



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 07:59 AM UTC

PDB ID : 8G3D / pdb_00008g3d
EMDB ID : EMD-29692
Title : 48-nm doublet microtubule from Tetrahymena thermophila strain K40R
Authors : Black, C.S.; Kubo, S.; Yang, S.K.; Bui, K.H.
Deposited on : 2023-02-07
Resolution : 3.70 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

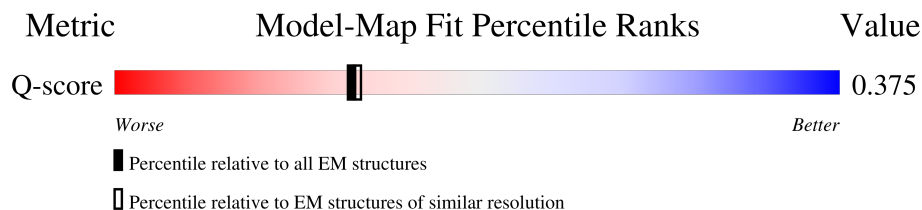
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



Metric	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	11569 (3.20 - 4.20)

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

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 1324599 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 RIB27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0A	152	Total	C	N	O	S	0	0
			1229	776	224	228	1		
1	1A	152	Total	C	N	O	S	0	0
			1229	776	224	228	1		
1	2A	152	Total	C	N	O	S	0	0
			1229	776	224	228	1		
1	3A	152	Total	C	N	O	S	0	0
			1229	776	224	228	1		

- Molecule 2 is a protein called RIB38.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0B	321	Total	C	N	O	S	0	0
			2614	1633	472	503	6		

- Molecule 3 is a protein called CFAM166B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0C	95	Total	C	N	O	S	0	0
			747	471	131	143	2		
3	1C	95	Total	C	N	O	S	0	0
			747	471	131	143	2		

- Molecule 4 is a protein called CFAM166A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	0D	202	Total	C	N	O	S	1	0
			1621	1019	293	307	2		
4	1D	202	Total	C	N	O	S	1	0
			1621	1019	293	307	2		
4	2D	202	Total	C	N	O	S	1	0
			1621	1019	293	307	2		

- Molecule 5 is a protein called RIB22.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	0E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		
5	1E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		
5	2E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		
5	3E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		

- Molecule 6 is a protein called CFAM166C.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	0F	206	Total	C	N	O	S	0	0
			1665	1048	300	314	3		

- Molecule 7 is a protein called CFAP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	0G	168	Total	C	N	O	S	0	0
			1378	872	237	265	4		
7	1G	133	Total	C	N	O	S	0	0
			1089	692	185	210	2		

- Molecule 8 is a protein called CFAP127.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	0H	116	Total	C	N	O	S	0	0
			1006	628	181	192	5		
8	1H	422	Total	C	N	O	S	0	0
			3687	2271	687	715	14		

- Molecule 9 is a protein called CFAP161A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0N	280	Total	C	N	O	S	0	0
			2305	1455	396	441	13		
9	1N	463	Total	C	N	O	S	0	0
			3805	2414	653	723	15		
9	2N	280	Total	C	N	O	S	0	0
			2305	1455	396	441	13		

- Molecule 10 is a protein called CFAP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	0Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	1Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	2Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	3Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	4Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	5Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
10	6Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		

- Molecule 11 is a protein called Parkin co-regulated protein PACRGA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	0S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		
11	1S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		
11	2S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		
11	3S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		

- Molecule 12 is a protein called IJ34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	0T	253	Total	C	N	O	S	0	0
			2056	1312	357	378	9		
12	1T	285	Total	C	N	O	S	0	0
			2321	1471	411	430	9		
12	2T	285	Total	C	N	O	S	0	0
			2321	1471	411	430	9		
12	3T	285	Total	C	N	O	S	0	0
			2321	1471	411	430	9		

- Molecule 13 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	0U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		
13	1U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		
13	2U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		
13	3U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		

- Molecule 14 is a protein called DNA polymerase delta C4-type zinc-finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	0V	212	Total	C	N	O	S	0	0
			1750	1095	317	332	6		
14	1V	263	Total	C	N	O	S	0	0
			2168	1359	388	412	9		
14	2V	263	Total	C	N	O	S	0	0
			2168	1359	388	412	9		
14	3V	263	Total	C	N	O	S	0	0
			2168	1359	388	412	9		

- Molecule 15 is a protein called RIB43A protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	0X	106	Total	C	N	O	S	0	0
			903	553	170	175	5		
15	1X	141	Total	C	N	O	S	0	0
			1205	736	229	234	6		
15	2X	141	Total	C	N	O	S	0	0
			1205	736	229	234	6		
15	3X	141	Total	C	N	O	S	0	0
			1205	736	229	234	6		
15	4X	141	Total	C	N	O	S	0	0
			1205	736	229	234	6		

- Molecule 16 is a protein called RIB57.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1B	498	Total	C	N	O	S	0	0
			4066	2598	692	768	8		
16	2B	295	Total	C	N	O	S	0	0
			2439	1553	416	464	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	3B	297	Total	C	N	O	S	0	0
			2449	1558	418	467	6		

- Molecule 17 is a protein called CFAP182A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1F	136	Total	C	N	O	S	0	0
			1093	696	184	208	5		

- Molecule 18 is a protein called CFAP143.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1I	188	Total	C	N	O	S	0	0
			1546	951	285	306	4		

- Molecule 19 is a protein called CFAP21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1J	370	Total	C	N	O	S	0	0
			3025	1901	534	579	11		

- Molecule 20 is a protein called Cilia- and flagella-associated protein 53.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1K	273	Total	C	N	O	S	0	0
			2391	1479	447	458	7		
20	2K	284	Total	C	N	O	S	0	0
			2465	1517	455	486	7		

- Molecule 21 is a protein called CFAP115.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1L	820	Total	C	N	O	S	0	0
			6841	4357	1186	1280	18		
21	2L	620	Total	C	N	O	S	0	0
			5181	3304	902	963	12		
21	3L	200	Total	C	N	O	S	0	0
			1660	1053	284	317	6		

- Molecule 22 is a protein called Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1M	369	Total	C	N	O	S	0	0
			2978	1910	501	552	15		
22	2M	369	Total	C	N	O	S	0	0
			2978	1910	501	552	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1O	235	Total	C	N	O	S	0	0
			1983	1235	350	386	12		
23	2O	370	Total	C	N	O	S	0	0
			3173	1948	595	617	13		
23	3O	275	Total	C	N	O	S	0	0
			2358	1447	451	456	4		

- Molecule 24 is a protein called CFAP210.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1P	351	Total	C	N	O	S	0	0
			3026	1869	567	582	8		
24	2P	186	Total	C	N	O	S	0	0
			1594	983	299	307	5		

- Molecule 25 is a protein called RIB72B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1R	508	Total	C	N	O	S	0	0
			4244	2744	711	777	12		
25	2R	508	Total	C	N	O	S	0	0
			4244	2744	711	777	12		
25	3R	508	Total	C	N	O	S	0	0
			4244	2744	711	777	12		

- Molecule 26 is a protein called Protofilament ribbon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1W	220	Total	C	N	O	S	0	0
			1888	1143	372	364	9		
26	2W	111	Total	C	N	O	S	0	0
			949	585	183	176	5		

- Molecule 27 is a protein called RIB35.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2C	300	Total	C	N	O	S	0	0
			2467	1581	417	464	5		
27	3C	300	Total	C	N	O	S	0	0
			2467	1581	417	464	5		
27	4C	300	Total	C	N	O	S	0	0
			2467	1581	417	464	5		

- Molecule 28 is a protein called CFAP182B.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2F	87	Total	C	N	O	S	0	0
			746	469	136	137	4		

- Molecule 29 is a protein called Flagellar FliJ protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2G	99	Total	C	N	O	S	0	0
			848	536	153	155	4		

- Molecule 30 is a protein called RIB27B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2H	61	Total	C	N	O	S	0	0
			501	313	92	94	2		
30	3H	61	Total	C	N	O	S	0	0
			501	313	92	94	2		
30	4H	61	Total	C	N	O	S	0	0
			501	313	92	94	2		

- Molecule 31 is a protein called STPG2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2I	140	Total	C	N	O	S	0	0
			1132	726	198	207	1		
31	3I	87	Total	C	N	O	S	0	0
			712	451	130	127	4		

- Molecule 32 is a protein called RIB26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3D	237	Total	C	N	O	S	0	0
			1835	1174	310	340	11		

- Molecule 33 is a protein called CFAP129.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	4F	200	Total	C	N	O	S	0	0
			1623	1022	286	313	2		

- Molecule 34 is a protein called Flagellar microtubule protofilament ribbon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		
34	5R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		
34	6R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		
34	7R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		

- Molecule 35 is a protein called Parkin co-regulated protein PACRGB.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4S	188	Total	C	N	O	S	0	0
			1537	999	251	279	8		
35	5S	188	Total	C	N	O	S	0	0
			1537	999	251	279	8		

- Molecule 36 is a protein called OJ2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	5A	157	Total	C	N	O	S	0	0
			1261	795	234	229	3		
36	5B	157	Total	C	N	O	S	0	0
			1261	795	234	229	3		
36	5C	157	Total	C	N	O	S	0	0
			1261	795	234	229	3		
36	5D	109	Total	C	N	O	S	0	0
			872	551	157	161	3		

- Molecule 37 is a protein called CFAP77A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	5E	185	Total	C	N	O	S	0	0
			1543	977	278	283	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
37	5F	210	Total	C	N	O	S	0	0
			1750	1107	316	322	5		
37	5G	210	Total	C	N	O	S	0	0
			1750	1107	316	322	5		
37	5H	139	Total	C	N	O	S	0	0
			1146	725	207	210	4		

- Molecule 38 is a protein called OJ3.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	5I	99	Total	C	N	O	0	0
			495	297	99	99		
38	5J	109	Total	C	N	O	0	0
			545	327	109	109		
38	5K	76	Total	C	N	O	0	0
			380	228	76	76		

- Molecule 39 is a protein called SB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	6F	132	Total	C	N	O	S	0	0
			1141	718	197	222	4		

- Molecule 40 is a protein called STPG1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	6G	216	Total	C	N	O	S	0	0
			1769	1128	303	333	5		

- Molecule 41 is a protein called Nebulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	6H	165	Total	C	N	O	S	0	0
			1361	856	232	267	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6H	198	HIS	MET	conflict	UNP Q231B6
6H	199	MET	GLN	conflict	UNP Q231B6

- Molecule 42 is a protein called B5B6_fMIP.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	8L	385	Total	C	N	O	0	0
			1925	1155	385	385		
42	8N	358	Total	C	N	O	0	0
			1790	1074	358	358		

- Molecule 43 is a protein called CFAP112A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	8P	363	Total	C	N	O	0	0
			1815	1089	363	363		

- Molecule 44 is a protein called B2B3_fMIP.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	8R	361	Total	C	N	O	0	0
			2022	1269	361	392		

- Molecule 45 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	AC	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	AE	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	AG	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	AI	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	AK	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	AM	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	BA	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BC	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BE	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BG	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	BI	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BK	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	BM	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	CA	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	CC	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	CE	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	CG	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	CI	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	CK	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	CM	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	DA	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	DC	436	Total	C	N	O	S	0	0
			3391	2143	578	648	22		
45	DE	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	DG	436	Total	C	N	O	S	0	0
			3391	2143	578	648	22		
45	DI	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	DK	436	Total	C	N	O	S	0	0
			3391	2143	578	648	22		
45	DM	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	EA	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	EC	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	EE	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	EG	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	EI	439	Total 3410	C 2155	N 581	O 652	S 22	0	0
45	EK	439	Total 3410	C 2155	N 581	O 652	S 22	0	0
45	EM	439	Total 3410	C 2155	N 581	O 652	S 22	0	0
45	FA	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
45	FC	432	Total 3364	C 2129	N 571	O 642	S 22	0	0
45	FE	434	Total 3376	C 2135	N 573	O 646	S 22	0	0
45	FG	439	Total 3410	C 2155	N 581	O 652	S 22	0	0
45	FI	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
45	FK	432	Total 3364	C 2129	N 571	O 642	S 22	0	0
45	FM	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
45	GA	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
45	GC	431	Total 3358	C 2126	N 570	O 640	S 22	0	0
45	GE	431	Total 3358	C 2126	N 570	O 640	S 22	0	0
45	GG	431	Total 3358	C 2126	N 570	O 640	S 22	0	0
45	GI	431	Total 3358	C 2126	N 570	O 640	S 22	0	0
45	GK	439	Total 3410	C 2155	N 581	O 652	S 22	0	0
45	GM	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
45	HA	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	HC	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	HE	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	HG	431	Total 3356	C 2125	N 570	O 639	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	HI	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	HK	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	HM	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	IA	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	IC	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	IE	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	IG	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	II	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	IK	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	IM	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	JA	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	JC	434	Total	C	N	O	S	0	0
			3376	2135	573	646	22		
45	JE	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	JG	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	JI	439	Total	C	N	O	S	0	0
			3406	2151	581	652	22		
45	JK	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	JM	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	KA	434	Total	C	N	O	S	0	0
			3376	2135	573	646	22		
45	KC	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	KE	435	Total	C	N	O	S	0	0
			3387	2141	577	647	22		
45	KG	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	KI	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	KK	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	KM	434	Total	C	N	O	S	0	0
			3376	2135	573	646	22		
45	LA	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	LC	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	LE	438	Total	C	N	O	S	0	0
			3402	2149	580	651	22		
45	LG	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	LI	434	Total	C	N	O	S	0	0
			3383	2139	576	646	22		
45	LK	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	LM	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	MA	436	Total	C	N	O	S	0	0
			3394	2145	578	649	22		
45	MC	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	ME	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
45	MG	437	Total	C	N	O	S	0	0
			3402	2151	579	650	22		
45	MI	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	MK	436	Total	C	N	O	S	0	0
			3384	2139	575	648	22		
45	MM	436	Total	C	N	O	S	0	0
			3394	2145	578	649	22		
45	NA	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	NC	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	NE	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	NG	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	NI	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	NK	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
45	NM	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	OA	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OC	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OE	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OG	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OI	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OK	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	OM	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
45	PA	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PC	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PE	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PG	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PI	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PK	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	PM	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
45	QA	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	QC	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	QE	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	QG	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	QI	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	QK	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	QM	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	RA	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	RC	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	RE	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	RG	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	RI	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	RK	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	RM	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	SA	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	SC	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	SE	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	SG	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	SI	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	SK	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	SM	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	TA	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	TC	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	TE	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	TG	430	Total 3350	C 2122	N 569	O 637	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	TI	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	TK	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	TM	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
45	UA	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	UC	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	UE	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	UG	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	UI	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	UK	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	UM	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	VA	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
45	VC	439	Total 3410	C 2155	N 581	O 652	S 22	0	0
45	VE	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
45	VG	439	Total 3410	C 2155	N 581	O 652	S 22	0	0
45	VI	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
45	VK	439	Total 3410	C 2155	N 581	O 652	S 22	0	0
45	VM	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
45	WA	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	WC	439	Total 3410	C 2155	N 581	O 652	S 22	0	0
45	WE	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
45	WG	439	Total 3410	C 2155	N 581	O 652	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	WI	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
45	WK	439	Total	C	N	O	S	0	0
			3410	2155	581	652	22		
45	WM	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		

There are 161 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	40	ARG	LYS	variant	UNP P41351
AC	40	ARG	LYS	variant	UNP P41351
AE	40	ARG	LYS	variant	UNP P41351
AG	40	ARG	LYS	variant	UNP P41351
AI	40	ARG	LYS	variant	UNP P41351
AK	40	ARG	LYS	variant	UNP P41351
AM	40	ARG	LYS	variant	UNP P41351
BA	40	ARG	LYS	variant	UNP P41351
BC	40	ARG	LYS	variant	UNP P41351
BE	40	ARG	LYS	variant	UNP P41351
BG	40	ARG	LYS	variant	UNP P41351
BI	40	ARG	LYS	variant	UNP P41351
BK	40	ARG	LYS	variant	UNP P41351
BM	40	ARG	LYS	variant	UNP P41351
CA	40	ARG	LYS	variant	UNP P41351
CC	40	ARG	LYS	variant	UNP P41351
CE	40	ARG	LYS	variant	UNP P41351
CG	40	ARG	LYS	variant	UNP P41351
CI	40	ARG	LYS	variant	UNP P41351
CK	40	ARG	LYS	variant	UNP P41351
CM	40	ARG	LYS	variant	UNP P41351
DA	40	ARG	LYS	variant	UNP P41351
DC	40	ARG	LYS	variant	UNP P41351
DE	40	ARG	LYS	variant	UNP P41351
DG	40	ARG	LYS	variant	UNP P41351
DI	40	ARG	LYS	variant	UNP P41351
DK	40	ARG	LYS	variant	UNP P41351
DM	40	ARG	LYS	variant	UNP P41351
EA	40	ARG	LYS	variant	UNP P41351
EC	40	ARG	LYS	variant	UNP P41351
EE	40	ARG	LYS	variant	UNP P41351
EG	40	ARG	LYS	variant	UNP P41351

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Chain	Residue	Modelled	Actual	Comment	Reference
EI	40	ARG	LYS	variant	UNP P41351
EK	40	ARG	LYS	variant	UNP P41351
EM	40	ARG	LYS	variant	UNP P41351
FA	40	ARG	LYS	variant	UNP P41351
FC	40	ARG	LYS	variant	UNP P41351
FE	40	ARG	LYS	variant	UNP P41351
FG	40	ARG	LYS	variant	UNP P41351
FI	40	ARG	LYS	variant	UNP P41351
FK	40	ARG	LYS	variant	UNP P41351
FM	40	ARG	LYS	variant	UNP P41351
GA	40	ARG	LYS	variant	UNP P41351
GC	40	ARG	LYS	variant	UNP P41351
GE	40	ARG	LYS	variant	UNP P41351
GG	40	ARG	LYS	variant	UNP P41351
GI	40	ARG	LYS	variant	UNP P41351
GK	40	ARG	LYS	variant	UNP P41351
GM	40	ARG	LYS	variant	UNP P41351
HA	40	ARG	LYS	variant	UNP P41351
HC	40	ARG	LYS	variant	UNP P41351
HE	40	ARG	LYS	variant	UNP P41351
HG	40	ARG	LYS	variant	UNP P41351
HI	40	ARG	LYS	variant	UNP P41351
HK	40	ARG	LYS	variant	UNP P41351
HM	40	ARG	LYS	variant	UNP P41351
IA	40	ARG	LYS	variant	UNP P41351
IC	40	ARG	LYS	variant	UNP P41351
IE	40	ARG	LYS	variant	UNP P41351
IG	40	ARG	LYS	variant	UNP P41351
II	40	ARG	LYS	variant	UNP P41351
IK	40	ARG	LYS	variant	UNP P41351
IM	40	ARG	LYS	variant	UNP P41351
JA	40	ARG	LYS	variant	UNP P41351
JC	40	ARG	LYS	variant	UNP P41351
JE	40	ARG	LYS	variant	UNP P41351
JG	40	ARG	LYS	variant	UNP P41351
JI	40	ARG	LYS	variant	UNP P41351
JK	40	ARG	LYS	variant	UNP P41351
JM	40	ARG	LYS	variant	UNP P41351
KA	40	ARG	LYS	variant	UNP P41351
KC	40	ARG	LYS	variant	UNP P41351
KE	40	ARG	LYS	variant	UNP P41351
KG	40	ARG	LYS	variant	UNP P41351

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Chain	Residue	Modelled	Actual	Comment	Reference
KI	40	ARG	LYS	variant	UNP P41351
KK	40	ARG	LYS	variant	UNP P41351
KM	40	ARG	LYS	variant	UNP P41351
LA	40	ARG	LYS	variant	UNP P41351
LC	40	ARG	LYS	variant	UNP P41351
LE	40	ARG	LYS	variant	UNP P41351
LG	40	ARG	LYS	variant	UNP P41351
LI	40	ARG	LYS	variant	UNP P41351
LK	40	ARG	LYS	variant	UNP P41351
LM	40	ARG	LYS	variant	UNP P41351
MA	40	ARG	LYS	variant	UNP P41351
MC	40	ARG	LYS	variant	UNP P41351
ME	40	ARG	LYS	variant	UNP P41351
MG	40	ARG	LYS	variant	UNP P41351
MI	40	ARG	LYS	variant	UNP P41351
MK	40	ARG	LYS	variant	UNP P41351
MM	40	ARG	LYS	variant	UNP P41351
NA	40	ARG	LYS	variant	UNP P41351
NC	40	ARG	LYS	variant	UNP P41351
NE	40	ARG	LYS	variant	UNP P41351
NG	40	ARG	LYS	variant	UNP P41351
NI	40	ARG	LYS	variant	UNP P41351
NK	40	ARG	LYS	variant	UNP P41351
NM	40	ARG	LYS	variant	UNP P41351
OA	40	ARG	LYS	variant	UNP P41351
OC	40	ARG	LYS	variant	UNP P41351
OE	40	ARG	LYS	variant	UNP P41351
OG	40	ARG	LYS	variant	UNP P41351
OI	40	ARG	LYS	variant	UNP P41351
OK	40	ARG	LYS	variant	UNP P41351
OM	40	ARG	LYS	variant	UNP P41351
PA	40	ARG	LYS	variant	UNP P41351
PC	40	ARG	LYS	variant	UNP P41351
PE	40	ARG	LYS	variant	UNP P41351
PG	40	ARG	LYS	variant	UNP P41351
PI	40	ARG	LYS	variant	UNP P41351
PK	40	ARG	LYS	variant	UNP P41351
PM	40	ARG	LYS	variant	UNP P41351
QA	40	ARG	LYS	variant	UNP P41351
QC	40	ARG	LYS	variant	UNP P41351
QE	40	ARG	LYS	variant	UNP P41351
QG	40	ARG	LYS	variant	UNP P41351

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Chain	Residue	Modelled	Actual	Comment	Reference
QI	40	ARG	LYS	variant	UNP P41351
QK	40	ARG	LYS	variant	UNP P41351
QM	40	ARG	LYS	variant	UNP P41351
RA	40	ARG	LYS	variant	UNP P41351
RC	40	ARG	LYS	variant	UNP P41351
RE	40	ARG	LYS	variant	UNP P41351
RG	40	ARG	LYS	variant	UNP P41351
RI	40	ARG	LYS	variant	UNP P41351
RK	40	ARG	LYS	variant	UNP P41351
RM	40	ARG	LYS	variant	UNP P41351
SA	40	ARG	LYS	variant	UNP P41351
SC	40	ARG	LYS	variant	UNP P41351
SE	40	ARG	LYS	variant	UNP P41351
SG	40	ARG	LYS	variant	UNP P41351
SI	40	ARG	LYS	variant	UNP P41351
SK	40	ARG	LYS	variant	UNP P41351
SM	40	ARG	LYS	variant	UNP P41351
TA	40	ARG	LYS	variant	UNP P41351
TC	40	ARG	LYS	variant	UNP P41351
TE	40	ARG	LYS	variant	UNP P41351
TG	40	ARG	LYS	variant	UNP P41351
TI	40	ARG	LYS	variant	UNP P41351
TK	40	ARG	LYS	variant	UNP P41351
TM	40	ARG	LYS	variant	UNP P41351
UA	40	ARG	LYS	variant	UNP P41351
UC	40	ARG	LYS	variant	UNP P41351
UE	40	ARG	LYS	variant	UNP P41351
UG	40	ARG	LYS	variant	UNP P41351
UI	40	ARG	LYS	variant	UNP P41351
UK	40	ARG	LYS	variant	UNP P41351
UM	40	ARG	LYS	variant	UNP P41351
VA	40	ARG	LYS	variant	UNP P41351
VC	40	ARG	LYS	variant	UNP P41351
VE	40	ARG	LYS	variant	UNP P41351
VG	40	ARG	LYS	variant	UNP P41351
VI	40	ARG	LYS	variant	UNP P41351
VK	40	ARG	LYS	variant	UNP P41351
VM	40	ARG	LYS	variant	UNP P41351
WA	40	ARG	LYS	variant	UNP P41351
WC	40	ARG	LYS	variant	UNP P41351
WE	40	ARG	LYS	variant	UNP P41351
WG	40	ARG	LYS	variant	UNP P41351

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Chain	Residue	Modelled	Actual	Comment	Reference
WI	40	ARG	LYS	variant	UNP P41351
WK	40	ARG	LYS	variant	UNP P41351
WM	40	ARG	LYS	variant	UNP P41351

- Molecule 46 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	AN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BB	423	Total	C	N	O	S	0	0
			3304	2074	564	638	28		
46	BD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	BN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	CH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	CJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	CL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	CN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	DB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	DD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	DF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	DH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	DJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	DL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	DN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	EB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	ED	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	EF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	EH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	EJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	EL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	EN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	FB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	FD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	FF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	FH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	FJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	FL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	FN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	GB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	GD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	GF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	GH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	GJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	GL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	GN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	HB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	HD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	HF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	HH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	HJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	HL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	HN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	IB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	ID	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	IF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	IH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	IJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	IL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	IN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	JB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	JD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	JF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	JH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	JJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	JL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	JN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	KB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	KD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	KF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	KH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	KJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	KL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	KN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	LB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	LD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	LF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	LH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	LJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	LL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	LN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	MB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	MD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	MF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	MH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	MJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	ML	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	MN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	NB	423	Total 3304	C 2079	N 562	O 635	S 28	0	0
46	ND	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	NF	423	Total 3304	C 2079	N 562	O 635	S 28	0	0
46	NH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	NJ	423	Total 3304	C 2079	N 562	O 635	S 28	0	0
46	NL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	NN	423	Total 3304	C 2079	N 562	O 635	S 28	0	0
46	OB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	OD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	OF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	OH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	OJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	OL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	ON	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	PB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	PD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	PF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	PH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	PJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	PL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	PN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	QB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	QD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	QF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	QH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	QJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	QL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	QN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	RB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	RD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	RF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	RH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0

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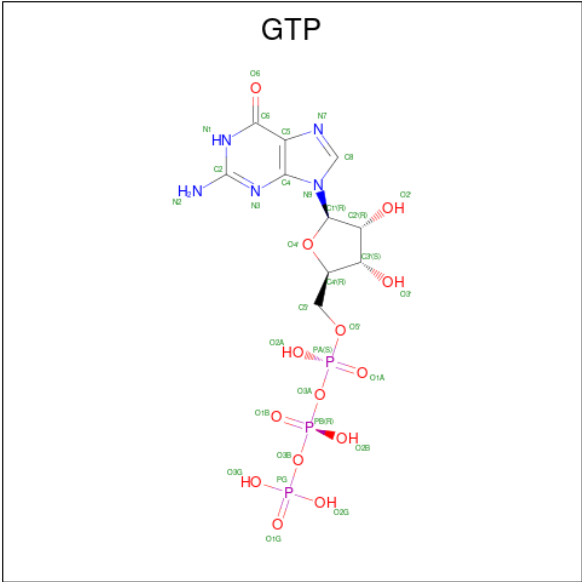
Mol	Chain	Residues	Atoms					AltConf	Trace
46	RJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	RL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	RN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	SB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	SD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	SF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	SH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	SJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	SL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	SN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	TB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	TD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	TF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	TH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	TJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	TL	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	TN	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	UB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	UD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	UF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
46	UH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
46	UJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	UL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	UN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	VN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
46	WN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

- Molecule 47 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
47	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	AM	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BA	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BC	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BI	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BK	1	Total	C	N	O	P	0
			32	10	5	14	3	
47	BM	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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Mol	Chain	Residues	Atoms					AltConf
47	FA	1	Total 32	C 10	N 5	O 14	P 3	0
47	FC	1	Total 32	C 10	N 5	O 14	P 3	0
47	FE	1	Total 32	C 10	N 5	O 14	P 3	0
47	FG	1	Total 32	C 10	N 5	O 14	P 3	0
47	FI	1	Total 32	C 10	N 5	O 14	P 3	0
47	FK	1	Total 32	C 10	N 5	O 14	P 3	0
47	FM	1	Total 32	C 10	N 5	O 14	P 3	0
47	GA	1	Total 32	C 10	N 5	O 14	P 3	0
47	GC	1	Total 32	C 10	N 5	O 14	P 3	0
47	GE	1	Total 32	C 10	N 5	O 14	P 3	0
47	GG	1	Total 32	C 10	N 5	O 14	P 3	0
47	GI	1	Total 32	C 10	N 5	O 14	P 3	0
47	GK	1	Total 32	C 10	N 5	O 14	P 3	0
47	GM	1	Total 32	C 10	N 5	O 14	P 3	0
47	HA	1	Total 32	C 10	N 5	O 14	P 3	0
47	HC	1	Total 32	C 10	N 5	O 14	P 3	0
47	HE	1	Total 32	C 10	N 5	O 14	P 3	0
47	HG	1	Total 32	C 10	N 5	O 14	P 3	0
47	HI	1	Total 32	C 10	N 5	O 14	P 3	0
47	HK	1	Total 32	C 10	N 5	O 14	P 3	0
47	HM	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
47	IA	1	Total 32	C 10	N 5	O 14	P 3	0
47	IC	1	Total 32	C 10	N 5	O 14	P 3	0
47	IE	1	Total 32	C 10	N 5	O 14	P 3	0
47	IG	1	Total 32	C 10	N 5	O 14	P 3	0
47	II	1	Total 32	C 10	N 5	O 14	P 3	0
47	IK	1	Total 32	C 10	N 5	O 14	P 3	0
47	IM	1	Total 32	C 10	N 5	O 14	P 3	0
47	JA	1	Total 32	C 10	N 5	O 14	P 3	0
47	JC	1	Total 32	C 10	N 5	O 14	P 3	0
47	JE	1	Total 32	C 10	N 5	O 14	P 3	0
47	JG	1	Total 32	C 10	N 5	O 14	P 3	0
47	JI	1	Total 32	C 10	N 5	O 14	P 3	0
47	JK	1	Total 32	C 10	N 5	O 14	P 3	0
47	JM	1	Total 32	C 10	N 5	O 14	P 3	0
47	KA	1	Total 32	C 10	N 5	O 14	P 3	0
47	KC	1	Total 32	C 10	N 5	O 14	P 3	0
47	KE	1	Total 32	C 10	N 5	O 14	P 3	0
47	KG	1	Total 32	C 10	N 5	O 14	P 3	0
47	KI	1	Total 32	C 10	N 5	O 14	P 3	0
47	KK	1	Total 32	C 10	N 5	O 14	P 3	0
47	KM	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
47	LA	1	Total 32	C 10	N 5	O 14	P 3	0
47	LC	1	Total 32	C 10	N 5	O 14	P 3	0
47	LE	1	Total 32	C 10	N 5	O 14	P 3	0
47	LG	1	Total 32	C 10	N 5	O 14	P 3	0
47	LI	1	Total 32	C 10	N 5	O 14	P 3	0
47	LK	1	Total 32	C 10	N 5	O 14	P 3	0
47	LM	1	Total 32	C 10	N 5	O 14	P 3	0
47	MA	1	Total 32	C 10	N 5	O 14	P 3	0
47	MC	1	Total 32	C 10	N 5	O 14	P 3	0
47	ME	1	Total 32	C 10	N 5	O 14	P 3	0
47	MG	1	Total 32	C 10	N 5	O 14	P 3	0
47	MI	1	Total 32	C 10	N 5	O 14	P 3	0
47	MK	1	Total 32	C 10	N 5	O 14	P 3	0
47	MM	1	Total 32	C 10	N 5	O 14	P 3	0
47	NA	1	Total 32	C 10	N 5	O 14	P 3	0
47	NC	1	Total 32	C 10	N 5	O 14	P 3	0
47	NE	1	Total 32	C 10	N 5	O 14	P 3	0
47	NG	1	Total 32	C 10	N 5	O 14	P 3	0
47	NI	1	Total 32	C 10	N 5	O 14	P 3	0
47	NK	1	Total 32	C 10	N 5	O 14	P 3	0
47	NM	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
47	OA	1	Total 32	C 10	N 5	O 14	P 3	0
47	OC	1	Total 32	C 10	N 5	O 14	P 3	0
47	OE	1	Total 32	C 10	N 5	O 14	P 3	0
47	OG	1	Total 32	C 10	N 5	O 14	P 3	0
47	OI	1	Total 32	C 10	N 5	O 14	P 3	0
47	OK	1	Total 32	C 10	N 5	O 14	P 3	0
47	OM	1	Total 32	C 10	N 5	O 14	P 3	0
47	PA	1	Total 32	C 10	N 5	O 14	P 3	0
47	PC	1	Total 32	C 10	N 5	O 14	P 3	0
47	PE	1	Total 32	C 10	N 5	O 14	P 3	0
47	PG	1	Total 32	C 10	N 5	O 14	P 3	0
47	PI	1	Total 32	C 10	N 5	O 14	P 3	0
47	PK	1	Total 32	C 10	N 5	O 14	P 3	0
47	PM	1	Total 32	C 10	N 5	O 14	P 3	0
47	QA	1	Total 32	C 10	N 5	O 14	P 3	0
47	QC	1	Total 32	C 10	N 5	O 14	P 3	0
47	QE	1	Total 32	C 10	N 5	O 14	P 3	0
47	QG	1	Total 32	C 10	N 5	O 14	P 3	0
47	QI	1	Total 32	C 10	N 5	O 14	P 3	0
47	QK	1	Total 32	C 10	N 5	O 14	P 3	0
47	QM	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
47	RA	1	Total 32	C 10	N 5	O 14	P 3	0
47	RC	1	Total 32	C 10	N 5	O 14	P 3	0
47	RE	1	Total 32	C 10	N 5	O 14	P 3	0
47	RG	1	Total 32	C 10	N 5	O 14	P 3	0
47	RI	1	Total 32	C 10	N 5	O 14	P 3	0
47	RK	1	Total 32	C 10	N 5	O 14	P 3	0
47	RM	1	Total 32	C 10	N 5	O 14	P 3	0
47	SA	1	Total 32	C 10	N 5	O 14	P 3	0
47	SC	1	Total 32	C 10	N 5	O 14	P 3	0
47	SE	1	Total 32	C 10	N 5	O 14	P 3	0
47	SG	1	Total 32	C 10	N 5	O 14	P 3	0
47	SI	1	Total 32	C 10	N 5	O 14	P 3	0
47	SK	1	Total 32	C 10	N 5	O 14	P 3	0
47	SM	1	Total 32	C 10	N 5	O 14	P 3	0
47	TA	1	Total 32	C 10	N 5	O 14	P 3	0
47	TC	1	Total 32	C 10	N 5	O 14	P 3	0
47	TE	1	Total 32	C 10	N 5	O 14	P 3	0
47	TG	1	Total 32	C 10	N 5	O 14	P 3	0
47	TI	1	Total 32	C 10	N 5	O 14	P 3	0
47	TK	1	Total 32	C 10	N 5	O 14	P 3	0
47	TM	1	Total 32	C 10	N 5	O 14	P 3	0

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

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
48	AA	1	Total 1	Mg 1	0
48	AC	1	Total 1	Mg 1	0
48	AE	1	Total 1	Mg 1	0
48	AG	1	Total 1	Mg 1	0
48	AI	1	Total 1	Mg 1	0
48	AL	1	Total 1	Mg 1	0
48	AM	1	Total 1	Mg 1	0
48	BB	1	Total 1	Mg 1	0
48	BC	1	Total 1	Mg 1	0
48	BE	1	Total 1	Mg 1	0
48	BG	1	Total 1	Mg 1	0
48	BI	1	Total 1	Mg 1	0
48	BK	1	Total 1	Mg 1	0
48	BM	1	Total 1	Mg 1	0
48	CA	1	Total 1	Mg 1	0
48	CC	1	Total 1	Mg 1	0
48	CE	1	Total 1	Mg 1	0
48	CG	1	Total 1	Mg 1	0
48	CI	1	Total 1	Mg 1	0
48	CK	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
48	CM	1	Total 1	Mg 1	0
48	DA	1	Total 1	Mg 1	0
48	DC	1	Total 1	Mg 1	0
48	DE	1	Total 1	Mg 1	0
48	DG	1	Total 1	Mg 1	0
48	DI	1	Total 1	Mg 1	0
48	DK	1	Total 1	Mg 1	0
48	DM	1	Total 1	Mg 1	0
48	EA	1	Total 1	Mg 1	0
48	EC	1	Total 1	Mg 1	0
48	EE	1	Total 1	Mg 1	0
48	EG	1	Total 1	Mg 1	0
48	EI	1	Total 1	Mg 1	0
48	EK	1	Total 1	Mg 1	0
48	EM	1	Total 1	Mg 1	0
48	FA	1	Total 1	Mg 1	0
48	FC	1	Total 1	Mg 1	0
48	FE	1	Total 1	Mg 1	0
48	FG	1	Total 1	Mg 1	0
48	FI	1	Total 1	Mg 1	0
48	FK	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
48	FM	1	Total 1	Mg 1	0
48	GB	1	Total 1	Mg 1	0
48	GC	1	Total 1	Mg 1	0
48	GE	1	Total 1	Mg 1	0
48	GG	1	Total 1	Mg 1	0
48	GI	1	Total 1	Mg 1	0
48	GK	1	Total 1	Mg 1	0
48	GM	1	Total 1	Mg 1	0
48	HA	1	Total 1	Mg 1	0
48	HC	1	Total 1	Mg 1	0
48	HE	1	Total 1	Mg 1	0
48	HG	1	Total 1	Mg 1	0
48	HI	1	Total 1	Mg 1	0
48	HK	1	Total 1	Mg 1	0
48	HM	1	Total 1	Mg 1	0
48	IA	1	Total 1	Mg 1	0
48	IC	1	Total 1	Mg 1	0
48	IE	1	Total 1	Mg 1	0
48	IG	1	Total 1	Mg 1	0
48	II	1	Total 1	Mg 1	0
48	IK	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
48	IM	1	Total 1	Mg 1	0
48	JA	1	Total 1	Mg 1	0
48	JC	1	Total 1	Mg 1	0
48	JE	1	Total 1	Mg 1	0
48	JG	1	Total 1	Mg 1	0
48	JI	1	Total 1	Mg 1	0
48	JK	1	Total 1	Mg 1	0
48	JM	1	Total 1	Mg 1	0
48	KA	1	Total 1	Mg 1	0
48	KC	1	Total 1	Mg 1	0
48	KE	1	Total 1	Mg 1	0
48	KG	1	Total 1	Mg 1	0
48	KI	1	Total 1	Mg 1	0
48	KK	1	Total 1	Mg 1	0
48	KM	1	Total 1	Mg 1	0
48	LA	1	Total 1	Mg 1	0
48	LC	1	Total 1	Mg 1	0
48	LE	1	Total 1	Mg 1	0
48	LG	1	Total 1	Mg 1	0
48	LI	1	Total 1	Mg 1	0
48	LK	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
48	LM	1	Total 1	Mg 1	0
48	MA	1	Total 1	Mg 1	0
48	MC	1	Total 1	Mg 1	0
48	ME	1	Total 1	Mg 1	0
48	MG	1	Total 1	Mg 1	0
48	MI	1	Total 1	Mg 1	0
48	MK	1	Total 1	Mg 1	0
48	MM	1	Total 1	Mg 1	0
48	NB	1	Total 1	Mg 1	0
48	NC	1	Total 1	Mg 1	0
48	NE	1	Total 1	Mg 1	0
48	NG	1	Total 1	Mg 1	0
48	NI	1	Total 1	Mg 1	0
48	NK	1	Total 1	Mg 1	0
48	NM	1	Total 1	Mg 1	0
48	OA	1	Total 1	Mg 1	0
48	OC	1	Total 1	Mg 1	0
48	OE	1	Total 1	Mg 1	0
48	OG	1	Total 1	Mg 1	0
48	OI	1	Total 1	Mg 1	0
48	OK	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
48	OM	1	Total 1	Mg 1	0
48	PA	1	Total 1	Mg 1	0
48	PC	1	Total 1	Mg 1	0
48	PE	1	Total 1	Mg 1	0
48	PG	1	Total 1	Mg 1	0
48	PI	1	Total 1	Mg 1	0
48	PK	1	Total 1	Mg 1	0
48	PM	1	Total 1	Mg 1	0
48	QA	1	Total 1	Mg 1	0
48	QC	1	Total 1	Mg 1	0
48	QE	1	Total 1	Mg 1	0
48	QG	1	Total 1	Mg 1	0
48	QI	1	Total 1	Mg 1	0
48	QK	1	Total 1	Mg 1	0
48	QM	1	Total 1	Mg 1	0
48	RA	1	Total 1	Mg 1	0
48	RC	1	Total 1	Mg 1	0
48	RE	1	Total 1	Mg 1	0
48	RF	1	Total 1	Mg 1	0
48	RI	1	Total 1	Mg 1	0
48	RK	1	Total 1	Mg 1	0

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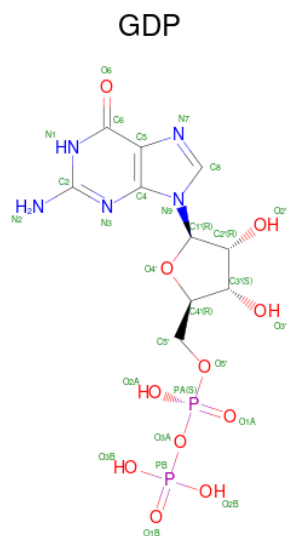
Mol	Chain	Residues	Atoms		AltConf
48	RM	1	Total 1	Mg 1	0
48	SA	1	Total 1	Mg 1	0
48	SB	1	Total 1	Mg 1	0
48	SE	1	Total 1	Mg 1	0
48	SG	1	Total 1	Mg 1	0
48	SI	1	Total 1	Mg 1	0
48	SK	1	Total 1	Mg 1	0
48	SM	1	Total 1	Mg 1	0
48	TA	1	Total 1	Mg 1	0
48	TC	1	Total 1	Mg 1	0
48	TE	1	Total 1	Mg 1	0
48	TG	1	Total 1	Mg 1	0
48	TI	1	Total 1	Mg 1	0
48	TK	1	Total 1	Mg 1	0
48	TM	1	Total 1	Mg 1	0
48	UA	1	Total 1	Mg 1	0
48	UC	1	Total 1	Mg 1	0
48	UE	1	Total 1	Mg 1	0
48	UG	1	Total 1	Mg 1	0
48	UI	1	Total 1	Mg 1	0
48	UK	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
48	UM	1	Total 1	Mg 1	0
48	VA	1	Total 1	Mg 1	0
48	VC	1	Total 1	Mg 1	0
48	VE	1	Total 1	Mg 1	0
48	VG	1	Total 1	Mg 1	0
48	VI	1	Total 1	Mg 1	0
48	VK	1	Total 1	Mg 1	0
48	VM	1	Total 1	Mg 1	0
48	WA	1	Total 1	Mg 1	0
48	WC	1	Total 1	Mg 1	0
48	WE	1	Total 1	Mg 1	0
48	WG	1	Total 1	Mg 1	0
48	WI	1	Total 1	Mg 1	0
48	WK	1	Total 1	Mg 1	0
48	WM	1	Total 1	Mg 1	0

- Molecule 49 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
49	AB	1	Total 28	C 10	N 5	O 11	P 2	0
49	AD	1	Total 28	C 10	N 5	O 11	P 2	0
49	AF	1	Total 28	C 10	N 5	O 11	P 2	0
49	AH	1	Total 28	C 10	N 5	O 11	P 2	0
49	AJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	AL	1	Total 28	C 10	N 5	O 11	P 2	0
49	AN	1	Total 28	C 10	N 5	O 11	P 2	0
49	BB	1	Total 28	C 10	N 5	O 11	P 2	0
49	BD	1	Total 28	C 10	N 5	O 11	P 2	0
49	BF	1	Total 28	C 10	N 5	O 11	P 2	0
49	BH	1	Total 28	C 10	N 5	O 11	P 2	0
49	BJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	BL	1	Total 28	C 10	N 5	O 11	P 2	0
49	BN	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
49	CB	1	Total 28	C 10	N 5	O 11	P 2	0
49	CD	1	Total 28	C 10	N 5	O 11	P 2	0
49	CF	1	Total 28	C 10	N 5	O 11	P 2	0
49	CH	1	Total 28	C 10	N 5	O 11	P 2	0
49	CJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	CL	1	Total 28	C 10	N 5	O 11	P 2	0
49	CN	1	Total 28	C 10	N 5	O 11	P 2	0
49	DB	1	Total 28	C 10	N 5	O 11	P 2	0
49	DD	1	Total 28	C 10	N 5	O 11	P 2	0
49	DF	1	Total 28	C 10	N 5	O 11	P 2	0
49	DH	1	Total 28	C 10	N 5	O 11	P 2	0
49	DJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	DL	1	Total 28	C 10	N 5	O 11	P 2	0
49	DN	1	Total 28	C 10	N 5	O 11	P 2	0
49	EB	1	Total 28	C 10	N 5	O 11	P 2	0
49	ED	1	Total 28	C 10	N 5	O 11	P 2	0
49	EF	1	Total 28	C 10	N 5	O 11	P 2	0
49	EH	1	Total 28	C 10	N 5	O 11	P 2	0
49	EJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	EL	1	Total 28	C 10	N 5	O 11	P 2	0
49	EN	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
49	FB	1	Total 28	C 10	N 5	O 11	P 2	0
49	FD	1	Total 28	C 10	N 5	O 11	P 2	0
49	FF	1	Total 28	C 10	N 5	O 11	P 2	0
49	FH	1	Total 28	C 10	N 5	O 11	P 2	0
49	FJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	FL	1	Total 28	C 10	N 5	O 11	P 2	0
49	FN	1	Total 28	C 10	N 5	O 11	P 2	0
49	GB	1	Total 28	C 10	N 5	O 11	P 2	0
49	GD	1	Total 28	C 10	N 5	O 11	P 2	0
49	GF	1	Total 28	C 10	N 5	O 11	P 2	0
49	GH	1	Total 28	C 10	N 5	O 11	P 2	0
49	GJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	GL	1	Total 28	C 10	N 5	O 11	P 2	0
49	GN	1	Total 28	C 10	N 5	O 11	P 2	0
49	HB	1	Total 28	C 10	N 5	O 11	P 2	0
49	HD	1	Total 28	C 10	N 5	O 11	P 2	0
49	HF	1	Total 28	C 10	N 5	O 11	P 2	0
49	HH	1	Total 28	C 10	N 5	O 11	P 2	0
49	HJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	HL	1	Total 28	C 10	N 5	O 11	P 2	0
49	HN	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
49	IB	1	Total 28	C 10	N 5	O 11	P 2	0
49	ID	1	Total 28	C 10	N 5	O 11	P 2	0
49	IF	1	Total 28	C 10	N 5	O 11	P 2	0
49	IH	1	Total 28	C 10	N 5	O 11	P 2	0
49	IJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	IL	1	Total 28	C 10	N 5	O 11	P 2	0
49	IN	1	Total 28	C 10	N 5	O 11	P 2	0
49	JB	1	Total 28	C 10	N 5	O 11	P 2	0
49	JD	1	Total 28	C 10	N 5	O 11	P 2	0
49	JF	1	Total 28	C 10	N 5	O 11	P 2	0
49	JH	1	Total 28	C 10	N 5	O 11	P 2	0
49	JJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	JL	1	Total 28	C 10	N 5	O 11	P 2	0
49	JN	1	Total 28	C 10	N 5	O 11	P 2	0
49	KB	1	Total 28	C 10	N 5	O 11	P 2	0
49	KD	1	Total 28	C 10	N 5	O 11	P 2	0
49	KF	1	Total 28	C 10	N 5	O 11	P 2	0
49	KH	1	Total 28	C 10	N 5	O 11	P 2	0
49	KJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	KL	1	Total 28	C 10	N 5	O 11	P 2	0
49	KN	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
49	LB	1	Total 28	C 10	N 5	O 11	P 2	0
49	LD	1	Total 28	C 10	N 5	O 11	P 2	0
49	LF	1	Total 28	C 10	N 5	O 11	P 2	0
49	LH	1	Total 28	C 10	N 5	O 11	P 2	0
49	LJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	LL	1	Total 28	C 10	N 5	O 11	P 2	0
49	LN	1	Total 28	C 10	N 5	O 11	P 2	0
49	MB	1	Total 28	C 10	N 5	O 11	P 2	0
49	MD	1	Total 28	C 10	N 5	O 11	P 2	0
49	MF	1	Total 28	C 10	N 5	O 11	P 2	0
49	MH	1	Total 28	C 10	N 5	O 11	P 2	0
49	MJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	ML	1	Total 28	C 10	N 5	O 11	P 2	0
49	MN	1	Total 28	C 10	N 5	O 11	P 2	0
49	NB	1	Total 28	C 10	N 5	O 11	P 2	0
49	ND	1	Total 28	C 10	N 5	O 11	P 2	0
49	NF	1	Total 28	C 10	N 5	O 11	P 2	0
49	NH	1	Total 28	C 10	N 5	O 11	P 2	0
49	NJ	1	Total 28	C 10	N 5	O 11	P 2	0
49	NL	1	Total 28	C 10	N 5	O 11	P 2	0
49	NN	1	Total 28	C 10	N 5	O 11	P 2	0

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	RB	1	28	10	5	11	2	0
49	RD	1	28	10	5	11	2	0
49	RF	1	28	10	5	11	2	0
49	RH	1	28	10	5	11	2	0
49	RJ	1	28	10	5	11	2	0
49	RL	1	28	10	5	11	2	0
49	RN	1	28	10	5	11	2	0
49	SB	1	28	10	5	11	2	0
49	SD	1	28	10	5	11	2	0
49	SF	1	28	10	5	11	2	0
49	SH	1	28	10	5	11	2	0
49	SJ	1	28	10	5	11	2	0
49	SL	1	28	10	5	11	2	0
49	SN	1	28	10	5	11	2	0
49	TB	1	28	10	5	11	2	0
49	TD	1	28	10	5	11	2	0
49	TF	1	28	10	5	11	2	0
49	TH	1	28	10	5	11	2	0
49	TJ	1	28	10	5	11	2	0
49	TL	1	28	10	5	11	2	0
49	TN	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
49	UB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	UN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	VN	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WB	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WD	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WF	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WH	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WL	1	Total	C	N	O	P	0
			28	10	5	11	2	
49	WN	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	182355	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.387	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	701.44, 701.44, 701.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.37, 1.37, 1.37	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 483 ligands modelled in this entry, 161 are monoatomic - leaving 322 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	GDP	FD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	JK	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	TA	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	DE	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	NC	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	KG	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	SH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	UC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	HJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	JN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	FE	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	AD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	PD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	LD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	FN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	QG	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	GA	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	JE	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.61	9 (18%)
47	GTP	TE	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	SN	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	7 (15%)
49	GDP	VJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	CI	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	WF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	EL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	TN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	LE	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	FI	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	8 (16%)
47	GTP	FG	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	HE	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	OM	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	LA	501	48	33,34,34	0.98	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	PE	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.61	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	GDP	QN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	IJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	VL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	VC	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.62	9 (18%)
47	GTP	UE	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	NI	501	48	33,34,34	0.97	2 (6%)	50,54,54	1.57	8 (16%)
49	GDP	SJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	GM	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	MD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	RG	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
47	GTP	QI	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	GI	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	GJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	DD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	WN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	SG	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	KA	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	HC	501	48	33,34,34	0.99	2 (6%)	50,54,54	1.61	9 (18%)
47	GTP	OI	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.56	9 (18%)
47	GTP	OG	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.57	8 (16%)
49	GDP	HB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	VF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	AG	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	OF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	VA	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	DG	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	UA	501	48	33,34,34	0.99	2 (6%)	50,54,54	1.57	9 (18%)
47	GTP	MK	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	GD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	BA	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	KH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	OK	501	48	33,34,34	0.96	2 (6%)	50,54,54	1.58	9 (18%)
49	GDP	AH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	SM	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.61	9 (18%)
47	GTP	TC	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	GTP	SK	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.56	8 (16%)
49	GDP	FL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	CC	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.61	9 (18%)
49	GDP	DJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	AL	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	ME	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	WA	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.56	9 (18%)
47	GTP	LM	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	VN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	SF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	BG	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
49	GDP	CN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	NL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	NG	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.56	9 (18%)
47	GTP	JA	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	PC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	UI	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	EF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	TD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	QD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	EN	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.77	7 (15%)
47	GTP	HM	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	GN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	GL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	BH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	BE	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.58	8 (16%)
47	GTP	MI	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	CF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
47	GTP	MG	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	IH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	DN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	8 (17%)
47	GTP	IK	502	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	UM	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	LH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	EJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	GDP	ID	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	UF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	VB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	WH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
47	GTP	MC	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	TF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	UD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	GH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	NK	501	48	33,34,34	0.97	2 (6%)	50,54,54	1.57	9 (18%)
47	GTP	NM	501	48	33,34,34	0.98	2 (6%)	50,54,54	1.57	8 (16%)
49	GDP	PB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	LK	501	48	33,34,34	0.96	2 (6%)	50,54,54	1.57	9 (18%)
47	GTP	AA	501	48	33,34,34	0.98	2 (6%)	50,54,54	1.59	9 (18%)
49	GDP	QH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	DH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	JH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	6 (13%)
47	GTP	QM	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	WJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	FF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	SC	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	DM	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	MM	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	EC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	TG	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.56	9 (18%)
49	GDP	HF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
47	GTP	BC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	AC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	UG	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
47	GTP	JI	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	VK	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	EI	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	SD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	BN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	UL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	MA	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	GTP	IG	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	HK	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	KC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	HG	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	QA	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	SE	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.56	9 (18%)
47	GTP	CM	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	AE	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	FH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	RE	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	KM	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	VD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	KJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	RM	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	PH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	JJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	VM	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
47	GTP	IA	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	RJ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	QC	501	48	33,34,34	0.98	2 (6%)	50,54,54	1.60	9 (18%)
49	GDP	NF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	NN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	EG	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	LC	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	8 (16%)
49	GDP	CL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	PK	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	OB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	CG	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	LN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	PG	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	OJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	CK	501	48	33,34,34	0.99	2 (6%)	50,54,54	1.59	9 (18%)
49	GDP	OD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	WD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	JM	501	48	33,34,34	0.99	3 (9%)	50,54,54	1.59	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	GDP	GF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	UJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	PJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	BI	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	SL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	IL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	FJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	JG	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	FB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	HA	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	KI	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	GE	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.62	9 (18%)
49	GDP	BB	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	DK	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
47	GTP	EE	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	JC	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	FA	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	WK	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	VH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
47	GTP	RC	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	NA	501	48	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
47	GTP	NE	501	48	33,34,34	0.97	2 (6%)	50,54,54	1.57	8 (16%)
47	GTP	FK	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	MB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	CA	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	FM	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.65	9 (18%)
47	GTP	AI	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	IE	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	JD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	QJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	EH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	MH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	OL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	NJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	JF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	GTP	II	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	ND	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	LL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
49	GDP	RB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	GB	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	SI	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	TB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	DA	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	EM	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	BL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	QK	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	WB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	IN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	TL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	RD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	PA	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	DB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	AN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	SB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	TH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	ED	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
47	GTP	LI	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	HN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	KN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
49	GDP	BD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	DL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	EB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	KB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	FC	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	NH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	DF	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.76	7 (15%)
49	GDP	AB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	QF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	RL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	UN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	GTP	IM	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	WL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	TK	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
49	GDP	JL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
47	GTP	VE	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	JB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	RF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	UH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
47	GTP	GK	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	ML	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	VG	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.61	9 (18%)
49	GDP	KF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	GC	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	LF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	LG	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	LJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	KD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	TJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	NB	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
47	GTP	OA	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	UB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	VI	501	48	33,34,34	0.98	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	MN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
47	GTP	HI	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	AJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	BM	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	RK	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	AM	501	48	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	UK	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	OC	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	PI	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	DC	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	KE	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
47	GTP	DI	501	48	33,34,34	0.98	3 (9%)	50,54,54	1.61	9 (18%)
47	GTP	KK	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	GDP	IB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	GG	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
47	GTP	OE	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	LB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	MF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	PM	501	48	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	IF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
49	GDP	RN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	HD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
49	GDP	CB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	QL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	EA	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.56	9 (18%)
47	GTP	CE	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	WI	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	HL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	RA	501	48	33,34,34	0.98	1 (3%)	50,54,54	1.60	9 (18%)
49	GDP	KL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	SA	501	48	33,34,34	0.98	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	PL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
49	GDP	OH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	IC	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.61	9 (18%)
47	GTP	WG	501	48	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
47	GTP	AK	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
49	GDP	QB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	CD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	PF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
47	GTP	WE	501	48	33,34,34	0.95	2 (6%)	50,54,54	1.58	8 (16%)
49	GDP	BF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.73	7 (15%)
47	GTP	EK	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	AF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	BK	501	48	33,34,34	0.96	2 (6%)	50,54,54	1.58	9 (18%)
47	GTP	QE	501	48	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
49	GDP	BJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	HH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
49	GDP	ON	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	GTP	TI	501	48	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
47	GTP	WC	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
47	GTP	WM	501	48	33,34,34	0.98	2 (6%)	50,54,54	1.58	10 (20%)
47	GTP	RI	501	48	33,34,34	0.96	1 (3%)	50,54,54	1.61	9 (18%)
49	GDP	RH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	PN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	CH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
47	GTP	TM	501	48	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
49	GDP	MJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
49	GDP	CJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	GDP	FD	501	-	-	0/16/32/32	0/3/3/3
47	GTP	JK	501	48	-	6/22/38/38	0/3/3/3
47	GTP	TA	501	48	-	8/22/38/38	0/3/3/3
47	GTP	DE	501	48	-	7/22/38/38	0/3/3/3
47	GTP	NC	501	48	-	5/22/38/38	0/3/3/3
47	GTP	KG	501	48	-	7/22/38/38	0/3/3/3
49	GDP	SH	501	-	-	0/16/32/32	0/3/3/3
47	GTP	UC	501	48	-	7/22/38/38	0/3/3/3
49	GDP	HJ	501	-	-	0/16/32/32	0/3/3/3
49	GDP	JN	501	-	-	1/16/32/32	0/3/3/3
47	GTP	FE	501	48	-	9/22/38/38	0/3/3/3
49	GDP	AD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	PD	501	-	-	0/16/32/32	0/3/3/3
49	GDP	LD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	FN	501	-	-	1/16/32/32	0/3/3/3
47	GTP	QG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	GA	501	48	-	7/22/38/38	0/3/3/3
47	GTP	JE	501	48	-	6/22/38/38	0/3/3/3
47	GTP	TE	501	48	-	9/22/38/38	0/3/3/3
49	GDP	SN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	VJ	501	-	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	CI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	WF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	EL	501	-	-	1/16/32/32	0/3/3/3
49	GDP	TN	501	-	-	1/16/32/32	0/3/3/3
47	GTP	LE	501	48	-	8/22/38/38	0/3/3/3
47	GTP	FI	501	48	-	5/22/38/38	0/3/3/3
47	GTP	FG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	HE	501	48	-	8/22/38/38	0/3/3/3
47	GTP	OM	501	48	-	3/22/38/38	0/3/3/3
47	GTP	LA	501	48	-	5/22/38/38	0/3/3/3
47	GTP	PE	501	48	-	8/22/38/38	0/3/3/3
49	GDP	QN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	IJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	VL	501	-	-	1/16/32/32	0/3/3/3
47	GTP	VC	501	48	-	7/22/38/38	0/3/3/3
47	GTP	UE	501	48	-	8/22/38/38	0/3/3/3
47	GTP	NI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	SJ	501	-	-	1/16/32/32	0/3/3/3
47	GTP	GM	501	48	-	6/22/38/38	0/3/3/3
49	GDP	MD	501	-	-	2/16/32/32	0/3/3/3
47	GTP	RG	501	48	-	7/22/38/38	0/3/3/3
47	GTP	QI	501	48	-	5/22/38/38	0/3/3/3
47	GTP	GI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	GJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	DD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	WN	501	-	-	0/16/32/32	0/3/3/3
47	GTP	SG	501	48	-	4/22/38/38	0/3/3/3
47	GTP	KA	501	48	-	7/22/38/38	0/3/3/3
47	GTP	HC	501	48	-	5/22/38/38	0/3/3/3
47	GTP	OI	501	48	-	4/22/38/38	0/3/3/3
47	GTP	OG	501	48	-	5/22/38/38	0/3/3/3
49	GDP	HB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	VF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	AG	501	48	-	6/22/38/38	0/3/3/3
49	GDP	OF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	VA	501	48	-	5/22/38/38	0/3/3/3
47	GTP	DG	501	48	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	UA	501	48	-	5/22/38/38	0/3/3/3
47	GTP	MK	501	48	-	8/22/38/38	0/3/3/3
49	GDP	GD	501	-	-	1/16/32/32	0/3/3/3
47	GTP	BA	501	48	-	7/22/38/38	0/3/3/3
49	GDP	KH	501	-	-	1/16/32/32	0/3/3/3
47	GTP	OK	501	48	-	5/22/38/38	0/3/3/3
49	GDP	AH	501	-	-	1/16/32/32	0/3/3/3
47	GTP	SM	501	48	-	8/22/38/38	0/3/3/3
47	GTP	TC	501	48	-	9/22/38/38	0/3/3/3
47	GTP	SK	501	48	-	5/22/38/38	0/3/3/3
49	GDP	FL	501	-	-	1/16/32/32	0/3/3/3
47	GTP	CC	501	48	-	5/22/38/38	0/3/3/3
49	GDP	DJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	AL	502	-	-	1/16/32/32	0/3/3/3
47	GTP	ME	501	48	-	8/22/38/38	0/3/3/3
47	GTP	WA	501	48	-	8/22/38/38	0/3/3/3
47	GTP	LM	501	48	-	6/22/38/38	0/3/3/3
49	GDP	VN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	SF	501	-	-	2/16/32/32	0/3/3/3
47	GTP	BG	501	48	-	8/22/38/38	0/3/3/3
49	GDP	CN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	NL	501	-	-	3/16/32/32	0/3/3/3
47	GTP	NG	501	48	-	6/22/38/38	0/3/3/3
47	GTP	JA	501	48	-	5/22/38/38	0/3/3/3
47	GTP	PC	501	48	-	7/22/38/38	0/3/3/3
47	GTP	UI	501	48	-	5/22/38/38	0/3/3/3
49	GDP	EF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	TD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	QD	501	-	-	0/16/32/32	0/3/3/3
49	GDP	EN	501	-	-	0/16/32/32	0/3/3/3
47	GTP	HM	501	48	-	8/22/38/38	0/3/3/3
49	GDP	GN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	GL	501	-	-	0/16/32/32	0/3/3/3
49	GDP	BH	501	-	-	1/16/32/32	0/3/3/3
47	GTP	BE	501	48	-	5/22/38/38	0/3/3/3
47	GTP	MI	501	48	-	8/22/38/38	0/3/3/3
49	GDP	CF	501	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	MG	501	48	-	7/22/38/38	0/3/3/3
49	GDP	IH	501	-	-	2/16/32/32	0/3/3/3
49	GDP	DN	501	-	-	1/16/32/32	0/3/3/3
47	GTP	IK	502	48	-	7/22/38/38	0/3/3/3
47	GTP	UM	501	48	-	7/22/38/38	0/3/3/3
49	GDP	LH	501	-	-	2/16/32/32	0/3/3/3
49	GDP	EJ	501	-	-	2/16/32/32	0/3/3/3
49	GDP	ID	501	-	-	0/16/32/32	0/3/3/3
49	GDP	UF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	VB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	WH	501	-	-	2/16/32/32	0/3/3/3
47	GTP	MC	501	48	-	7/22/38/38	0/3/3/3
49	GDP	TF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	UD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	GH	501	-	-	0/16/32/32	0/3/3/3
47	GTP	NK	501	48	-	6/22/38/38	0/3/3/3
47	GTP	NM	501	48	-	8/22/38/38	0/3/3/3
49	GDP	PB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	LK	501	48	-	5/22/38/38	0/3/3/3
47	GTP	AA	501	48	-	4/22/38/38	0/3/3/3
49	GDP	QH	501	-	-	0/16/32/32	0/3/3/3
49	GDP	DH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	JH	501	-	-	1/16/32/32	0/3/3/3
47	GTP	QM	501	48	-	8/22/38/38	0/3/3/3
49	GDP	WJ	501	-	-	0/16/32/32	0/3/3/3
49	GDP	FF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	SC	501	48	-	6/22/38/38	0/3/3/3
47	GTP	DM	501	48	-	6/22/38/38	0/3/3/3
47	GTP	MM	501	48	-	6/22/38/38	0/3/3/3
47	GTP	EC	501	48	-	8/22/38/38	0/3/3/3
47	GTP	TG	501	48	-	7/22/38/38	0/3/3/3
49	GDP	HF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	BC	501	48	-	8/22/38/38	0/3/3/3
47	GTP	AC	501	48	-	9/22/38/38	0/3/3/3
47	GTP	UG	501	48	-	7/22/38/38	0/3/3/3
47	GTP	JI	501	48	-	7/22/38/38	0/3/3/3
47	GTP	VK	501	48	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	EI	501	48	-	5/22/38/38	0/3/3/3
49	GDP	SD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	BN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	UL	501	-	-	1/16/32/32	0/3/3/3
47	GTP	MA	501	48	-	7/22/38/38	0/3/3/3
47	GTP	IG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	HK	501	48	-	5/22/38/38	0/3/3/3
47	GTP	KC	501	48	-	5/22/38/38	0/3/3/3
47	GTP	HG	501	48	-	4/22/38/38	0/3/3/3
47	GTP	QA	501	48	-	8/22/38/38	0/3/3/3
47	GTP	SE	501	48	-	5/22/38/38	0/3/3/3
47	GTP	CM	501	48	-	8/22/38/38	0/3/3/3
47	GTP	AE	501	48	-	5/22/38/38	0/3/3/3
49	GDP	FH	501	-	-	1/16/32/32	0/3/3/3
47	GTP	RE	501	48	-	7/22/38/38	0/3/3/3
47	GTP	KM	501	48	-	5/22/38/38	0/3/3/3
49	GDP	VD	501	-	-	0/16/32/32	0/3/3/3
49	GDP	KJ	501	-	-	1/16/32/32	0/3/3/3
47	GTP	RM	501	48	-	7/22/38/38	0/3/3/3
49	GDP	PH	501	-	-	0/16/32/32	0/3/3/3
49	GDP	JJ	501	-	-	2/16/32/32	0/3/3/3
47	GTP	VM	501	48	-	5/22/38/38	0/3/3/3
47	GTP	IA	501	48	-	7/22/38/38	0/3/3/3
49	GDP	RJ	501	-	-	1/16/32/32	0/3/3/3
47	GTP	QC	501	48	-	7/22/38/38	0/3/3/3
49	GDP	NF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	NN	501	-	-	1/16/32/32	0/3/3/3
47	GTP	EG	501	48	-	4/22/38/38	0/3/3/3
47	GTP	LC	501	48	-	7/22/38/38	0/3/3/3
49	GDP	CL	501	-	-	1/16/32/32	0/3/3/3
47	GTP	PK	501	48	-	7/22/38/38	0/3/3/3
49	GDP	OB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	CG	501	48	-	7/22/38/38	0/3/3/3
49	GDP	LN	501	-	-	0/16/32/32	0/3/3/3
47	GTP	PG	501	48	-	8/22/38/38	0/3/3/3
49	GDP	OJ	501	-	-	0/16/32/32	0/3/3/3
47	GTP	CK	501	48	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	GDP	OD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	WD	501	-	-	0/16/32/32	0/3/3/3
47	GTP	JM	501	48	-	6/22/38/38	0/3/3/3
49	GDP	GF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	UJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	PJ	501	-	-	1/16/32/32	0/3/3/3
47	GTP	BI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	SL	501	-	-	3/16/32/32	0/3/3/3
49	GDP	IL	501	-	-	1/16/32/32	0/3/3/3
49	GDP	FJ	501	-	-	1/16/32/32	0/3/3/3
47	GTP	JG	501	48	-	8/22/38/38	0/3/3/3
49	GDP	FB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	HA	501	48	-	6/22/38/38	0/3/3/3
47	GTP	KI	501	48	-	5/22/38/38	0/3/3/3
47	GTP	GE	501	48	-	5/22/38/38	0/3/3/3
49	GDP	BB	502	-	-	0/16/32/32	0/3/3/3
47	GTP	DK	501	48	-	6/22/38/38	0/3/3/3
47	GTP	EE	501	48	-	9/22/38/38	0/3/3/3
47	GTP	JC	501	48	-	6/22/38/38	0/3/3/3
47	GTP	FA	501	48	-	8/22/38/38	0/3/3/3
47	GTP	WK	501	48	-	8/22/38/38	0/3/3/3
49	GDP	VH	501	-	-	0/16/32/32	0/3/3/3
47	GTP	RC	501	48	-	7/22/38/38	0/3/3/3
47	GTP	NA	501	48	-	8/22/38/38	0/3/3/3
47	GTP	NE	501	48	-	5/22/38/38	0/3/3/3
47	GTP	FK	501	48	-	7/22/38/38	0/3/3/3
49	GDP	MB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	CA	501	48	-	6/22/38/38	0/3/3/3
47	GTP	FM	501	48	-	6/22/38/38	0/3/3/3
47	GTP	AI	501	48	-	9/22/38/38	0/3/3/3
47	GTP	IE	501	48	-	8/22/38/38	0/3/3/3
49	GDP	JD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	QJ	501	-	-	0/16/32/32	0/3/3/3
49	GDP	EH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	MH	501	-	-	3/16/32/32	0/3/3/3
49	GDP	OL	501	-	-	0/16/32/32	0/3/3/3
49	GDP	NJ	501	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	GDP	JF	501	-	-	2/16/32/32	0/3/3/3
47	GTP	II	501	48	-	8/22/38/38	0/3/3/3
49	GDP	ND	501	-	-	1/16/32/32	0/3/3/3
49	GDP	LL	501	-	-	1/16/32/32	0/3/3/3
49	GDP	RB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	GB	502	-	-	1/16/32/32	0/3/3/3
47	GTP	SI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	TB	501	-	-	1/16/32/32	0/3/3/3
47	GTP	DA	501	48	-	5/22/38/38	0/3/3/3
47	GTP	EM	501	48	-	8/22/38/38	0/3/3/3
49	GDP	BL	501	-	-	1/16/32/32	0/3/3/3
47	GTP	QK	501	48	-	7/22/38/38	0/3/3/3
49	GDP	WB	501	-	-	1/16/32/32	0/3/3/3
49	GDP	IN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	TL	501	-	-	1/16/32/32	0/3/3/3
49	GDP	RD	501	-	-	1/16/32/32	0/3/3/3
47	GTP	PA	501	48	-	8/22/38/38	0/3/3/3
49	GDP	DB	501	-	-	1/16/32/32	0/3/3/3
49	GDP	AN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	SB	501	-	-	3/16/32/32	0/3/3/3
49	GDP	TH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	ED	501	-	-	2/16/32/32	0/3/3/3
47	GTP	LI	501	48	-	7/22/38/38	0/3/3/3
49	GDP	HN	501	-	-	1/16/32/32	0/3/3/3
49	GDP	KN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	BD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	DL	501	-	-	0/16/32/32	0/3/3/3
49	GDP	EB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	KB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	FC	501	48	-	7/22/38/38	0/3/3/3
49	GDP	NH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	DF	501	-	-	0/16/32/32	0/3/3/3
49	GDP	AB	501	-	-	1/16/32/32	0/3/3/3
49	GDP	QF	501	-	-	0/16/32/32	0/3/3/3
49	GDP	RL	501	-	-	1/16/32/32	0/3/3/3
49	GDP	UN	501	-	-	1/16/32/32	0/3/3/3
47	GTP	IM	501	48	-	9/22/38/38	0/3/3/3
49	GDP	WL	501	-	-	1/16/32/32	0/3/3/3
47	GTP	TK	501	48	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	GDP	JL	501	-	-	2/16/32/32	0/3/3/3
47	GTP	VE	501	48	-	6/22/38/38	0/3/3/3
49	GDP	JB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	RF	501	-	-	3/16/32/32	0/3/3/3
49	GDP	UH	501	-	-	1/16/32/32	0/3/3/3
47	GTP	GK	501	48	-	7/22/38/38	0/3/3/3
49	GDP	ML	501	-	-	3/16/32/32	0/3/3/3
47	GTP	VG	501	48	-	8/22/38/38	0/3/3/3
49	GDP	KF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	GC	501	48	-	5/22/38/38	0/3/3/3
49	GDP	LF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	LG	501	48	-	8/22/38/38	0/3/3/3
49	GDP	LJ	501	-	-	2/16/32/32	0/3/3/3
49	GDP	KD	501	-	-	0/16/32/32	0/3/3/3
49	GDP	TJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	NB	502	-	-	0/16/32/32	0/3/3/3
47	GTP	OA	501	48	-	3/22/38/38	0/3/3/3
49	GDP	UB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	VI	501	48	-	8/22/38/38	0/3/3/3
49	GDP	MN	501	-	-	2/16/32/32	0/3/3/3
47	GTP	HI	501	48	-	4/22/38/38	0/3/3/3
49	GDP	AJ	501	-	-	0/16/32/32	0/3/3/3
47	GTP	BM	501	48	-	8/22/38/38	0/3/3/3
47	GTP	RK	501	48	-	7/22/38/38	0/3/3/3
47	GTP	AM	501	48	-	4/22/38/38	0/3/3/3
47	GTP	UK	501	48	-	5/22/38/38	0/3/3/3
47	GTP	OC	501	48	-	2/22/38/38	0/3/3/3
47	GTP	PI	501	48	-	6/22/38/38	0/3/3/3
47	GTP	DC	501	48	-	6/22/38/38	0/3/3/3
47	GTP	KE	501	48	-	7/22/38/38	0/3/3/3
47	GTP	DI	501	48	-	6/22/38/38	0/3/3/3
47	GTP	KK	501	48	-	4/22/38/38	0/3/3/3
49	GDP	IB	501	-	-	0/16/32/32	0/3/3/3
47	GTP	GG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	OE	501	48	-	3/22/38/38	0/3/3/3
49	GDP	LB	501	-	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	GDP	MF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	PM	501	48	-	8/22/38/38	0/3/3/3
49	GDP	IF	501	-	-	1/16/32/32	0/3/3/3
49	GDP	RN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	HD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	CB	501	-	-	1/16/32/32	0/3/3/3
49	GDP	QL	501	-	-	0/16/32/32	0/3/3/3
47	GTP	EA	501	48	-	6/22/38/38	0/3/3/3
47	GTP	CE	501	48	-	7/22/38/38	0/3/3/3
47	GTP	WI	501	48	-	6/22/38/38	0/3/3/3
49	GDP	HL	501	-	-	0/16/32/32	0/3/3/3
47	GTP	RA	501	48	-	7/22/38/38	0/3/3/3
49	GDP	KL	501	-	-	1/16/32/32	0/3/3/3
47	GTP	SA	501	48	-	6/22/38/38	0/3/3/3
49	GDP	PL	501	-	-	1/16/32/32	0/3/3/3
49	GDP	OH	501	-	-	1/16/32/32	0/3/3/3
47	GTP	IC	501	48	-	8/22/38/38	0/3/3/3
47	GTP	WG	501	48	-	8/22/38/38	0/3/3/3
47	GTP	AK	501	48	-	9/22/38/38	0/3/3/3
49	GDP	QB	501	-	-	0/16/32/32	0/3/3/3
49	GDP	CD	501	-	-	1/16/32/32	0/3/3/3
49	GDP	PF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	WE	501	48	-	3/22/38/38	0/3/3/3
49	GDP	BF	501	-	-	1/16/32/32	0/3/3/3
47	GTP	EK	501	48	-	6/22/38/38	0/3/3/3
49	GDP	AF	501	-	-	0/16/32/32	0/3/3/3
47	GTP	BK	501	48	-	4/22/38/38	0/3/3/3
47	GTP	QE	501	48	-	7/22/38/38	0/3/3/3
49	GDP	BJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	HH	501	-	-	1/16/32/32	0/3/3/3
49	GDP	ON	501	-	-	0/16/32/32	0/3/3/3
47	GTP	TI	501	48	-	9/22/38/38	0/3/3/3
47	GTP	WC	501	48	-	6/22/38/38	0/3/3/3
47	GTP	WM	501	48	-	3/22/38/38	0/3/3/3
47	GTP	RI	501	48	-	8/22/38/38	0/3/3/3
49	GDP	RH	501	-	-	0/16/32/32	0/3/3/3
49	GDP	PN	501	-	-	0/16/32/32	0/3/3/3
49	GDP	CH	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	GTP	TM	501	48	-	8/22/38/38	0/3/3/3
49	GDP	MJ	501	-	-	1/16/32/32	0/3/3/3
49	GDP	CJ	501	-	-	1/16/32/32	0/3/3/3

The worst 5 of 663 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	DN	501	GDP	C5-C4	3.20	1.47	1.38
49	UB	501	GDP	C5-C4	3.20	1.47	1.38
49	SB	501	GDP	C5-C4	3.19	1.47	1.38
49	JB	501	GDP	C5-C4	3.18	1.47	1.38
49	IB	501	GDP	C5-C4	3.18	1.47	1.38

The worst 5 of 2563 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	SN	501	GDP	C5-C4-N3	-6.30	118.36	128.39
49	NB	502	GDP	C5-C4-N3	-6.26	118.43	128.39
49	DB	501	GDP	C5-C4-N3	-6.26	118.43	128.39
49	DH	501	GDP	C5-C4-N3	-6.26	118.43	128.39
49	HF	501	GDP	C5-C4-N3	-6.24	118.45	128.39

There are no chirality outliers.

5 of 1178 torsion outliers are listed below:

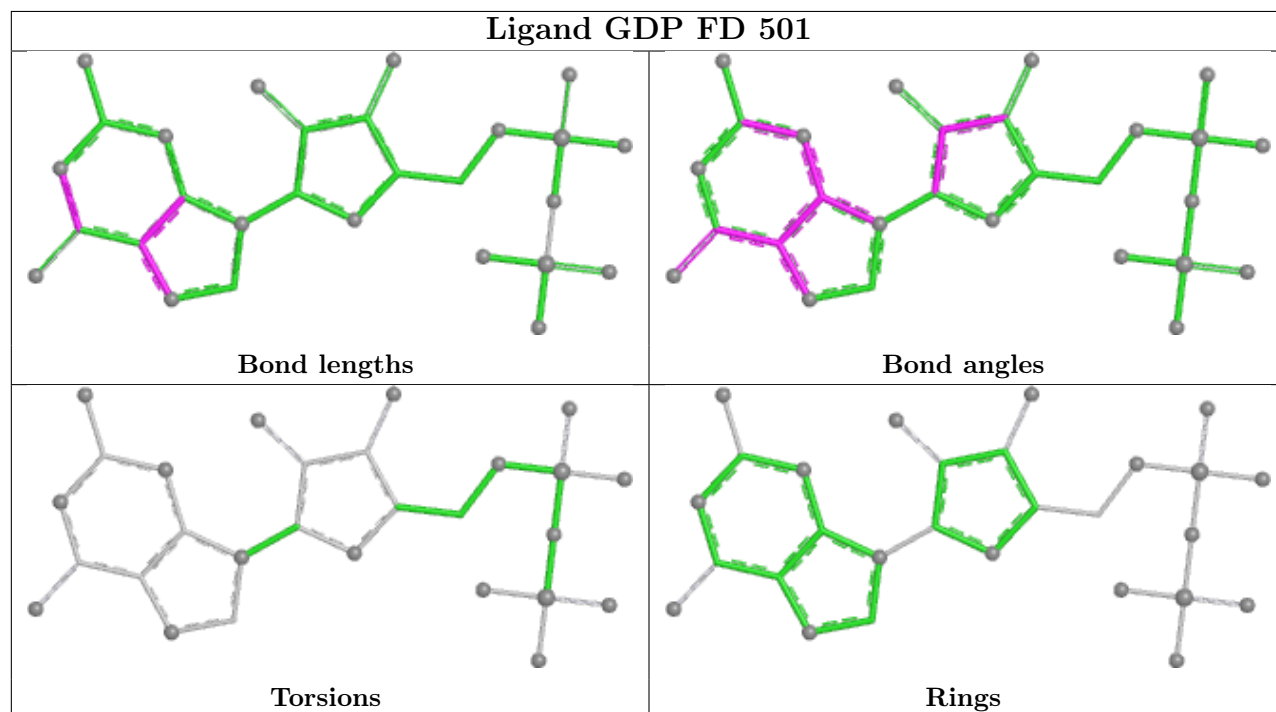
Mol	Chain	Res	Type	Atoms
47	AC	501	GTP	C5'-O5'-PA-O3A
47	AC	501	GTP	C5'-O5'-PA-O1A
47	AC	501	GTP	C5'-O5'-PA-O2A
47	AG	501	GTP	PB-O3A-PA-O5'
47	AI	501	GTP	PB-O3A-PA-O5'

There are no ring outliers.

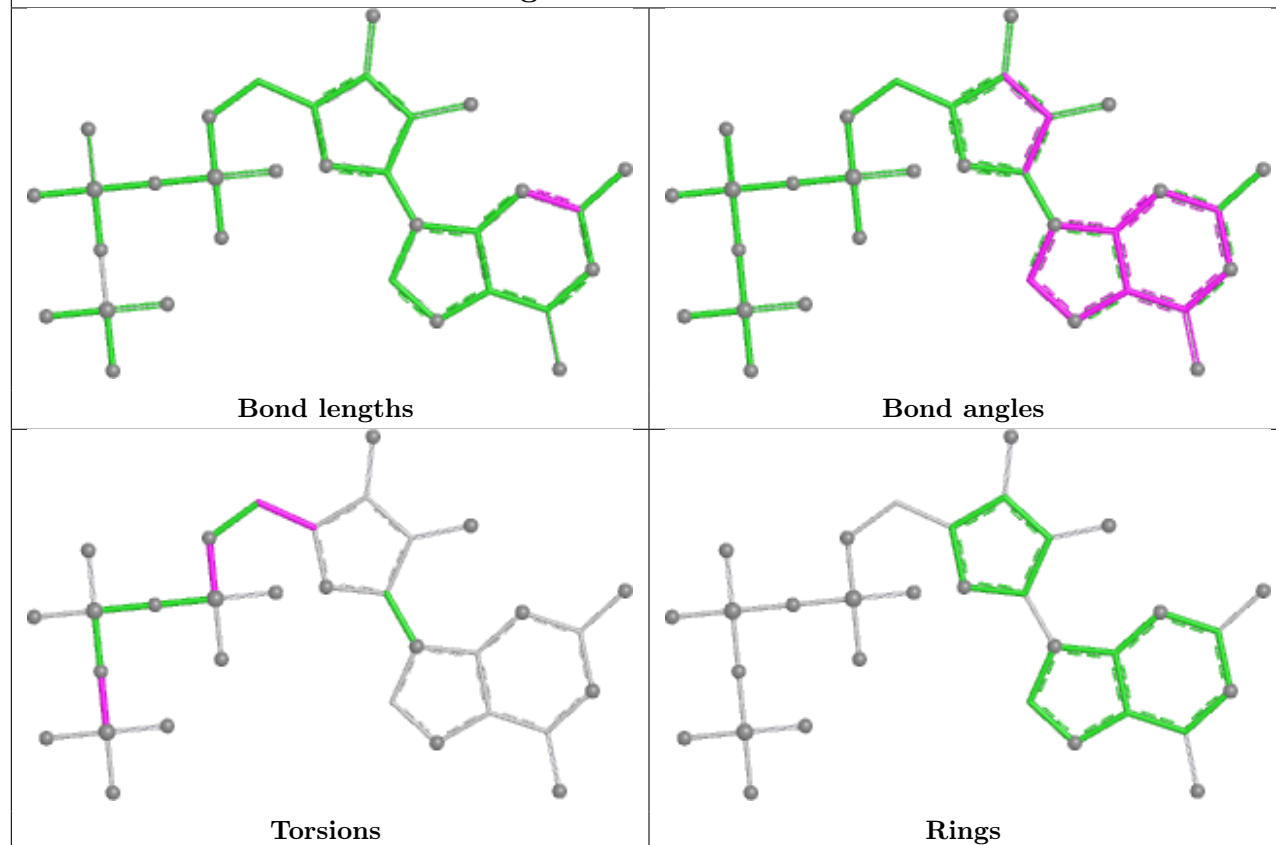
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

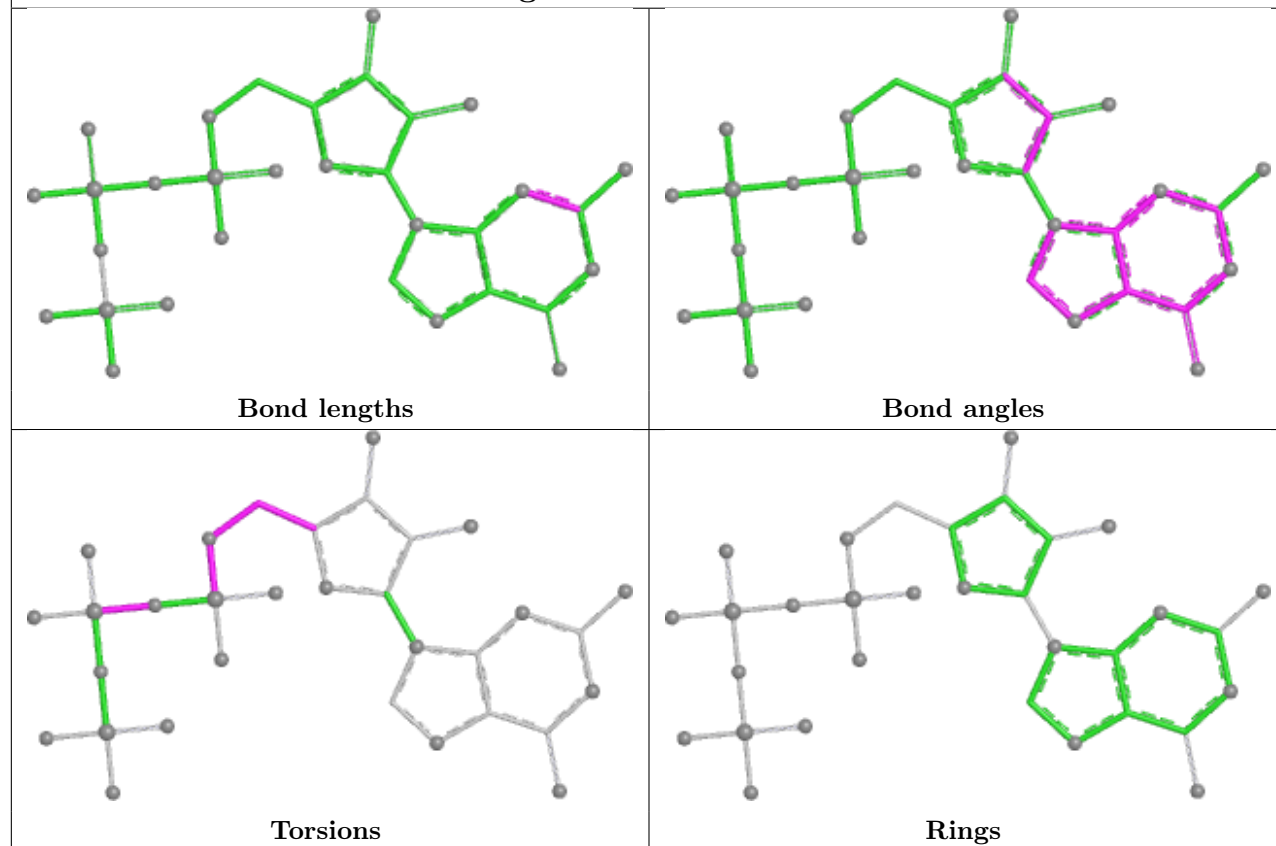
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



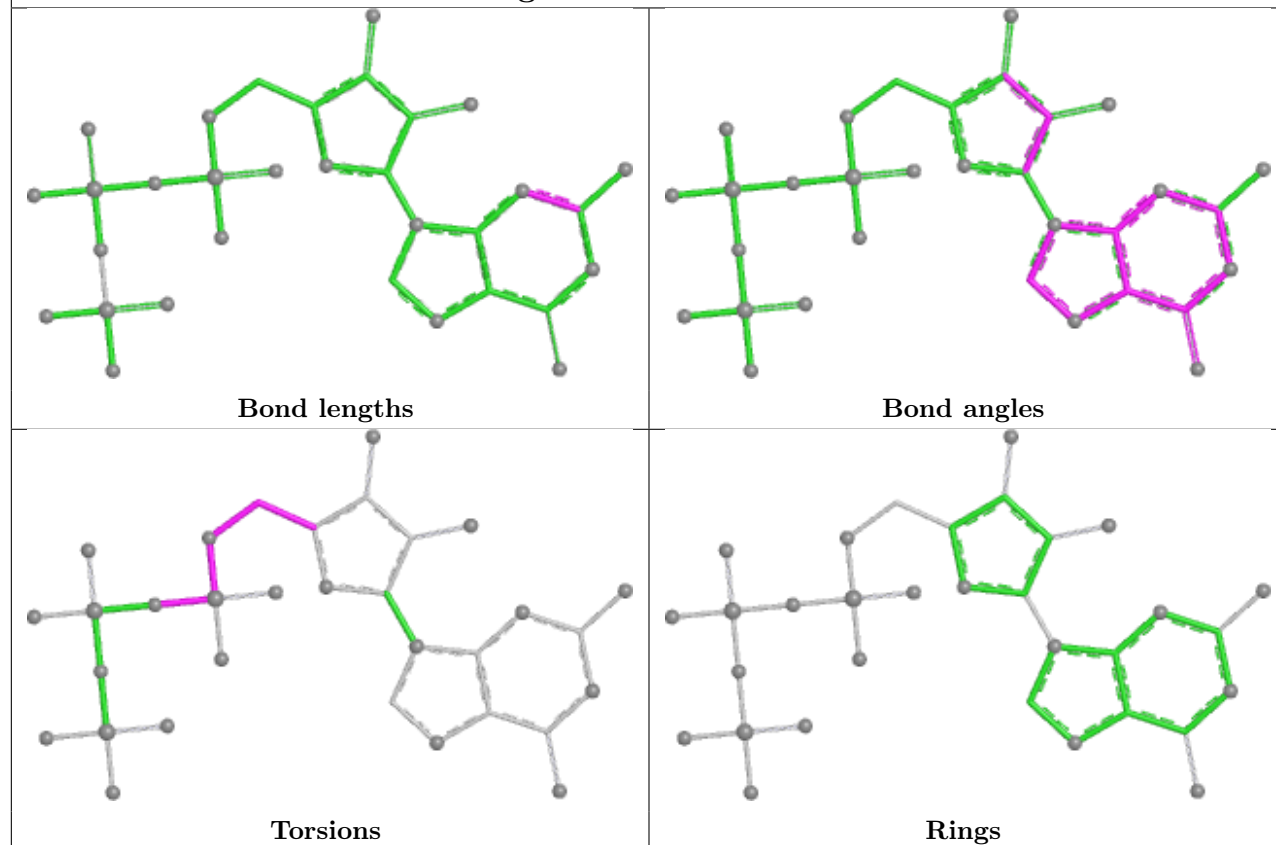
Ligand GTP JK 501



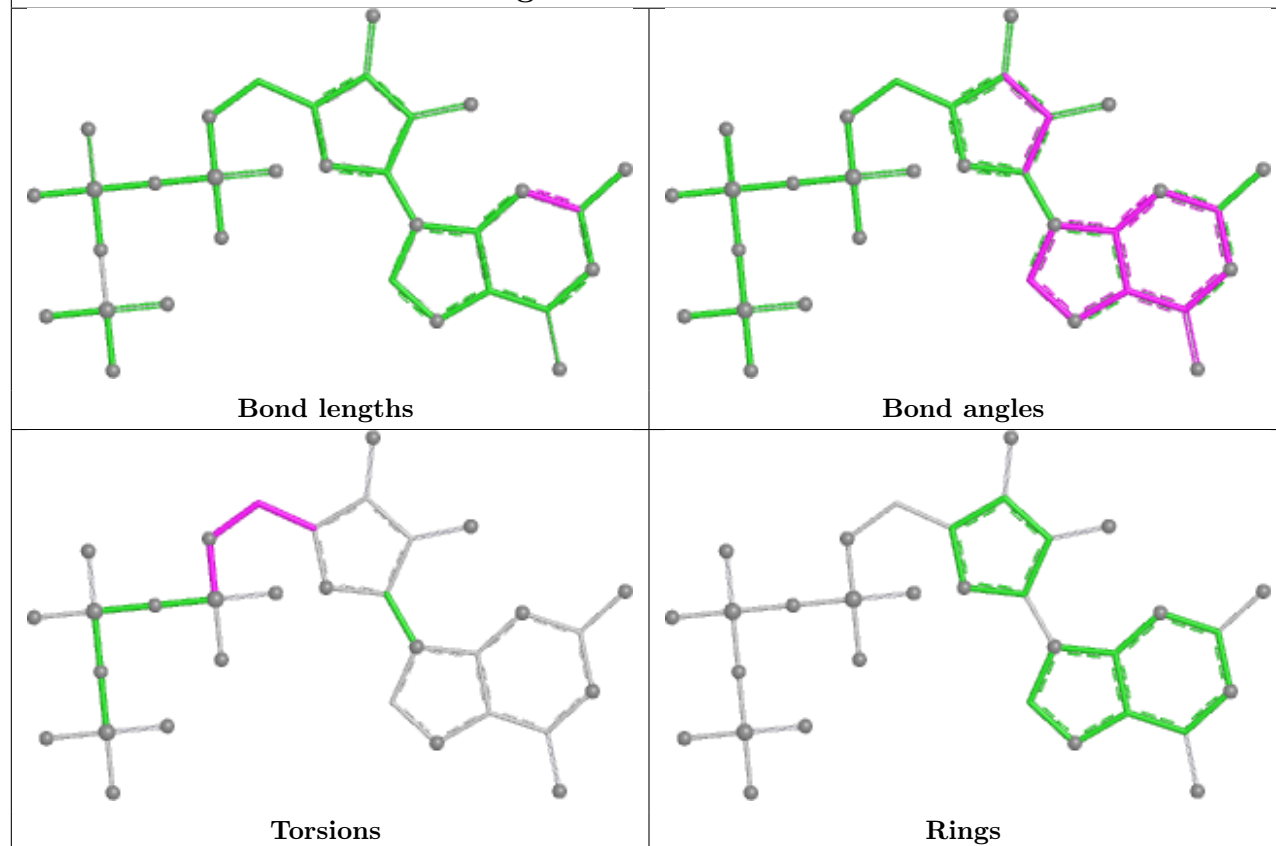
Ligand GTP TA 501

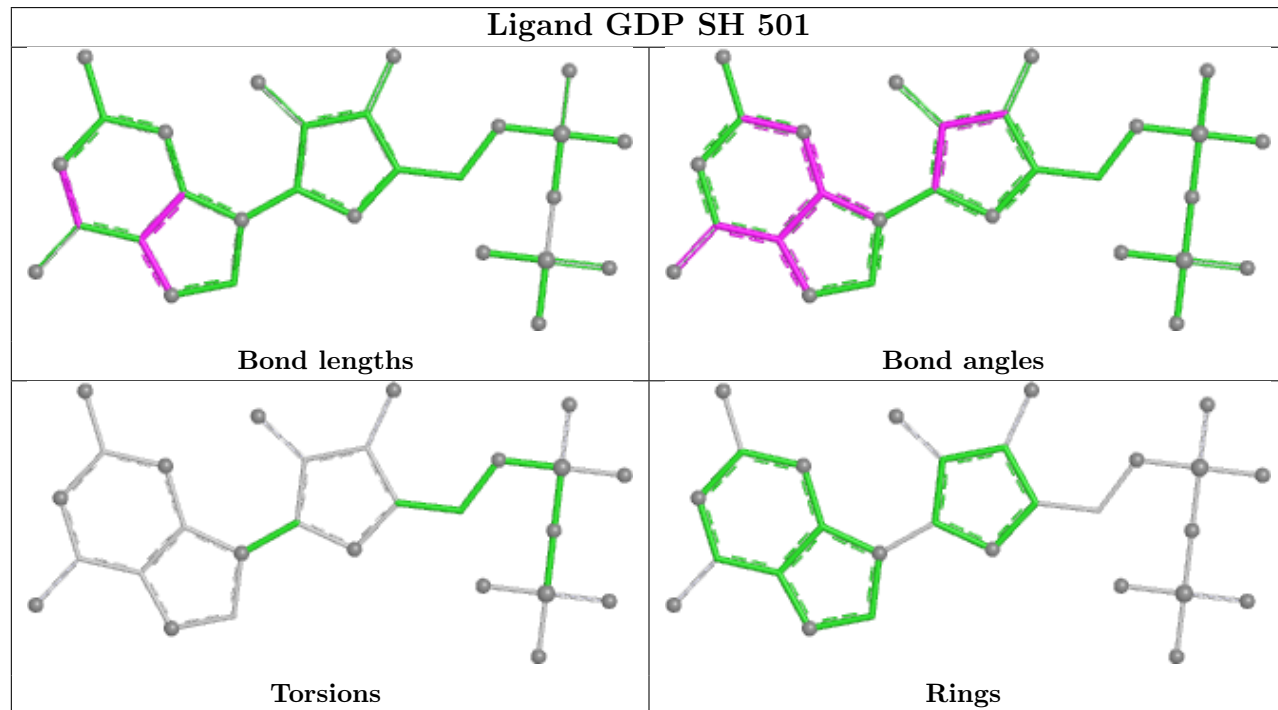
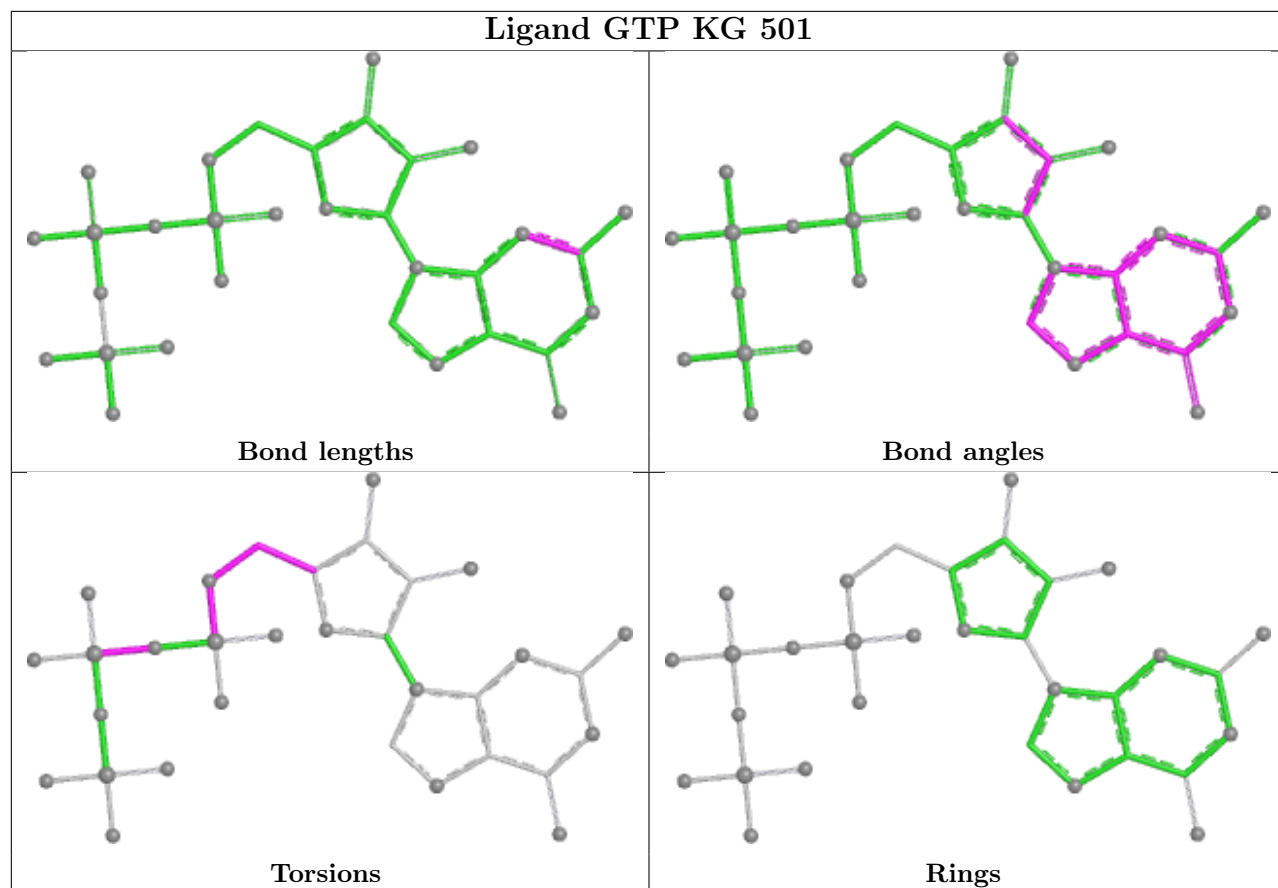


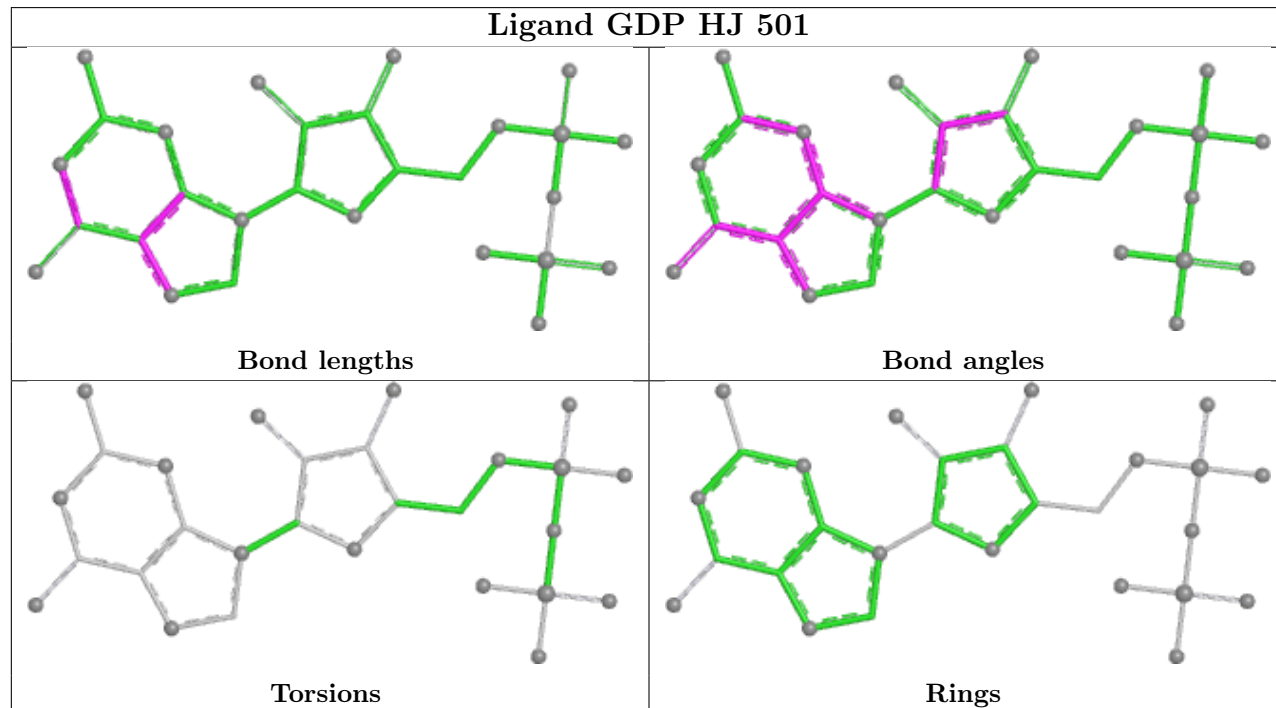
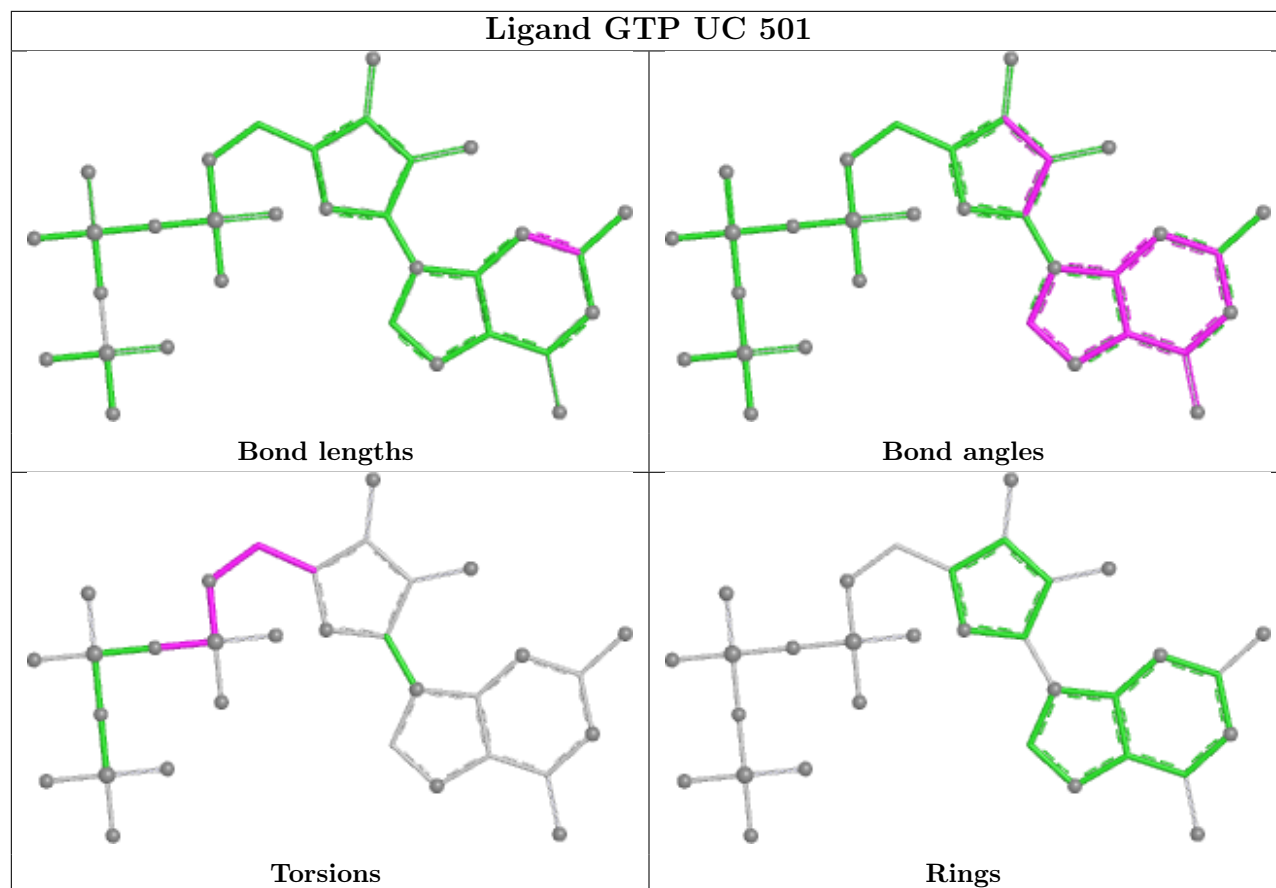
Ligand GTP DE 501

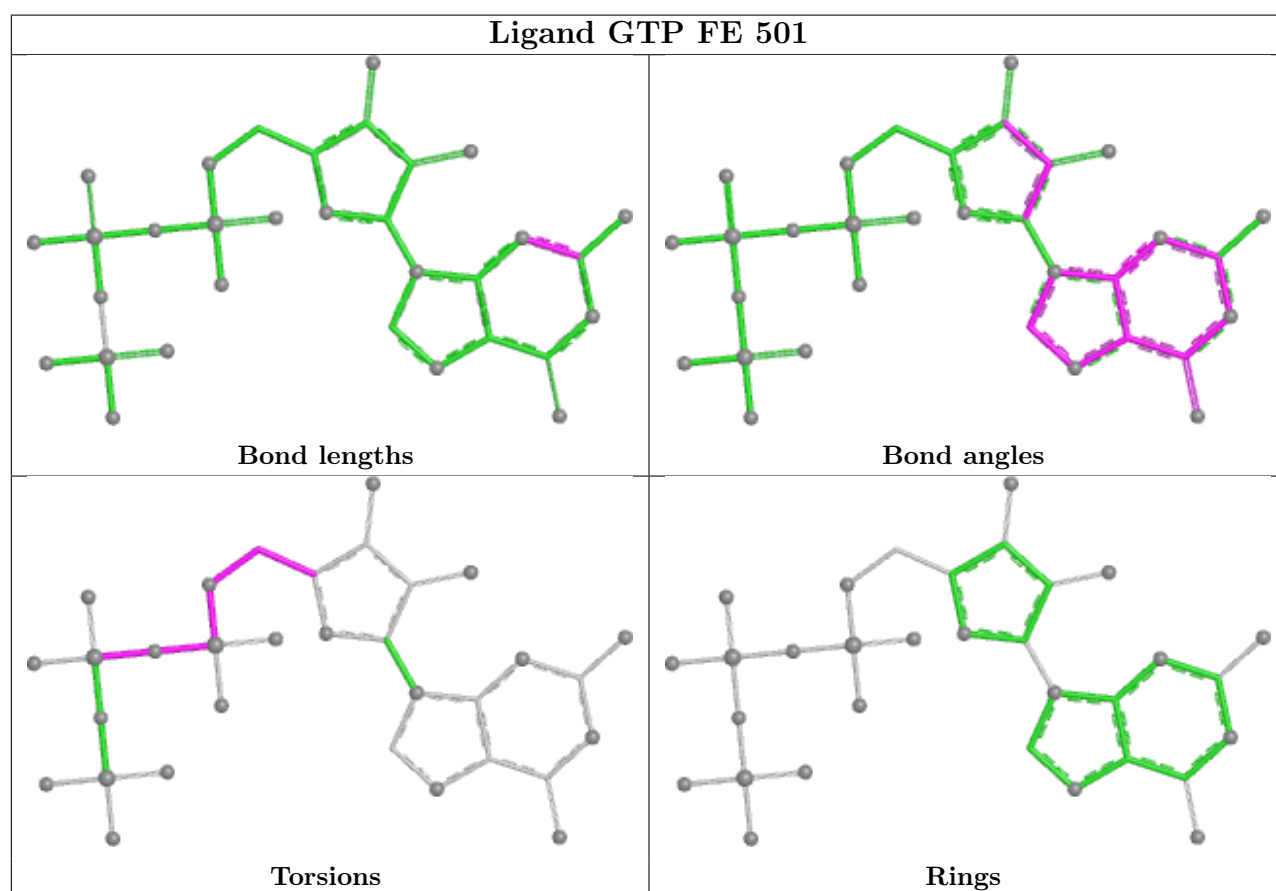
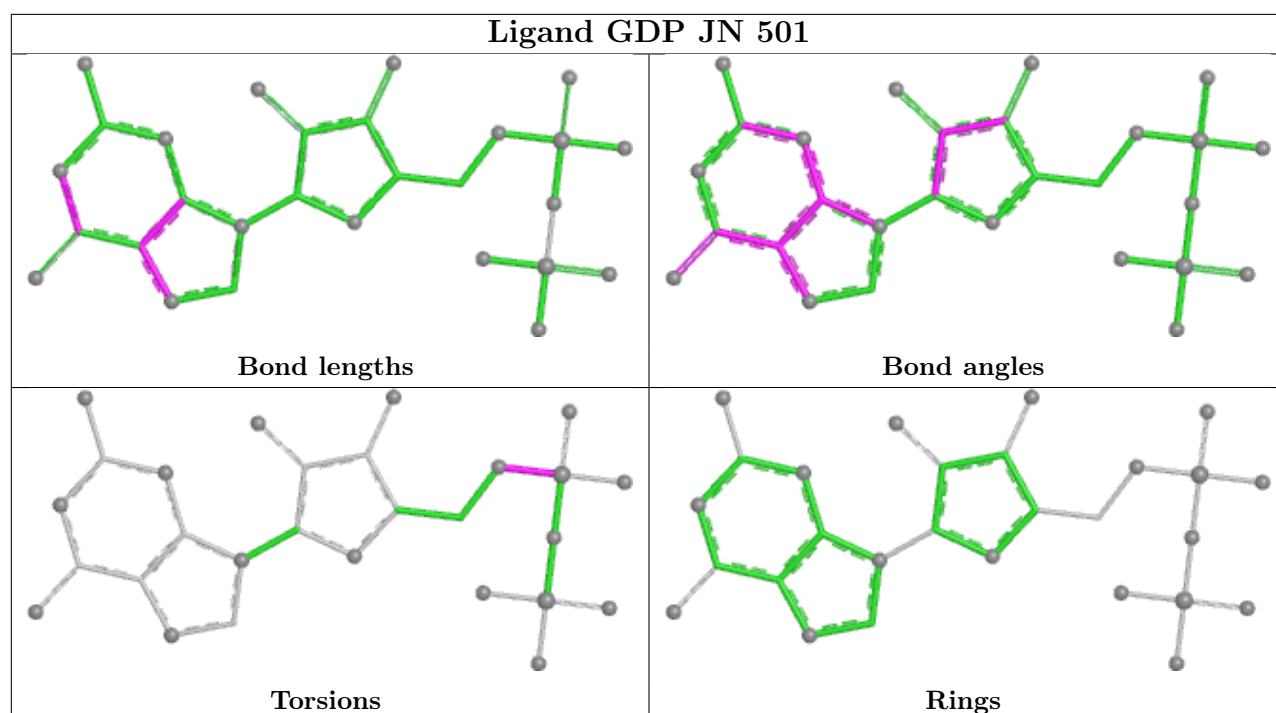


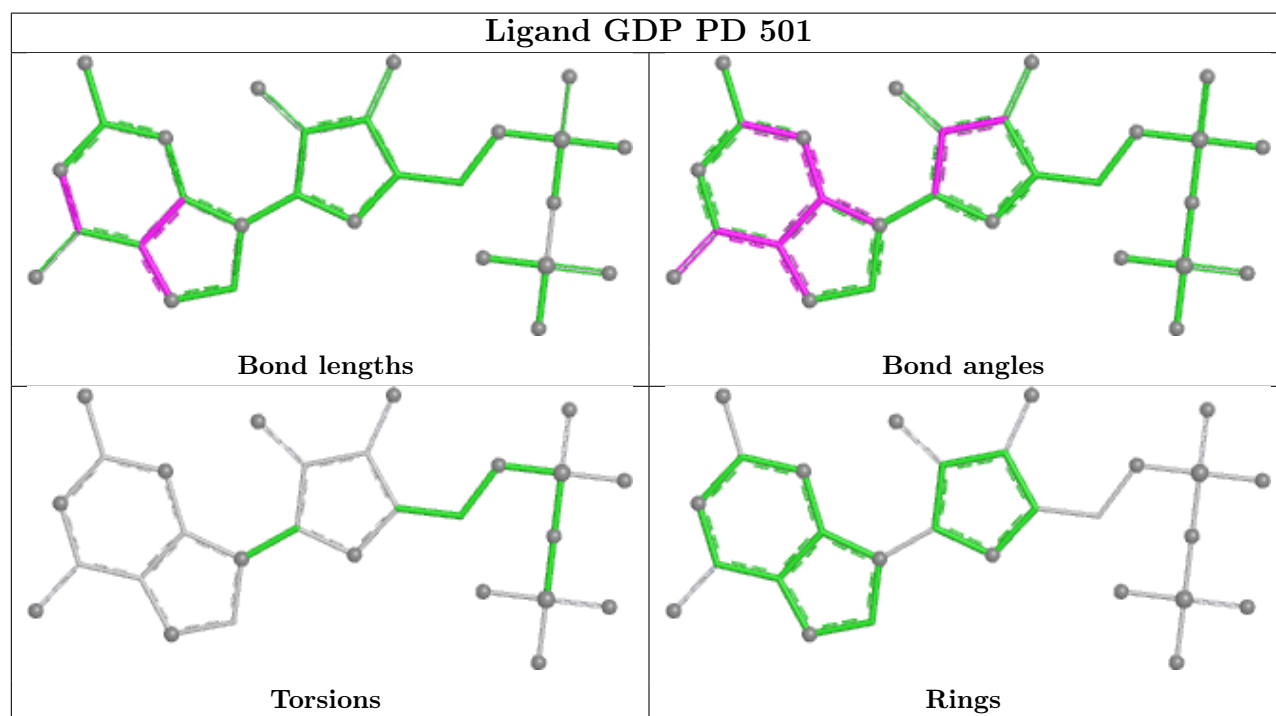
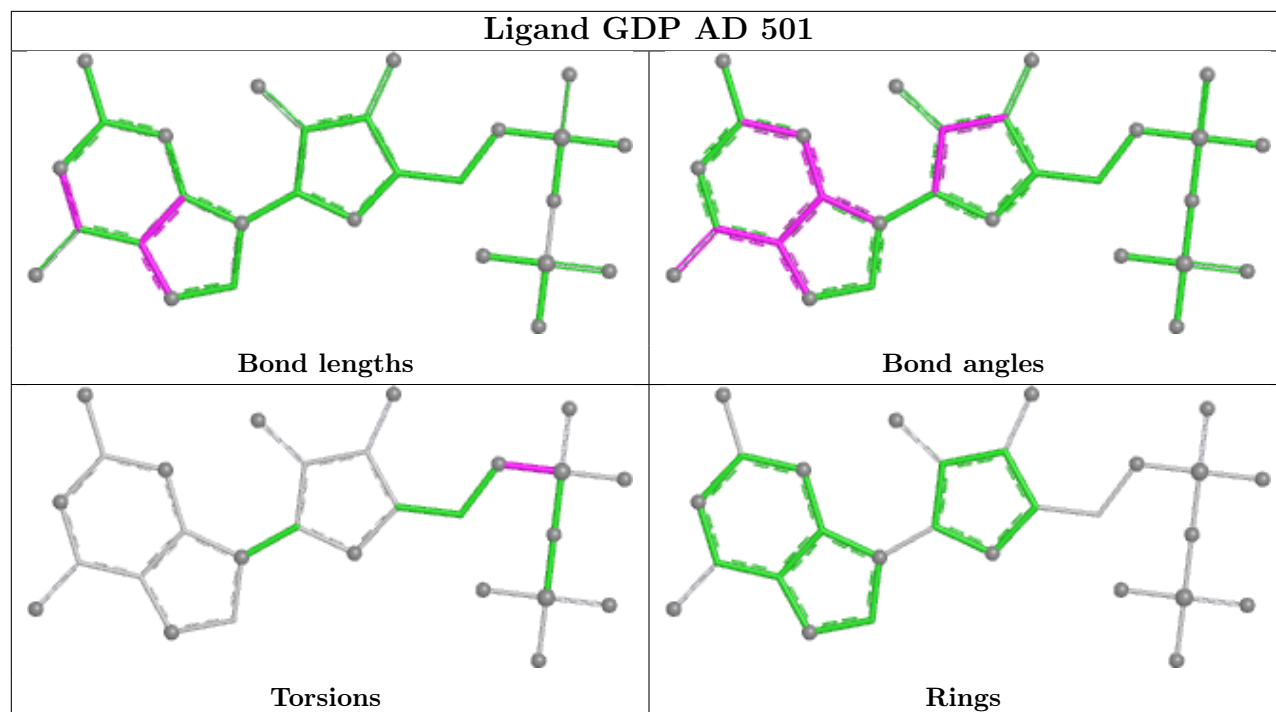
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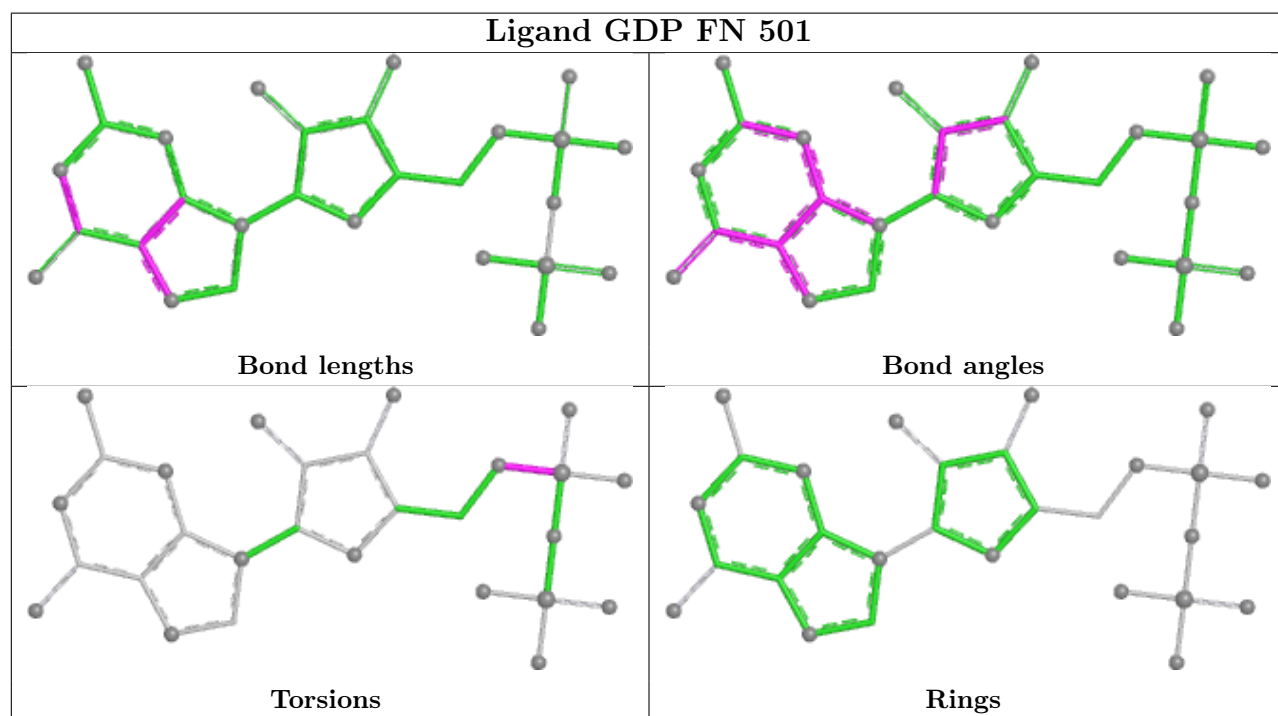
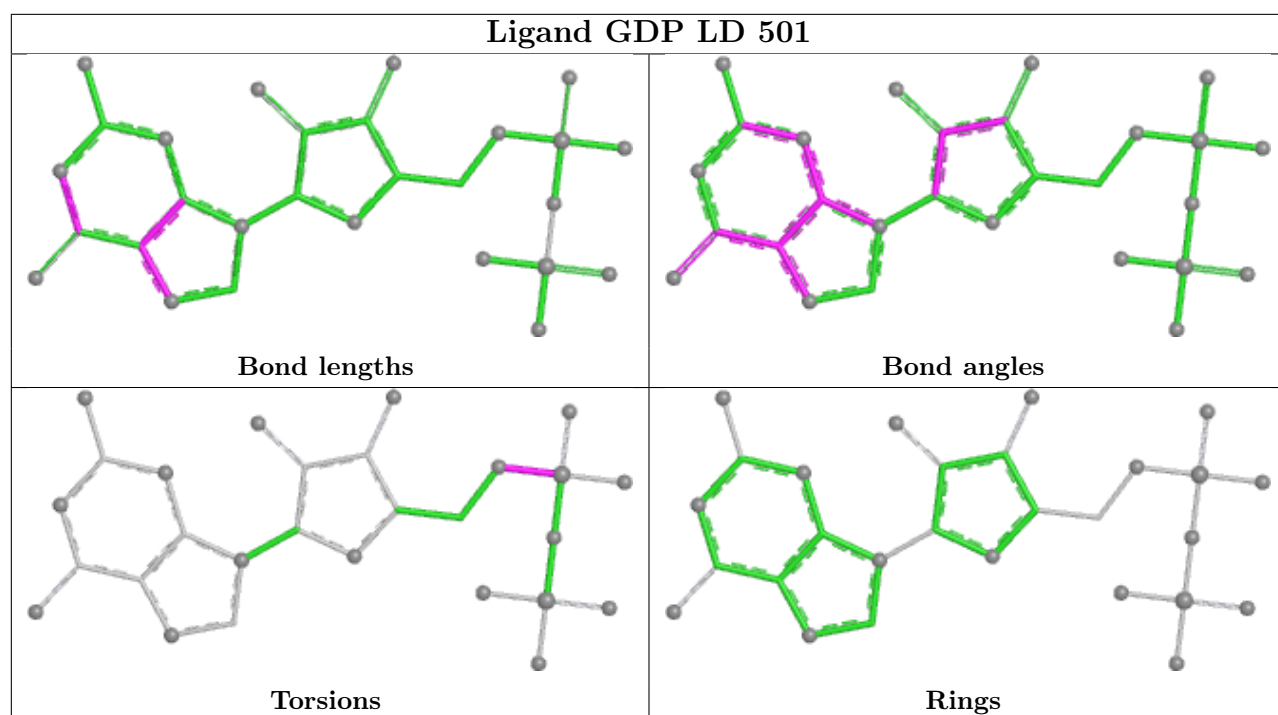




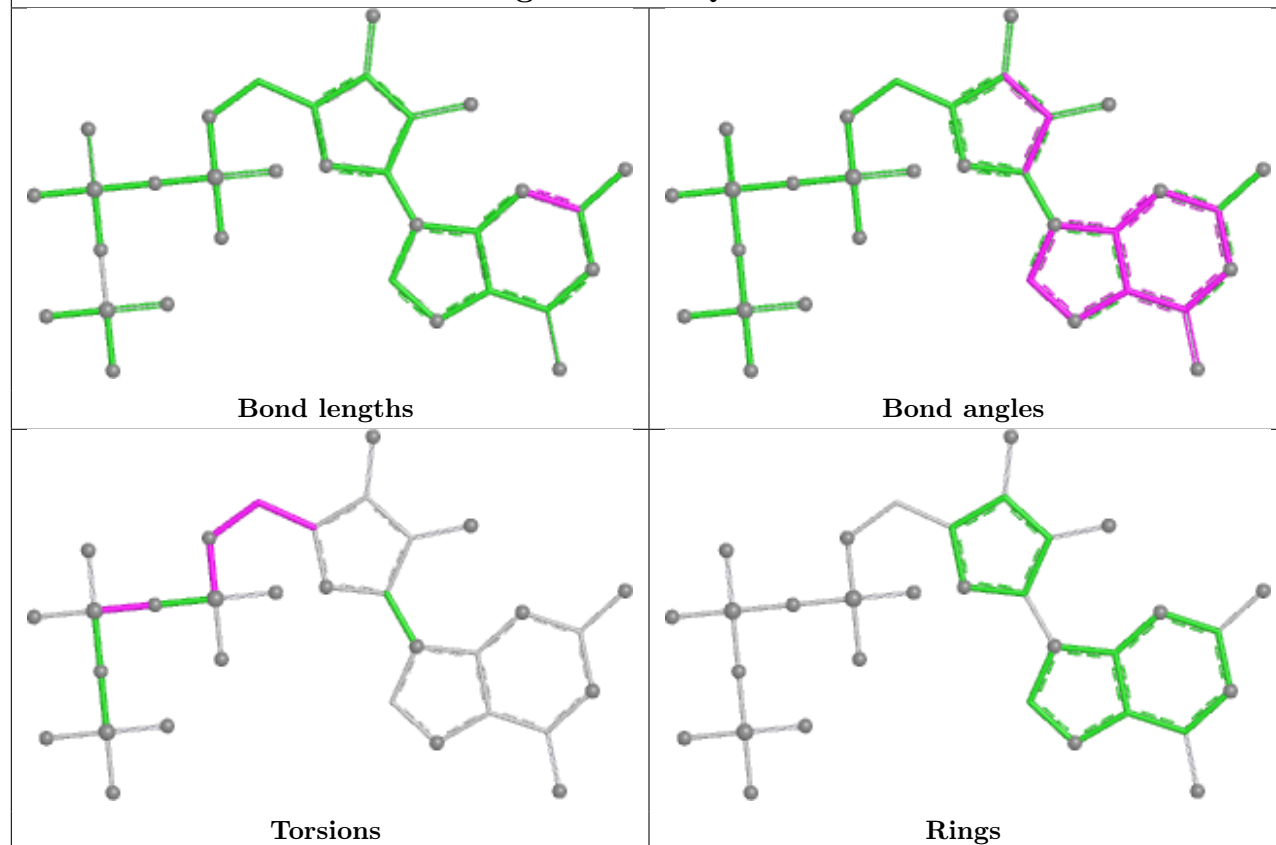




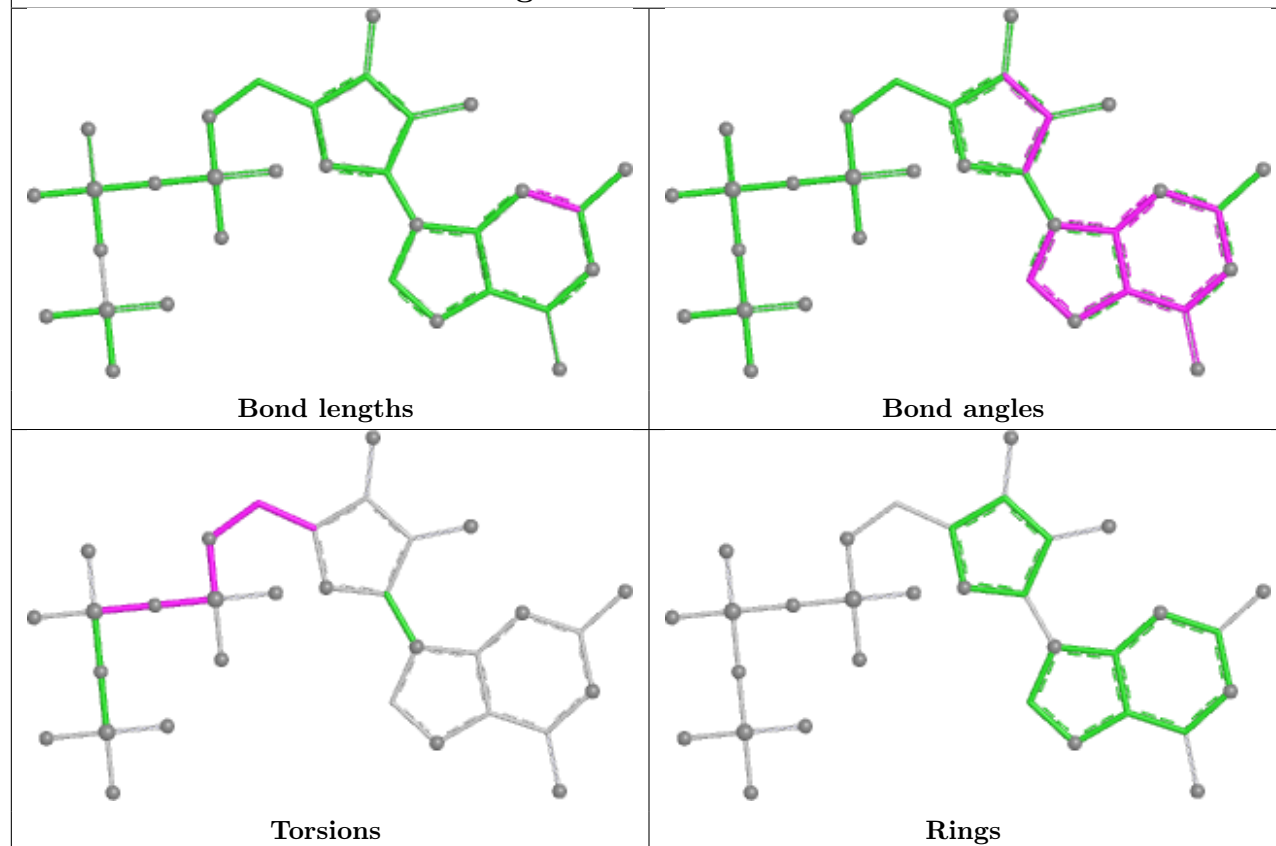


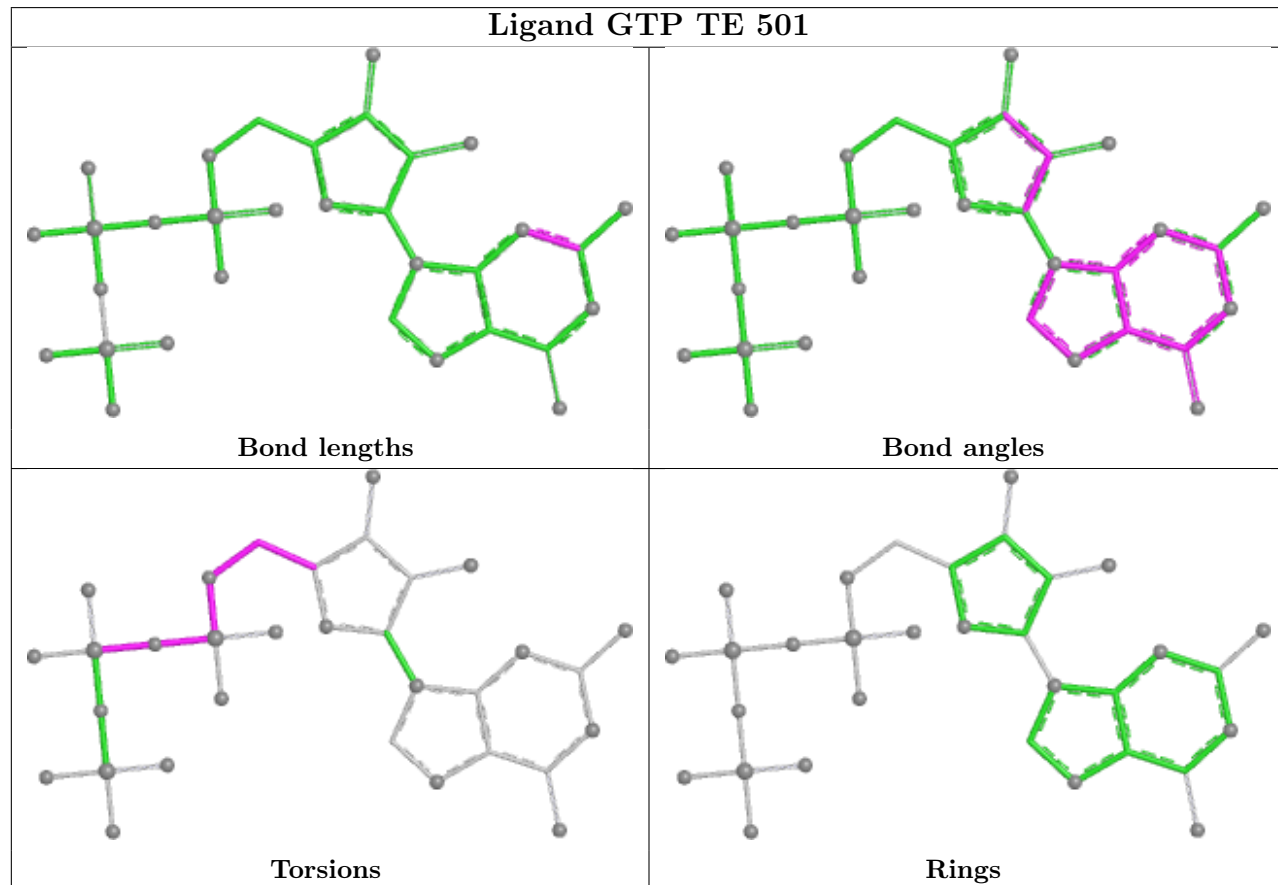
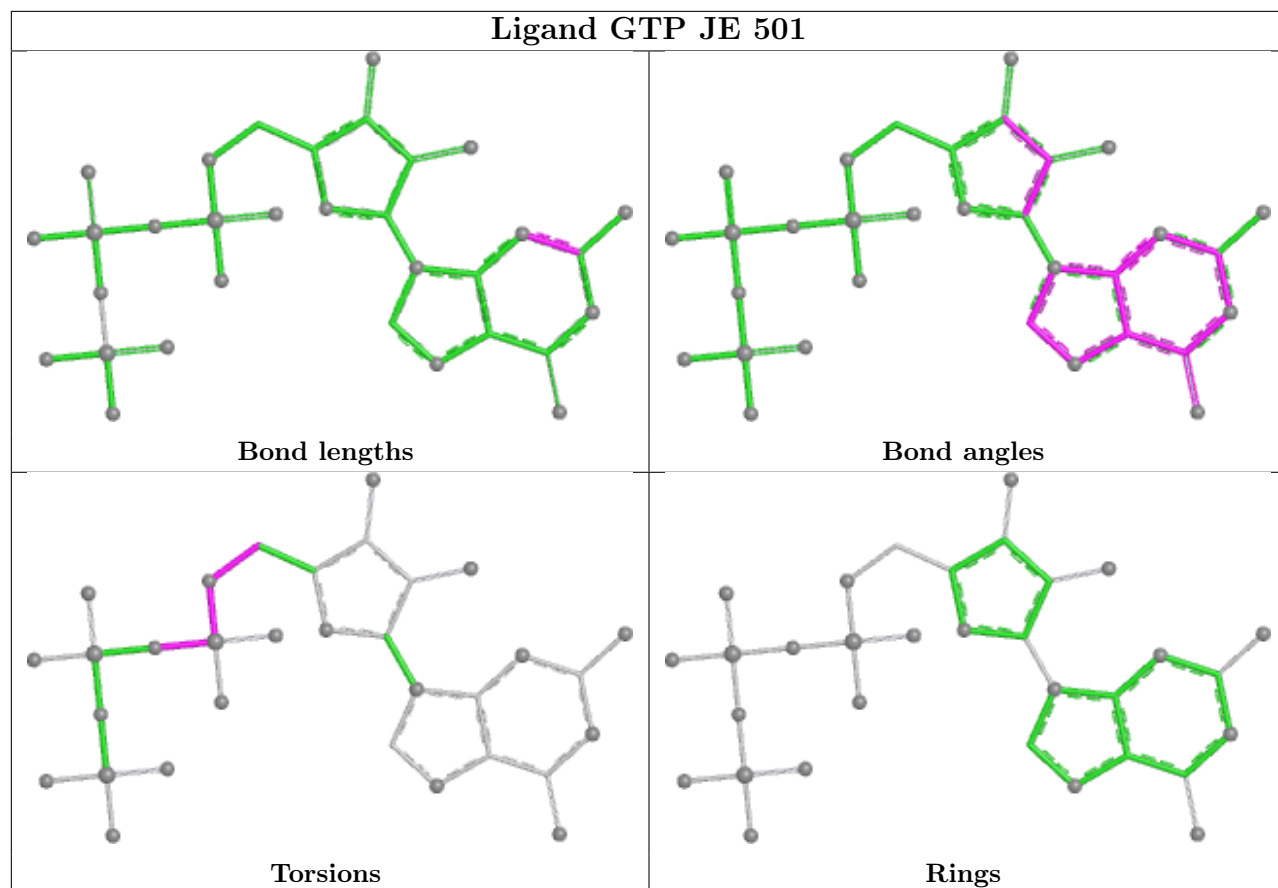


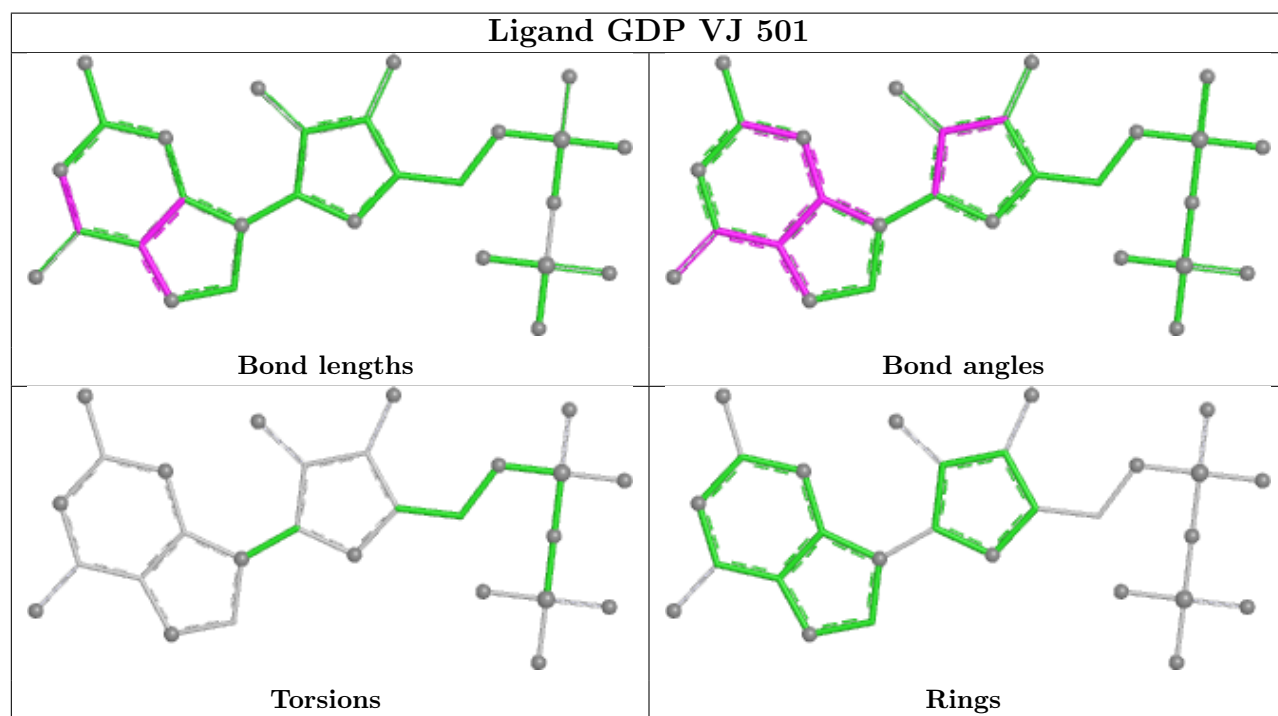
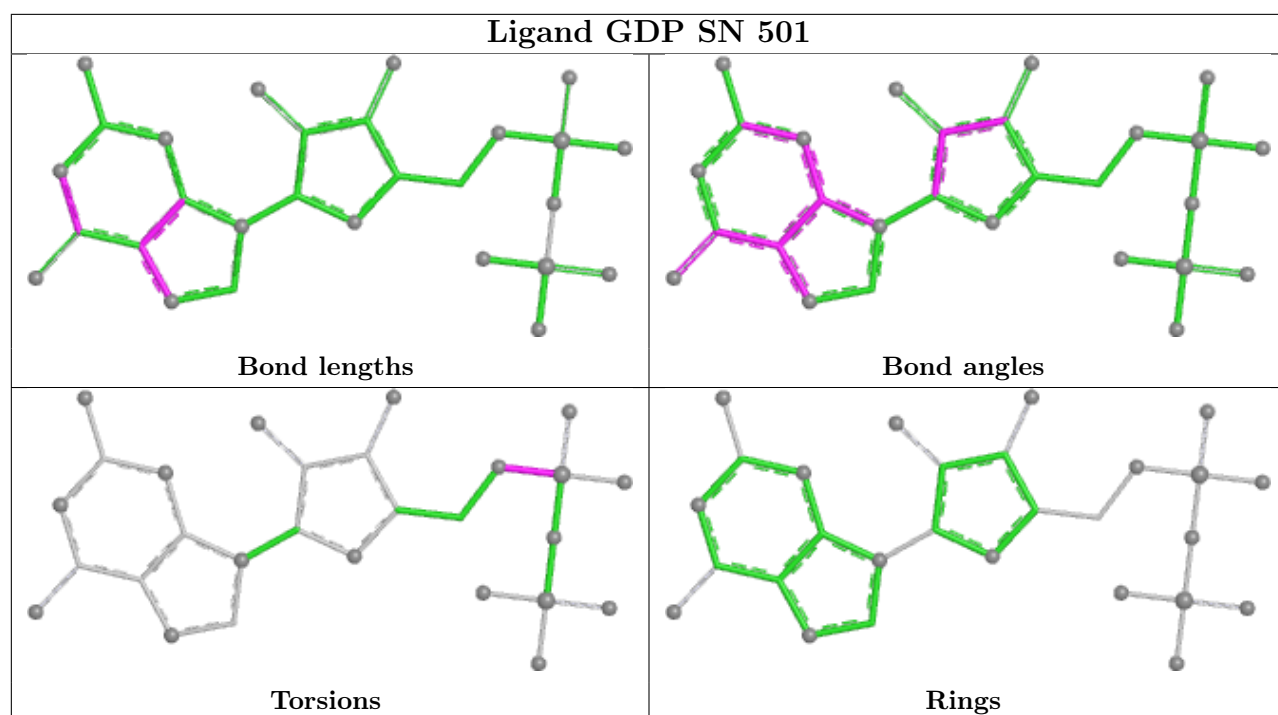
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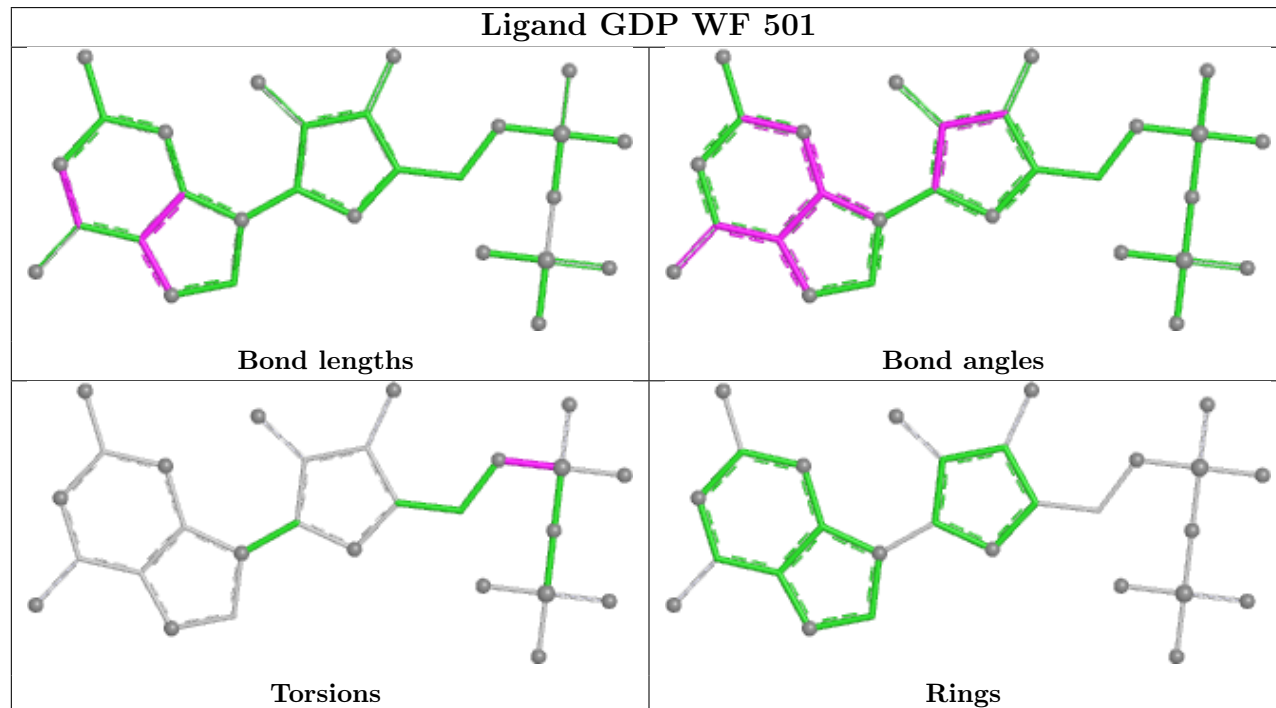
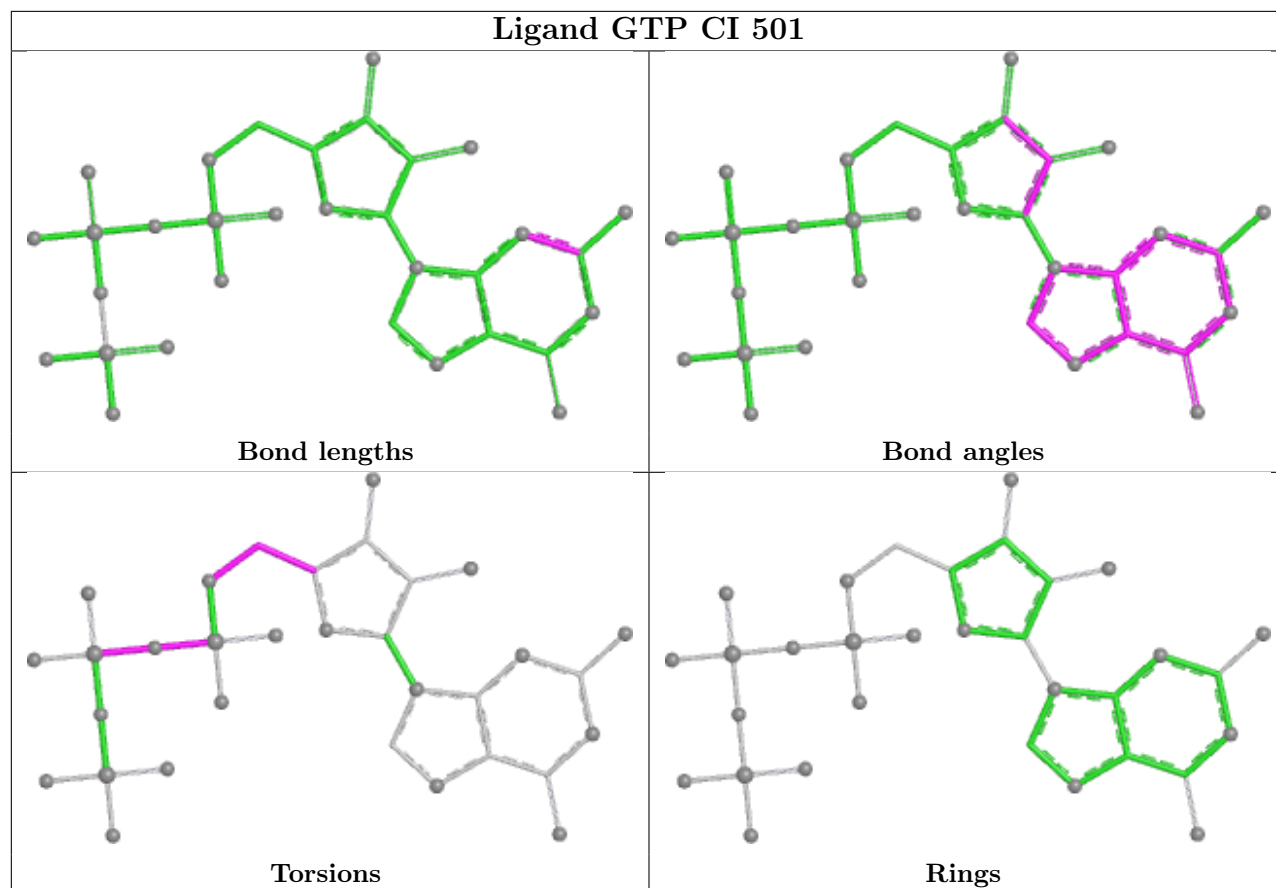


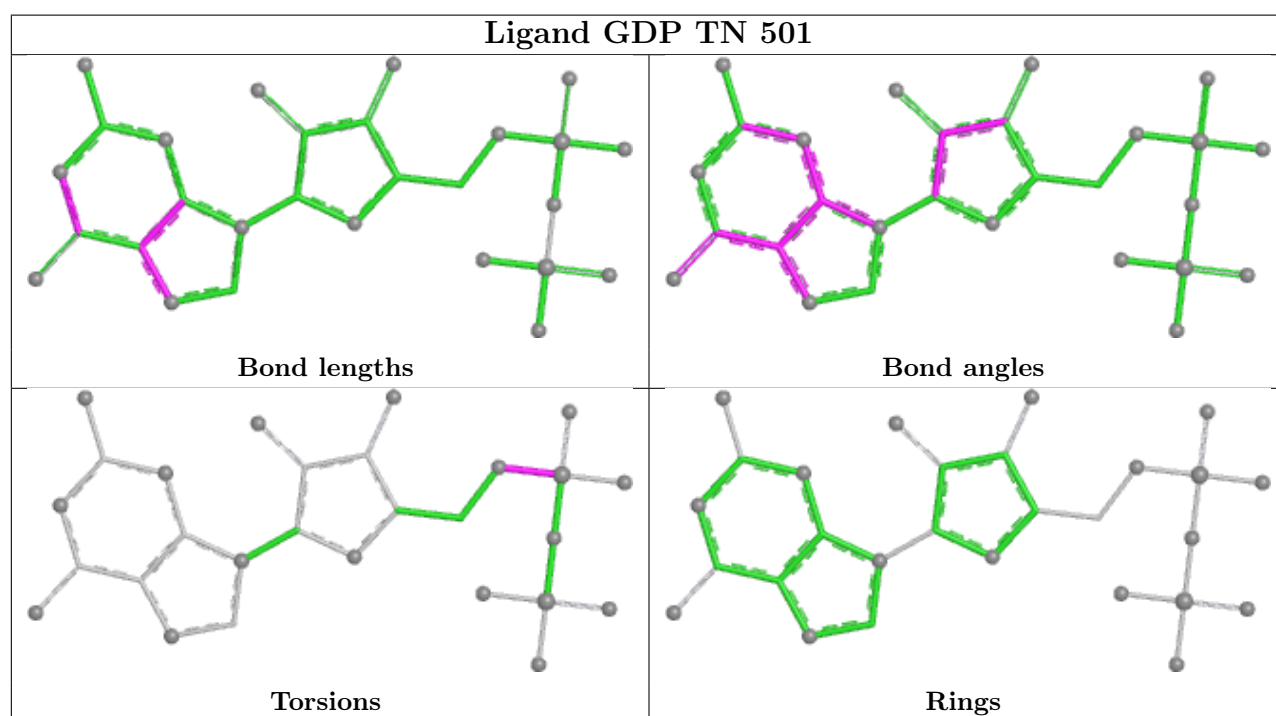
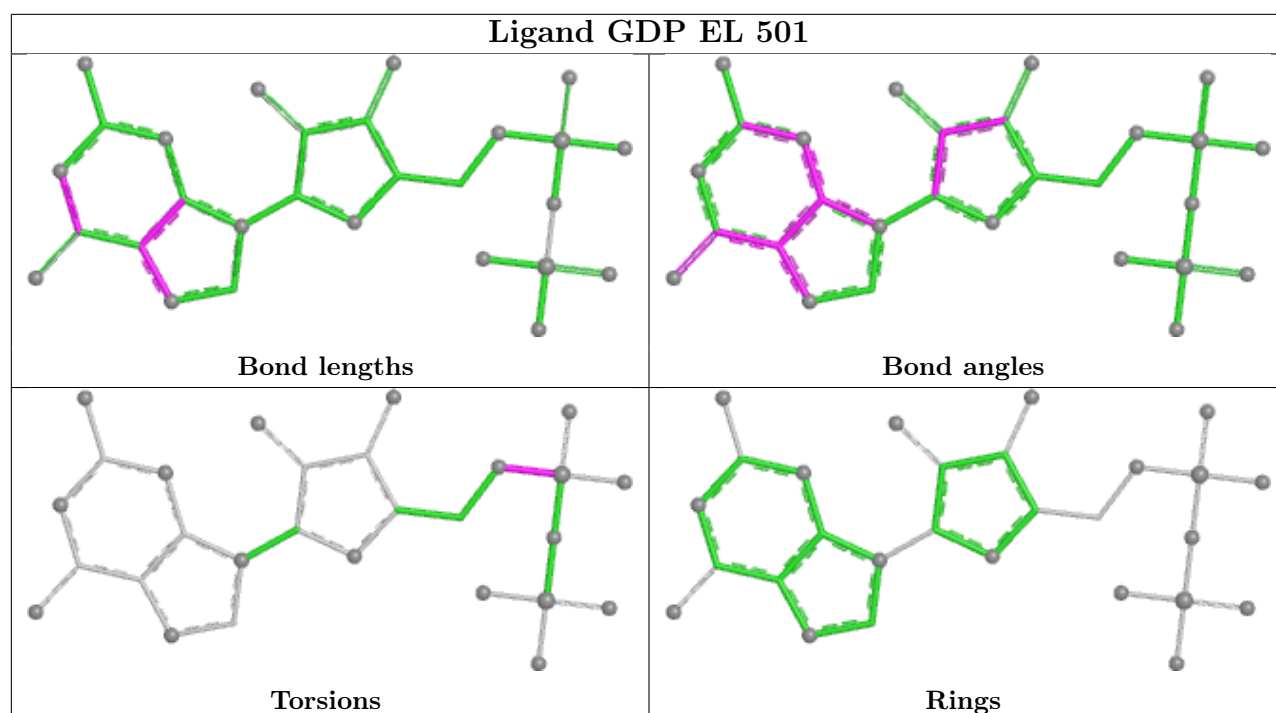
Ligand GTP GA 501



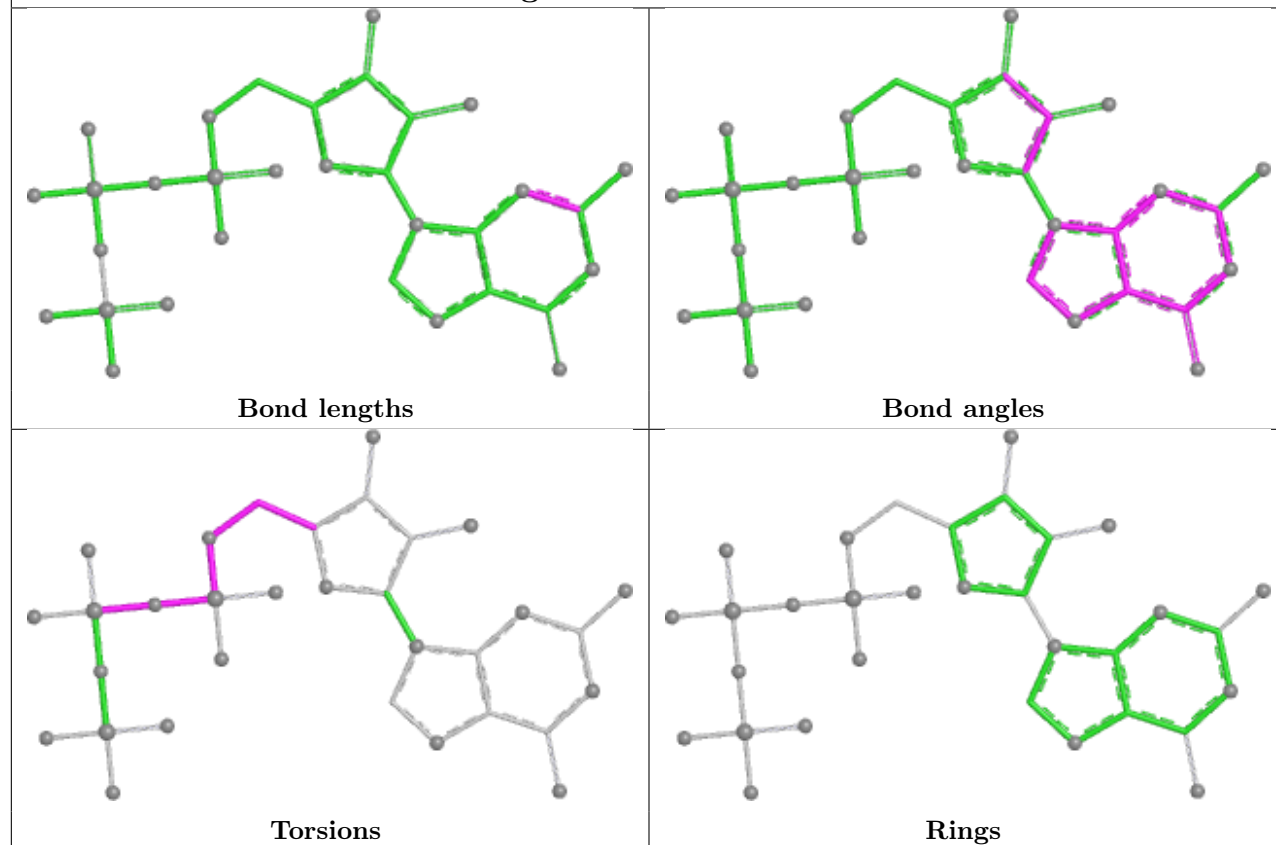




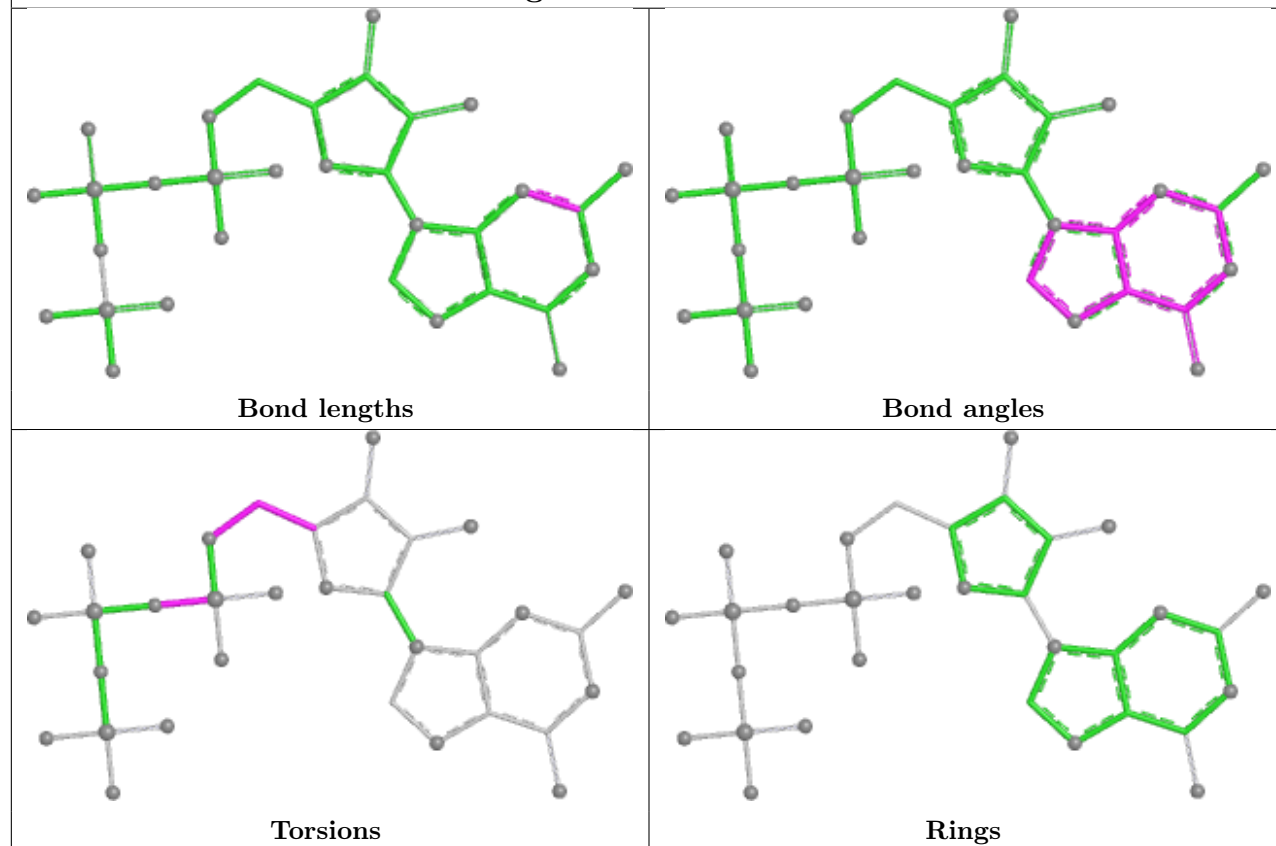




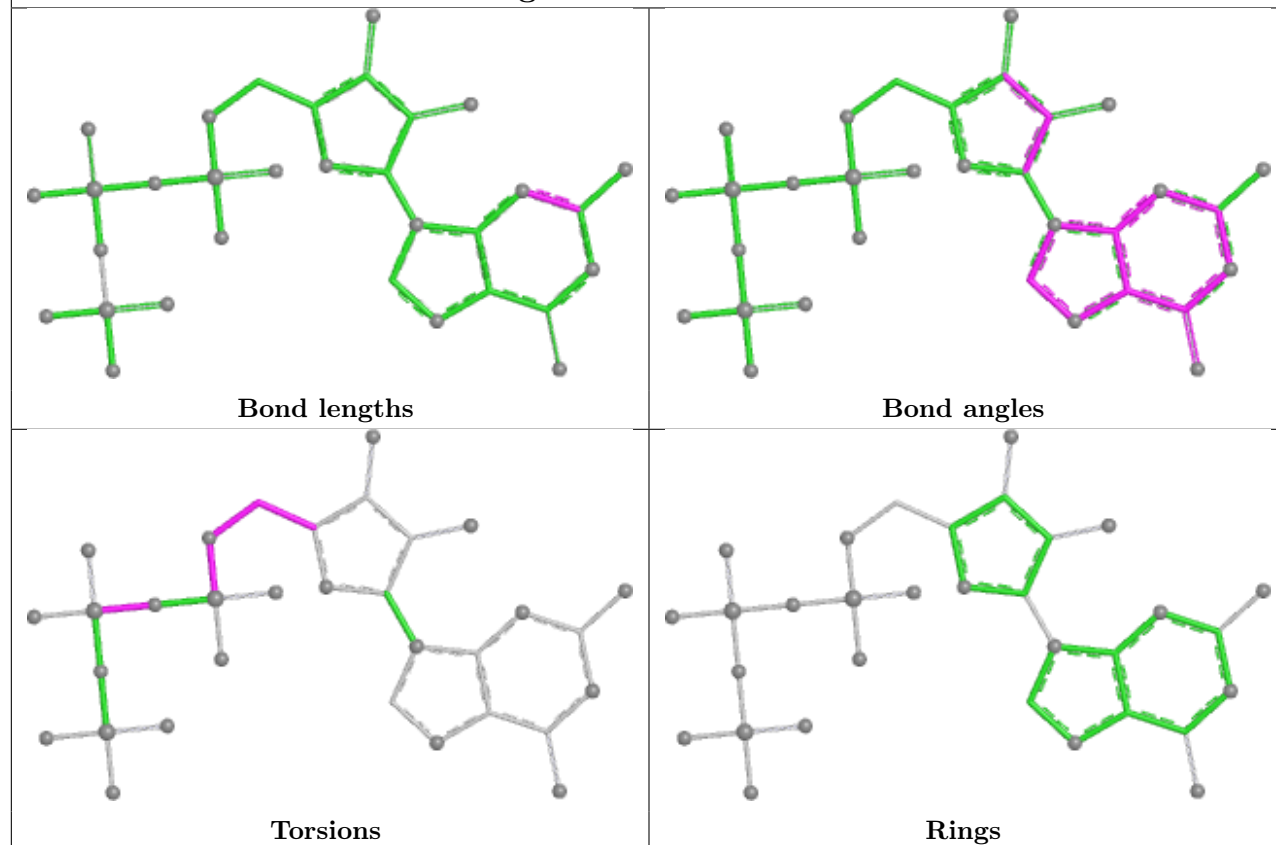
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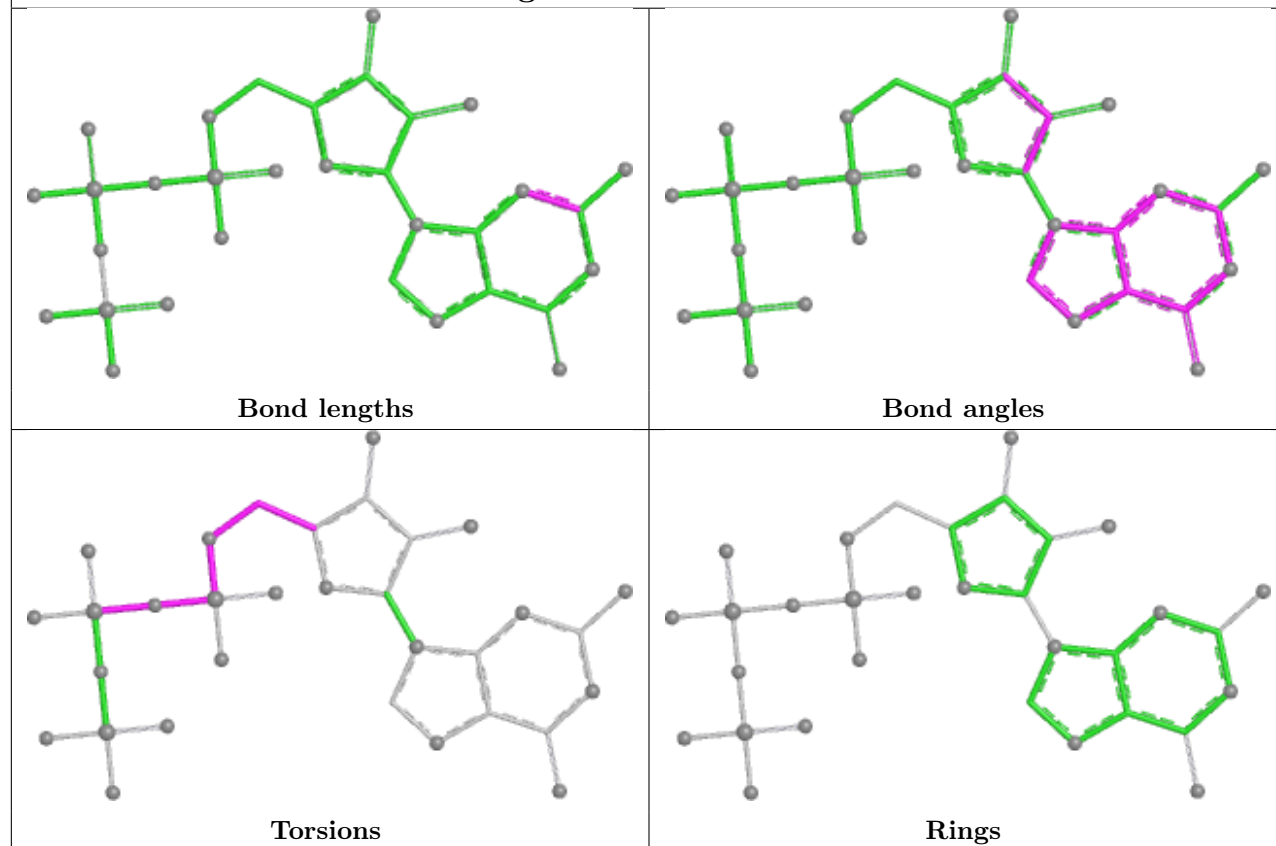
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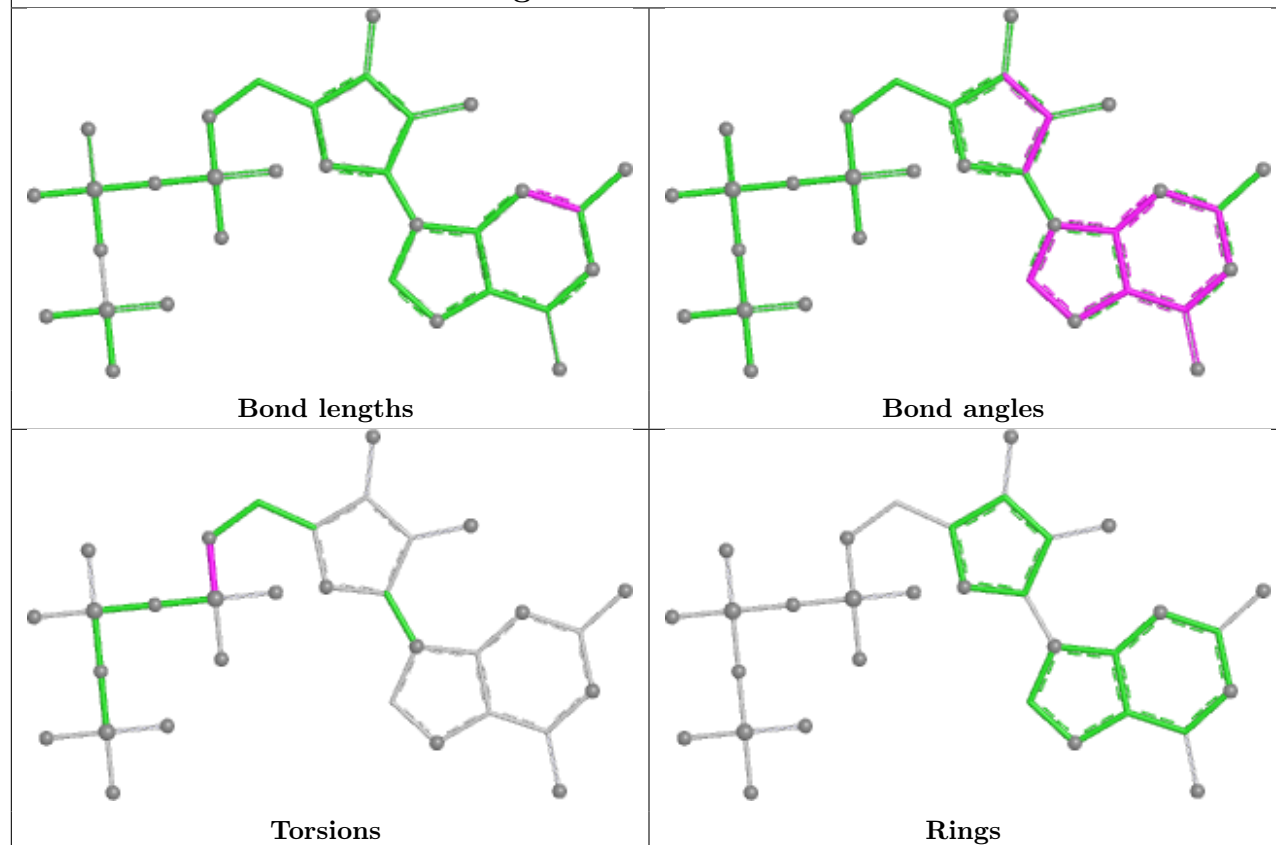
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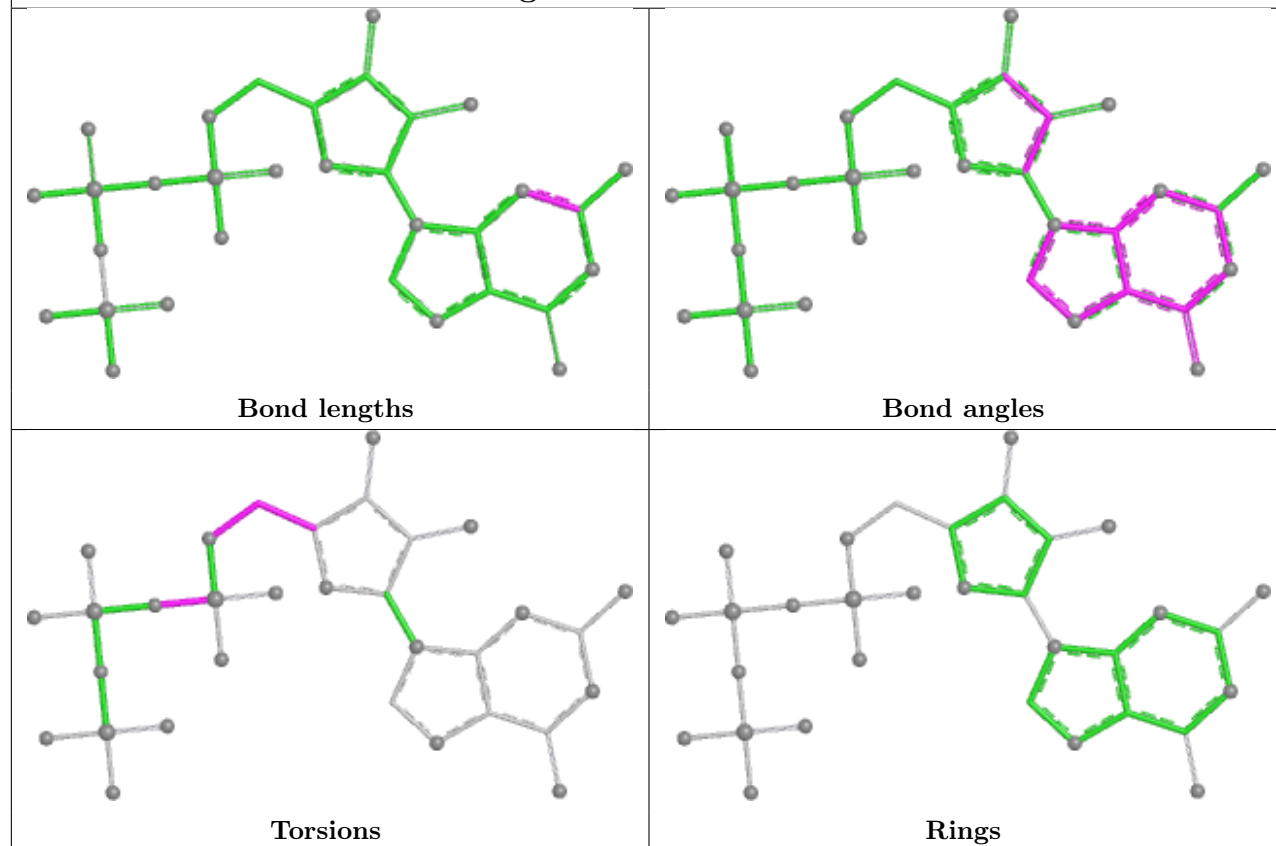
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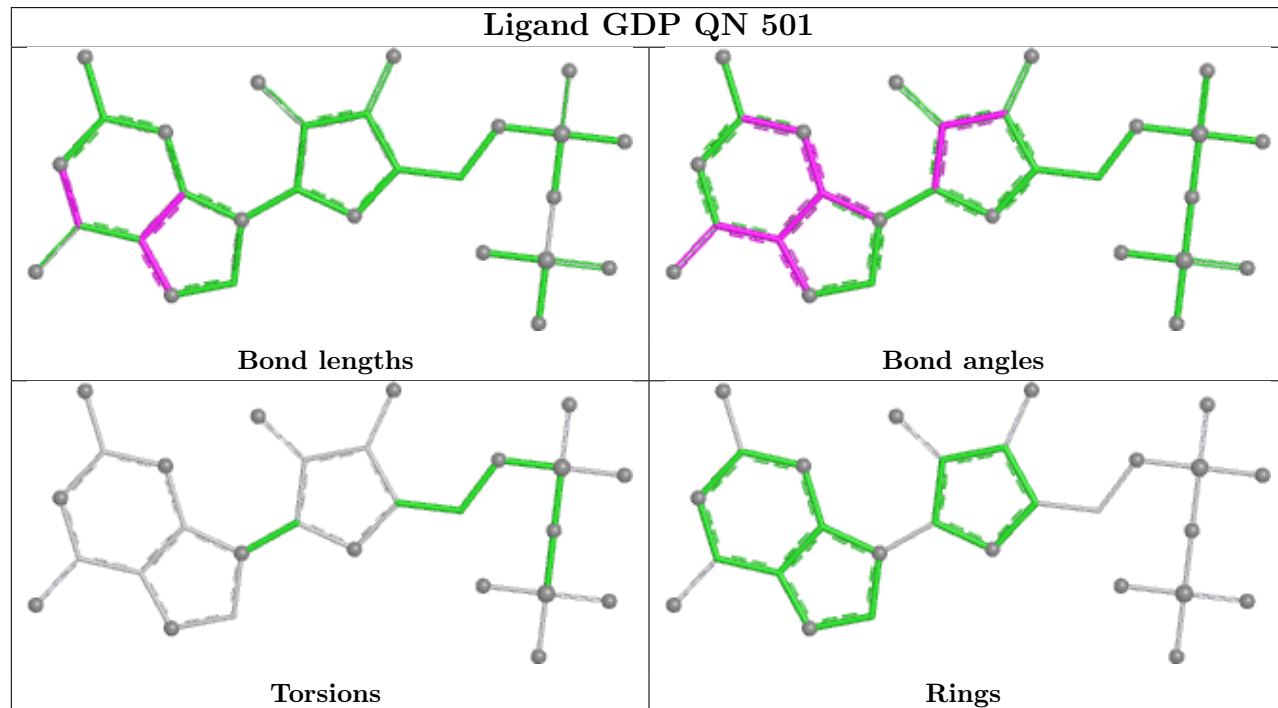
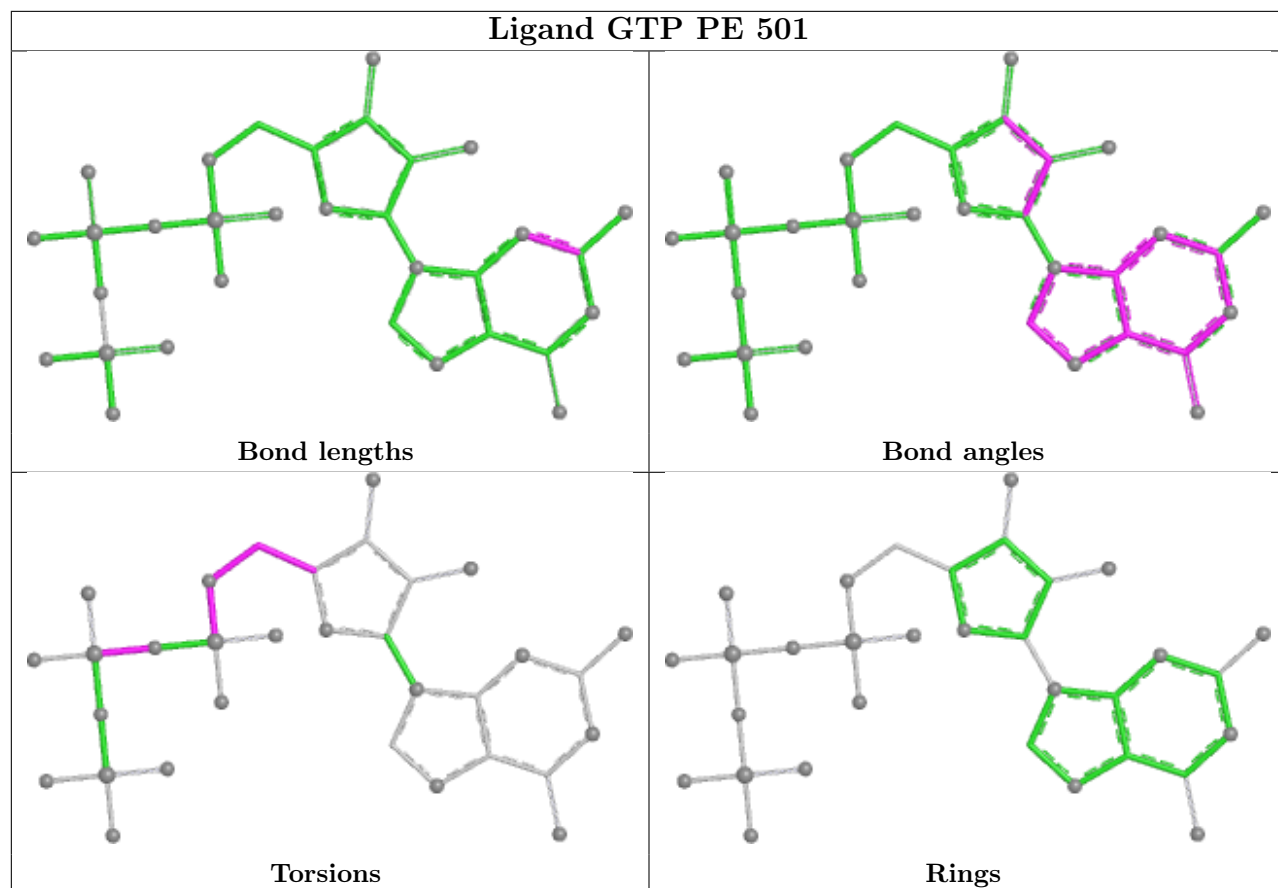


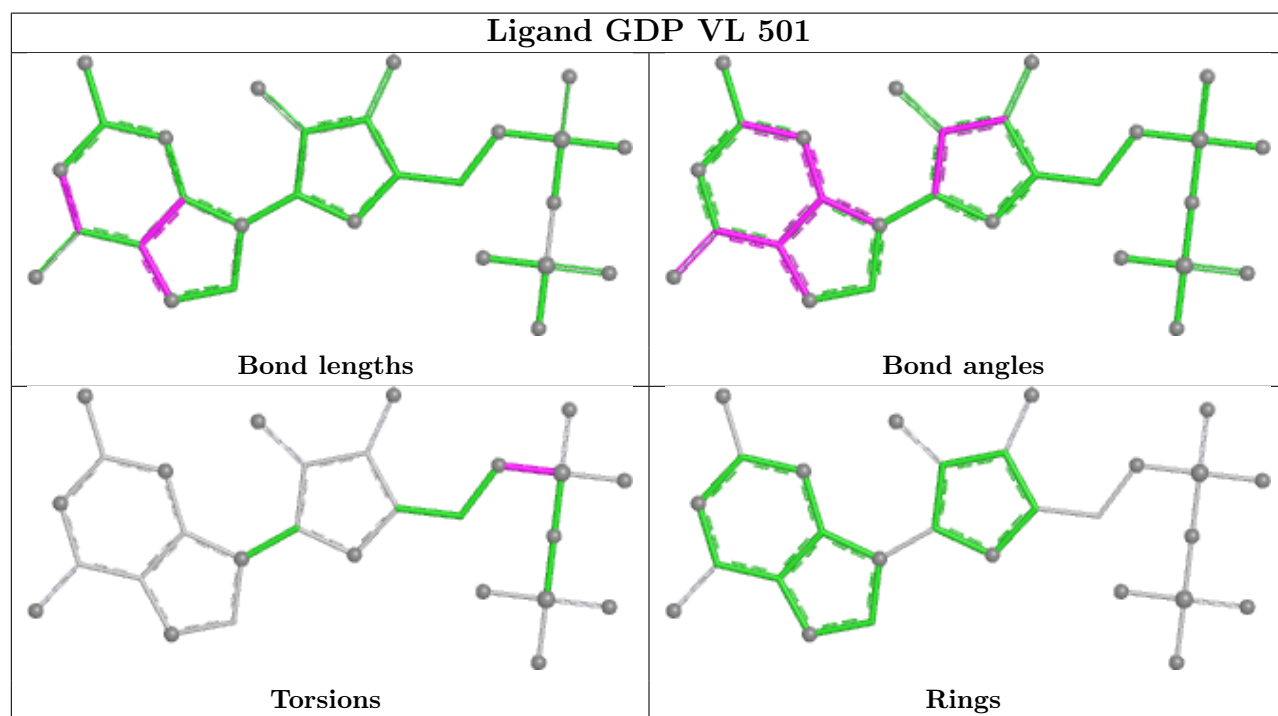
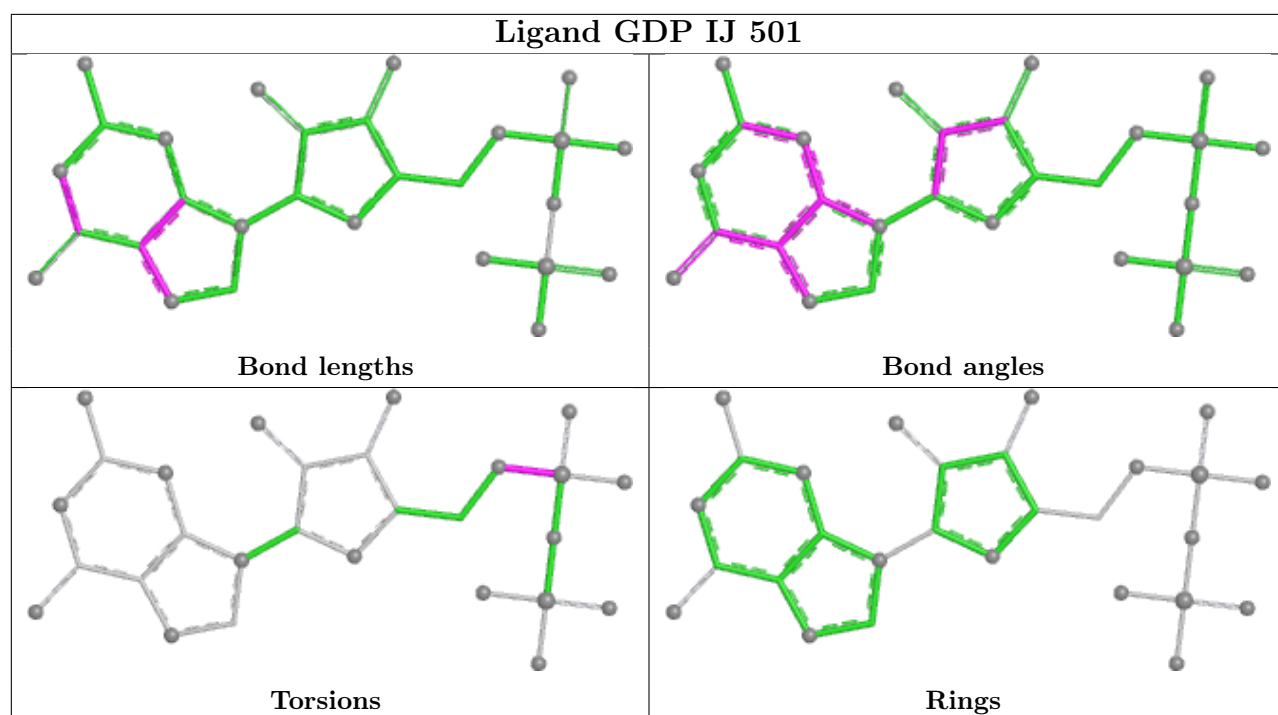
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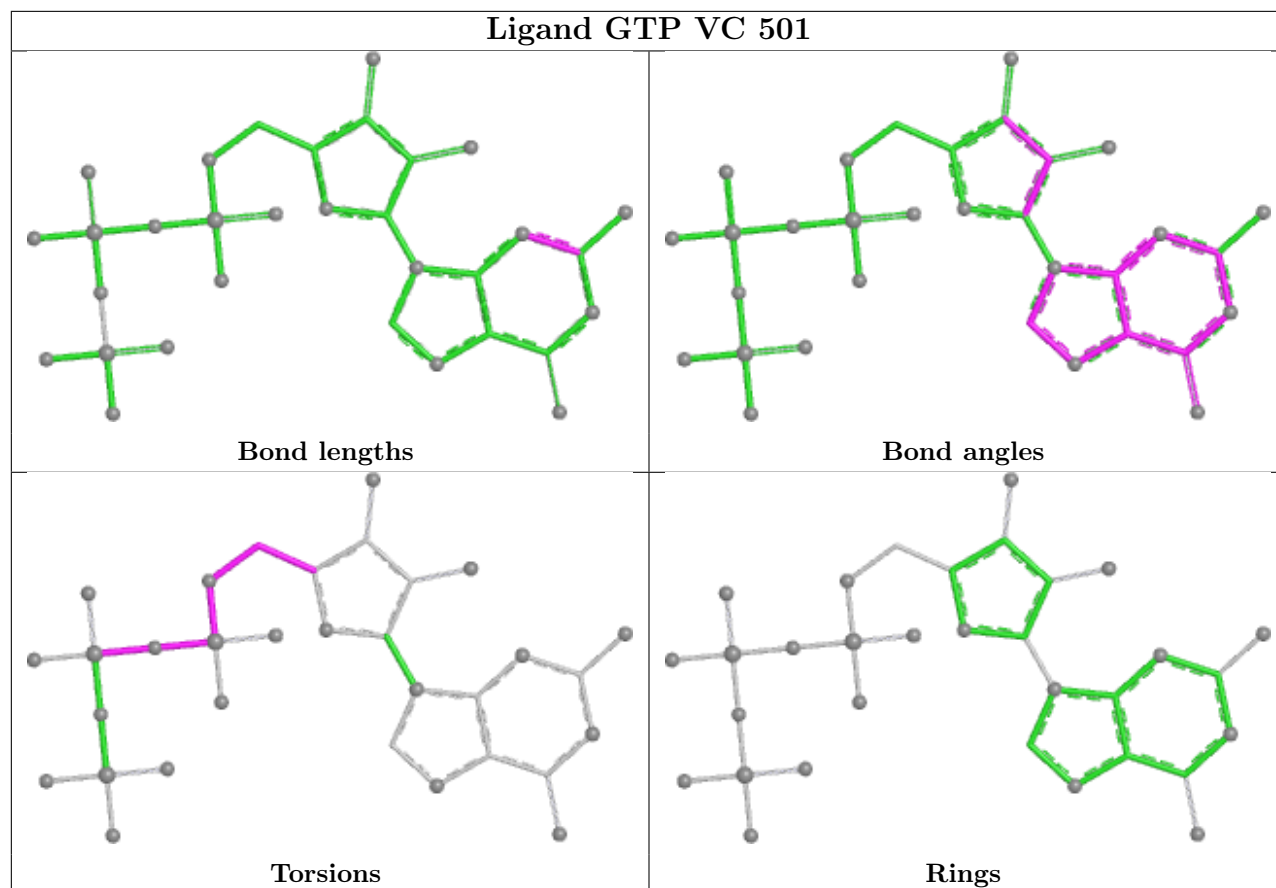
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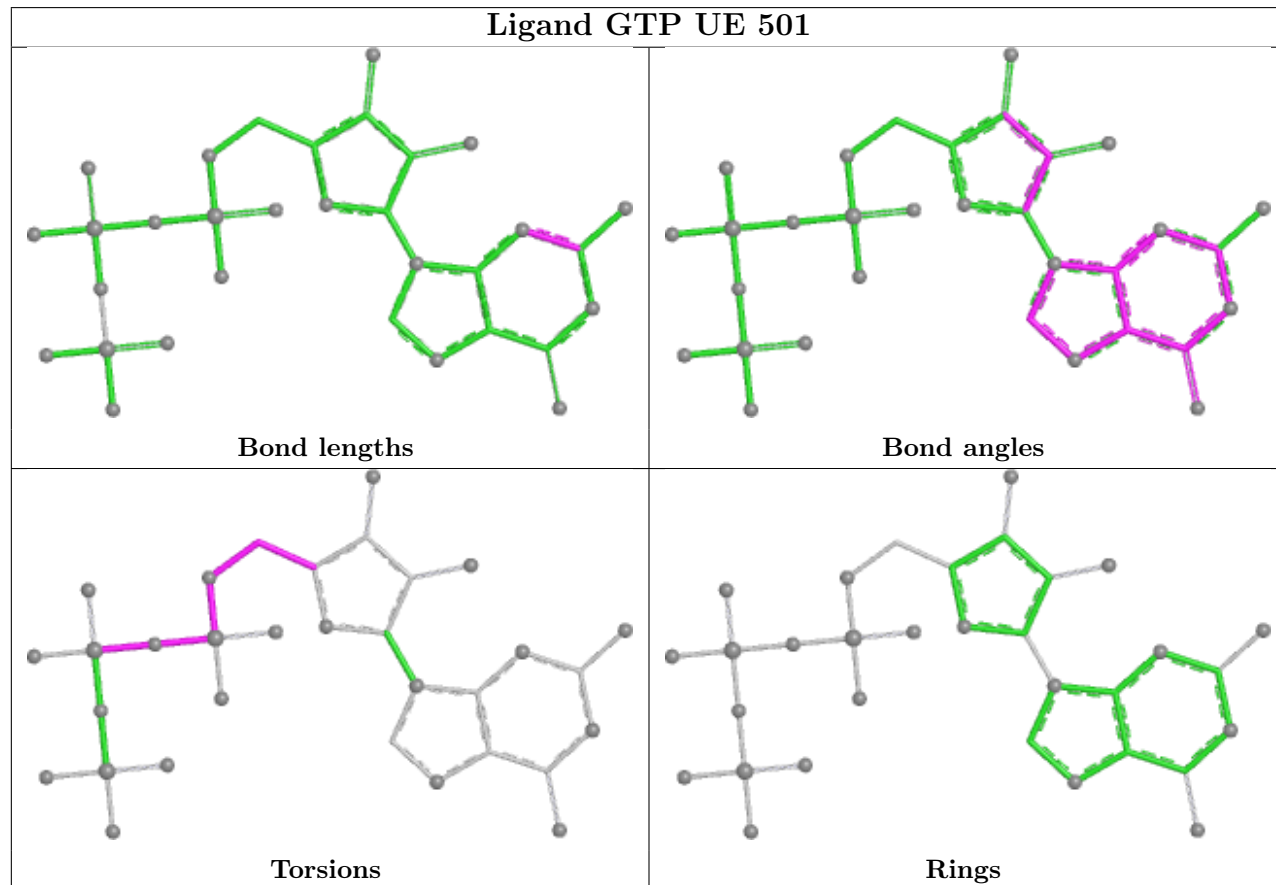


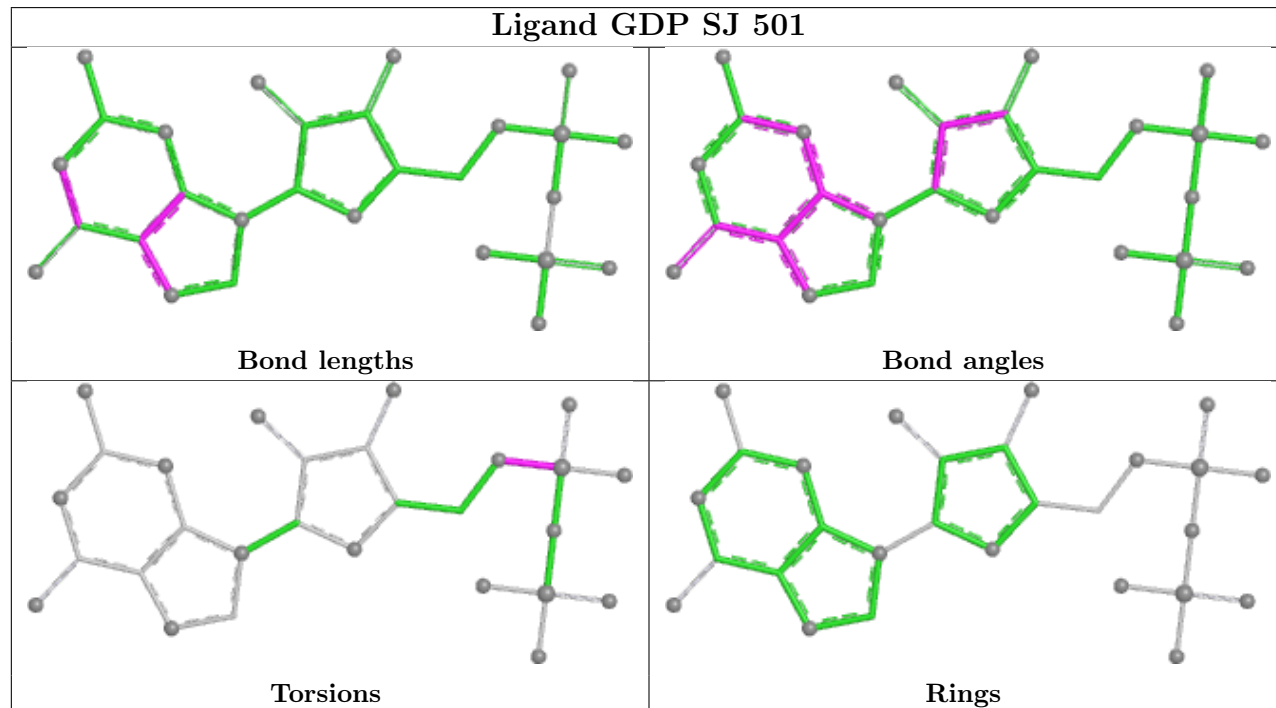
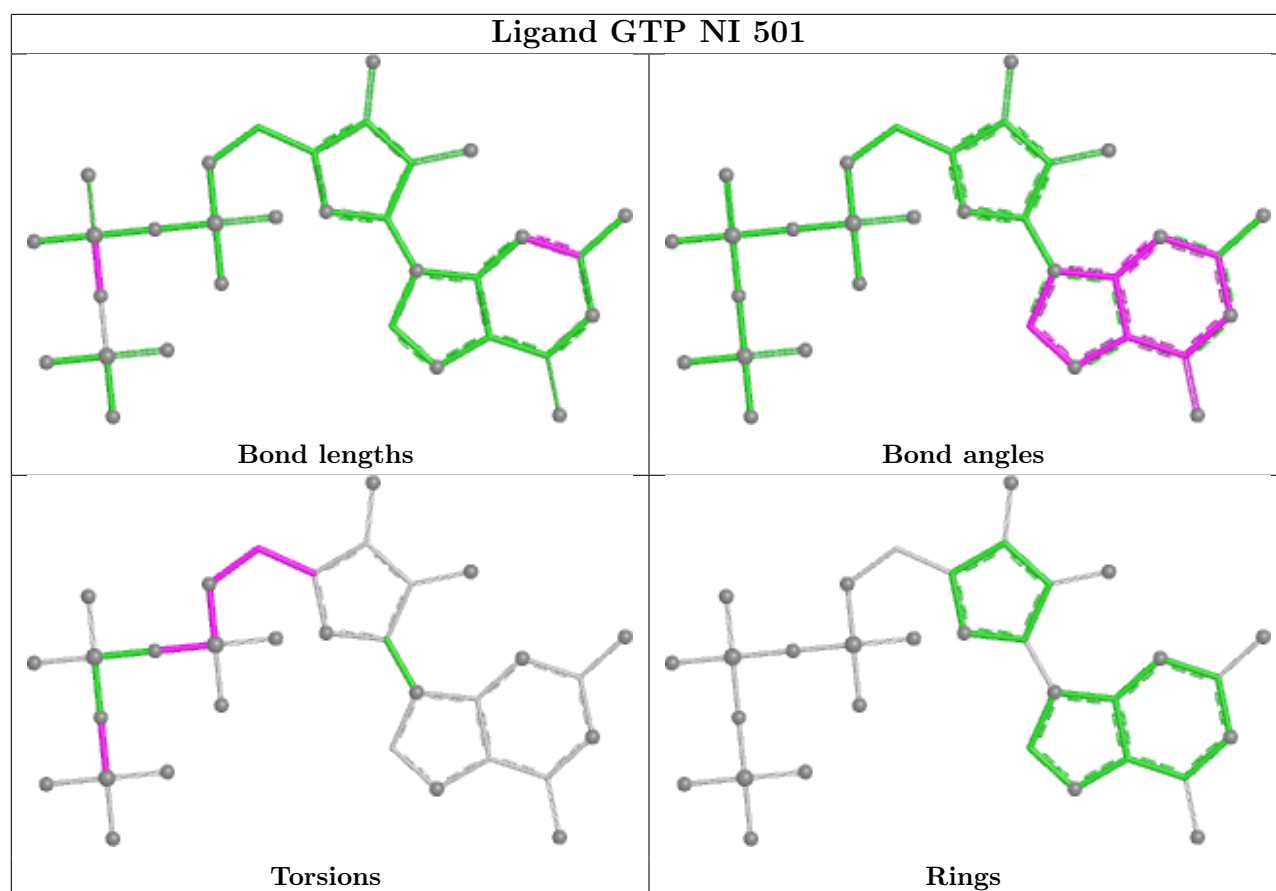


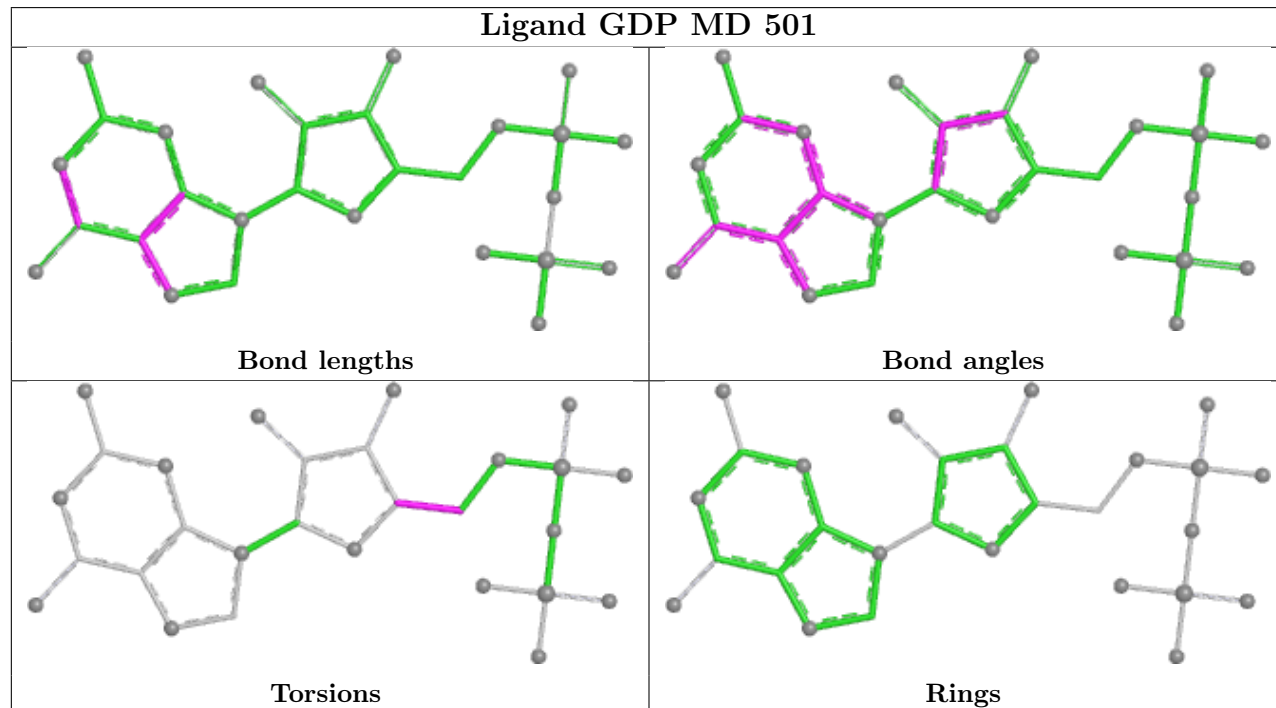
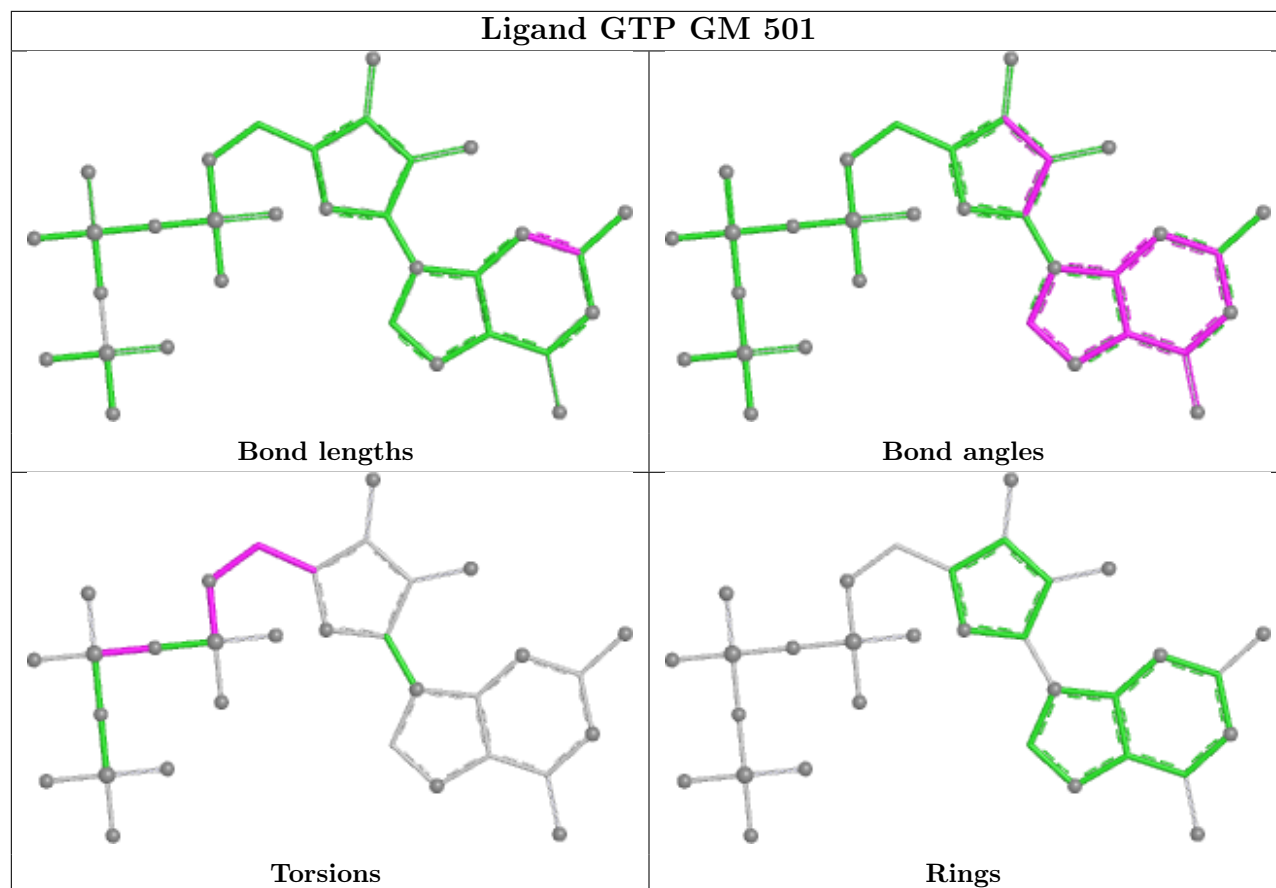
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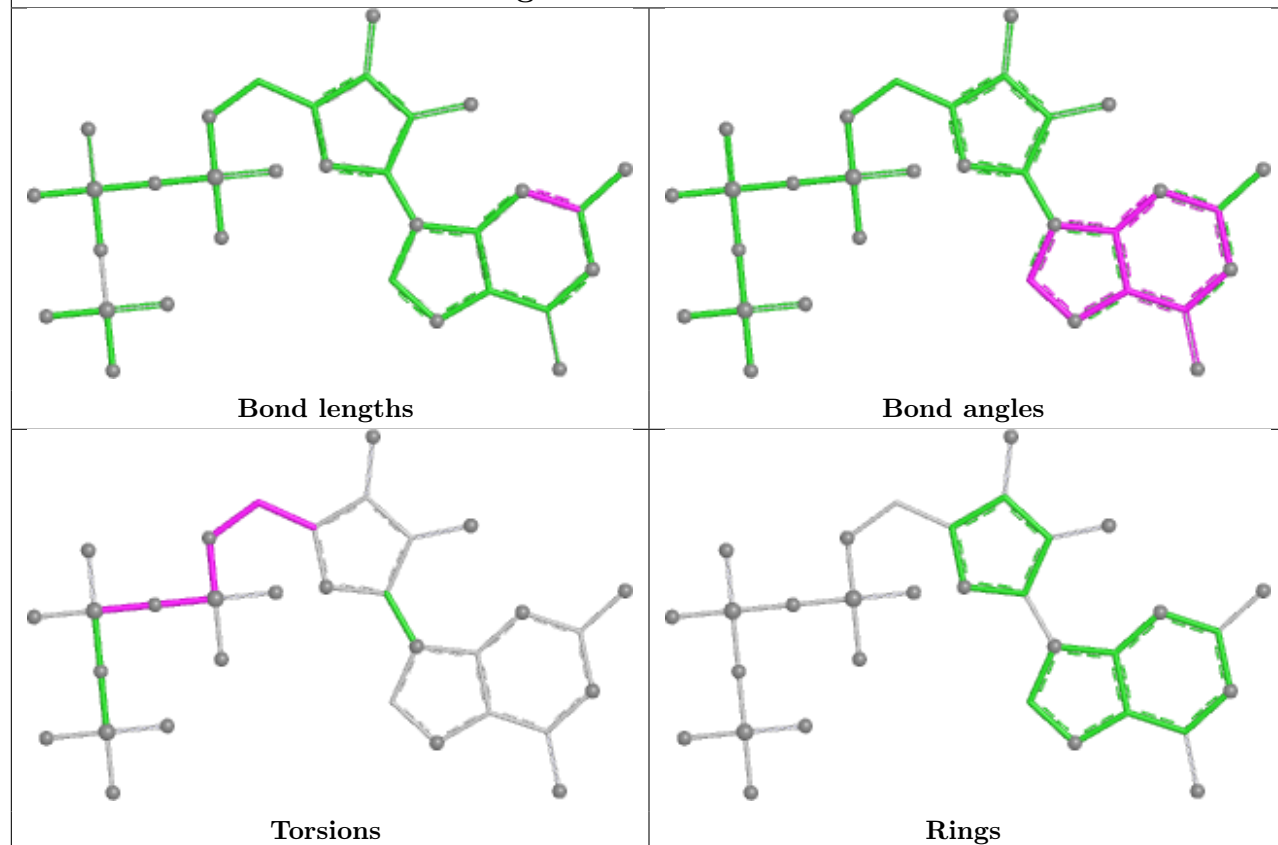
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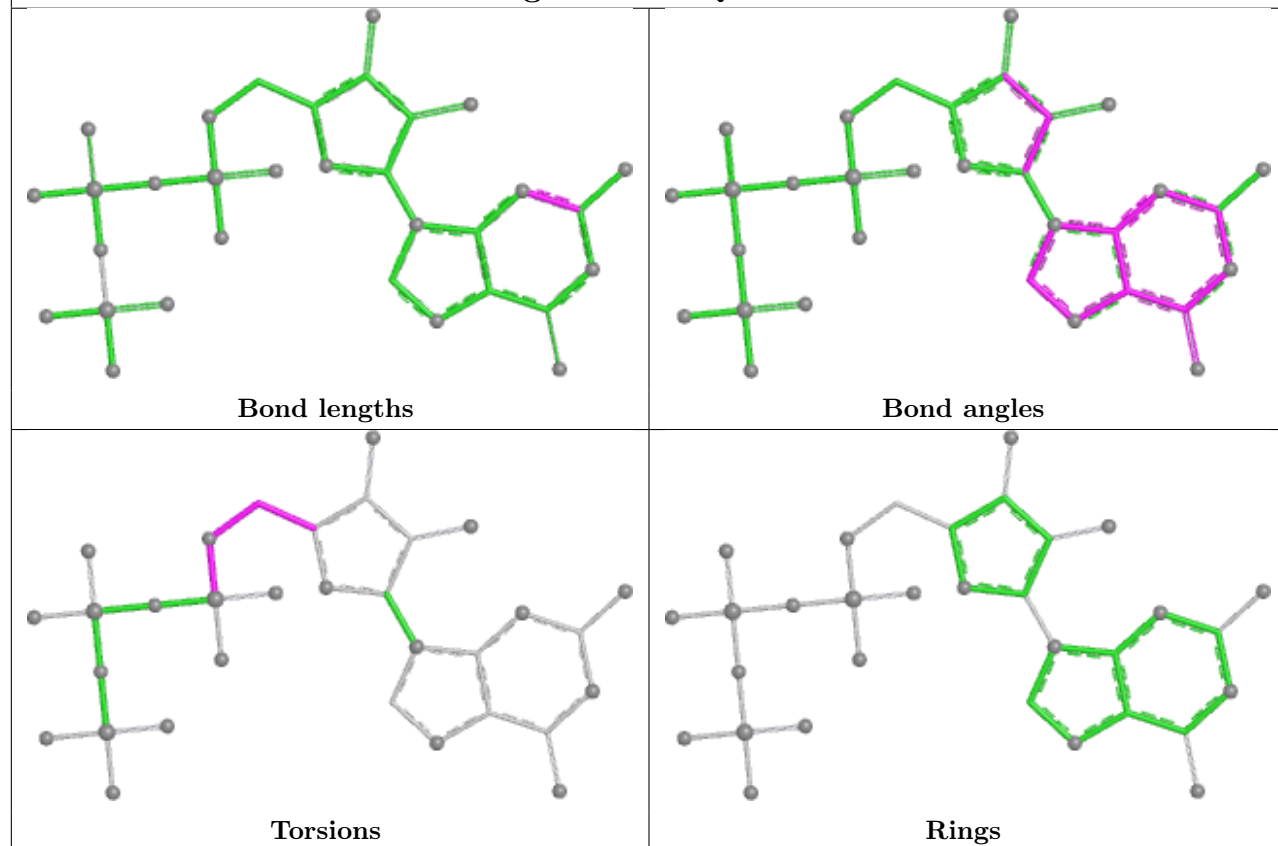


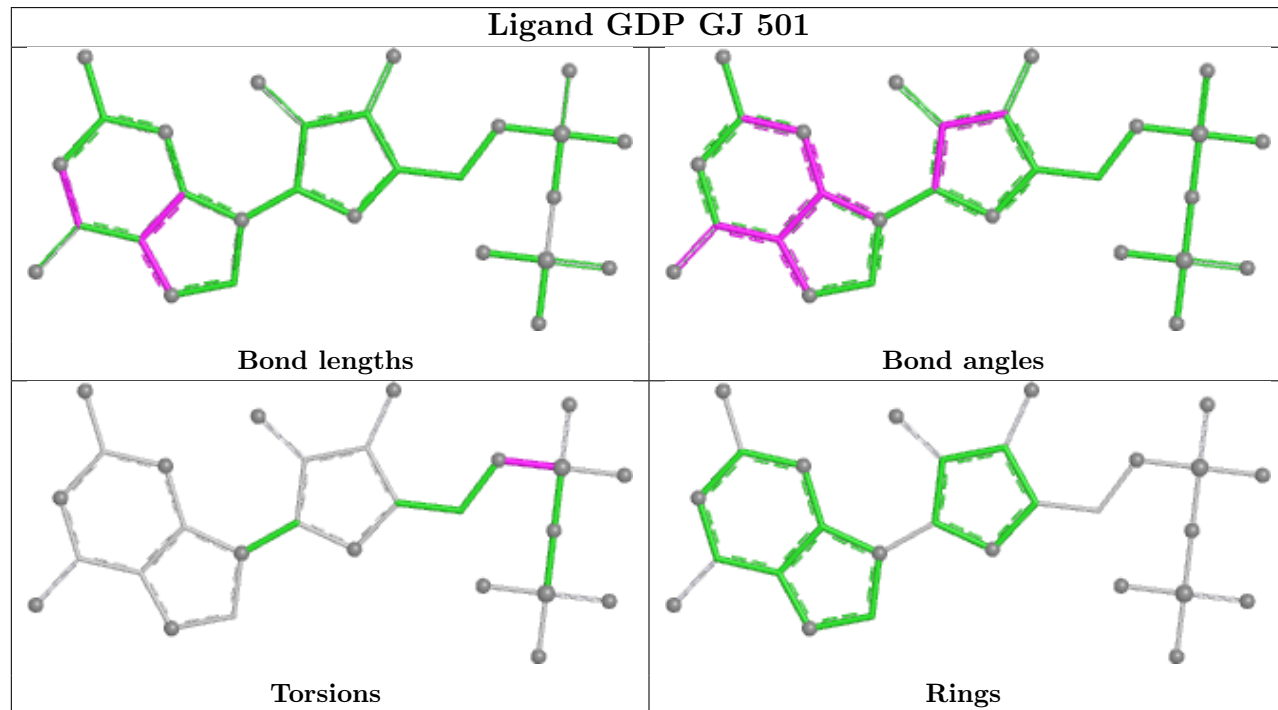
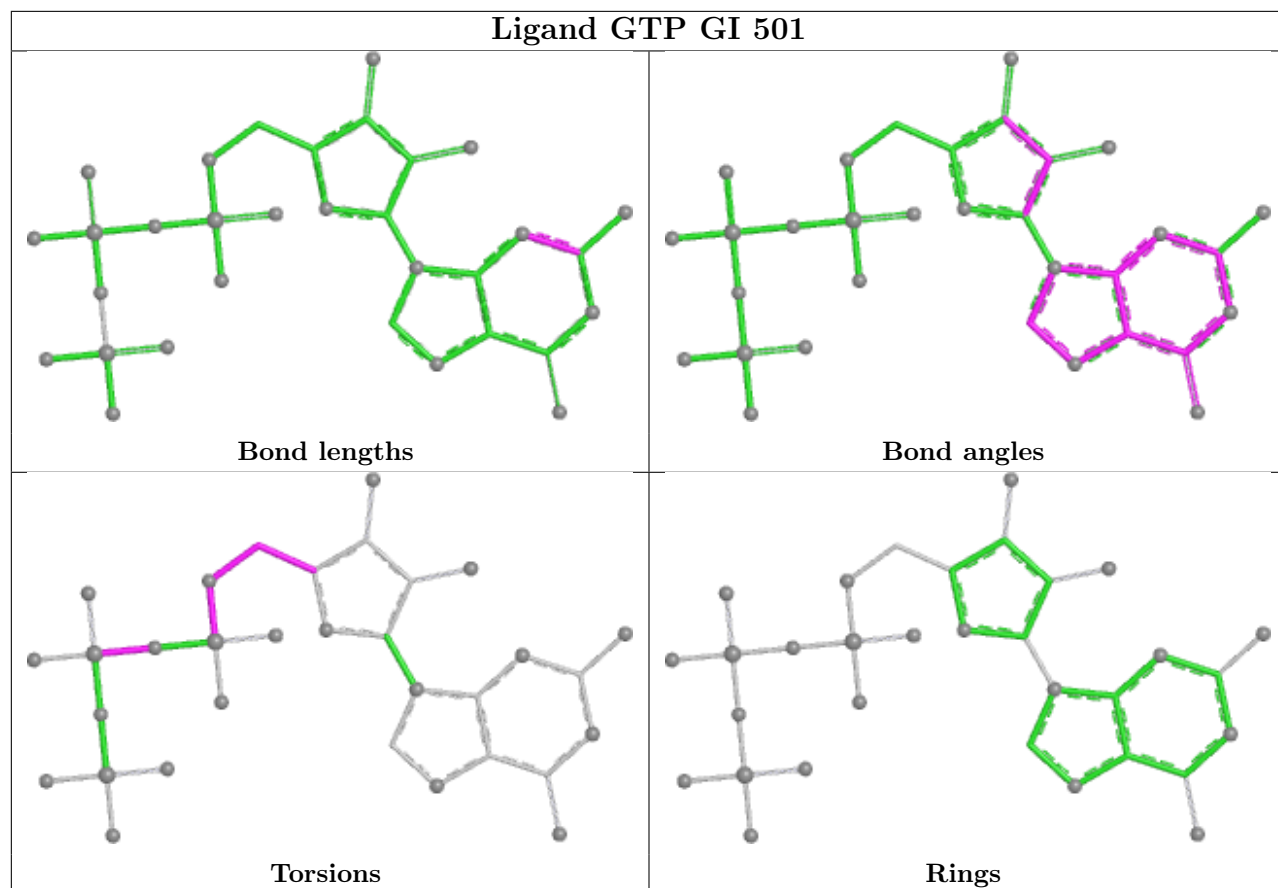


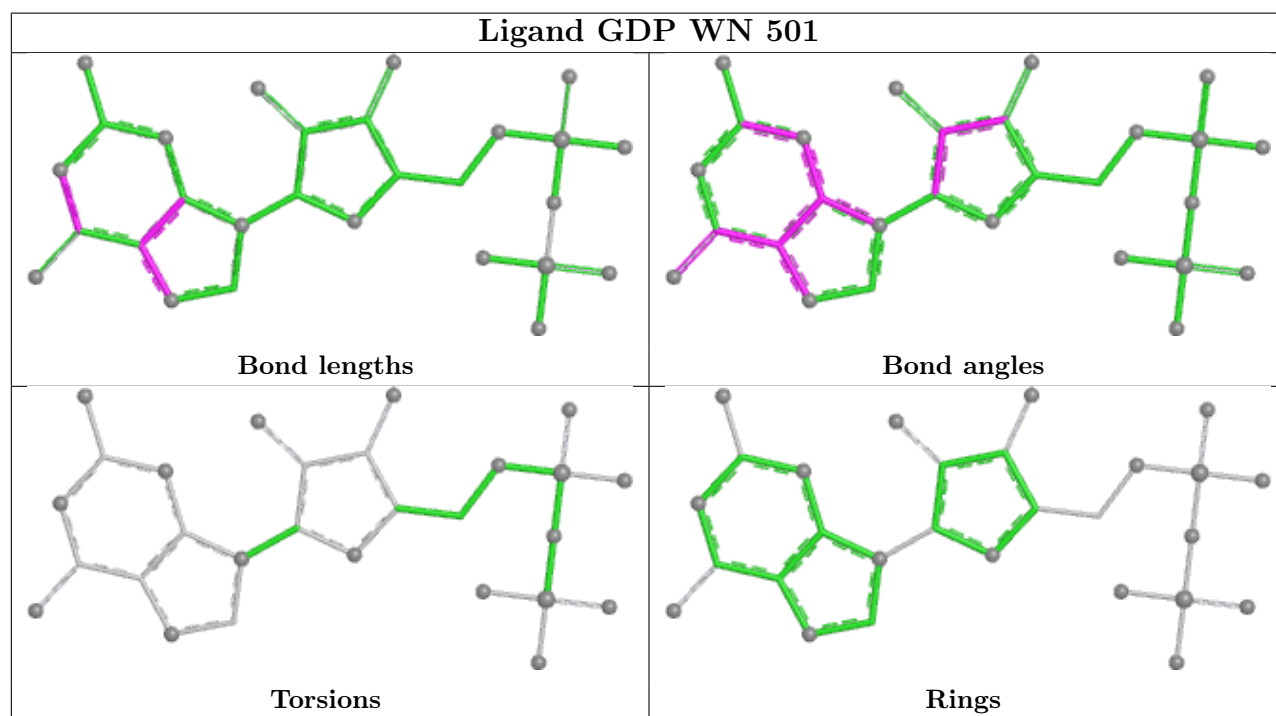
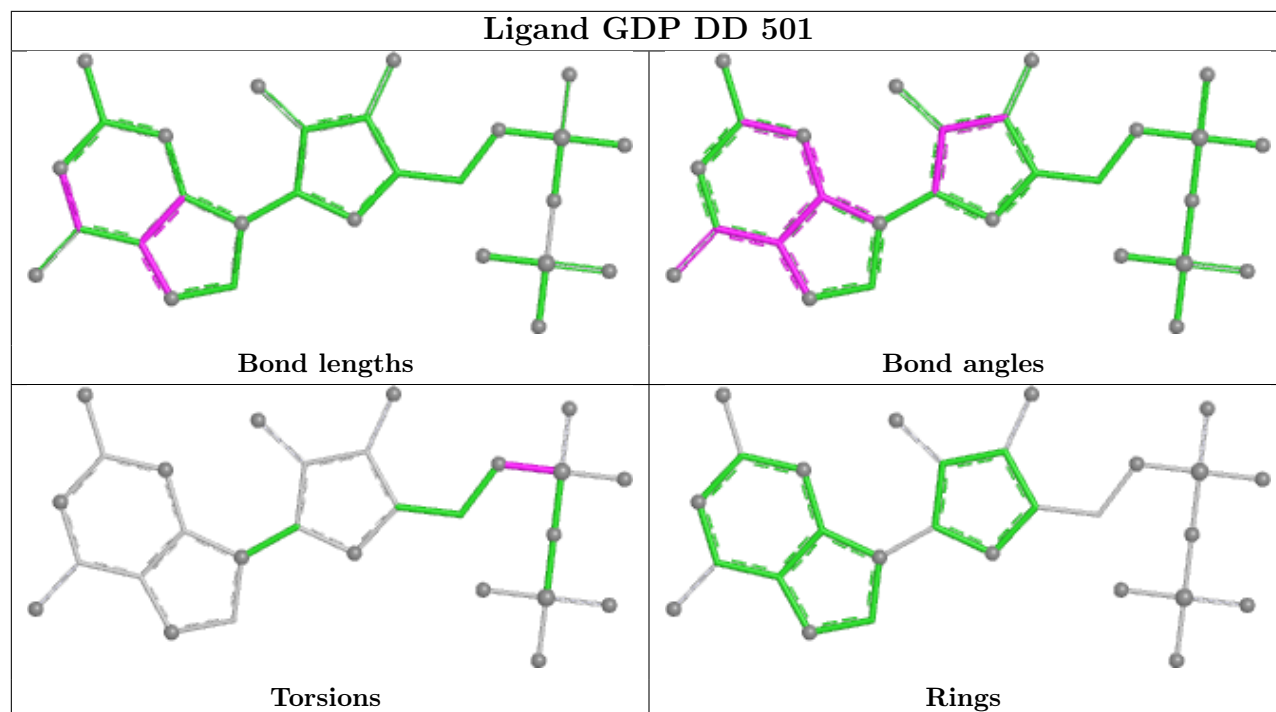
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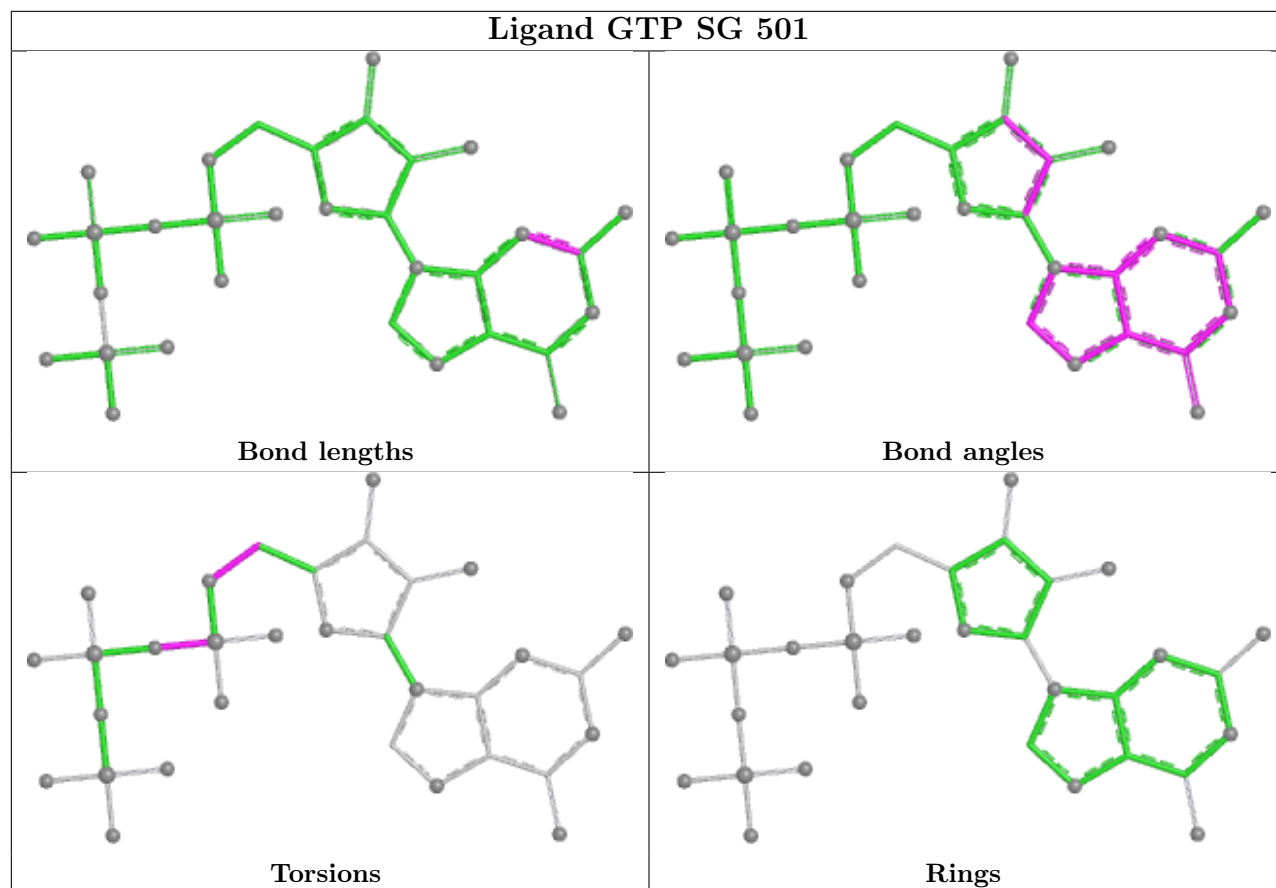
Ligand GTP QI 501



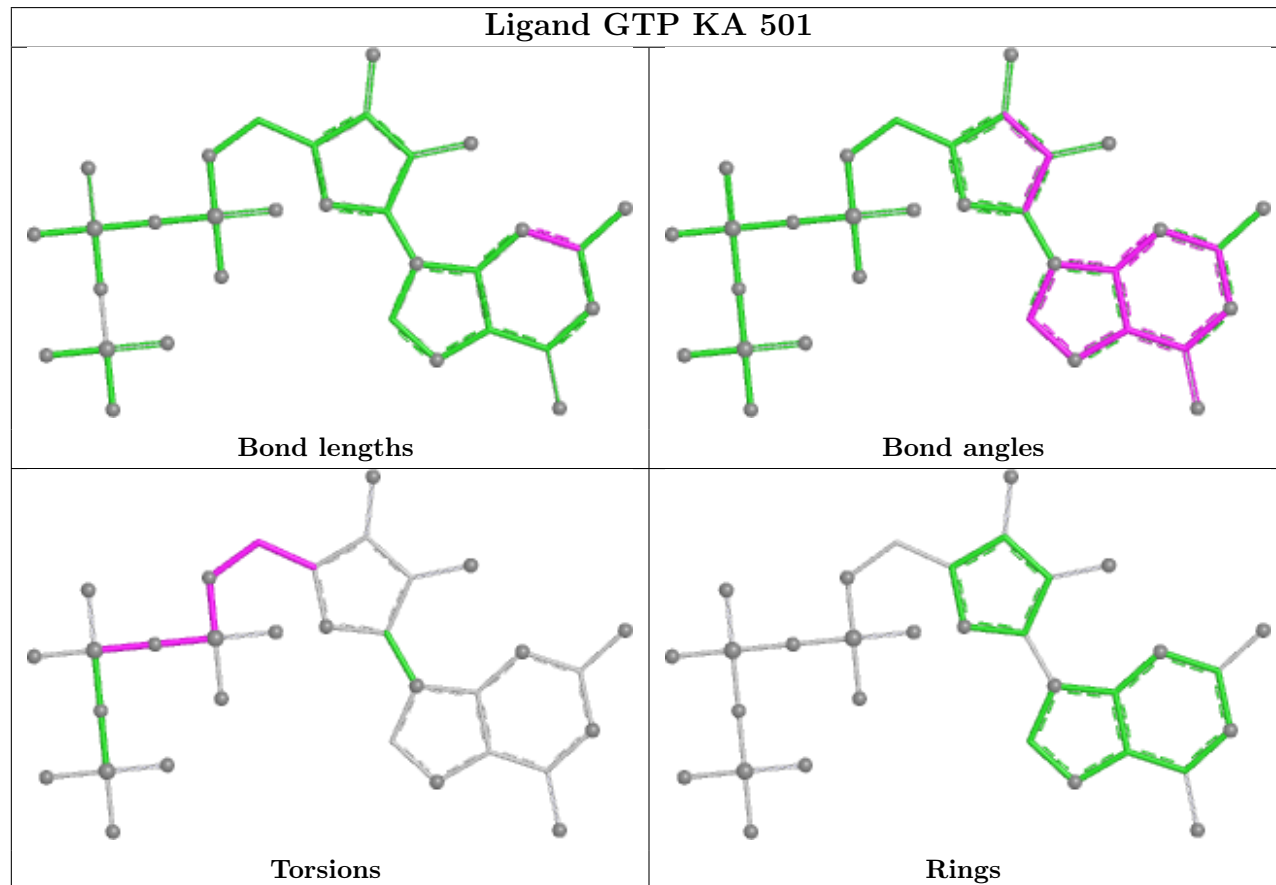




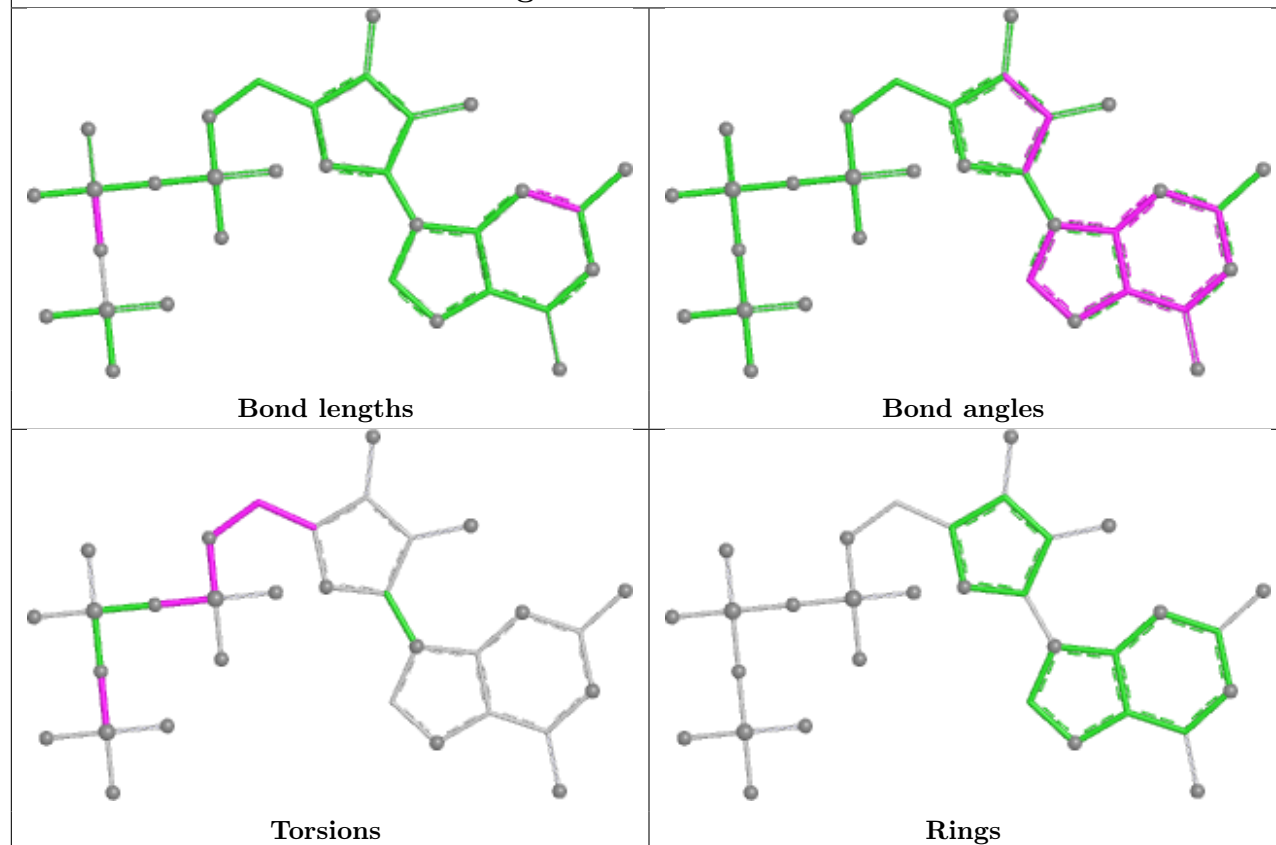
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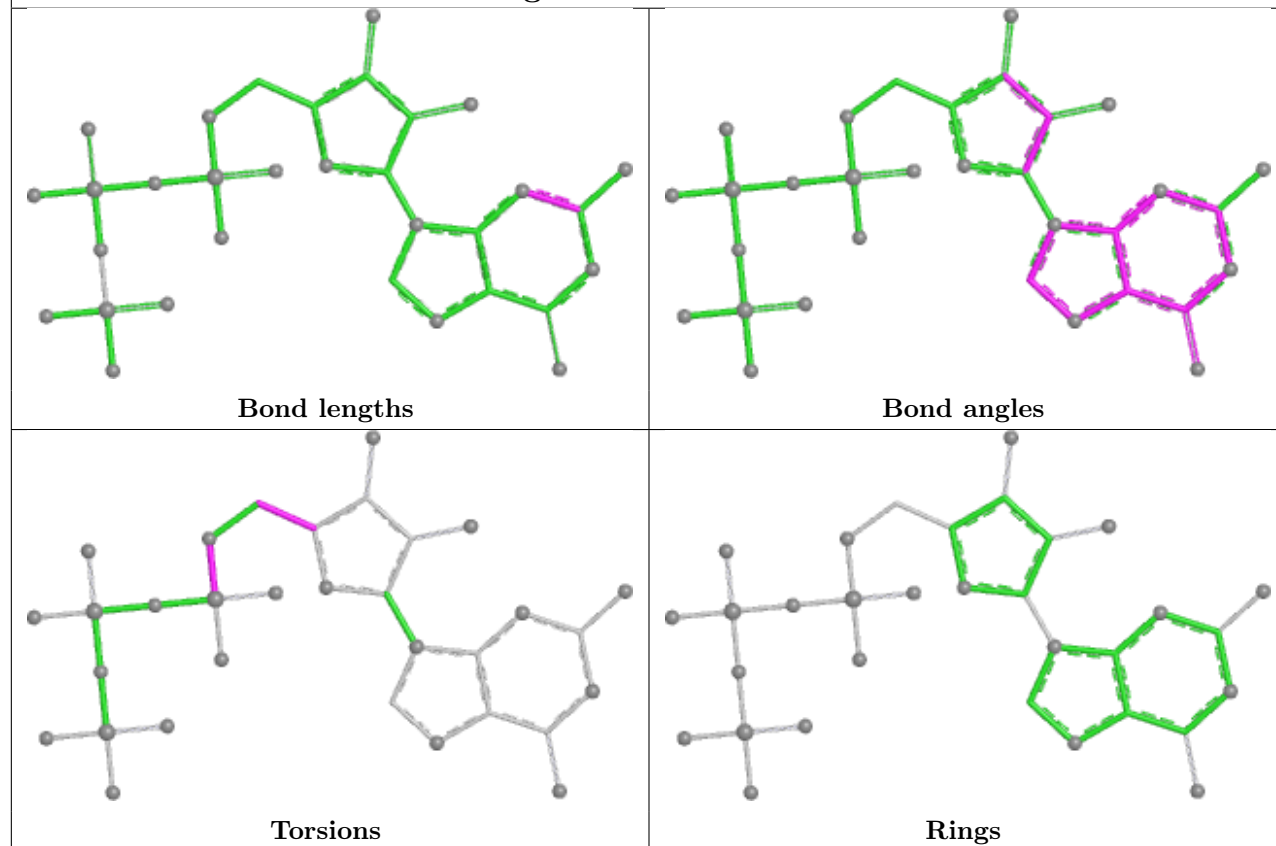
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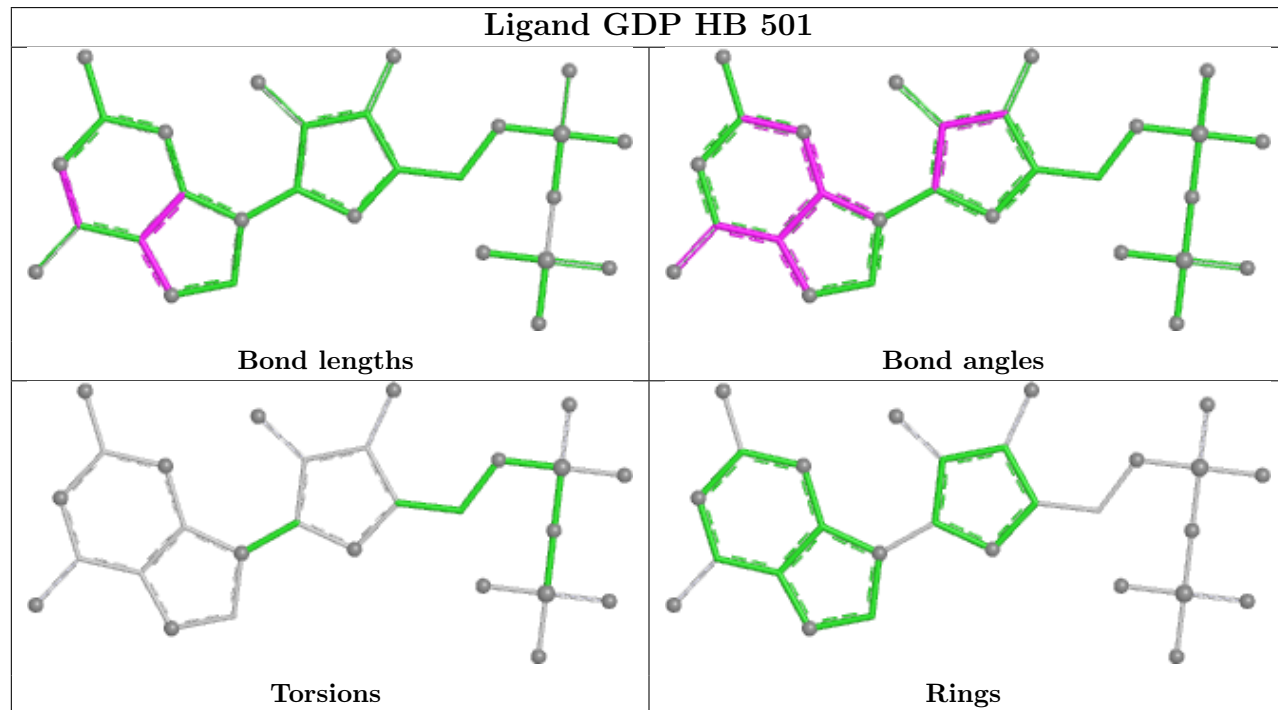
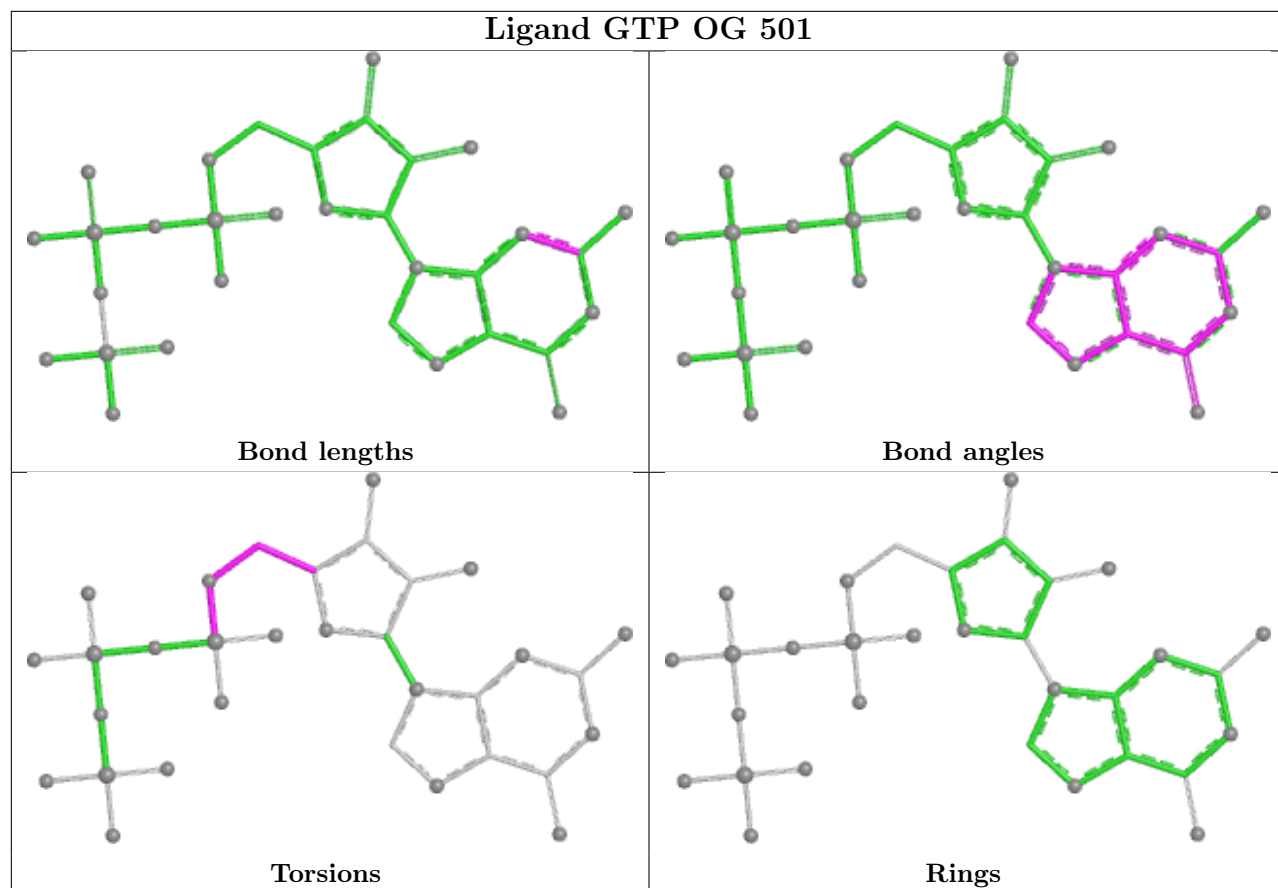


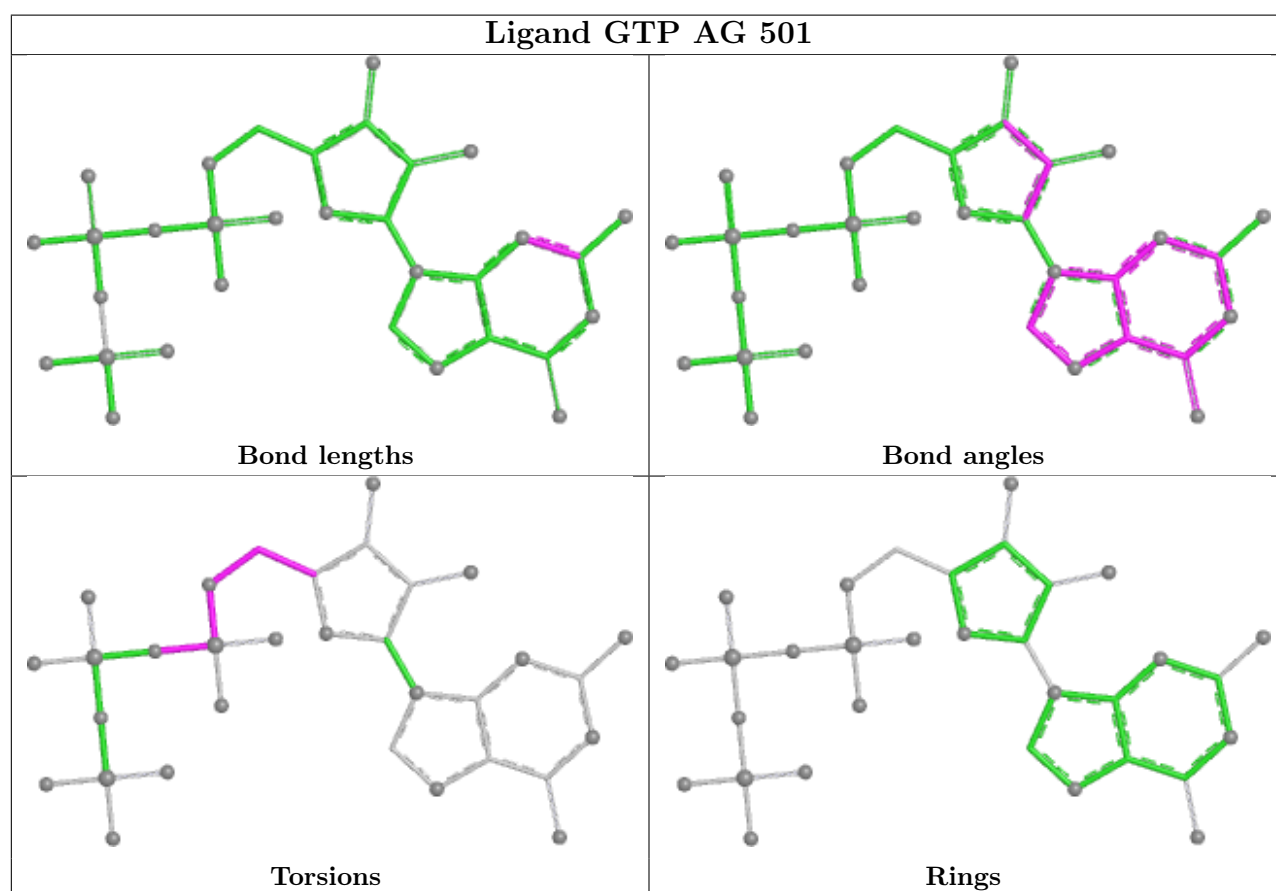
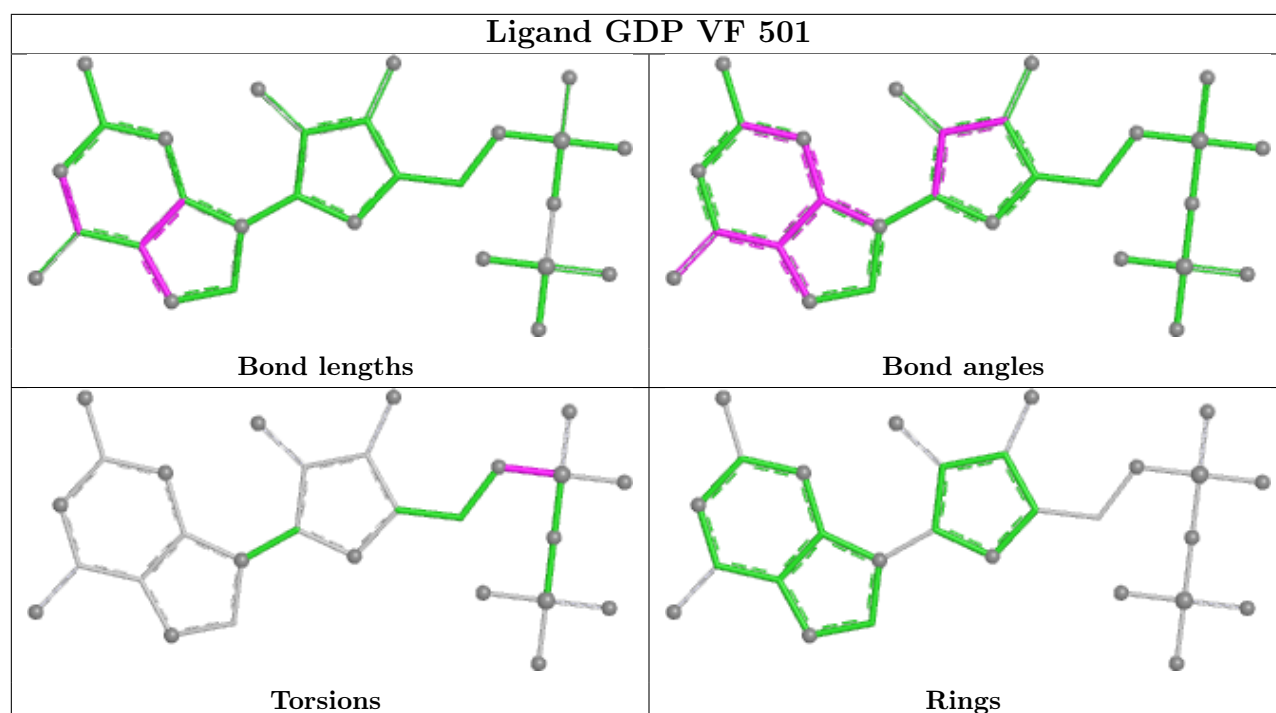
Ligand GTP HC 501

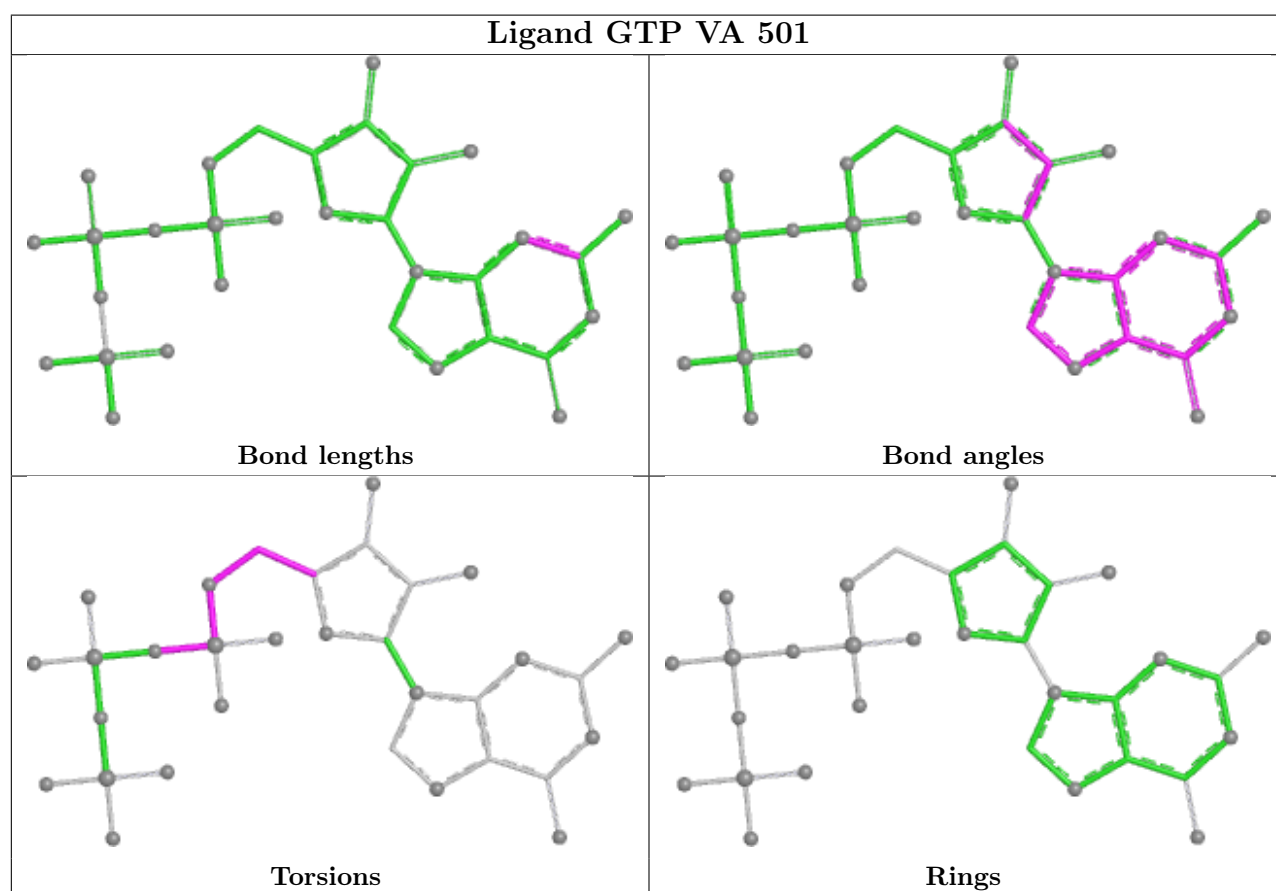
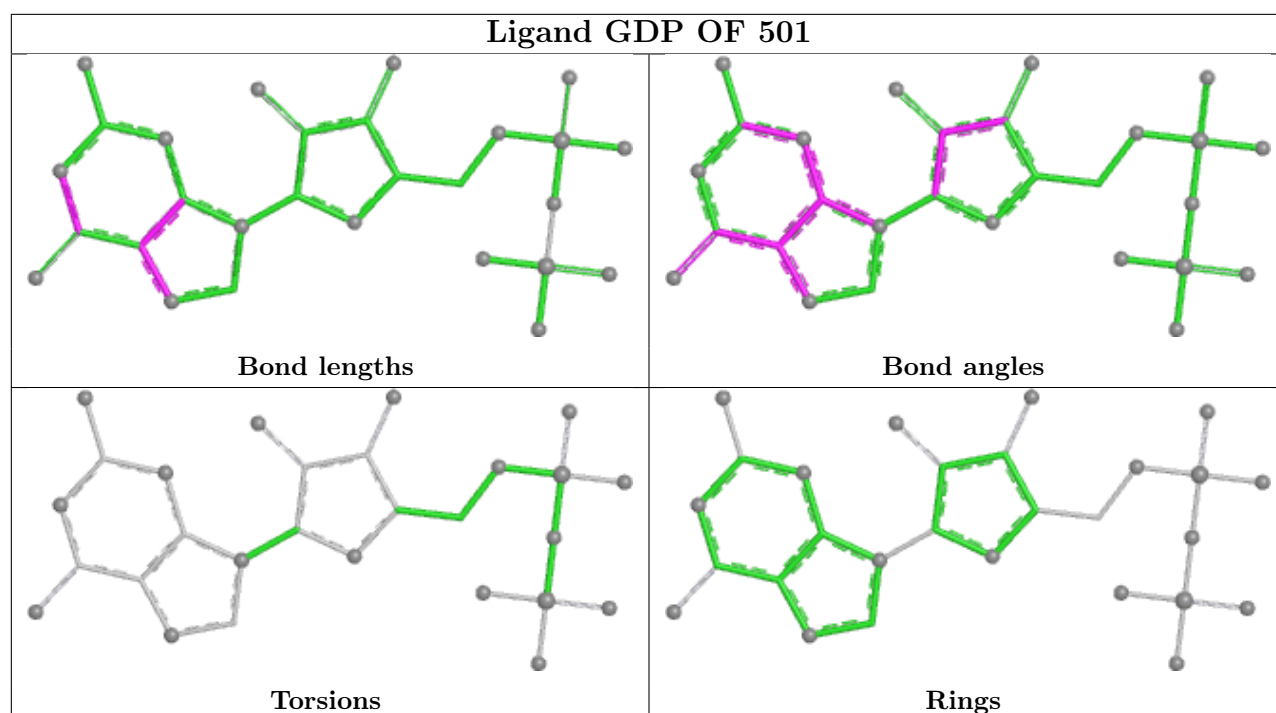


Ligand GTP OI 501

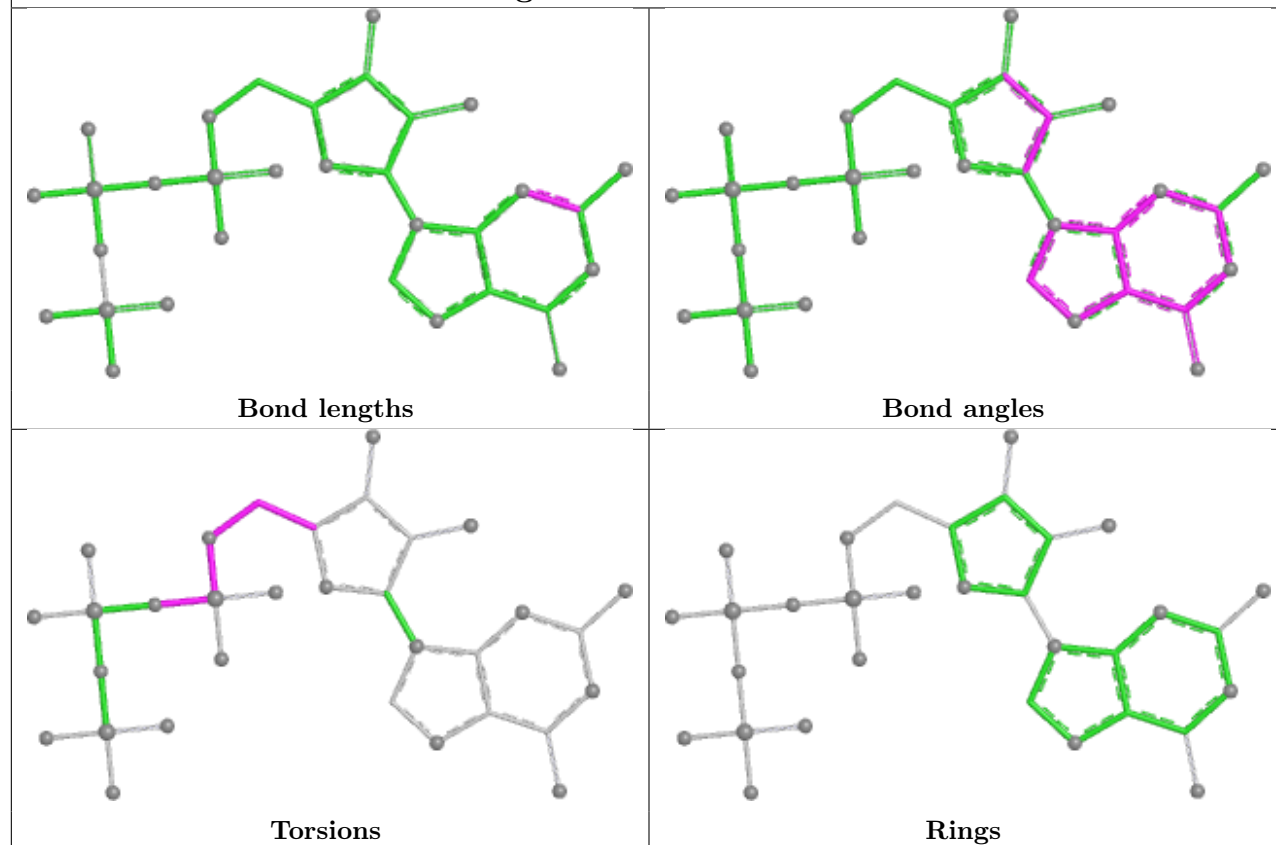




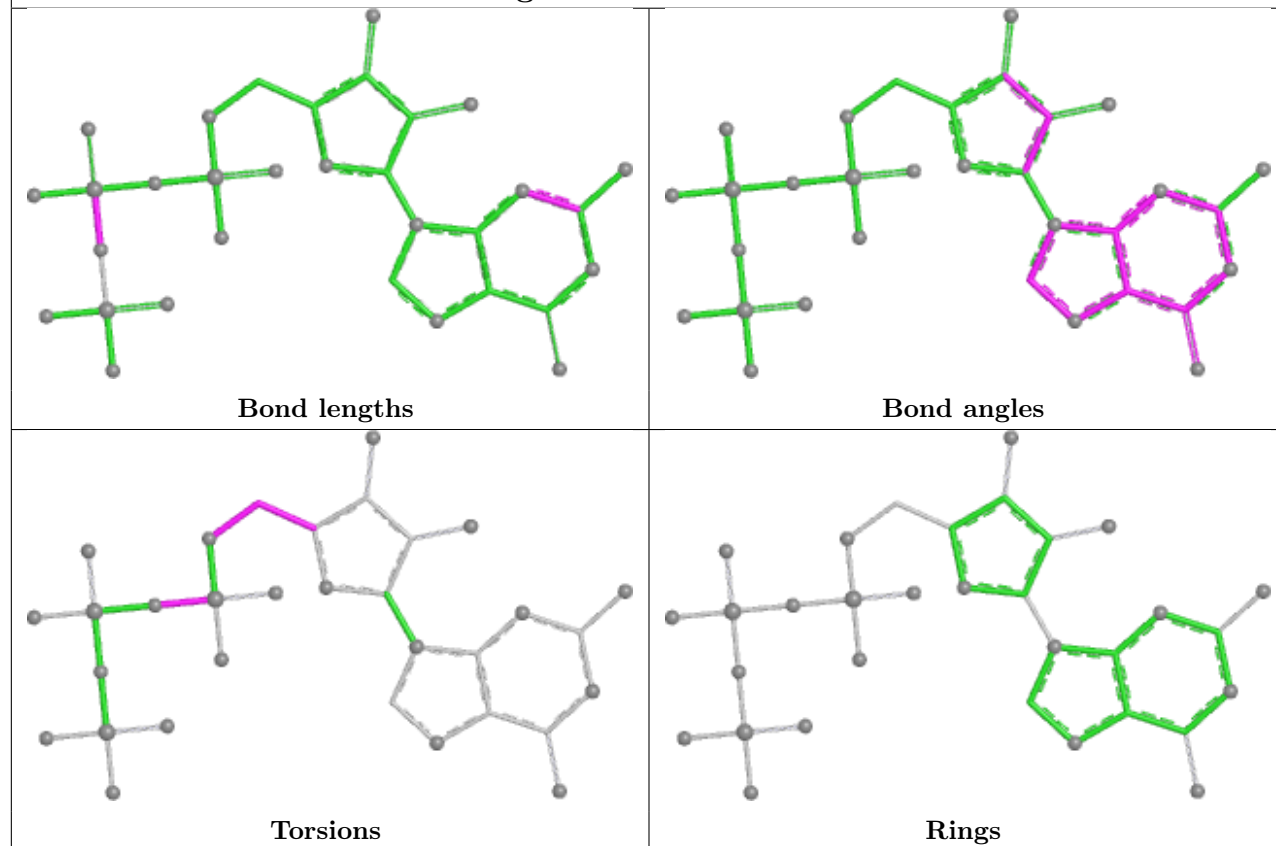




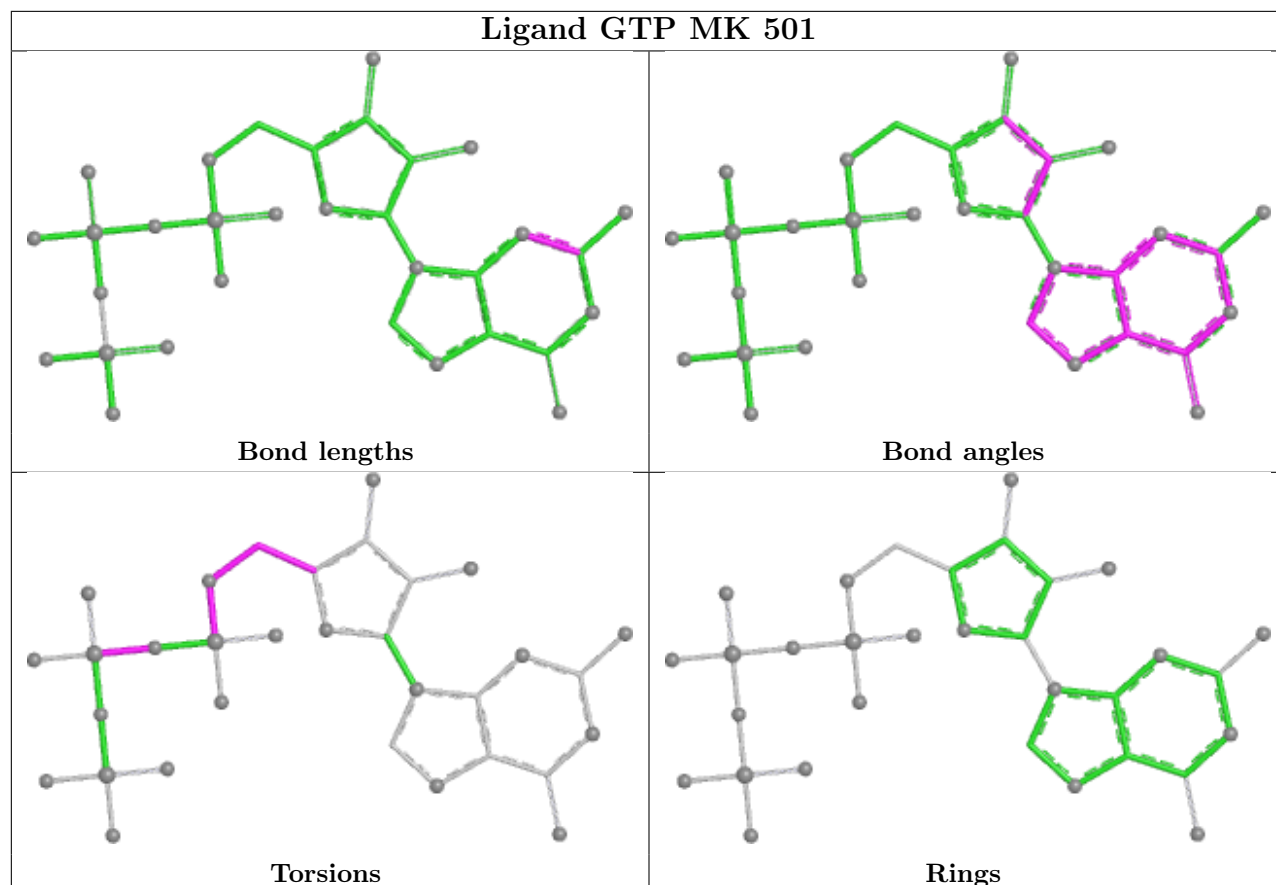
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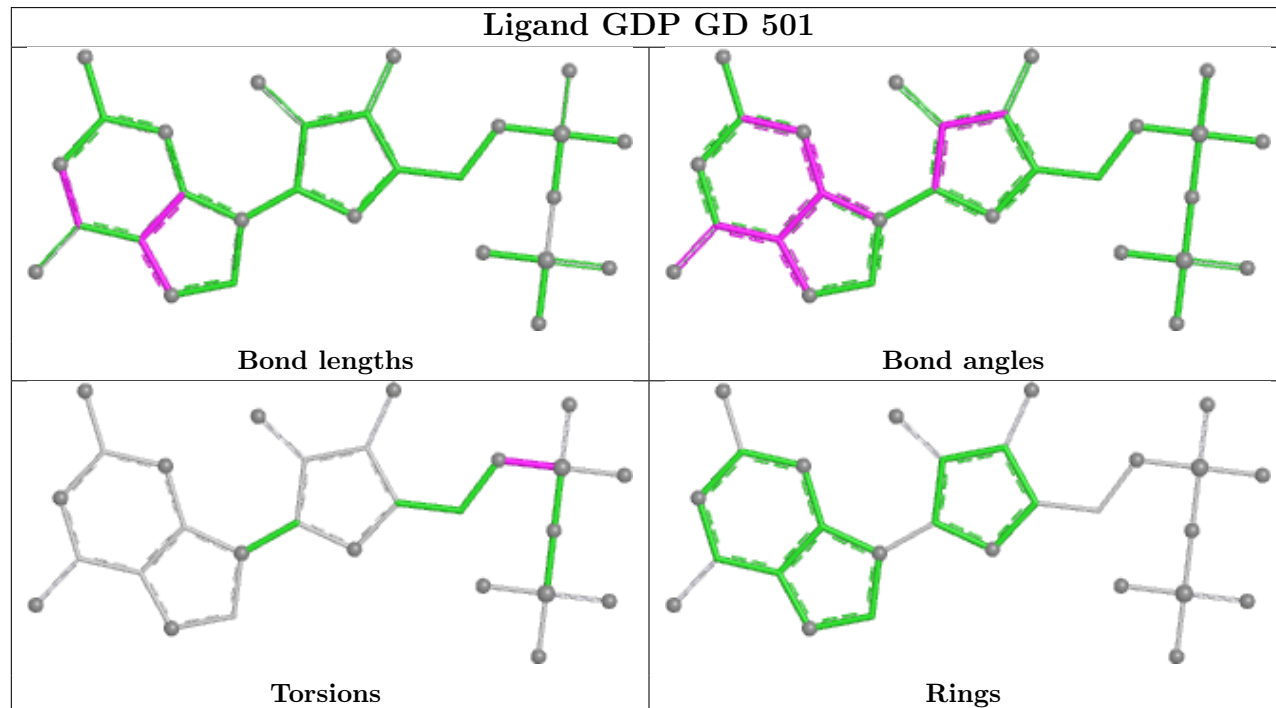
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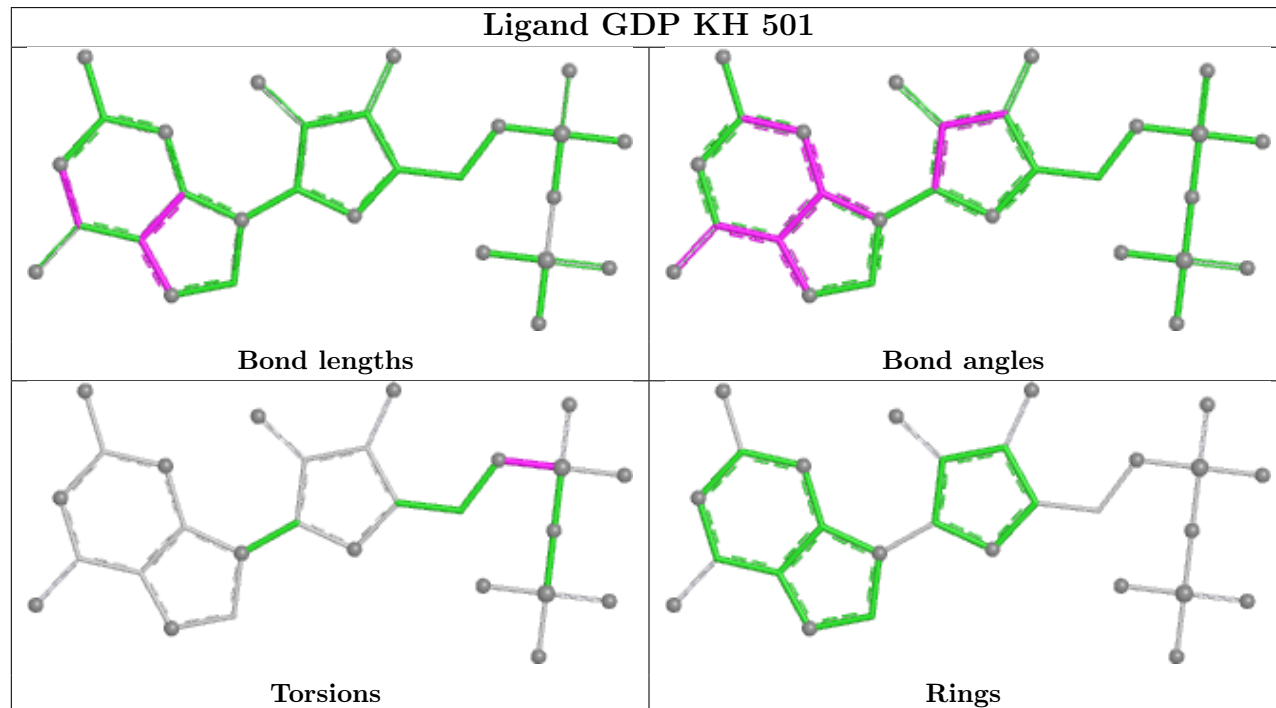
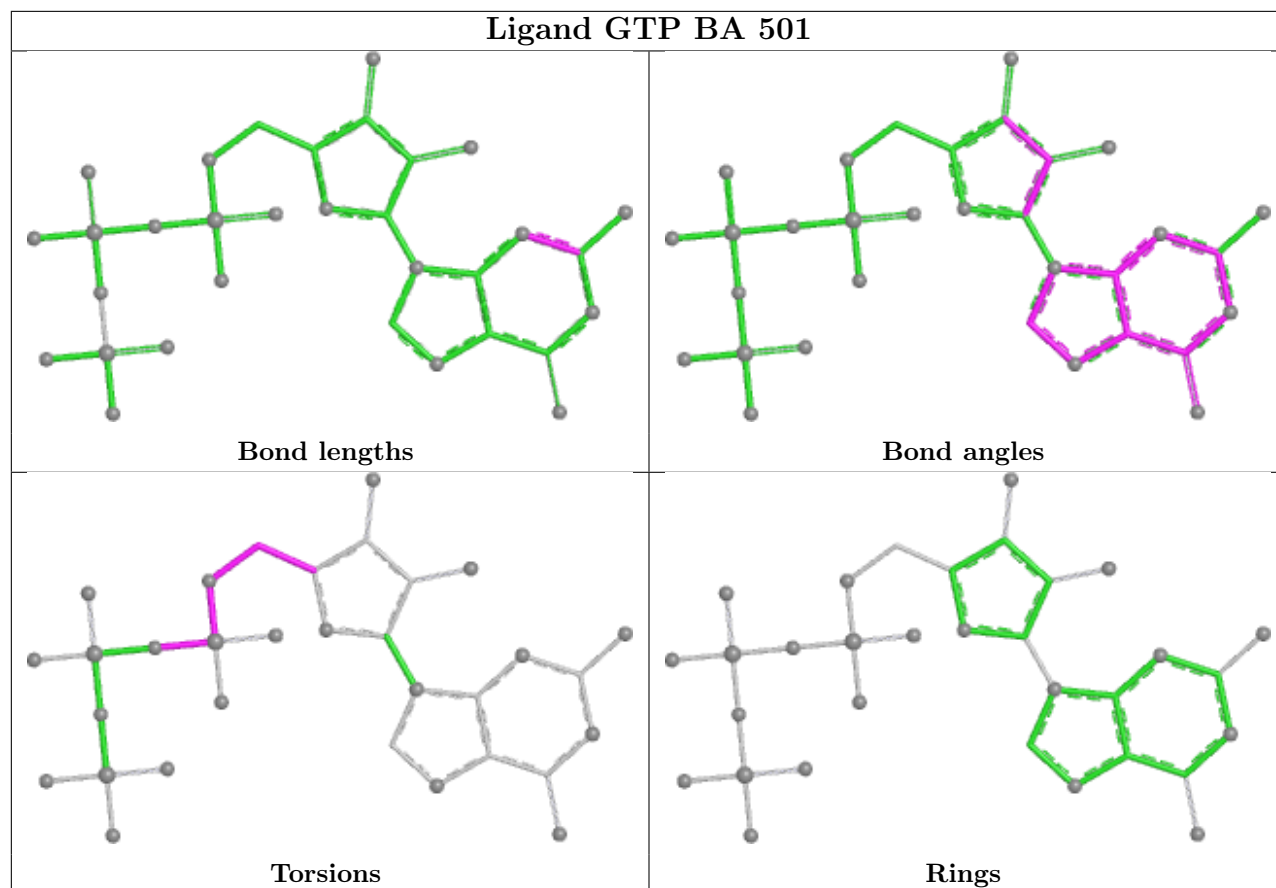


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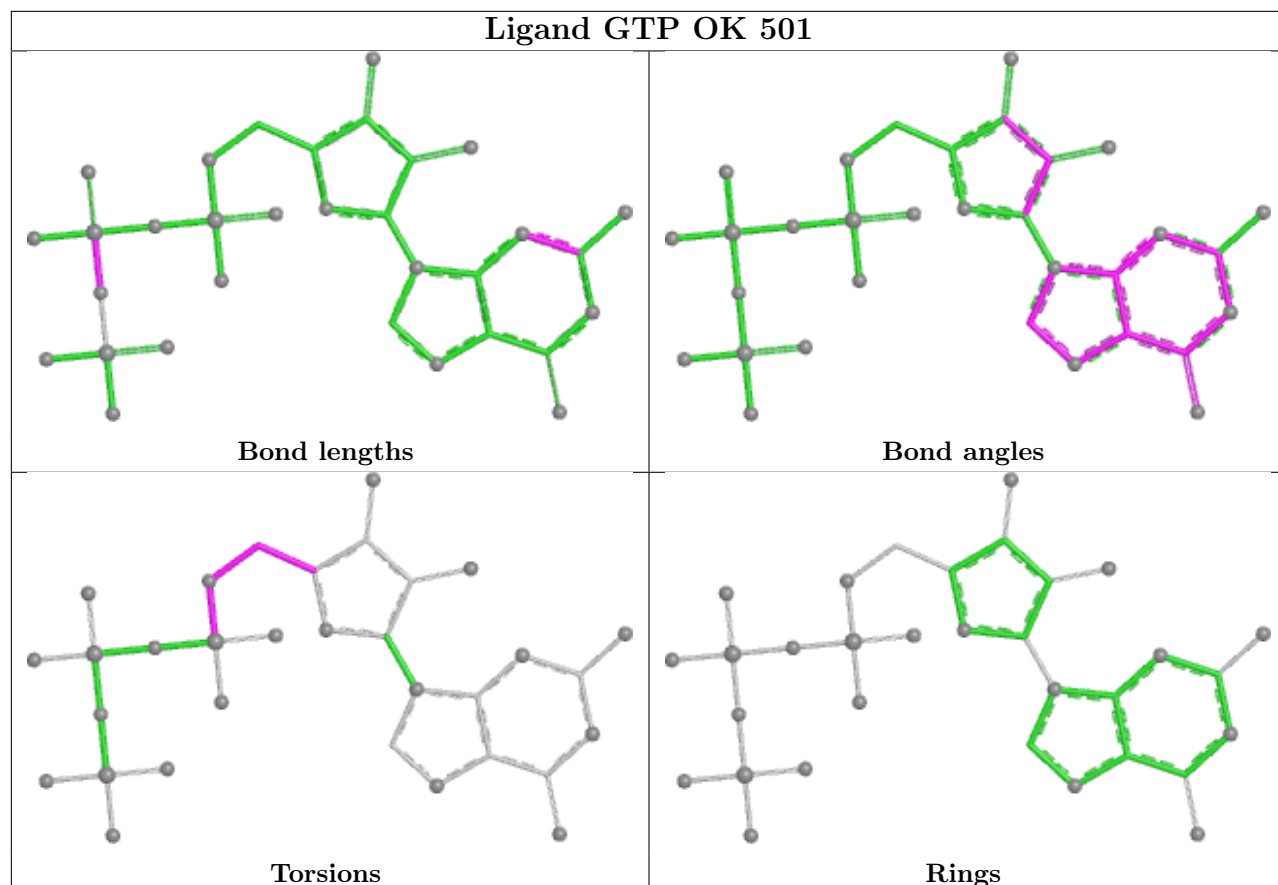


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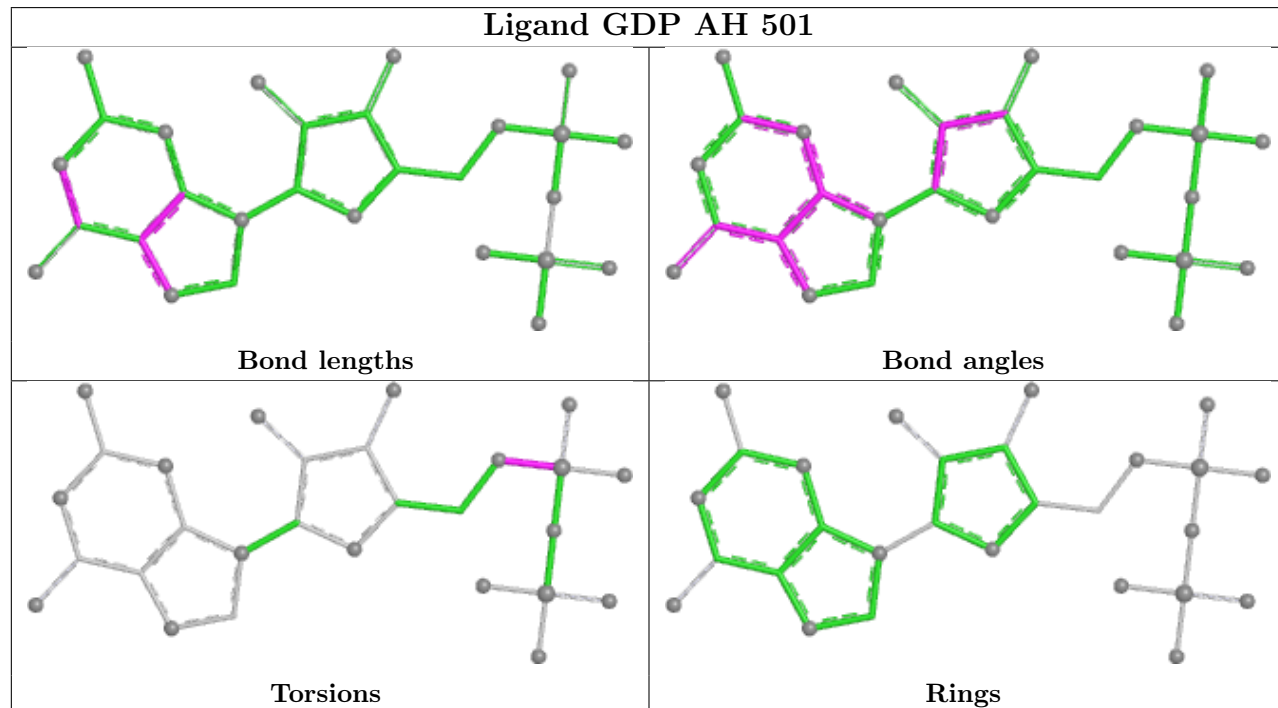




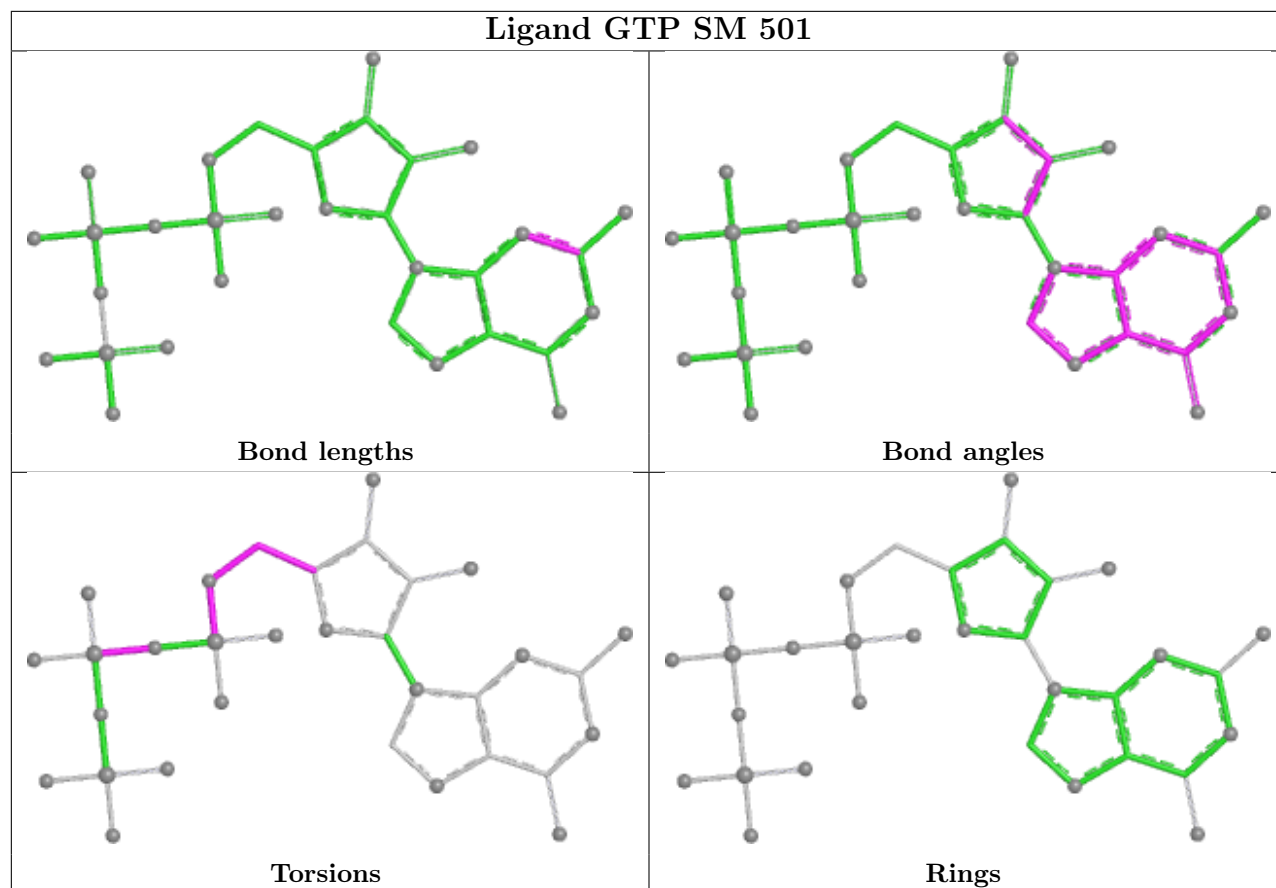
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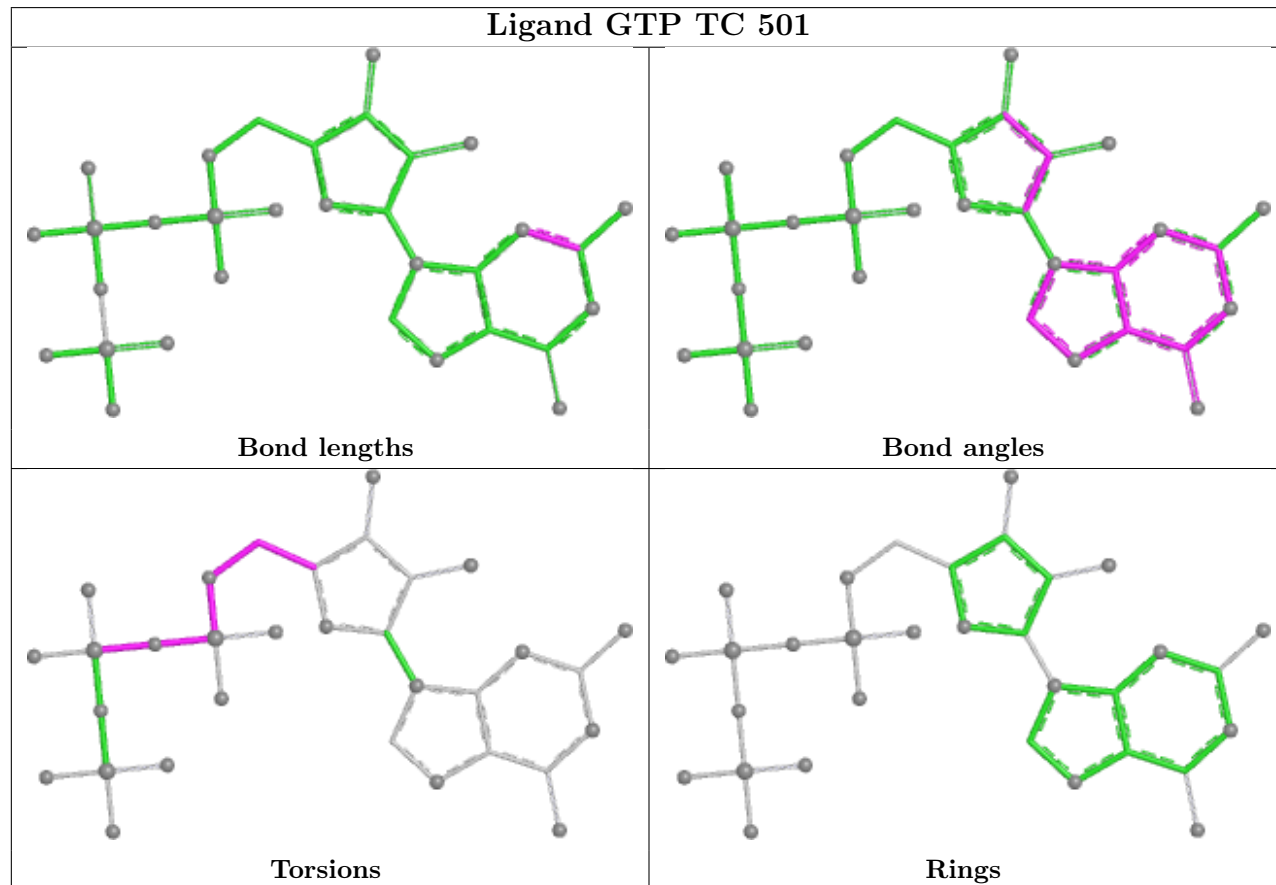
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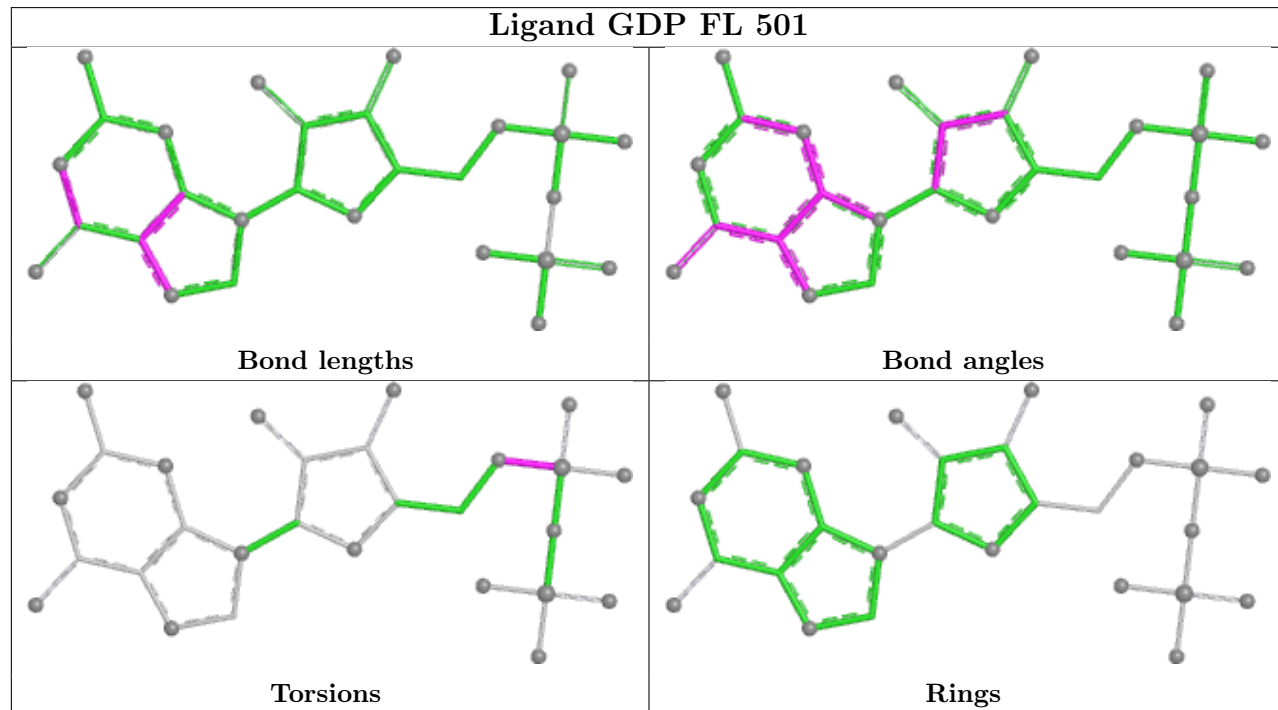
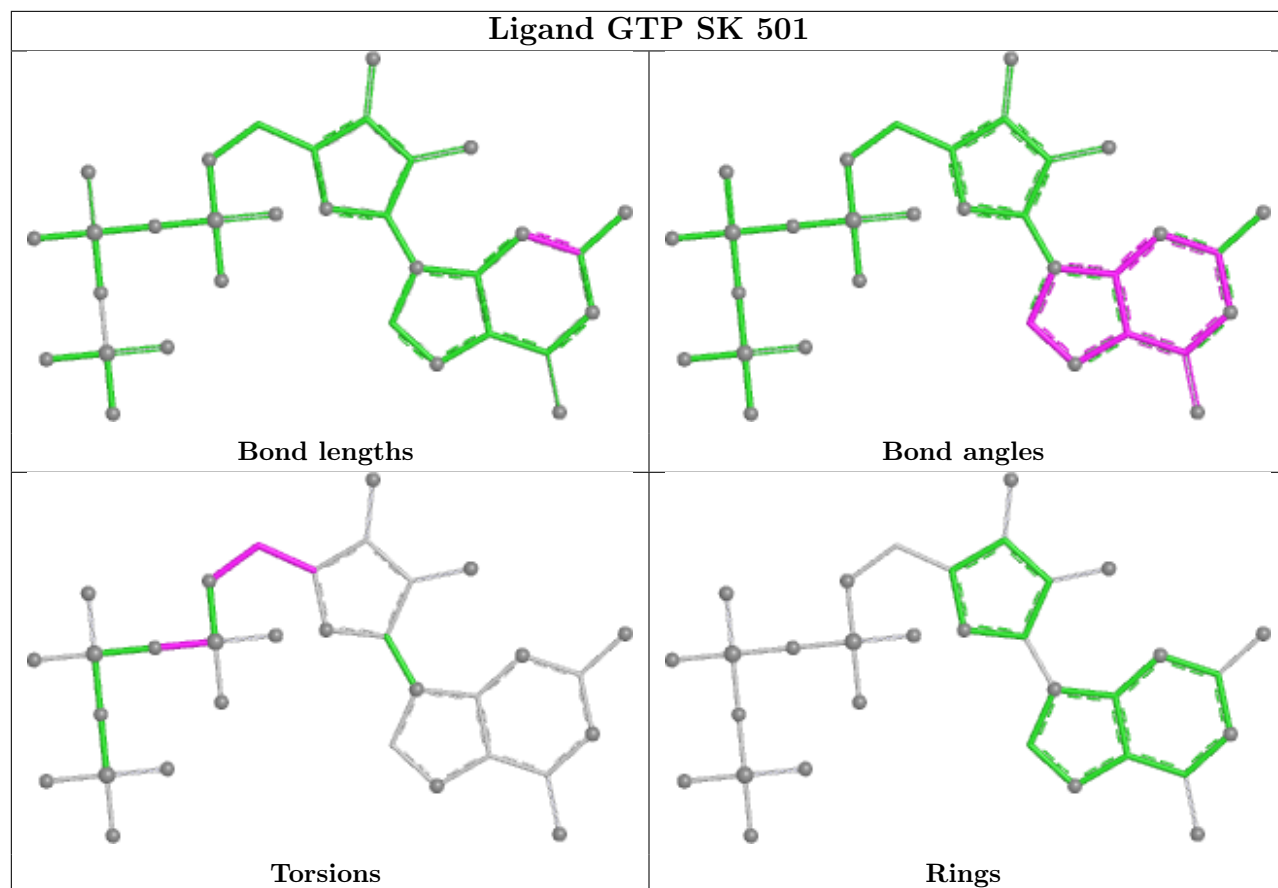


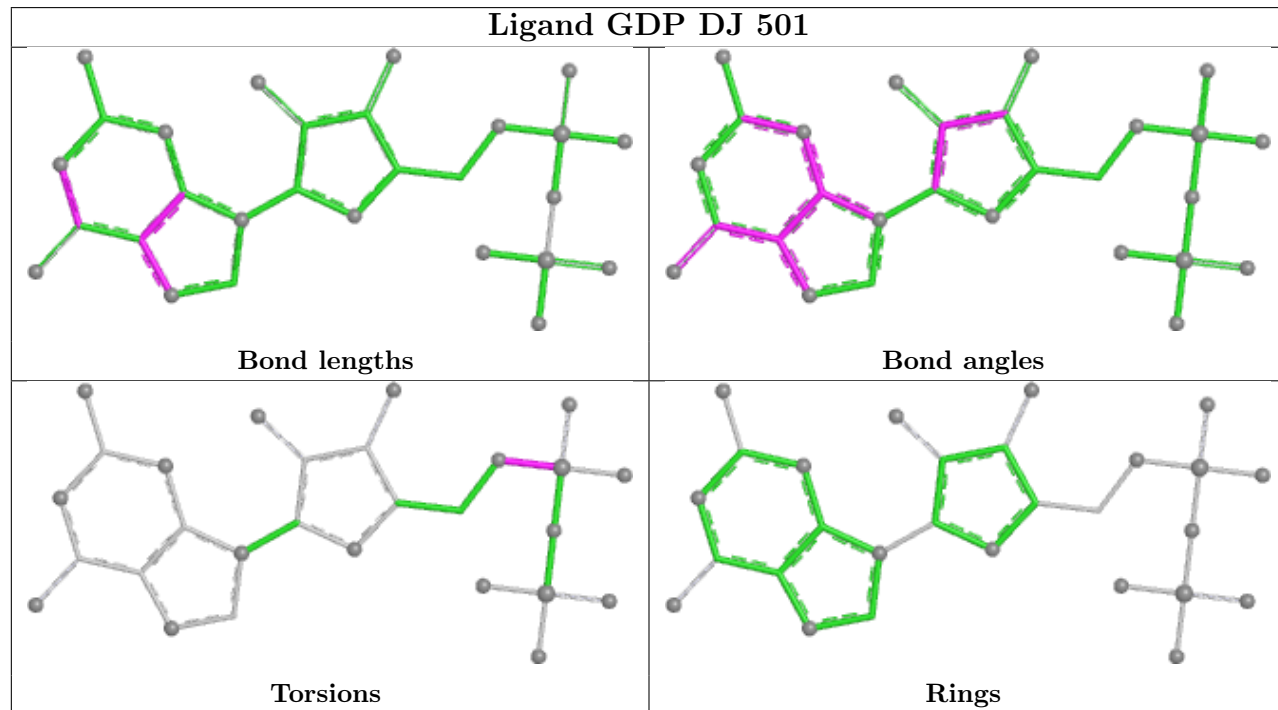
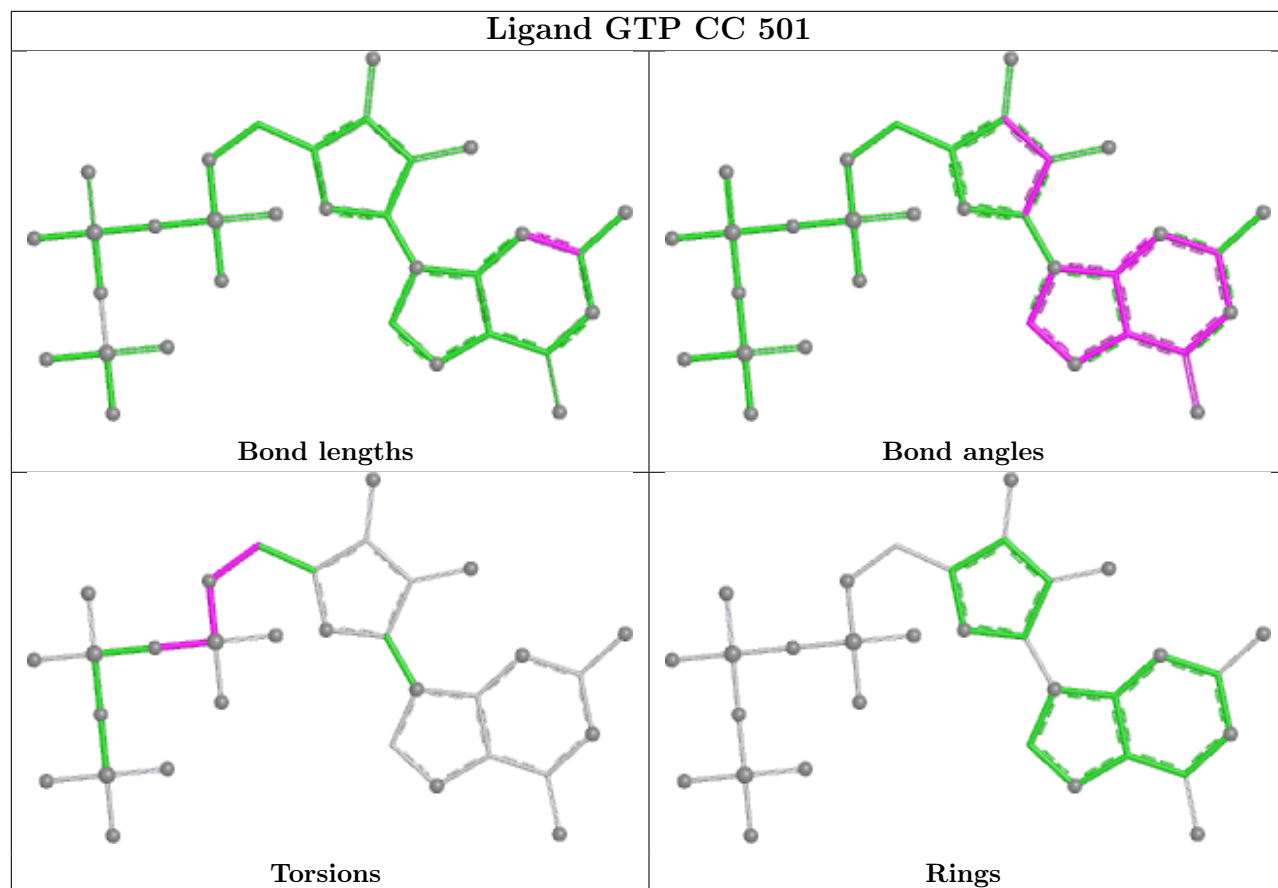
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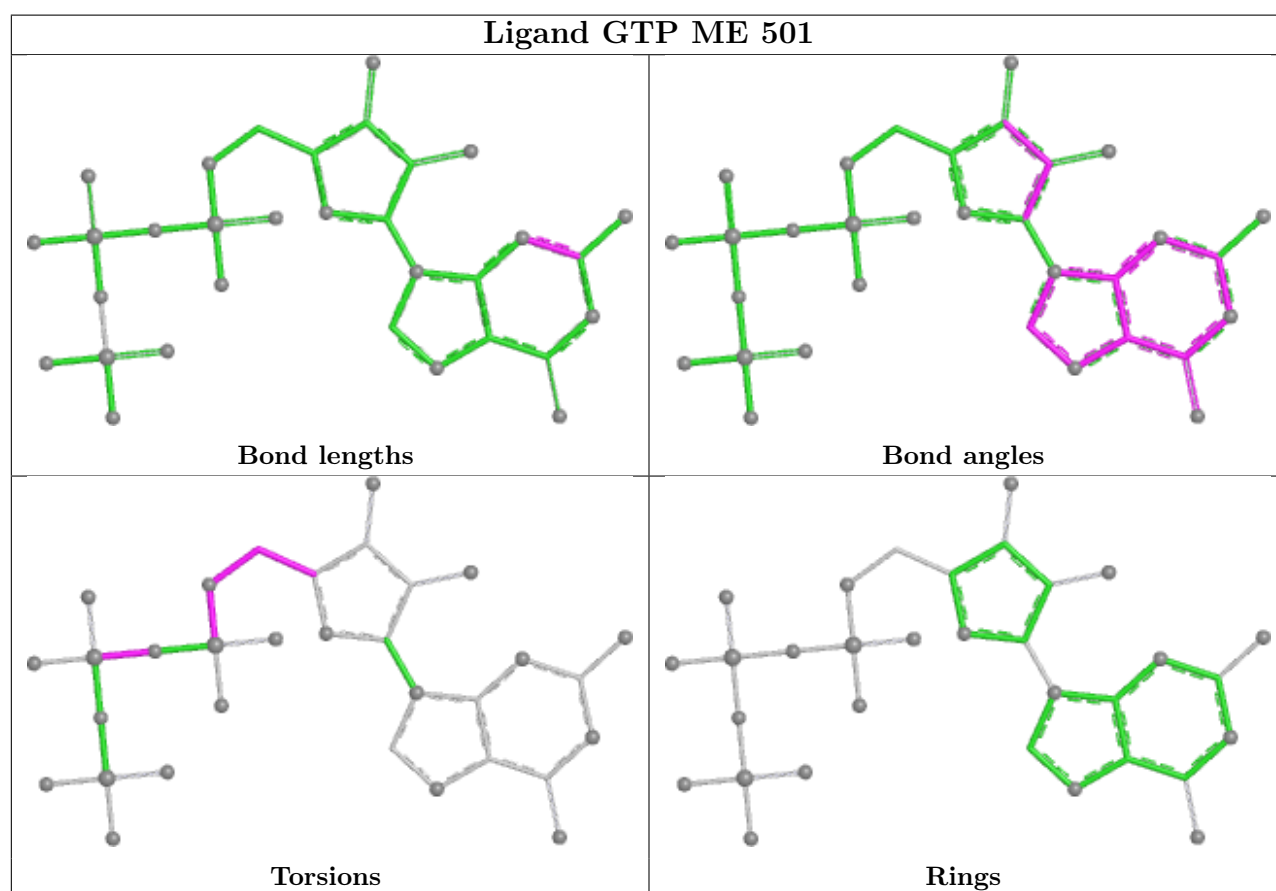
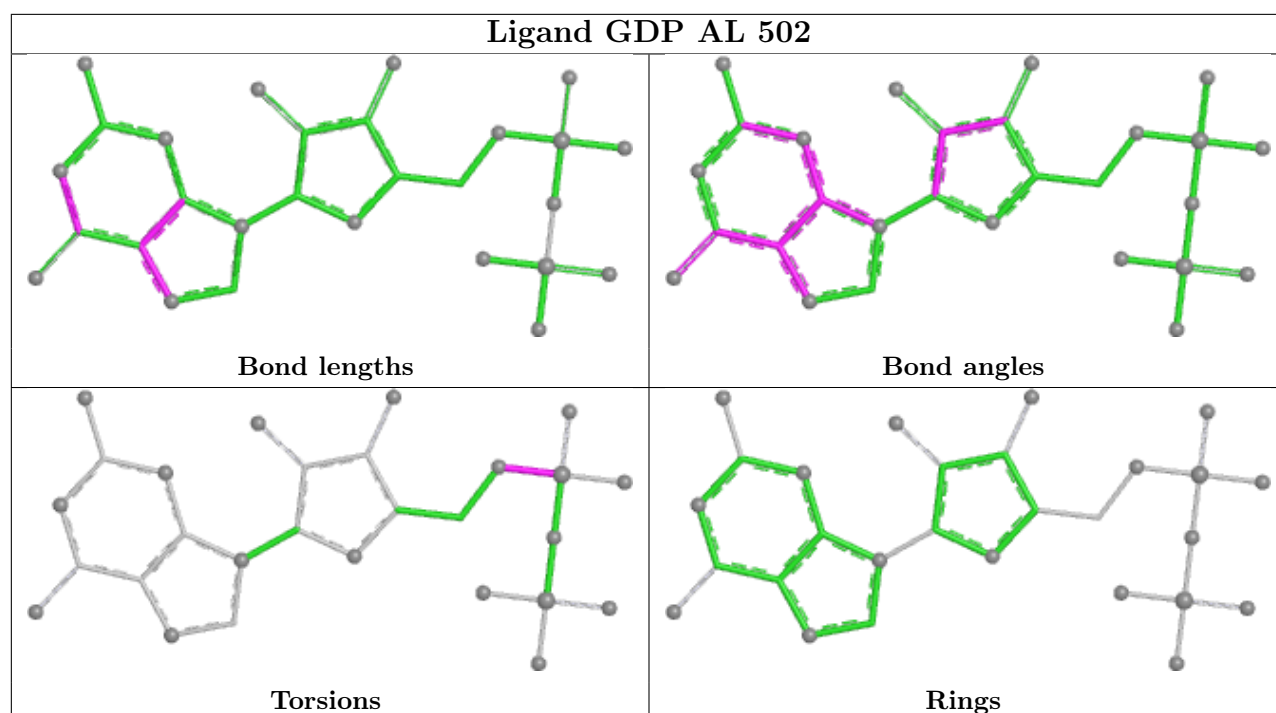


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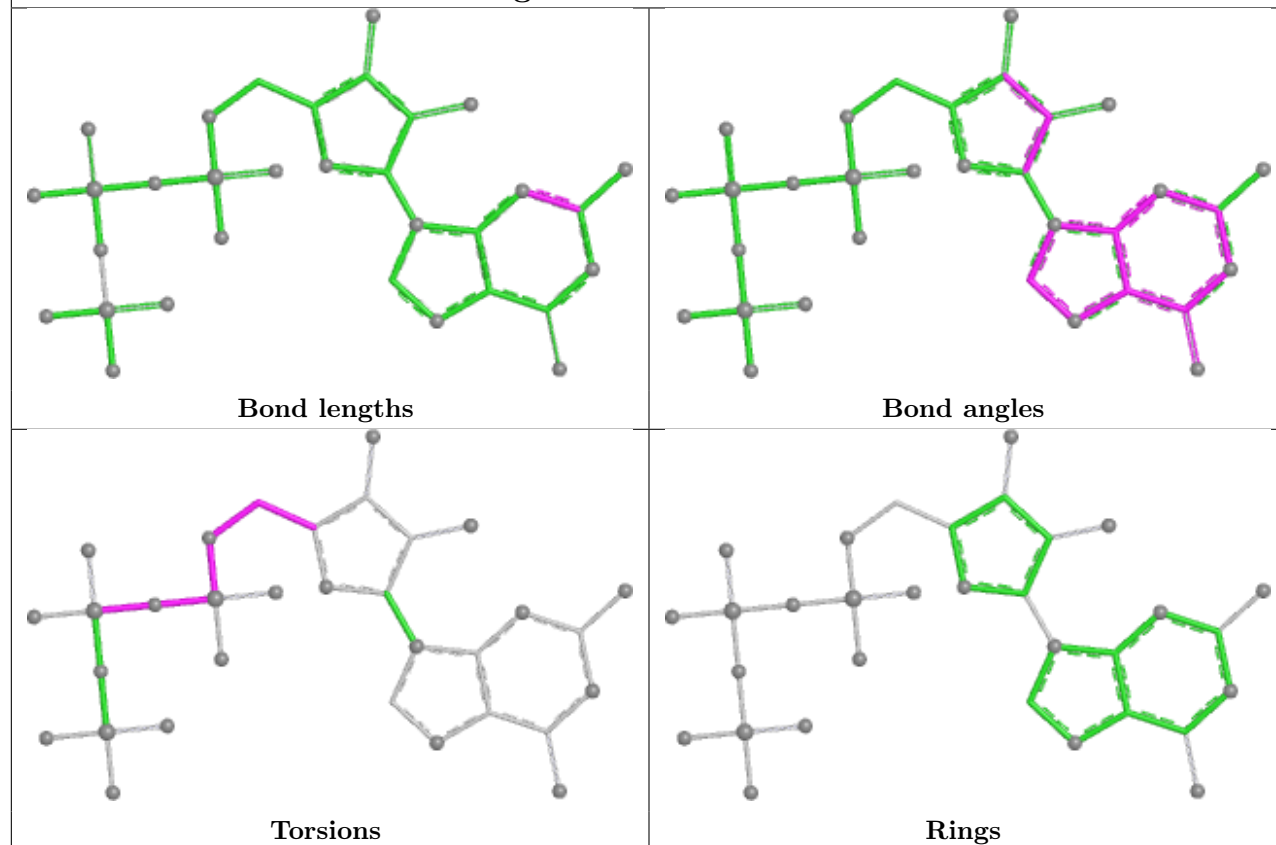




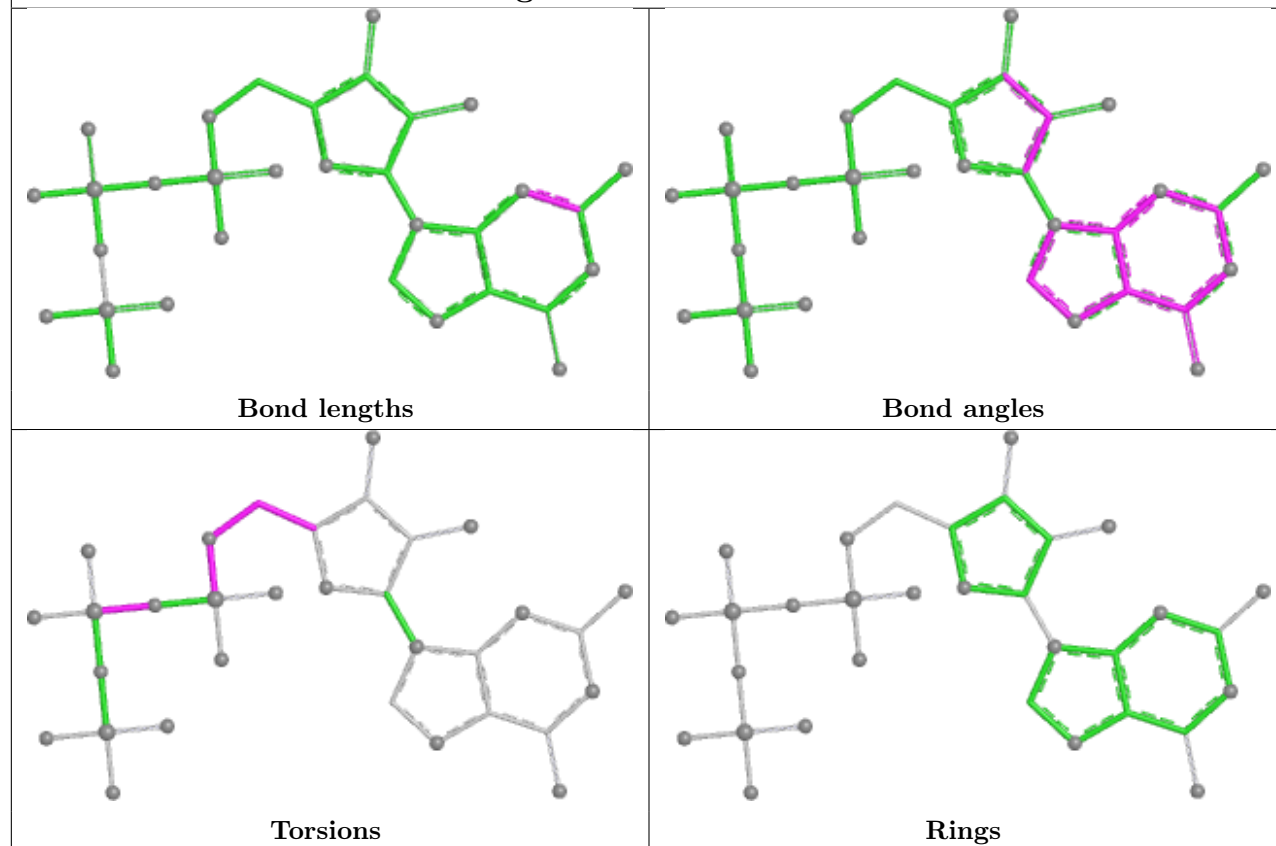


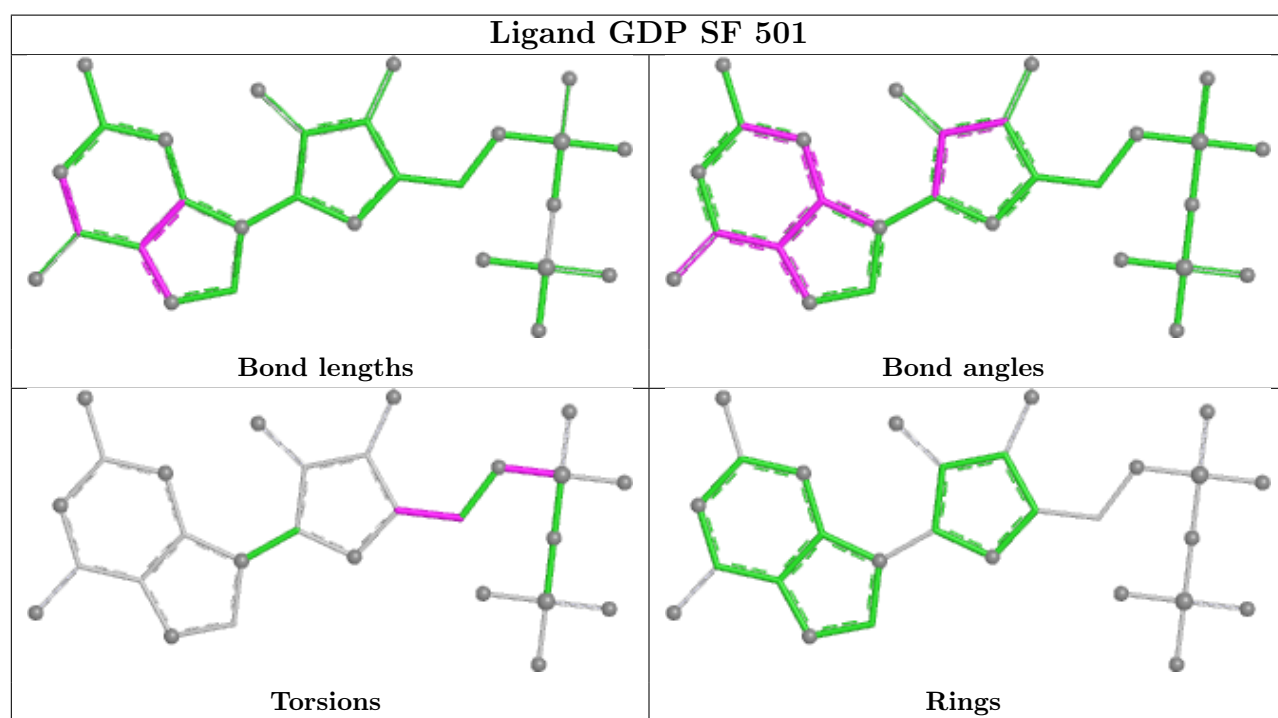
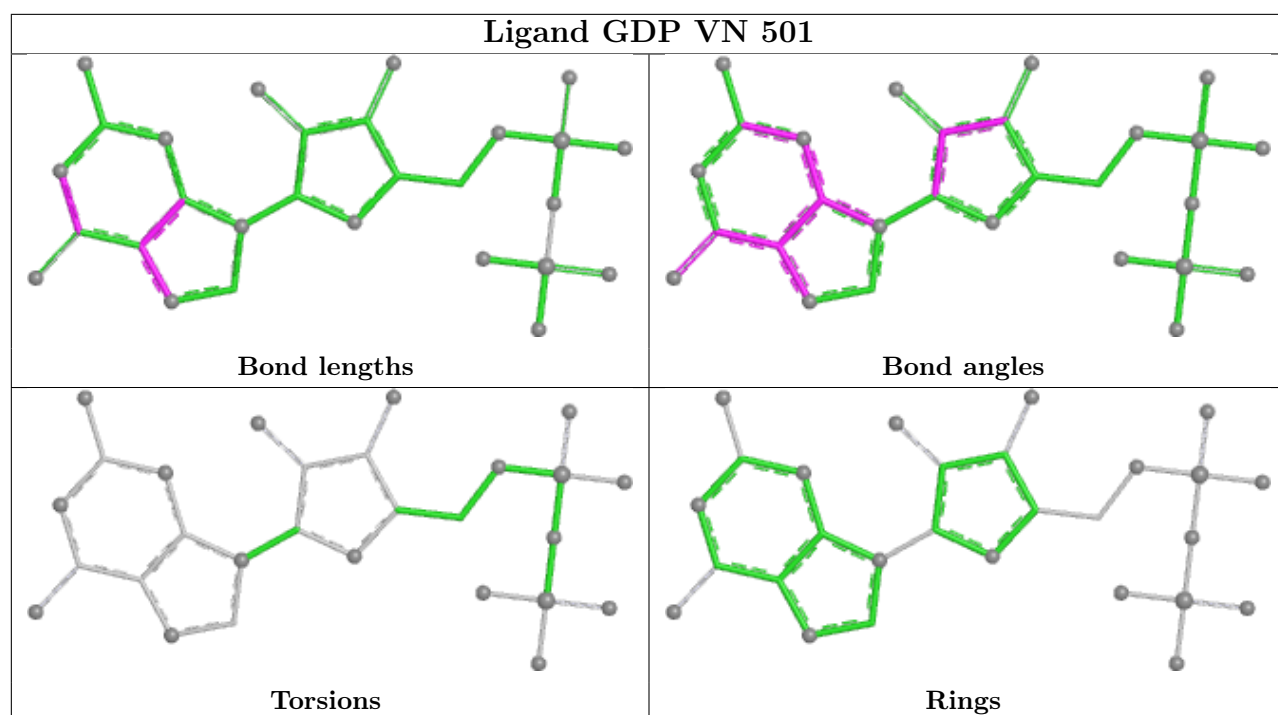


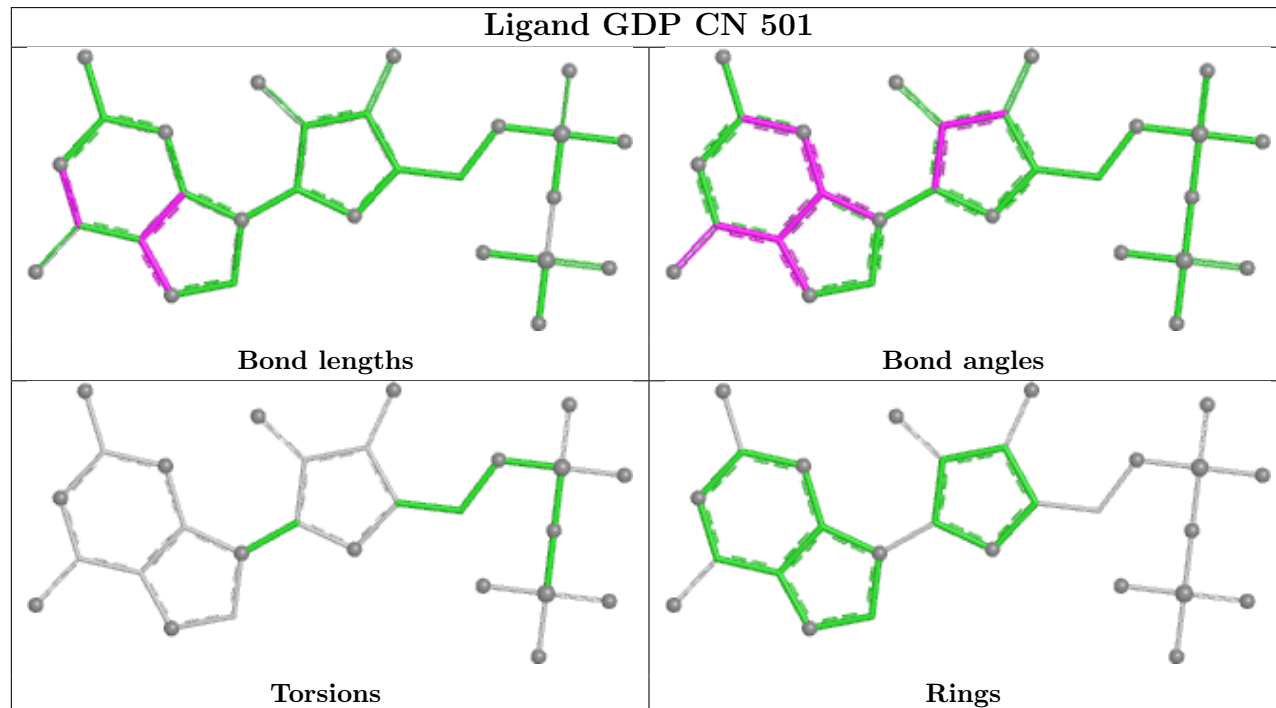
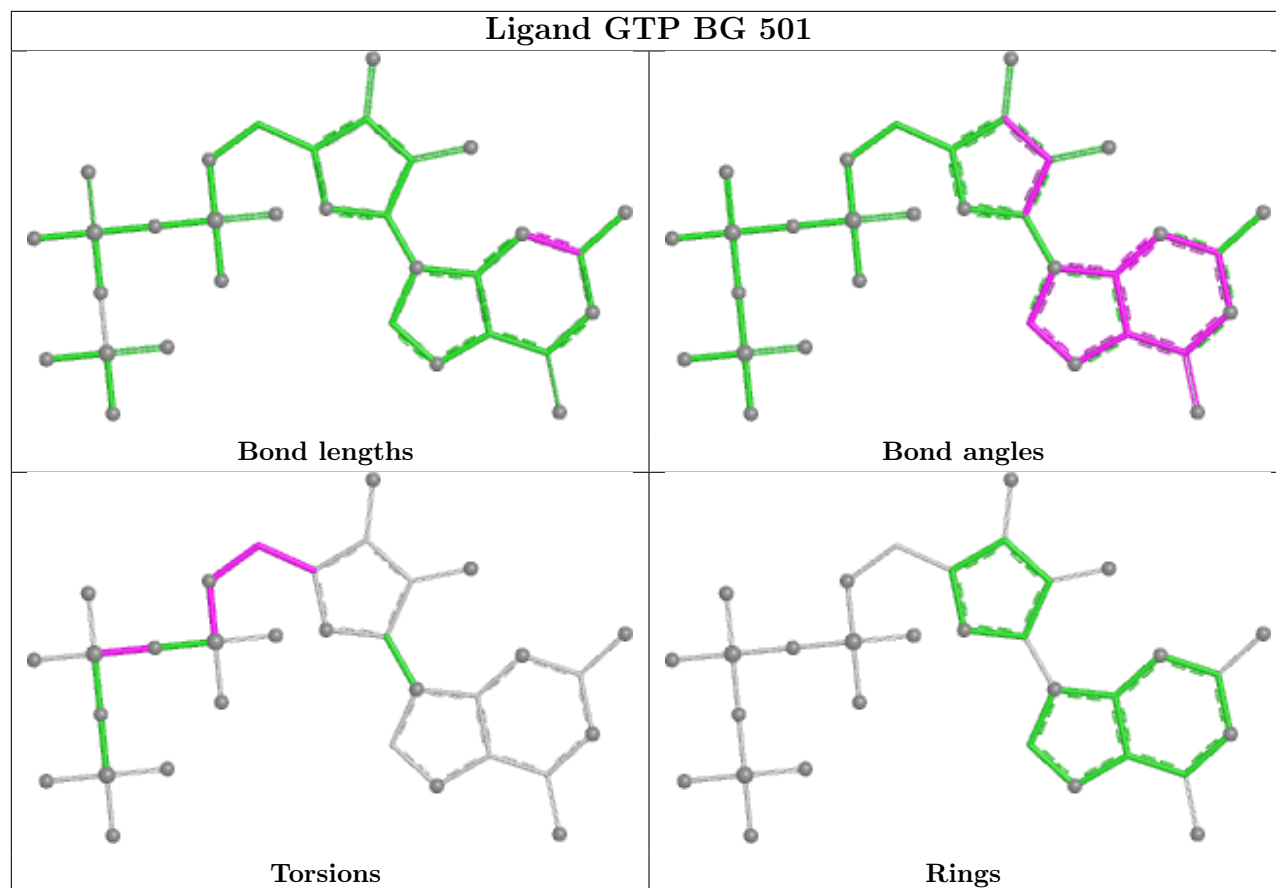
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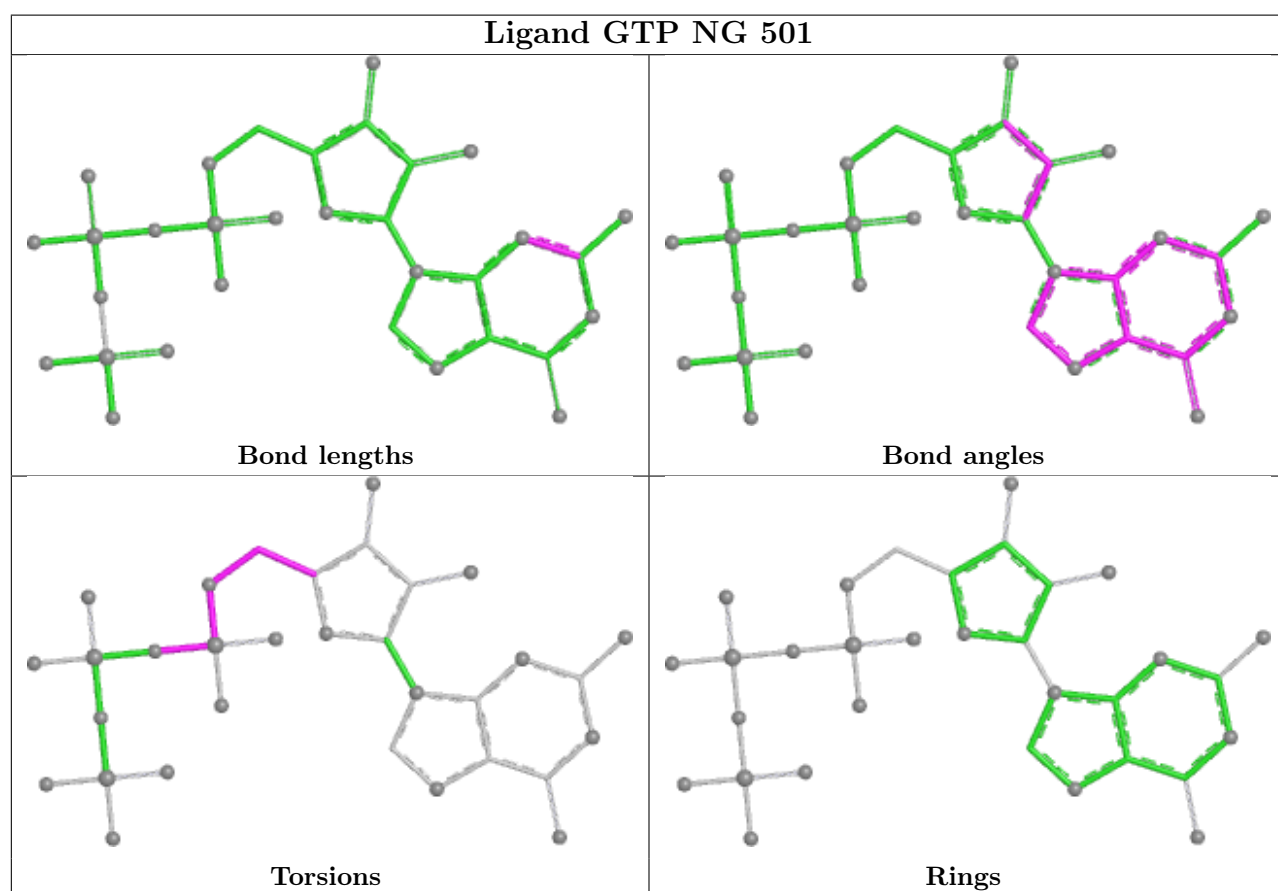
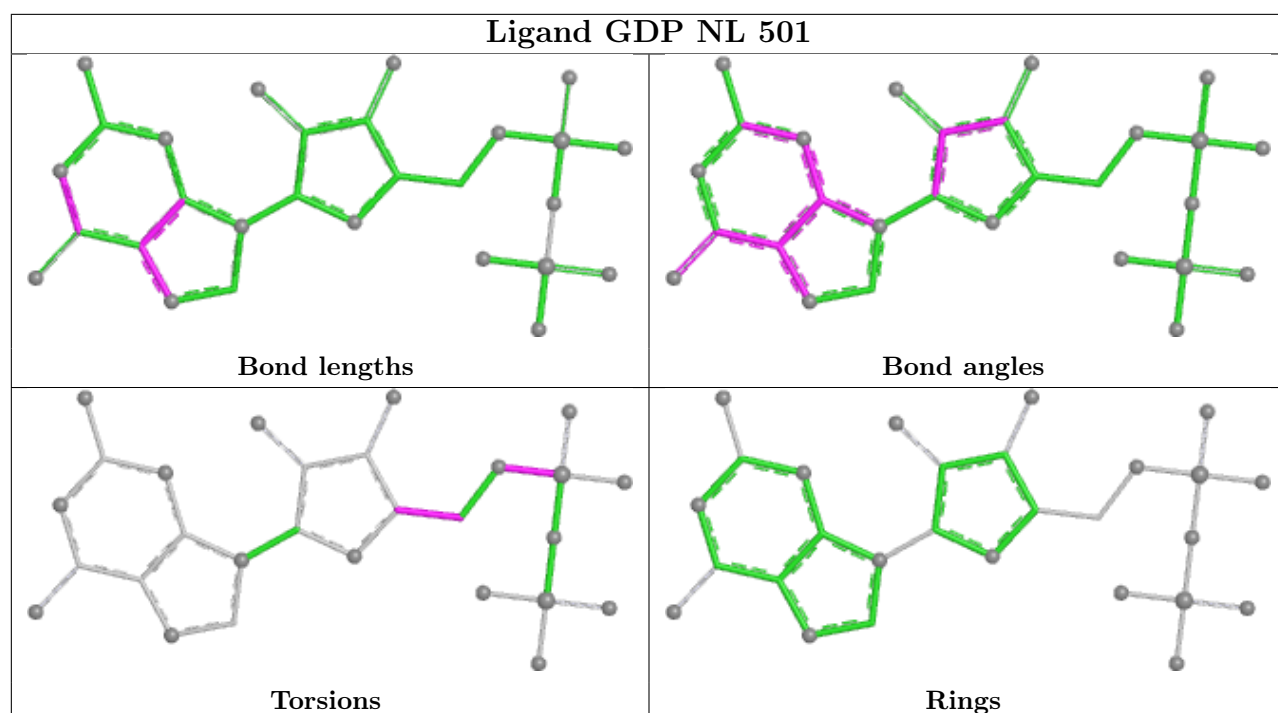


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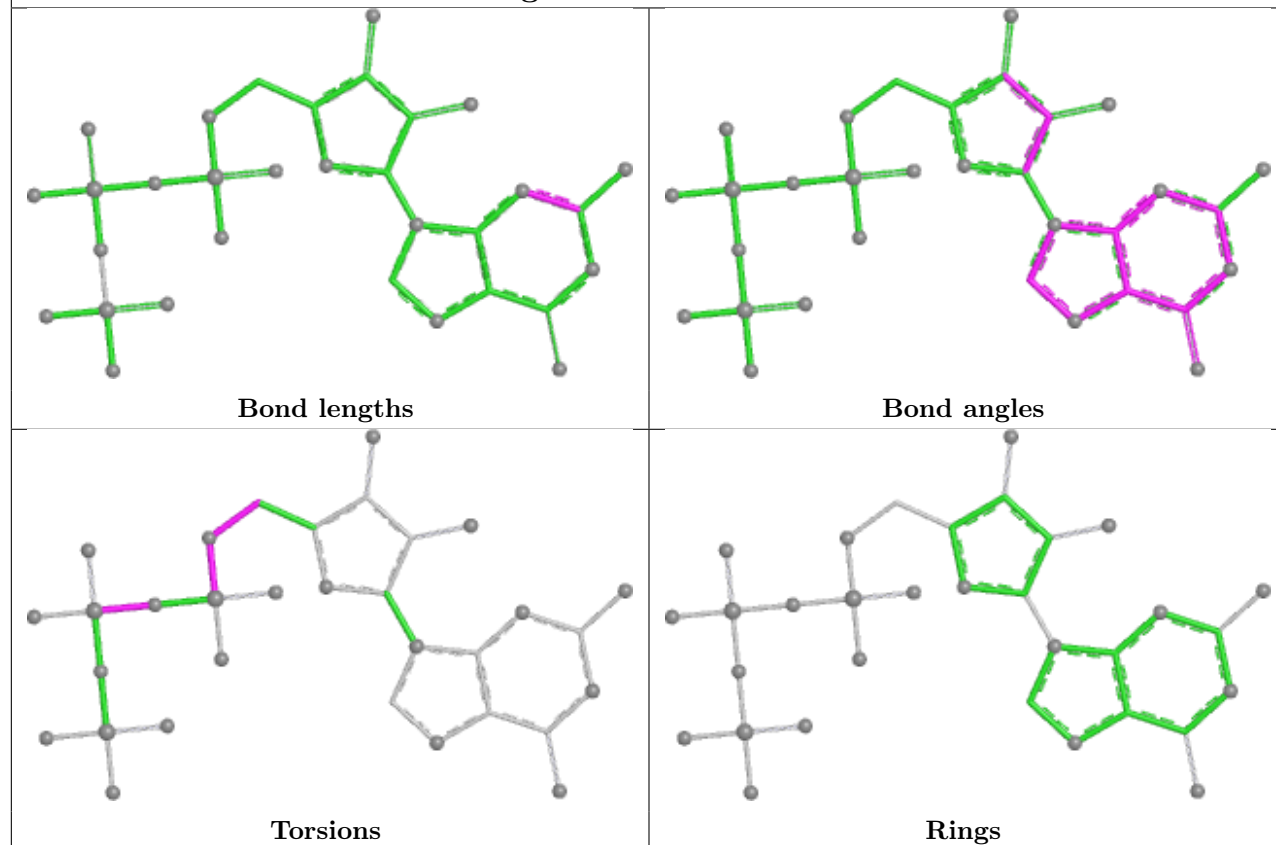




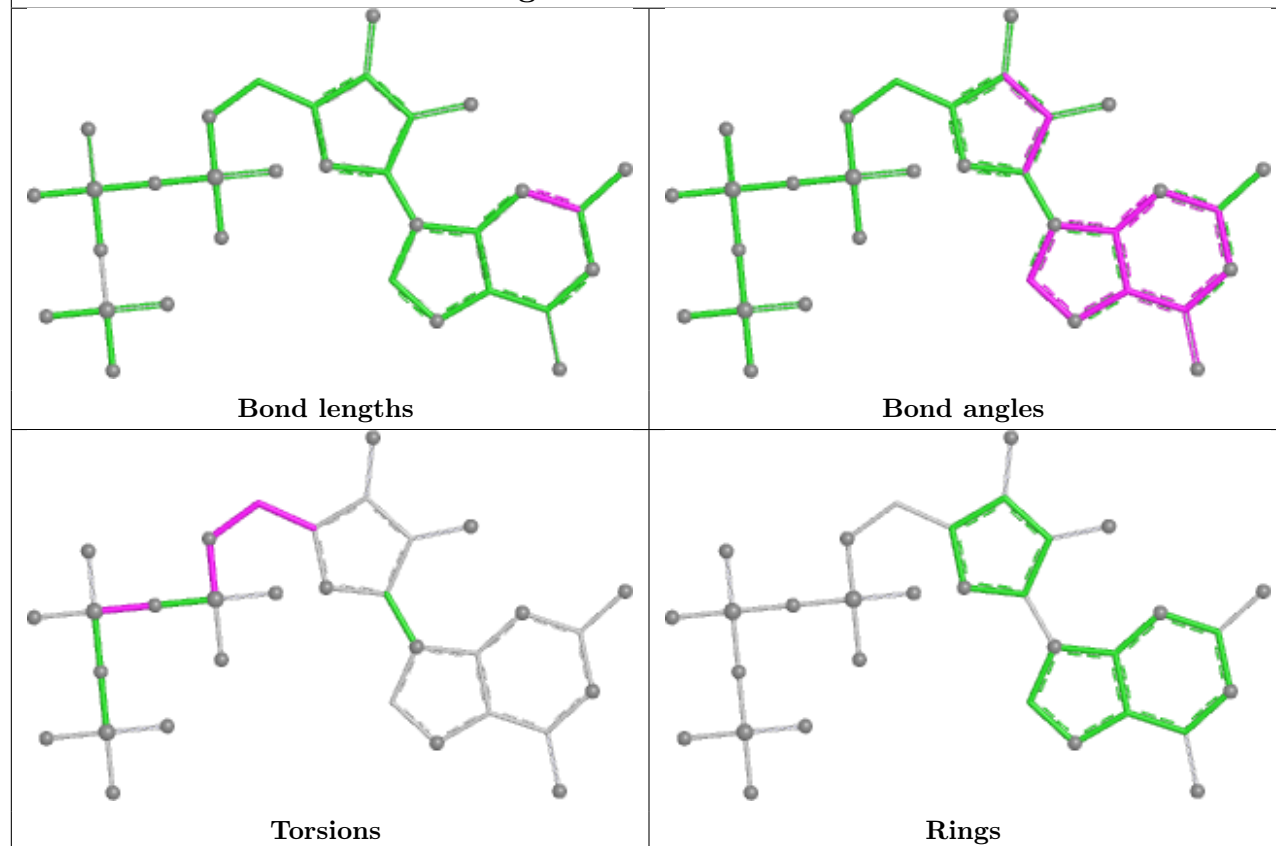


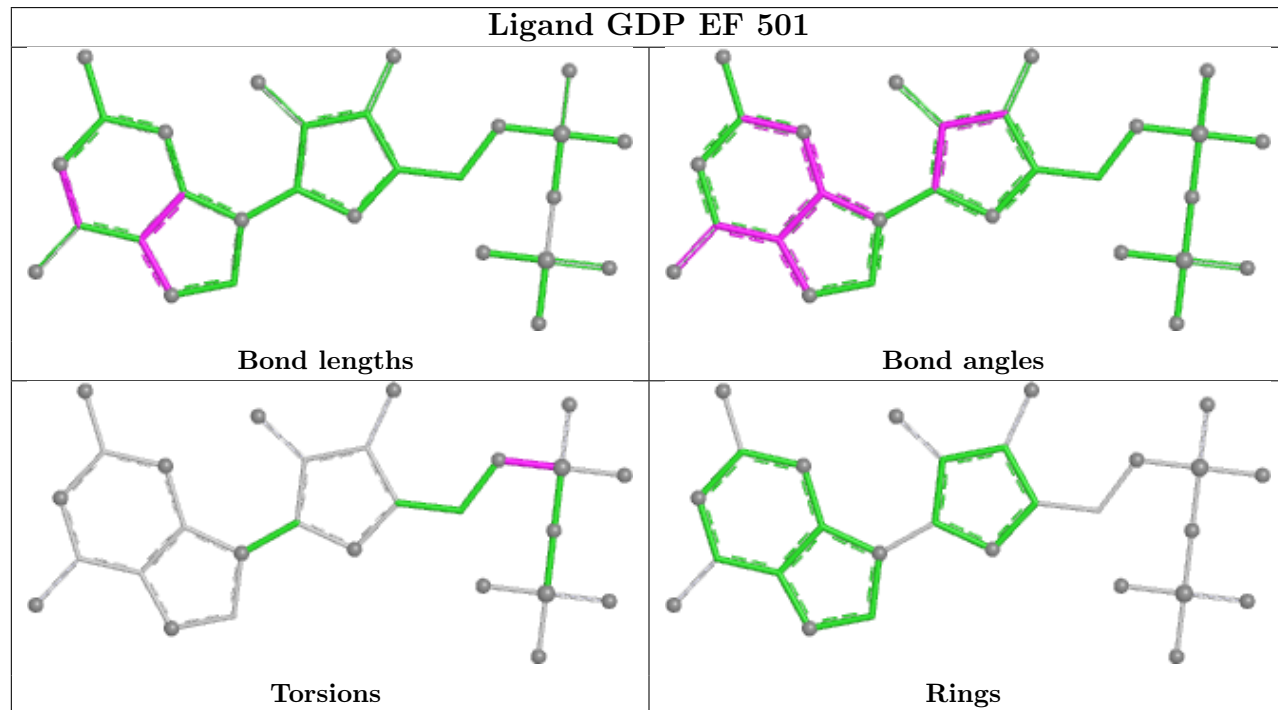
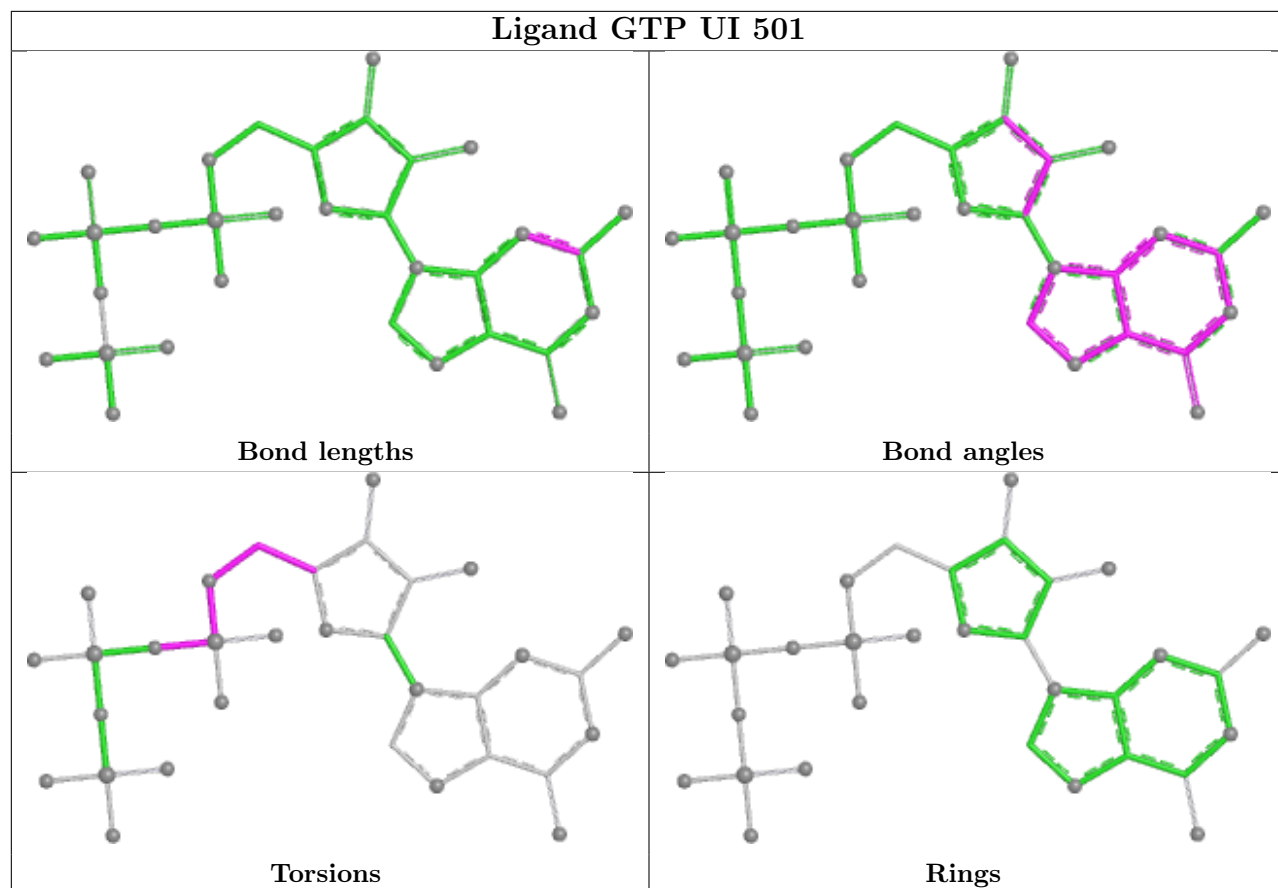


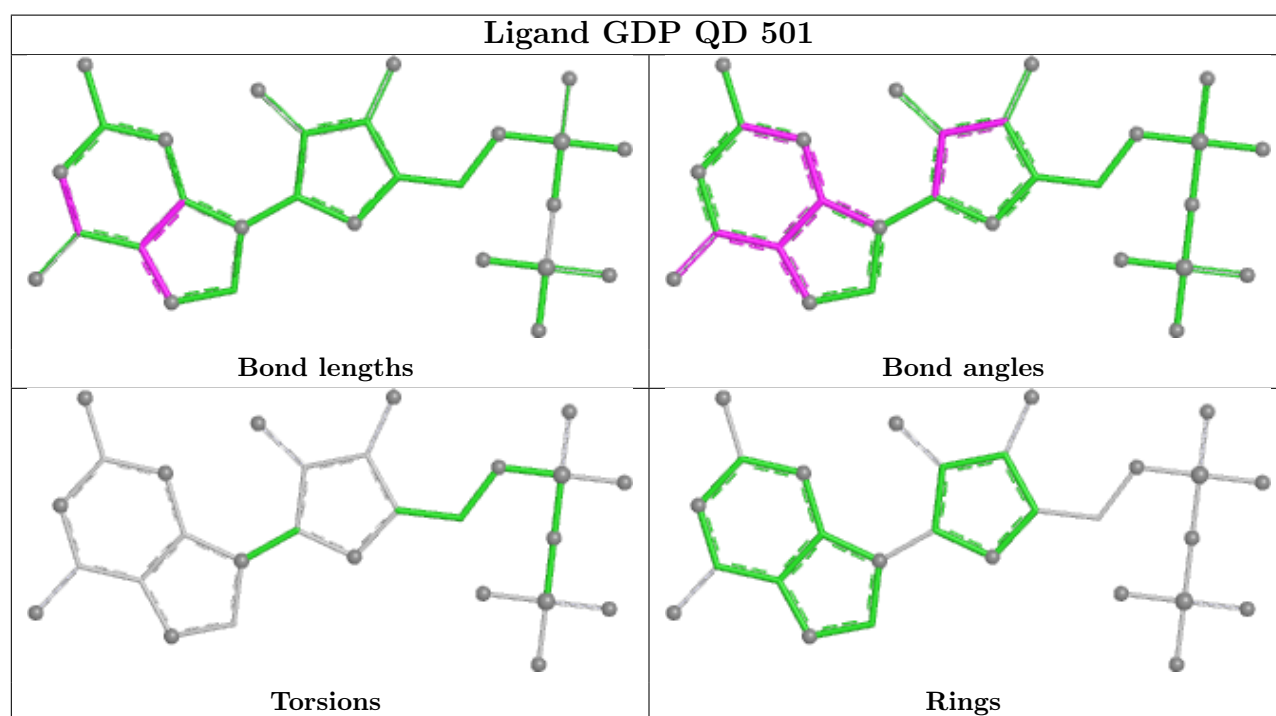
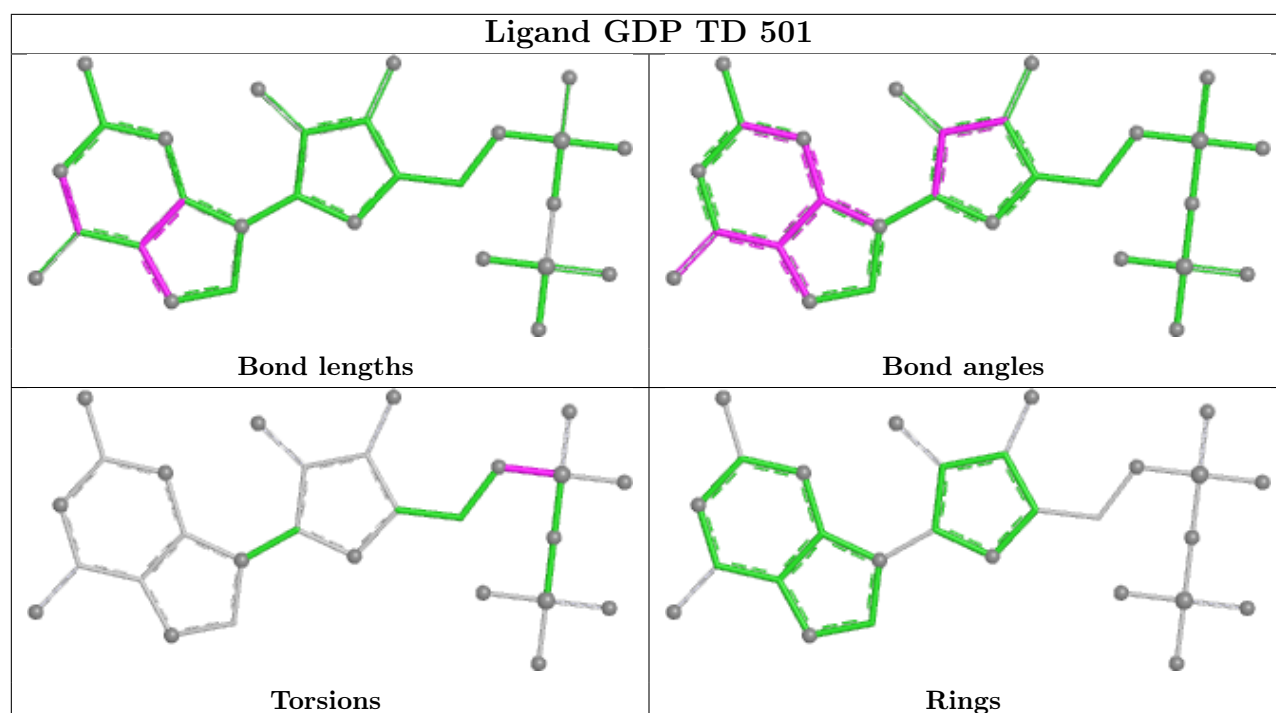
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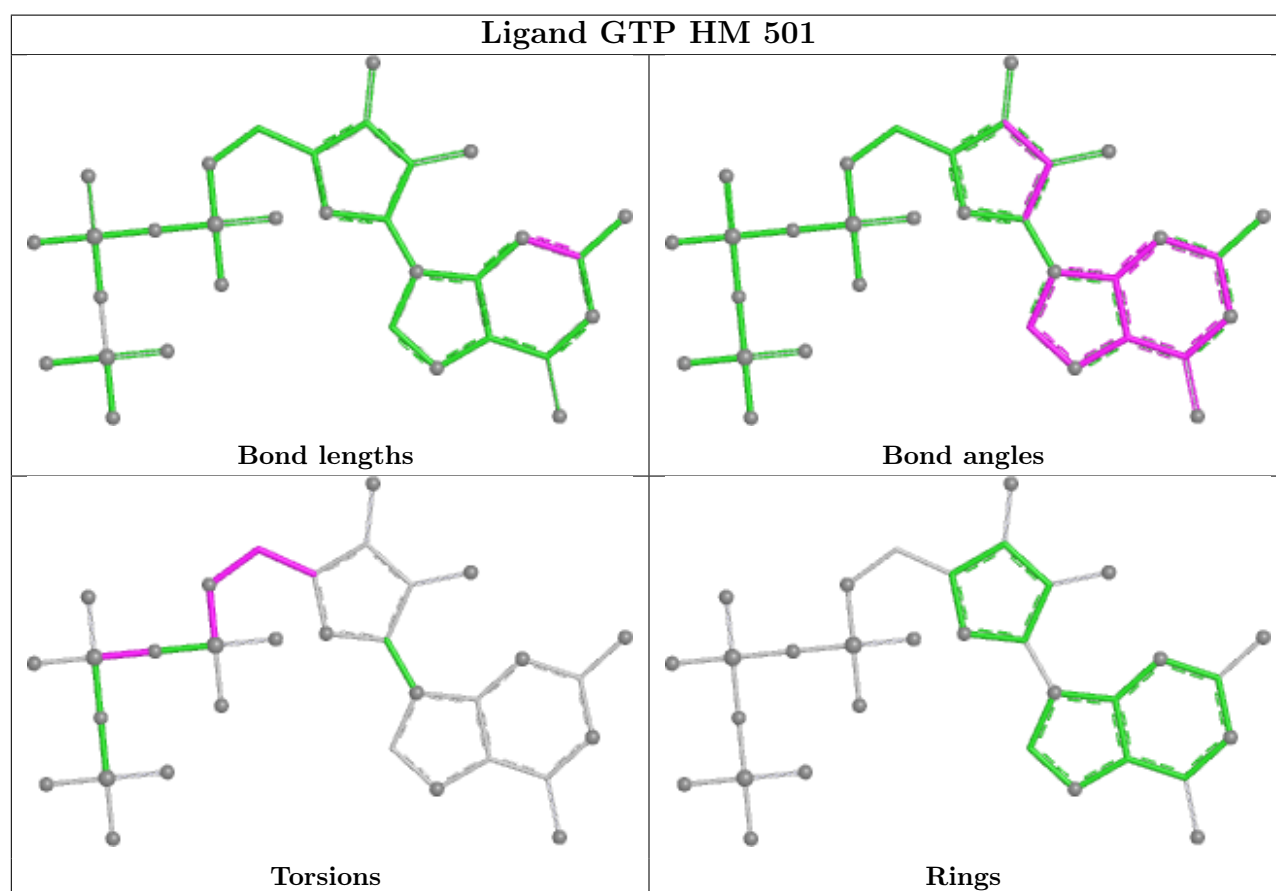
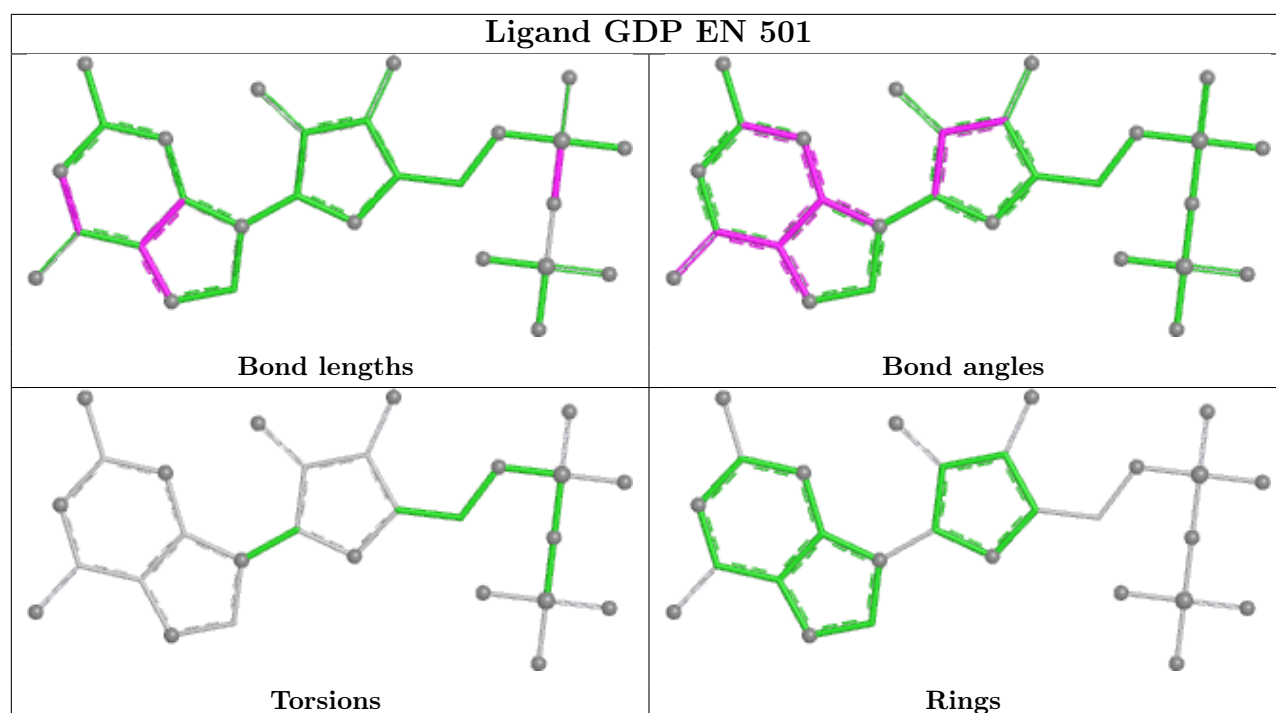


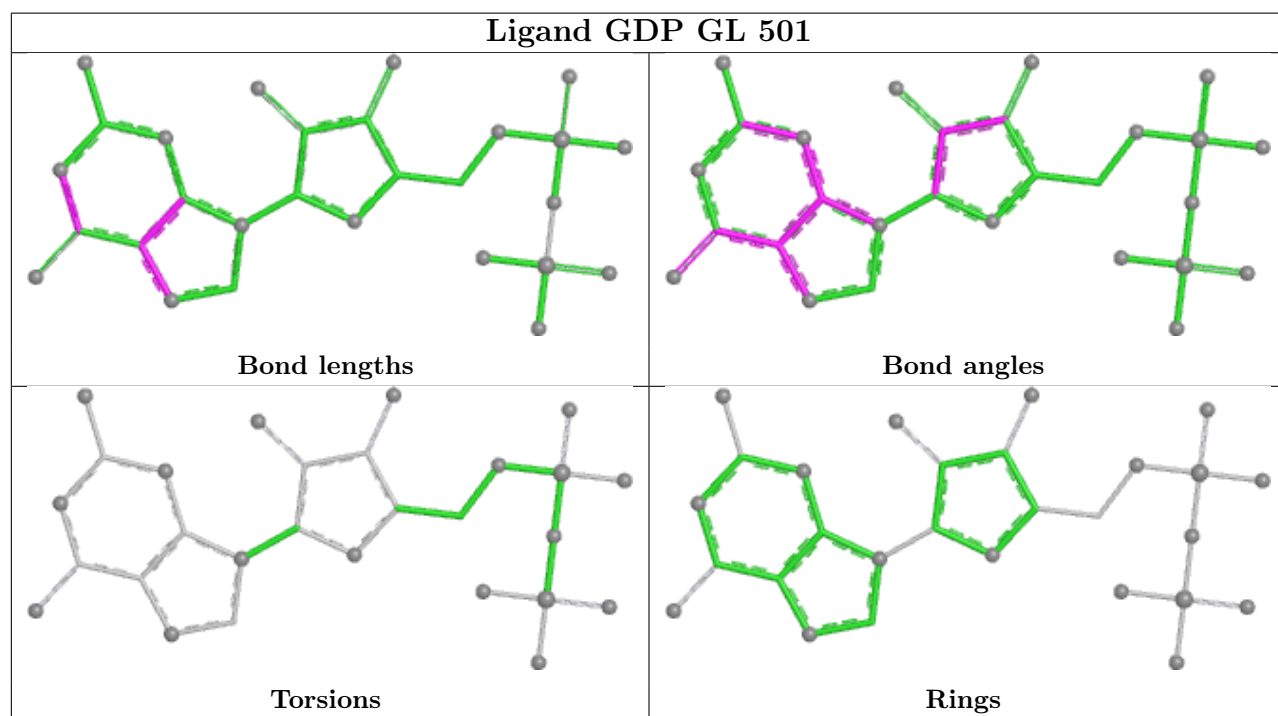
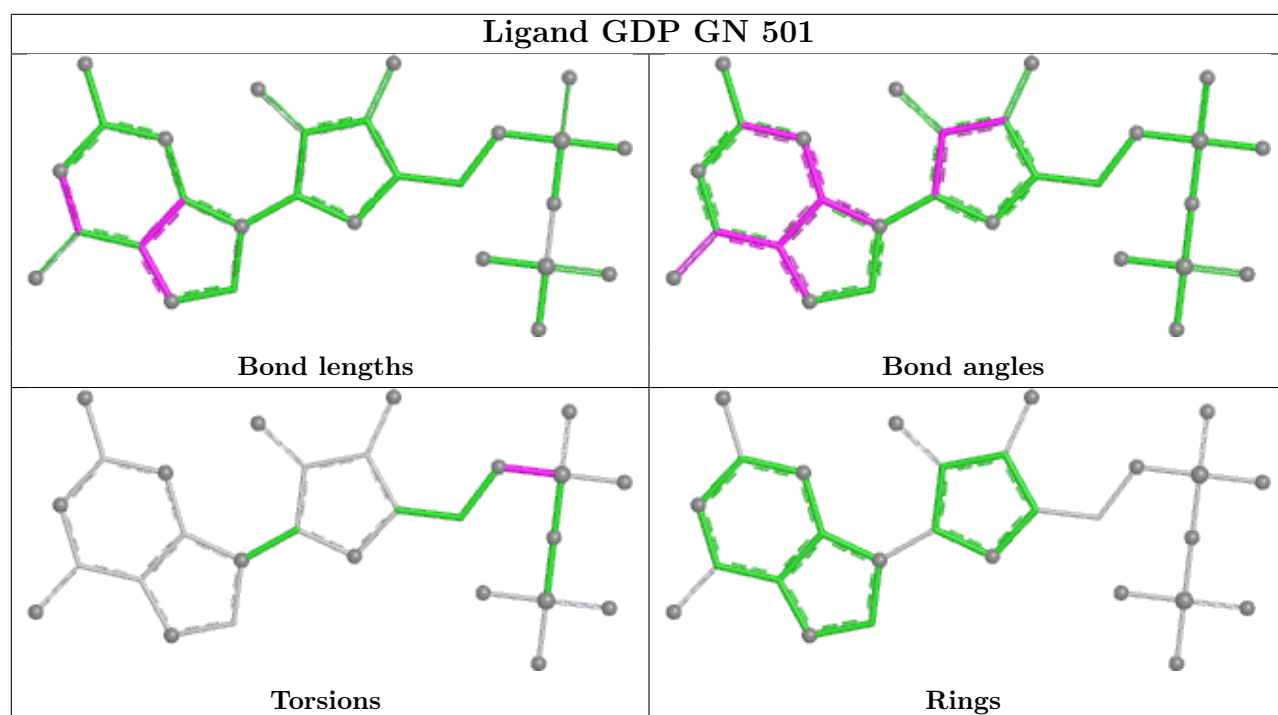
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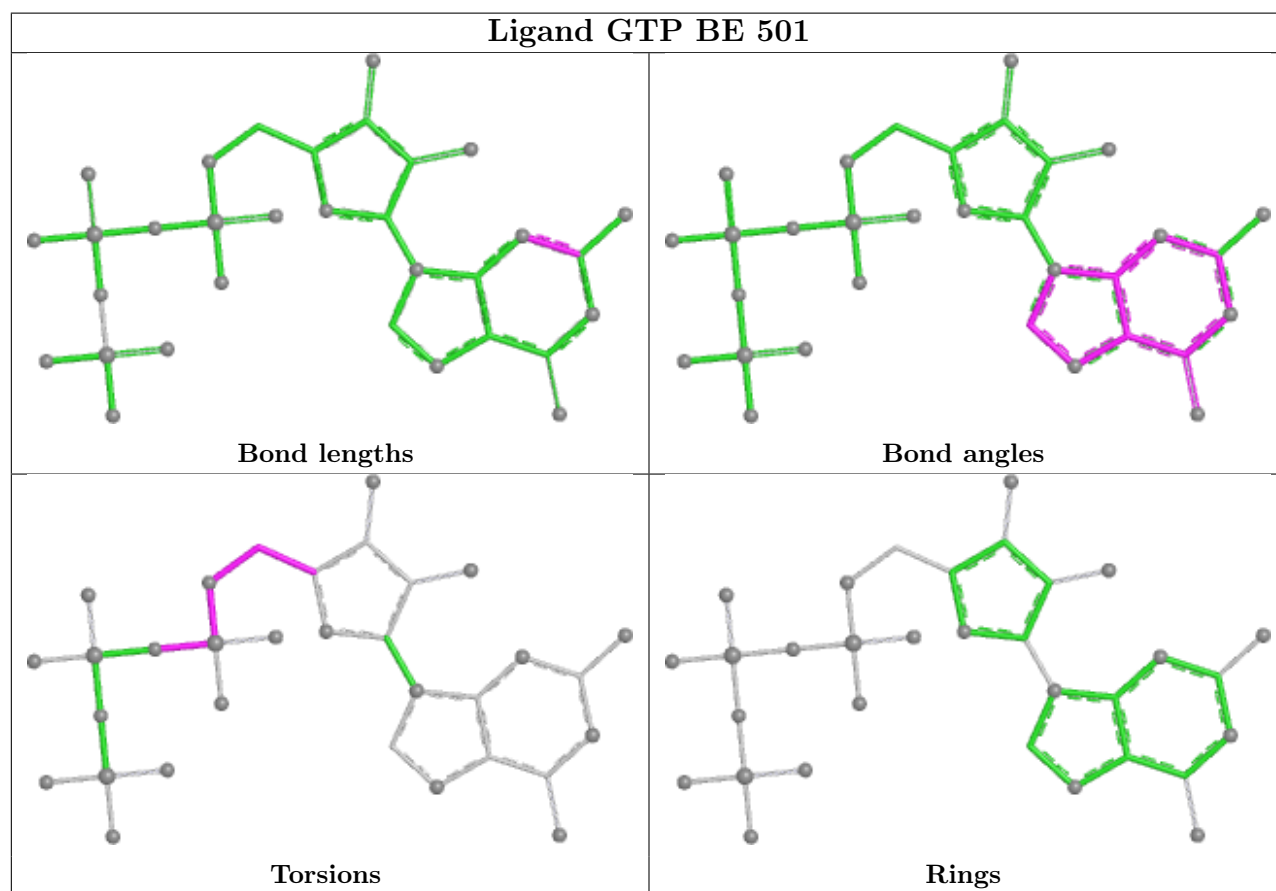
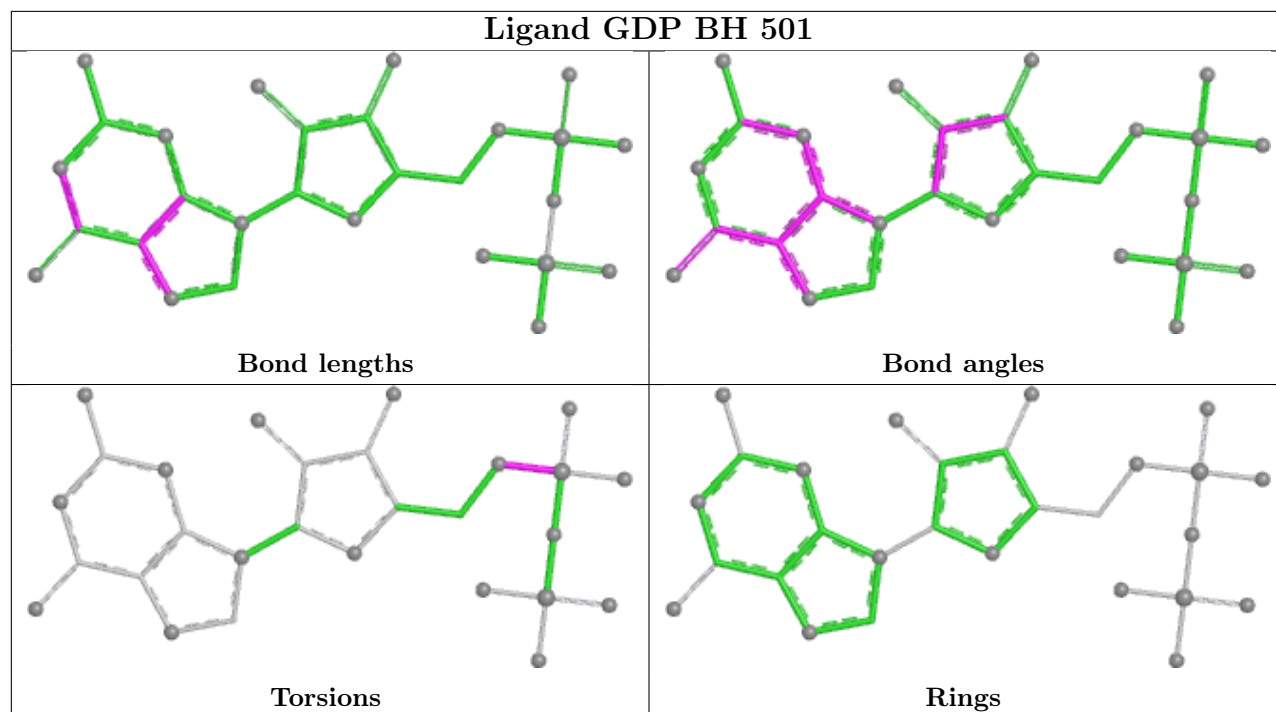


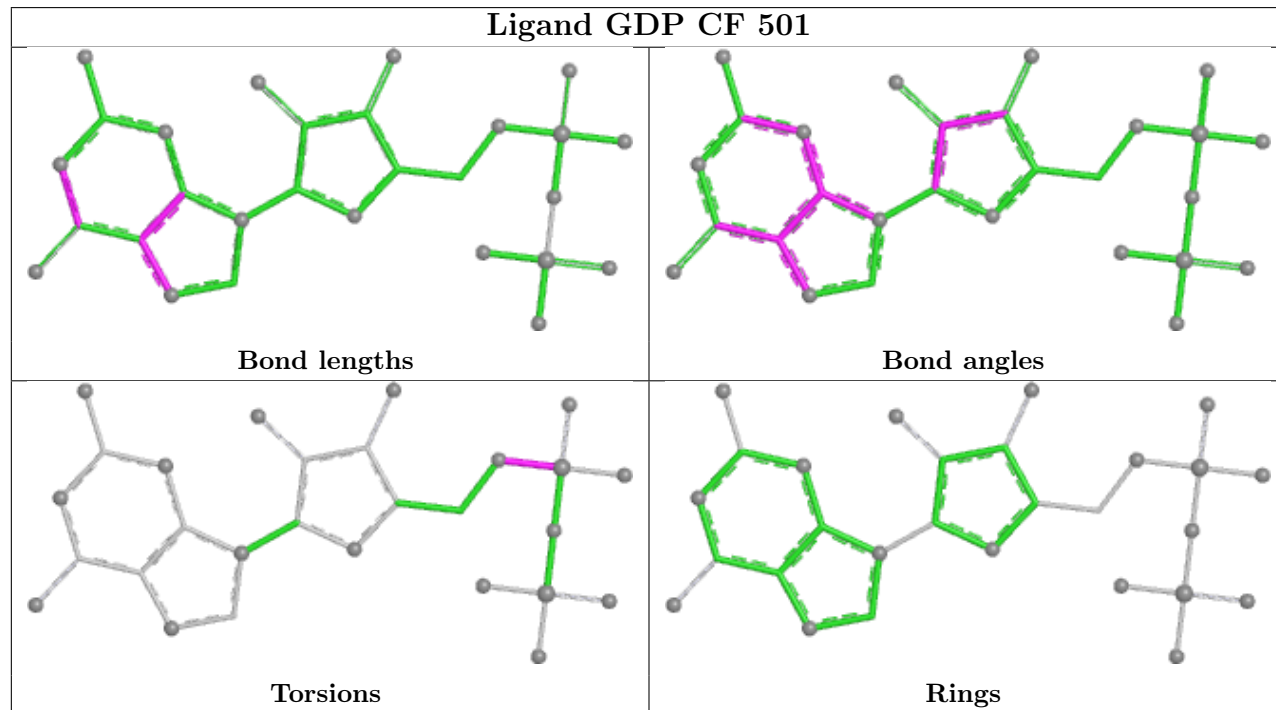
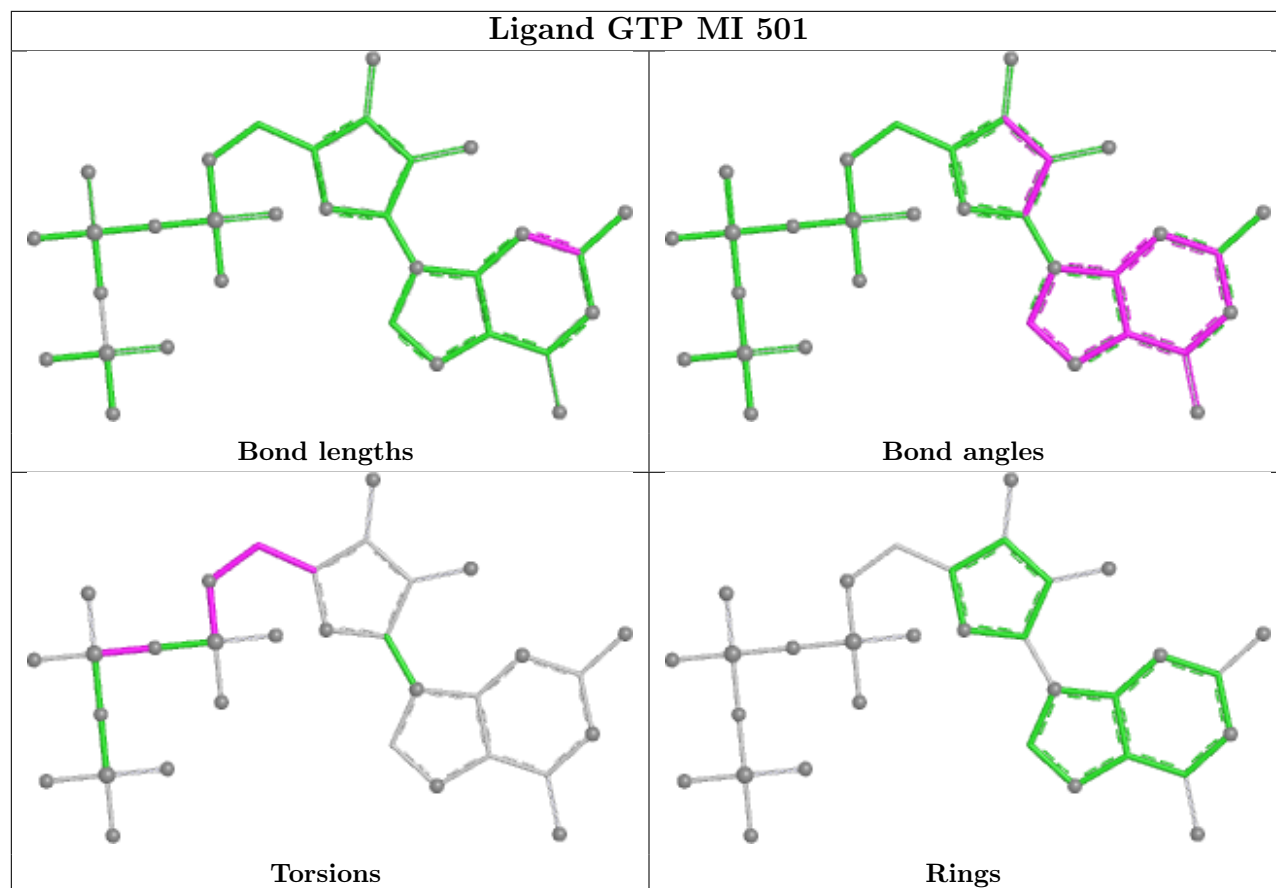




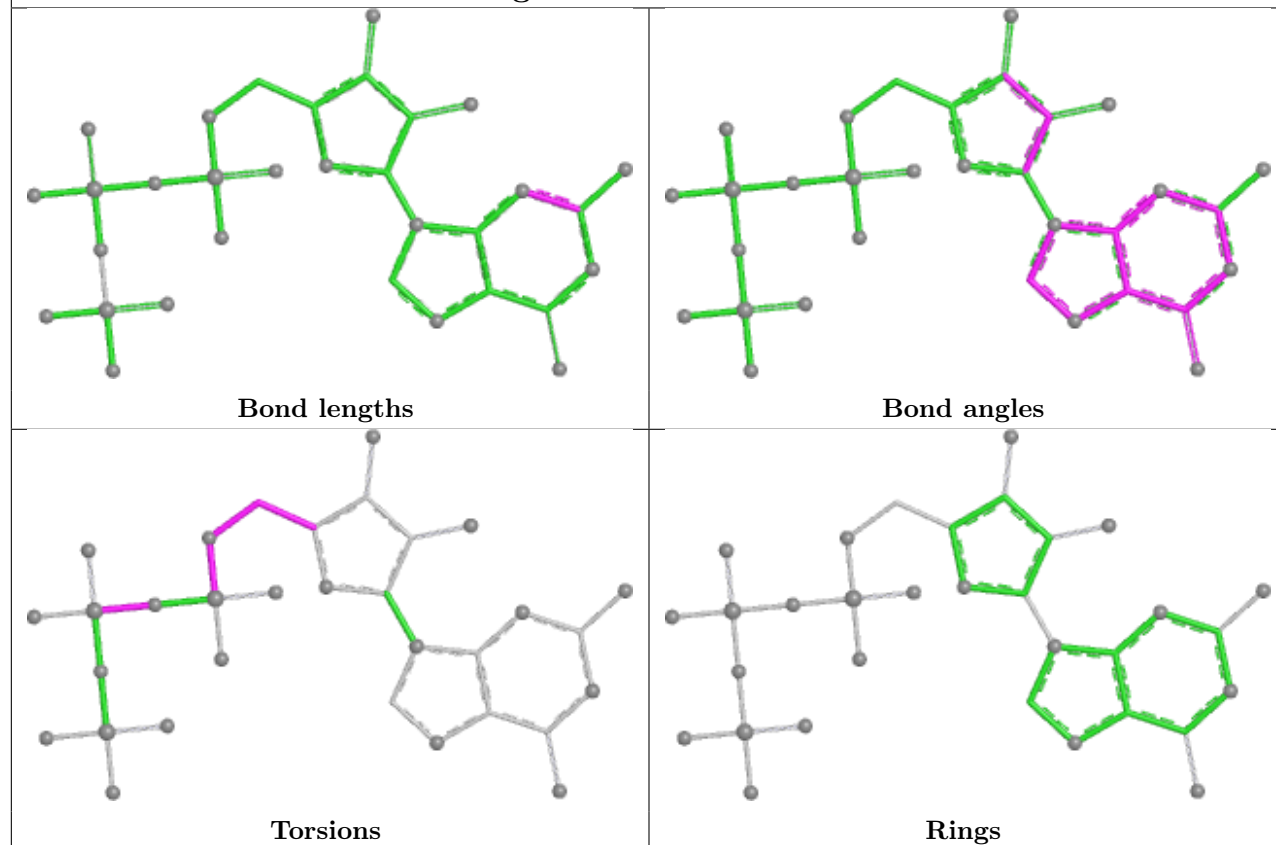




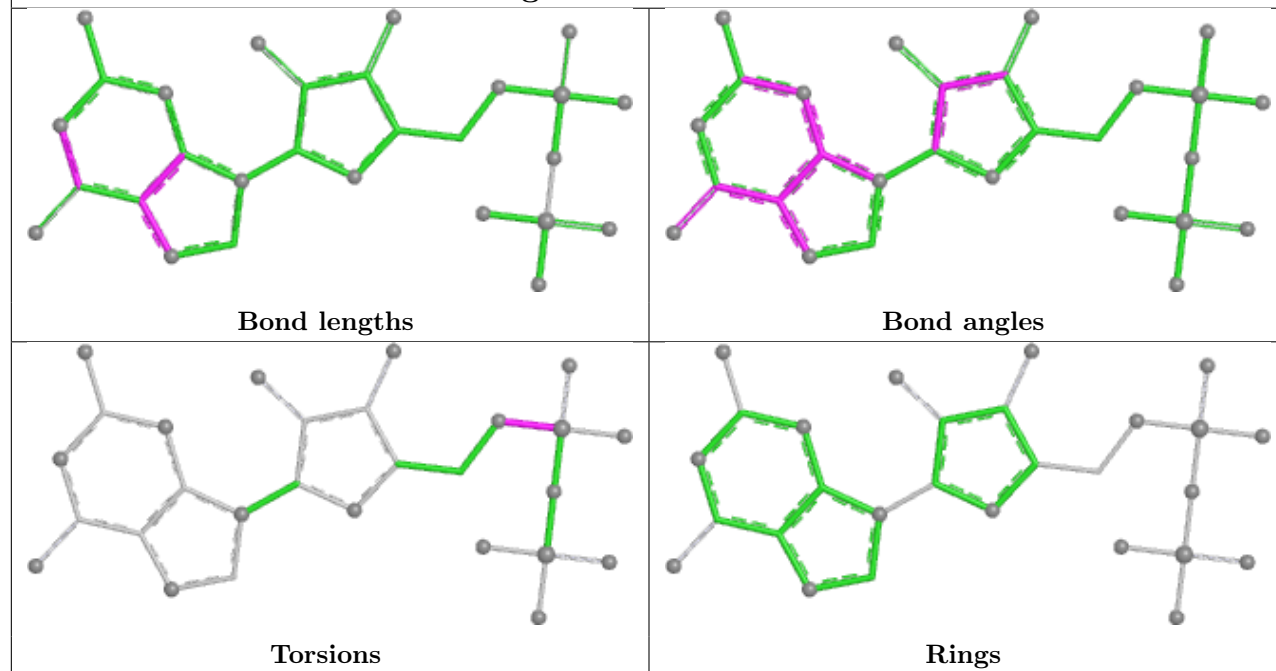


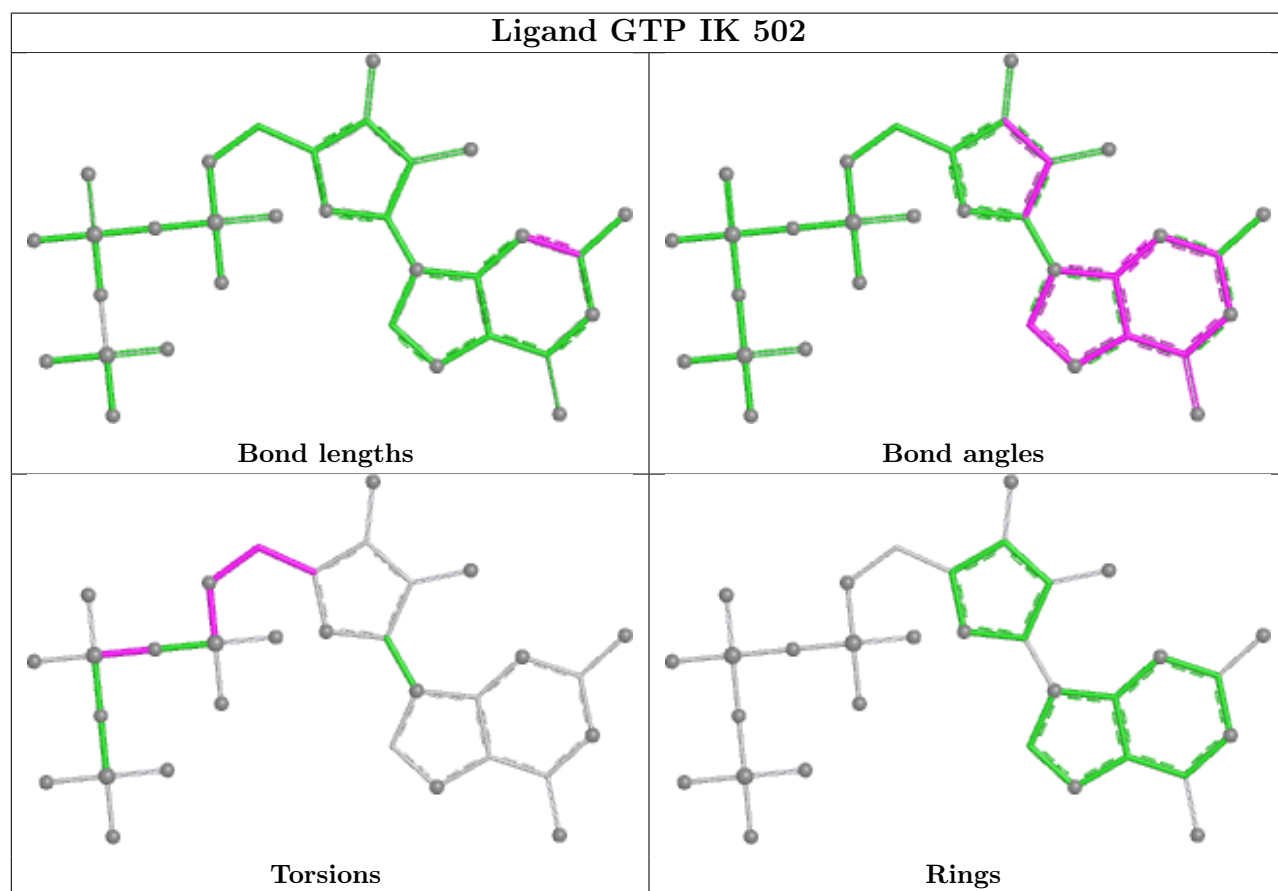
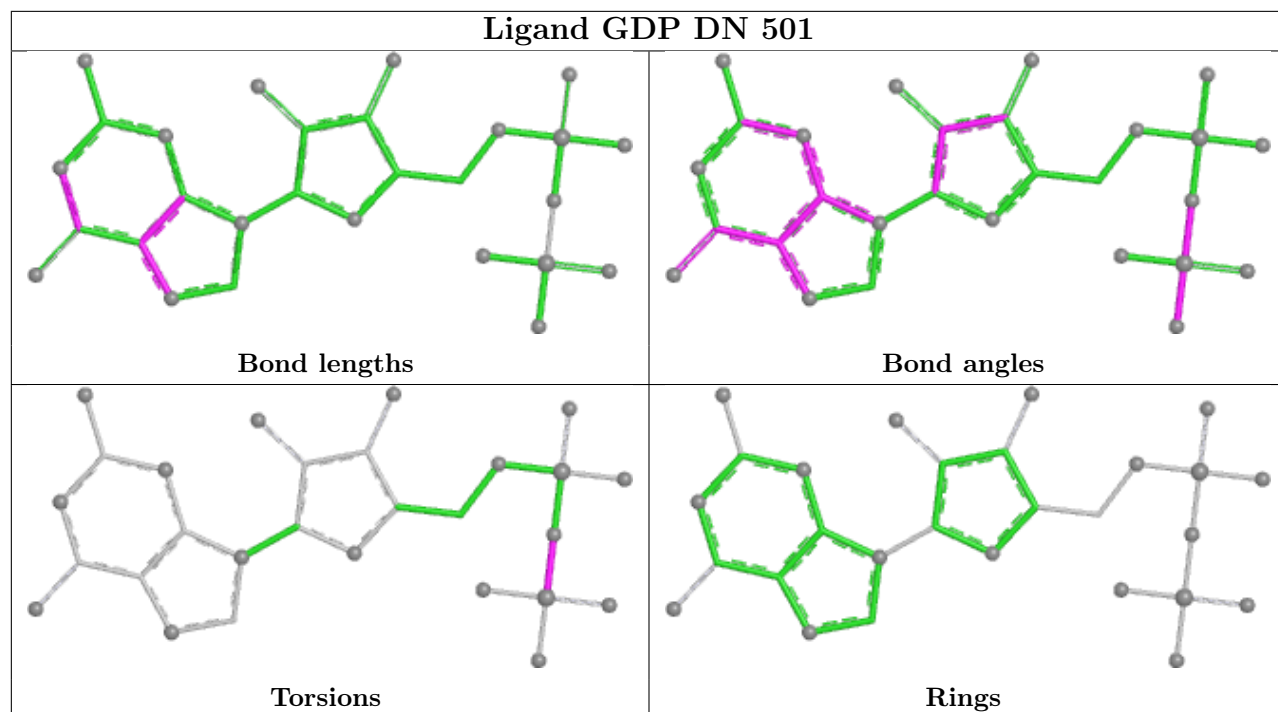


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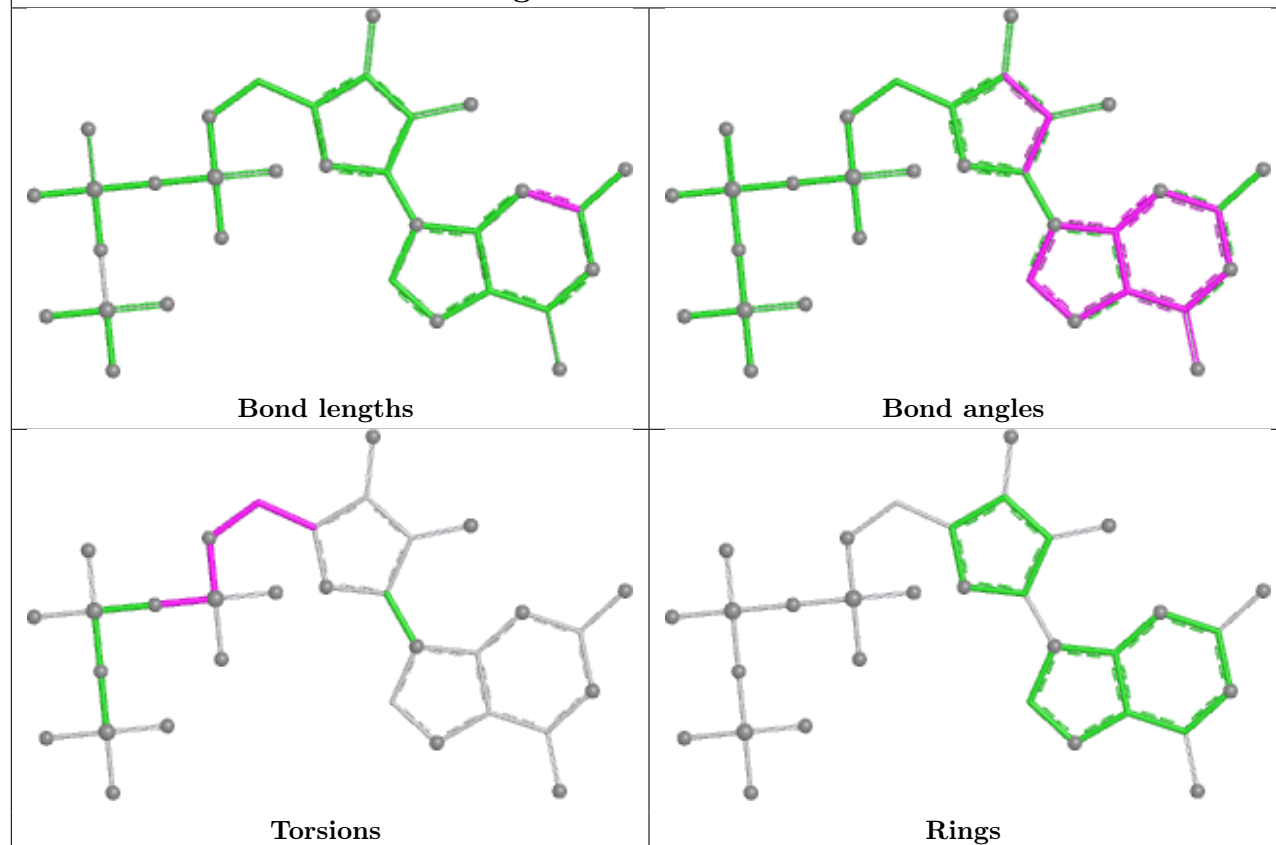


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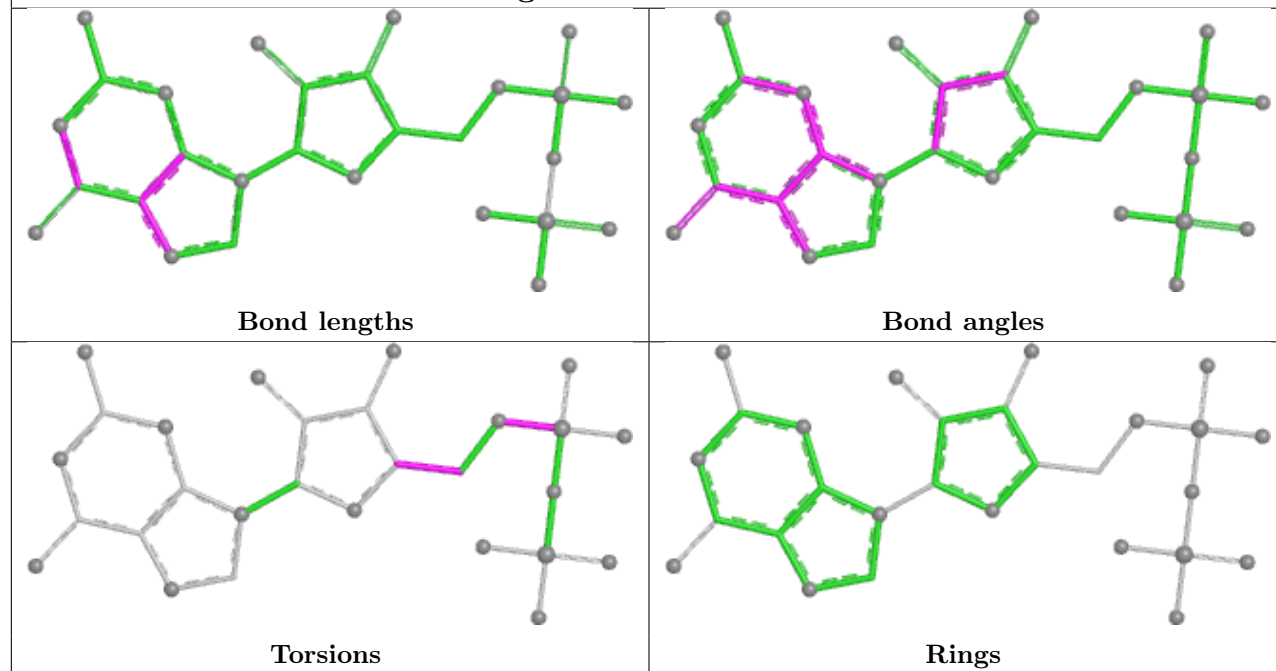


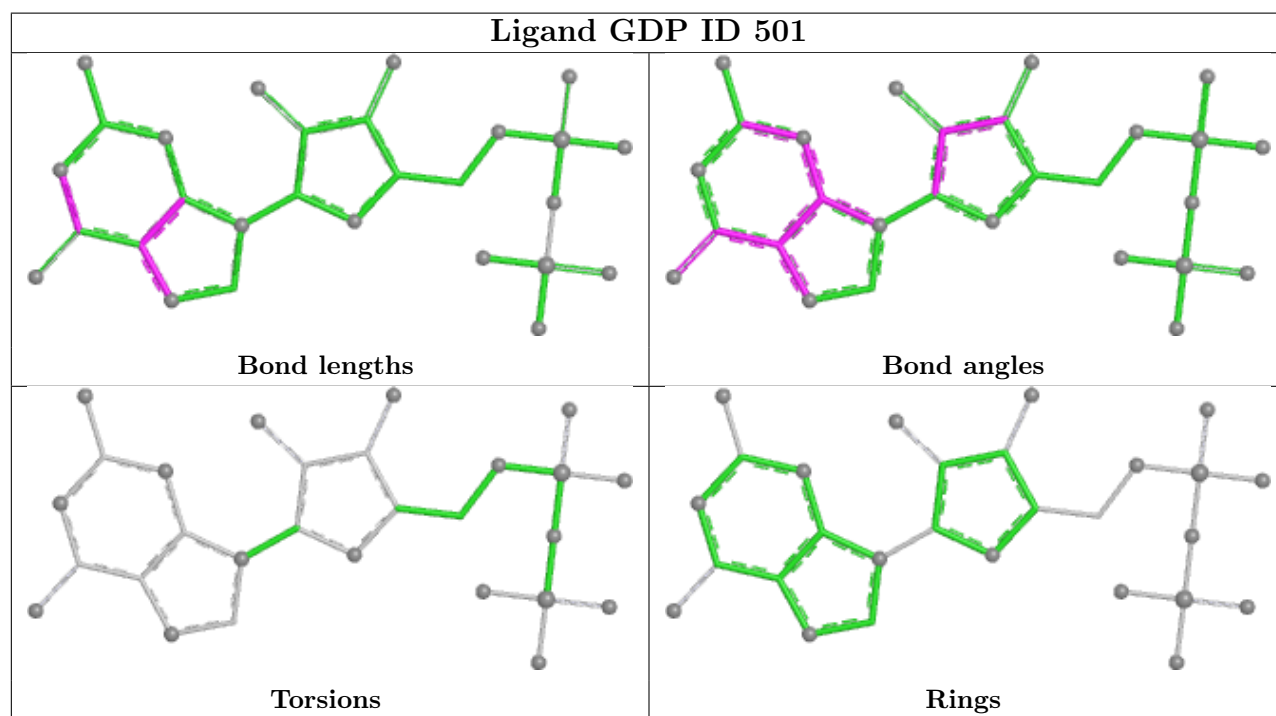
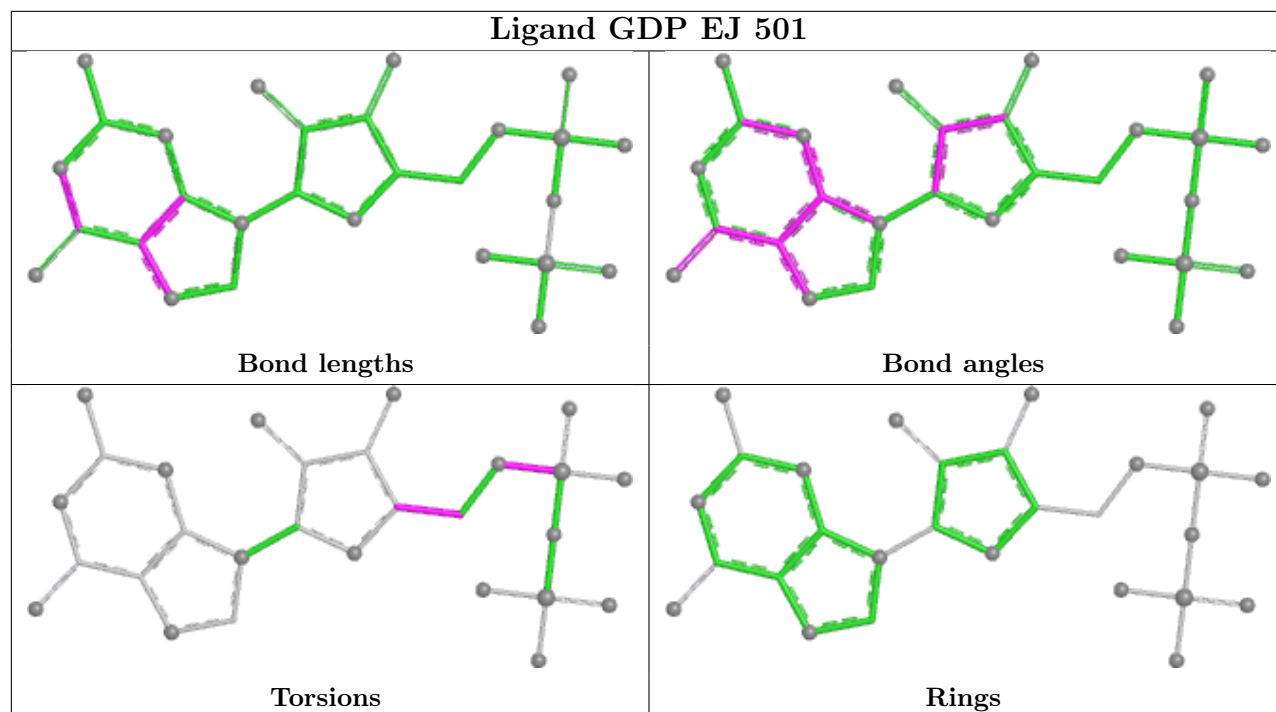


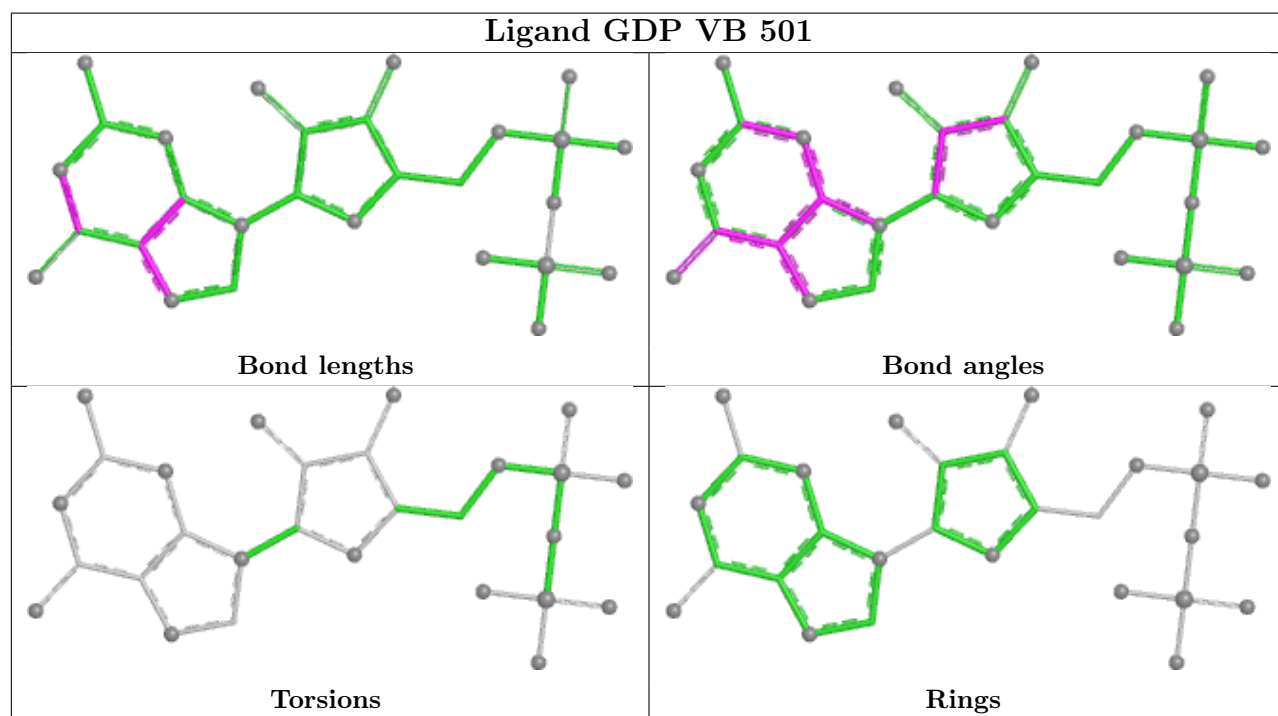
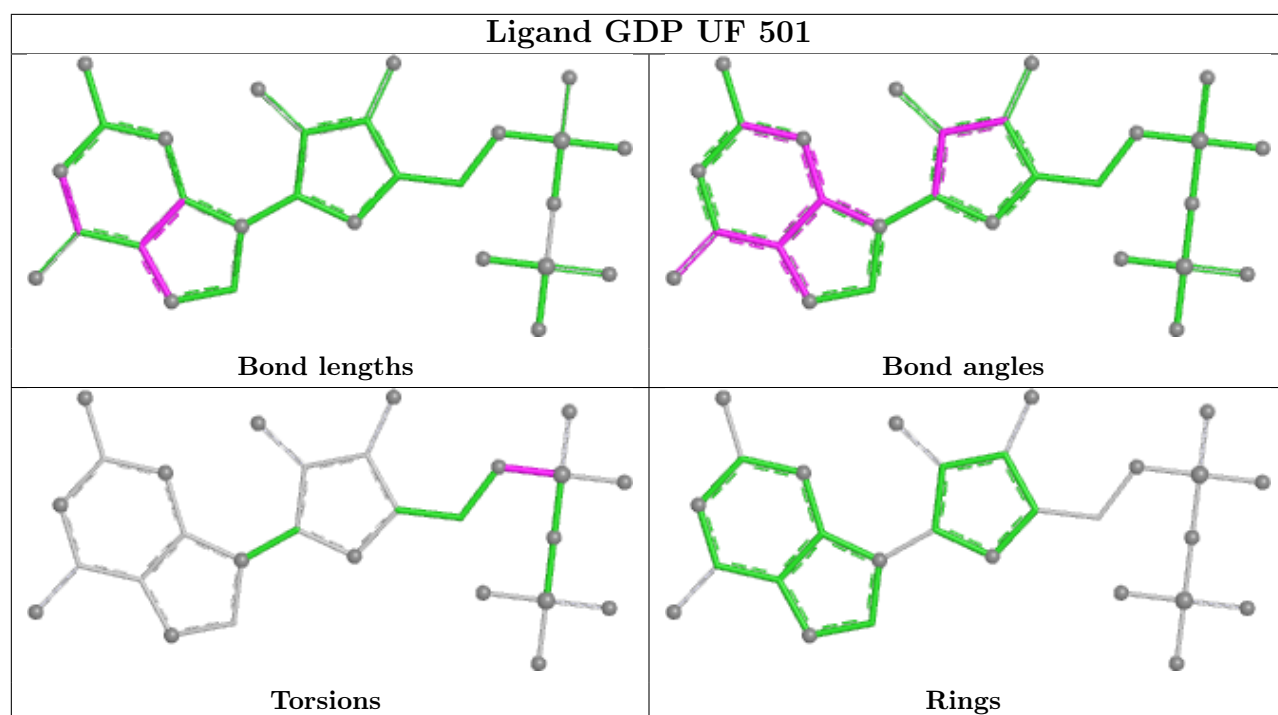
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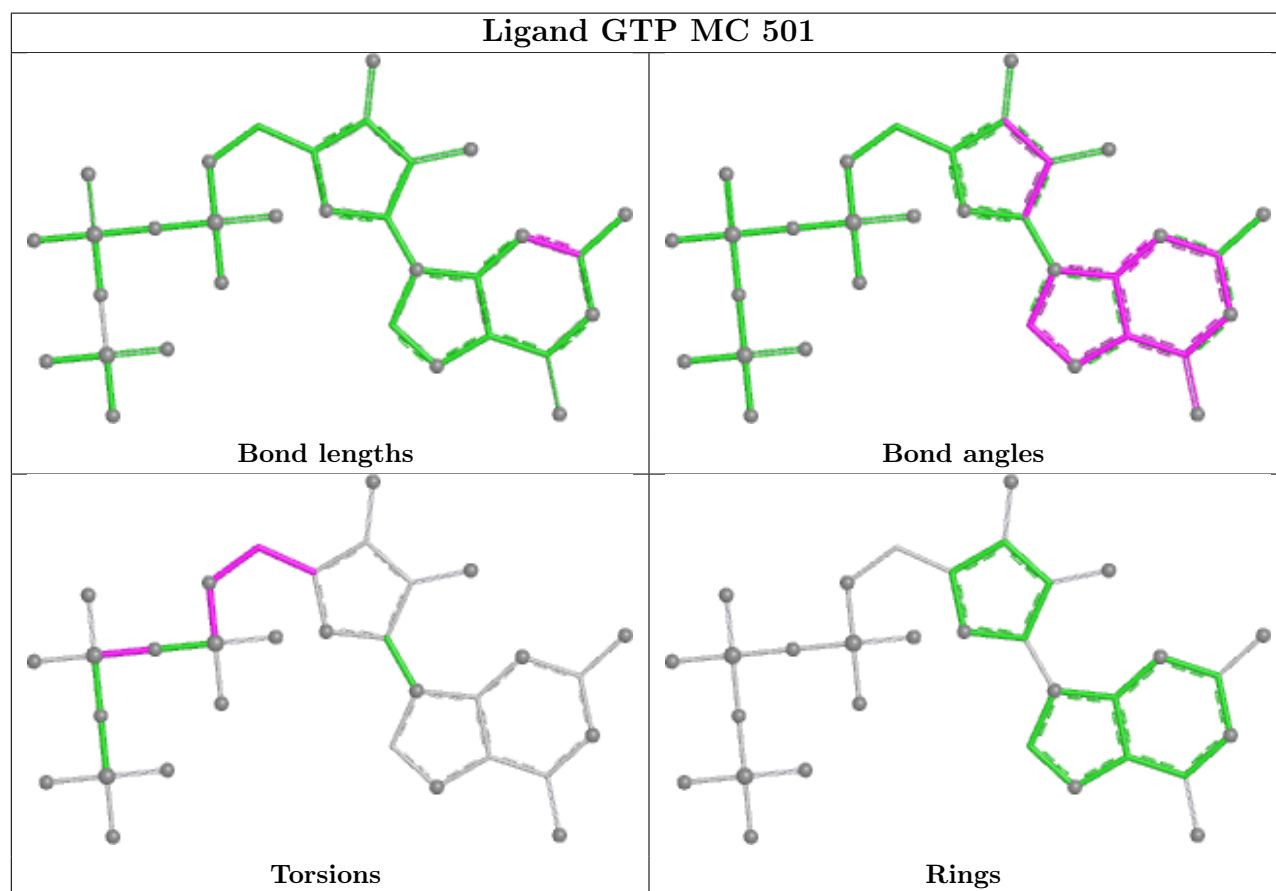
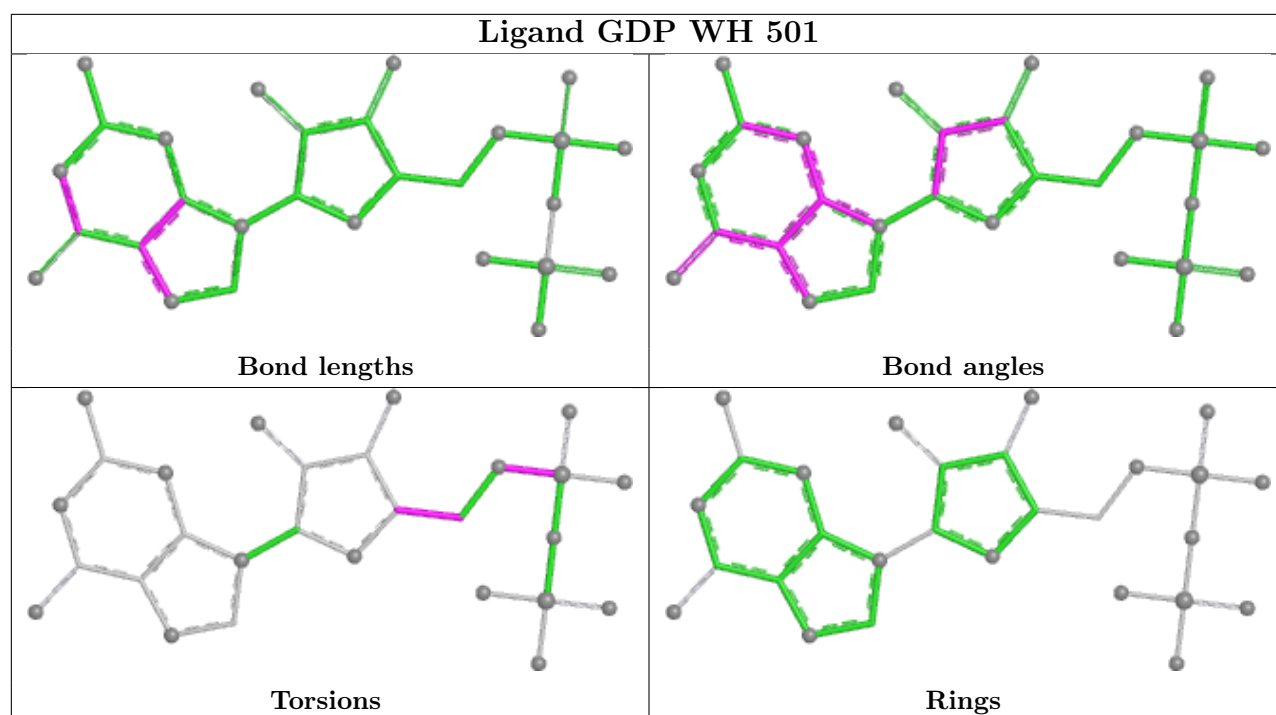


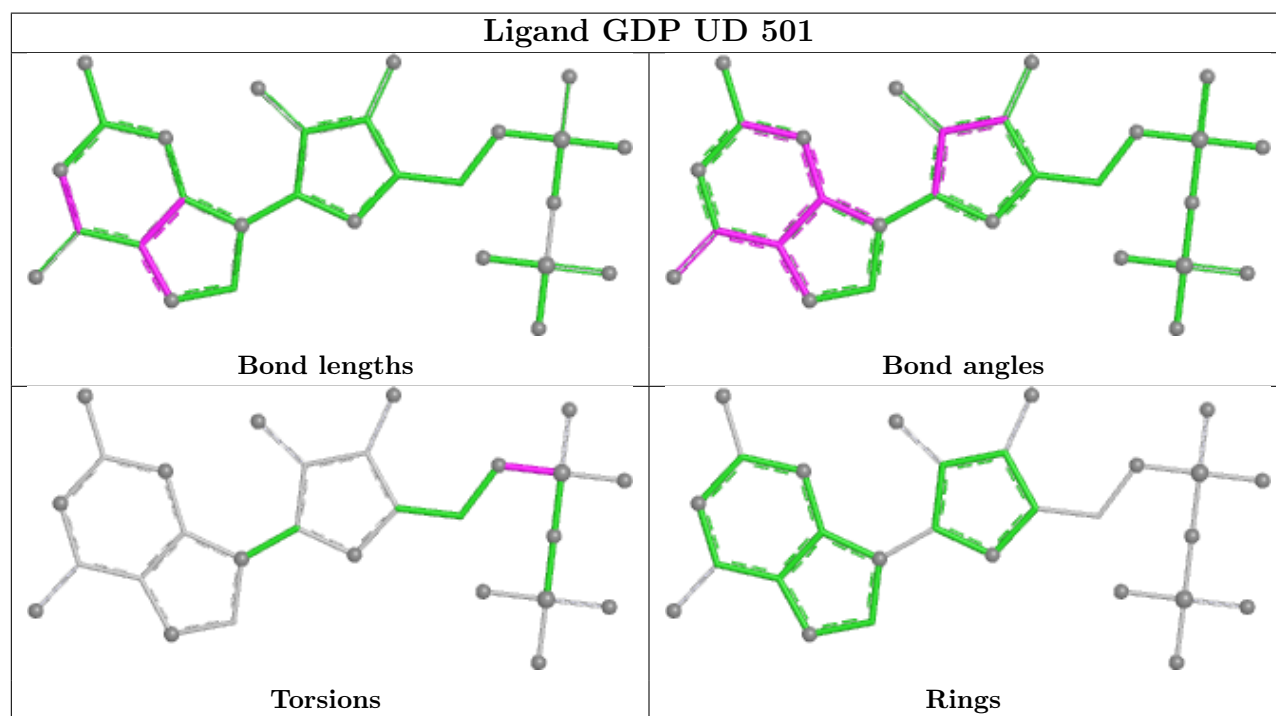
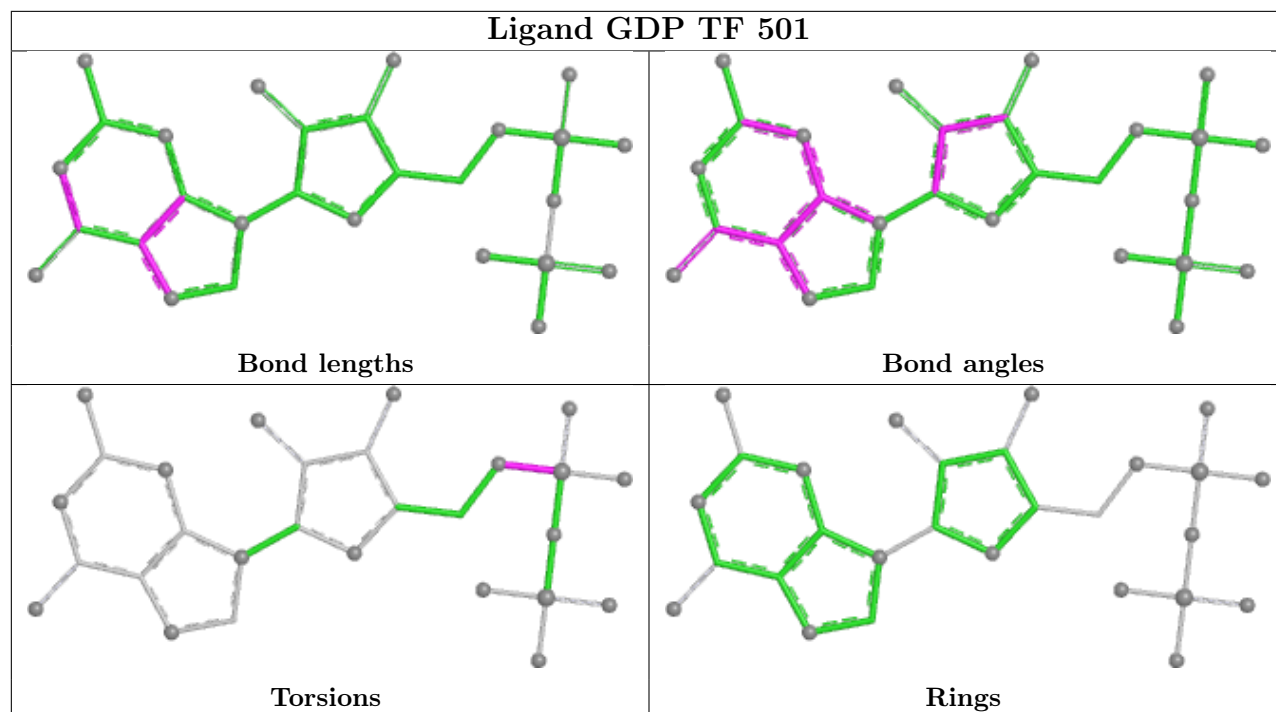
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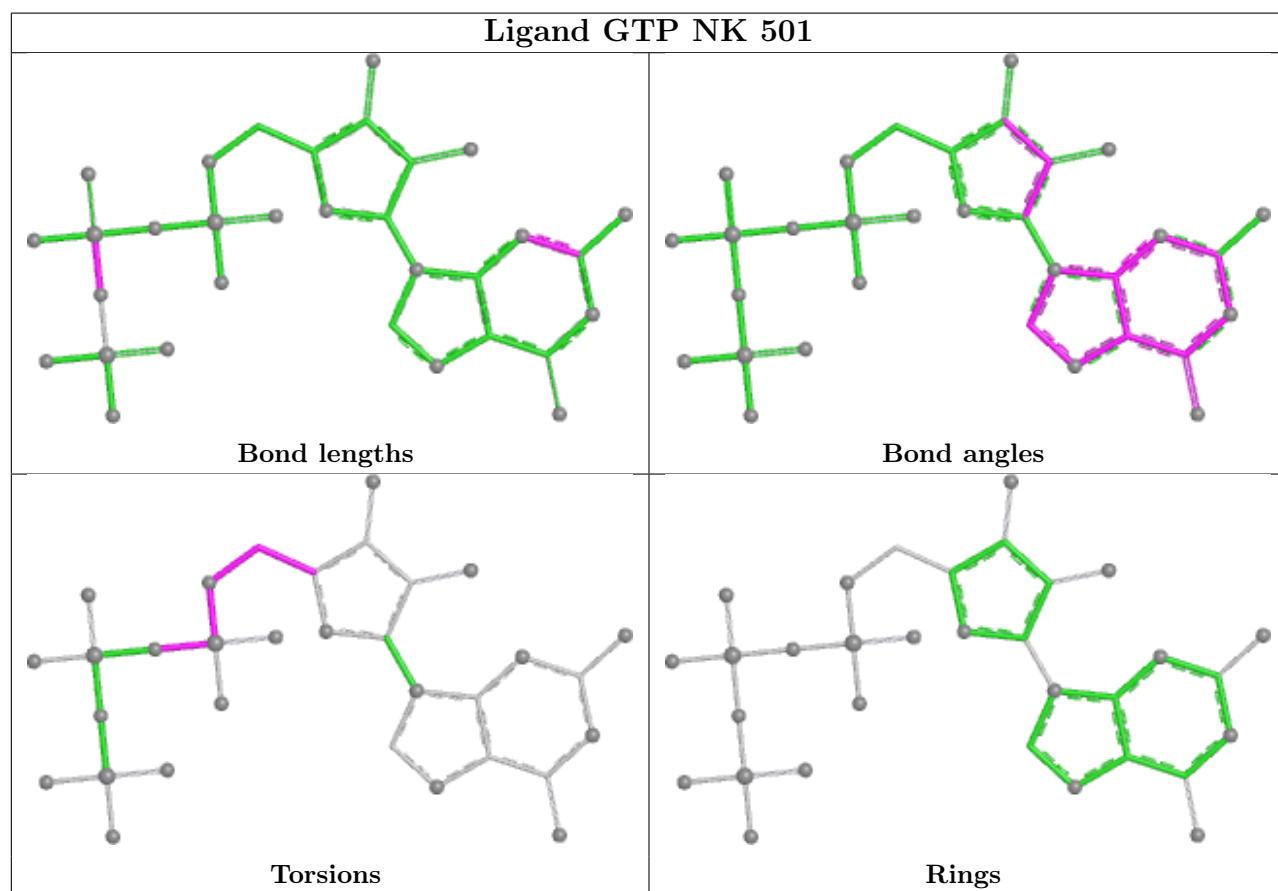
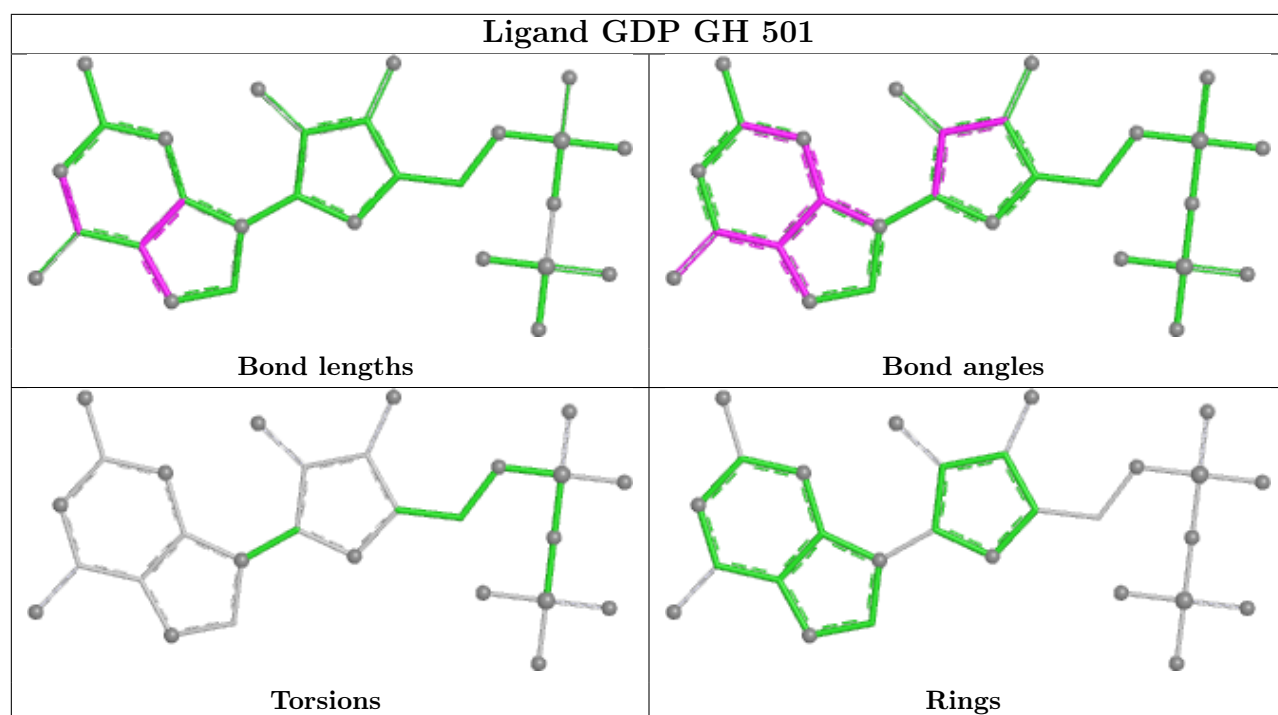




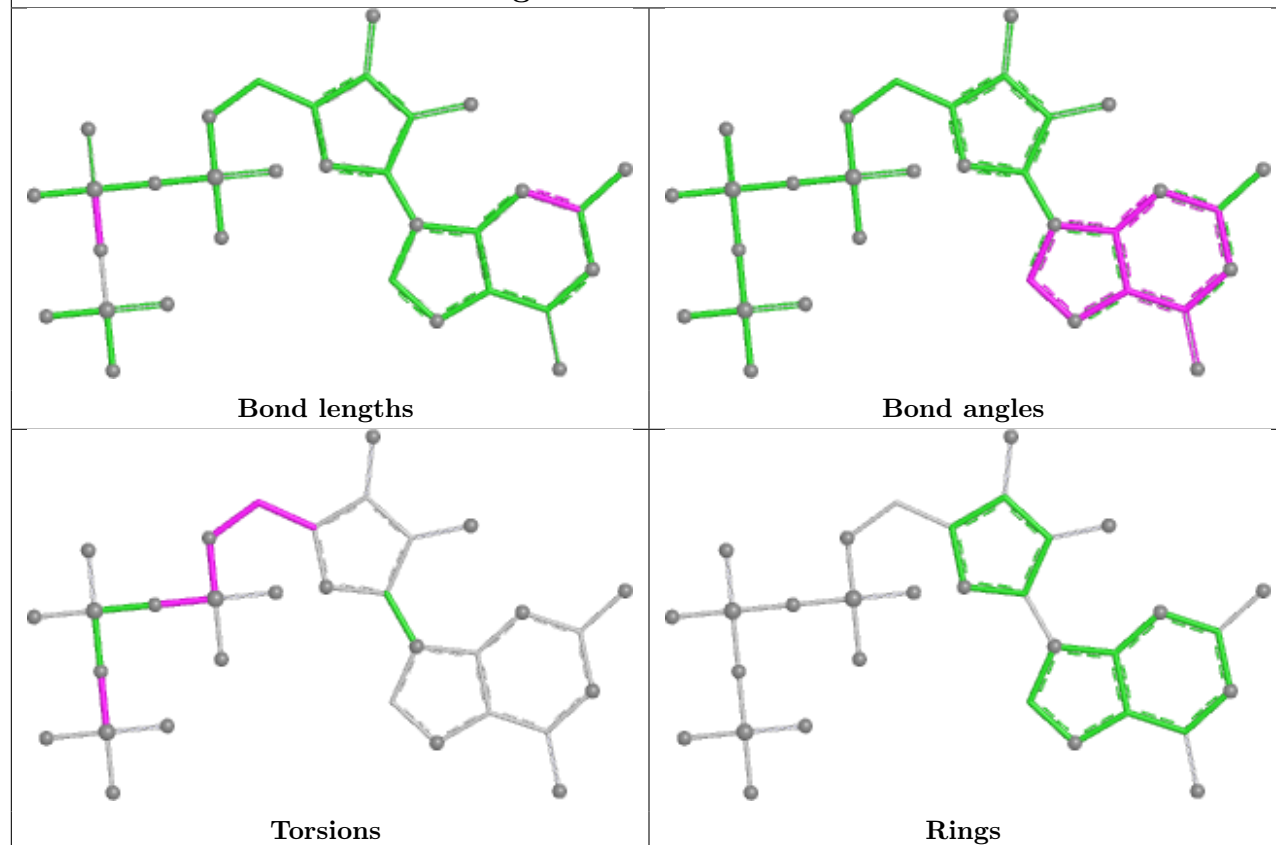




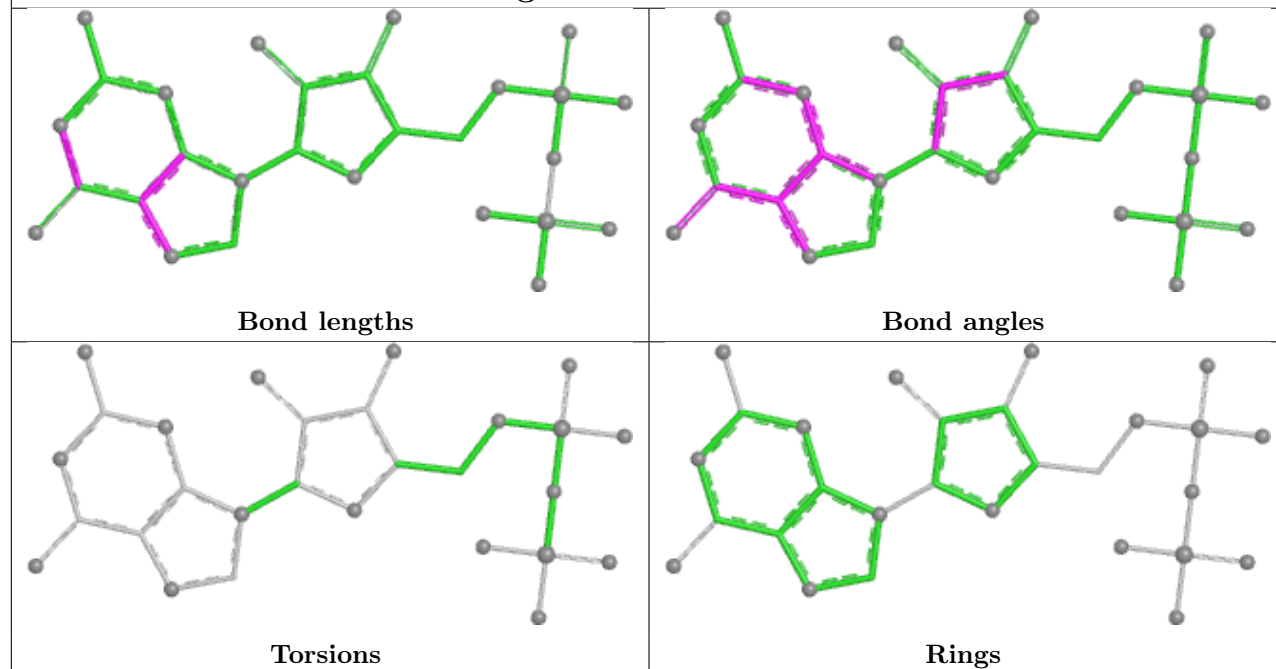




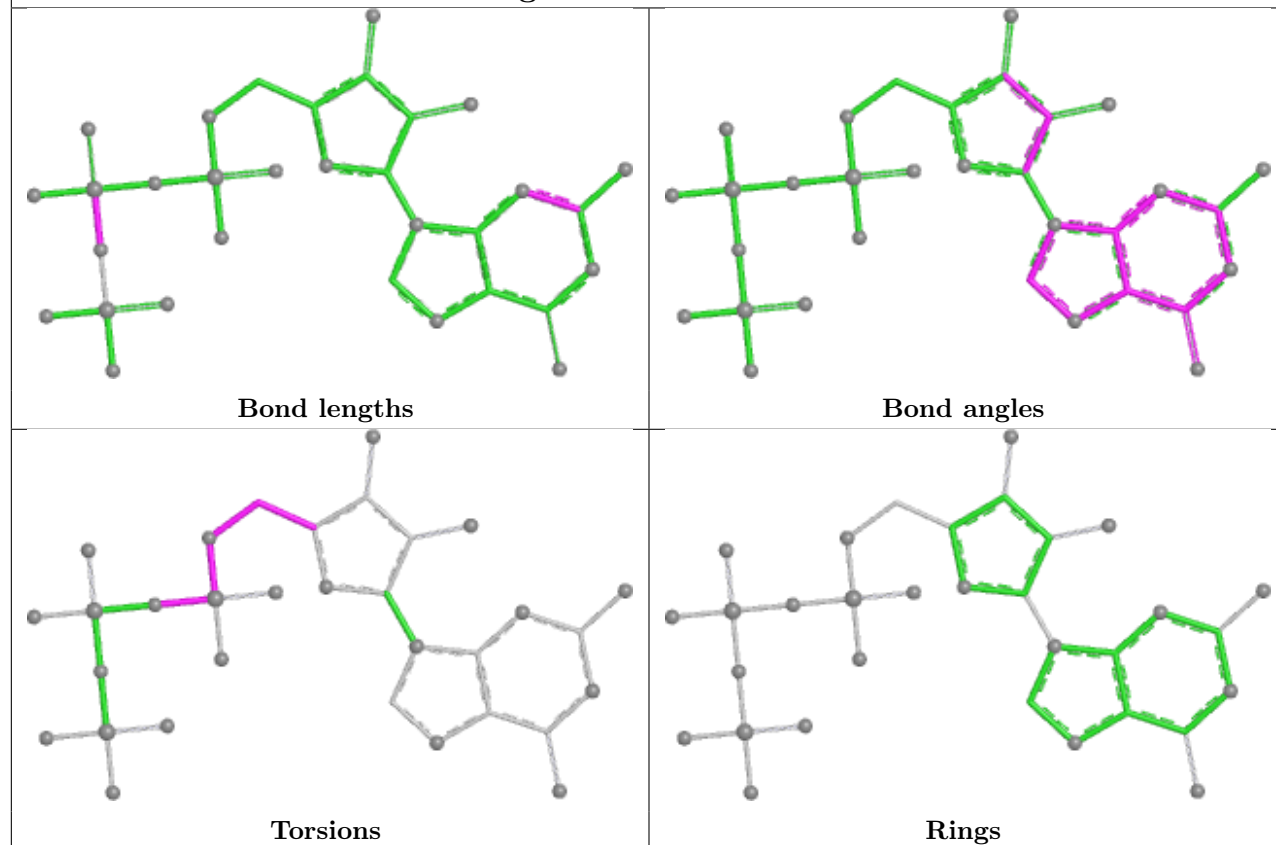
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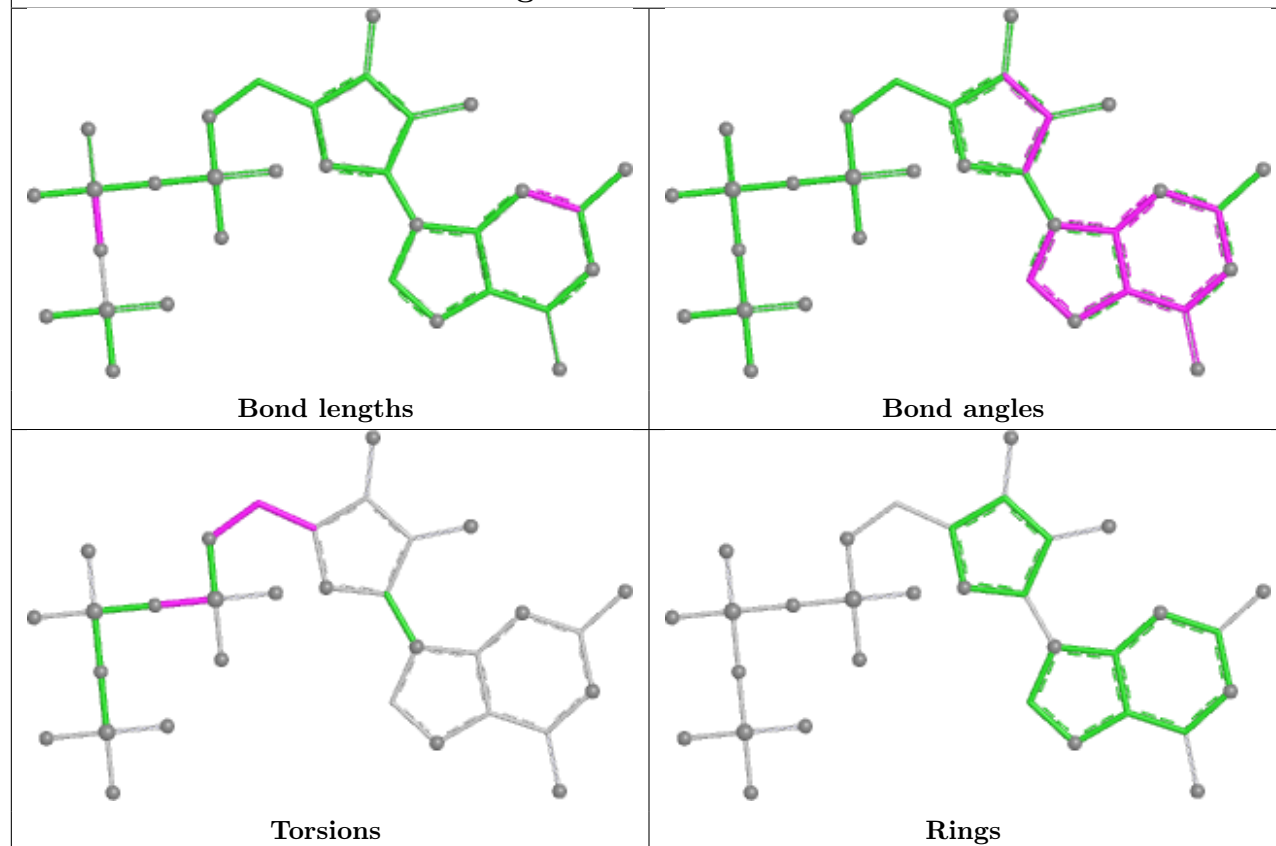
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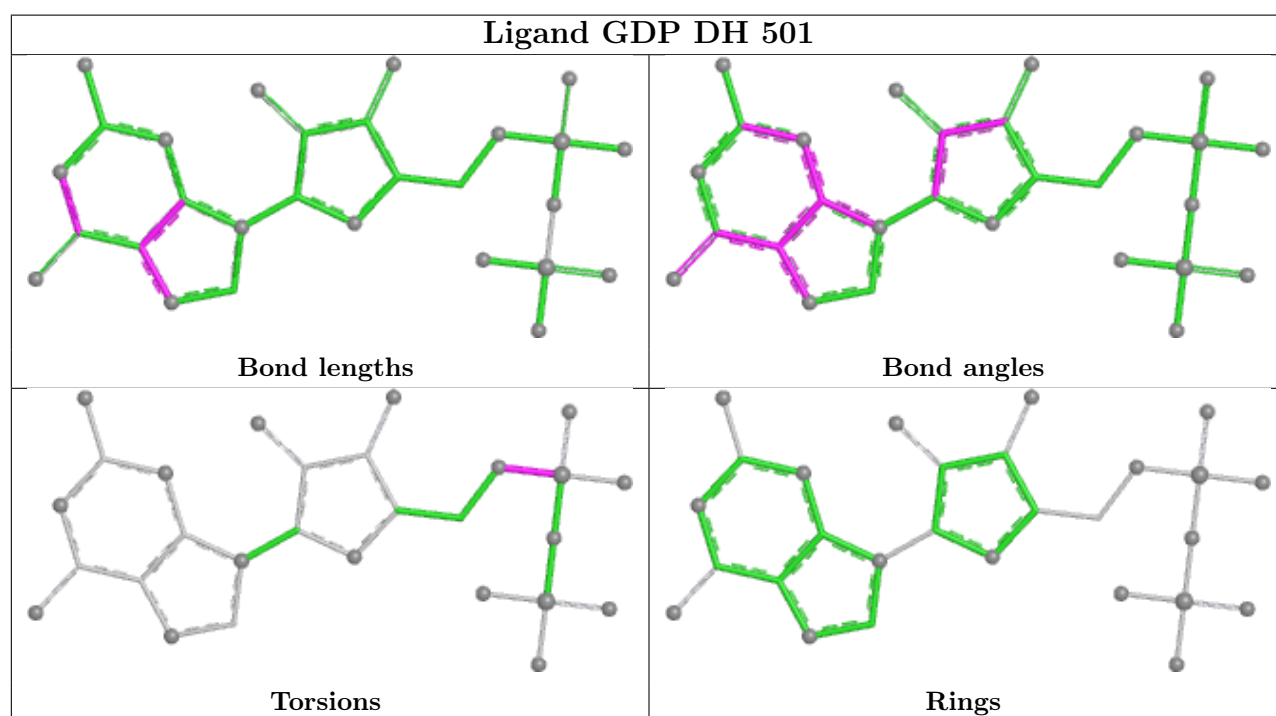
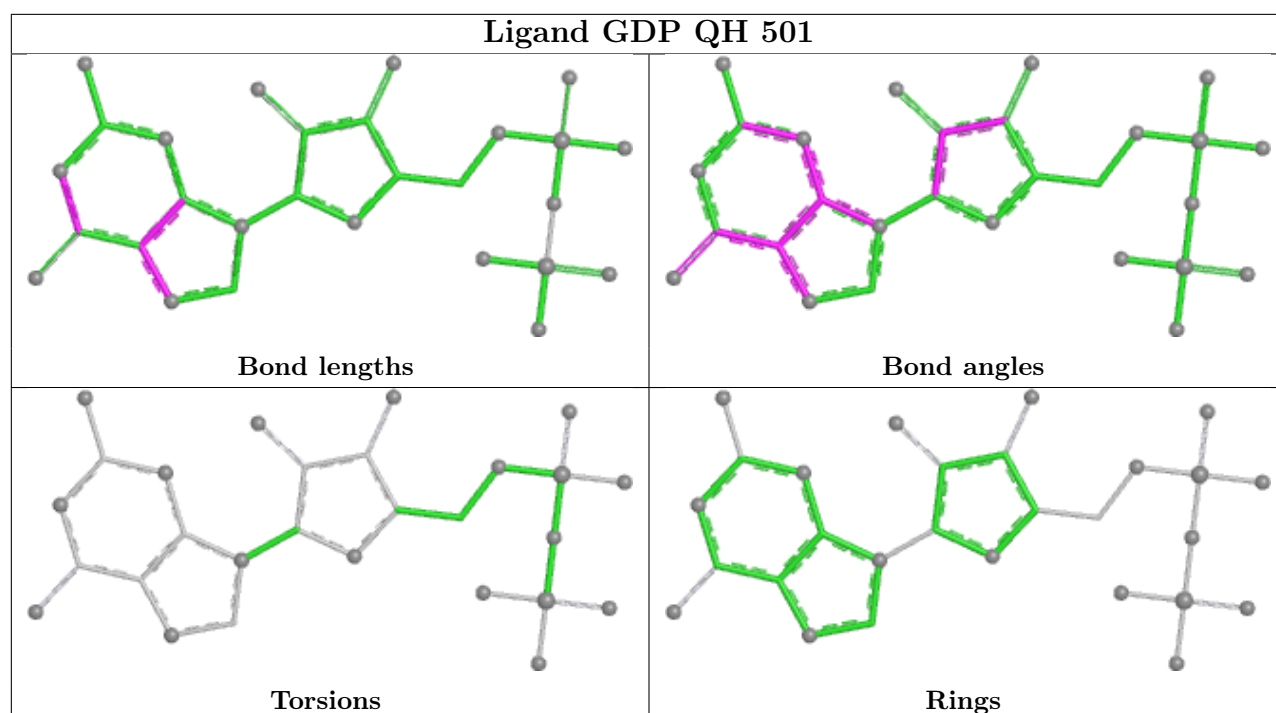


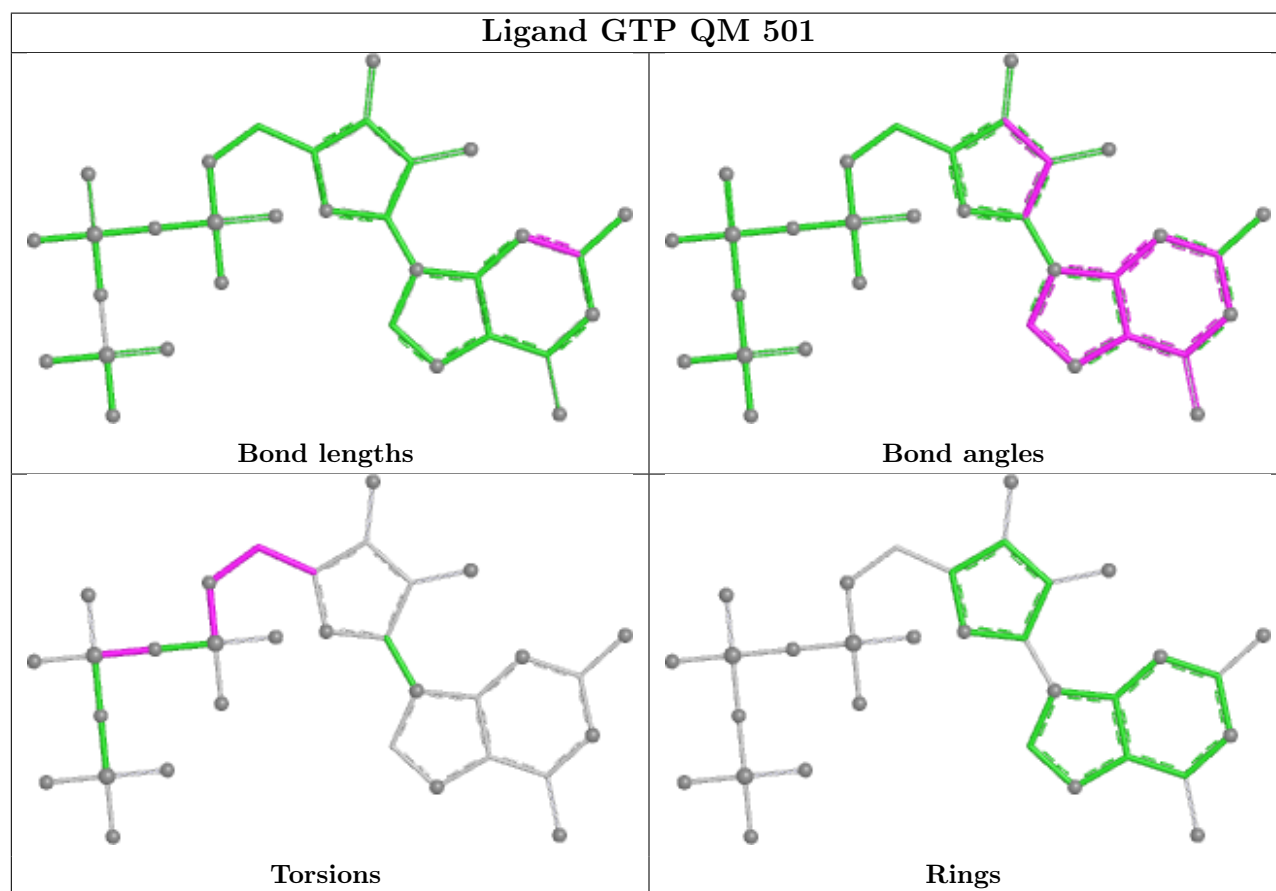
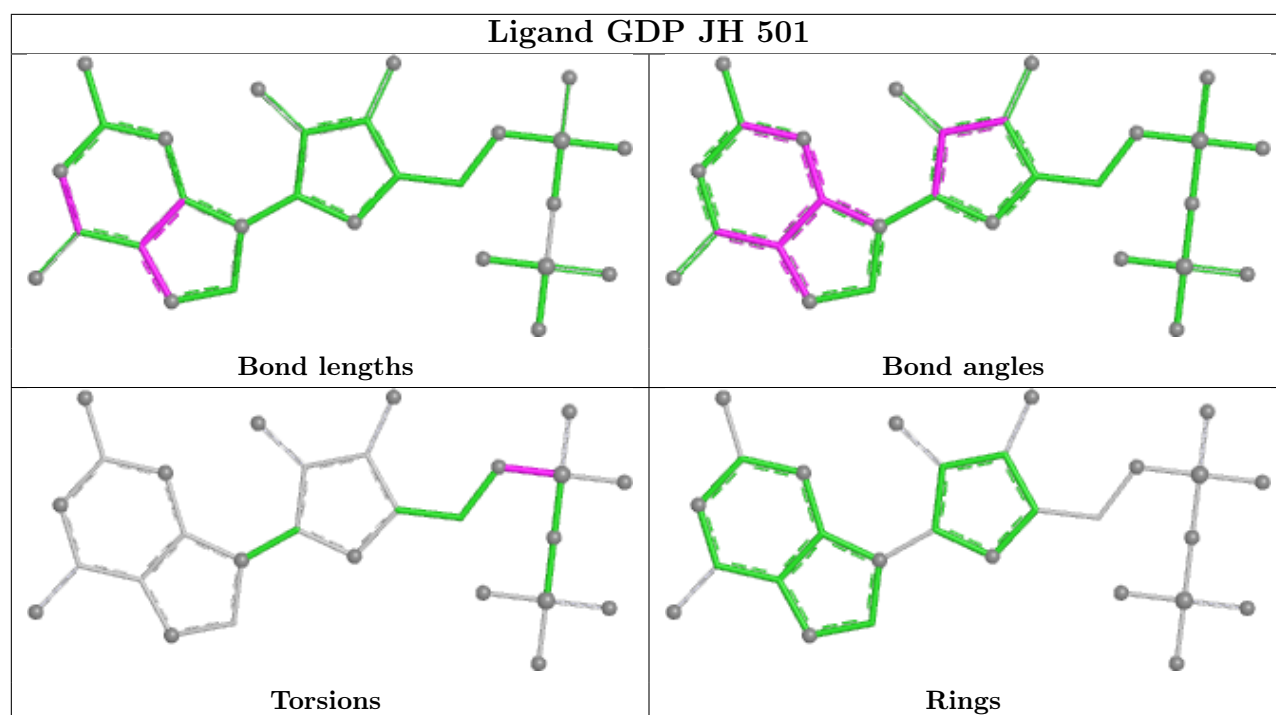
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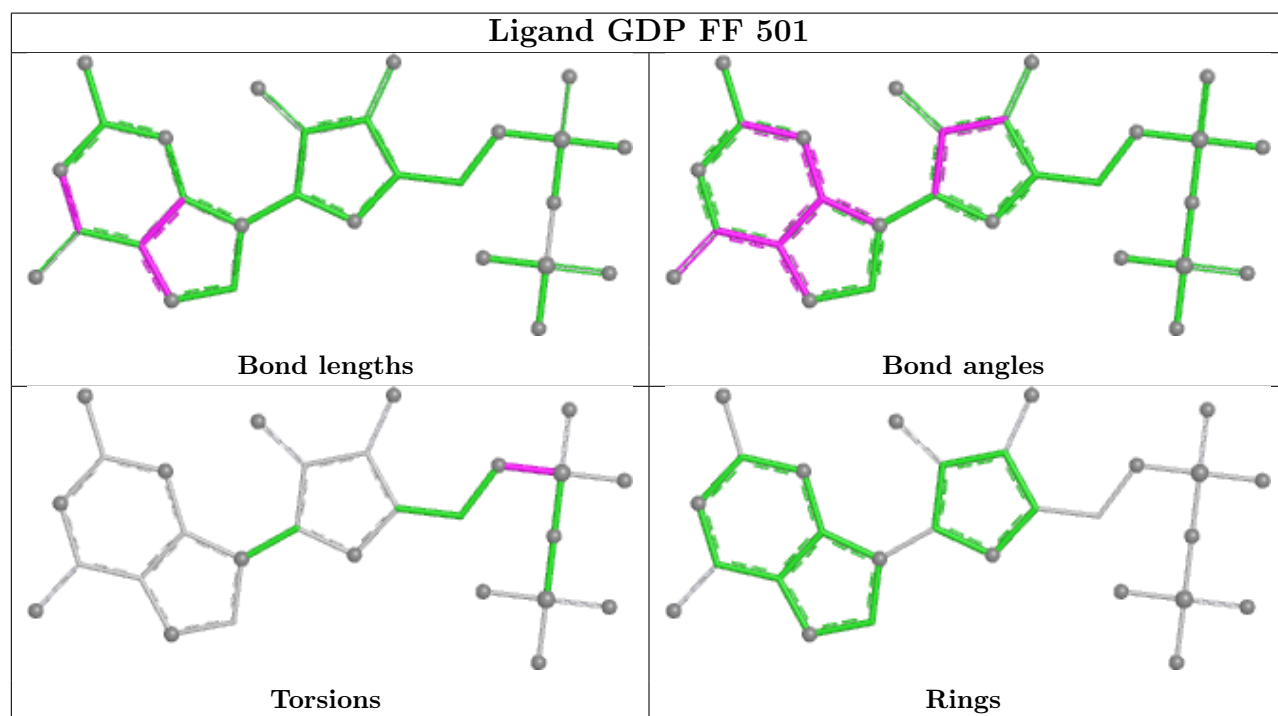
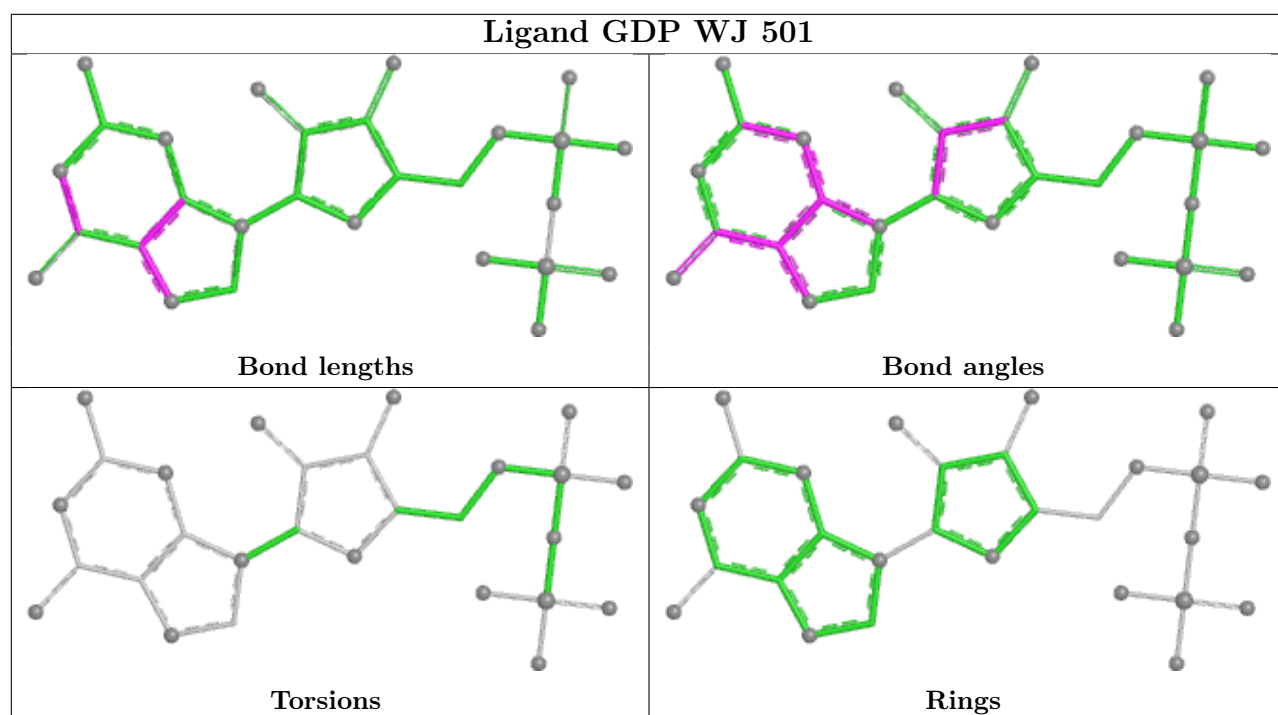


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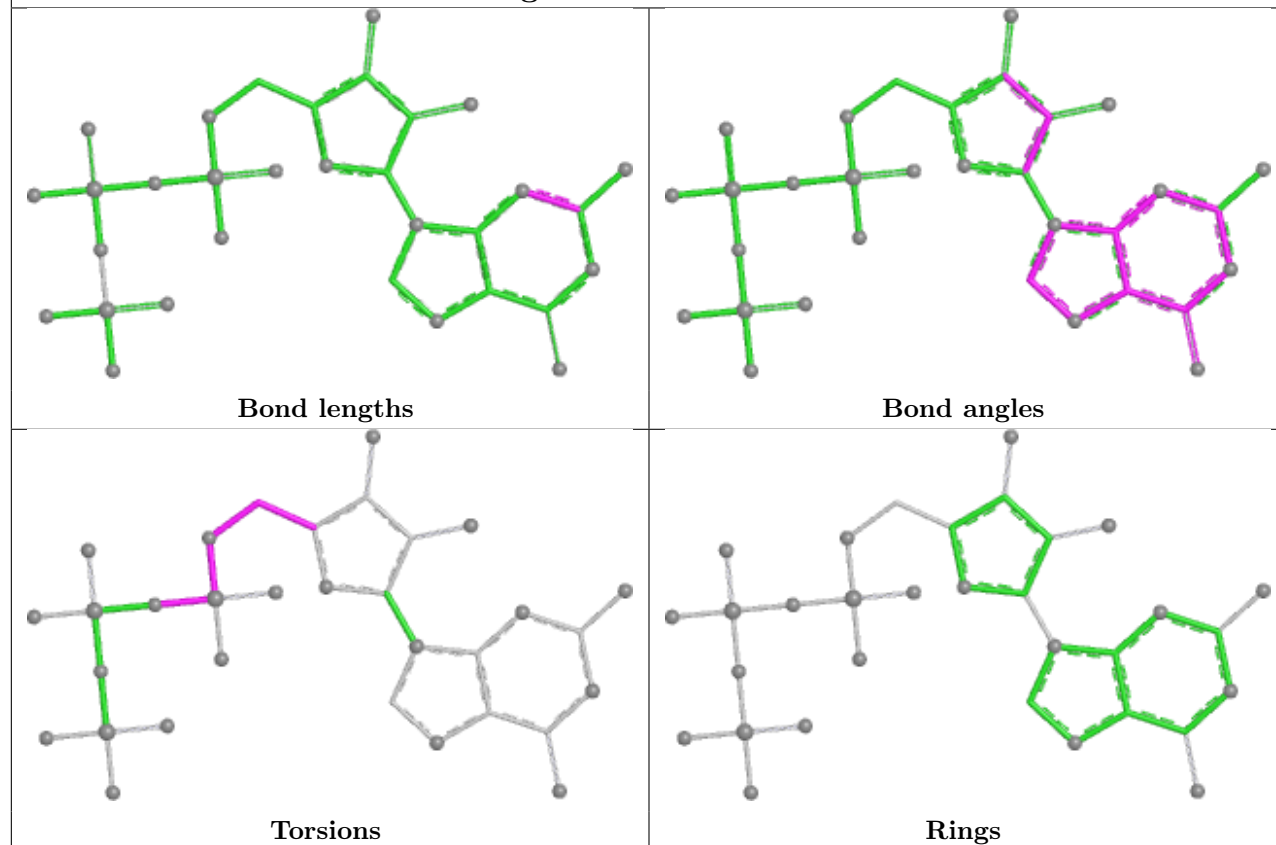




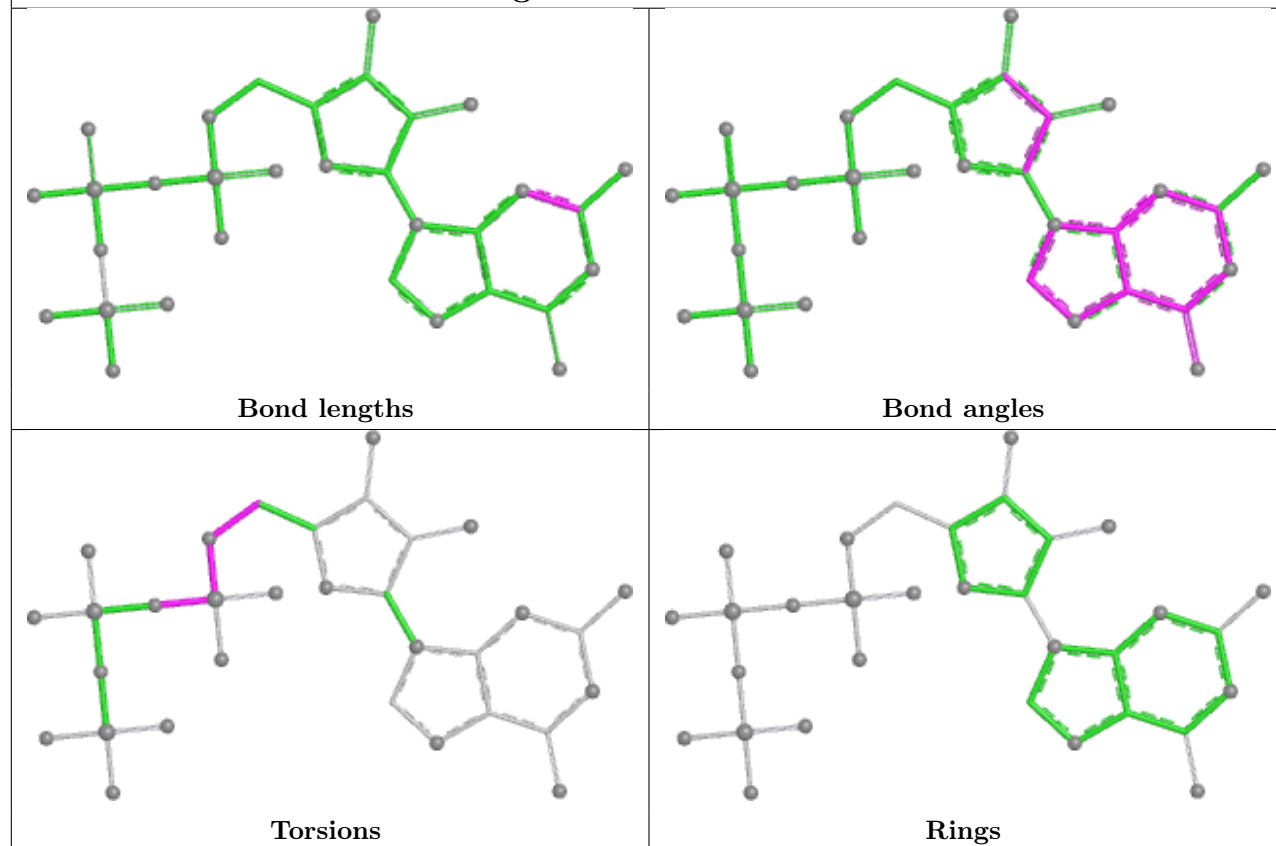


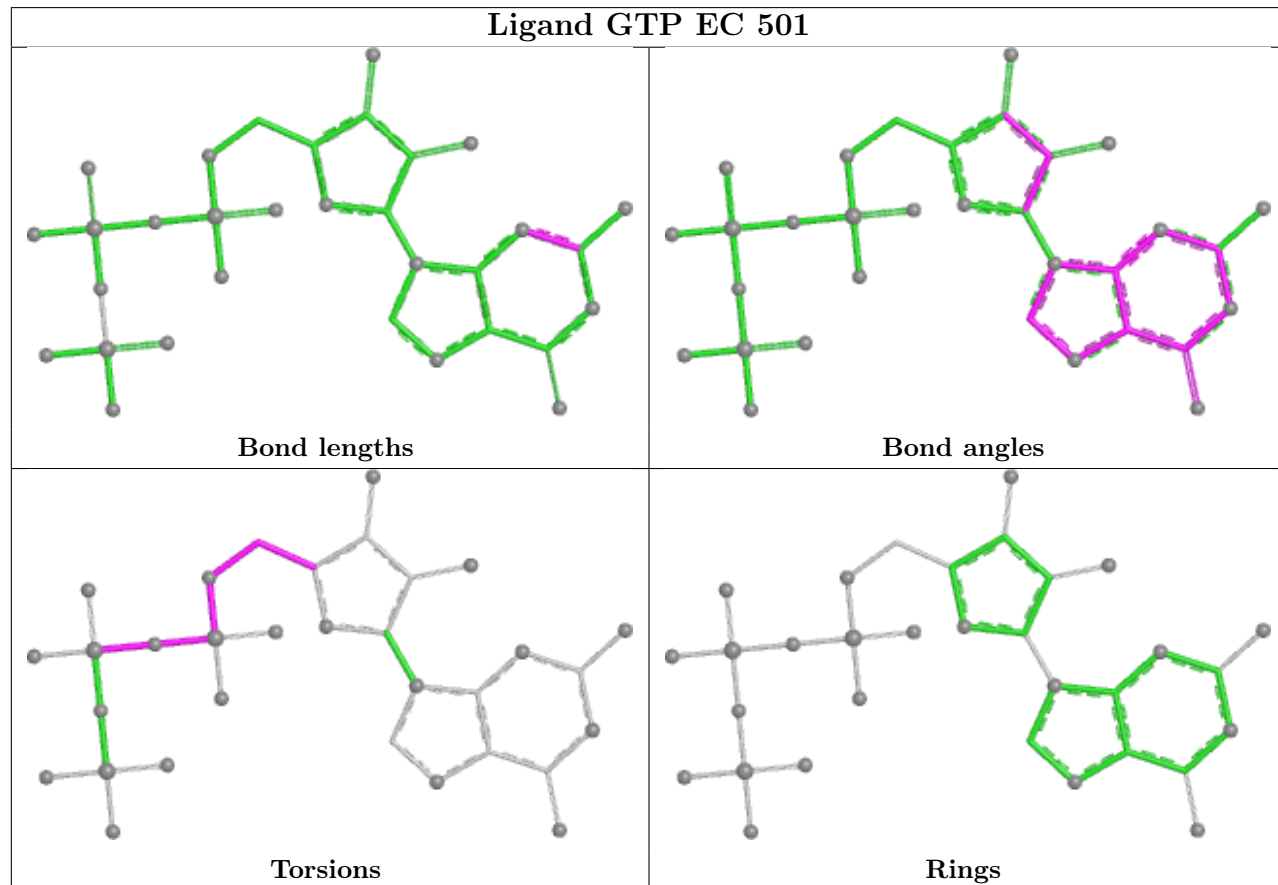
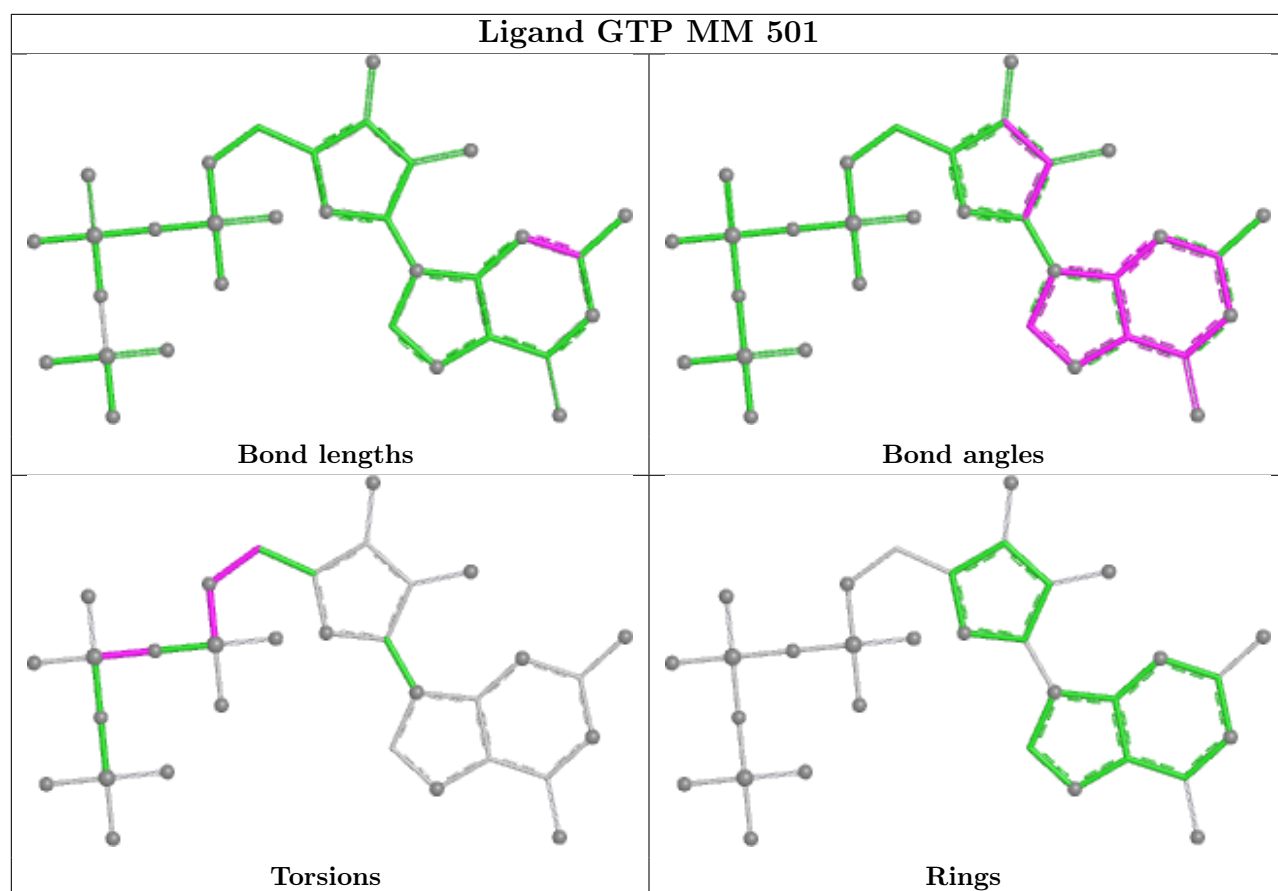


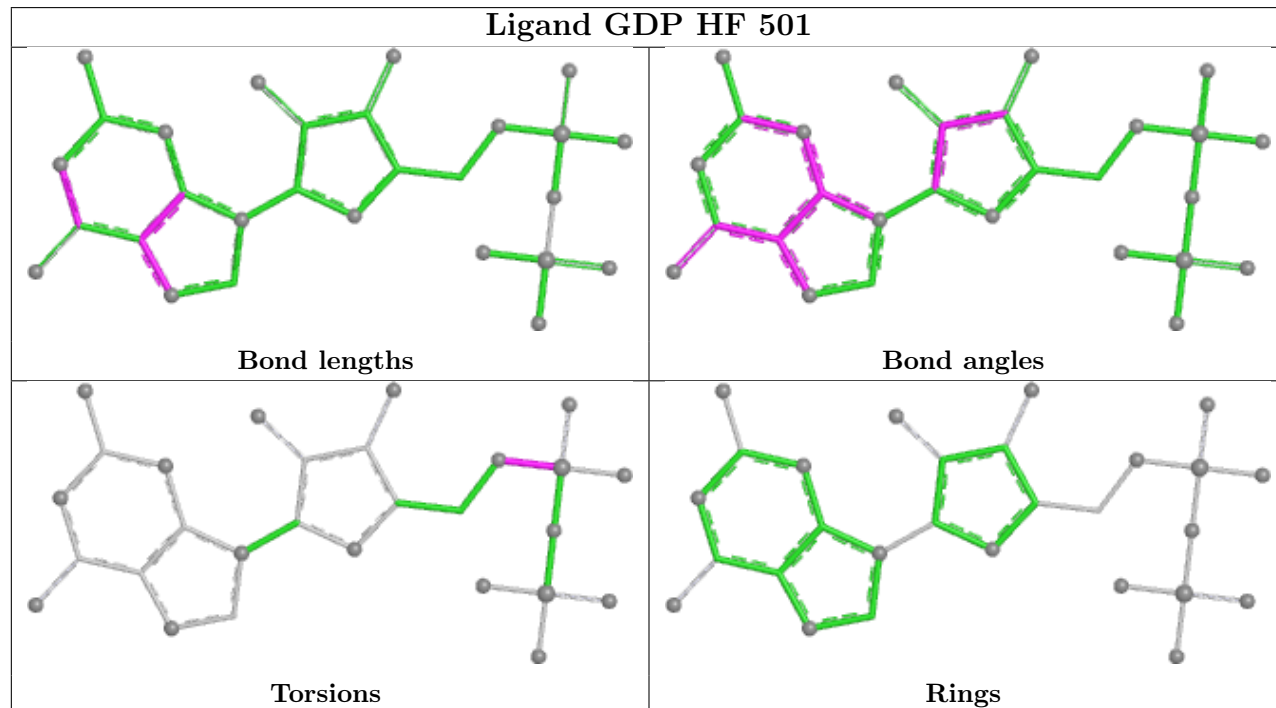
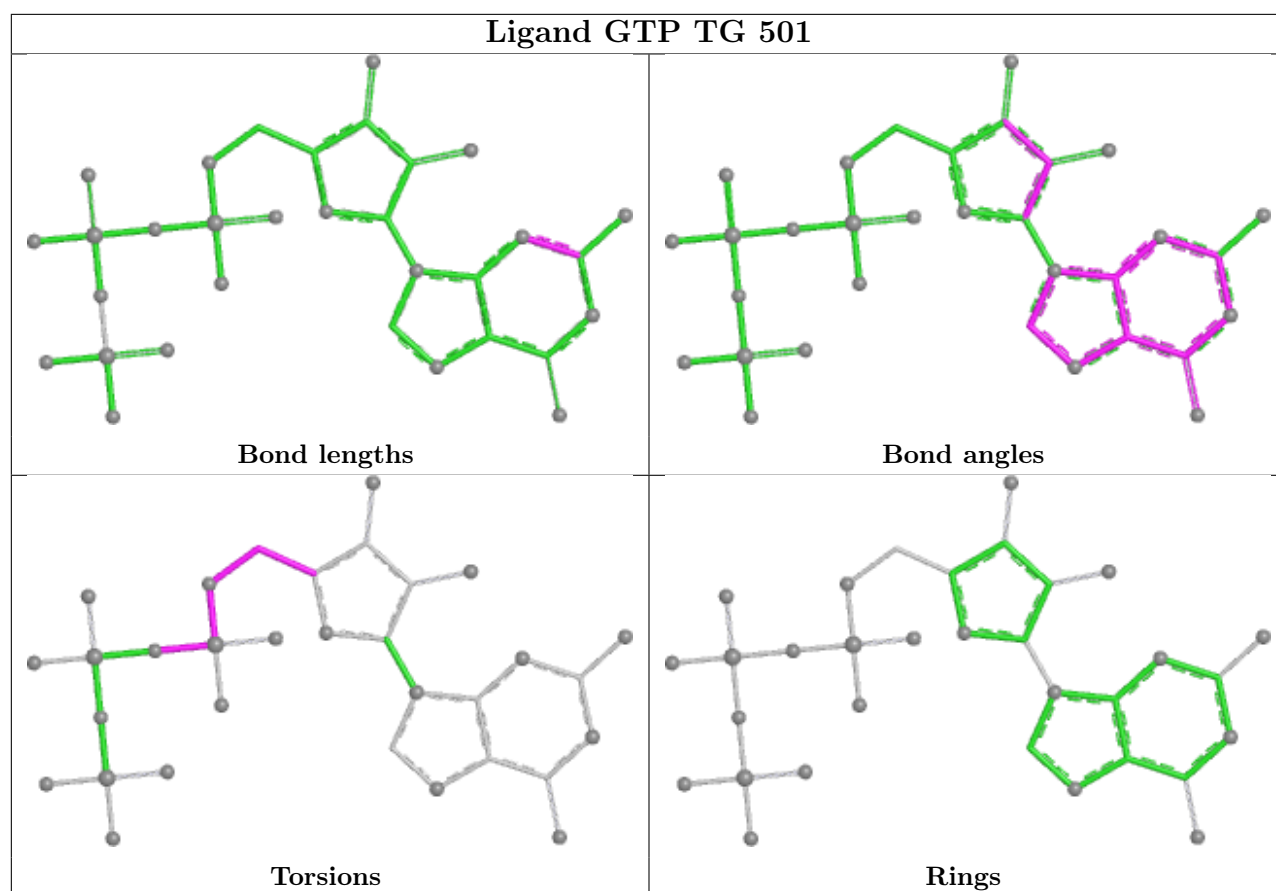
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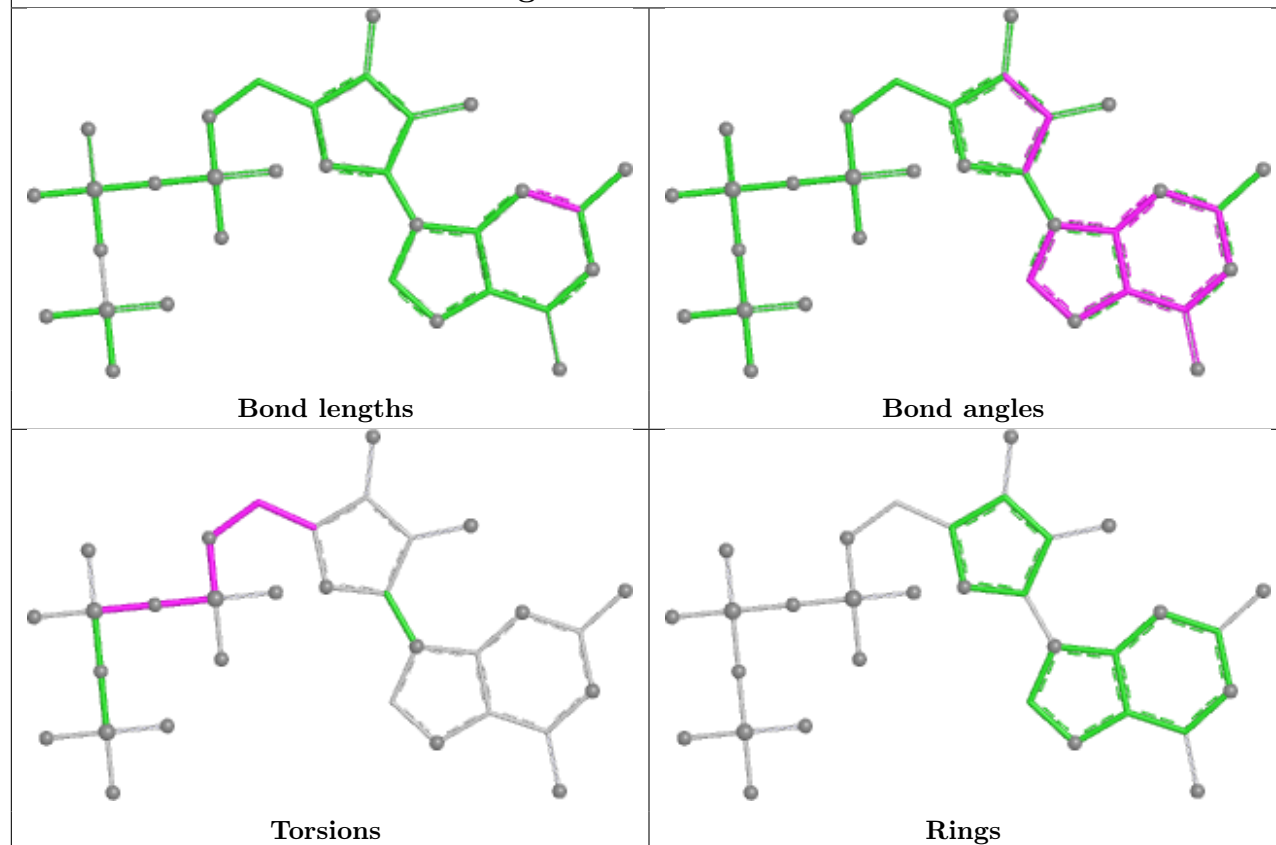
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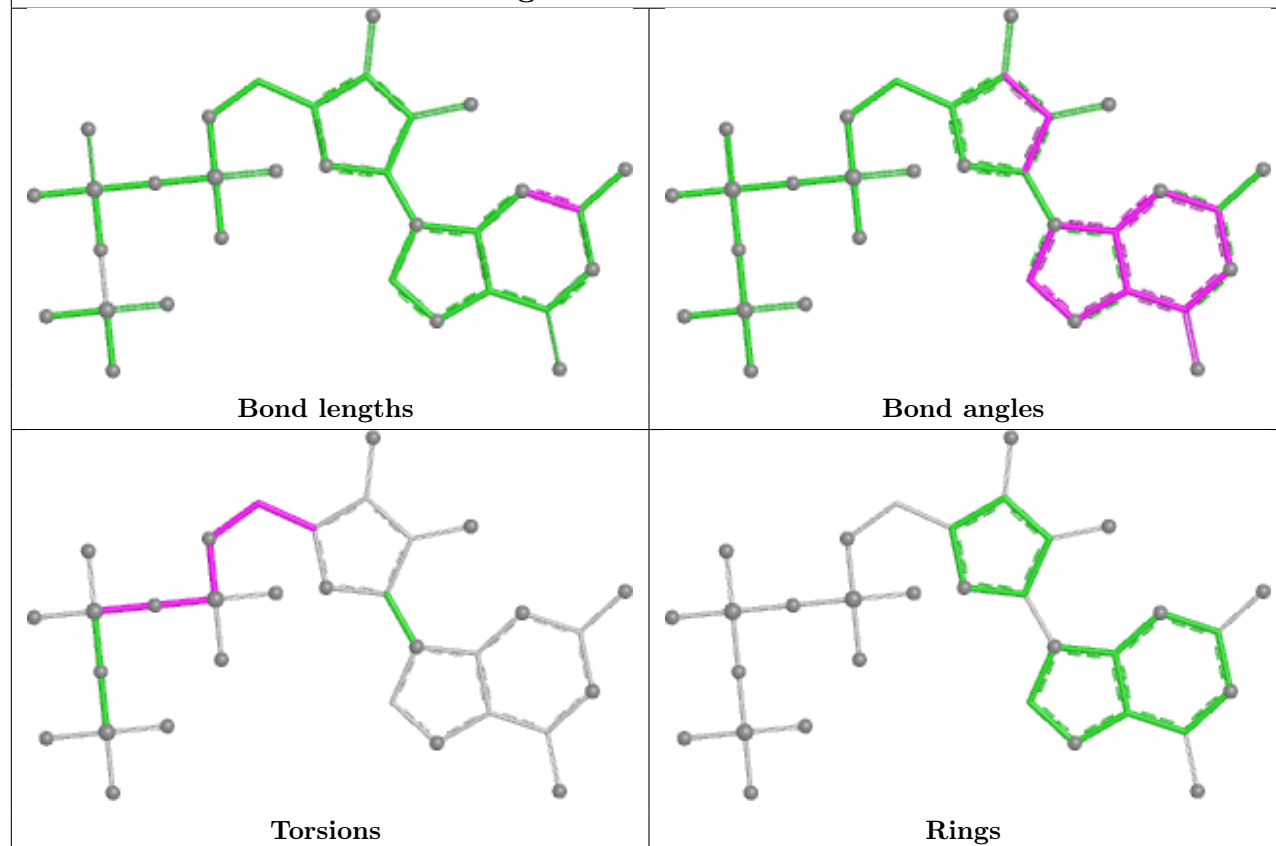




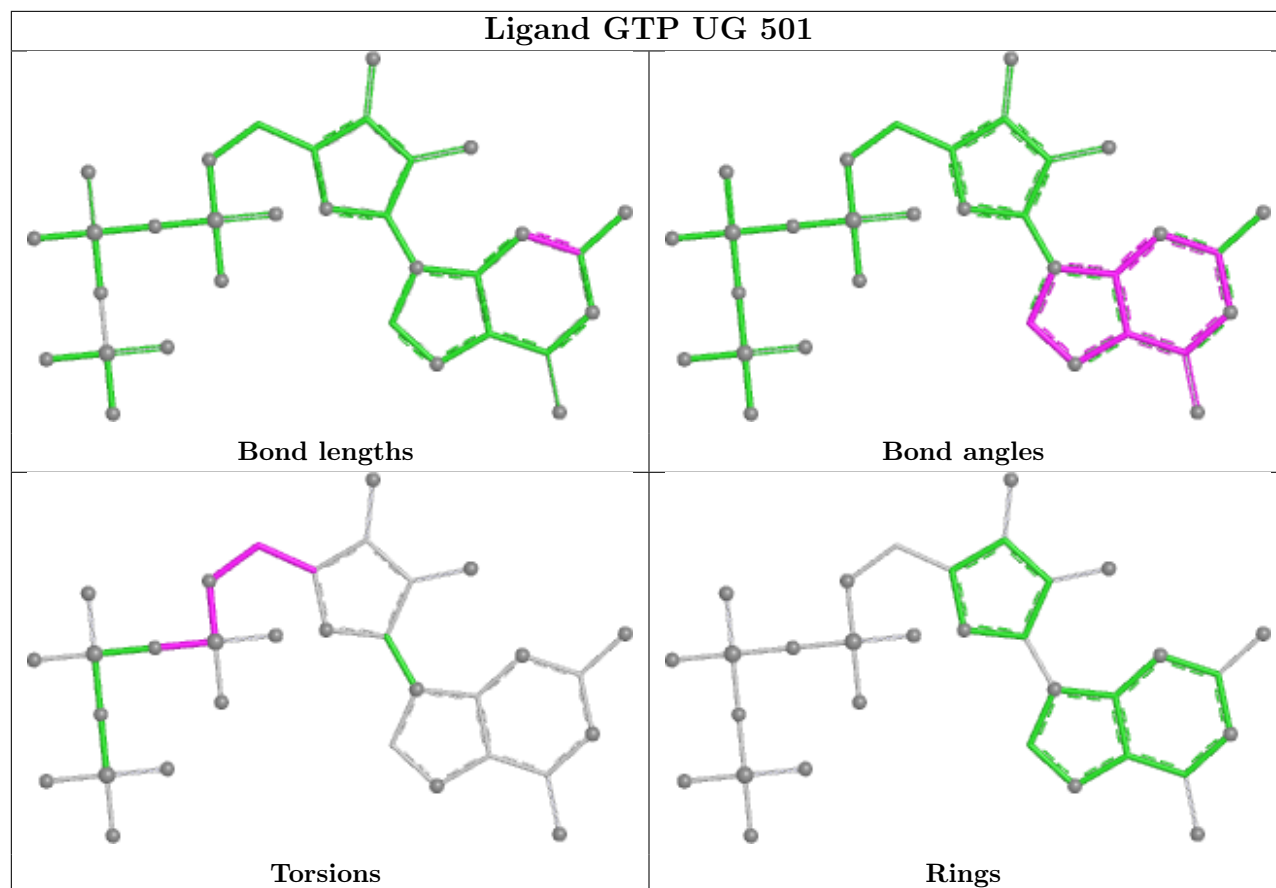
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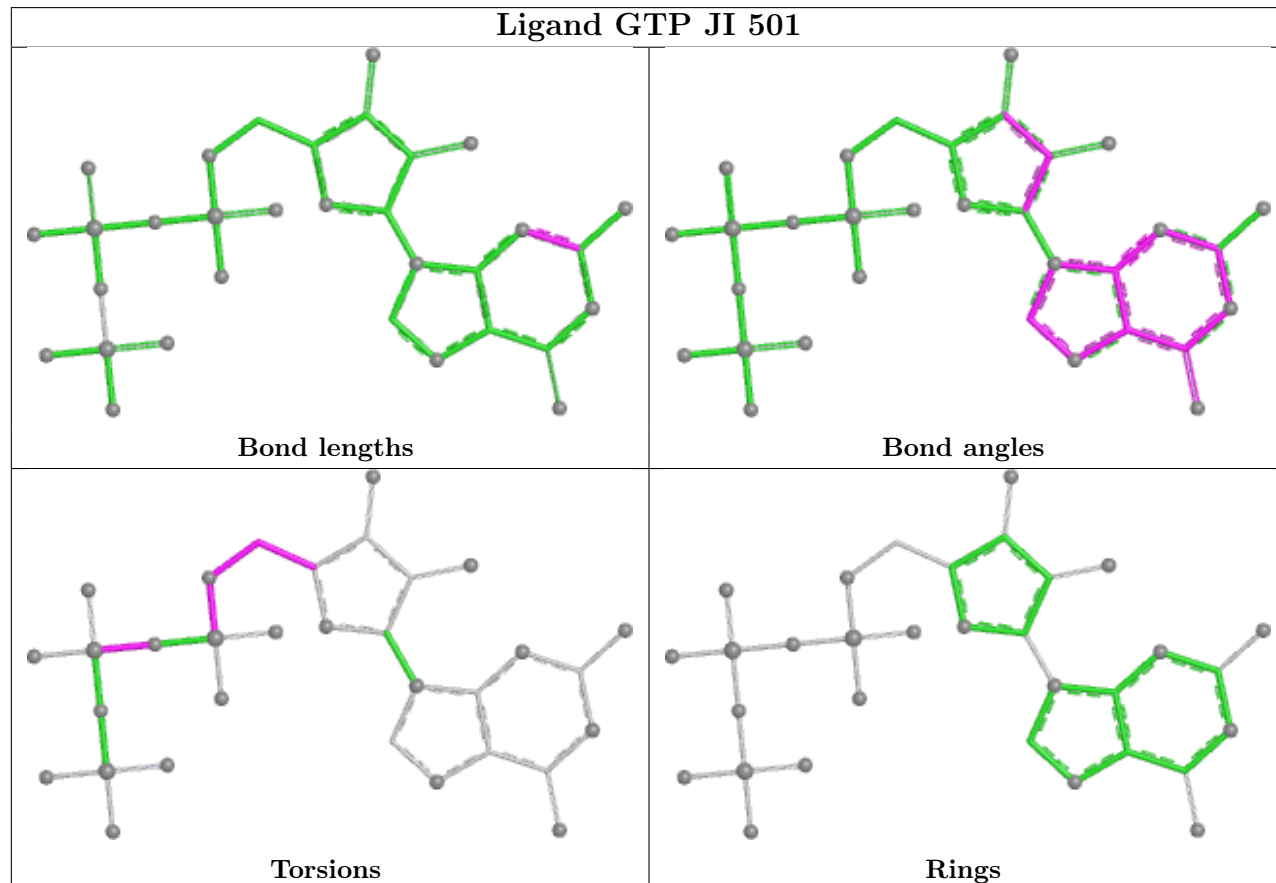
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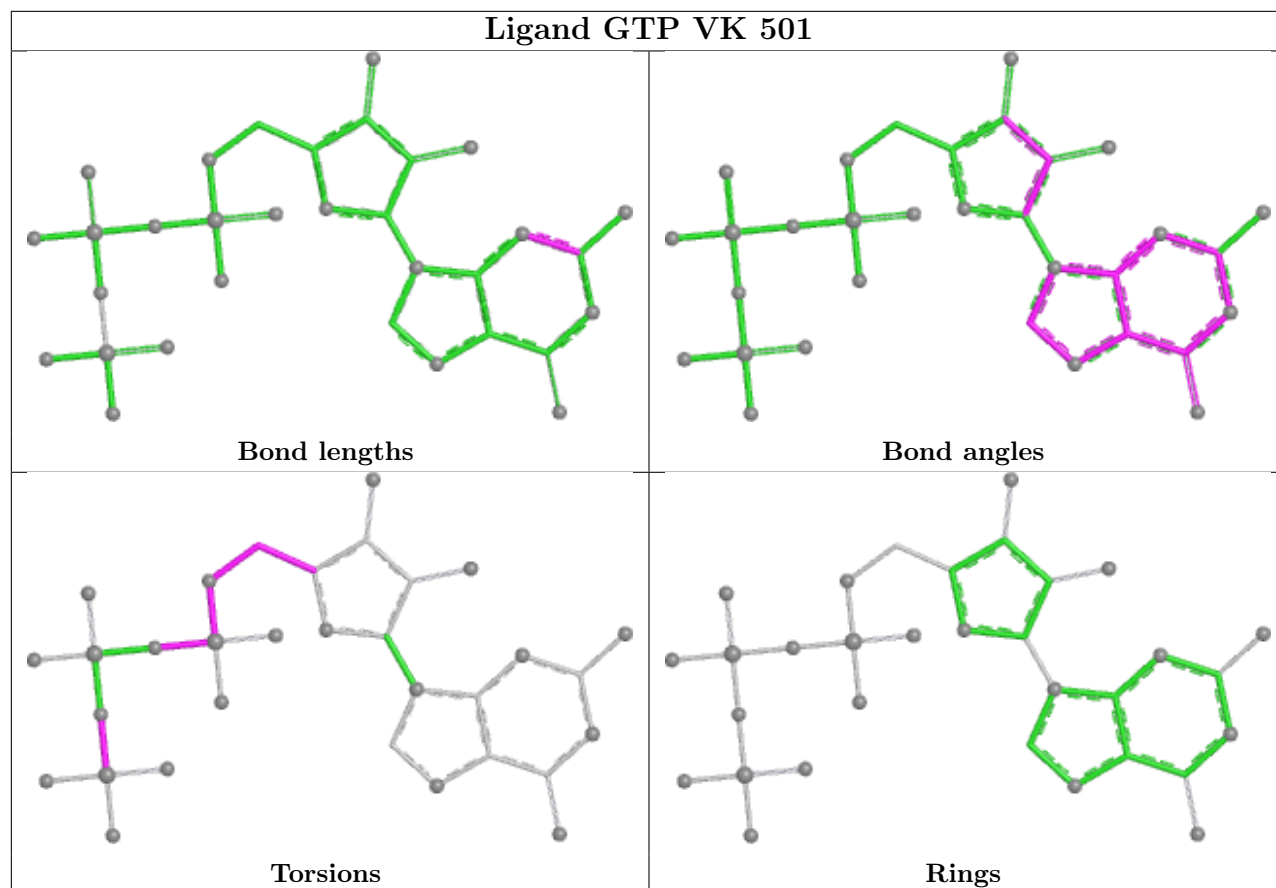
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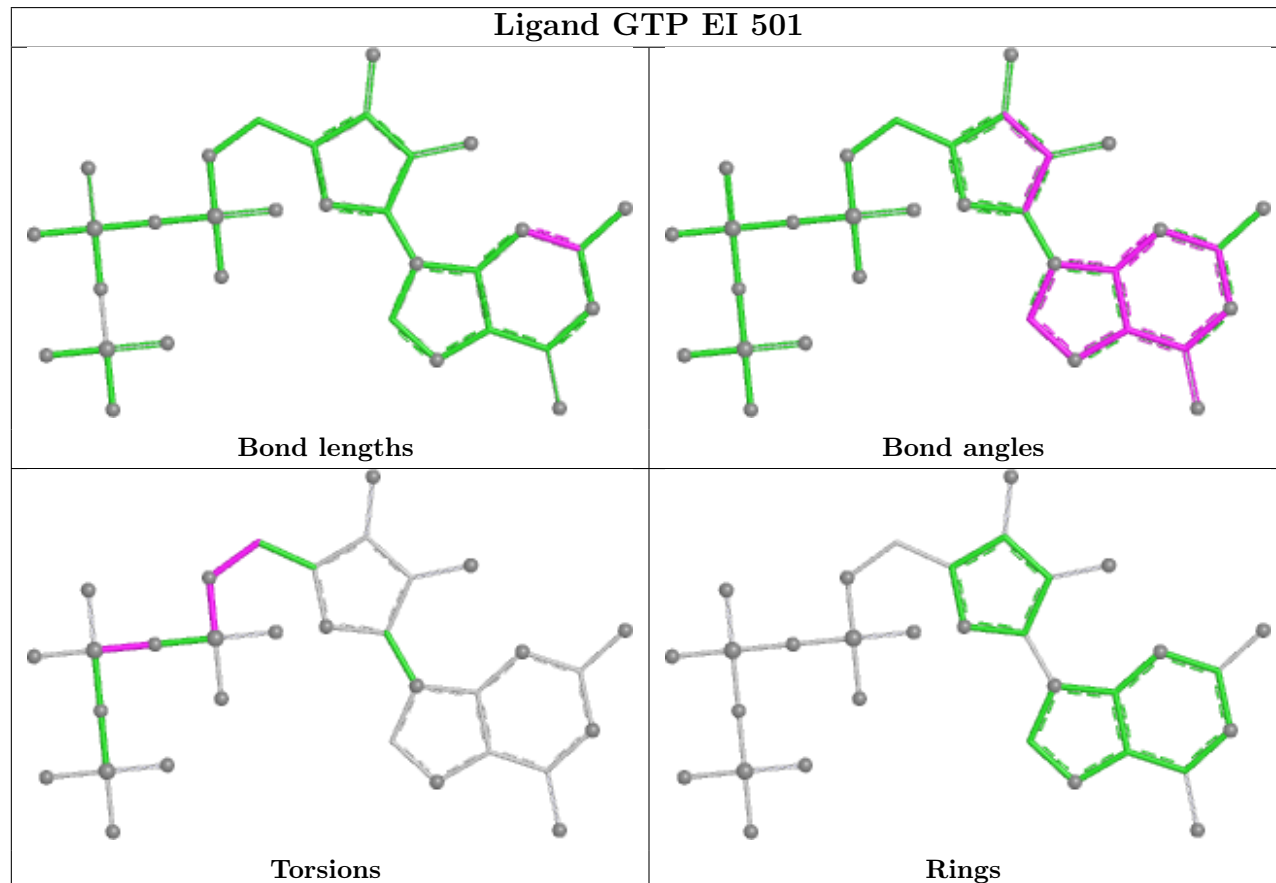
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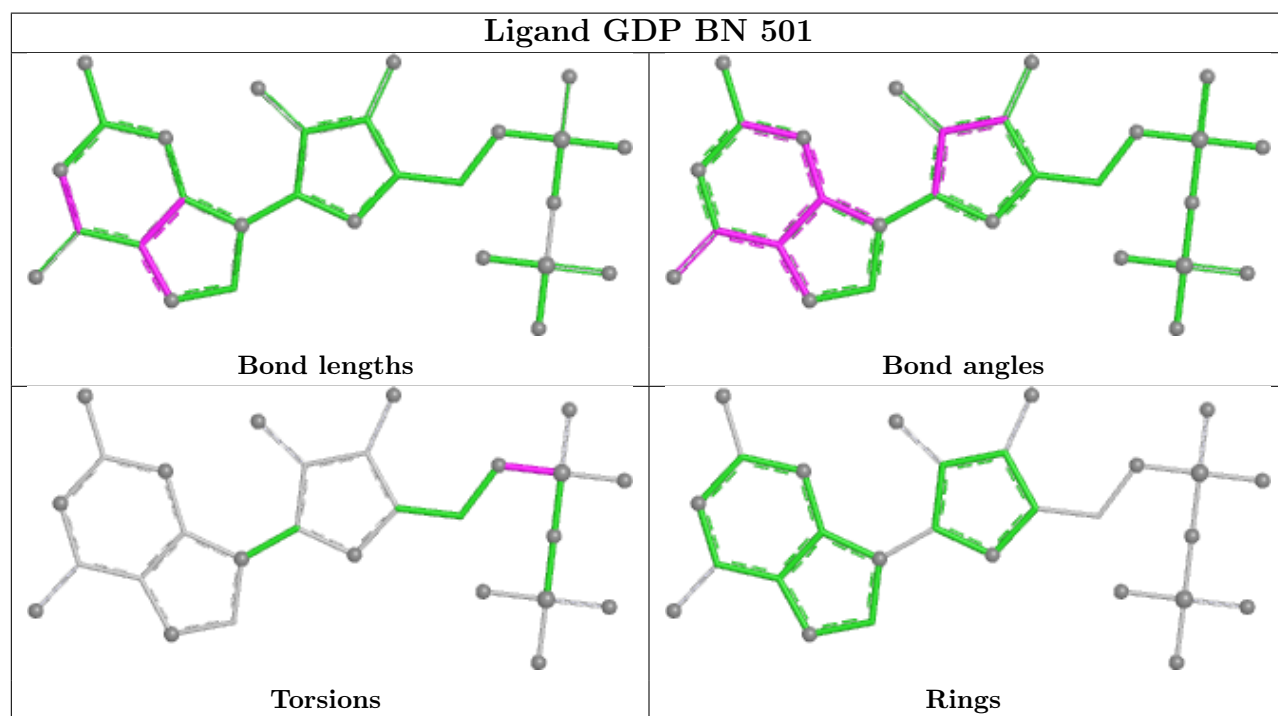
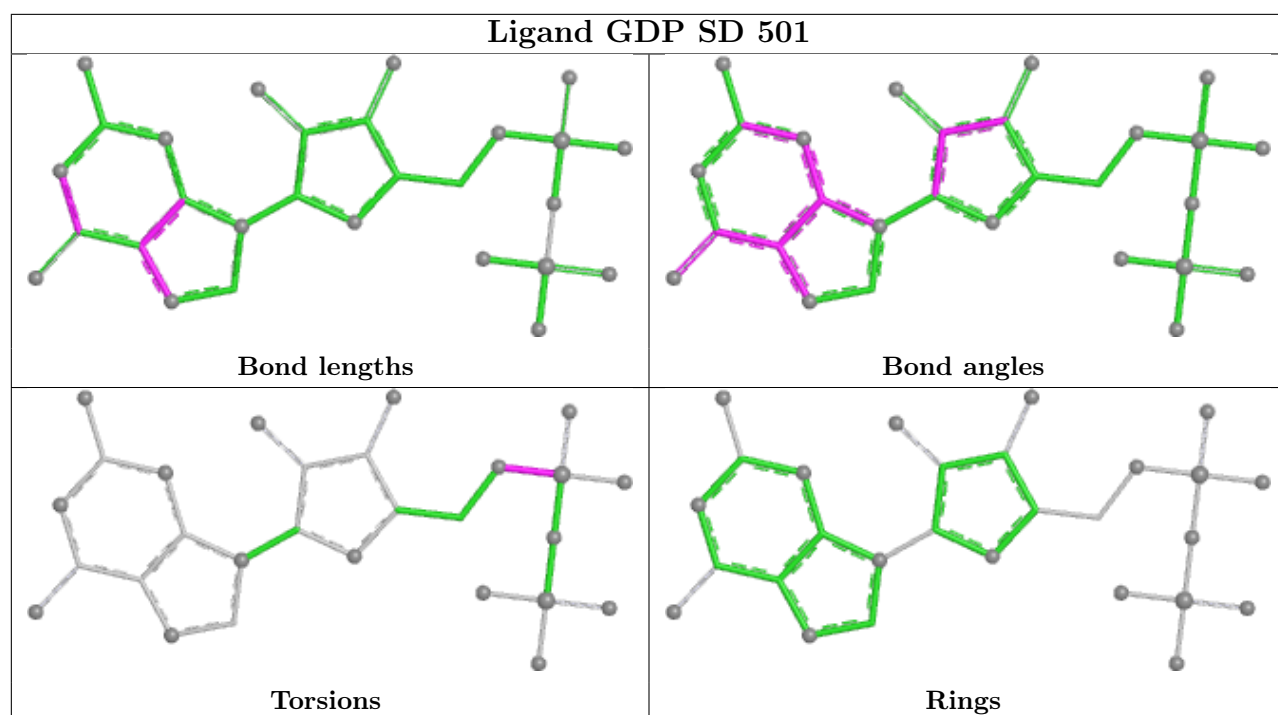


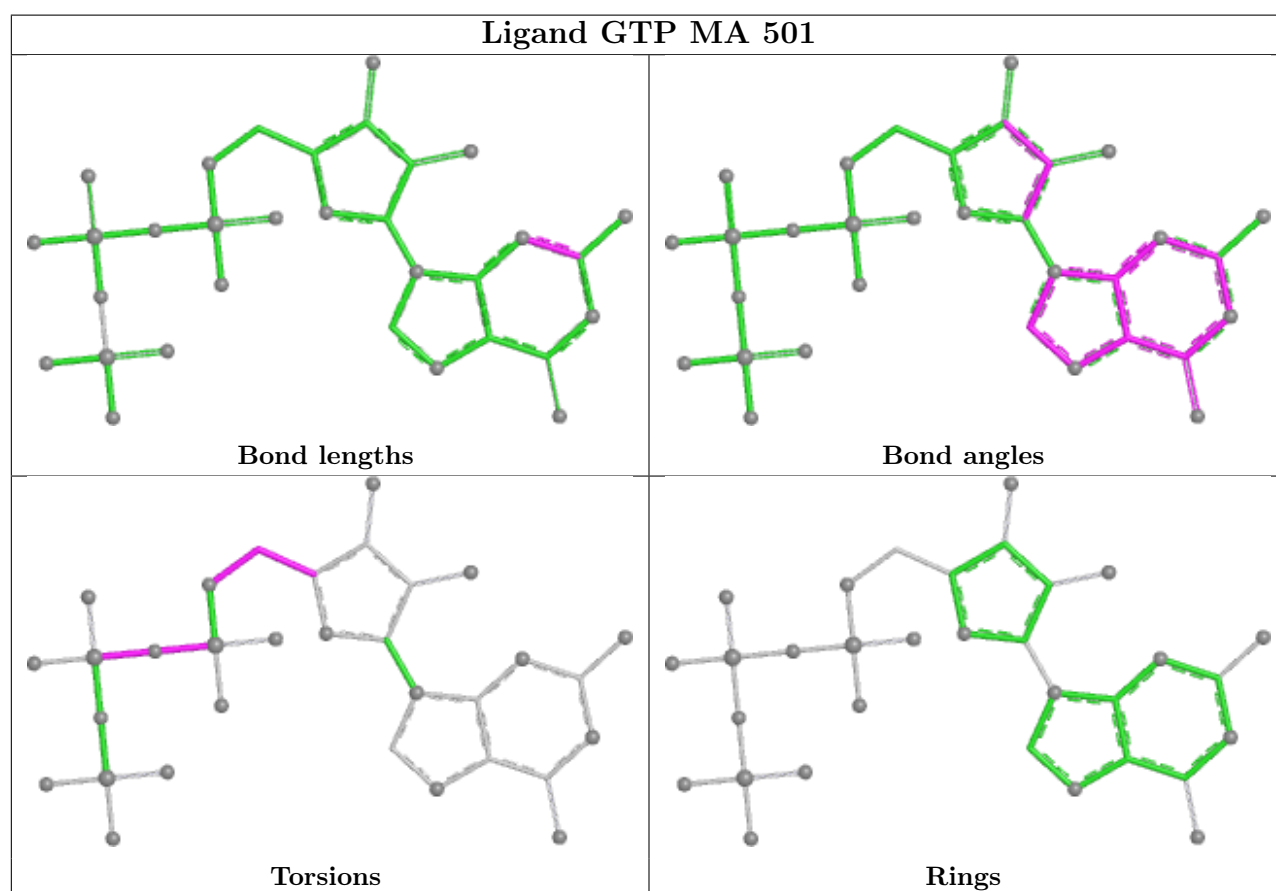
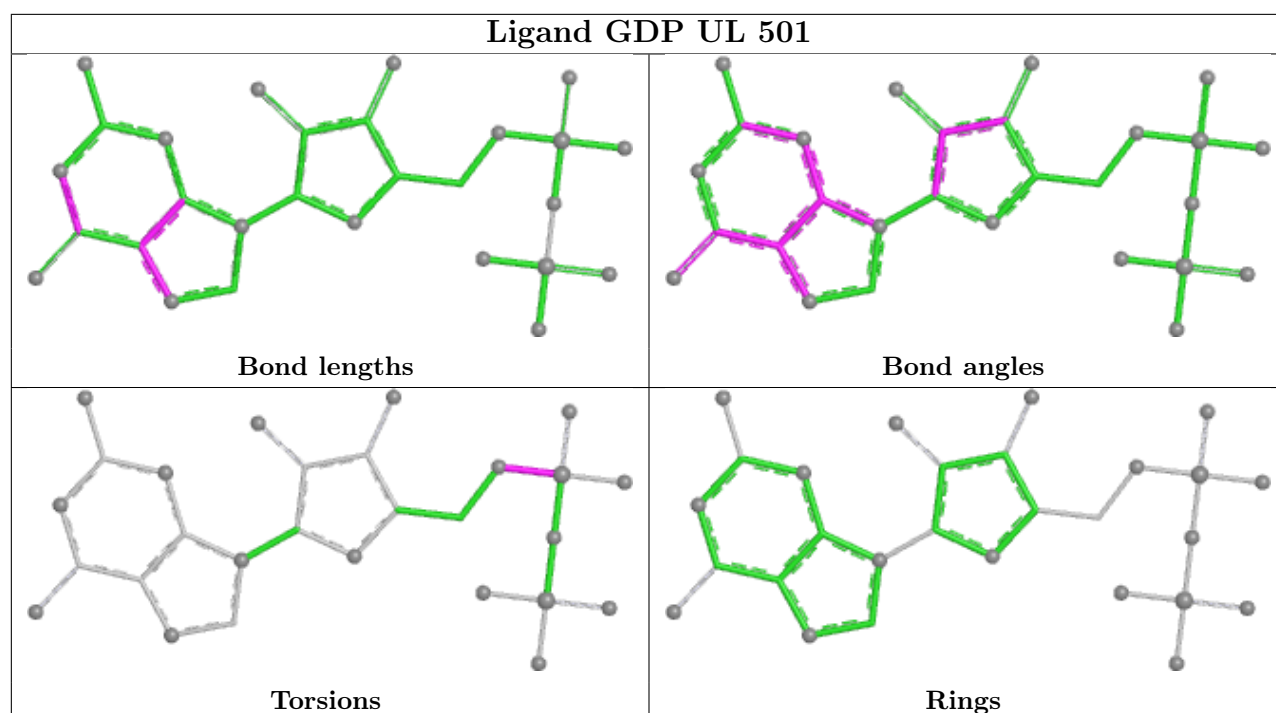
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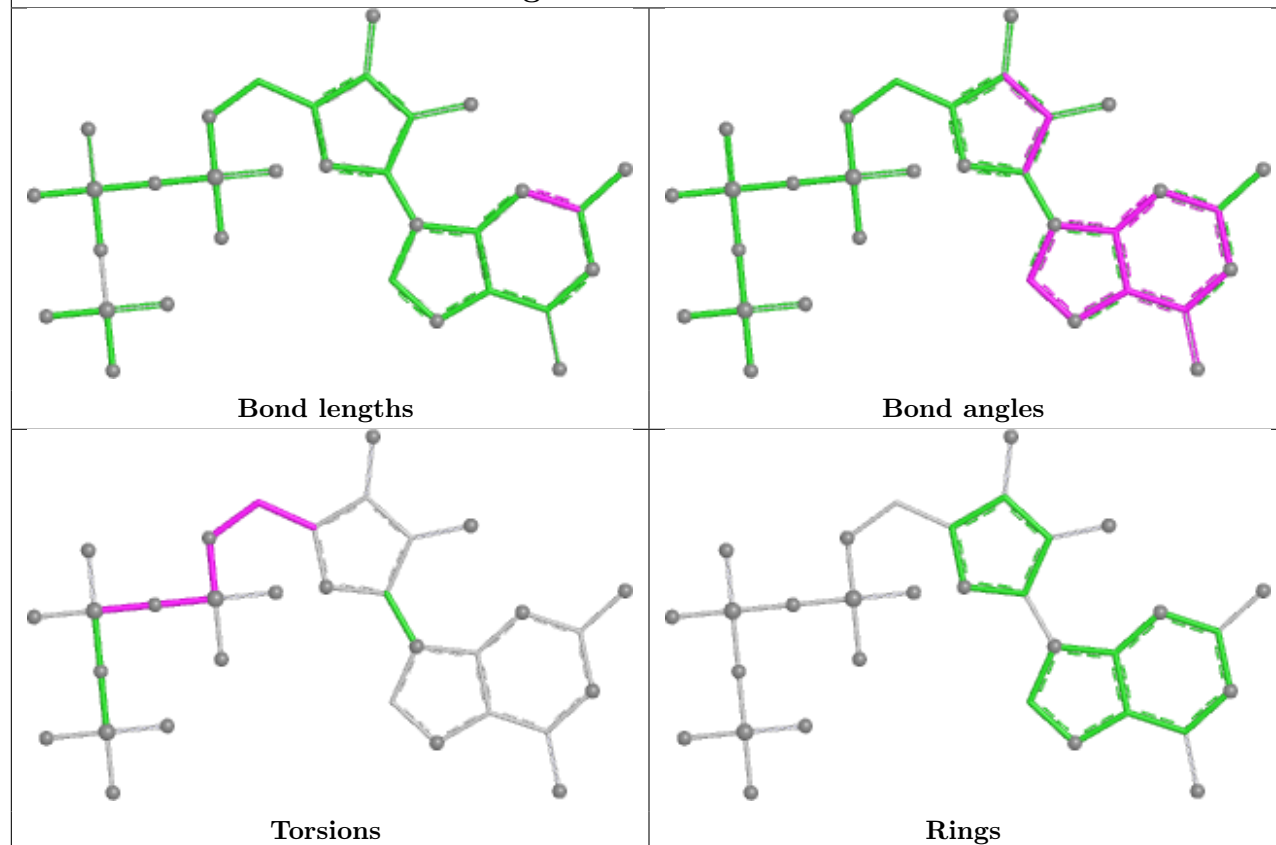
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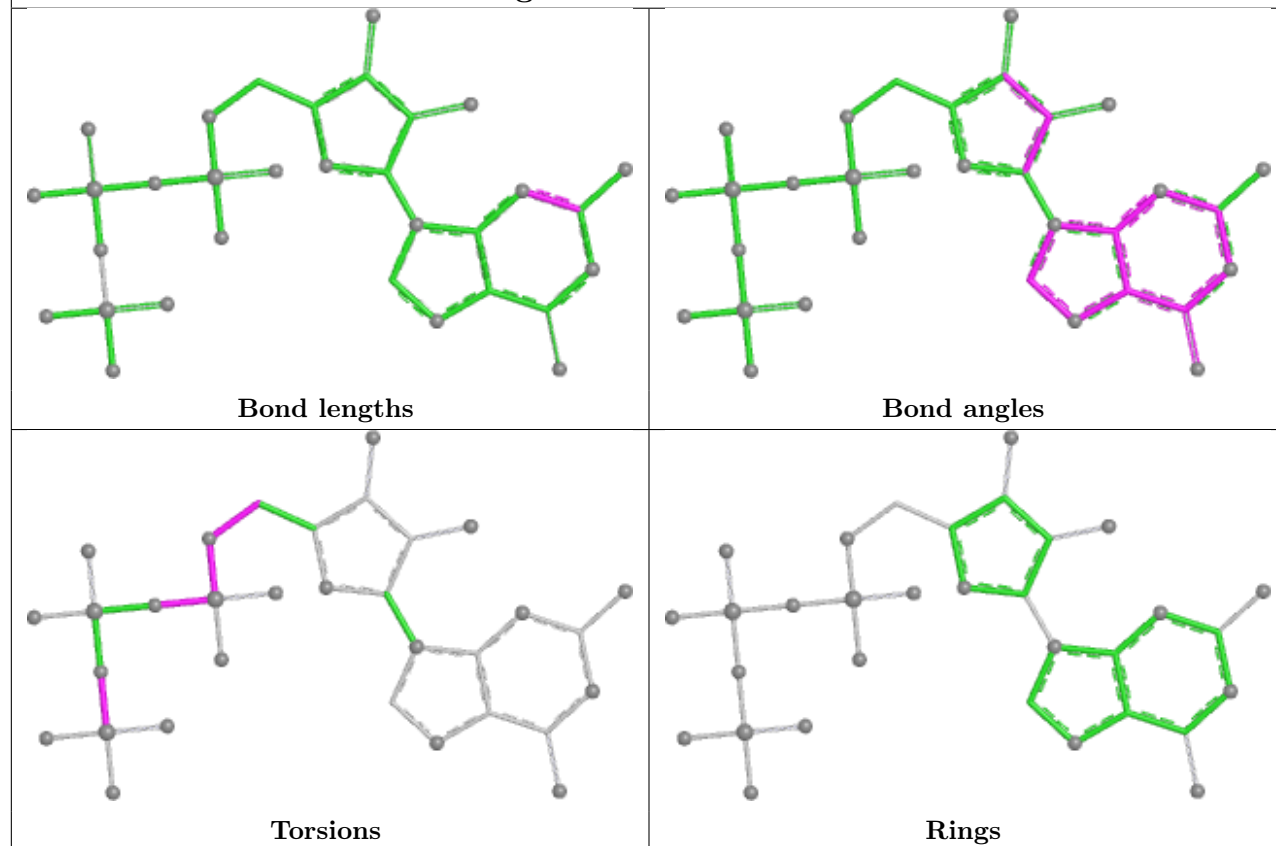




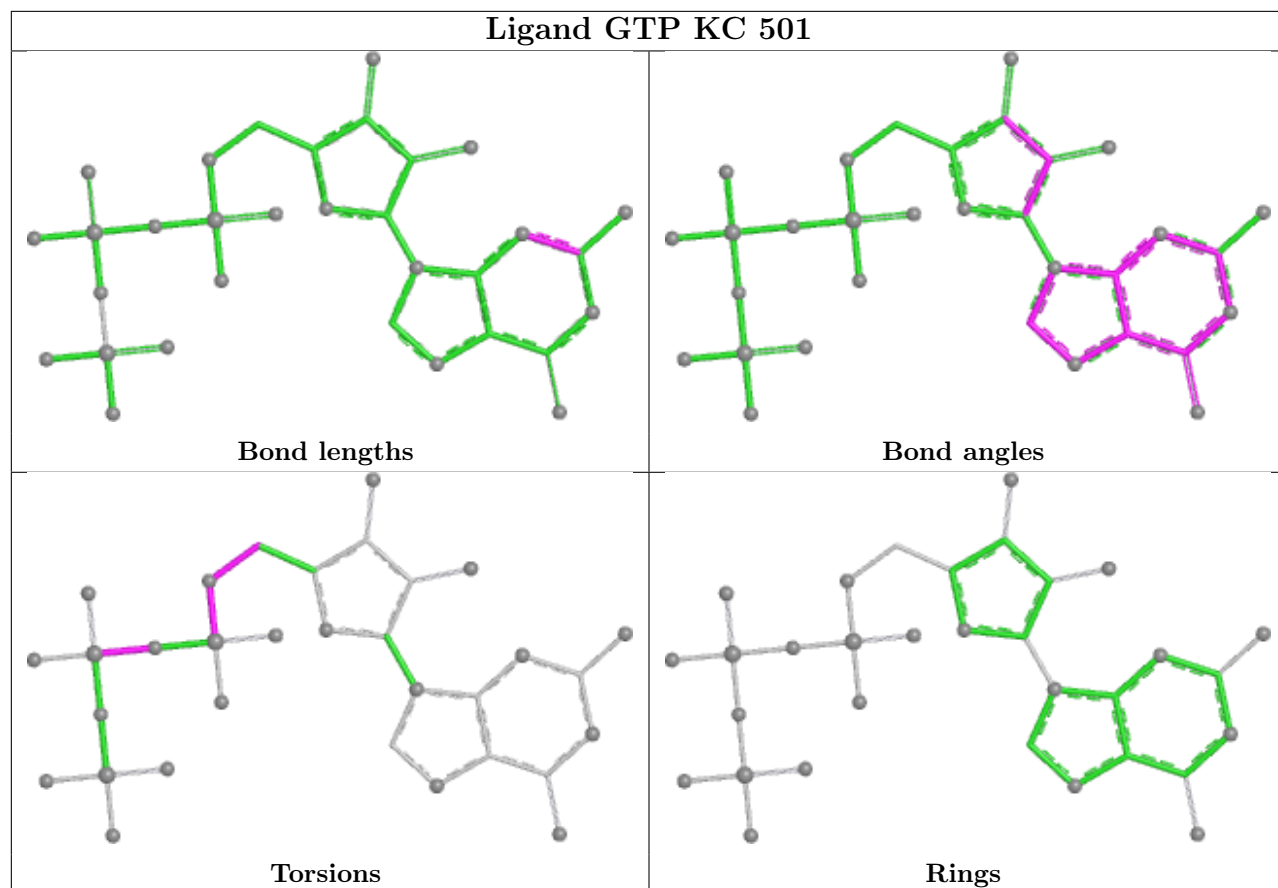
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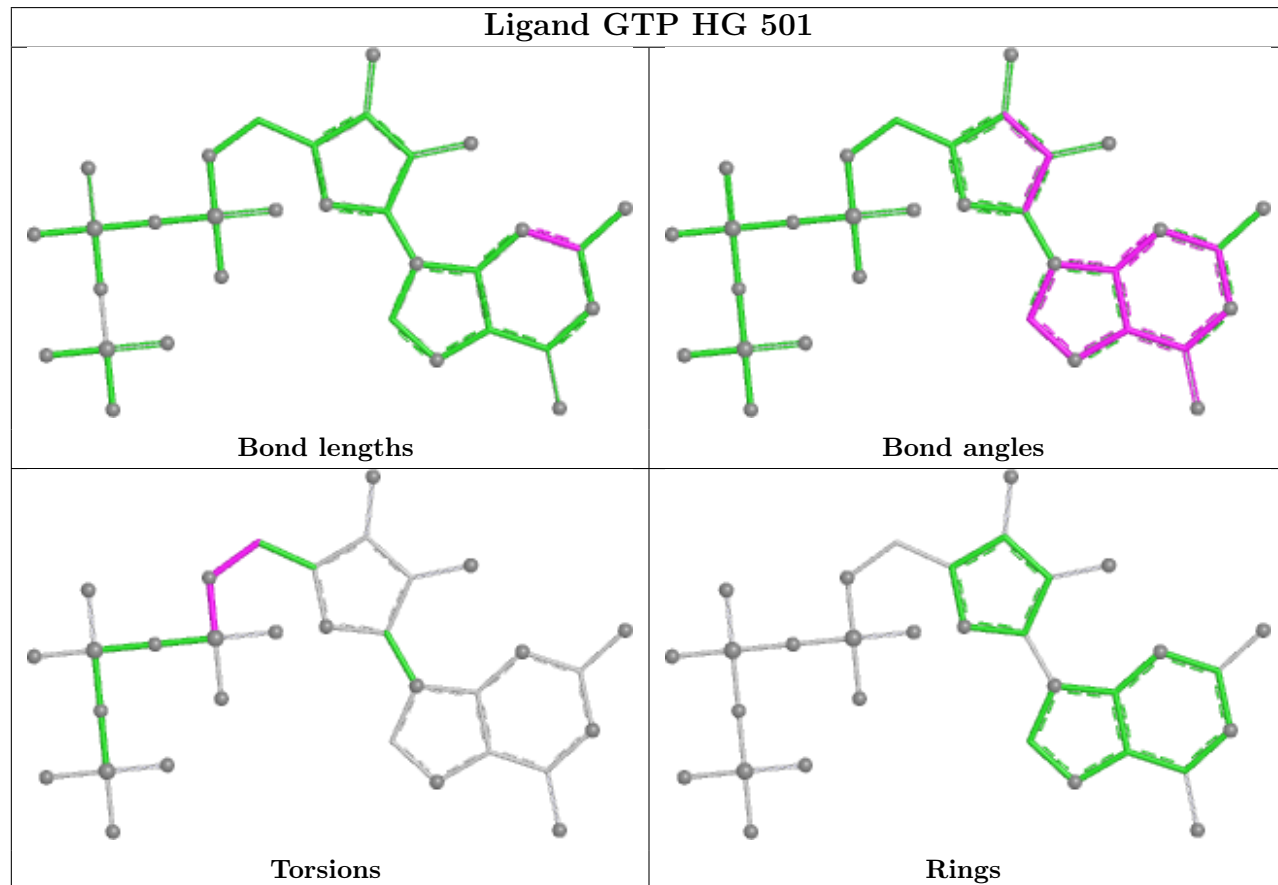
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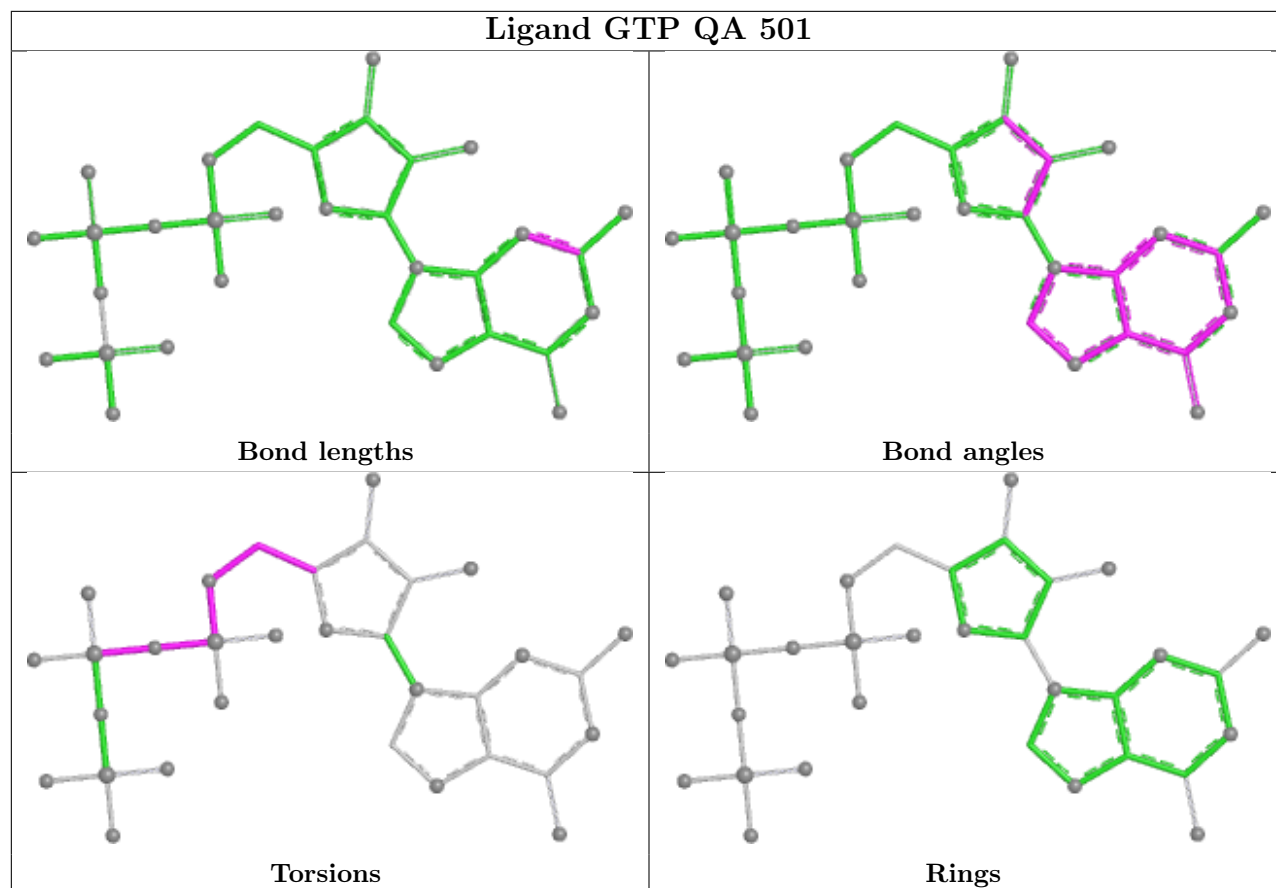
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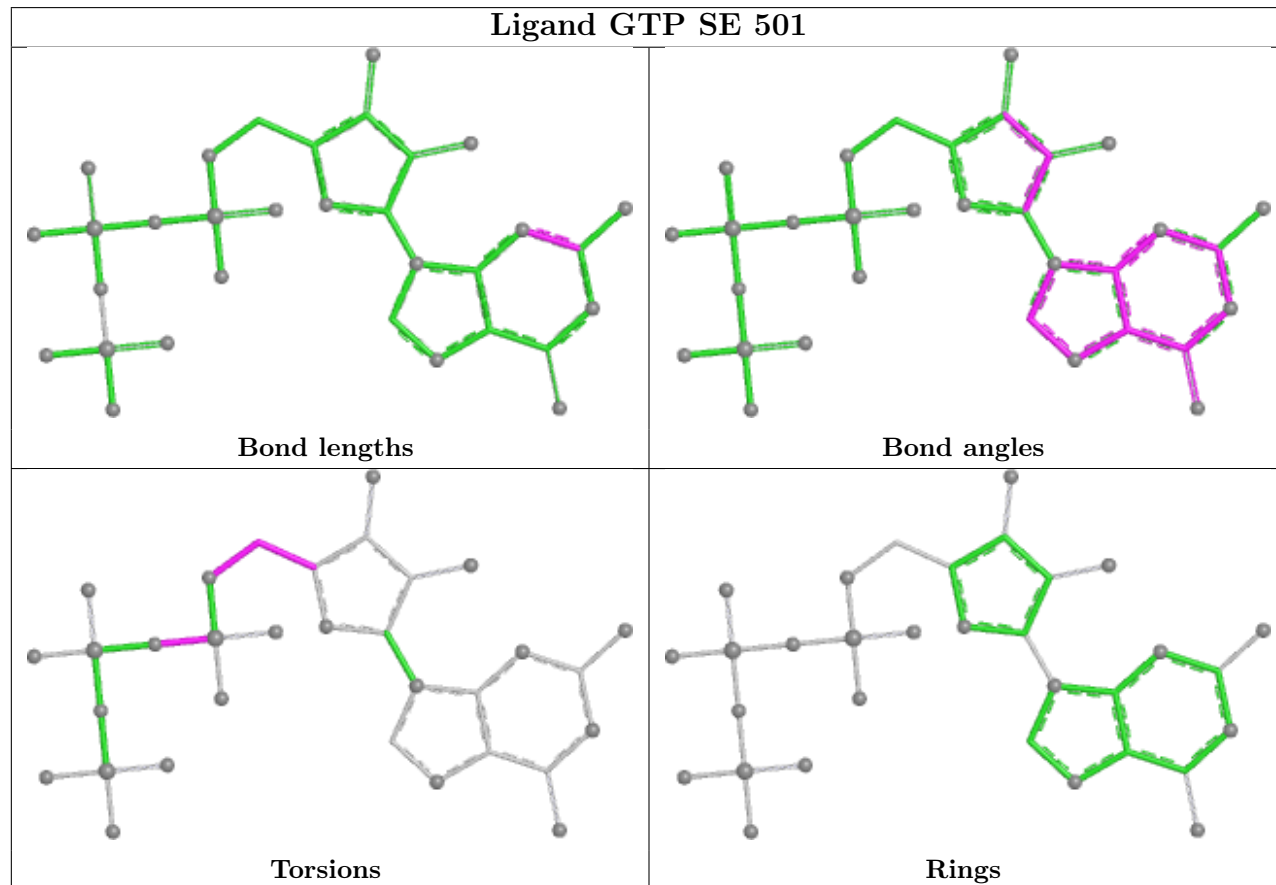
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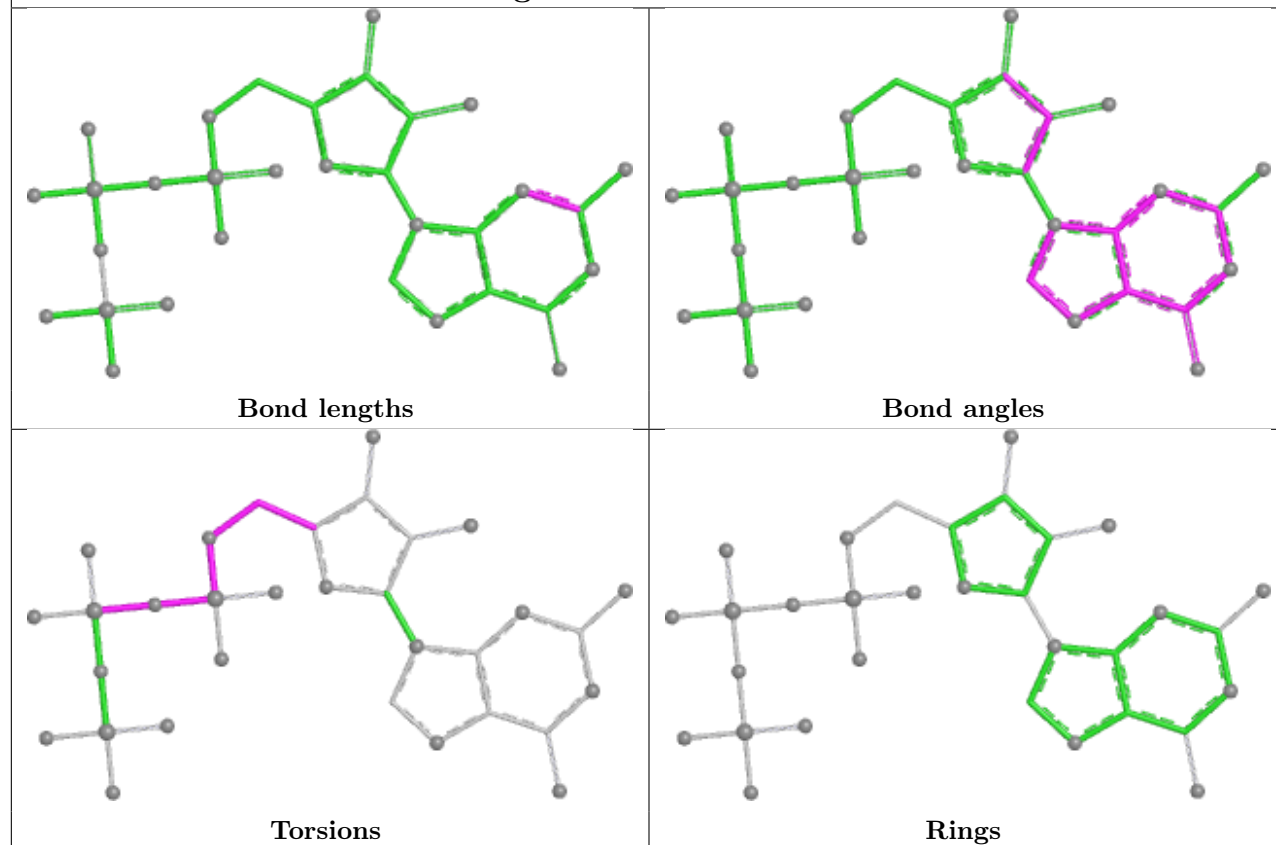
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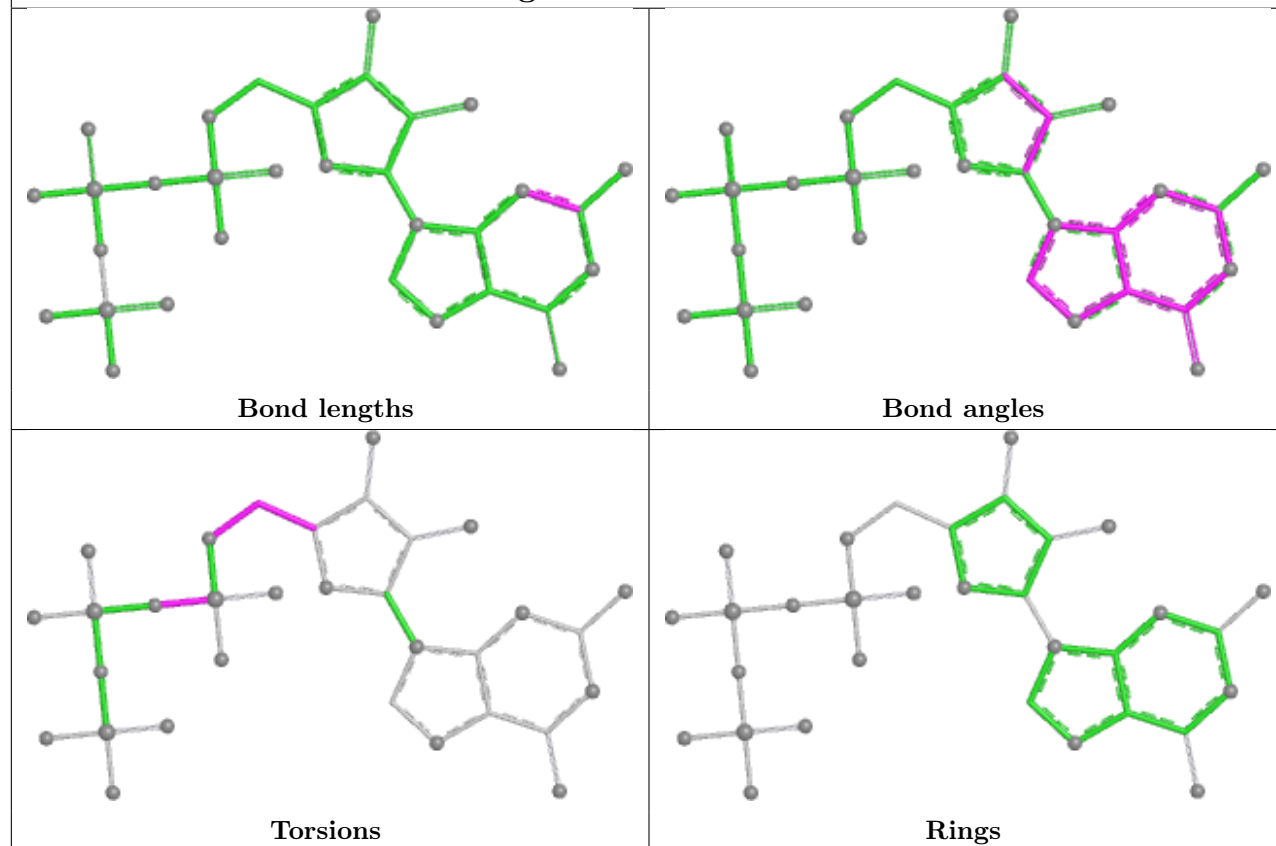
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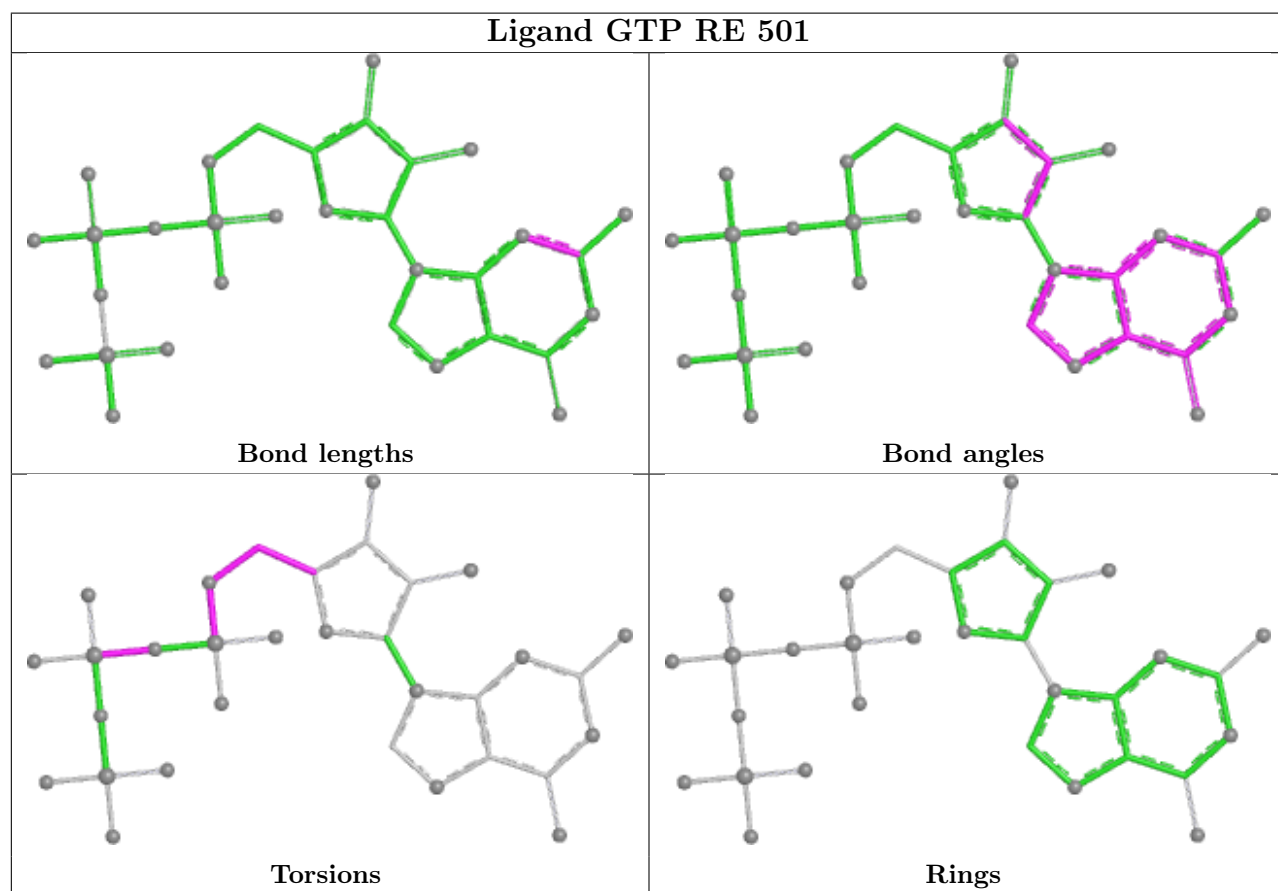
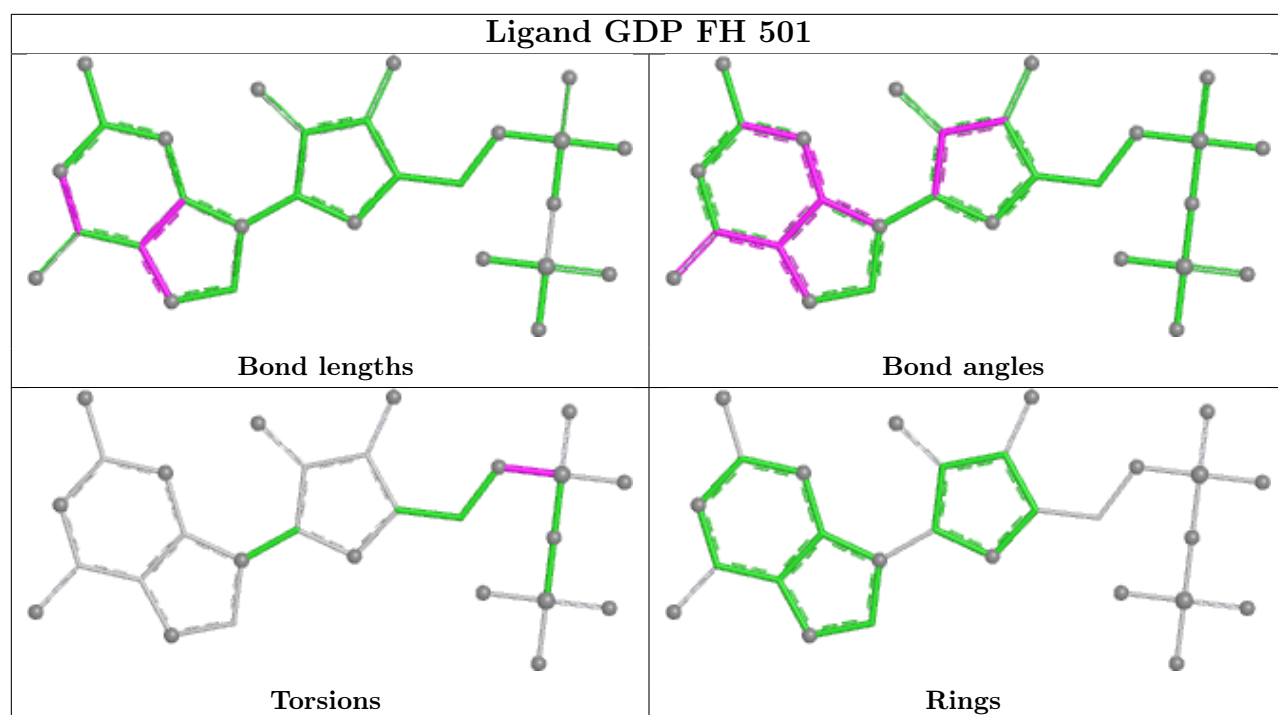


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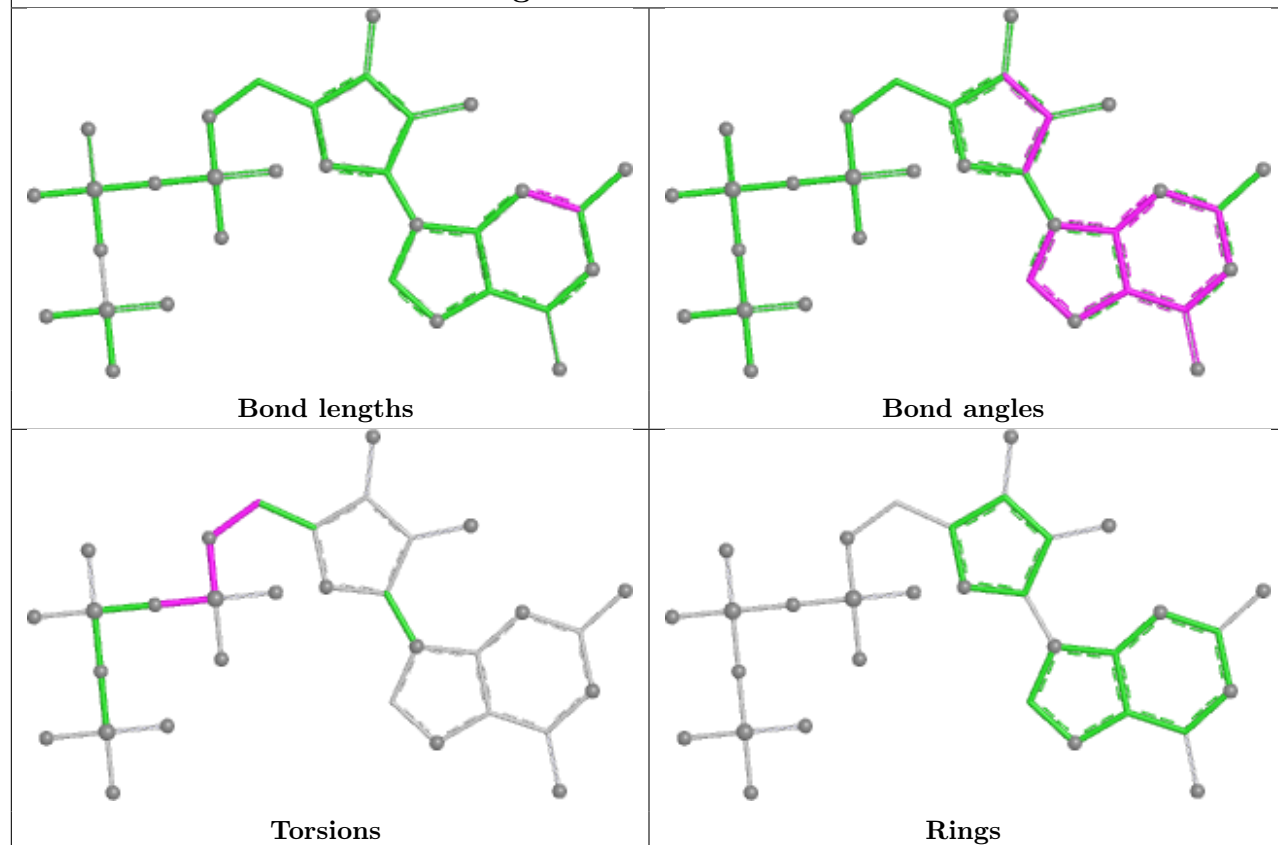


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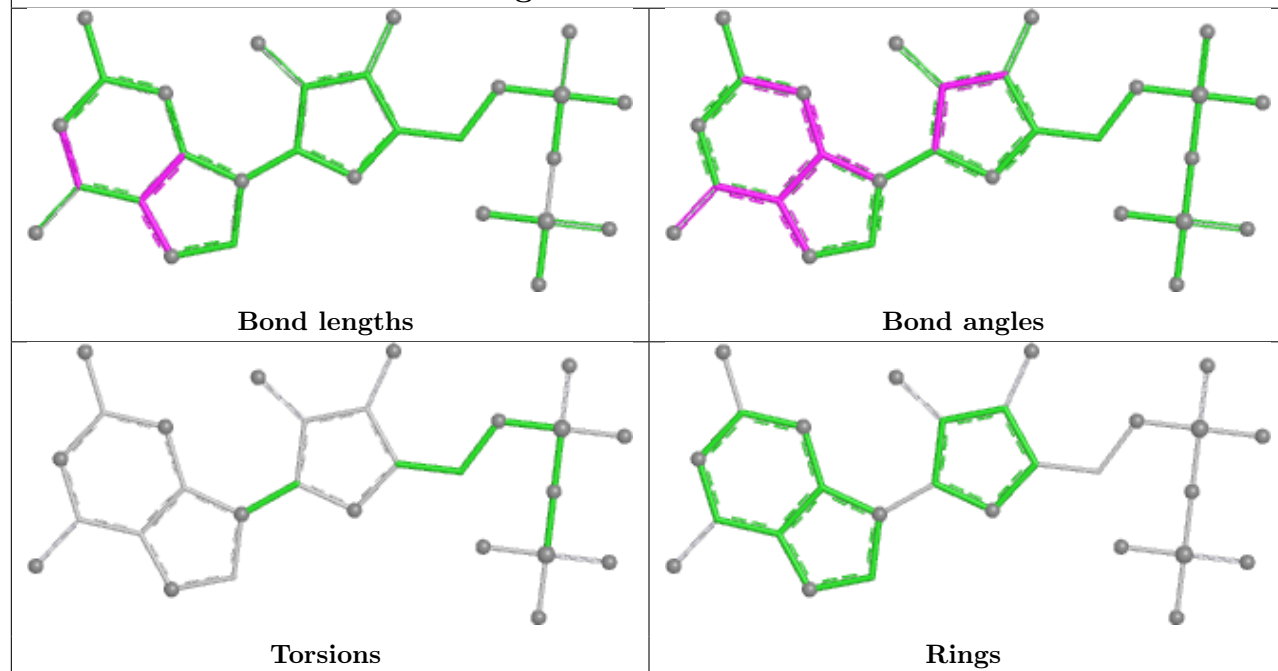


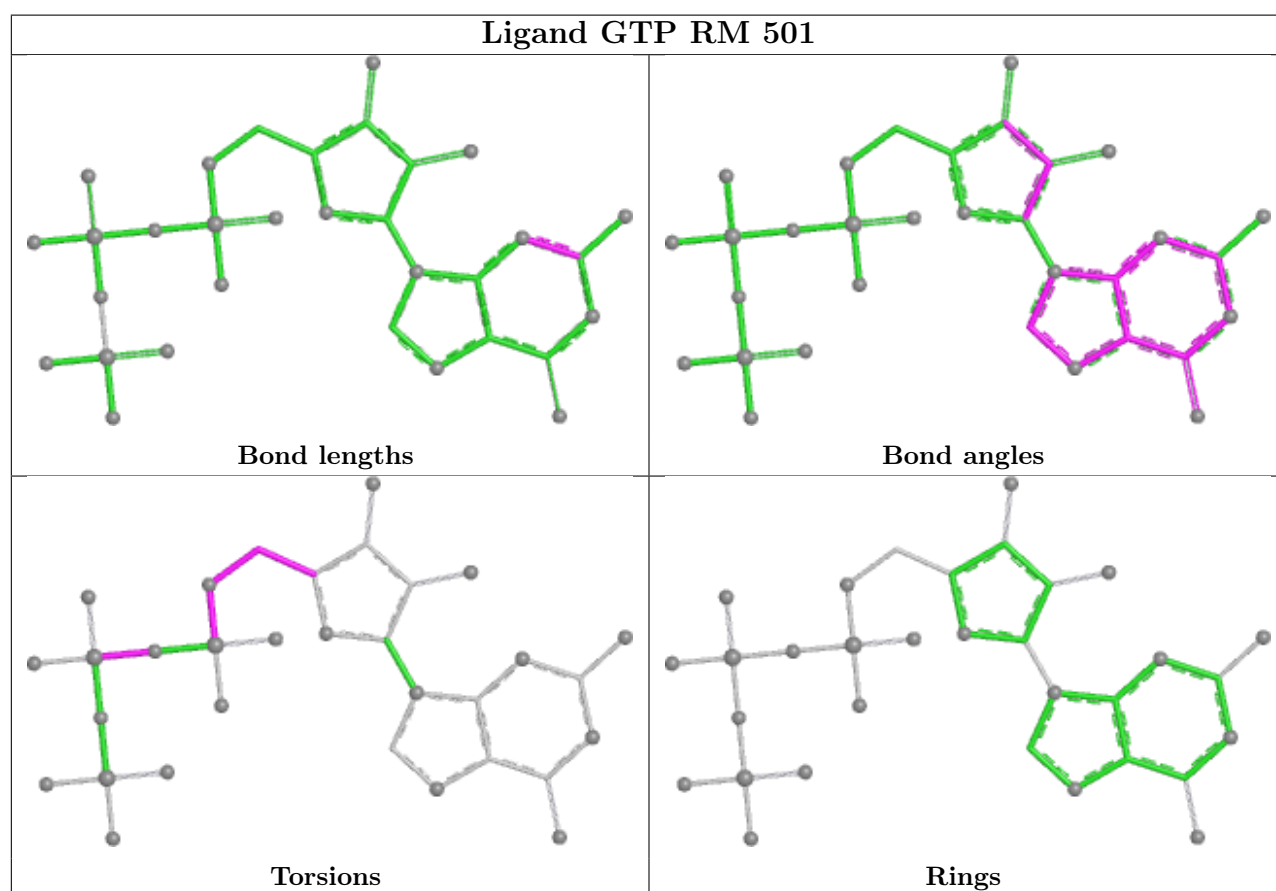
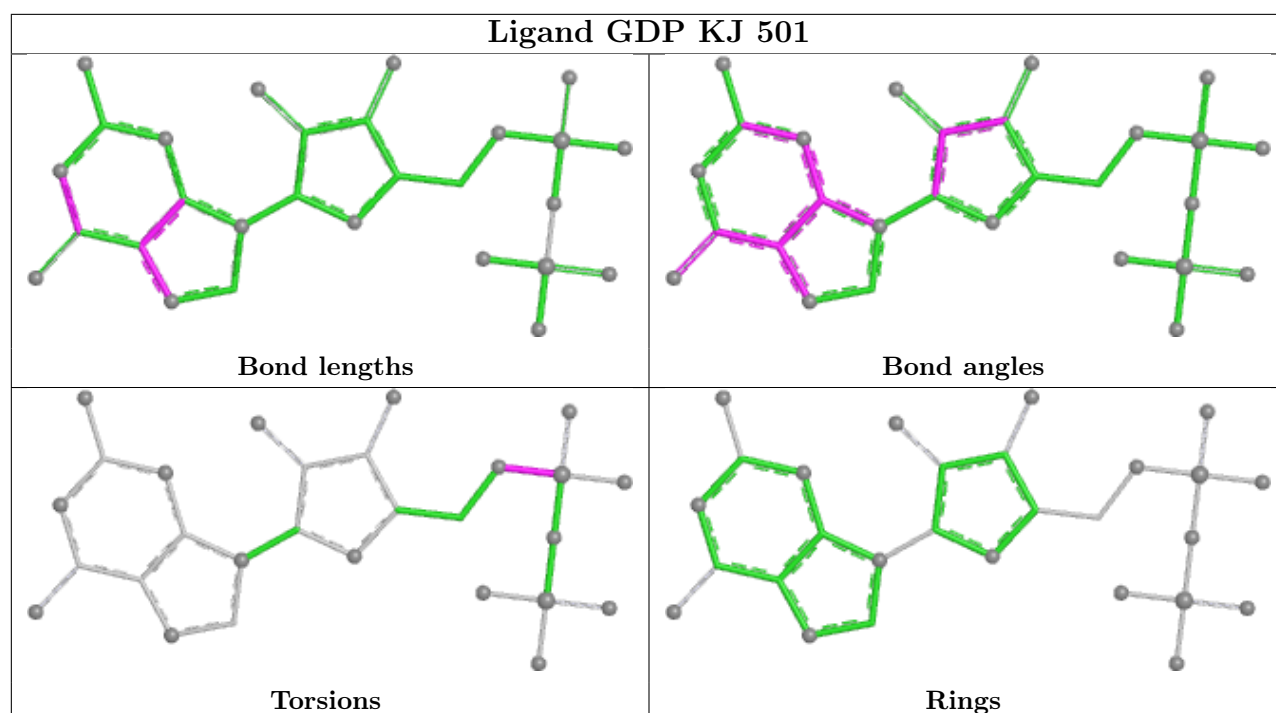


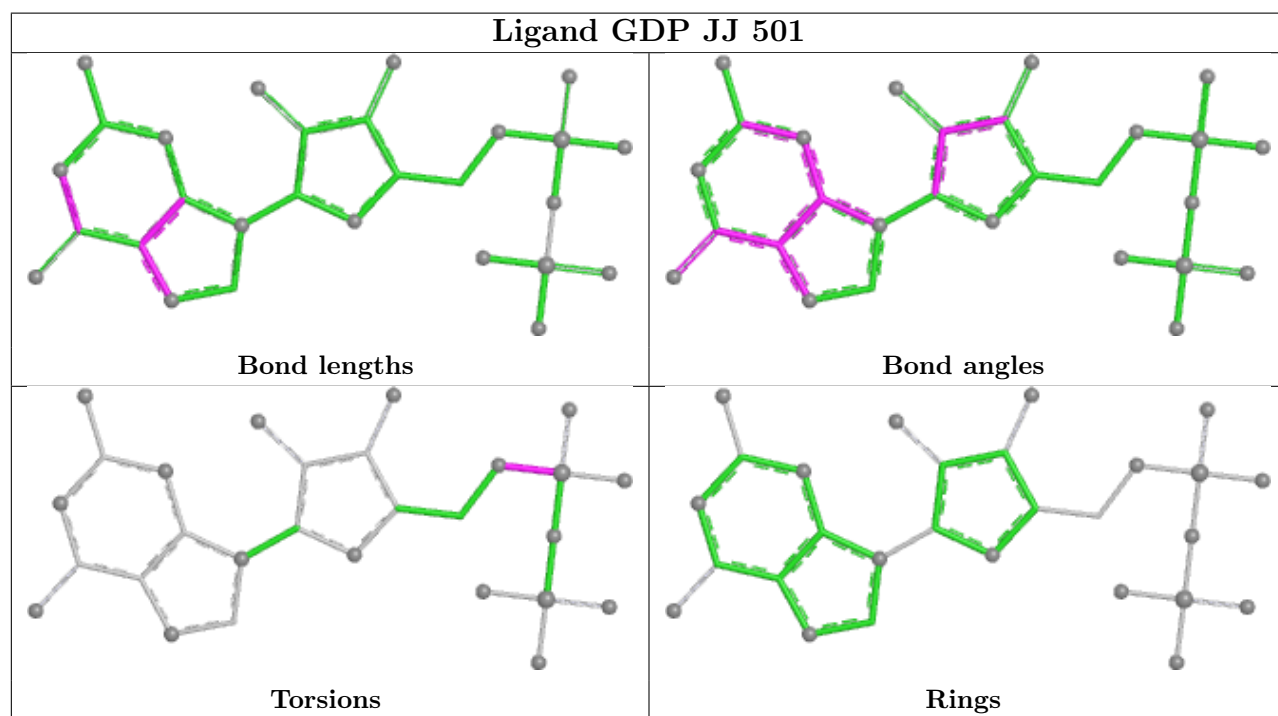
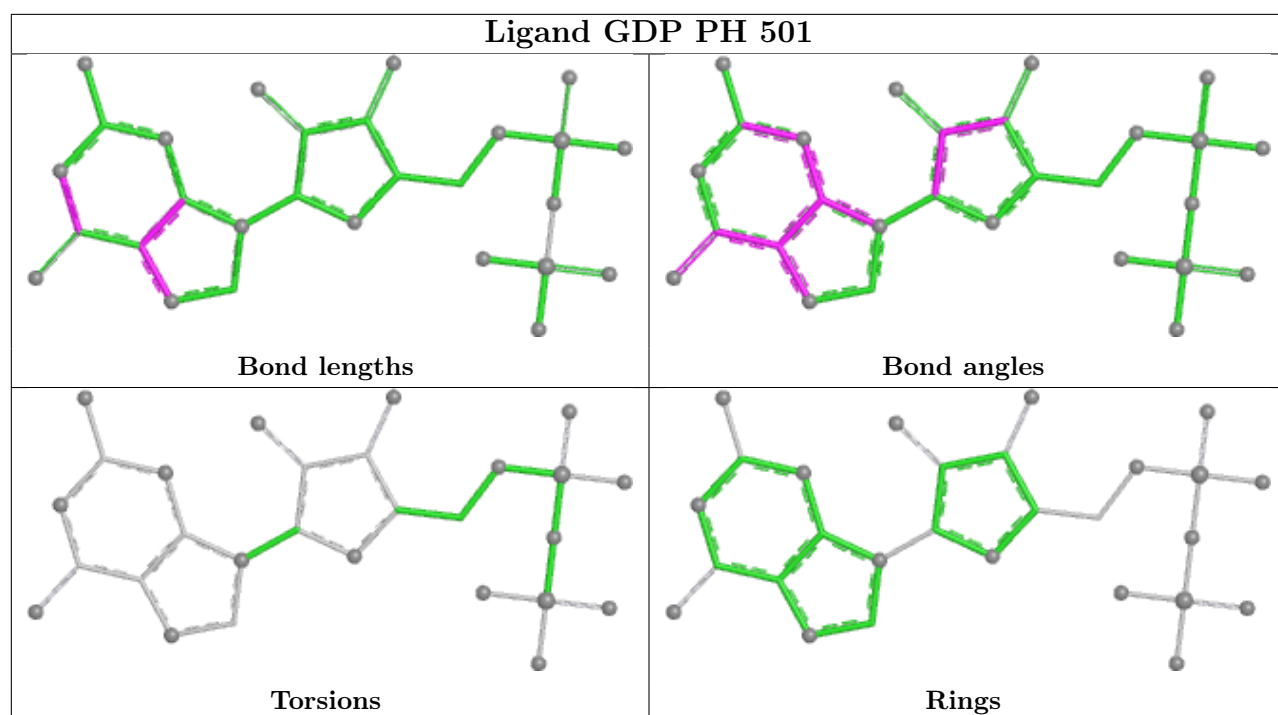
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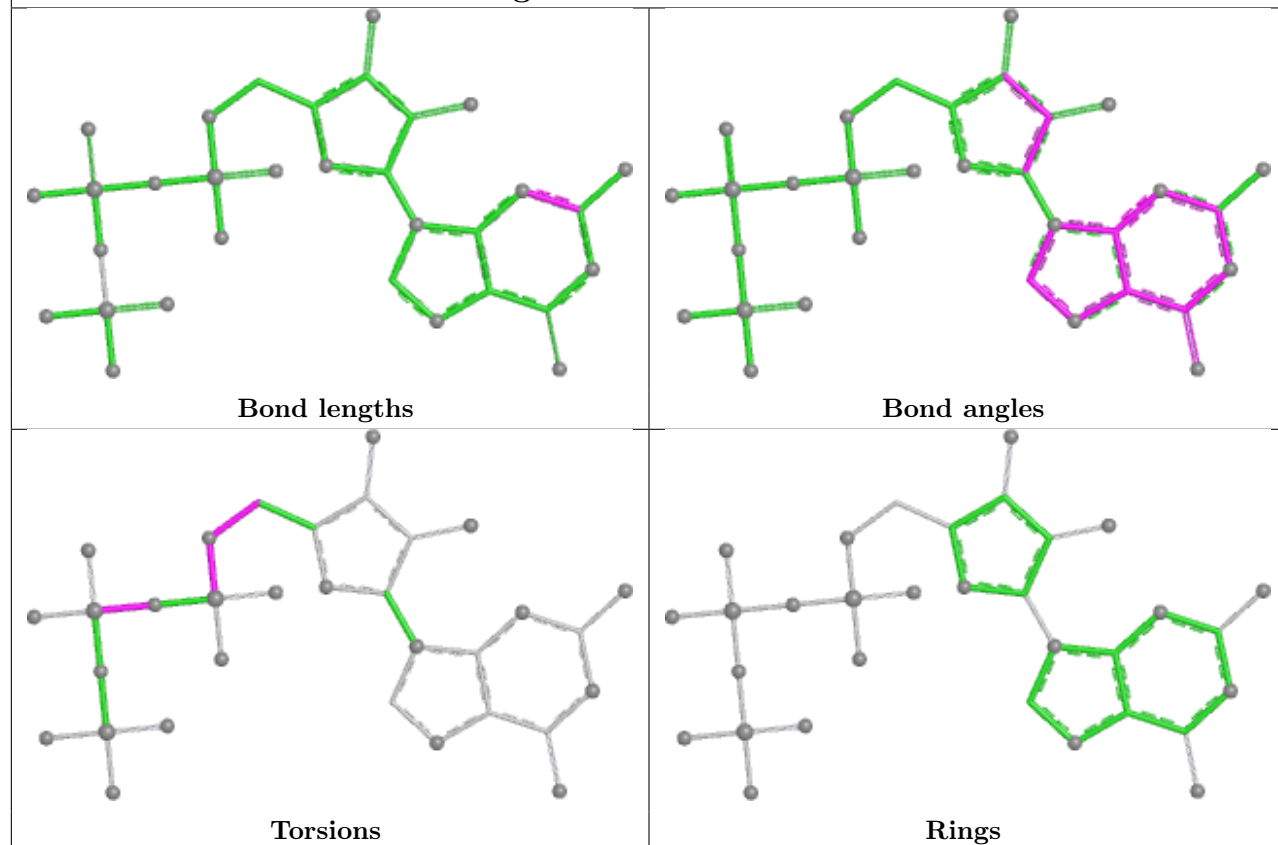
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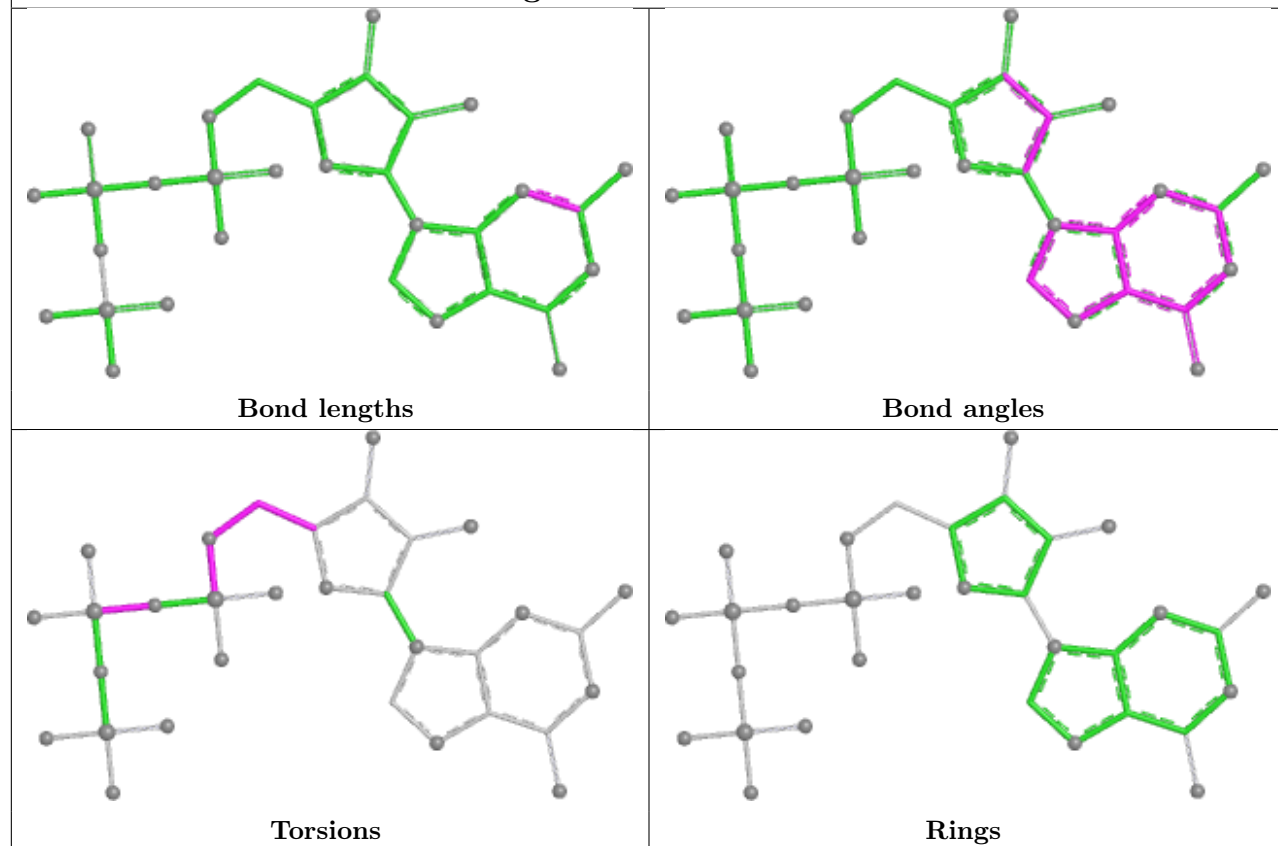


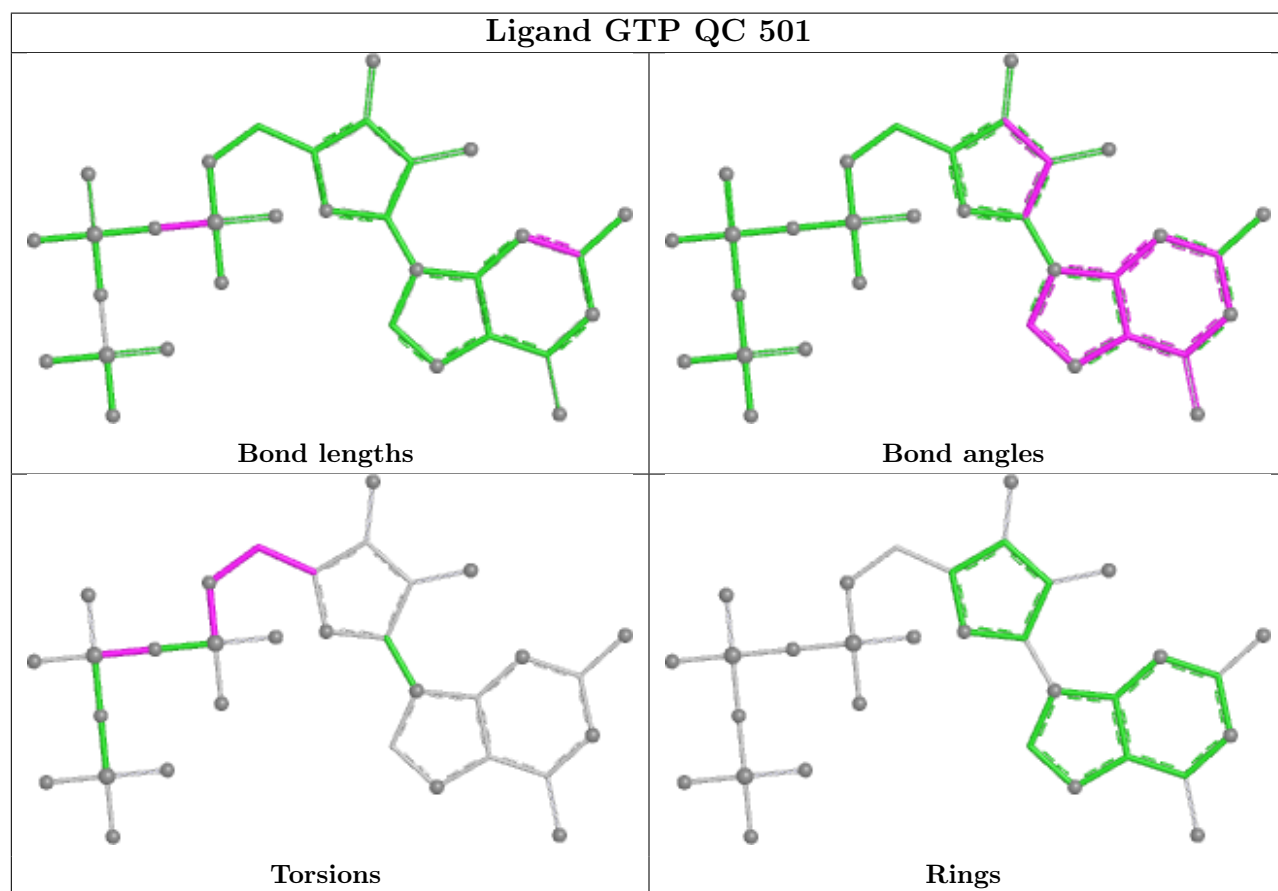
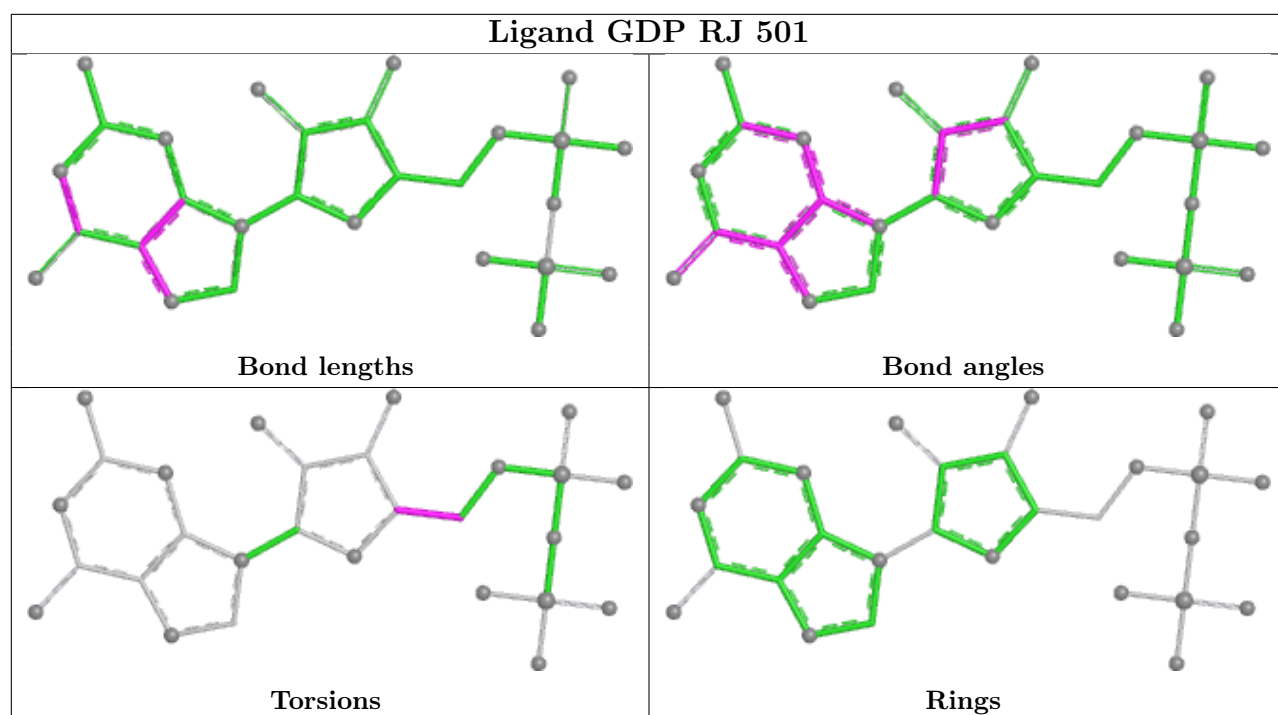


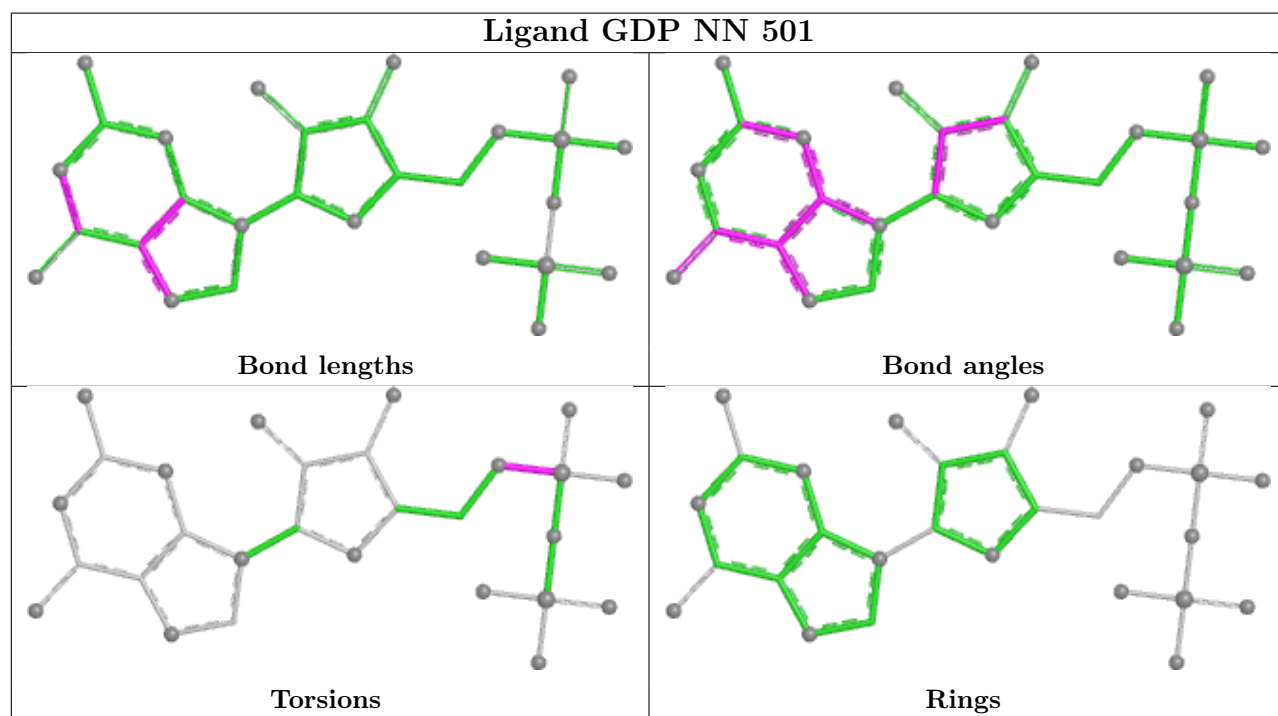
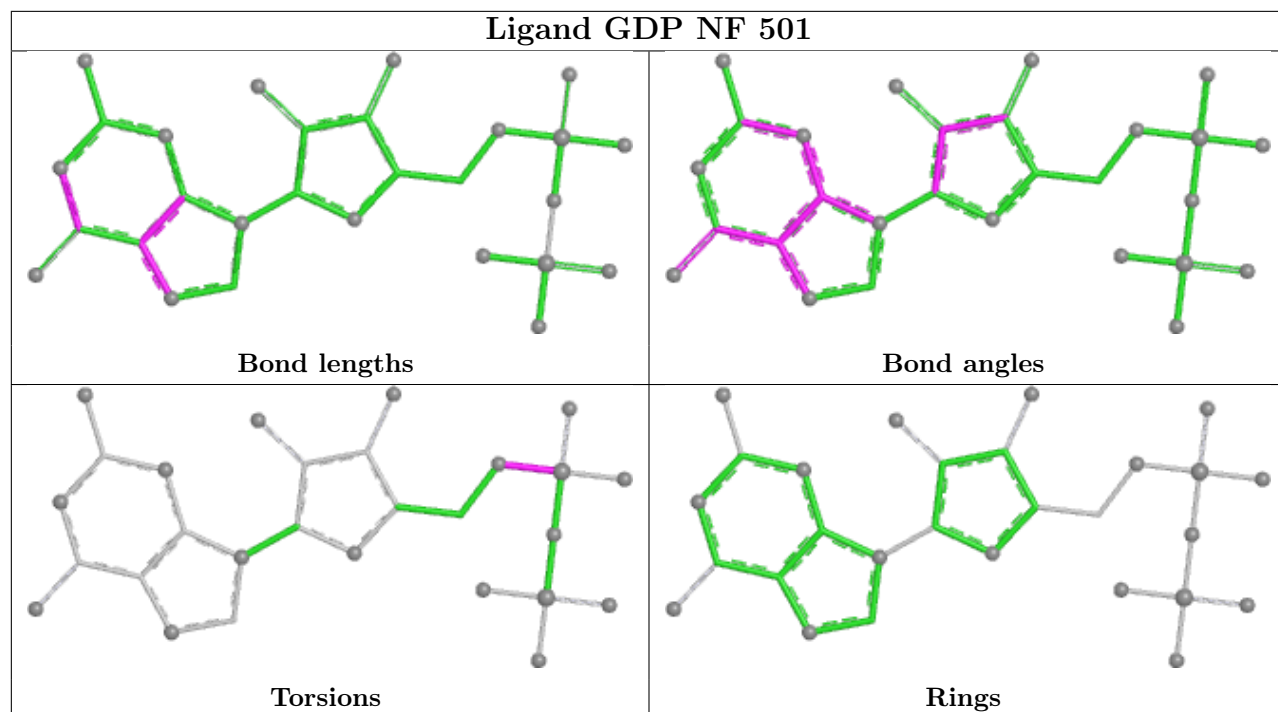
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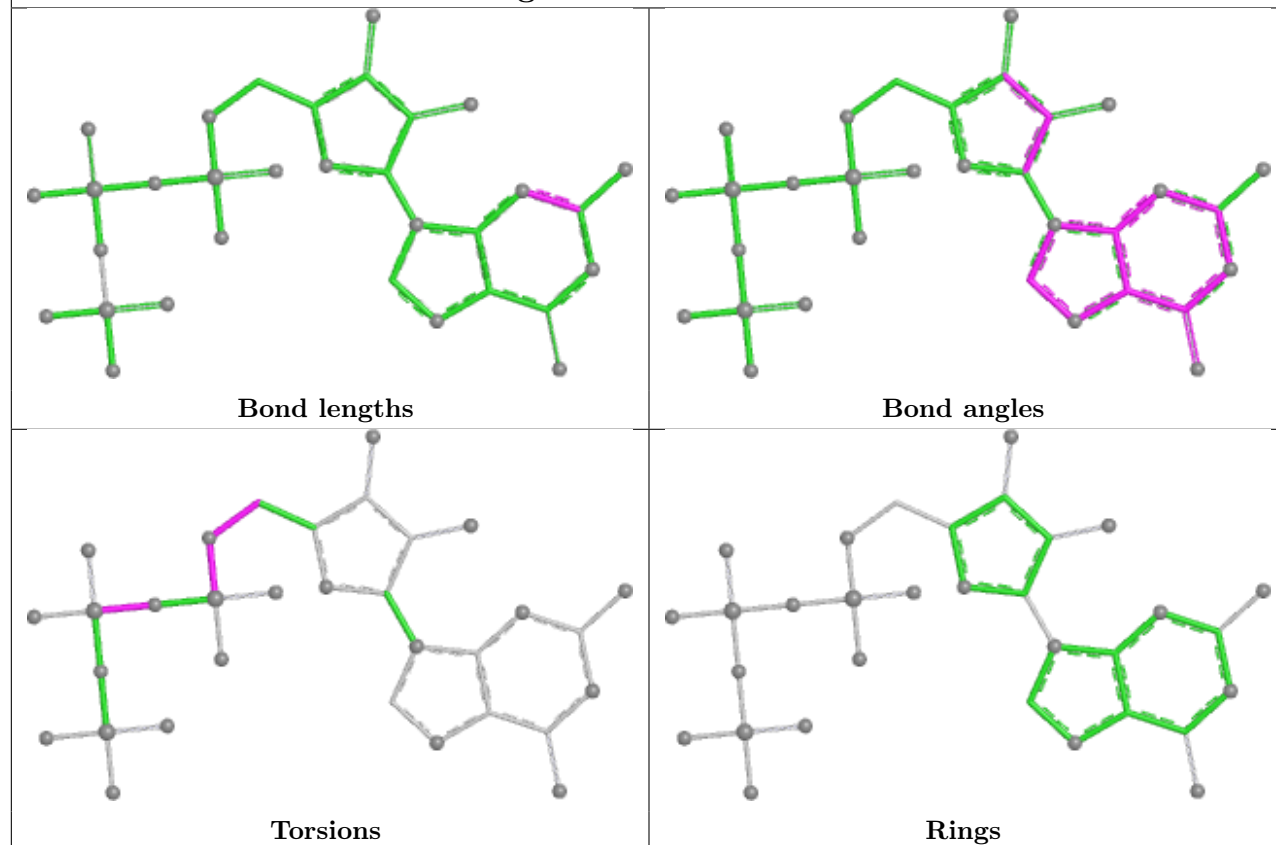
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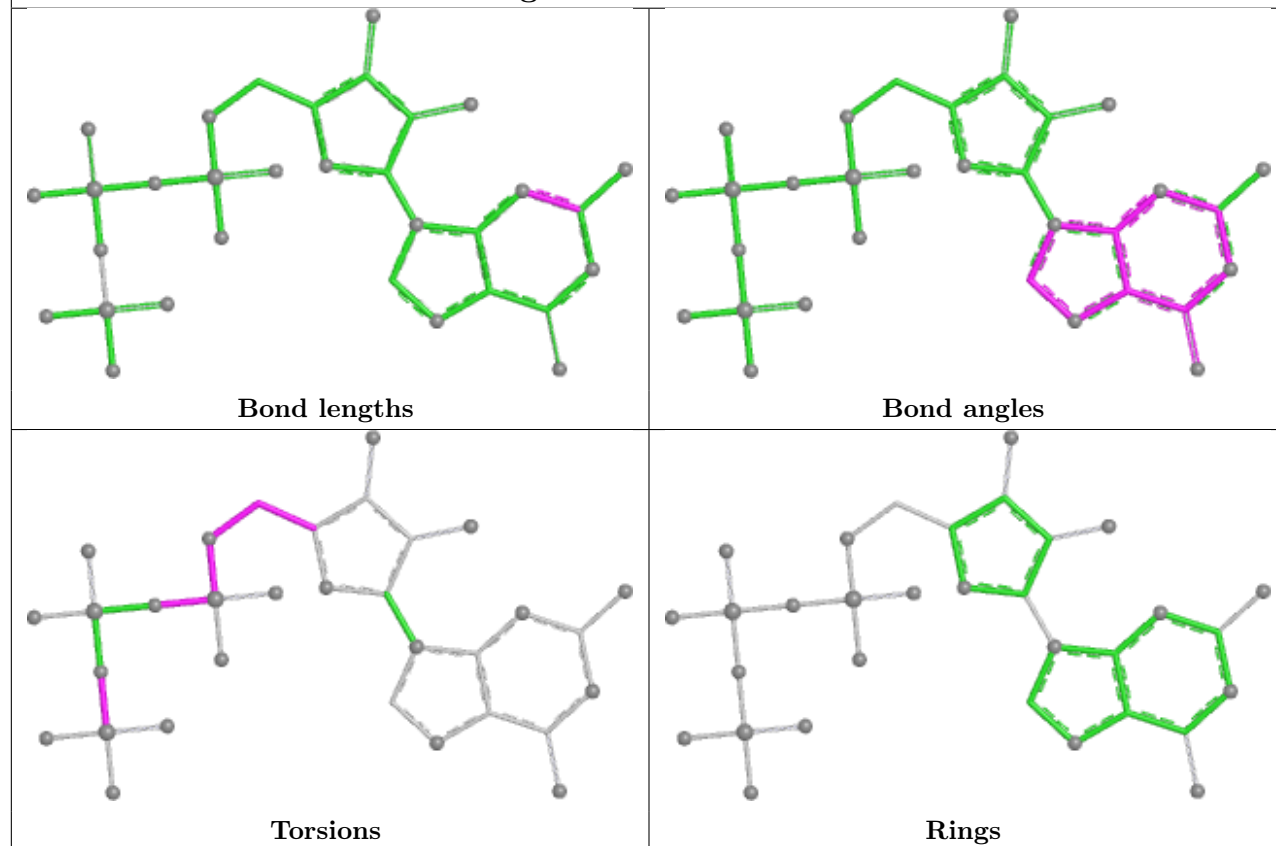


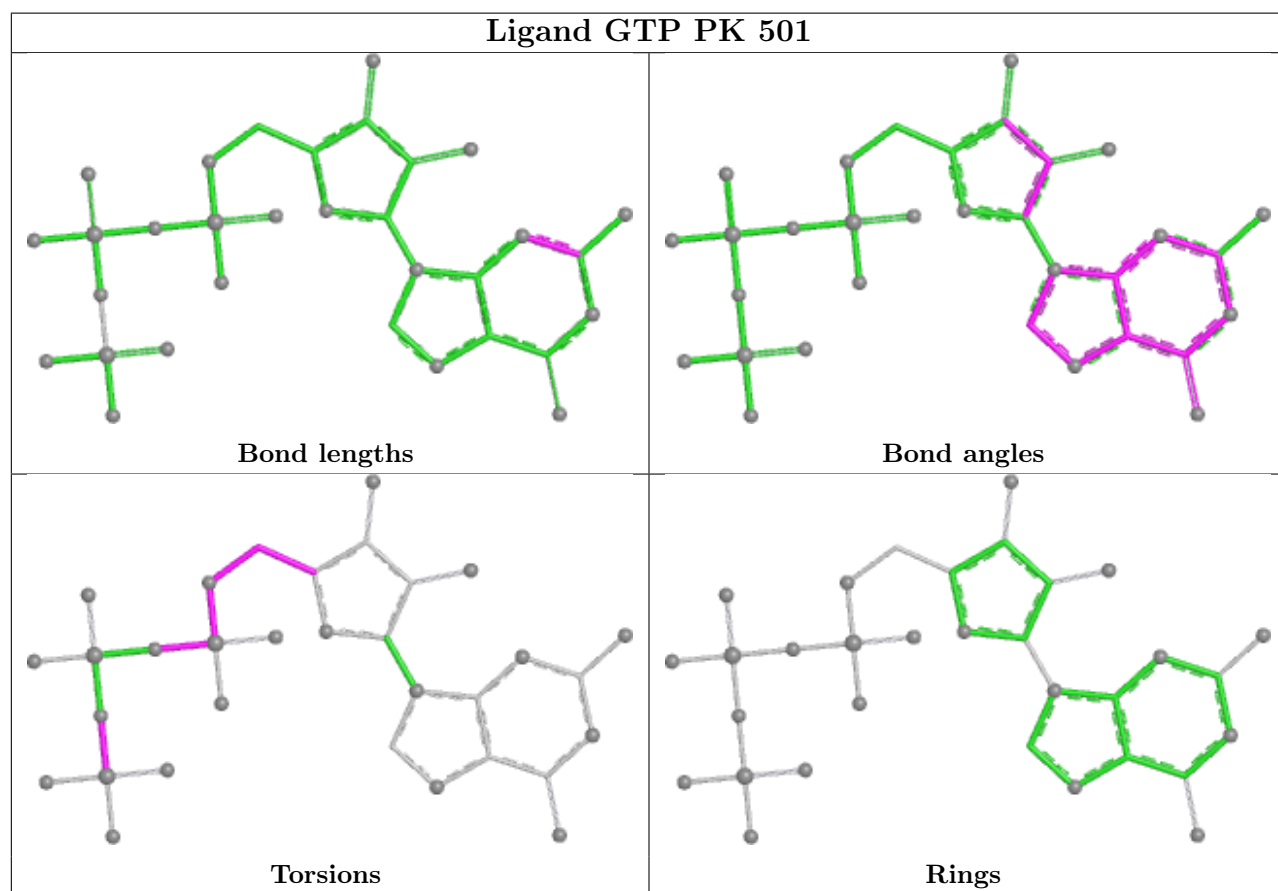
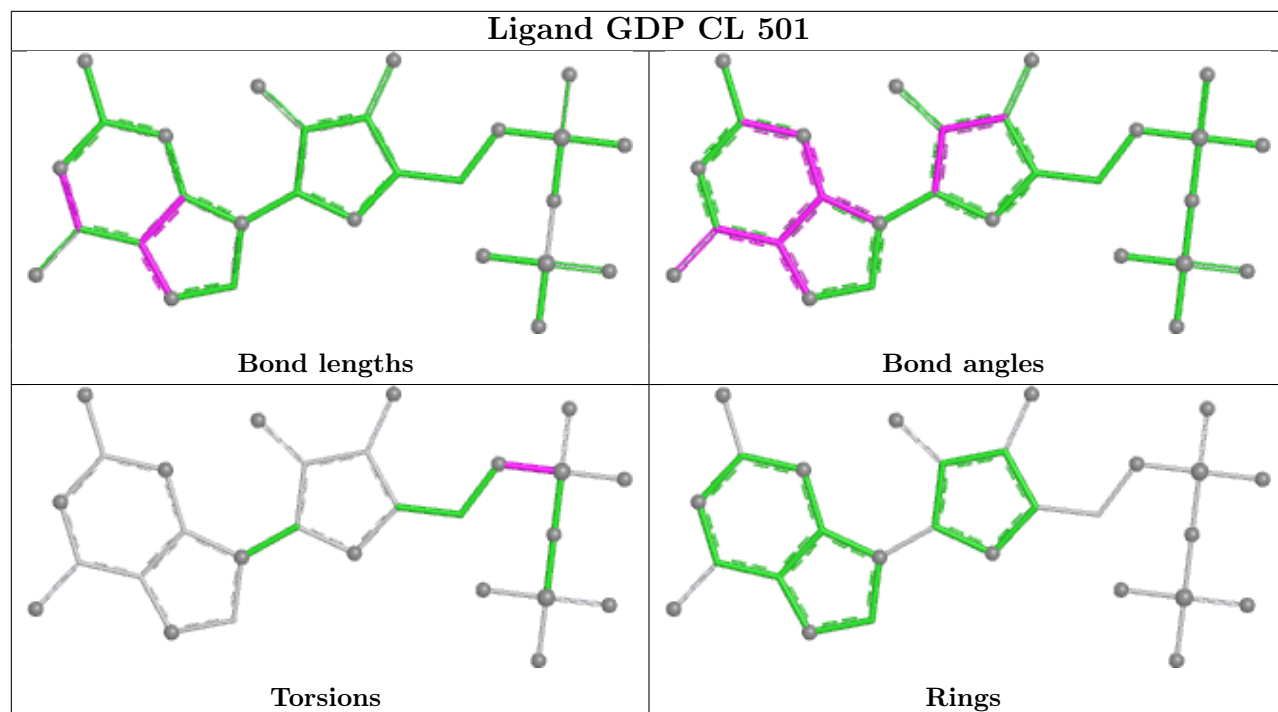


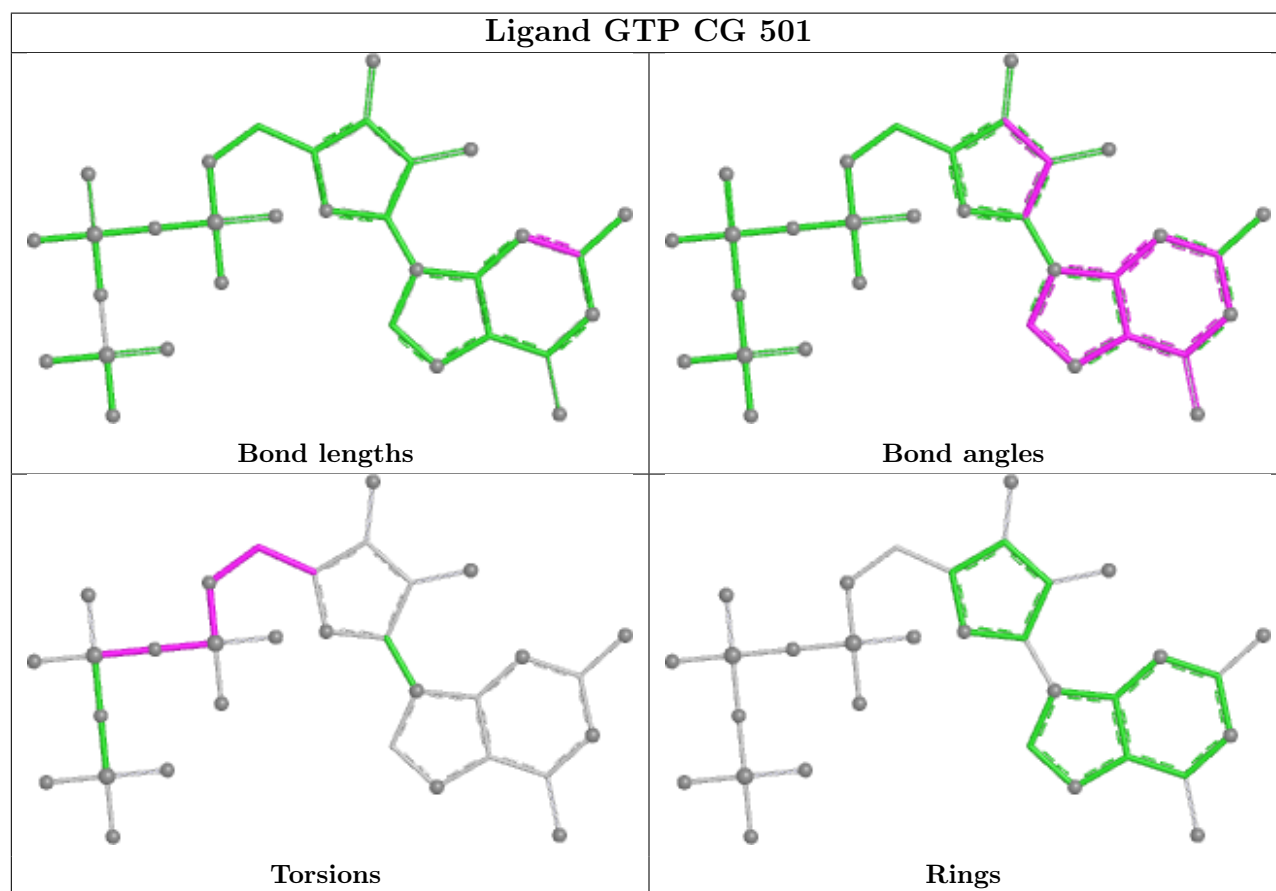
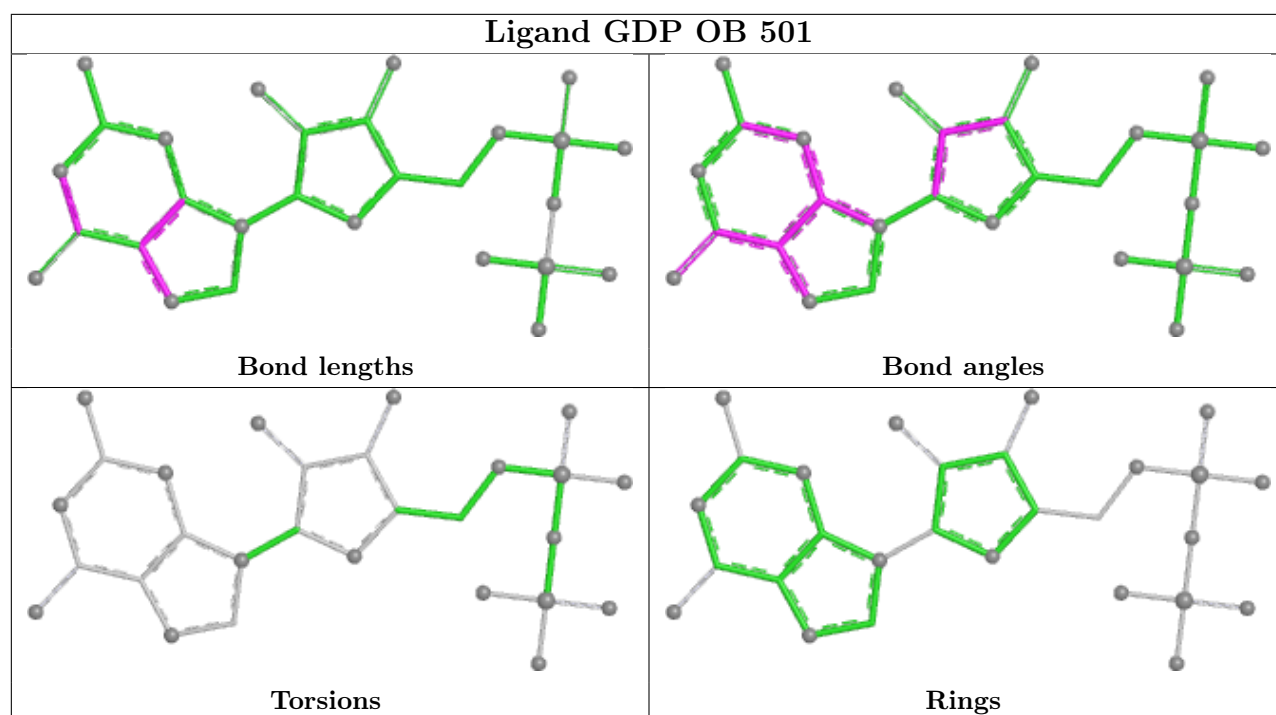
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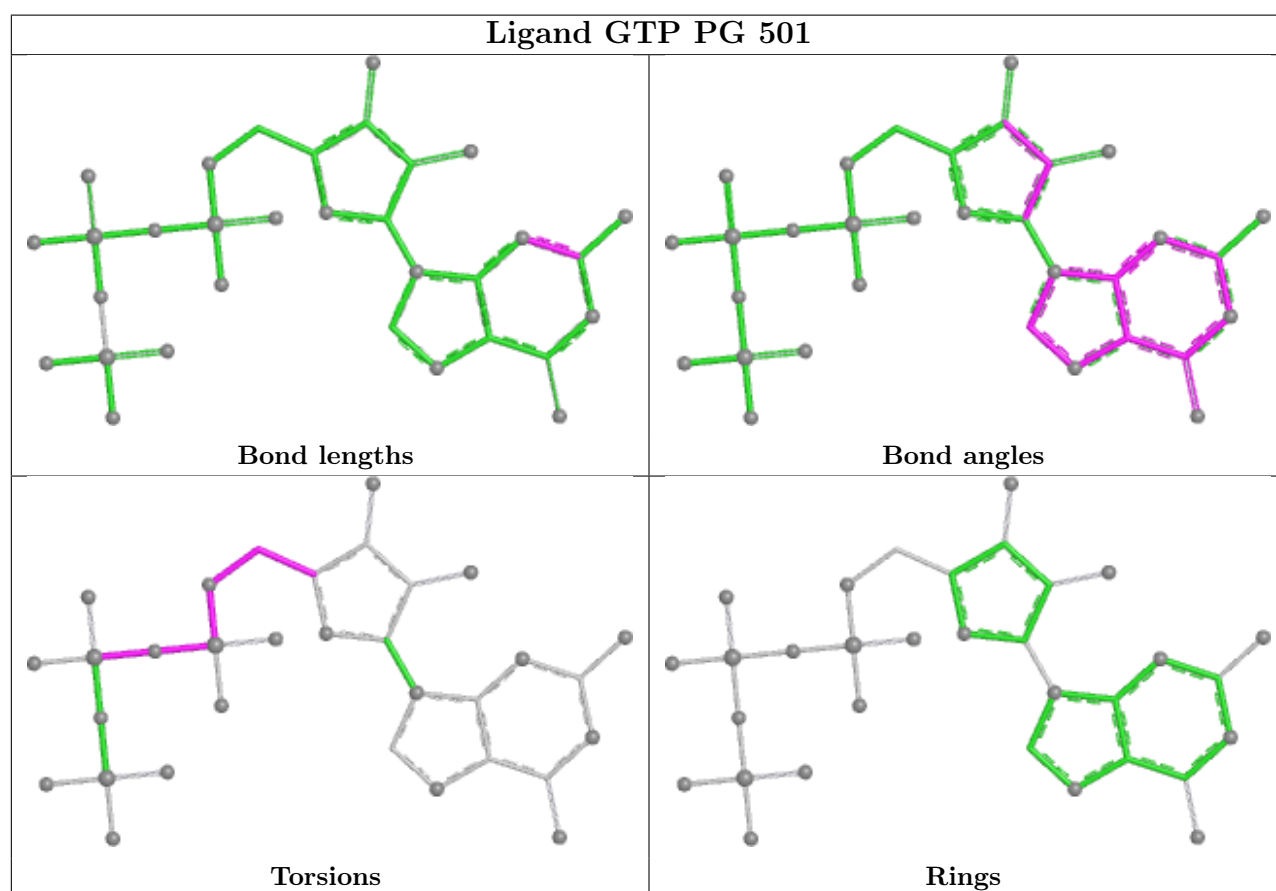
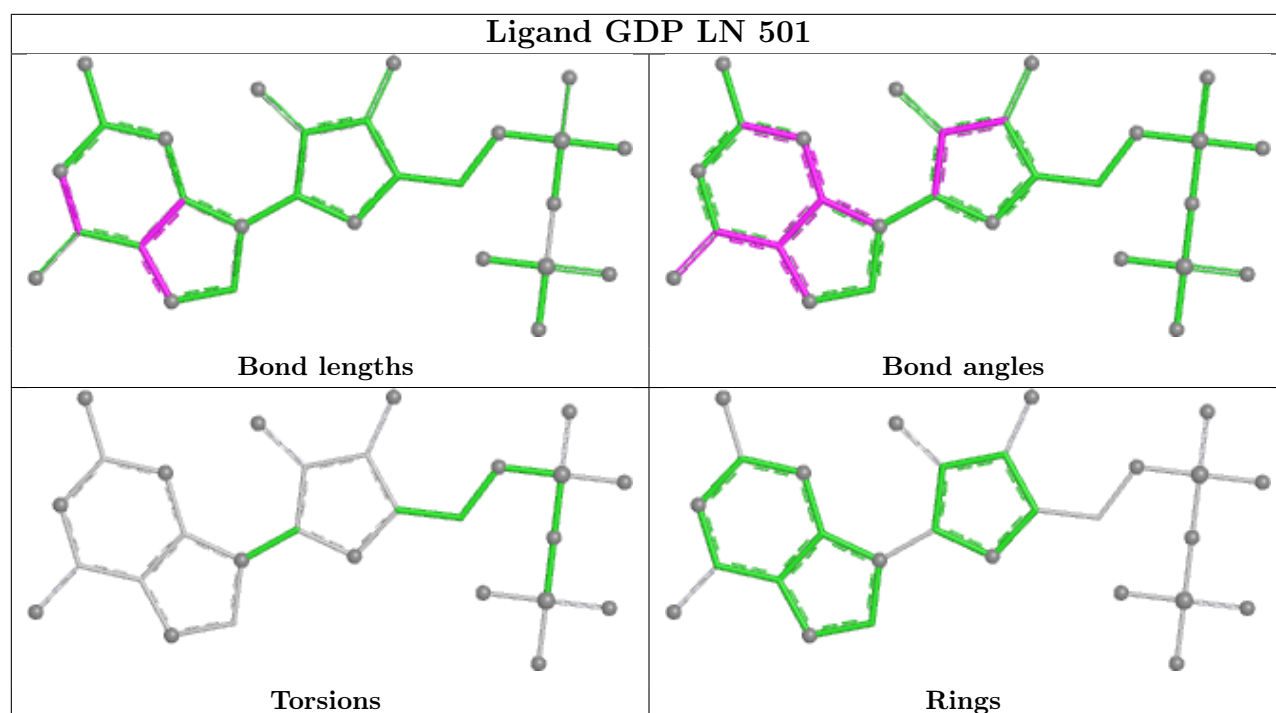


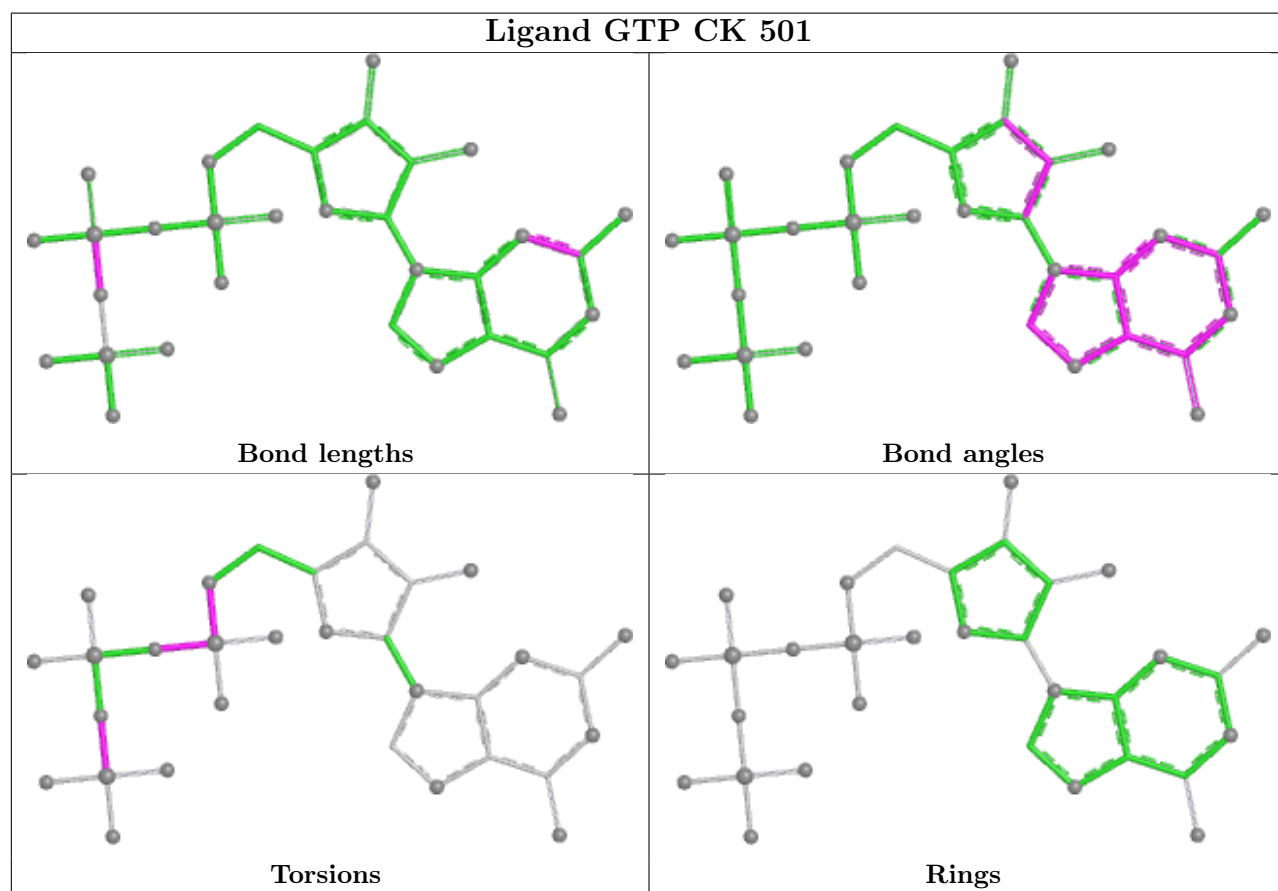
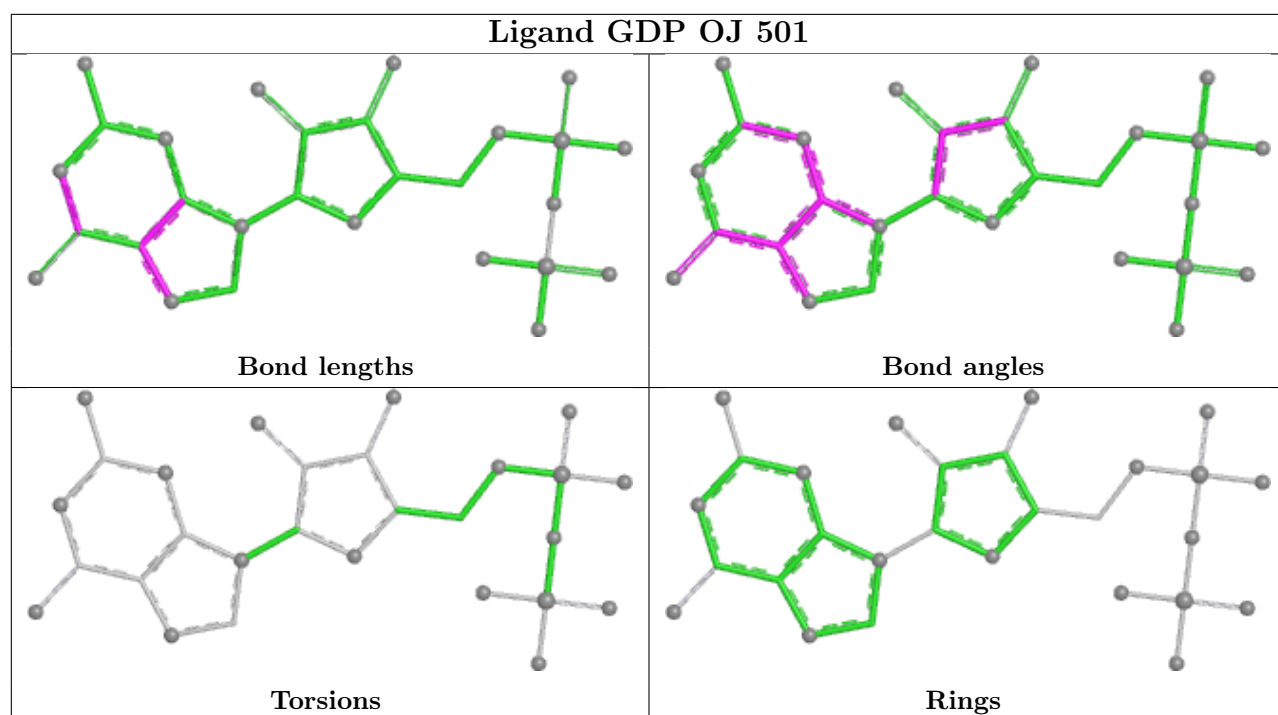
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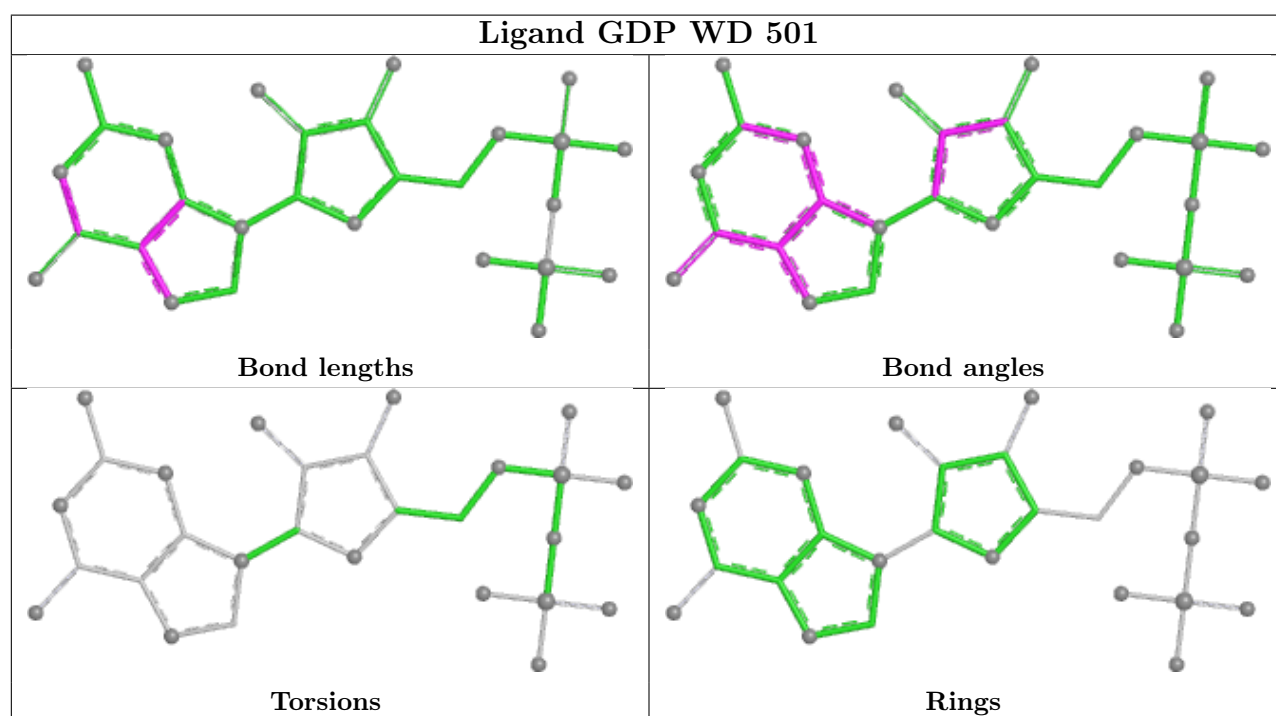
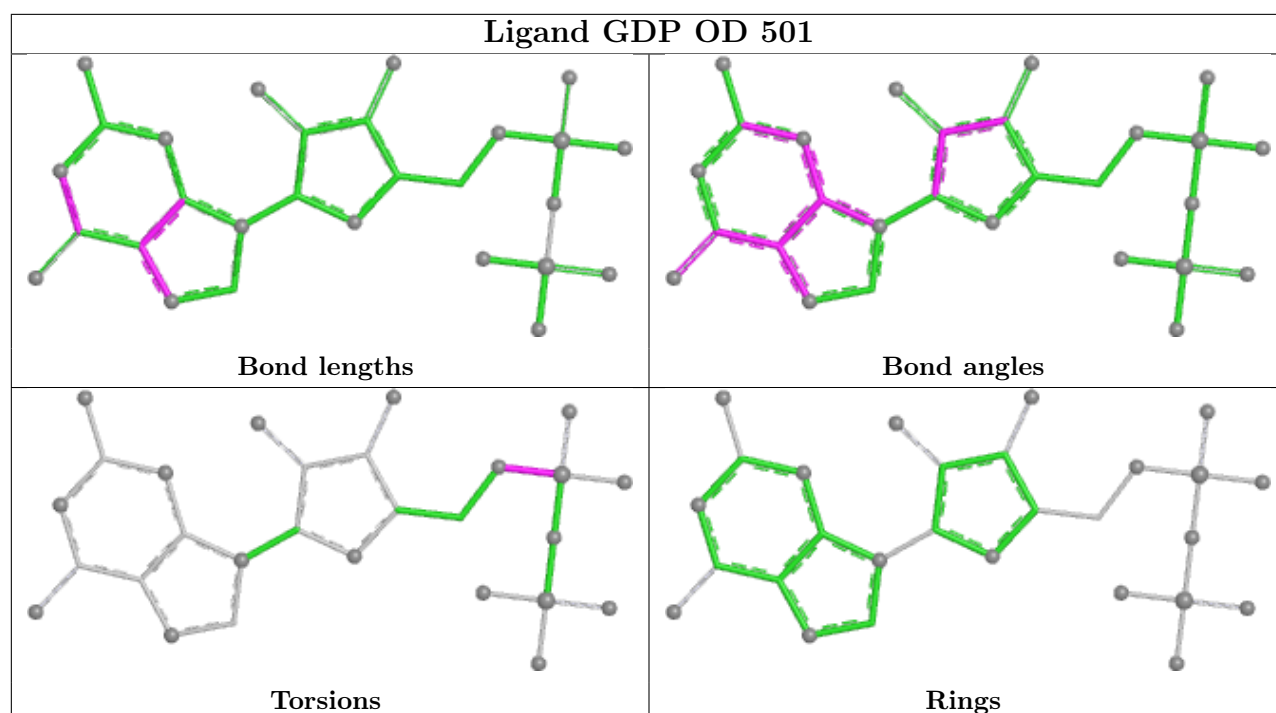


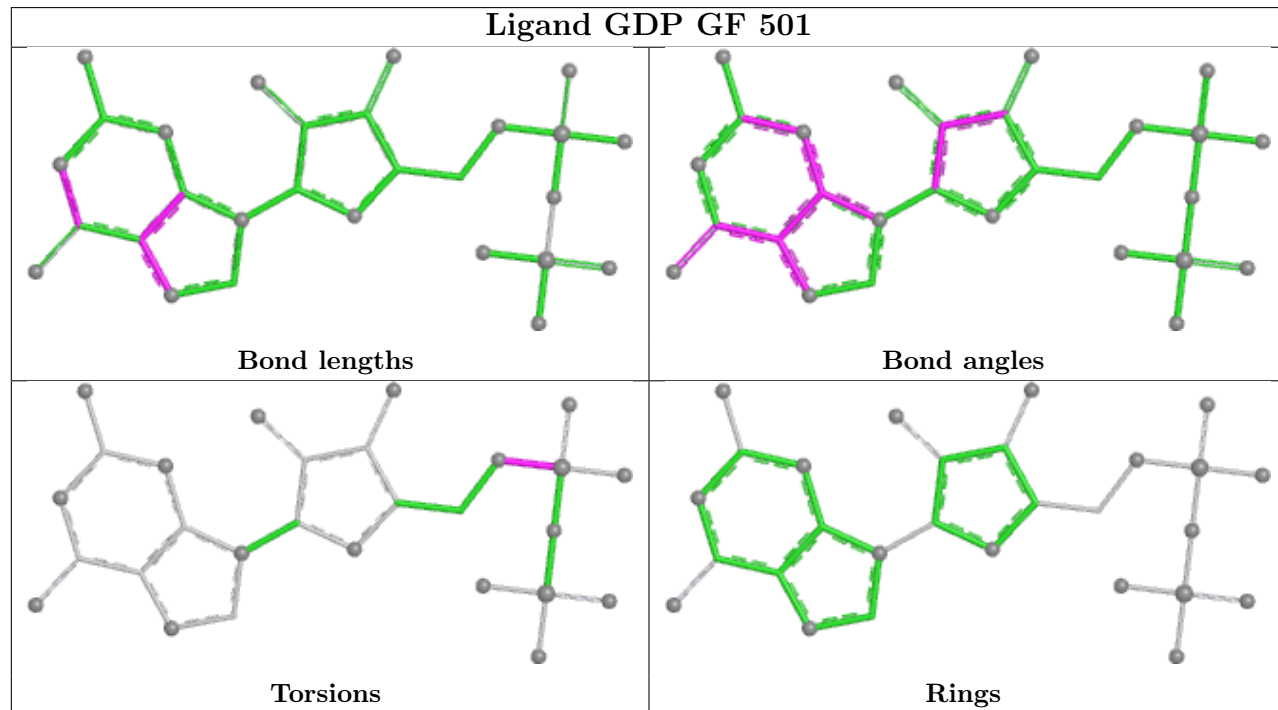
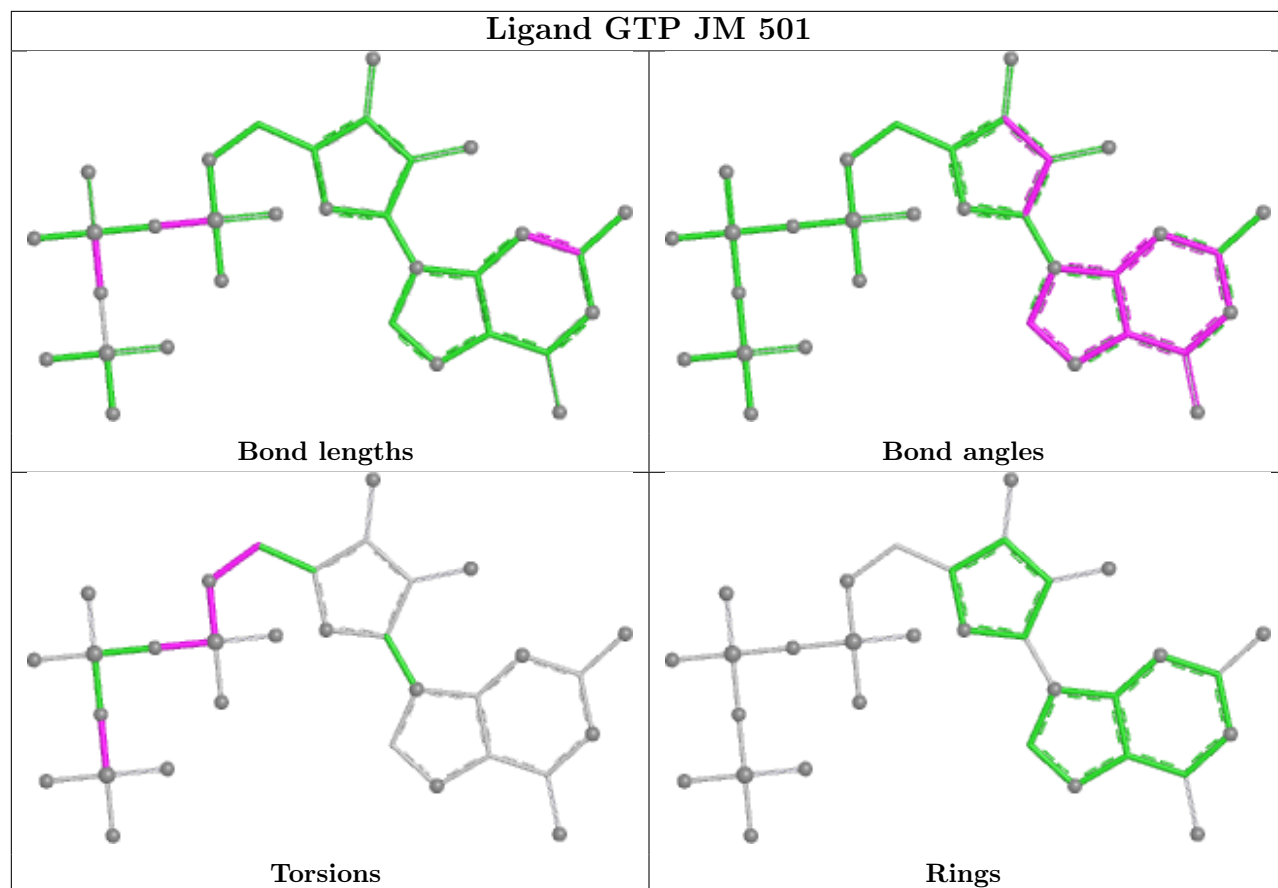


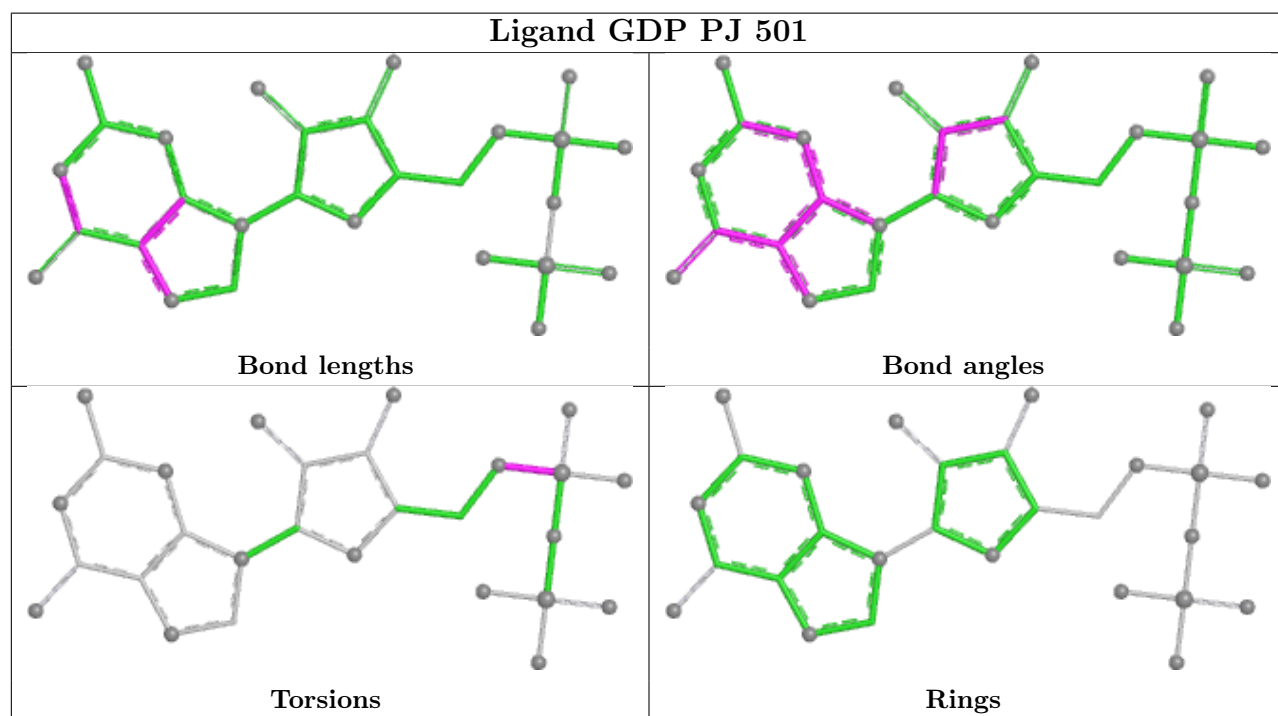
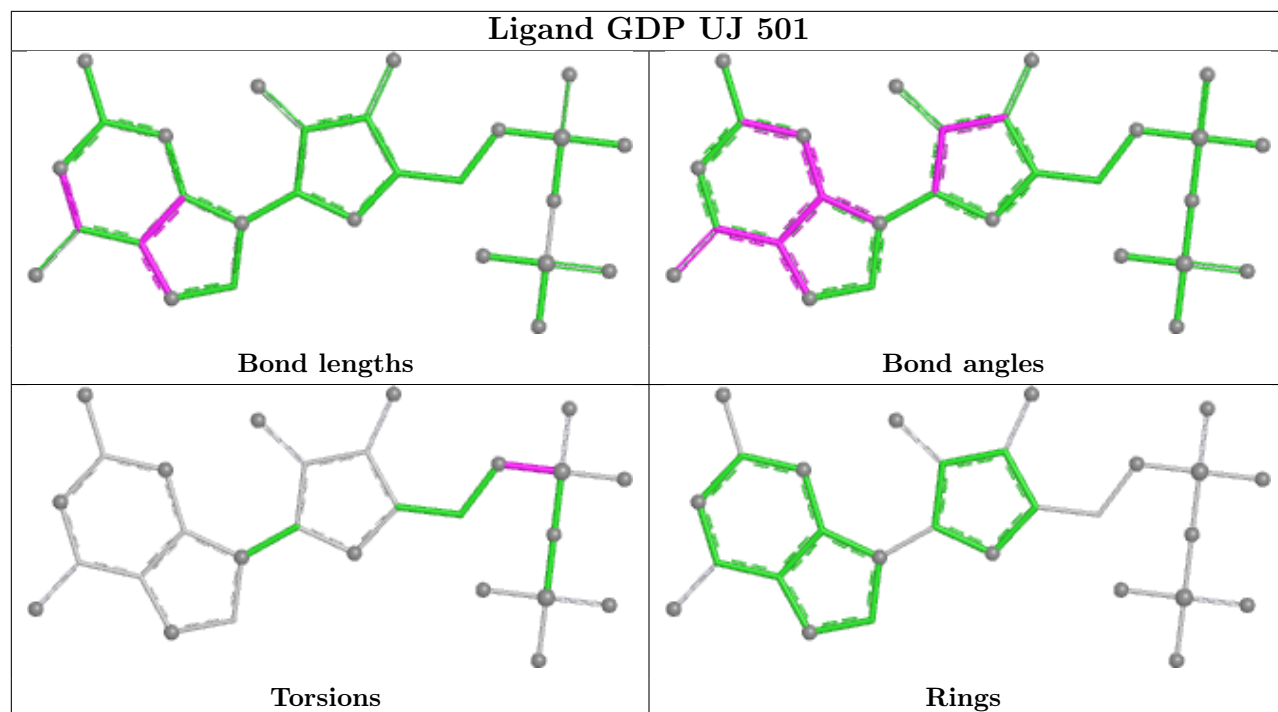


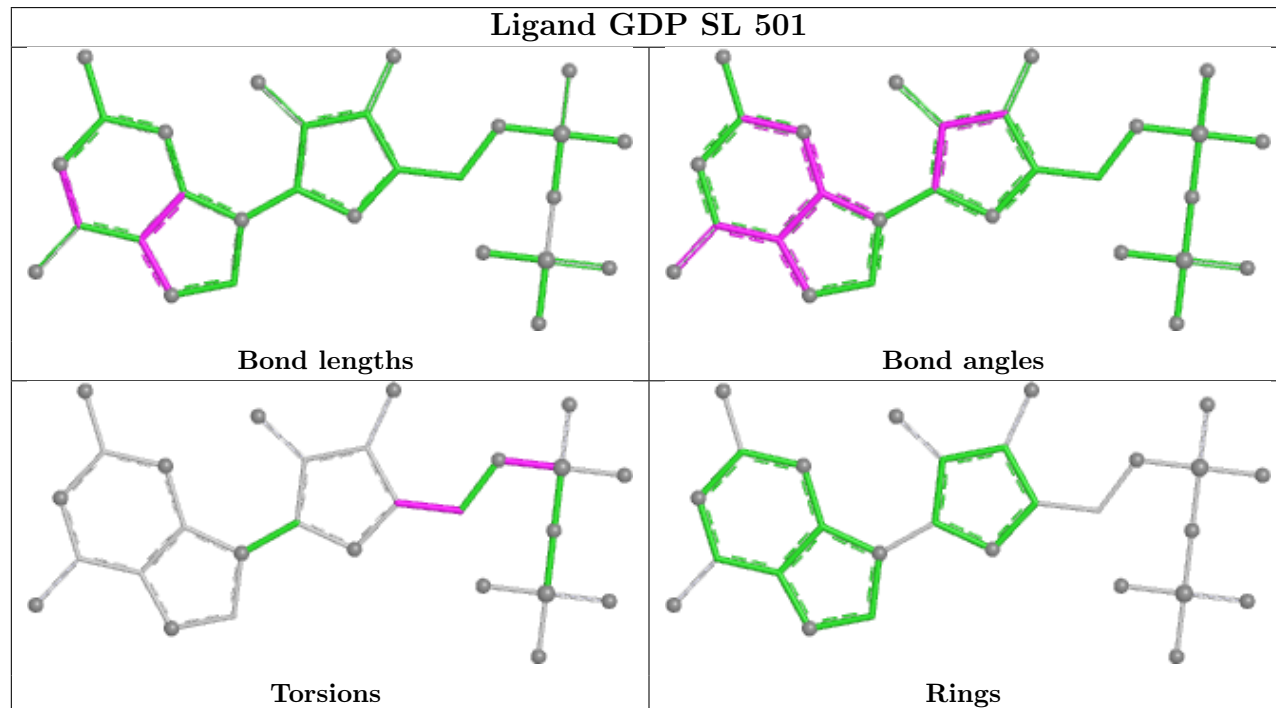
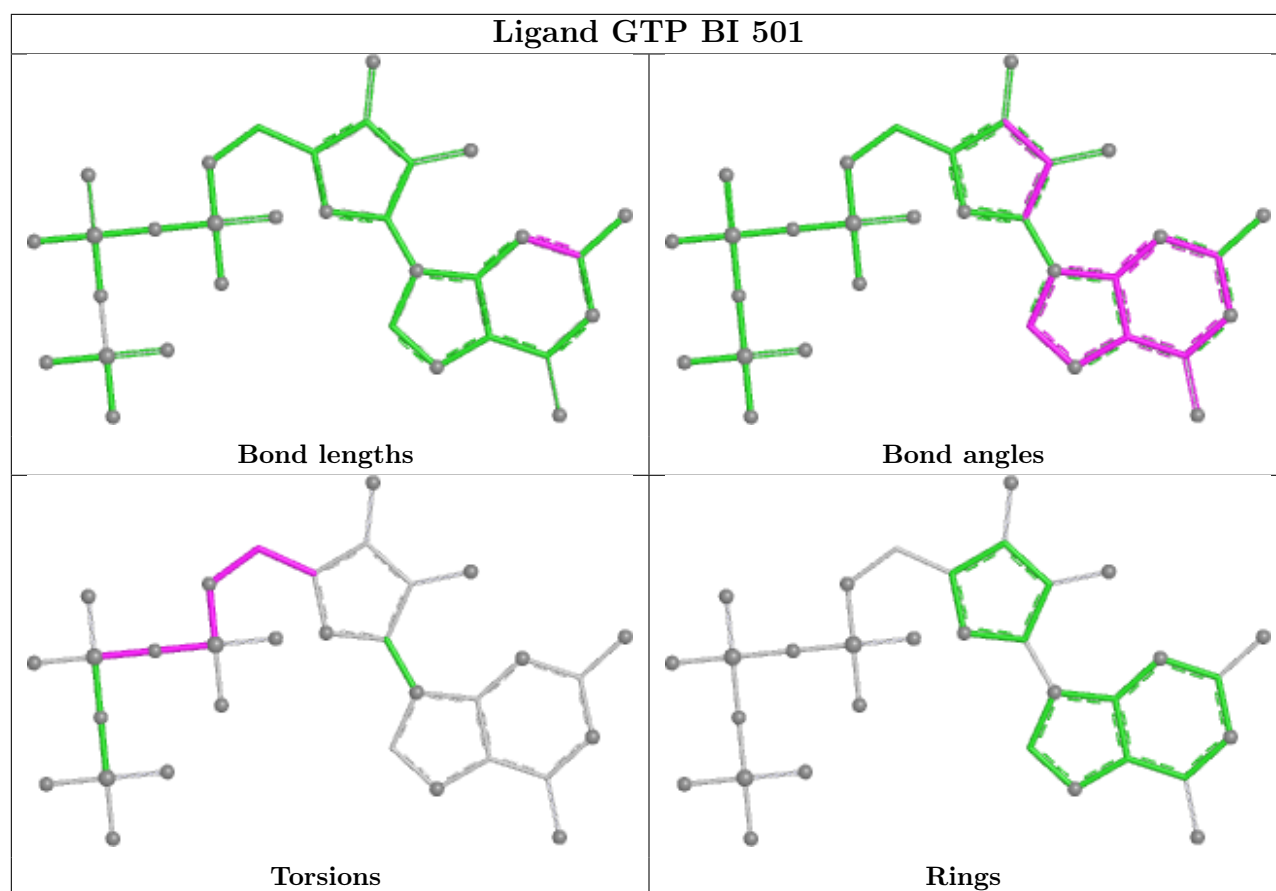


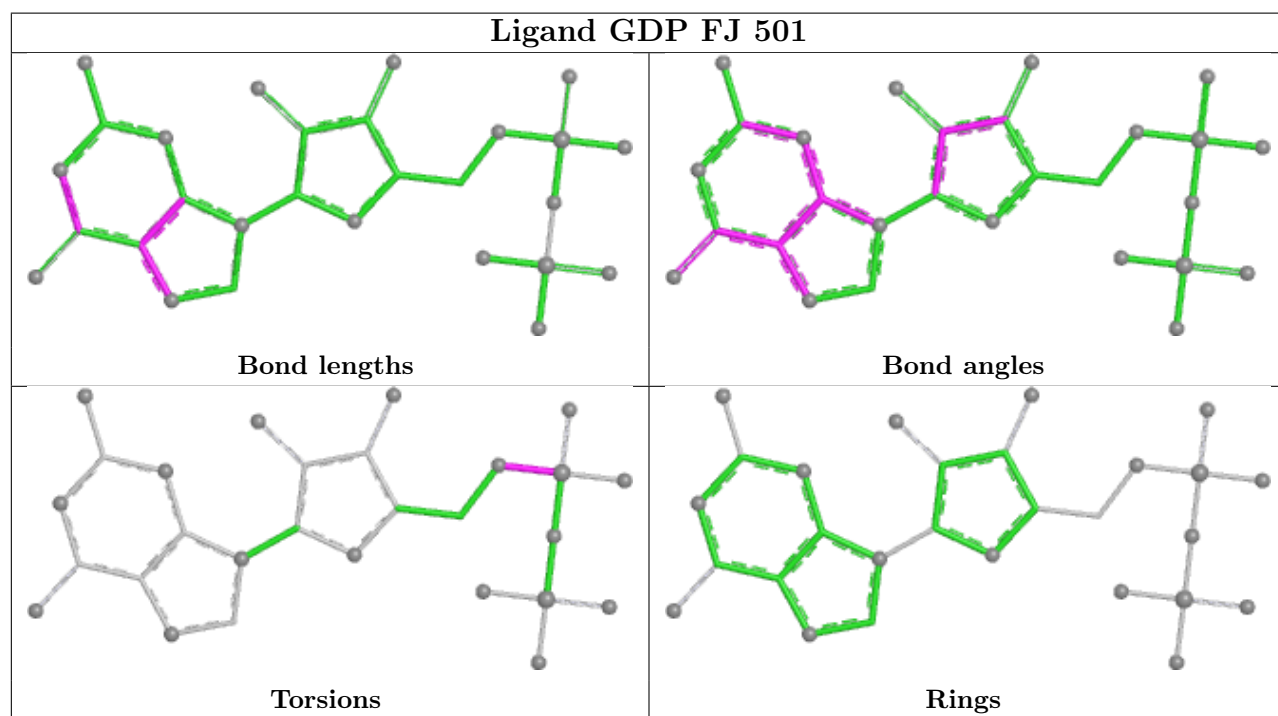
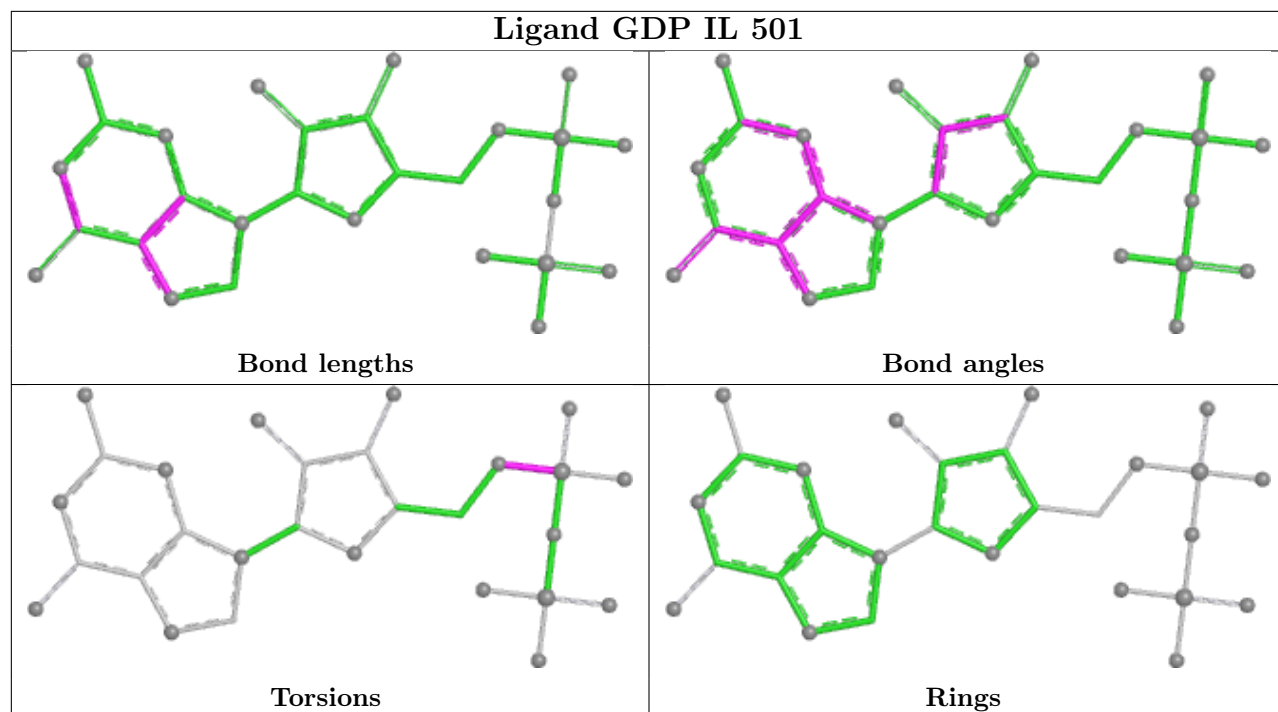


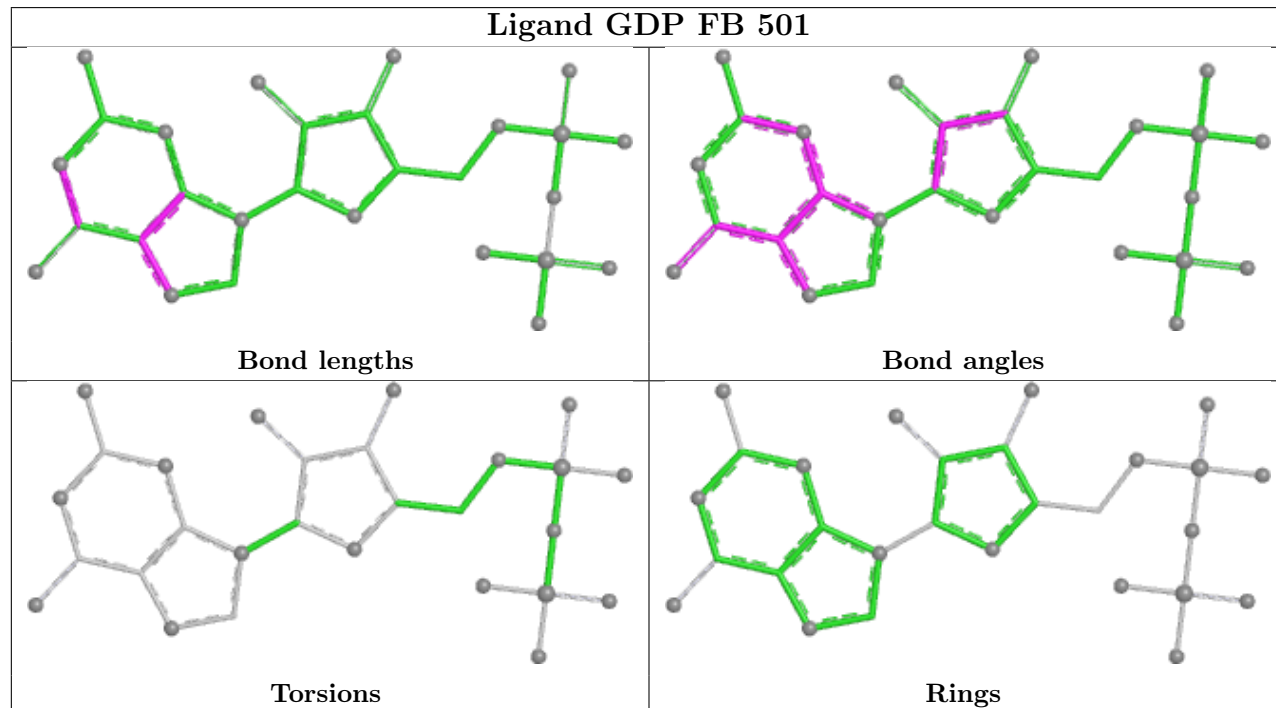
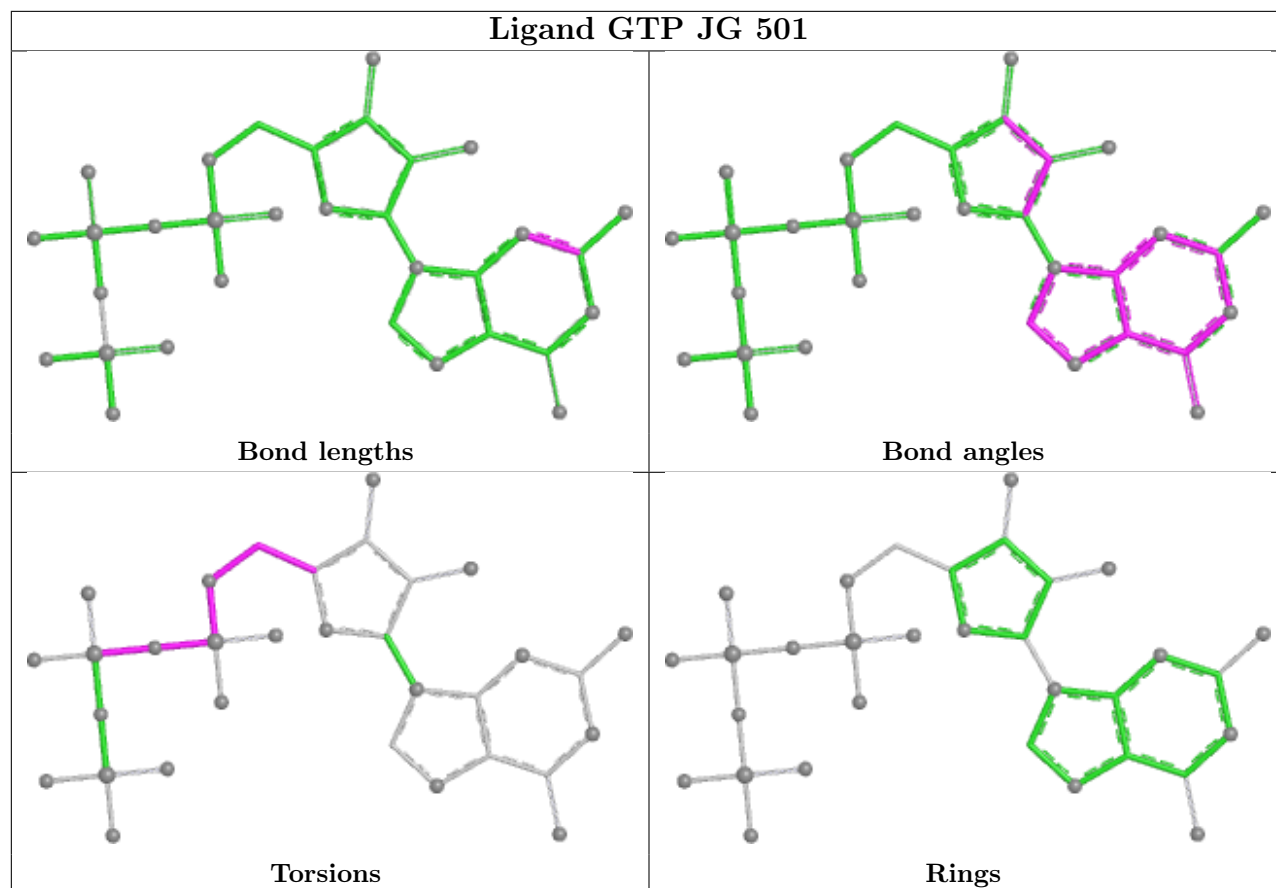




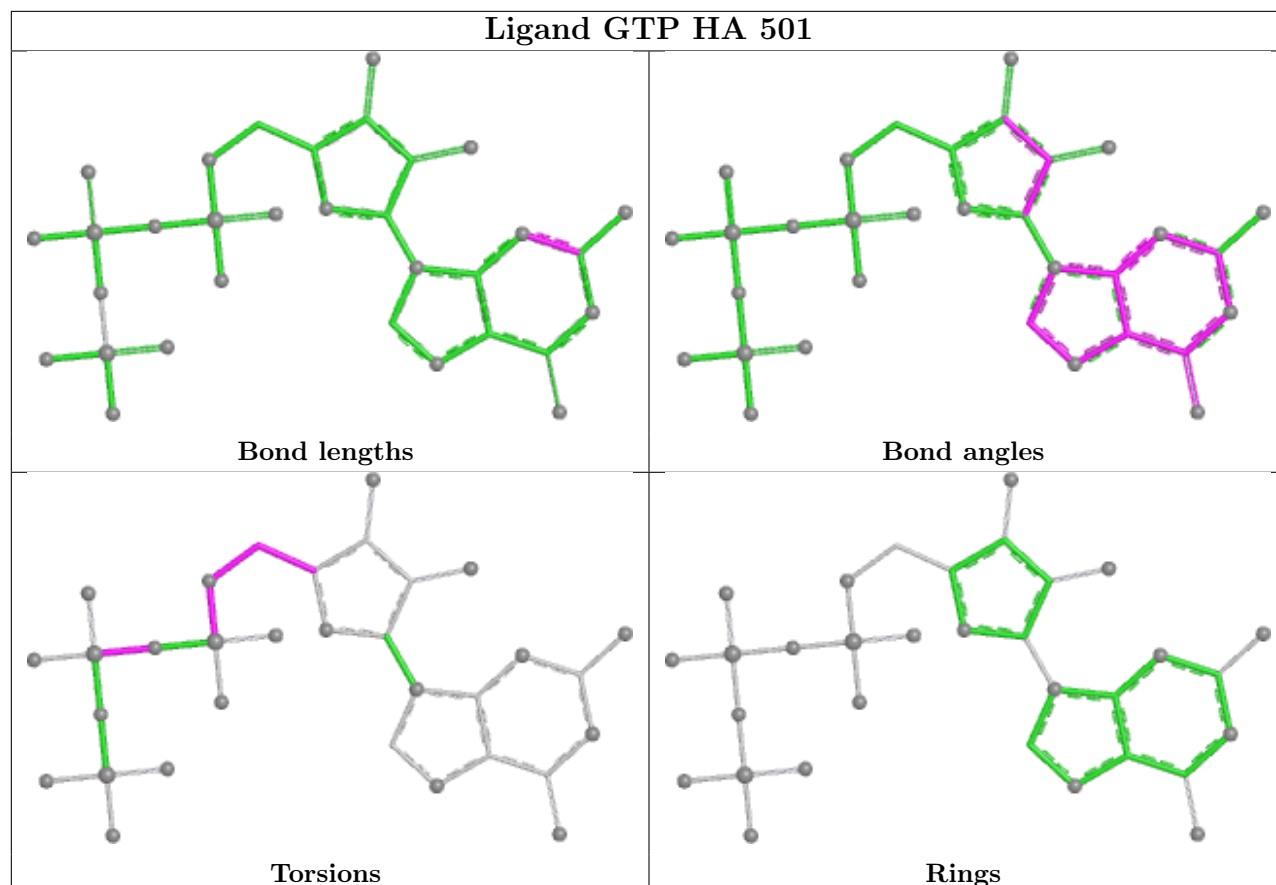




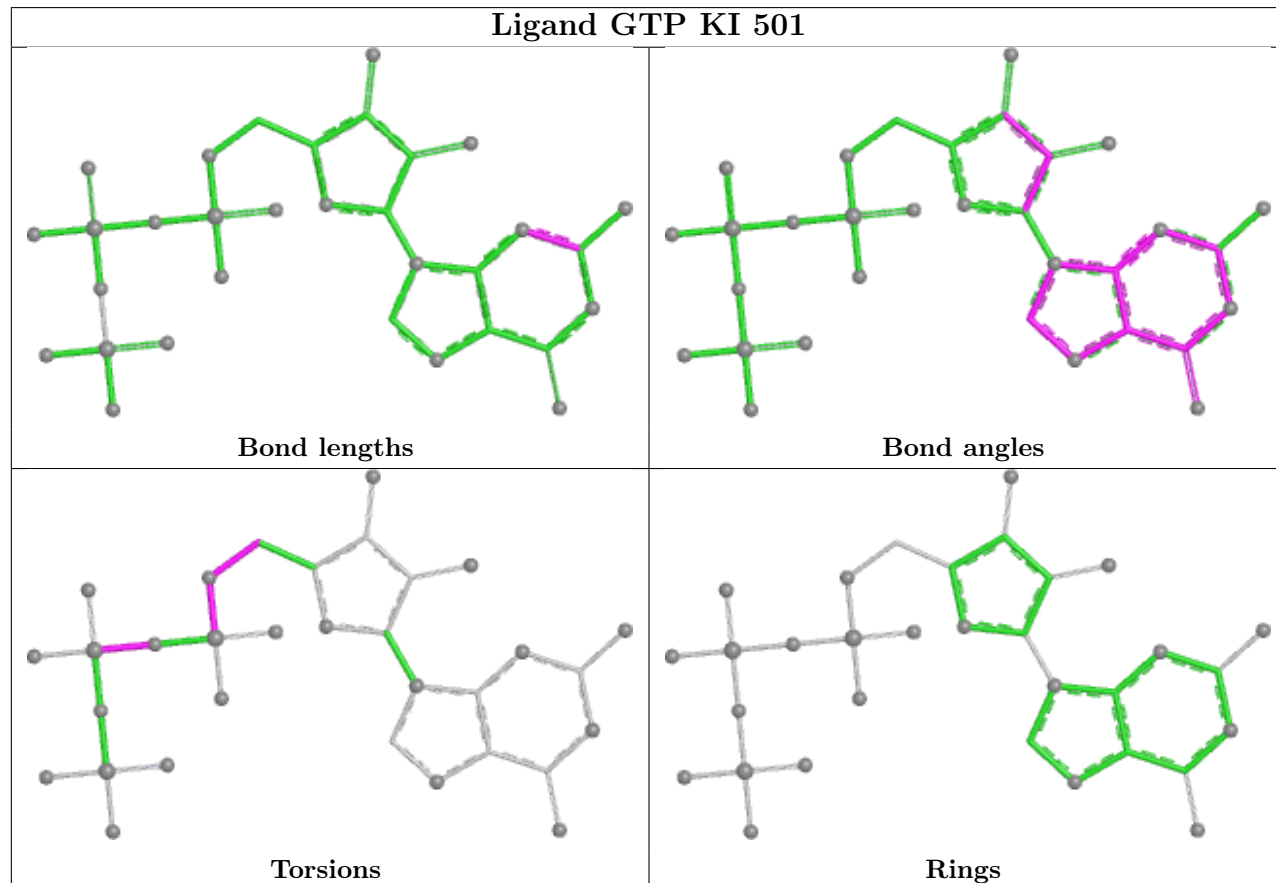


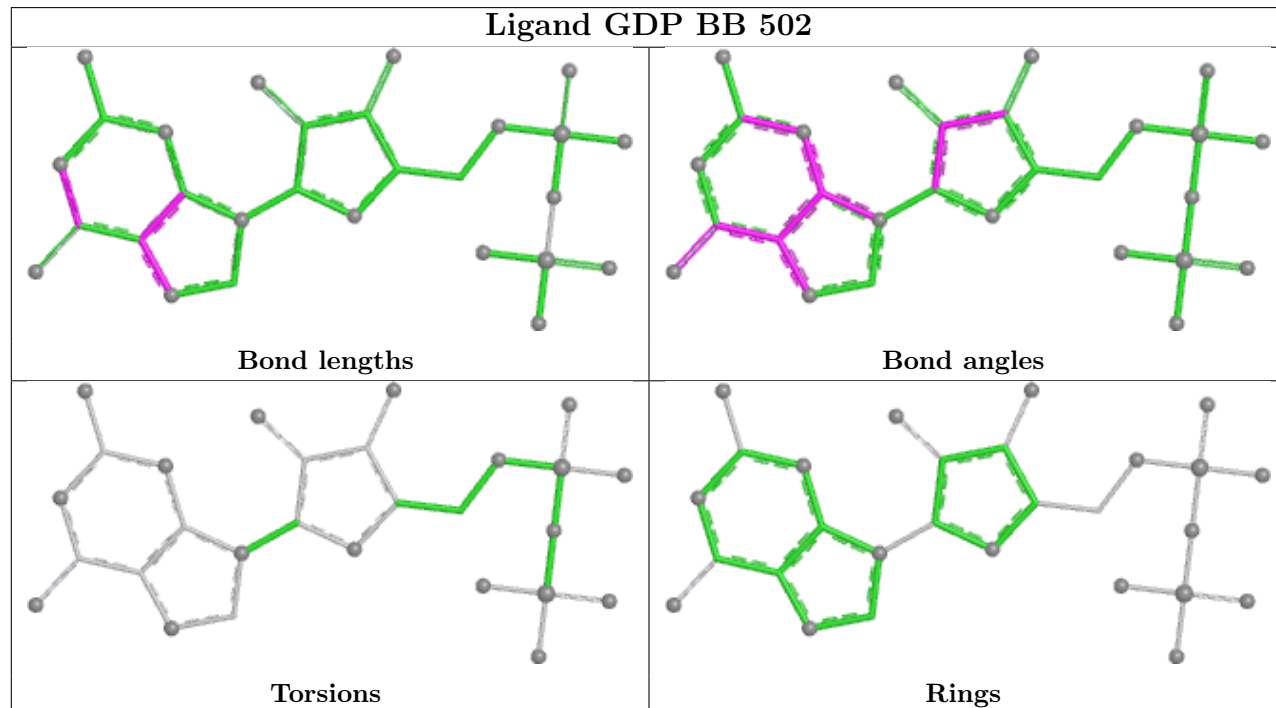
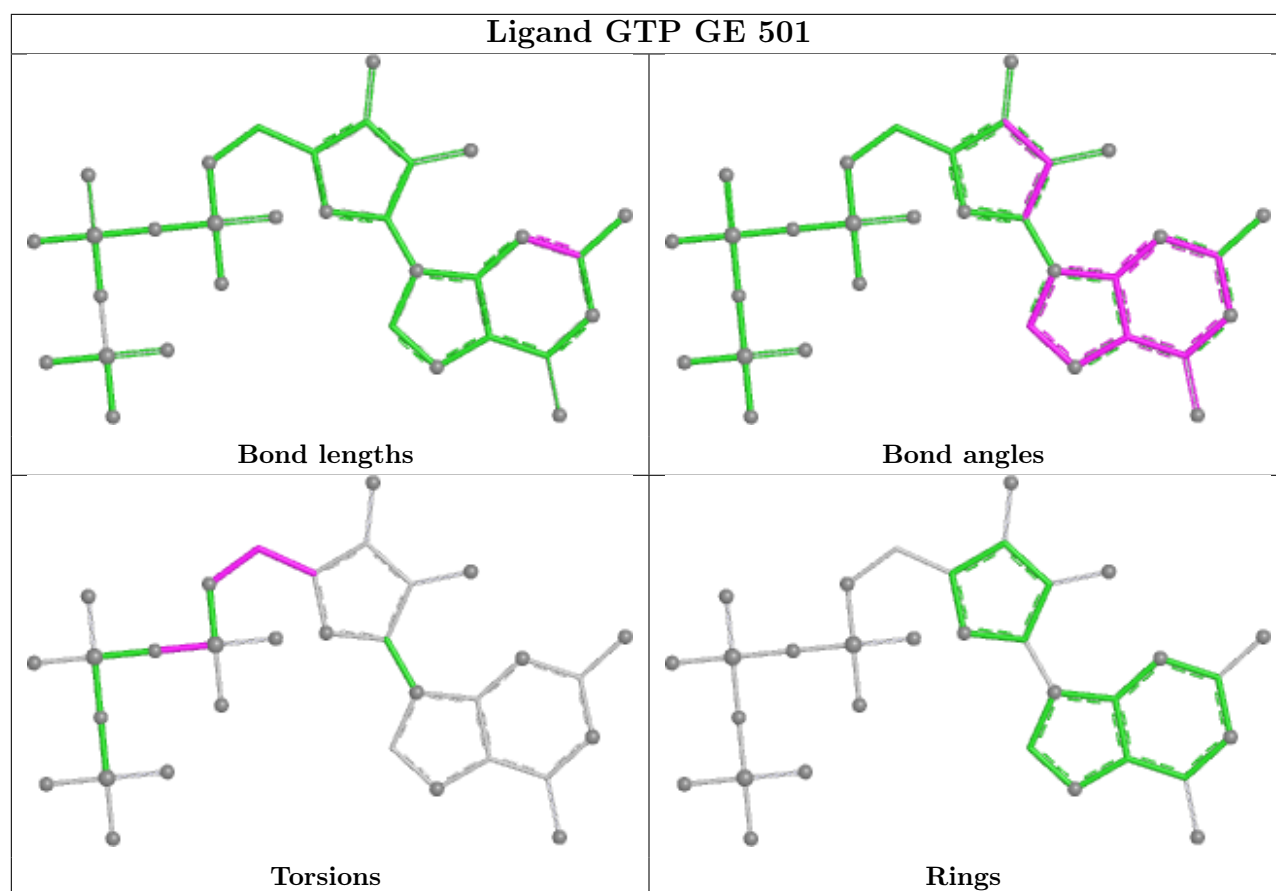


Ligand GTP HA 501

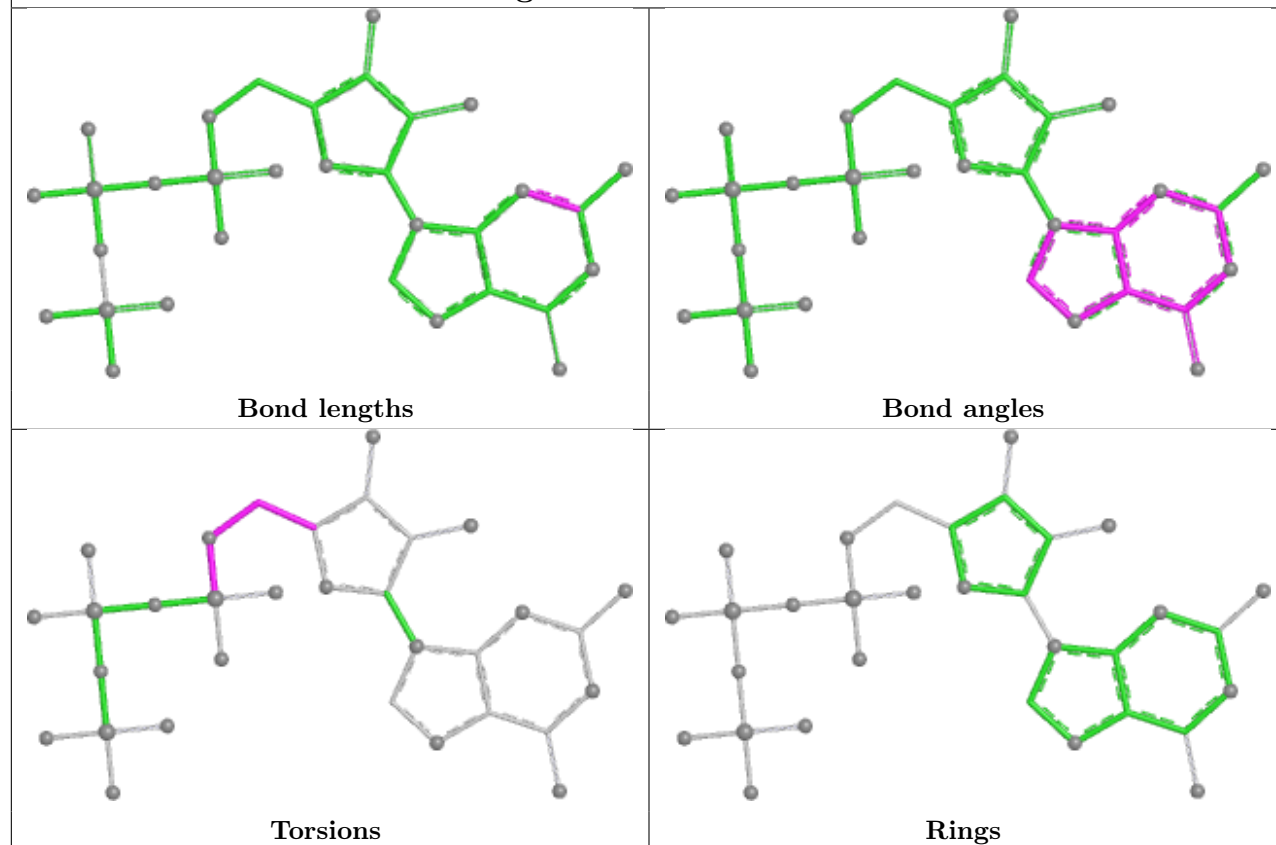


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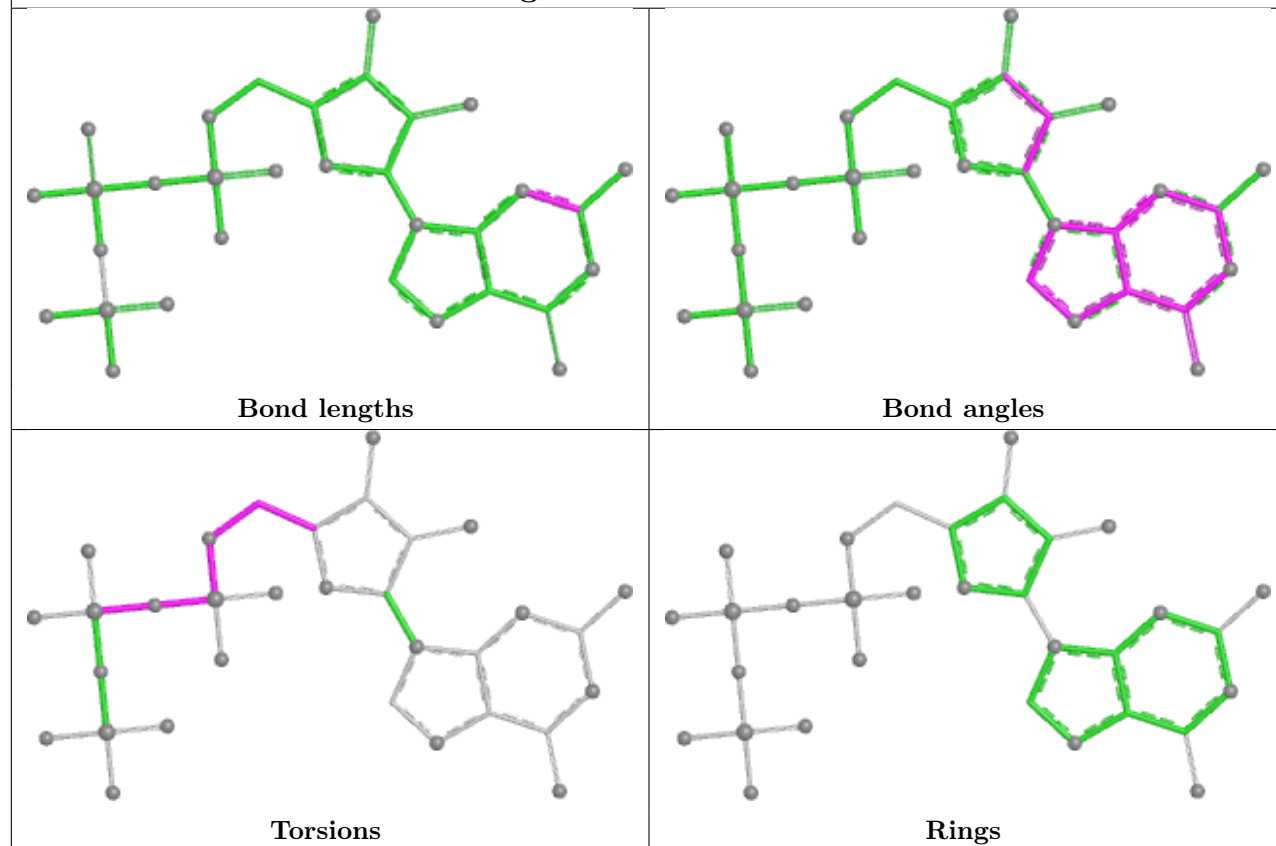




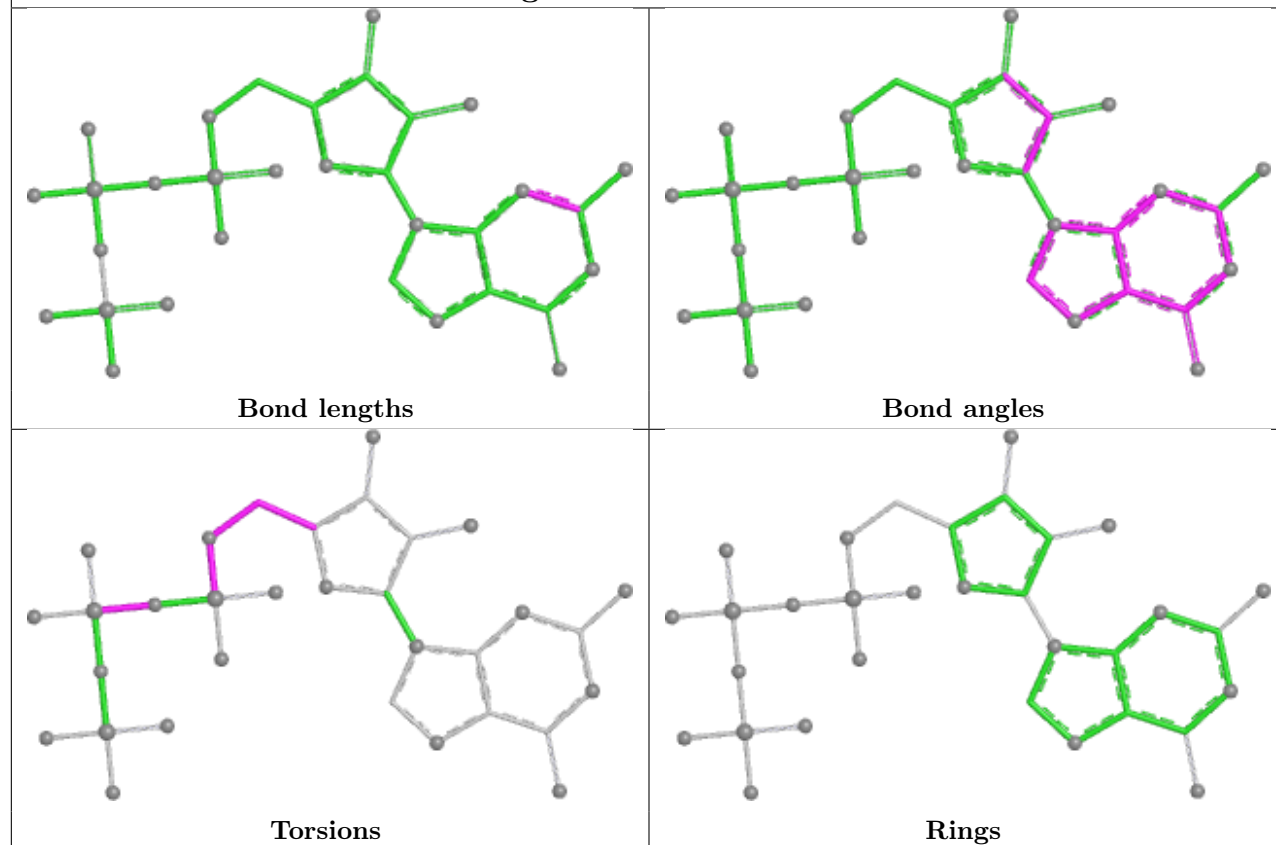
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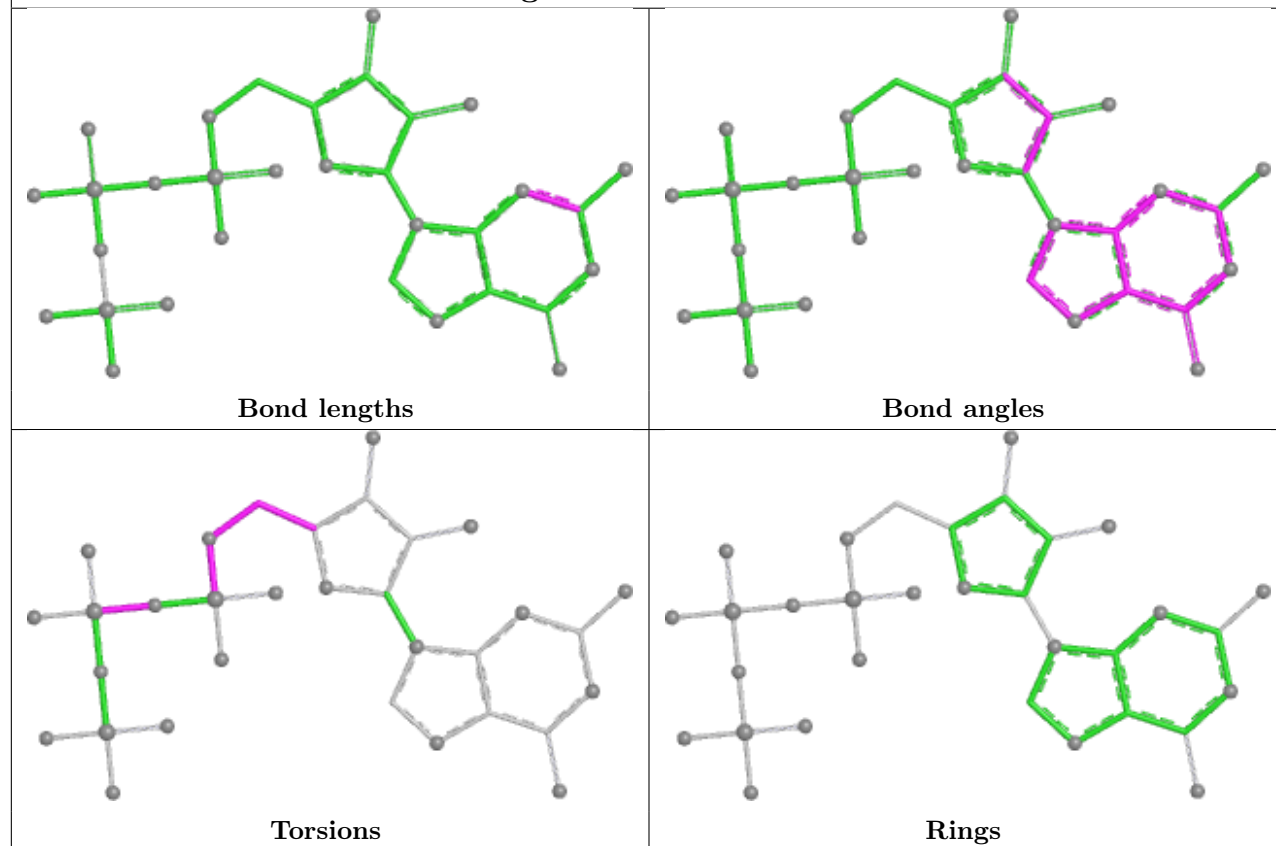
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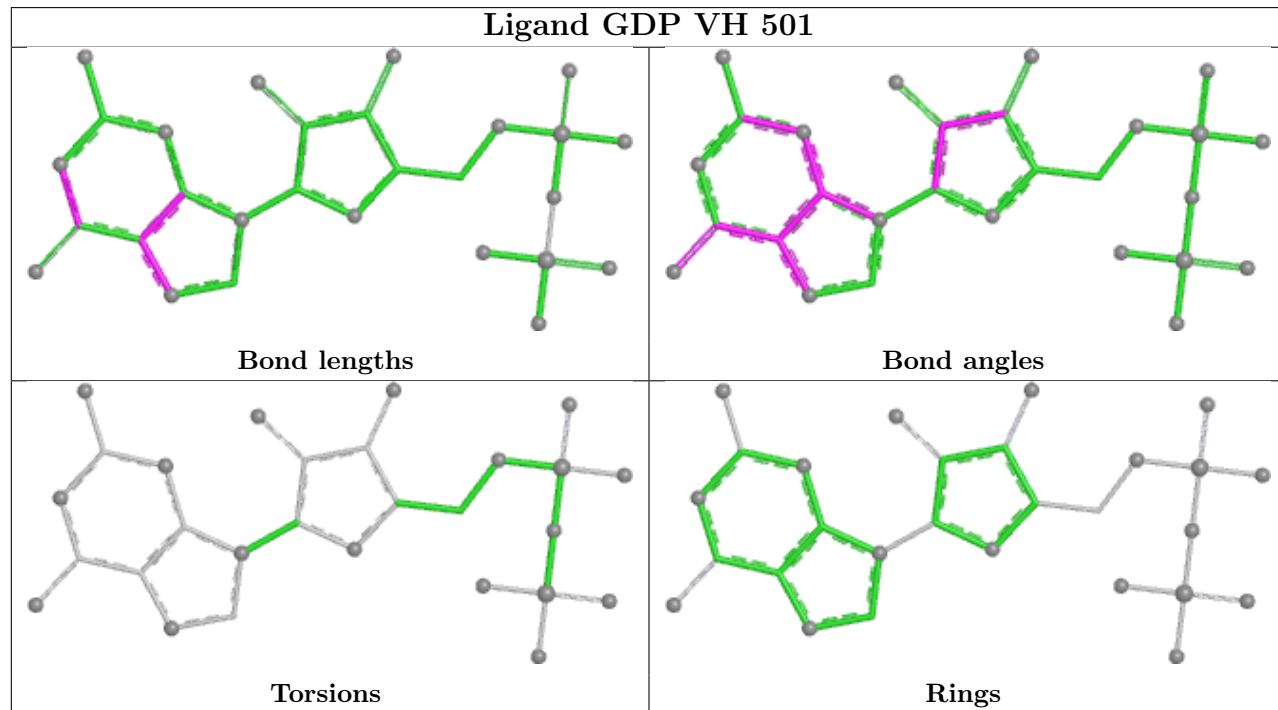
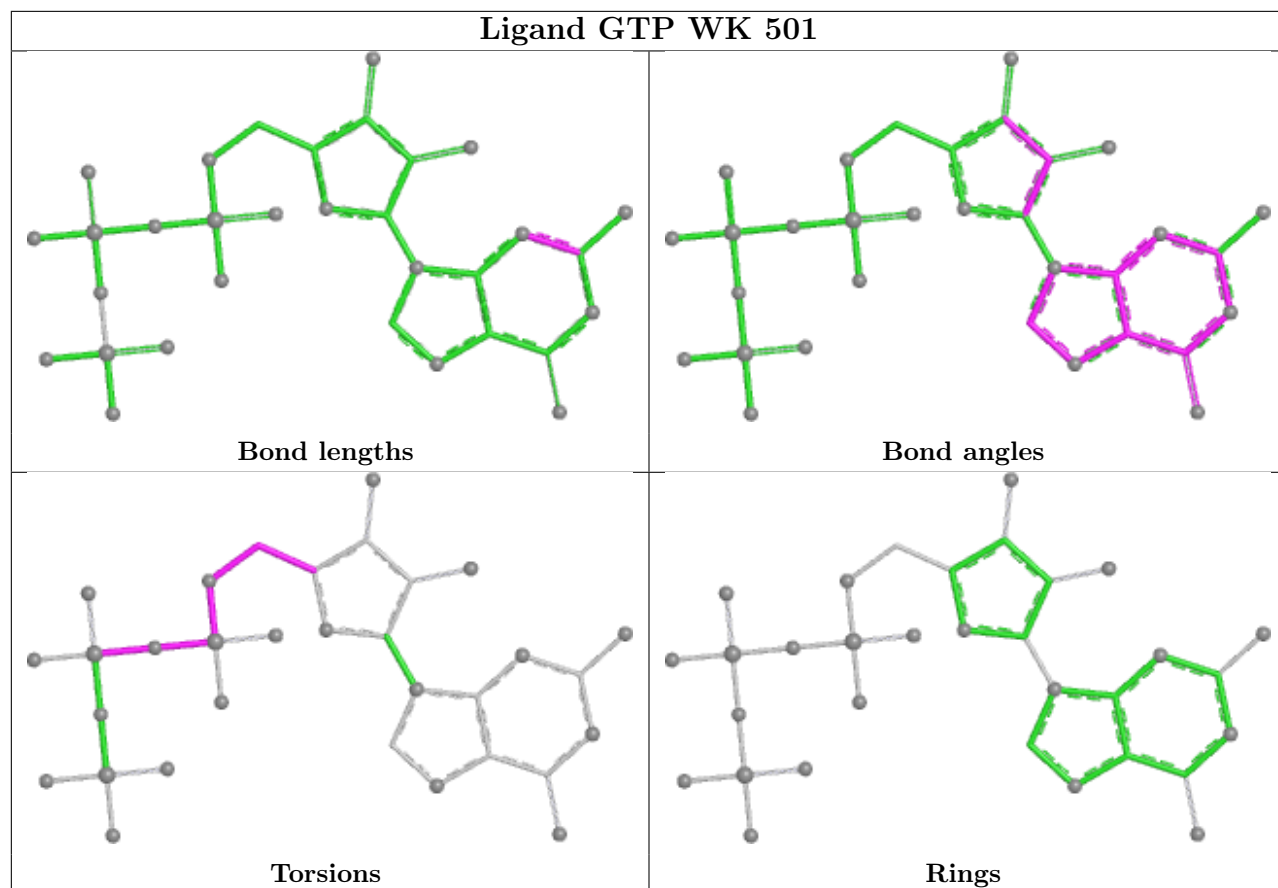


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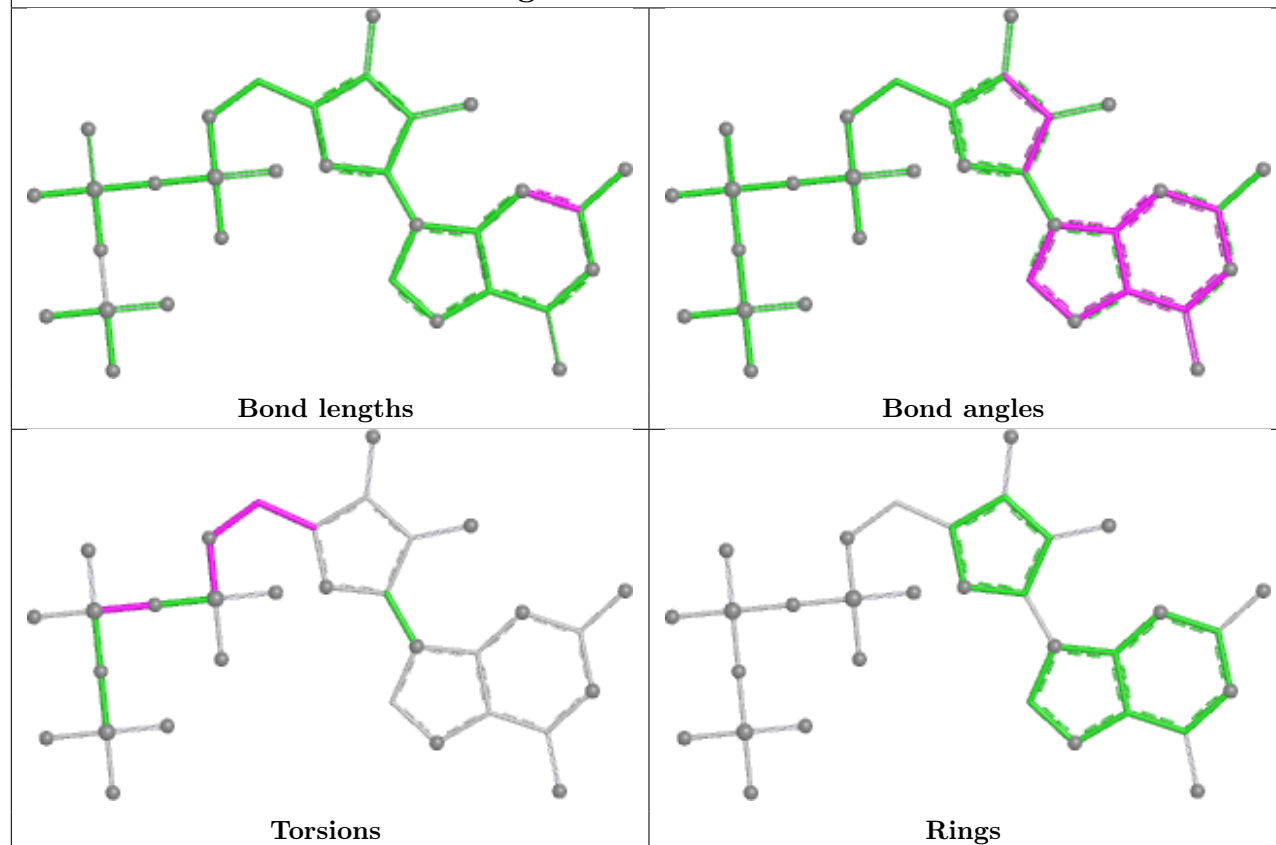


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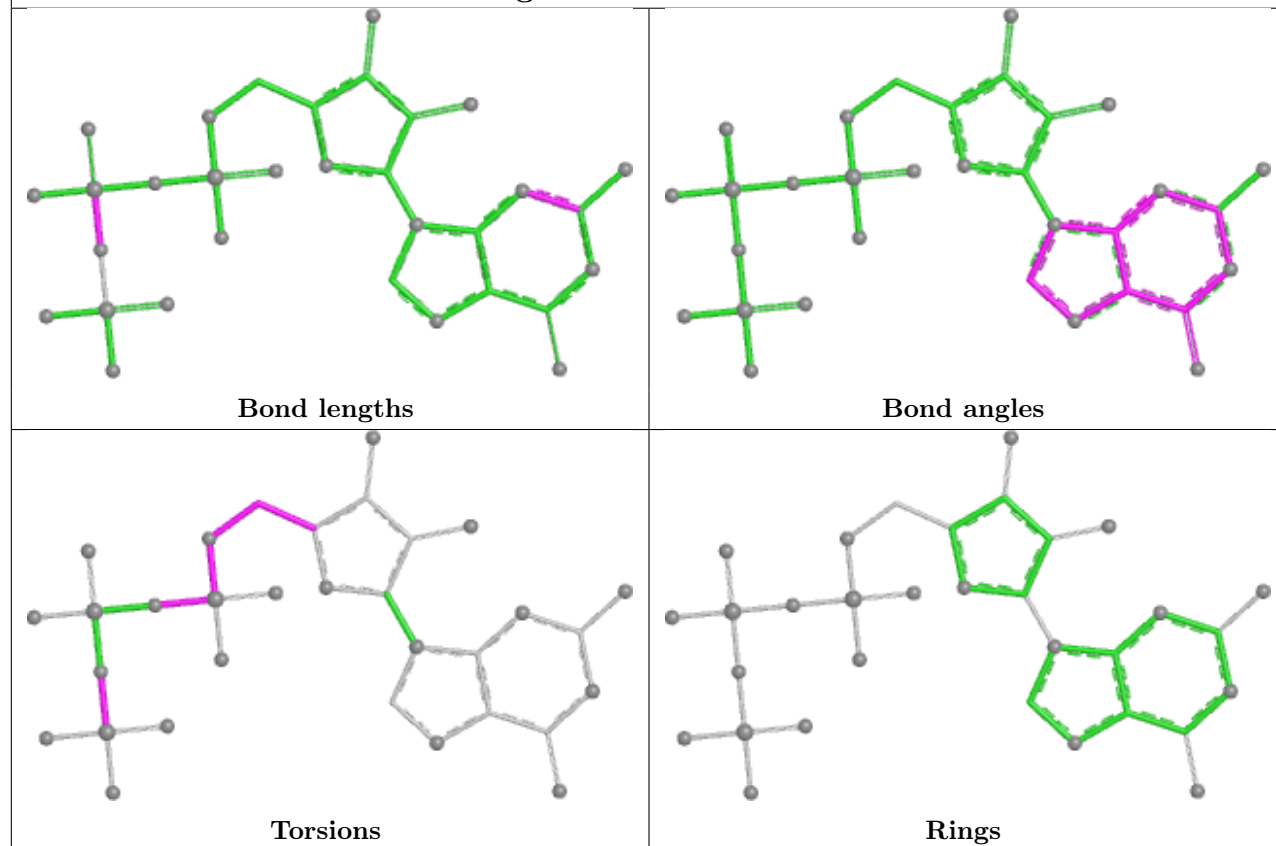




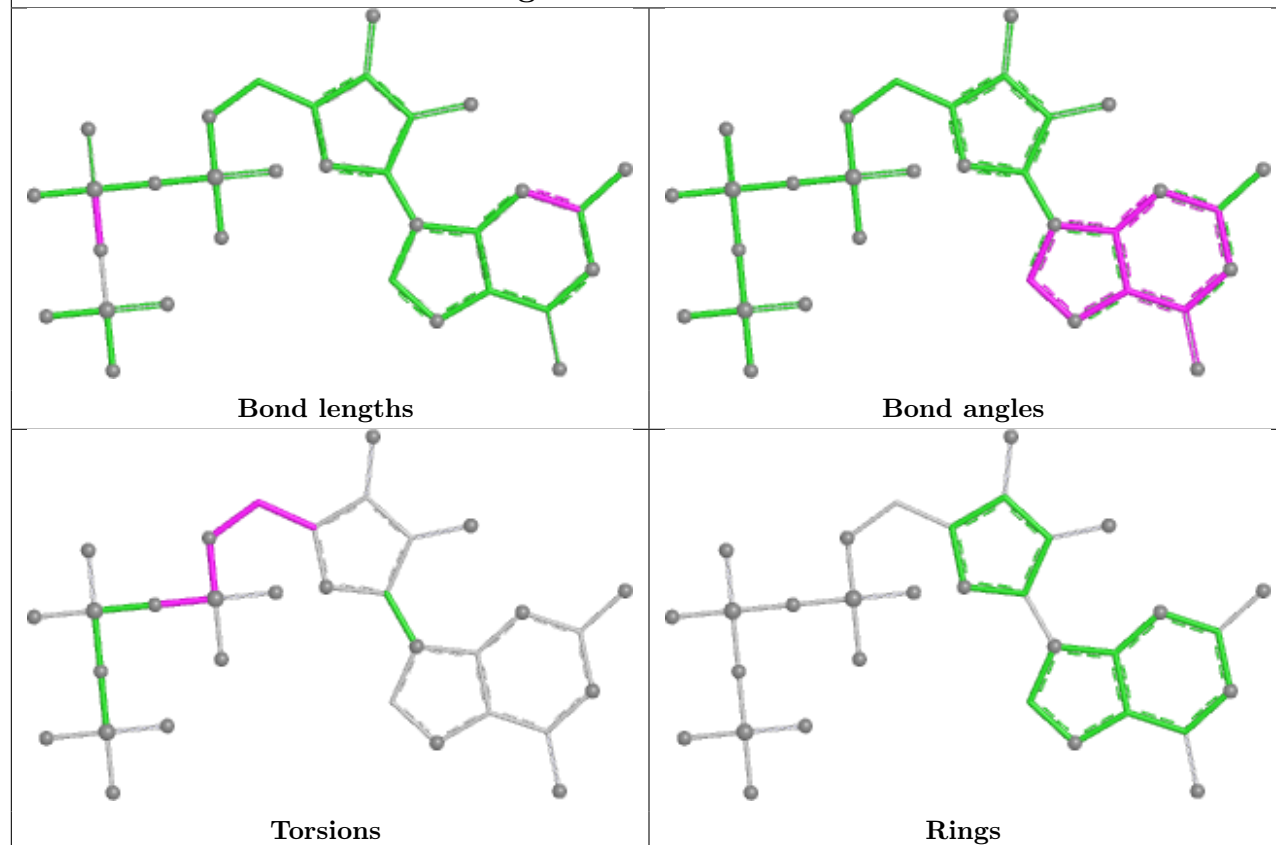
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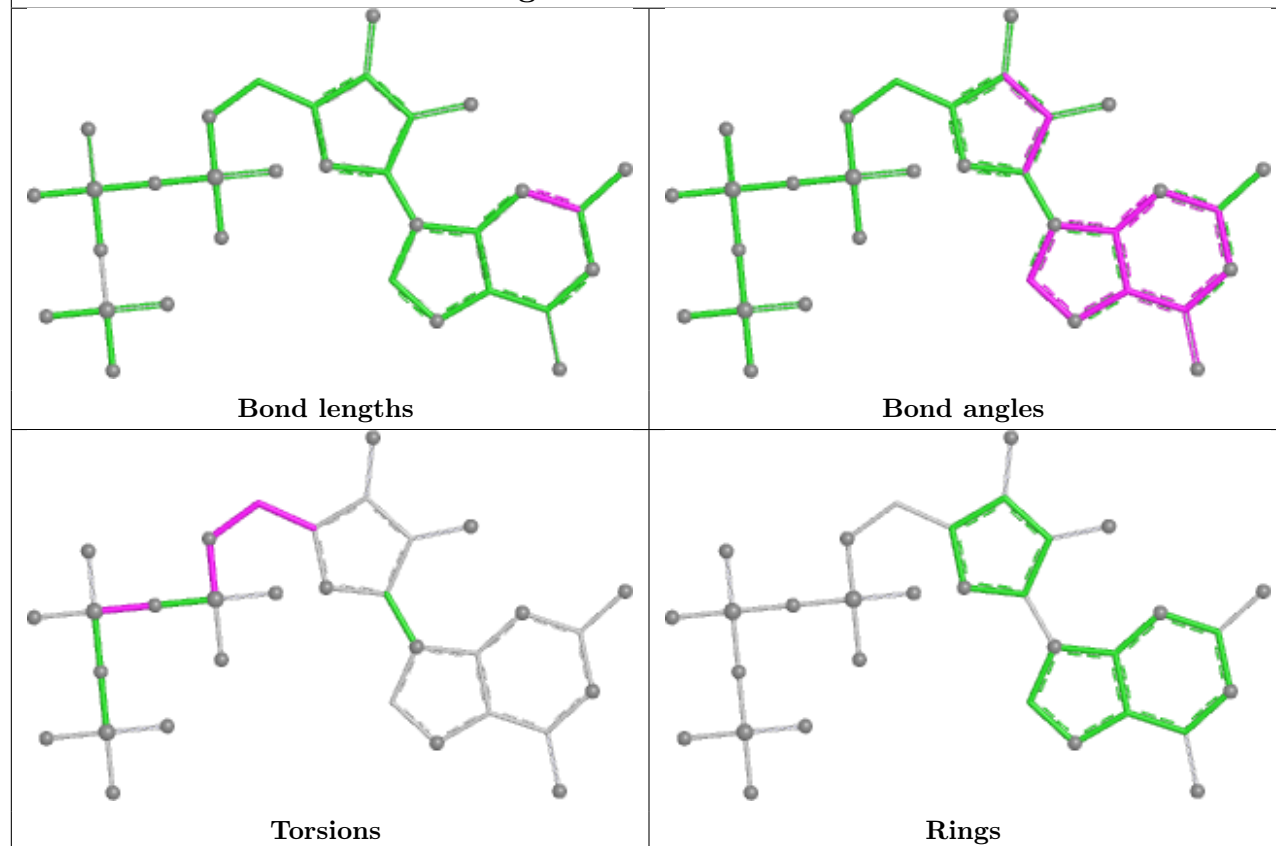
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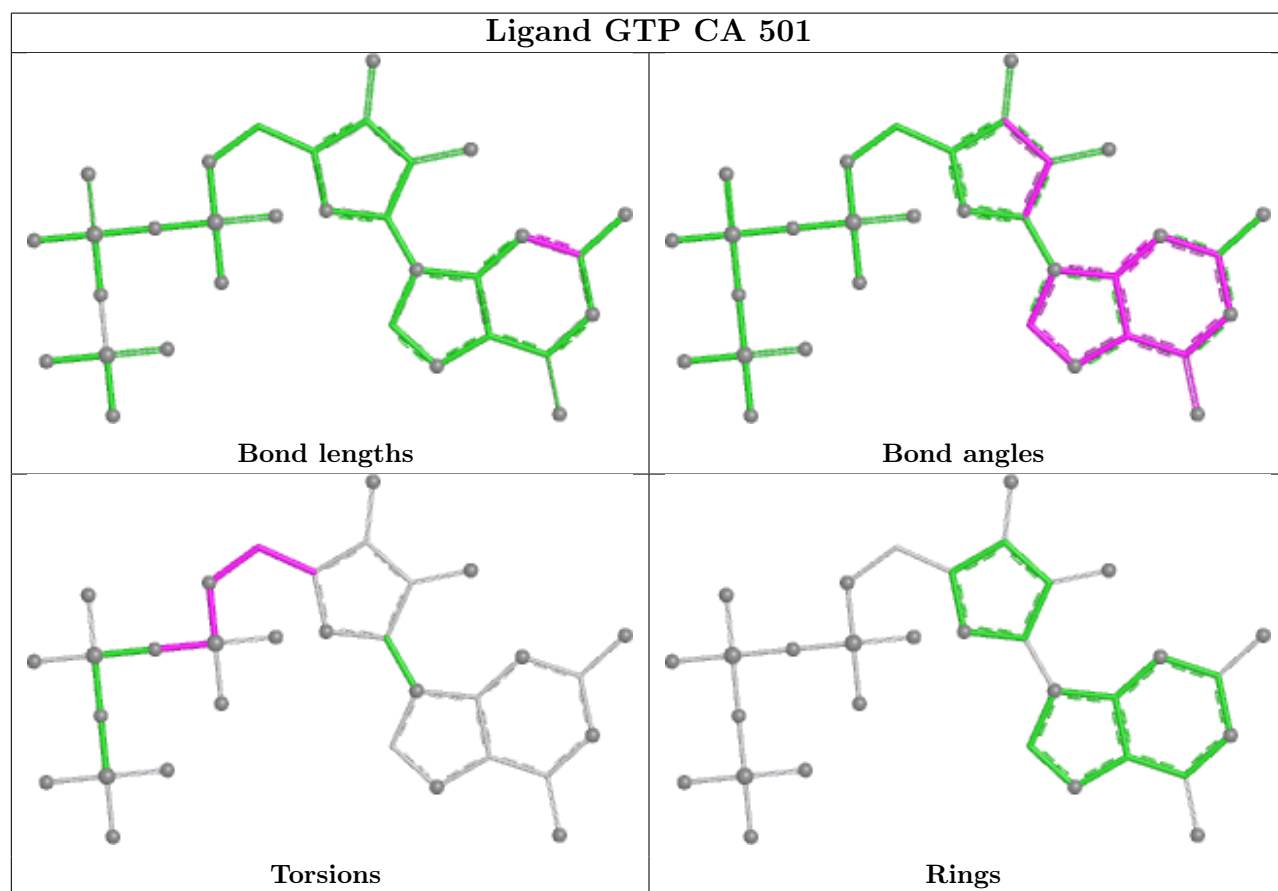
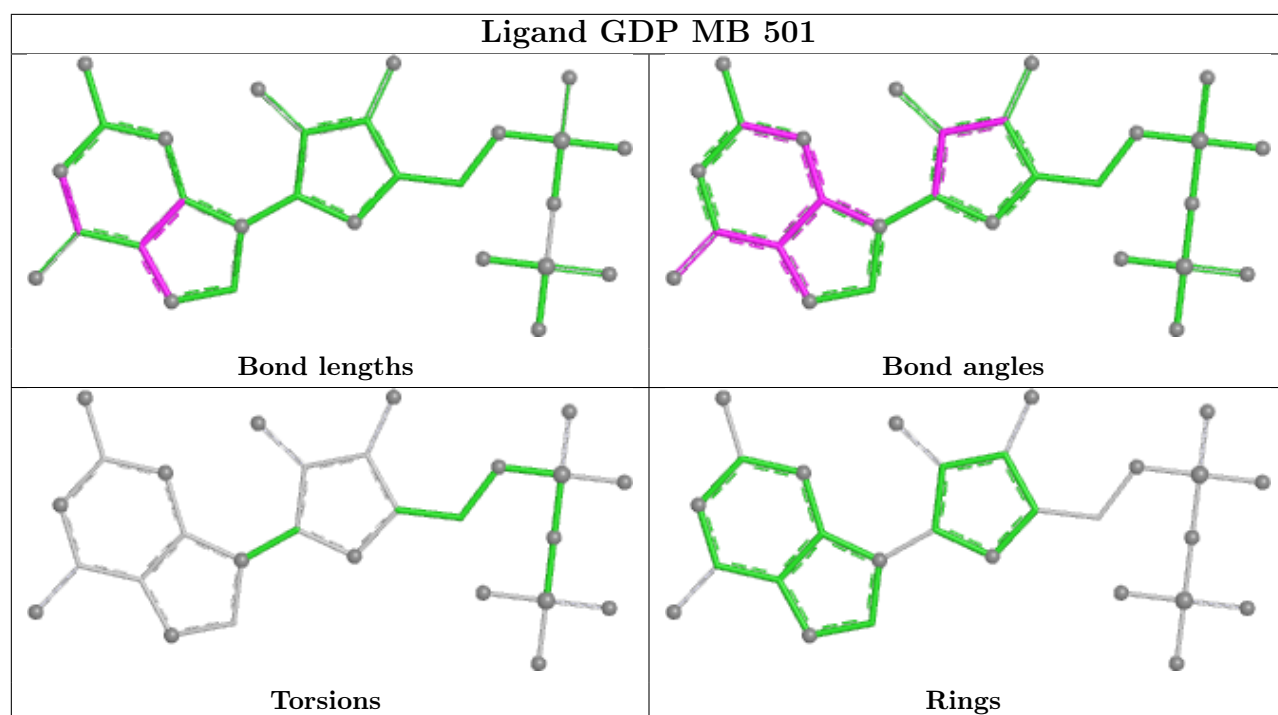


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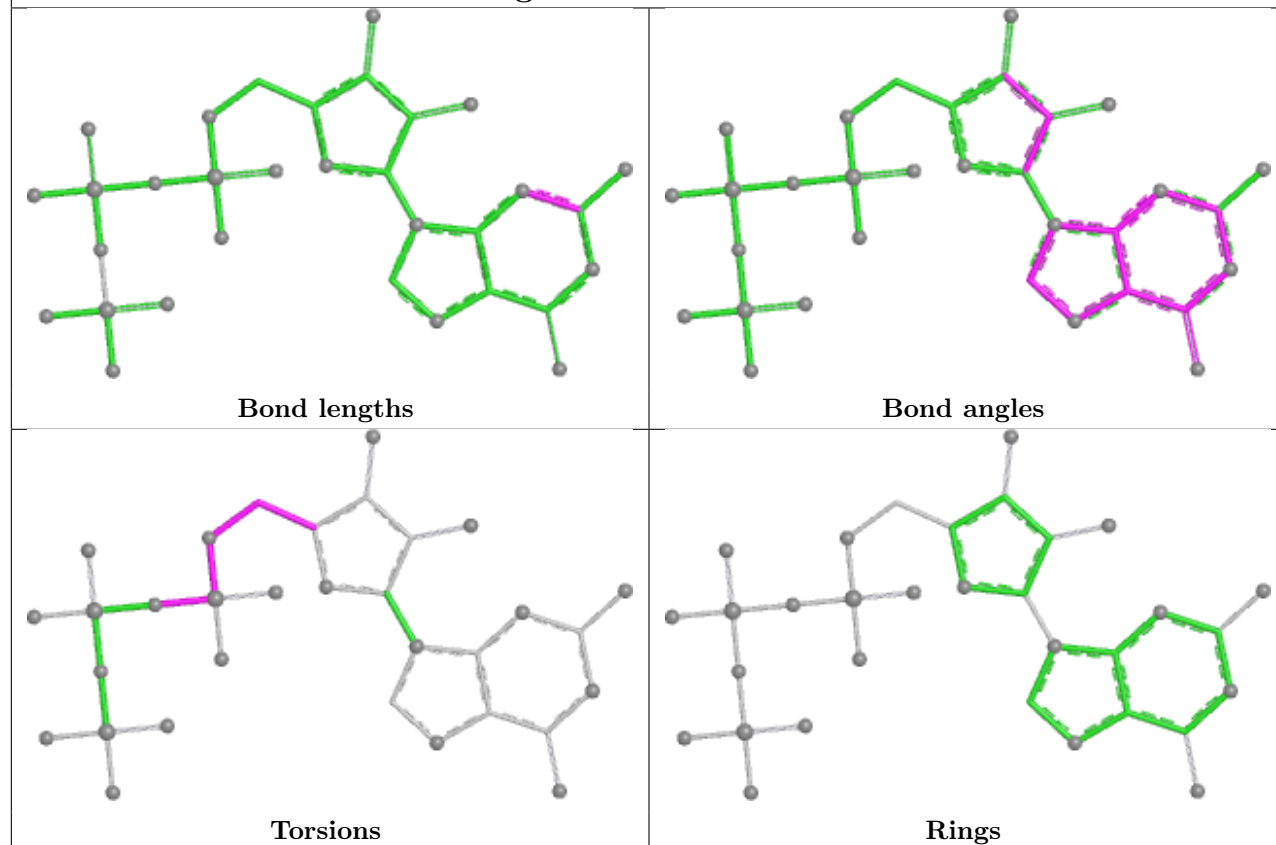


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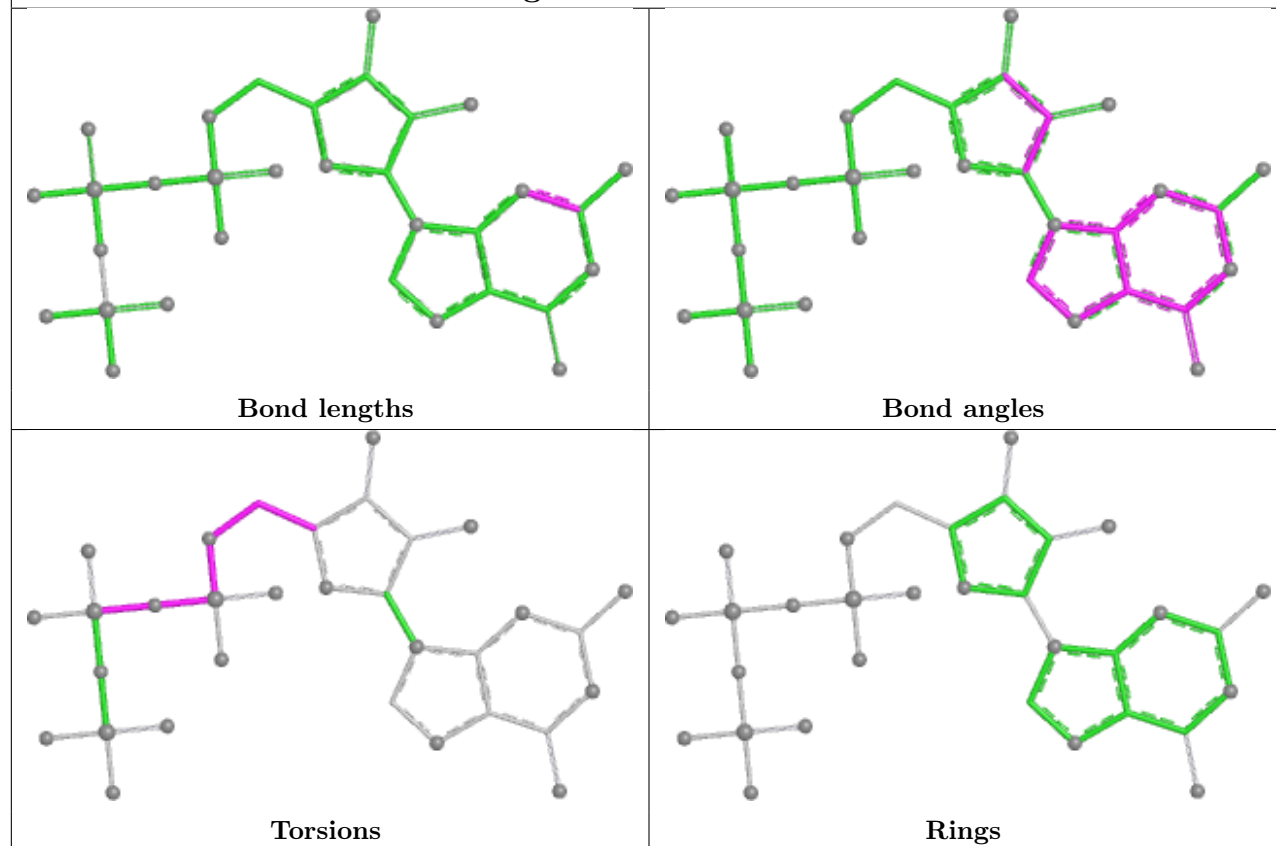


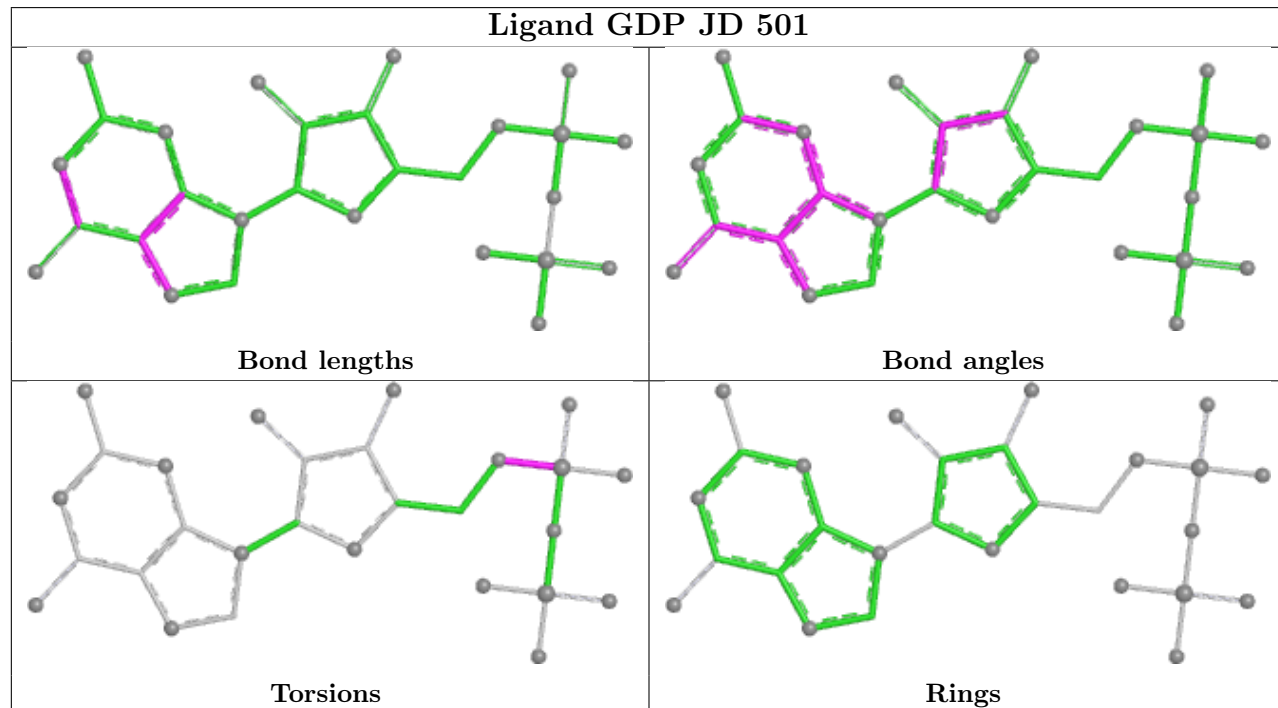
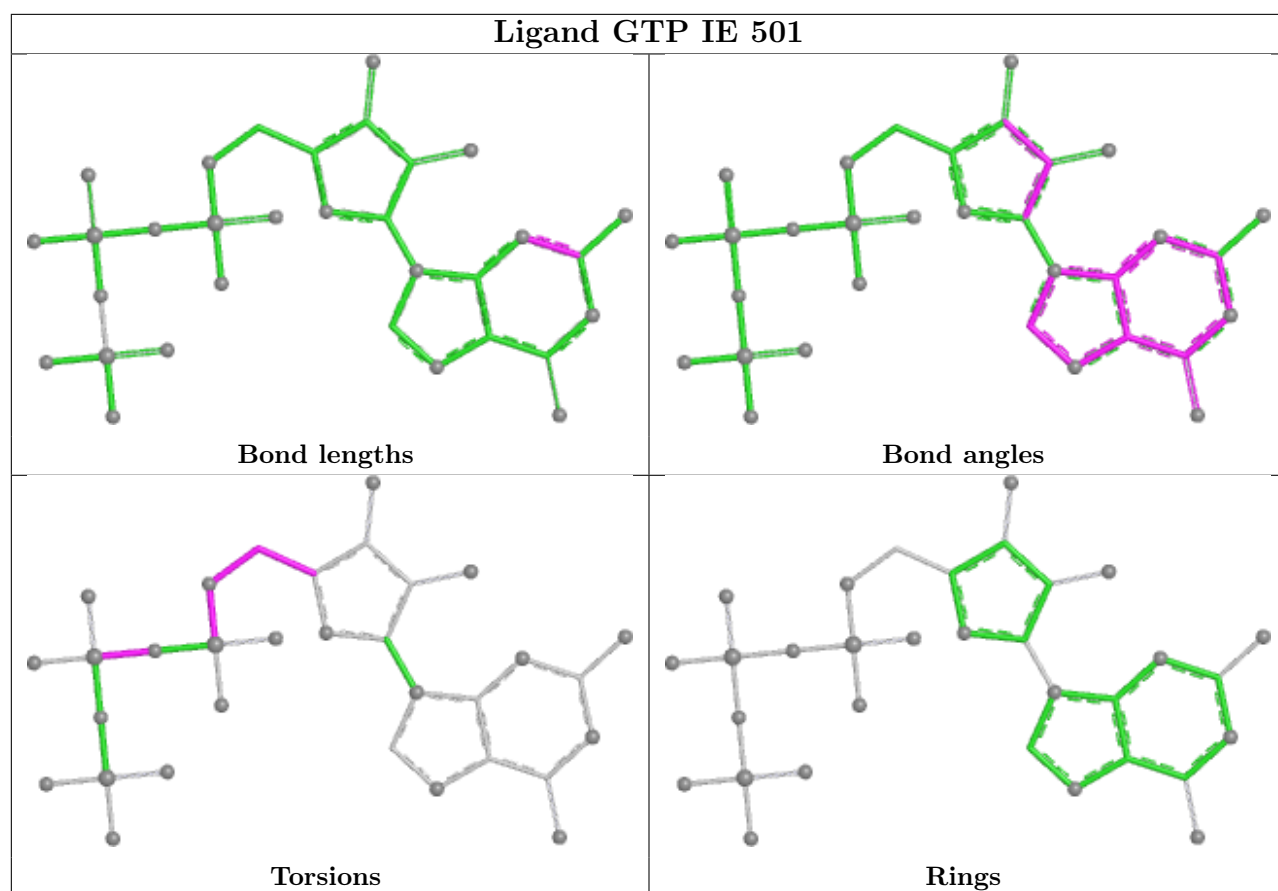


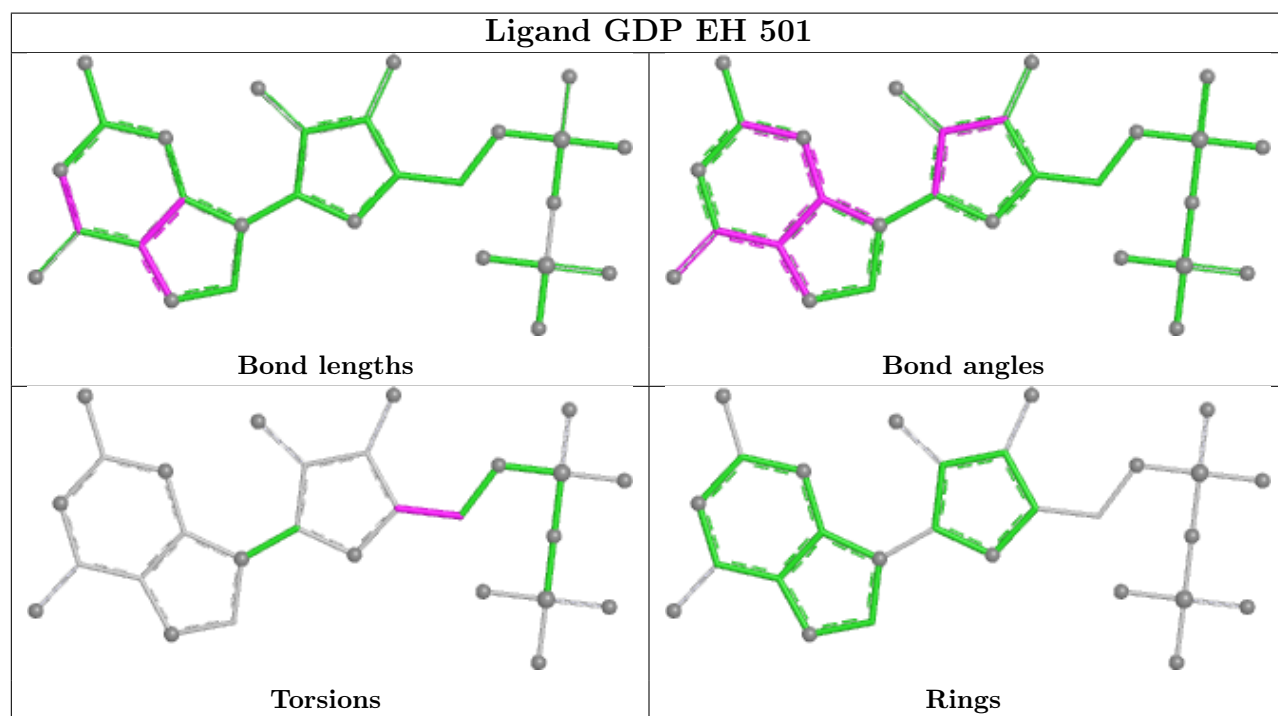
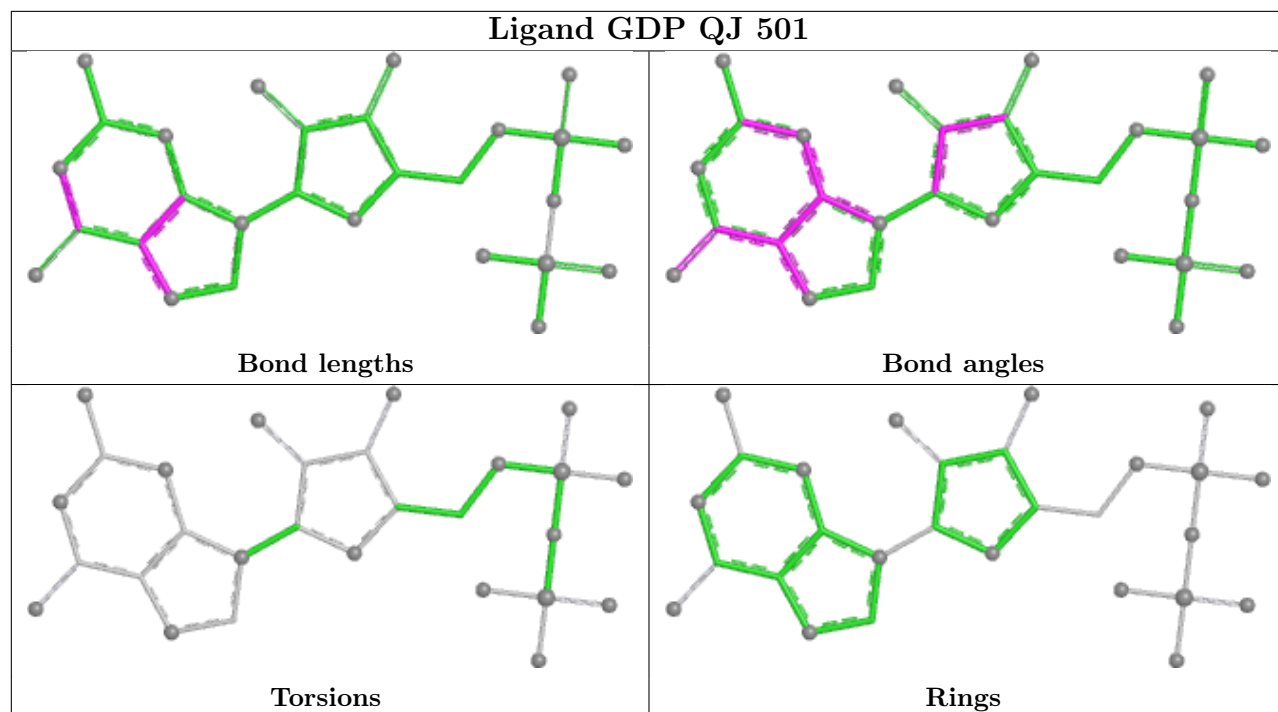
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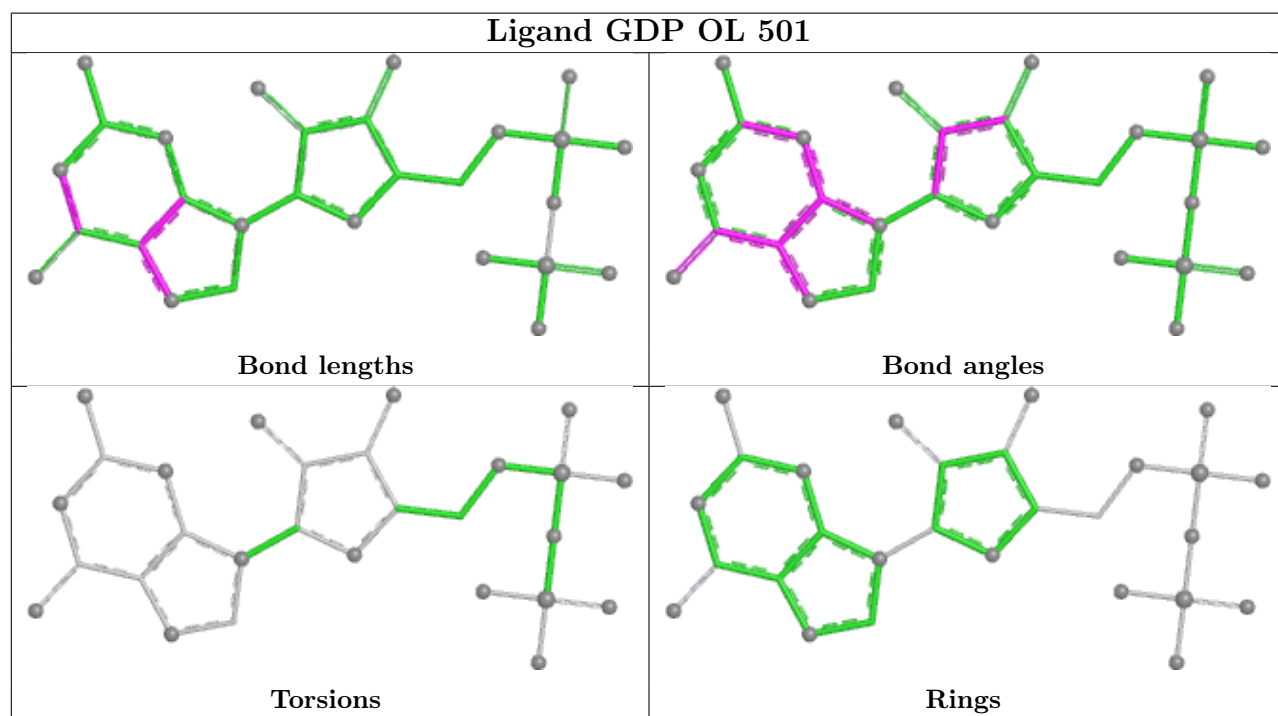
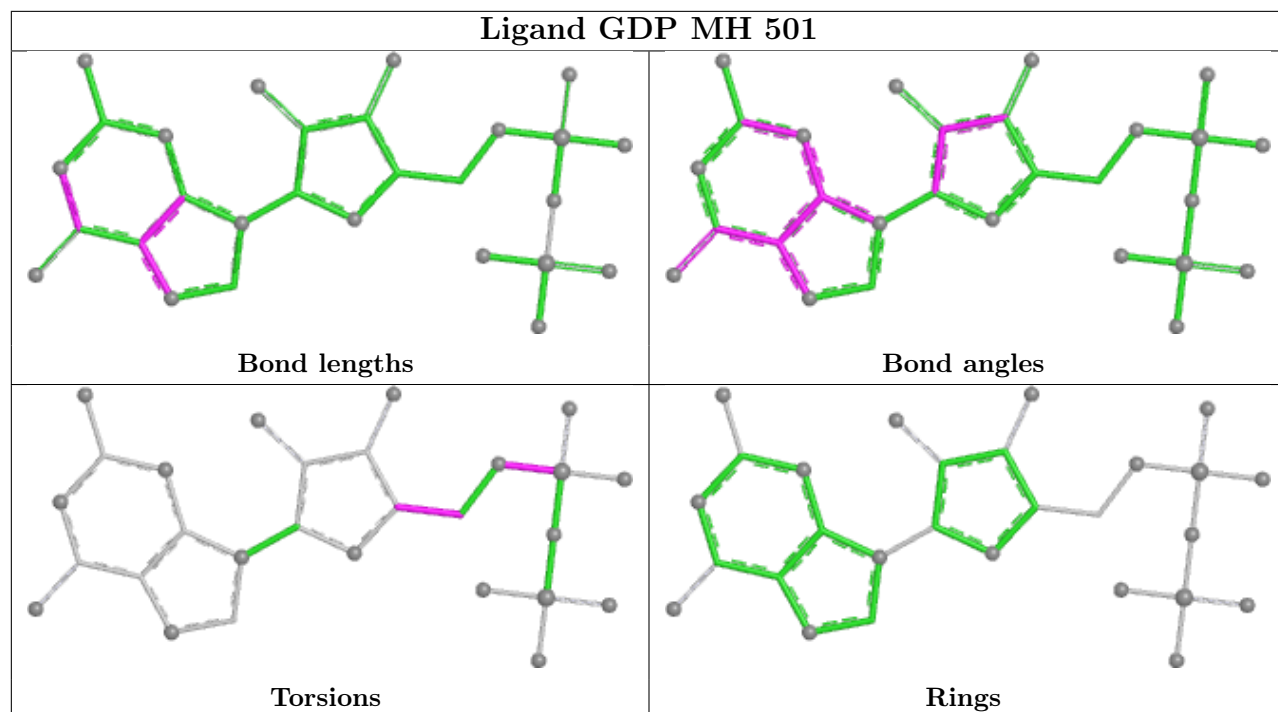


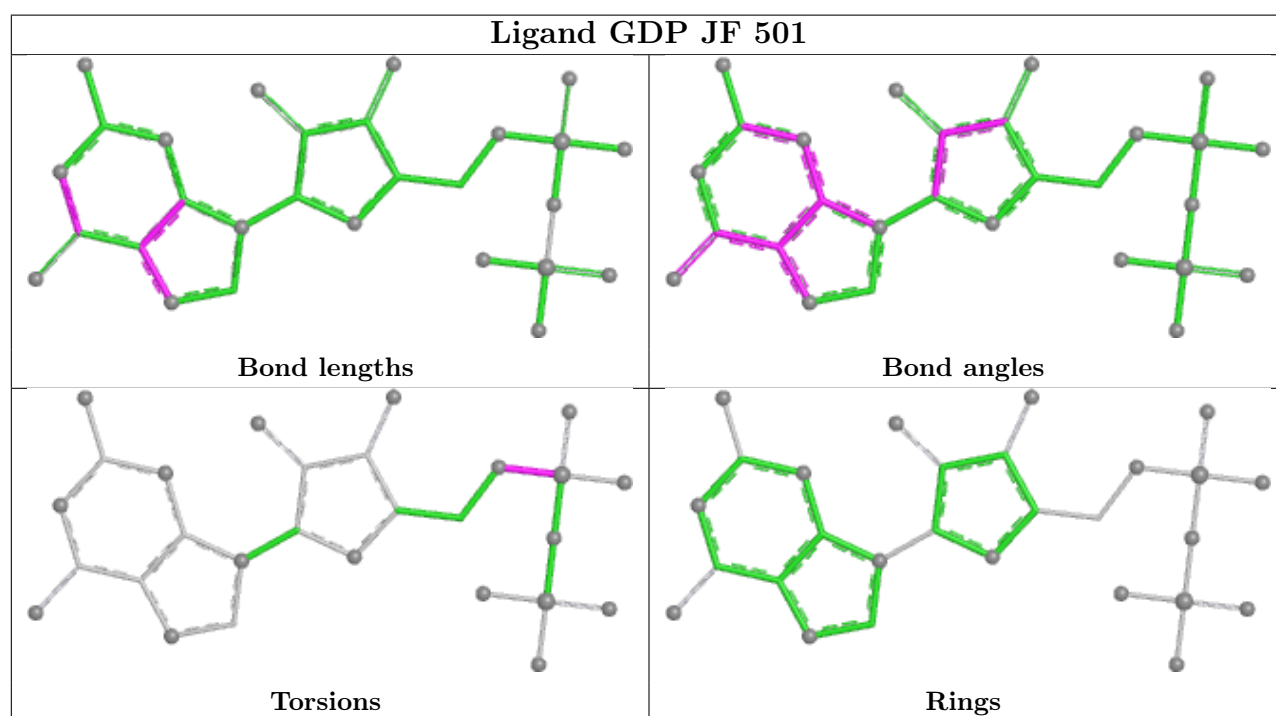
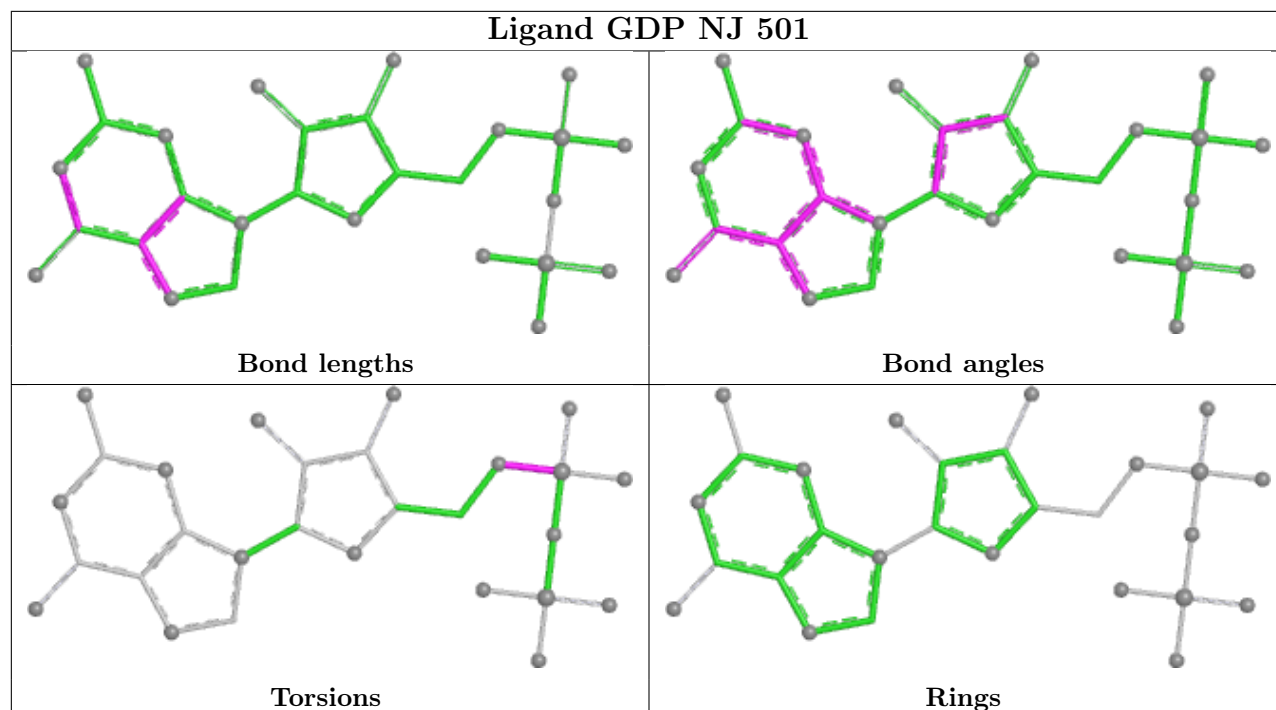
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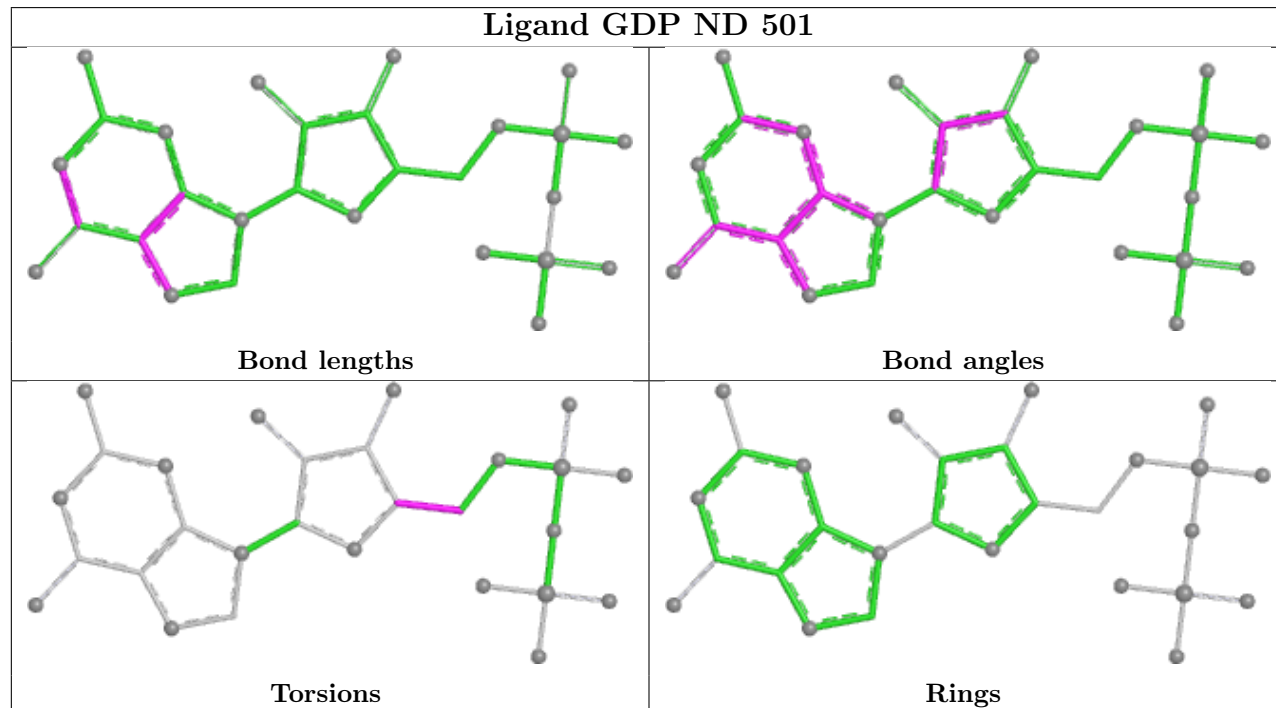
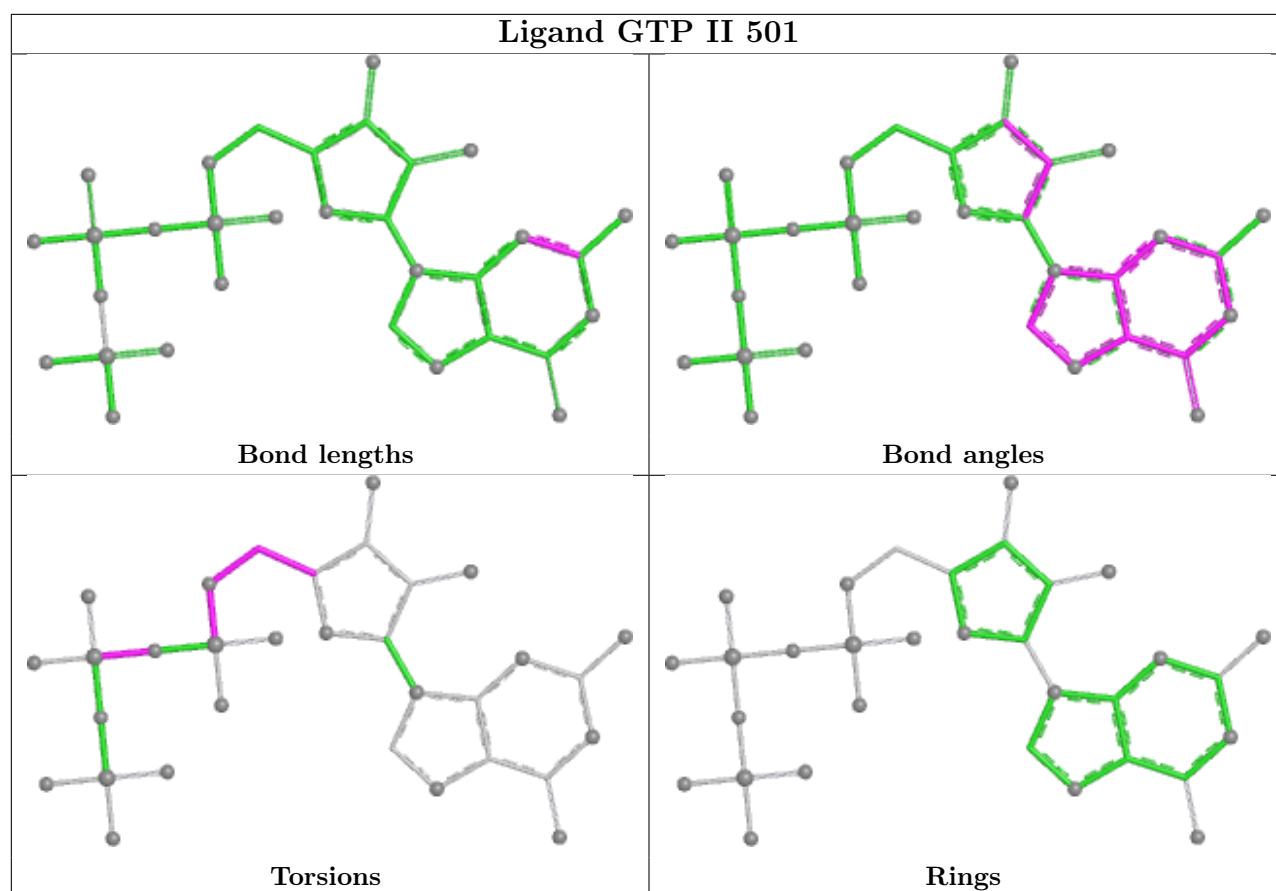


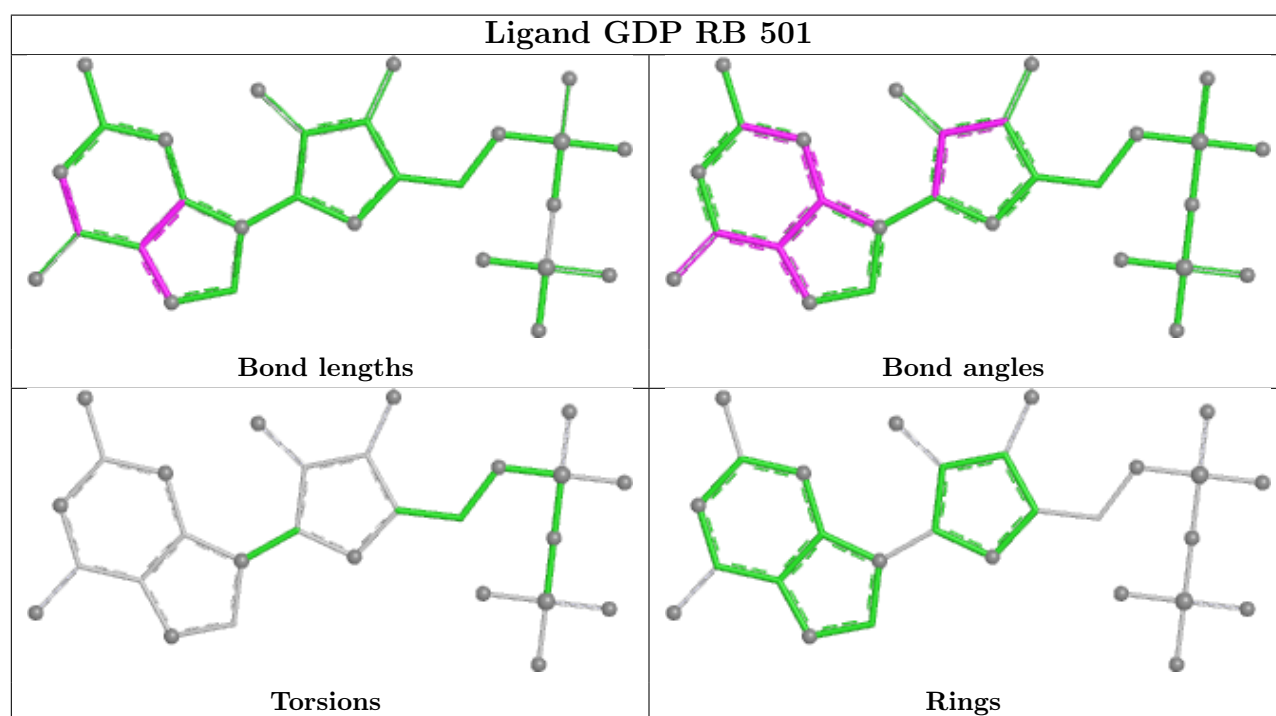
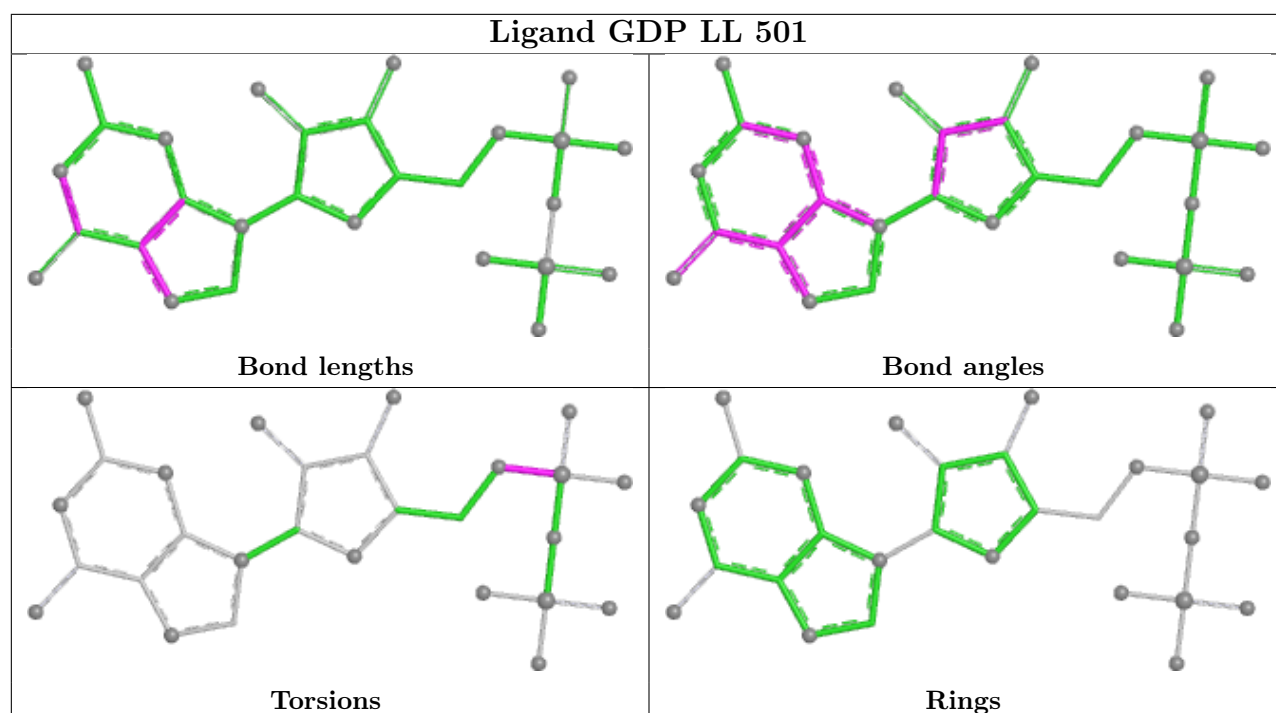


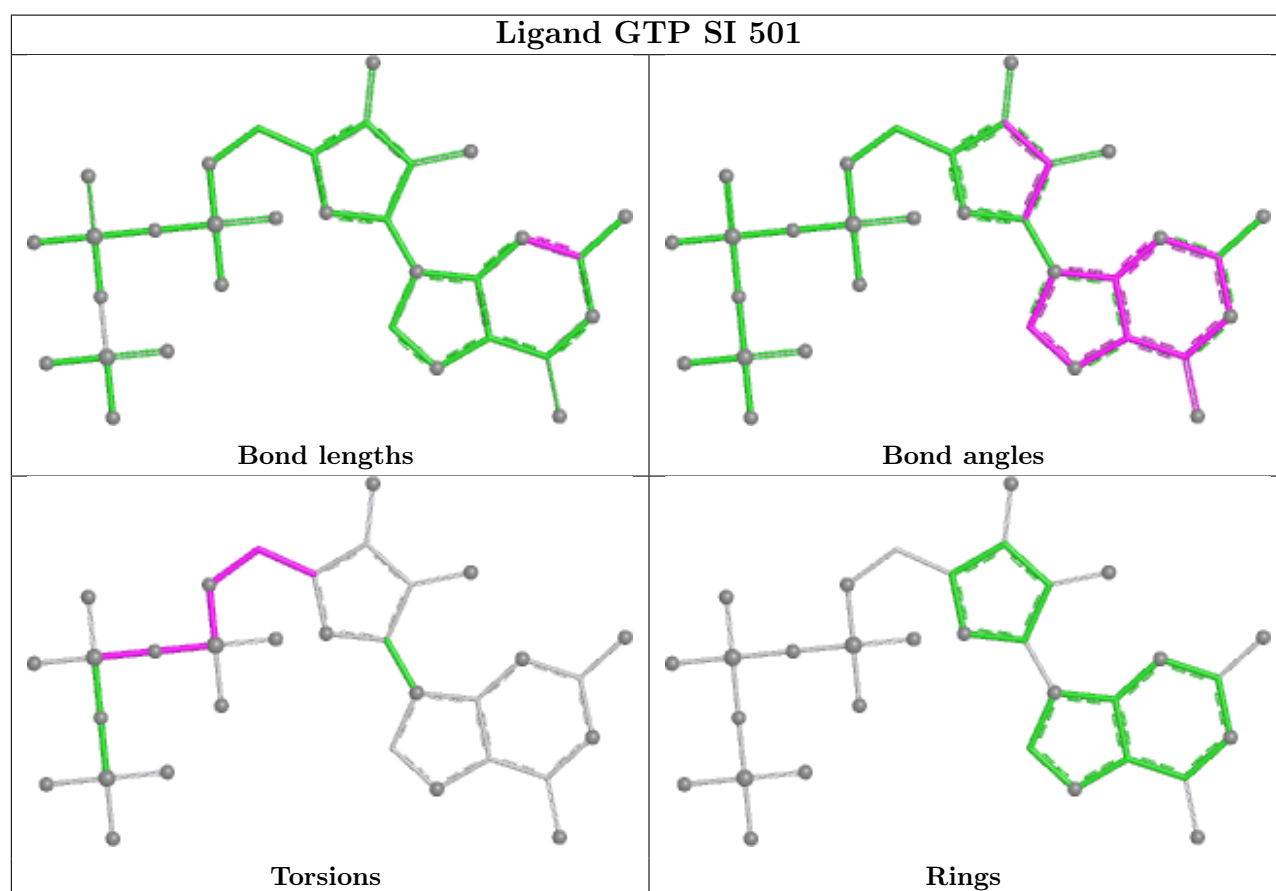
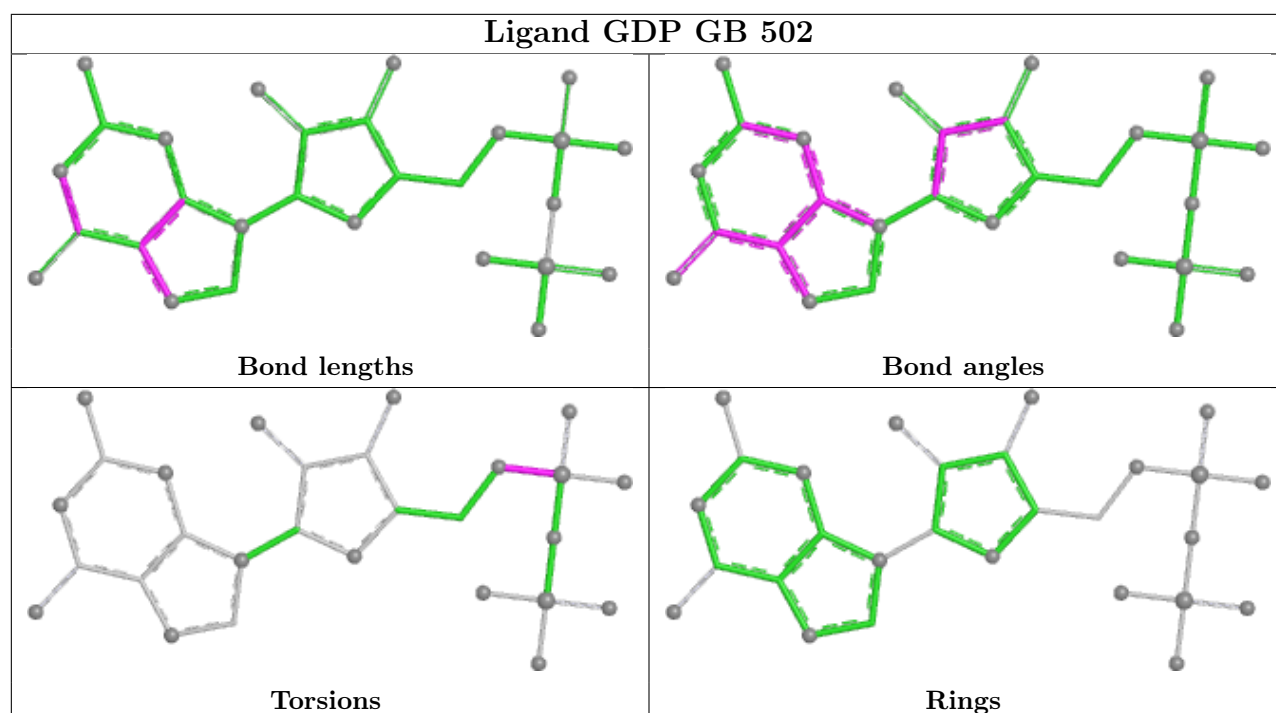


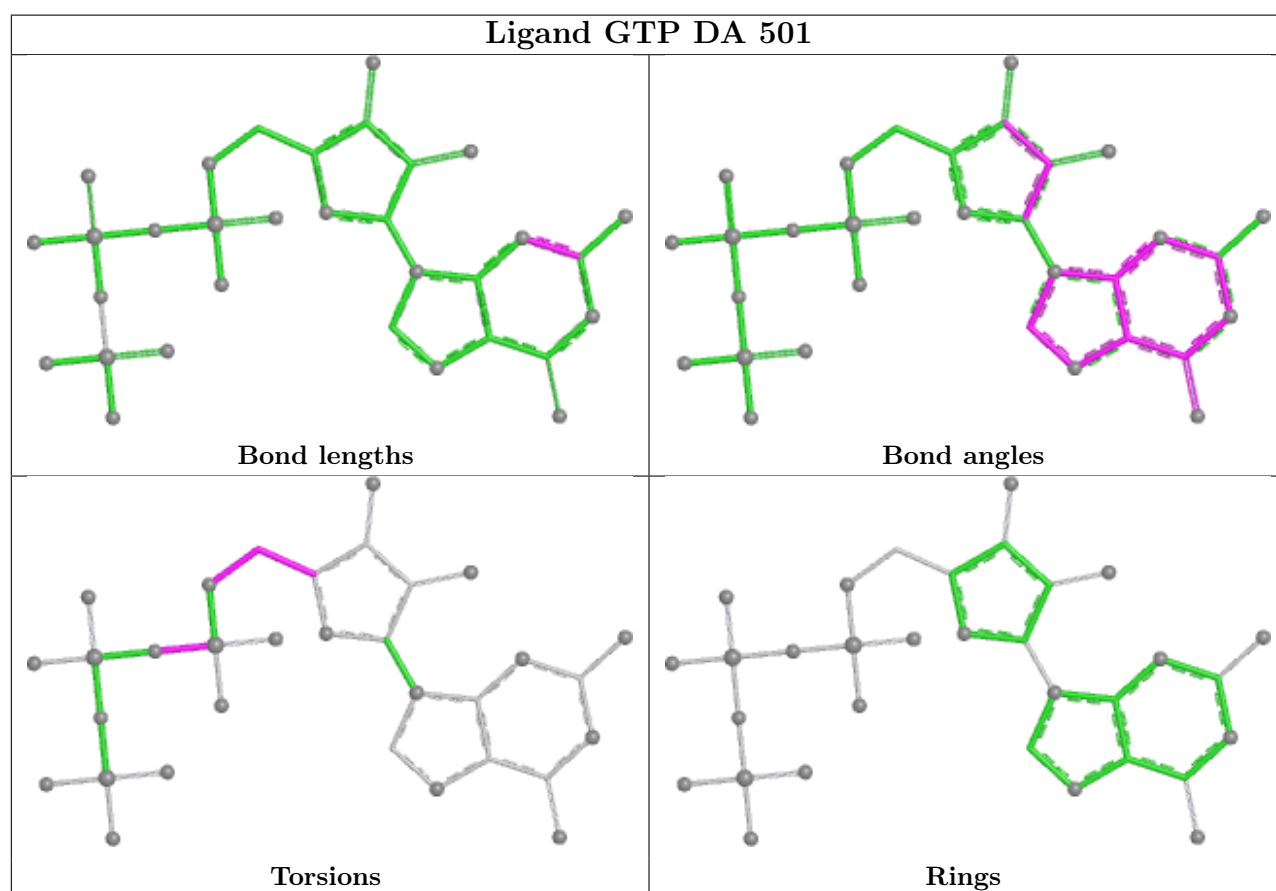
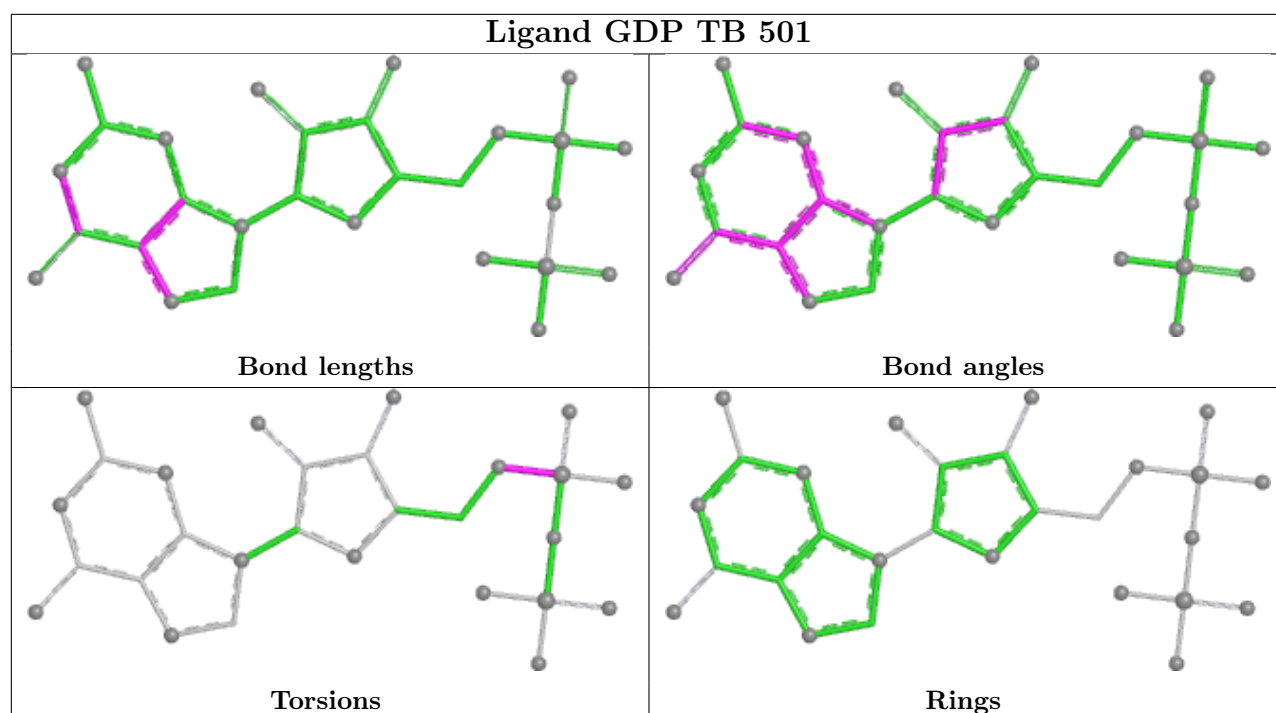




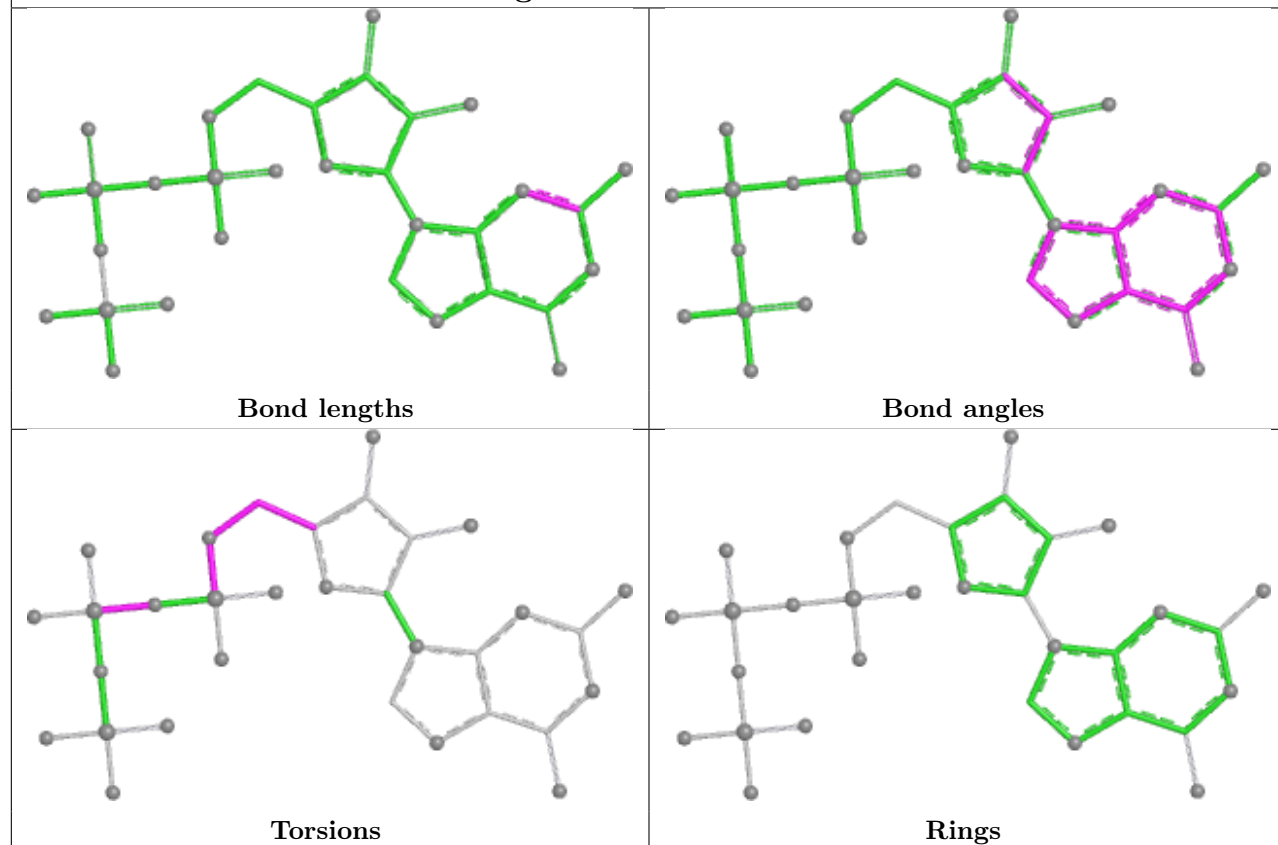




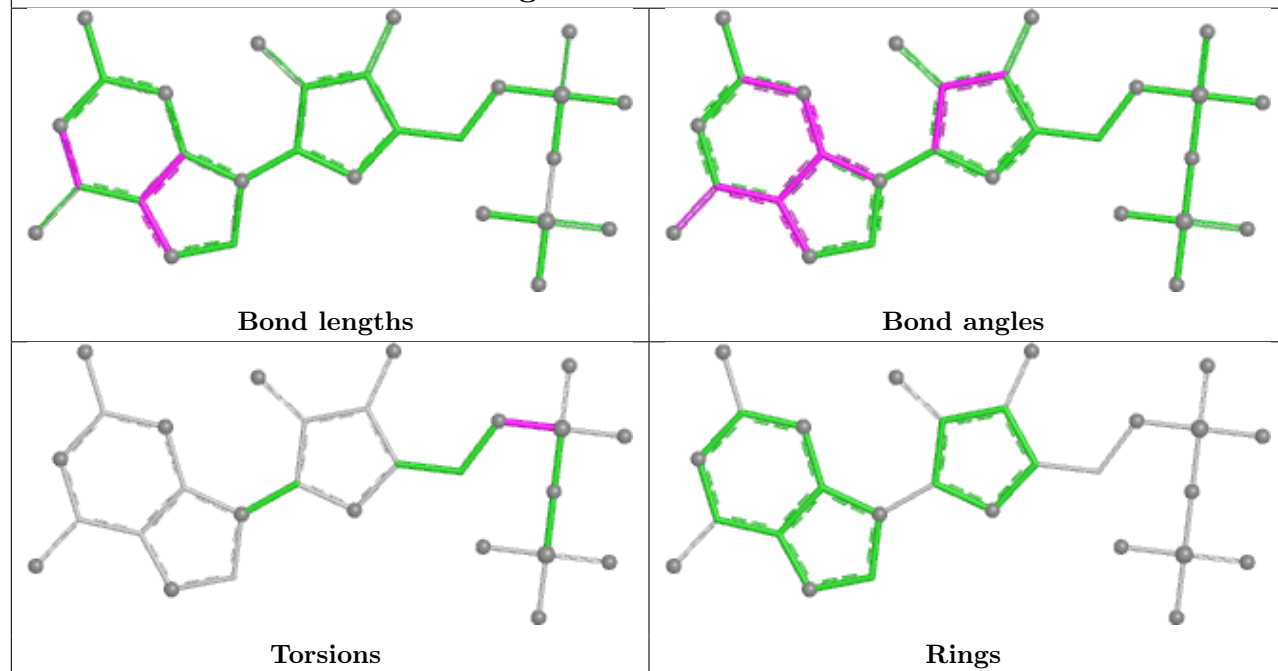




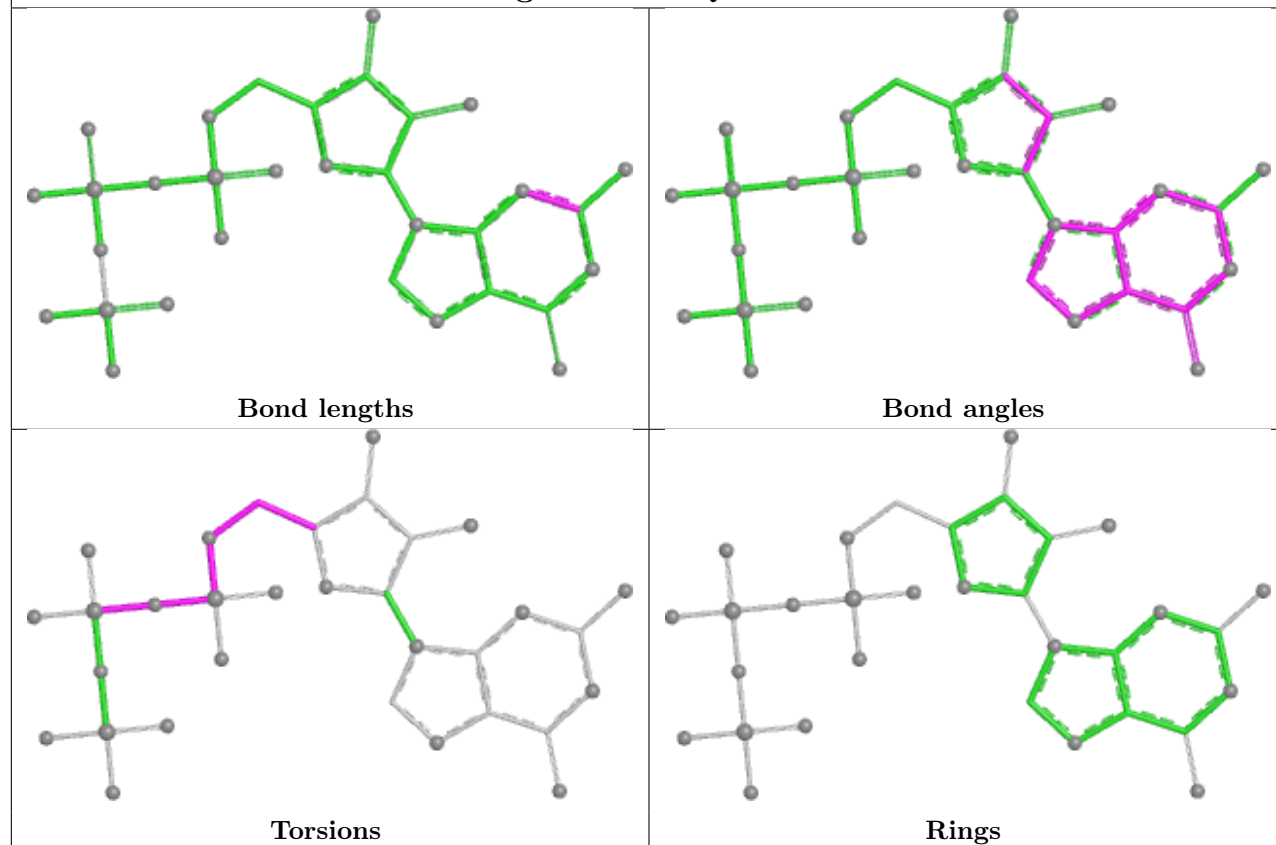
Ligand GTP EM 501



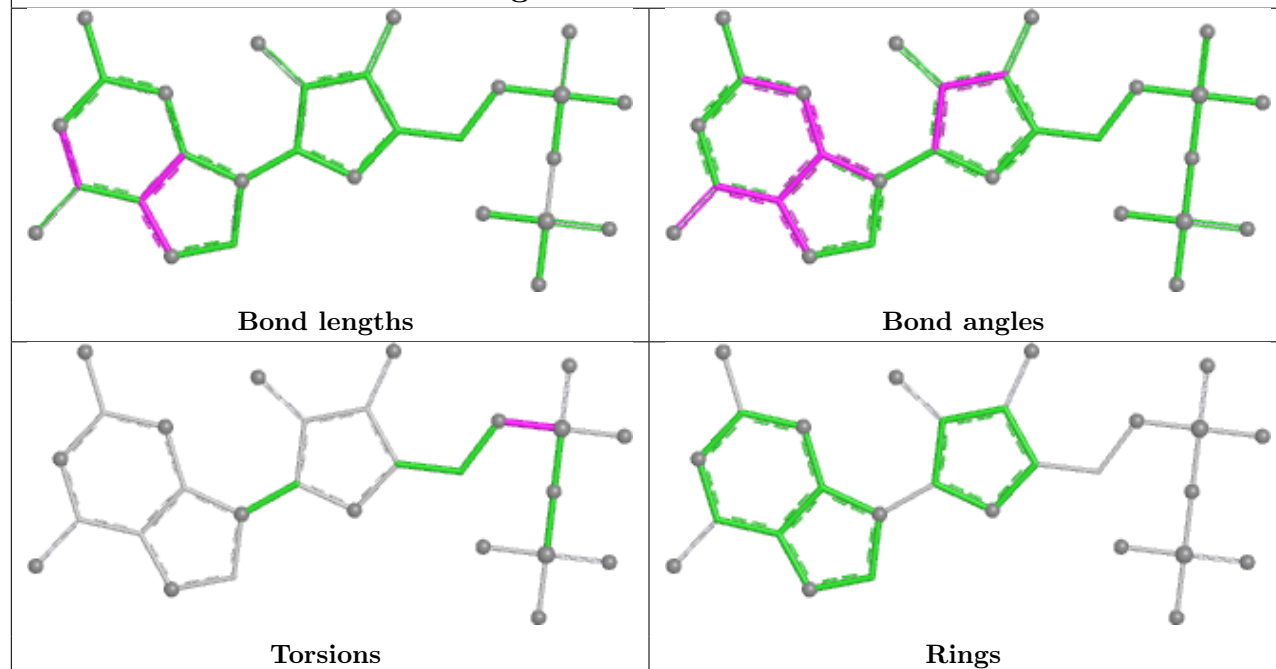
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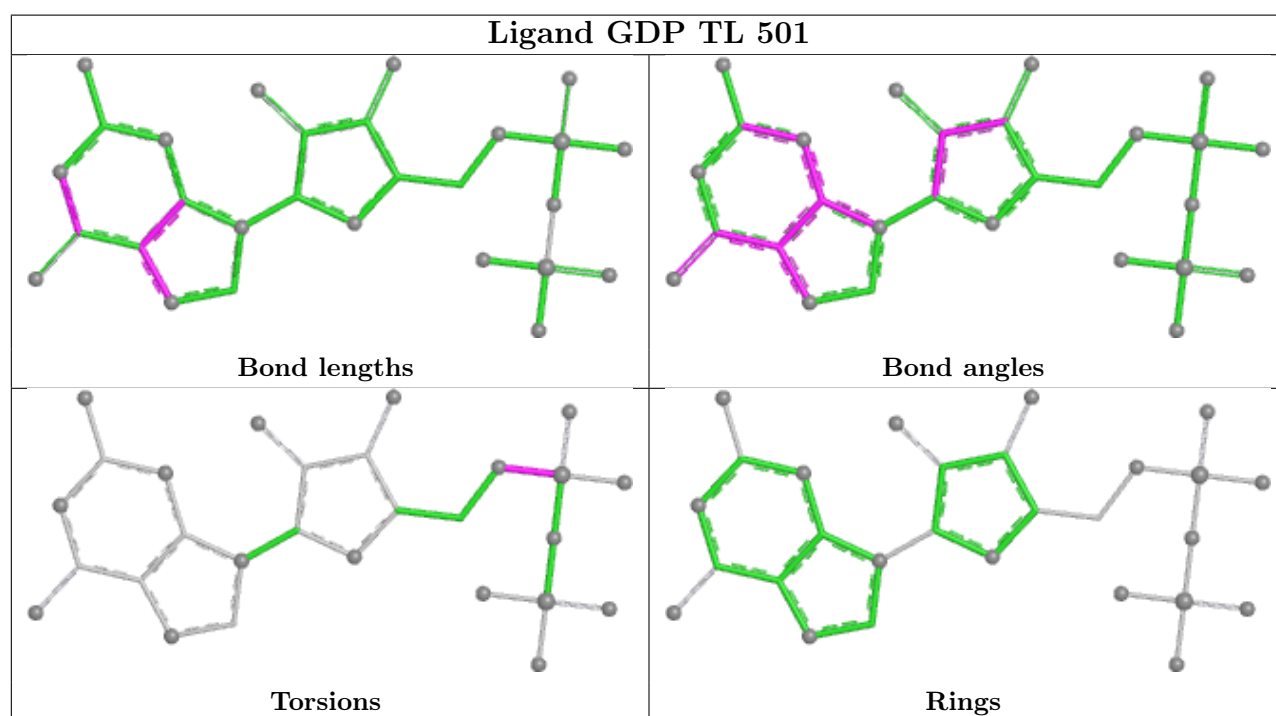
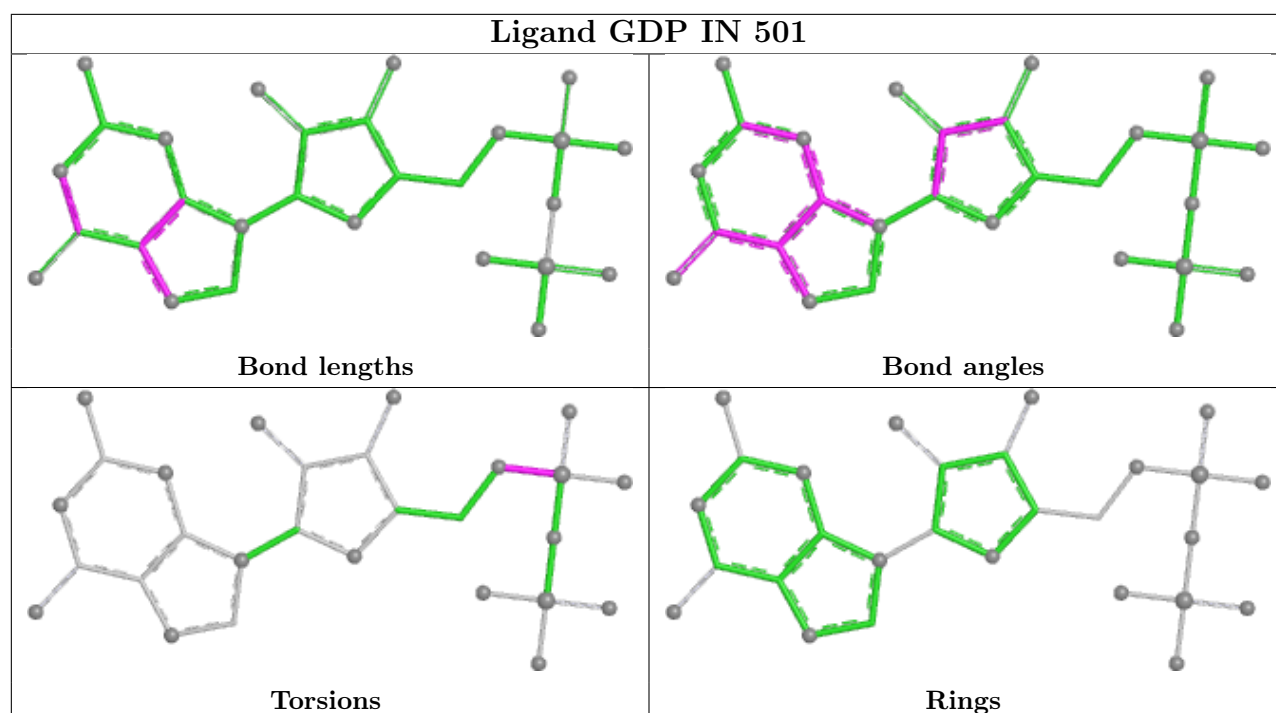


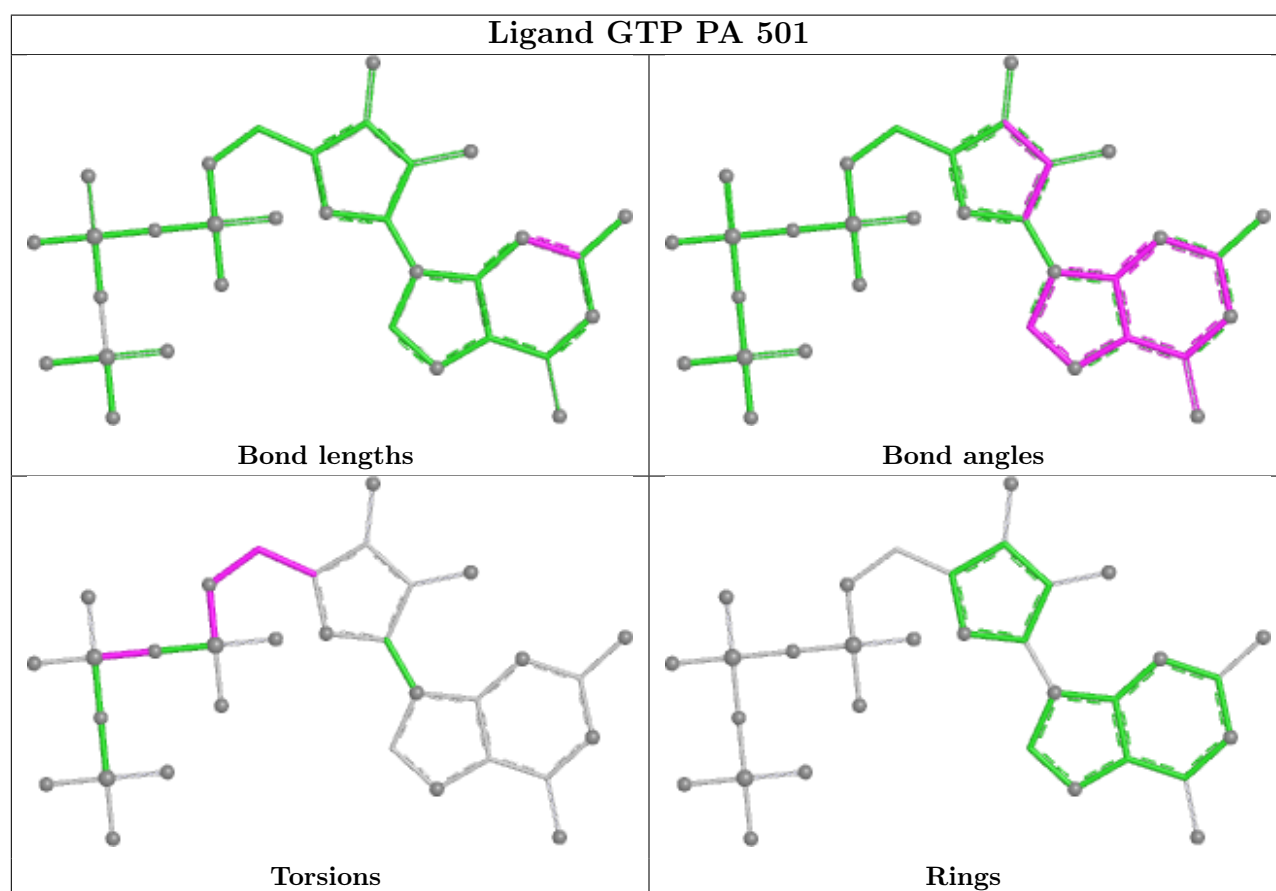
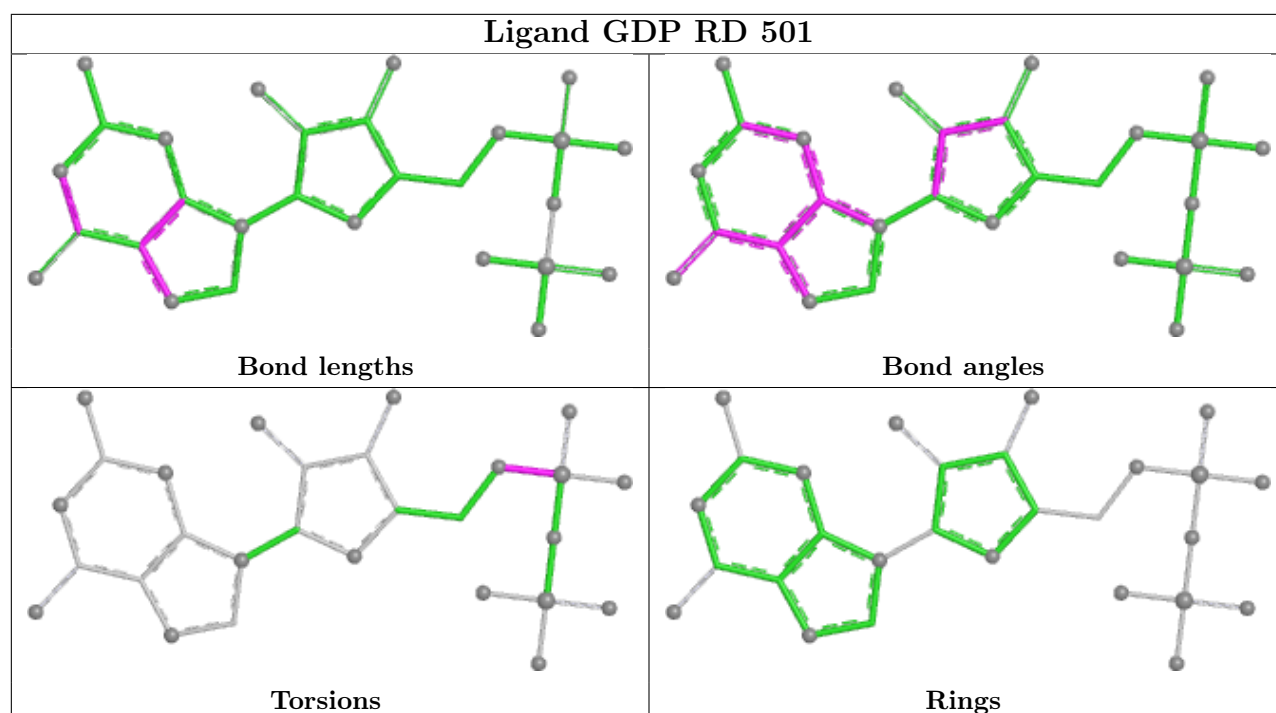
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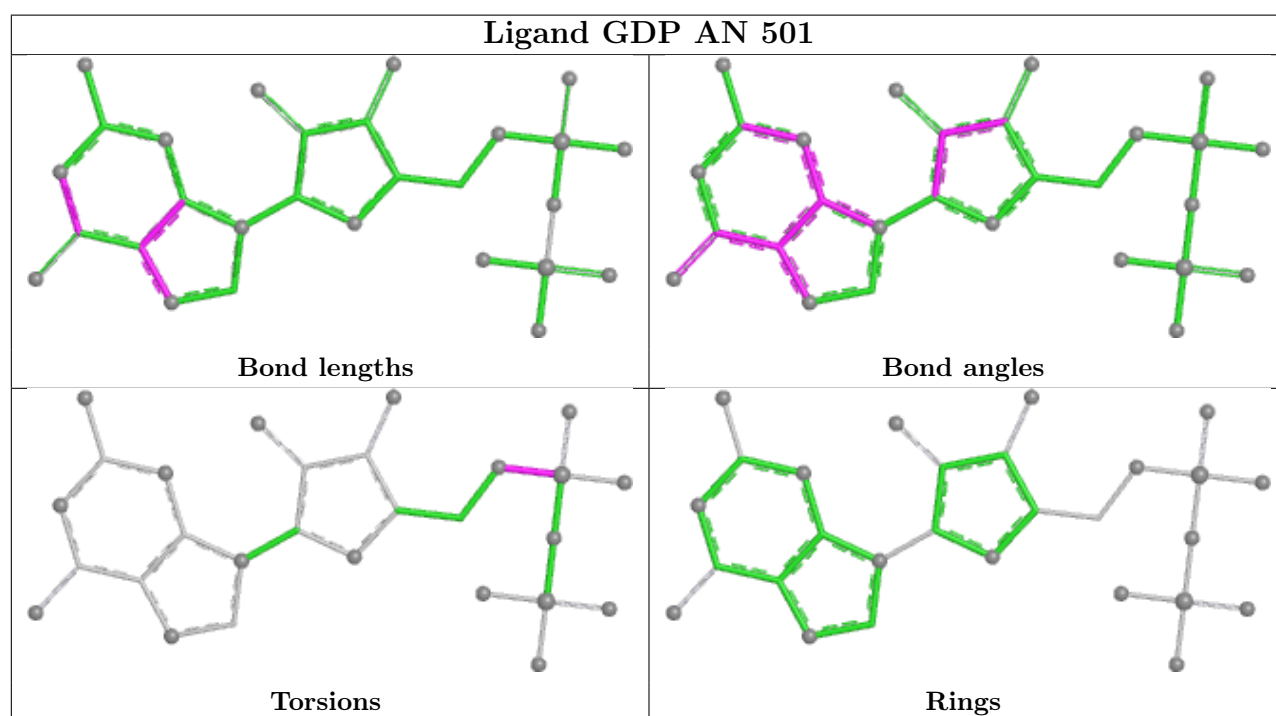
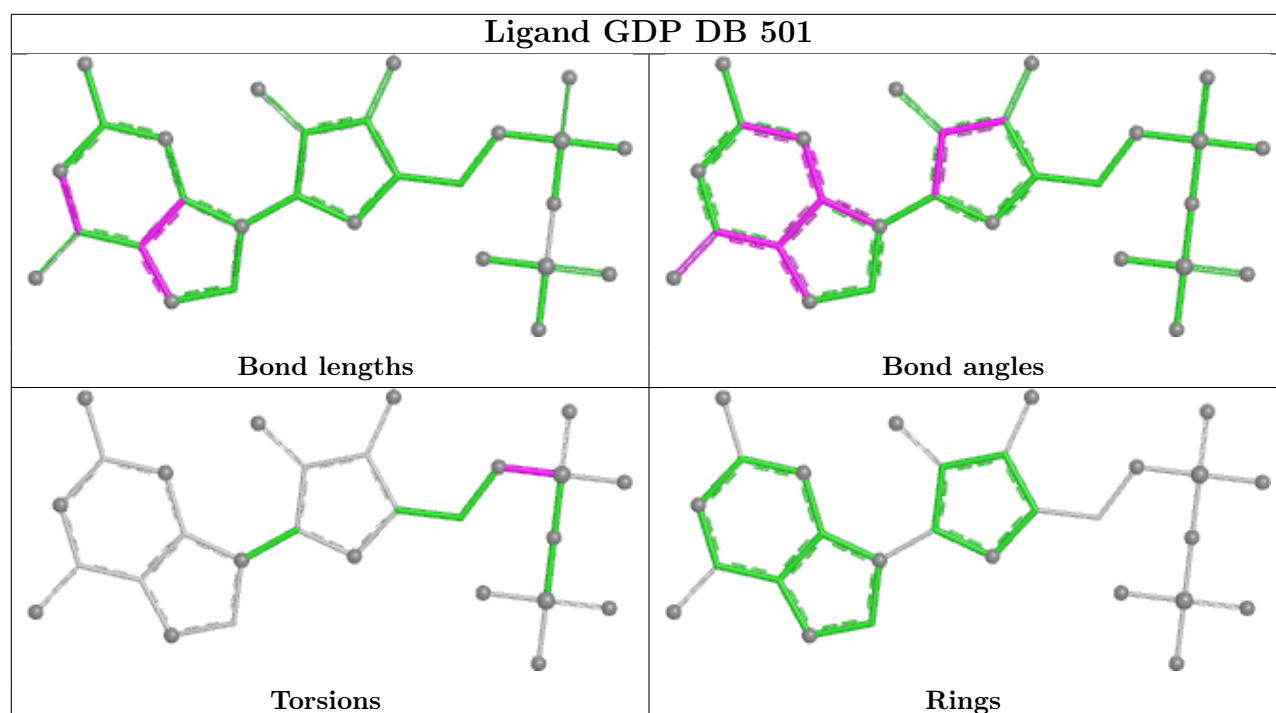


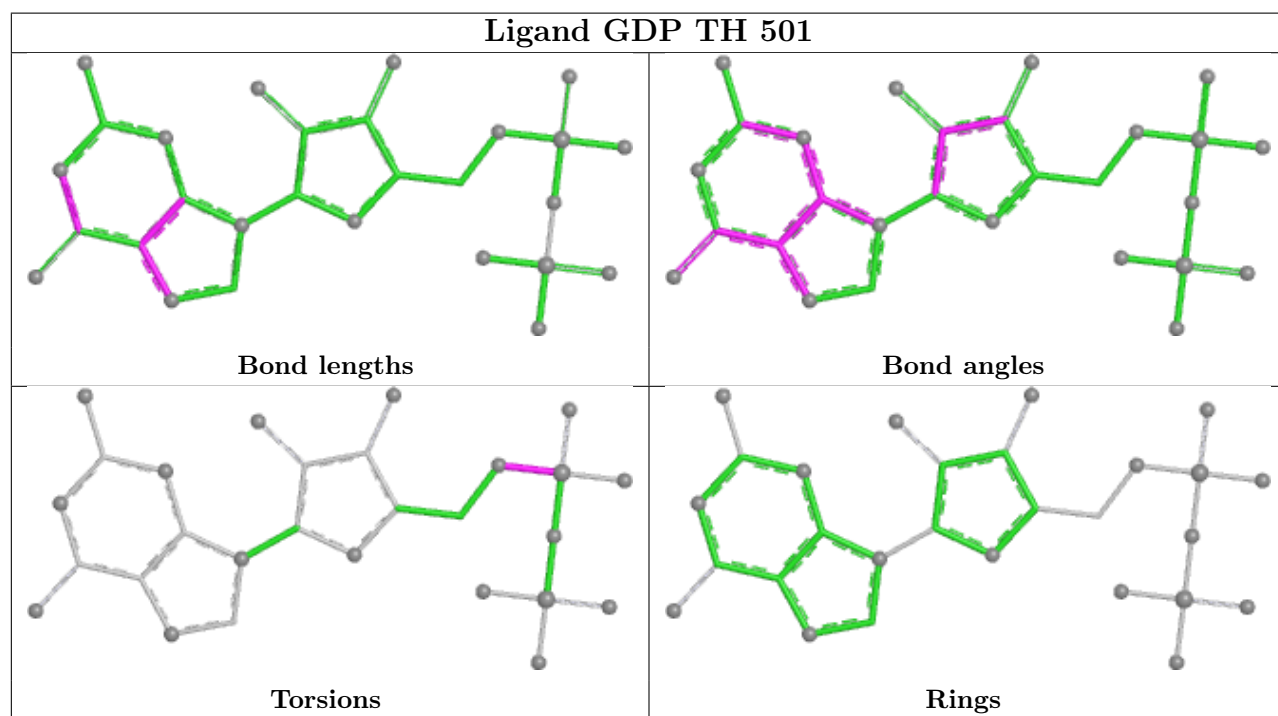
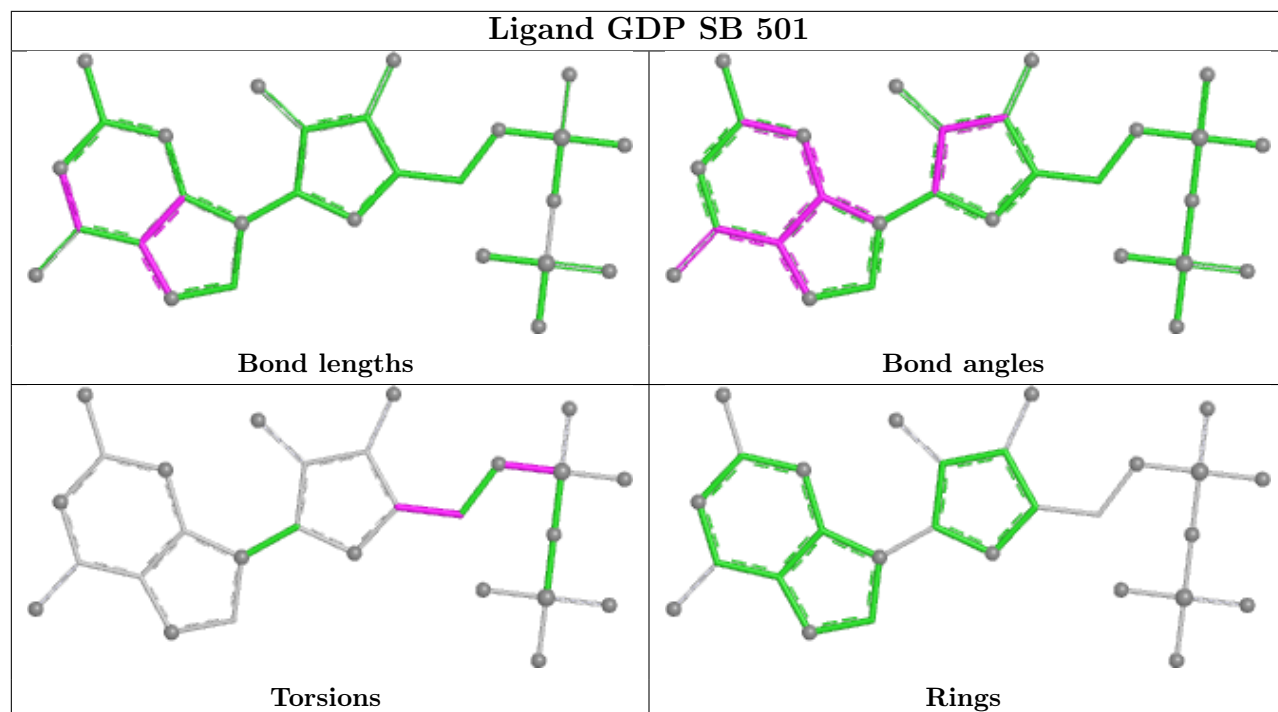
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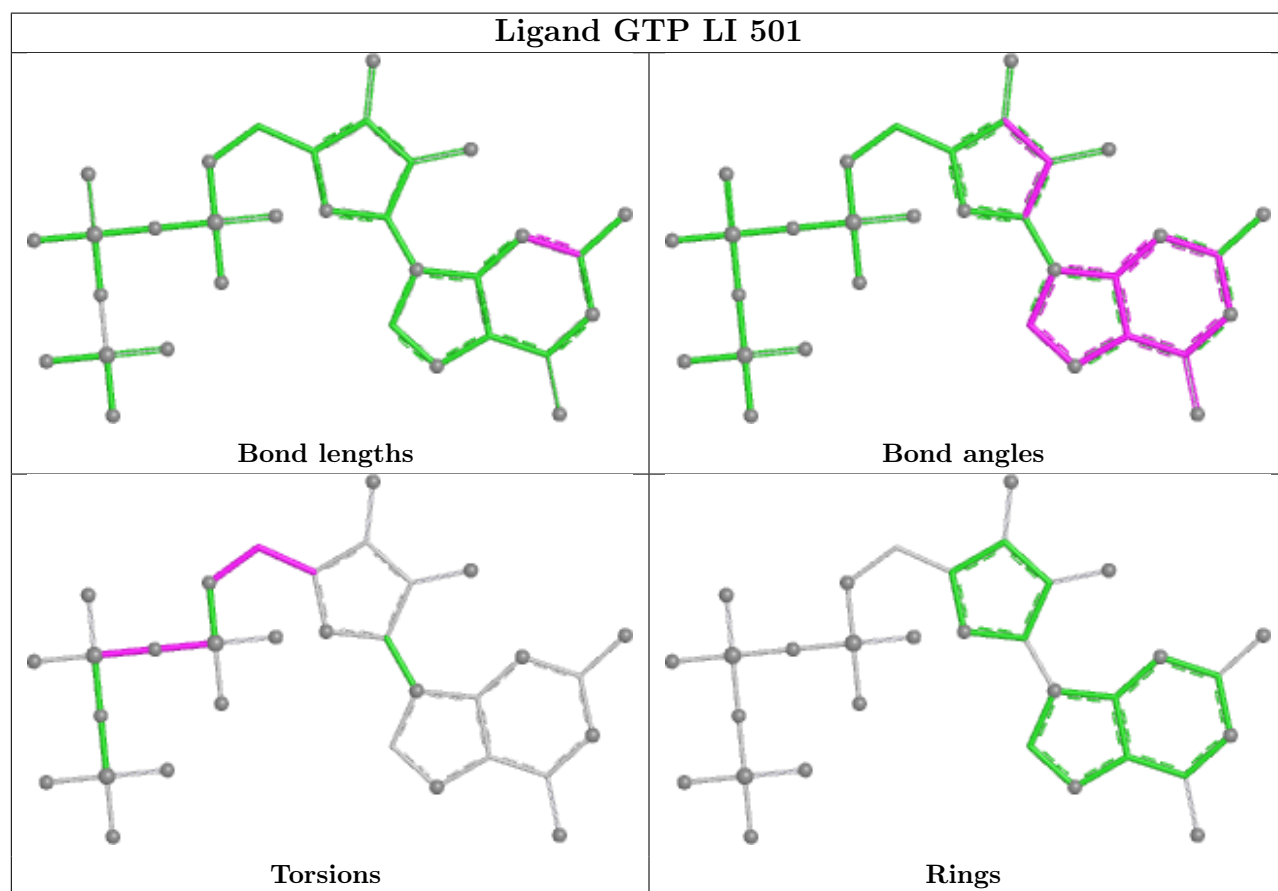
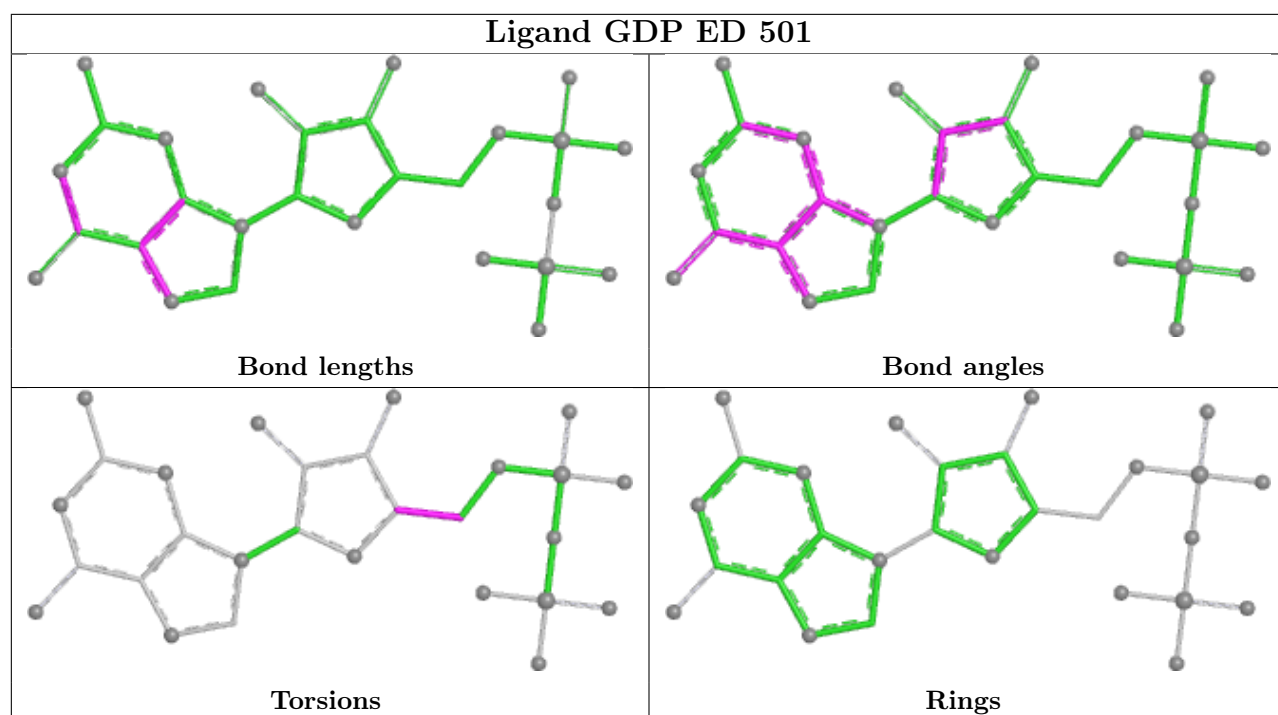


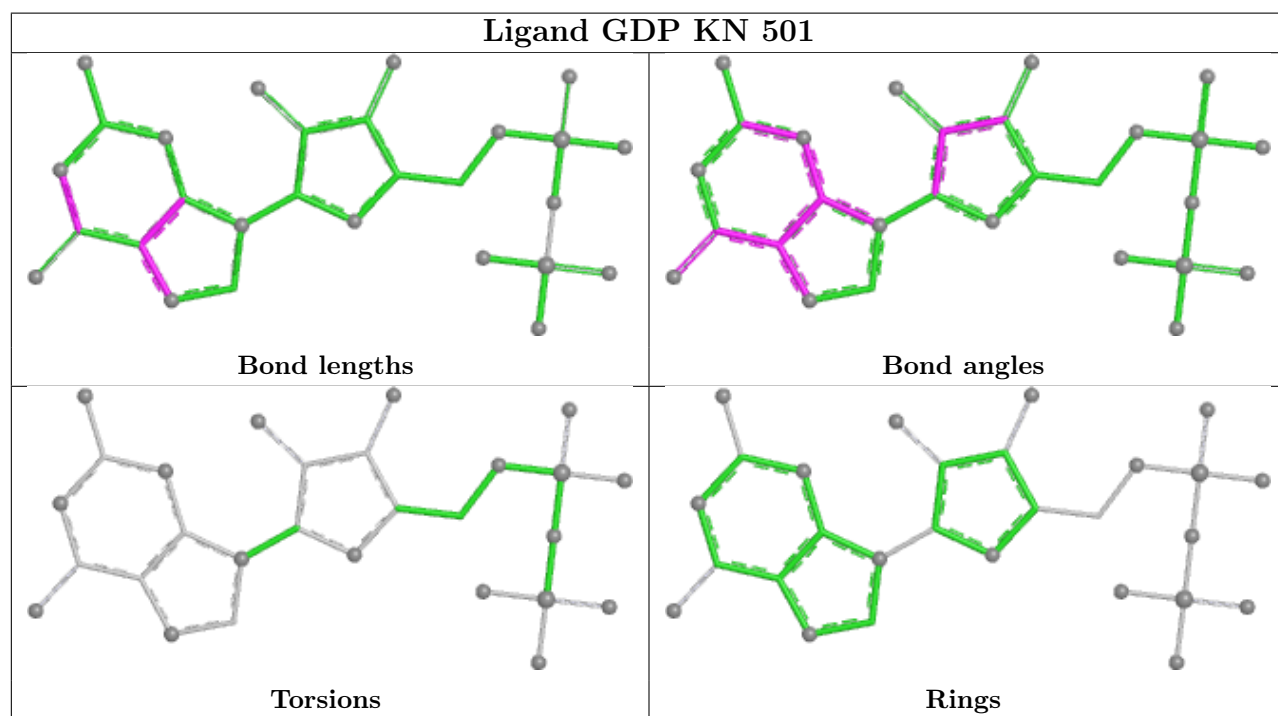
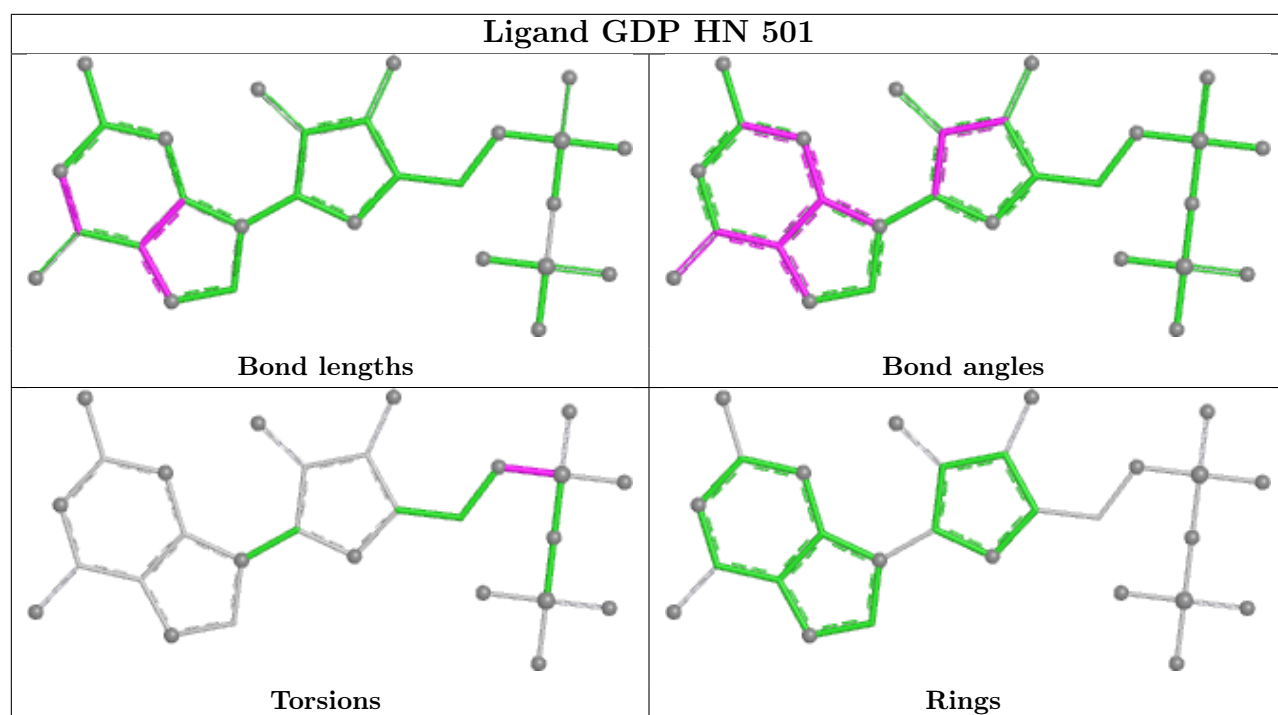


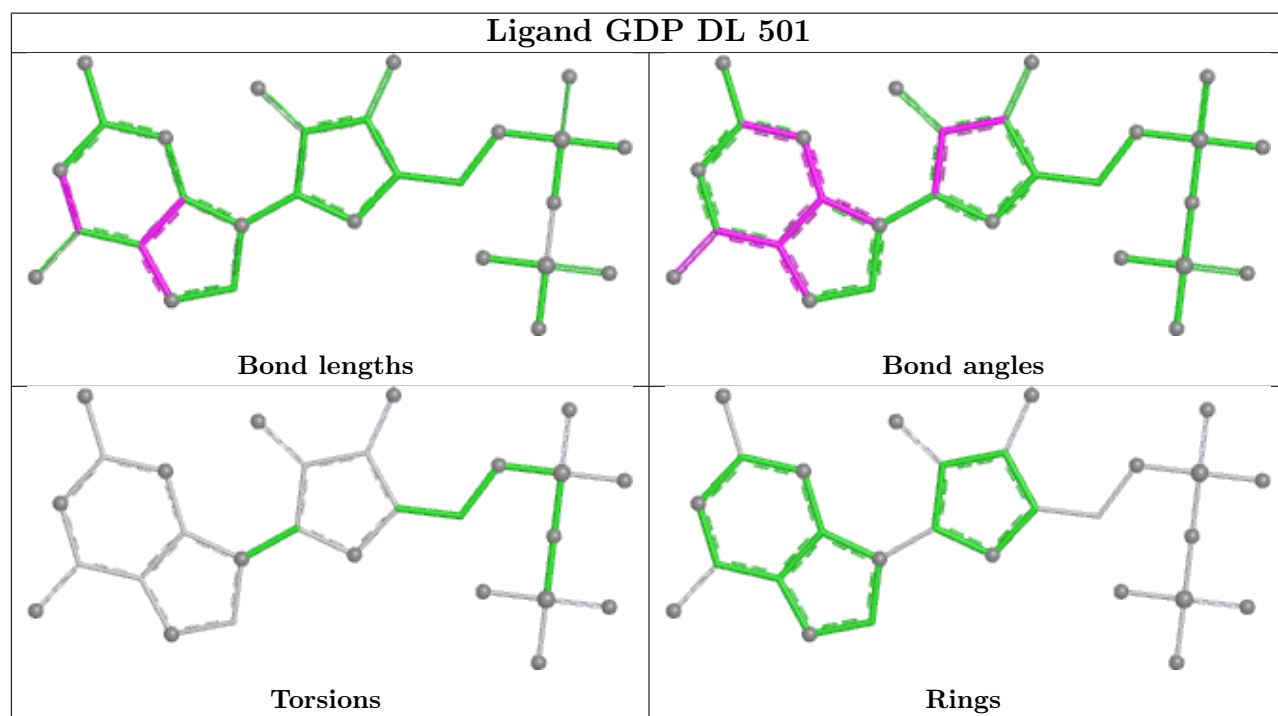
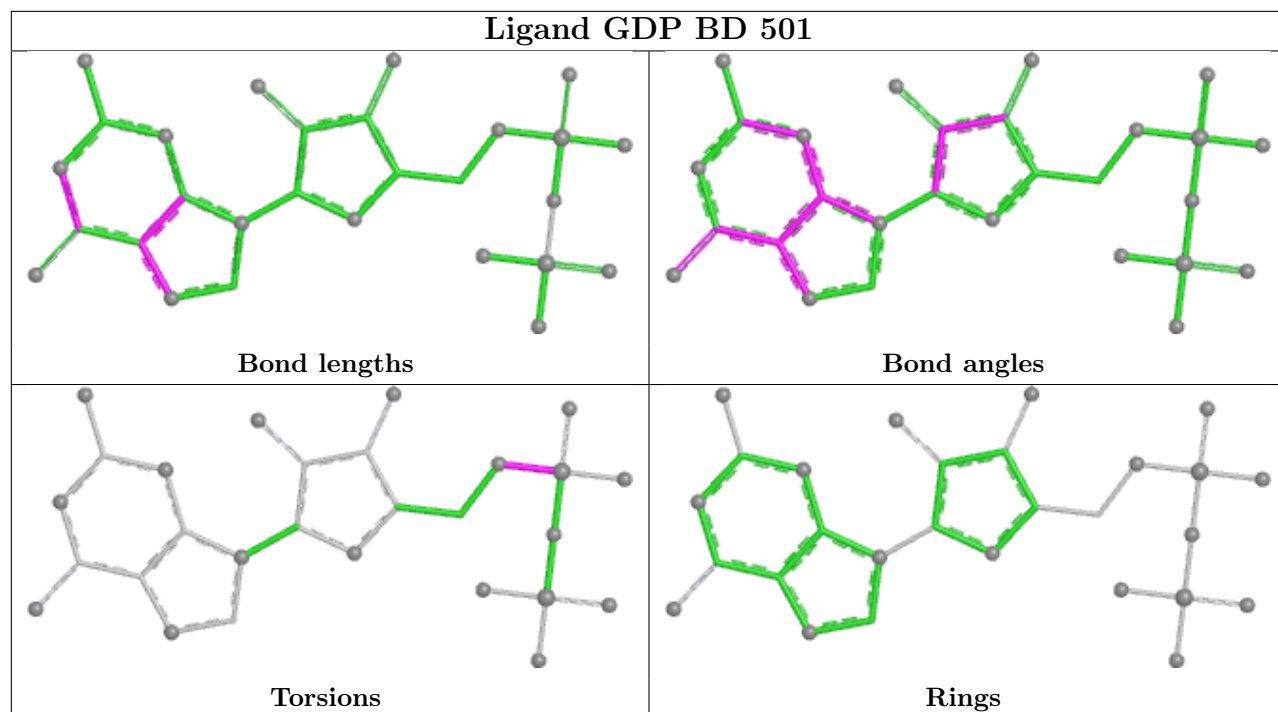


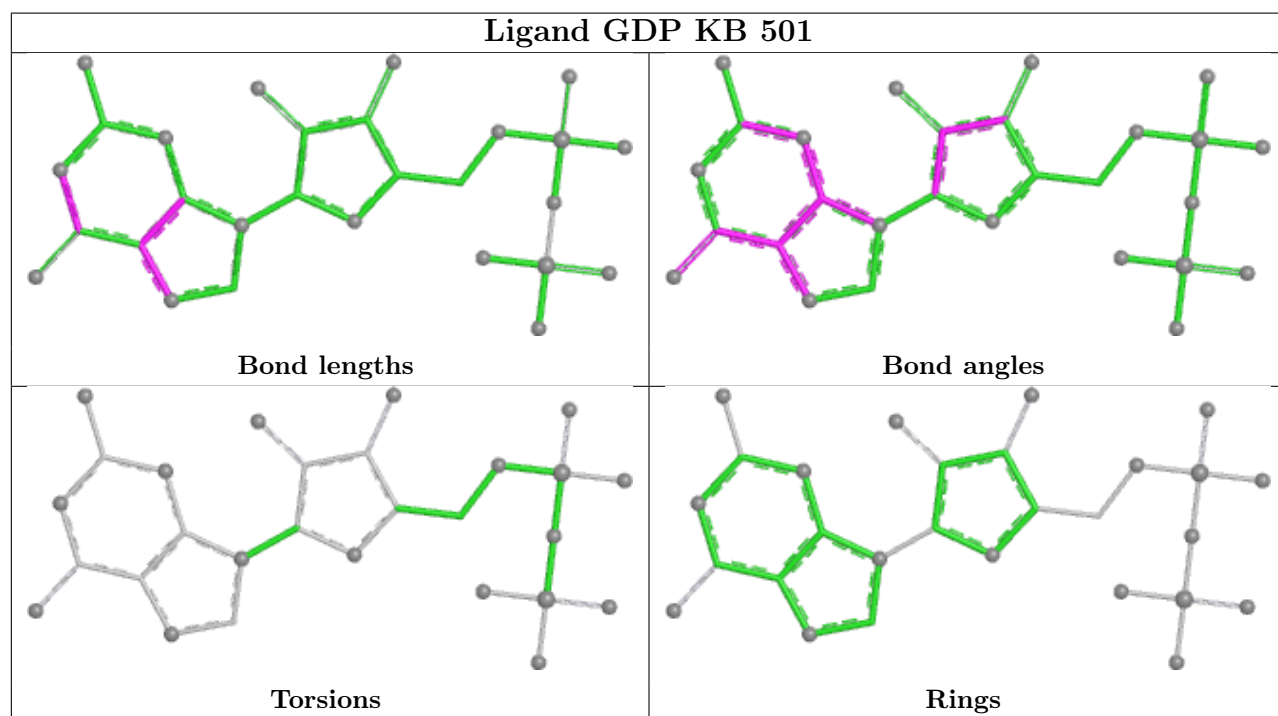
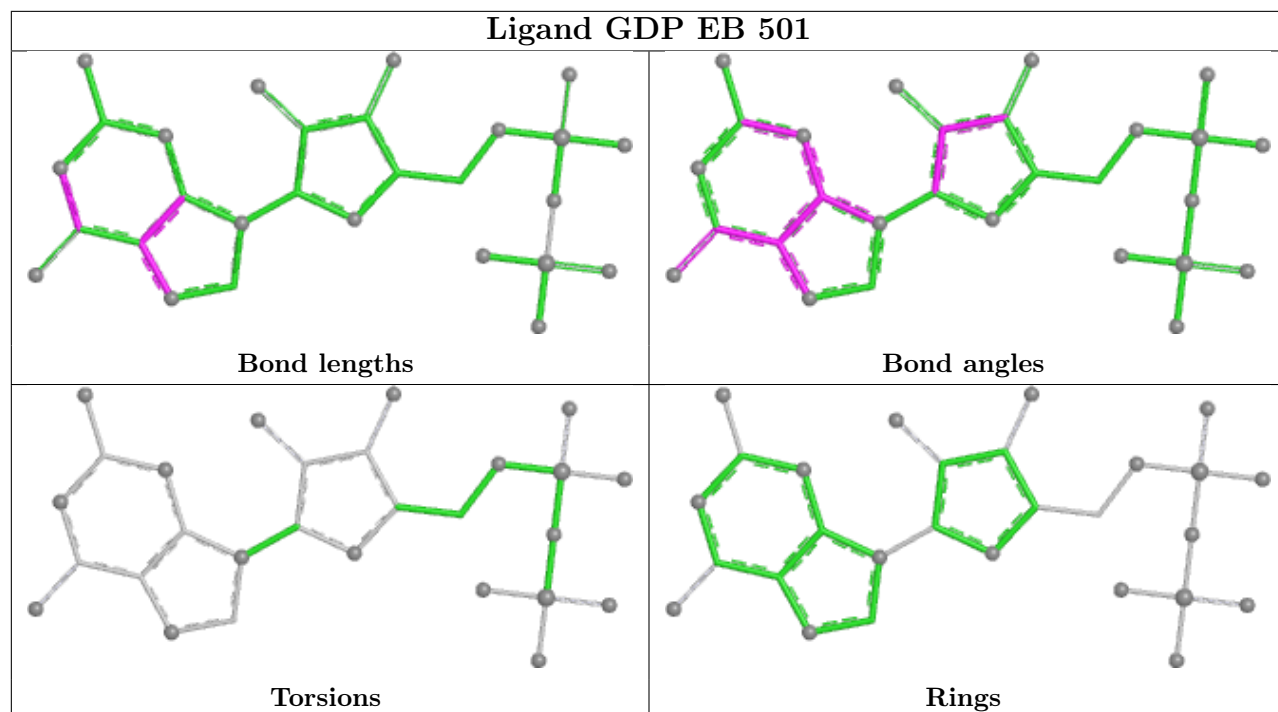


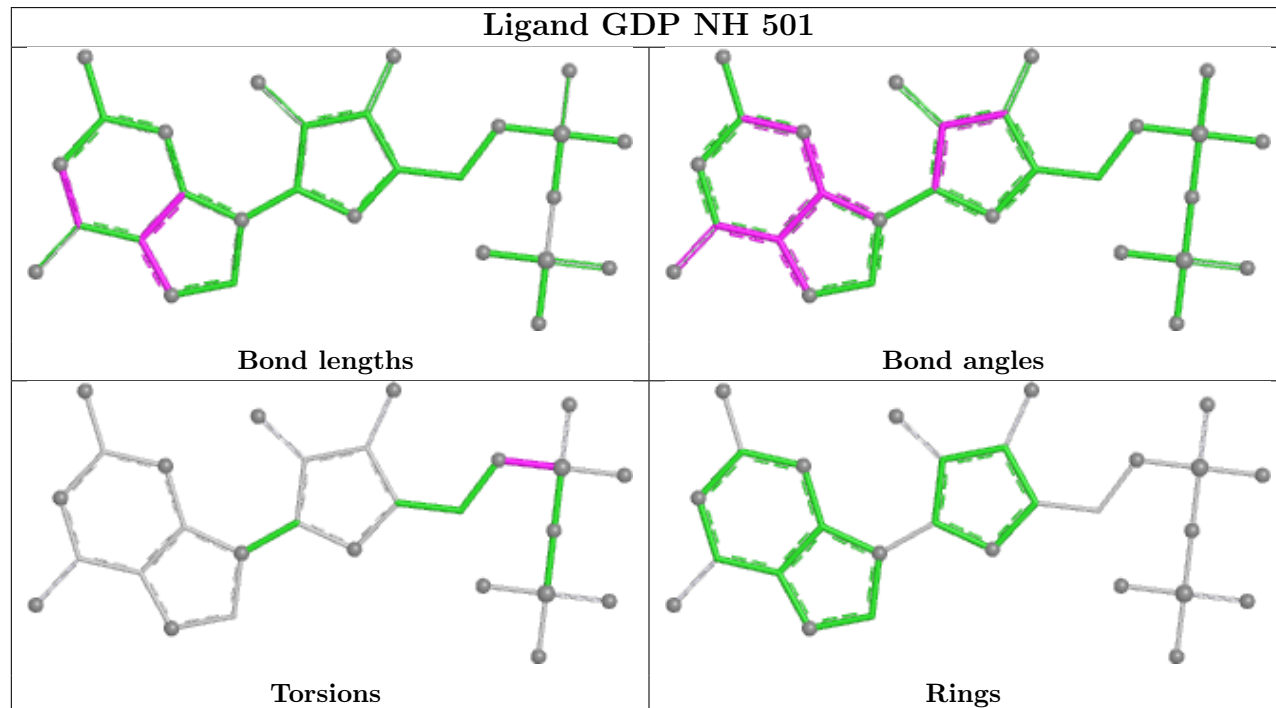
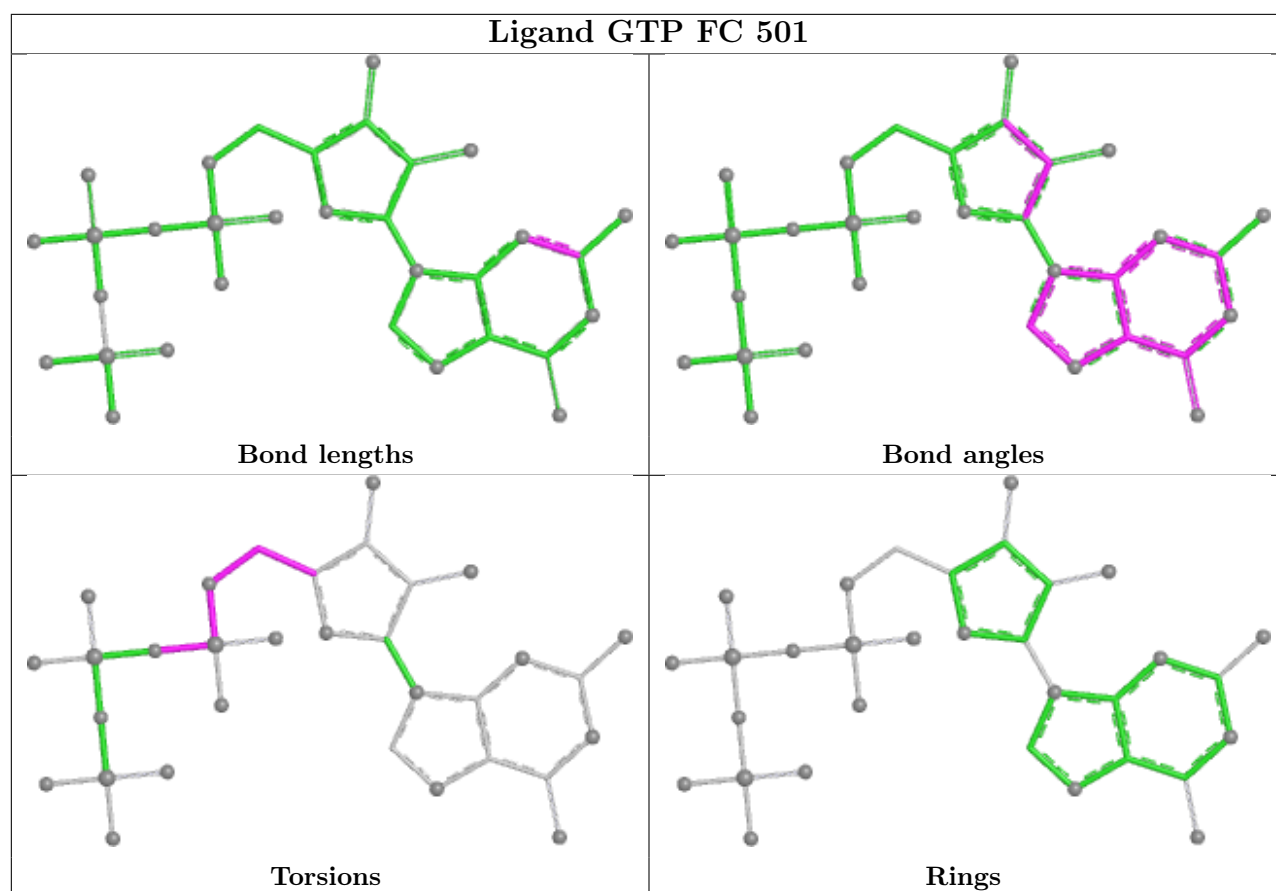


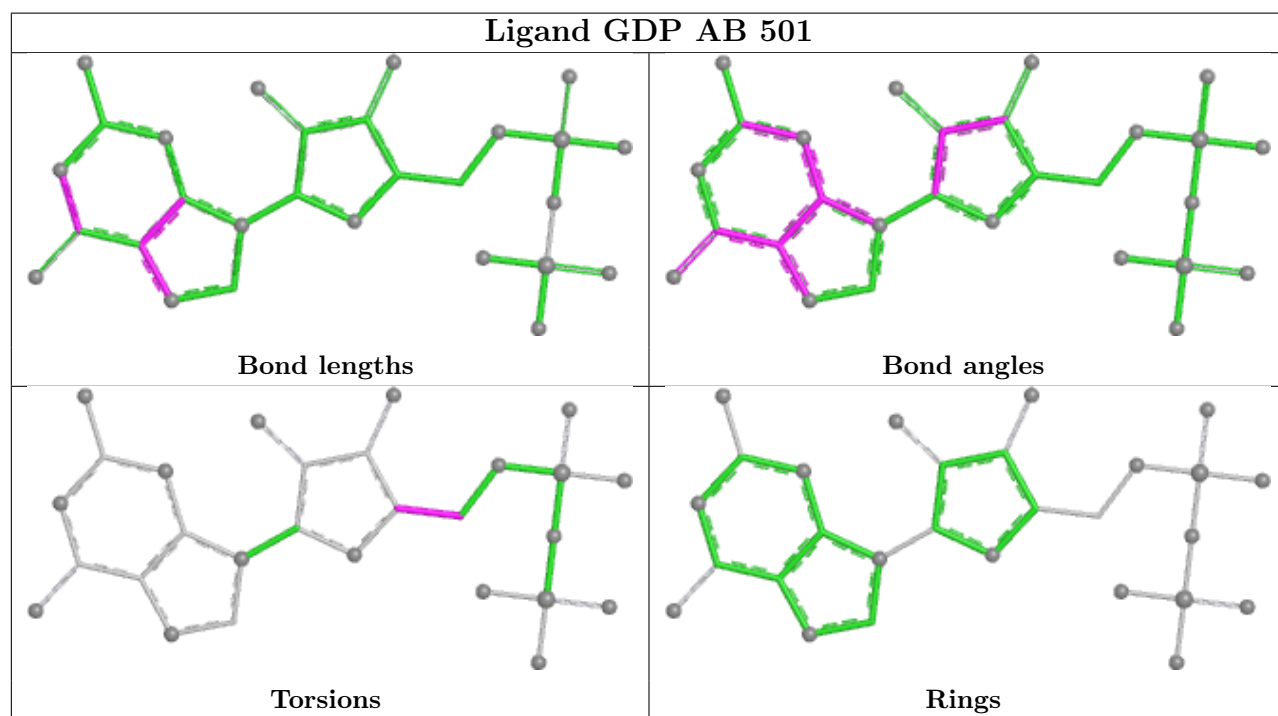
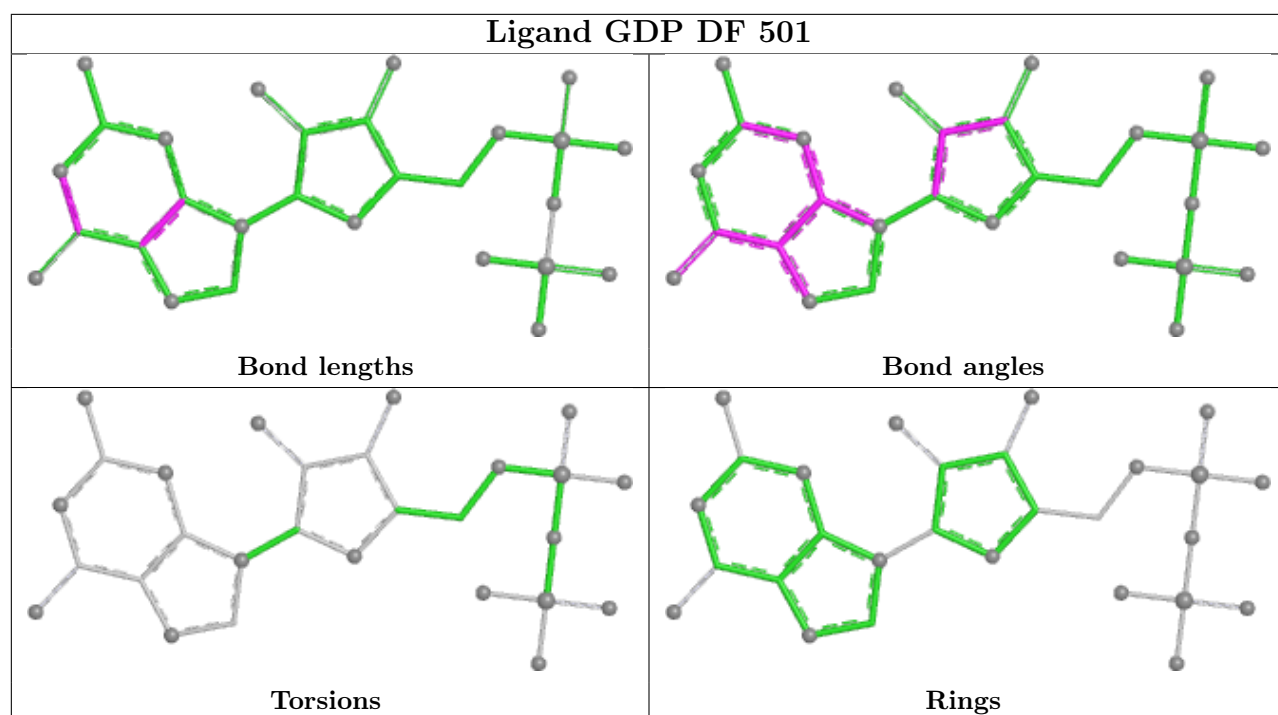


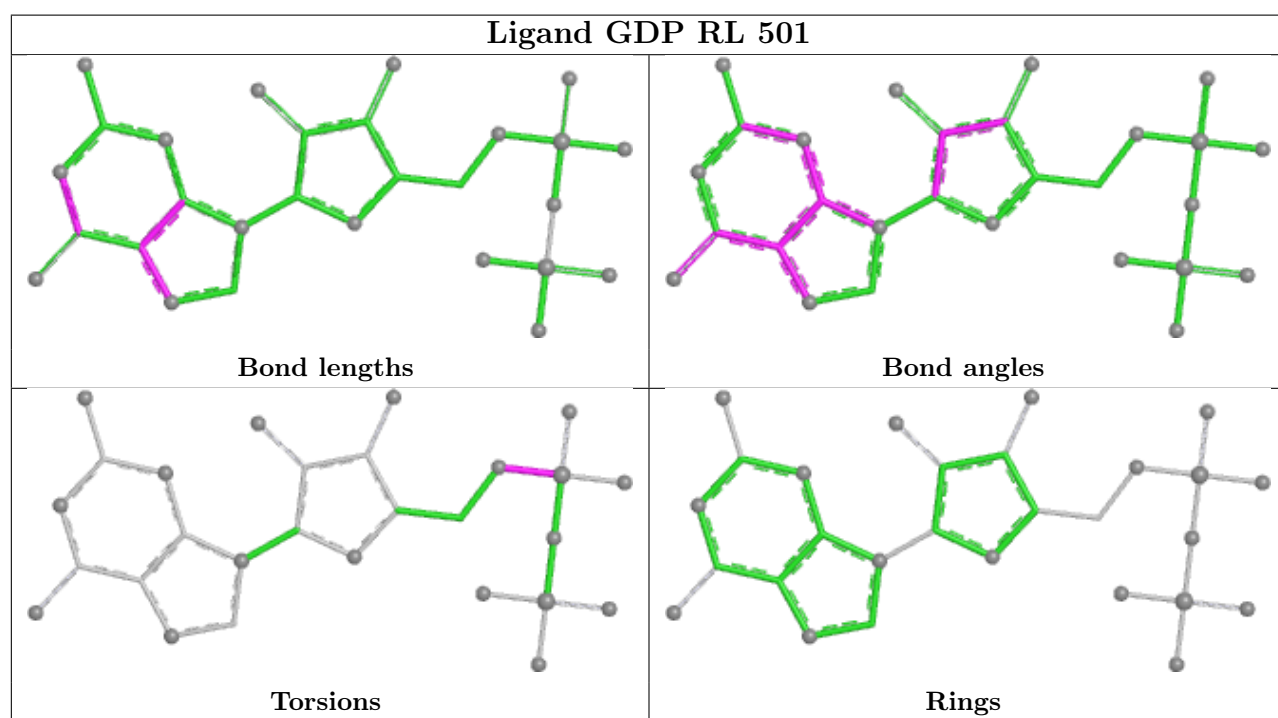
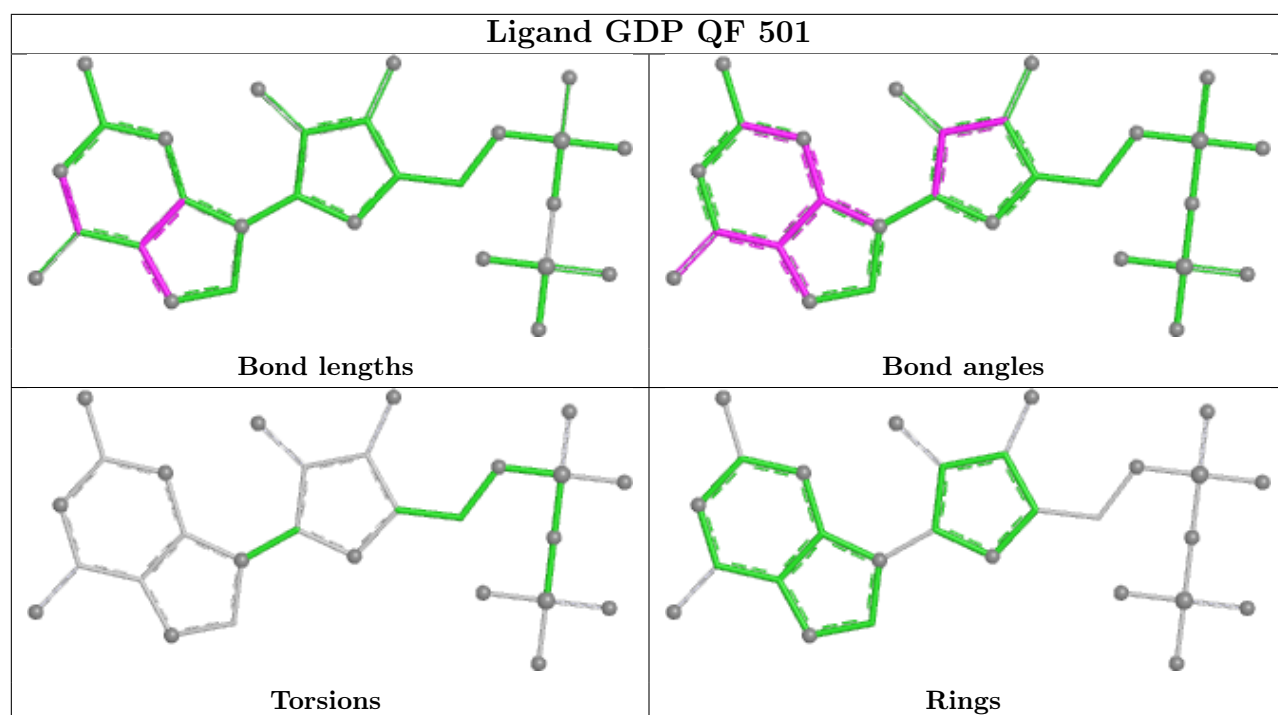


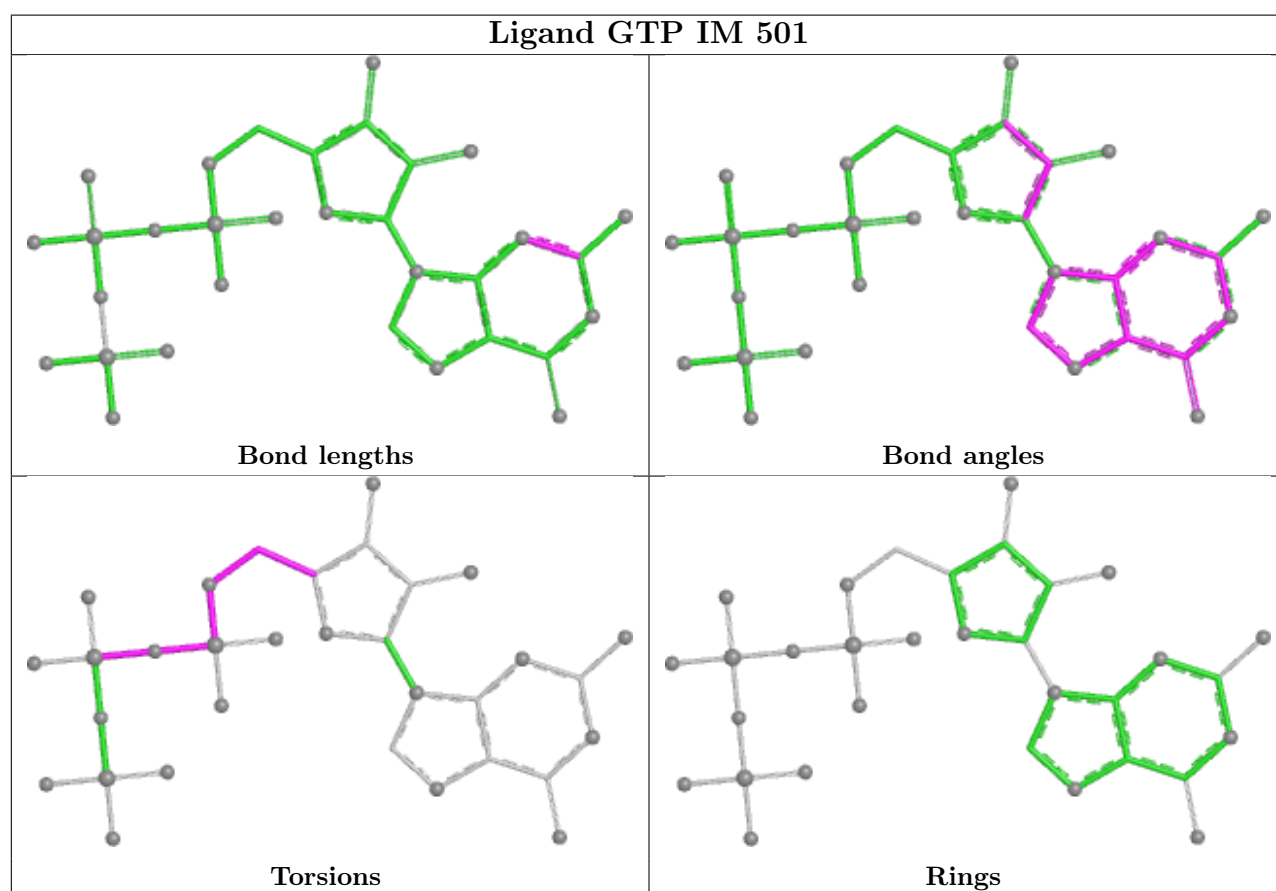
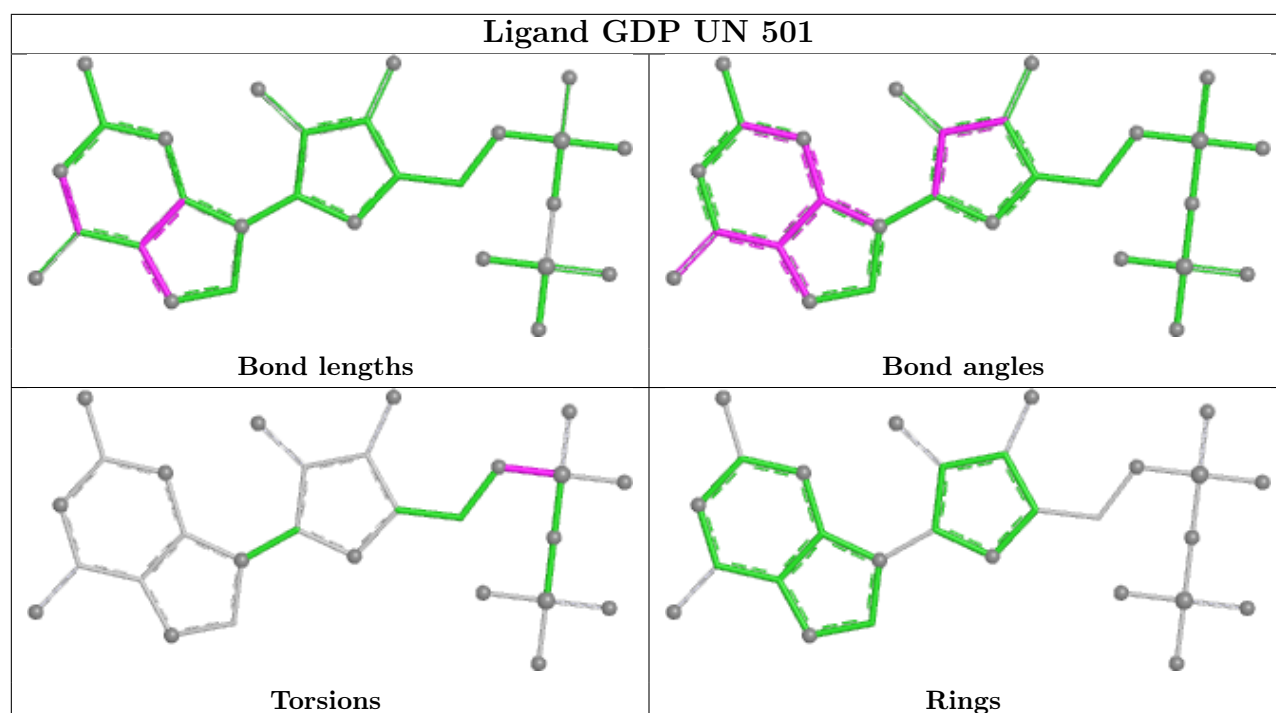


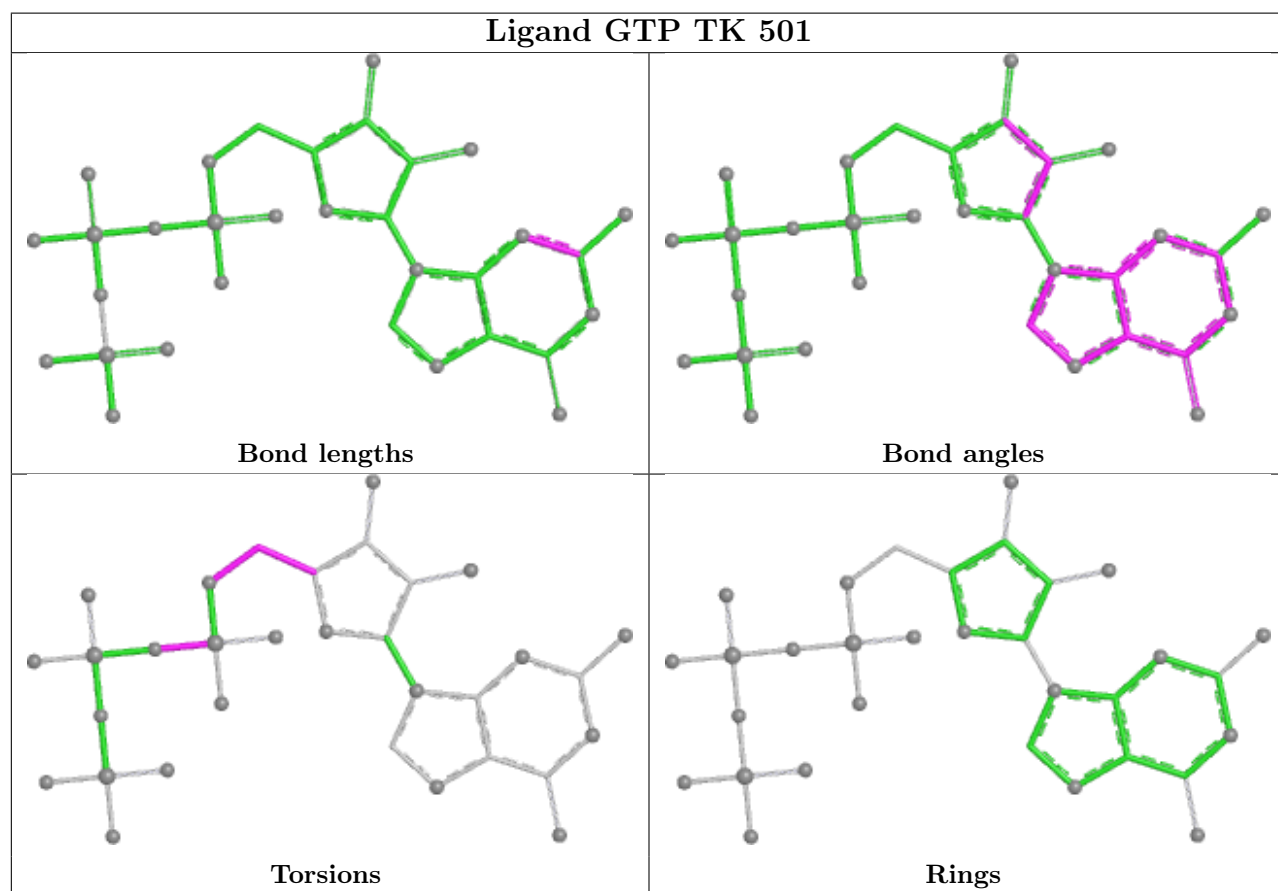
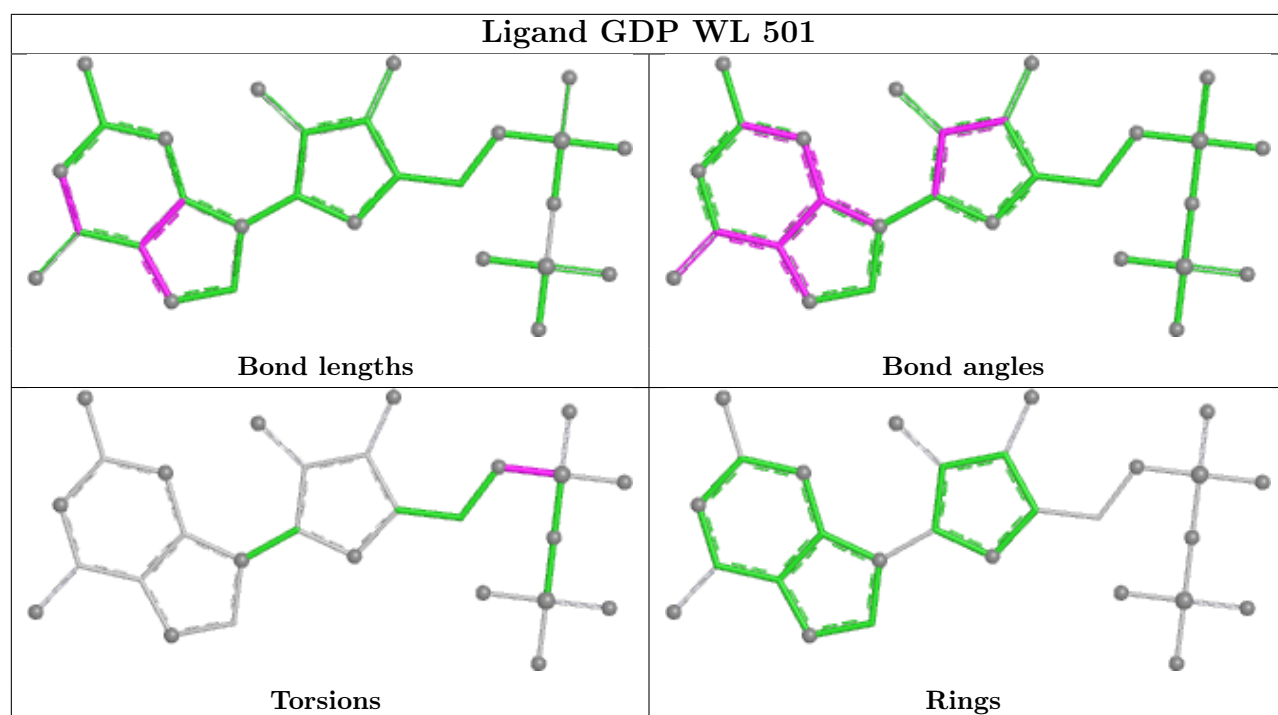


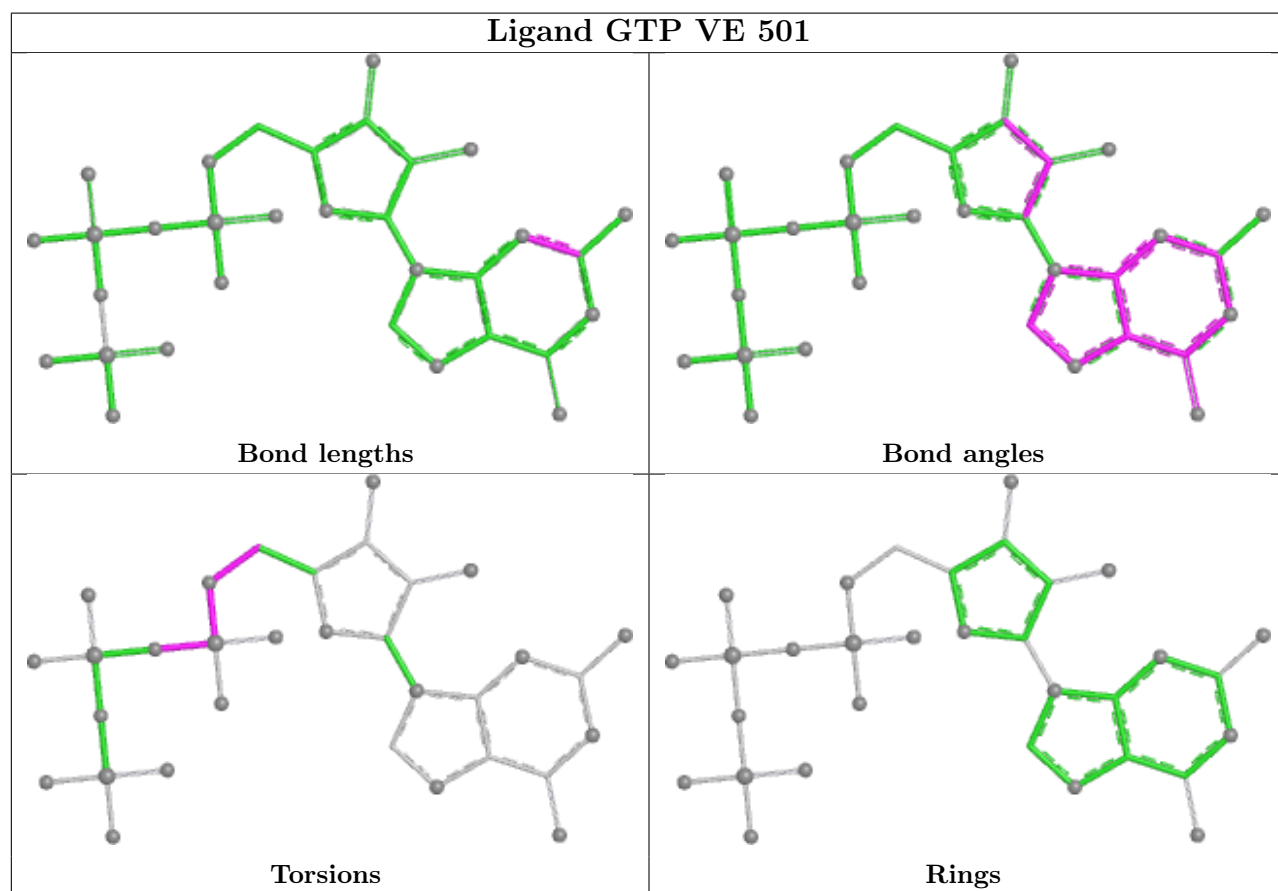
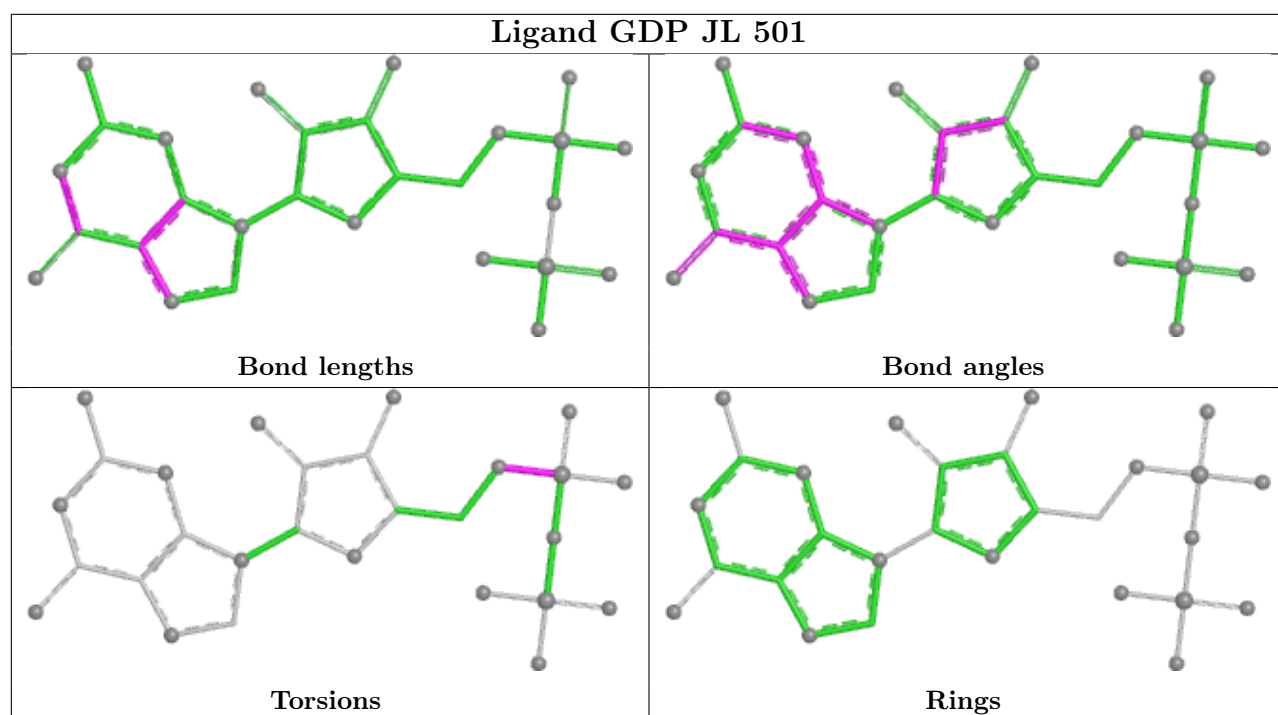


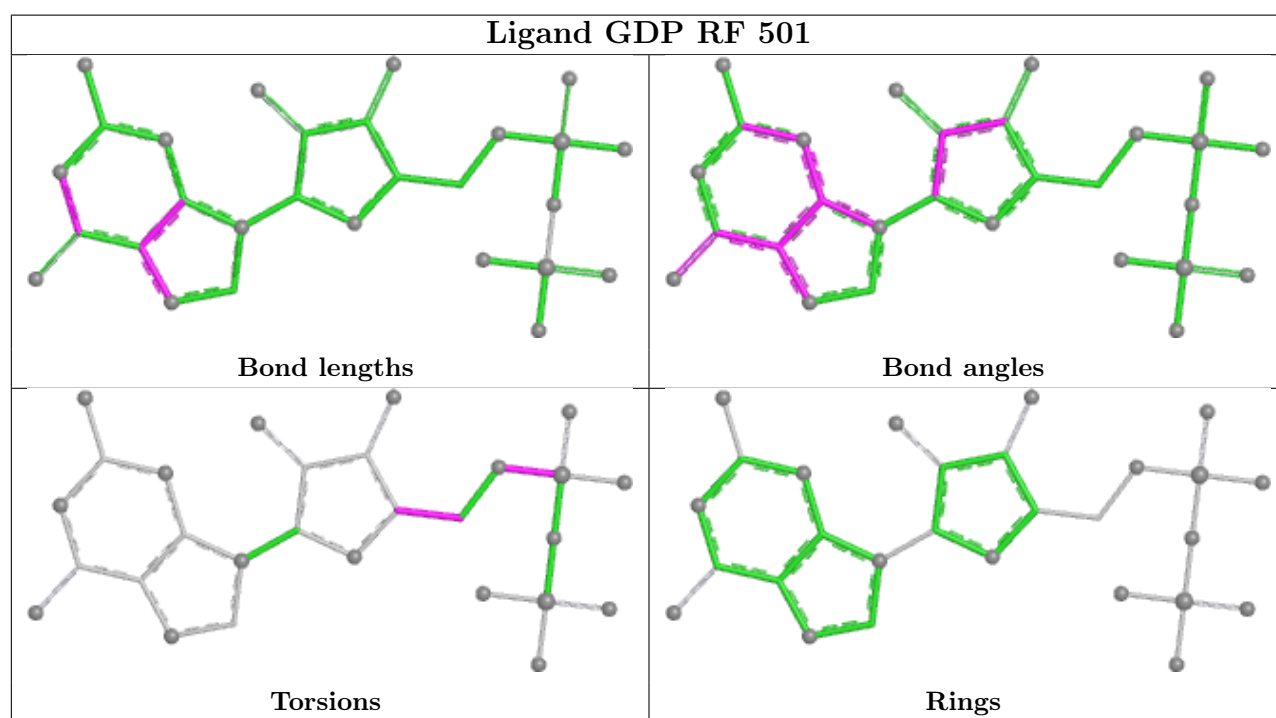
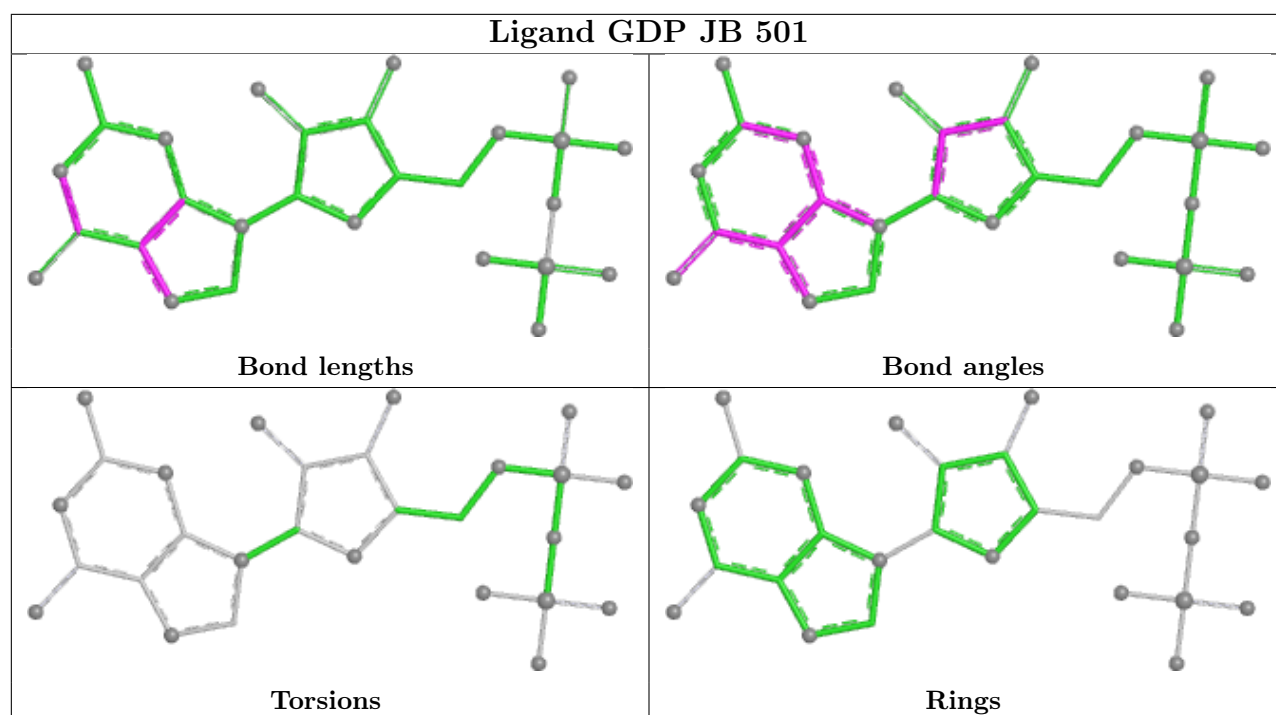


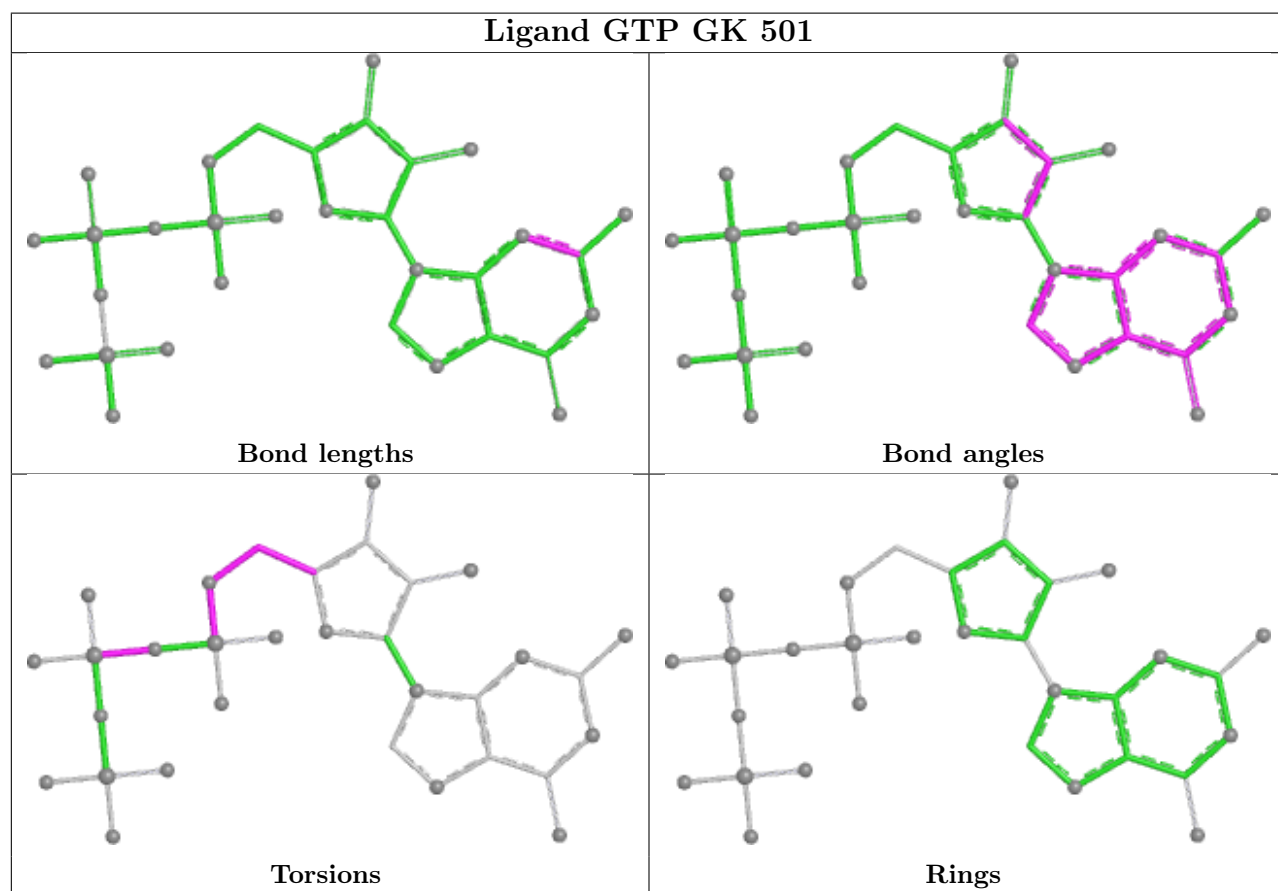
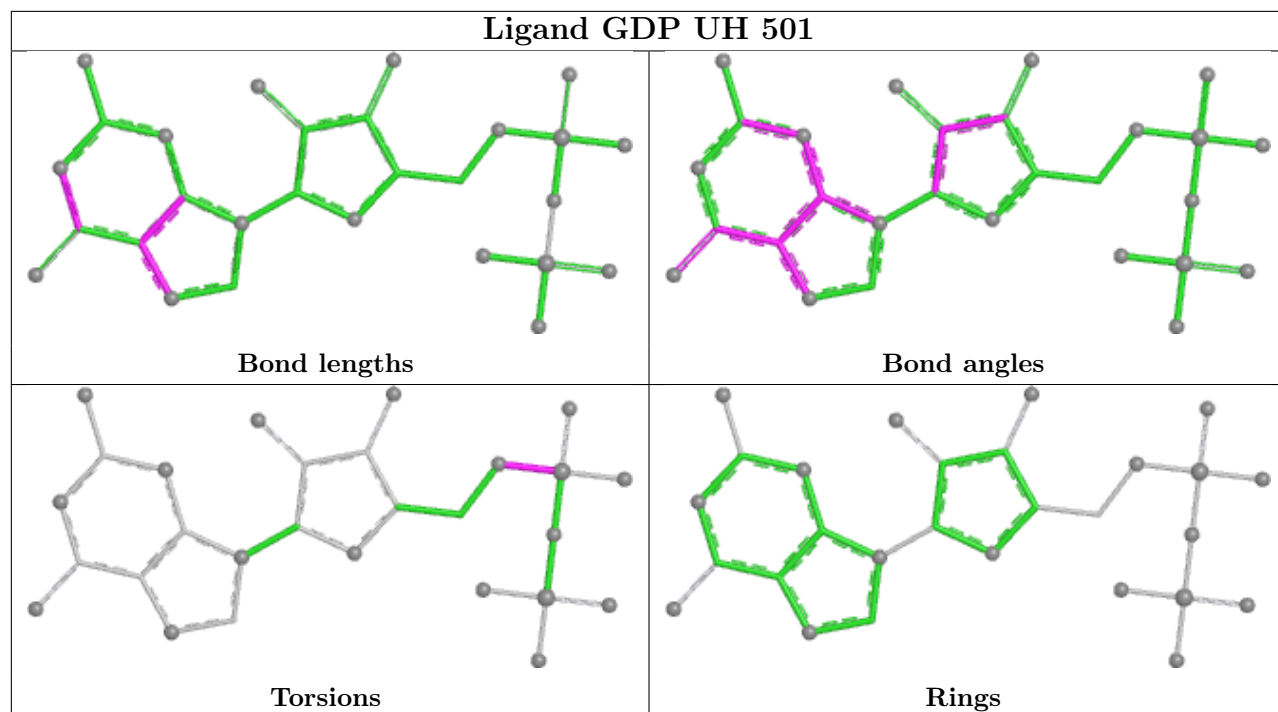


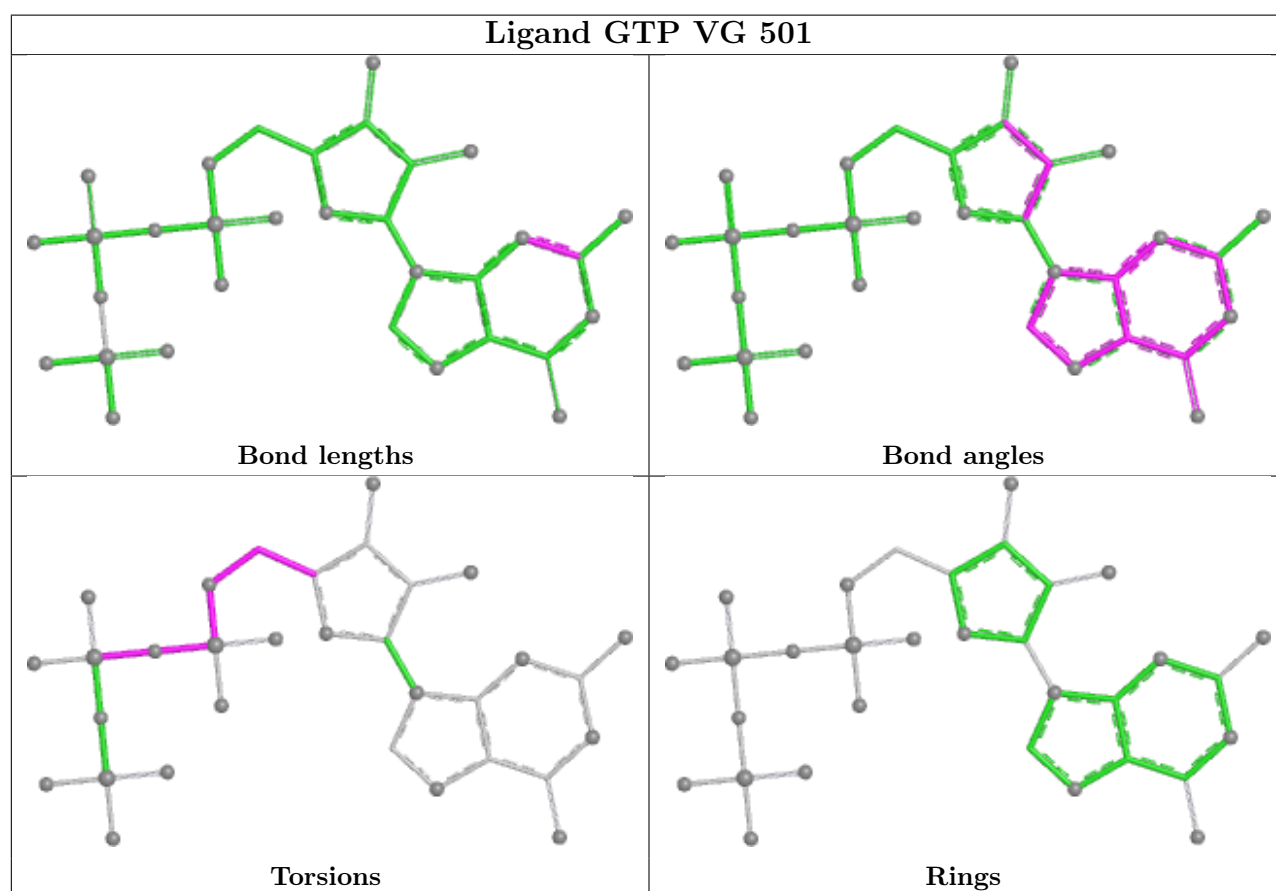
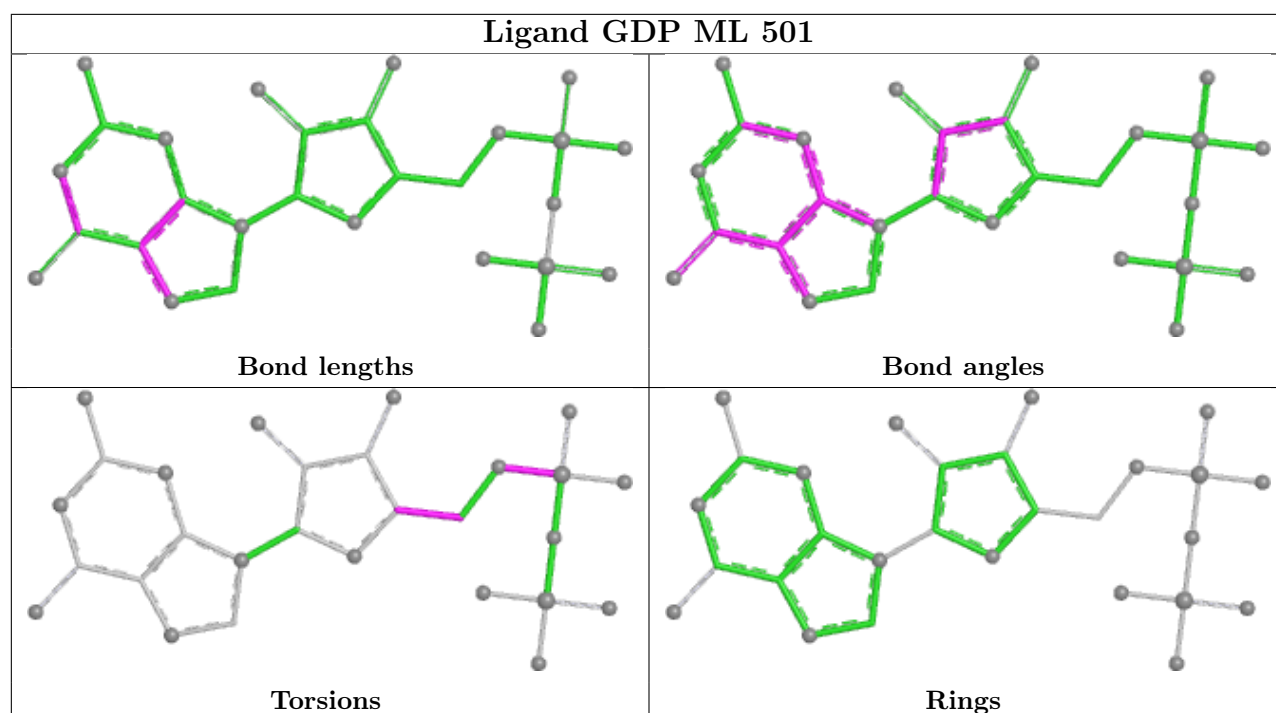


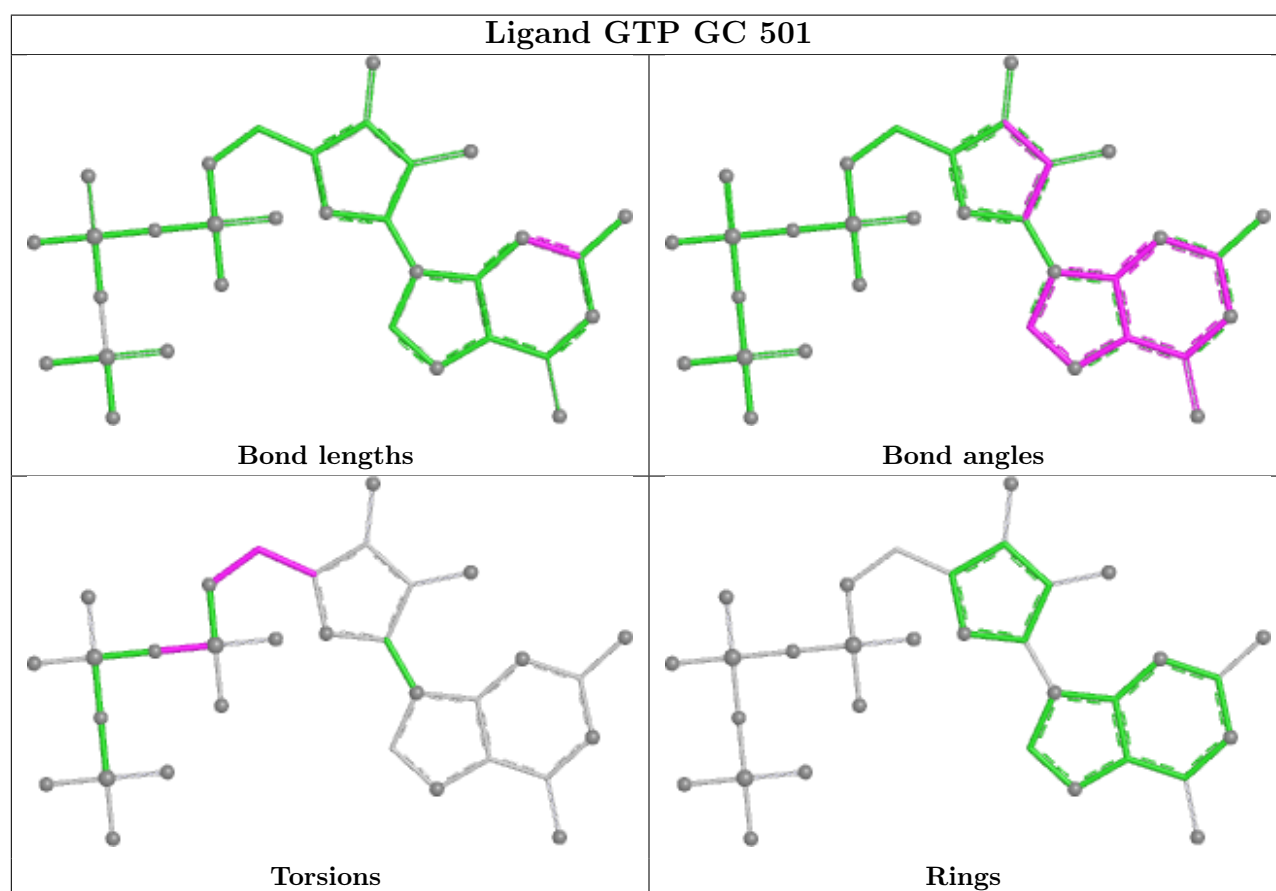
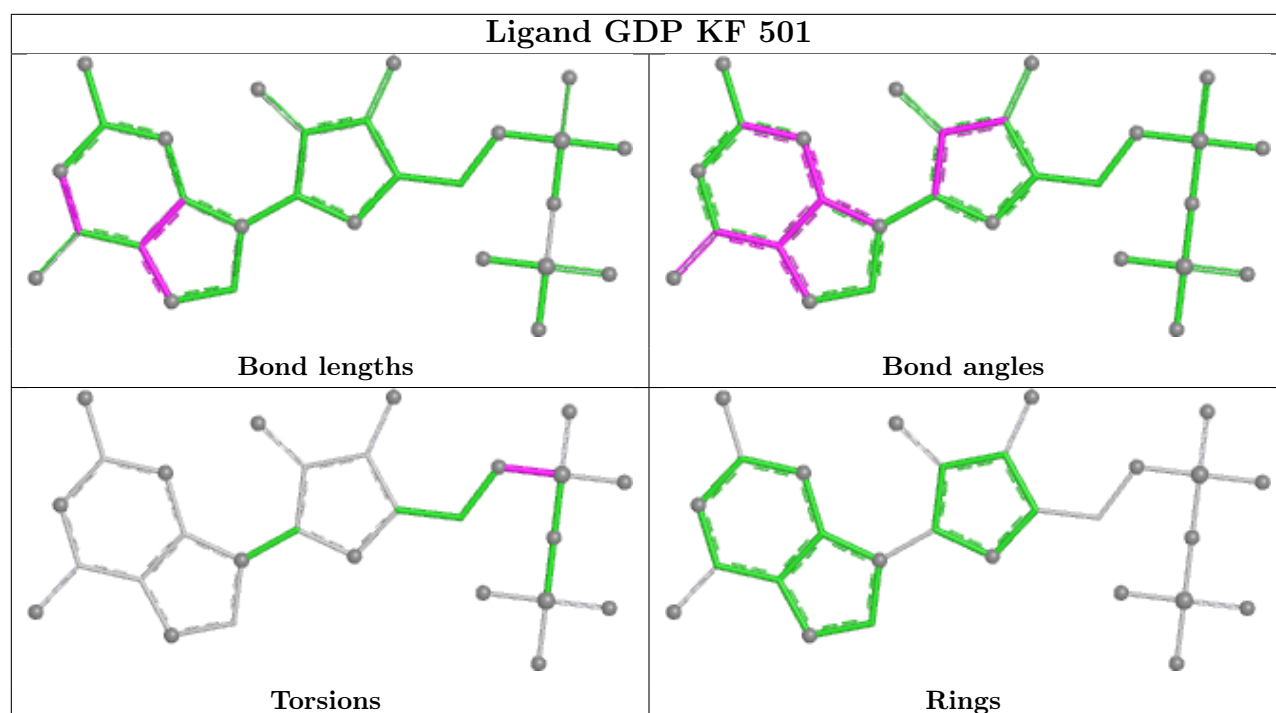


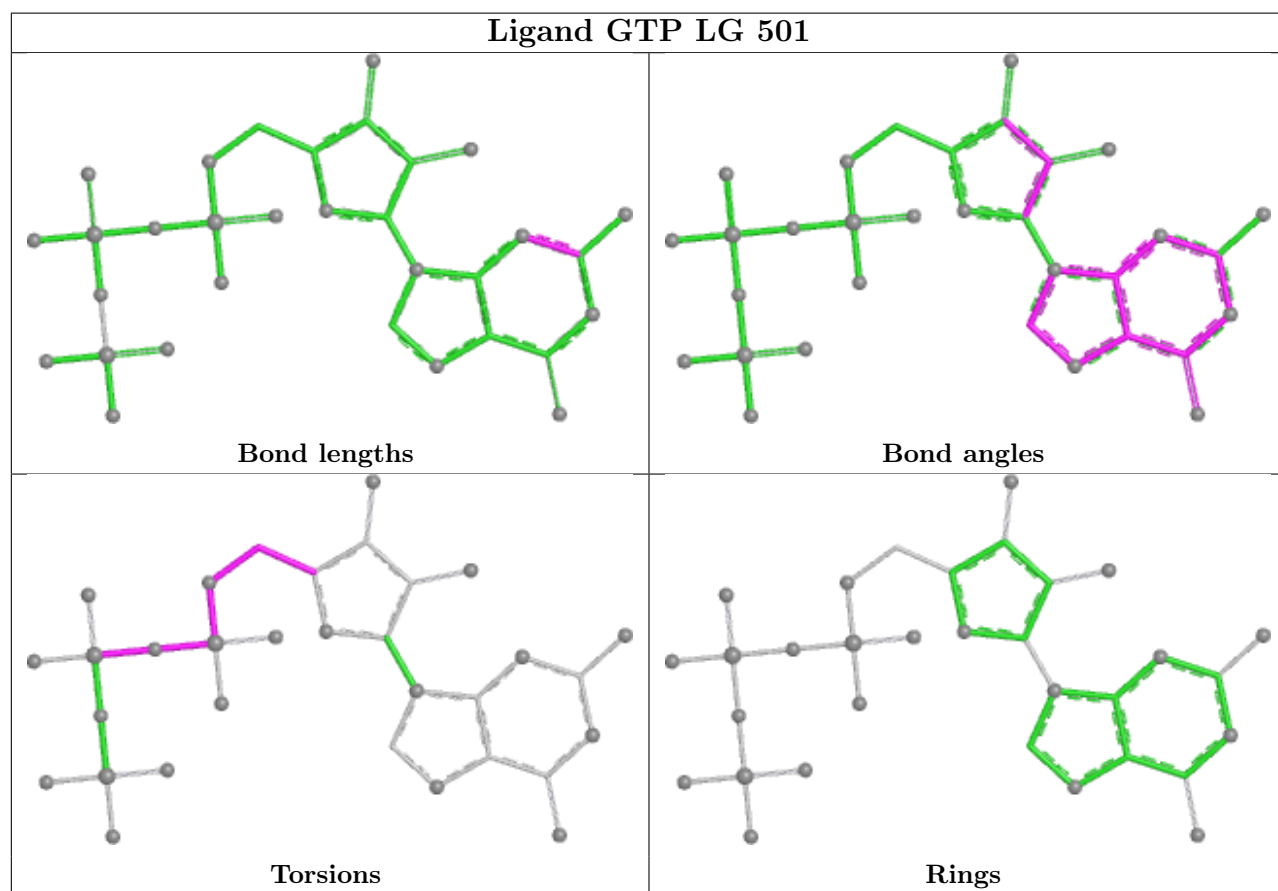
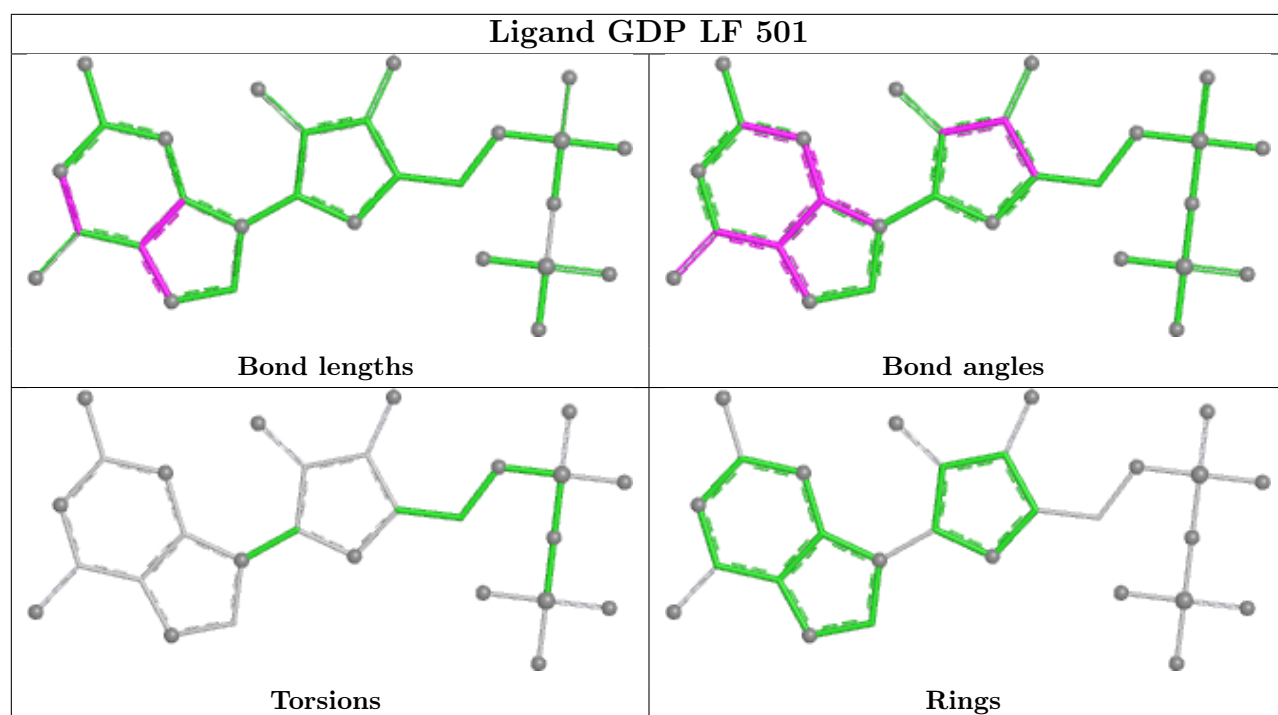


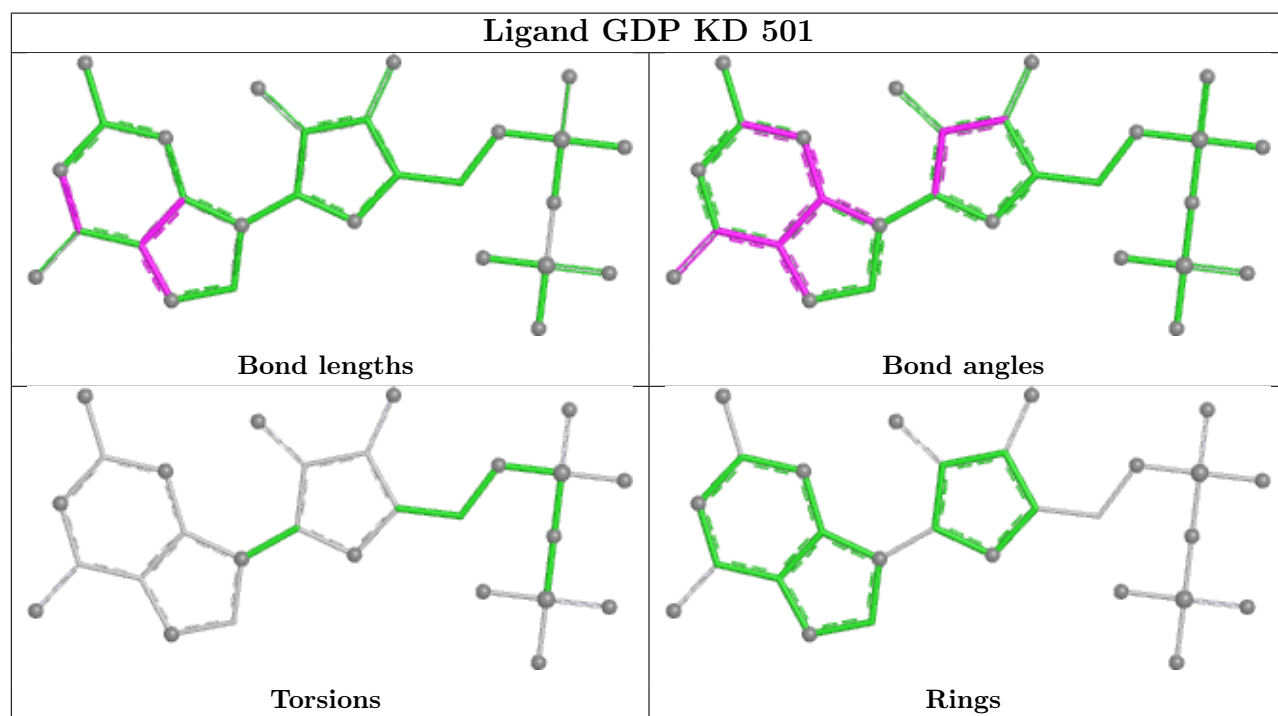
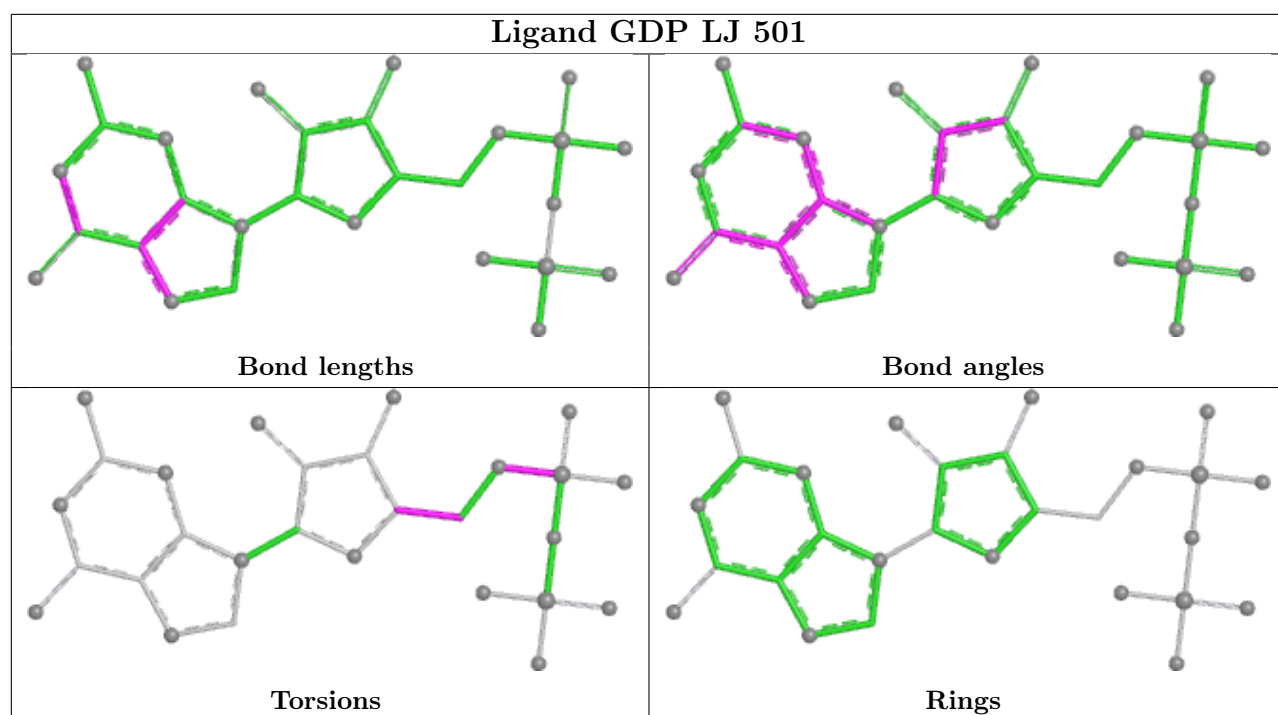


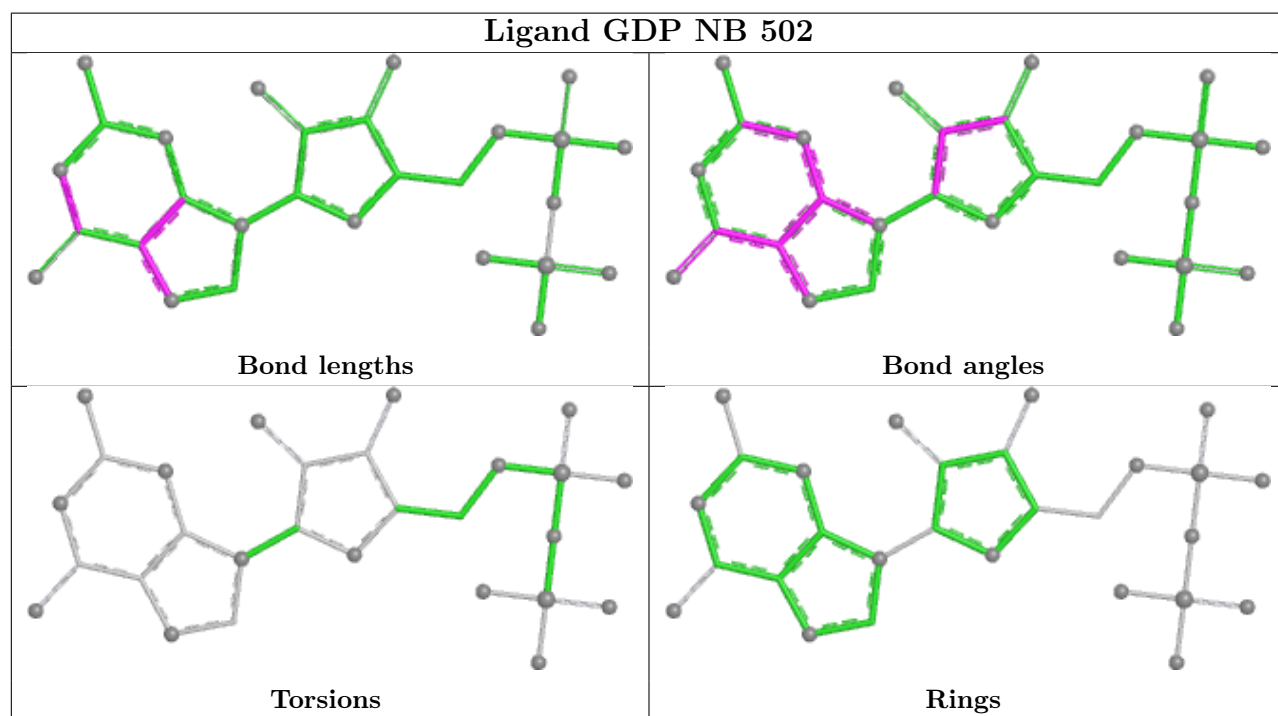
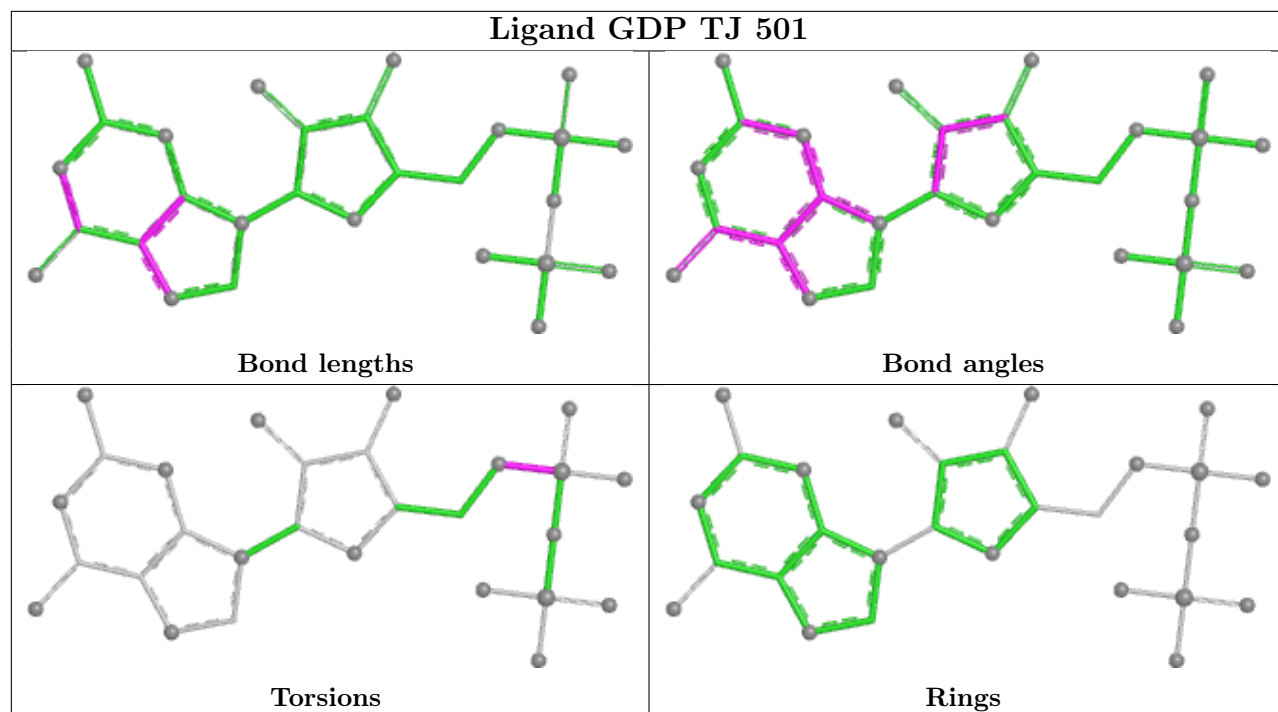




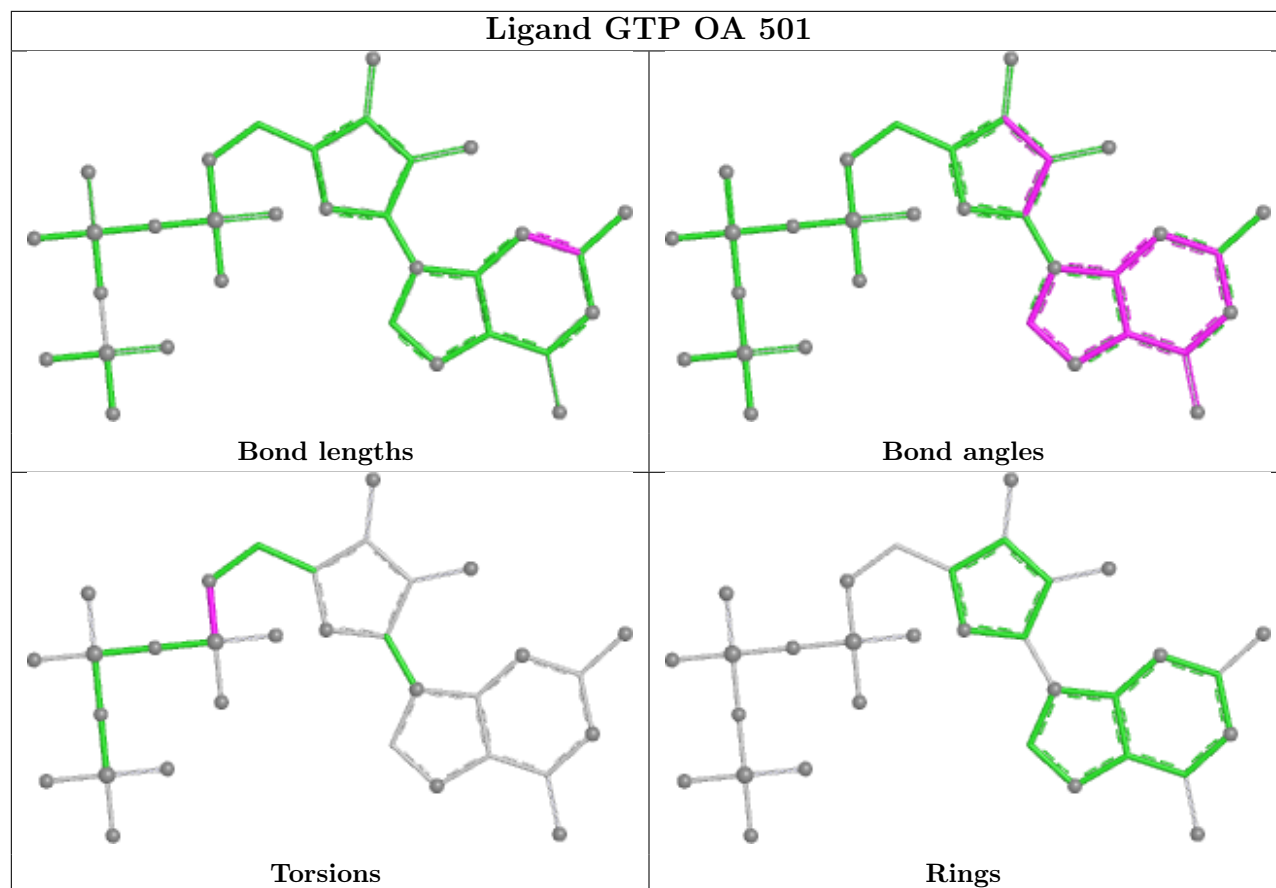




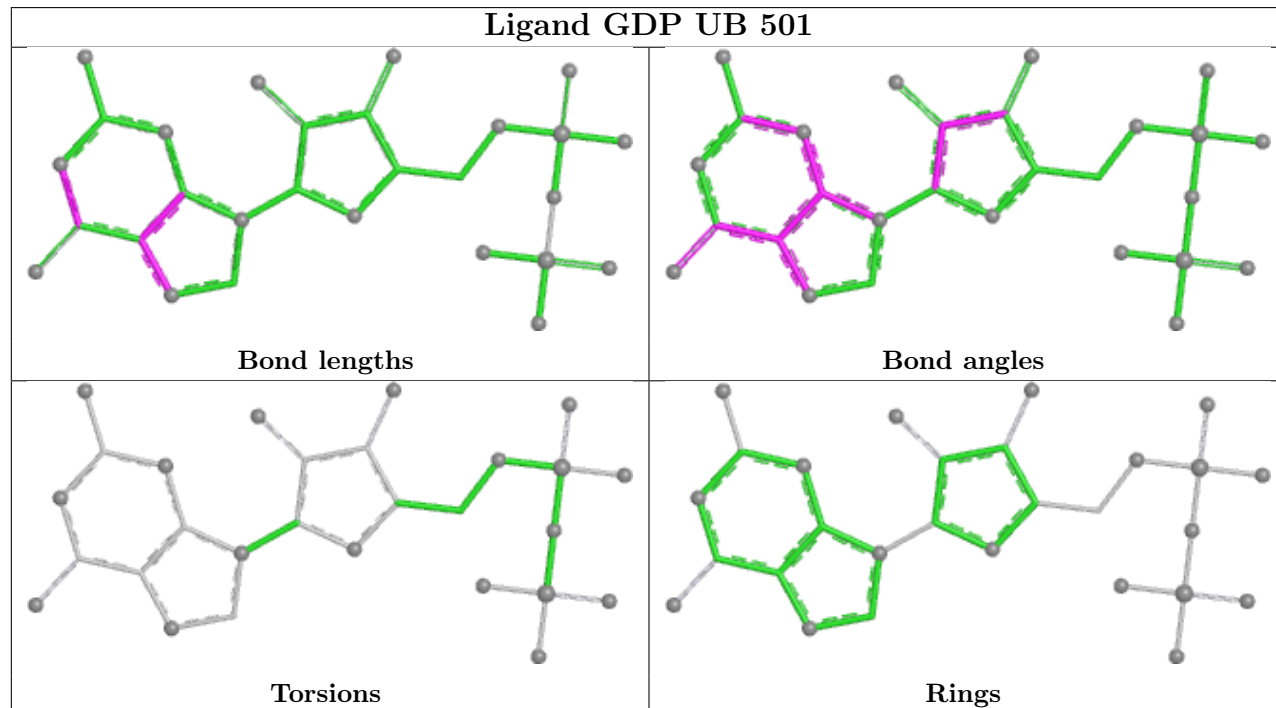


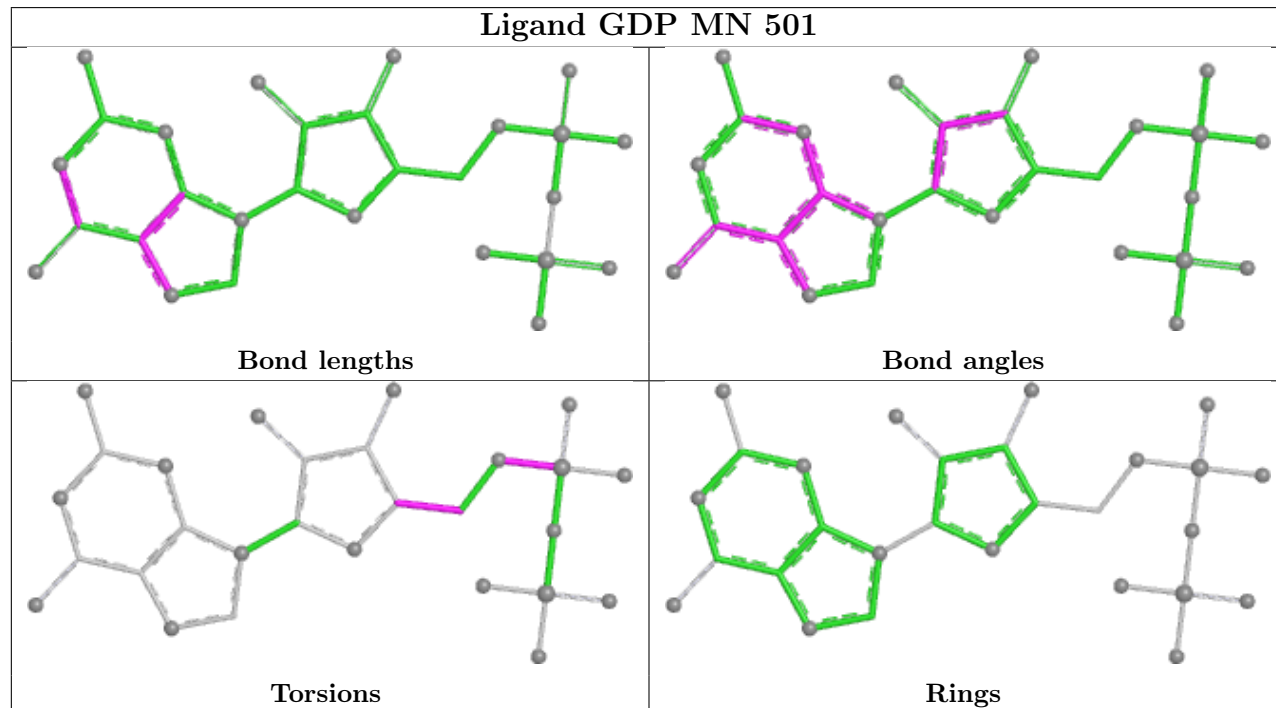
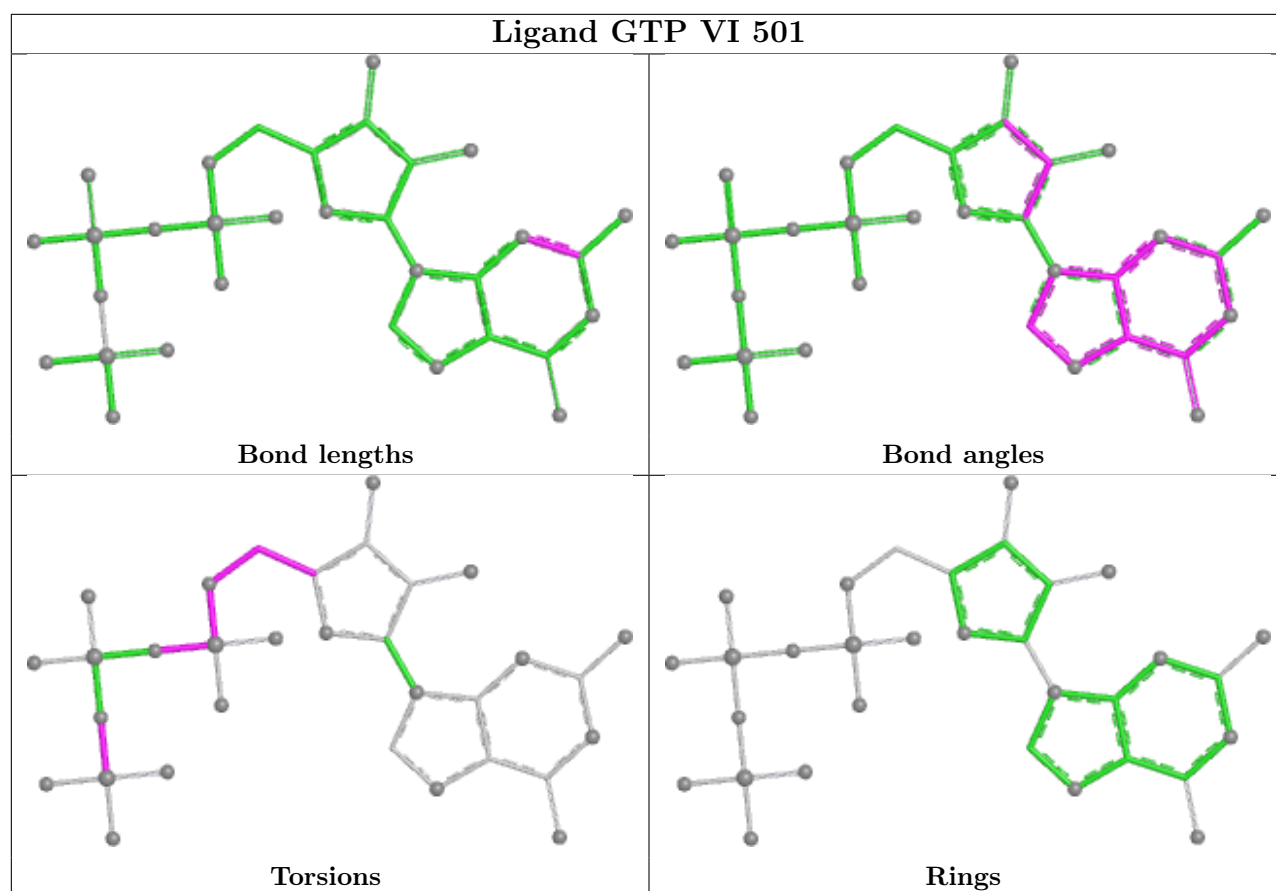


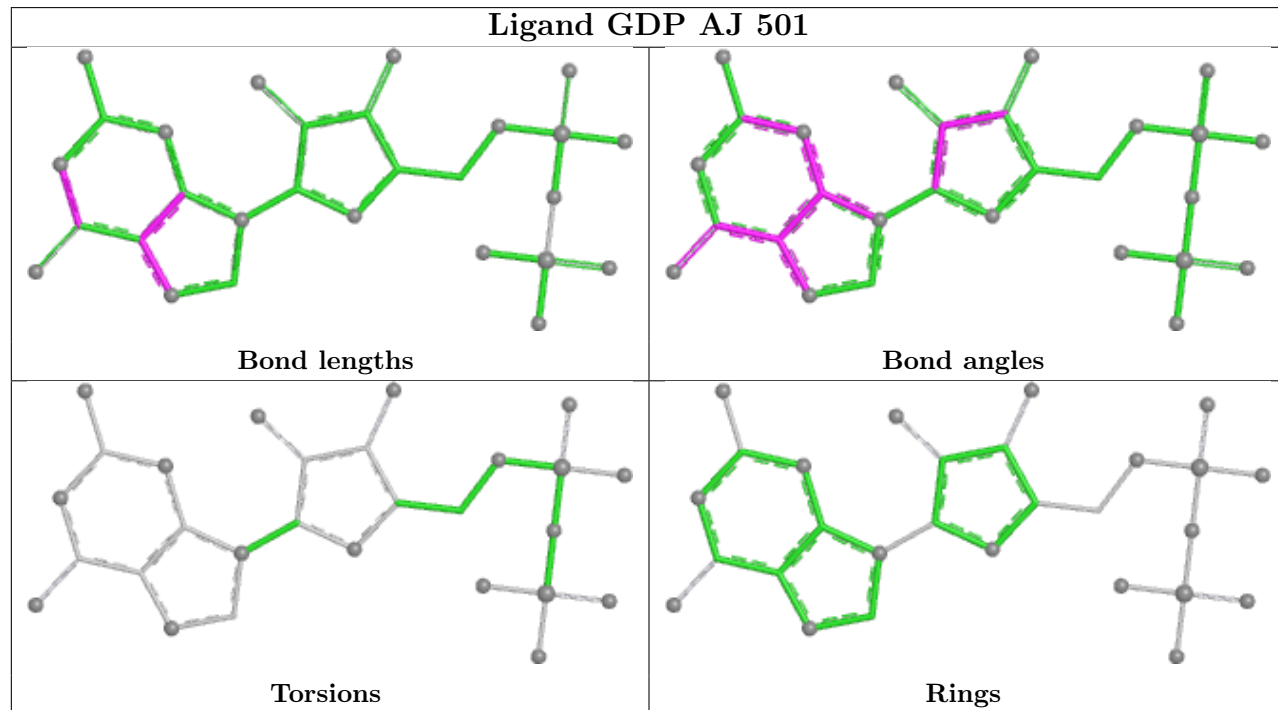
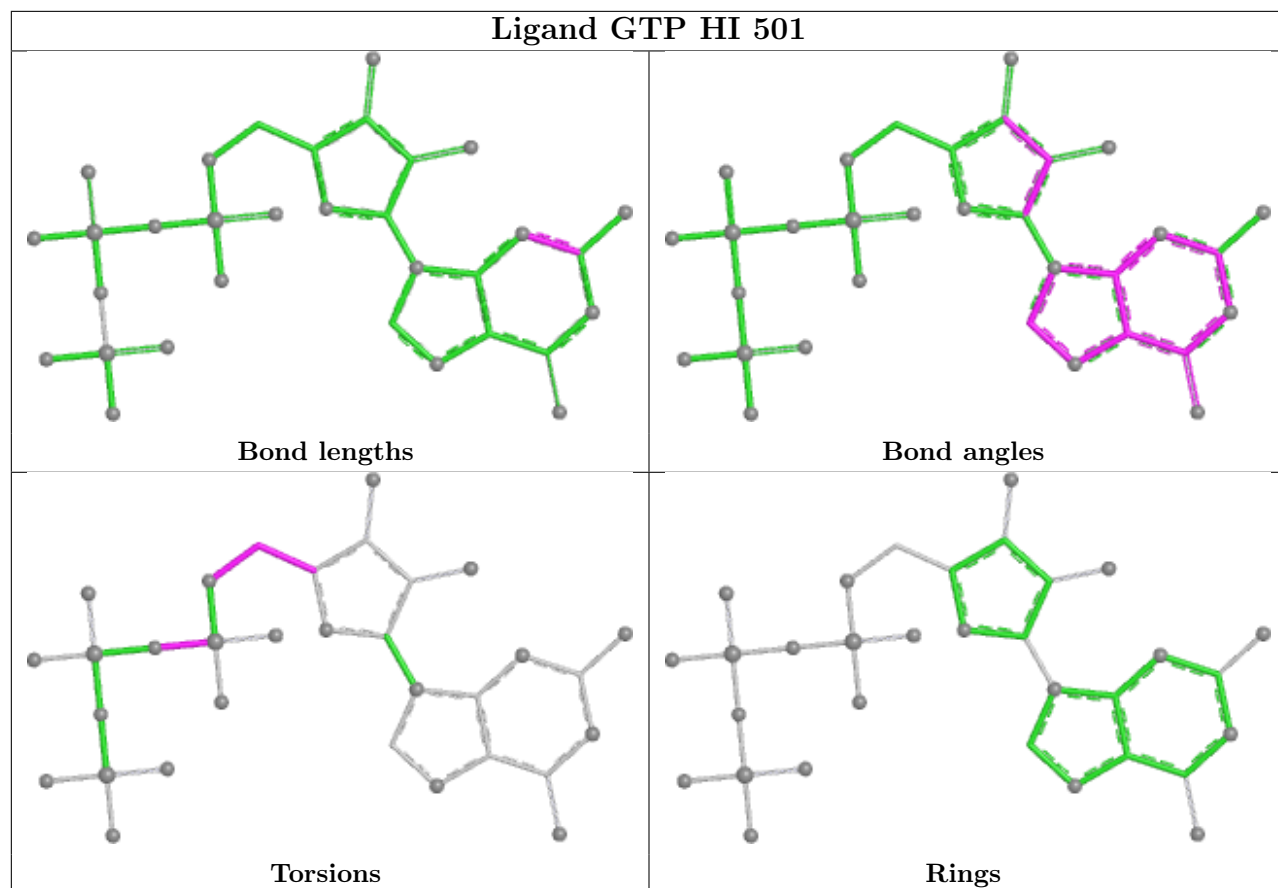
Ligand GTP OA 501



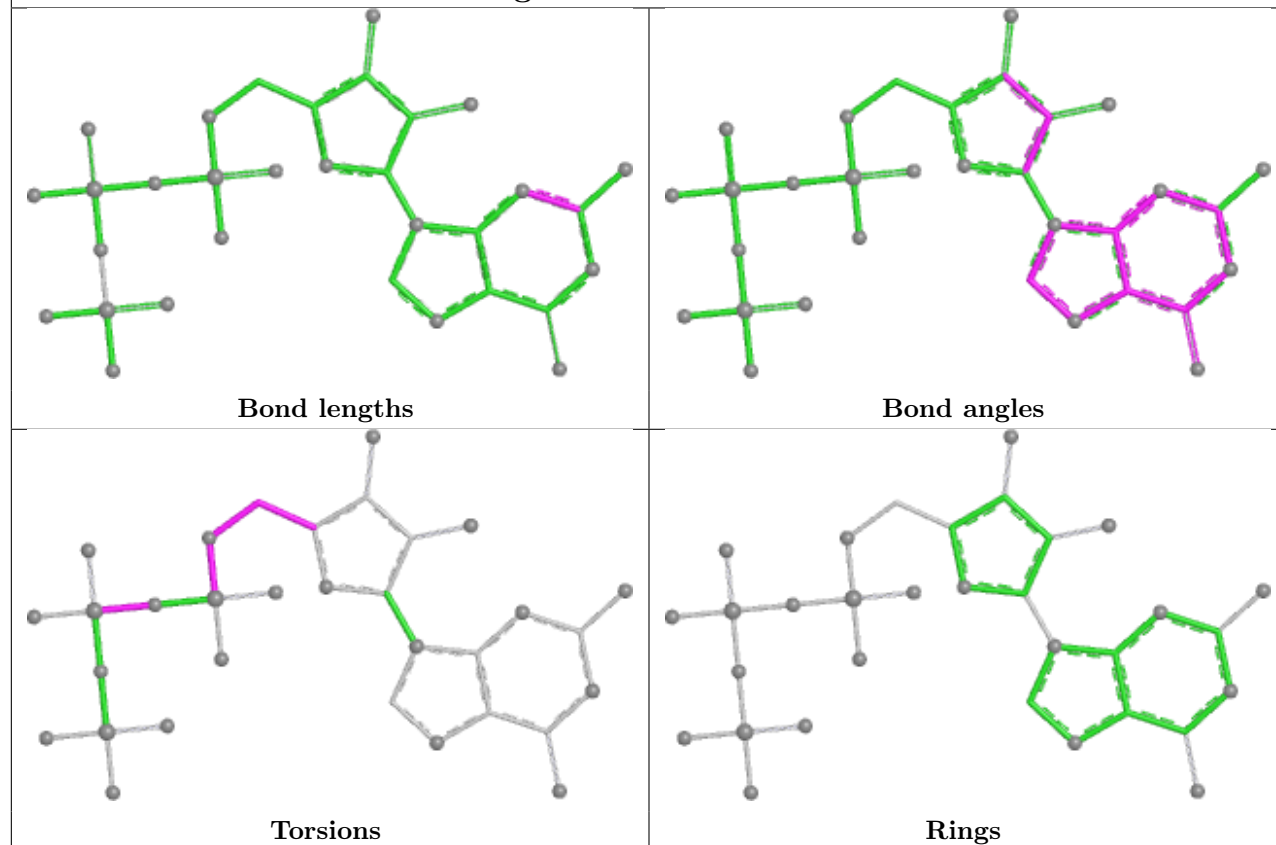
Ligand GDP UB 501



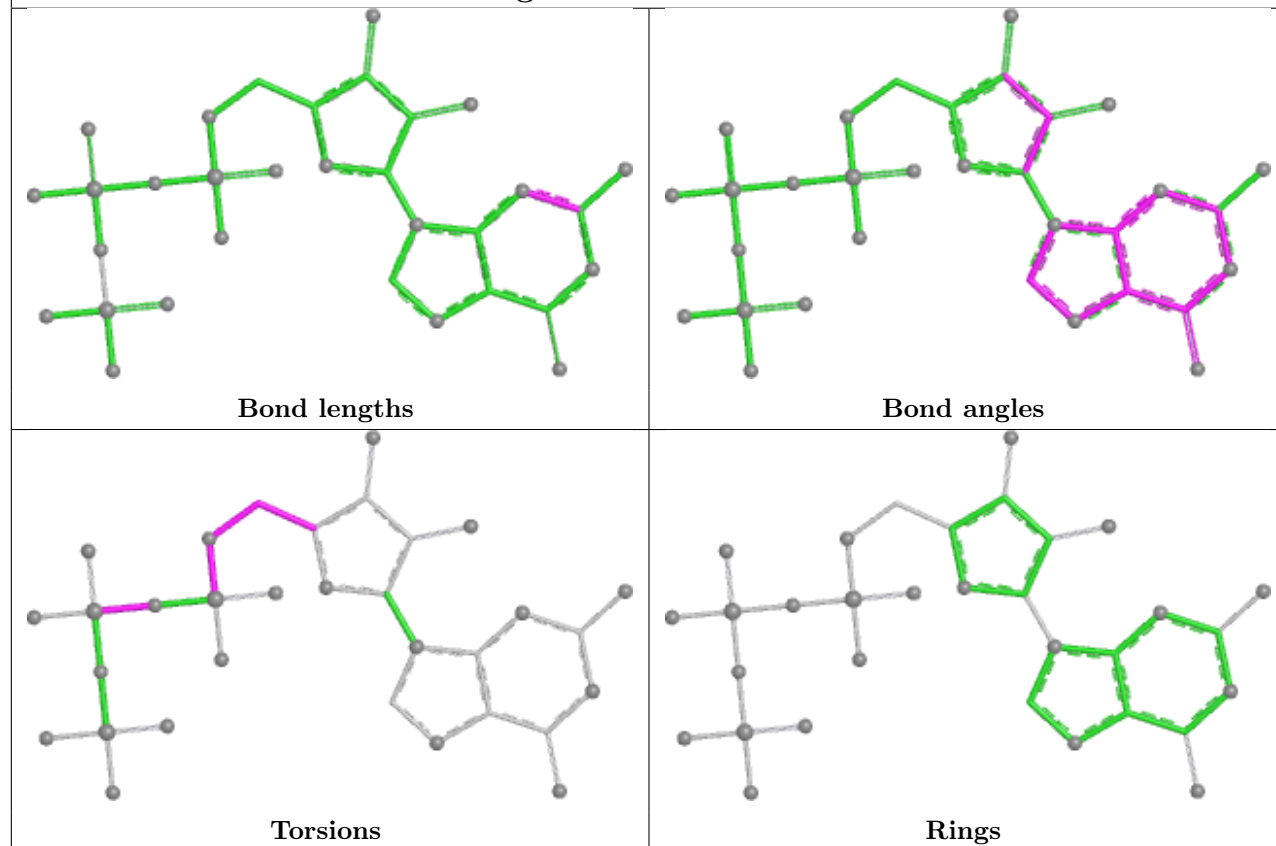




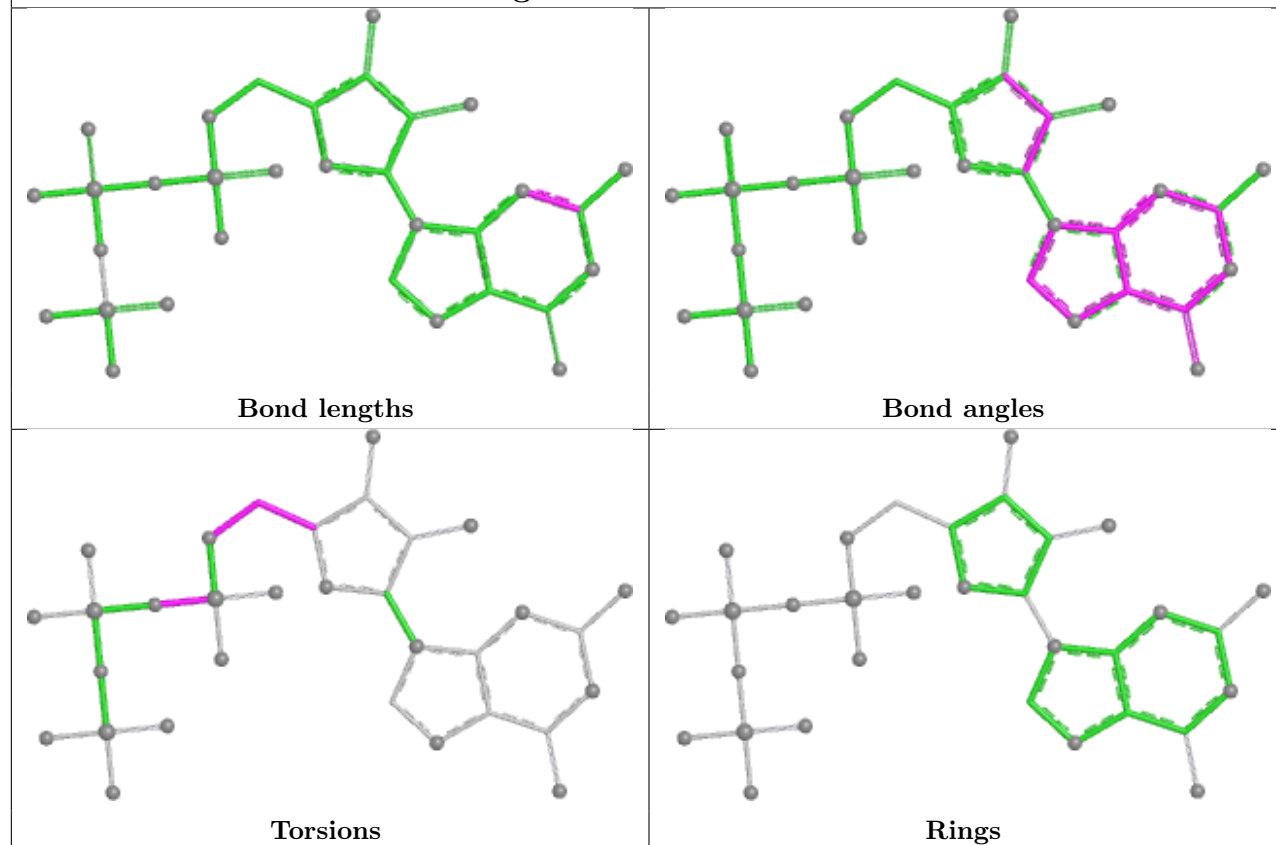
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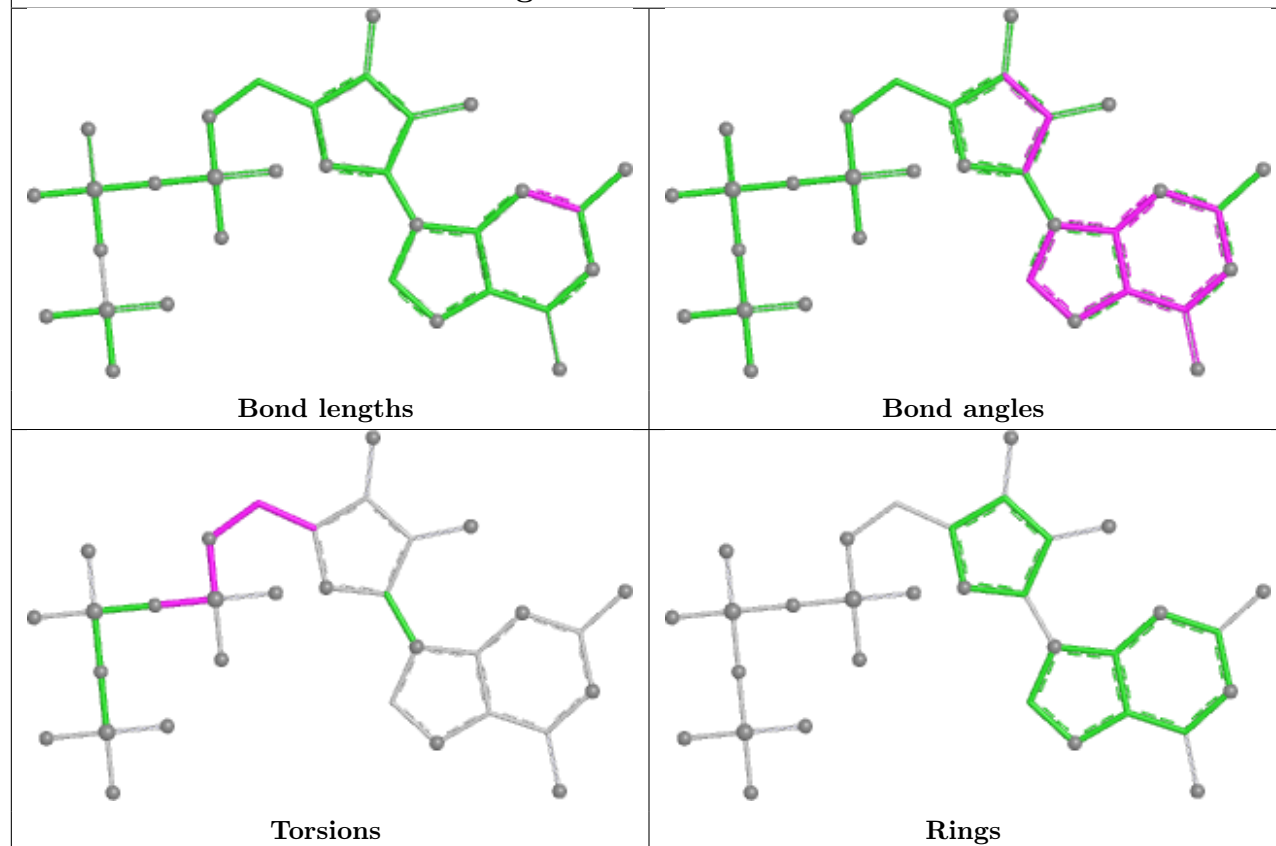
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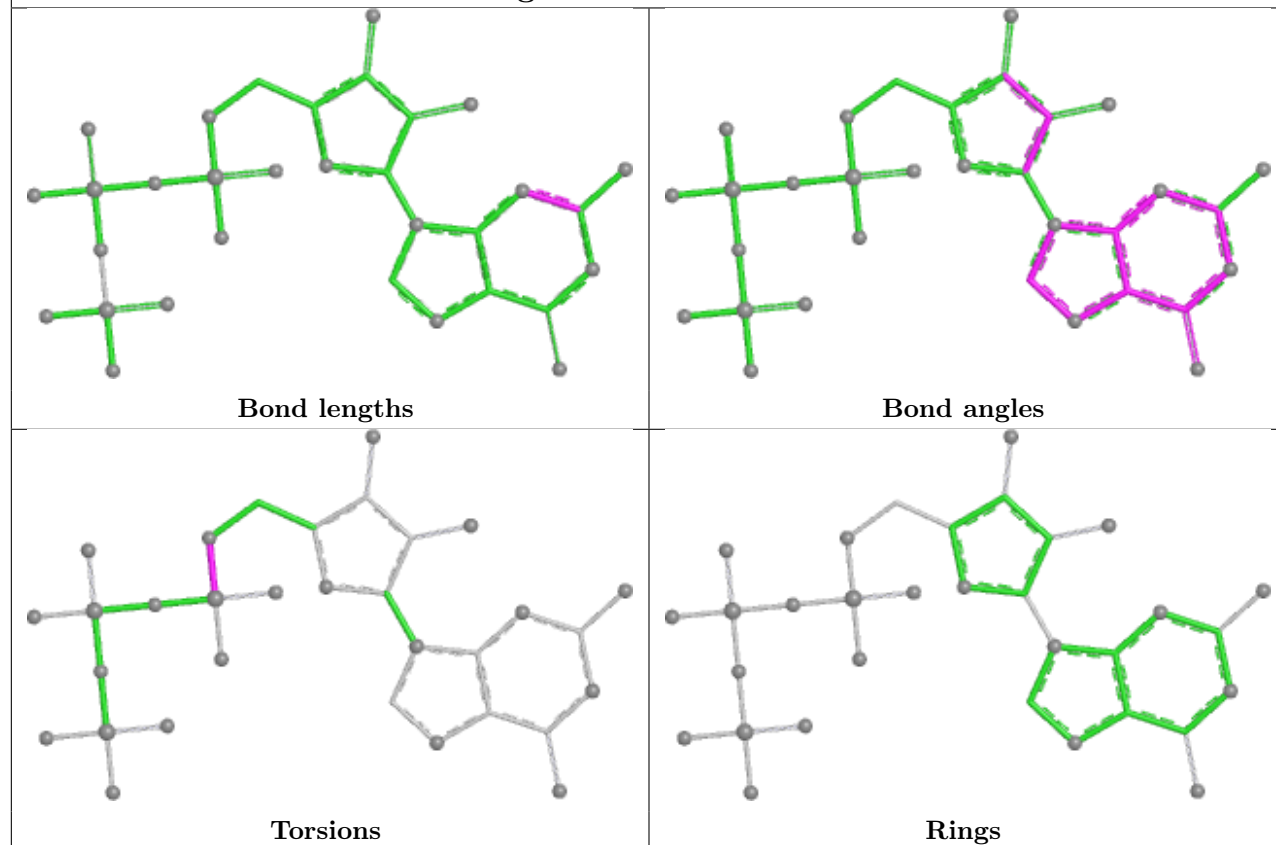
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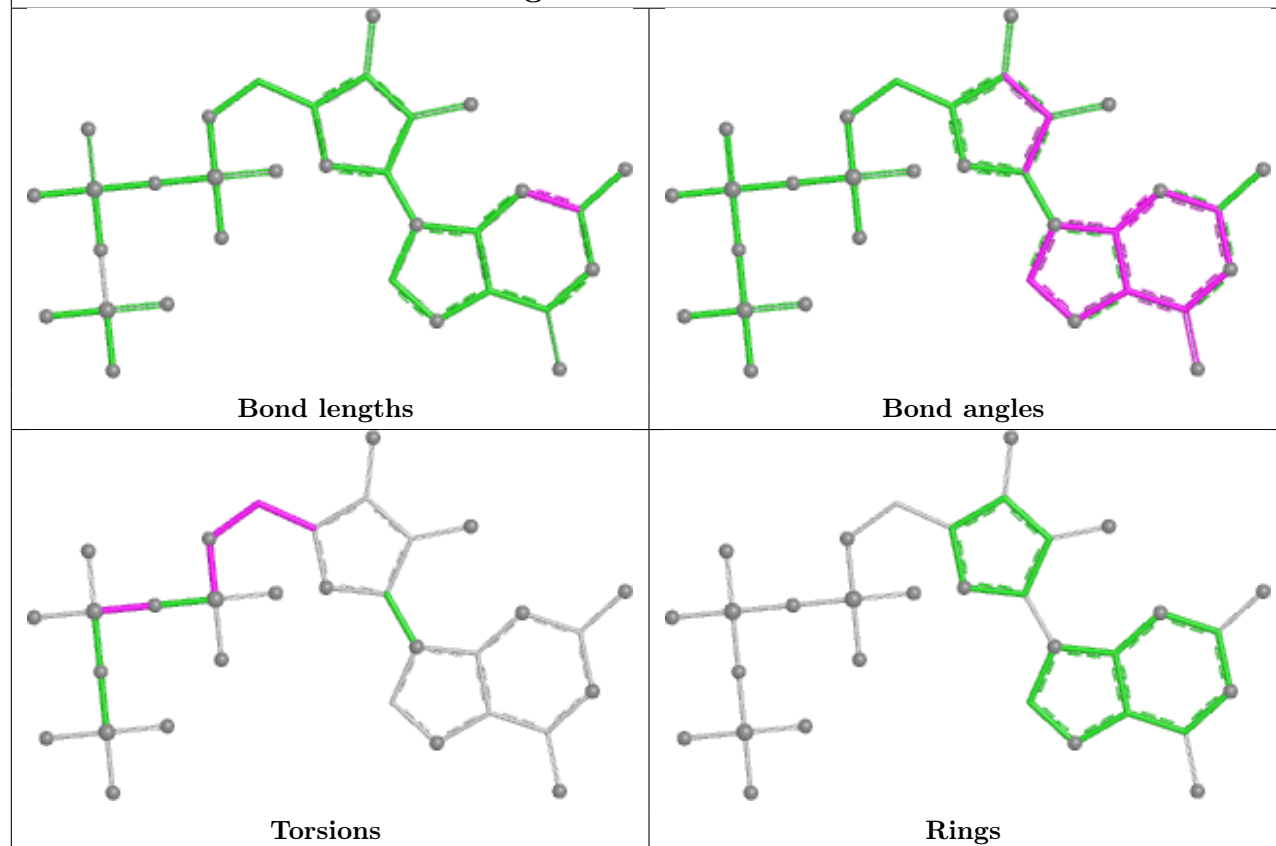
Ligand GTP UK 501



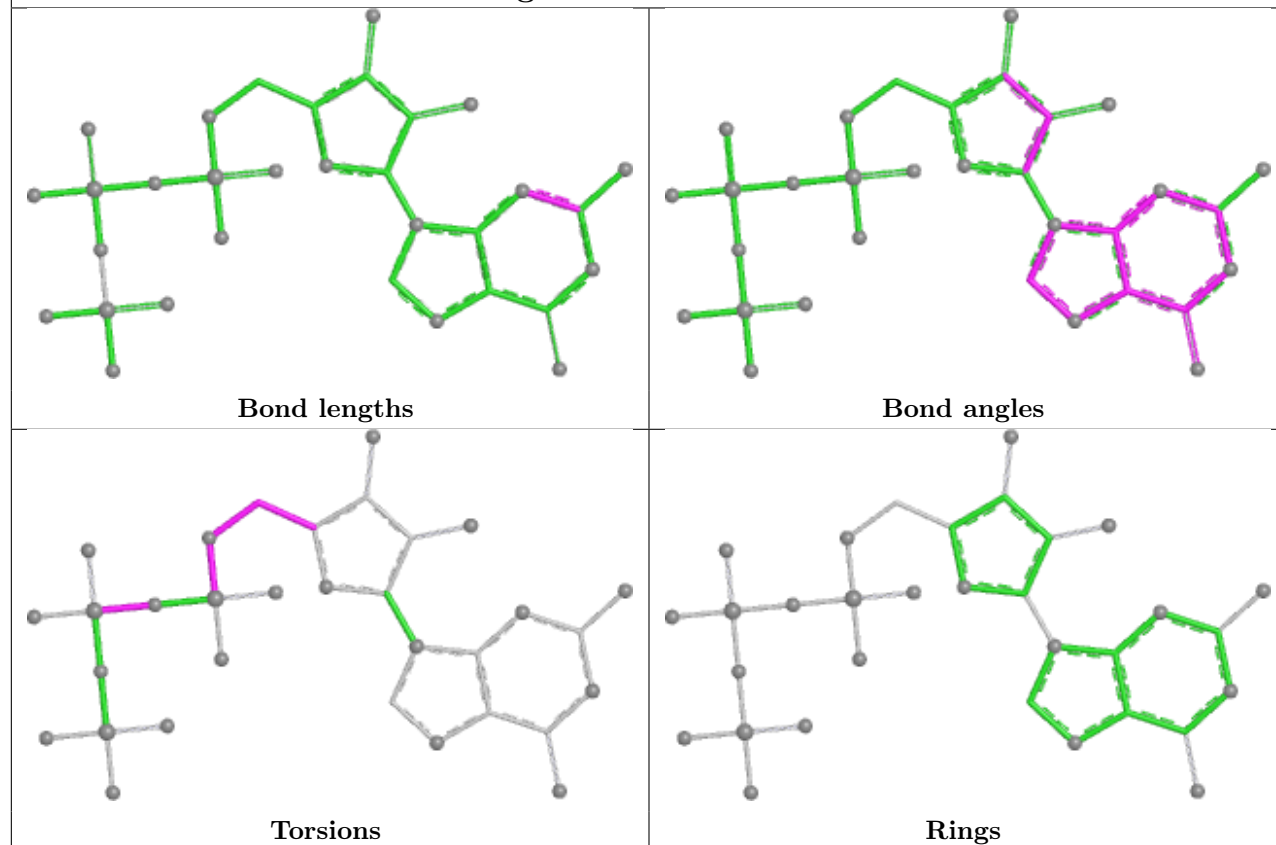
Ligand GTP OC 501



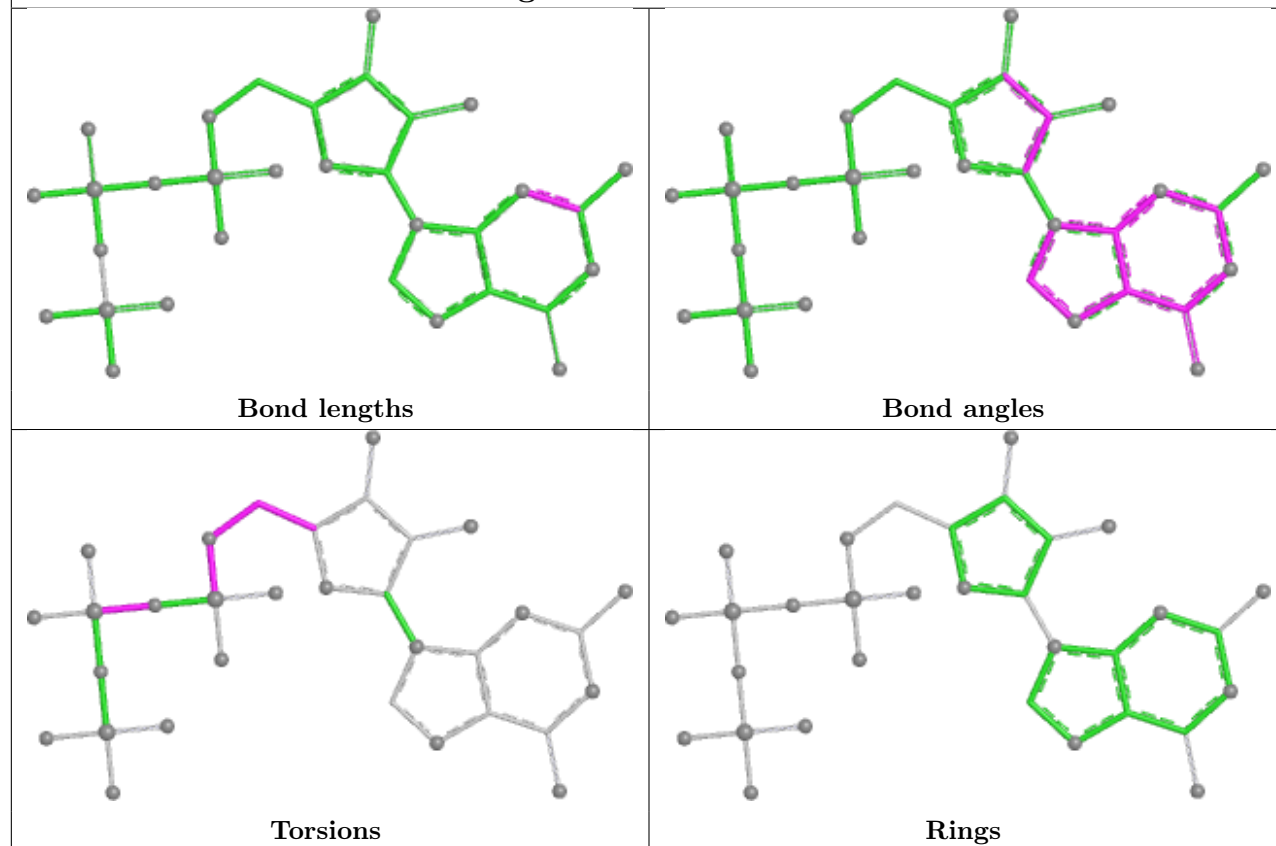
Ligand GTP PI 501



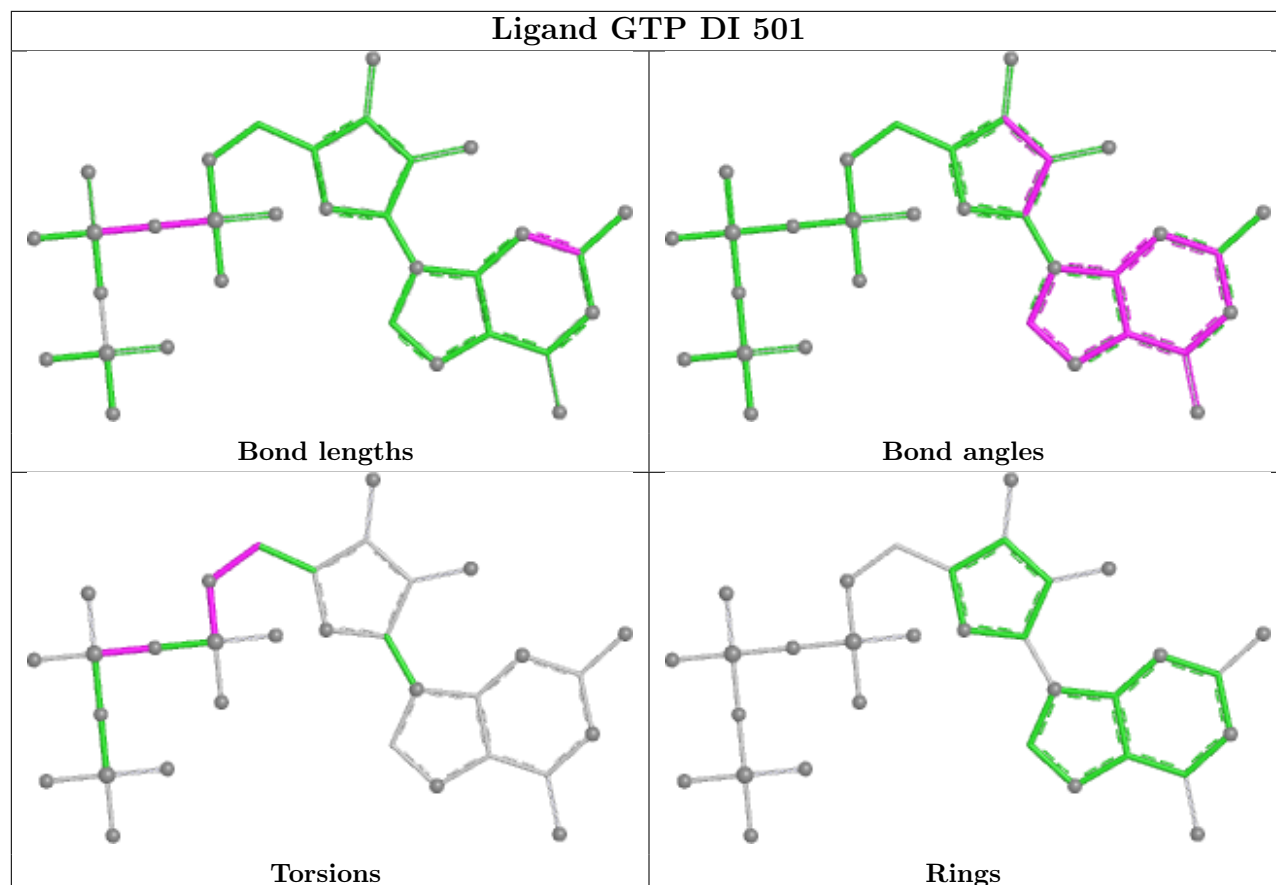
Ligand GTP DC 501



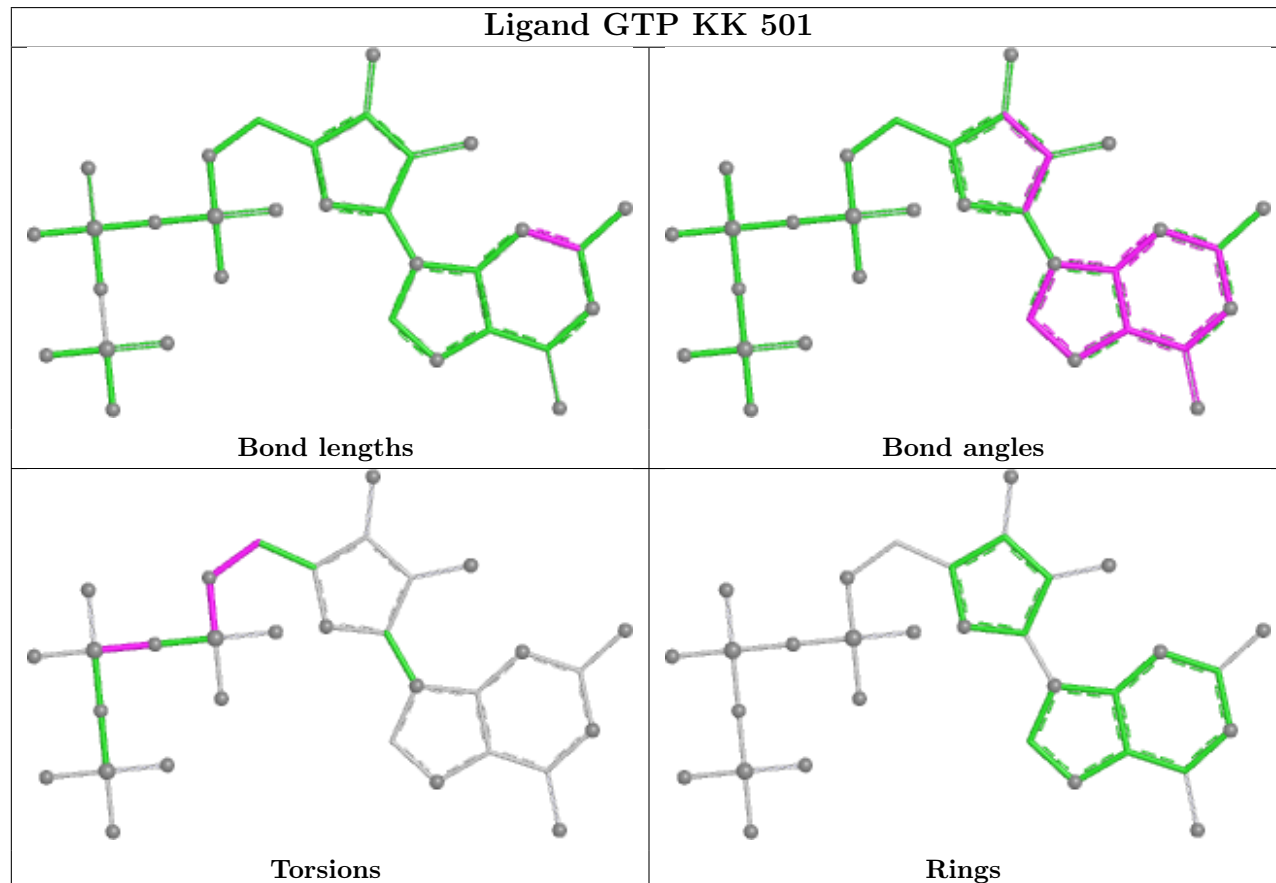
Ligand GTP KE 501

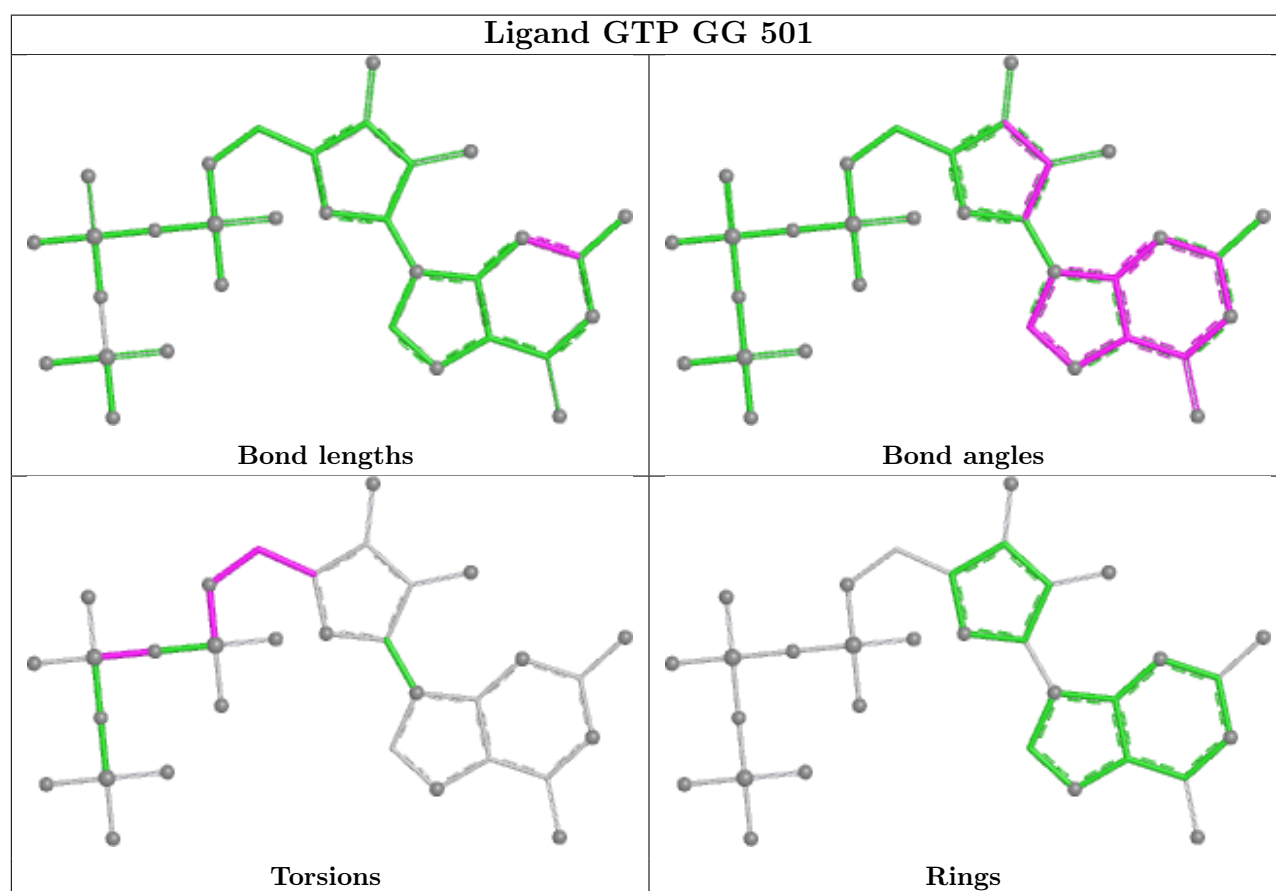
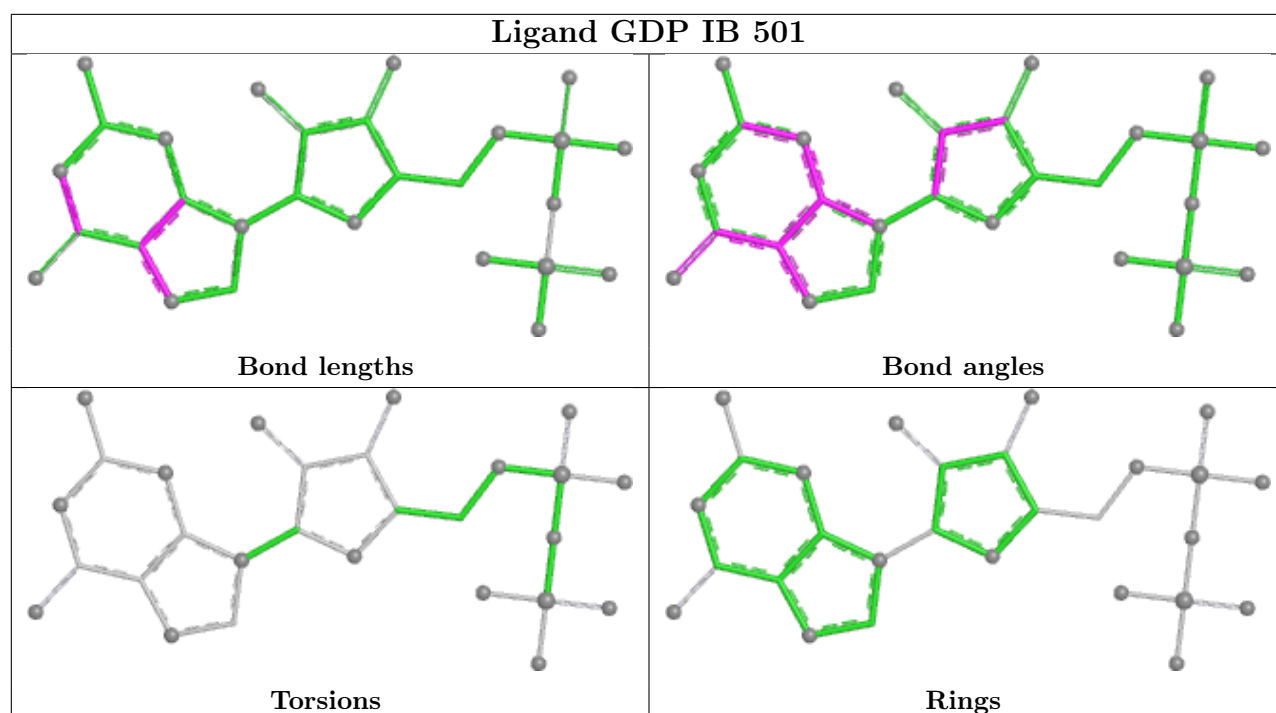


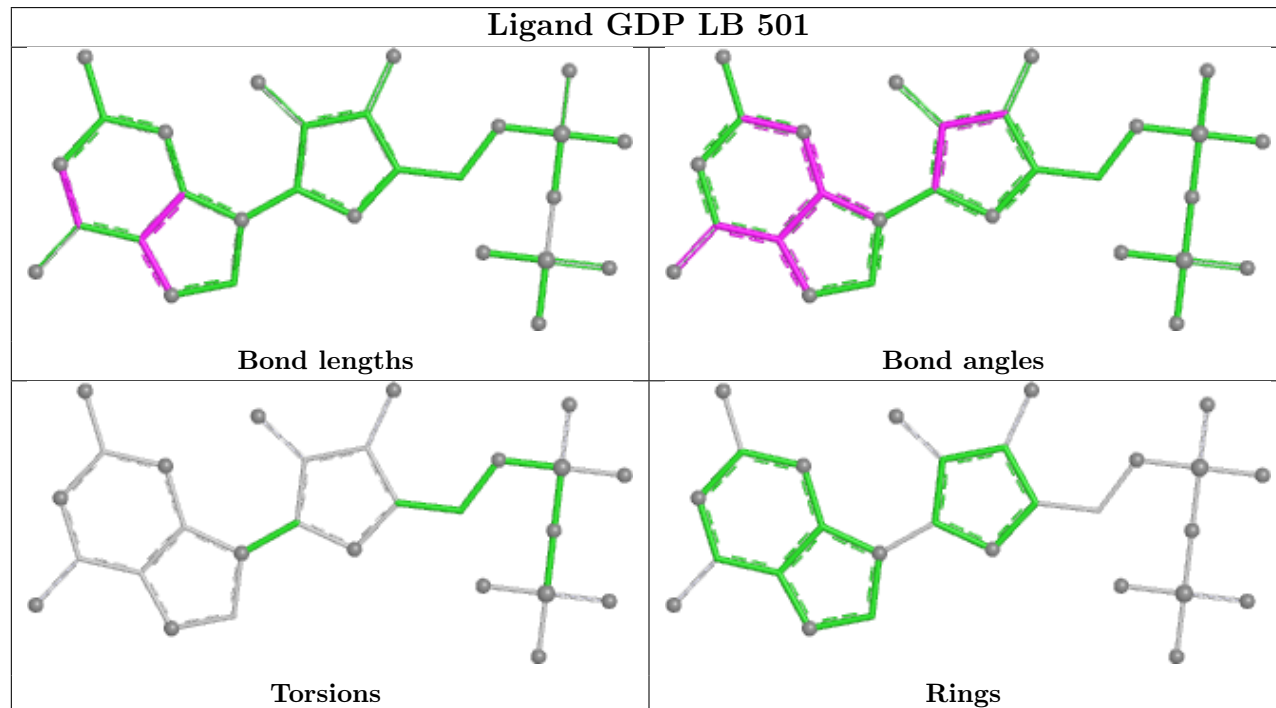
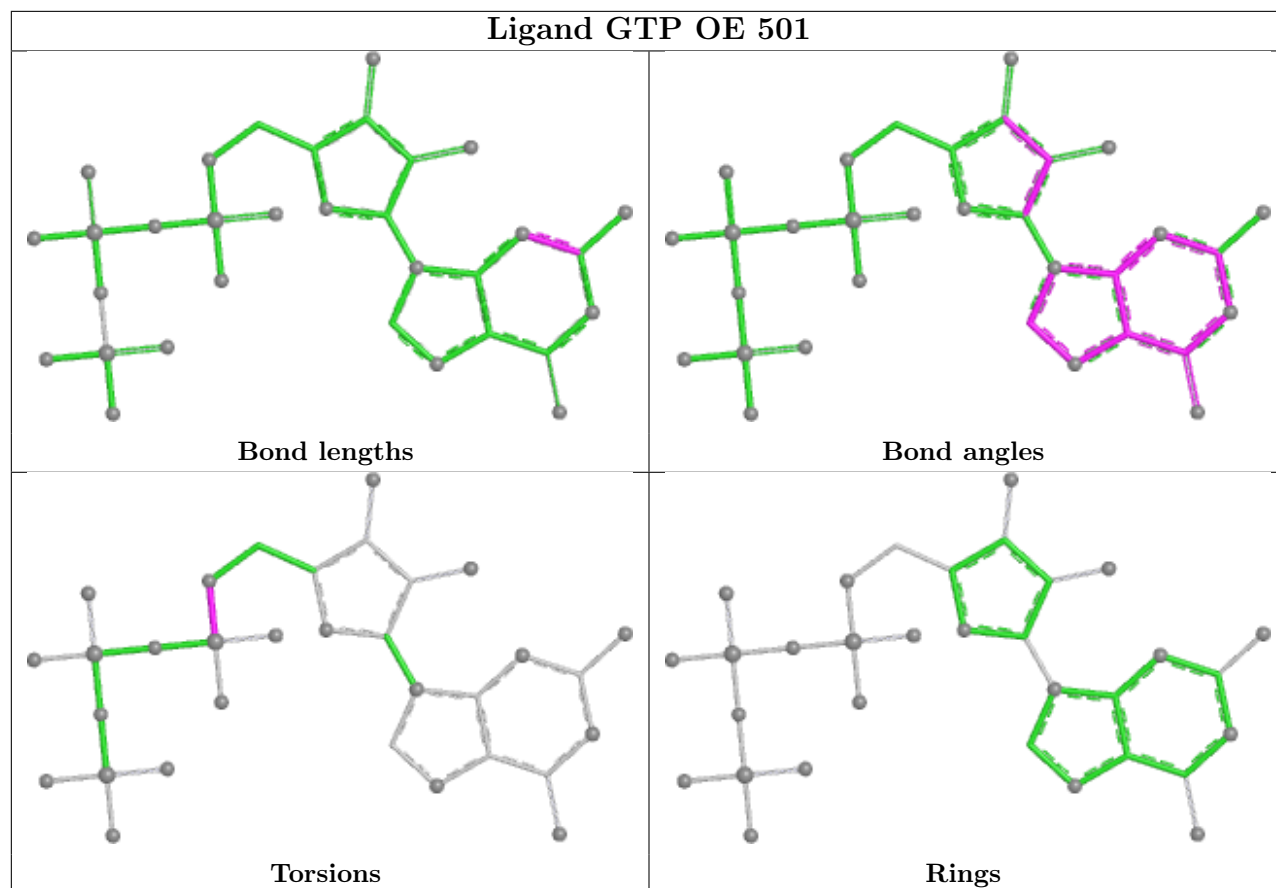
Ligand GTP DI 501

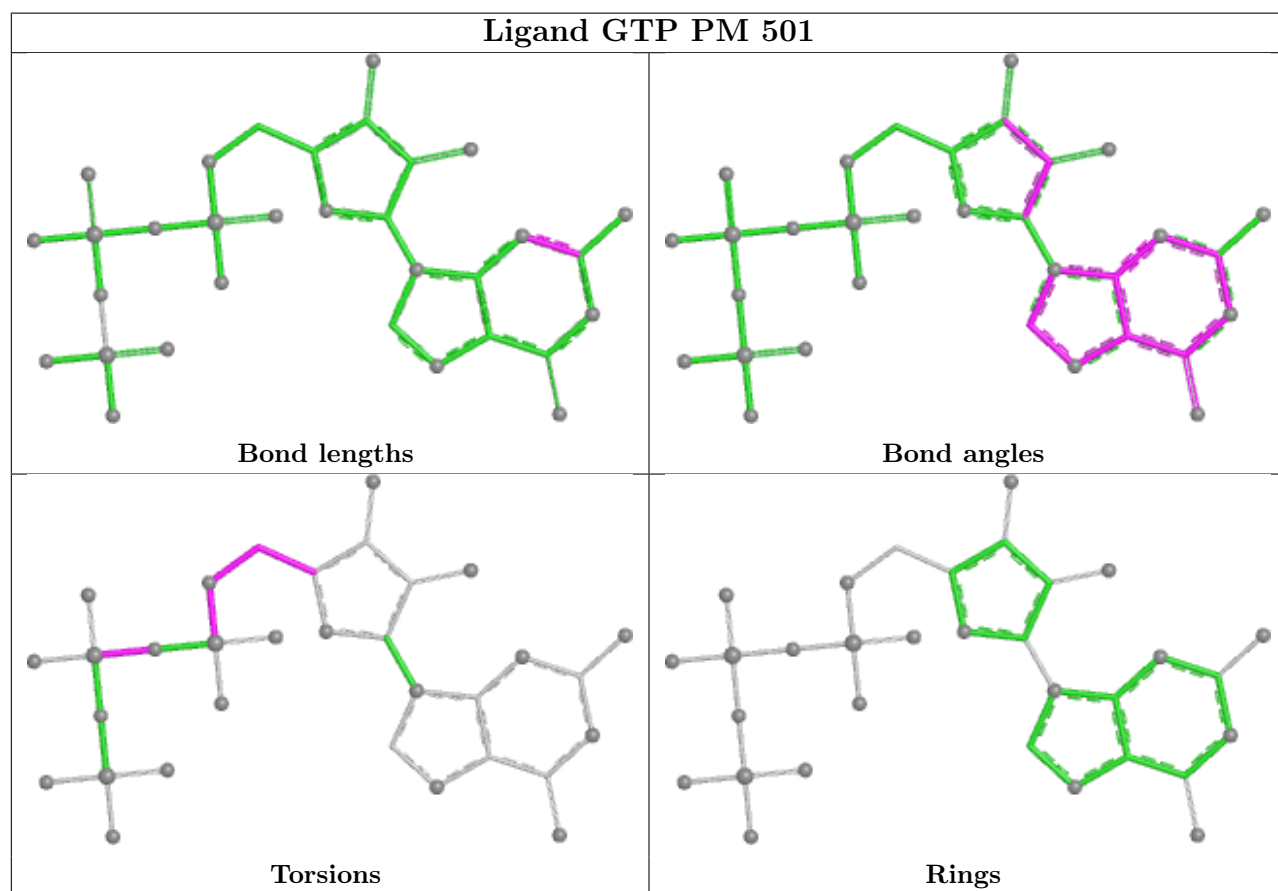
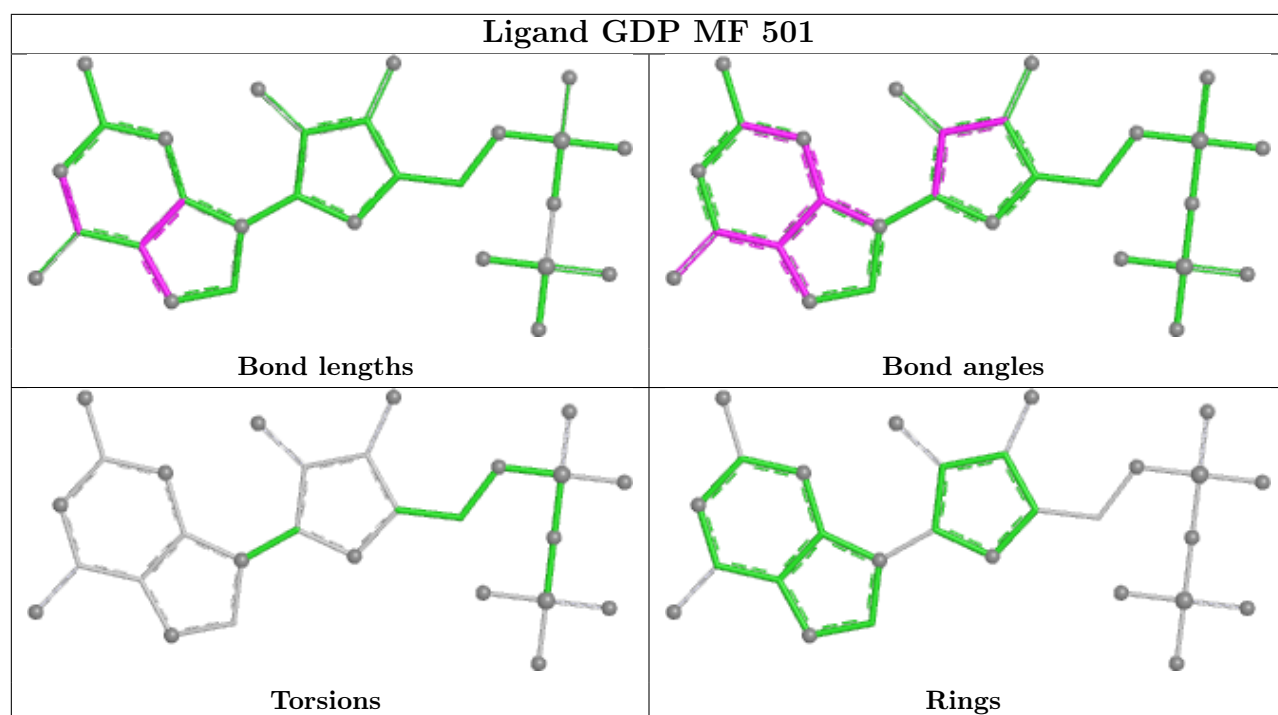


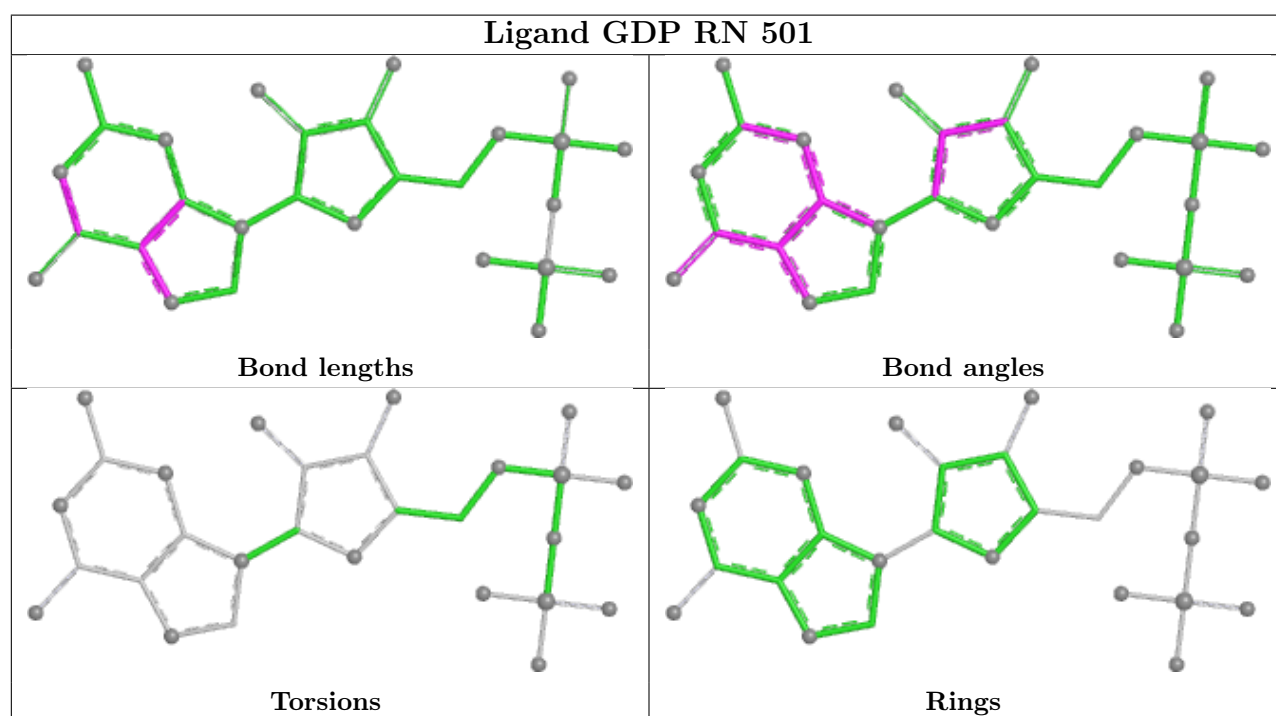
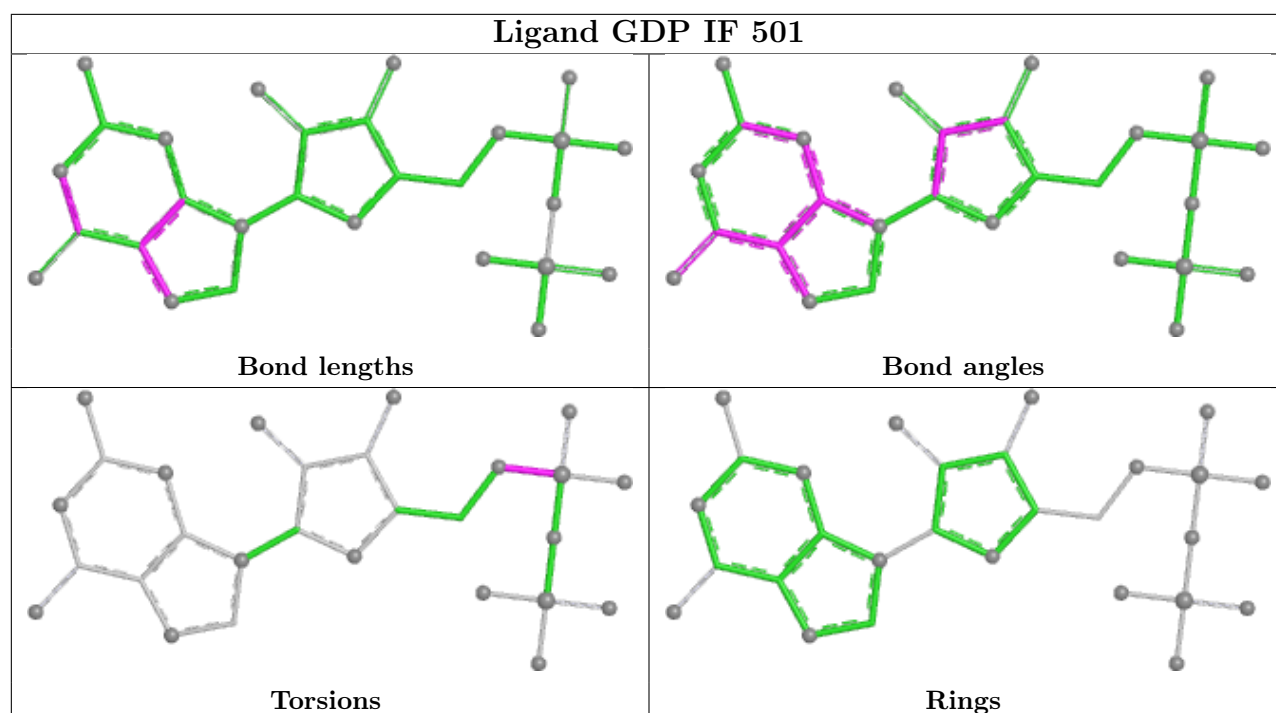
Ligand GTP KK 501

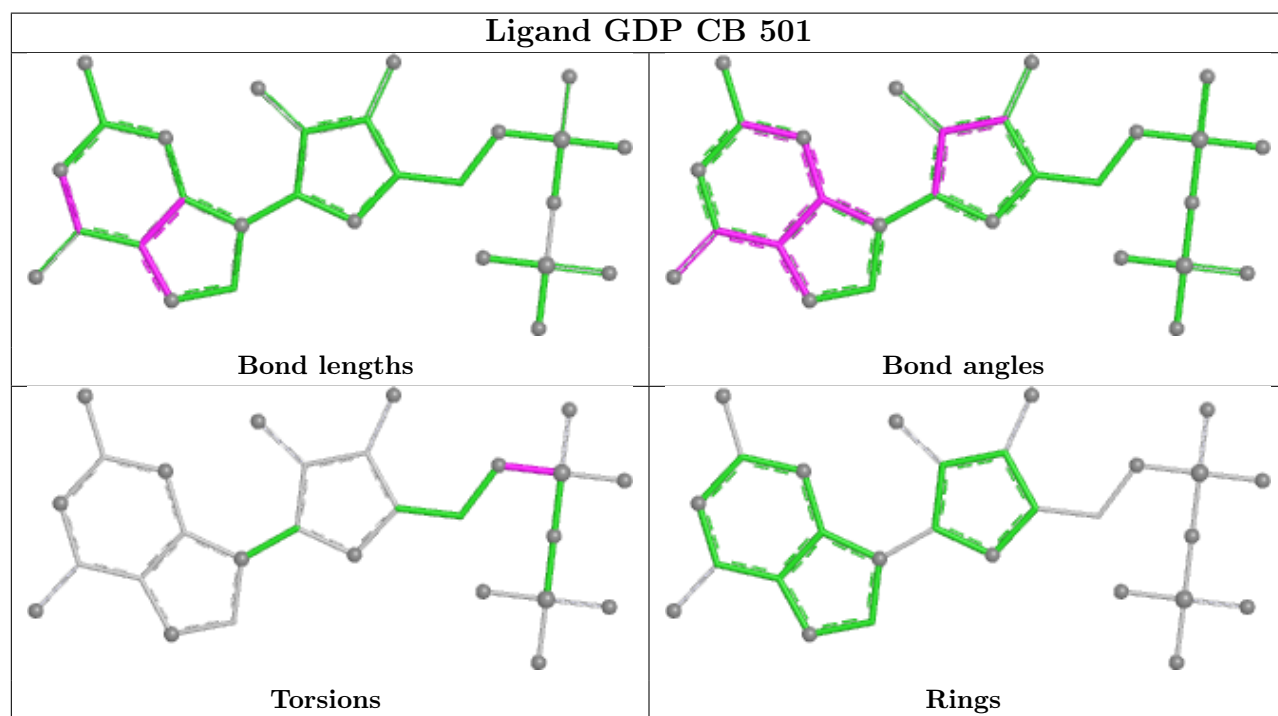
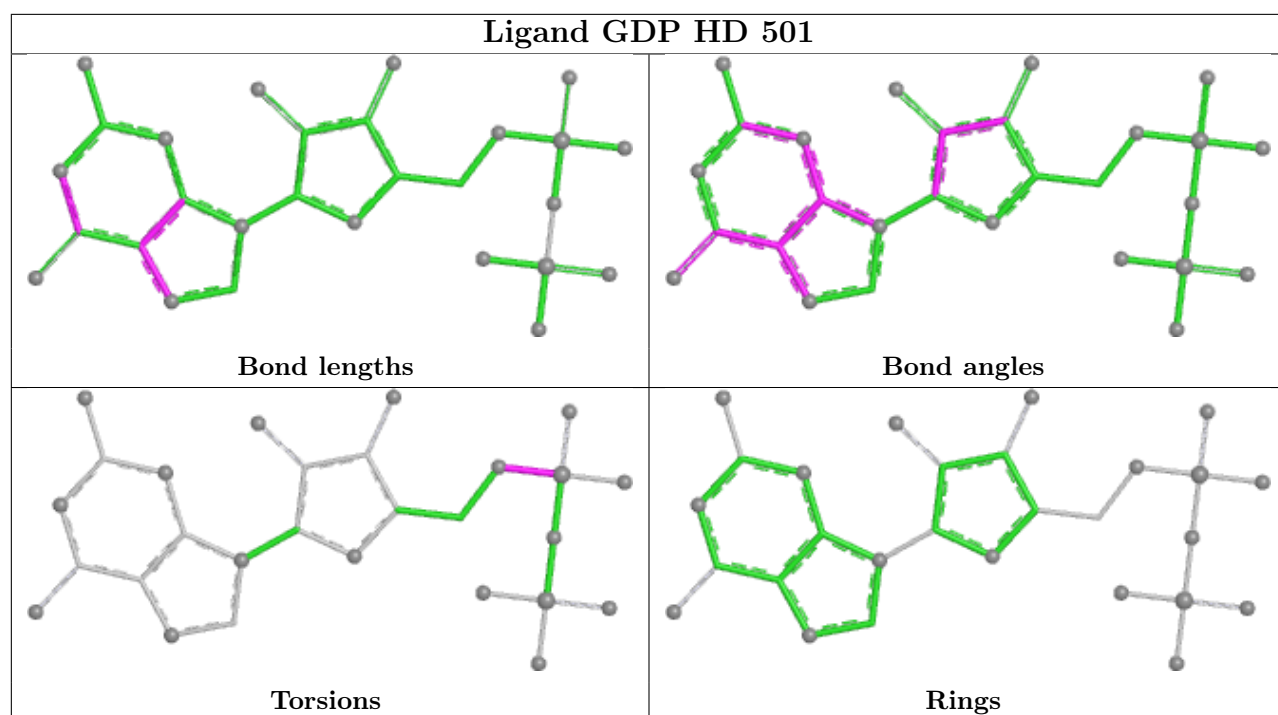


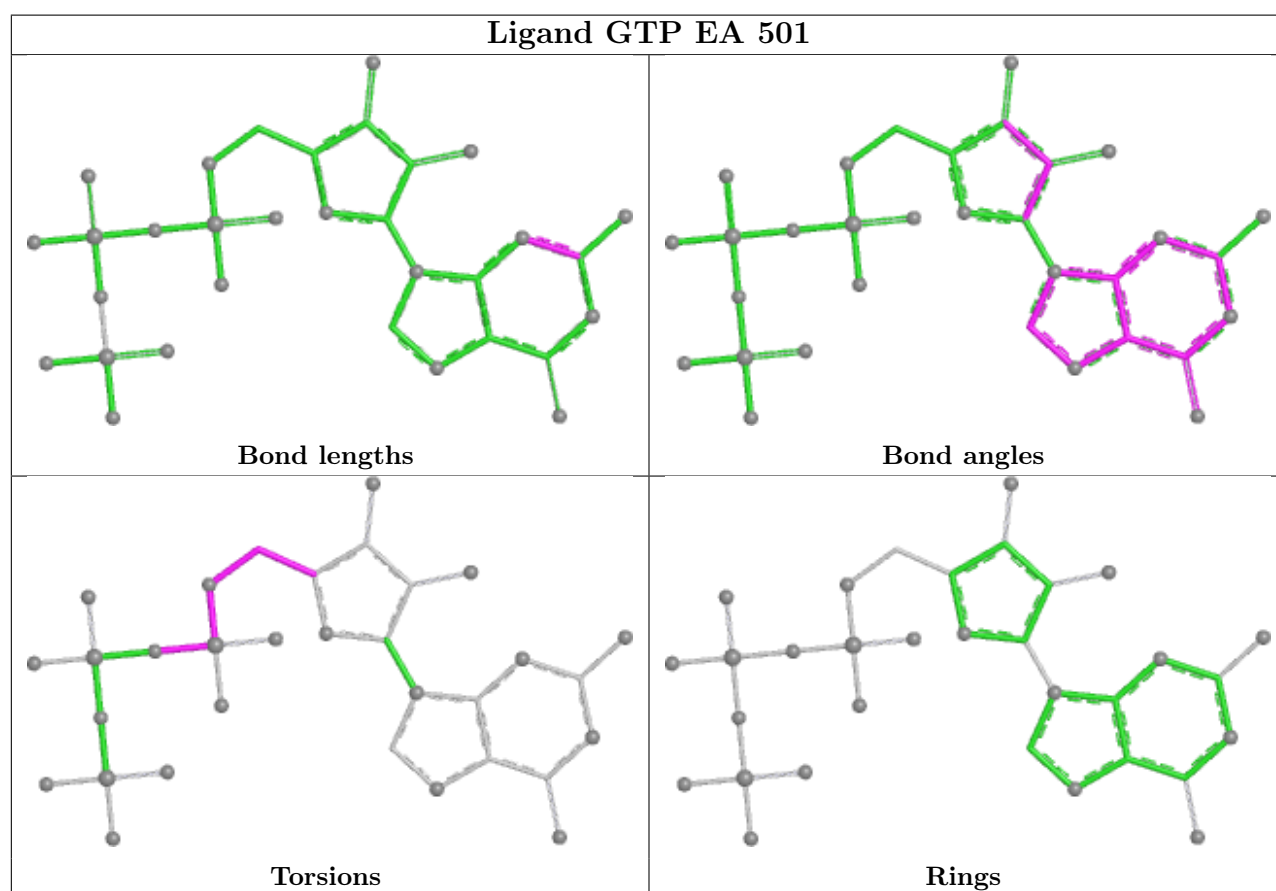
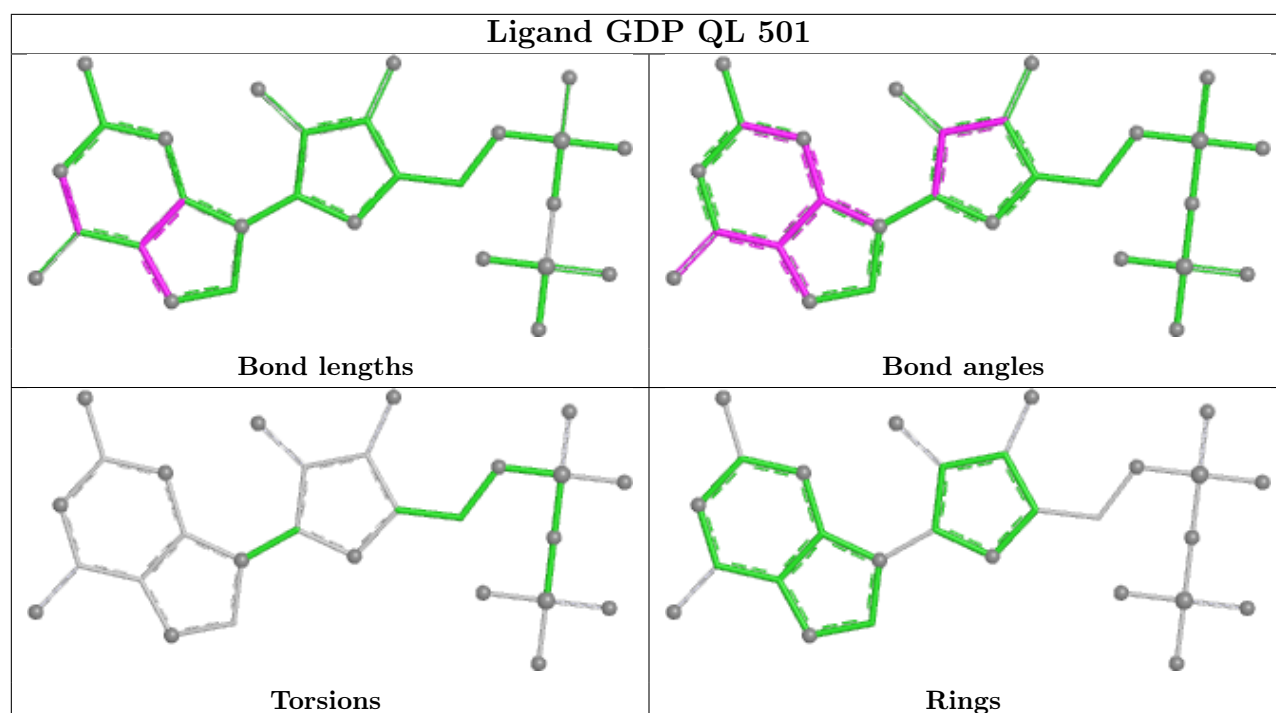




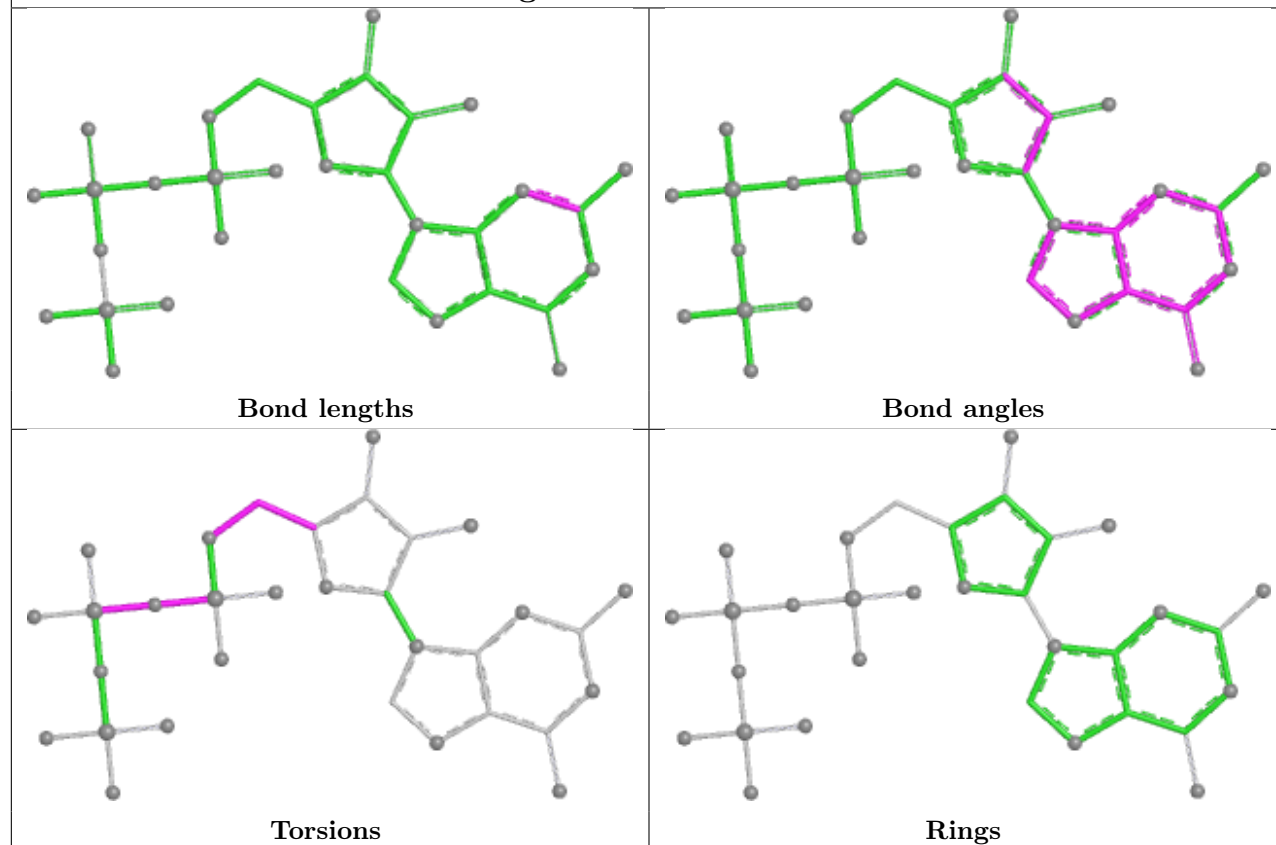




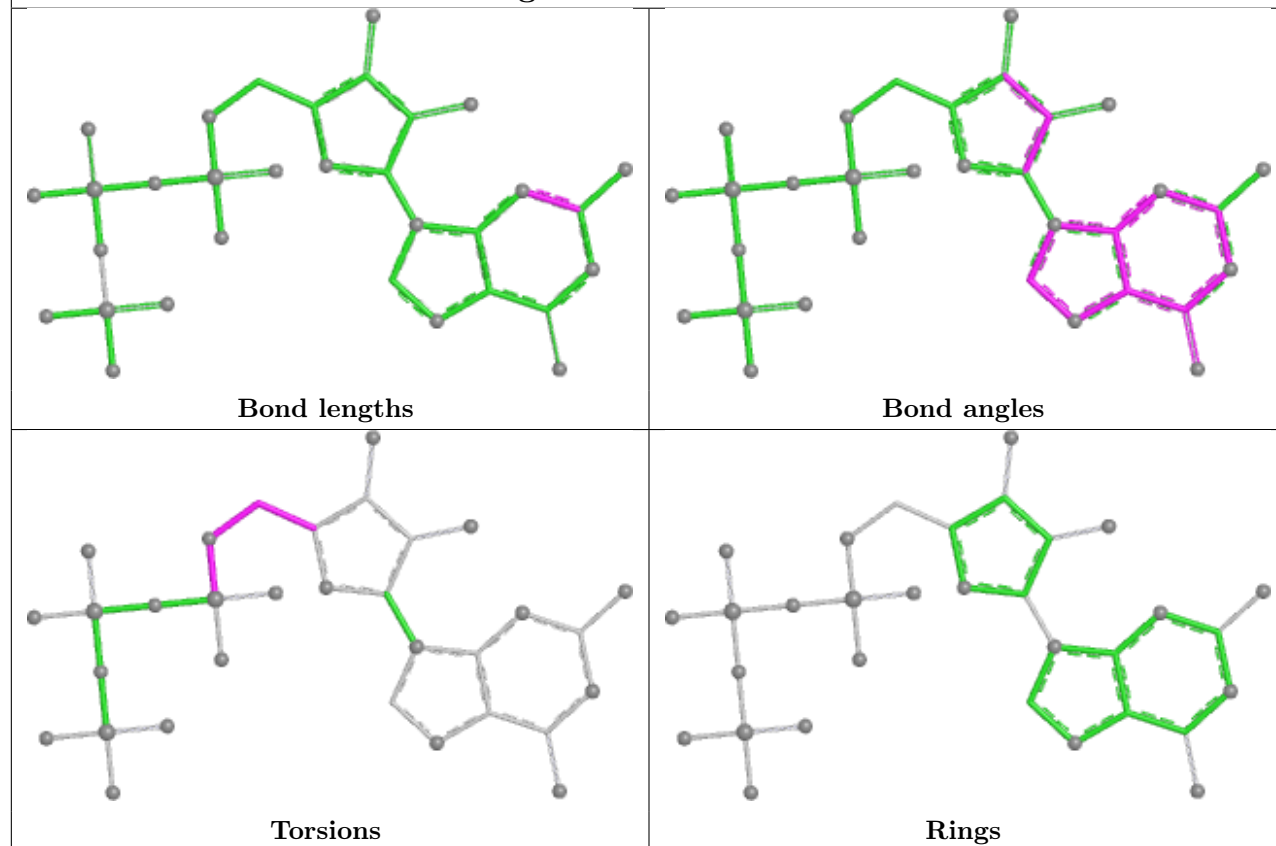


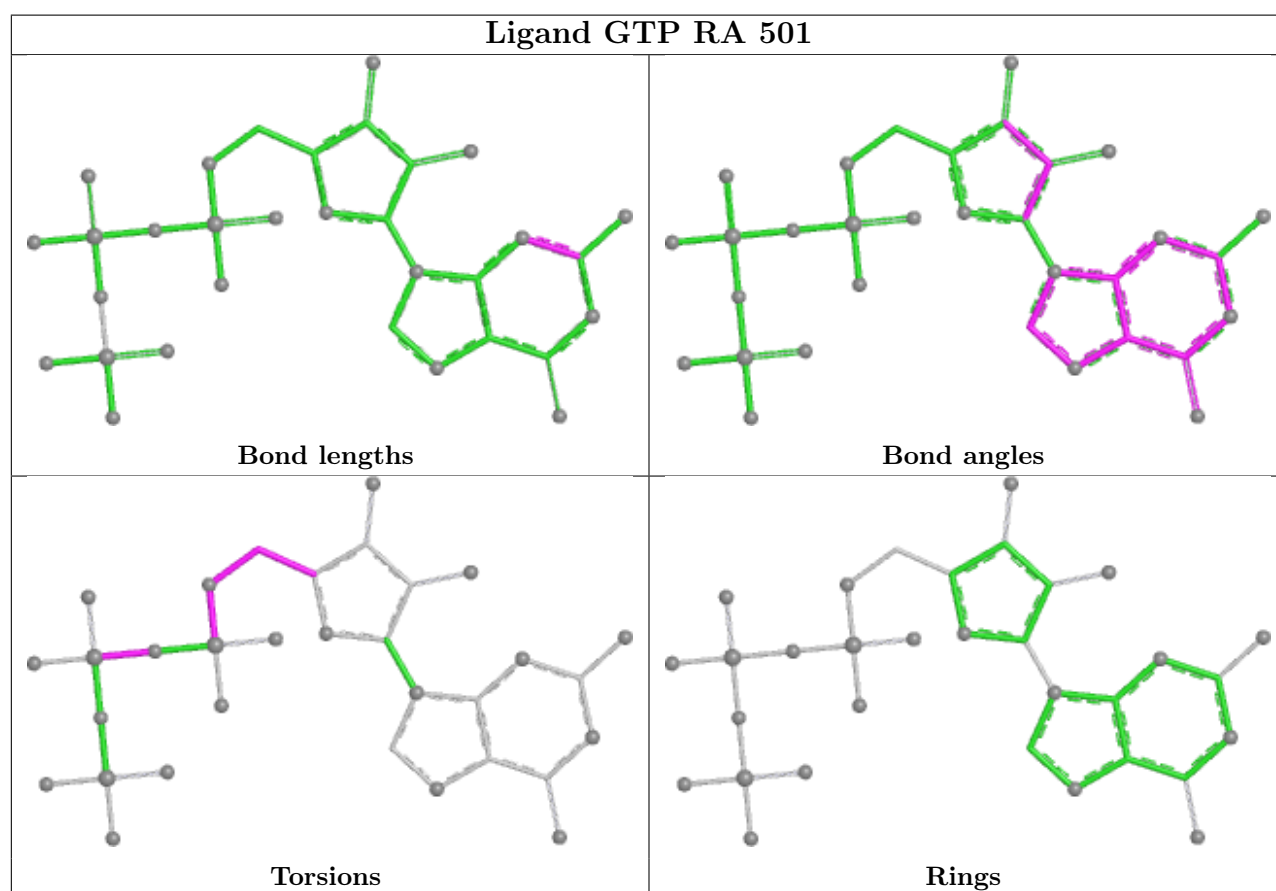
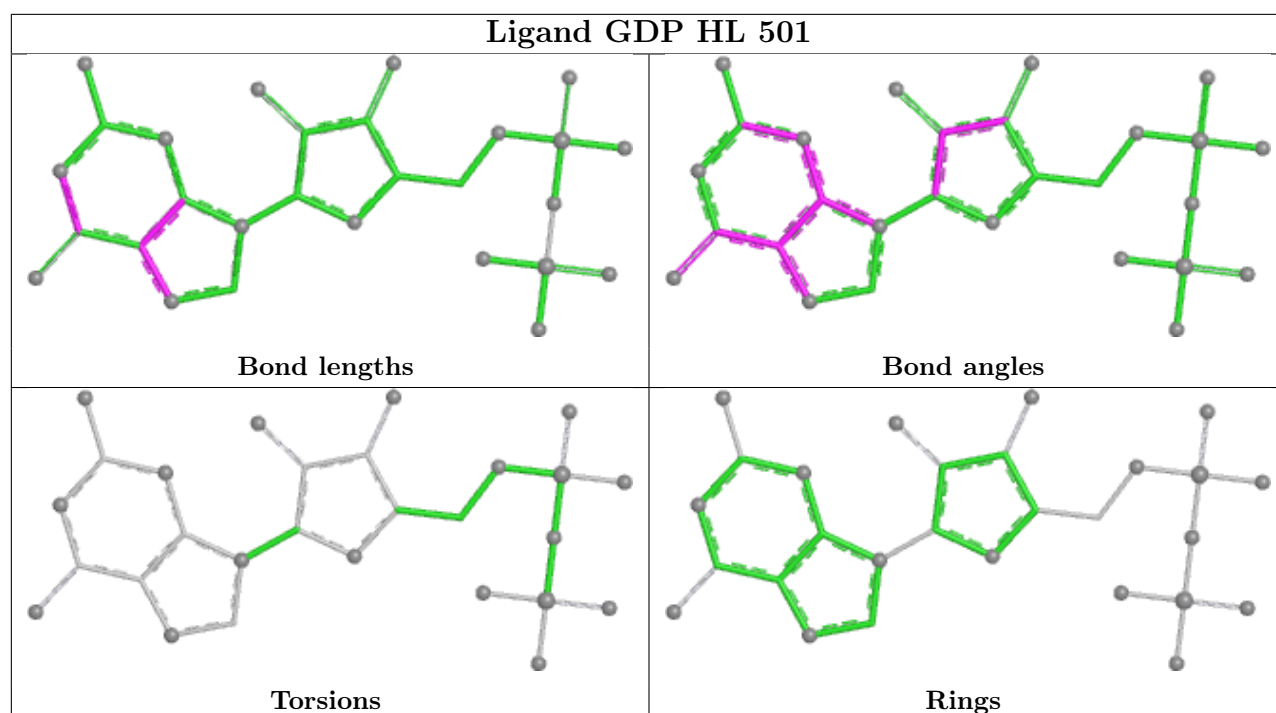


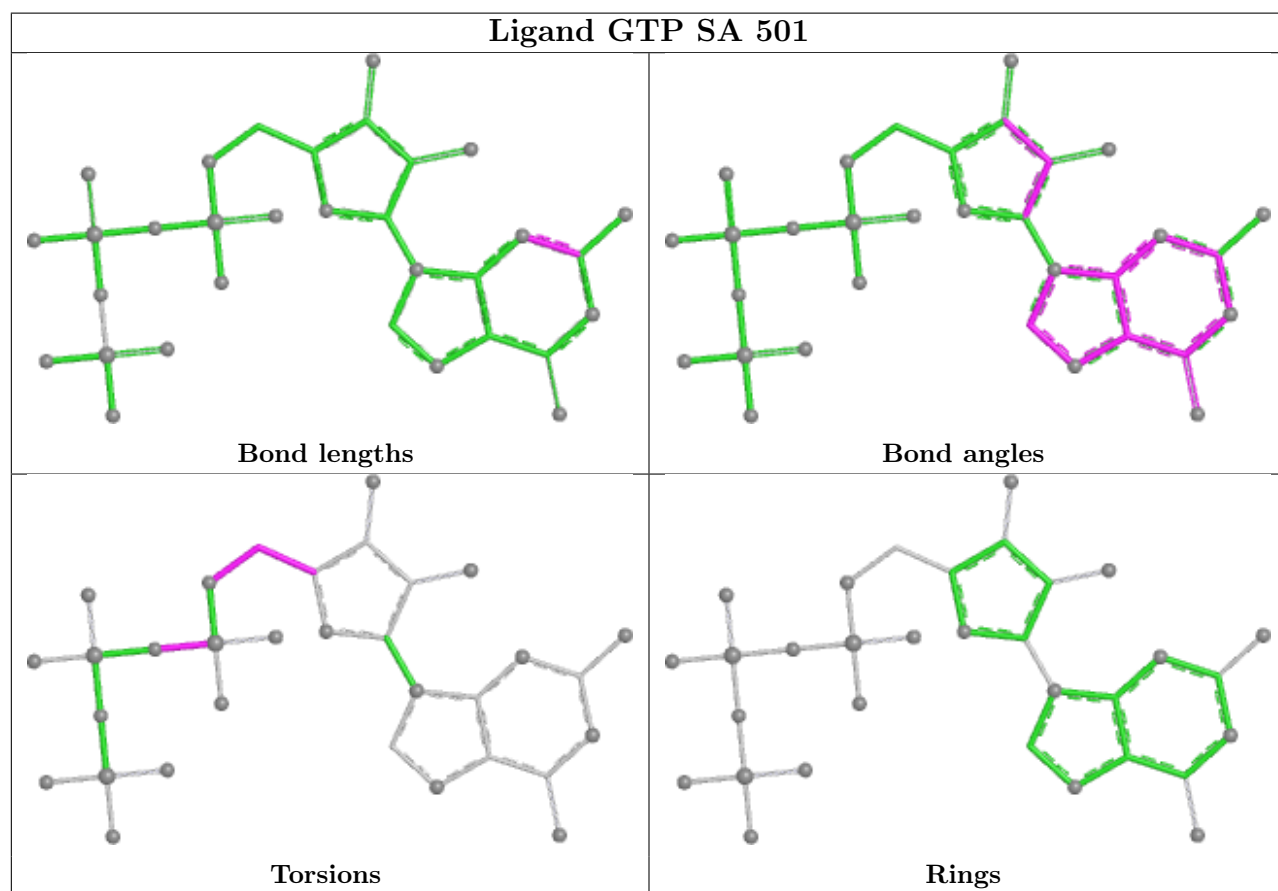
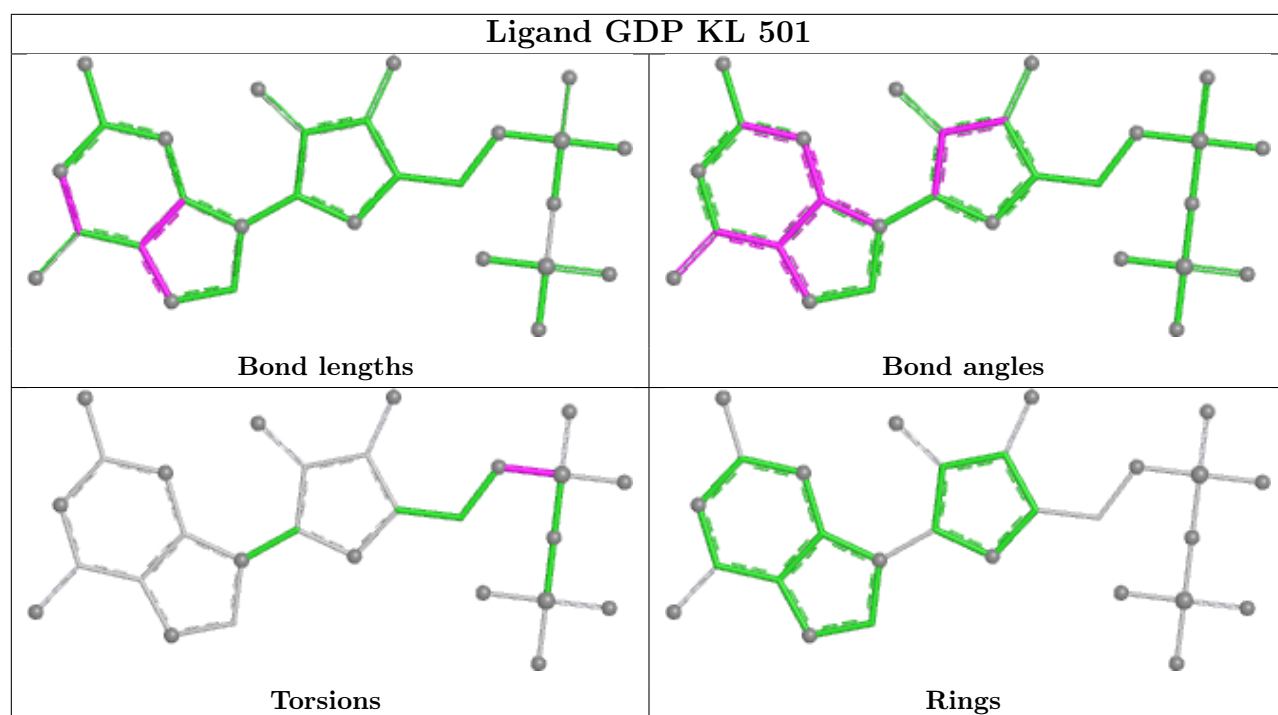
Ligand GTP CE 501

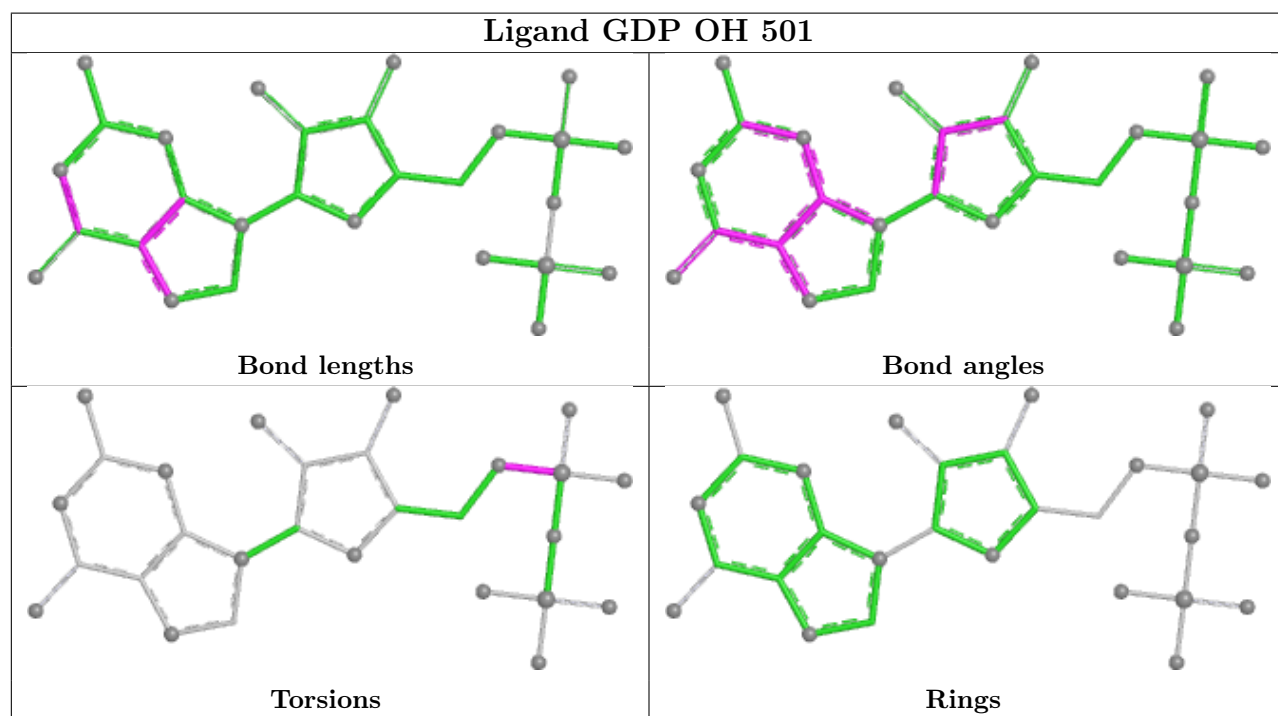
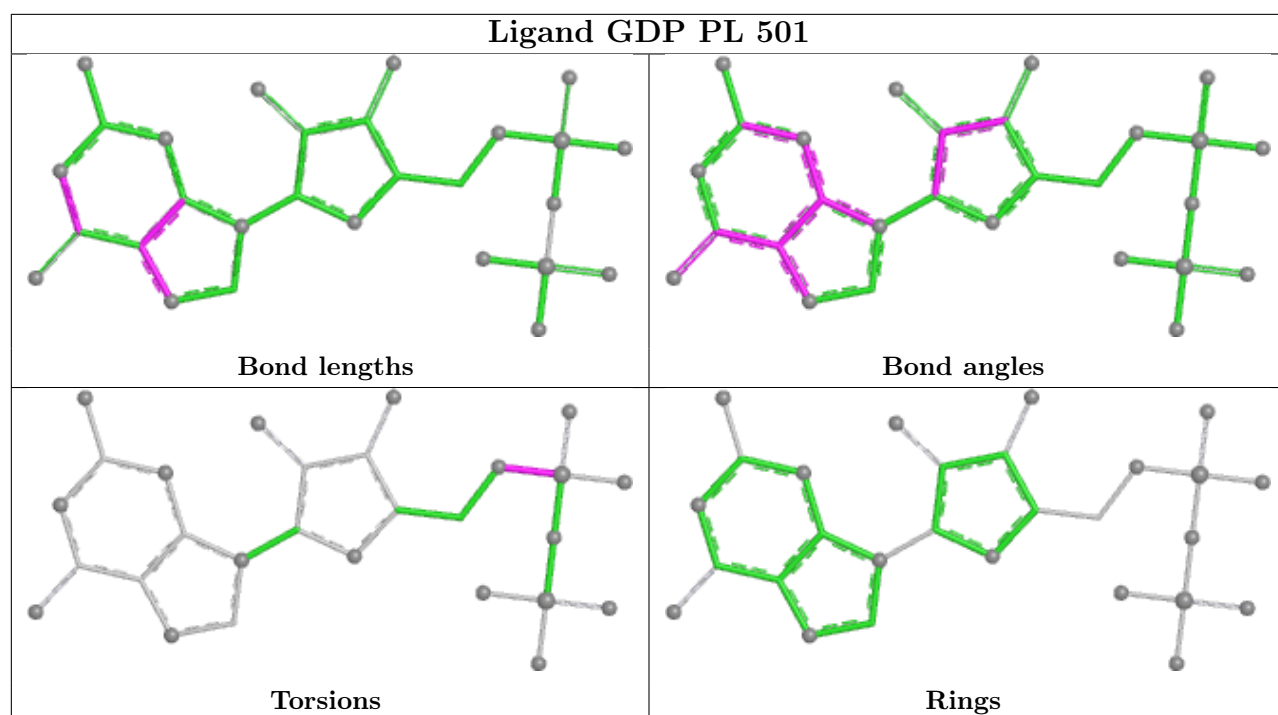


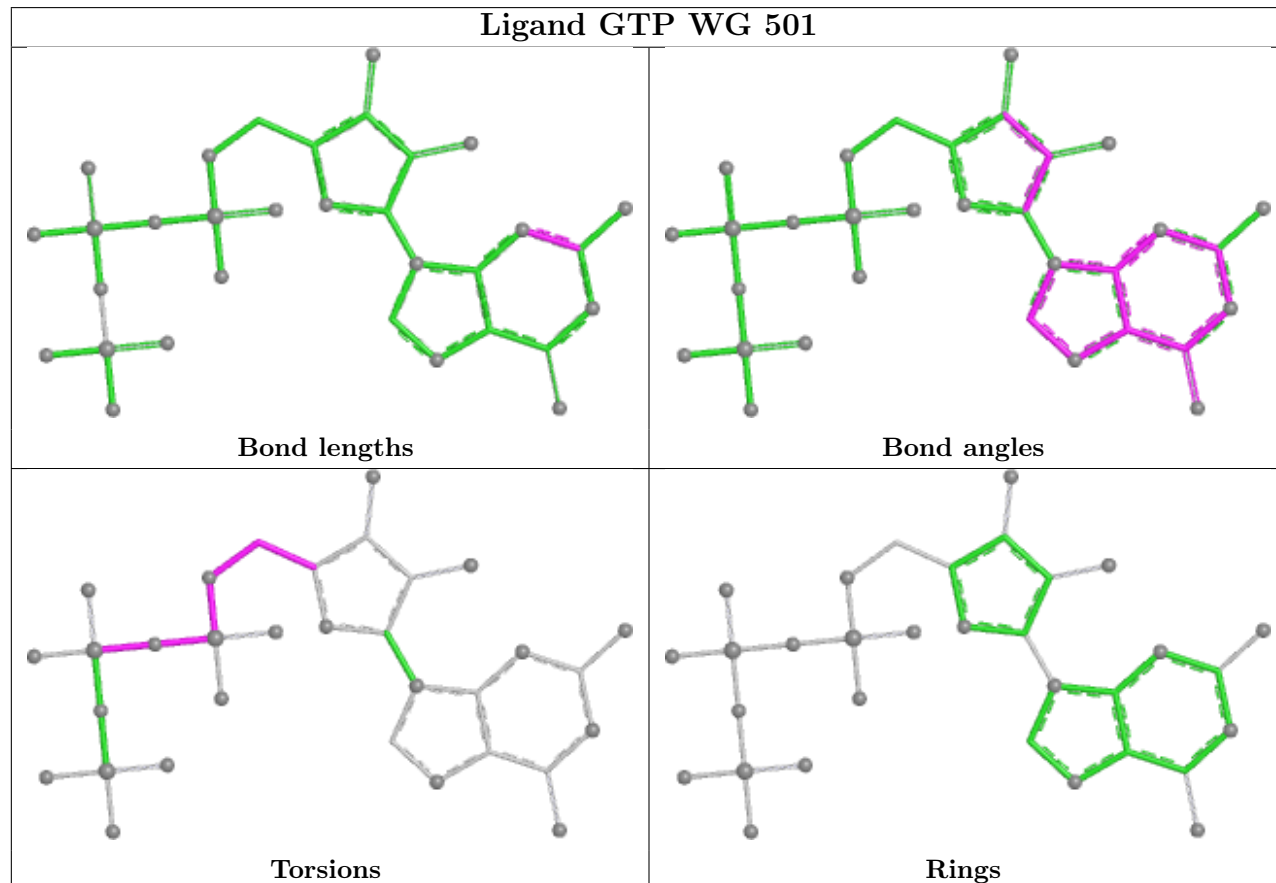
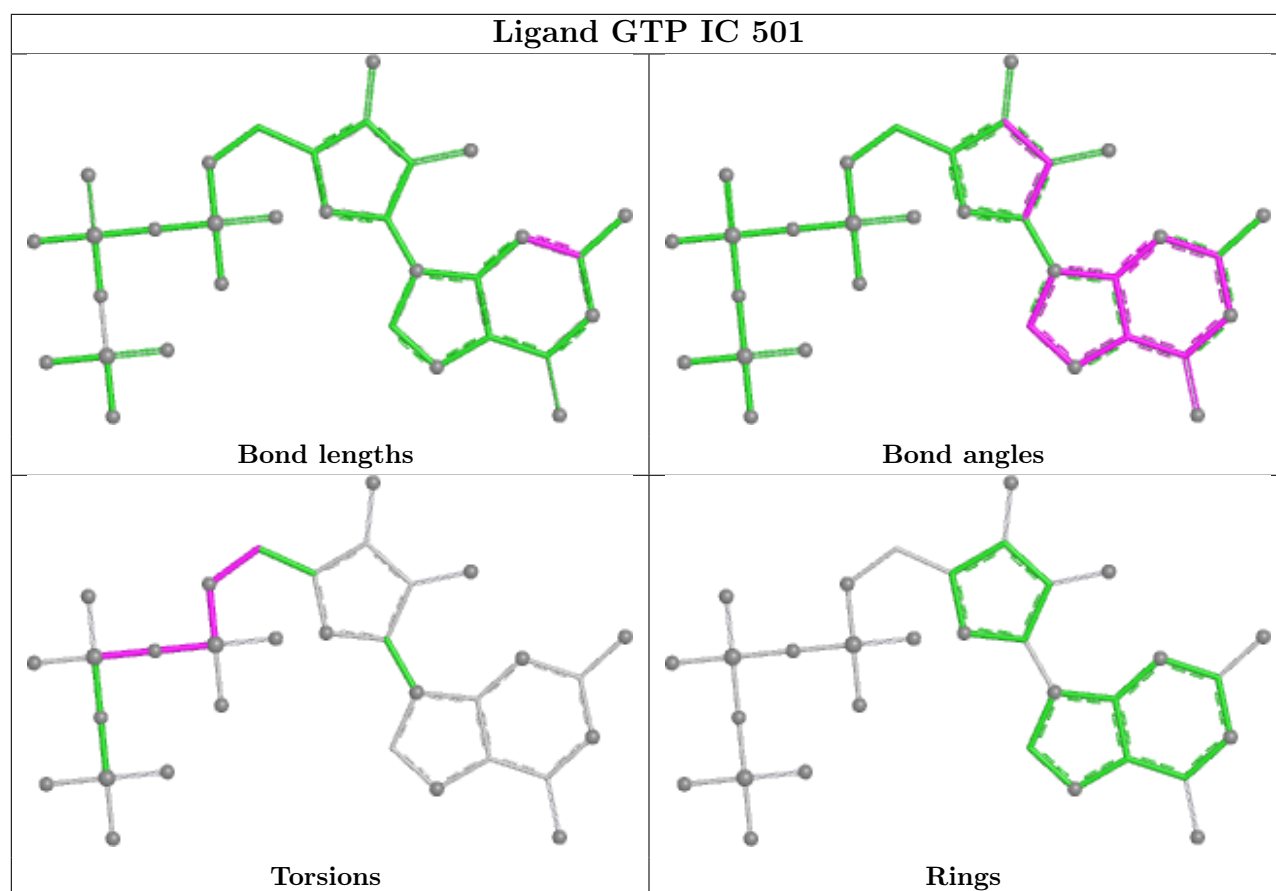
Ligand GTP WI 501



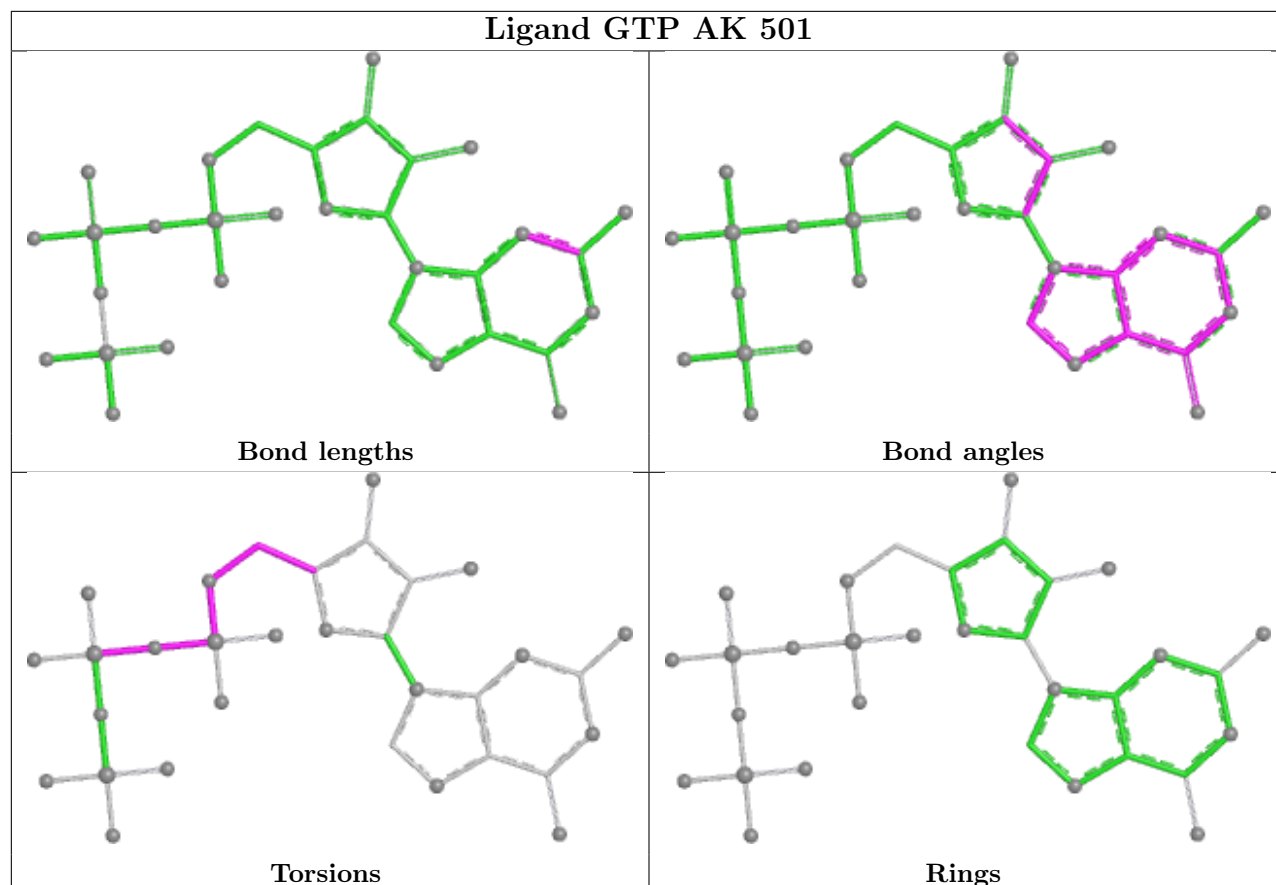




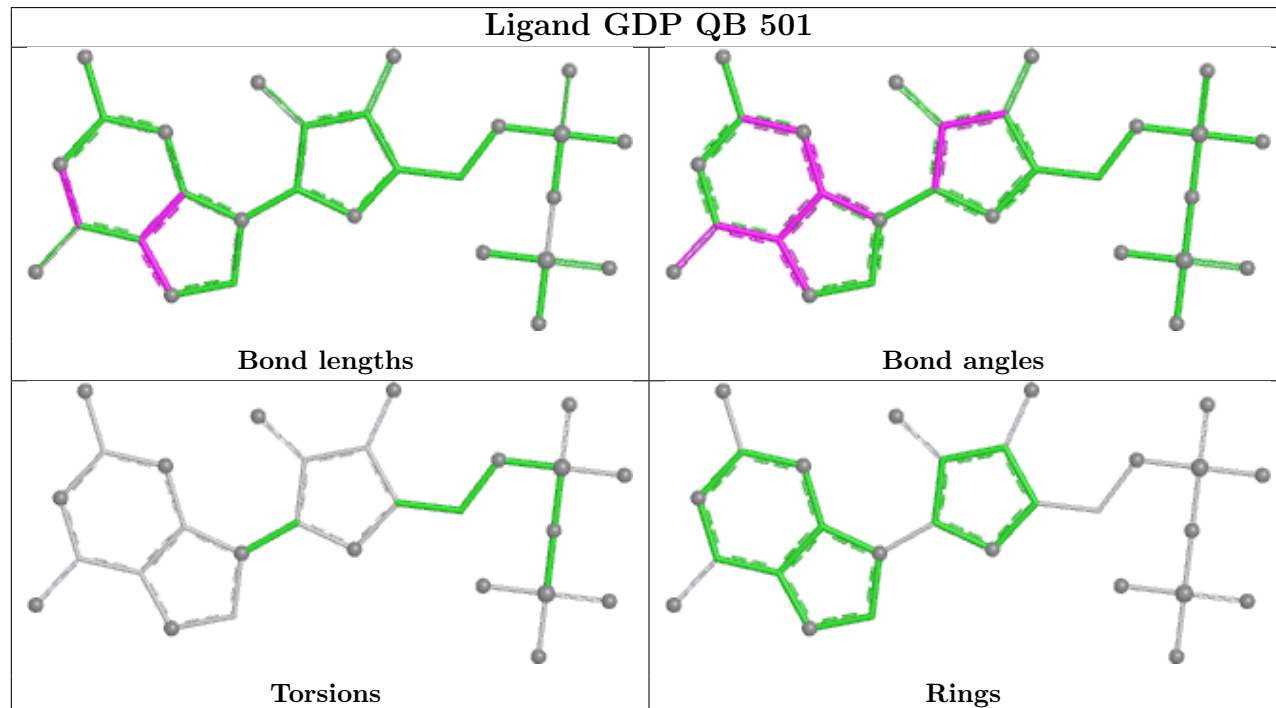


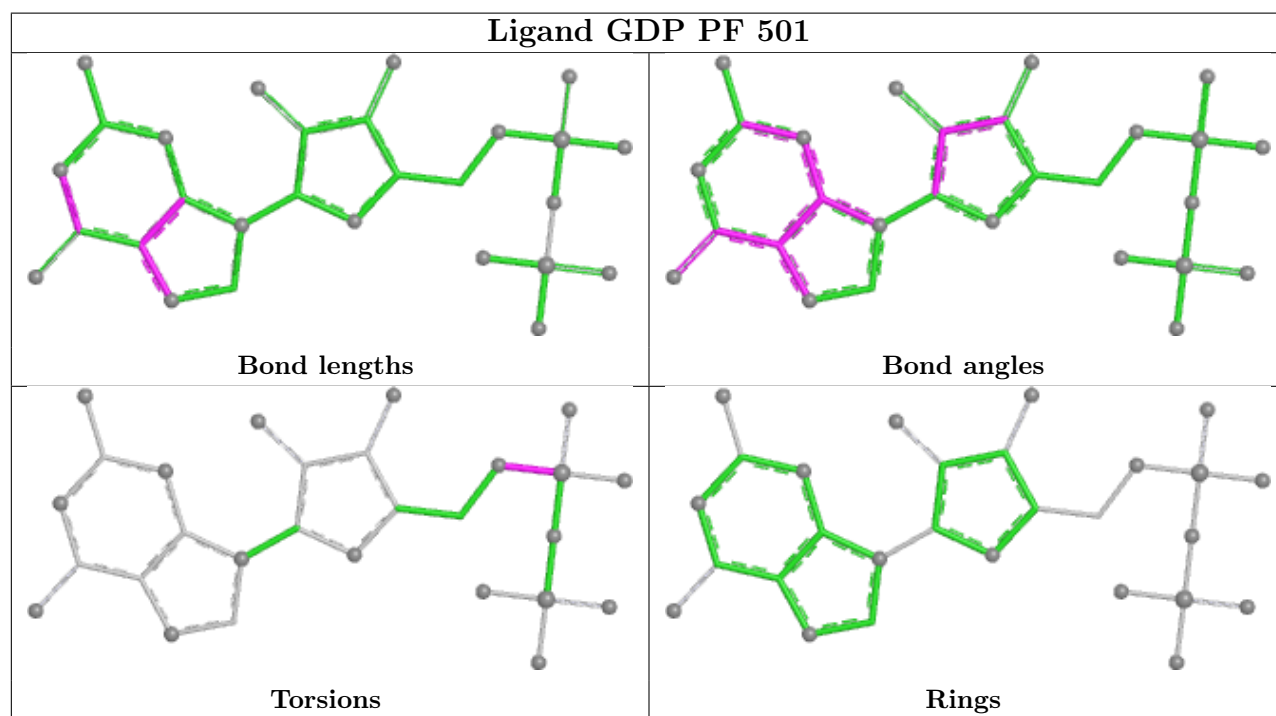
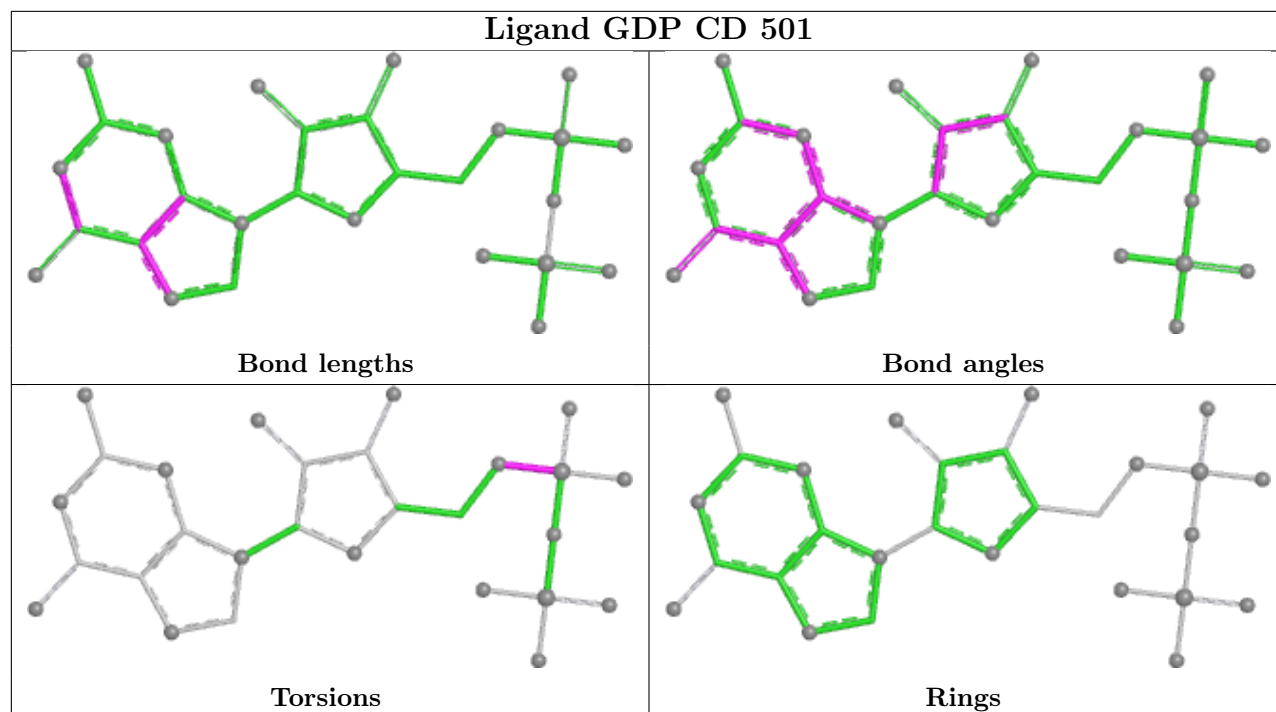


Ligand GTP AK 501

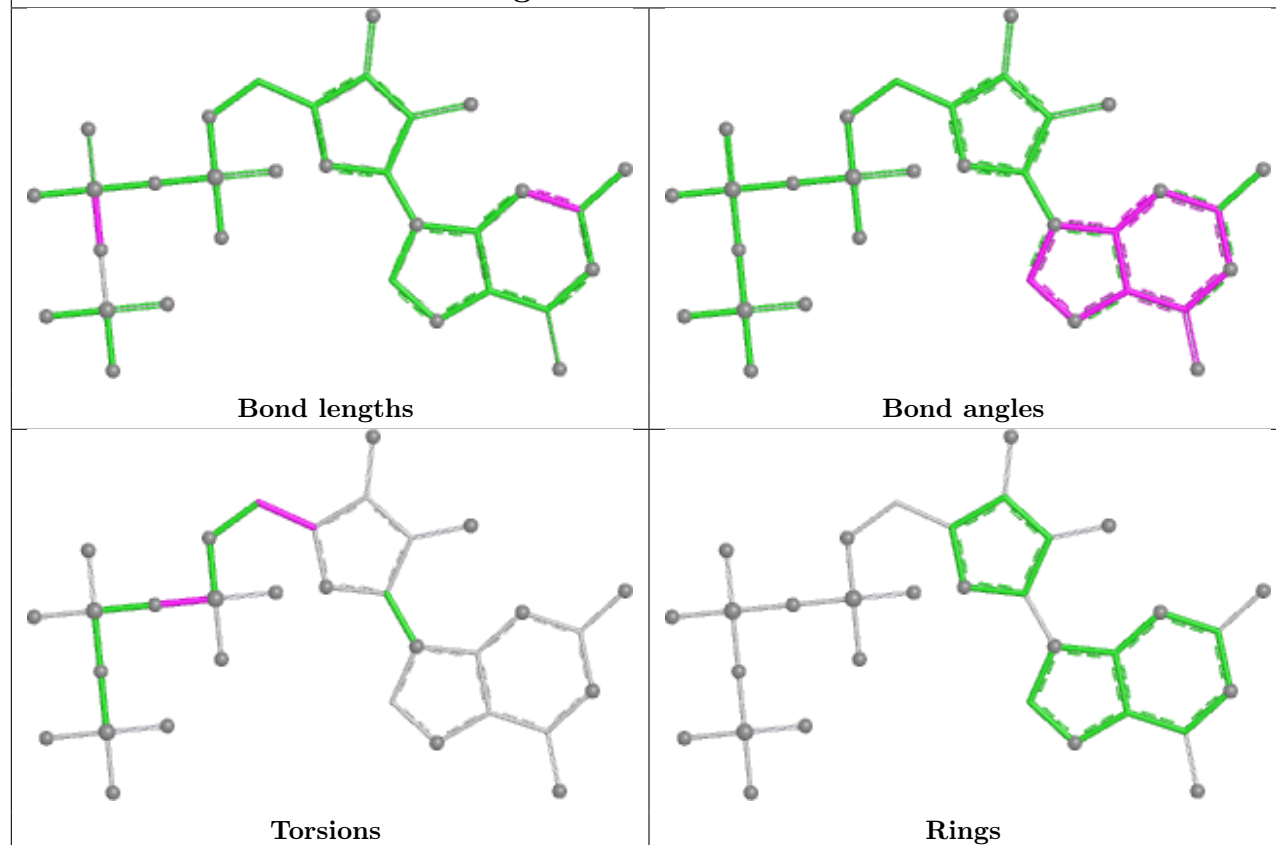


Ligand GDP QB 501

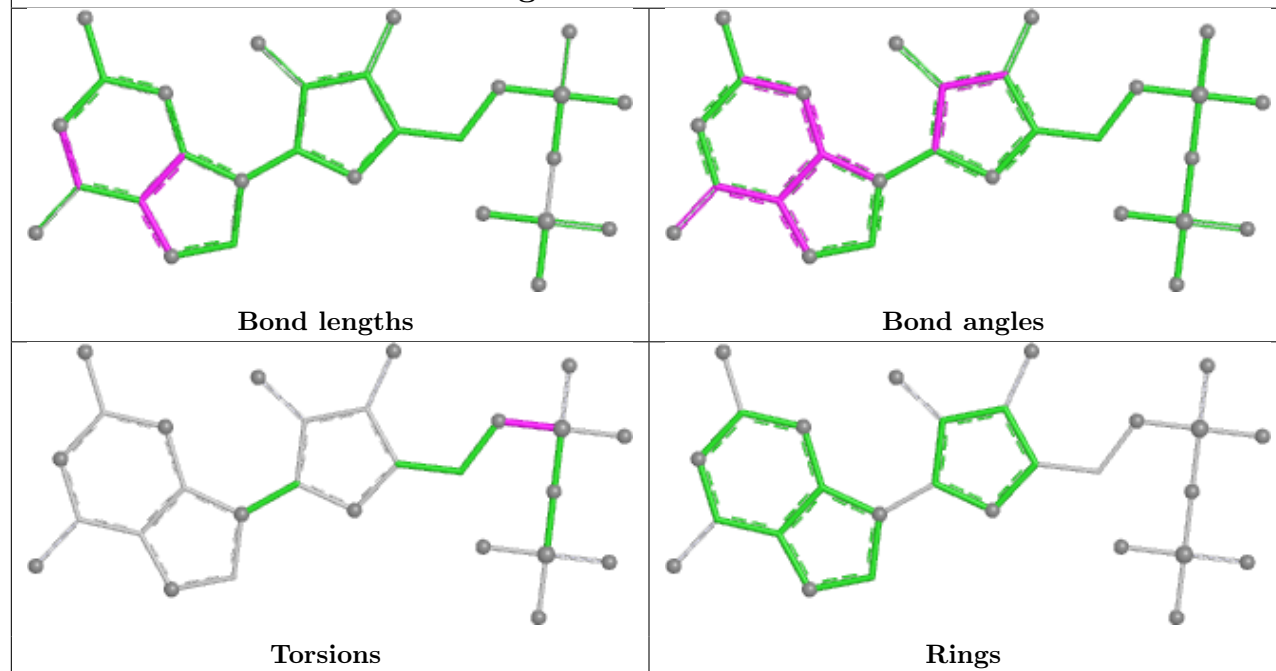


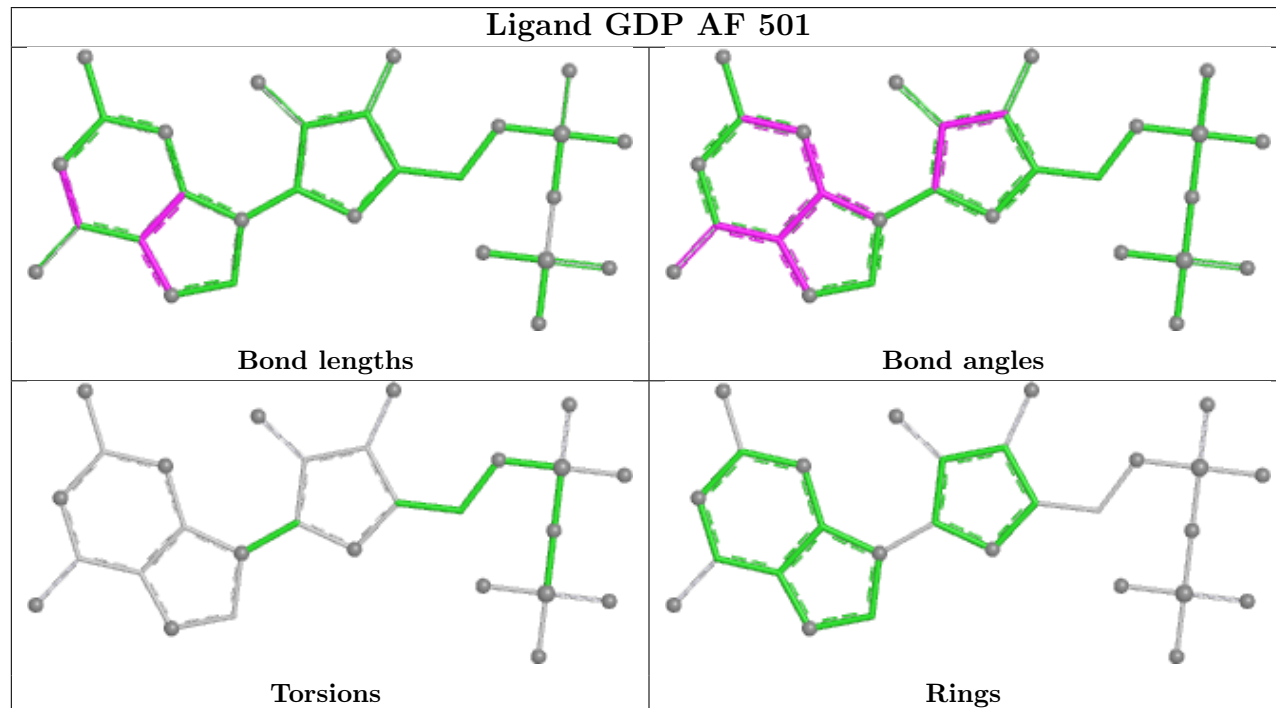
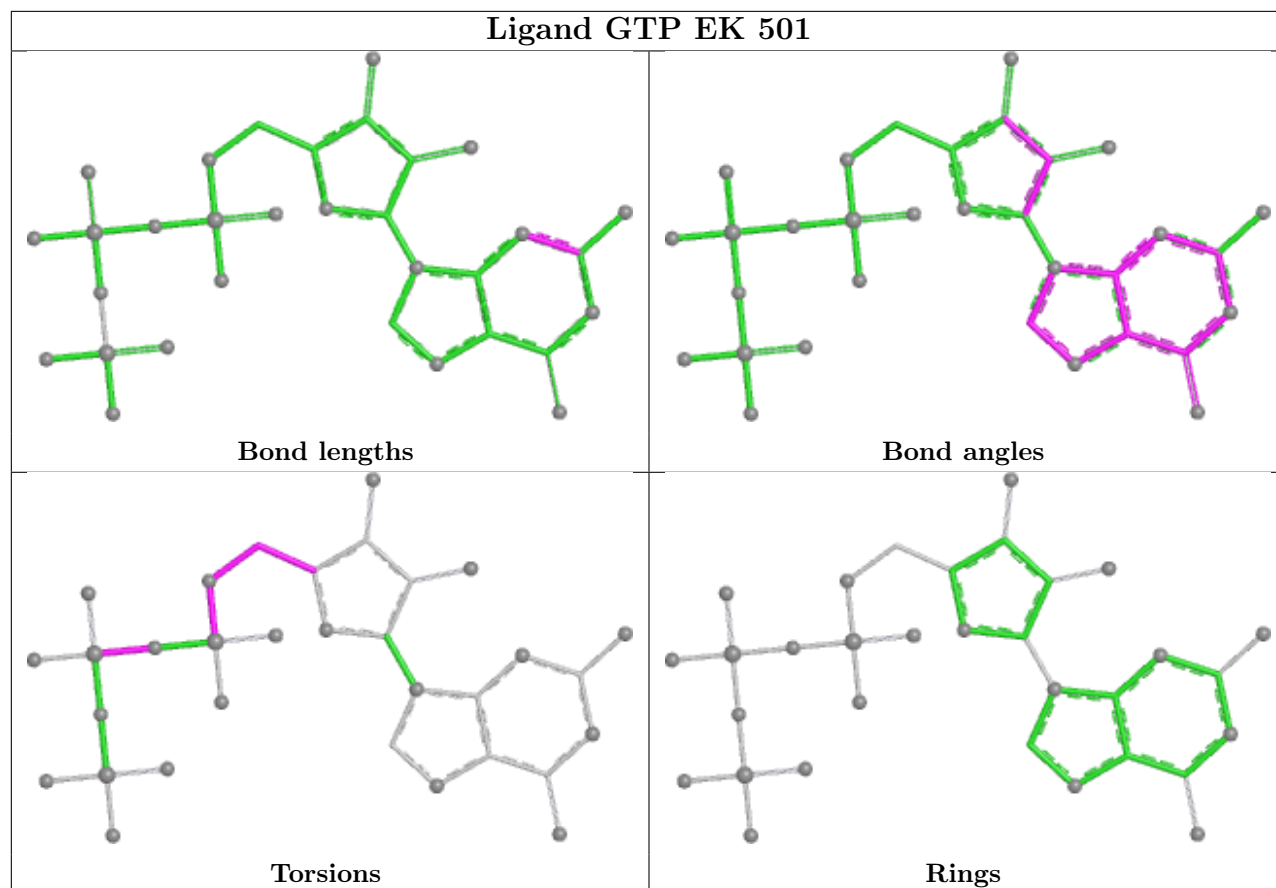


Ligand GTP WE 501

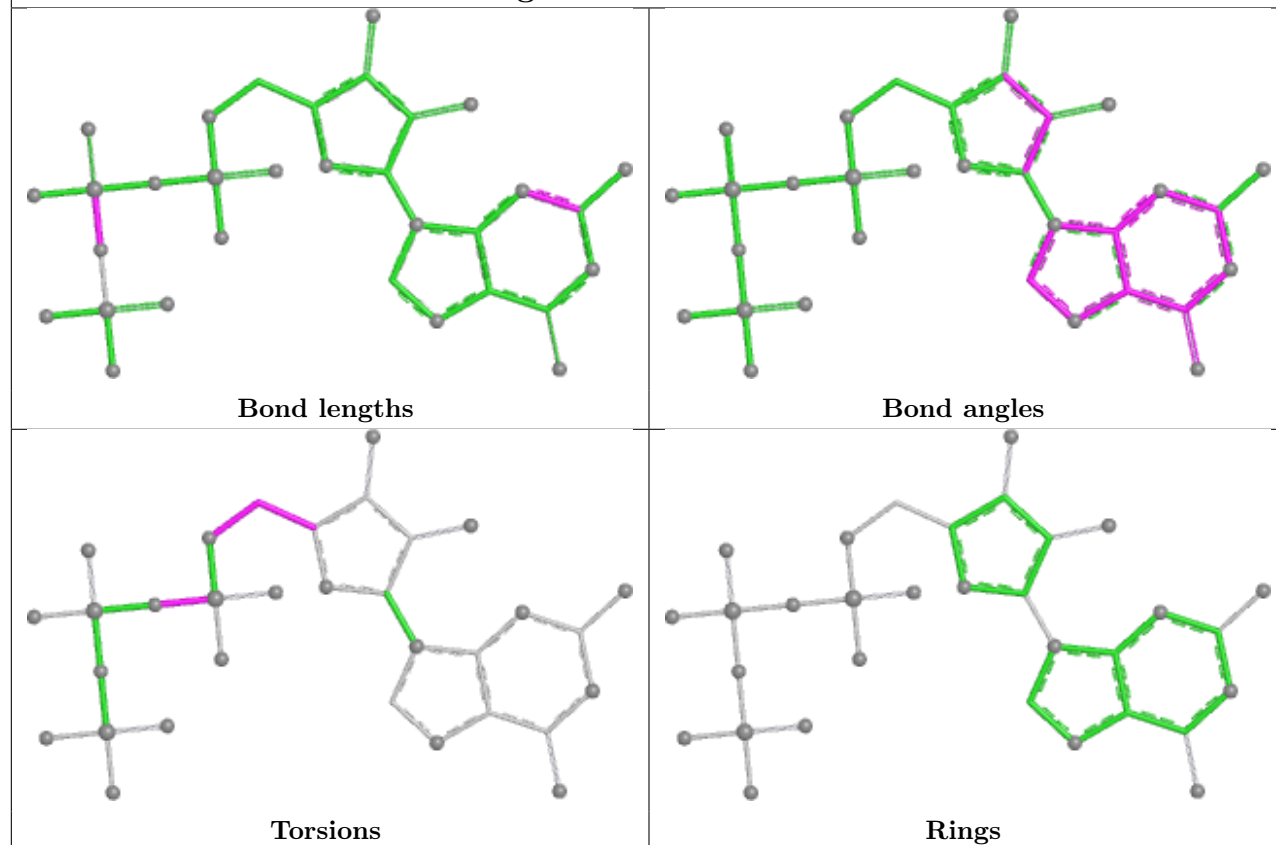


Ligand GDP BF 501

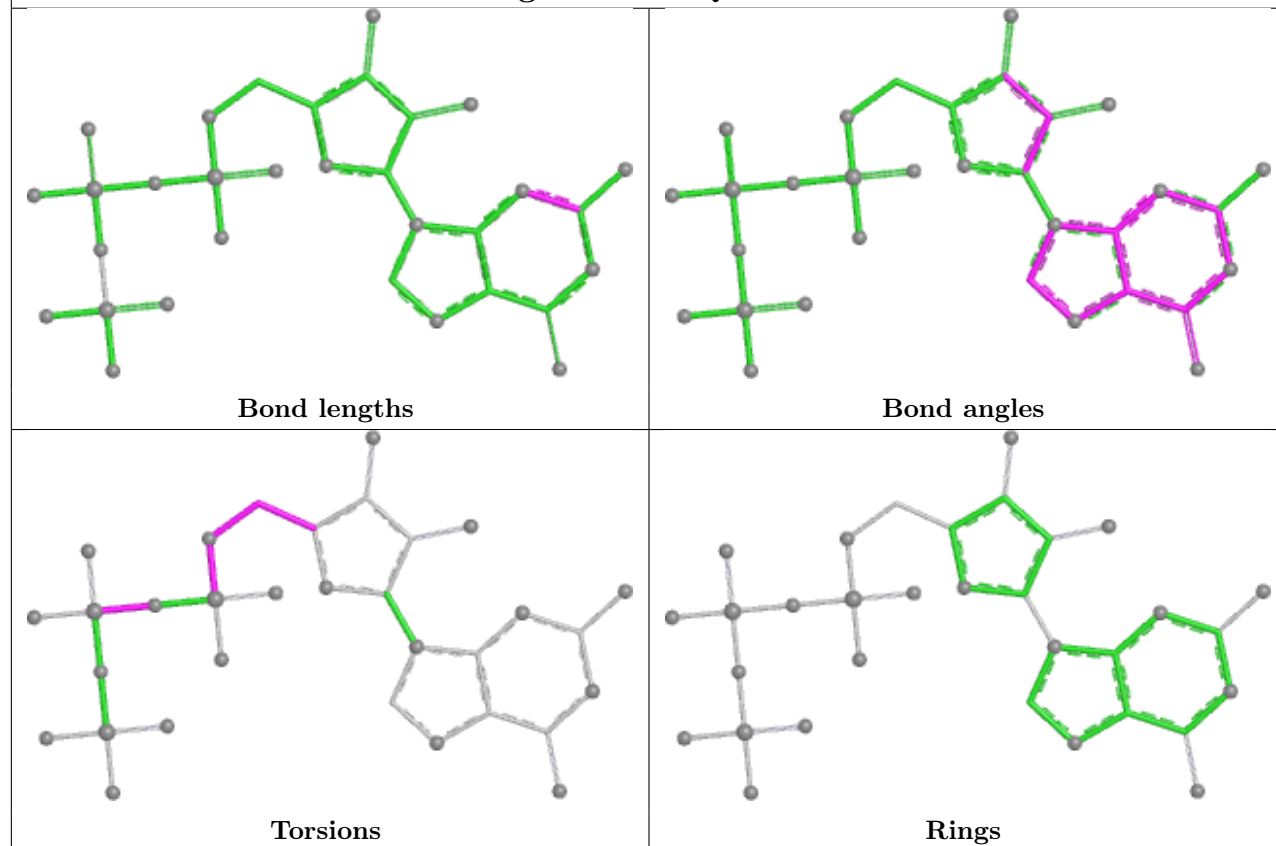


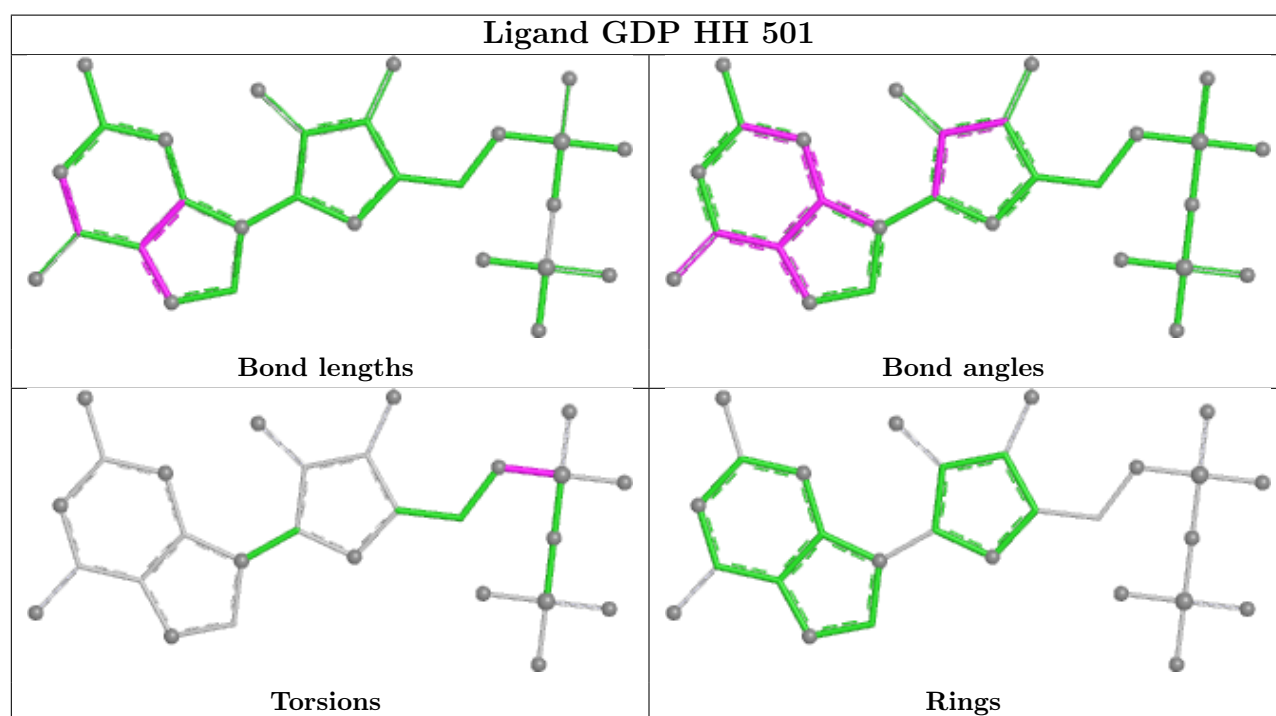
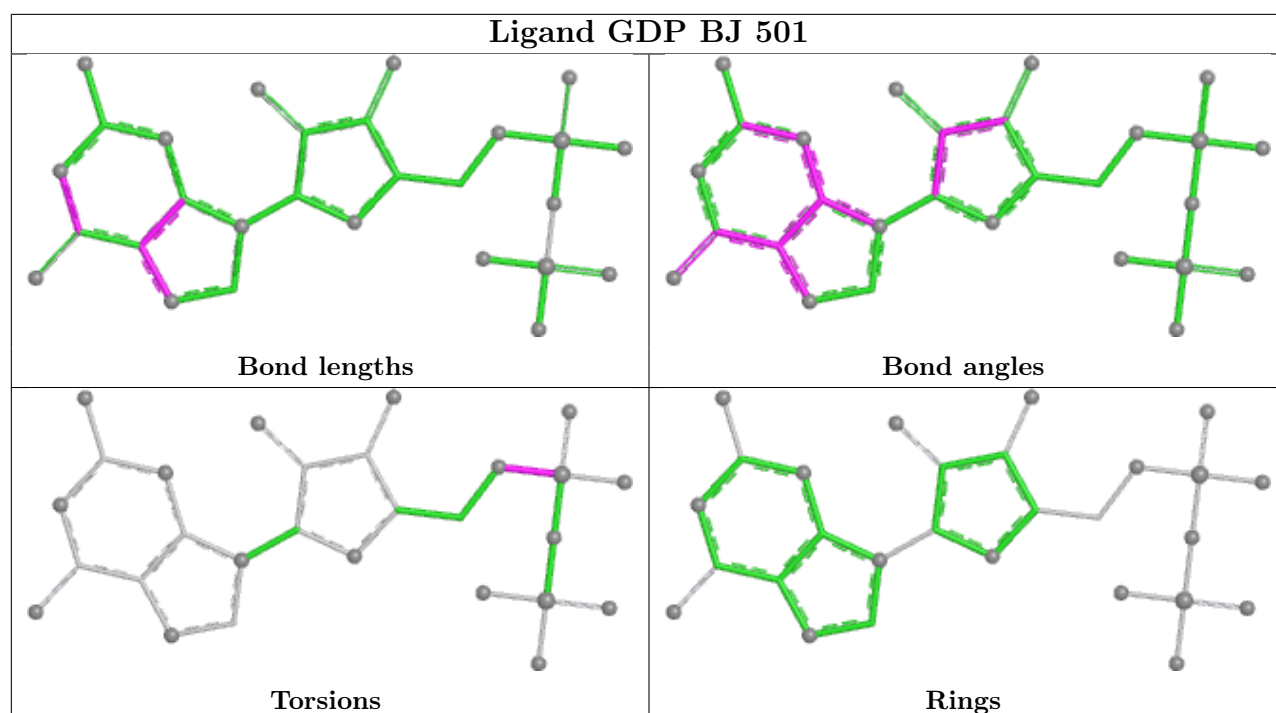


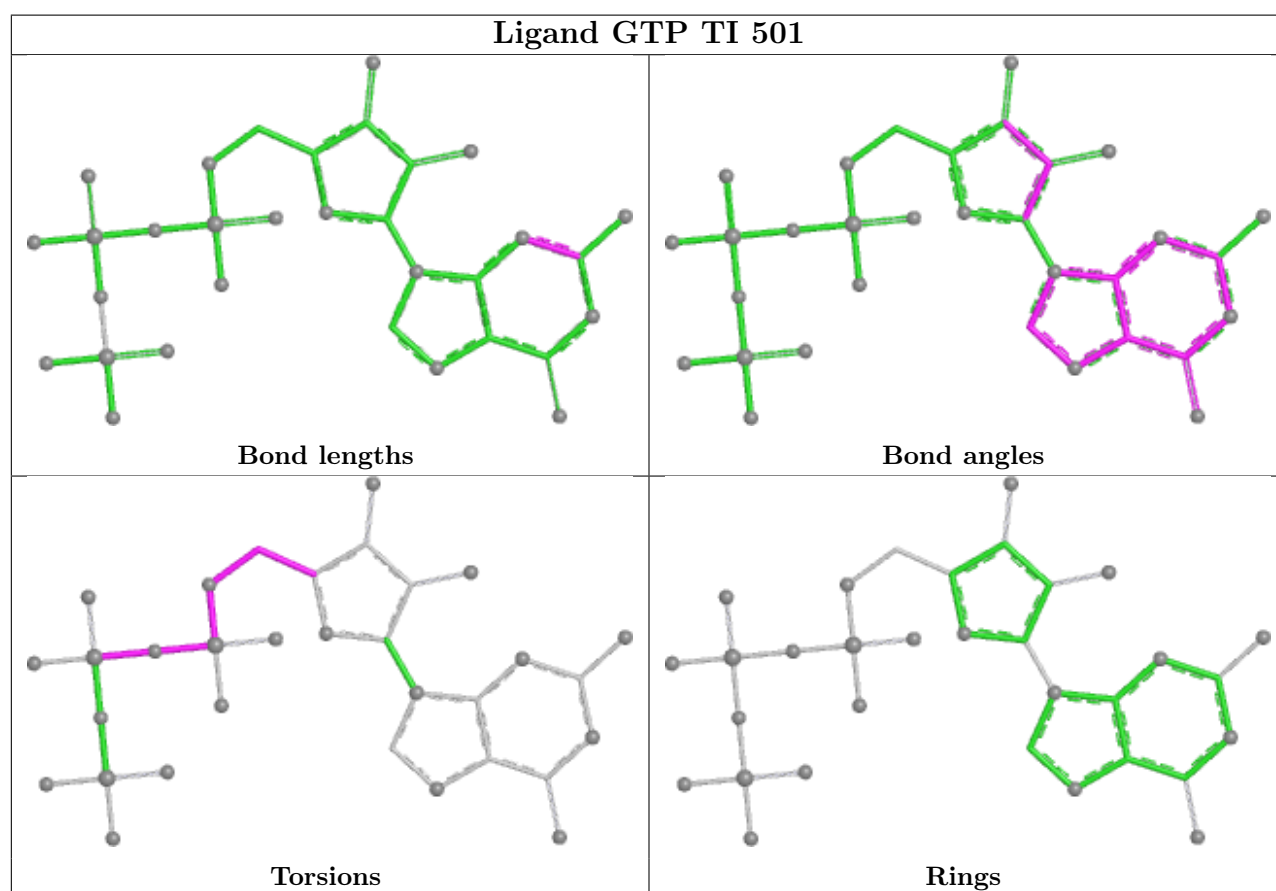
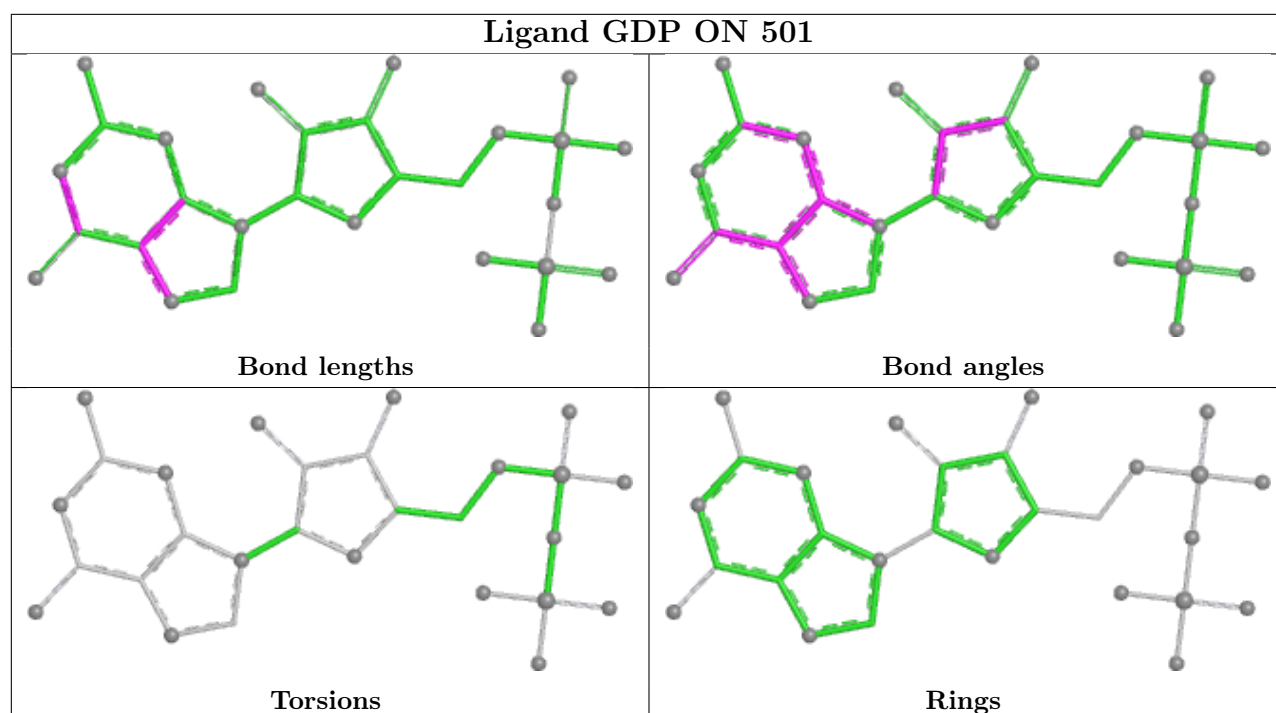
Ligand GTP BK 501



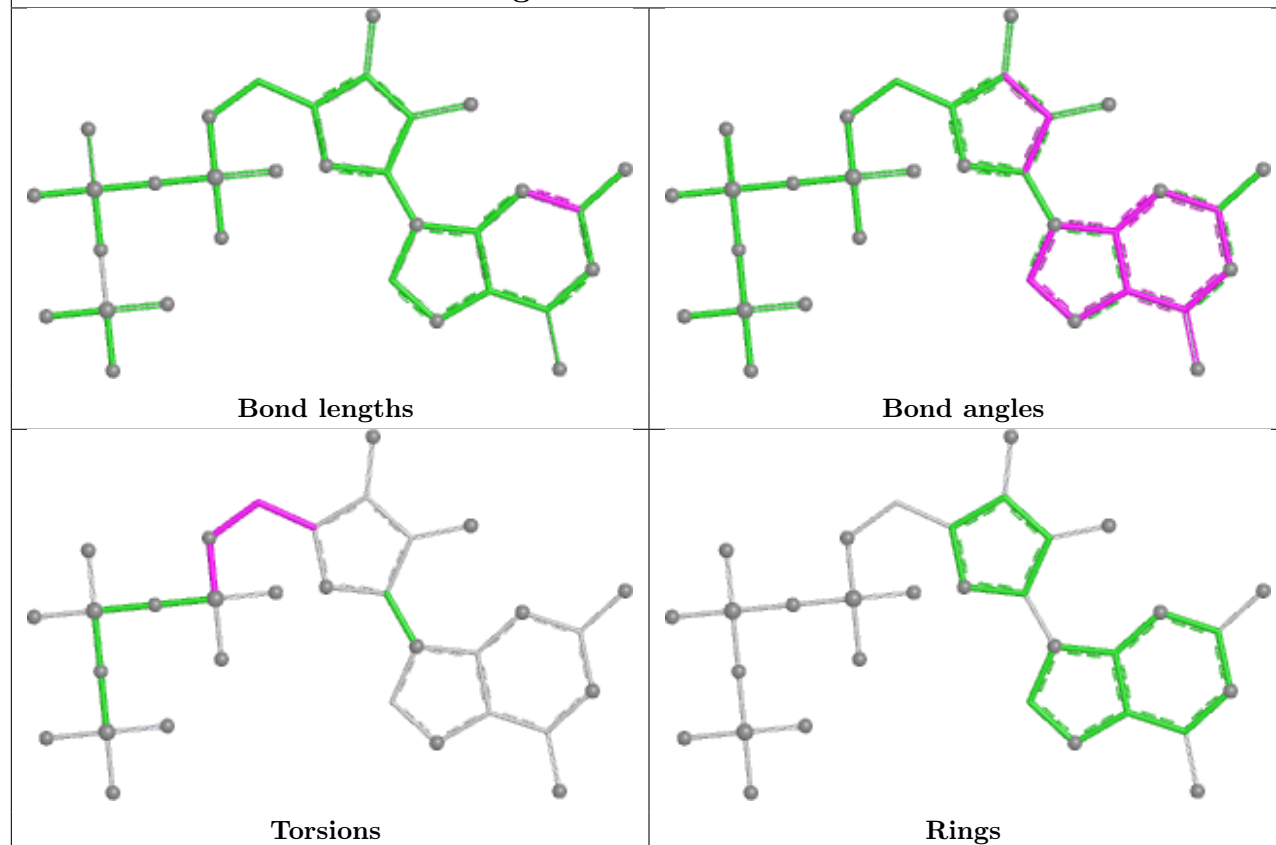
Ligand GTP QE 501



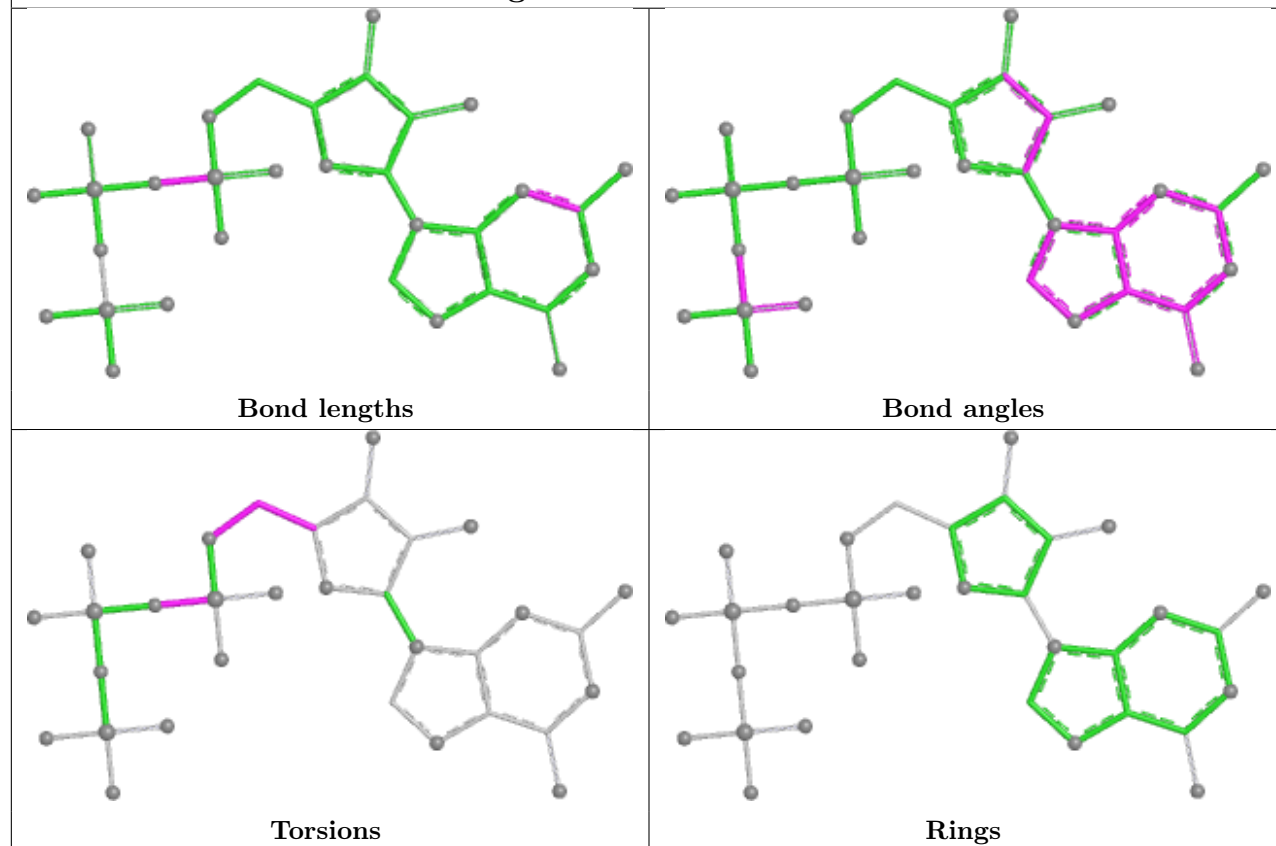


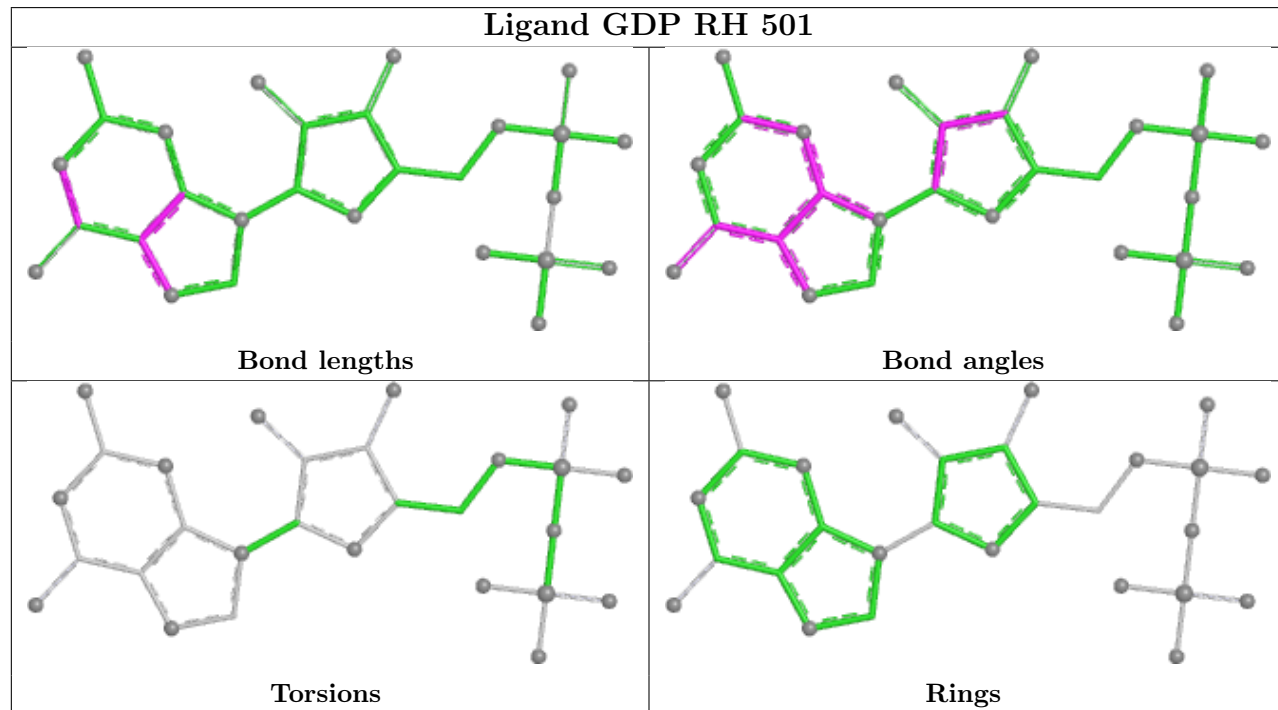
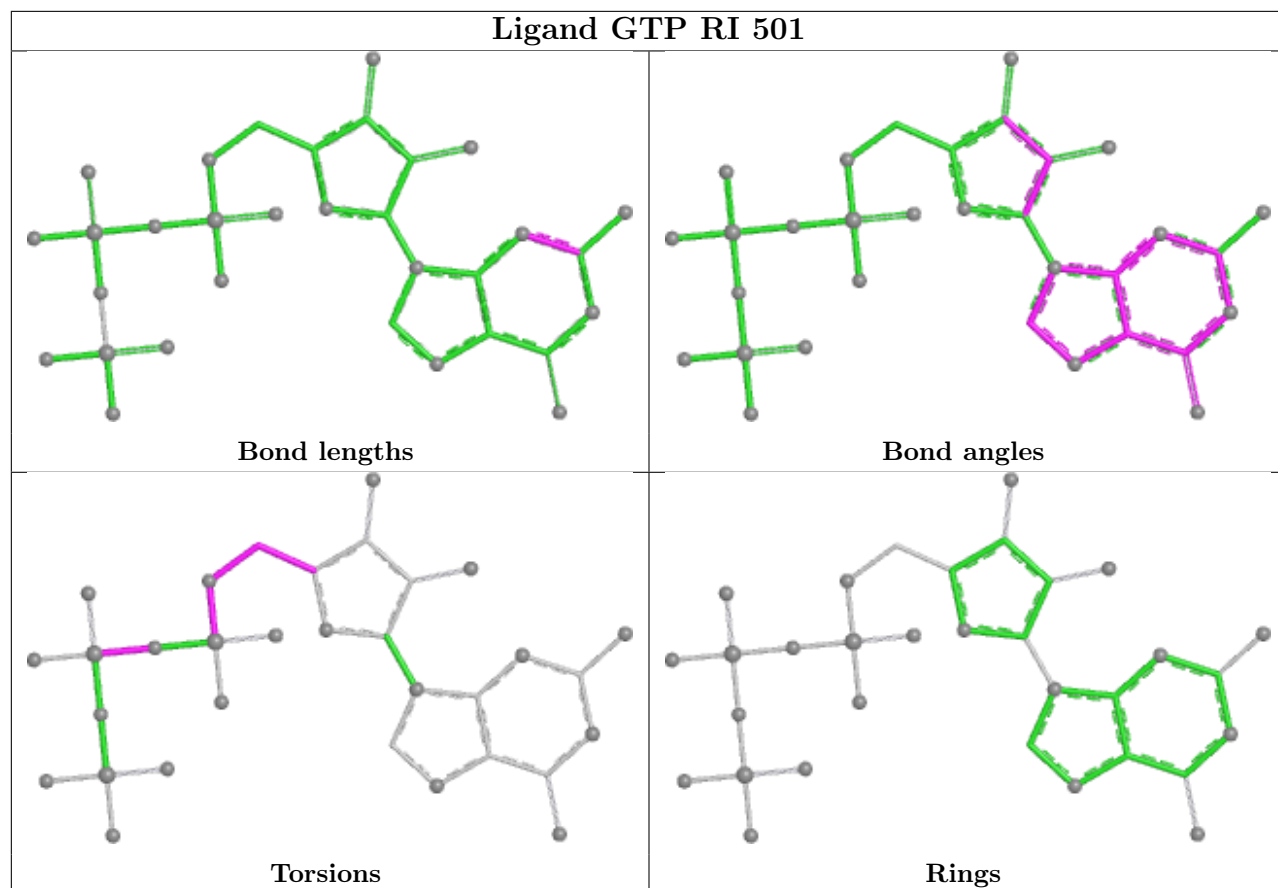


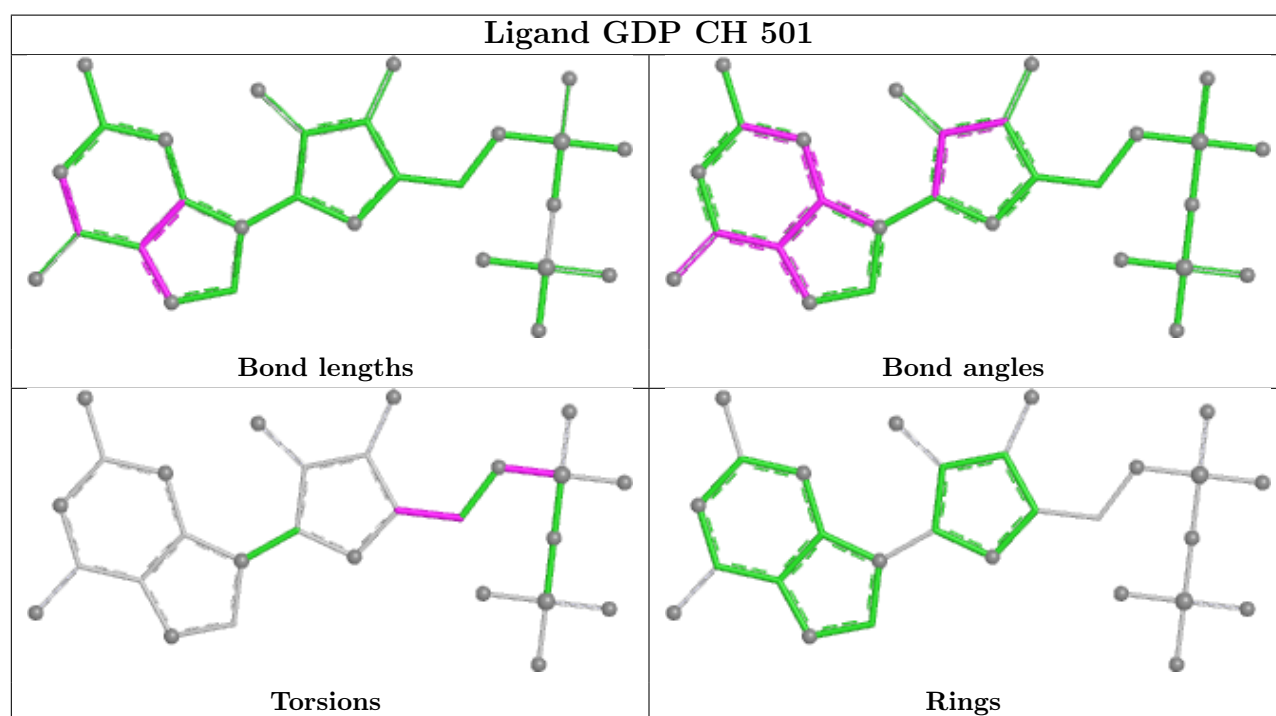
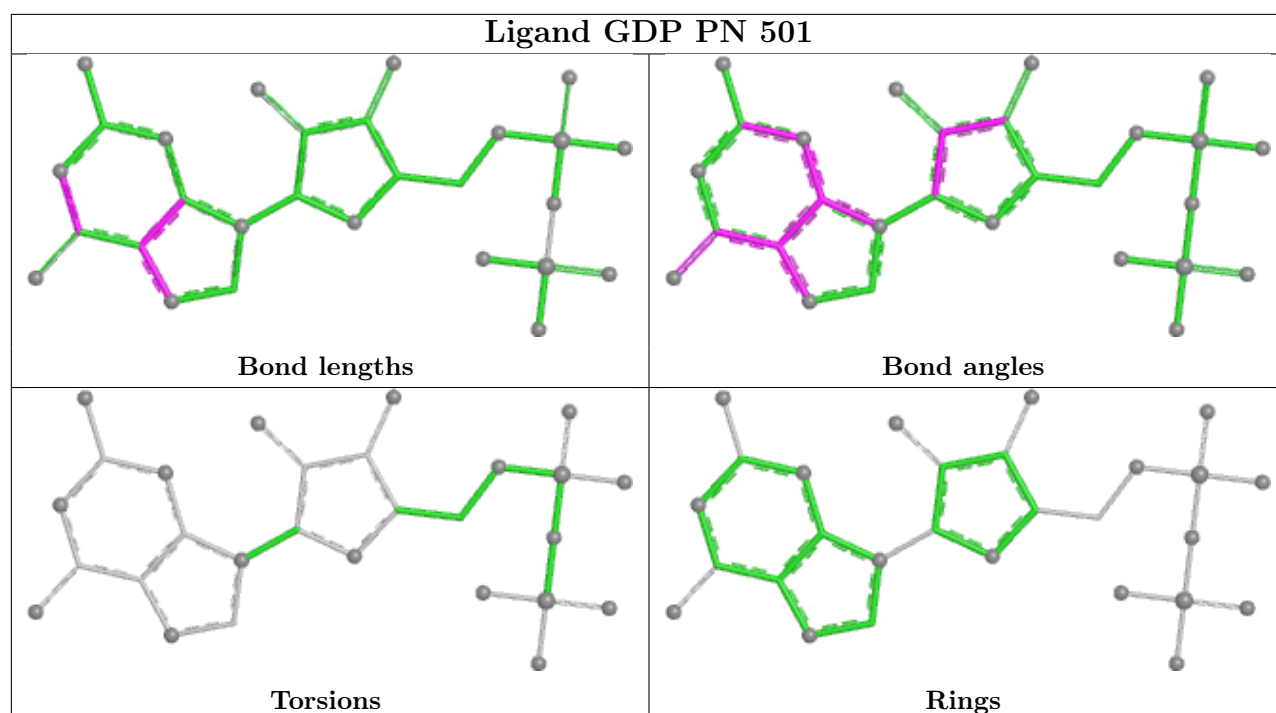
Ligand GTP WC 501



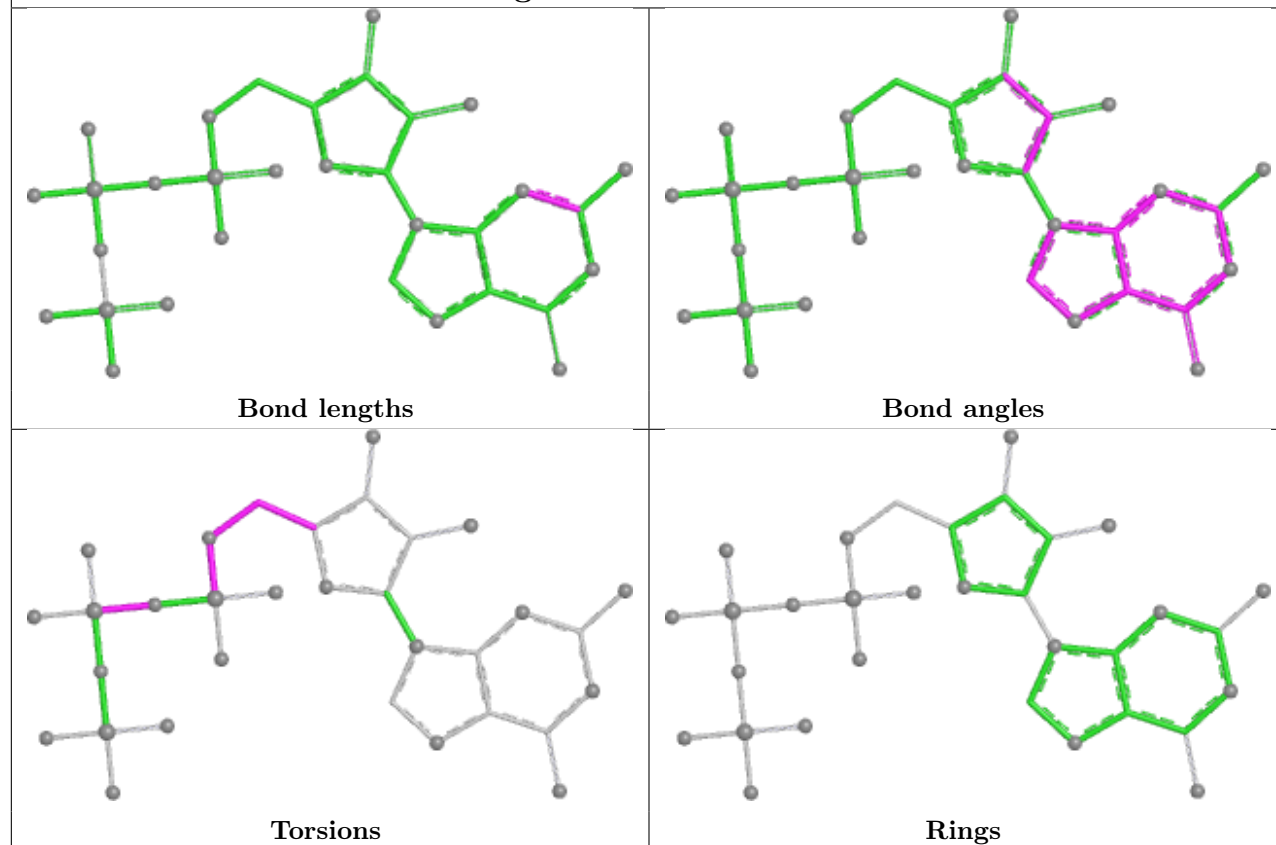
Ligand GTP WM 501



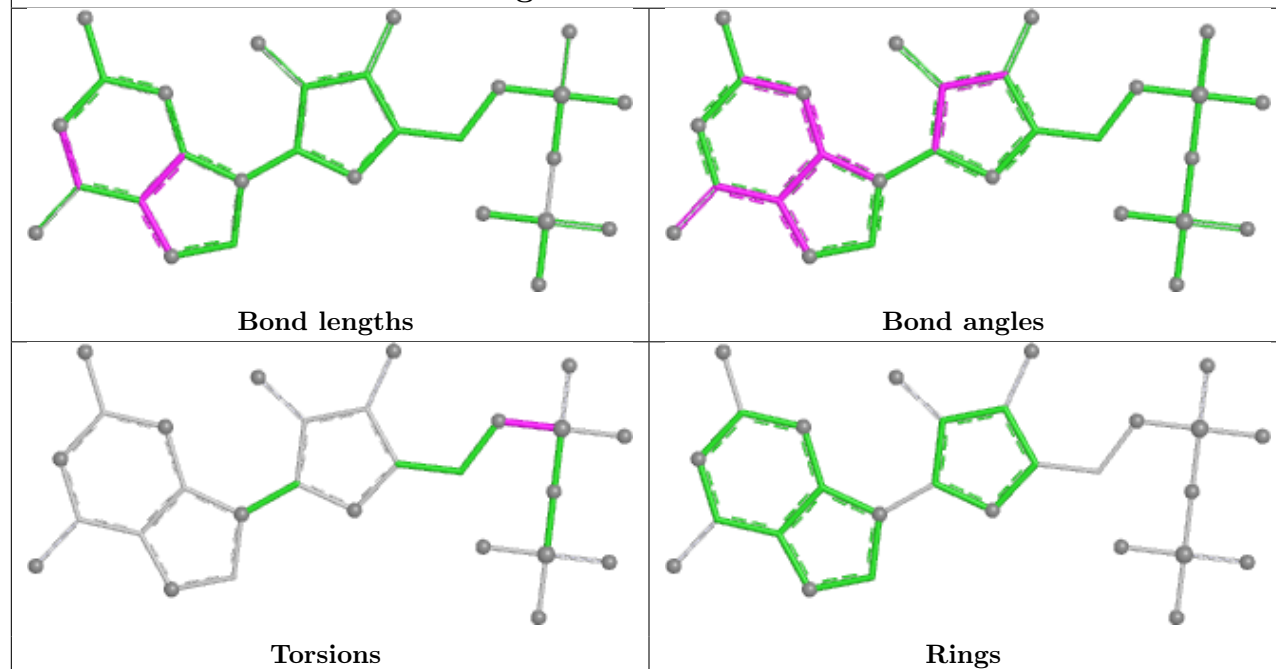


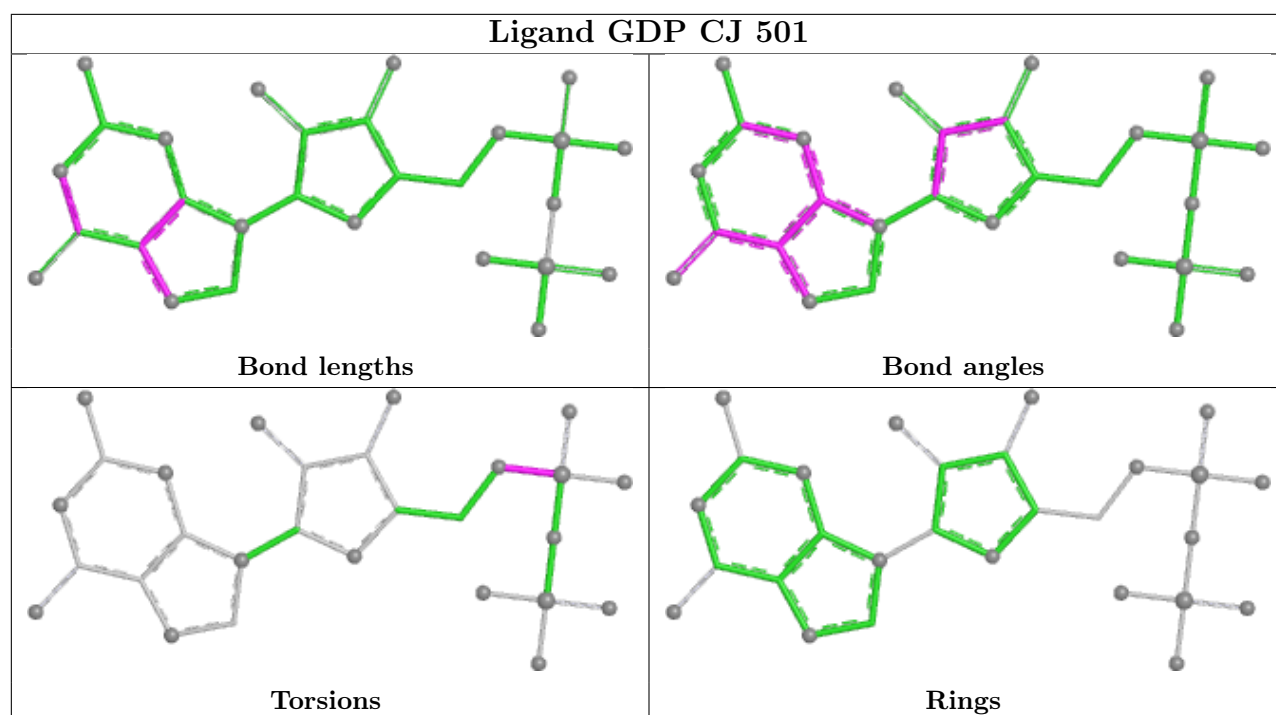


Ligand GTP TM 501



Ligand GDP MJ 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.

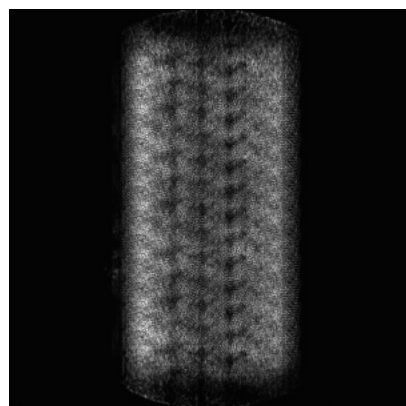
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29692. These allow visual inspection of the internal detail of the map and identification of artifacts.

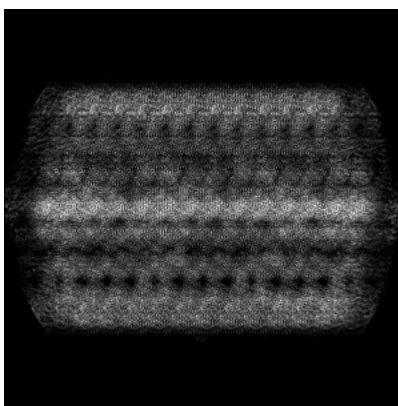
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

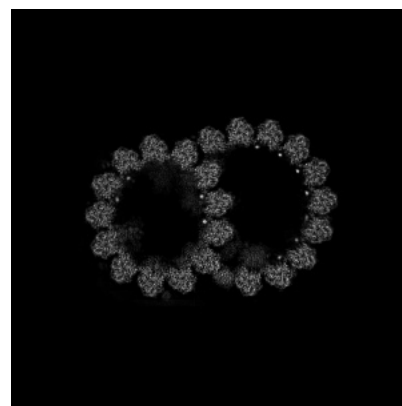
5.1.1 Primary map



X

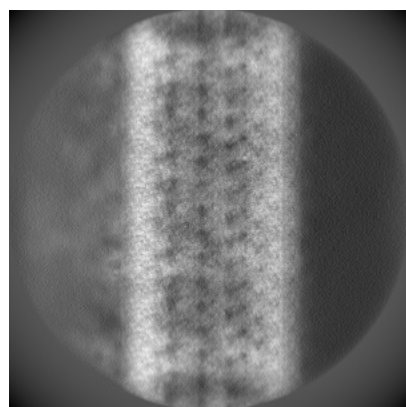


Y

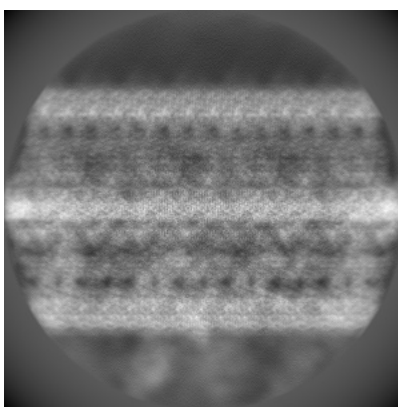


Z

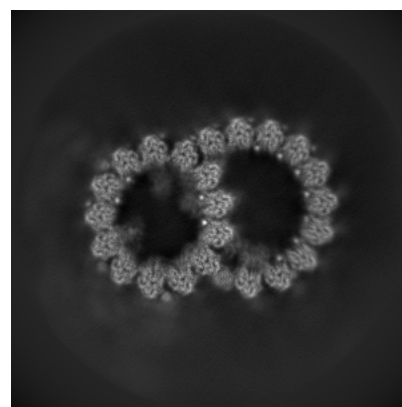
5.1.2 Raw map



X



Y

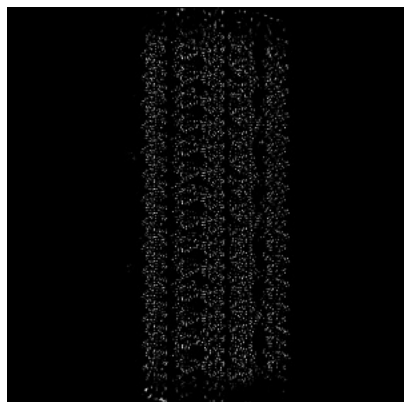


Z

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

5.2 Central slices [i](#)

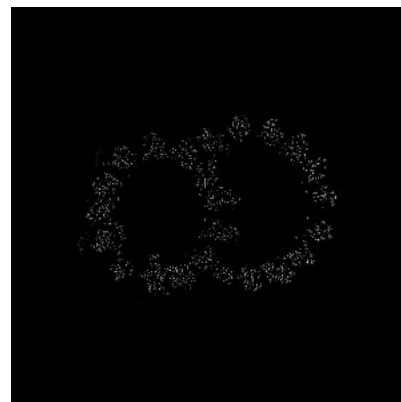
5.2.1 Primary map



X Index: 256

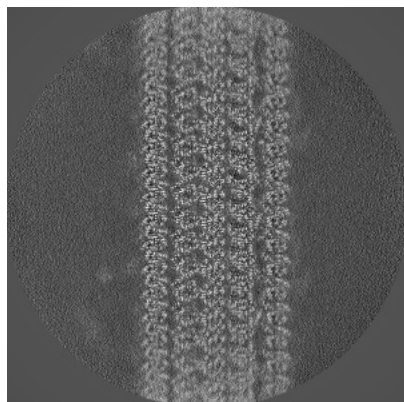


Y Index: 256

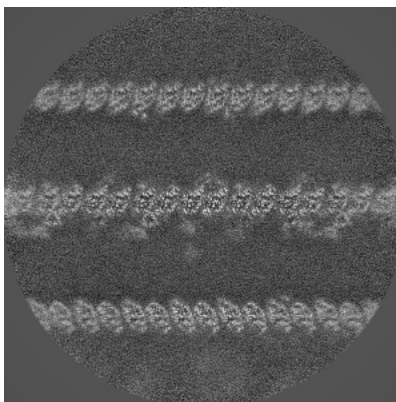


Z Index: 256

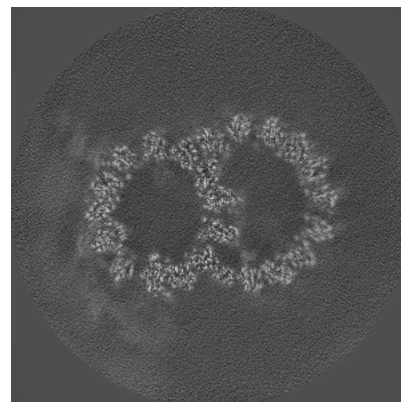
5.2.2 Raw map



X Index: 256



Y Index: 256

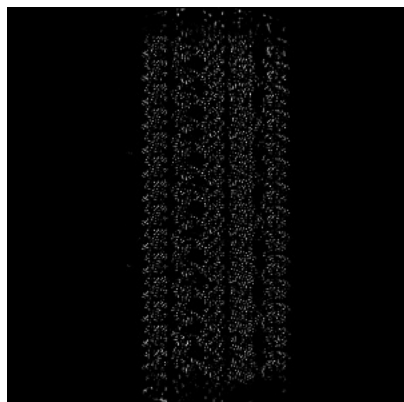


Z Index: 256

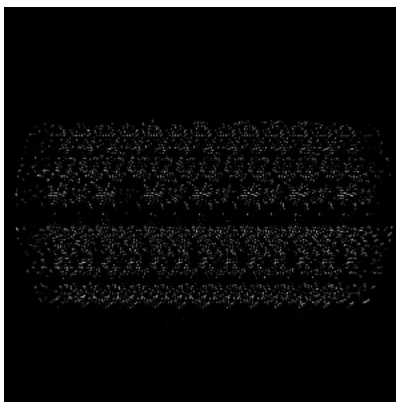
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

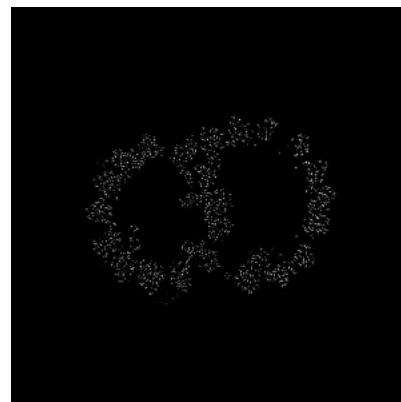
5.3.1 Primary map



X Index: 255

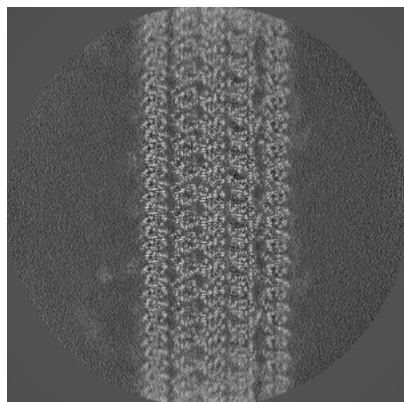


Y Index: 172

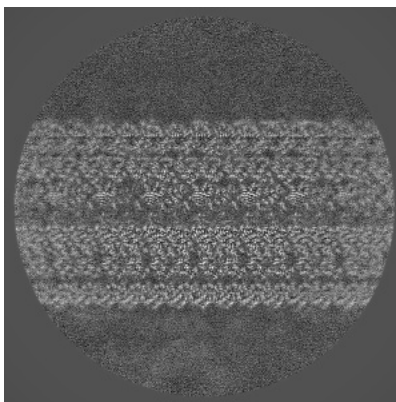


Z Index: 421

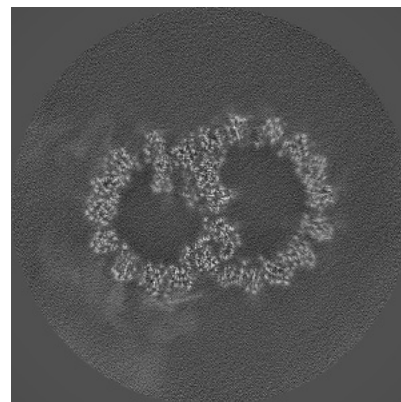
5.3.2 Raw map



X Index: 256



Y Index: 172

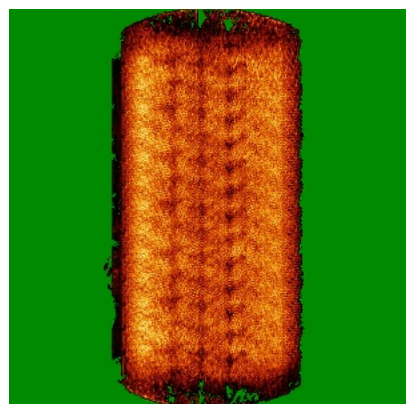


Z Index: 228

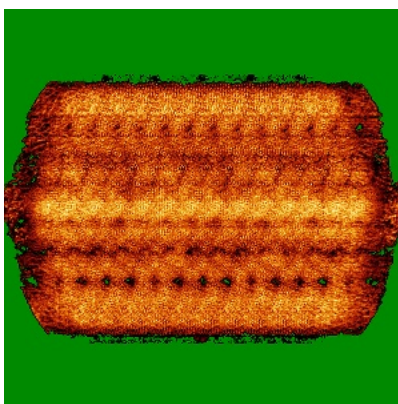
The images above show the largest variance slices of the map in three orthogonal directions.

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

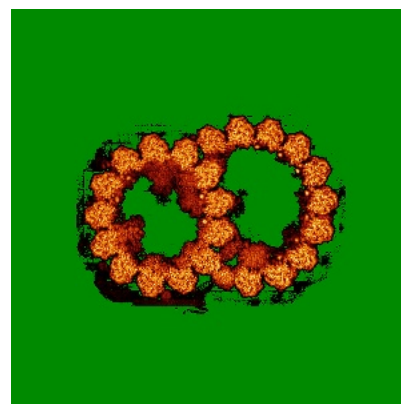
5.4.1 Primary map



X

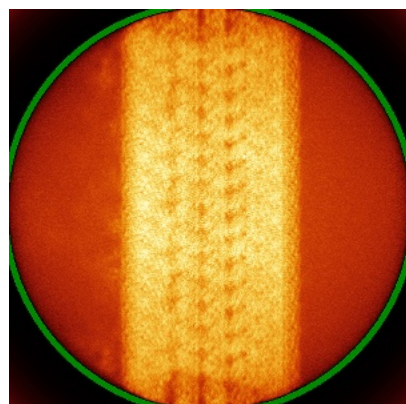


Y

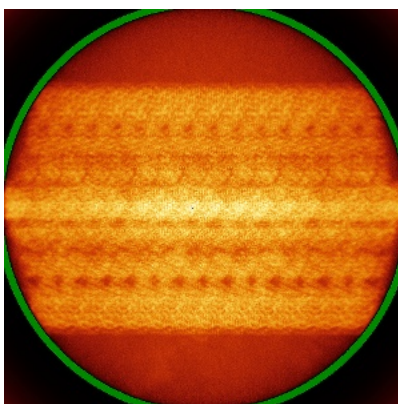


Z

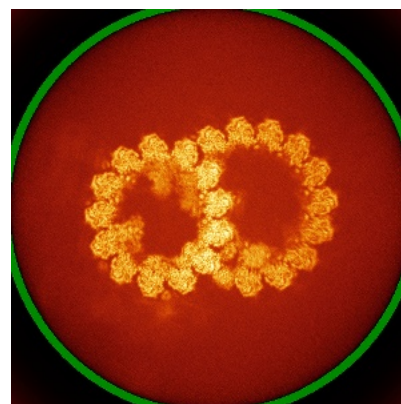
5.4.2 Raw map



X



Y

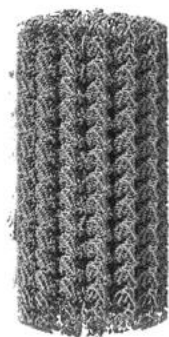


Z

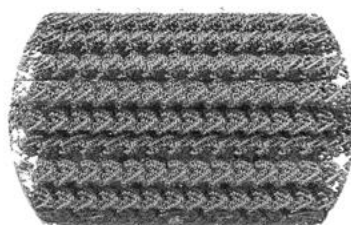
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

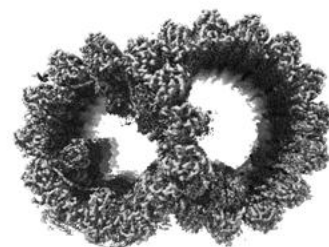
5.5.1 Primary map



X



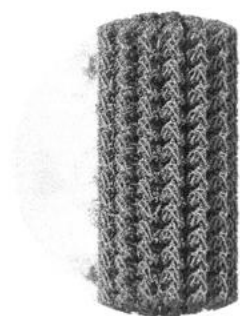
Y



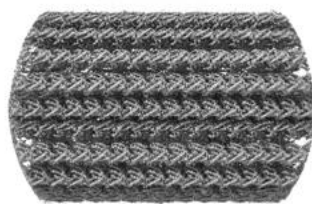
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

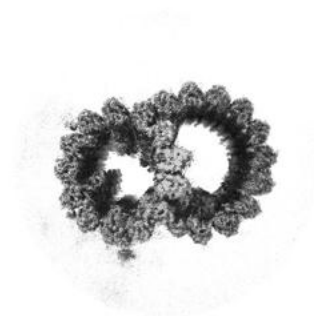
5.5.2 Raw map



X



Y



Z

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

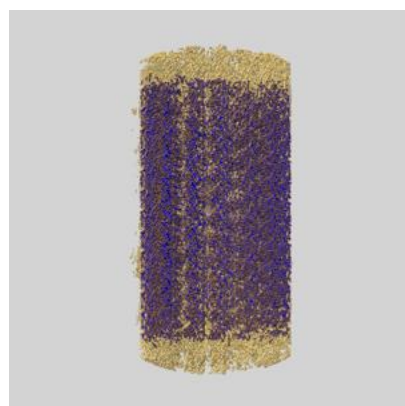
5.6 Mask visualisation [i](#)

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

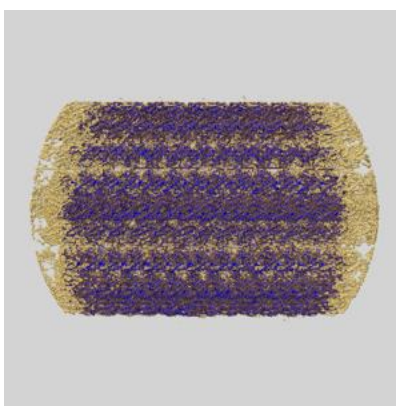
A mask typically either:

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

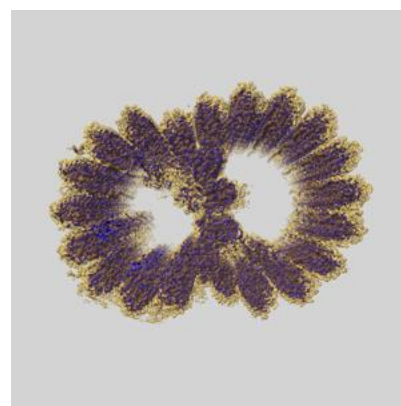
5.6.1 emd_29692_msk_1.map [i](#)



X



Y

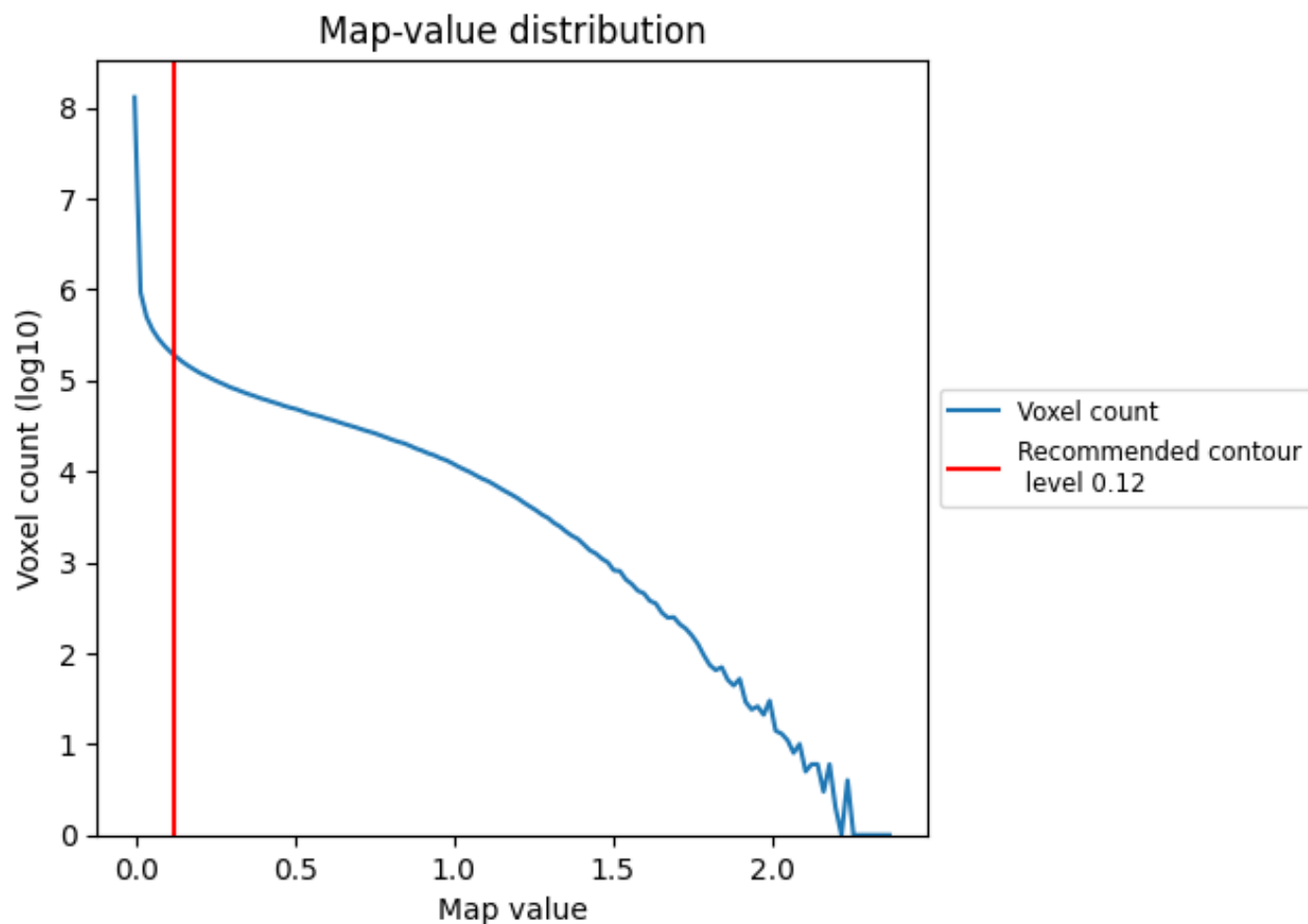


Z

6 Map analysis [i](#)

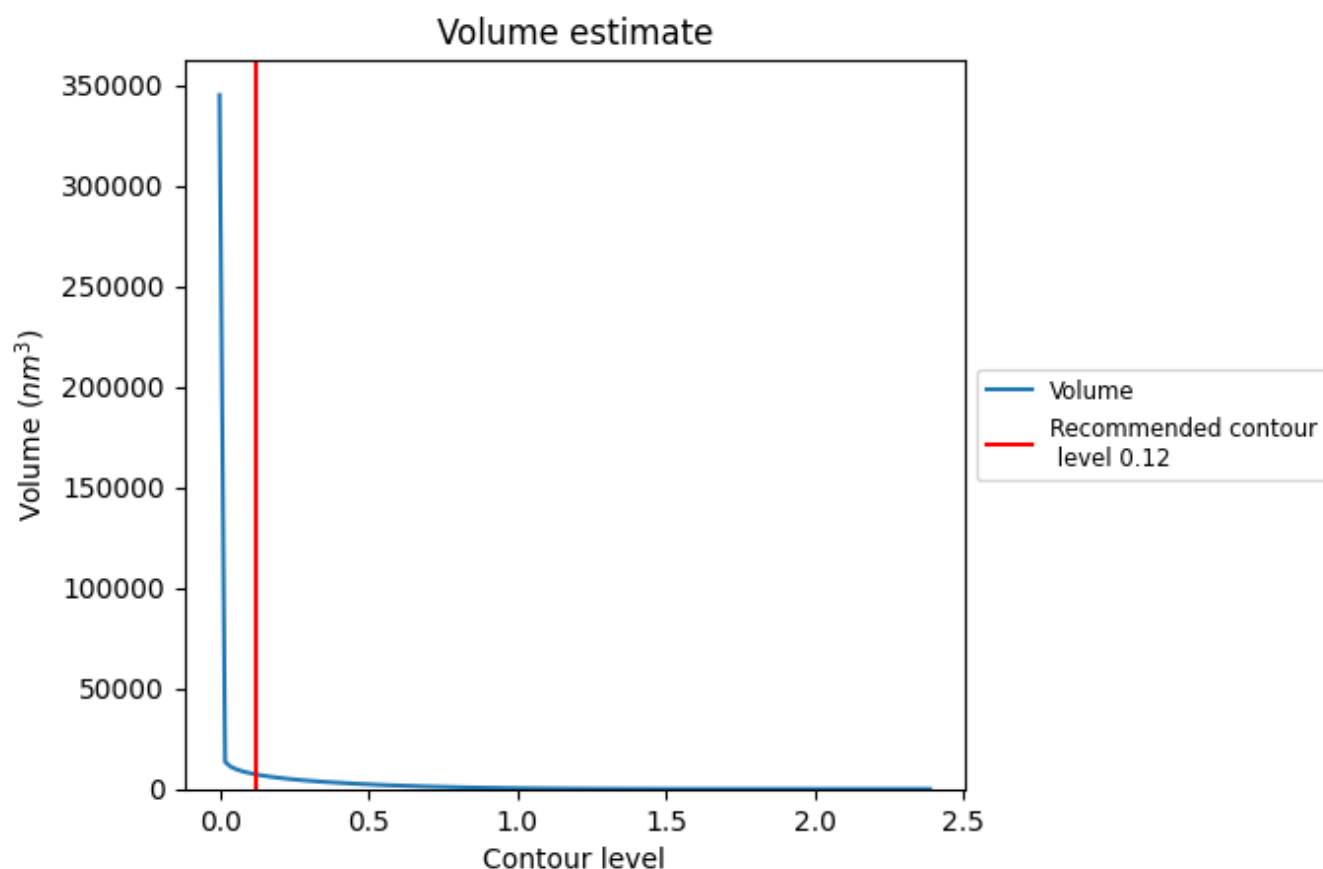
This section contains the results of statistical analysis of the map.

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.

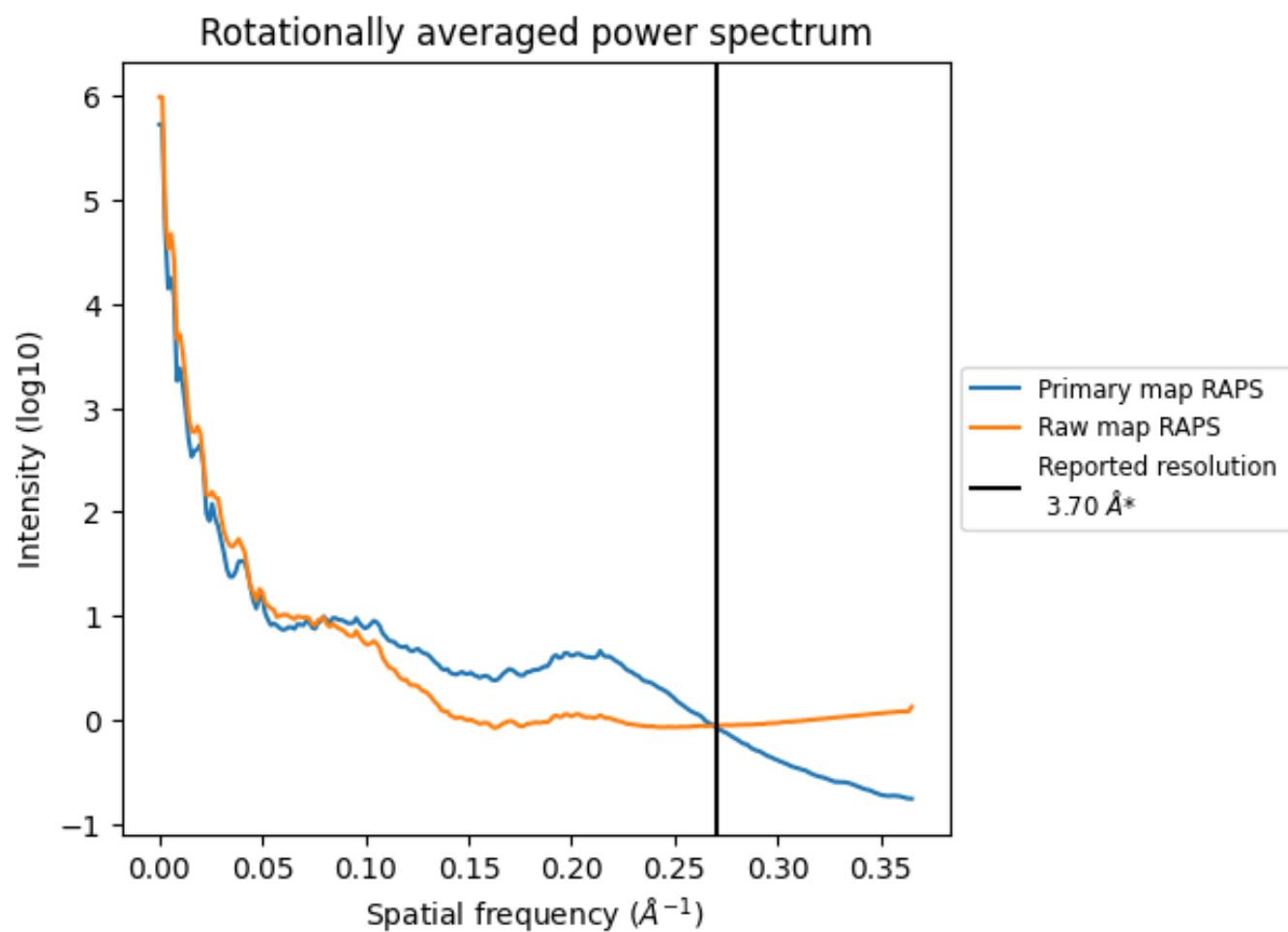
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 7236 nm^3 ; this corresponds to an approximate mass of 6536 kDa.

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

6.3 Rotationally averaged power spectrum [i](#)

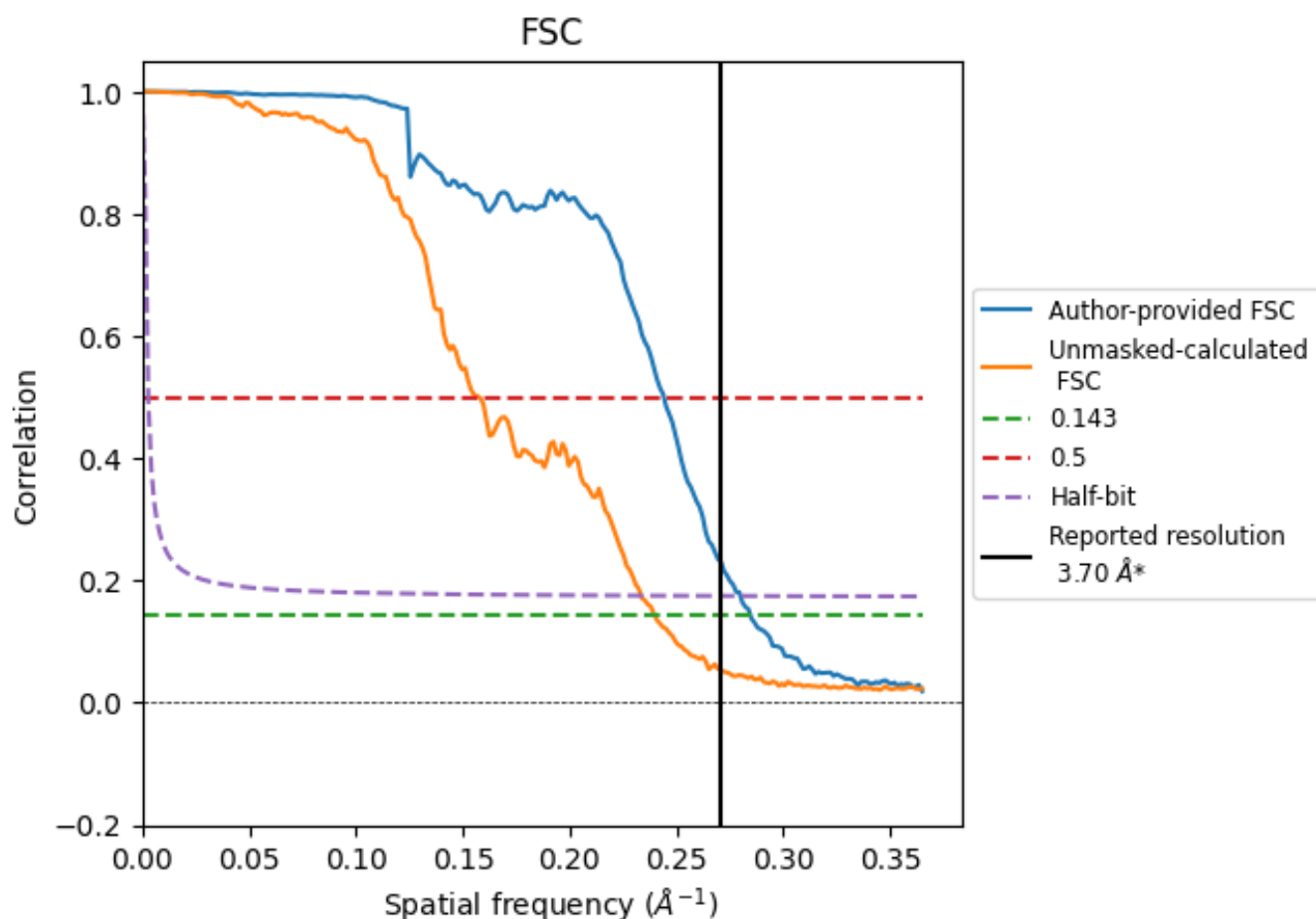


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

7.2 Resolution estimates [i](#)

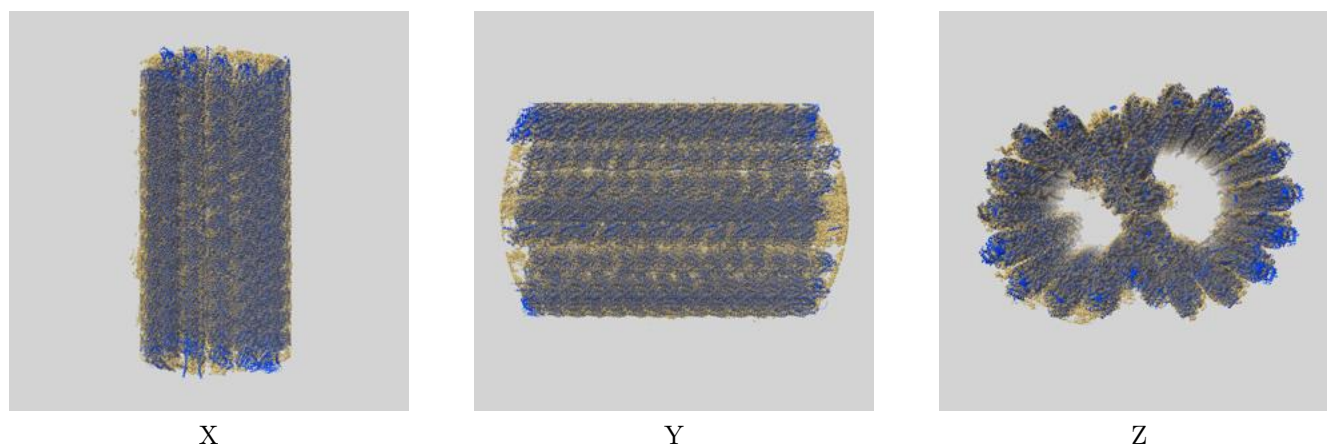
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.51	4.10	3.57
Unmasked-calculated*	4.17	6.34	4.28

*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 4.17 differs from the reported value 3.7 by more than 10 %

8 Map-model fit [i](#)

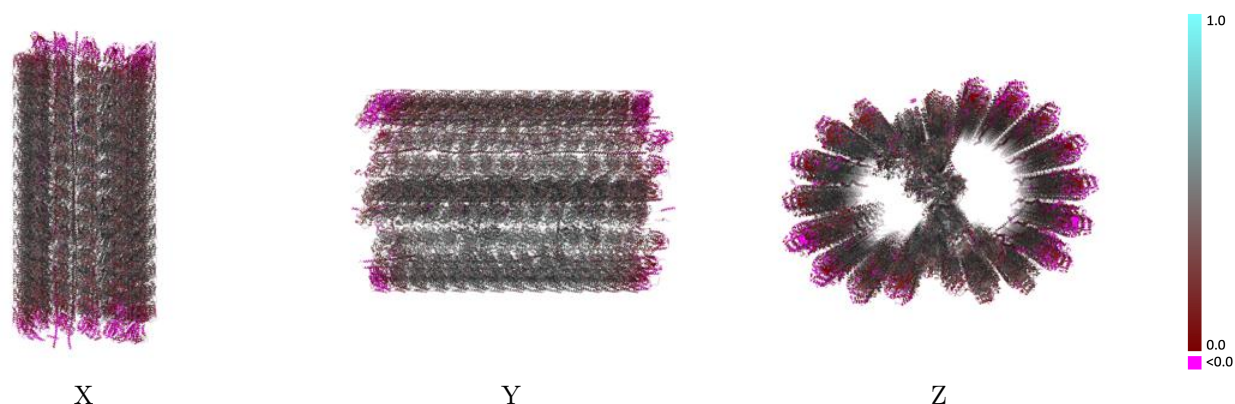
This section contains information regarding the fit between EMDB map EMD-29692 and PDB model 8G3D. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



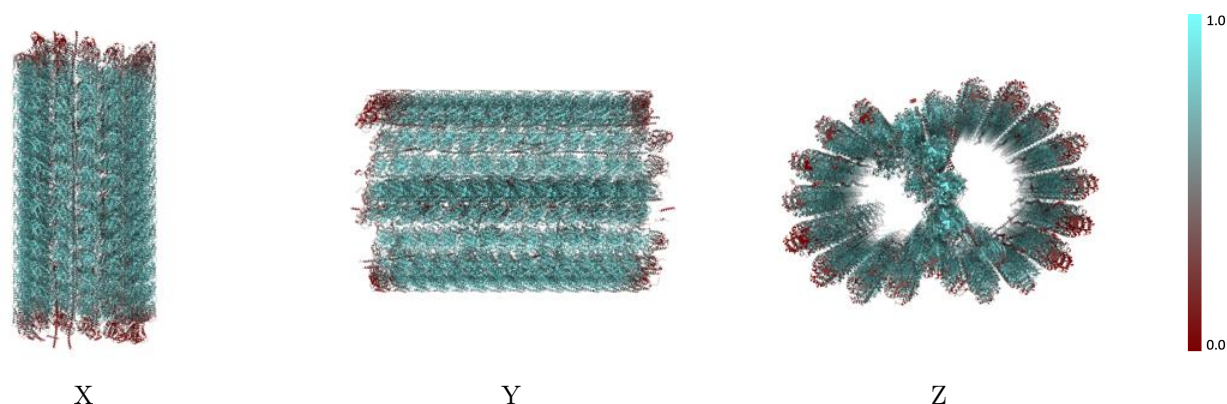
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



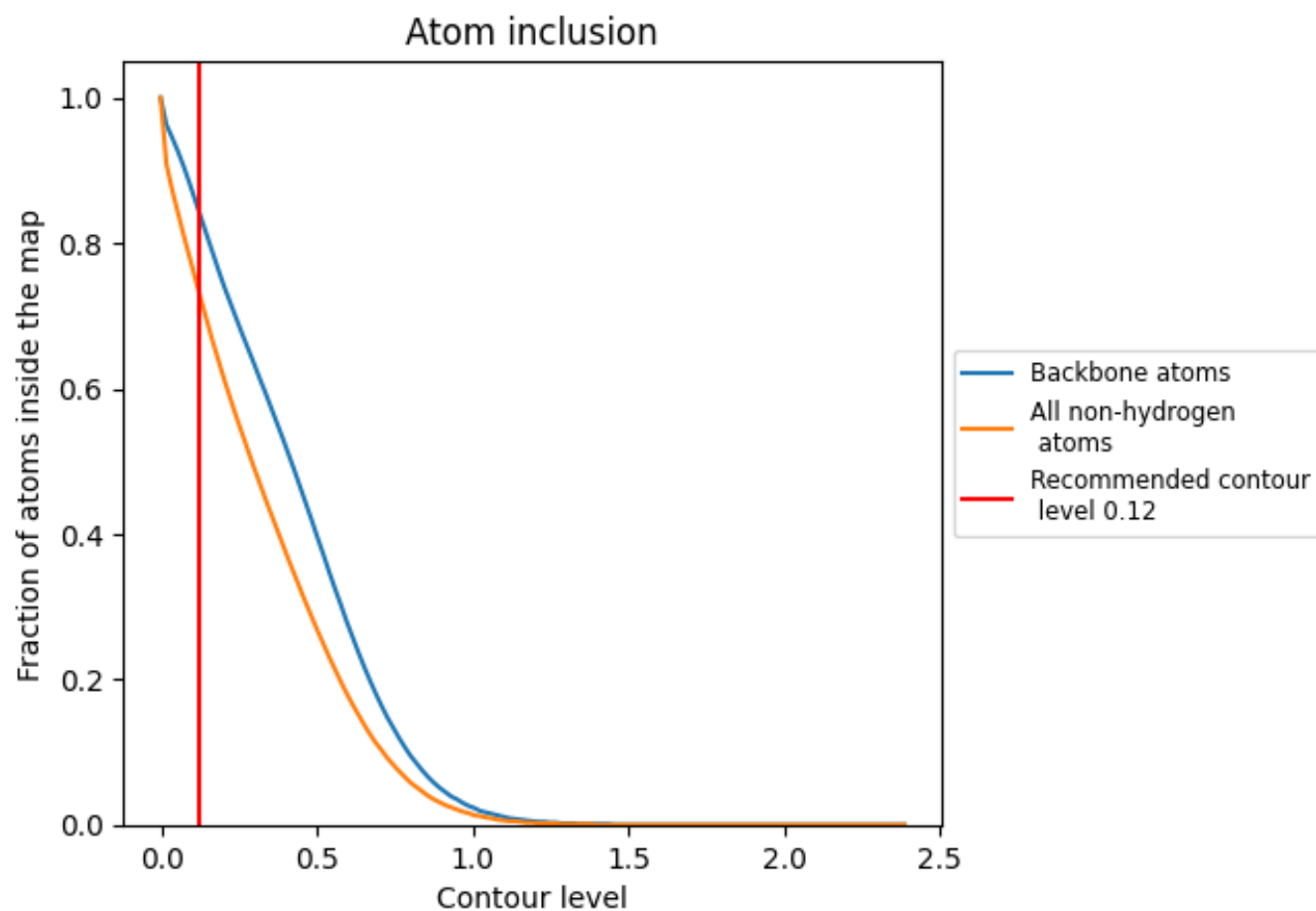
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

8.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 73% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7330	 0.3750
0A	 0.6480	 0.3110
0B	 0.6760	 0.4100
0C	 0.7220	 0.3910
0D	 0.6170	 0.2560
0E	 0.5970	 0.2200
0F	 0.7420	 0.3900
0G	 0.6560	 0.3440
0H	 0.4610	 0.1240
0N	 0.7200	 0.3390
0Q	 0.7640	 0.3630
0S	 0.4210	 0.2380
0T	 0.5000	 0.2970
0U	 0.6910	 0.3150
0V	 0.3380	 0.1270
0X	 0.7270	 0.4000
1A	 0.6510	 0.3700
1B	 0.6980	 0.3840
1C	 0.7160	 0.3200
1D	 0.6440	 0.3160
1E	 0.6600	 0.3320
1F	 0.7210	 0.4220
1G	 0.6060	 0.2790
1H	 0.4680	 0.1810
1I	 0.7620	 0.4350
1J	 0.6640	 0.3700
1K	 0.6190	 0.3230
1L	 0.6440	 0.3360
1M	 0.8170	 0.4520
1N	 0.7590	 0.4500
1O	 0.3520	 0.1010
1P	 0.4340	 0.1370
1Q	 0.8080	 0.4410
1R	 0.7860	 0.4410
1S	 0.7500	 0.4240



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Chain	Atom inclusion	Q-score
1T	 0.7500	 0.4370
1U	 0.7610	 0.3980
1V	 0.5250	 0.2990
1W	 0.7070	 0.4040
1X	 0.7480	 0.4440
2A	 0.6810	 0.3780
2B	 0.4370	 0.2970
2C	 0.5630	 0.2820
2D	 0.6260	 0.2940
2E	 0.6860	 0.3580
2F	 0.7180	 0.4100
2G	 0.7240	 0.4260
2H	 0.6420	 0.3780
2I	 0.5970	 0.3360
2K	 0.5270	 0.2680
2L	 0.4680	 0.2170
2M	 0.8120	 0.4580
2N	 0.6260	 0.2640
2O	 0.3730	 0.0880
2P	 0.4590	 0.1770
2Q	 0.7920	 0.4350
2R	 0.7720	 0.4480
2S	 0.7480	 0.4140
2T	 0.7600	 0.4300
2U	 0.7670	 0.3900
2V	 0.5640	 0.3040
2W	 0.4770	 0.2110
2X	 0.7470	 0.4330
3A	 0.6610	 0.3380
3B	 0.3860	 0.2130
3C	 0.7240	 0.3560
3D	 0.7610	 0.4200
3E	 0.4810	 0.1490
3H	 0.6240	 0.3980
3I	 0.7050	 0.4080
3L	 0.4770	 0.1650
3O	 0.3560	 0.1200
3Q	 0.8000	 0.4350
3R	 0.7770	 0.4320
3S	 0.7380	 0.3850
3T	 0.7400	 0.4020
3U	 0.7210	 0.3300

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Chain	Atom inclusion	Q-score
3V	 0.5190	 0.2670
3X	 0.6780	 0.3790
4C	 0.6980	 0.3540
4F	 0.7090	 0.4140
4H	 0.6840	 0.4140
4Q	 0.7980	 0.4300
4R	 0.7760	 0.4350
4S	 0.7180	 0.3780
4X	 0.5340	 0.3180
5A	 0.4880	 0.2770
5B	 0.6180	 0.3920
5C	 0.5970	 0.3620
5D	 0.5640	 0.3170
5E	 0.3540	 0.1830
5F	 0.5020	 0.2980
5G	 0.4920	 0.2900
5H	 0.5040	 0.2600
5I	 0.2930	 0.1980
5J	 0.3450	 0.3140
5K	 0.2470	 0.1430
5Q	 0.7900	 0.4150
5R	 0.7940	 0.4460
5S	 0.7240	 0.4110
6F	 0.7330	 0.4310
6G	 0.6600	 0.3210
6H	 0.6700	 0.3570
6Q	 0.7490	 0.3690
6R	 0.6920	 0.3330
7R	 0.6850	 0.3280
8L	 0.7020	 0.2430
8N	 0.6540	 0.1780
8P	 0.6670	 0.2070
8R	 0.6250	 0.2020
AA	 0.8240	 0.4360
AB	 0.6240	 0.3510
AC	 0.8310	 0.4750
AD	 0.8350	 0.4700
AE	 0.8360	 0.4850
AF	 0.8340	 0.4850
AG	 0.8320	 0.4890
AH	 0.8400	 0.4870
AI	 0.8420	 0.4910

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Chain	Atom inclusion	Q-score
AJ	 0.8300	 0.4790
AK	 0.8340	 0.4780
AL	 0.8270	 0.4770
AM	 0.8190	 0.4300
AN	 0.8320	 0.4640
BA	 0.7480	 0.3540
BB	 0.4340	 0.1290
BC	 0.8210	 0.4480
BD	 0.8260	 0.4330
BE	 0.8210	 0.4600
BF	 0.8170	 0.4580
BG	 0.8210	 0.4550
BH	 0.8240	 0.4630
BI	 0.8280	 0.4650
BJ	 0.8200	 0.4580
BK	 0.8280	 0.4590
BL	 0.8330	 0.4710
BM	 0.8120	 0.4080
BN	 0.8240	 0.4350
CA	 0.4990	 0.1790
CB	 0.7800	 0.3760
CC	 0.7950	 0.4090
CD	 0.8250	 0.4470
CE	 0.8190	 0.4500
CF	 0.8090	 0.4510
CG	 0.8190	 0.4460
CH	 0.8230	 0.4580
CI	 0.8320	 0.4600
CJ	 0.8350	 0.4630
CK	 0.8370	 0.4550
CL	 0.8220	 0.4170
CM	 0.7680	 0.3560
CN	 0.4020	 0.0980
DA	 0.3160	 0.0290
DB	 0.6960	 0.2900
DC	 0.7790	 0.3630
DD	 0.8360	 0.4470
DE	 0.8330	 0.4480
DF	 0.8260	 0.4520
DG	 0.8190	 0.4470
DH	 0.8340	 0.4570
DI	 0.8150	 0.4390

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Chain	Atom inclusion	Q-score
DJ	 0.8310	 0.4440
DK	 0.8170	 0.4260
DL	 0.7970	 0.3900
DM	 0.7310	 0.3280
DN	 0.3610	 0.0690
EA	 0.2500	 0.0270
EB	 0.5730	 0.2210
EC	 0.7810	 0.3580
ED	 0.8160	 0.4220
EE	 0.8260	 0.4430
EF	 0.8070	 0.4320
EG	 0.8090	 0.4340
EH	 0.8080	 0.4250
EI	 0.8150	 0.4350
EJ	 0.8050	 0.4310
EK	 0.8140	 0.4390
EL	 0.7970	 0.3970
EM	 0.7650	 0.3550
EN	 0.4180	 0.1220
FA	 0.7740	 0.3540
FB	 0.5270	 0.2070
FC	 0.8240	 0.4540
FD	 0.8270	 0.4300
FE	 0.8220	 0.4590
FF	 0.8200	 0.4510
FG	 0.8130	 0.4470
FH	 0.8270	 0.4600
FI	 0.8260	 0.4620
FJ	 0.8400	 0.4620
FK	 0.8200	 0.4220
FL	 0.8170	 0.4360
FM	 0.1680	 -0.0030
FN	 0.5420	 0.2460
GA	 0.7520	 0.3390
GB	 0.4480	 0.1510
GC	 0.8260	 0.4610
GD	 0.8300	 0.4350
GE	 0.8340	 0.4780
GF	 0.8340	 0.4730
GG	 0.8280	 0.4700
GH	 0.8280	 0.4750
GI	 0.8300	 0.4700

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Chain	Atom inclusion	Q-score
GJ	 0.8310	 0.4750
GK	 0.8280	 0.4440
GL	 0.8250	 0.4570
GM	 0.3100	 0.0560
GN	 0.7090	 0.3620
HA	 0.7590	 0.3620
HB	 0.4410	 0.1400
HC	 0.8130	 0.4600
HD	 0.8240	 0.4410
HE	 0.8390	 0.4850
HF	 0.8370	 0.4710
HG	 0.8140	 0.4680
HH	 0.8210	 0.4600
HI	 0.8290	 0.4740
HJ	 0.8230	 0.4680
HK	 0.8320	 0.4620
HL	 0.8250	 0.4700
HM	 0.5100	 0.2400
HN	 0.7870	 0.4130
IA	 0.7770	 0.3670
IB	 0.4800	 0.2120
IC	 0.8220	 0.4570
ID	 0.8320	 0.4480
IE	 0.8370	 0.4840
IF	 0.8360	 0.4800
IG	 0.8290	 0.4790
IH	 0.8570	 0.4890
II	 0.8400	 0.4890
IJ	 0.8530	 0.4950
IK	 0.8390	 0.4740
IL	 0.8370	 0.4730
IM	 0.7080	 0.3950
IN	 0.8320	 0.4500
JA	 0.8230	 0.4340
JB	 0.8090	 0.3960
JC	 0.8370	 0.4780
JD	 0.8500	 0.4750
JE	 0.8350	 0.4790
JF	 0.8410	 0.4830
JG	 0.8280	 0.4700
JH	 0.8360	 0.4760
JI	 0.8370	 0.4660

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Chain	Atom inclusion	Q-score
JJ	 0.8400	 0.4720
JK	 0.8140	 0.4440
JL	 0.8400	 0.4780
JM	 0.5030	 0.2960
JN	 0.8170	 0.4350
KA	 0.8420	 0.4500
KB	 0.8240	 0.4080
KC	 0.8410	 0.4840
KD	 0.8530	 0.4830
KE	 0.8390	 0.4820
KF	 0.8540	 0.4910
KG	 0.8310	 0.4730
KH	 0.8350	 0.4810
KI	 0.8300	 0.4750
KJ	 0.8470	 0.4840
KK	 0.8480	 0.4830
KL	 0.8460	 0.4920
KM	 0.7500	 0.4160
KN	 0.8550	 0.4690
LA	 0.8170	 0.4420
LB	 0.7960	 0.4120
LC	 0.8350	 0.4860
LD	 0.8460	 0.4800
LE	 0.8310	 0.4840
LF	 0.8360	 0.4850
LG	 0.8410	 0.4860
LH	 0.8420	 0.4890
LI	 0.8260	 0.4790
LJ	 0.8420	 0.4860
LK	 0.8330	 0.4860
LL	 0.8340	 0.4790
LM	 0.7960	 0.4180
LN	 0.8400	 0.4650
MA	 0.8200	 0.4430
MB	 0.8050	 0.4240
MC	 0.8410	 0.4960
MD	 0.8450	 0.4950
ME	 0.8230	 0.4870
MF	 0.8410	 0.4960
MG	 0.8320	 0.4850
MH	 0.8350	 0.4870
MI	 0.8210	 0.4700

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Chain	Atom inclusion	Q-score
MJ	 0.8470	 0.4940
MK	 0.8330	 0.4820
ML	 0.8180	 0.4790
MM	 0.8070	 0.4250
MN	 0.8460	 0.4840
NA	 0.7420	 0.3530
NB	 0.6380	 0.2690
NC	 0.8010	 0.4360
ND	 0.7780	 0.4050
NE	 0.7930	 0.4360
NF	 0.7850	 0.4310
NG	 0.7950	 0.4290
NH	 0.7680	 0.4160
NI	 0.7780	 0.4210
NJ	 0.8000	 0.4330
NK	 0.7900	 0.4210
NL	 0.7710	 0.4220
NM	 0.5910	 0.3350
NN	 0.7700	 0.4070
OA	 0.6790	 0.2760
OB	 0.4700	 0.1150
OC	 0.8070	 0.4110
OD	 0.7980	 0.3820
OE	 0.8110	 0.4340
OF	 0.8220	 0.4310
OG	 0.8110	 0.4220
OH	 0.7990	 0.4140
OI	 0.8100	 0.4250
OJ	 0.8110	 0.4200
OK	 0.8040	 0.4120
OL	 0.8020	 0.4200
OM	 0.5880	 0.2970
ON	 0.7930	 0.3800
PA	 0.5030	 0.1510
PB	 0.3080	 0.0130
PC	 0.7860	 0.3730
PD	 0.7300	 0.3180
PE	 0.7950	 0.3900
PF	 0.7950	 0.3900
PG	 0.7910	 0.3970
PH	 0.7910	 0.3930
PI	 0.7980	 0.4000

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Chain	Atom inclusion	Q-score
PJ	 0.7890	 0.3890
PK	 0.8010	 0.3900
PL	 0.7910	 0.3910
PM	 0.5140	 0.2230
PN	 0.7570	 0.3380
QA	 0.3770	 0.0860
QB	 0.7180	 0.3050
QC	 0.7650	 0.3460
QD	 0.7860	 0.3760
QE	 0.7760	 0.3730
QF	 0.7910	 0.3780
QG	 0.7740	 0.3670
QH	 0.7850	 0.3820
QI	 0.7850	 0.3670
QJ	 0.7870	 0.3710
QK	 0.7650	 0.3570
QL	 0.7160	 0.3020
QM	 0.4560	 0.1380
QN	 0.1310	 -0.0040
RA	 0.2780	 0.0410
RB	 0.6570	 0.2830
RC	 0.7570	 0.3470
RD	 0.7580	 0.3640
RE	 0.7600	 0.3720
RF	 0.7620	 0.3690
RG	 0.7660	 0.3710
RH	 0.7650	 0.3650
RI	 0.7480	 0.3600
RJ	 0.7530	 0.3560
RK	 0.7420	 0.3370
RL	 0.6520	 0.2620
RM	 0.4230	 0.0620
RN	 0.1440	 -0.0230
SA	 0.2440	 0.0110
SB	 0.6460	 0.2670
SC	 0.7760	 0.3420
SD	 0.7810	 0.3690
SE	 0.7840	 0.3820
SF	 0.7810	 0.3840
SG	 0.7980	 0.3860
SH	 0.7810	 0.3770
SI	 0.7850	 0.3860

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Chain	Atom inclusion	Q-score
SJ	 0.7720	 0.3620
SK	 0.7750	 0.3550
SL	 0.7650	 0.3220
SM	 0.6080	 0.2230
SN	 0.2210	 -0.0100
TA	 0.2060	 0.0060
TB	 0.5180	 0.2280
TC	 0.7400	 0.3240
TD	 0.7860	 0.3630
TE	 0.7860	 0.3820
TF	 0.7910	 0.3800
TG	 0.7690	 0.3650
TH	 0.7640	 0.3540
TI	 0.7680	 0.3650
TJ	 0.7790	 0.3660
TK	 0.7790	 0.3590
TL	 0.7530	 0.3100
TM	 0.6470	 0.2460
TN	 0.2170	 0.0080
UA	 0.2230	 0.0110
UB	 0.5200	 0.2270
UC	 0.7490	 0.3300
UD	 0.7910	 0.3850
UE	 0.8030	 0.4130
UF	 0.8020	 0.4060
UG	 0.8020	 0.4020
UH	 0.7790	 0.3880
UI	 0.8030	 0.4010
UJ	 0.7860	 0.3910
UK	 0.8020	 0.3930
UL	 0.7510	 0.3400
UM	 0.7120	 0.2950
UN	 0.3860	 0.1030
VA	 0.7890	 0.3830
VB	 0.6350	 0.3080
VC	 0.8070	 0.4370
VD	 0.8140	 0.4240
VE	 0.8160	 0.4290
VF	 0.8030	 0.4260
VG	 0.7910	 0.4090
VH	 0.7920	 0.4140
VI	 0.8090	 0.4190

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Chain	Atom inclusion	Q-score
VJ	 0.8040	 0.4170
VK	 0.7860	 0.3700
VL	 0.8010	 0.3930
VM	 0.3210	 0.0300
VN	 0.6710	 0.2870
WA	 0.7860	 0.3850
WB	 0.6300	 0.3150
WC	 0.8060	 0.4280
WD	 0.8160	 0.4310
WE	 0.8050	 0.4250
WF	 0.8010	 0.4340
WG	 0.7970	 0.4080
WH	 0.7990	 0.4240
WI	 0.8030	 0.4300
WJ	 0.8050	 0.4280
WK	 0.7980	 0.3840
WL	 0.7990	 0.4100
WM	 0.4440	 0.1380
WN	 0.7340	 0.3270