



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2026 – 03:51 AM UTC

PDB ID : 9CPC / pdb_00009cpc
EMDB ID : EMD-45802
Title : Atomic model of porcine brain ventricles cilia doublet microtubule (48-nm periodicity)
Authors : Sun, C.; Zeng, J.; Zhang, R.
Deposited on : 2024-07-18
Resolution : 3.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

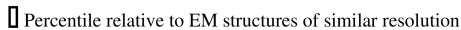
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 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

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ELECTRON MICROSCOPY

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.



11564 (3.15 - 4.15)

WORLDWIDE
PDB
PROTEIN DATA BANK

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 1114625 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 protein 4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	587	Total	C	N	O	S	0	0
			4498	2806	817	843	32		
1	1B	149	Total	C	N	O	S	0	0
			1135	698	212	217	8		

- Molecule 2 is a protein called Outer dynein arm-docking complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1C	211	Total	C	N	O	S	0	0
			1699	1076	297	317	9		
2	1D	211	Total	C	N	O	S	0	0
			1699	1076	297	317	9		

- Molecule 3 is a protein called EF-hand calcium binding domain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1F	171	Total	C	N	O	S	0	0
			1375	887	219	255	14		
3	1G	171	Total	C	N	O	S	0	0
			1375	887	219	255	14		

- Molecule 4 is a protein called Coiled-coil domain-containing protein 114 isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1H	195	Total	C	N	O	S	0	0
			1633	1001	326	299	7		
4	1I	88	Total	C	N	O	S	0	0
			727	439	150	134	4		
4	1J	115	Total	C	N	O	S	0	0
			973	601	189	180	3		

- Molecule 5 is a protein called Outer dynein arm docking complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1L	155	Total 1306	C 801	N 247	O 253	S 5	0	0
5	1M	248	Total 2086	C 1287	N 392	O 402	S 5	0	0
5	1N	103	Total 865	C 539	N 164	O 162		0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1L	478	ALA	-	insertion	UNP A0A5G2RIE6
1L	479	ASP	-	insertion	UNP A0A5G2RIE6
1L	480	SER	-	insertion	UNP A0A5G2RIE6
1L	481	ALA	-	insertion	UNP A0A5G2RIE6
1L	482	PRO	-	insertion	UNP A0A5G2RIE6
1L	483	GLU	-	insertion	UNP A0A5G2RIE6
1L	484	GLU	-	insertion	UNP A0A5G2RIE6
1L	485	ALA	-	insertion	UNP A0A5G2RIE6
1L	486	PRO	-	insertion	UNP A0A5G2RIE6
1L	487	PRO	-	insertion	UNP A0A5G2RIE6
1L	488	ARG	-	insertion	UNP A0A5G2RIE6
1L	489	ALA	-	insertion	UNP A0A5G2RIE6
1L	490	PRO	-	insertion	UNP A0A5G2RIE6
1L	491	GLN	-	insertion	UNP A0A5G2RIE6
1L	492	ASP	-	insertion	UNP A0A5G2RIE6
1L	493	VAL	-	insertion	UNP A0A5G2RIE6
1L	494	ARG	-	insertion	UNP A0A5G2RIE6
1L	495	GLY	-	insertion	UNP A0A5G2RIE6
1L	496	SER	-	insertion	UNP A0A5G2RIE6
1L	497	SER	-	insertion	UNP A0A5G2RIE6
1L	498	THR	-	insertion	UNP A0A5G2RIE6
1L	499	ILE	-	insertion	UNP A0A5G2RIE6
1L	500	THR	-	insertion	UNP A0A5G2RIE6
1L	501	GLN	-	insertion	UNP A0A5G2RIE6
1M	478	ALA	-	insertion	UNP A0A5G2RIE6
1M	479	ASP	-	insertion	UNP A0A5G2RIE6
1M	480	SER	-	insertion	UNP A0A5G2RIE6
1M	481	ALA	-	insertion	UNP A0A5G2RIE6
1M	482	PRO	-	insertion	UNP A0A5G2RIE6
1M	483	GLU	-	insertion	UNP A0A5G2RIE6
1M	484	GLU	-	insertion	UNP A0A5G2RIE6
1M	485	ALA	-	insertion	UNP A0A5G2RIE6
1M	486	PRO	-	insertion	UNP A0A5G2RIE6

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Chain	Residue	Modelled	Actual	Comment	Reference
1M	487	PRO	-	insertion	UNP A0A5G2RIE6
1M	488	ARG	-	insertion	UNP A0A5G2RIE6
1M	489	ALA	-	insertion	UNP A0A5G2RIE6
1M	490	PRO	-	insertion	UNP A0A5G2RIE6
1M	491	GLN	-	insertion	UNP A0A5G2RIE6
1M	492	ASP	-	insertion	UNP A0A5G2RIE6
1M	493	VAL	-	insertion	UNP A0A5G2RIE6
1M	494	ARG	-	insertion	UNP A0A5G2RIE6
1M	495	GLY	-	insertion	UNP A0A5G2RIE6
1M	496	SER	-	insertion	UNP A0A5G2RIE6
1M	497	SER	-	insertion	UNP A0A5G2RIE6
1M	498	THR	-	insertion	UNP A0A5G2RIE6
1M	499	ILE	-	insertion	UNP A0A5G2RIE6
1M	500	THR	-	insertion	UNP A0A5G2RIE6
1M	501	GLN	-	insertion	UNP A0A5G2RIE6
1N	478	ALA	-	insertion	UNP A0A5G2RIE6
1N	479	ASP	-	insertion	UNP A0A5G2RIE6
1N	480	SER	-	insertion	UNP A0A5G2RIE6
1N	481	ALA	-	insertion	UNP A0A5G2RIE6
1N	482	PRO	-	insertion	UNP A0A5G2RIE6
1N	483	GLU	-	insertion	UNP A0A5G2RIE6
1N	484	GLU	-	insertion	UNP A0A5G2RIE6
1N	485	ALA	-	insertion	UNP A0A5G2RIE6
1N	486	PRO	-	insertion	UNP A0A5G2RIE6
1N	487	PRO	-	insertion	UNP A0A5G2RIE6
1N	488	ARG	-	insertion	UNP A0A5G2RIE6
1N	489	ALA	-	insertion	UNP A0A5G2RIE6
1N	490	PRO	-	insertion	UNP A0A5G2RIE6
1N	491	GLN	-	insertion	UNP A0A5G2RIE6
1N	492	ASP	-	insertion	UNP A0A5G2RIE6
1N	493	VAL	-	insertion	UNP A0A5G2RIE6
1N	494	ARG	-	insertion	UNP A0A5G2RIE6
1N	495	GLY	-	insertion	UNP A0A5G2RIE6
1N	496	SER	-	insertion	UNP A0A5G2RIE6
1N	497	SER	-	insertion	UNP A0A5G2RIE6
1N	498	THR	-	insertion	UNP A0A5G2RIE6
1N	499	ILE	-	insertion	UNP A0A5G2RIE6
1N	500	THR	-	insertion	UNP A0A5G2RIE6
1N	501	GLN	-	insertion	UNP A0A5G2RIE6

- Molecule 6 is a protein called EFCAB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1P	84	Total	C	N	O	S	0	0
			704	456	126	119	3		
6	1Q	81	Total	C	N	O	S	0	0
			675	436	122	114	3		

- Molecule 7 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1S	611	Total	C	N	O	S	0	0
			4712	2983	817	883	29		
7	1T	611	Total	C	N	O	S	0	0
			4712	2983	817	883	29		
7	1U	611	Total	C	N	O	S	0	0
			4712	2983	817	883	29		

- Molecule 8 is a protein called Cilia- and flagella-associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1W	316	Total	C	N	O	S	0	0
			2722	1643	539	528	12		
8	1X	275	Total	C	N	O	S	0	0
			2293	1398	427	452	16		
8	1Y	162	Total	C	N	O	S	0	0
			1331	819	242	260	10		
8	1Z	196	Total	C	N	O	S	0	0
			1680	1016	338	323	3		

- Molecule 9 is a protein called Cilia and flagella associated protein 210.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2B	373	Total	C	N	O	S	0	0
			3205	1994	606	596	9		
9	2C	80	Total	C	N	O	S	0	0
			665	413	122	127	3		

- Molecule 10 is a protein called Cilia and flagella associated protein 276.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	2E	115	Total	C	N	O	S	0	0
			930	577	173	177	3		
10	2F	115	Total	C	N	O	S	0	0
			930	577	173	177	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	2G	115	Total	C	N	O	S	0	0
			930	577	173	177	3		

- Molecule 11 is a protein called Enkurin.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2I	247	Total	C	N	O	S	0	0
			2024	1294	350	373	7		
11	2J	247	Total	C	N	O	S	0	0
			2027	1296	350	373	8		
11	2K	237	Total	C	N	O	S	0	0
			1947	1244	336	359	8		

- Molecule 12 is a protein called Parkin coregulated.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2M	219	Total	C	N	O	S	0	0
			1767	1144	297	316	10		
12	2N	219	Total	C	N	O	S	0	0
			1767	1144	297	316	10		
12	2O	219	Total	C	N	O	S	0	0
			1767	1144	297	316	10		
12	2P	219	Total	C	N	O	S	0	0
			1767	1144	297	316	10		
12	2Q	219	Total	C	N	O	S	0	0
			1767	1144	297	316	10		
12	2R	219	Total	C	N	O	S	0	0
			1767	1144	297	316	10		

- Molecule 13 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2T	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
13	2U	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
13	2V	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
13	2W	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		
13	2X	185	Total	C	N	O	S	0	0
			1540	990	269	274	7		

- Molecule 14 is a protein called Protein Flattop.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3A	118	Total	C	N	O	S	0	0
			924	586	170	166	2		
14	3B	118	Total	C	N	O	S	0	0
			924	586	170	166	2		
14	3C	118	Total	C	N	O	S	0	0
			924	586	170	166	2		

- Molecule 15 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3E	394	Total	C	N	O	S	0	0
			3216	1989	591	627	9		
15	3F	397	Total	C	N	O	S	0	0
			3241	2006	595	631	9		
15	3G	136	Total	C	N	O	S	0	0
			1096	675	207	211	3		
15	3H	298	Total	C	N	O	S	0	0
			2451	1517	447	481	6		

- Molecule 16 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3J	397	Total	C	N	O	S	0	0
			3234	1990	599	629	16		
16	3K	316	Total	C	N	O	S	0	0
			2559	1578	463	503	15		
16	3L	397	Total	C	N	O	S	0	0
			3234	1990	599	629	16		
16	3M	114	Total	C	N	O	S	0	0
			939	572	184	181	2		

- Molecule 17 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3O	391	Total	C	N	O	S	0	0
			3180	1957	581	627	15		
17	3P	391	Total	C	N	O	S	0	0
			3180	1957	581	627	15		
17	3Q	131	Total	C	N	O	S	0	0
			1058	654	192	207	5		
17	3R	264	Total	C	N	O	S	0	0
			2149	1319	393	428	9		

- Molecule 18 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3T	398	Total	C	N	O	S	0	0
			3284	2024	605	637	18		
18	3U	399	Total	C	N	O	S	0	0
			3289	2027	606	638	18		
18	3V	170	Total	C	N	O	S	0	0
			1405	863	255	280	7		
18	3W	259	Total	C	N	O	S	0	0
			2121	1310	398	402	11		

- Molecule 19 is a protein called RIB43A domain with coiled-coils 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3Y	356	Total	C	N	O	S	0	0
			2977	1815	580	571	11		
19	3Z	22	Total	C	N	O	S	0	0
			194	121	33	39	1		

- Molecule 20 is a protein called RIB43A-like with coiled-coils protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4A	181	Total	C	N	O	S	0	0
			1485	891	294	286	14		
20	4B	115	Total	C	N	O	S	0	0
			943	561	185	193	4		

- Molecule 21 is a protein called EF-hand domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4D	468	Total	C	N	O	S	0	0
			3844	2478	648	702	16		
21	4E	468	Total	C	N	O	S	0	0
			3844	2478	648	702	16		
21	4F	468	Total	C	N	O	S	0	0
			3844	2478	648	702	16		

- Molecule 22 is a protein called EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4H	354	Total	C	N	O	S	0	0
			2895	1866	483	532	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
22	4I	612	Total	C	N	O	S	0	0
			5027	3227	847	926	27		
22	4J	615	Total	C	N	O	S	0	0
			5055	3247	851	930	27		
22	4K	242	Total	C	N	O	S	0	0
			1983	1268	340	363	12		

- Molecule 23 is a protein called Ciliary microtubule inner protein 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4M	170	Total	C	N	O	S	0	0
			1330	859	229	235	7		
23	4N	170	Total	C	N	O	S	0	0
			1320	853	228	234	5		
23	4P	87	Total	C	N	O	S	0	0
			705	457	121	124	3		
23	4Q	136	Total	C	N	O	S	0	0
			1070	687	186	193	4		
23	4R	167	Total	C	N	O	S	0	0
			1319	851	229	232	7		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4M	271	ALA	-	insertion	UNP A0A8D1CRM3
4M	?	-	SER	deletion	UNP A0A8D1CRM3
4N	271	ALA	-	insertion	UNP A0A8D1CRM3
4N	?	-	SER	deletion	UNP A0A8D1CRM3
4P	271	ALA	-	insertion	UNP A0A8D1CRM3
4P	?	-	SER	deletion	UNP A0A8D1CRM3
4Q	271	ALA	-	insertion	UNP A0A8D1CRM3
4Q	?	-	SER	deletion	UNP A0A8D1CRM3
4R	271	ALA	-	insertion	UNP A0A8D1CRM3
4R	?	-	SER	deletion	UNP A0A8D1CRM3

- Molecule 24 is a protein called Ciliary microtubule inner protein 2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	4O	87	Total	C	N	O	S	0	0
			702	455	121	124	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4O	271	ALA	-	insertion	UNP A0A8D1QC18

- Molecule 25 is a protein called Sperm-associated antigen 8 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4T	162	Total	C	N	O	S	0	0
			1320	825	245	243	7		

- Molecule 26 is a protein called Nucleoside diphosphate kinase homolog 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4V	373	Total	C	N	O	S	0	0
			2946	1876	500	548	22		
26	4W	373	Total	C	N	O	S	0	0
			2946	1876	500	548	22		

- Molecule 27 is a protein called Cilia and flagella associated protein 161.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4Y	267	Total	C	N	O	S	0	0
			2145	1359	378	395	13		
27	4Z	270	Total	C	N	O	S	0	0
			2160	1369	380	398	13		

- Molecule 28 is a protein called Chromosome 1 C9orf135 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5B	200	Total	C	N	O	S	0	0
			1625	1030	278	311	6		

- Molecule 29 is a protein called Piercer of microtubule wall 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5D	84	Total	C	N	O	S	0	0
			697	442	125	127	3		
29	5E	33	Total	C	N	O	S	0	0
			280	180	47	52	1		

- Molecule 30 is a protein called Chromosome 1 C15orf65 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5G	93	Total	C	N	O	S	0	0
			708	445	123	136	4		

- Molecule 31 is a protein called EF-hand domain family member B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5I	443	Total	C	N	O	S	0	0
			3576	2284	630	653	9		
31	5J	112	Total	C	N	O	S	0	0
			898	563	161	172	2		

- Molecule 32 is a protein called Cilia and flagella associated protein 141.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5L	92	Total	C	N	O	S	0	0
			736	460	140	130	6		

- Molecule 33 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5N	334	Total	C	N	O	S	0	0
			2883	1791	520	556	16		
33	5O	151	Total	C	N	O	S	0	0
			1277	783	242	245	7		

- Molecule 34 is a protein called Cilia- and flagella-associated protein 53.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	5Q	262	Total	C	N	O	S	0	0
			2216	1361	412	433	10		
34	5R	198	Total	C	N	O	S	0	0
			1671	1019	319	326	7		

- Molecule 35 is a protein called CFAP107/C1orf158.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	5T	135	Total	C	N	O	S	0	0
			1118	732	196	188	2		
35	5U	28	Total	C	N	O		0	0
			223	141	41	41			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5T	40F	UNK	THR	conflict	UNP A0A8D1WB49
5U	46	UNK	THR	conflict	UNP A0A8D1WB49

- Molecule 36 is a protein called Cilia and flagella associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5W	231	Total	C	N	O	S	0	0
			1868	1186	349	325	8		
36	5X	231	Total	C	N	O	S	0	0
			1868	1186	349	325	8		
36	5Y	185	Total	C	N	O	S	0	0
			1487	942	277	262	6		
36	5Z	59	Total	C	N	O	S	0	0
			488	310	93	83	2		

- Molecule 37 is a protein called Cilia and flagella associated protein 144.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	6A	116	Total	C	N	O	S	0	0
			992	626	184	180	2		

- Molecule 38 is a protein called Cilia-and flagella-associated protein 96.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	6C	212	Total	C	N	O	S	0	0
			1698	1086	290	315	7		
38	6D	65	Total	C	N	O	S	0	0
			495	318	87	87	3		

- Molecule 39 is a protein called Sperm acrosome associated 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	6F	157	Total	C	N	O	S	0	0
			1264	789	229	236	10		
39	6G	157	Total	C	N	O	S	0	0
			1264	789	229	236	10		
39	6H	141	Total	C	N	O	S	0	0
			1134	710	202	213	9		
39	6I	157	Total	C	N	O	S	0	0
			1264	789	229	236	10		
39	6J	157	Total	C	N	O	S	0	0
			1264	789	229	236	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
39	6K	157	Total	C	N	O	S	0	0
			1264	789	229	236	10		
39	6L	137	Total	C	N	O	S	0	0
			1095	694	190	204	7		

- Molecule 40 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AA	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	AE	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	AF	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	AG	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	AH	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	BA	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	BE	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	BF	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	BG	432	Total	C	N	O	S	0	0
			3392	2148	576	646	22		
40	BH	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	BI	373	Total	C	N	O	S	0	0
			2932	1855	501	555	21		
40	CA	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	CE	440	Total	C	N	O	S	0	0
			3438	2174	584	658	22		
40	CF	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	CG	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	CH	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	CI	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
40	DA	432	Total	C	N	O	S	0	0
			3390	2147	576	645	22		
40	DE	435	Total	C	N	O	S	0	0
			3410	2157	579	652	22		
40	DF	432	Total	C	N	O	S	0	0
			3390	2147	576	645	22		
40	DG	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	DH	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	DI	432	Total	C	N	O	S	0	0
			3390	2147	576	645	22		
40	EA	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	EE	435	Total	C	N	O	S	0	0
			3415	2161	580	652	22		
40	EF	435	Total	C	N	O	S	0	0
			3415	2161	580	652	22		
40	EG	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	EH	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	EI	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	FA	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	FE	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	FF	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	FG	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	FH	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	FI	434	Total	C	N	O	S	0	0
			3402	2152	577	651	22		
40	GA	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	GE	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	GF	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
40	GG	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	GH	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	GI	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	HA	435	Total	C	N	O	S	0	0
			3410	2157	579	652	22		
40	HE	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	HF	432	Total	C	N	O	S	0	0
			3392	2148	576	646	22		
40	HG	434	Total	C	N	O	S	0	0
			3402	2153	578	649	22		
40	HH	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	HI	435	Total	C	N	O	S	0	0
			3415	2161	580	652	22		
40	IA	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	IE	420	Total	C	N	O	S	0	0
			3286	2074	557	633	22		
40	IF	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	IG	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	IH	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	II	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	JA	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	JD	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	JE	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	JF	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	JG	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	JH	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
40	KA	434	Total 3406	C 2155	N 578	O 651	S 22	0	0
40	KD	433	Total 3398	C 2151	N 577	O 648	S 22	0	0
40	KE	434	Total 3402	C 2153	N 578	O 649	S 22	0	0
40	KF	434	Total 3406	C 2155	N 578	O 651	S 22	0	0
40	KG	440	Total 3442	C 2177	N 585	O 658	S 22	0	0
40	KH	440	Total 3442	C 2177	N 585	O 658	S 22	0	0
40	LA	440	Total 3442	C 2177	N 585	O 658	S 22	0	0
40	LD	433	Total 3398	C 2151	N 577	O 648	S 22	0	0
40	LE	440	Total 3442	C 2177	N 585	O 658	S 22	0	0
40	LF	433	Total 3398	C 2151	N 577	O 648	S 22	0	0
40	LG	434	Total 3406	C 2155	N 578	O 651	S 22	0	0
40	LH	434	Total 3406	C 2155	N 578	O 651	S 22	0	0
40	MA	432	Total 3392	C 2148	N 576	O 646	S 22	0	0
40	MD	434	Total 3406	C 2155	N 578	O 651	S 22	0	0
40	ME	434	Total 3406	C 2155	N 578	O 651	S 22	0	0
40	MF	433	Total 3398	C 2151	N 577	O 648	S 22	0	0
40	MG	433	Total 3398	C 2151	N 577	O 648	S 22	0	0
40	MH	433	Total 3398	C 2151	N 577	O 648	S 22	0	0
40	NA	432	Total 3392	C 2148	N 576	O 646	S 22	0	0
40	ND	433	Total 3398	C 2151	N 577	O 648	S 22	0	0
40	NE	434	Total 3402	C 2153	N 578	O 649	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
40	NF	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	NG	432	Total	C	N	O	S	0	0
			3392	2148	576	646	22		
40	NH	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	OA	436	Total	C	N	O	S	0	0
			3422	2165	581	654	22		
40	OD	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	OE	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	OF	436	Total	C	N	O	S	0	0
			3419	2163	581	653	22		
40	OG	436	Total	C	N	O	S	0	0
			3415	2160	580	653	22		
40	OH	436	Total	C	N	O	S	0	0
			3419	2163	581	653	22		
40	PA	432	Total	C	N	O	S	0	0
			3392	2148	576	646	22		
40	PD	408	Total	C	N	O	S	0	0
			3196	2023	543	610	20		
40	PE	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	PF	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	PG	431	Total	C	N	O	S	0	0
			3384	2144	575	643	22		
40	PH	431	Total	C	N	O	S	0	0
			3384	2144	575	643	22		
40	QA	432	Total	C	N	O	S	0	0
			3392	2148	576	646	22		
40	QE	431	Total	C	N	O	S	0	0
			3384	2144	575	643	22		
40	QF	431	Total	C	N	O	S	0	0
			3384	2144	575	643	22		
40	QG	432	Total	C	N	O	S	0	0
			3390	2147	576	645	22		
40	QH	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	RA	432	Total	C	N	O	S	0	0
			3390	2147	576	645	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
40	RE	431	Total	C	N	O	S	0	0
			3384	2144	575	643	22		
40	RF	431	Total	C	N	O	S	0	0
			3384	2144	575	643	22		
40	RG	432	Total	C	N	O	S	0	0
			3390	2147	576	645	22		
40	RH	431	Total	C	N	O	S	0	0
			3384	2144	575	643	22		
40	RI	376	Total	C	N	O	S	0	0
			2962	1875	505	562	20		
40	SA	432	Total	C	N	O	S	0	0
			3390	2147	576	645	22		
40	SE	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	SF	432	Total	C	N	O	S	0	0
			3390	2147	576	645	22		
40	SG	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	SH	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	SI	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	TA	432	Total	C	N	O	S	0	0
			3390	2147	576	645	22		
40	TE	432	Total	C	N	O	S	0	0
			3392	2148	576	646	22		
40	TF	432	Total	C	N	O	S	0	0
			3392	2148	576	646	22		
40	TG	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	TH	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	TI	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	UA	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	UE	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	UF	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	UG	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
40	UH	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	UI	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	VA	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	VF	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	VG	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	VH	434	Total	C	N	O	S	0	0
			3406	2155	578	651	22		
40	VI	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	VJ	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	WA	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	WE	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	WF	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		
40	WG	432	Total	C	N	O	S	0	0
			3390	2147	576	645	22		
40	WH	440	Total	C	N	O	S	0	0
			3442	2177	585	658	22		
40	WI	433	Total	C	N	O	S	0	0
			3398	2151	577	648	22		

- Molecule 41 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AB	428	Total	C	N	O	S	0	0
			3341	2098	577	639	27		
41	AL	428	Total	C	N	O	S	0	0
			3341	2098	577	639	27		
41	AM	428	Total	C	N	O	S	0	0
			3341	2098	577	639	27		
41	AN	428	Total	C	N	O	S	0	0
			3341	2098	577	639	27		
41	AO	428	Total	C	N	O	S	0	0
			3341	2098	577	639	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	AP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	BB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	BL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	BM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	BN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	BO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	BP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	CB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	CL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	CM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	CN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	CO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	CP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	DB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	DL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	DM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	DN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	DO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	DP	428	Total 3337	C 2096	N 577	O 637	S 27	0	0
41	EB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	EL	364	Total 2826	C 1775	N 489	O 538	S 24	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	EM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	EN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	EO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	EP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	FB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	FM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	FN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	FO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	FP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	GB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	GM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	GN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	GO	428	Total 3335	C 2095	N 574	O 639	S 27	0	0
41	GP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	HB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	HM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	HN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	HO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	HP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	HQ	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	IB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	IM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	IN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	IO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	IP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	IQ	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	JB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	JL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	JM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	JN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	JO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	KB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	KL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	KM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	KN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	KO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	KP	386	Total 3007	C 1892	N 519	O 573	S 23	0	0
41	LB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	LL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	LM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	LN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	LO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	LP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	MB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	ML	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	MM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	MN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	MO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	MP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	NB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	NL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	NM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	NN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	NO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	NP	418	Total 3264	C 2052	N 565	O 621	S 26	0	0
41	OB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	OL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	OM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	ON	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	OO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	OP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	PB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	PL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	PM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	PN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	PO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	PP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	QB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	QL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	QM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	QN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	QO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	QP	428	Total 3327	C 2090	N 575	O 636	S 26	0	0
41	RB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	RL	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	RM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	RN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	RO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	RP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	SB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	SL	381	Total 2964	C 1861	N 512	O 567	S 24	0	0
41	SM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	SN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	SO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0

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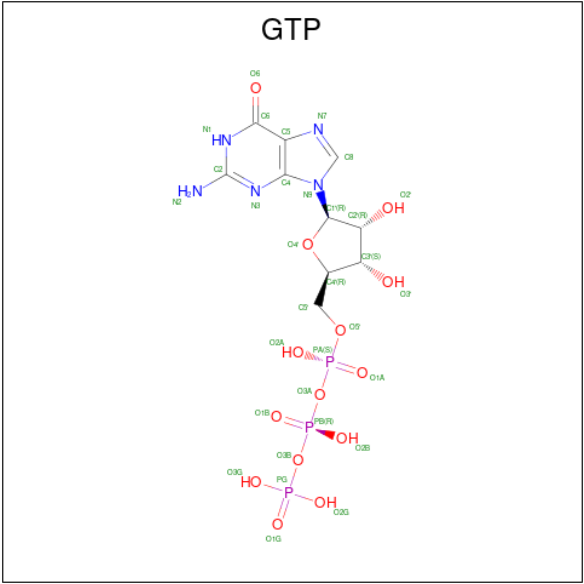
Mol	Chain	Residues	Atoms					AltConf	Trace
41	SP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	TB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	TL	387	Total 3019	C 1899	N 521	O 576	S 23	0	0
41	TM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	TN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	TO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	TP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	UB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	UM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	UN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	UO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	UP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	VB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	VN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	VO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	VP	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	VQ	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	WB	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	WM	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	WN	428	Total 3341	C 2098	N 577	O 639	S 27	0	0
41	WO	428	Total 3341	C 2098	N 577	O 639	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	WP	428	Total	C	N	O	S	0	0
			3341	2098	577	639	27		
41	WQ	421	Total	C	N	O	S	0	0
			3285	2065	569	625	26		

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
42	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
42	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
42	AF	1	Total	C	N	O	P	0
			32	10	5	14	3	
42	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	
42	AH	1	Total	C	N	O	P	0
			32	10	5	14	3	
42	BA	1	Total	C	N	O	P	0
			32	10	5	14	3	
42	BF	1	Total	C	N	O	P	0
			32	10	5	14	3	
42	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
42	BH	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
42	BI	1	Total 32	C 10	N 5	O 14	P 3	0
42	BL	1	Total 32	C 10	N 5	O 14	P 3	0
42	CA	1	Total 32	C 10	N 5	O 14	P 3	0
42	CE	1	Total 32	C 10	N 5	O 14	P 3	0
42	CF	1	Total 32	C 10	N 5	O 14	P 3	0
42	CG	1	Total 32	C 10	N 5	O 14	P 3	0
42	CH	1	Total 32	C 10	N 5	O 14	P 3	0
42	CI	1	Total 32	C 10	N 5	O 14	P 3	0
42	DA	1	Total 32	C 10	N 5	O 14	P 3	0
42	DE	1	Total 32	C 10	N 5	O 14	P 3	0
42	DF	1	Total 32	C 10	N 5	O 14	P 3	0
42	DG	1	Total 32	C 10	N 5	O 14	P 3	0
42	DH	1	Total 32	C 10	N 5	O 14	P 3	0
42	DI	1	Total 32	C 10	N 5	O 14	P 3	0
42	EA	1	Total 32	C 10	N 5	O 14	P 3	0
42	EF	1	Total 32	C 10	N 5	O 14	P 3	0
42	EG	1	Total 32	C 10	N 5	O 14	P 3	0
42	EH	1	Total 32	C 10	N 5	O 14	P 3	0
42	EI	1	Total 32	C 10	N 5	O 14	P 3	0
42	EL	1	Total 32	C 10	N 5	O 14	P 3	0
42	FB	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
42	FE	1	Total 32	C 10	N 5	O 14	P 3	0
42	FI	1	Total 32	C 10	N 5	O 14	P 3	0
42	FM	1	Total 32	C 10	N 5	O 14	P 3	0
42	FN	1	Total 32	C 10	N 5	O 14	P 3	0
42	FO	1	Total 32	C 10	N 5	O 14	P 3	0
42	GA	1	Total 32	C 10	N 5	O 14	P 3	0
42	GB	1	Total 32	C 10	N 5	O 14	P 3	0
42	GE	1	Total 32	C 10	N 5	O 14	P 3	0
42	GF	1	Total 32	C 10	N 5	O 14	P 3	0
42	GH	1	Total 32	C 10	N 5	O 14	P 3	0
42	GP	1	Total 32	C 10	N 5	O 14	P 3	0
42	HA	1	Total 32	C 10	N 5	O 14	P 3	0
42	HB	1	Total 32	C 10	N 5	O 14	P 3	0
42	HE	1	Total 32	C 10	N 5	O 14	P 3	0
42	HH	1	Total 32	C 10	N 5	O 14	P 3	0
42	HM	1	Total 32	C 10	N 5	O 14	P 3	0
42	HP	1	Total 32	C 10	N 5	O 14	P 3	0
42	IA	1	Total 32	C 10	N 5	O 14	P 3	0
42	IE	1	Total 32	C 10	N 5	O 14	P 3	0
42	IF	1	Total 32	C 10	N 5	O 14	P 3	0
42	IG	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
42	IH	1	Total 32	C 10	N 5	O 14	P 3	0
42	II	1	Total 32	C 10	N 5	O 14	P 3	0
42	JA	1	Total 32	C 10	N 5	O 14	P 3	0
42	JB	1	Total 32	C 10	N 5	O 14	P 3	0
42	JD	1	Total 32	C 10	N 5	O 14	P 3	0
42	JE	1	Total 32	C 10	N 5	O 14	P 3	0
42	JF	1	Total 32	C 10	N 5	O 14	P 3	0
42	JO	1	Total 32	C 10	N 5	O 14	P 3	0
42	KB	1	Total 32	C 10	N 5	O 14	P 3	0
42	KD	1	Total 32	C 10	N 5	O 14	P 3	0
42	KE	1	Total 32	C 10	N 5	O 14	P 3	0
42	KM	1	Total 32	C 10	N 5	O 14	P 3	0
42	KN	1	Total 32	C 10	N 5	O 14	P 3	0
42	KO	1	Total 32	C 10	N 5	O 14	P 3	0
42	LA	1	Total 32	C 10	N 5	O 14	P 3	0
42	LB	1	Total 32	C 10	N 5	O 14	P 3	0
42	LD	1	Total 32	C 10	N 5	O 14	P 3	0
42	LL	1	Total 32	C 10	N 5	O 14	P 3	0
42	LM	1	Total 32	C 10	N 5	O 14	P 3	0
42	LO	1	Total 32	C 10	N 5	O 14	P 3	0
42	MB	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
42	MD	1	Total 32	C 10	N 5	O 14	P 3	0
42	MH	1	Total 32	C 10	N 5	O 14	P 3	0
42	ML	1	Total 32	C 10	N 5	O 14	P 3	0
42	MM	1	Total 32	C 10	N 5	O 14	P 3	0
42	MN	1	Total 32	C 10	N 5	O 14	P 3	0
42	ND	1	Total 32	C 10	N 5	O 14	P 3	0
42	NE	1	Total 32	C 10	N 5	O 14	P 3	0
42	NG	1	Total 32	C 10	N 5	O 14	P 3	0
42	NM	1	Total 32	C 10	N 5	O 14	P 3	0
42	NN	1	Total 32	C 10	N 5	O 14	P 3	0
42	NO	1	Total 32	C 10	N 5	O 14	P 3	0
42	OB	1	Total 32	C 10	N 5	O 14	P 3	0
42	OD	1	Total 32	C 10	N 5	O 14	P 3	0
42	OL	1	Total 32	C 10	N 5	O 14	P 3	0
42	OM	1	Total 32	C 10	N 5	O 14	P 3	0
42	ON	1	Total 32	C 10	N 5	O 14	P 3	0
42	OO	1	Total 32	C 10	N 5	O 14	P 3	0
42	PB	1	Total 32	C 10	N 5	O 14	P 3	0
42	PD	1	Total 32	C 10	N 5	O 14	P 3	0
42	PE	1	Total 32	C 10	N 5	O 14	P 3	0
42	PM	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
42	PN	1	Total 32	C 10	N 5	O 14	P 3	0
42	PO	1	Total 32	C 10	N 5	O 14	P 3	0
42	QF	1	Total 32	C 10	N 5	O 14	P 3	0
42	QG	1	Total 32	C 10	N 5	O 14	P 3	0
42	QL	1	Total 32	C 10	N 5	O 14	P 3	0
42	QN	1	Total 32	C 10	N 5	O 14	P 3	0
42	QO	1	Total 32	C 10	N 5	O 14	P 3	0
42	RE	1	Total 32	C 10	N 5	O 14	P 3	0
42	RF	1	Total 32	C 10	N 5	O 14	P 3	0
42	RG	1	Total 32	C 10	N 5	O 14	P 3	0
42	RN	1	Total 32	C 10	N 5	O 14	P 3	0
42	RO	1	Total 32	C 10	N 5	O 14	P 3	0
42	RP	1	Total 32	C 10	N 5	O 14	P 3	0
42	SG	1	Total 32	C 10	N 5	O 14	P 3	0
42	SH	1	Total 32	C 10	N 5	O 14	P 3	0
42	SL	1	Total 32	C 10	N 5	O 14	P 3	0
42	SM	1	Total 32	C 10	N 5	O 14	P 3	0
42	SN	1	Total 32	C 10	N 5	O 14	P 3	0
42	SP	1	Total 32	C 10	N 5	O 14	P 3	0
42	TF	1	Total 32	C 10	N 5	O 14	P 3	0
42	TG	1	Total 32	C 10	N 5	O 14	P 3	0

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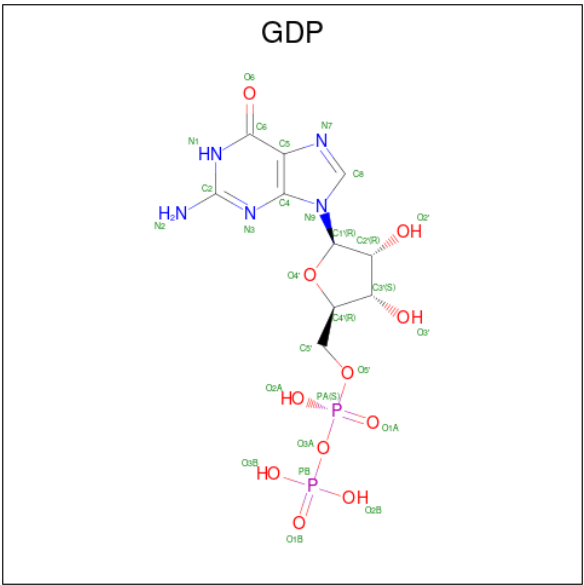
Mol	Chain	Residues	Atoms					AltConf
42	TH	1	Total 32	C 10	N 5	O 14	P 3	0
42	TI	1	Total 32	C 10	N 5	O 14	P 3	0
42	TL	1	Total 32	C 10	N 5	O 14	P 3	0
42	TN	1	Total 32	C 10	N 5	O 14	P 3	0
42	UA	1	Total 32	C 10	N 5	O 14	P 3	0
42	UB	1	Total 32	C 10	N 5	O 14	P 3	0
42	UE	1	Total 32	C 10	N 5	O 14	P 3	0
42	UI	1	Total 32	C 10	N 5	O 14	P 3	0
42	UM	1	Total 32	C 10	N 5	O 14	P 3	0
42	UO	1	Total 32	C 10	N 5	O 14	P 3	0
42	VA	1	Total 32	C 10	N 5	O 14	P 3	0
42	VB	1	Total 32	C 10	N 5	O 14	P 3	0
42	VF	1	Total 32	C 10	N 5	O 14	P 3	0
42	VN	1	Total 32	C 10	N 5	O 14	P 3	0
42	VP	1	Total 32	C 10	N 5	O 14	P 3	0
42	VQ	1	Total 32	C 10	N 5	O 14	P 3	0
42	WA	1	Total 32	C 10	N 5	O 14	P 3	0
42	WE	1	Total 32	C 10	N 5	O 14	P 3	0
42	WF	1	Total 32	C 10	N 5	O 14	P 3	0
42	WG	1	Total 32	C 10	N 5	O 14	P 3	0
42	WI	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
42	WO	1	32	10	5	14	3	0

- Molecule 43 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
43	AB	1	Total 28	10	5	11	2	0
43	AL	1	Total 28	10	5	11	2	0
43	AM	1	Total 28	10	5	11	2	0
43	AN	1	Total 28	10	5	11	2	0
43	AO	1	Total 28	10	5	11	2	0
43	AP	1	Total 28	10	5	11	2	0
43	BB	1	Total 28	10	5	11	2	0
43	BL	1	Total 28	10	5	11	2	0
43	BM	1	Total 28	10	5	11	2	0
43	BN	1	Total 28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
43	BO	1	Total 28	C 10	N 5	O 11	P 2	0
43	BP	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	CL	1	Total 28	C 10	N 5	O 11	P 2	0
43	CM	1	Total 28	C 10	N 5	O 11	P 2	0
43	CN	1	Total 28	C 10	N 5	O 11	P 2	0
43	CO	1	Total 28	C 10	N 5	O 11	P 2	0
43	CP	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	DL	1	Total 28	C 10	N 5	O 11	P 2	0
43	DM	1	Total 28	C 10	N 5	O 11	P 2	0
43	DN	1	Total 28	C 10	N 5	O 11	P 2	0
43	DO	1	Total 28	C 10	N 5	O 11	P 2	0
43	DP	1	Total 28	C 10	N 5	O 11	P 2	0
43	EB	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	EM	1	Total 28	C 10	N 5	O 11	P 2	0
43	EN	1	Total 28	C 10	N 5	O 11	P 2	0
43	EO	1	Total 28	C 10	N 5	O 11	P 2	0
43	EP	1	Total 28	C 10	N 5	O 11	P 2	0
43	FB	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
43	FM	1	Total 28	C 10	N 5	O 11	P 2	0
43	FN	1	Total 28	C 10	N 5	O 11	P 2	0
43	FO	1	Total 28	C 10	N 5	O 11	P 2	0
43	FP	1	Total 28	C 10	N 5	O 11	P 2	0
43	GB	1	Total 28	C 10	N 5	O 11	P 2	0
43	GM	1	Total 28	C 10	N 5	O 11	P 2	0
43	GN	1	Total 28	C 10	N 5	O 11	P 2	0
43	GO	1	Total 28	C 10	N 5	O 11	P 2	0
43	GP	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	HM	1	Total 28	C 10	N 5	O 11	P 2	0
43	HN	1	Total 28	C 10	N 5	O 11	P 2	0
43	HO	1	Total 28	C 10	N 5	O 11	P 2	0
43	HP	1	Total 28	C 10	N 5	O 11	P 2	0
43	HQ	1	Total 28	C 10	N 5	O 11	P 2	0
43	IB	1	Total 28	C 10	N 5	O 11	P 2	0
43	IM	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	IO	1	Total 28	C 10	N 5	O 11	P 2	0
43	IP	1	Total 28	C 10	N 5	O 11	P 2	0
43	IQ	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
43	JB	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
43	JM	1	Total 28	C 10	N 5	O 11	P 2	0
43	JN	1	Total 28	C 10	N 5	O 11	P 2	0
43	JO	1	Total 28	C 10	N 5	O 11	P 2	0
43	KB	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	KM	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	KO	1	Total 28	C 10	N 5	O 11	P 2	0
43	KP	1	Total 28	C 10	N 5	O 11	P 2	0
43	LB	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	LM	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	LO	1	Total 28	C 10	N 5	O 11	P 2	0
43	LP	1	Total 28	C 10	N 5	O 11	P 2	0
43	MB	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	MM	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

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Mol	Chain	Residues	Atoms					AltConf
43	MO	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	MP	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	NB	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	NL	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	NM	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	NN	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	NO	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	NP	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	OB	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	OL	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	OM	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	ON	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	OO	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	OP	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	PB	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	PL	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	PM	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	PN	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	PO	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	PP	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	QB	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
43	QL	1	Total 28	C 10	N 5	O 11	P 2	0
43	QM	1	Total 28	C 10	N 5	O 11	P 2	0
43	QN	1	Total 28	C 10	N 5	O 11	P 2	0
43	QO	1	Total 28	C 10	N 5	O 11	P 2	0
43	QP	1	Total 28	C 10	N 5	O 11	P 2	0
43	RB	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	RM	1	Total 28	C 10	N 5	O 11	P 2	0
43	RN	1	Total 28	C 10	N 5	O 11	P 2	0
43	RO	1	Total 28	C 10	N 5	O 11	P 2	0
43	RP	1	Total 28	C 10	N 5	O 11	P 2	0
43	SB	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	SM	1	Total 28	C 10	N 5	O 11	P 2	0
43	SN	1	Total 28	C 10	N 5	O 11	P 2	0
43	SO	1	Total 28	C 10	N 5	O 11	P 2	0
43	SP	1	Total 28	C 10	N 5	O 11	P 2	0
43	TB	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	TM	1	Total 28	C 10	N 5	O 11	P 2	0
43	TN	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
43	TO	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	TP	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	UB	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	UM	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	UN	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	UO	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	UP	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	VB	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	VN	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	VO	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	VP	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	VQ	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	WB	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	WM	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	
43	WO	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	WP	1	Total	C	N	O	P	0
			28	10	5	11	2	
43	WQ	1	Total	C	N	O	P	0
			28	10	5	11	2	

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

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113809	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	2.382	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.35	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](#)

269 ligands are modelled in this entry.

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
42	GTP	FE	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
42	GTP	NO	501	-	33,34,34	1.00	1 (3%)	50,54,54	1.63	10 (20%)
42	GTP	LL	501	-	33,34,34	1.17	3 (9%)	50,54,54	1.97	10 (20%)
43	GDP	LO	502	-	29,30,30	1.10	2 (6%)	45,47,47	2.00	9 (20%)
42	GTP	VQ	501	-	33,34,34	1.02	2 (6%)	50,54,54	1.58	10 (20%)
42	GTP	SH	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.69	10 (20%)
42	GTP	GE	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.55	9 (18%)
43	GDP	FN	502	-	29,30,30	1.05	3 (10%)	45,47,47	2.51	8 (17%)
42	GTP	AE	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.56	8 (16%)
43	GDP	QL	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.87	9 (20%)
43	GDP	WB	501	-	29,30,30	1.10	2 (6%)	45,47,47	1.96	9 (20%)
43	GDP	HM	502	-	29,30,30	1.07	2 (6%)	45,47,47	2.11	8 (17%)
43	GDP	QM	501	-	29,30,30	1.09	2 (6%)	45,47,47	2.12	8 (17%)
43	GDP	WO	502	-	29,30,30	1.11	2 (6%)	45,47,47	2.02	9 (20%)
42	GTP	CA	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.60	10 (20%)
43	GDP	NL	501	-	29,30,30	1.11	3 (10%)	45,47,47	1.86	9 (20%)
42	GTP	DH	501	-	33,34,34	1.46	7 (21%)	50,54,54	2.47	15 (30%)
42	GTP	SP	501	-	33,34,34	1.01	3 (9%)	50,54,54	1.67	10 (20%)
42	GTP	EF	501	-	33,34,34	1.00	1 (3%)	50,54,54	1.69	10 (20%)
42	GTP	KE	501	-	33,34,34	1.05	3 (9%)	50,54,54	1.62	10 (20%)
42	GTP	UA	501	-	33,34,34	1.49	8 (24%)	50,54,54	2.49	16 (32%)
42	GTP	GA	501	-	33,34,34	1.40	5 (15%)	50,54,54	1.99	13 (26%)
42	GTP	IE	501	-	33,34,34	1.04	3 (9%)	50,54,54	1.65	10 (20%)
42	GTP	ND	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.53	9 (18%)
43	GDP	HB	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.96	9 (20%)
43	GDP	HN	501	-	29,30,30	1.10	2 (6%)	45,47,47	1.95	9 (20%)
42	GTP	WF	501	-	33,34,34	1.08	4 (12%)	50,54,54	1.69	10 (20%)
43	GDP	AB	501	-	29,30,30	1.08	2 (6%)	45,47,47	2.08	9 (20%)
42	GTP	CF	501	-	33,34,34	1.07	4 (12%)	50,54,54	1.68	10 (20%)
42	GTP	QN	501	-	33,34,34	1.27	5 (15%)	50,54,54	1.66	10 (20%)
43	GDP	FB	501	-	29,30,30	1.10	2 (6%)	45,47,47	2.01	9 (20%)
42	GTP	ON	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.62	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	GDP	QP	501	-	29,30,30	1.10	1 (3%)	45,47,47	2.83	13 (28%)
43	GDP	MP	501	-	29,30,30	1.08	2 (6%)	45,47,47	2.12	9 (20%)
43	GDP	TL	502	-	29,30,30	1.12	3 (10%)	45,47,47	3.06	12 (26%)
42	GTP	KM	501	-	33,34,34	1.32	4 (12%)	50,54,54	2.33	14 (28%)
42	GTP	CH	501	-	33,34,34	1.01	2 (6%)	50,54,54	1.67	10 (20%)
43	GDP	DM	501	-	29,30,30	1.03	2 (6%)	45,47,47	2.10	9 (20%)
42	GTP	NN	501	-	33,34,34	1.03	1 (3%)	50,54,54	1.69	10 (20%)
43	GDP	SO	501	-	29,30,30	1.05	2 (6%)	45,47,47	2.13	10 (22%)
43	GDP	JM	501	-	29,30,30	1.09	2 (6%)	45,47,47	1.98	9 (20%)
42	GTP	EA	501	-	33,34,34	1.03	3 (9%)	50,54,54	1.61	9 (18%)
43	GDP	IN	501	-	29,30,30	1.11	2 (6%)	45,47,47	1.94	8 (17%)
43	GDP	KN	502	-	29,30,30	1.06	2 (6%)	45,47,47	2.05	9 (20%)
43	GDP	SL	502	-	29,30,30	1.11	2 (6%)	45,47,47	2.36	11 (24%)
42	GTP	BA	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.60	9 (18%)
42	GTP	HB	502	-	33,34,34	0.99	2 (6%)	50,54,54	1.60	9 (18%)
43	GDP	JN	501	-	29,30,30	1.10	2 (6%)	45,47,47	1.93	9 (20%)
42	GTP	BF	501	-	33,34,34	1.04	3 (9%)	50,54,54	1.68	10 (20%)
43	GDP	QO	502	-	29,30,30	1.11	3 (10%)	45,47,47	1.98	9 (20%)
42	GTP	PE	501	-	33,34,34	1.06	2 (6%)	50,54,54	1.70	10 (20%)
43	GDP	SB	501	-	29,30,30	1.03	2 (6%)	45,47,47	2.42	11 (24%)
42	GTP	VN	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.61	10 (20%)
43	GDP	TN	502	-	29,30,30	1.10	3 (10%)	45,47,47	2.01	9 (20%)
42	GTP	WE	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.63	9 (18%)
43	GDP	DN	501	-	29,30,30	1.10	3 (10%)	45,47,47	2.03	9 (20%)
43	GDP	GP	502	-	29,30,30	1.09	1 (3%)	45,47,47	2.81	15 (33%)
42	GTP	UB	502	-	33,34,34	1.03	2 (6%)	50,54,54	1.66	10 (20%)
42	GTP	JB	502	-	33,34,34	1.32	5 (15%)	50,54,54	2.40	14 (28%)
43	GDP	KP	501	-	29,30,30	1.06	2 (6%)	45,47,47	2.11	9 (20%)
43	GDP	NB	501	-	29,30,30	1.11	2 (6%)	45,47,47	1.98	9 (20%)
43	GDP	JB	501	-	29,30,30	1.07	2 (6%)	45,47,47	2.07	8 (17%)
42	GTP	IA	501	-	33,34,34	1.01	1 (3%)	50,54,54	1.62	10 (20%)
43	GDP	KM	502	-	29,30,30	1.10	2 (6%)	45,47,47	1.99	9 (20%)
43	GDP	VO	501	-	29,30,30	1.07	2 (6%)	45,47,47	2.00	8 (17%)
42	GTP	BH	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.61	10 (20%)
42	GTP	EI	501	-	33,34,34	1.07	4 (12%)	50,54,54	1.68	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	GDP	CL	501	-	29,30,30	1.09	3 (10%)	45,47,47	1.93	9 (20%)
42	GTP	IF	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.63	10 (20%)
42	GTP	KO	501	-	33,34,34	1.53	7 (21%)	50,54,54	2.52	17 (34%)
42	GTP	GP	501	-	33,34,34	1.22	4 (12%)	50,54,54	2.11	12 (24%)
42	GTP	LM	501	-	33,34,34	1.08	2 (6%)	50,54,54	1.68	10 (20%)
42	GTP	UE	501	-	33,34,34	1.08	4 (12%)	50,54,54	1.61	10 (20%)
42	GTP	FI	501	-	33,34,34	1.03	2 (6%)	50,54,54	1.88	12 (24%)
43	GDP	OM	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.86	8 (17%)
42	GTP	LD	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.61	9 (18%)
42	GTP	UI	501	-	33,34,34	1.08	4 (12%)	50,54,54	1.75	11 (22%)
43	GDP	TB	501	-	29,30,30	1.07	2 (6%)	45,47,47	2.50	15 (33%)
42	GTP	MH	501	-	33,34,34	1.10	3 (9%)	50,54,54	1.82	12 (24%)
42	GTP	EH	501	-	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
42	GTP	CE	501	-	33,34,34	1.16	3 (9%)	50,54,54	1.71	10 (20%)
42	GTP	CI	501	-	33,34,34	0.97	0	50,54,54	1.56	10 (20%)
43	GDP	AP	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
43	GDP	BO	501	-	29,30,30	1.11	2 (6%)	45,47,47	1.94	9 (20%)
43	GDP	JO	502	-	29,30,30	1.09	2 (6%)	45,47,47	1.92	9 (20%)
42	GTP	RN	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.64	10 (20%)
43	GDP	IO	501	-	29,30,30	1.11	3 (10%)	45,47,47	1.93	9 (20%)
42	GTP	AG	501	-	33,34,34	0.94	1 (3%)	50,54,54	1.62	10 (20%)
42	GTP	II	501	-	33,34,34	1.06	2 (6%)	50,54,54	1.67	9 (18%)
42	GTP	BI	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.64	10 (20%)
43	GDP	RM	501	-	29,30,30	1.07	2 (6%)	45,47,47	2.23	10 (22%)
42	GTP	EG	501	-	33,34,34	1.32	5 (15%)	50,54,54	1.94	10 (20%)
42	GTP	HA	501	-	33,34,34	1.01	2 (6%)	50,54,54	1.60	11 (22%)
43	GDP	MN	502	-	29,30,30	1.10	3 (10%)	45,47,47	1.99	9 (20%)
43	GDP	WM	501	-	29,30,30	1.08	2 (6%)	45,47,47	2.13	9 (20%)
42	GTP	LB	502	-	33,34,34	1.04	2 (6%)	50,54,54	1.67	10 (20%)
42	GTP	HH	501	-	33,34,34	0.99	3 (9%)	50,54,54	1.64	8 (16%)
43	GDP	IB	501	-	29,30,30	1.11	2 (6%)	45,47,47	2.02	10 (22%)
43	GDP	UO	502	-	29,30,30	1.07	2 (6%)	45,47,47	1.98	9 (20%)
43	GDP	VN	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.92	8 (17%)
43	GDP	WP	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.92	8 (17%)
42	GTP	VA	501	-	33,34,34	1.08	3 (9%)	50,54,54	1.68	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	GTP	JE	501	-	33,34,34	0.99	2 (6%)	50,54,54	1.63	12 (24%)
42	GTP	QG	501	-	33,34,34	1.06	3 (9%)	50,54,54	1.60	11 (22%)
43	GDP	CO	501	-	29,30,30	1.07	2 (6%)	45,47,47	2.13	9 (20%)
42	GTP	WO	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.65	10 (20%)
42	GTP	JF	501	-	33,34,34	1.01	2 (6%)	50,54,54	1.74	12 (24%)
42	GTP	JA	501	-	33,34,34	1.32	4 (12%)	50,54,54	1.74	12 (24%)
42	GTP	TL	501	-	33,34,34	1.16	4 (12%)	50,54,54	1.75	11 (22%)
43	GDP	ML	502	-	29,30,30	1.10	2 (6%)	45,47,47	1.98	9 (20%)
43	GDP	VQ	502	-	29,30,30	1.09	2 (6%)	45,47,47	2.15	9 (20%)
43	GDP	PM	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.90	9 (20%)
43	GDP	CN	501	-	29,30,30	1.06	2 (6%)	45,47,47	2.14	8 (17%)
42	GTP	FN	501	-	33,34,34	1.07	4 (12%)	50,54,54	1.64	11 (22%)
42	GTP	QL	501	-	33,34,34	1.55	8 (24%)	50,54,54	2.47	19 (38%)
42	GTP	NE	501	-	33,34,34	1.04	2 (6%)	50,54,54	1.75	11 (22%)
42	GTP	WI	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.68	10 (20%)
43	GDP	OP	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.89	9 (20%)
42	GTP	IH	501	-	33,34,34	1.12	3 (9%)	50,54,54	1.70	11 (22%)
42	GTP	MD	501	-	33,34,34	1.20	4 (12%)	50,54,54	1.99	13 (26%)
42	GTP	MB	502	-	33,34,34	1.32	5 (15%)	50,54,54	1.91	11 (22%)
42	GTP	QO	501	-	33,34,34	1.01	2 (6%)	50,54,54	1.60	10 (20%)
43	GDP	EO	501	-	29,30,30	1.11	3 (10%)	45,47,47	1.85	8 (17%)
43	GDP	MM	502	-	29,30,30	1.08	2 (6%)	45,47,47	2.00	9 (20%)
42	GTP	UM	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.62	8 (16%)
43	GDP	MO	501	-	29,30,30	1.10	2 (6%)	45,47,47	2.00	9 (20%)
43	GDP	PP	501	-	29,30,30	1.10	2 (6%)	45,47,47	2.00	8 (17%)
43	GDP	EL	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.88	9 (20%)
42	GTP	TN	501	-	33,34,34	1.13	4 (12%)	50,54,54	1.67	9 (18%)
42	GTP	JD	501	-	33,34,34	1.18	3 (9%)	50,54,54	1.87	11 (22%)
43	GDP	CB	501	-	29,30,30	1.09	2 (6%)	45,47,47	2.04	9 (20%)
43	GDP	BB	501	-	29,30,30	1.09	2 (6%)	45,47,47	2.01	9 (20%)
43	GDP	IQ	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.84	9 (20%)
43	GDP	TP	501	-	29,30,30	1.10	3 (10%)	45,47,47	2.96	13 (28%)
43	GDP	UB	501	-	29,30,30	1.08	3 (10%)	45,47,47	1.89	8 (17%)
43	GDP	PL	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.99	9 (20%)
43	GDP	JL	501	-	29,30,30	1.09	3 (10%)	45,47,47	3.00	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	GDP	VP	502	-	29,30,30	1.09	2 (6%)	45,47,47	2.06	9 (20%)
42	GTP	AA	501	-	33,34,34	1.04	4 (12%)	50,54,54	1.60	9 (18%)
43	GDP	DP	501	-	29,30,30	1.11	3 (10%)	45,47,47	1.87	8 (17%)
43	GDP	PN	502	-	29,30,30	1.09	2 (6%)	45,47,47	2.00	9 (20%)
43	GDP	RB	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.96	9 (20%)
42	GTP	DI	501	-	33,34,34	1.23	3 (9%)	50,54,54	2.11	12 (24%)
42	GTP	GH	501	-	33,34,34	1.01	2 (6%)	50,54,54	1.76	11 (22%)
43	GDP	AN	501	-	29,30,30	1.08	2 (6%)	45,47,47	2.09	9 (20%)
43	GDP	DL	501	-	29,30,30	1.18	3 (10%)	45,47,47	2.96	14 (31%)
43	GDP	LB	501	-	29,30,30	1.09	3 (10%)	45,47,47	1.96	9 (20%)
42	GTP	JO	501	-	33,34,34	1.12	2 (6%)	50,54,54	1.79	11 (22%)
42	GTP	HE	501	-	33,34,34	1.05	2 (6%)	50,54,54	1.62	10 (20%)
42	GTP	SM	501	-	33,34,34	1.01	1 (3%)	50,54,54	1.76	11 (22%)
43	GDP	GO	501	-	29,30,30	1.10	2 (6%)	45,47,47	2.01	9 (20%)
42	GTP	EL	501	-	33,34,34	1.02	2 (6%)	50,54,54	1.59	10 (20%)
42	GTP	OM	501	-	33,34,34	1.02	3 (9%)	50,54,54	1.59	8 (16%)
43	GDP	EP	501	-	29,30,30	1.03	2 (6%)	45,47,47	2.77	12 (26%)
43	GDP	NO	502	-	29,30,30	1.10	2 (6%)	45,47,47	1.94	9 (20%)
43	GDP	OB	501	-	29,30,30	1.11	2 (6%)	45,47,47	2.00	8 (17%)
43	GDP	QB	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.83	8 (17%)
42	GTP	GF	501	-	33,34,34	1.15	5 (15%)	50,54,54	1.75	11 (22%)
42	GTP	WA	501	-	33,34,34	1.00	3 (9%)	50,54,54	1.66	11 (22%)
42	GTP	PM	501	-	33,34,34	1.01	1 (3%)	50,54,54	1.66	9 (18%)
43	GDP	LM	502	-	29,30,30	1.07	2 (6%)	45,47,47	2.15	9 (20%)
42	GTP	RG	501	-	33,34,34	0.98	1 (3%)	50,54,54	1.58	9 (18%)
42	GTP	BG	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.54	9 (18%)
43	GDP	KL	501	-	29,30,30	1.11	2 (6%)	45,47,47	1.95	9 (20%)
42	GTP	CG	501	-	33,34,34	1.07	3 (9%)	50,54,54	1.77	10 (20%)
42	GTP	BL	501	-	33,34,34	0.98	1 (3%)	50,54,54	1.61	9 (18%)
43	GDP	VB	501	-	29,30,30	1.09	3 (10%)	45,47,47	1.91	8 (17%)
43	GDP	AO	501	-	29,30,30	1.09	2 (6%)	45,47,47	1.98	9 (20%)
43	GDP	UM	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.81	7 (15%)
42	GTP	OO	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.68	10 (20%)
43	GDP	UP	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.96	10 (22%)
42	GTP	PO	501	-	33,34,34	1.07	2 (6%)	50,54,54	1.73	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	GTP	VB	502	-	33,34,34	1.02	2 (6%)	50,54,54	1.68	11 (22%)
42	GTP	MN	501	-	33,34,34	1.07	3 (9%)	50,54,54	1.68	9 (18%)
43	GDP	GB	501	-	29,30,30	1.09	3 (10%)	45,47,47	1.93	9 (20%)
43	GDP	SP	502	-	29,30,30	1.13	2 (6%)	45,47,47	1.84	6 (13%)
43	GDP	SN	502	-	29,30,30	1.05	3 (10%)	45,47,47	3.11	12 (26%)
42	GTP	SN	501	-	33,34,34	1.28	5 (15%)	50,54,54	2.16	16 (32%)
42	GTP	UO	501	-	33,34,34	1.01	2 (6%)	50,54,54	1.68	10 (20%)
43	GDP	LN	501	-	29,30,30	1.09	3 (10%)	45,47,47	1.91	9 (20%)
43	GDP	OO	502	-	29,30,30	1.11	2 (6%)	45,47,47	1.91	8 (17%)
43	GDP	LP	501	-	29,30,30	1.09	2 (6%)	45,47,47	1.94	9 (20%)
43	GDP	RL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.85	9 (20%)
43	GDP	BM	501	-	29,30,30	1.08	2 (6%)	45,47,47	2.03	8 (17%)
43	GDP	AL	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.89	9 (20%)
42	GTP	OB	502	-	33,34,34	1.08	3 (9%)	50,54,54	1.74	10 (20%)
43	GDP	DO	501	-	29,30,30	1.07	2 (6%)	45,47,47	1.96	8 (17%)
43	GDP	PB	501	-	29,30,30	1.10	2 (6%)	45,47,47	2.00	9 (20%)
43	GDP	HO	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.90	9 (20%)
42	GTP	KD	501	-	33,34,34	1.09	2 (6%)	50,54,54	1.76	10 (20%)
43	GDP	TM	501	-	29,30,30	1.09	2 (6%)	45,47,47	2.02	8 (17%)
42	GTP	FB	502	-	33,34,34	0.95	1 (3%)	50,54,54	1.62	9 (18%)
43	GDP	AM	501	-	29,30,30	1.07	2 (6%)	45,47,47	2.17	8 (17%)
43	GDP	LL	502	-	29,30,30	1.10	3 (10%)	45,47,47	1.83	8 (17%)
43	GDP	IP	501	-	29,30,30	1.12	2 (6%)	45,47,47	1.93	9 (20%)
42	GTP	HM	501	-	33,34,34	1.09	3 (9%)	50,54,54	1.72	11 (22%)
42	GTP	ML	501	-	33,34,34	1.15	3 (9%)	50,54,54	2.02	13 (26%)
43	GDP	KO	502	-	29,30,30	1.06	3 (10%)	45,47,47	2.50	10 (22%)
42	GTP	DE	501	-	33,34,34	1.00	2 (6%)	50,54,54	1.67	9 (18%)
43	GDP	CP	501	-	29,30,30	1.12	2 (6%)	45,47,47	1.99	9 (20%)
42	GTP	WG	501	-	33,34,34	1.03	3 (9%)	50,54,54	1.66	11 (22%)
43	GDP	MB	501	-	29,30,30	1.08	2 (6%)	45,47,47	2.06	9 (20%)
42	GTP	GB	502	-	33,34,34	0.97	2 (6%)	50,54,54	1.80	11 (22%)
42	GTP	LA	501	-	33,34,34	0.98	1 (3%)	50,54,54	1.65	10 (20%)
42	GTP	NM	501	-	33,34,34	1.04	2 (6%)	50,54,54	1.64	9 (18%)
43	GDP	RP	502	-	29,30,30	1.00	3 (10%)	45,47,47	3.40	14 (31%)
42	GTP	PD	501	-	33,34,34	1.01	1 (3%)	50,54,54	1.58	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	GDP	FO	502	-	29,30,30	1.09	2 (6%)	45,47,47	1.95	8 (17%)
42	GTP	RF	501	-	33,34,34	0.96	2 (6%)	50,54,54	1.47	7 (14%)
43	GDP	DB	501	-	29,30,30	1.09	2 (6%)	45,47,47	1.98	10 (22%)
43	GDP	UN	501	-	29,30,30	1.12	2 (6%)	45,47,47	1.91	9 (20%)
42	GTP	DG	501	-	33,34,34	1.16	4 (12%)	50,54,54	1.81	12 (24%)
43	GDP	CM	501	-	29,30,30	1.09	2 (6%)	45,47,47	2.04	9 (20%)
42	GTP	RO	501	-	33,34,34	0.97	2 (6%)	50,54,54	1.66	11 (22%)
43	GDP	OL	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.94	9 (20%)
43	GDP	GN	501	-	29,30,30	1.08	2 (6%)	45,47,47	2.12	9 (20%)
43	GDP	HQ	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.83	8 (17%)
43	GDP	IM	501	-	29,30,30	1.10	2 (6%)	45,47,47	1.95	9 (20%)
42	GTP	PB	502	-	33,34,34	1.07	4 (12%)	50,54,54	1.66	11 (22%)
42	GTP	AF	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.61	10 (20%)
43	GDP	QN	502	-	29,30,30	1.08	2 (6%)	45,47,47	1.99	9 (20%)
42	GTP	DA	501	-	33,34,34	1.13	4 (12%)	50,54,54	1.86	13 (26%)
42	GTP	LO	501	-	33,34,34	1.04	3 (9%)	50,54,54	1.77	10 (20%)
42	GTP	VP	501	-	33,34,34	1.03	2 (6%)	50,54,54	1.72	10 (20%)
43	GDP	ON	502	-	29,30,30	1.10	3 (10%)	45,47,47	2.12	8 (17%)
42	GTP	PN	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)
43	GDP	BL	502	-	29,30,30	1.10	2 (6%)	45,47,47	1.96	9 (20%)
43	GDP	RO	502	-	29,30,30	1.09	2 (6%)	45,47,47	1.95	8 (17%)
42	GTP	HP	501	-	33,34,34	1.11	5 (15%)	50,54,54	1.68	9 (18%)
42	GTP	VF	501	-	33,34,34	1.01	3 (9%)	50,54,54	1.63	11 (22%)
43	GDP	NP	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.87	8 (17%)
42	GTP	RE	501	-	33,34,34	0.98	1 (3%)	50,54,54	1.63	9 (18%)
42	GTP	RP	501	-	33,34,34	0.93	1 (3%)	50,54,54	1.64	9 (18%)
42	GTP	IG	501	-	33,34,34	1.05	2 (6%)	50,54,54	1.65	8 (16%)
42	GTP	SL	501	-	33,34,34	1.13	4 (12%)	50,54,54	1.92	13 (26%)
42	GTP	TG	501	-	33,34,34	1.16	4 (12%)	50,54,54	2.00	12 (24%)
43	GDP	GM	501	-	29,30,30	1.08	2 (6%)	45,47,47	2.08	8 (17%)
43	GDP	HP	502	-	29,30,30	1.10	3 (10%)	45,47,47	1.89	8 (17%)
42	GTP	TF	501	-	33,34,34	1.19	4 (12%)	50,54,54	2.02	15 (30%)
42	GTP	QF	501	-	33,34,34	1.06	4 (12%)	50,54,54	1.60	10 (20%)
42	GTP	DF	501	-	33,34,34	1.10	4 (12%)	50,54,54	1.68	9 (18%)
42	GTP	MM	501	-	33,34,34	1.20	3 (9%)	50,54,54	1.99	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	GTP	KB	502	-	33,34,34	1.07	2 (6%)	50,54,54	1.79	12 (24%)
43	GDP	EM	501	-	29,30,30	1.09	3 (10%)	45,47,47	2.44	10 (22%)
42	GTP	OD	501	-	33,34,34	1.05	4 (12%)	50,54,54	1.65	11 (22%)
42	GTP	FM	501	-	33,34,34	1.14	4 (12%)	50,54,54	1.87	13 (26%)
42	GTP	TH	501	-	33,34,34	1.08	3 (9%)	50,54,54	1.66	10 (20%)
43	GDP	BP	501	-	29,30,30	1.09	2 (6%)	45,47,47	2.10	9 (20%)
42	GTP	TI	501	-	33,34,34	1.37	4 (12%)	50,54,54	2.26	14 (28%)
43	GDP	EN	501	-	29,30,30	1.07	3 (10%)	45,47,47	2.45	9 (20%)
43	GDP	KB	501	-	29,30,30	1.09	2 (6%)	45,47,47	1.93	9 (20%)
43	GDP	WN	501	-	29,30,30	1.09	2 (6%)	45,47,47	2.01	9 (20%)
43	GDP	WQ	501	-	29,30,30	1.10	3 (10%)	45,47,47	1.90	9 (20%)
43	GDP	FP	501	-	29,30,30	1.08	1 (3%)	45,47,47	2.78	13 (28%)
42	GTP	FO	501	-	33,34,34	1.12	4 (12%)	50,54,54	1.87	11 (22%)
43	GDP	TO	501	-	29,30,30	1.06	2 (6%)	45,47,47	2.36	11 (24%)
42	GTP	SG	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.65	10 (20%)
43	GDP	FM	502	-	29,30,30	1.11	3 (10%)	45,47,47	1.91	9 (20%)
42	GTP	AH	501	-	33,34,34	1.02	2 (6%)	50,54,54	1.58	9 (18%)
42	GTP	OL	501	-	33,34,34	1.00	1 (3%)	50,54,54	1.69	11 (22%)
43	GDP	BN	501	-	29,30,30	1.08	2 (6%)	45,47,47	2.14	9 (20%)
43	GDP	RN	502	-	29,30,30	1.12	3 (10%)	45,47,47	3.00	12 (26%)
43	GDP	PO	502	-	29,30,30	1.11	2 (6%)	45,47,47	2.02	9 (20%)
42	GTP	KN	501	-	33,34,34	1.23	5 (15%)	50,54,54	2.04	15 (30%)
43	GDP	EB	501	-	29,30,30	1.09	2 (6%)	45,47,47	1.93	8 (17%)
42	GTP	NG	501	-	33,34,34	1.05	2 (6%)	50,54,54	1.64	9 (18%)
43	GDP	SM	502	-	29,30,30	1.12	3 (10%)	45,47,47	1.98	10 (22%)
43	GDP	NN	502	-	29,30,30	1.11	1 (3%)	45,47,47	2.67	14 (31%)
43	GDP	NM	502	-	29,30,30	1.08	2 (6%)	45,47,47	2.02	9 (20%)

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
42	GTP	FE	501	-	-	5/22/38/38	0/3/3/3
42	GTP	NO	501	-	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	LL	501	-	-	6/22/38/38	0/3/3/3
43	GDP	LO	502	-	-	4/16/32/32	0/3/3/3
42	GTP	VQ	501	-	-	9/22/38/38	0/3/3/3
42	GTP	SH	501	-	-	5/22/38/38	0/3/3/3
42	GTP	GE	501	-	-	4/22/38/38	0/3/3/3
43	GDP	FN	502	-	-	2/16/32/32	0/3/3/3
42	GTP	AE	501	-	-	5/22/38/38	0/3/3/3
43	GDP	QL	502	-	-	4/16/32/32	0/3/3/3
43	GDP	WB	501	-	-	4/16/32/32	0/3/3/3
43	GDP	HM	502	-	-	4/16/32/32	0/3/3/3
43	GDP	QM	501	-	-	4/16/32/32	0/3/3/3
43	GDP	WO	502	-	-	4/16/32/32	0/3/3/3
42	GTP	CA	501	-	-	8/22/38/38	0/3/3/3
43	GDP	NL	501	-	-	4/16/32/32	0/3/3/3
42	GTP	DH	501	-	-	7/22/38/38	0/3/3/3
42	GTP	SP	501	-	-	4/22/38/38	0/3/3/3
42	GTP	EF	501	-	-	8/22/38/38	0/3/3/3
42	GTP	KE	501	-	-	8/22/38/38	0/3/3/3
42	GTP	UA	501	-	-	4/22/38/38	0/3/3/3
42	GTP	GA	501	-	-	3/22/38/38	0/3/3/3
42	GTP	IE	501	-	-	7/22/38/38	0/3/3/3
42	GTP	ND	501	-	-	6/22/38/38	0/3/3/3
43	GDP	HB	501	-	-	4/16/32/32	0/3/3/3
43	GDP	HN	501	-	-	5/16/32/32	0/3/3/3
42	GTP	WF	501	-	-	6/22/38/38	0/3/3/3
43	GDP	AB	501	-	-	4/16/32/32	0/3/3/3
42	GTP	CF	501	-	-	8/22/38/38	0/3/3/3
42	GTP	QN	501	-	-	5/22/38/38	0/3/3/3
43	GDP	FB	501	-	-	5/16/32/32	0/3/3/3
42	GTP	ON	501	-	-	6/22/38/38	0/3/3/3
43	GDP	QP	501	-	-	2/16/32/32	0/3/3/3
43	GDP	MP	501	-	-	2/16/32/32	0/3/3/3
43	GDP	TL	502	-	-	4/16/32/32	0/3/3/3
42	GTP	KM	501	-	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	CH	501	-	-	6/22/38/38	0/3/3/3
43	GDP	DM	501	-	-	2/16/32/32	0/3/3/3
42	GTP	NN	501	-	-	5/22/38/38	0/3/3/3
43	GDP	SO	501	-	-	2/16/32/32	0/3/3/3
43	GDP	JM	501	-	-	4/16/32/32	0/3/3/3
42	GTP	EA	501	-	-	5/22/38/38	0/3/3/3
43	GDP	IN	501	-	-	4/16/32/32	0/3/3/3
43	GDP	KN	502	-	-	4/16/32/32	0/3/3/3
43	GDP	SL	502	-	-	2/16/32/32	0/3/3/3
42	GTP	BA	501	-	-	8/22/38/38	0/3/3/3
42	GTP	HB	502	-	-	5/22/38/38	0/3/3/3
43	GDP	JN	501	-	-	4/16/32/32	0/3/3/3
42	GTP	BF	501	-	-	7/22/38/38	0/3/3/3
43	GDP	QO	502	-	-	4/16/32/32	0/3/3/3
42	GTP	PE	501	-	-	6/22/38/38	0/3/3/3
43	GDP	SB	501	-	-	2/16/32/32	0/3/3/3
42	GTP	VN	501	-	-	6/22/38/38	0/3/3/3
43	GDP	TN	502	-	-	3/16/32/32	0/3/3/3
42	GTP	WE	501	-	-	6/22/38/38	0/3/3/3
43	GDP	DN	501	-	-	3/16/32/32	0/3/3/3
43	GDP	GP	502	-	-	4/16/32/32	0/3/3/3
42	GTP	UB	502	-	-	3/22/38/38	0/3/3/3
42	GTP	JB	502	-	-	6/22/38/38	0/3/3/3
43	GDP	KP	501	-	-	3/16/32/32	0/3/3/3
43	GDP	NB	501	-	-	4/16/32/32	0/3/3/3
43	GDP	JB	501	-	-	4/16/32/32	0/3/3/3
42	GTP	IA	501	-	-	4/22/38/38	0/3/3/3
43	GDP	KM	502	-	-	4/16/32/32	0/3/3/3
43	GDP	VO	501	-	-	4/16/32/32	0/3/3/3
42	GTP	BH	501	-	-	8/22/38/38	0/3/3/3
42	GTP	EI	501	-	-	3/22/38/38	0/3/3/3
43	GDP	CL	501	-	-	3/16/32/32	0/3/3/3
42	GTP	IF	501	-	-	6/22/38/38	0/3/3/3
42	GTP	KO	501	-	-	10/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	GP	501	-	-	6/22/38/38	0/3/3/3
42	GTP	LM	501	-	-	2/22/38/38	0/3/3/3
42	GTP	UE	501	-	-	7/22/38/38	0/3/3/3
42	GTP	FI	501	-	-	6/22/38/38	0/3/3/3
43	GDP	OM	502	-	-	4/16/32/32	0/3/3/3
42	GTP	LD	501	-	-	8/22/38/38	0/3/3/3
42	GTP	UI	501	-	-	8/22/38/38	0/3/3/3
43	GDP	TB	501	-	-	3/16/32/32	0/3/3/3
42	GTP	MH	501	-	-	8/22/38/38	0/3/3/3
42	GTP	EH	501	-	-	7/22/38/38	0/3/3/3
42	GTP	CE	501	-	-	8/22/38/38	0/3/3/3
42	GTP	CI	501	-	-	7/22/38/38	0/3/3/3
43	GDP	AP	501	-	-	4/16/32/32	0/3/3/3
43	GDP	BO	501	-	-	4/16/32/32	0/3/3/3
43	GDP	JO	502	-	-	4/16/32/32	0/3/3/3
42	GTP	RN	501	-	-	9/22/38/38	0/3/3/3
43	GDP	IO	501	-	-	4/16/32/32	0/3/3/3
42	GTP	AG	501	-	-	6/22/38/38	0/3/3/3
42	GTP	II	501	-	-	6/22/38/38	0/3/3/3
42	GTP	BI	501	-	-	6/22/38/38	0/3/3/3
43	GDP	RM	501	-	-	2/16/32/32	0/3/3/3
42	GTP	EG	501	-	-	8/22/38/38	0/3/3/3
42	GTP	HA	501	-	-	9/22/38/38	0/3/3/3
43	GDP	MN	502	-	-	4/16/32/32	0/3/3/3
43	GDP	WM	501	-	-	4/16/32/32	0/3/3/3
42	GTP	LB	502	-	-	4/22/38/38	0/3/3/3
42	GTP	HH	501	-	-	4/22/38/38	0/3/3/3
43	GDP	IB	501	-	-	4/16/32/32	0/3/3/3
43	GDP	UO	502	-	-	4/16/32/32	0/3/3/3
43	GDP	VN	502	-	-	4/16/32/32	0/3/3/3
43	GDP	WP	501	-	-	4/16/32/32	0/3/3/3
42	GTP	VA	501	-	-	7/22/38/38	0/3/3/3
42	GTP	JE	501	-	-	6/22/38/38	0/3/3/3
42	GTP	QG	501	-	-	8/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	GDP	CO	501	-	-	3/16/32/32	0/3/3/3
42	GTP	WO	501	-	-	7/22/38/38	0/3/3/3
42	GTP	JF	501	-	-	2/22/38/38	0/3/3/3
42	GTP	JA	501	-	-	4/22/38/38	0/3/3/3
42	GTP	TL	501	-	-	2/22/38/38	0/3/3/3
43	GDP	ML	502	-	-	4/16/32/32	0/3/3/3
43	GDP	VQ	502	-	-	4/16/32/32	0/3/3/3
43	GDP	PM	502	-	-	5/16/32/32	0/3/3/3
43	GDP	CN	501	-	-	3/16/32/32	0/3/3/3
42	GTP	FN	501	-	-	8/22/38/38	0/3/3/3
42	GTP	QL	501	-	-	7/22/38/38	0/3/3/3
42	GTP	NE	501	-	-	6/22/38/38	0/3/3/3
42	GTP	WI	501	-	-	6/22/38/38	0/3/3/3
43	GDP	OP	501	-	-	4/16/32/32	0/3/3/3
42	GTP	IH	501	-	-	7/22/38/38	0/3/3/3
42	GTP	MD	501	-	-	6/22/38/38	0/3/3/3
42	GTP	MB	502	-	-	7/22/38/38	0/3/3/3
42	GTP	QO	501	-	-	2/22/38/38	0/3/3/3
43	GDP	EO	501	-	-	3/16/32/32	0/3/3/3
43	GDP	MM	502	-	-	4/16/32/32	0/3/3/3
42	GTP	UM	501	-	-	2/22/38/38	0/3/3/3
43	GDP	MO	501	-	-	4/16/32/32	0/3/3/3
43	GDP	PP	501	-	-	3/16/32/32	0/3/3/3
43	GDP	EL	502	-	-	4/16/32/32	0/3/3/3
42	GTP	TN	501	-	-	5/22/38/38	0/3/3/3
42	GTP	JD	501	-	-	5/22/38/38	0/3/3/3
43	GDP	CB	501	-	-	2/16/32/32	0/3/3/3
43	GDP	BB	501	-	-	4/16/32/32	0/3/3/3
43	GDP	IQ	501	-	-	4/16/32/32	0/3/3/3
43	GDP	TP	501	-	-	3/16/32/32	0/3/3/3
43	GDP	UB	501	-	-	4/16/32/32	0/3/3/3
43	GDP	PL	501	-	-	4/16/32/32	0/3/3/3
43	GDP	JL	501	-	-	4/16/32/32	0/3/3/3
43	GDP	VP	502	-	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	AA	501	-	-	3/22/38/38	0/3/3/3
43	GDP	DP	501	-	-	2/16/32/32	0/3/3/3
43	GDP	PN	502	-	-	4/16/32/32	0/3/3/3
43	GDP	RB	501	-	-	3/16/32/32	0/3/3/3
42	GTP	DI	501	-	-	6/22/38/38	0/3/3/3
42	GTP	GH	501	-	-	6/22/38/38	0/3/3/3
43	GDP	AN	501	-	-	4/16/32/32	0/3/3/3
43	GDP	DL	501	-	-	4/16/32/32	0/3/3/3
43	GDP	LB	501	-	-	4/16/32/32	0/3/3/3
42	GTP	JO	501	-	-	6/22/38/38	0/3/3/3
42	GTP	HE	501	-	-	5/22/38/38	0/3/3/3
42	GTP	SM	501	-	-	4/22/38/38	0/3/3/3
43	GDP	GO	501	-	-	4/16/32/32	0/3/3/3
42	GTP	EL	501	-	-	5/22/38/38	0/3/3/3
42	GTP	OM	501	-	-	6/22/38/38	0/3/3/3
43	GDP	EP	501	-	-	2/16/32/32	0/3/3/3
43	GDP	NO	502	-	-	4/16/32/32	0/3/3/3
43	GDP	OB	501	-	-	4/16/32/32	0/3/3/3
43	GDP	QB	501	-	-	3/16/32/32	0/3/3/3
42	GTP	GF	501	-	-	7/22/38/38	0/3/3/3
42	GTP	WA	501	-	-	9/22/38/38	0/3/3/3
42	GTP	PM	501	-	-	6/22/38/38	0/3/3/3
43	GDP	LM	502	-	-	3/16/32/32	0/3/3/3
42	GTP	RG	501	-	-	8/22/38/38	0/3/3/3
42	GTP	BG	501	-	-	7/22/38/38	0/3/3/3
43	GDP	KL	501	-	-	4/16/32/32	0/3/3/3
42	GTP	CG	501	-	-	8/22/38/38	0/3/3/3
42	GTP	BL	501	-	-	2/22/38/38	0/3/3/3
43	GDP	VB	501	-	-	3/16/32/32	0/3/3/3
43	GDP	AO	501	-	-	4/16/32/32	0/3/3/3
43	GDP	UM	502	-	-	3/16/32/32	0/3/3/3
42	GTP	OO	501	-	-	6/22/38/38	0/3/3/3
43	GDP	UP	501	-	-	3/16/32/32	0/3/3/3
42	GTP	PO	501	-	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	VB	502	-	-	4/22/38/38	0/3/3/3
42	GTP	MN	501	-	-	5/22/38/38	0/3/3/3
43	GDP	GB	501	-	-	4/16/32/32	0/3/3/3
43	GDP	SP	502	-	-	4/16/32/32	0/3/3/3
43	GDP	SN	502	-	-	3/16/32/32	0/3/3/3
42	GTP	SN	501	-	-	8/22/38/38	0/3/3/3
42	GTP	UO	501	-	-	7/22/38/38	0/3/3/3
43	GDP	LN	501	-	-	4/16/32/32	0/3/3/3
43	GDP	OO	502	-	-	4/16/32/32	0/3/3/3
43	GDP	LP	501	-	-	4/16/32/32	0/3/3/3
43	GDP	RL	501	-	-	4/16/32/32	0/3/3/3
43	GDP	BM	501	-	-	4/16/32/32	0/3/3/3
43	GDP	AL	501	-	-	4/16/32/32	0/3/3/3
42	GTP	OB	502	-	-	8/22/38/38	0/3/3/3
43	GDP	DO	501	-	-	3/16/32/32	0/3/3/3
43	GDP	PB	501	-	-	4/16/32/32	0/3/3/3
43	GDP	HO	501	-	-	4/16/32/32	0/3/3/3
42	GTP	KD	501	-	-	7/22/38/38	0/3/3/3
43	GDP	TM	501	-	-	4/16/32/32	0/3/3/3
42	GTP	FB	502	-	-	6/22/38/38	0/3/3/3
43	GDP	AM	501	-	-	4/16/32/32	0/3/3/3
43	GDP	LL	502	-	-	4/16/32/32	0/3/3/3
43	GDP	IP	501	-	-	4/16/32/32	0/3/3/3
42	GTP	HM	501	-	-	6/22/38/38	0/3/3/3
42	GTP	ML	501	-	-	6/22/38/38	0/3/3/3
43	GDP	KO	502	-	-	2/16/32/32	0/3/3/3
42	GTP	DE	501	-	-	9/22/38/38	0/3/3/3
43	GDP	CP	501	-	-	4/16/32/32	0/3/3/3
42	GTP	WG	501	-	-	8/22/38/38	0/3/3/3
43	GDP	MB	501	-	-	4/16/32/32	0/3/3/3
42	GTP	GB	502	-	-	9/22/38/38	0/3/3/3
42	GTP	LA	501	-	-	4/22/38/38	0/3/3/3
42	GTP	NM	501	-	-	5/22/38/38	0/3/3/3
43	GDP	RP	502	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	PD	501	-	-	3/22/38/38	0/3/3/3
43	GDP	FO	502	-	-	3/16/32/32	0/3/3/3
42	GTP	RF	501	-	-	7/22/38/38	0/3/3/3
43	GDP	DB	501	-	-	3/16/32/32	0/3/3/3
43	GDP	UN	501	-	-	4/16/32/32	0/3/3/3
42	GTP	DG	501	-	-	8/22/38/38	0/3/3/3
43	GDP	CM	501	-	-	2/16/32/32	0/3/3/3
42	GTP	RO	501	-	-	7/22/38/38	0/3/3/3
43	GDP	OL	502	-	-	4/16/32/32	0/3/3/3
43	GDP	GN	501	-	-	3/16/32/32	0/3/3/3
43	GDP	HQ	501	-	-	3/16/32/32	0/3/3/3
43	GDP	IM	501	-	-	4/16/32/32	0/3/3/3
42	GTP	PB	502	-	-	6/22/38/38	0/3/3/3
42	GTP	AF	501	-	-	7/22/38/38	0/3/3/3
43	GDP	QN	502	-	-	4/16/32/32	0/3/3/3
42	GTP	DA	501	-	-	8/22/38/38	0/3/3/3
42	GTP	LO	501	-	-	9/22/38/38	0/3/3/3
42	GTP	VP	501	-	-	3/22/38/38	0/3/3/3
43	GDP	ON	502	-	-	4/16/32/32	0/3/3/3
42	GTP	PN	501	-	-	8/22/38/38	0/3/3/3
43	GDP	BL	502	-	-	3/16/32/32	0/3/3/3
43	GDP	RO	502	-	-	3/16/32/32	0/3/3/3
42	GTP	HP	501	-	-	8/22/38/38	0/3/3/3
42	GTP	VF	501	-	-	10/22/38/38	0/3/3/3
43	GDP	NP	501	-	-	5/16/32/32	0/3/3/3
42	GTP	RE	501	-	-	7/22/38/38	0/3/3/3
42	GTP	RP	501	-	-	4/22/38/38	0/3/3/3
42	GTP	IG	501	-	-	6/22/38/38	0/3/3/3
42	GTP	SL	501	-	-	5/22/38/38	0/3/3/3
42	GTP	TG	501	-	-	6/22/38/38	0/3/3/3
43	GDP	GM	501	-	-	3/16/32/32	0/3/3/3
43	GDP	HP	502	-	-	4/16/32/32	0/3/3/3
42	GTP	TF	501	-	-	6/22/38/38	0/3/3/3
42	GTP	QF	501	-	-	9/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	DF	501	-	-	3/22/38/38	0/3/3/3
42	GTP	MM	501	-	-	7/22/38/38	0/3/3/3
42	GTP	KB	502	-	-	7/22/38/38	0/3/3/3
43	GDP	EM	501	-	-	2/16/32/32	0/3/3/3
42	GTP	OD	501	-	-	8/22/38/38	0/3/3/3
42	GTP	FM	501	-	-	9/22/38/38	0/3/3/3
42	GTP	TH	501	-	-	4/22/38/38	0/3/3/3
43	GDP	BP	501	-	-	4/16/32/32	0/3/3/3
42	GTP	TI	501	-	-	7/22/38/38	0/3/3/3
43	GDP	EN	501	-	-	2/16/32/32	0/3/3/3
43	GDP	KB	501	-	-	3/16/32/32	0/3/3/3
43	GDP	WN	501	-	-	4/16/32/32	0/3/3/3
43	GDP	WQ	501	-	-	4/16/32/32	0/3/3/3
43	GDP	FP	501	-	-	2/16/32/32	0/3/3/3
42	GTP	FO	501	-	-	2/22/38/38	0/3/3/3
43	GDP	TO	501	-	-	3/16/32/32	0/3/3/3
42	GTP	SG	501	-	-	6/22/38/38	0/3/3/3
43	GDP	FM	502	-	-	2/16/32/32	0/3/3/3
42	GTP	AH	501	-	-	4/22/38/38	0/3/3/3
42	GTP	OL	501	-	-	10/22/38/38	0/3/3/3
43	GDP	BN	501	-	-	4/16/32/32	0/3/3/3
43	GDP	RN	502	-	-	2/16/32/32	0/3/3/3
43	GDP	PO	502	-	-	4/16/32/32	0/3/3/3
42	GTP	KN	501	-	-	4/22/38/38	0/3/3/3
43	GDP	EB	501	-	-	3/16/32/32	0/3/3/3
42	GTP	NG	501	-	-	2/22/38/38	0/3/3/3
43	GDP	SM	502	-	-	3/16/32/32	0/3/3/3
43	GDP	NN	502	-	-	3/16/32/32	0/3/3/3
43	GDP	NM	502	-	-	3/16/32/32	0/3/3/3

The worst 5 of 682 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	JA	501	GTP	PB-O3B	4.67	1.64	1.59
42	KO	501	GTP	C2-N3	4.35	1.43	1.33
42	EG	501	GTP	PB-O3B	4.25	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	DH	501	GTP	C2-N3	4.17	1.43	1.33
42	QL	501	GTP	C2-N3	4.16	1.43	1.33

The worst 5 of 2670 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	RP	502	GDP	C5-C4-N3	-11.54	110.03	128.39
43	JL	501	GDP	C5-C4-N3	-10.35	111.92	128.39
43	TP	501	GDP	C5-C4-N3	-10.02	112.45	128.39
43	TL	502	GDP	C5-C4-N3	-9.93	112.59	128.39
43	SN	502	GDP	C5-C4-N3	-9.91	112.62	128.39

There are no chirality outliers.

5 of 1290 torsion outliers are listed below:

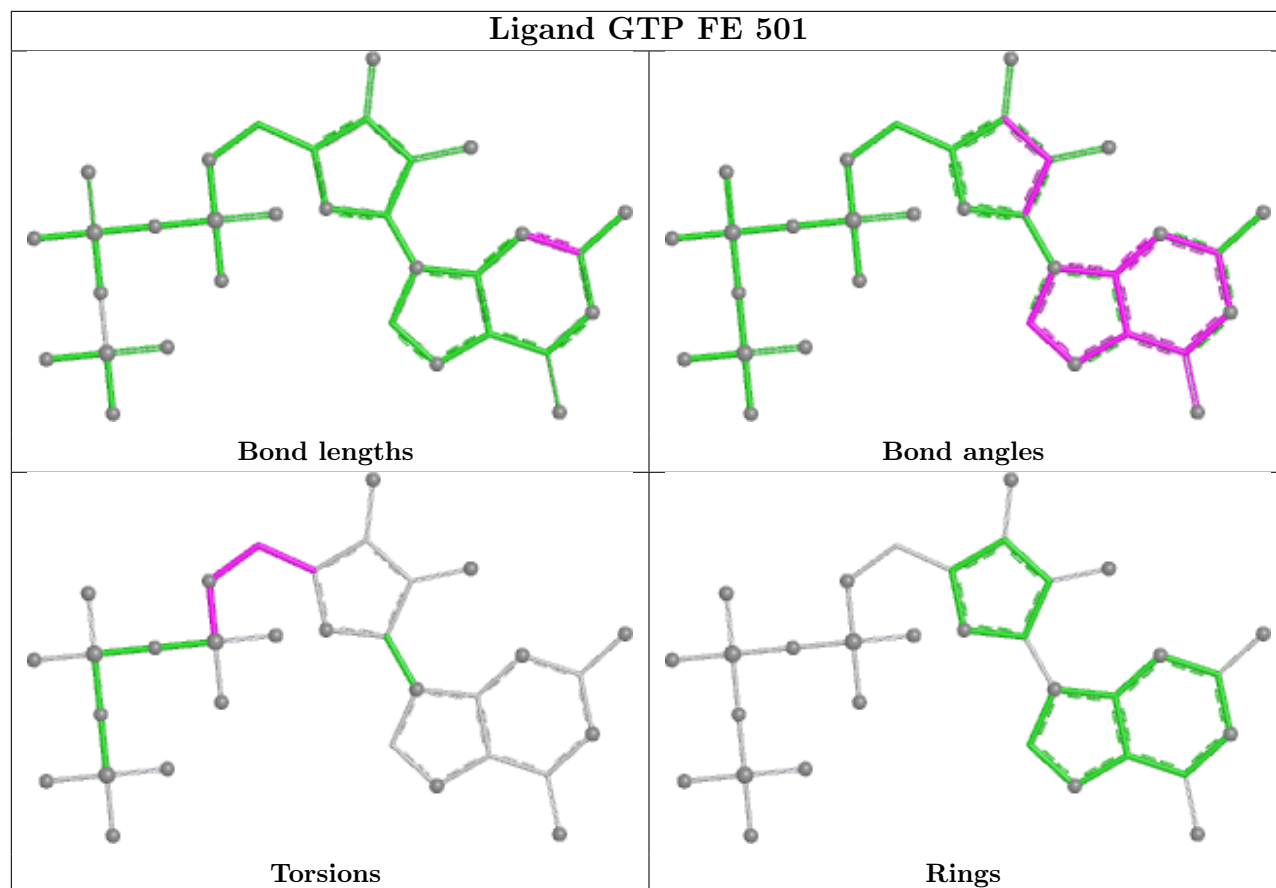
Mol	Chain	Res	Type	Atoms
42	AA	501	GTP	O4'-C4'-C5'-O5'
42	AE	501	GTP	C5'-O5'-PA-O3A
42	AE	501	GTP	C5'-O5'-PA-O1A
42	AE	501	GTP	C5'-O5'-PA-O2A
42	AF	501	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

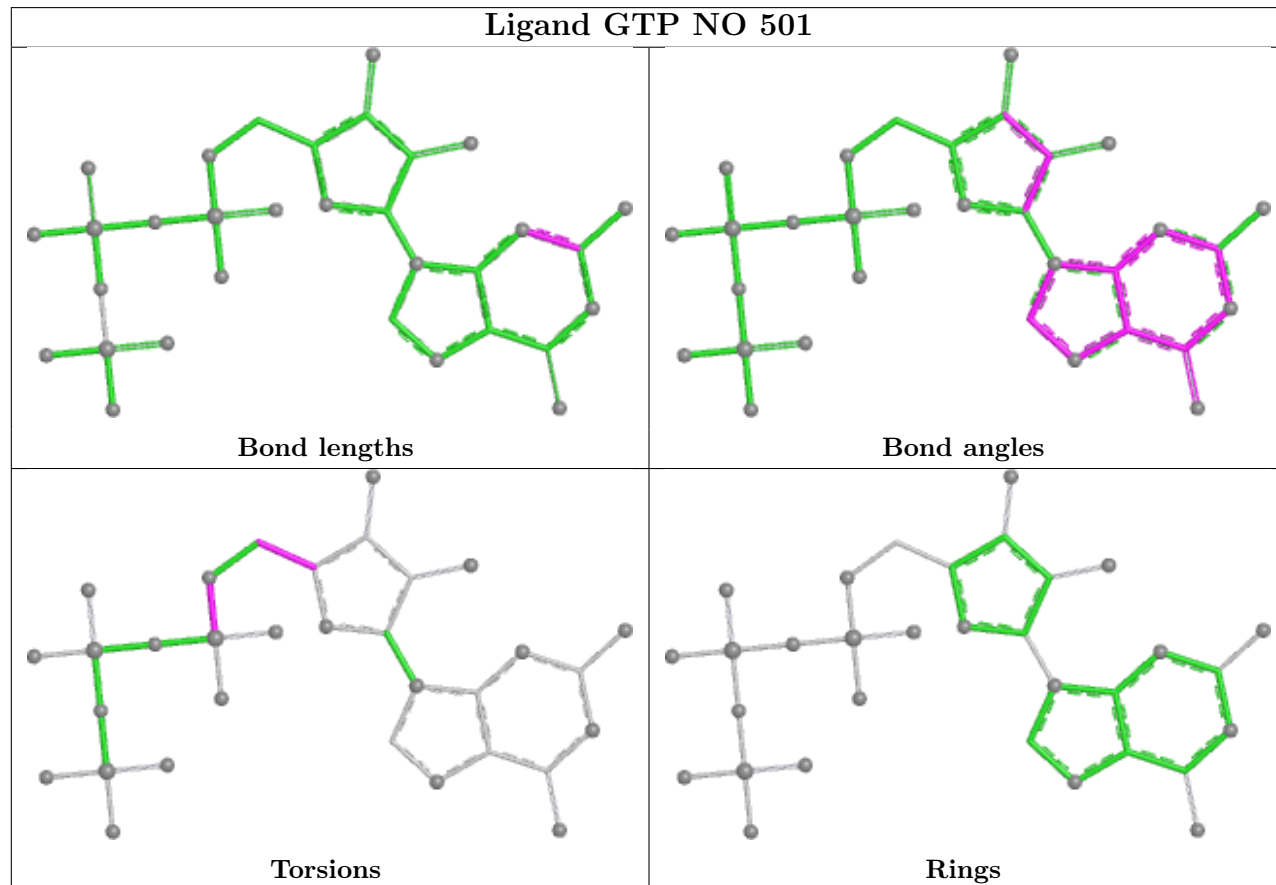
No monomer is involved in short contacts.

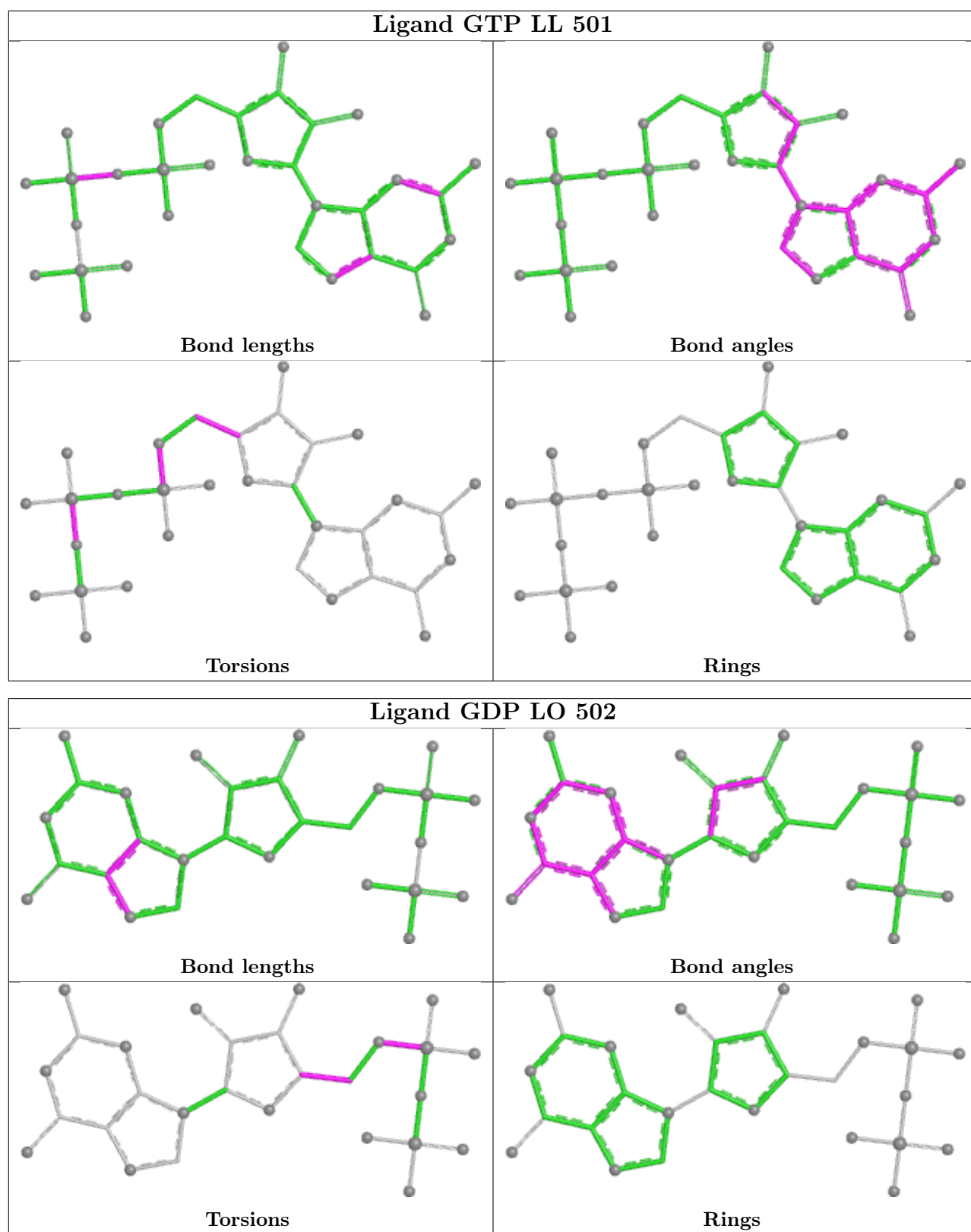
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP FE 501

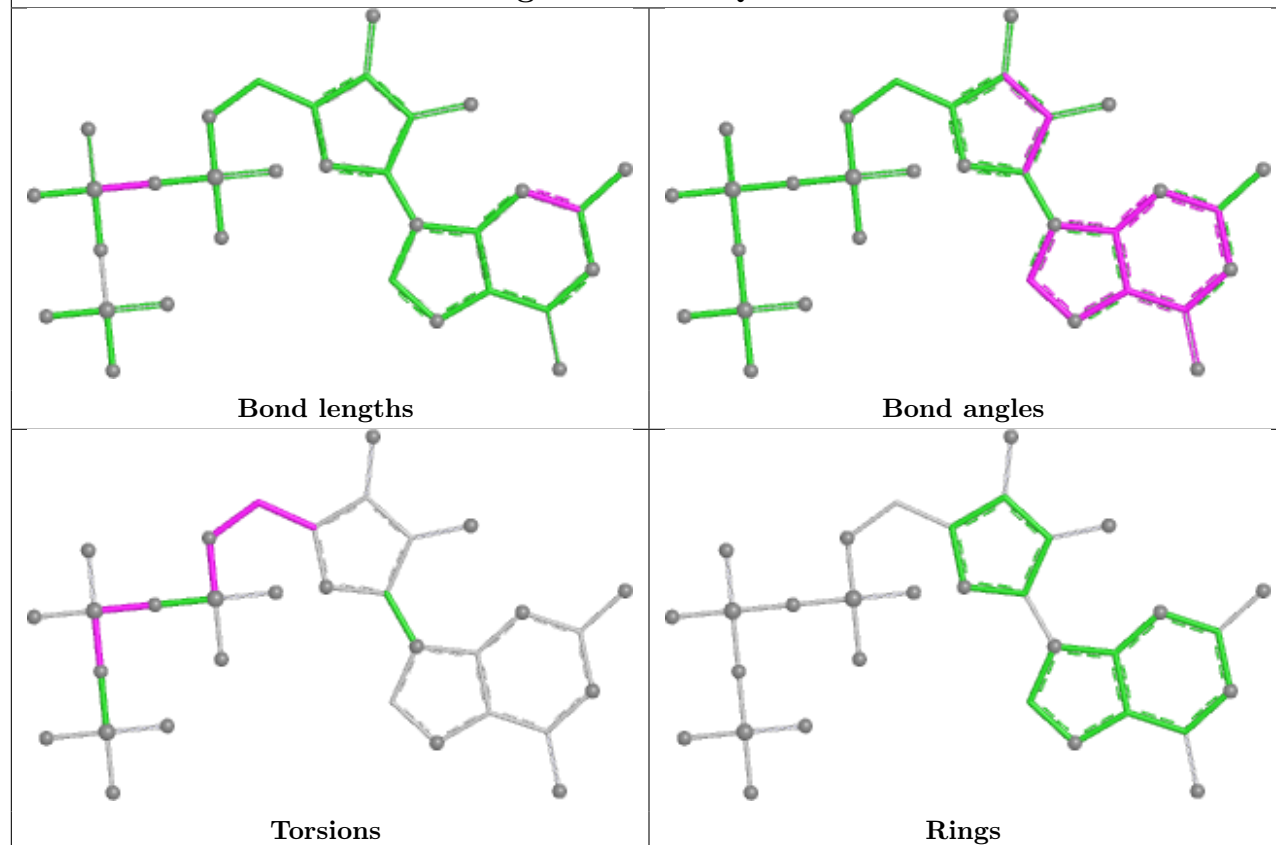


Ligand GTP NO 501

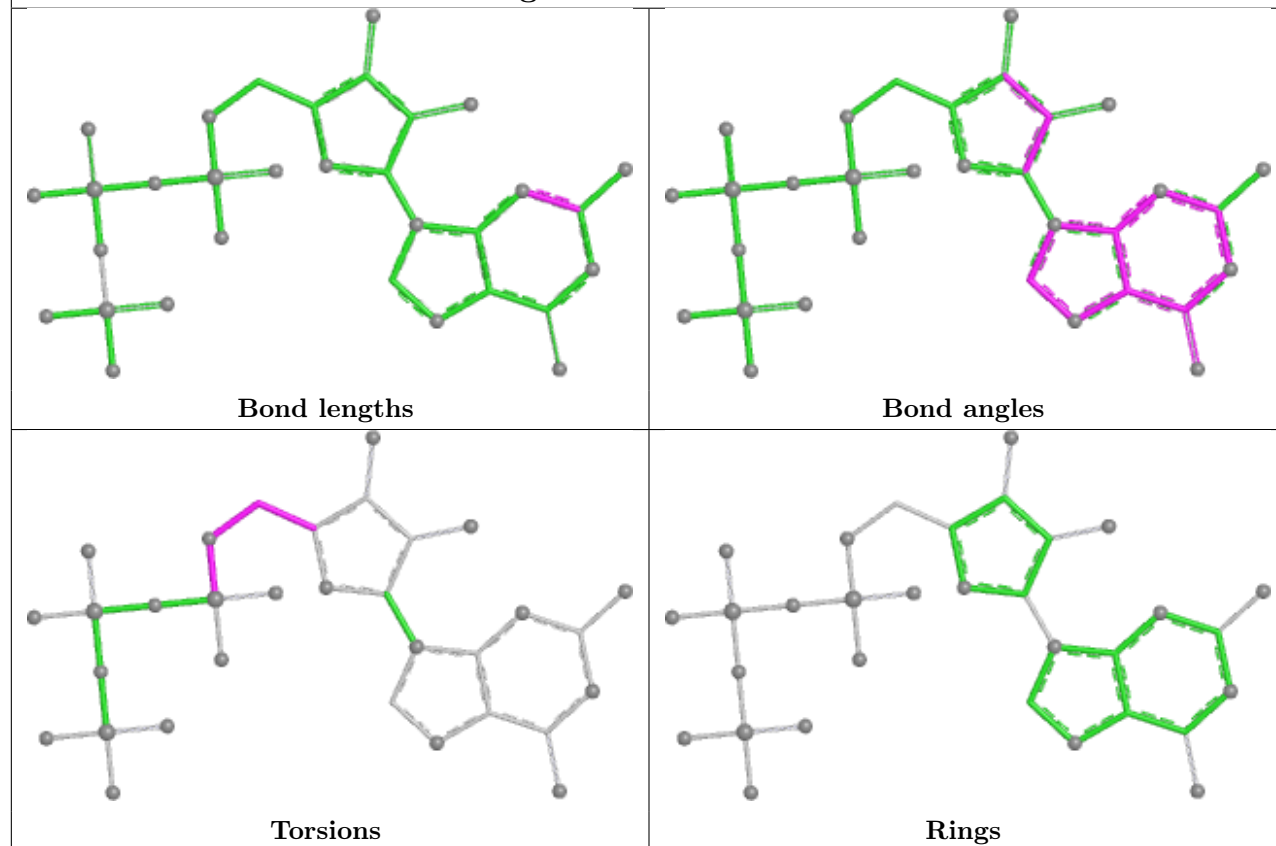


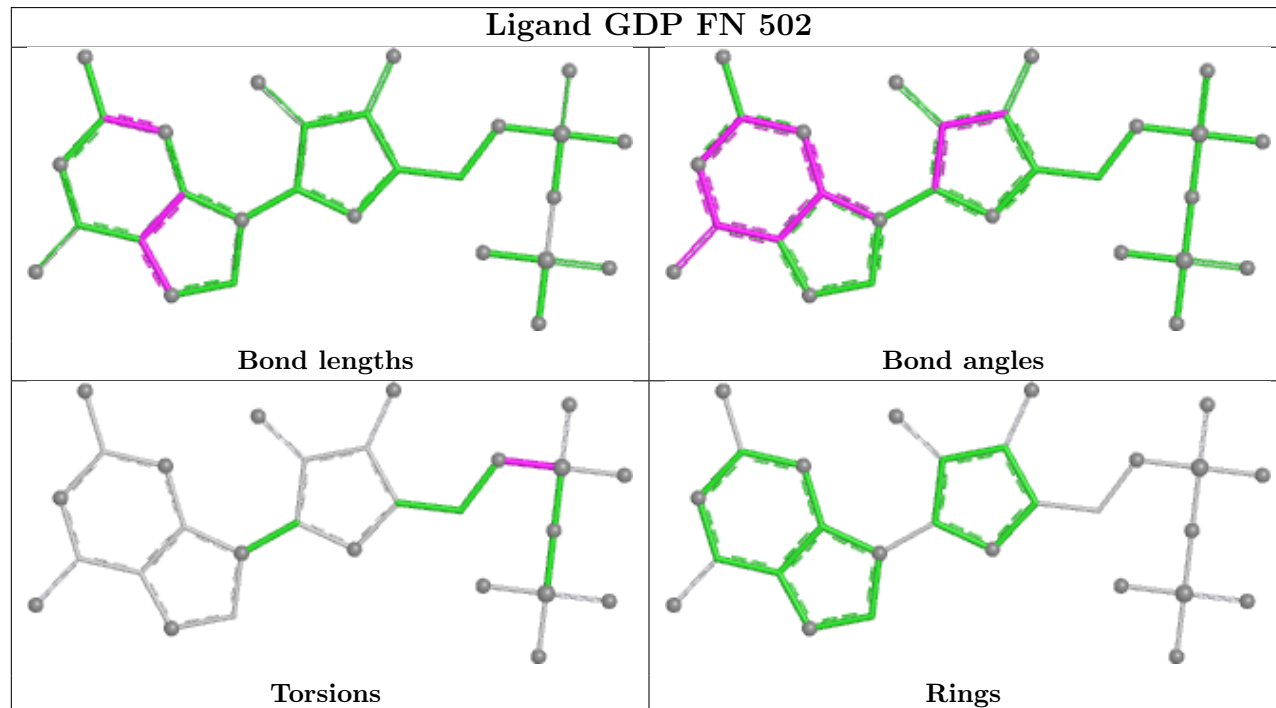
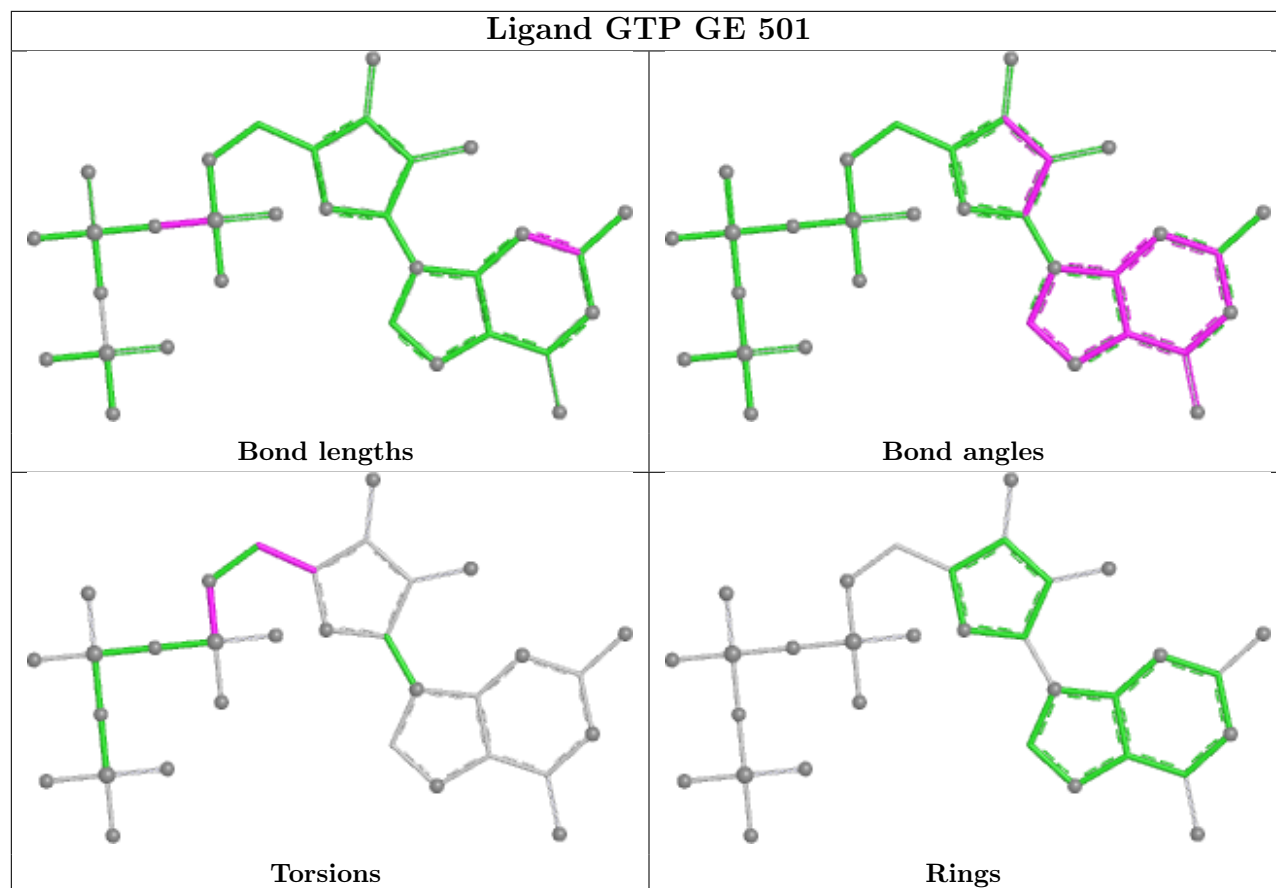


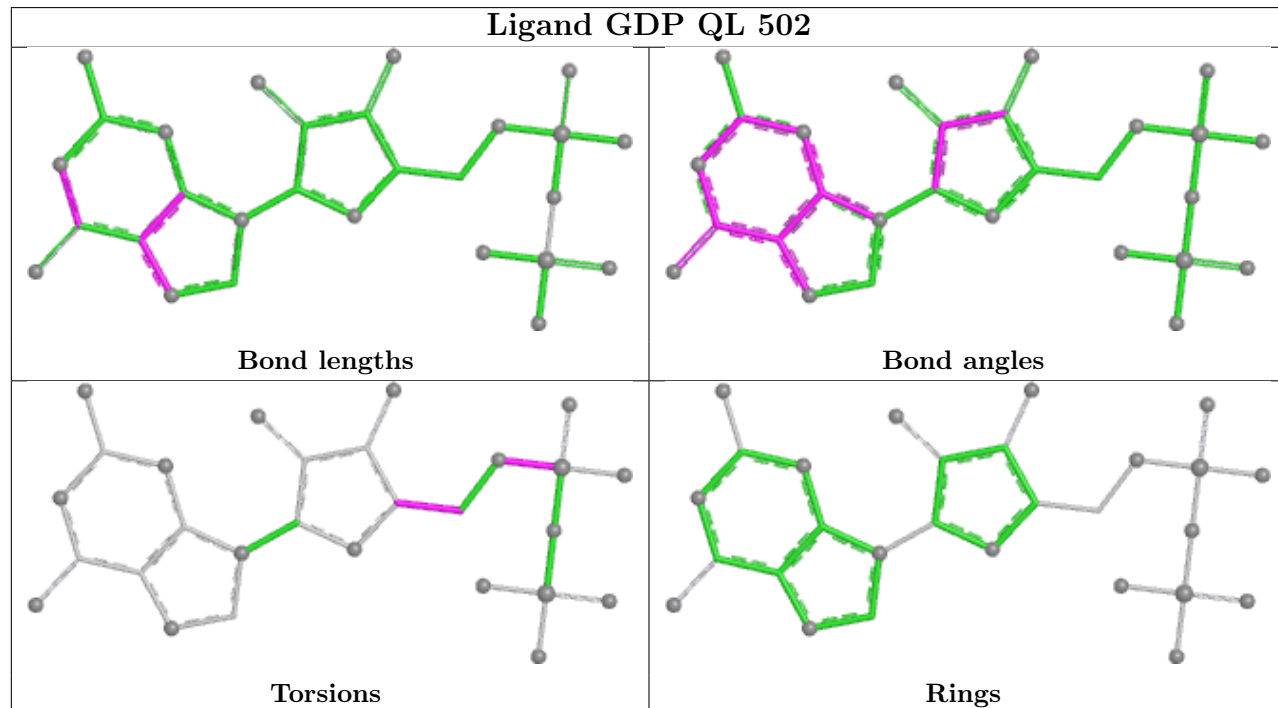
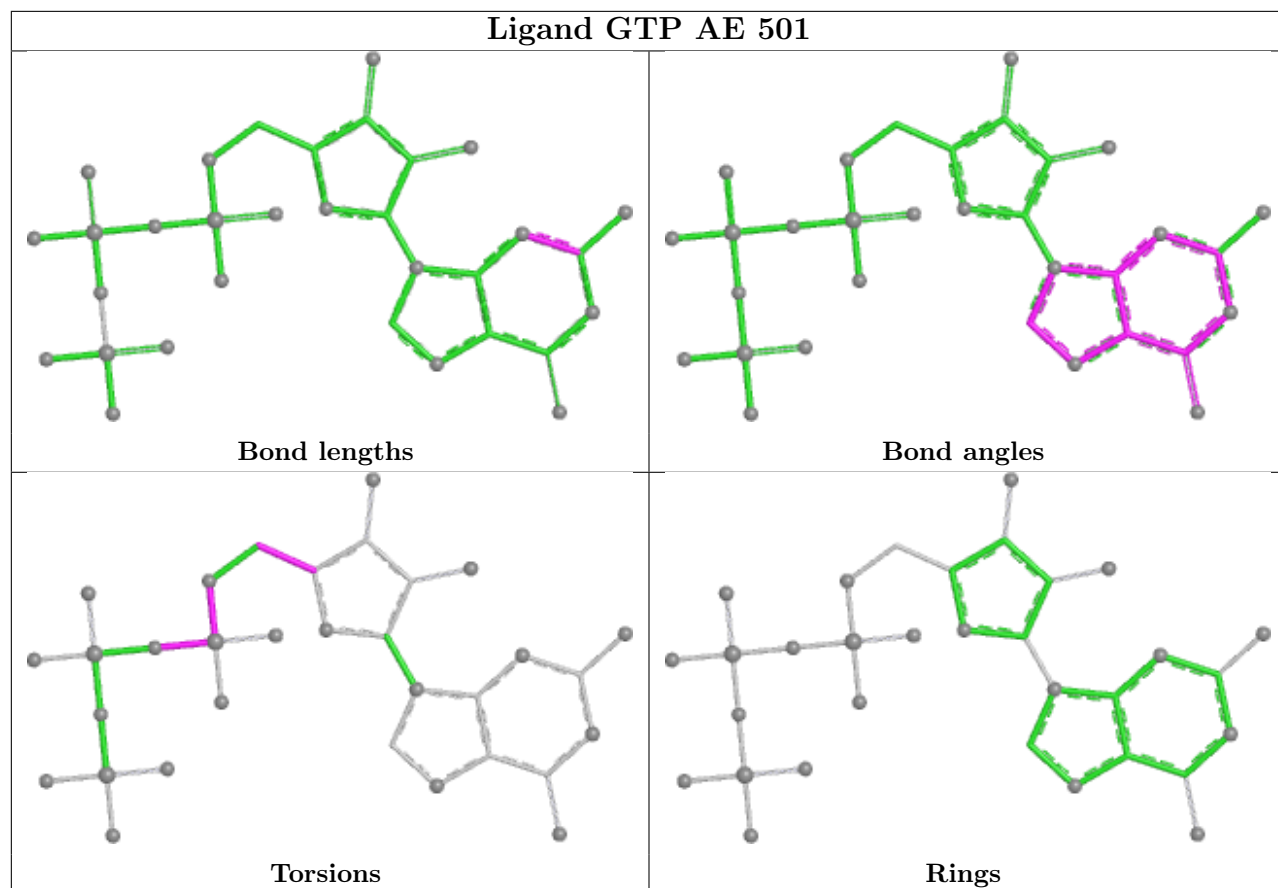
Ligand GTP VQ 501

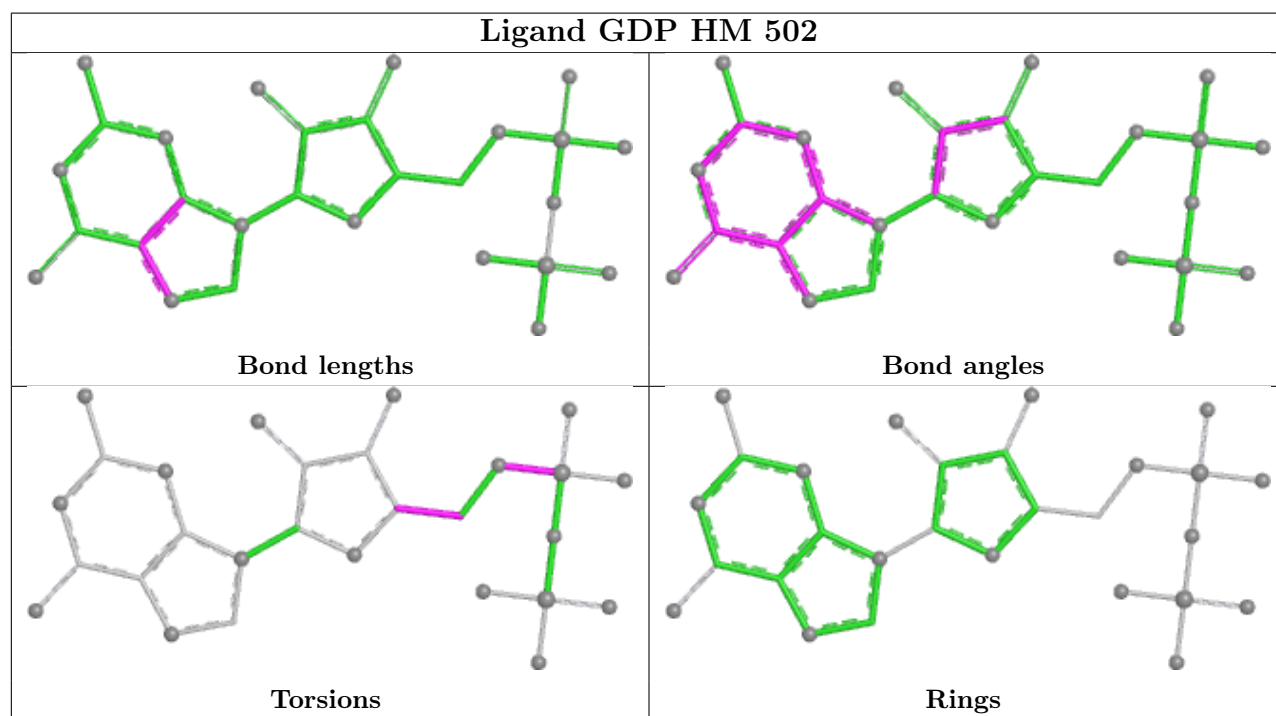
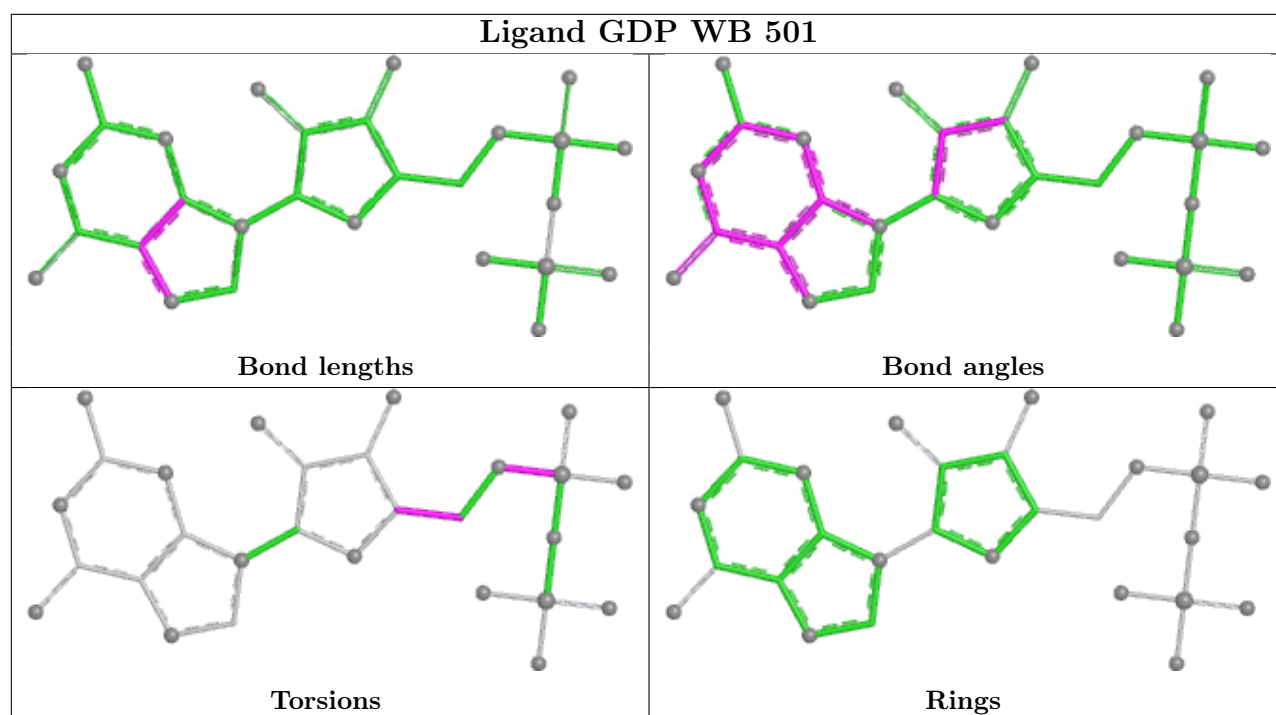


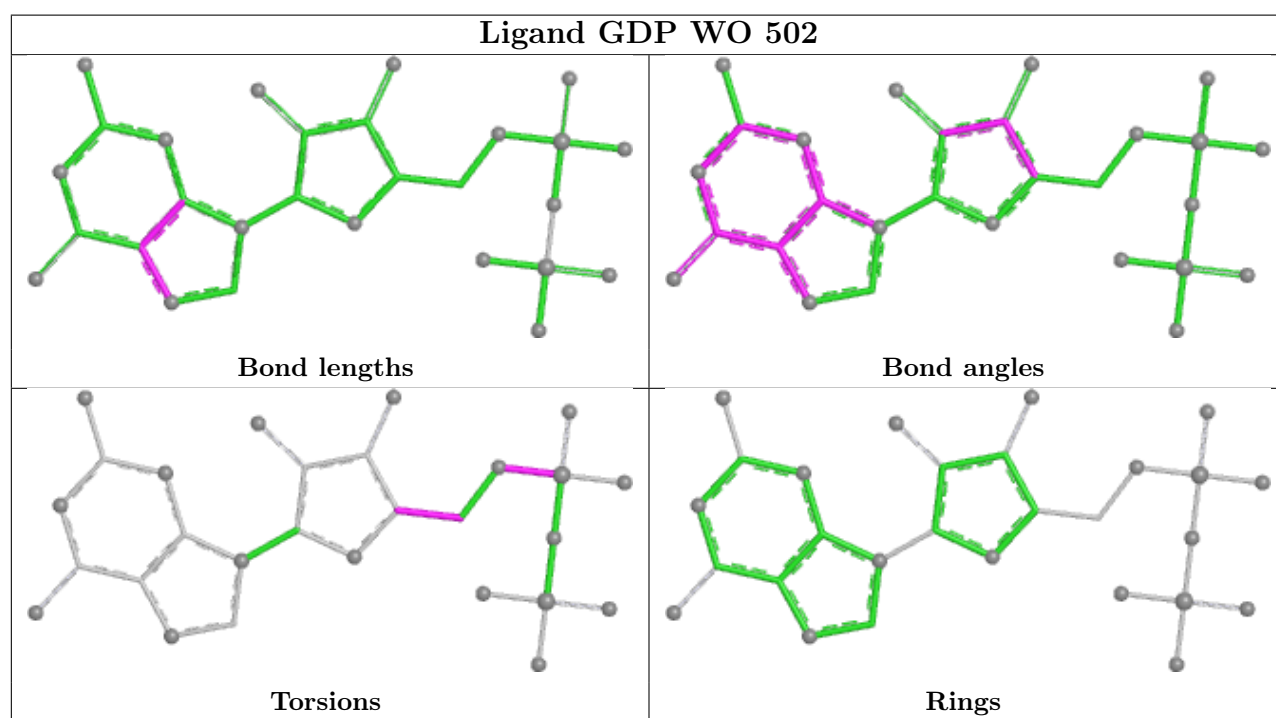
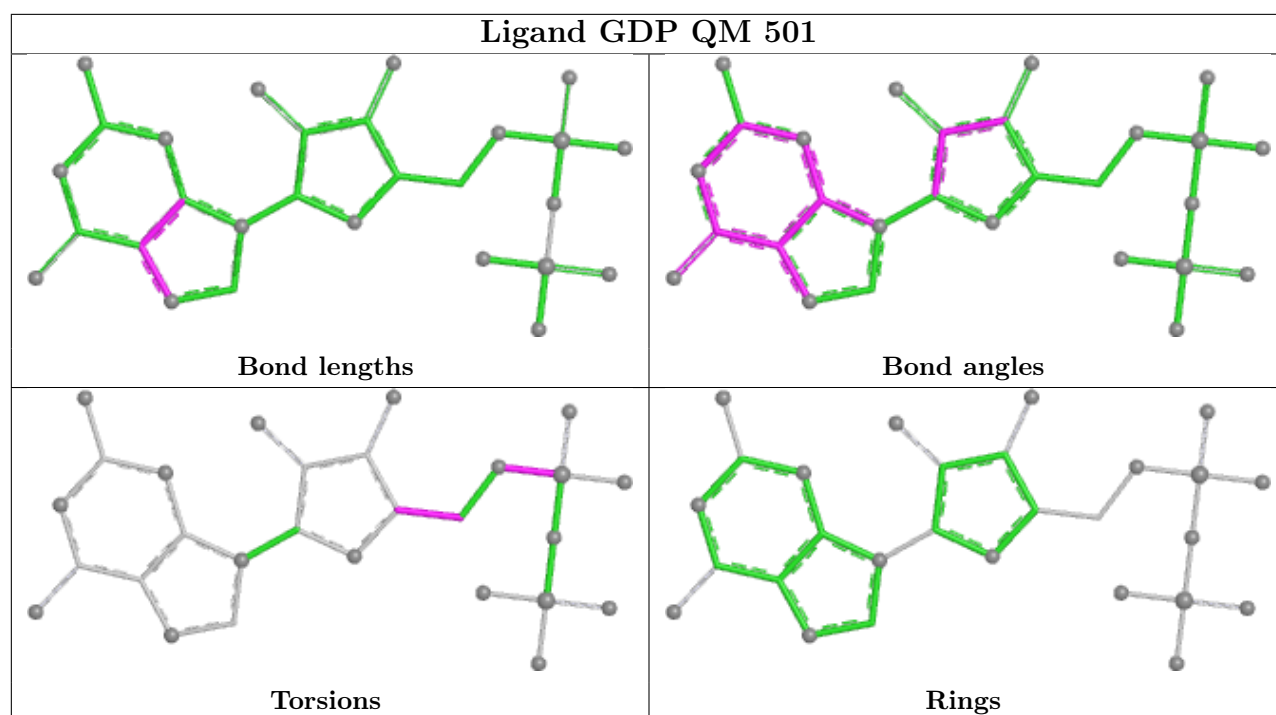
Ligand GTP SH 501

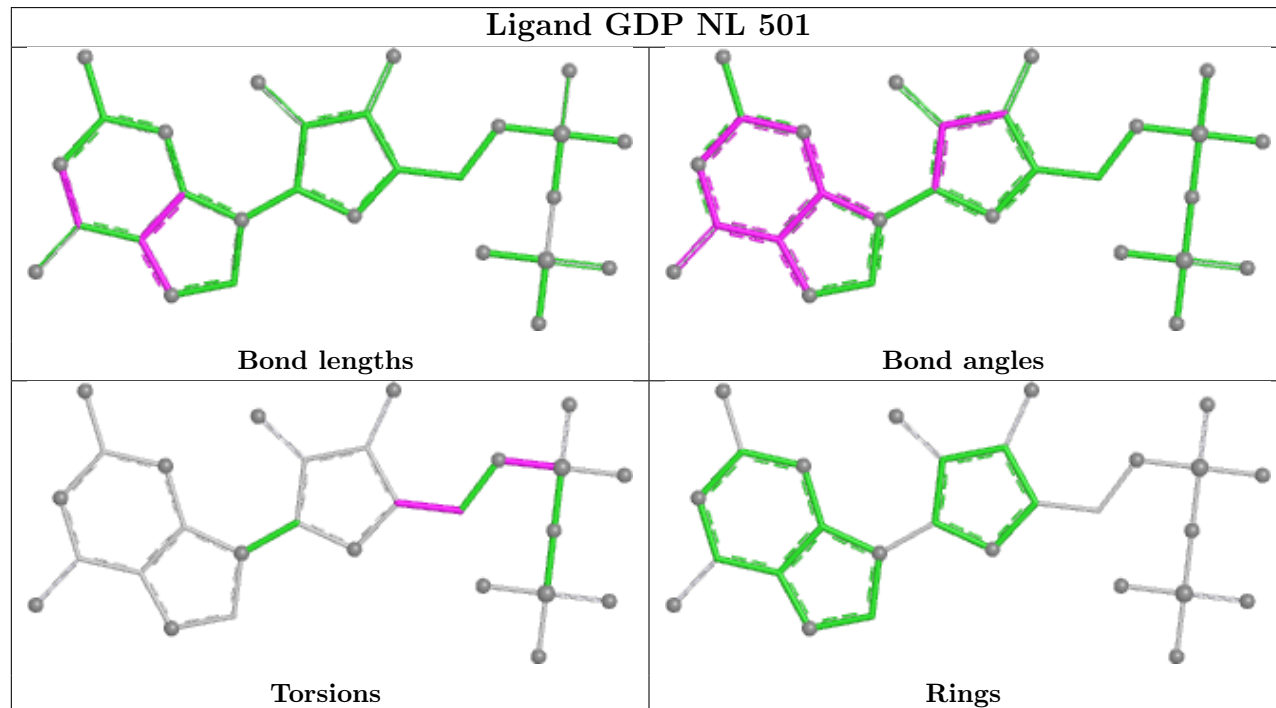
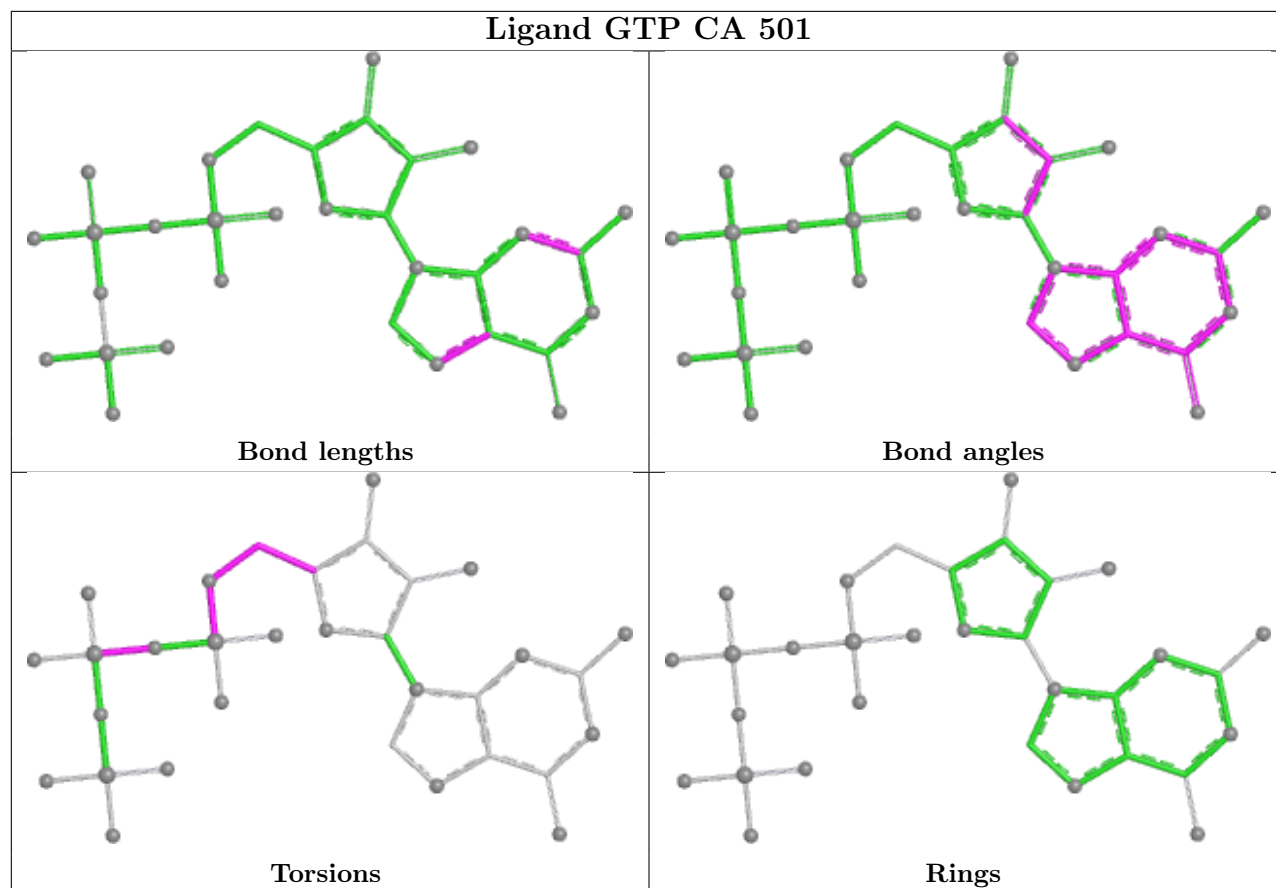




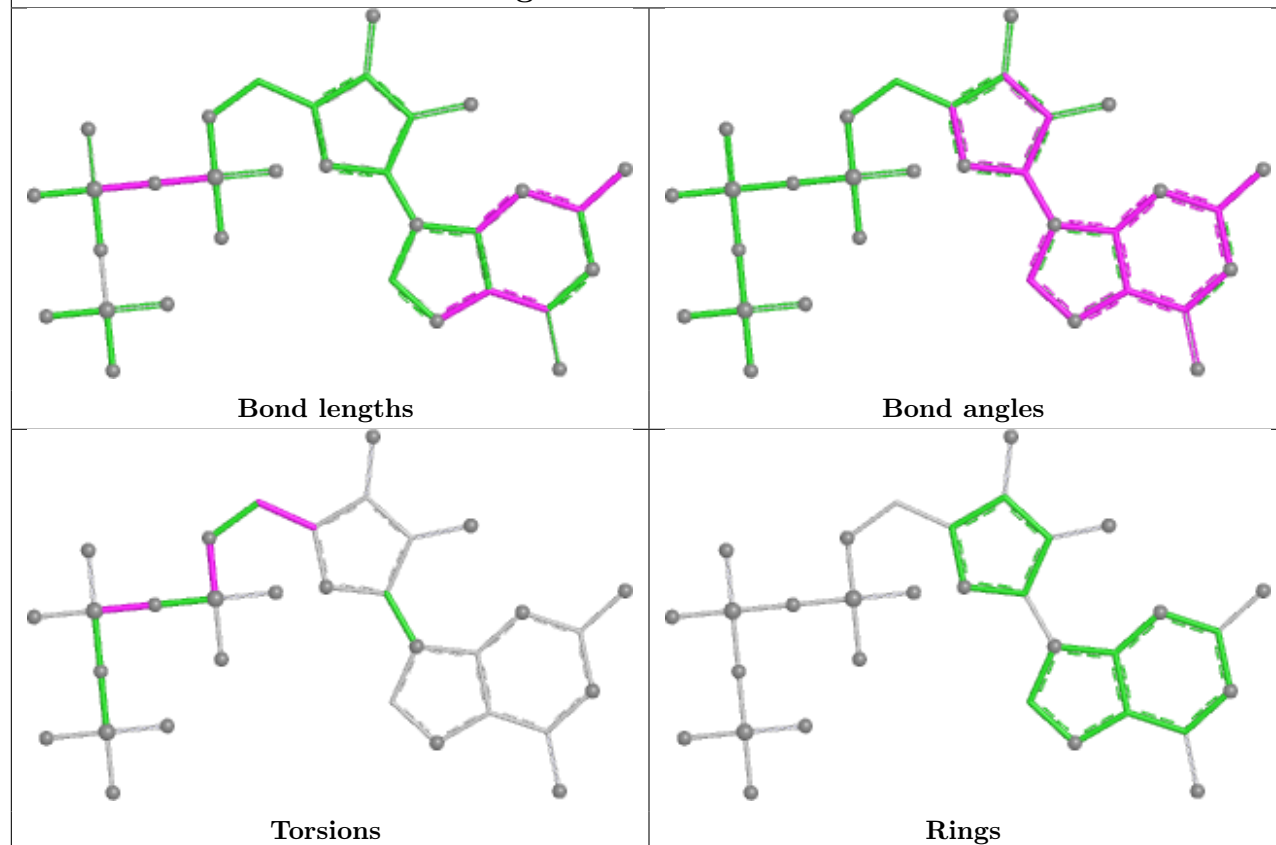




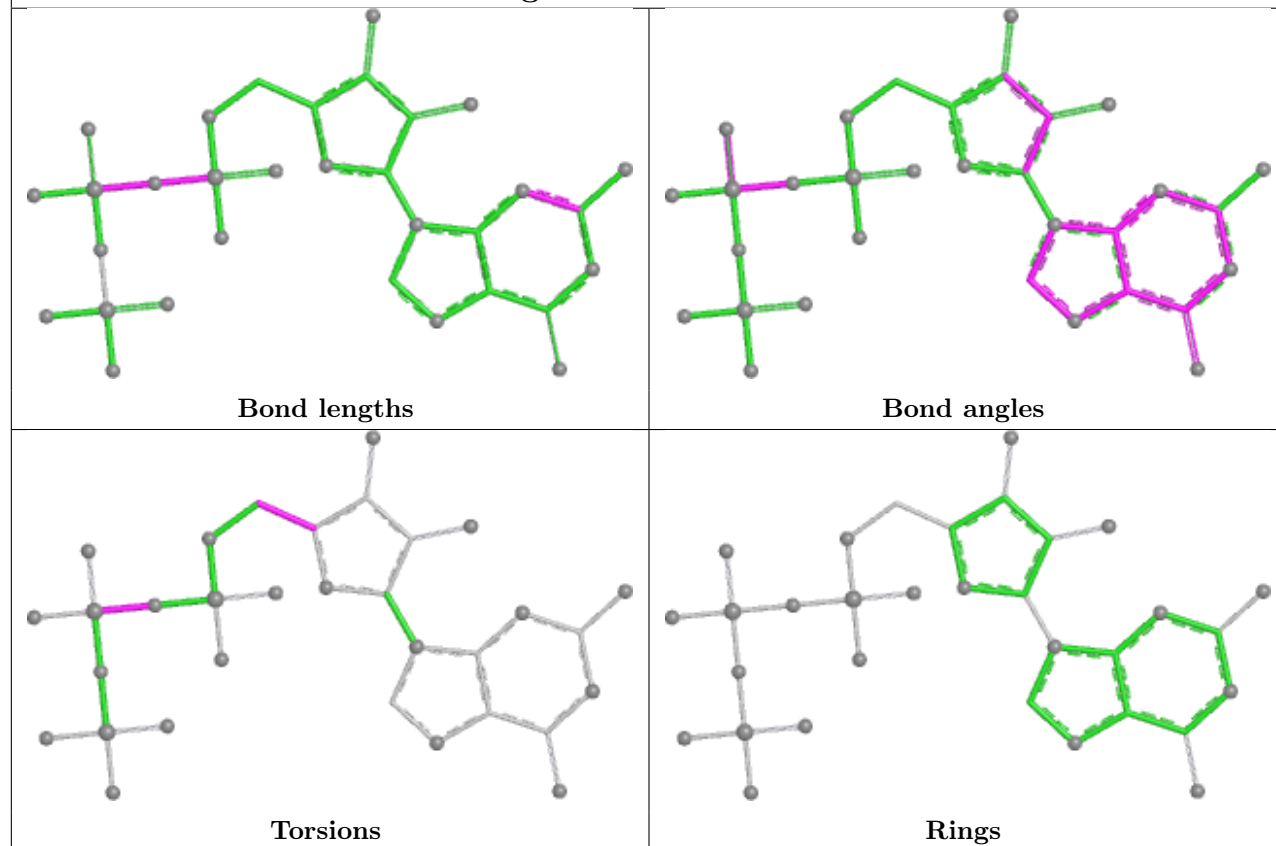




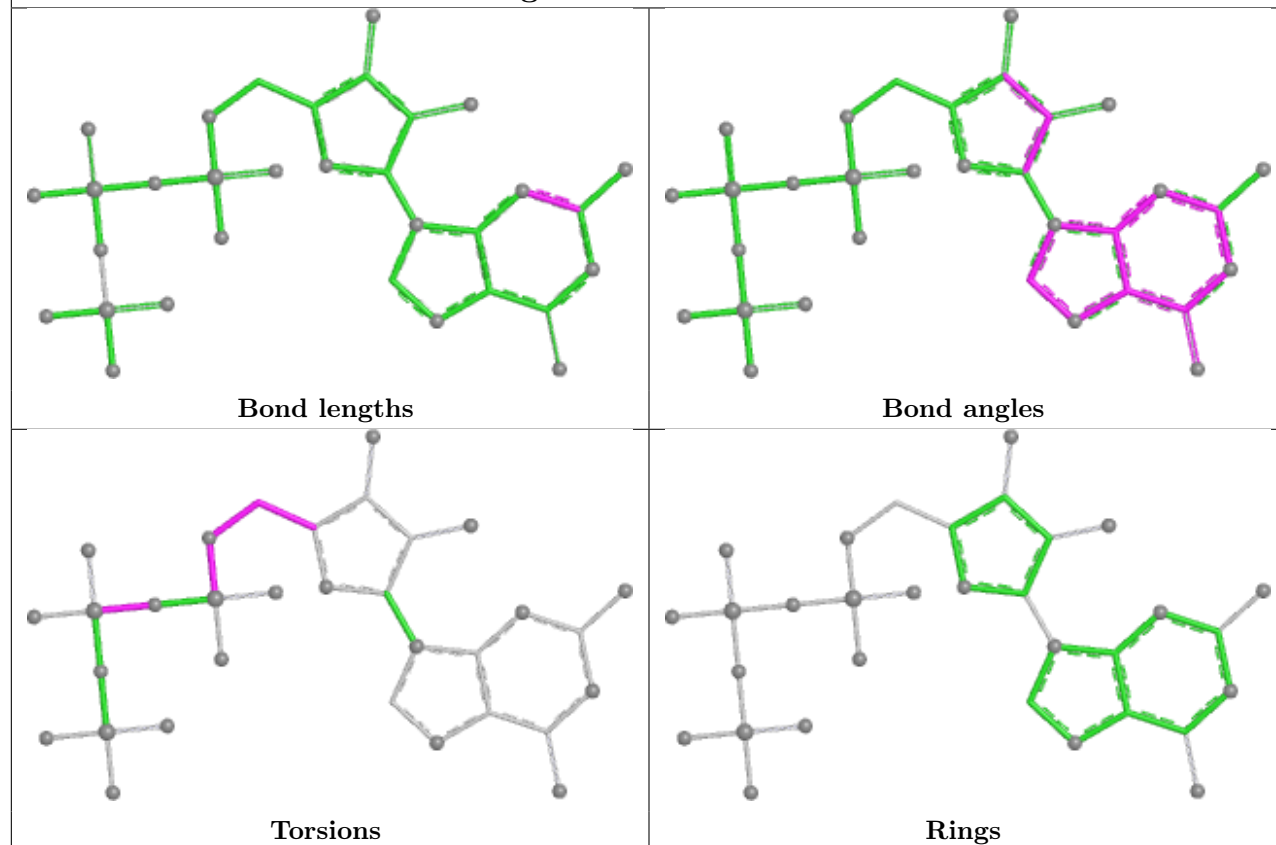
Ligand GTP DH 501



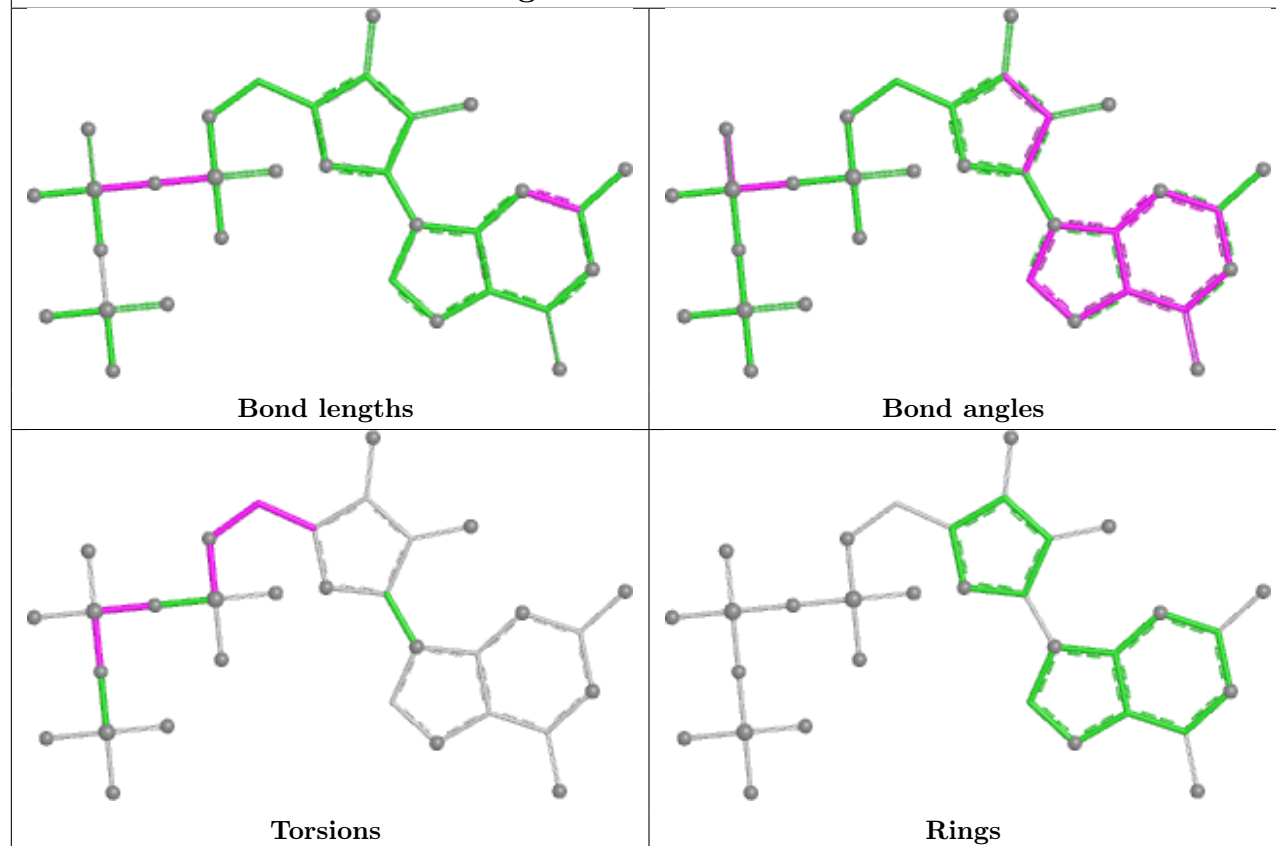
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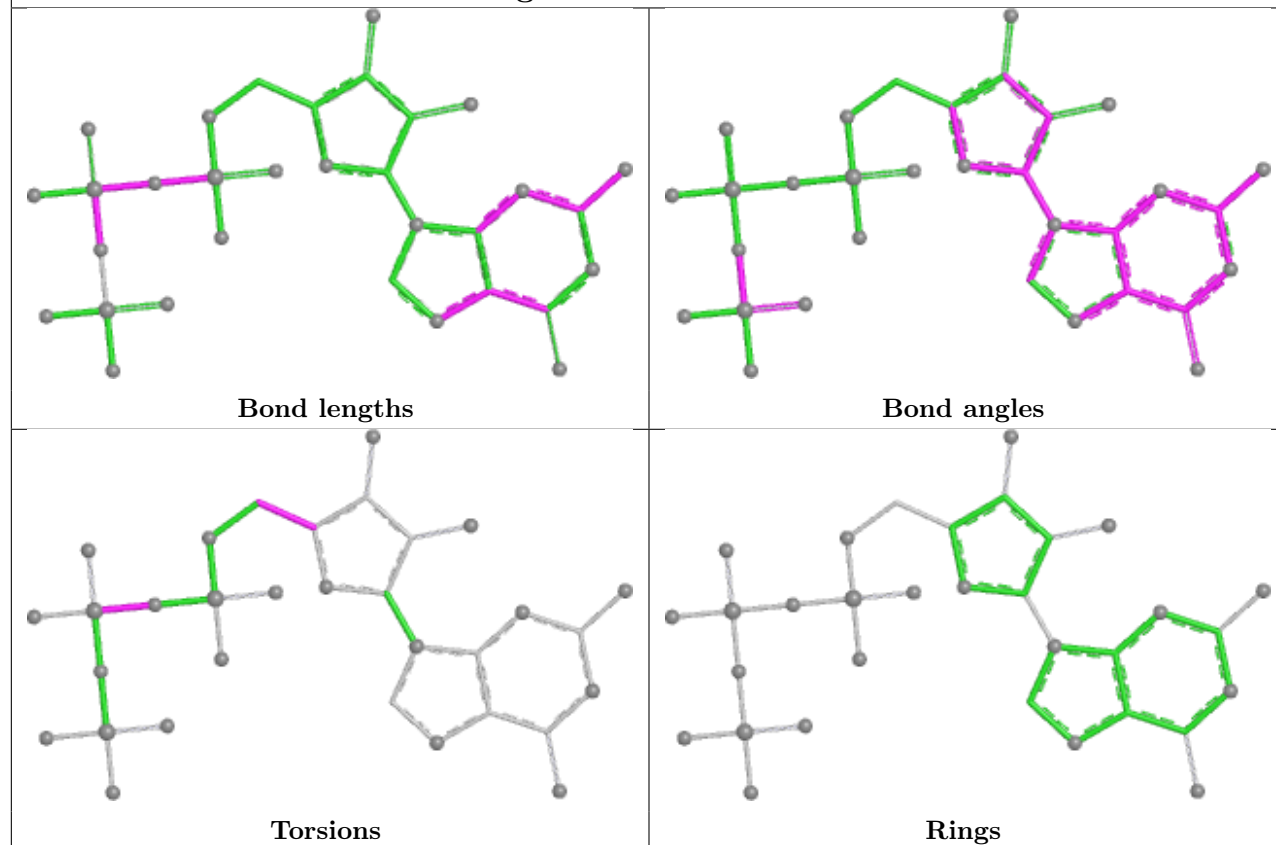
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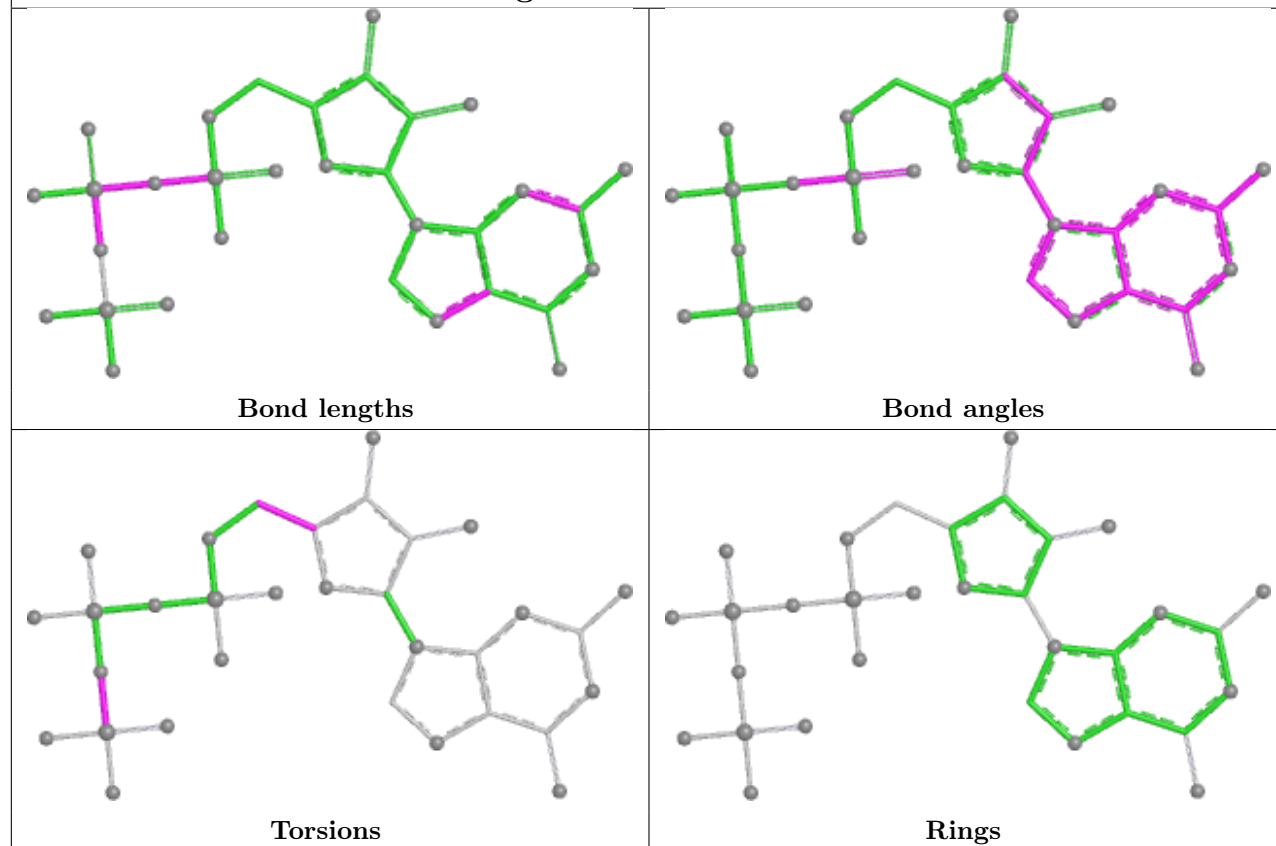
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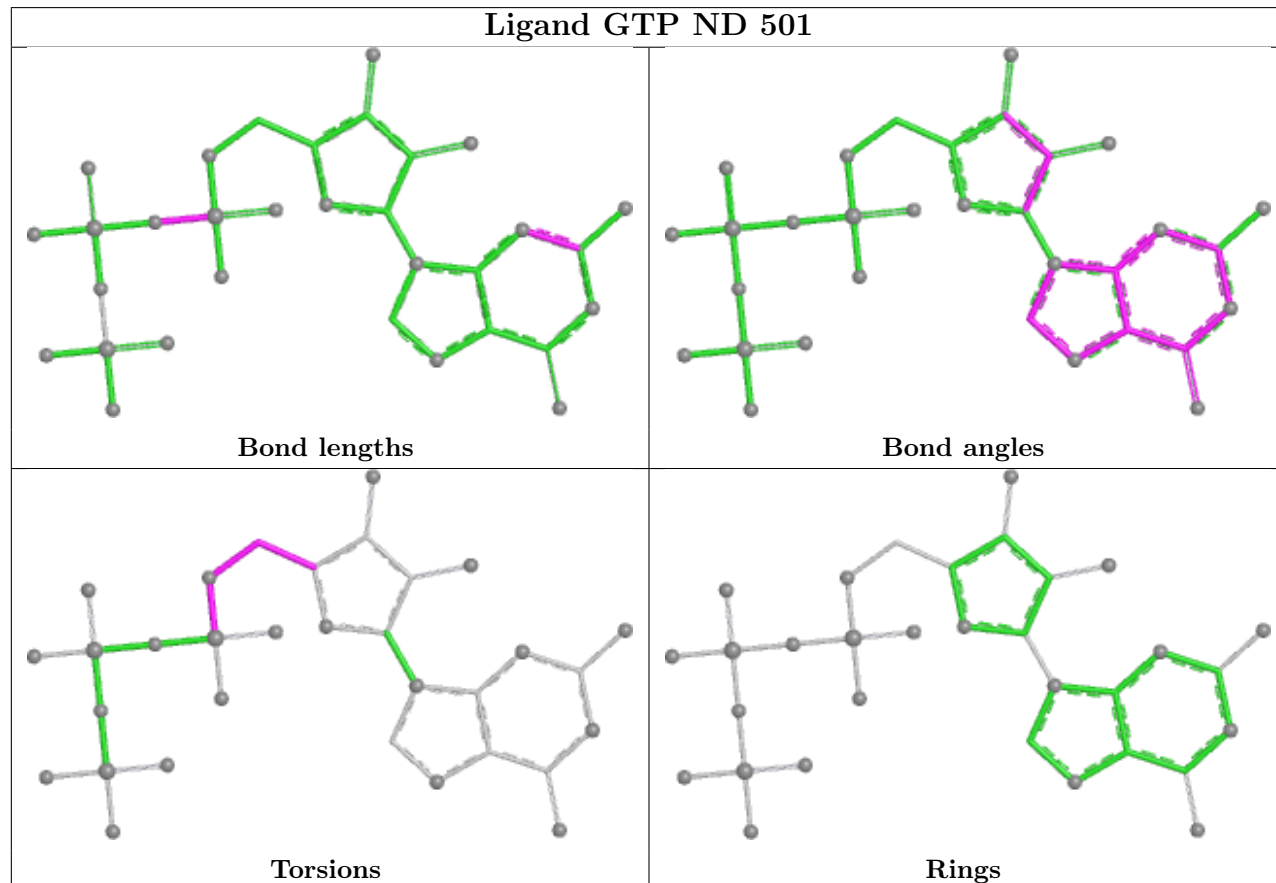
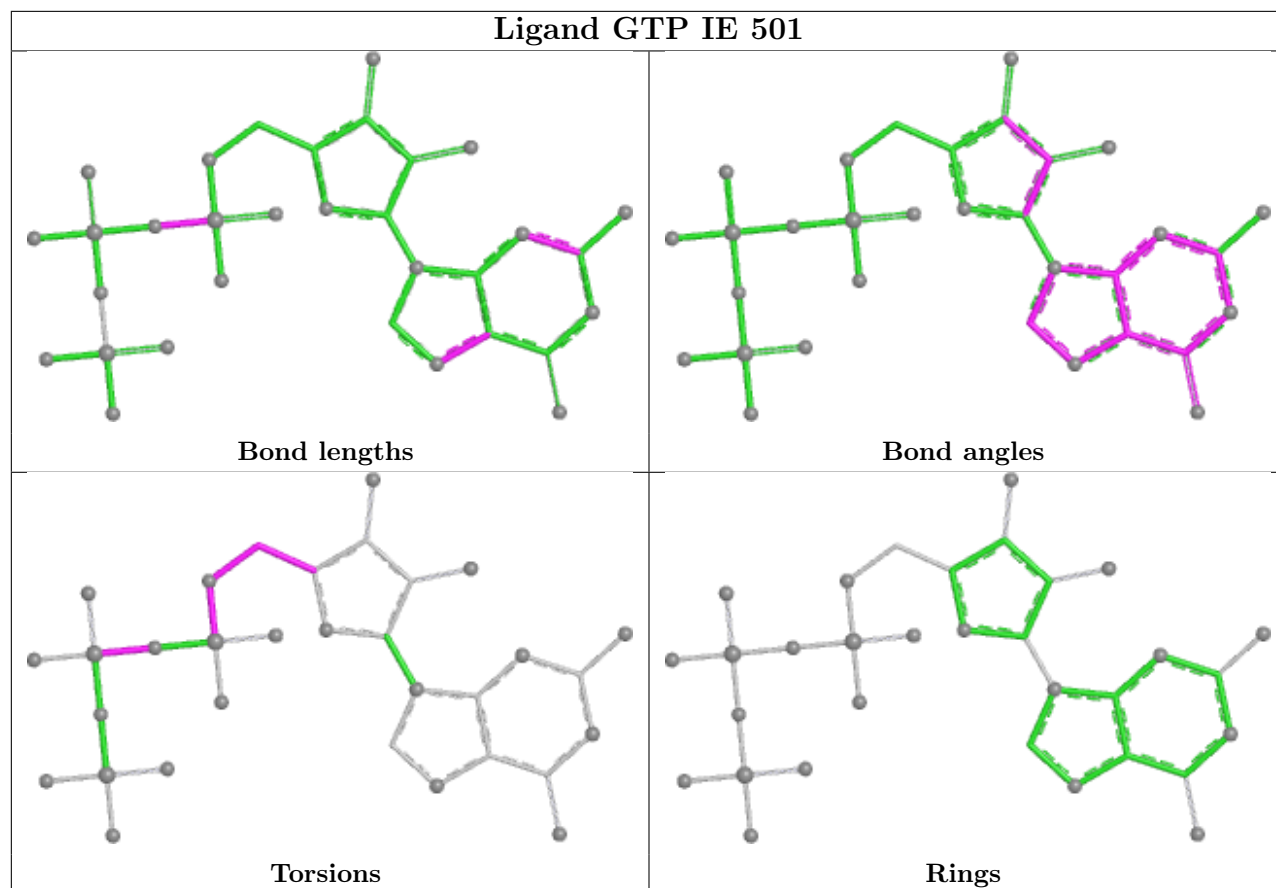


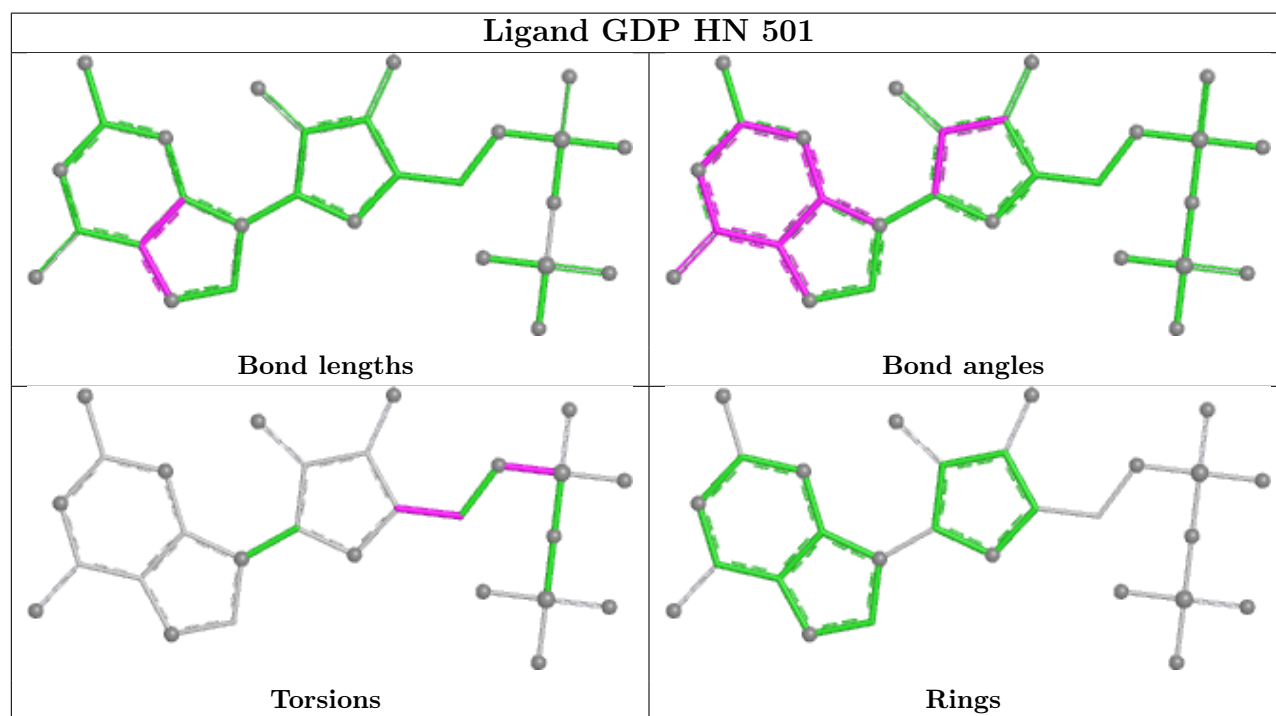
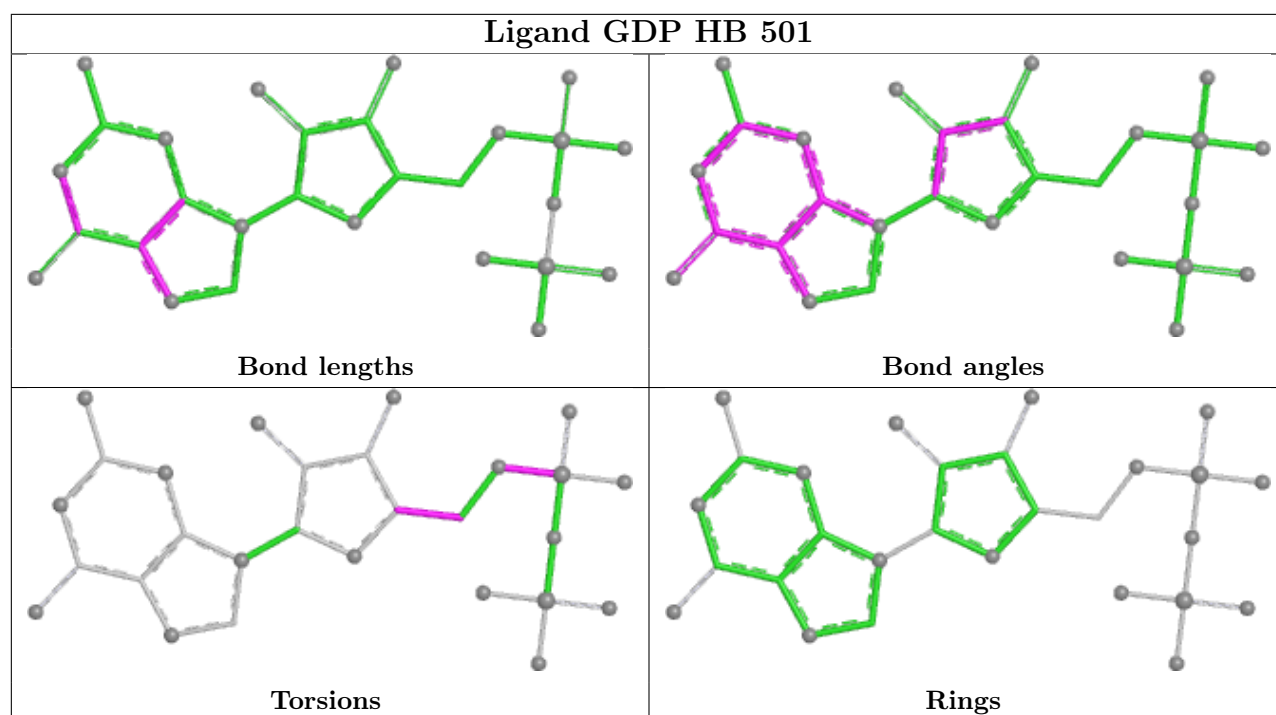
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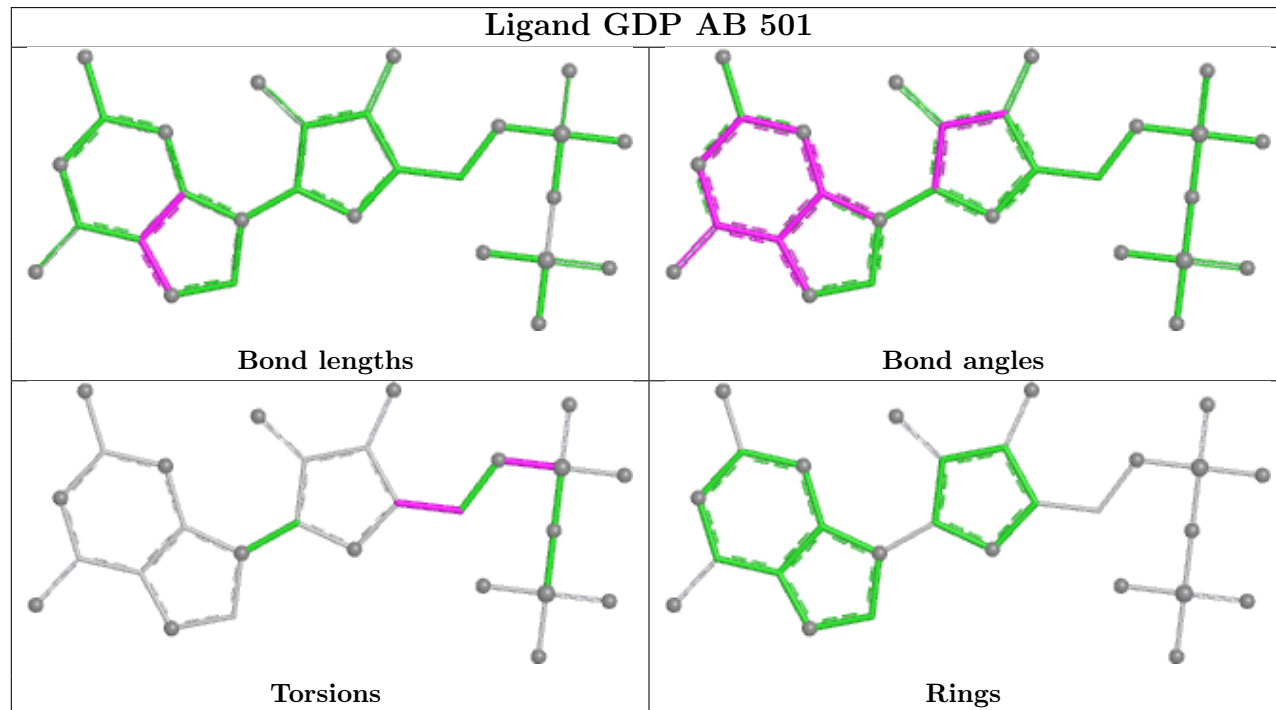
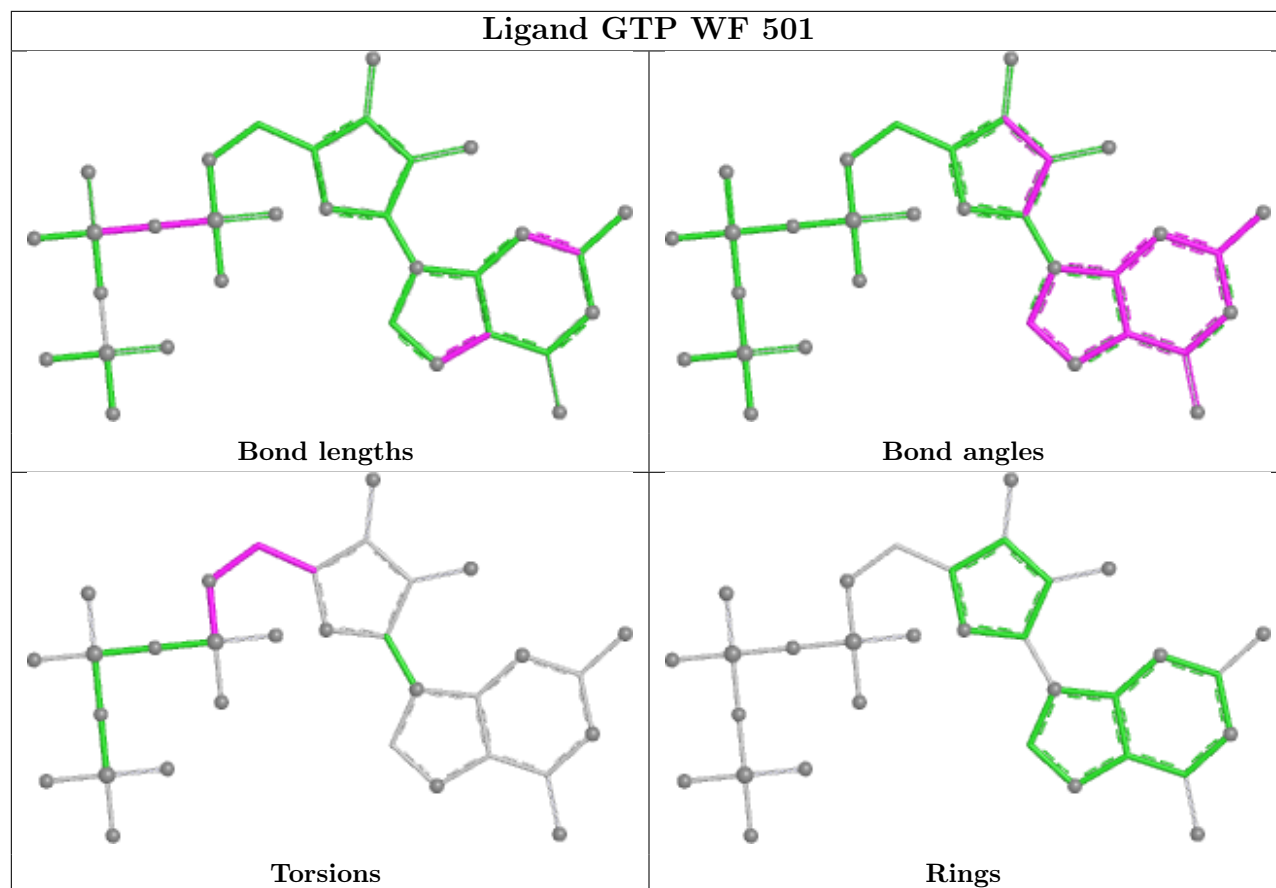


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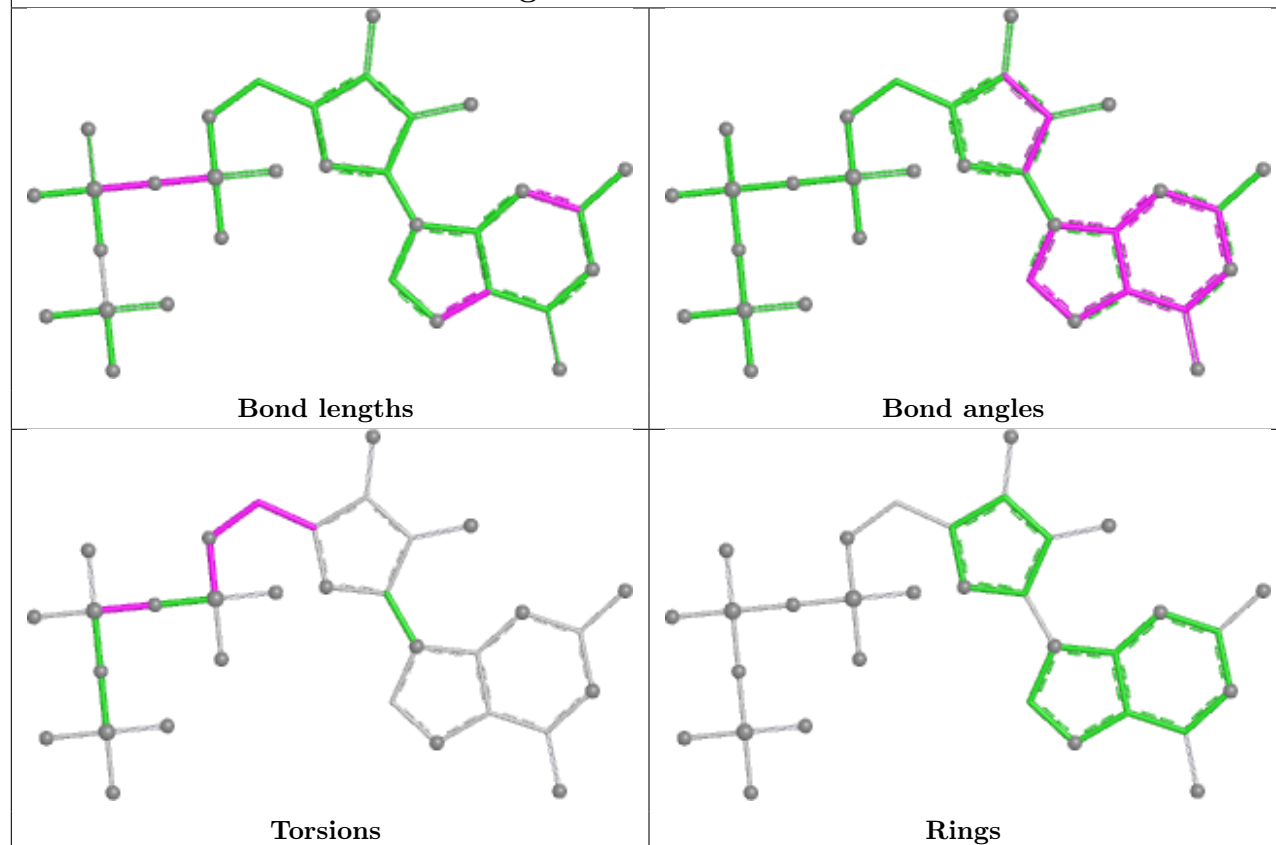




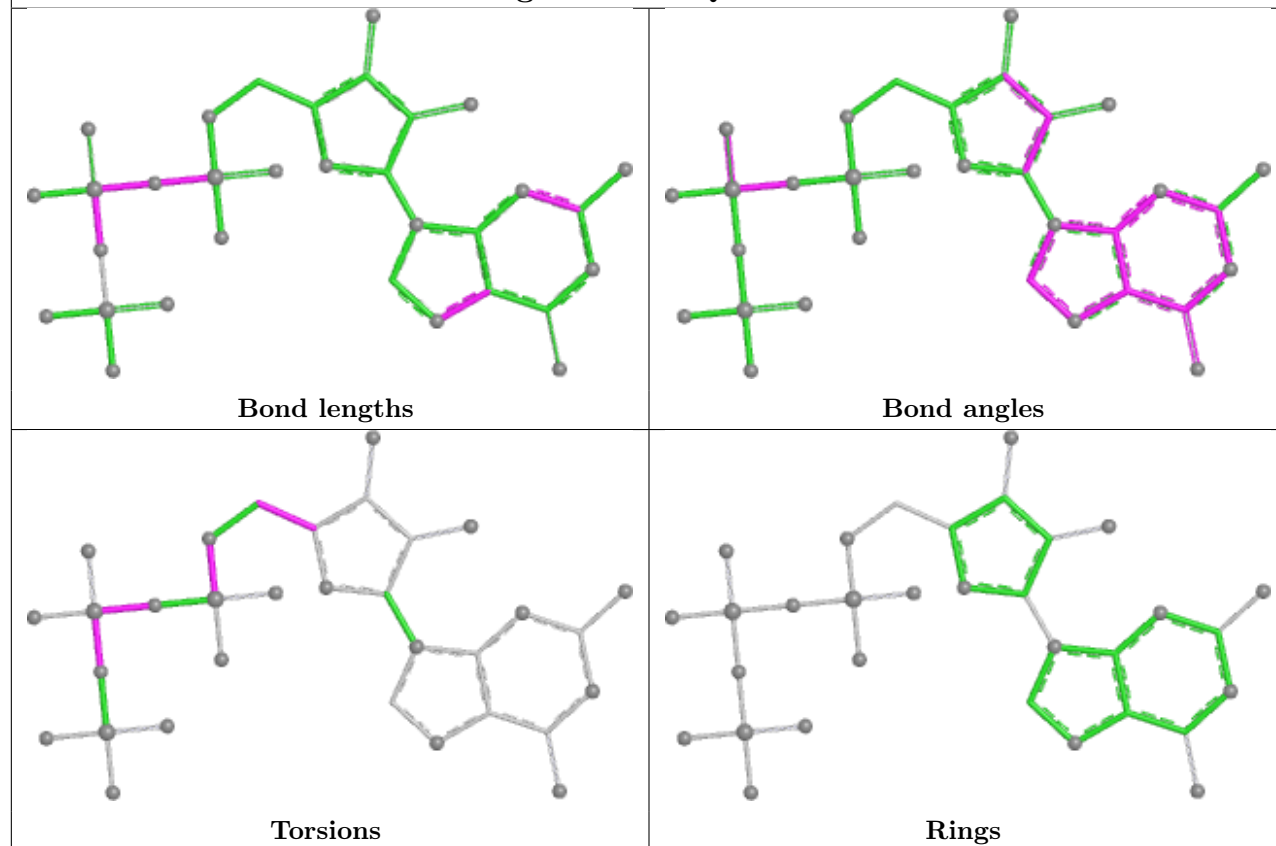


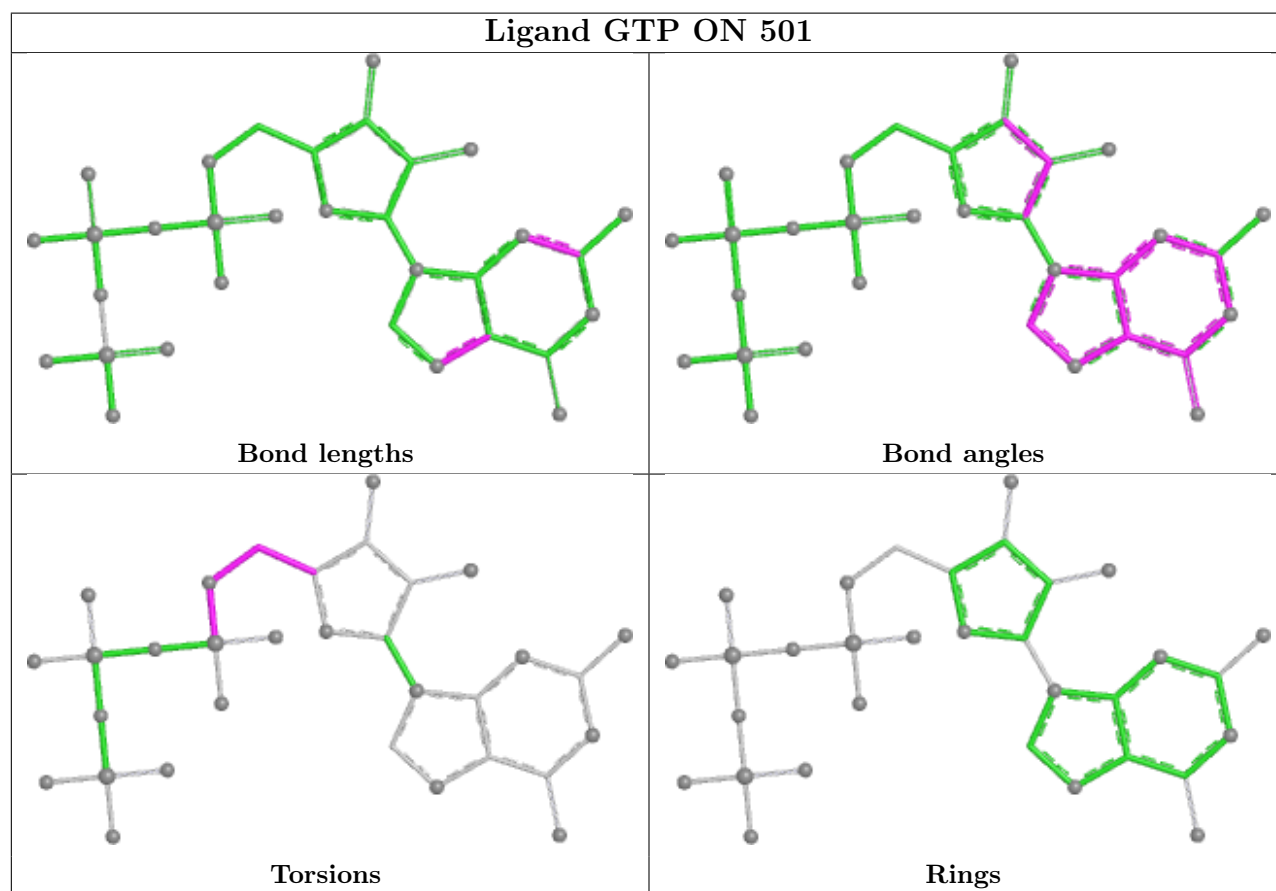
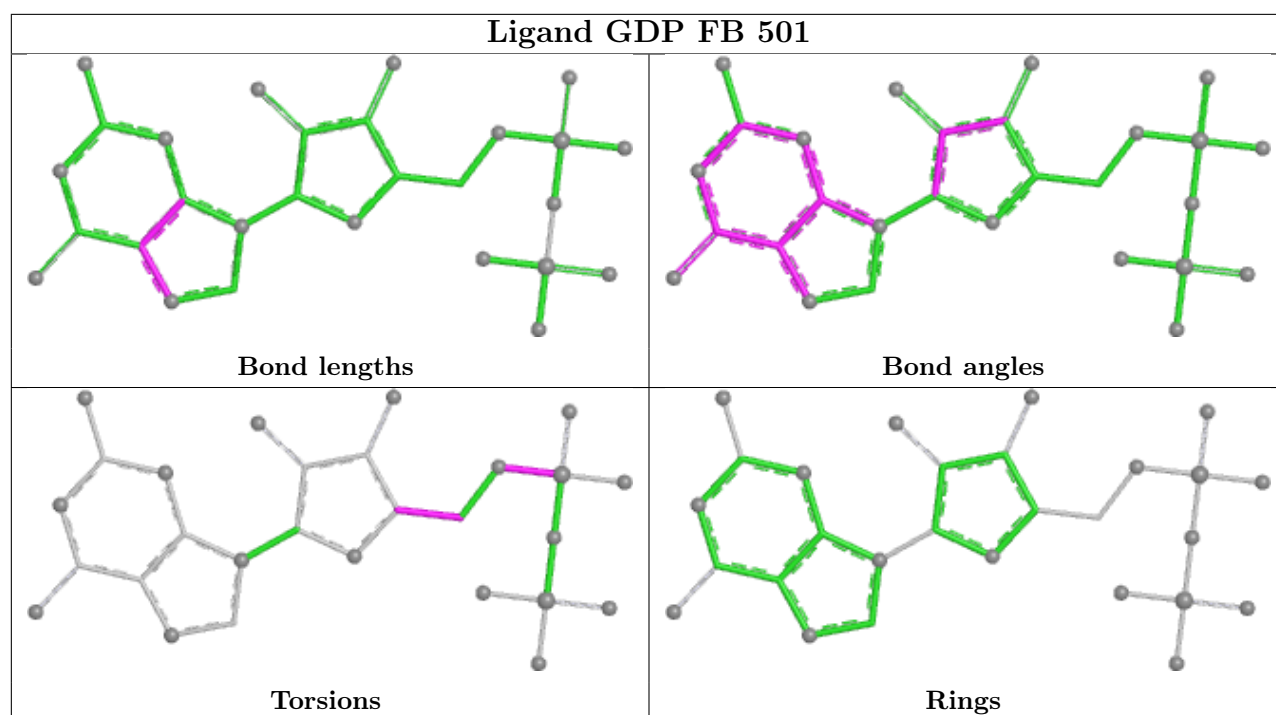


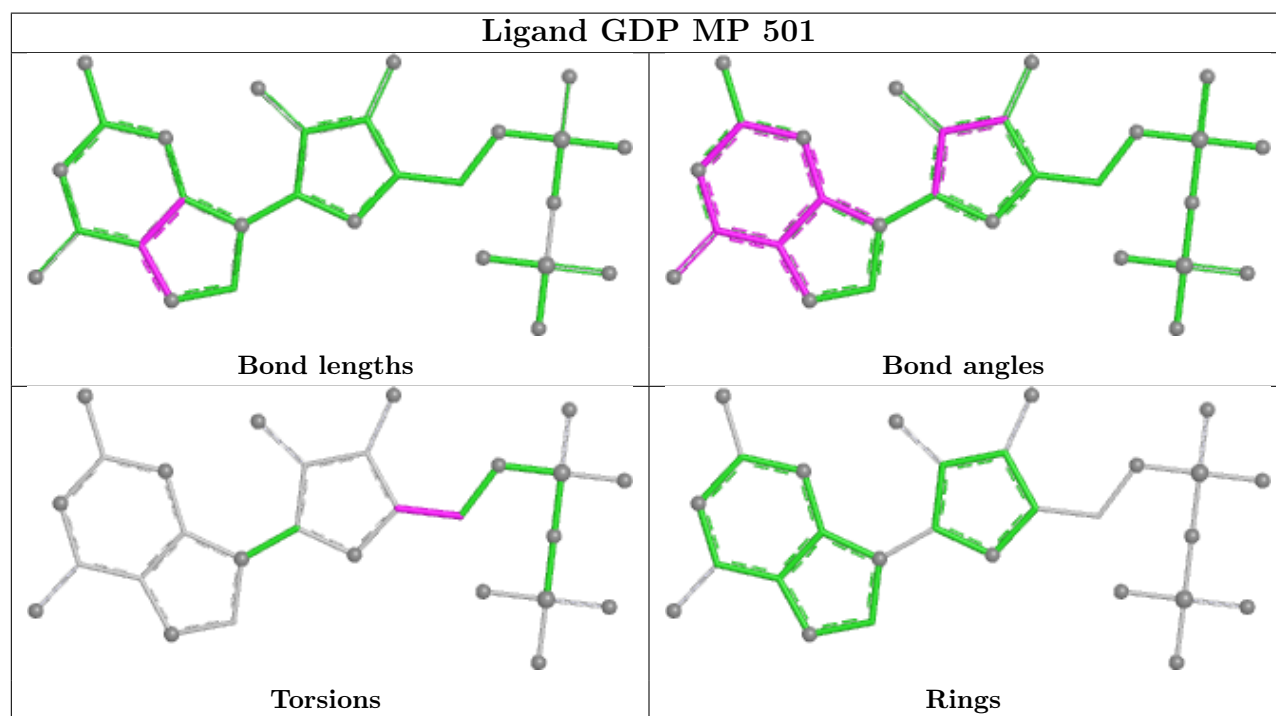
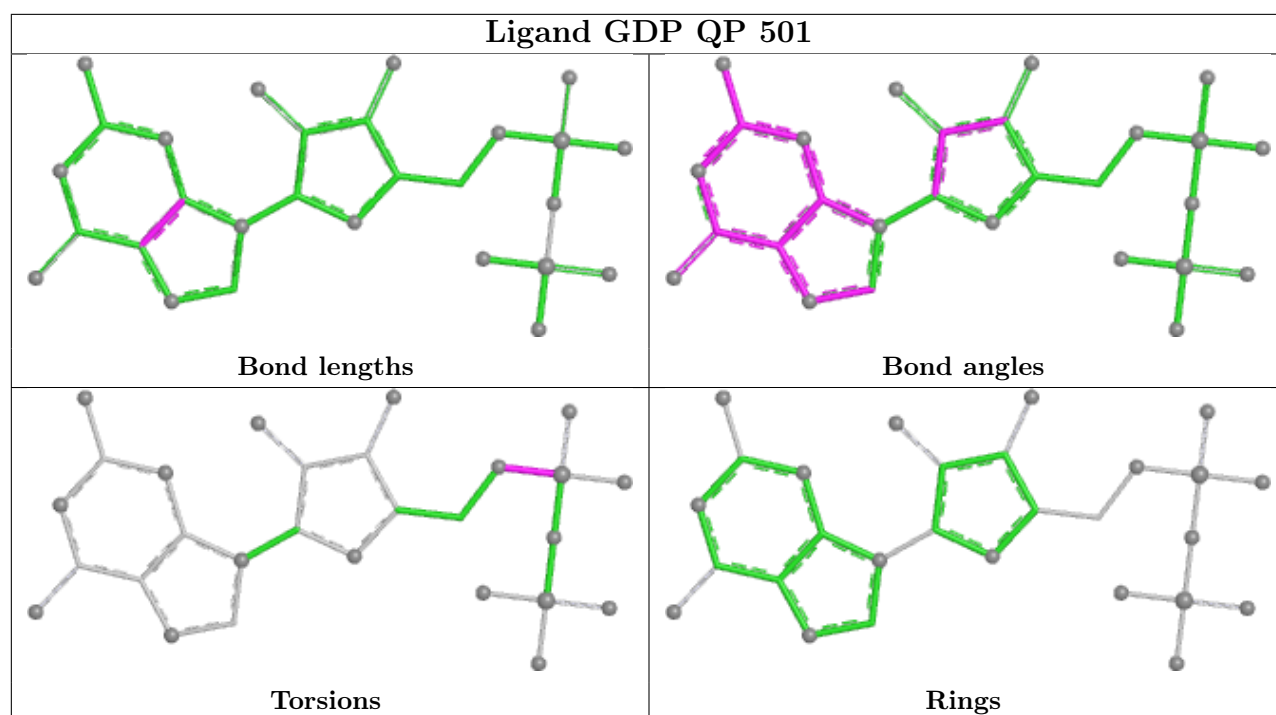
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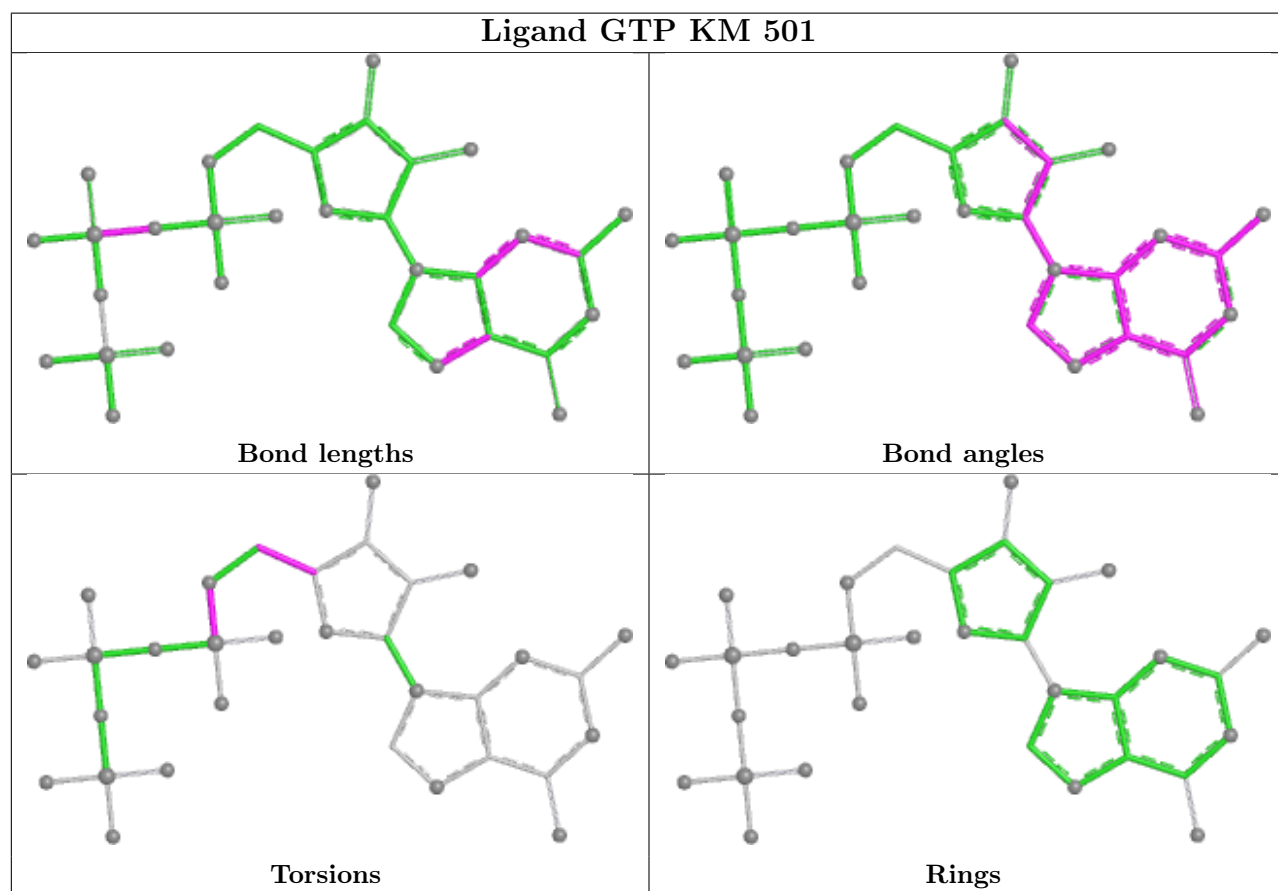
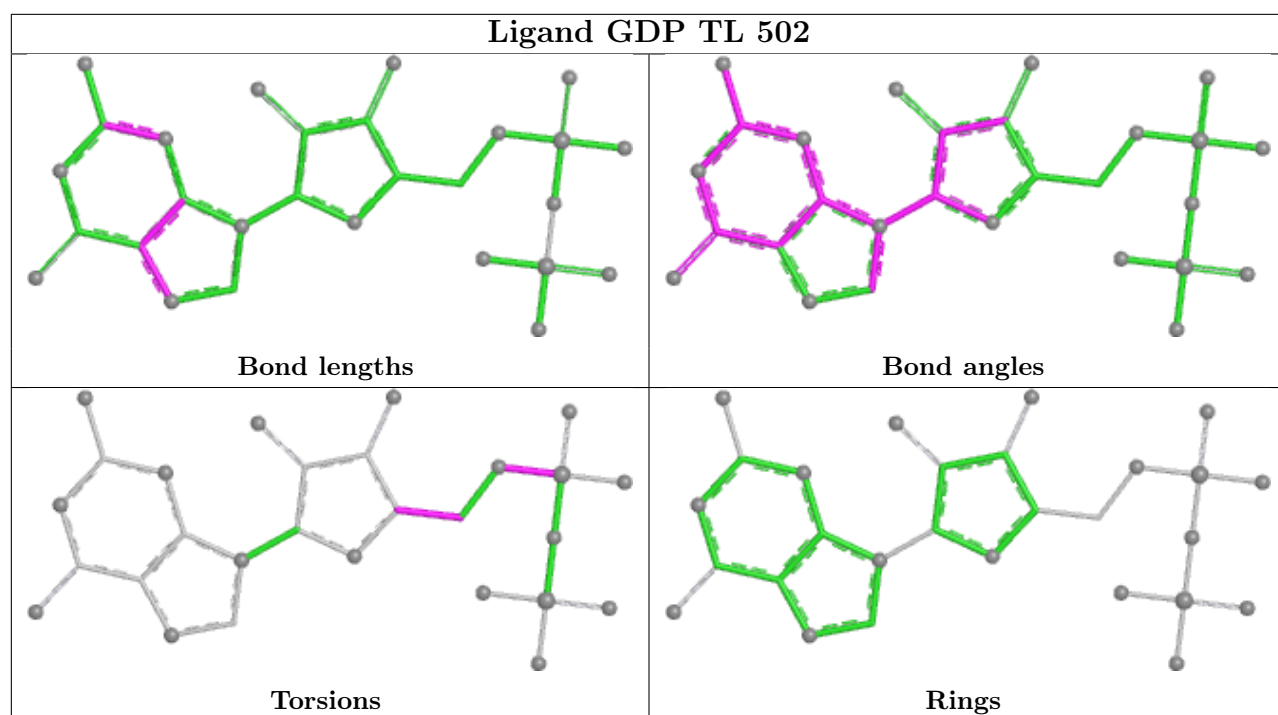


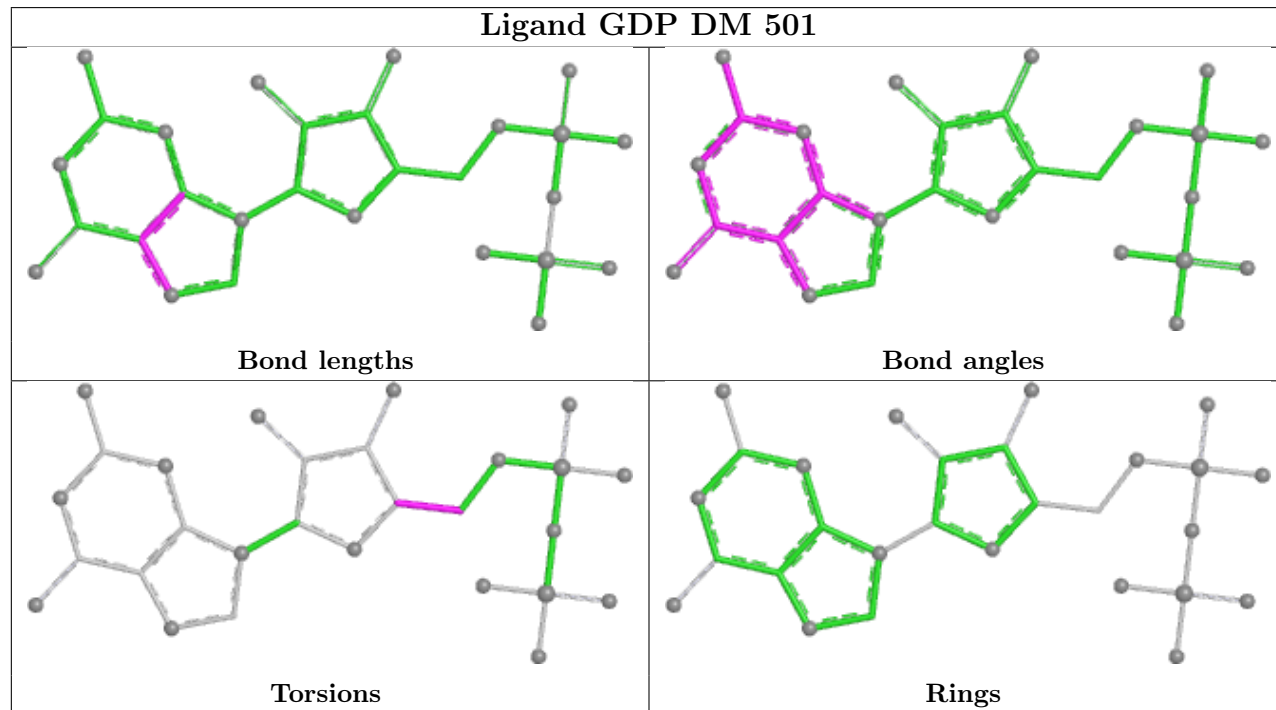
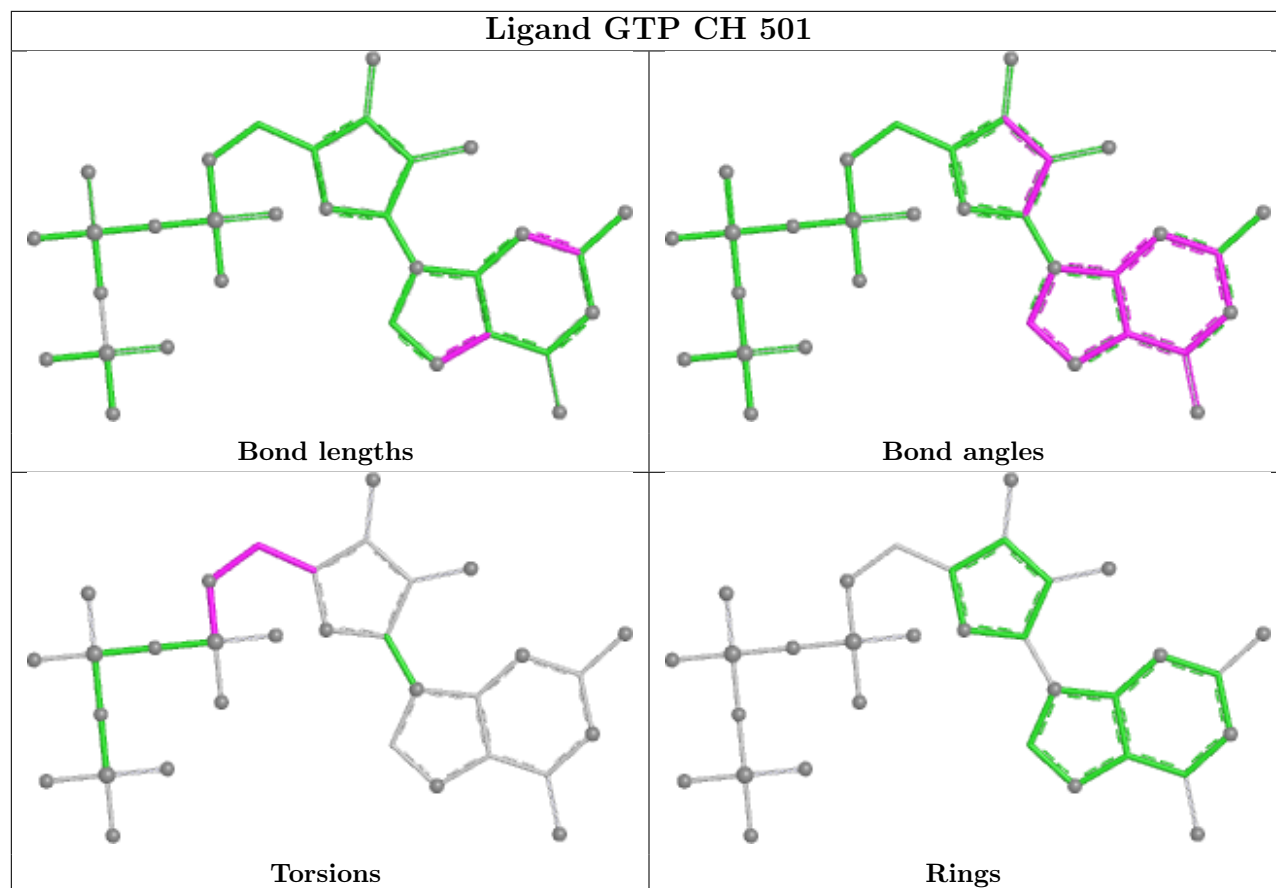
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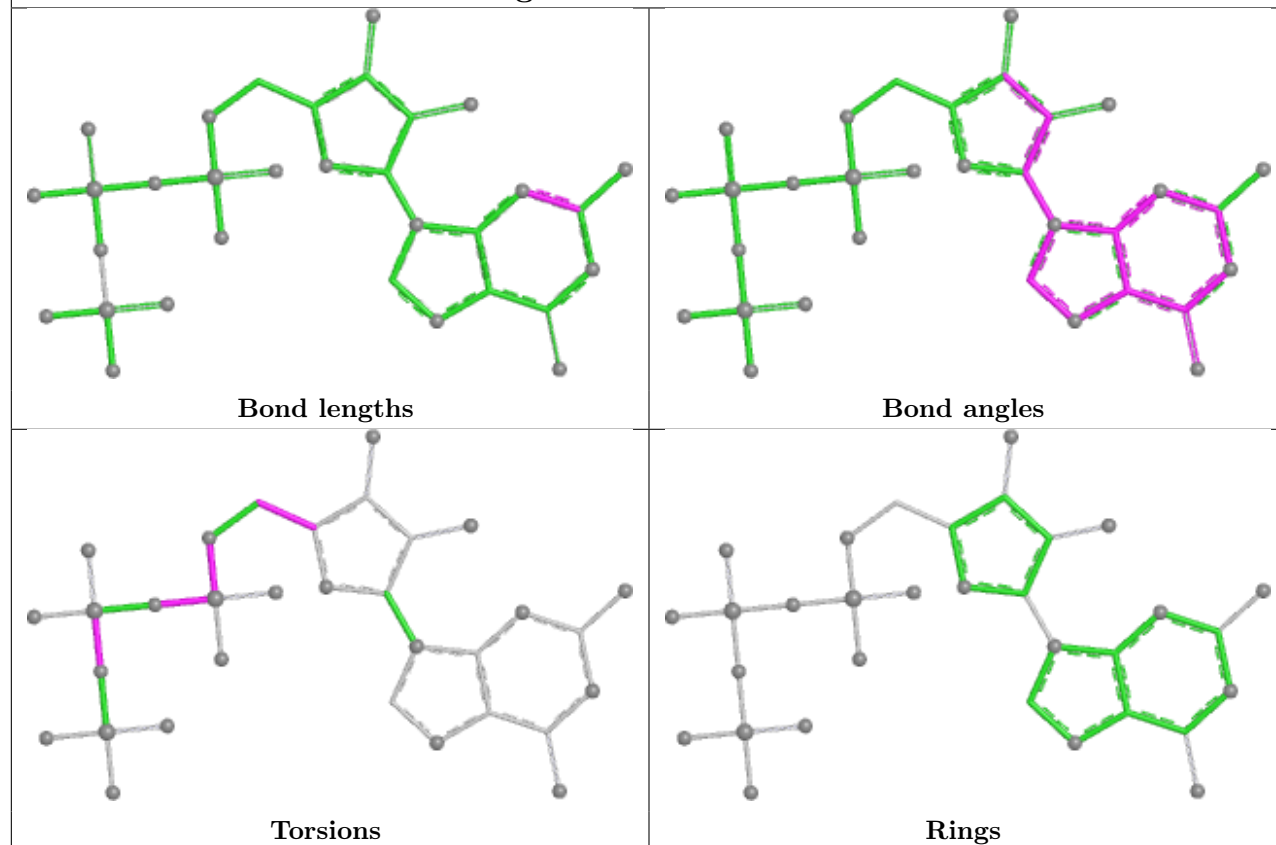




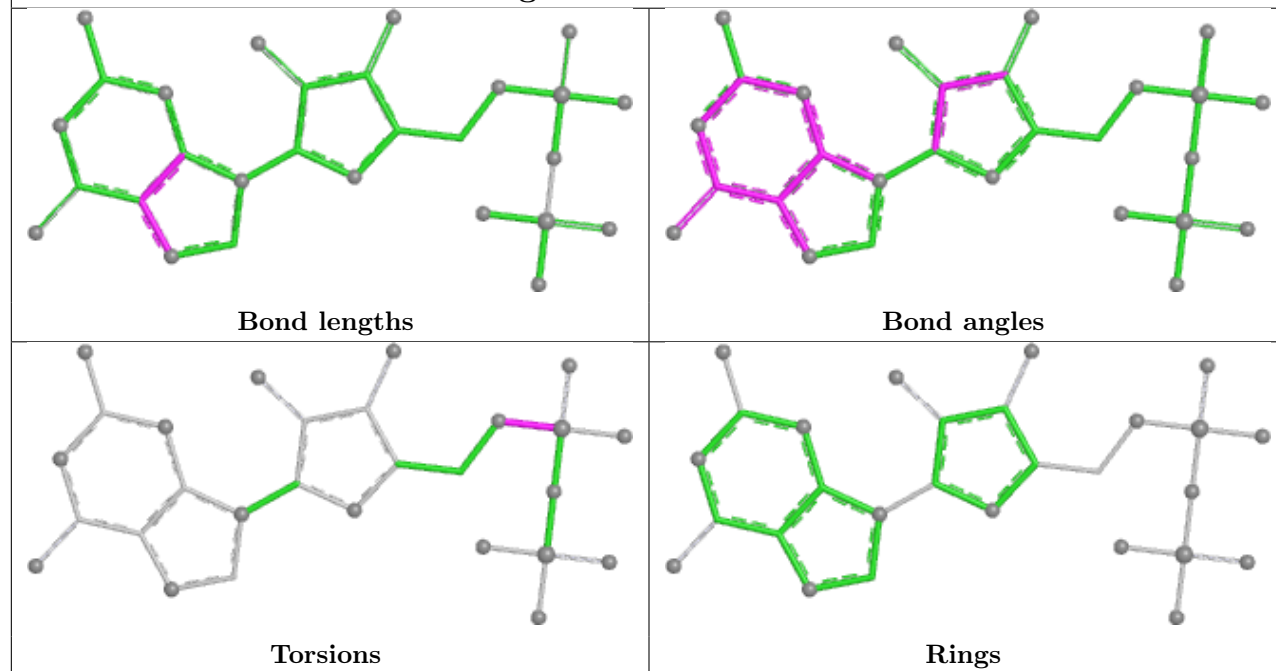


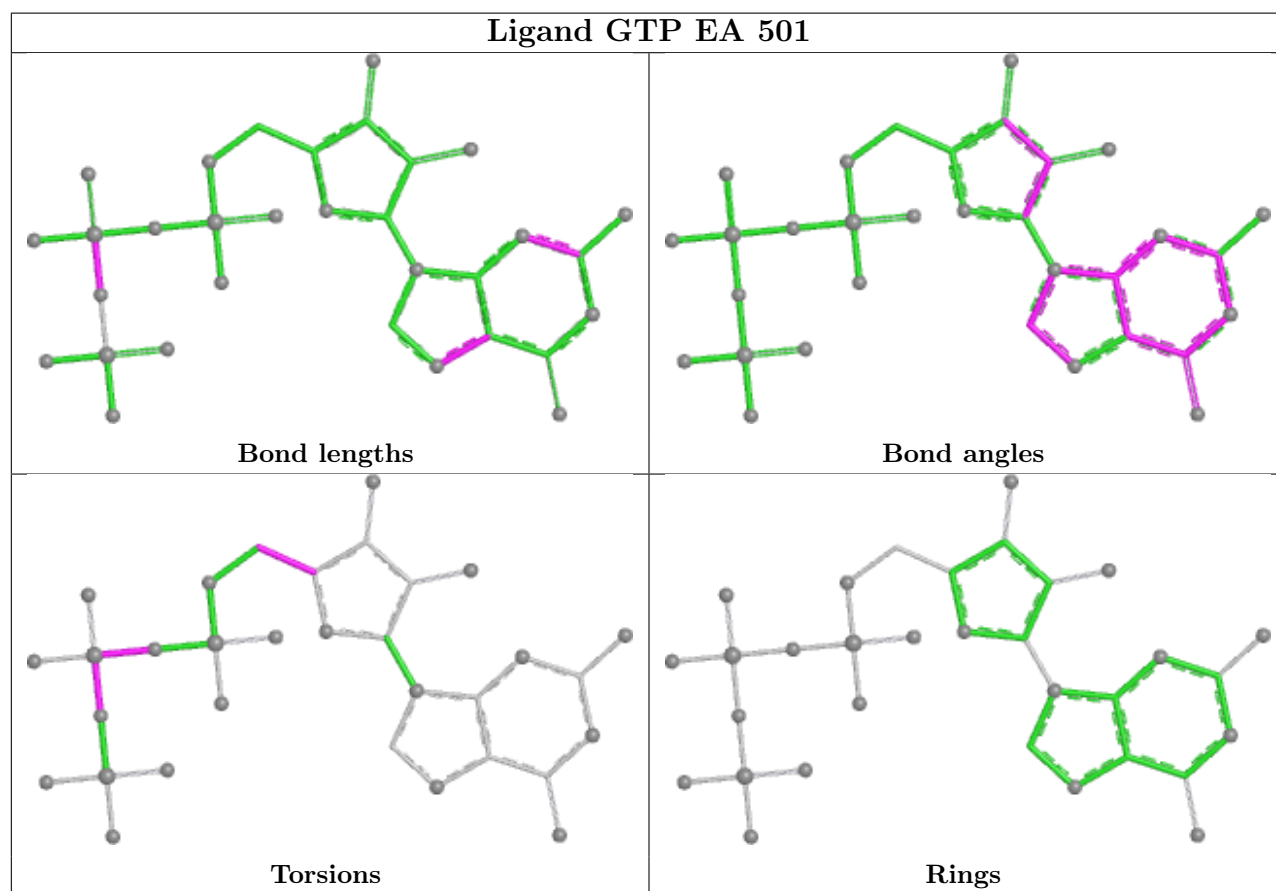
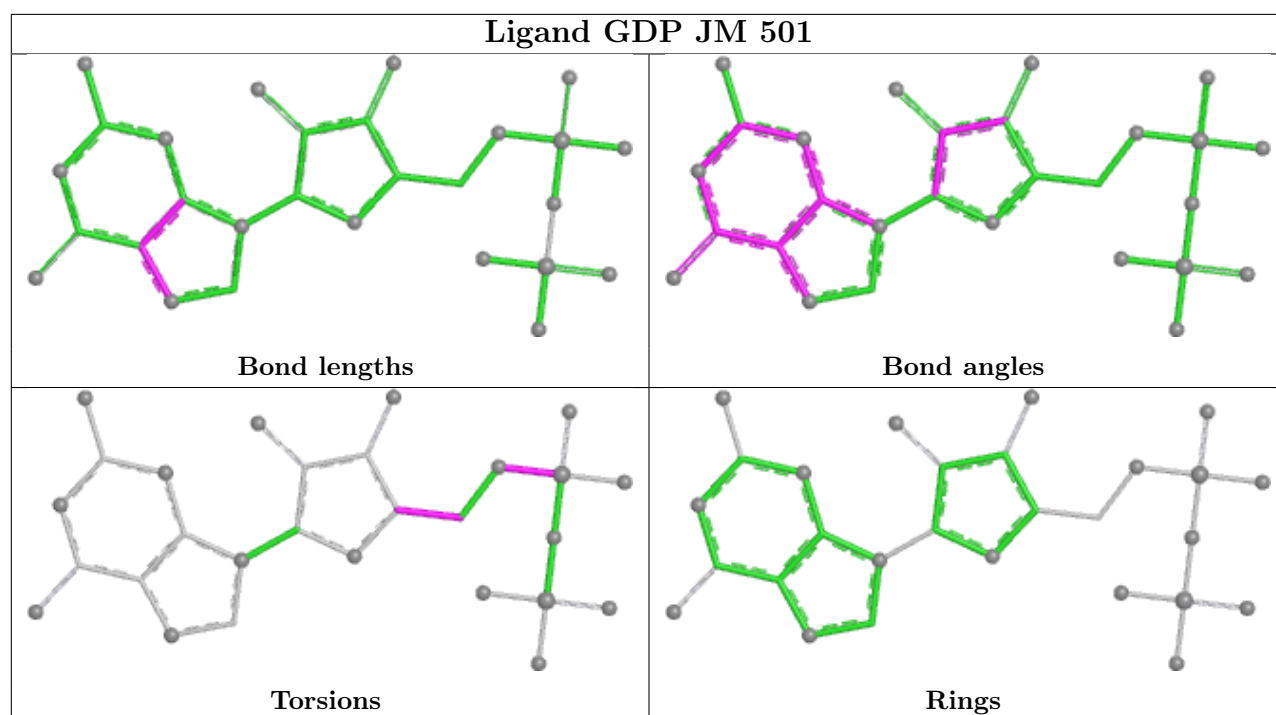


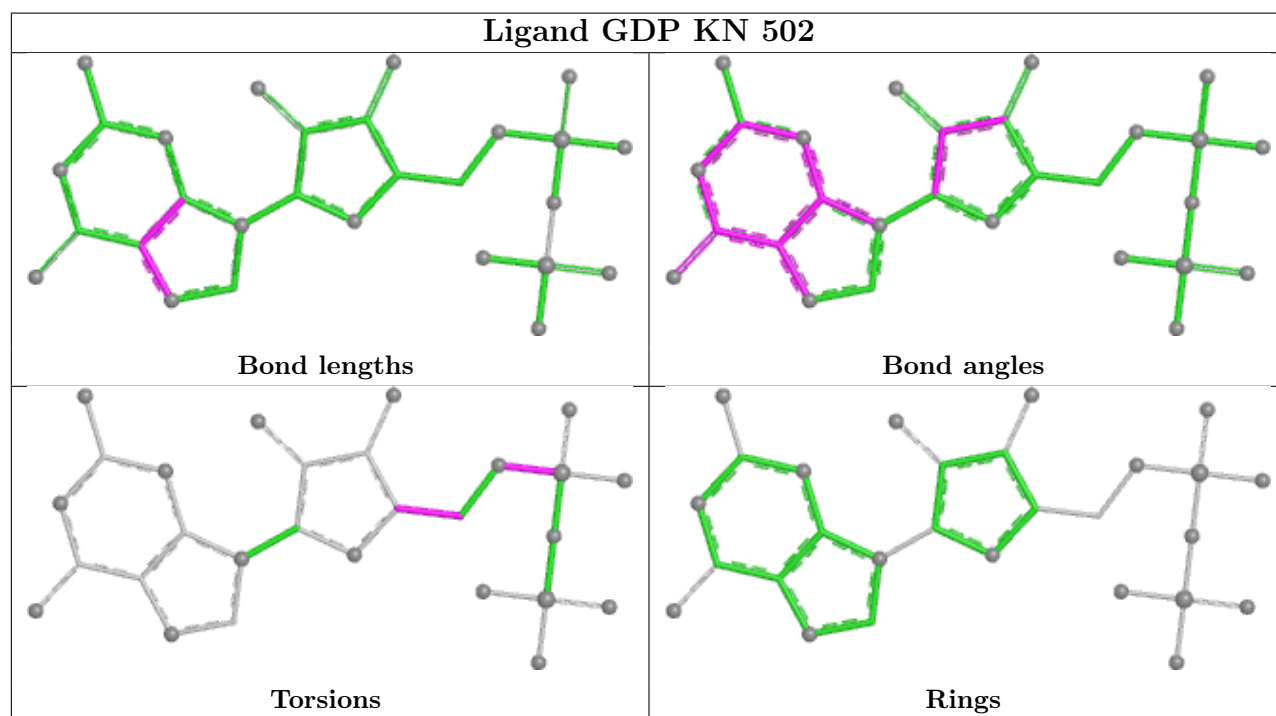
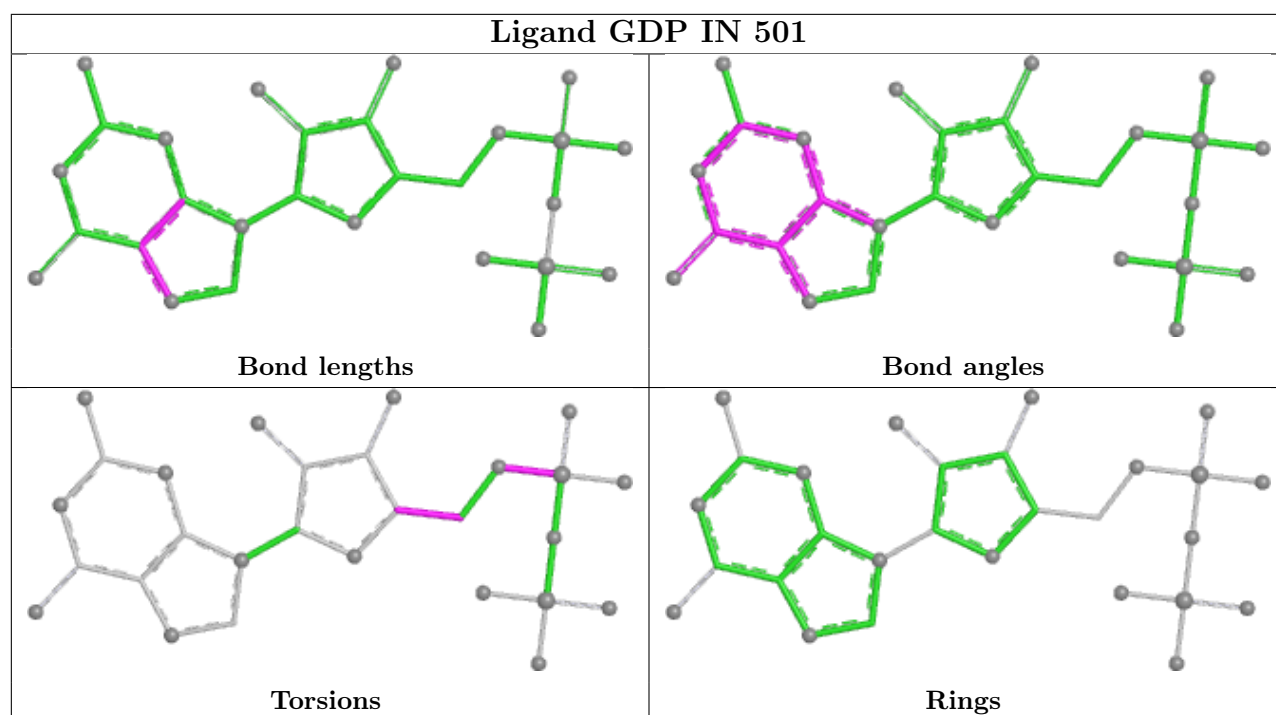
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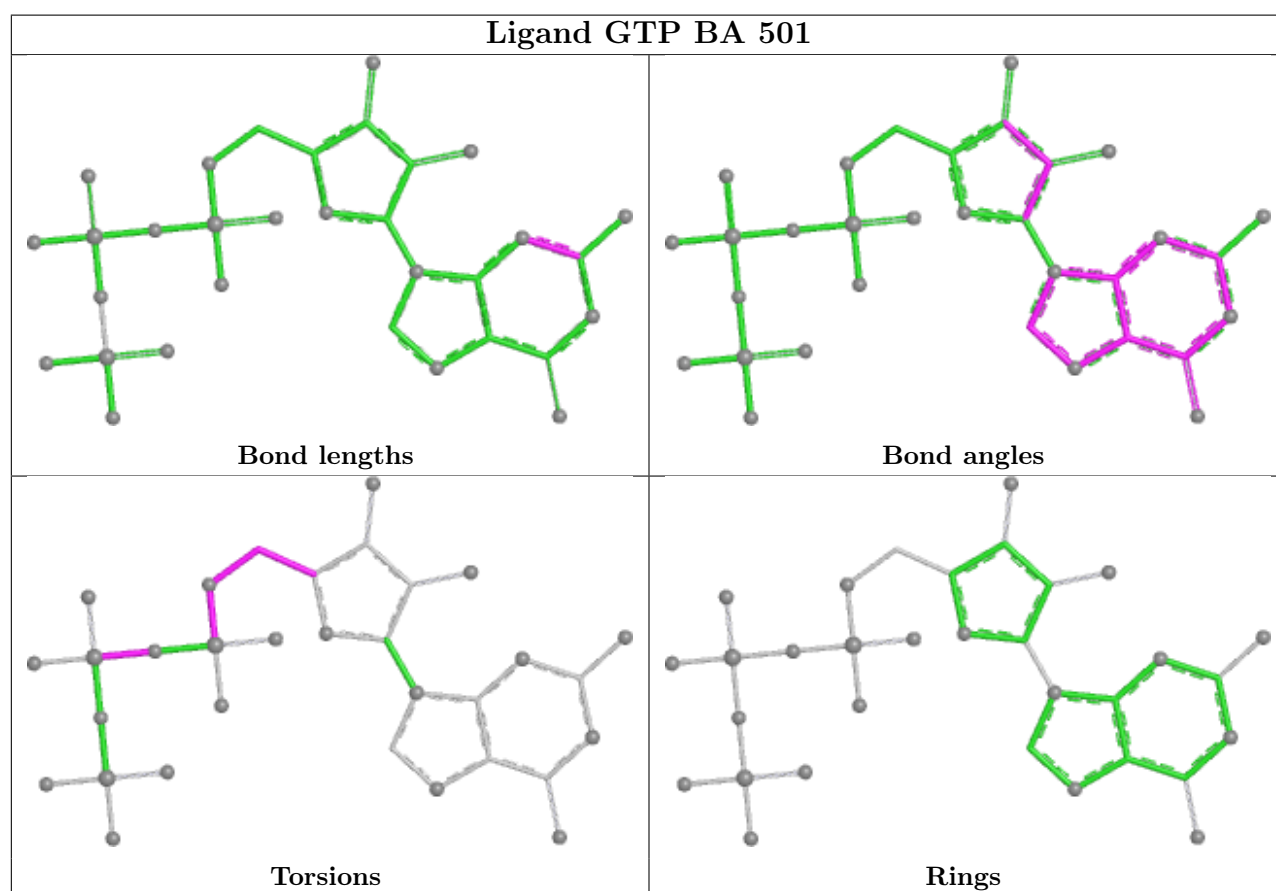
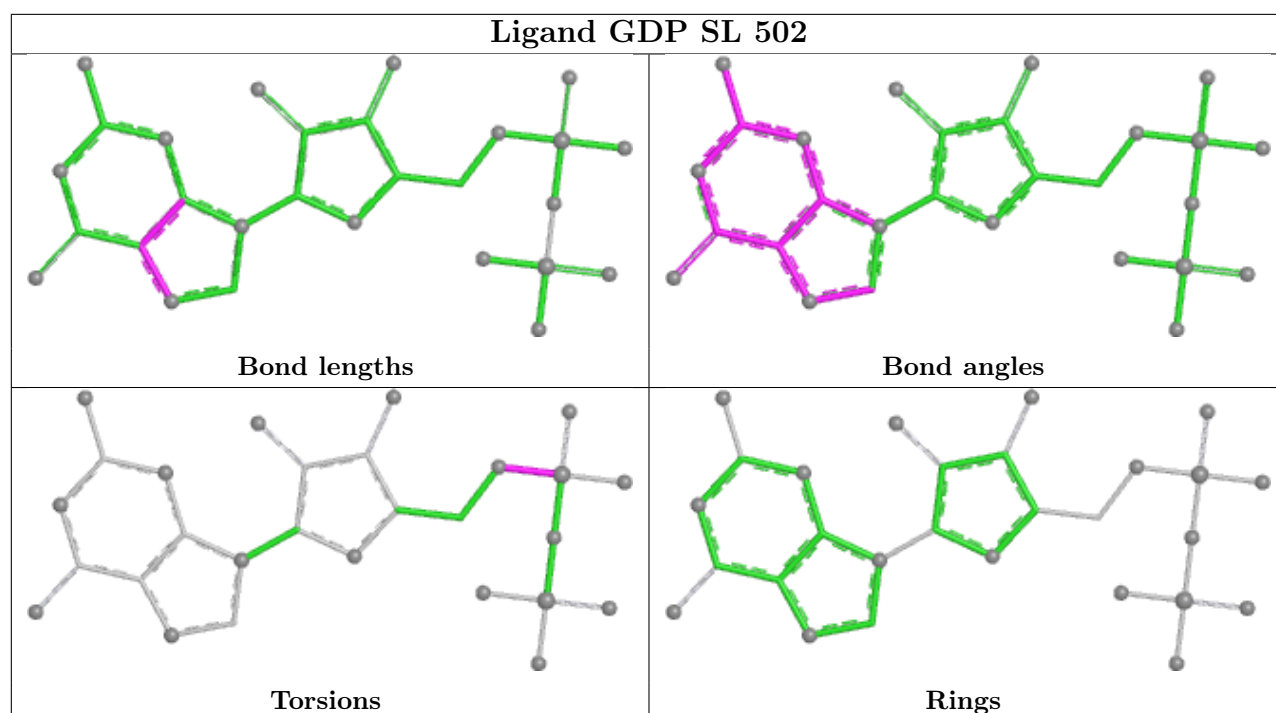


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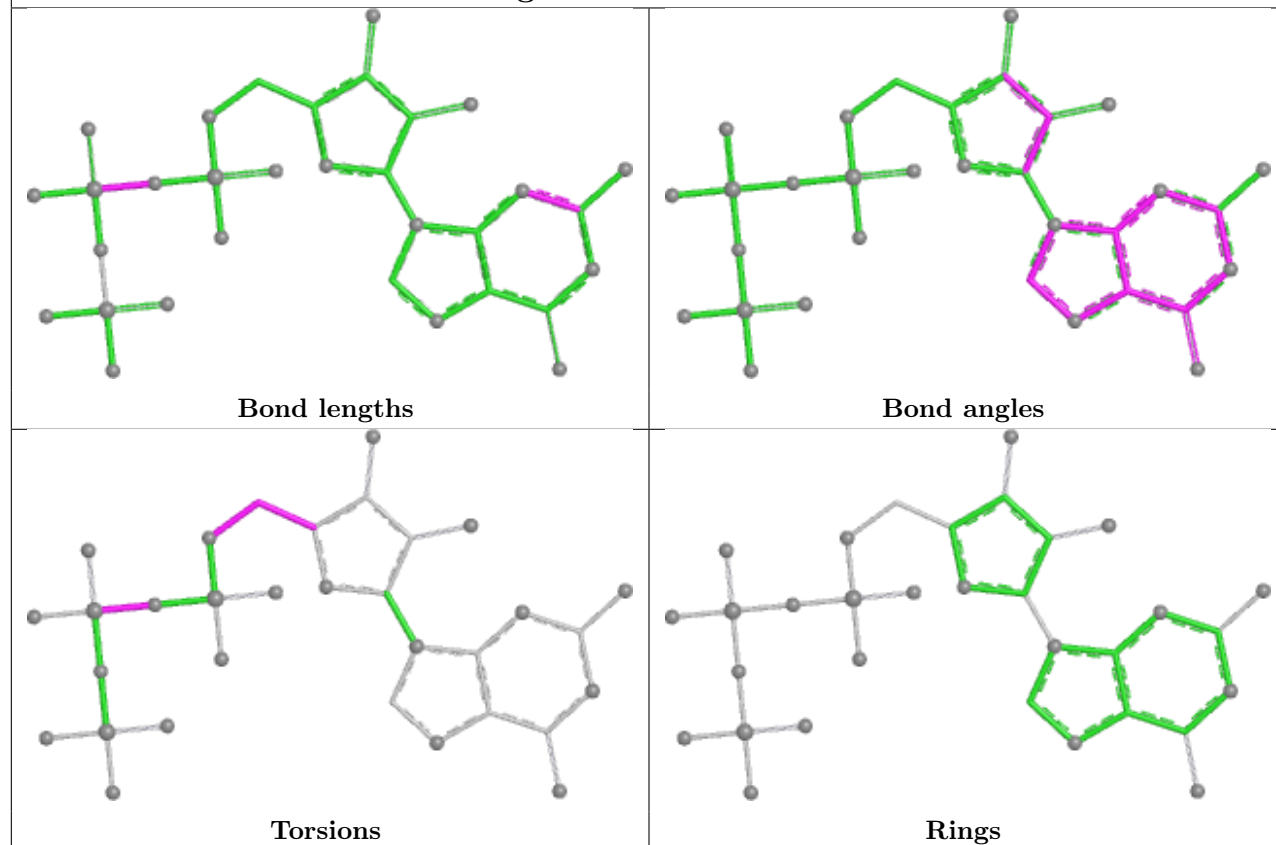




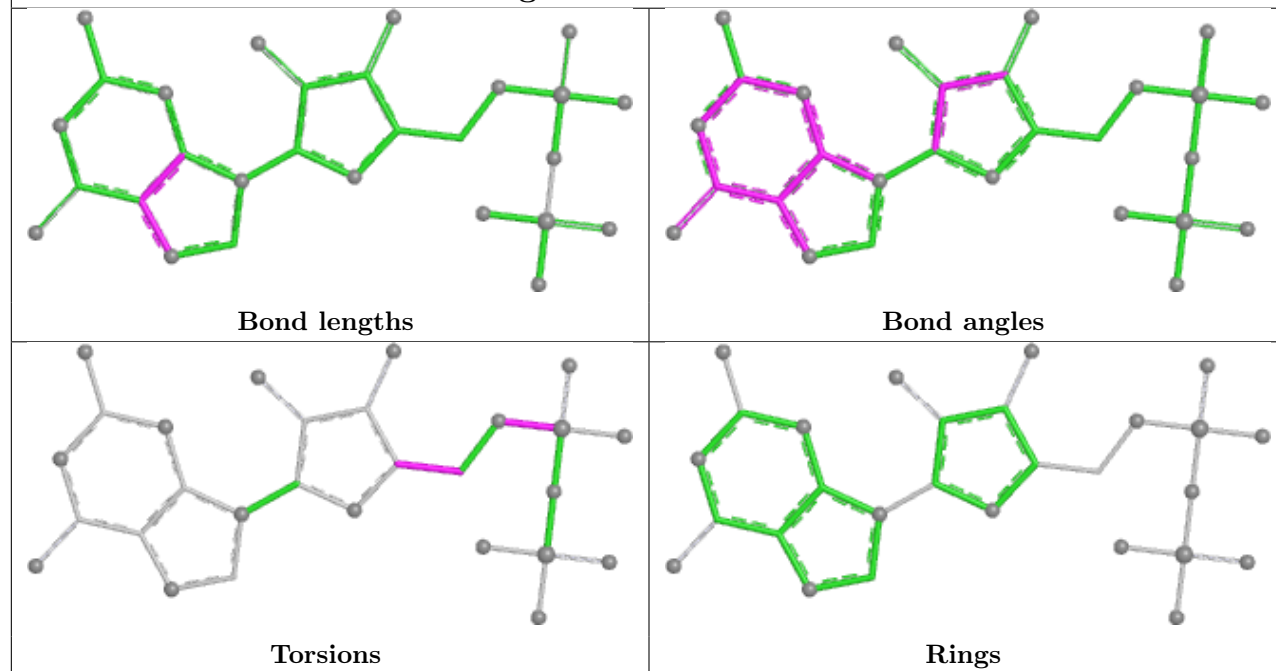


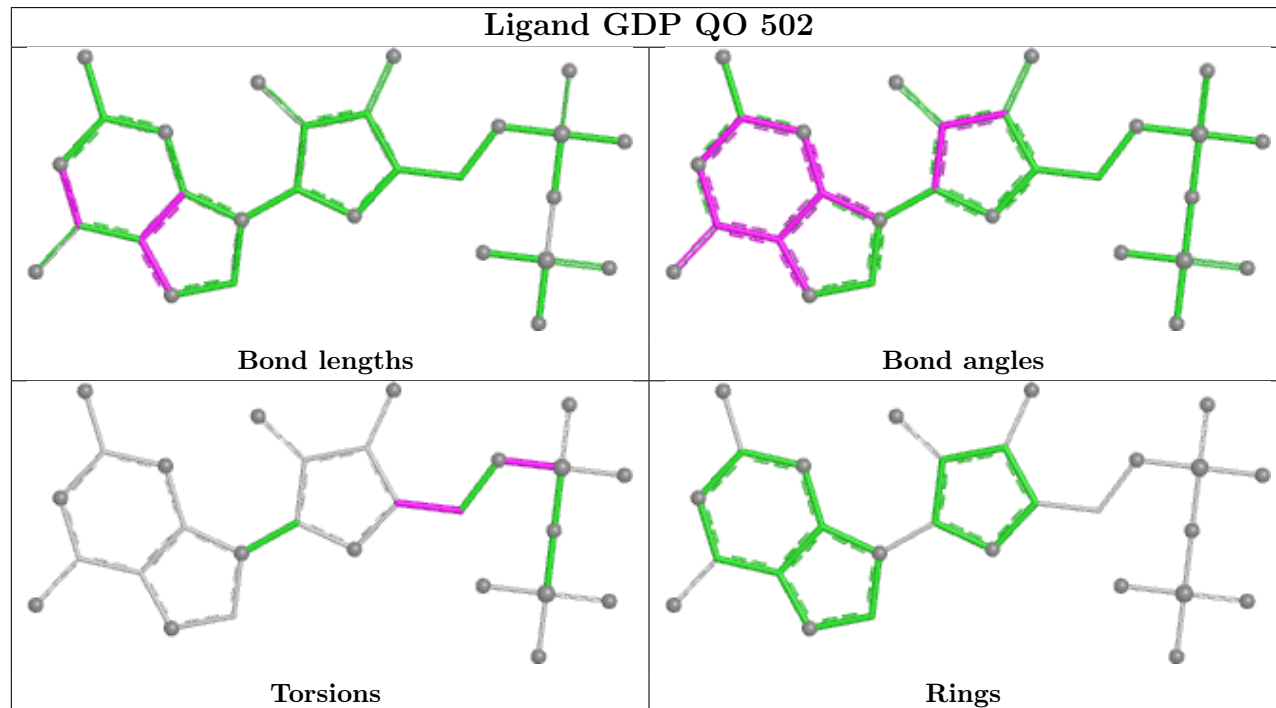
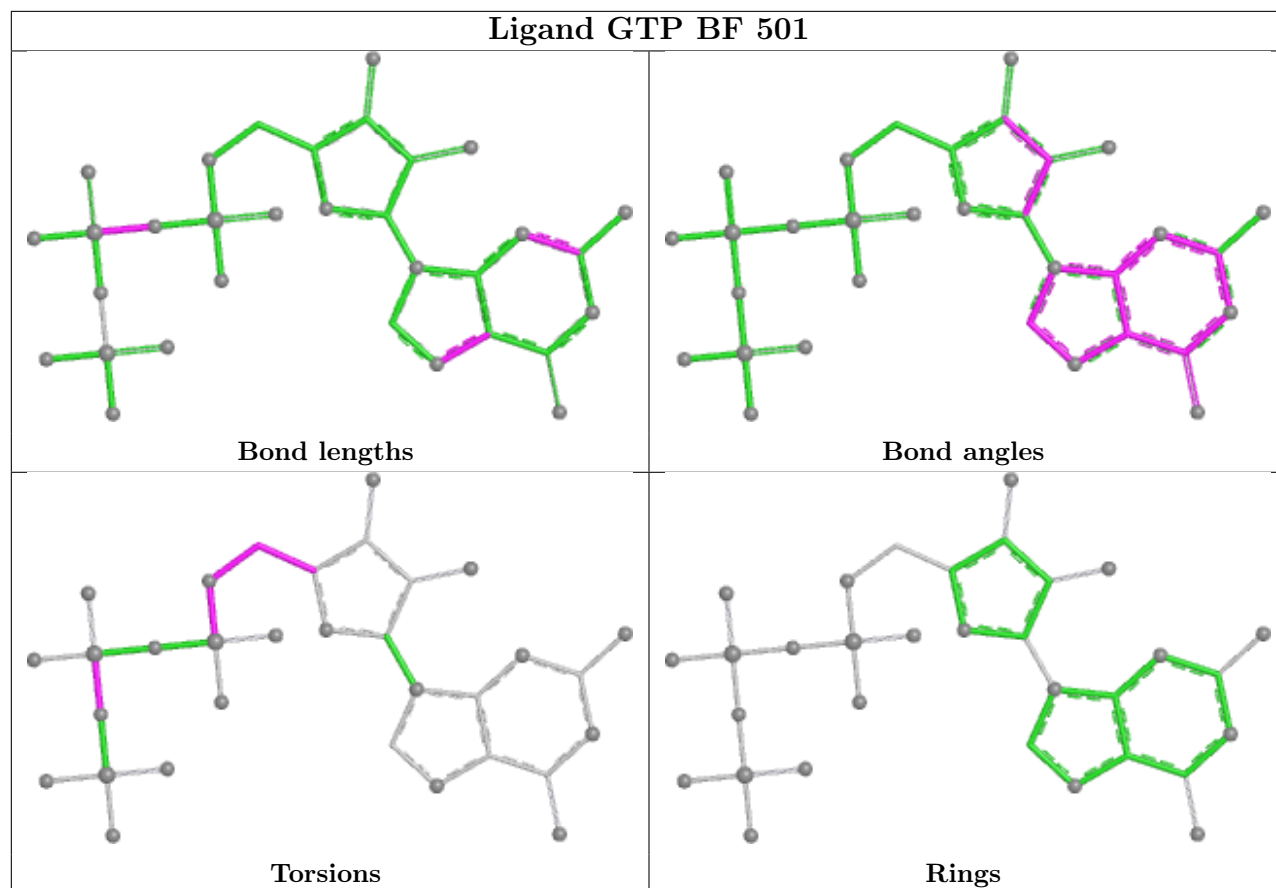


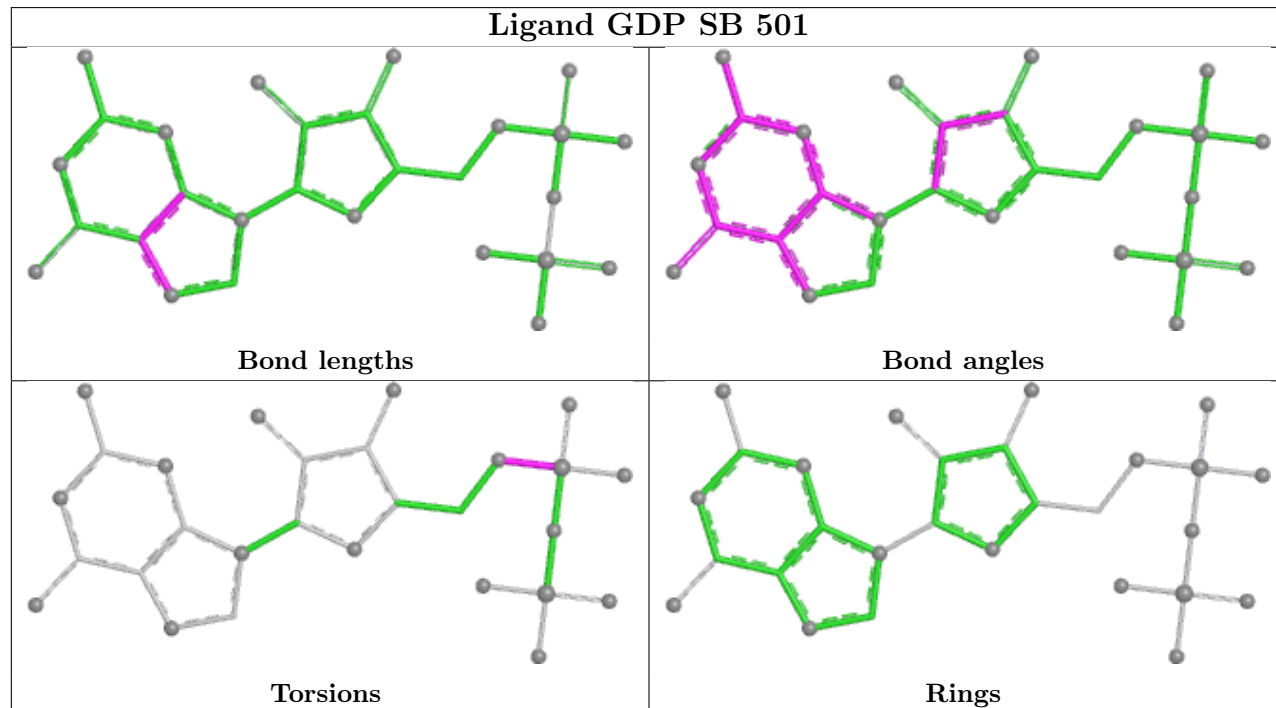
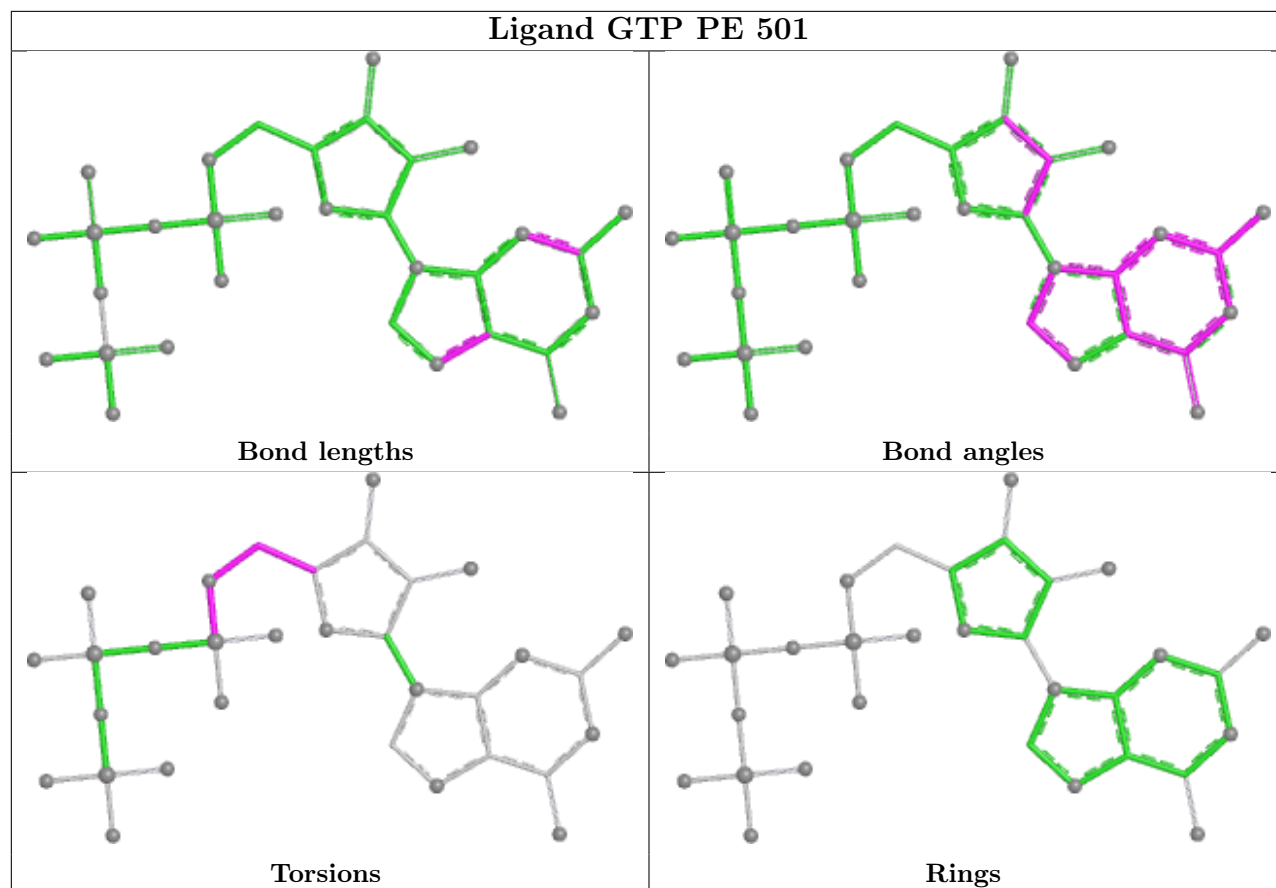
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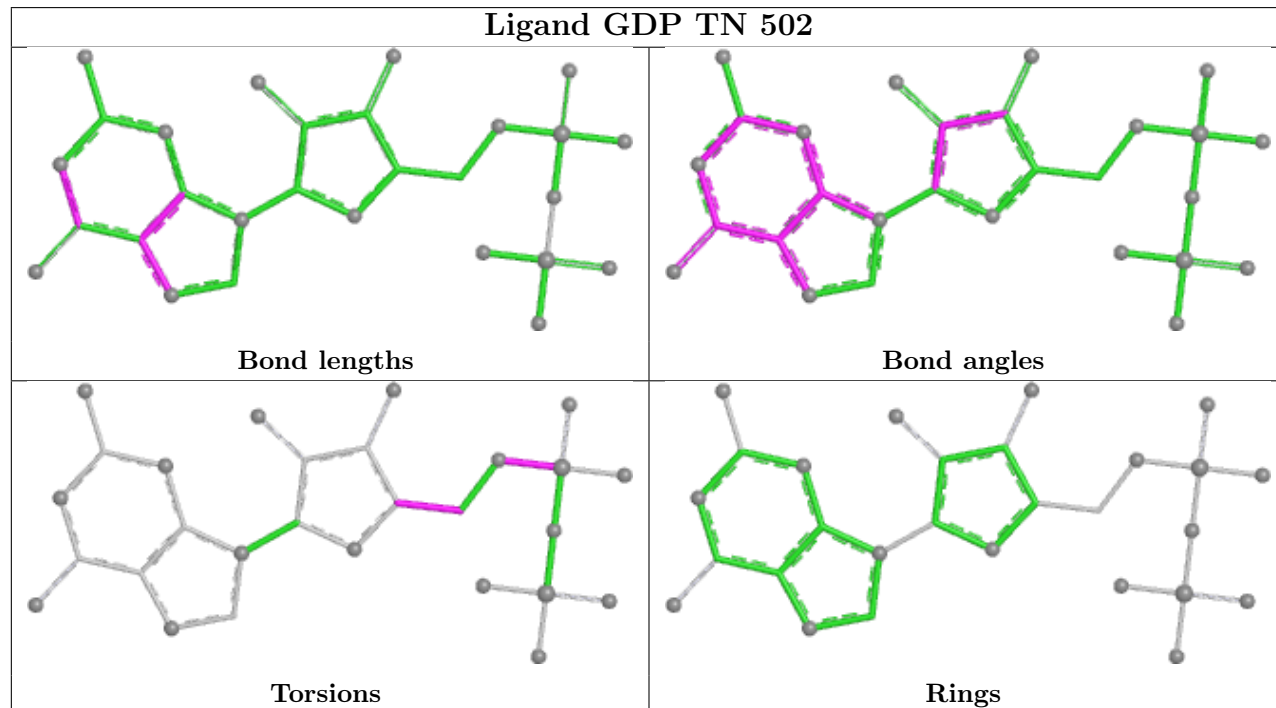
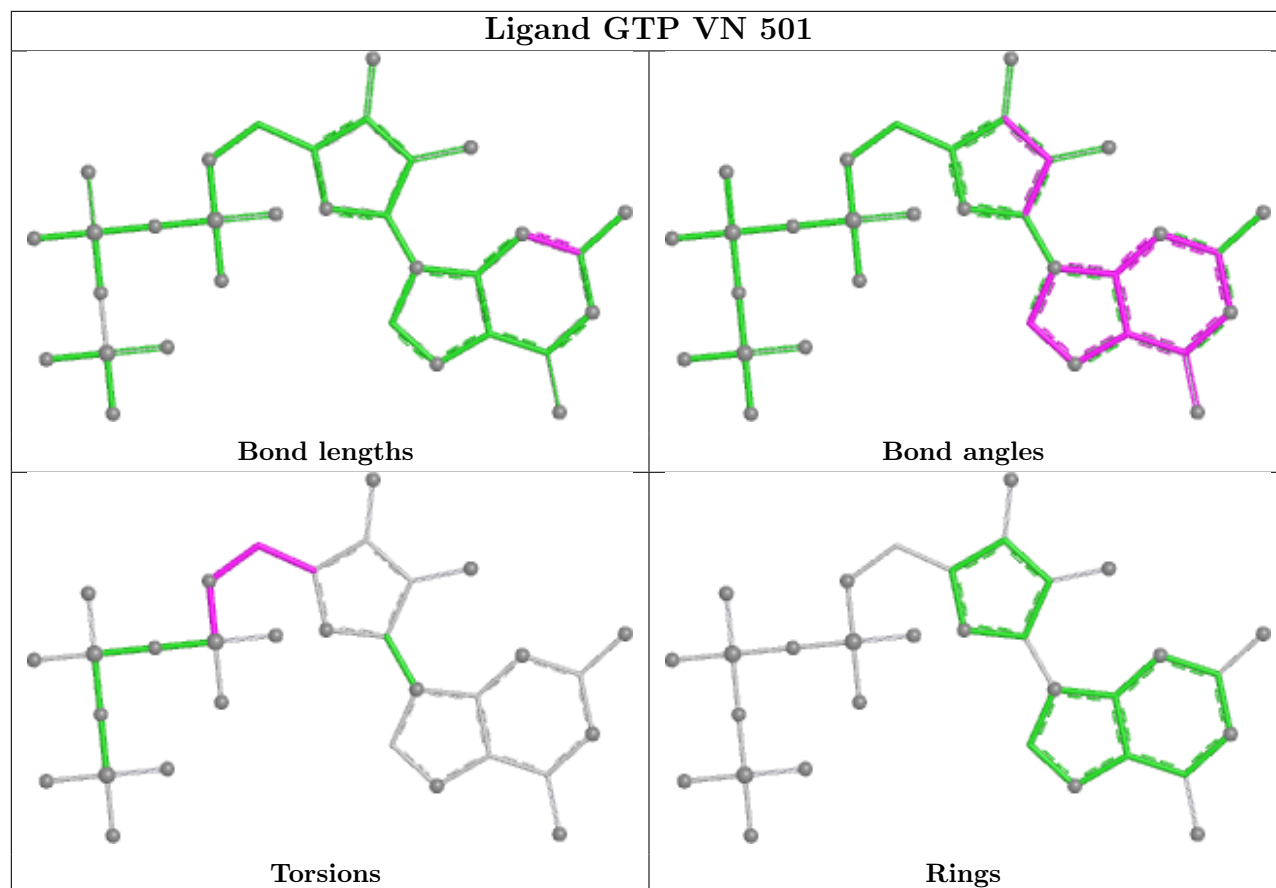


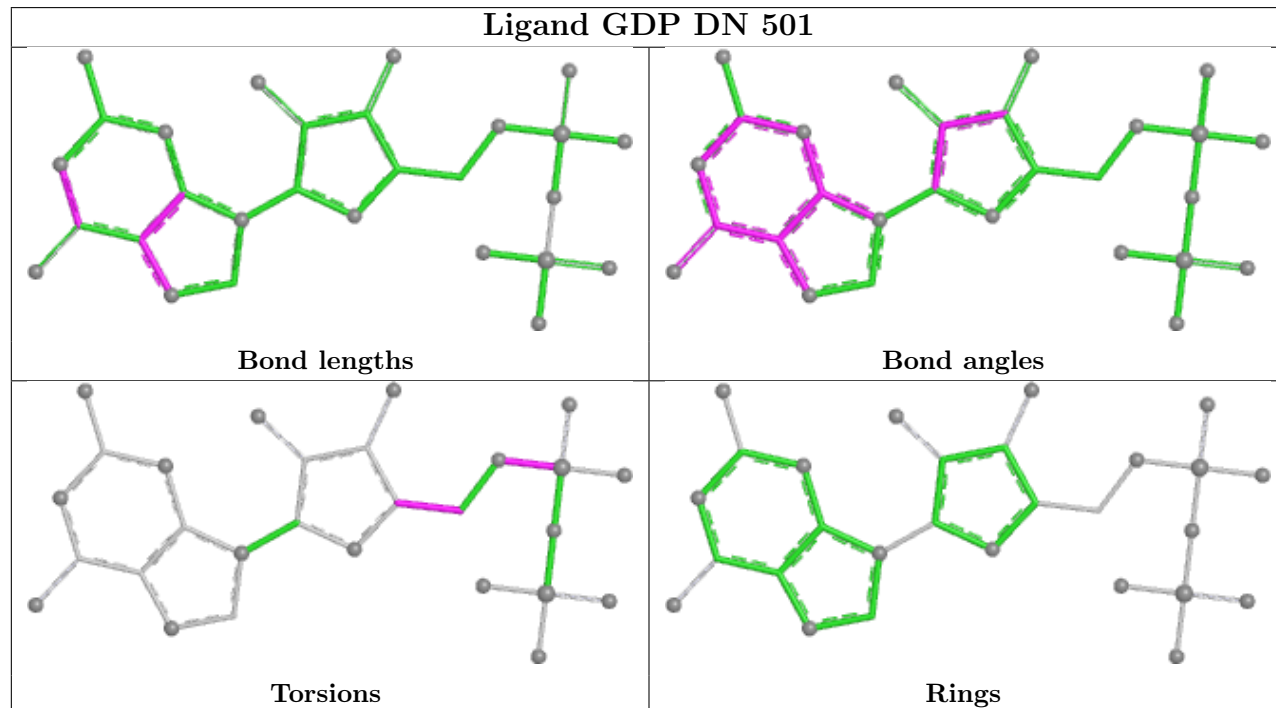
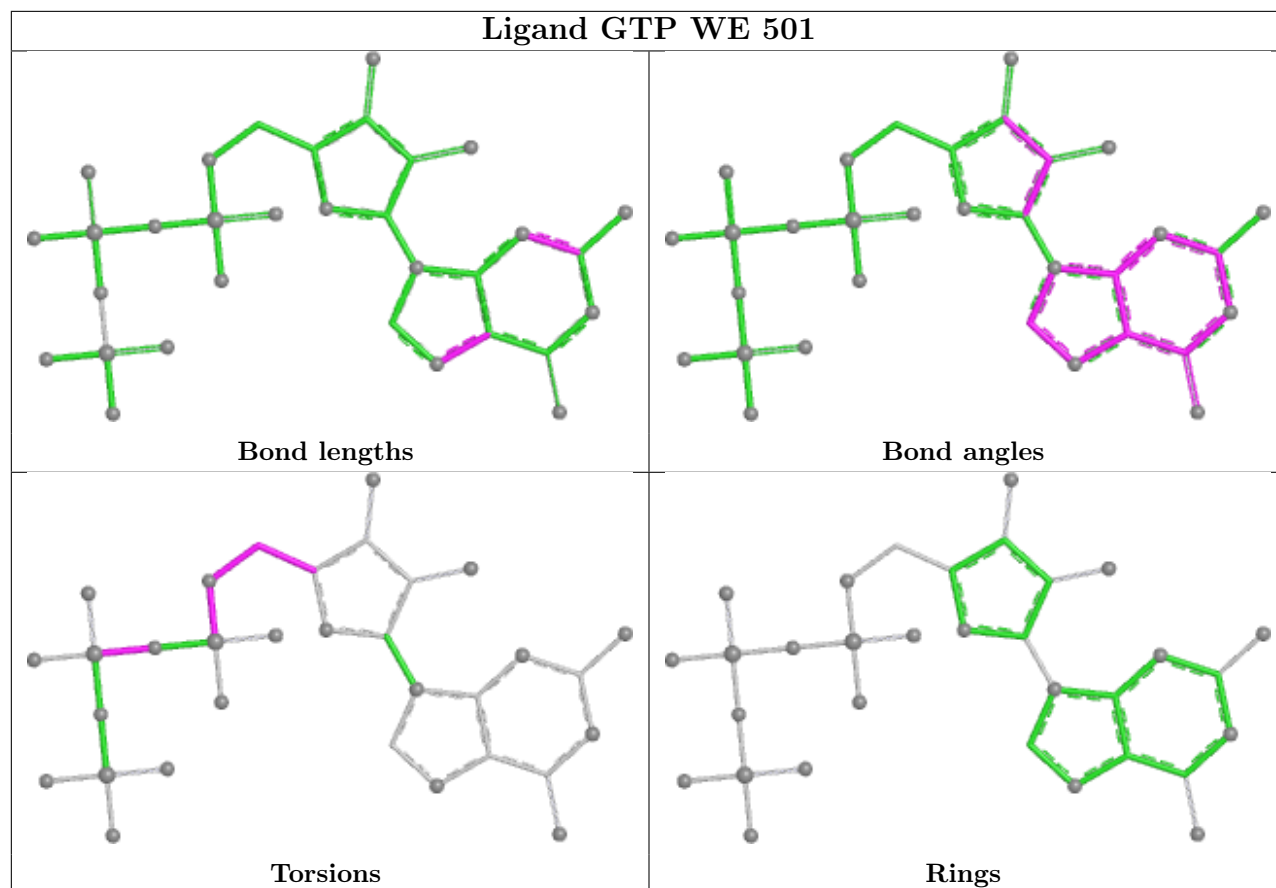
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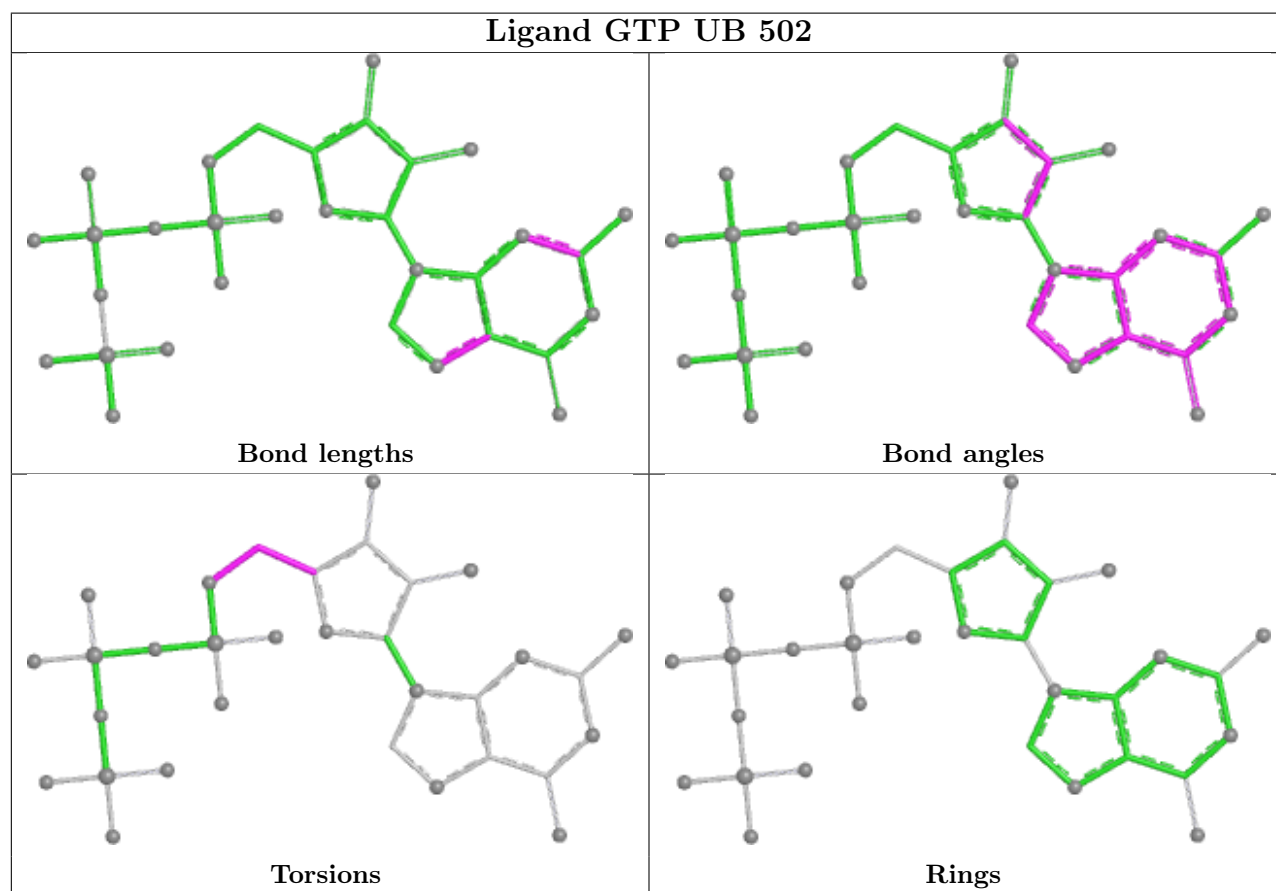
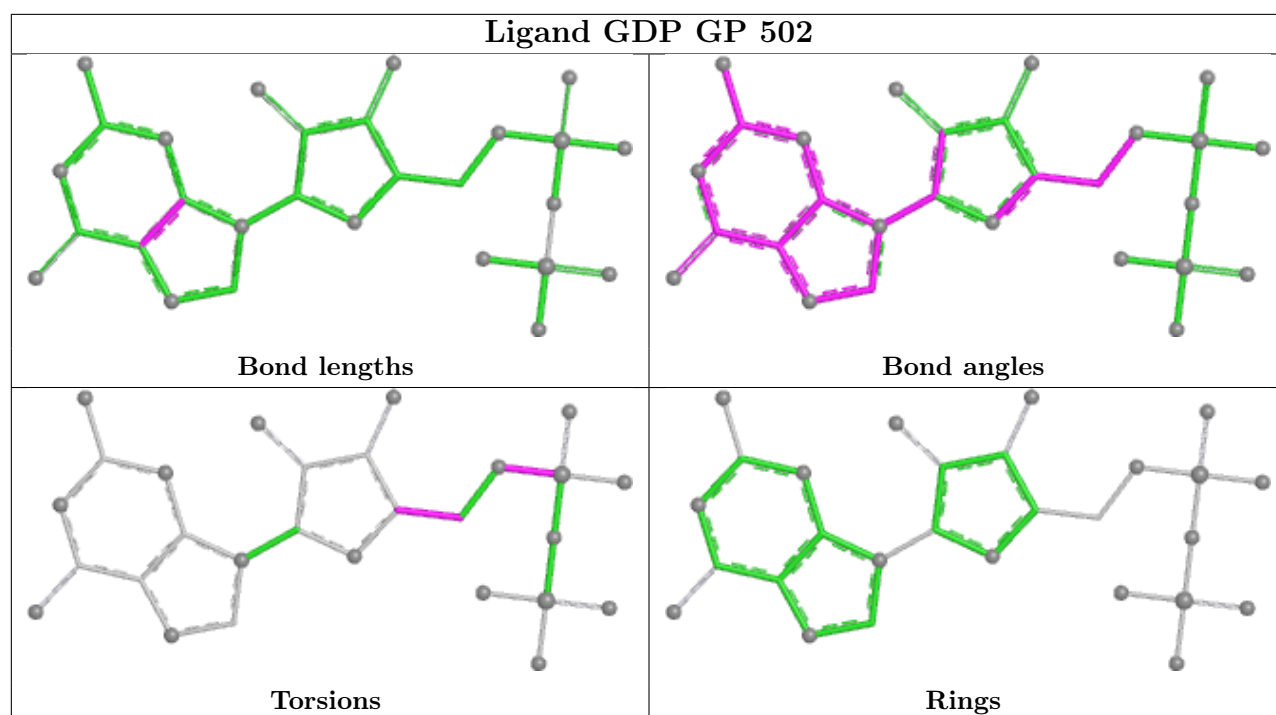


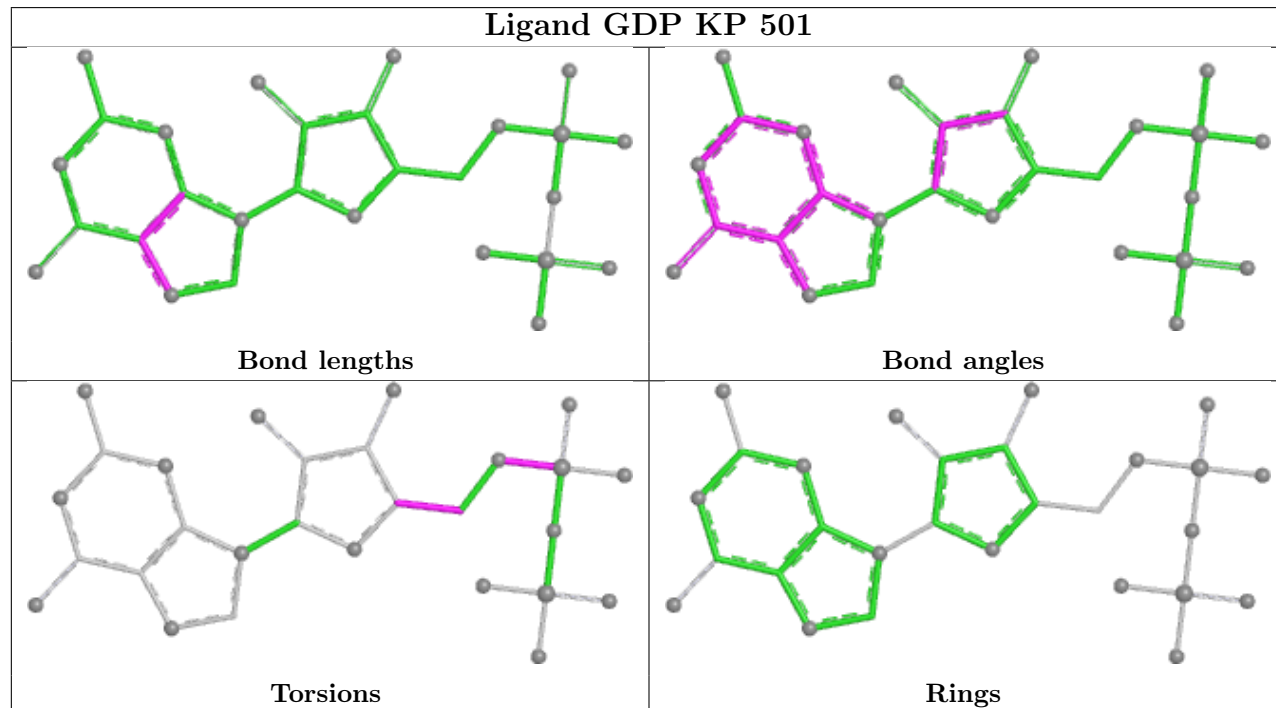
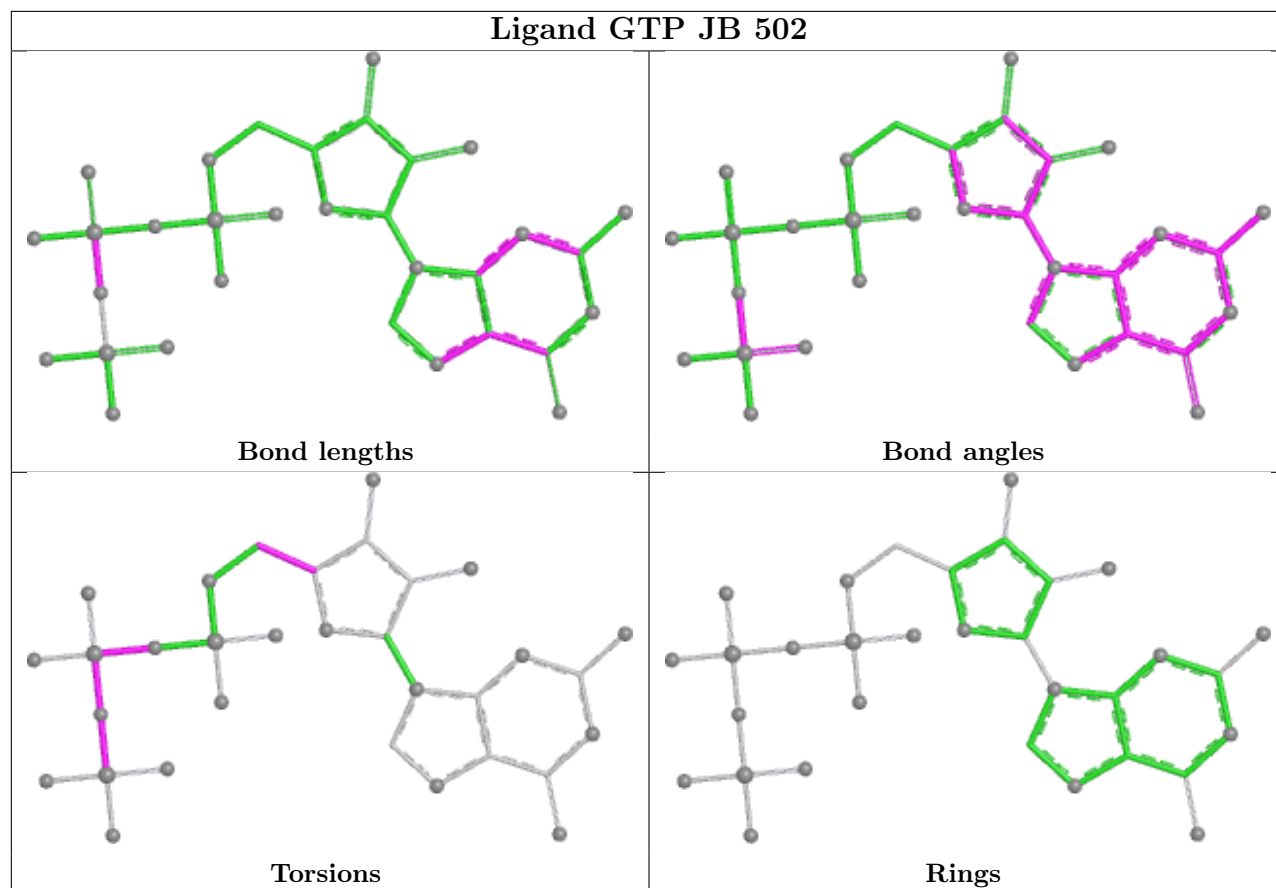


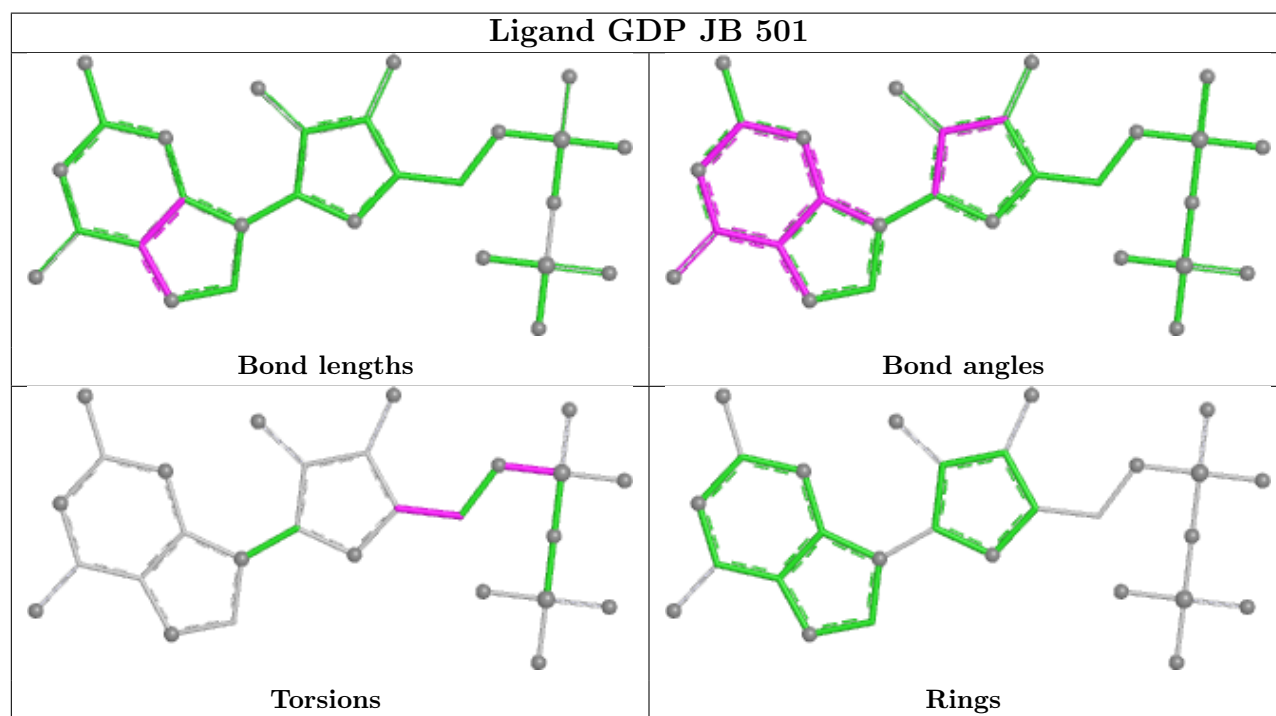
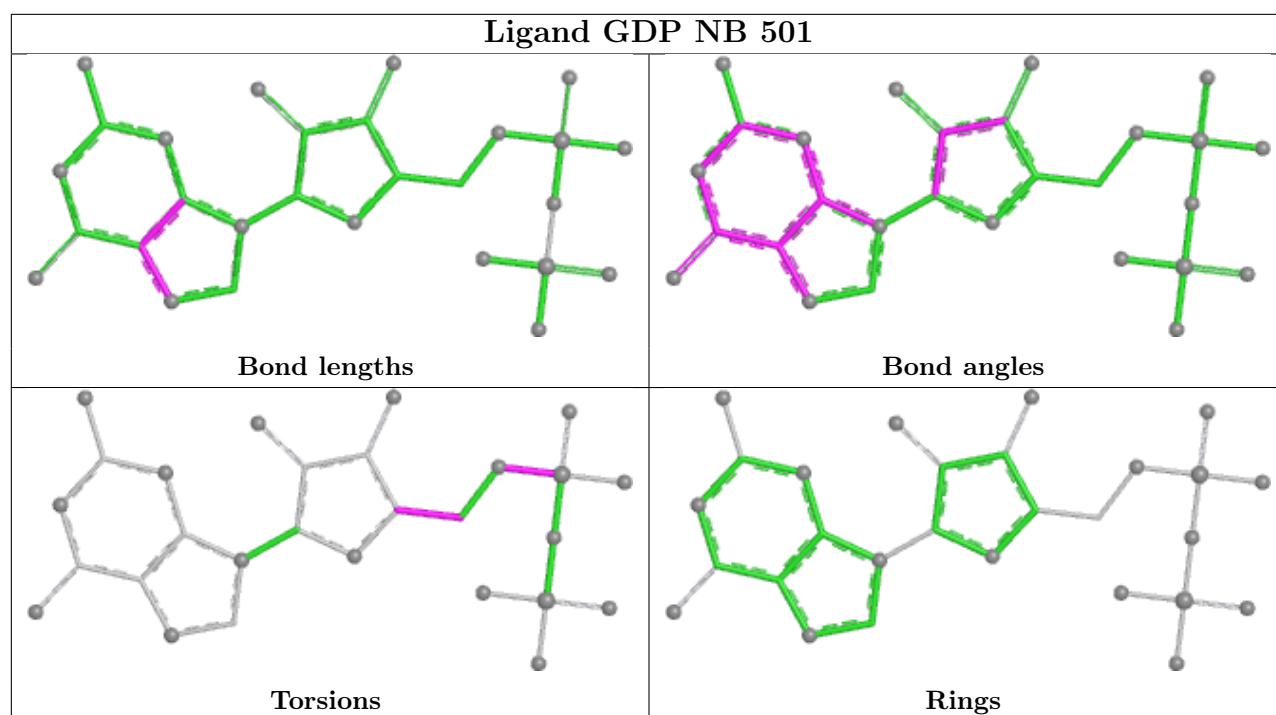


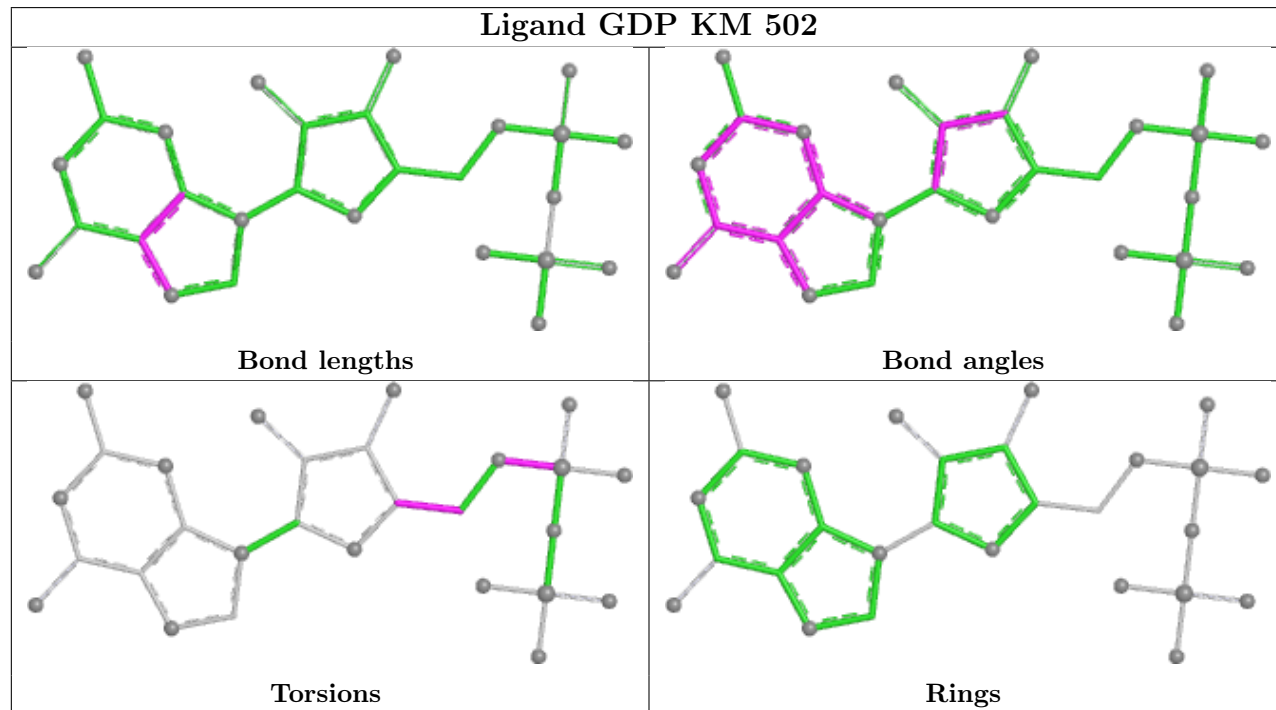
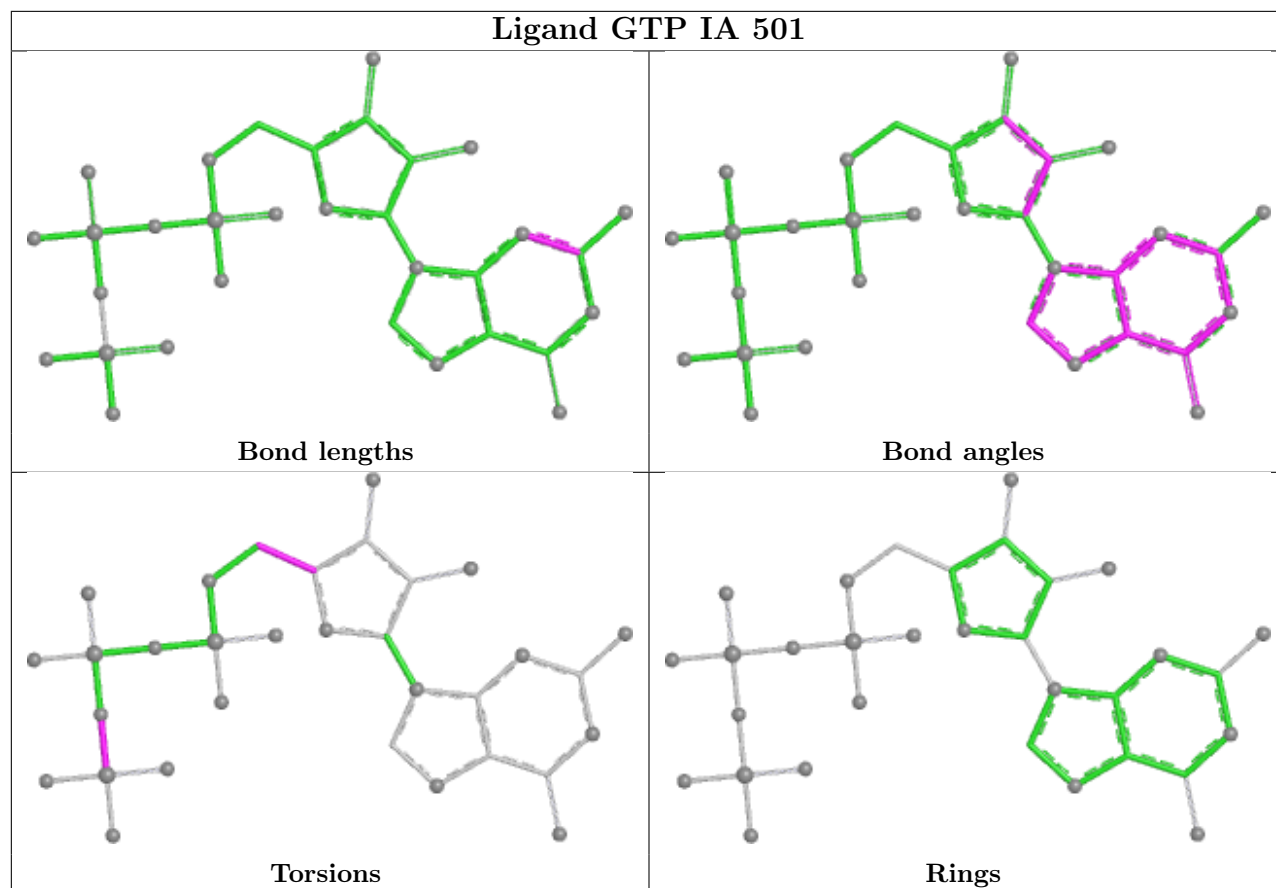


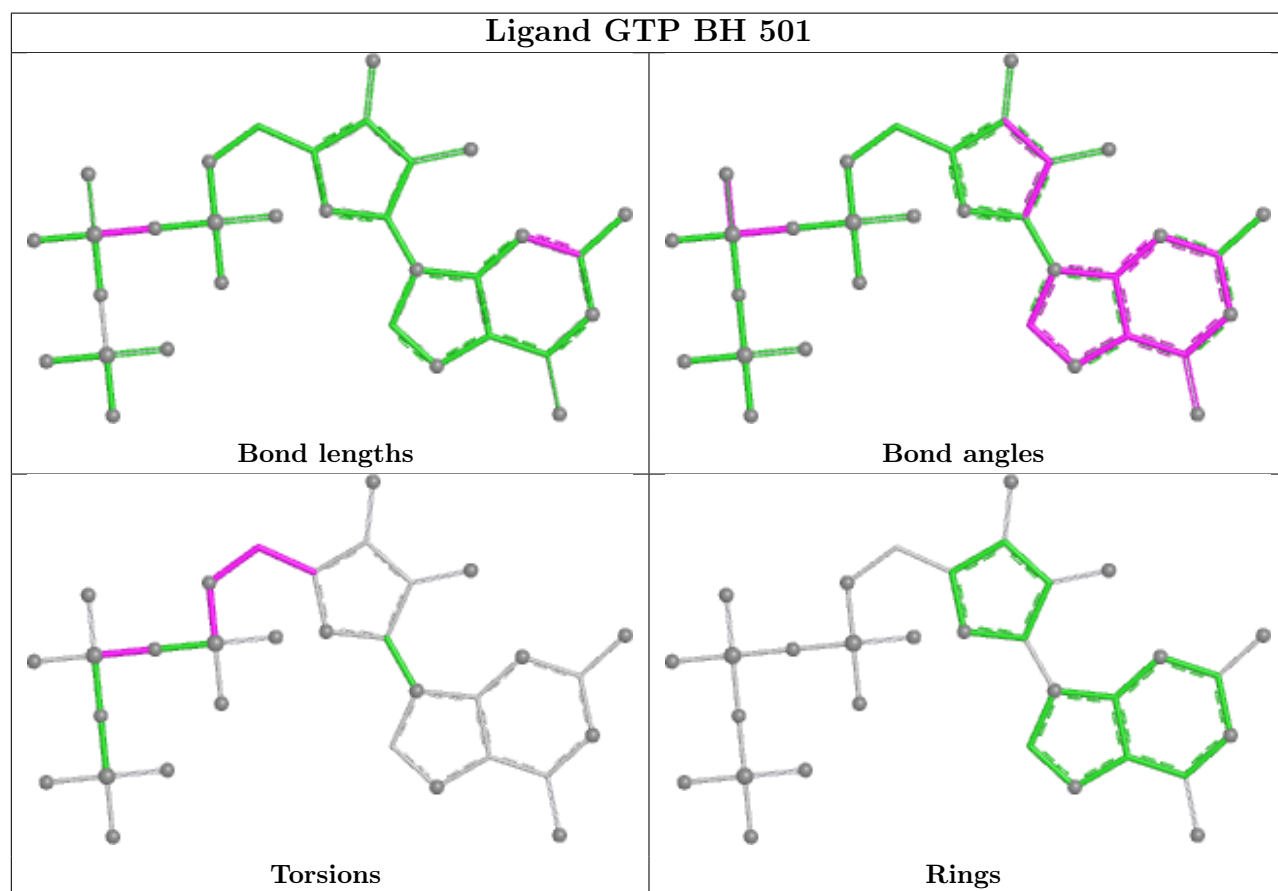
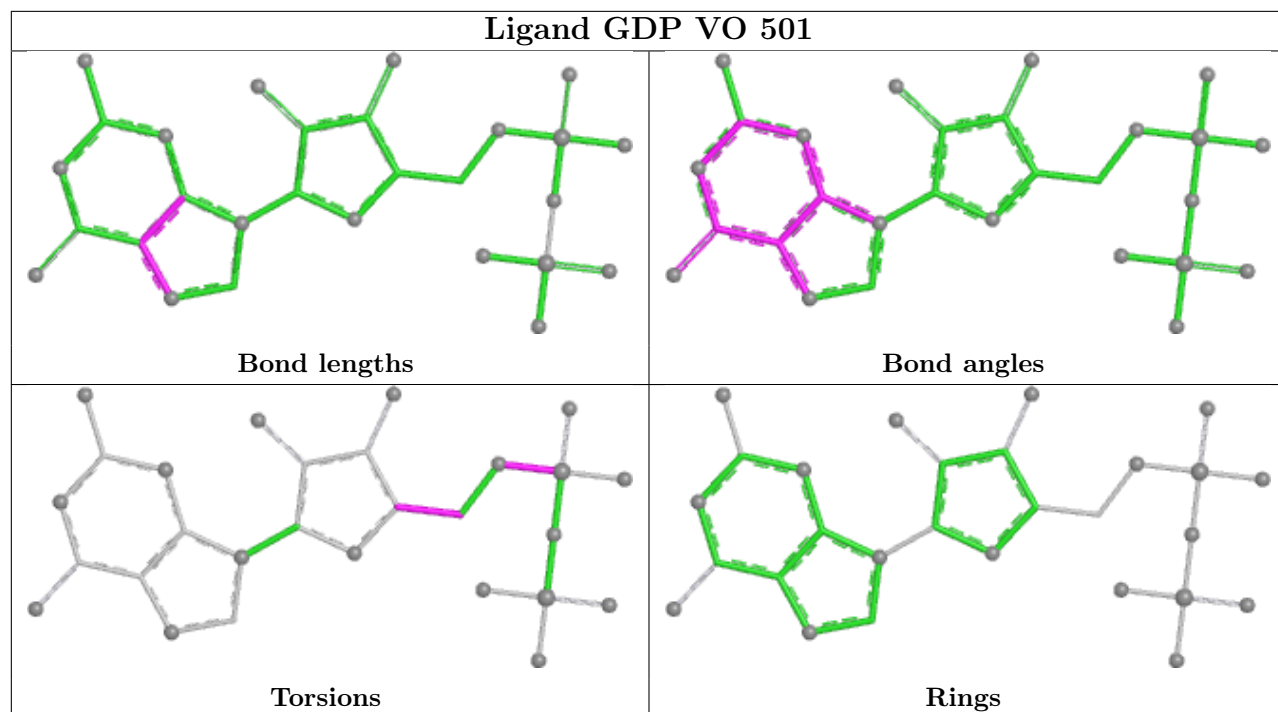


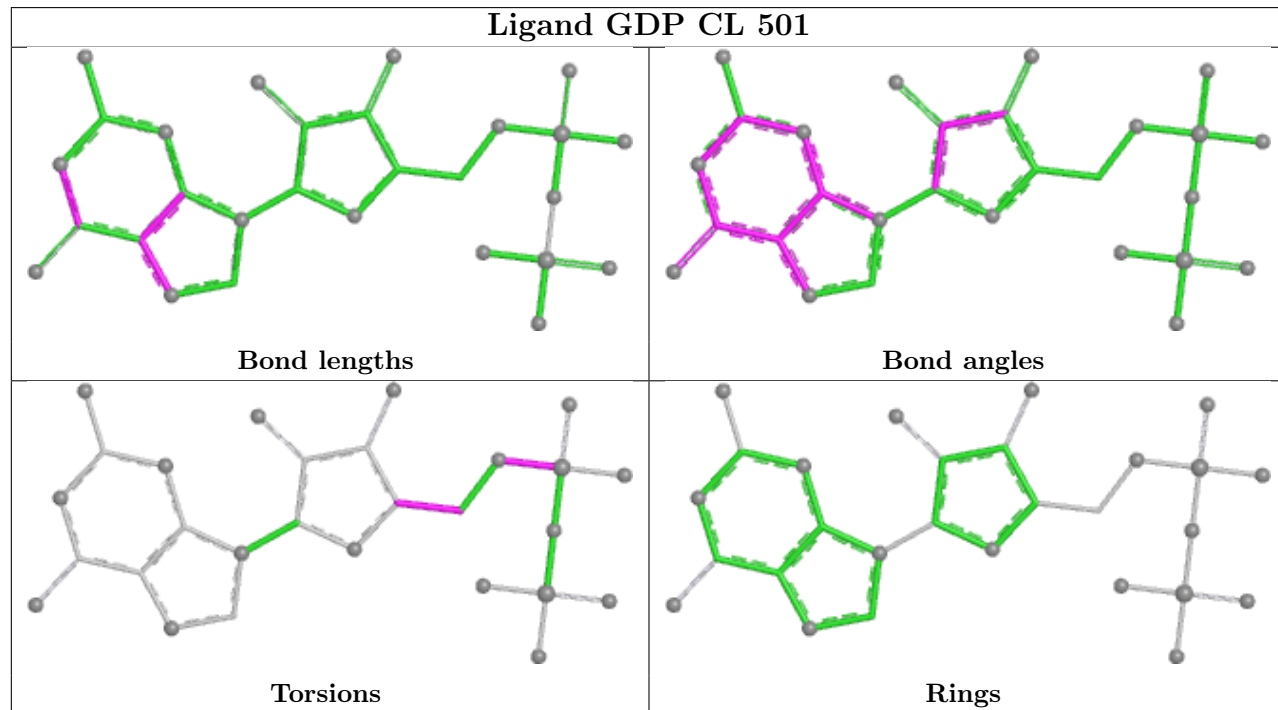
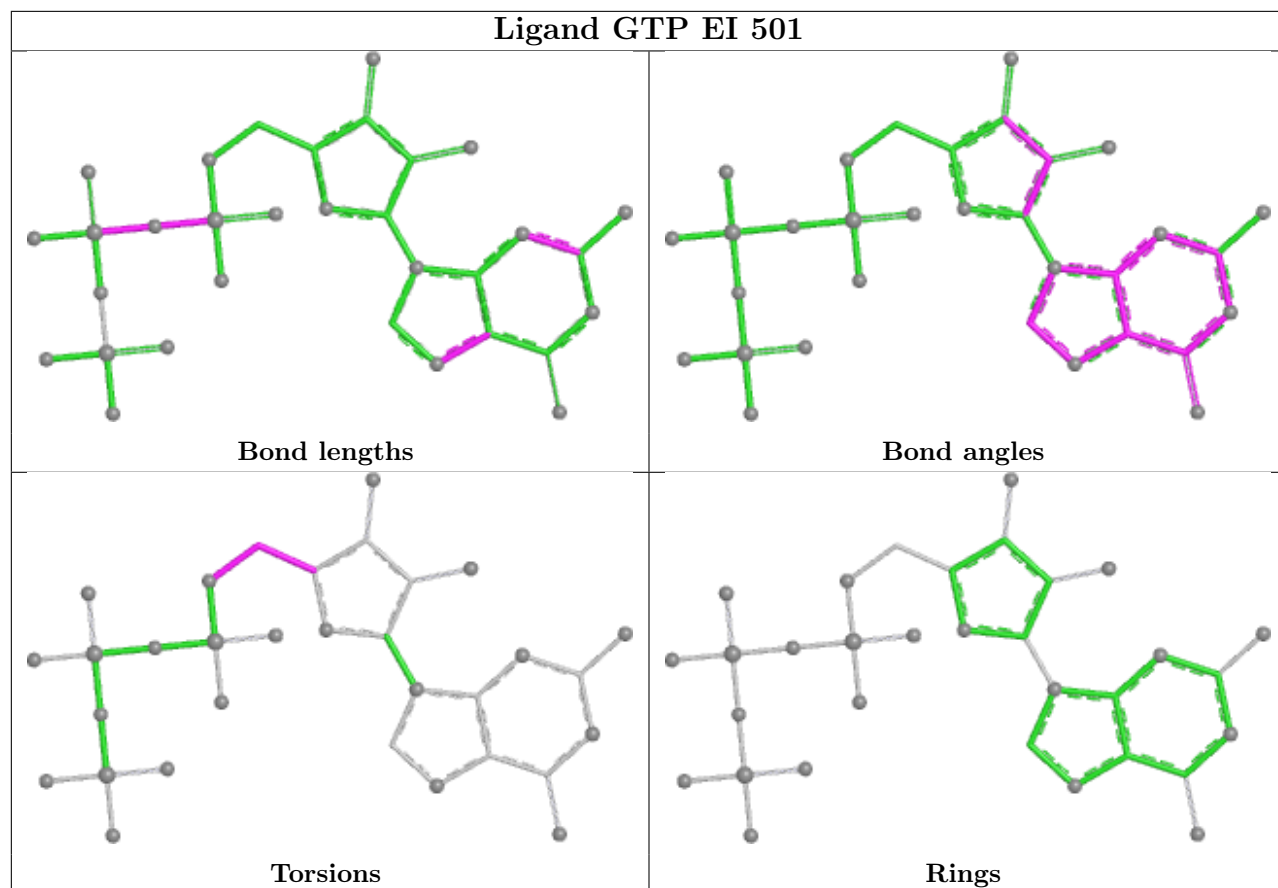


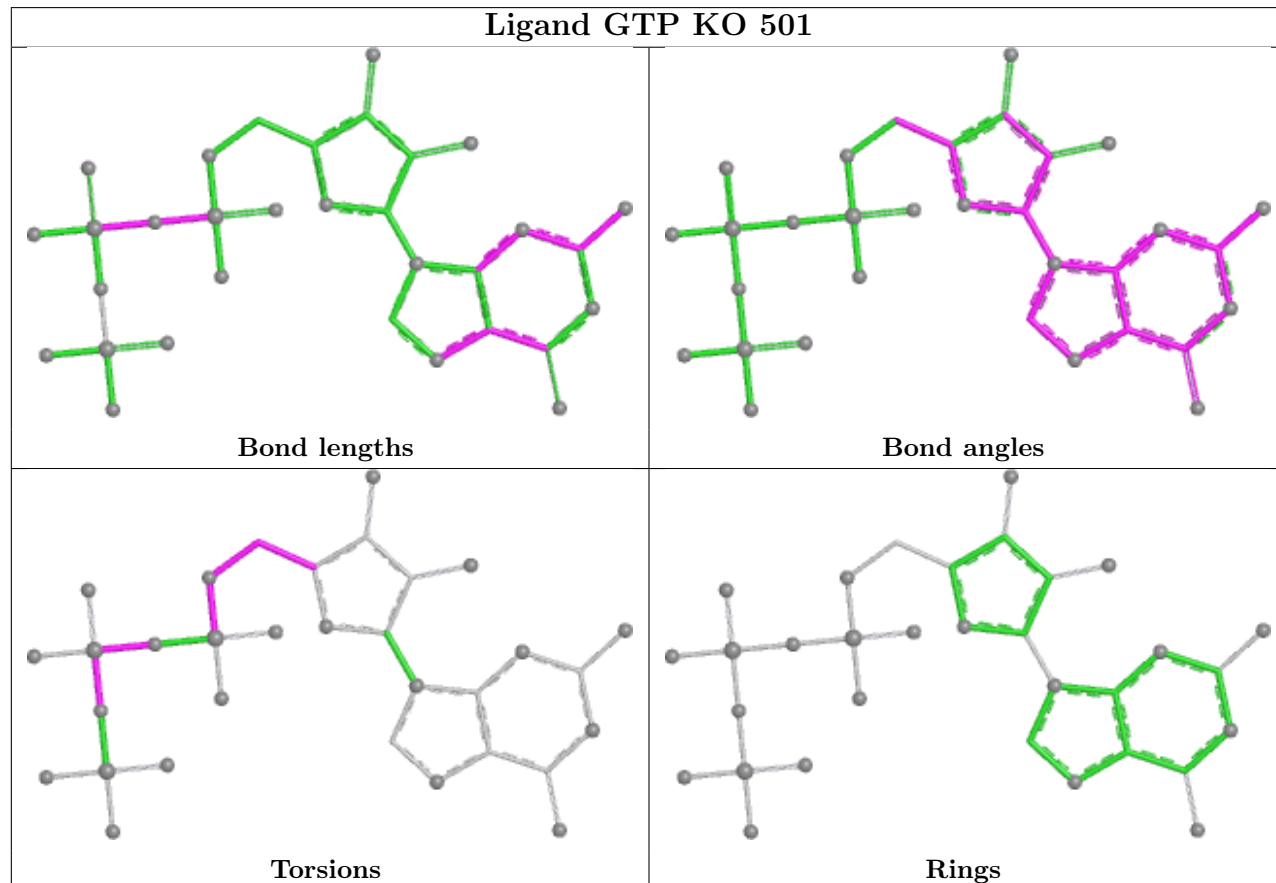
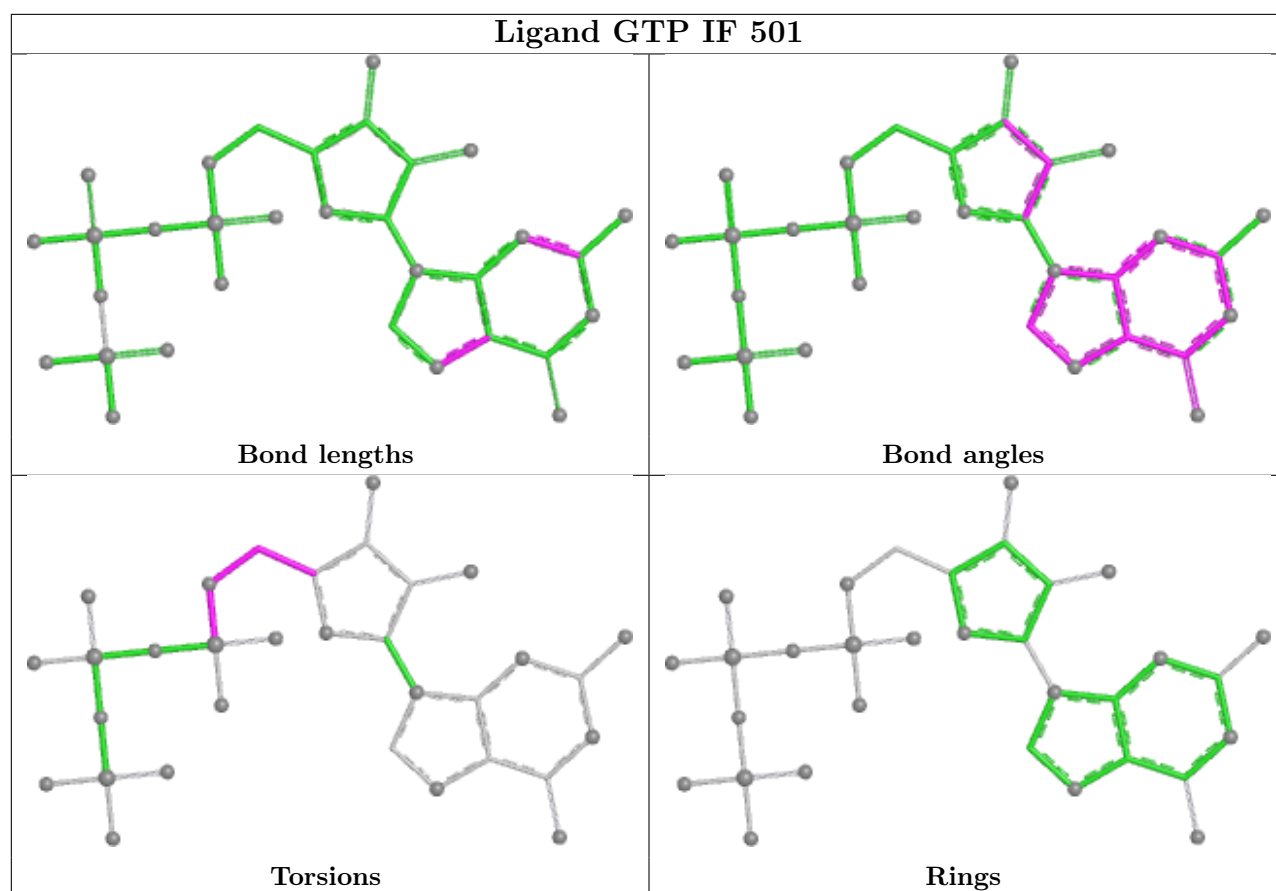




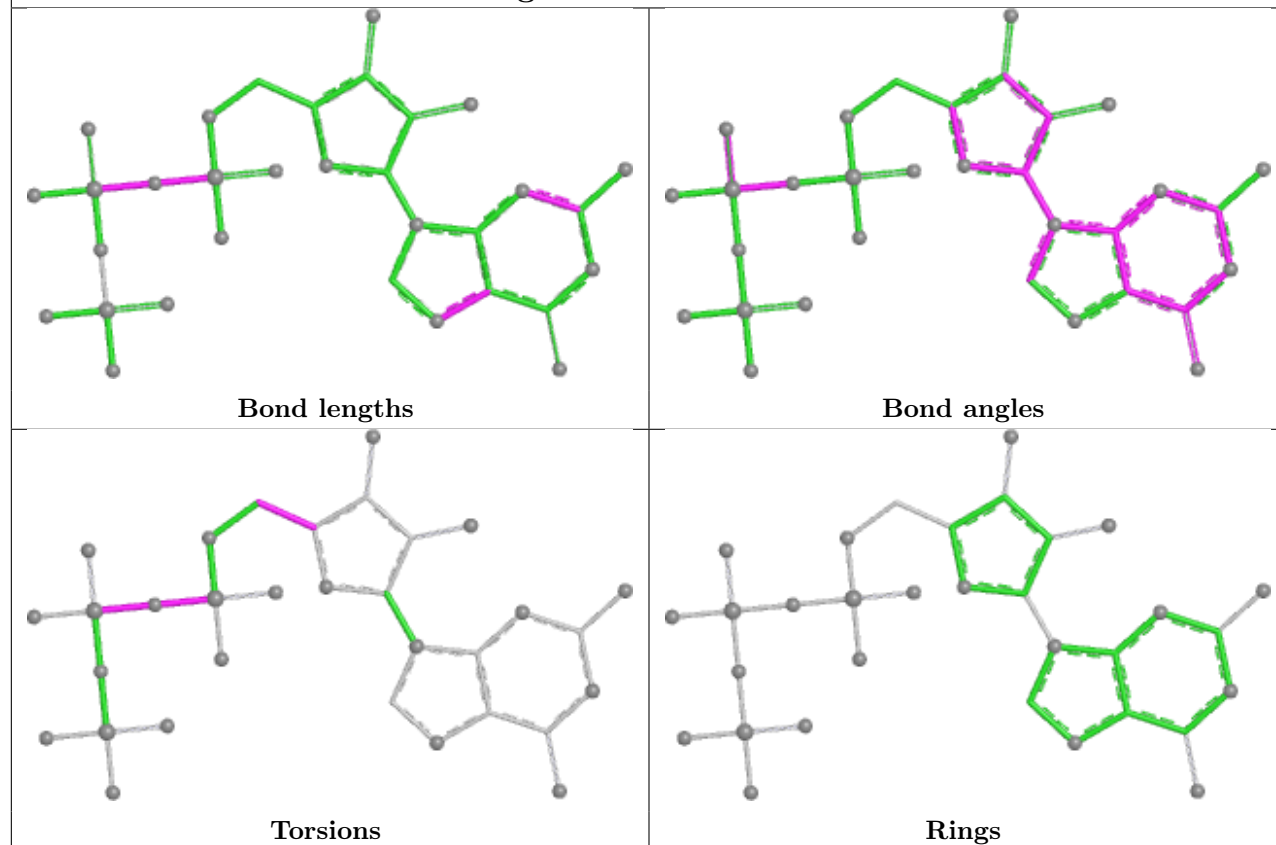




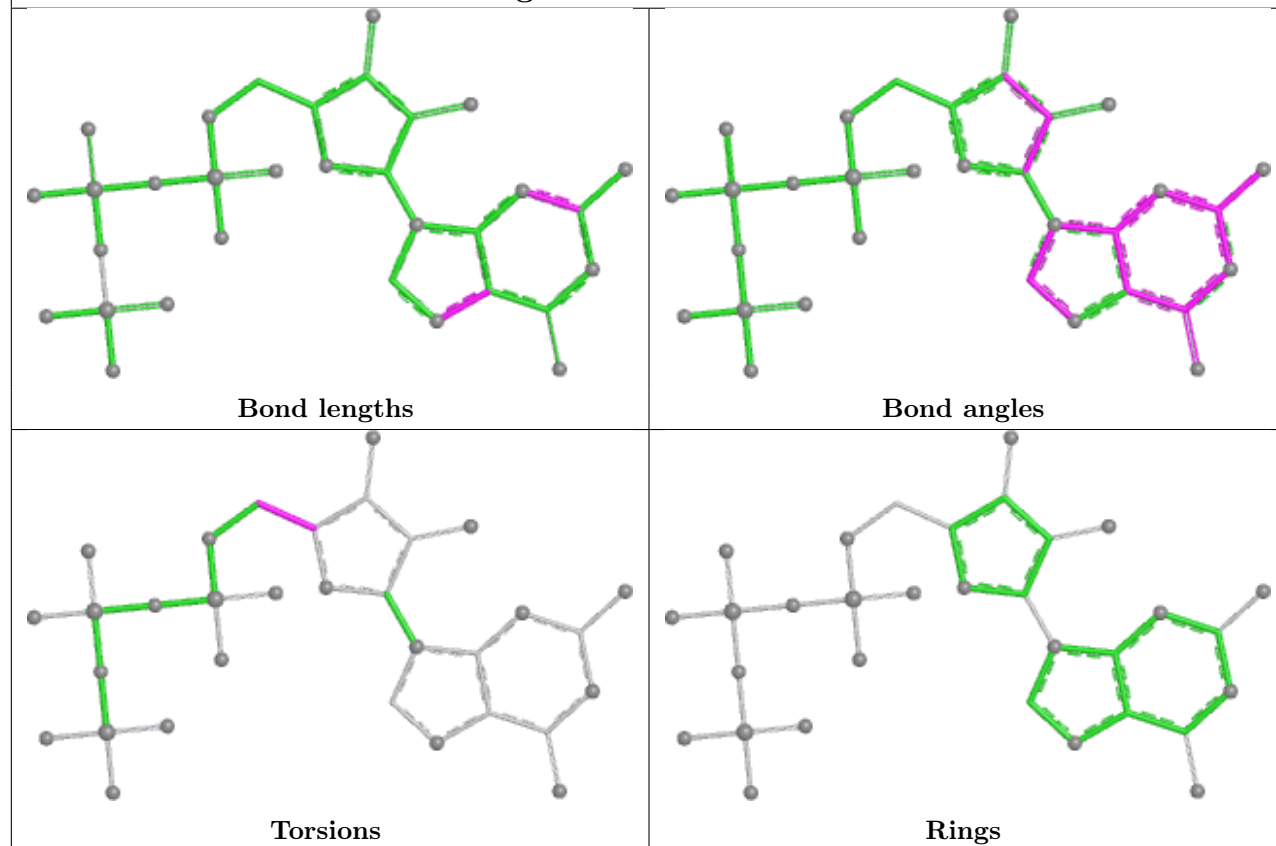




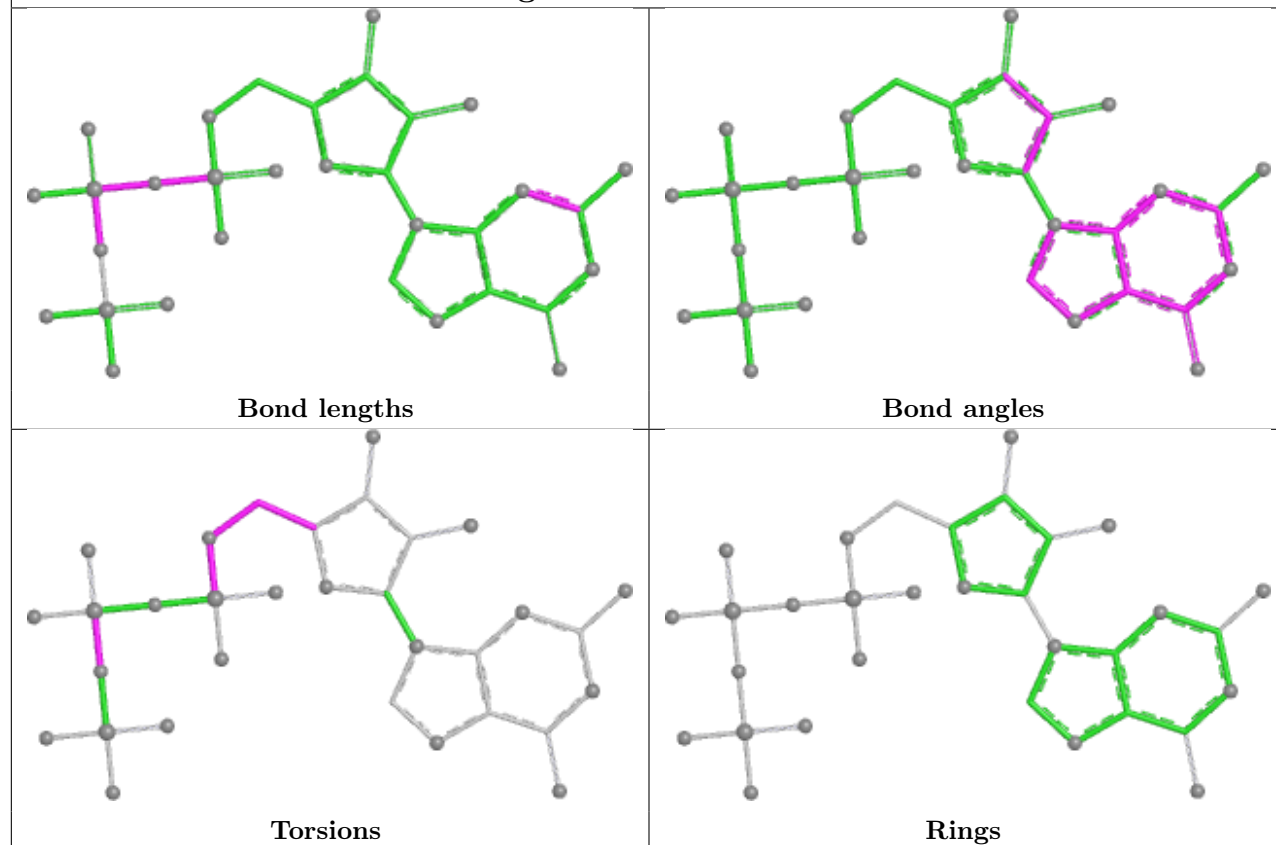
Ligand GTP GP 501



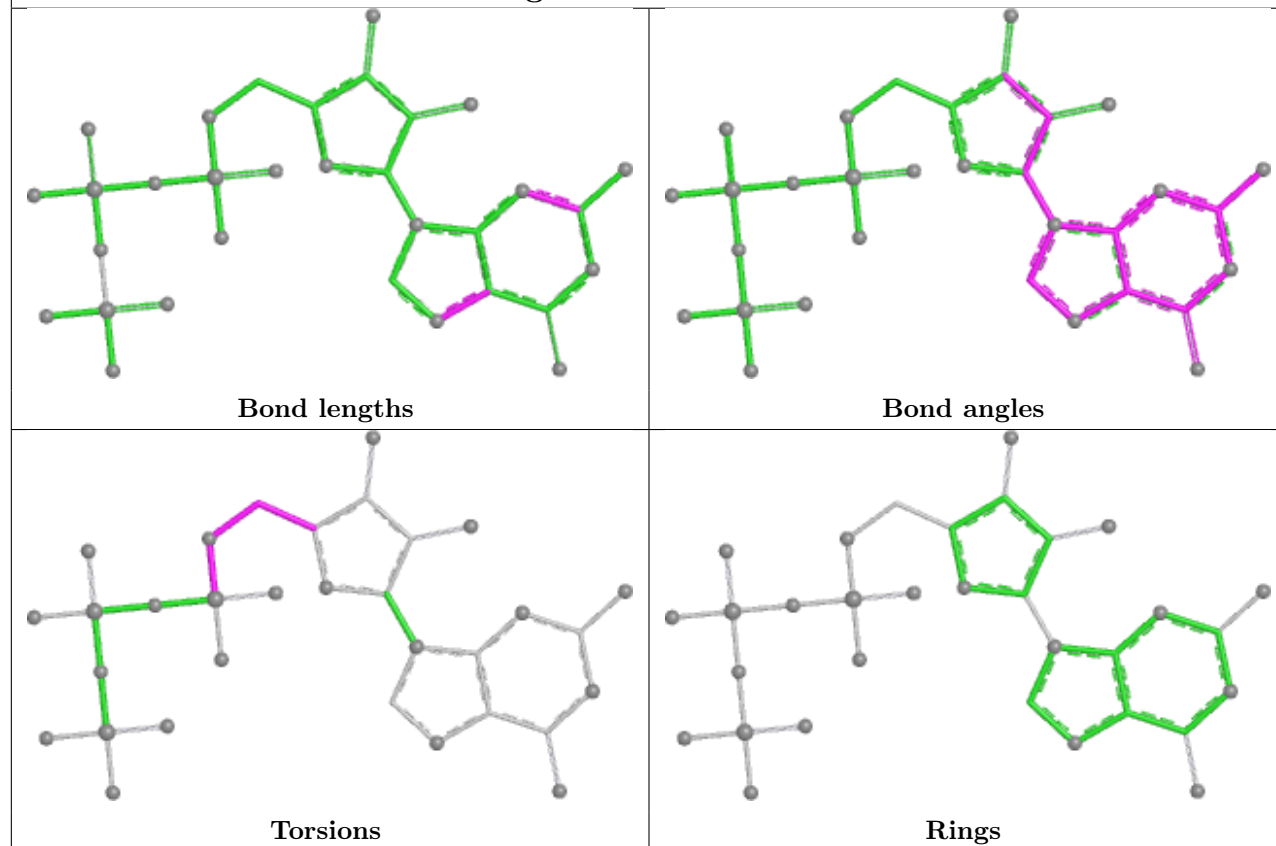
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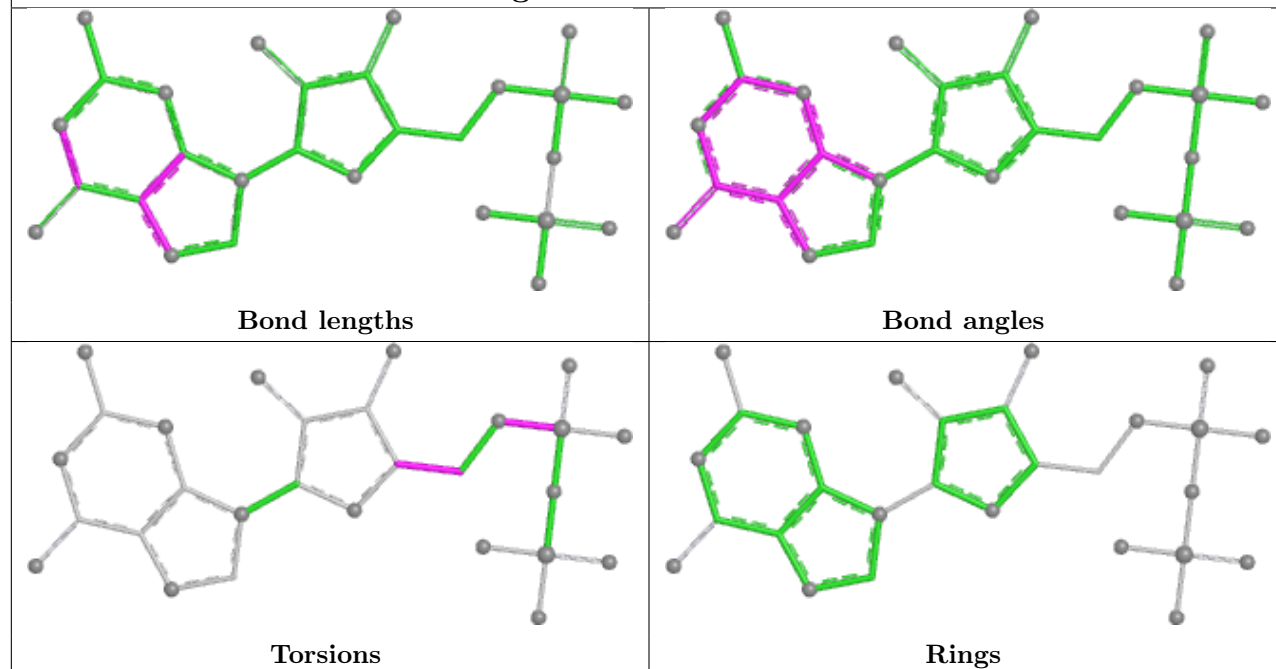
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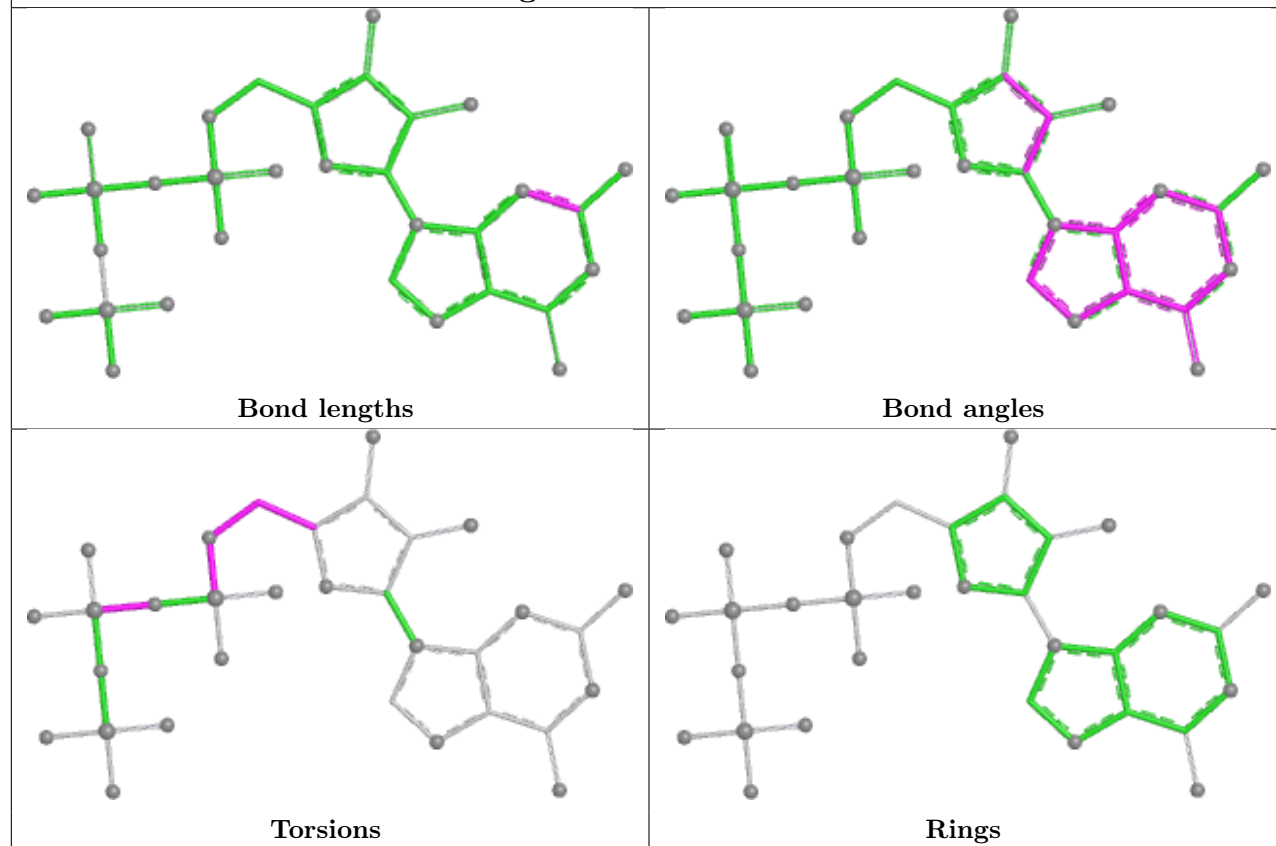
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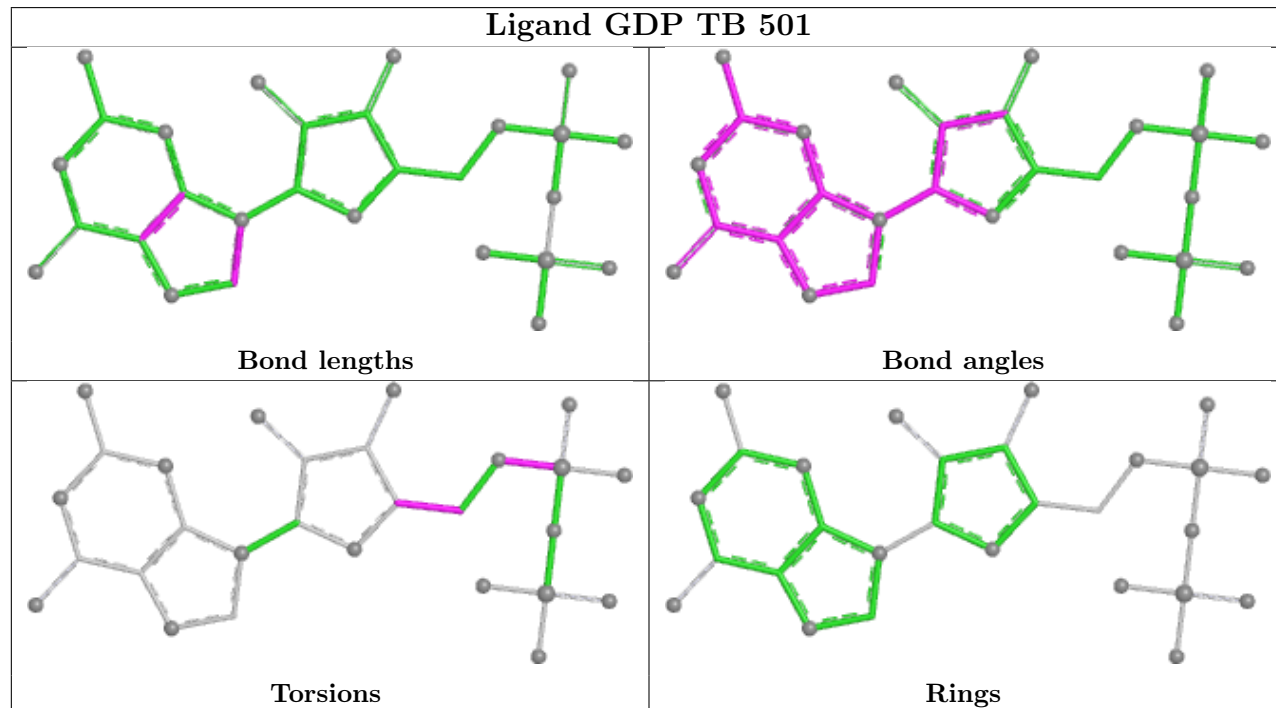
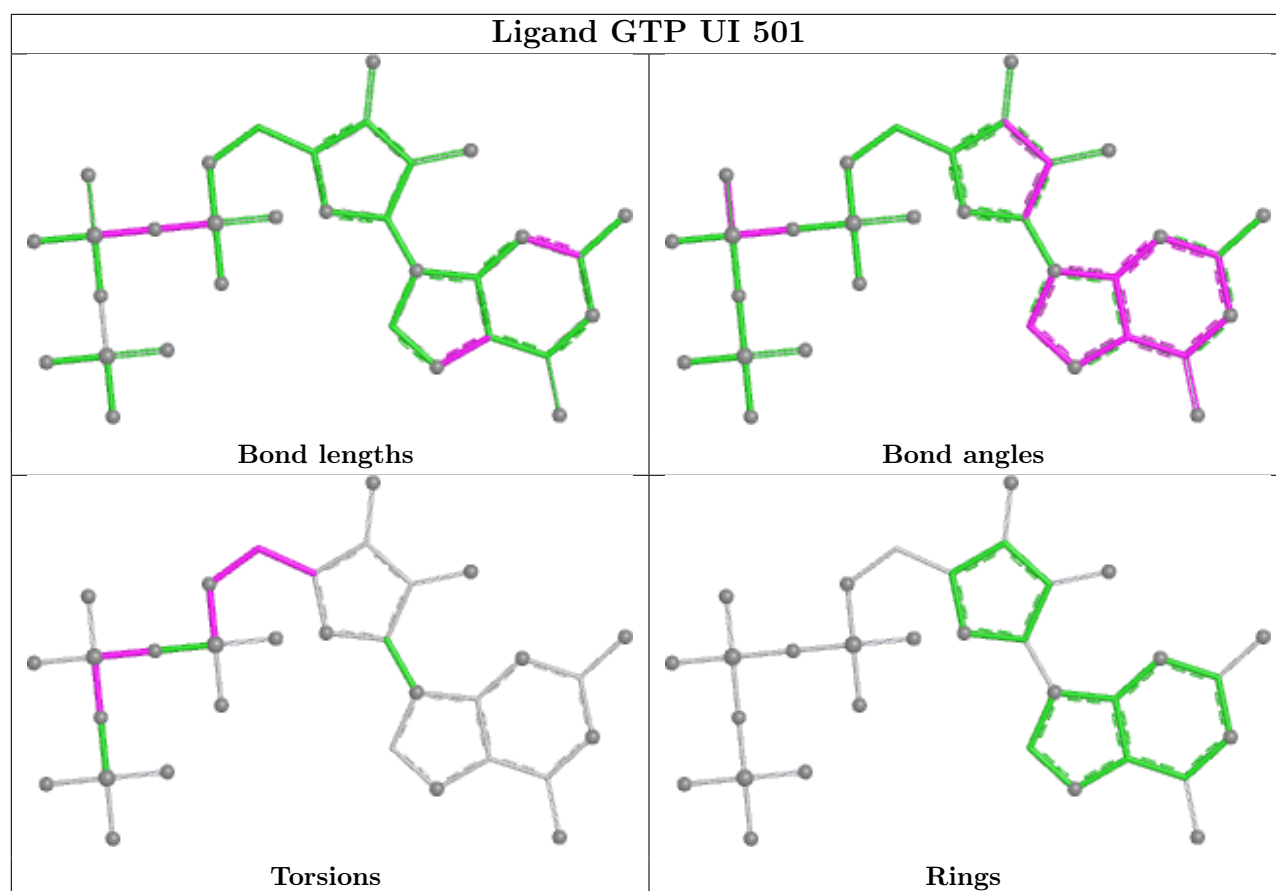


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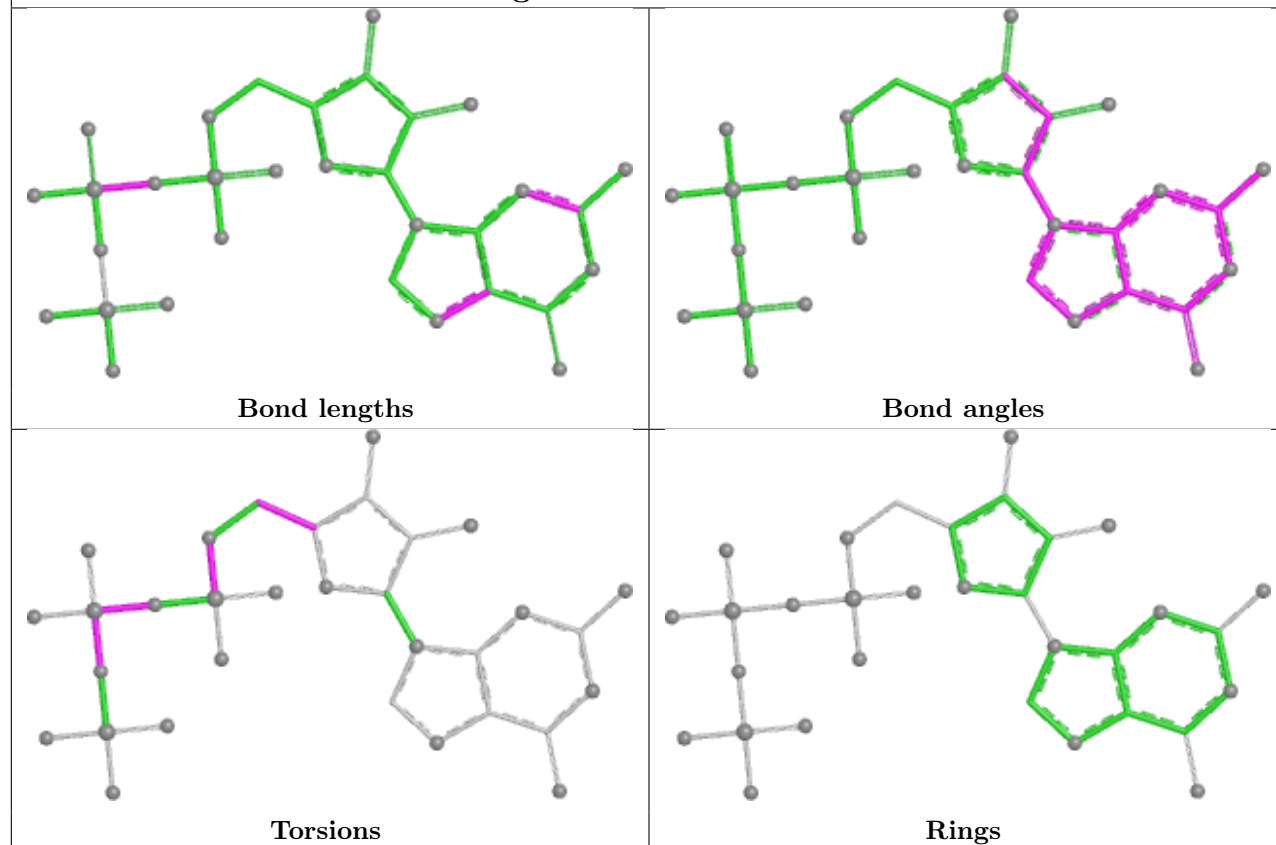


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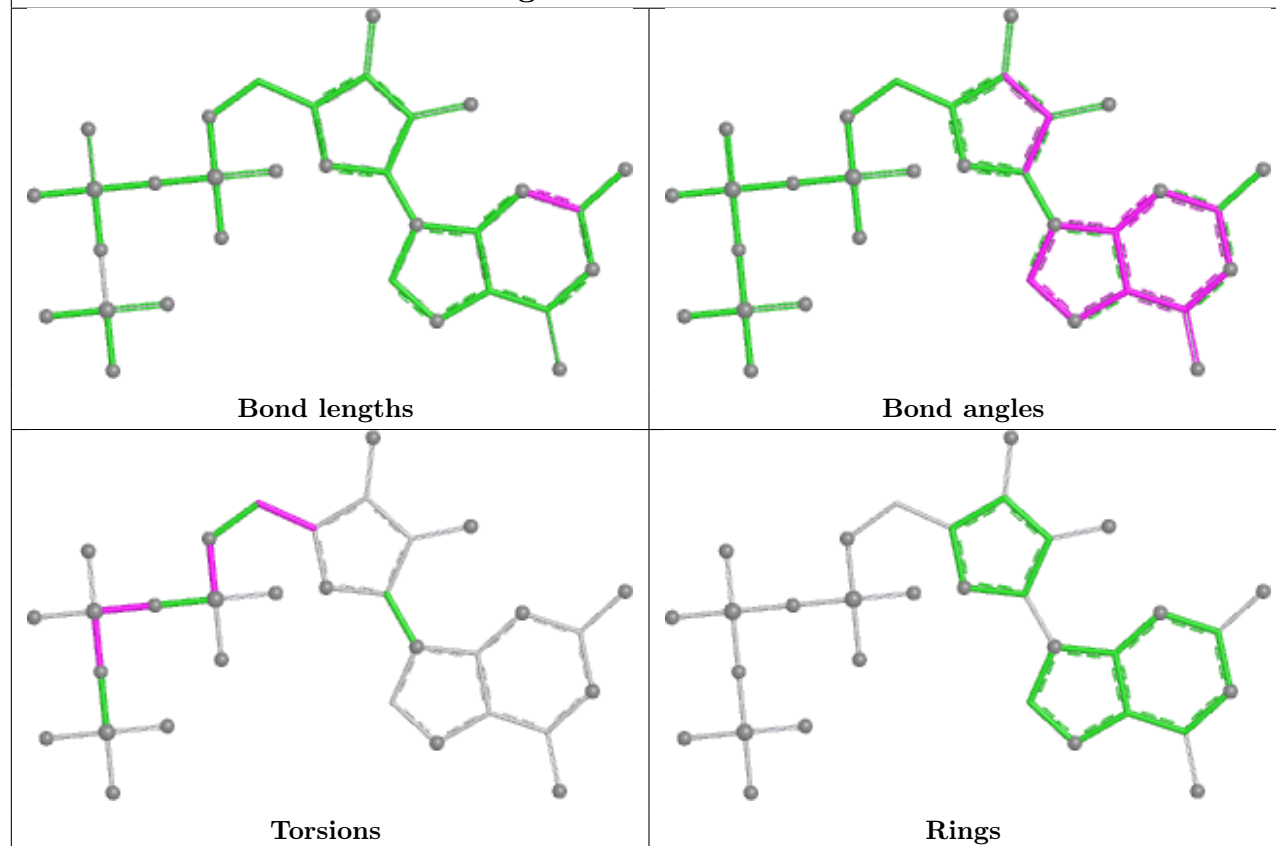




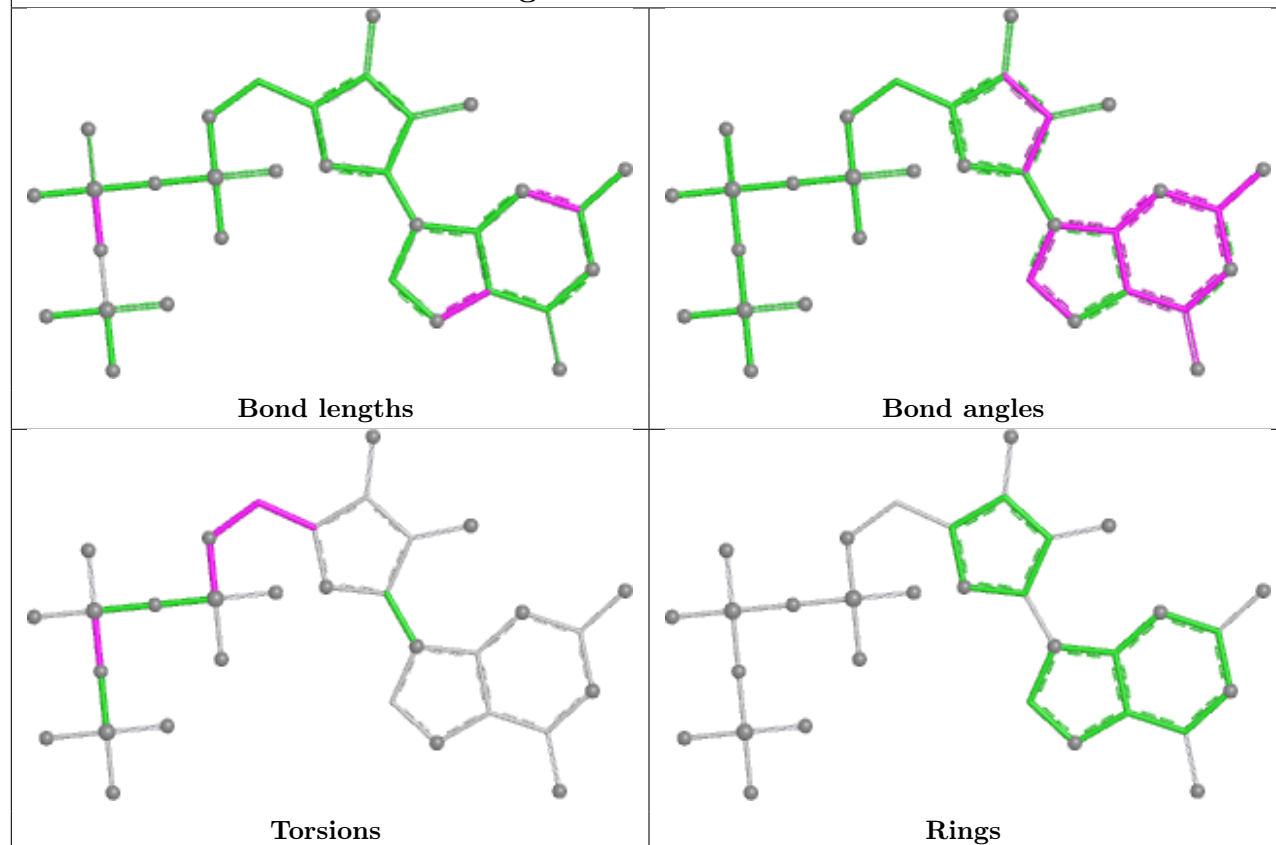
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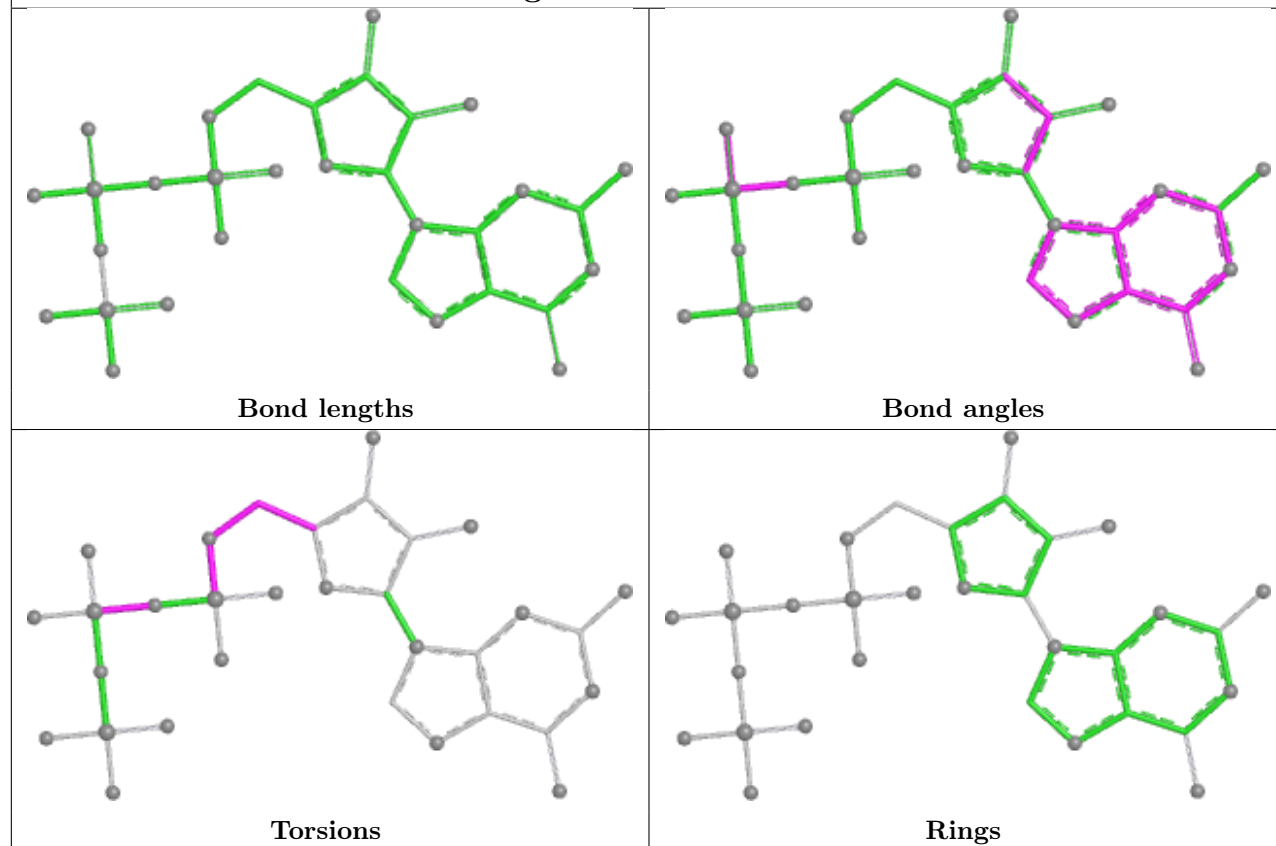
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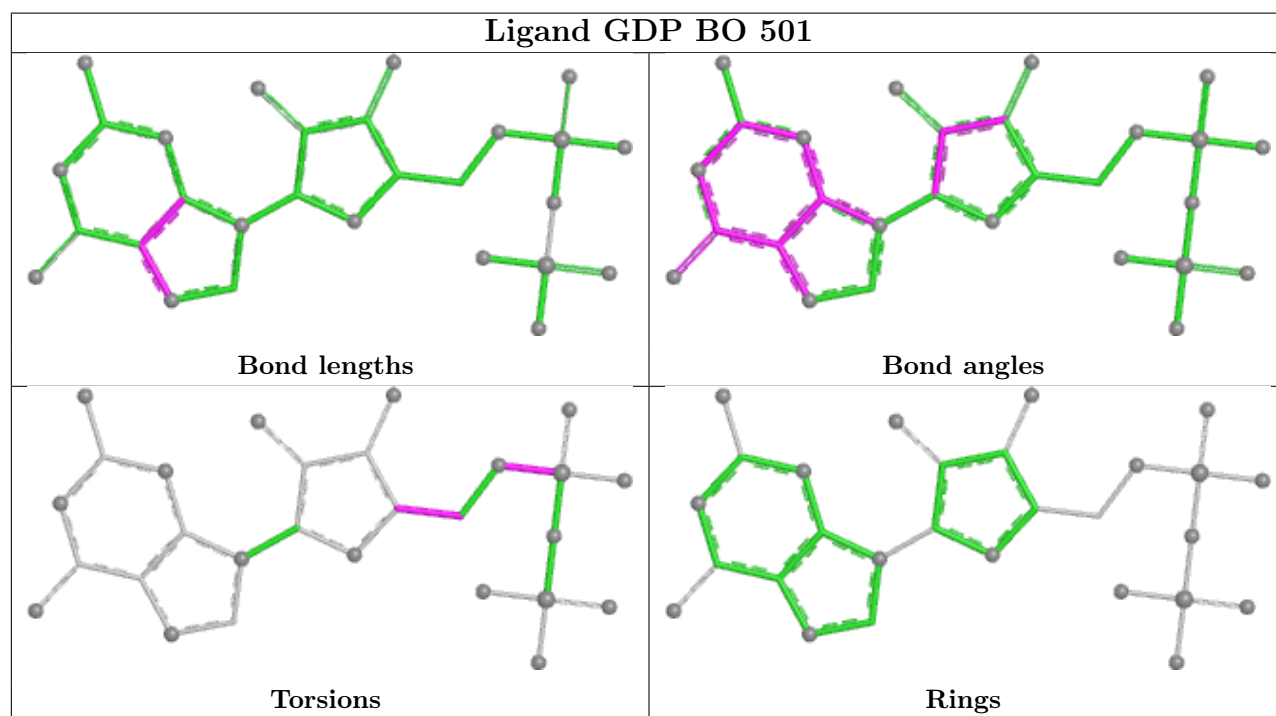
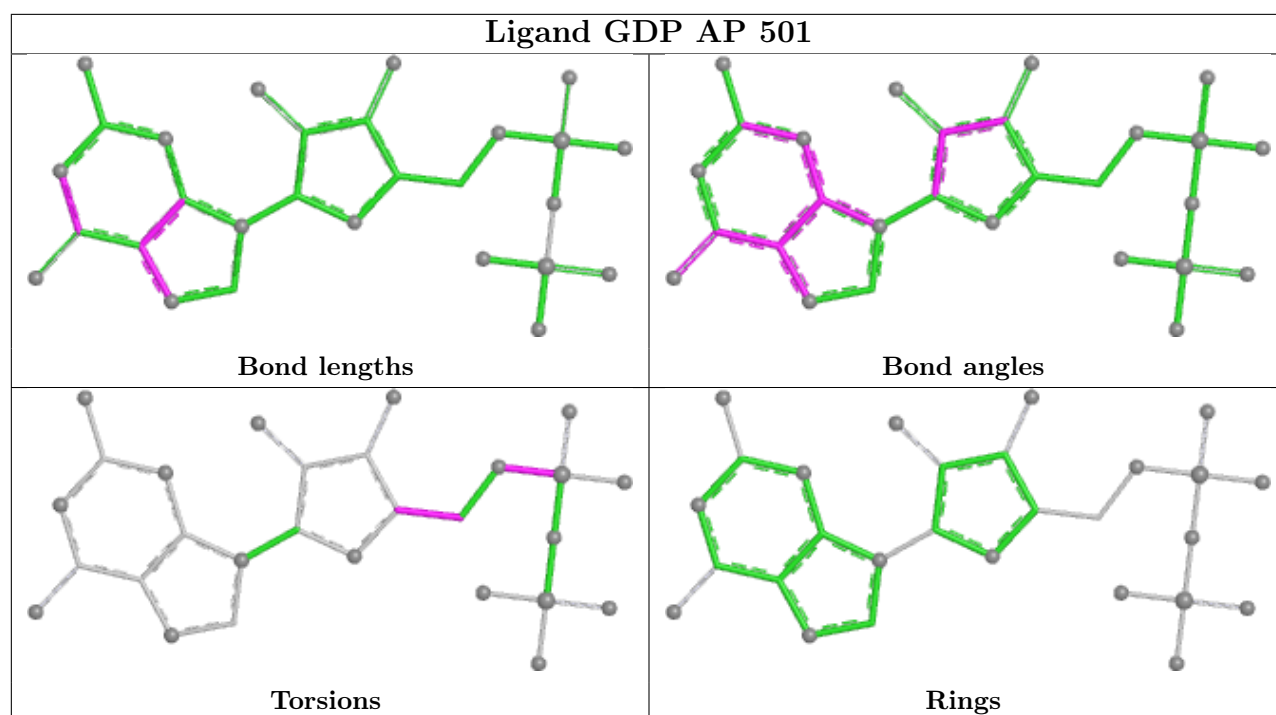


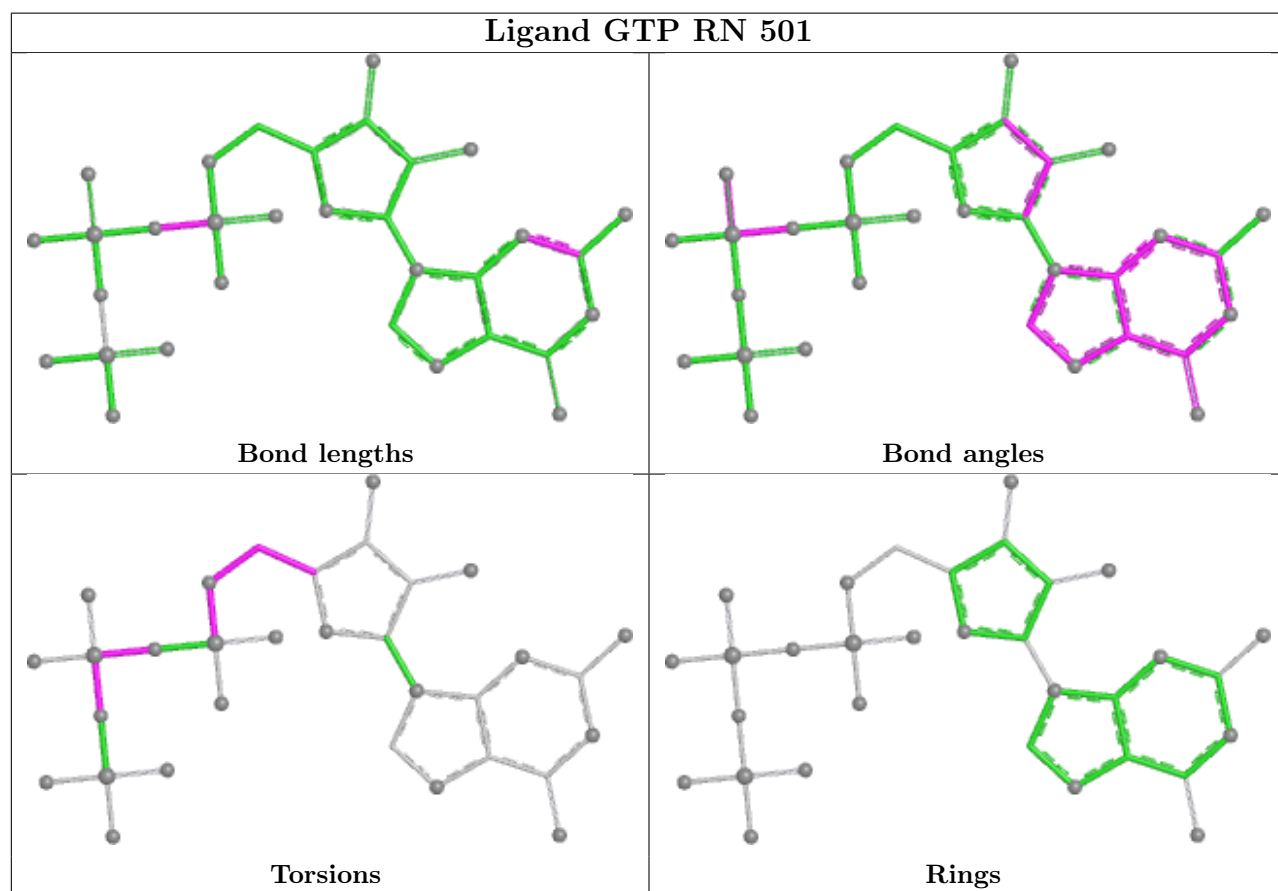
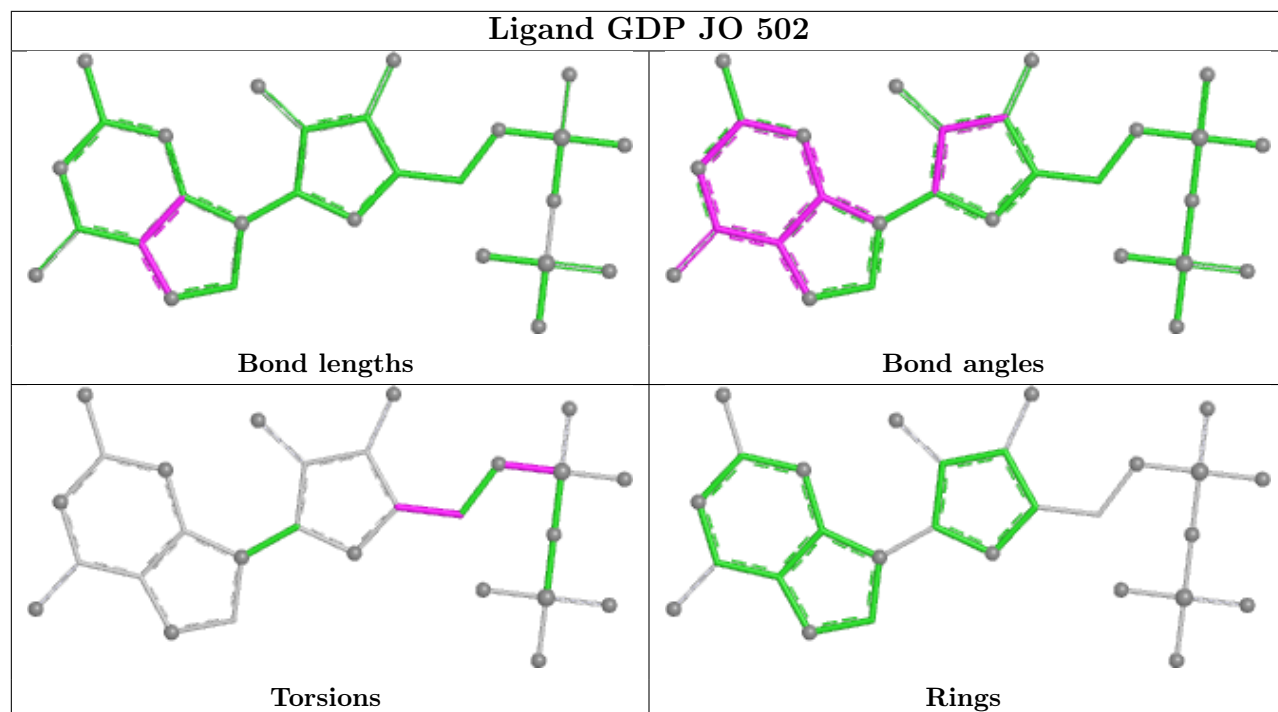
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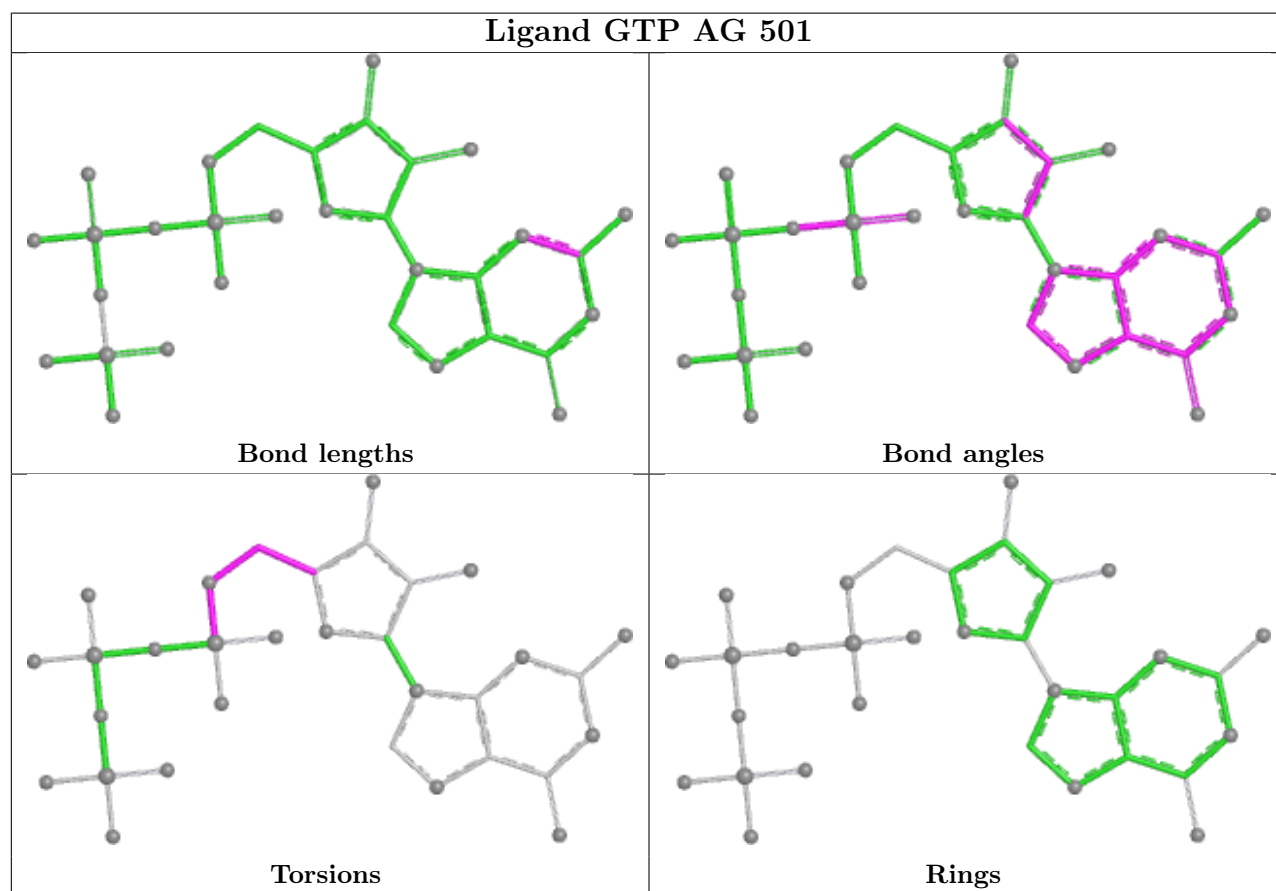
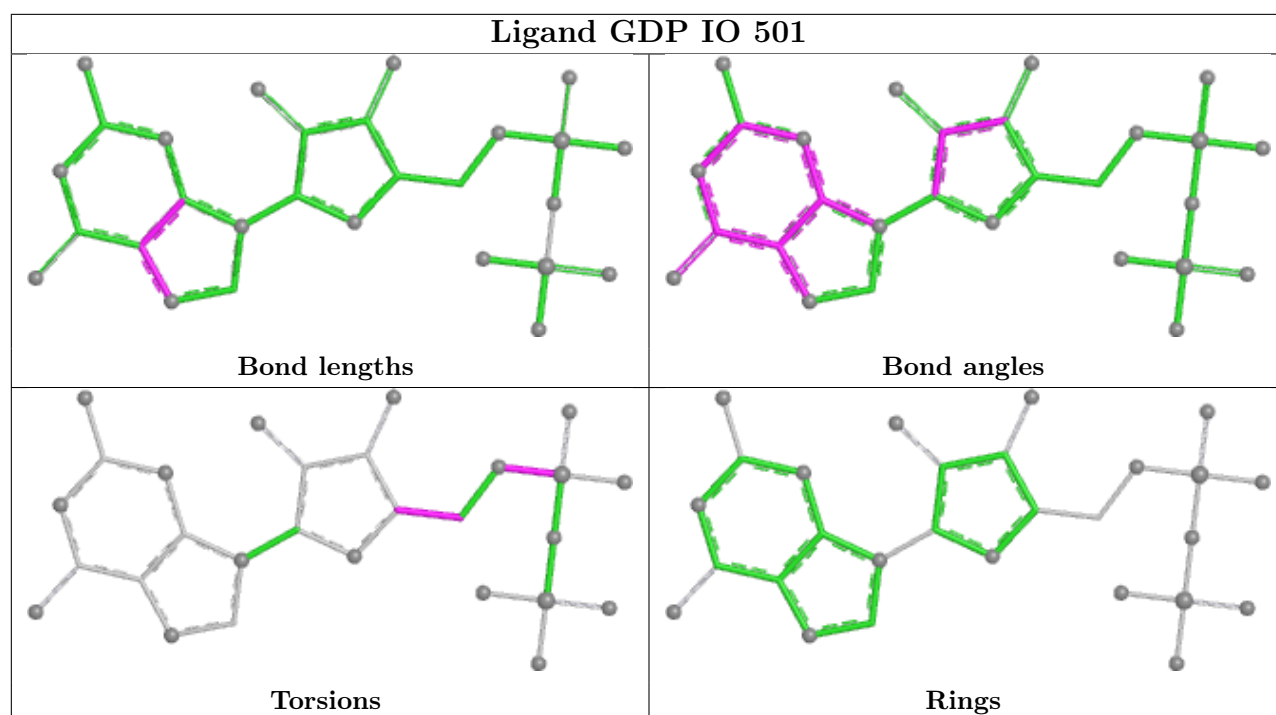


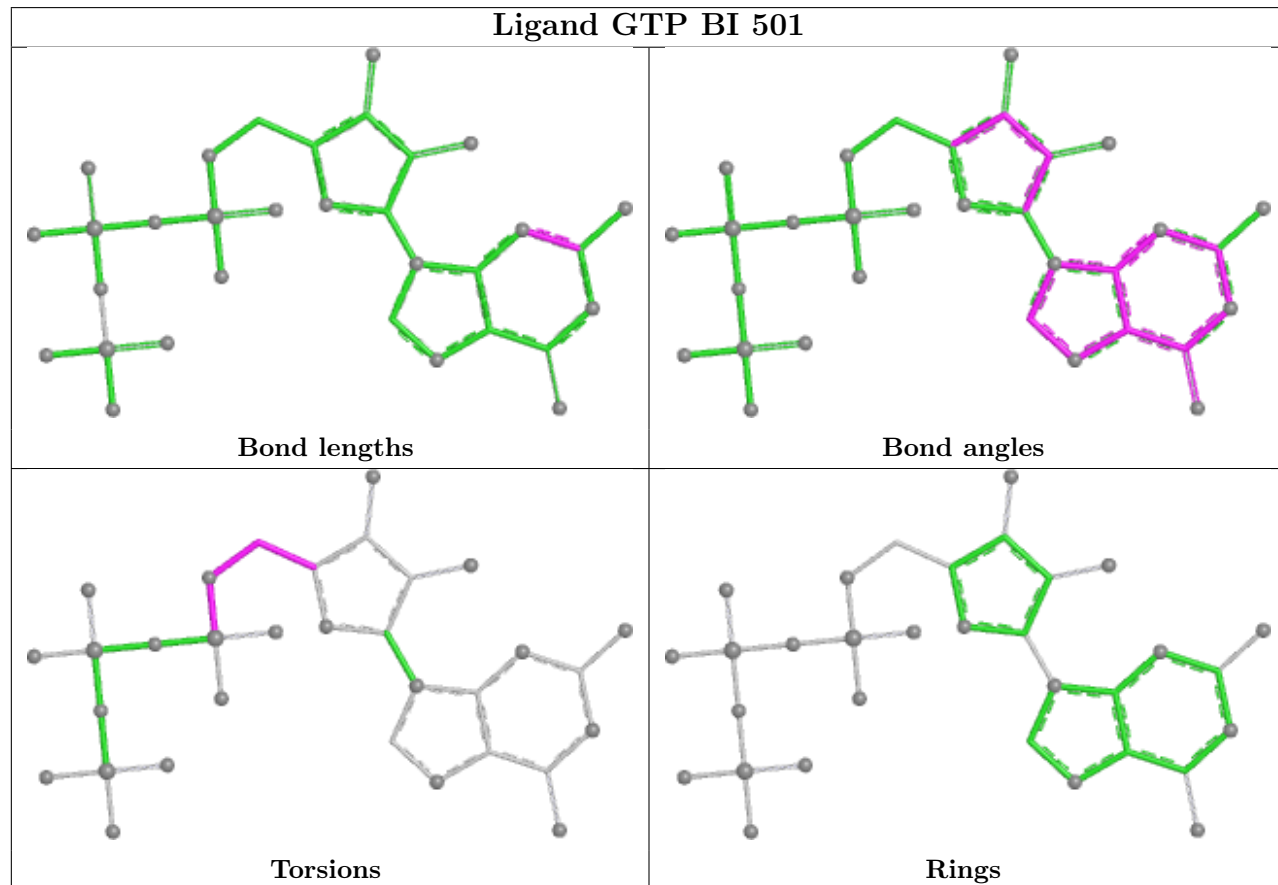
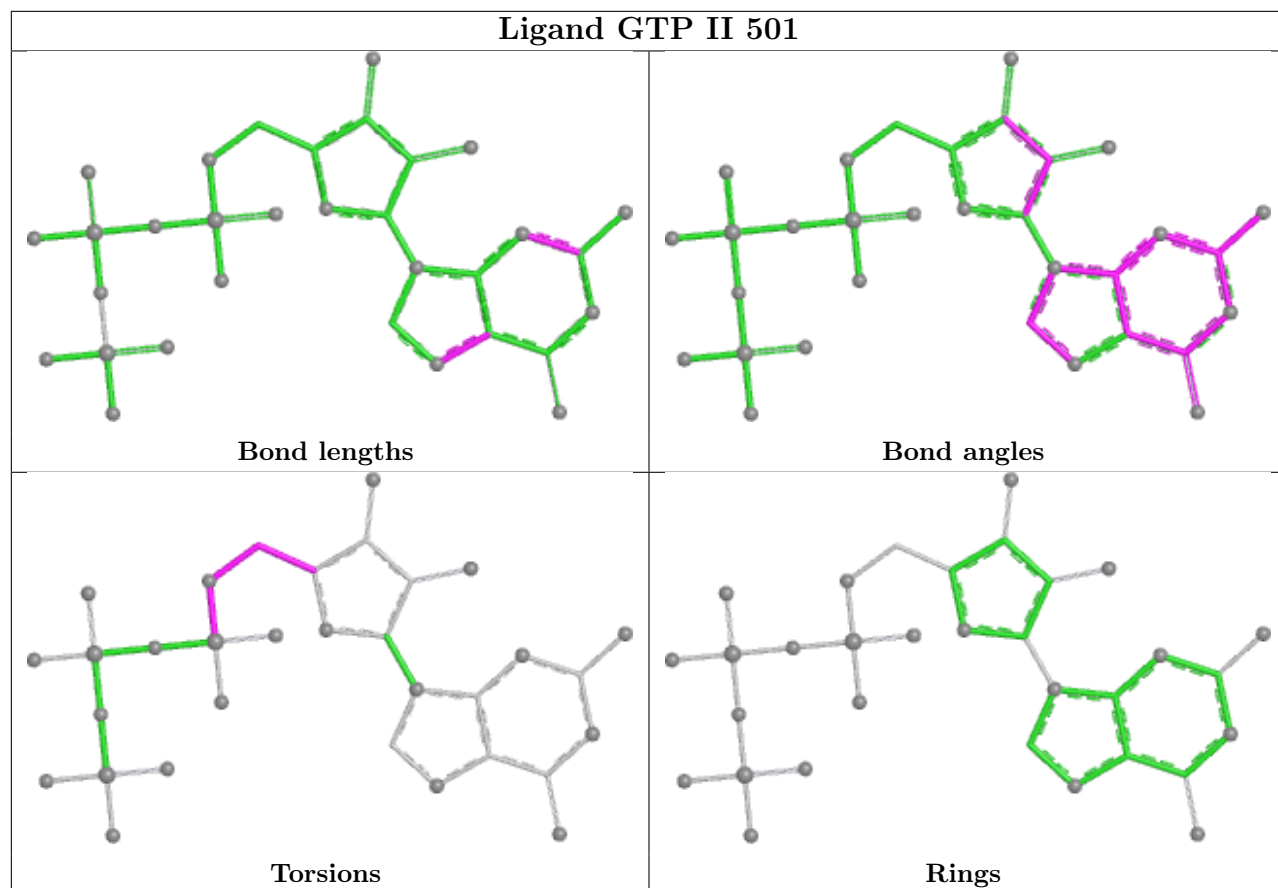
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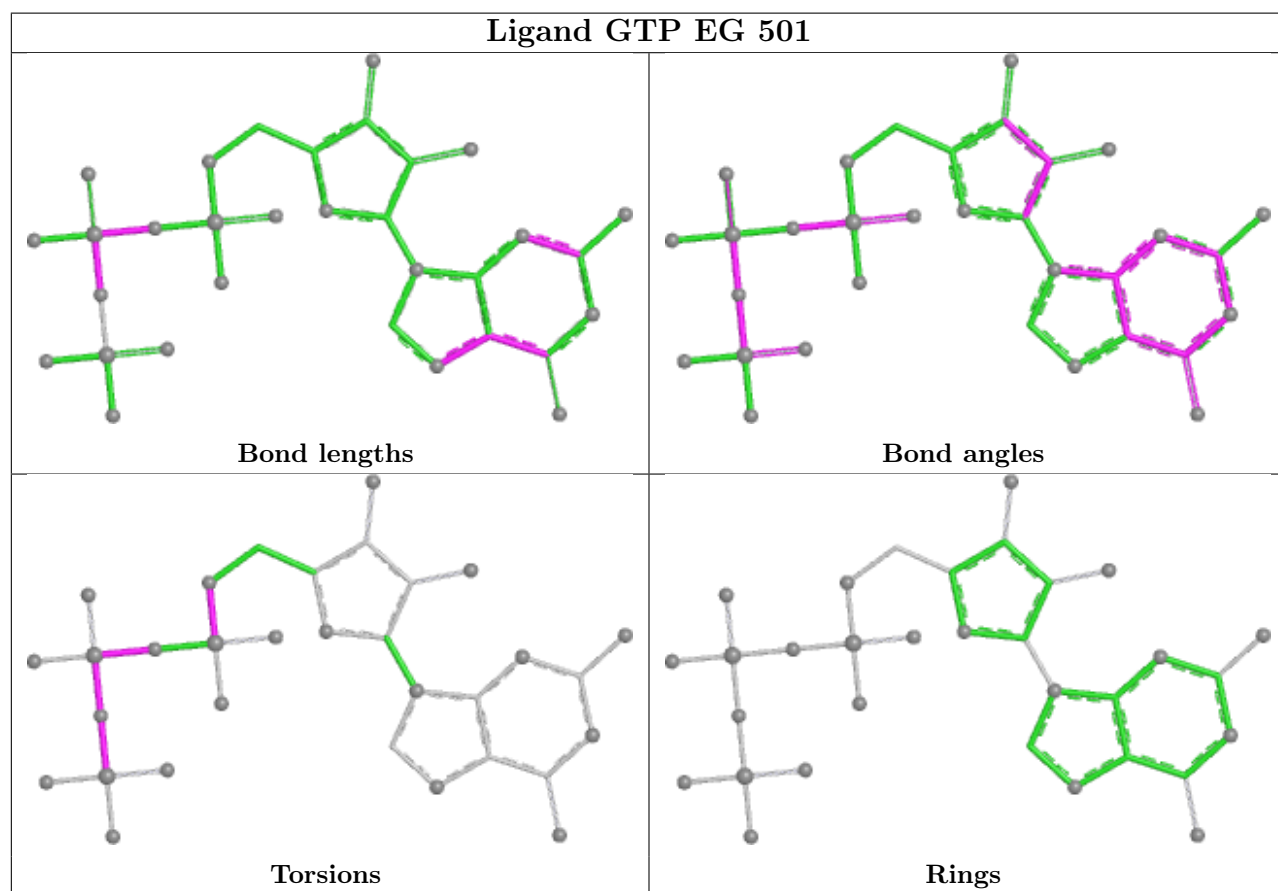
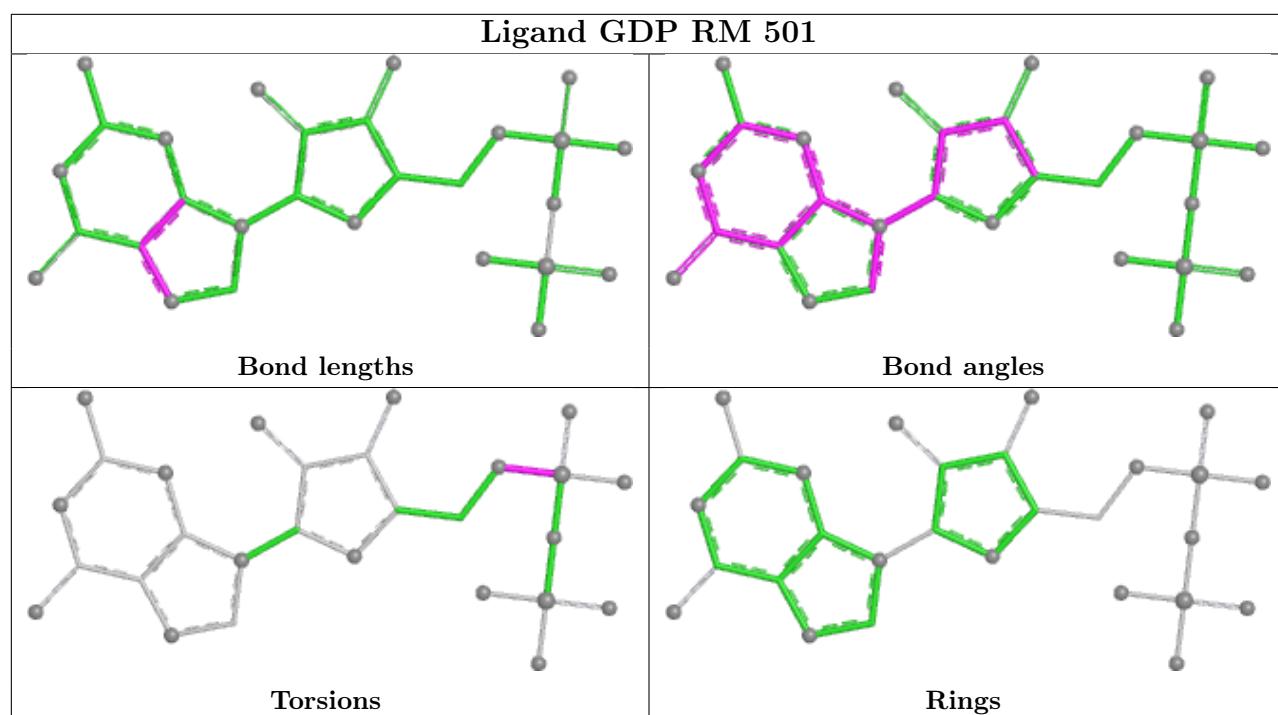


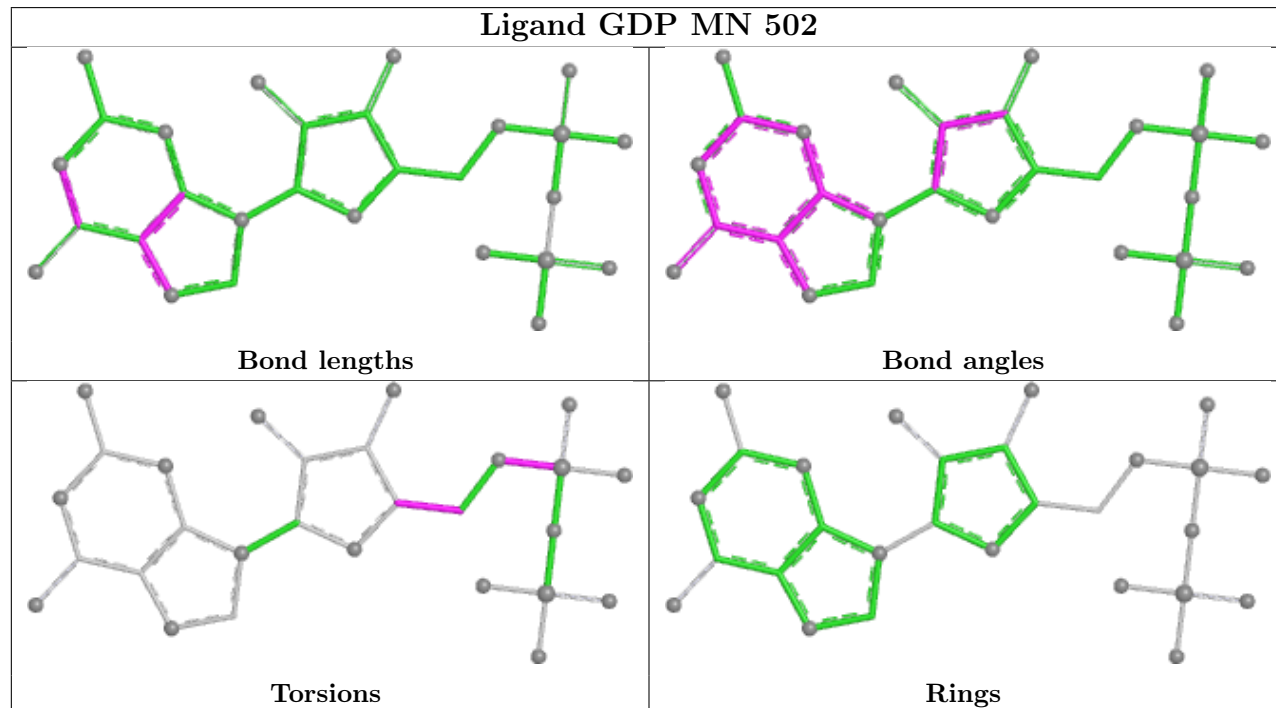
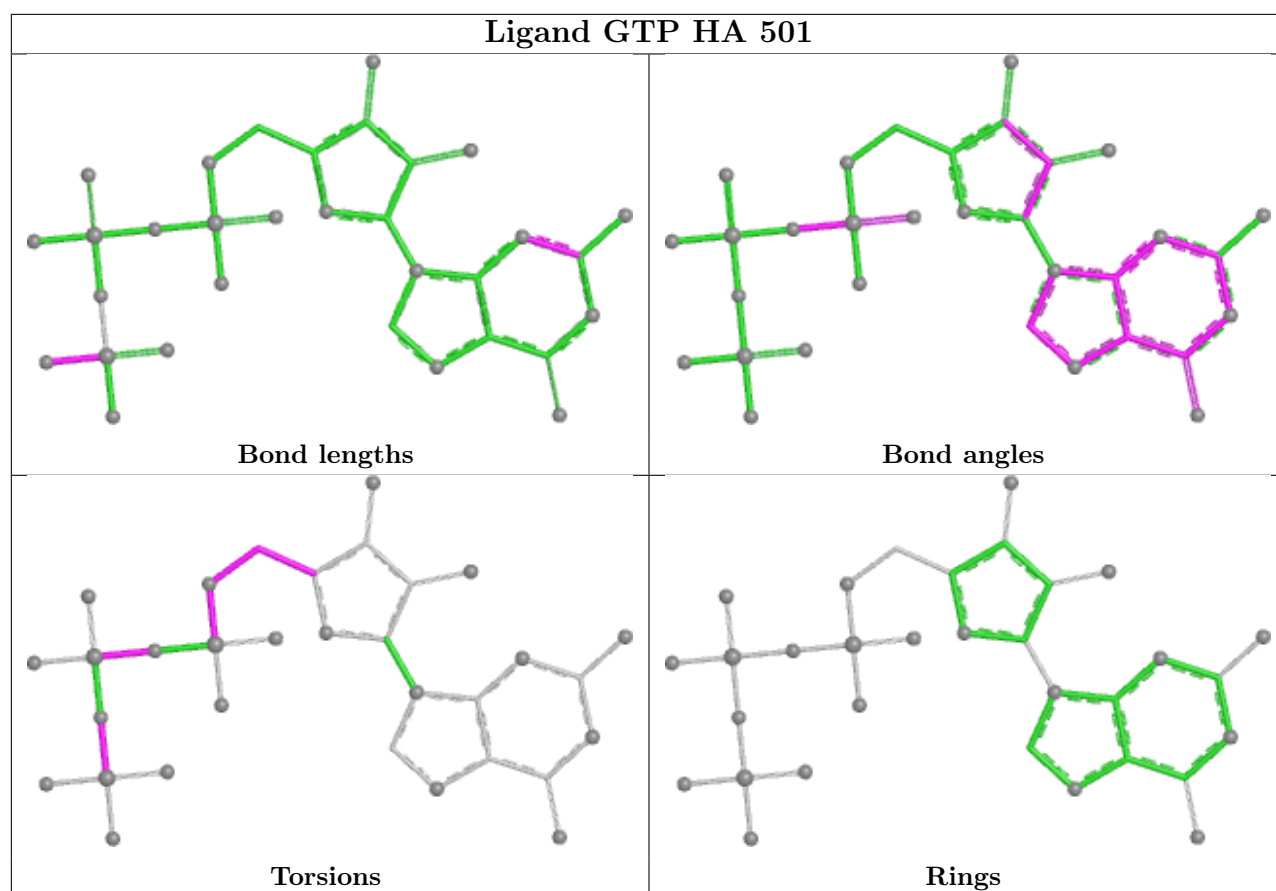




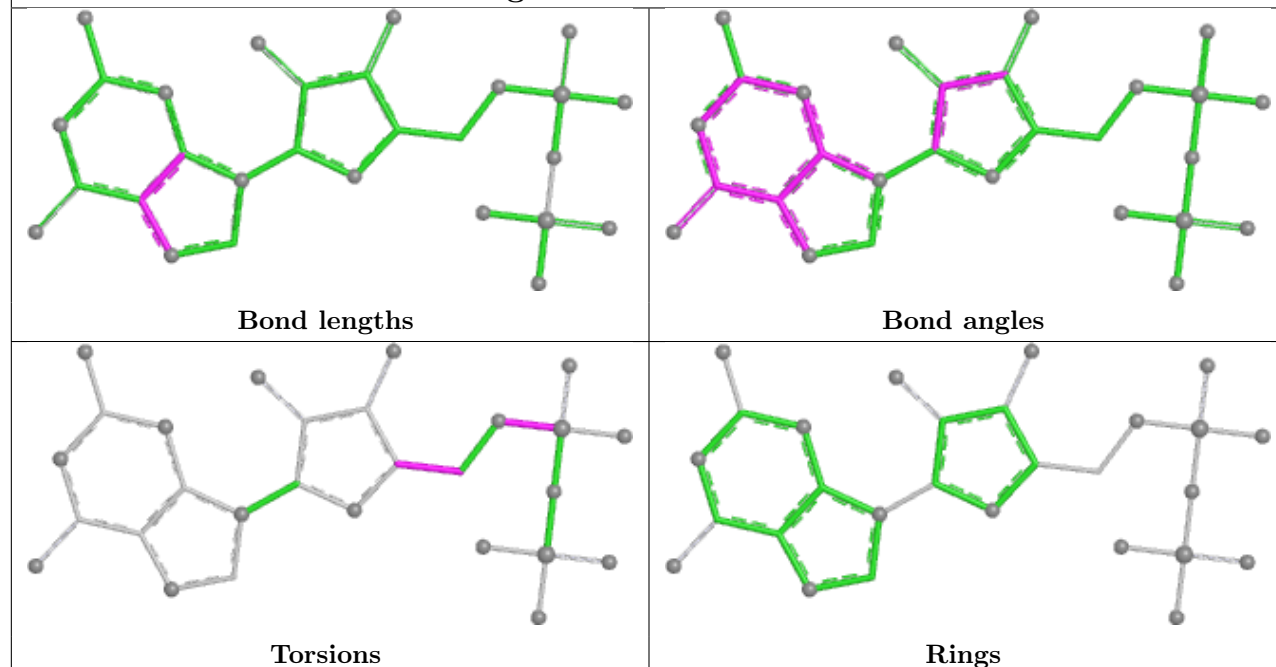




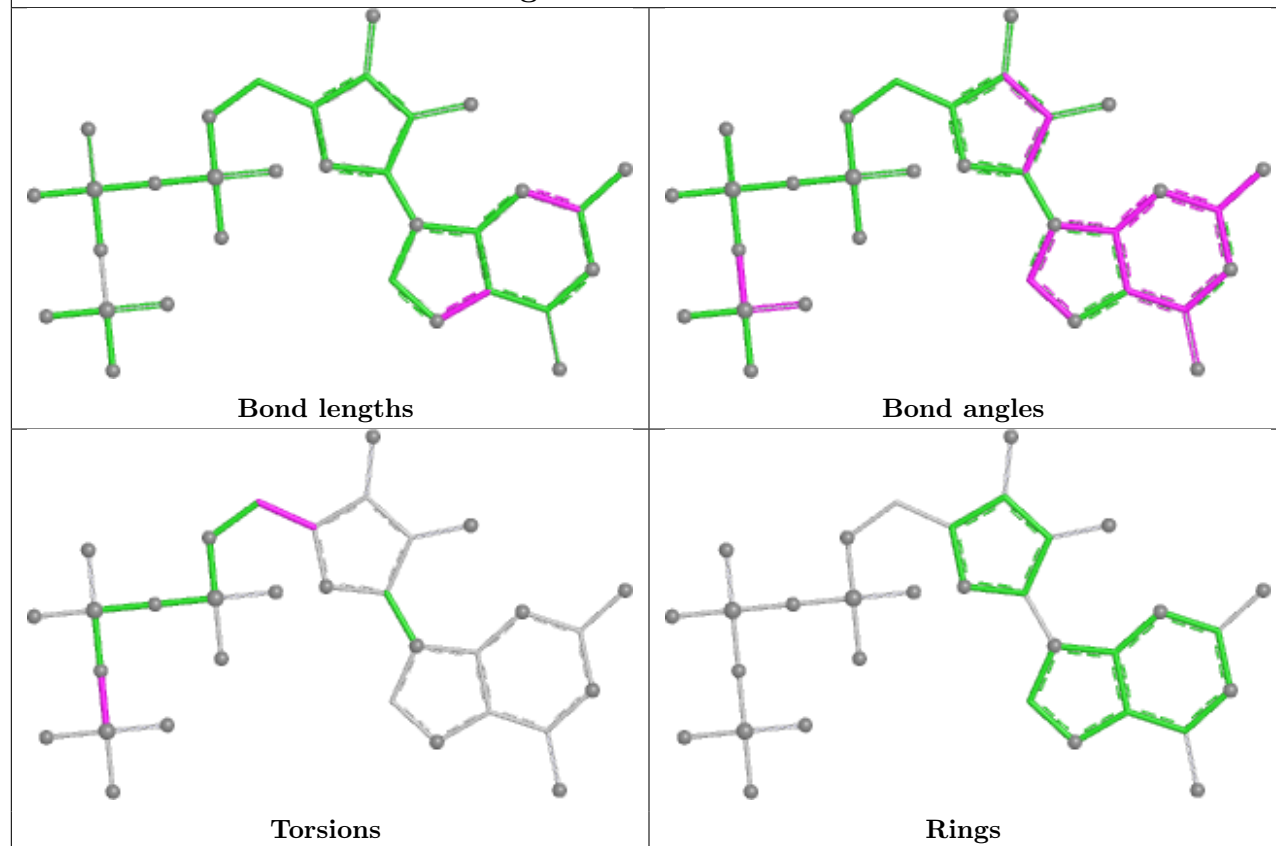




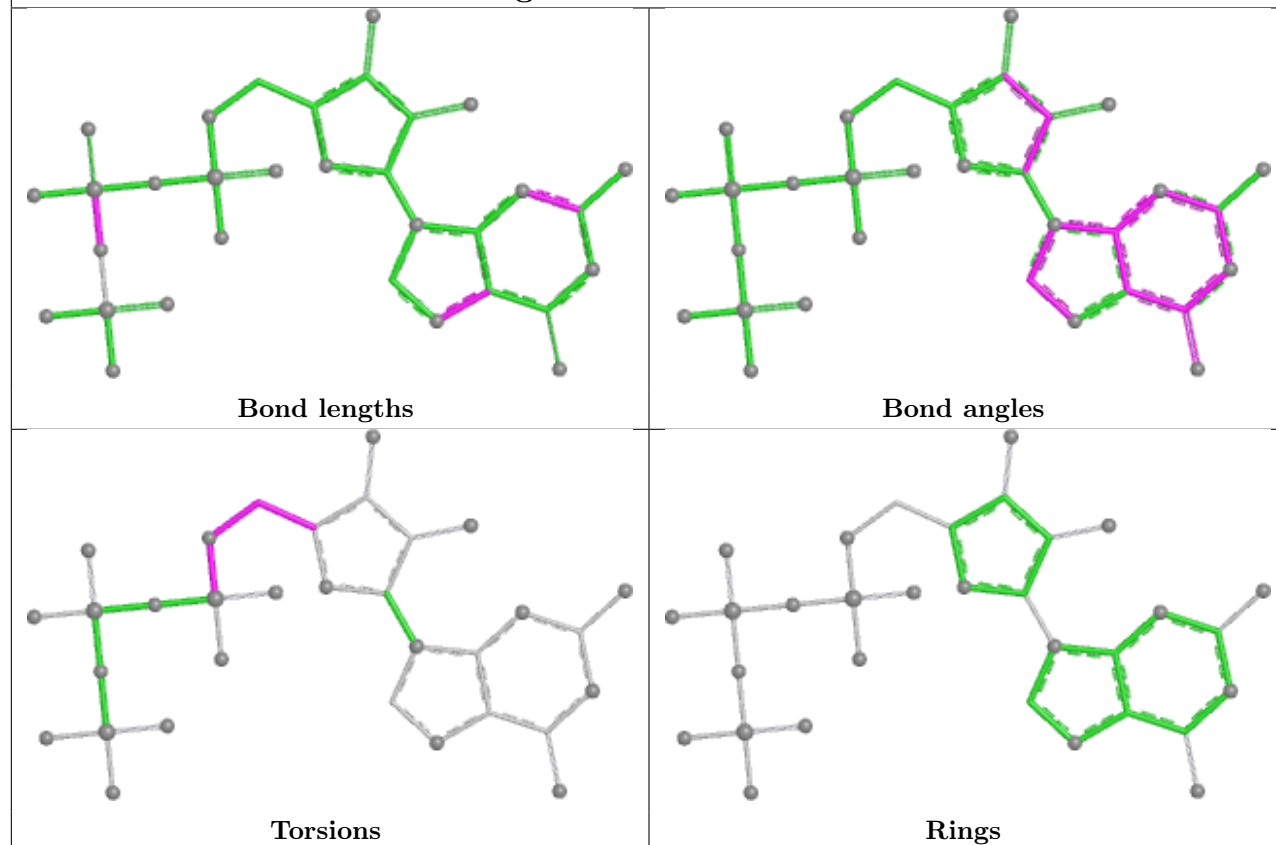
Ligand GDP WM 501



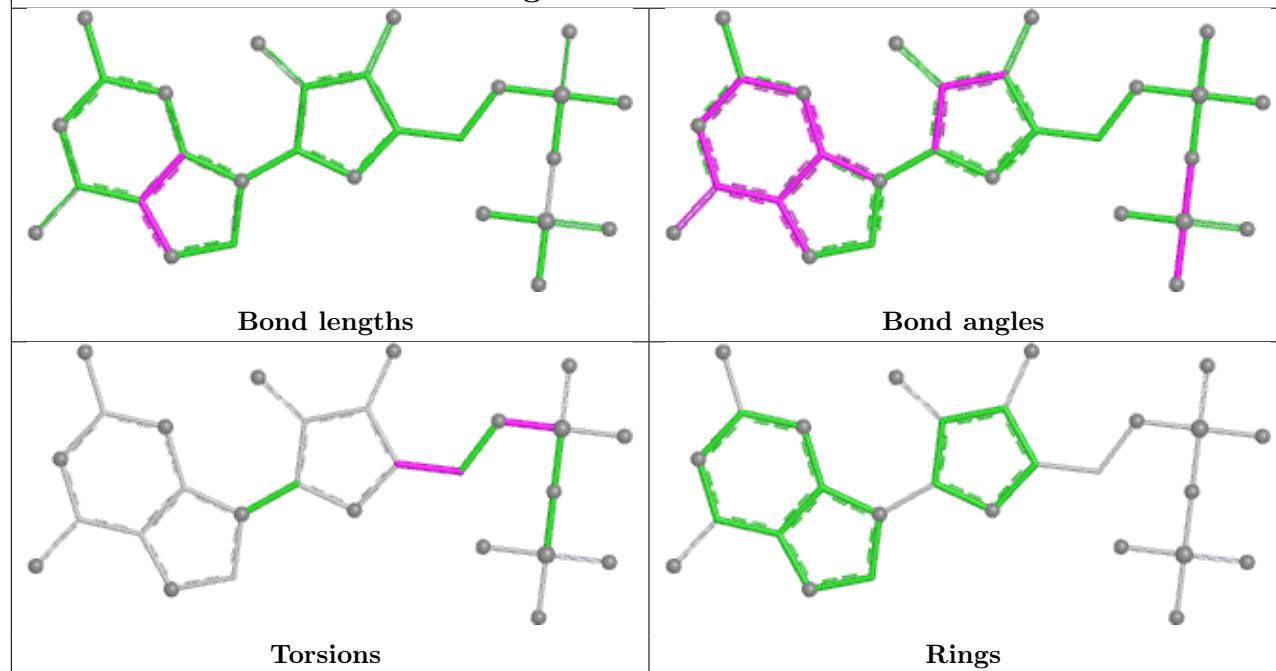
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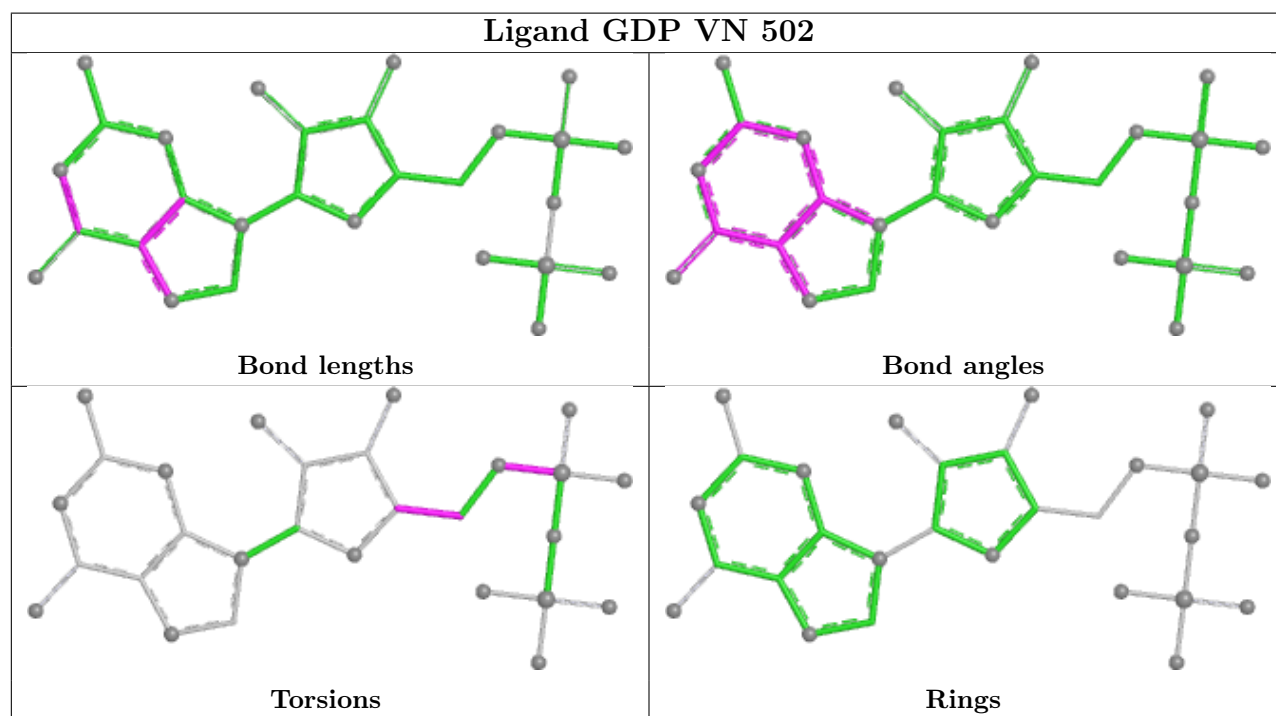
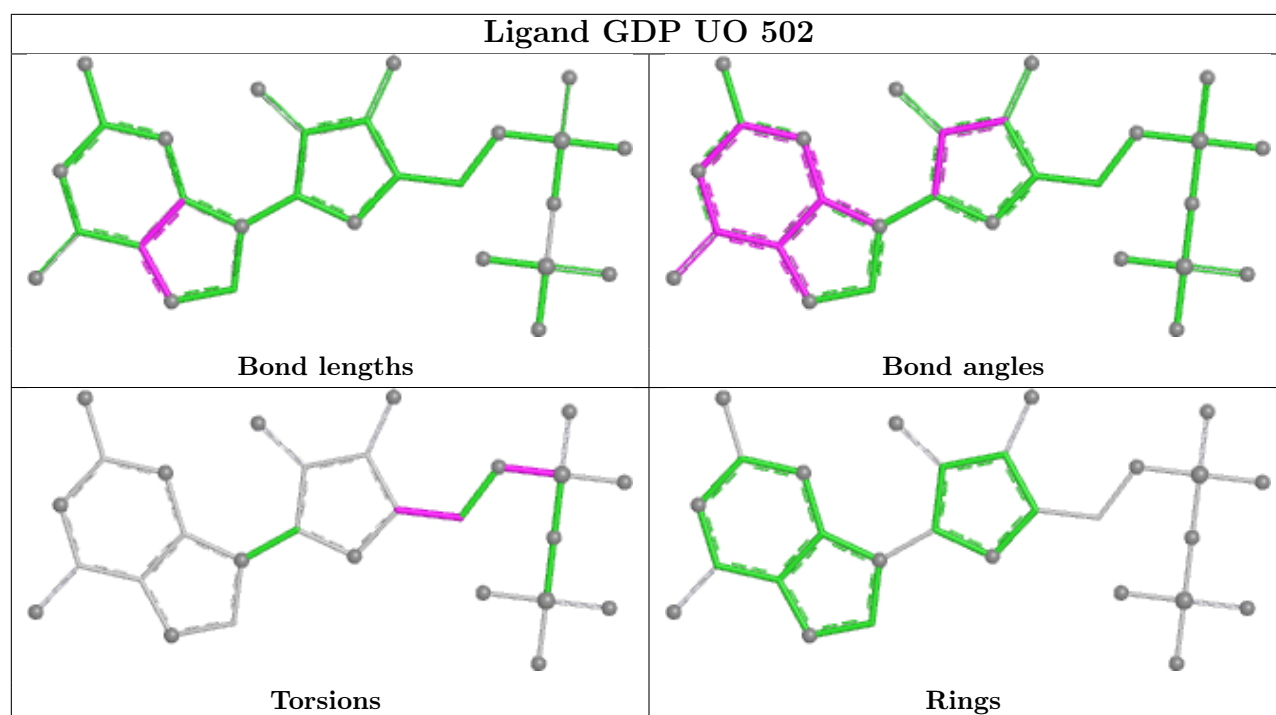


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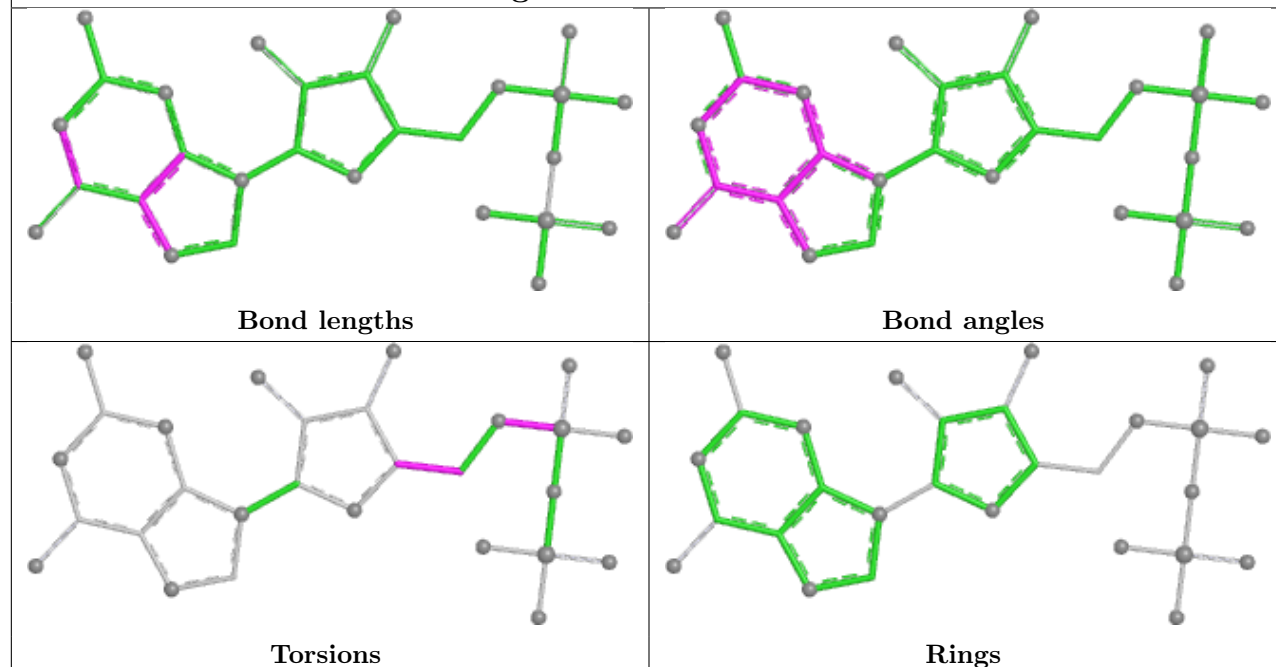


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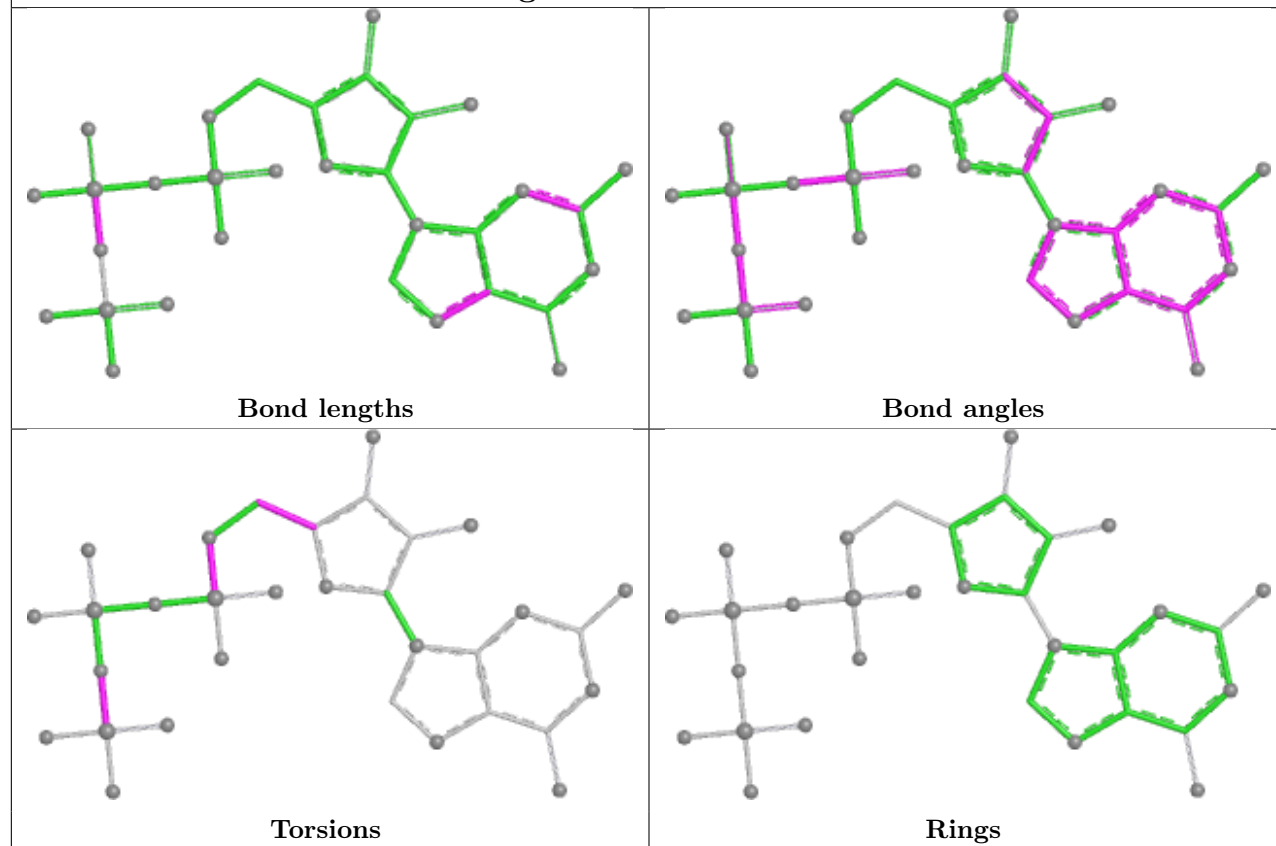




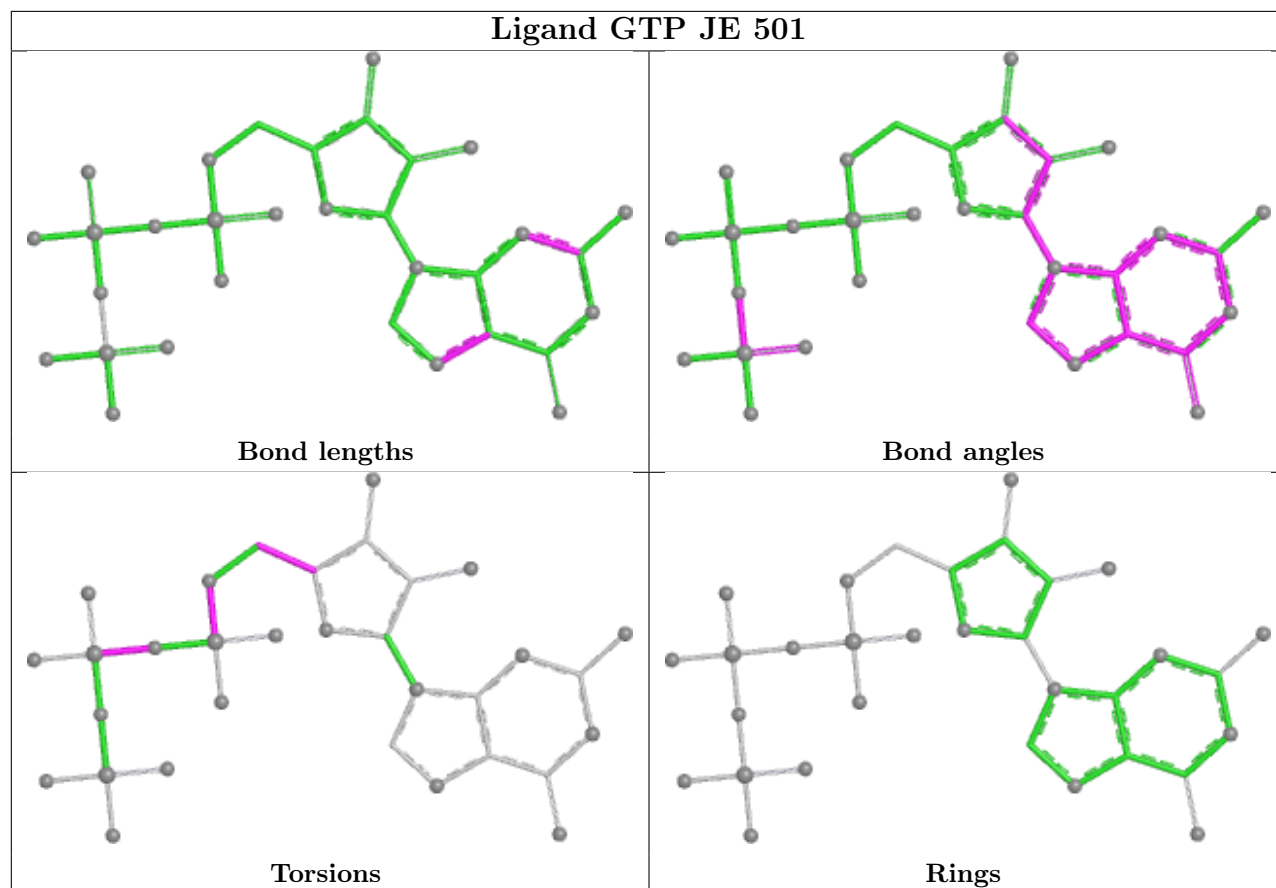
Ligand GDP WP 501



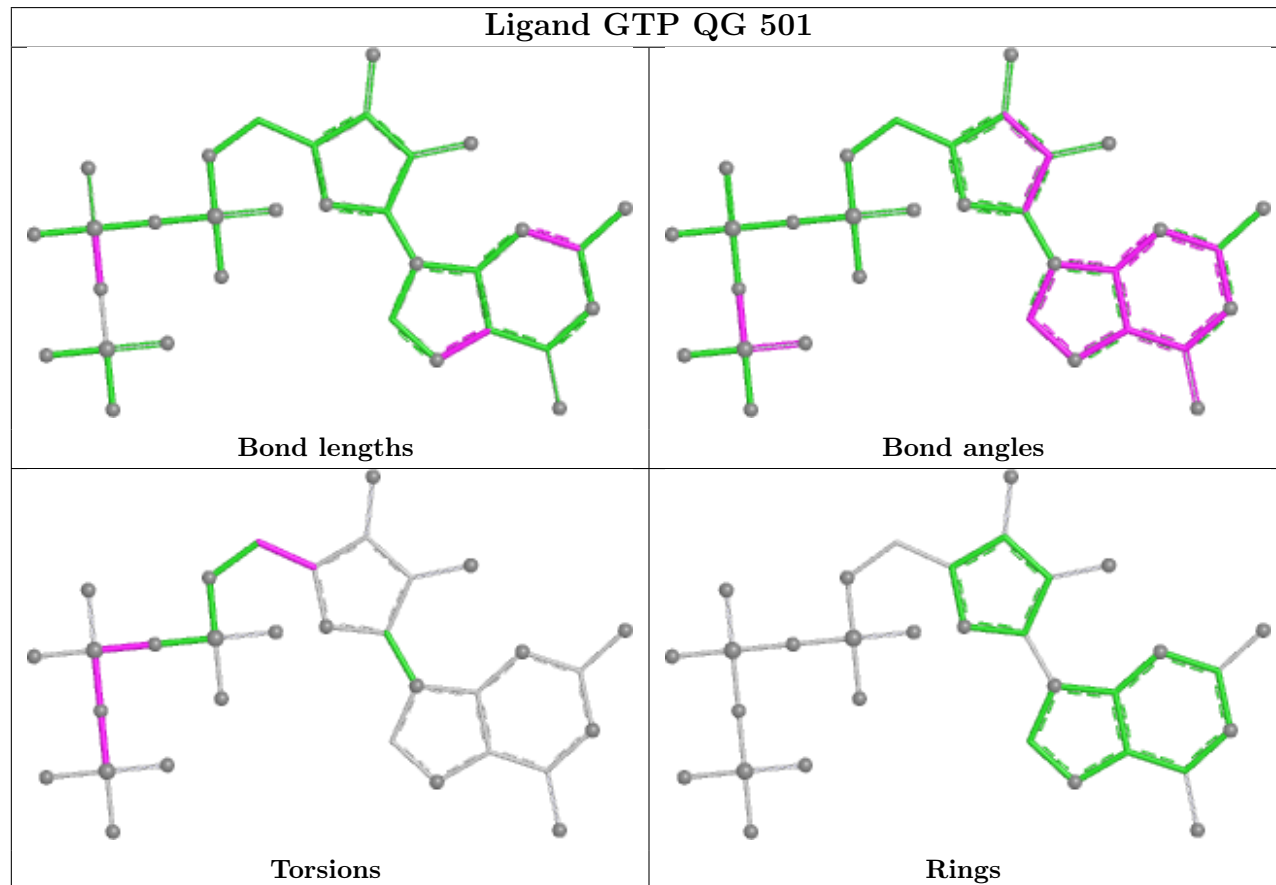
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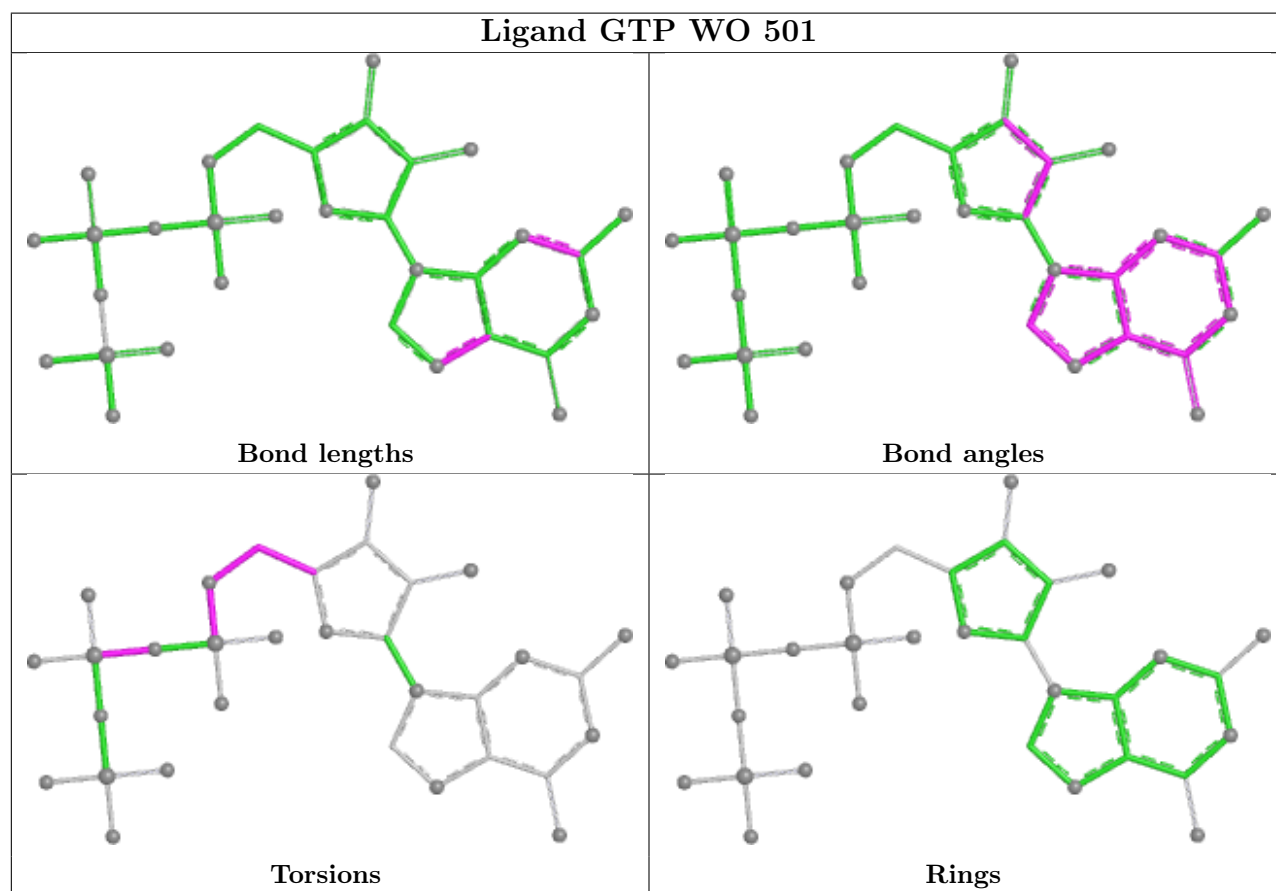
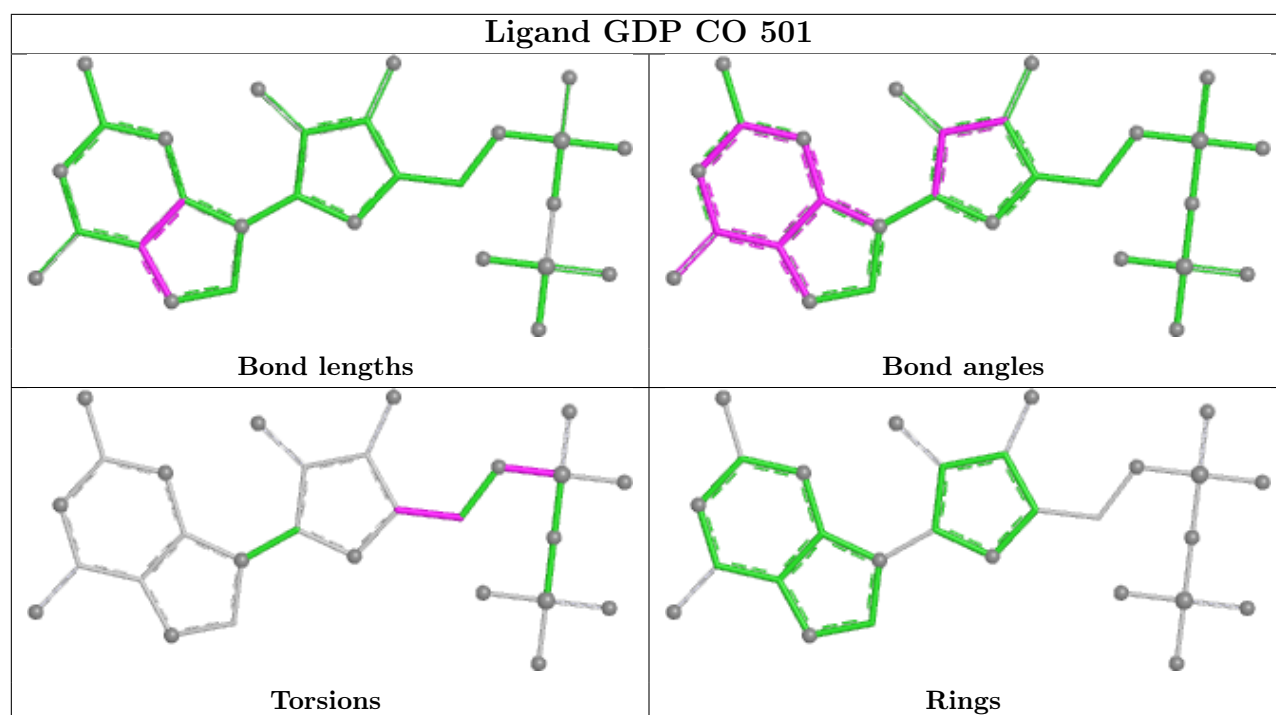


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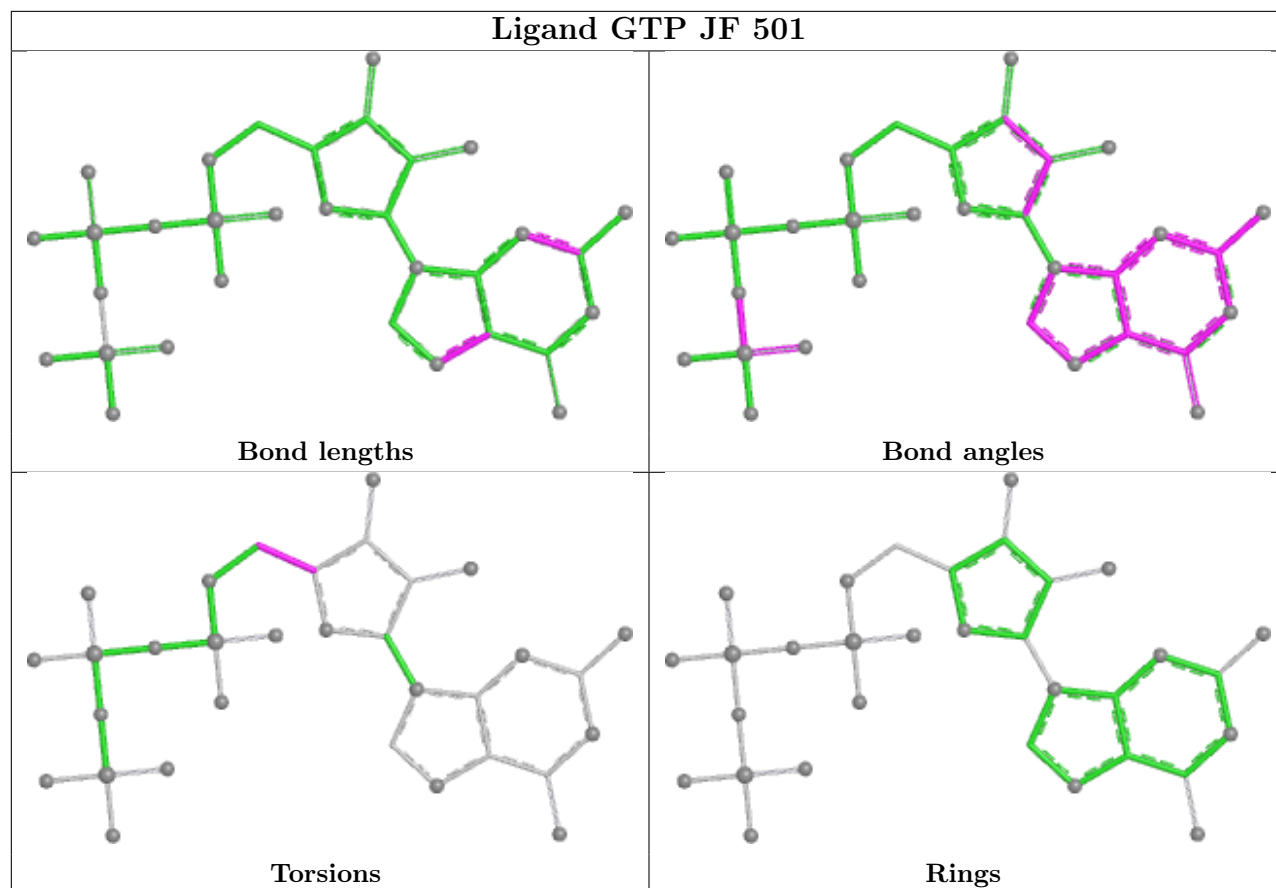


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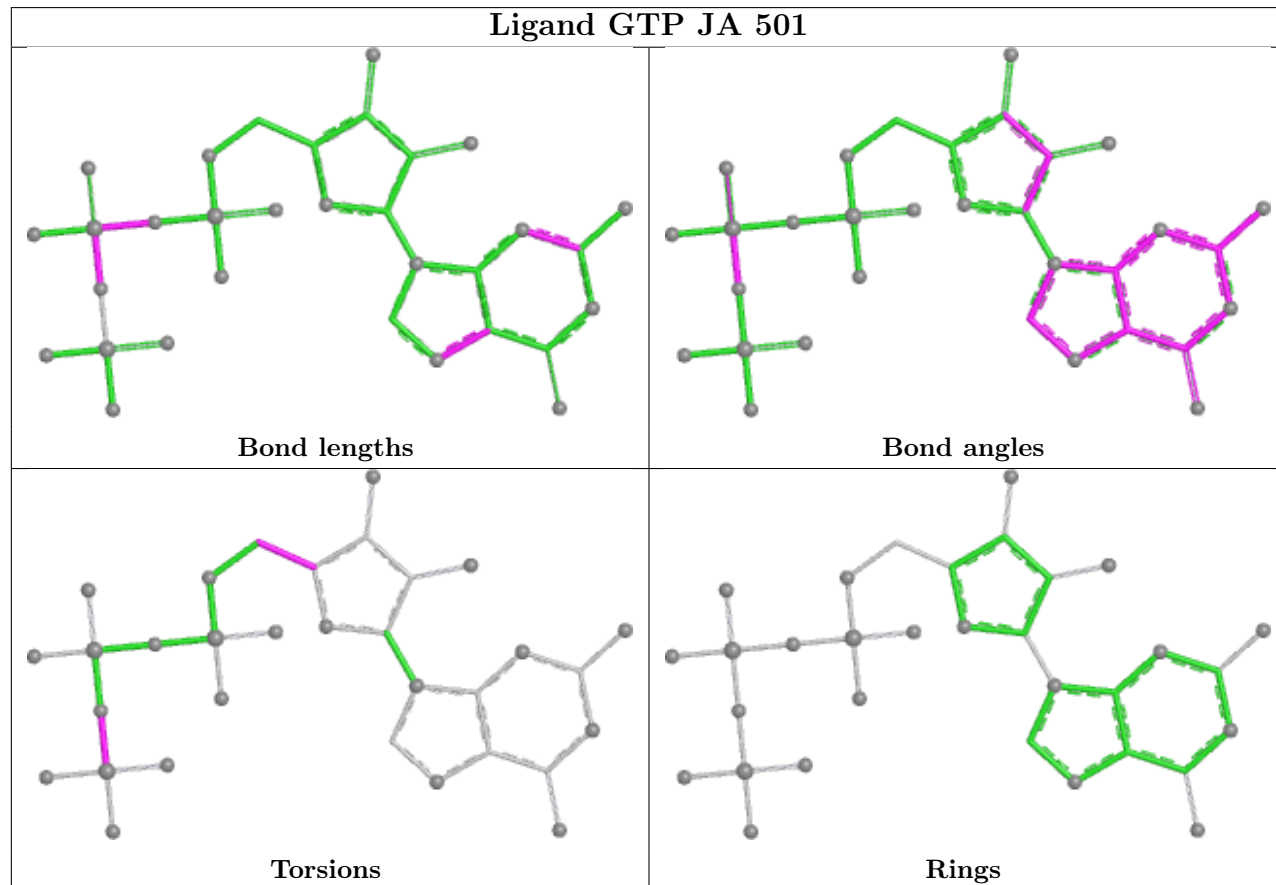


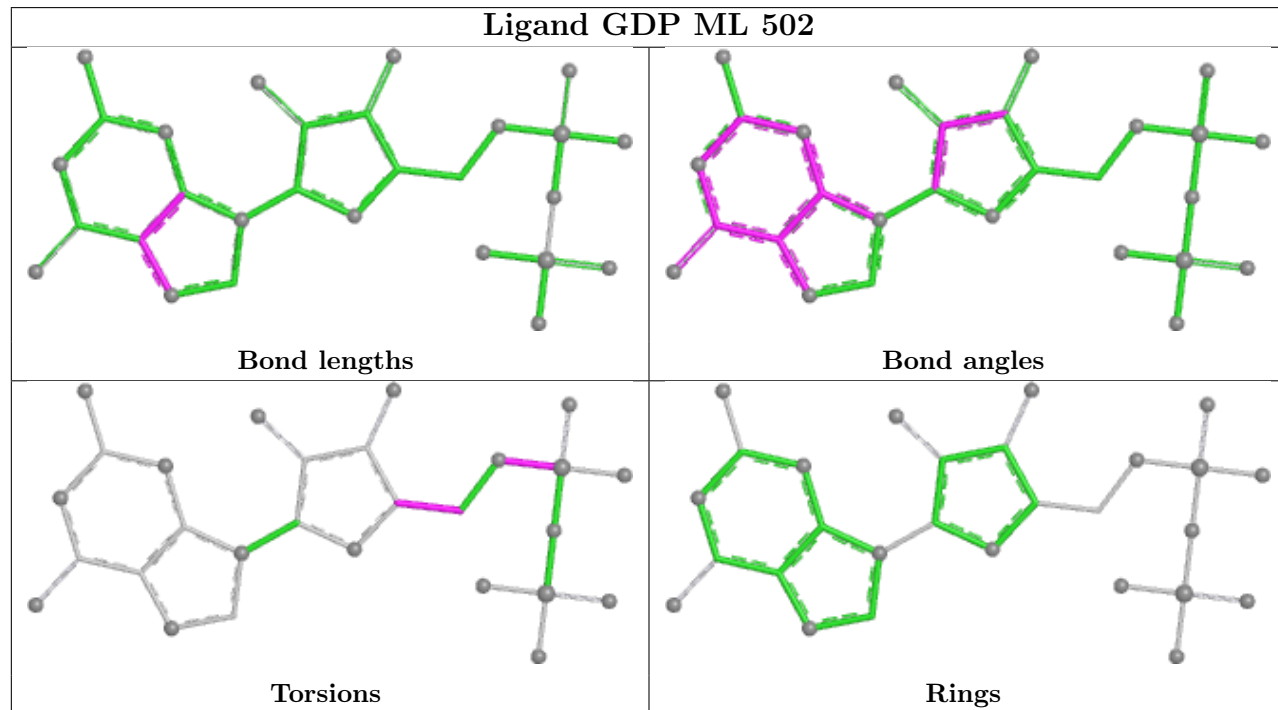
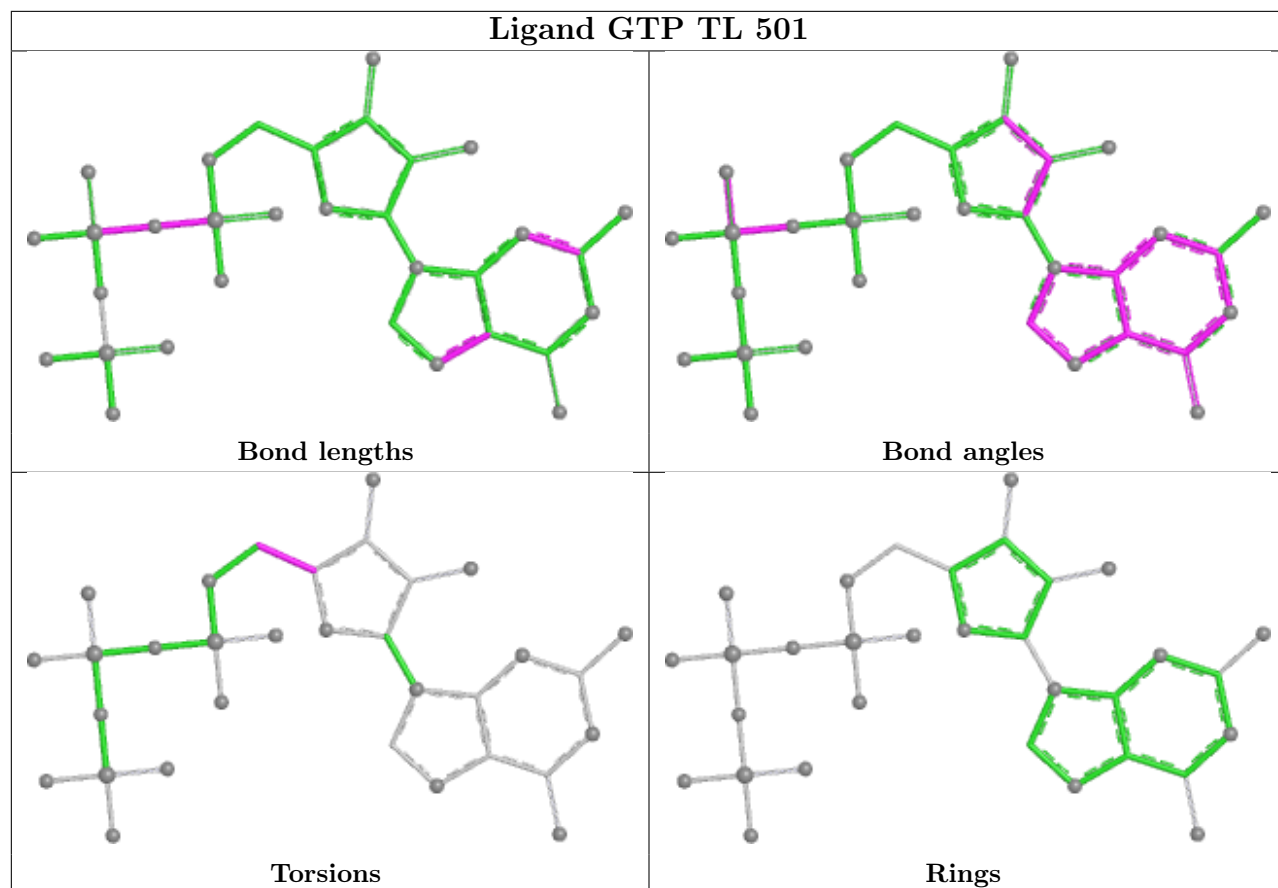


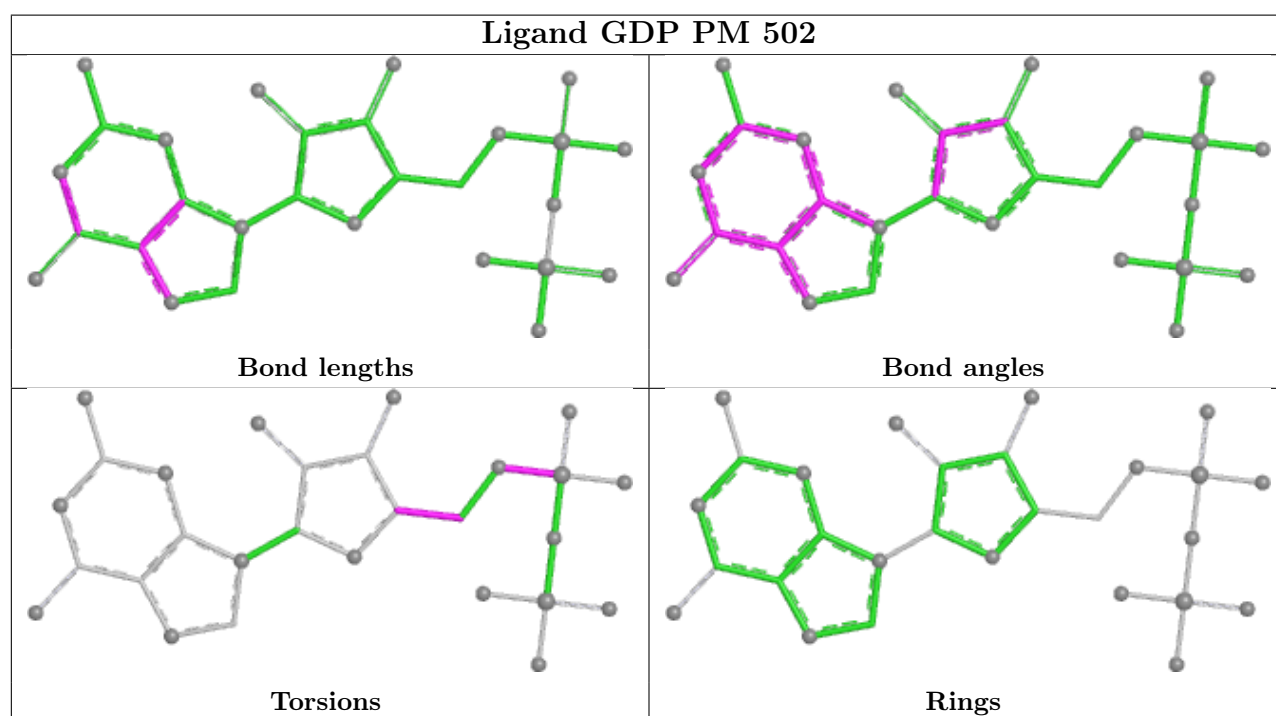
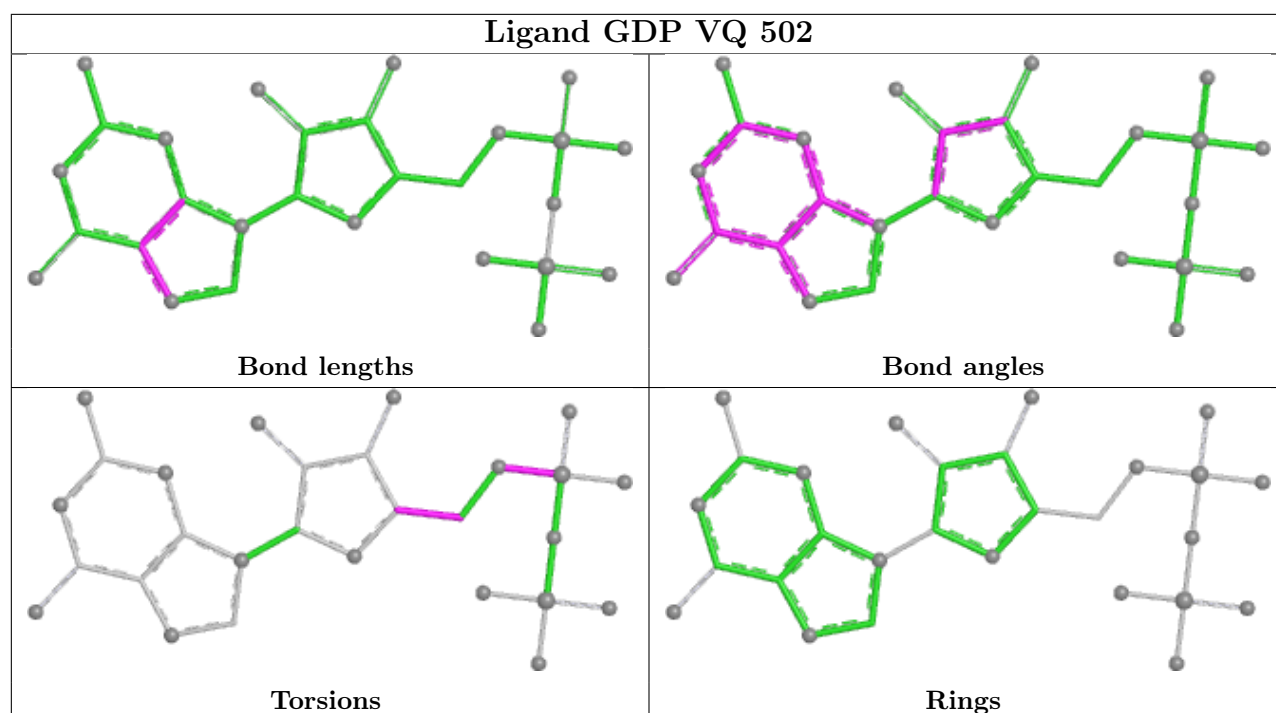
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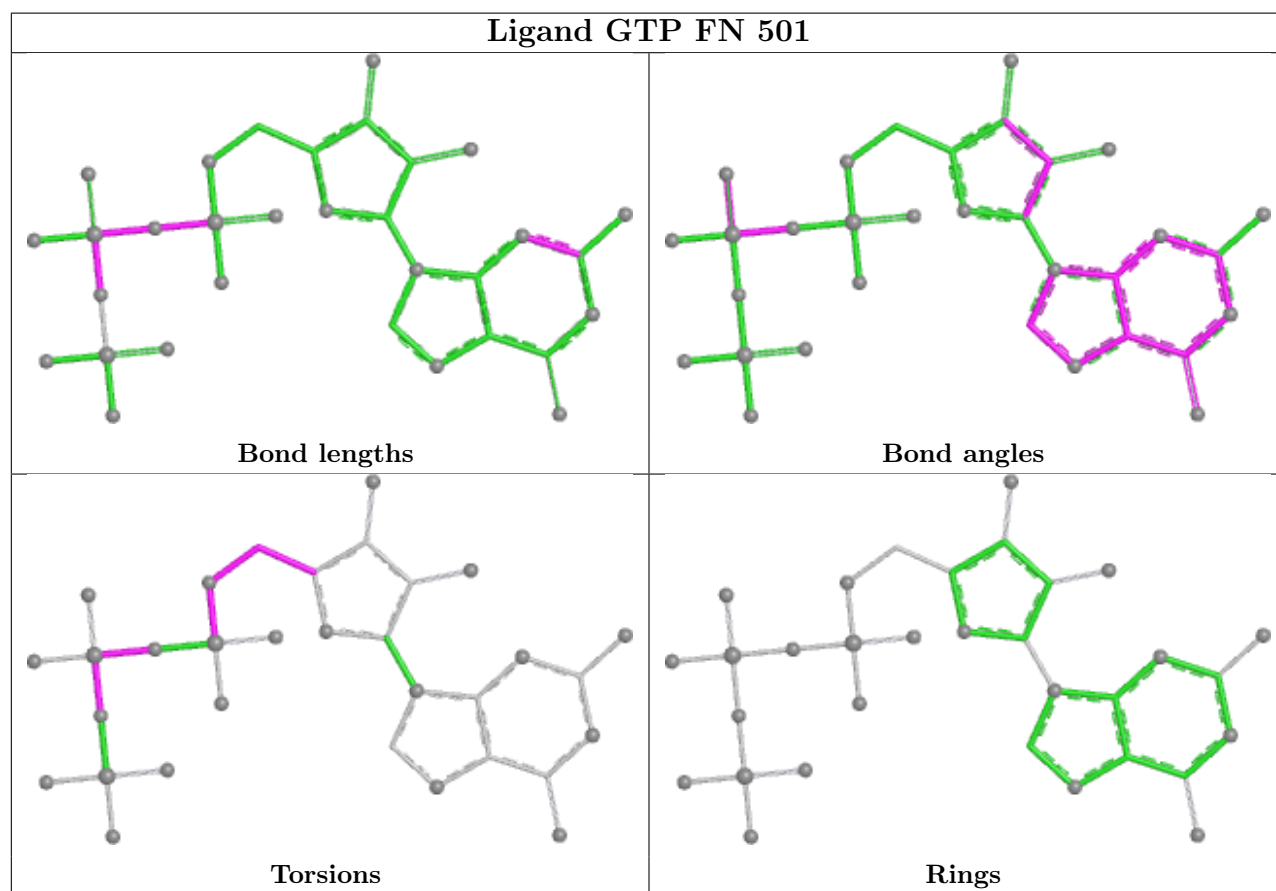
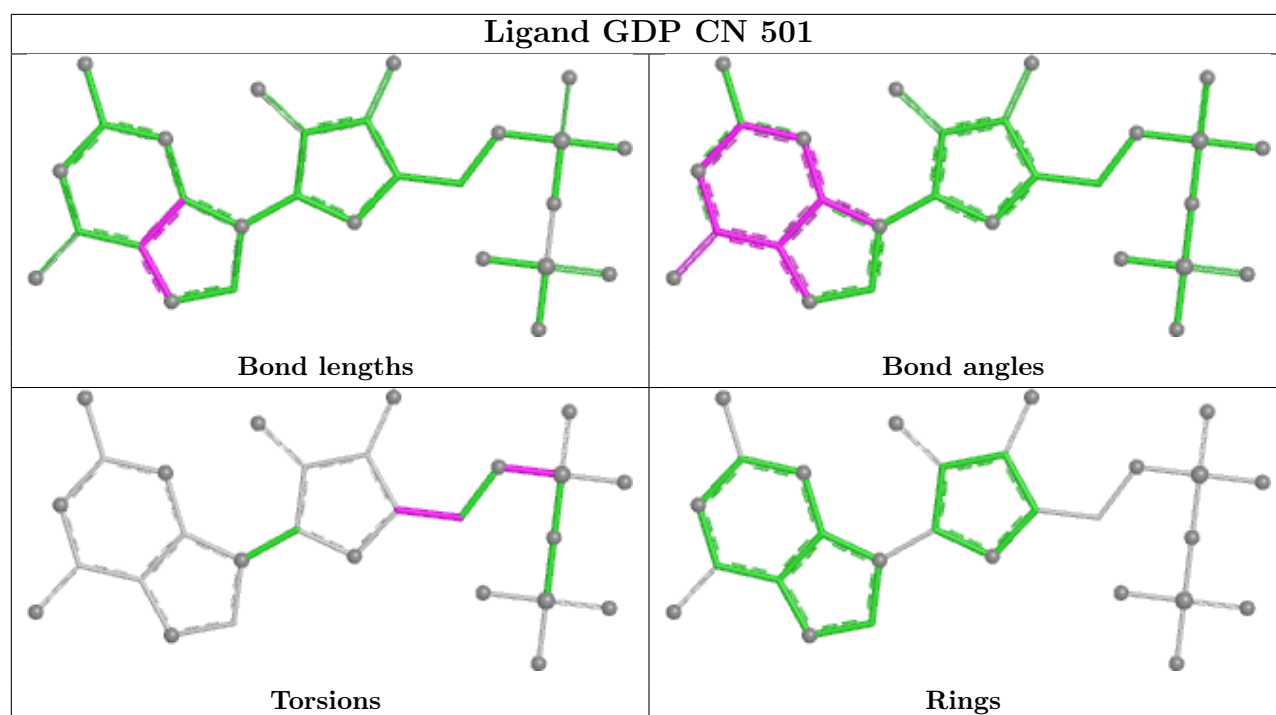


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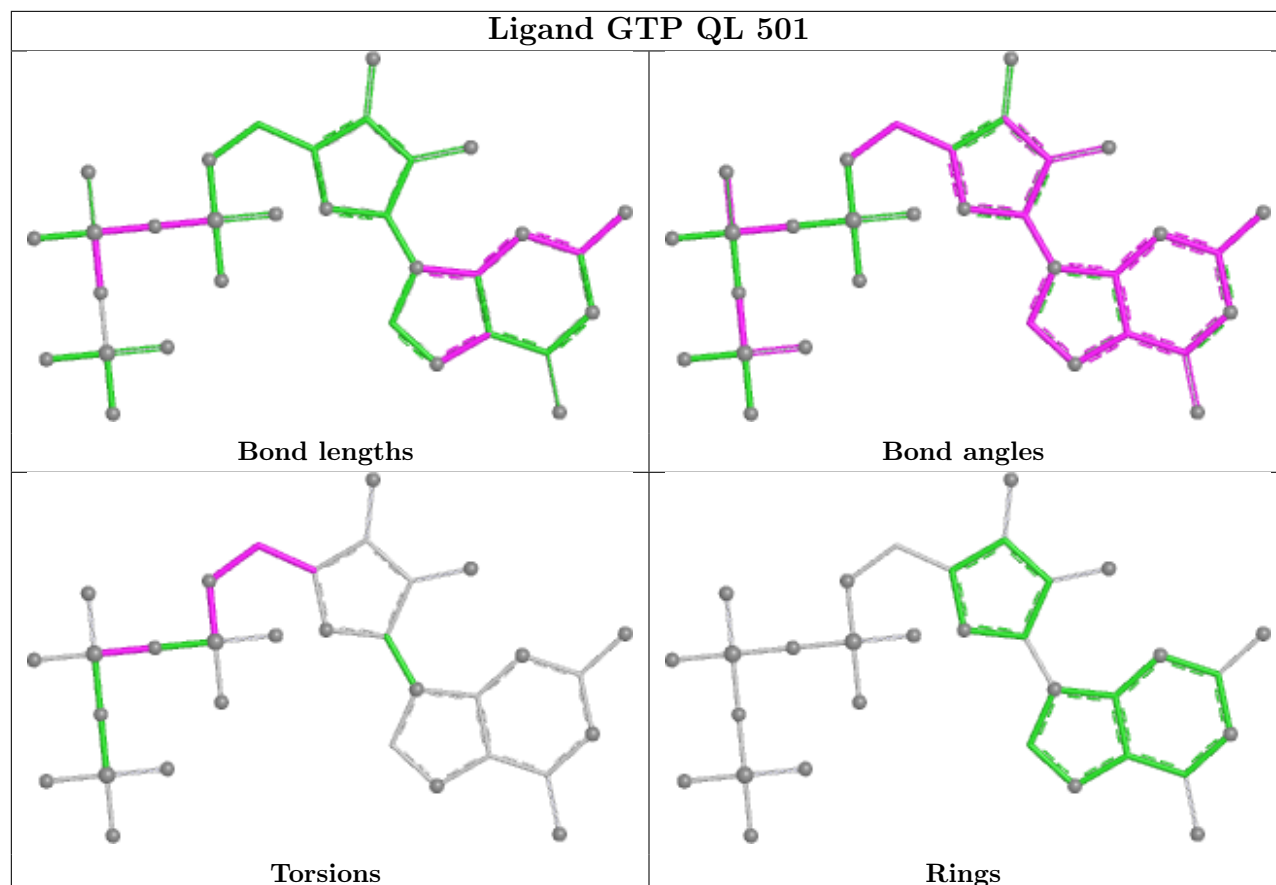




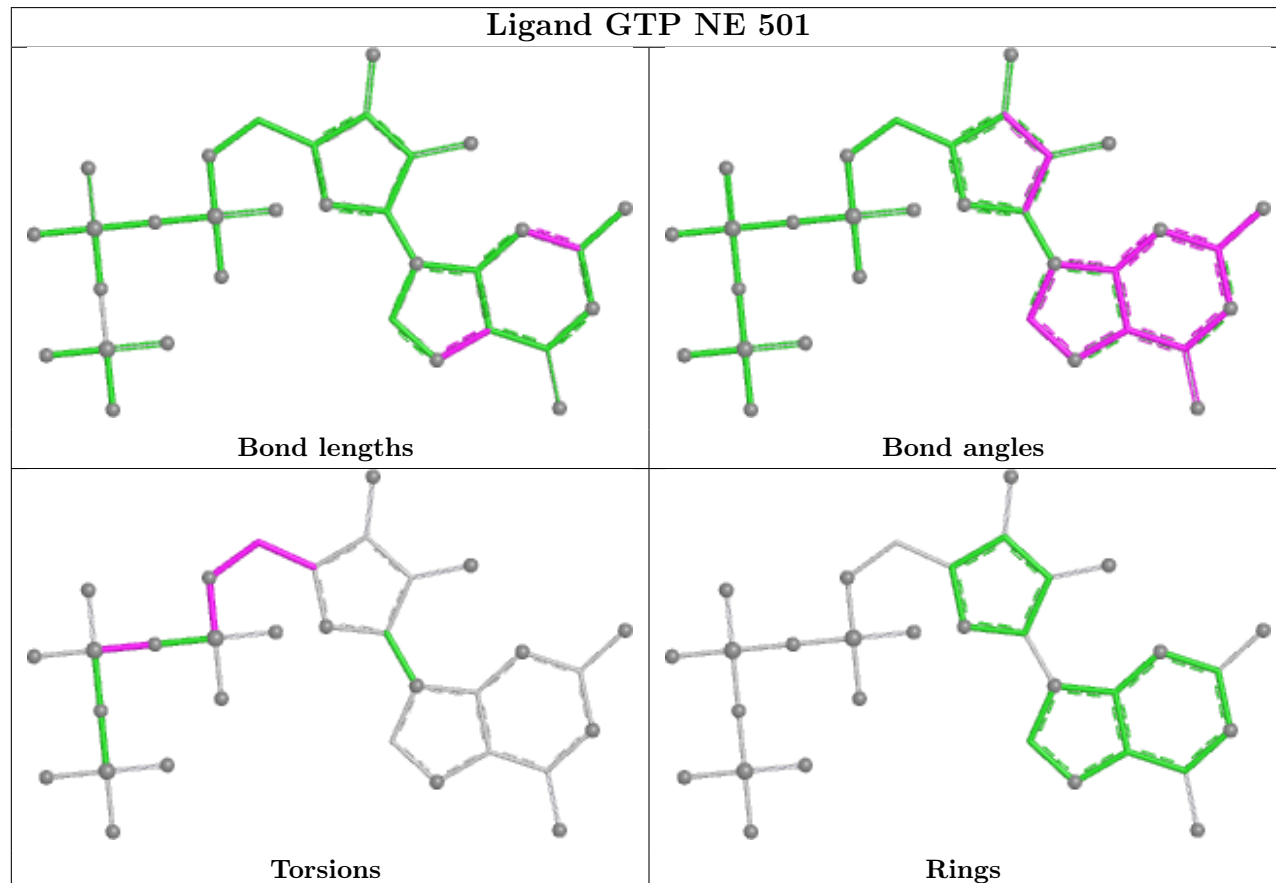


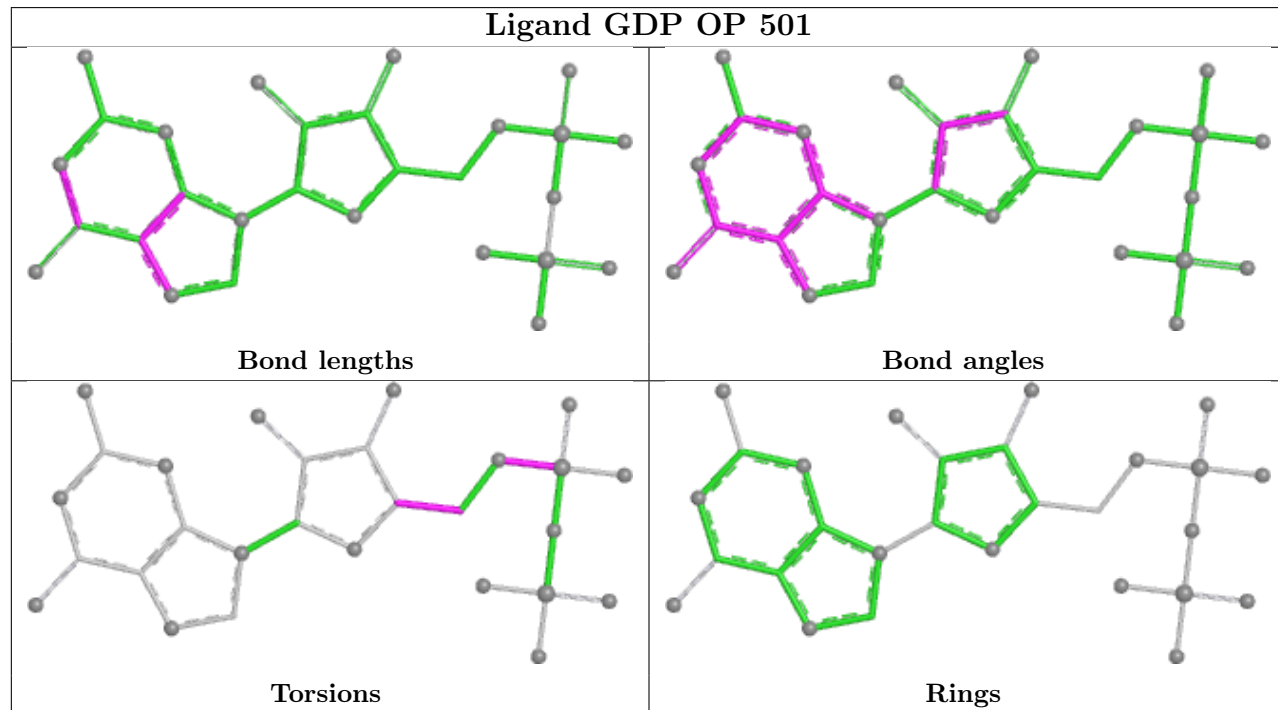
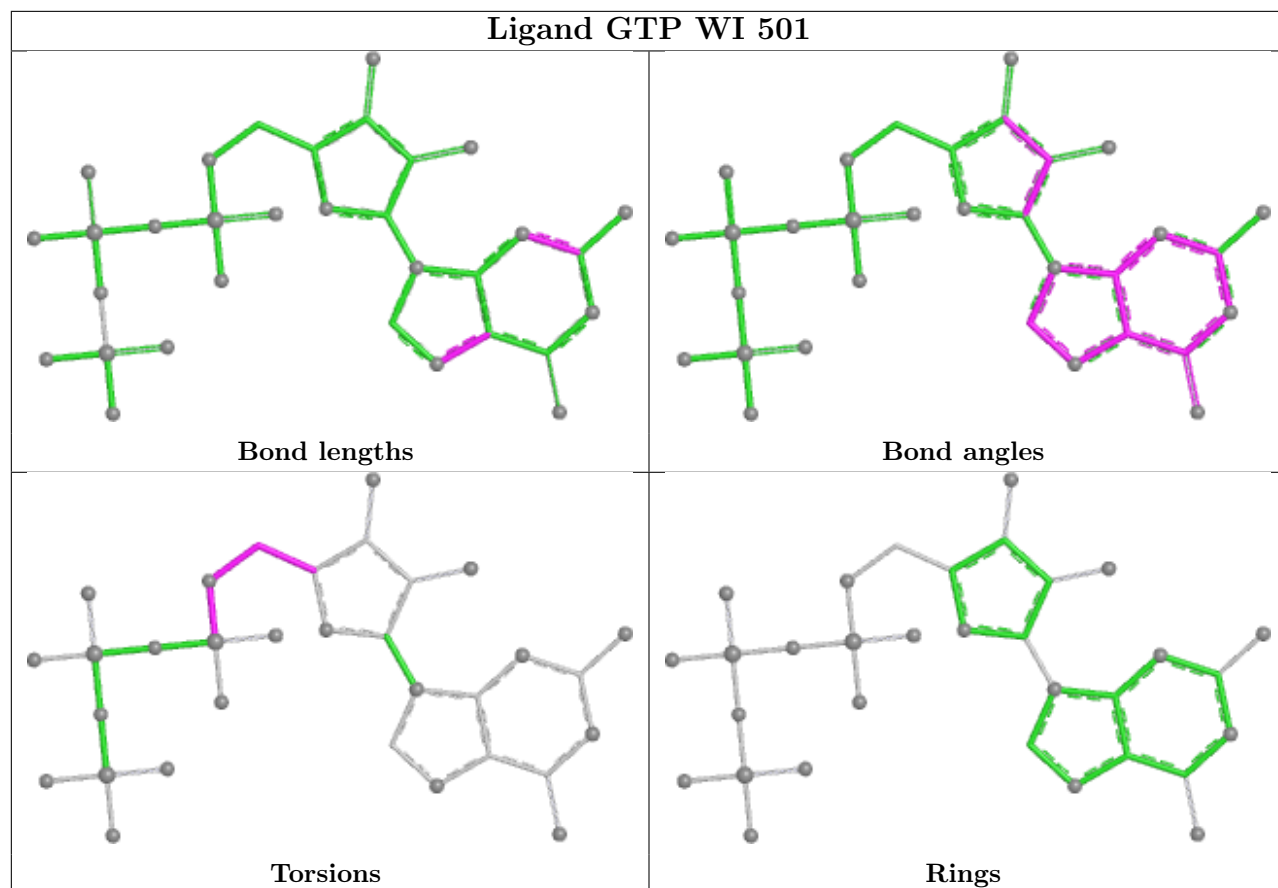


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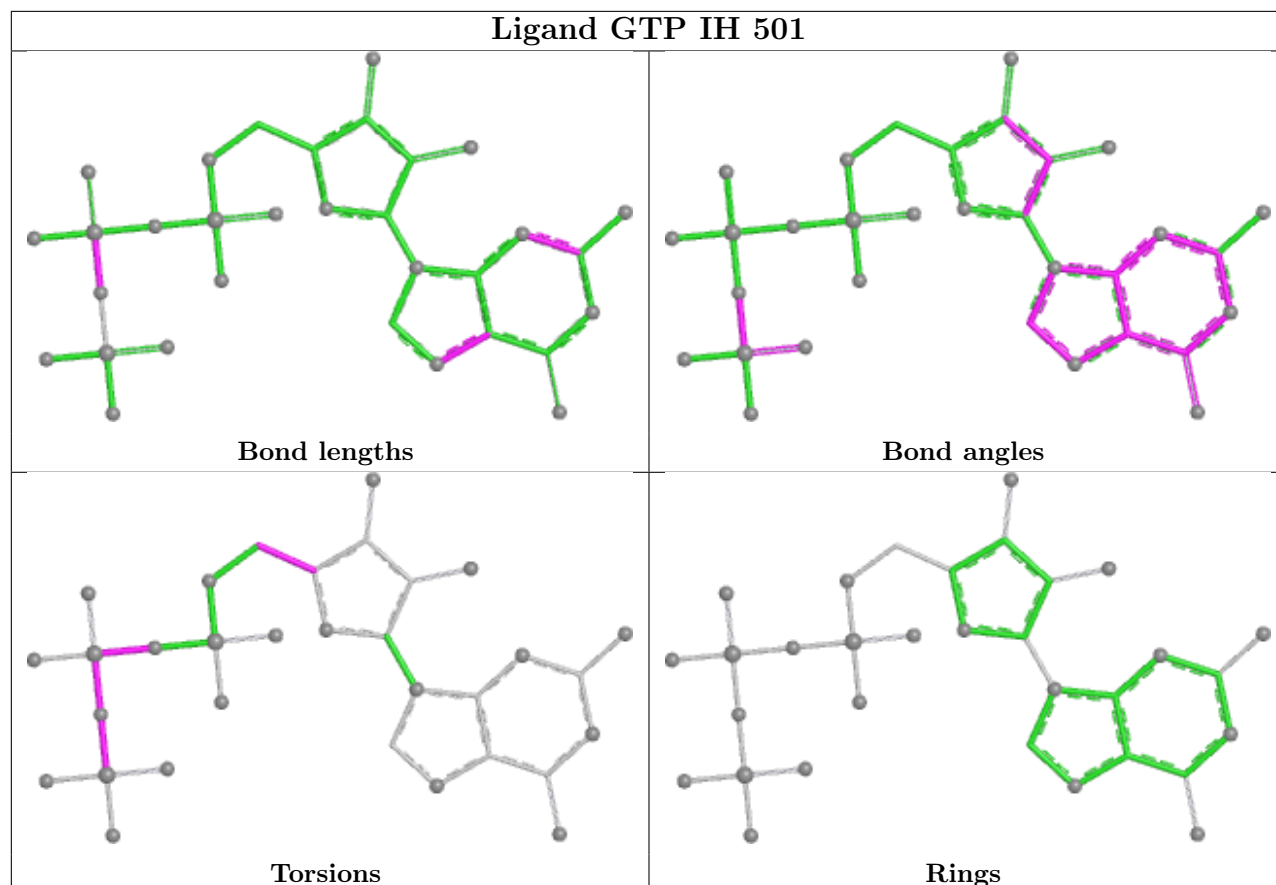


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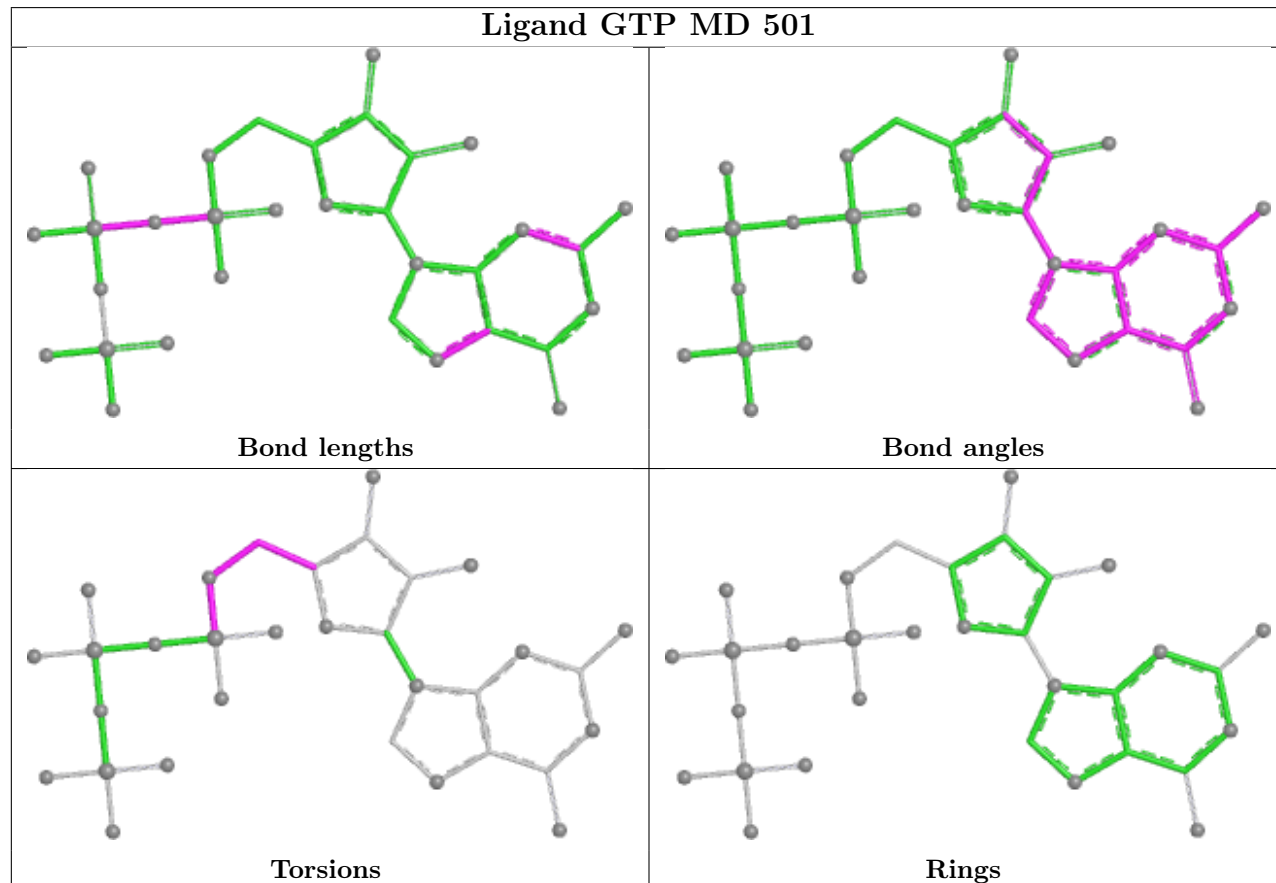




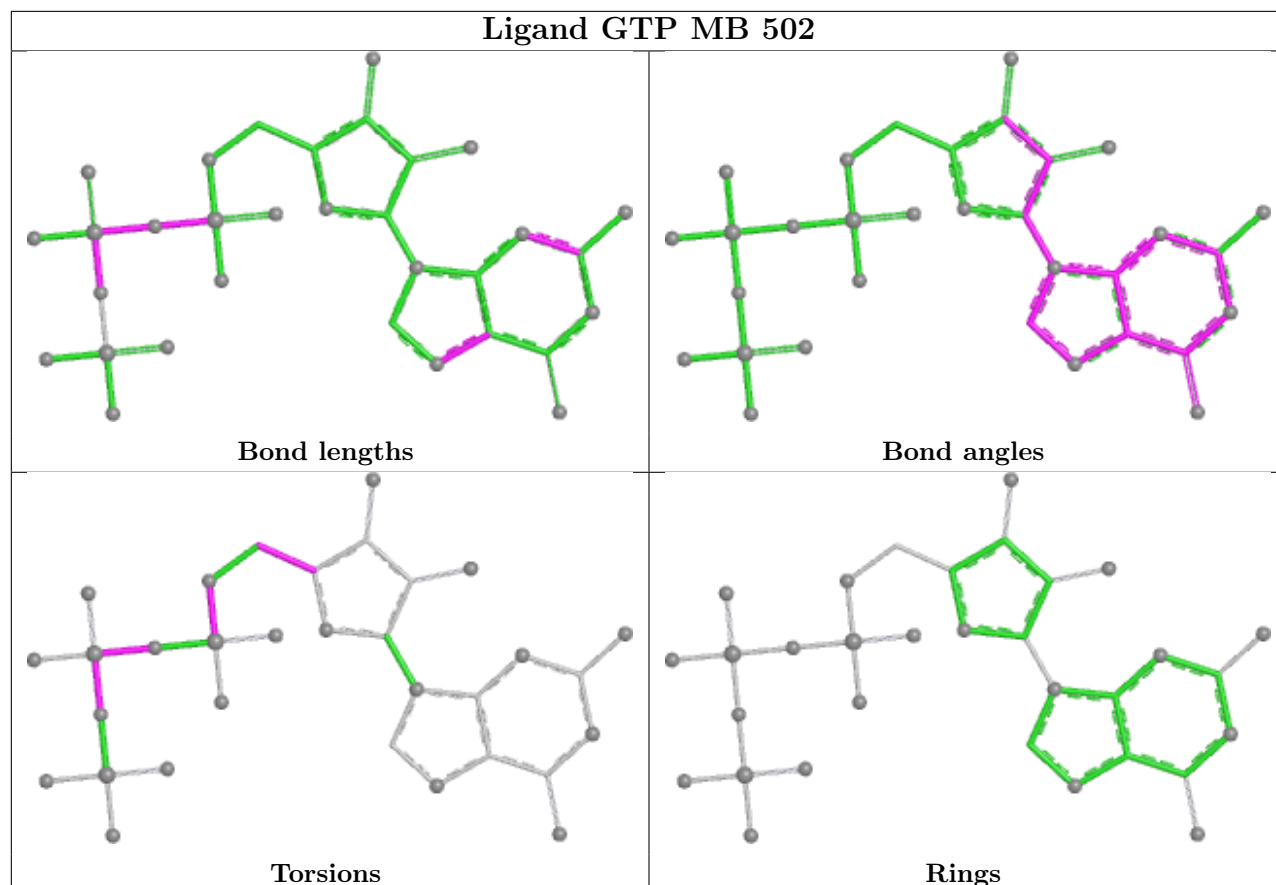
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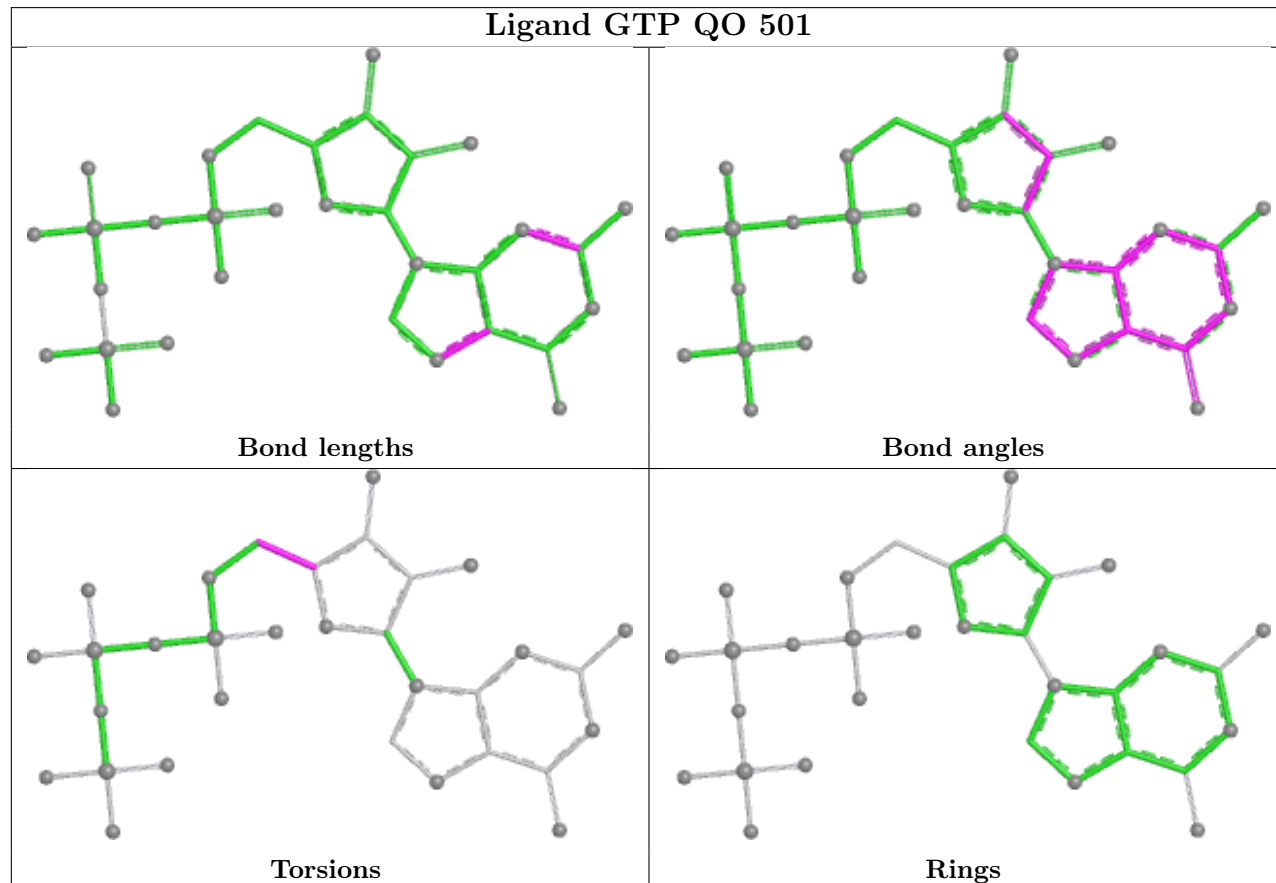
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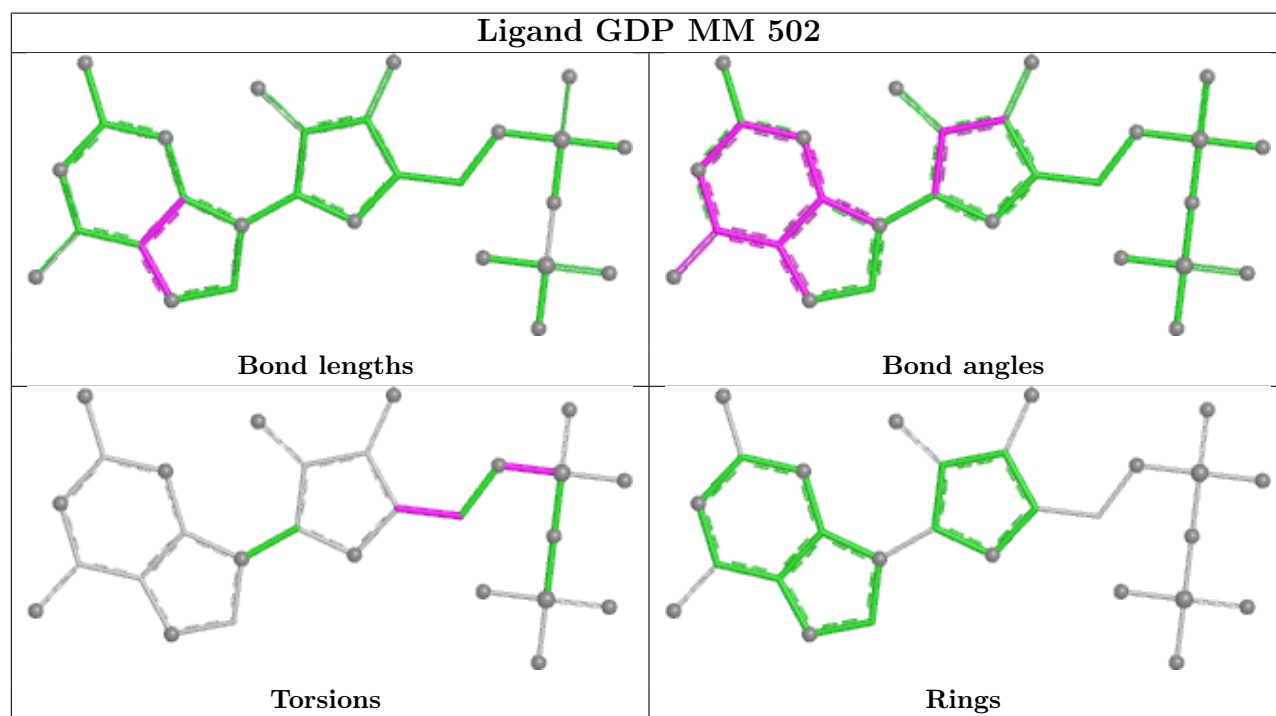
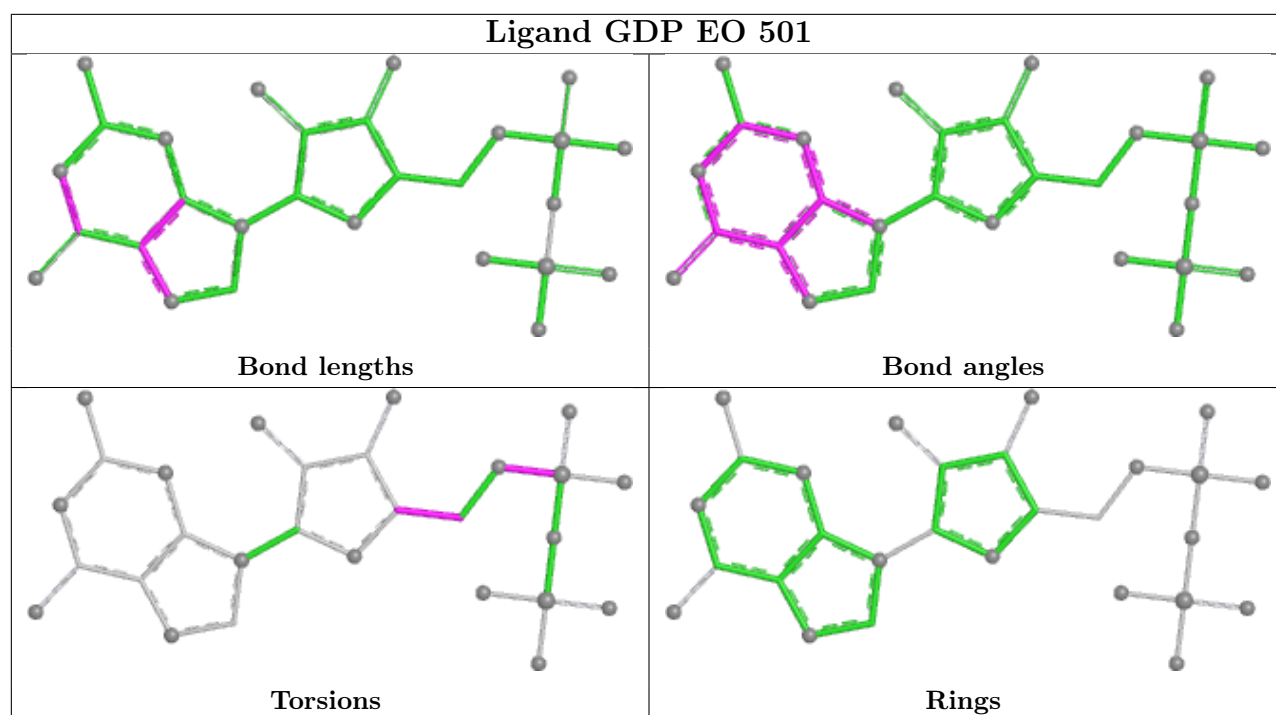


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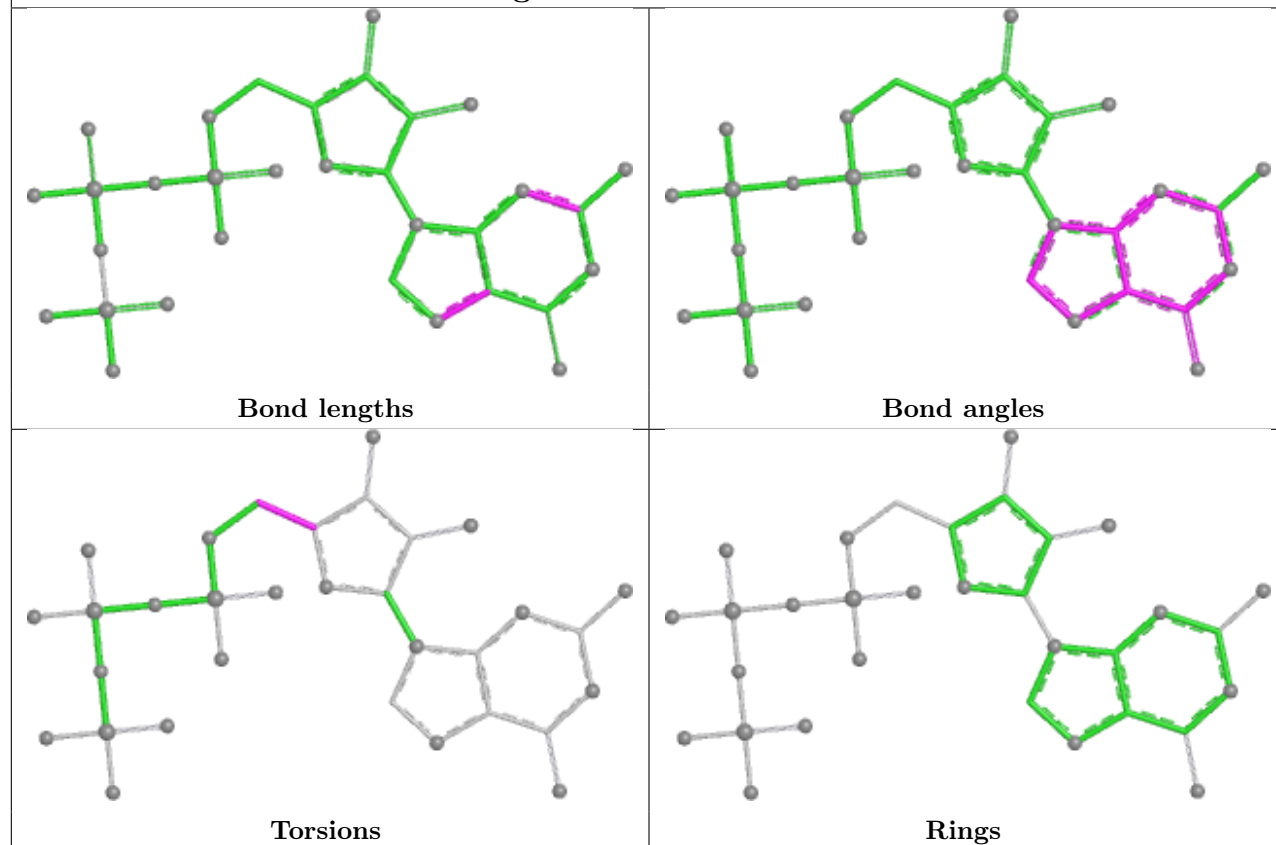


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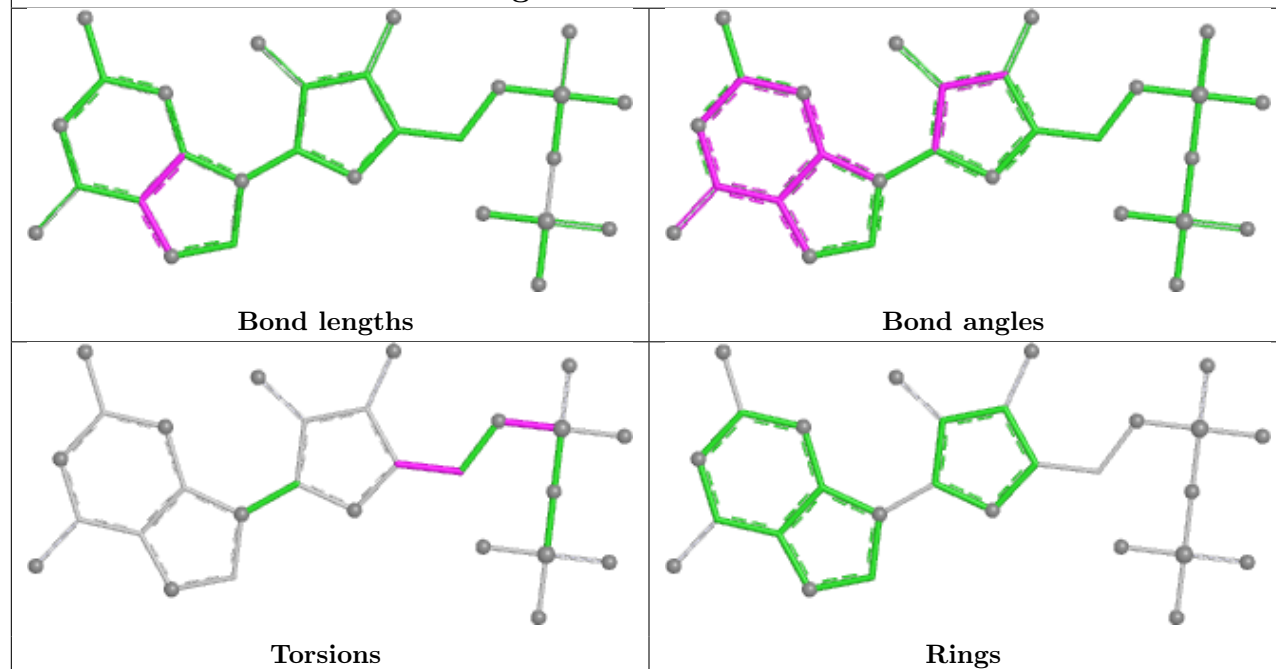


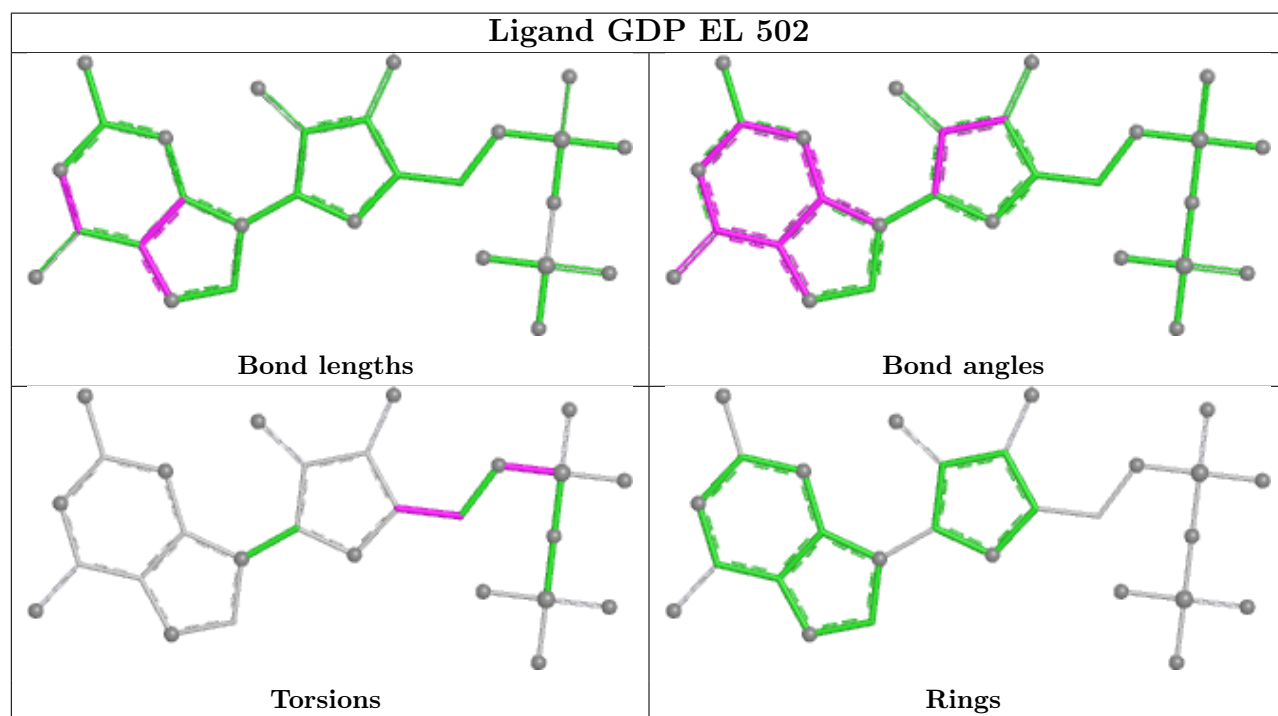
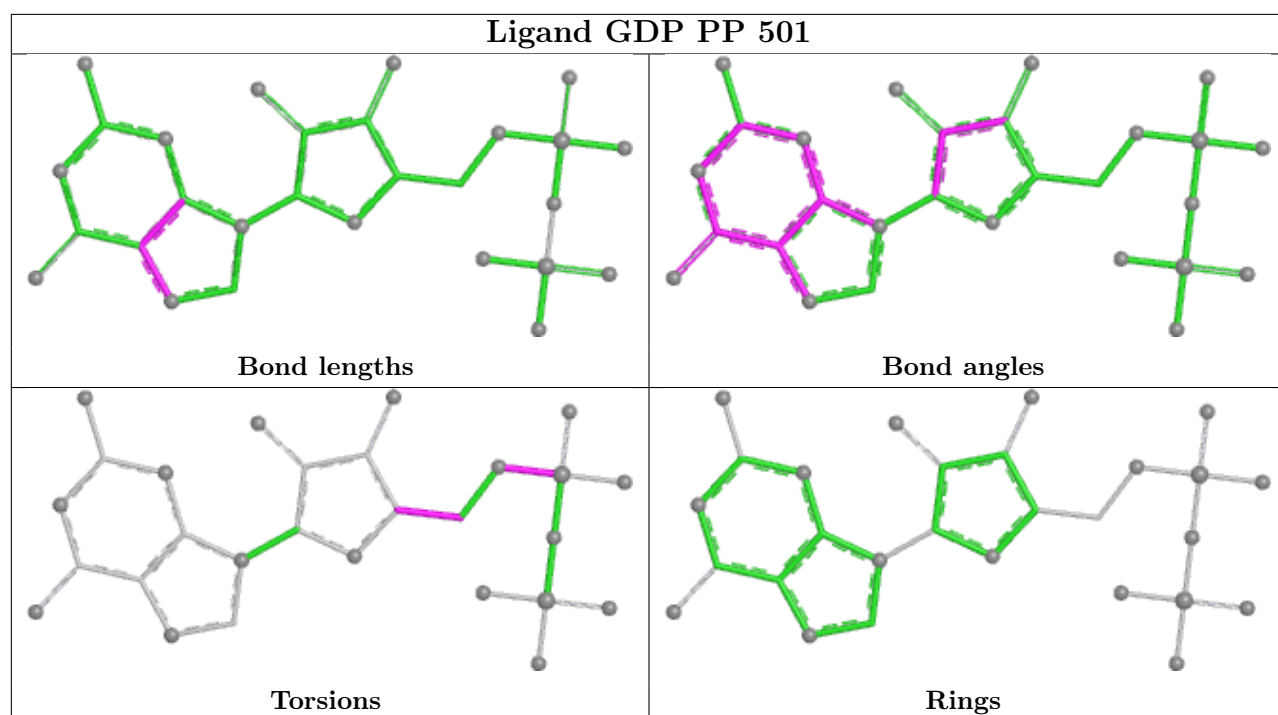


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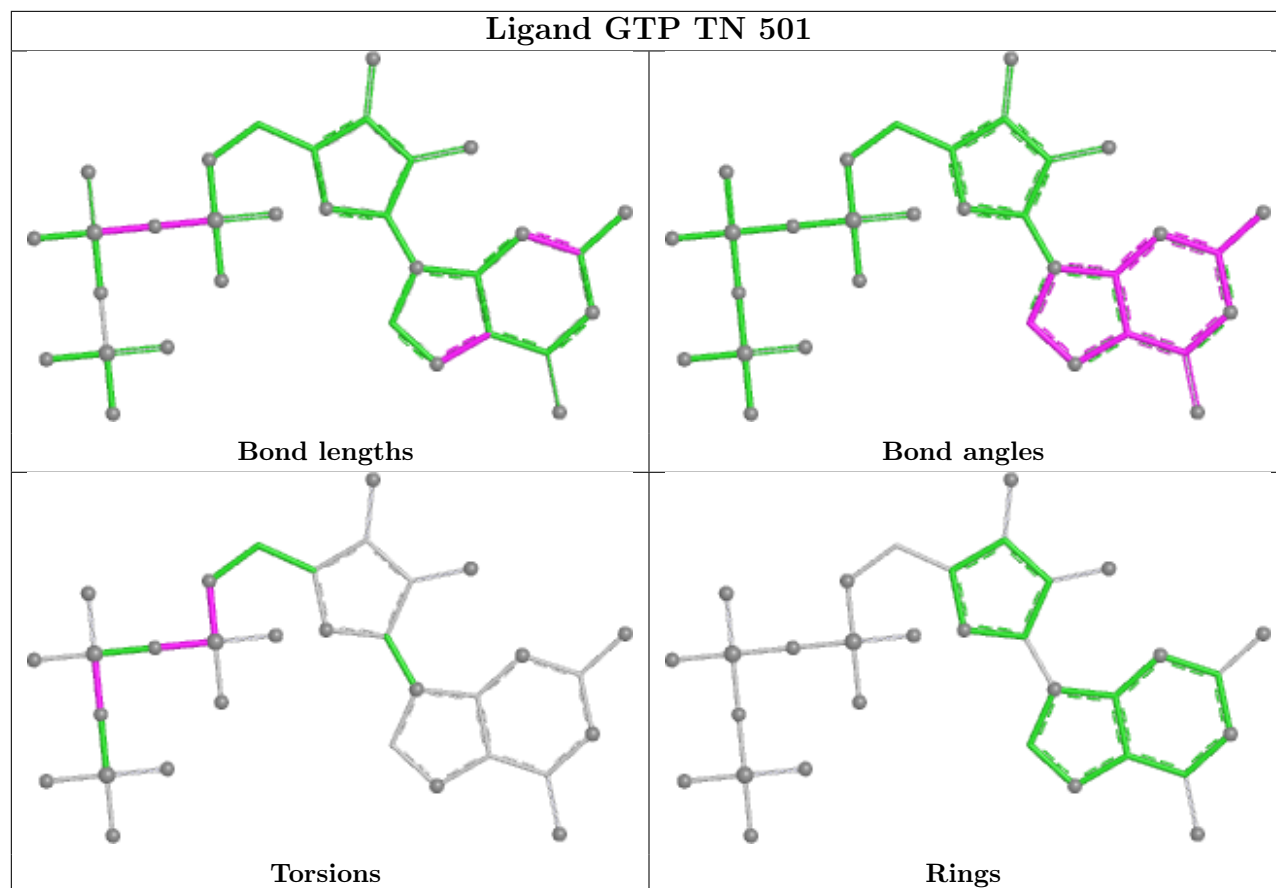


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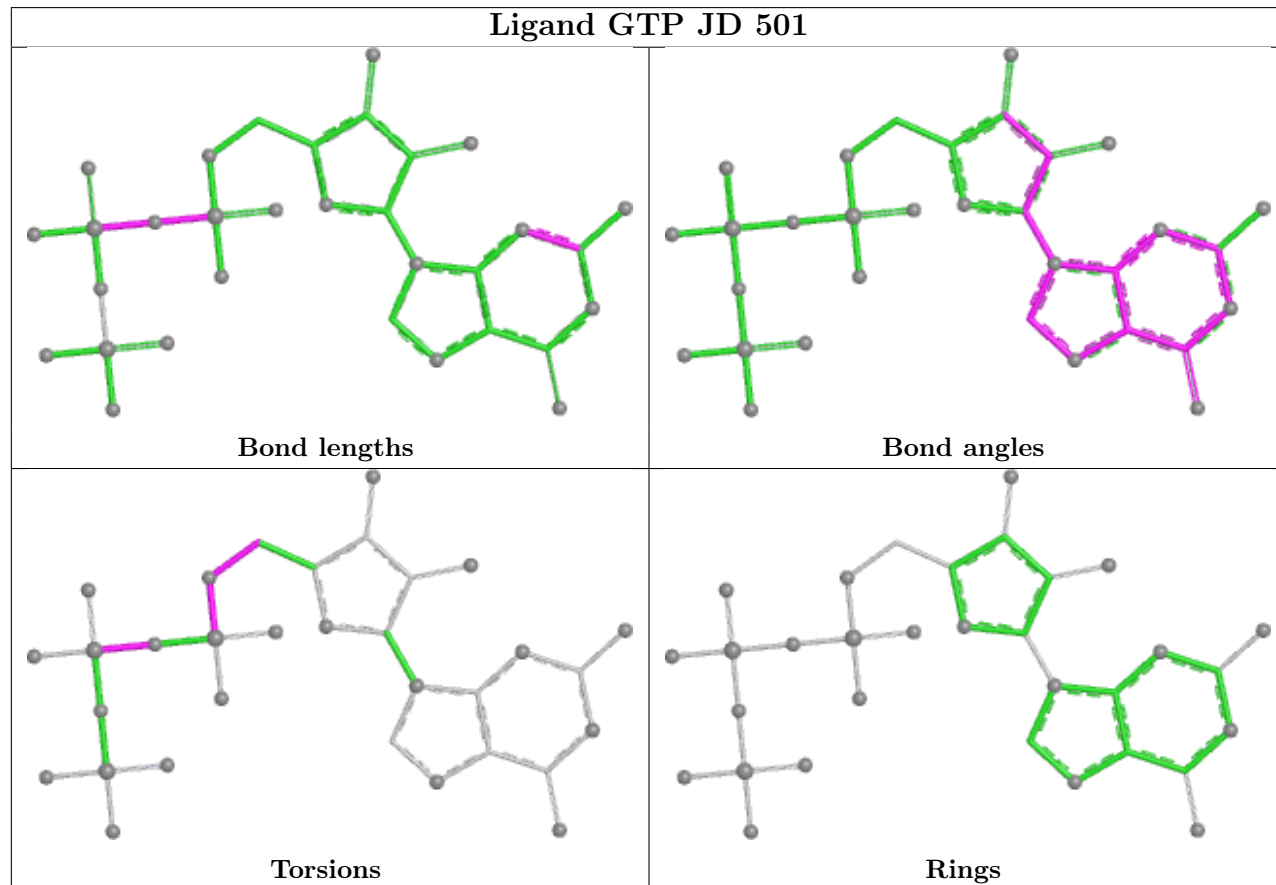


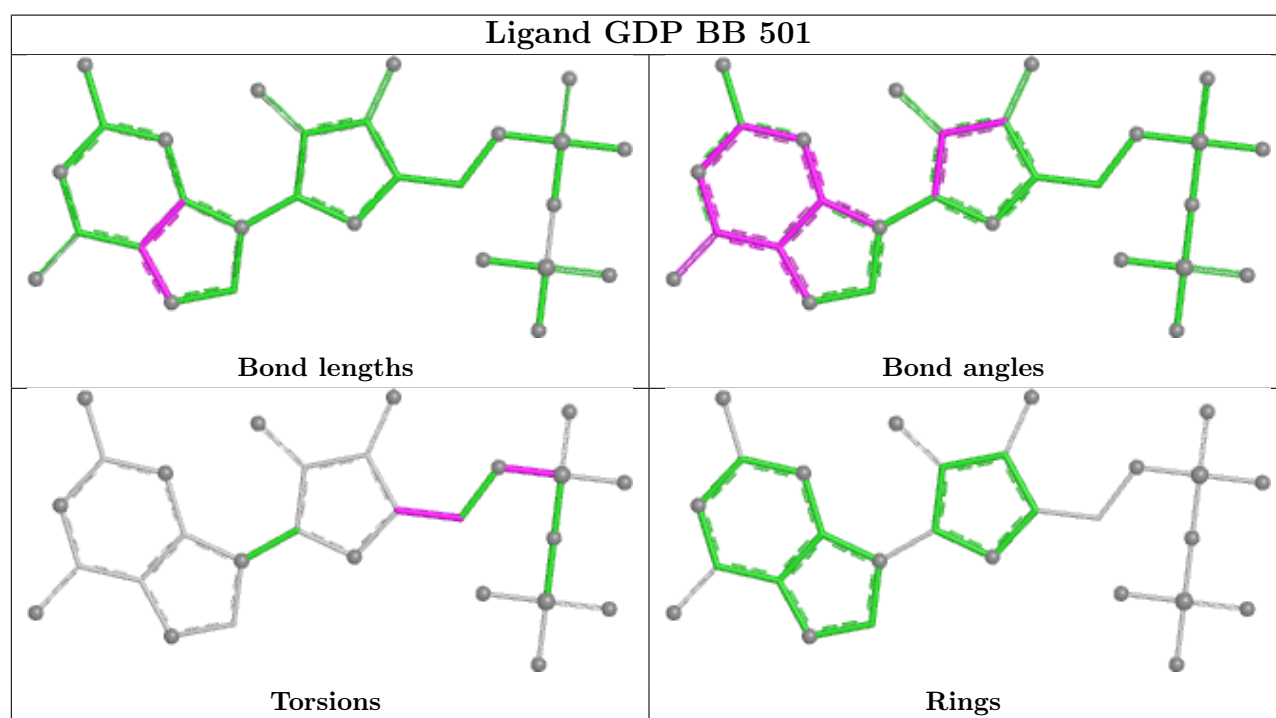
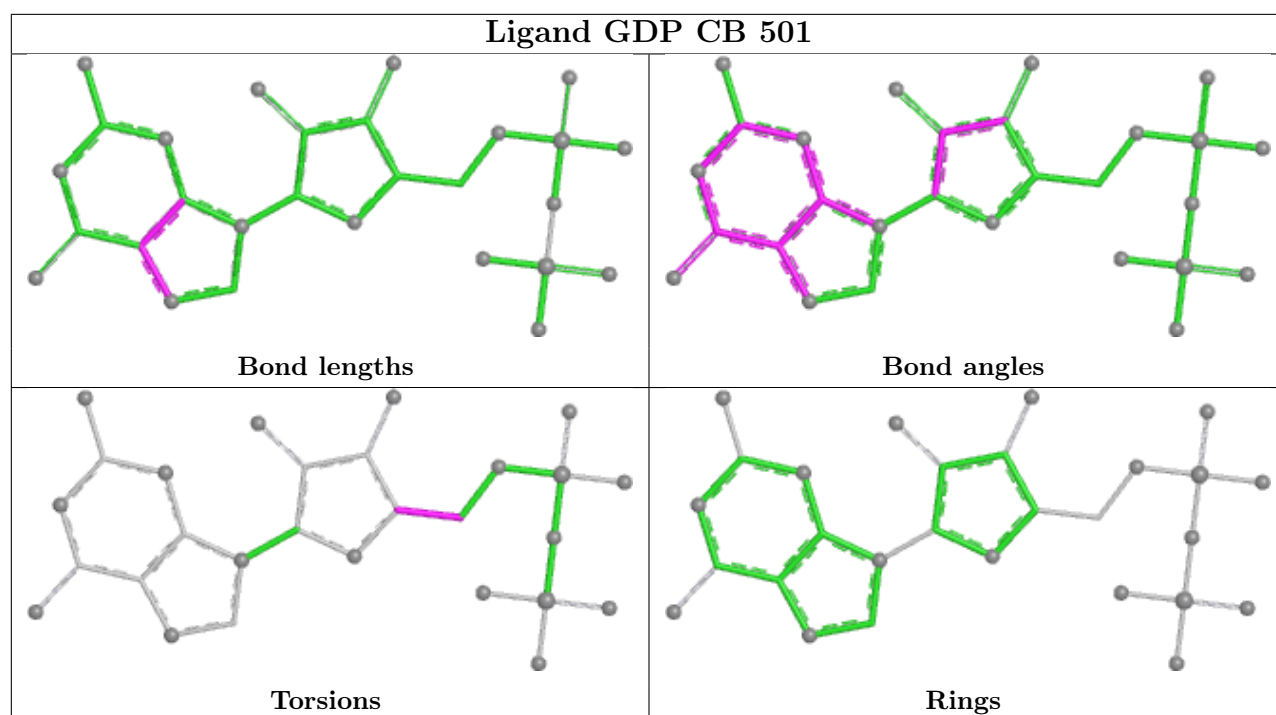


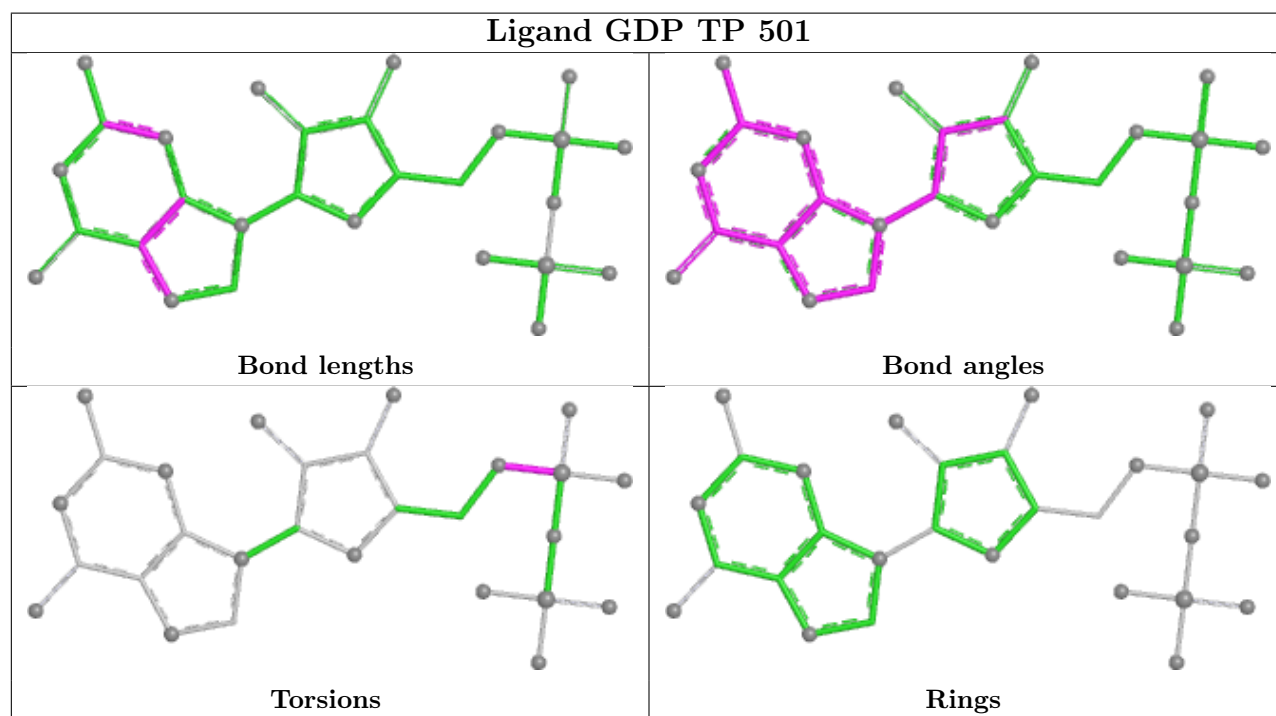
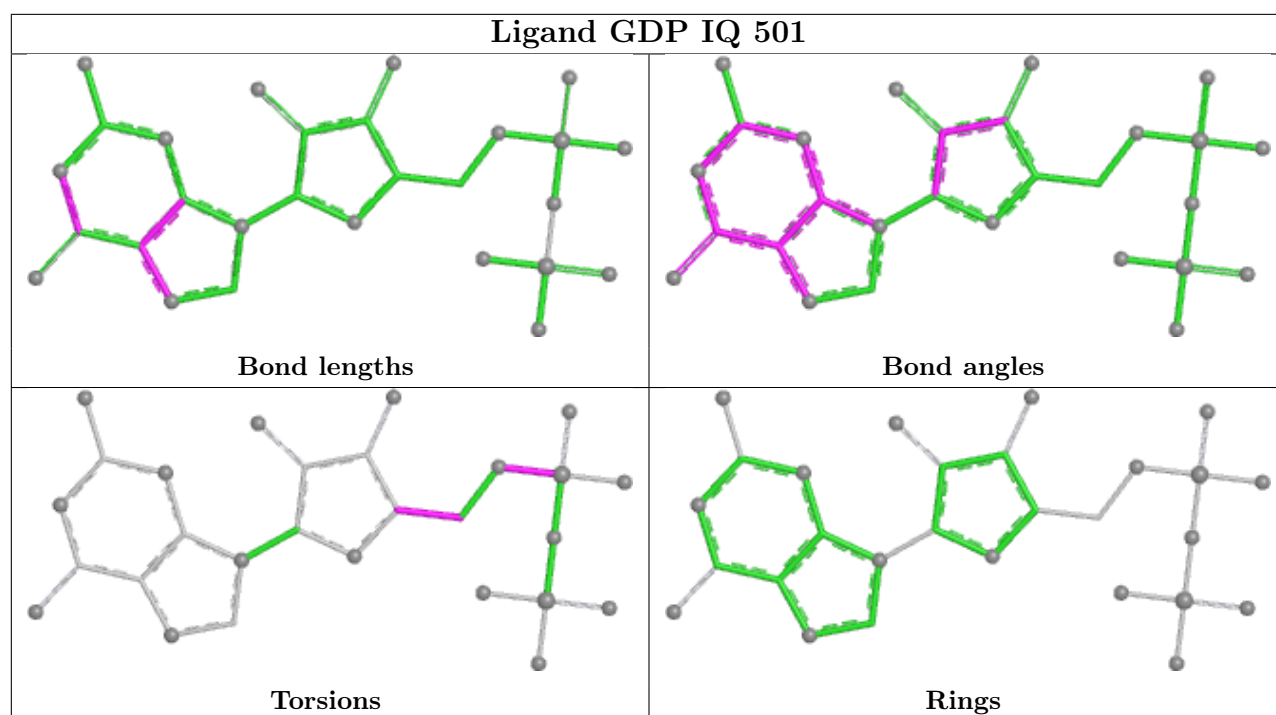
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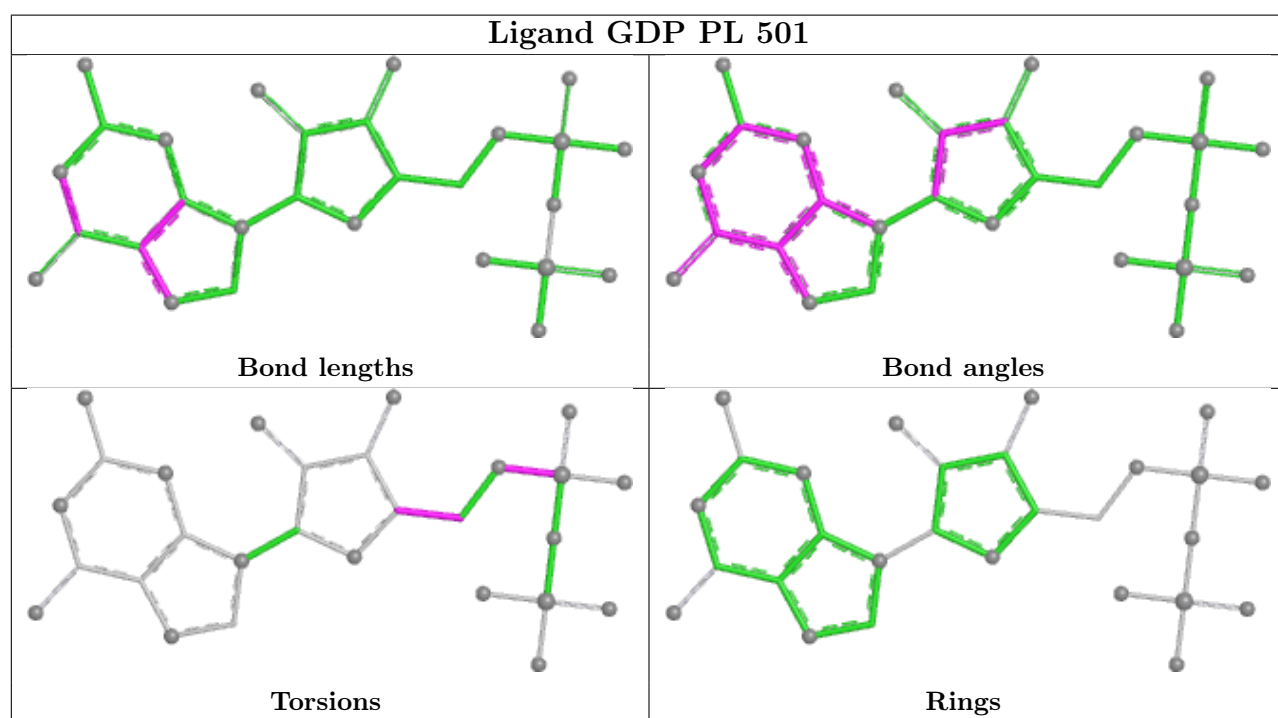
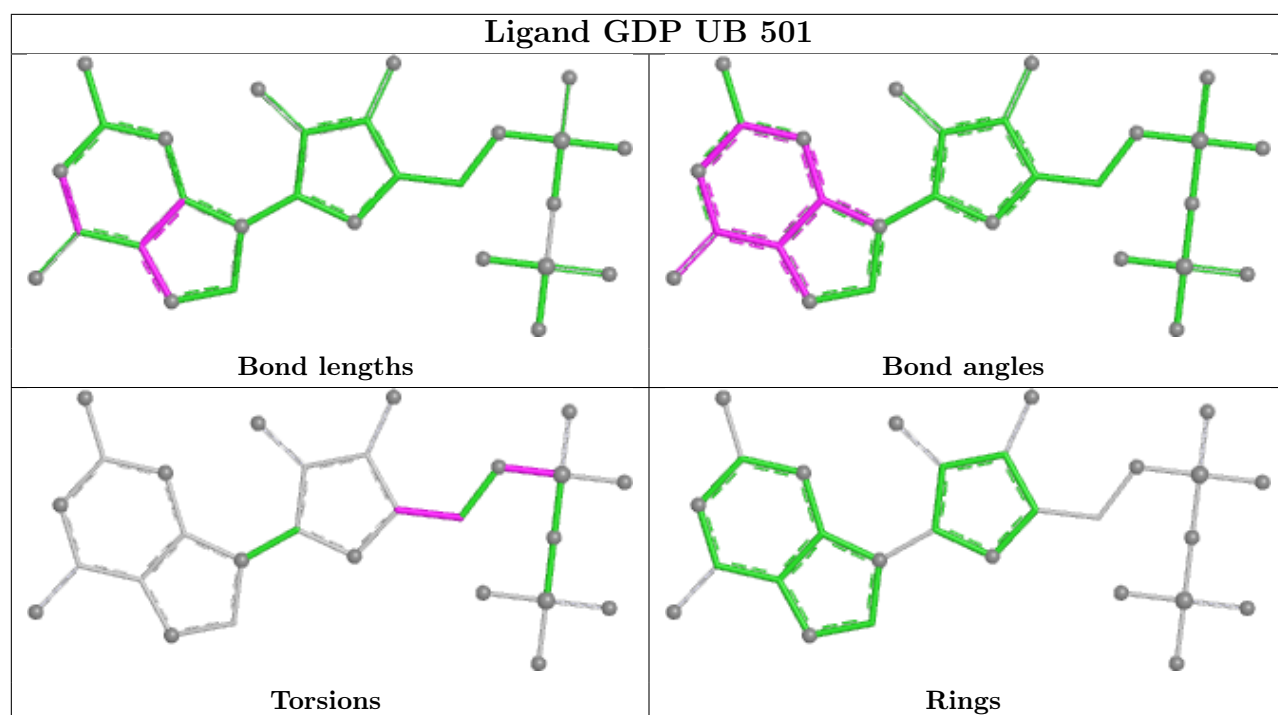


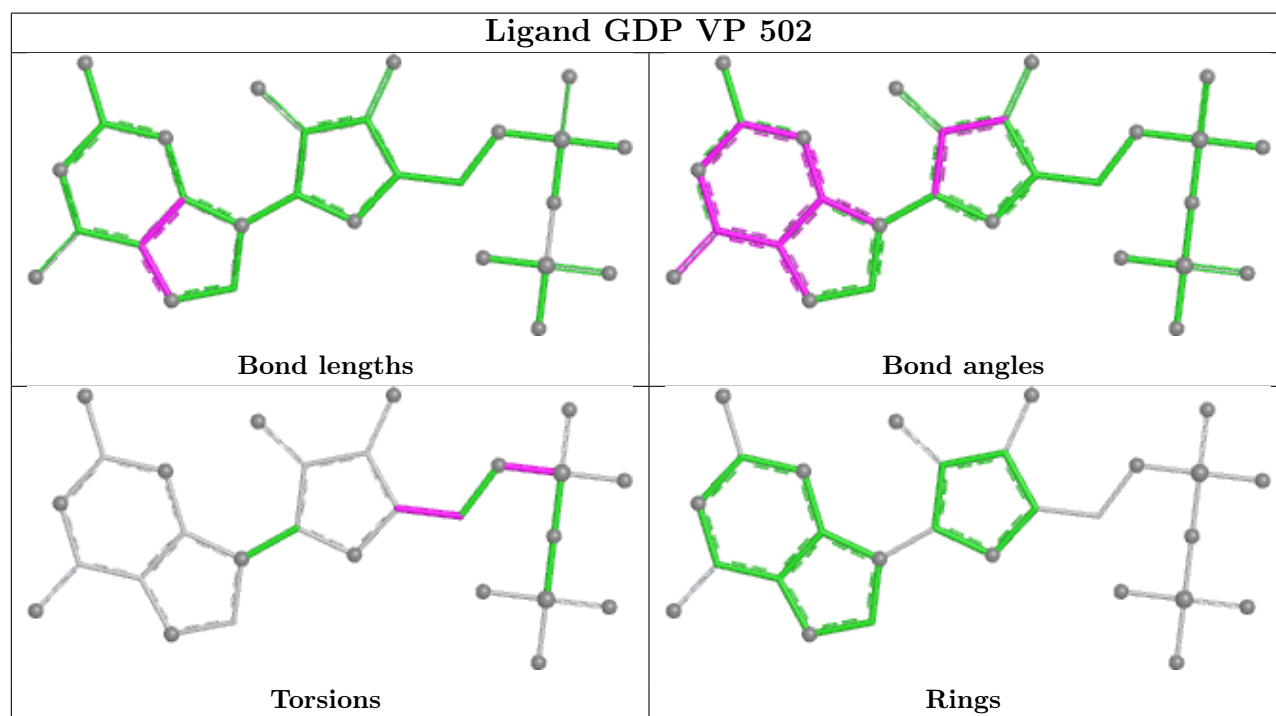
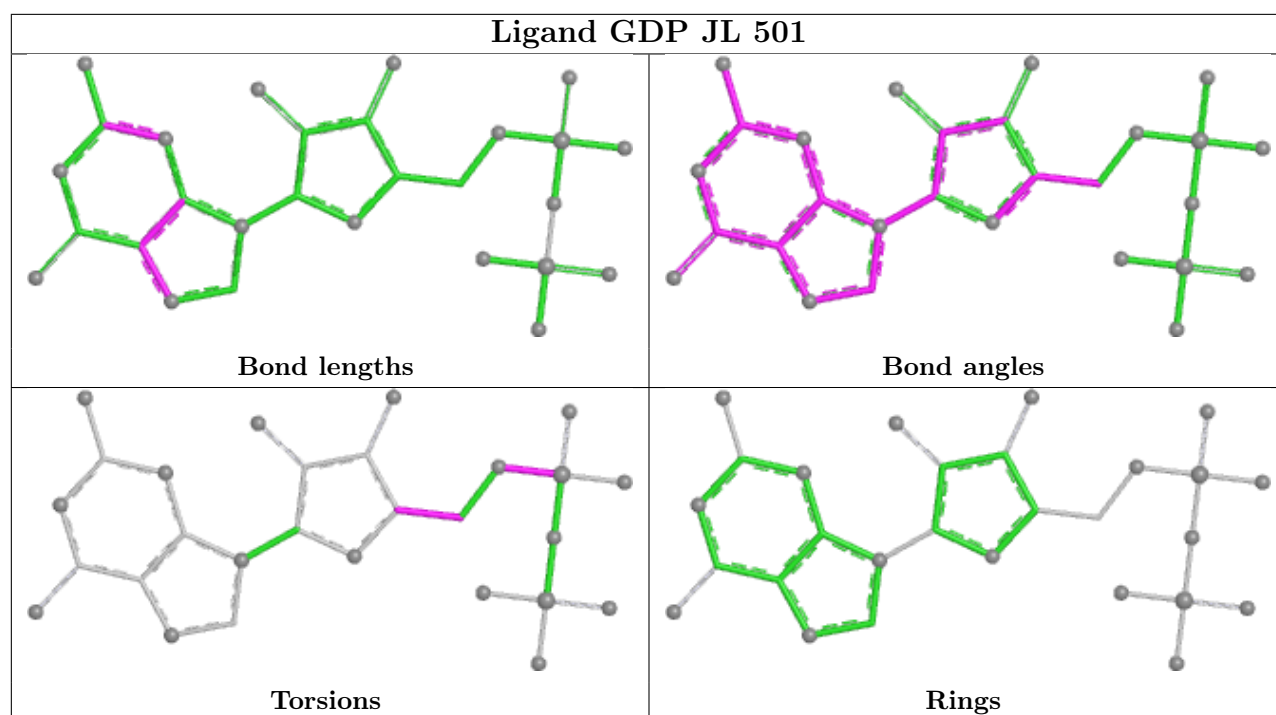
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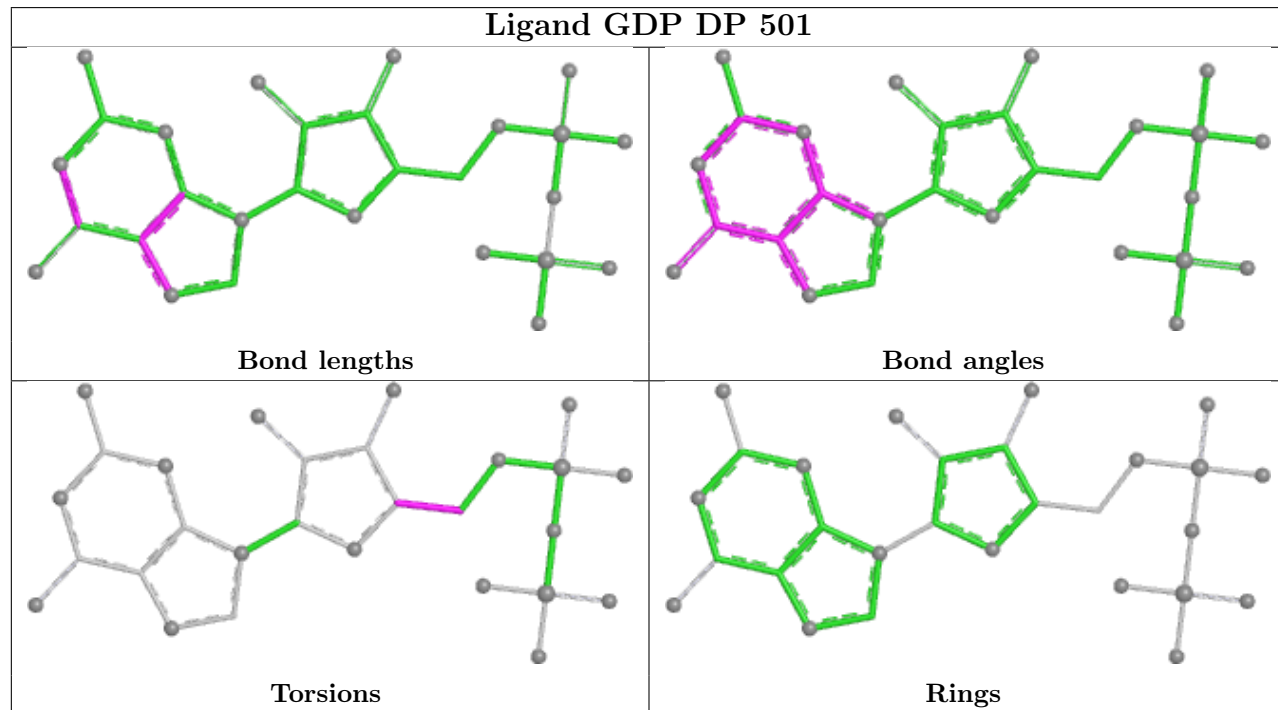
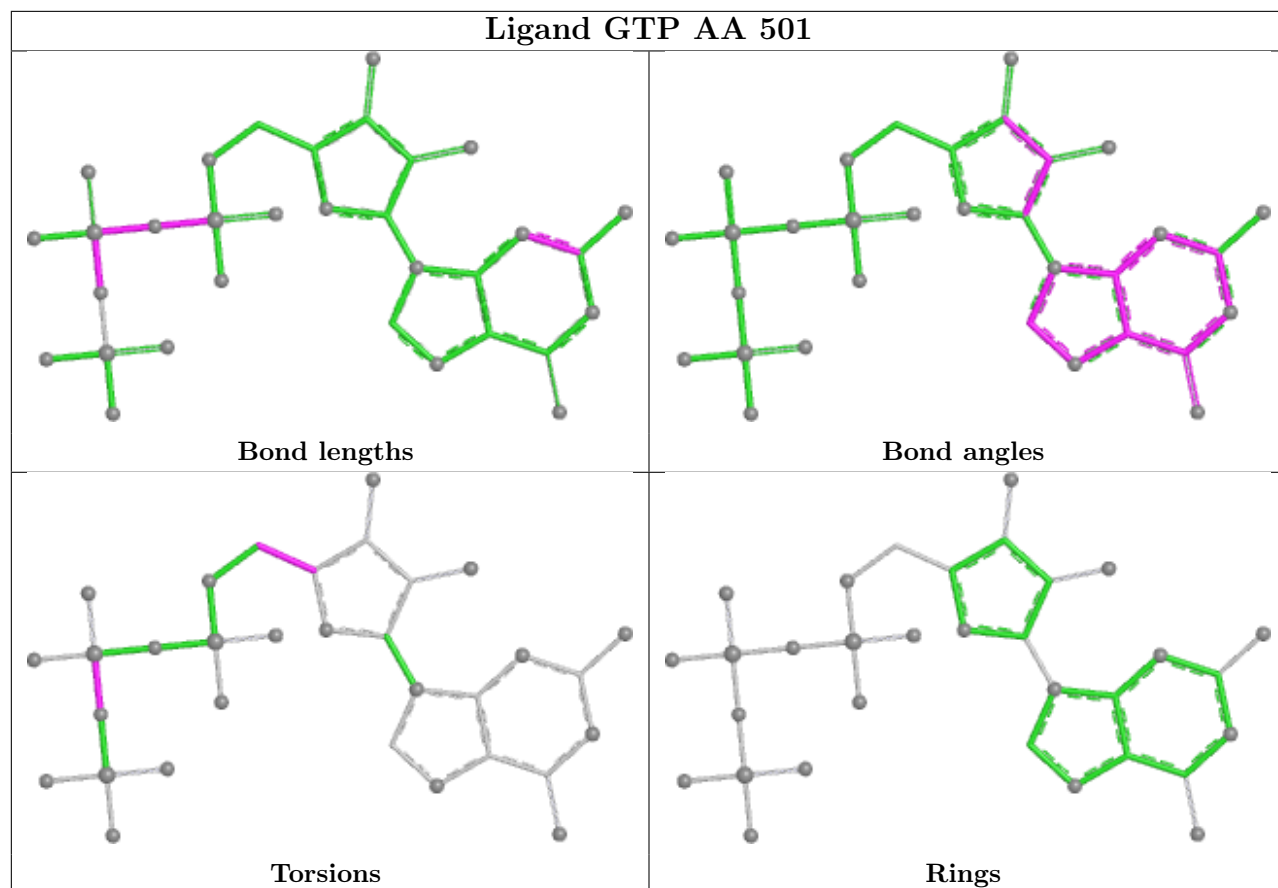


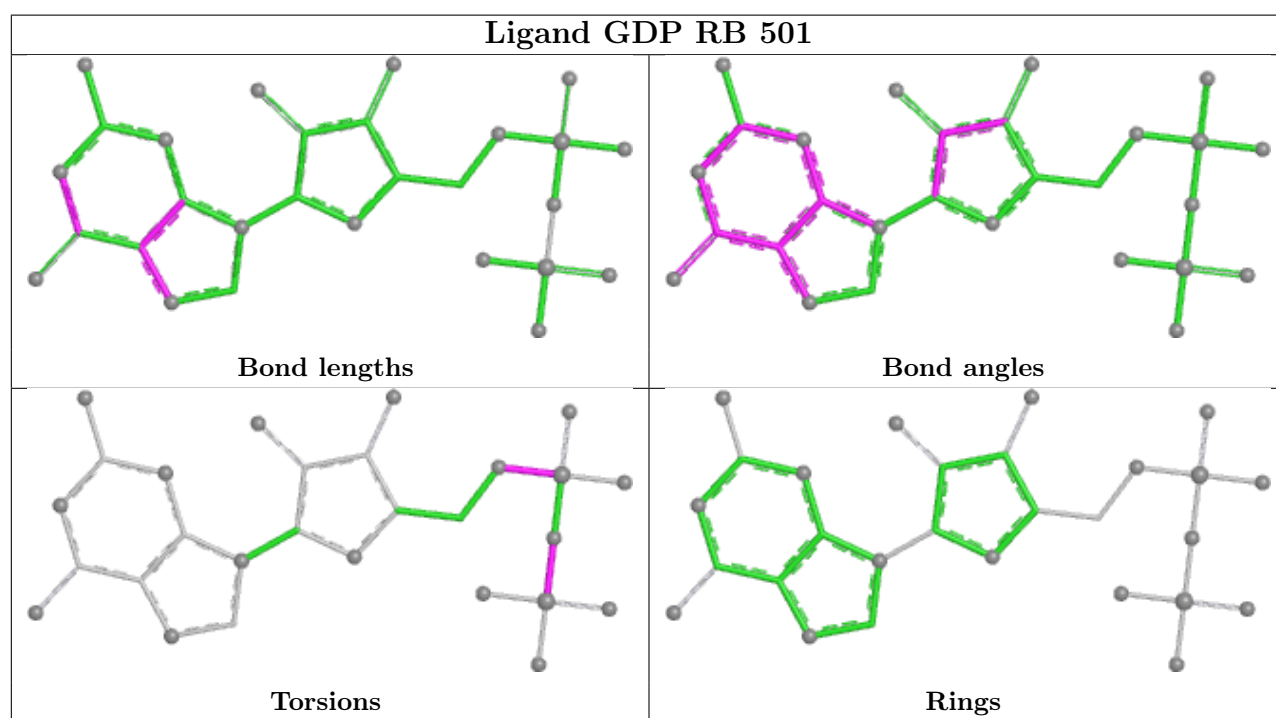
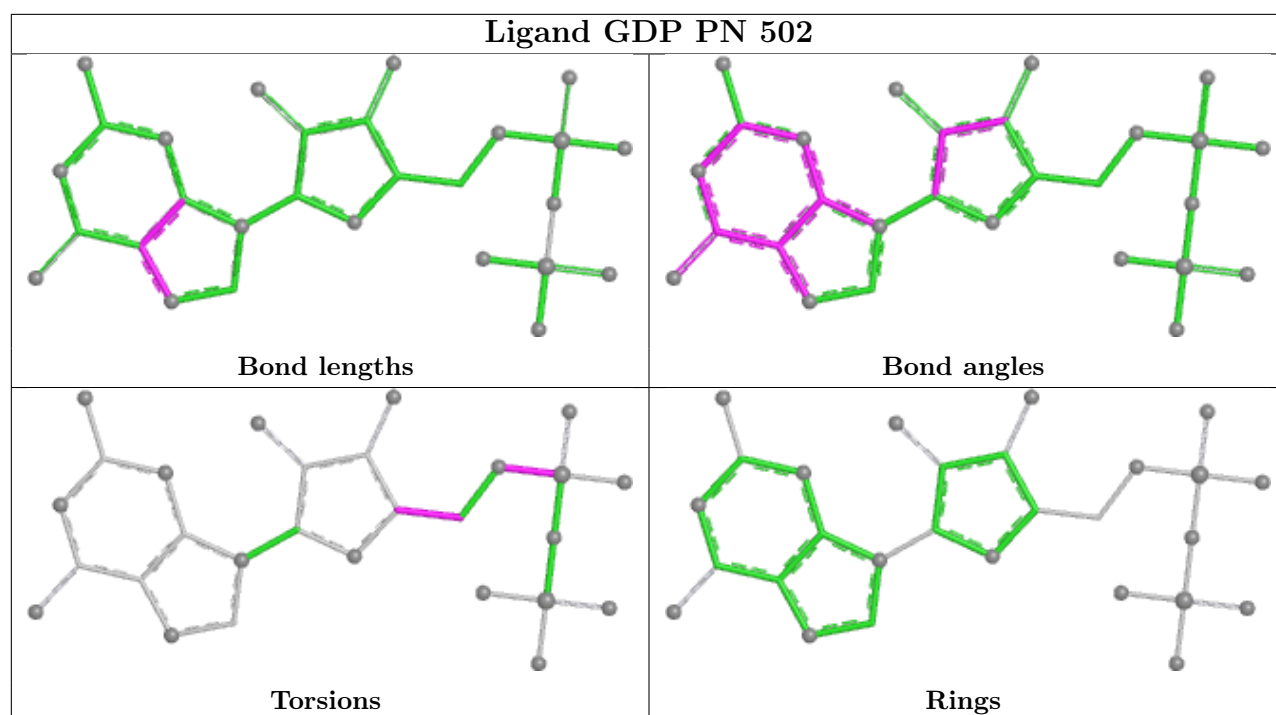


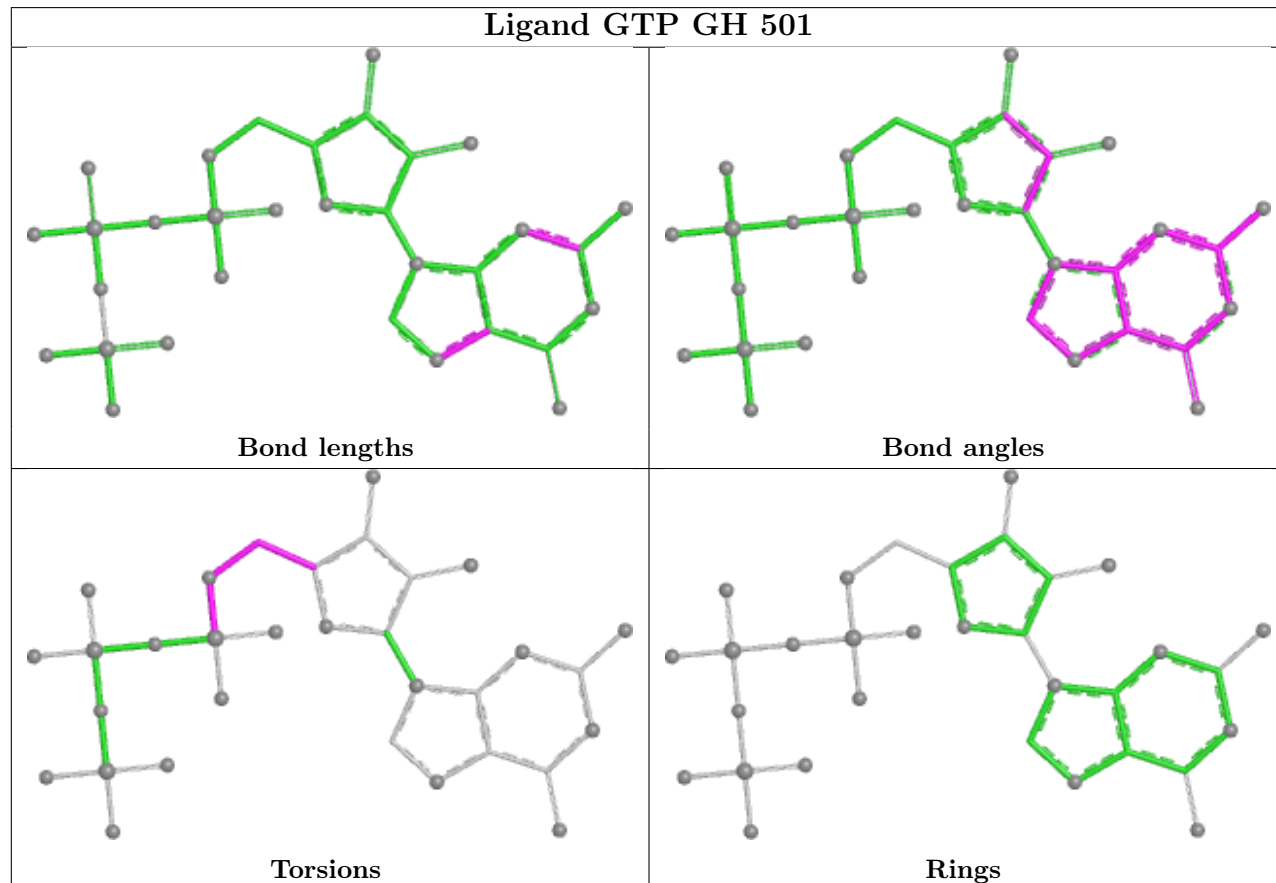
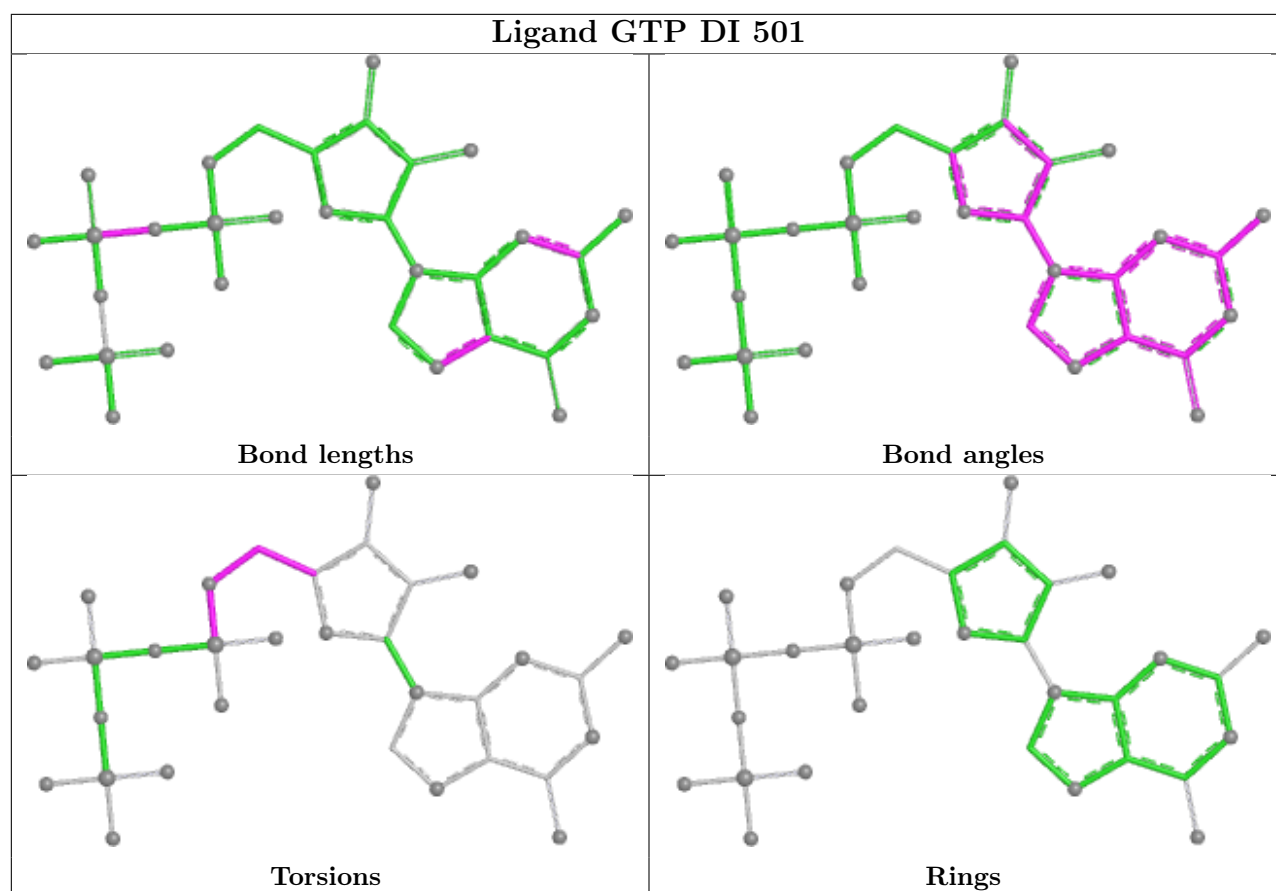


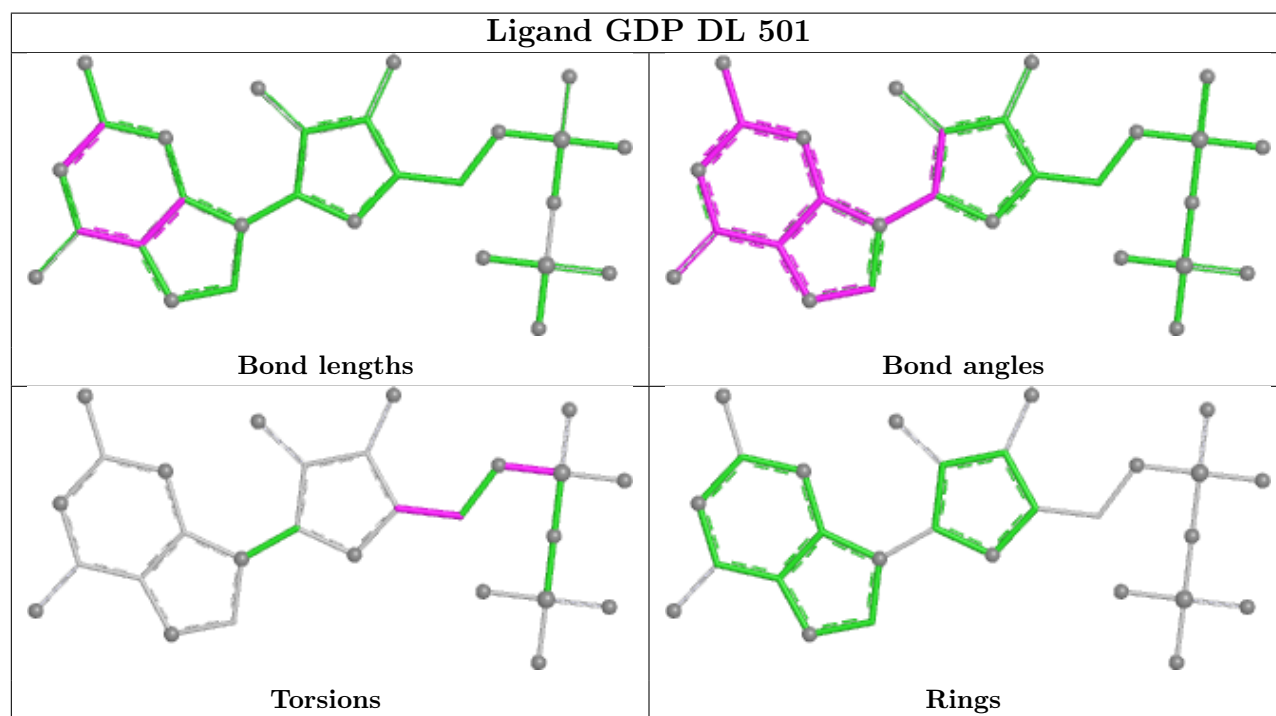
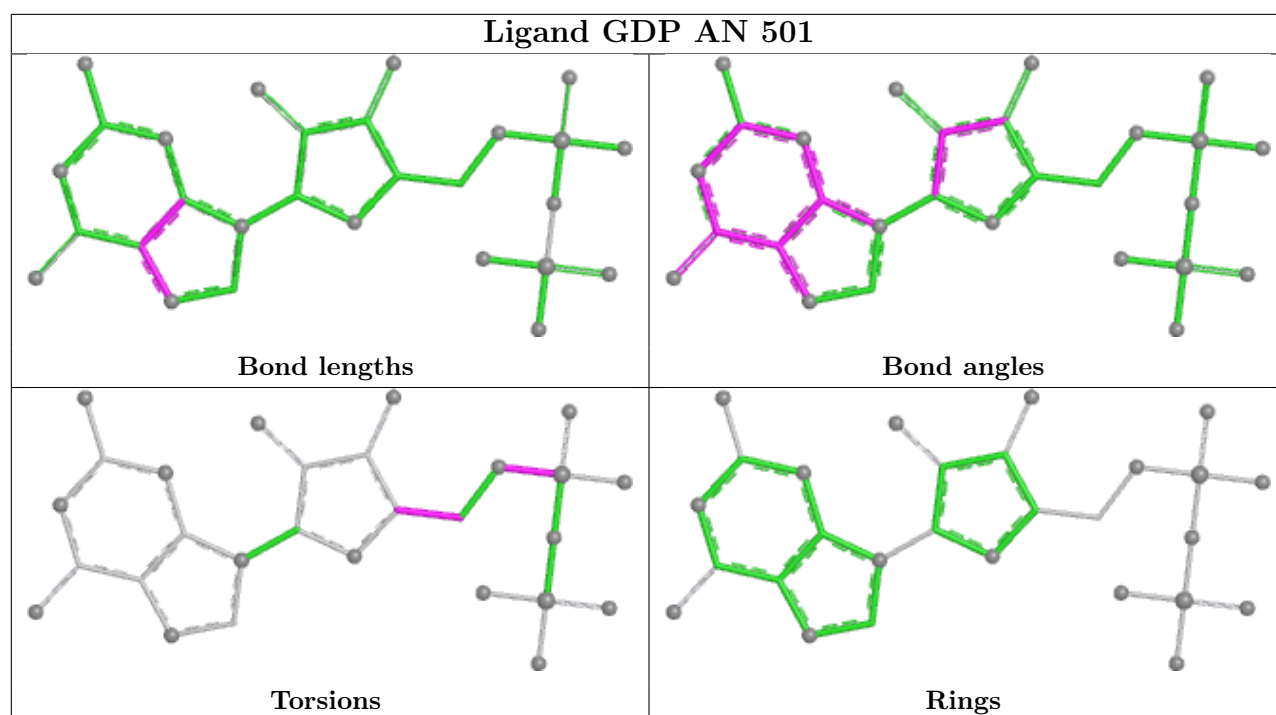


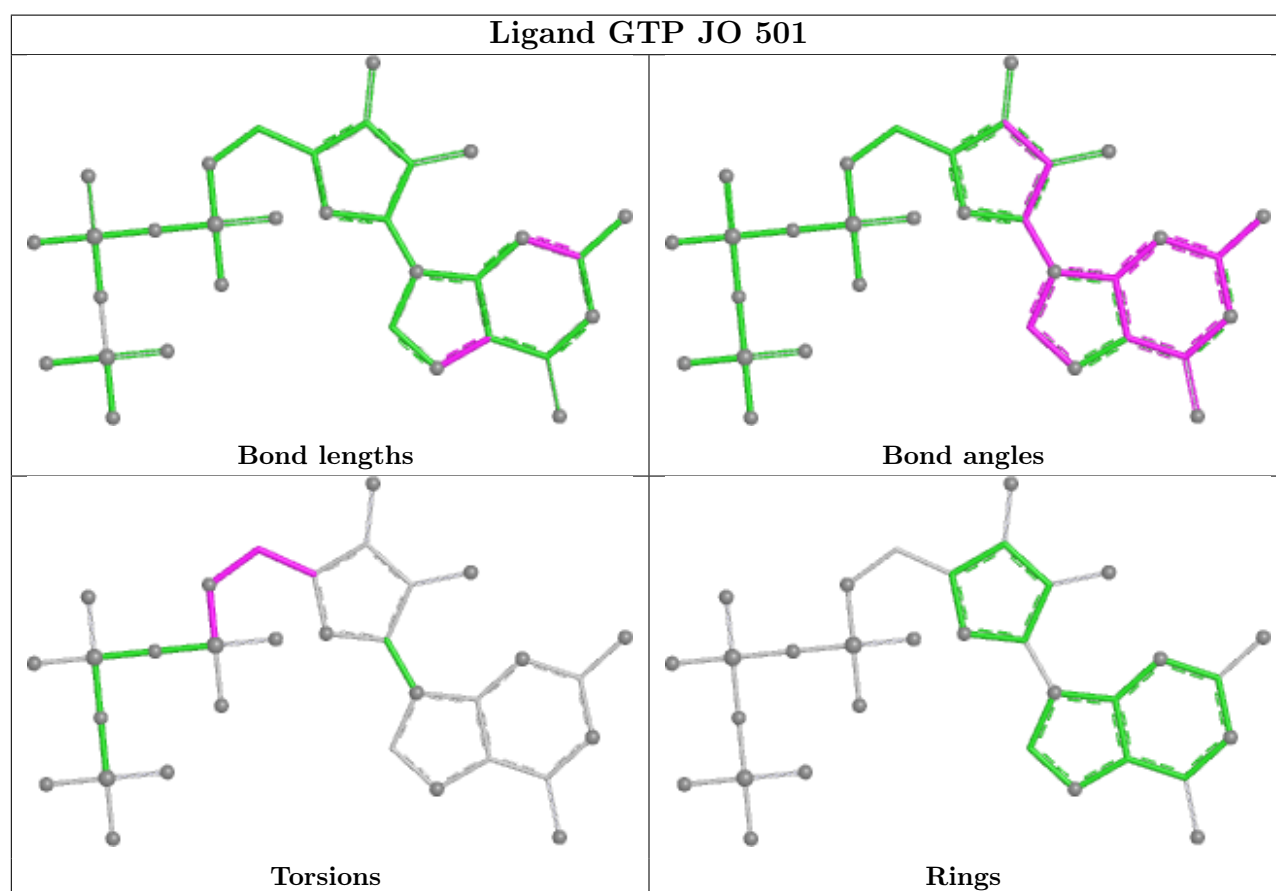
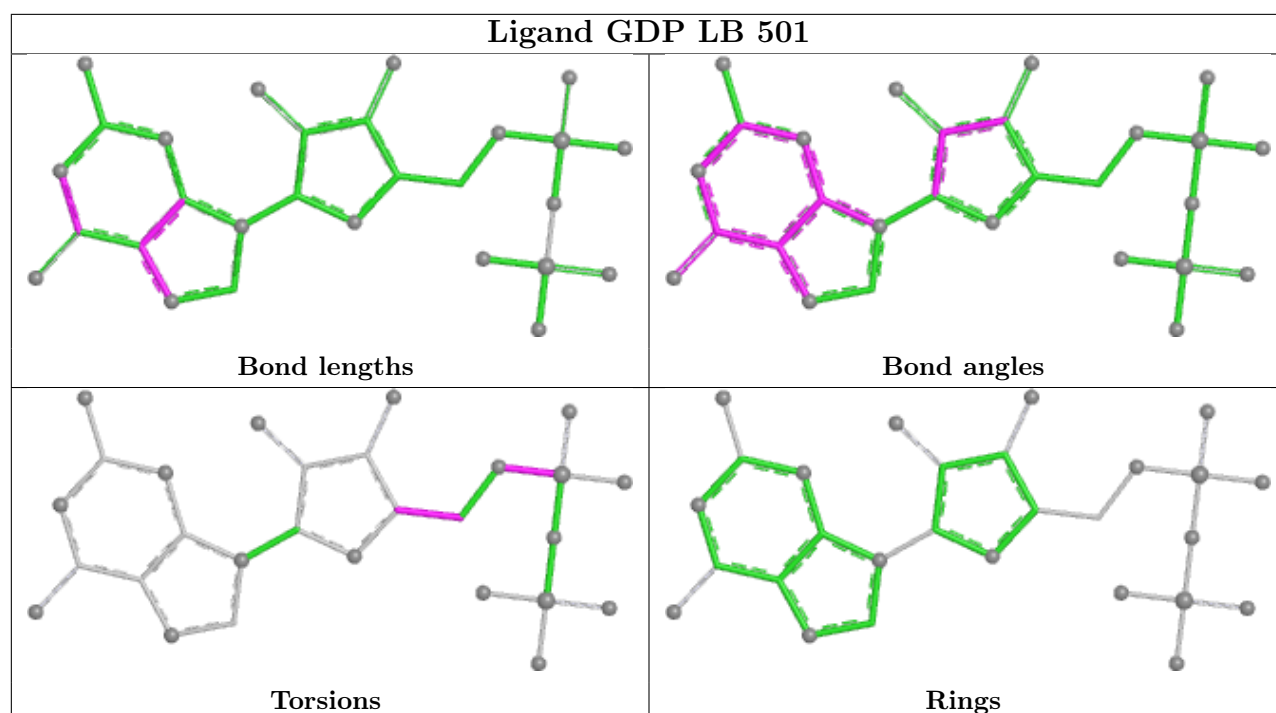




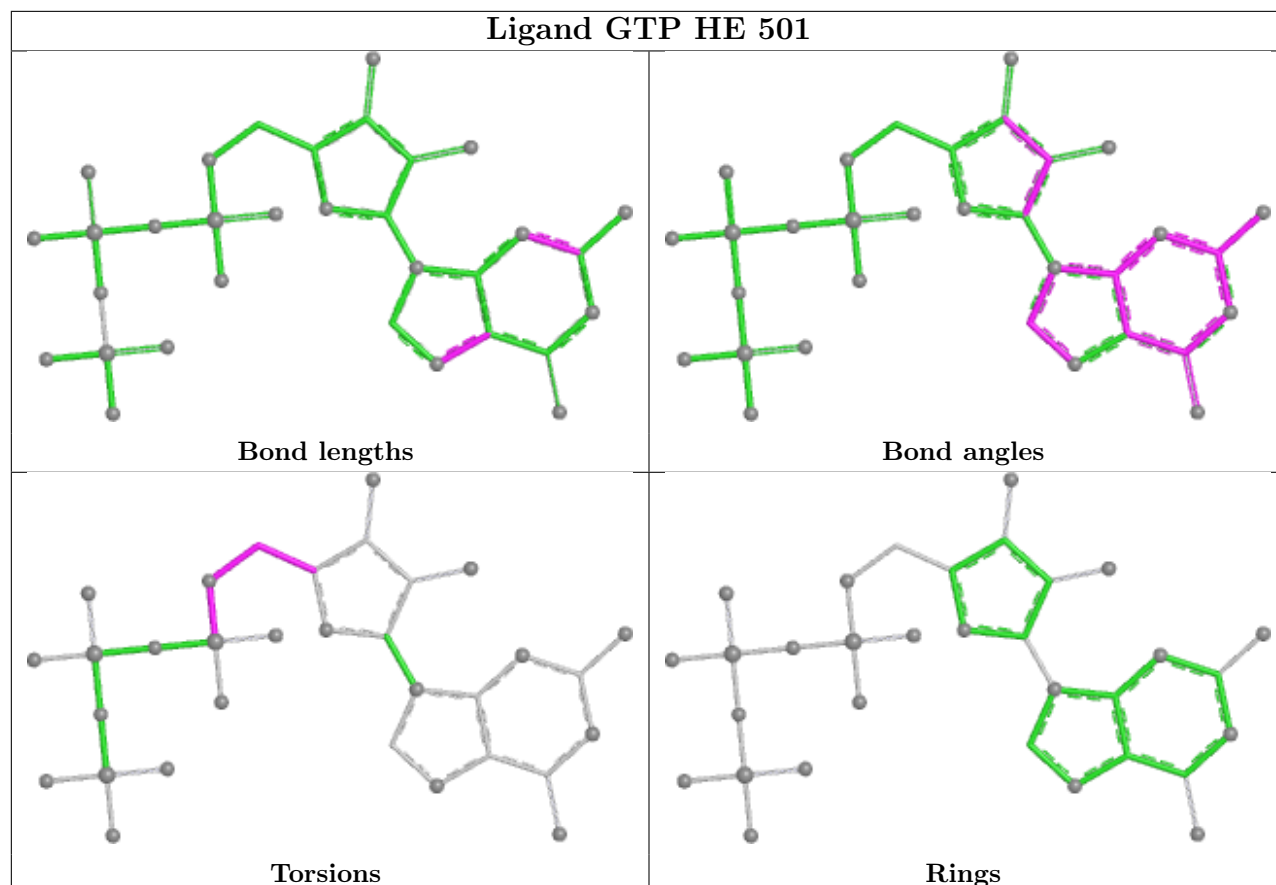




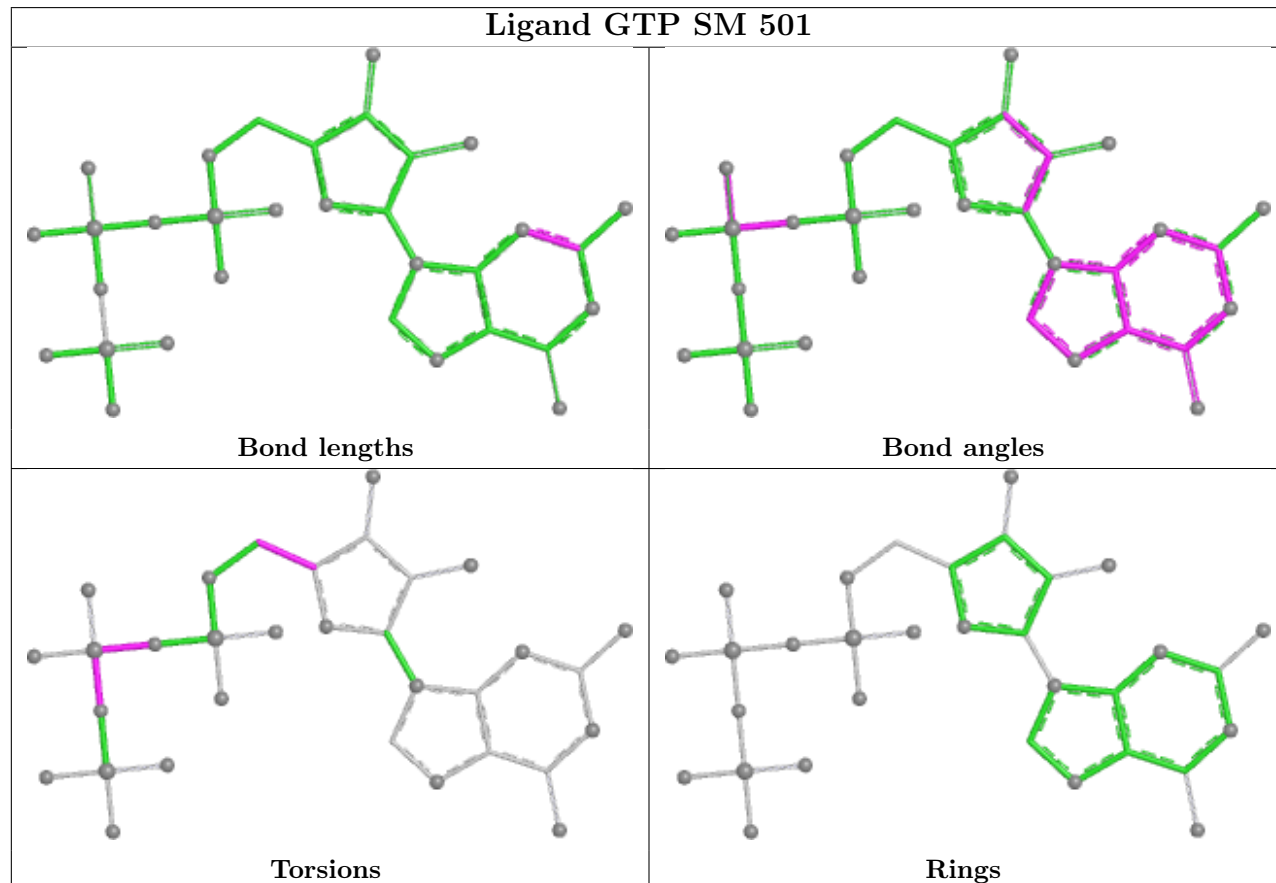


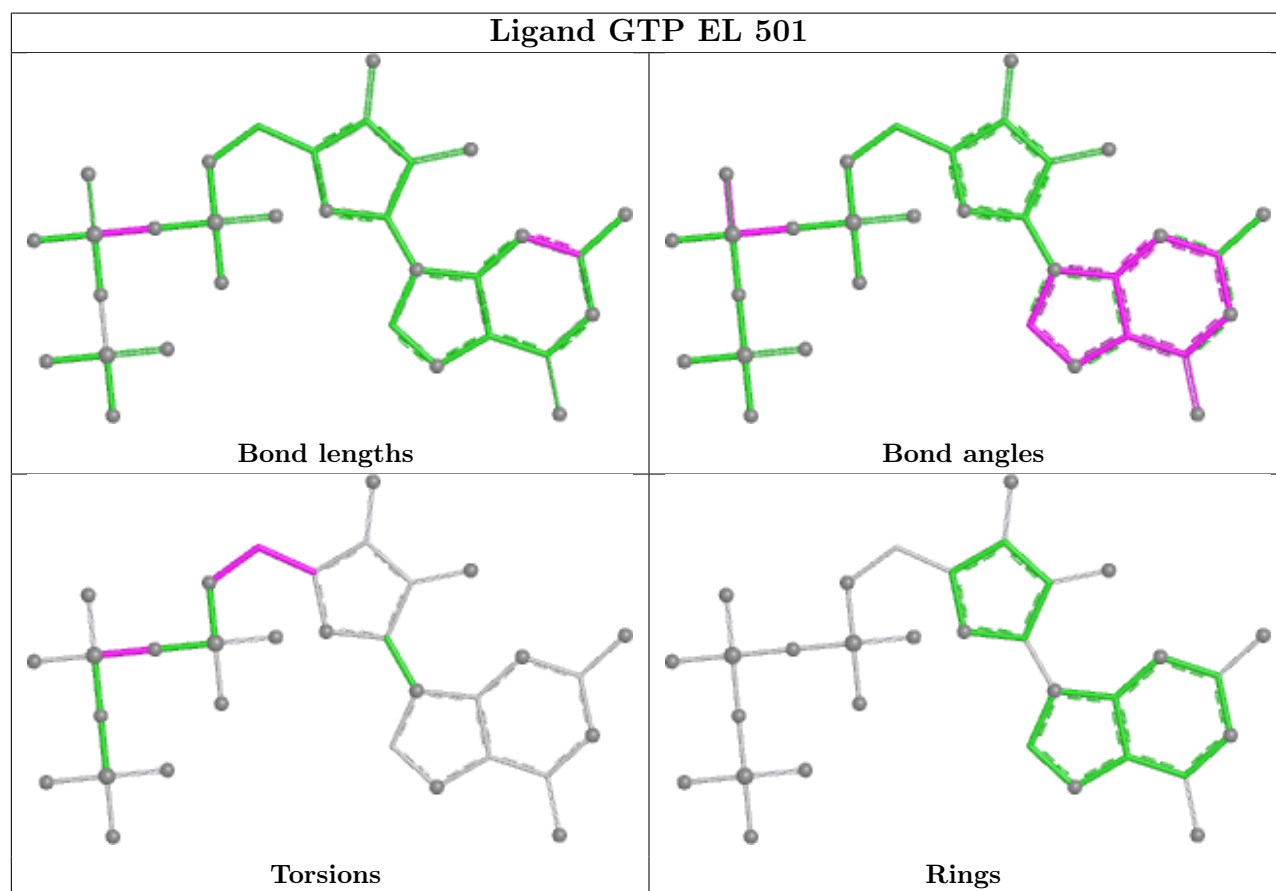
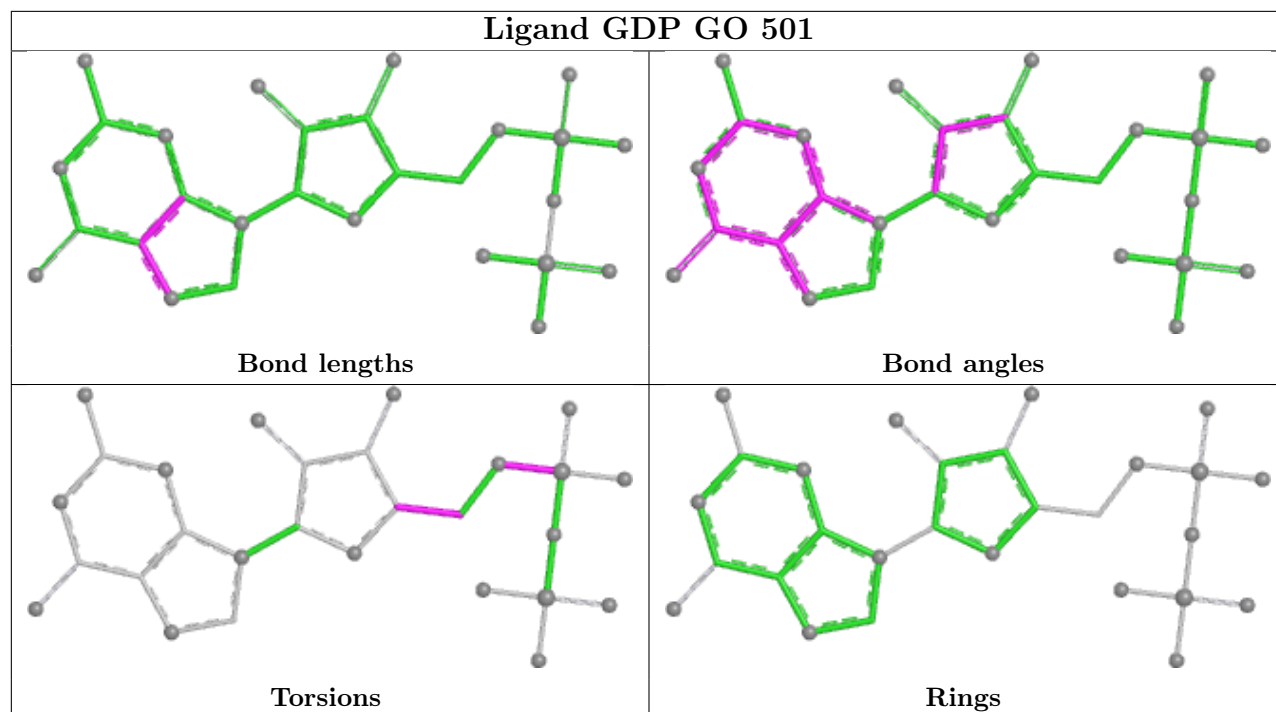


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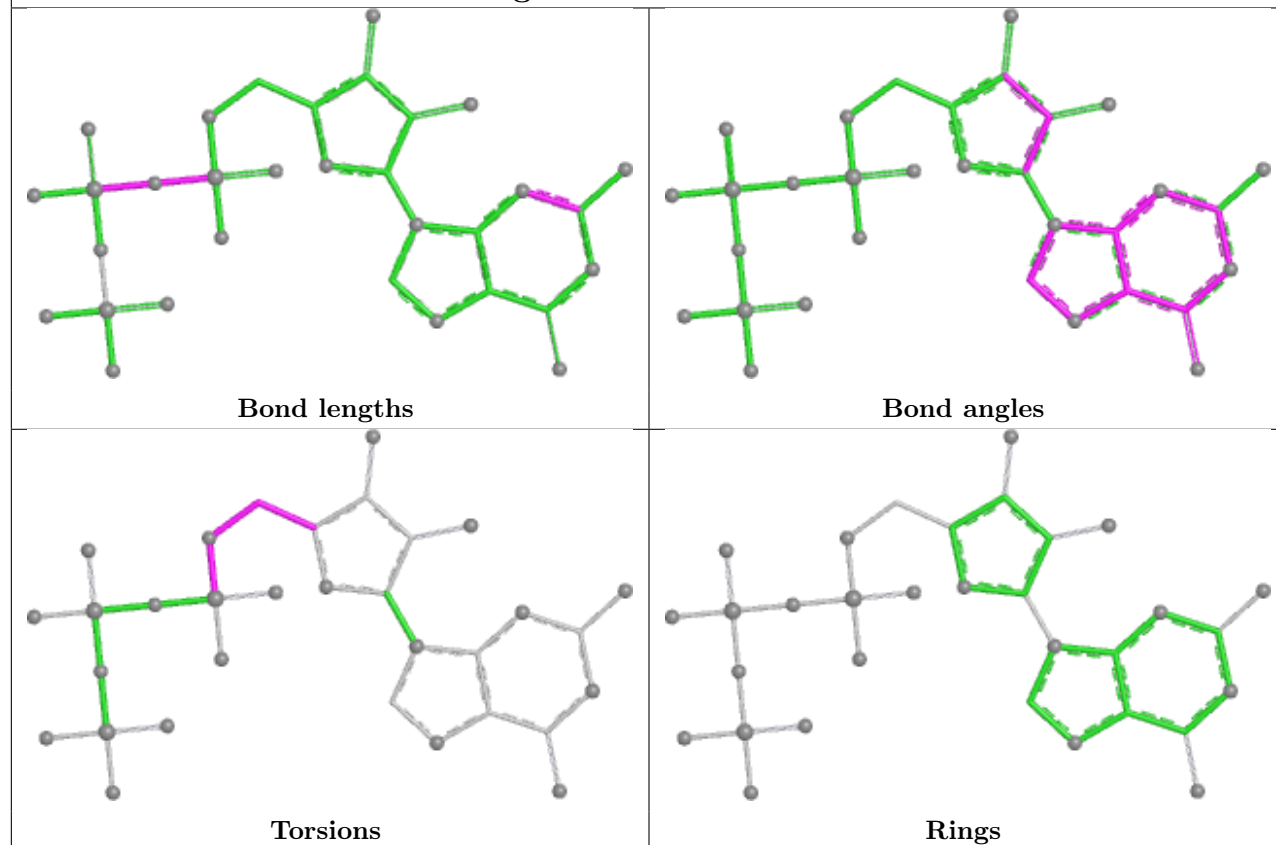


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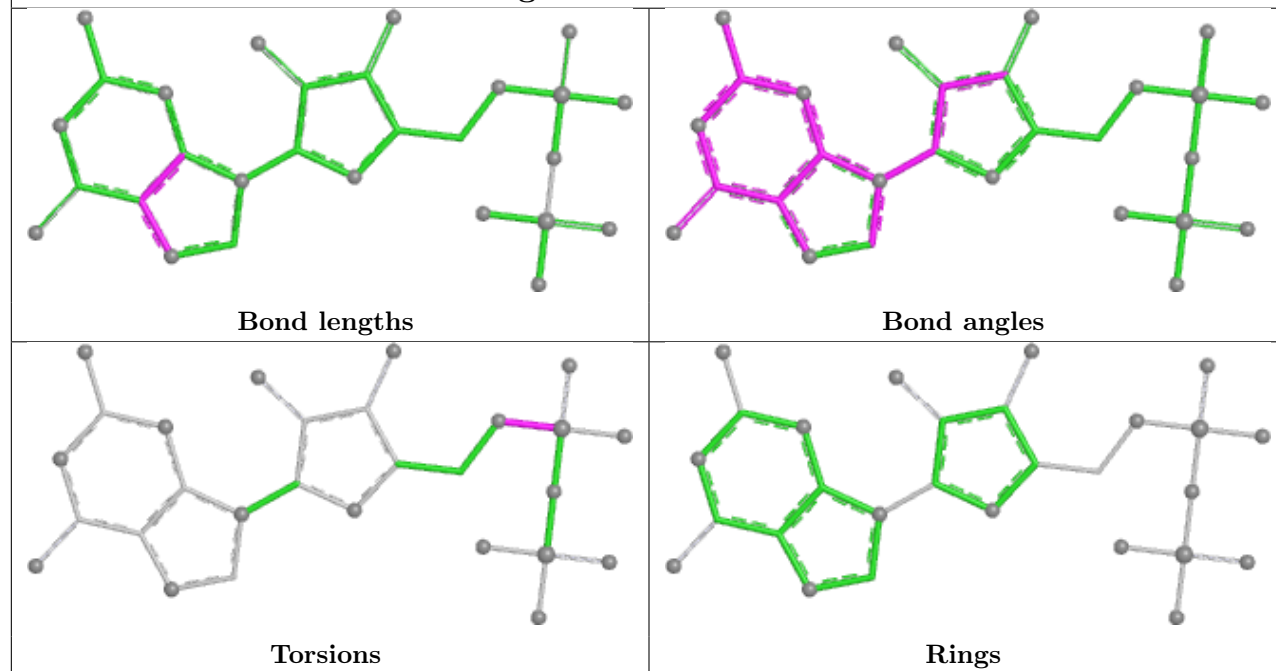


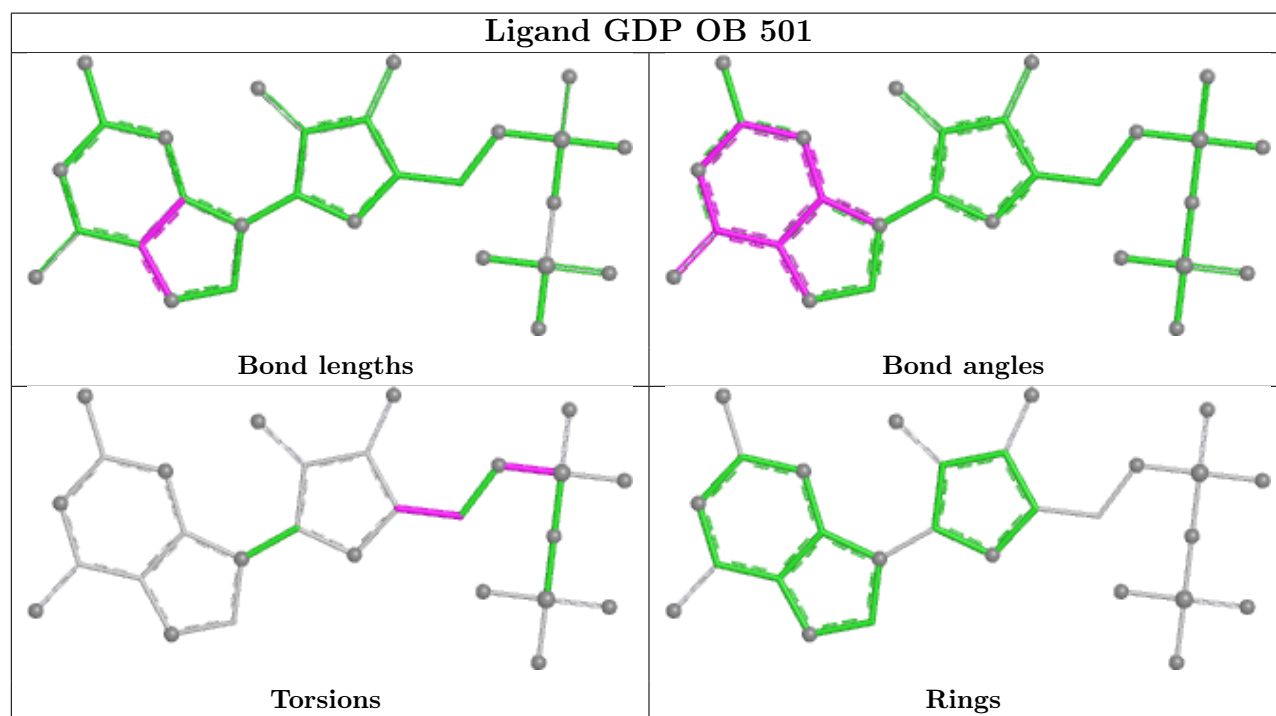
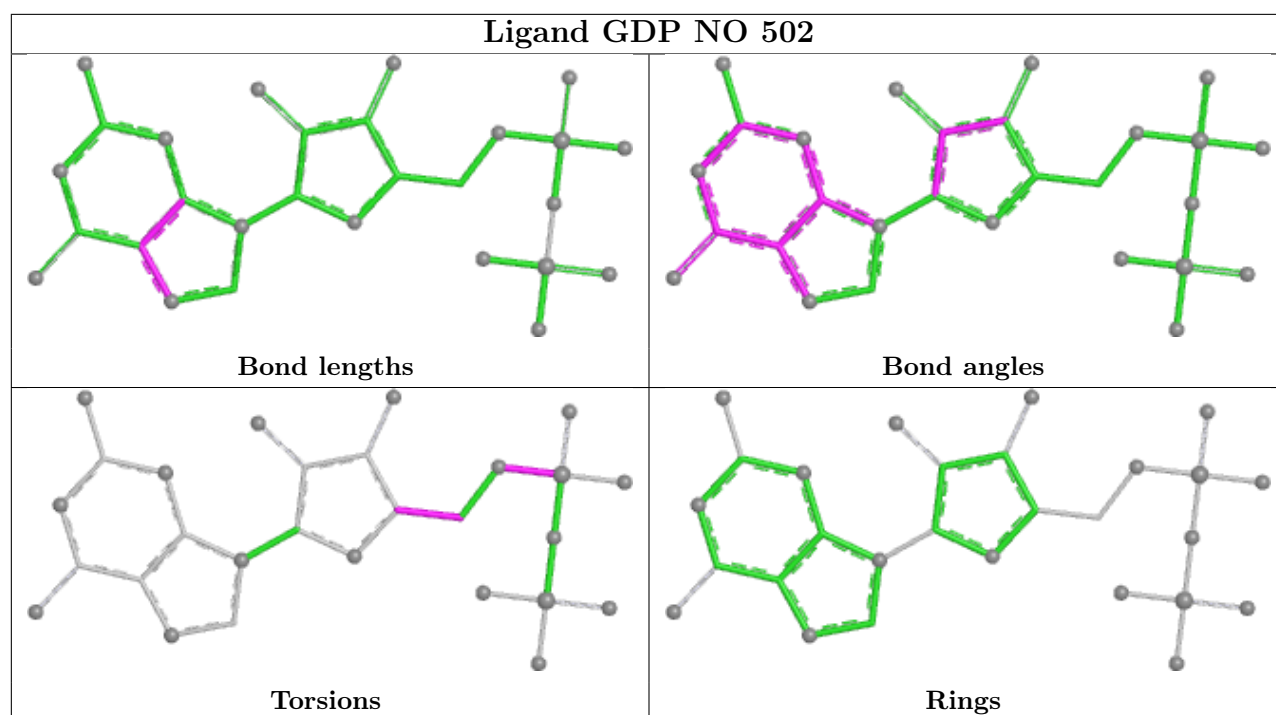


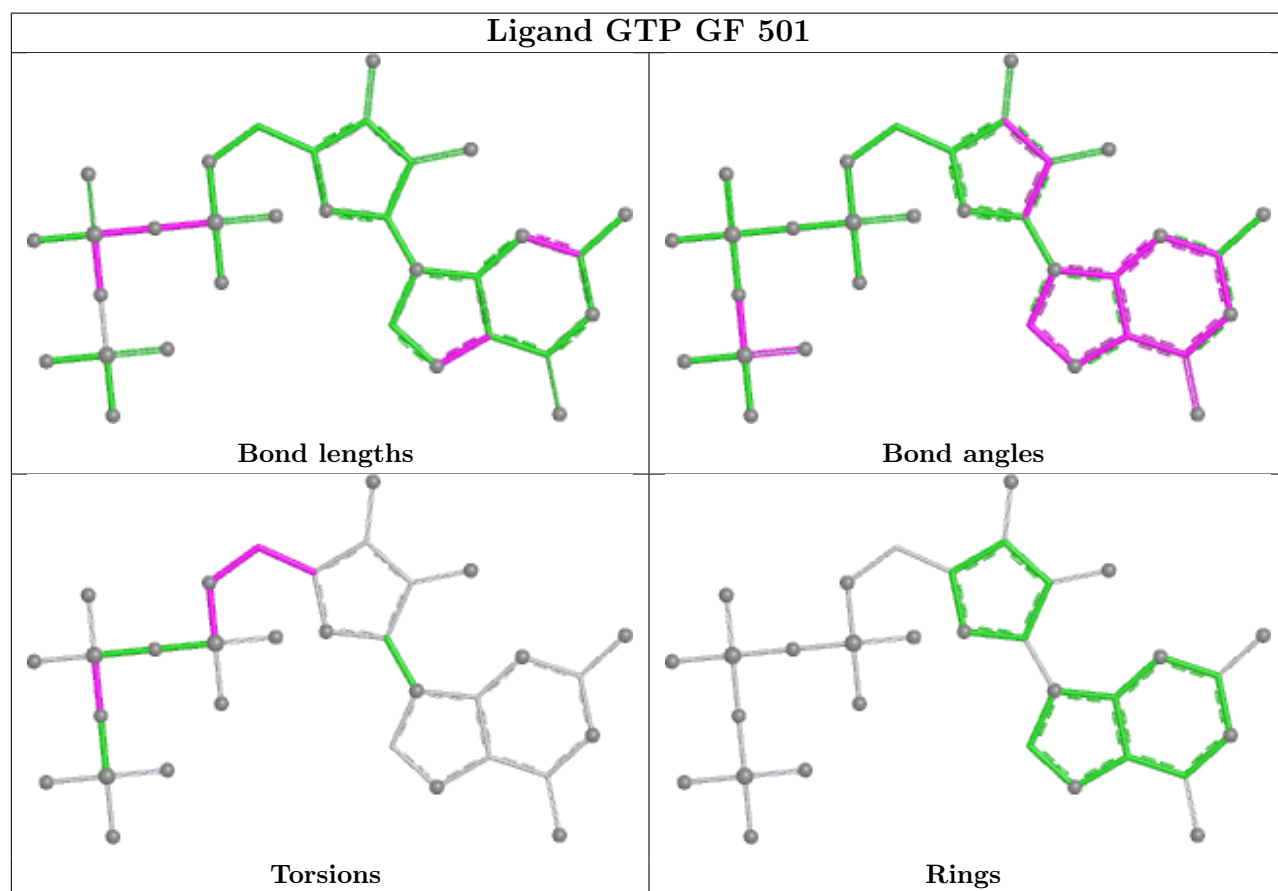
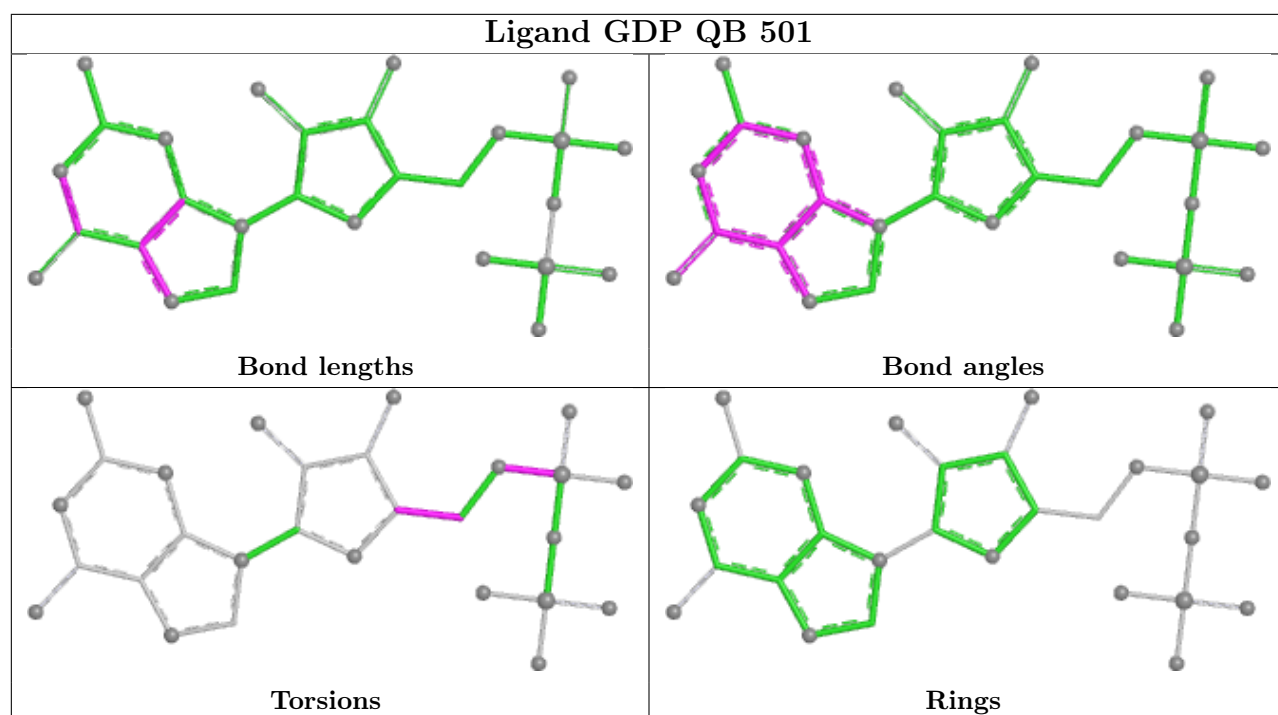
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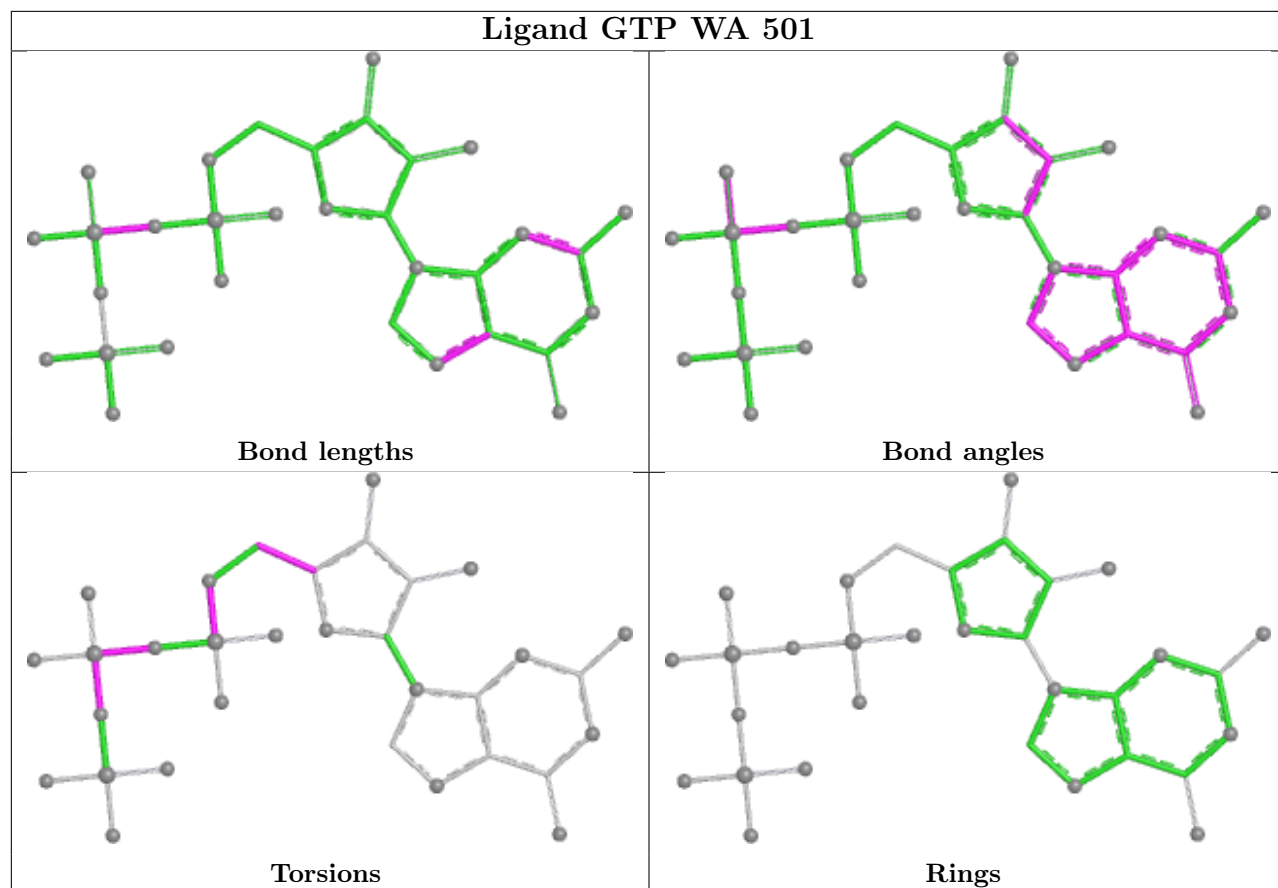
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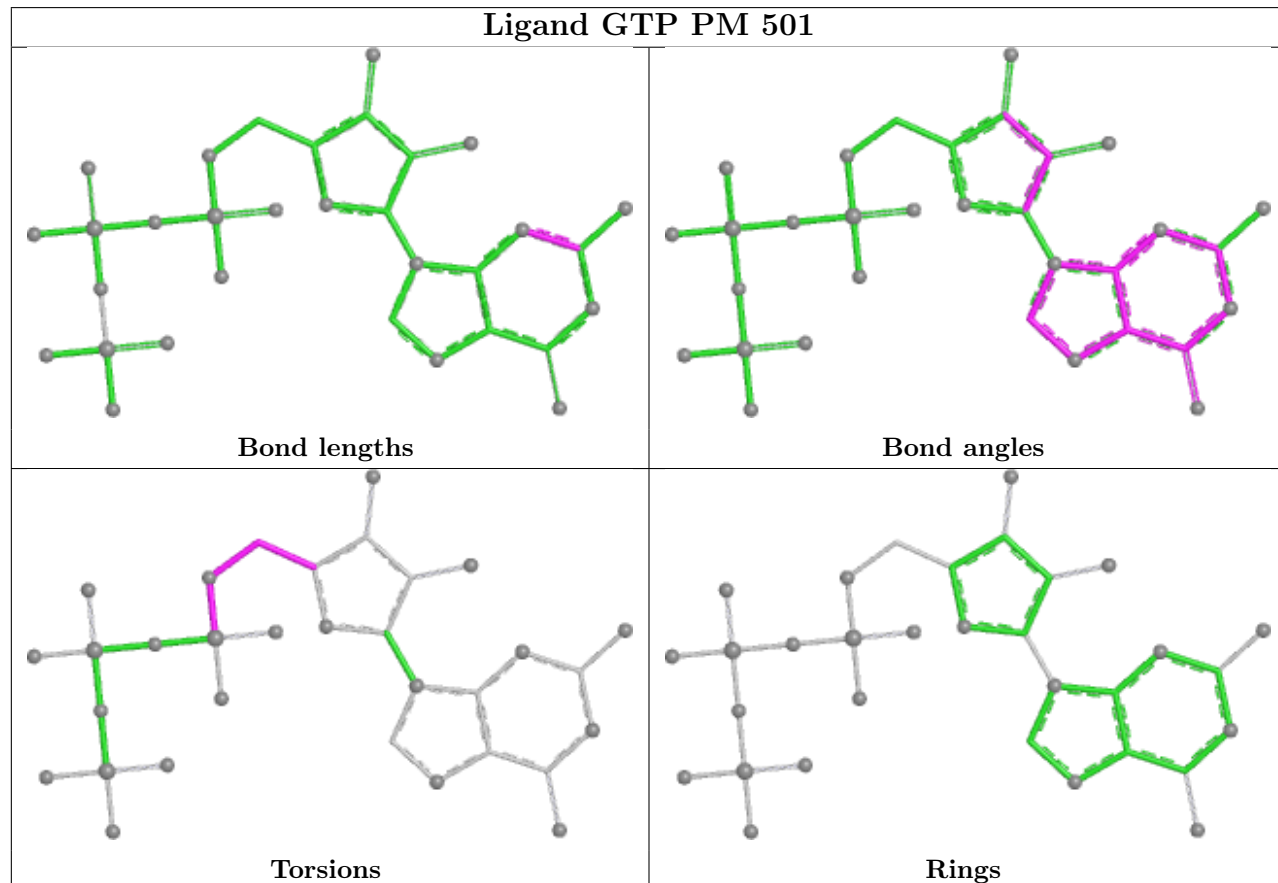


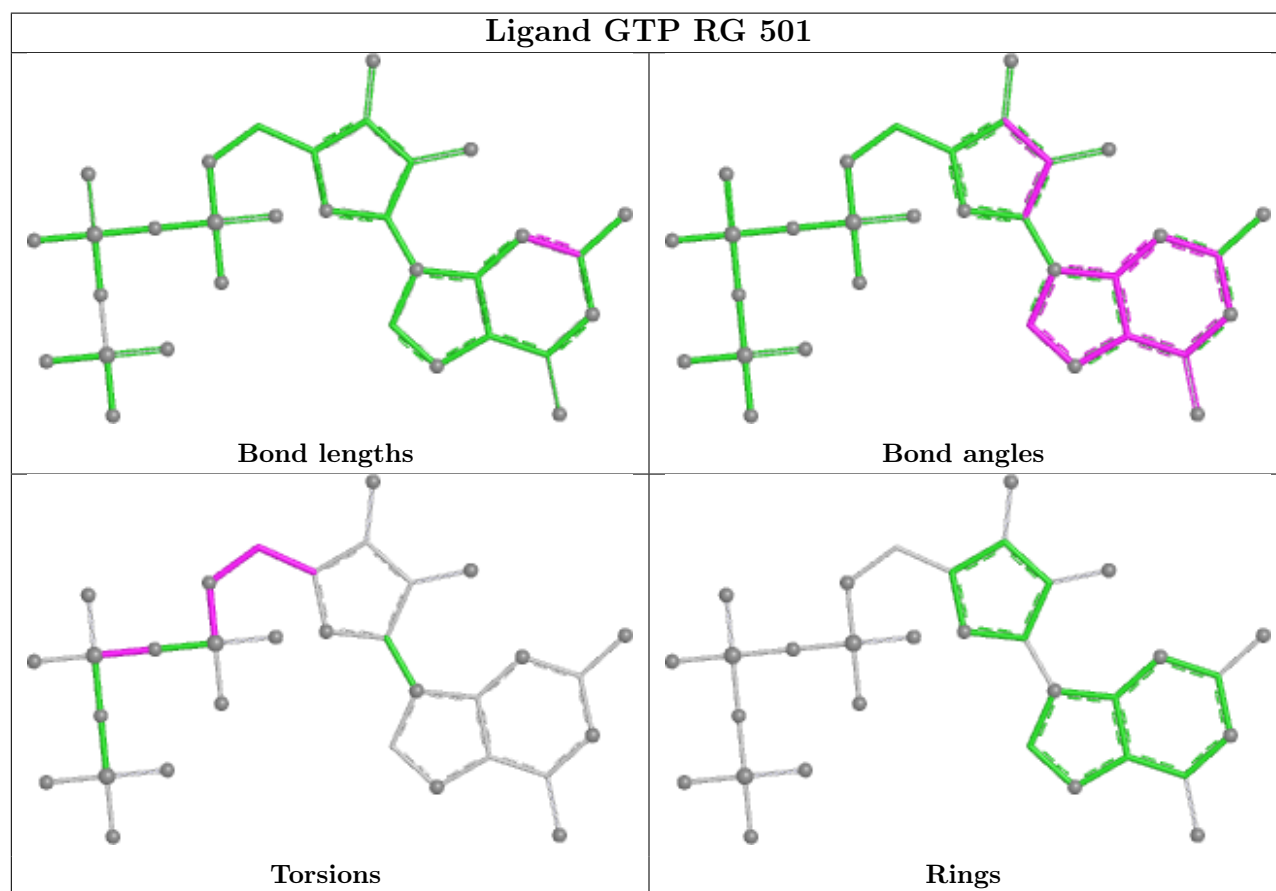
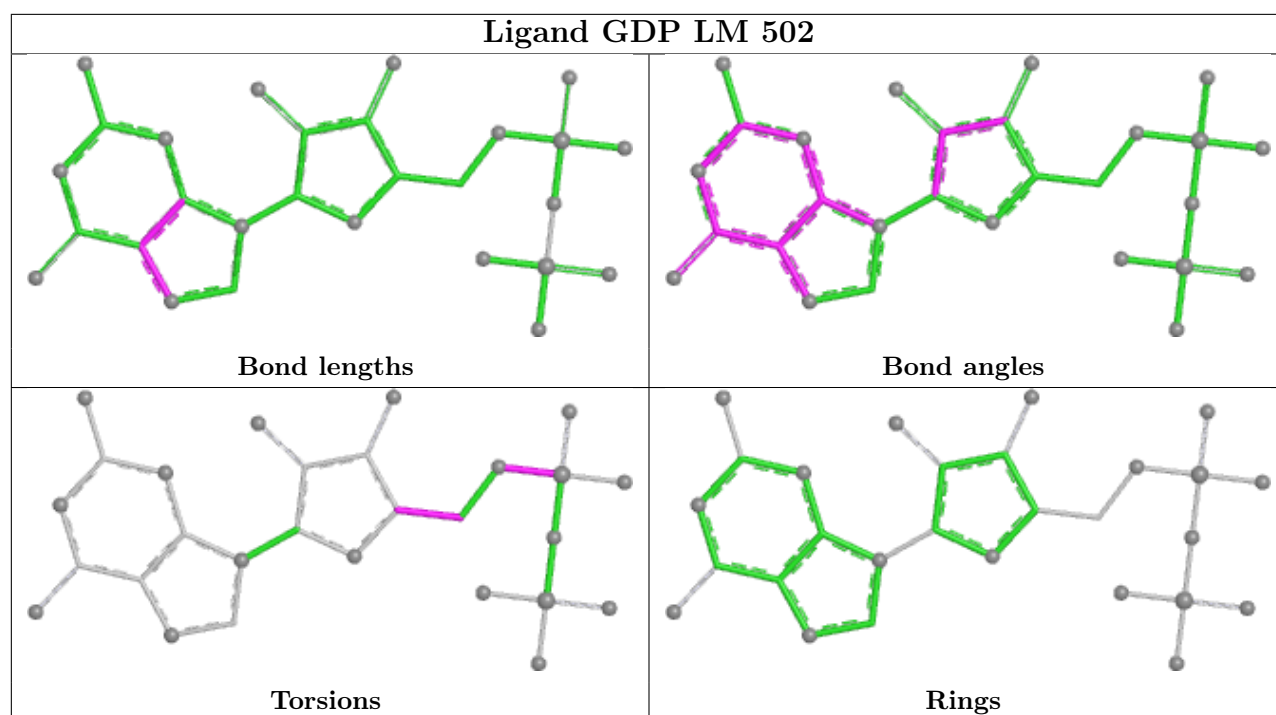


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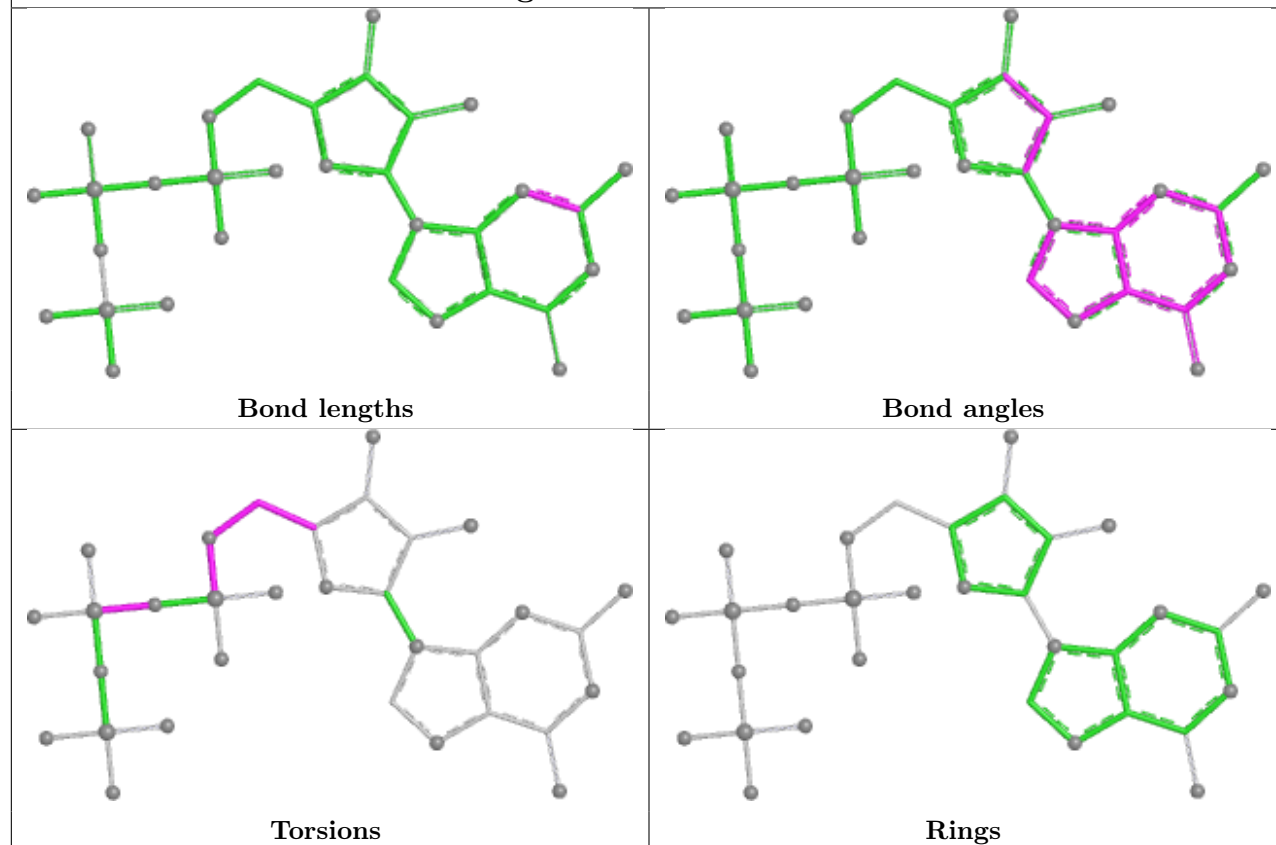


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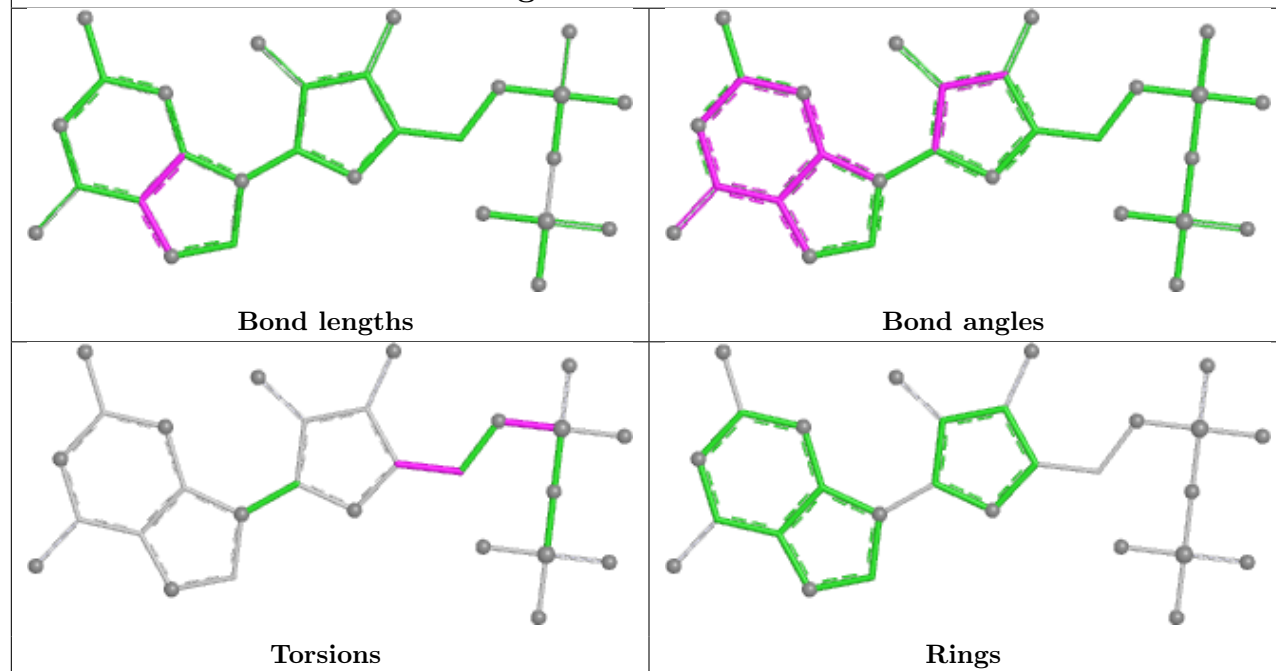




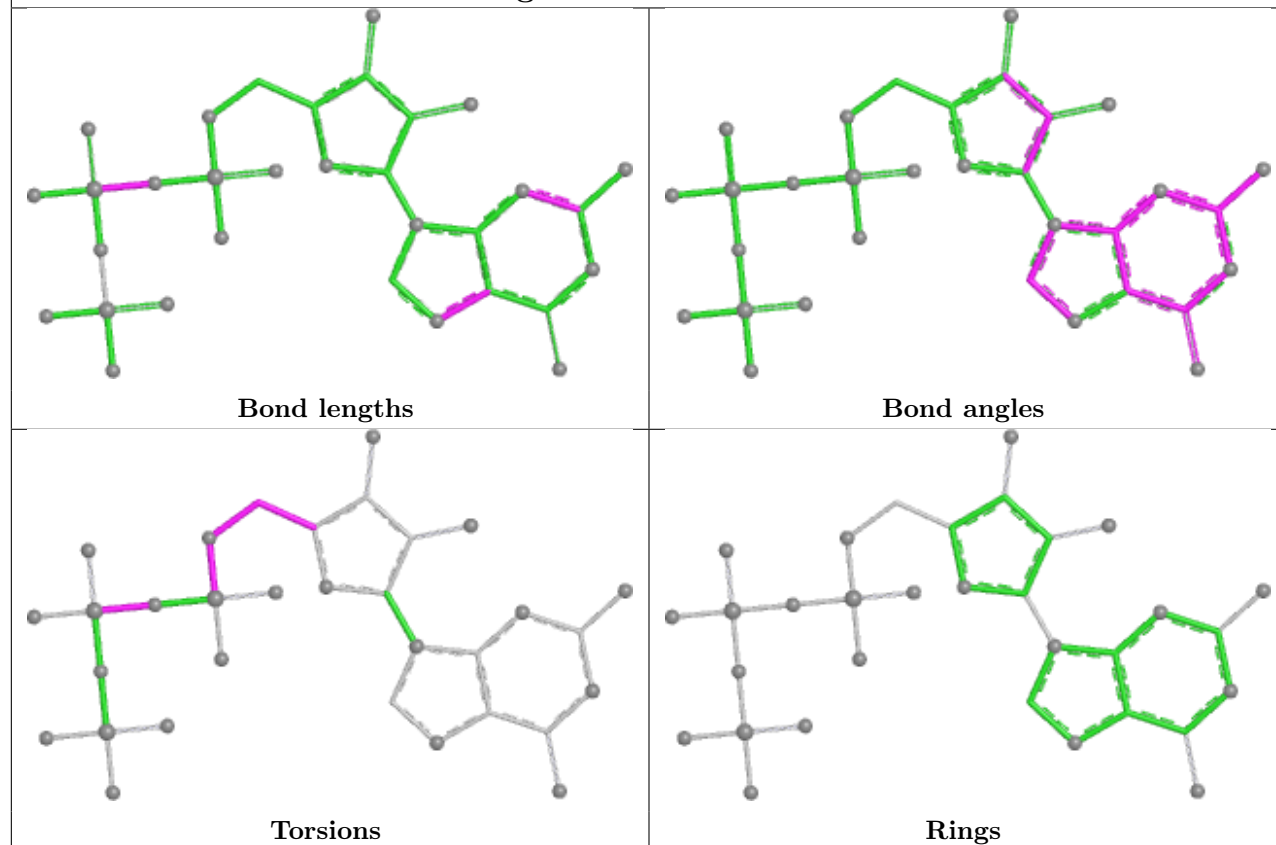
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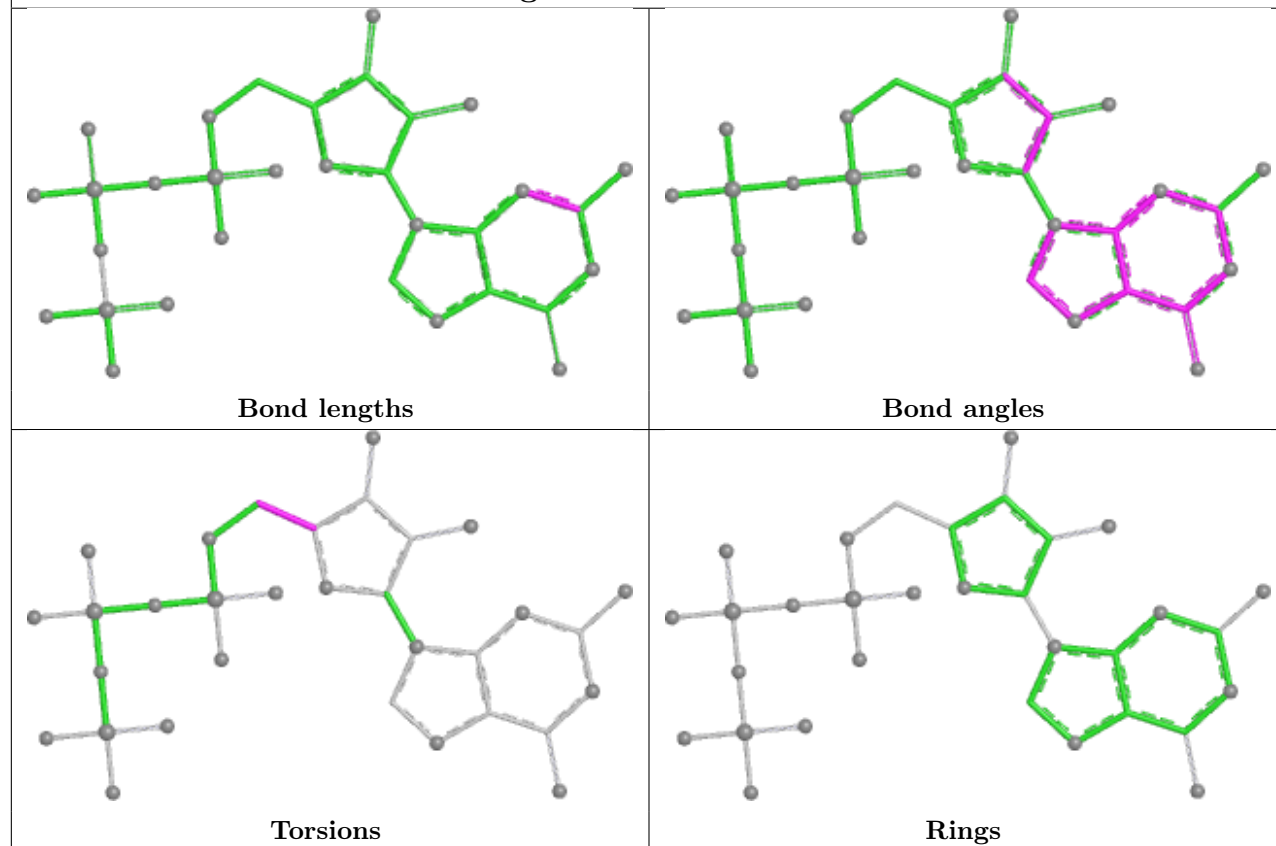
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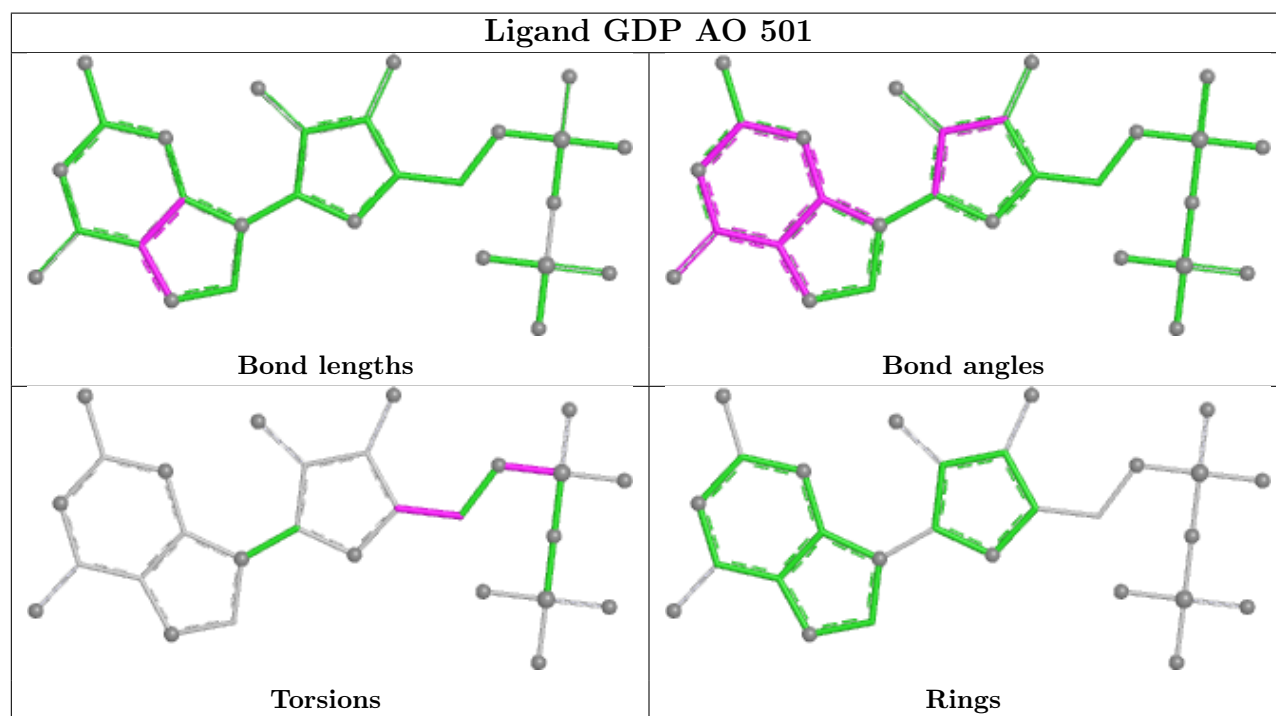
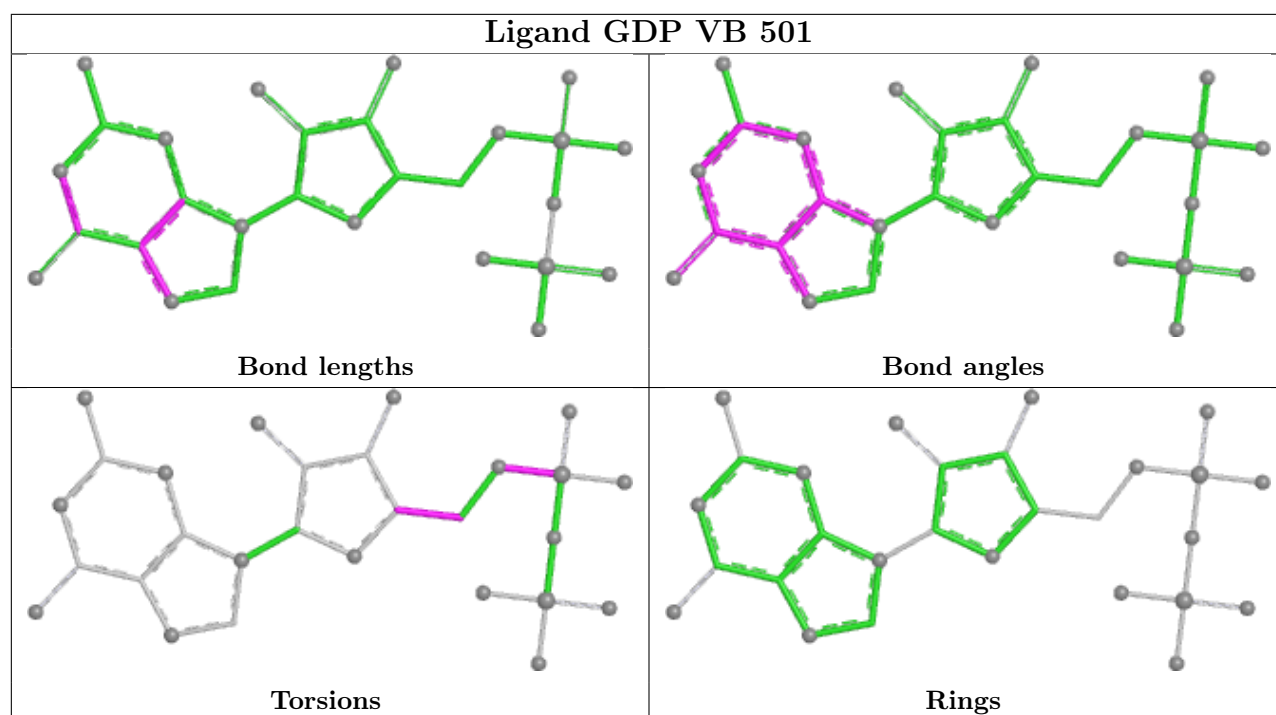


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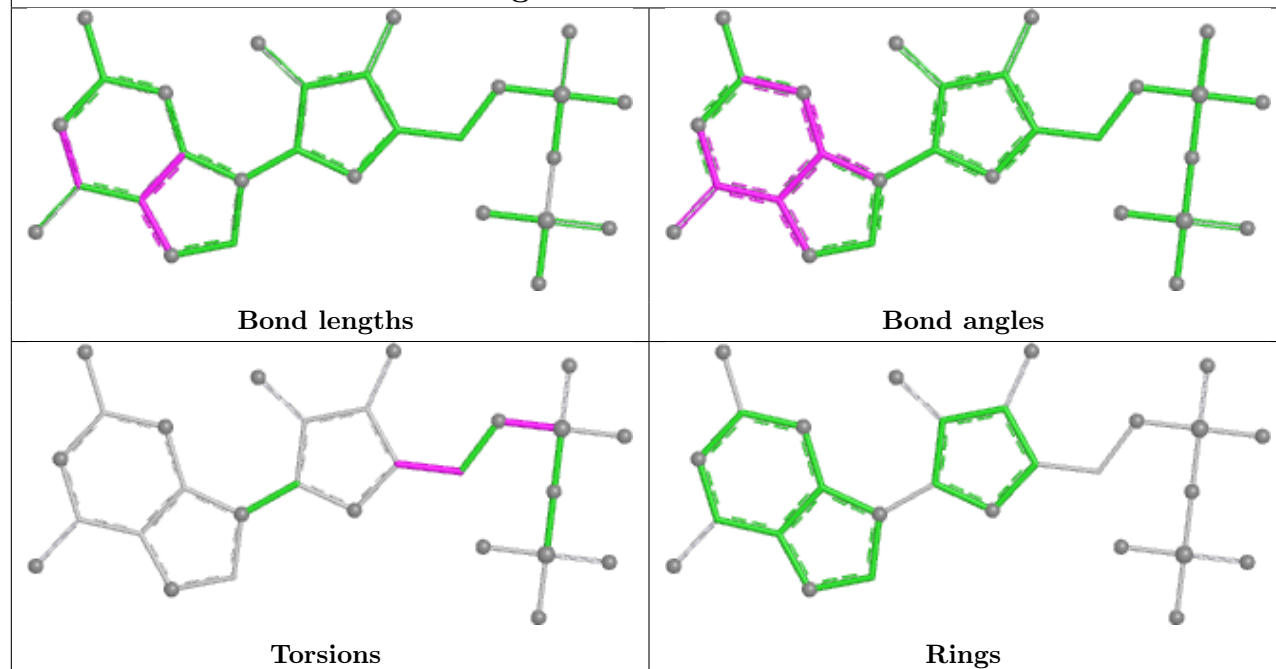


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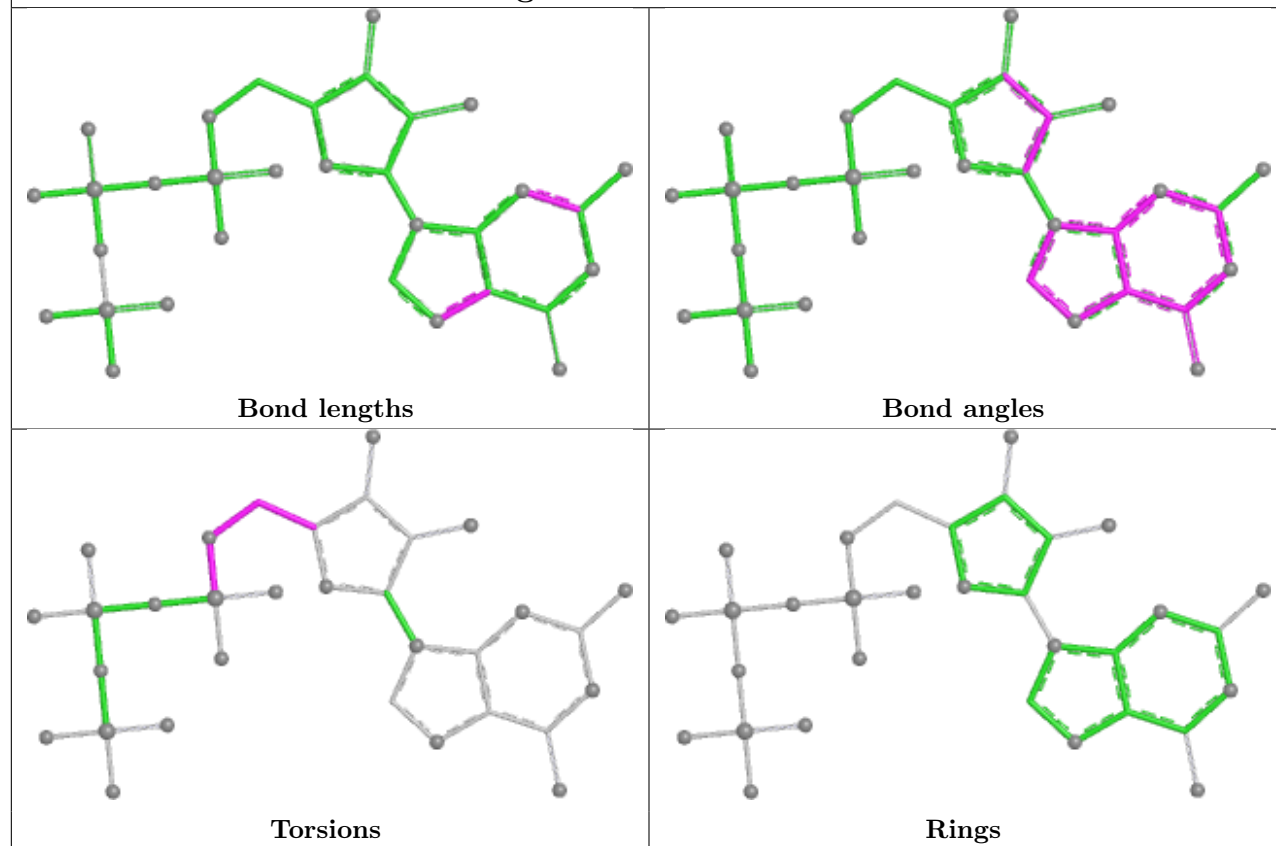


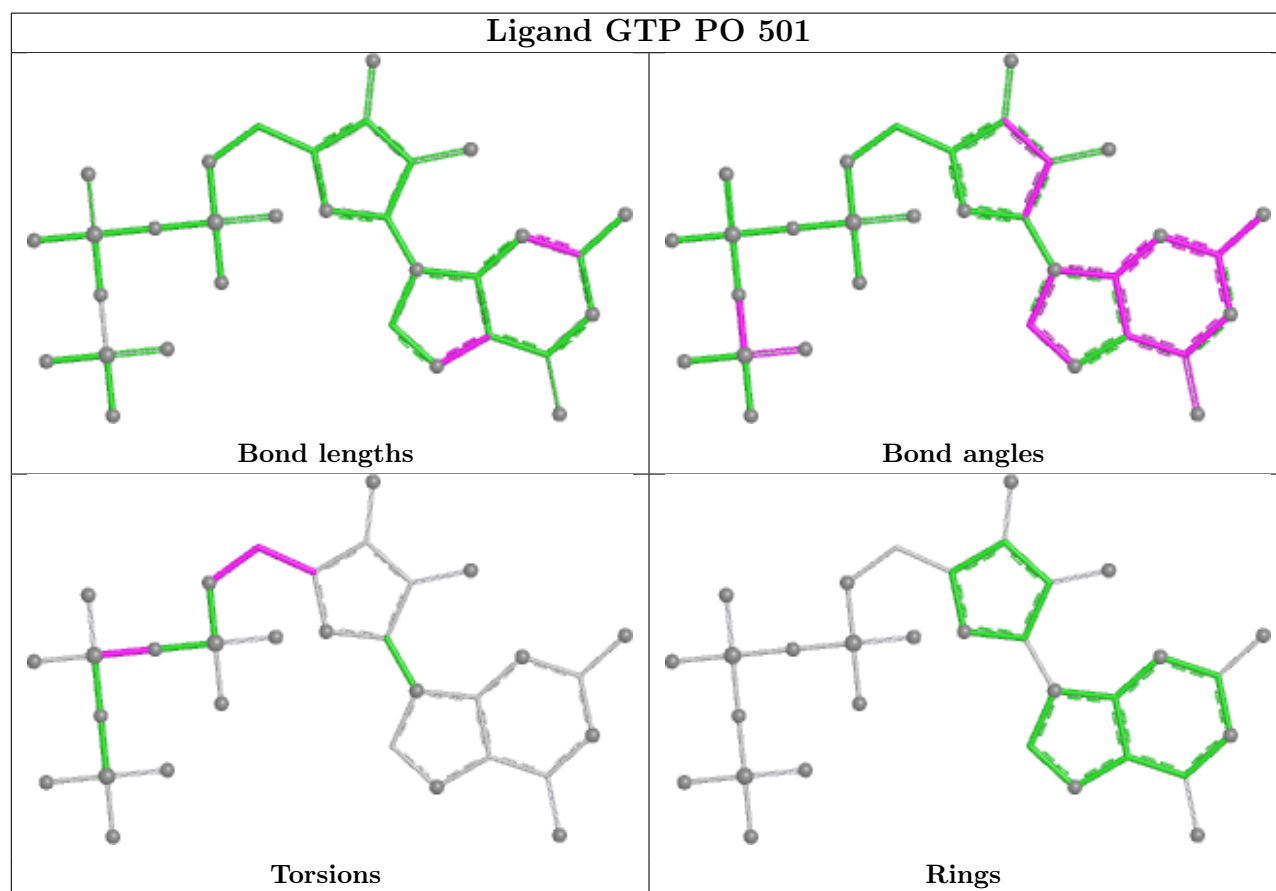
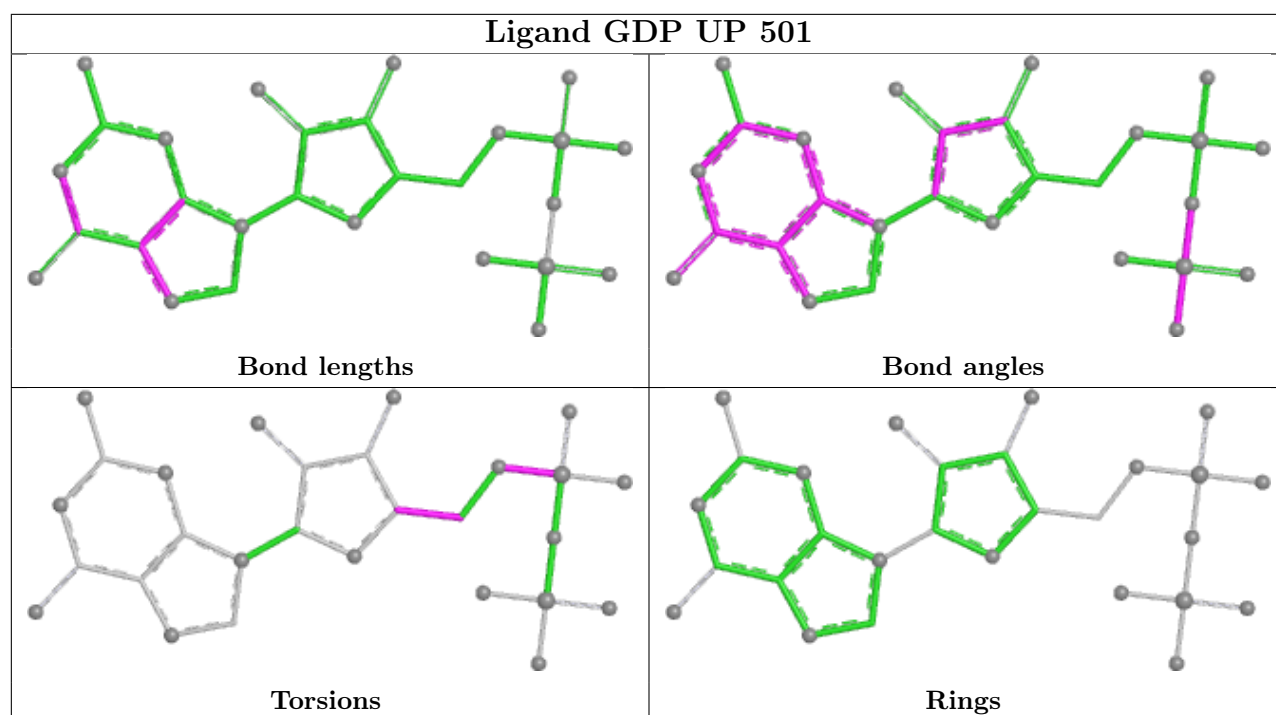


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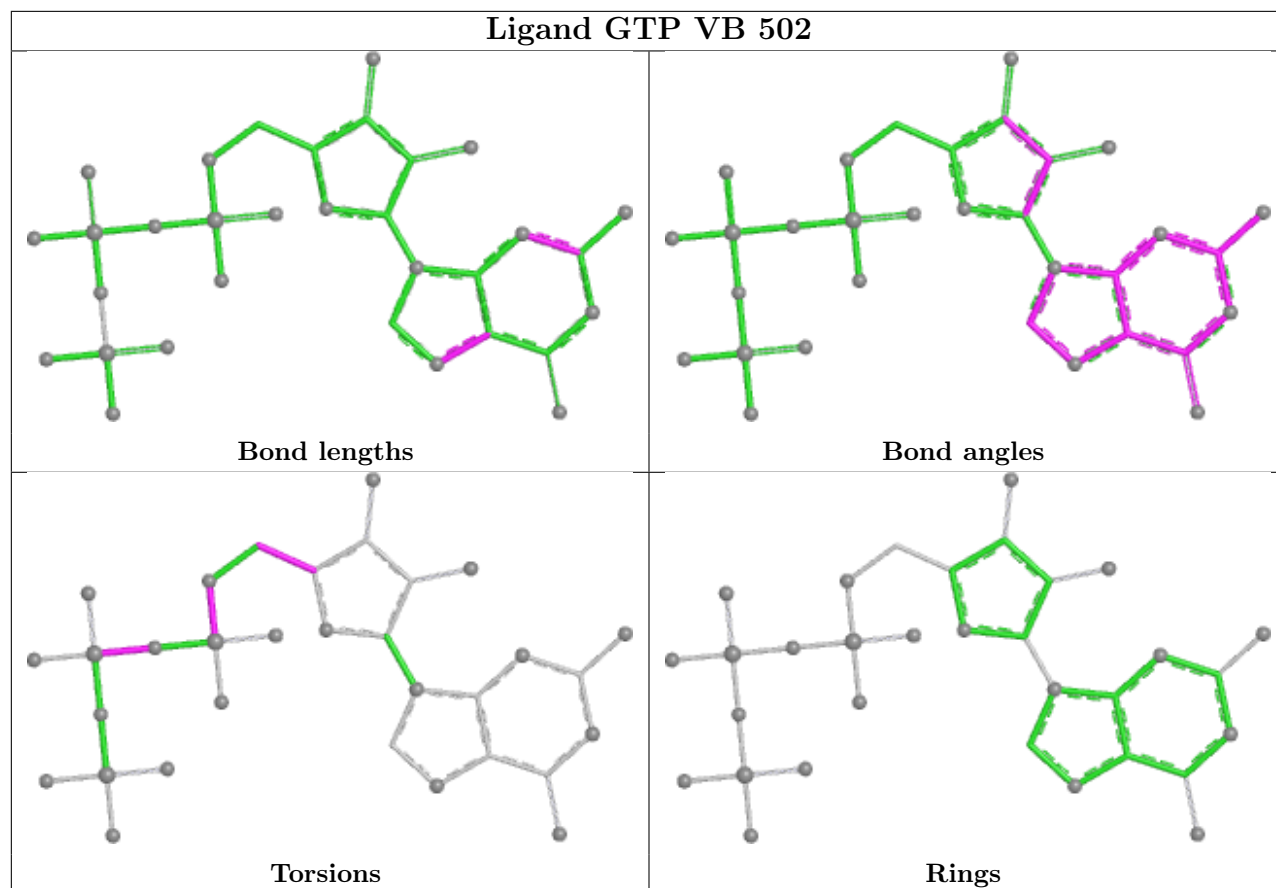


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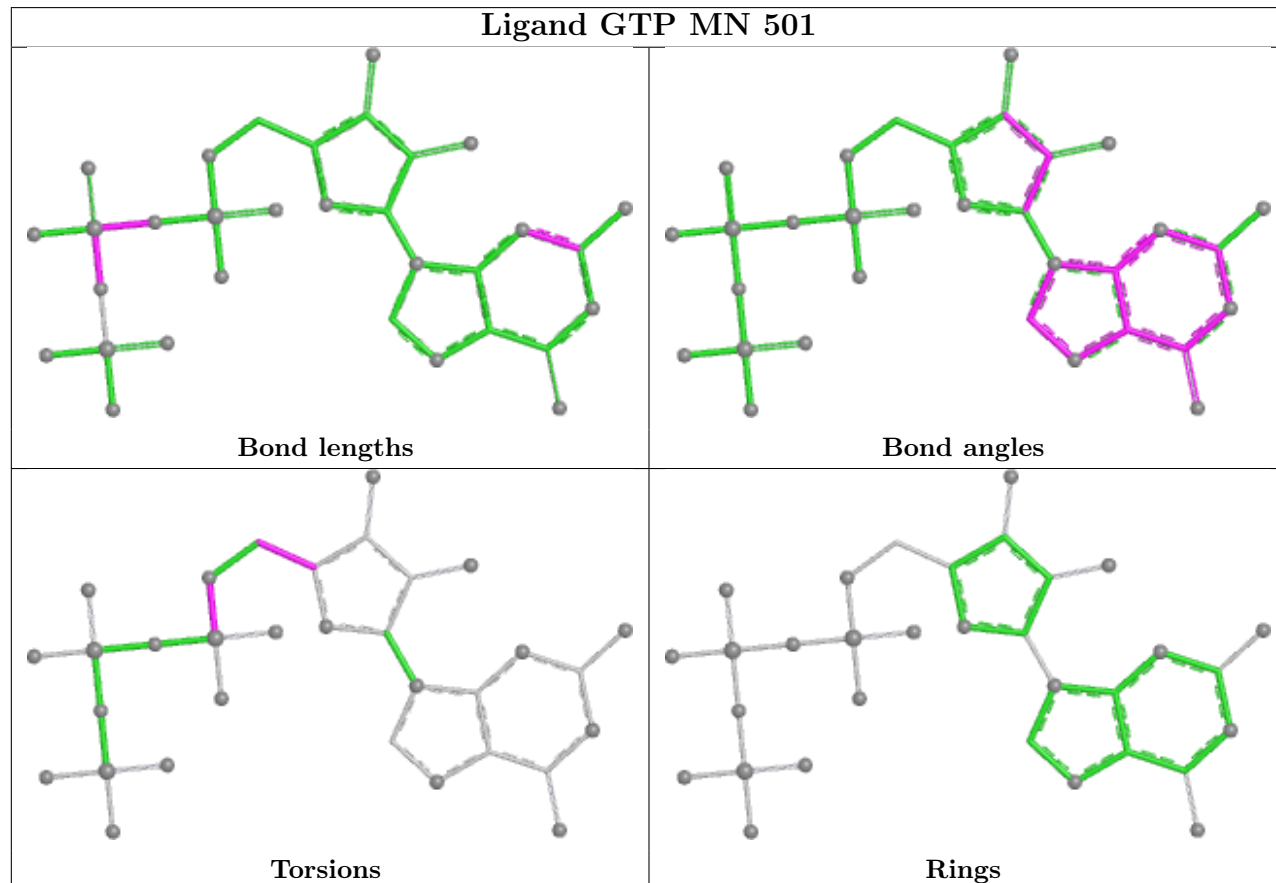


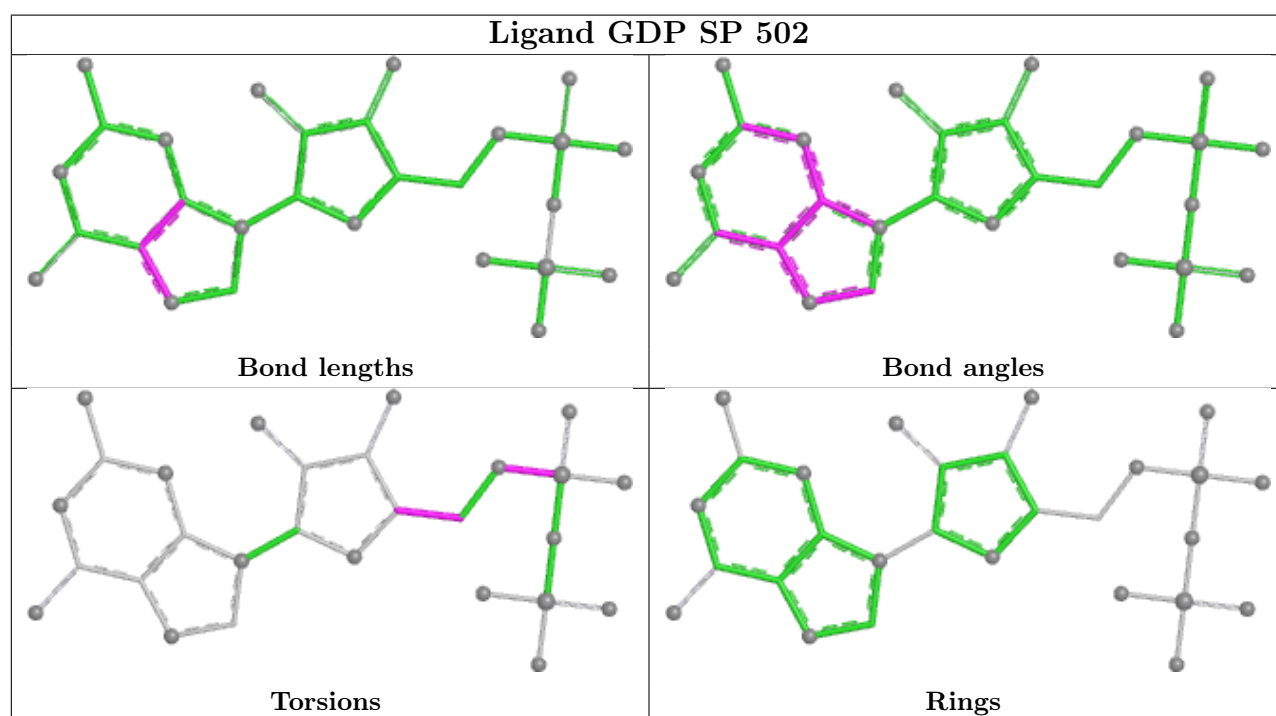
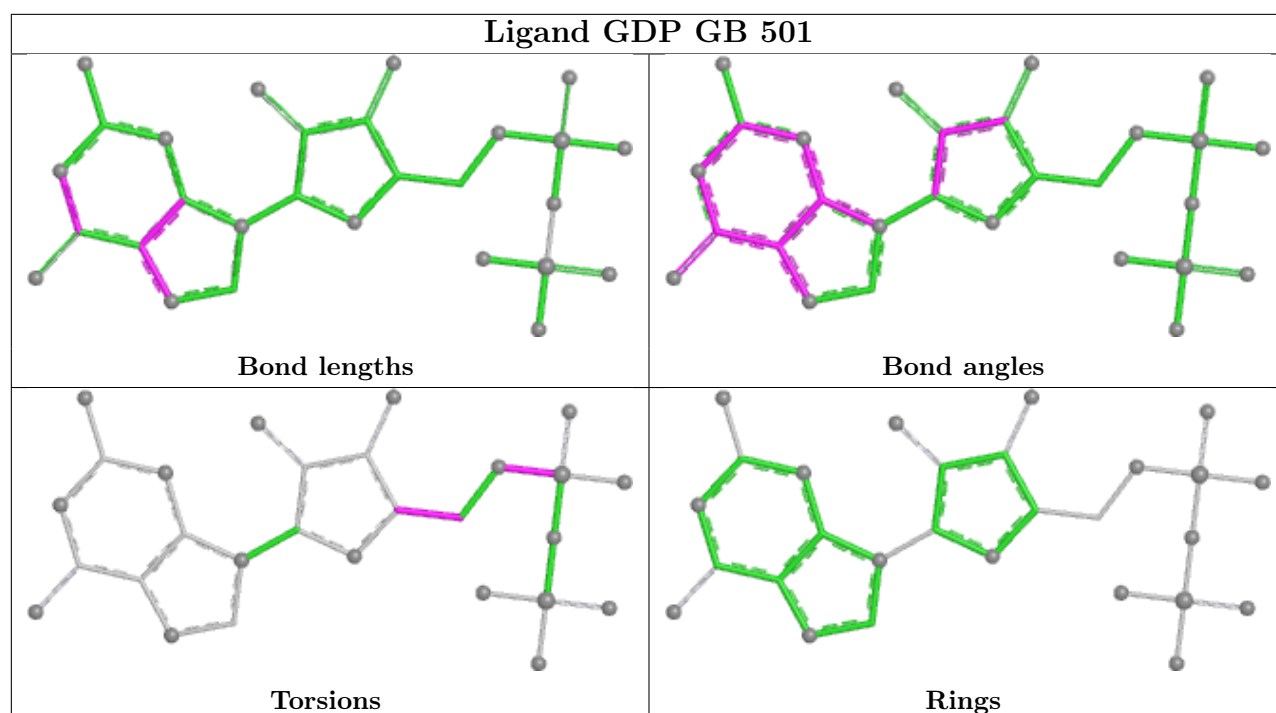


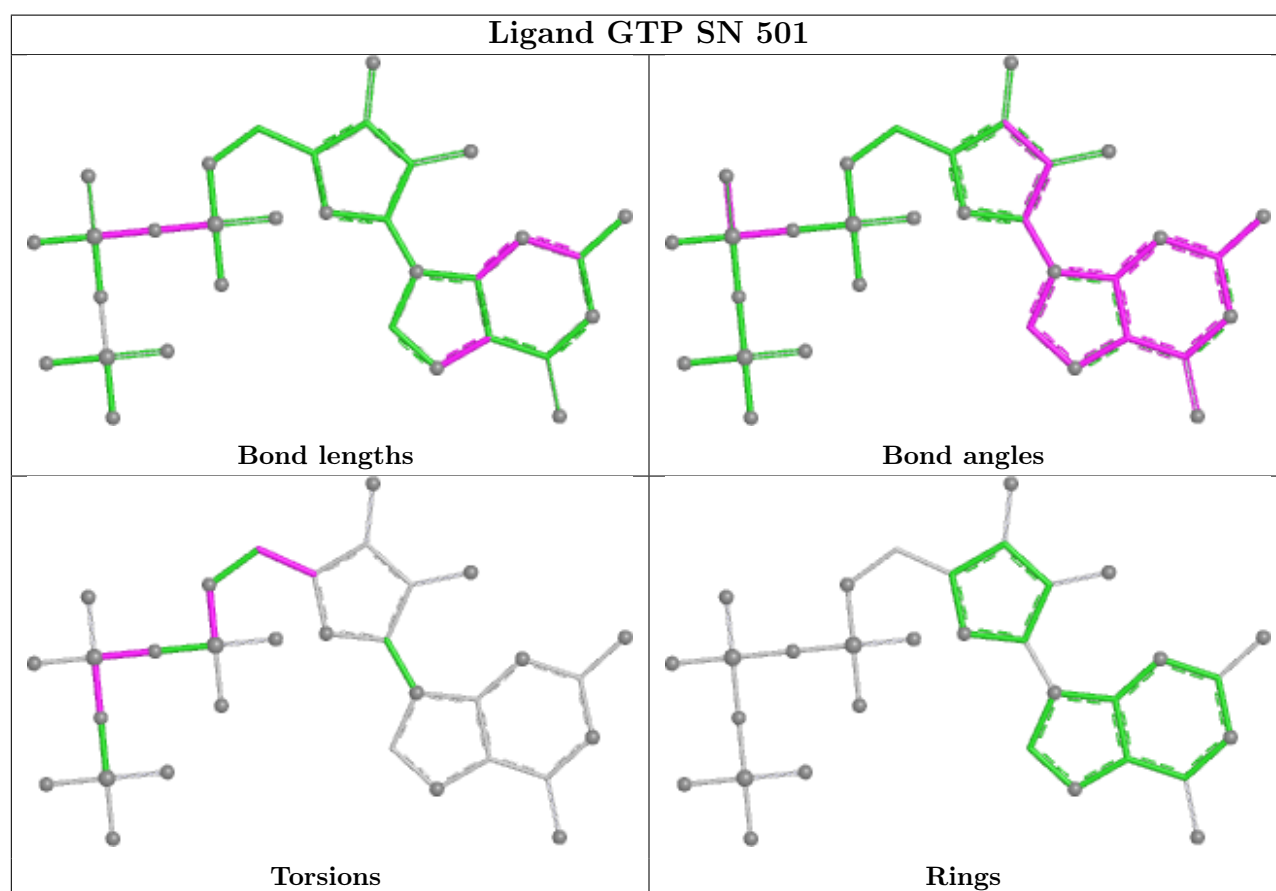
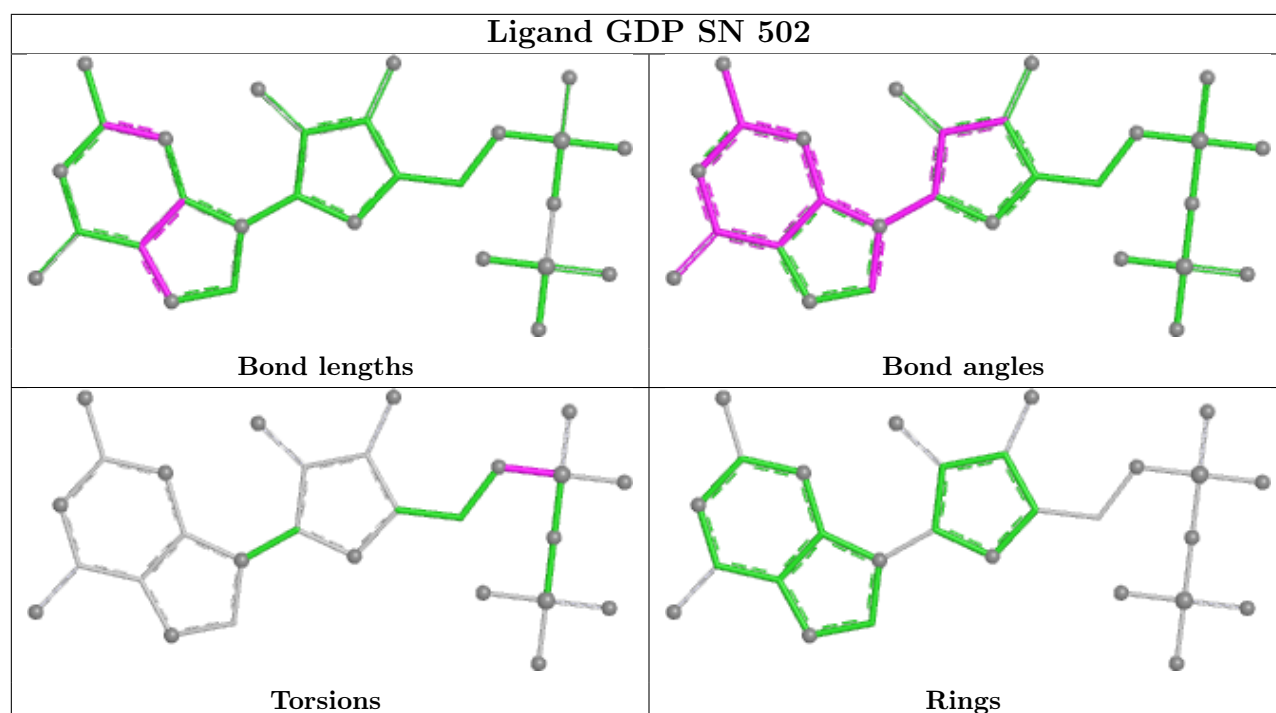
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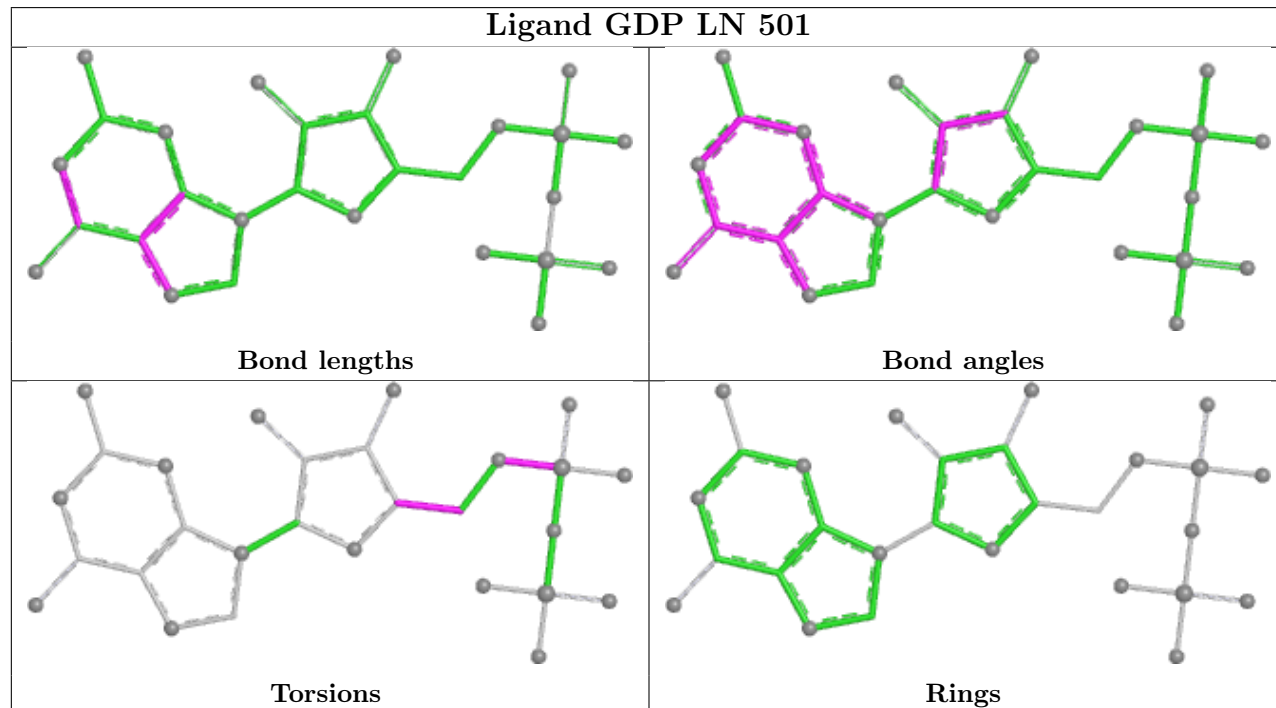
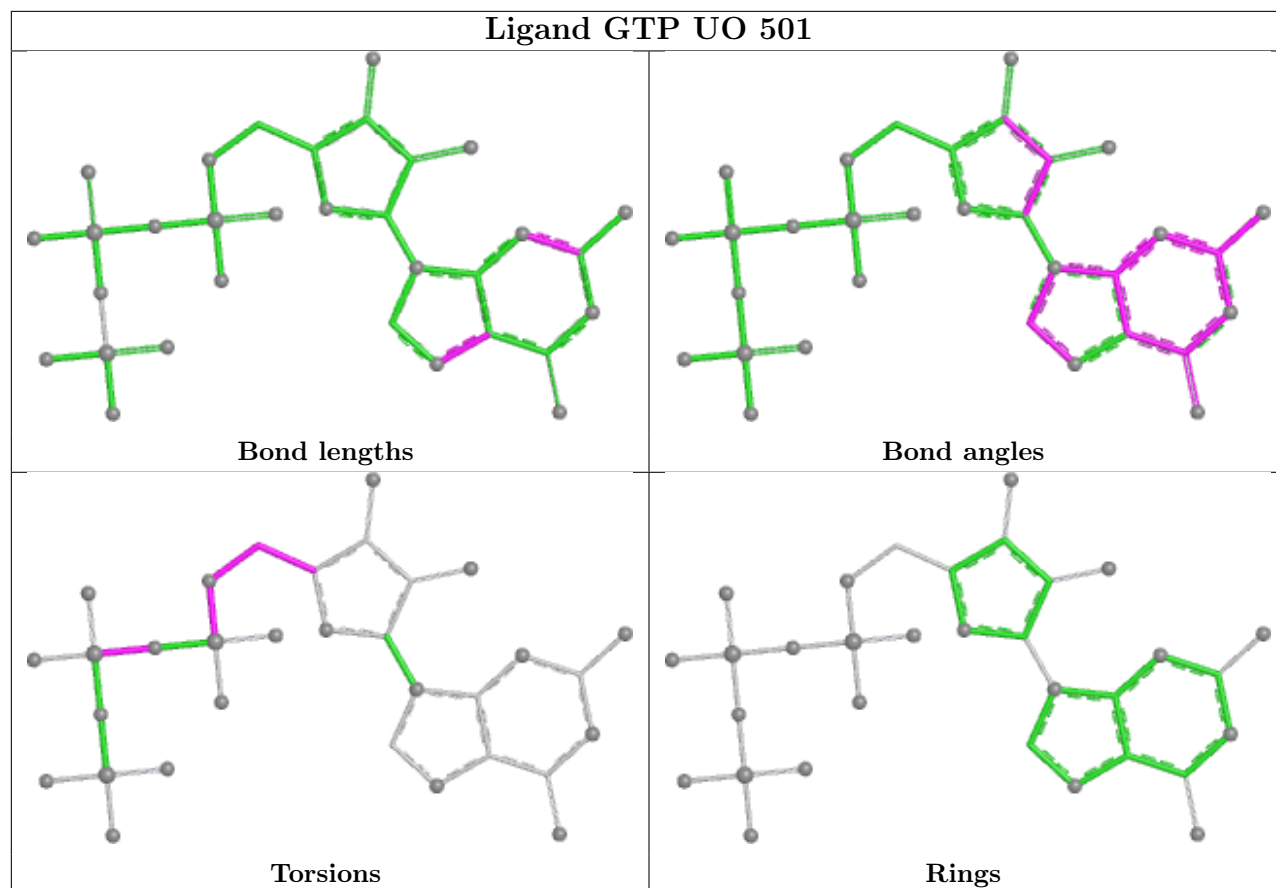


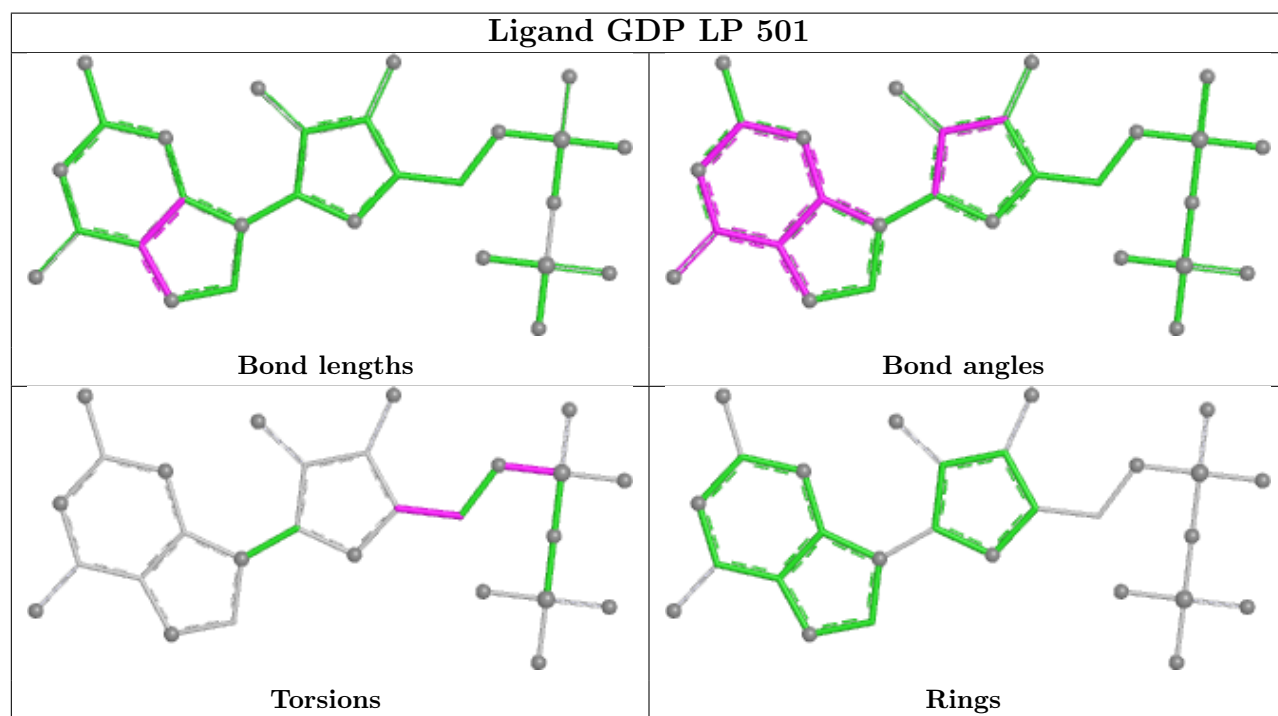
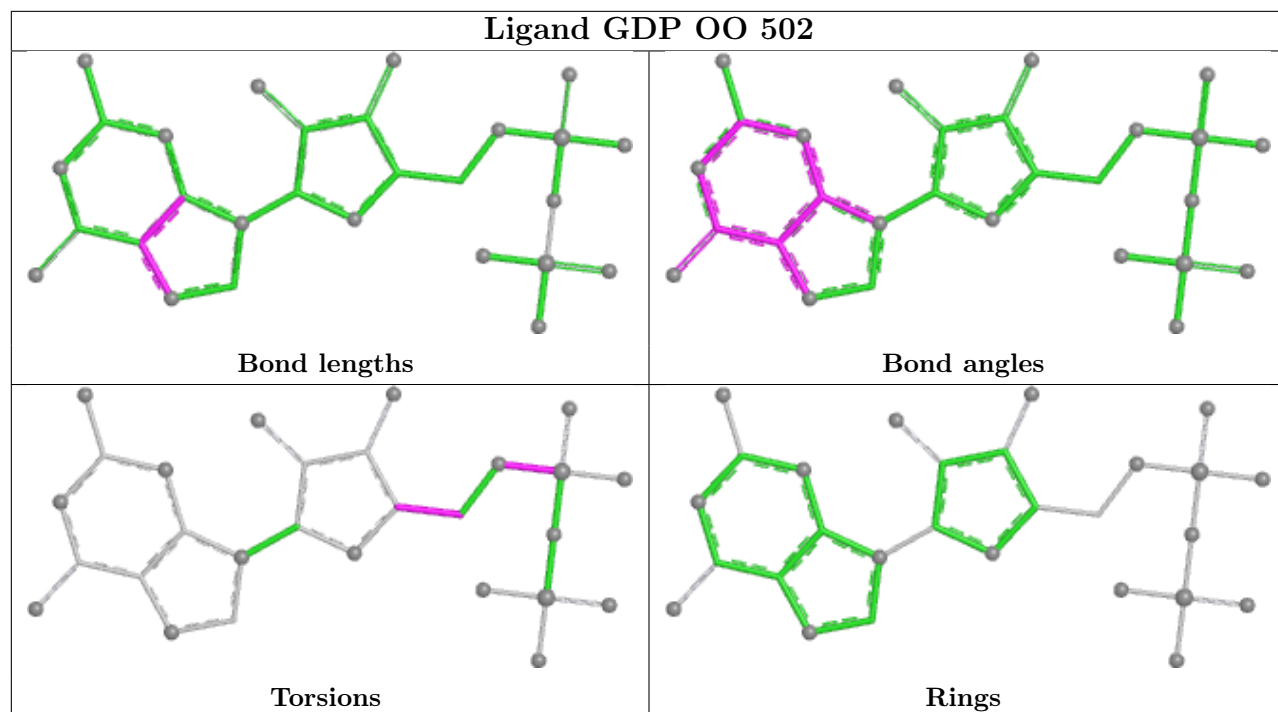
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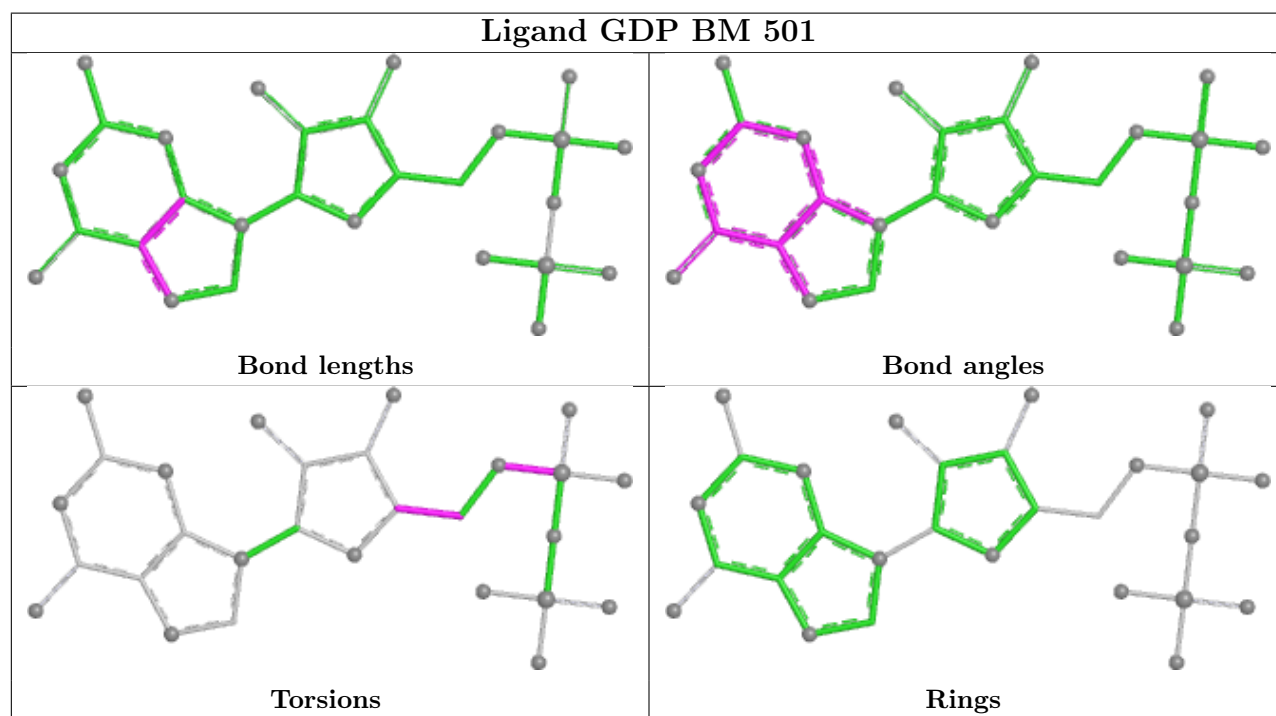
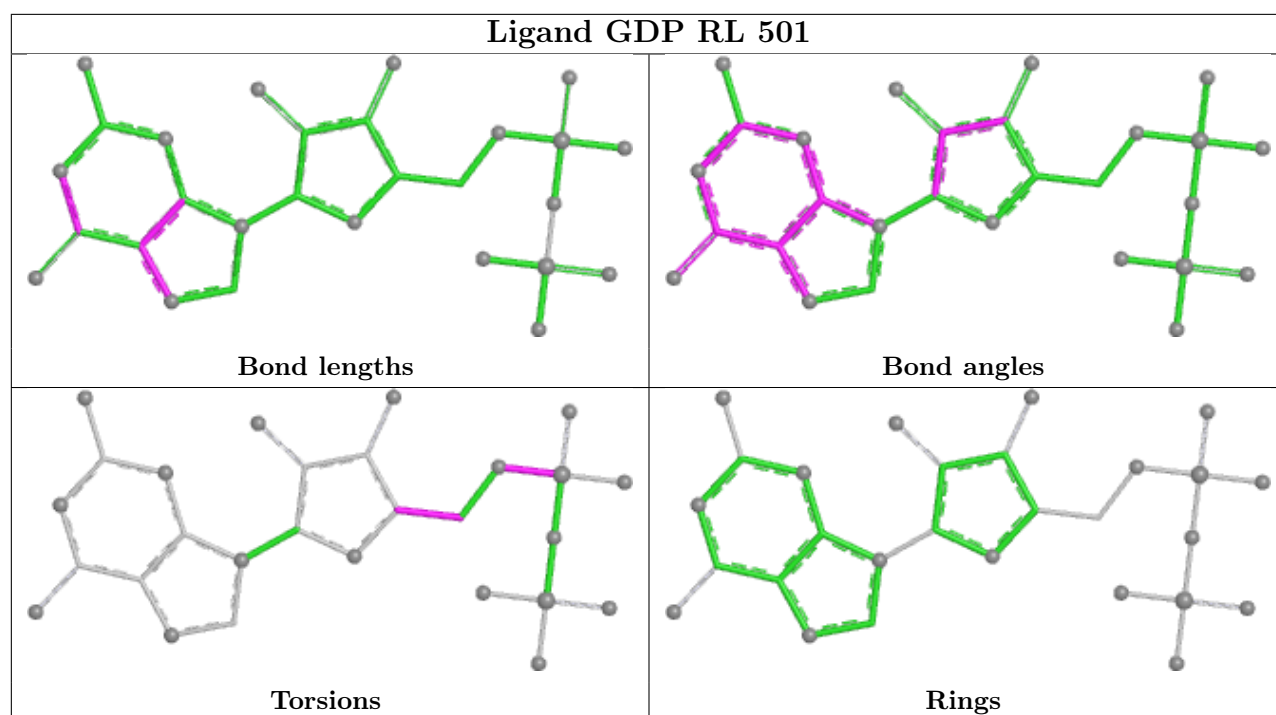


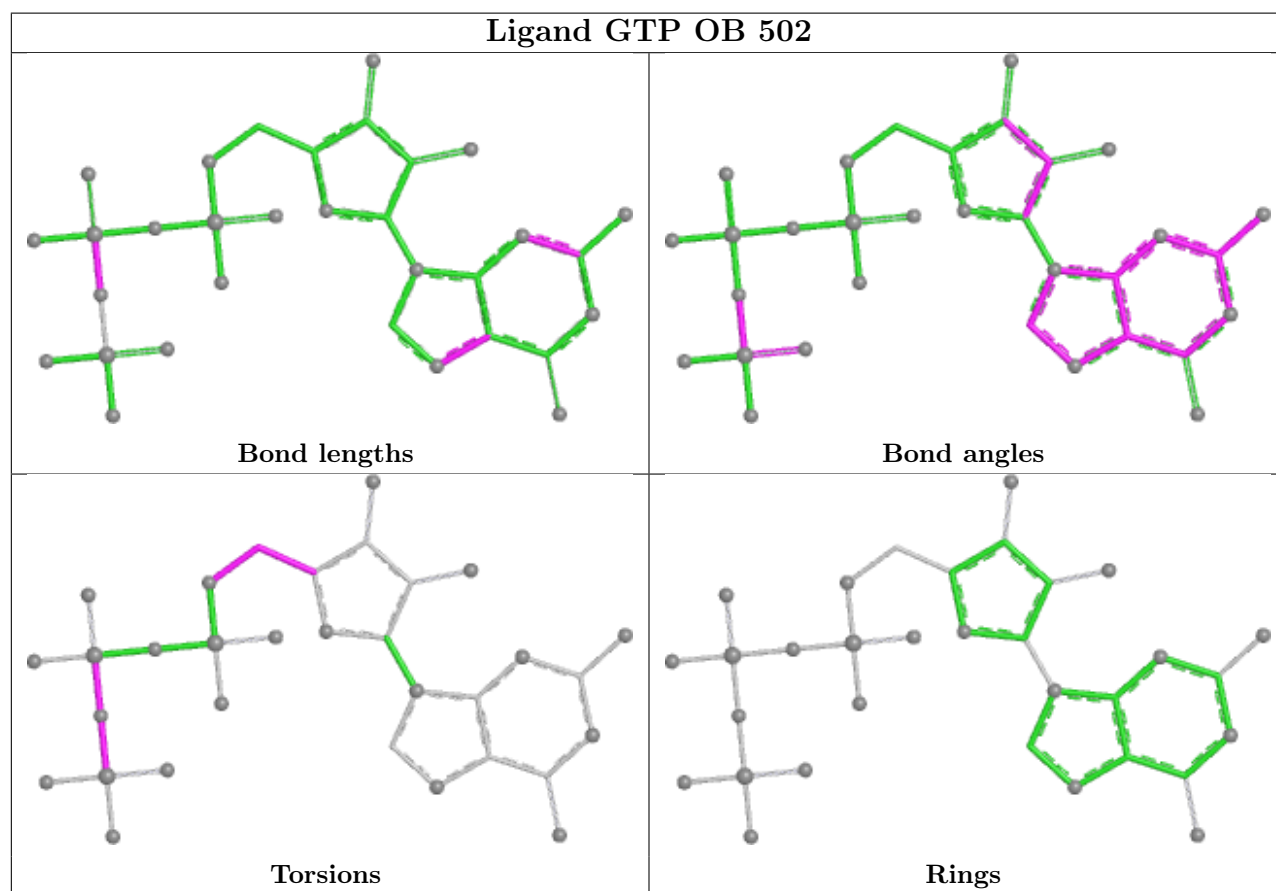
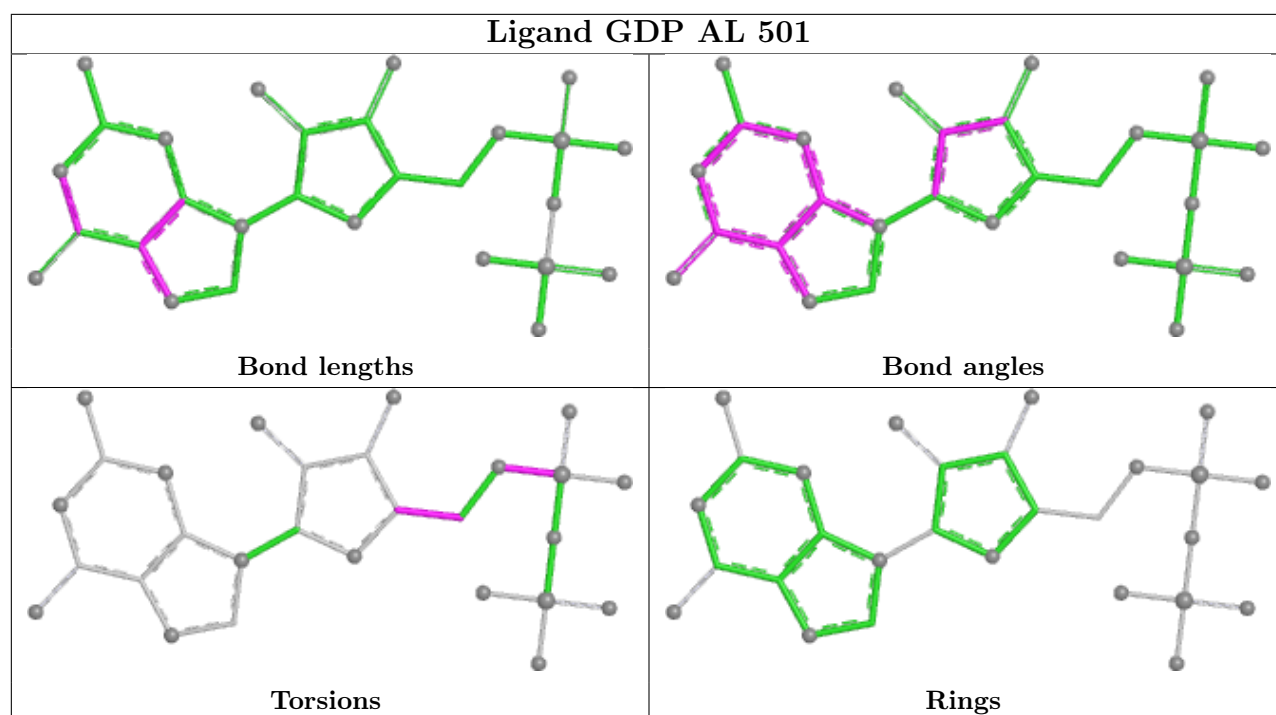


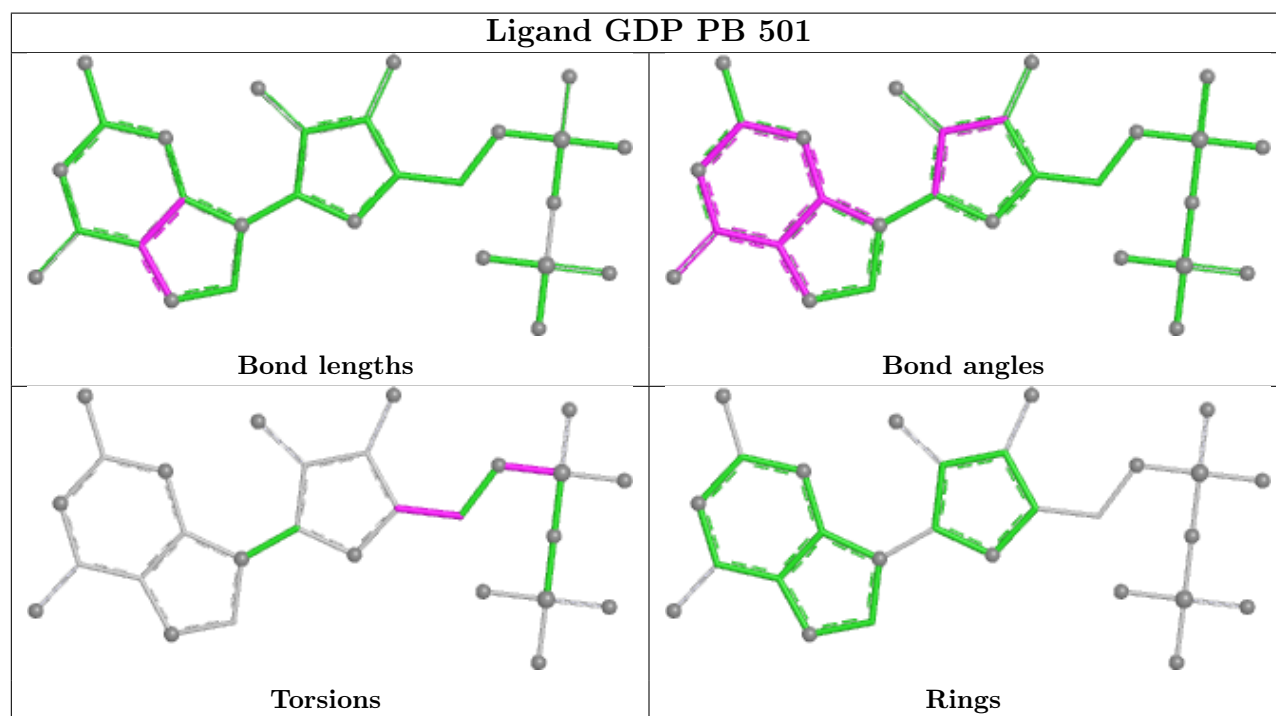
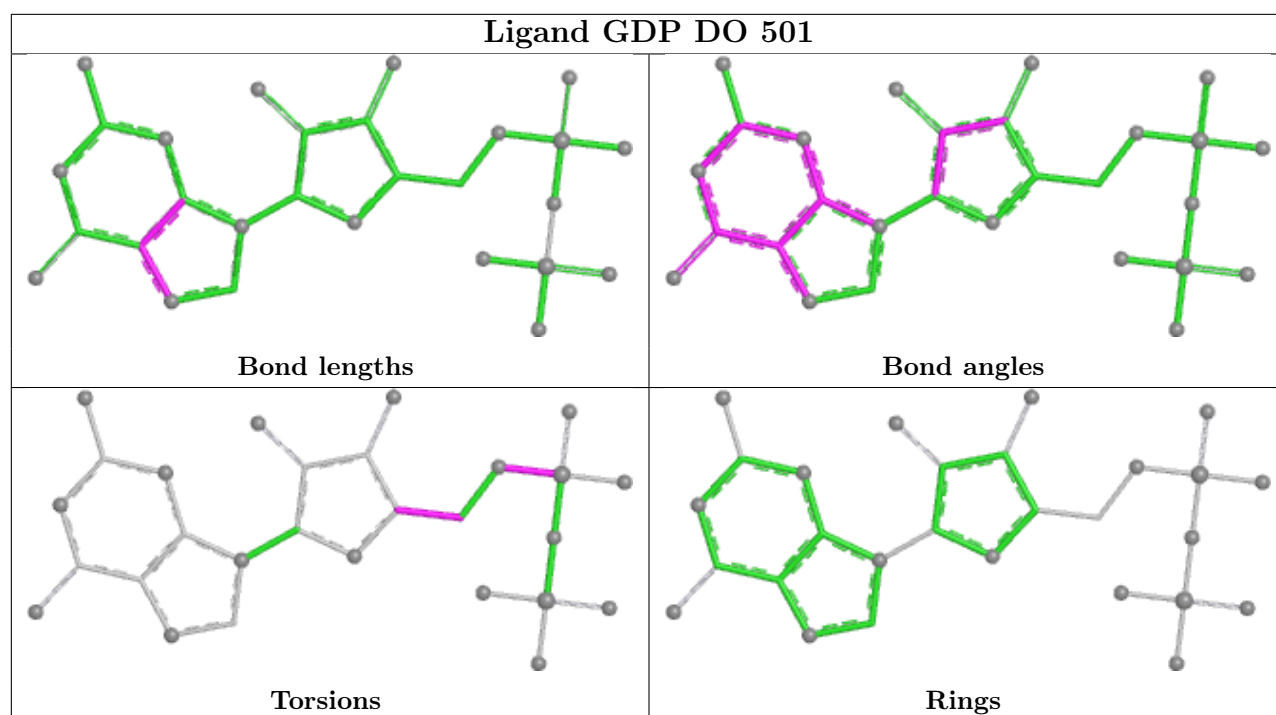


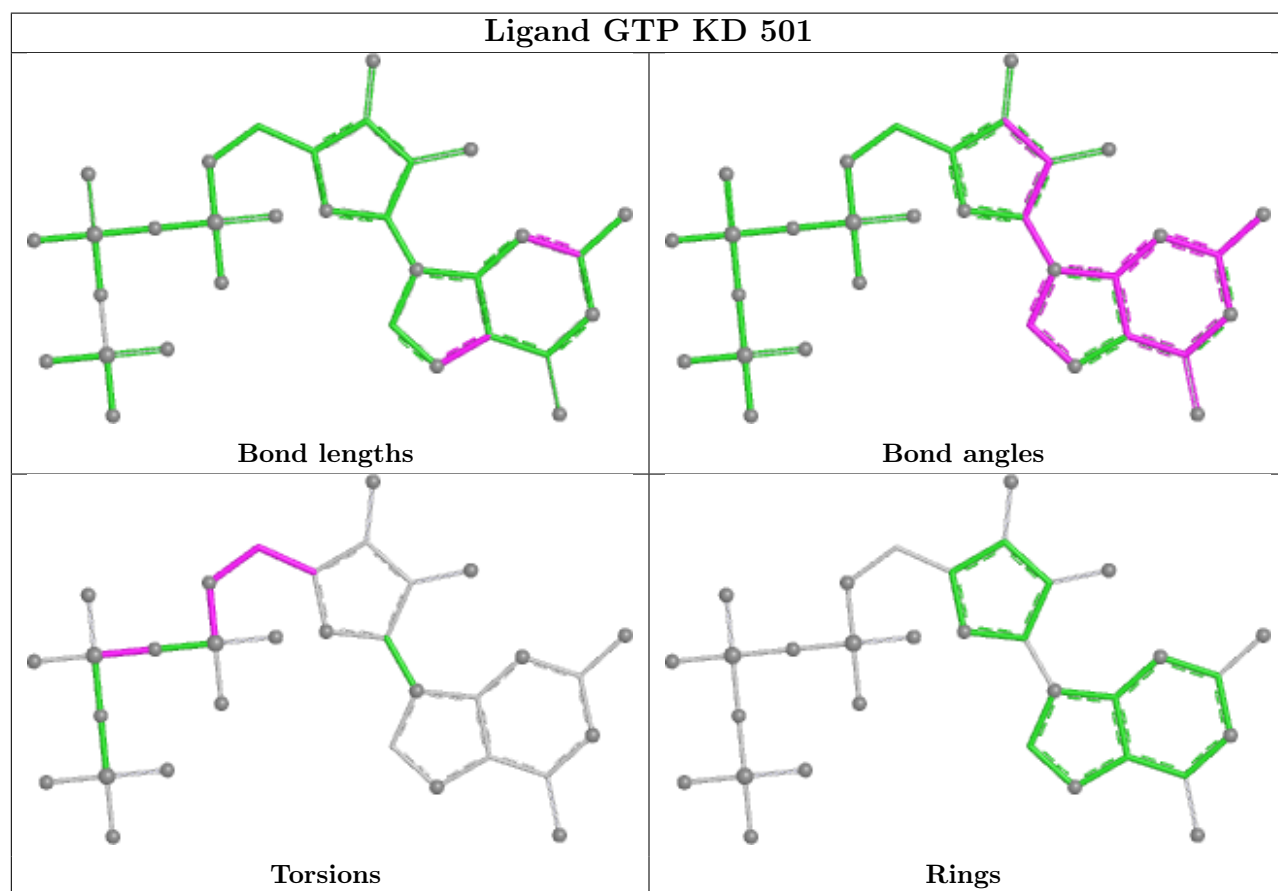
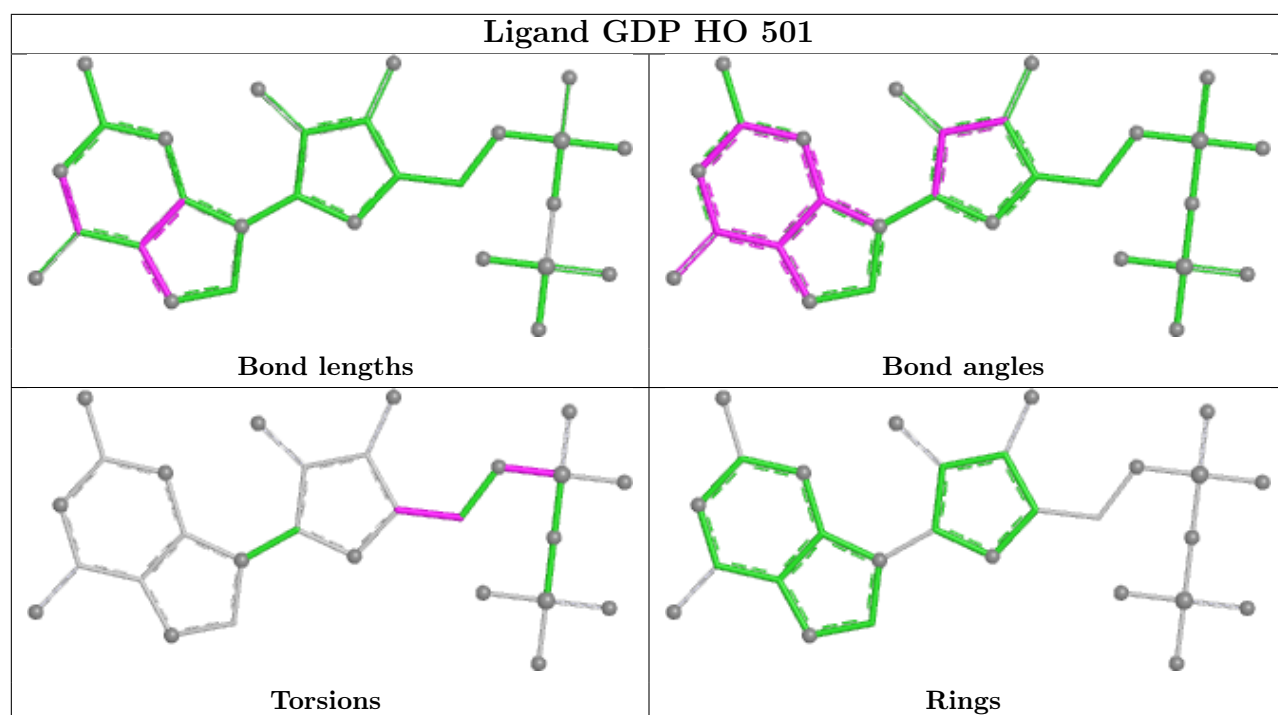


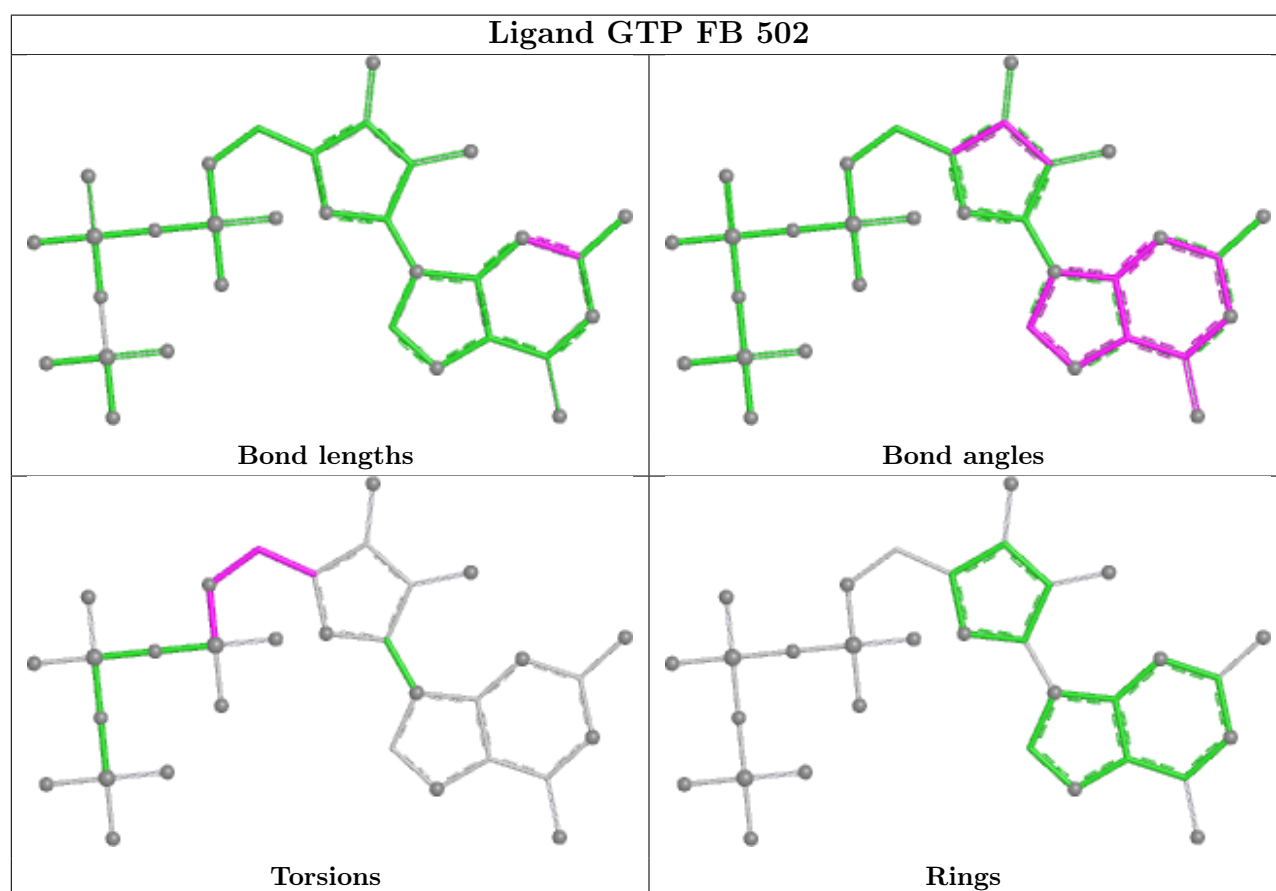
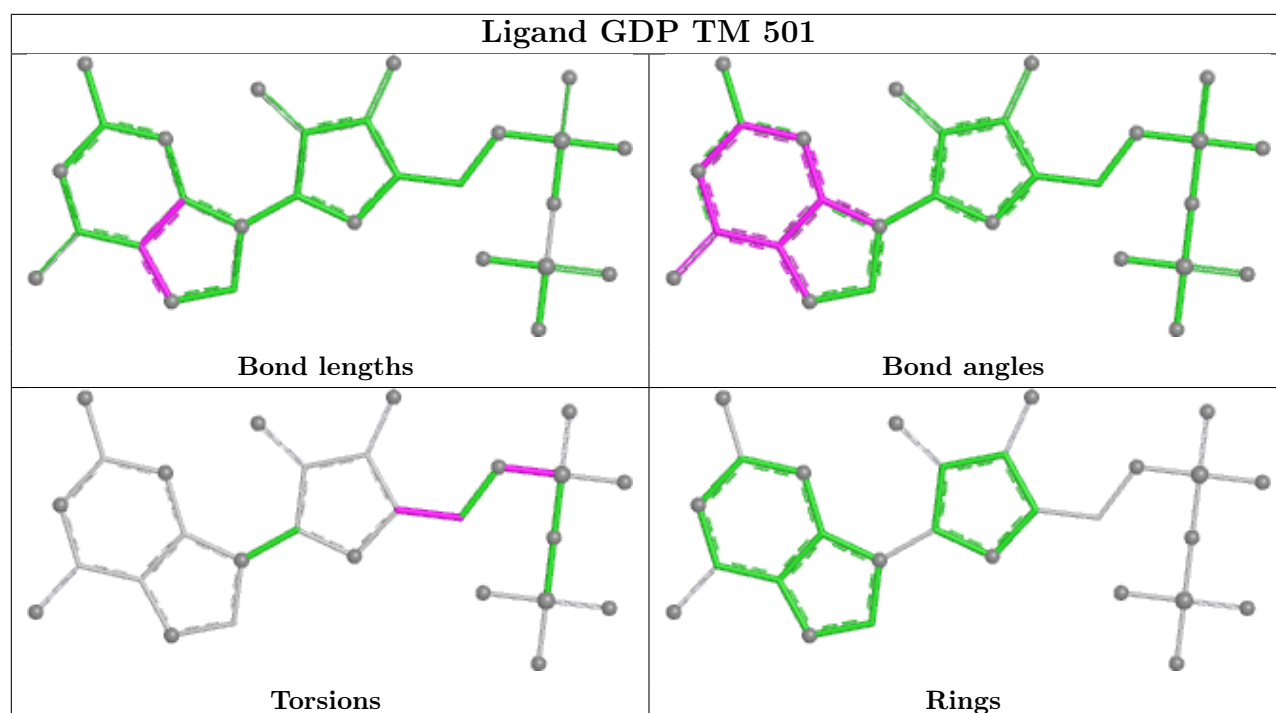


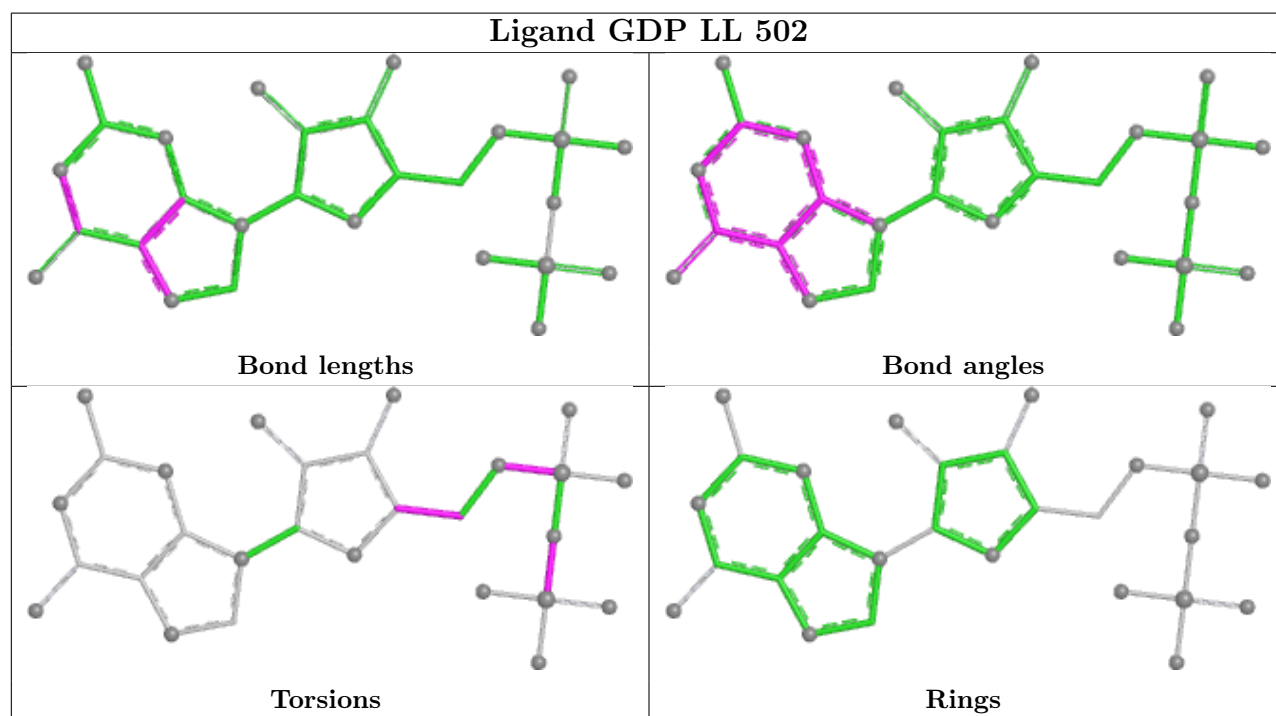
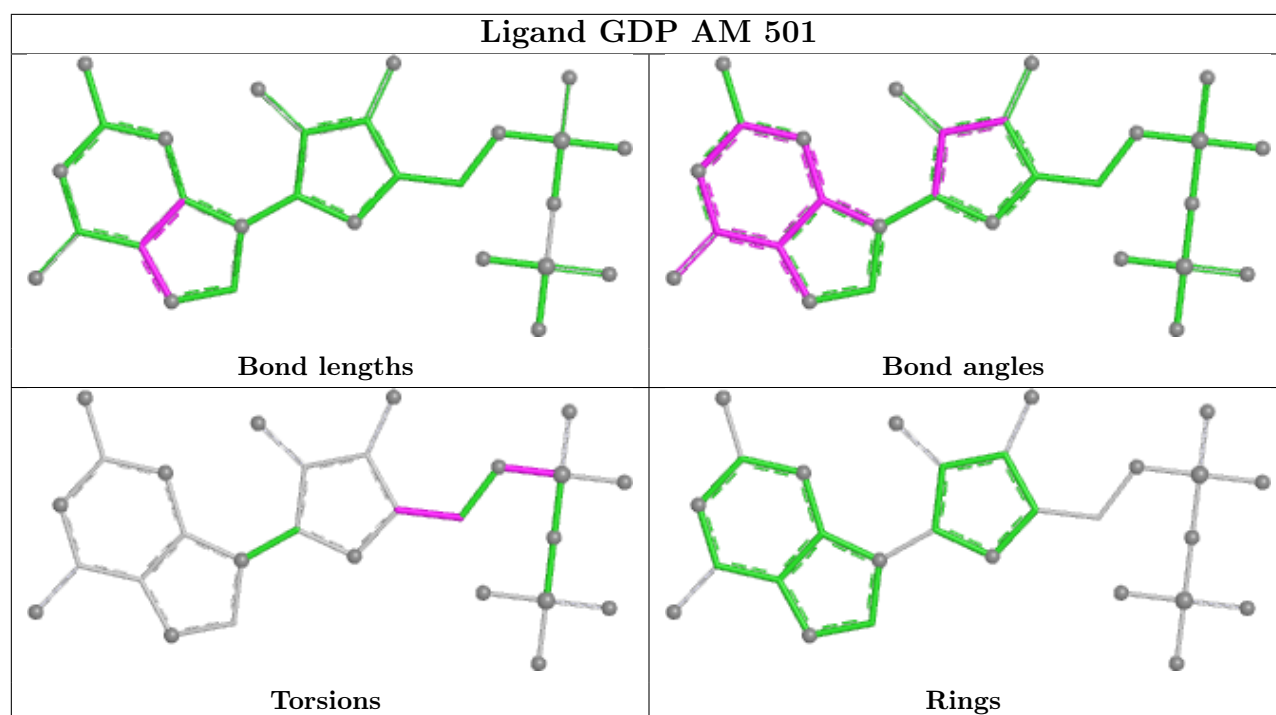


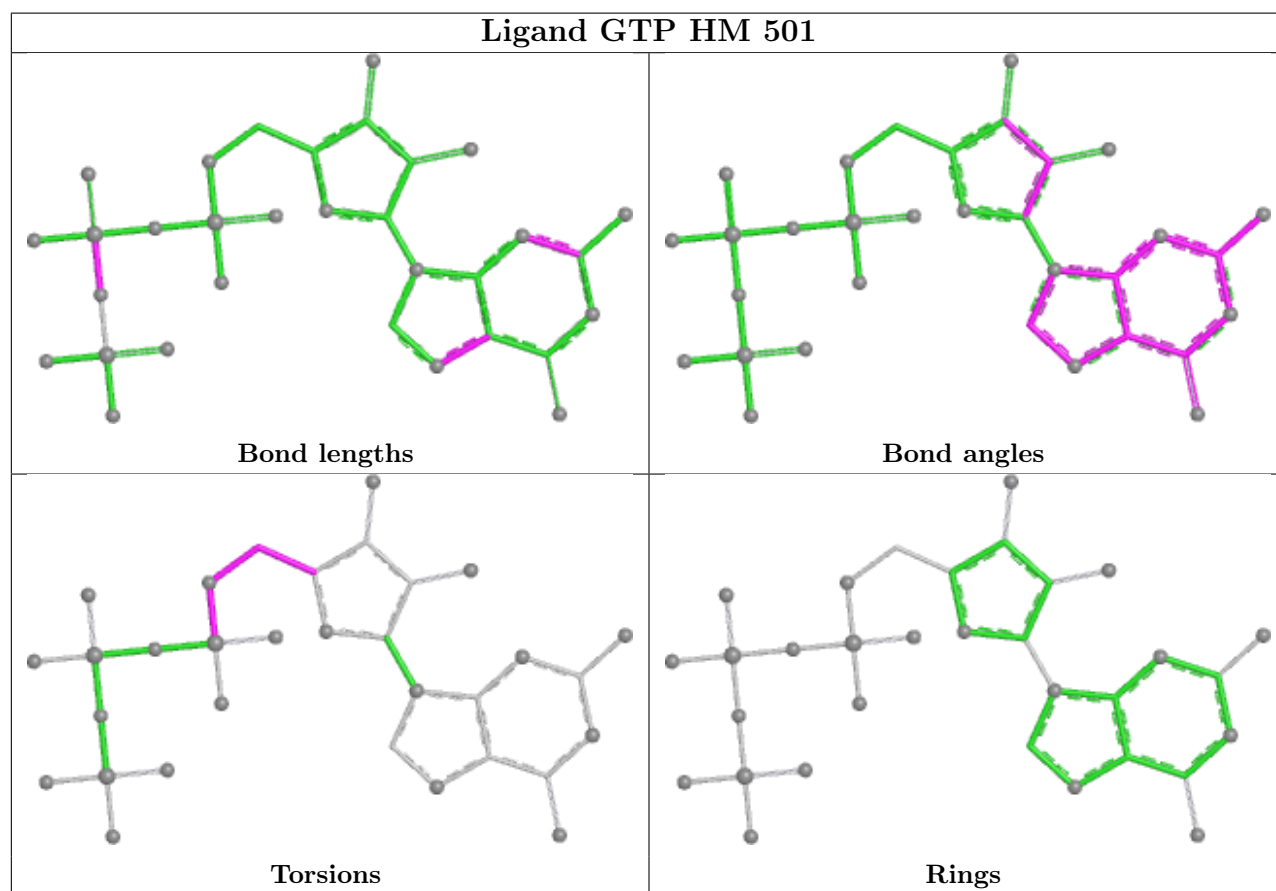
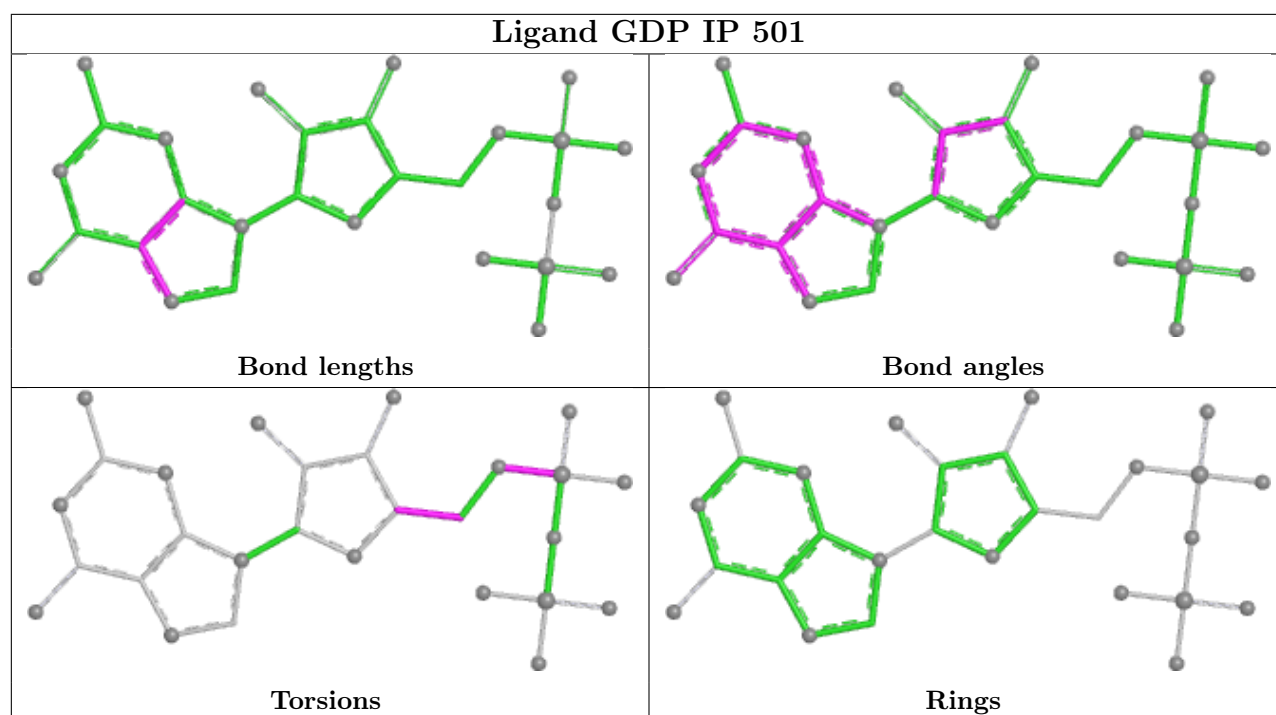




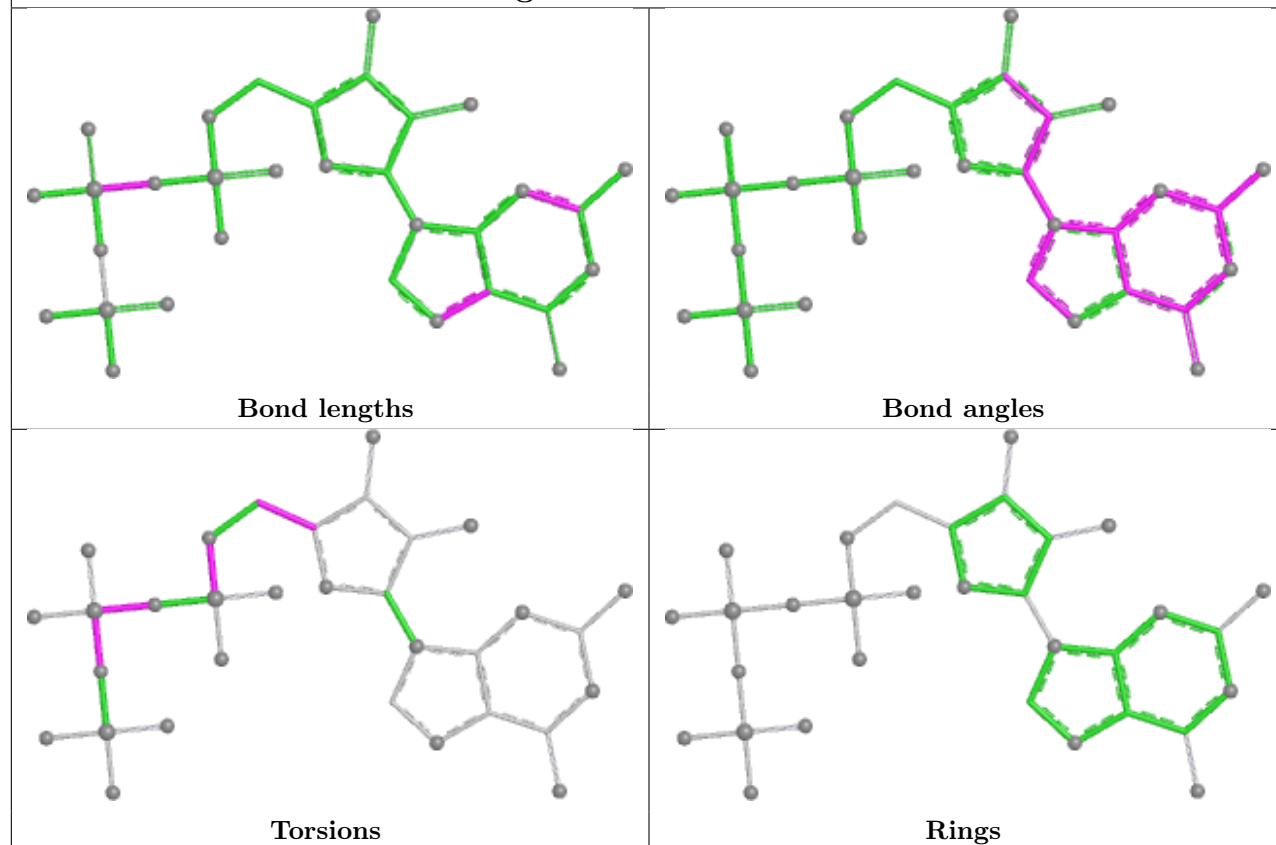




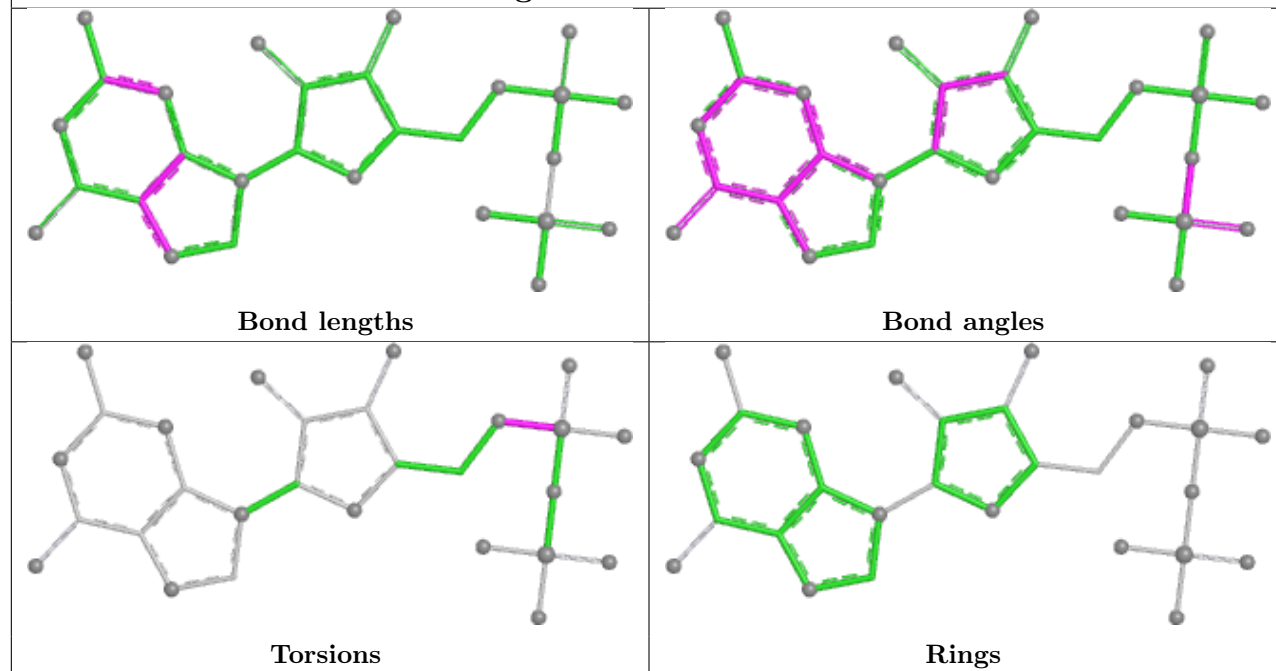


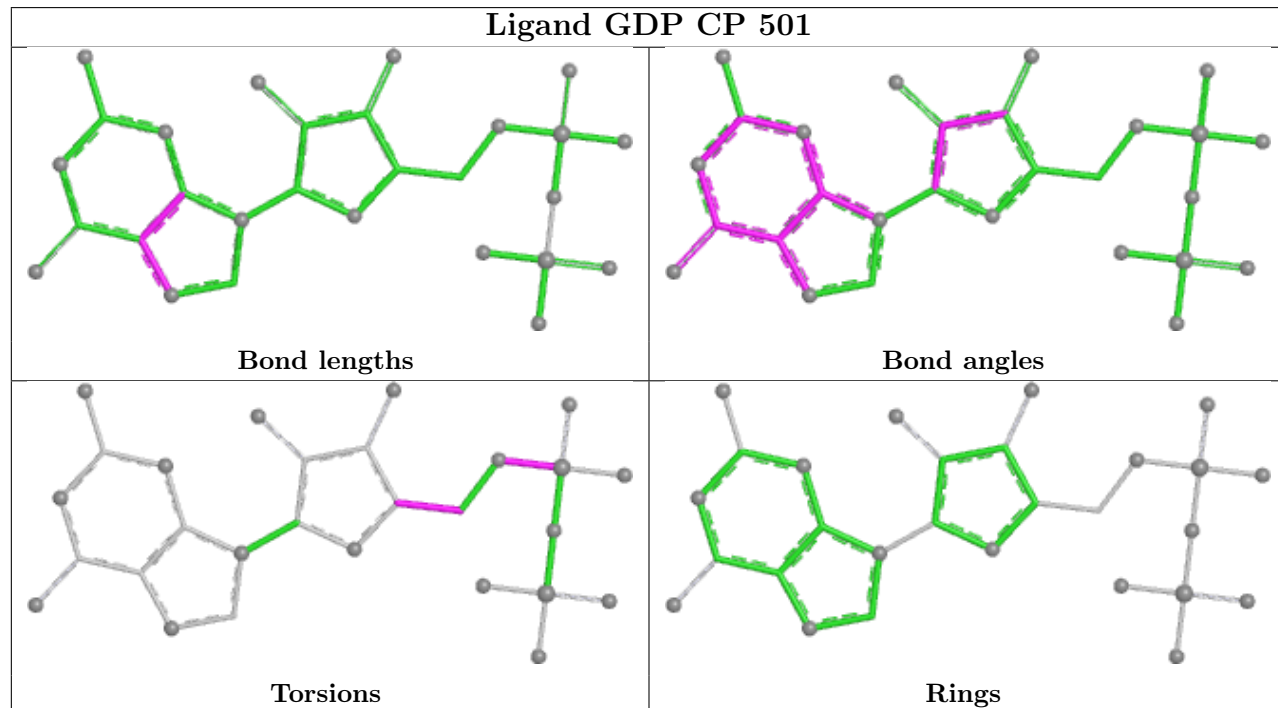
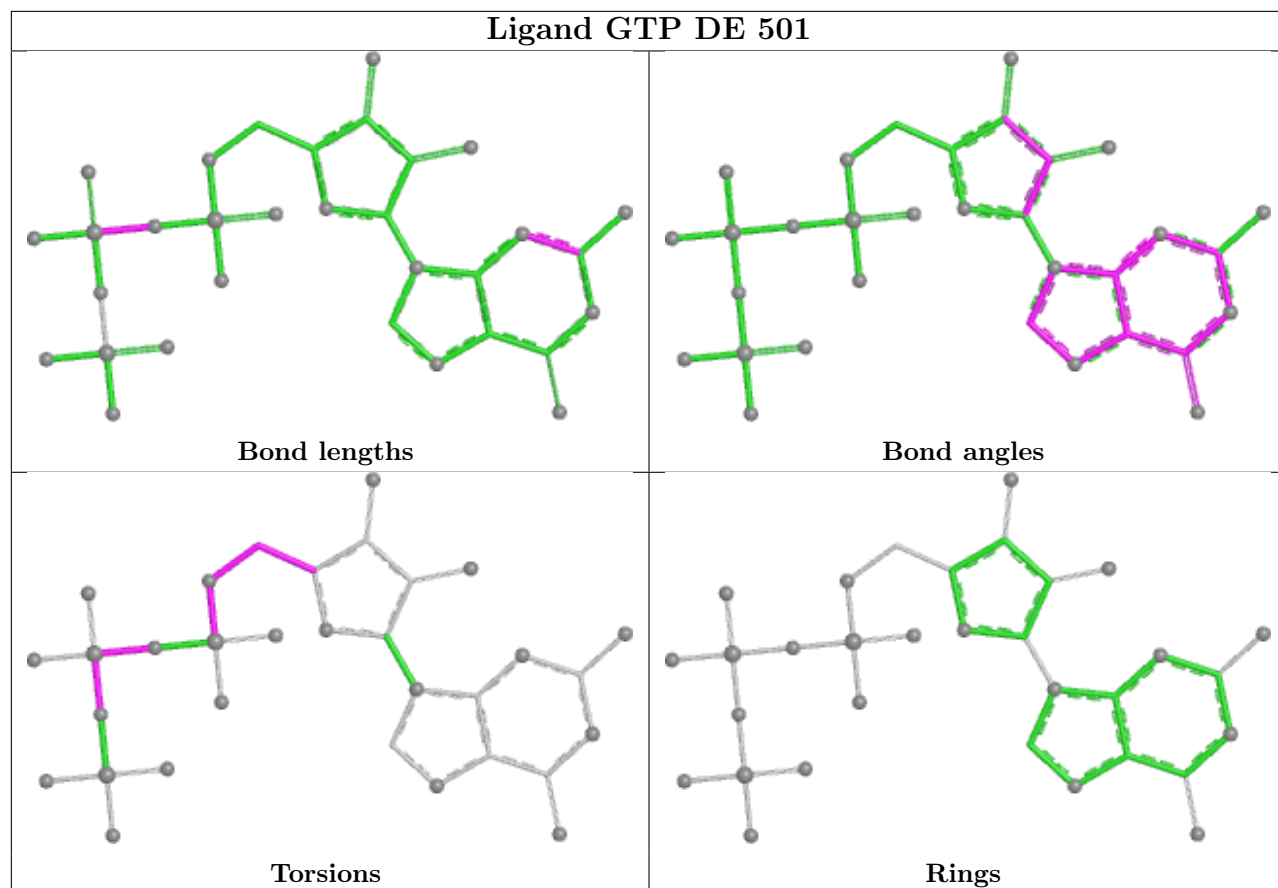


Ligand GTP ML 501

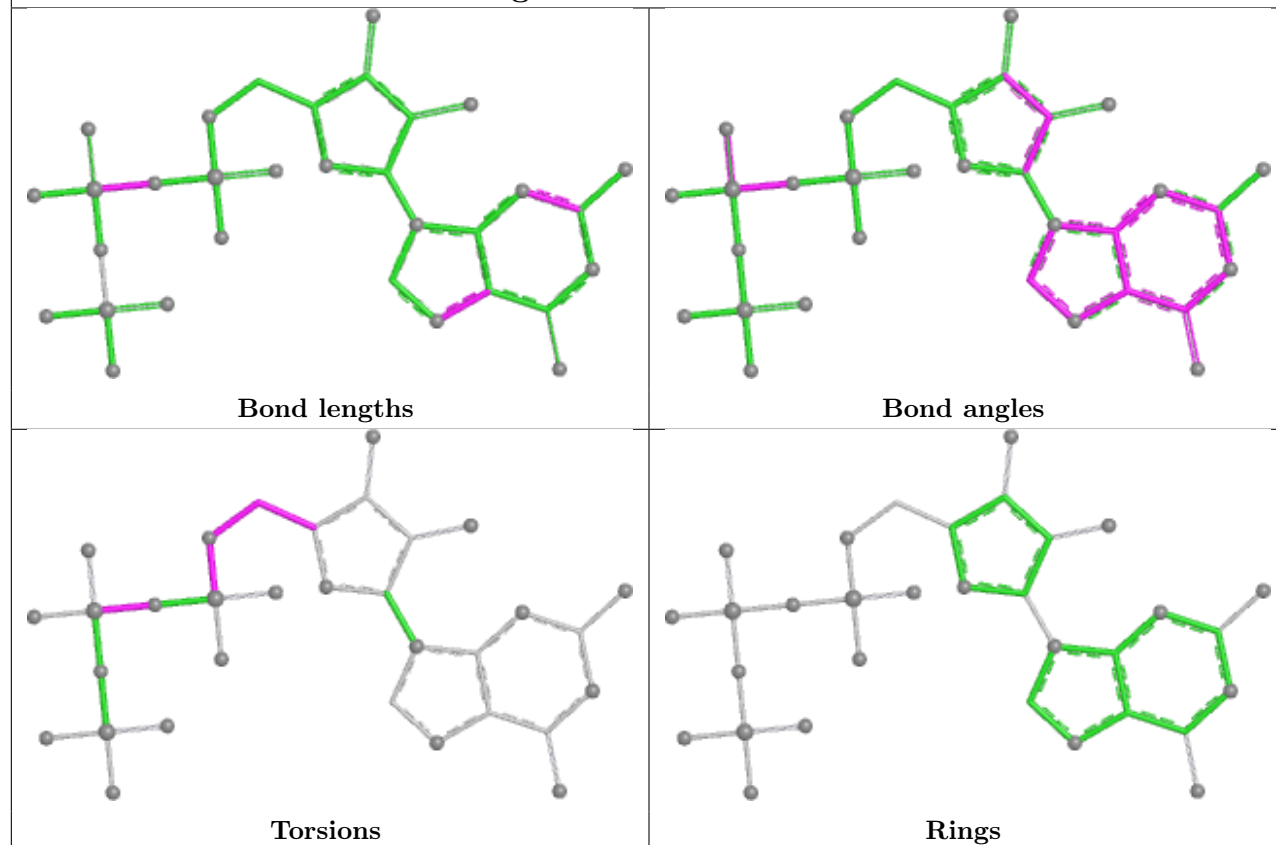


Ligand GDP KO 502

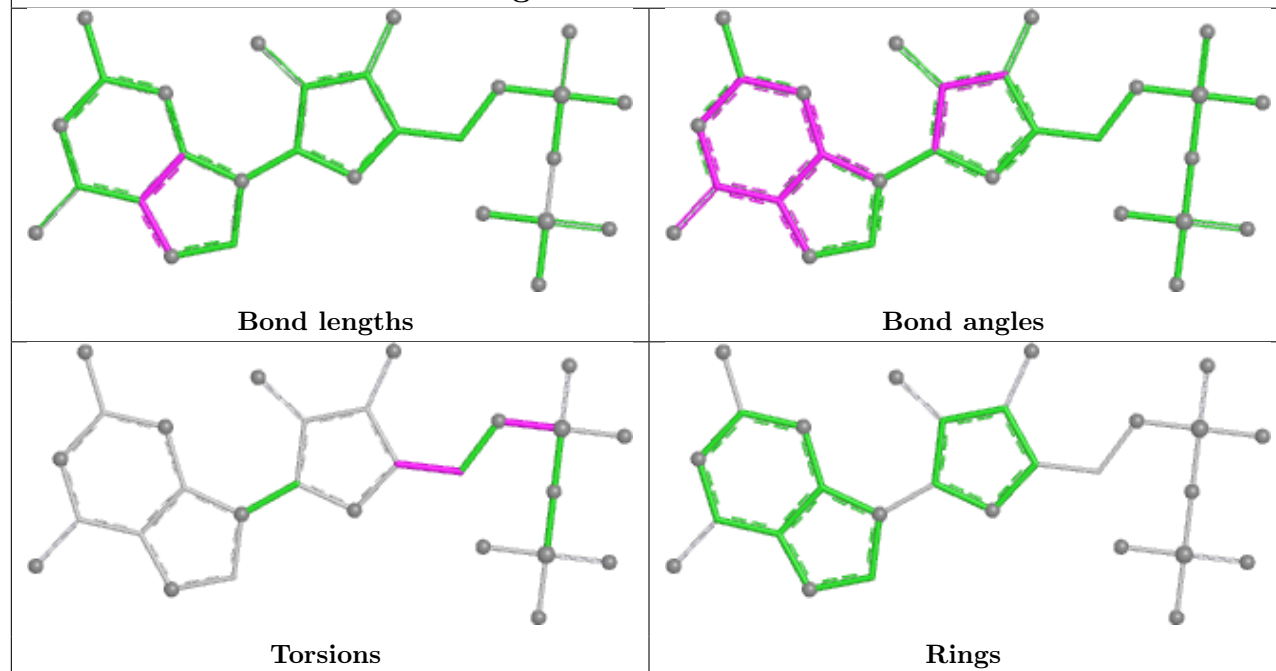




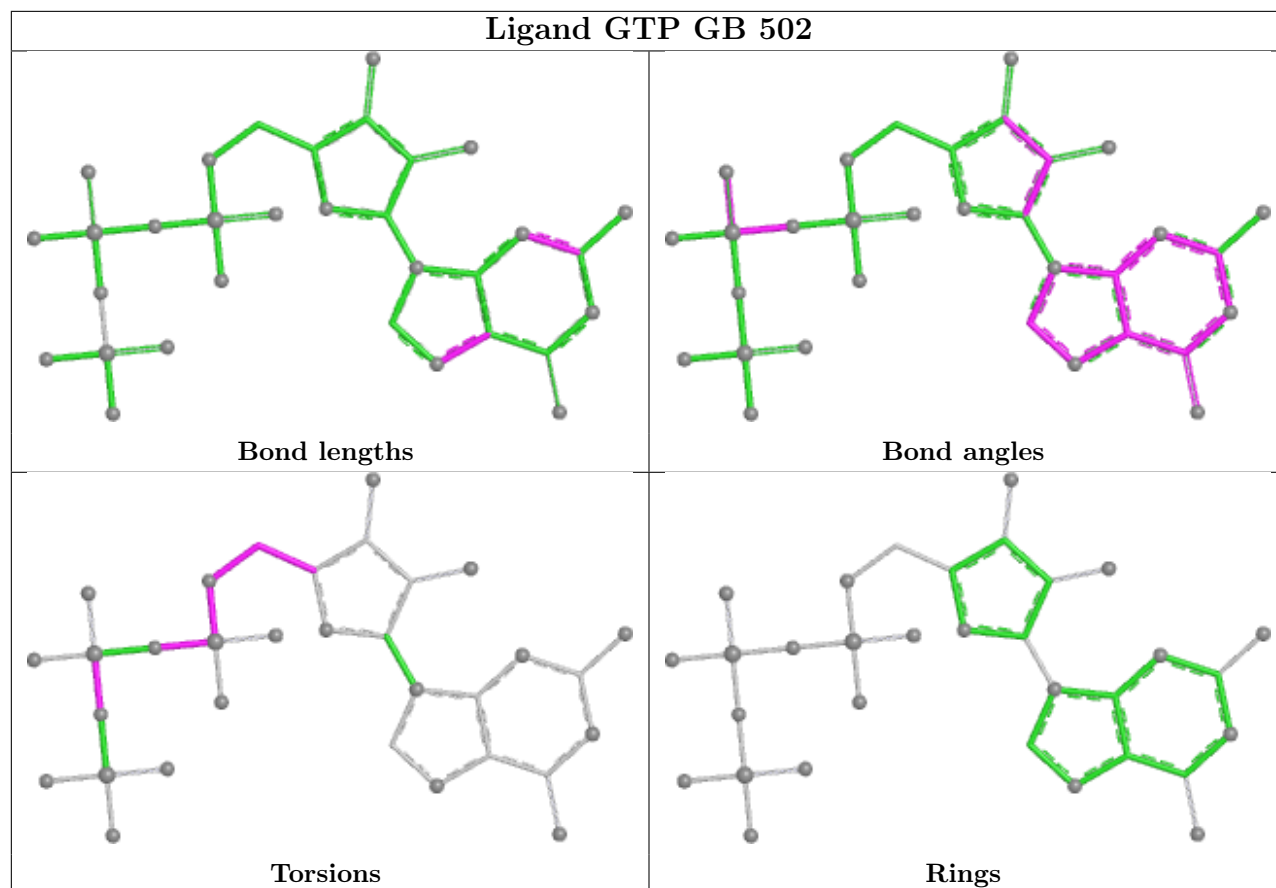
Ligand GTP WG 501



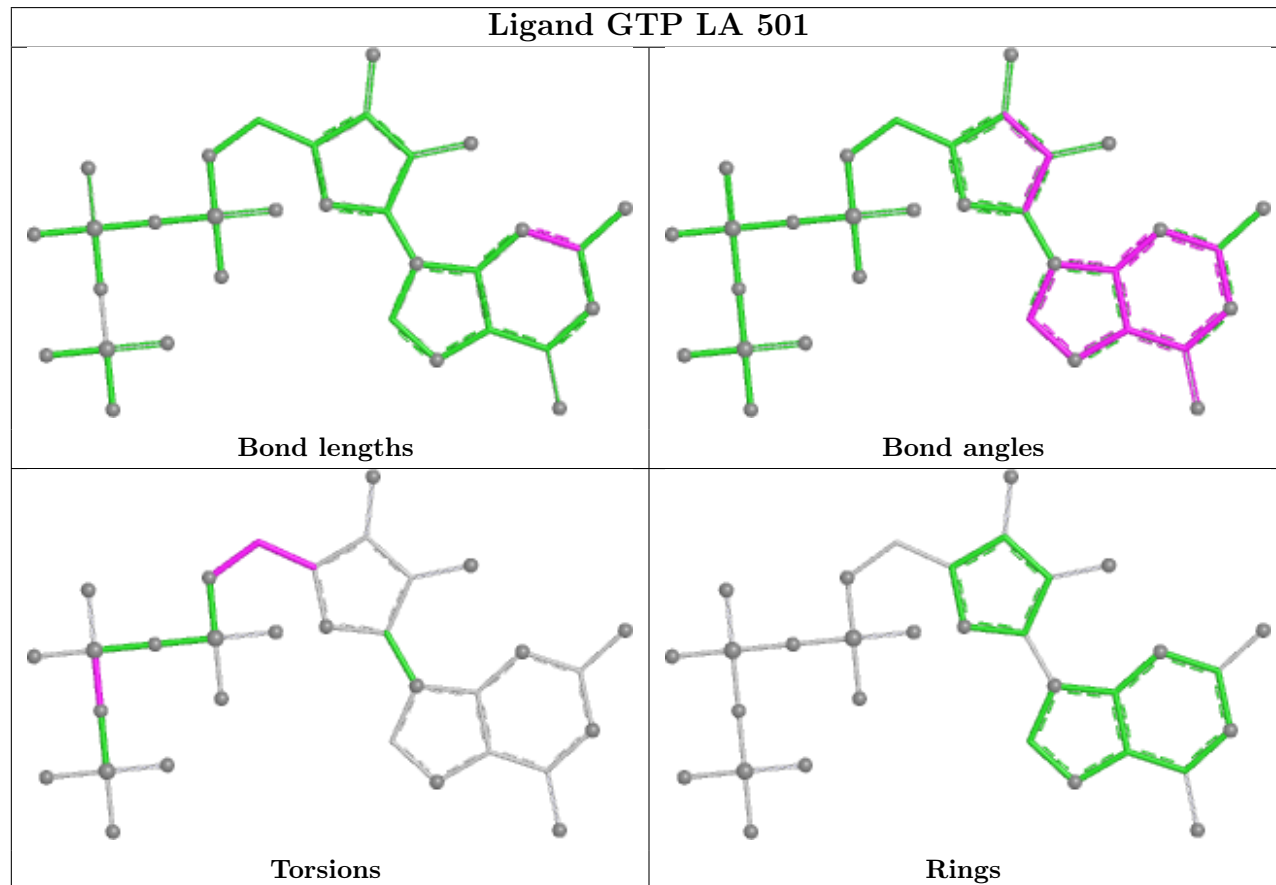
Ligand GDP MB 501



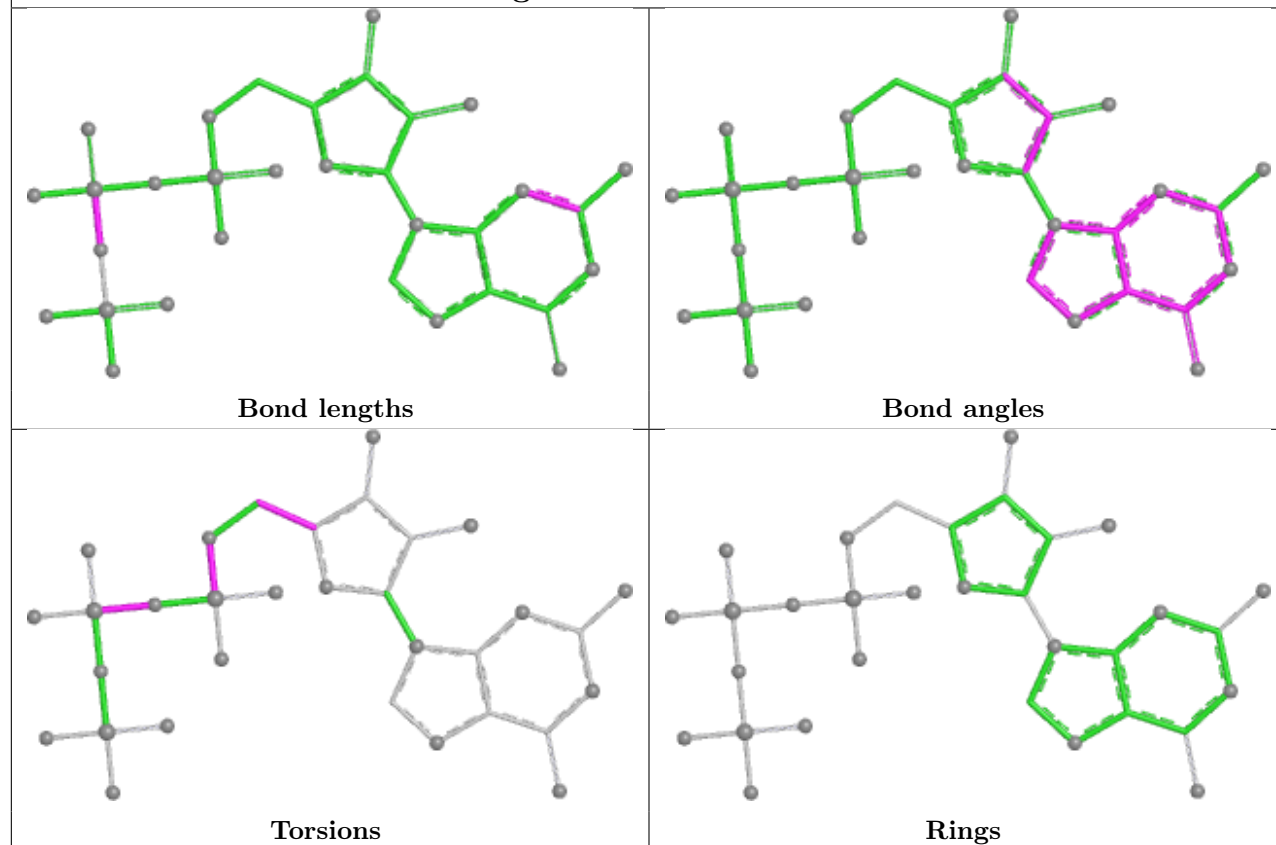
Ligand GTP GB 502



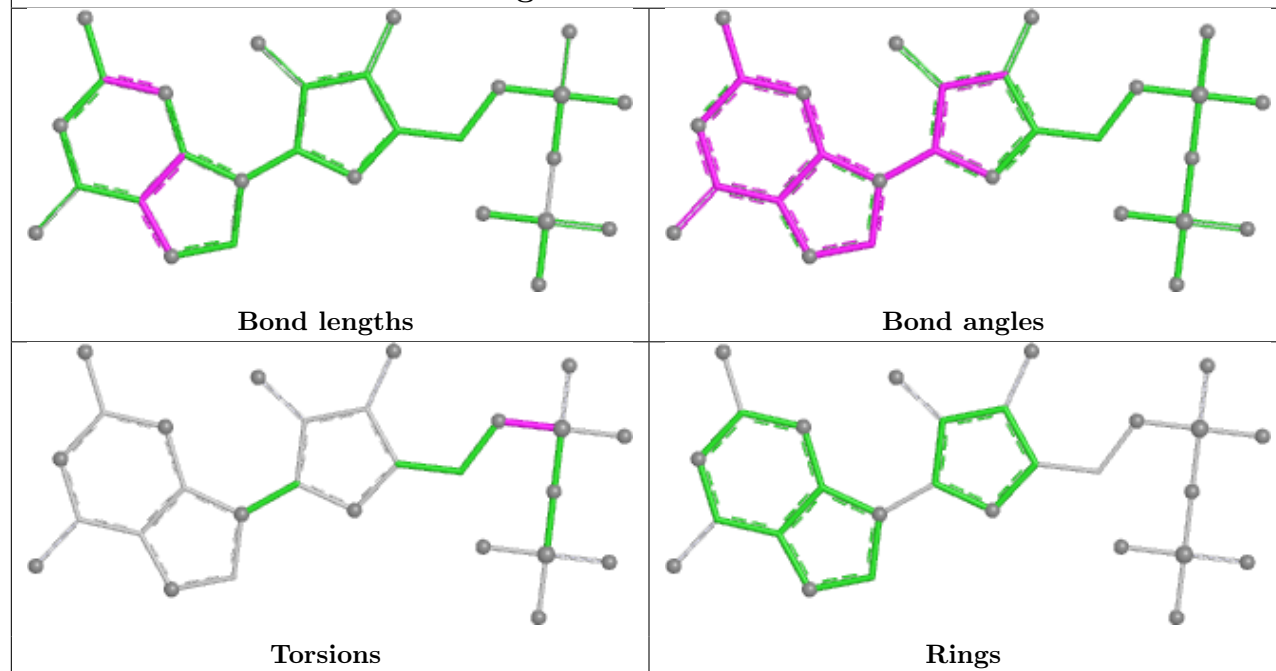
Ligand GTP LA 501

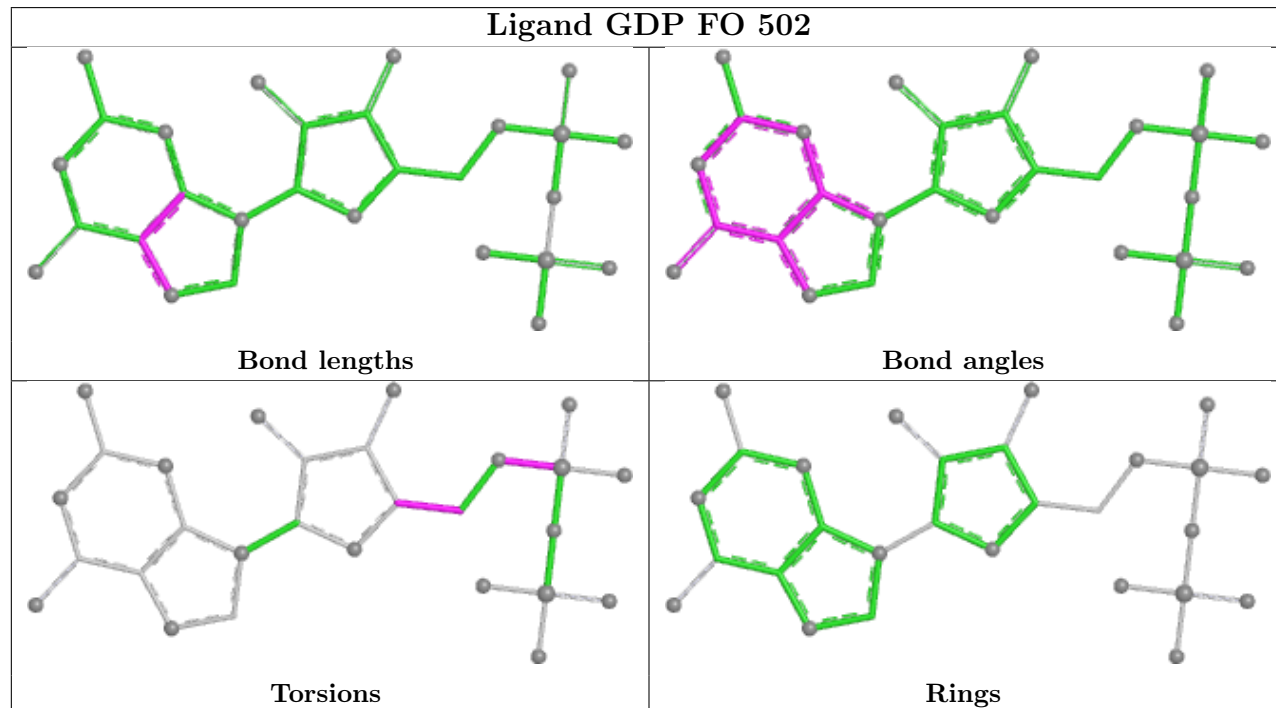
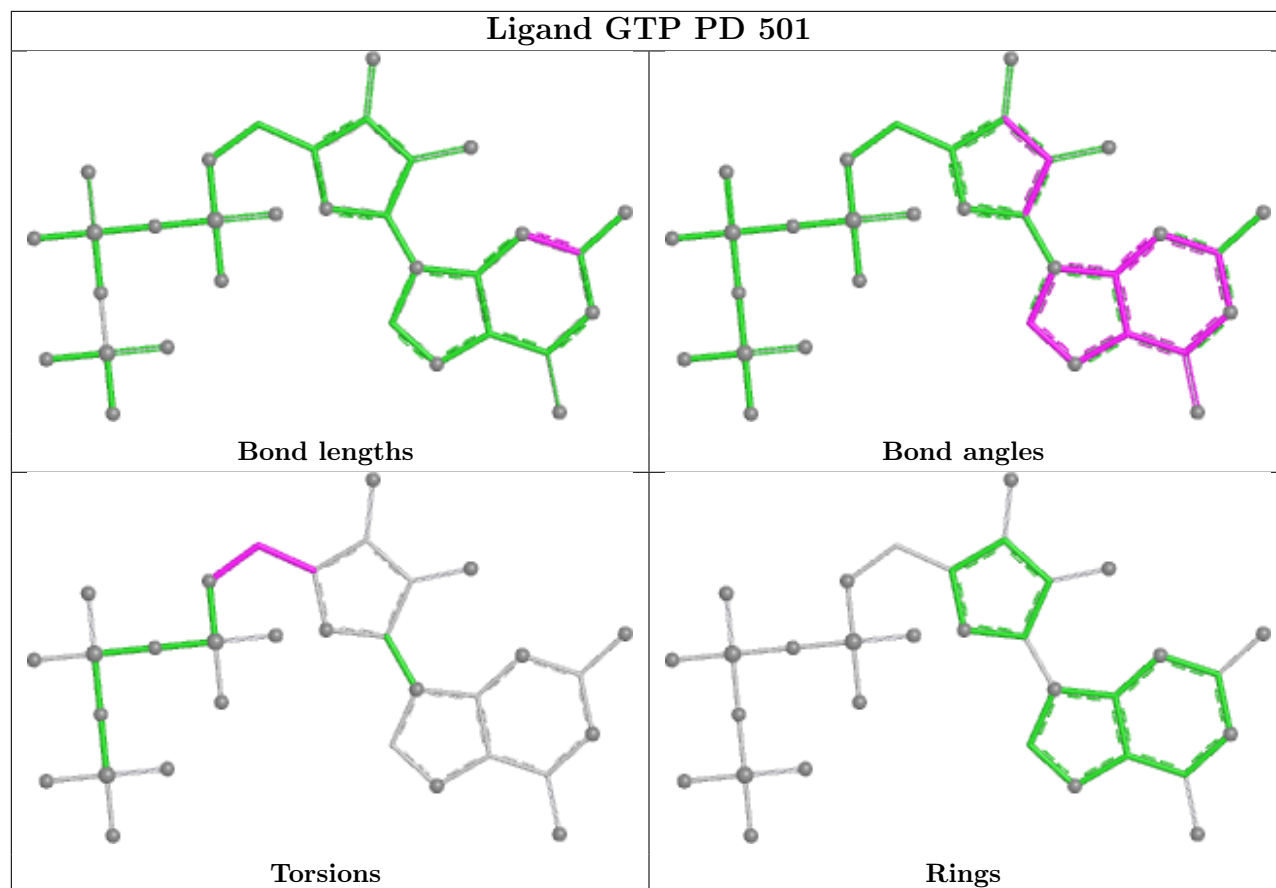


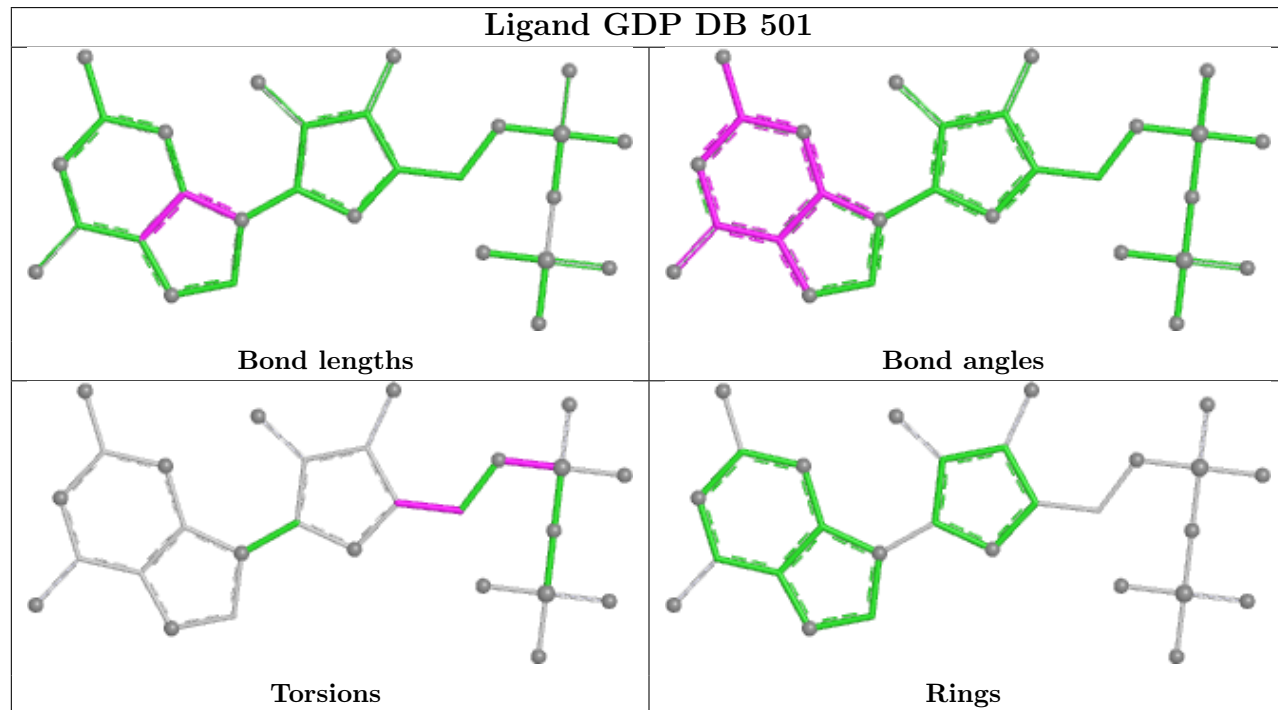
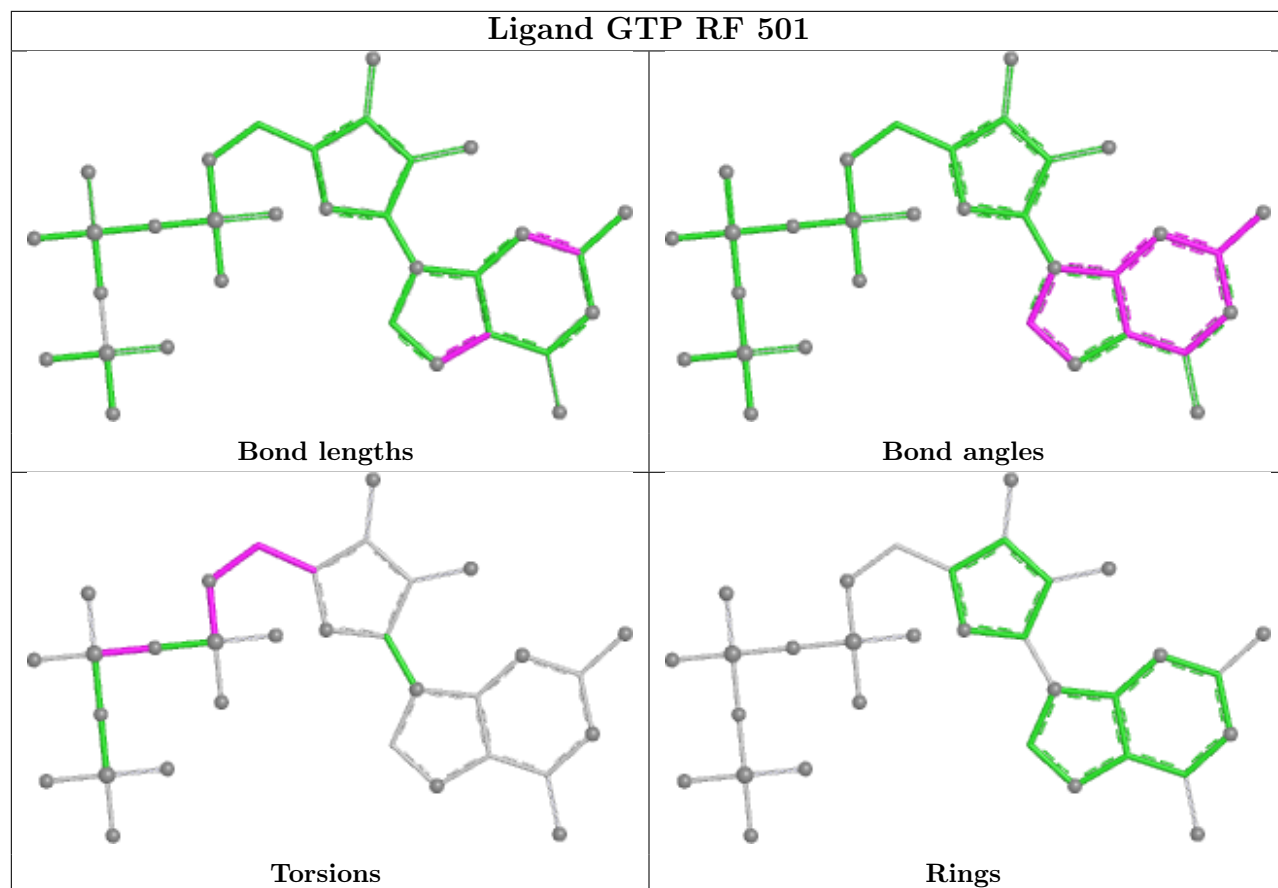
Ligand GTP NM 501

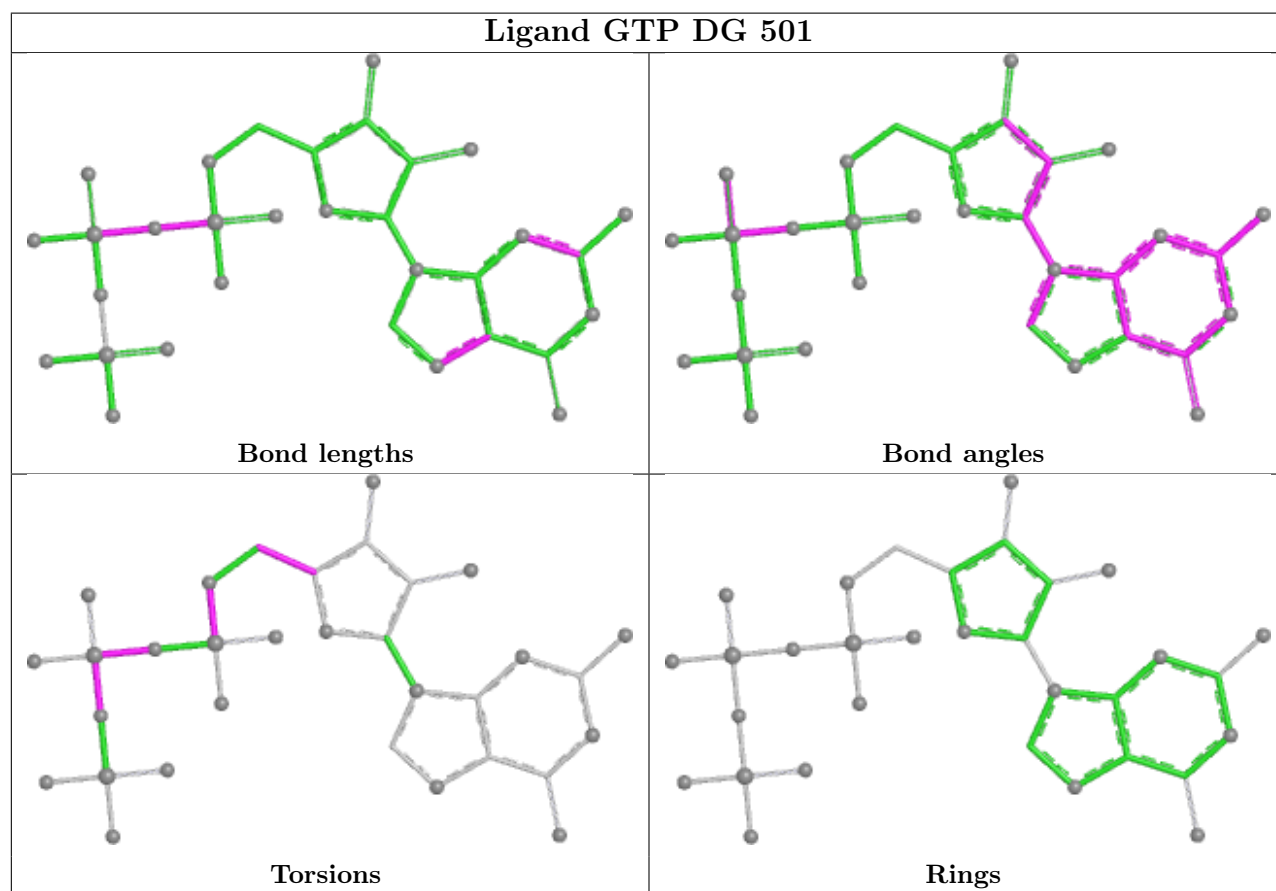
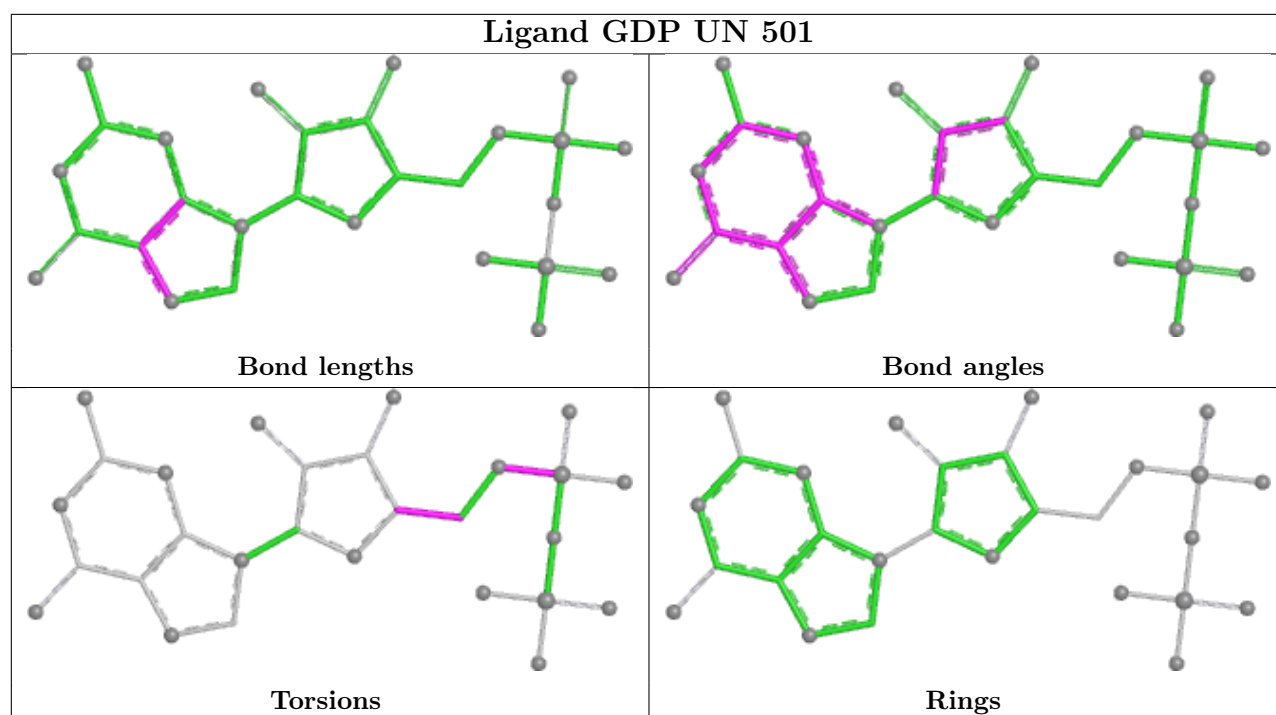


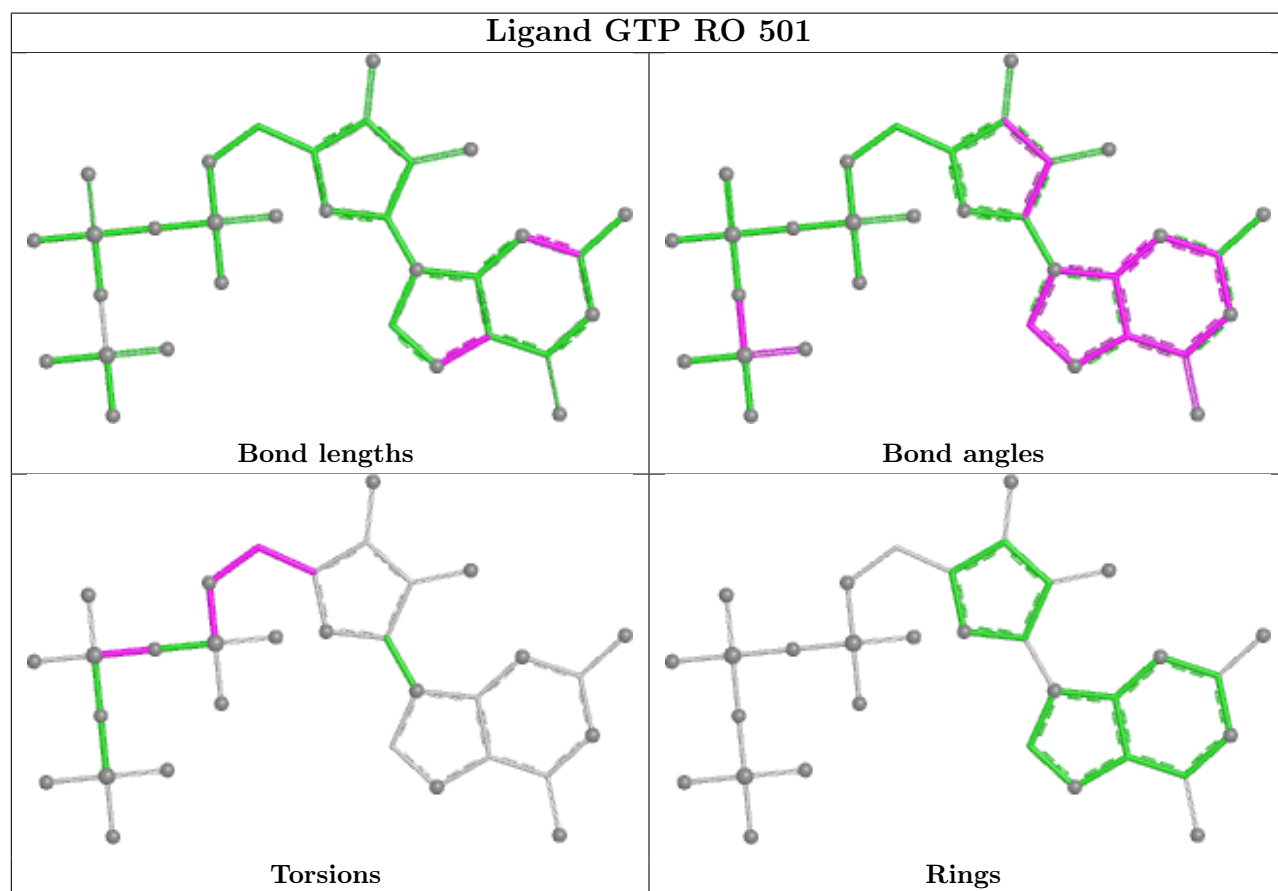
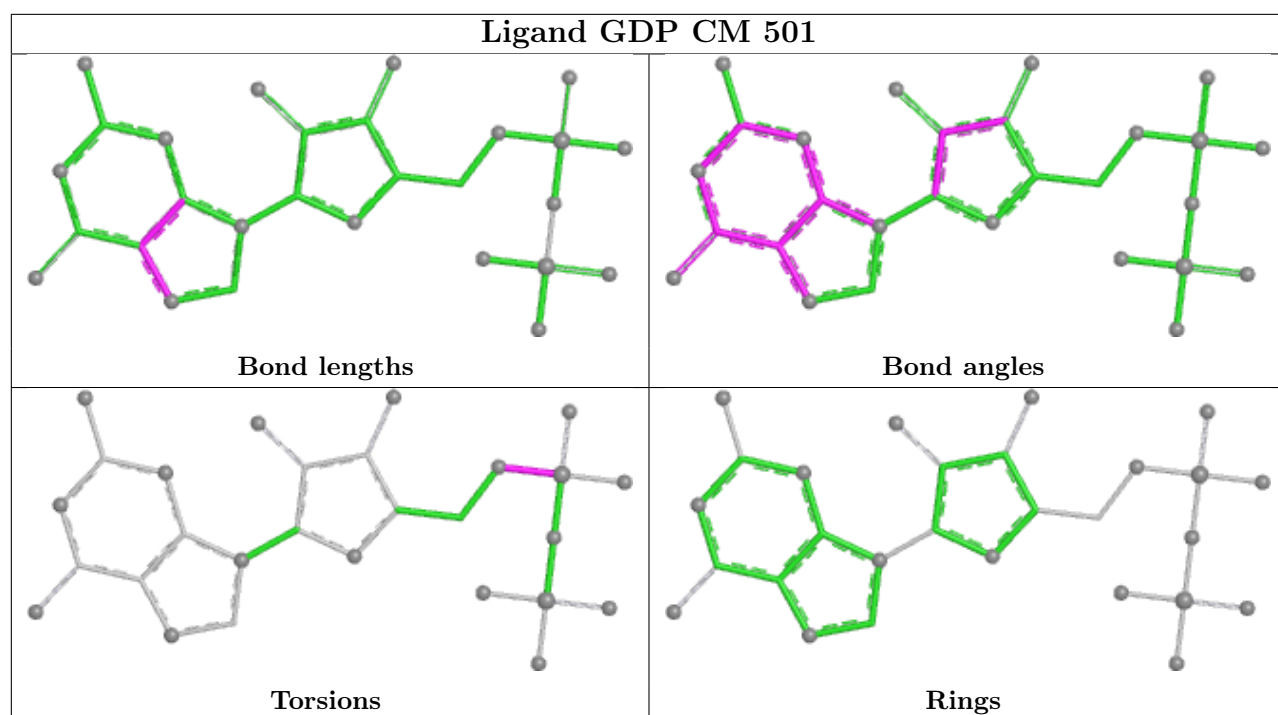
Ligand GDP RP 502

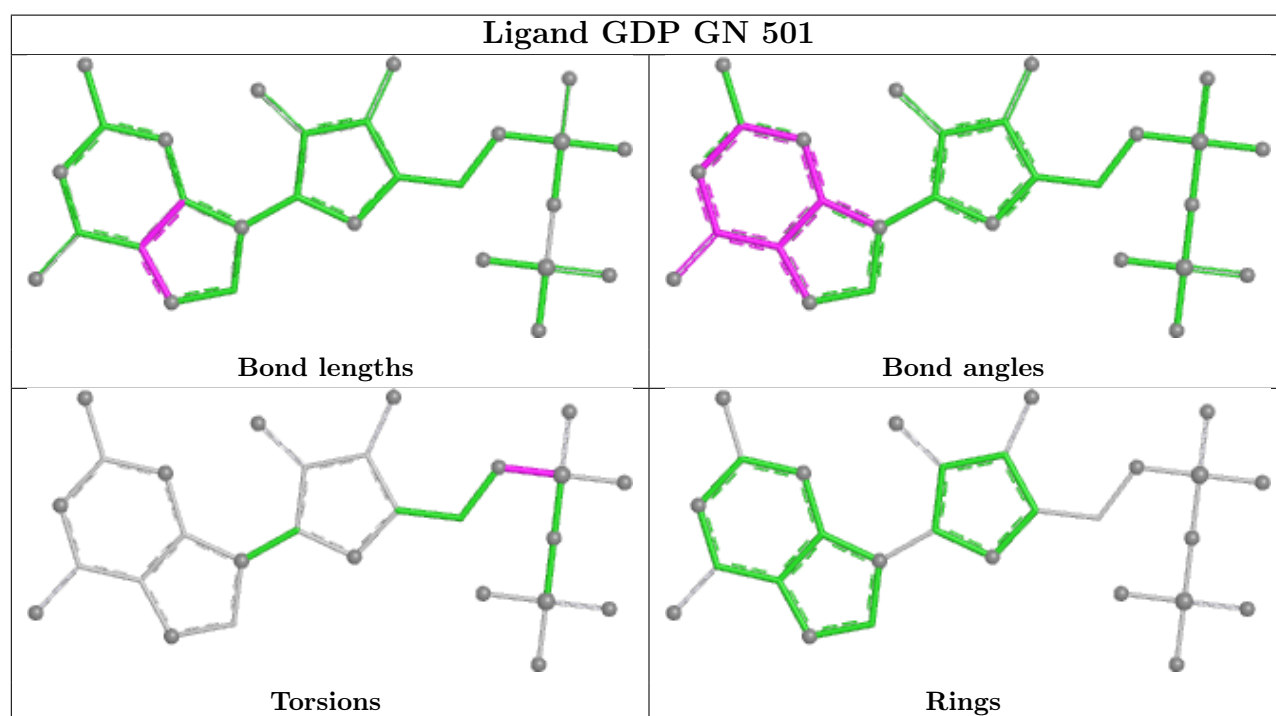
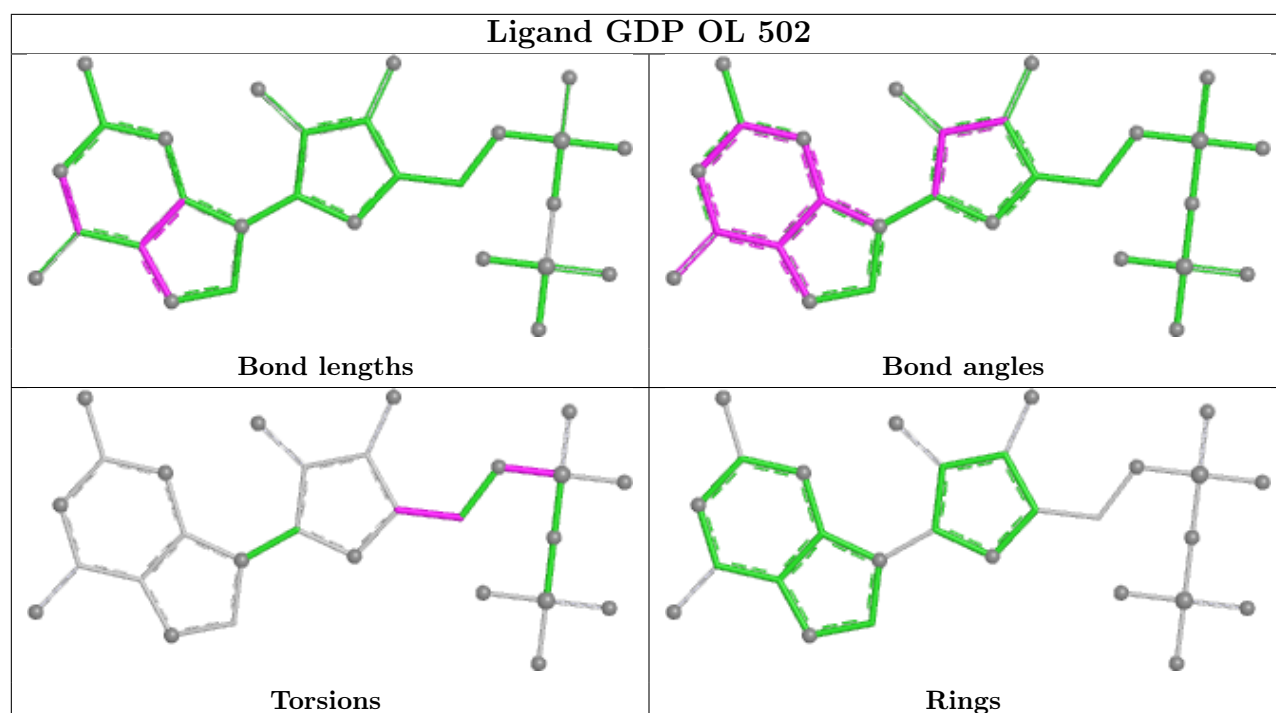


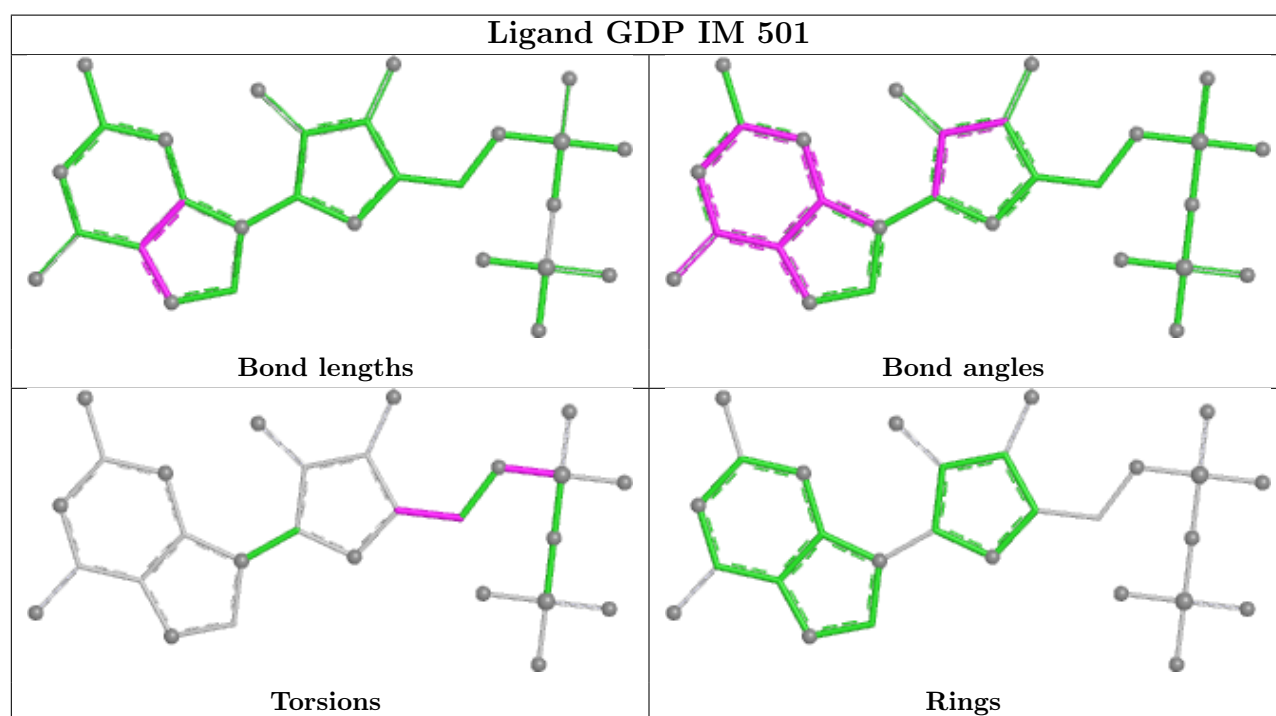
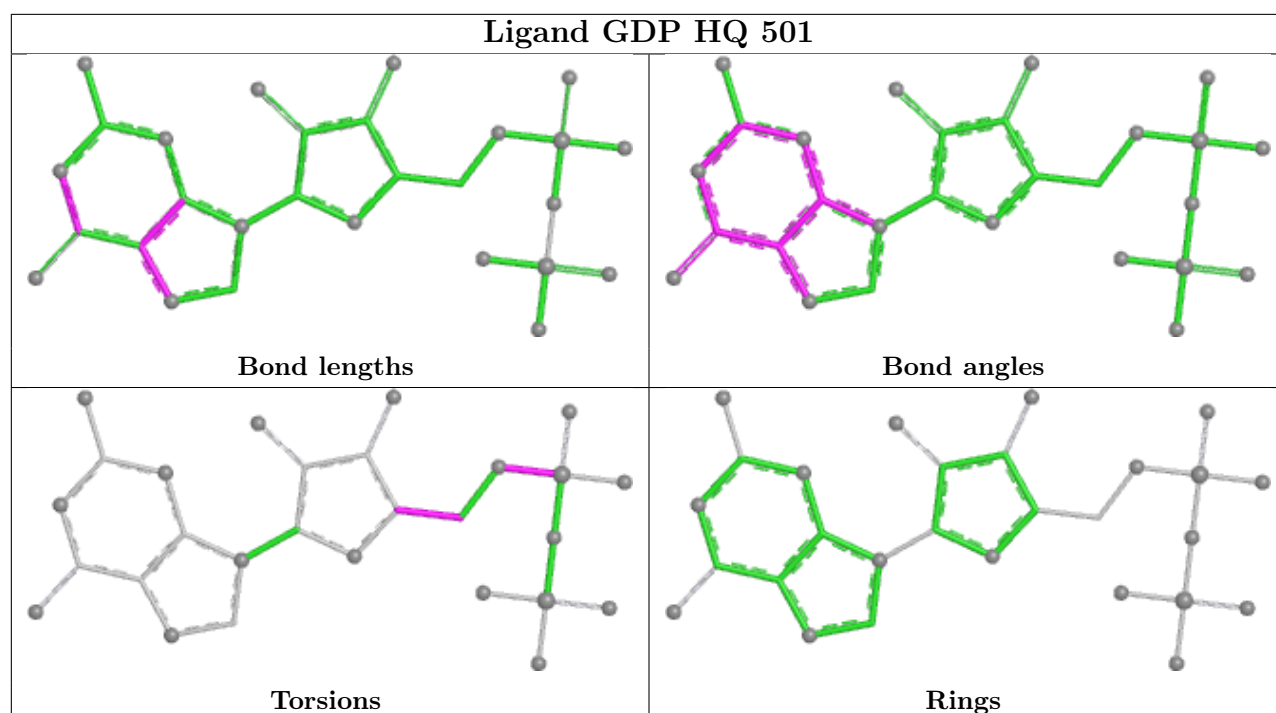




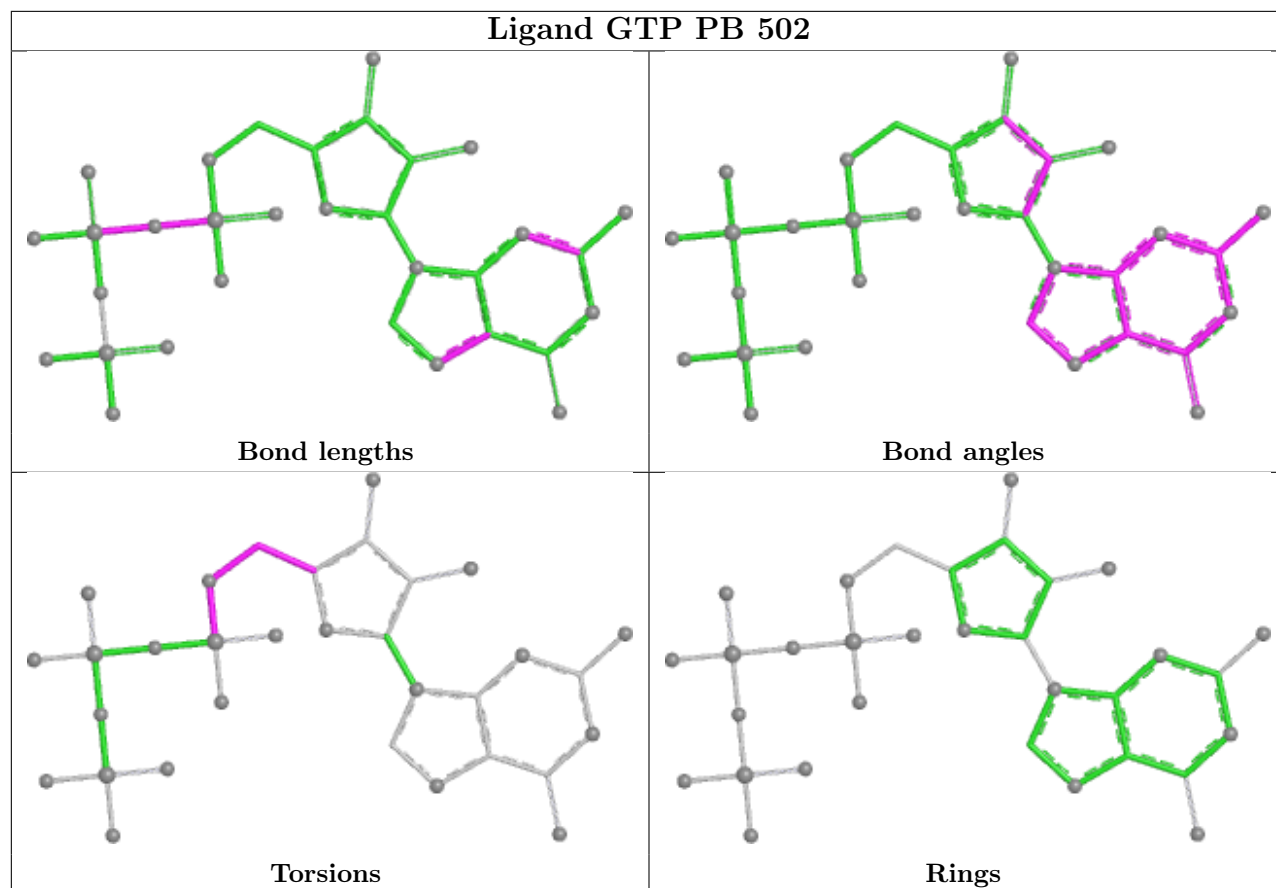




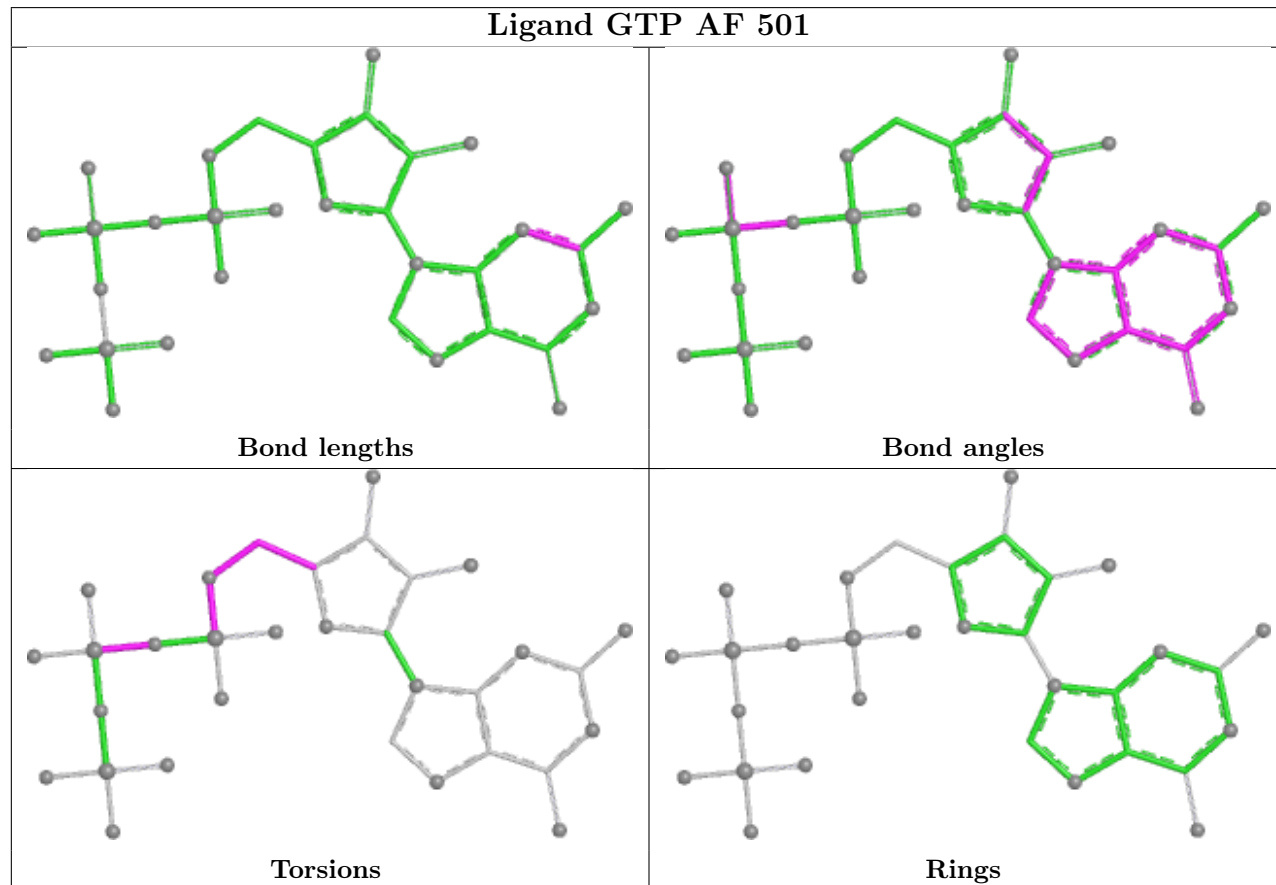


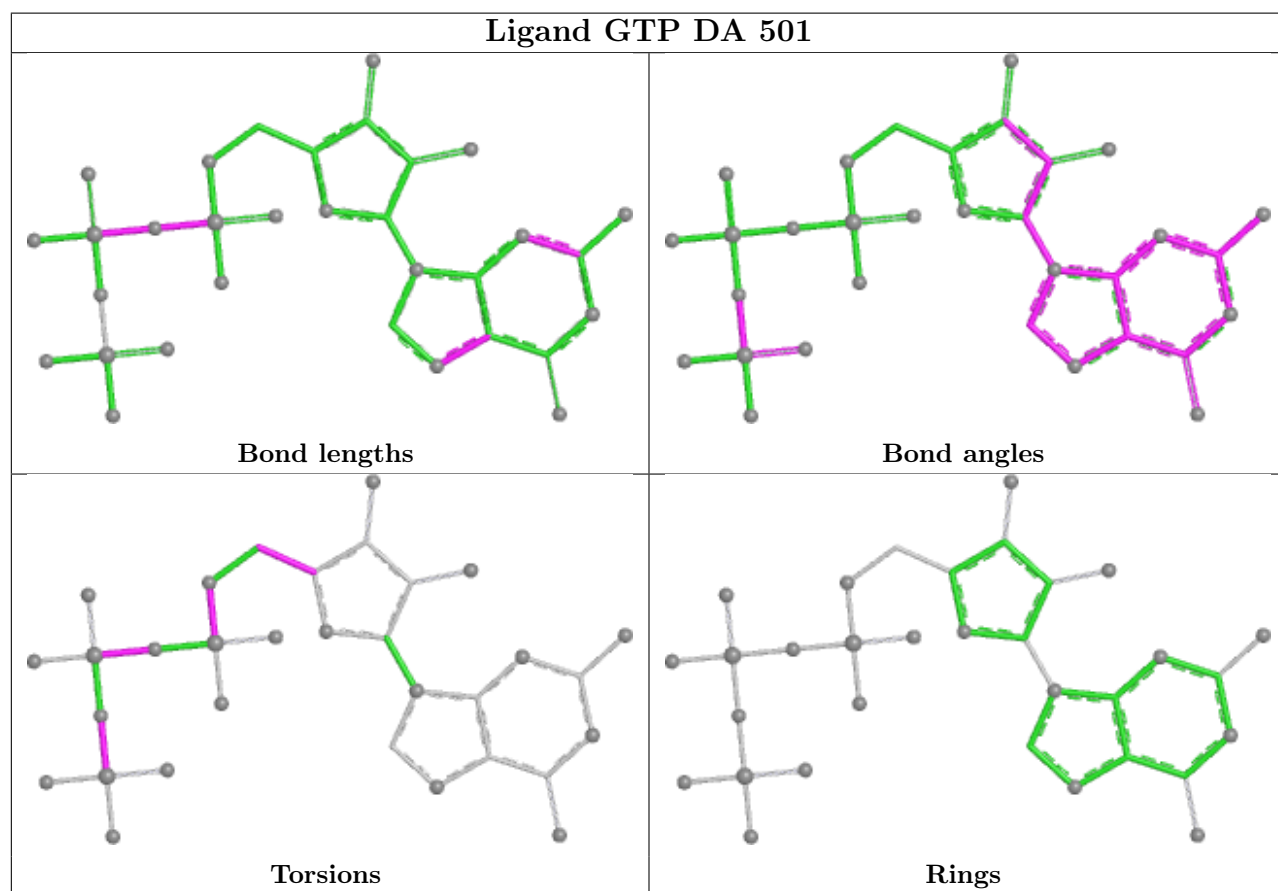
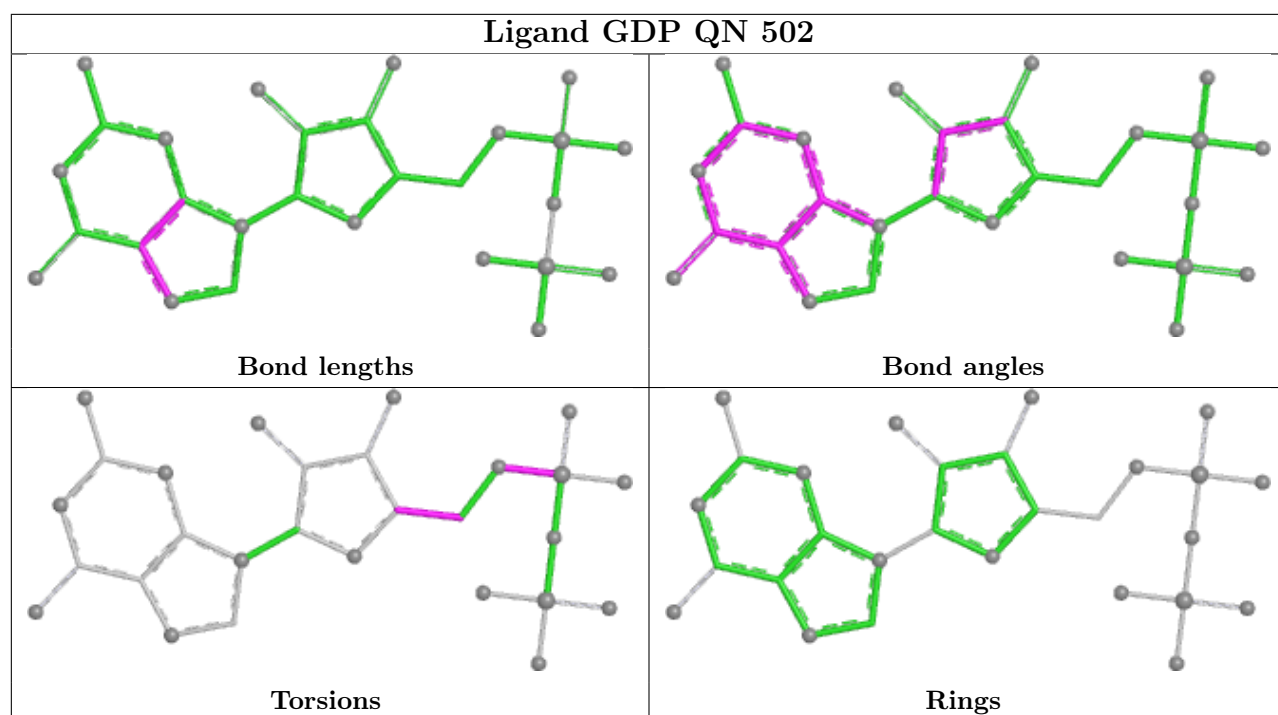


Ligand GTP PB 502

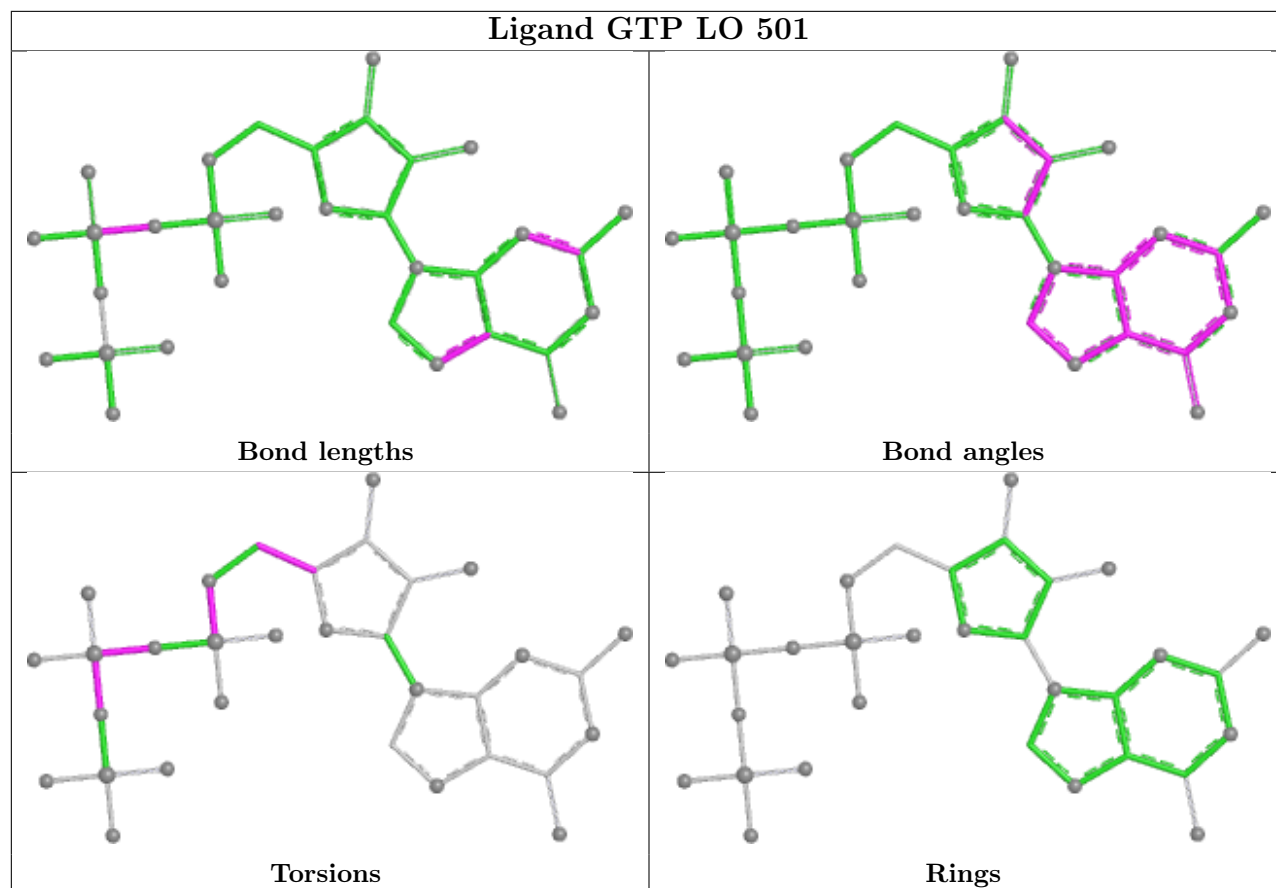


Ligand GTP AF 501

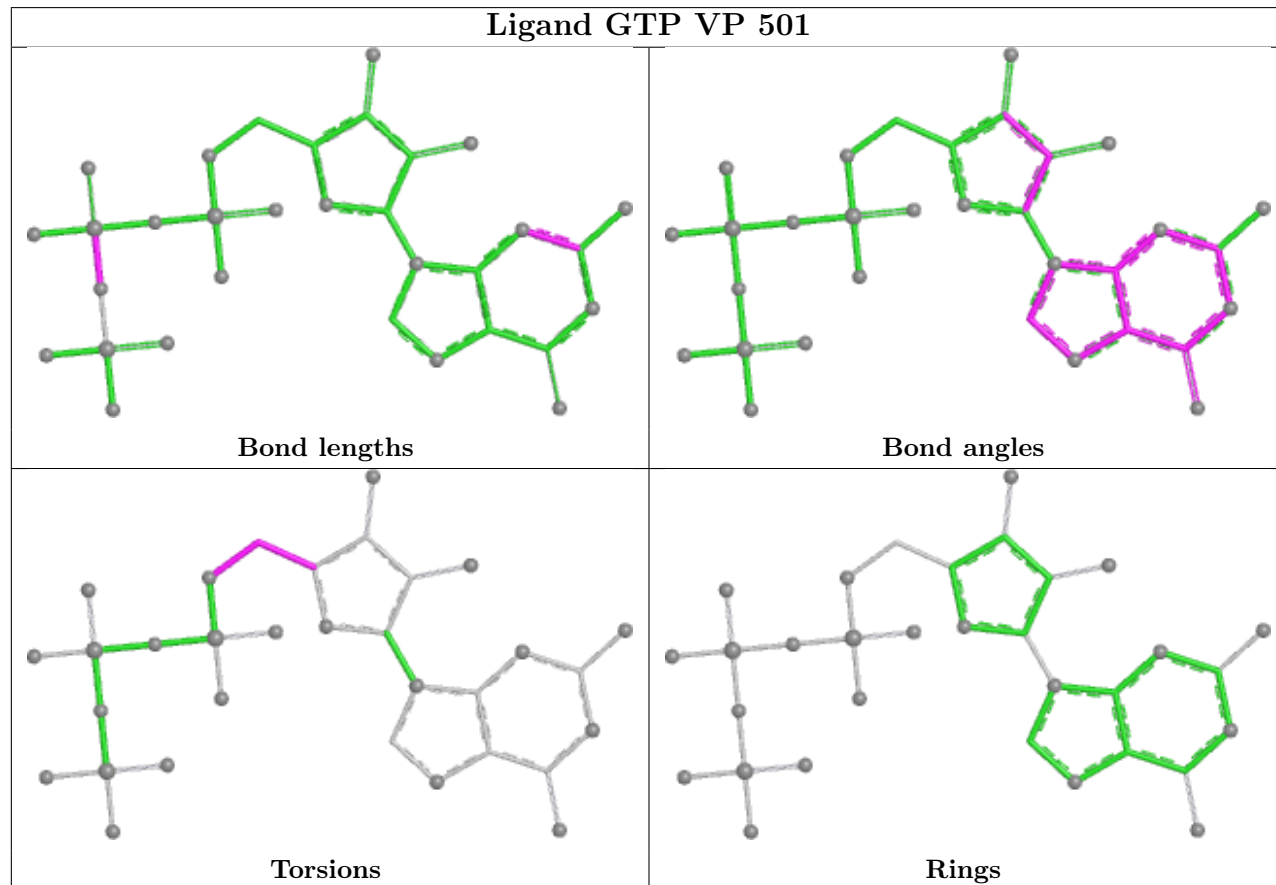


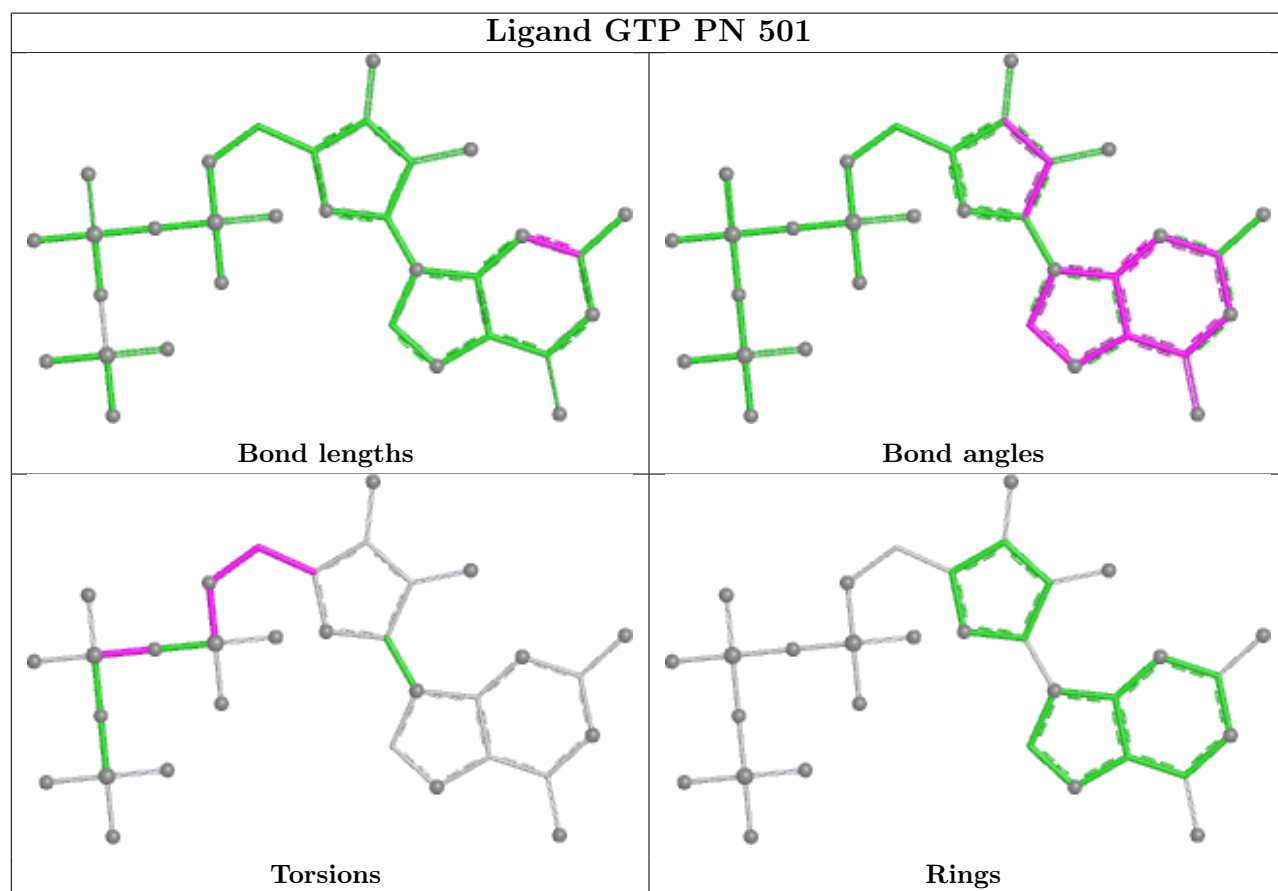
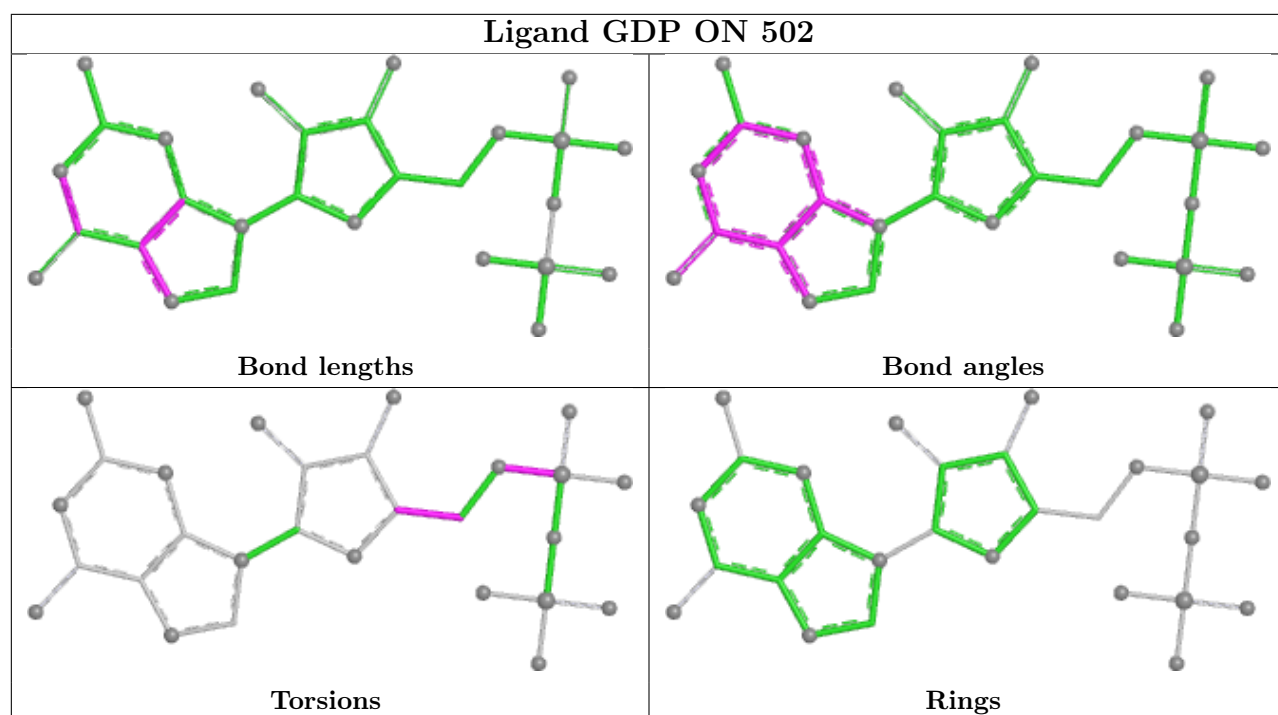


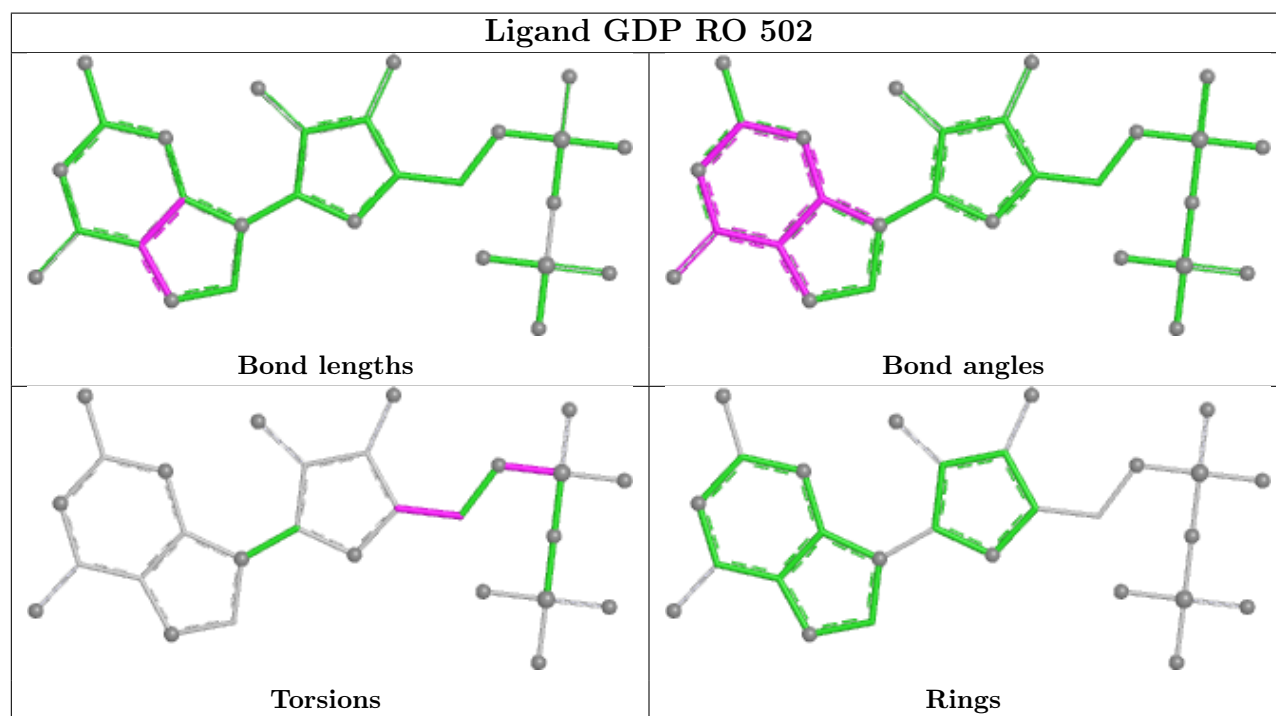
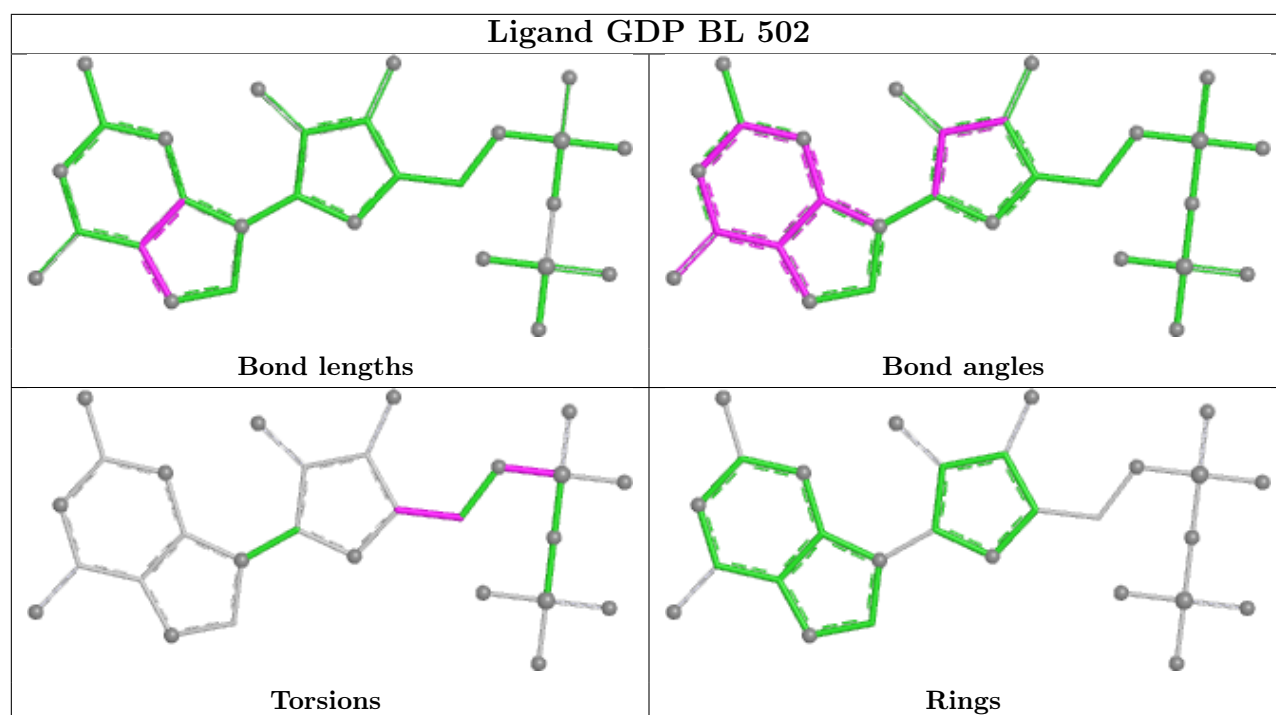
Ligand GTP LO 501



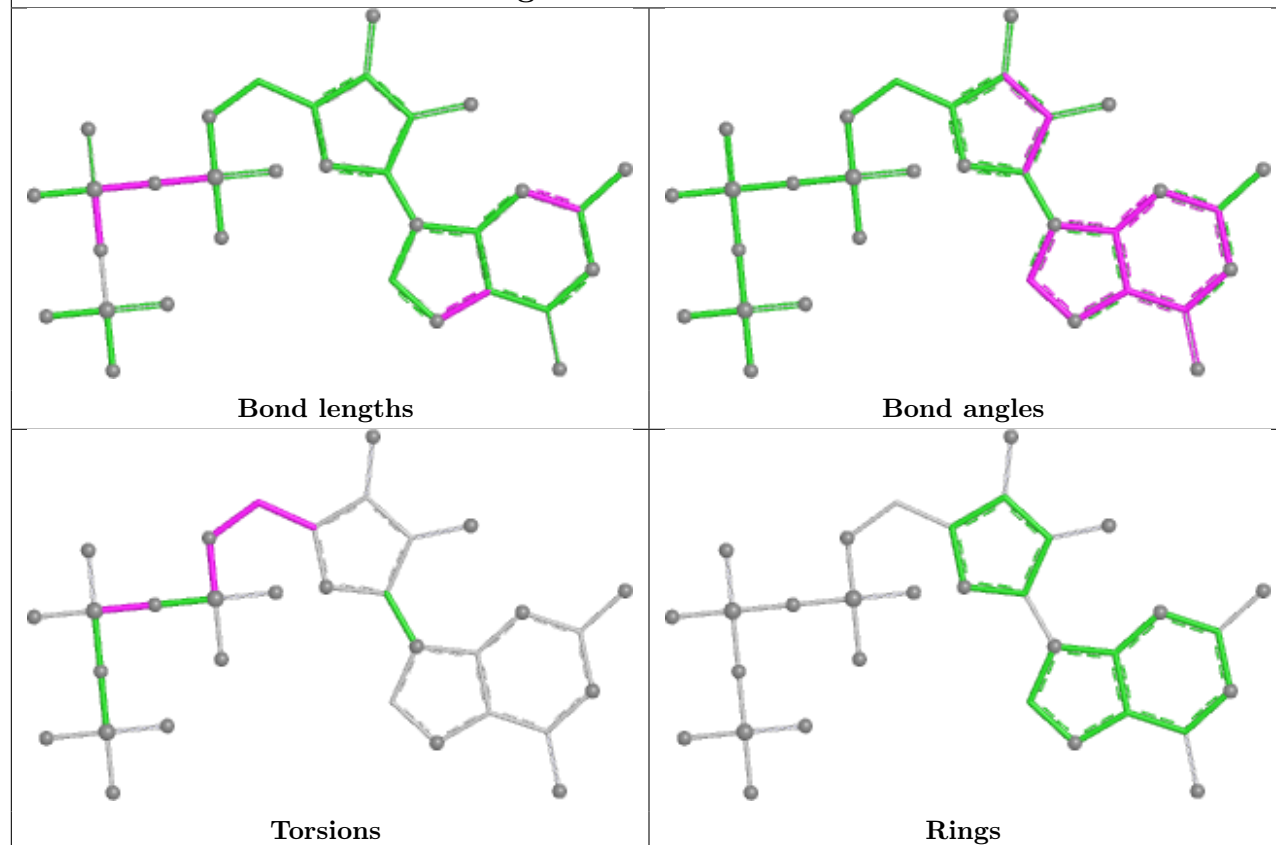
Ligand GTP VP 501



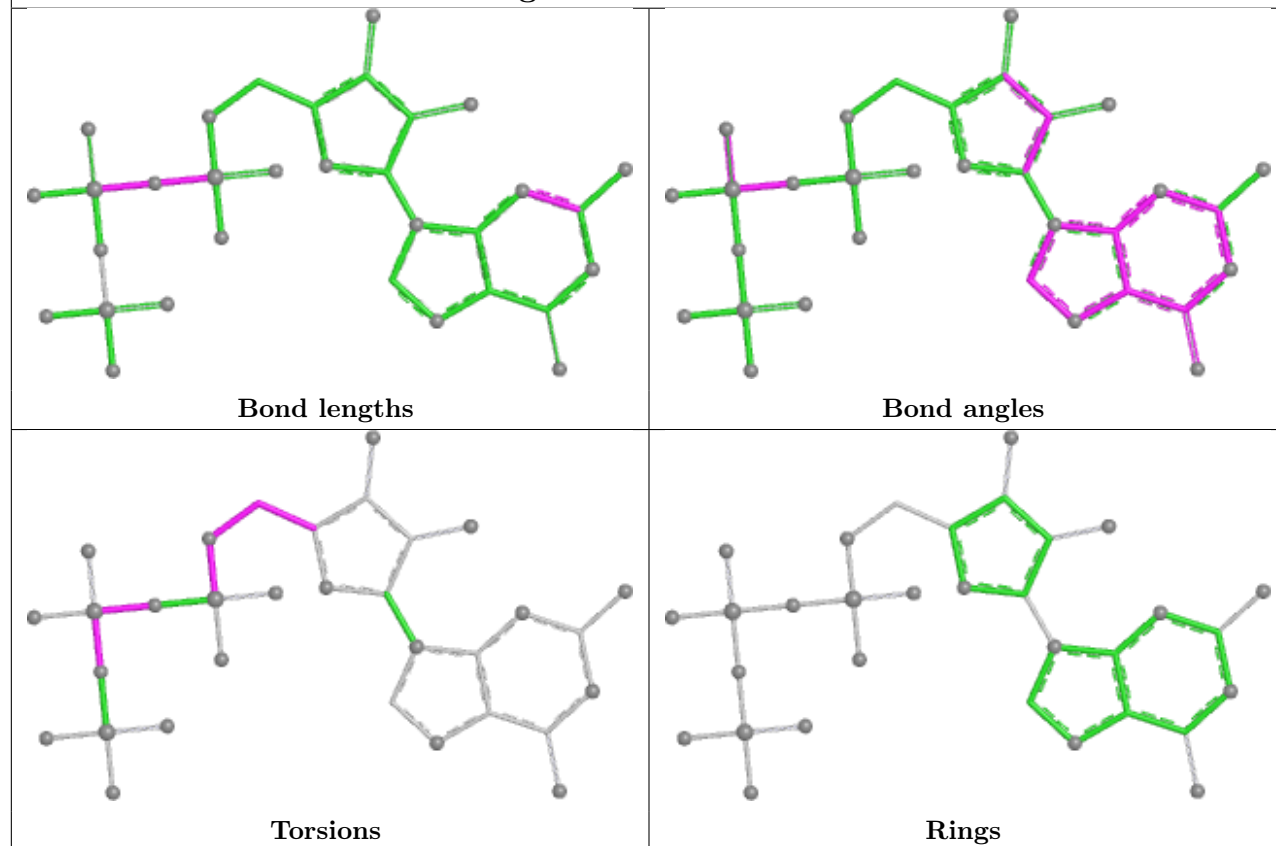


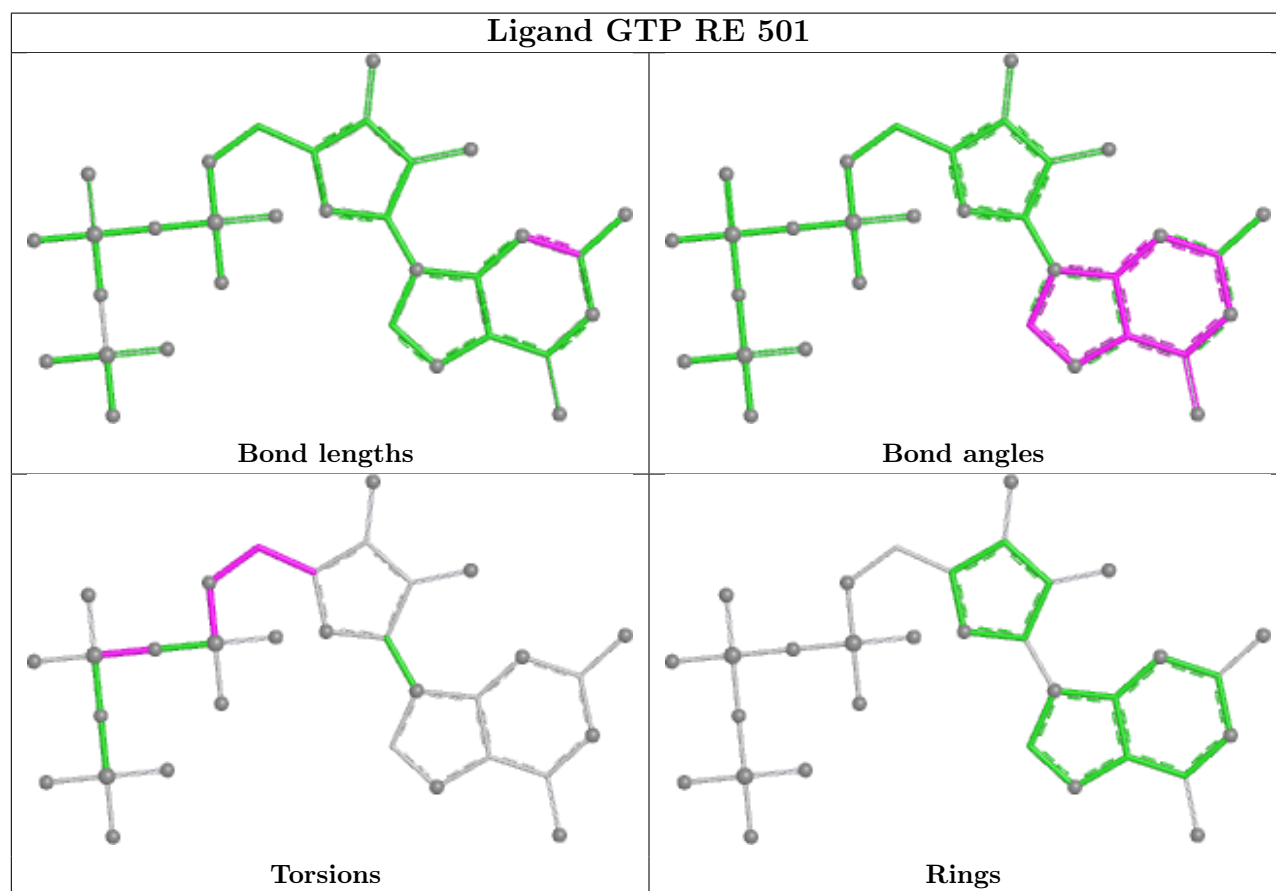
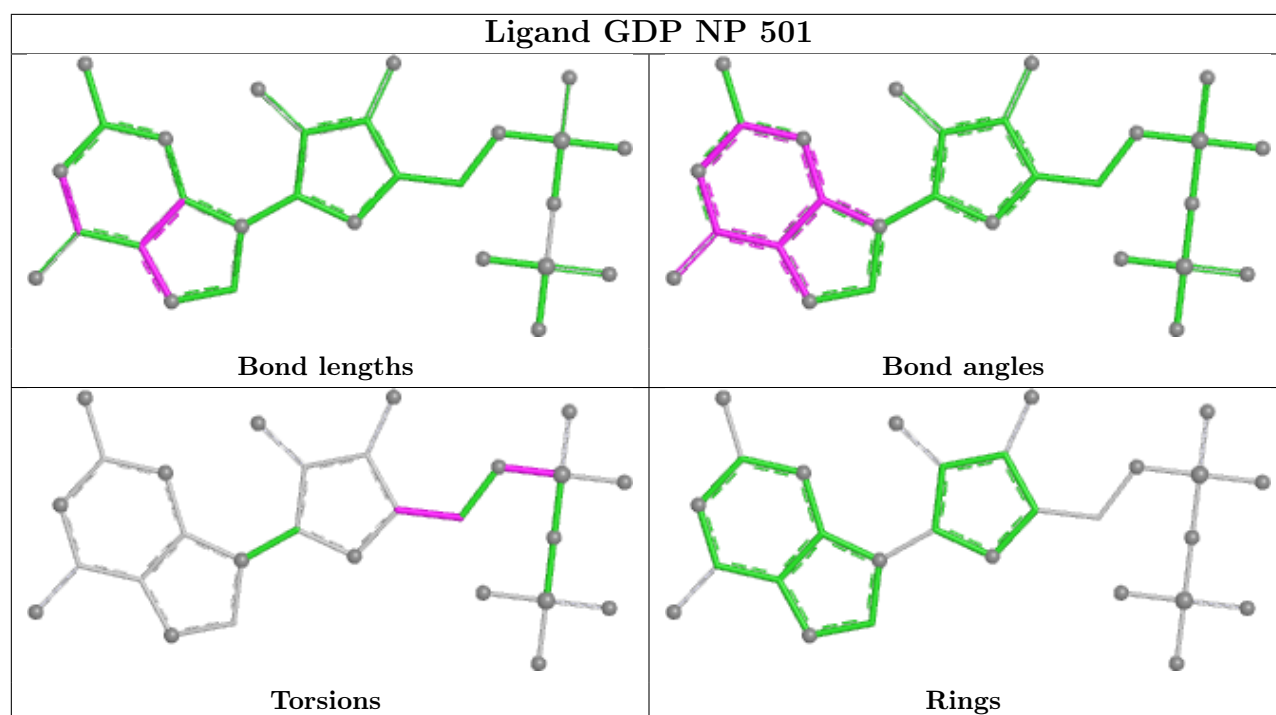


Ligand GTP HP 501

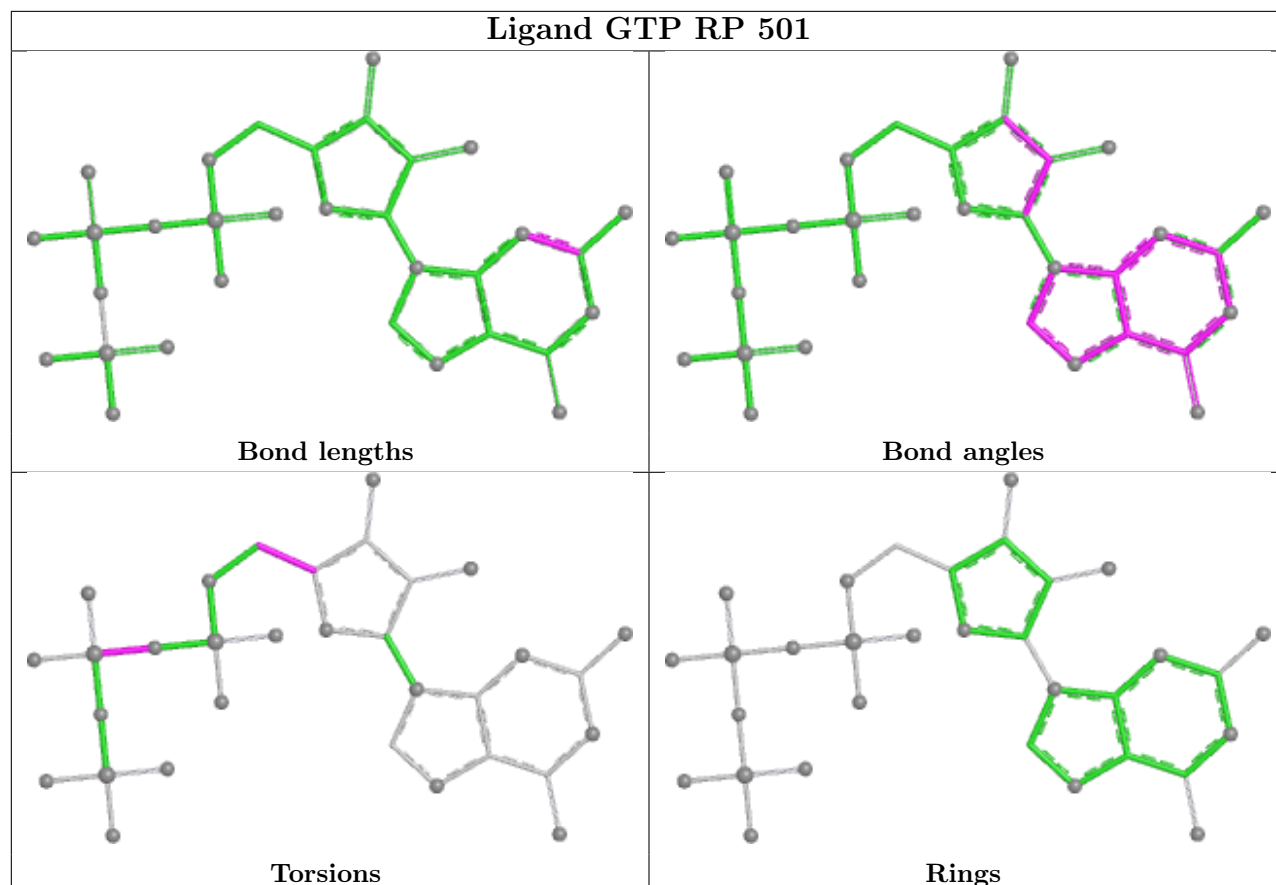


Ligand GTP VF 501

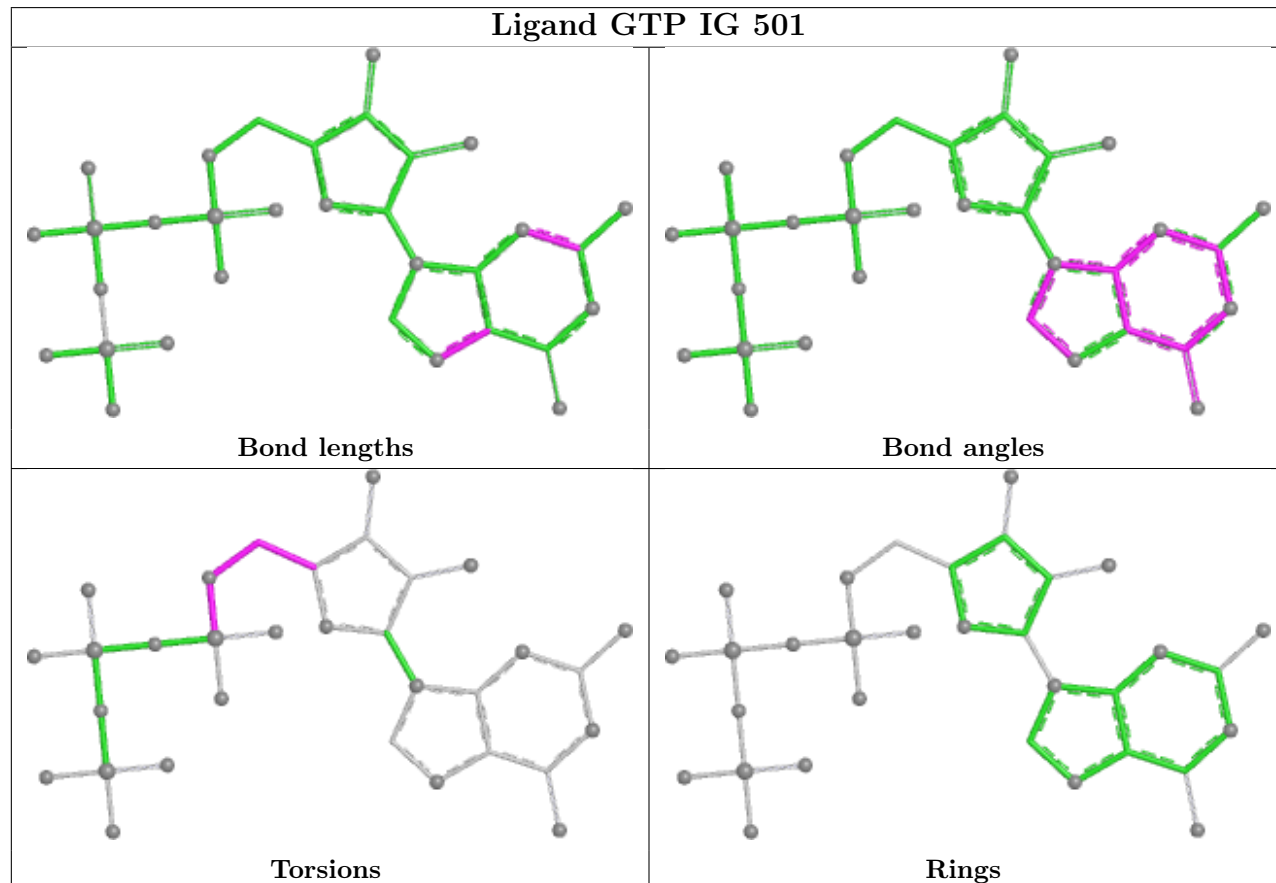




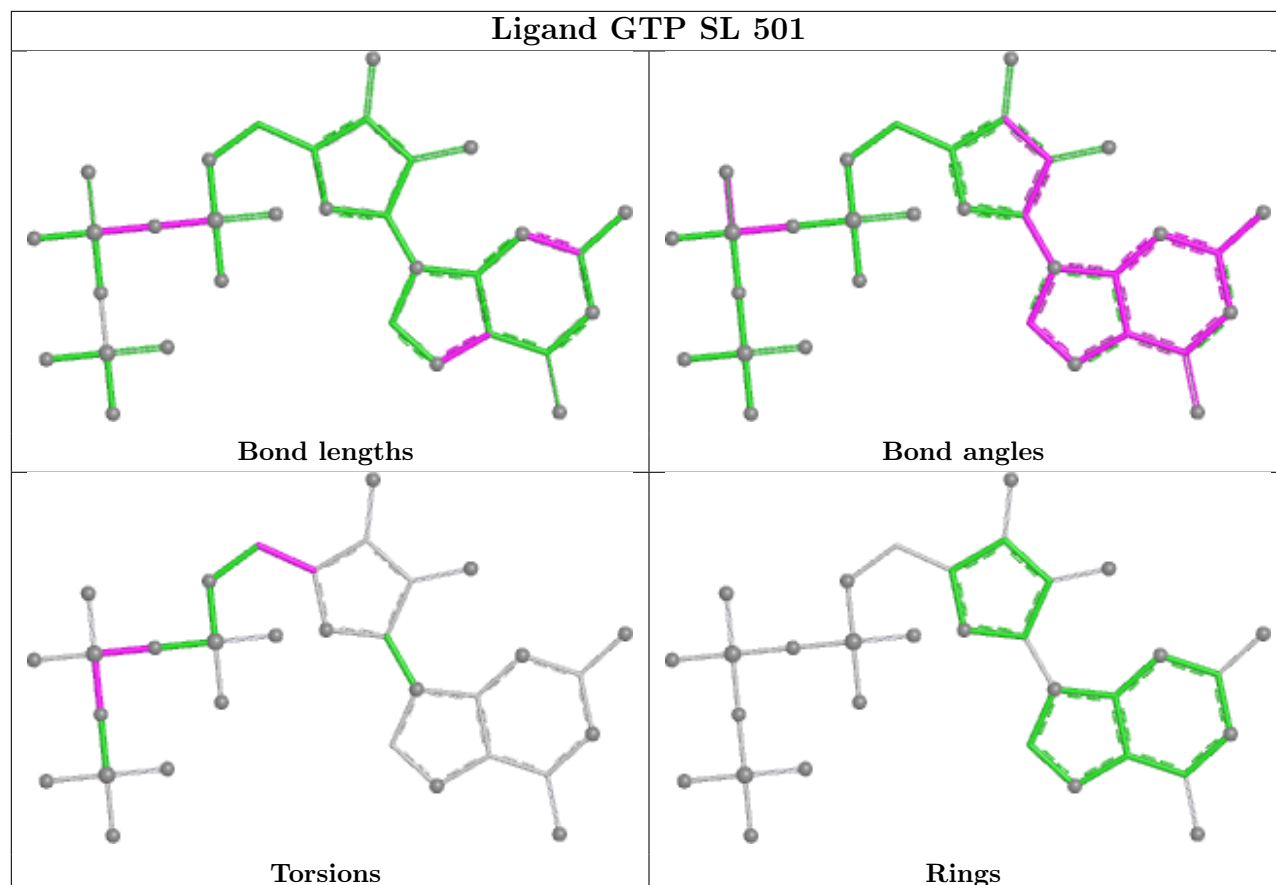
Ligand GTP RP 501



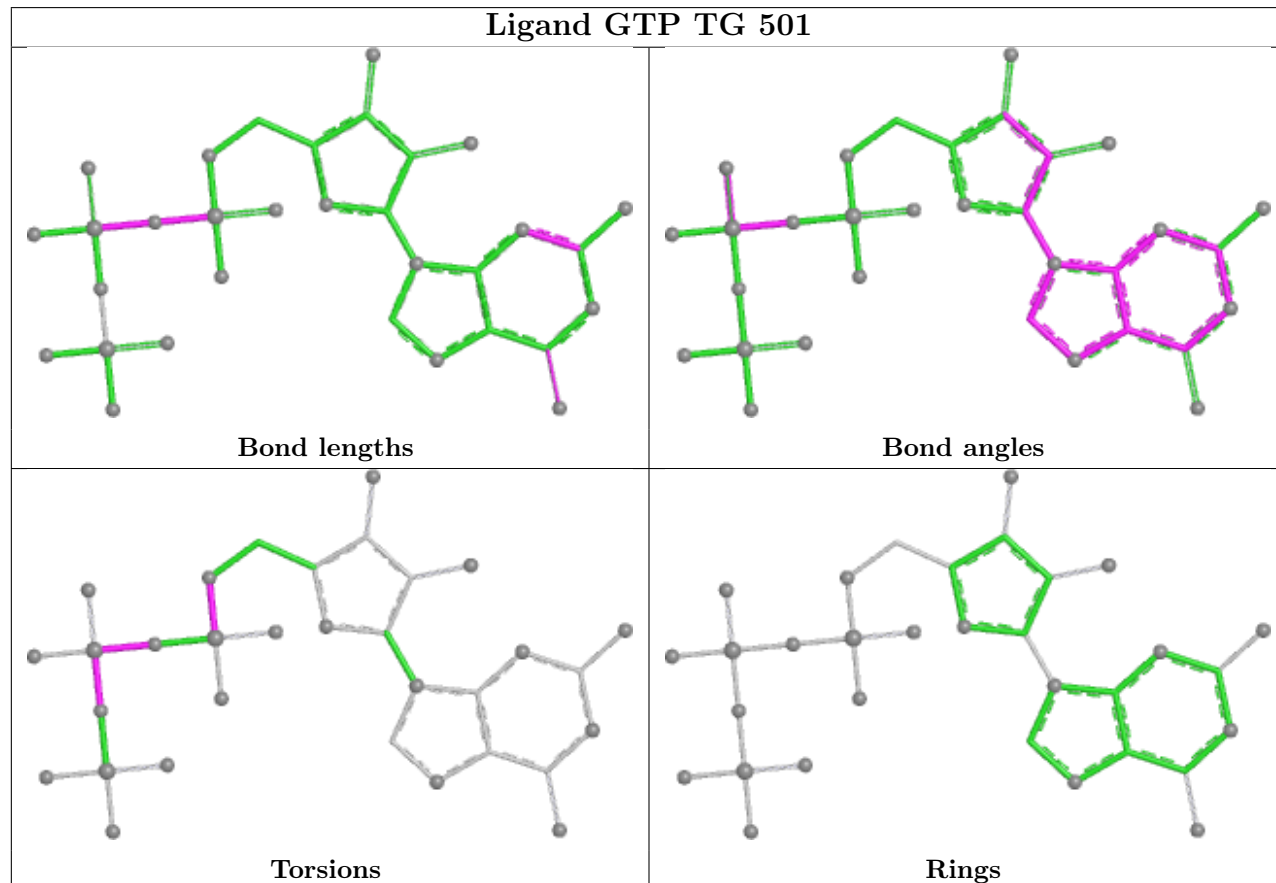
Ligand GTP IG 501

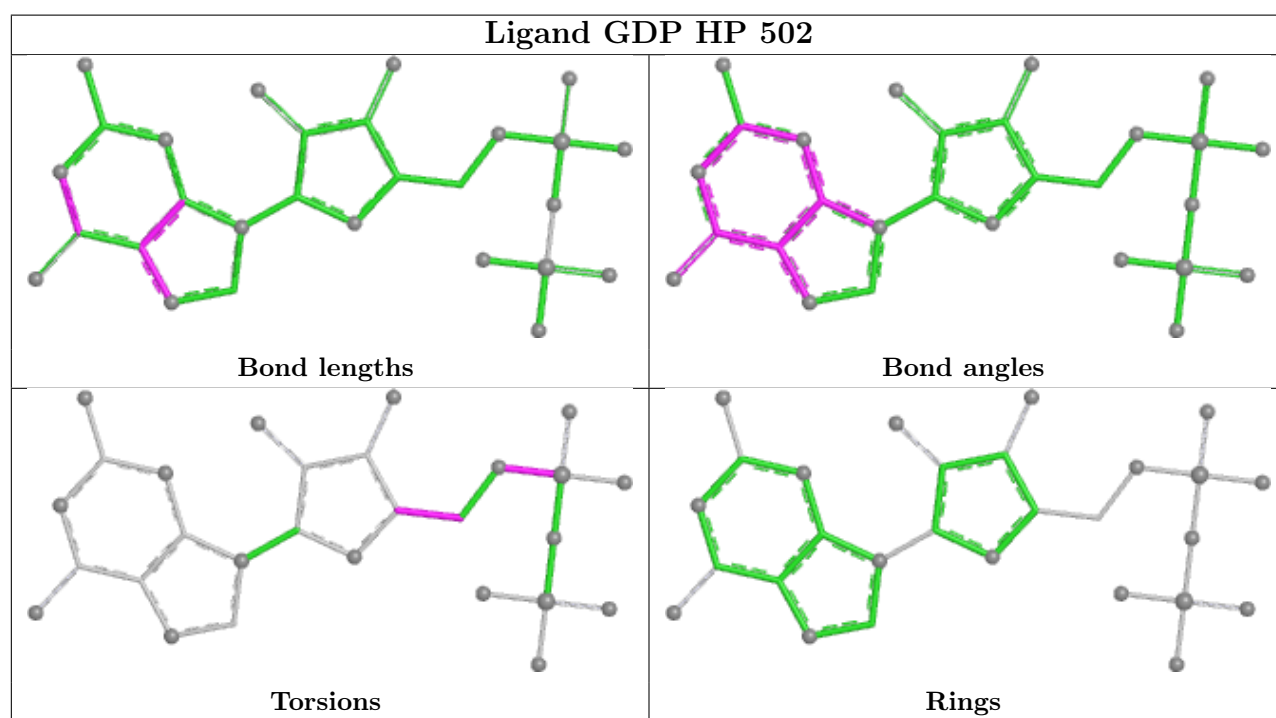
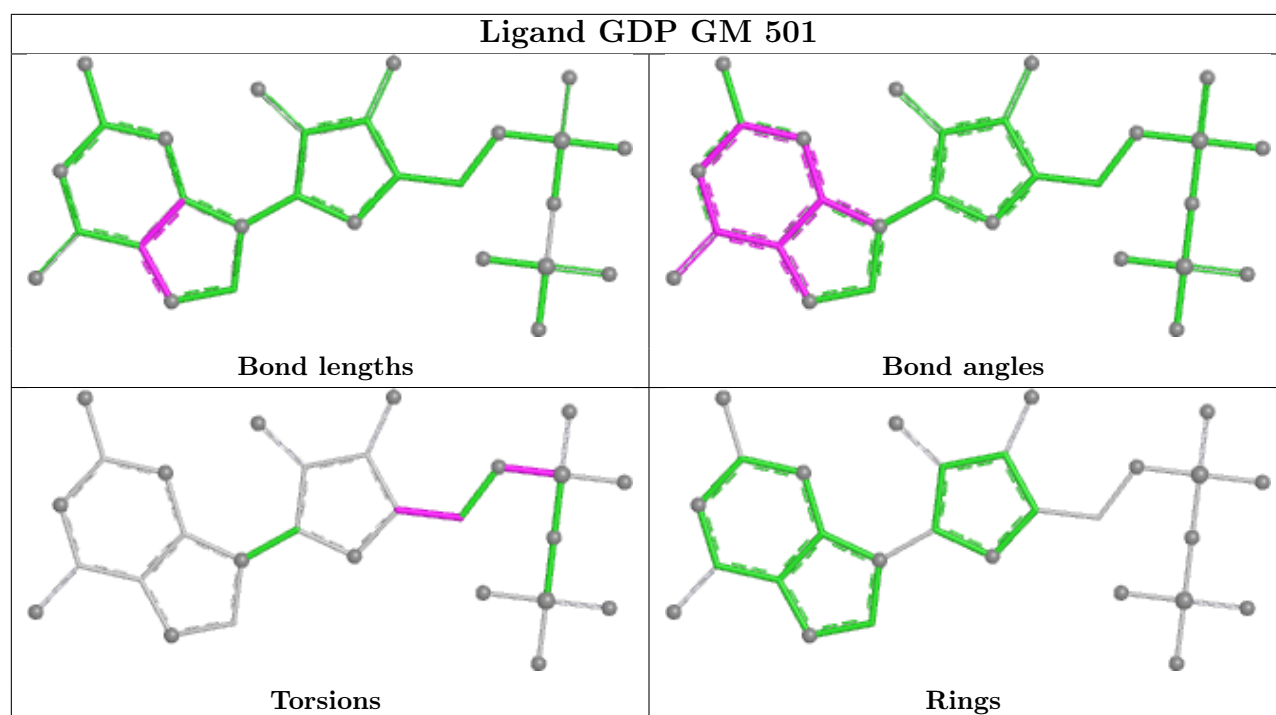


Ligand GTP SL 501

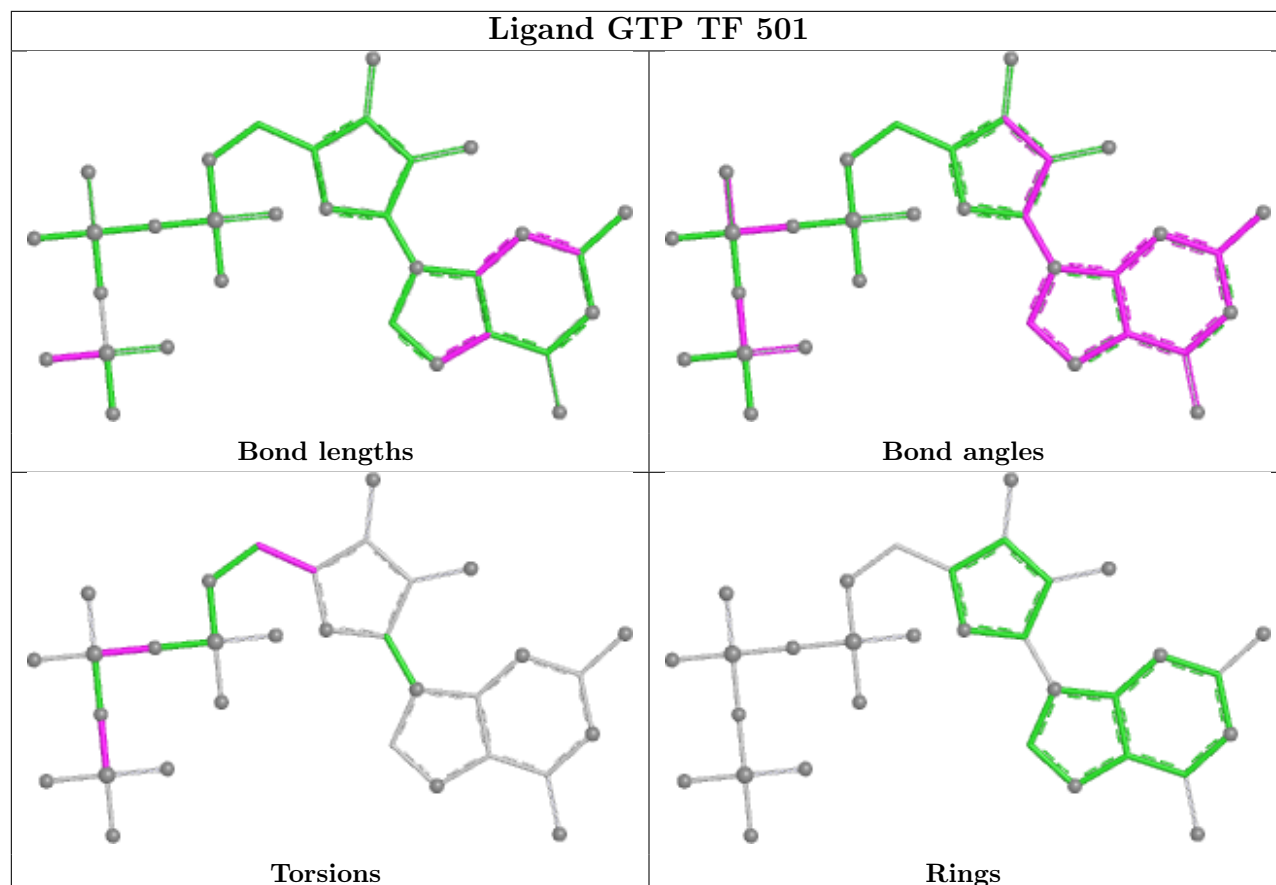


Ligand GTP TG 501

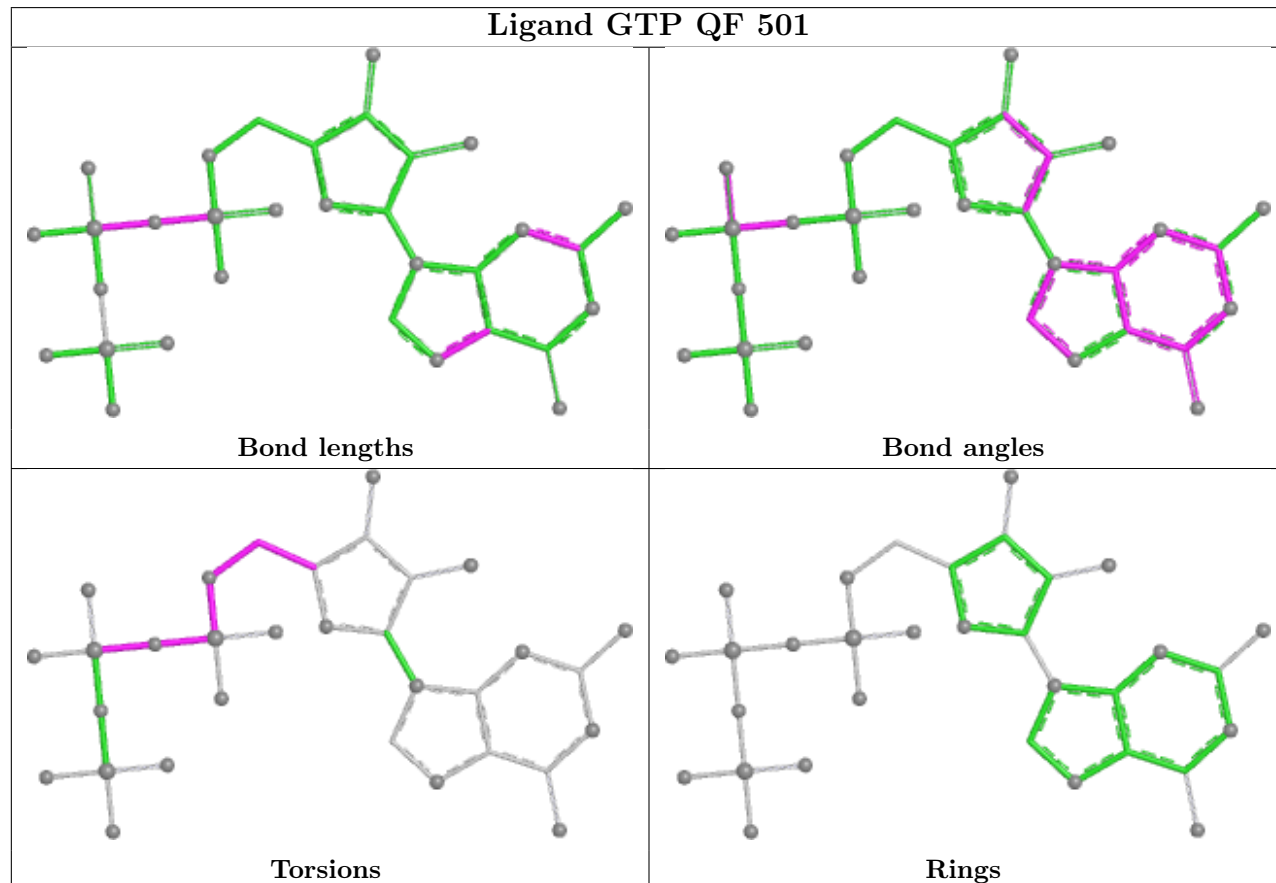




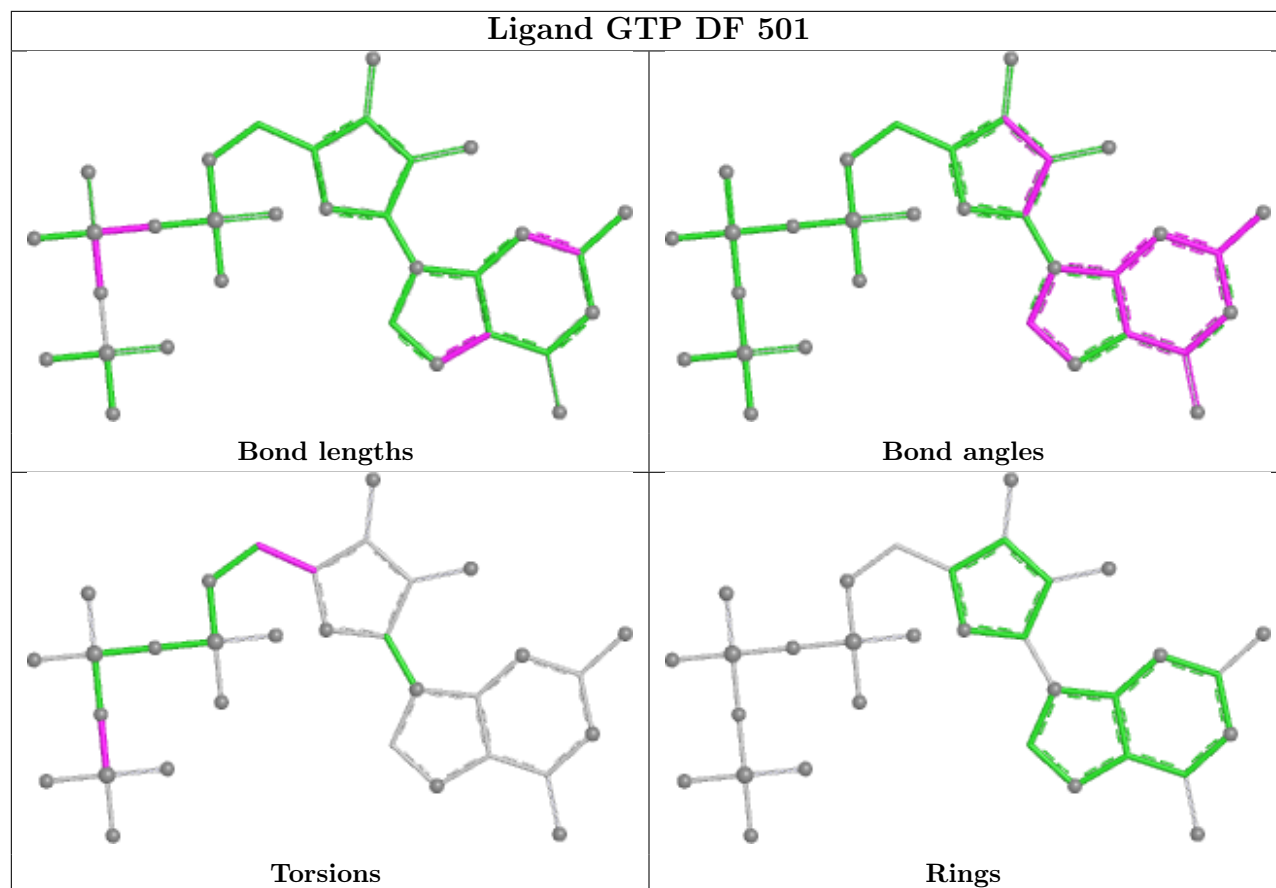
Ligand GTP TF 501



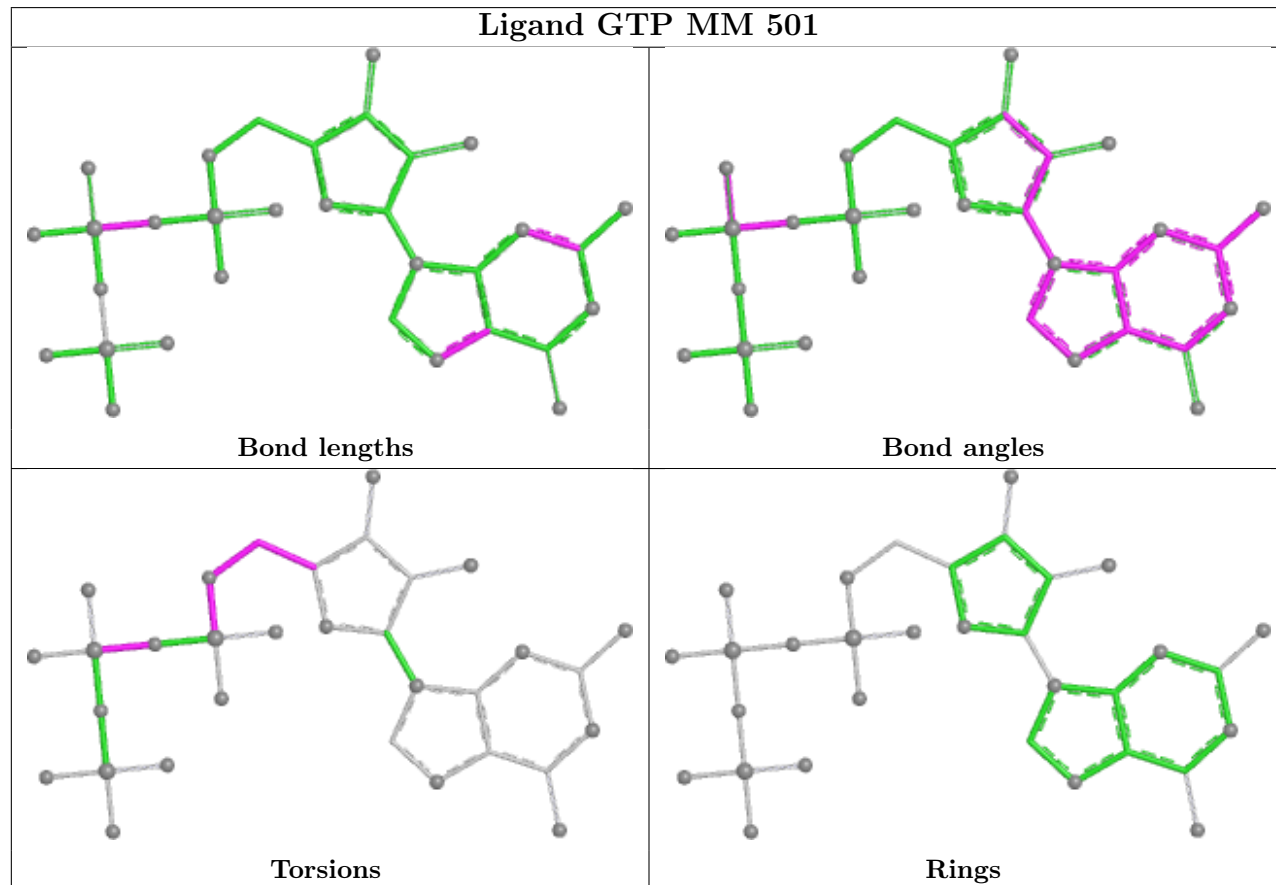
Ligand GTP QF 501

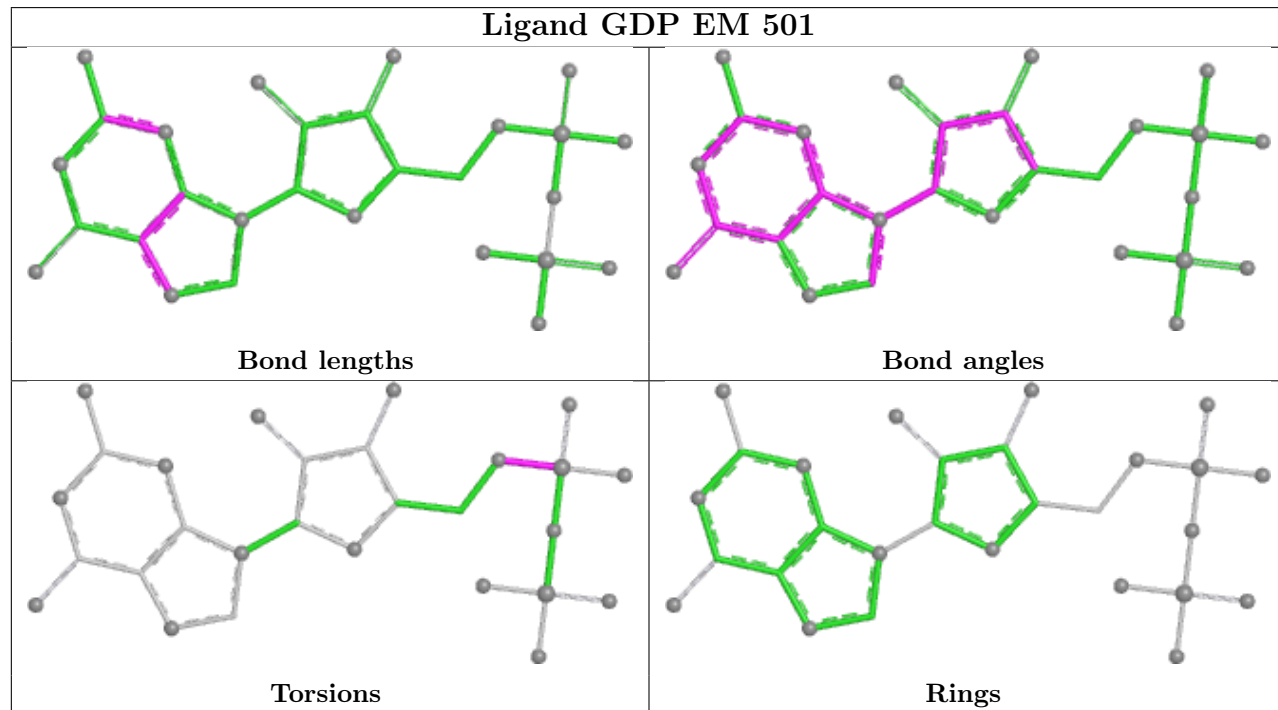
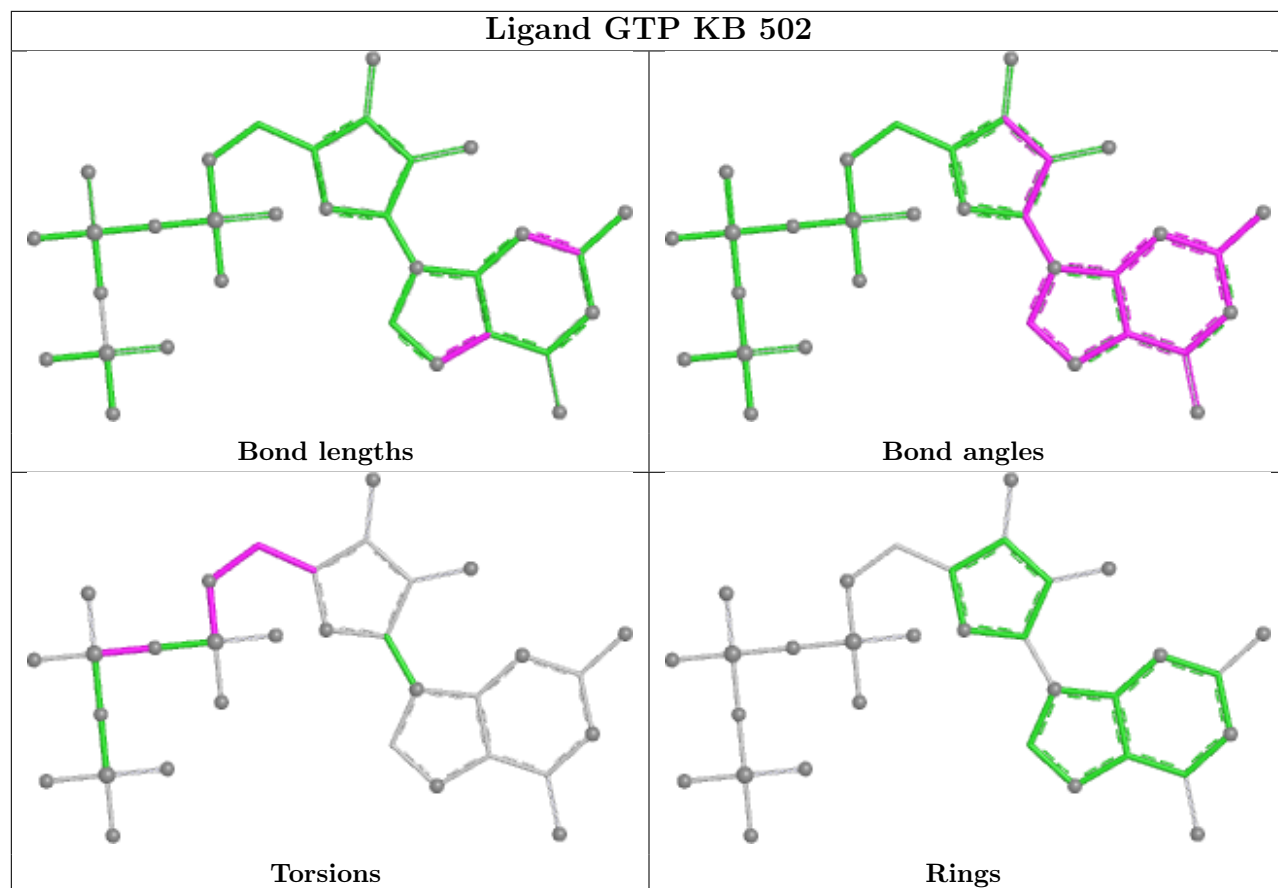


Ligand GTP DF 501

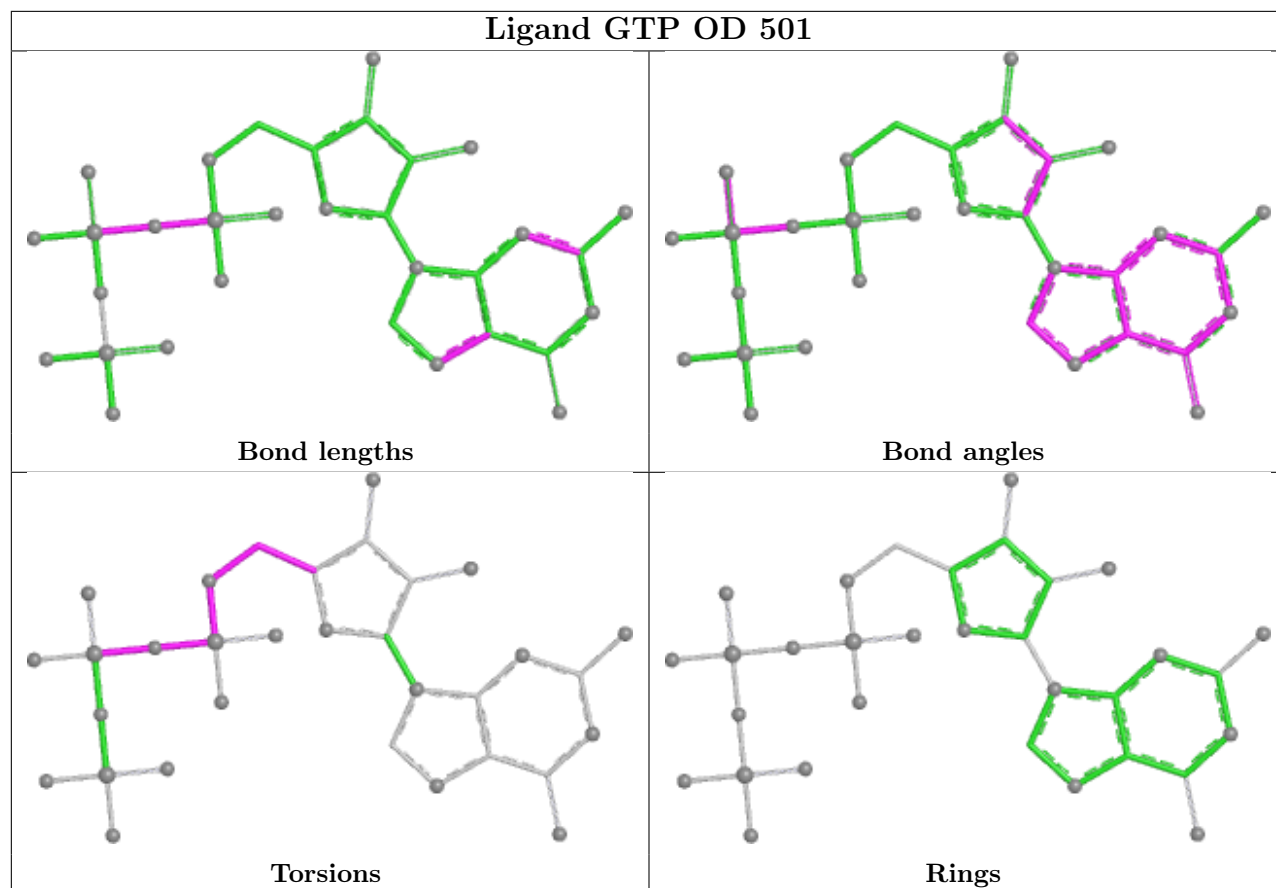


Ligand GTP MM 501

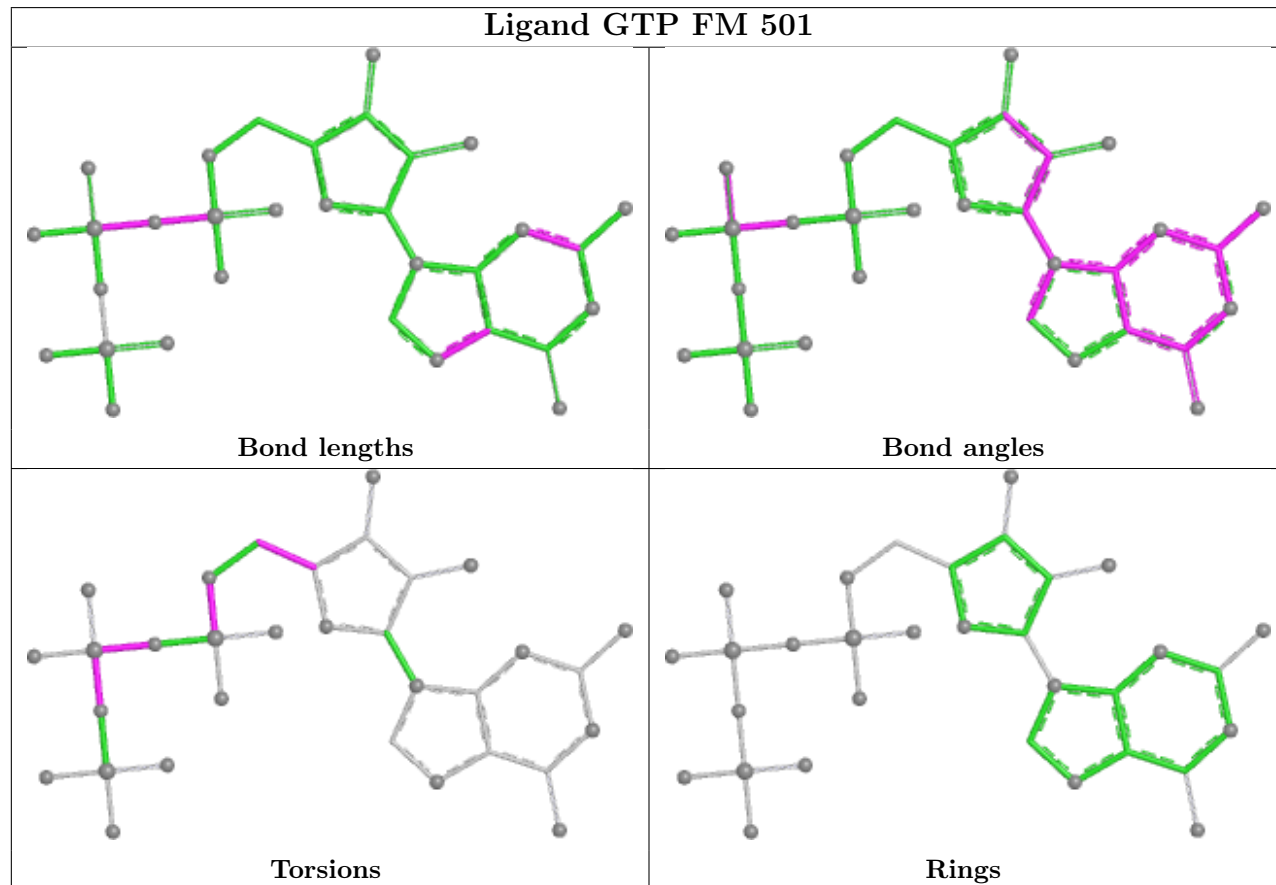


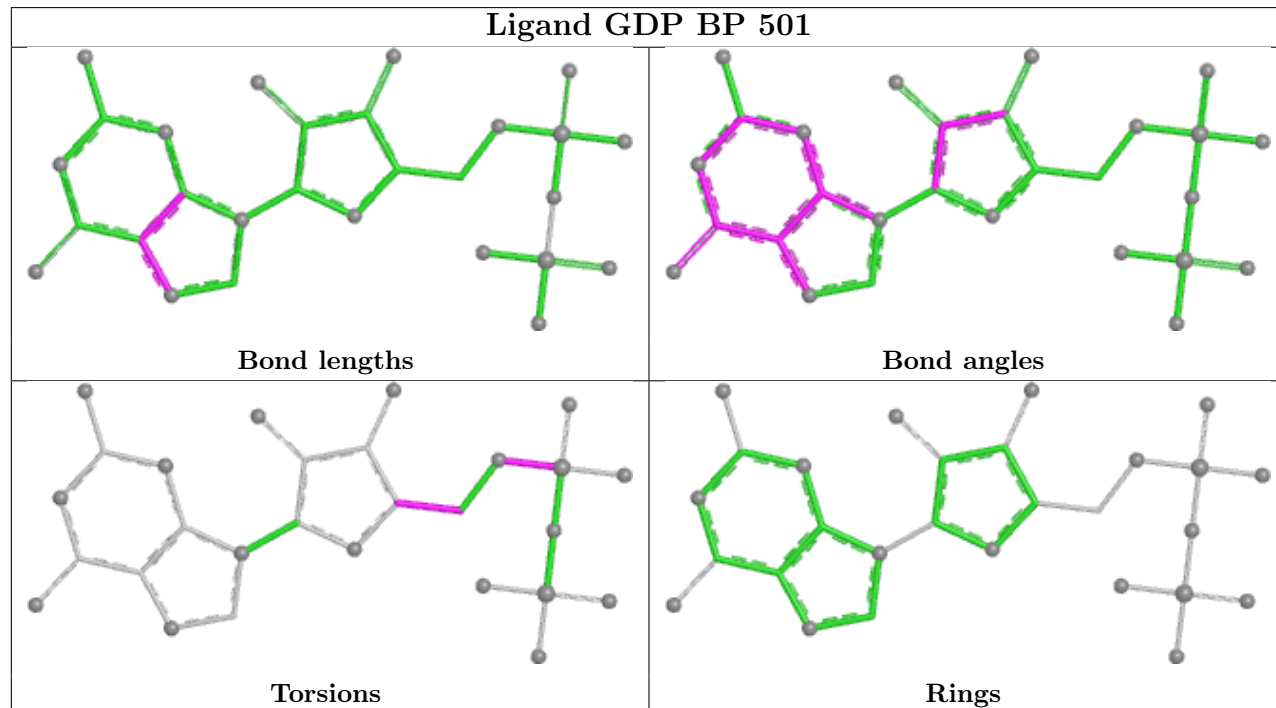
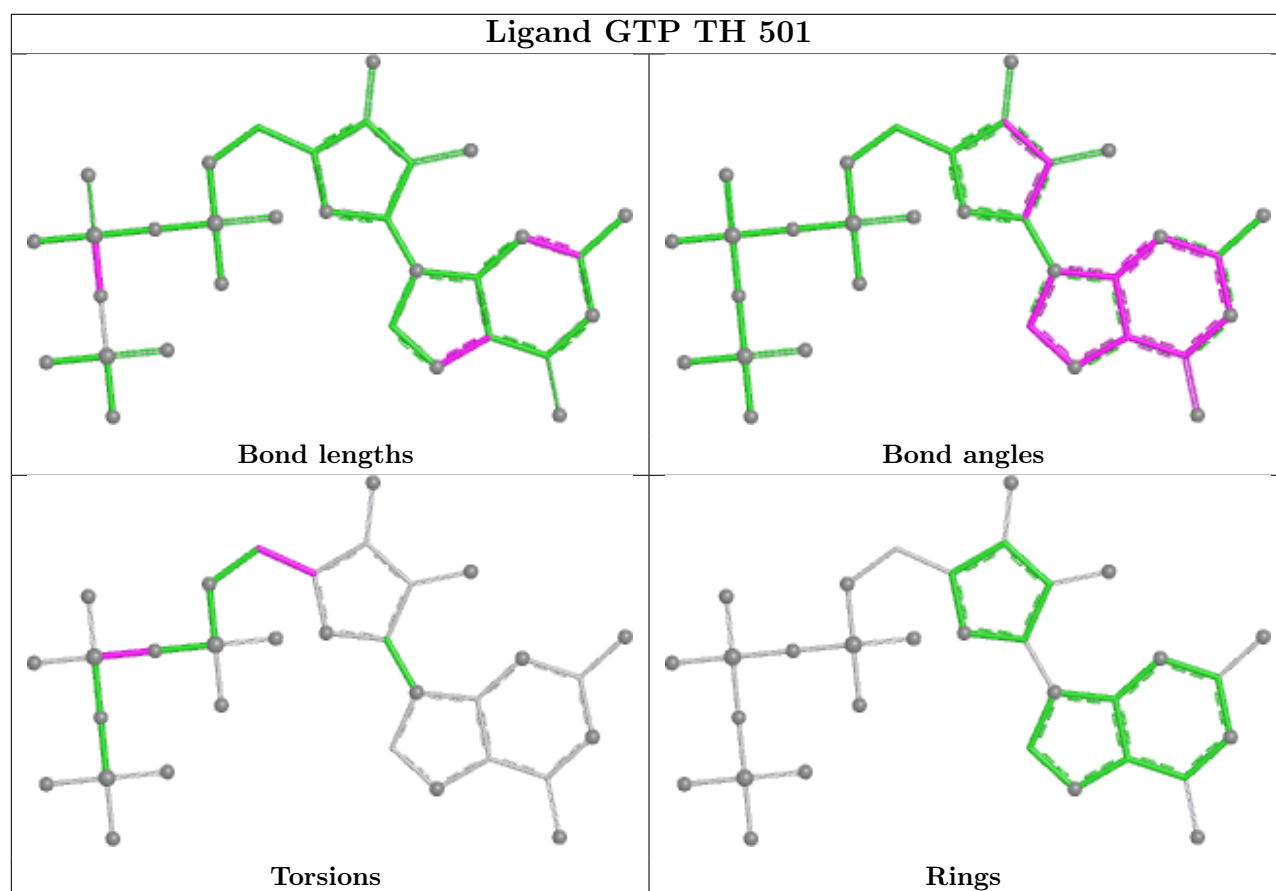


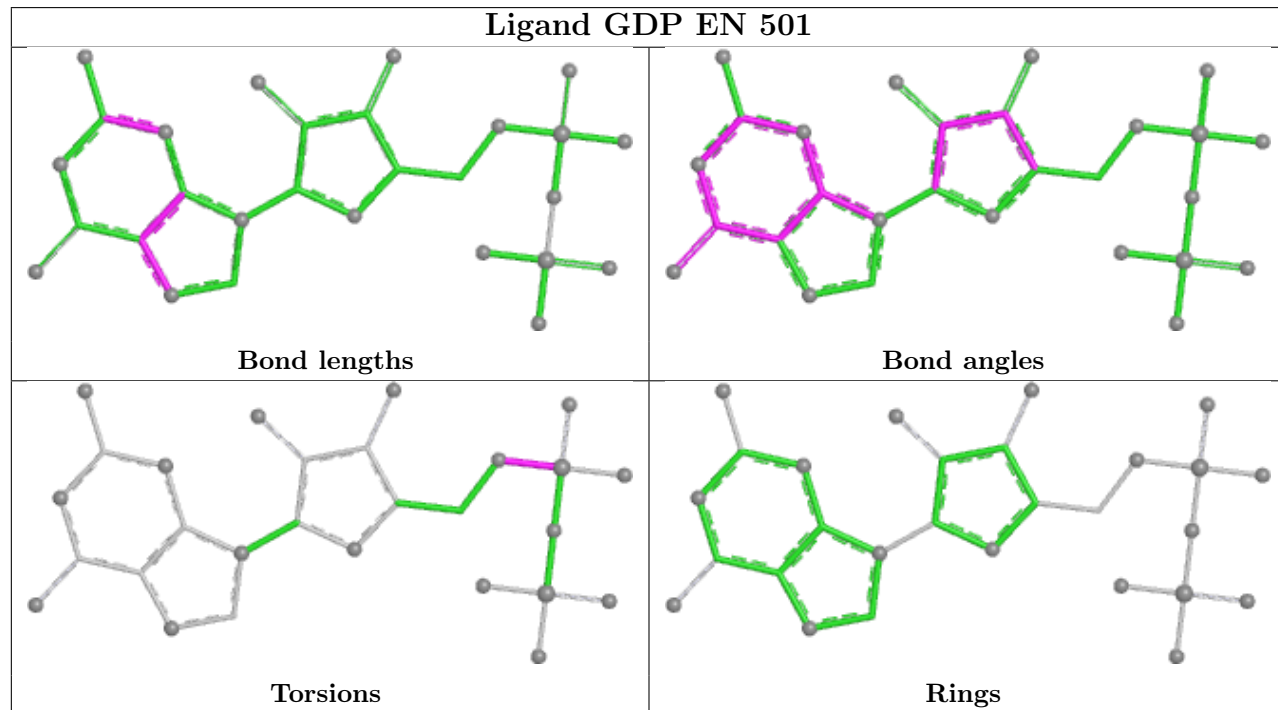
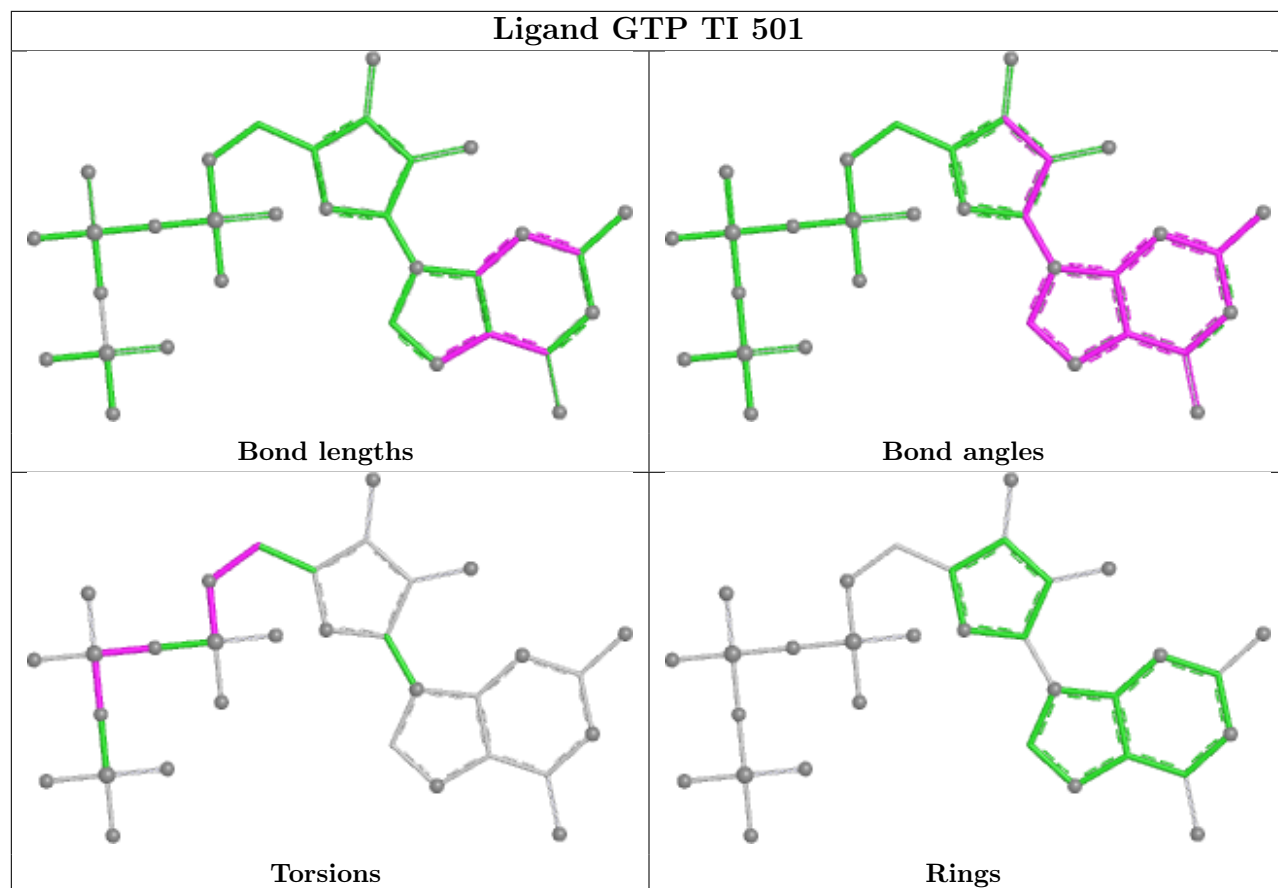
Ligand GTP OD 501

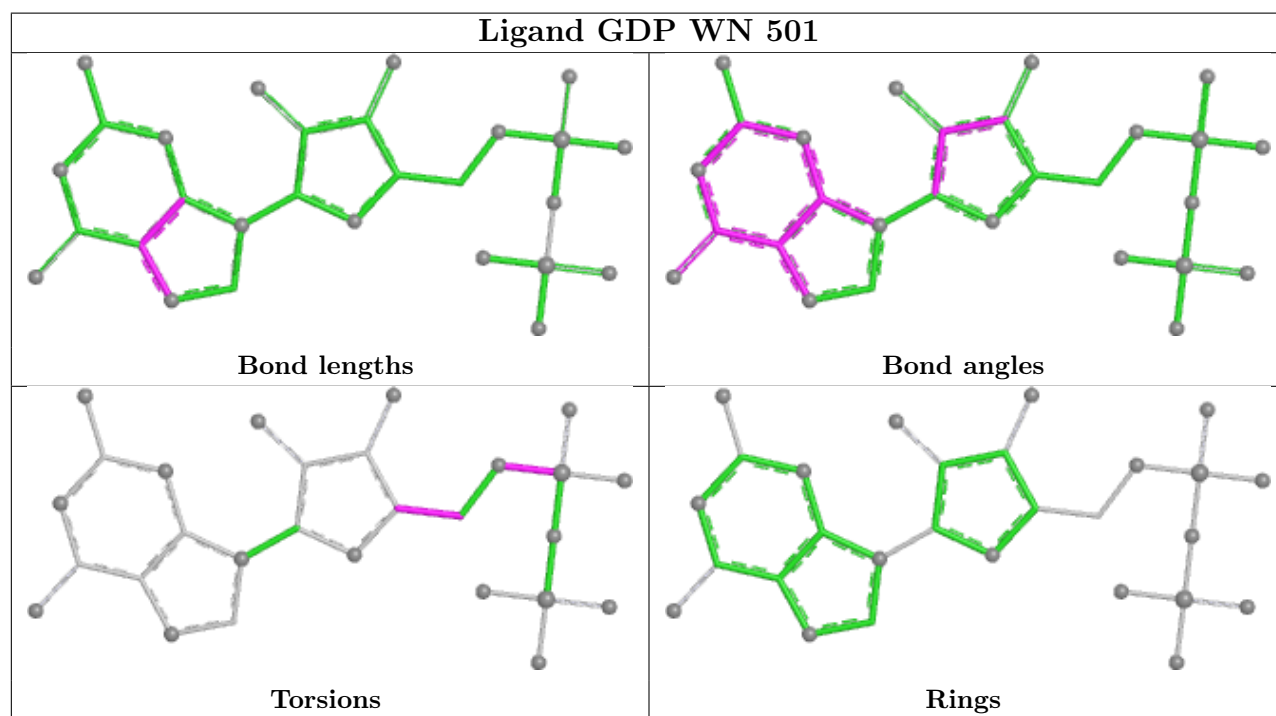
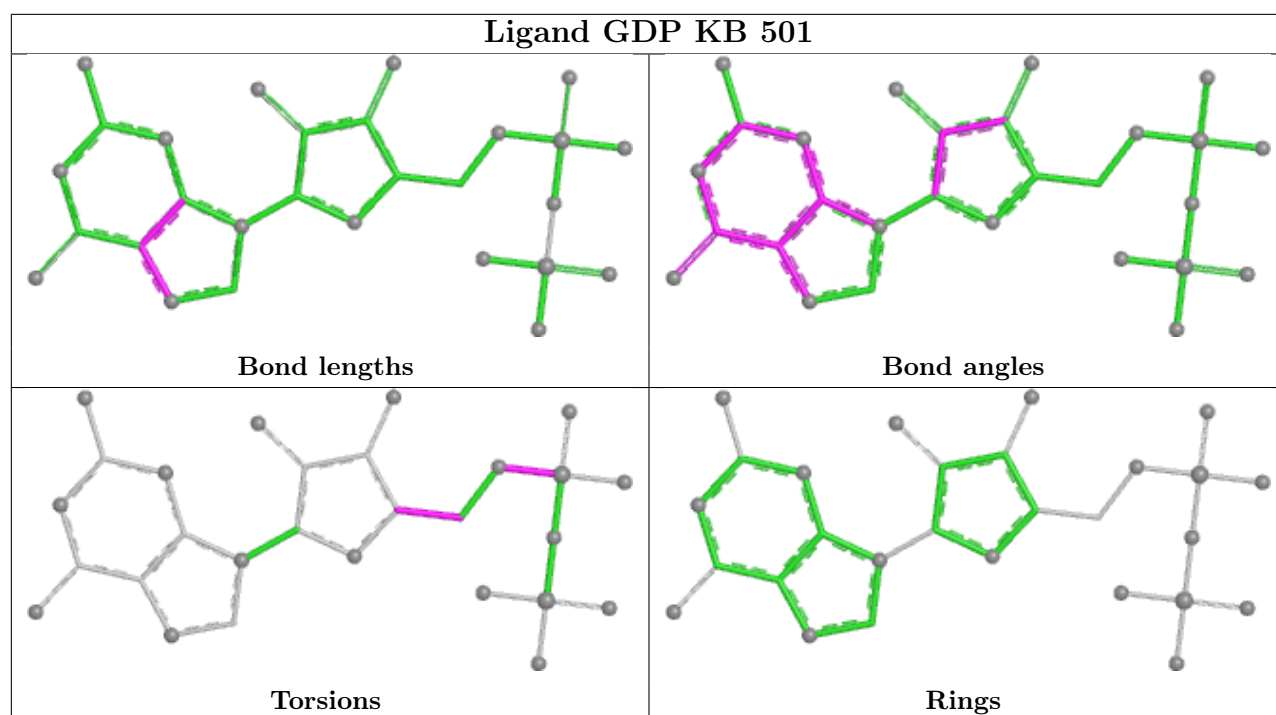


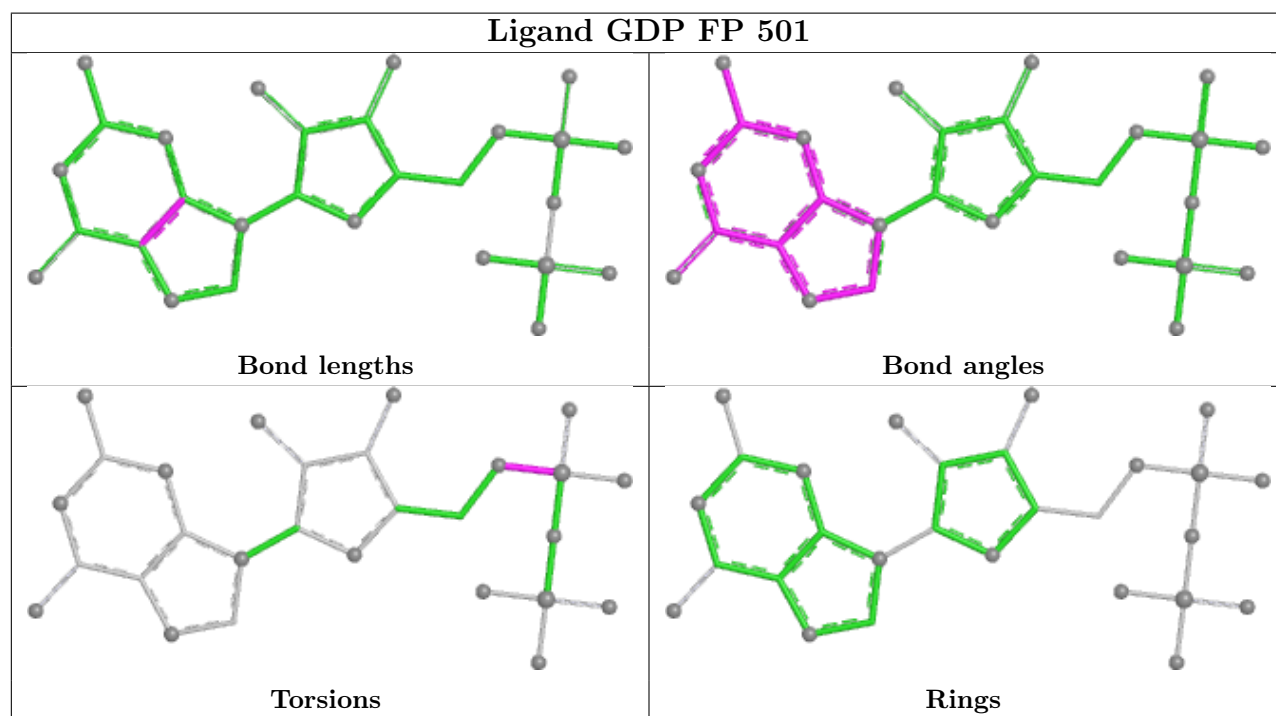
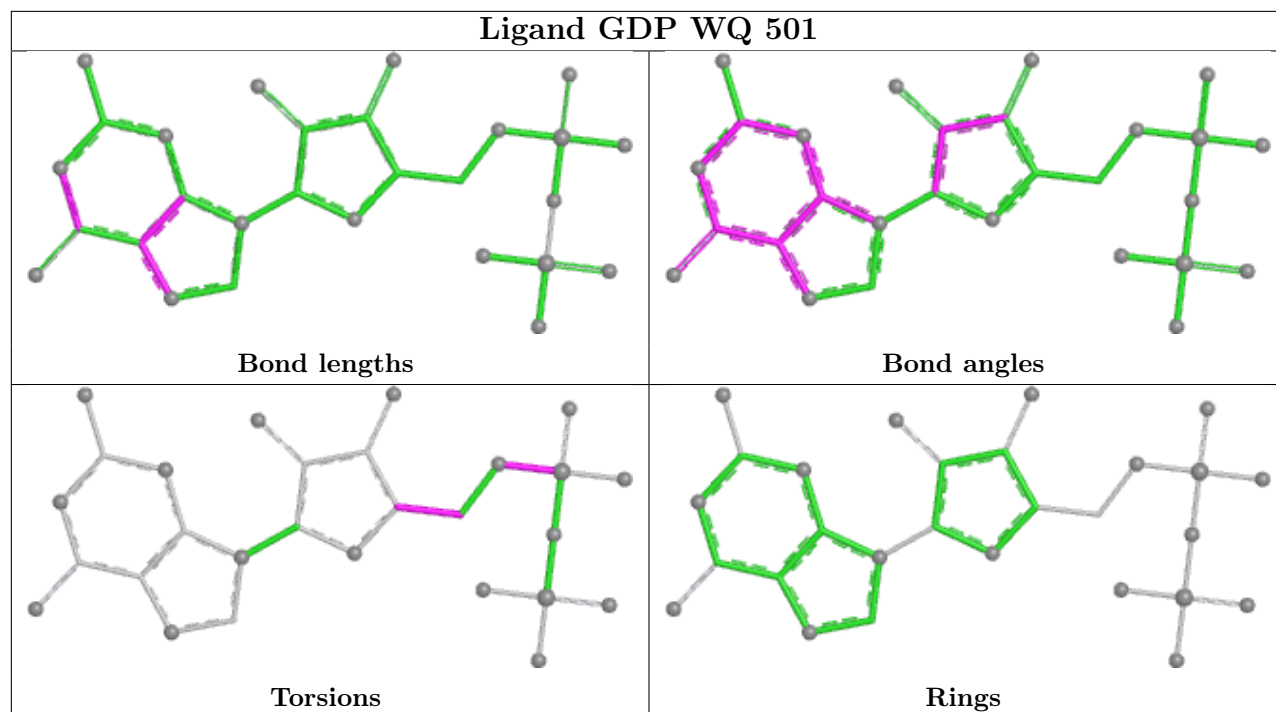
Ligand GTP FM 501

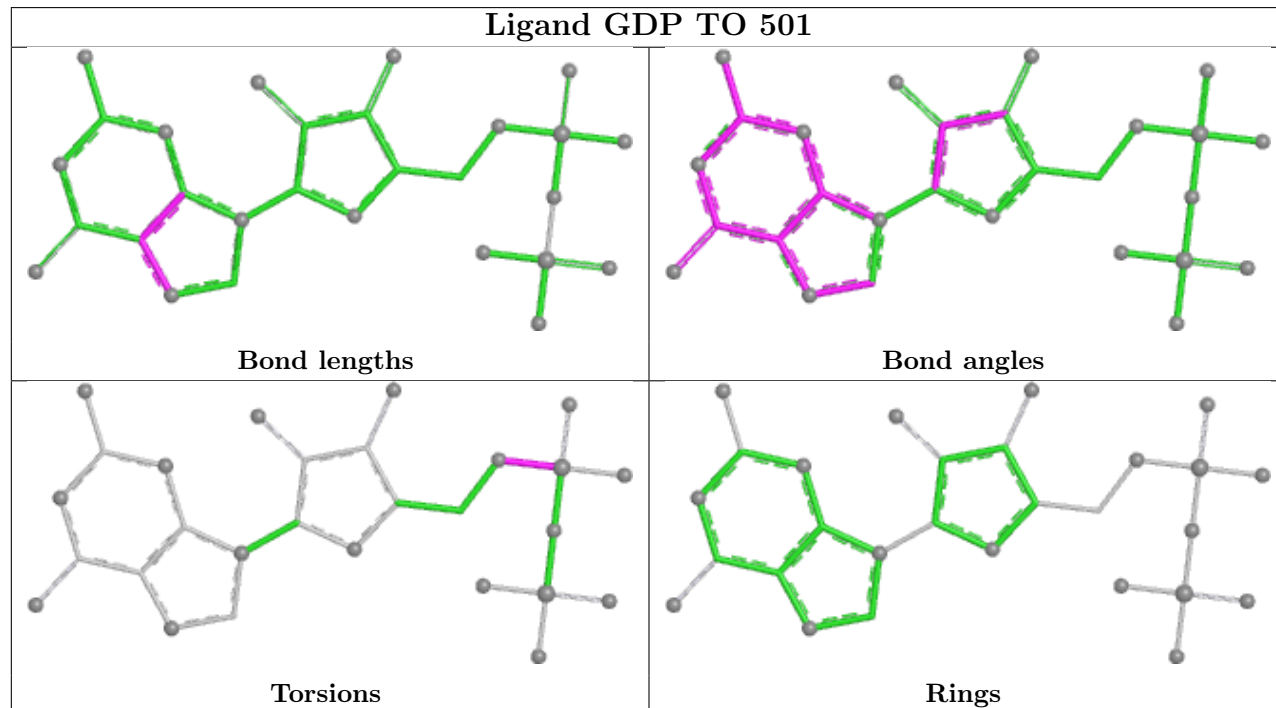
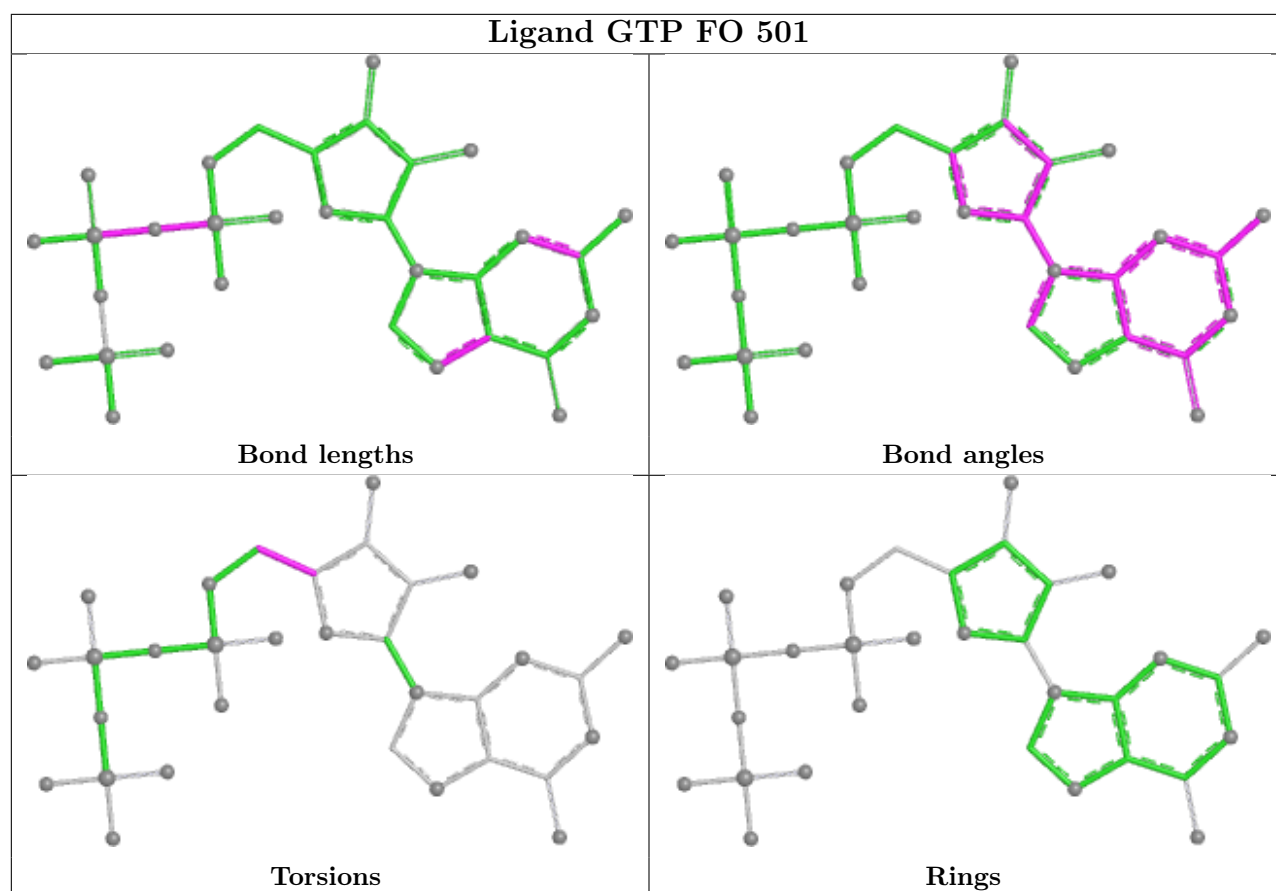


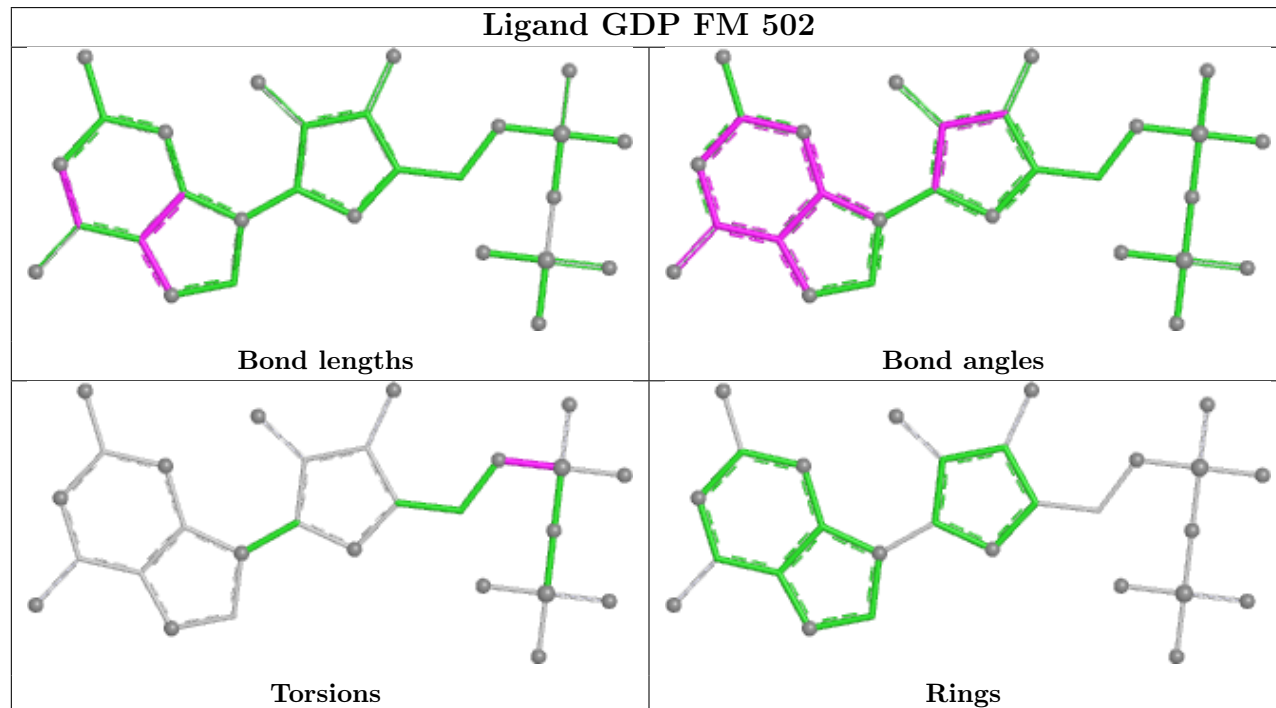
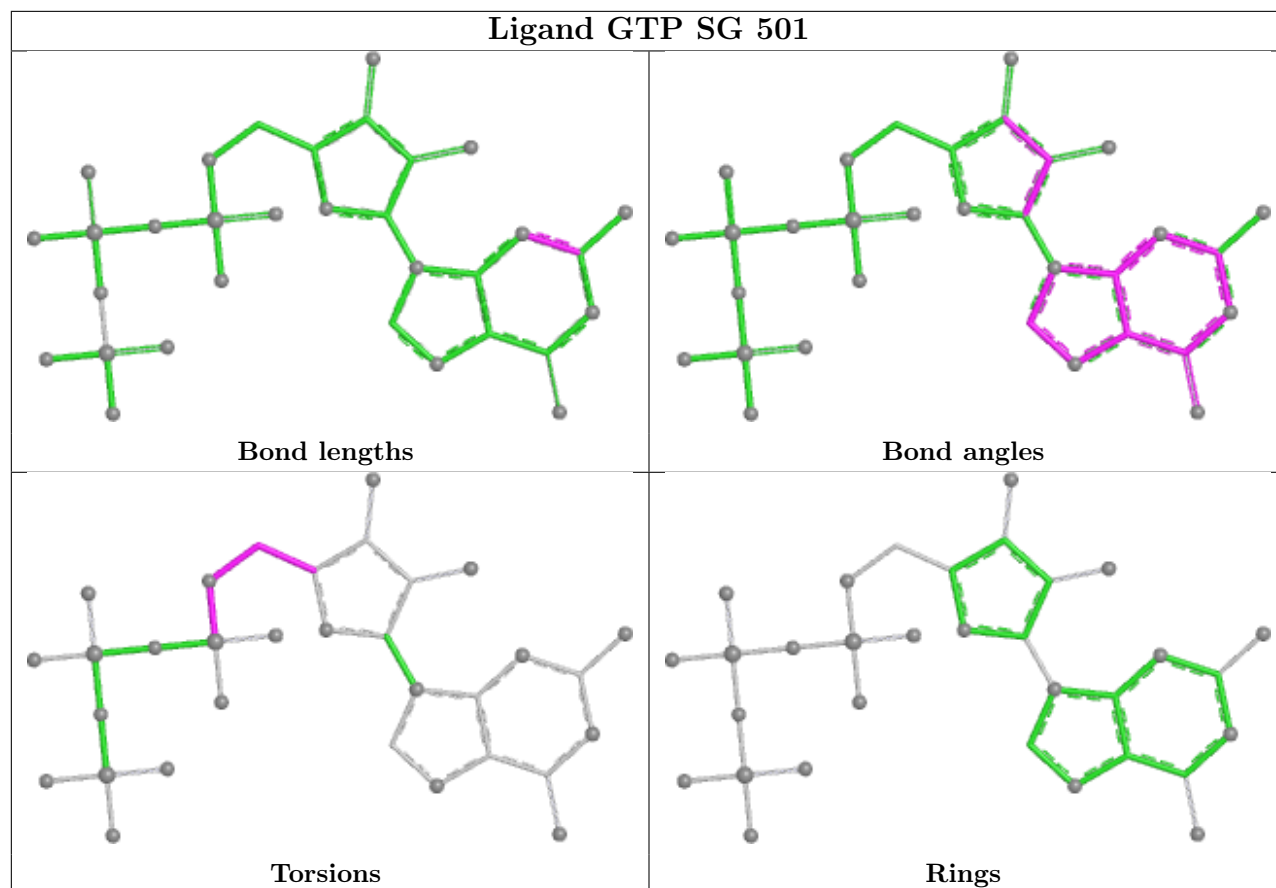




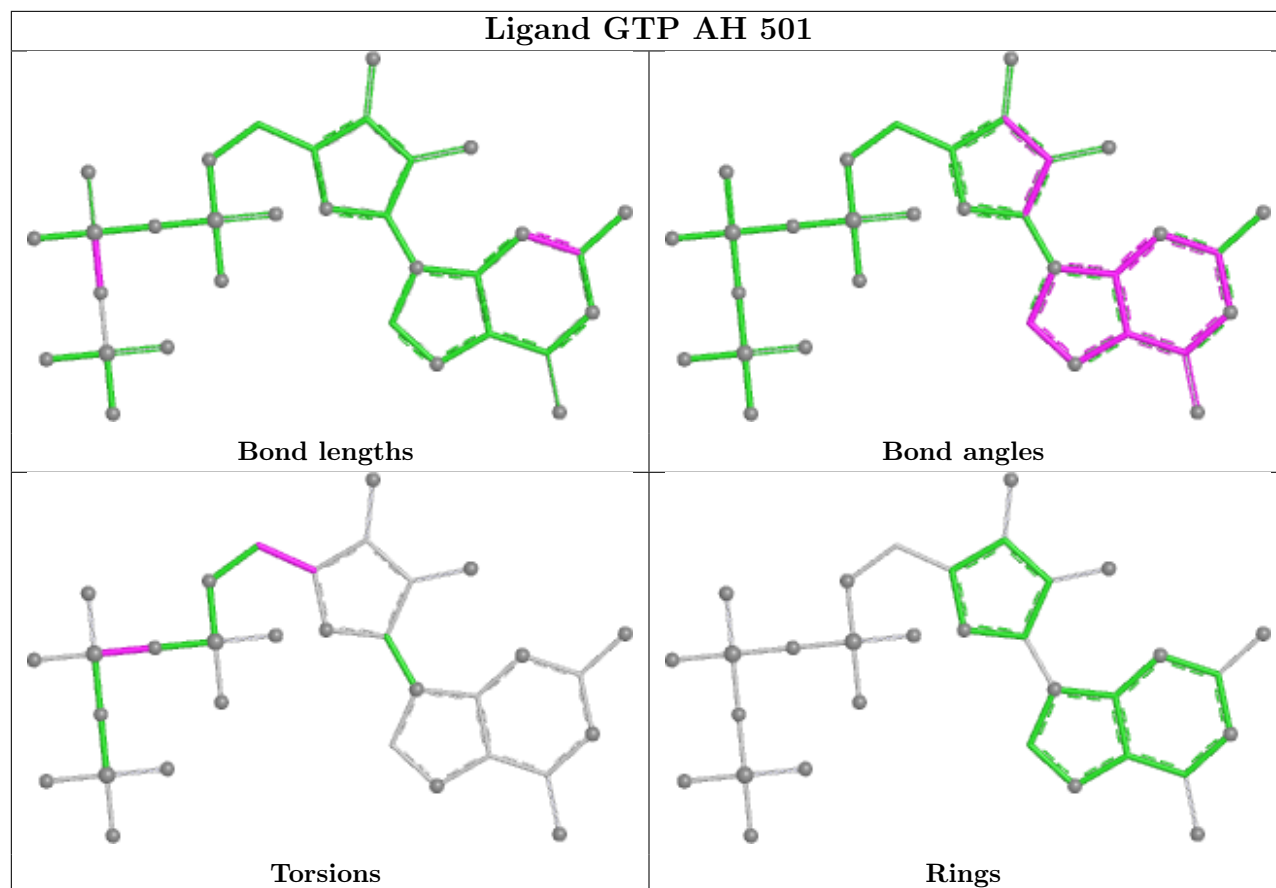




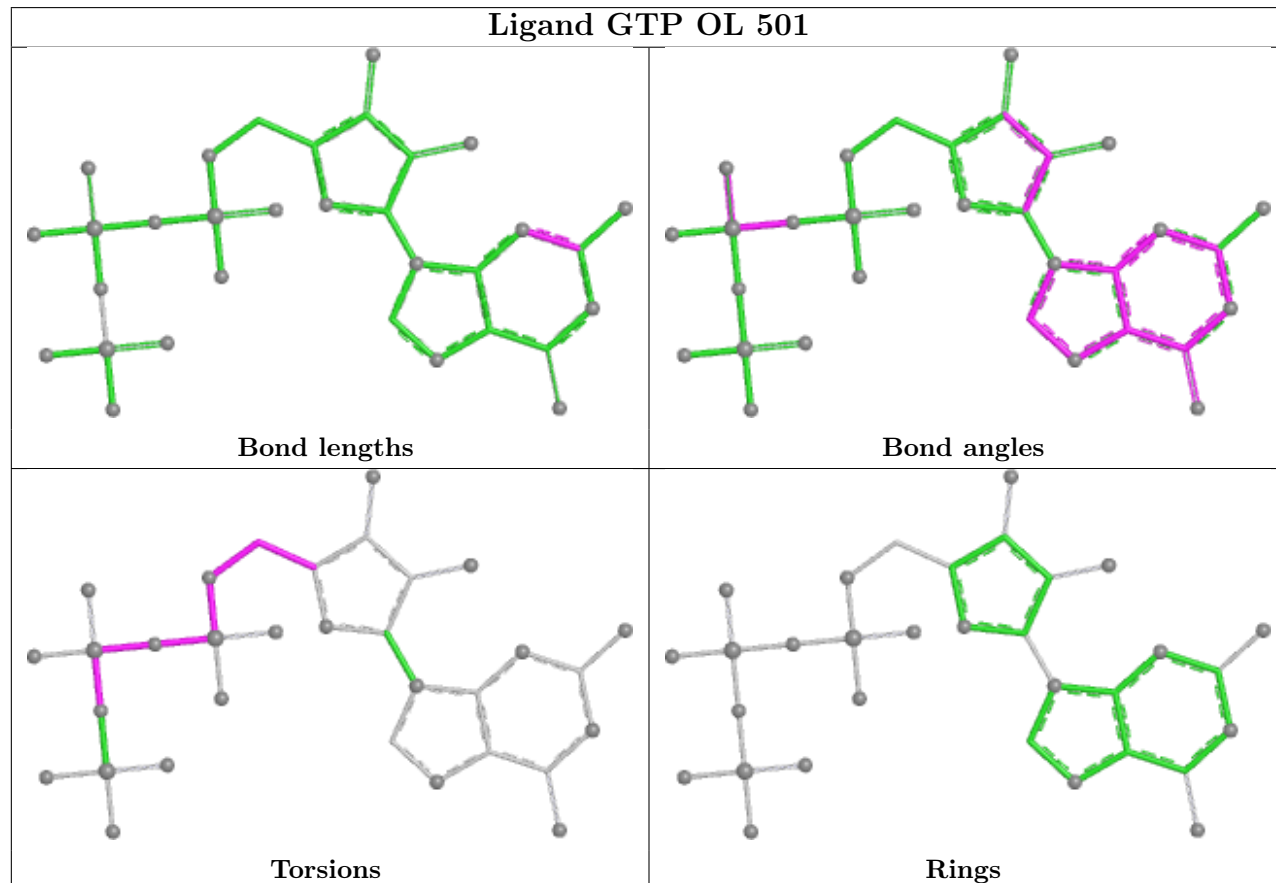


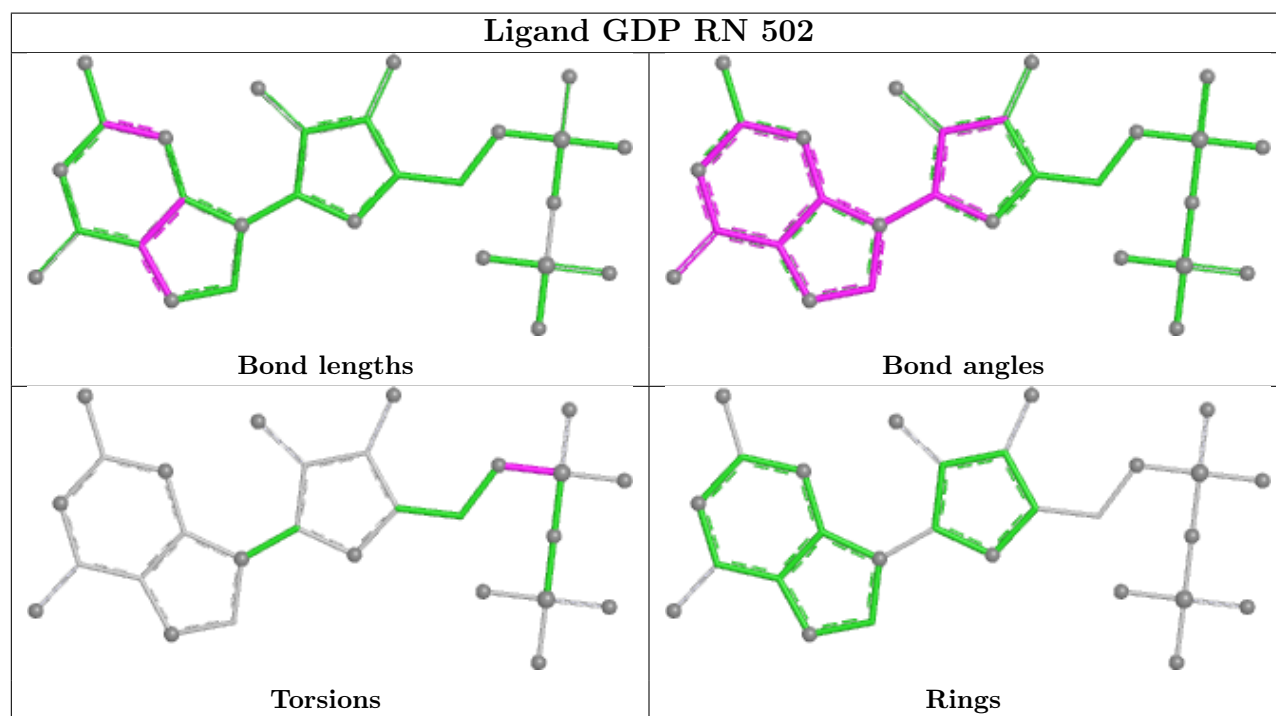
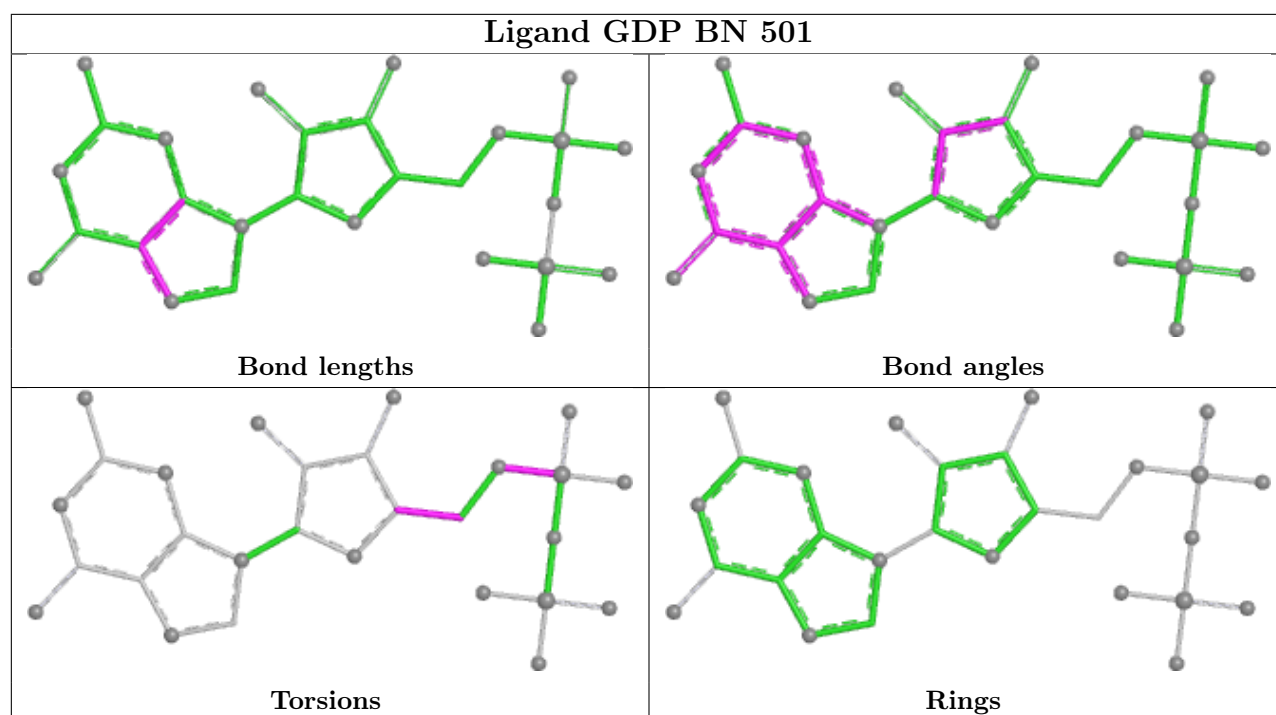


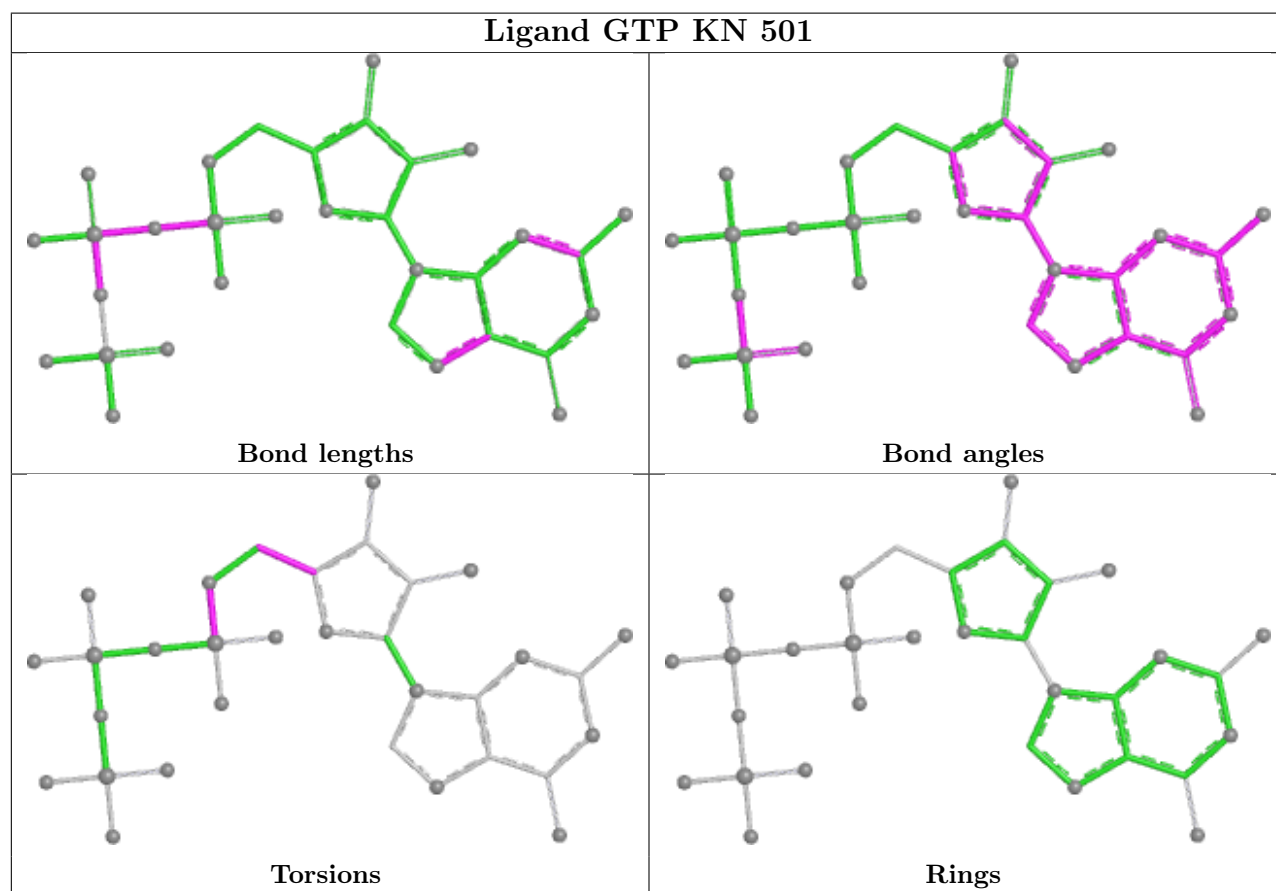
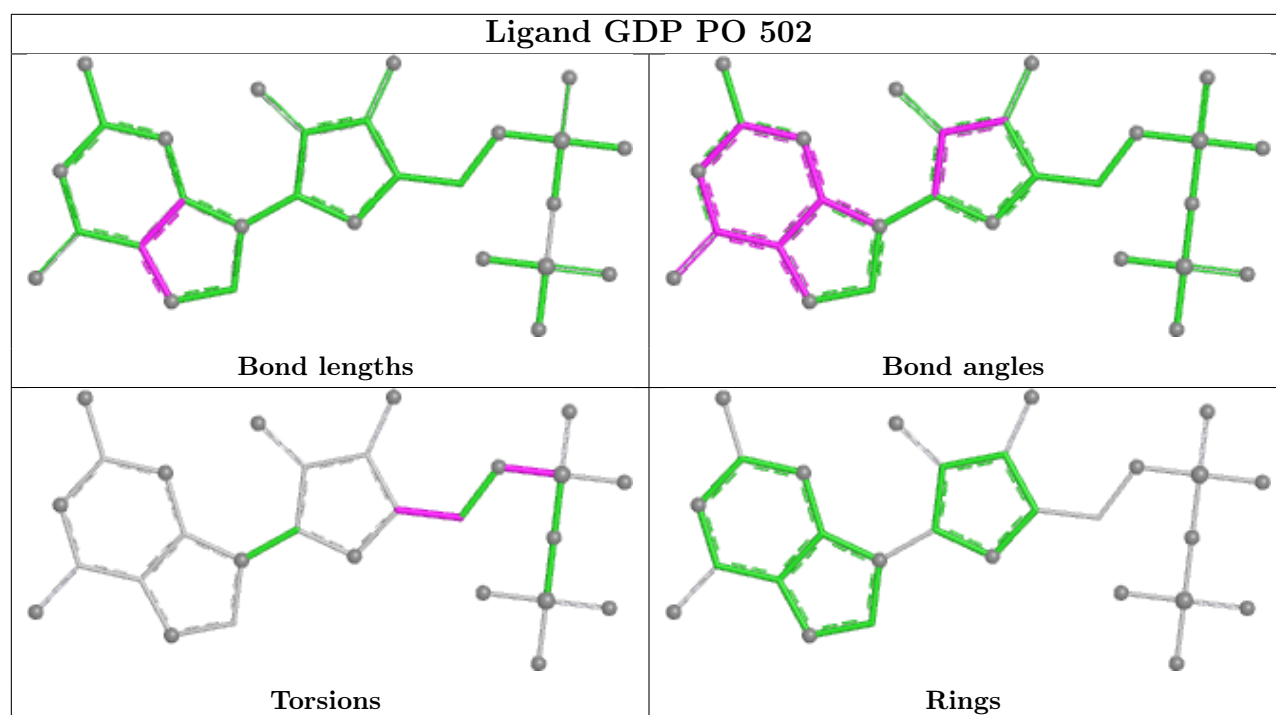
Ligand GTP AH 501

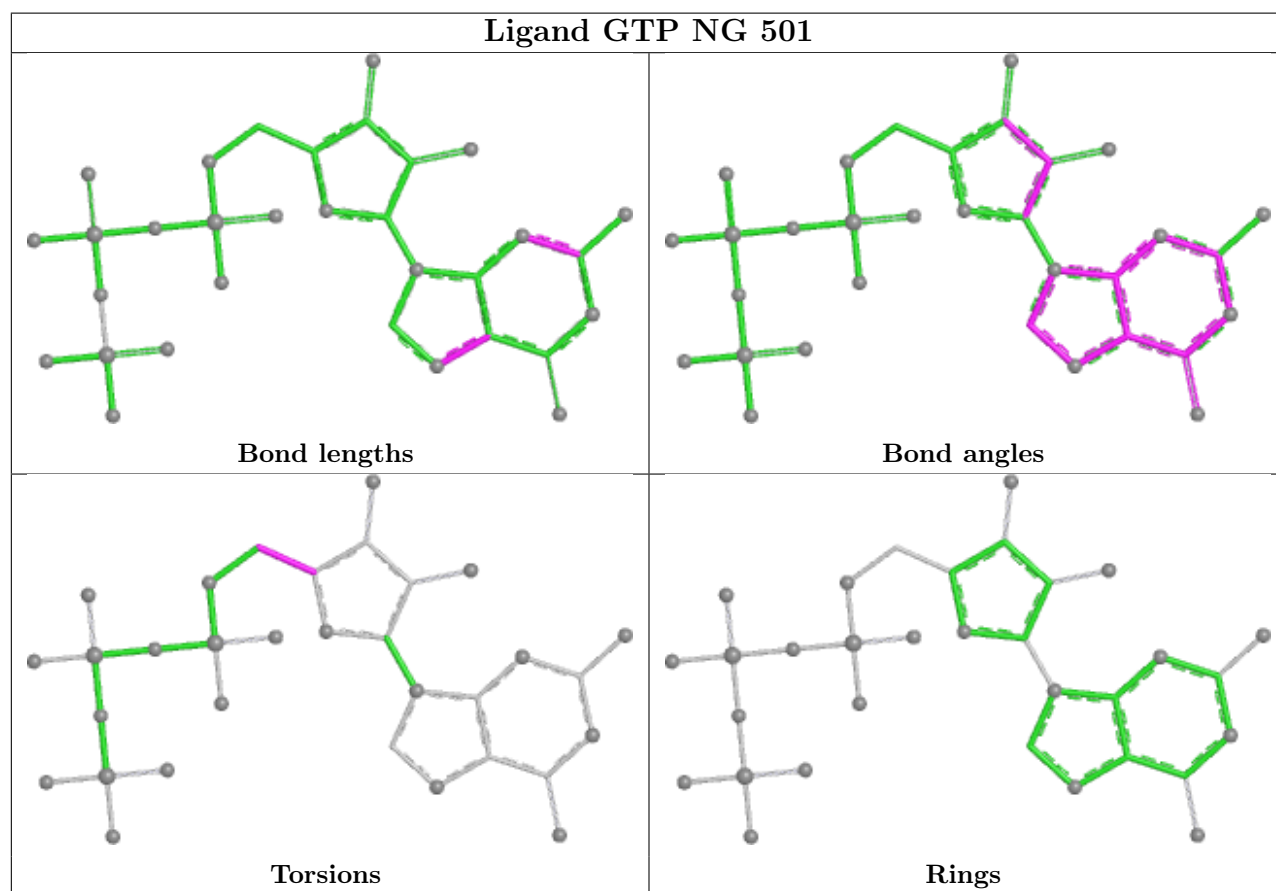
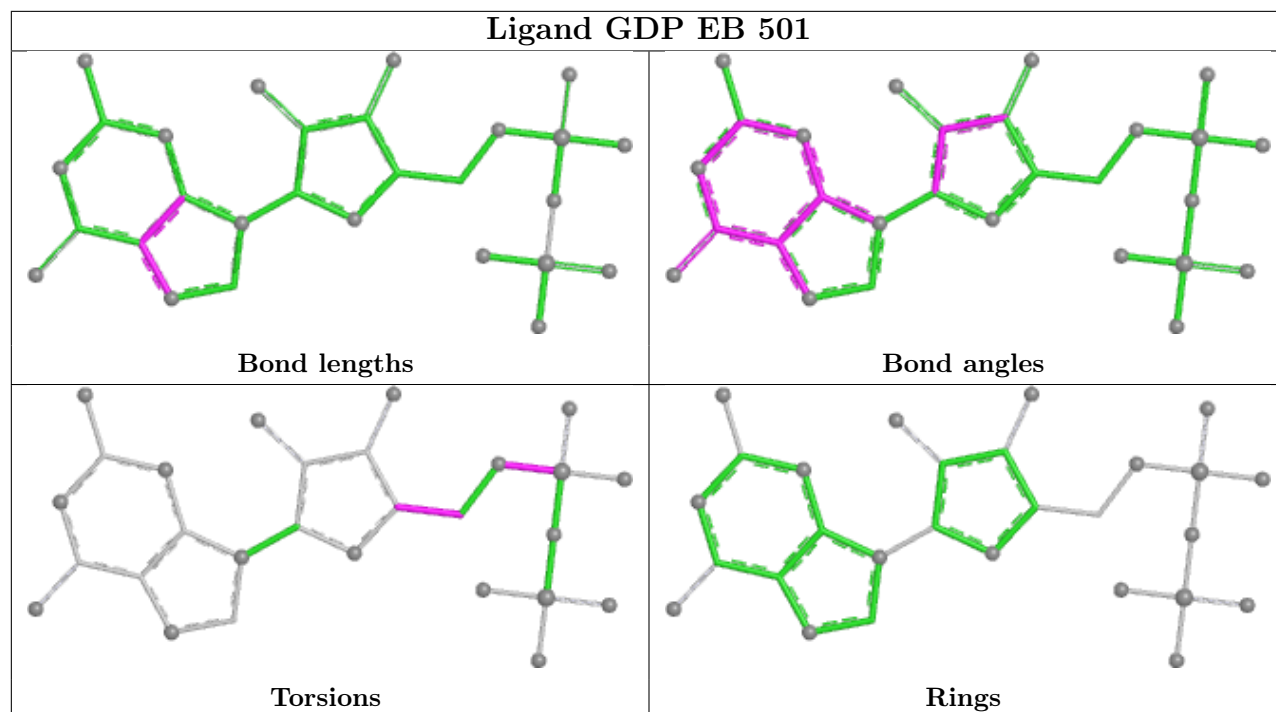


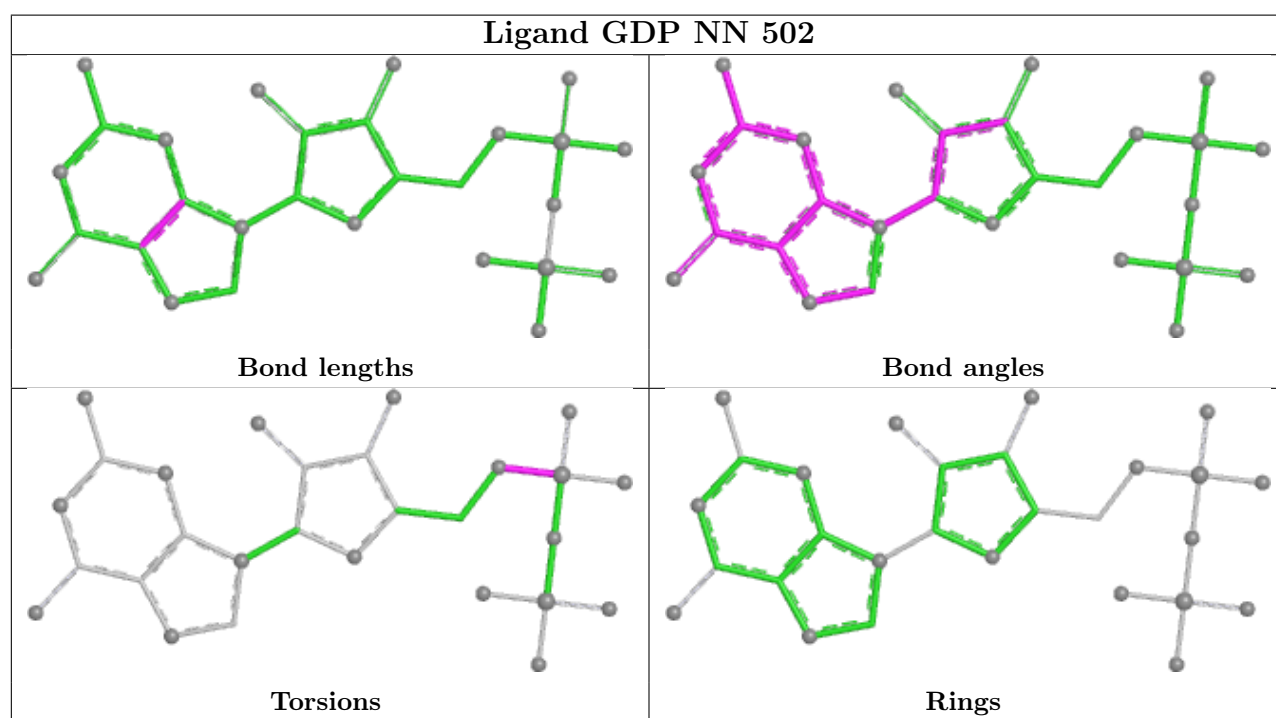
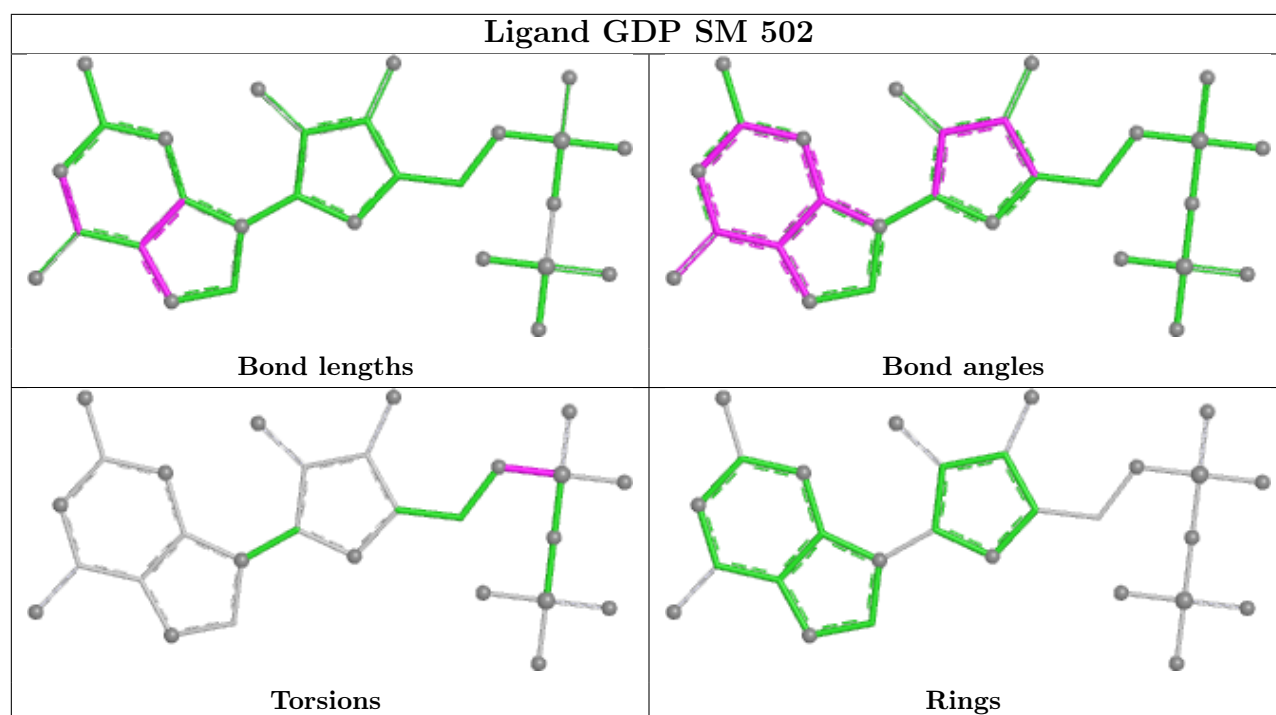
Ligand GTP OL 501

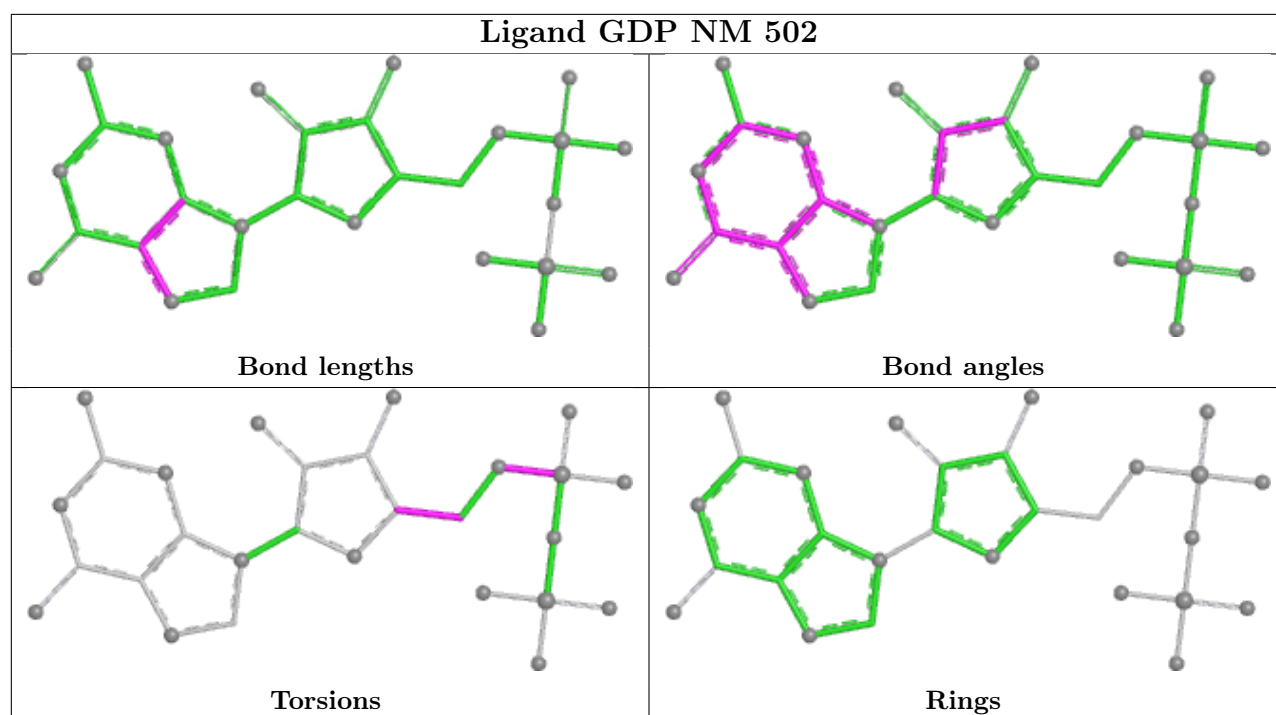












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

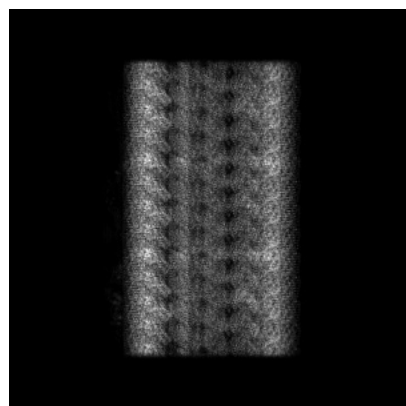
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45802. These allow visual inspection of the internal detail of the map and identification of artifacts.

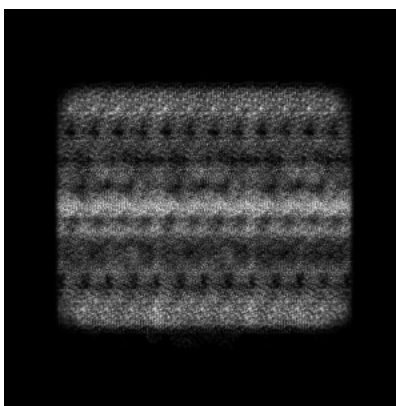
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

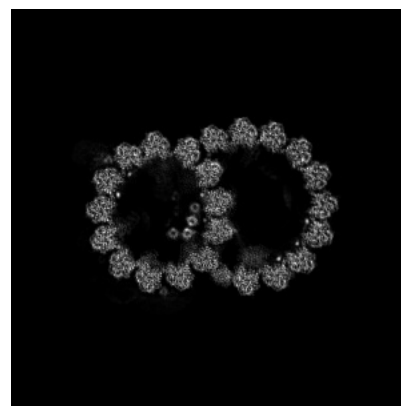
5.1.1 Primary map



X

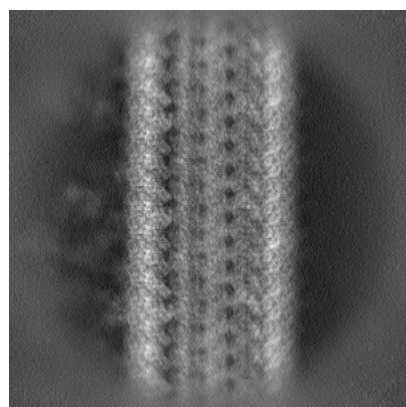


Y

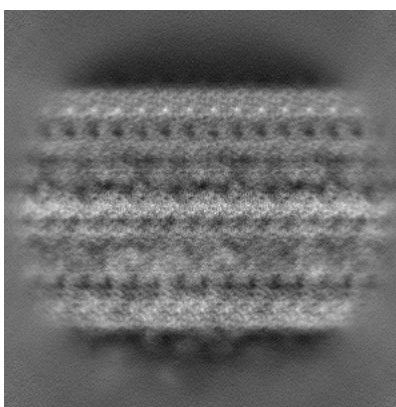


Z

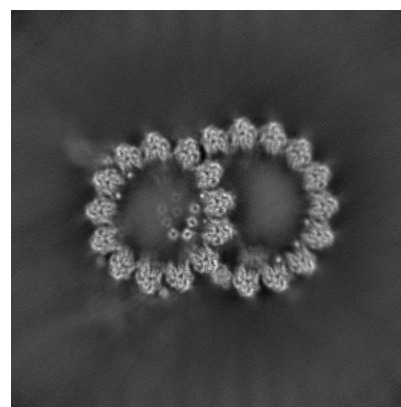
5.1.2 Raw map



X



Y

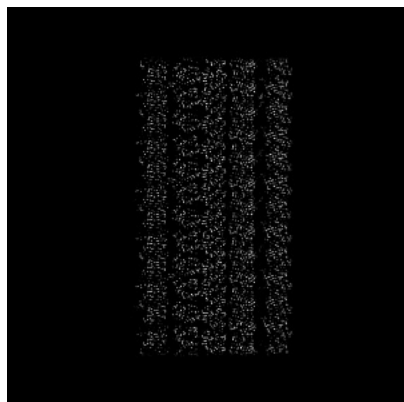


Z

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

5.2 Central slices [i](#)

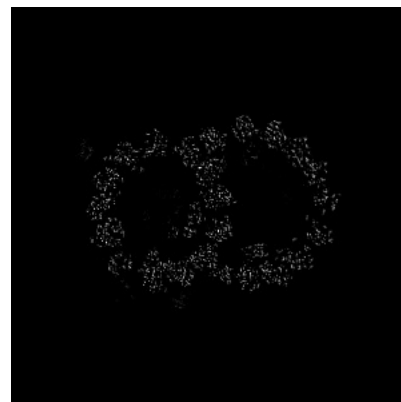
5.2.1 Primary map



X Index: 256

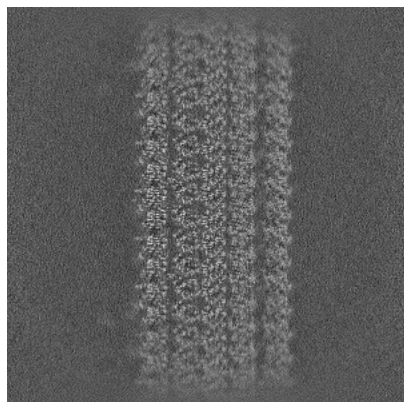


Y Index: 256

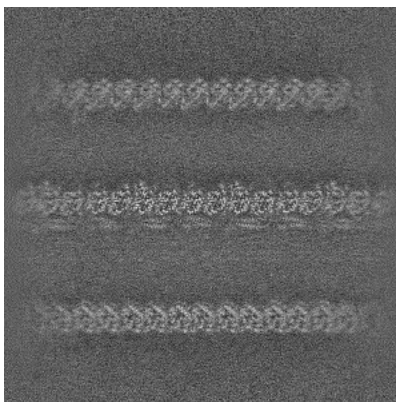


Z Index: 256

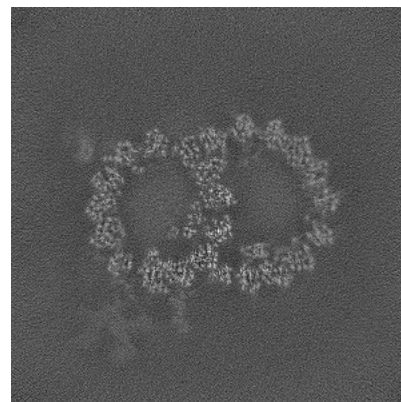
5.2.2 Raw map



X Index: 256



Y Index: 256

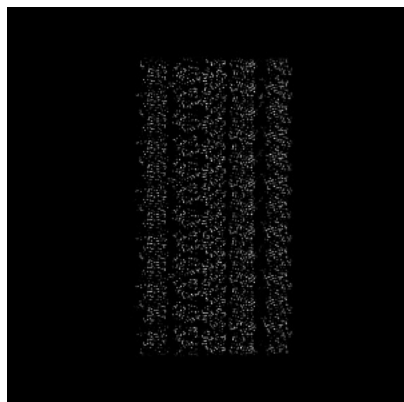


Z Index: 256

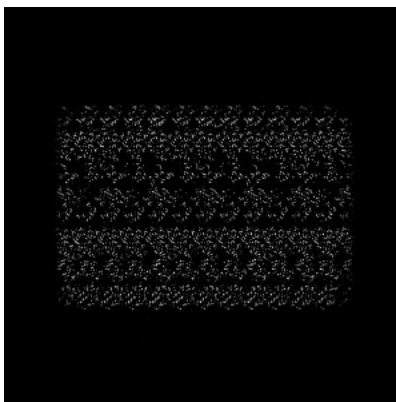
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

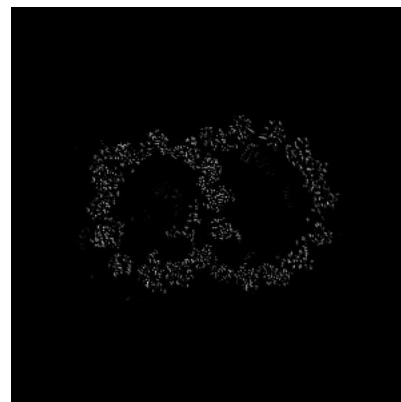
5.3.1 Primary map



X Index: 256

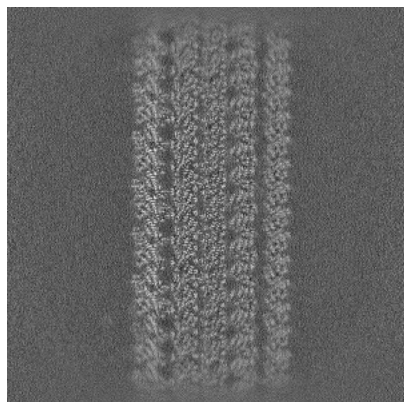


Y Index: 177

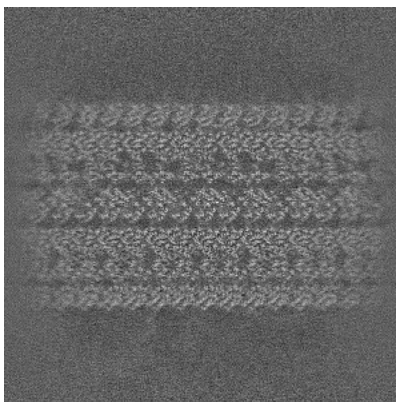


Z Index: 197

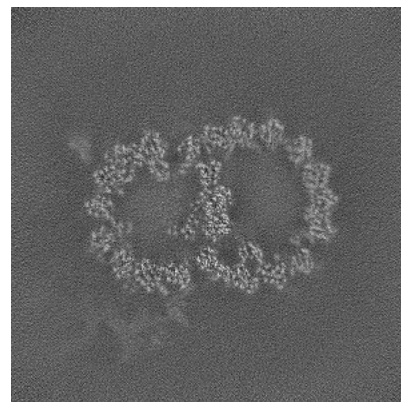
5.3.2 Raw map



X Index: 261



Y Index: 177

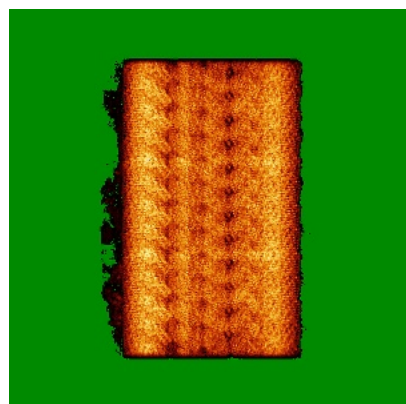


Z Index: 266

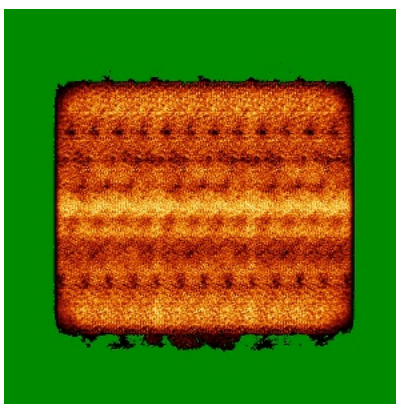
The images above show the largest variance slices of the map in three orthogonal directions.

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

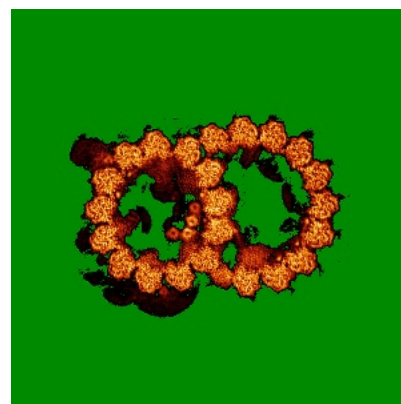
5.4.1 Primary map



X

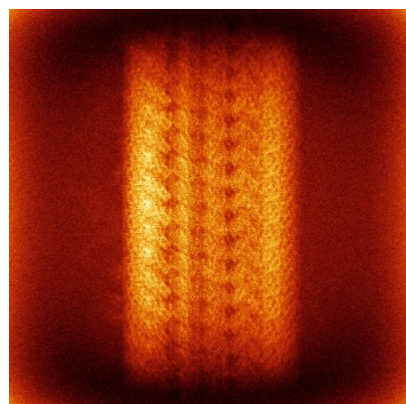


Y

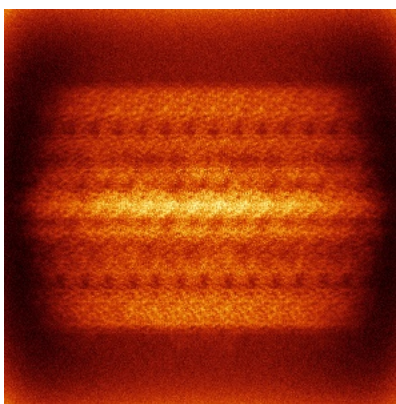


Z

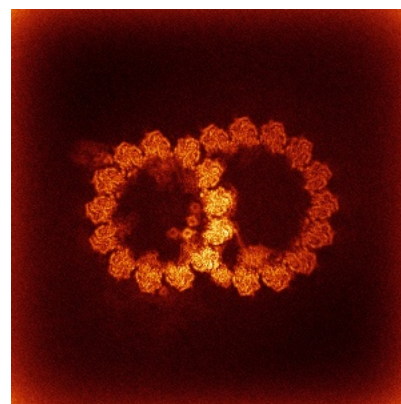
5.4.2 Raw map



X



Y

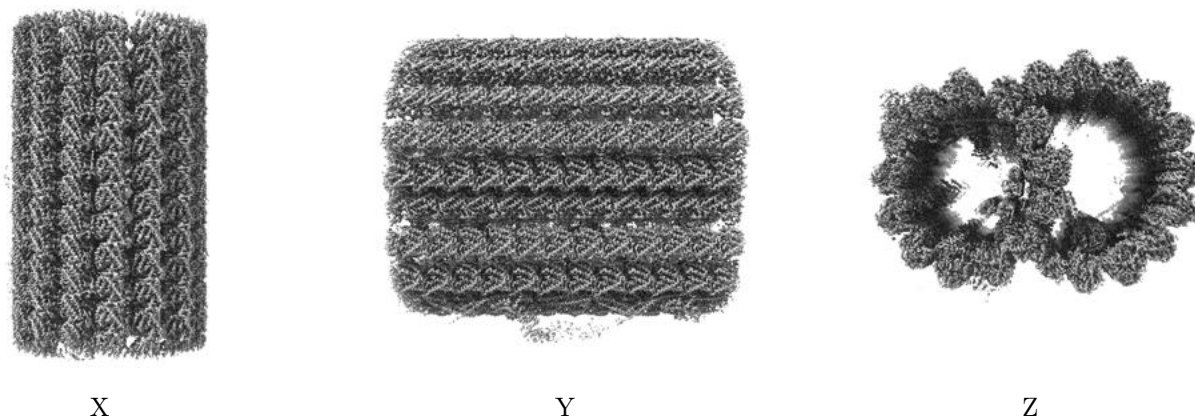


Z

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.

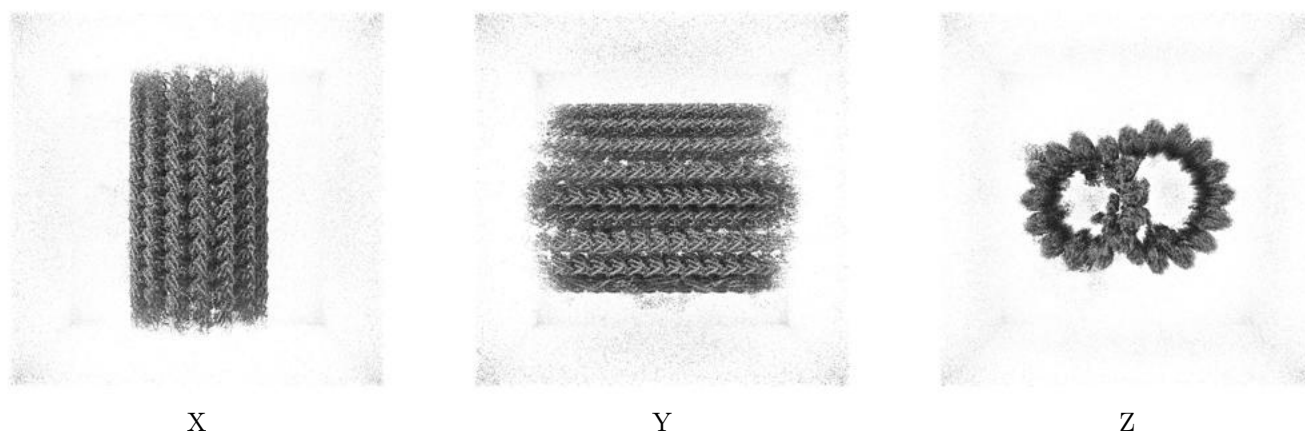
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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



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.

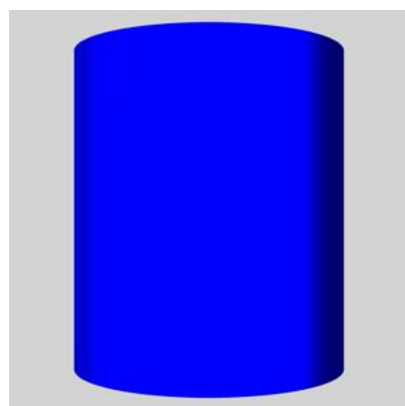
5.6 Mask visualisation [i](#)

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

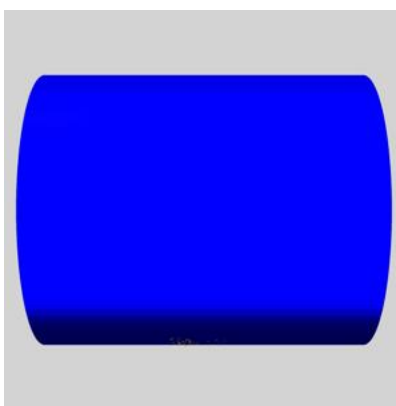
A mask typically either:

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

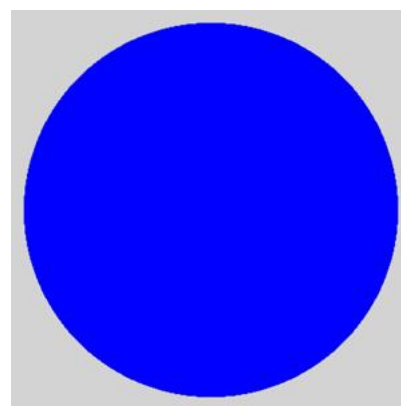
5.6.1 emd_45802_msk_1.map [i](#)



X



Y

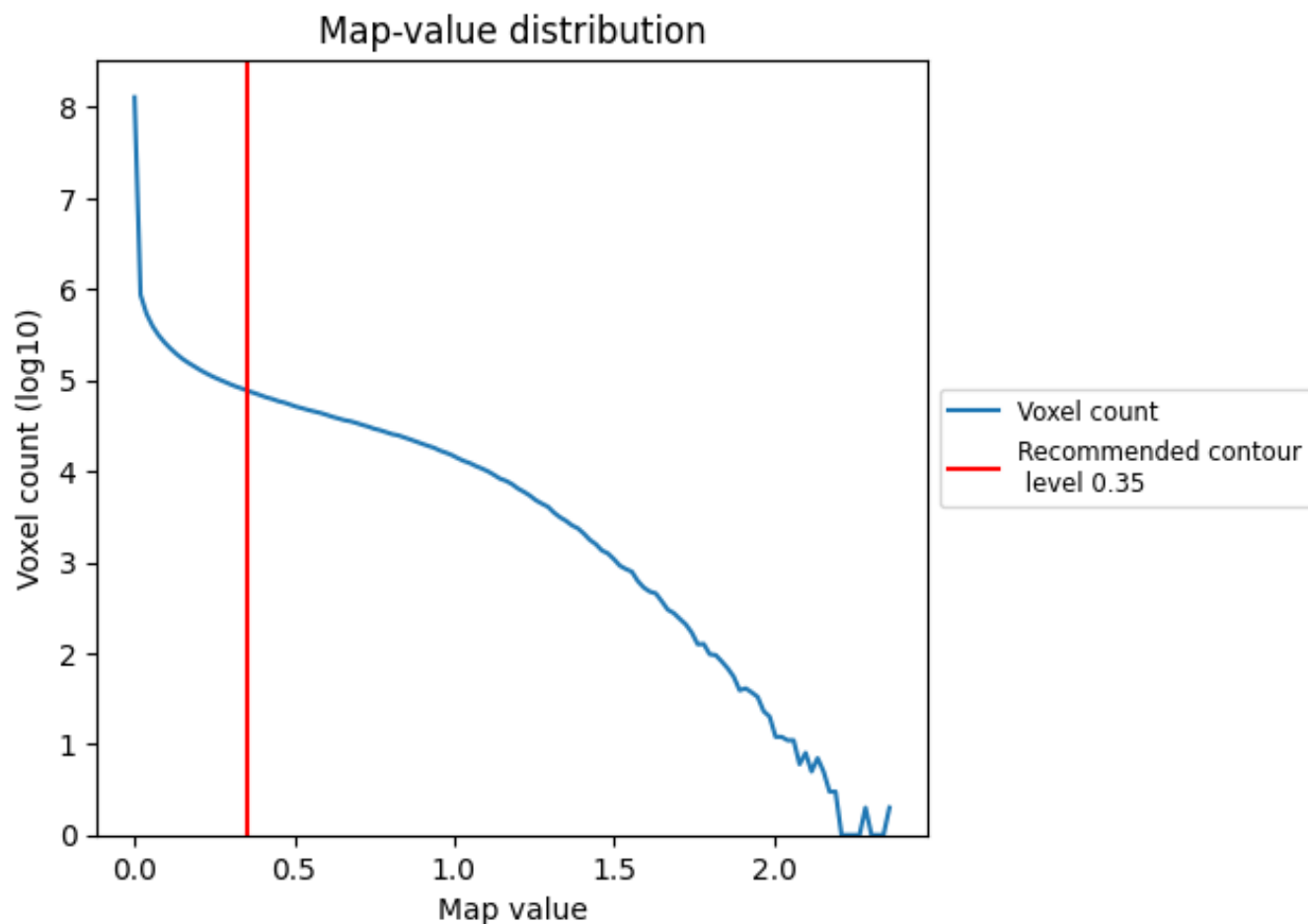


Z

6 Map analysis [i](#)

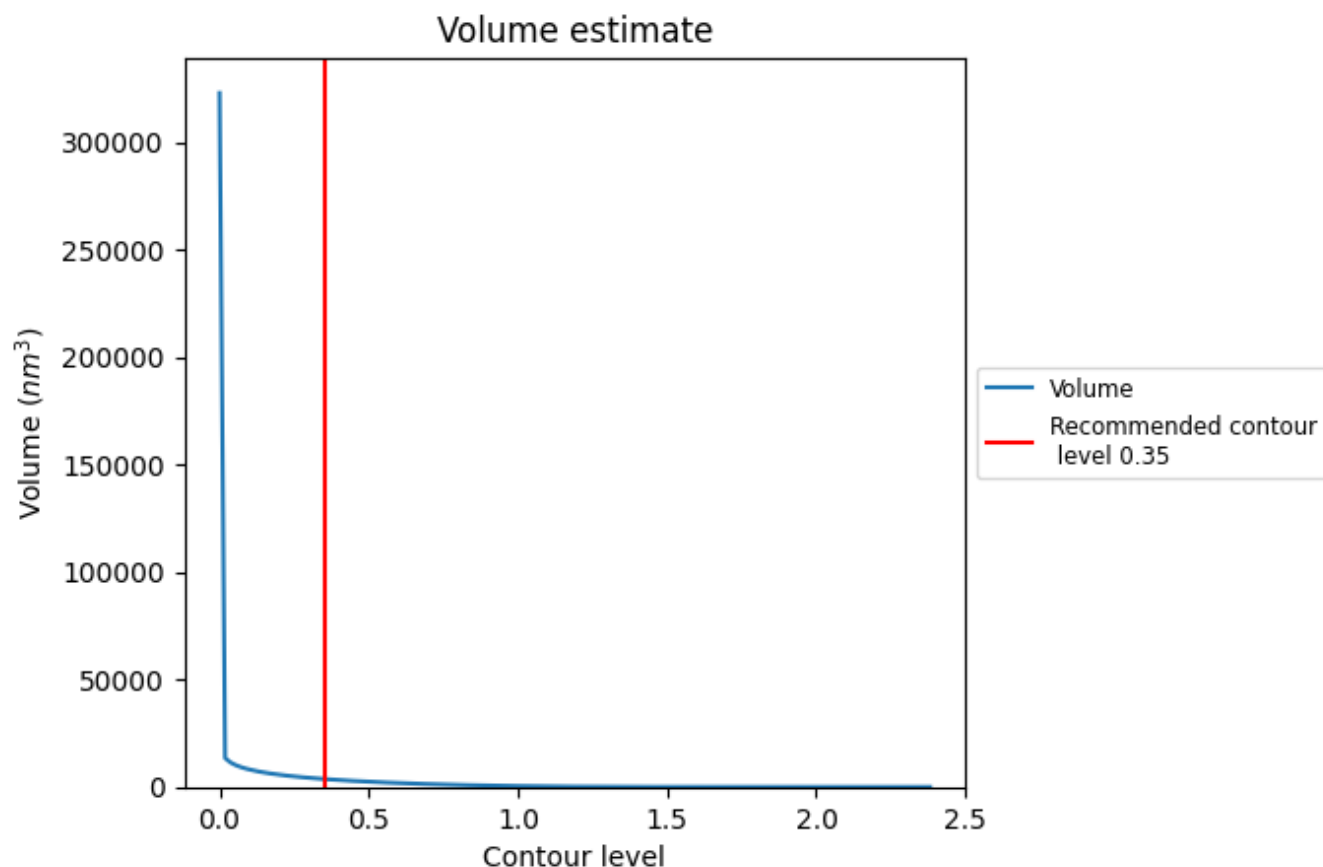
This section contains the results of statistical analysis of the map.

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.

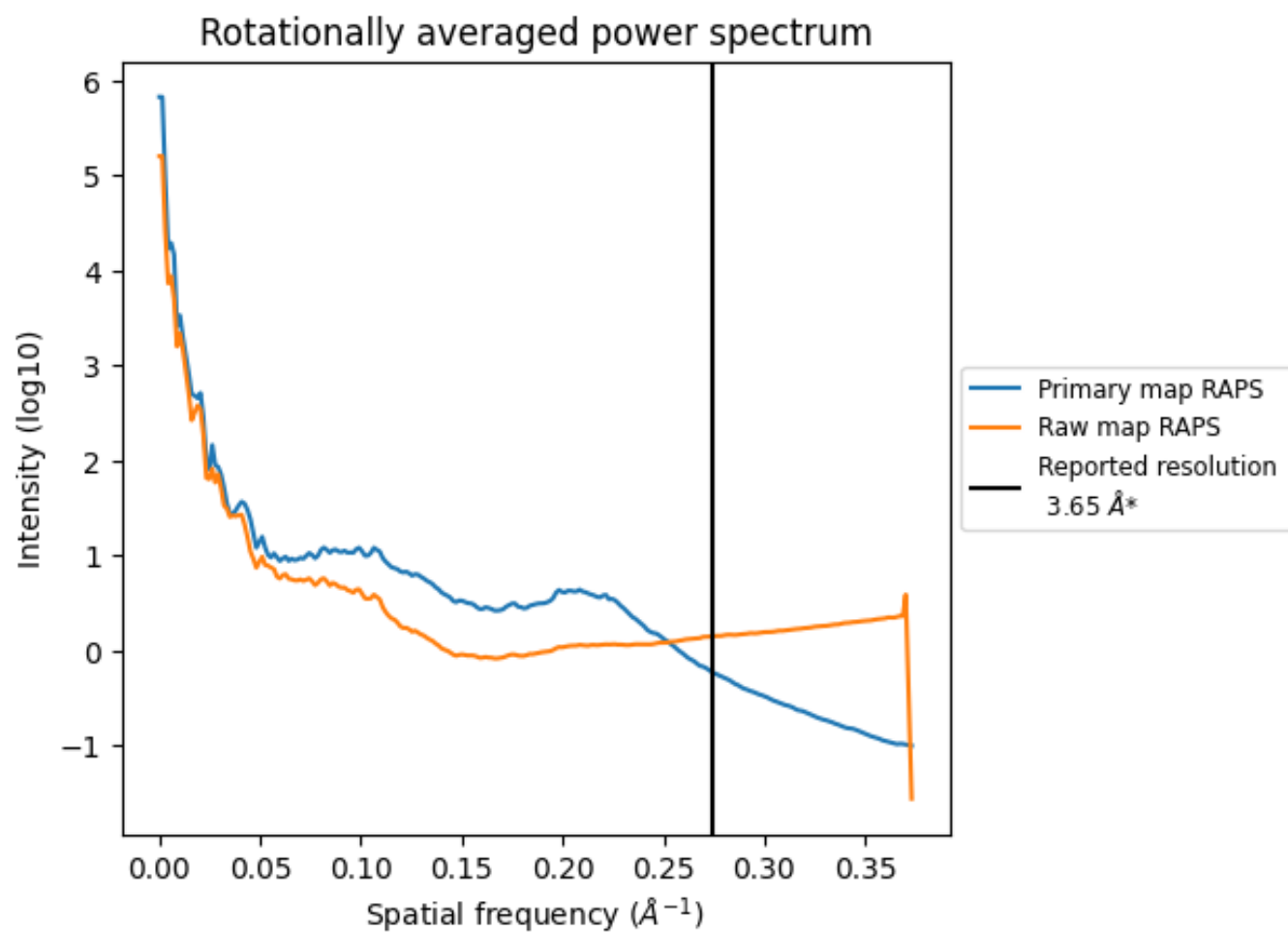
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 3691 nm^3 ; this corresponds to an approximate mass of 3334 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 ⓘ

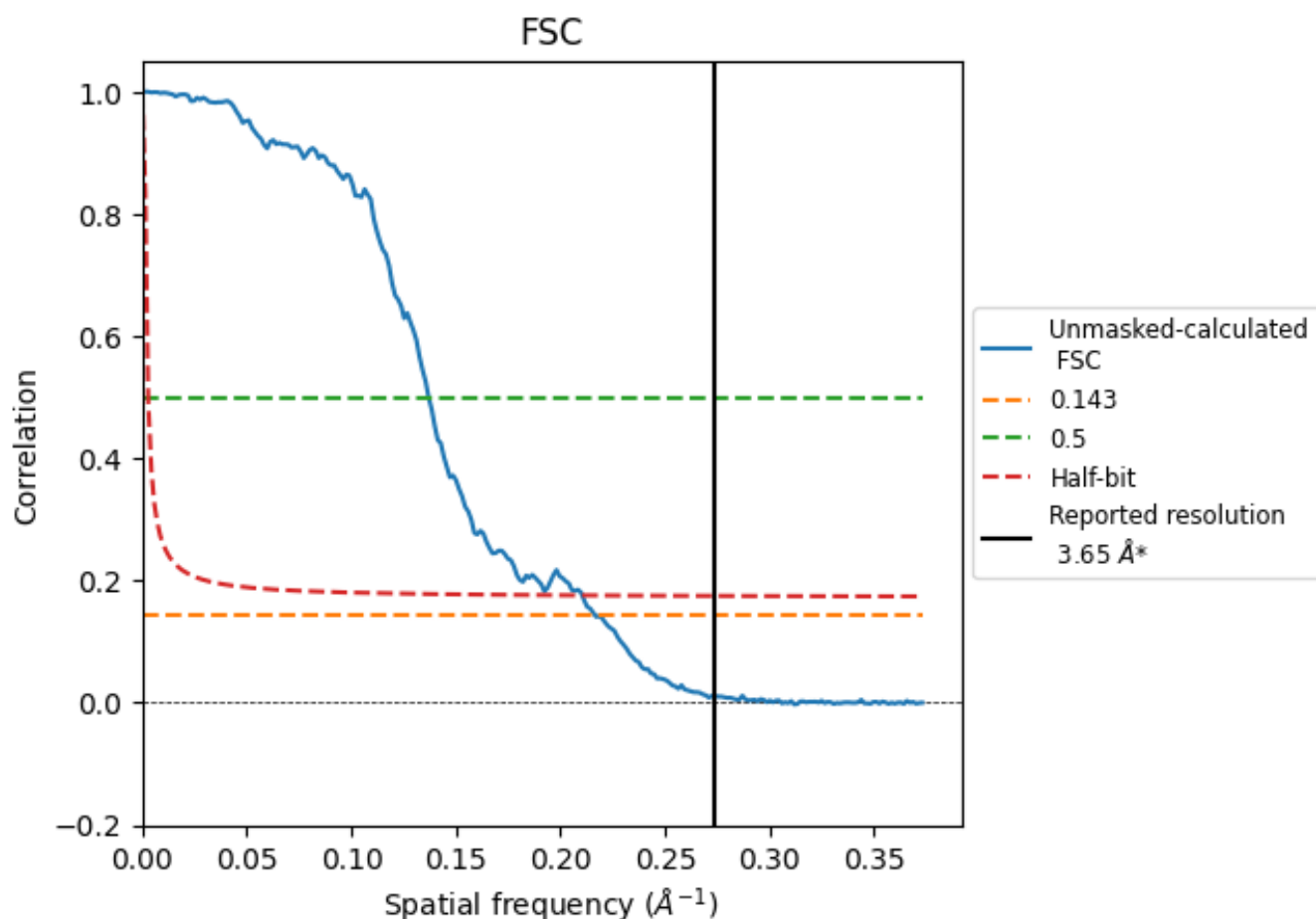


*Reported resolution corresponds to spatial frequency of $0.274 \text{ \AA}^{-1}$

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 0.274 Å⁻¹

7.2 Resolution estimates [i](#)

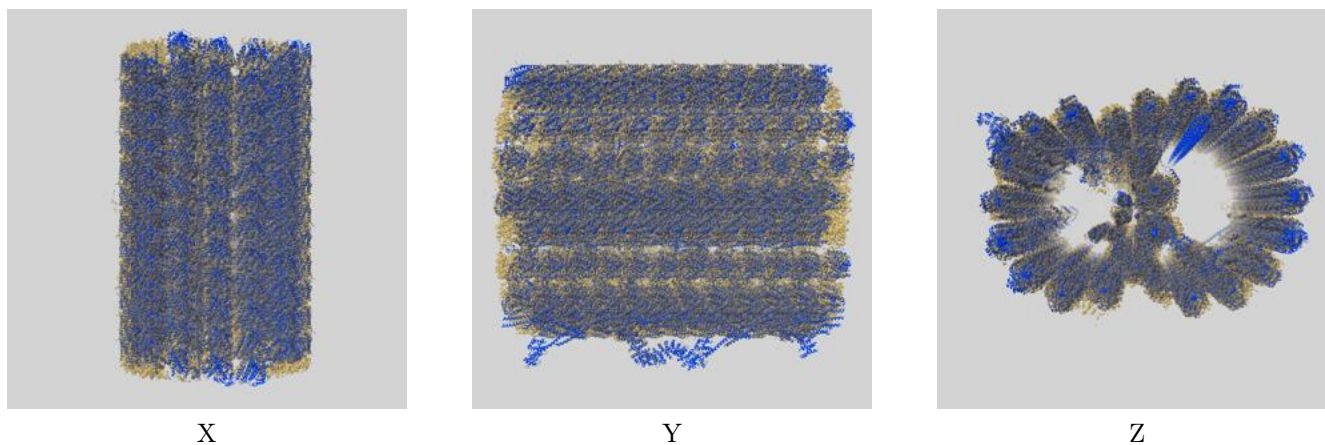
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.62	7.30	4.75

*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 4.62 differs from the reported value 3.65 by more than 10 %

8 Map-model fit [i](#)

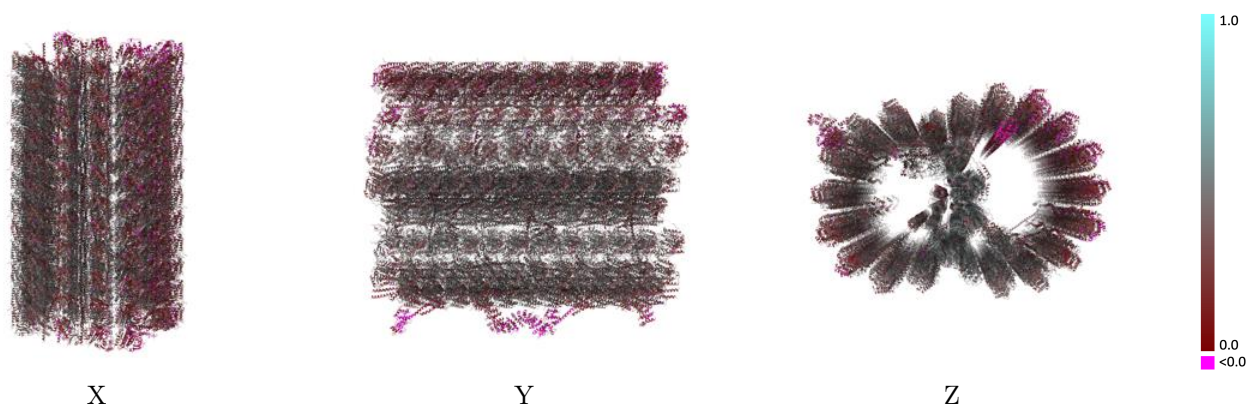
This section contains information regarding the fit between EMDB map EMD-45802 and PDB model 9CPC. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



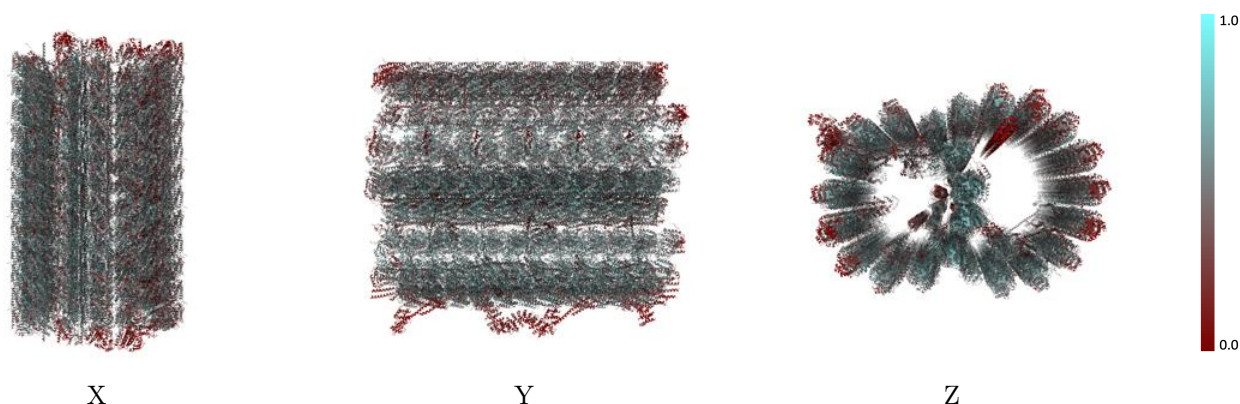
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



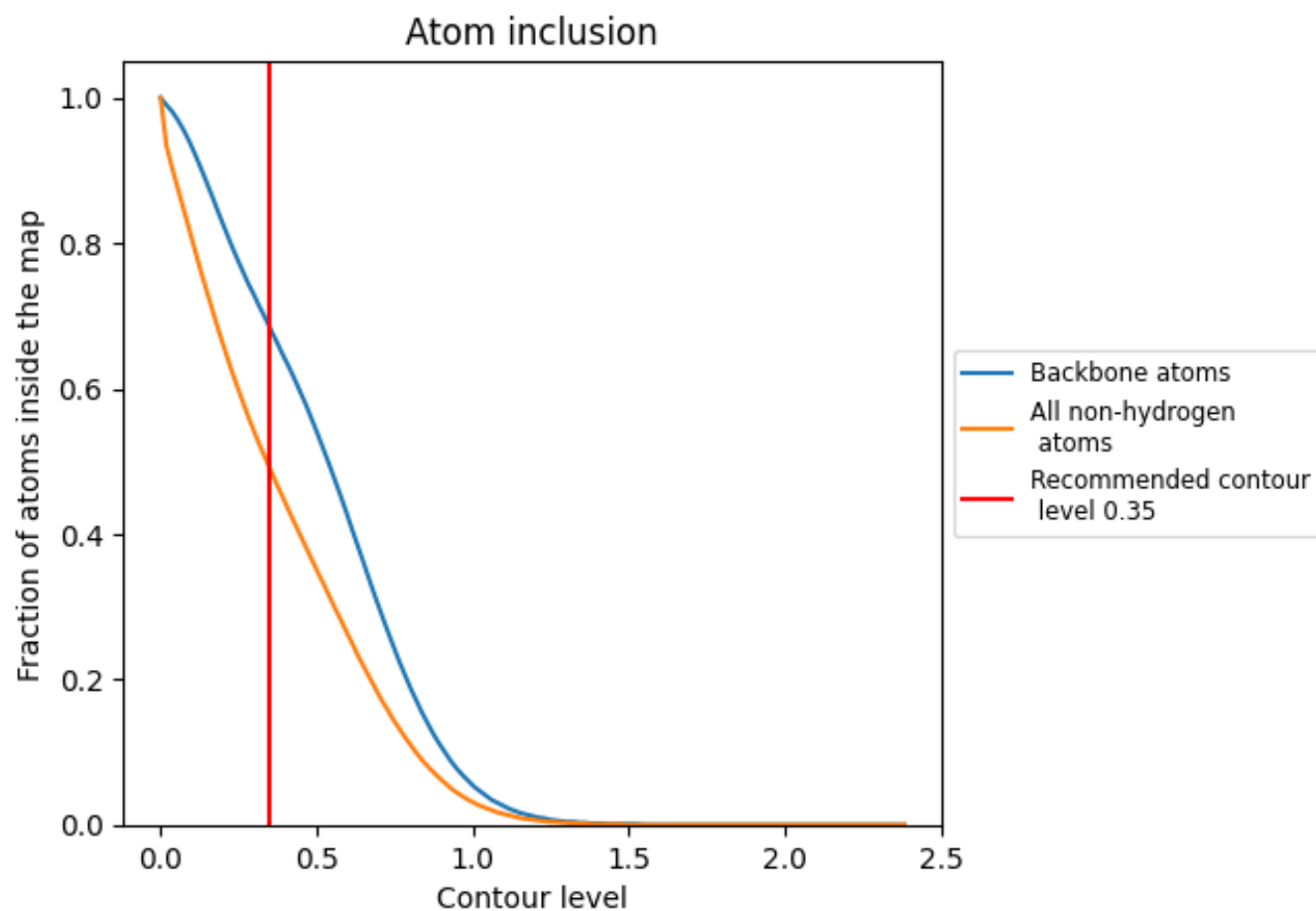
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

8.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 49% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4900	 0.3780
1A	 0.0730	 0.0860
1B	 0.0630	 0.1520
1C	 0.2910	 0.2880
1D	 0.3500	 0.2990
1F	 0.0070	 0.0710
1G	 0.0000	 -0.0110
1H	 0.3100	 0.3130
1I	 0.1710	 0.2420
1J	 0.2620	 0.2890
1L	 0.2220	 0.2360
1M	 0.2940	 0.2650
1N	 0.1930	 0.2080
1P	 0.1300	 0.3070
1Q	 0.0110	 0.1820
1S	 0.5180	 0.4400
1T	 0.5280	 0.4460
1U	 0.5340	 0.4410
1W	 0.3090	 0.2320
1X	 0.2830	 0.2480
1Y	 0.2890	 0.2670
1Z	 0.2870	 0.2150
2B	 0.3750	 0.2300
2C	 0.4330	 0.2440
2E	 0.4630	 0.3970
2F	 0.4240	 0.3860
2G	 0.4500	 0.3830
2I	 0.4350	 0.3860
2J	 0.4120	 0.3660
2K	 0.4110	 0.3890
2M	 0.4280	 0.4350
2N	 0.5240	 0.4490
2O	 0.5070	 0.4500
2P	 0.5450	 0.4500
2Q	 0.5370	 0.4550



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Chain	Atom inclusion	Q-score
2R	 0.1760	 0.3480
2T	 0.5600	 0.4740
2U	 0.5580	 0.4550
2V	 0.5540	 0.4770
2W	 0.5730	 0.4740
2X	 0.5600	 0.4710
3A	 0.5670	 0.4520
3B	 0.5620	 0.4420
3C	 0.5640	 0.4650
3E	 0.5440	 0.4600
3F	 0.5360	 0.4560
3G	 0.4730	 0.4520
3H	 0.5210	 0.4400
3J	 0.5240	 0.4470
3K	 0.5000	 0.4260
3L	 0.5370	 0.4390
3M	 0.4660	 0.4220
3O	 0.3050	 0.3780
3P	 0.3370	 0.3810
3Q	 0.3360	 0.3640
3R	 0.2840	 0.3220
3T	 0.2770	 0.3520
3U	 0.2980	 0.3680
3V	 0.1410	 0.2510
3W	 0.2030	 0.3110
3Y	 0.5140	 0.4460
3Z	 0.4790	 0.4300
4A	 0.1910	 0.3050
4B	 0.2790	 0.3260
4D	 0.4750	 0.4210
4E	 0.4810	 0.3980
4F	 0.4660	 0.3800
4H	 0.3990	 0.3710
4I	 0.4030	 0.3690
4J	 0.4010	 0.3520
4K	 0.0980	 0.2030
4M	 0.3630	 0.3850
4N	 0.3990	 0.3680
4O	 0.2340	 0.2680
4P	 0.1590	 0.2620
4Q	 0.1800	 0.3250
4R	 0.2890	 0.3370

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Chain	Atom inclusion	Q-score
4T	 0.3790	 0.3560
4V	 0.4440	 0.3870
4W	 0.3460	 0.3280
4Y	 0.4880	 0.4110
4Z	 0.5130	 0.4140
5B	 0.3820	 0.3630
5D	 0.4460	 0.3890
5E	 0.3090	 0.2930
5G	 0.0790	 0.2220
5I	 0.4110	 0.3740
5J	 0.2560	 0.2900
5L	 0.4270	 0.3700
5N	 0.3500	 0.2920
5O	 0.3890	 0.2990
5Q	 0.3820	 0.3020
5R	 0.4030	 0.3080
5T	 0.0660	 0.2300
5U	 0.0470	 0.1580
5W	 0.3770	 0.3360
5X	 0.3650	 0.3300
5Y	 0.3720	 0.3050
5Z	 0.3570	 0.3570
6A	 0.4110	 0.3070
6C	 0.3790	 0.3170
6D	 0.4490	 0.3790
6F	 0.0740	 0.1900
6G	 0.0470	 0.1490
6H	 0.0320	 0.1080
6I	 0.0790	 0.1960
6J	 0.0220	 0.1330
6K	 0.0560	 0.1620
6L	 0.0110	 0.0900
AA	 0.5760	 0.4780
AB	 0.5620	 0.4740
AE	 0.5820	 0.4890
AF	 0.6020	 0.4800
AG	 0.5920	 0.4820
AH	 0.5860	 0.4820
AL	 0.5960	 0.4760
AM	 0.5910	 0.4810
AN	 0.5810	 0.4770
AO	 0.5960	 0.4970

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Chain	Atom inclusion	Q-score
AP	 0.5780	 0.4730
BA	 0.5610	 0.4460
BB	 0.5600	 0.4630
BE	 0.5560	 0.4510
BF	 0.5780	 0.4310
BG	 0.5810	 0.4390
BH	 0.5670	 0.4600
BI	 0.4730	 0.4150
BL	 0.5320	 0.4160
BM	 0.5540	 0.4490
BN	 0.5470	 0.4280
BO	 0.5570	 0.4580
BP	 0.5680	 0.4520
CA	 0.5370	 0.4330
CB	 0.5300	 0.4050
CE	 0.5200	 0.3900
CF	 0.5390	 0.4010
CG	 0.5490	 0.4120
CH	 0.5480	 0.4430
CI	 0.4540	 0.3620
CL	 0.5000	 0.3930
CM	 0.5430	 0.4340
CN	 0.5610	 0.4310
CO	 0.5520	 0.4350
CP	 0.5510	 0.4240
DA	 0.5230	 0.3970
DB	 0.5370	 0.3940
DE	 0.4890	 0.3530
DF	 0.5150	 0.3800
DG	 0.5060	 0.3590
DH	 0.5150	 0.3880
DI	 0.4360	 0.3410
DL	 0.3490	 0.2960
DM	 0.5160	 0.3820
DN	 0.5440	 0.3920
DO	 0.5140	 0.3600
DP	 0.5280	 0.3800
EA	 0.5410	 0.3700
EB	 0.5520	 0.3760
EE	 0.4810	 0.3210
EF	 0.5380	 0.3670
EG	 0.5540	 0.3800

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Chain	Atom inclusion	Q-score
EH	 0.5610	 0.4080
EI	 0.4740	 0.3570
EL	 0.2490	 0.2560
EM	 0.5500	 0.4020
EN	 0.5480	 0.3600
EO	 0.5570	 0.3730
EP	 0.5400	 0.3920
FA	 0.5460	 0.4140
FB	 0.5470	 0.4050
FE	 0.4320	 0.3320
FF	 0.5290	 0.3890
FG	 0.5360	 0.4010
FH	 0.5220	 0.3970
FI	 0.4700	 0.3560
FM	 0.5210	 0.3820
FN	 0.5380	 0.3840
FO	 0.5550	 0.3950
FP	 0.5060	 0.3800
GA	 0.5330	 0.3940
GB	 0.5620	 0.4110
GE	 0.4500	 0.3690
GF	 0.5340	 0.4070
GG	 0.5520	 0.4180
GH	 0.5540	 0.4280
GI	 0.5260	 0.4040
GM	 0.5310	 0.3920
GN	 0.5660	 0.4160
GO	 0.5680	 0.3990
GP	 0.5380	 0.3990
HA	 0.5620	 0.4040
HB	 0.5640	 0.4220
HE	 0.4660	 0.3820
HF	 0.5480	 0.4160
HG	 0.5630	 0.4280
HH	 0.5550	 0.4200
HI	 0.5330	 0.3960
HM	 0.5470	 0.4050
HN	 0.5620	 0.4280
HO	 0.5650	 0.4160
HP	 0.5470	 0.4160
HQ	 0.4410	 0.3480
IA	 0.5510	 0.4050

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Chain	Atom inclusion	Q-score
IB	 0.5530	 0.4180
IE	 0.4250	 0.3490
IF	 0.5270	 0.4150
IG	 0.5460	 0.4180
IH	 0.5630	 0.4260
II	 0.5410	 0.4160
IM	 0.5310	 0.4080
IN	 0.5330	 0.4130
IO	 0.5530	 0.4190
IP	 0.5590	 0.4380
IQ	 0.5160	 0.4010
JA	 0.5480	 0.4040
JB	 0.5690	 0.4090
JD	 0.5190	 0.3820
JE	 0.5330	 0.4000
JF	 0.5510	 0.4120
JG	 0.5510	 0.4200
JH	 0.5480	 0.4070
JL	 0.5400	 0.4000
JM	 0.5780	 0.4280
JN	 0.5410	 0.4020
JO	 0.5660	 0.4230
KA	 0.5840	 0.4490
KB	 0.6030	 0.4490
KD	 0.5780	 0.4260
KE	 0.5840	 0.4430
KF	 0.5750	 0.4410
KG	 0.5810	 0.4420
KH	 0.5810	 0.4430
KL	 0.5980	 0.4610
KM	 0.5950	 0.4330
KN	 0.5780	 0.4450
KO	 0.5810	 0.4370
KP	 0.5080	 0.4090
LA	 0.5960	 0.4730
LB	 0.6310	 0.4820
LD	 0.6100	 0.4730
LE	 0.5960	 0.4710
LF	 0.6190	 0.5070
LG	 0.6170	 0.5000
LH	 0.6040	 0.4730
LL	 0.6070	 0.4780

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Chain	Atom inclusion	Q-score
LM	 0.6080	 0.4750
LN	 0.6110	 0.4880
LO	 0.6180	 0.4830
LP	 0.5880	 0.4670
MA	 0.6150	 0.5070
MB	 0.6100	 0.4820
MD	 0.5980	 0.4810
ME	 0.6050	 0.4790
MF	 0.6350	 0.5100
MG	 0.6300	 0.5130
MH	 0.6150	 0.5060
ML	 0.6240	 0.4920
MM	 0.6040	 0.4750
MN	 0.6130	 0.4920
MO	 0.6250	 0.5070
MP	 0.6050	 0.4720
NA	 0.5090	 0.3890
NB	 0.5210	 0.3810
ND	 0.4920	 0.3850
NE	 0.4920	 0.3830
NF	 0.5050	 0.3840
NG	 0.5000	 0.3810
NH	 0.4870	 0.3700
NL	 0.4920	 0.3800
NM	 0.5140	 0.3850
NN	 0.4920	 0.3810
NO	 0.4950	 0.3800
NP	 0.4230	 0.3260
OA	 0.5140	 0.3740
OB	 0.5190	 0.3580
OD	 0.4180	 0.3120
OE	 0.5060	 0.3710
OF	 0.5010	 0.3540
OG	 0.5050	 0.3600
OH	 0.5040	 0.3830
OL	 0.4930	 0.3560
OM	 0.5100	 0.3580
ON	 0.5130	 0.3730
OO	 0.5040	 0.3670
OP	 0.4400	 0.3000
PA	 0.4710	 0.3240
PB	 0.4550	 0.3050

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Chain	Atom inclusion	Q-score
PD	 0.2750	 0.1850
PE	 0.4470	 0.2930
PF	 0.4570	 0.2930
PG	 0.4600	 0.2910
PH	 0.4440	 0.2930
PL	 0.4270	 0.2790
PM	 0.4440	 0.2990
PN	 0.4790	 0.3150
PO	 0.4370	 0.2890
PP	 0.3980	 0.2380
QA	 0.4210	 0.2830
QB	 0.4740	 0.3250
QE	 0.3910	 0.2390
QF	 0.4510	 0.2710
QG	 0.4450	 0.2660
QH	 0.4010	 0.2650
QL	 0.3510	 0.2060
QM	 0.4210	 0.2700
QN	 0.4300	 0.2770
QO	 0.4100	 0.2730
QP	 0.4150	 0.2620
RA	 0.4340	 0.3000
RB	 0.4440	 0.2870
RE	 0.3900	 0.2440
RF	 0.4510	 0.2740
RG	 0.4580	 0.2840
RH	 0.4230	 0.2820
RI	 0.1670	 0.1800
RL	 0.3030	 0.2020
RM	 0.4270	 0.2730
RN	 0.4430	 0.2920
RO	 0.4390	 0.3000
RP	 0.3860	 0.2420
SA	 0.4680	 0.3240
SB	 0.4620	 0.3120
SE	 0.4080	 0.2640
SF	 0.4500	 0.2920
SG	 0.4690	 0.3070
SH	 0.4600	 0.3160
SI	 0.2480	 0.2280
SL	 0.2910	 0.2130
SM	 0.4470	 0.2910

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Chain	Atom inclusion	Q-score
SN	 0.4660	 0.2990
SO	 0.5010	 0.3430
SP	 0.4280	 0.2870
TA	 0.4800	 0.3310
TB	 0.4860	 0.3400
TE	 0.4050	 0.2780
TF	 0.4680	 0.3230
TG	 0.4760	 0.3270
TH	 0.5110	 0.3640
TI	 0.3740	 0.3020
TL	 0.2390	 0.2220
TM	 0.4740	 0.3270
TN	 0.5090	 0.3290
TO	 0.5200	 0.3530
TP	 0.4860	 0.3390
UA	 0.4940	 0.3600
UB	 0.5000	 0.3570
UE	 0.4290	 0.3000
UF	 0.4930	 0.3790
UG	 0.4750	 0.3500
UH	 0.5060	 0.3800
UI	 0.4810	 0.3670
UM	 0.4780	 0.3390
UN	 0.4950	 0.3340
UO	 0.5300	 0.3640
UP	 0.5190	 0.3870
VA	 0.5230	 0.4090
VB	 0.5440	 0.4240
VF	 0.5070	 0.4030
VG	 0.5510	 0.4280
VH	 0.5380	 0.4200
VI	 0.5300	 0.4260
VJ	 0.5150	 0.4000
VN	 0.5460	 0.4230
VO	 0.5430	 0.4090
VP	 0.5310	 0.3970
VQ	 0.5380	 0.4150
WA	 0.5270	 0.4180
WB	 0.5580	 0.4260
WE	 0.5240	 0.4130
WF	 0.5610	 0.4330
WG	 0.5570	 0.4360

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Chain	Atom inclusion	Q-score
WH	 0.5430	 0.4290
WI	 0.5440	 0.4330
WM	 0.5670	 0.4560
WN	 0.5700	 0.4460
WO	 0.5420	 0.4090
WP	 0.5590	 0.4400
WQ	 0.4940	 0.3860