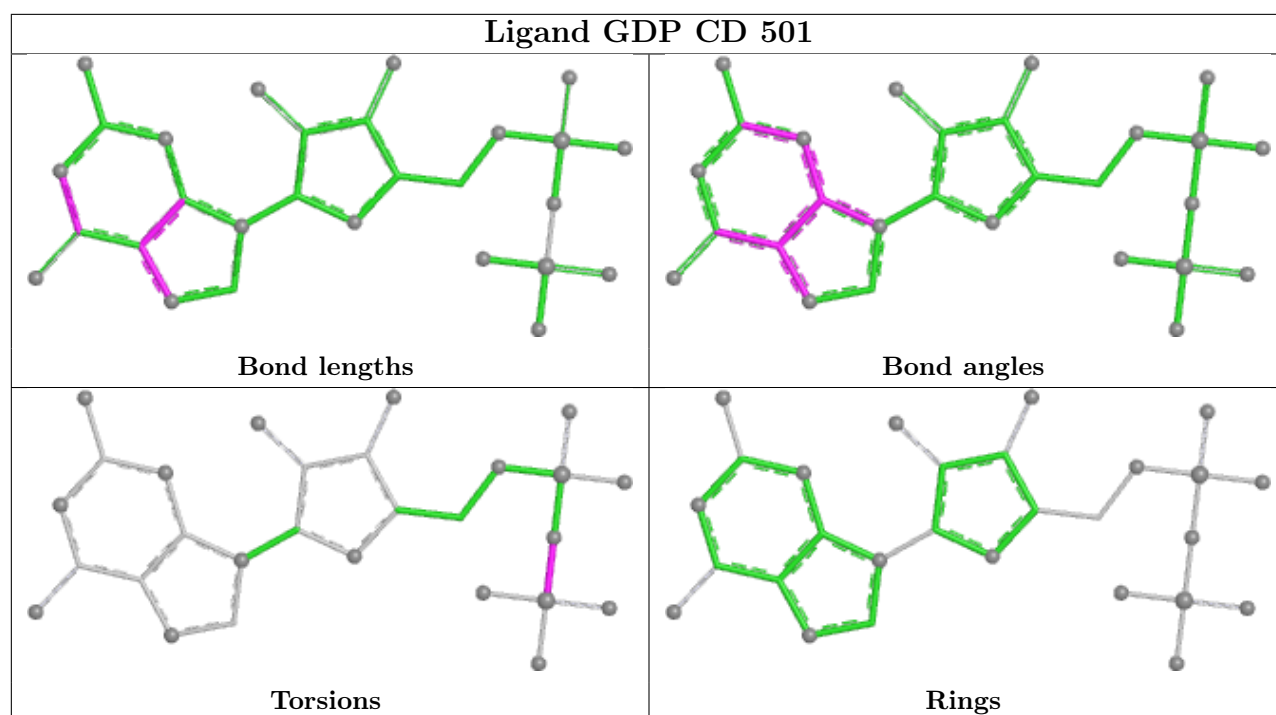




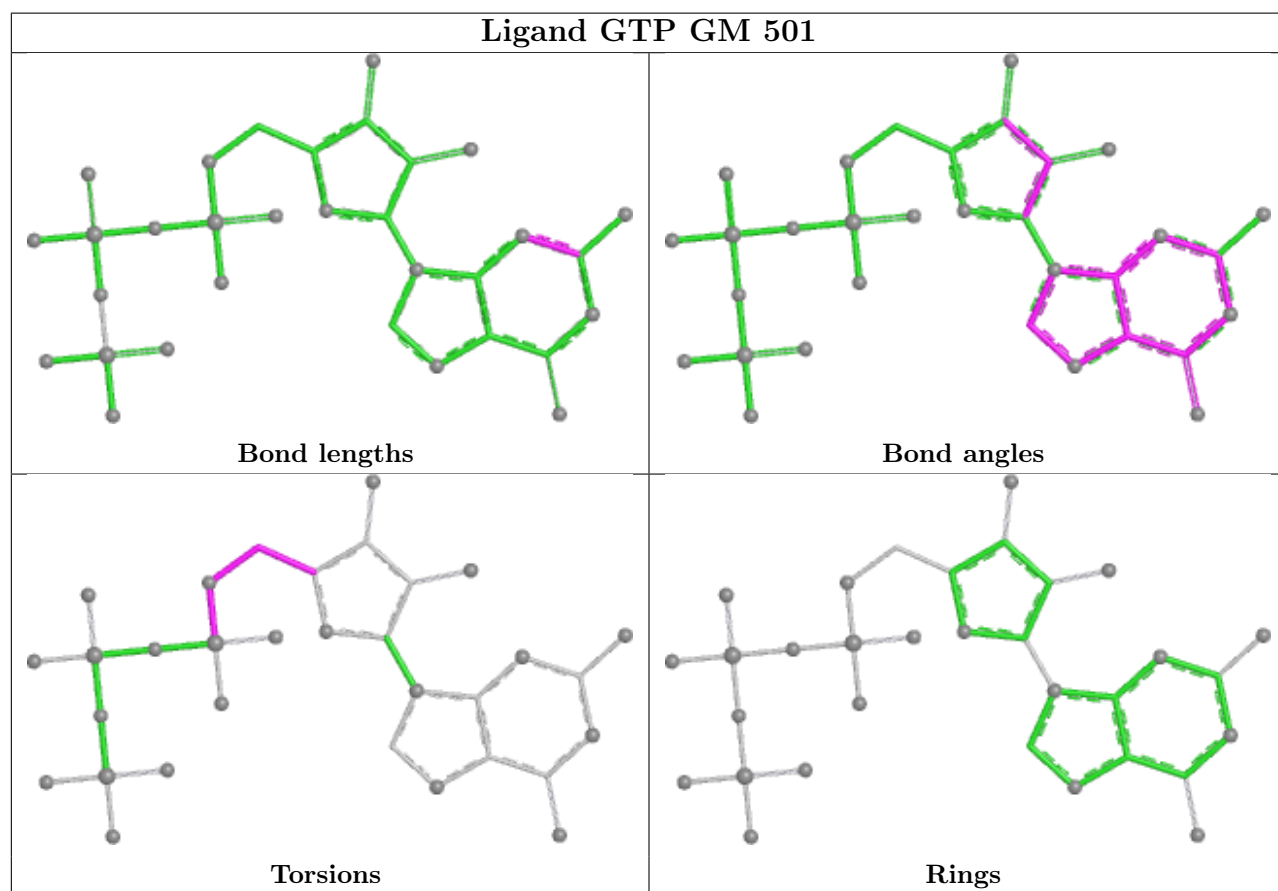
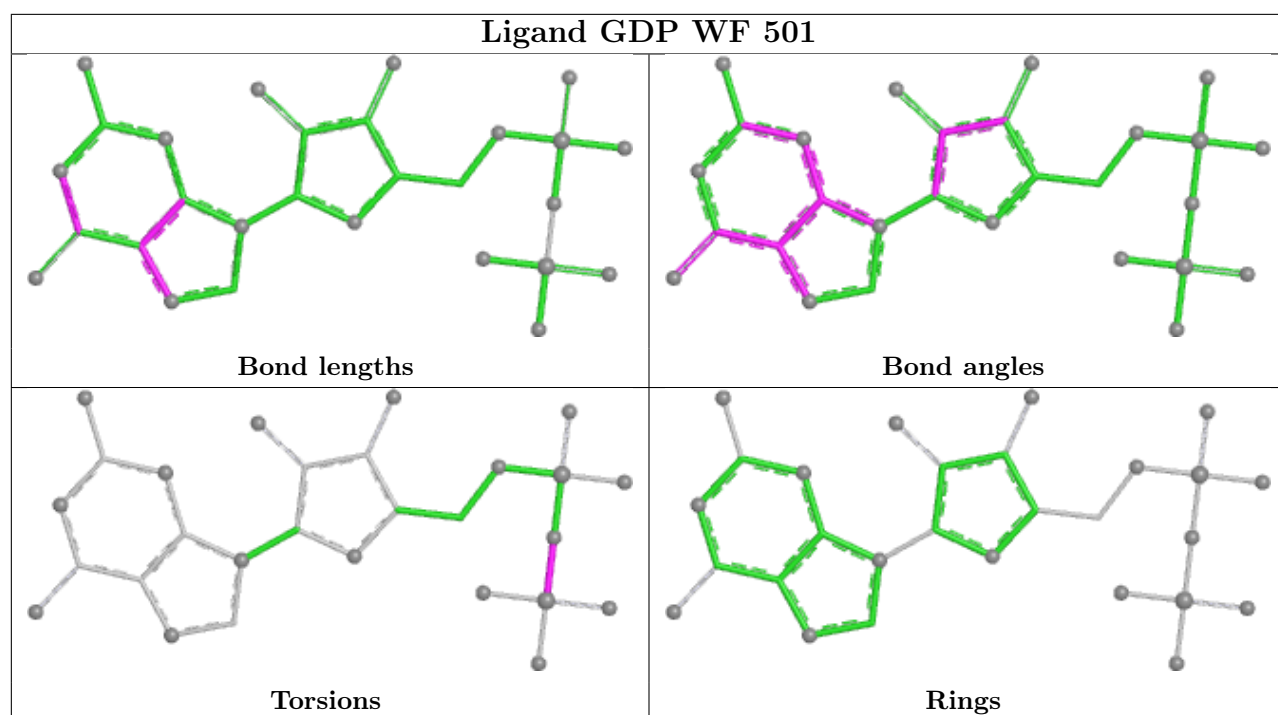




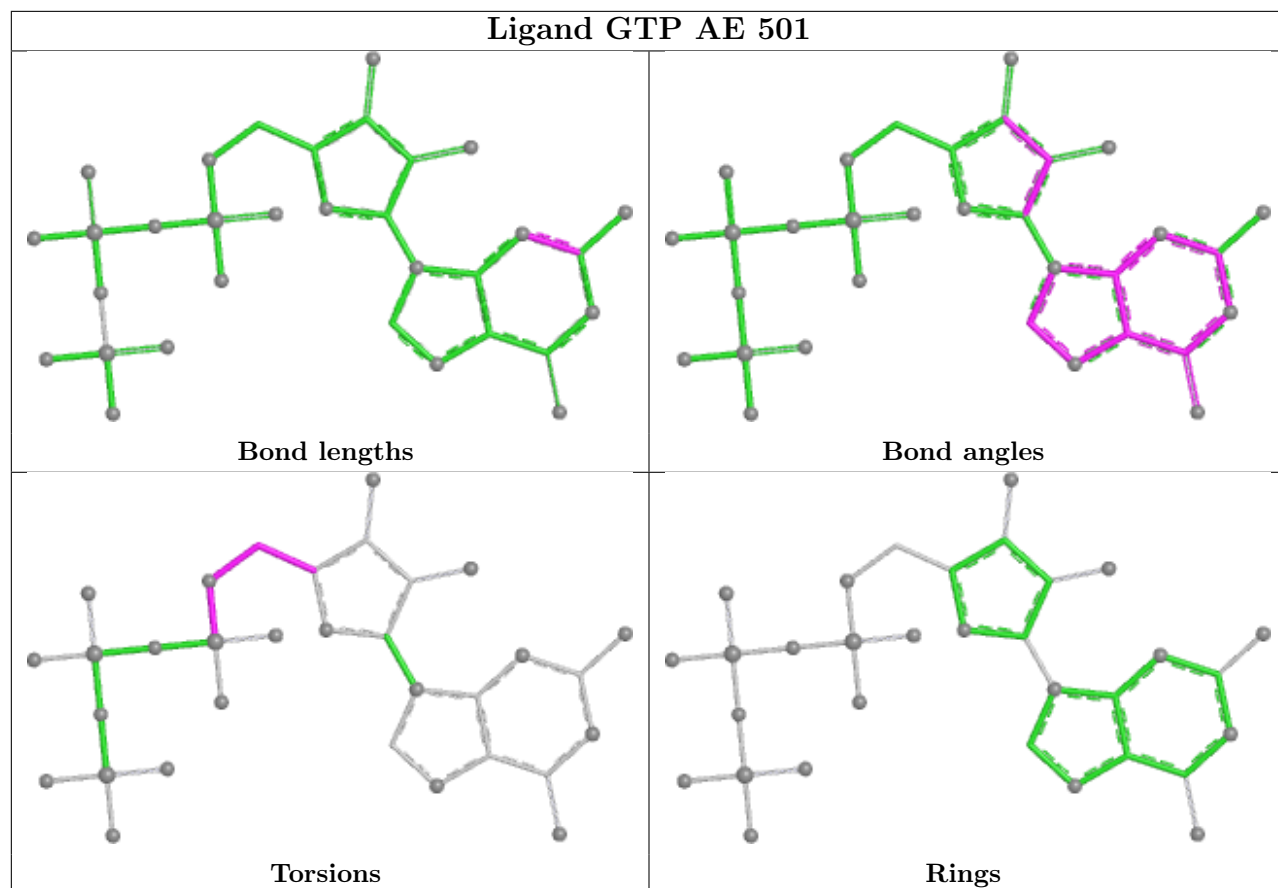




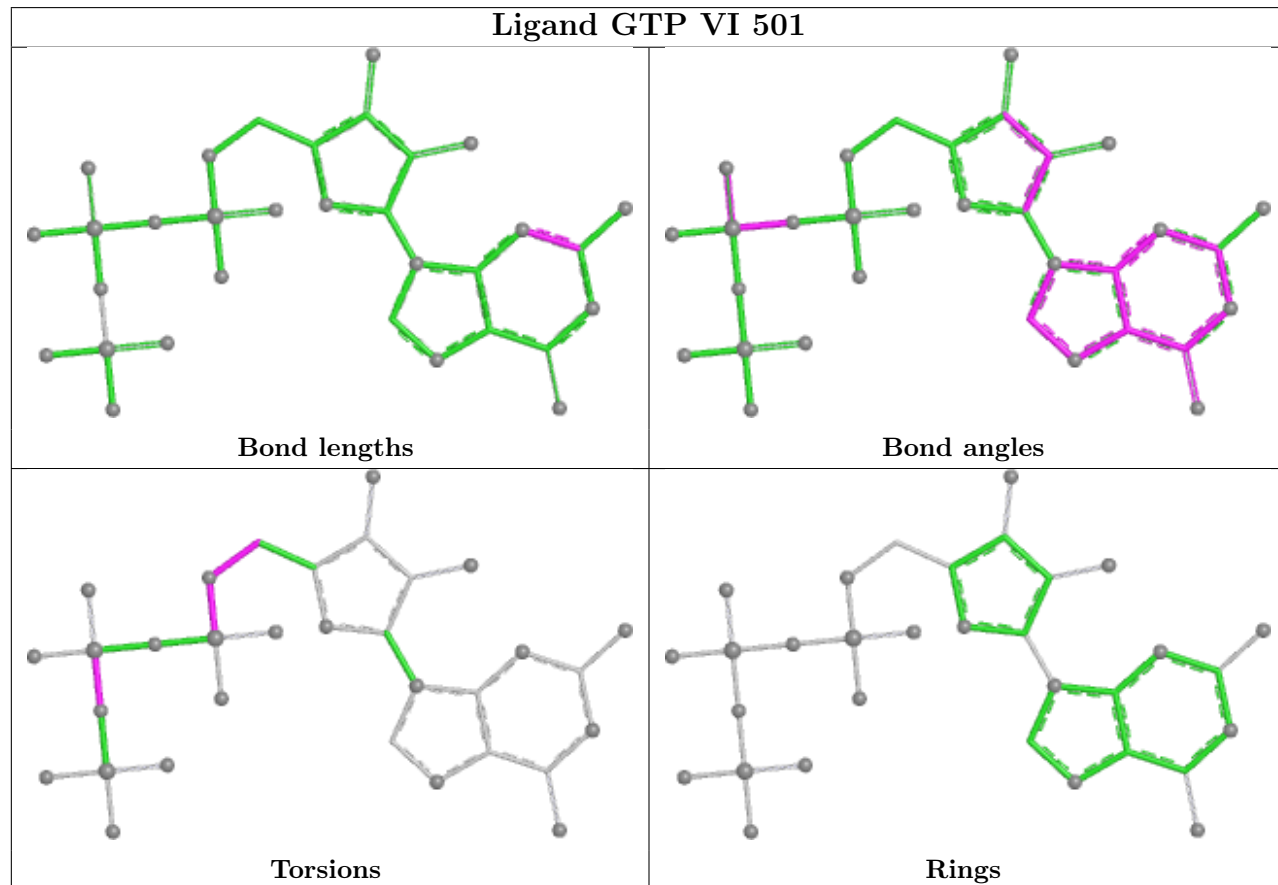


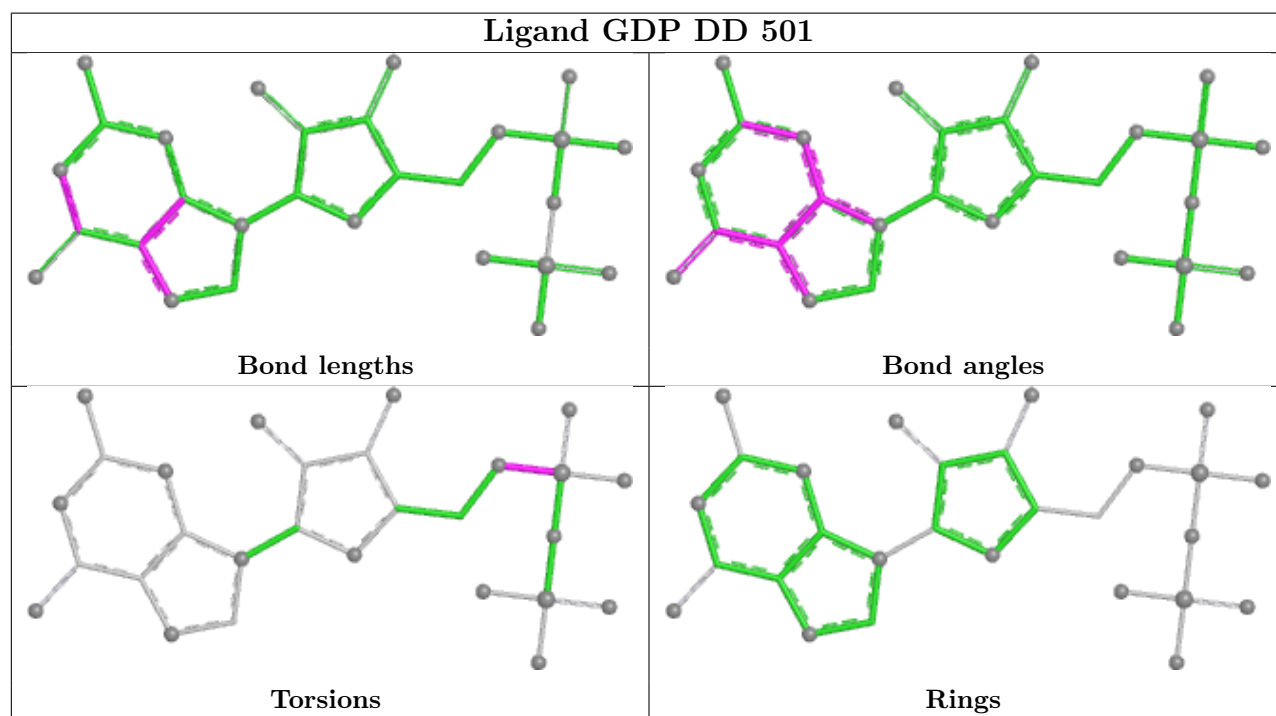
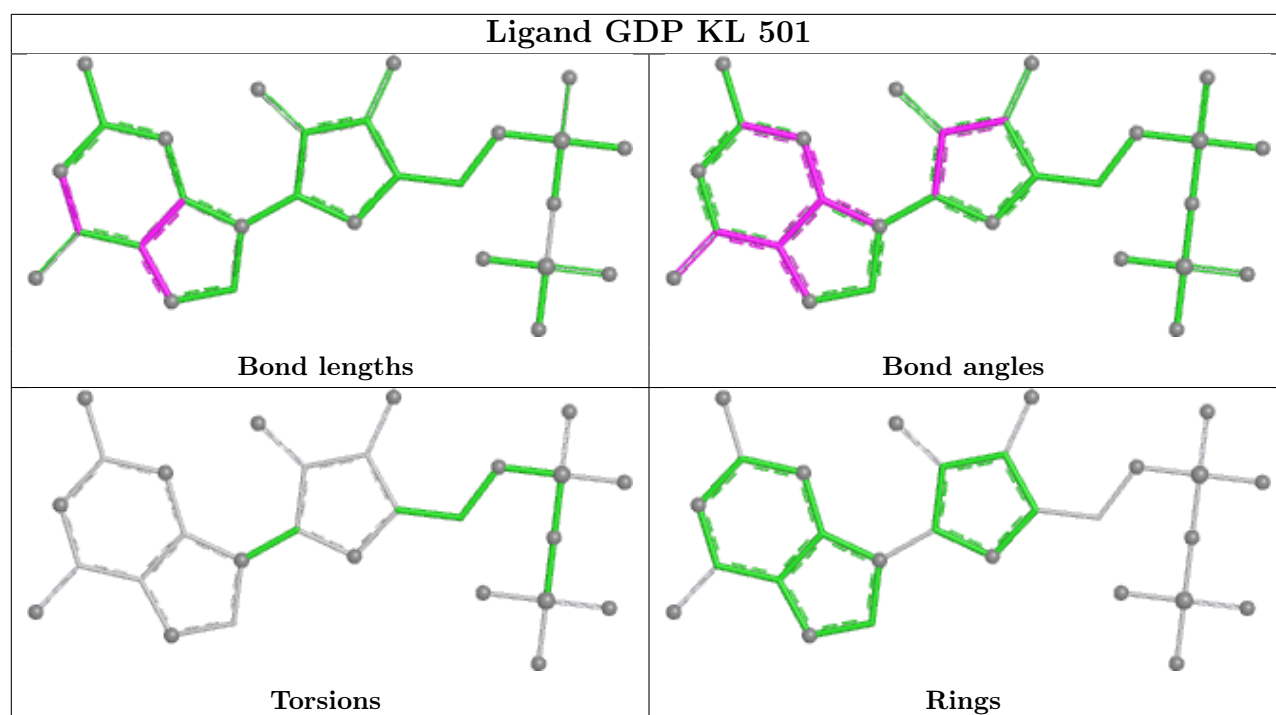


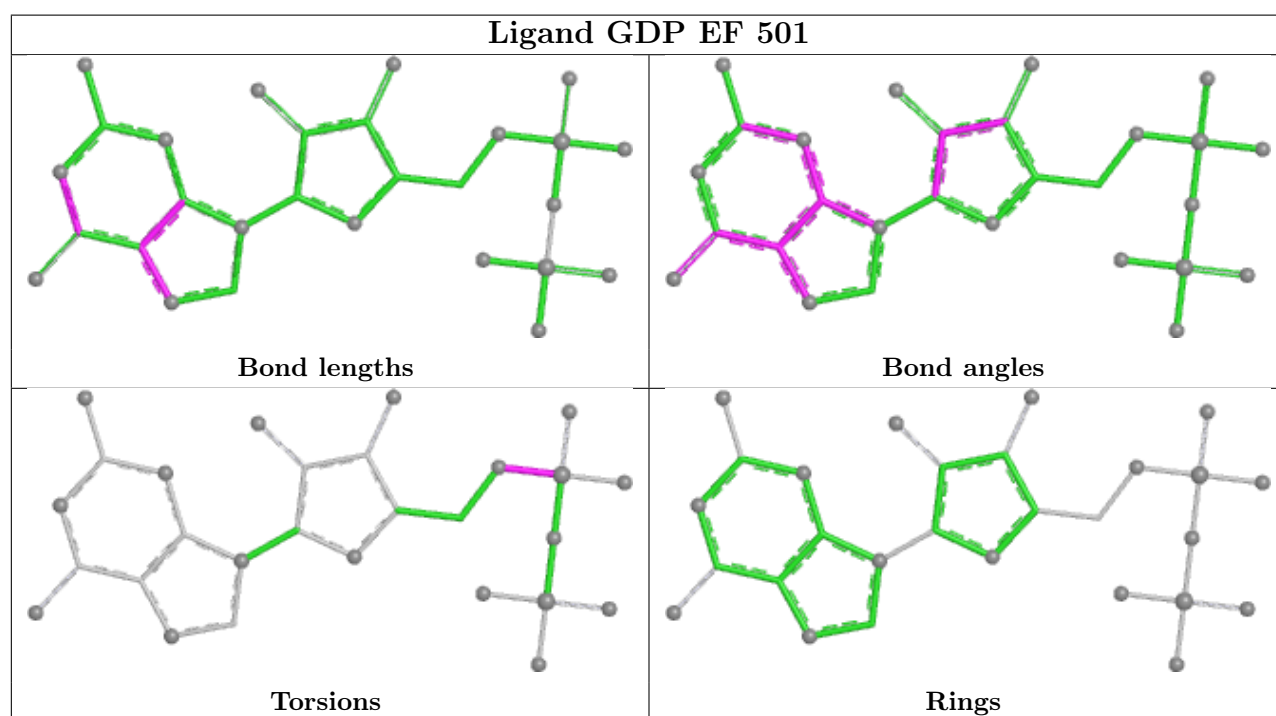
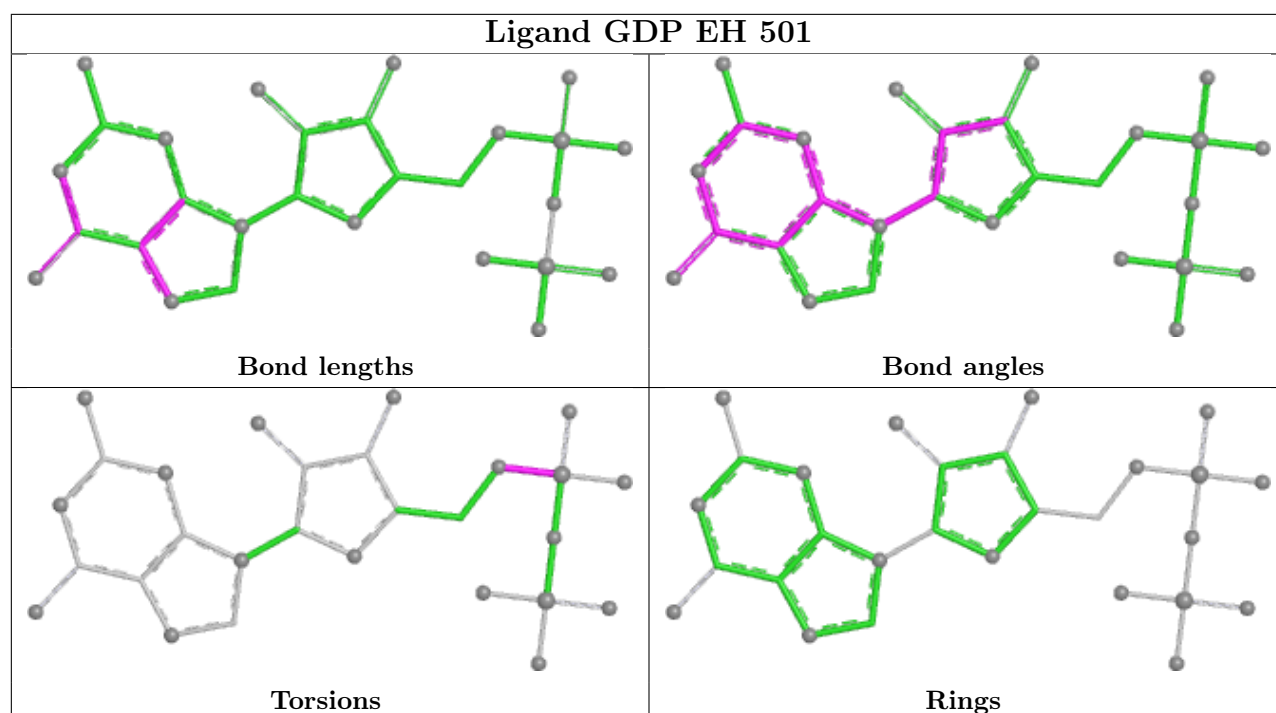
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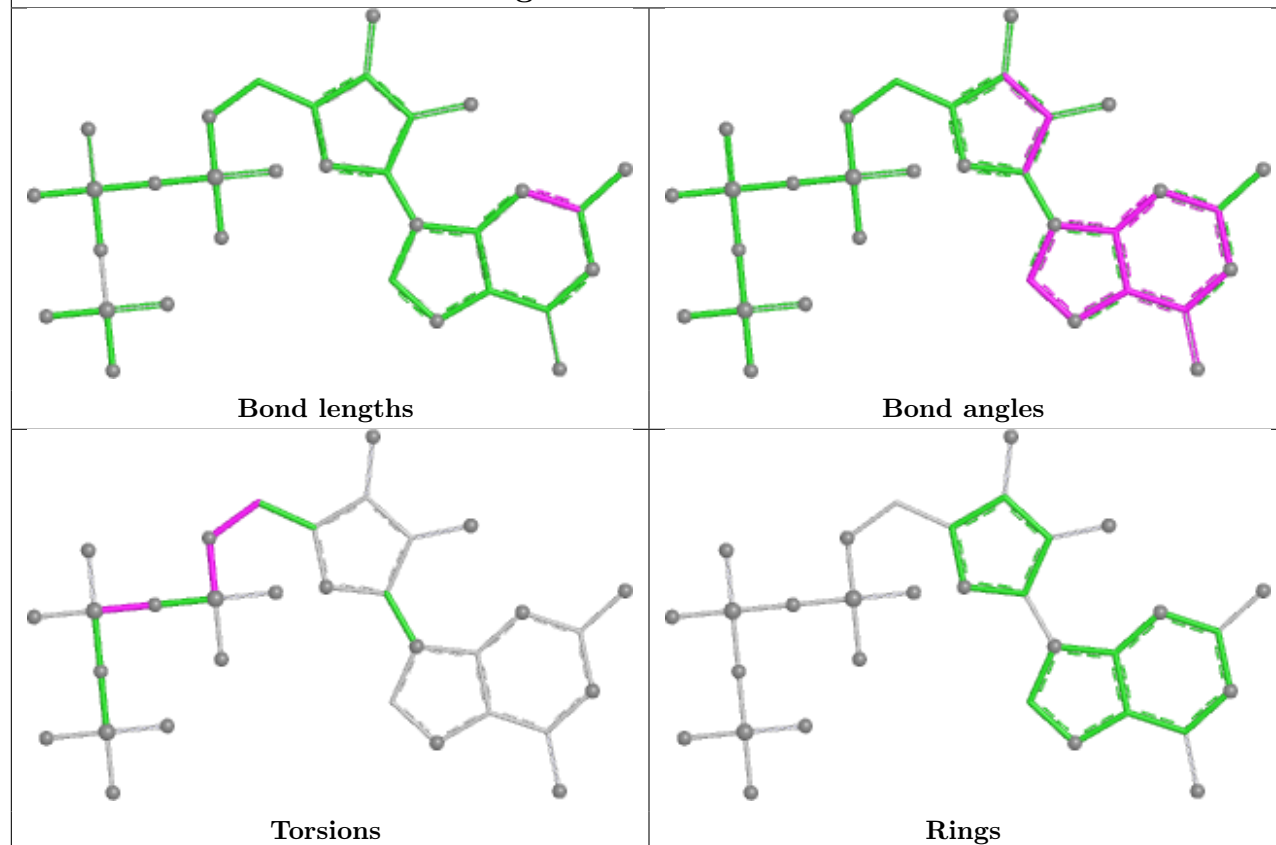
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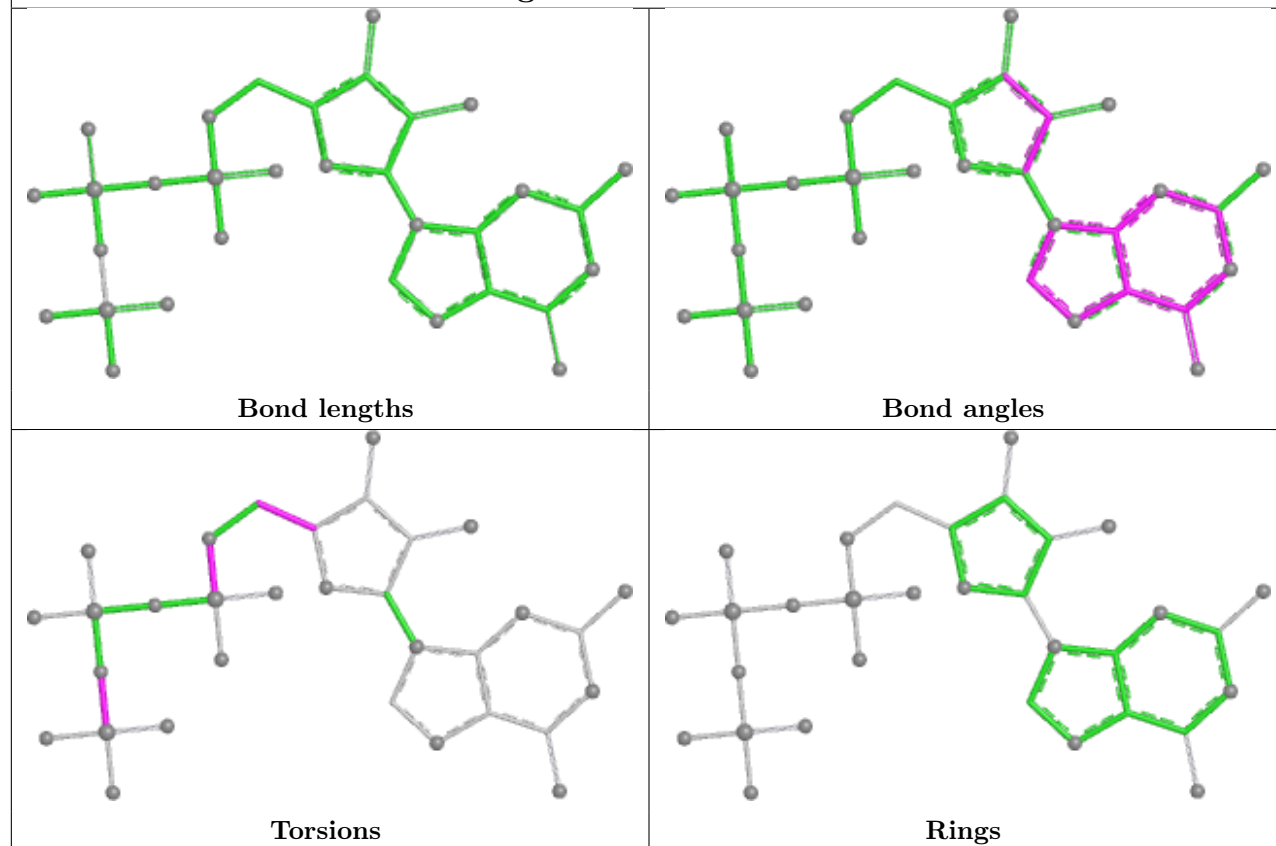


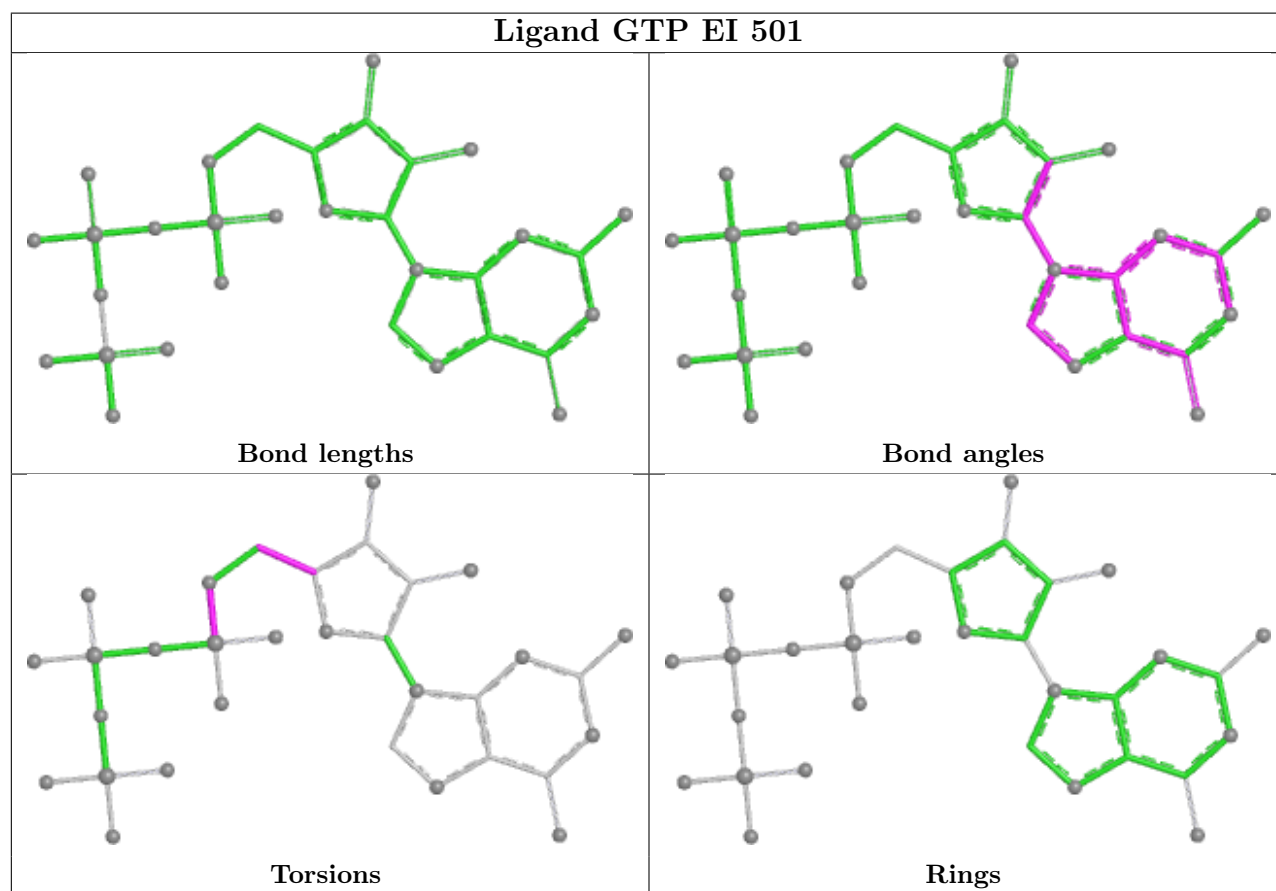
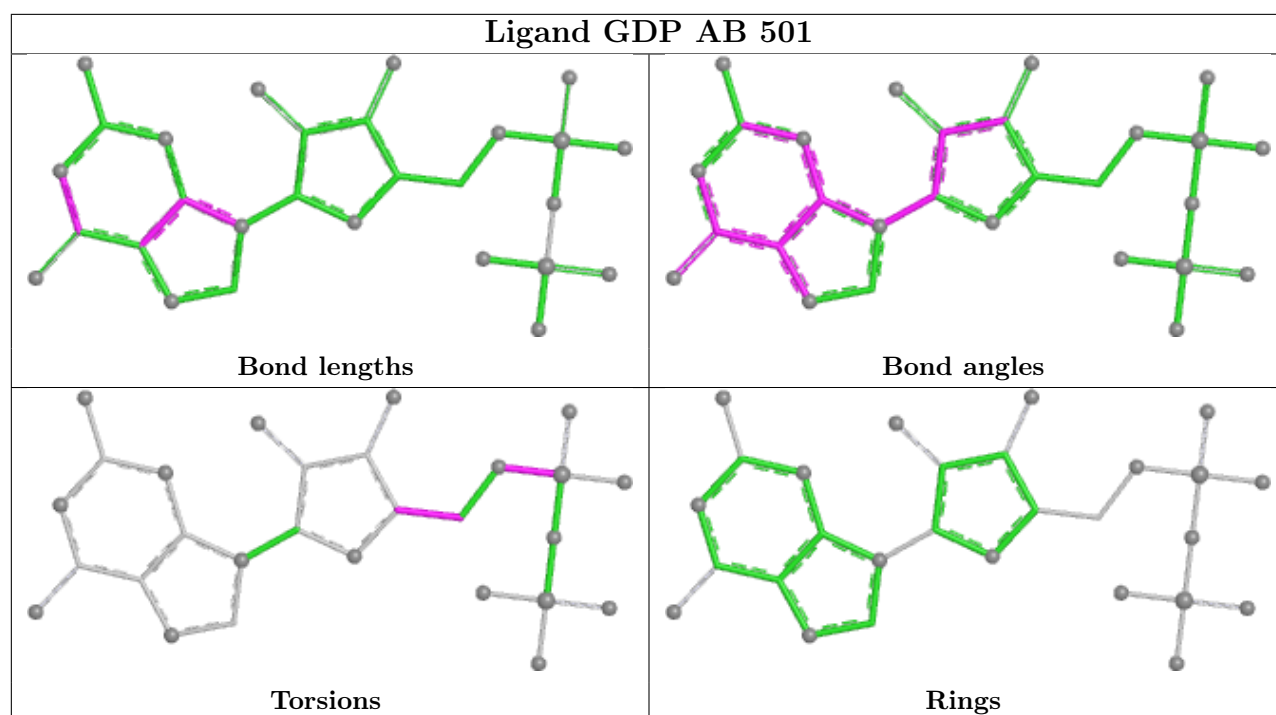


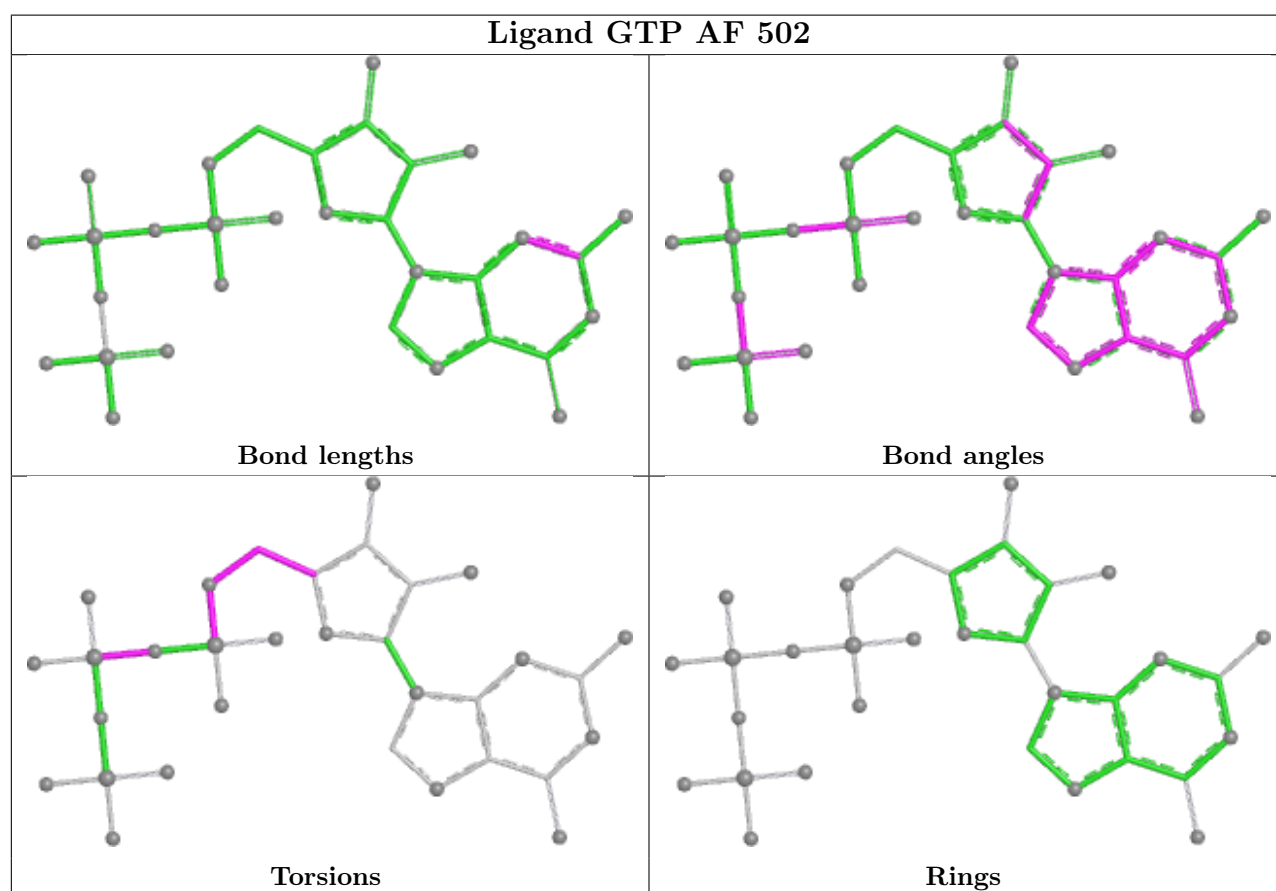
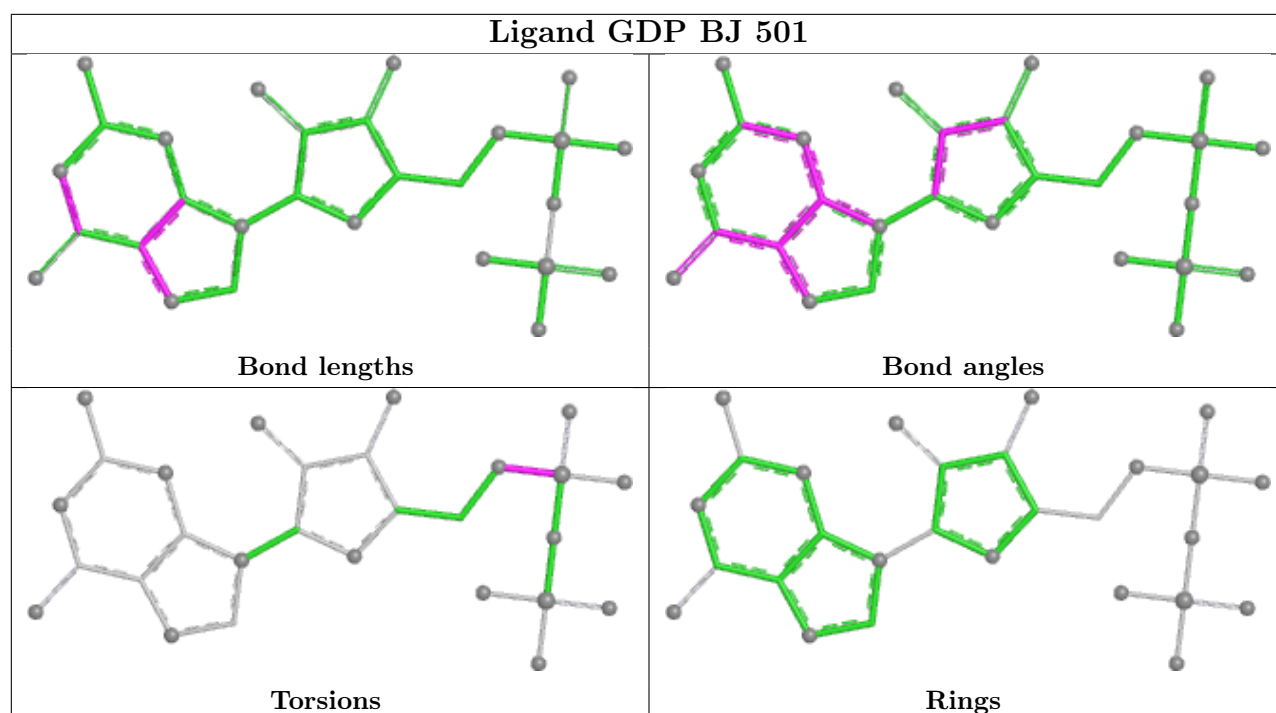
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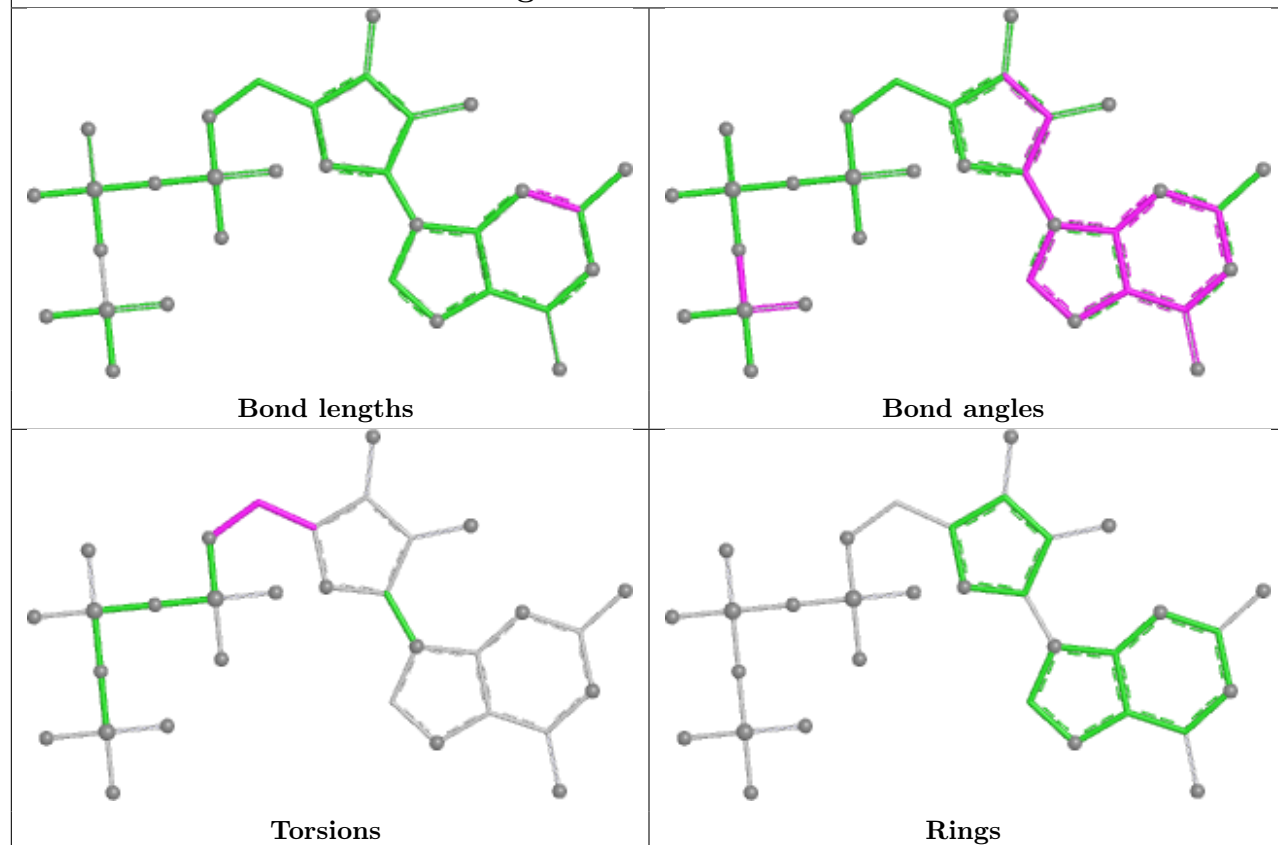
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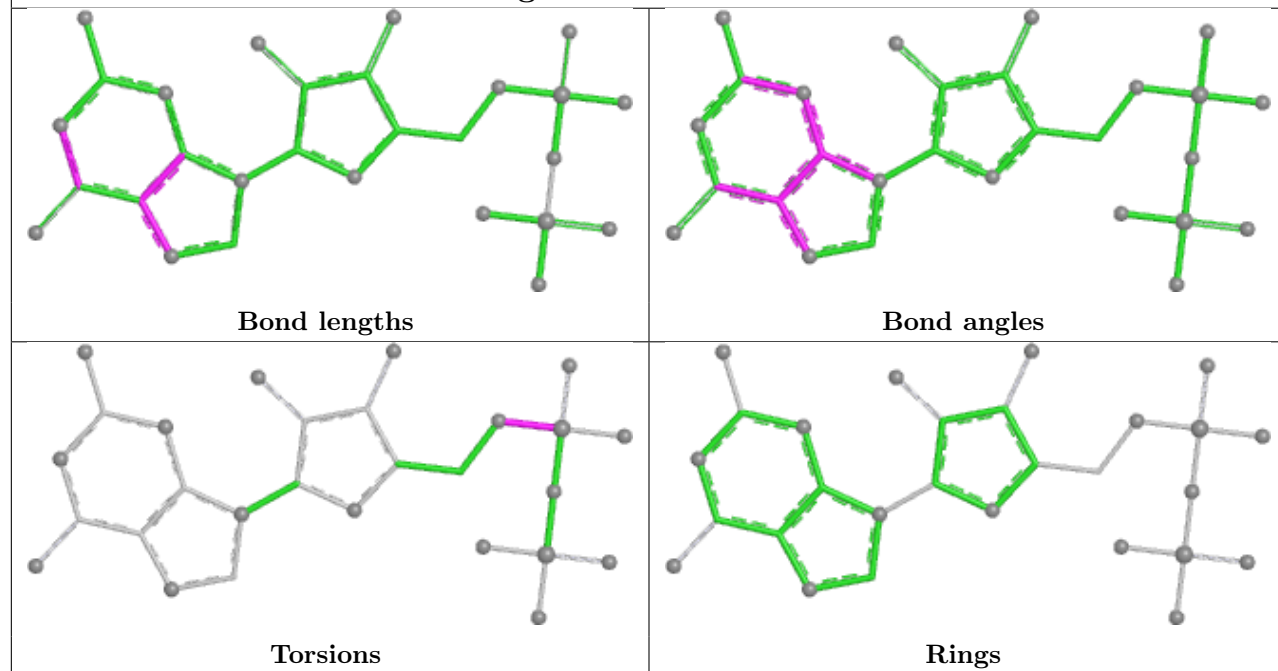




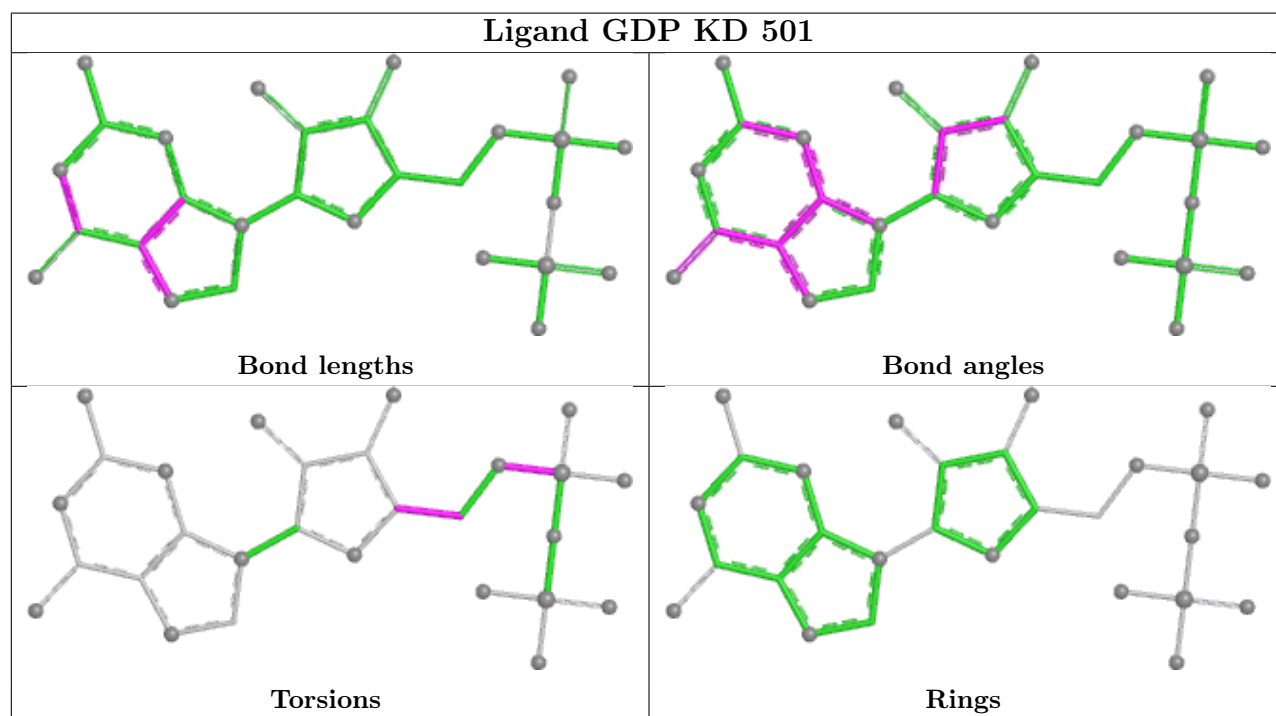
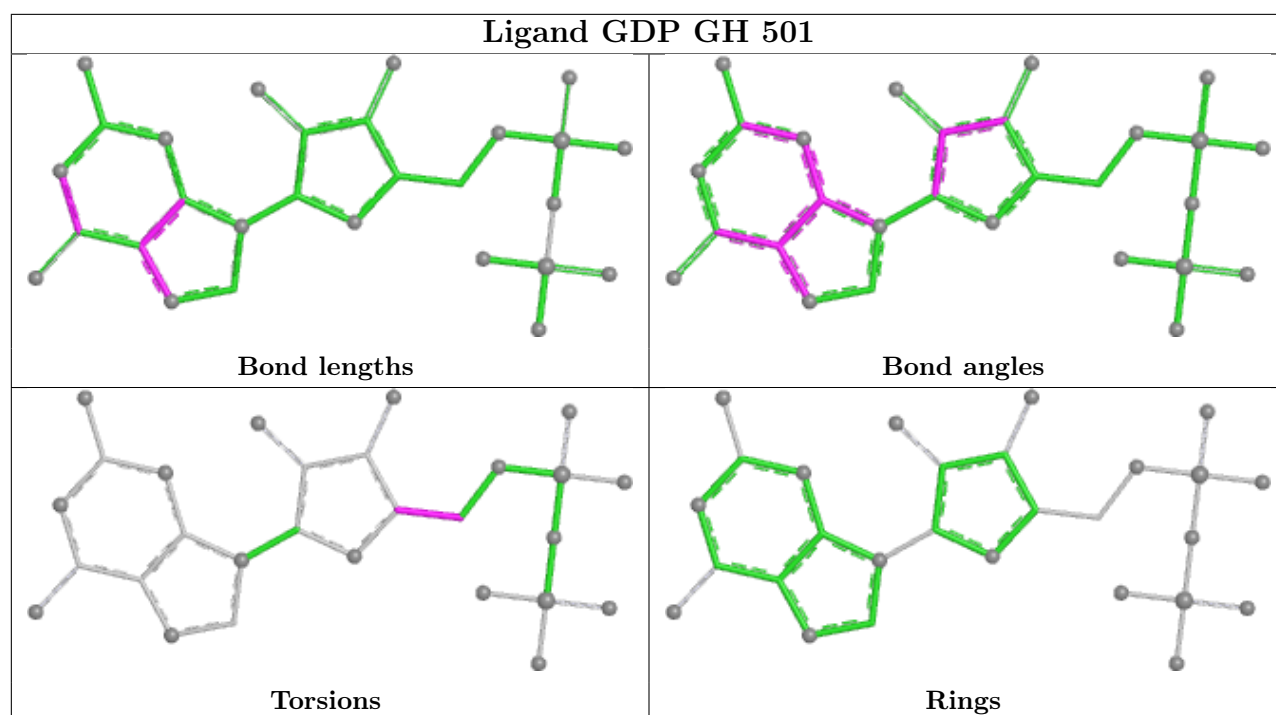
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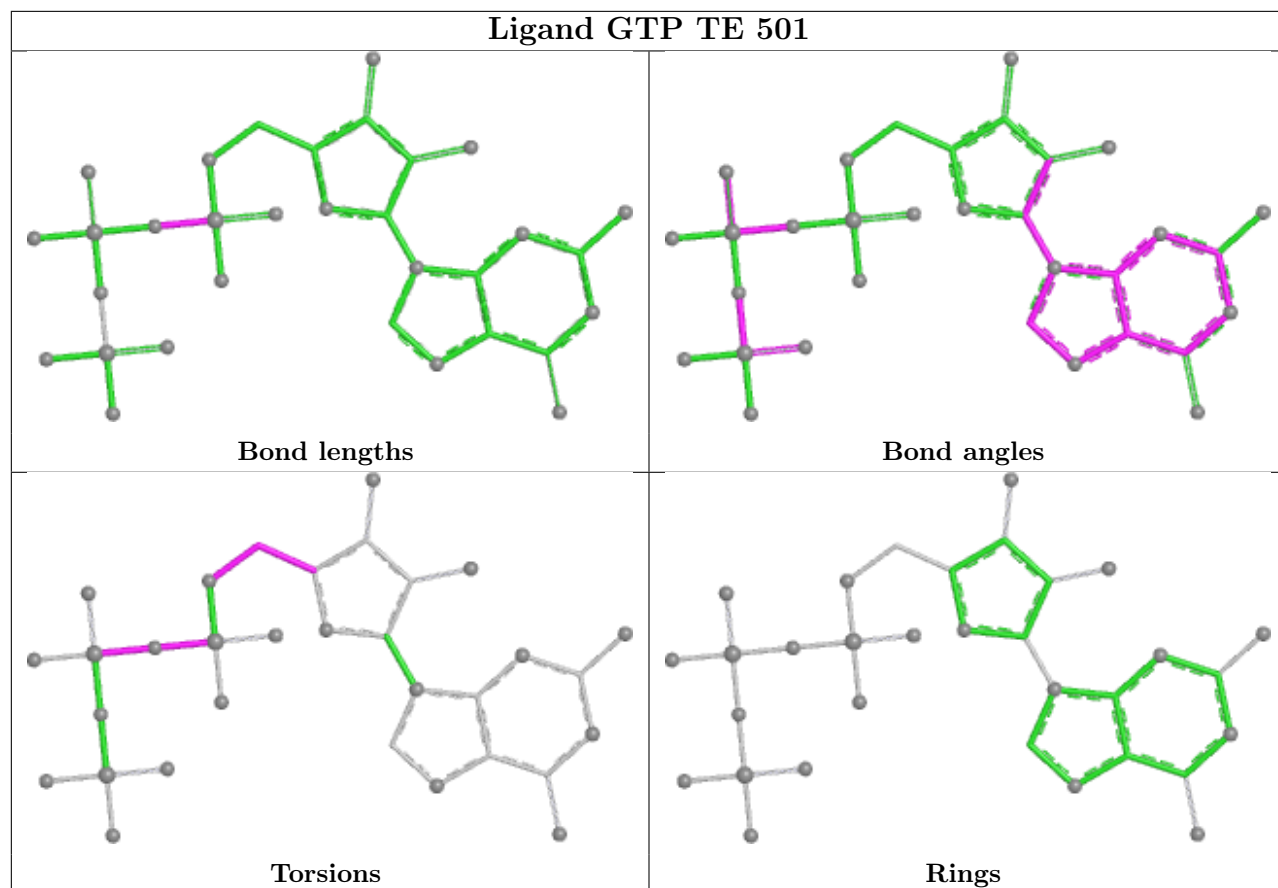
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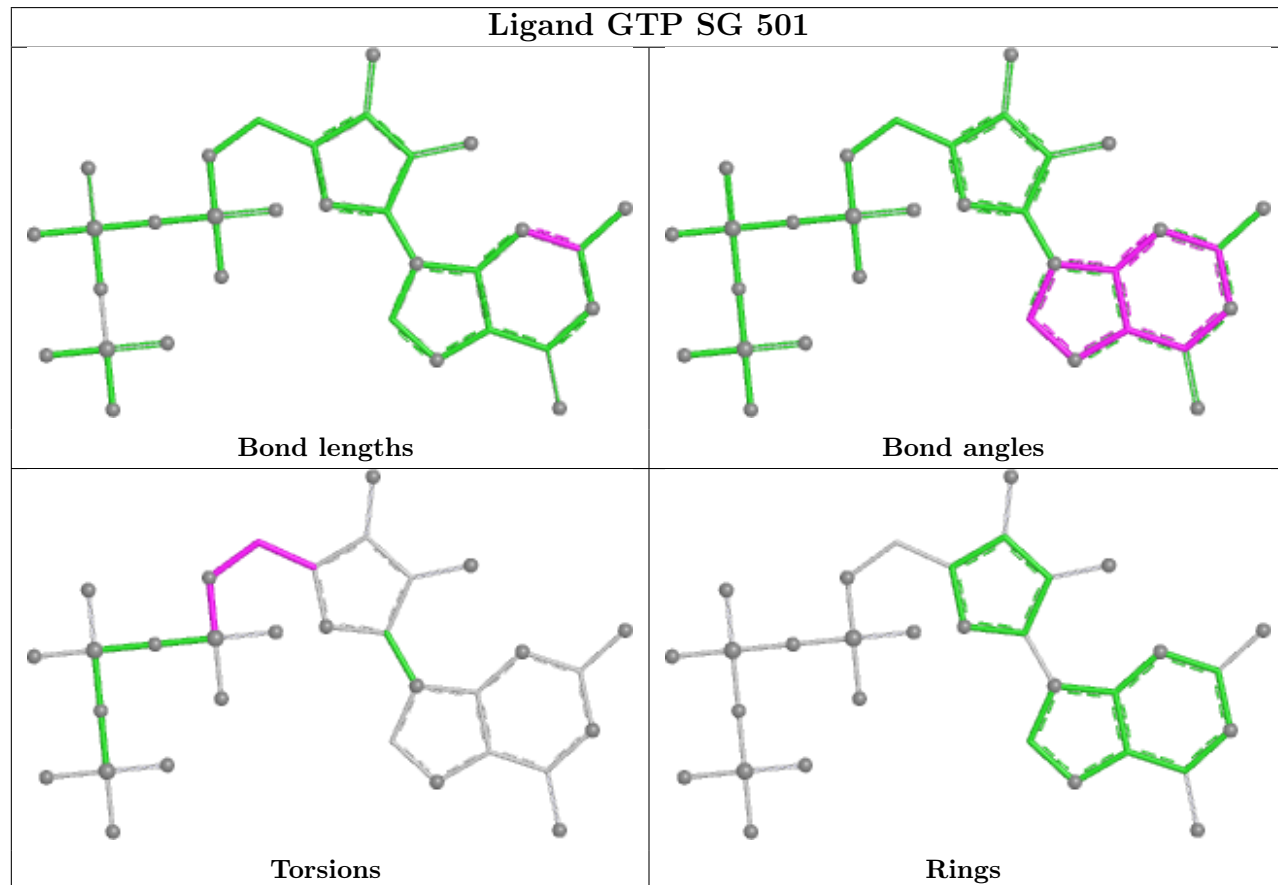




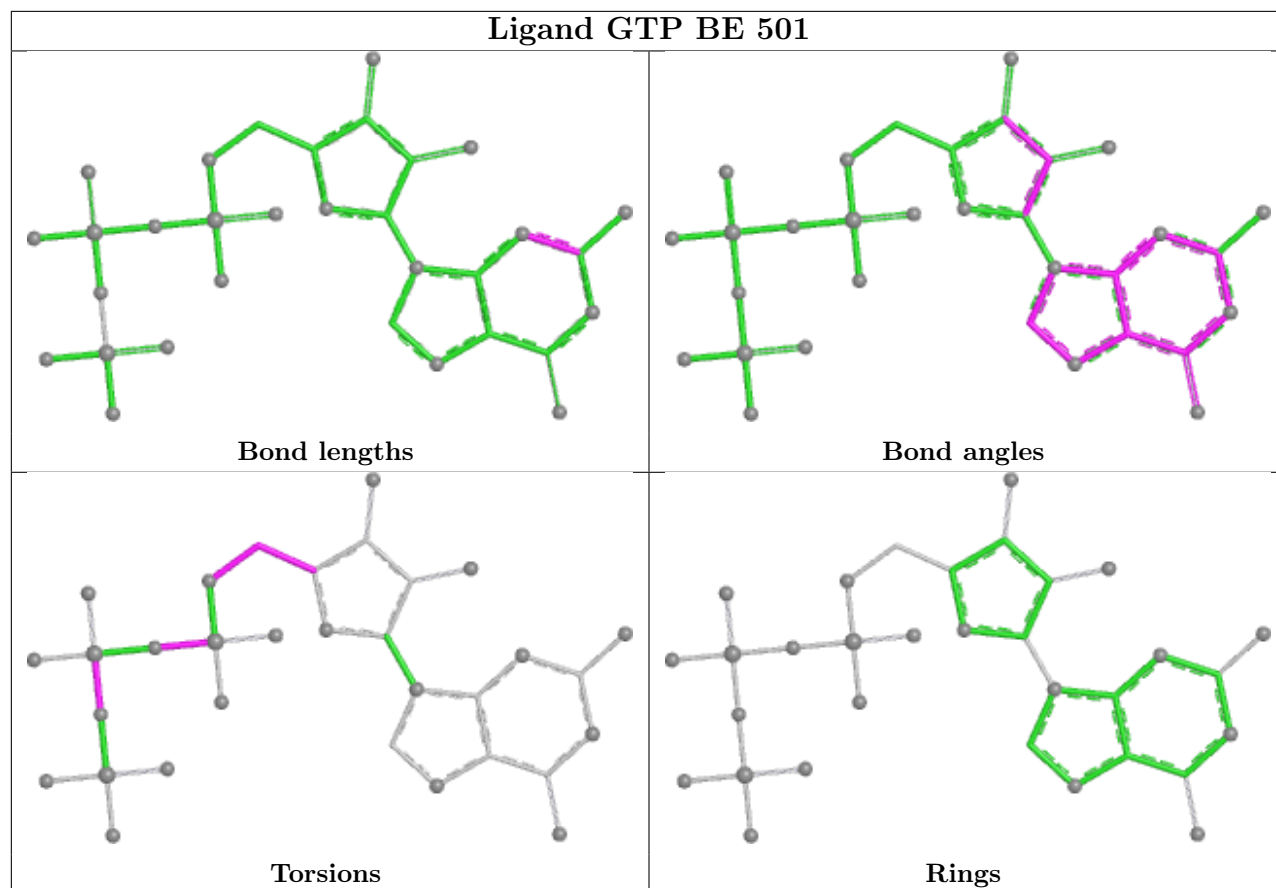
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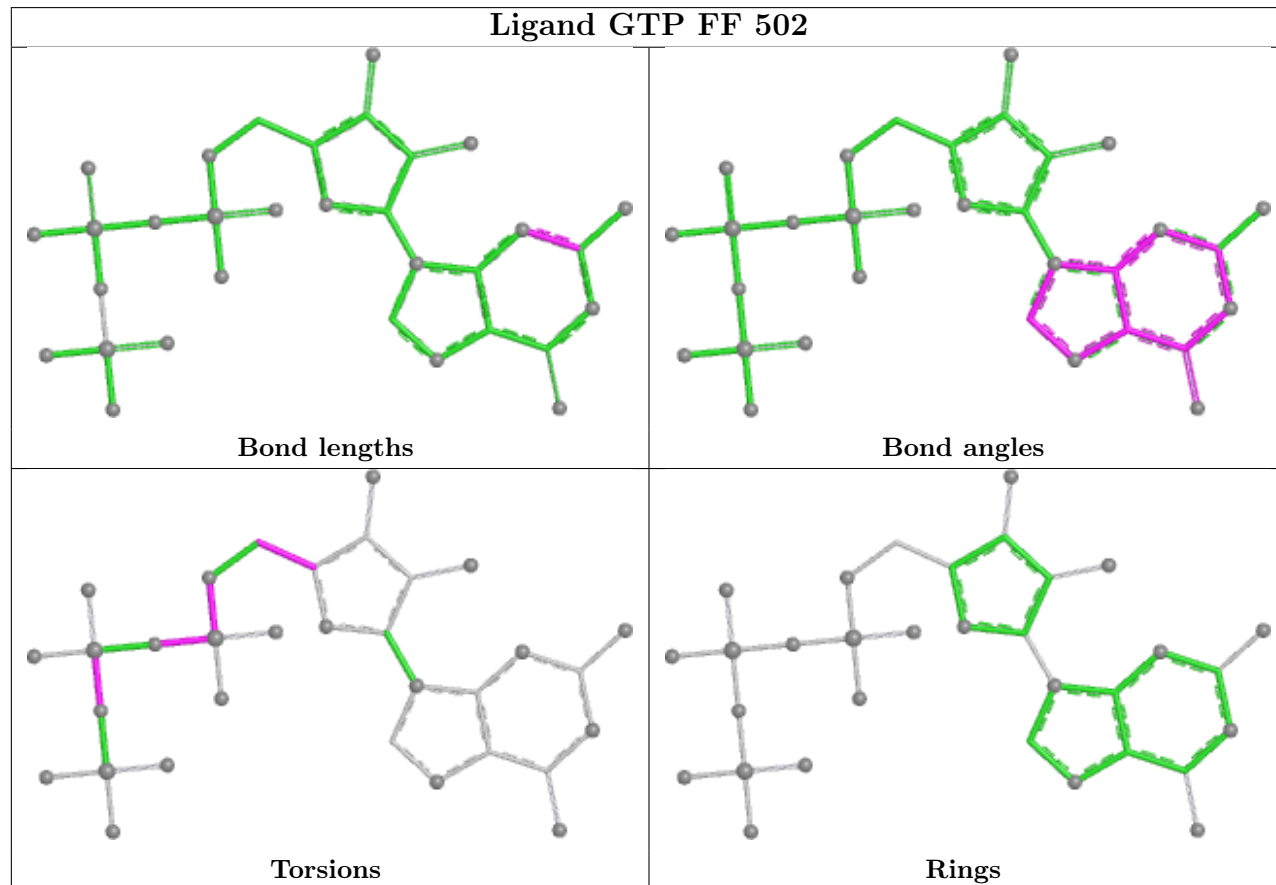
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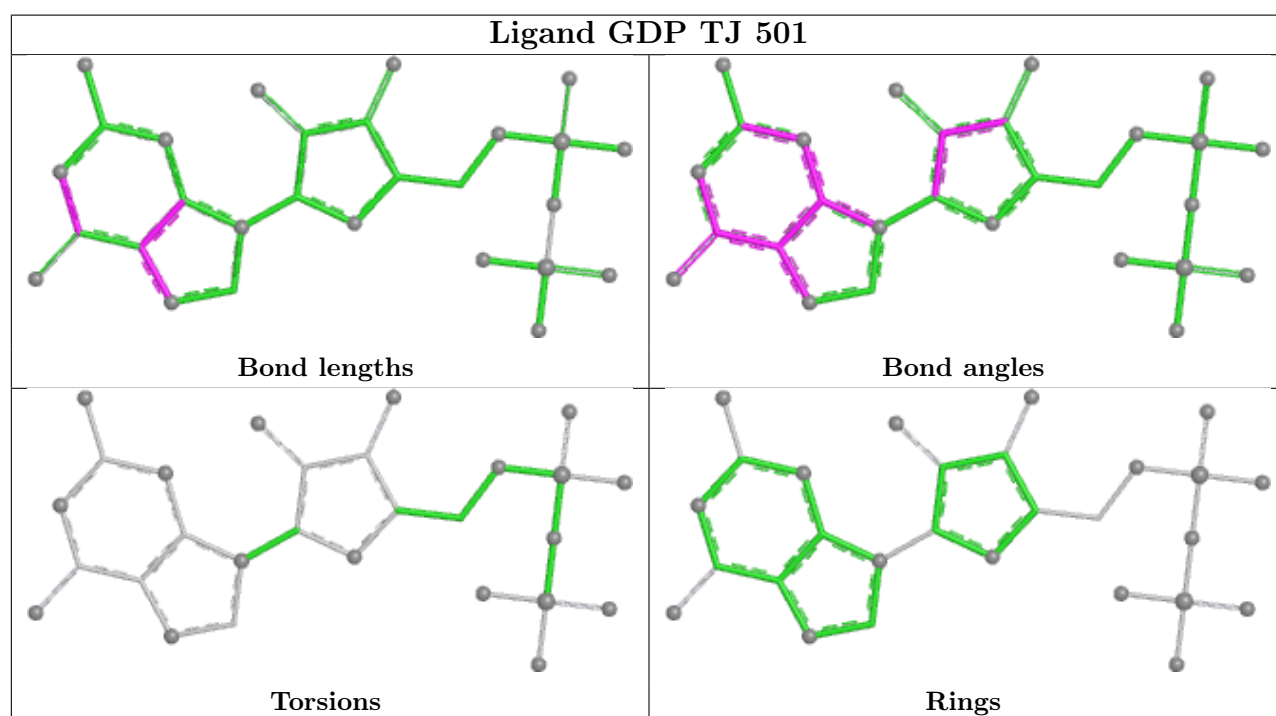
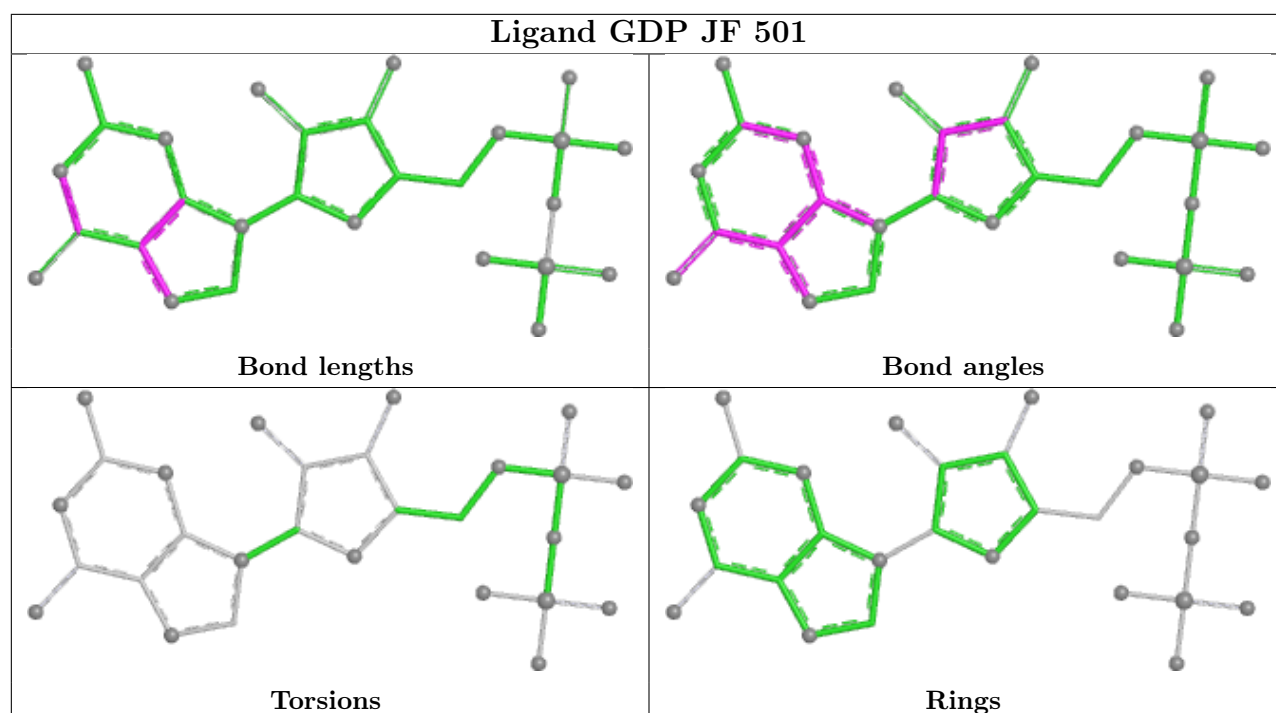


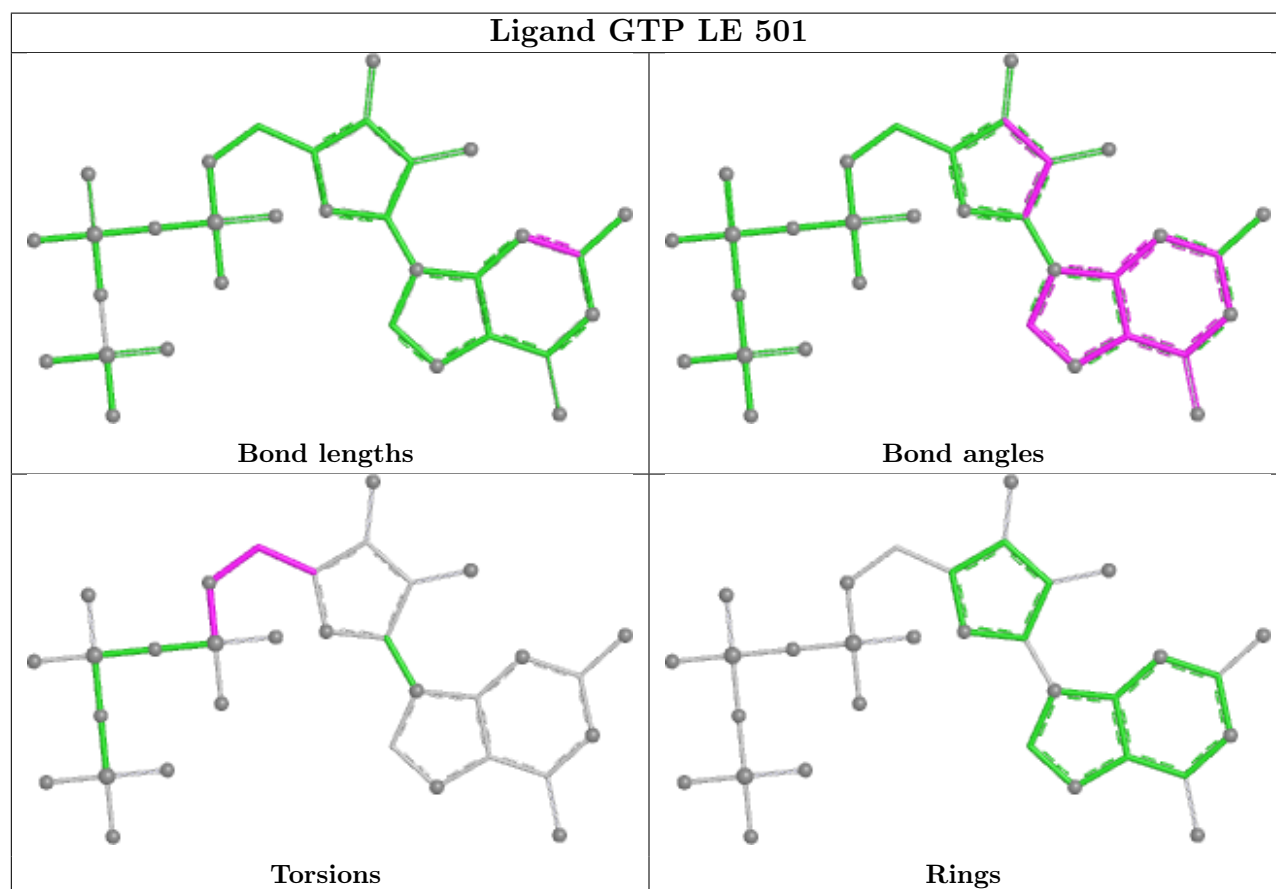
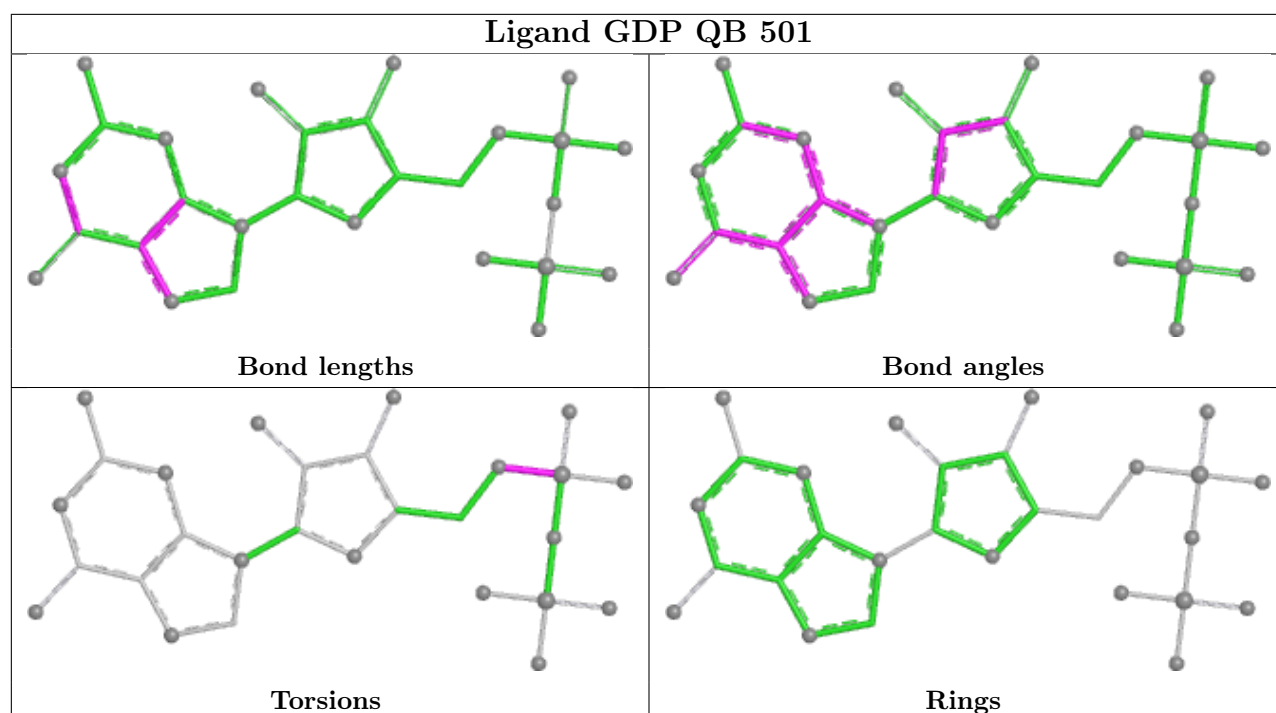
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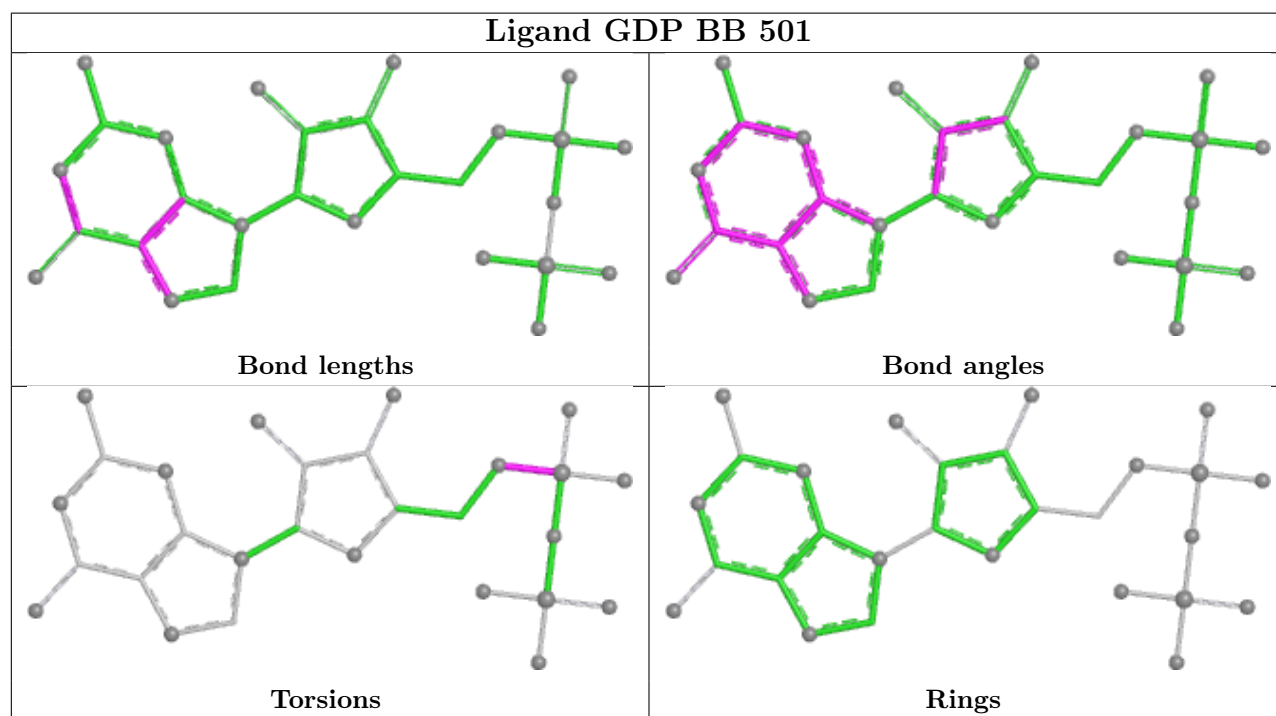
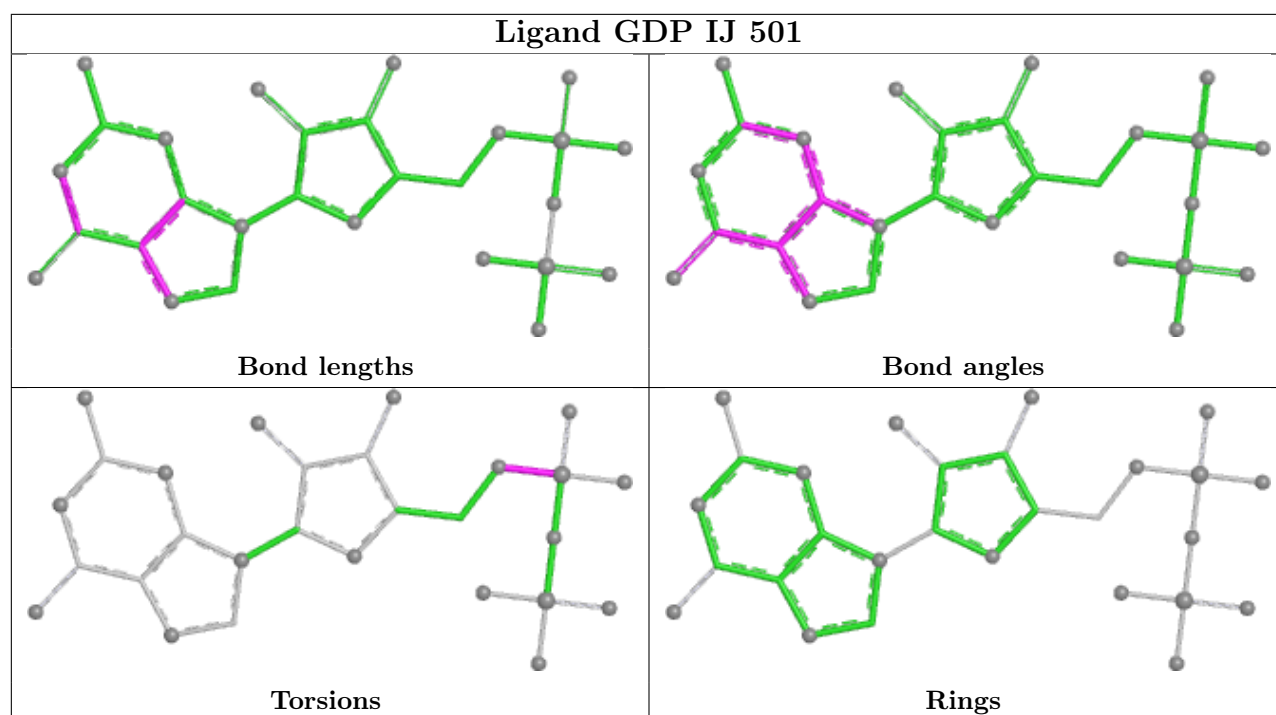


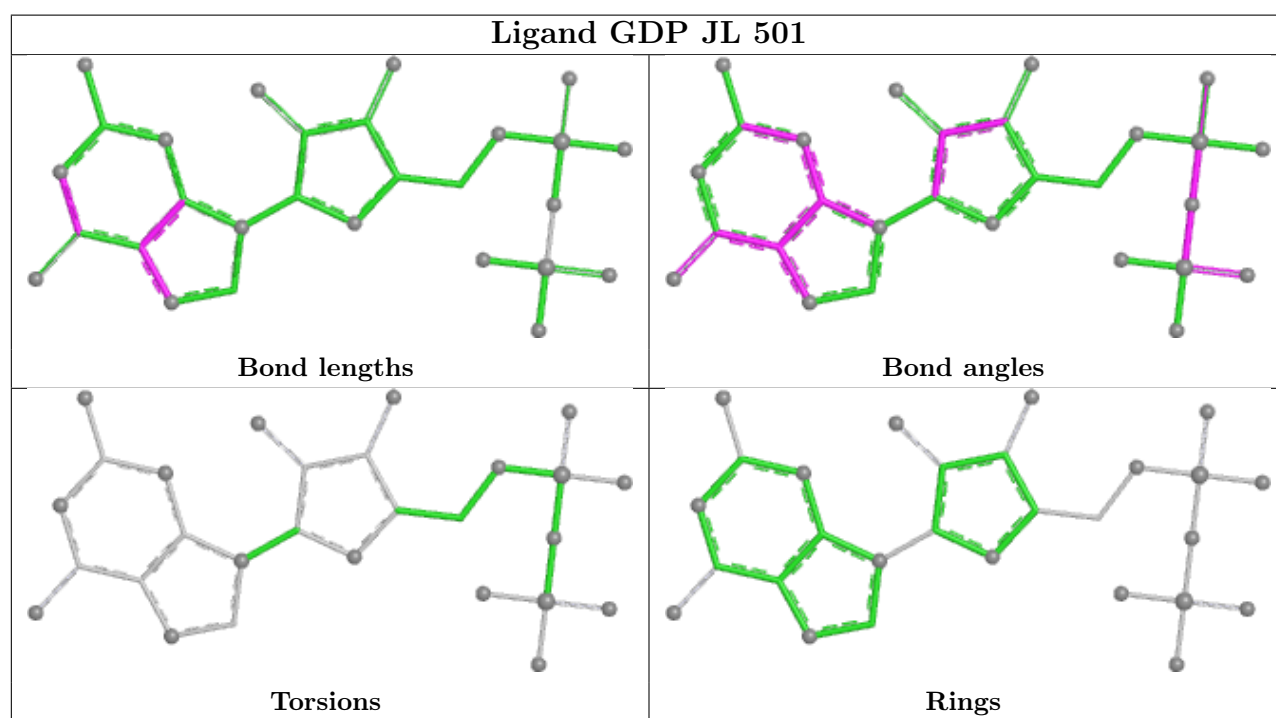
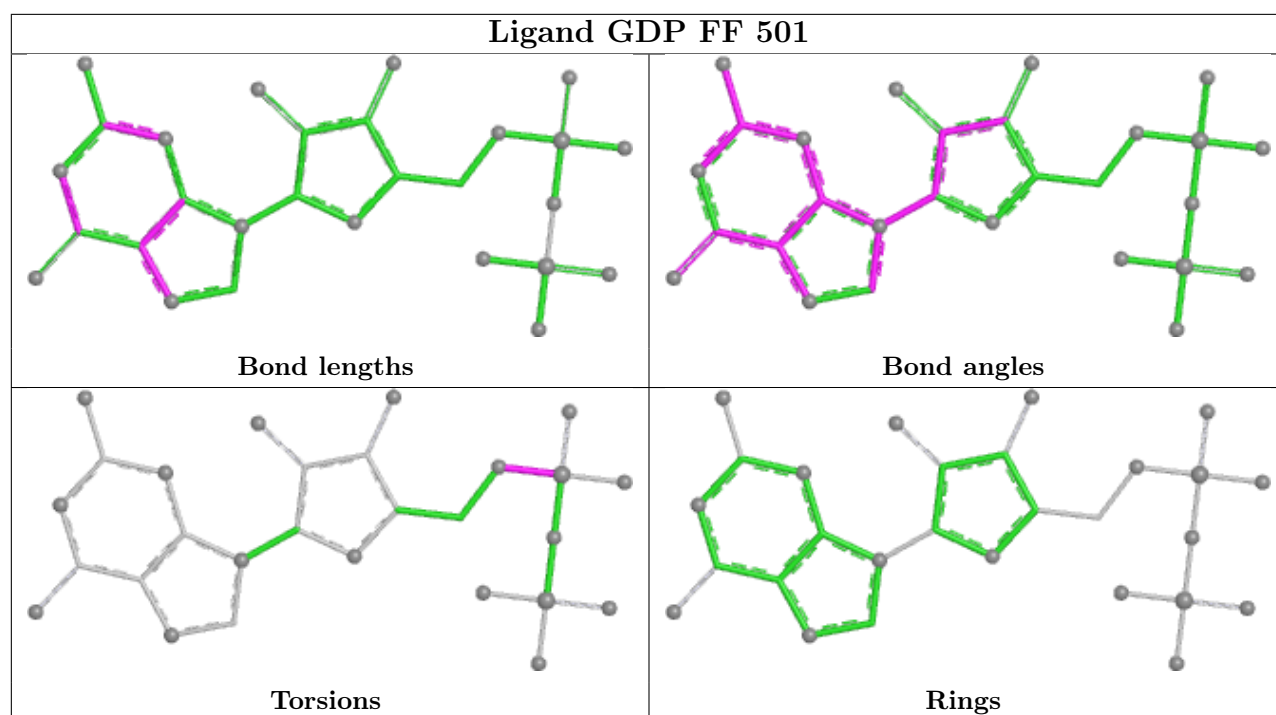
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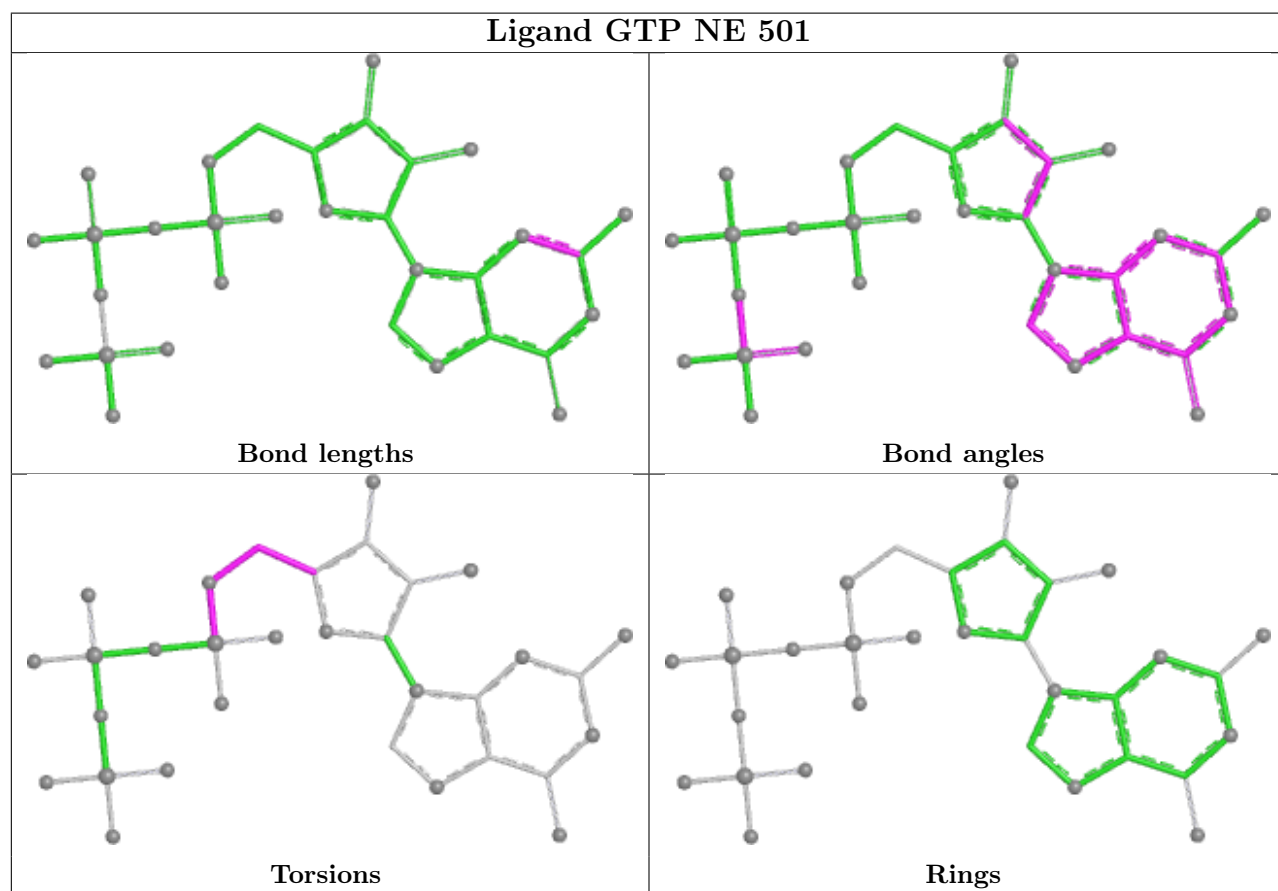
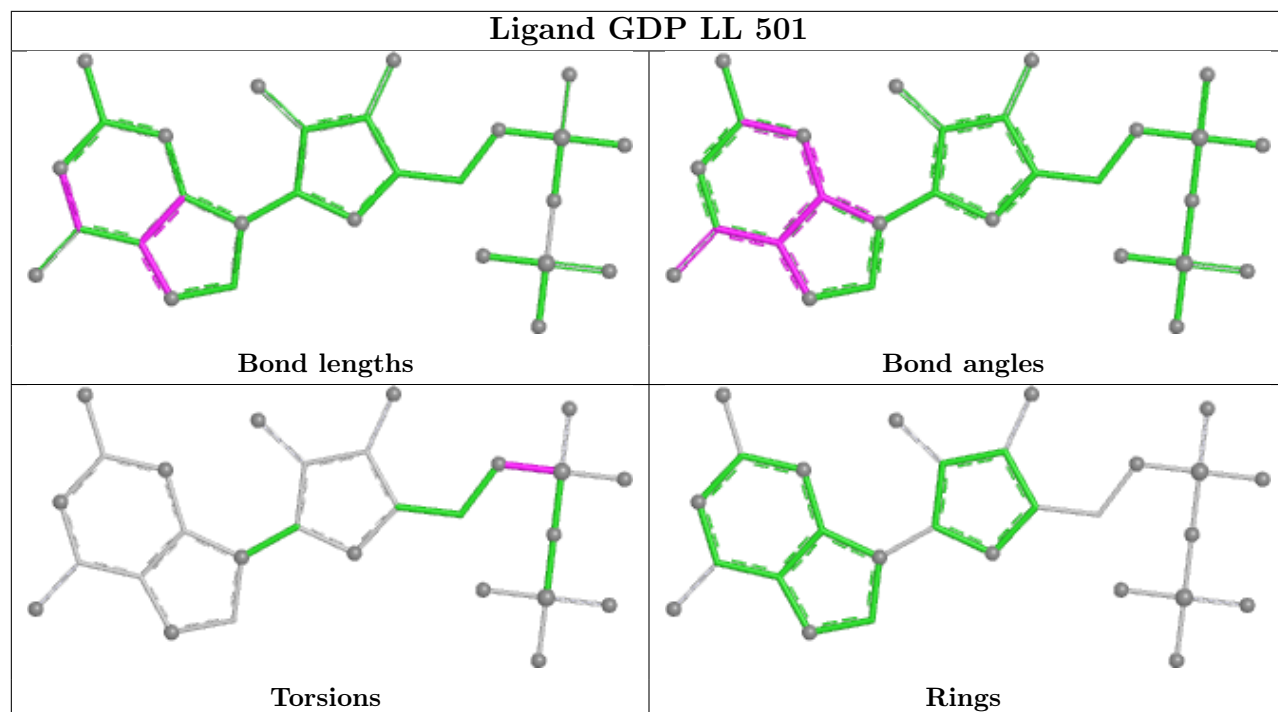




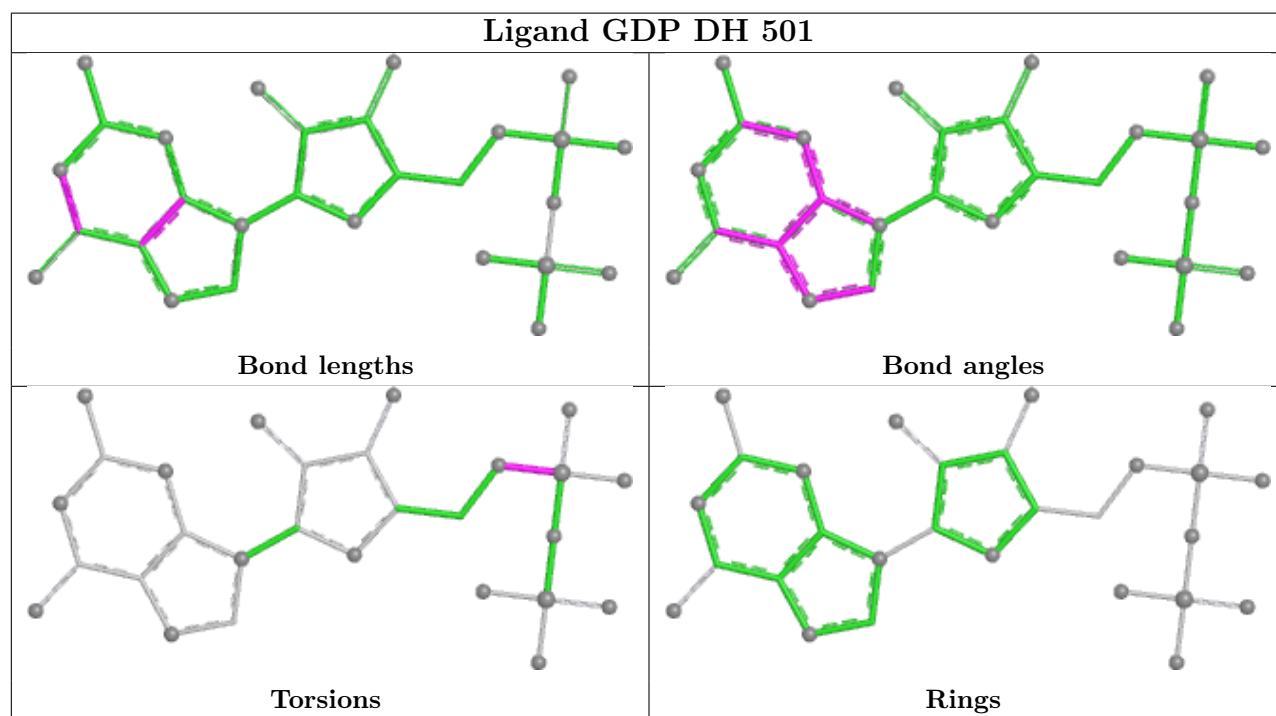
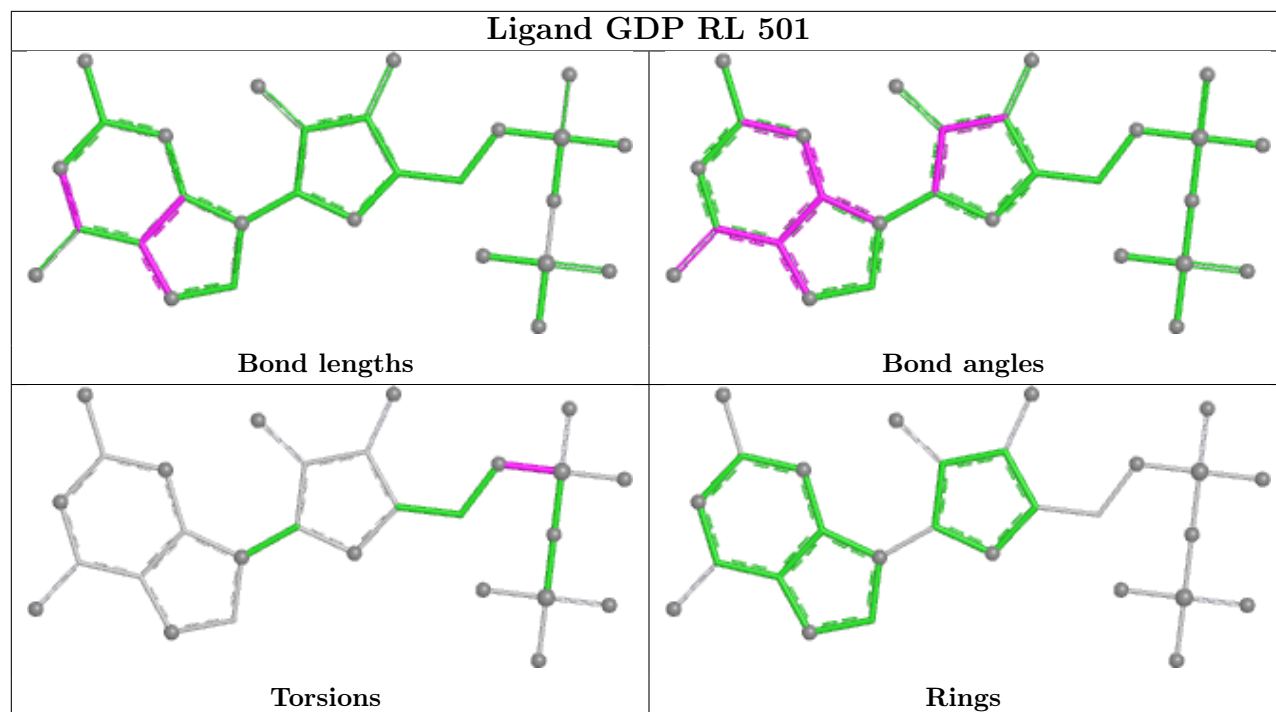


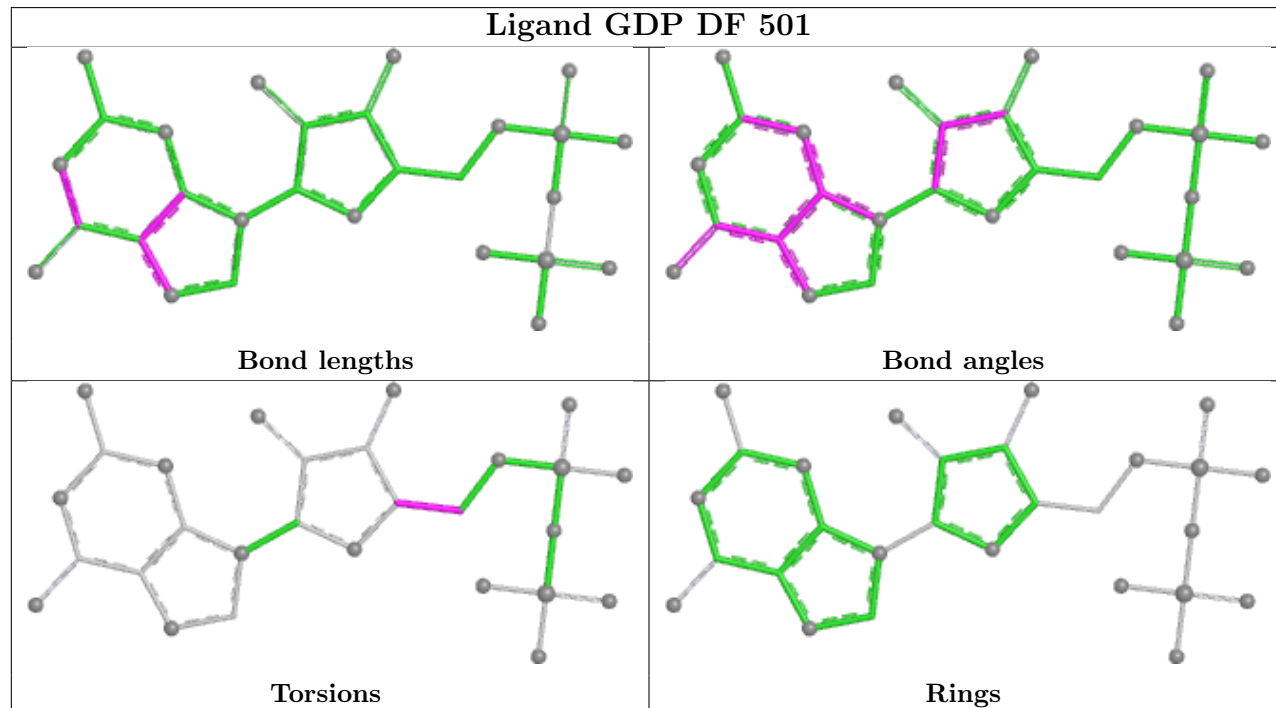
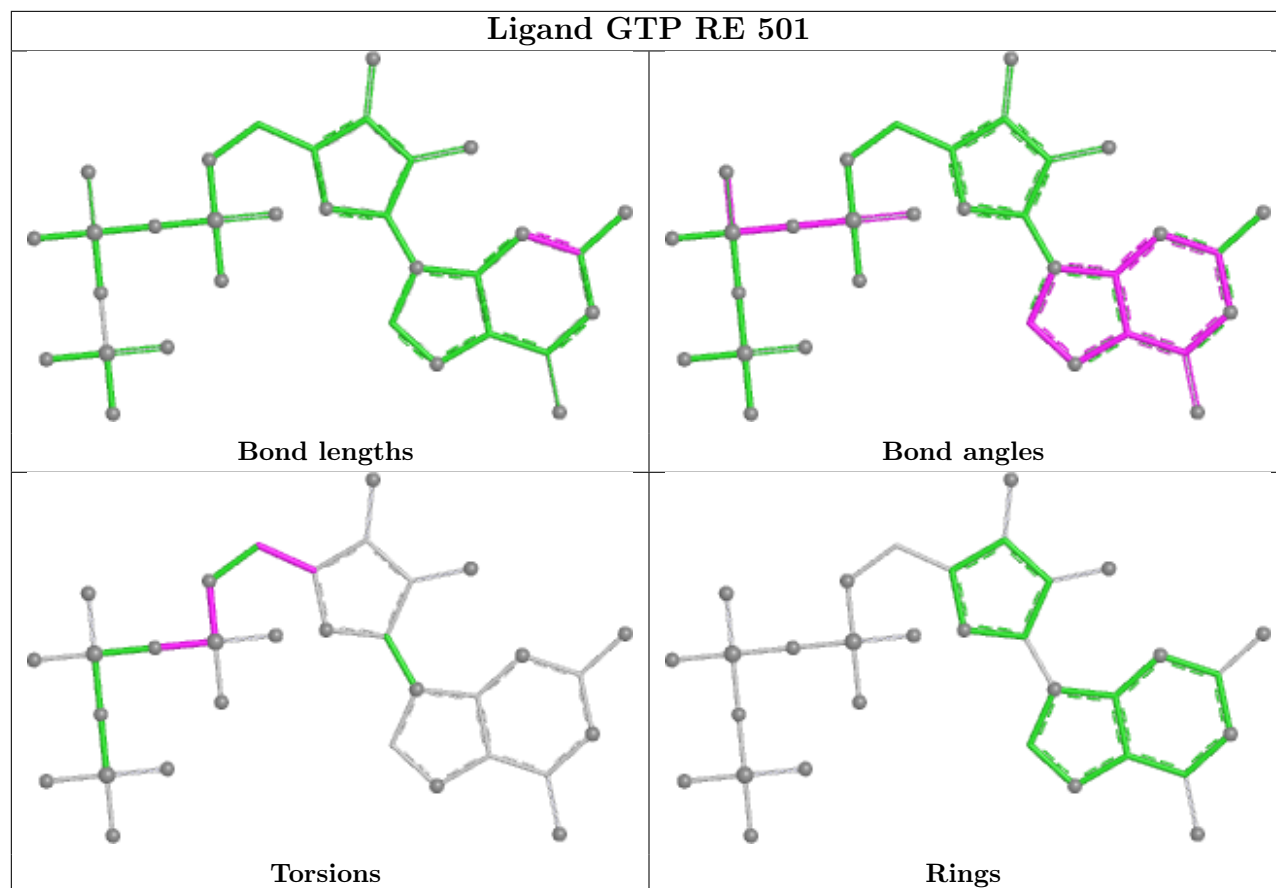


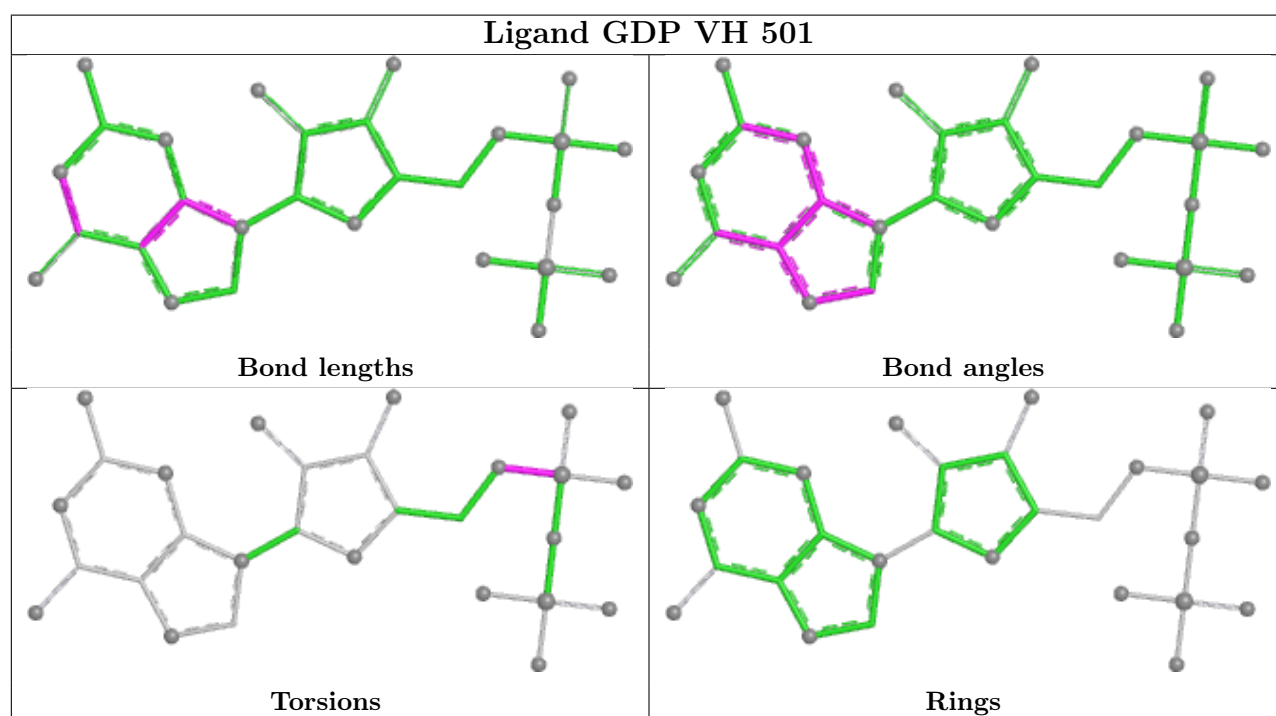
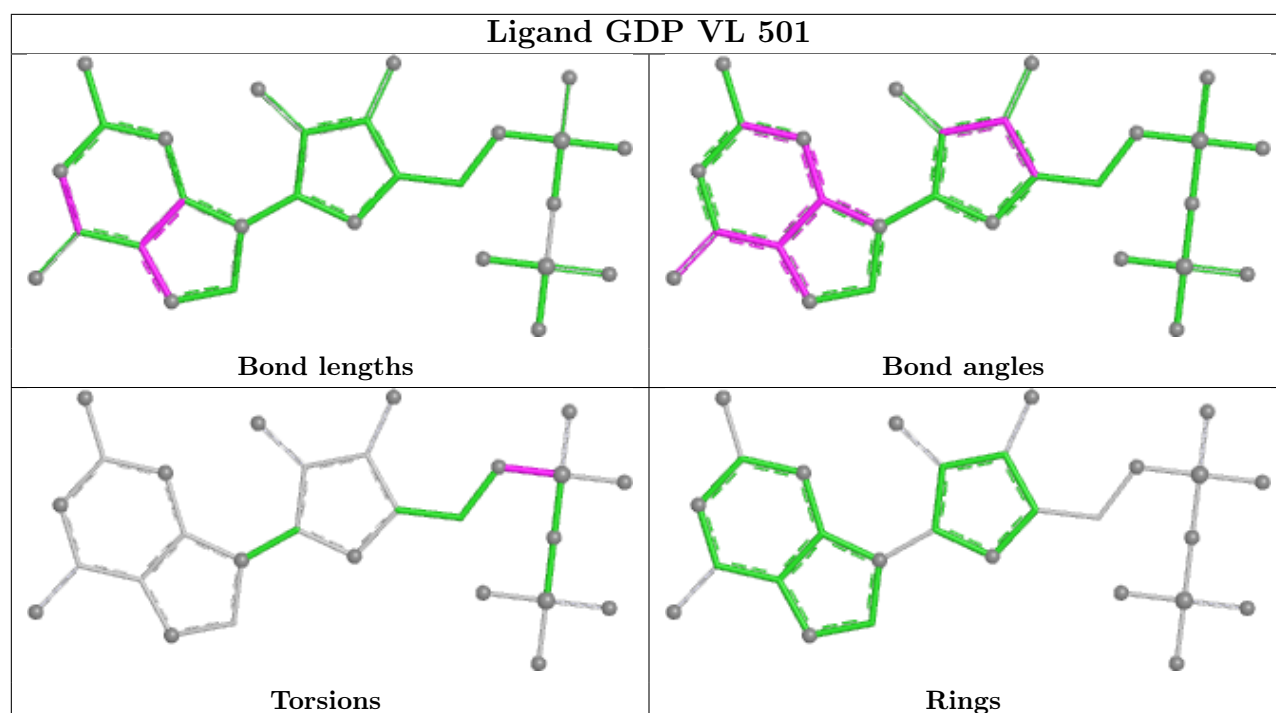




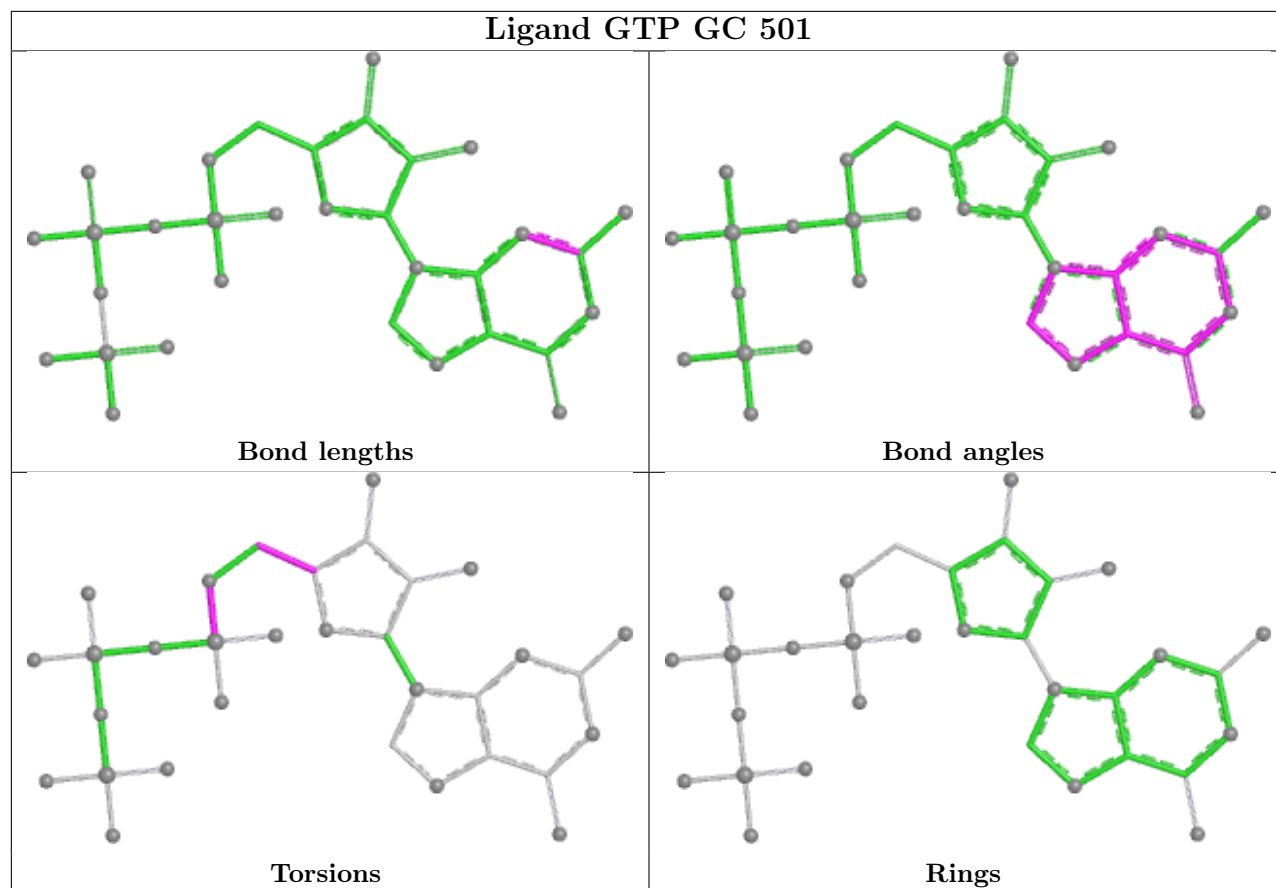




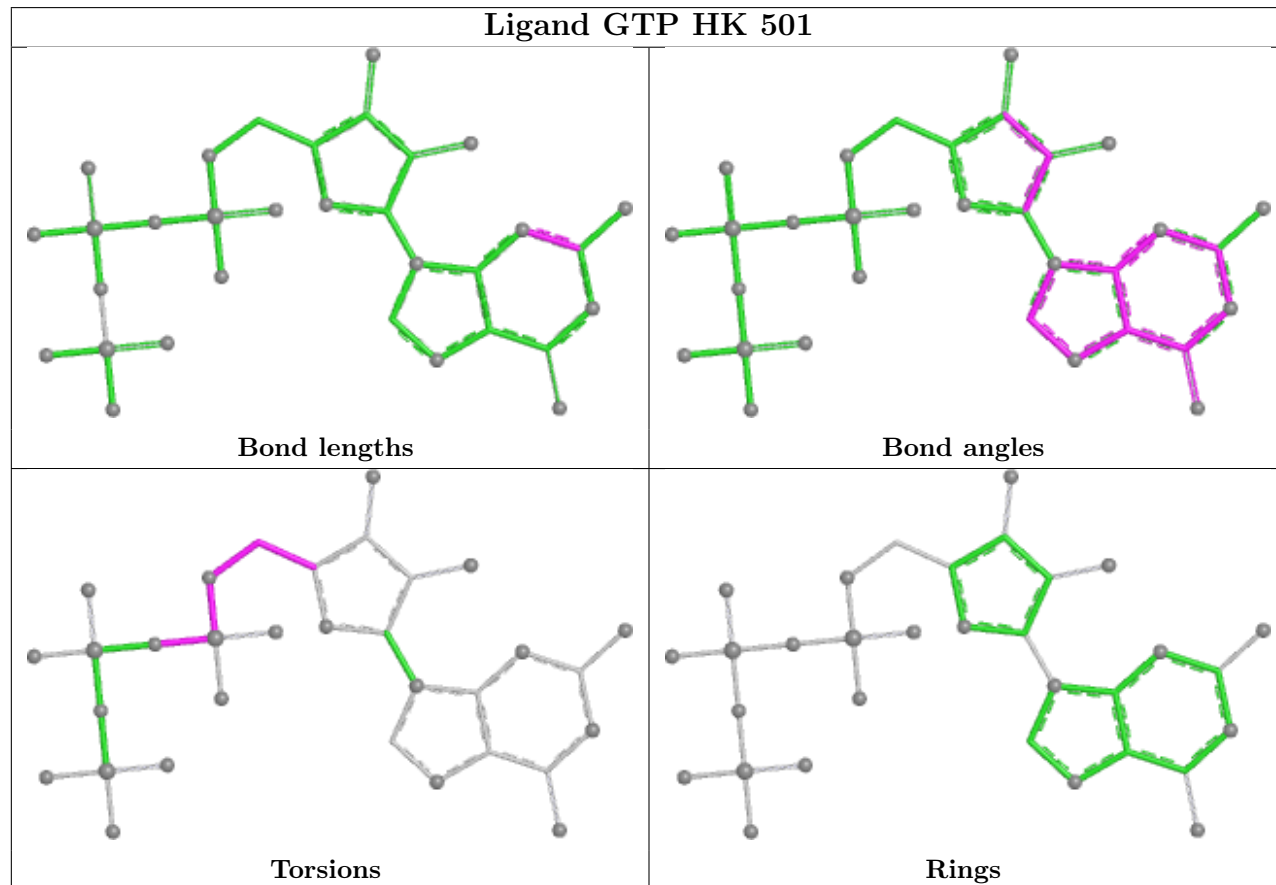


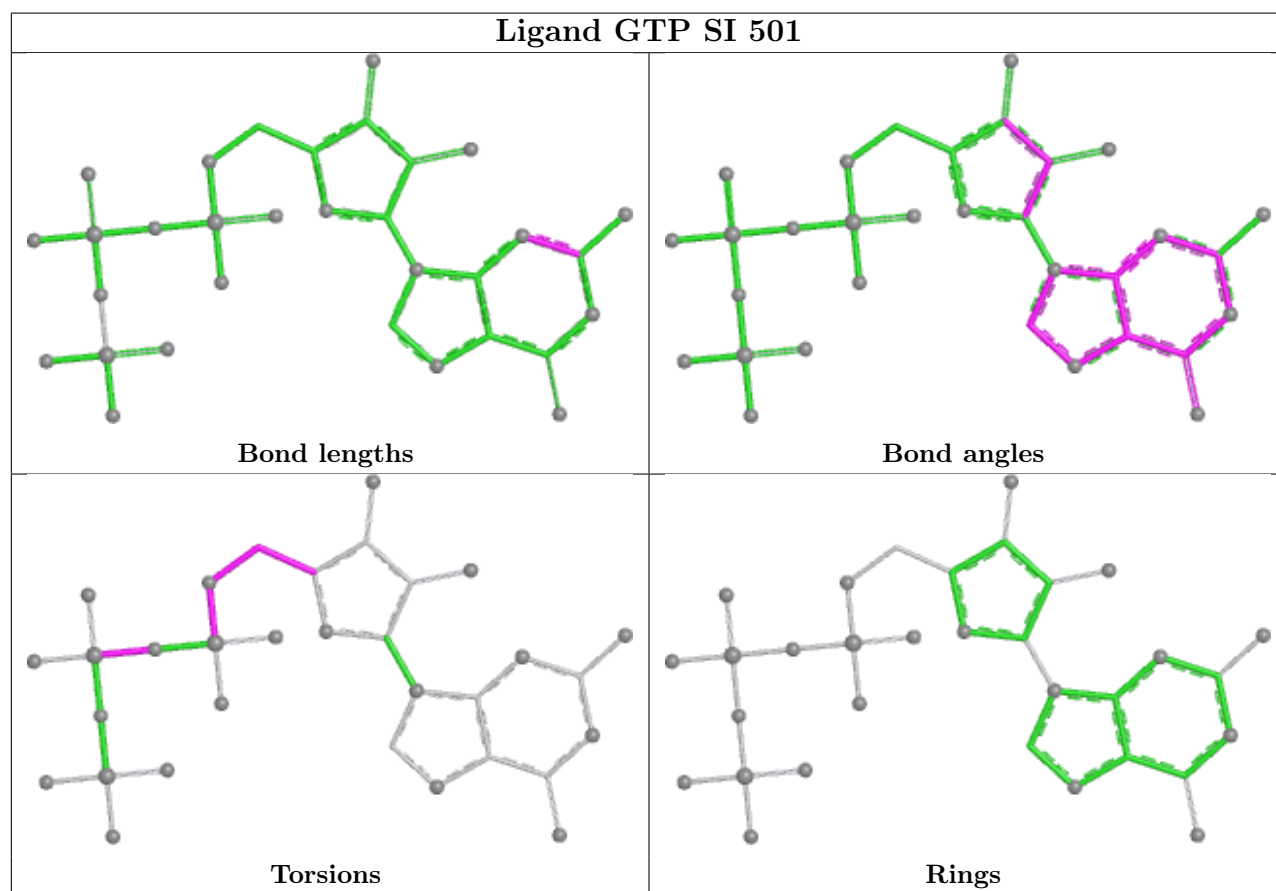
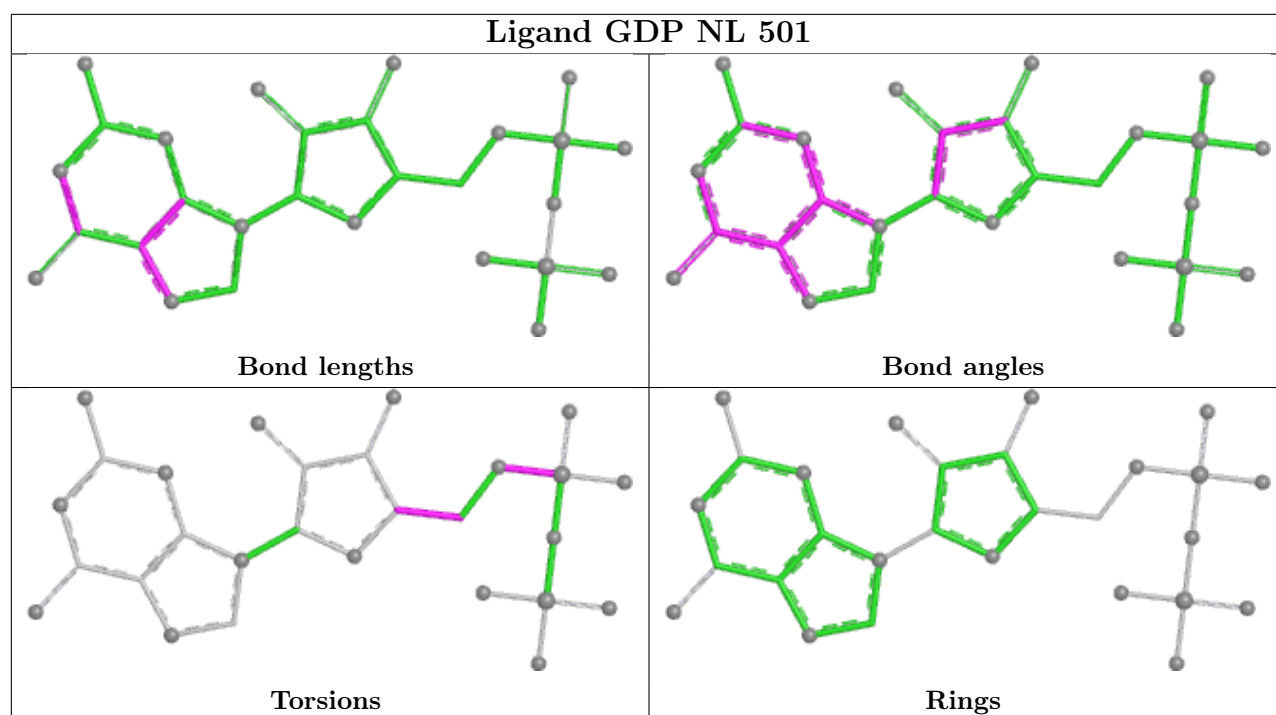


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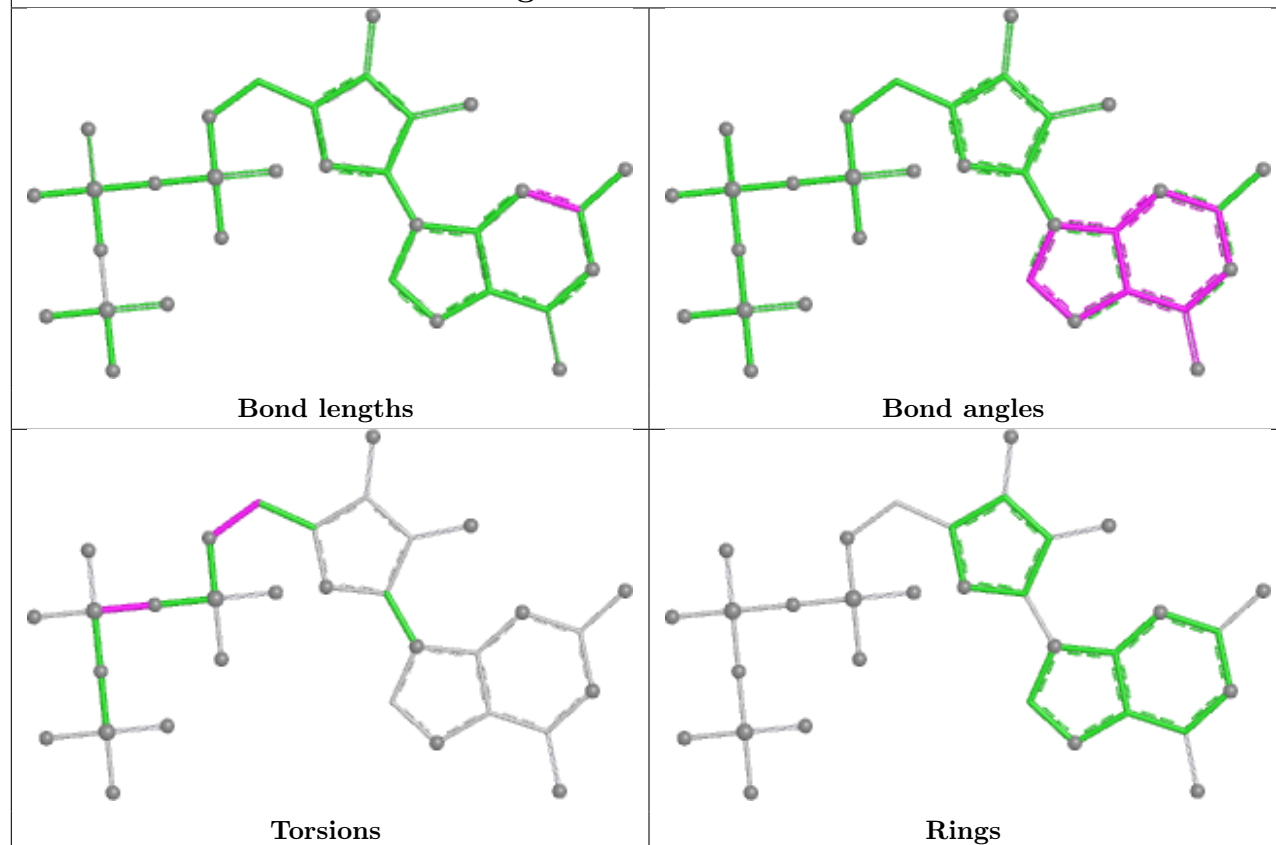


## Ligand GTP HK 501

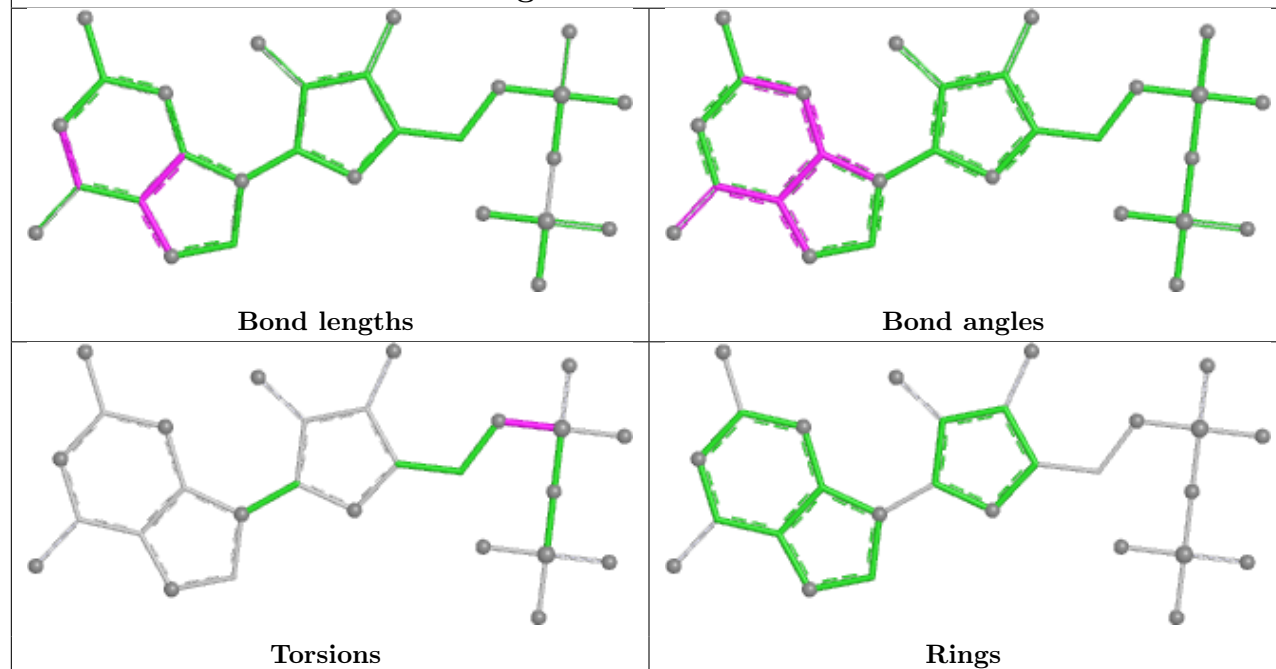


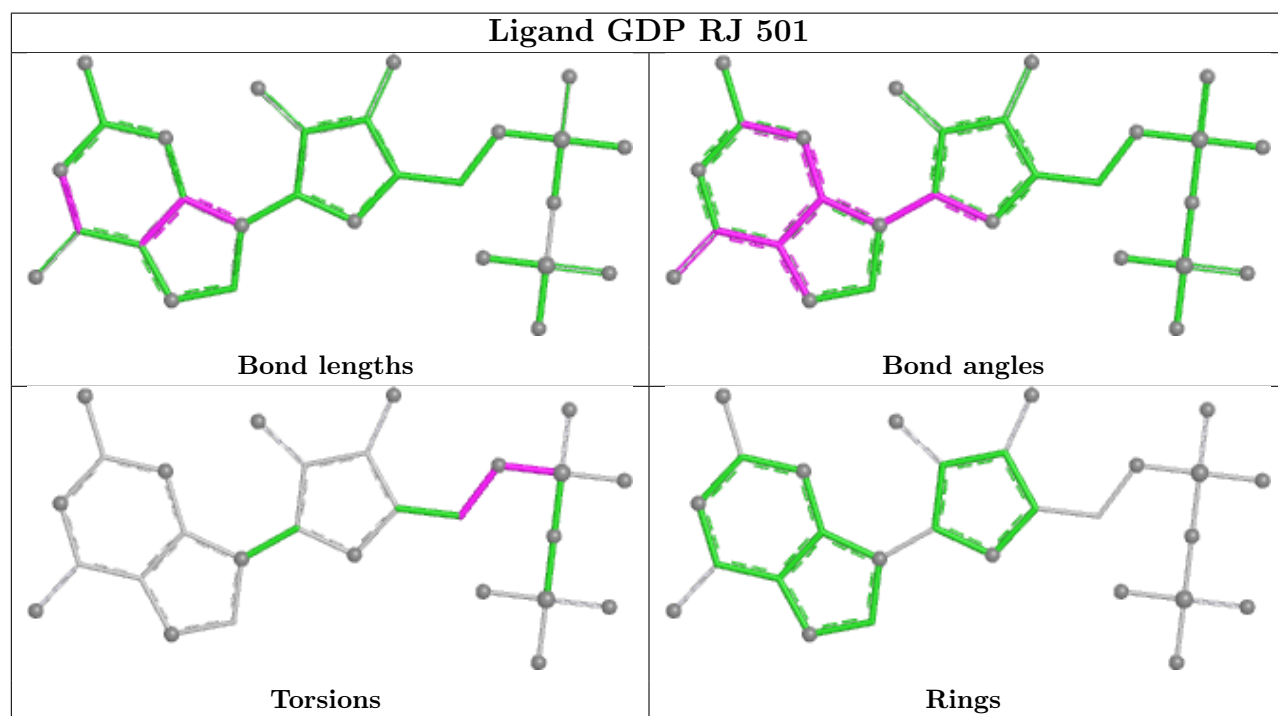
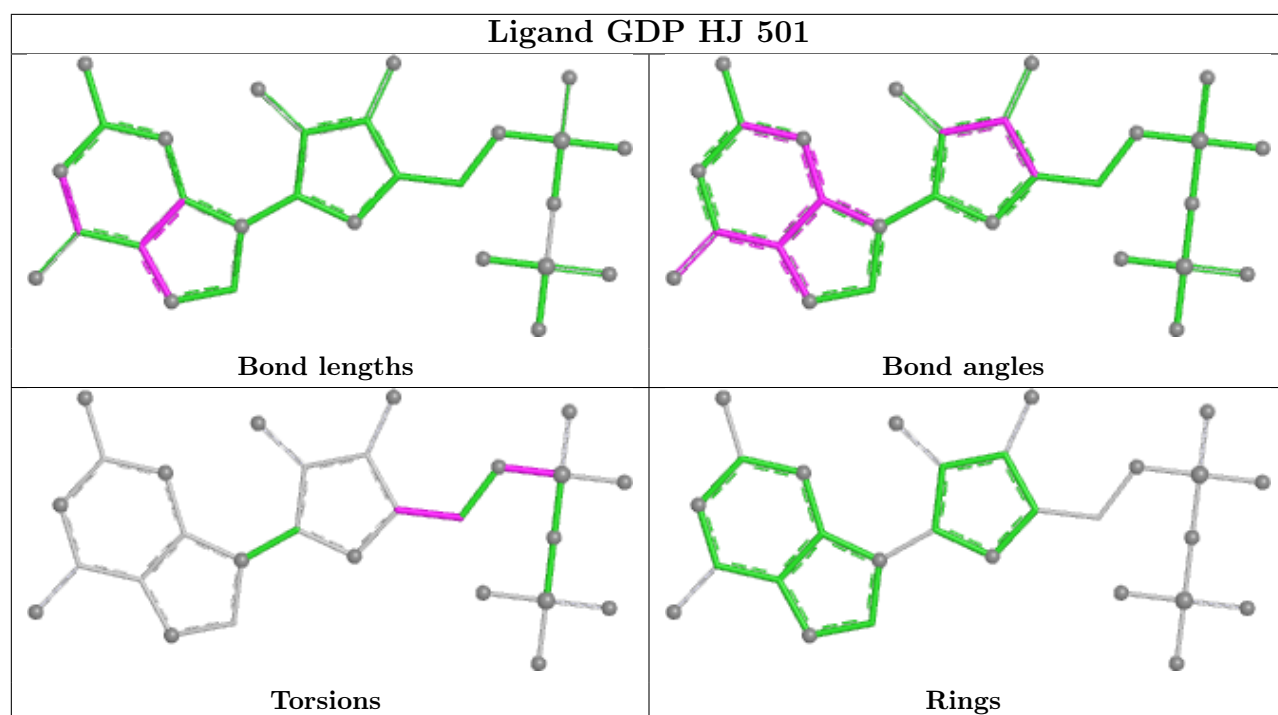


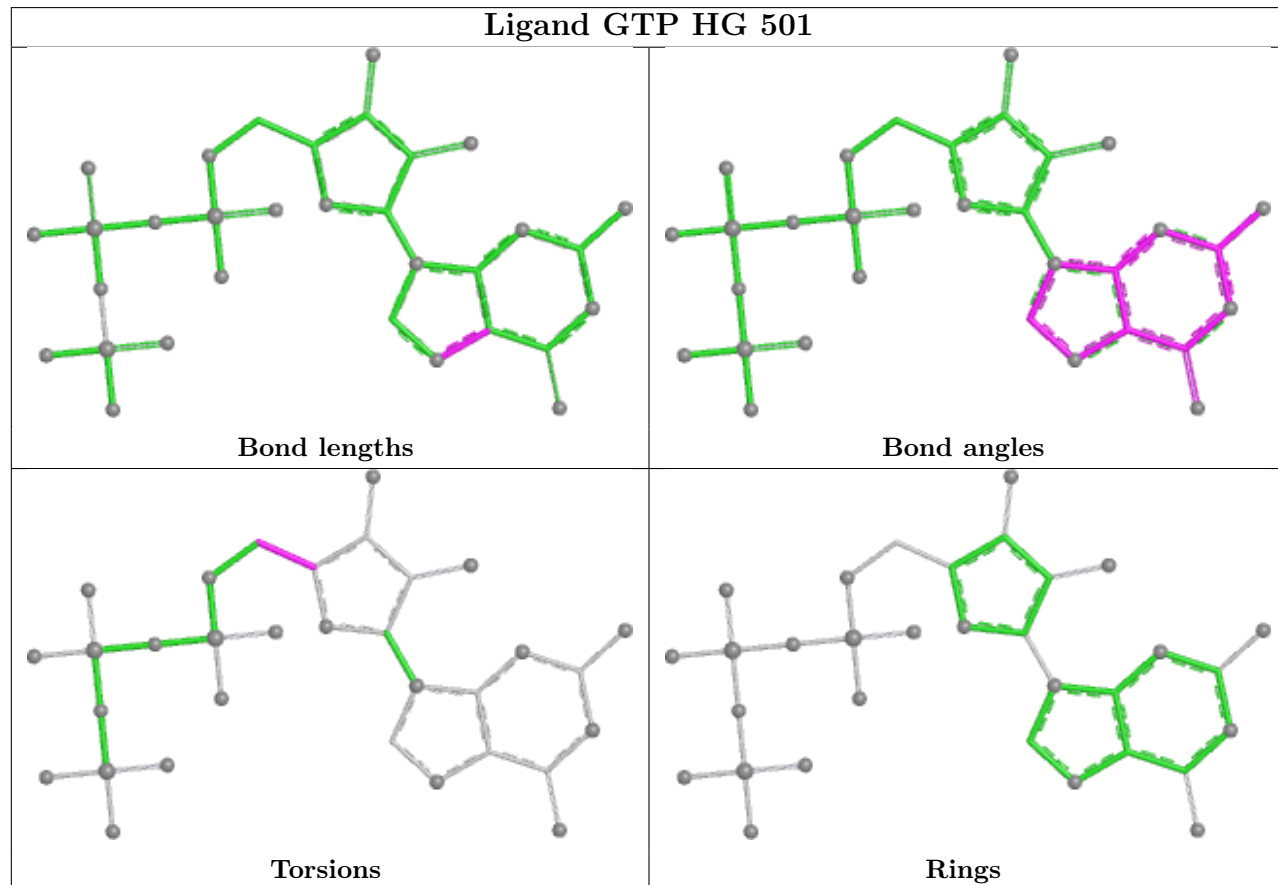
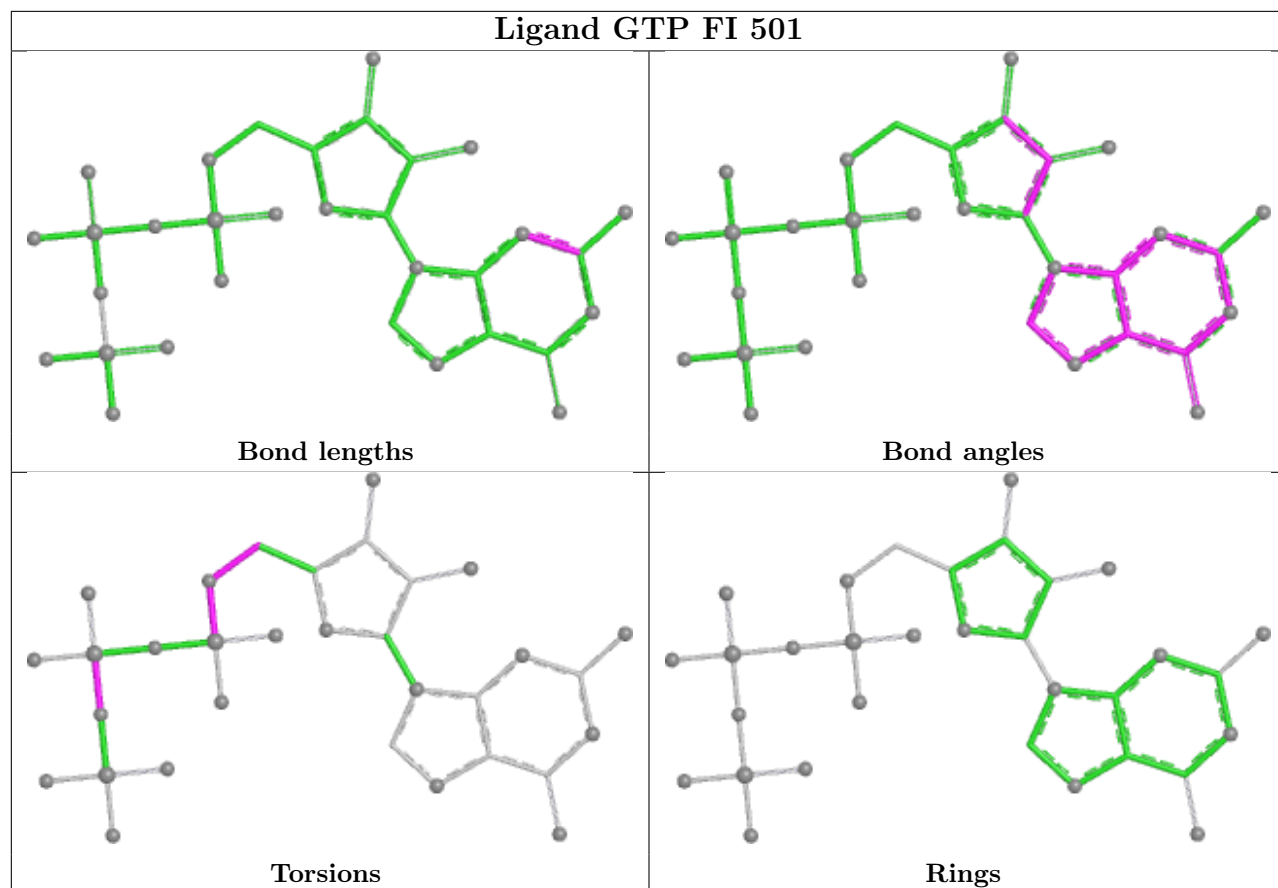
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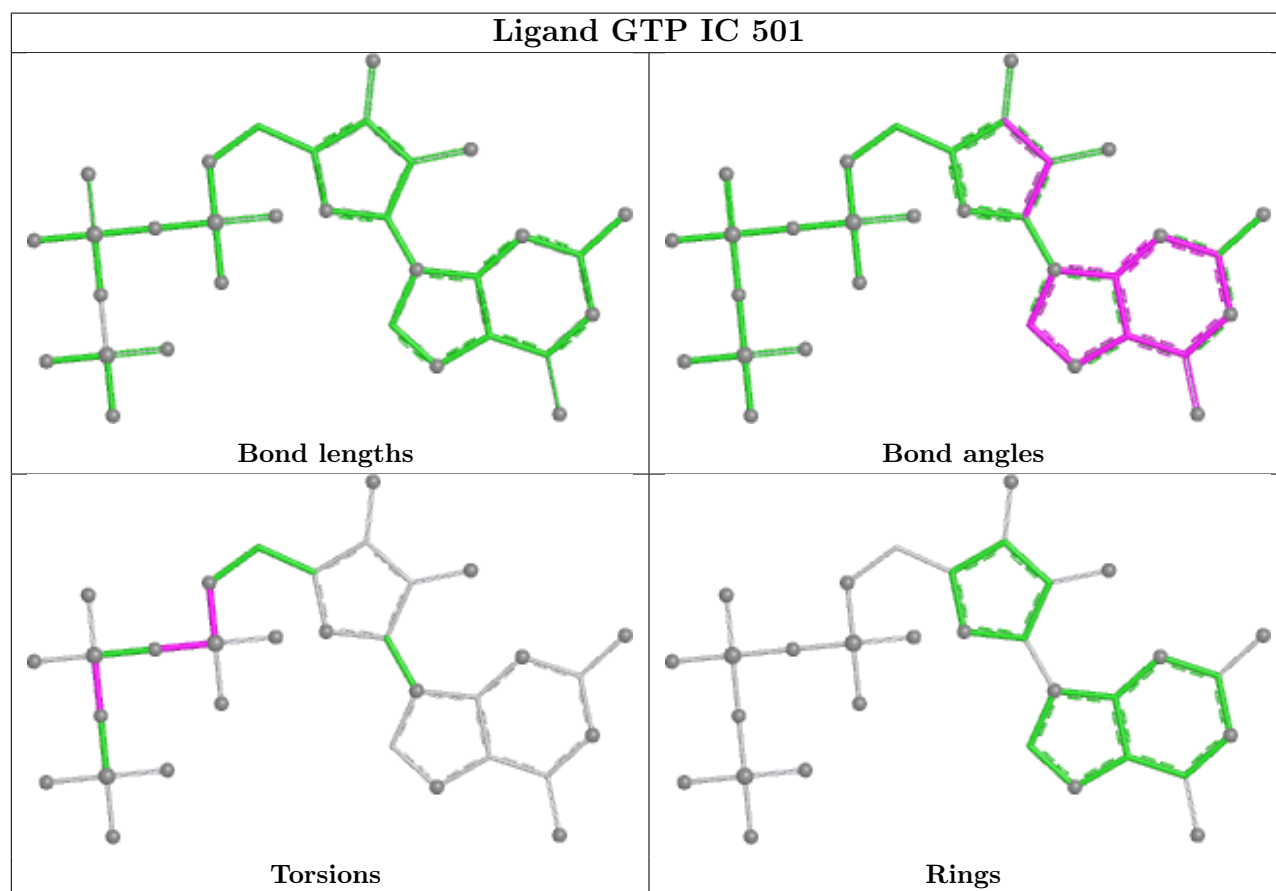
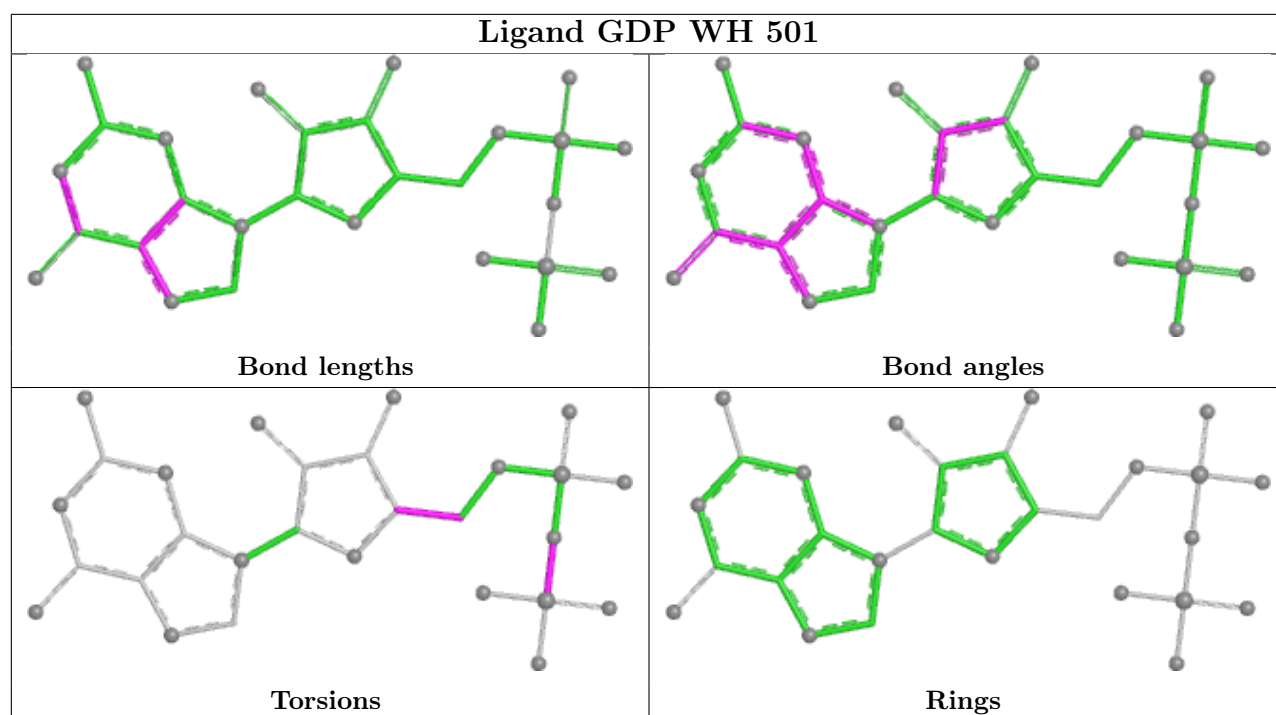
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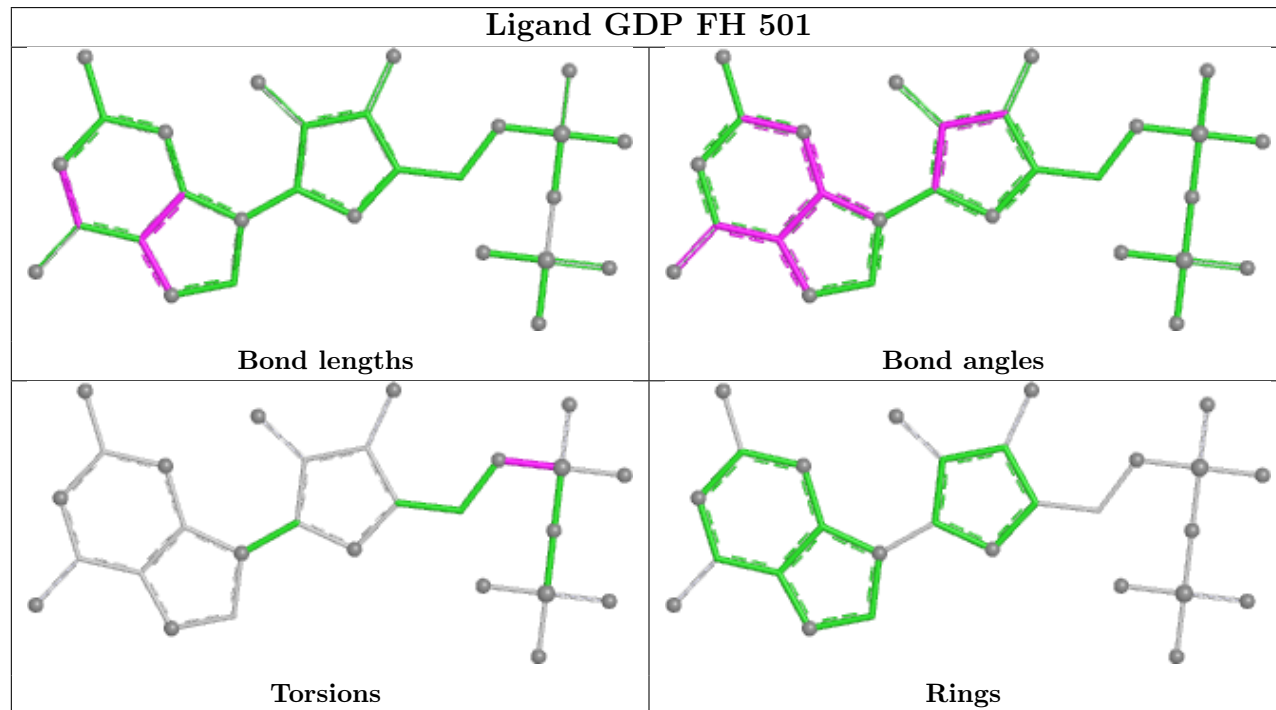
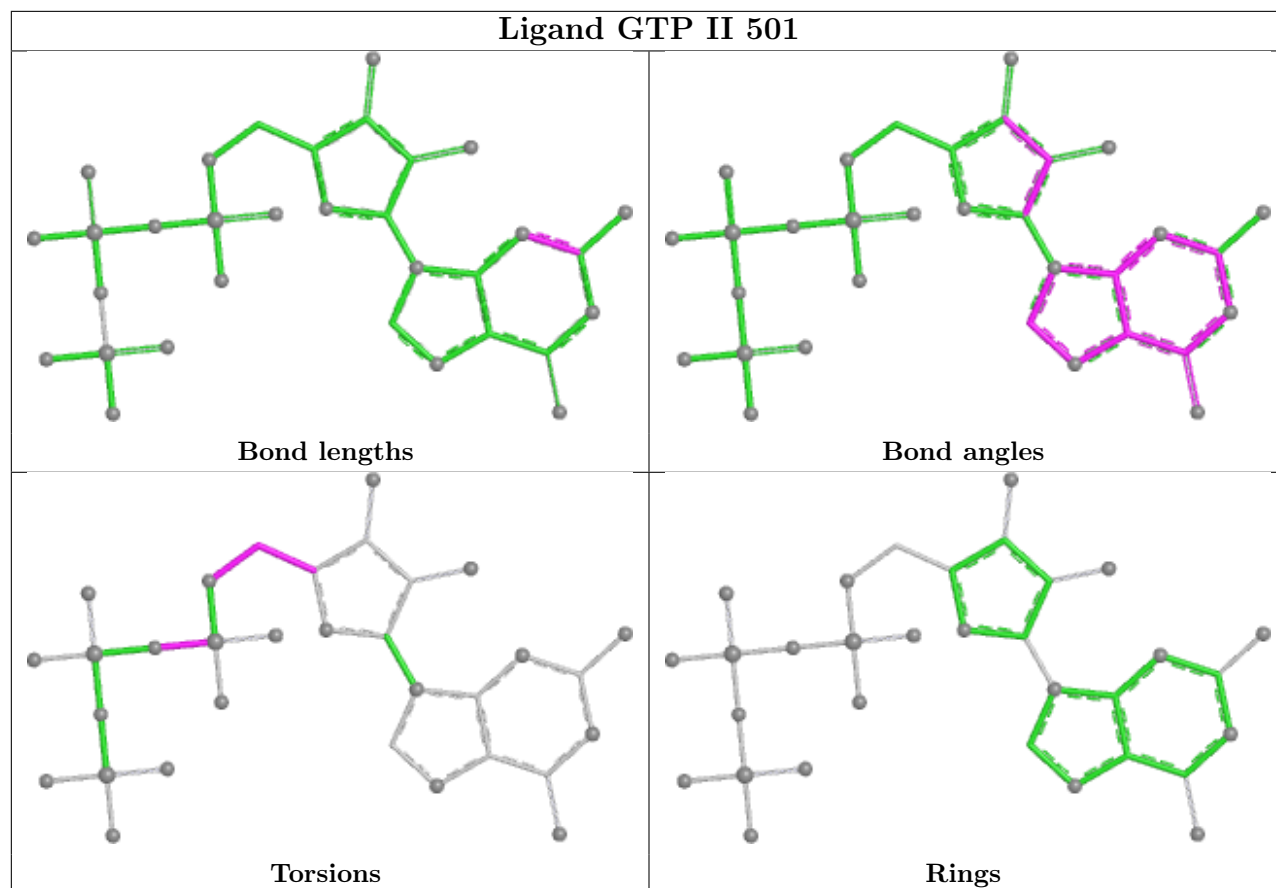


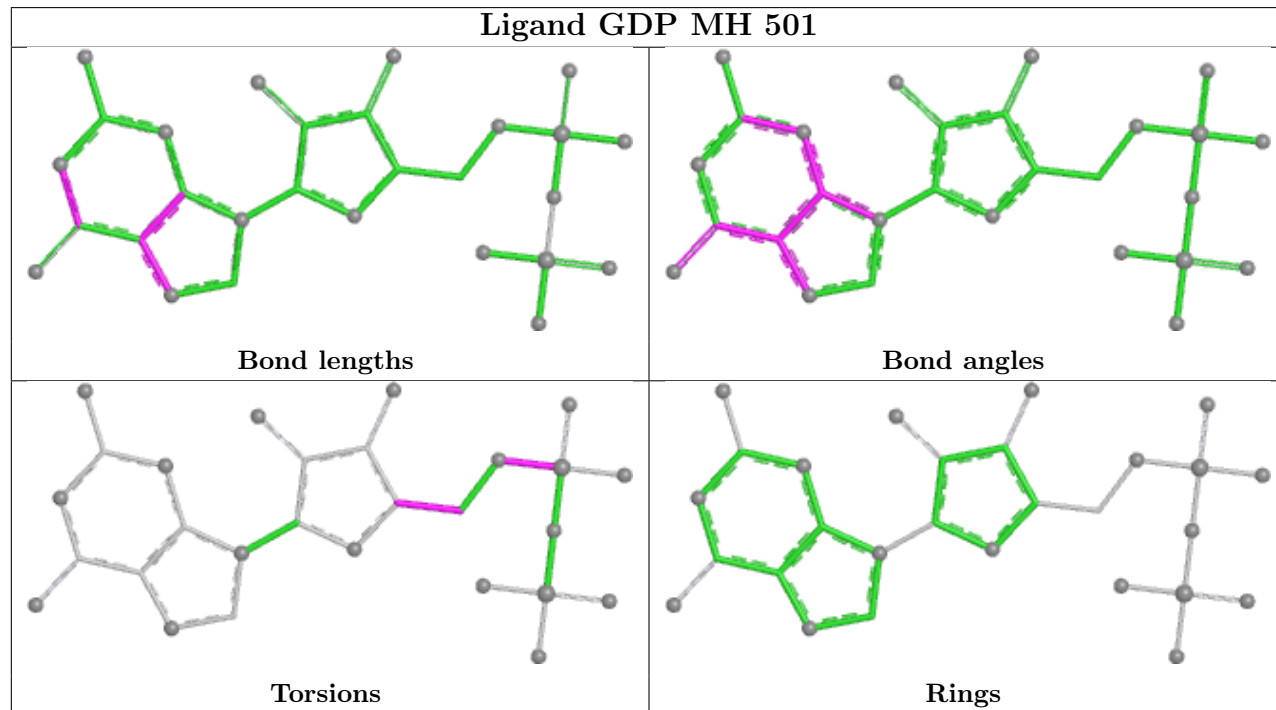
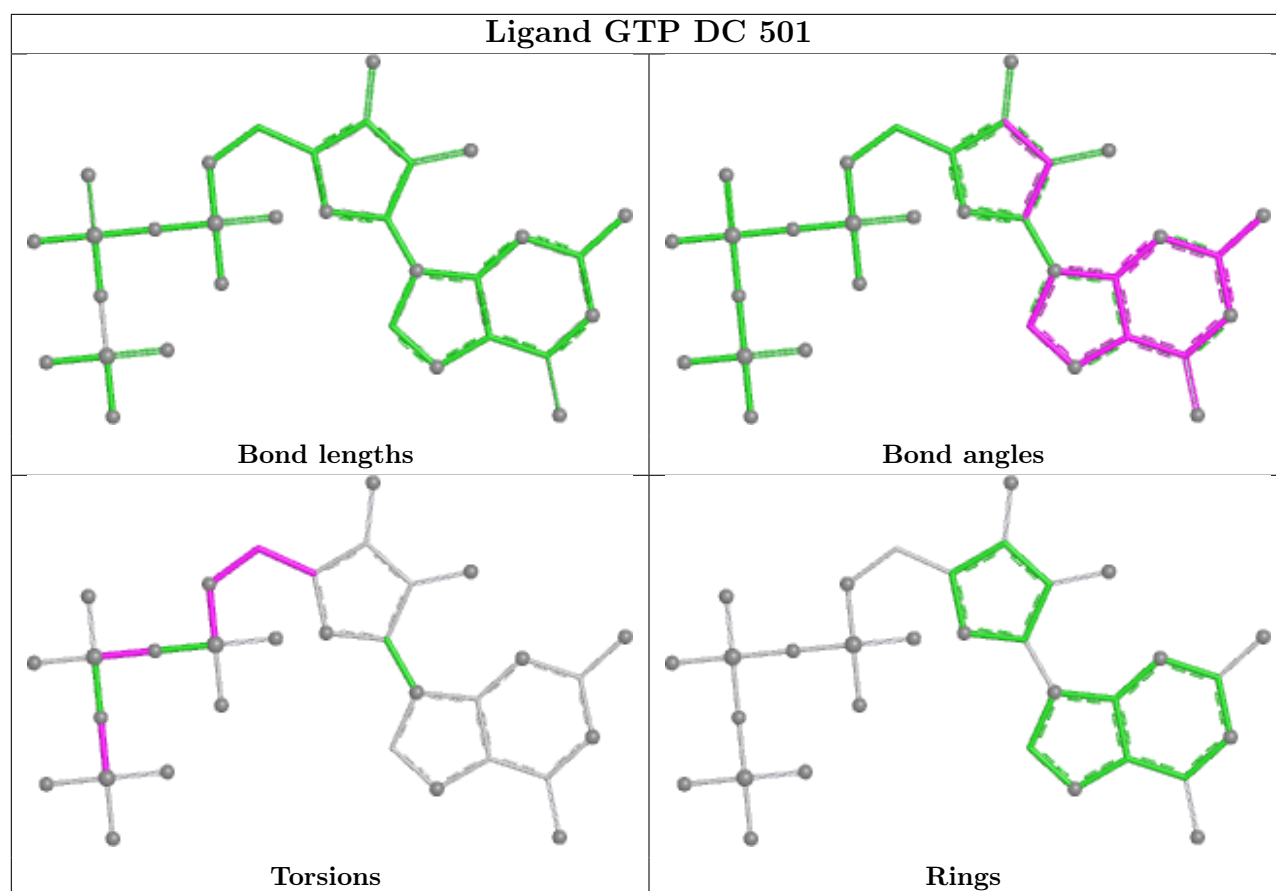


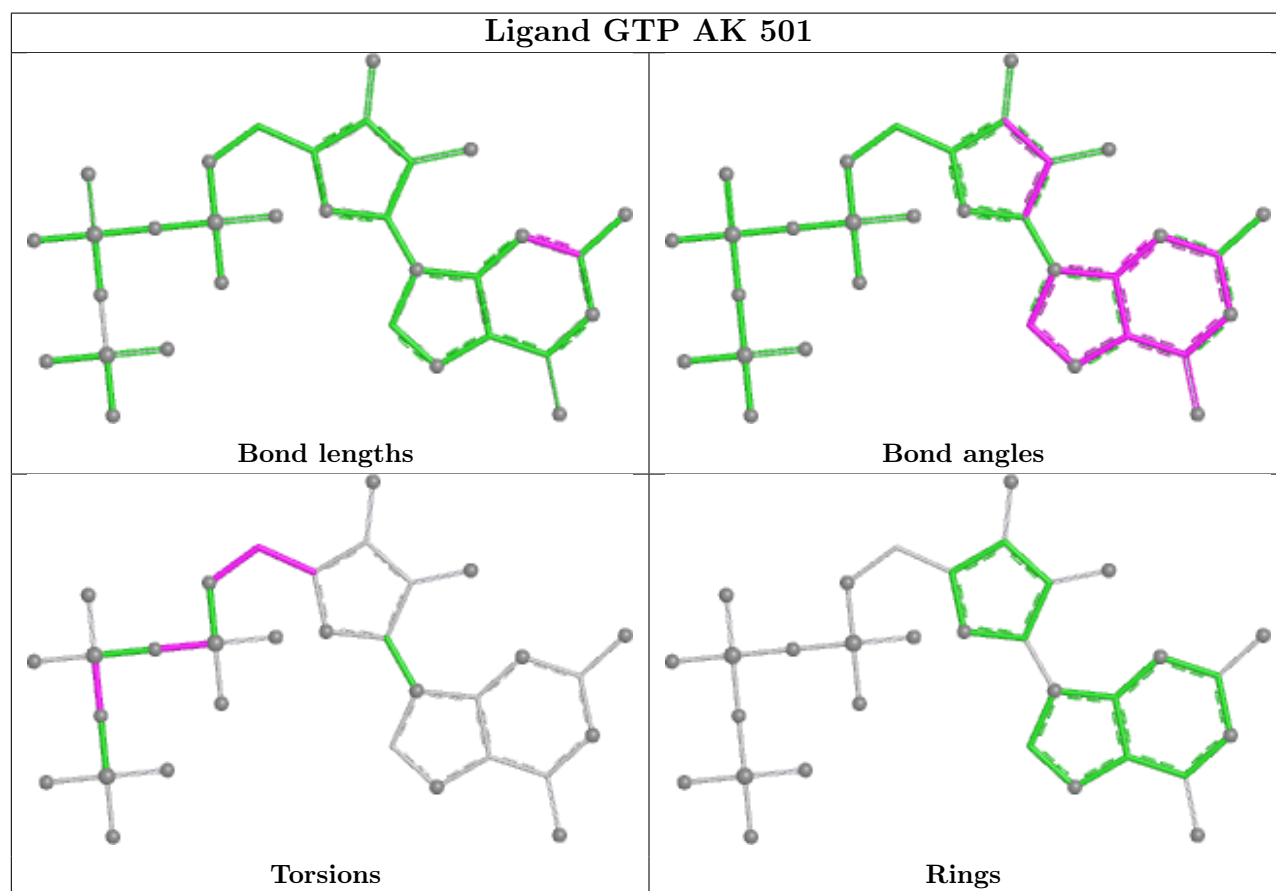
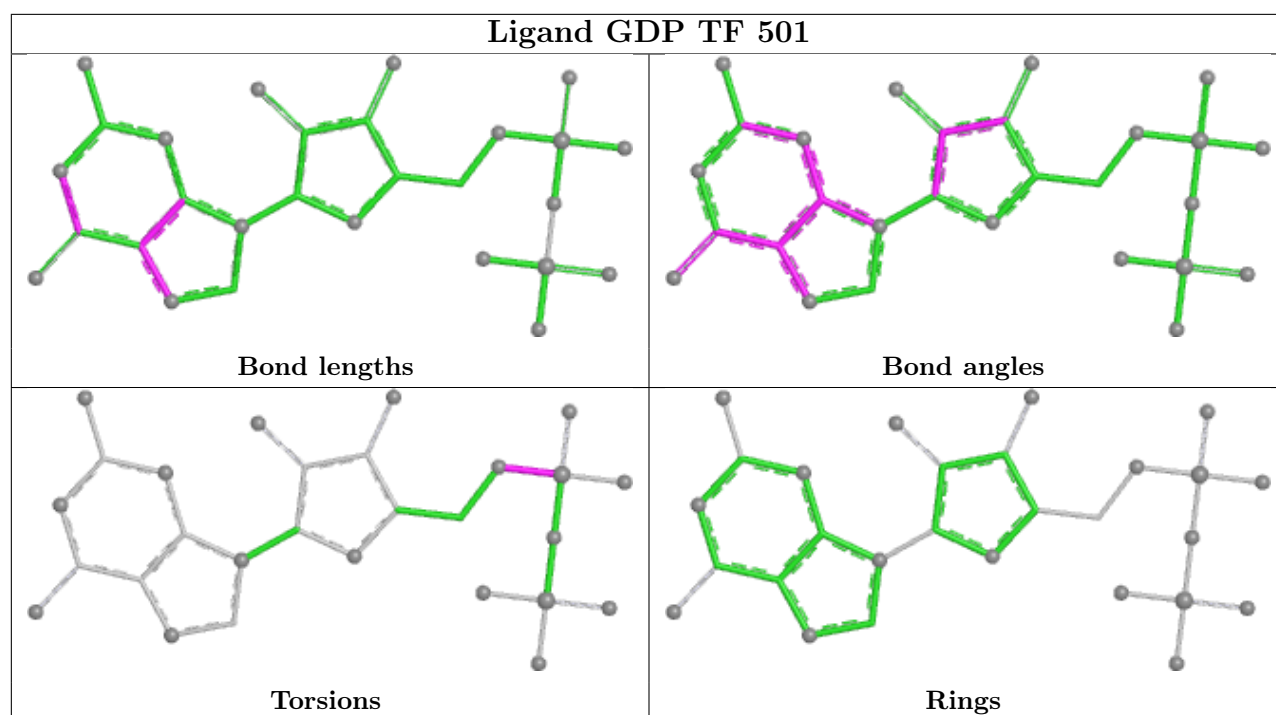




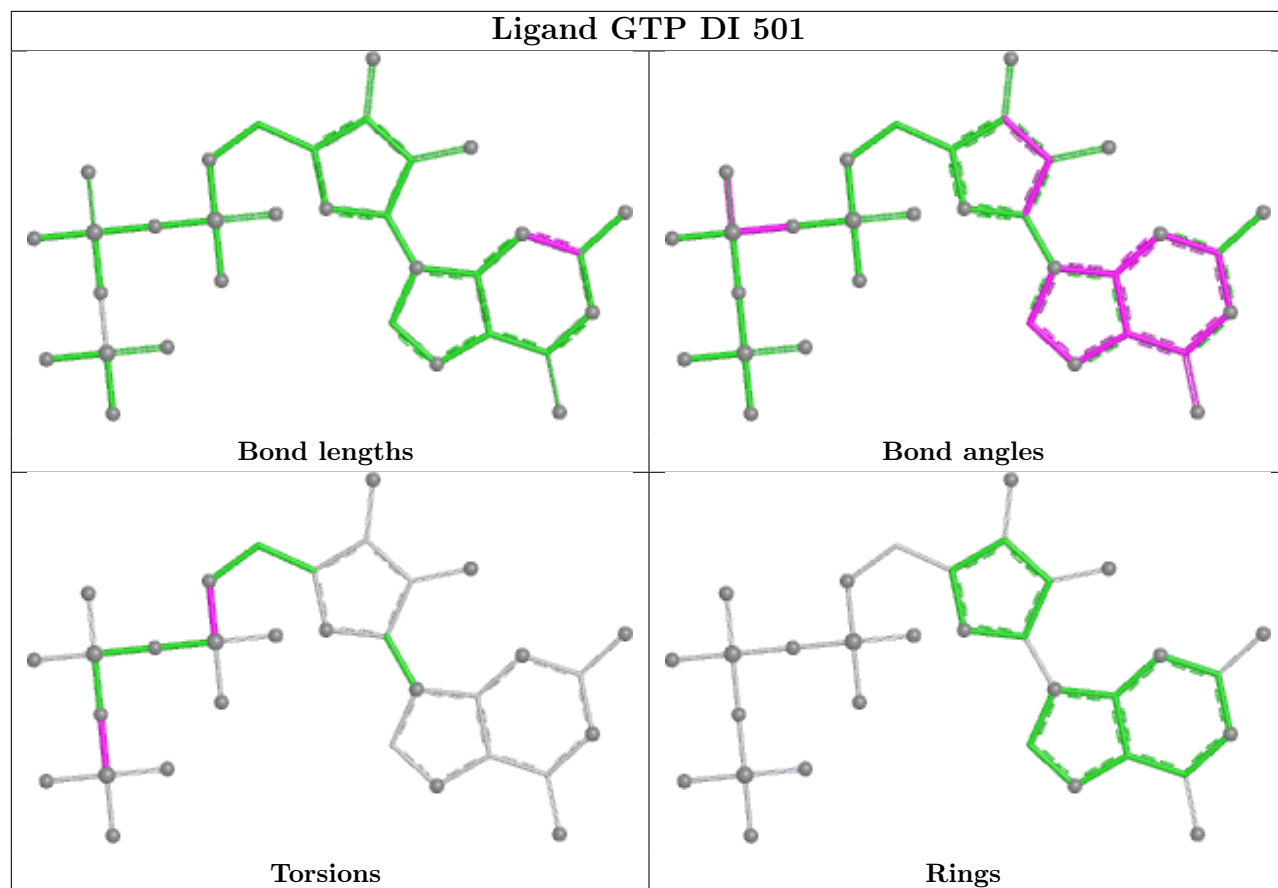




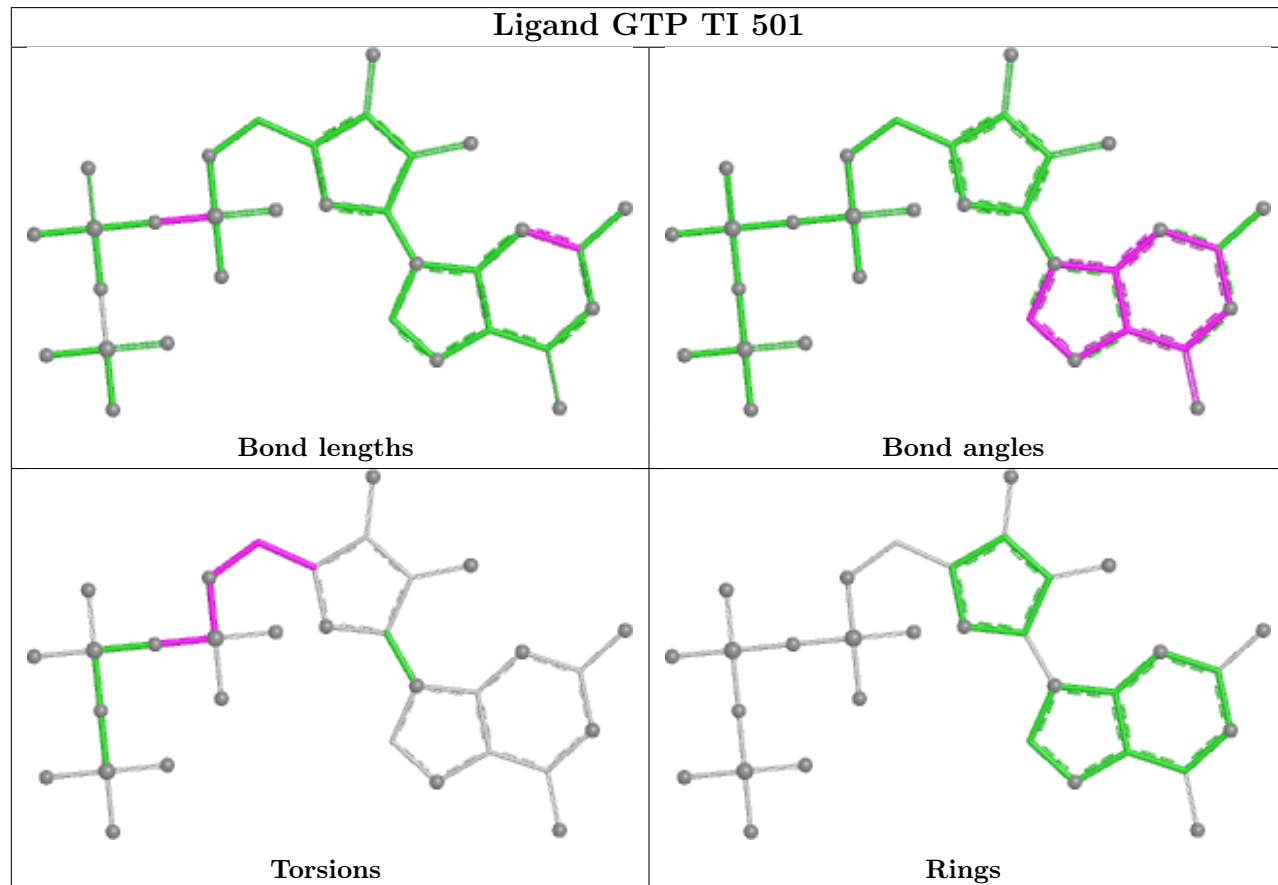


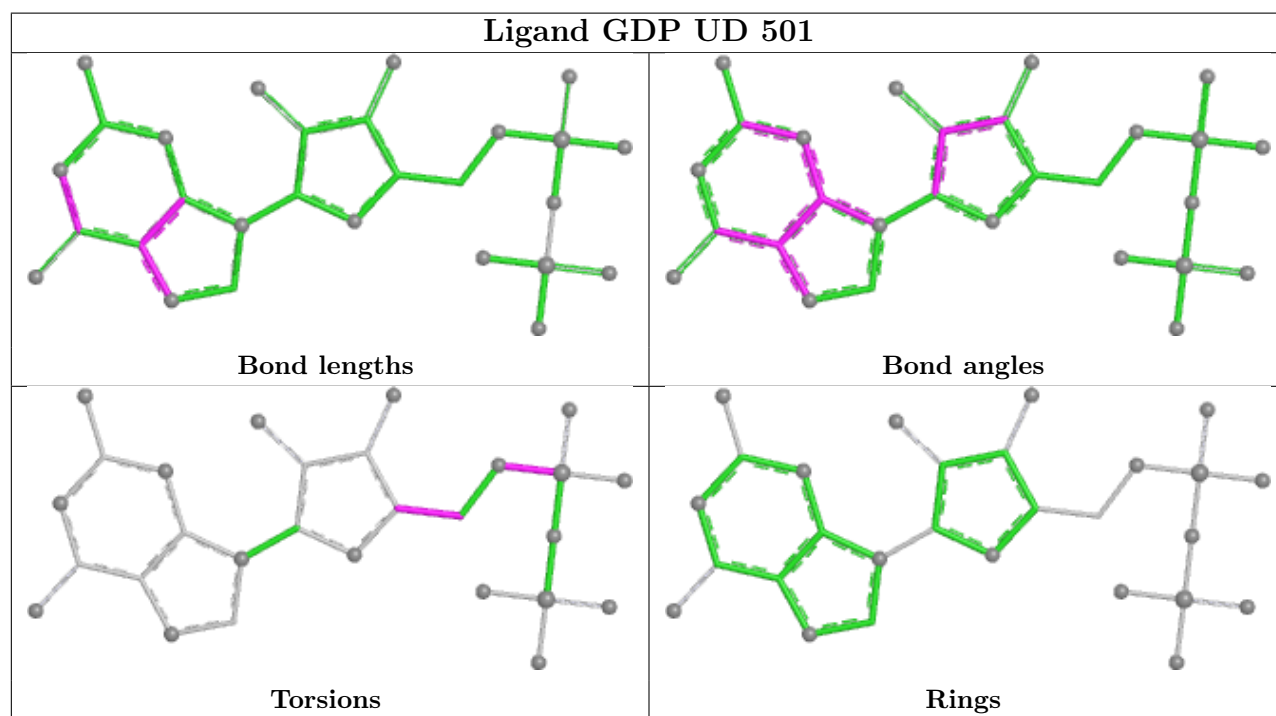
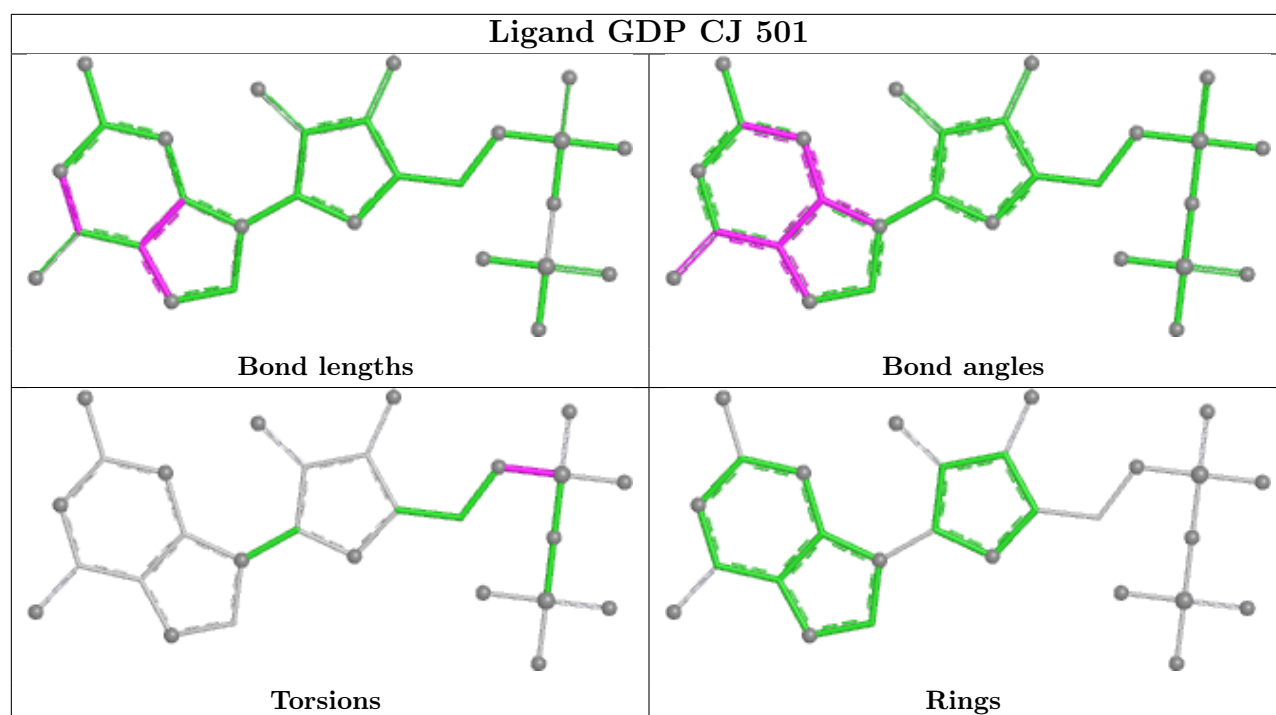


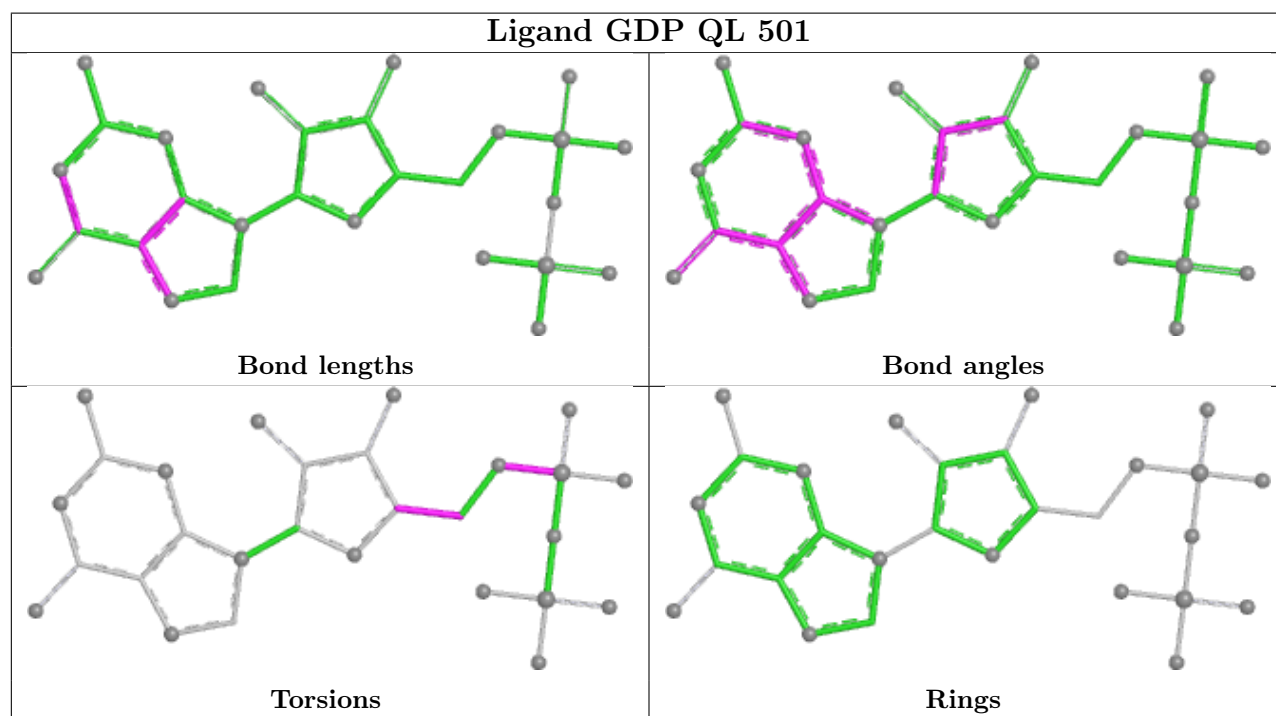
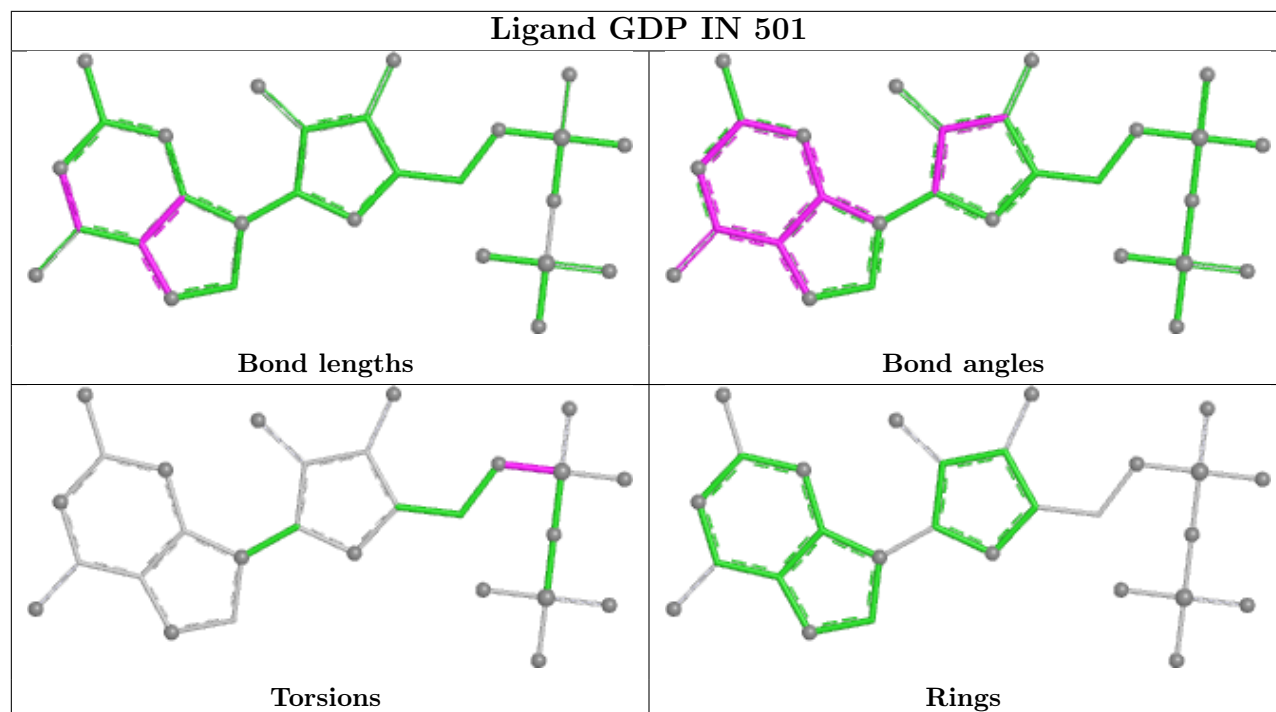
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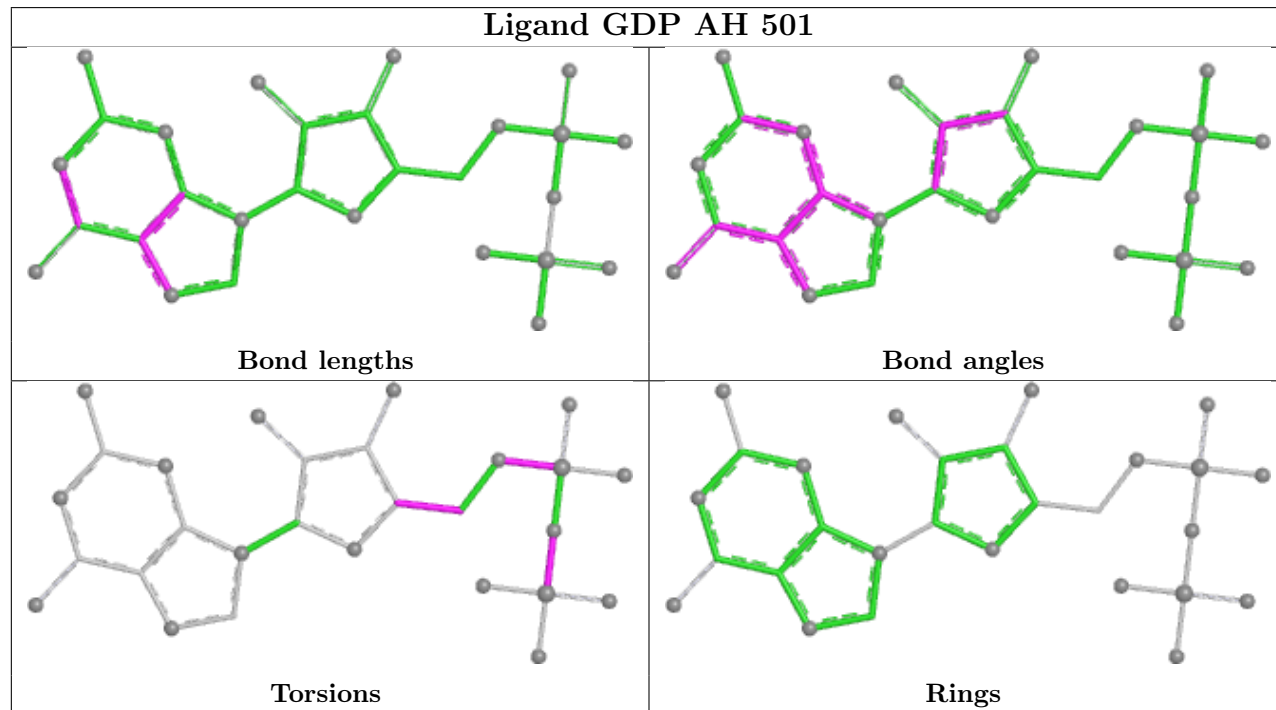
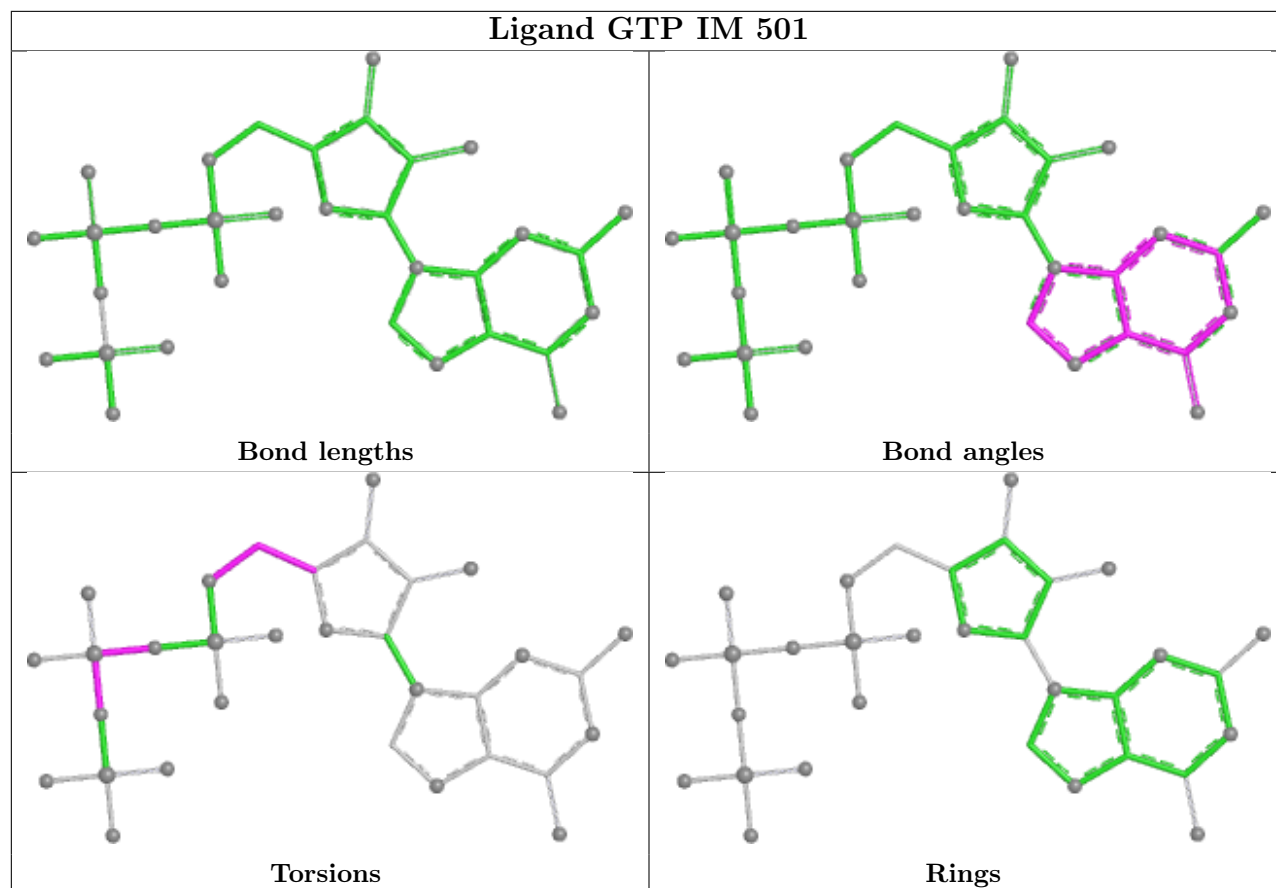


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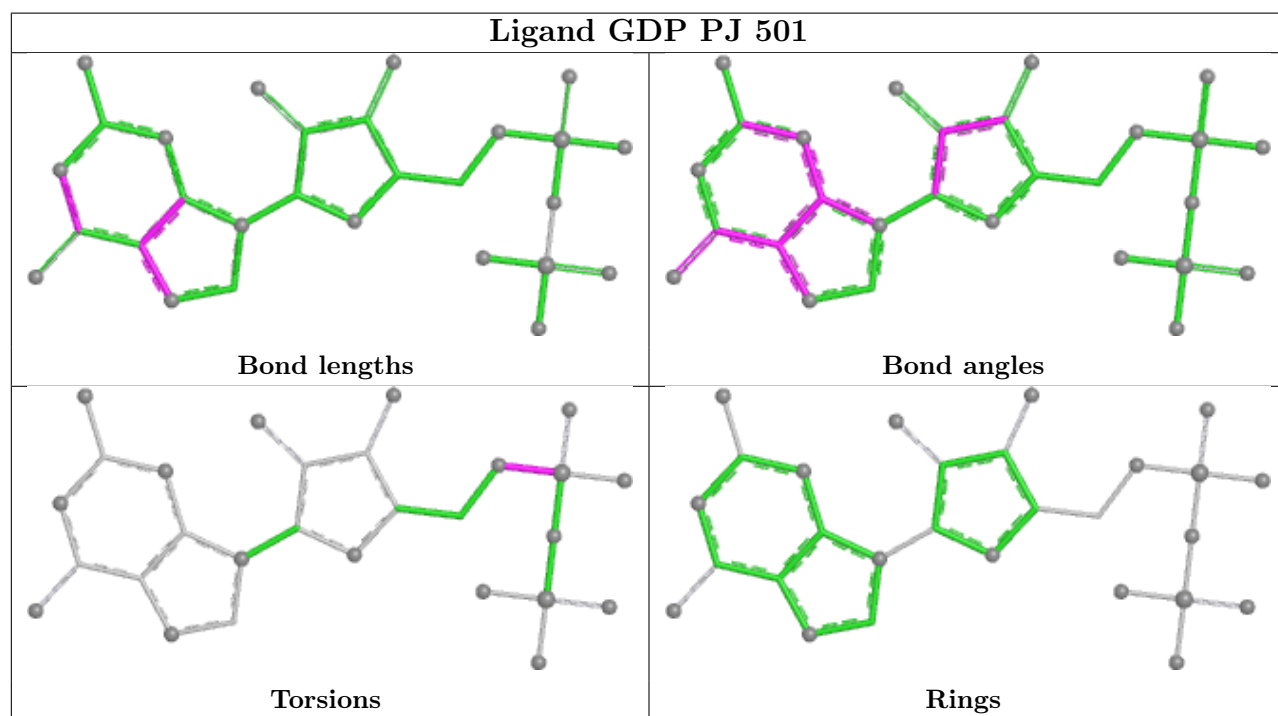
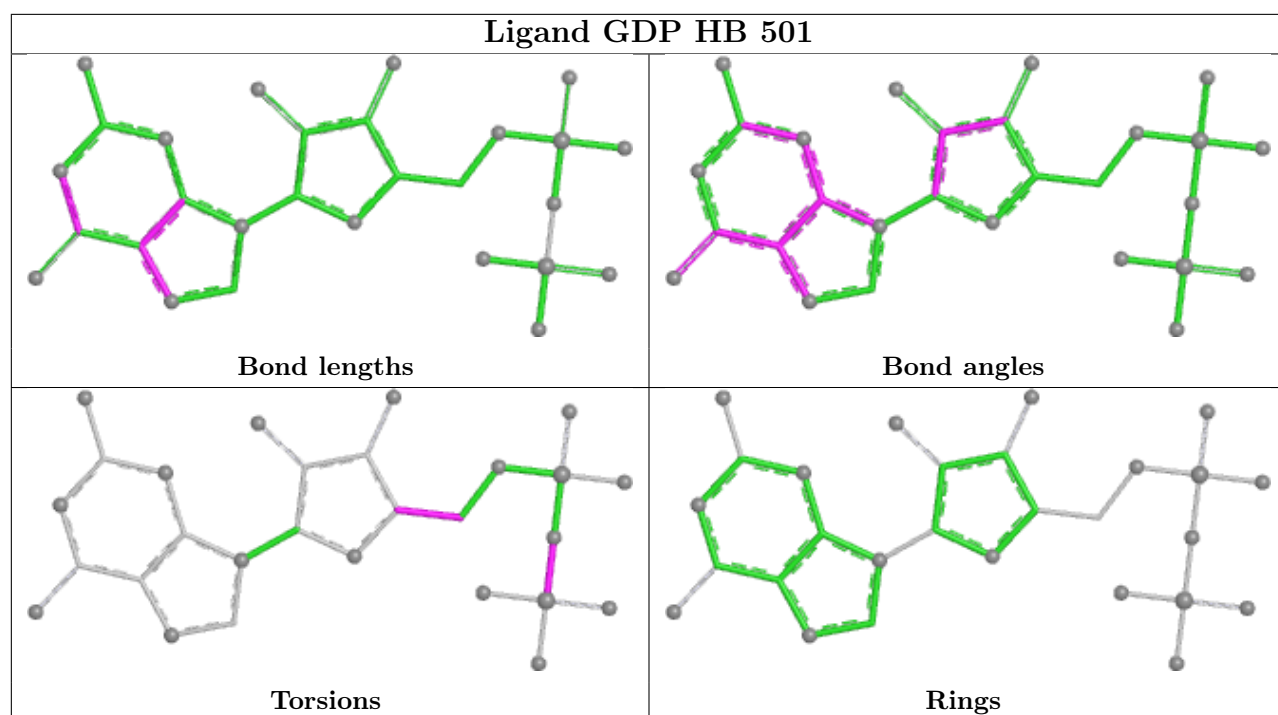




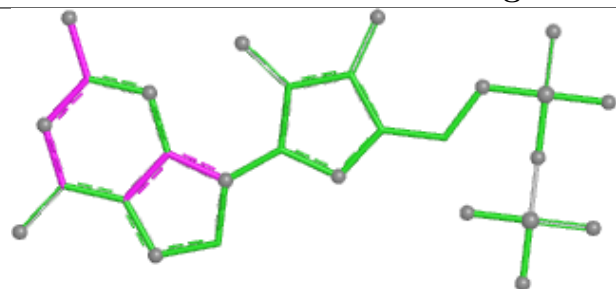




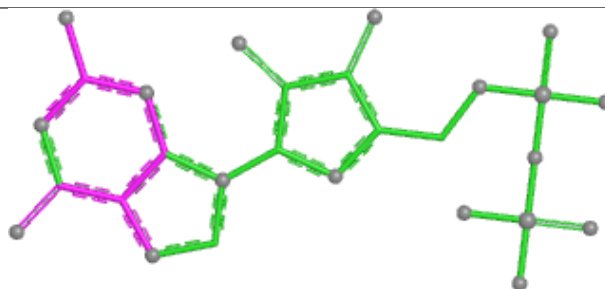




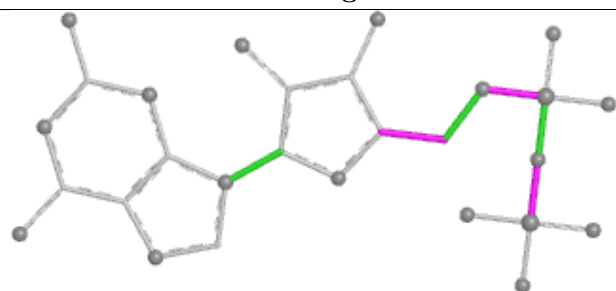
## Ligand GDP UJ 501



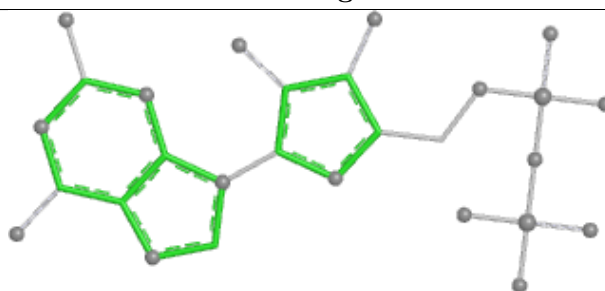
Bond lengths



Bond angles

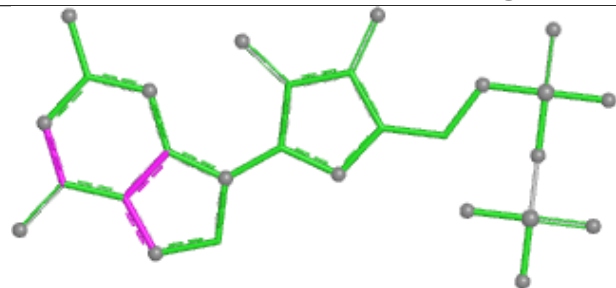


Torsions

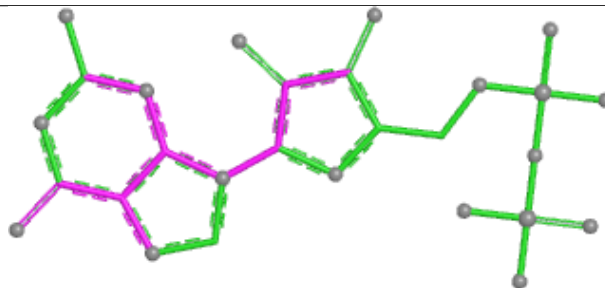


Rings

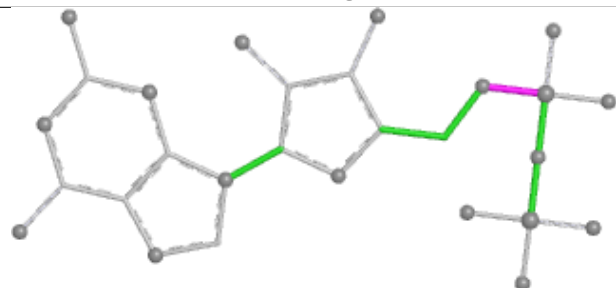
## Ligand GDP TH 501



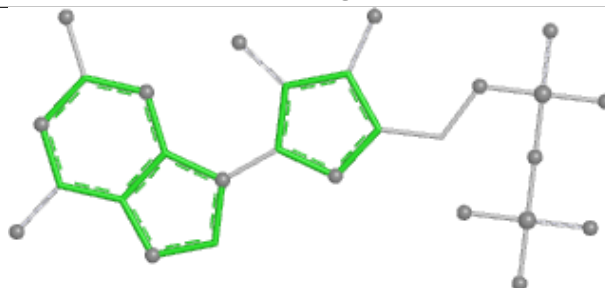
Bond lengths



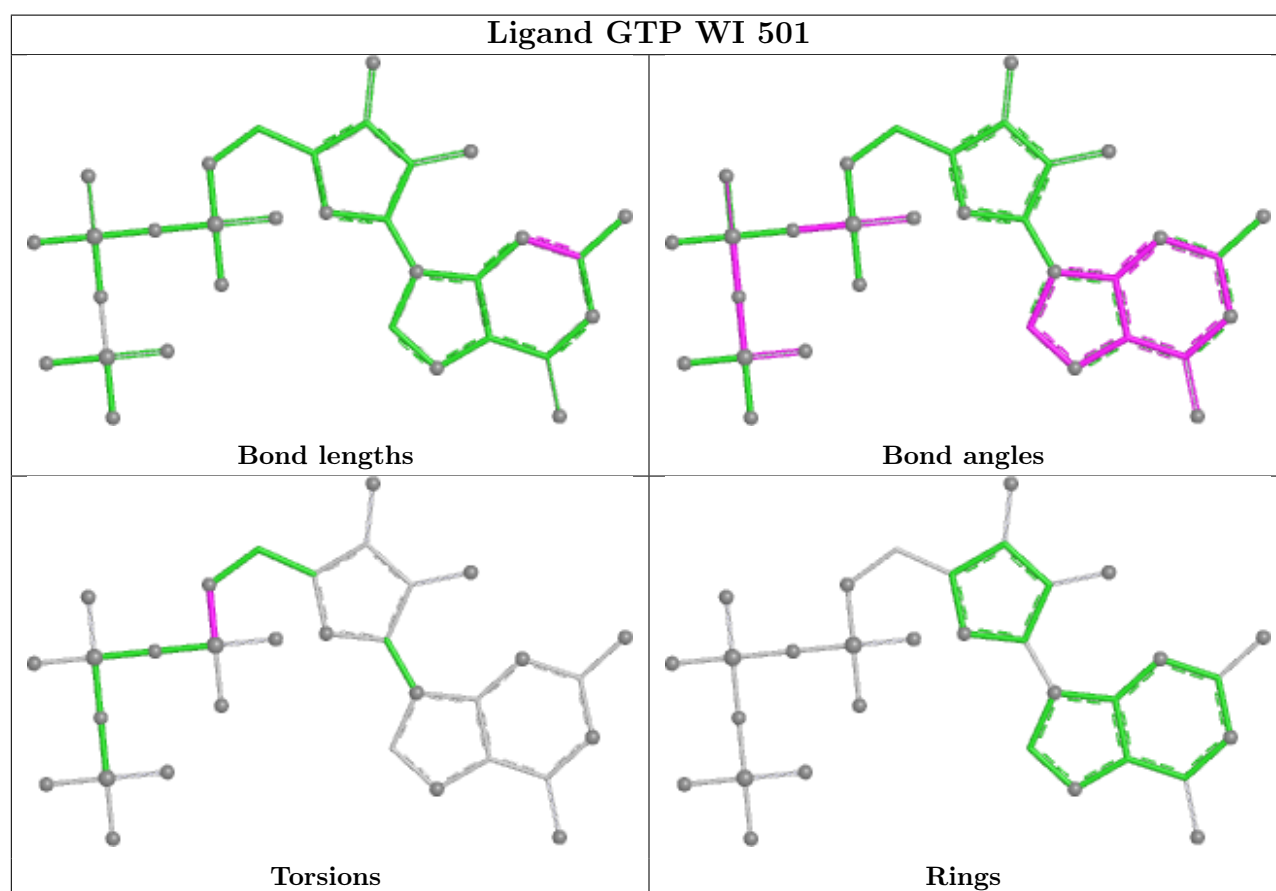
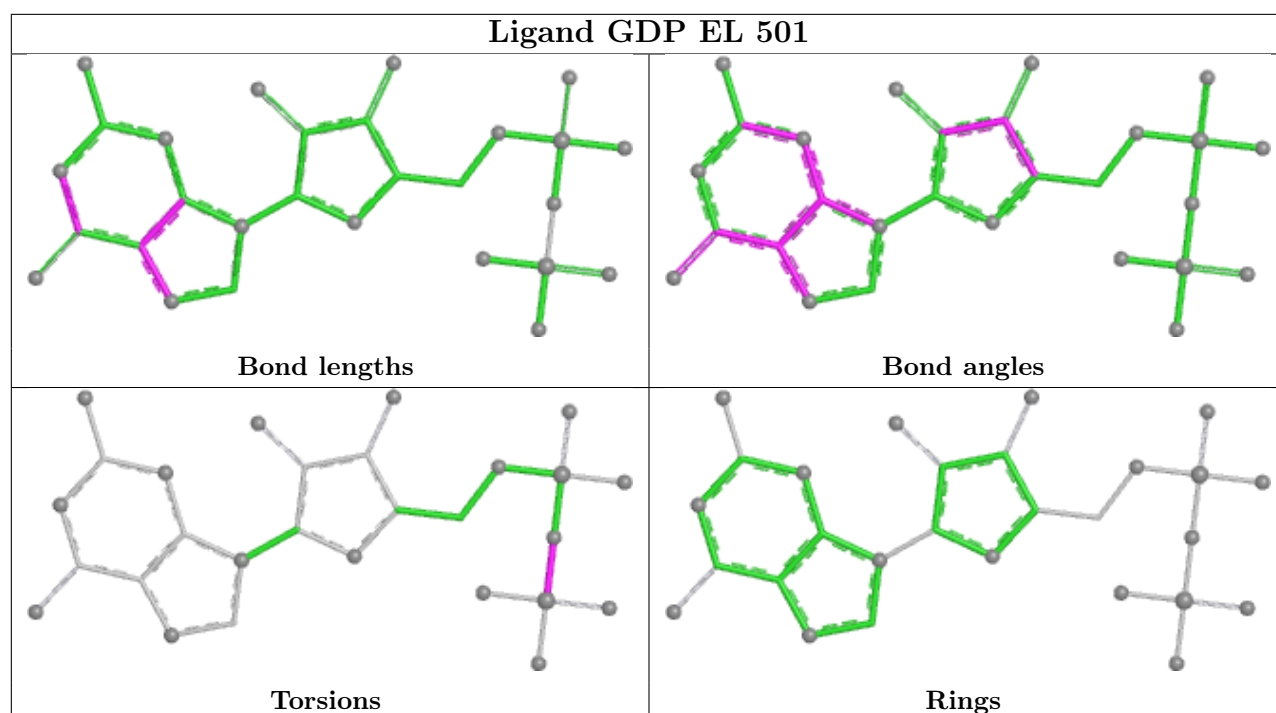
Bond angles



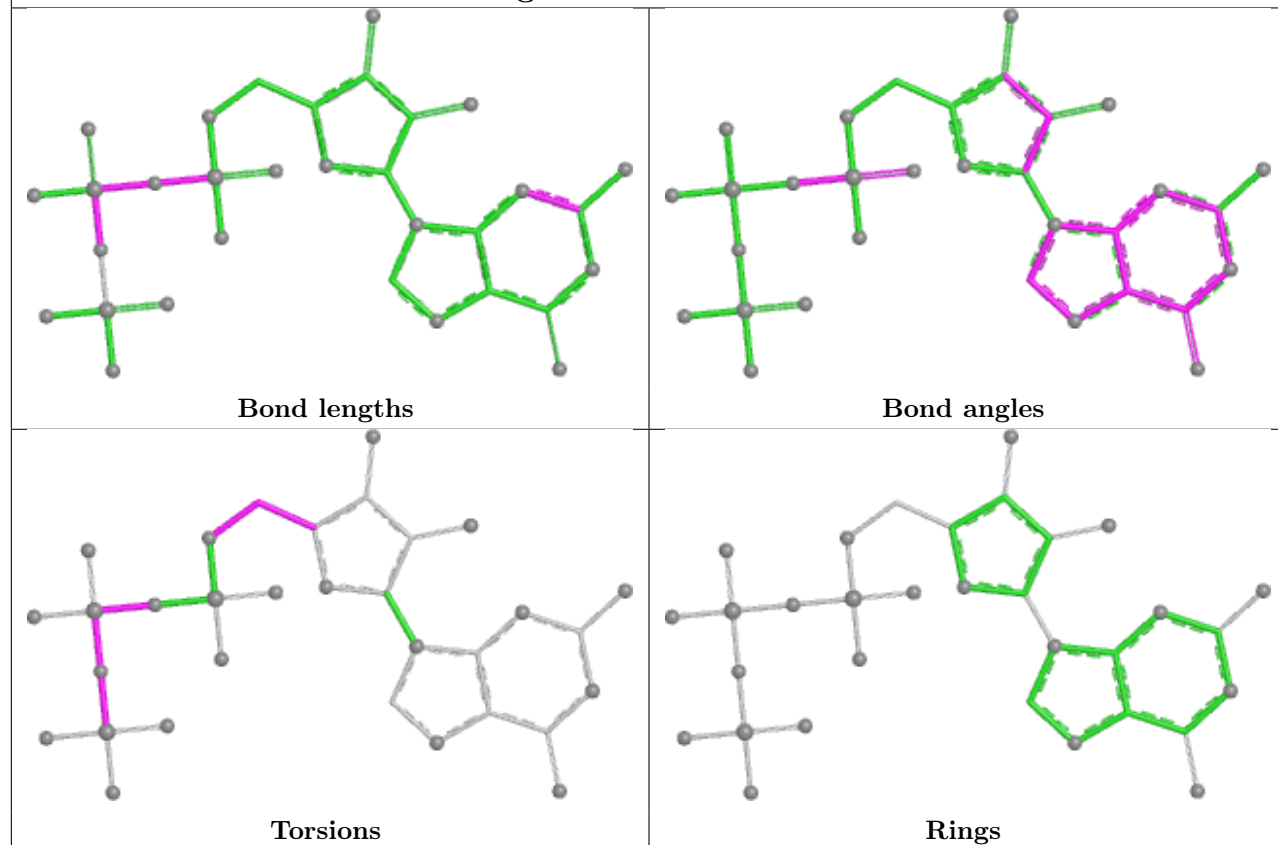
Torsions



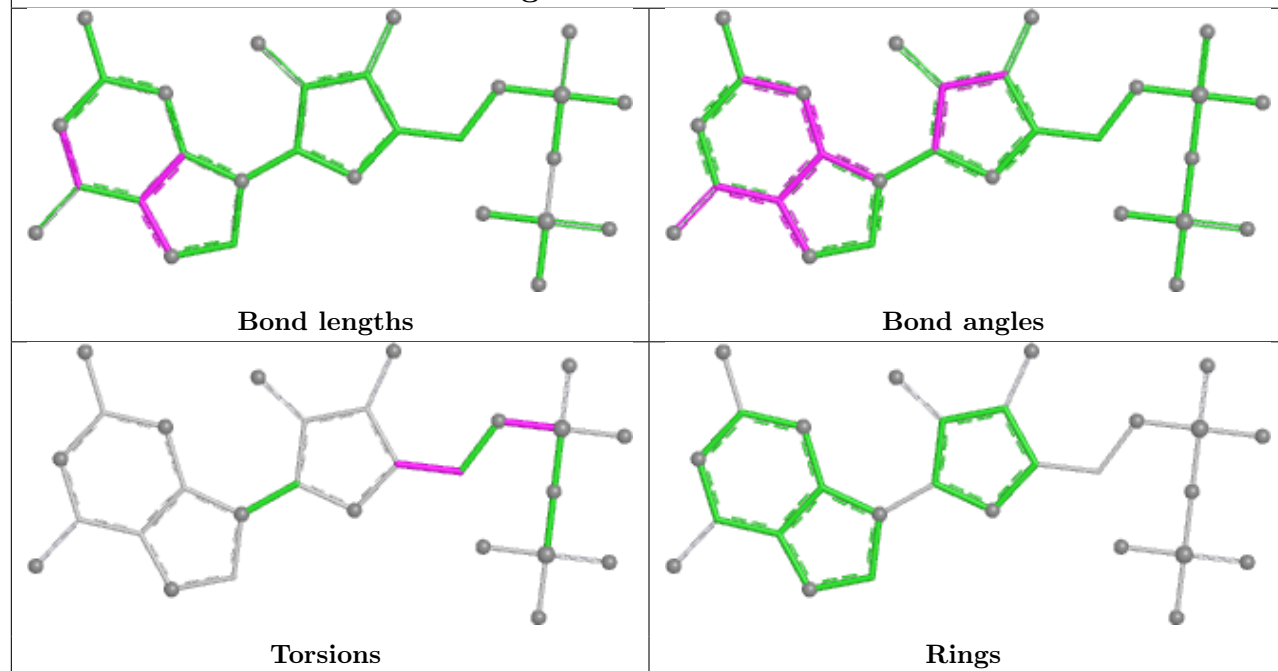
Rings

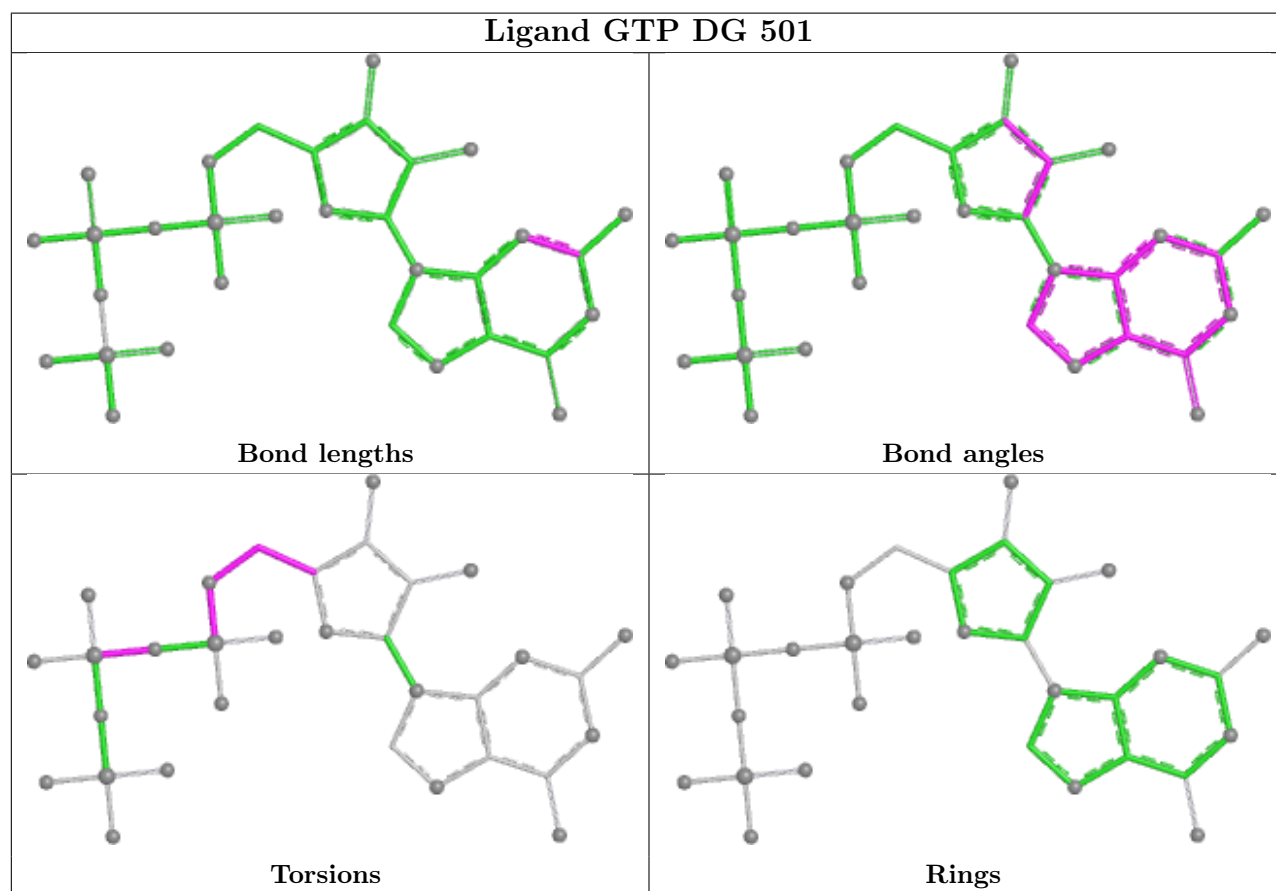
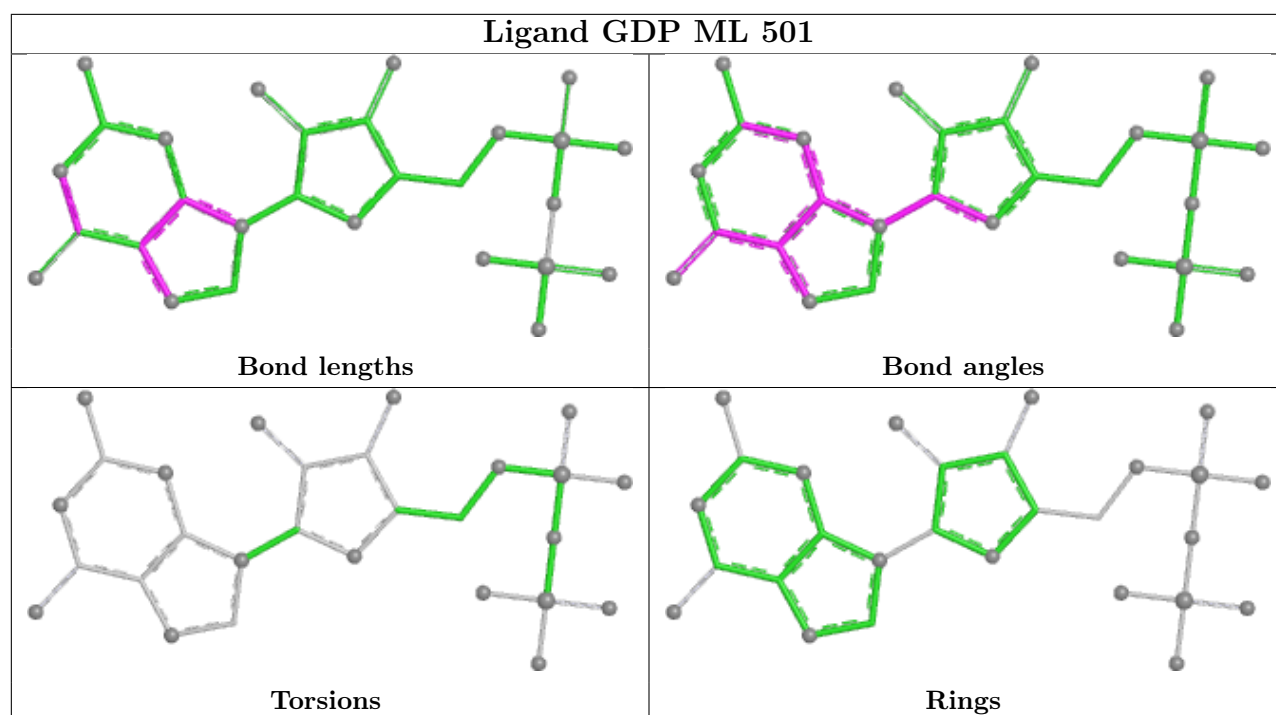


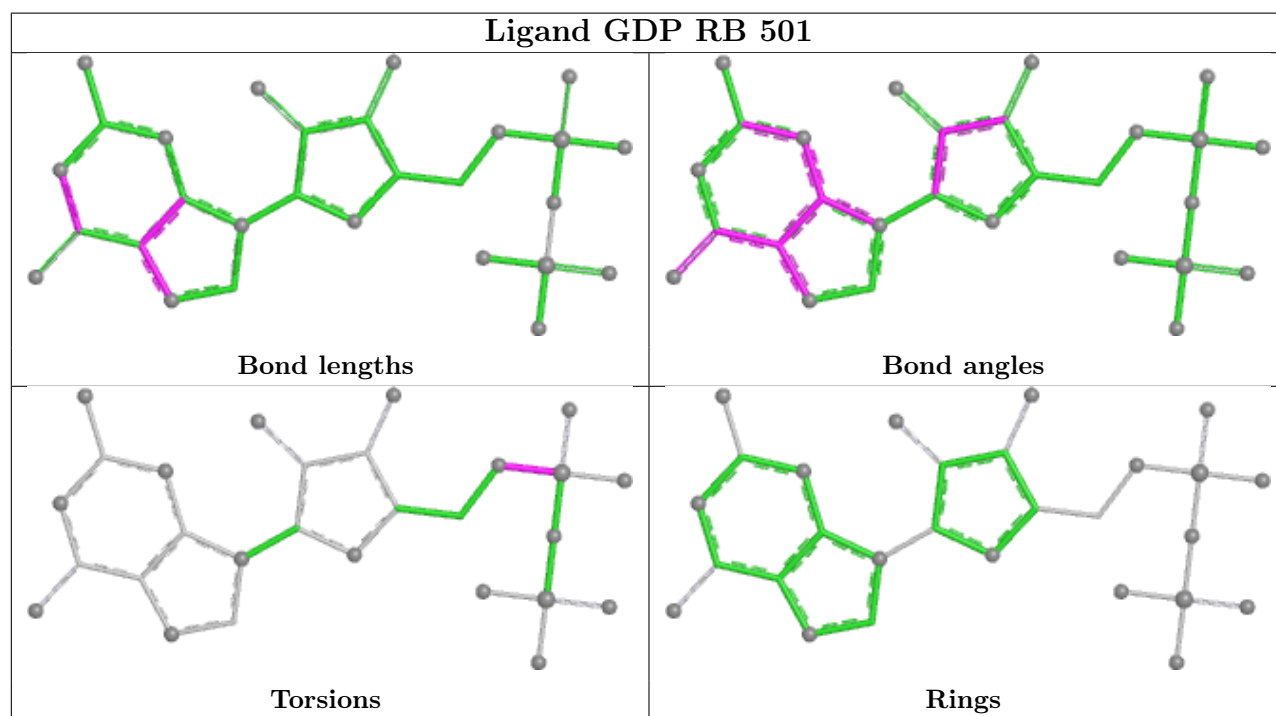
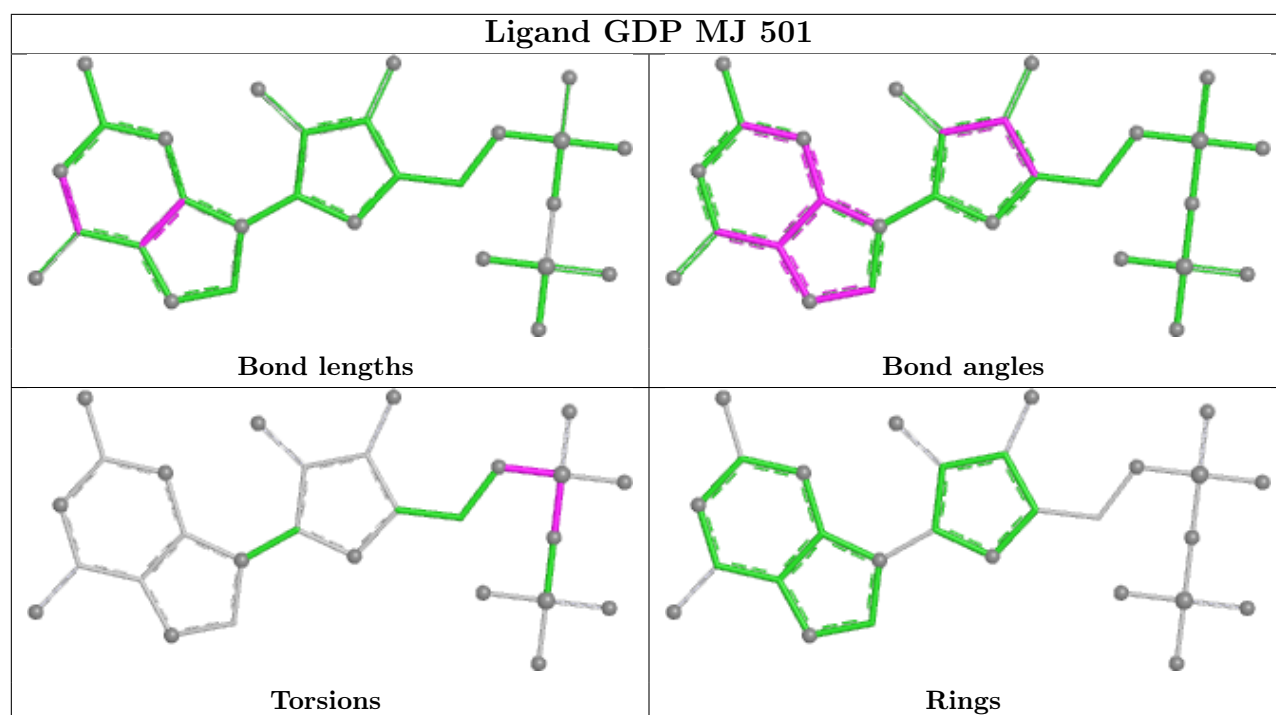
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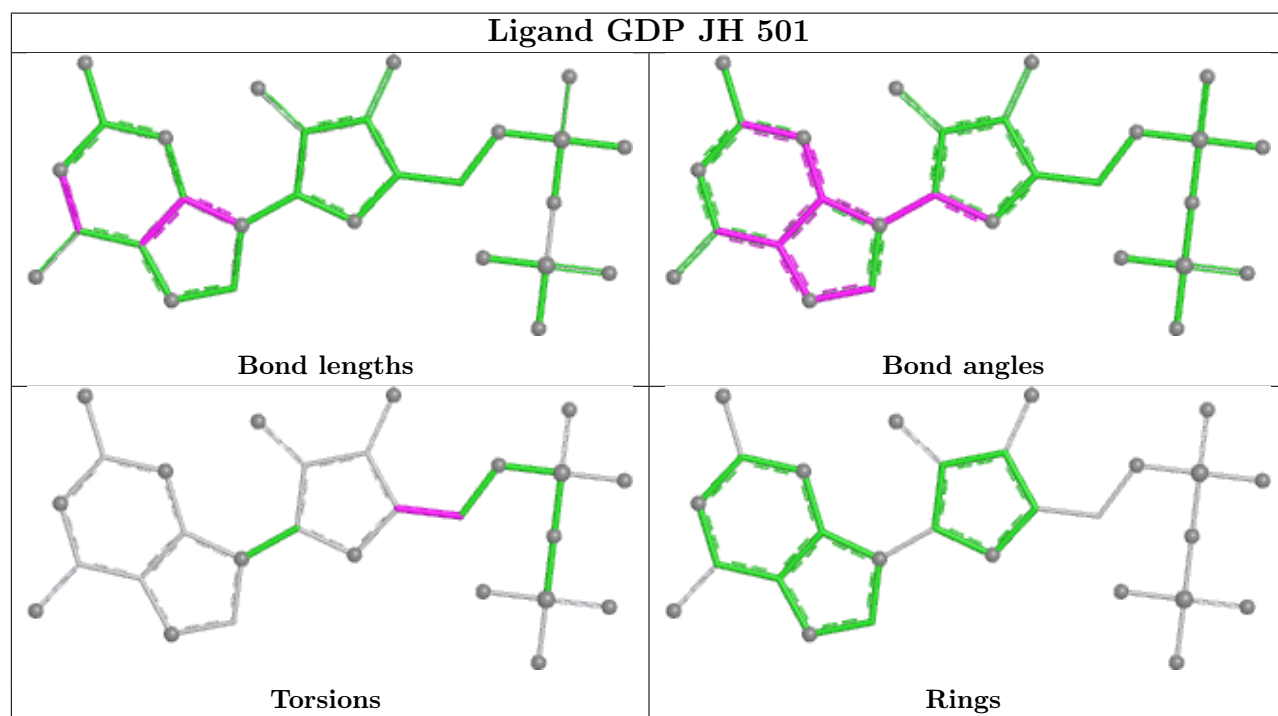
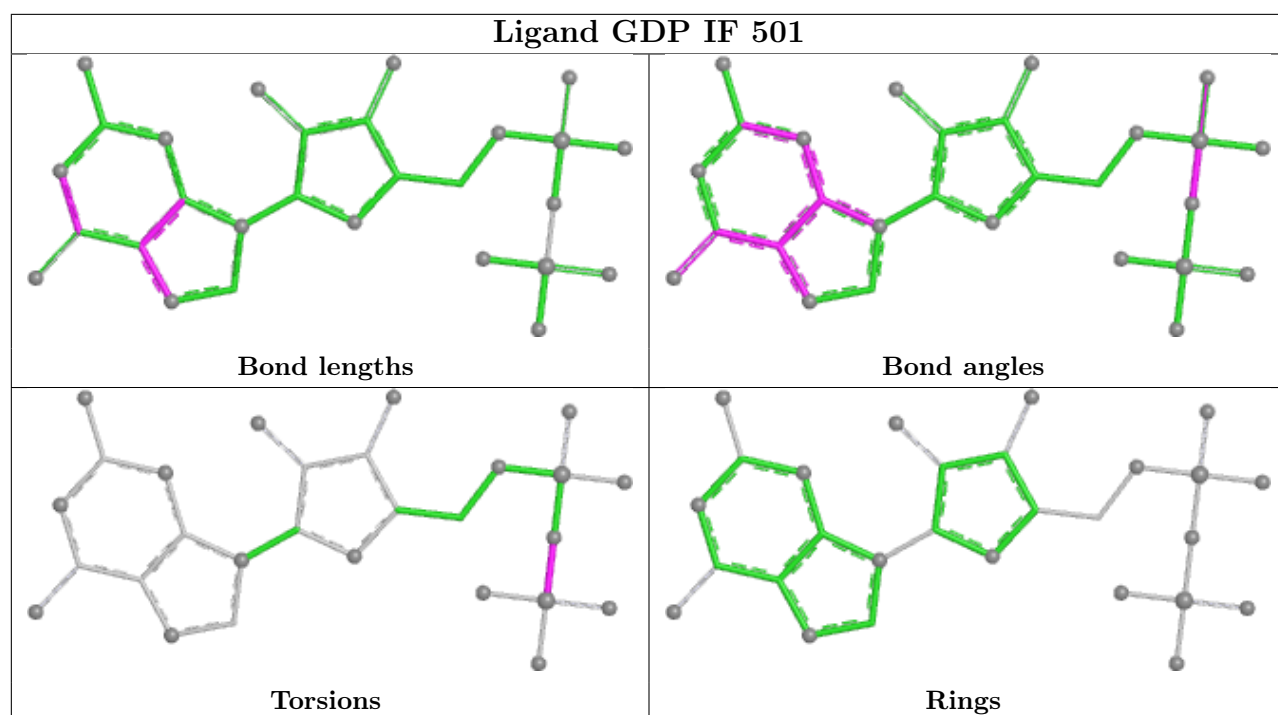


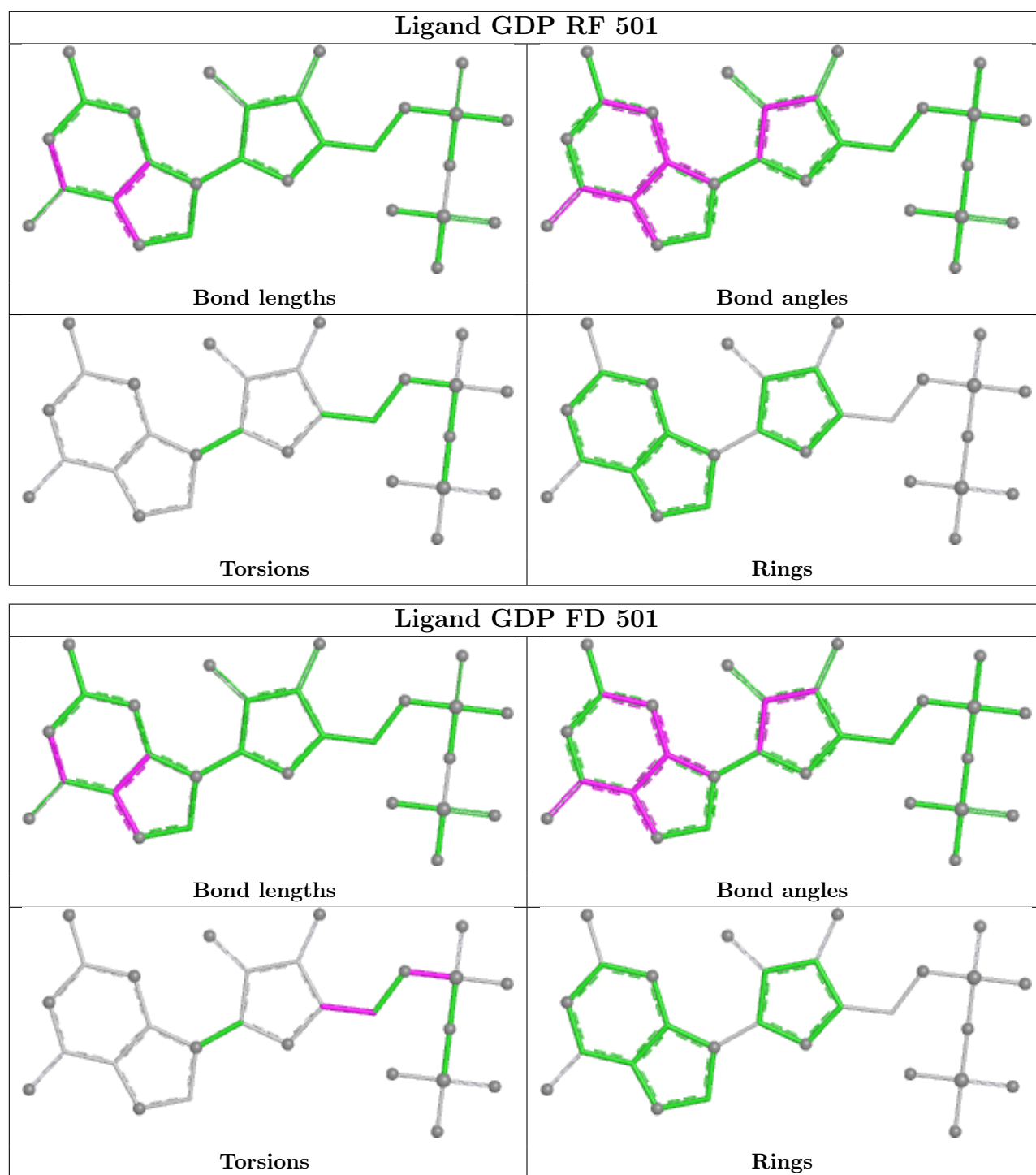
## Ligand GDP EJ 501



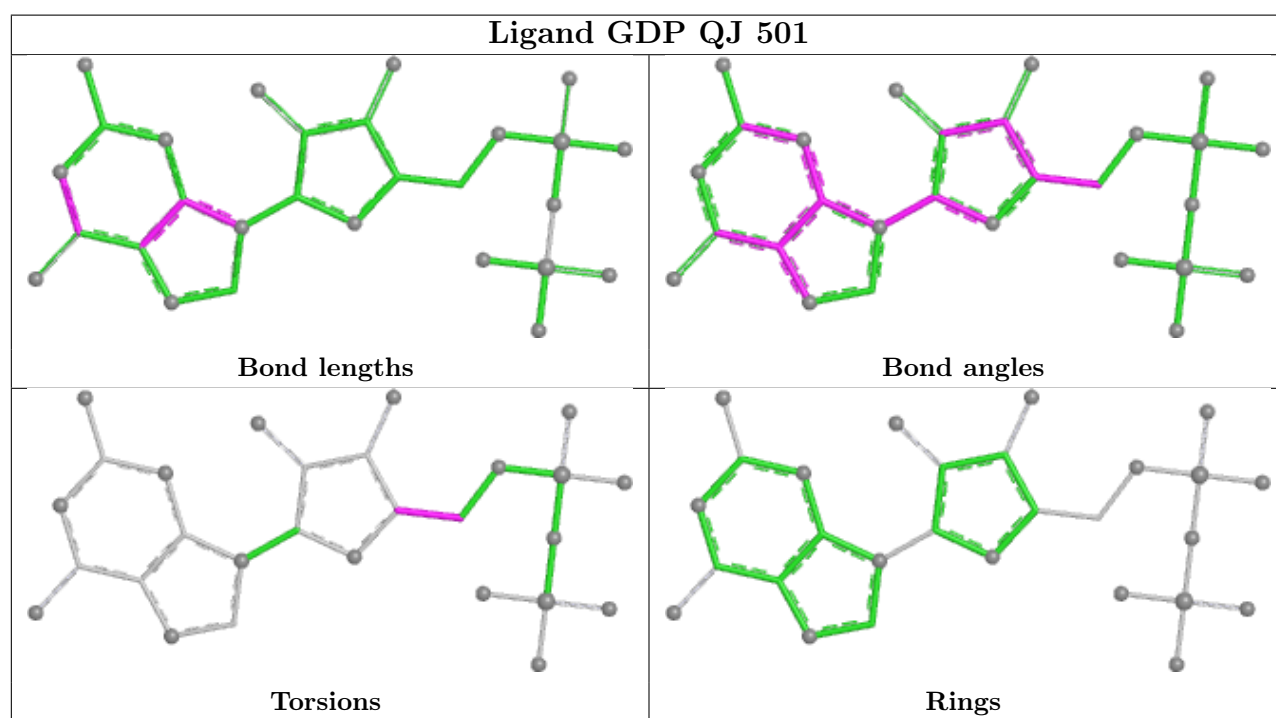
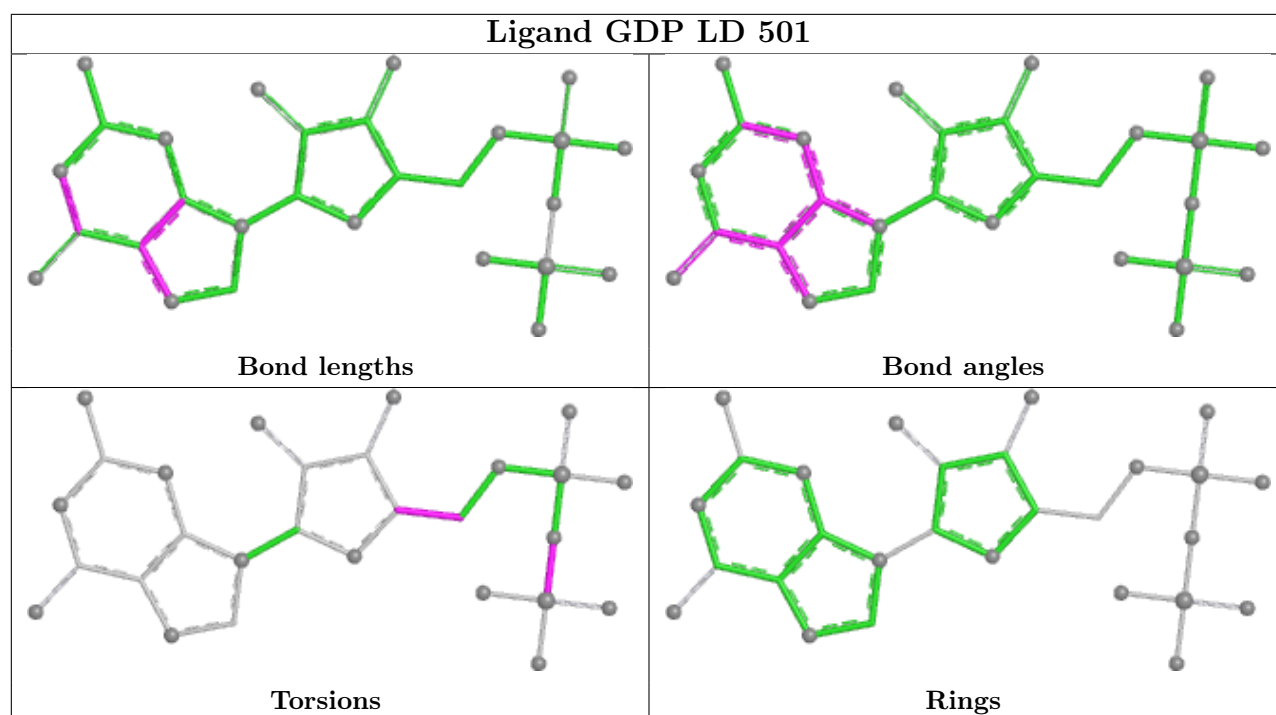


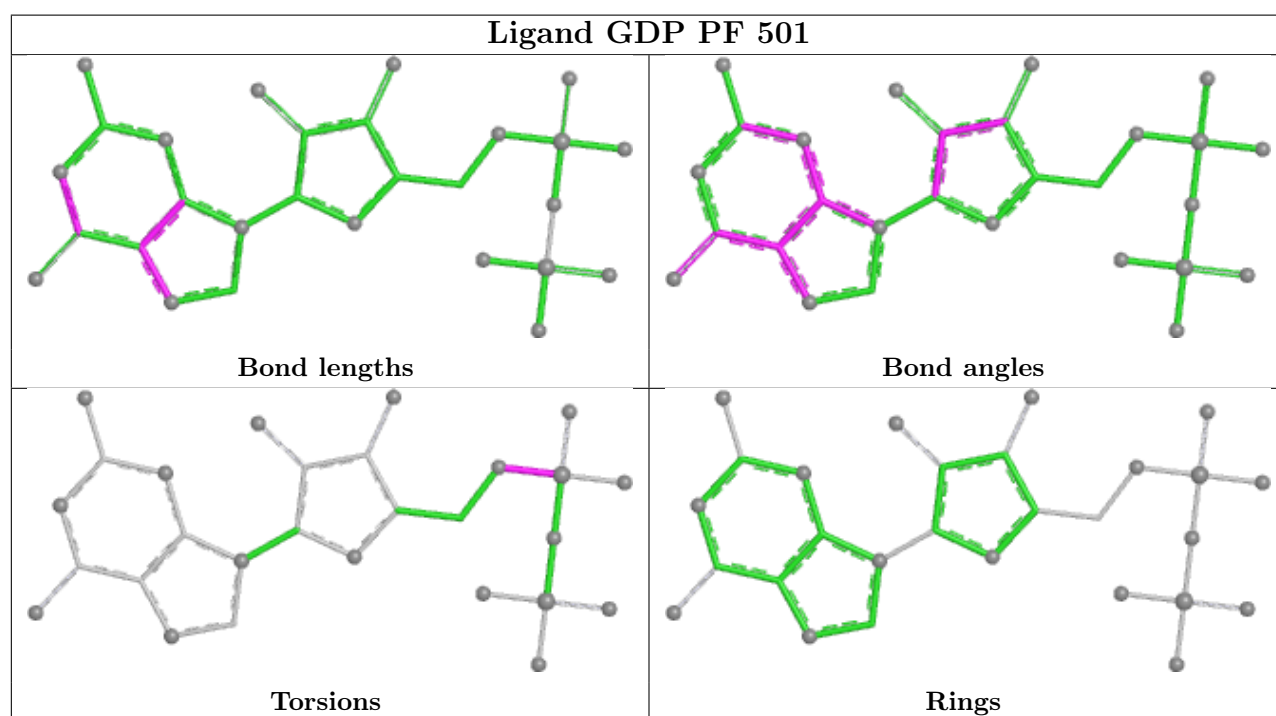
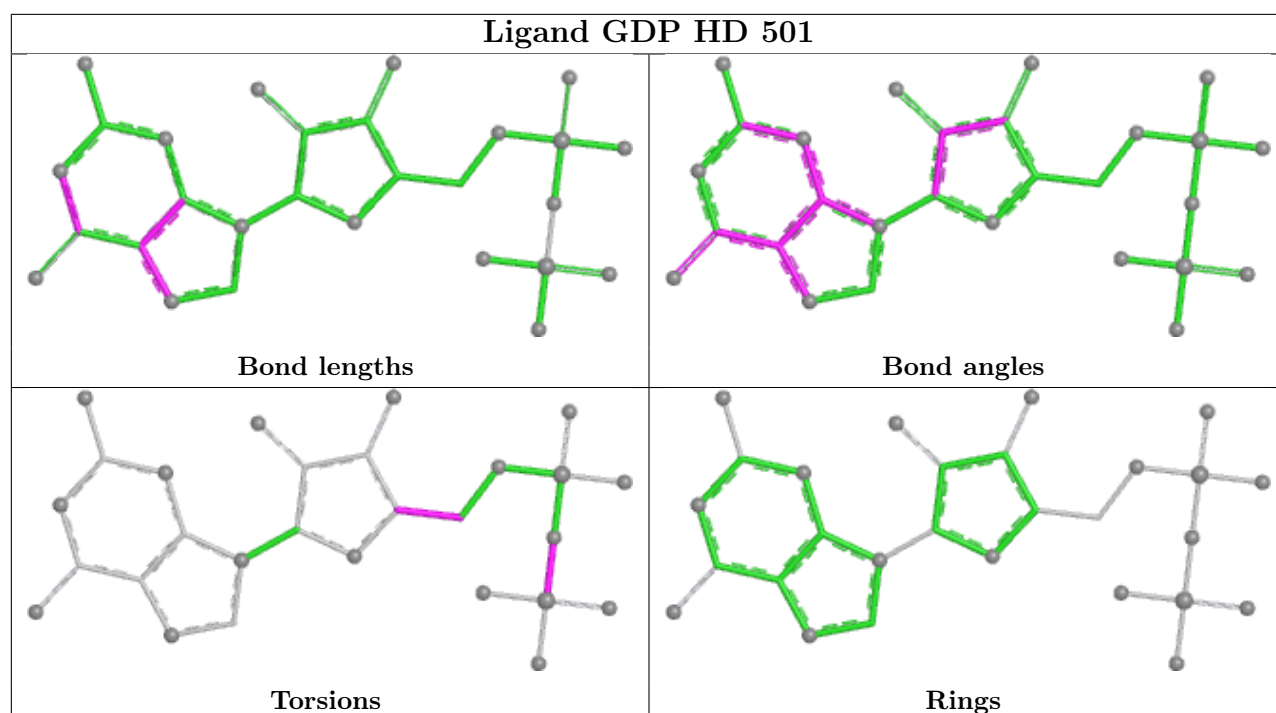




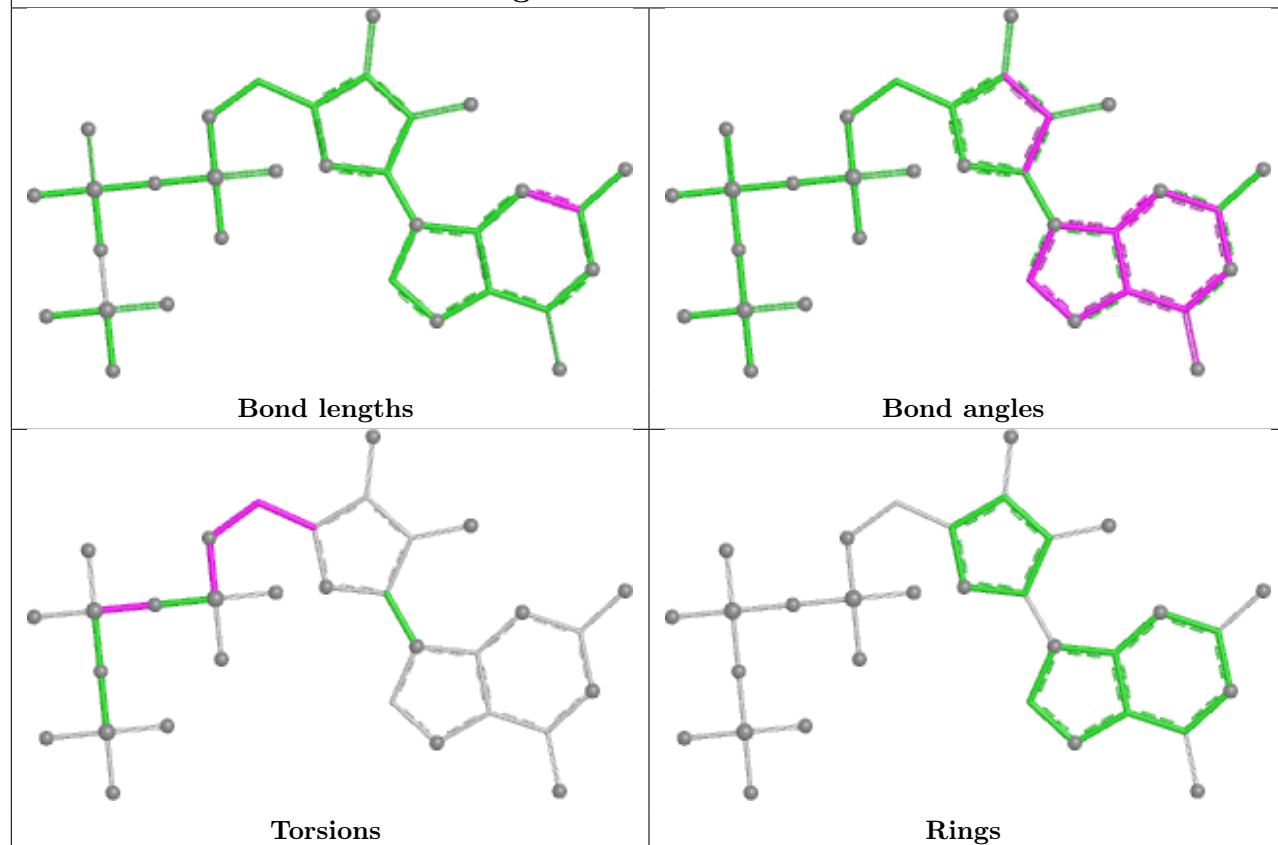




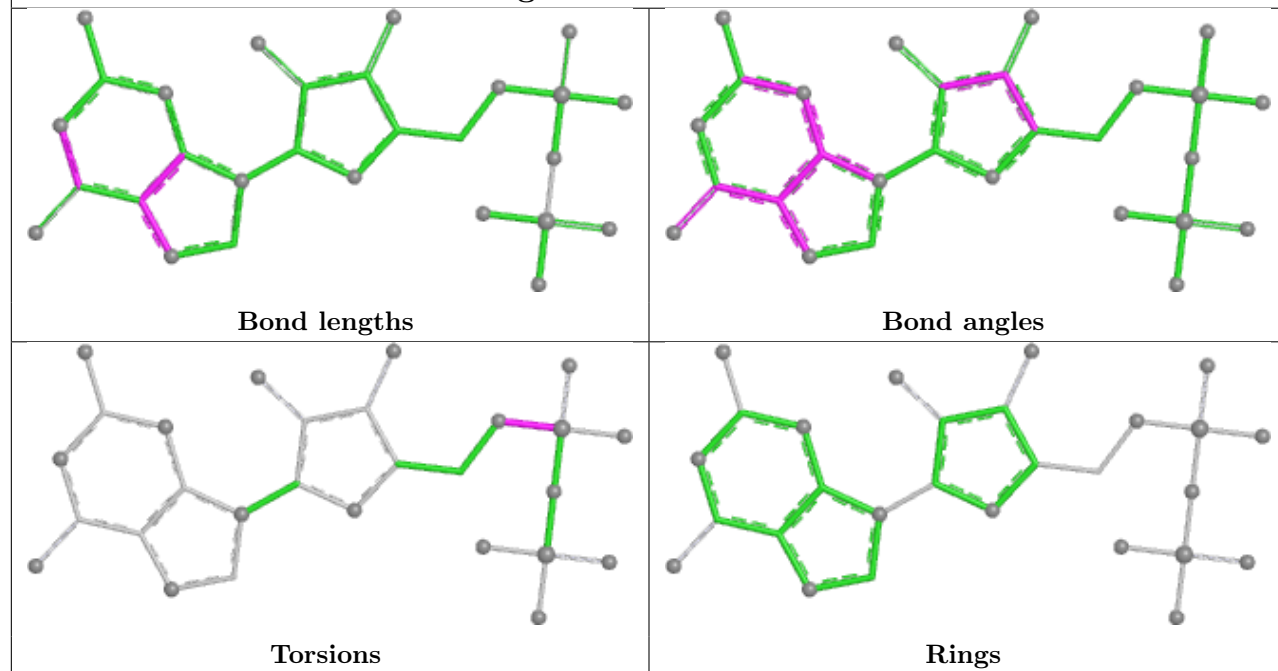


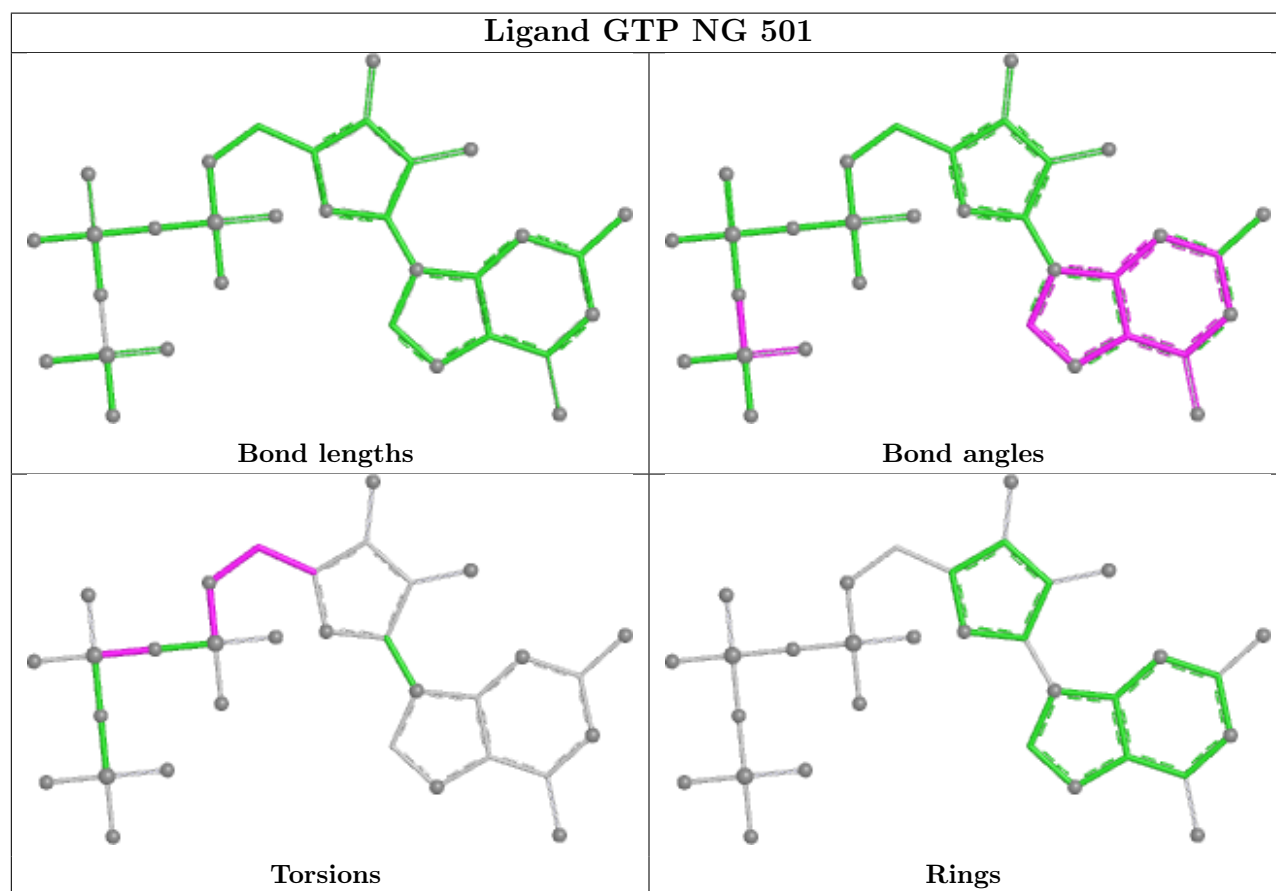
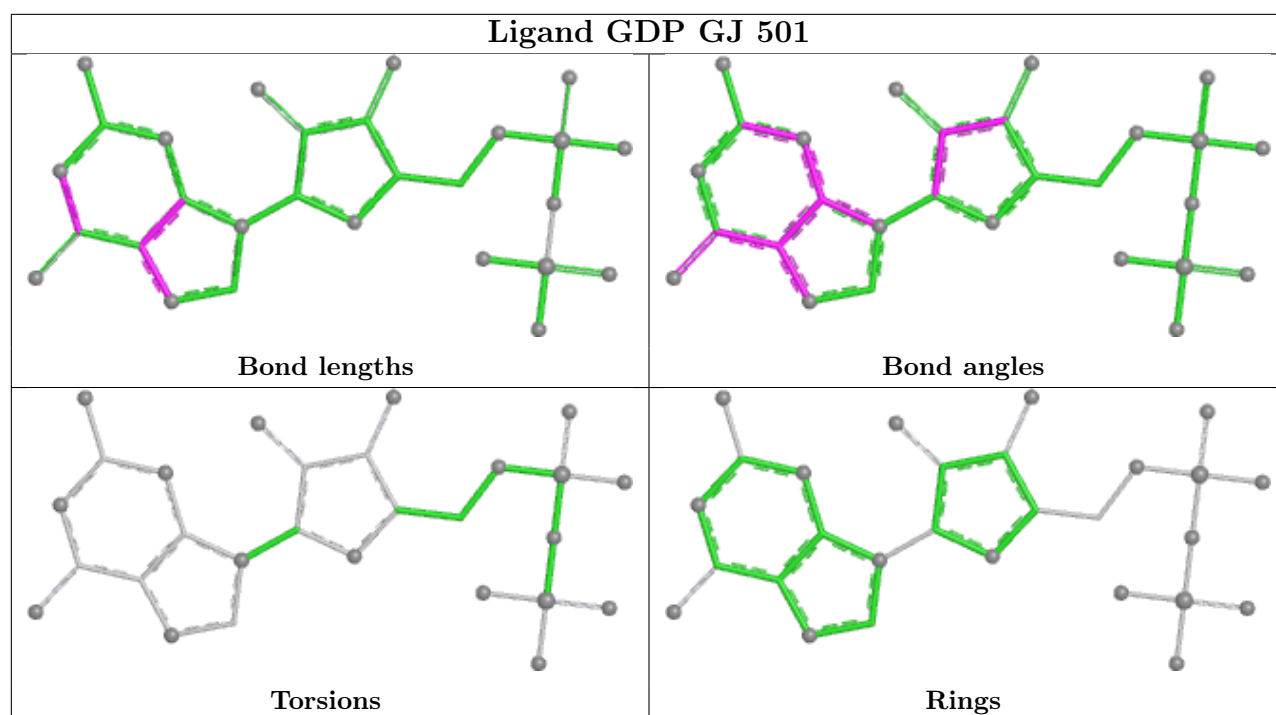


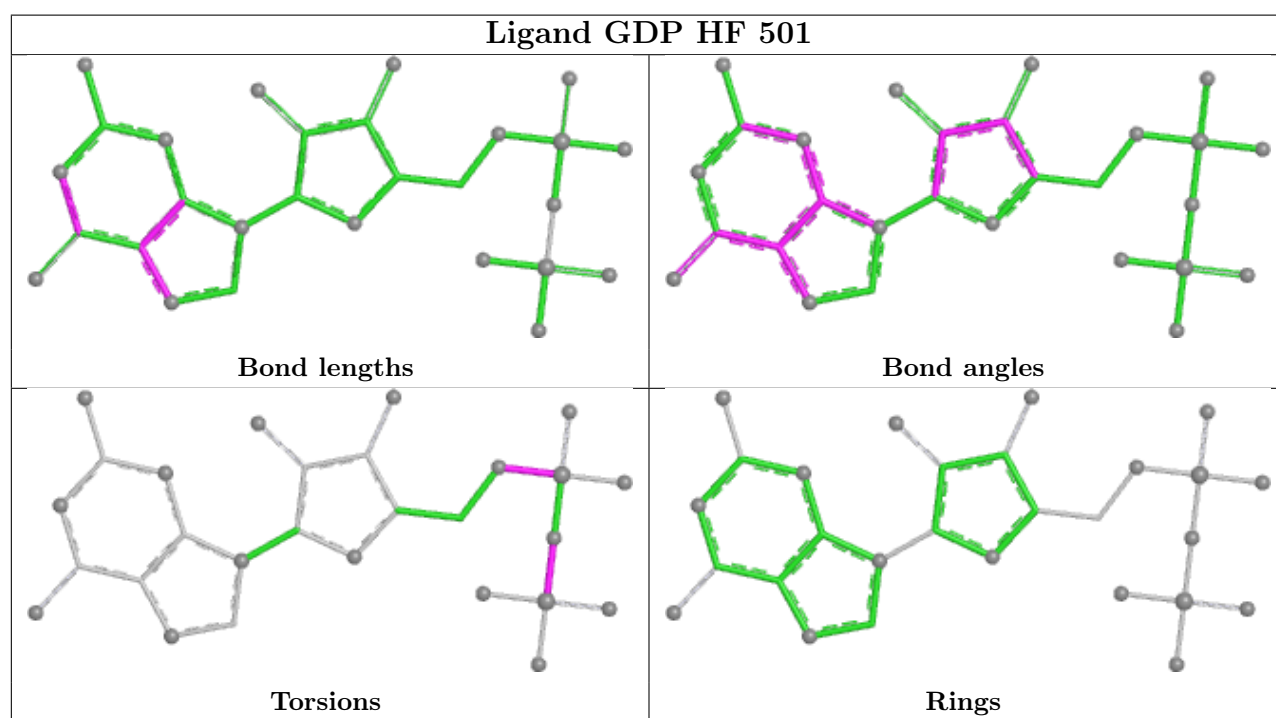
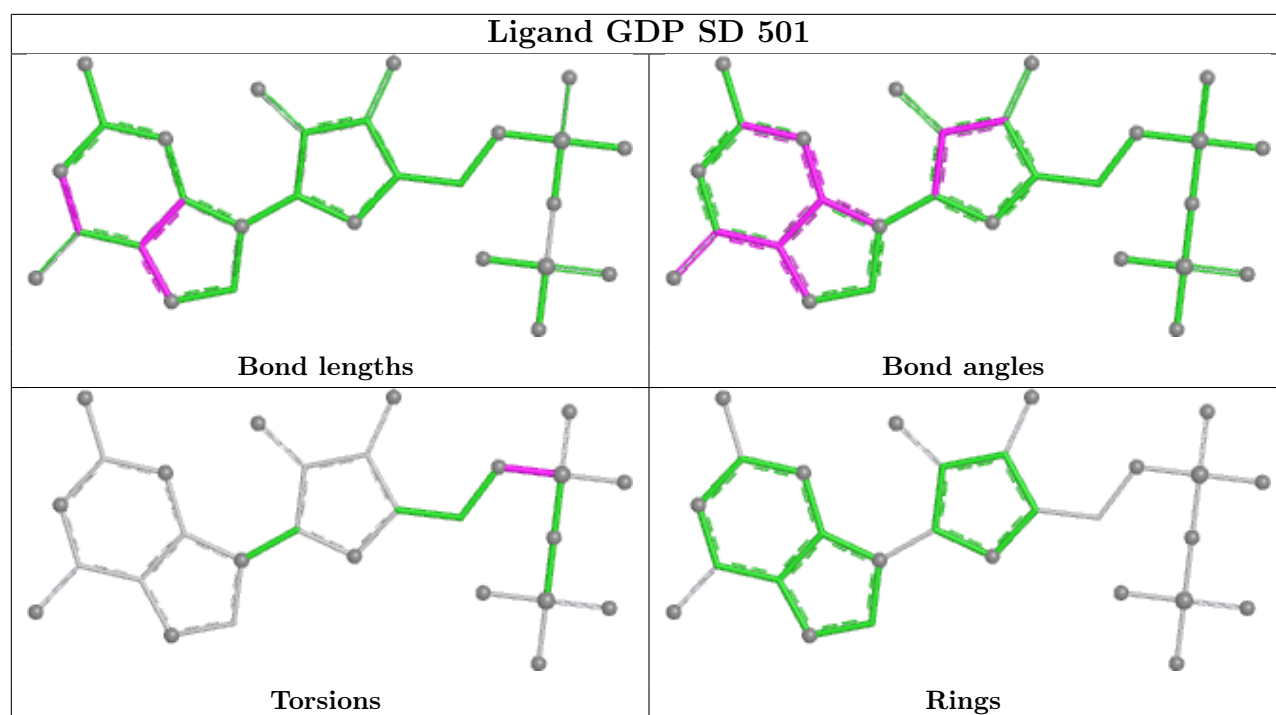
## Ligand GTP MK 501

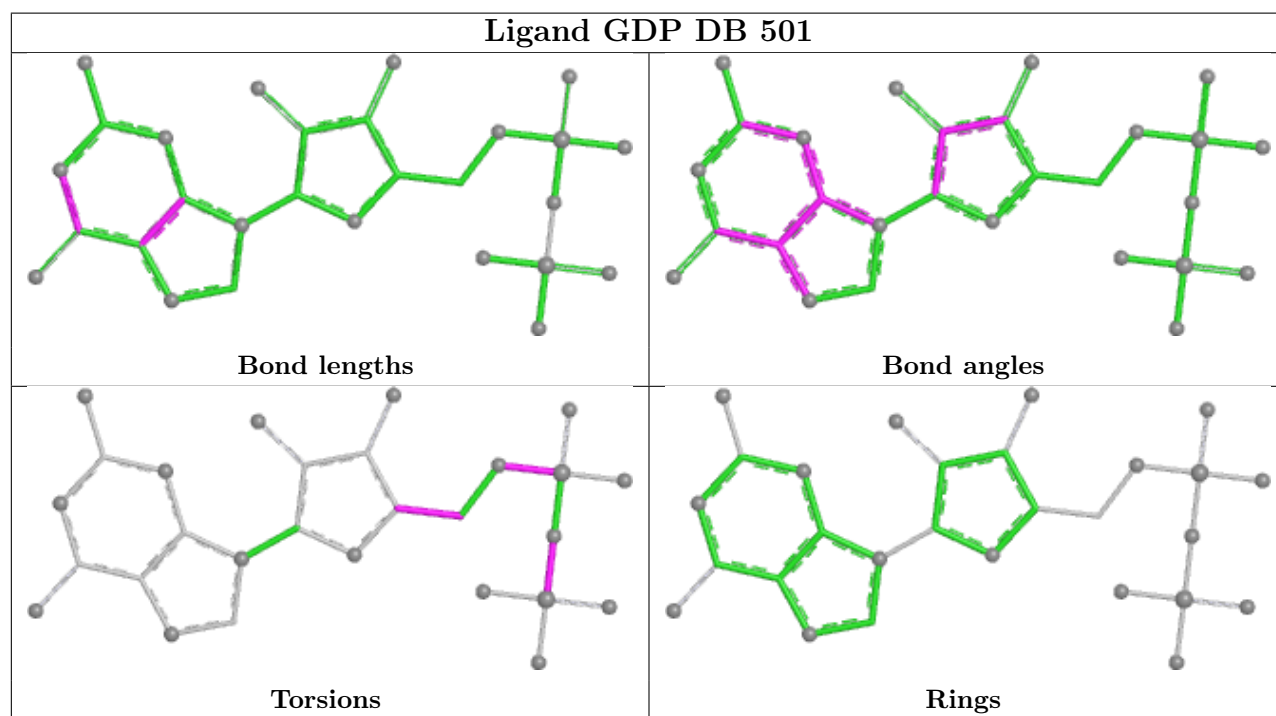
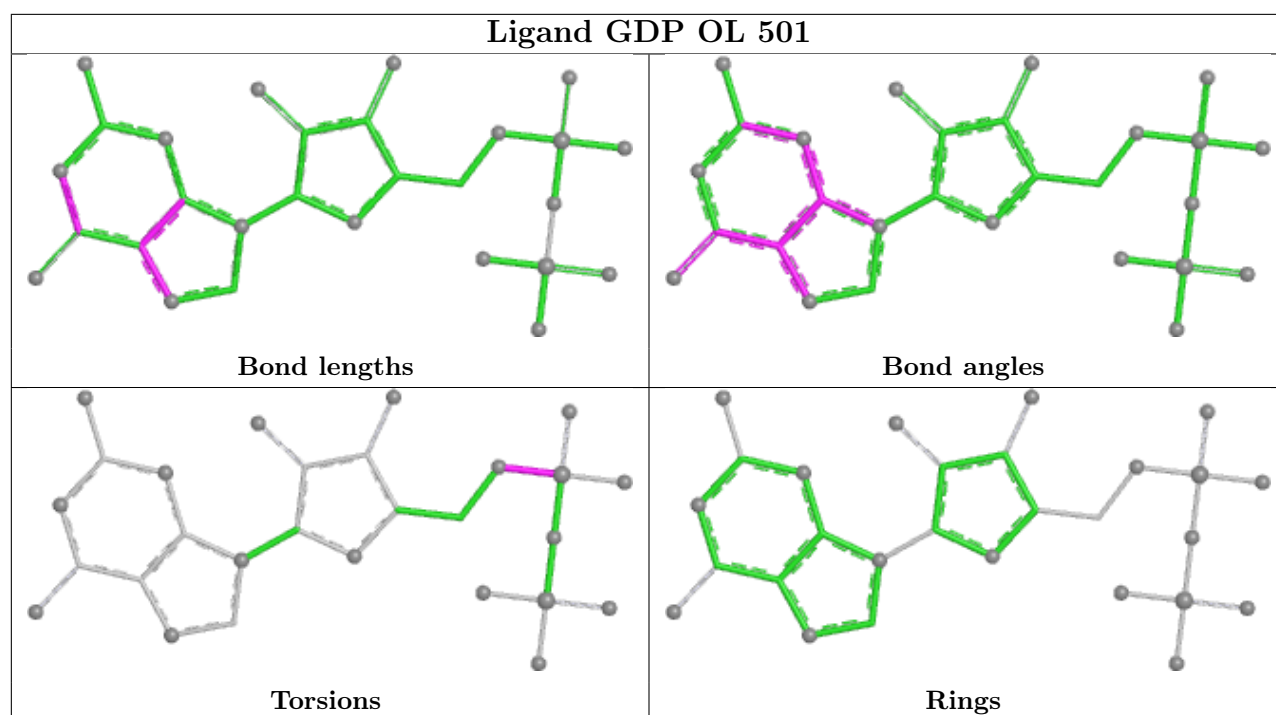


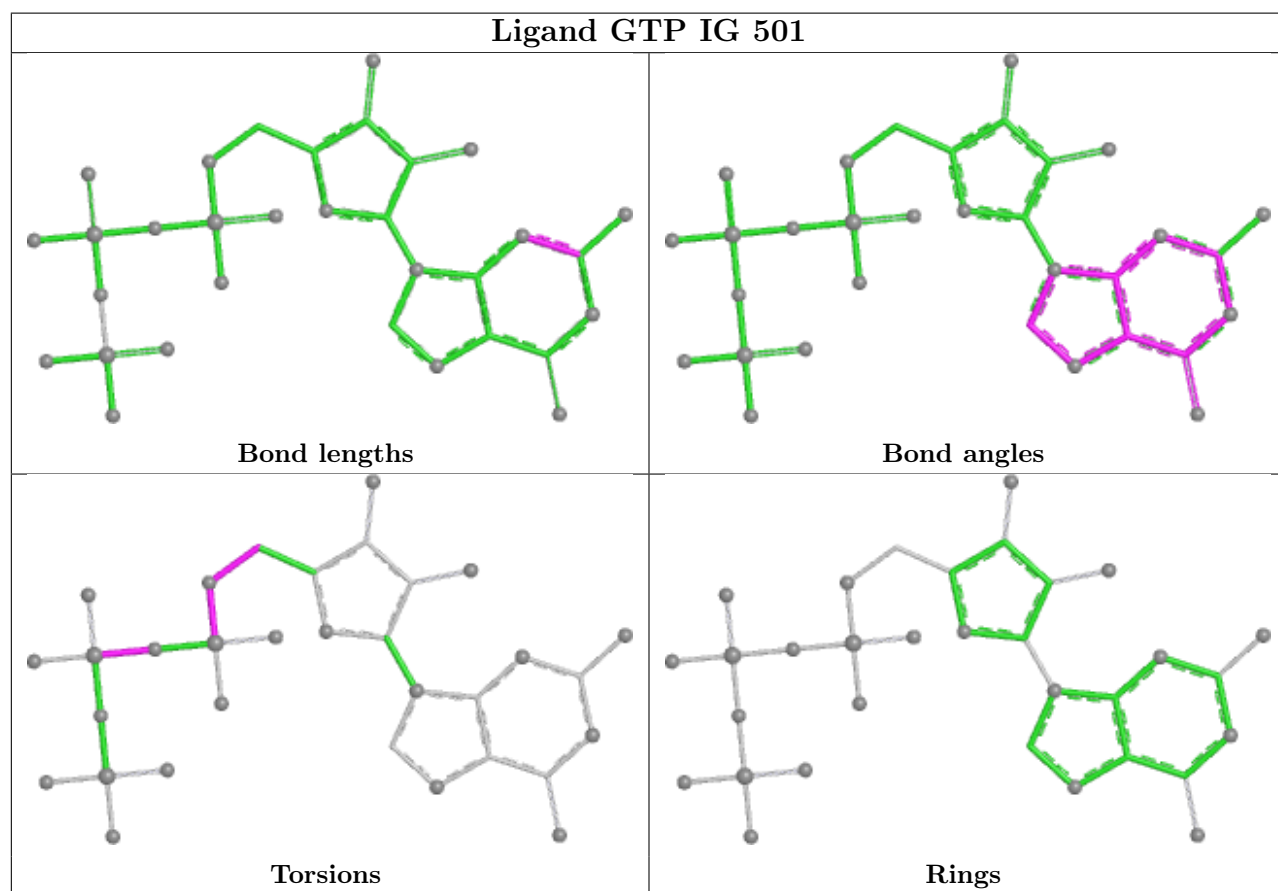
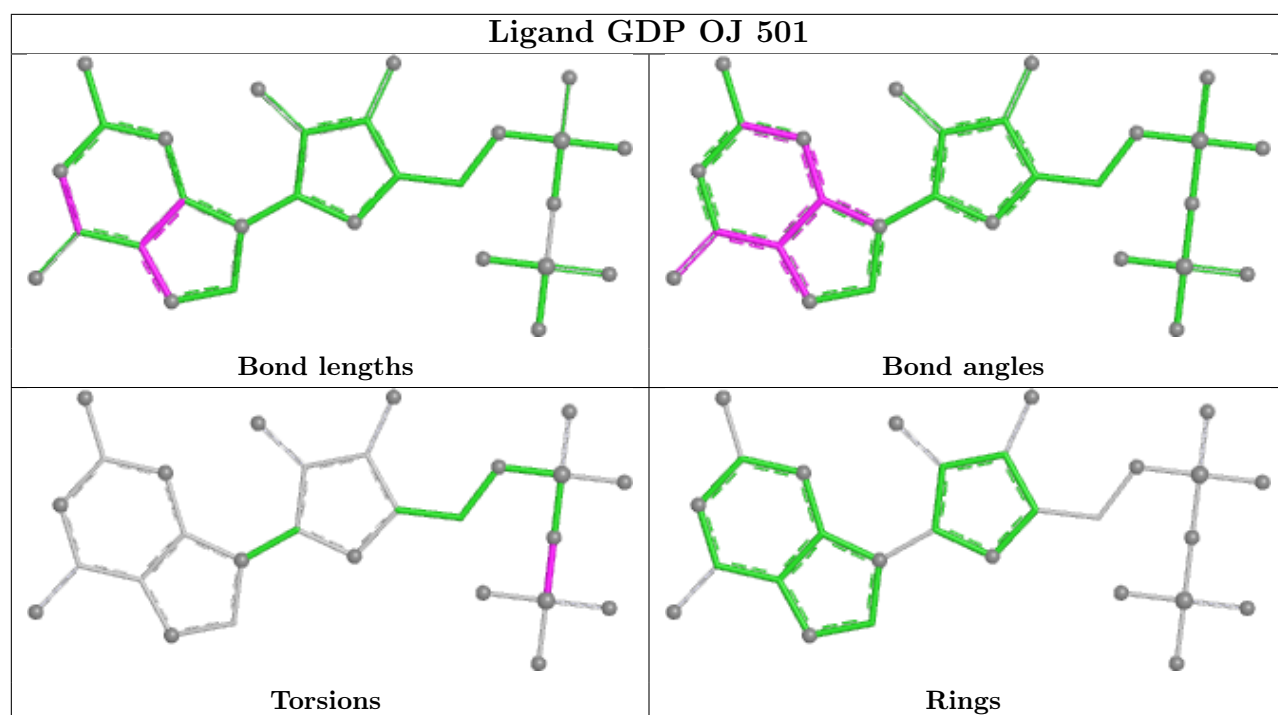
## Ligand GDP VF 501

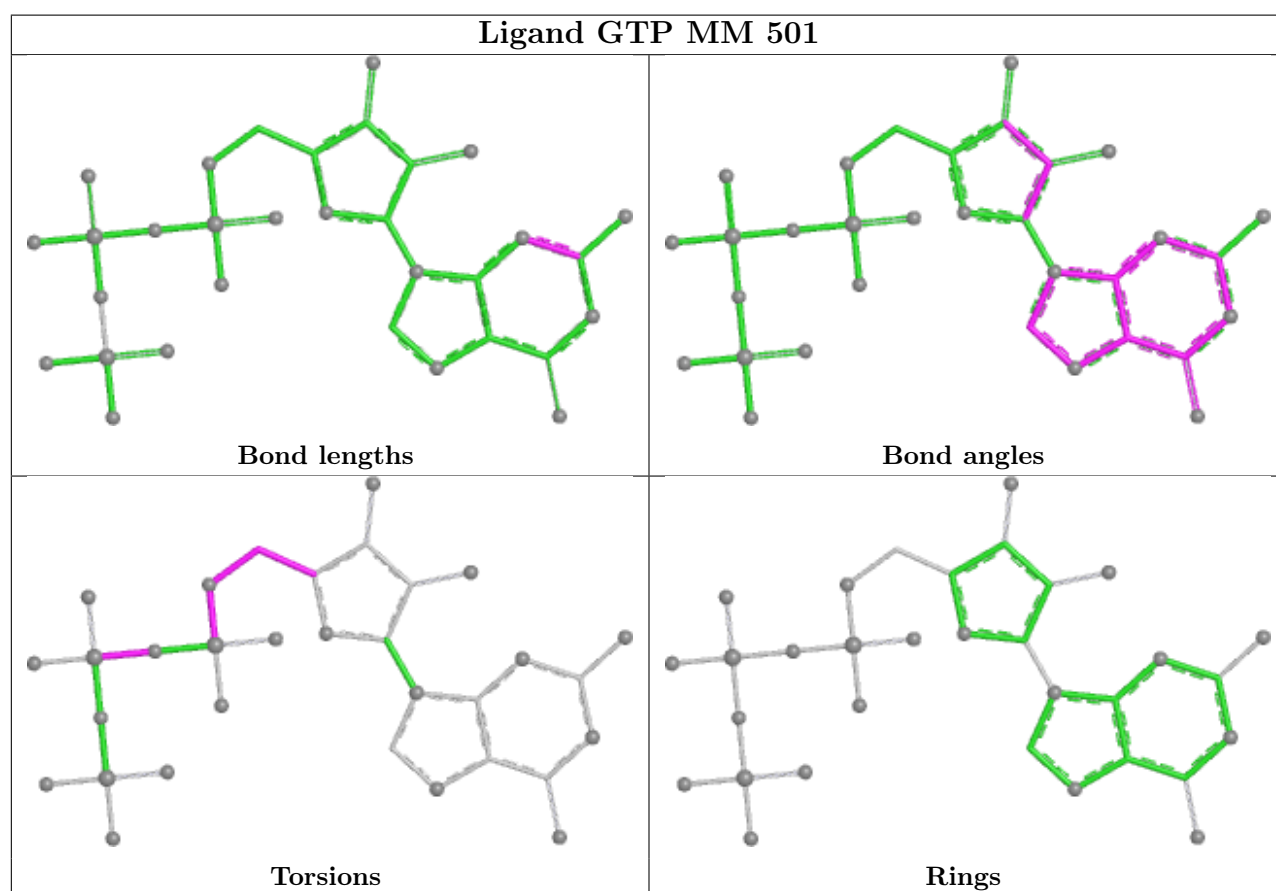
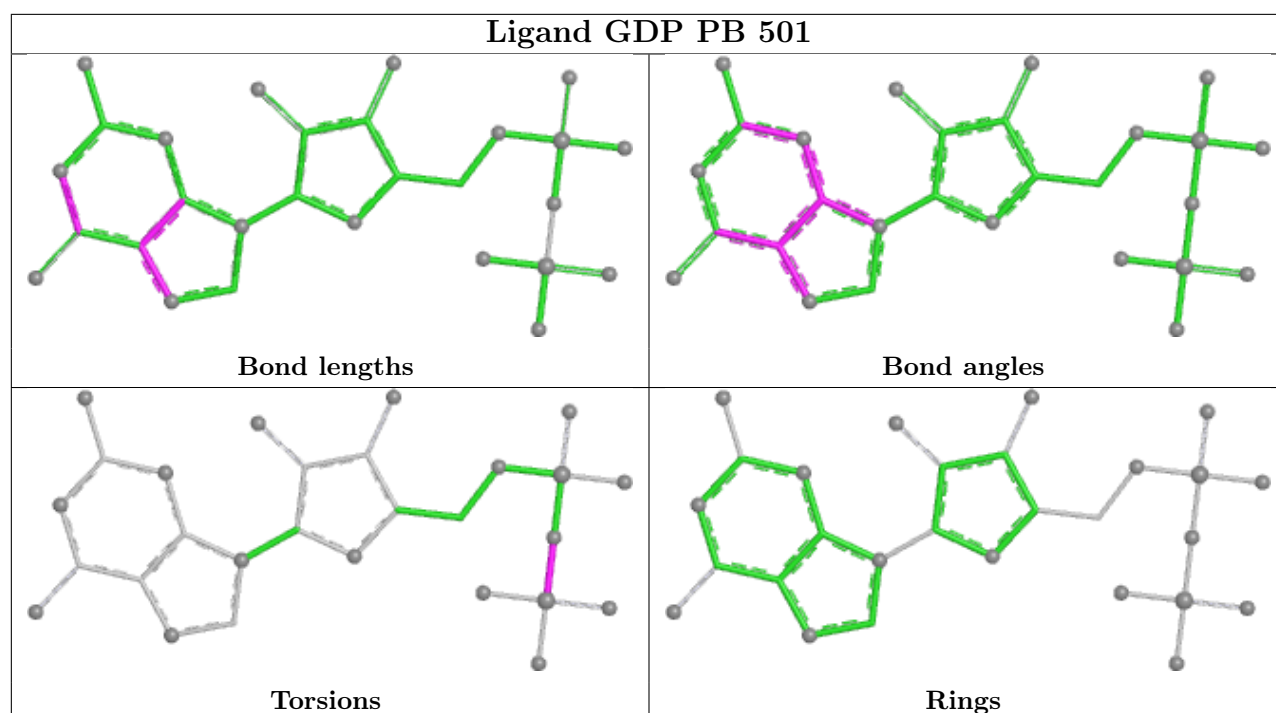






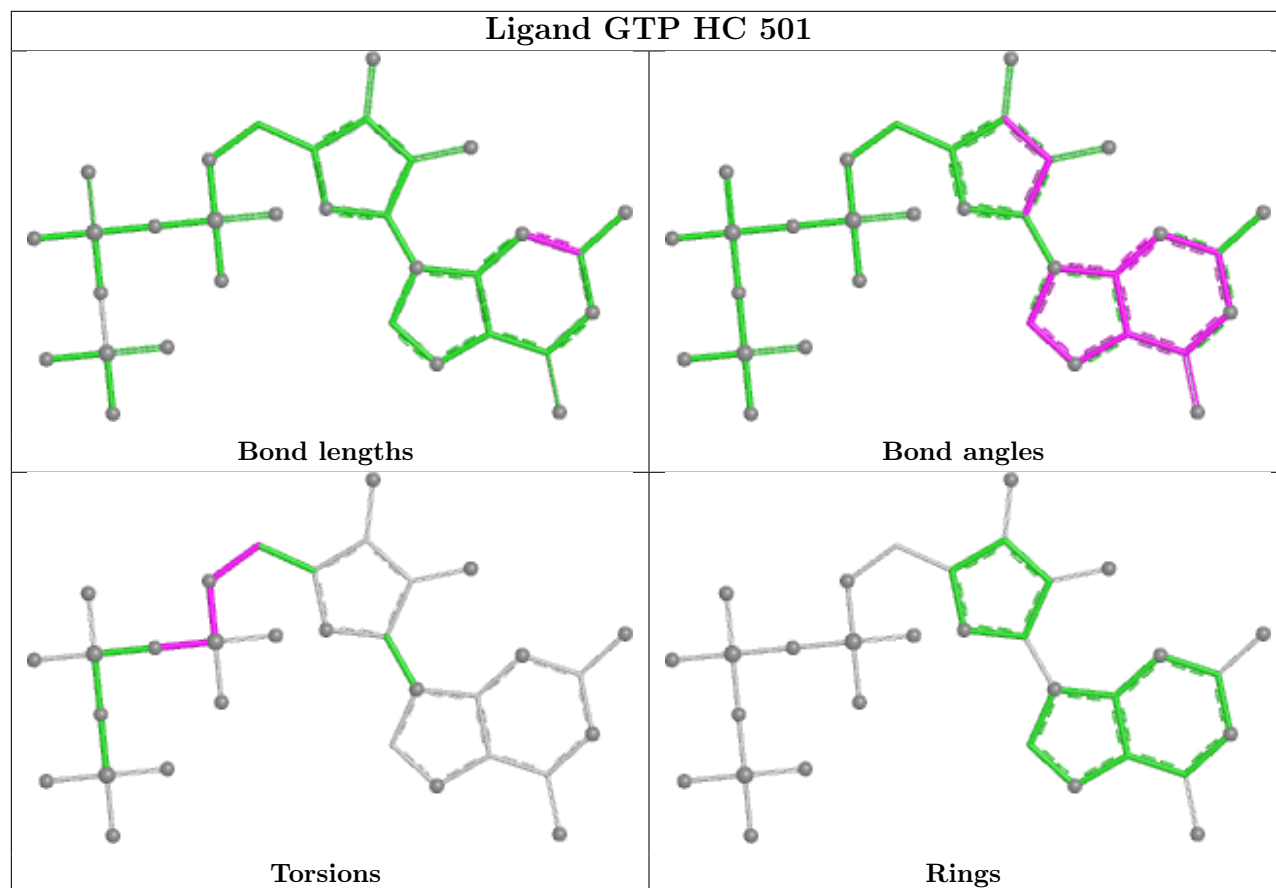




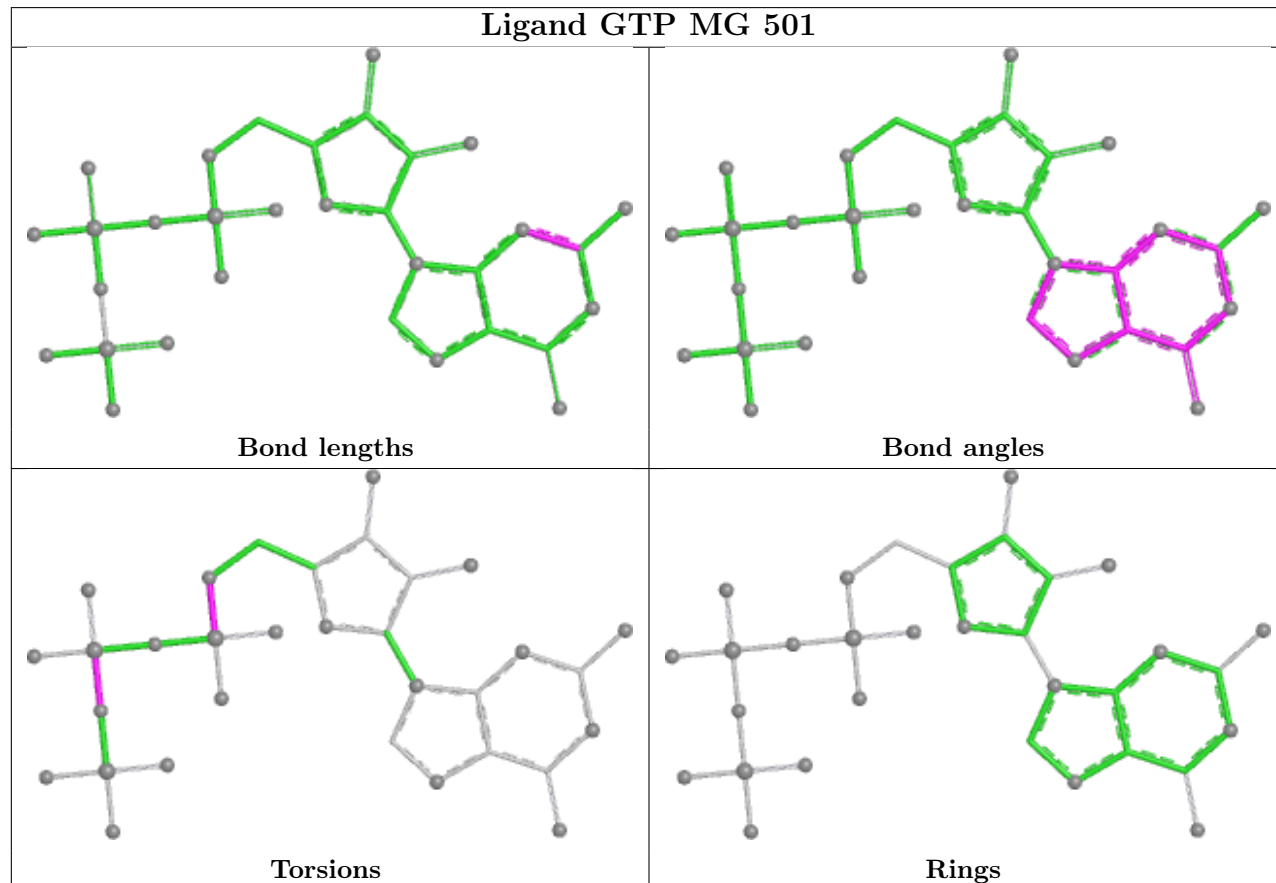




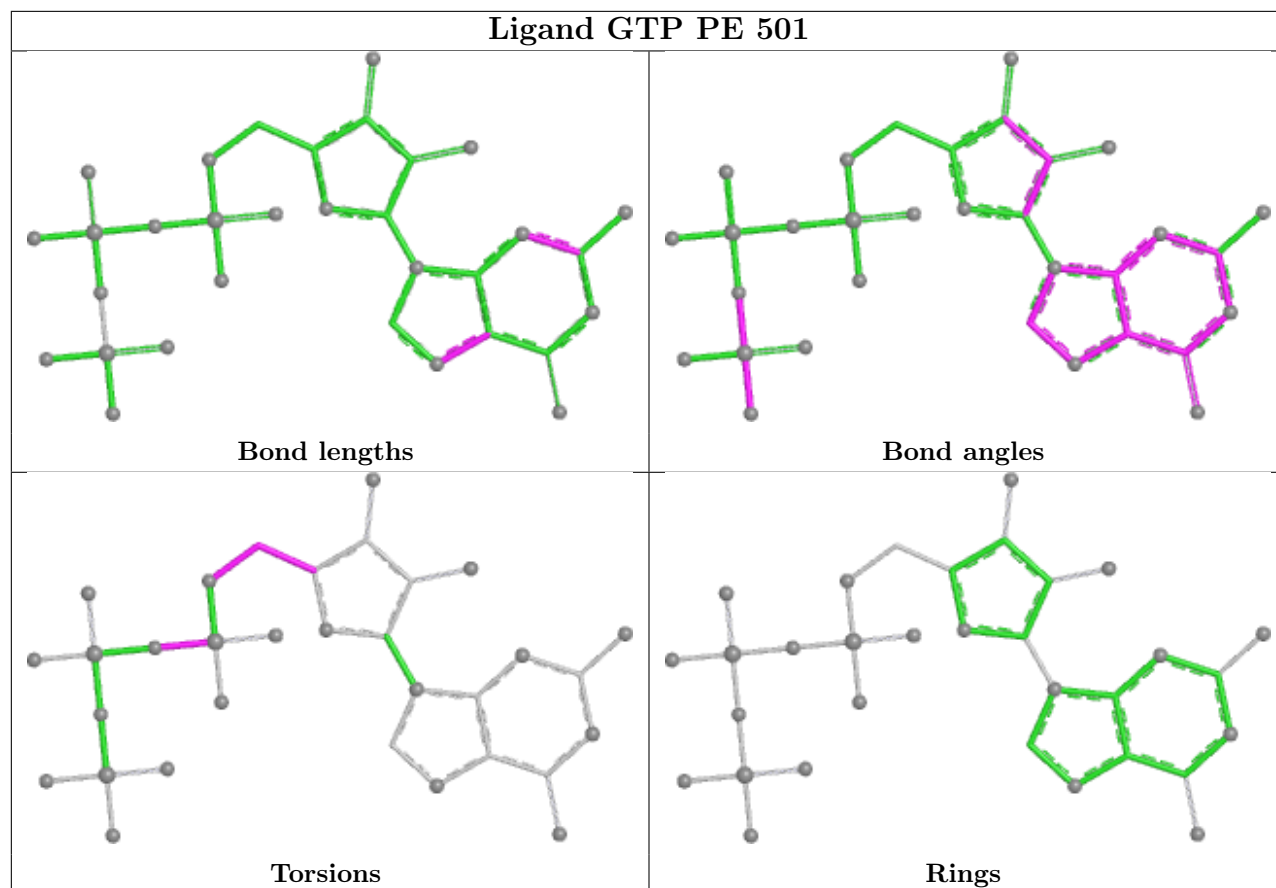
## Ligand GTP HC 501



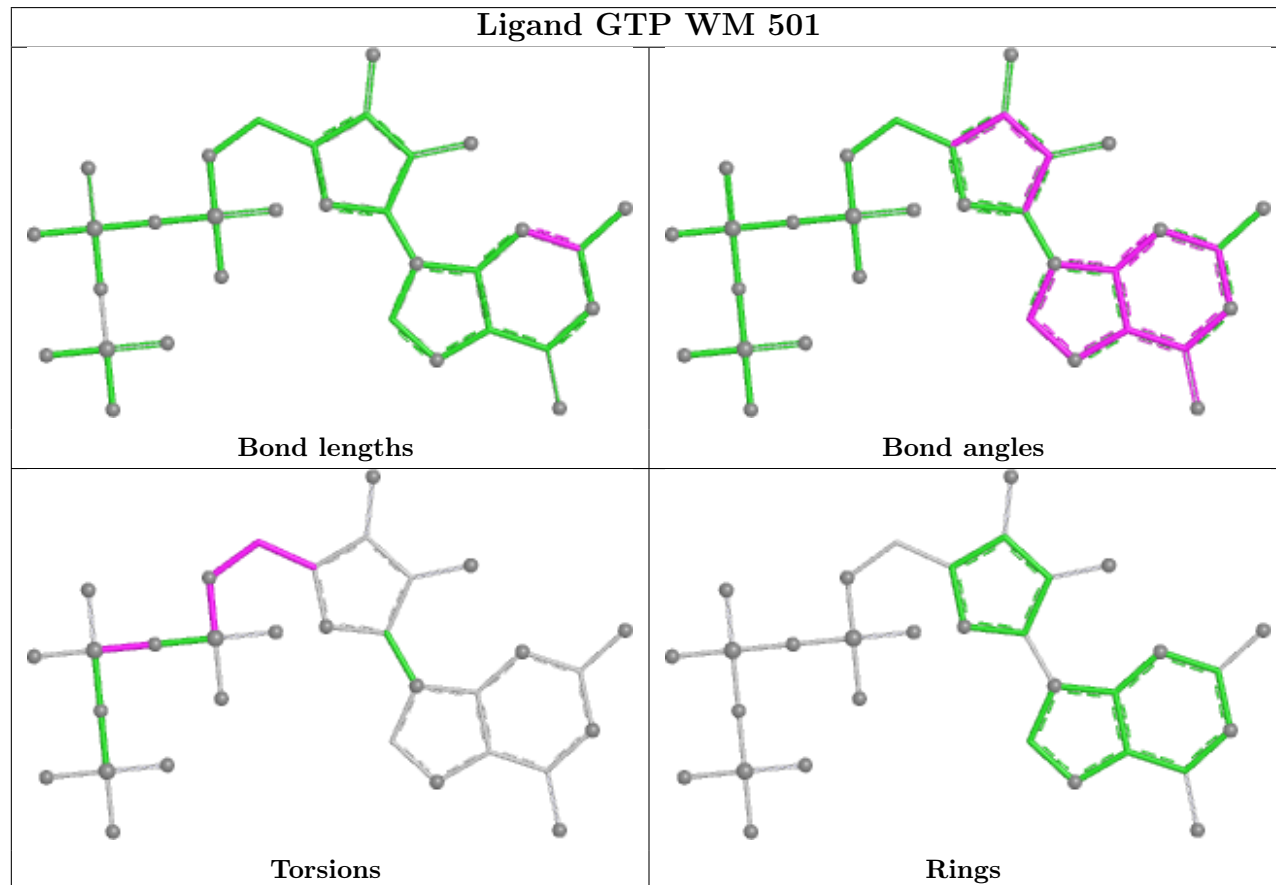
## Ligand GTP MG 501

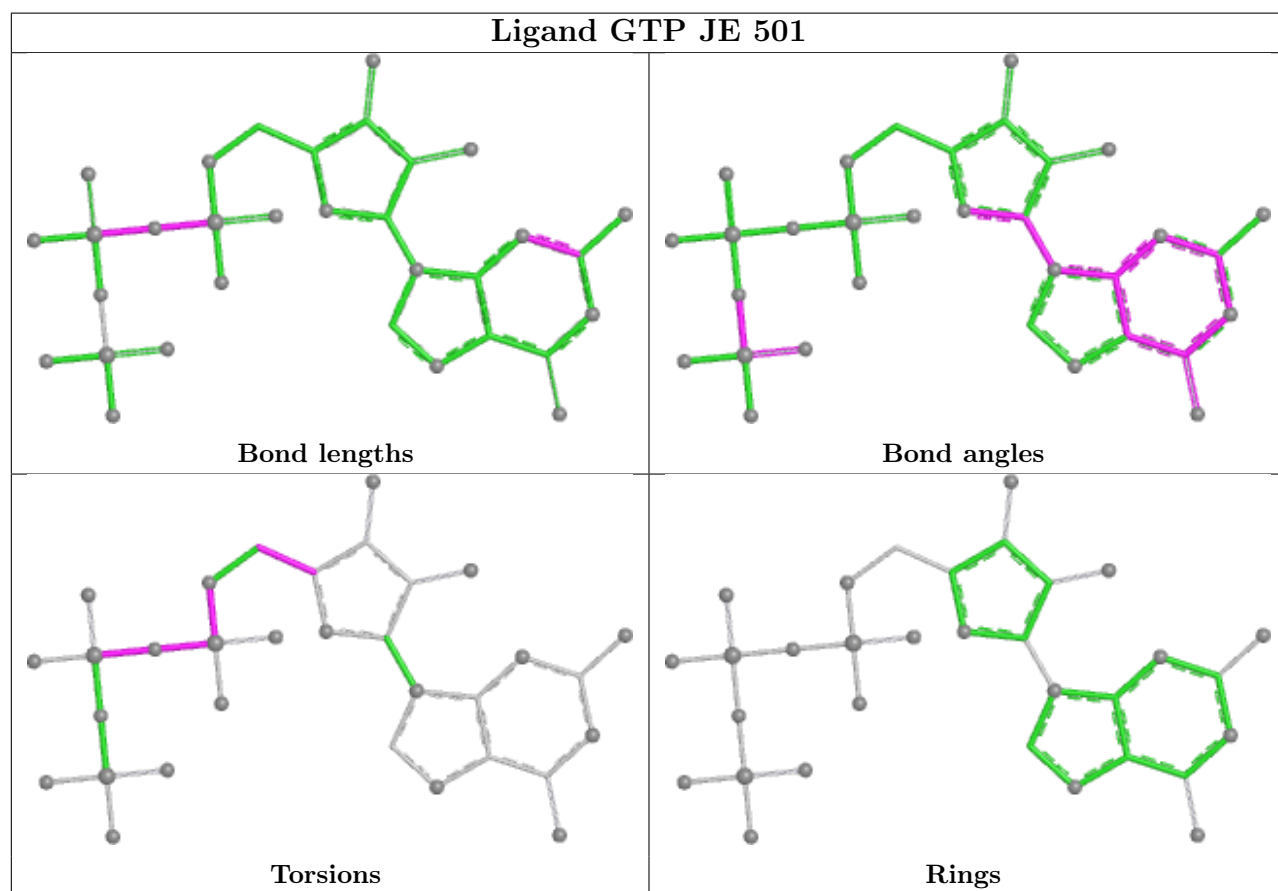
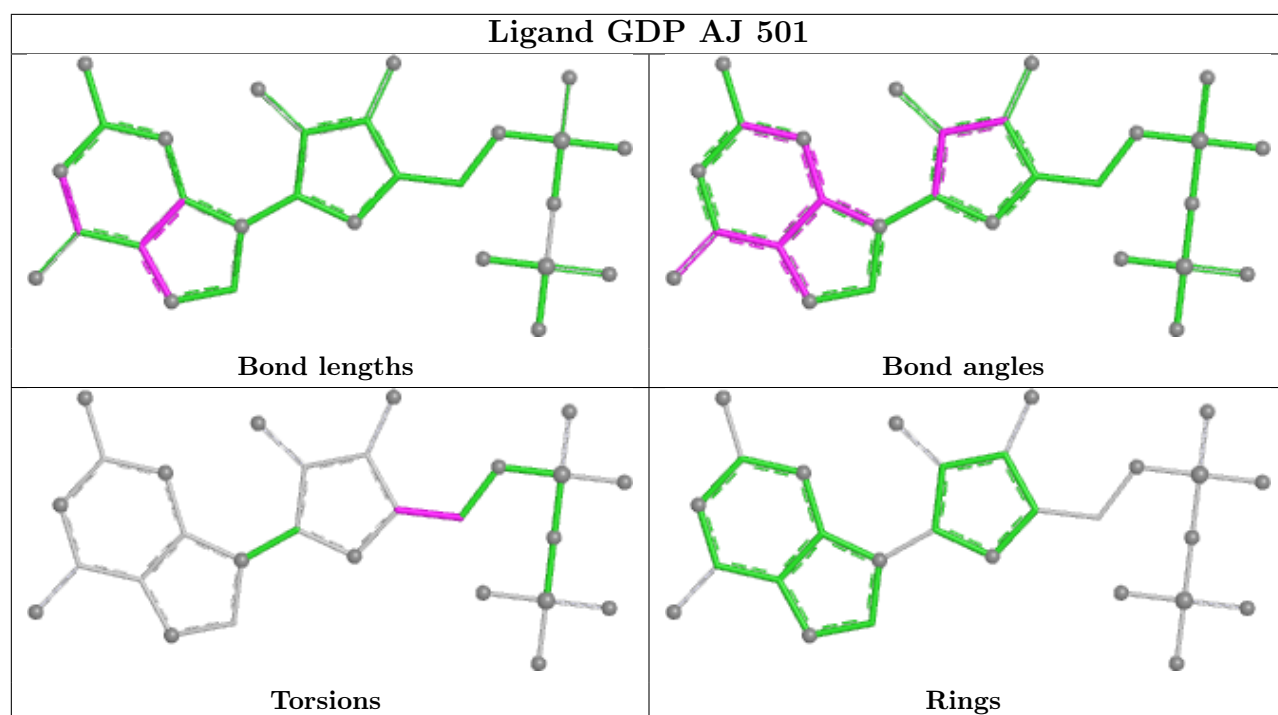


## Ligand GTP PE 501

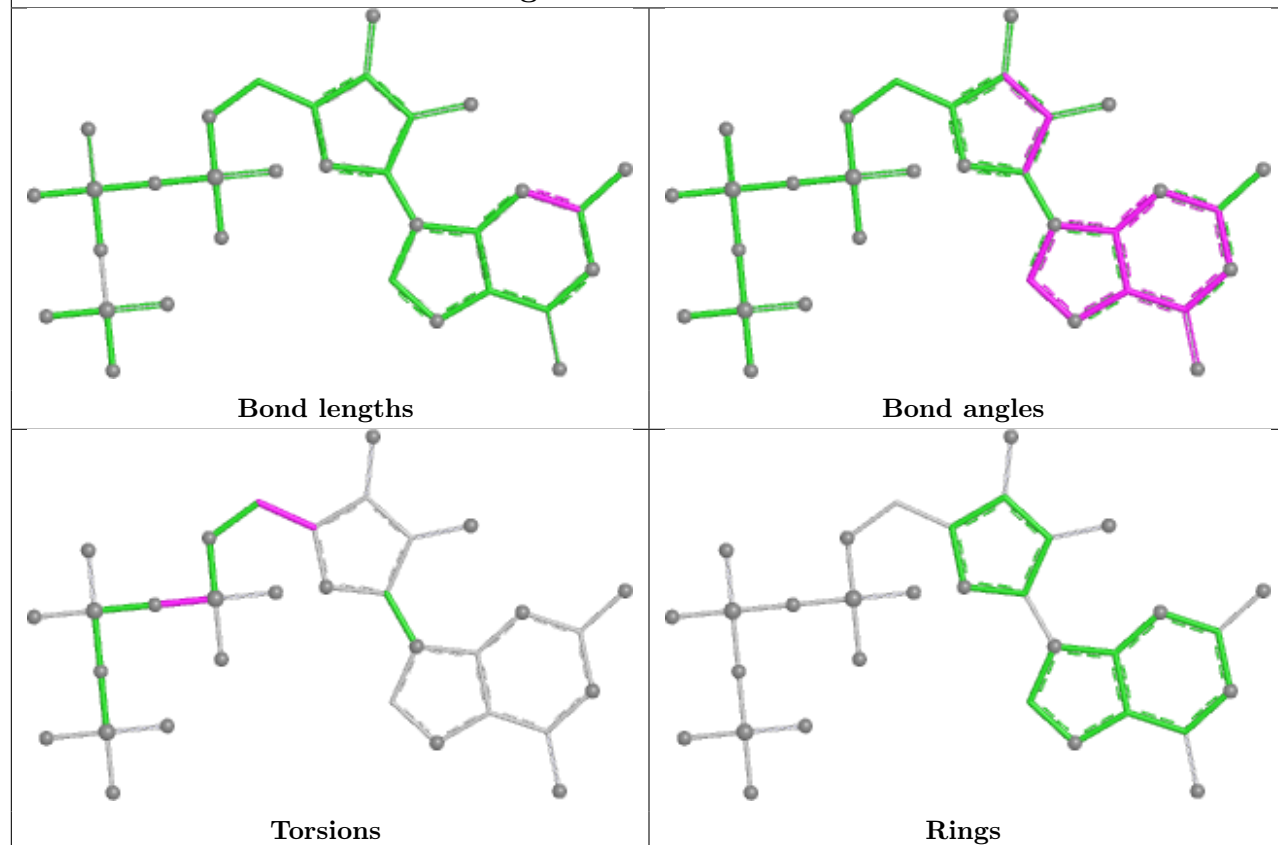


## Ligand GTP WM 501

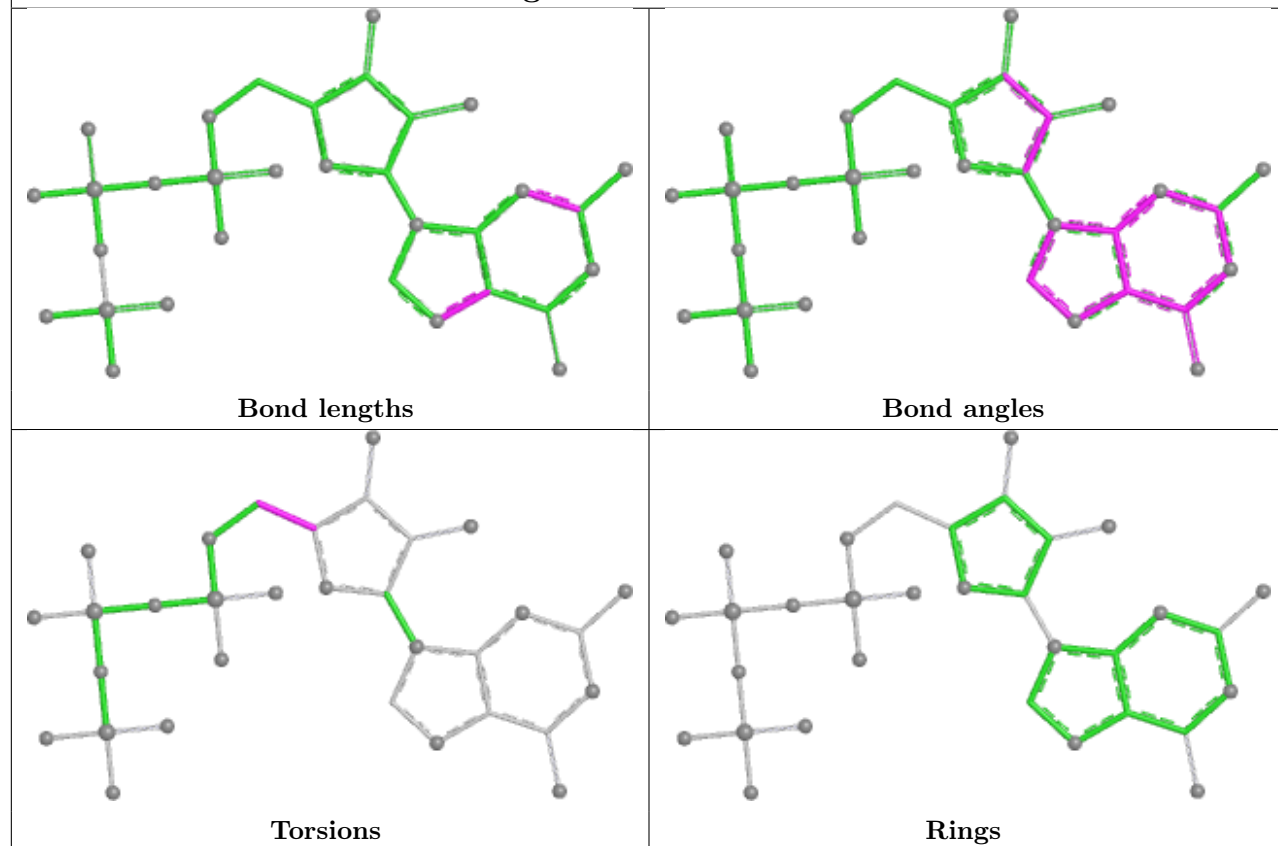


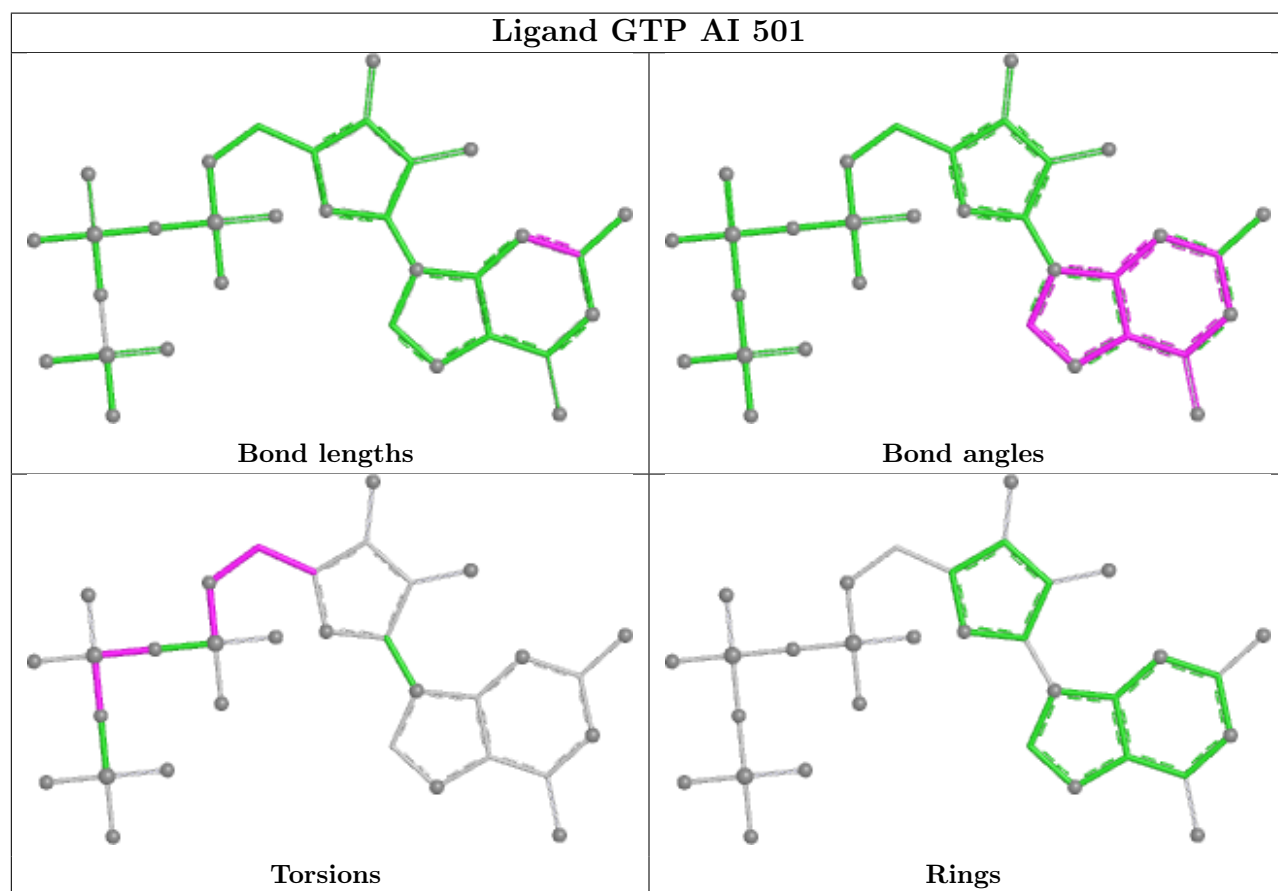
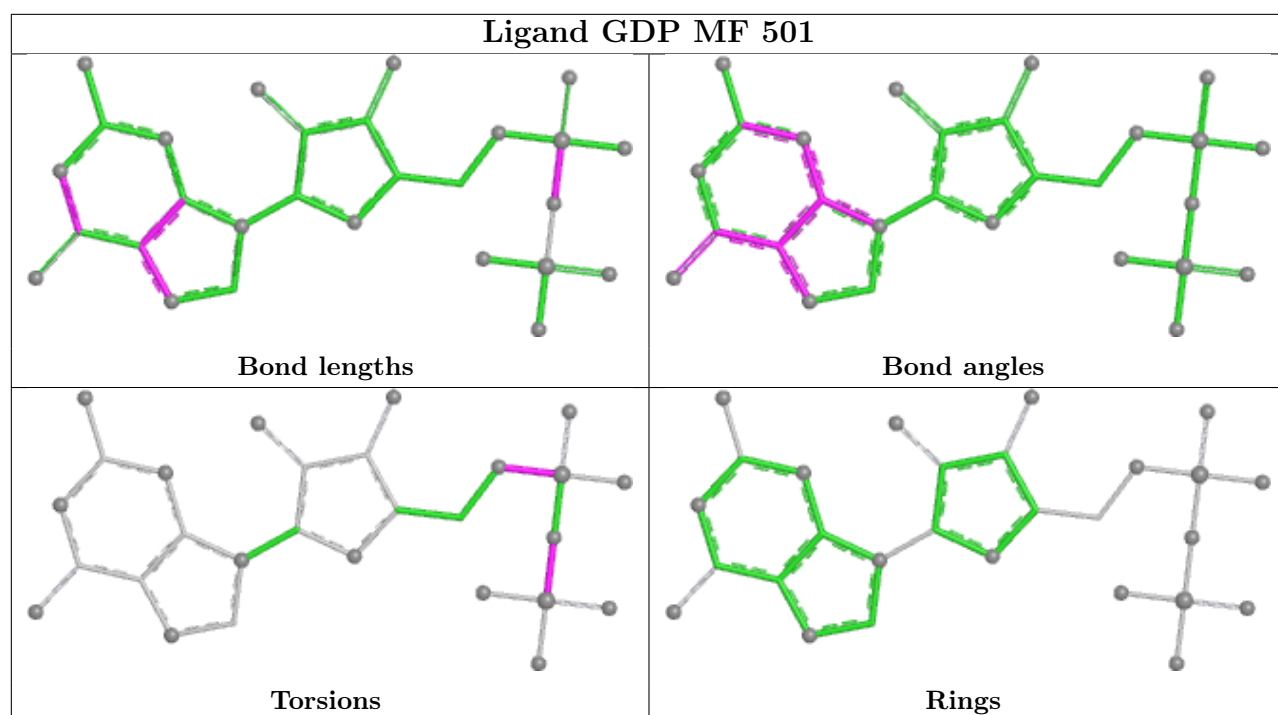


## Ligand GTP LC 501

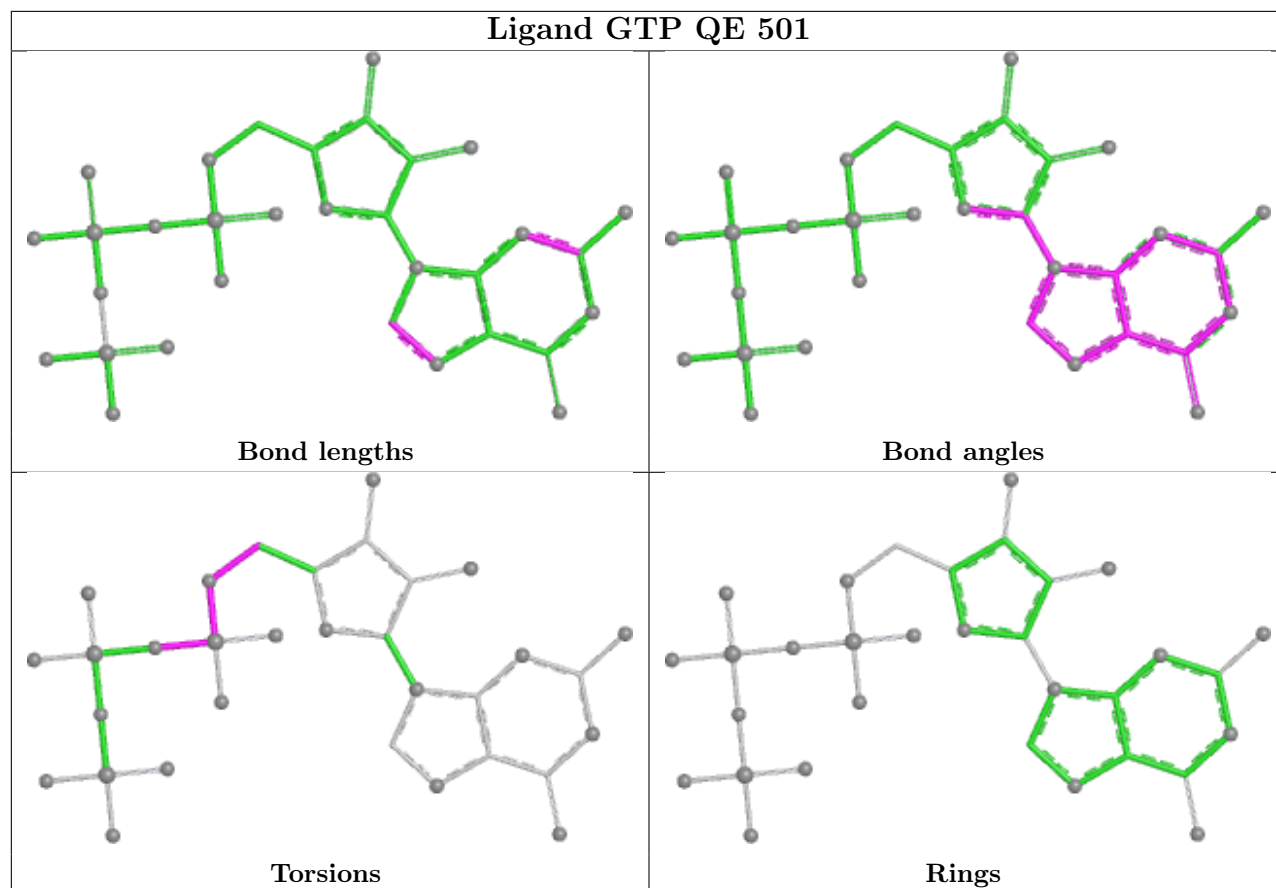


## Ligand GTP GI 501

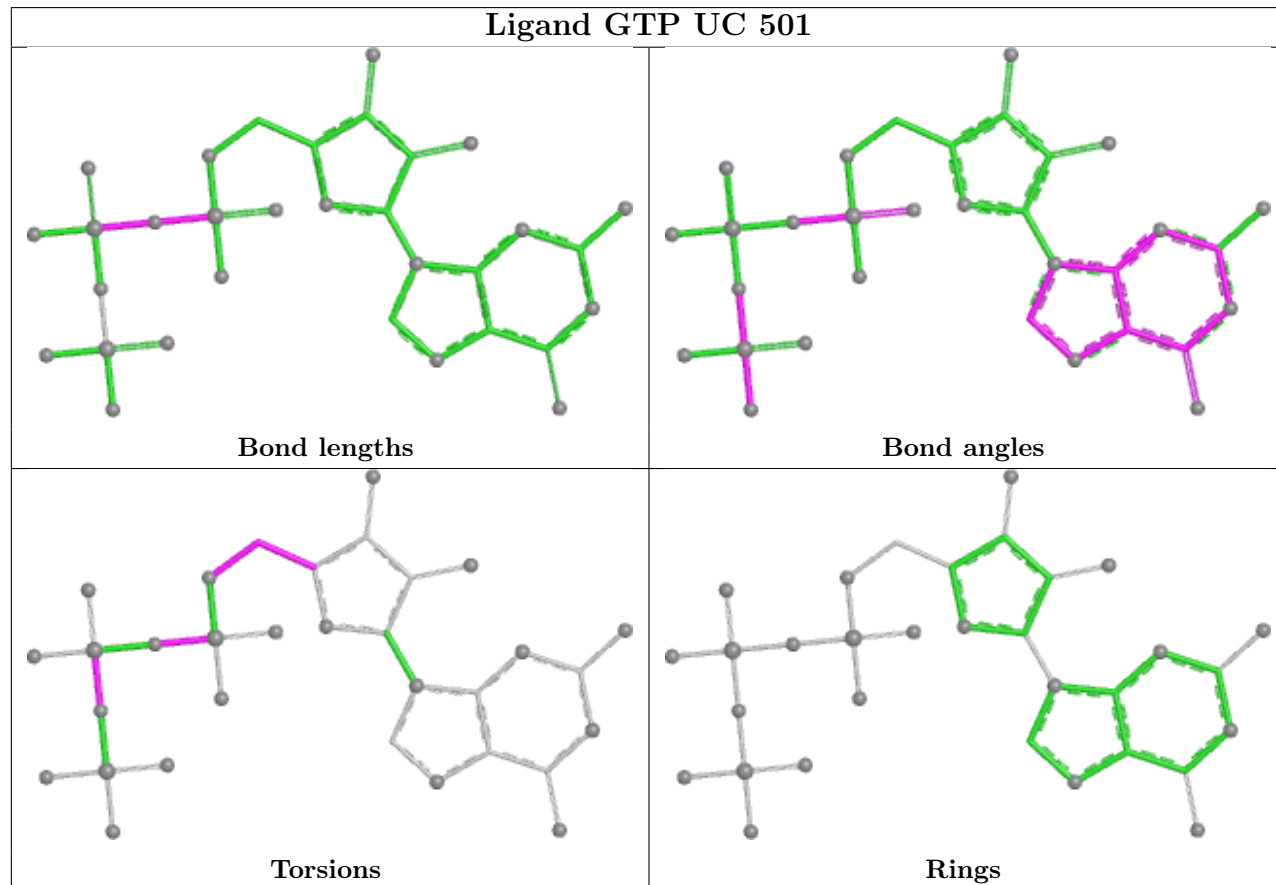


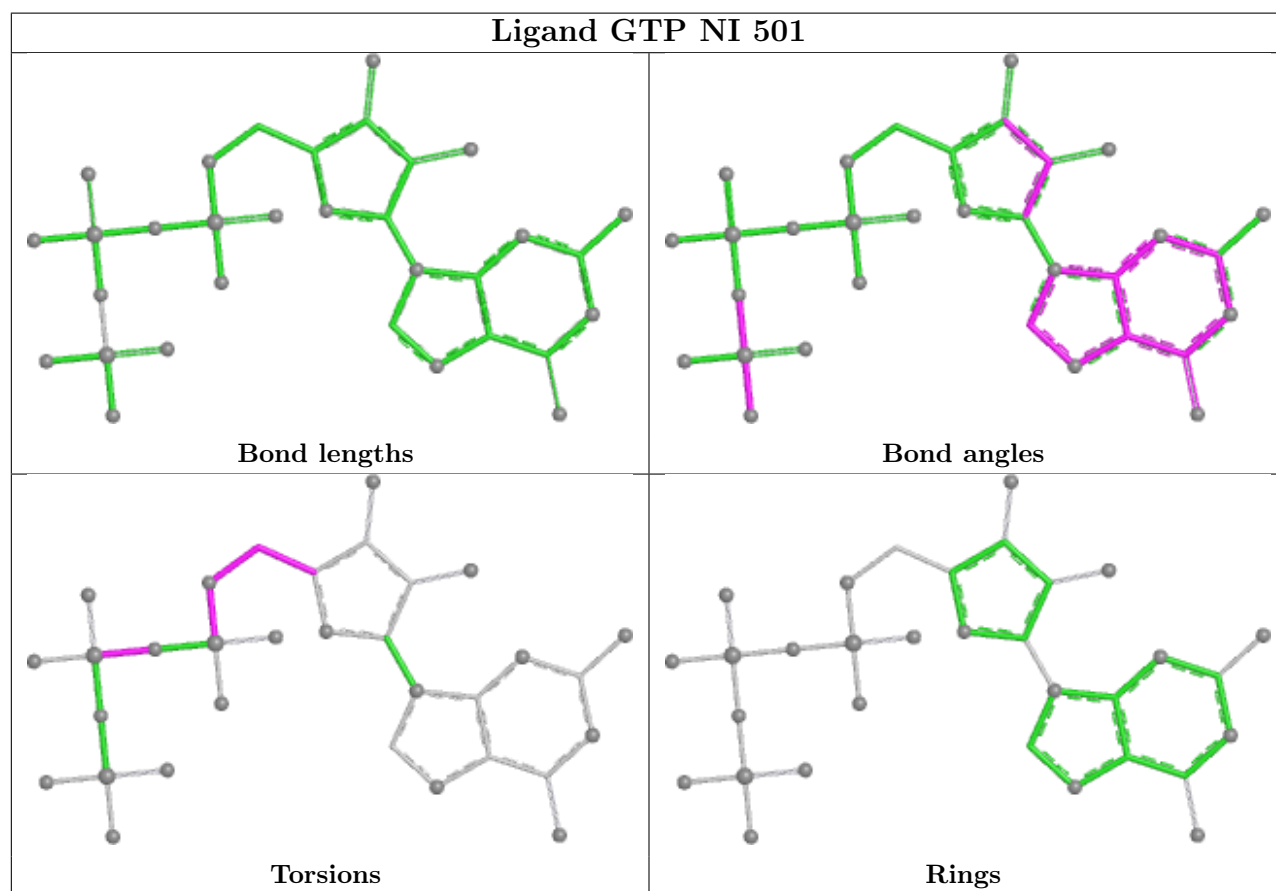
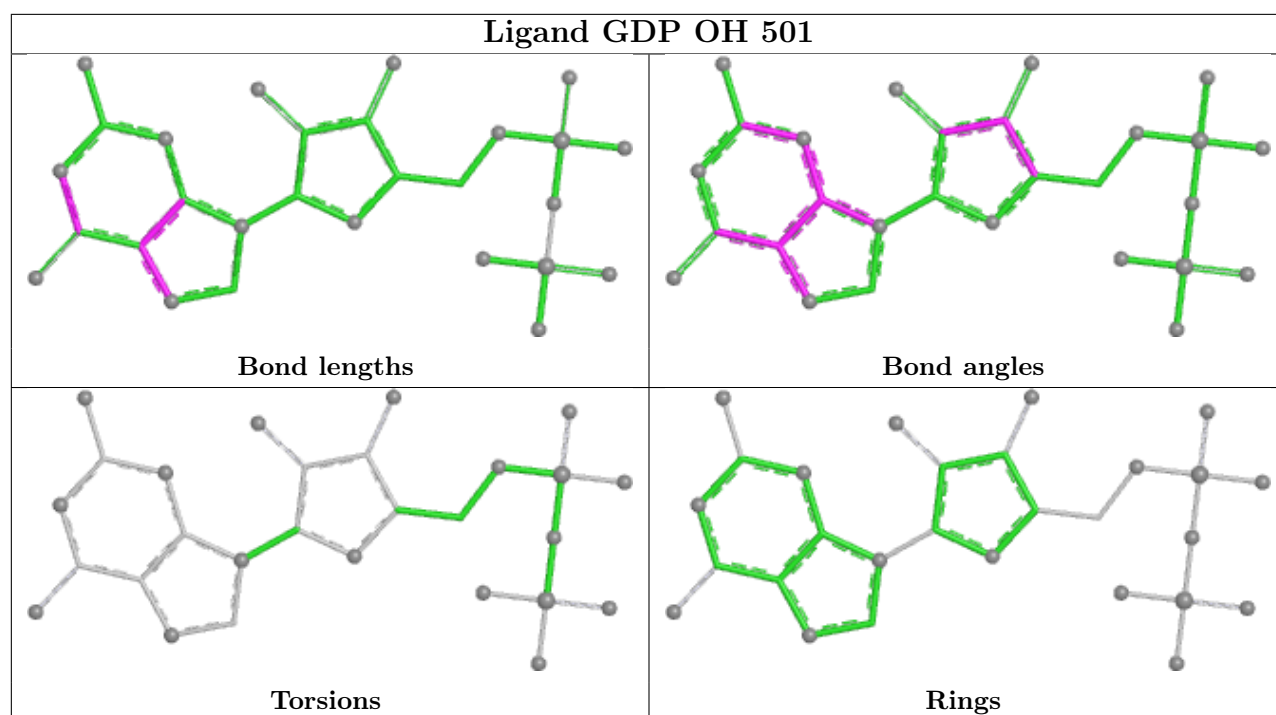


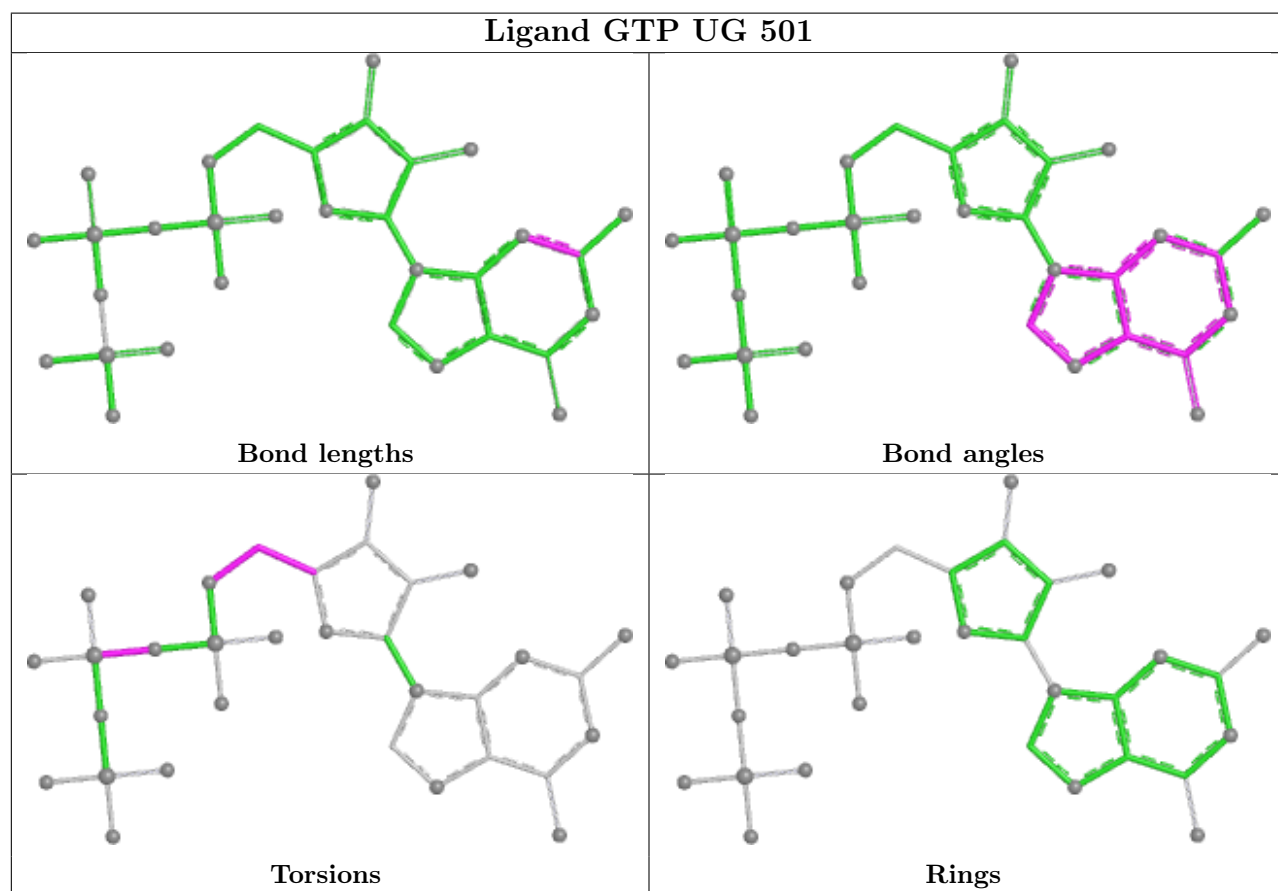
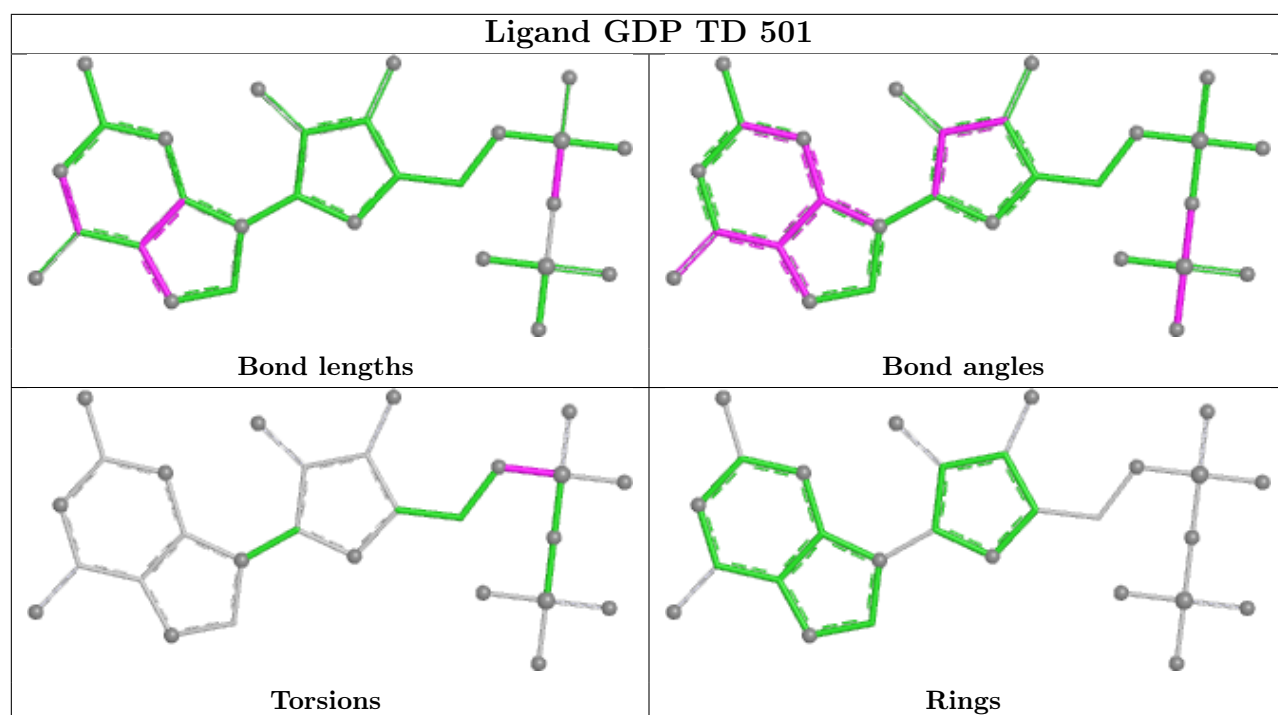
## Ligand GTP QE 501



## Ligand GTP UC 501

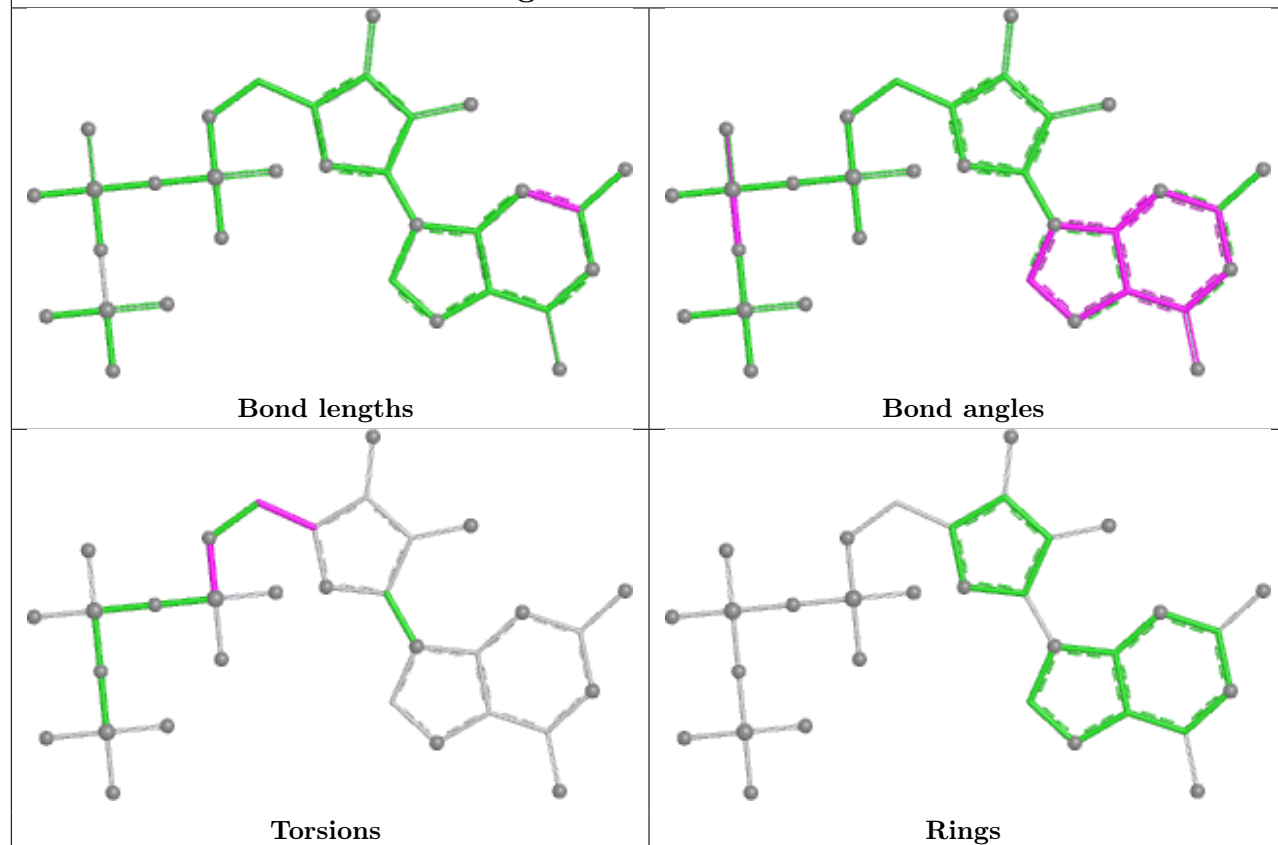




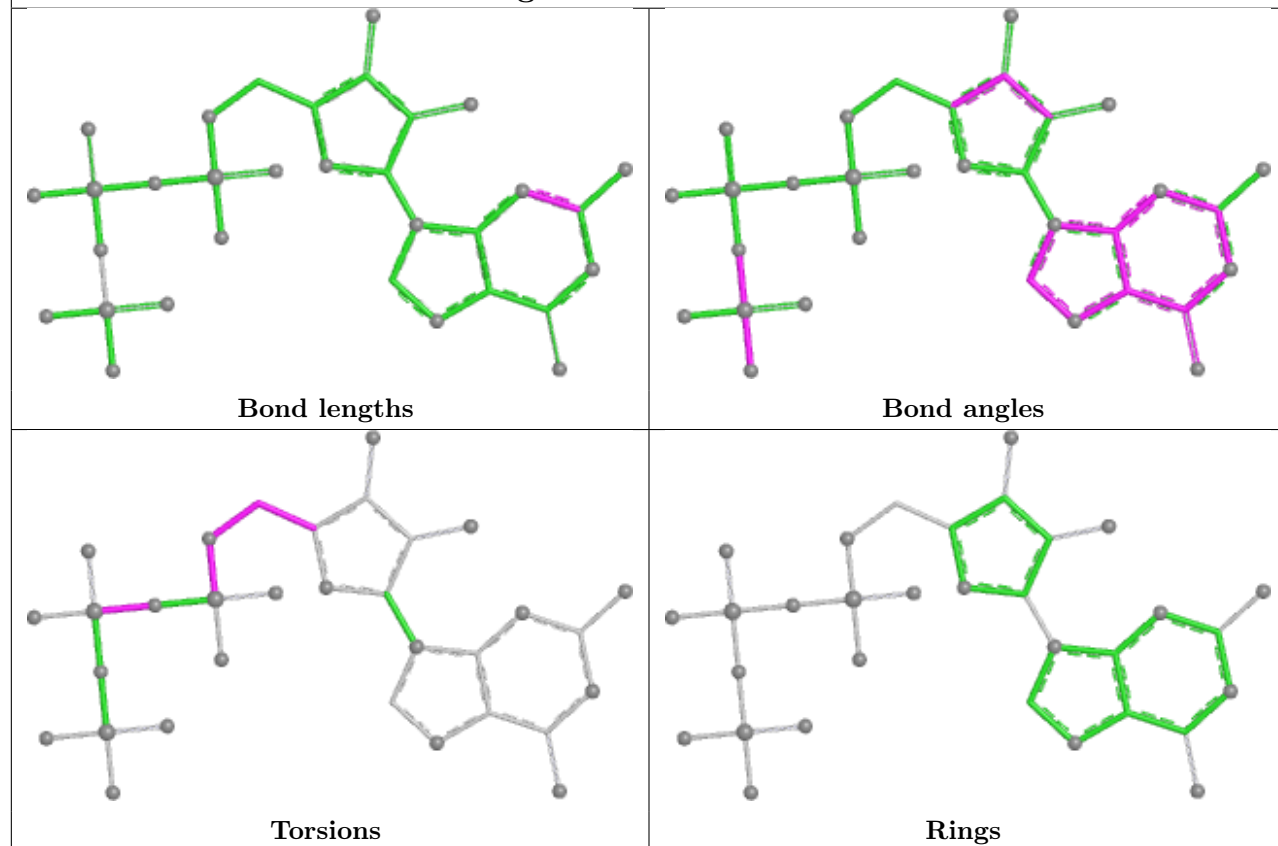




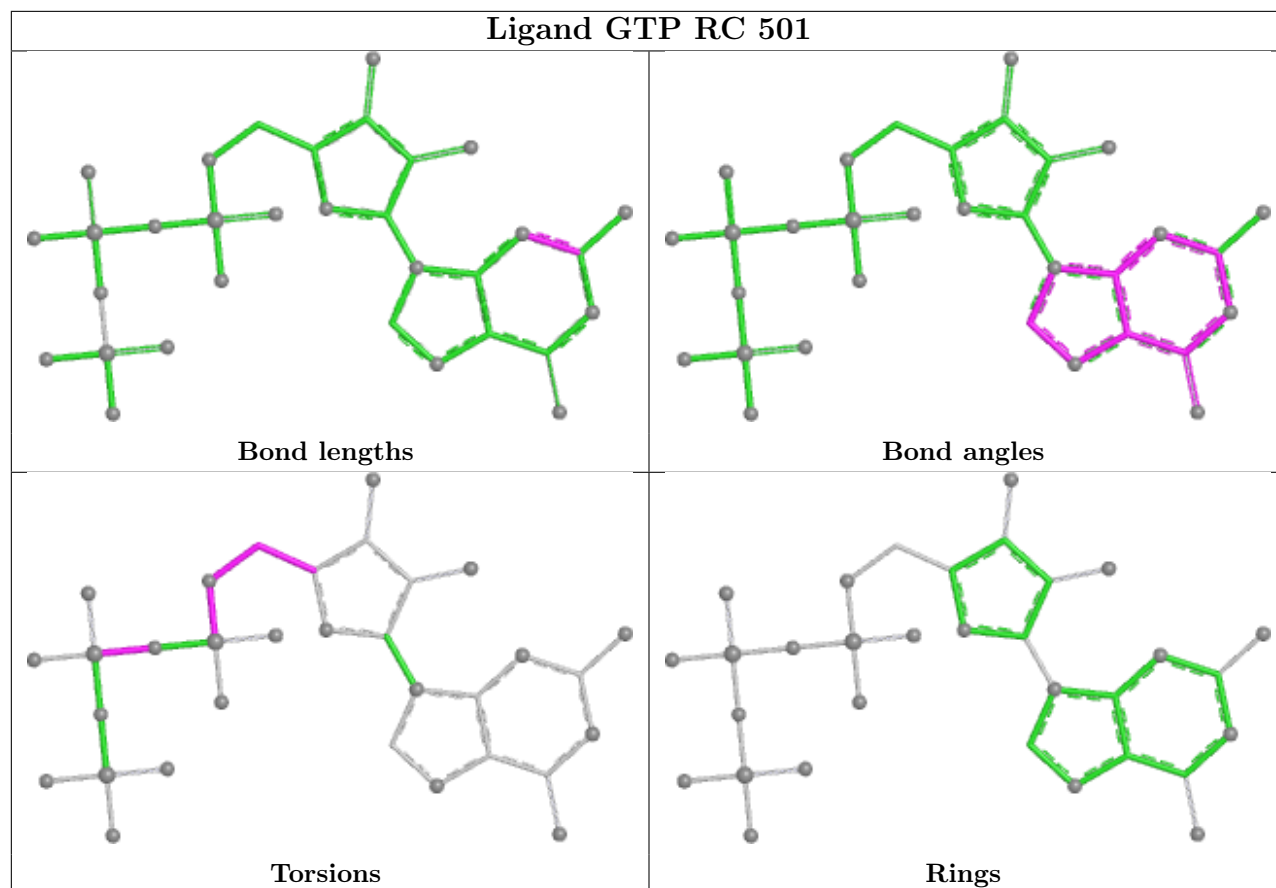
## Ligand GTP GE 501



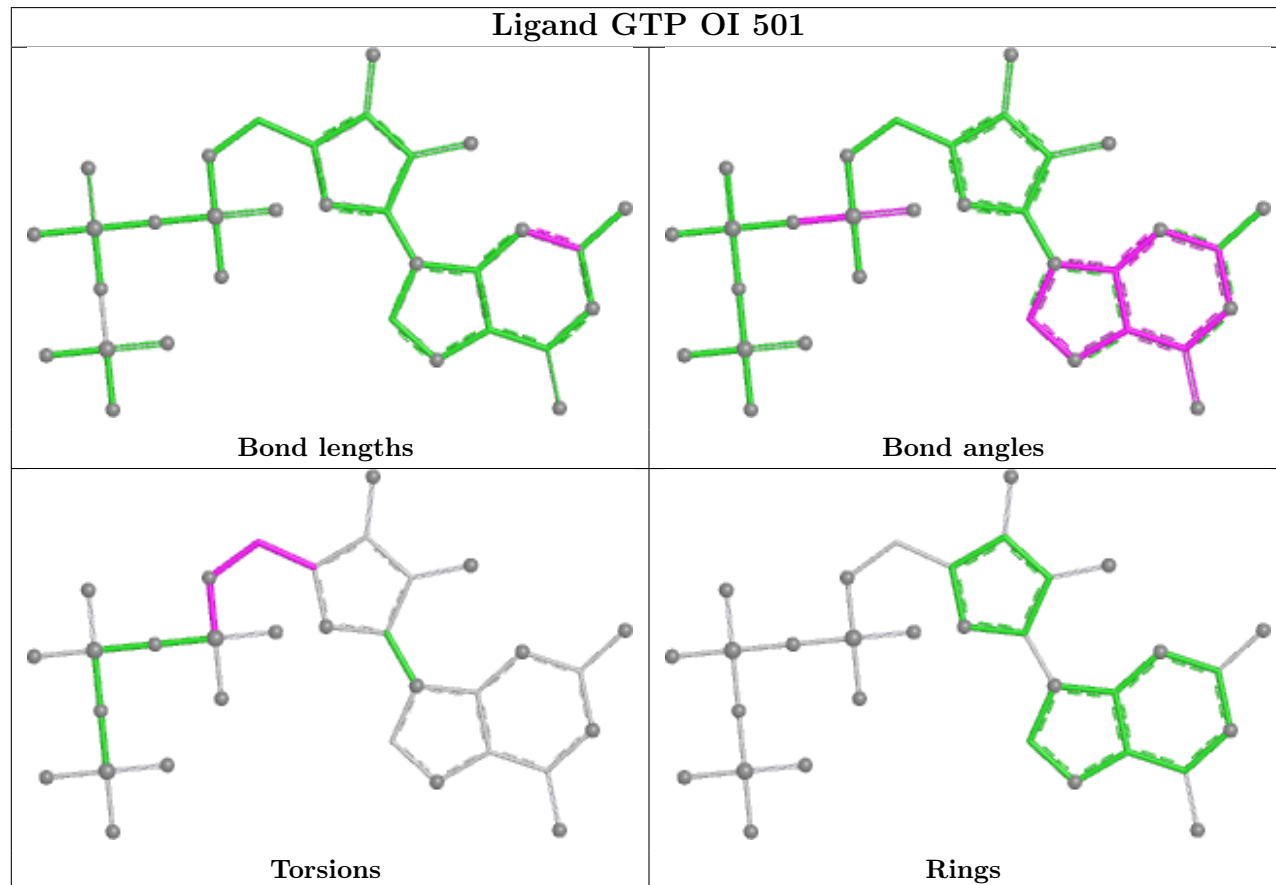
## Ligand GTP OC 501

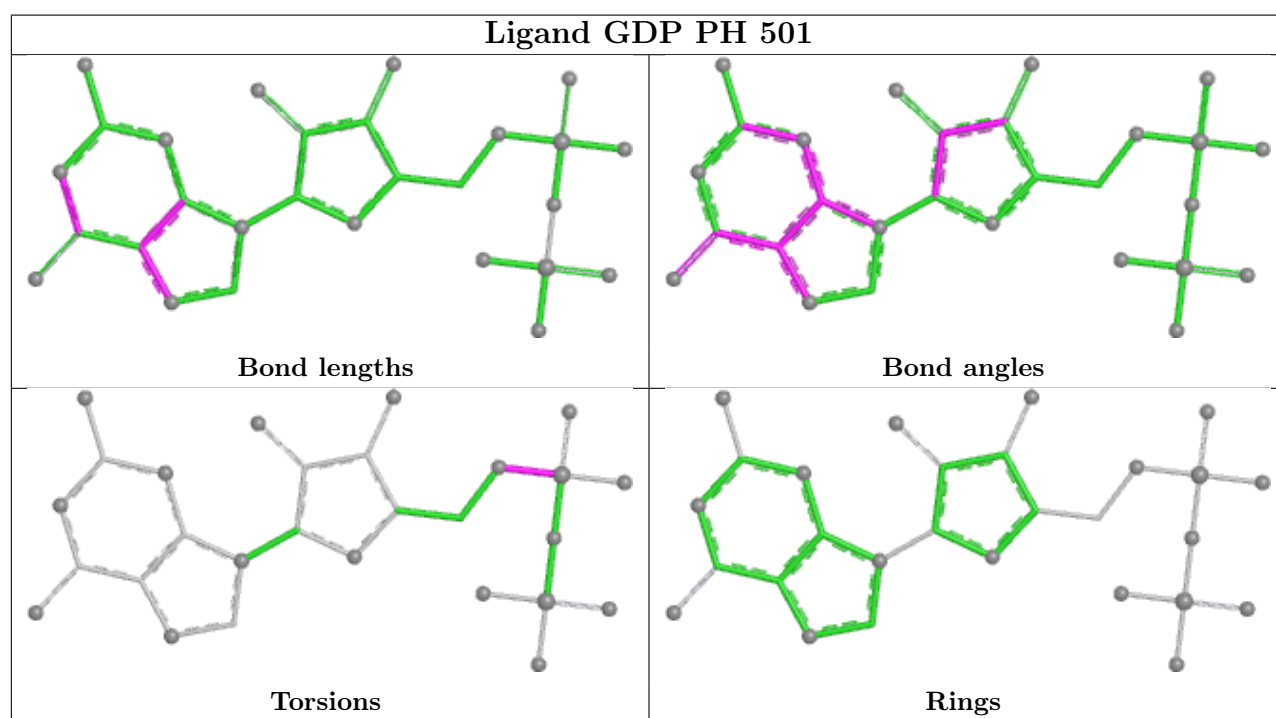
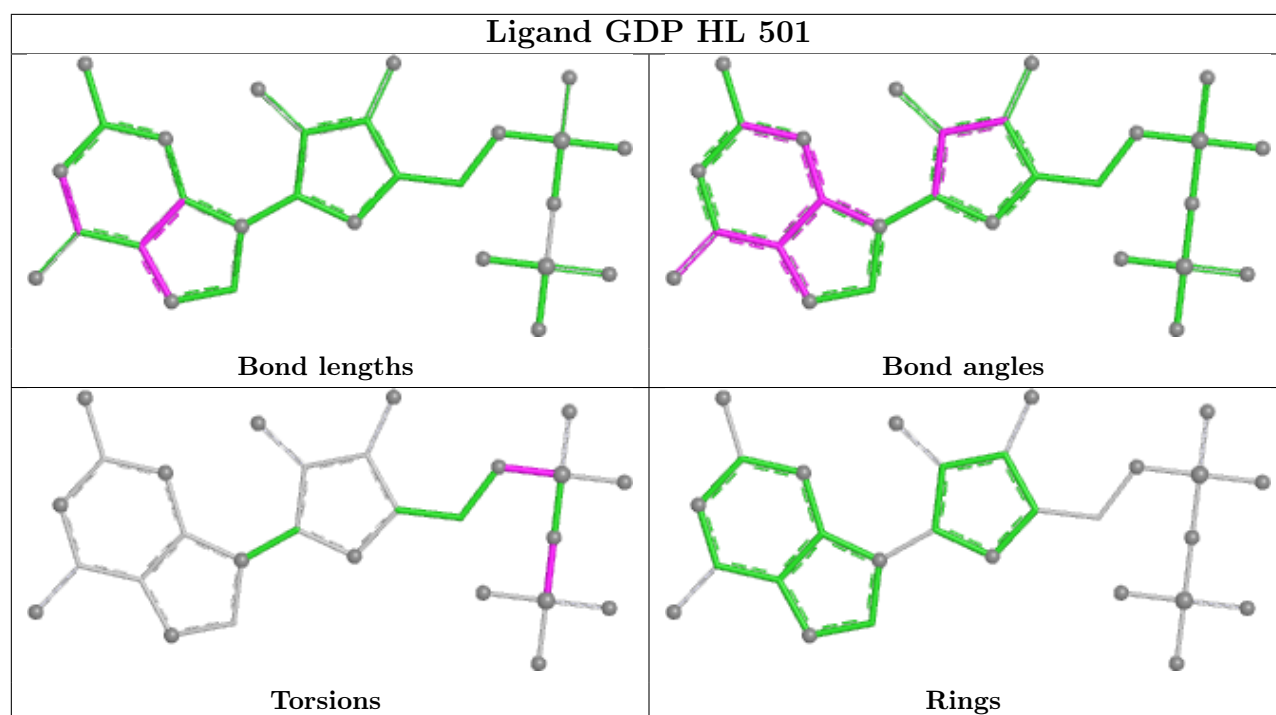


## Ligand GTP RC 501

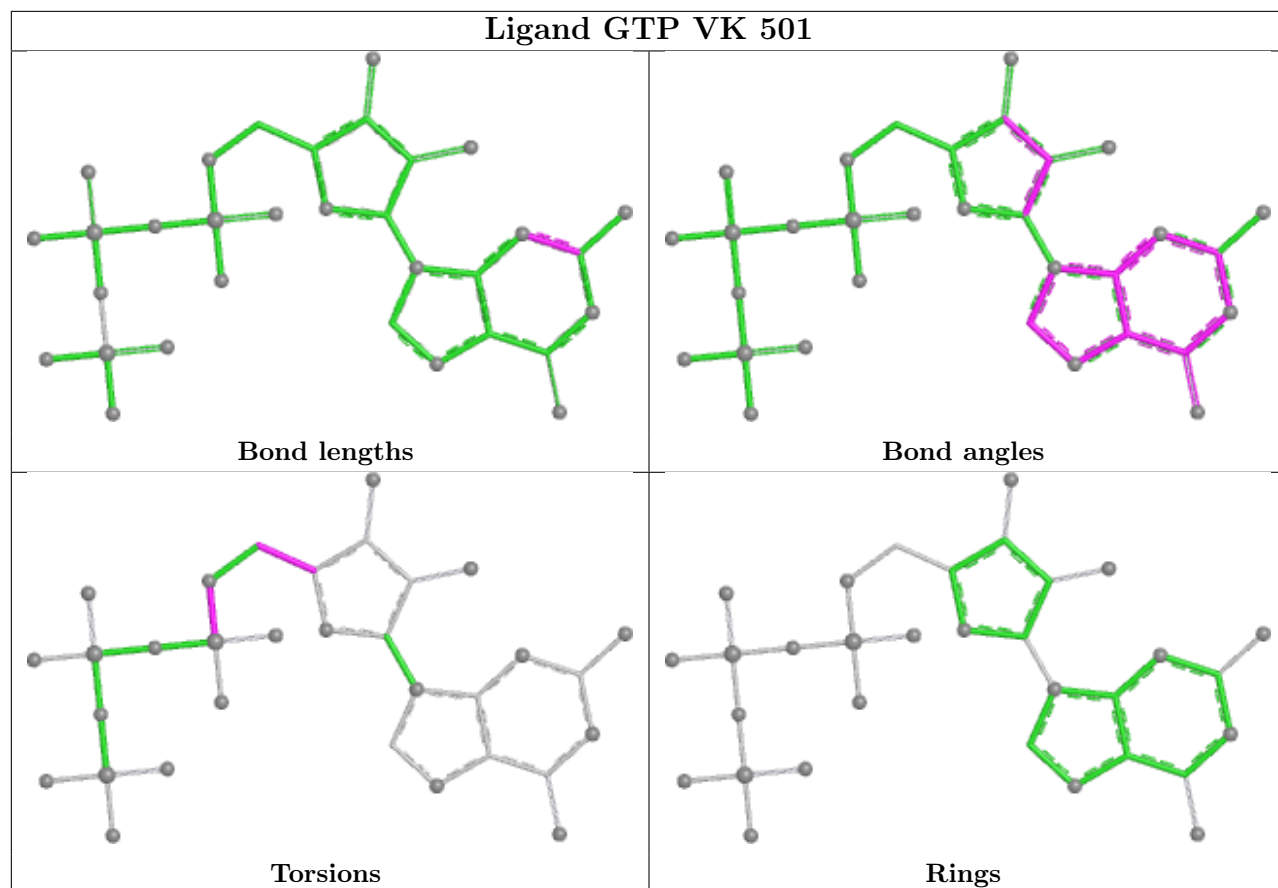


## Ligand GTP OI 501

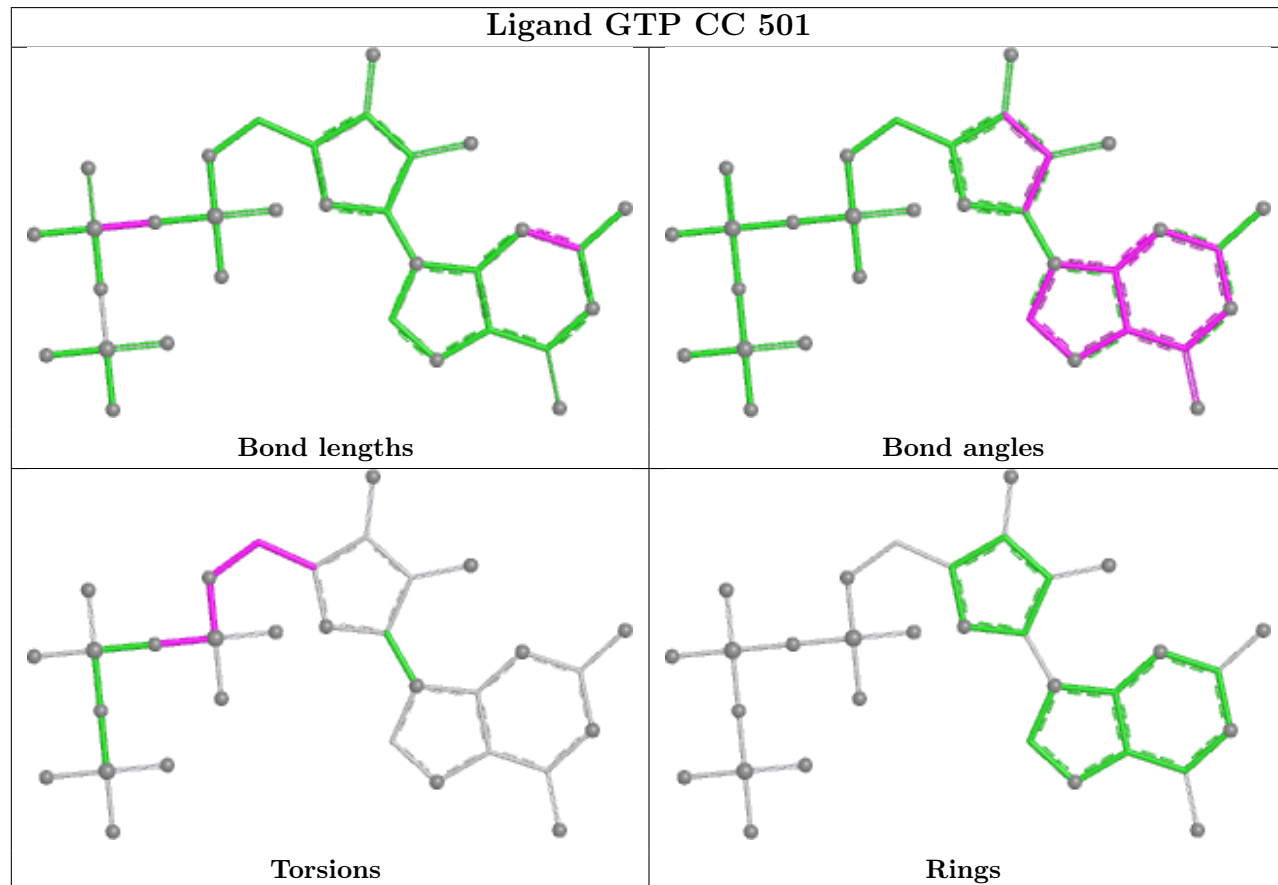


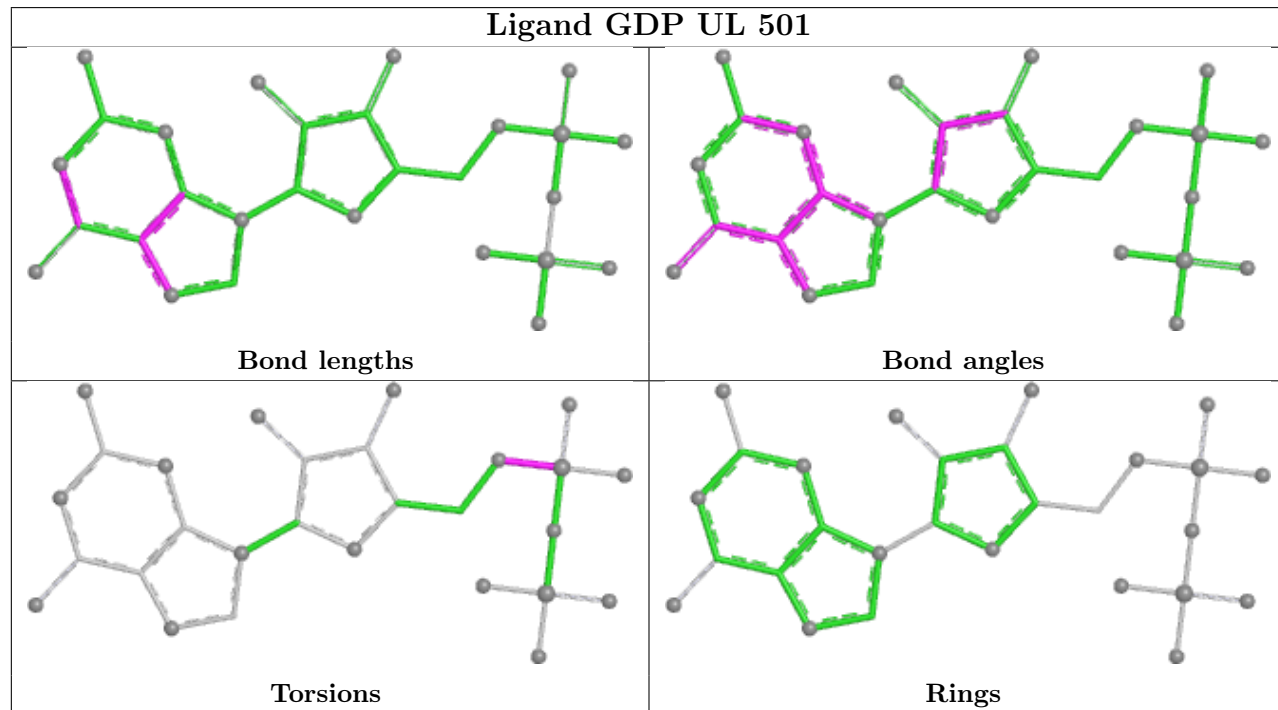
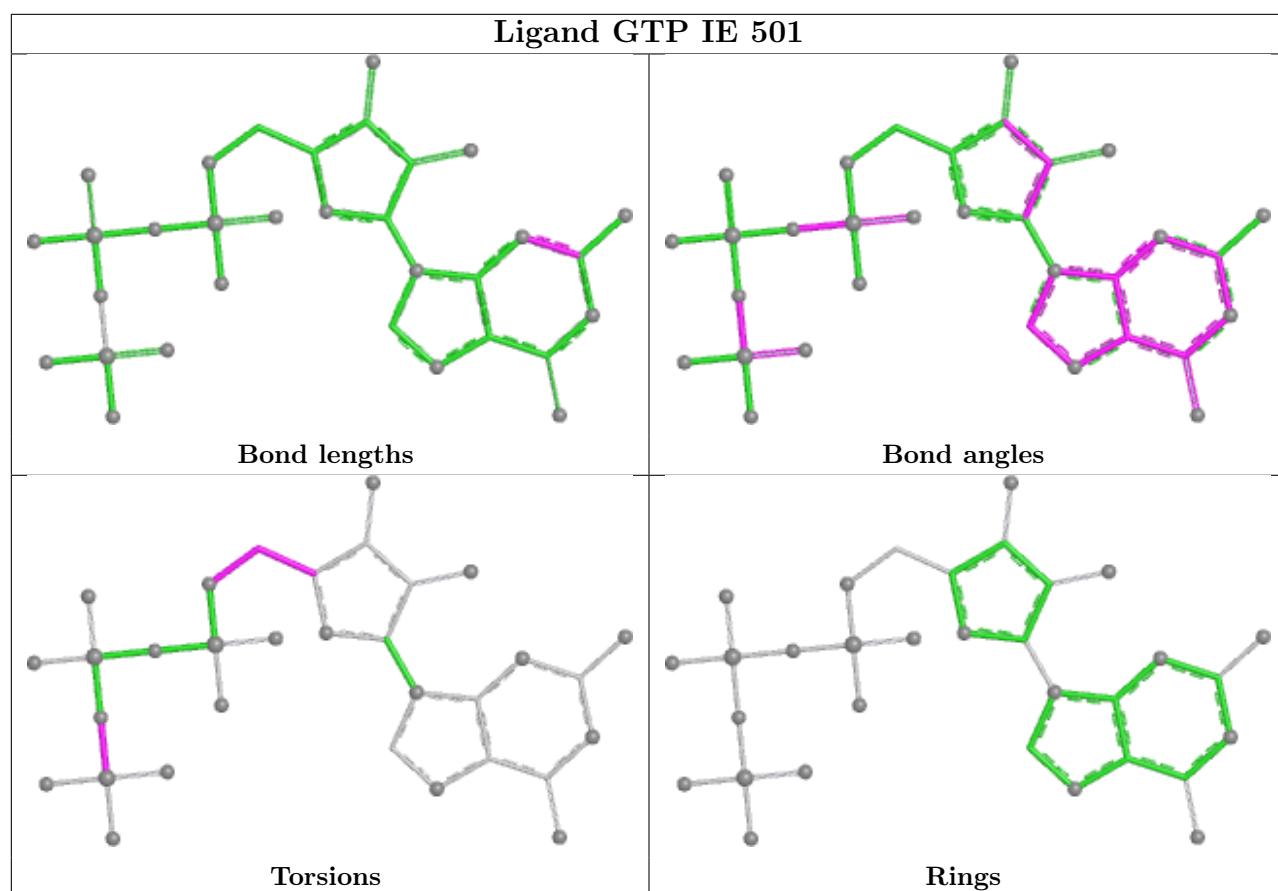


## Ligand GTP VK 501

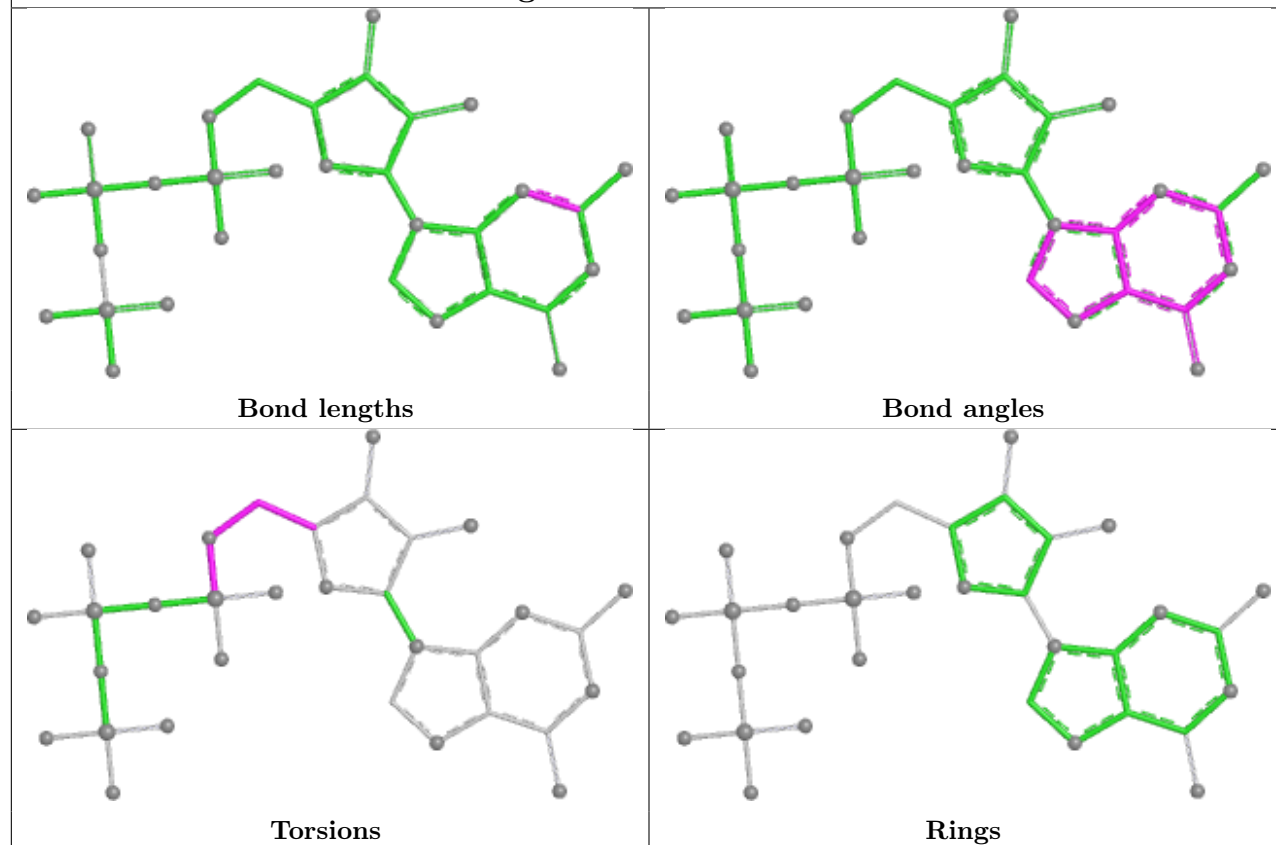


## Ligand GTP CC 501

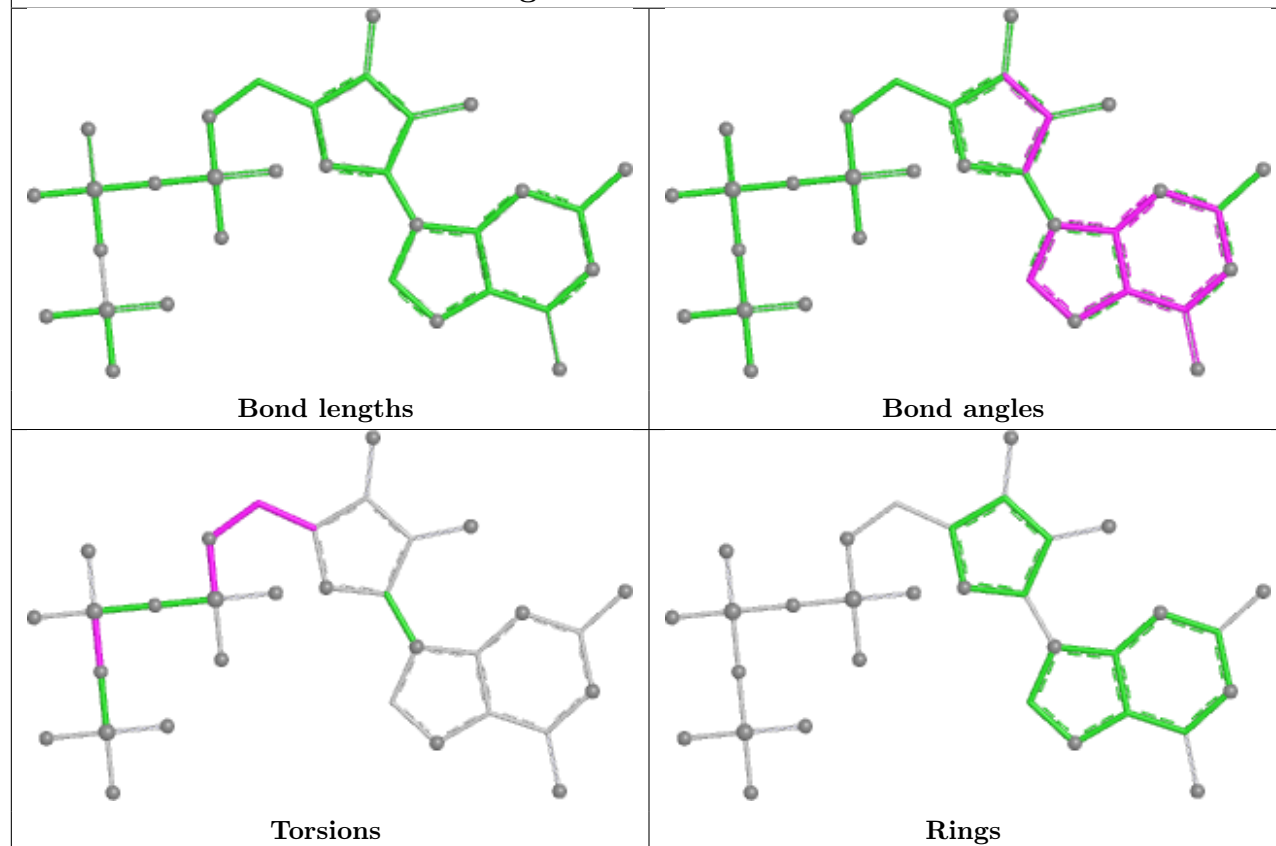


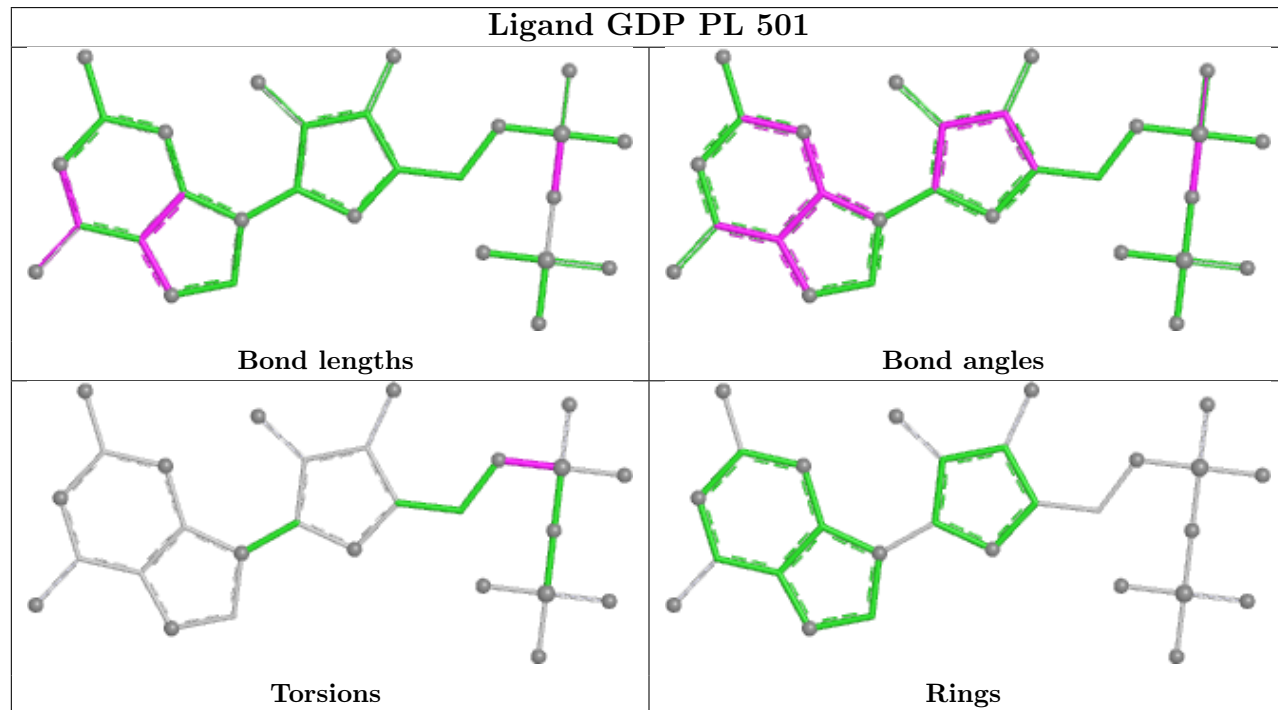
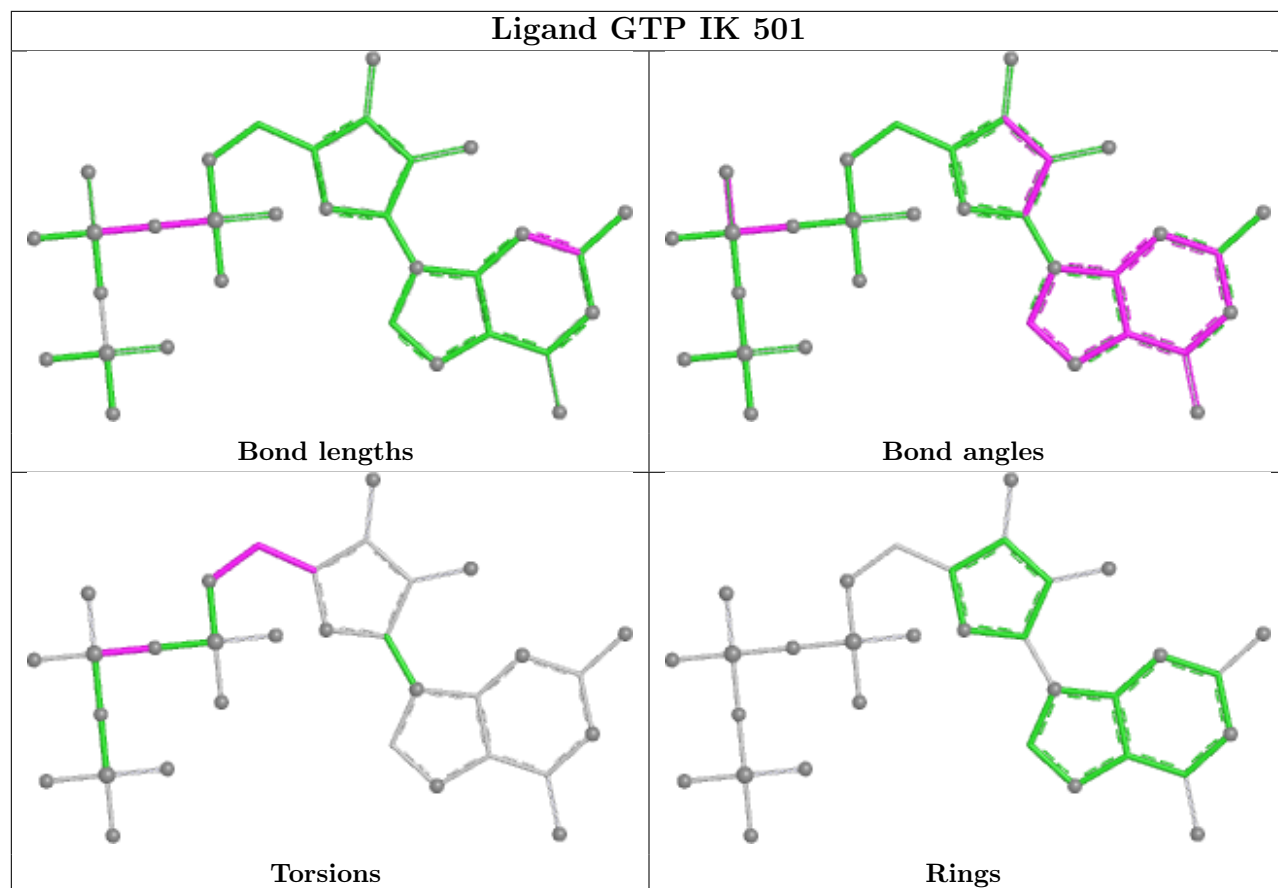


## Ligand GTP UE 501

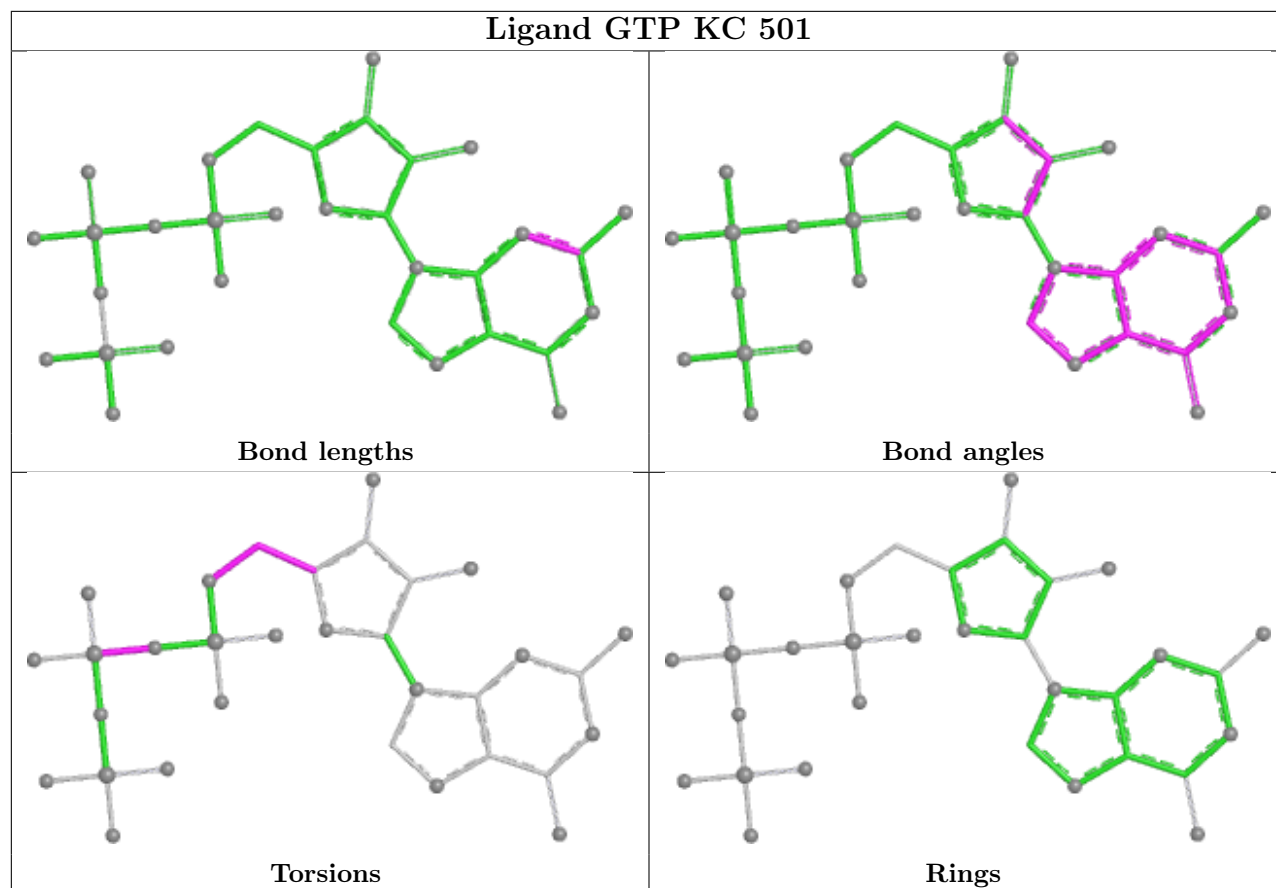


## Ligand GTP PA 501

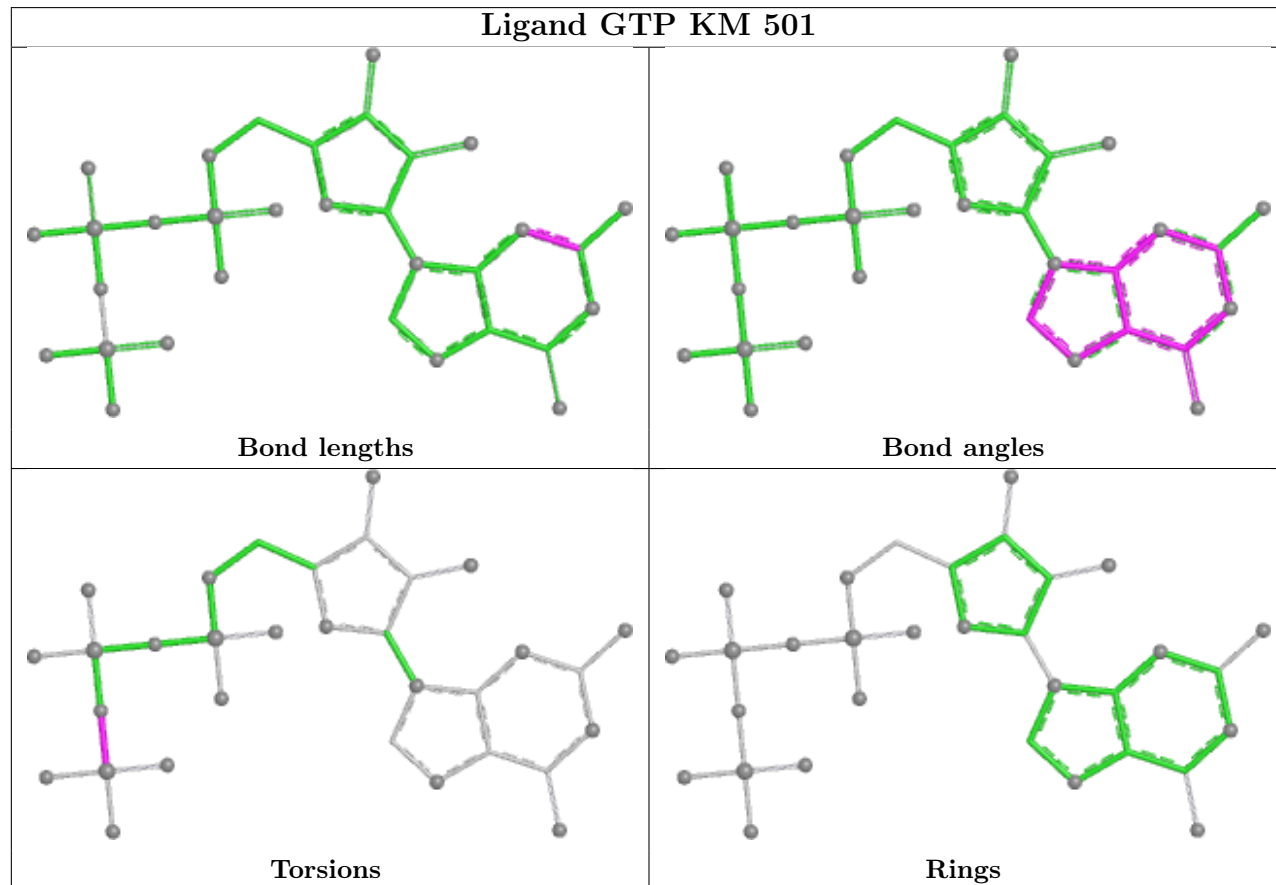




## Ligand GTP KC 501

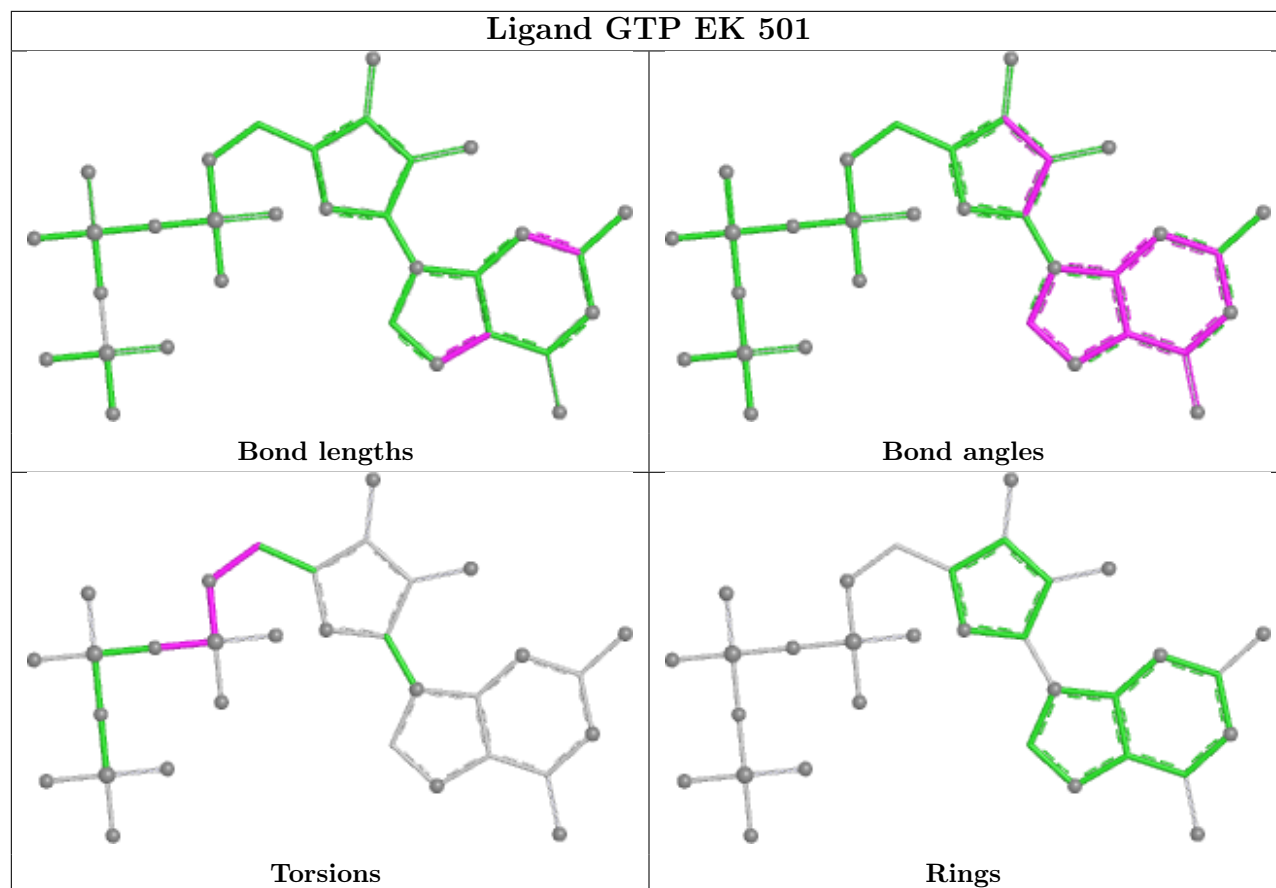


## Ligand GTP KM 501

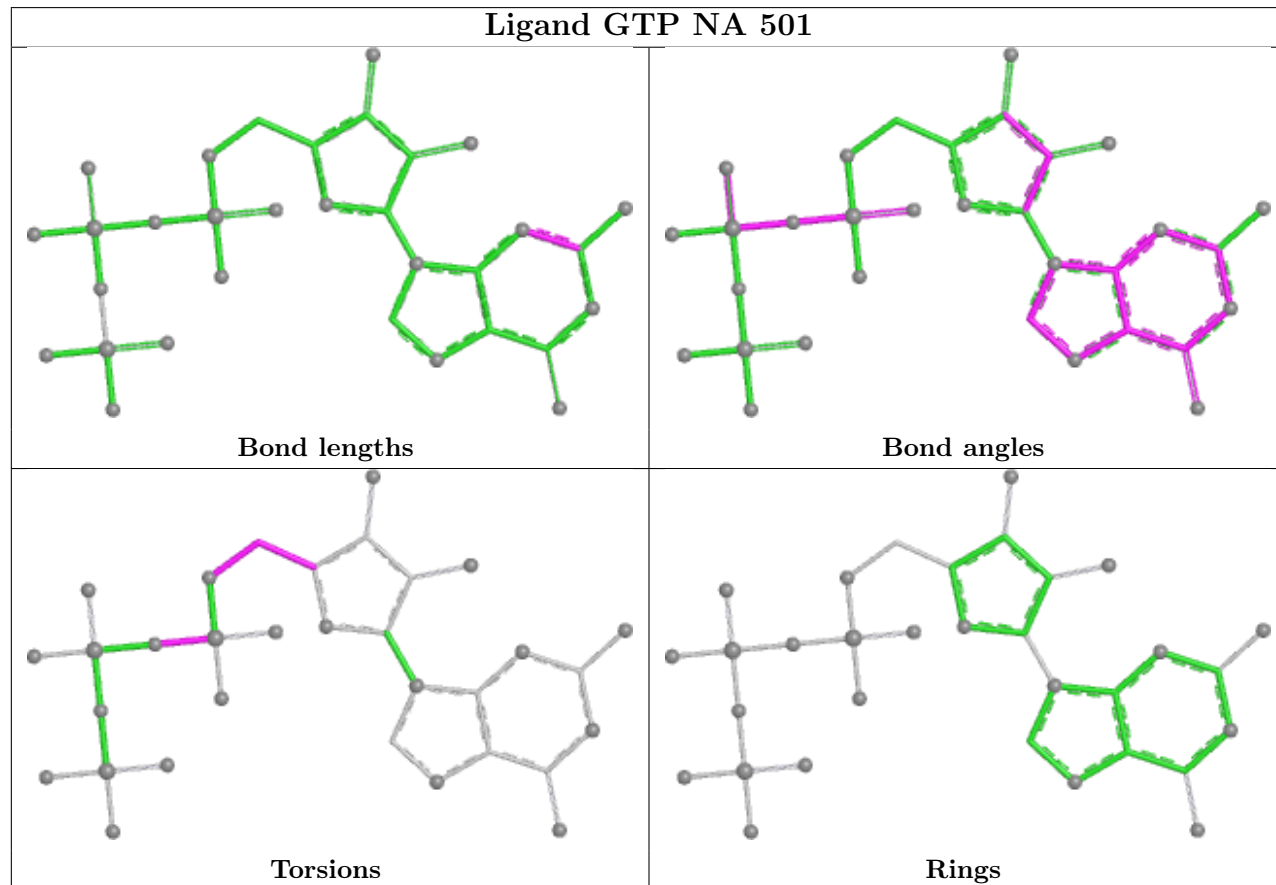


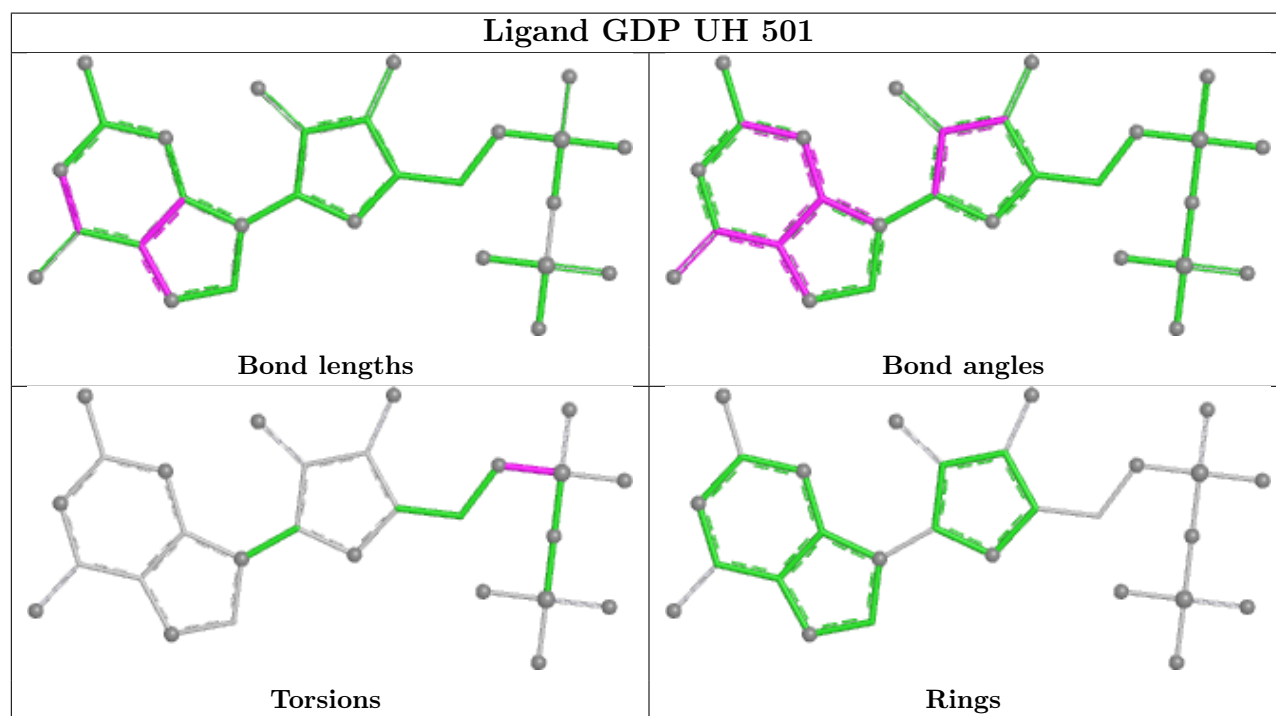
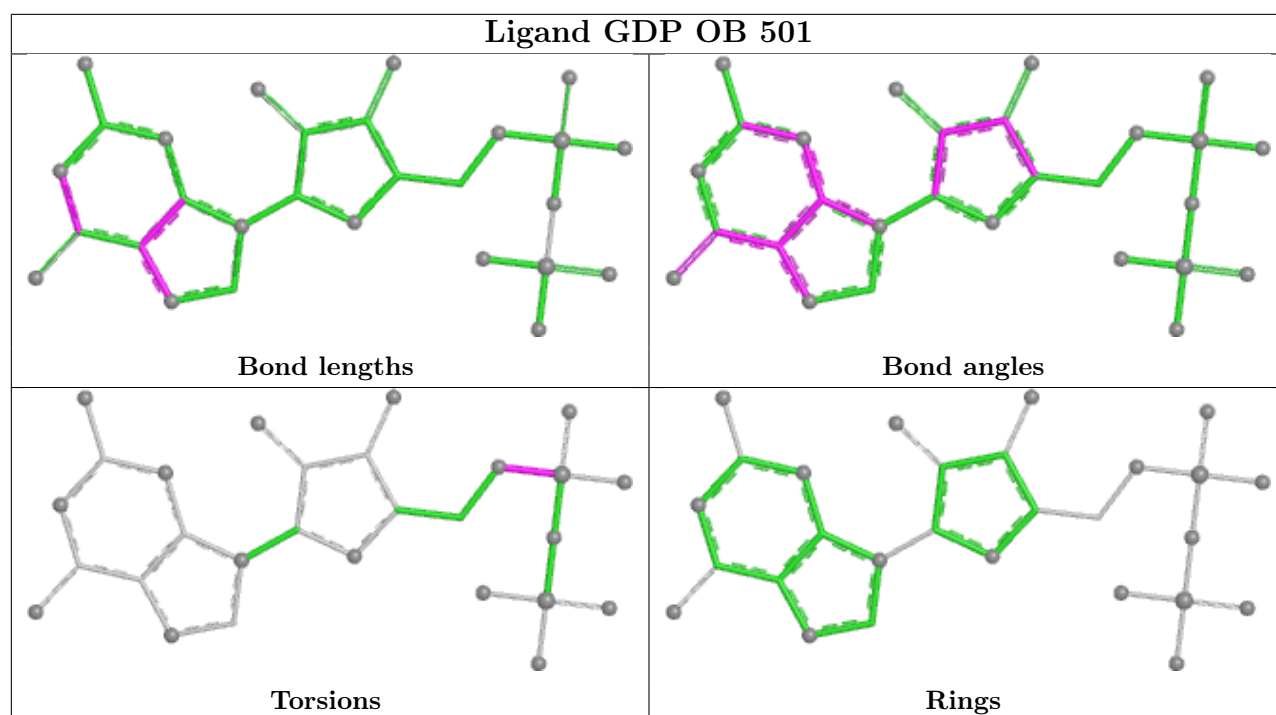


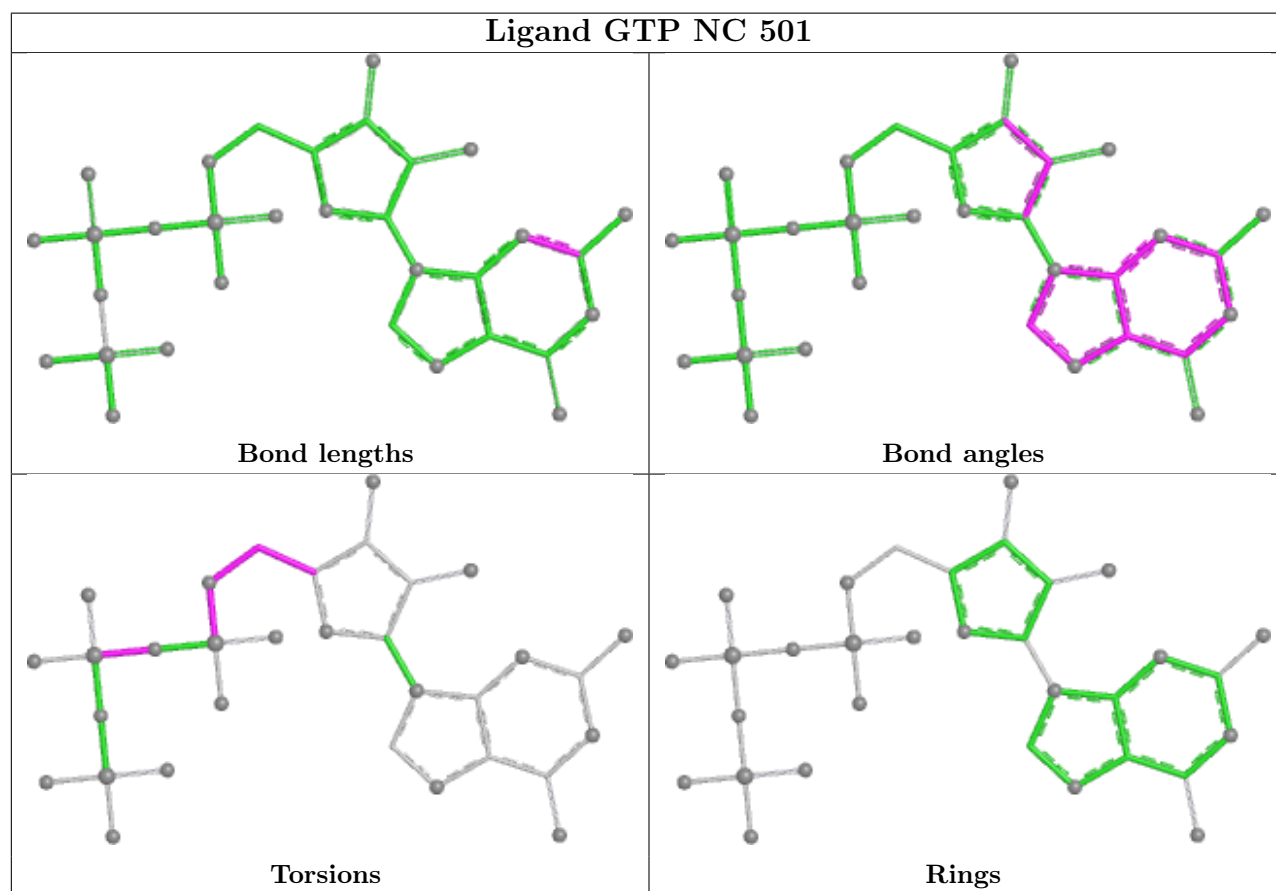
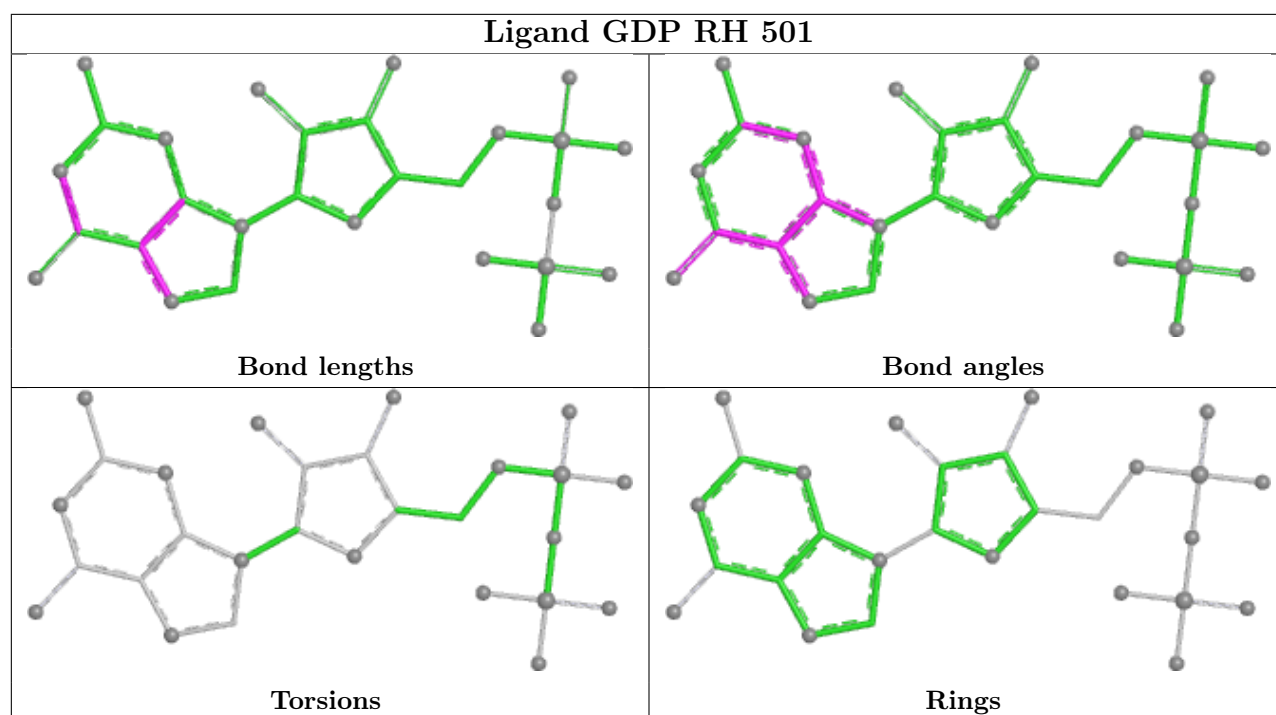
## Ligand GTP EK 501

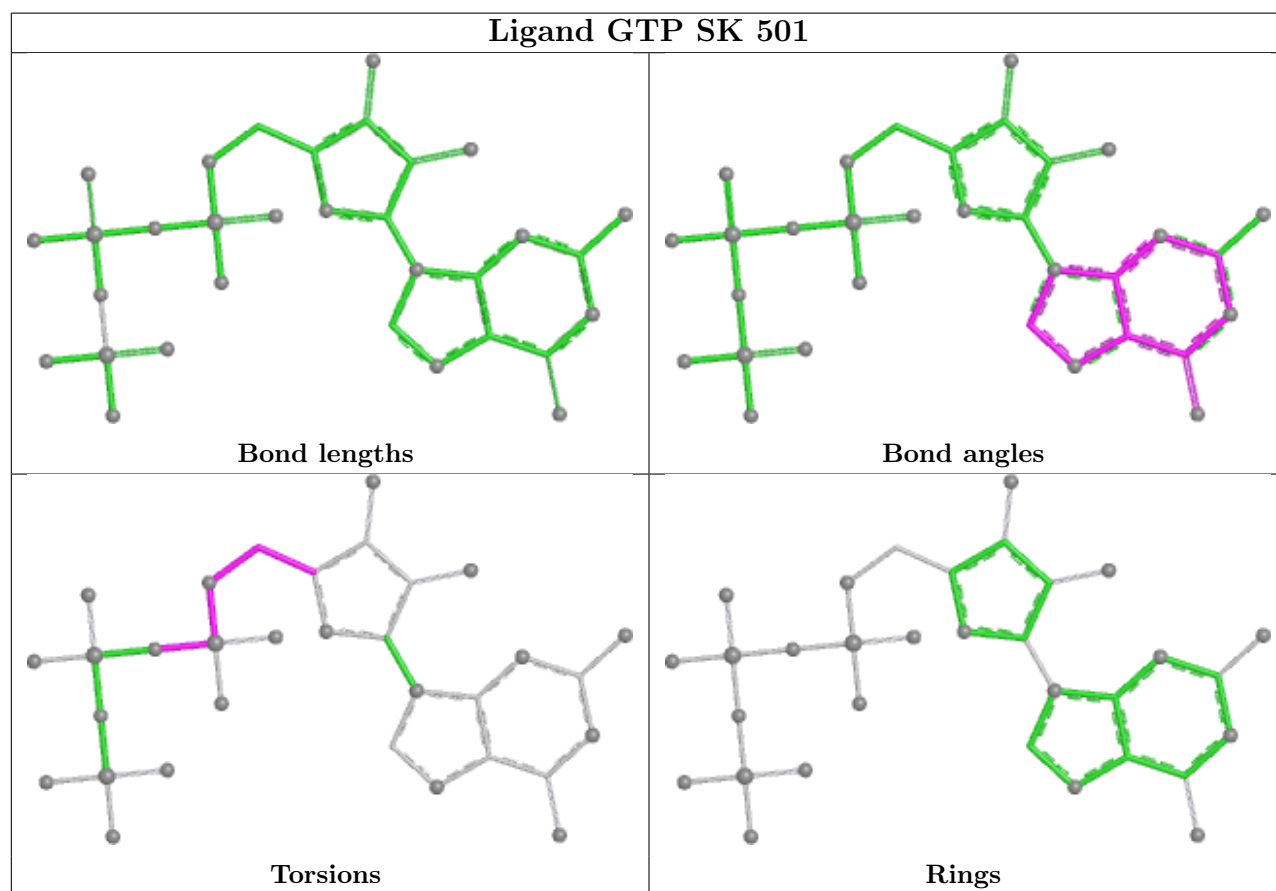
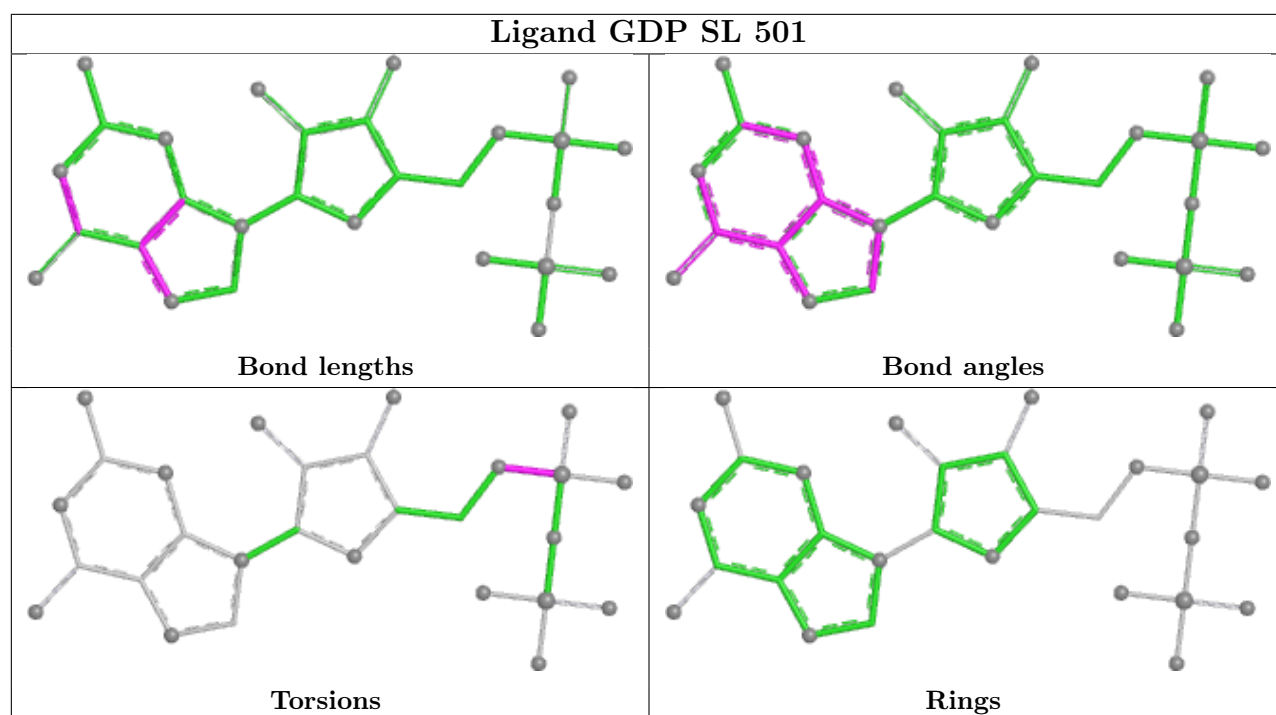


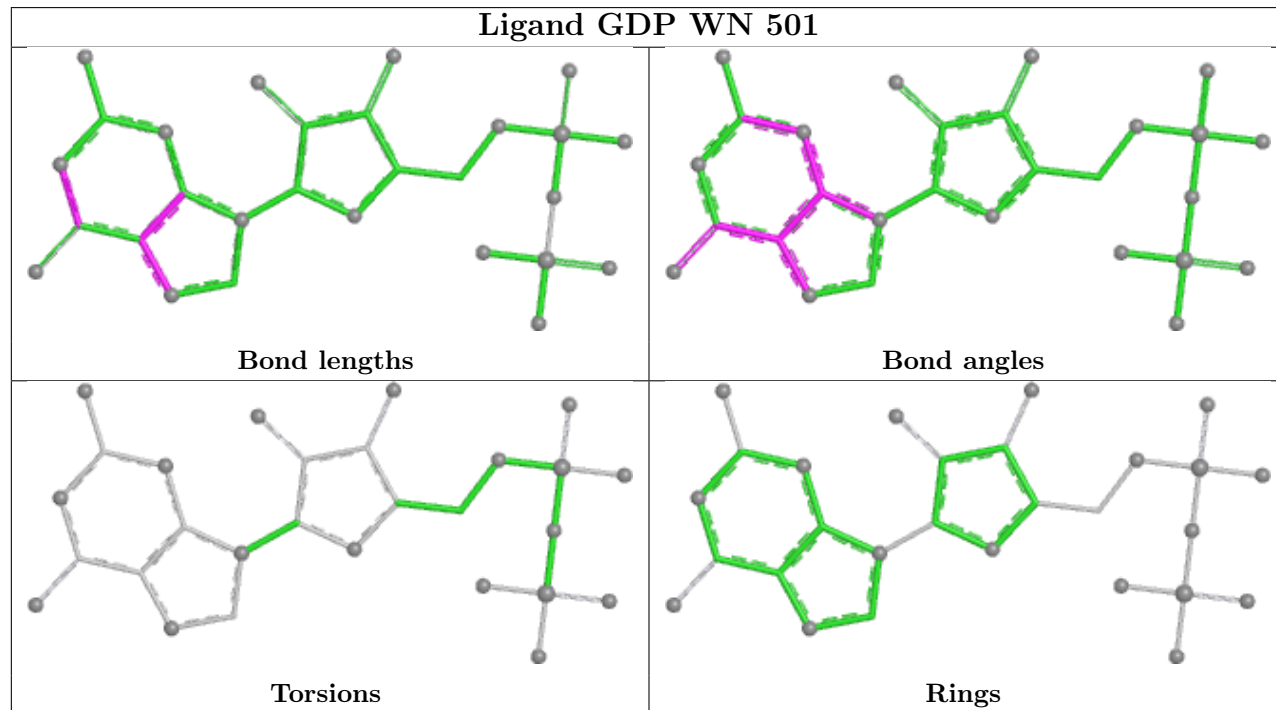
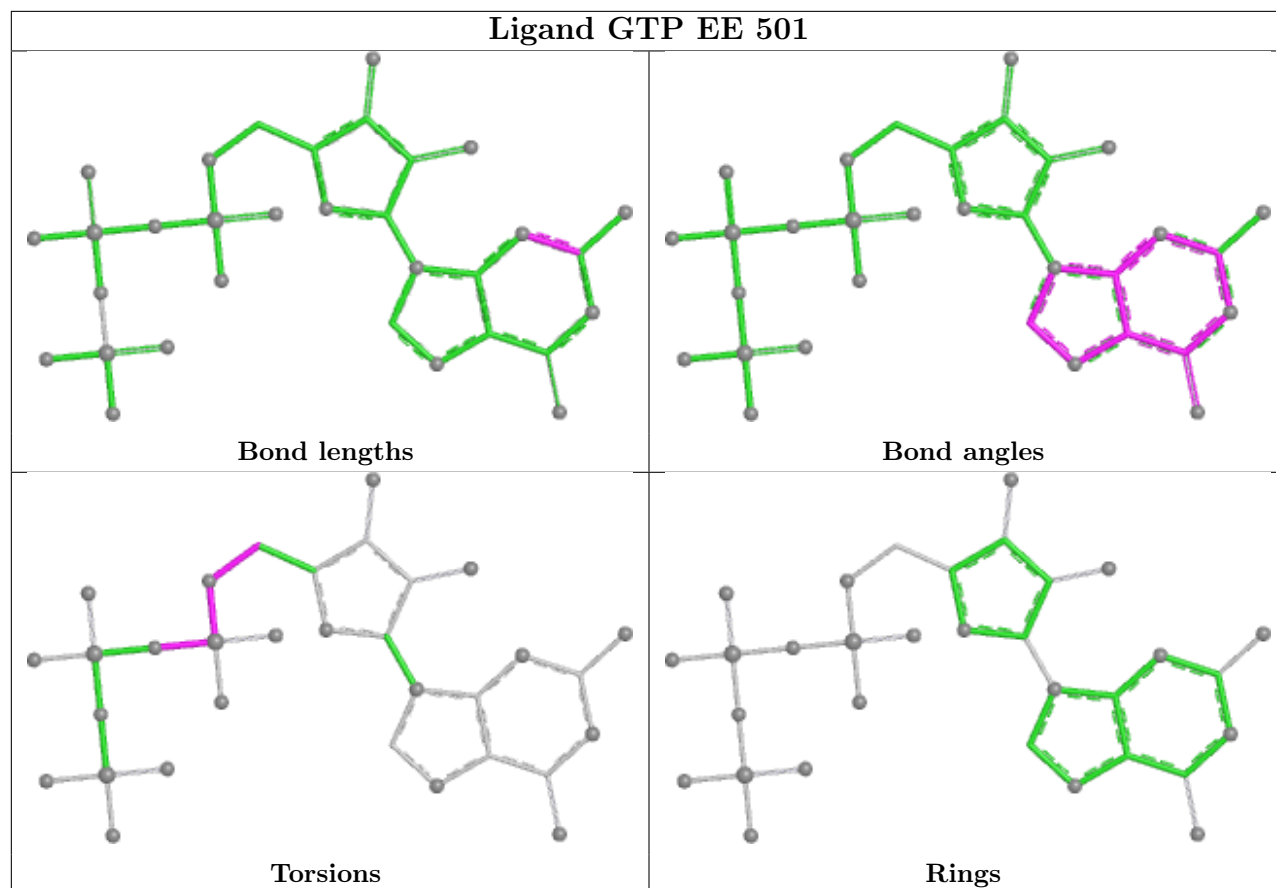
## Ligand GTP NA 501



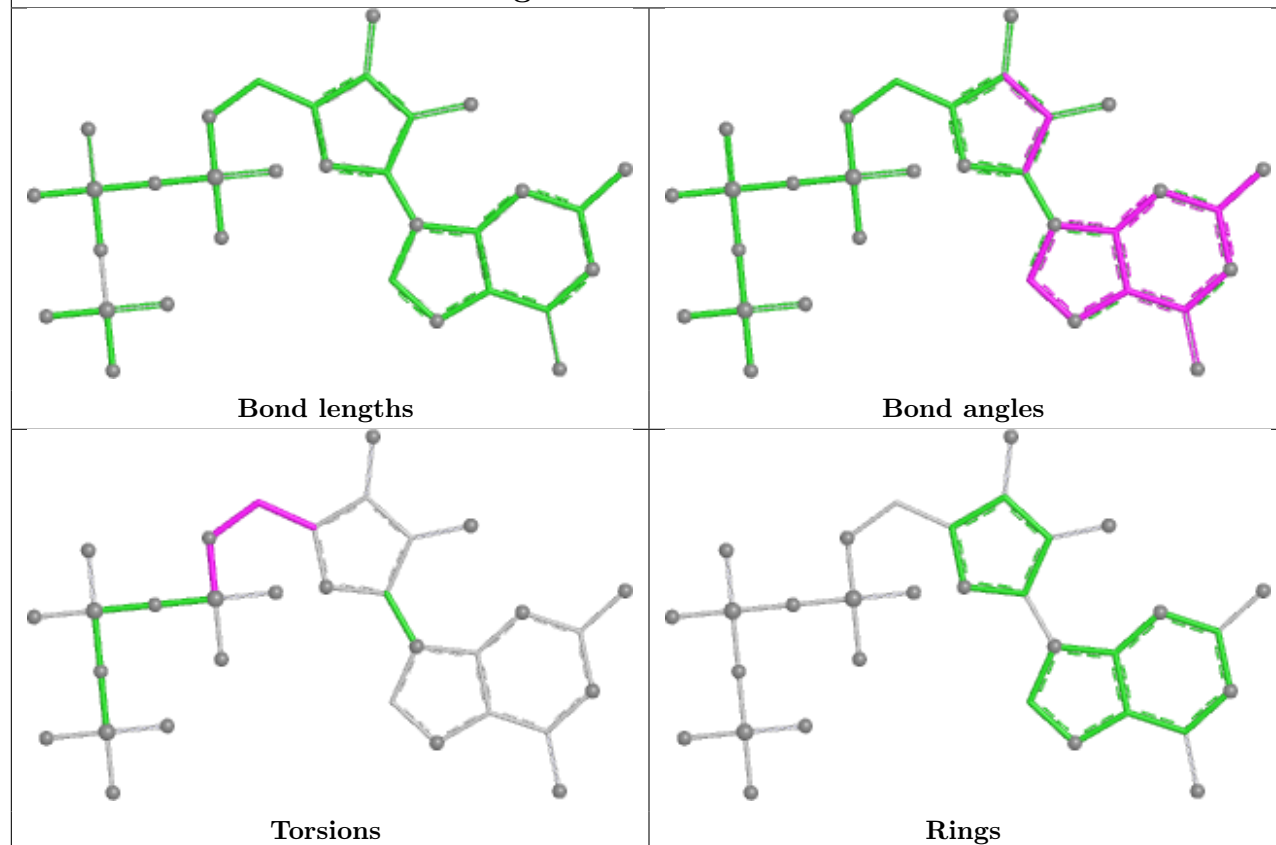




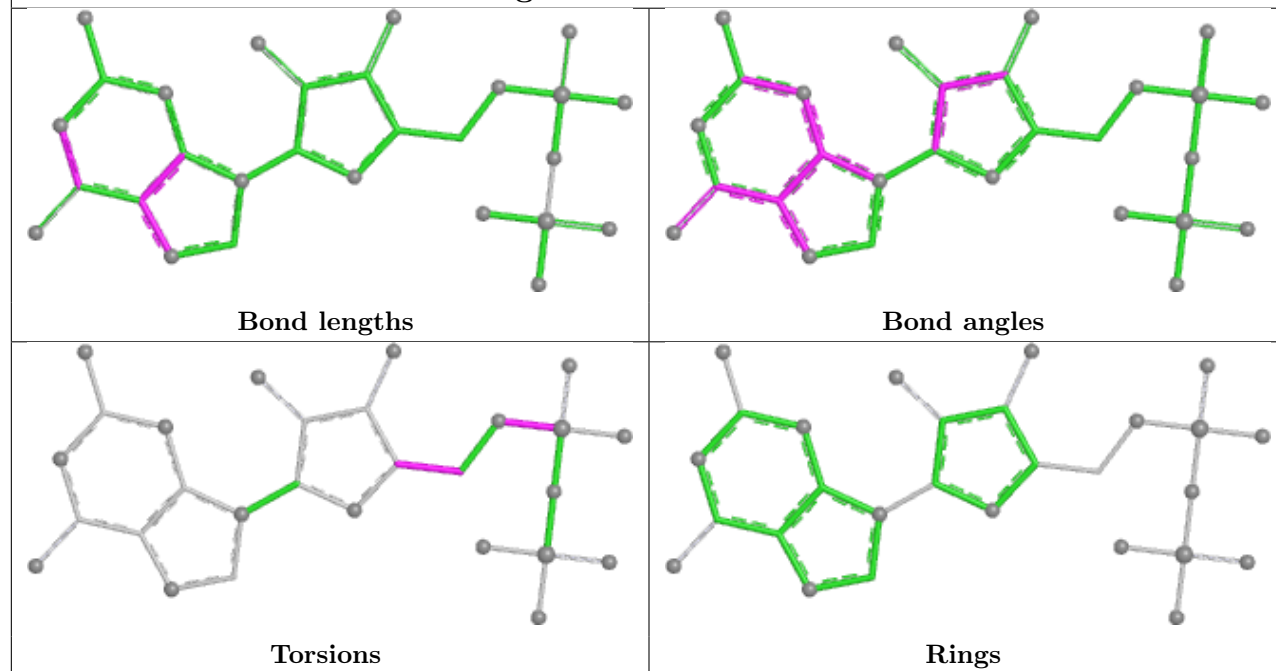


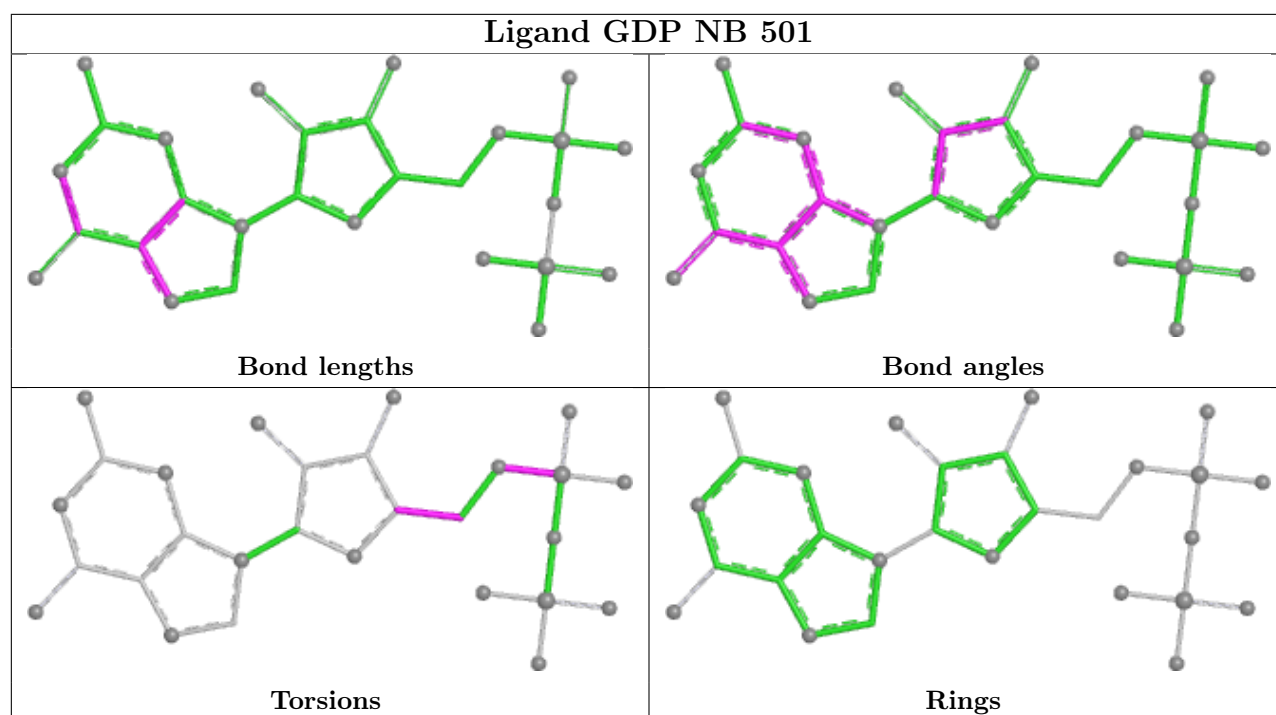


## Ligand GTP CM 501



## Ligand GDP BH 501





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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

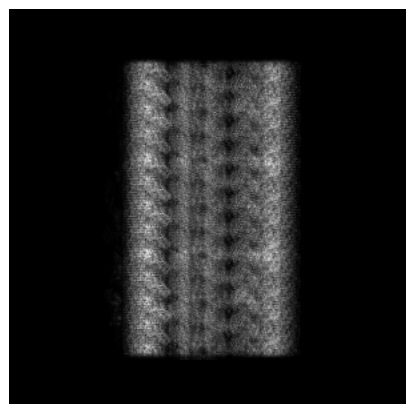
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45801. These allow visual inspection of the internal detail of the map and identification of artifacts.

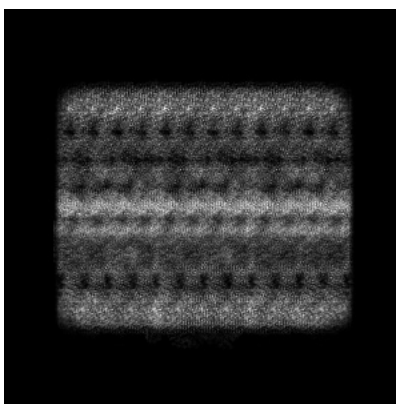
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

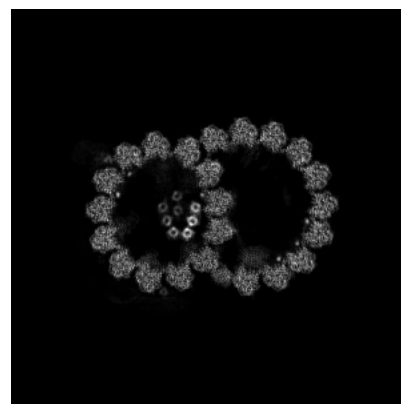
#### 5.1.1 Primary map



X

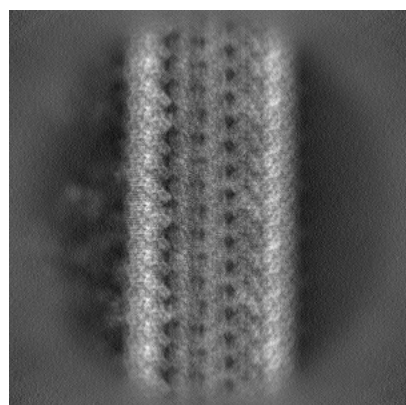


Y

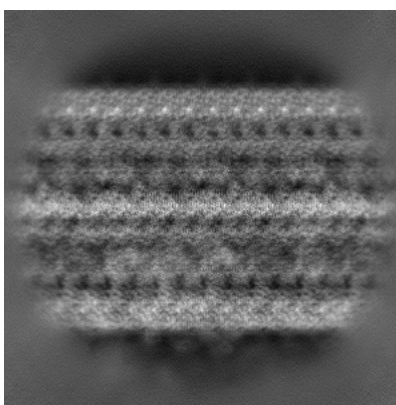


Z

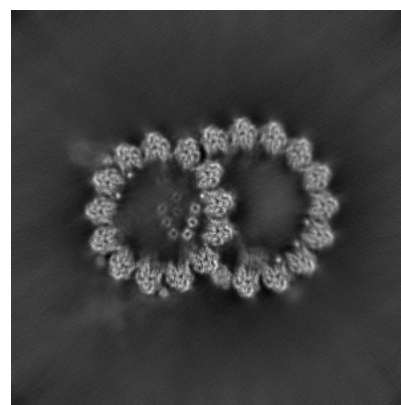
#### 5.1.2 Raw map



X



Y



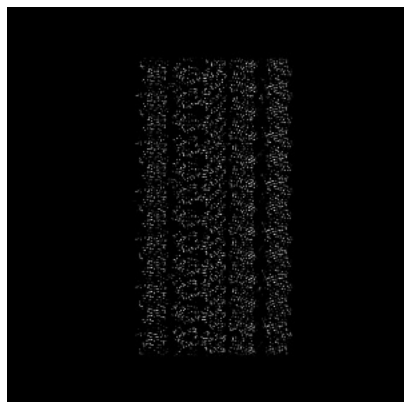
Z

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

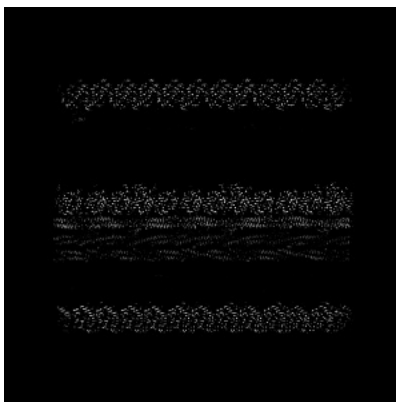


## 5.2 Central slices [i](#)

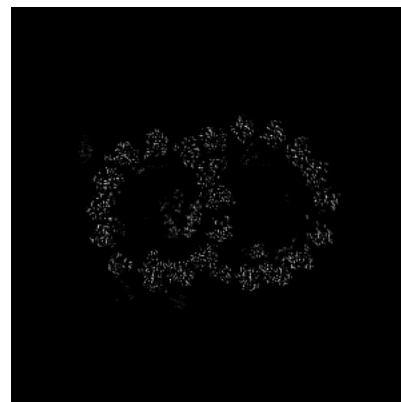
### 5.2.1 Primary map



X Index: 256

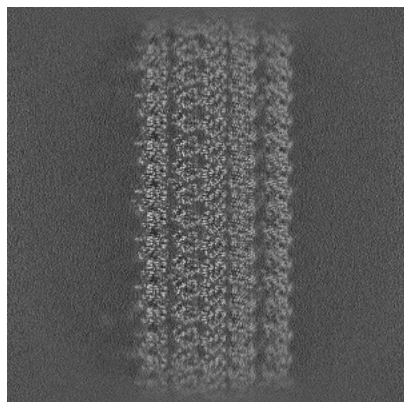


Y Index: 256

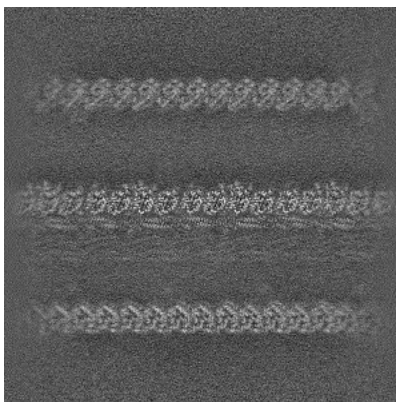


Z Index: 256

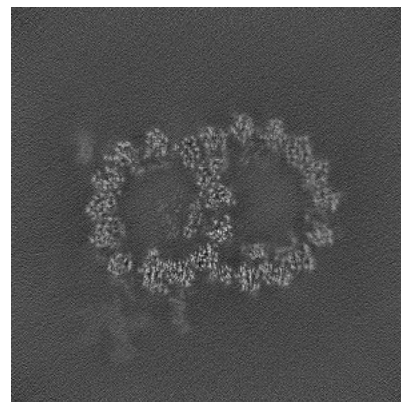
### 5.2.2 Raw map



X Index: 256



Y Index: 256

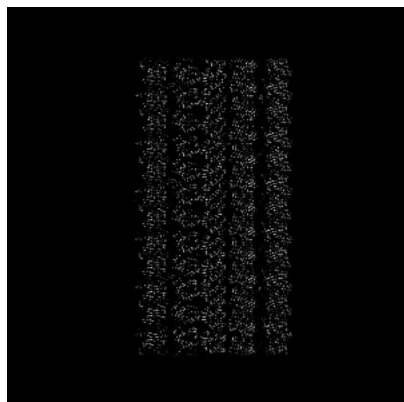


Z Index: 256

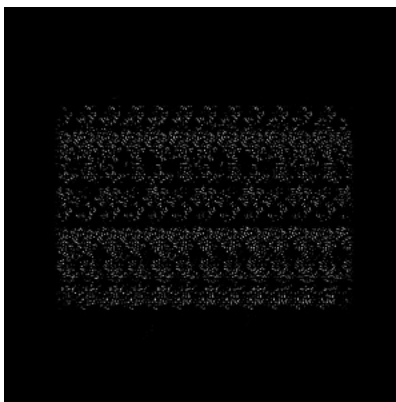
The images above show central slices of the map in three orthogonal directions.

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

### 5.3.1 Primary map



X Index: 256

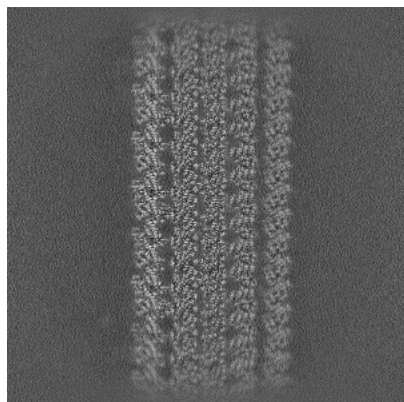


Y Index: 176

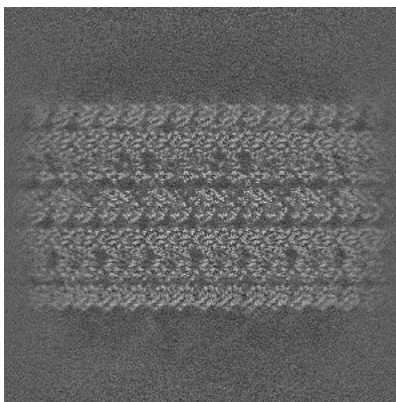


Z Index: 199

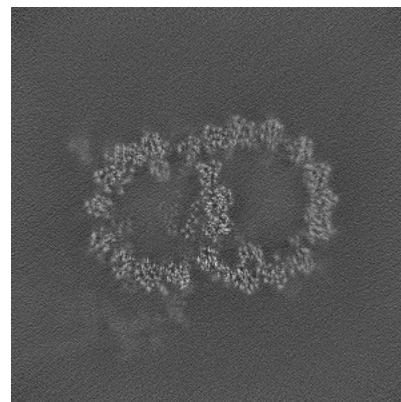
### 5.3.2 Raw map



X Index: 261



Y Index: 177

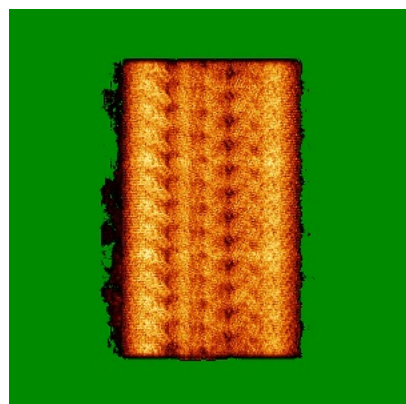


Z Index: 266

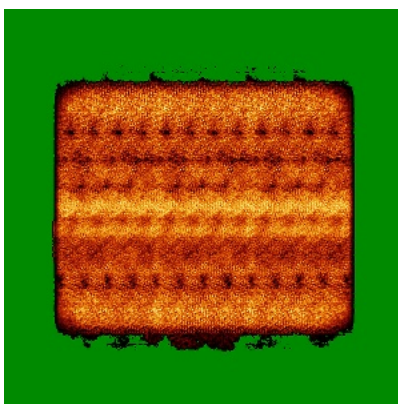
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 5.4.1 Primary map



X

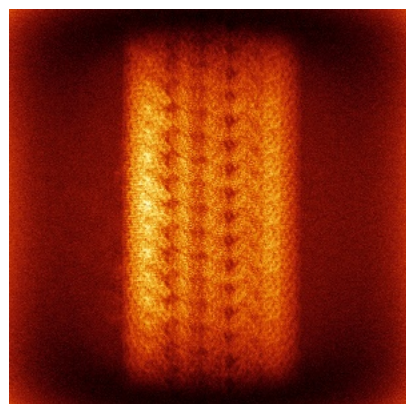


Y

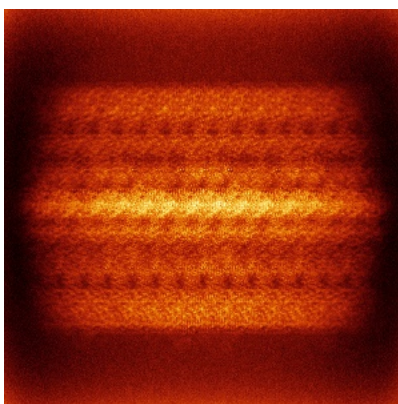


Z

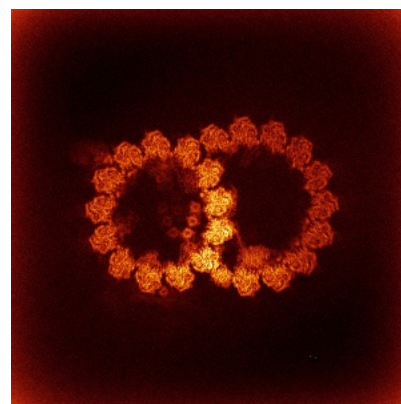
### 5.4.2 Raw map



X



Y



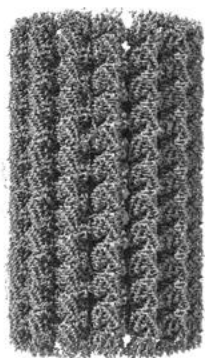
Z

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

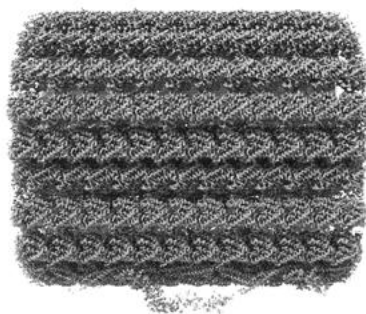


## 5.5 Orthogonal surface views [i](#)

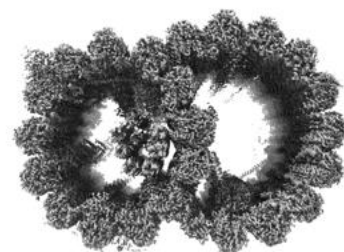
### 5.5.1 Primary map



X



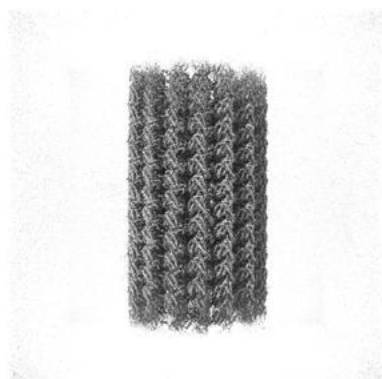
Y



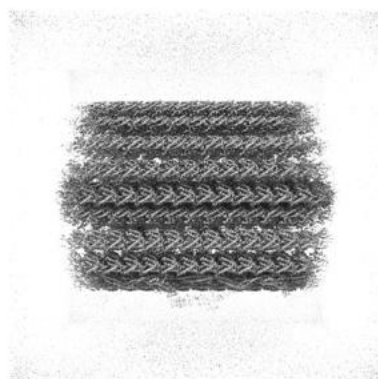
Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

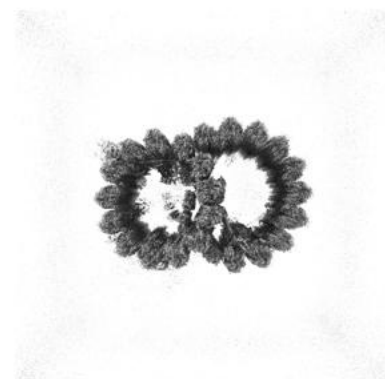
### 5.5.2 Raw map



X



Y



Z

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

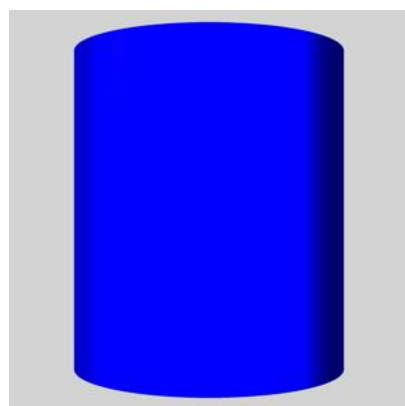
## 5.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

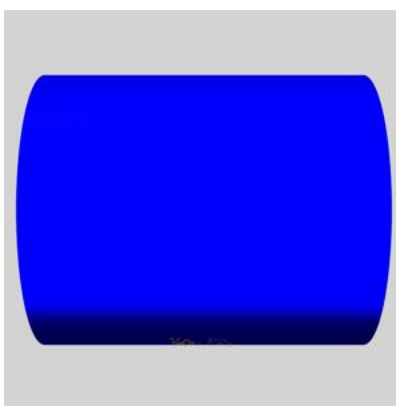
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

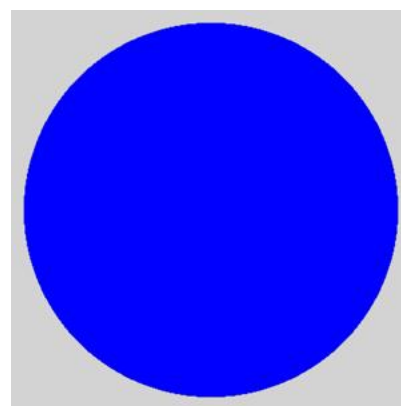
### 5.6.1 emd\_45801\_msk\_1.map [i](#)



X



Y

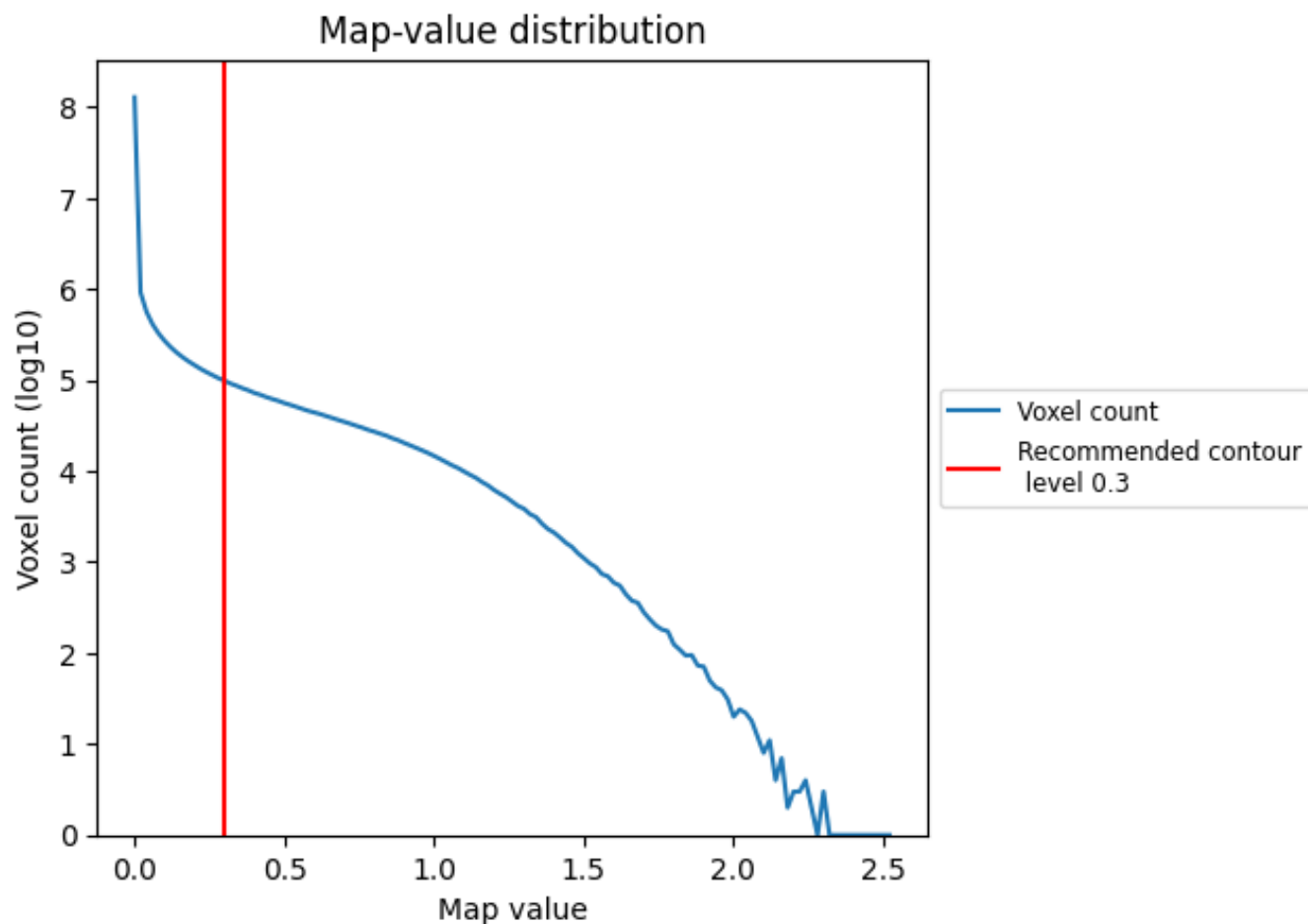


Z

## 6 Map analysis [i](#)

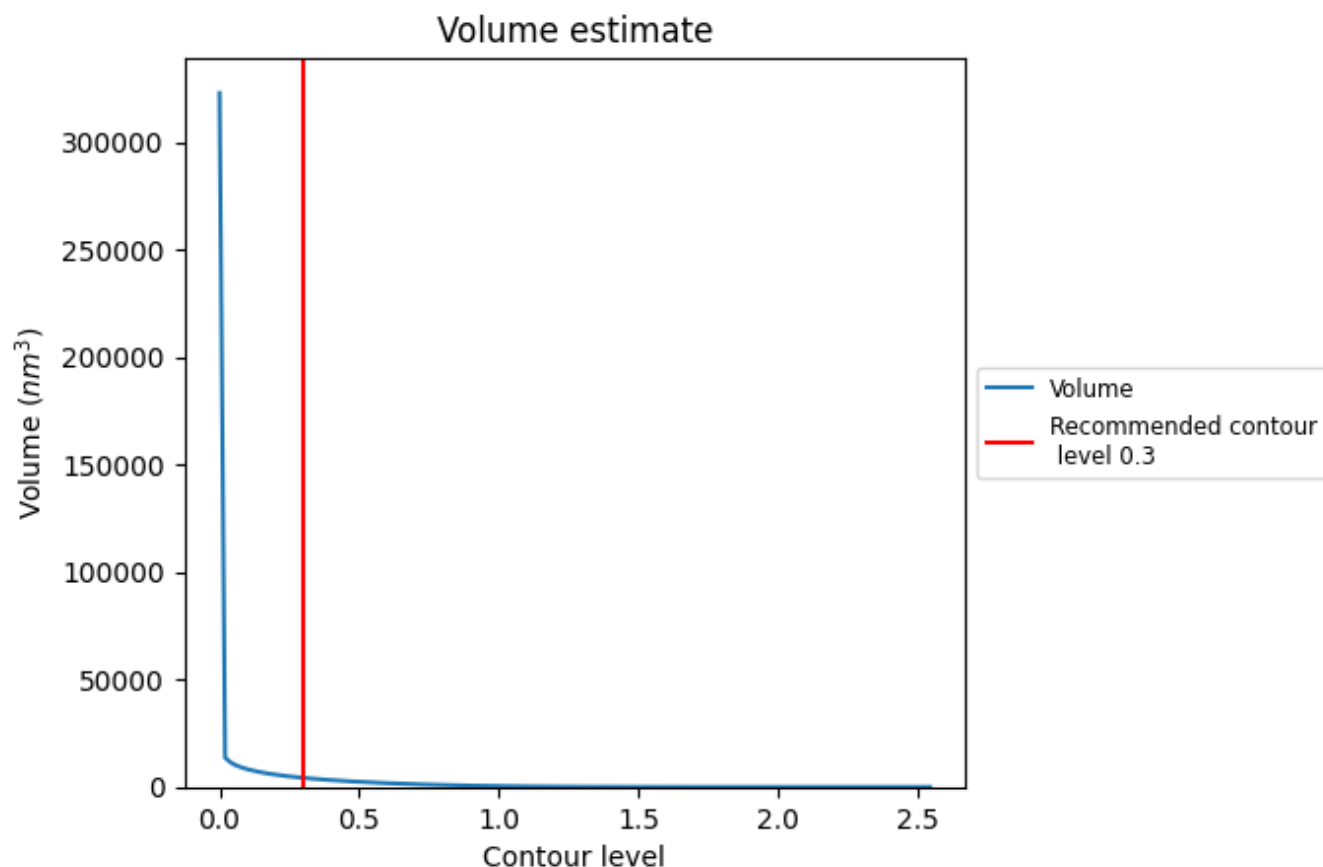
This section contains the results of statistical analysis of the map.

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



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

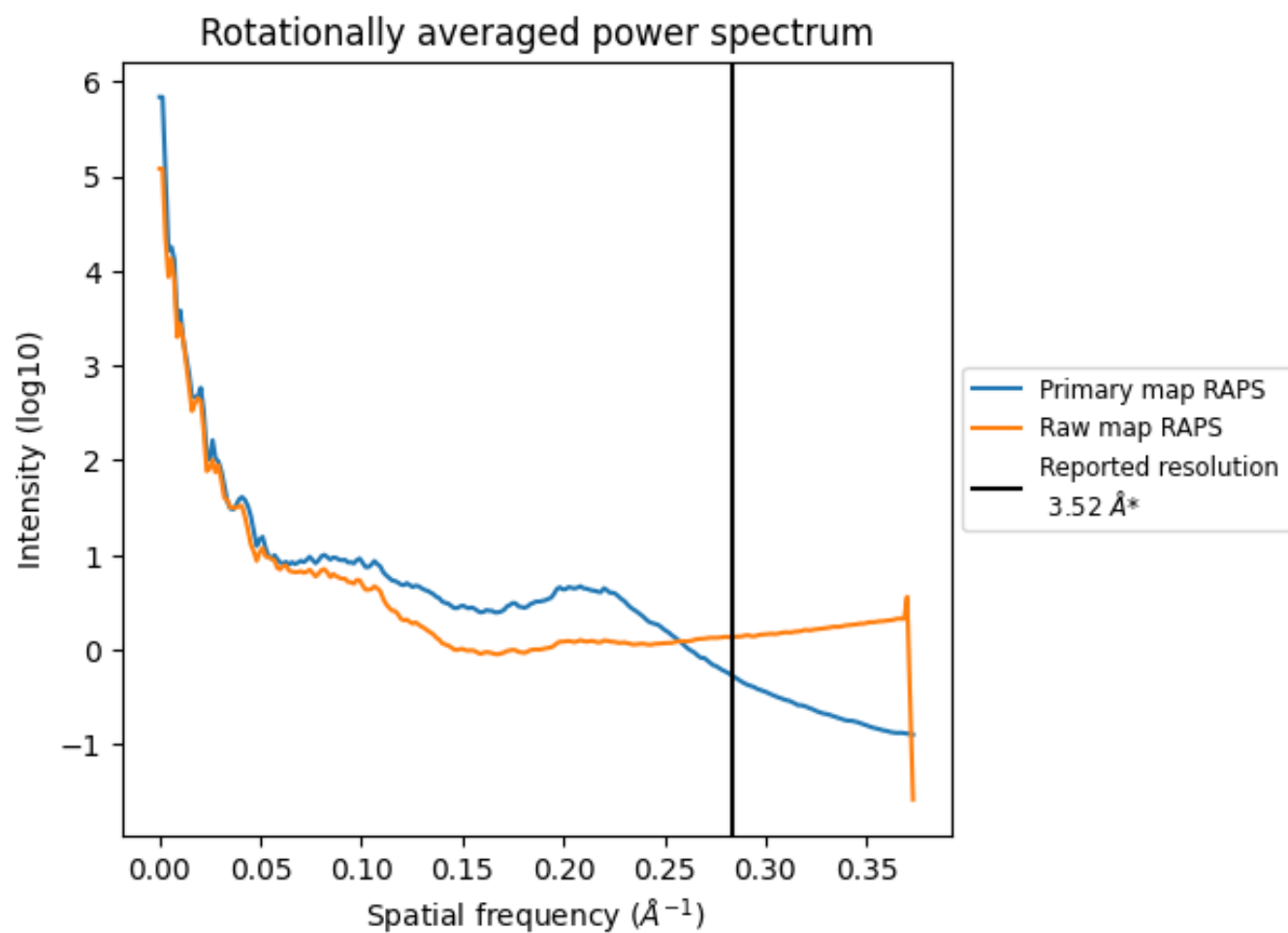
## 6.2 Volume estimate [i](#)



The volume at the recommended contour level is  $4225 \text{ nm}^3$ ; this corresponds to an approximate mass of 3816 kDa.

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

### 6.3 Rotationally averaged power spectrum ⓘ



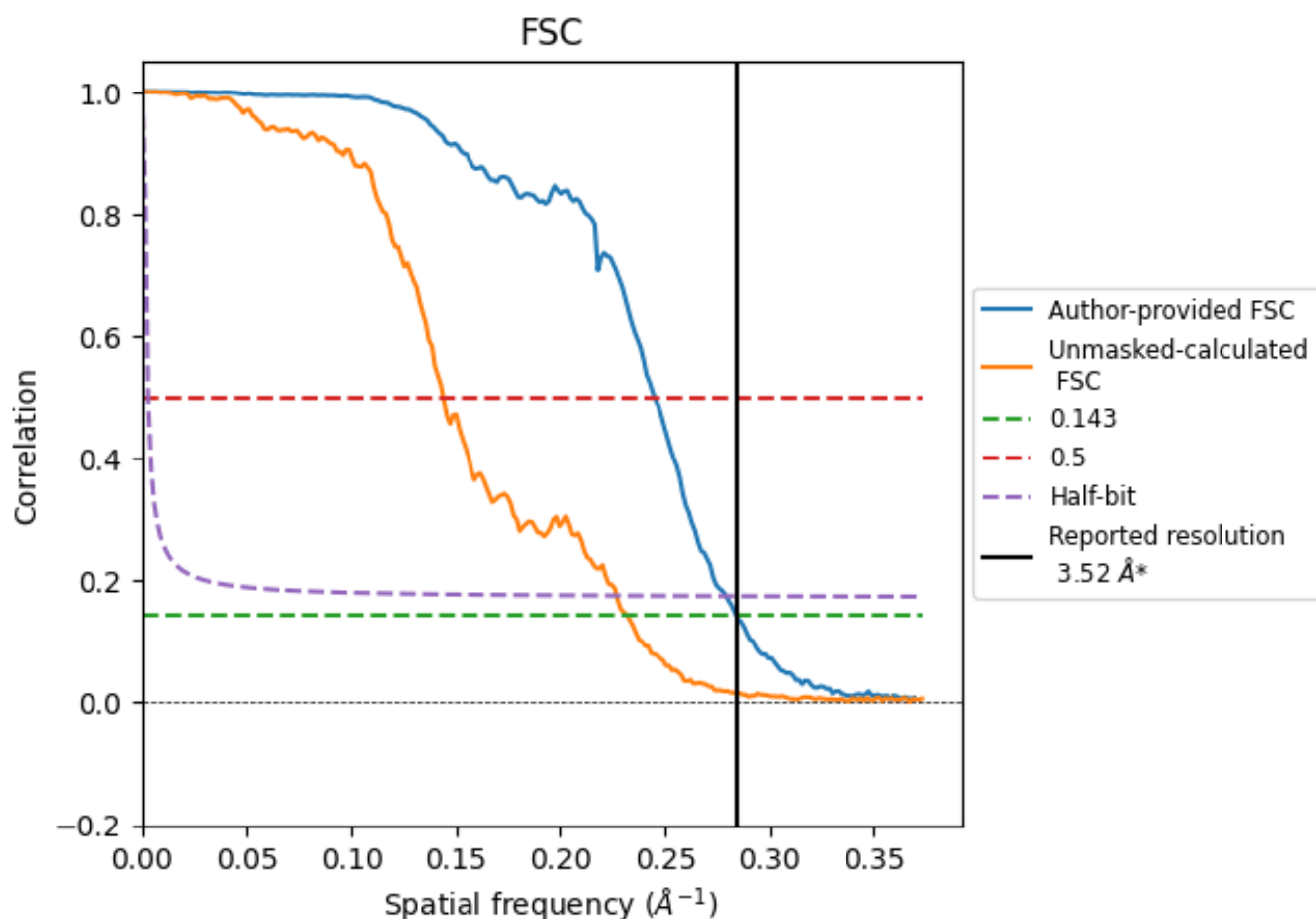
\*Reported resolution corresponds to spatial frequency of 0.284 Å<sup>-1</sup>



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

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

### 7.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.284  $\text{\AA}^{-1}$

## 7.2 Resolution estimates [i](#)

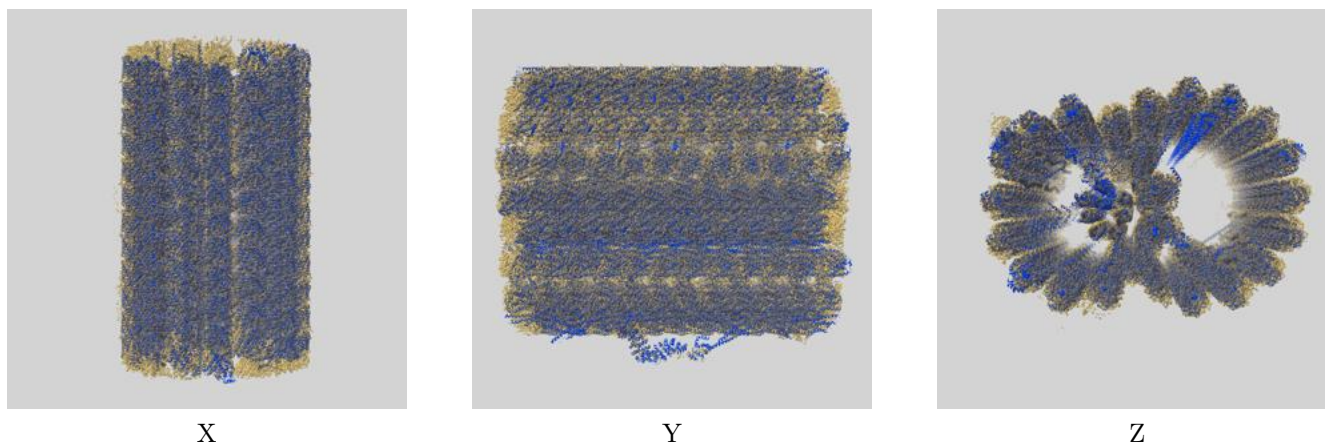
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	3.52	4.08	3.58
Unmasked-calculated*	4.31	6.95	4.41

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.52 by more than 10 %

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

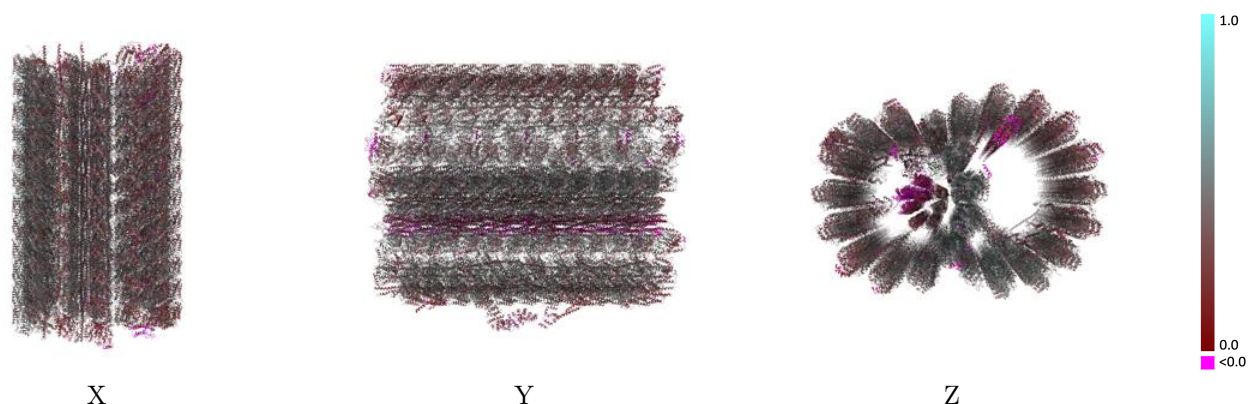
This section contains information regarding the fit between EMDB map EMD-45801 and PDB model 9CPB. Per-residue inclusion information can be found in section ?? on page ??.

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



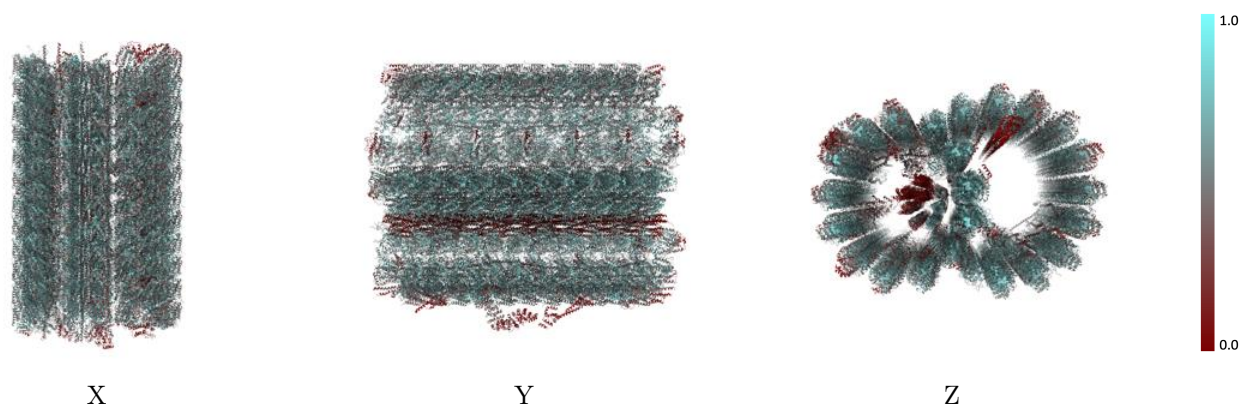
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



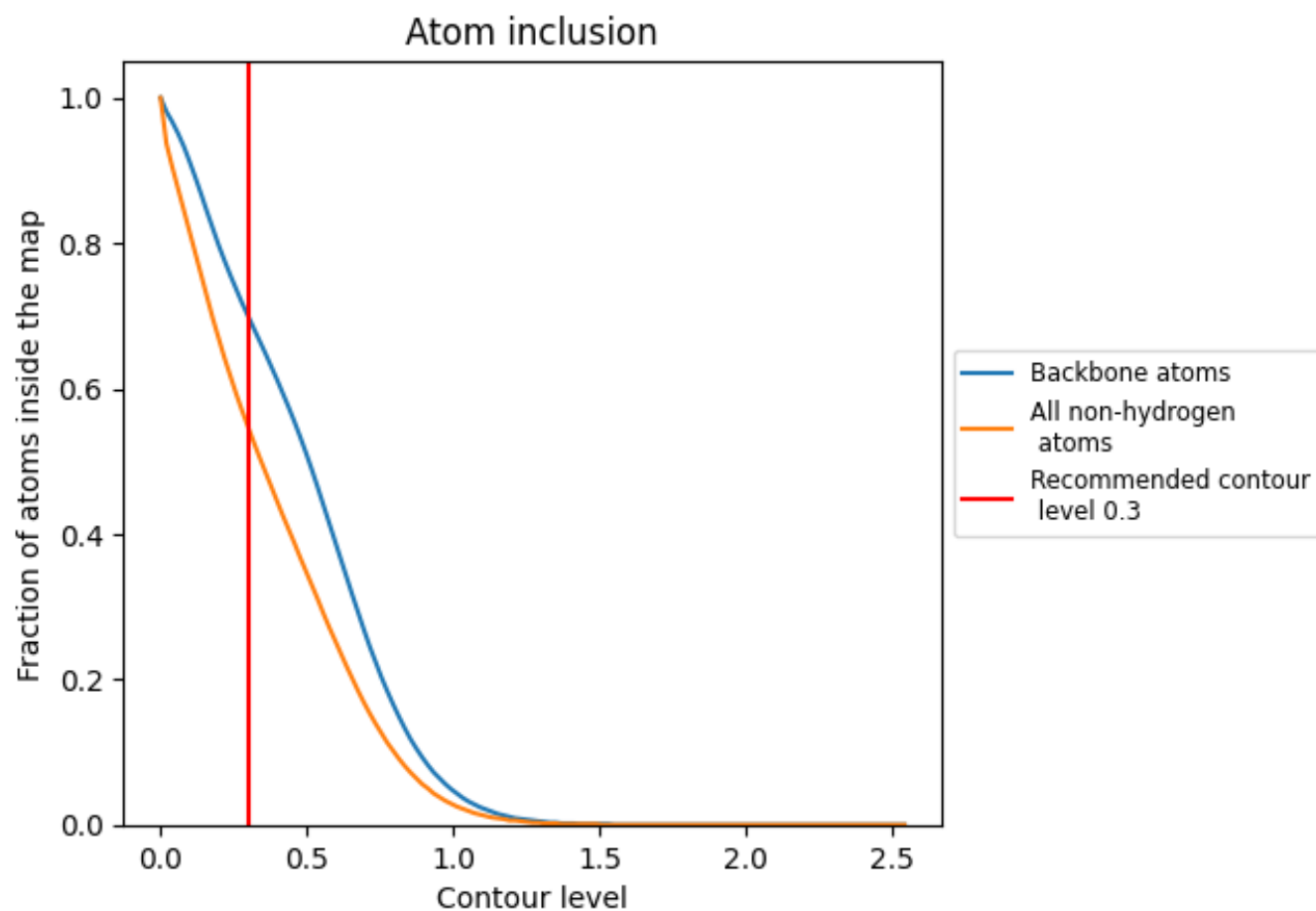
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).







































































## 8.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

## 8.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5460	 0.3920
1A	 0.2040	 0.2830
1D	 0.2740	 0.2720
1E	 0.3550	 0.3350
1F	 0.2100	 0.2710
1H	 0.5480	 0.3650
1I	 0.4580	 0.3370
1K	 0.3820	 0.2800
1L	 0.3540	 0.2590
1N	 0.6230	 0.4340
1O	 0.6220	 0.4400
1P	 0.6200	 0.4770
1R	 0.4690	 0.3600
1T	 0.5810	 0.4230
1U	 0.5540	 0.4450
1W	 0.5540	 0.4510
1X	 0.6030	 0.4470
1Y	 0.6210	 0.4540
1Z	 0.6040	 0.4540
2A	 0.5920	 0.4340
2B	 0.6040	 0.4330
2D	 0.2690	 0.2750
2E	 0.0250	 0.0980
2F	 0.5530	 0.4210
2G	 0.4940	 0.3720
2H	 0.4890	 0.3390
2J	 0.3500	 0.3190
2K	 0.3870	 0.3070
2L	 0.3080	 0.2520
2M	 0.3770	 0.2950
2O	 0.5800	 0.4570
2P	 0.5590	 0.4490
2Q	 0.5720	 0.4490
2S	 0.4100	 0.3040
2T	 0.4100	 0.2870























































































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Chain	Atom inclusion	Q-score
2V	 0.1390	 -0.0150
2W	 0.3370	 0.2550
2X	 0.3520	 0.2760
2Y	 0.3690	 0.2800
3A	 0.4000	 0.3830
3C	 0.4600	 0.3360
3D	 0.5340	 0.4000
3F	 0.0420	 0.2660
3H	 0.3180	 0.3930
3J	 0.5180	 0.4190
3K	 0.4680	 0.4010
3L	 0.4650	 0.3680
3N	 0.3920	 0.3480
3O	 0.4250	 0.3650
3P	 0.3700	 0.3330
3Q	 0.2450	 0.2160
3S	 0.5410	 0.4300
3T	 0.4850	 0.3910
3U	 0.4690	 0.3780
3V	 0.4470	 0.3350
3X	 0.0820	 0.2370
3Y	 0.4360	 0.4040
3Z	 0.3760	 0.3380
4A	 0.1380	 0.2790
4B	 0.3080	 0.2200
4C	 0.0020	 0.1020
4D	 0.4980	 0.3650
4F	 0.4550	 0.3510
4G	 0.3710	 0.3260
4I	 0.3360	 0.2280
4J	 0.4140	 0.3060
4K	 0.3390	 0.3180
4L	 0.3770	 0.3370
4M	 0.2750	 0.2790
4O	 0.5780	 0.4440
4P	 0.5660	 0.4490
4Q	 0.5820	 0.4590
4R	 0.5250	 0.4620
4S	 0.5690	 0.4270
4T	 0.3050	 0.3740
4V	 0.2690	 0.2540
4W	 0.5160	 0.3540

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Chain	Atom inclusion	Q-score
4Y	 0.3370	 0.3590
5A	 0.4910	 0.3610
5B	 0.5000	 0.3280
5D	 0.0520	 -0.0100
5E	 0.2100	 0.2210
5F	 0.0620	 0.1350
5G	 0.1220	 0.1700
5H	 0.0360	 0.1140
5I	 0.0320	 -0.0550
5J	 0.0310	 0.0560
5L	 0.6150	 0.3740
5M	 0.5970	 0.3530
5N	 0.6160	 0.3620
5O	 0.6040	 0.3500
5Q	 0.5450	 0.3690
5R	 0.6430	 0.3940
5S	 0.6420	 0.3740
5T	 0.6410	 0.3650
5V	 0.1370	 0.0700
5W	 0.1440	 0.0860
5X	 0.1630	 0.0950
5Y	 0.1310	 0.0650
6A	 0.2820	 0.2230
6B	 0.3180	 0.2350
6C	 0.3330	 0.2370
6D	 0.3040	 0.2120
6E	 0.0130	 0.0920
6F	 0.0340	 0.0620
6G	 0.0650	 0.0790
6H	 0.0390	 0.0820
6I	 0.0200	 0.1010
6J	 0.0090	 0.0610
6K	 0.0290	 0.0970
6L	 0.0500	 0.1060
6M	 0.0410	 0.1000
6N	 0.0390	 0.1450
6P	 0.4010	 0.2870
6Q	 0.5080	 0.2980
6R	 0.5000	 0.3070
6S	 0.4950	 0.2900
6T	 0.0350	 -0.0600
6U	 0.0700	 -0.0260

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Chain	Atom inclusion	Q-score
6V	 0.0620	 -0.0320
6W	 0.0520	 -0.0170
6Y	 0.4020	 0.3500
6Z	 0.4620	 0.3810
7C	 0.3440	 0.2210
7D	 0.4260	 0.2720
7E	 0.2640	 0.2970
7F	 0.3700	 0.3690
7H	 0.2210	 0.2830
7I	 0.2790	 0.3550
7K	 0.4600	 0.3700
7L	 0.3100	 0.3060
7N	 0.0510	 0.2710
AB	 0.5700	 0.4050
AC	 0.6350	 0.4920
AD	 0.6190	 0.4800
AE	 0.6340	 0.4870
AF	 0.6370	 0.4890
AG	 0.6320	 0.4980
AH	 0.6310	 0.5090
AI	 0.6310	 0.5080
AJ	 0.6310	 0.4870
AK	 0.6400	 0.5070
AL	 0.6180	 0.4780
BB	 0.5860	 0.4230
BC	 0.5780	 0.4410
BD	 0.6070	 0.4760
BE	 0.6200	 0.4480
BF	 0.6000	 0.4520
BG	 0.6220	 0.4610
BH	 0.6070	 0.4630
BI	 0.6350	 0.4850
BJ	 0.5630	 0.3930
BK	 0.6130	 0.4550
BL	 0.6010	 0.4380
CB	 0.5450	 0.3650
CC	 0.5940	 0.4470
CD	 0.5890	 0.4580
CE	 0.5820	 0.4060
CF	 0.6000	 0.4560
CG	 0.5930	 0.4600
CH	 0.5890	 0.4460





















































































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Chain	Atom inclusion	Q-score
CI	 0.6020	 0.4170
CJ	 0.5980	 0.4590
CK	 0.5940	 0.4520
CL	 0.5860	 0.4340
CM	 0.5100	 0.3960
DB	 0.4320	 0.3090
DC	 0.5410	 0.3610
DD	 0.5570	 0.3830
DE	 0.5670	 0.3890
DF	 0.5790	 0.3890
DG	 0.5780	 0.4020
DH	 0.5800	 0.4140
DI	 0.5720	 0.3900
DJ	 0.6020	 0.4180
DK	 0.5900	 0.4240
DL	 0.5820	 0.3930
DM	 0.5110	 0.3440
EC	 0.5670	 0.3550
ED	 0.6280	 0.4390
EE	 0.6350	 0.4520
EF	 0.6260	 0.4120
EG	 0.6360	 0.4370
EH	 0.5960	 0.3960
EI	 0.6240	 0.4170
EJ	 0.6070	 0.3850
EK	 0.6110	 0.4260
EL	 0.6030	 0.3990
EM	 0.5730	 0.4010
FC	 0.5500	 0.4020
FD	 0.6120	 0.4360
FE	 0.5840	 0.3870
FF	 0.5990	 0.3850
FG	 0.5760	 0.3780
FH	 0.5530	 0.3520
FI	 0.5670	 0.3660
FJ	 0.5830	 0.3680
FK	 0.5990	 0.4230
FL	 0.5940	 0.4330
FM	 0.5160	 0.3240
GC	 0.5030	 0.3490
GD	 0.5990	 0.4260
GE	 0.5940	 0.4020





















































































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Chain	Atom inclusion	Q-score
GF	 0.5980	 0.3900
GG	 0.5950	 0.4110
GH	 0.5920	 0.4030
GI	 0.5950	 0.4030
GJ	 0.6400	 0.4570
GK	 0.5790	 0.3990
GL	 0.5890	 0.3900
GM	 0.5880	 0.4340
HB	 0.5470	 0.4140
HC	 0.5640	 0.4120
HD	 0.6130	 0.4560
HE	 0.6020	 0.4030
HF	 0.5920	 0.4070
HG	 0.6210	 0.4610
HH	 0.6030	 0.4040
HI	 0.6230	 0.4700
HJ	 0.6300	 0.4650
HK	 0.5910	 0.4040
HL	 0.6130	 0.4590
HM	 0.6100	 0.4650
IC	 0.4960	 0.3630
ID	 0.5900	 0.4230
IE	 0.5980	 0.4560
IF	 0.5910	 0.4320
IG	 0.6060	 0.4190
IH	 0.6060	 0.4290
II	 0.6070	 0.4400
IJ	 0.5980	 0.4180
IK	 0.5890	 0.3910
IL	 0.5900	 0.4210
IM	 0.5900	 0.4270
IN	 0.5940	 0.4370
JC	 0.5970	 0.3990
JD	 0.6240	 0.4250
JE	 0.6160	 0.4260
JF	 0.6330	 0.4350
JG	 0.6290	 0.4430
JH	 0.5840	 0.3880
JI	 0.6010	 0.4120
JJ	 0.6350	 0.4320
JK	 0.6120	 0.4630
JL	 0.6090	 0.4530





















































































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Chain	Atom inclusion	Q-score
JM	 0.6200	 0.4530
KC	 0.6470	 0.4860
KD	 0.6560	 0.4770
KE	 0.6630	 0.5030
KF	 0.6560	 0.4950
KG	 0.6820	 0.5090
KH	 0.6590	 0.5010
KI	 0.6710	 0.5110
KJ	 0.6600	 0.5020
KK	 0.6740	 0.4970
KL	 0.6710	 0.5120
KM	 0.6560	 0.5100
KN	 0.6520	 0.4720
LC	 0.6600	 0.4890
LD	 0.6610	 0.5140
LE	 0.6550	 0.5040
LF	 0.6650	 0.5060
LG	 0.6770	 0.5200
LH	 0.6640	 0.5070
LI	 0.6520	 0.4980
LJ	 0.6770	 0.5080
LK	 0.6680	 0.5110
LL	 0.6570	 0.5070
LM	 0.6570	 0.4930
LN	 0.6240	 0.4670
MC	 0.6420	 0.4420
MD	 0.6520	 0.4940
ME	 0.6580	 0.4610
MF	 0.6540	 0.4700
MG	 0.6500	 0.4750
MH	 0.6400	 0.4680
MI	 0.6500	 0.4610
MJ	 0.6530	 0.4490
MK	 0.5810	 0.3820
ML	 0.6180	 0.4290
MM	 0.6300	 0.4280
MN	 0.4990	 0.3940
NA	 0.5850	 0.4170
NB	 0.5880	 0.4270
NC	 0.6010	 0.4600
ND	 0.6070	 0.4340
NE	 0.5810	 0.4280





















































































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Chain	Atom inclusion	Q-score
NF	 0.5930	 0.4390
NG	 0.5920	 0.4340
NH	 0.6030	 0.4250
NI	 0.5850	 0.4310
NJ	 0.5780	 0.4160
NK	 0.5920	 0.4240
NL	 0.5160	 0.3490
OA	 0.5470	 0.3810
OB	 0.5900	 0.4270
OC	 0.5890	 0.4240
OD	 0.5710	 0.3930
OE	 0.5850	 0.4070
OF	 0.5720	 0.4060
OG	 0.5790	 0.4250
OH	 0.5880	 0.4070
OI	 0.5980	 0.4170
OJ	 0.5710	 0.4120
OK	 0.5730	 0.4060
OL	 0.5520	 0.3660
PA	 0.4730	 0.3190
PB	 0.5660	 0.3680
PC	 0.5570	 0.3660
PD	 0.5720	 0.3760
PE	 0.5980	 0.3810
PF	 0.5710	 0.3790
PG	 0.6050	 0.4290
PH	 0.5920	 0.4070
PI	 0.6180	 0.4180
PJ	 0.5900	 0.4140
PK	 0.5620	 0.3790
PL	 0.5300	 0.3260
QB	 0.4960	 0.3060
QC	 0.5190	 0.3250
QD	 0.5360	 0.3380
QE	 0.5570	 0.3270
QF	 0.5300	 0.3290
QG	 0.5240	 0.3330
QH	 0.5330	 0.3380
QI	 0.5760	 0.3530
QJ	 0.5500	 0.3540
QK	 0.5290	 0.3560
QL	 0.4900	 0.3010



















































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Chain	Atom inclusion	Q-score
RB	 0.4370	 0.2990
RC	 0.5110	 0.3280
RD	 0.5640	 0.3630
RE	 0.5770	 0.3420
RF	 0.5690	 0.3590
RG	 0.5390	 0.3510
RH	 0.5480	 0.3450
RI	 0.5740	 0.3480
RJ	 0.5730	 0.3710
RK	 0.5380	 0.3490
RL	 0.4980	 0.3130
SC	 0.5320	 0.3420
SD	 0.5630	 0.3710
SE	 0.5790	 0.3810
SF	 0.5670	 0.3680
SG	 0.5580	 0.3760
SH	 0.5470	 0.3600
SI	 0.6040	 0.3840
SJ	 0.5610	 0.3610
SK	 0.5590	 0.3610
SL	 0.5360	 0.3540
SM	 0.3420	 0.2680
TC	 0.5040	 0.3190
TD	 0.5780	 0.3830
TE	 0.5620	 0.3820
TF	 0.5940	 0.3710
TG	 0.5440	 0.3610
TH	 0.5600	 0.3740
TI	 0.5710	 0.3790
TJ	 0.5910	 0.3880
TK	 0.5900	 0.4080
TL	 0.5680	 0.3900
TM	 0.4470	 0.2940
UC	 0.5560	 0.3890
UD	 0.5870	 0.4120
UE	 0.5780	 0.3990
UF	 0.6050	 0.4050
UG	 0.6000	 0.4160
UH	 0.5900	 0.4140
UI	 0.5850	 0.3980
UJ	 0.6150	 0.4180
UK	 0.5930	 0.4170

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Chain	Atom inclusion	Q-score
UL	 0.5880	 0.4190
UM	 0.5600	 0.3950
VC	 0.5880	 0.4470
VD	 0.5930	 0.4580
VE	 0.6060	 0.4660
VF	 0.6180	 0.4600
VG	 0.5950	 0.4540
VH	 0.6110	 0.4630
VI	 0.6100	 0.4620
VJ	 0.6150	 0.4410
VK	 0.5840	 0.4470
VL	 0.5990	 0.4640
VM	 0.5910	 0.4510
WC	 0.6050	 0.4720
WD	 0.6300	 0.4840
WE	 0.6230	 0.4850
WF	 0.6320	 0.4720
WG	 0.6190	 0.4750
WH	 0.6310	 0.4790
WI	 0.6330	 0.4820
WJ	 0.6290	 0.4780
WK	 0.6170	 0.4750
WL	 0.6350	 0.4870
WM	 0.6230	 0.4750
WN	 0.5790	 0.4420