



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2026 – 03:29 AM UTC

PDB ID : 8SF7 / pdb_00008sf7
EMDB ID : EMD-40436
Title : 48-nm doublet microtubule from Tetrahymena thermophila strain MEC17
Authors : Black, C.S.; Kubo, S.; Yang, S.K.; Bui, K.H.
Deposited on : 2023-04-10
Resolution : 4.10 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

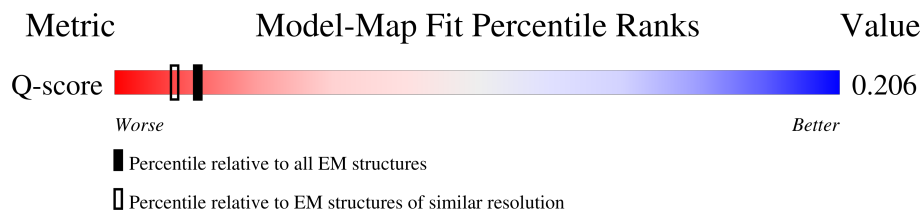
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 1334198 atoms, of which 10347 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 Nebulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	6H	166	Total	C	N	O	S	0	0
			1370	861	234	269	6		

- Molecule 2 is a protein called RIB27A.

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

- Molecule 3 is a protein called RIB38.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	0B	321	Total	C	N	O	S	0	0
			2614	1633	472	503	6		

- Molecule 4 is a protein called CFAM166B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	0C	95	Total	C	N	O	S	0	0
			747	471	131	143	2		
4	1C	95	Total	C	N	O	S	0	0
			747	471	131	143	2		

- Molecule 5 is a protein called CFAM166A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	0D	202	Total	C	N	O	S	1	0
			1621	1019	293	307	2		
5	1D	202	Total	C	N	O	S	1	0
			1621	1019	293	307	2		
5	2D	202	Total	C	N	O	S	1	0
			1621	1019	293	307	2		

- Molecule 6 is a protein called RIB22.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	0E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		
6	1E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		
6	2E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		
6	3E	189	Total	C	N	O	S	0	0
			1557	978	280	294	5		

- Molecule 7 is a protein called CFAM166C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	0F	206	Total	C	N	O	S	0	0
			1665	1048	300	314	3		

- Molecule 8 is a protein called CFAP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	0G	168	Total	C	N	O	S	0	0
			1378	872	237	265	4		
8	1G	133	Total	C	N	O	S	0	0
			1089	692	185	210	2		

- Molecule 9 is a protein called CFAP127.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	0H	111	Total	C	N	O	S	0	2
			949	591	172	183	3		
9	1H	418	Total	C	N	O	S	0	0
			3654	2250	680	710	14		

- Molecule 10 is a protein called CFAP161A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	0N	280	Total	C	N	O	S	0	0
			2305	1455	396	441	13		
10	1N	463	Total	C	N	O	S	0	0
			3805	2414	653	723	15		
10	2N	280	Total	C	N	O	S	0	0
			2305	1455	396	441	13		

- Molecule 11 is a protein called CFAP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	0Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
11	1Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
11	2Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
11	3Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
11	4Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
11	5Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		
11	6Q	186	Total	C	N	O	S	0	0
			1548	997	268	276	7		

- Molecule 12 is a protein called Parkin co-regulated protein PACRGA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	0S	281	Total	C	N	O	S	0	1
			2227	1430	383	408	6		
12	1S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		
12	2S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		
12	3S	288	Total	C	N	O	S	0	0
			2310	1485	397	422	6		

- Molecule 13 is a protein called IJ34.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	0T	226	Total	C	N	O	S	0	4
			1774	1138	305	322	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1T	285	Total	C	N	O	S	0	0
			2321	1471	411	430	9		
13	2T	285	Total	C	N	O	S	0	0
			2321	1471	411	430	9		
13	3T	285	Total	C	N	O	S	0	0
			2321	1471	411	430	9		

- Molecule 14 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	0U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		
14	1U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		
14	2U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		
14	3U	607	Total	C	N	O	S	0	0
			4774	3025	819	906	24		

- Molecule 15 is a protein called DNA polymerase delta C4-type zinc-finger protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
15	0V	212	Total 1750	C 1095	N 317	O 332	S 6	0	0	
15	1V	263	Total 3379	C 1359	H 1211	N 388	O 412	S 9	0	0
15	2V	263	Total 3379	C 1359	H 1211	N 388	O 412	S 9	0	0
15	3V	263	Total 3379	C 1359	H 1211	N 388	O 412	S 9	0	0

- Molecule 16 is a protein called RIB43A protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	0X	106	Total	C	N	O	S	0	0
			903	553	170	175	5		
16	1X	141	Total	C	N	O	S	0	0
			1205	736	229	234	6		
16	2X	141	Total	C	N	O	S	0	0
			1205	736	229	234	6		
16	3X	141	Total	C	N	O	S	0	0
			1205	736	229	234	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4X	141	Total	C	N	O	S	0	0
			1205	736	229	234	6		

- Molecule 17 is a protein called RIB57.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1B	498	Total	C	N	O	S	0	0
			4066	2598	692	768	8		
17	2B	295	Total	C	N	O	S	0	0
			2439	1553	416	464	6		
17	3B	297	Total	C	N	O	S	0	0
			2449	1558	418	467	6		

- Molecule 18 is a protein called CFAP182A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1F	136	Total	C	N	O	S	0	0
			1093	696	184	208	5		

- Molecule 19 is a protein called CFAP143.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1I	188	Total	C	N	O	S	0	0
			1546	951	285	306	4		

- Molecule 20 is a protein called CFAP21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1J	370	Total	C	N	O	S	0	0
			3025	1901	534	579	11		

- Molecule 21 is a protein called Cilia- and flagella-associated protein 53.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1K	269	Total	C	N	O	S	0	1
			2335	1441	440	447	7		
21	2K	278	Total	C	N	O	S	0	2
			2396	1473	443	473	7		

- Molecule 22 is a protein called CFAP115.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1L	820	Total	C	N	O	S	0	0
			6841	4357	1186	1280	18		
22	2L	620	Total	C	N	O	S	0	0
			5181	3304	902	963	12		
22	3L	200	Total	C	N	O	S	0	0
			1660	1053	284	317	6		

- Molecule 23 is a protein called Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	1M	369	Total	C	H	N	O	S	0	0
			5154	1910	2176	501	552	15		
23	2M	369	Total	C	H	N	O	S	0	0
			5169	1910	2191	501	552	15		

- Molecule 24 is a protein called Cilia- and flagella-associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	1O	235	Total	C	N	O	S	0	0	
			1983	1235	350	386	12			
24	2O	370	Total	C	N	O	S	0	0	
			3173	1948	595	617	13			
24	3O	269	Total	C	H	N	O	S	0	1
			4637	1404	2347	438	444	4		

- Molecule 25 is a protein called CFAP210.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1P	344	Total	C	N	O	S	0	0
			2958	1831	552	567	8		
25	2P	179	Total	C	N	O	S	0	2
			1507	928	282	293	4		

- Molecule 26 is a protein called RIB72B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1R	508	Total	C	N	O	S	0	0
			4244	2744	711	777	12		
26	2R	508	Total	C	N	O	S	0	0
			4244	2744	711	777	12		
26	3R	508	Total	C	N	O	S	0	0
			4244	2744	711	777	12		

- Molecule 27 is a protein called Protofilament ribbon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1W	216	Total	C	N	O	S	0	1
			1840	1113	365	353	9		
27	2W	105	Total	C	N	O	S	0	0
			890	550	171	164	5		

- Molecule 28 is a protein called RIB35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2C	300	Total	C	N	O	S	0	0
			2467	1581	417	464	5		
28	3C	300	Total	C	N	O	S	0	0
			2467	1581	417	464	5		
28	4C	300	Total	C	N	O	S	0	0
			2467	1581	417	464	5		

- Molecule 29 is a protein called CFAP182B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2F	87	Total	C	N	O	S	0	0
			746	469	136	137	4		

- Molecule 30 is a protein called Flagellar FliJ protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2G	99	Total	C	N	O	S	0	0
			848	536	153	155	4		

- Molecule 31 is a protein called RIB27B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2H	61	Total	C	N	O	S	0	0
			501	313	92	94	2		
31	3H	61	Total	C	N	O	S	0	0
			501	313	92	94	2		
31	4H	61	Total	C	N	O	S	0	0
			501	313	92	94	2		

- Molecule 32 is a protein called STPG2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	2I	136	Total	C	N	O	S	0	1
			1086	699	190	196	1		
32	3I	87	Total	C	N	O	S	0	0
			712	451	130	127	4		

- Molecule 33 is a protein called RIB26.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	3D	237	Total	C	N	O	S	0	0
			1835	1174	310	340	11		

- Molecule 34 is a protein called CFAP129.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4F	200	Total	C	N	O	S	0	0
			1622	1022	286	312	2		

- Molecule 35 is a protein called Flagellar microtubule protofilament ribbon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		
35	5R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		
35	6R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		
35	7R	609	Total	C	N	O	S	0	0
			5070	3267	847	932	24		

- Molecule 36 is a protein called Parkin co-regulated protein PACRGB.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	4S	188	Total	C	N	O	S	0	0
			1537	999	251	279	8		
36	5S	188	Total	C	N	O	S	0	0
			1537	999	251	279	8		

- Molecule 37 is a protein called OJ2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	5A	157	Total	C	N	O	S	0	0
			1261	795	234	229	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
37	5B	157	Total	C	N	O	S	0	0
			1261	795	234	229	3		
37	5C	157	Total	C	N	O	S	0	0
			1261	795	234	229	3		
37	5D	107	Total	C	N	O	S	0	1
			846	535	154	154	3		

- Molecule 38 is a protein called CFAP77A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5E	181	Total	C	N	O	S	0	1
			1500	949	272	274	5		
38	5F	210	Total	C	N	O	S	0	0
			1750	1107	316	322	5		
38	5G	210	Total	C	N	O	S	0	0
			1750	1107	316	322	5		
38	5H	132	Total	C	N	O	S	0	1
			1077	683	194	197	3		

- Molecule 39 is a protein called OJ3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5I	93	Total	C	N	O	S	0	1
			732	465	122	143	2		
39	5J	109	Total	C	N	O	S	0	0
			878	559	147	169	3		
39	5K	70	Total	C	N	O	S	0	0
			553	358	92	102	1		

- Molecule 40 is a protein called SB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	6F	132	Total	C	N	O	S	0	0
			1140	718	197	221	4		

- Molecule 41 is a protein called STPG1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	6G	216	Total	C	N	O	S	0	0
			1769	1128	303	333	5		

- Molecule 42 is a protein called CFAP112B.

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		
43	8R	361	Total	C	N	O	0	0
			2020	1269	361	390		

- Molecule 44 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AA	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	AC	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	AE	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	AG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	AI	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	AK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	AM	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	BA	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	BC	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	BE	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	BG	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	BI	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	BK	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	BM	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
44	CA	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	CC	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	CE	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	CG	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	CI	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	CK	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	CM	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	DA	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
44	DC	433	Total 3368	C 2131	N 572	O 643	S 22	0	0
44	DE	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
44	DG	436	Total 3389	C 2143	N 576	O 648	S 22	0	0
44	DI	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
44	DK	436	Total 3389	C 2143	N 576	O 648	S 22	0	0
44	DM	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
44	EA	439	Total 3397	C 2147	N 576	O 652	S 22	0	0
44	EC	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	EE	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	EG	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	EI	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	EK	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	EM	439	Total 3408	C 2155	N 579	O 652	S 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
44	FA	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
44	FC	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	FE	434	Total	C	N	O	S	0	0
			3376	2135	573	646	22		
44	FG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	FI	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
44	FK	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	FM	420	Total	C	N	O	S	0	4
			3239	2055	549	613	22		
44	GA	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
44	GC	431	Total	C	N	O	S	0	0
			3358	2126	570	640	22		
44	GE	431	Total	C	N	O	S	0	0
			3358	2126	570	640	22		
44	GG	431	Total	C	N	O	S	0	0
			3358	2126	570	640	22		
44	GI	431	Total	C	N	O	S	0	0
			3358	2126	570	640	22		
44	GK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	GM	429	Total	C	N	O	S	0	0
			3342	2118	568	634	22		
44	HA	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
44	HC	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
44	HE	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
44	HG	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
44	HI	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
44	HK	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		
44	HM	431	Total	C	N	O	S	0	0
			3356	2125	570	639	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
44	IA	432	Total 3364	C 2129	N 571	O 642	S 22	0	0
44	IC	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	IE	432	Total 3364	C 2129	N 571	O 642	S 22	0	0
44	IG	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	II	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	IK	432	Total 3364	C 2129	N 571	O 642	S 22	0	0
44	IM	432	Total 3364	C 2129	N 571	O 642	S 22	0	0
44	JA	432	Total 3364	C 2129	N 571	O 642	S 22	0	0
44	JC	434	Total 3376	C 2135	N 573	O 646	S 22	0	0
44	JE	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	JG	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	JI	439	Total 3404	C 2151	N 579	O 652	S 22	0	0
44	JK	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	JM	434	Total 3376	C 2135	N 573	O 646	S 22	0	0
44	KA	434	Total 3376	C 2135	N 573	O 646	S 22	0	0
44	KC	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
44	KE	435	Total 3385	C 2141	N 575	O 647	S 22	0	0
44	KG	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	KI	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	KK	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	KM	434	Total 3376	C 2135	N 573	O 646	S 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LA	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	LC	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	LE	438	Total	C	N	O	S	0	0
			3400	2149	578	651	22		
44	LG	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	LI	434	Total	C	N	O	S	0	0
			3381	2139	574	646	22		
44	LK	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	LM	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	MA	436	Total	C	N	O	S	0	0
			3392	2145	576	649	22		
44	MC	433	Total	C	N	O	S	0	0
			3368	2131	572	643	22		
44	ME	433	Total	C	N	O	S	0	0
			3372	2133	572	645	22		
44	MG	437	Total	C	N	O	S	0	0
			3400	2151	577	650	22		
44	MI	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	MK	436	Total	C	N	O	S	0	0
			3384	2139	575	648	22		
44	MM	436	Total	C	N	O	S	0	0
			3392	2145	576	649	22		
44	NA	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	NC	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	NE	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	NG	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	NI	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		
44	NK	432	Total	C	N	O	S	0	0
			3364	2129	571	642	22		
44	NM	439	Total	C	N	O	S	0	0
			3408	2155	579	652	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
44	OA	433	Total 3368	C 2131	N 572	O 643	S 22	0	0
44	OC	433	Total 3368	C 2131	N 572	O 643	S 22	0	0
44	OE	433	Total 3368	C 2131	N 572	O 643	S 22	0	0
44	OG	433	Total 3368	C 2131	N 572	O 643	S 22	0	0
44	OI	433	Total 3368	C 2131	N 572	O 643	S 22	0	0
44	OK	433	Total 3368	C 2131	N 572	O 643	S 22	0	0
44	OM	433	Total 3368	C 2131	N 572	O 643	S 22	0	0
44	PA	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
44	PC	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
44	PE	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
44	PG	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
44	PI	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
44	PK	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
44	PM	429	Total 3342	C 2118	N 568	O 634	S 22	0	0
44	QA	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	QC	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	QE	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	QG	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	QI	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	QK	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	QM	431	Total 3356	C 2125	N 570	O 639	S 22	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
44	UA	430	Total 3350	C 2122	N 569	O 637	S 22	0	0
44	UC	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	UE	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	UG	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	UI	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	UK	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	UM	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	VA	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
44	VC	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	VE	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
44	VG	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	VI	433	Total 3372	C 2133	N 572	O 645	S 22	0	0
44	VK	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	VM	433	Total 3365	C 2128	N 570	O 645	S 22	0	0
44	WA	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	WC	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	WE	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	WG	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	WI	431	Total 3356	C 2125	N 570	O 639	S 22	0	0
44	WK	439	Total 3408	C 2155	N 579	O 652	S 22	0	0
44	WM	431	Total 3356	C 2125	N 570	O 639	S 22	0	0

- Molecule 45 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AB	425	Total	C	N	O	S	0	1
			3291	2066	563	634	28		
45	AD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	AF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	AH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	AJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	AL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	AN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	BB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	BD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	BF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	BH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	BJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	BL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	BN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	CB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	CD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	CF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	CH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	CJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	CL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	CN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
45	PB	430	Total	C	N	O	S	0	0
			3351	2106	571	646	28		
45	PD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	PF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	PH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	PJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	PL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	PN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	QB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	QD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	QF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	QH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	QJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	QL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	QN	420	Total	C	N	O	S	0	3
			3244	2045	551	620	28		
45	RB	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	RD	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	RF	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	RH	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	RJ	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	RL	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		
45	RN	430	Total	C	N	O	S	0	0
			3366	2115	577	646	28		

Continued on next page...

Continued from previous page...

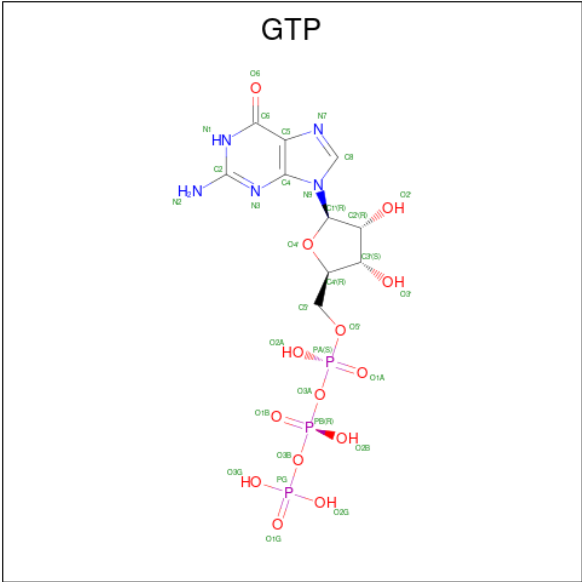
Mol	Chain	Residues	Atoms					AltConf	Trace
45	SB	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
45	SD	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
45	SF	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
45	SH	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
45	SJ	430	Total 3366	C 2115	N 577	O 646	S 28	0	0
45	SL	430	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 46 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 47 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
47	AB	1	Total 1	Mg 1	0
47	AC	1	Total 1	Mg 1	0
47	AE	1	Total 1	Mg 1	0
47	AG	1	Total 1	Mg 1	0
47	AI	1	Total 1	Mg 1	0
47	AL	1	Total 1	Mg 1	0
47	AM	1	Total 1	Mg 1	0
47	BA	1	Total 1	Mg 1	0
47	BD	1	Total 1	Mg 1	0
47	BF	1	Total 1	Mg 1	0
47	BH	1	Total 1	Mg 1	0
47	BJ	1	Total 1	Mg 1	0
47	BL	1	Total 1	Mg 1	0
47	BM	1	Total 1	Mg 1	0
47	CA	1	Total 1	Mg 1	0
47	CC	1	Total 1	Mg 1	0
47	CE	1	Total 1	Mg 1	0
47	CF	1	Total 1	Mg 1	0
47	CH	1	Total 1	Mg 1	0
47	CJ	1	Total 1	Mg 1	0
47	CM	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
47	DA	1	Total 1	Mg 1	0
47	DB	1	Total 1	Mg 1	0
47	DE	1	Total 1	Mg 1	0
47	DG	1	Total 1	Mg 1	0
47	DI	1	Total 1	Mg 1	0
47	DK	1	Total 1	Mg 1	0
47	DM	1	Total 1	Mg 1	0
47	EA	1	Total 1	Mg 1	0
47	EB	1	Total 1	Mg 1	0
47	EE	1	Total 1	Mg 1	0
47	EG	1	Total 1	Mg 1	0
47	EI	1	Total 1	Mg 1	0
47	EJ	1	Total 1	Mg 1	0
47	EL	1	Total 1	Mg 1	0
47	FA	1	Total 1	Mg 1	0
47	FD	1	Total 1	Mg 1	0
47	FF	1	Total 1	Mg 1	0
47	FG	1	Total 1	Mg 1	0
47	FI	1	Total 1	Mg 1	0
47	FK	1	Total 1	Mg 1	0
47	FM	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
47	GA	1	Total 1	Mg 1	0
47	GD	1	Total 1	Mg 1	0
47	GE	1	Total 1	Mg 1	0
47	GH	1	Total 1	Mg 1	0
47	GJ	1	Total 1	Mg 1	0
47	GK	1	Total 1	Mg 1	0
47	GM	1	Total 1	Mg 1	0
47	HA	1	Total 1	Mg 1	0
47	HC	1	Total 1	Mg 1	0
47	HF	1	Total 1	Mg 1	0
47	HG	1	Total 1	Mg 1	0
47	HI	1	Total 1	Mg 1	0
47	HL	1	Total 1	Mg 1	0
47	HM	1	Total 1	Mg 1	0
47	IA	1	Total 1	Mg 1	0
47	IC	1	Total 1	Mg 1	0
47	IE	1	Total 1	Mg 1	0
47	IH	1	Total 1	Mg 1	0
47	IJ	1	Total 1	Mg 1	0
47	IK	1	Total 1	Mg 1	0
47	IM	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
47	MA	1	Total 1	Mg 1	0
47	MC	1	Total 1	Mg 1	0
47	MF	1	Total 1	Mg 1	0
47	MG	1	Total 1	Mg 1	0
47	MJ	1	Total 1	Mg 1	0
47	MK	1	Total 1	Mg 1	0
47	MN	1	Total 1	Mg 1	0
47	NA	1	Total 1	Mg 1	0
47	NC	1	Total 1	Mg 1	0
47	NE	1	Total 1	Mg 1	0
47	NG	1	Total 1	Mg 1	0
47	NI	1	Total 1	Mg 1	0
47	NK	1	Total 1	Mg 1	0
47	NM	1	Total 1	Mg 1	0
47	OA	1	Total 1	Mg 1	0
47	OD	1	Total 1	Mg 1	0
47	OE	1	Total 1	Mg 1	0
47	OG	1	Total 1	Mg 1	0
47	OI	1	Total 1	Mg 1	0
47	OK	1	Total 1	Mg 1	0
47	OM	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
47	PA	1	Total 1	Mg 1	0
47	PD	1	Total 1	Mg 1	0
47	PE	1	Total 1	Mg 1	0
47	PG	1	Total 1	Mg 1	0
47	PI	1	Total 1	Mg 1	0
47	PK	1	Total 1	Mg 1	0
47	PM	1	Total 1	Mg 1	0
47	QA	1	Total 1	Mg 1	0
47	QC	1	Total 1	Mg 1	0
47	QD	1	Total 1	Mg 1	0
47	QG	1	Total 1	Mg 1	0
47	QI	1	Total 1	Mg 1	0
47	QJ	1	Total 1	Mg 1	0
47	QM	1	Total 1	Mg 1	0
47	RA	1	Total 1	Mg 1	0
47	RC	1	Total 1	Mg 1	0
47	RE	1	Total 1	Mg 1	0
47	RG	1	Total 1	Mg 1	0
47	RH	1	Total 1	Mg 1	0
47	RK	1	Total 1	Mg 1	0
47	RM	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

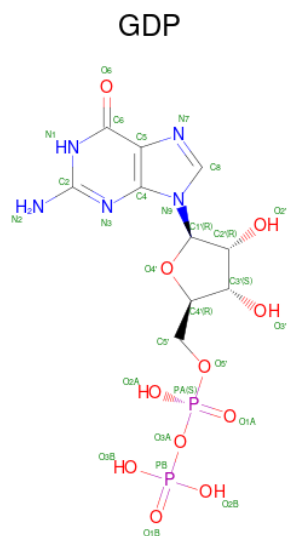
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
47	SA	1	1	1	0
47	SC	1	1	1	0
47	SE	1	1	1	0
47	SG	1	1	1	0
47	SI	1	1	1	0
47	SK	1	1	1	0
47	SM	1	1	1	0
47	TA	1	1	1	0
47	TC	1	1	1	0
47	TE	1	1	1	0
47	TG	1	1	1	0
47	TI	1	1	1	0
47	TK	1	1	1	0
47	TM	1	1	1	0
47	UA	1	1	1	0
47	UC	1	1	1	0
47	UE	1	1	1	0
47	UG	1	1	1	0
47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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
47	VB	1	Total 1	Mg 1	0
47	VC	1	Total 1	Mg 1	0
47	VE	1	Total 1	Mg 1	0
47	VG	1	Total 1	Mg 1	0
47	VI	1	Total 1	Mg 1	0
47	VK	1	Total 1	Mg 1	0
47	VM	1	Total 1	Mg 1	0
47	WA	1	Total 1	Mg 1	0
47	WC	1	Total 1	Mg 1	0
47	WE	1	Total 1	Mg 1	0
47	WG	1	Total 1	Mg 1	0
47	WJ	1	Total 1	Mg 1	0
47	WK	1	Total 1	Mg 1	0
47	WM	1	Total 1	Mg 1	0

- Molecule 48 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
48	AB	1	Total 28	C 10	N 5	O 11	P 2	0
48	AD	1	Total 28	C 10	N 5	O 11	P 2	0
48	AF	1	Total 28	C 10	N 5	O 11	P 2	0
48	AH	1	Total 28	C 10	N 5	O 11	P 2	0
48	AJ	1	Total 28	C 10	N 5	O 11	P 2	0
48	AL	1	Total 28	C 10	N 5	O 11	P 2	0
48	AN	1	Total 28	C 10	N 5	O 11	P 2	0
48	BB	1	Total 28	C 10	N 5	O 11	P 2	0
48	BD	1	Total 28	C 10	N 5	O 11	P 2	0
48	BF	1	Total 28	C 10	N 5	O 11	P 2	0
48	BH	1	Total 28	C 10	N 5	O 11	P 2	0
48	BJ	1	Total 28	C 10	N 5	O 11	P 2	0
48	BL	1	Total 28	C 10	N 5	O 11	P 2	0
48	BN	1	Total 28	C 10	N 5	O 11	P 2	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
48	UB	1	Total 28	C 10	N 5	O 11	P 2	0
48	UD	1	Total 28	C 10	N 5	O 11	P 2	0
48	UF	1	Total 28	C 10	N 5	O 11	P 2	0
48	UH	1	Total 28	C 10	N 5	O 11	P 2	0
48	UJ	1	Total 28	C 10	N 5	O 11	P 2	0
48	UL	1	Total 28	C 10	N 5	O 11	P 2	0
48	UN	1	Total 28	C 10	N 5	O 11	P 2	0
48	VB	1	Total 28	C 10	N 5	O 11	P 2	0
48	VD	1	Total 28	C 10	N 5	O 11	P 2	0
48	VF	1	Total 28	C 10	N 5	O 11	P 2	0
48	VH	1	Total 28	C 10	N 5	O 11	P 2	0
48	VJ	1	Total 28	C 10	N 5	O 11	P 2	0
48	VL	1	Total 28	C 10	N 5	O 11	P 2	0
48	VN	1	Total 28	C 10	N 5	O 11	P 2	0
48	WB	1	Total 28	C 10	N 5	O 11	P 2	0
48	WD	1	Total 28	C 10	N 5	O 11	P 2	0
48	WF	1	Total 28	C 10	N 5	O 11	P 2	0
48	WH	1	Total 28	C 10	N 5	O 11	P 2	0
48	WJ	1	Total 28	C 10	N 5	O 11	P 2	0
48	WL	1	Total 28	C 10	N 5	O 11	P 2	0
48	WN	1	Total 28	C 10	N 5	O 11	P 2	0

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

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39417	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	2.579	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.15	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
46	GTP	LM	501	47	33,34,34	0.93	2 (6%)	50,54,54	1.56	9 (18%)
46	GTP	WK	501	47	33,34,34	0.97	0	50,54,54	1.57	8 (16%)
46	GTP	BA	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.60	9 (18%)
48	GDP	FF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
46	GTP	GD	501	47	33,34,34	0.92	2 (6%)	50,54,54	1.58	10 (20%)
46	GTP	PA	501	47	33,34,34	0.87	1 (3%)	50,54,54	1.57	9 (18%)
48	GDP	LF	501	-	29,30,30	1.12	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	GH	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	6 (13%)
48	GDP	CJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	RJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	OF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
48	GDP	VJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	7 (15%)
46	GTP	GL	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	LE	501	47	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
46	GTP	EG	501	47	33,34,34	0.84	1 (3%)	50,54,54	1.56	9 (18%)
48	GDP	EL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	IF	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.74	6 (13%)
46	GTP	RK	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
48	GDP	HN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
46	GTP	FK	501	47	33,34,34	0.90	2 (6%)	50,54,54	1.58	9 (18%)
46	GTP	NK	501	47	33,34,34	0.94	1 (3%)	50,54,54	1.56	8 (16%)
46	GTP	MG	501	47	33,34,34	0.92	2 (6%)	50,54,54	1.57	9 (18%)
48	GDP	IB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
48	GDP	UN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
46	GTP	SI	501	47	33,34,34	0.95	1 (3%)	50,54,54	1.56	8 (16%)
46	GTP	JM	501	47	33,34,34	0.86	1 (3%)	50,54,54	1.56	9 (18%)
46	GTP	PK	501	47	33,34,34	0.96	3 (9%)	50,54,54	1.60	9 (18%)
48	GDP	VF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	7 (15%)
48	GDP	WH	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	GN	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.77	7 (15%)
46	GTP	QI	501	47	33,34,34	0.89	2 (6%)	50,54,54	1.58	9 (18%)
48	GDP	SL	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.75	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	GDP	EH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
48	GDP	PD	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	7 (15%)
48	GDP	HL	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	EN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
46	GTP	BI	501	47	33,34,34	0.98	1 (3%)	50,54,54	1.59	9 (18%)
48	GDP	WJ	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.81	7 (15%)
48	GDP	KB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
46	GTP	TI	501	47	33,34,34	0.95	2 (6%)	50,54,54	1.57	9 (18%)
48	GDP	PN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	FG	501	47	33,34,34	0.92	1 (3%)	50,54,54	1.60	9 (18%)
48	GDP	NF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	WL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	SN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
48	GDP	SB	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.72	7 (15%)
48	GDP	DF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
48	GDP	AL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	DJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	SH	501	-	29,30,30	1.13	4 (13%)	45,47,47	1.68	6 (13%)
46	GTP	EI	501	47	33,34,34	0.90	1 (3%)	50,54,54	1.57	9 (18%)
48	GDP	AJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	KF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
46	GTP	RC	501	47	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
46	GTP	BG	501	47	33,34,34	0.90	2 (6%)	50,54,54	1.62	9 (18%)
48	GDP	FD	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	DL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	TD	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.76	7 (15%)
48	GDP	EF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	7 (15%)
48	GDP	ID	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	LH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
46	GTP	DE	501	47	33,34,34	0.97	0	50,54,54	1.57	9 (18%)
46	GTP	OA	501	47	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
48	GDP	FJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	BH	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
46	GTP	DB	502	47	33,34,34	0.94	1 (3%)	50,54,54	1.55	8 (16%)
46	GTP	TC	501	47	33,34,34	1.01	3 (9%)	50,54,54	1.56	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	GTP	CE	501	47	33,34,34	0.99	3 (9%)	50,54,54	1.60	9 (18%)
48	GDP	ED	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	VD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	FL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	NJ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	PH	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.79	7 (15%)
46	GTP	WA	501	47	33,34,34	0.94	1 (3%)	50,54,54	1.61	9 (18%)
46	GTP	VK	501	47	33,34,34	0.94	2 (6%)	50,54,54	1.56	9 (18%)
48	GDP	WB	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.78	7 (15%)
48	GDP	GF	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	VL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
46	GTP	PI	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.56	8 (16%)
46	GTP	FM	501	47	33,34,34	0.97	1 (3%)	50,54,54	1.56	9 (18%)
46	GTP	BK	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.60	8 (16%)
46	GTP	EE	501	47	33,34,34	0.87	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	VG	501	47	33,34,34	1.00	4 (12%)	50,54,54	1.61	9 (18%)
48	GDP	MF	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	KK	501	47	33,34,34	0.89	2 (6%)	50,54,54	1.60	9 (18%)
48	GDP	HB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	7 (15%)
48	GDP	OJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
48	GDP	RF	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	6 (13%)
46	GTP	DA	501	47	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)
48	GDP	JL	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	RL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	WN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
46	GTP	AG	501	47	33,34,34	0.90	1 (3%)	50,54,54	1.57	8 (16%)
46	GTP	KC	501	47	33,34,34	0.86	0	50,54,54	1.57	9 (18%)
48	GDP	GD	503	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
48	GDP	GJ	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
48	GDP	KL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	LJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
46	GTP	VI	501	47	33,34,34	0.94	2 (6%)	50,54,54	1.60	8 (16%)
48	GDP	KN	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.71	7 (15%)
46	GTP	SA	501	47	33,34,34	1.04	4 (12%)	50,54,54	1.54	8 (16%)
48	GDP	TF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	GTP	MK	501	47	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
48	GDP	ML	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
46	GTP	DI	501	47	33,34,34	0.87	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	AC	501	47	33,34,34	0.92	2 (6%)	50,54,54	1.62	9 (18%)
46	GTP	VC	501	47	33,34,34	0.96	0	50,54,54	1.60	9 (18%)
46	GTP	HM	501	47	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
48	GDP	DB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
48	GDP	AD	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	HJ	501	-	29,30,30	1.24	4 (13%)	45,47,47	1.77	7 (15%)
48	GDP	NB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
46	GTP	HG	501	47	33,34,34	0.93	1 (3%)	50,54,54	1.58	9 (18%)
48	GDP	BL	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
46	GTP	IK	501	47	33,34,34	0.92	2 (6%)	50,54,54	1.56	9 (18%)
46	GTP	JG	501	47	33,34,34	0.91	0	50,54,54	1.56	10 (20%)
46	GTP	AM	501	47	33,34,34	0.88	1 (3%)	50,54,54	1.59	9 (18%)
46	GTP	FI	501	47	33,34,34	0.90	0	50,54,54	1.55	9 (18%)
46	GTP	NA	501	47	33,34,34	0.98	0	50,54,54	1.55	9 (18%)
48	GDP	EJ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	7 (15%)
48	GDP	QD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	EM	501	47	33,34,34	0.92	1 (3%)	50,54,54	1.57	9 (18%)
48	GDP	QF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	NL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
46	GTP	UG	501	47	33,34,34	0.96	2 (6%)	50,54,54	1.62	9 (18%)
46	GTP	VE	501	47	33,34,34	0.96	2 (6%)	50,54,54	1.60	8 (16%)
48	GDP	NH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	UJ	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.80	7 (15%)
46	GTP	RA	501	47	33,34,34	0.95	1 (3%)	50,54,54	1.56	9 (18%)
46	GTP	QK	501	47	33,34,34	0.87	1 (3%)	50,54,54	1.58	9 (18%)
48	GDP	JB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
46	GTP	OG	501	47	33,34,34	0.89	0	50,54,54	1.62	8 (16%)
48	GDP	DN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
48	GDP	ND	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
46	GTP	RI	501	47	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)
46	GTP	II	501	47	33,34,34	0.88	0	50,54,54	1.59	9 (18%)
46	GTP	GG	501	47	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	GTP	CC	501	47	33,34,34	0.99	1 (3%)	50,54,54	1.59	9 (18%)
46	GTP	NM	501	47	33,34,34	0.98	1 (3%)	50,54,54	1.57	9 (18%)
46	GTP	SC	501	47	33,34,34	0.92	0	50,54,54	1.56	8 (16%)
48	GDP	NN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
48	GDP	DH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	VH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
48	GDP	CL	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
48	GDP	PL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
46	GTP	GB	501	47	33,34,34	0.96	1 (3%)	50,54,54	1.53	9 (18%)
48	GDP	LL	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	OL	501	47	33,34,34	0.93	1 (3%)	50,54,54	1.64	10 (20%)
46	GTP	WM	501	47	33,34,34	0.99	2 (6%)	50,54,54	1.60	9 (18%)
48	GDP	KJ	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	QM	501	47	33,34,34	1.00	3 (9%)	50,54,54	1.59	9 (18%)
48	GDP	IL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	SF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
46	GTP	MA	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
46	GTP	QC	501	-	33,34,34	0.98	3 (9%)	50,54,54	1.58	9 (18%)
48	GDP	RB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	UB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
46	GTP	PG	501	47	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
46	GTP	JE	501	47	33,34,34	0.89	2 (6%)	50,54,54	1.61	9 (18%)
48	GDP	WF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	8 (17%)
46	GTP	DG	501	47	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	KE	501	47	33,34,34	0.89	0	50,54,54	1.59	9 (18%)
46	GTP	NE	501	47	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
46	GTP	FE	501	47	33,34,34	0.95	0	50,54,54	1.56	9 (18%)
48	GDP	OD	502	-	29,30,30	1.19	4 (13%)	45,47,47	1.76	7 (15%)
48	GDP	CF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
46	GTP	UA	501	47	33,34,34	0.97	1 (3%)	50,54,54	1.56	9 (18%)
46	GTP	OM	501	47	33,34,34	0.93	1 (3%)	50,54,54	1.61	9 (18%)
48	GDP	RN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
46	GTP	SE	501	47	33,34,34	0.88	2 (6%)	50,54,54	1.58	9 (18%)
48	GDP	UF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
46	GTP	PM	501	47	33,34,34	0.95	1 (3%)	50,54,54	1.59	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	GTP	EK	501	47	33,34,34	0.86	1 (3%)	50,54,54	1.57	9 (18%)
46	GTP	TA	501	47	33,34,34	0.97	1 (3%)	50,54,54	1.53	9 (18%)
48	GDP	MN	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
46	GTP	HK	501	47	33,34,34	0.88	2 (6%)	50,54,54	1.58	9 (18%)
46	GTP	AK	501	47	33,34,34	0.94	2 (6%)	50,54,54	1.59	8 (16%)
48	GDP	UD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
46	GTP	MI	501	47	33,34,34	0.88	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	FC	501	47	33,34,34	0.90	2 (6%)	50,54,54	1.60	9 (18%)
48	GDP	UH	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.73	6 (13%)
46	GTP	RG	501	47	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
48	GDP	ON	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.78	7 (15%)
48	GDP	GL	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	HF	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
46	GTP	JA	501	47	33,34,34	0.85	1 (3%)	50,54,54	1.64	10 (20%)
46	GTP	PC	501	47	33,34,34	0.90	1 (3%)	50,54,54	1.56	9 (18%)
48	GDP	CN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
48	GDP	BJ	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
48	GDP	OB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
48	GDP	FB	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
46	GTP	SM	501	47	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
46	GTP	AA	501	47	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
46	GTP	BC	501	47	33,34,34	0.90	2 (6%)	50,54,54	1.63	9 (18%)
48	GDP	TB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
46	GTP	BM	501	47	33,34,34	0.95	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	HC	501	47	33,34,34	0.90	2 (6%)	50,54,54	1.62	9 (18%)
48	GDP	QN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	AN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	PB	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
46	GTP	EA	501	47	33,34,34	0.99	3 (9%)	50,54,54	1.58	9 (18%)
48	GDP	AF	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	HI	501	47	33,34,34	0.95	2 (6%)	50,54,54	1.46	7 (14%)
46	GTP	ID	501	47	33,34,34	0.94	1 (3%)	50,54,54	1.58	8 (16%)
46	GTP	LK	501	-	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
48	GDP	GB	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
46	GTP	GM	501	47	33,34,34	1.00	1 (3%)	50,54,54	1.60	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	GDP	RD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	AB	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	MM	501	47	33,34,34	0.92	2 (6%)	50,54,54	1.59	9 (18%)
48	GDP	VB	502	-	29,30,30	1.21	3 (10%)	45,47,47	1.83	7 (15%)
46	GTP	TE	501	47	33,34,34	0.96	2 (6%)	50,54,54	1.70	10 (20%)
48	GDP	TJ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
46	GTP	AE	501	47	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
46	GTP	MC	501	47	33,34,34	0.89	0	50,54,54	1.60	9 (18%)
46	GTP	CM	501	47	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	LB	501	47	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
46	GTP	JI	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.60	9 (18%)
46	GTP	OC	501	47	33,34,34	0.95	1 (3%)	50,54,54	1.62	8 (16%)
46	GTP	UK	501	47	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	QA	501	47	33,34,34	0.99	3 (9%)	50,54,54	1.60	9 (18%)
48	GDP	JH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
46	GTP	AI	501	47	33,34,34	0.88	2 (6%)	50,54,54	1.59	9 (18%)
46	GTP	CK	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.57	9 (18%)
46	GTP	KM	501	47	33,34,34	0.92	2 (6%)	50,54,54	1.58	9 (18%)
46	GTP	NI	501	47	33,34,34	0.94	0	50,54,54	1.56	8 (16%)
46	GTP	SG	501	47	33,34,34	0.89	0	50,54,54	1.58	10 (20%)
48	GDP	EB	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	7 (15%)
46	GTP	QG	501	47	33,34,34	1.01	4 (12%)	50,54,54	1.60	8 (16%)
48	GDP	BF	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
48	GDP	QL	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.73	6 (13%)
48	GDP	OL	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
46	GTP	IA	501	47	33,34,34	0.92	0	50,54,54	1.60	9 (18%)
46	GTP	OE	501	47	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	CA	501	47	33,34,34	0.94	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	DM	501	47	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
48	GDP	JN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
46	GTP	FA	501	47	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
48	GDP	KH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	QH	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	UI	501	47	33,34,34	0.98	3 (9%)	50,54,54	1.52	9 (18%)
46	GTP	DK	501	47	33,34,34	0.90	1 (3%)	50,54,54	1.56	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	GDP	DD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
46	GTP	RM	501	47	33,34,34	0.96	3 (9%)	50,54,54	1.64	9 (18%)
46	GTP	BE	501	47	33,34,34	0.90	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	IG	501	47	33,34,34	0.87	0	50,54,54	1.57	9 (18%)
46	GTP	CI	501	47	33,34,34	0.93	2 (6%)	50,54,54	1.58	9 (18%)
46	GTP	IE	501	47	33,34,34	0.92	1 (3%)	50,54,54	1.59	8 (16%)
48	GDP	JJ	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.72	6 (13%)
46	GTP	TG	501	47	33,34,34	0.97	2 (6%)	50,54,54	1.58	8 (16%)
48	GDP	OH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	QB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
48	GDP	MB	501	-	29,30,30	1.18	4 (13%)	45,47,47	1.78	7 (15%)
46	GTP	CG	501	47	33,34,34	0.92	2 (6%)	50,54,54	1.57	9 (18%)
48	GDP	TH	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.78	7 (15%)
48	GDP	VN	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.79	8 (17%)
46	GTP	IM	501	-	33,34,34	0.98	2 (6%)	50,54,54	1.58	9 (18%)
48	GDP	WD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
48	GDP	BB	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	TN	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.78	7 (15%)
48	GDP	CB	501	-	29,30,30	1.27	4 (13%)	45,47,47	2.20	12 (26%)
48	GDP	HH	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.73	7 (15%)
46	GTP	HA	501	-	33,34,34	1.01	2 (6%)	50,54,54	1.58	9 (18%)
46	GTP	UC	501	47	33,34,34	0.96	1 (3%)	50,54,54	1.59	8 (16%)
48	GDP	RH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
46	GTP	KJ	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.56	9 (18%)
46	GTP	LI	501	47	33,34,34	0.88	1 (3%)	50,54,54	1.54	9 (18%)
48	GDP	SJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	7 (15%)
48	GDP	AH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	7 (15%)
46	GTP	OI	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
48	GDP	MJ	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
46	GTP	WE	501	47	33,34,34	0.93	1 (3%)	50,54,54	1.61	10 (20%)
48	GDP	IJ	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	SK	501	47	33,34,34	0.90	1 (3%)	50,54,54	1.55	9 (18%)
46	GTP	NC	501	47	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
46	GTP	TM	501	47	33,34,34	0.90	1 (3%)	50,54,54	1.61	10 (20%)
46	GTP	LG	501	47	33,34,34	0.92	2 (6%)	50,54,54	1.57	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	GTP	GE	501	47	33,34,34	0.91	1 (3%)	50,54,54	1.58	9 (18%)
46	GTP	PE	501	47	33,34,34	0.96	3 (9%)	50,54,54	1.59	9 (18%)
48	GDP	CD	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
46	GTP	RE	501	47	33,34,34	0.92	2 (6%)	50,54,54	1.58	9 (18%)
46	GTP	TK	501	47	33,34,34	0.91	0	50,54,54	1.55	9 (18%)
48	GDP	LN	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
46	GTP	JC	501	-	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
46	GTP	KA	501	47	33,34,34	0.91	1 (3%)	50,54,54	1.57	9 (18%)
48	GDP	FN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
46	GTP	WG	501	47	33,34,34	1.02	3 (9%)	50,54,54	1.63	8 (16%)
46	GTP	VA	501	47	33,34,34	1.00	3 (9%)	50,54,54	1.63	9 (18%)
46	GTP	QE	501	47	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)
46	GTP	EC	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.57	9 (18%)
48	GDP	TL	501	-	29,30,30	1.17	2 (6%)	45,47,47	1.82	7 (15%)
48	GDP	UL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	7 (15%)
48	GDP	JD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
48	GDP	JF	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	HD	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.81	6 (13%)
46	GTP	JK	501	47	33,34,34	0.97	2 (6%)	50,54,54	1.58	9 (18%)
48	GDP	LB	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
48	GDP	MD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	PJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
46	GTP	VM	501	47	33,34,34	0.98	2 (6%)	50,54,54	1.58	9 (18%)
46	GTP	LC	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
48	GDP	QJ	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	6 (13%)
48	GDP	BD	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	LD	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	KG	501	47	33,34,34	0.91	2 (6%)	50,54,54	1.58	8 (16%)
48	GDP	KD	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	PF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
48	GDP	MH	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
48	GDP	CH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
48	GDP	IH	502	-	29,30,30	1.13	3 (10%)	45,47,47	1.73	7 (15%)
48	GDP	IN	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
46	GTP	NG	501	47	33,34,34	0.91	0	50,54,54	1.59	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	GDP	SD	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.72	7 (15%)
46	GTP	WC	501	47	33,34,34	0.96	2 (6%)	50,54,54	1.61	9 (18%)
48	GDP	FH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
46	GTP	UE	501	47	33,34,34	0.99	2 (6%)	50,54,54	1.57	9 (18%)
46	GTP	UM	501	47	33,34,34	0.89	2 (6%)	50,54,54	1.62	9 (18%)
46	GTP	GI	501	47	33,34,34	0.90	2 (6%)	50,54,54	1.59	10 (20%)
46	GTP	ME	501	47	33,34,34	0.89	1 (3%)	50,54,54	1.61	9 (18%)
46	GTP	HE	501	47	33,34,34	0.92	1 (3%)	50,54,54	1.62	8 (16%)
48	GDP	BN	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.77	7 (15%)
46	GTP	WI	501	47	33,34,34	0.93	1 (3%)	50,54,54	1.60	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	GTP	LM	501	47	-	6/22/38/38	0/3/3/3
46	GTP	WK	501	47	-	5/22/38/38	0/3/3/3
46	GTP	BA	501	-	-	6/22/38/38	0/3/3/3
48	GDP	FF	502	-	-	2/16/32/32	0/3/3/3
46	GTP	GD	501	47	-	3/22/38/38	0/3/3/3
46	GTP	PA	501	47	-	4/22/38/38	0/3/3/3
48	GDP	LF	501	-	-	3/16/32/32	0/3/3/3
48	GDP	GH	502	-	-	2/16/32/32	0/3/3/3
48	GDP	CJ	501	-	-	2/16/32/32	0/3/3/3
48	GDP	RJ	501	-	-	1/16/32/32	0/3/3/3
48	GDP	OF	501	-	-	1/16/32/32	0/3/3/3
48	GDP	VJ	501	-	-	1/16/32/32	0/3/3/3
46	GTP	GL	501	47	-	5/22/38/38	0/3/3/3
46	GTP	LE	501	47	-	7/22/38/38	0/3/3/3
46	GTP	EG	501	47	-	8/22/38/38	0/3/3/3
48	GDP	EL	501	-	-	0/16/32/32	0/3/3/3
48	GDP	IF	501	-	-	1/16/32/32	0/3/3/3
46	GTP	RK	501	47	-	7/22/38/38	0/3/3/3
48	GDP	HN	501	-	-	1/16/32/32	0/3/3/3
46	GTP	FK	501	47	-	5/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	GTP	NK	501	47	-	5/22/38/38	0/3/3/3
46	GTP	MG	501	47	-	5/22/38/38	0/3/3/3
48	GDP	IB	501	-	-	0/16/32/32	0/3/3/3
48	GDP	UN	501	-	-	0/16/32/32	0/3/3/3
46	GTP	SI	501	47	-	7/22/38/38	0/3/3/3
46	GTP	JM	501	47	-	2/22/38/38	0/3/3/3
46	GTP	PK	501	47	-	4/22/38/38	0/3/3/3
48	GDP	VF	501	-	-	2/16/32/32	0/3/3/3
48	GDP	WH	501	-	-	0/16/32/32	0/3/3/3
48	GDP	GN	501	-	-	0/16/32/32	0/3/3/3
46	GTP	QI	501	47	-	6/22/38/38	0/3/3/3
48	GDP	SL	501	-	-	1/16/32/32	0/3/3/3
48	GDP	EH	501	-	-	2/16/32/32	0/3/3/3
48	GDP	PD	502	-	-	1/16/32/32	0/3/3/3
48	GDP	HL	502	-	-	1/16/32/32	0/3/3/3
48	GDP	EN	501	-	-	4/16/32/32	0/3/3/3
46	GTP	BI	501	47	-	4/22/38/38	0/3/3/3
48	GDP	WJ	502	-	-	0/16/32/32	0/3/3/3
48	GDP	KB	501	-	-	0/16/32/32	0/3/3/3
46	GTP	TI	501	47	-	6/22/38/38	0/3/3/3
48	GDP	PN	501	-	-	0/16/32/32	0/3/3/3
46	GTP	FG	501	47	-	8/22/38/38	0/3/3/3
48	GDP	NF	501	-	-	1/16/32/32	0/3/3/3
48	GDP	WL	501	-	-	0/16/32/32	0/3/3/3
48	GDP	SN	501	-	-	1/16/32/32	0/3/3/3
48	GDP	SB	501	-	-	1/16/32/32	0/3/3/3
48	GDP	DF	501	-	-	3/16/32/32	0/3/3/3
48	GDP	AL	502	-	-	0/16/32/32	0/3/3/3
48	GDP	DJ	501	-	-	1/16/32/32	0/3/3/3
48	GDP	SH	501	-	-	0/16/32/32	0/3/3/3
46	GTP	EI	501	47	-	7/22/38/38	0/3/3/3
48	GDP	AJ	501	-	-	0/16/32/32	0/3/3/3
48	GDP	KF	502	-	-	1/16/32/32	0/3/3/3
46	GTP	RC	501	47	-	4/22/38/38	0/3/3/3
46	GTP	BG	501	47	-	2/22/38/38	0/3/3/3
48	GDP	FD	502	-	-	0/16/32/32	0/3/3/3
48	GDP	DL	501	-	-	3/16/32/32	0/3/3/3
48	GDP	TD	501	-	-	0/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	GDP	EF	501	-	-	0/16/32/32	0/3/3/3
48	GDP	ID	502	-	-	1/16/32/32	0/3/3/3
48	GDP	LH	501	-	-	0/16/32/32	0/3/3/3
46	GTP	DE	501	47	-	7/22/38/38	0/3/3/3
46	GTP	OA	501	47	-	4/22/38/38	0/3/3/3
48	GDP	FJ	501	-	-	0/16/32/32	0/3/3/3
48	GDP	BH	502	-	-	1/16/32/32	0/3/3/3
46	GTP	DB	502	47	-	5/22/38/38	0/3/3/3
46	GTP	TC	501	47	-	4/22/38/38	0/3/3/3
46	GTP	CE	501	47	-	4/22/38/38	0/3/3/3
48	GDP	ED	501	-	-	2/16/32/32	0/3/3/3
48	GDP	VD	501	-	-	0/16/32/32	0/3/3/3
48	GDP	FL	501	-	-	2/16/32/32	0/3/3/3
48	GDP	NJ	501	-	-	0/16/32/32	0/3/3/3
48	GDP	PH	501	-	-	0/16/32/32	0/3/3/3
46	GTP	WA	501	47	-	3/22/38/38	0/3/3/3
46	GTP	VK	501	47	-	7/22/38/38	0/3/3/3
48	GDP	WB	501	-	-	1/16/32/32	0/3/3/3
48	GDP	GF	501	-	-	1/16/32/32	0/3/3/3
48	GDP	VL	501	-	-	2/16/32/32	0/3/3/3
46	GTP	PI	501	47	-	7/22/38/38	0/3/3/3
46	GTP	FM	501	47	-	3/22/38/38	0/3/3/3
46	GTP	BK	501	47	-	5/22/38/38	0/3/3/3
46	GTP	EE	501	47	-	5/22/38/38	0/3/3/3
46	GTP	VG	501	47	-	4/22/38/38	0/3/3/3
48	GDP	MF	502	-	-	3/16/32/32	0/3/3/3
46	GTP	KK	501	47	-	3/22/38/38	0/3/3/3
48	GDP	HB	501	-	-	1/16/32/32	0/3/3/3
48	GDP	OJ	501	-	-	2/16/32/32	0/3/3/3
48	GDP	RF	501	-	-	3/16/32/32	0/3/3/3
46	GTP	DA	501	47	-	5/22/38/38	0/3/3/3
48	GDP	JL	501	-	-	2/16/32/32	0/3/3/3
48	GDP	RL	501	-	-	1/16/32/32	0/3/3/3
48	GDP	WN	501	-	-	1/16/32/32	0/3/3/3
46	GTP	AG	501	47	-	4/22/38/38	0/3/3/3
46	GTP	KC	501	47	-	4/22/38/38	0/3/3/3
48	GDP	GD	503	-	-	1/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	GDP	GJ	502	-	-	3/16/32/32	0/3/3/3
48	GDP	KL	501	-	-	1/16/32/32	0/3/3/3
48	GDP	LJ	501	-	-	2/16/32/32	0/3/3/3
46	GTP	VI	501	47	-	9/22/38/38	0/3/3/3
48	GDP	KN	501	-	-	1/16/32/32	0/3/3/3
46	GTP	SA	501	47	-	8/22/38/38	0/3/3/3
48	GDP	TF	501	-	-	2/16/32/32	0/3/3/3
46	GTP	MK	501	47	-	3/22/38/38	0/3/3/3
48	GDP	ML	501	-	-	2/16/32/32	0/3/3/3
46	GTP	DI	501	47	-	7/22/38/38	0/3/3/3
46	GTP	AC	501	47	-	1/22/38/38	0/3/3/3
46	GTP	VC	501	47	-	4/22/38/38	0/3/3/3
46	GTP	HM	501	47	-	4/22/38/38	0/3/3/3
48	GDP	DB	501	-	-	1/16/32/32	0/3/3/3
48	GDP	AD	501	-	-	0/16/32/32	0/3/3/3
48	GDP	HJ	501	-	-	1/16/32/32	0/3/3/3
48	GDP	NB	501	-	-	2/16/32/32	0/3/3/3
46	GTP	HG	501	47	-	7/22/38/38	0/3/3/3
48	GDP	BL	502	-	-	3/16/32/32	0/3/3/3
46	GTP	IK	501	47	-	8/22/38/38	0/3/3/3
46	GTP	JG	501	47	-	8/22/38/38	0/3/3/3
46	GTP	AM	501	47	-	7/22/38/38	0/3/3/3
46	GTP	FI	501	47	-	4/22/38/38	0/3/3/3
46	GTP	NA	501	47	-	9/22/38/38	0/3/3/3
48	GDP	EJ	501	-	-	2/16/32/32	0/3/3/3
48	GDP	QD	501	-	-	1/16/32/32	0/3/3/3
46	GTP	EM	501	47	-	6/22/38/38	0/3/3/3
48	GDP	QF	501	-	-	0/16/32/32	0/3/3/3
48	GDP	NL	501	-	-	3/16/32/32	0/3/3/3
46	GTP	UG	501	47	-	8/22/38/38	0/3/3/3
46	GTP	VE	501	47	-	6/22/38/38	0/3/3/3
48	GDP	NH	501	-	-	3/16/32/32	0/3/3/3
48	GDP	UJ	501	-	-	3/16/32/32	0/3/3/3
46	GTP	RA	501	47	-	4/22/38/38	0/3/3/3
46	GTP	QK	501	47	-	6/22/38/38	0/3/3/3
48	GDP	JB	501	-	-	1/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	GTP	OG	501	47	-	2/22/38/38	0/3/3/3
48	GDP	DN	501	-	-	0/16/32/32	0/3/3/3
48	GDP	ND	501	-	-	0/16/32/32	0/3/3/3
46	GTP	RI	501	47	-	2/22/38/38	0/3/3/3
46	GTP	II	501	47	-	7/22/38/38	0/3/3/3
46	GTP	GG	501	47	-	1/22/38/38	0/3/3/3
46	GTP	CC	501	47	-	4/22/38/38	0/3/3/3
46	GTP	NM	501	47	-	3/22/38/38	0/3/3/3
46	GTP	SC	501	47	-	4/22/38/38	0/3/3/3
48	GDP	NN	501	-	-	3/16/32/32	0/3/3/3
48	GDP	DH	501	-	-	1/16/32/32	0/3/3/3
48	GDP	VH	501	-	-	1/16/32/32	0/3/3/3
48	GDP	CL	501	-	-	0/16/32/32	0/3/3/3
48	GDP	PL	501	-	-	2/16/32/32	0/3/3/3
46	GTP	GB	501	47	-	4/22/38/38	0/3/3/3
48	GDP	LL	501	-	-	0/16/32/32	0/3/3/3
46	GTP	OL	501	47	-	3/22/38/38	0/3/3/3
46	GTP	WM	501	47	-	4/22/38/38	0/3/3/3
48	GDP	KJ	502	-	-	0/16/32/32	0/3/3/3
46	GTP	QM	501	47	-	5/22/38/38	0/3/3/3
48	GDP	IL	501	-	-	1/16/32/32	0/3/3/3
48	GDP	SF	501	-	-	3/16/32/32	0/3/3/3
46	GTP	MA	501	47	-	6/22/38/38	0/3/3/3
46	GTP	QC	501	-	-	6/22/38/38	0/3/3/3
48	GDP	RB	501	-	-	0/16/32/32	0/3/3/3
48	GDP	UB	501	-	-	3/16/32/32	0/3/3/3
46	GTP	PG	501	47	-	6/22/38/38	0/3/3/3
46	GTP	JE	501	47	-	1/22/38/38	0/3/3/3
48	GDP	WF	501	-	-	0/16/32/32	0/3/3/3
46	GTP	DG	501	47	-	2/22/38/38	0/3/3/3
46	GTP	KE	501	47	-	2/22/38/38	0/3/3/3
46	GTP	NE	501	47	-	6/22/38/38	0/3/3/3
46	GTP	FE	501	47	-	4/22/38/38	0/3/3/3
48	GDP	OD	502	-	-	3/16/32/32	0/3/3/3
48	GDP	CF	501	-	-	1/16/32/32	0/3/3/3
46	GTP	UA	501	47	-	4/22/38/38	0/3/3/3
46	GTP	OM	501	47	-	3/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	GDP	RN	501	-	-	0/16/32/32	0/3/3/3
46	GTP	SE	501	47	-	6/22/38/38	0/3/3/3
48	GDP	UF	501	-	-	1/16/32/32	0/3/3/3
46	GTP	PM	501	47	-	7/22/38/38	0/3/3/3
46	GTP	EK	501	47	-	2/22/38/38	0/3/3/3
46	GTP	TA	501	47	-	8/22/38/38	0/3/3/3
48	GDP	MN	502	-	-	1/16/32/32	0/3/3/3
46	GTP	HK	501	47	-	1/22/38/38	0/3/3/3
46	GTP	AK	501	47	-	6/22/38/38	0/3/3/3
48	GDP	UD	501	-	-	0/16/32/32	0/3/3/3
46	GTP	MI	501	47	-	6/22/38/38	0/3/3/3
46	GTP	FC	501	47	-	5/22/38/38	0/3/3/3
48	GDP	UH	501	-	-	0/16/32/32	0/3/3/3
46	GTP	RG	501	47	-	6/22/38/38	0/3/3/3
48	GDP	ON	501	-	-	1/16/32/32	0/3/3/3
48	GDP	GL	502	-	-	4/16/32/32	0/3/3/3
48	GDP	HF	502	-	-	1/16/32/32	0/3/3/3
46	GTP	JA	501	47	-	1/22/38/38	0/3/3/3
46	GTP	PC	501	47	-	4/22/38/38	0/3/3/3
48	GDP	CN	501	-	-	1/16/32/32	0/3/3/3
48	GDP	BJ	502	-	-	1/16/32/32	0/3/3/3
48	GDP	OB	501	-	-	2/16/32/32	0/3/3/3
48	GDP	FB	501	-	-	1/16/32/32	0/3/3/3
46	GTP	SM	501	47	-	9/22/38/38	0/3/3/3
46	GTP	AA	501	47	-	7/22/38/38	0/3/3/3
46	GTP	BC	501	47	-	4/22/38/38	0/3/3/3
48	GDP	TB	501	-	-	0/16/32/32	0/3/3/3
46	GTP	BM	501	47	-	5/22/38/38	0/3/3/3
46	GTP	HC	501	47	-	6/22/38/38	0/3/3/3
48	GDP	QN	501	-	-	1/16/32/32	0/3/3/3
48	GDP	AN	501	-	-	2/16/32/32	0/3/3/3
48	GDP	PB	501	-	-	1/16/32/32	0/3/3/3
46	GTP	EA	501	47	-	4/22/38/38	0/3/3/3
48	GDP	AF	501	-	-	1/16/32/32	0/3/3/3
46	GTP	HI	501	47	-	9/22/38/38	0/3/3/3
46	GTP	ID	501	47	-	8/22/38/38	0/3/3/3
46	GTP	LK	501	-	-	6/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	GDP	GB	502	-	-	0/16/32/32	0/3/3/3
46	GTP	GM	501	47	-	7/22/38/38	0/3/3/3
48	GDP	RD	501	-	-	0/16/32/32	0/3/3/3
48	GDP	AB	502	-	-	1/16/32/32	0/3/3/3
46	GTP	MM	501	47	-	8/22/38/38	0/3/3/3
48	GDP	VB	502	-	-	1/16/32/32	0/3/3/3
46	GTP	TE	501	47	-	5/22/38/38	0/3/3/3
48	GDP	TJ	501	-	-	2/16/32/32	0/3/3/3
46	GTP	AE	501	47	-	7/22/38/38	0/3/3/3
46	GTP	MC	501	47	-	5/22/38/38	0/3/3/3
46	GTP	CM	501	47	-	6/22/38/38	0/3/3/3
46	GTP	LB	501	47	-	6/22/38/38	0/3/3/3
46	GTP	JI	501	47	-	8/22/38/38	0/3/3/3
46	GTP	OC	501	47	-	5/22/38/38	0/3/3/3
46	GTP	UK	501	47	-	6/22/38/38	0/3/3/3
46	GTP	QA	501	47	-	9/22/38/38	0/3/3/3
48	GDP	JH	501	-	-	2/16/32/32	0/3/3/3
46	GTP	AI	501	47	-	5/22/38/38	0/3/3/3
46	GTP	CK	501	47	-	6/22/38/38	0/3/3/3
46	GTP	KM	501	47	-	6/22/38/38	0/3/3/3
46	GTP	NI	501	47	-	4/22/38/38	0/3/3/3
46	GTP	SG	501	47	-	6/22/38/38	0/3/3/3
48	GDP	EB	501	-	-	0/16/32/32	0/3/3/3
46	GTP	QG	501	47	-	6/22/38/38	0/3/3/3
48	GDP	BF	502	-	-	1/16/32/32	0/3/3/3
48	GDP	QL	501	-	-	0/16/32/32	0/3/3/3
48	GDP	OL	502	-	-	1/16/32/32	0/3/3/3
46	GTP	IA	501	47	-	5/22/38/38	0/3/3/3
46	GTP	OE	501	47	-	3/22/38/38	0/3/3/3
46	GTP	CA	501	47	-	2/22/38/38	0/3/3/3
46	GTP	DM	501	47	-	4/22/38/38	0/3/3/3
48	GDP	JN	501	-	-	3/16/32/32	0/3/3/3
46	GTP	FA	501	47	-	1/22/38/38	0/3/3/3
48	GDP	KH	501	-	-	0/16/32/32	0/3/3/3
48	GDP	QH	501	-	-	1/16/32/32	0/3/3/3
46	GTP	UI	501	47	-	6/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	GTP	DK	501	47	-	2/22/38/38	0/3/3/3
48	GDP	DD	501	-	-	3/16/32/32	0/3/3/3
46	GTP	RM	501	47	-	5/22/38/38	0/3/3/3
46	GTP	BE	501	47	-	8/22/38/38	0/3/3/3
46	GTP	IG	501	47	-	5/22/38/38	0/3/3/3
46	GTP	CI	501	47	-	7/22/38/38	0/3/3/3
46	GTP	IE	501	47	-	8/22/38/38	0/3/3/3
48	GDP	JJ	501	-	-	0/16/32/32	0/3/3/3
46	GTP	TG	501	47	-	6/22/38/38	0/3/3/3
48	GDP	OH	501	-	-	1/16/32/32	0/3/3/3
48	GDP	QB	501	-	-	0/16/32/32	0/3/3/3
48	GDP	MB	501	-	-	6/16/32/32	0/3/3/3
46	GTP	CG	501	47	-	6/22/38/38	0/3/3/3
48	GDP	TH	501	-	-	0/16/32/32	0/3/3/3
48	GDP	VN	501	-	-	1/16/32/32	0/3/3/3
46	GTP	IM	501	-	-	5/22/38/38	0/3/3/3
48	GDP	WD	501	-	-	1/16/32/32	0/3/3/3
48	GDP	BB	501	-	-	1/16/32/32	0/3/3/3
48	GDP	TN	501	-	-	1/16/32/32	0/3/3/3
48	GDP	CB	501	-	-	6/16/32/32	0/3/3/3
48	GDP	HH	501	-	-	1/16/32/32	0/3/3/3
46	GTP	HA	501	-	-	9/22/38/38	0/3/3/3
46	GTP	UC	501	47	-	8/22/38/38	0/3/3/3
48	GDP	RH	501	-	-	1/16/32/32	0/3/3/3
46	GTP	KJ	501	47	-	7/22/38/38	0/3/3/3
46	GTP	LI	501	47	-	2/22/38/38	0/3/3/3
48	GDP	SJ	501	-	-	2/16/32/32	0/3/3/3
48	GDP	AH	501	-	-	0/16/32/32	0/3/3/3
46	GTP	OI	501	47	-	4/22/38/38	0/3/3/3
48	GDP	MJ	502	-	-	2/16/32/32	0/3/3/3
46	GTP	WE	501	47	-	6/22/38/38	0/3/3/3
48	GDP	IJ	502	-	-	3/16/32/32	0/3/3/3
46	GTP	SK	501	47	-	4/22/38/38	0/3/3/3
46	GTP	NC	501	47	-	3/22/38/38	0/3/3/3
46	GTP	TM	501	47	-	7/22/38/38	0/3/3/3
46	GTP	LG	501	47	-	4/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	GTP	GE	501	47	-	4/22/38/38	0/3/3/3
46	GTP	PE	501	47	-	6/22/38/38	0/3/3/3
48	GDP	CD	501	-	-	0/16/32/32	0/3/3/3
46	GTP	RE	501	47	-	6/22/38/38	0/3/3/3
46	GTP	TK	501	47	-	8/22/38/38	0/3/3/3
48	GDP	LN	502	-	-	2/16/32/32	0/3/3/3
46	GTP	JC	501	-	-	6/22/38/38	0/3/3/3
46	GTP	KA	501	47	-	7/22/38/38	0/3/3/3
48	GDP	FN	501	-	-	2/16/32/32	0/3/3/3
46	GTP	WG	501	47	-	7/22/38/38	0/3/3/3
46	GTP	VA	501	47	-	6/22/38/38	0/3/3/3
46	GTP	QE	501	47	-	7/22/38/38	0/3/3/3
46	GTP	EC	501	47	-	4/22/38/38	0/3/3/3
48	GDP	TL	501	-	-	0/16/32/32	0/3/3/3
48	GDP	UL	501	-	-	1/16/32/32	0/3/3/3
48	GDP	JD	501	-	-	4/16/32/32	0/3/3/3
48	GDP	JF	501	-	-	0/16/32/32	0/3/3/3
48	GDP	HD	501	-	-	0/16/32/32	0/3/3/3
46	GTP	JK	501	47	-	5/22/38/38	0/3/3/3
48	GDP	LB	502	-	-	1/16/32/32	0/3/3/3
48	GDP	MD	501	-	-	1/16/32/32	0/3/3/3
48	GDP	PJ	501	-	-	1/16/32/32	0/3/3/3
46	GTP	VM	501	47	-	8/22/38/38	0/3/3/3
46	GTP	LC	501	47	-	2/22/38/38	0/3/3/3
48	GDP	QJ	501	-	-	1/16/32/32	0/3/3/3
48	GDP	BD	502	-	-	0/16/32/32	0/3/3/3
48	GDP	LD	501	-	-	3/16/32/32	0/3/3/3
46	GTP	KG	501	47	-	3/22/38/38	0/3/3/3
48	GDP	KD	501	-	-	0/16/32/32	0/3/3/3
48	GDP	PF	501	-	-	1/16/32/32	0/3/3/3
48	GDP	MH	501	-	-	1/16/32/32	0/3/3/3
48	GDP	CH	501	-	-	1/16/32/32	0/3/3/3
48	GDP	IH	502	-	-	0/16/32/32	0/3/3/3
48	GDP	IN	501	-	-	3/16/32/32	0/3/3/3
46	GTP	NG	501	47	-	5/22/38/38	0/3/3/3
48	GDP	SD	501	-	-	1/16/32/32	0/3/3/3
46	GTP	WC	501	47	-	5/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	GDP	FH	501	-	-	2/16/32/32	0/3/3/3
46	GTP	UE	501	47	-	6/22/38/38	0/3/3/3
46	GTP	UM	501	47	-	5/22/38/38	0/3/3/3
46	GTP	GI	501	47	-	8/22/38/38	0/3/3/3
46	GTP	ME	501	47	-	5/22/38/38	0/3/3/3
46	GTP	HE	501	47	-	5/22/38/38	0/3/3/3
48	GDP	BN	501	-	-	1/16/32/32	0/3/3/3
46	GTP	WI	501	47	-	10/22/38/38	0/3/3/3

The worst 5 of 704 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	CB	501	GDP	C5-C4	3.43	1.48	1.38
48	PB	501	GDP	C5-C4	3.19	1.47	1.38
48	TB	501	GDP	C5-C4	3.19	1.47	1.38
48	OB	501	GDP	C5-C4	3.18	1.47	1.38
48	SN	501	GDP	C5-C4	3.18	1.47	1.38

The worst 5 of 2545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	CB	501	GDP	C5-C4-N3	-7.62	116.26	128.39
48	VB	502	GDP	C5-C4-N3	-6.56	117.95	128.39
48	VN	501	GDP	C5-C4-N3	-6.46	118.11	128.39
48	WJ	502	GDP	C5-C4-N3	-6.43	118.15	128.39
48	ND	501	GDP	C5-C4-N3	-6.34	118.30	128.39

There are no chirality outliers.

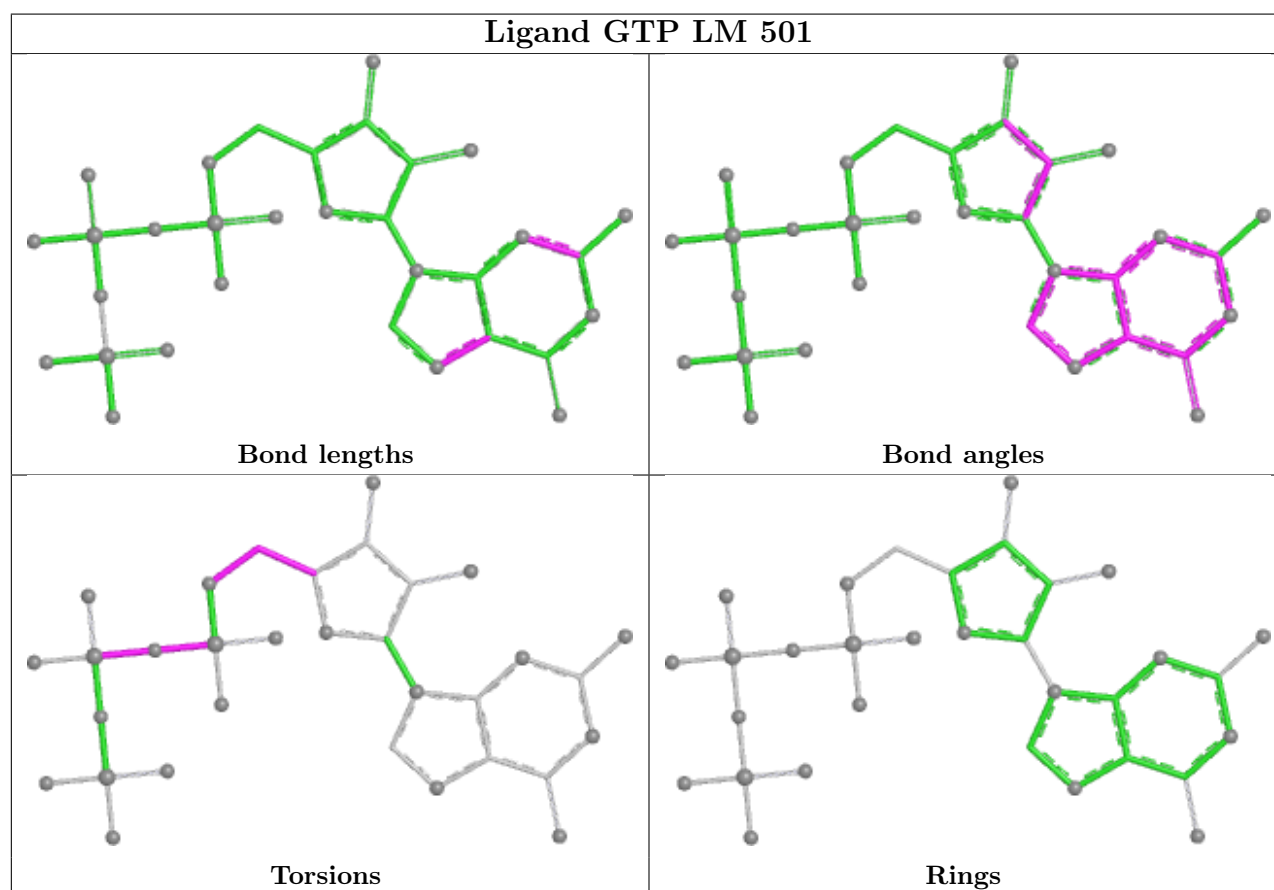
5 of 1042 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	AA	501	GTP	PB-O3B-PG-O3G
46	AA	501	GTP	C5'-O5'-PA-O3A
46	AC	501	GTP	C4'-C5'-O5'-PA
46	AE	501	GTP	PB-O3A-PA-O5'
46	AG	501	GTP	C5'-O5'-PA-O3A

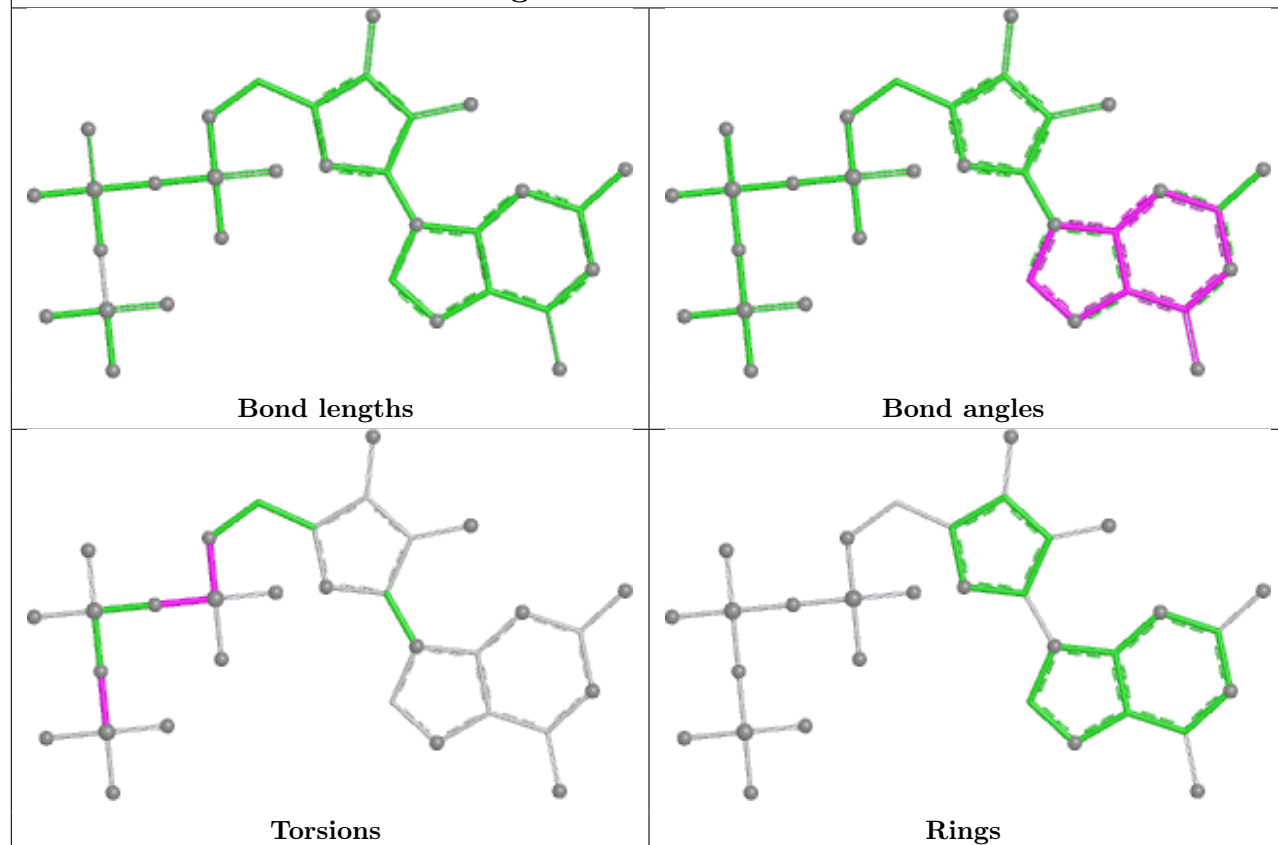
There are no ring outliers.

No monomer is involved in short contacts.

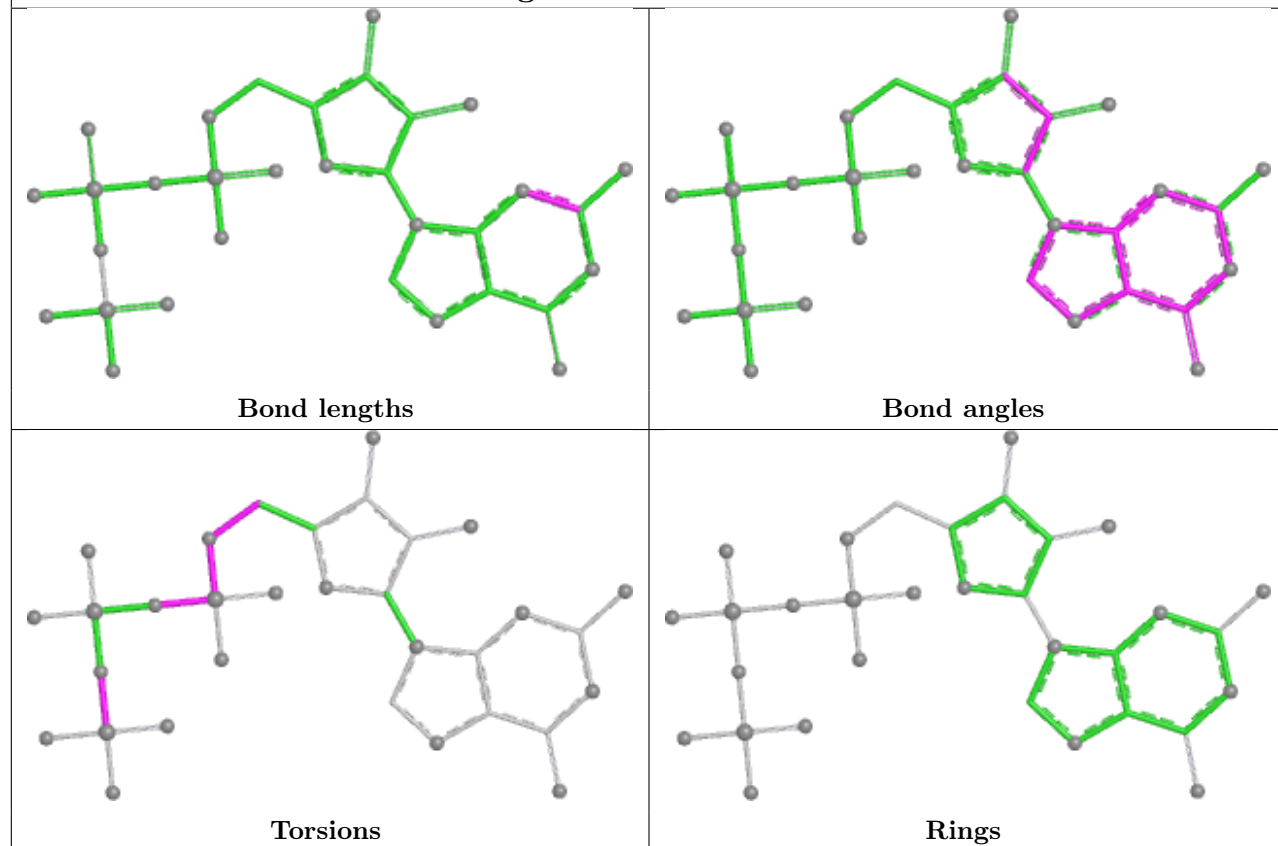
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

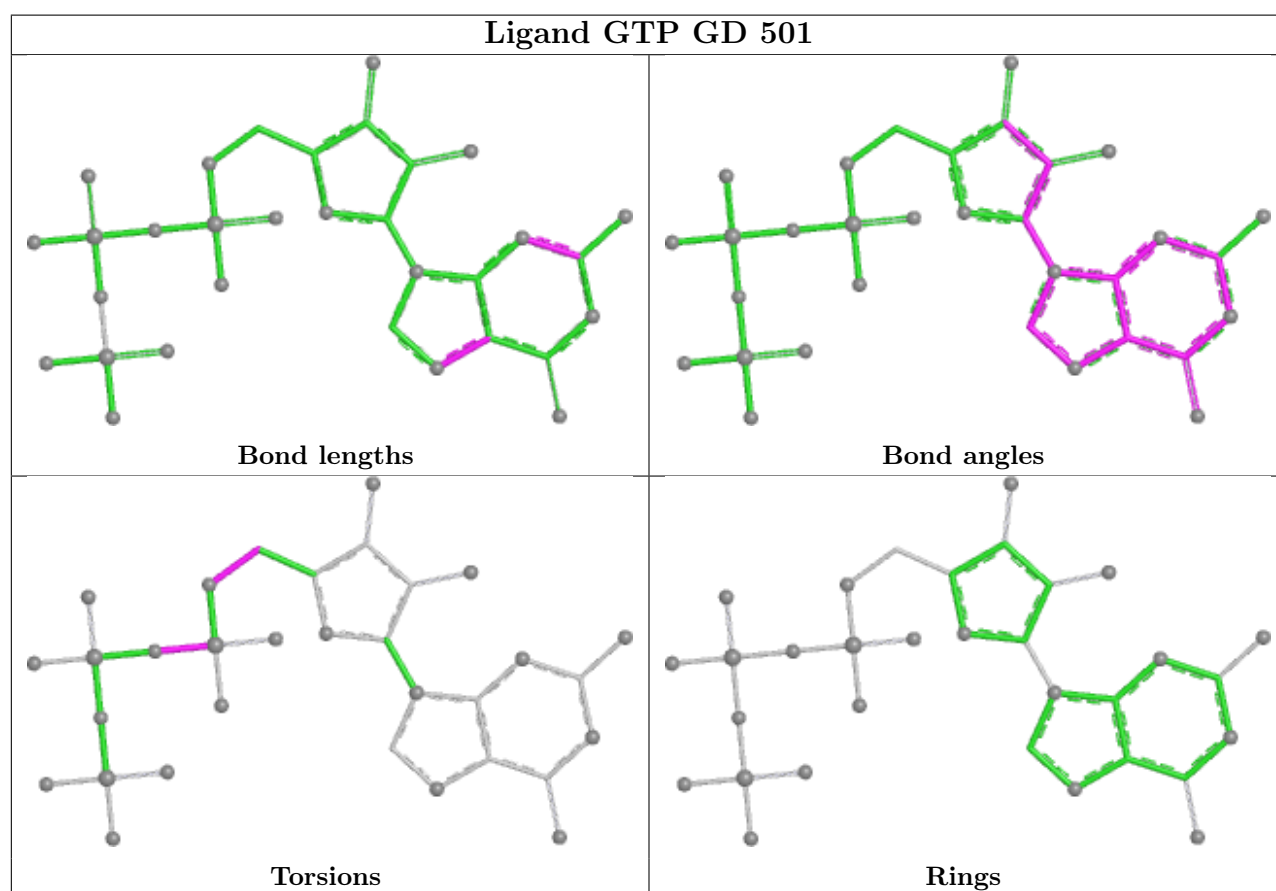
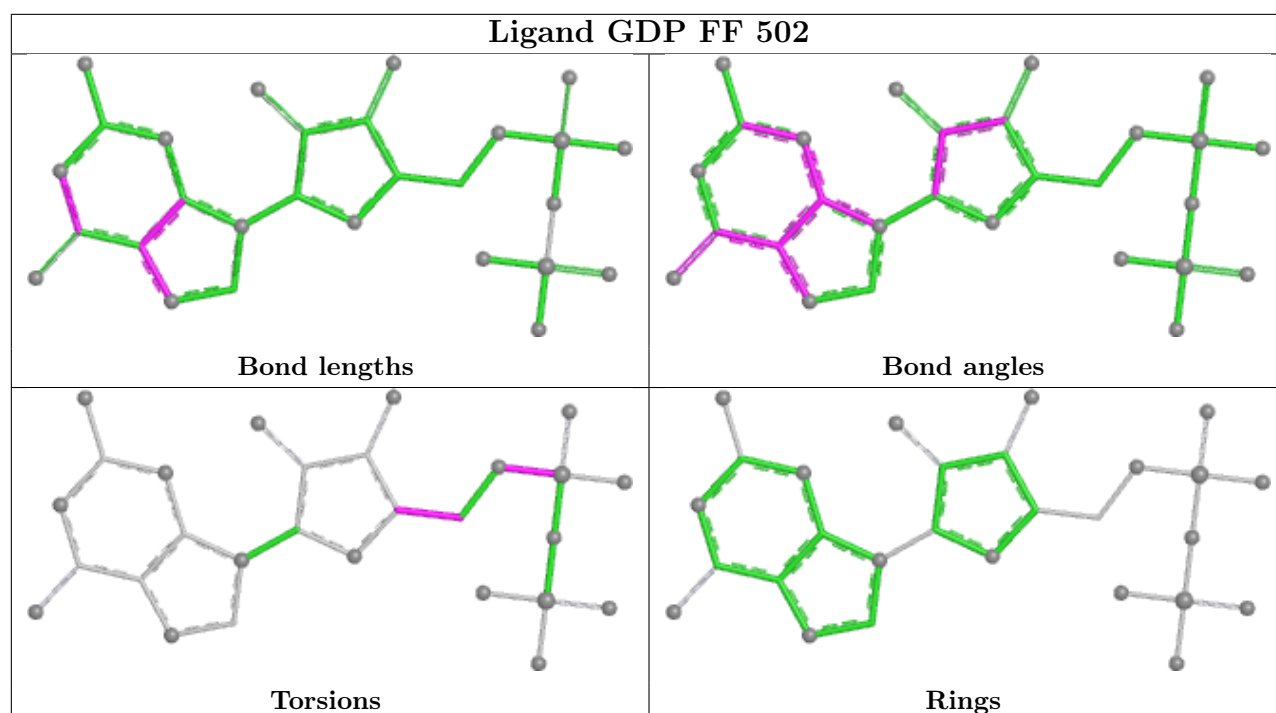


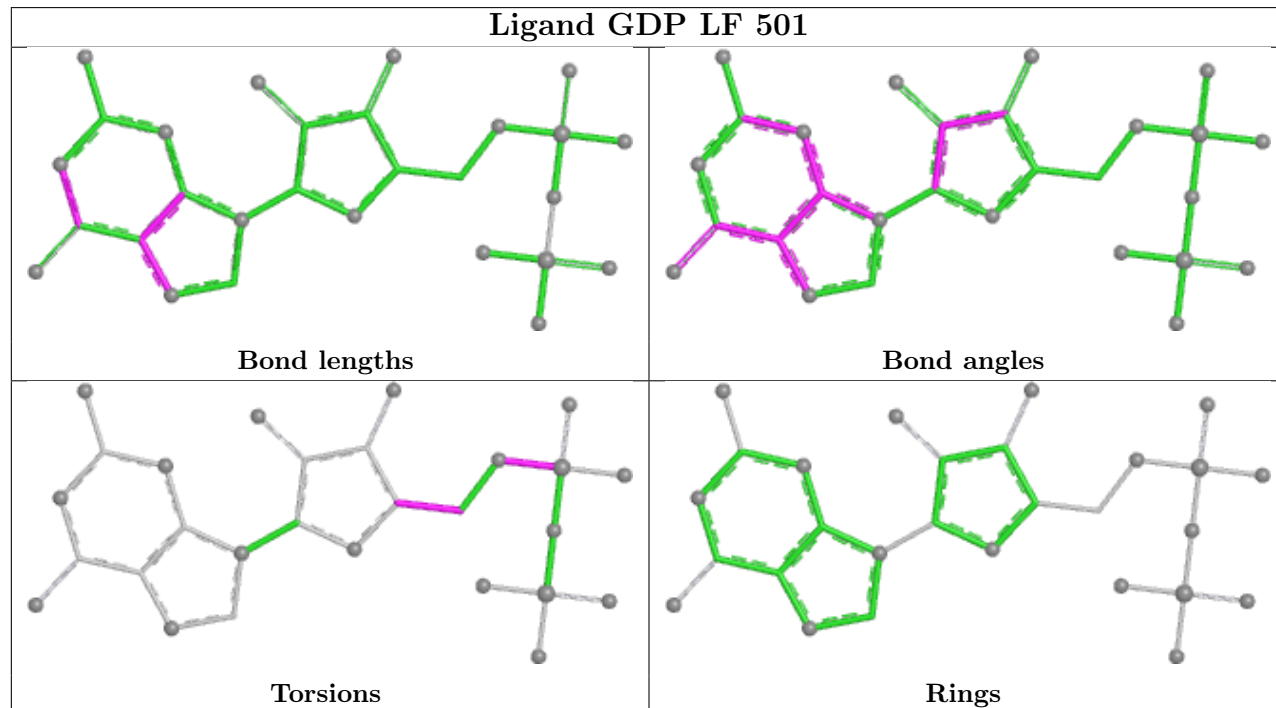
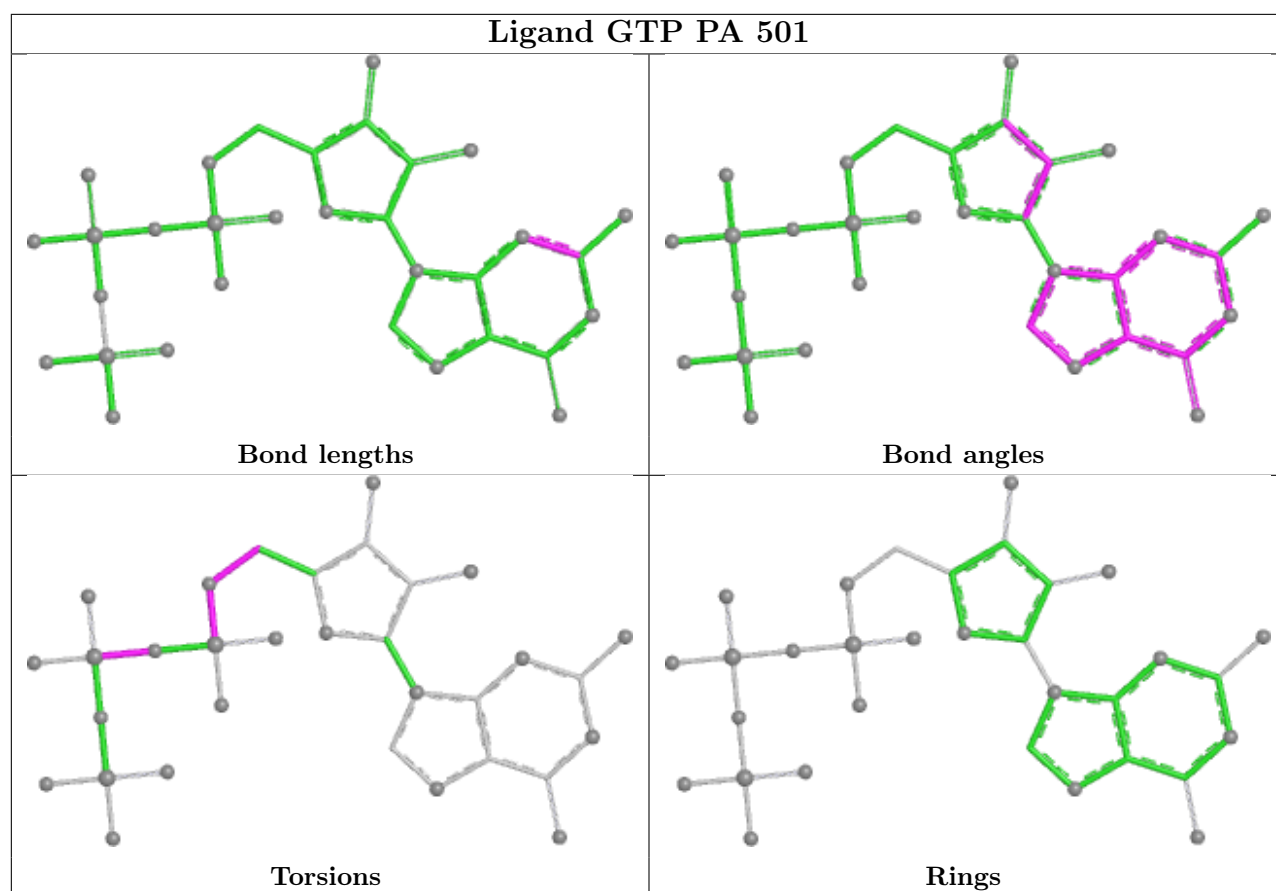
Ligand GTP WK 501

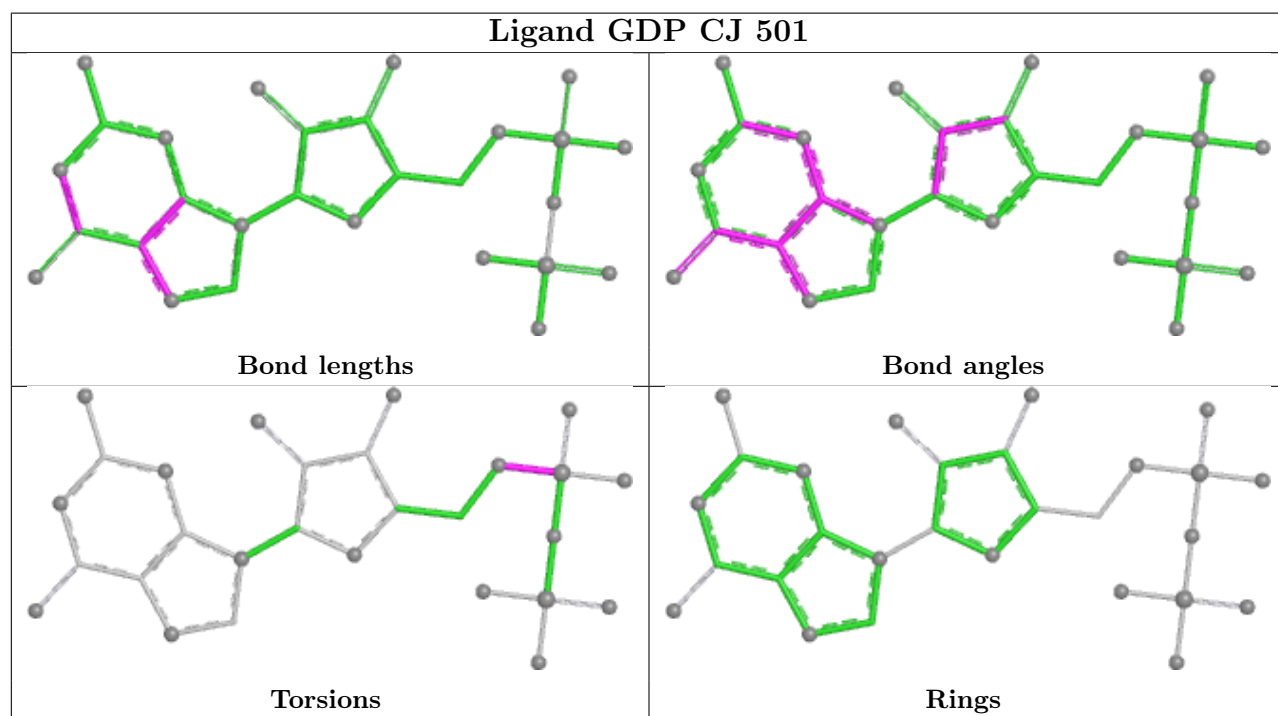
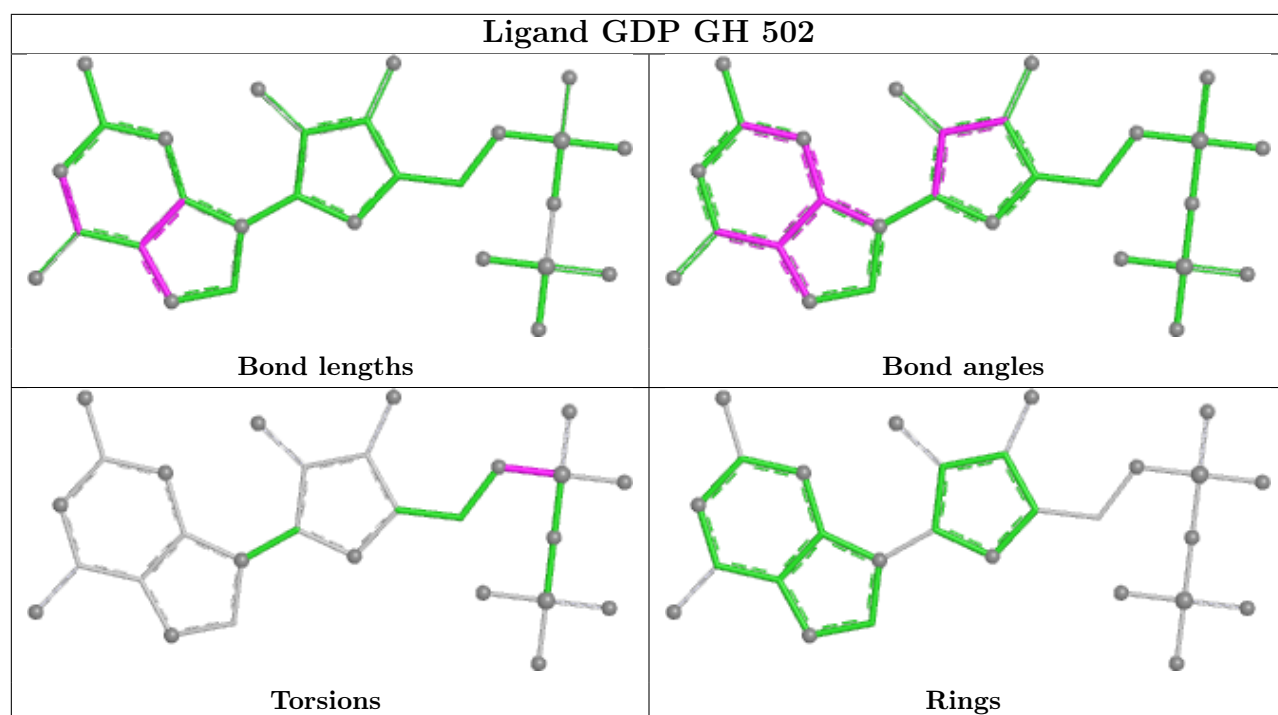


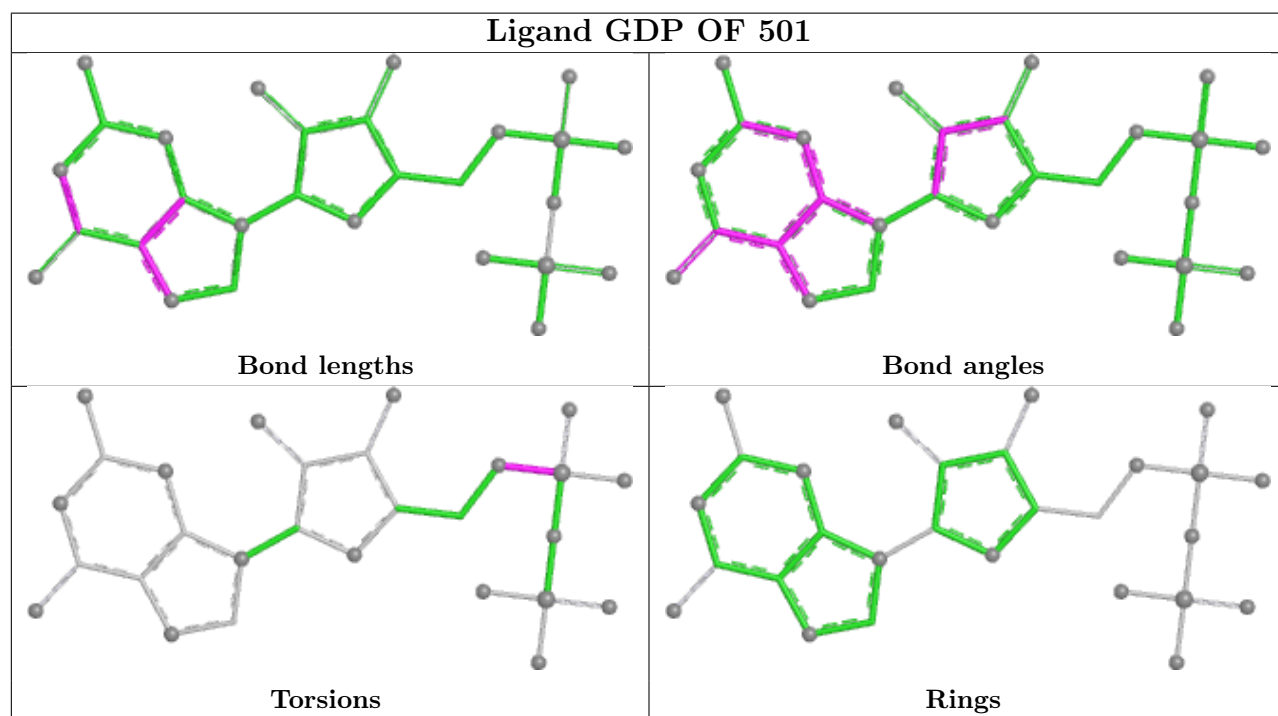
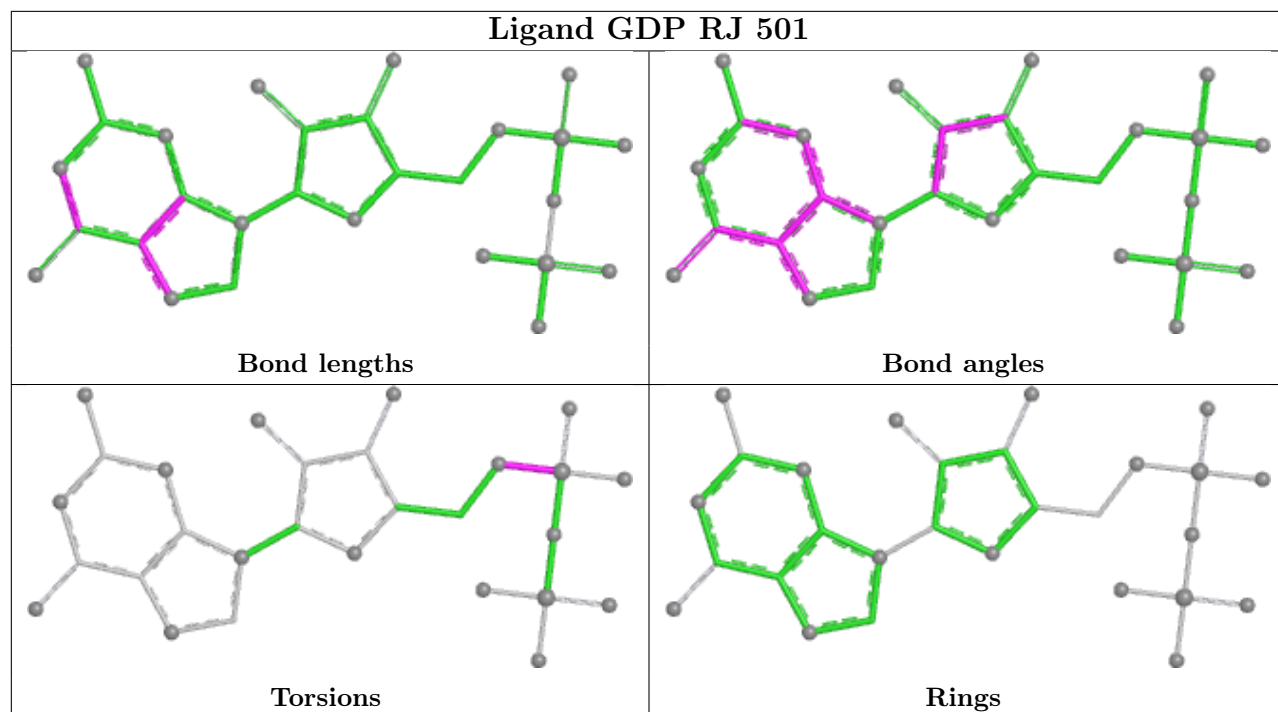
Ligand GTP BA 501

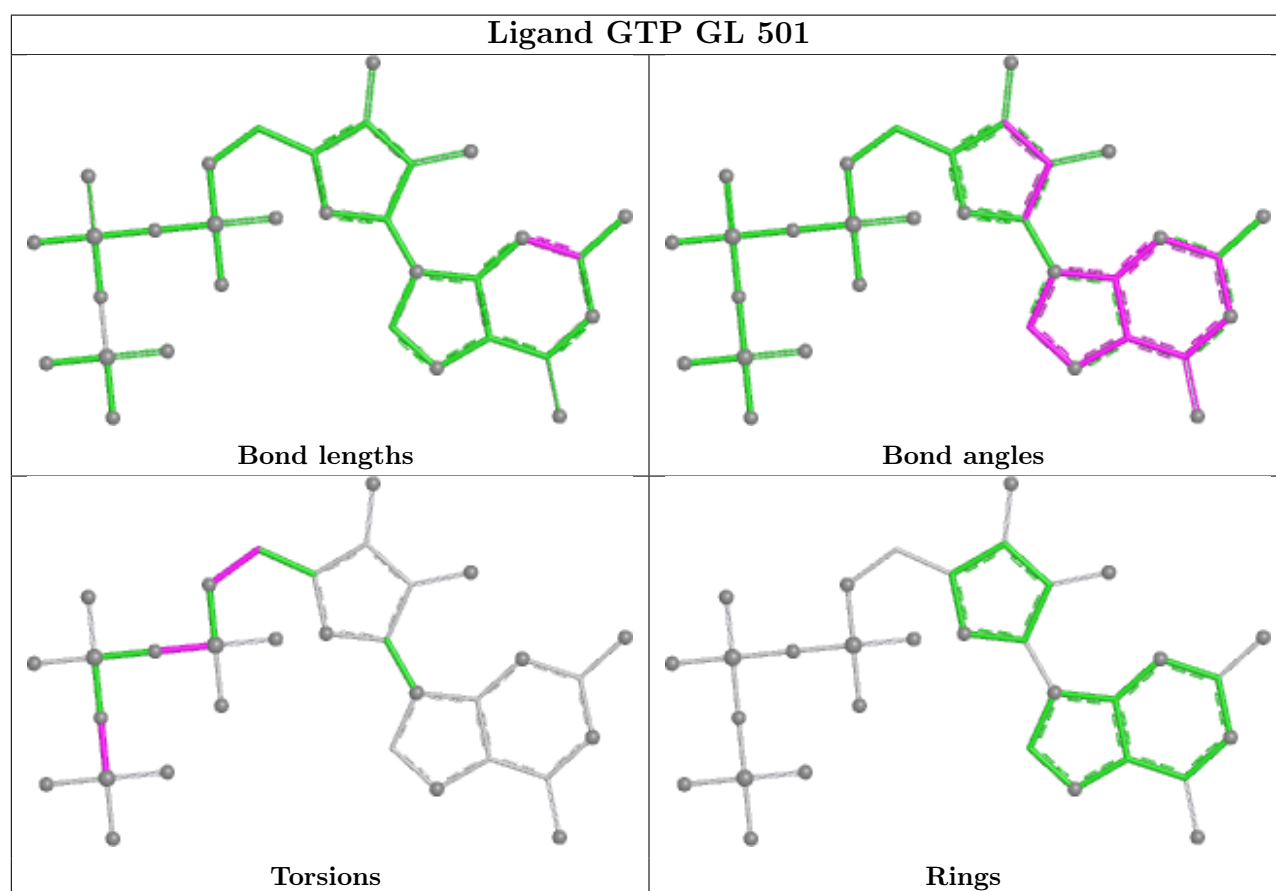
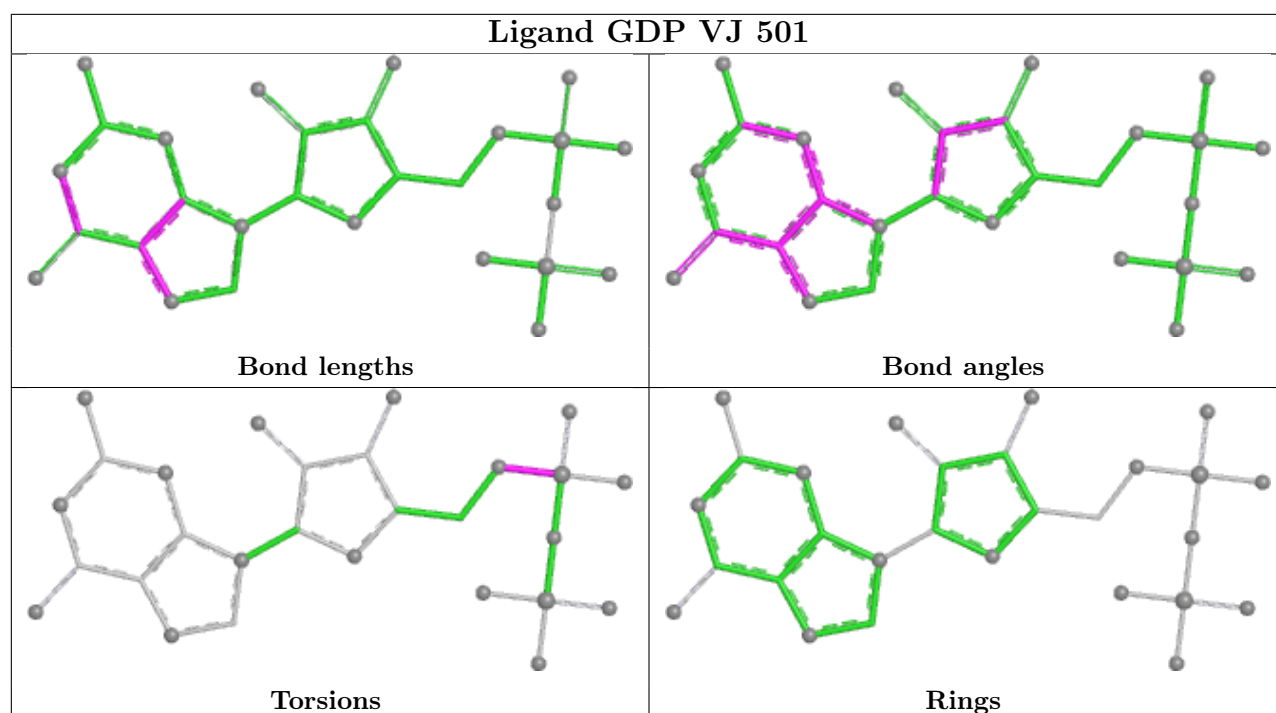




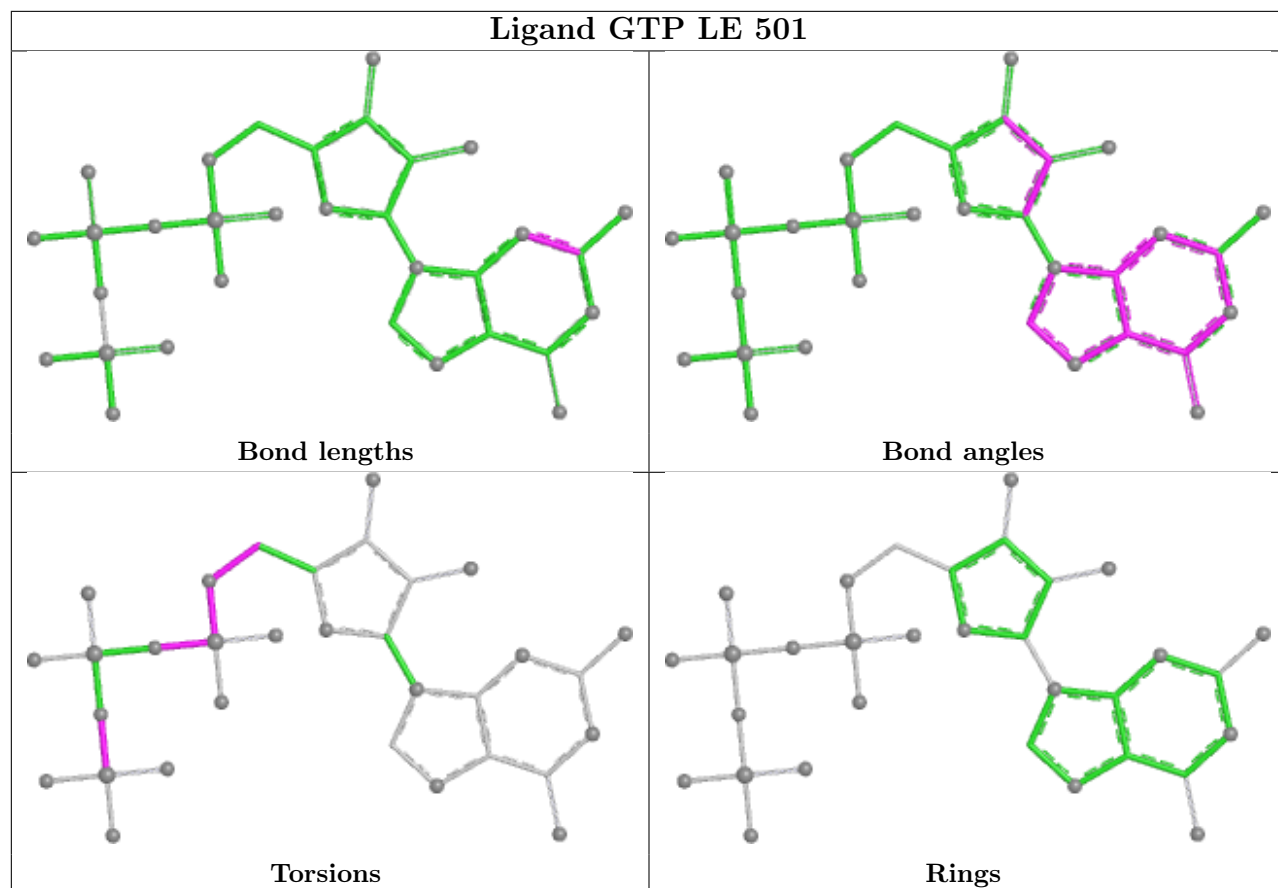




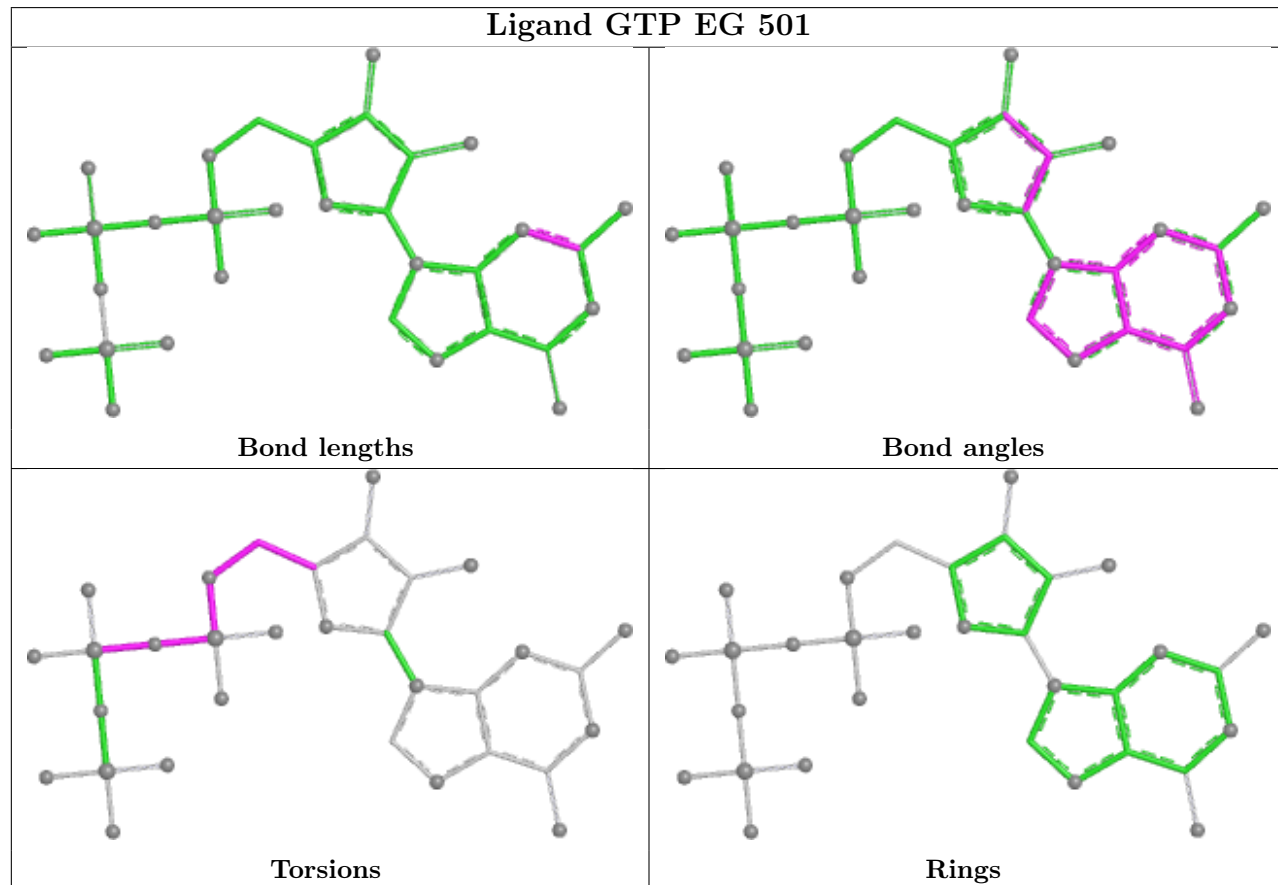


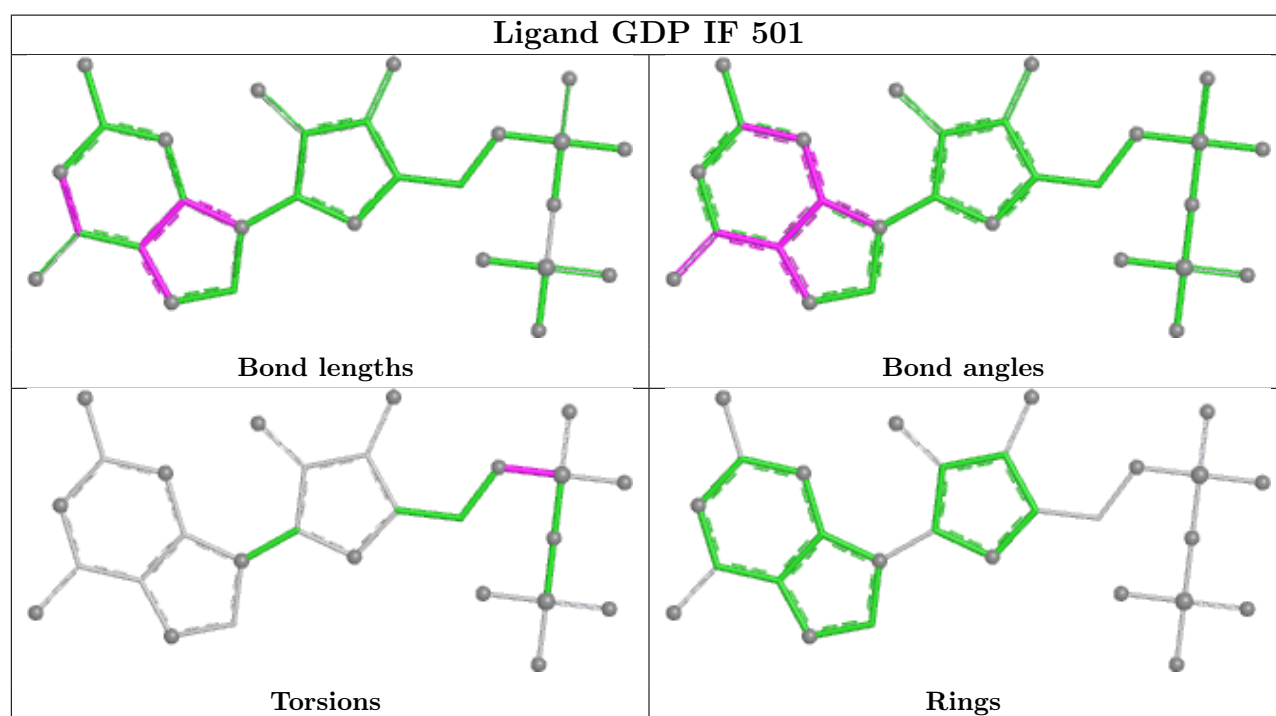
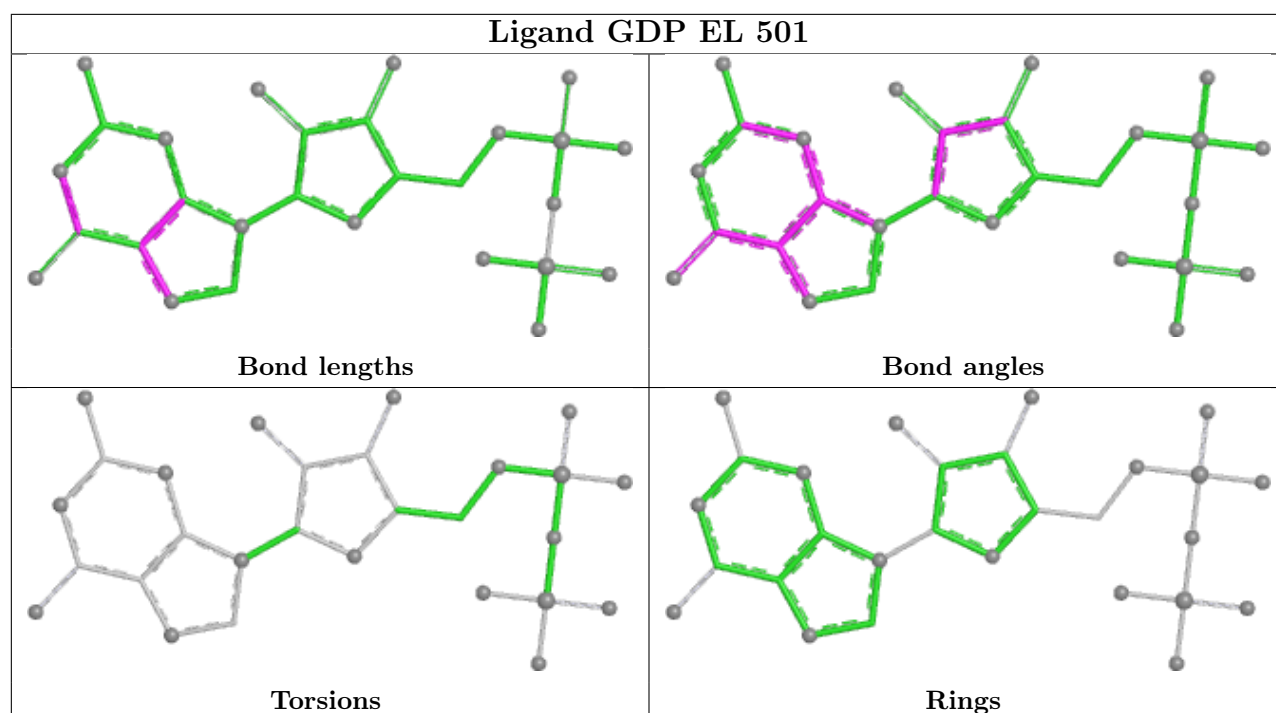


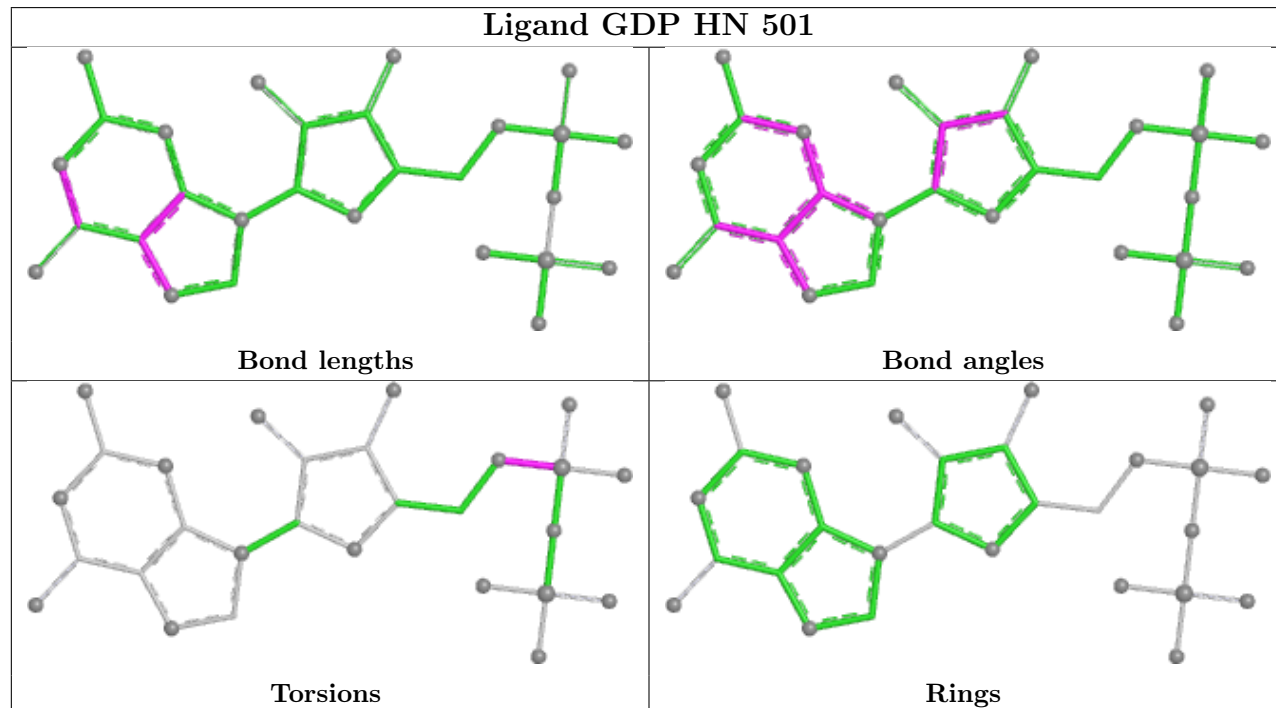
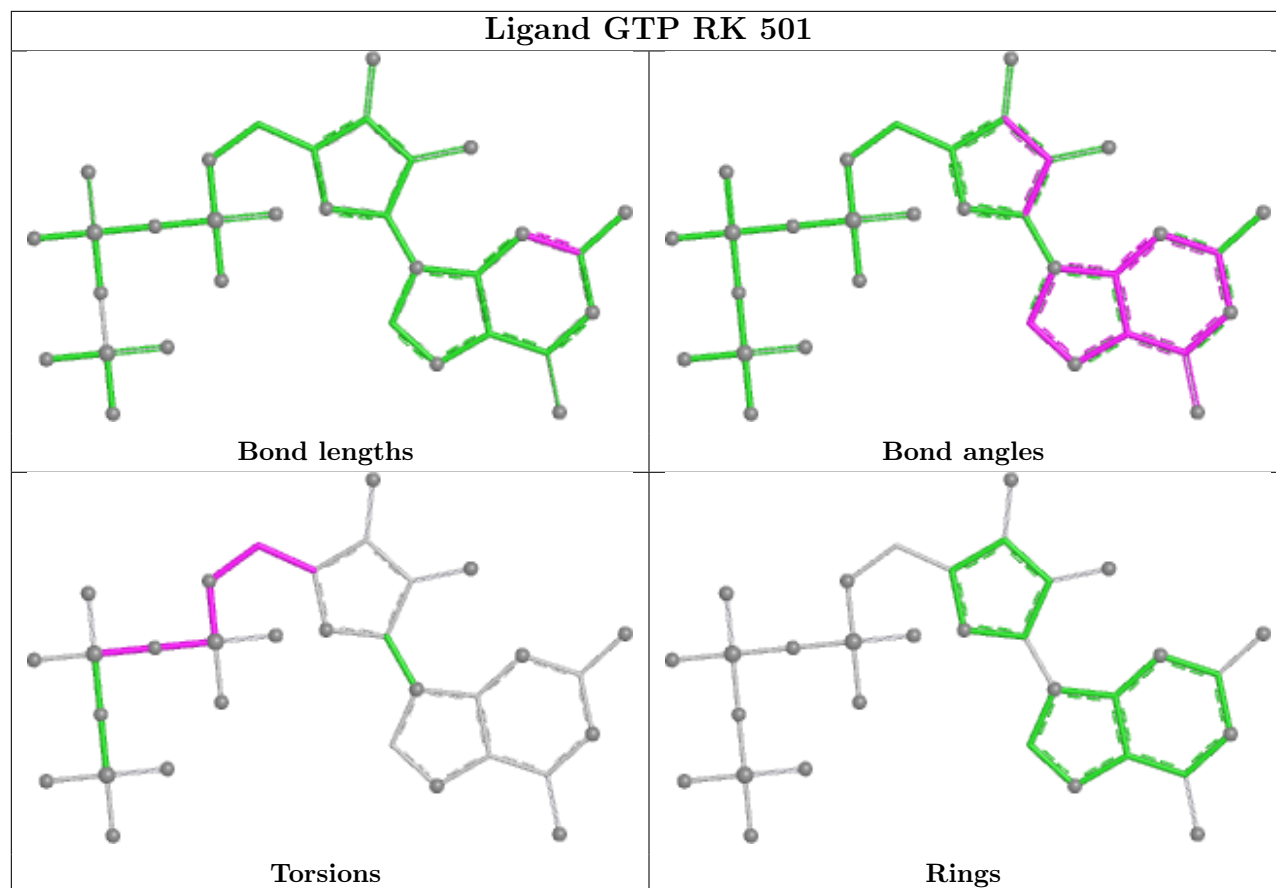
Ligand GTP LE 501



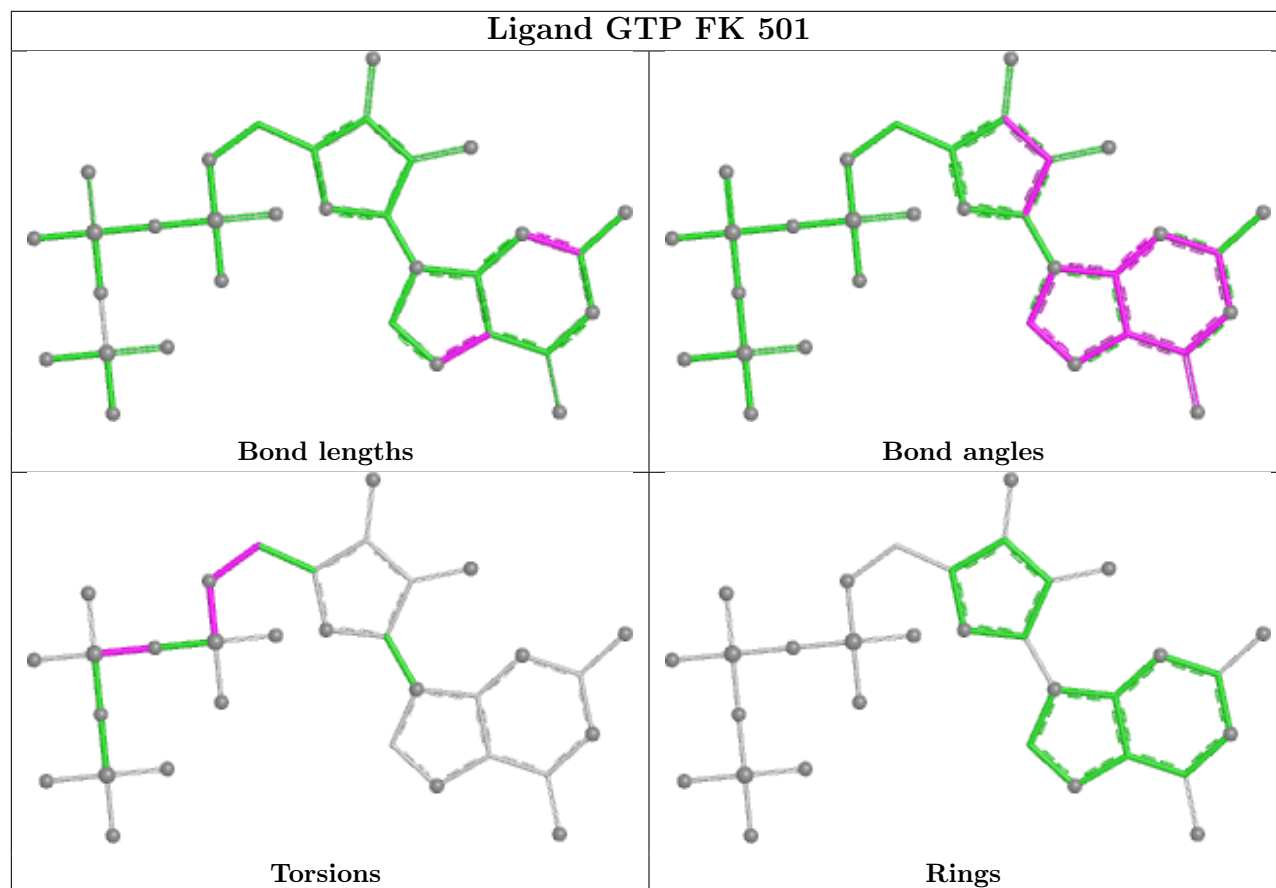
Ligand GTP EG 501



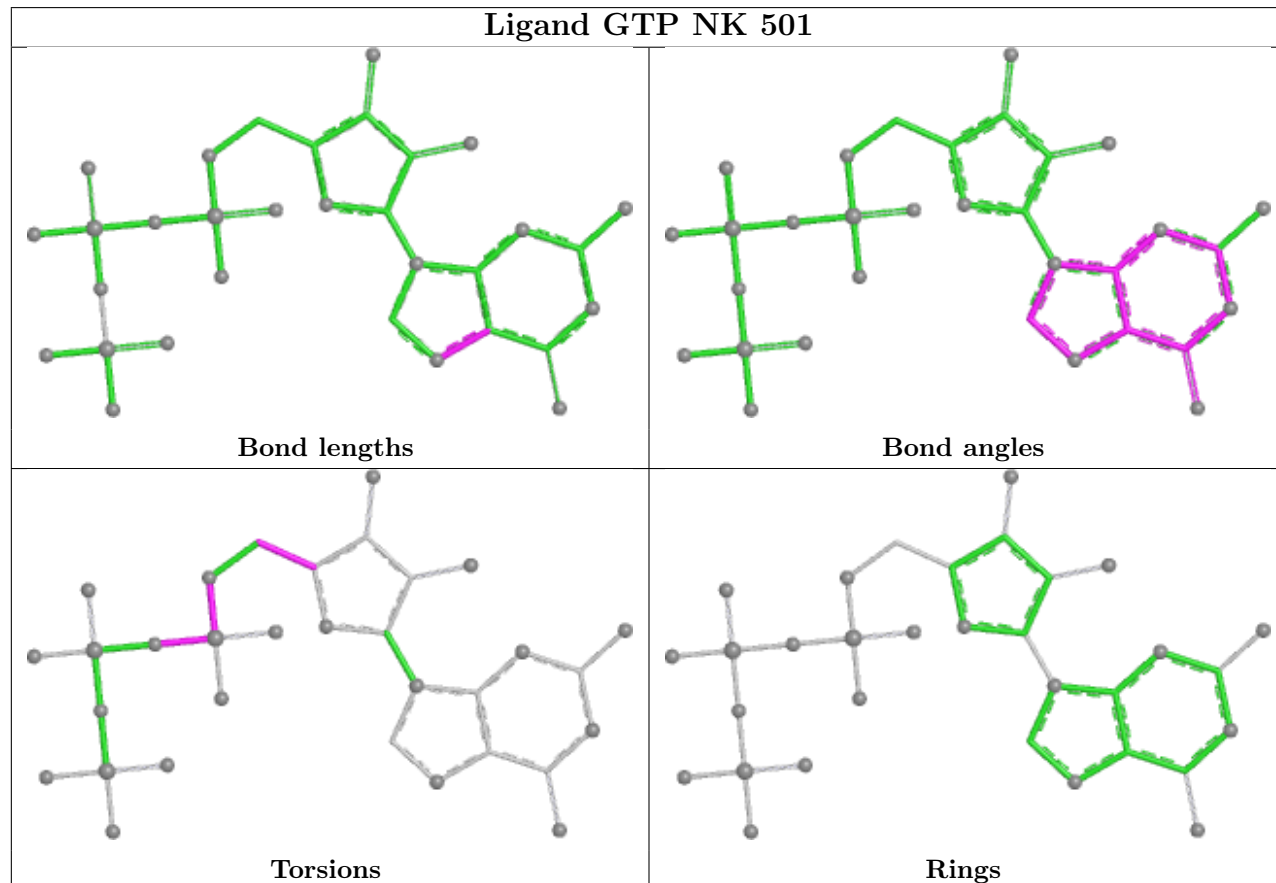




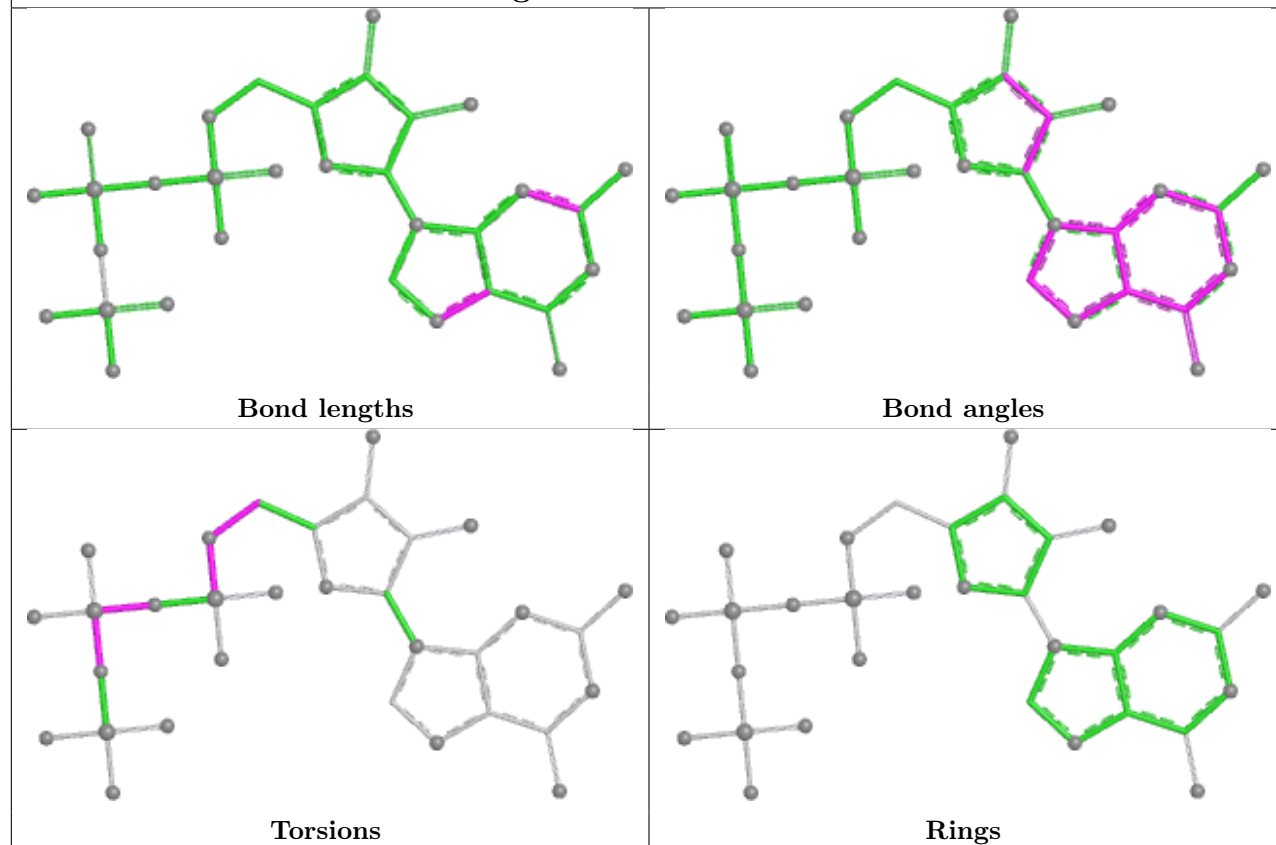
Ligand GTP FK 501



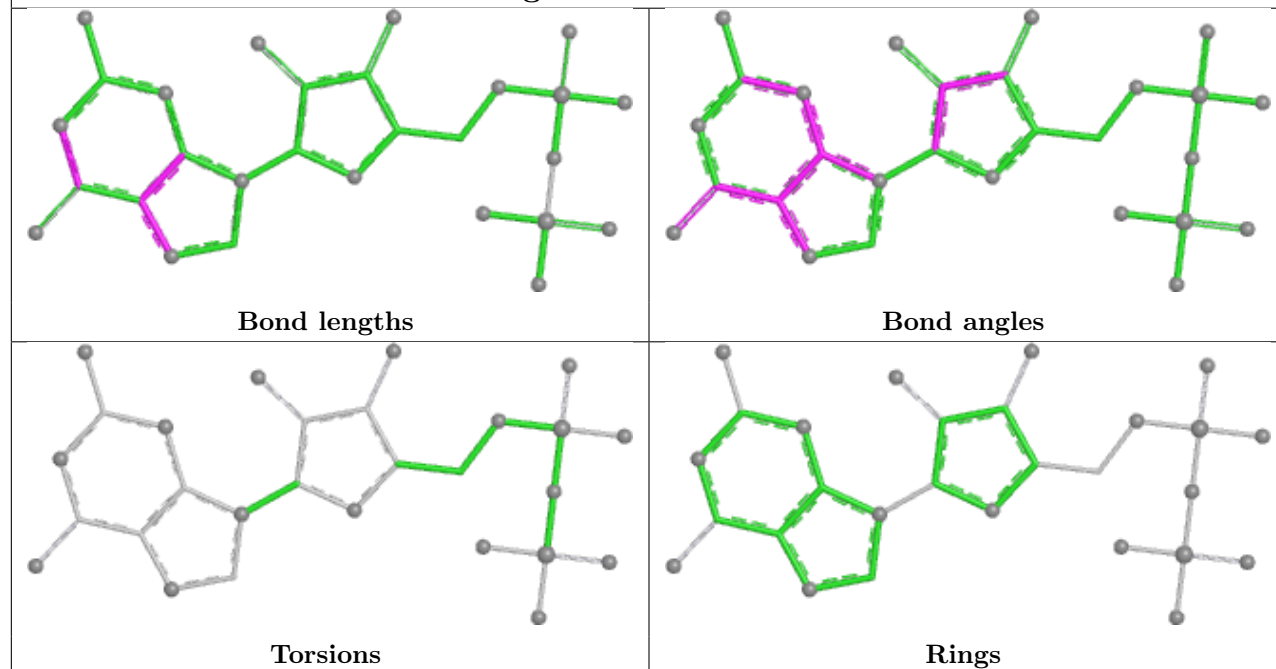
Ligand GTP NK 501

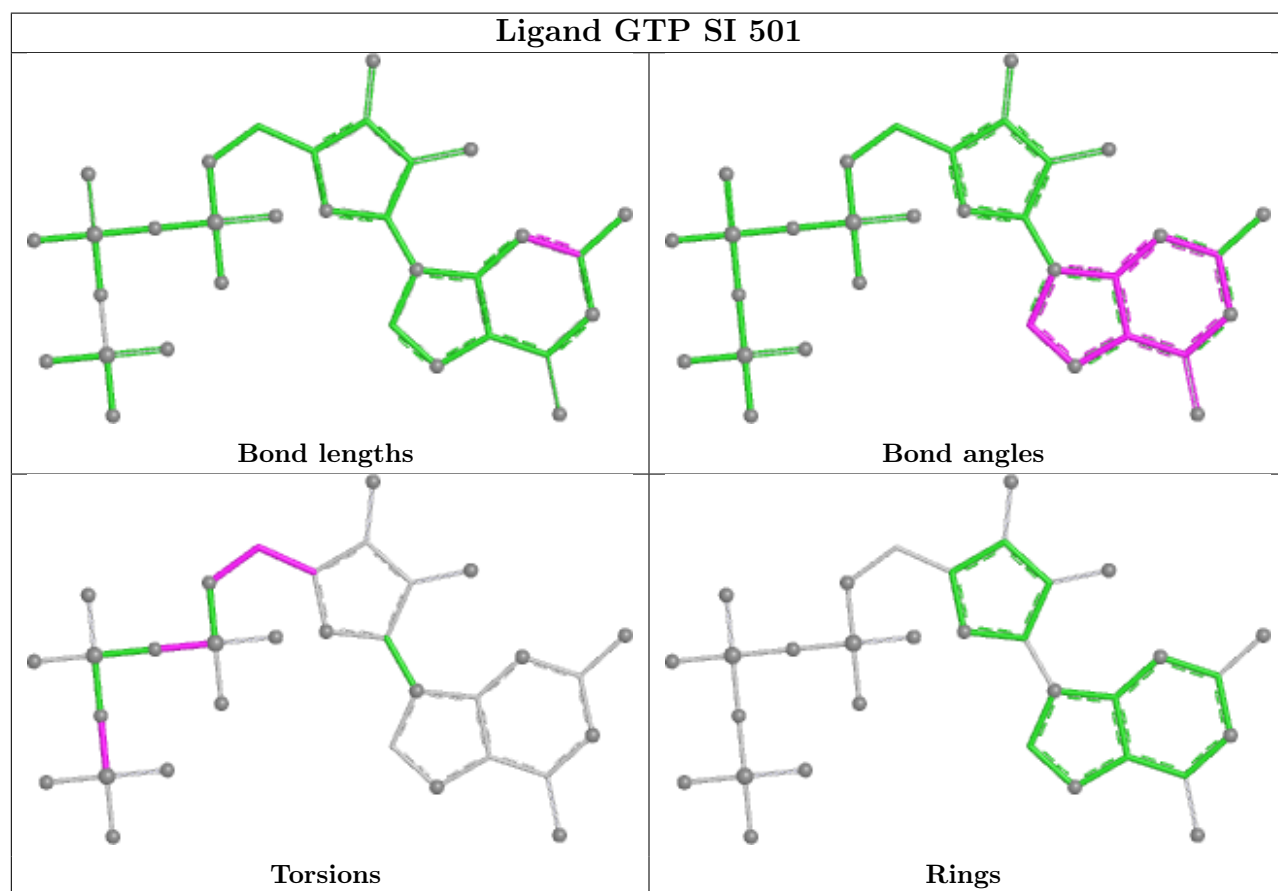
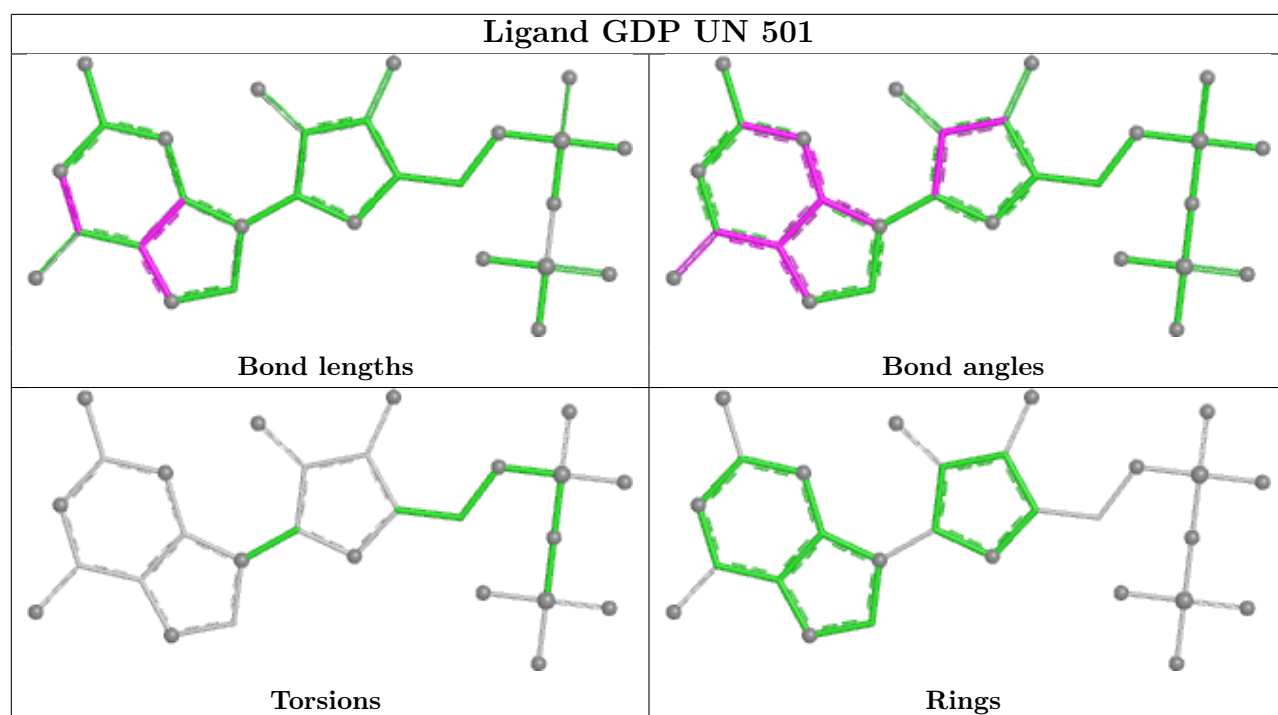


Ligand GTP MG 501

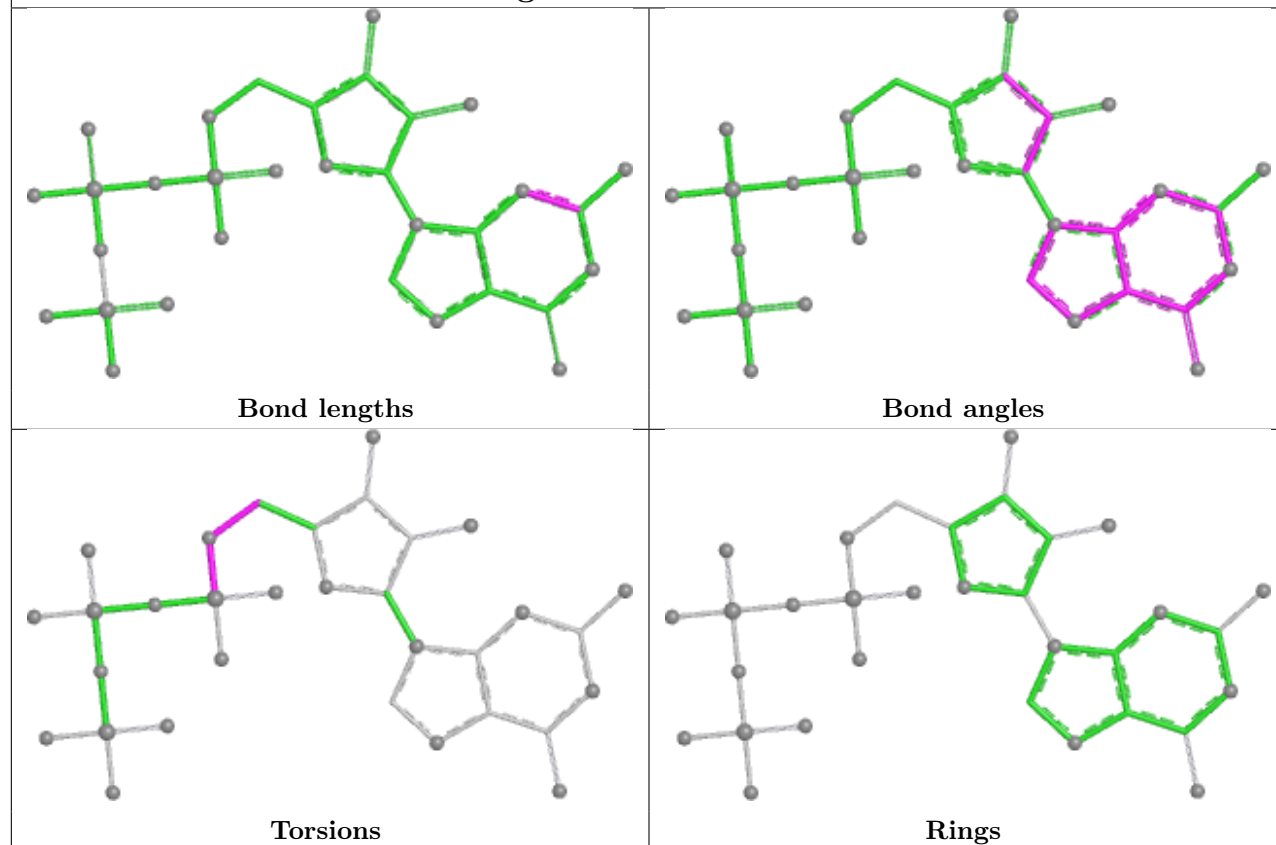


Ligand GDP IB 501

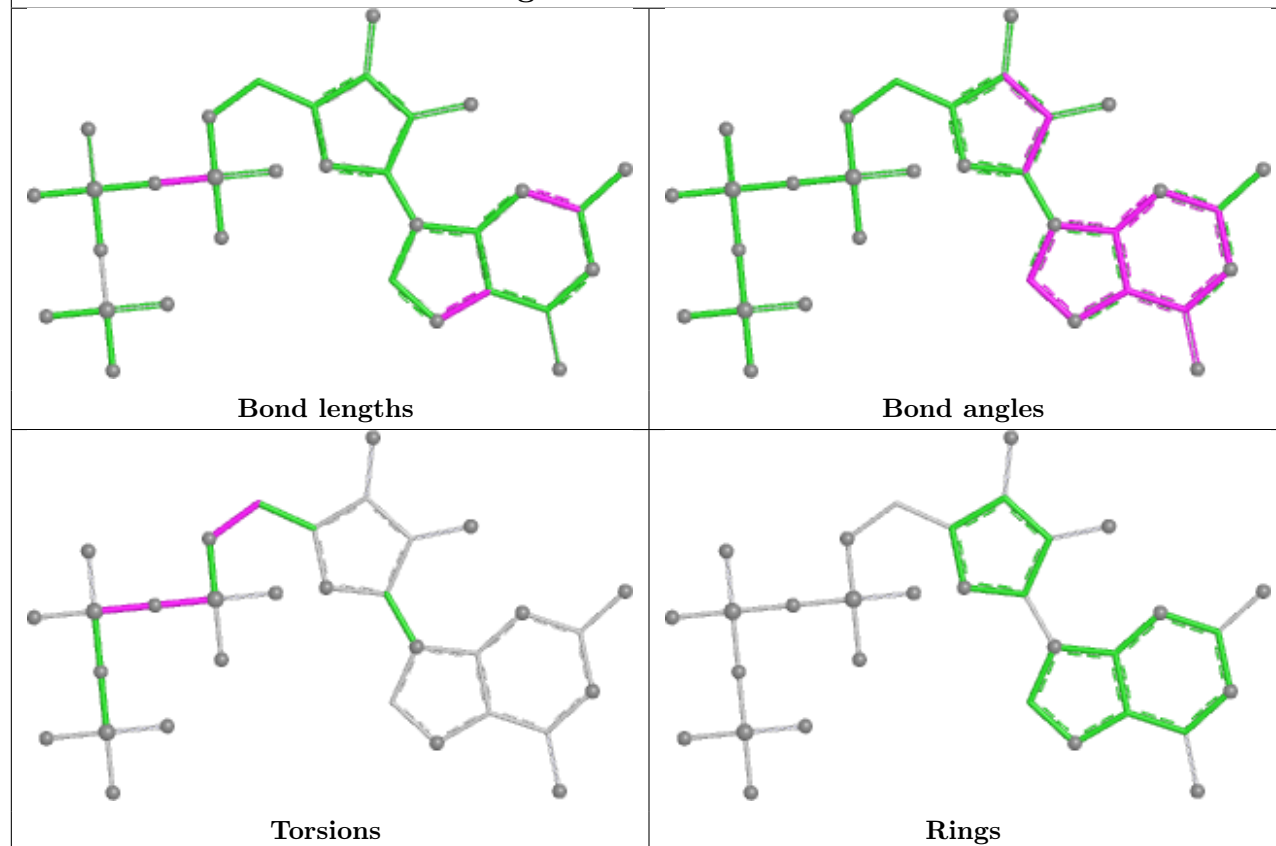


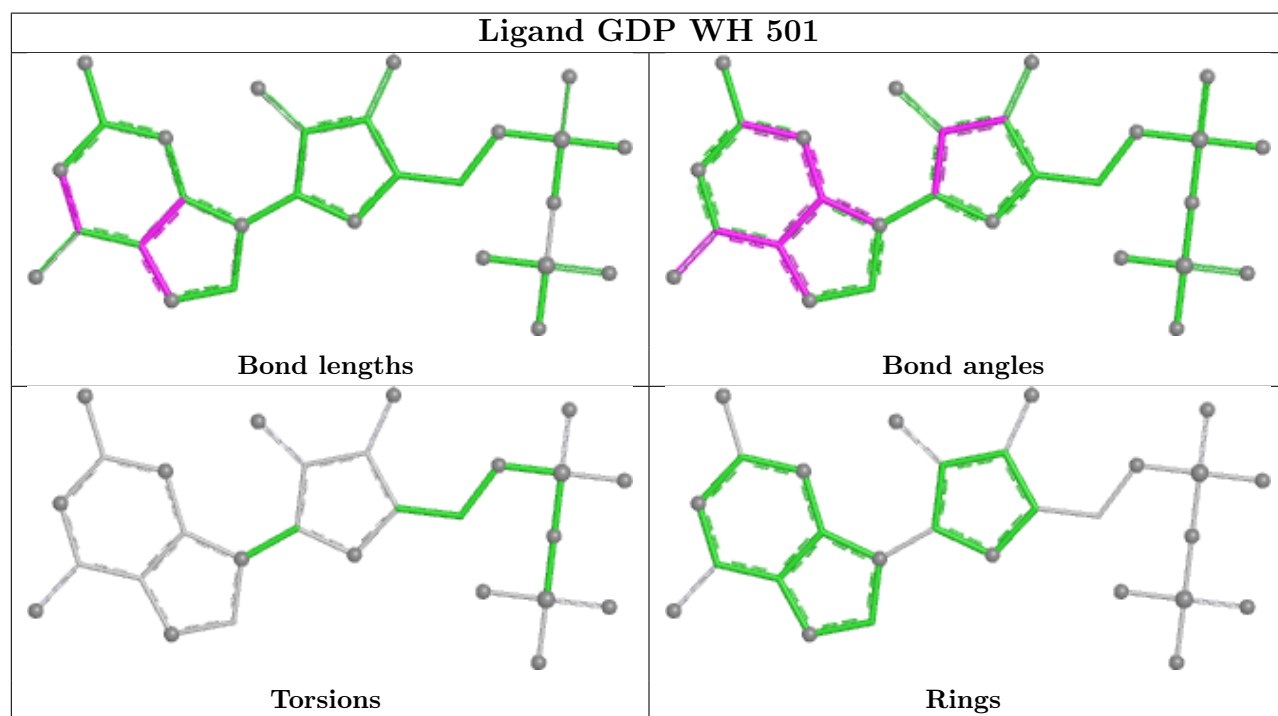
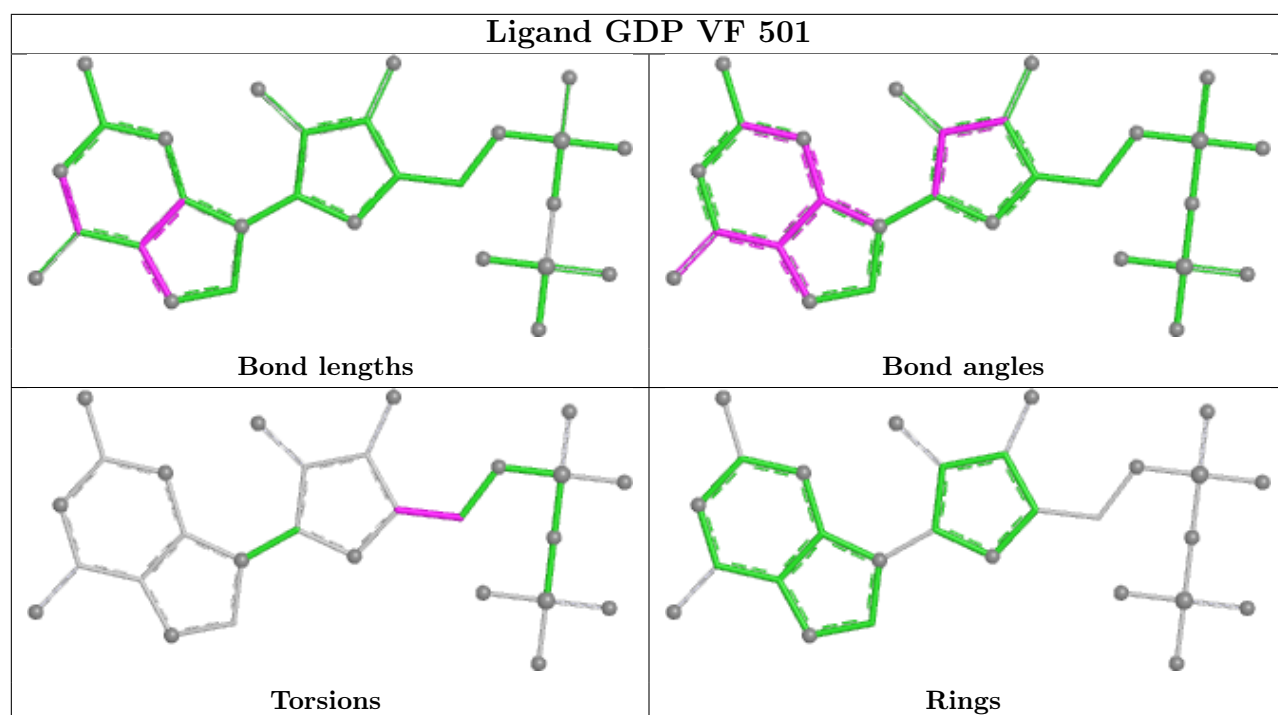


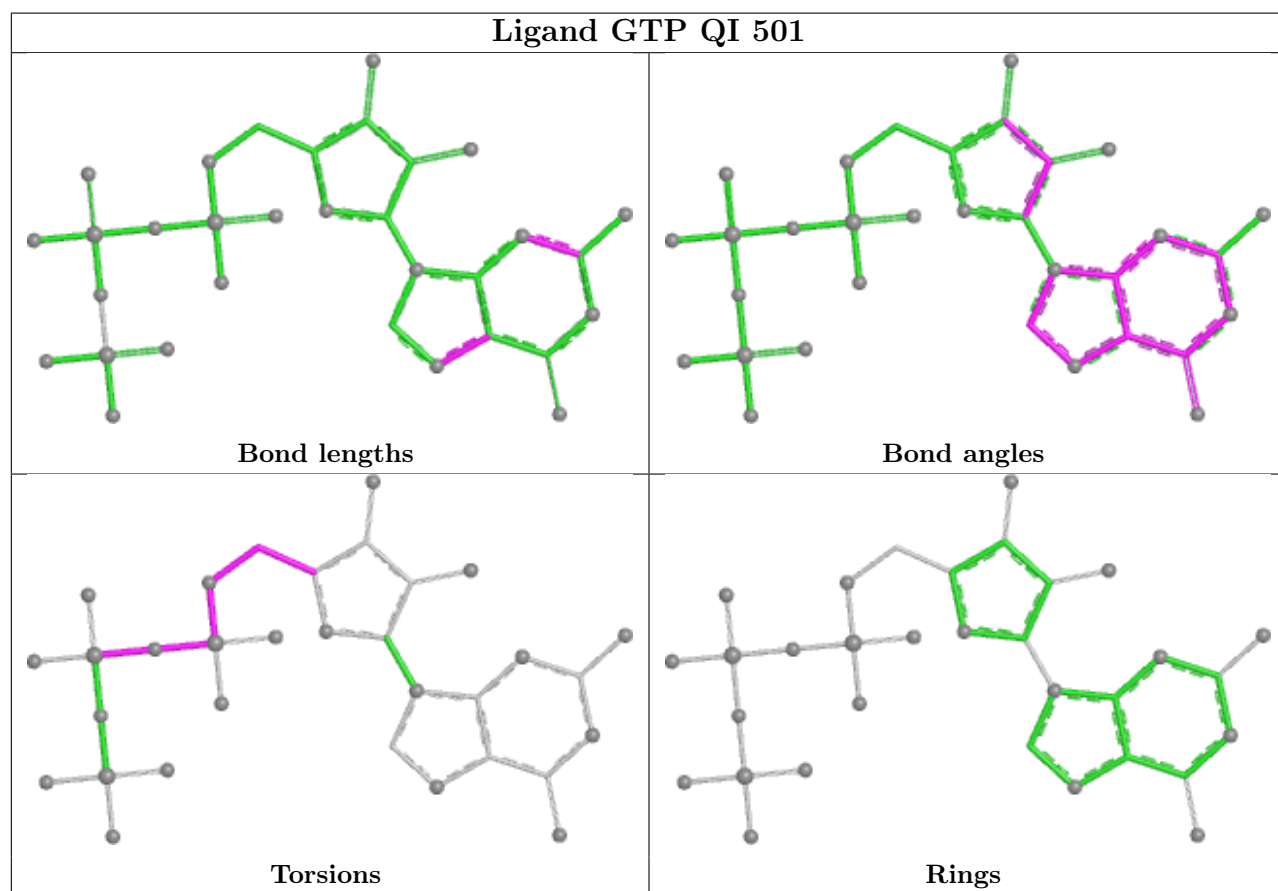
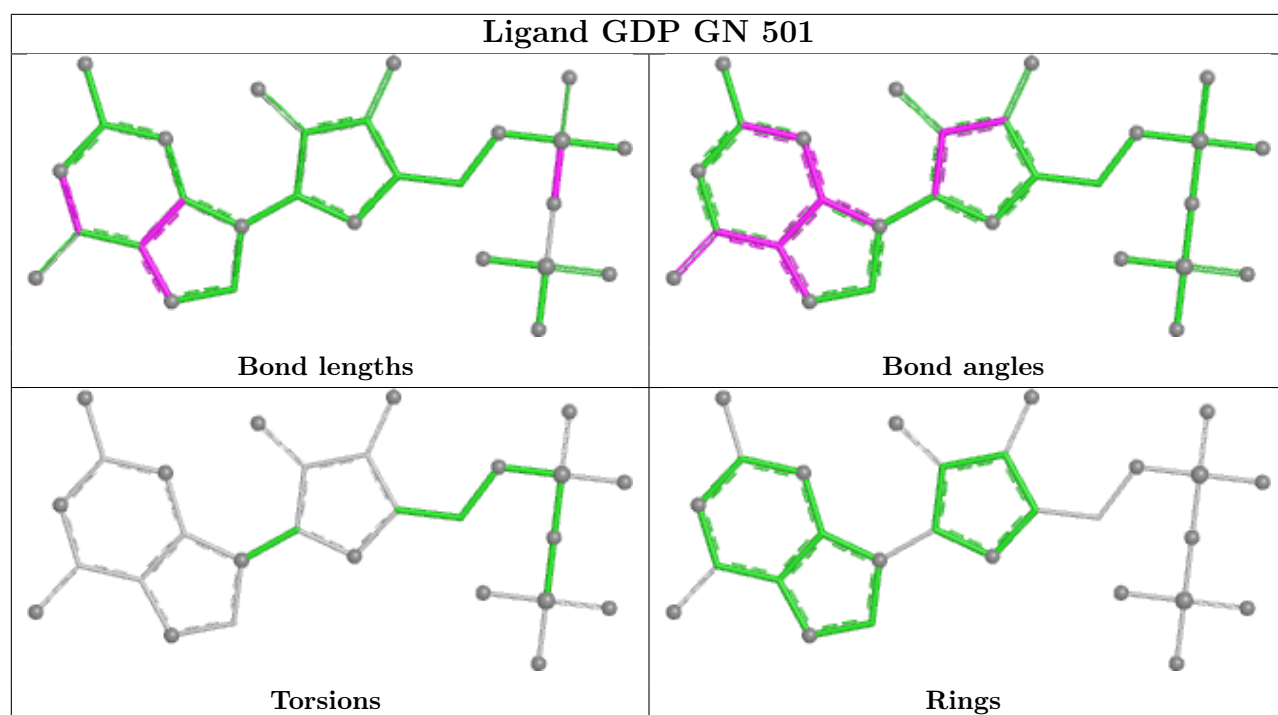
Ligand GTP JM 501

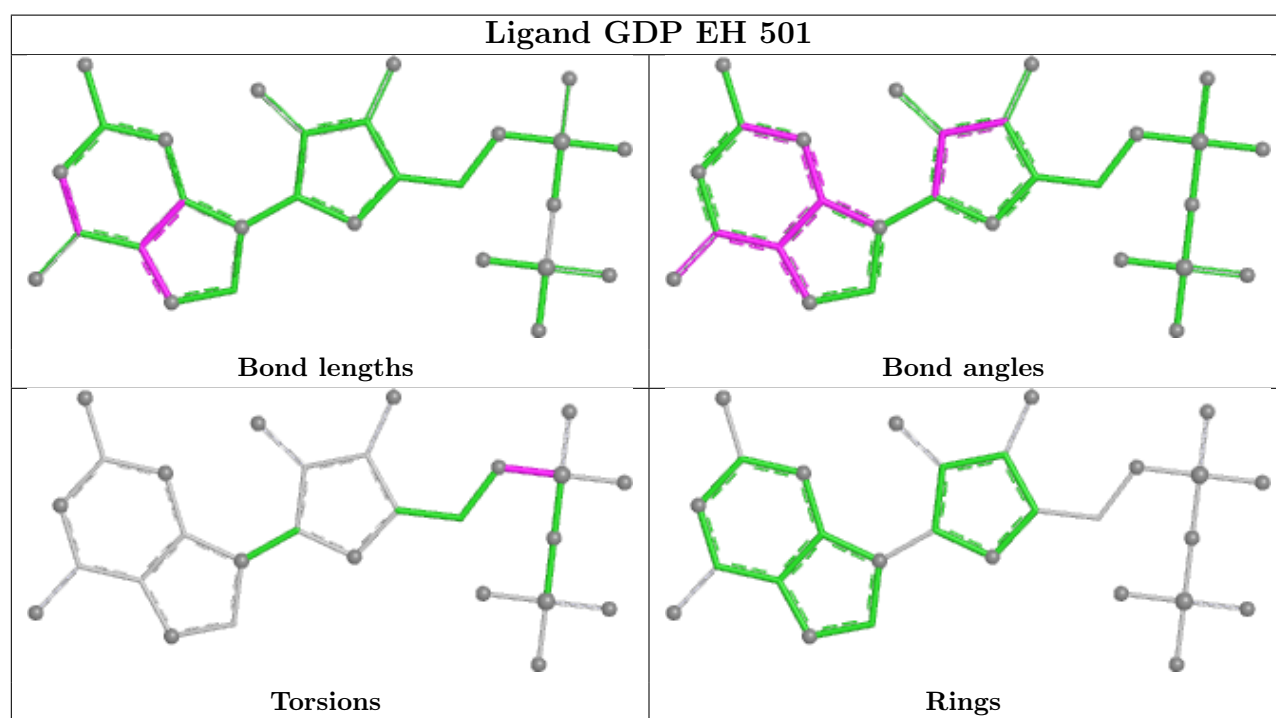
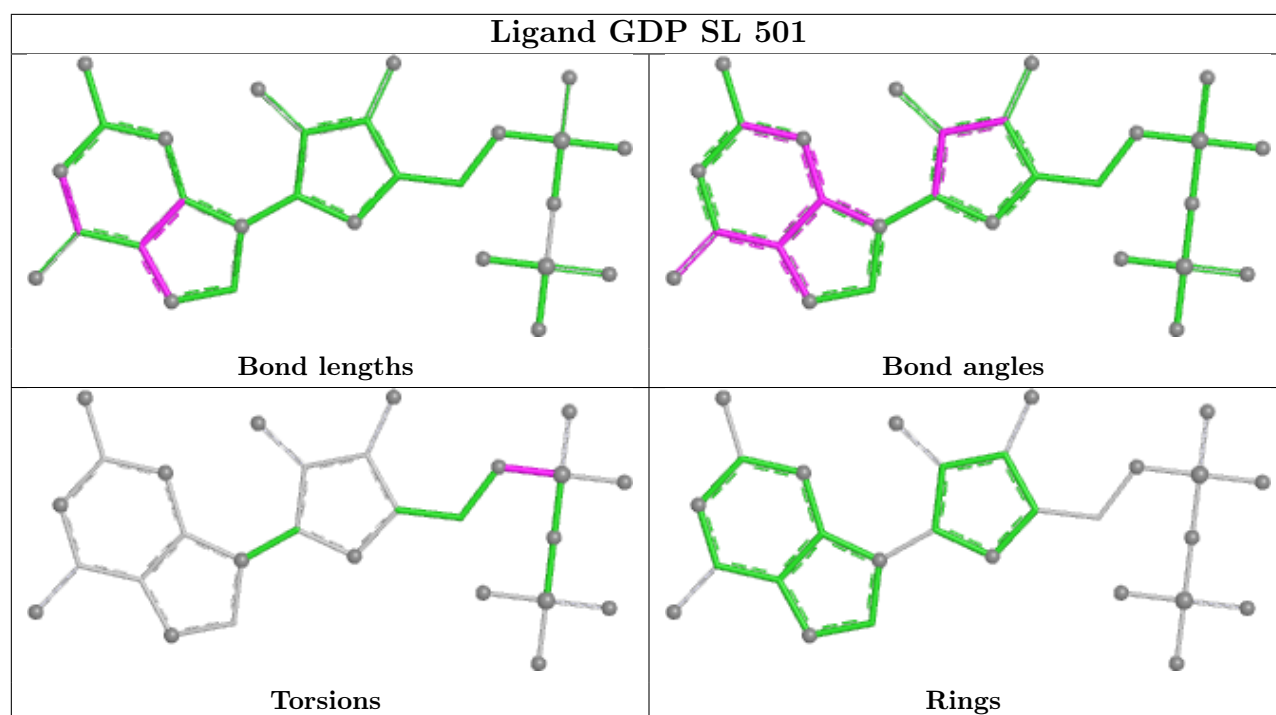


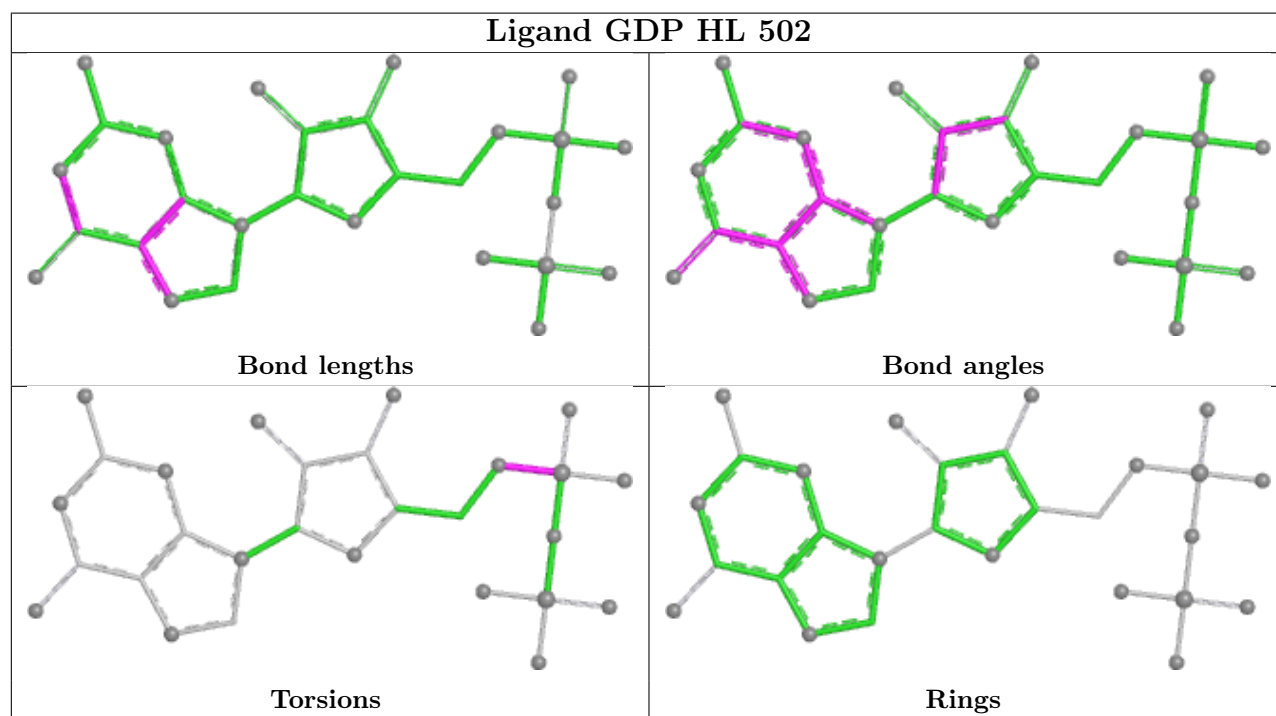
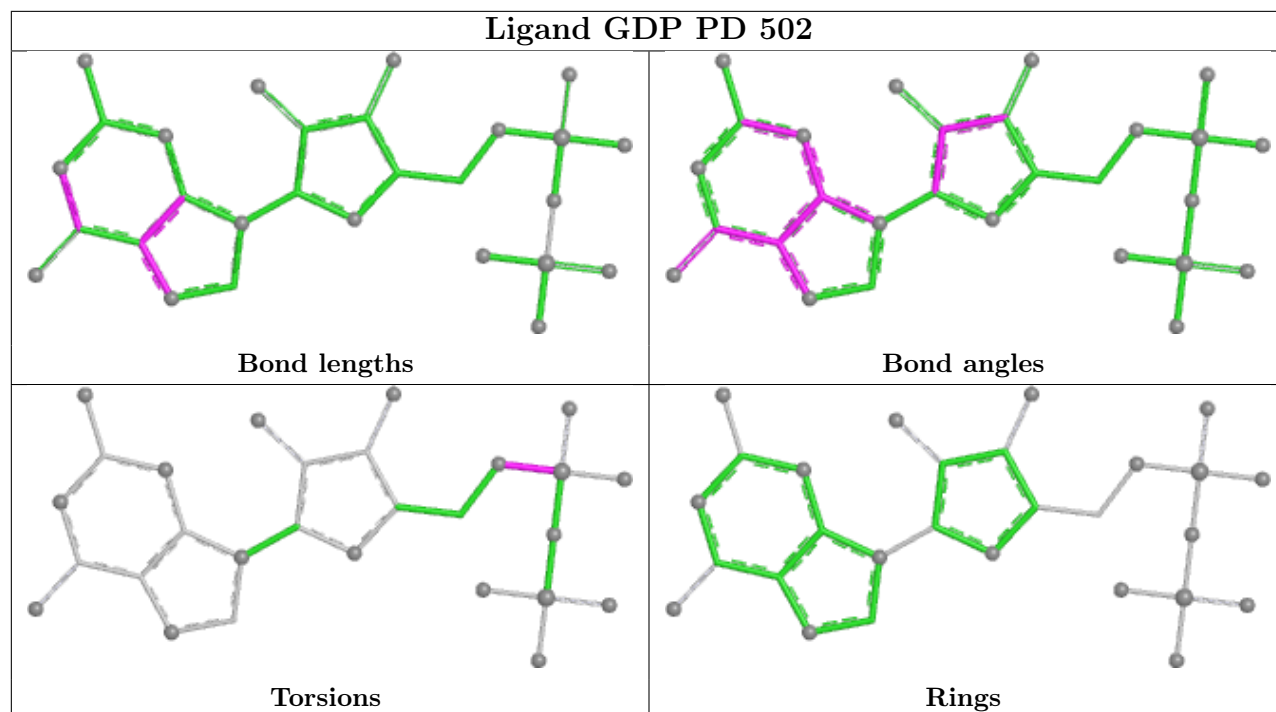
Ligand GTP PK 501

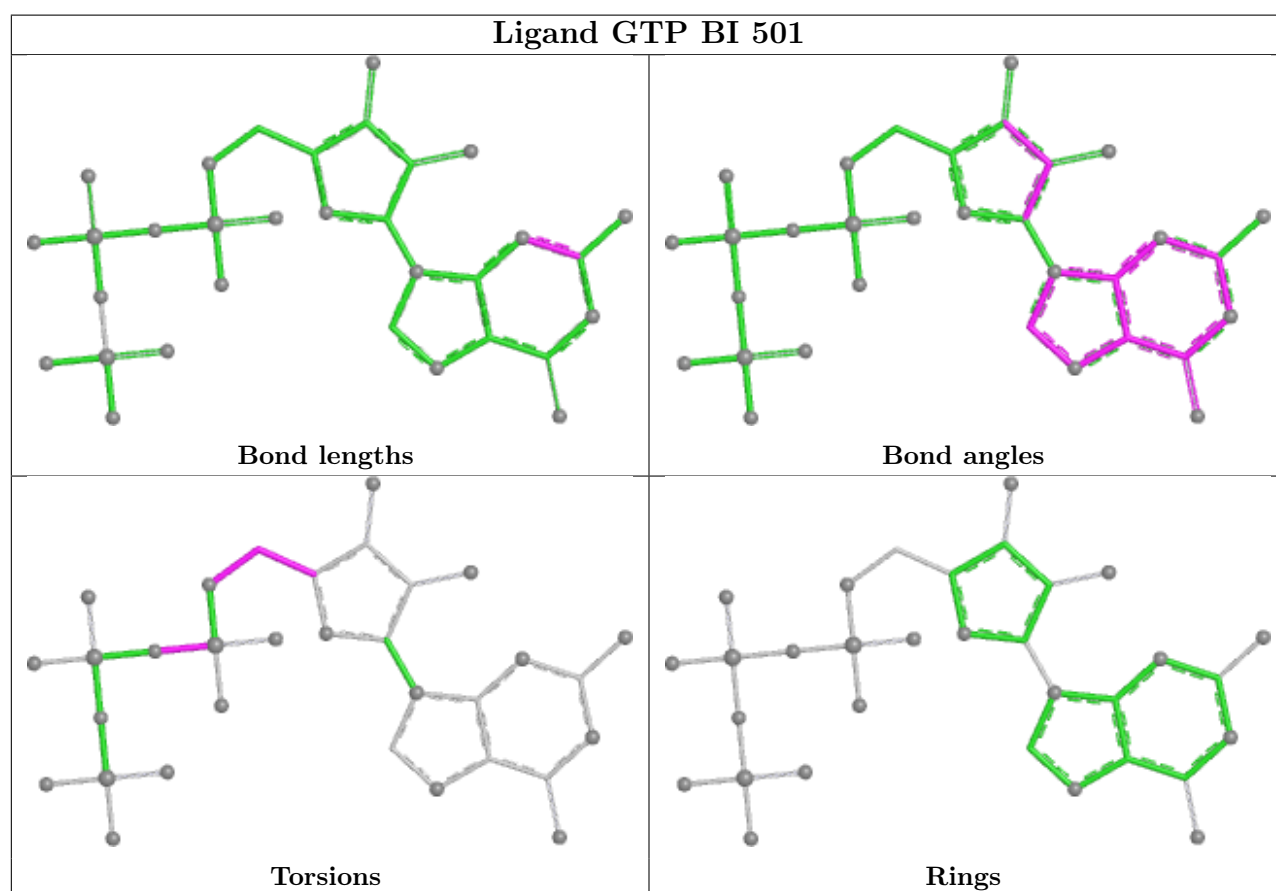
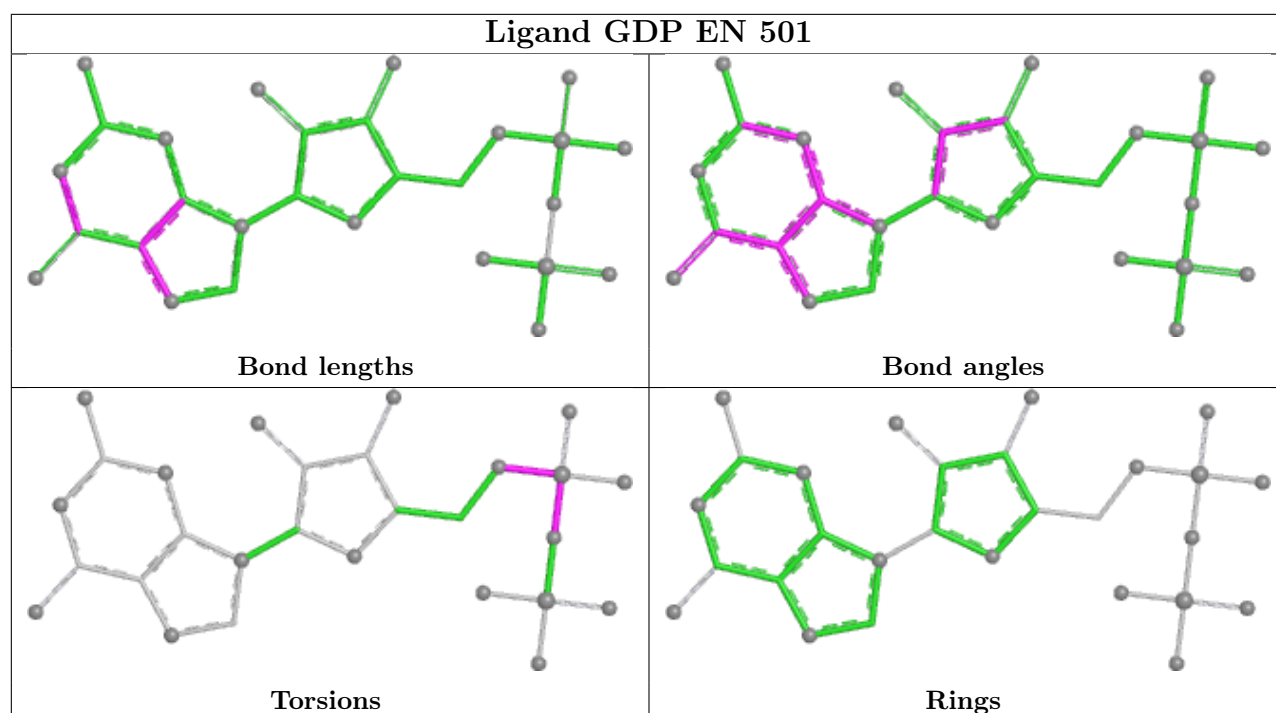


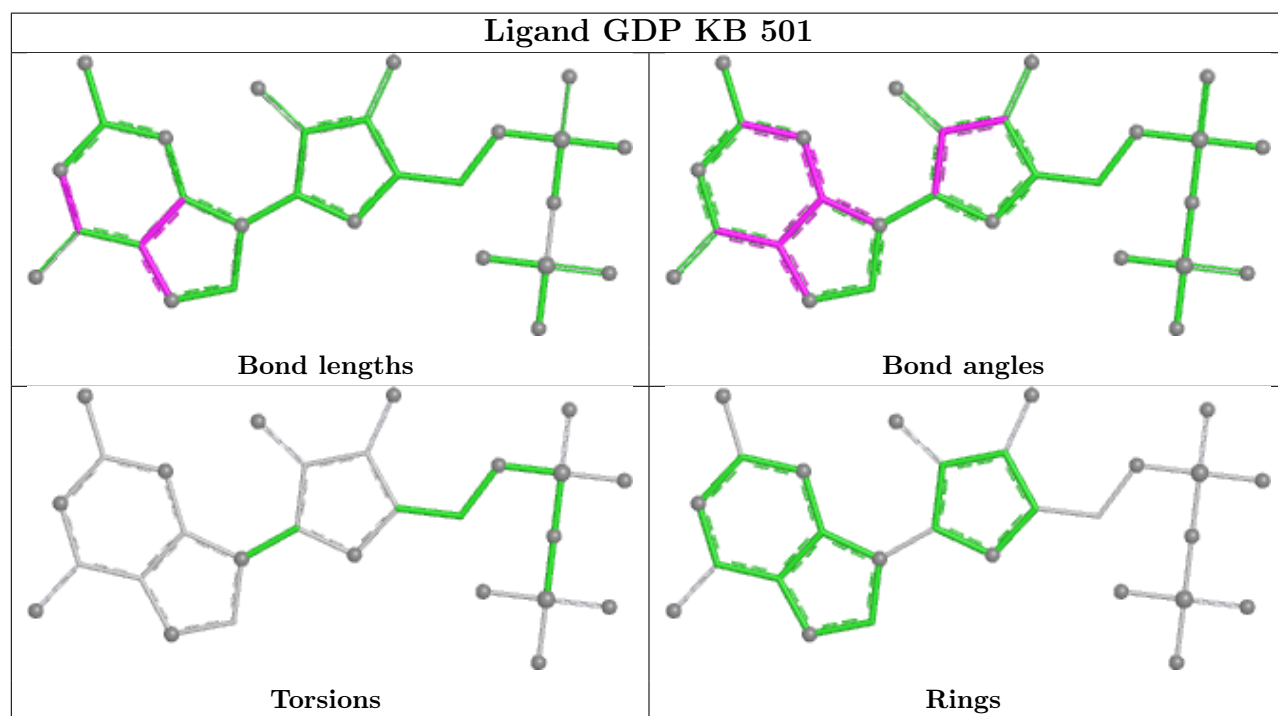
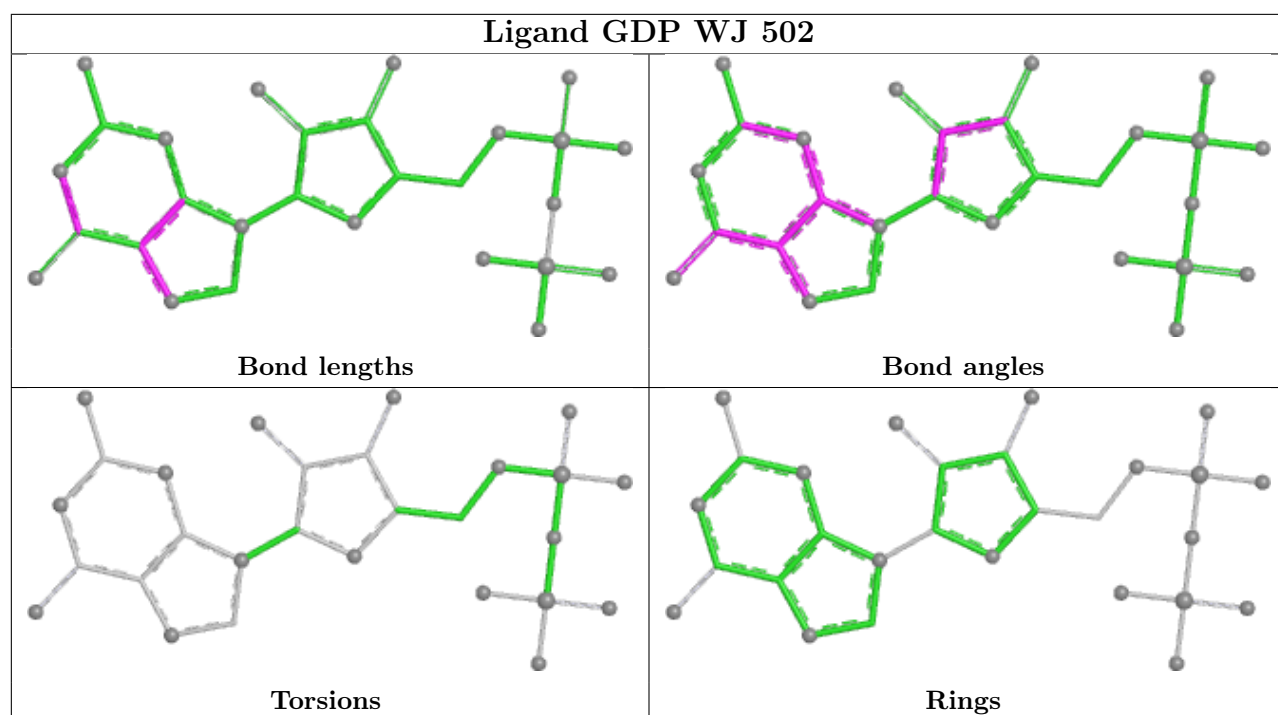


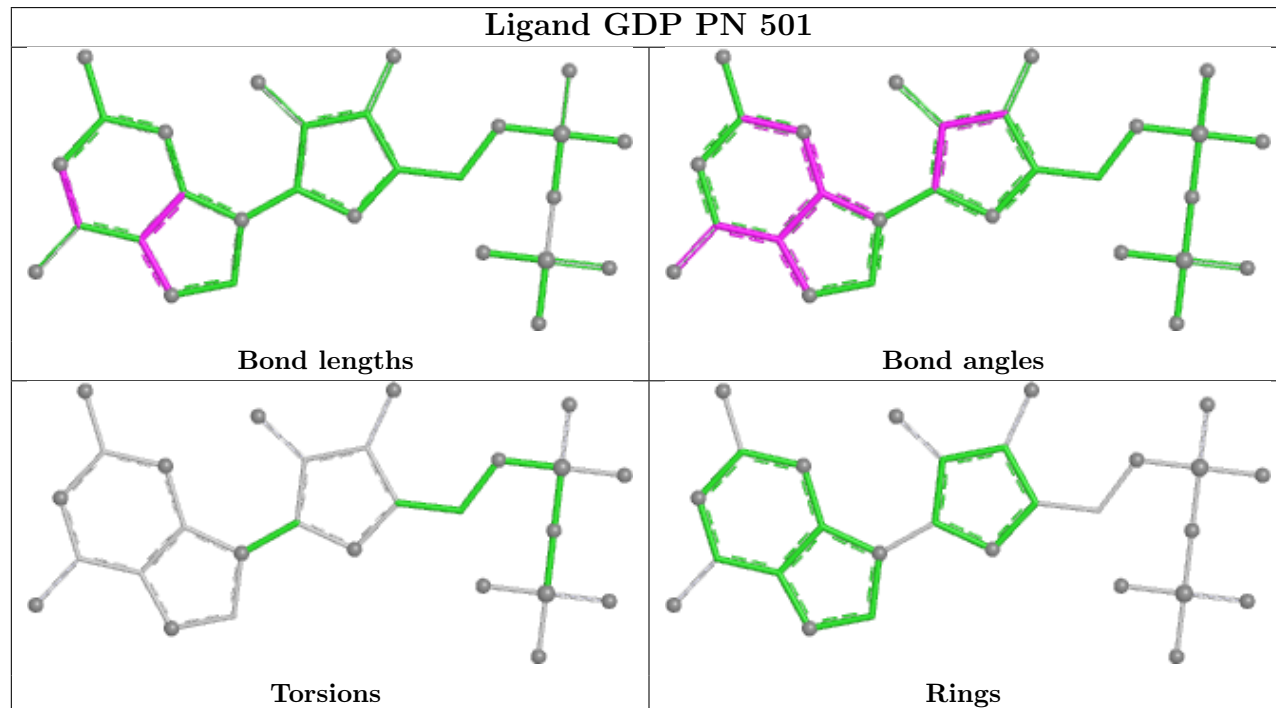
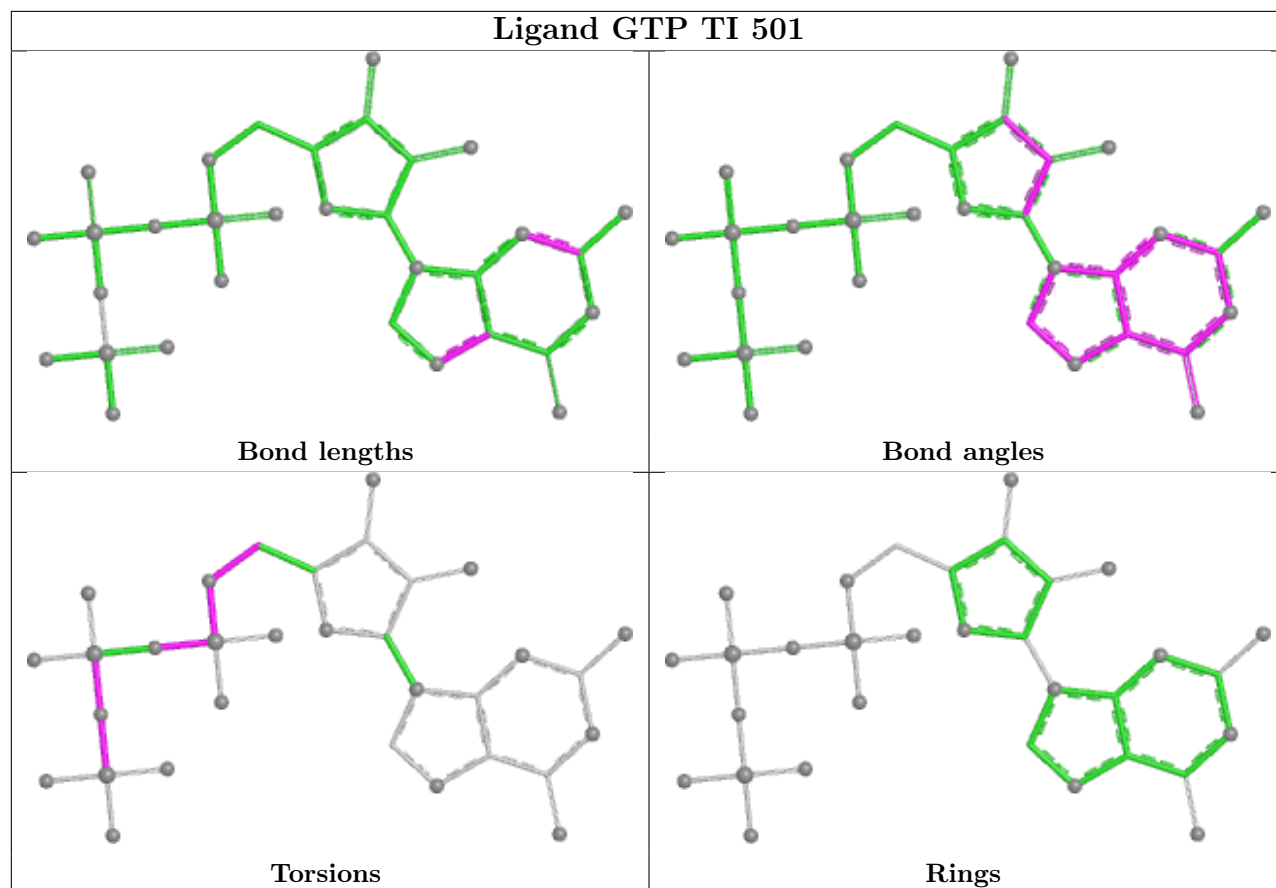


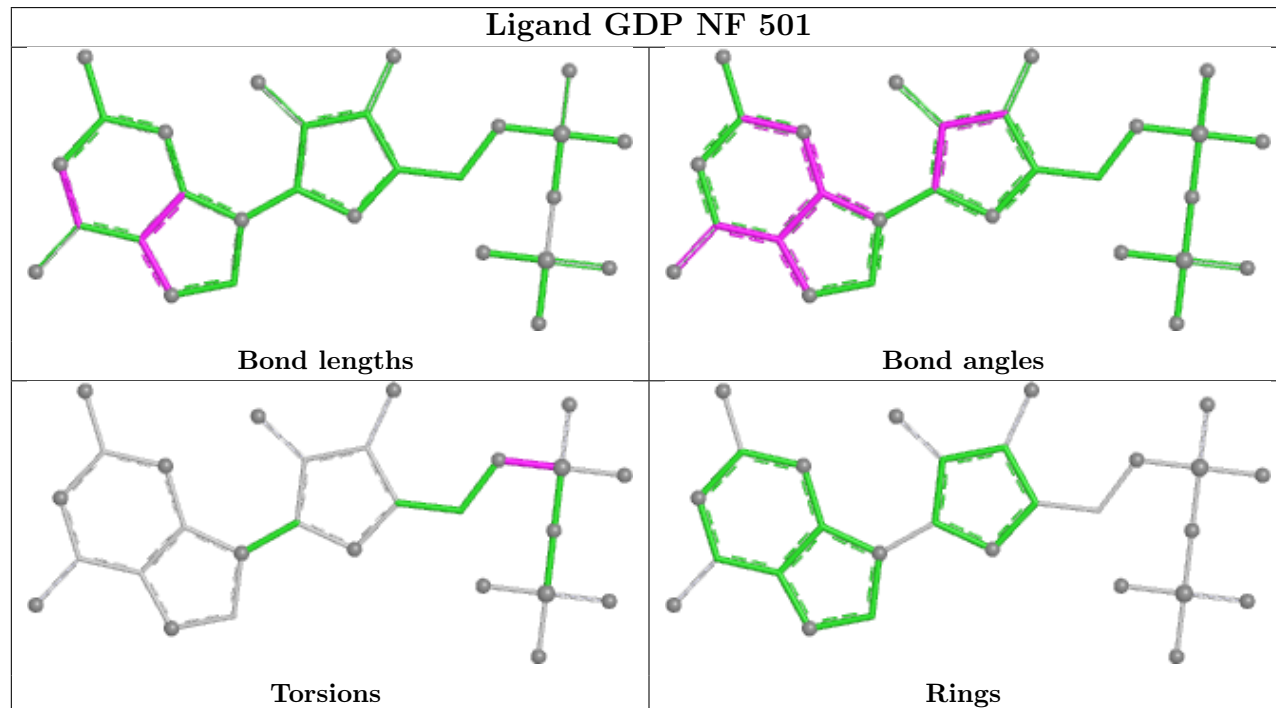
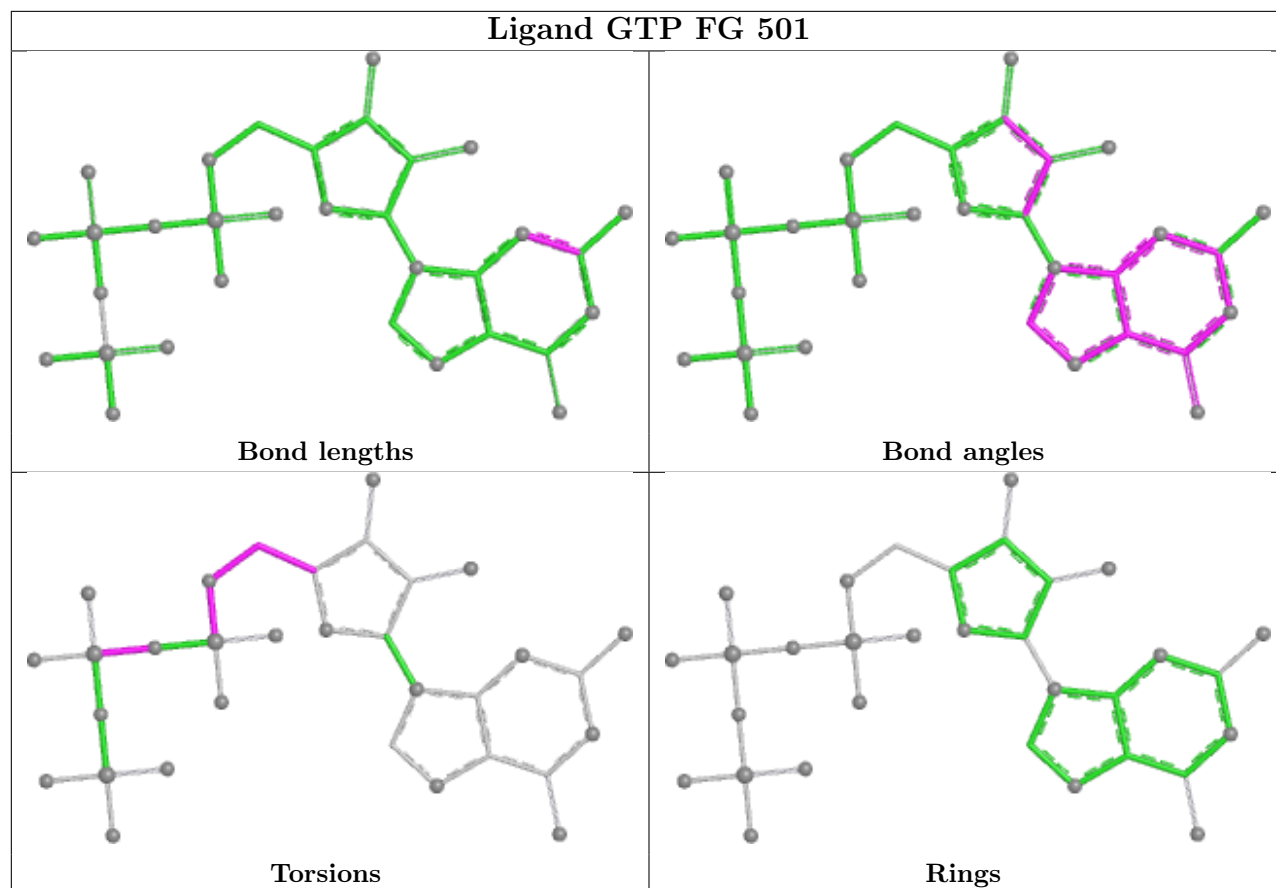


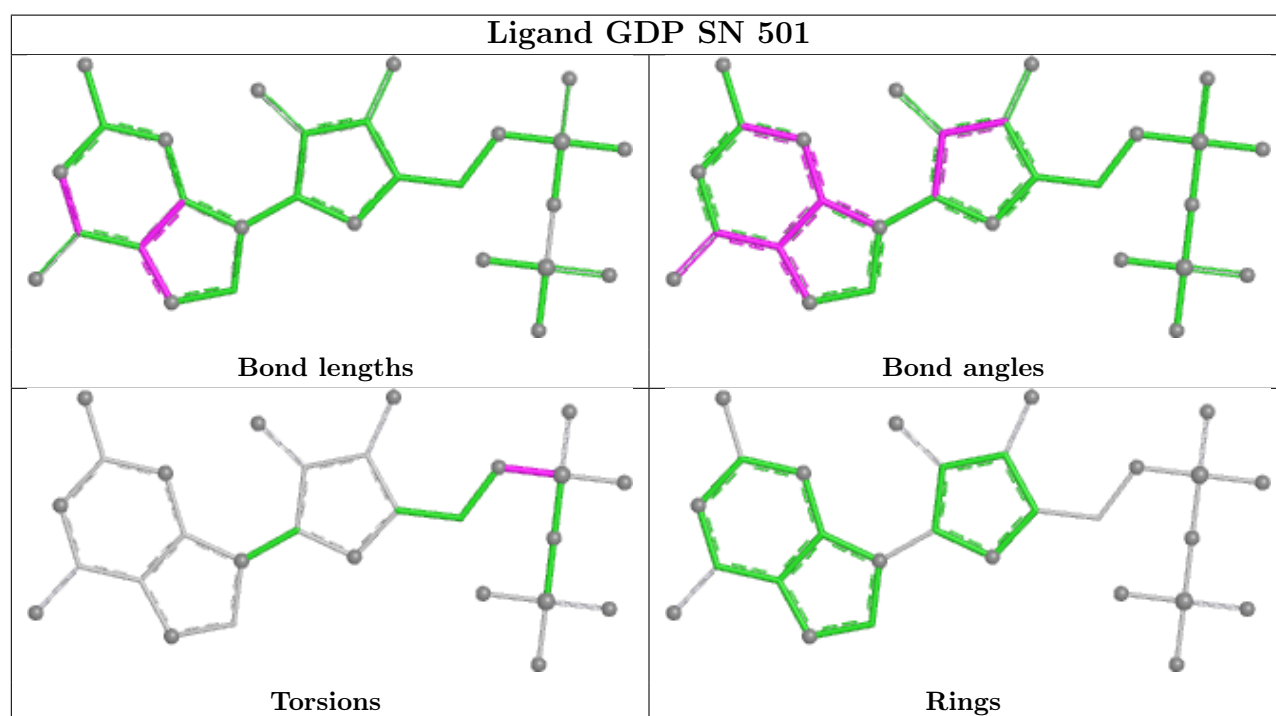
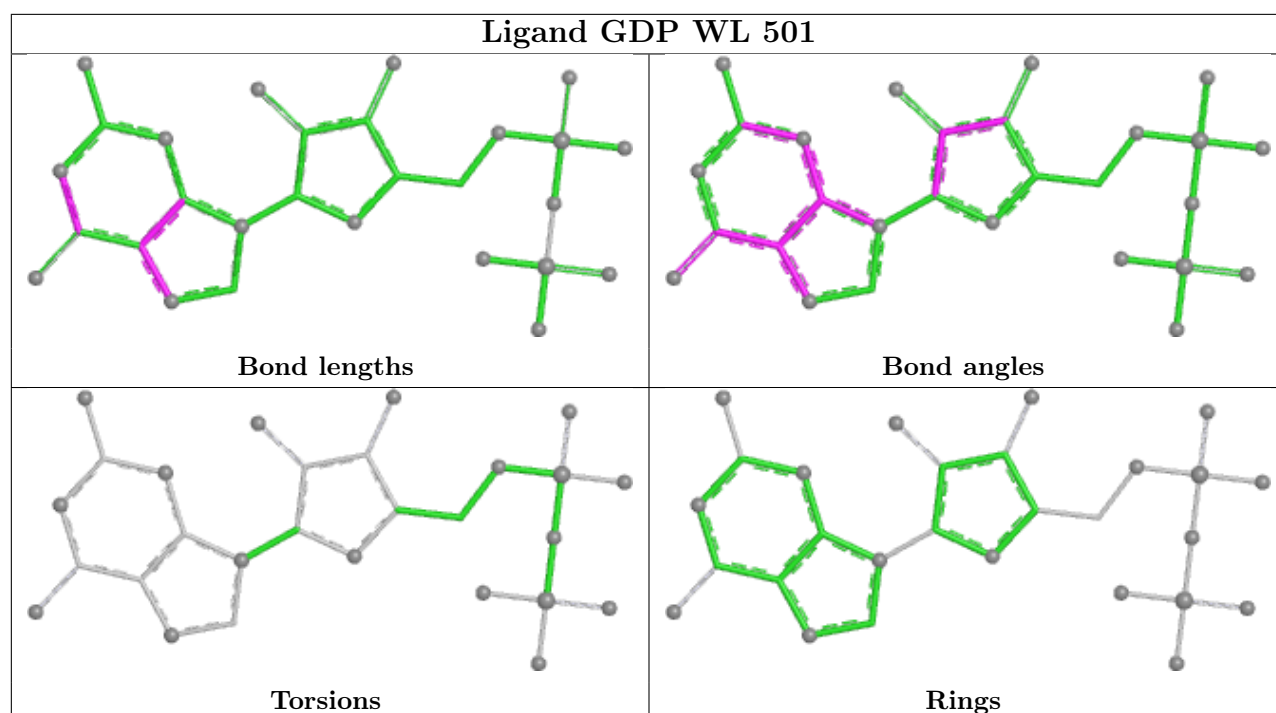


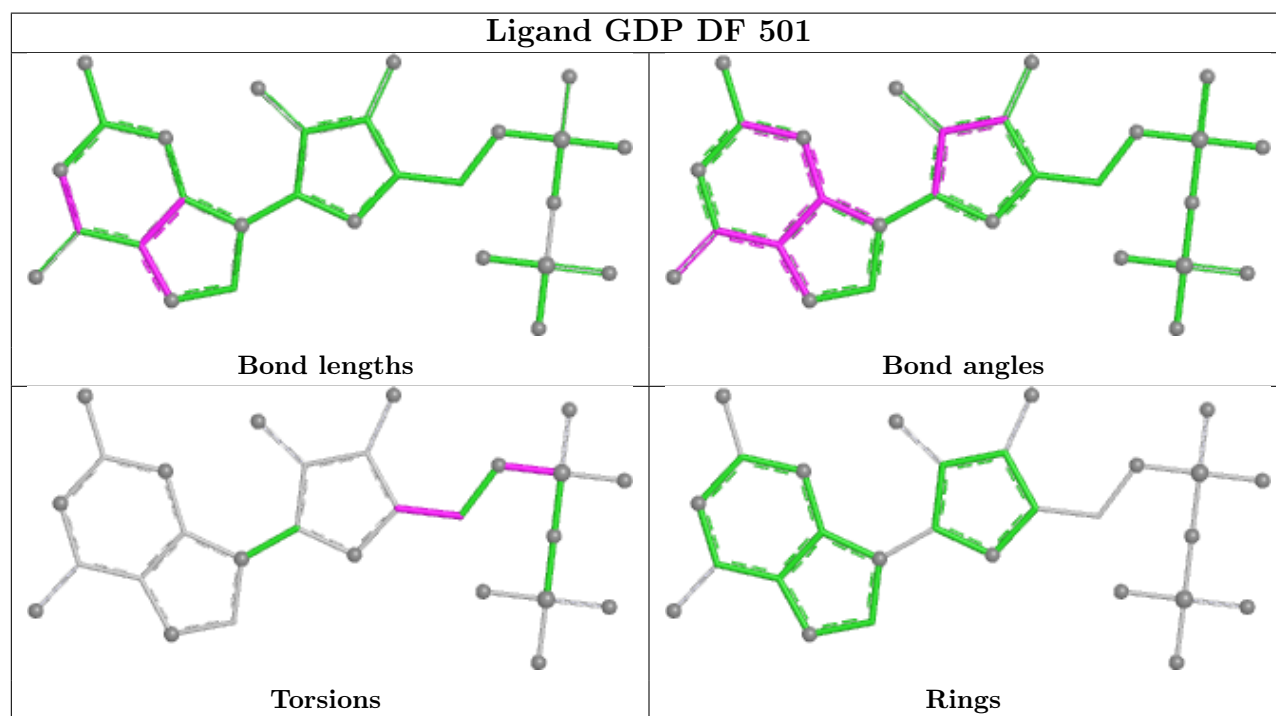
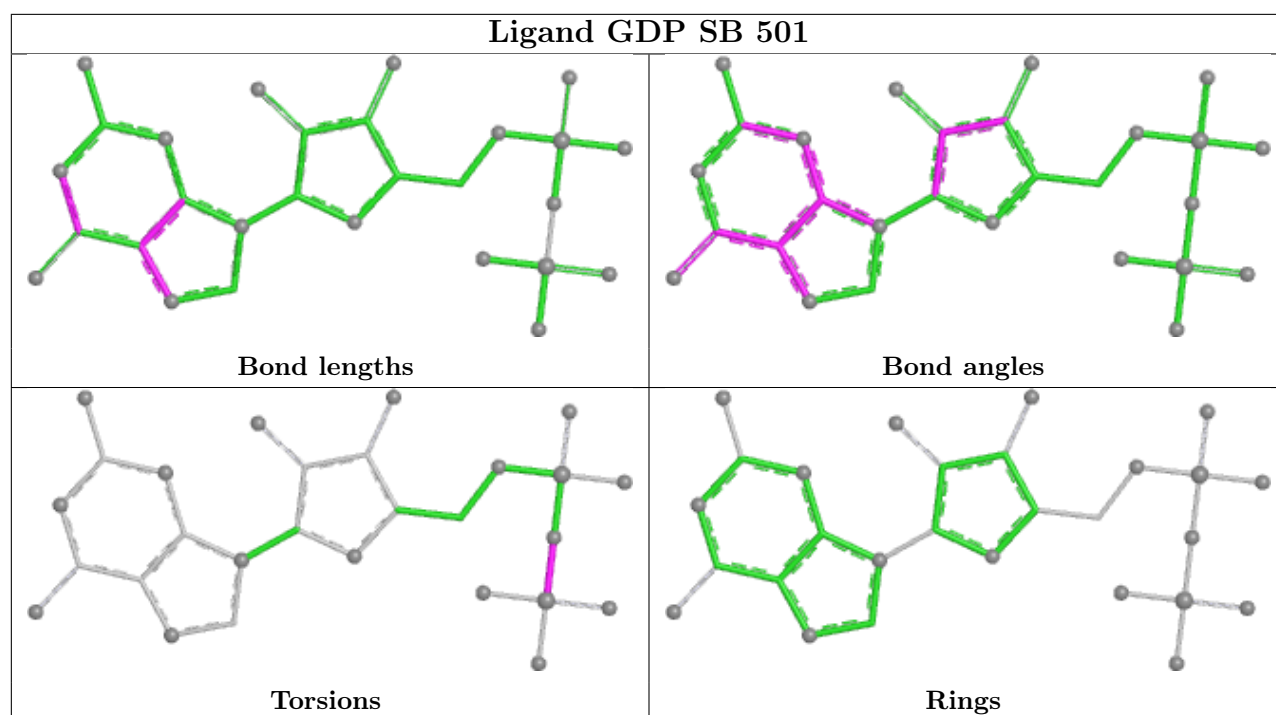


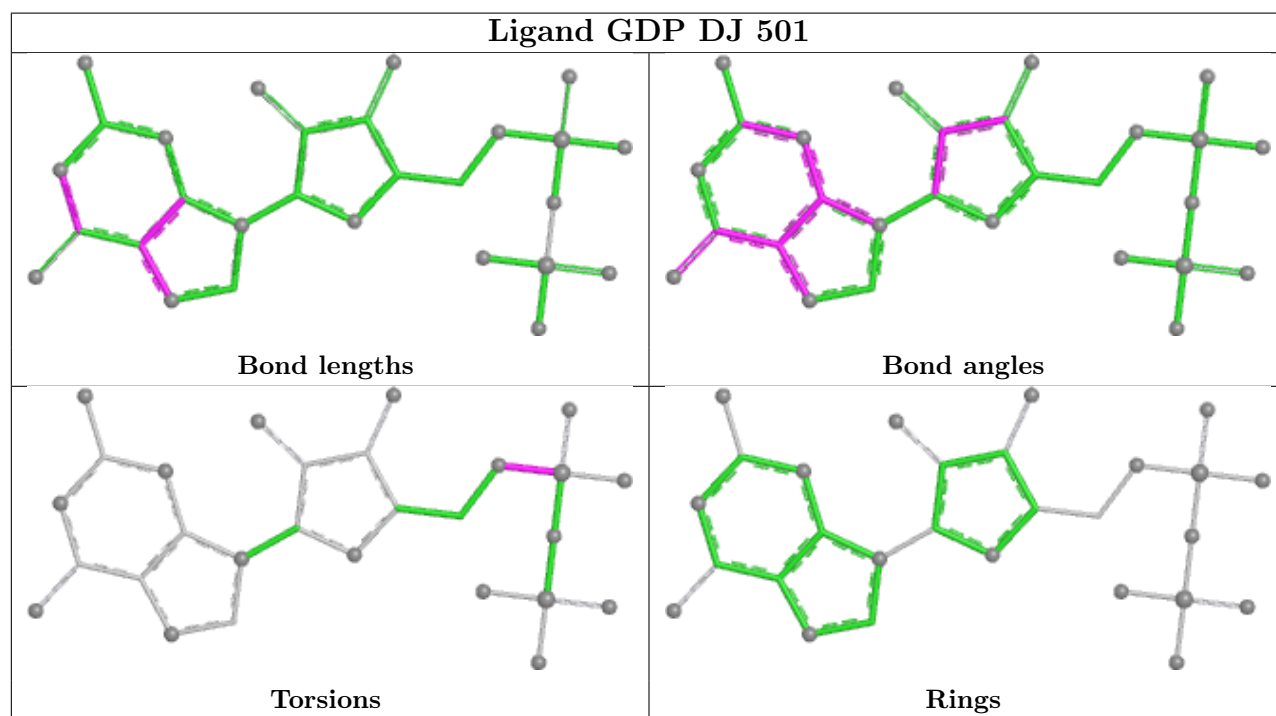
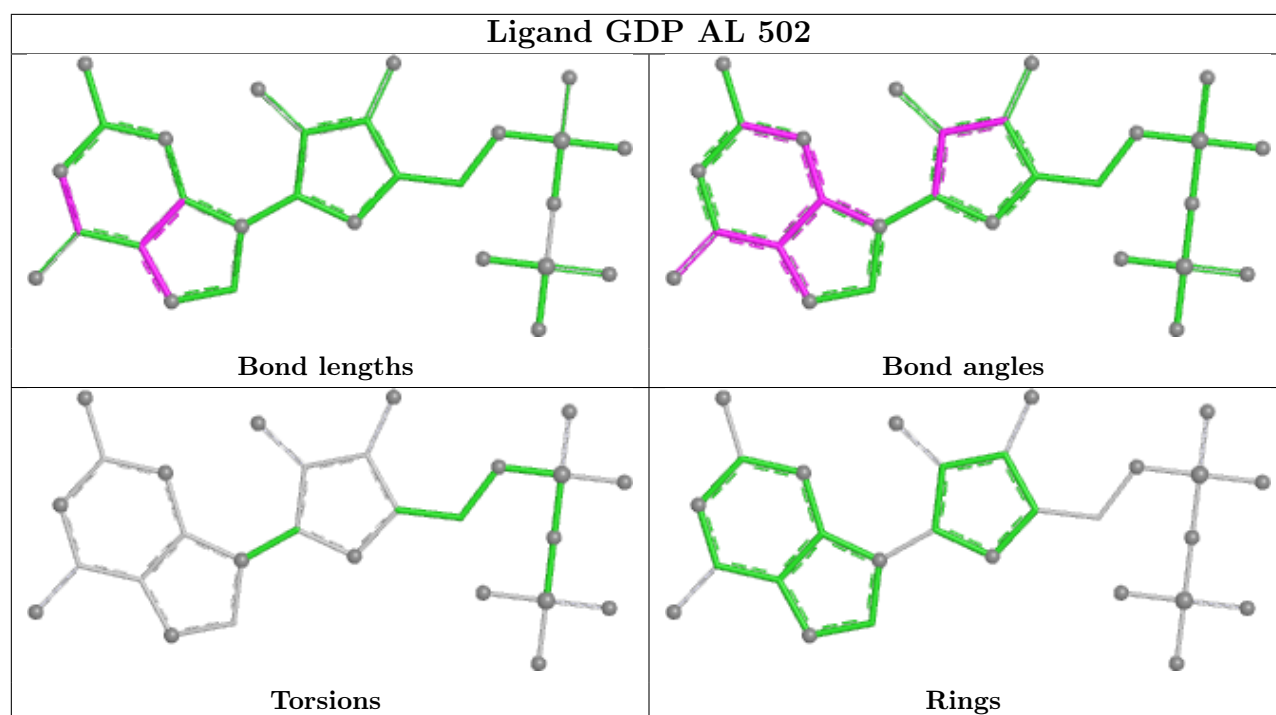


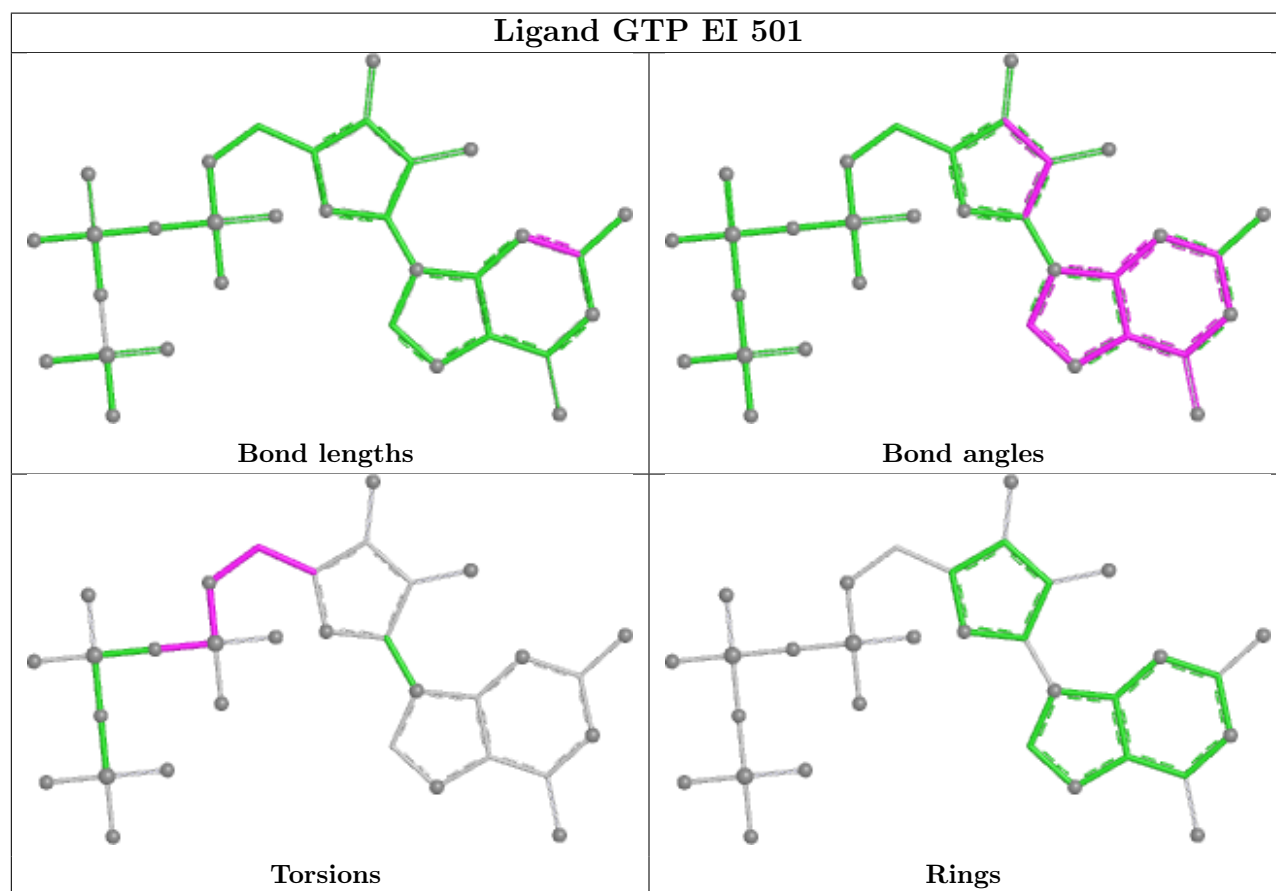
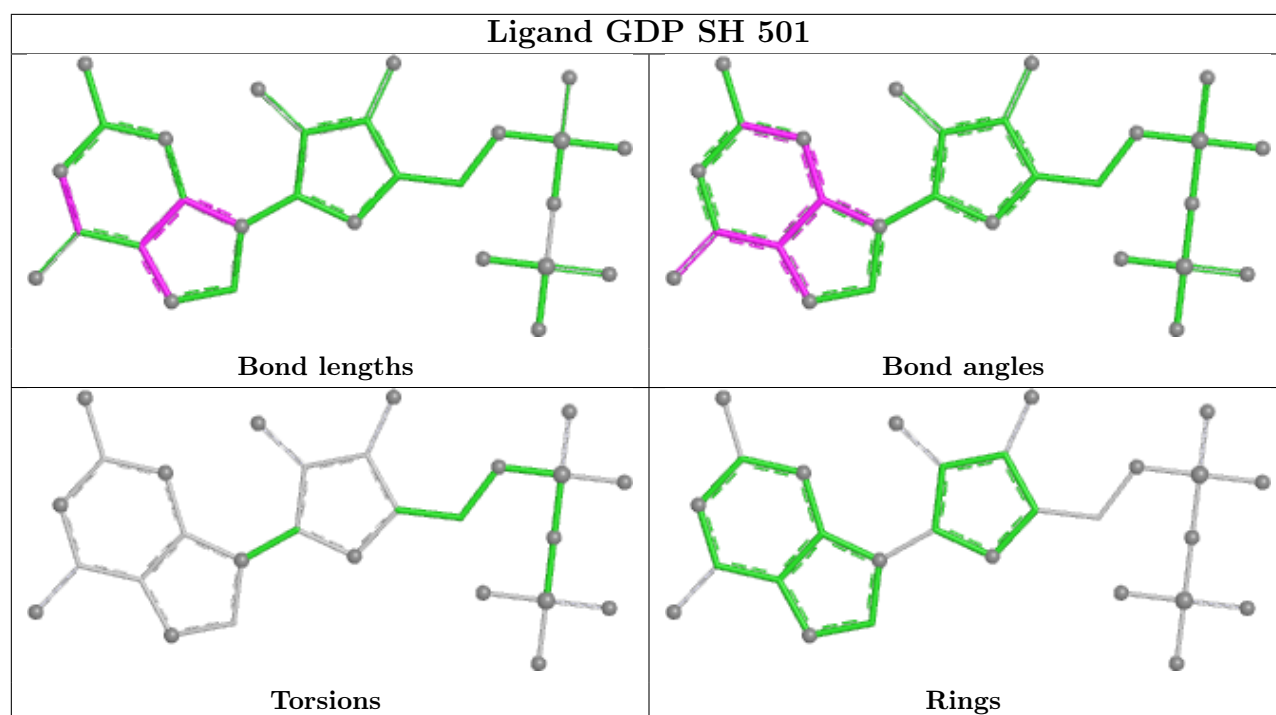


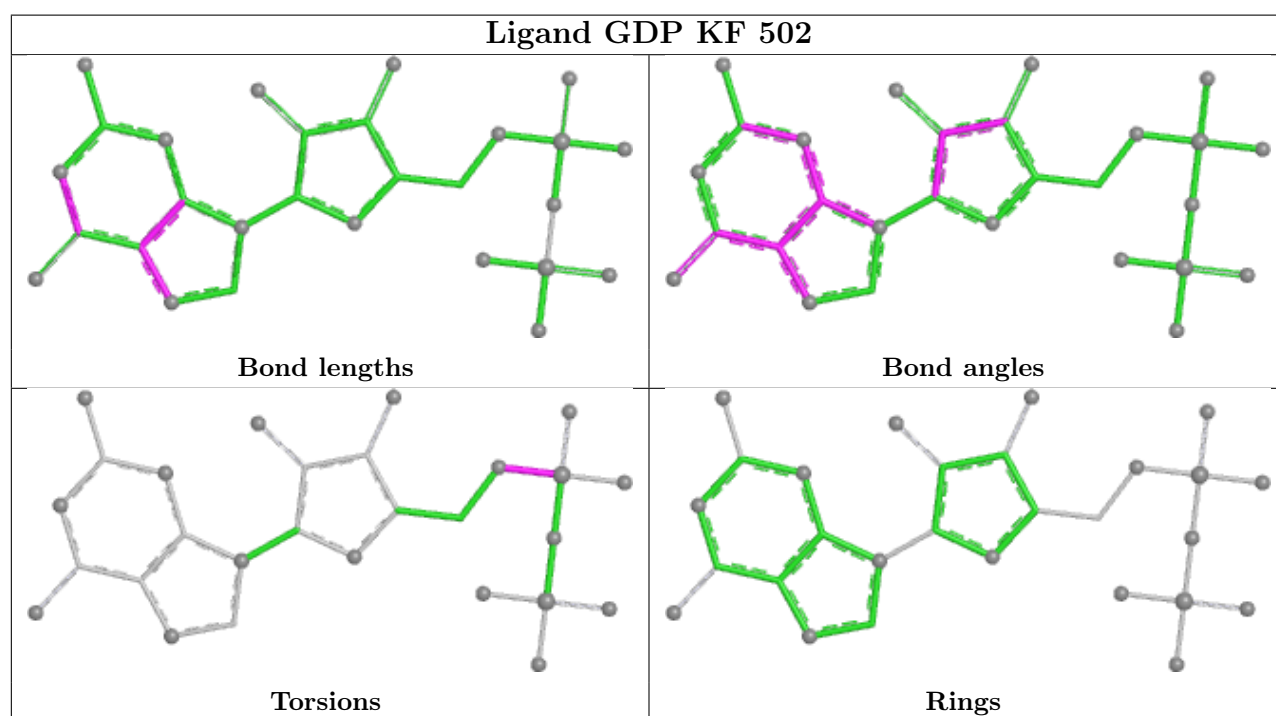
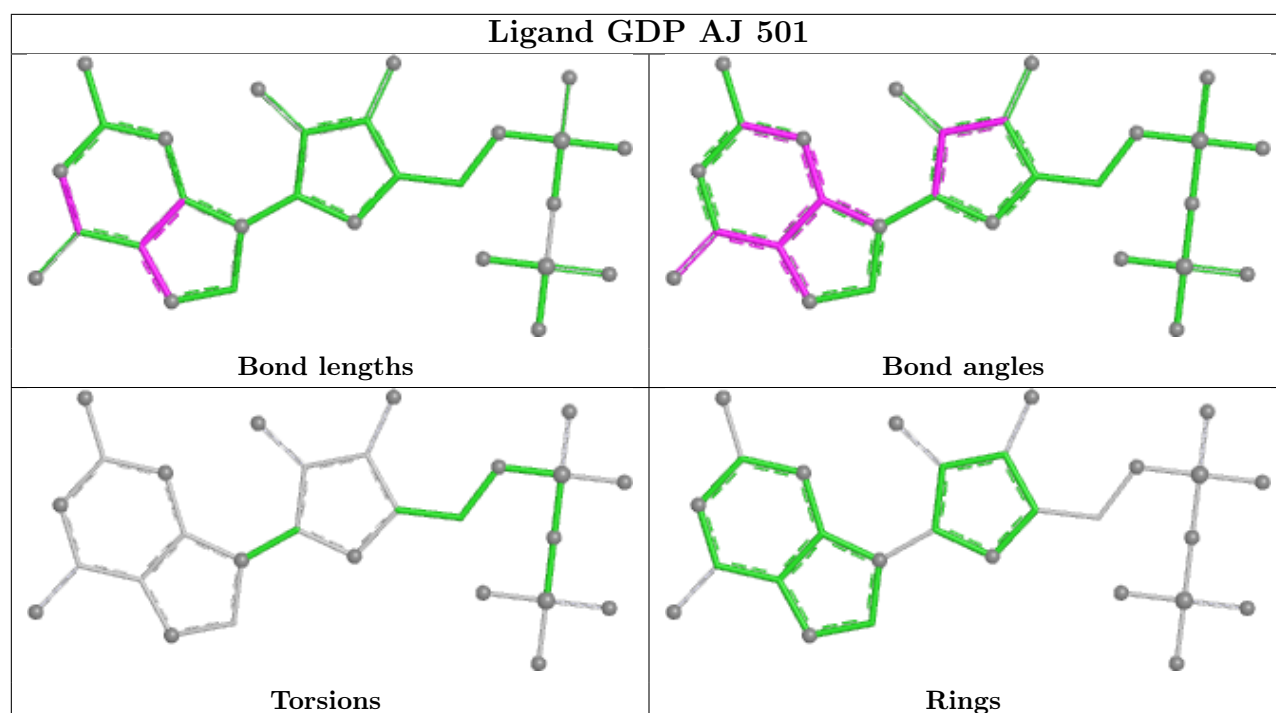




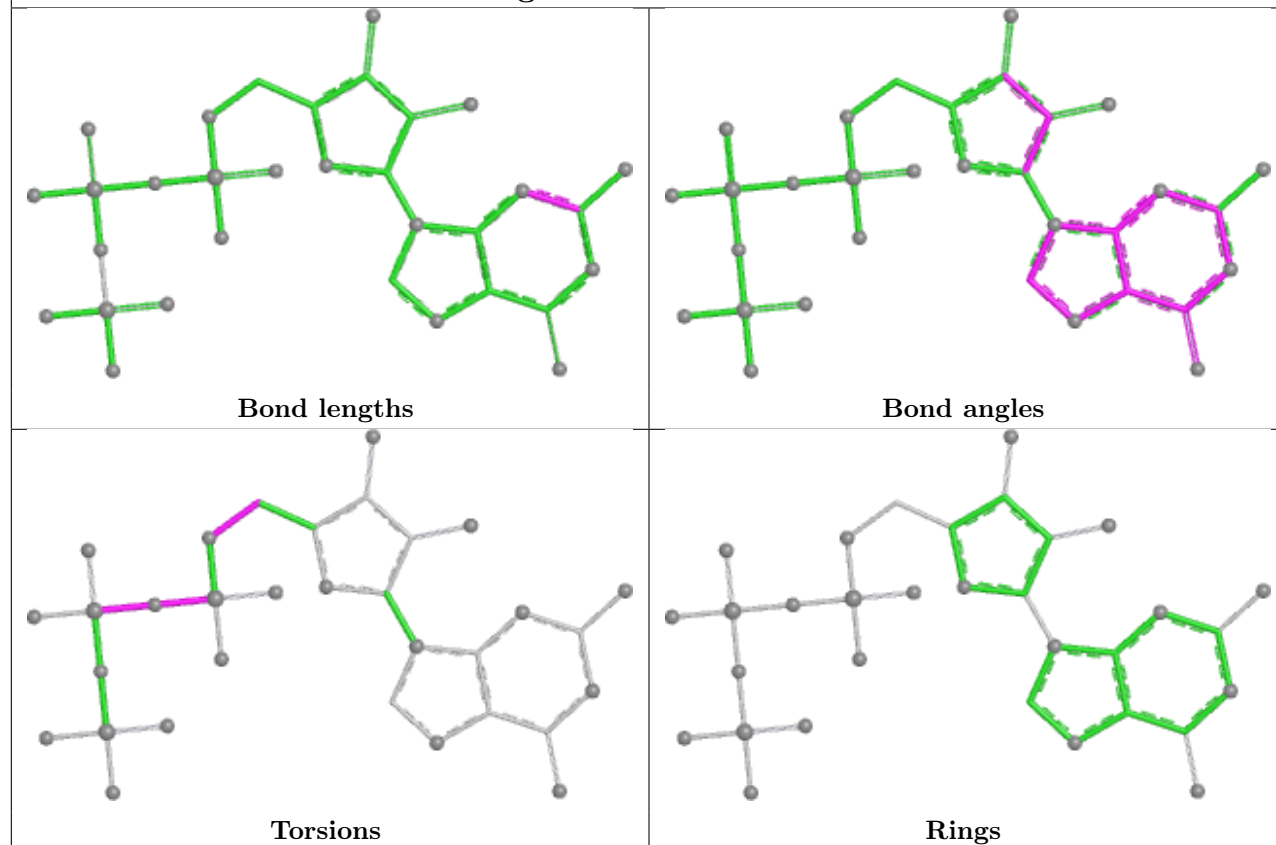




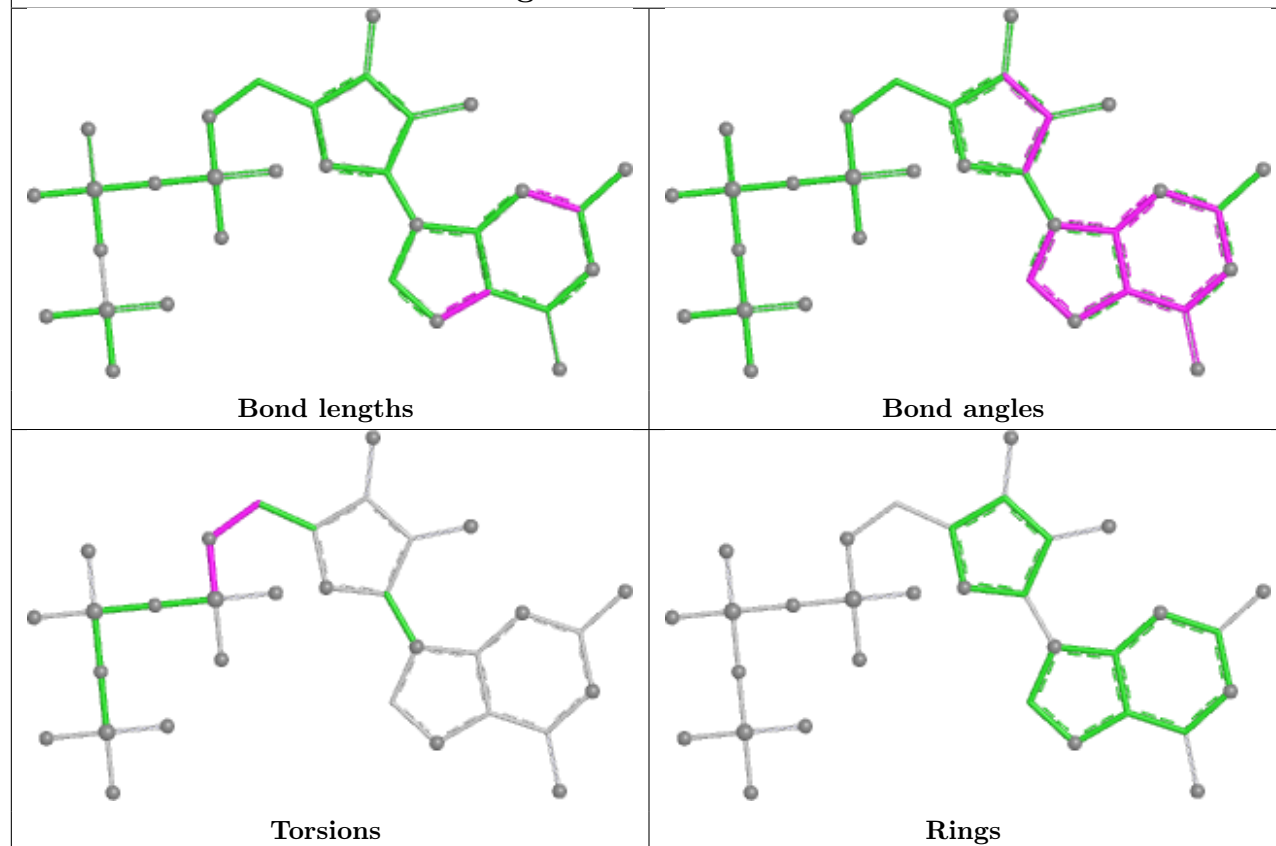


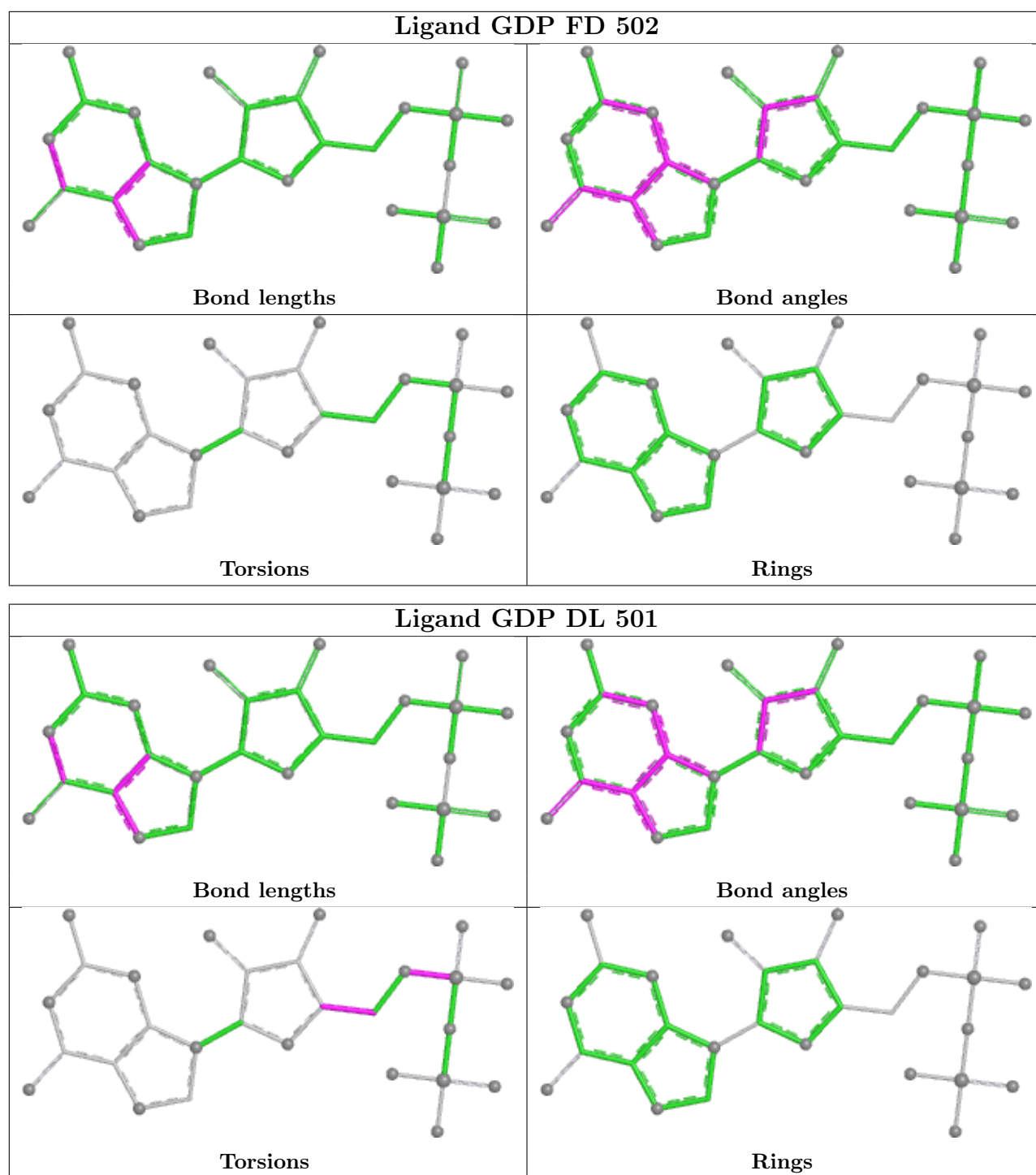


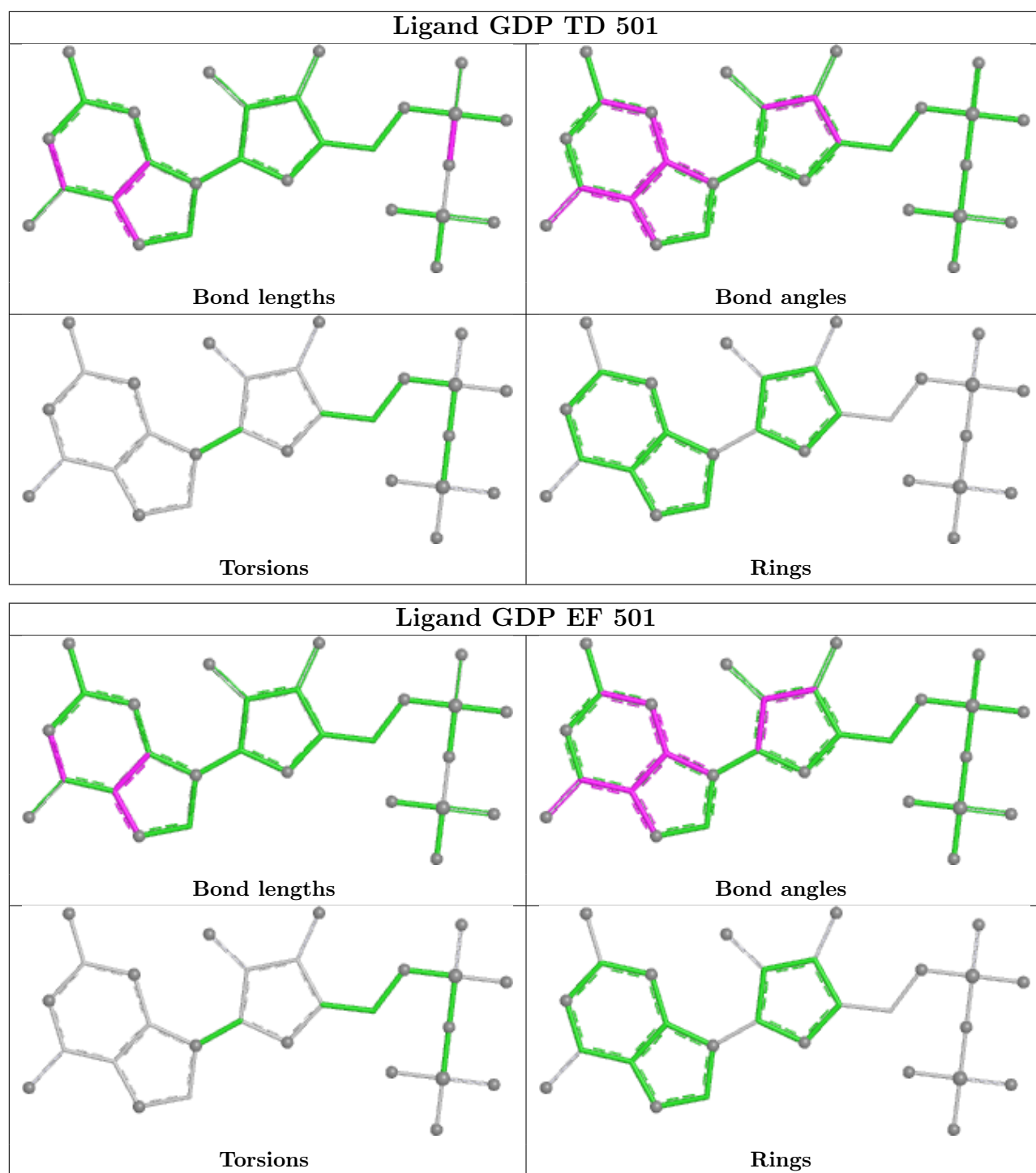
Ligand GTP RC 501

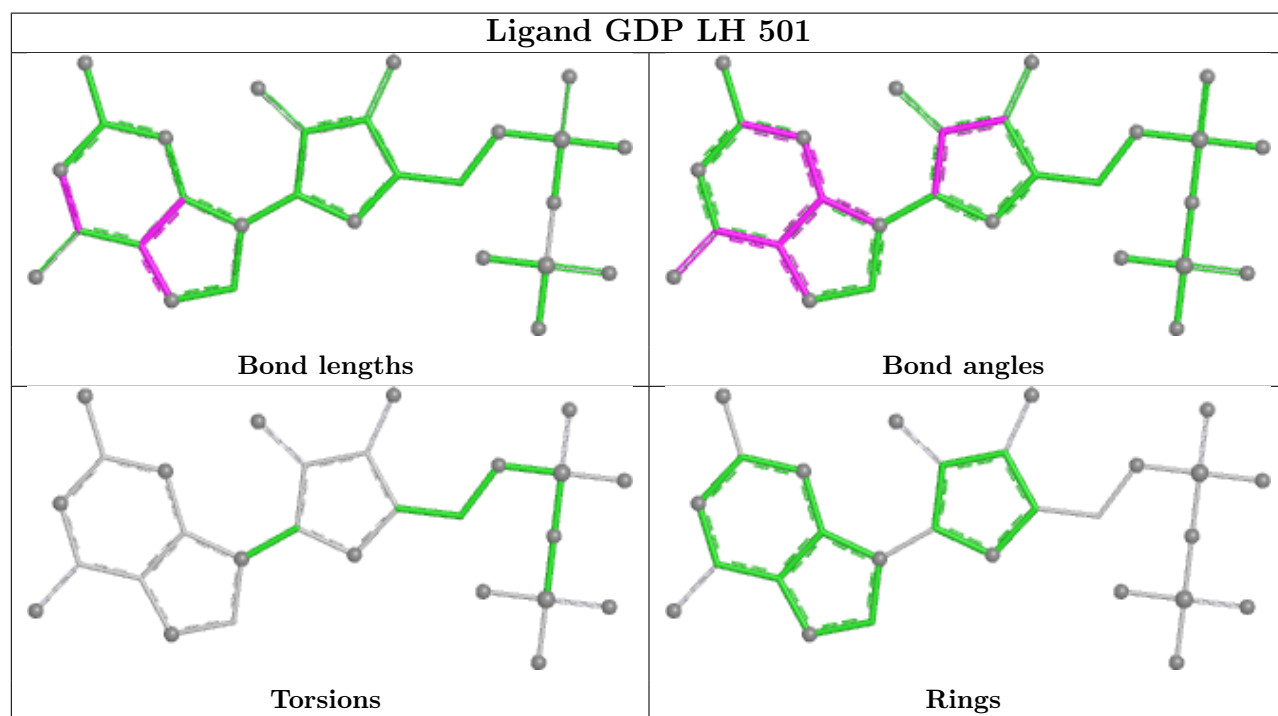
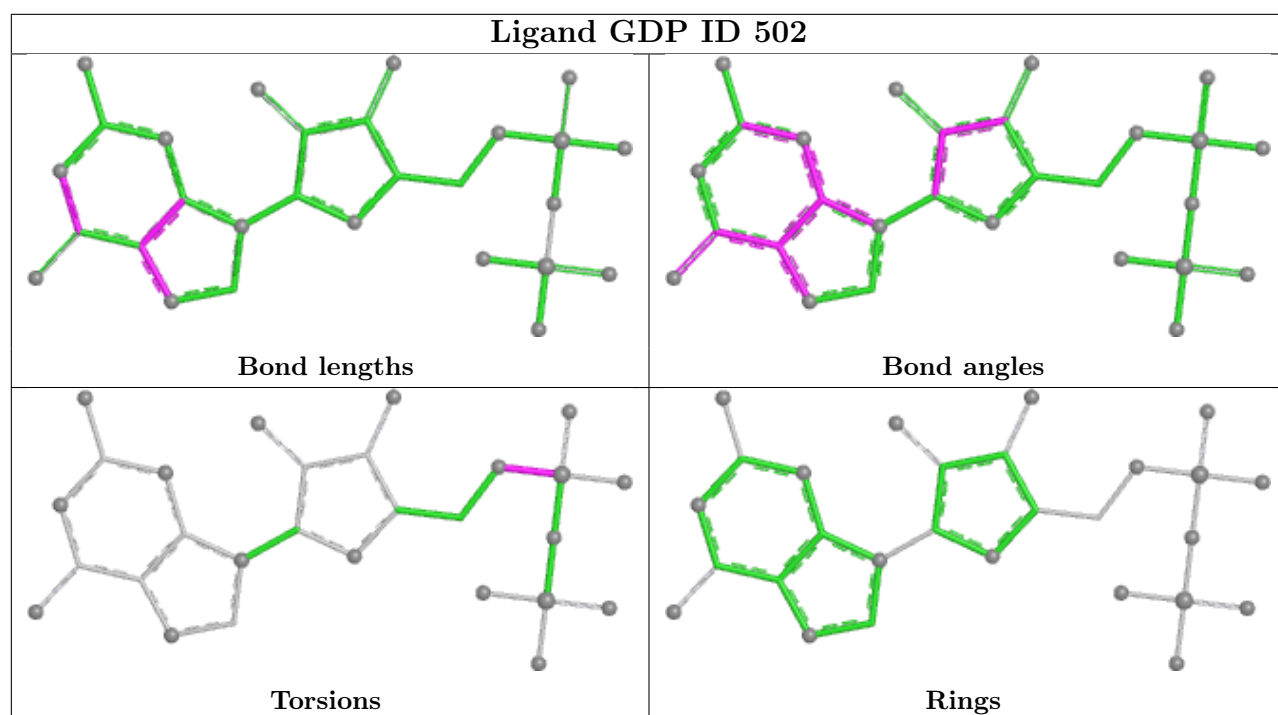


Ligand GTP BG 501

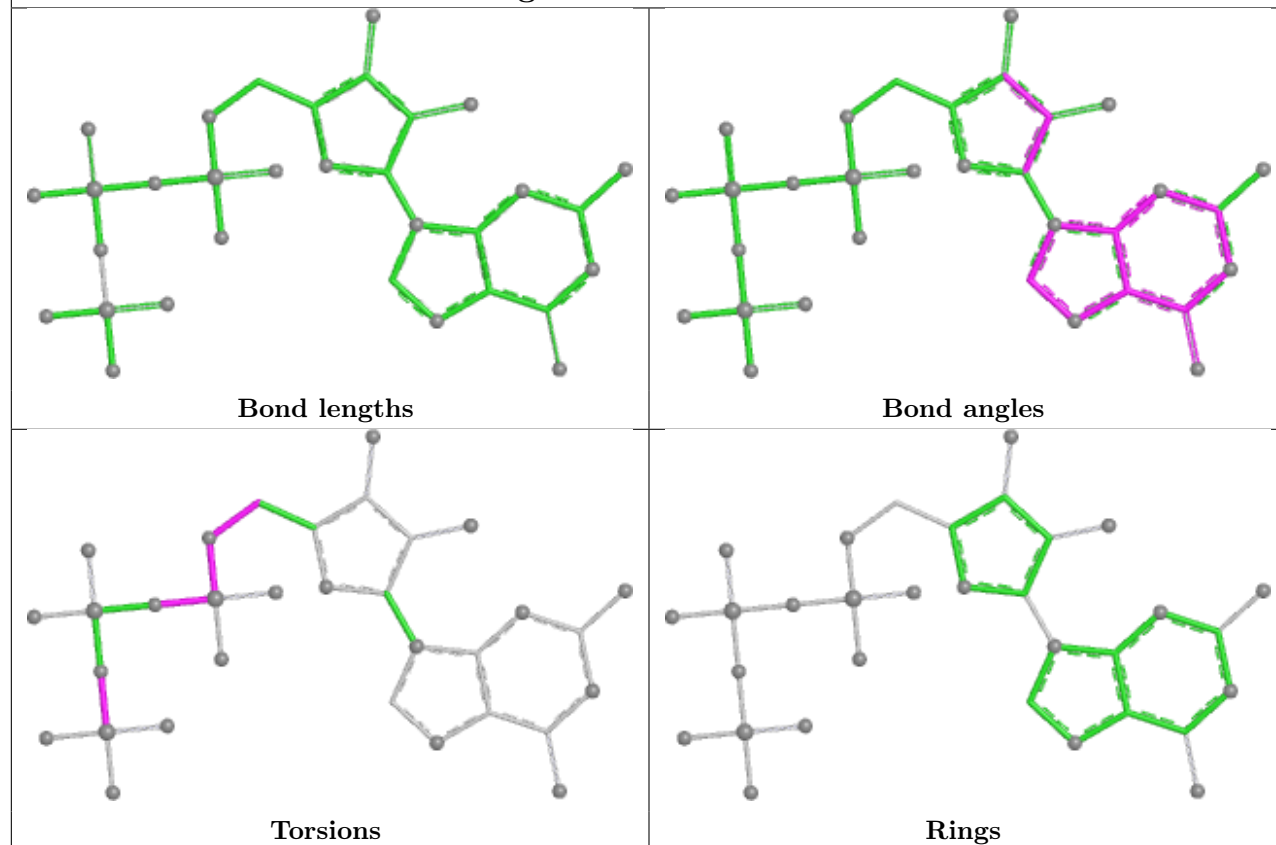




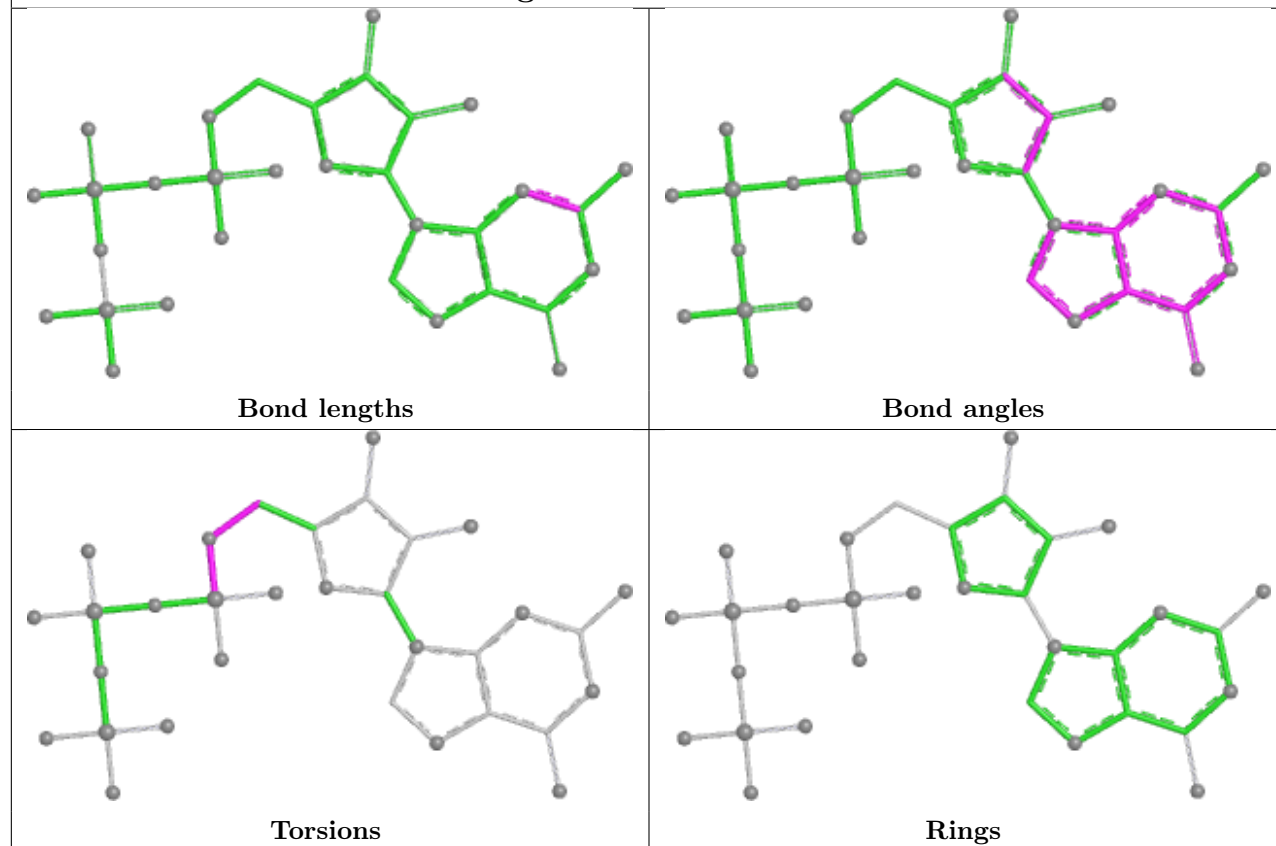


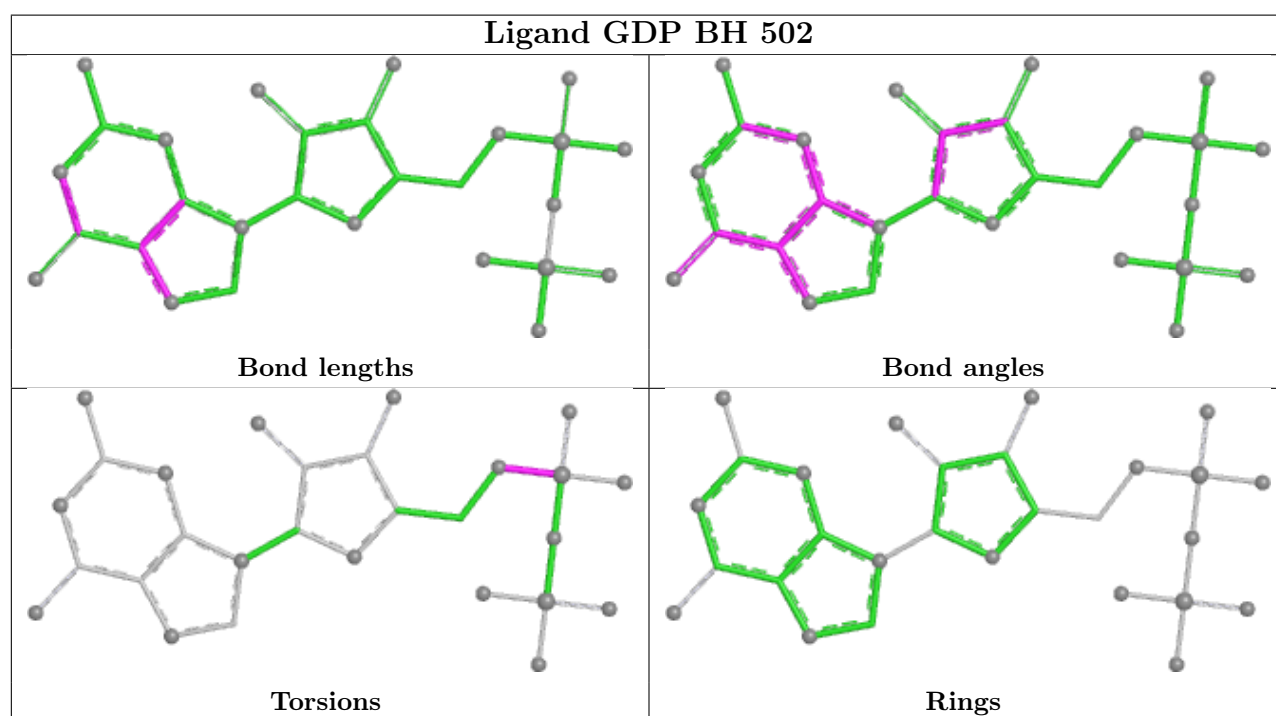
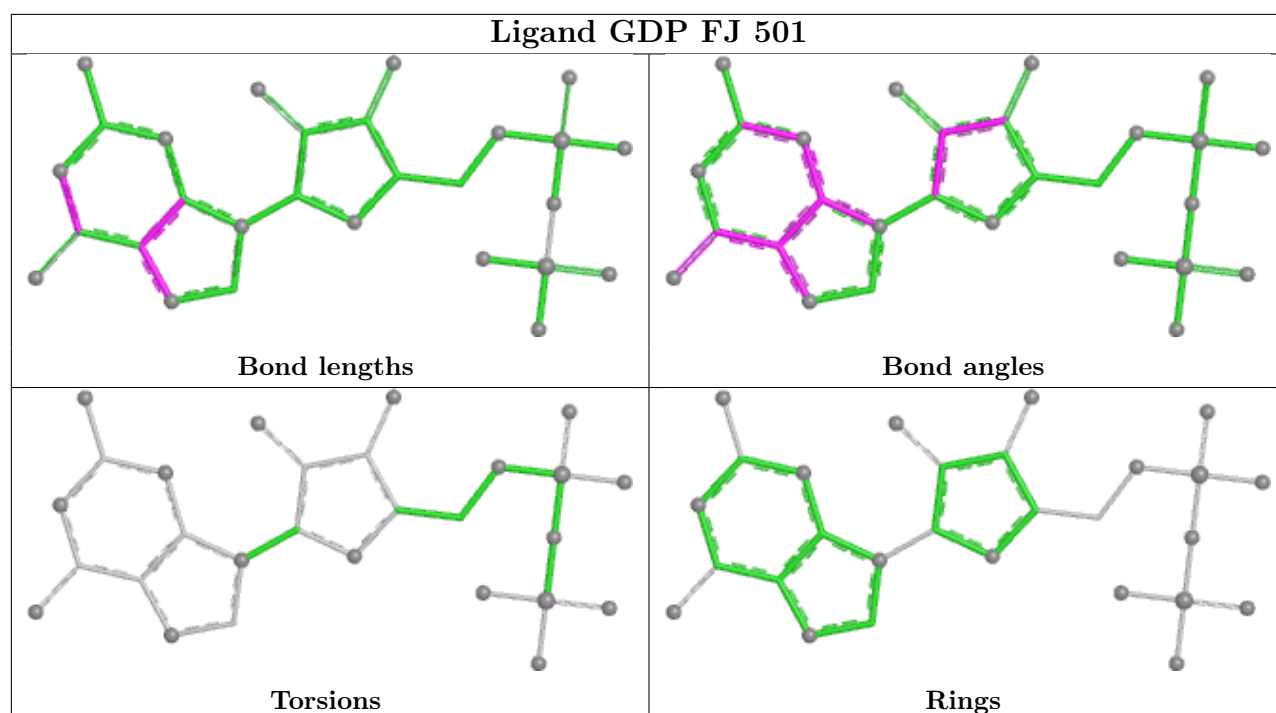


Ligand GTP DE 501

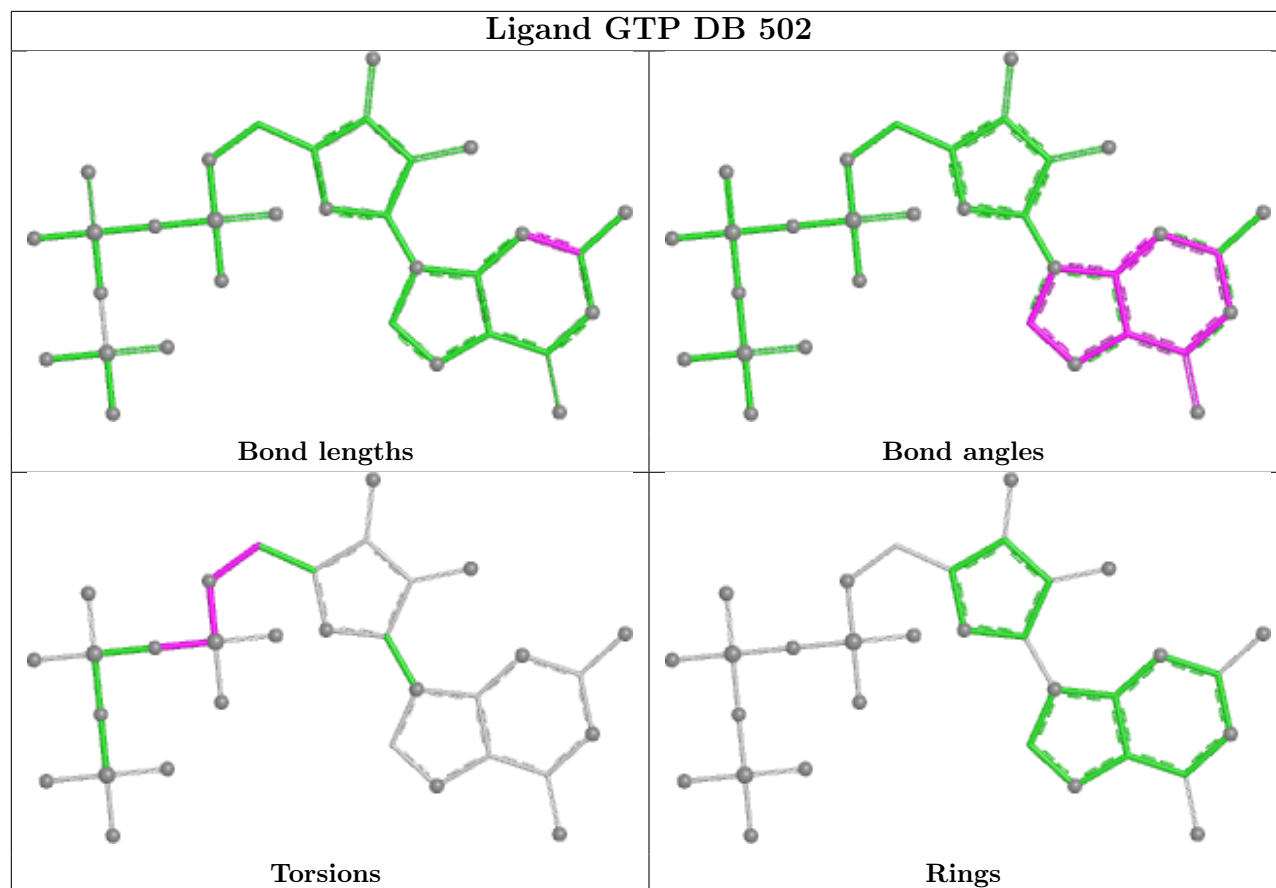


Ligand GTP OA 501

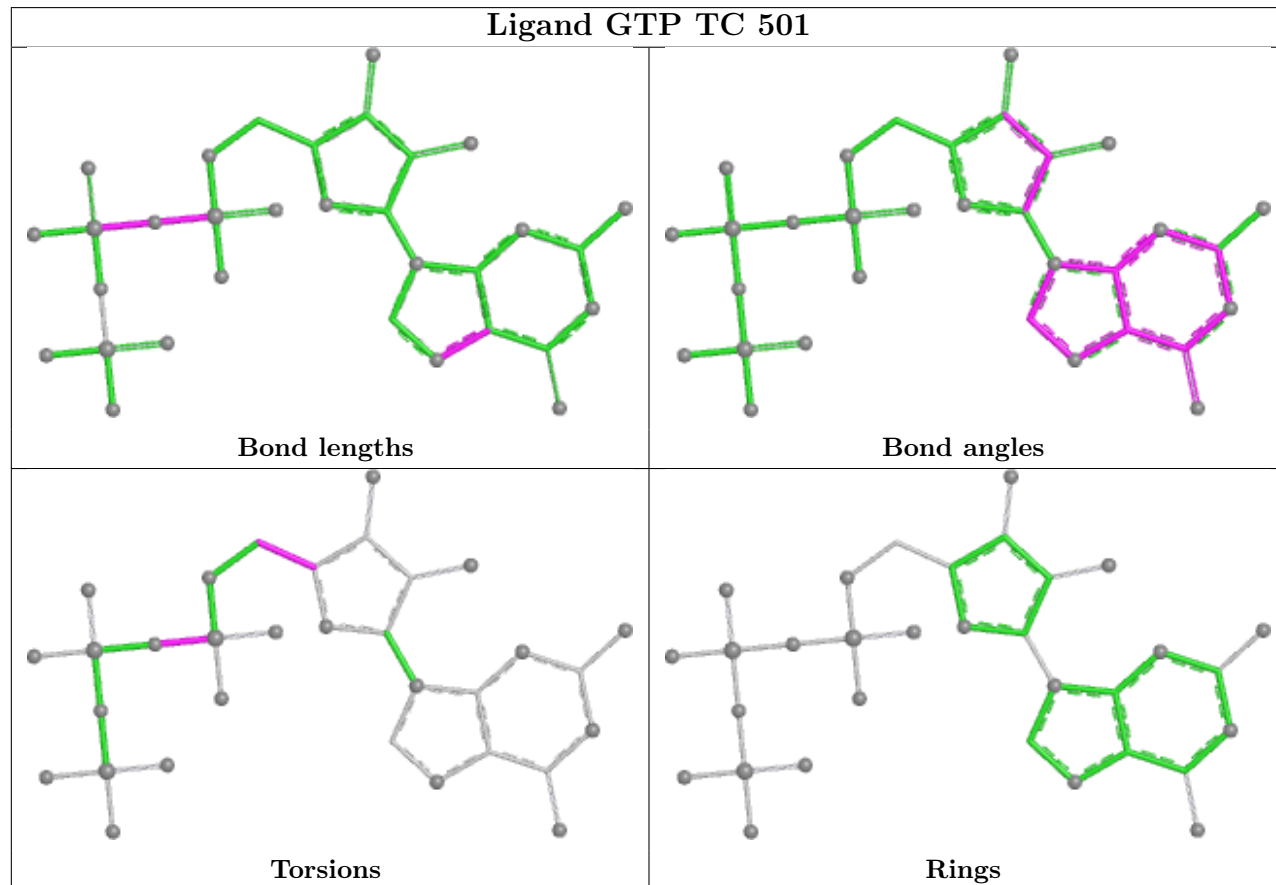


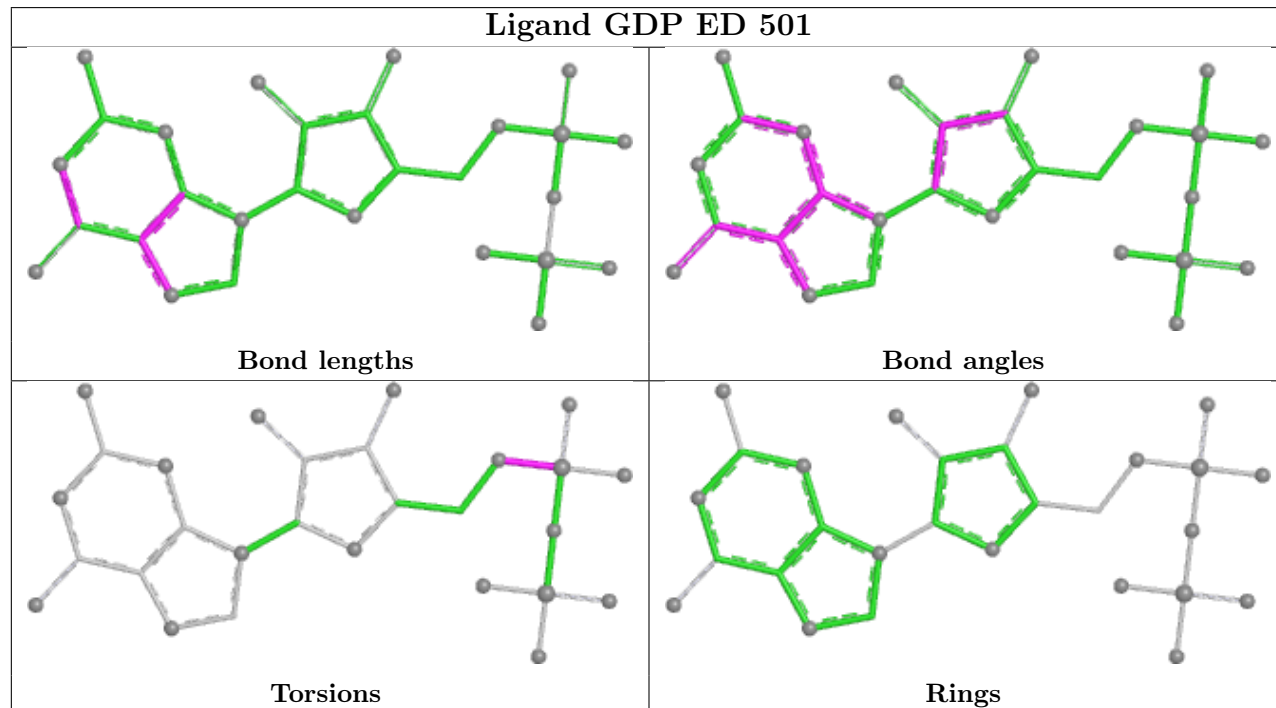
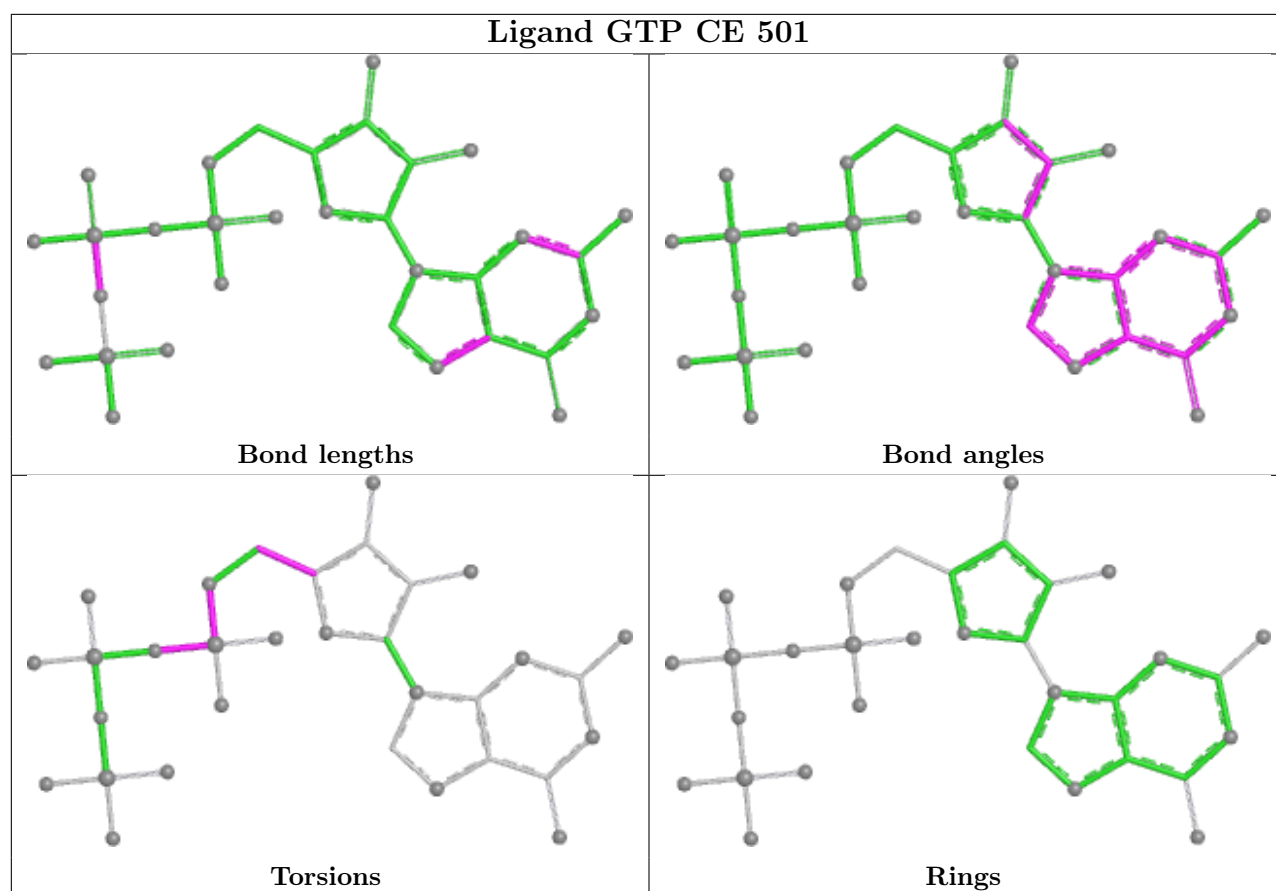


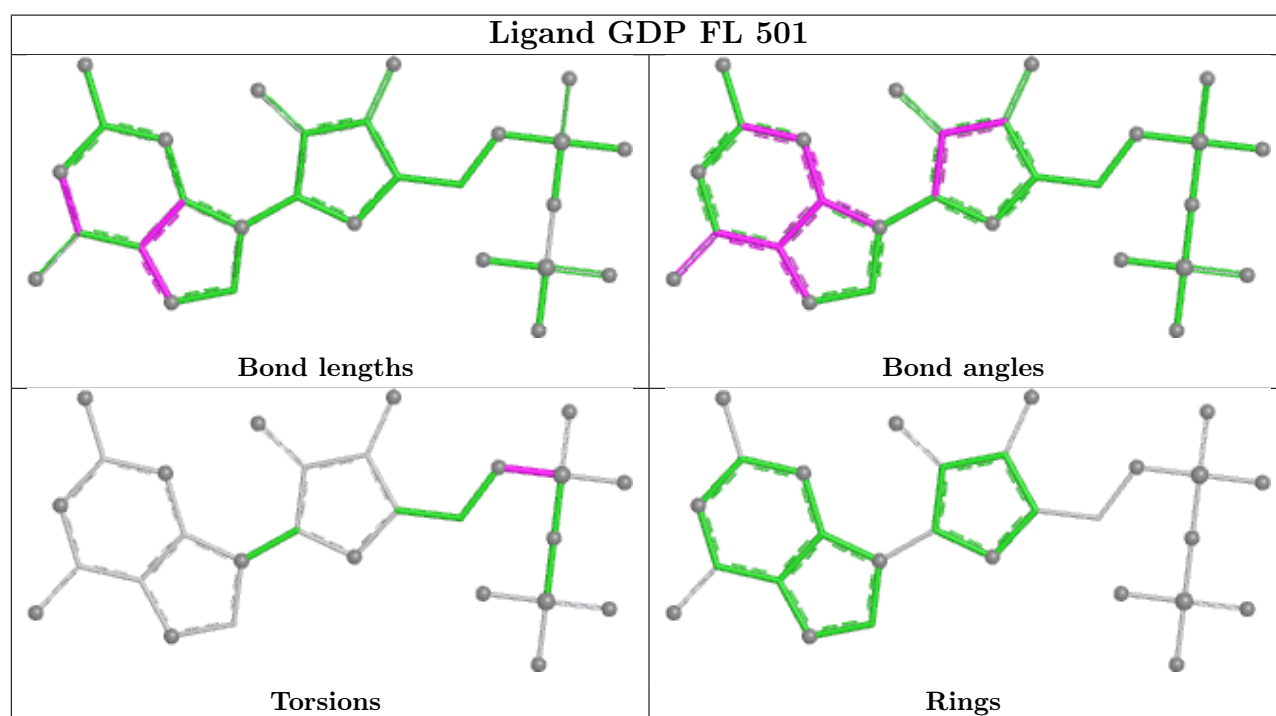
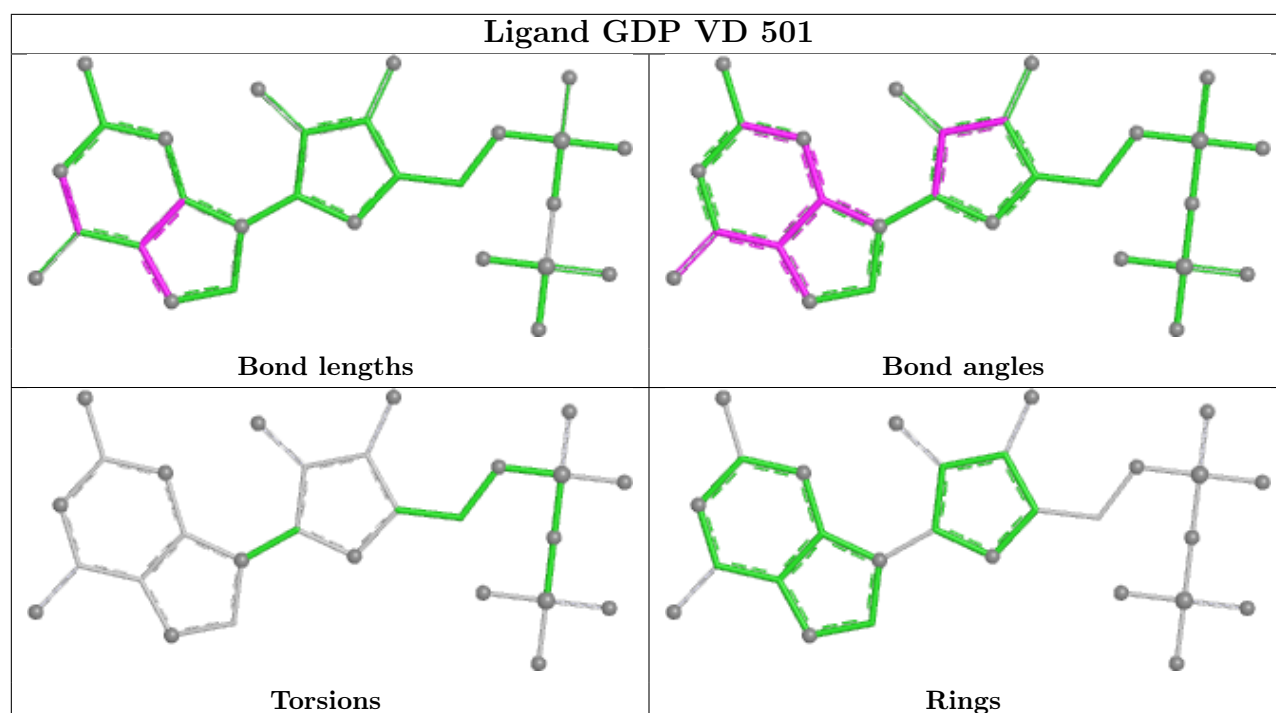
Ligand GTP DB 502

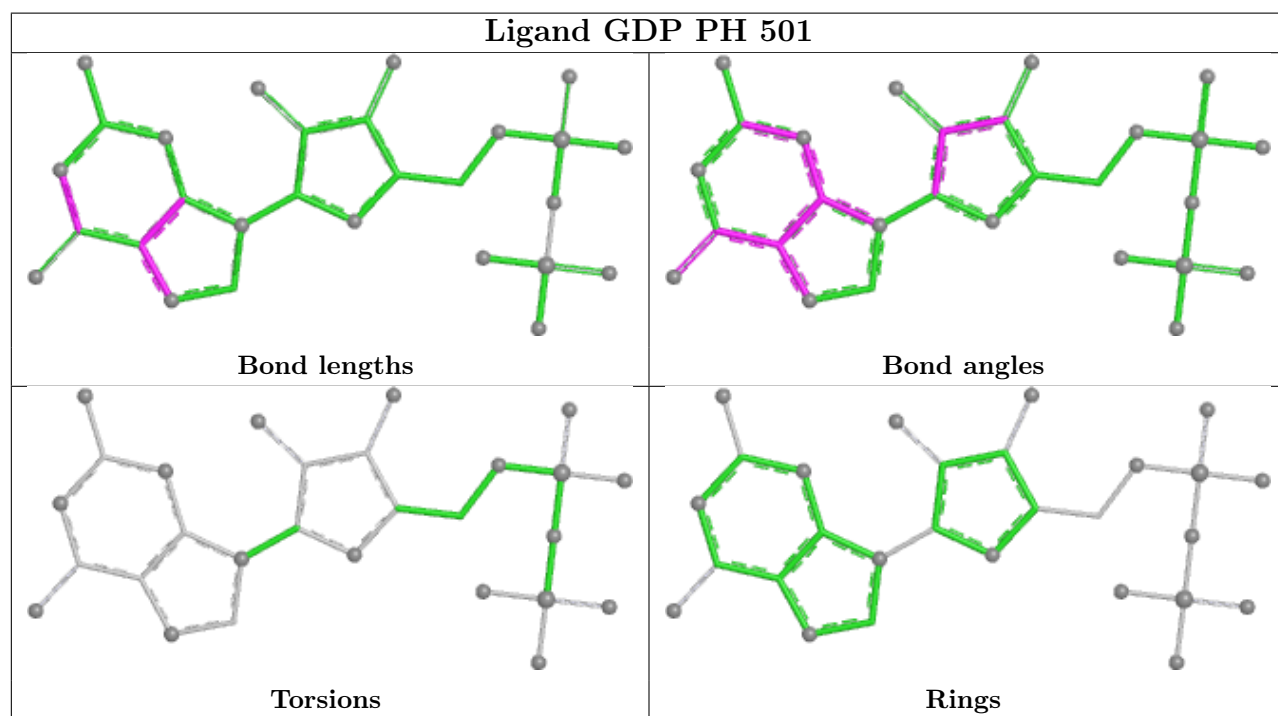
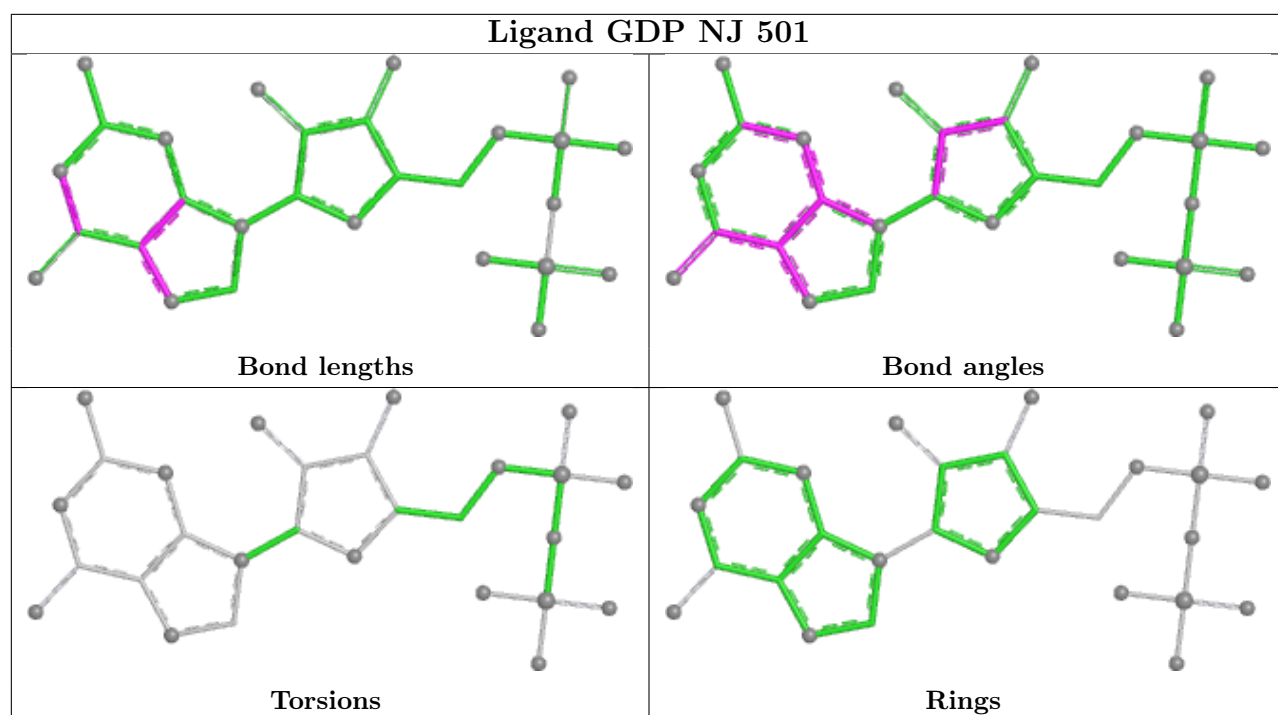


Ligand GTP TC 501

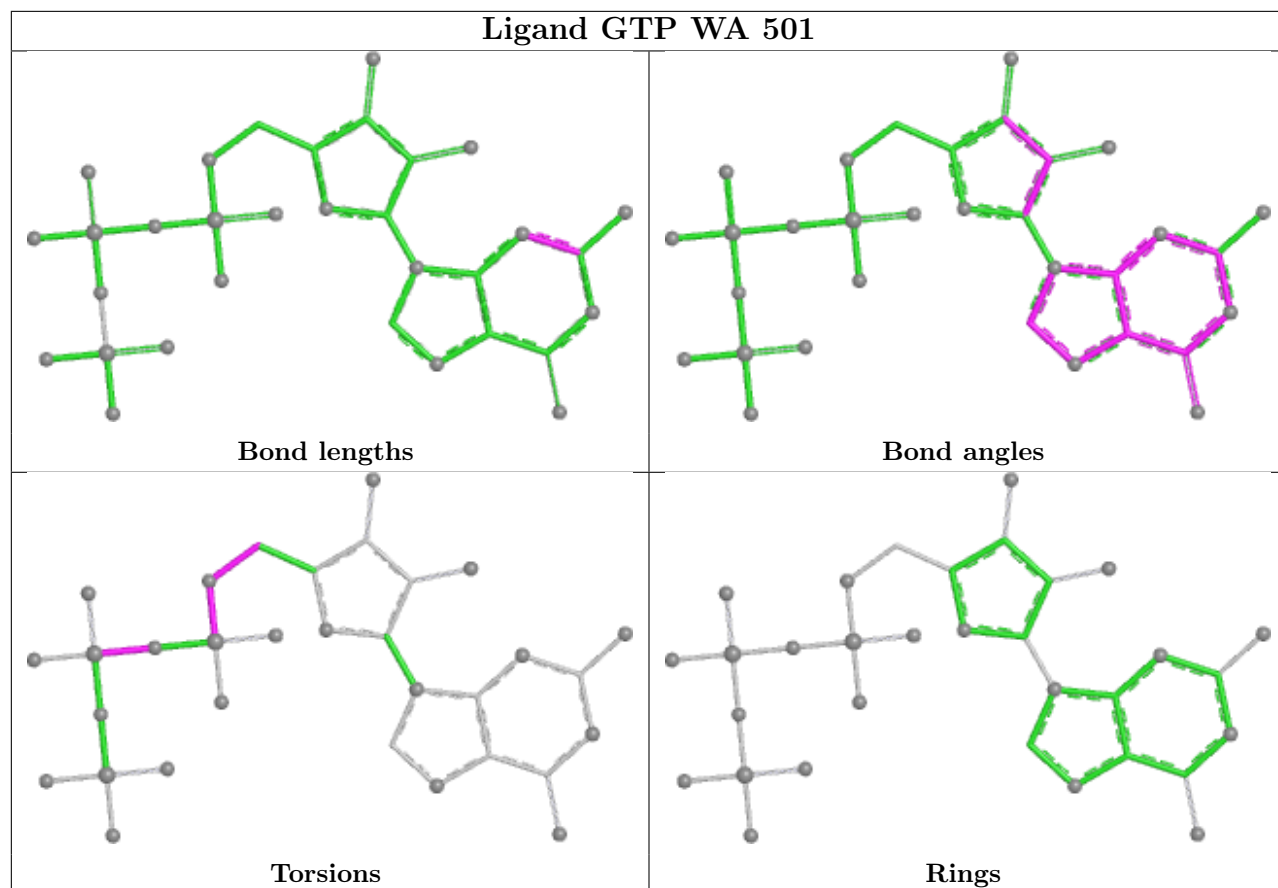




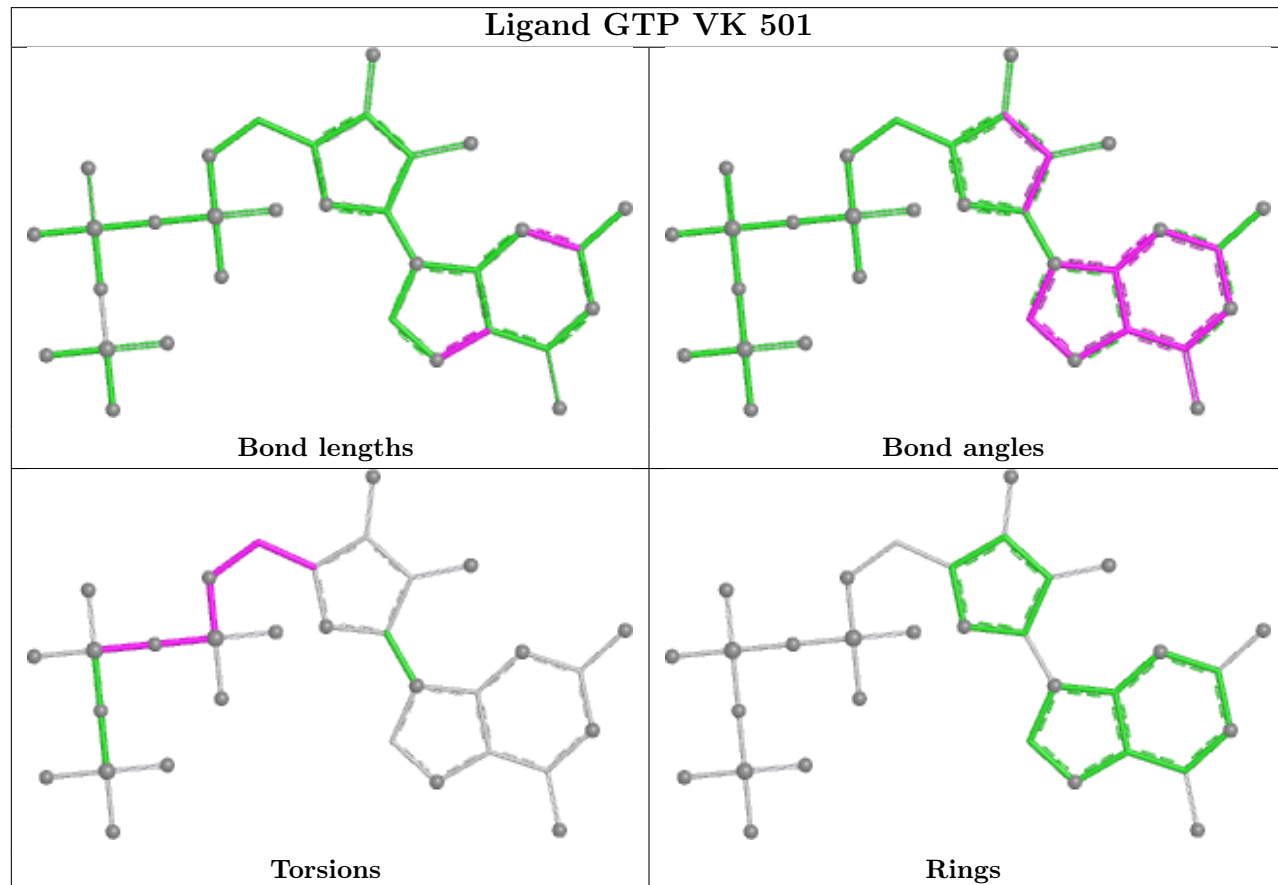


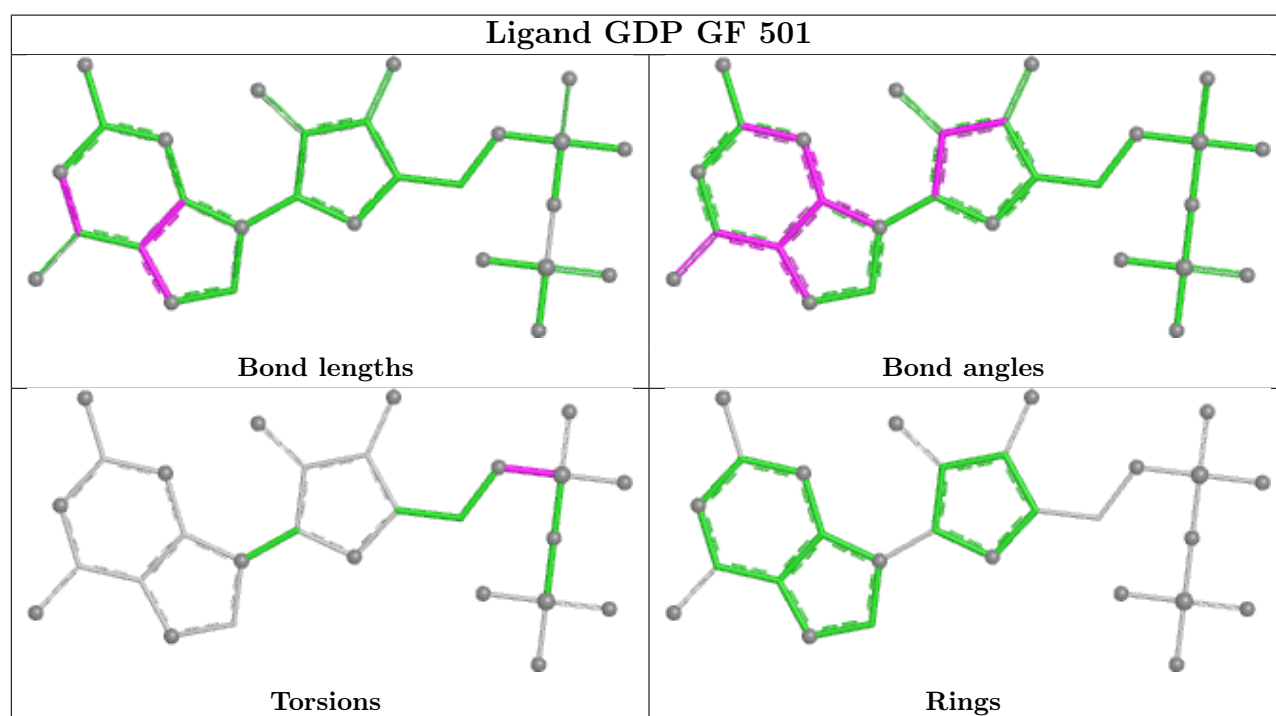
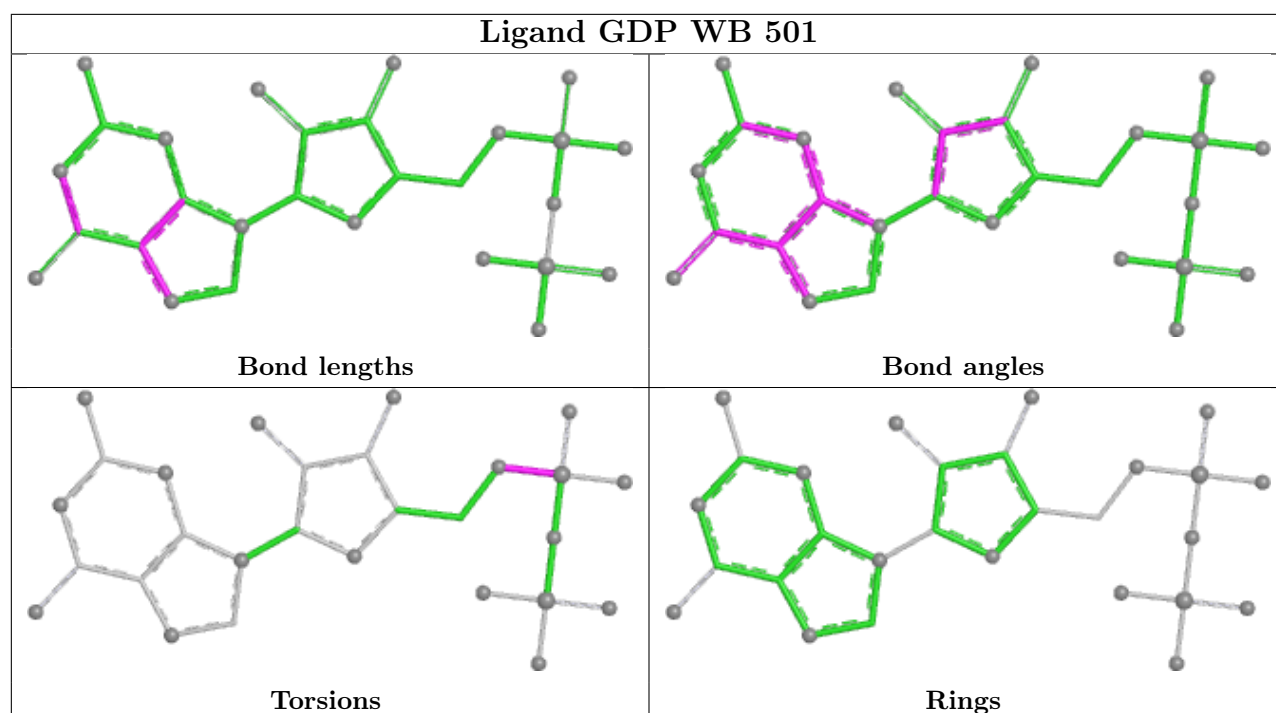


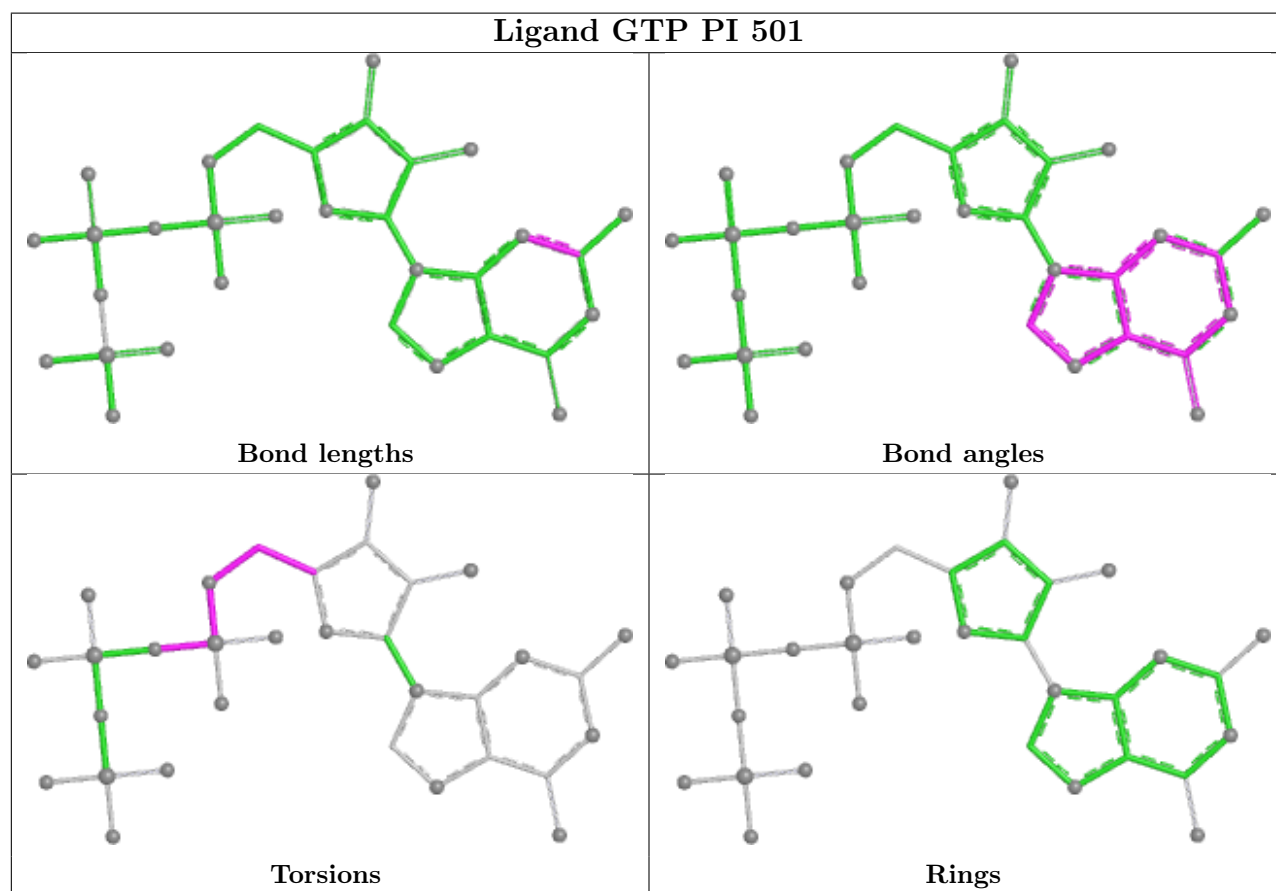
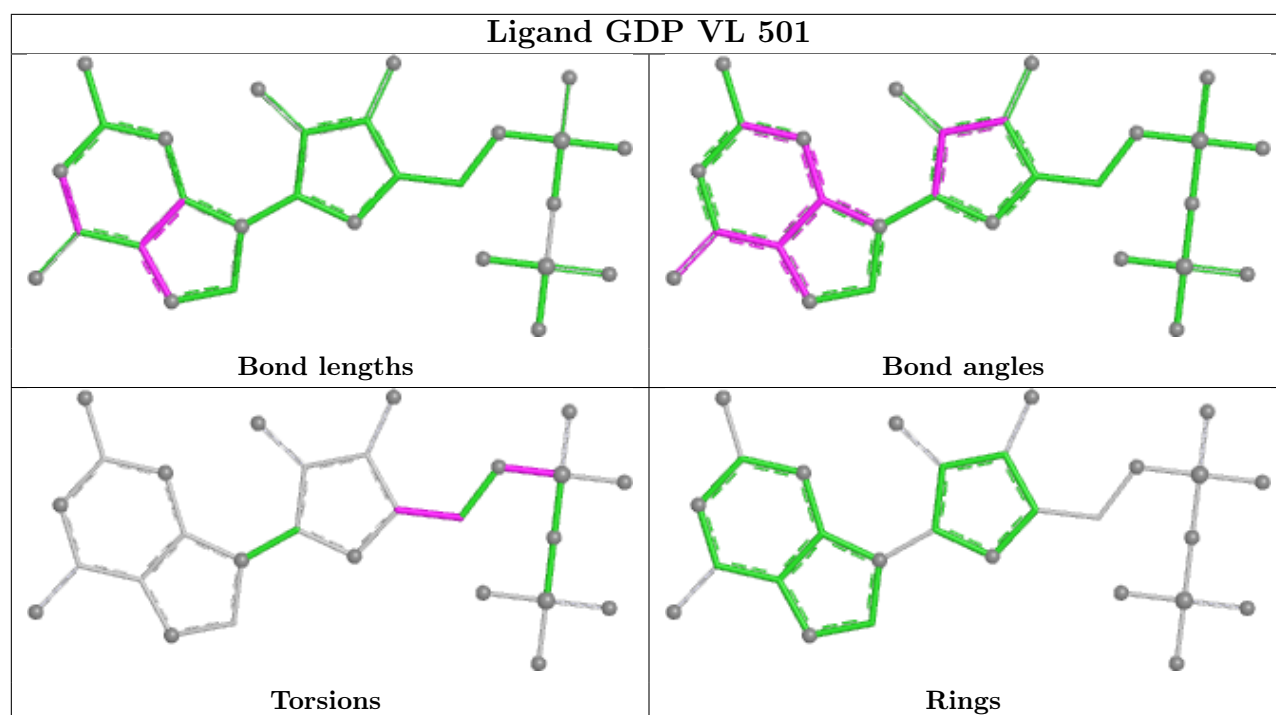
Ligand GTP WA 501



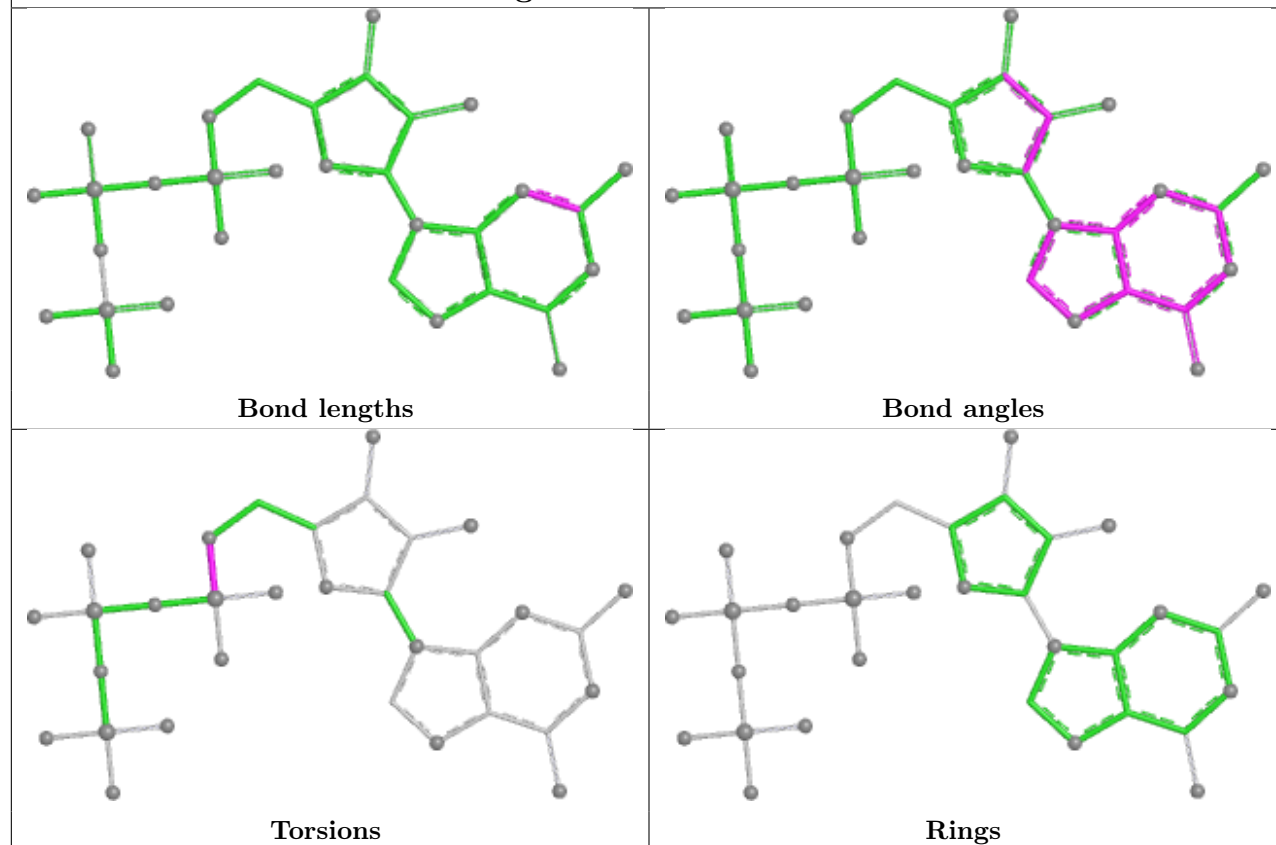
Ligand GTP VK 501



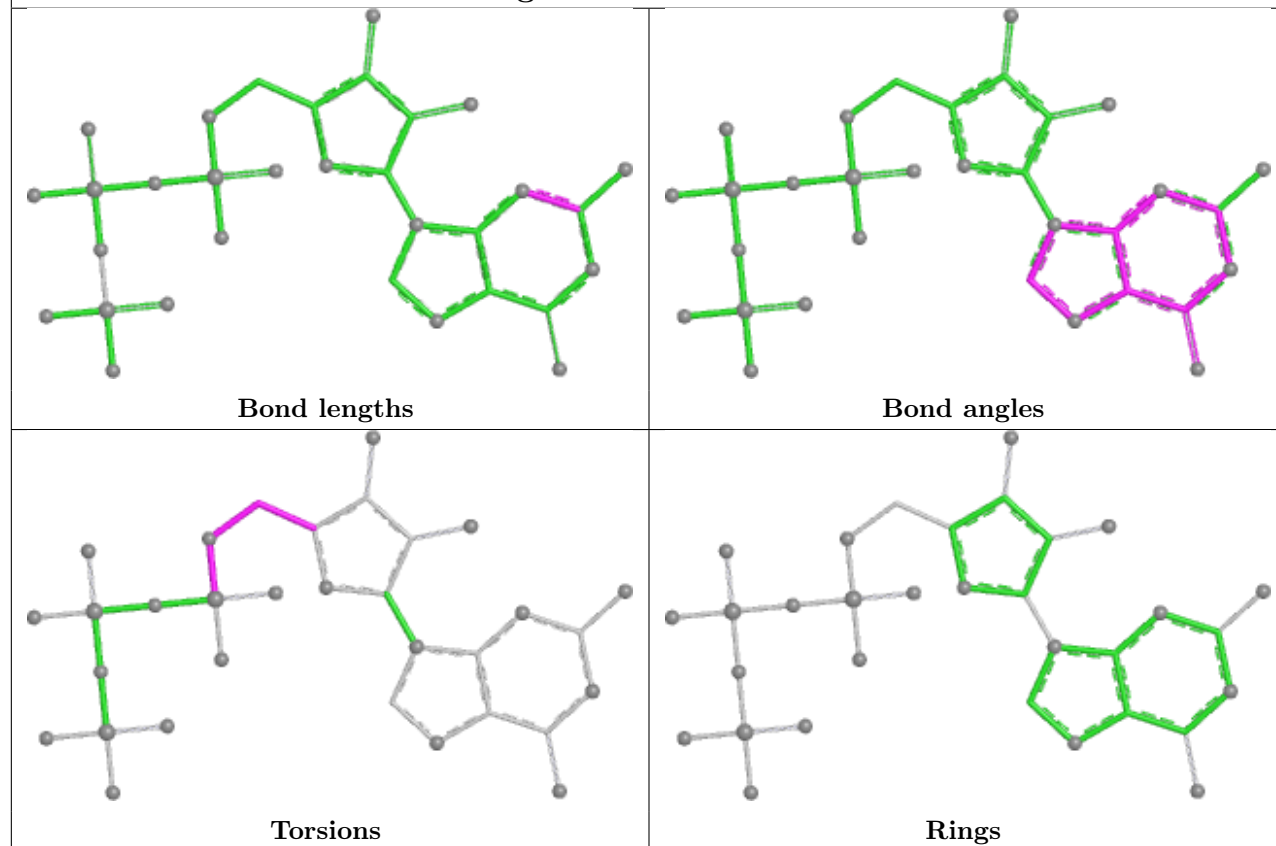




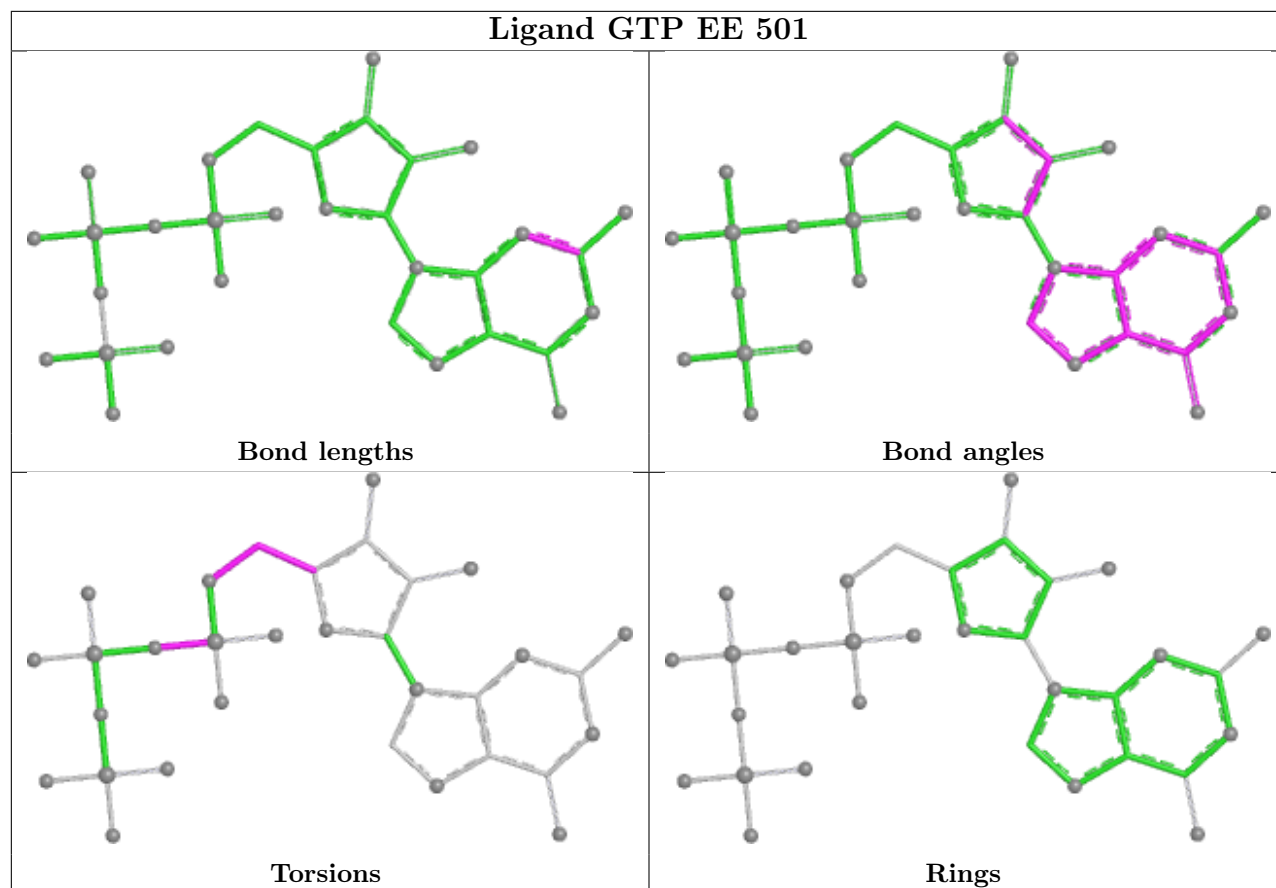
Ligand GTP FM 501



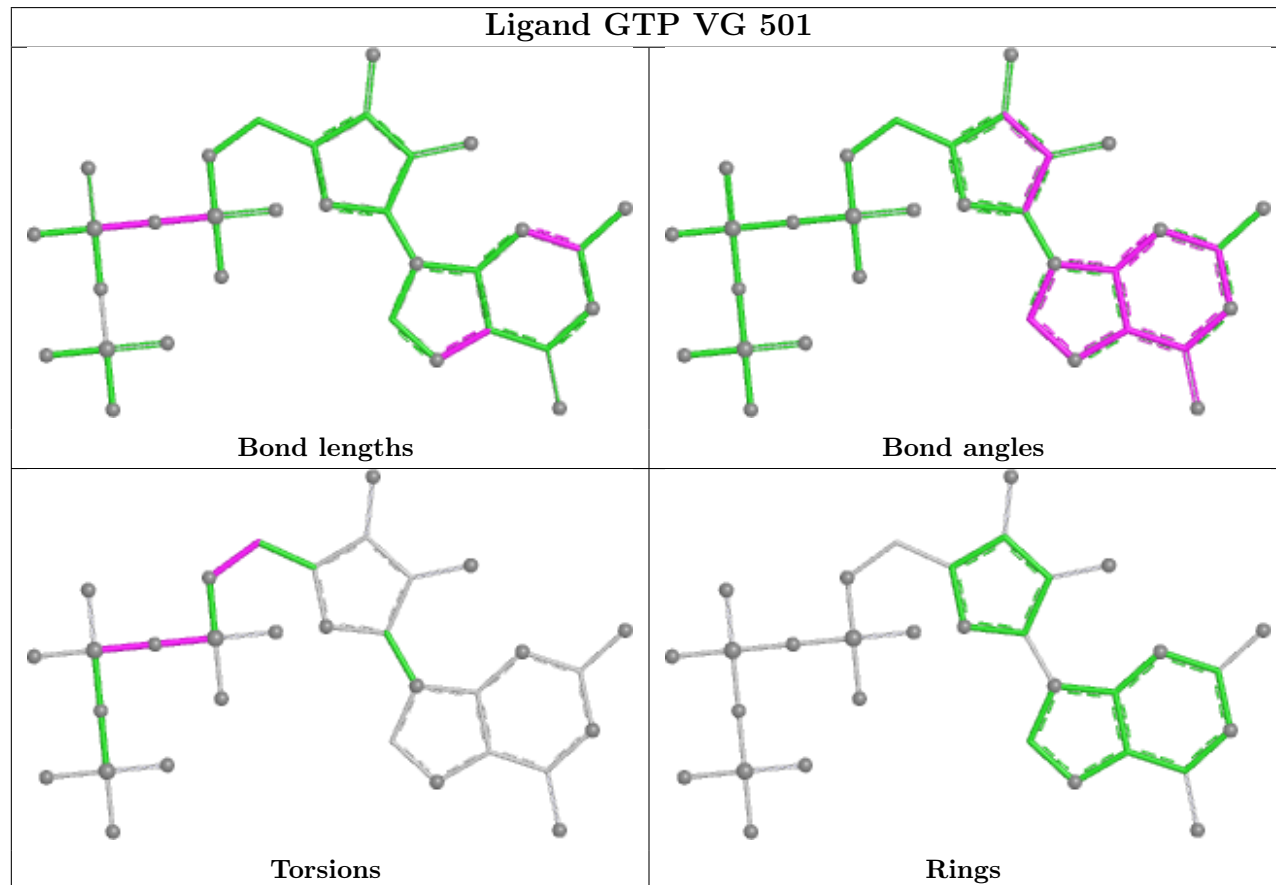
Ligand GTP BK 501

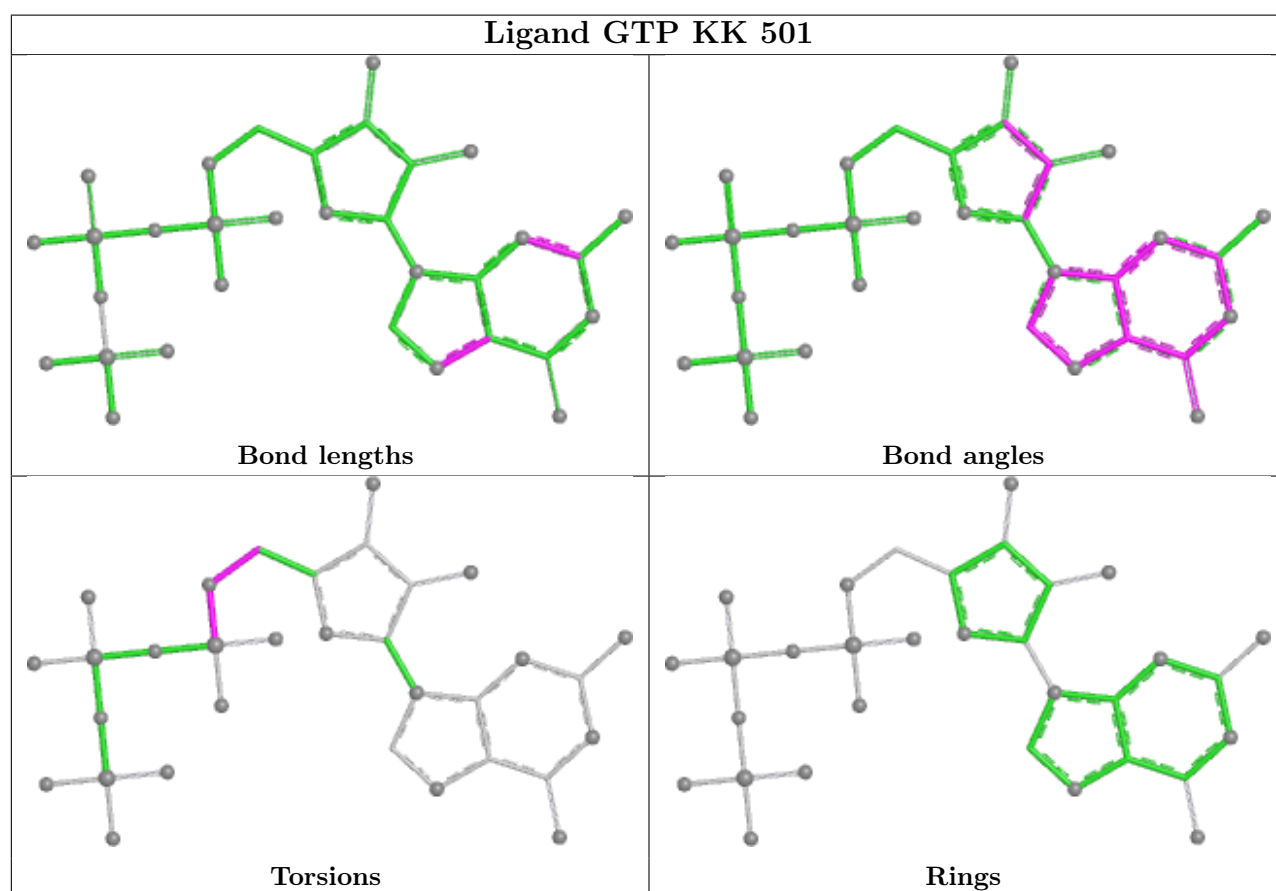
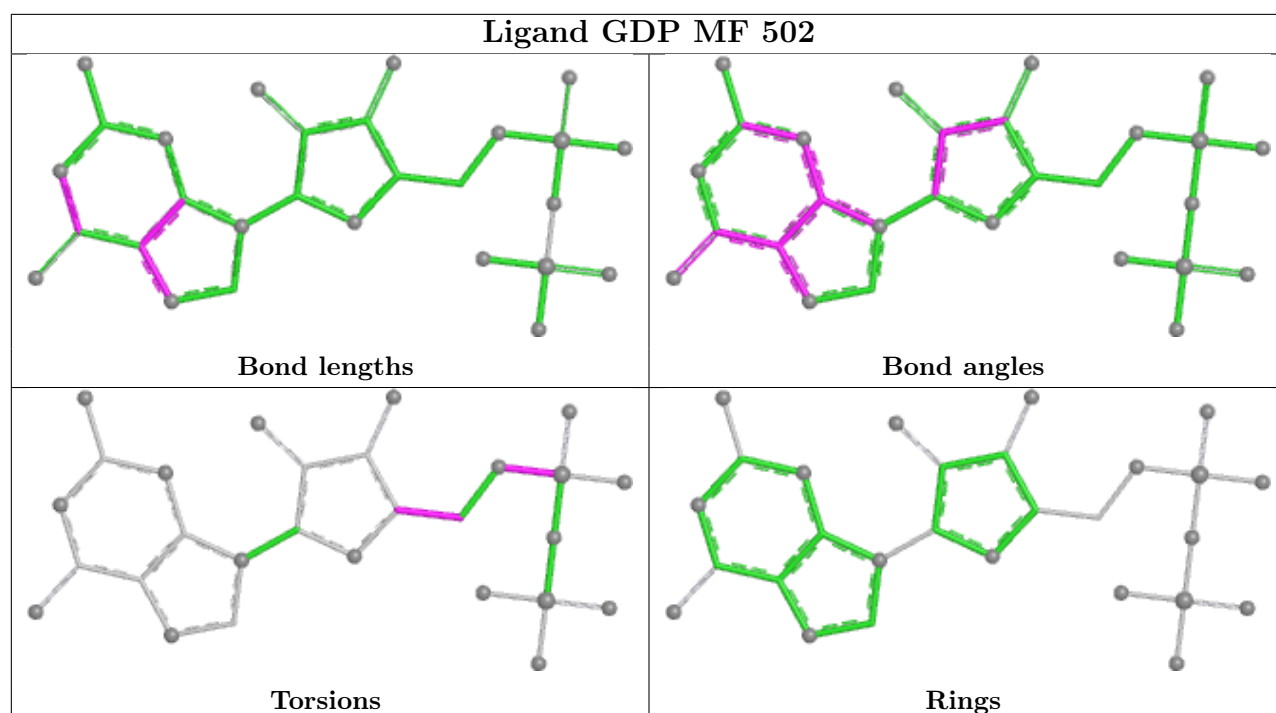


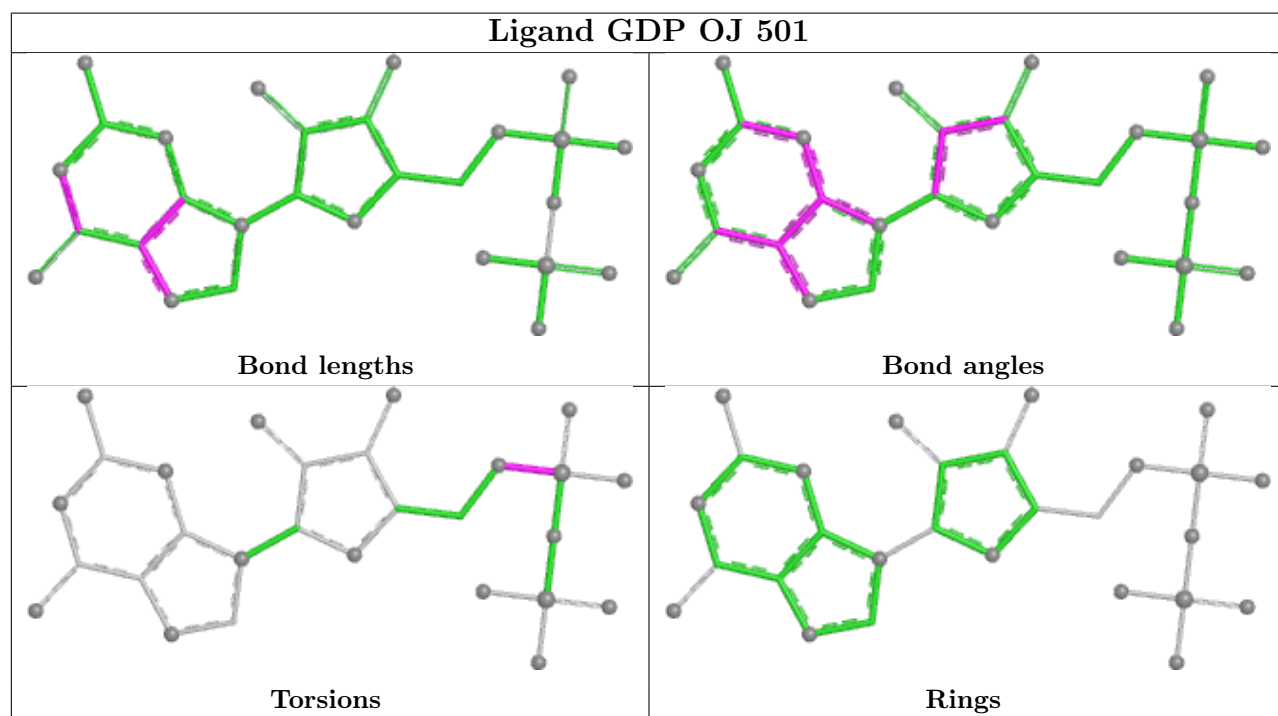
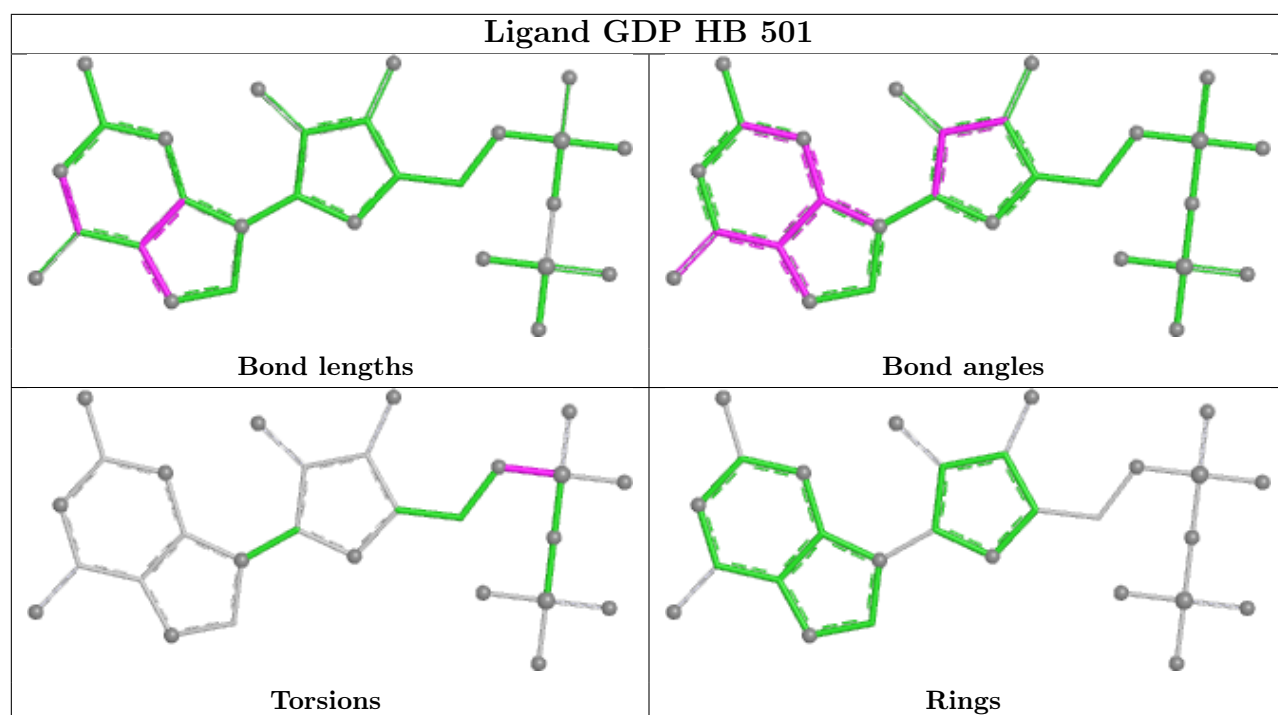
Ligand GTP EE 501

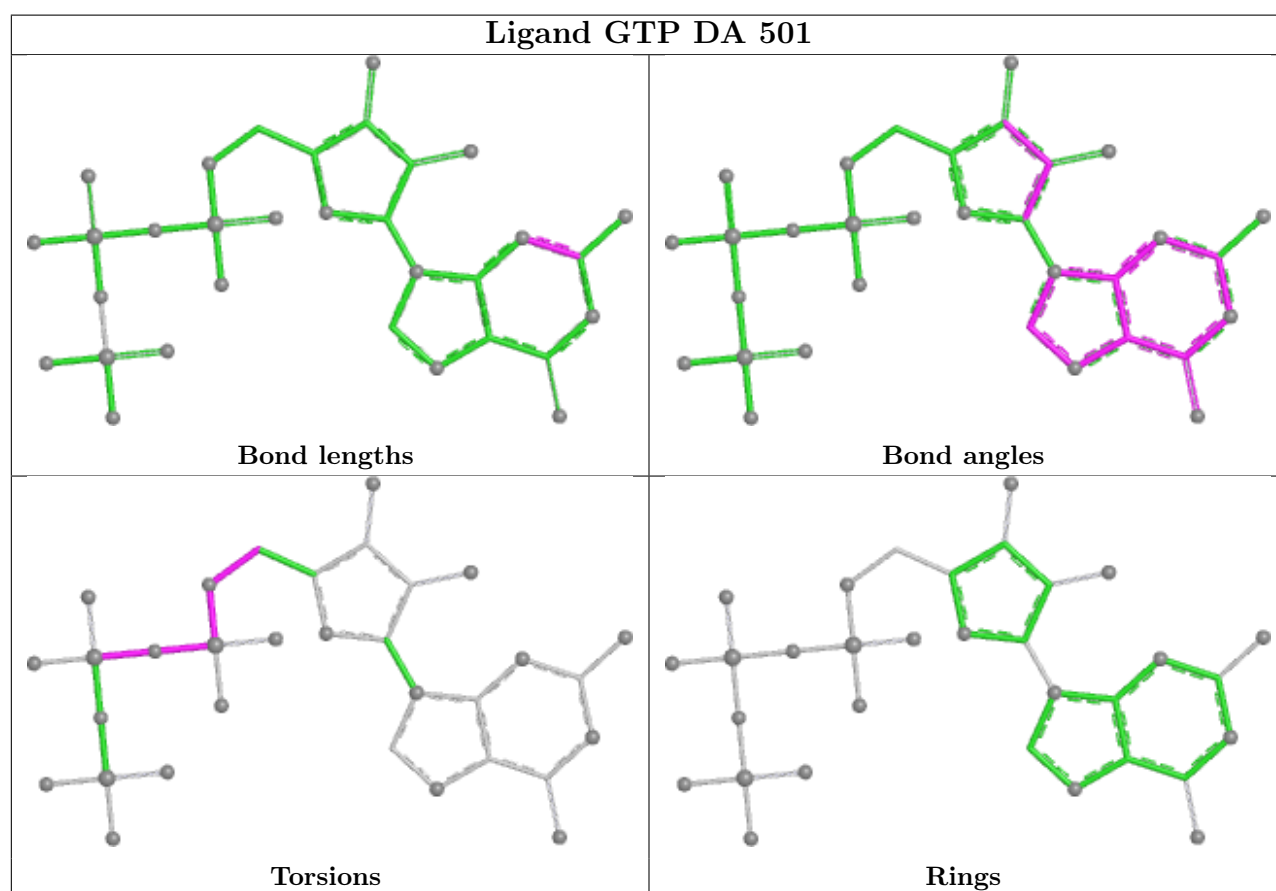
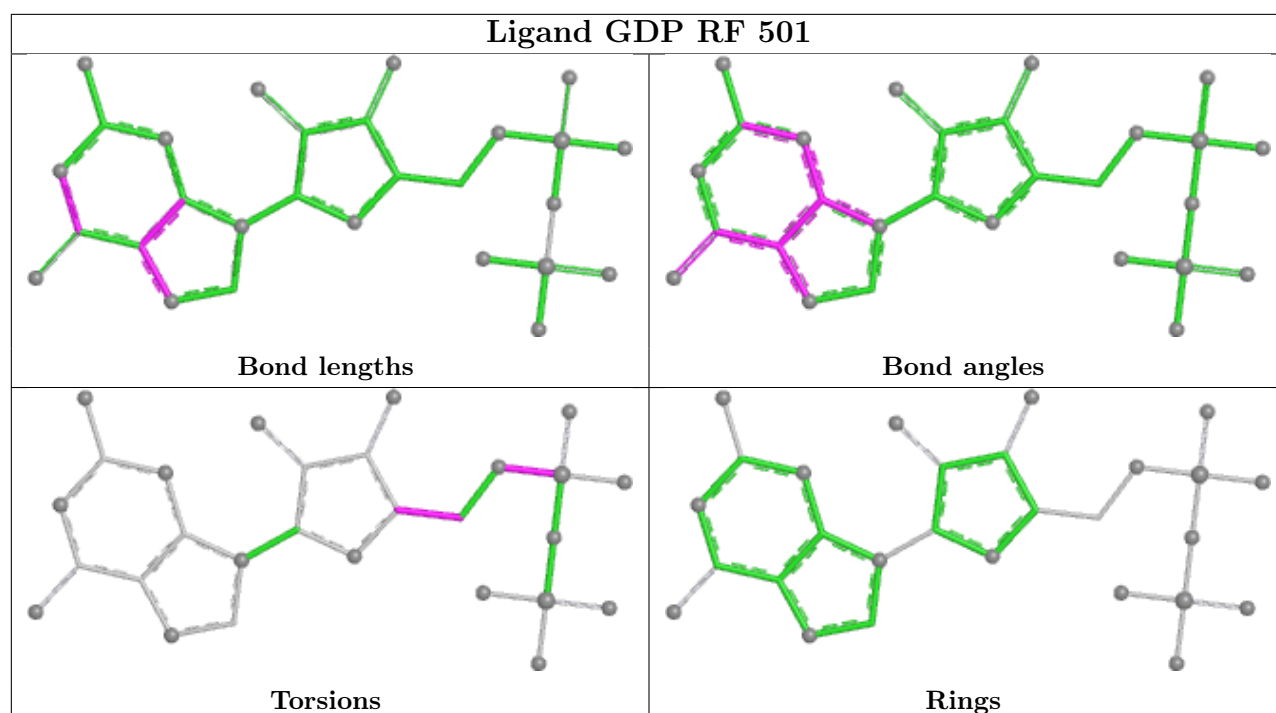


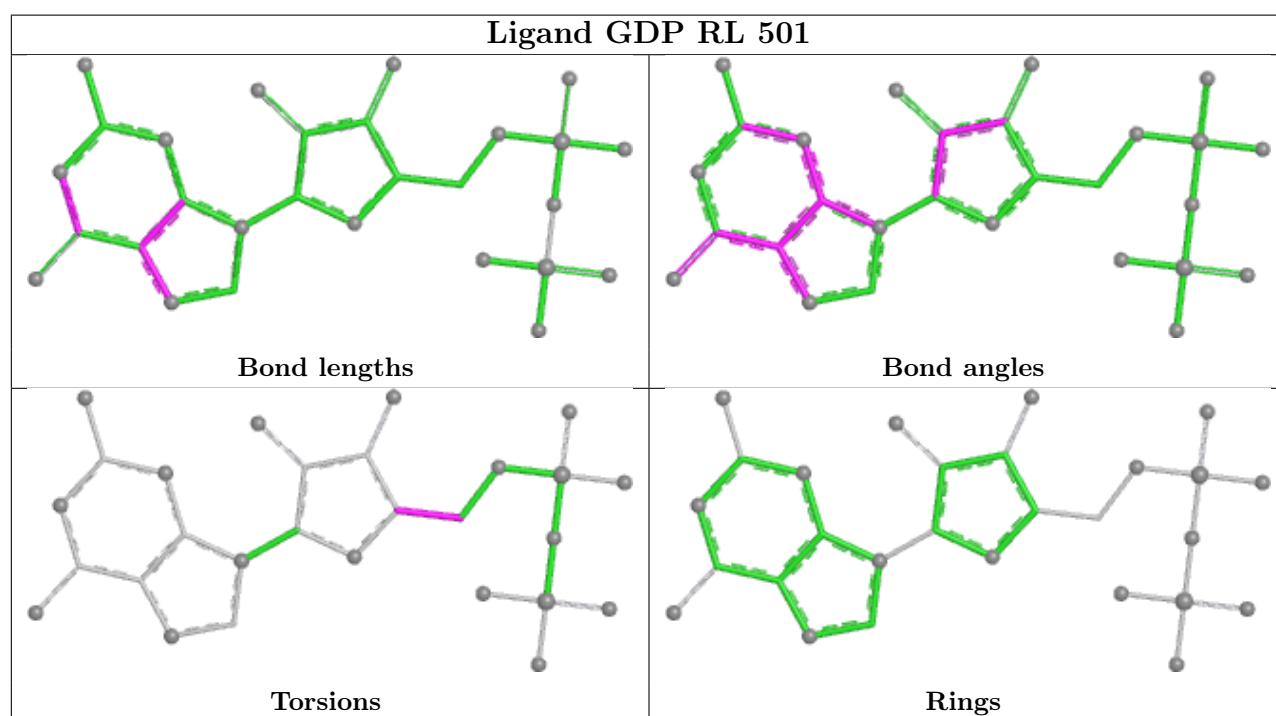
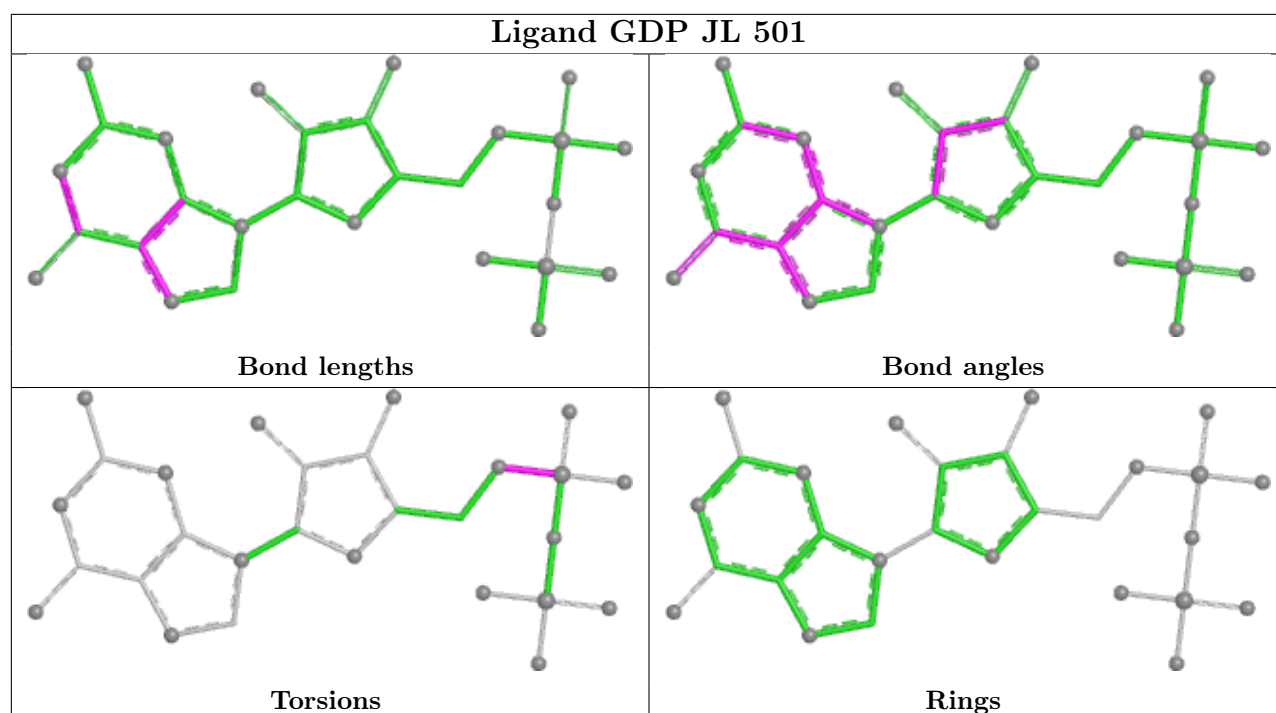
Ligand GTP VG 501

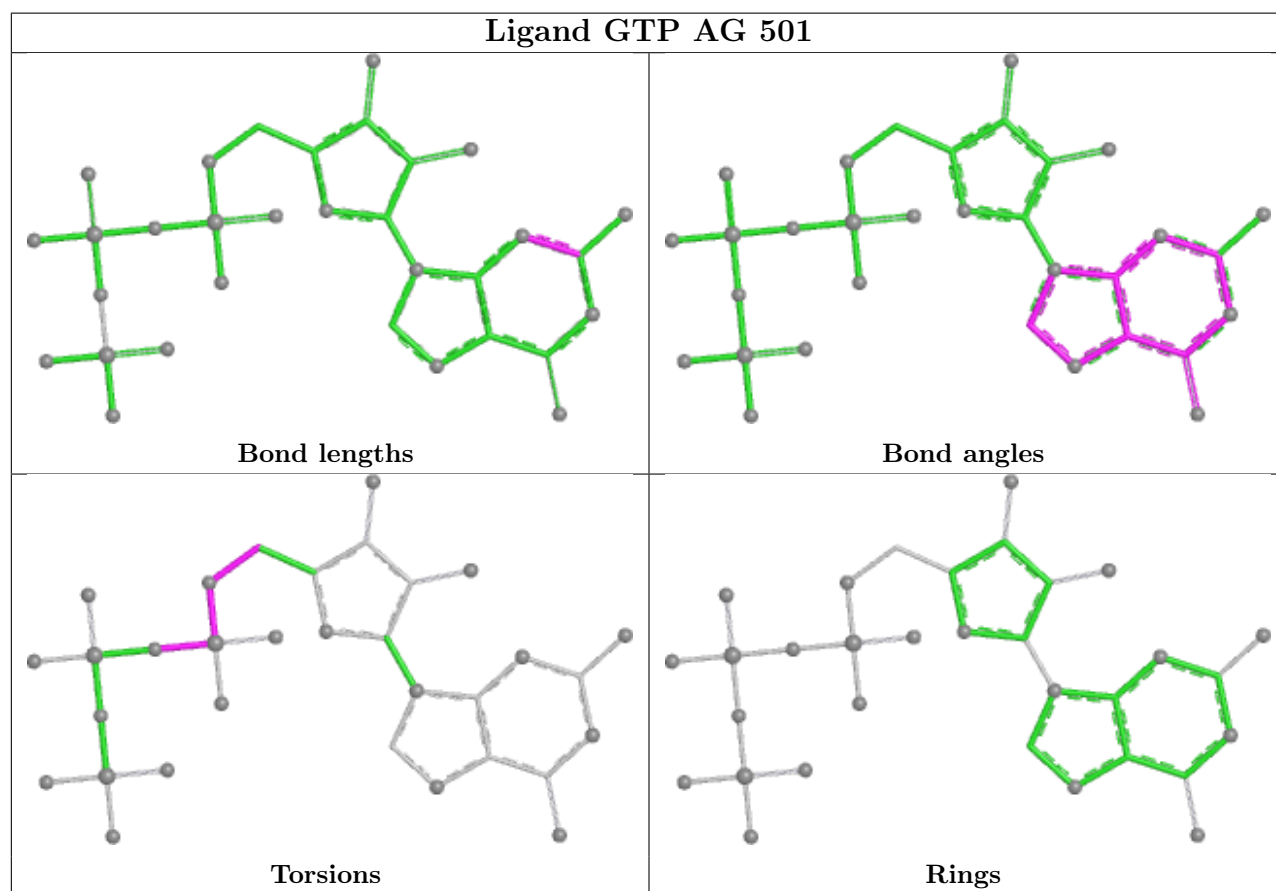
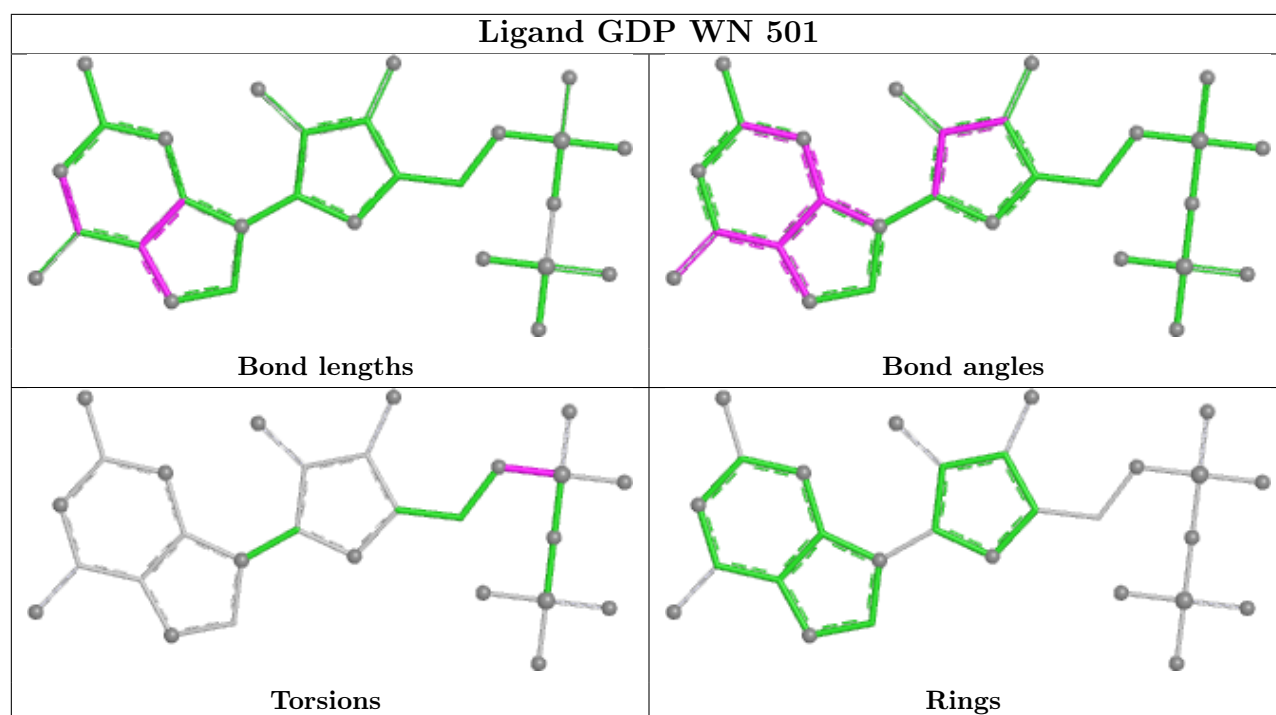


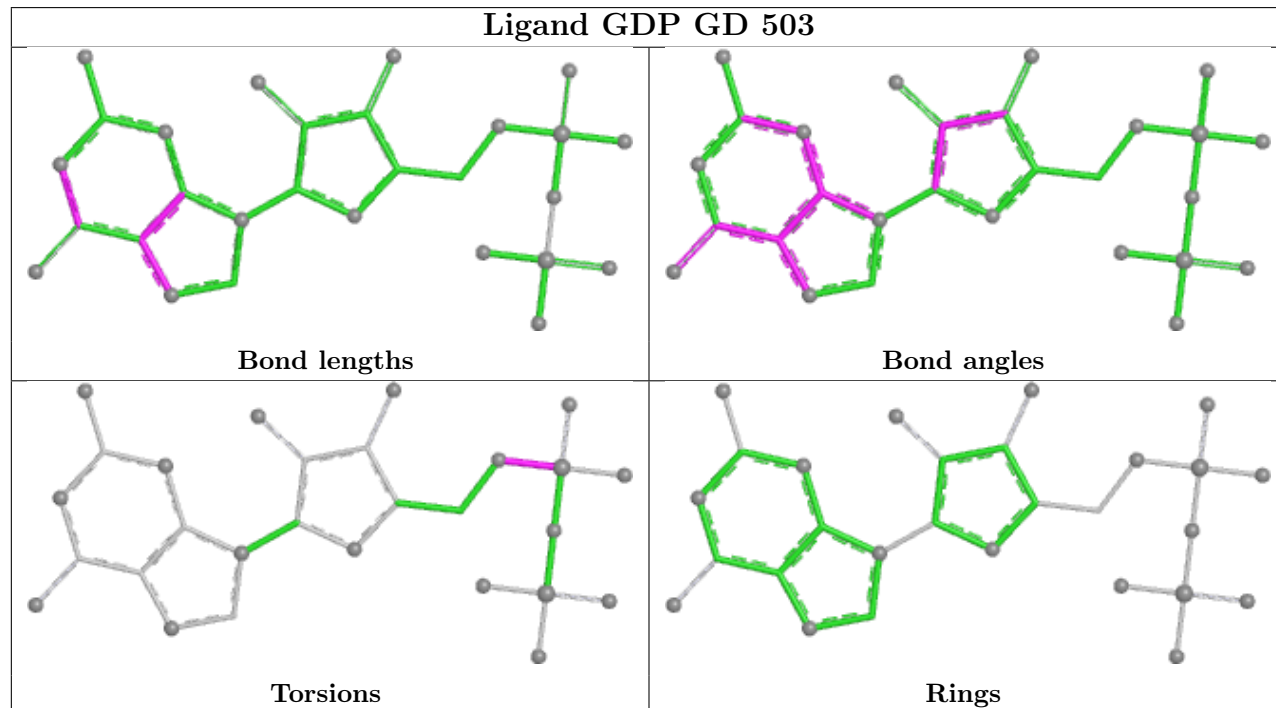
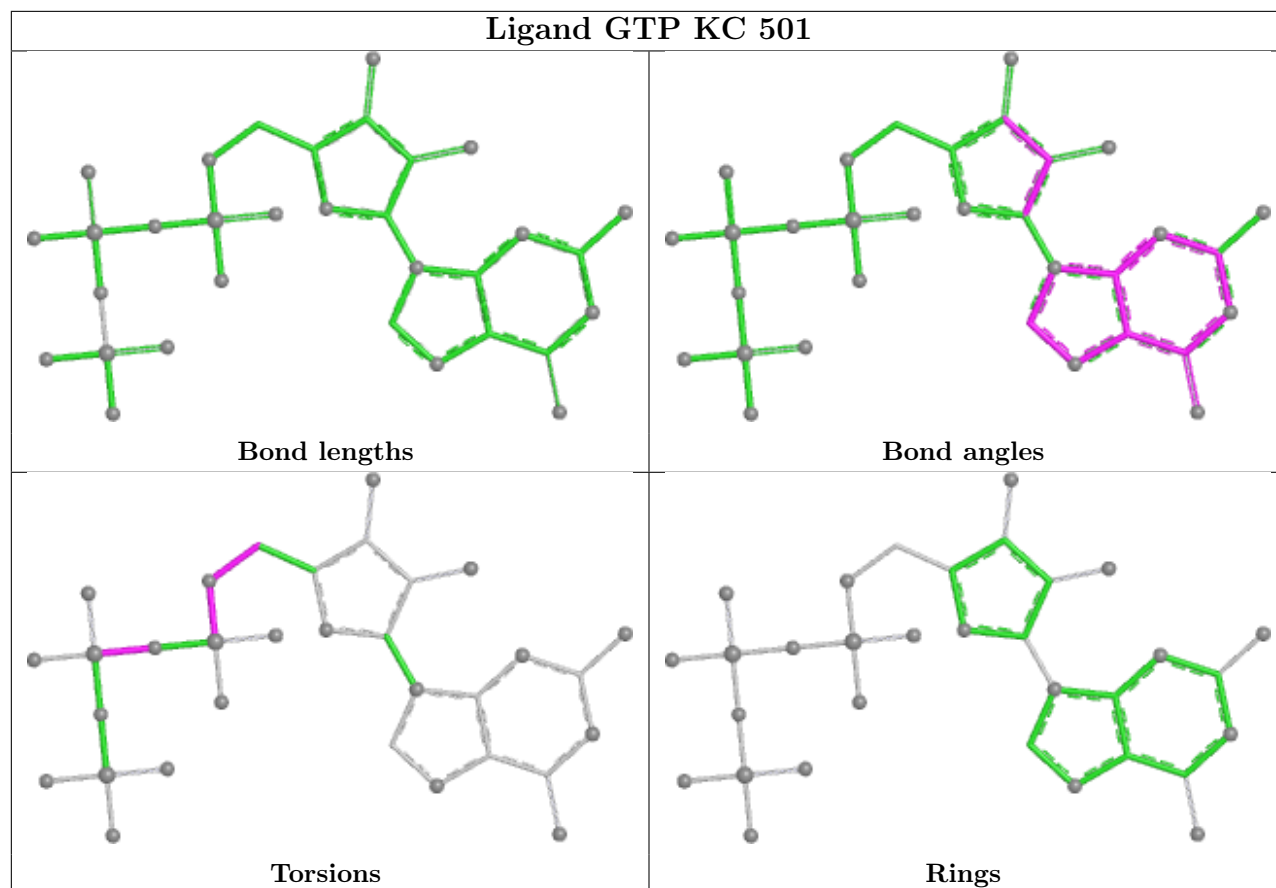


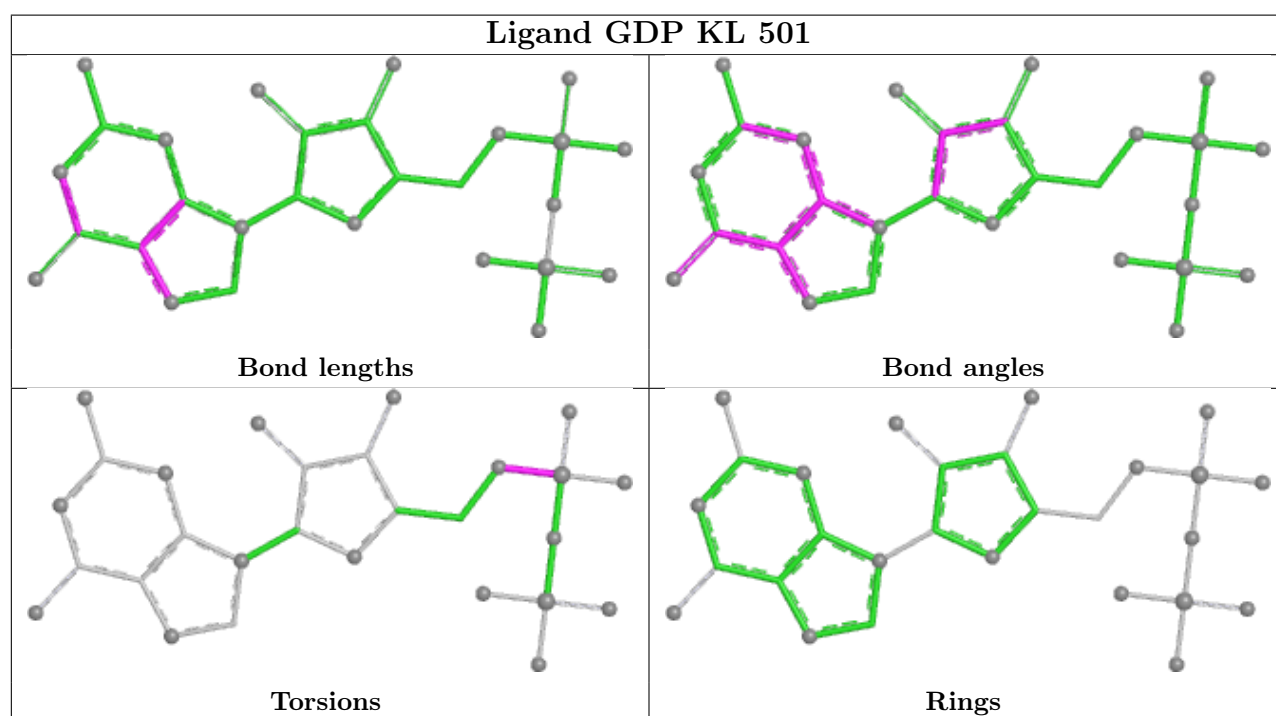
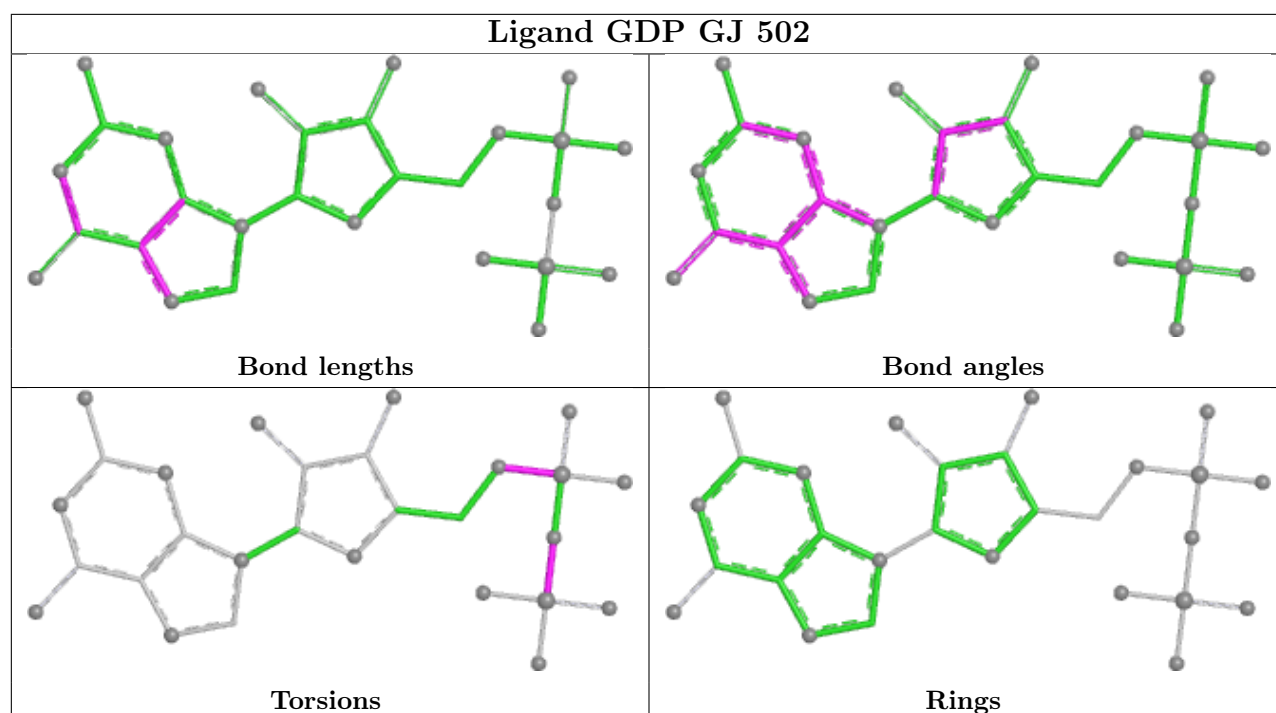


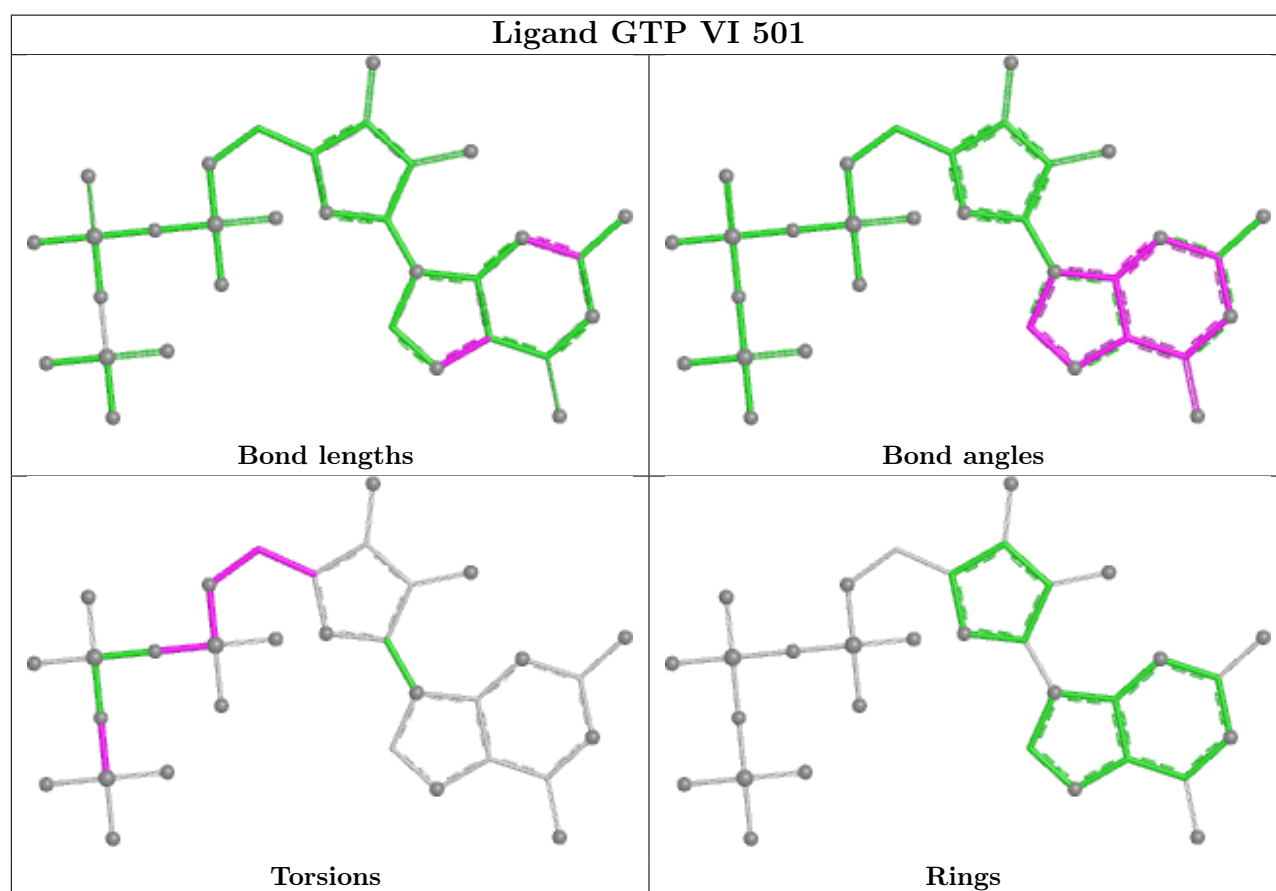
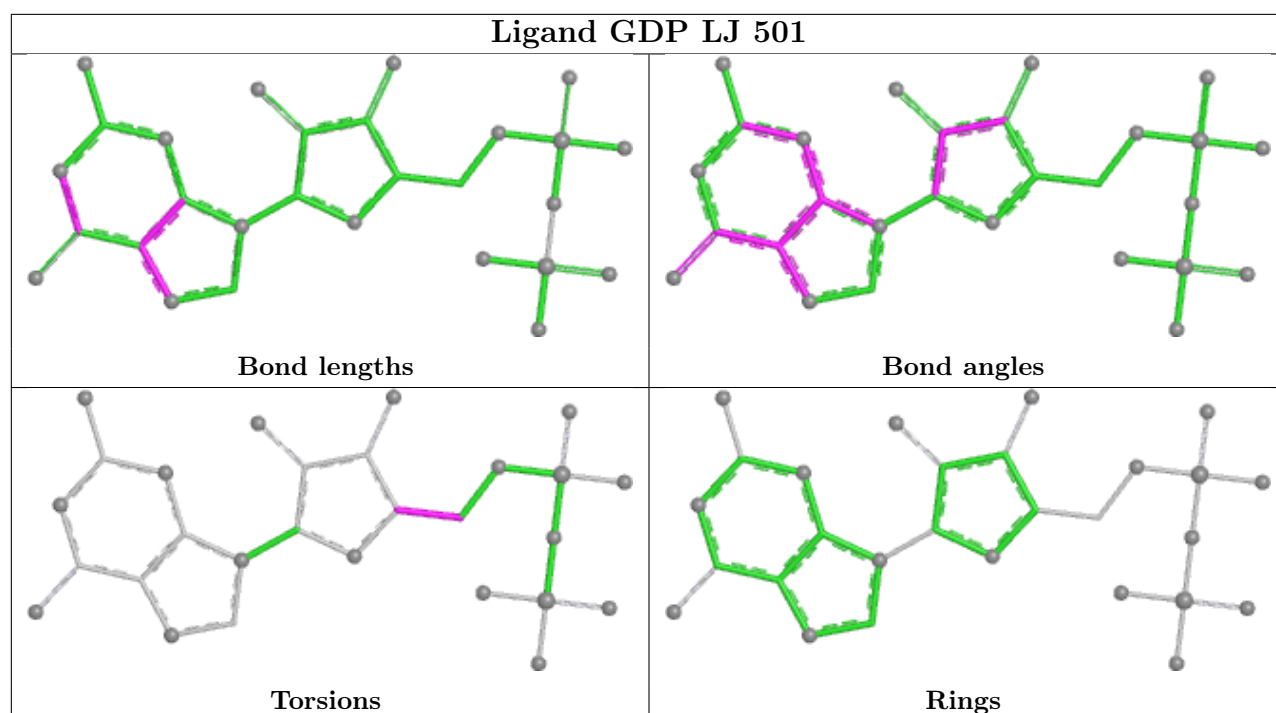


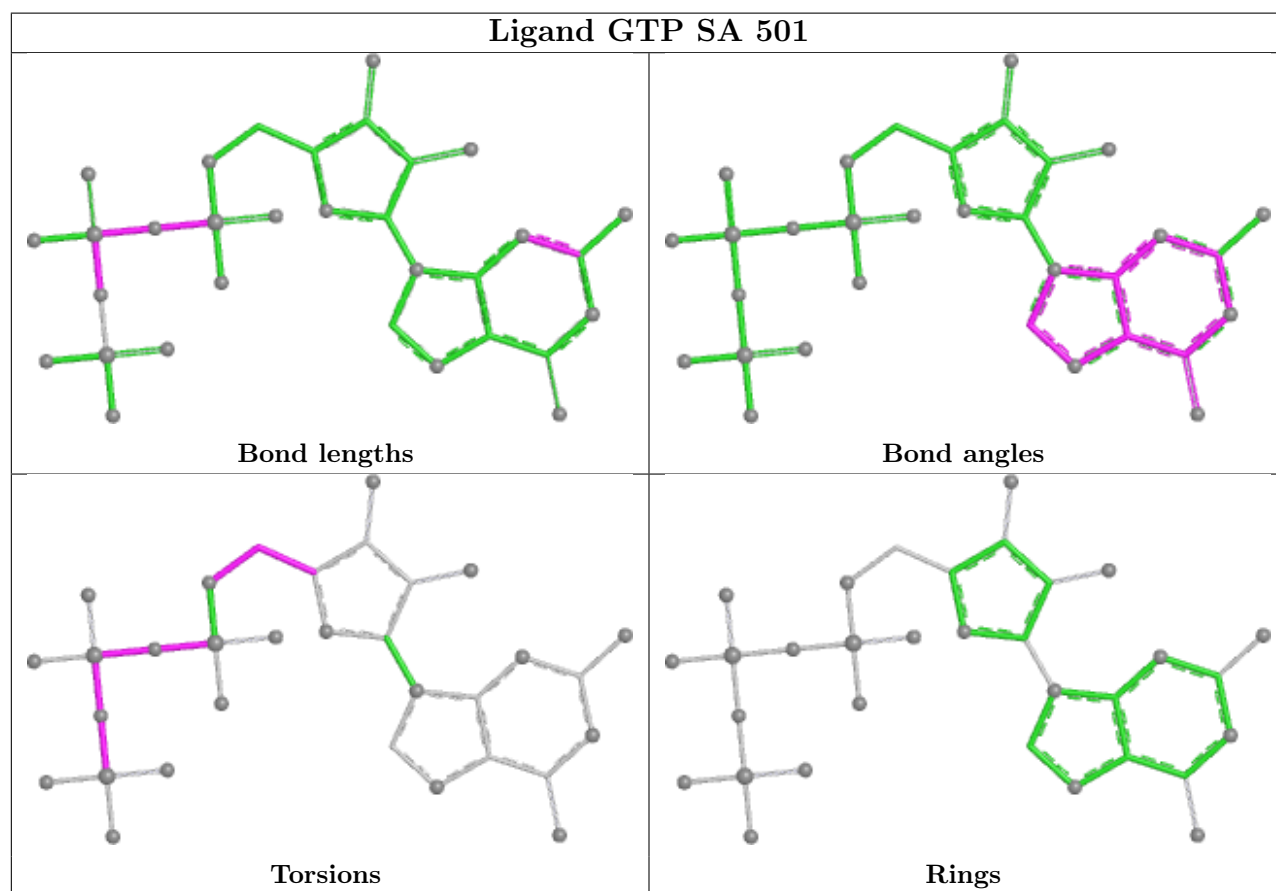
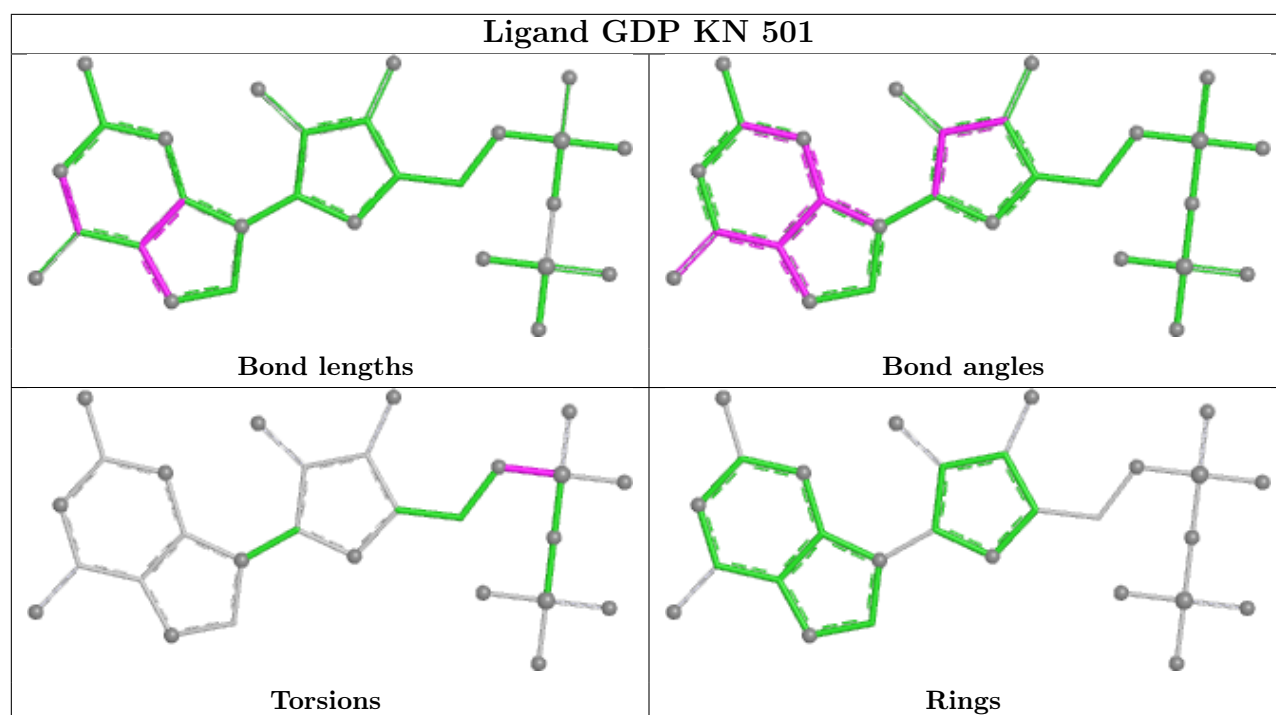


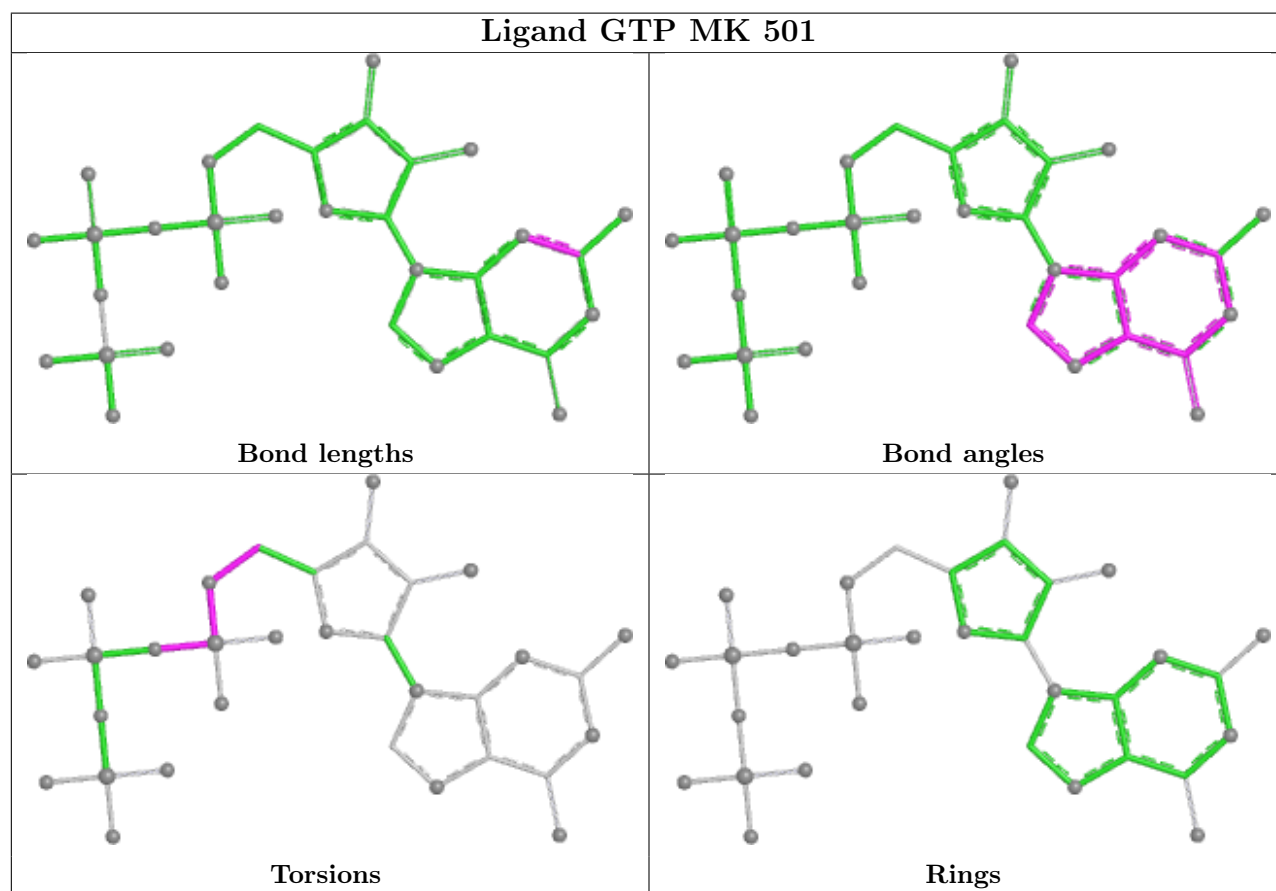
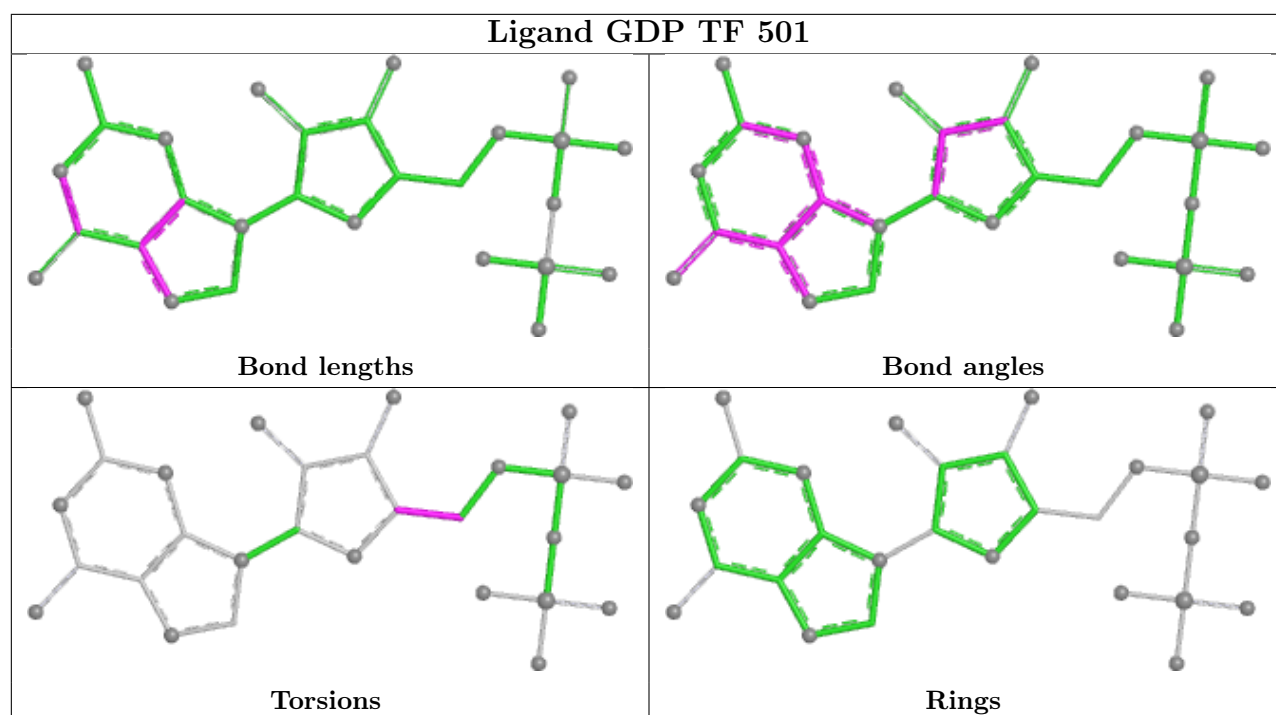


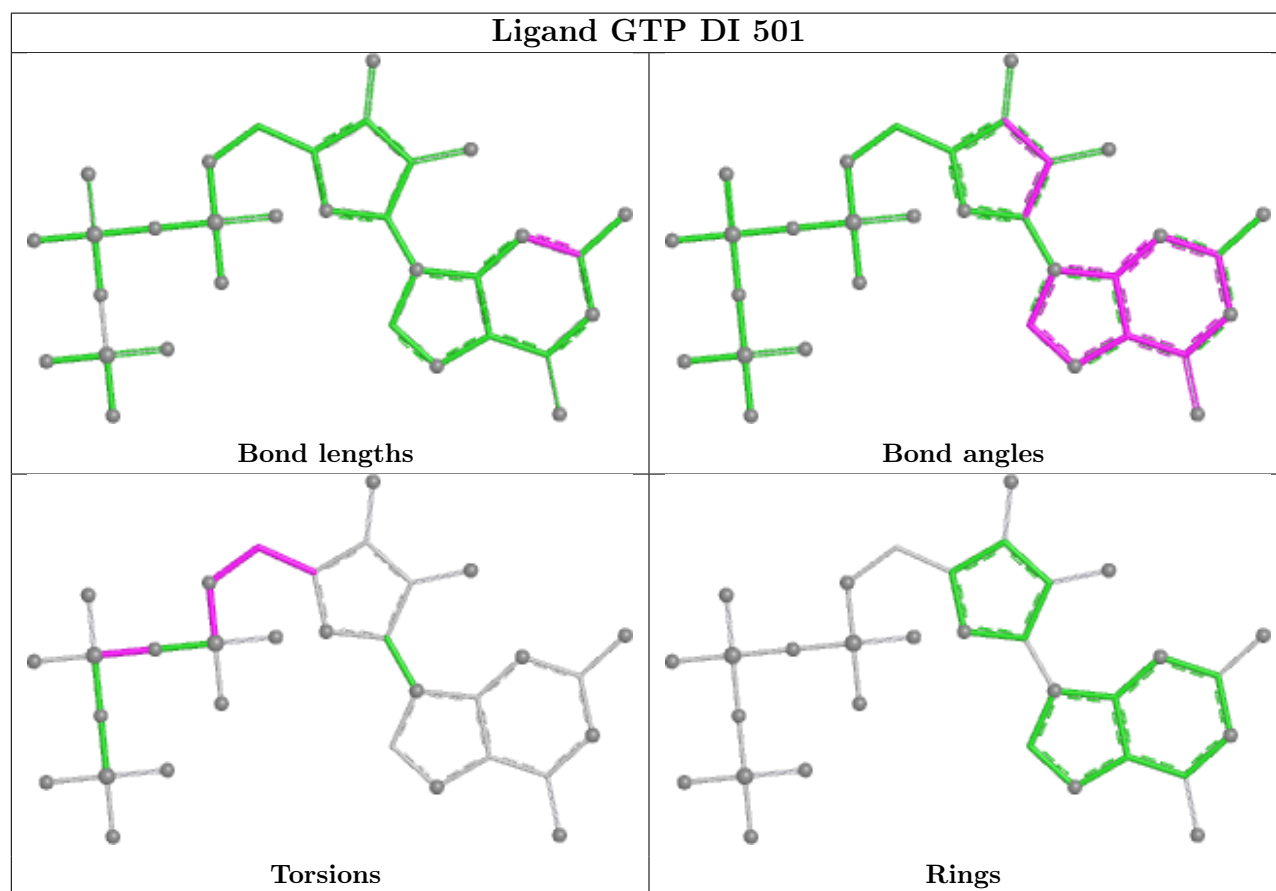
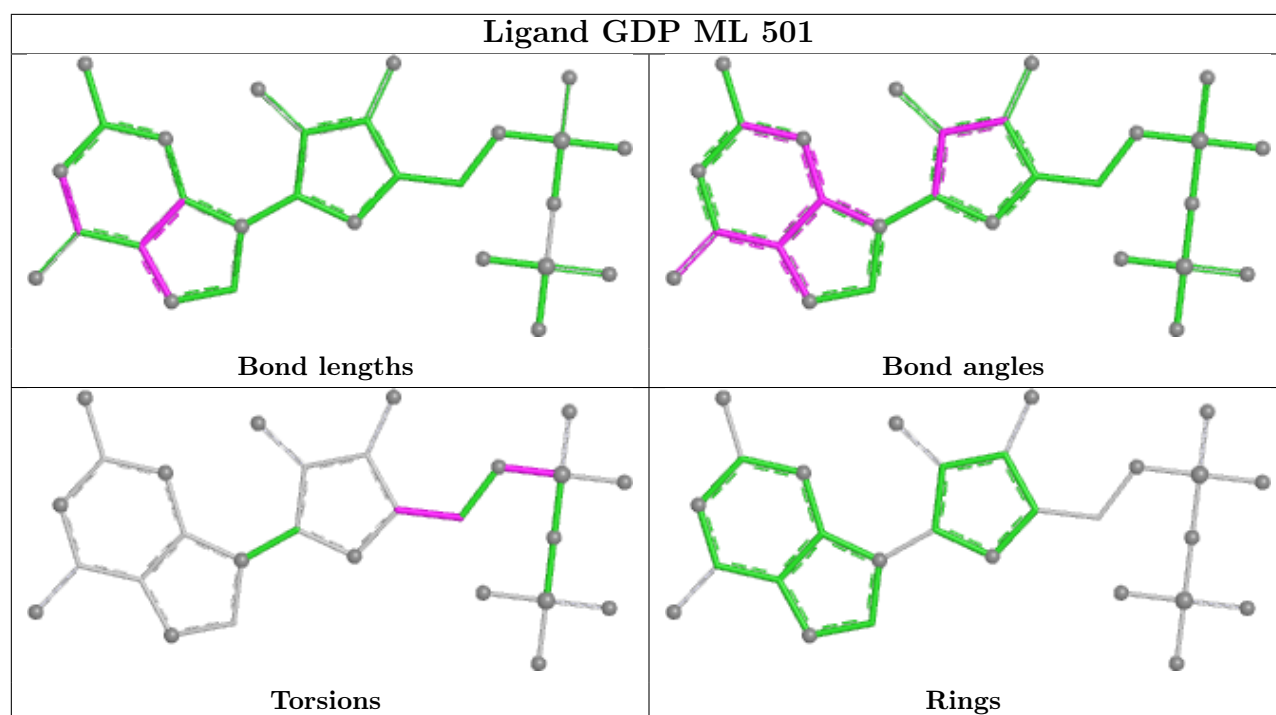




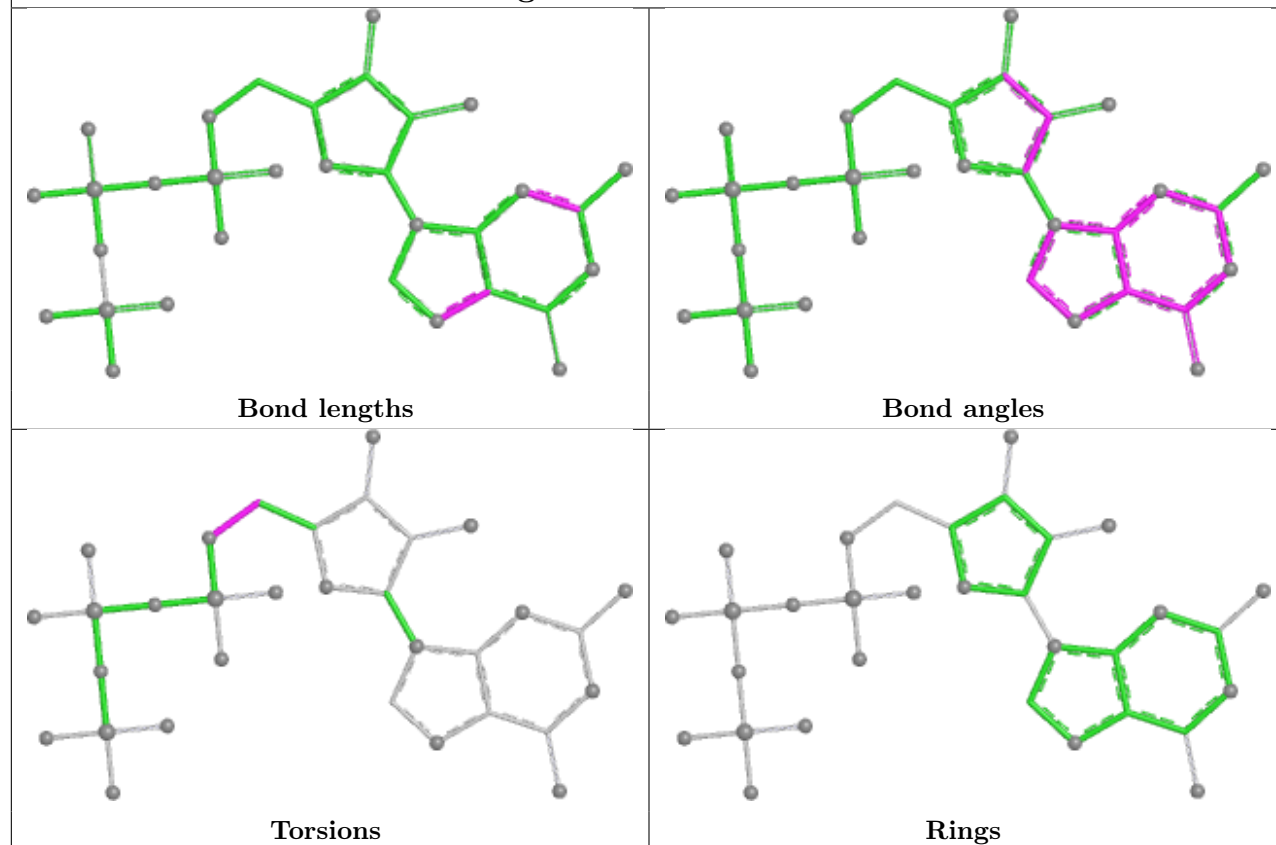




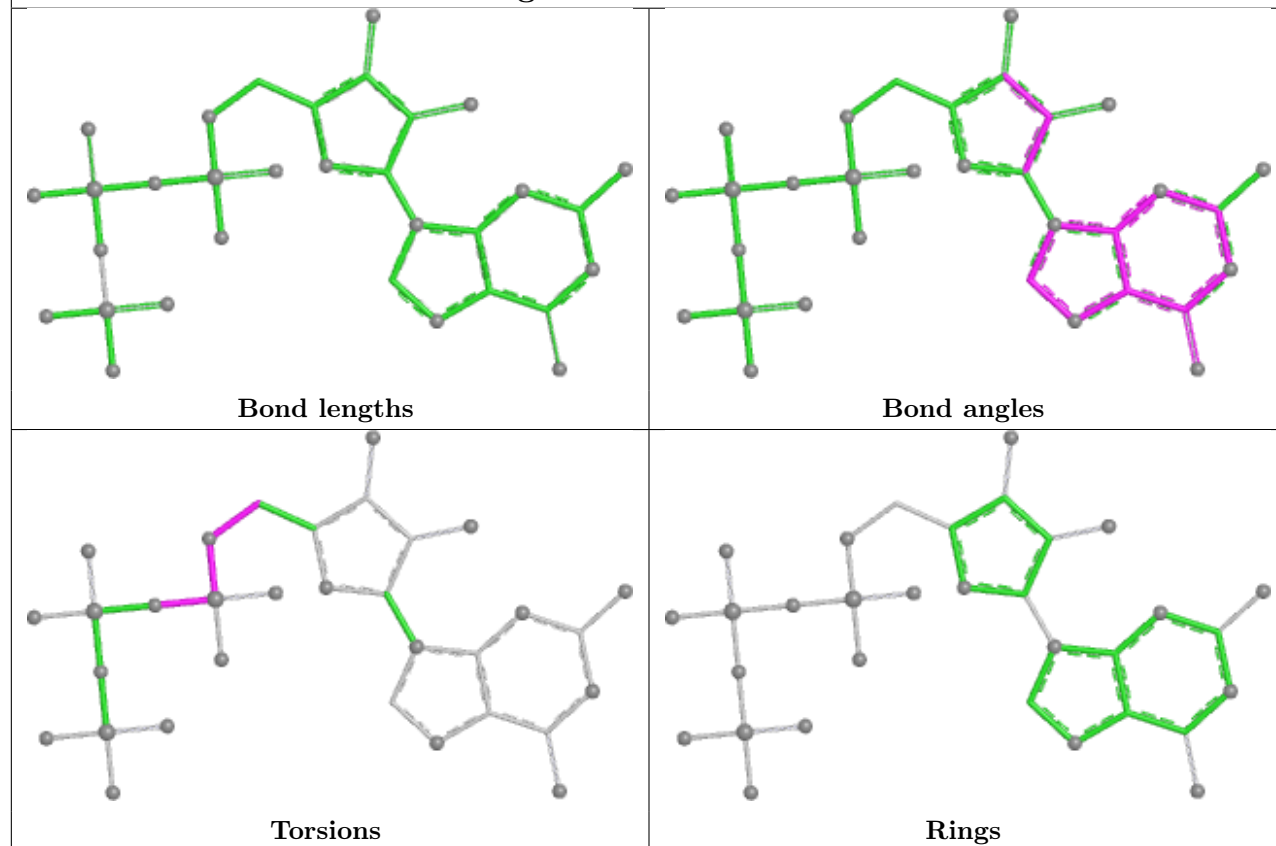




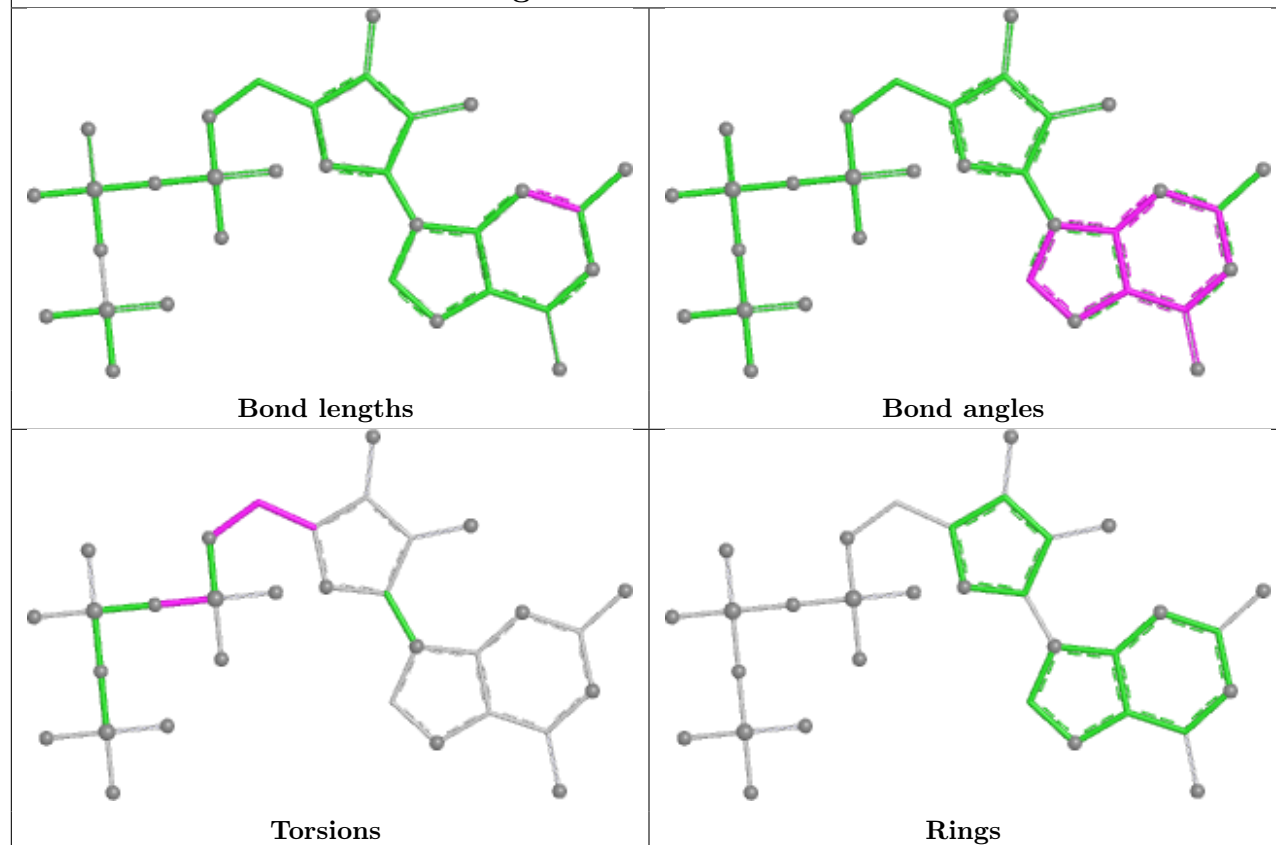
Ligand GTP AC 501



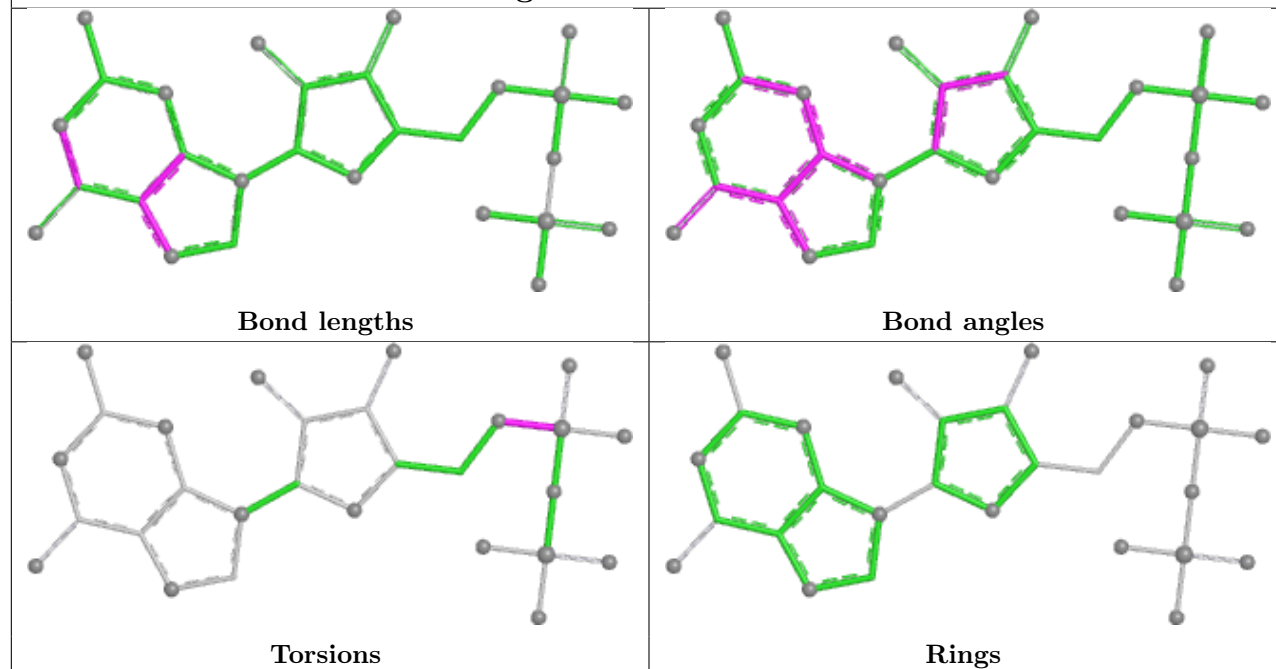
Ligand GTP VC 501

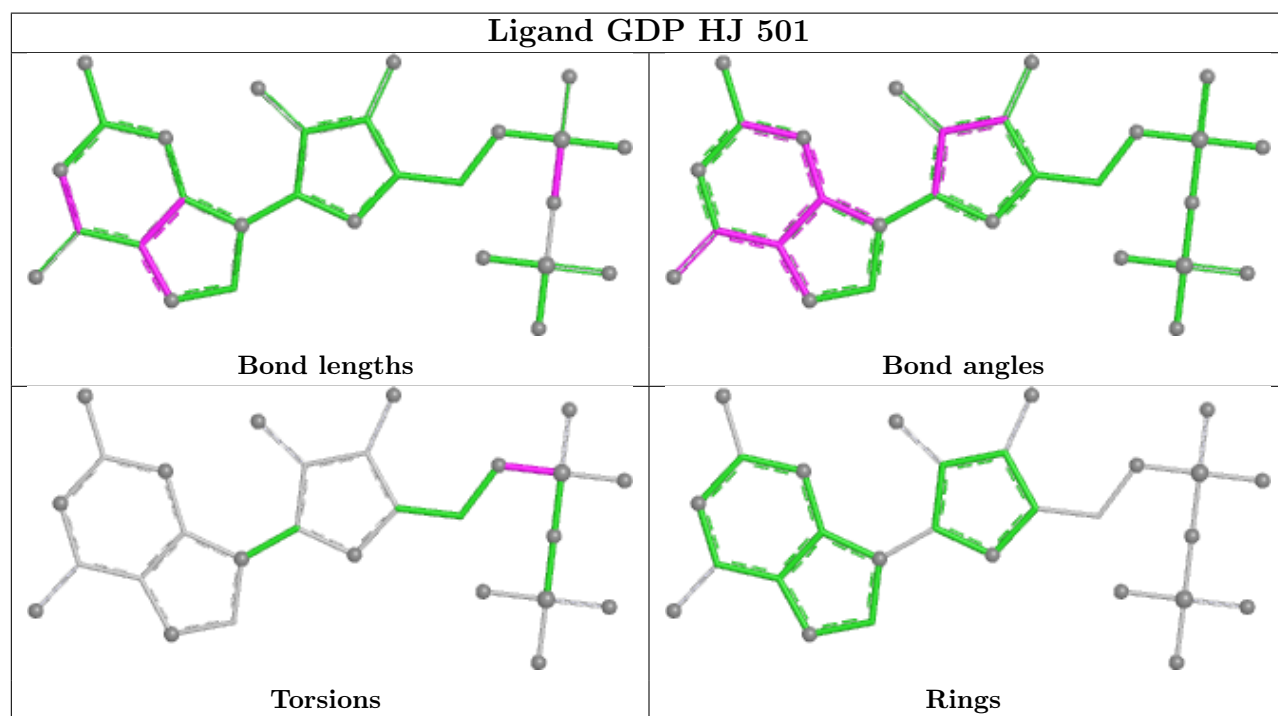
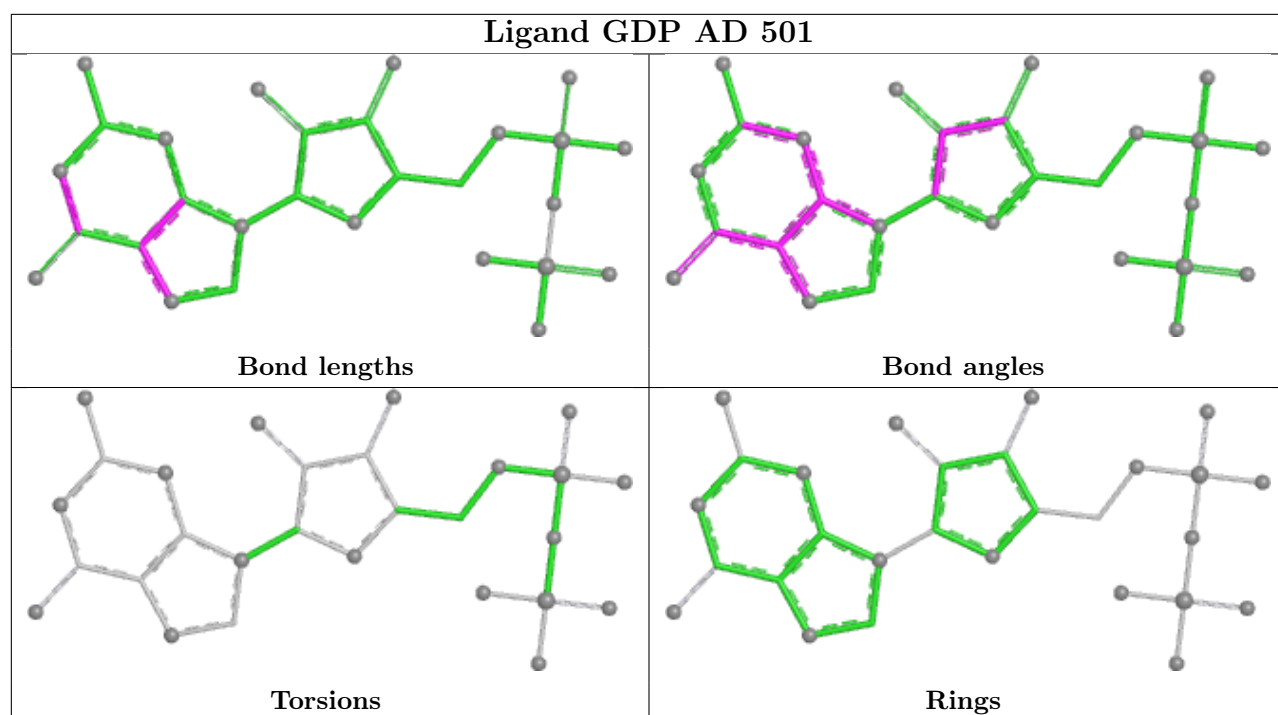


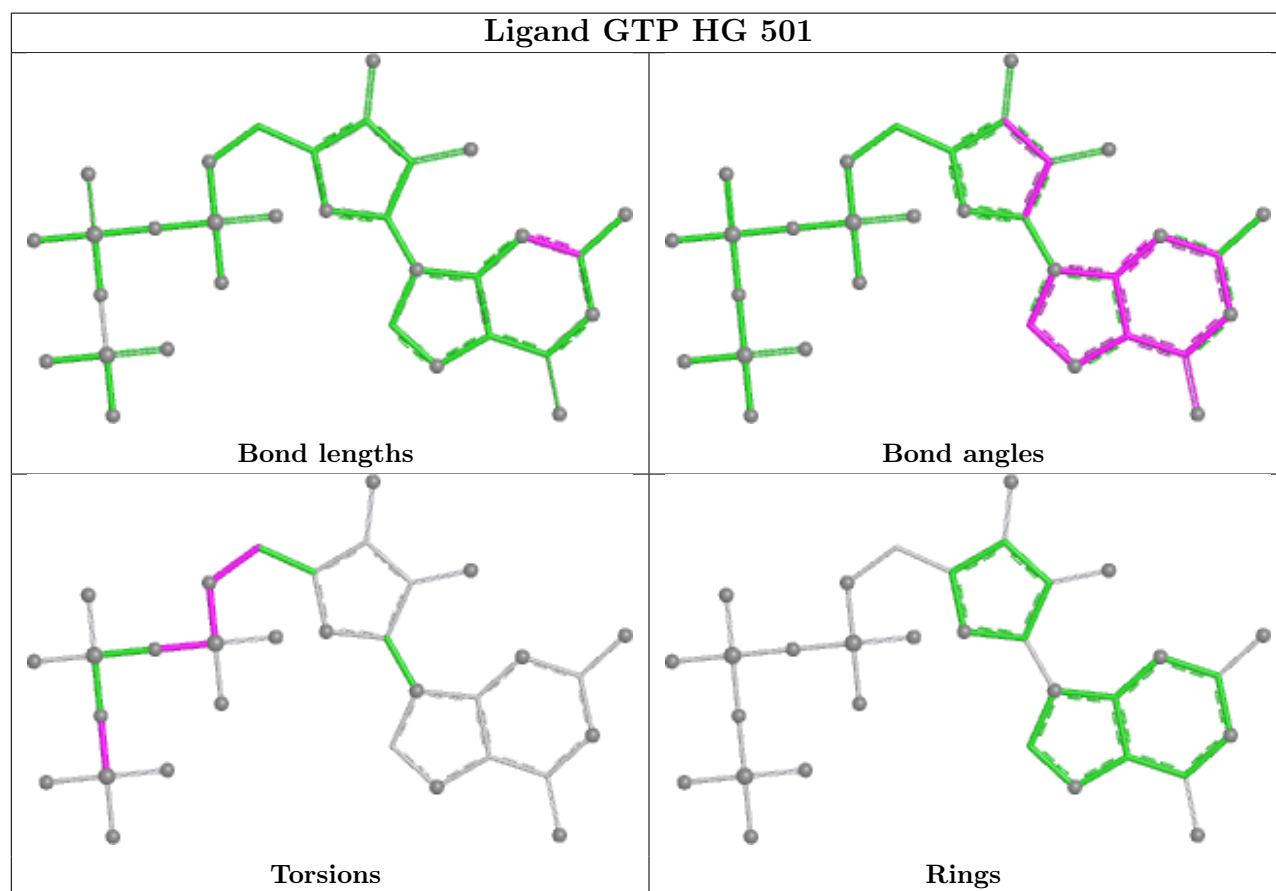
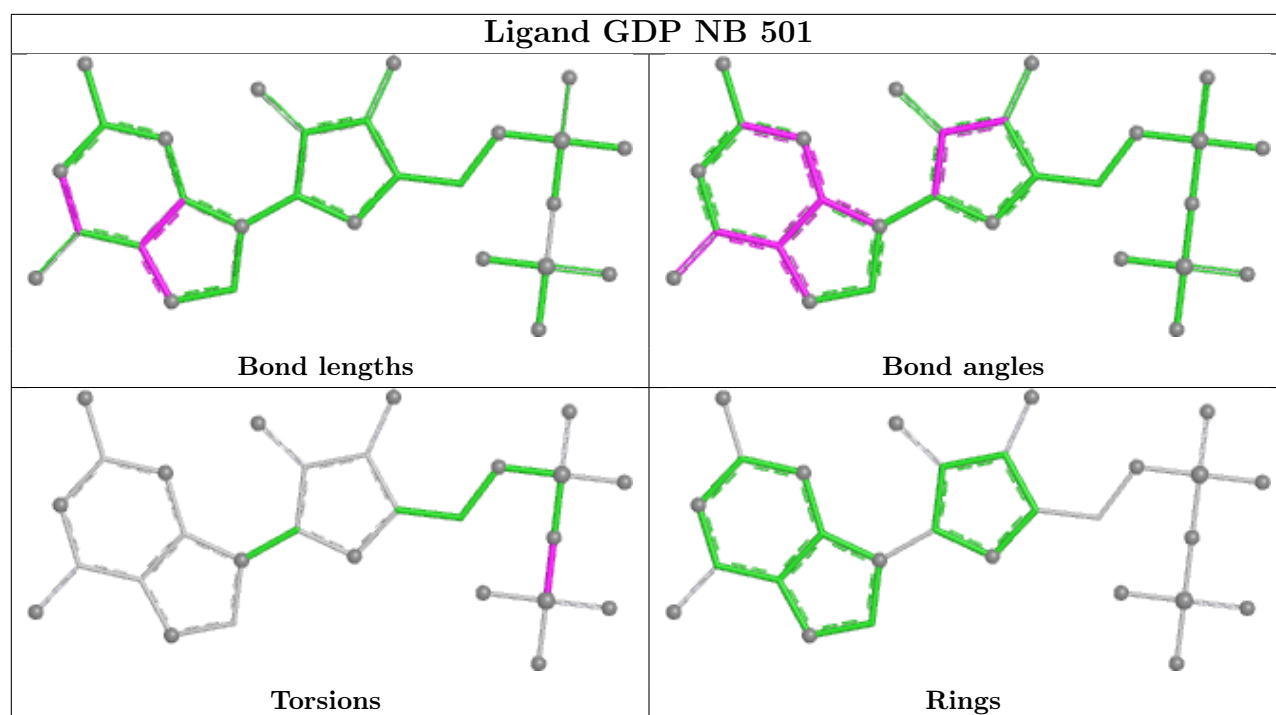
Ligand GTP HM 501



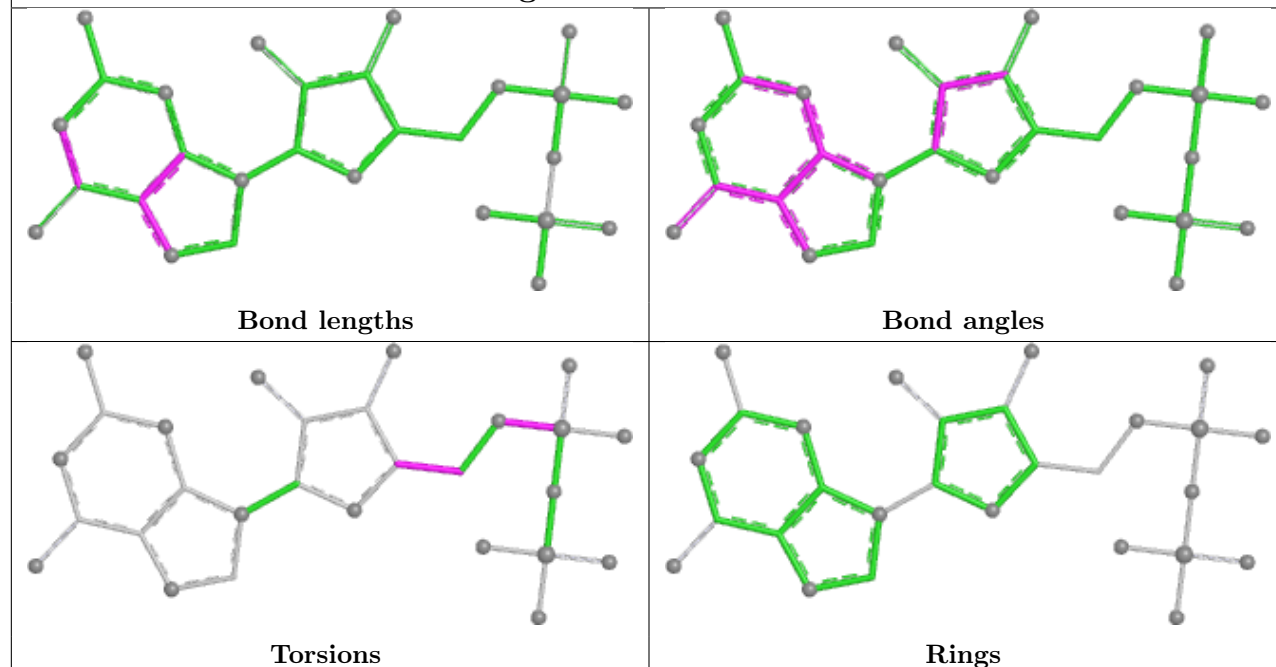
Ligand GDP DB 501



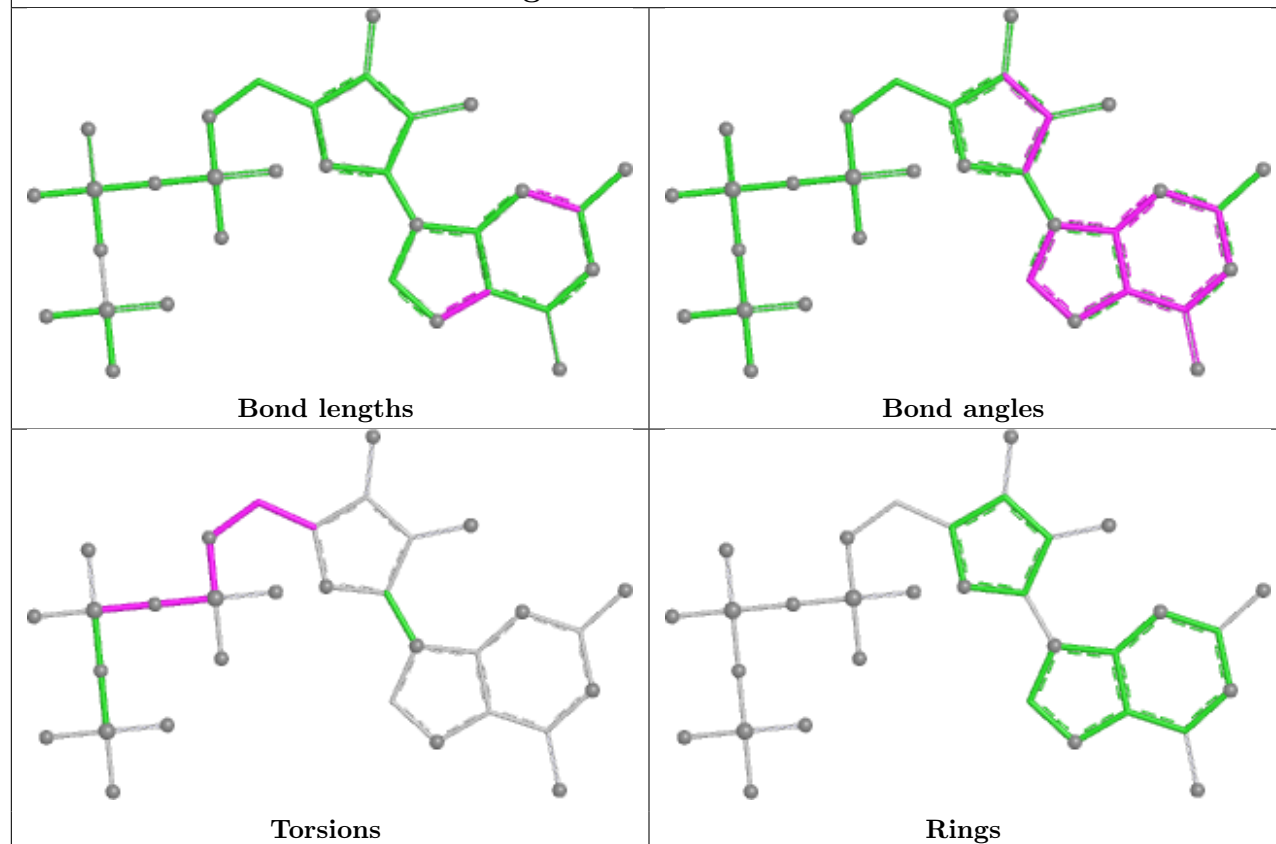




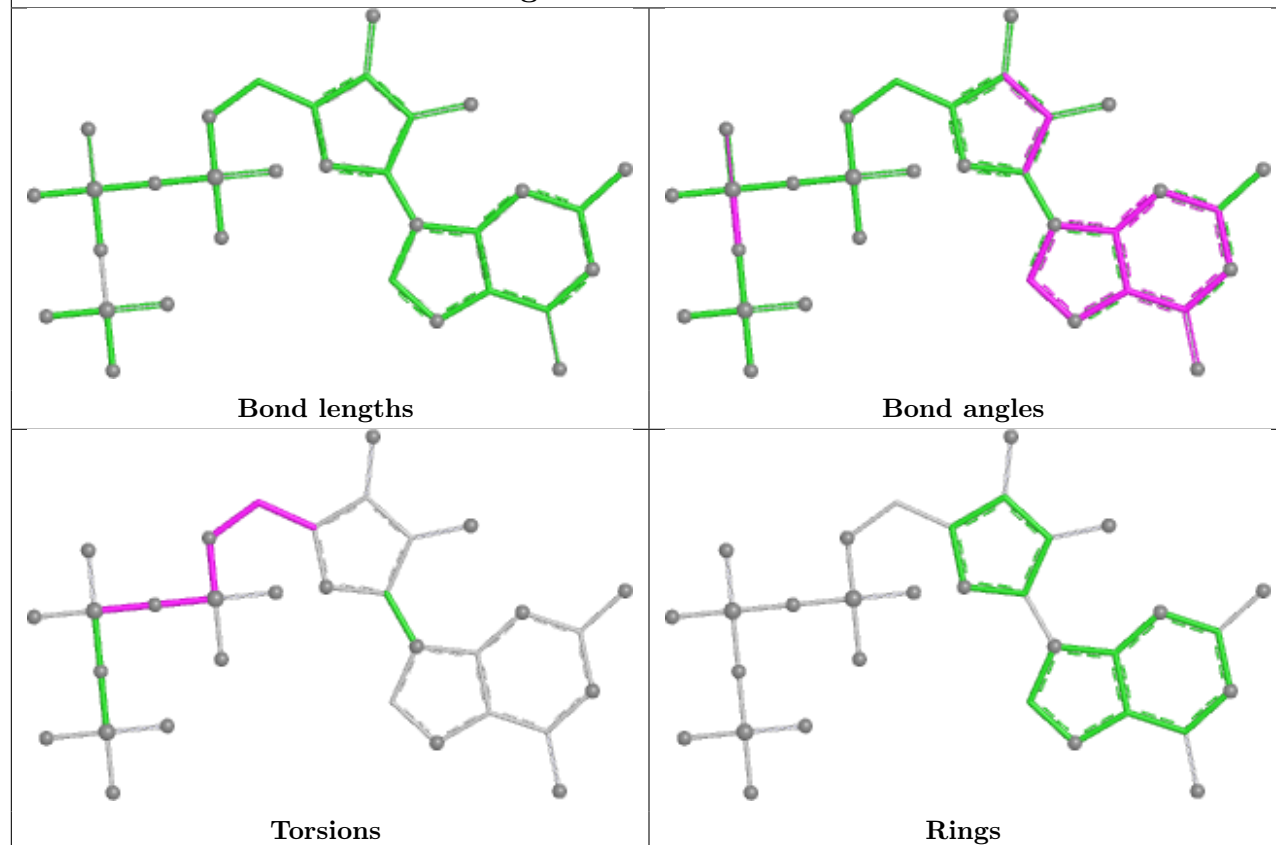
Ligand GDP BL 502



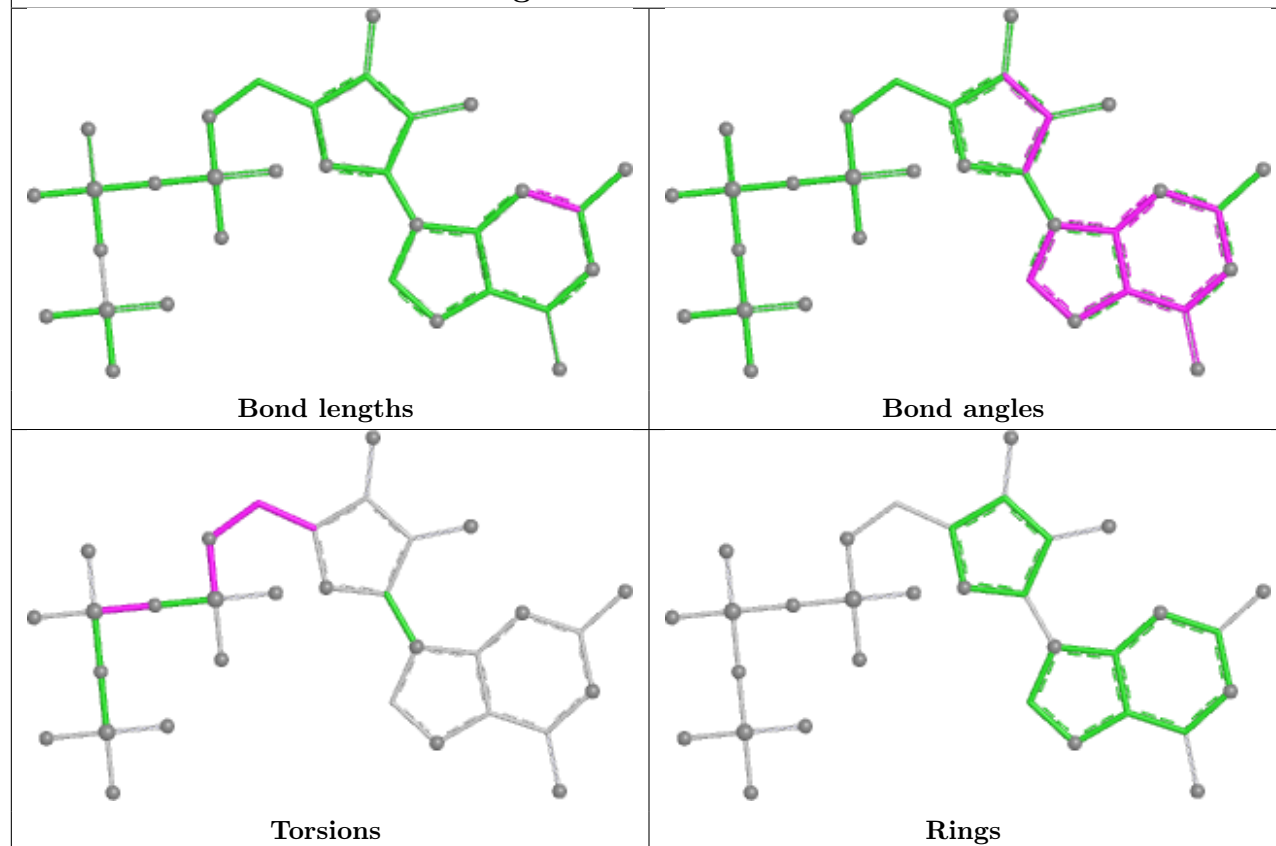
Ligand GTP IK 501

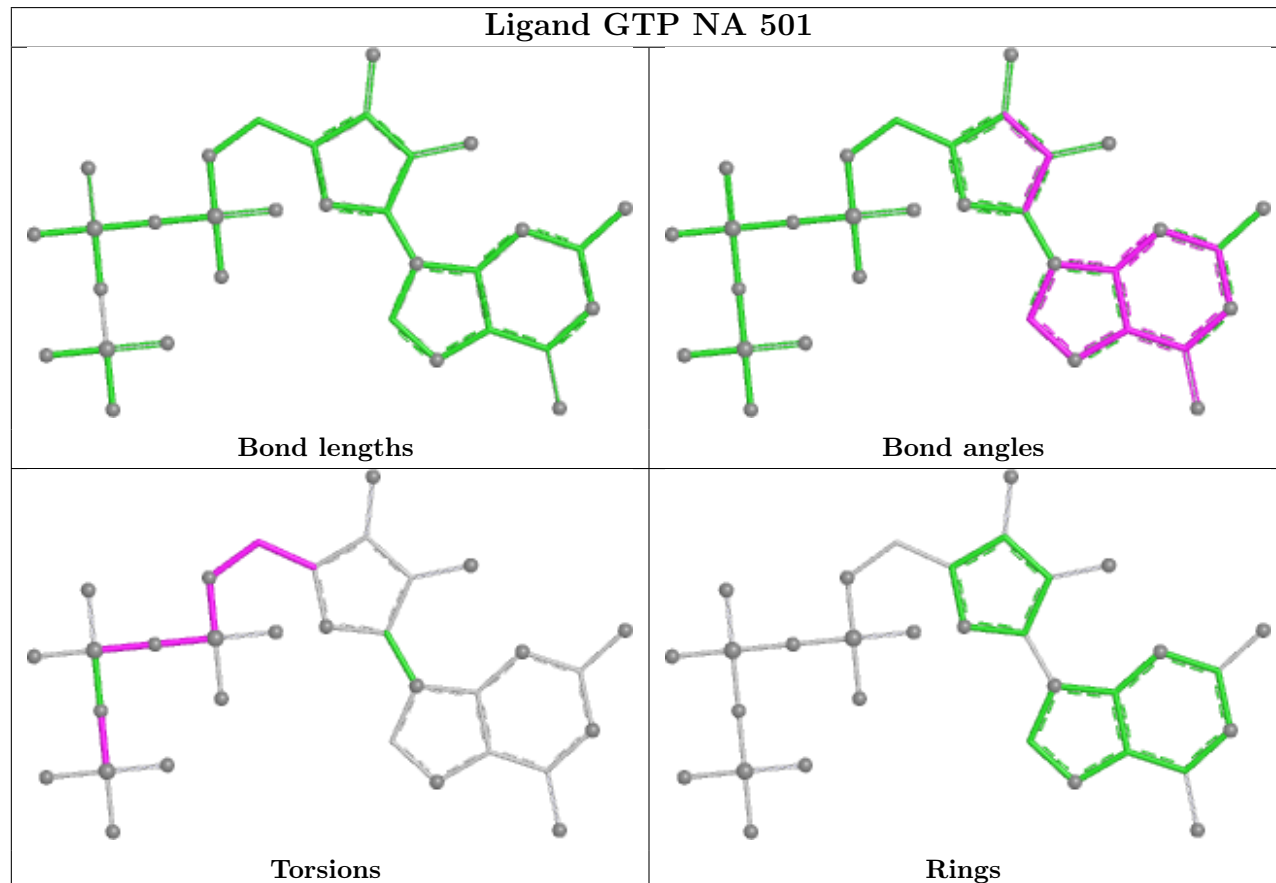
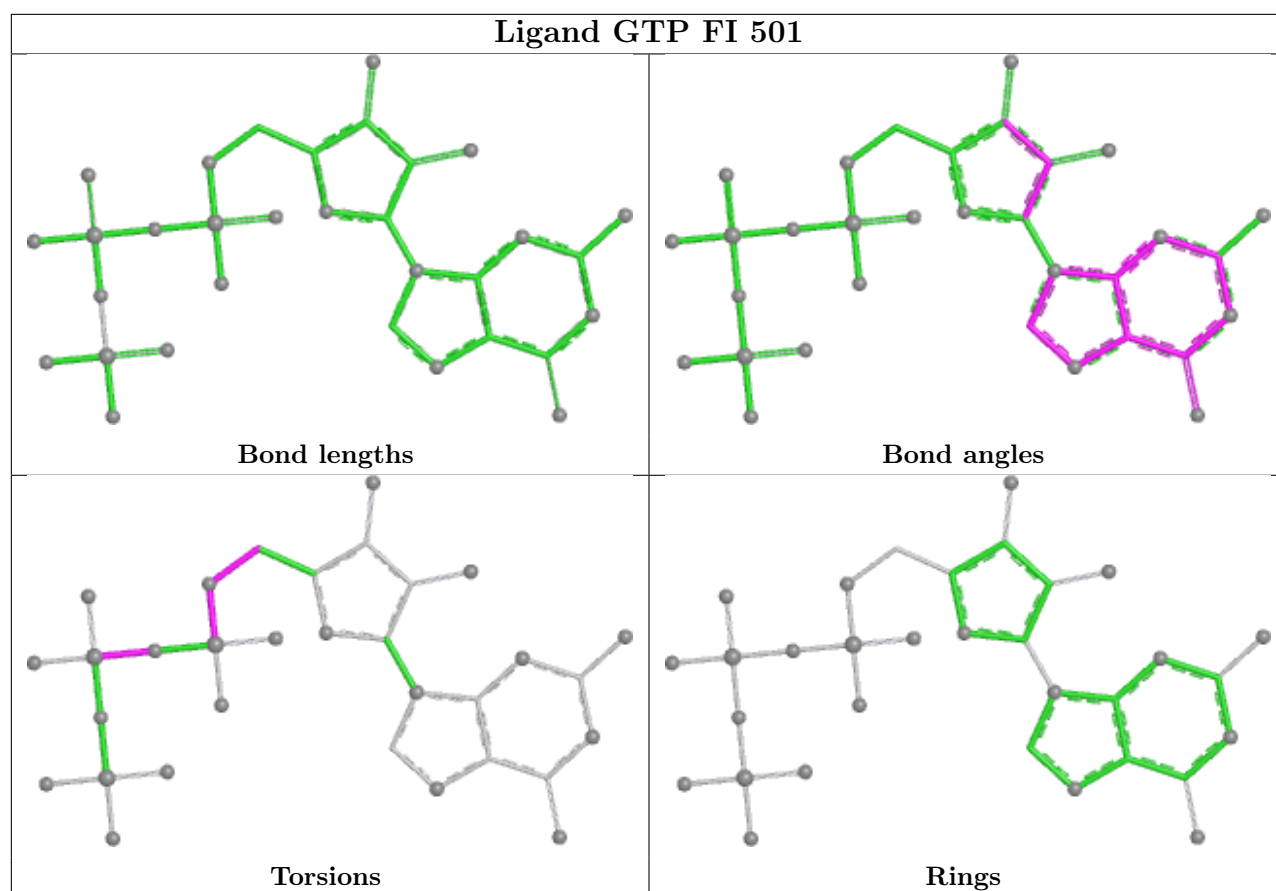


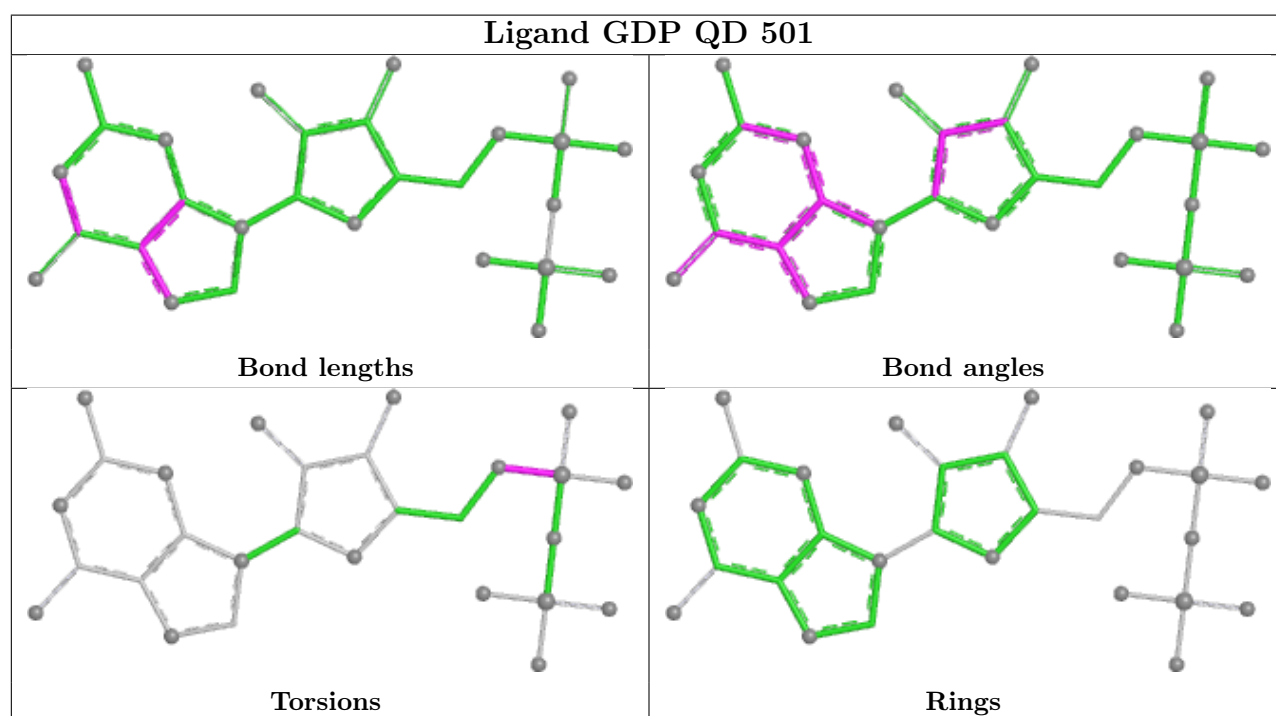
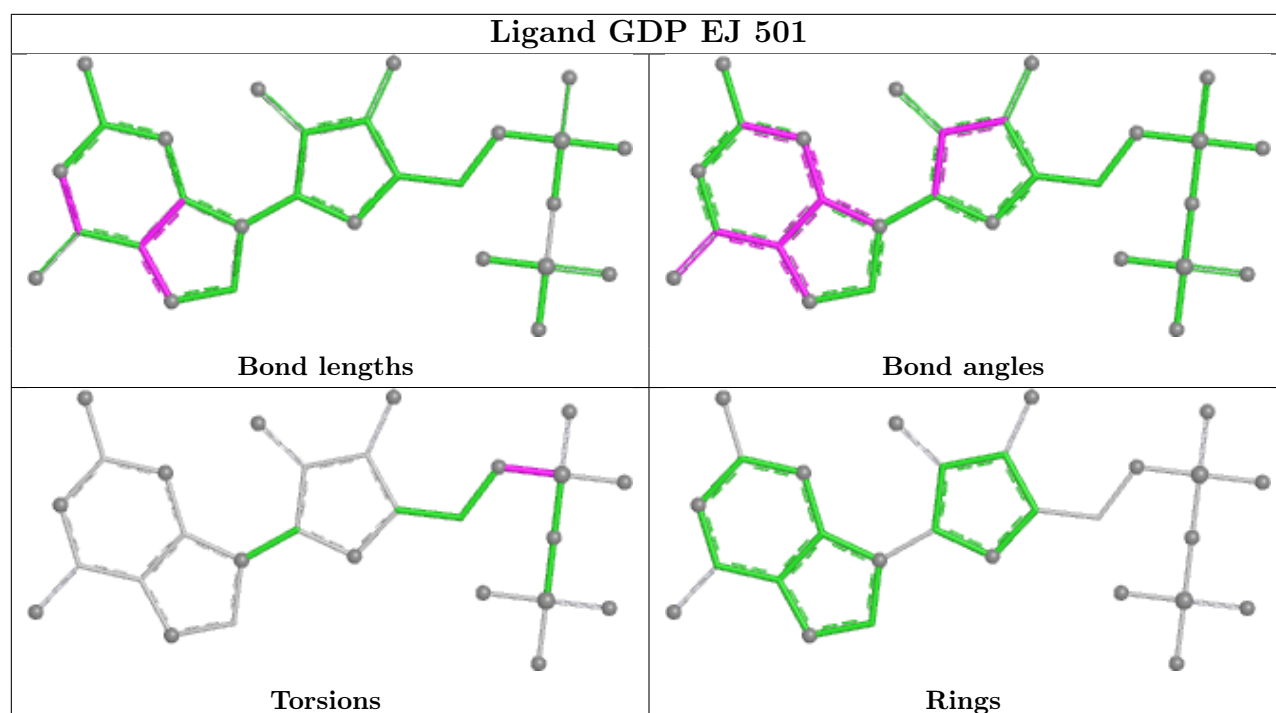
Ligand GTP JG 501



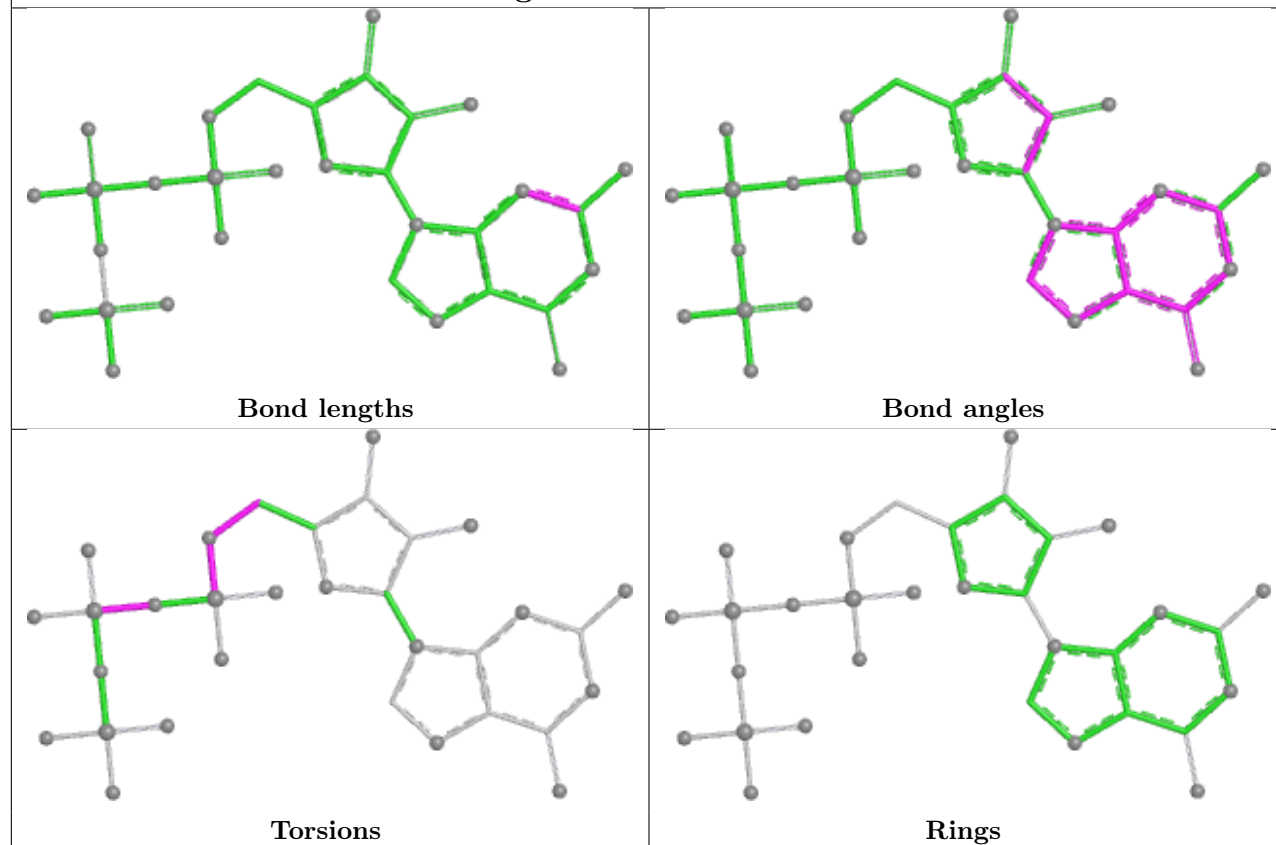
Ligand GTP AM 501



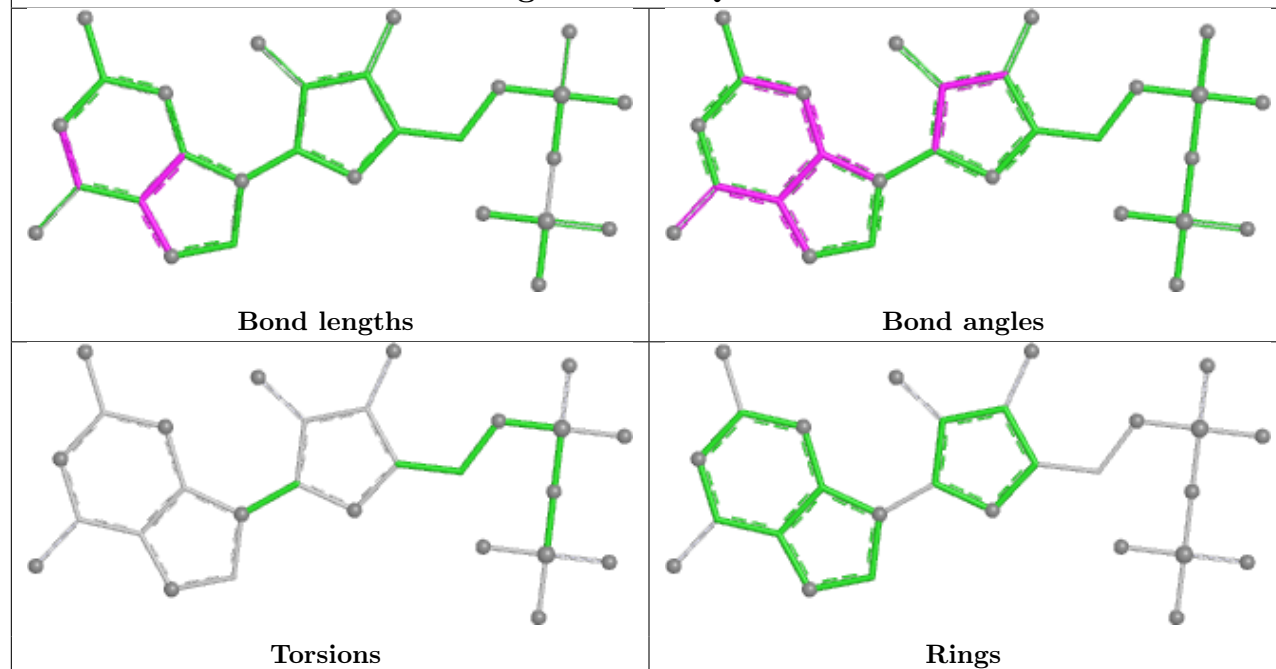


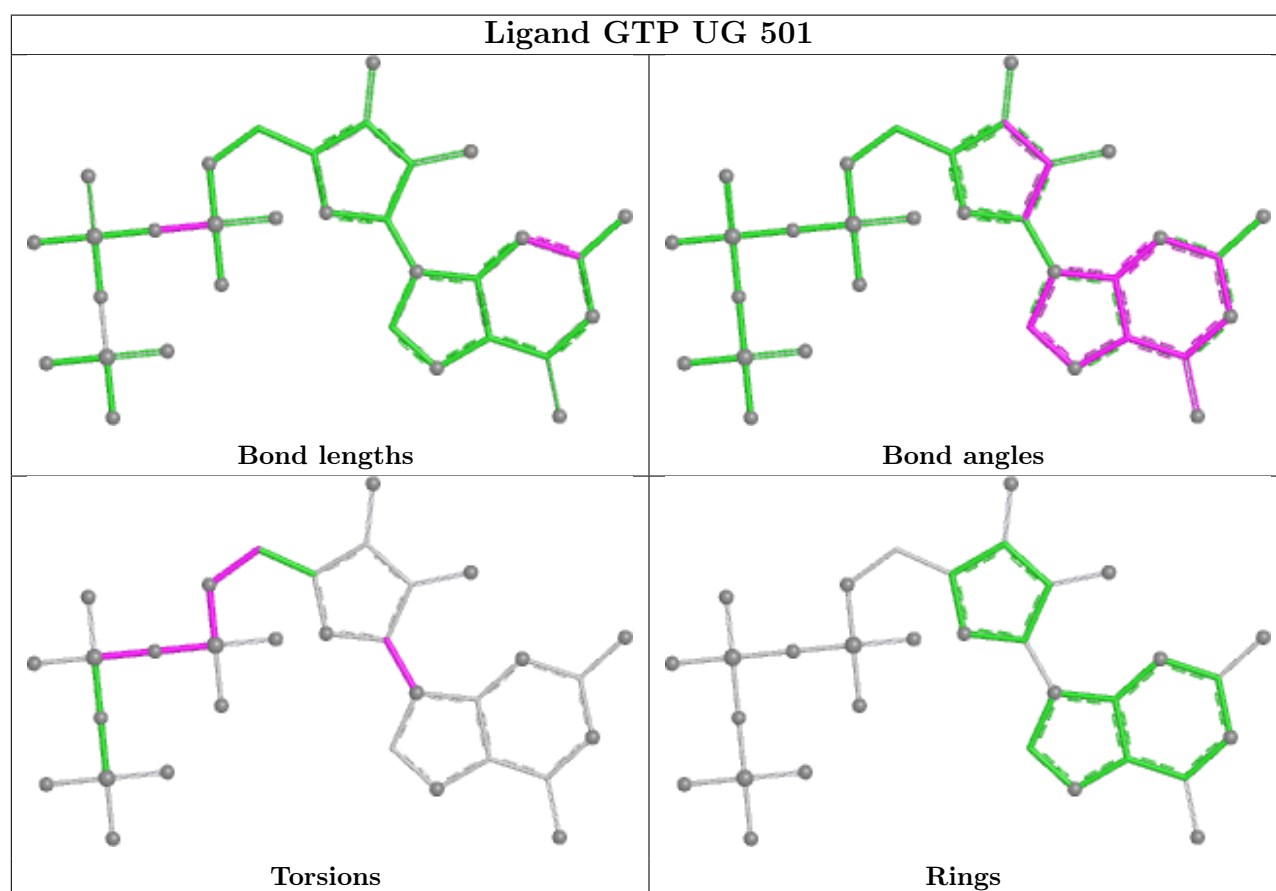
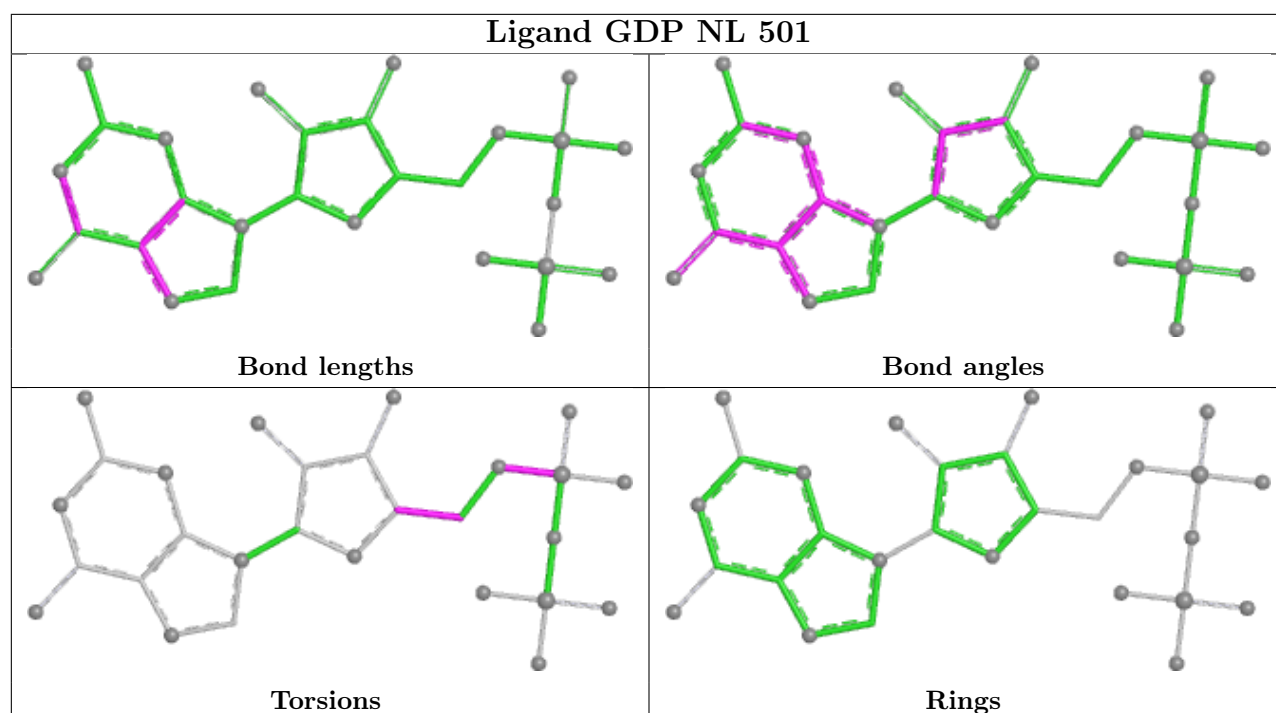


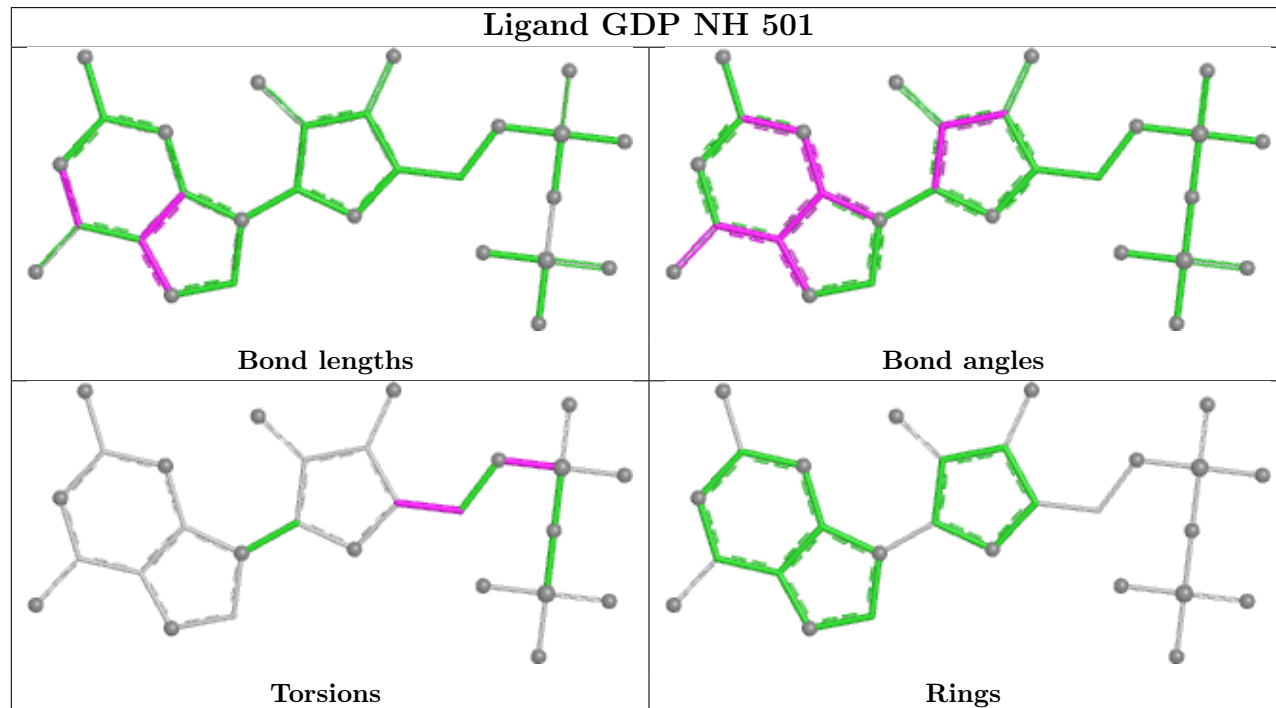
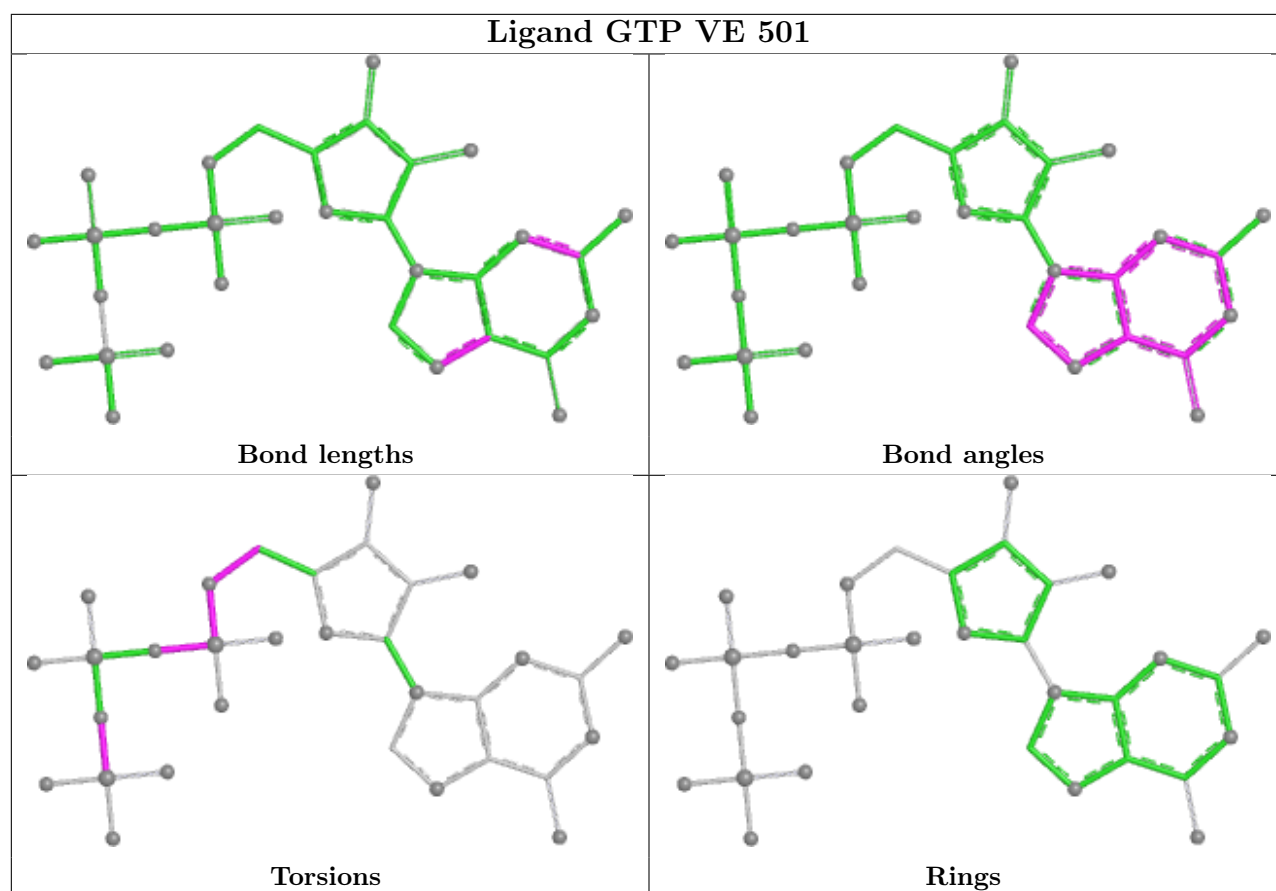
Ligand GTP EM 501

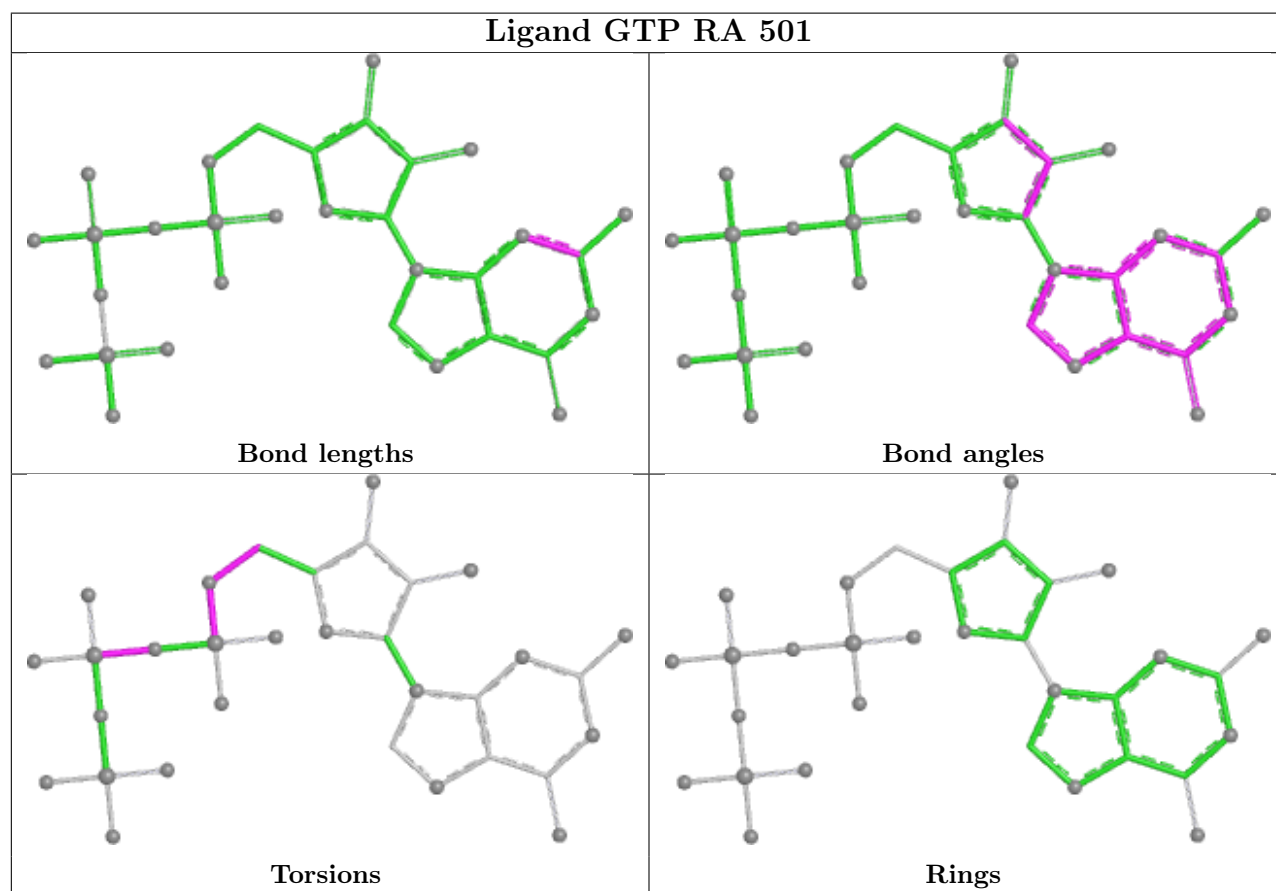
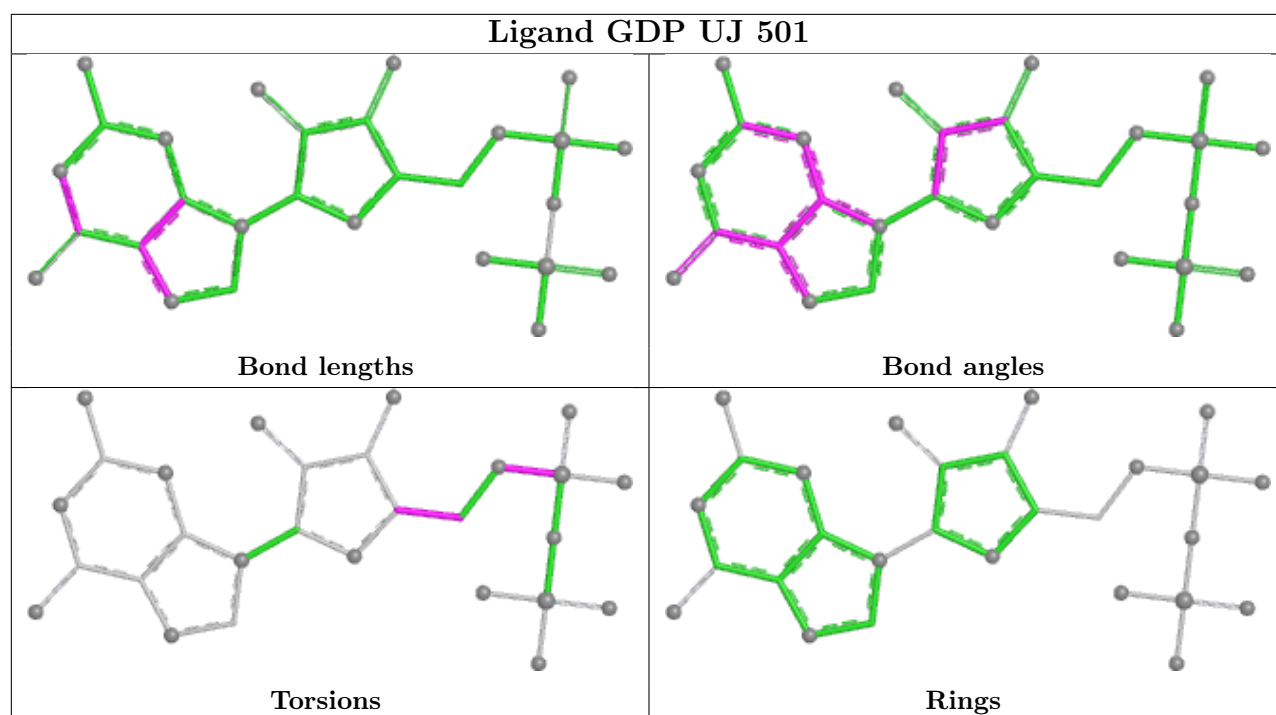


Ligand GDP QF 501

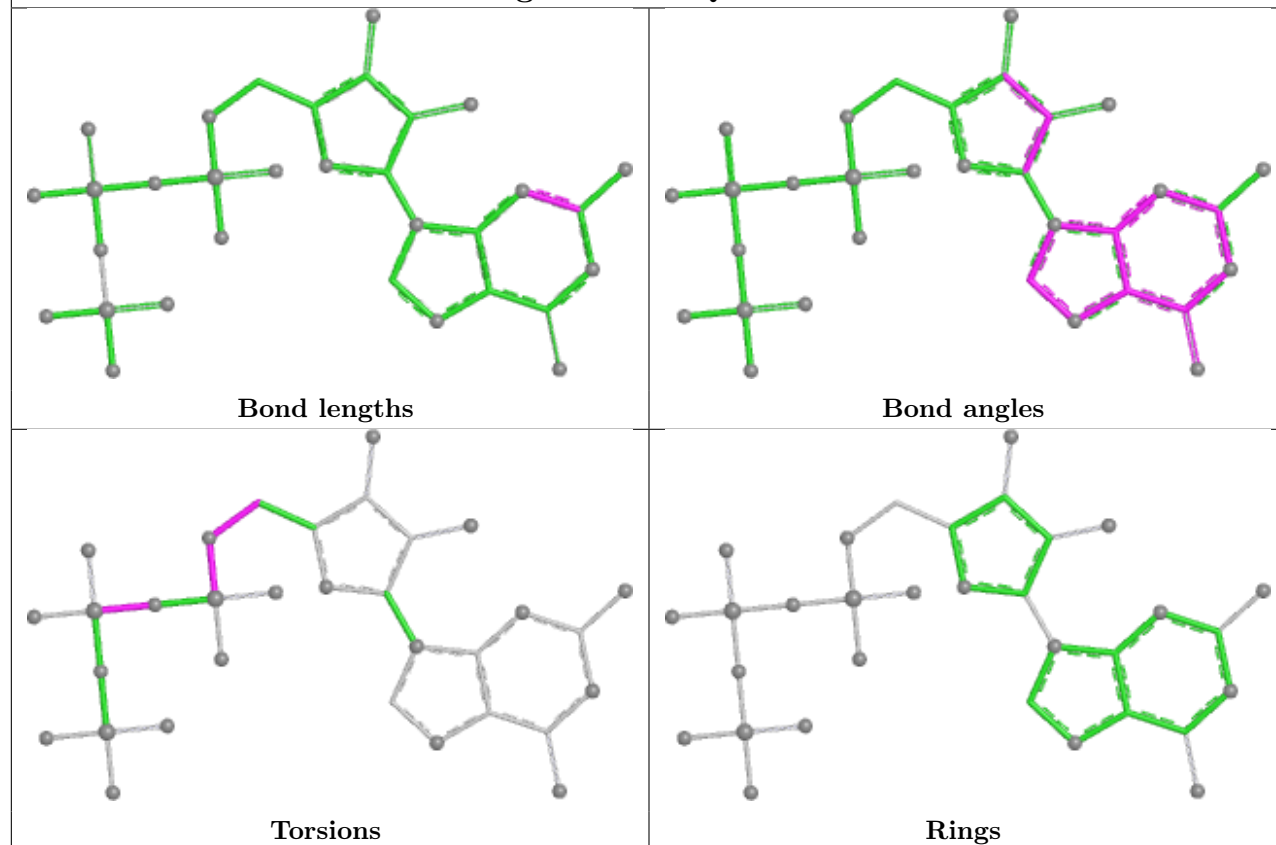




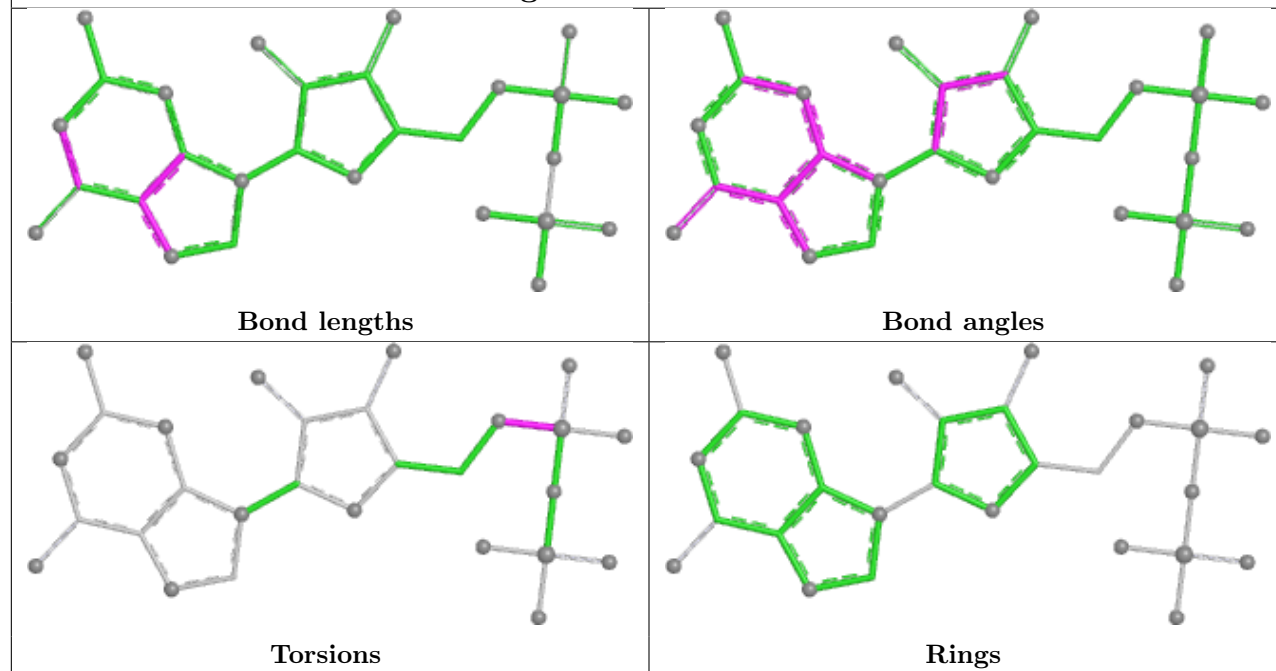


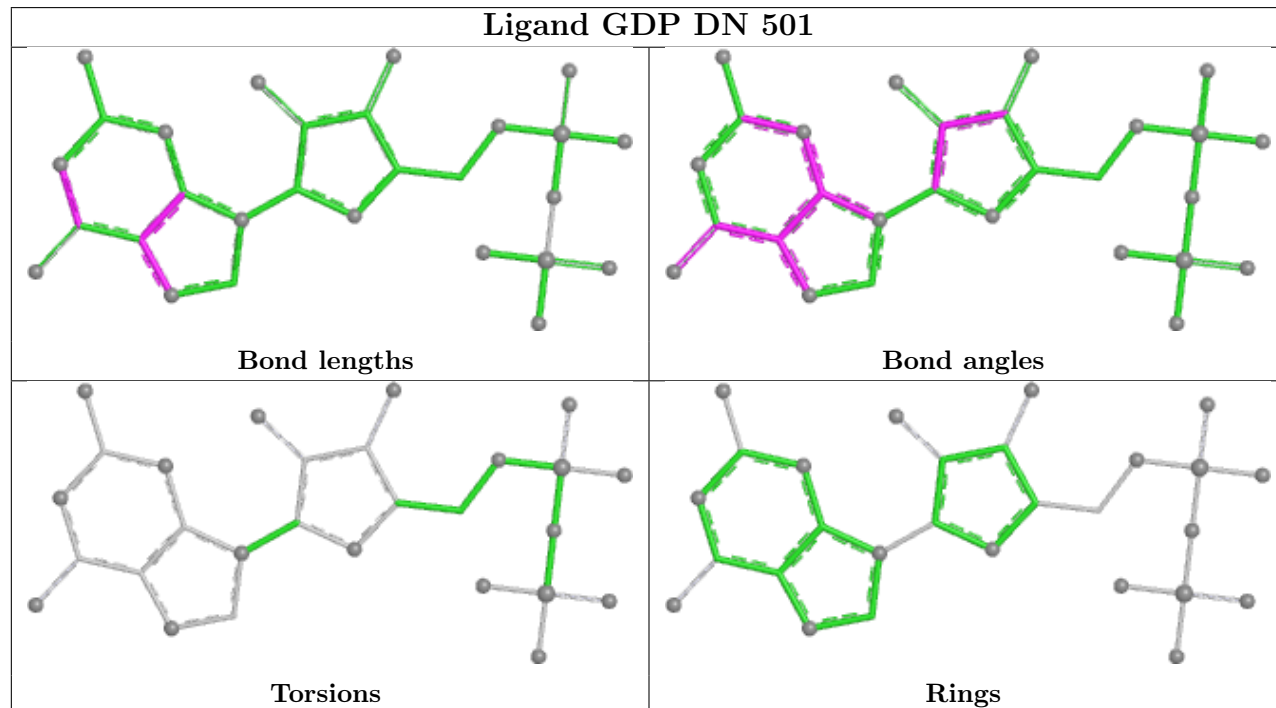
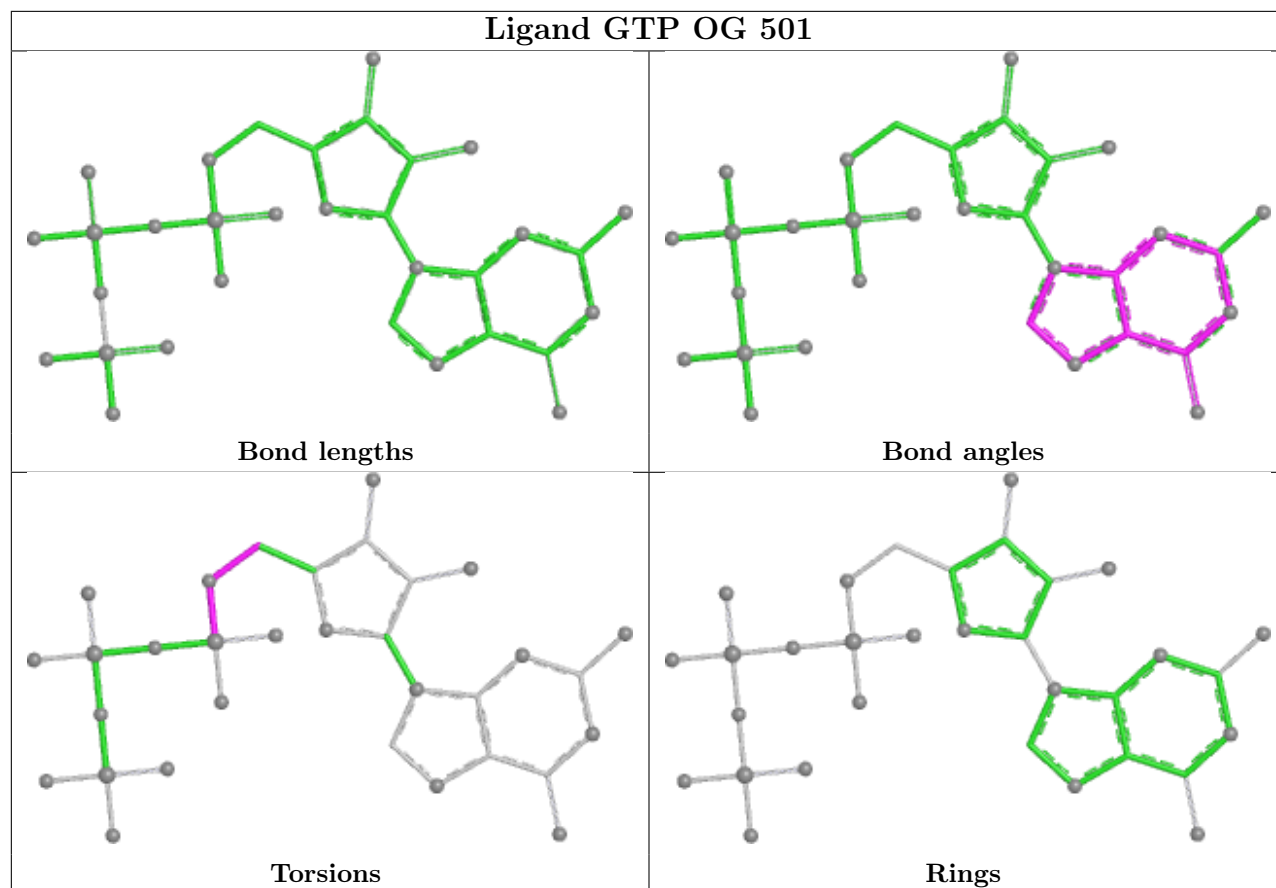


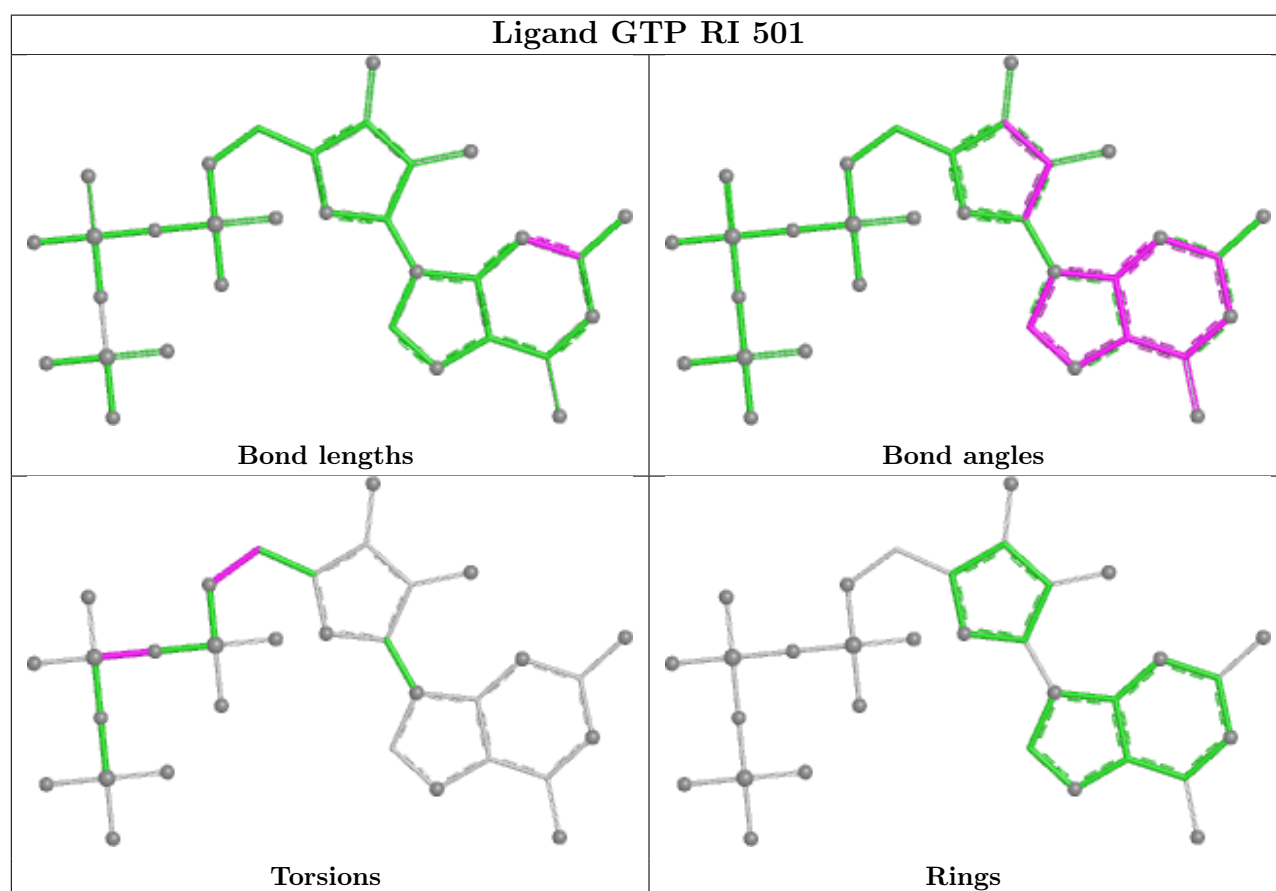
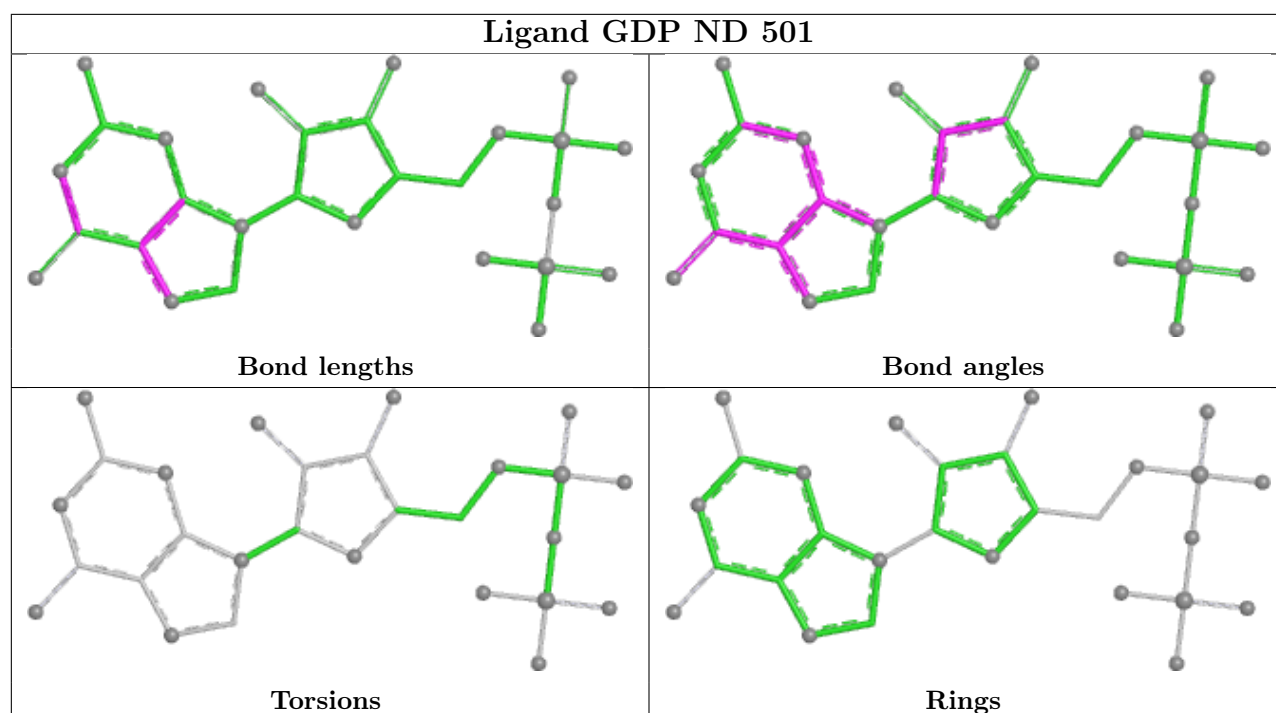
Ligand GTP QK 501

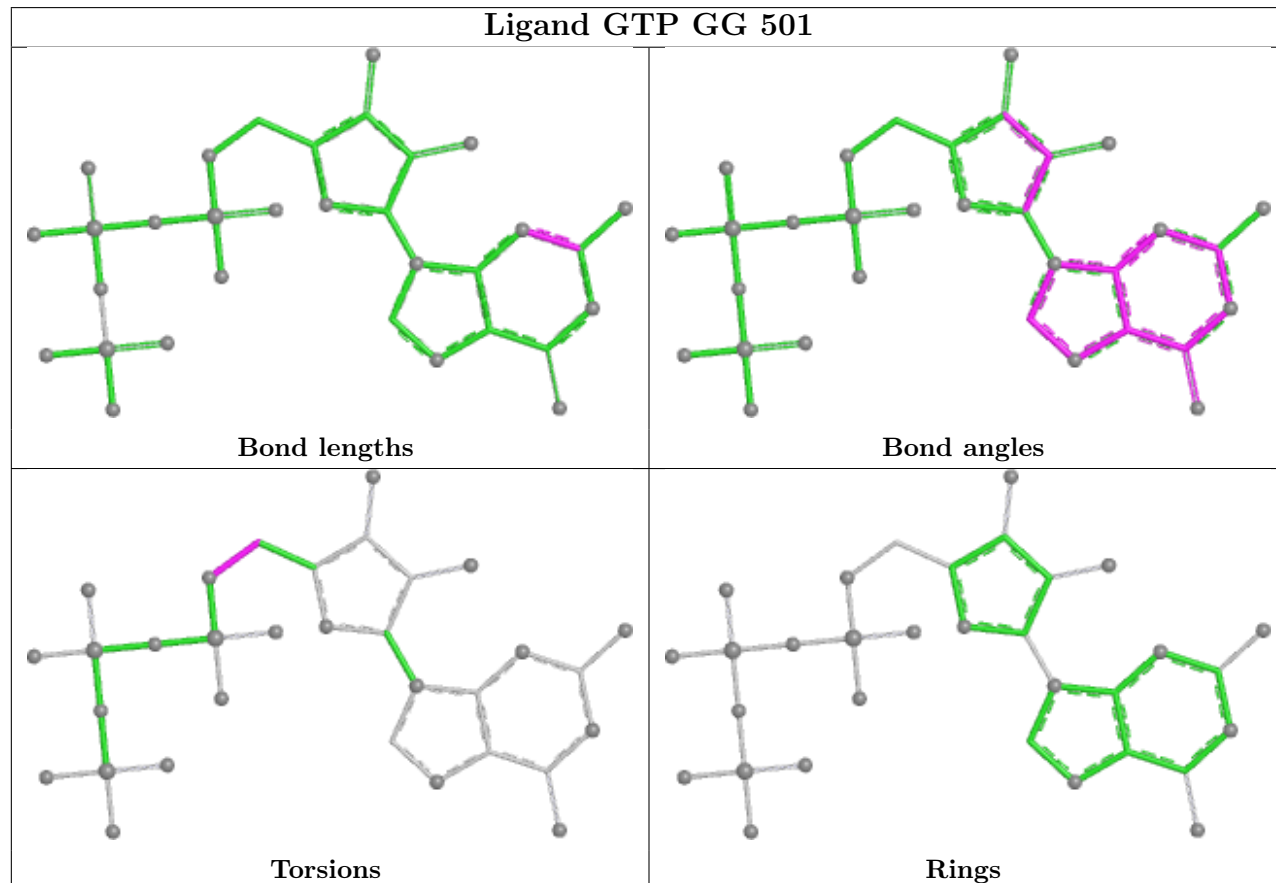
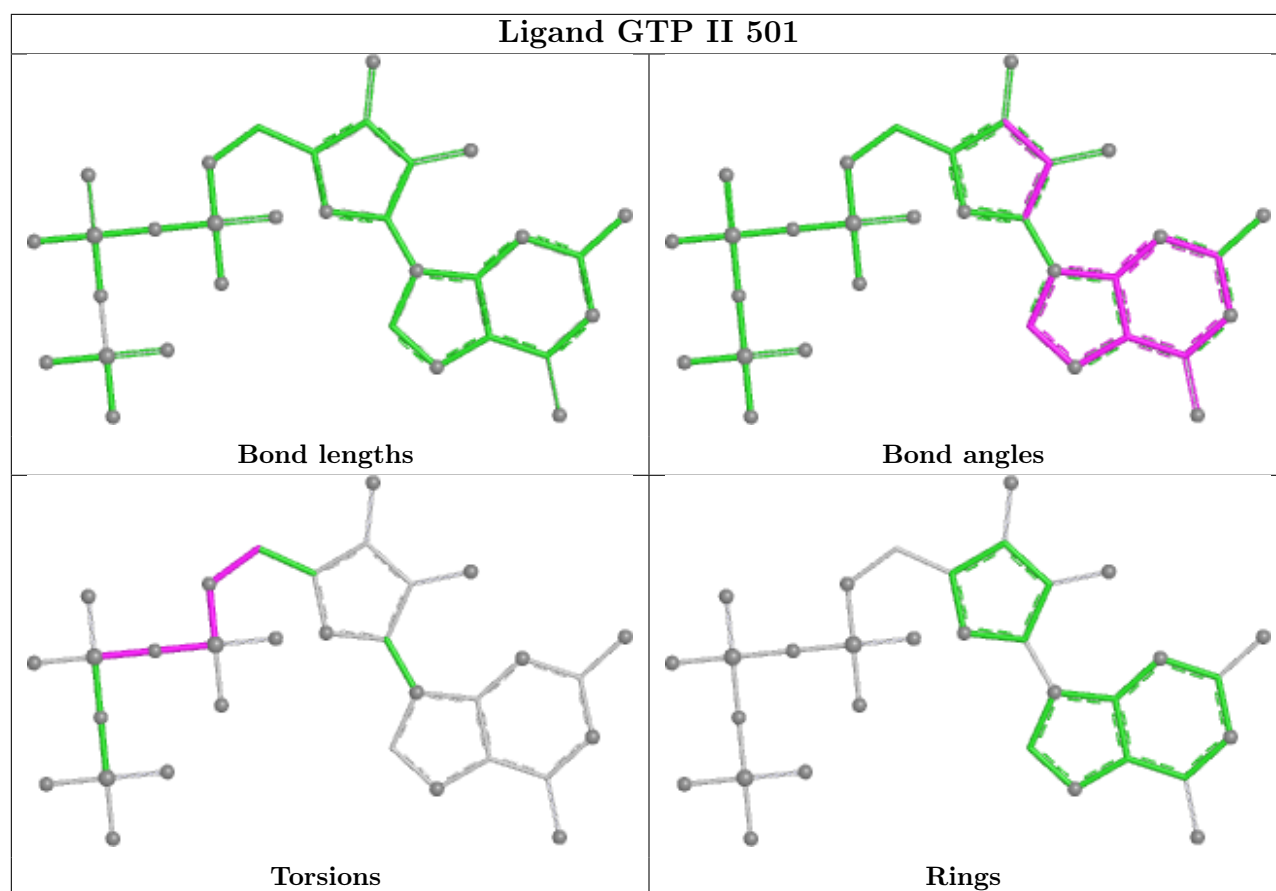


Ligand GDP JB 501

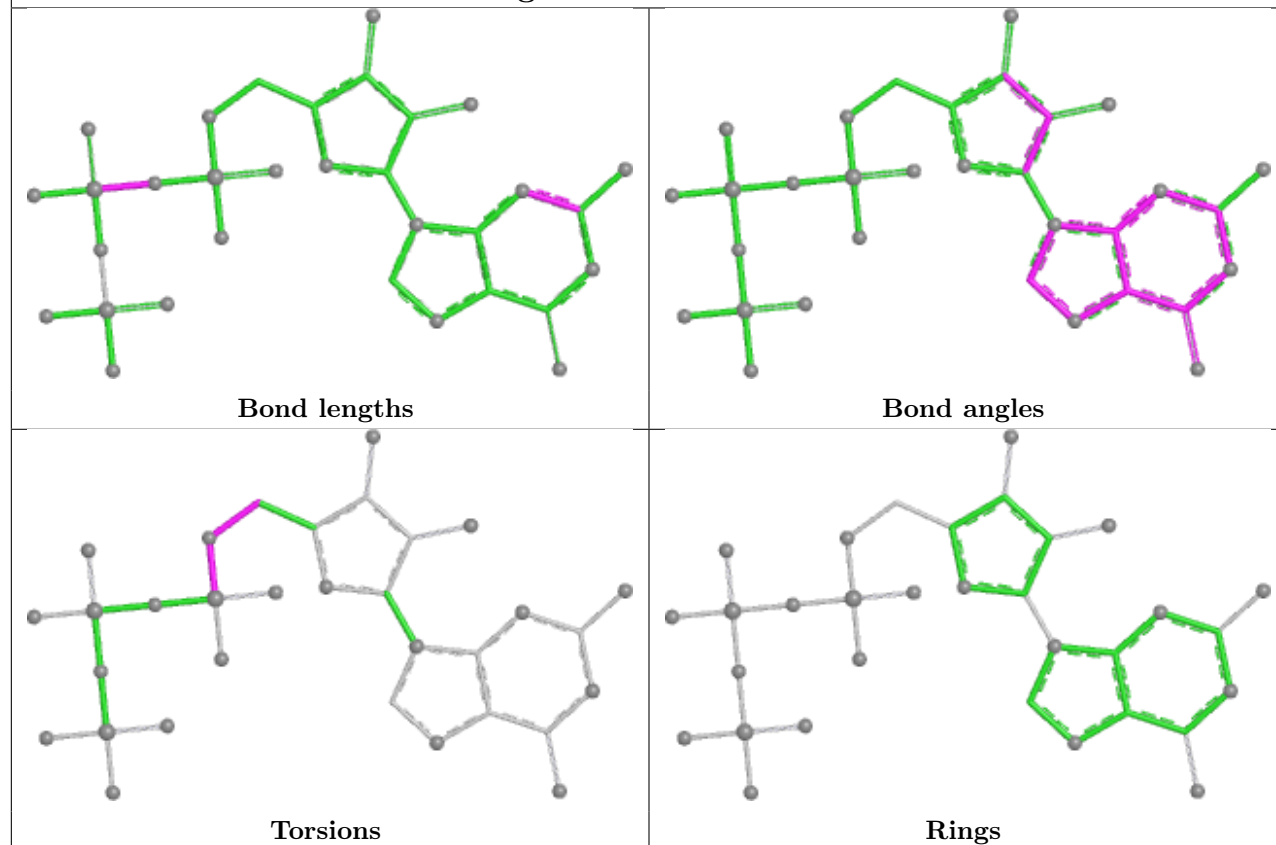




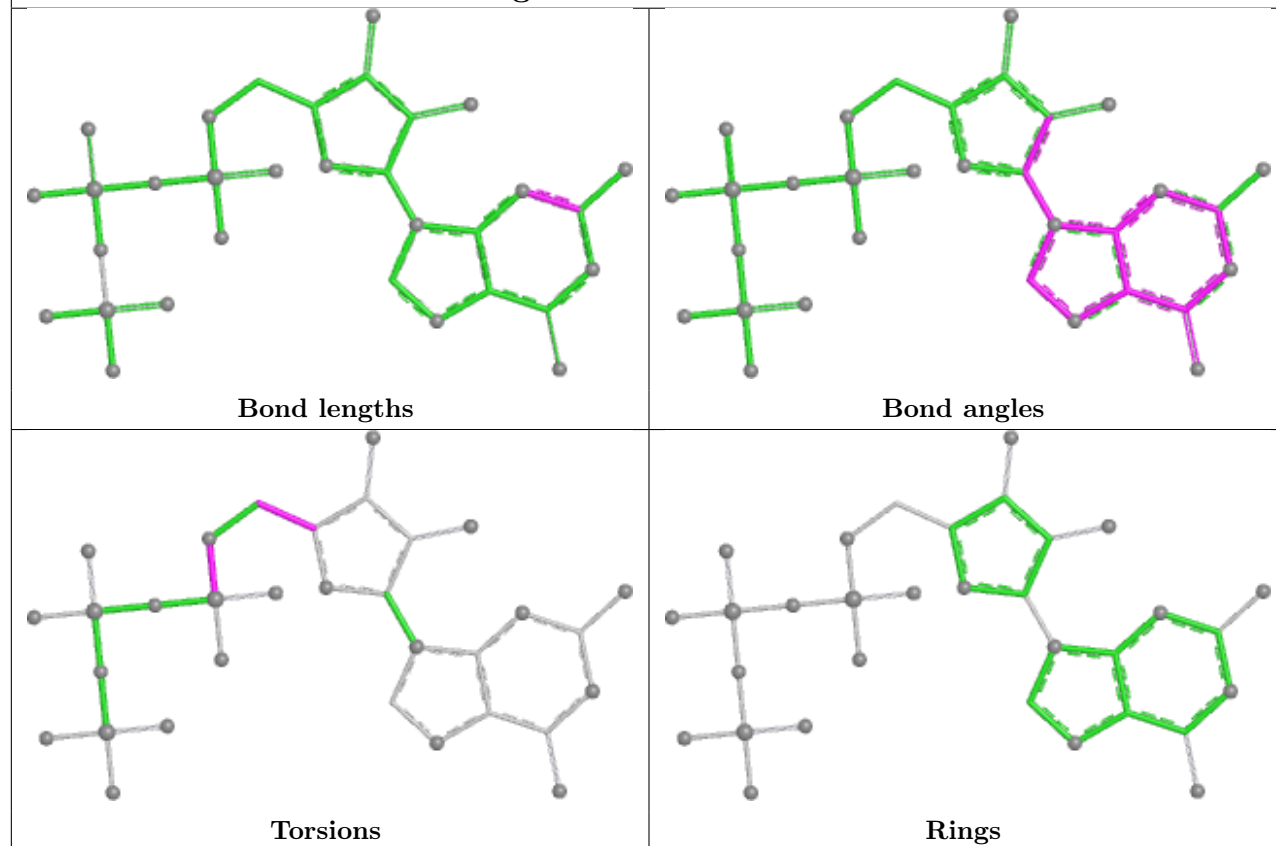


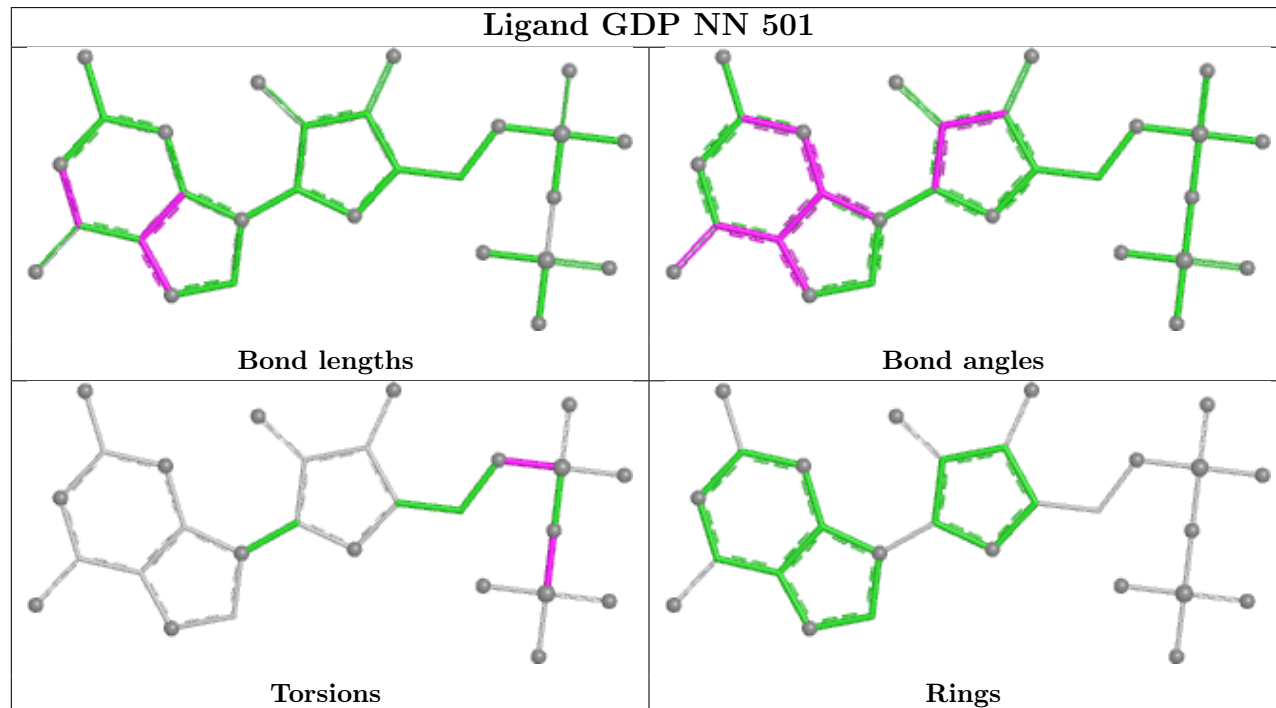
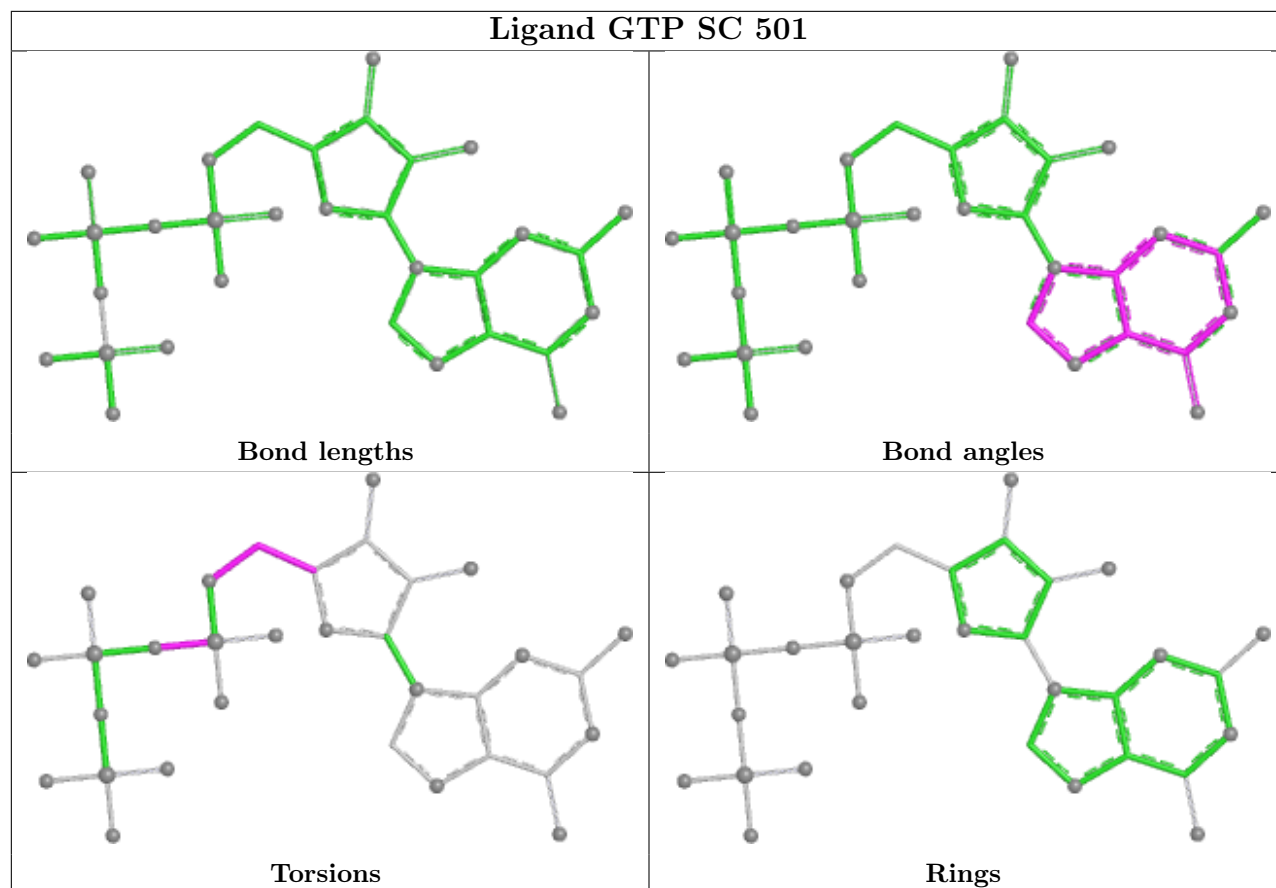


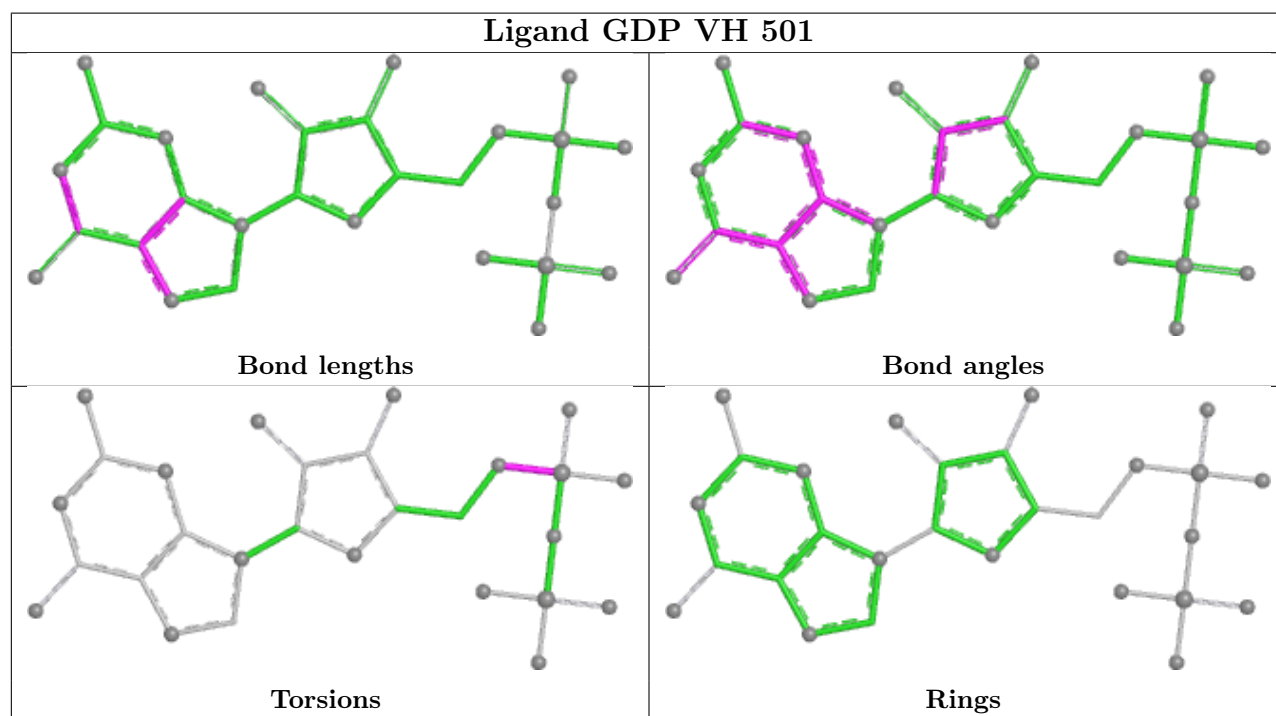
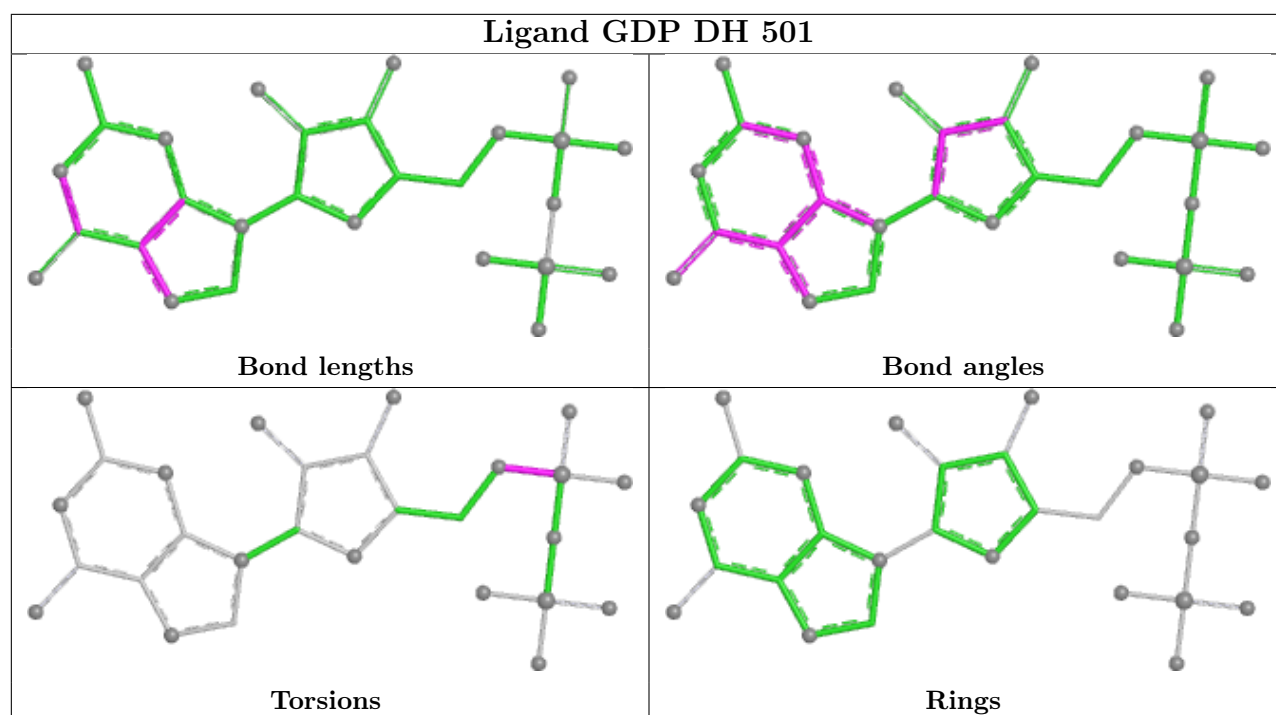
Ligand GTP CC 501

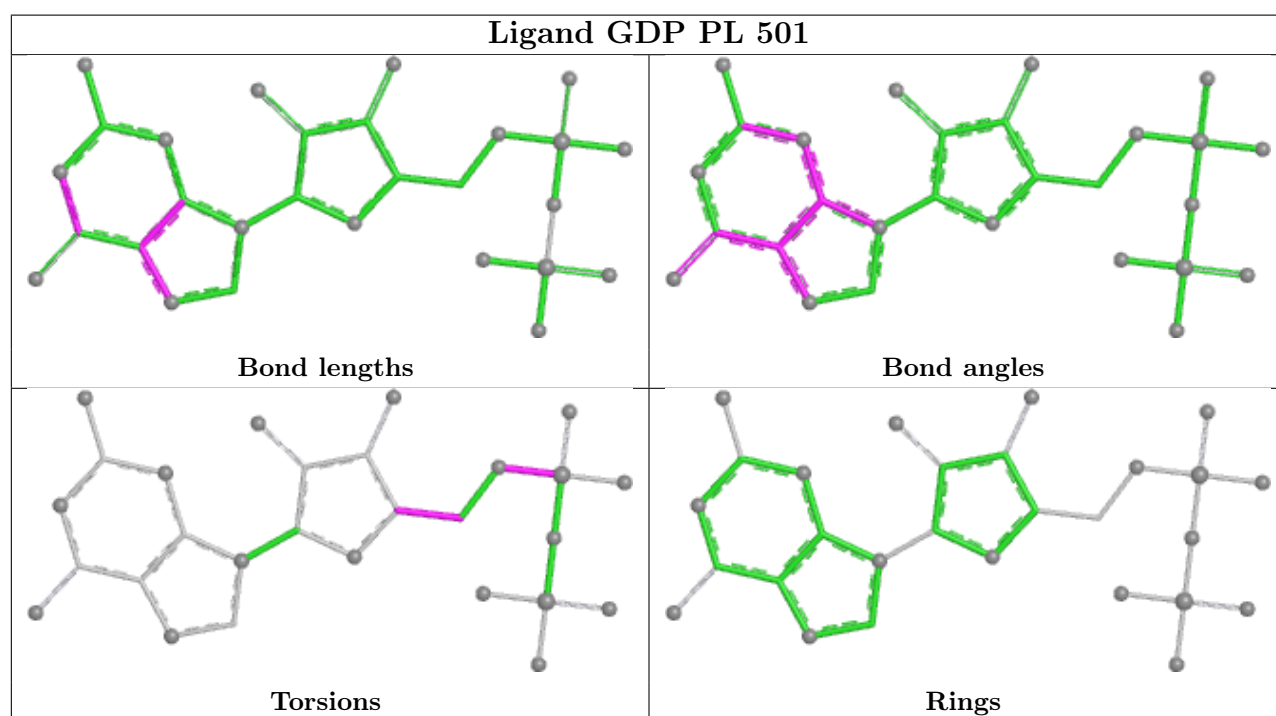
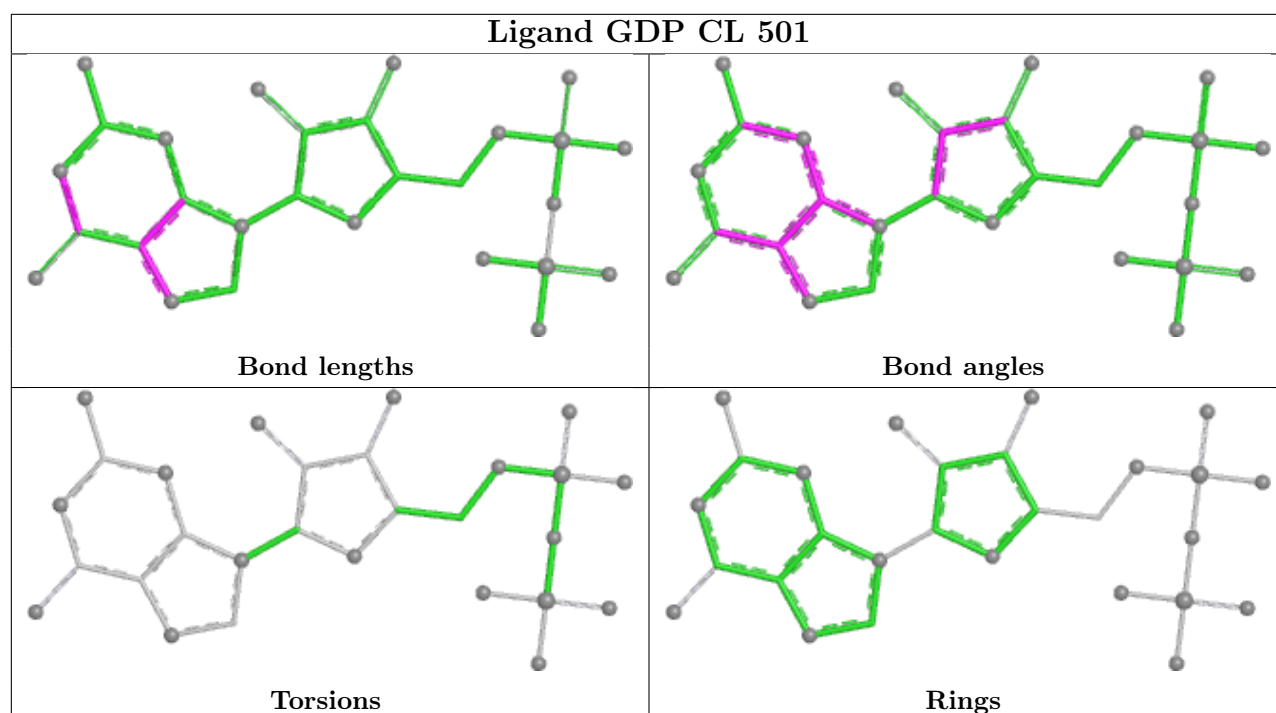


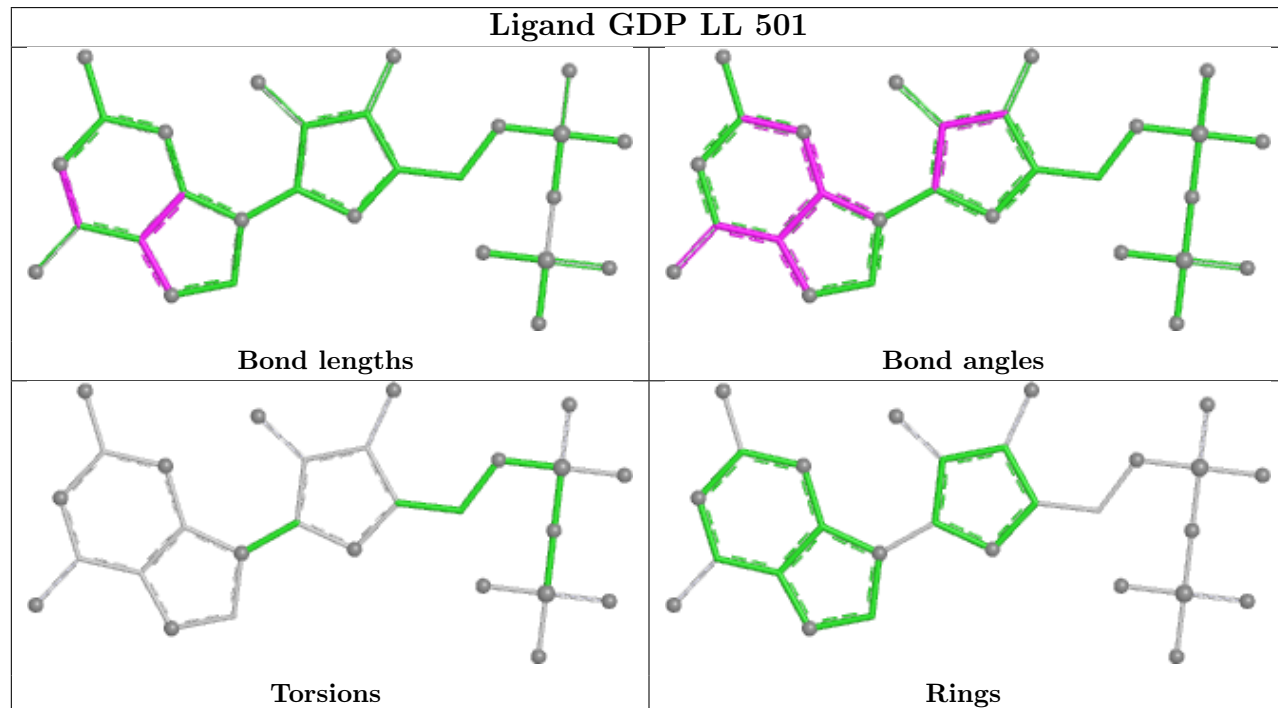
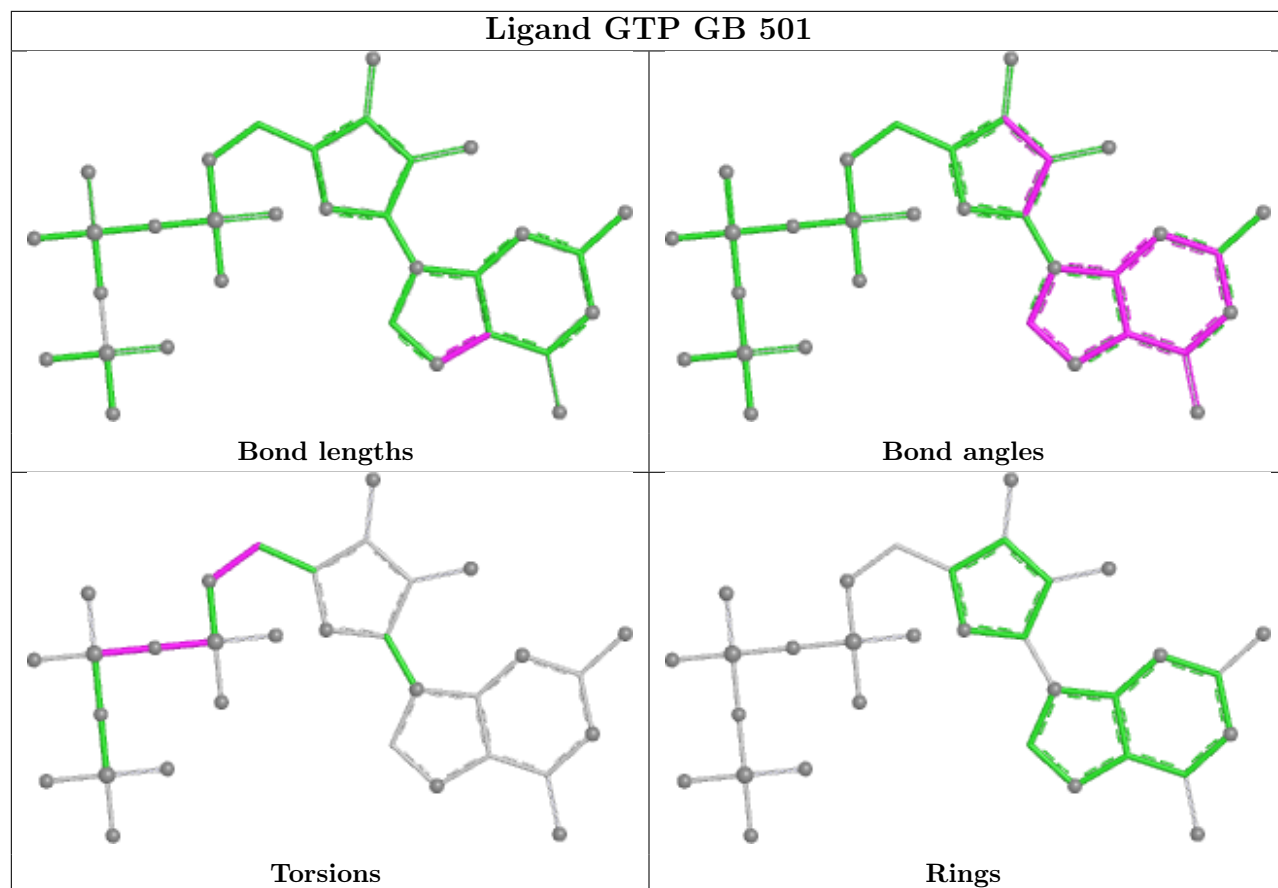
Ligand GTP NM 501



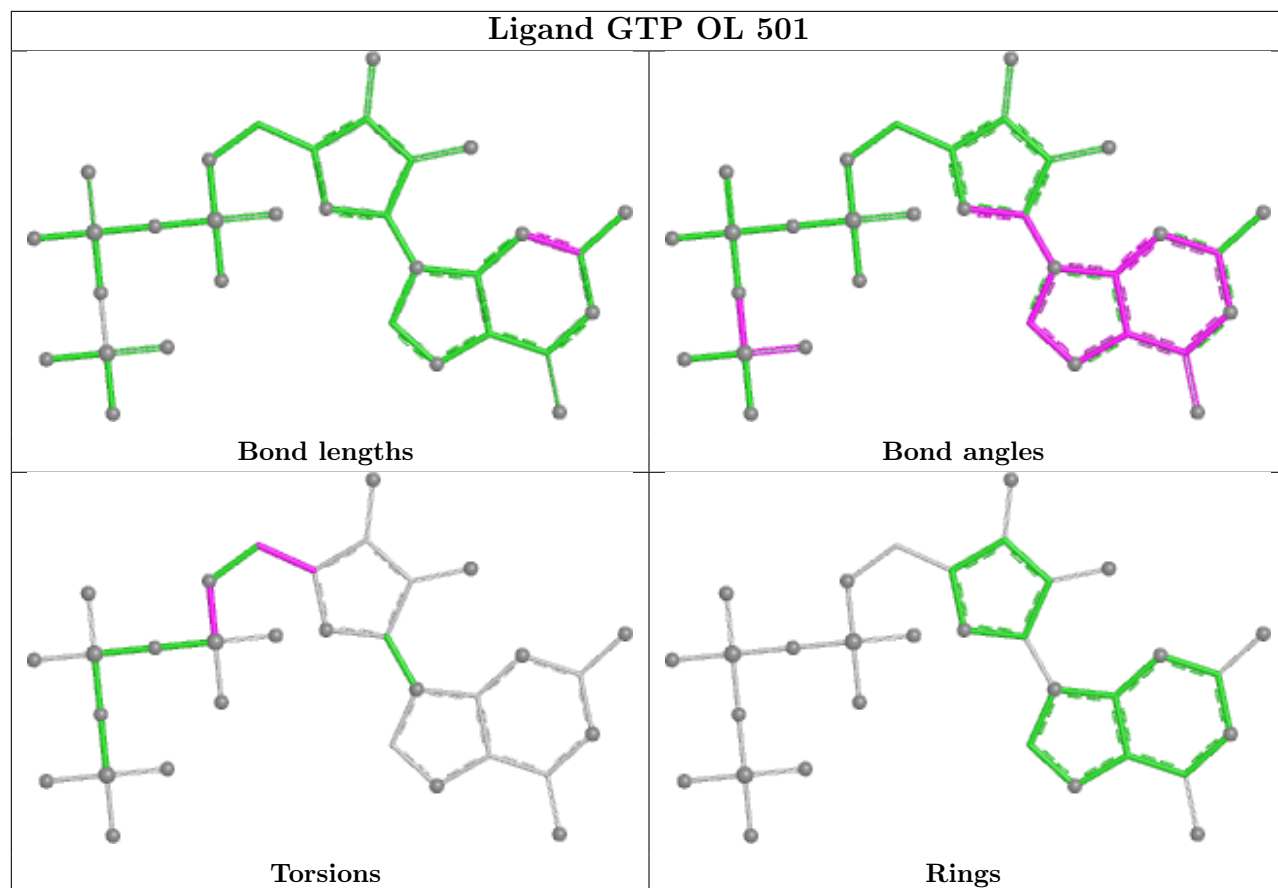




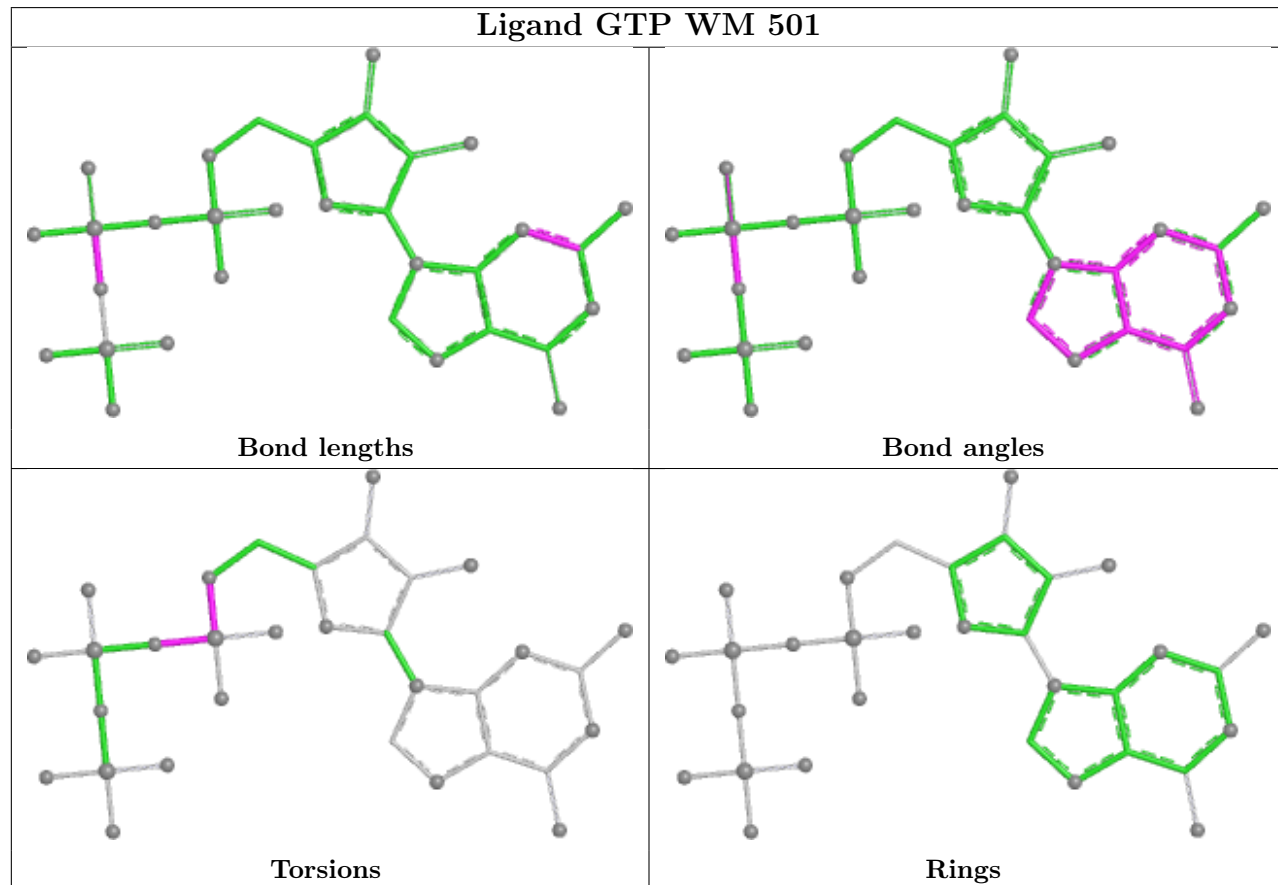


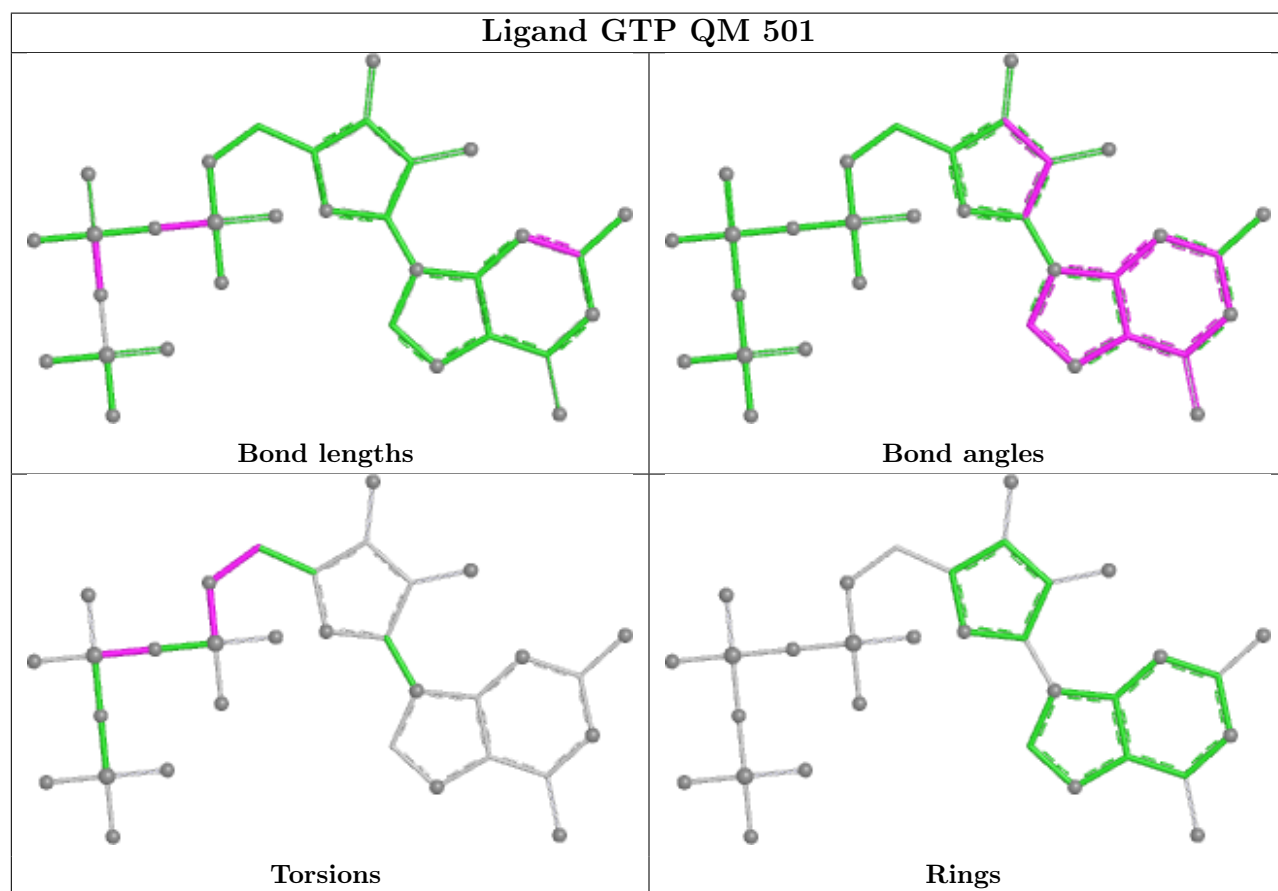
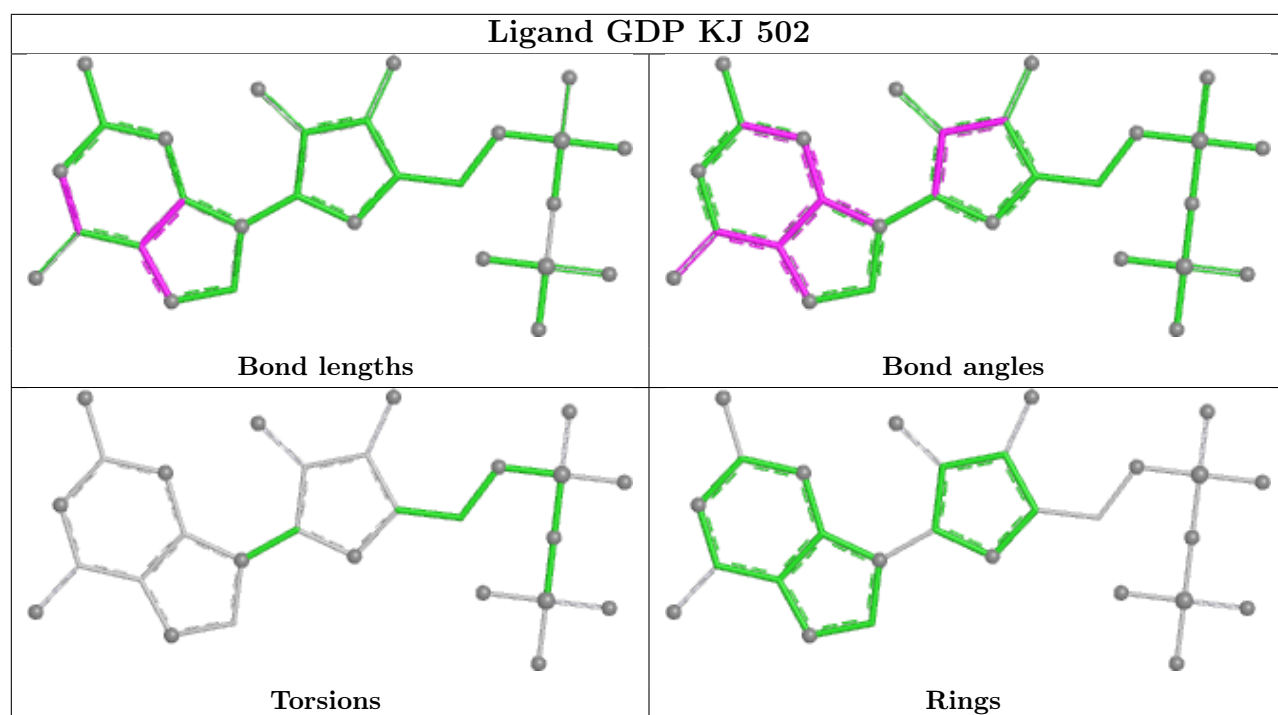


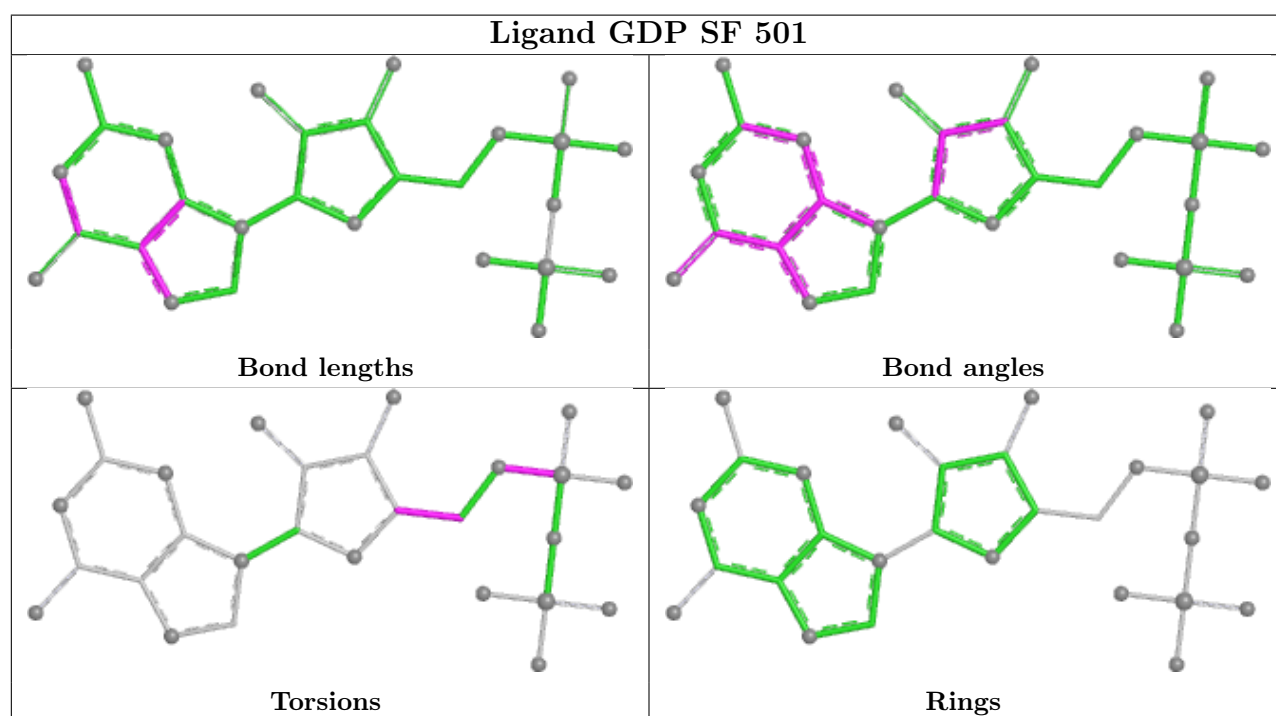
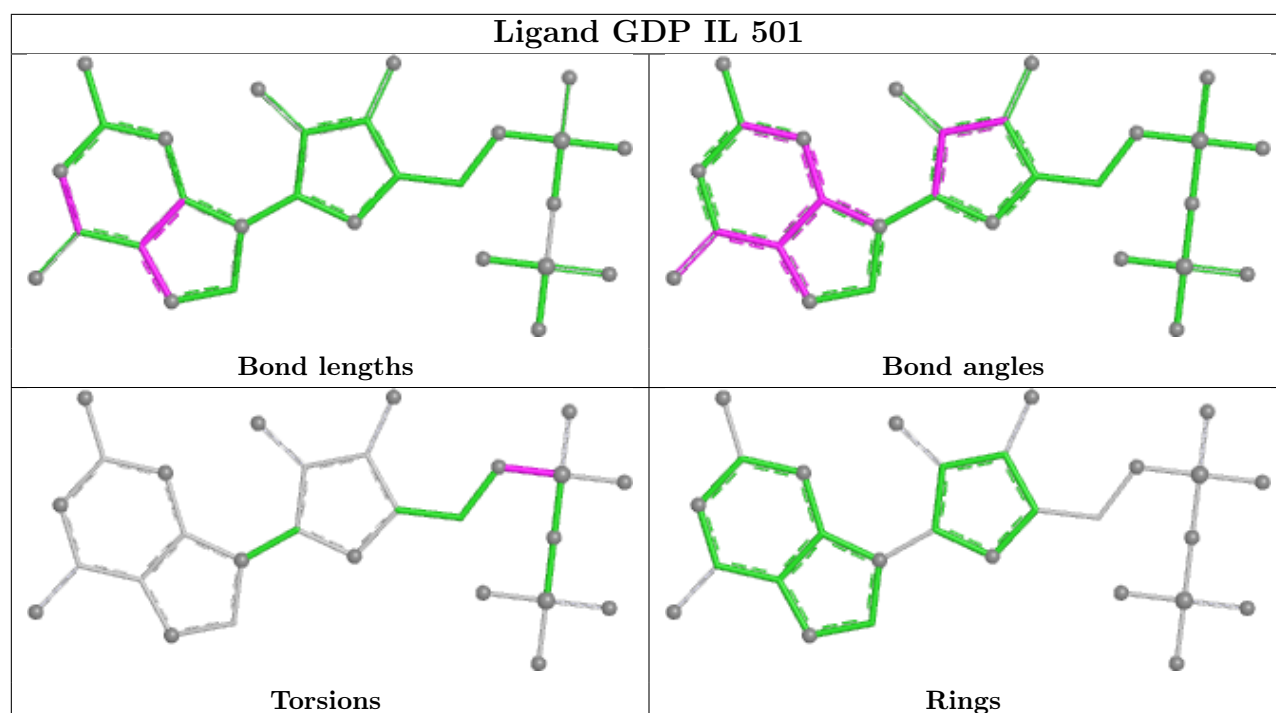
Ligand GTP OL 501



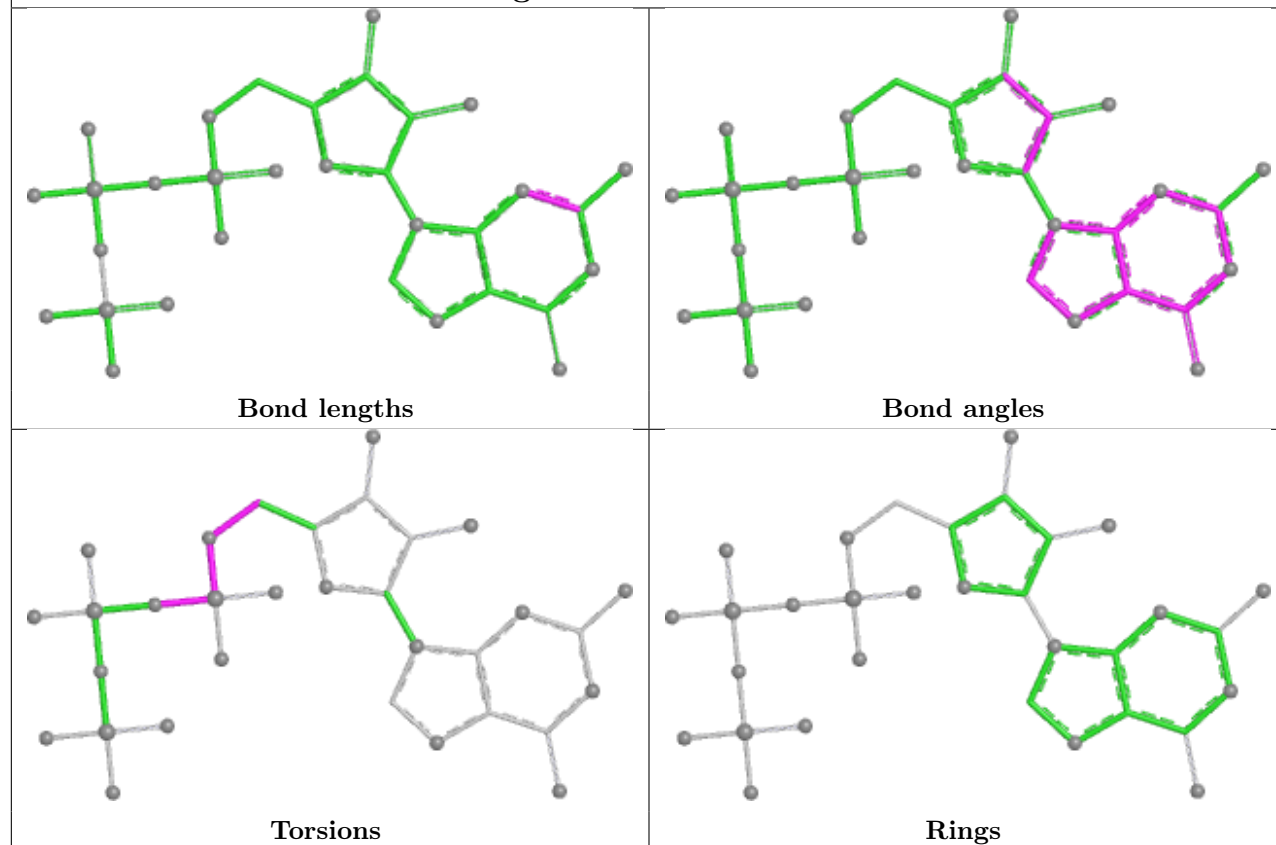
Ligand GTP WM 501



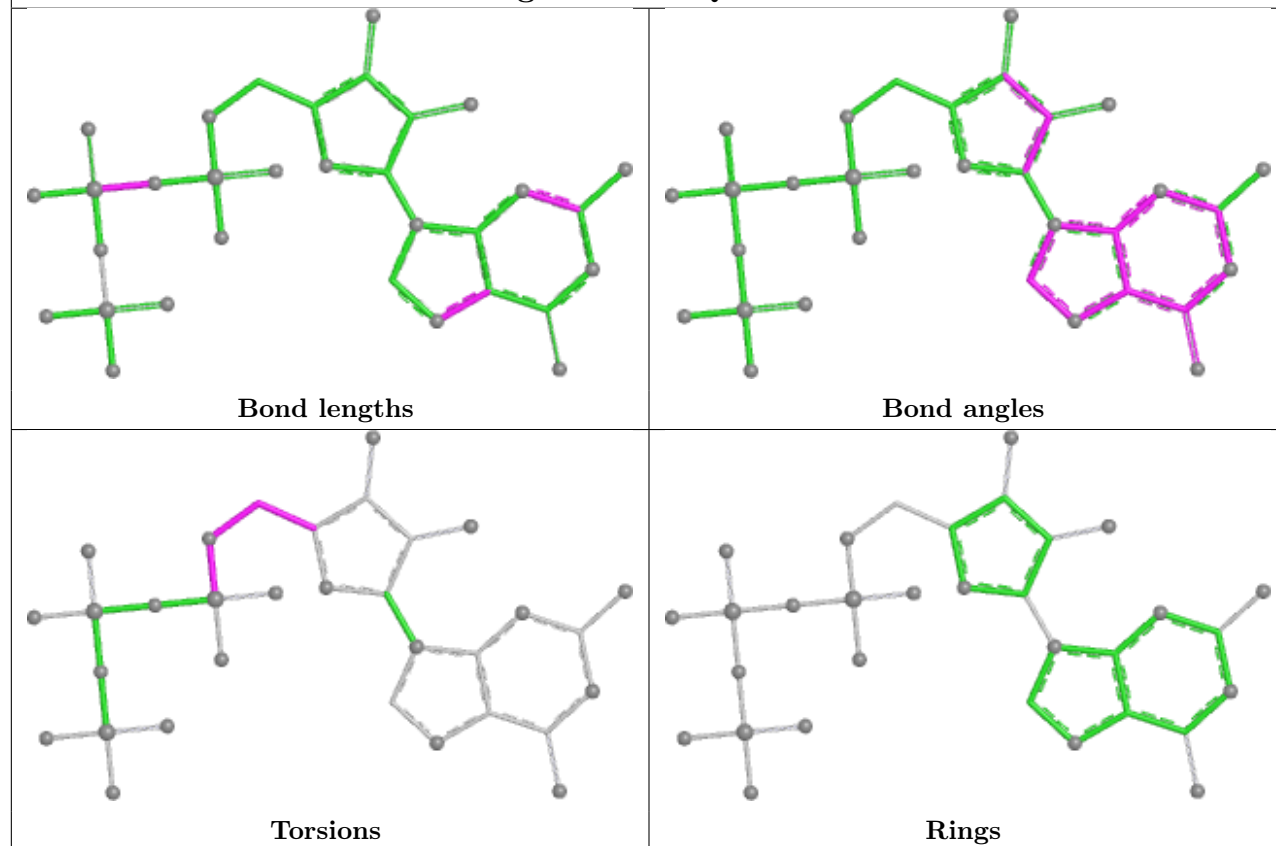


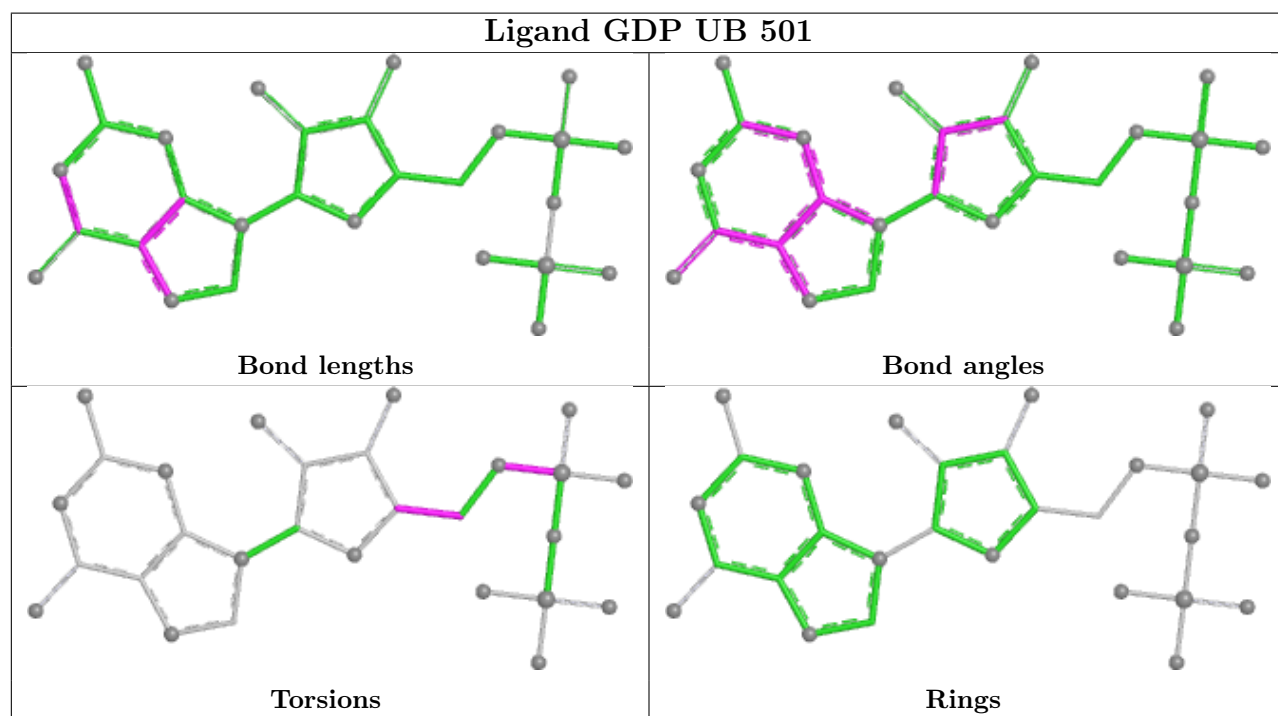
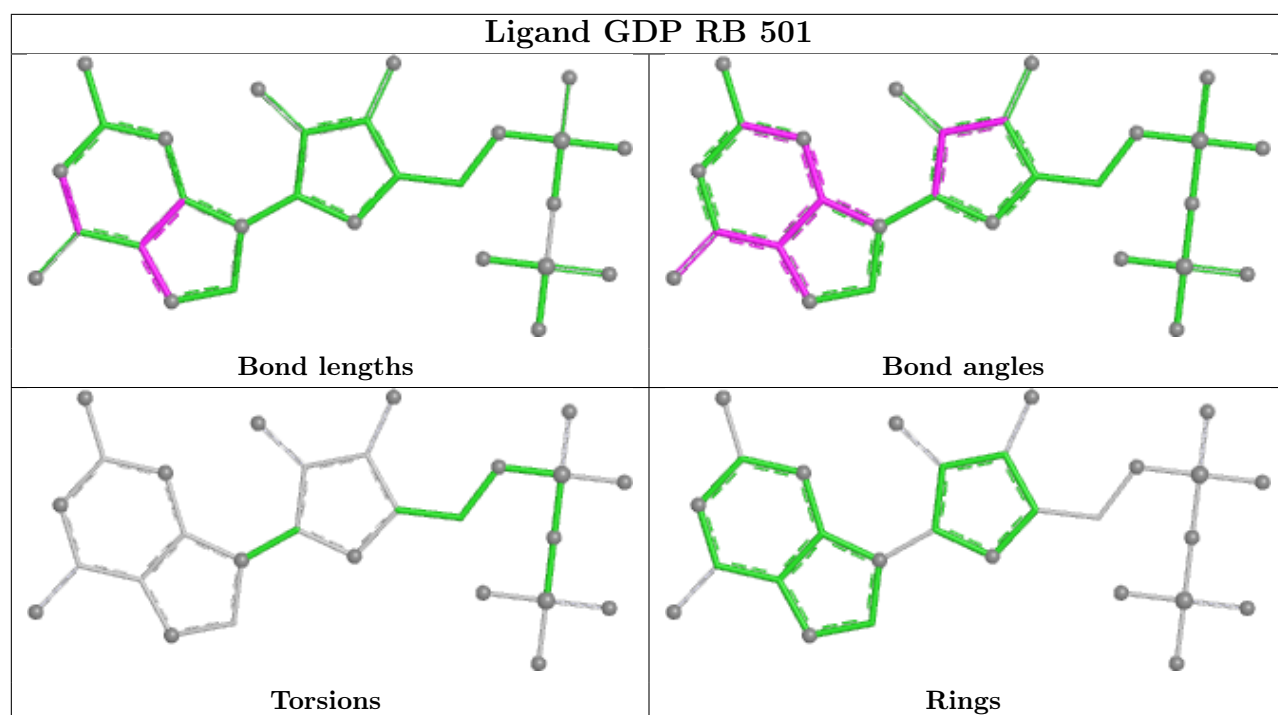


Ligand GTP MA 501

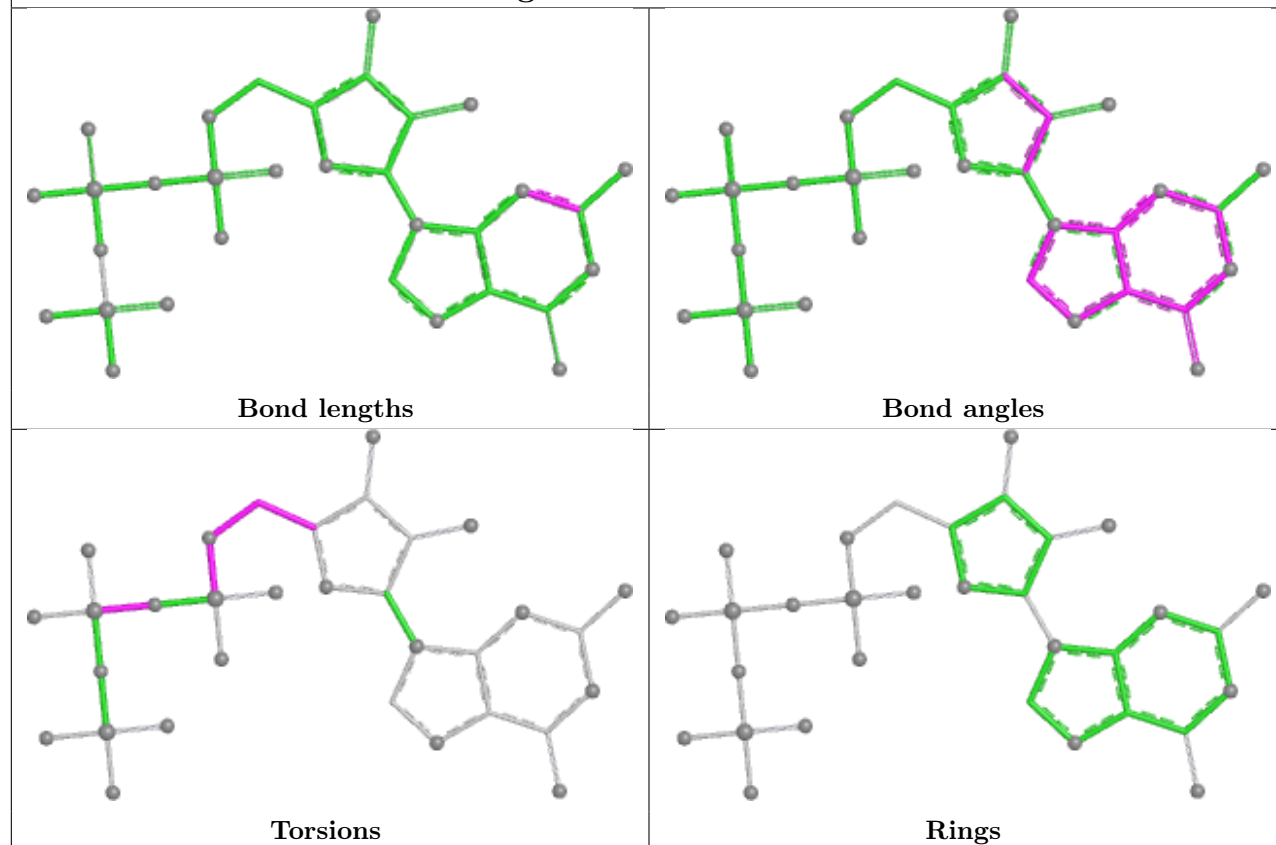


Ligand GTP QC 501

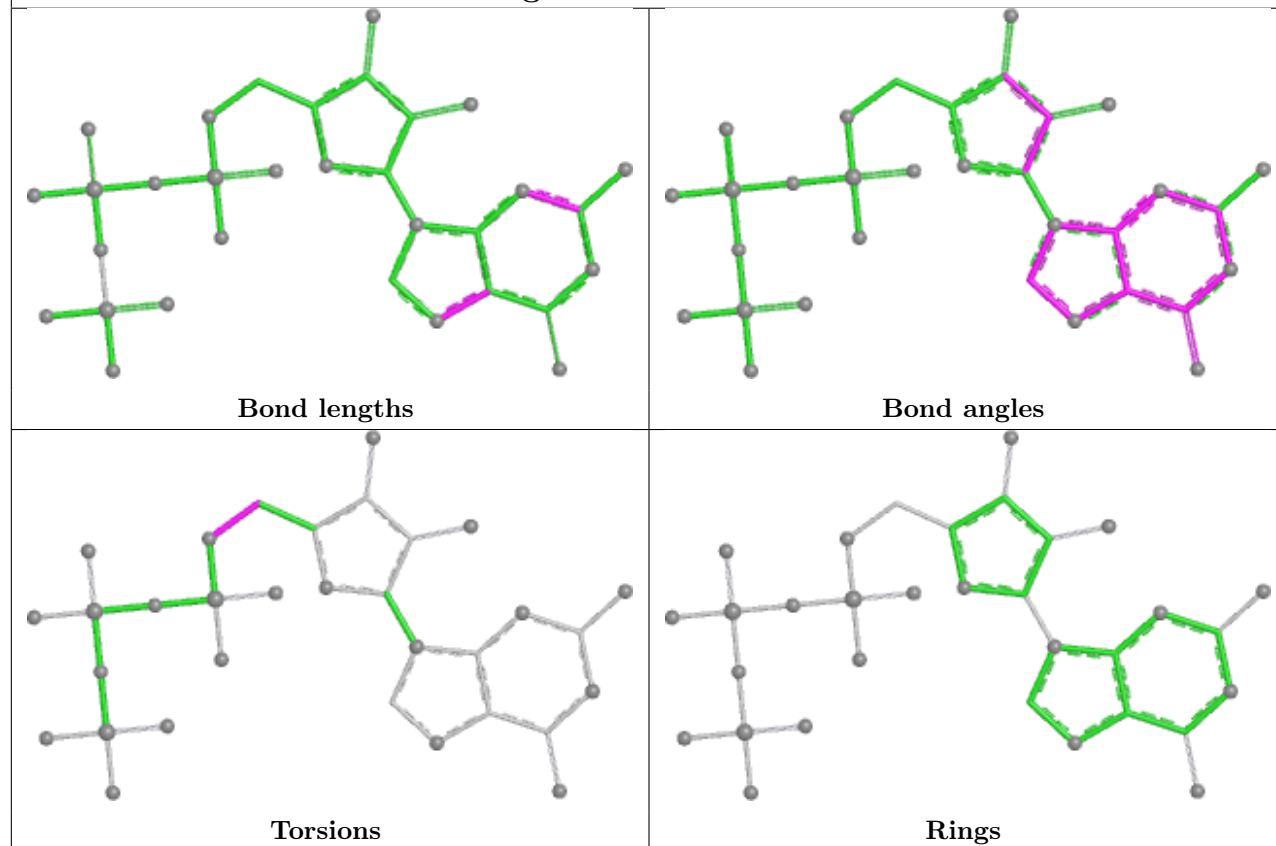


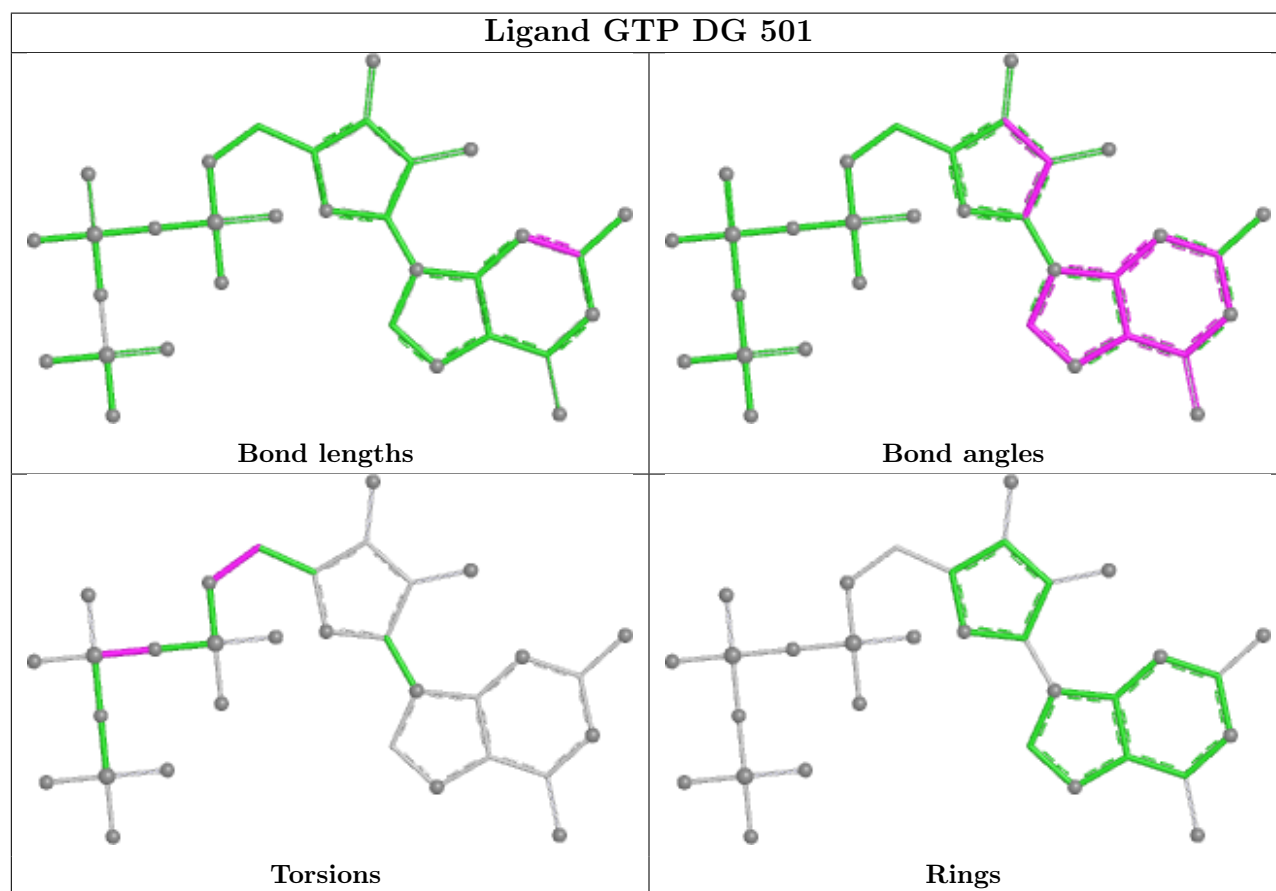
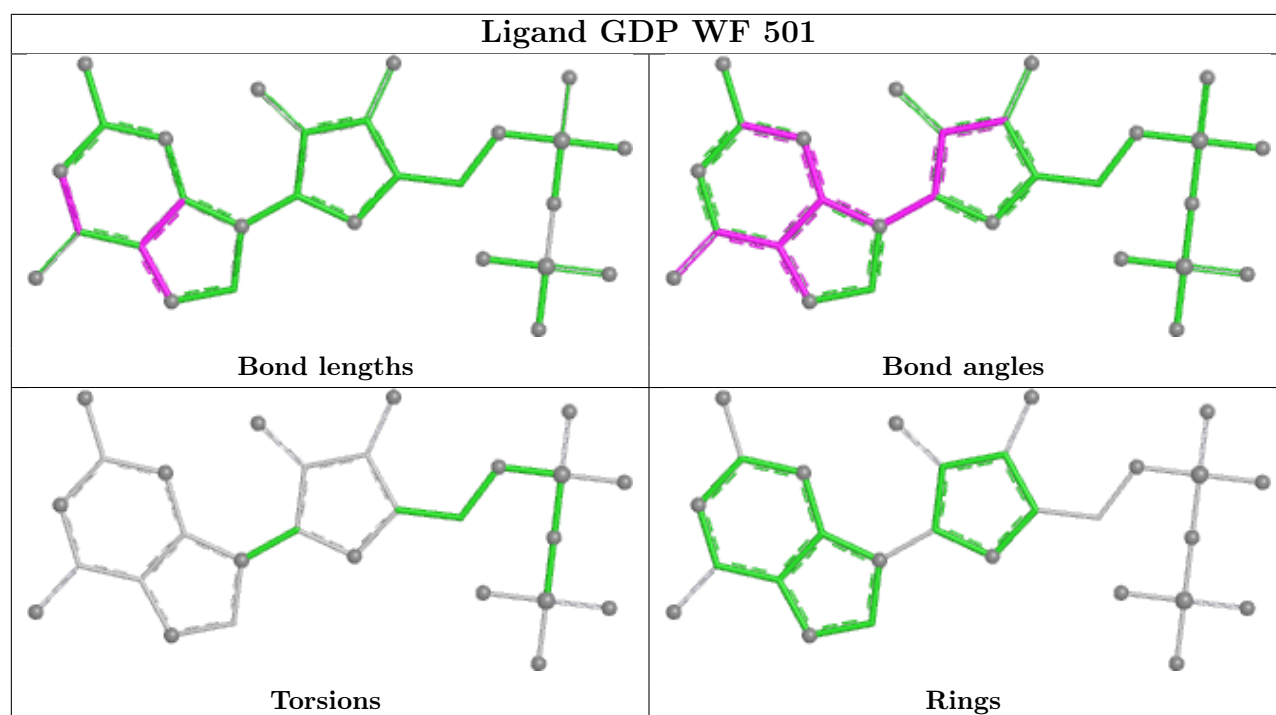


Ligand GTP PG 501

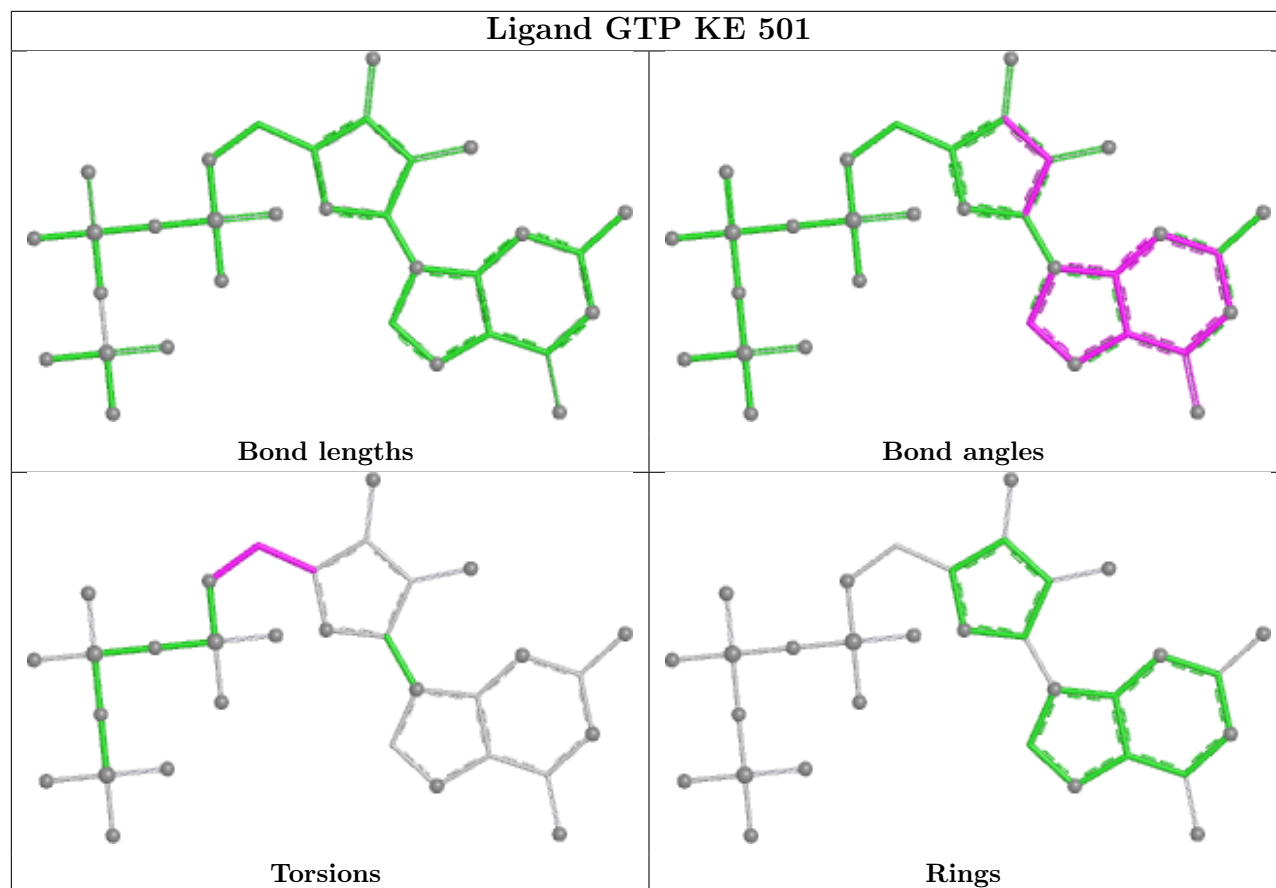


Ligand GTP JE 501

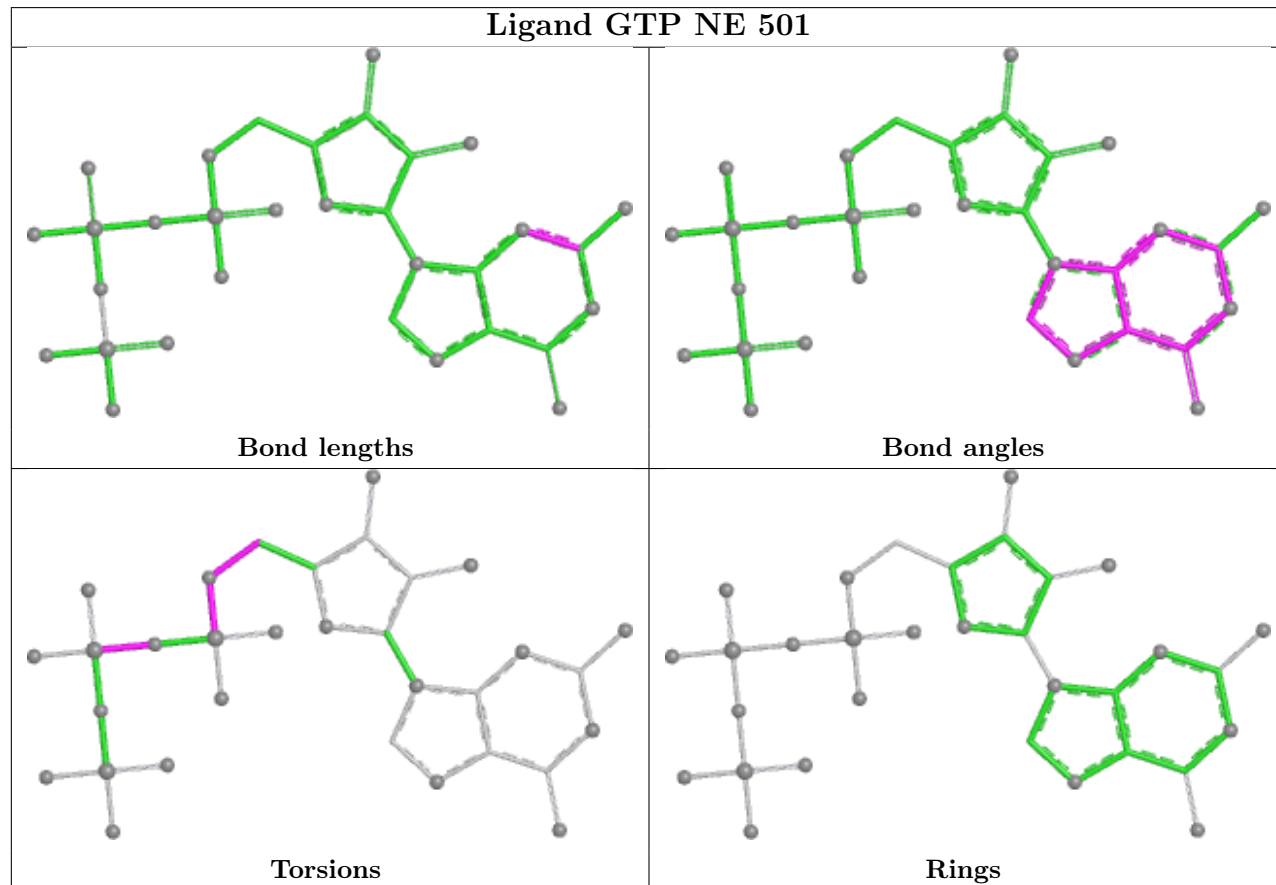


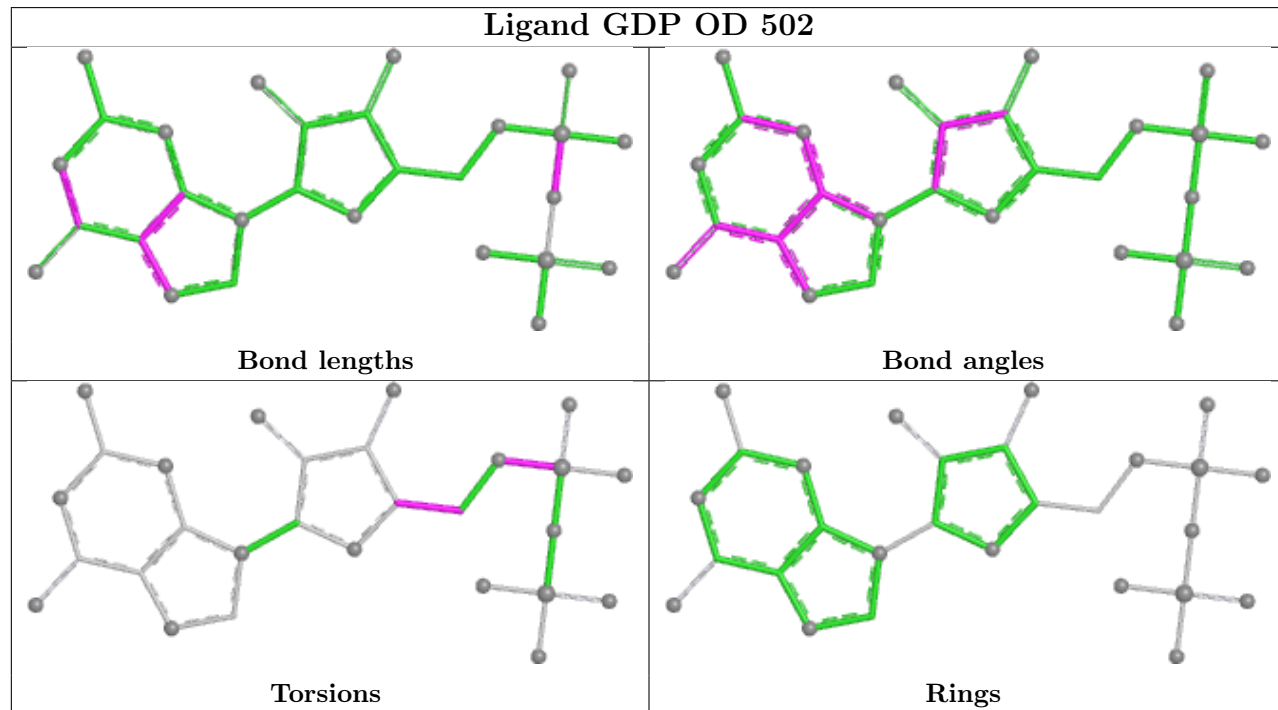
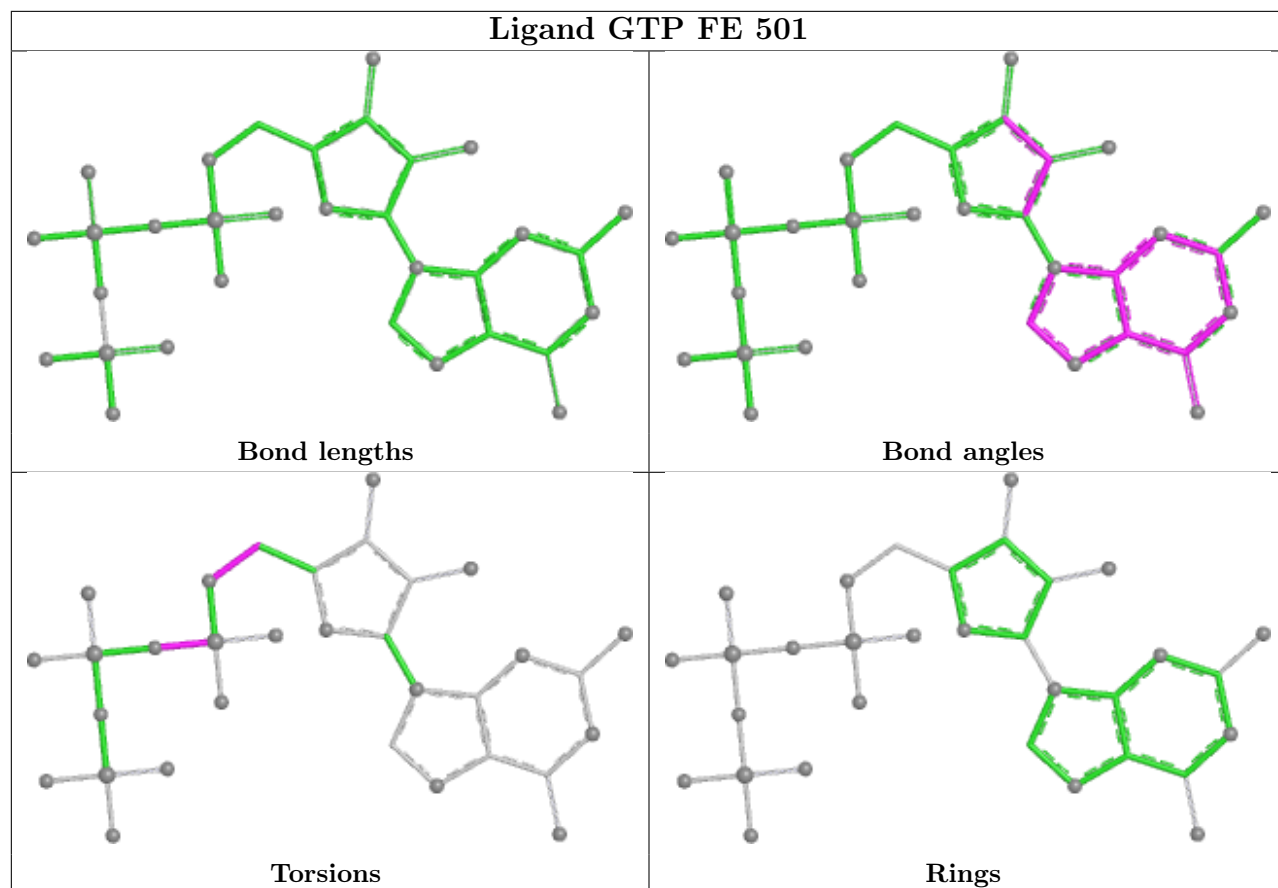


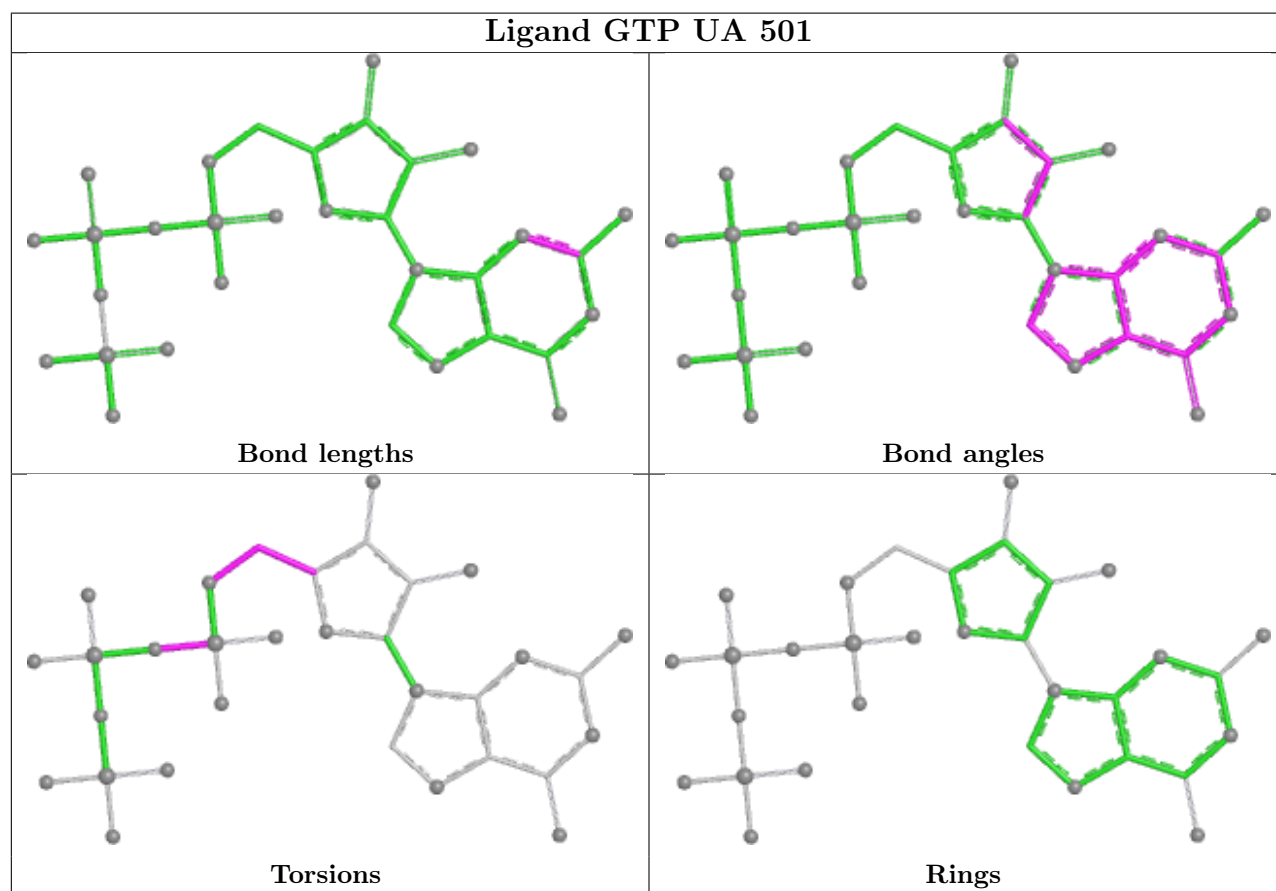
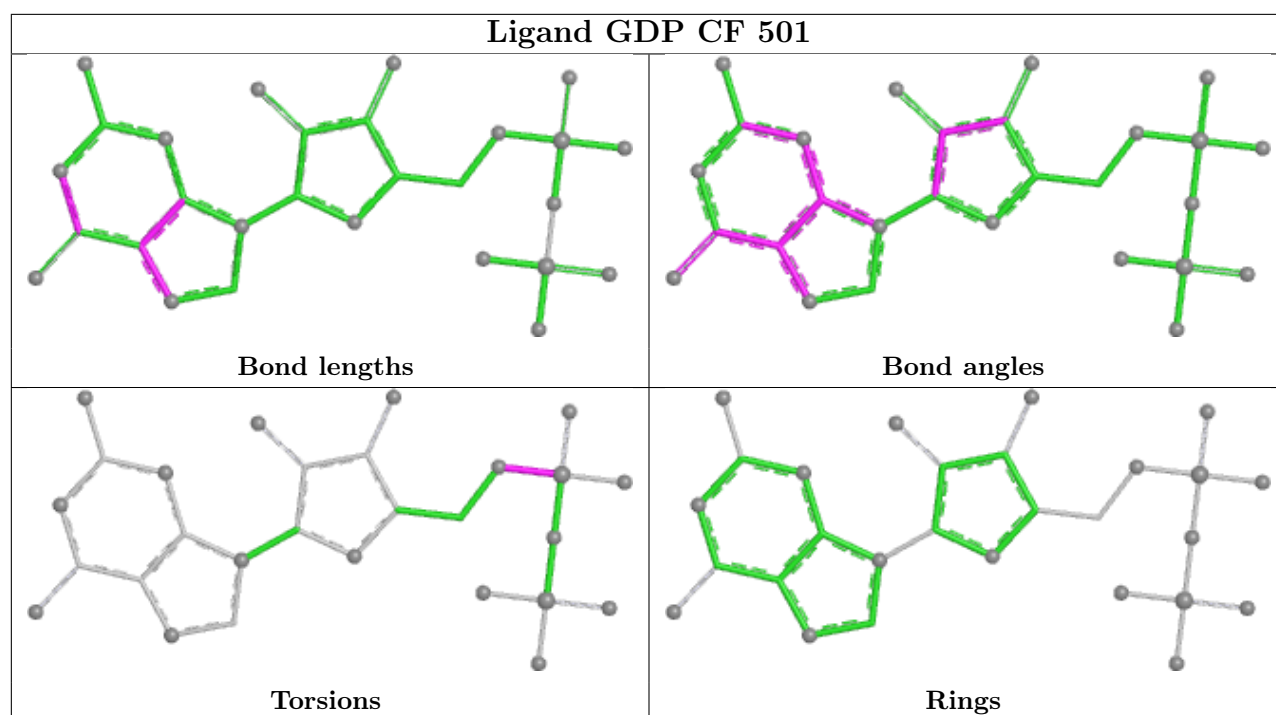
Ligand GTP KE 501

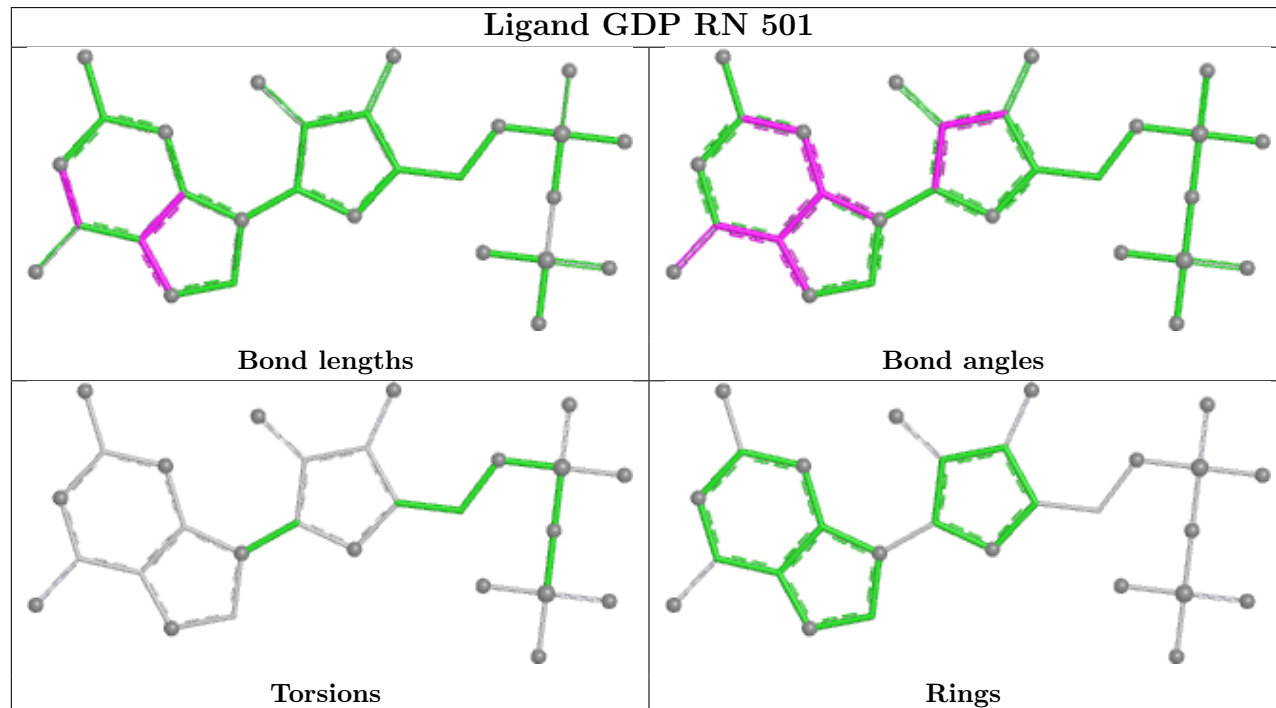
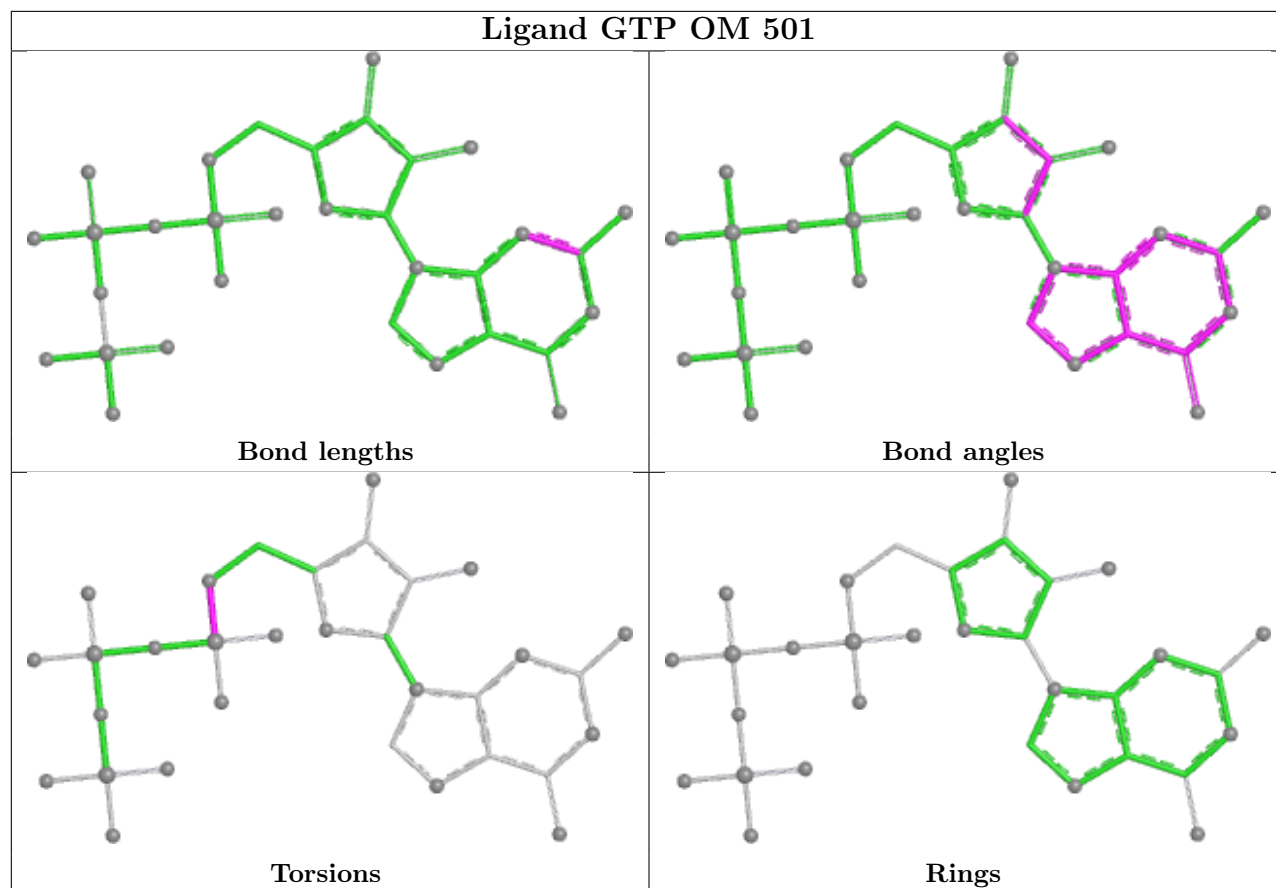


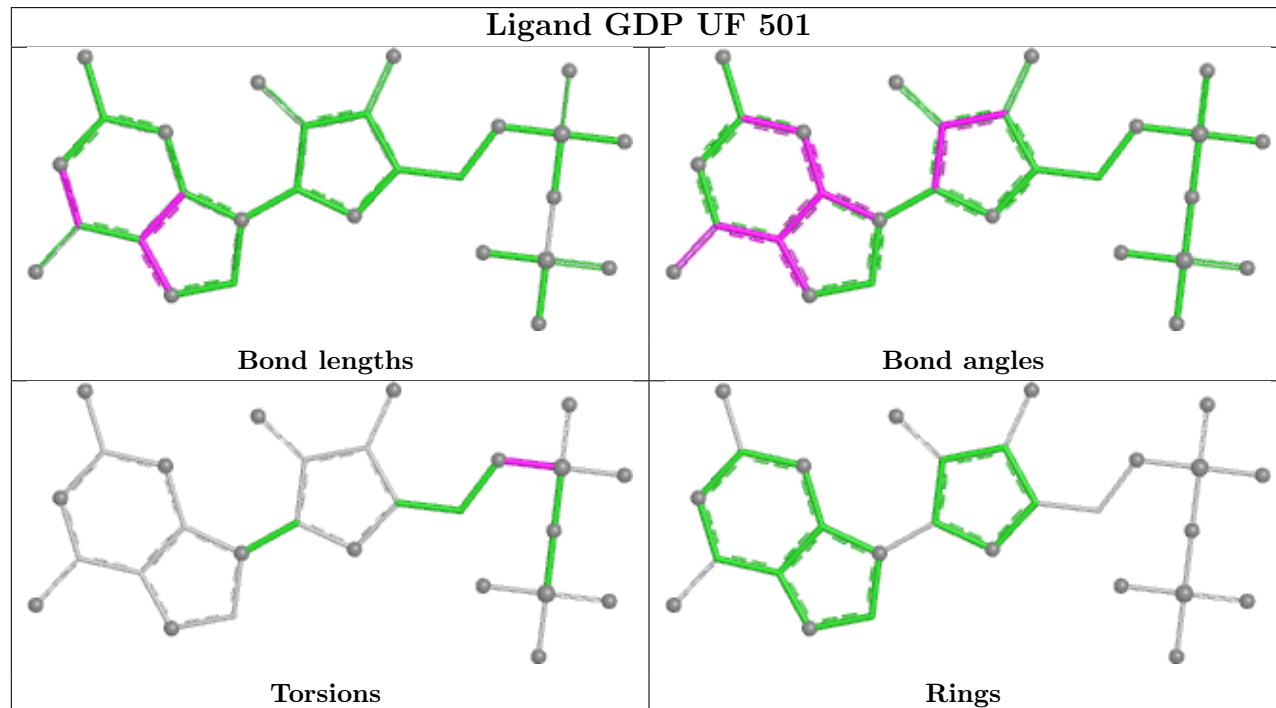
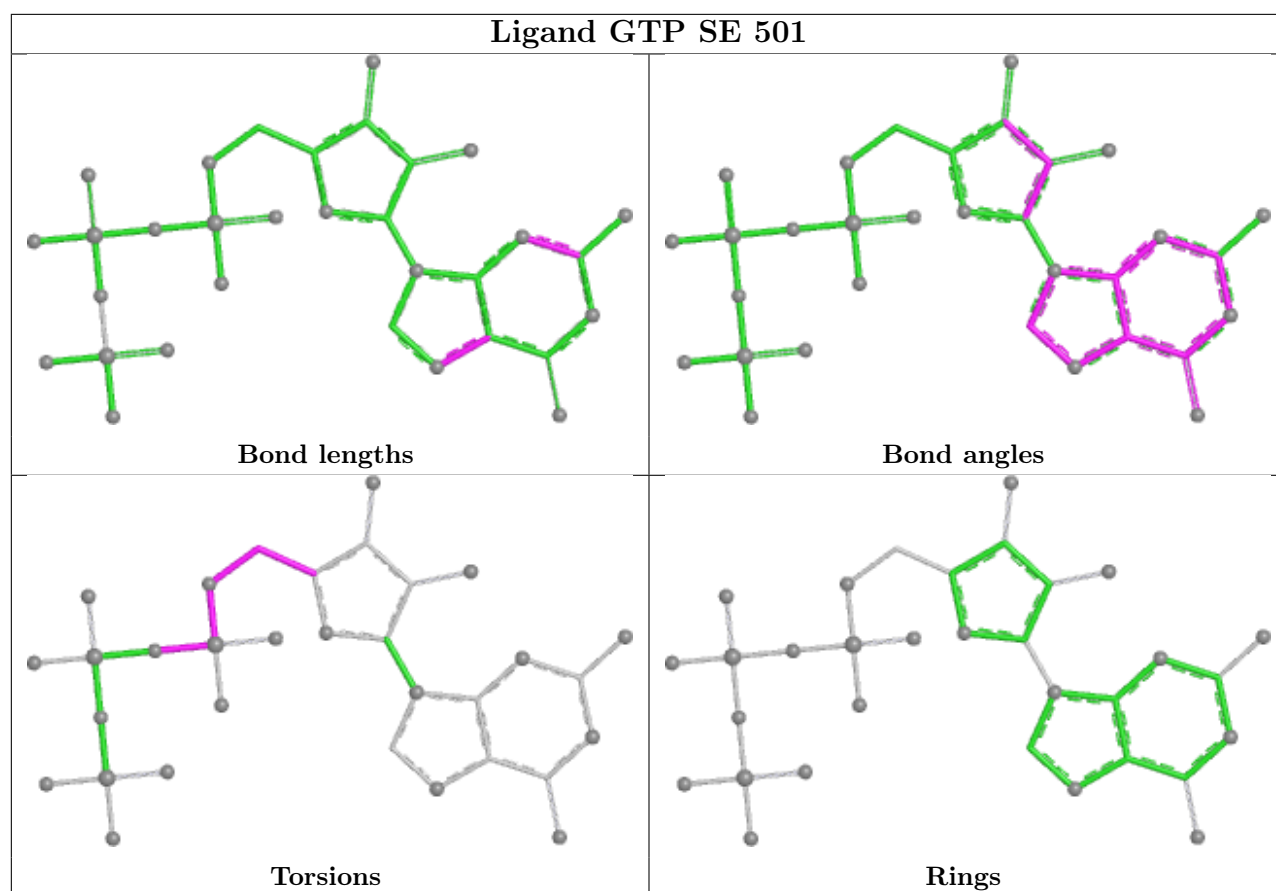
Ligand GTP NE 501



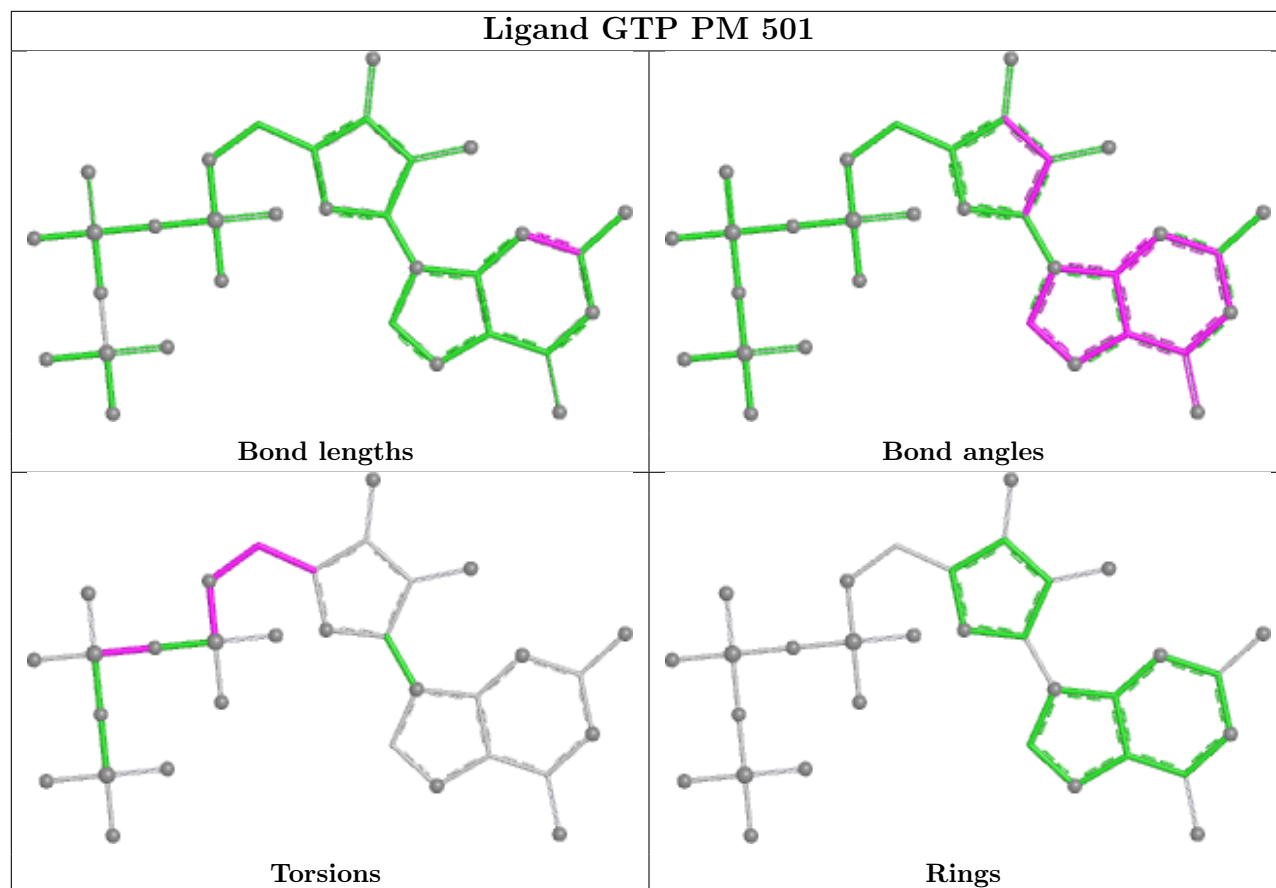




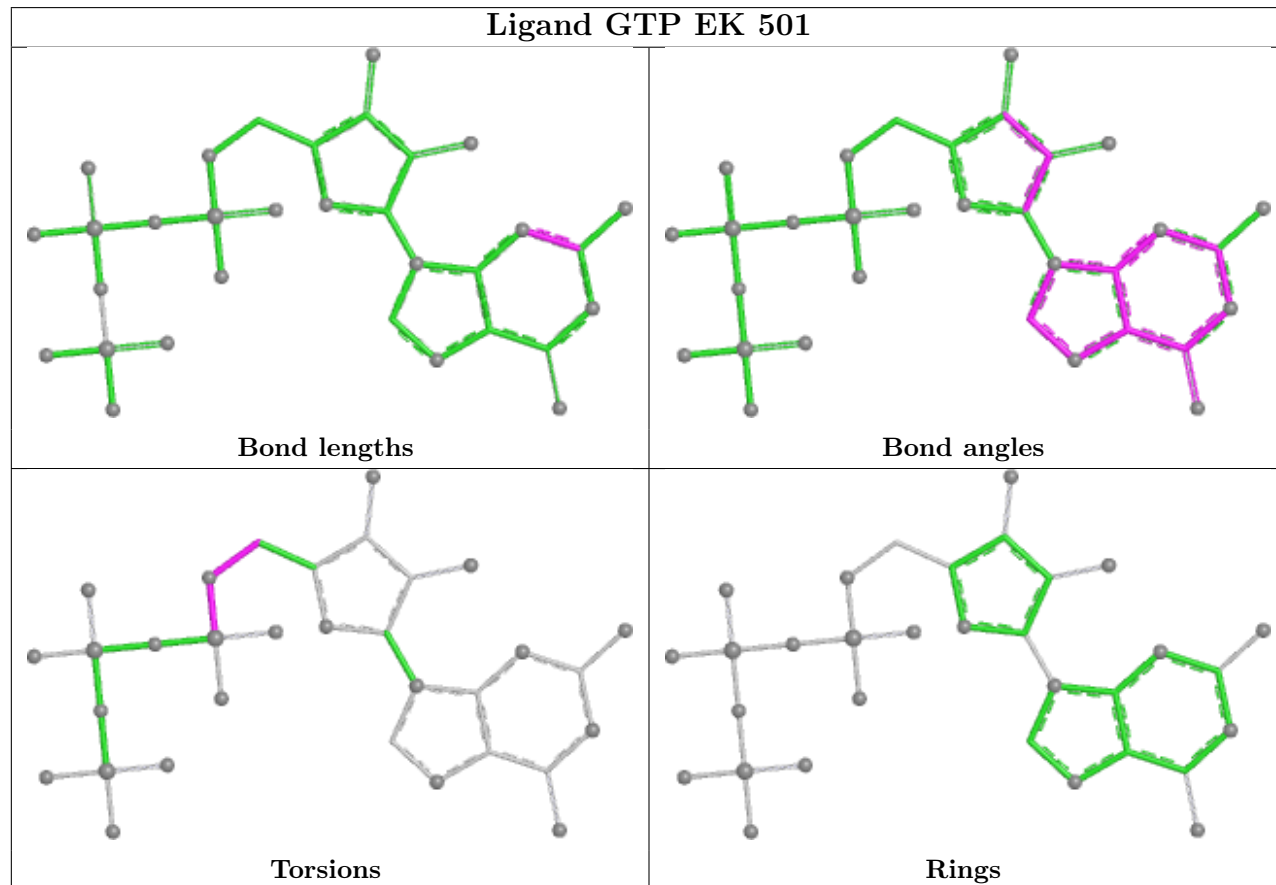




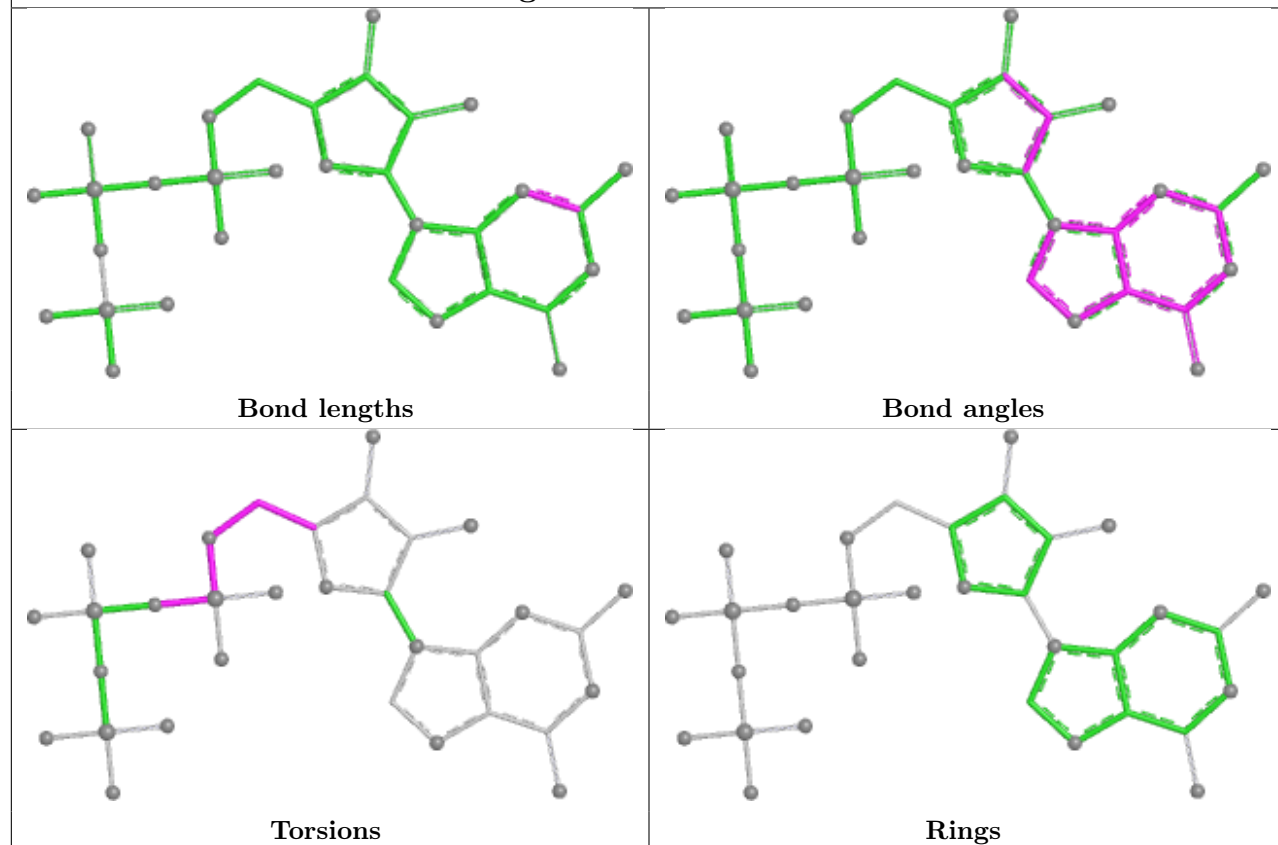
Ligand GTP PM 501



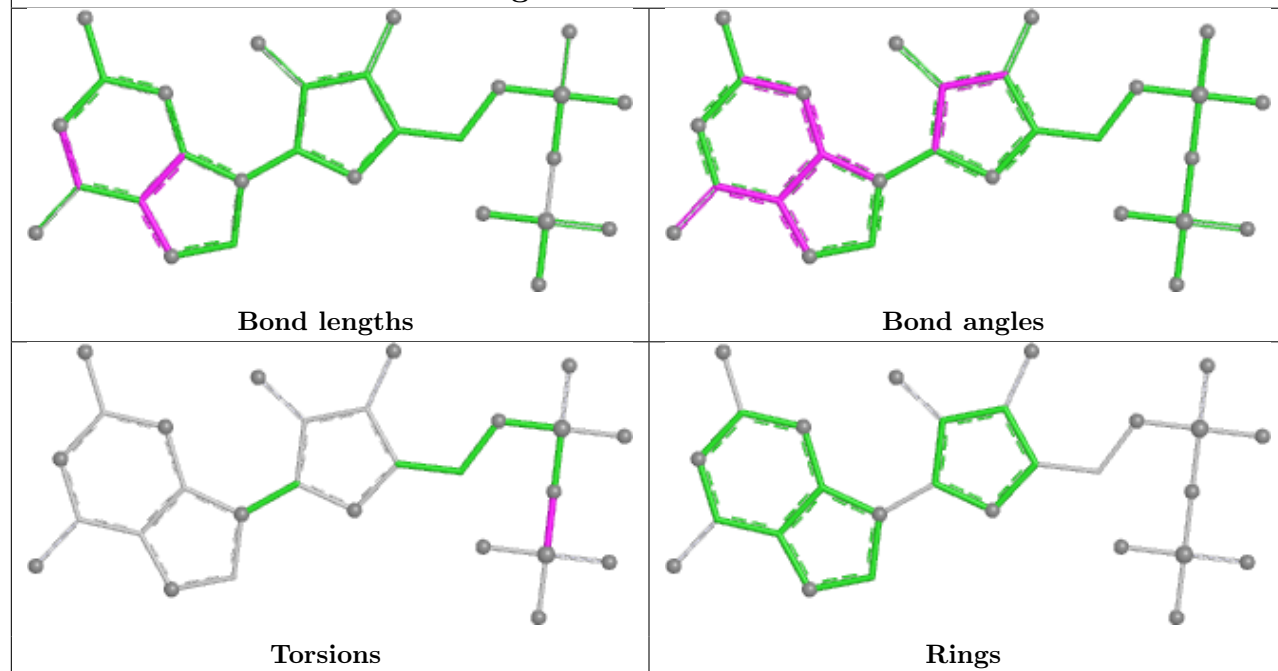
Ligand GTP EK 501



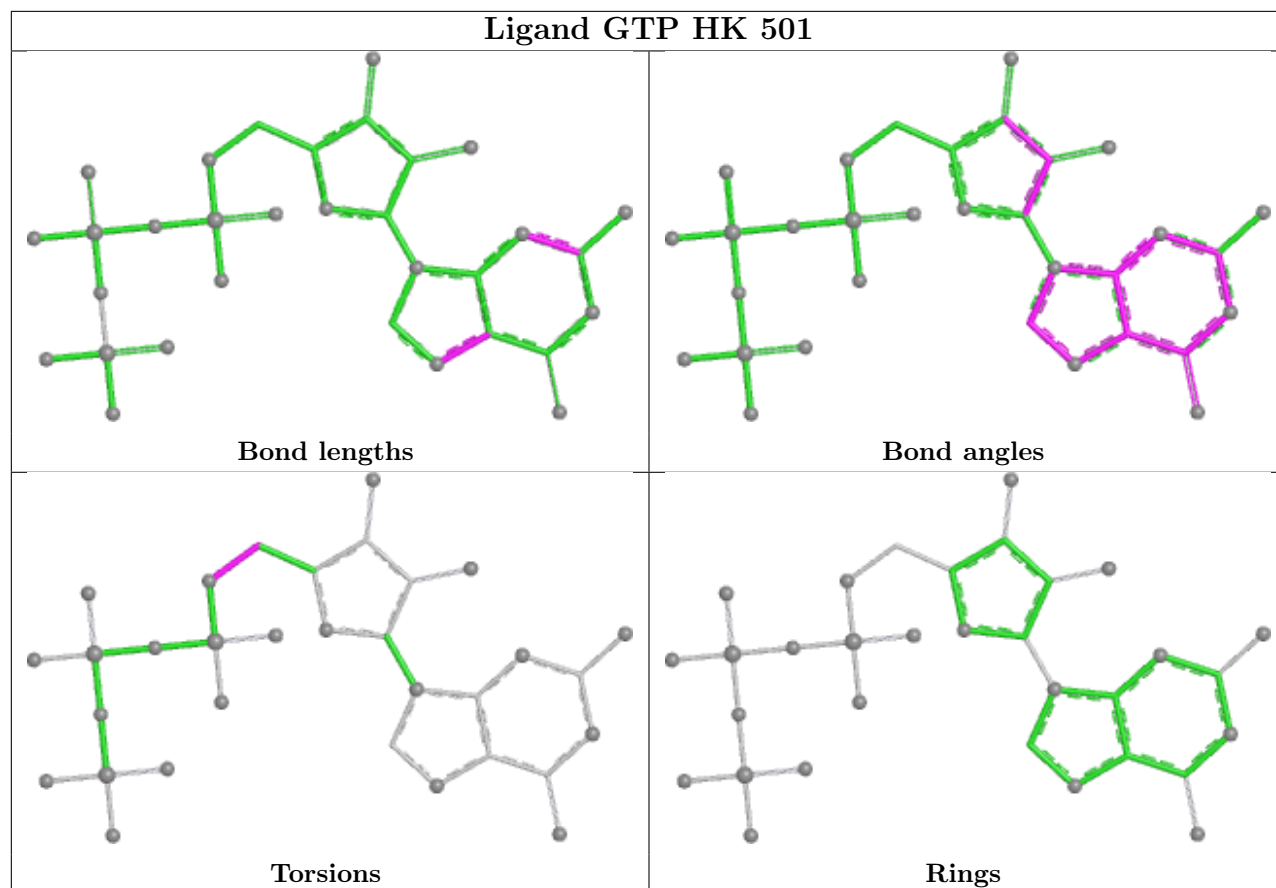
Ligand GTP TA 501



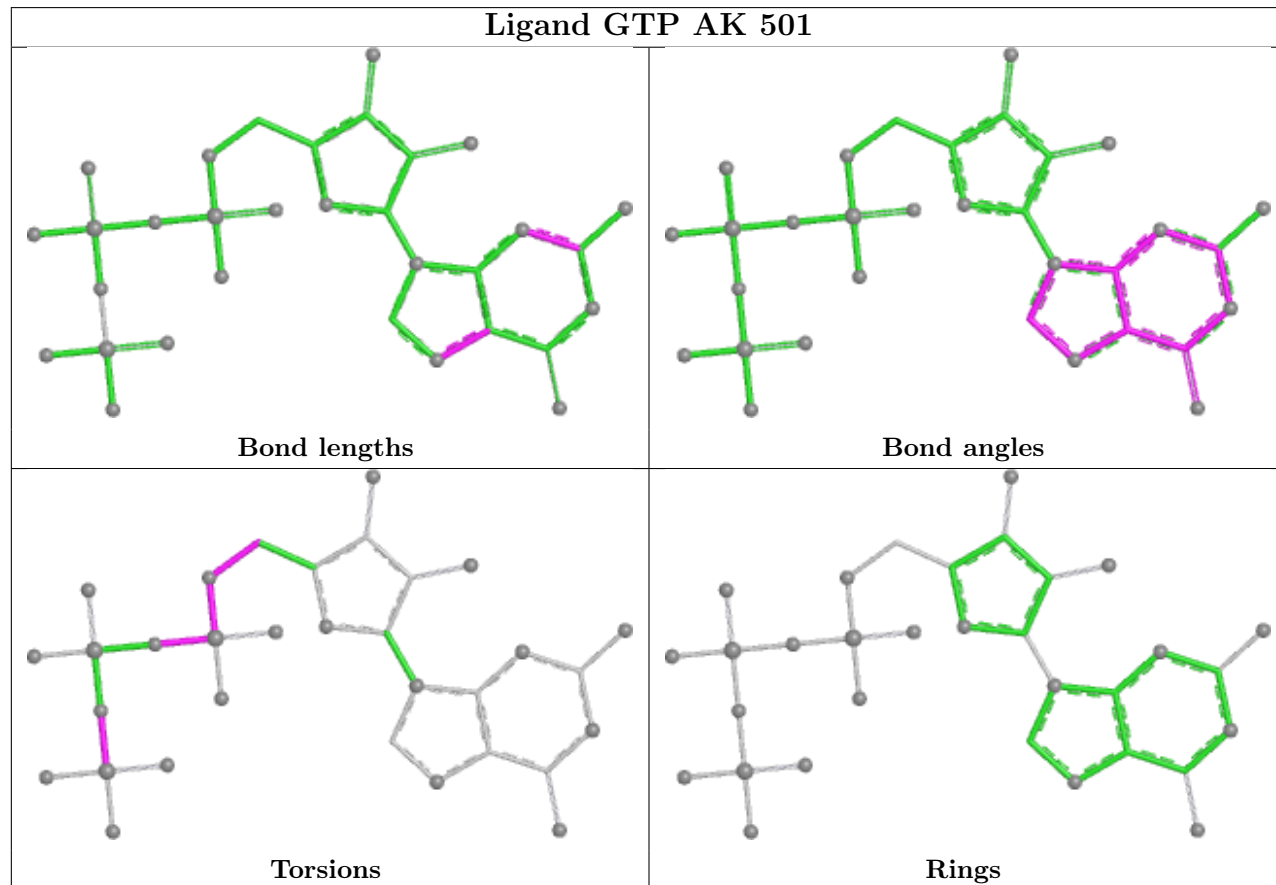
Ligand GDP MN 502

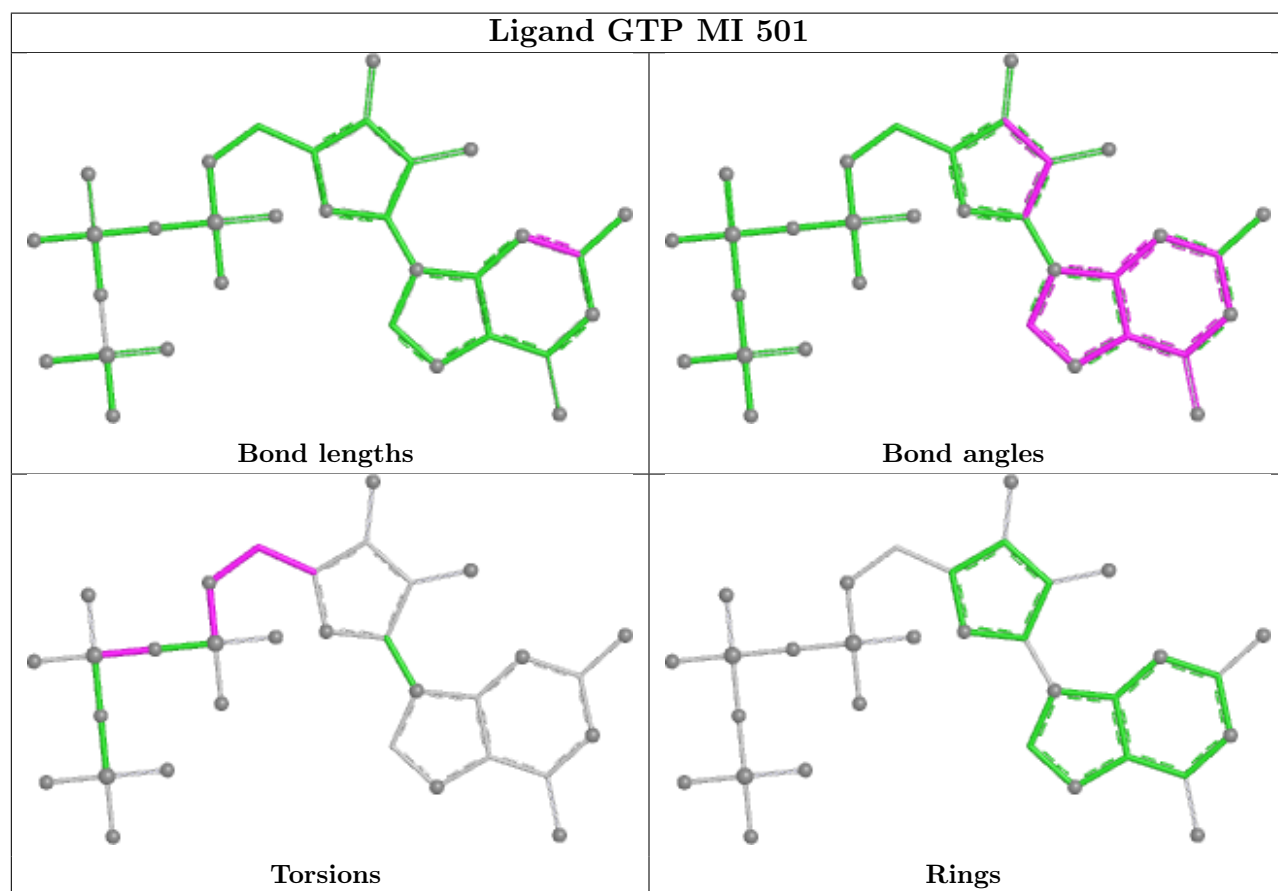
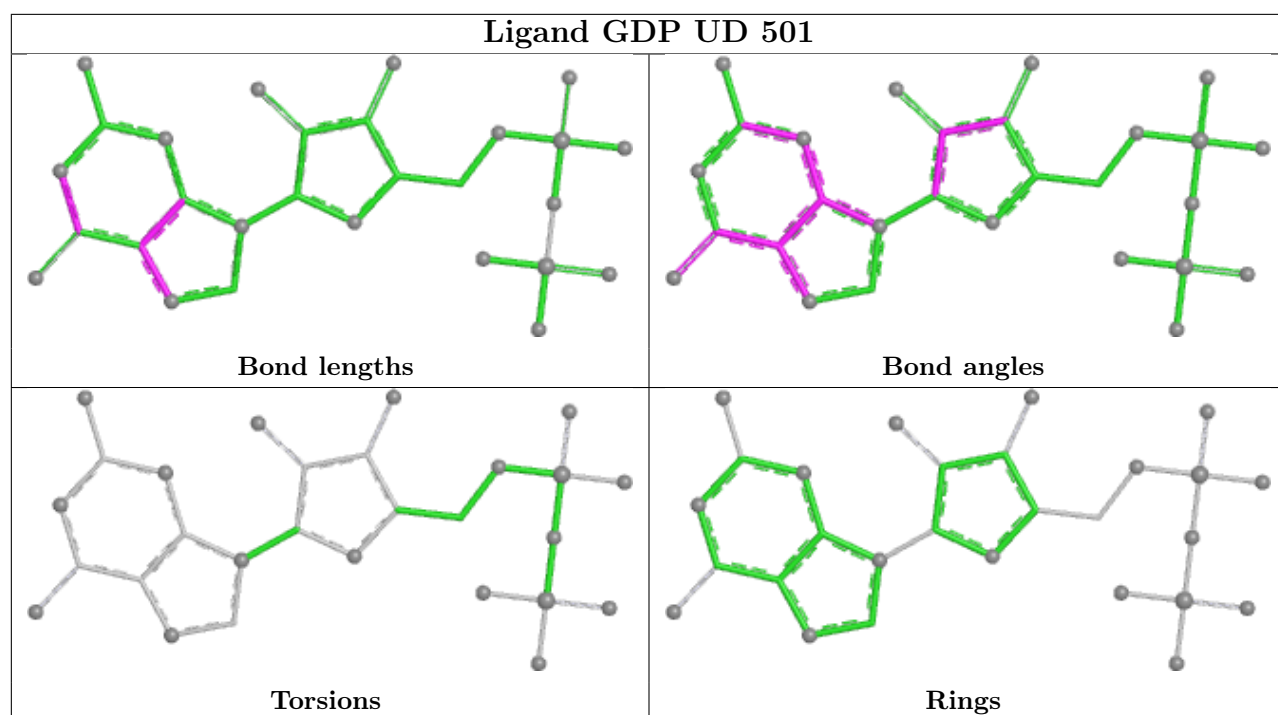


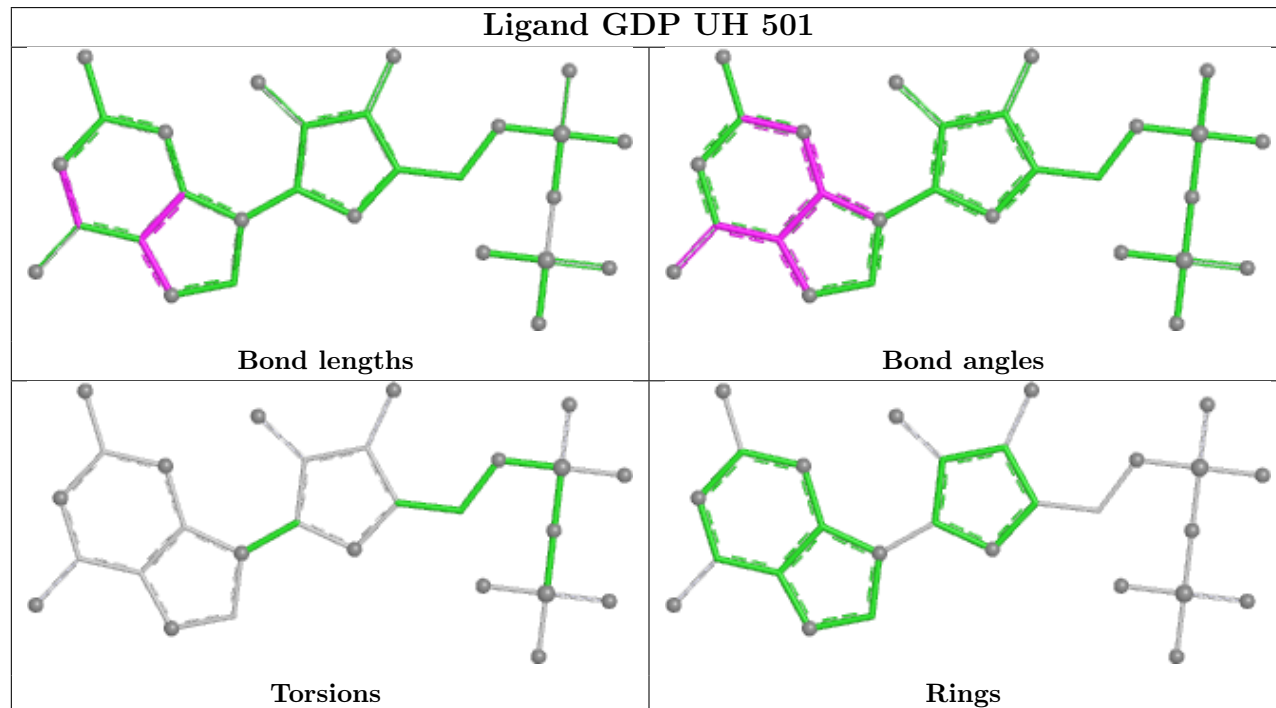
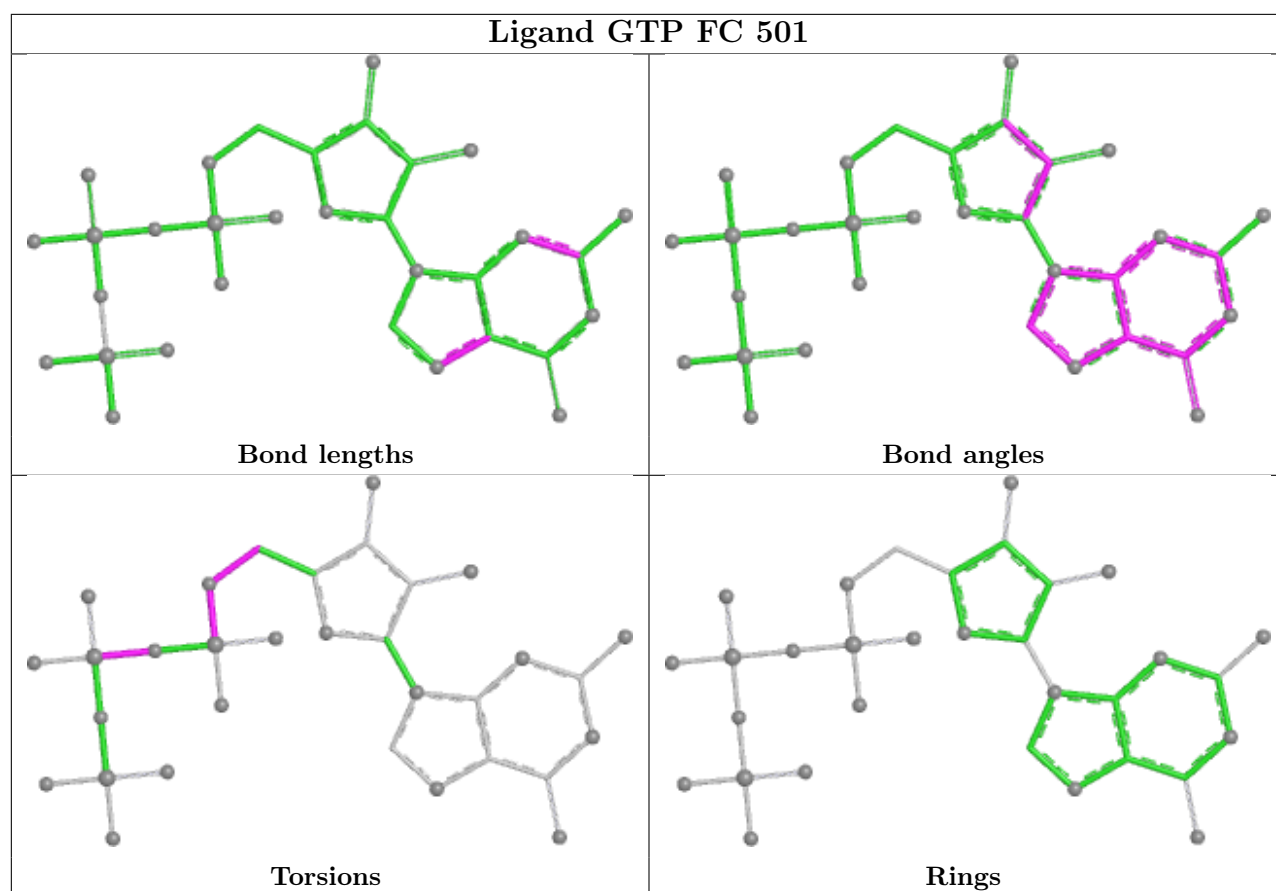
Ligand GTP HK 501



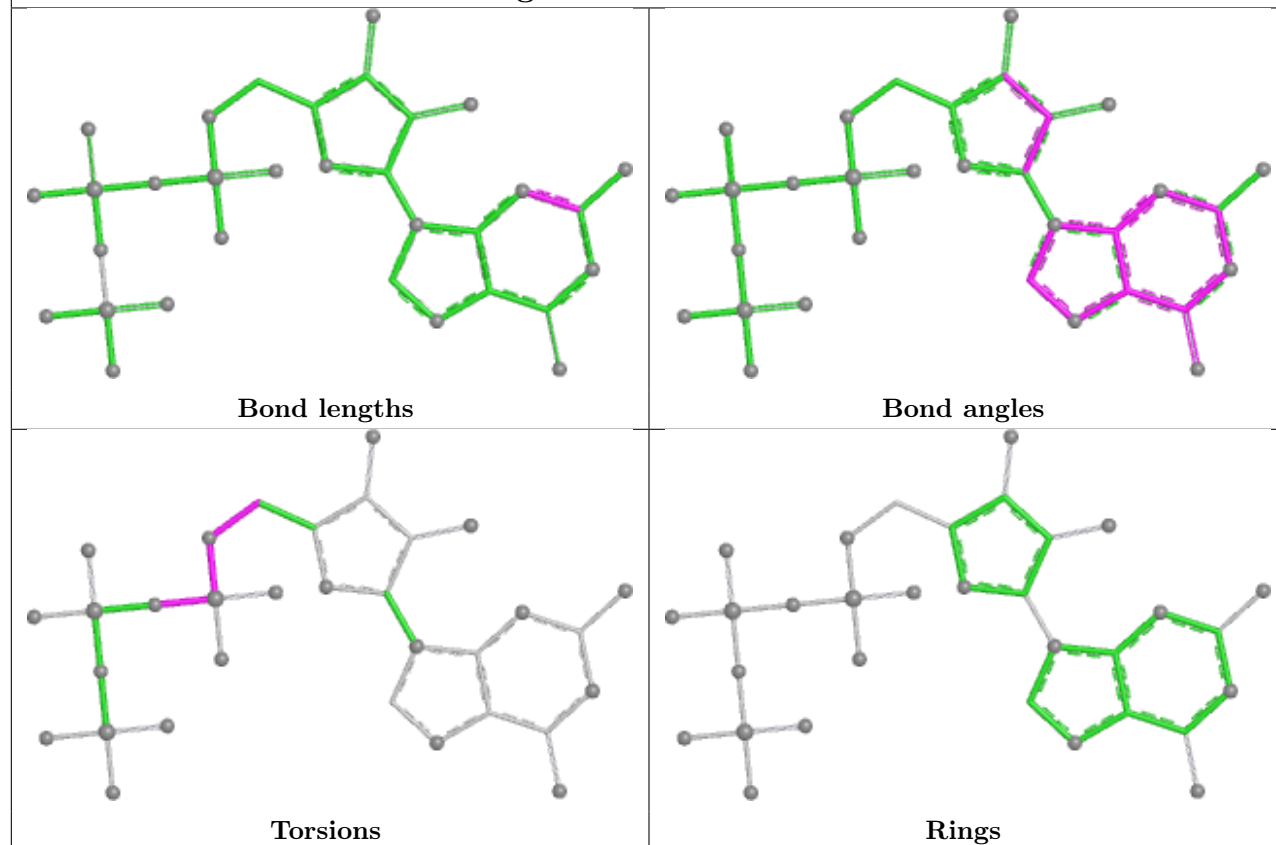
Ligand GTP AK 501



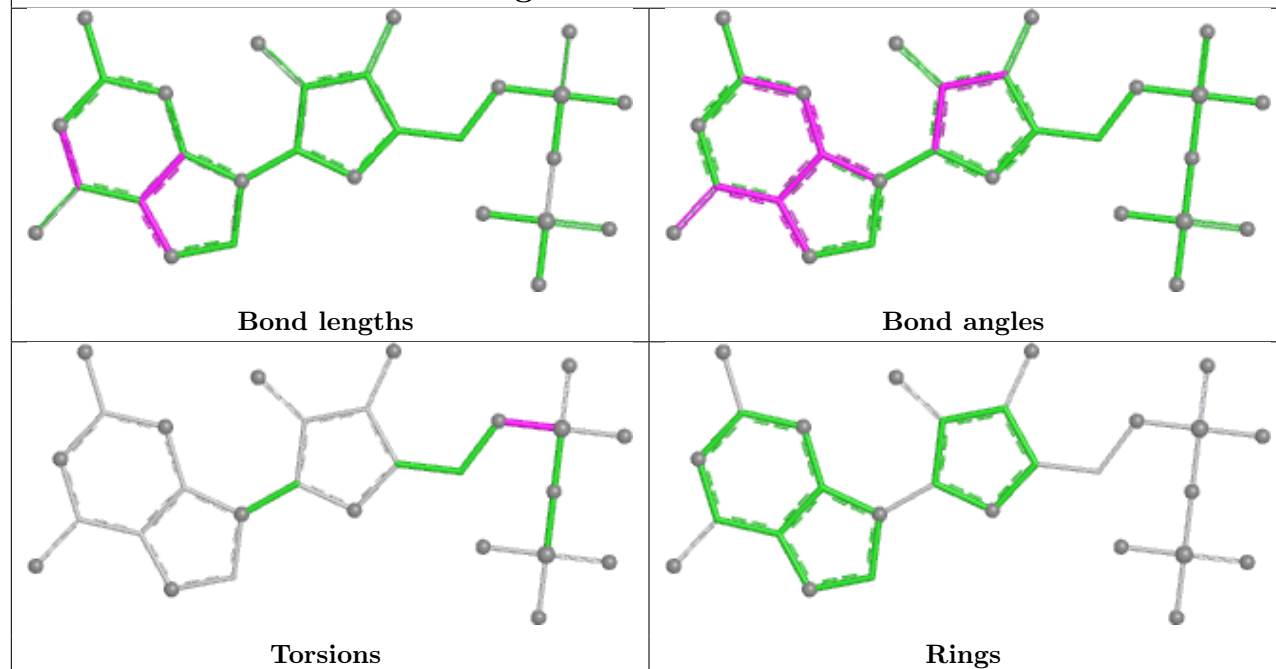


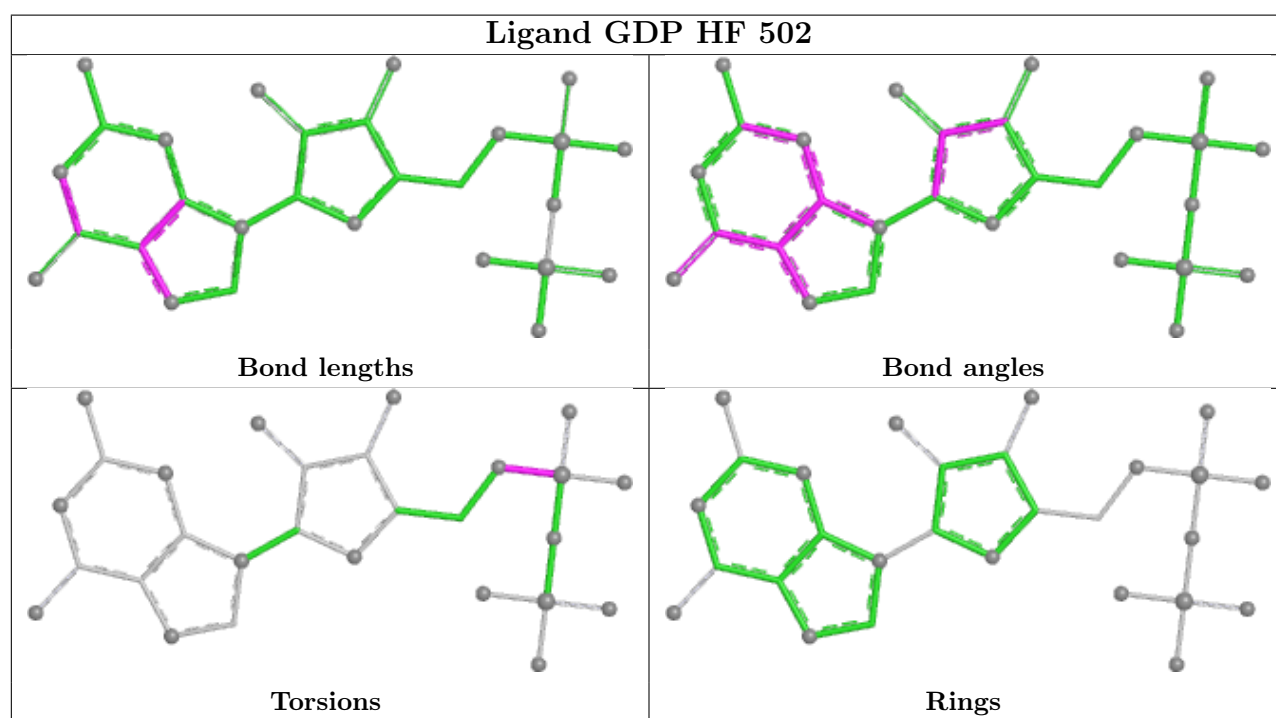
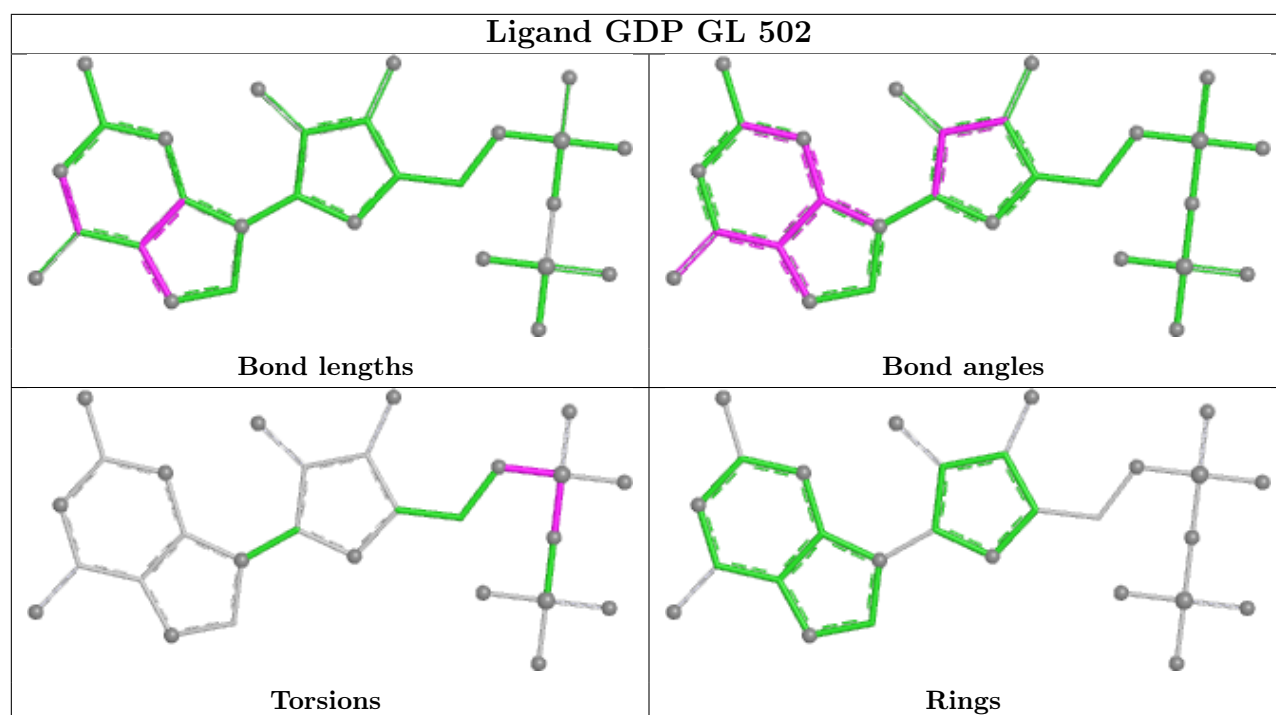


Ligand GTP RG 501

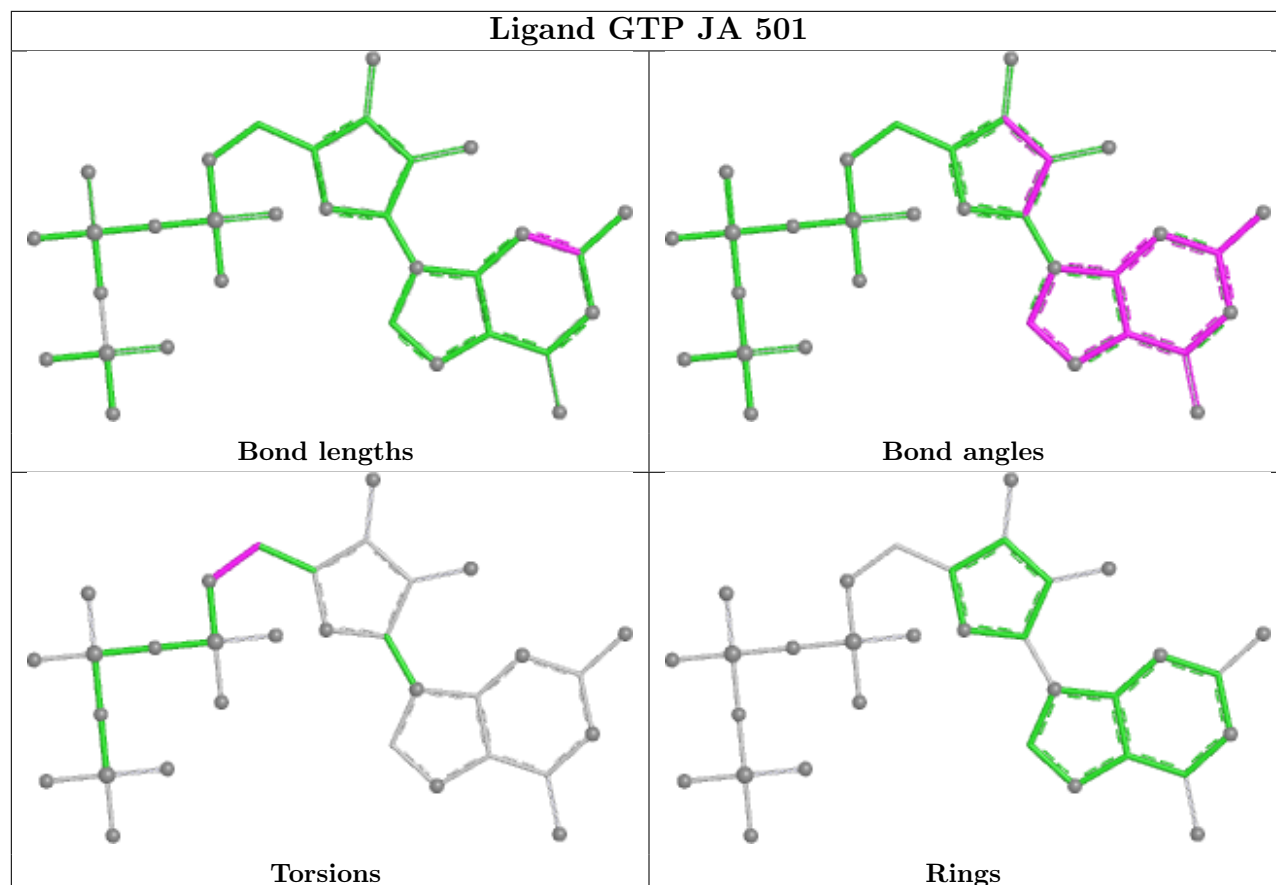


Ligand GDP ON 501

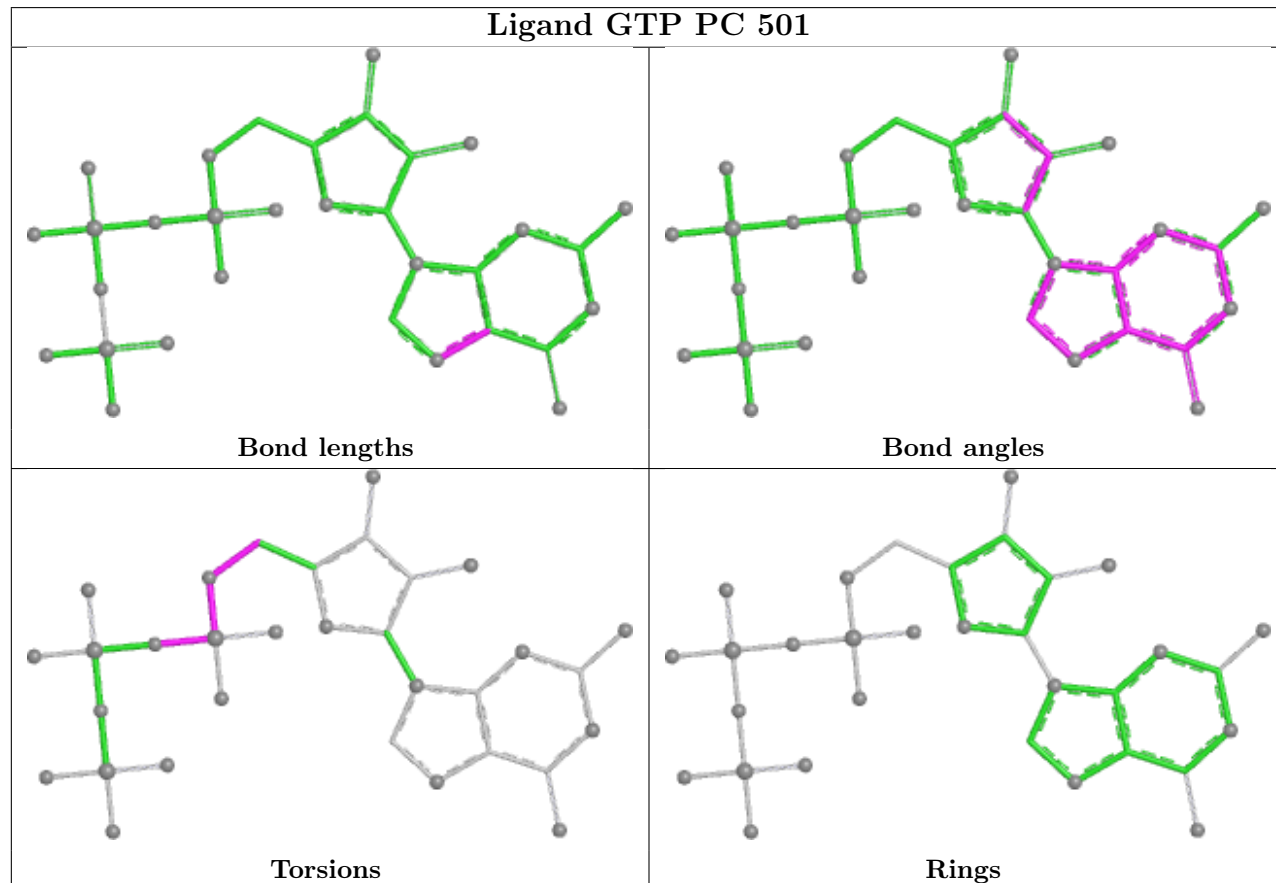


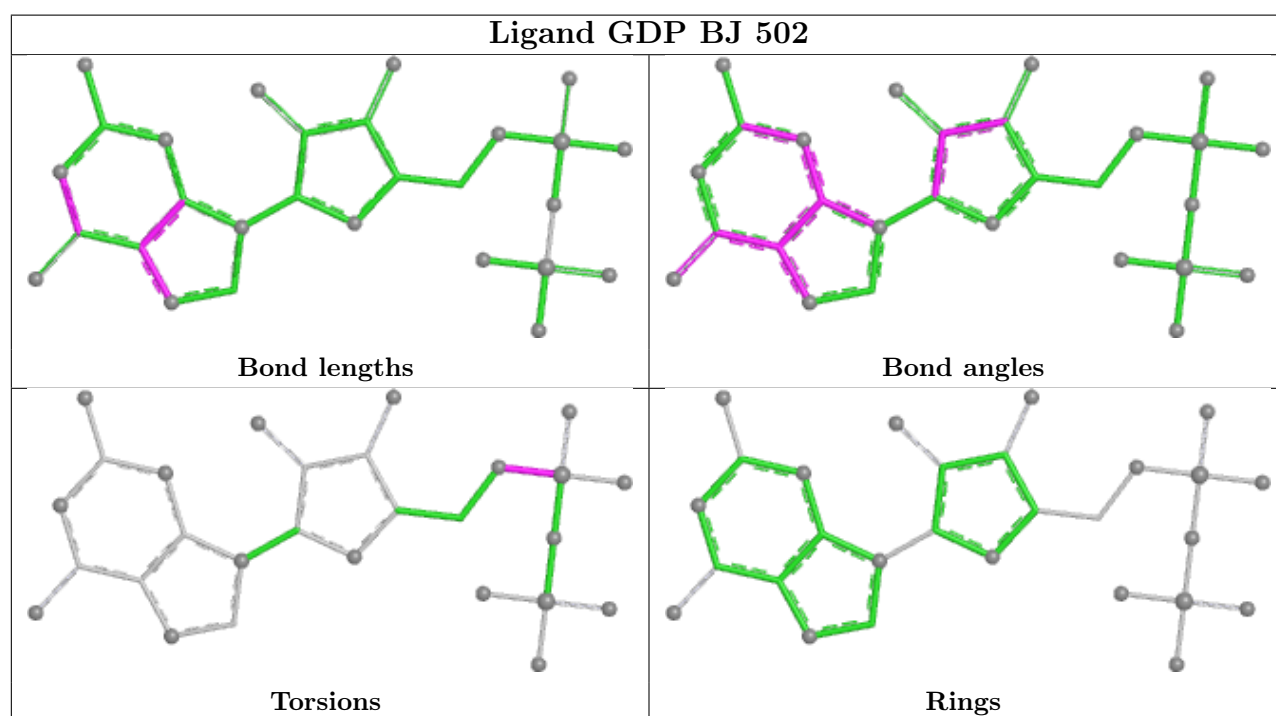
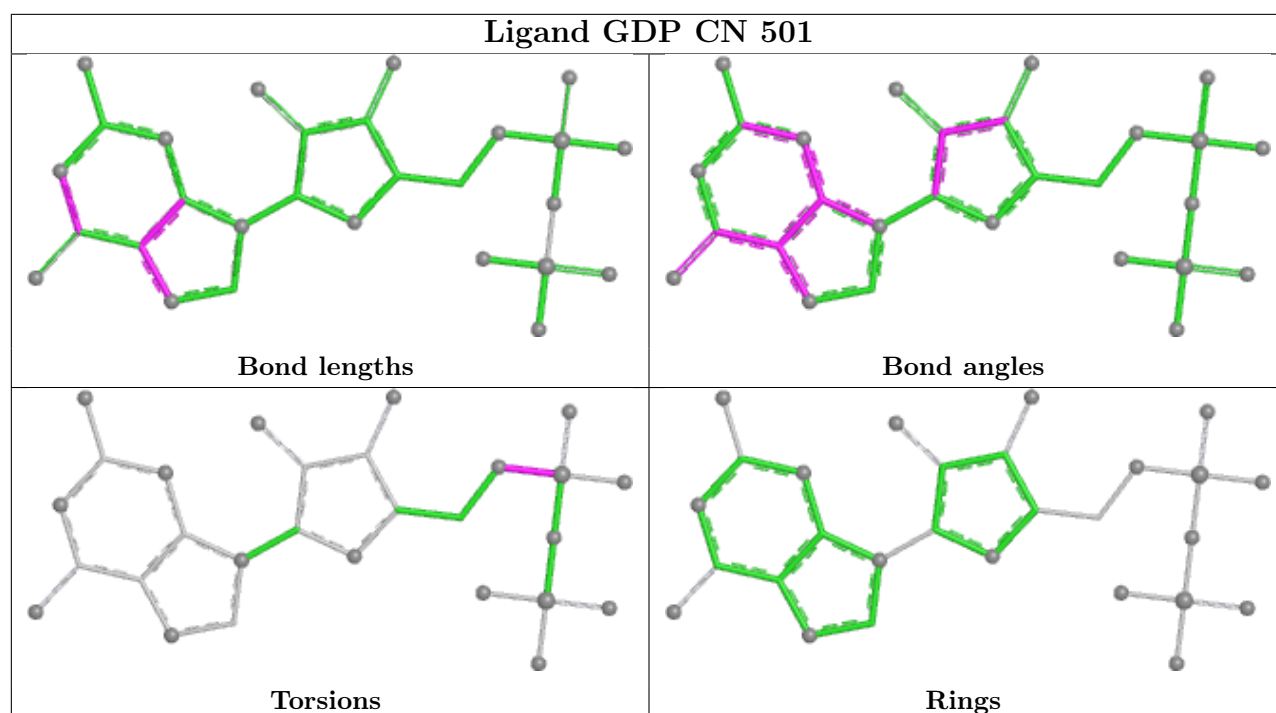


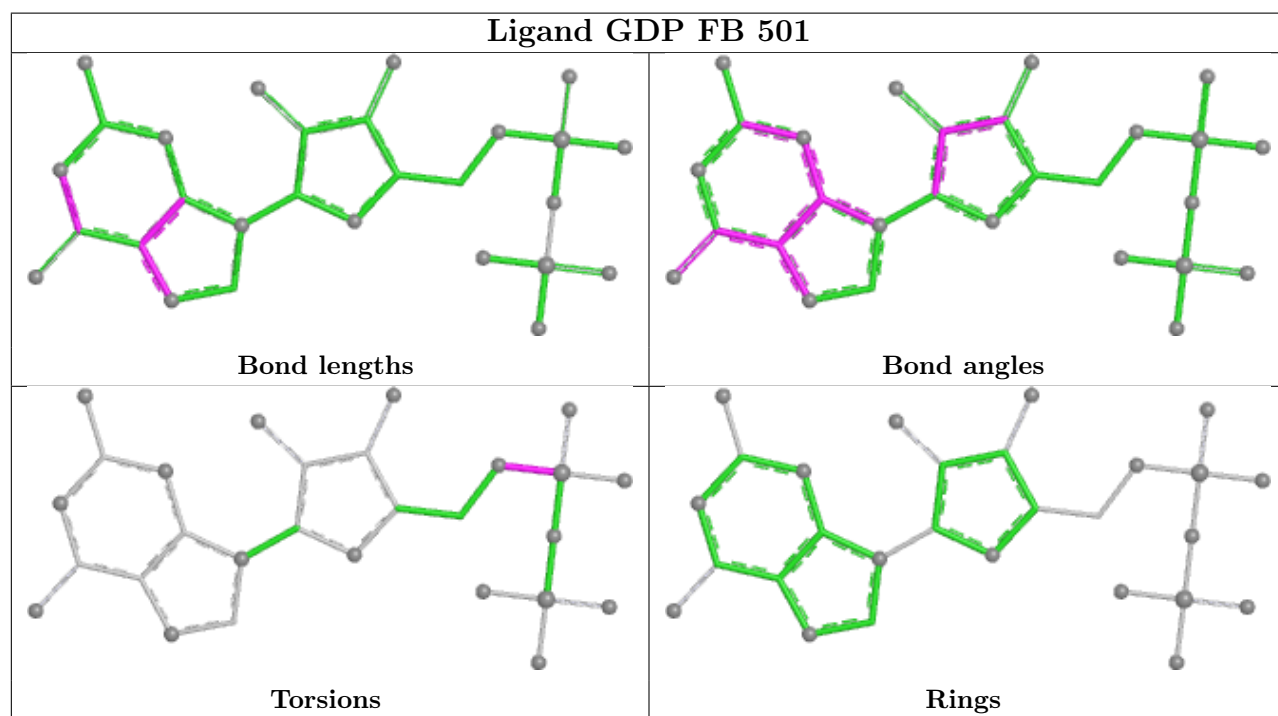
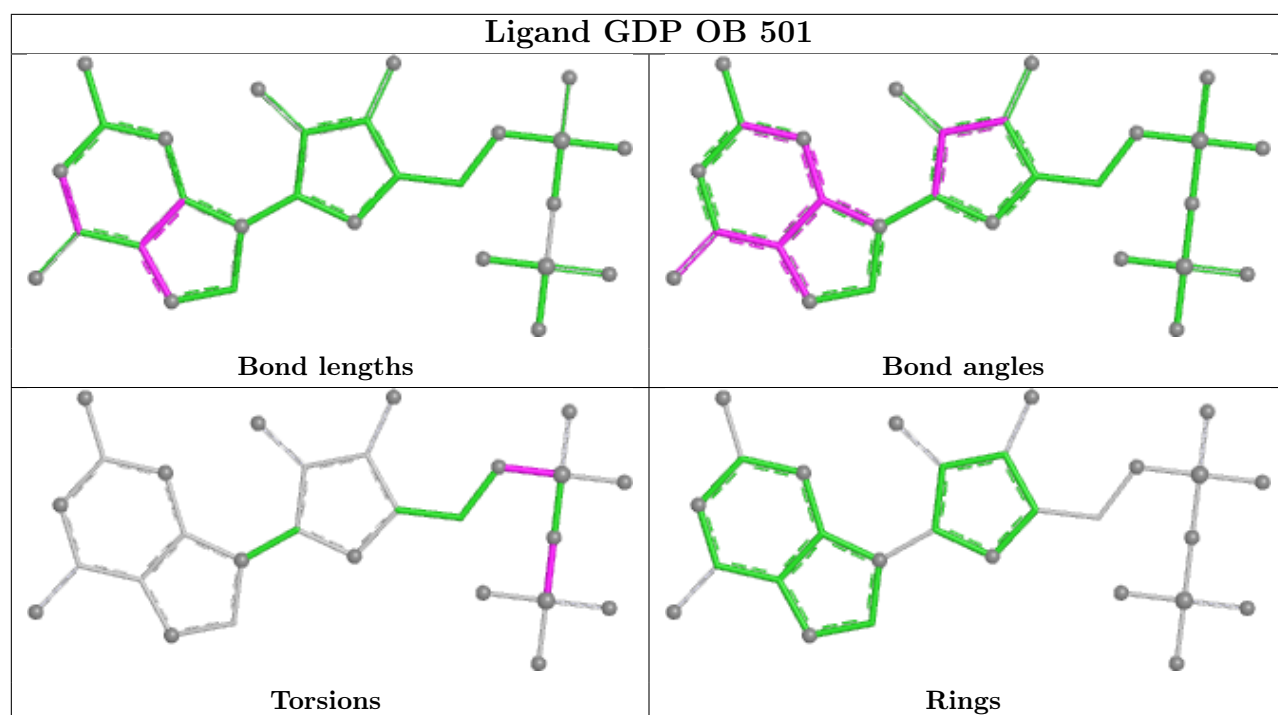
Ligand GTP JA 501



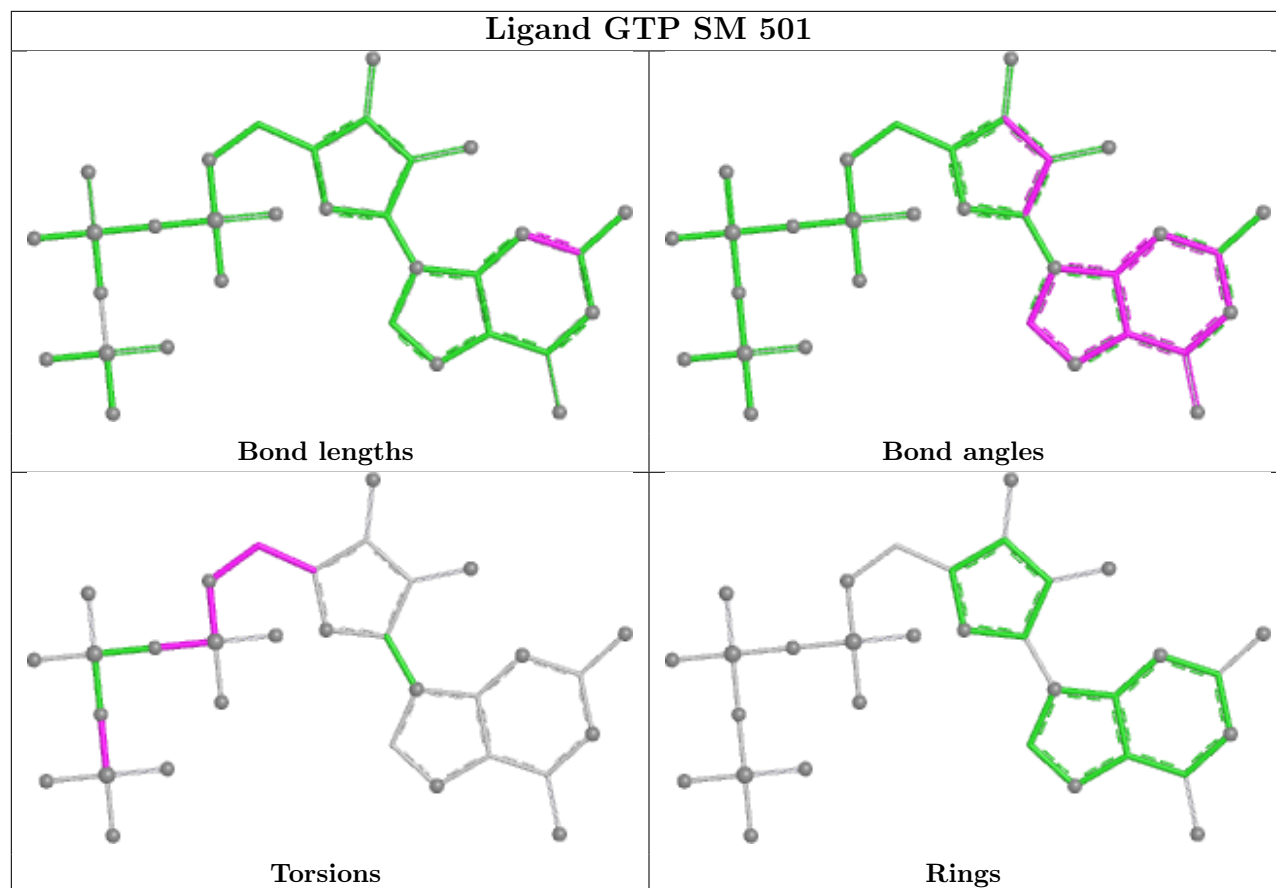
Ligand GTP PC 501



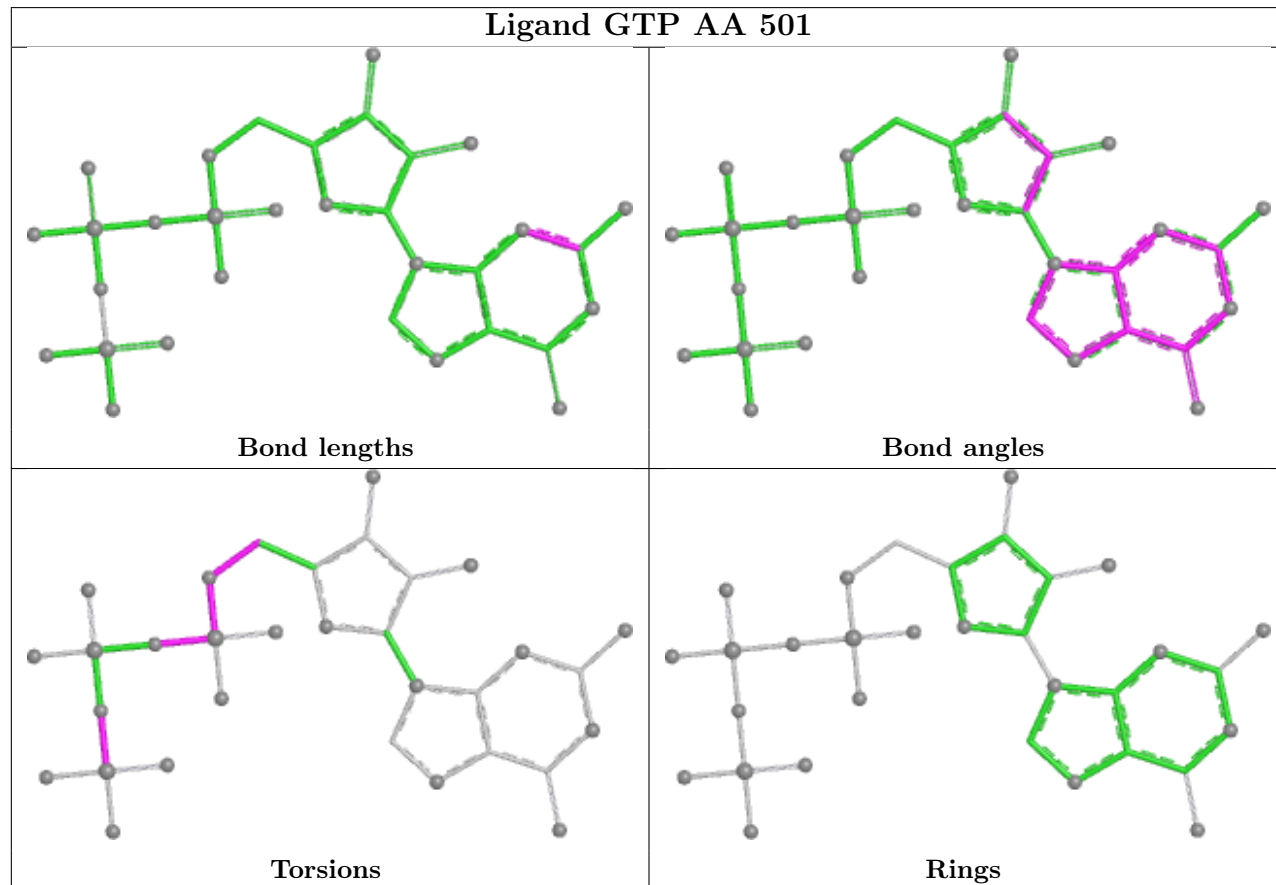


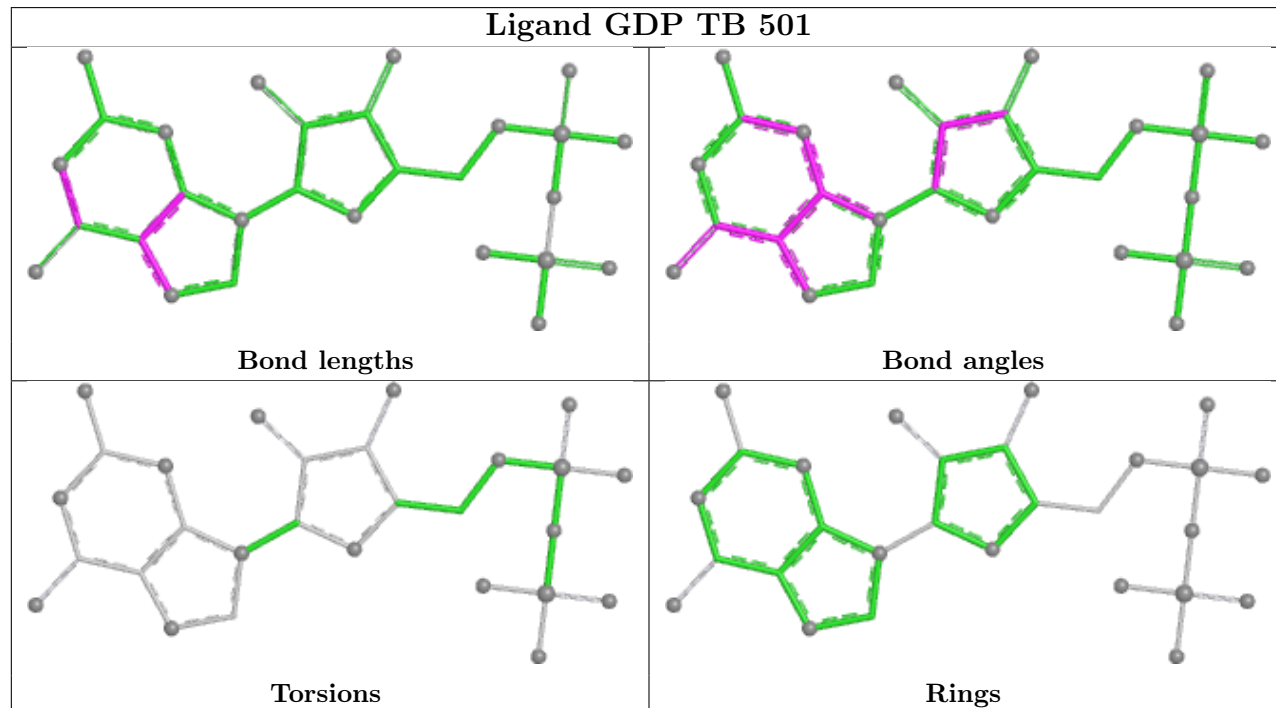
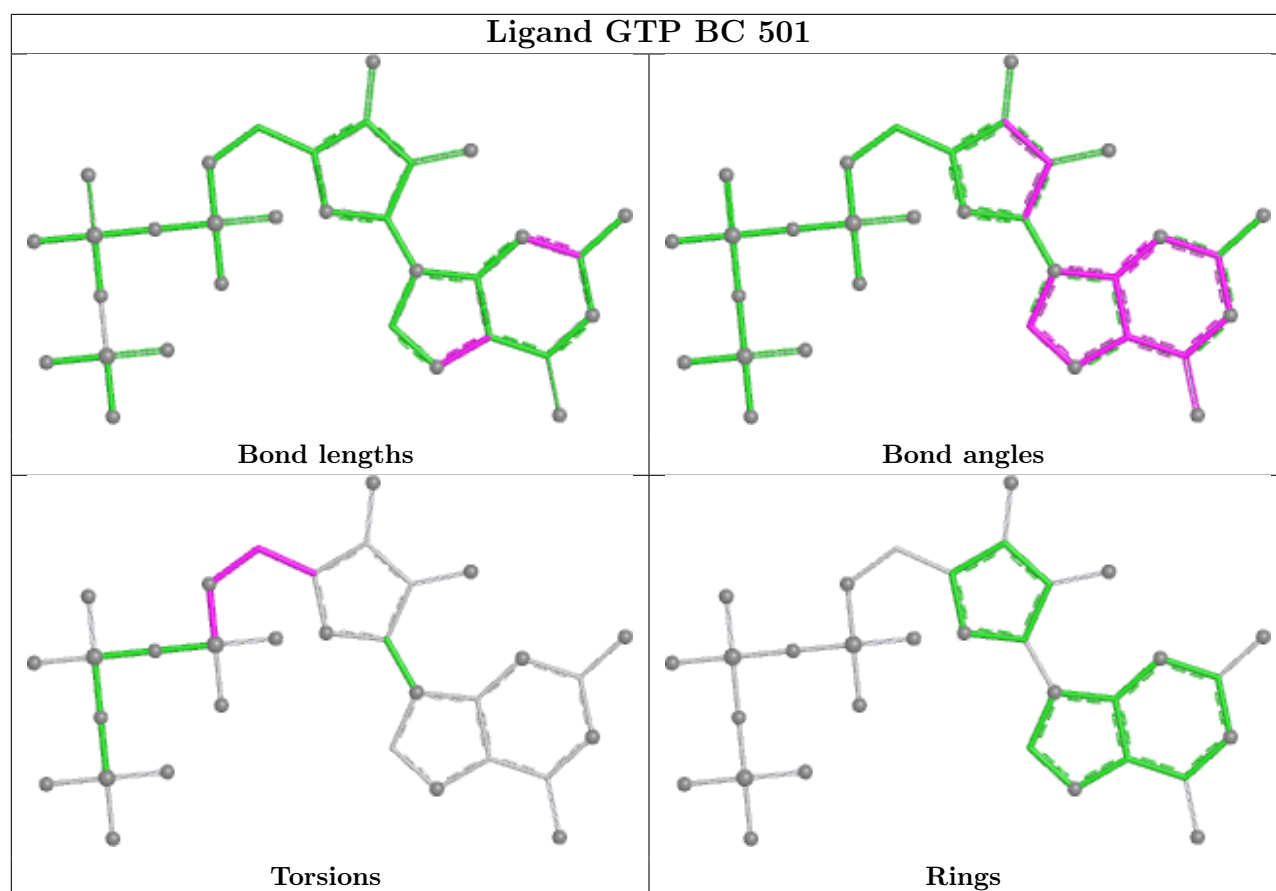


Ligand GTP SM 501

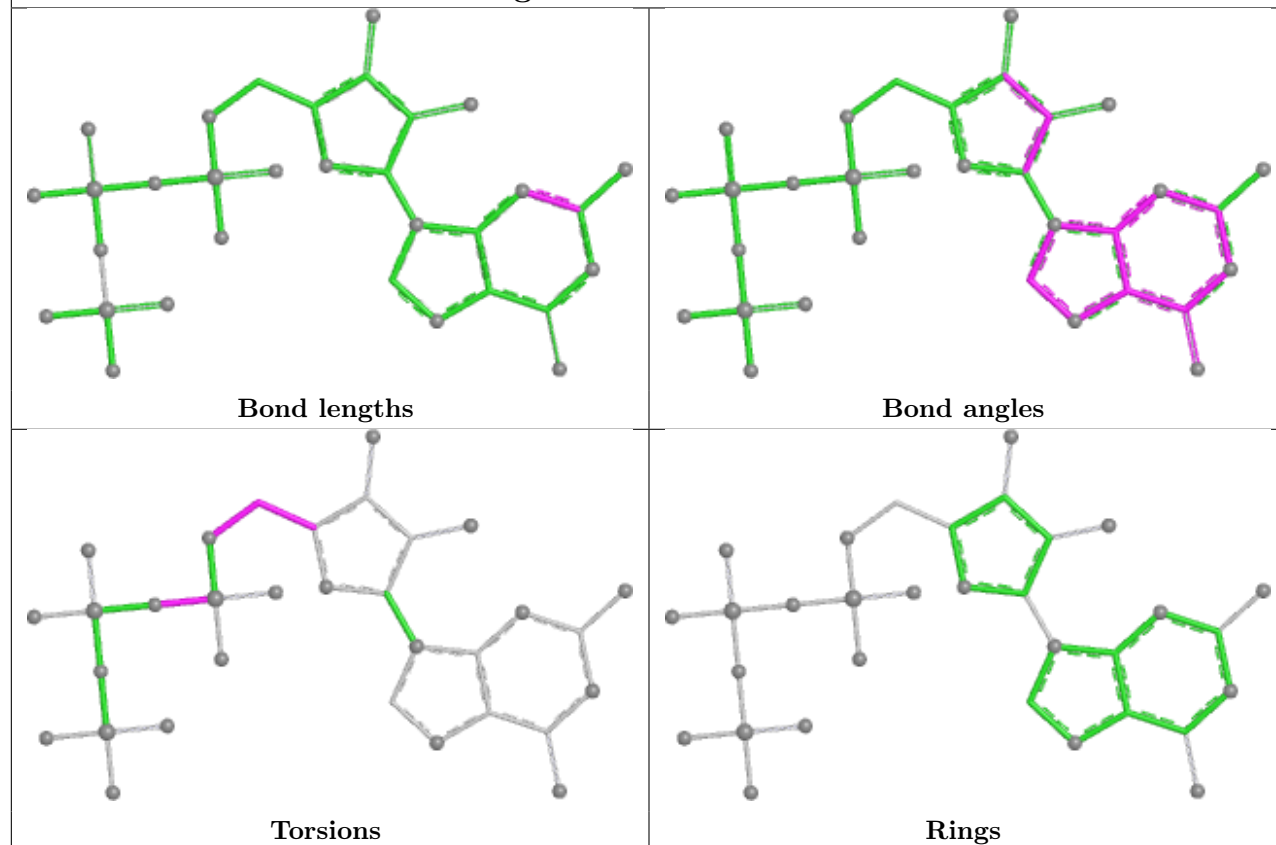


Ligand GTP AA 501

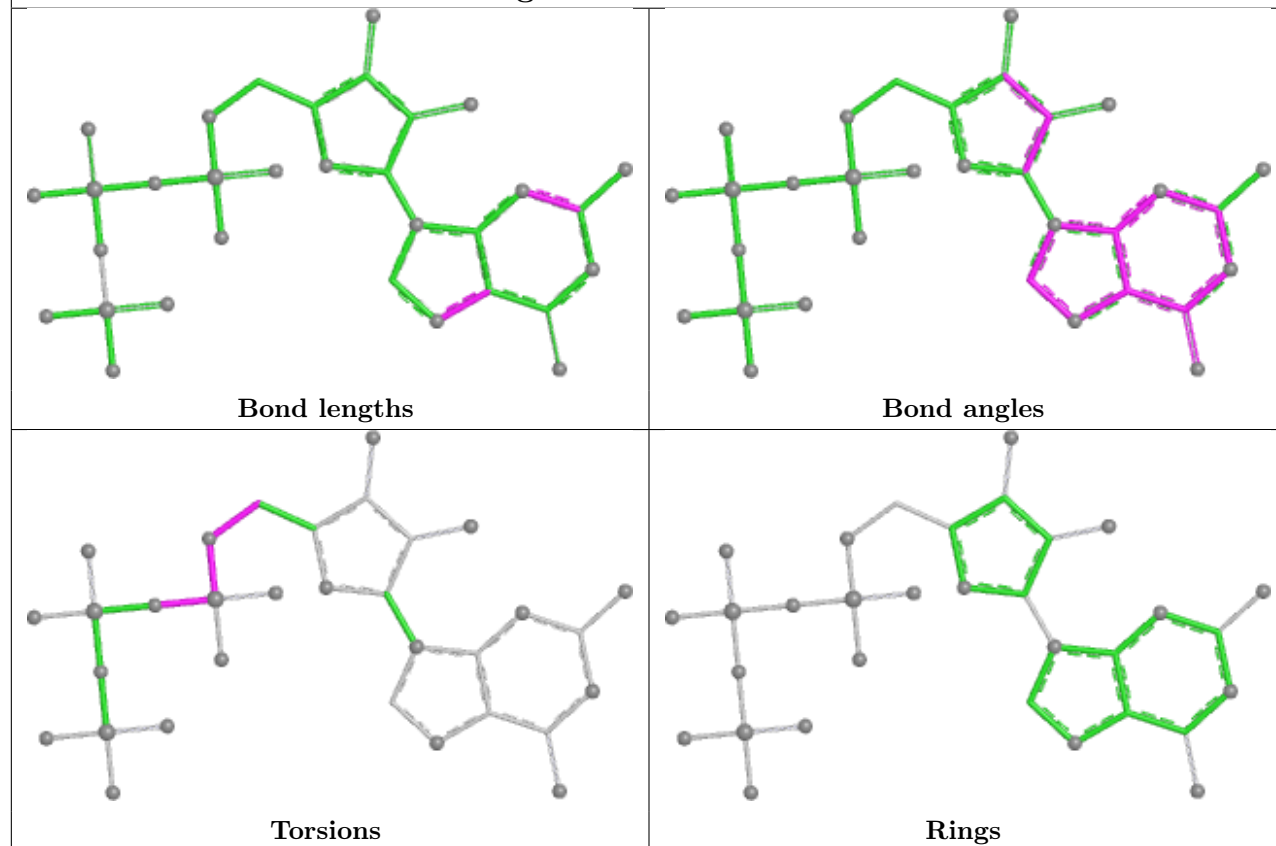


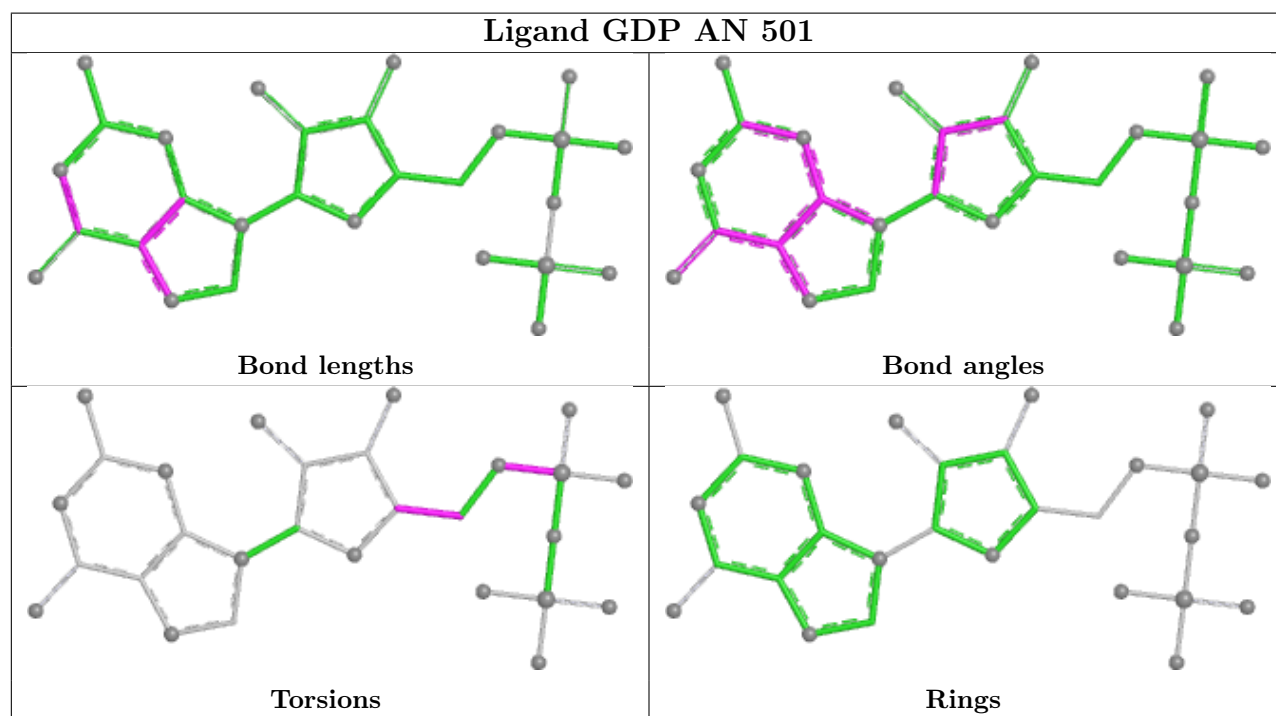
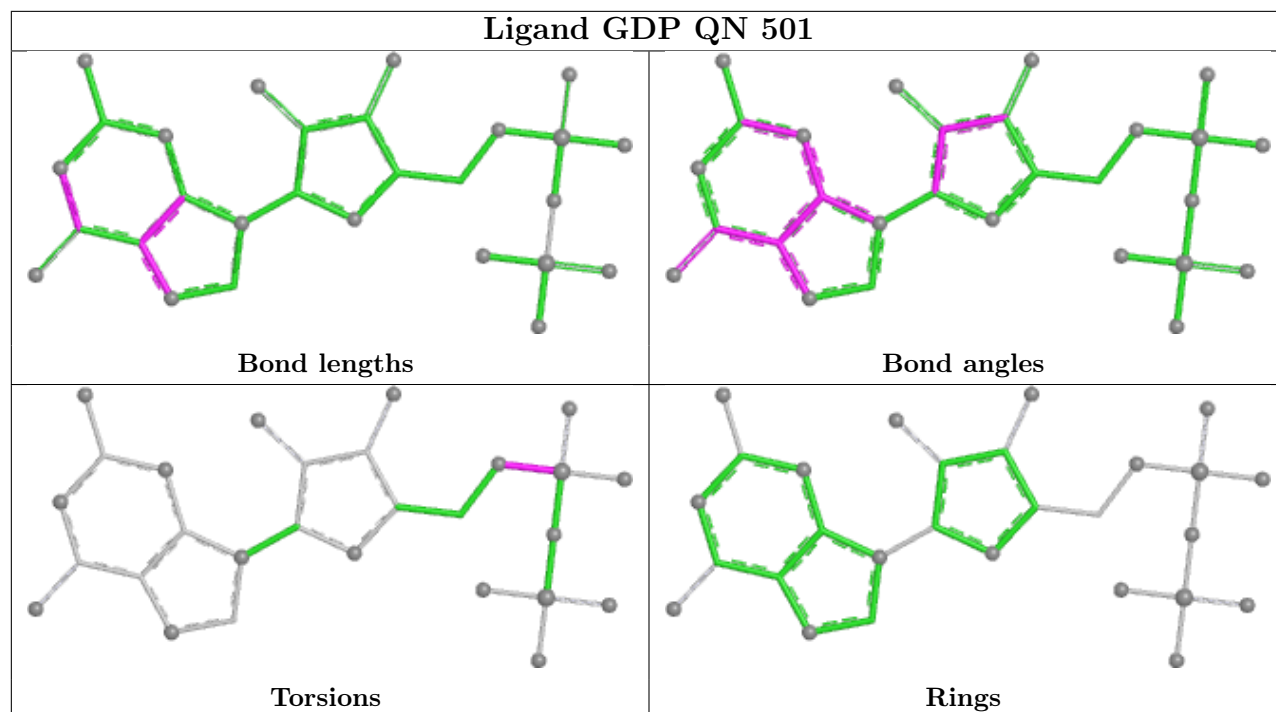


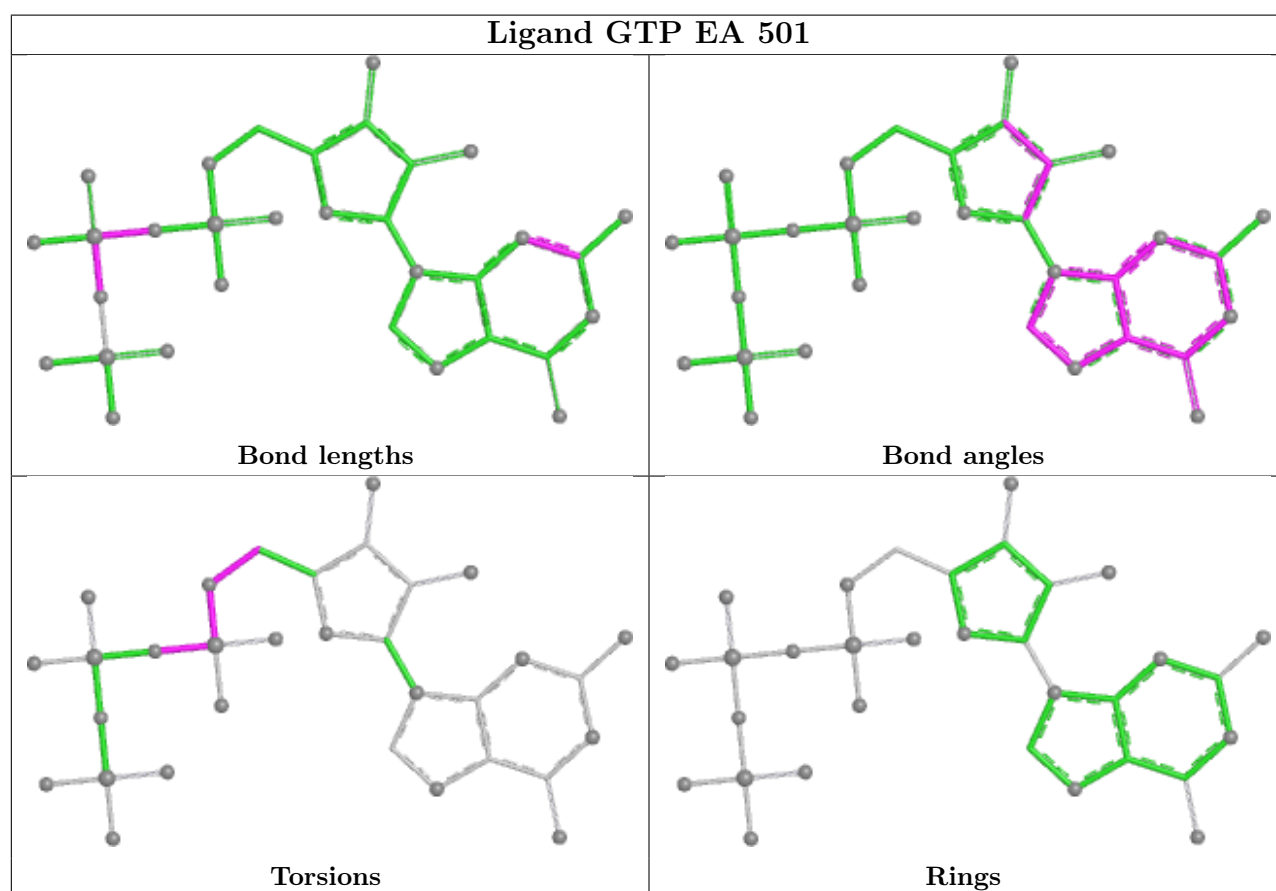
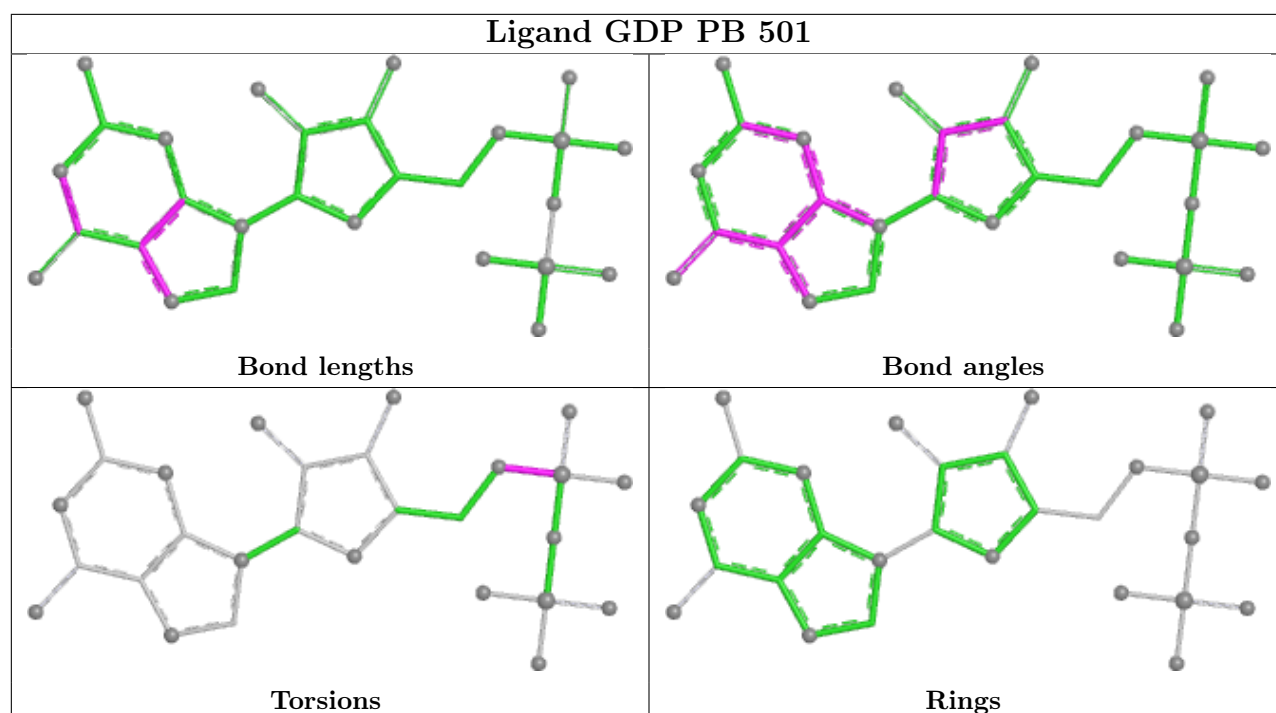
Ligand GTP BM 501

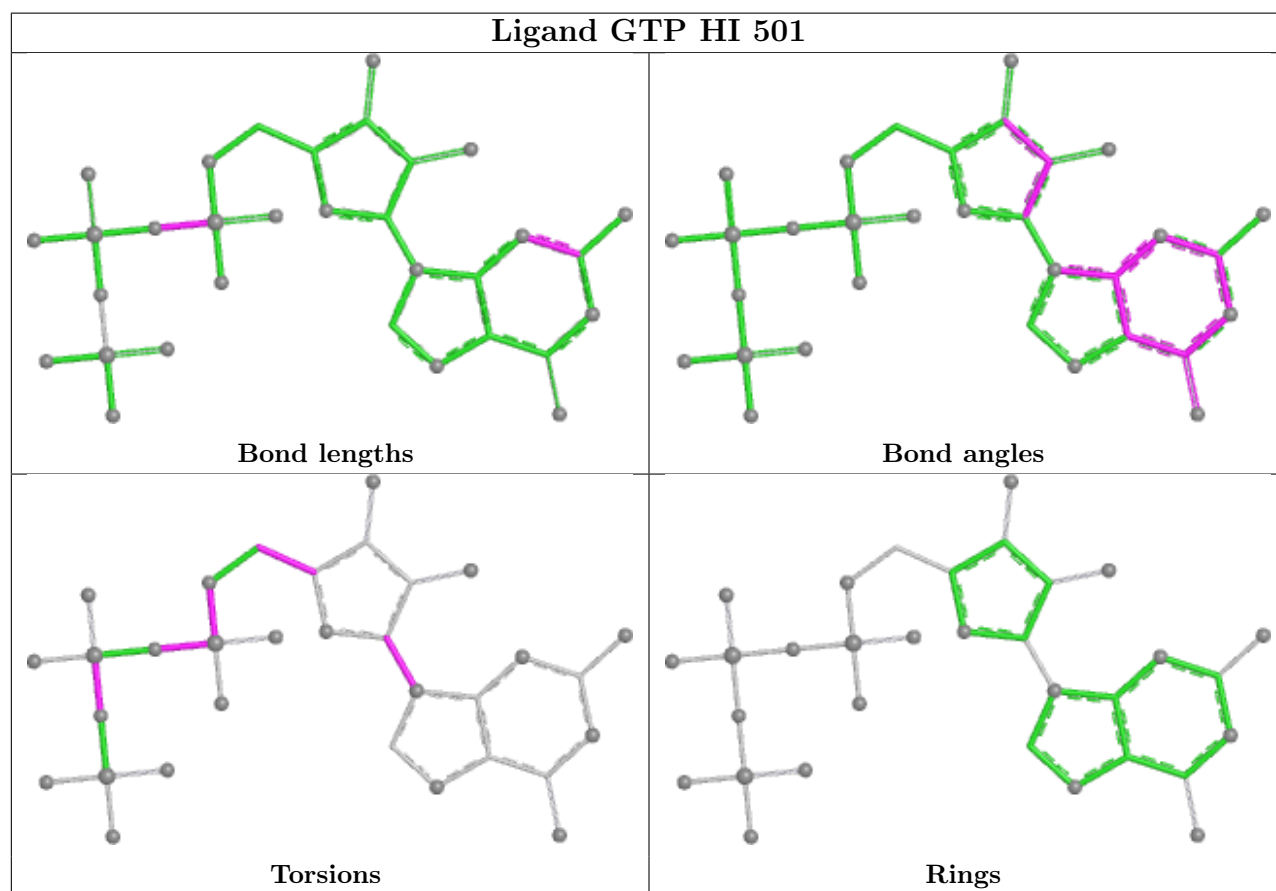
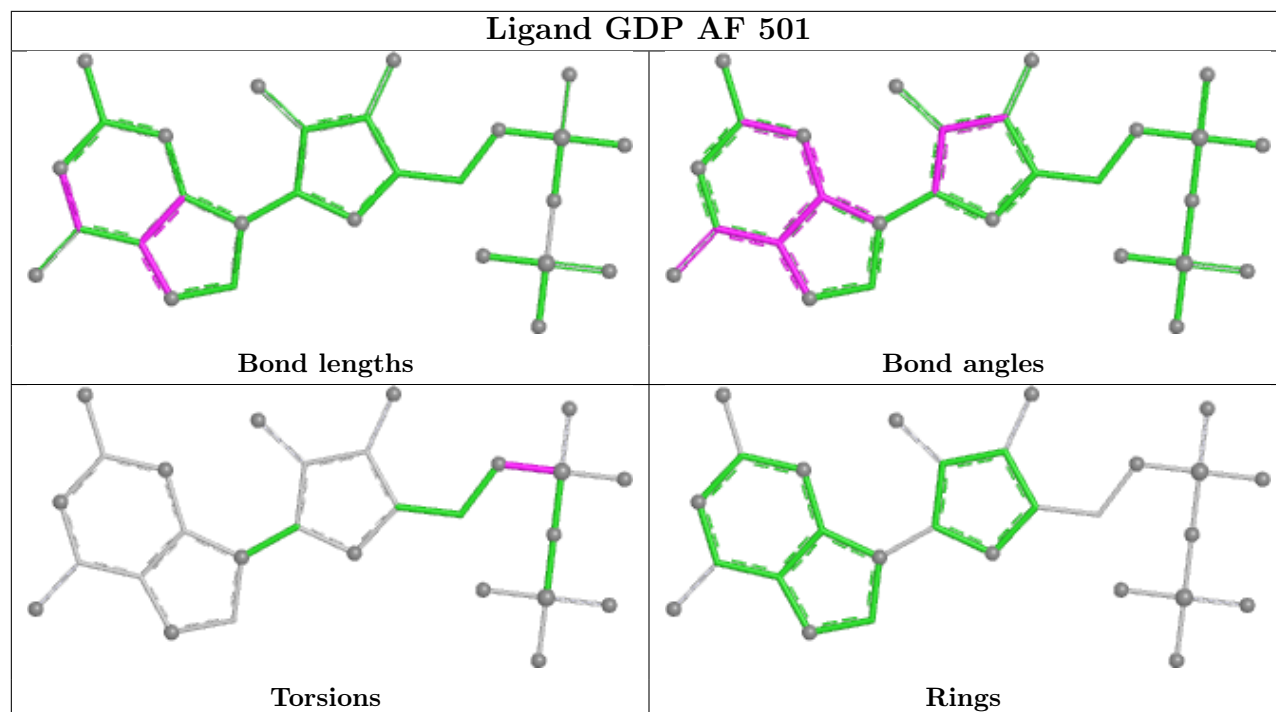


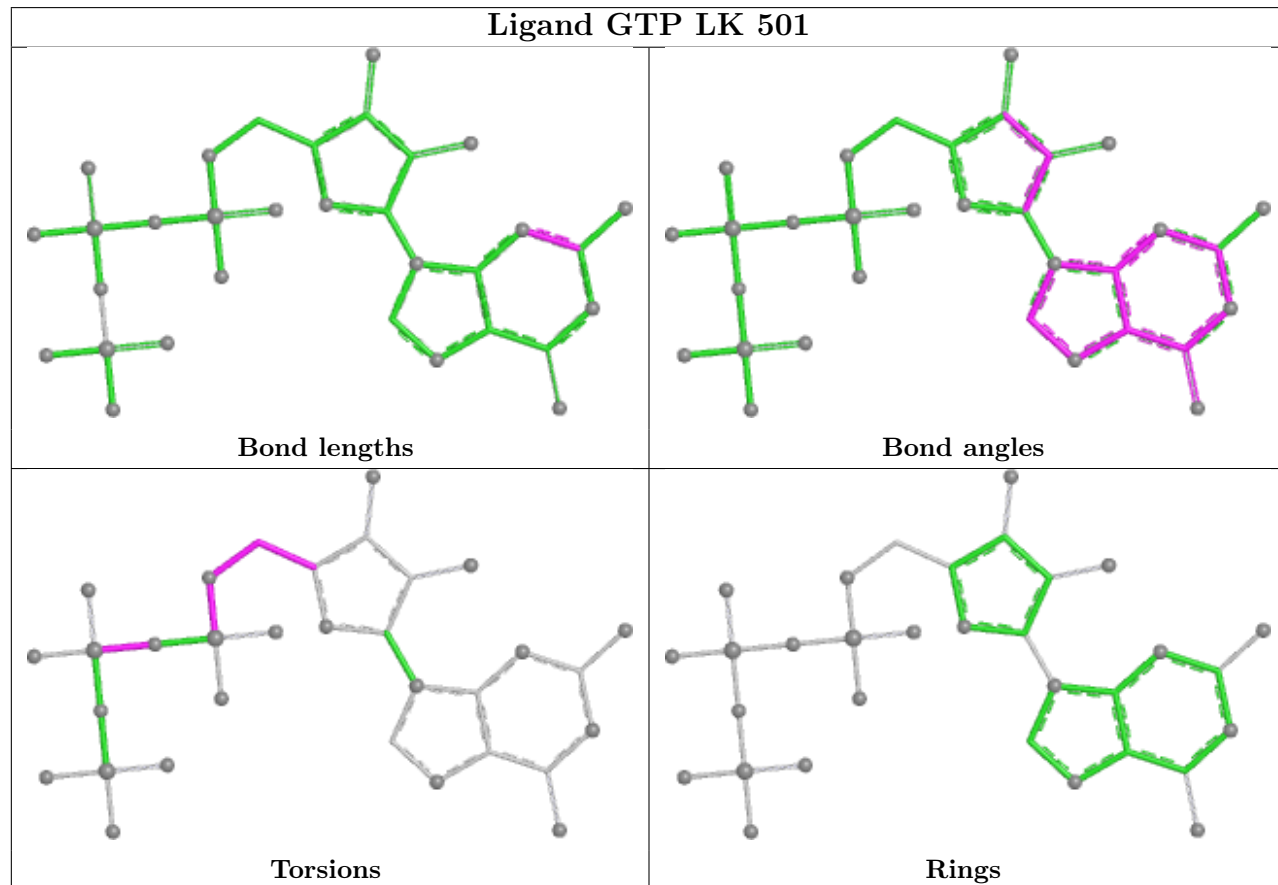
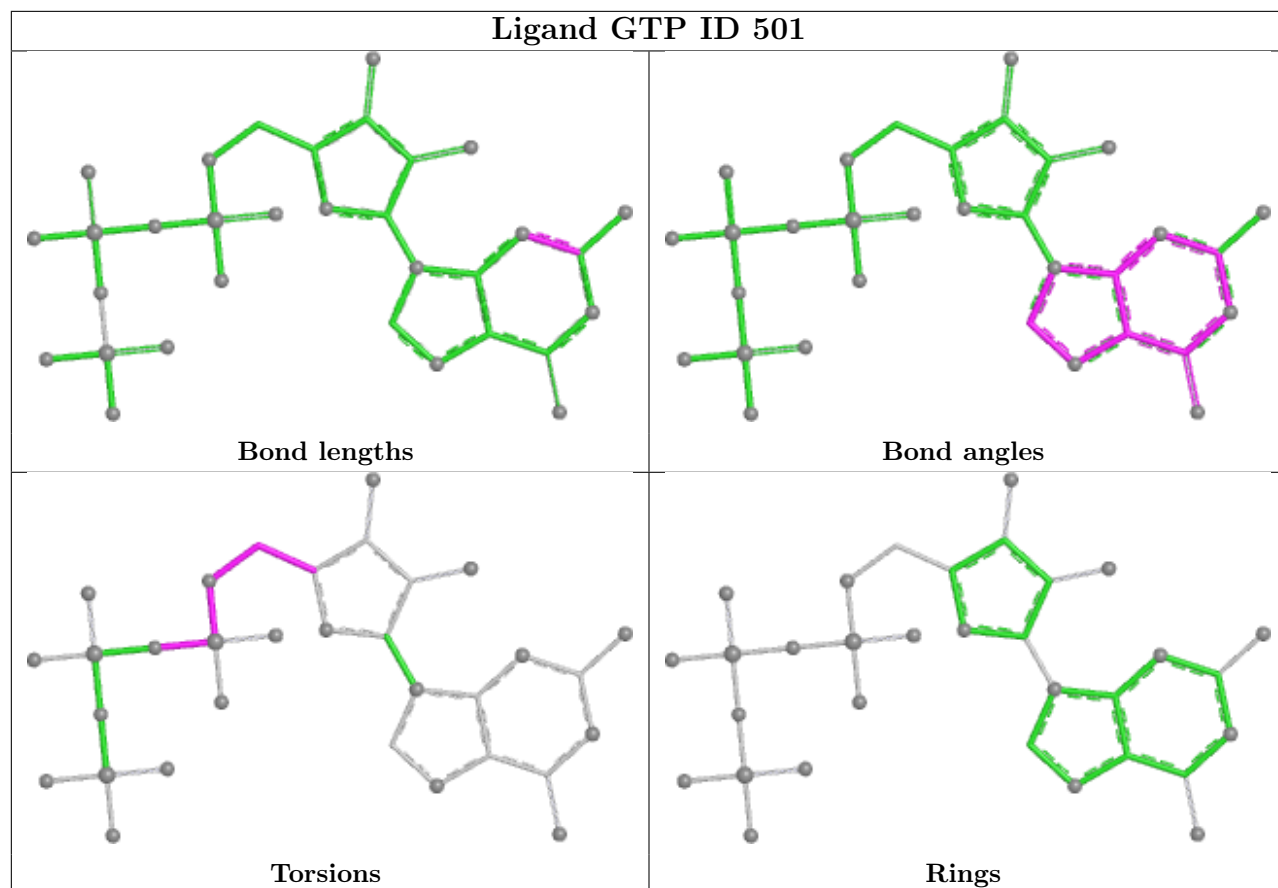
Ligand GTP HC 501

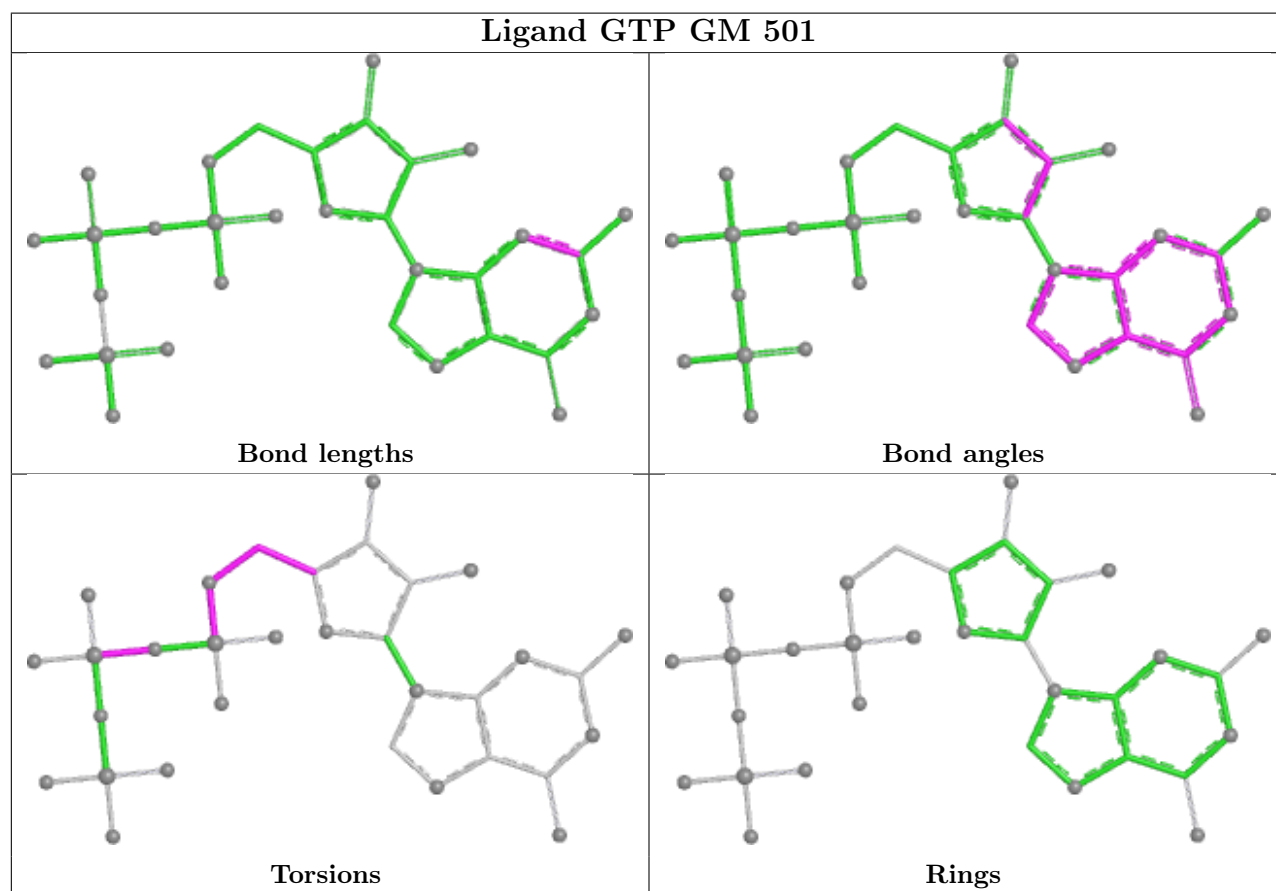
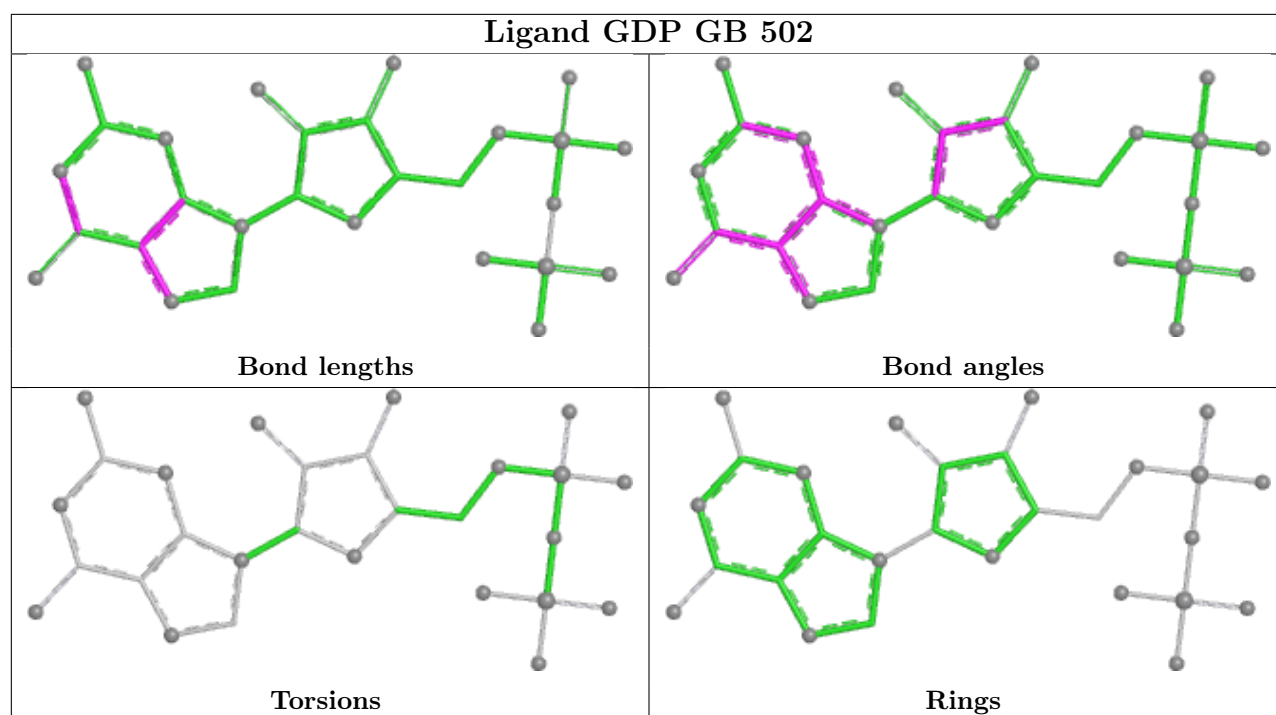


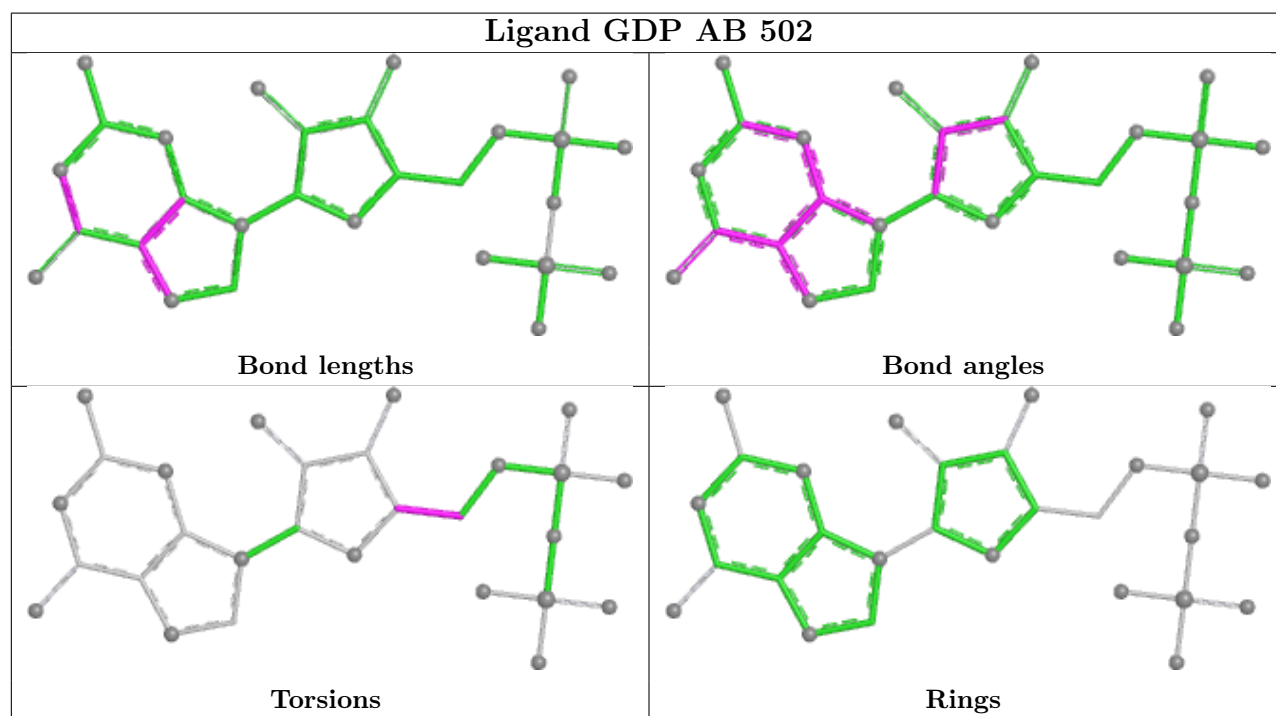
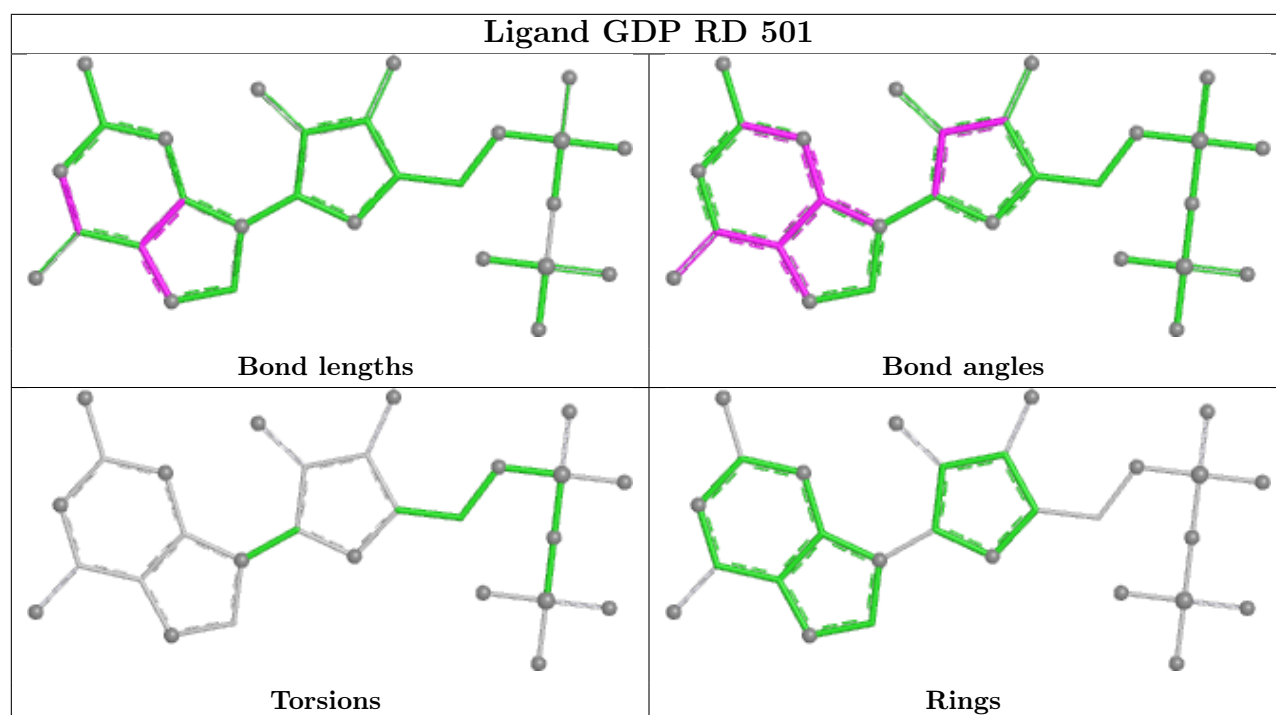


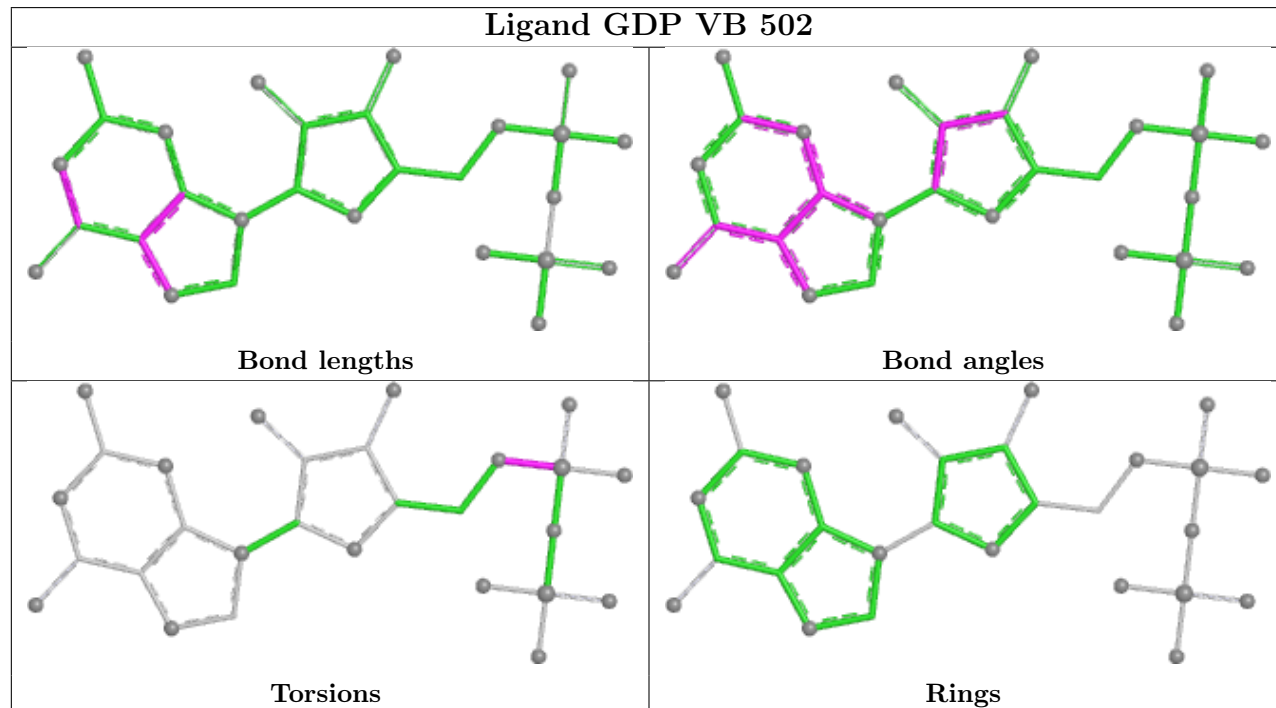
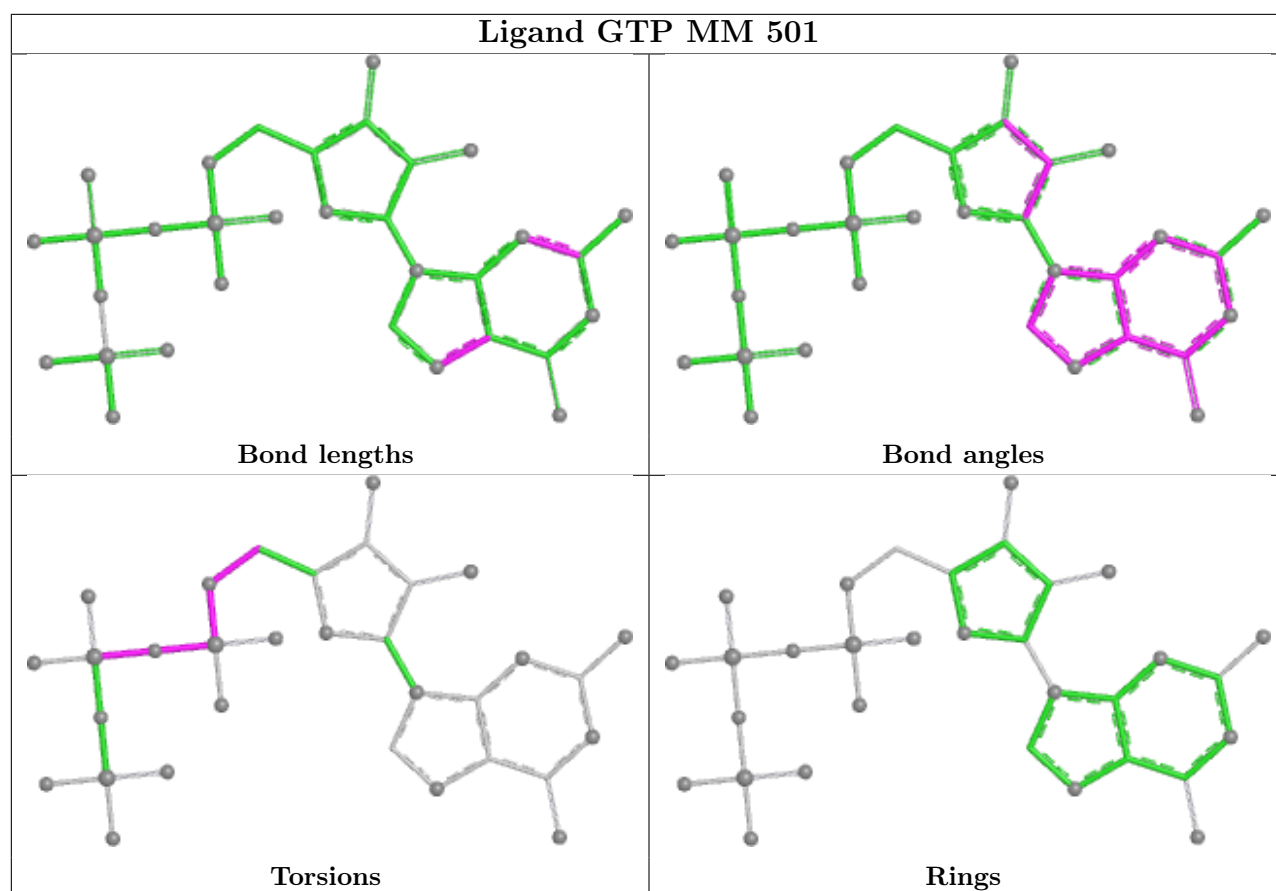




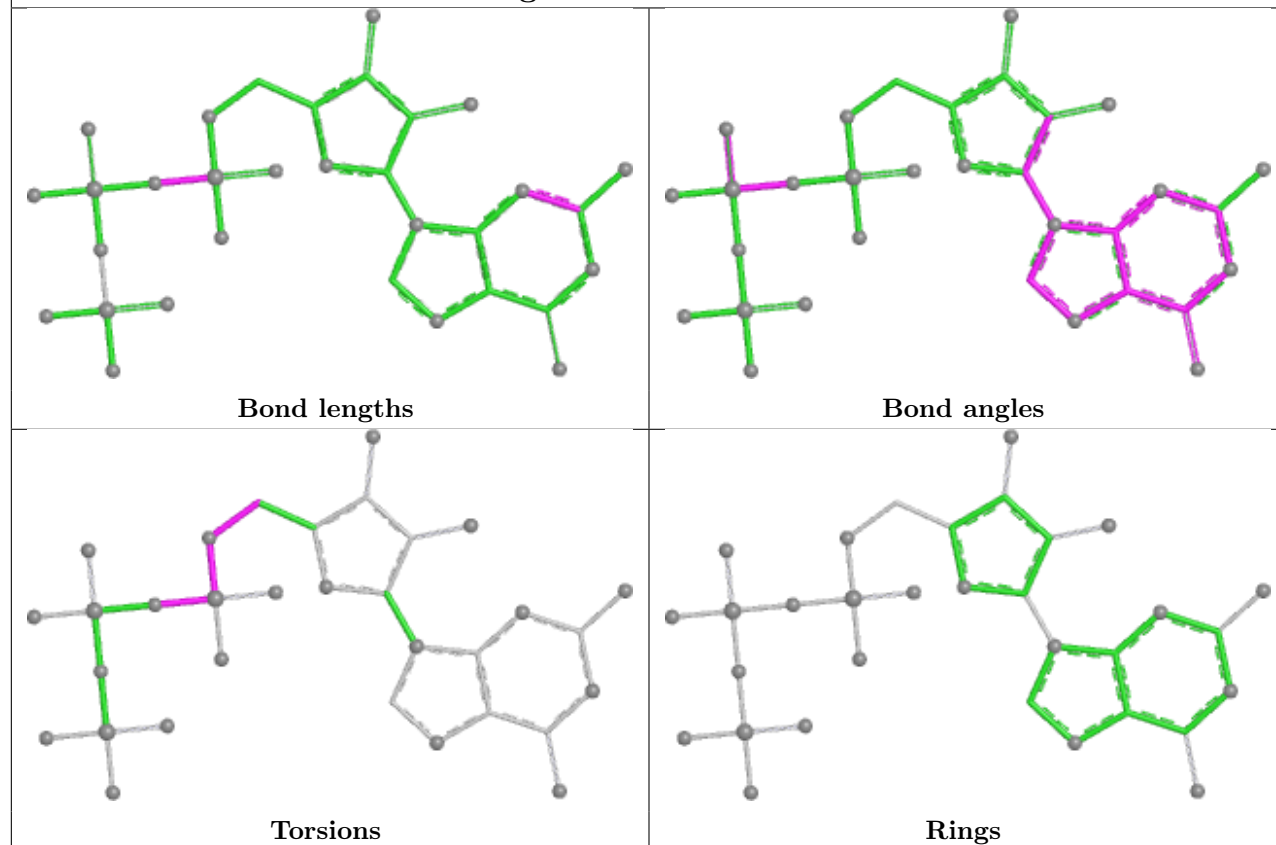




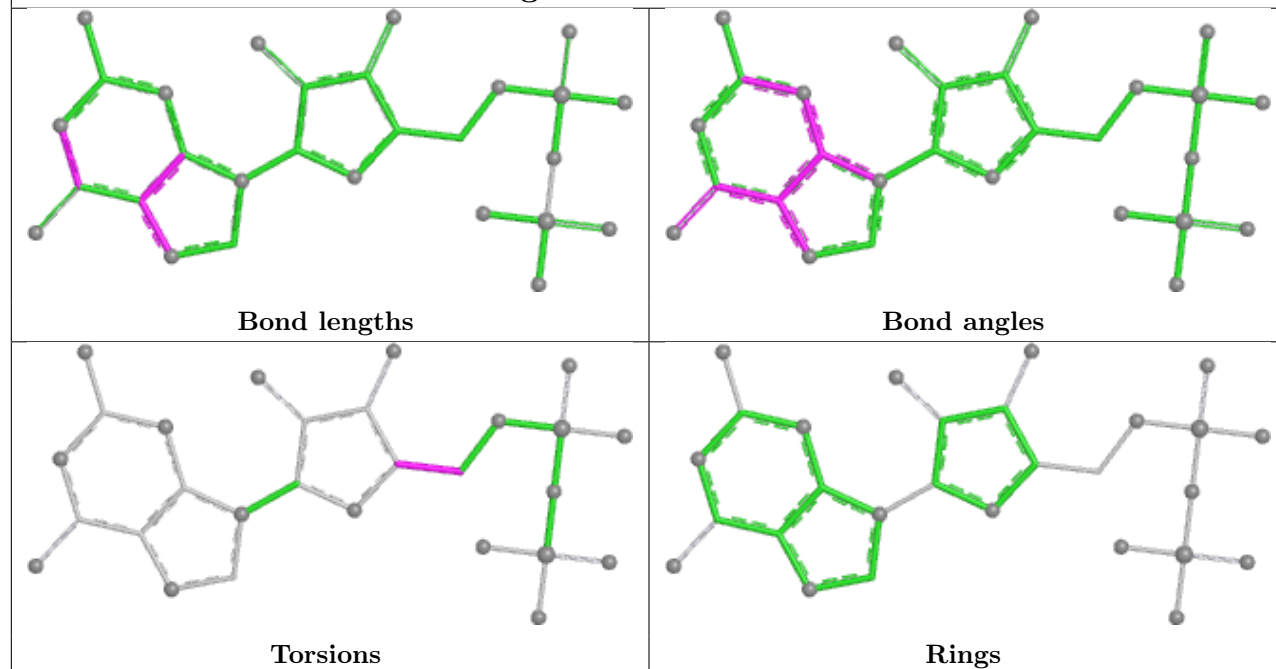




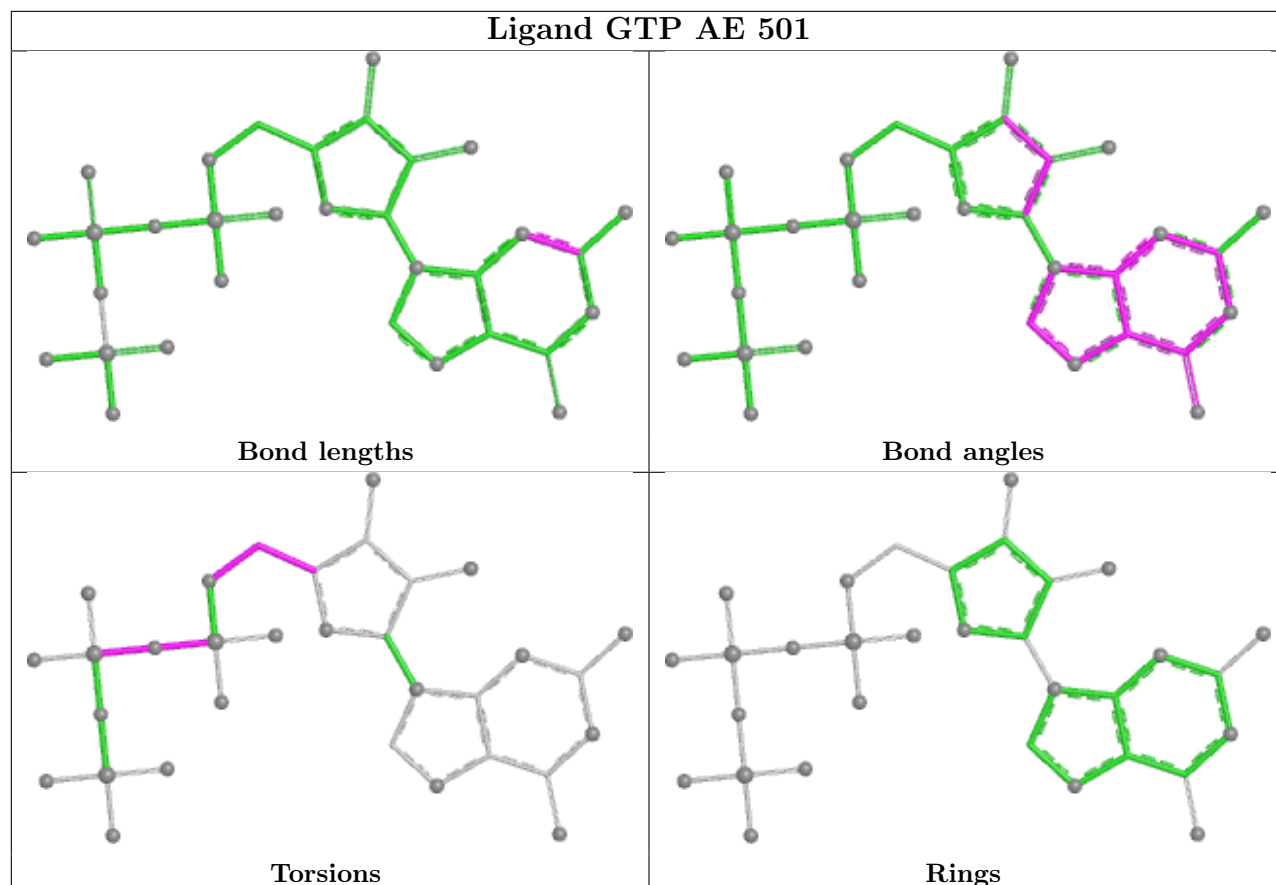
Ligand GTP TE 501



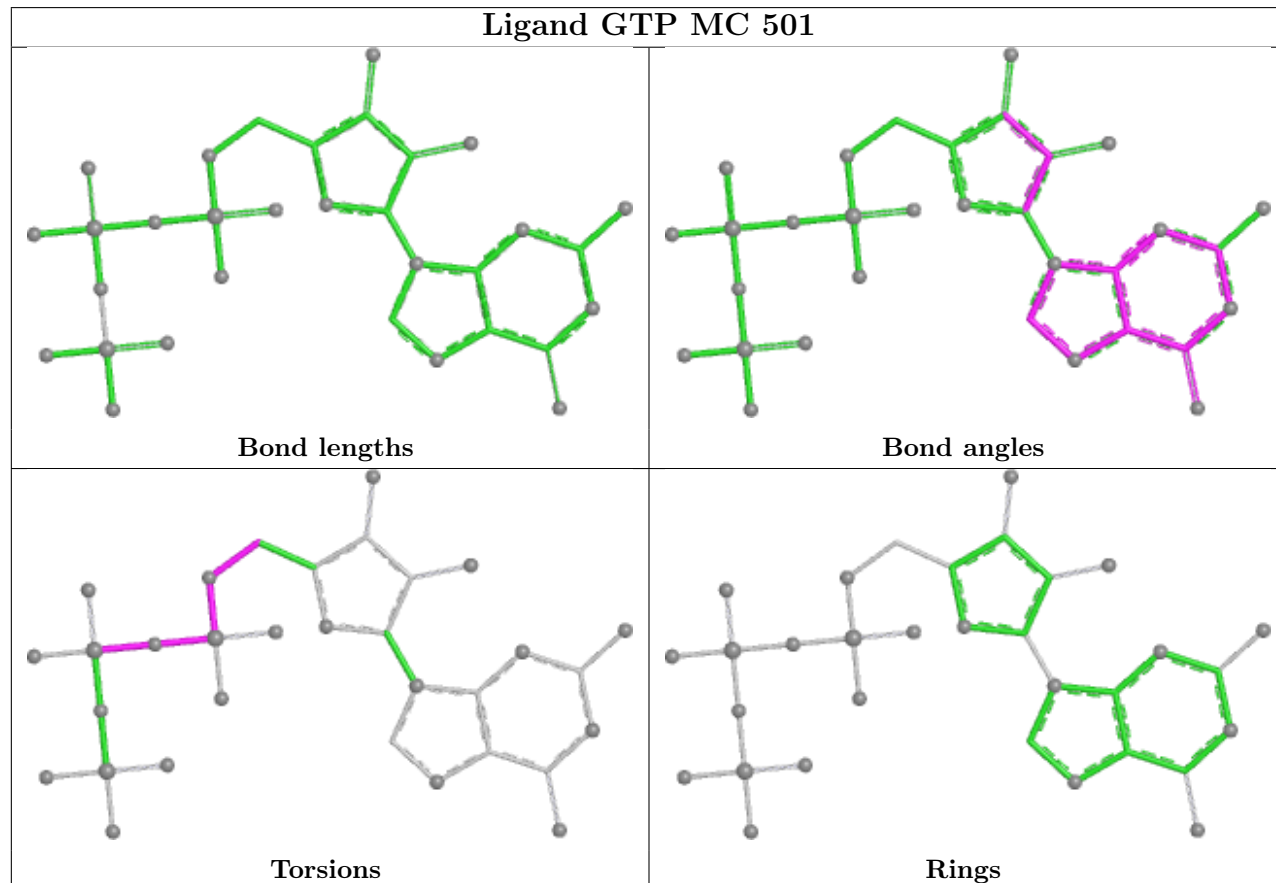
Ligand GDP TJ 501



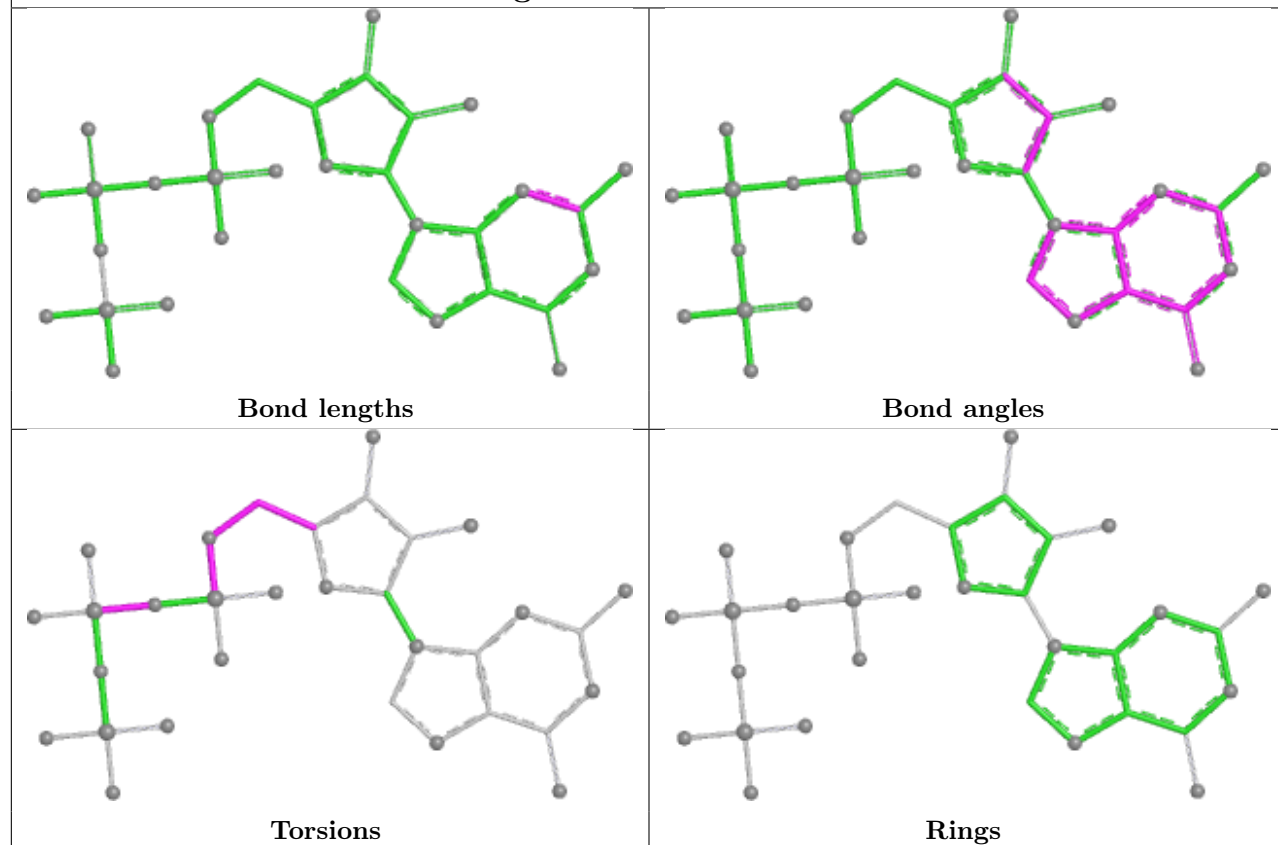
Ligand GTP AE 501



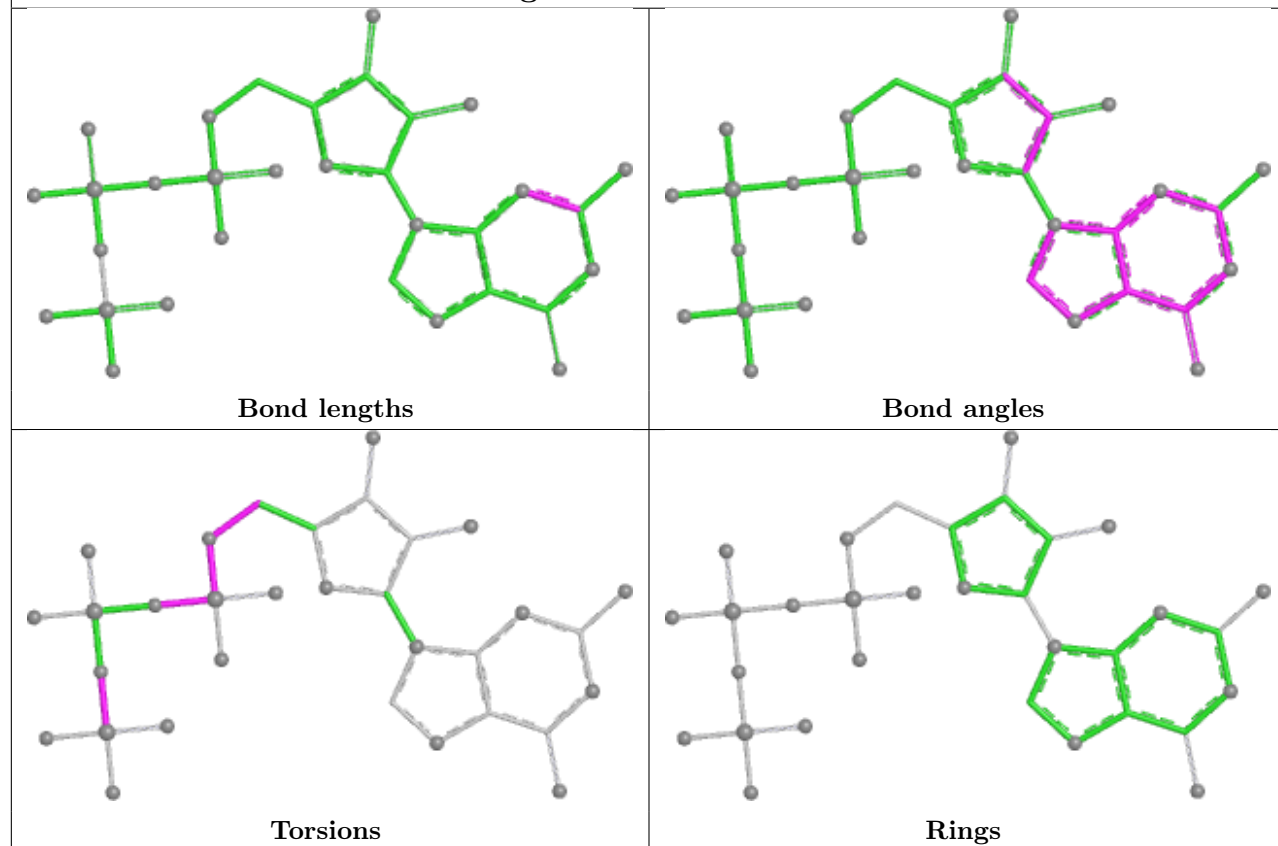
Ligand GTP MC 501

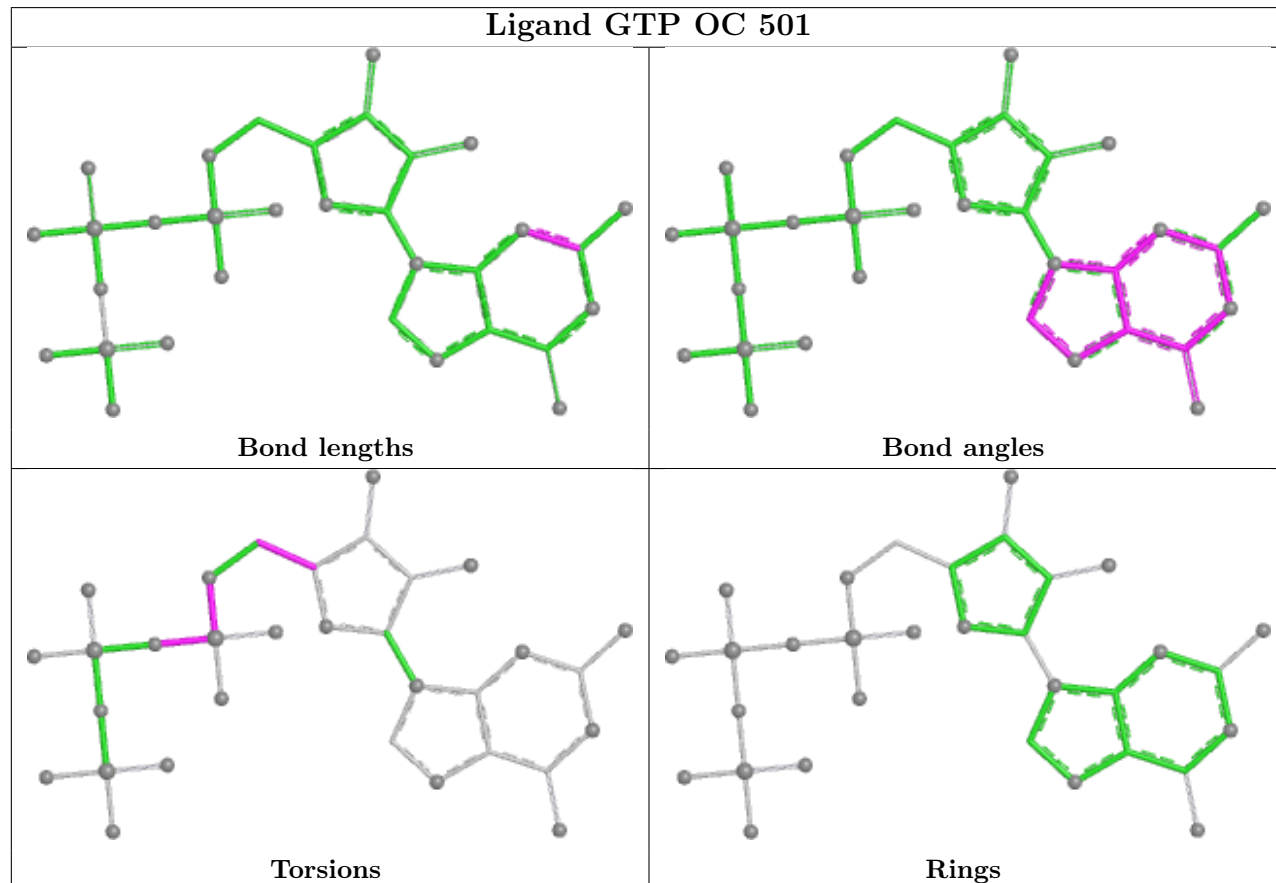
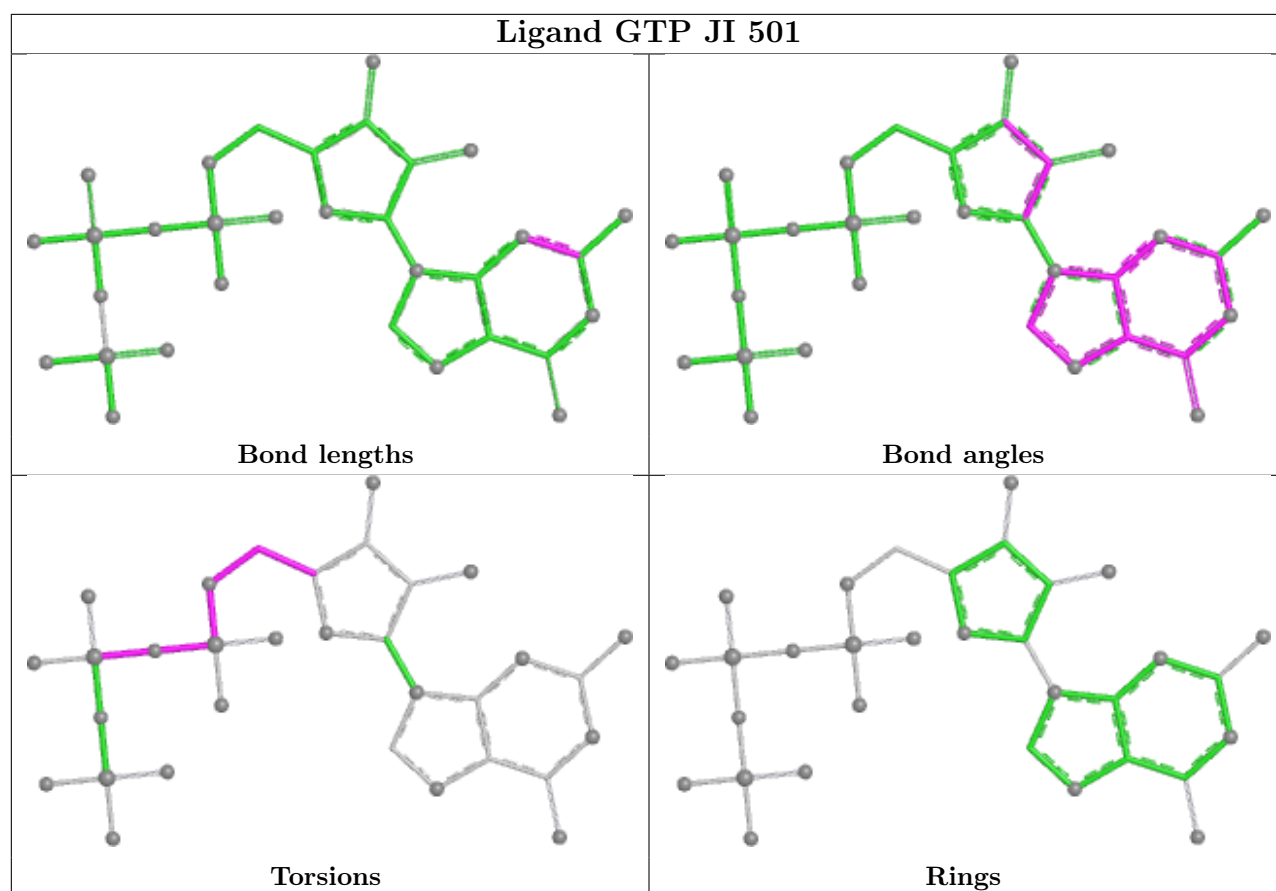


Ligand GTP CM 501

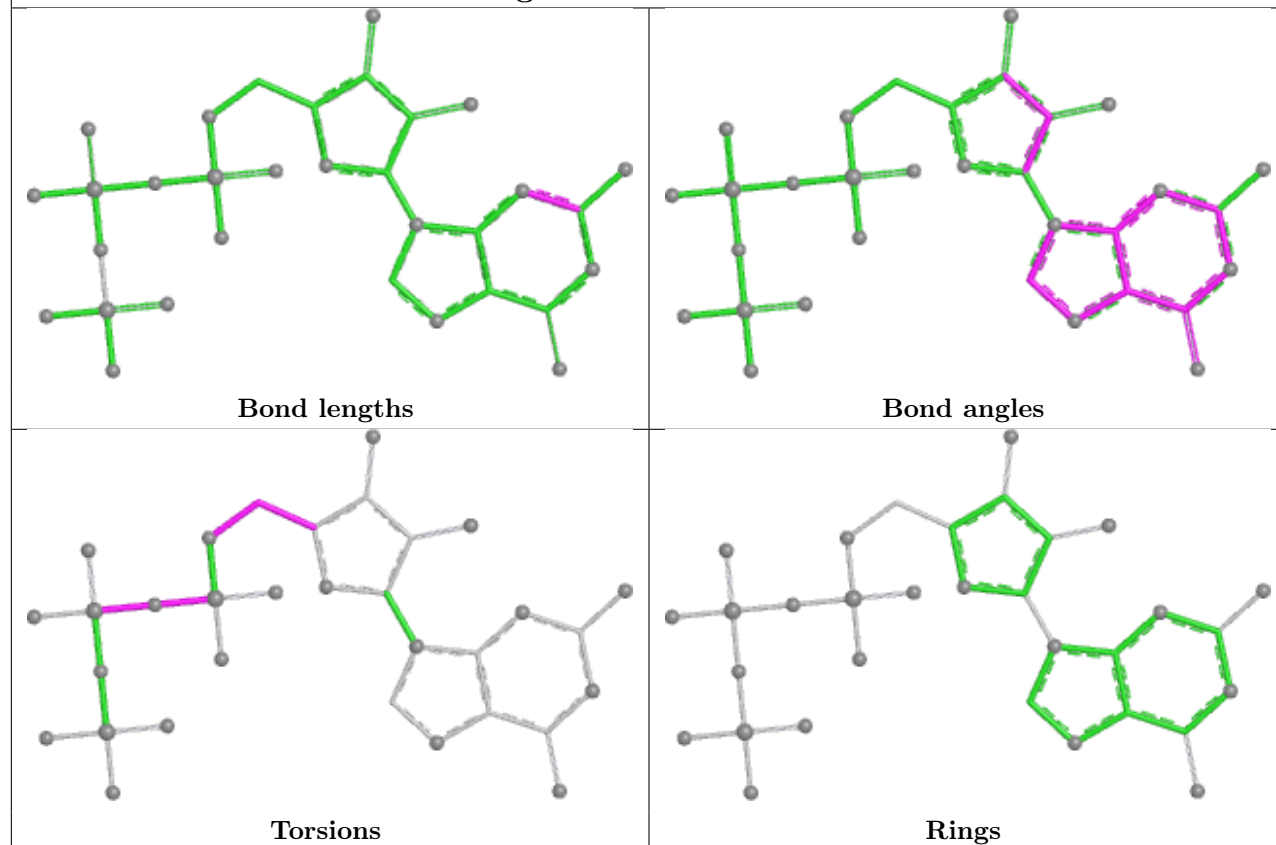


Ligand GTP LB 501

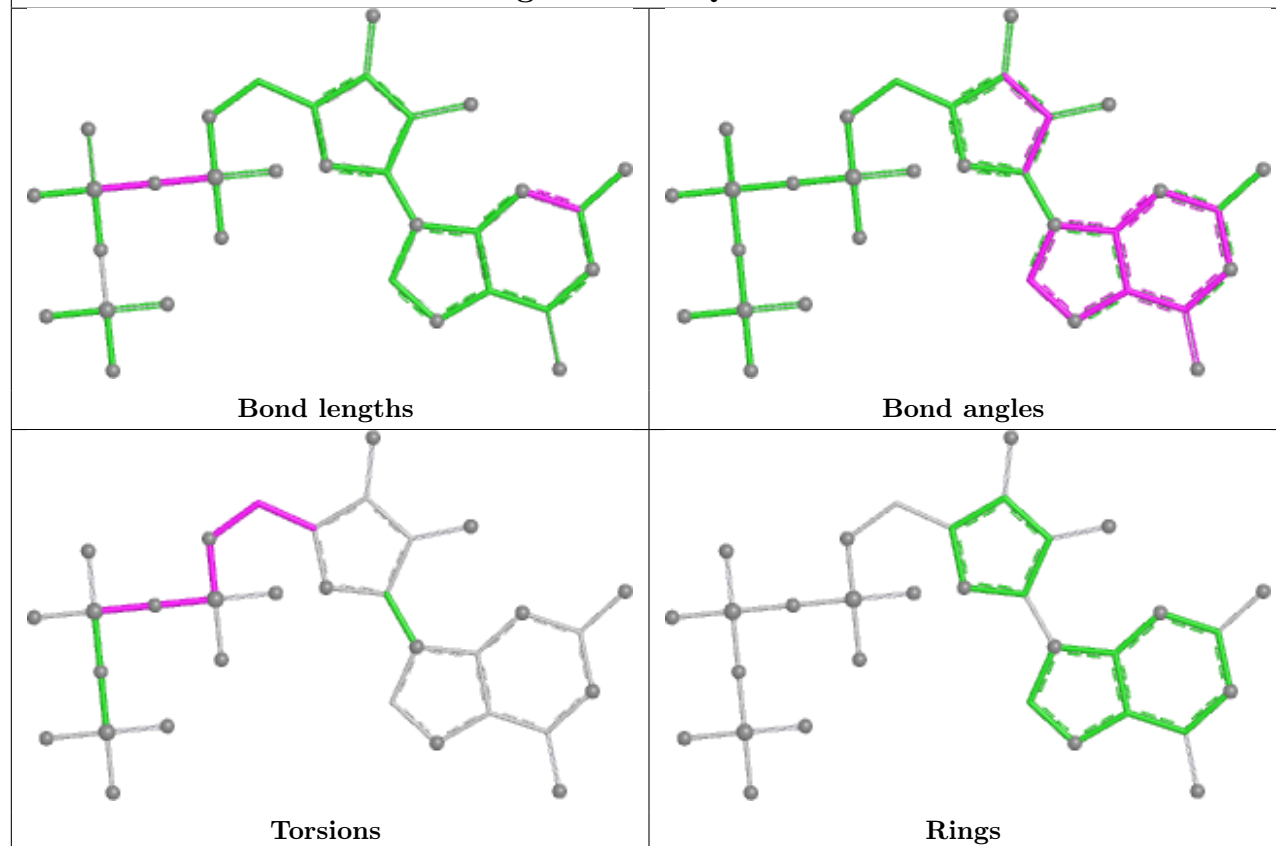


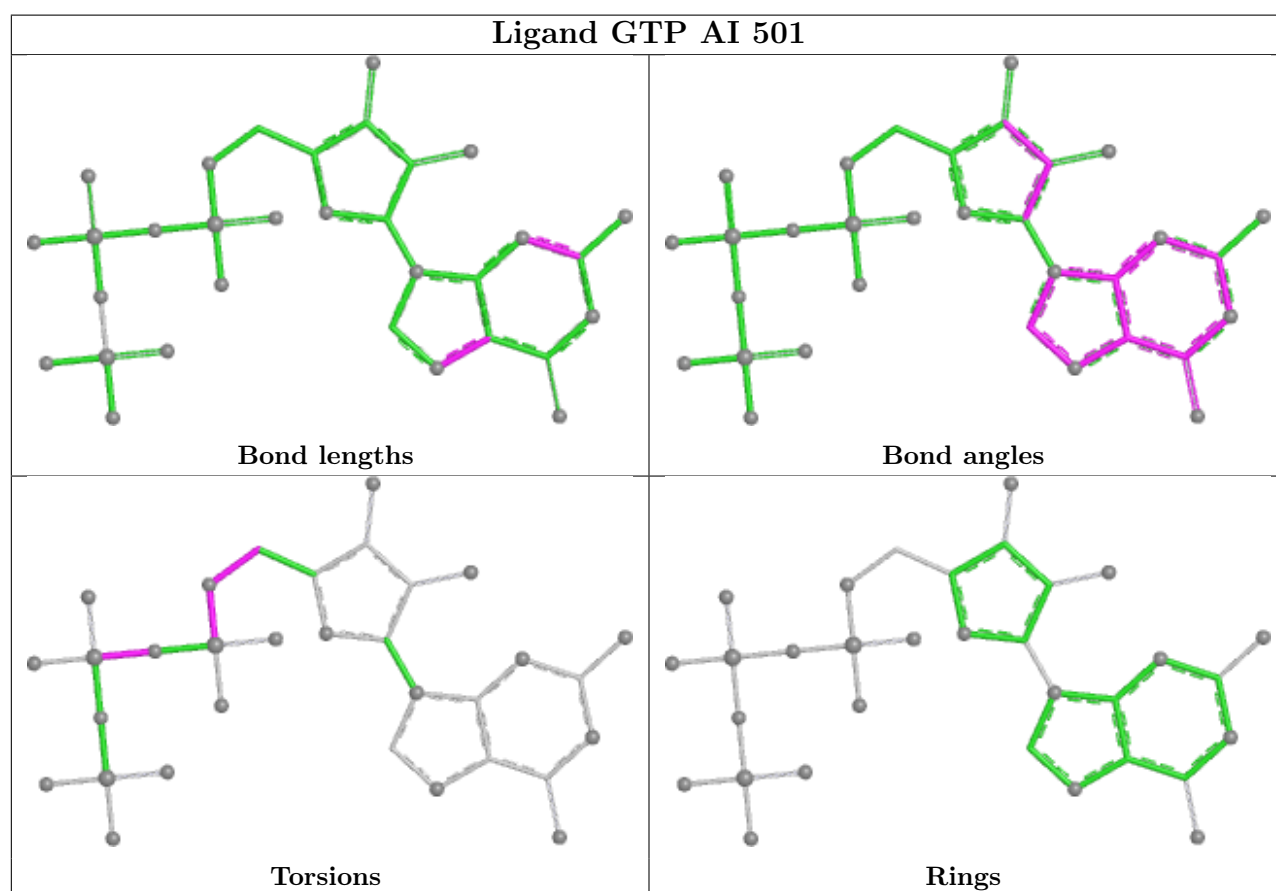
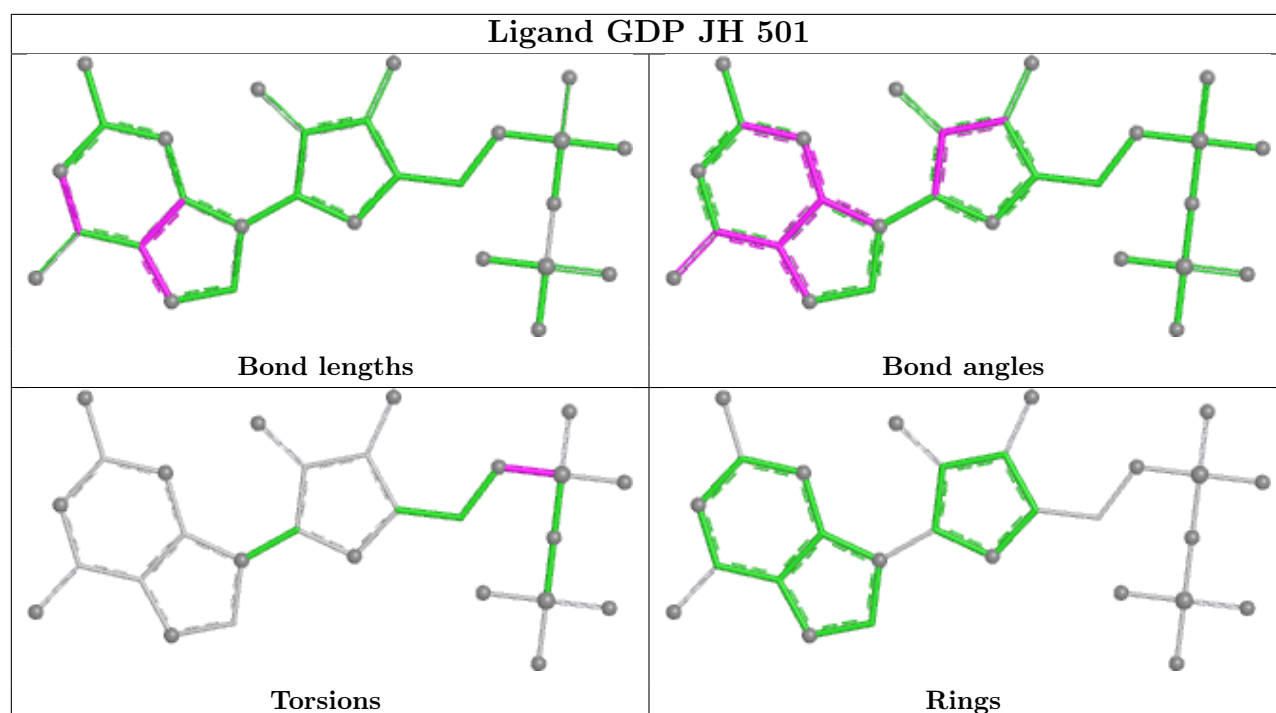


Ligand GTP UK 501

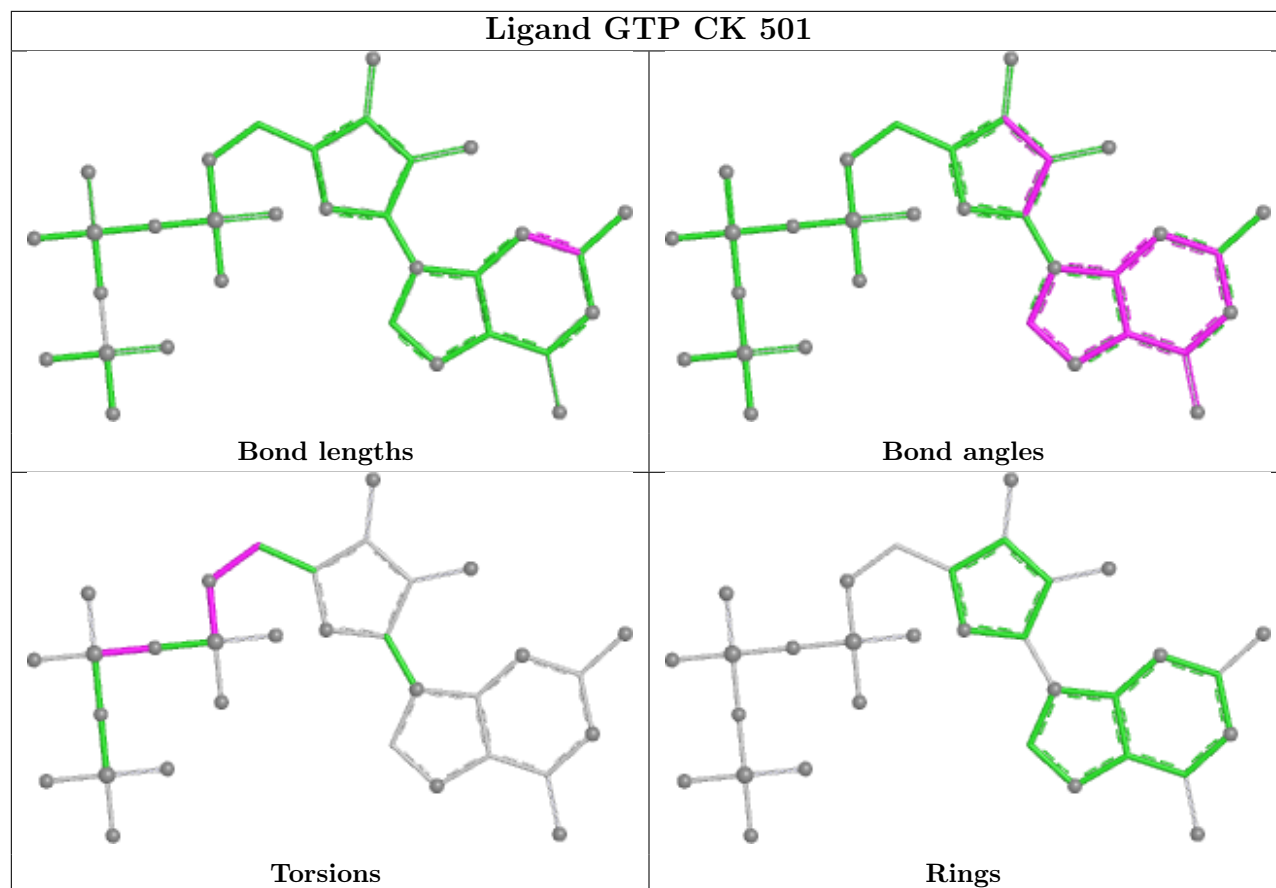


Ligand GTP QA 501

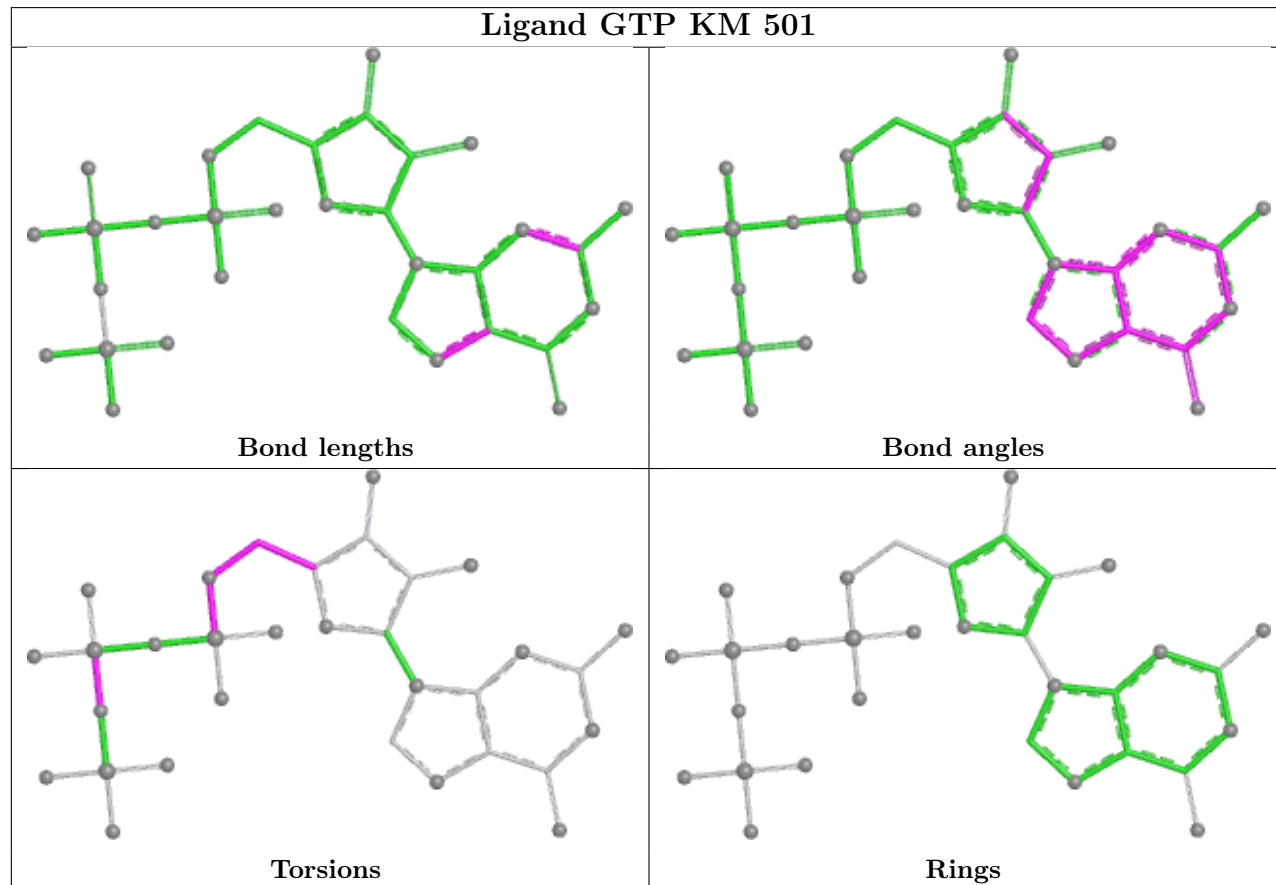




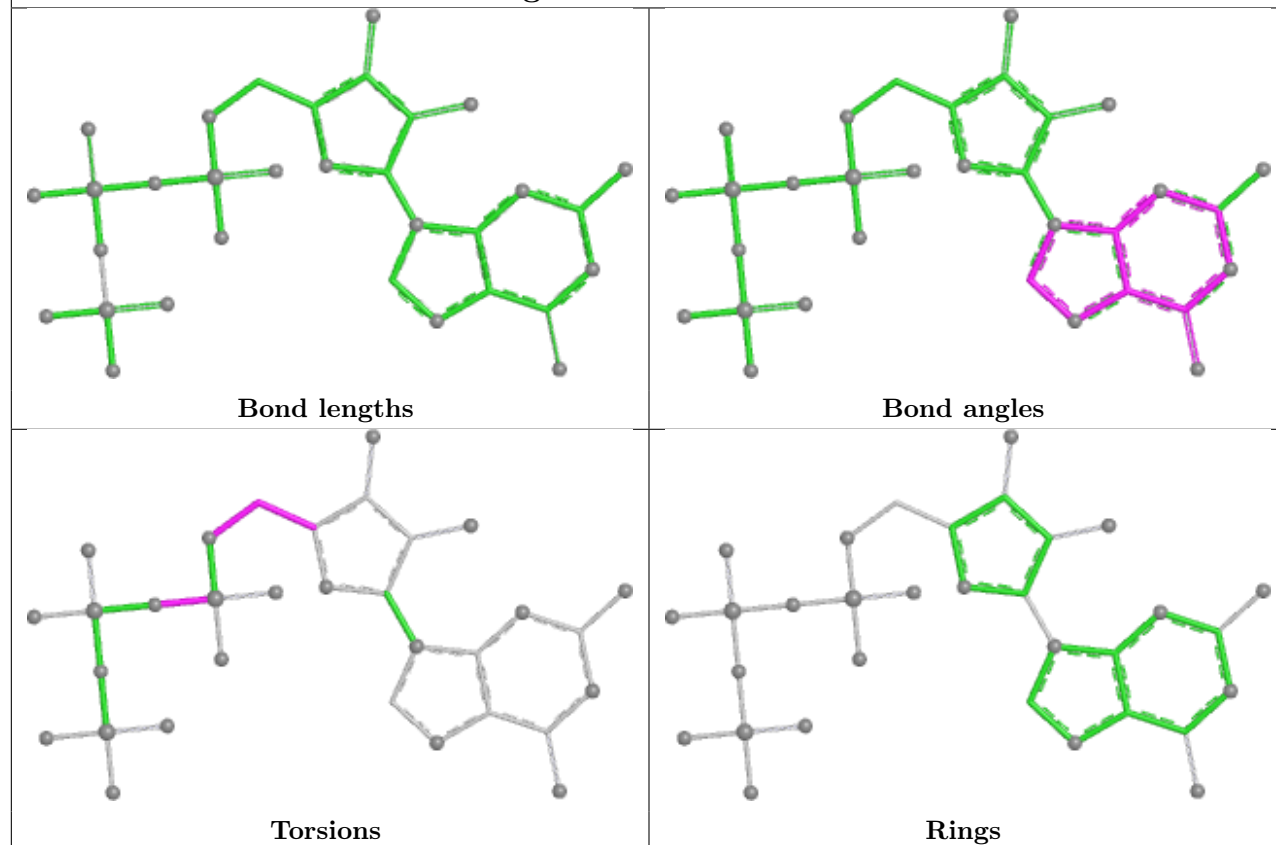
Ligand GTP CK 501



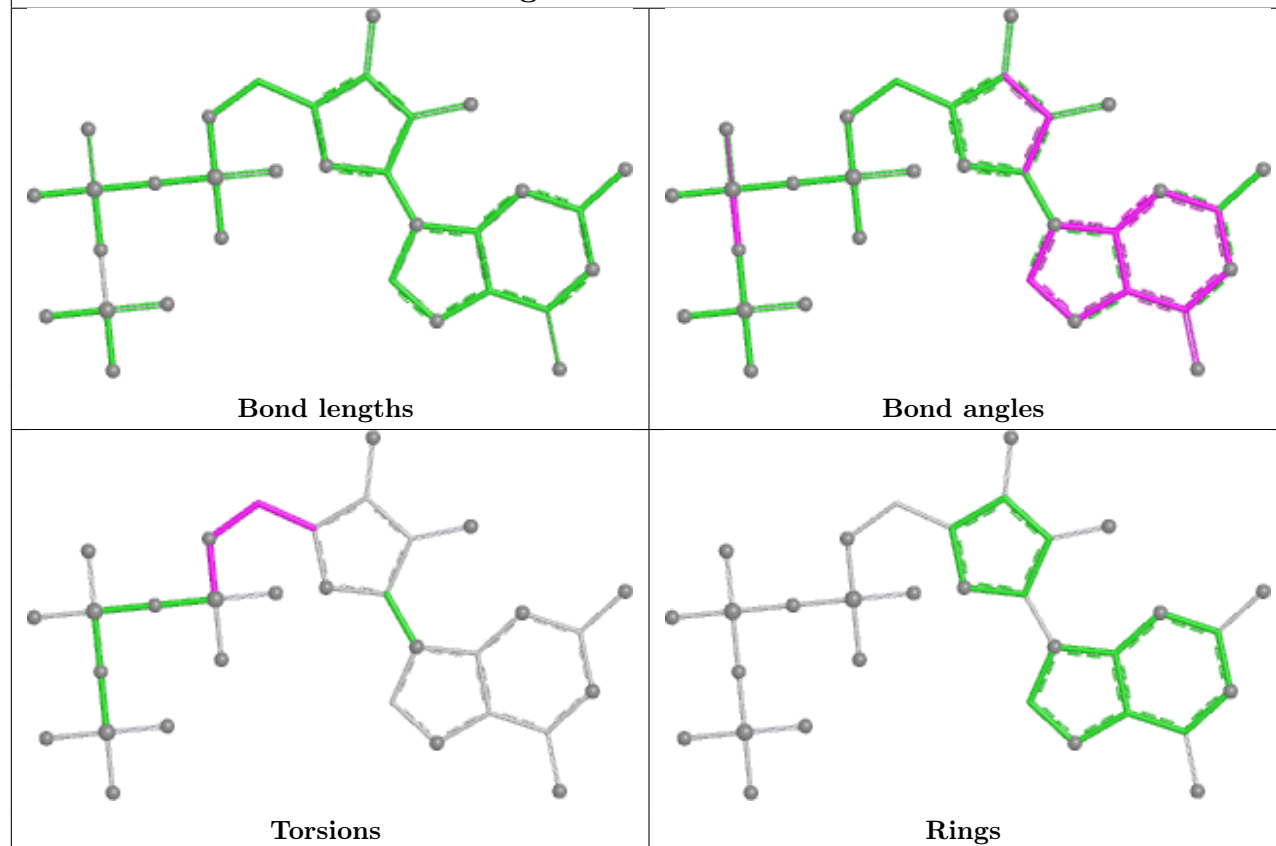
Ligand GTP KM 501

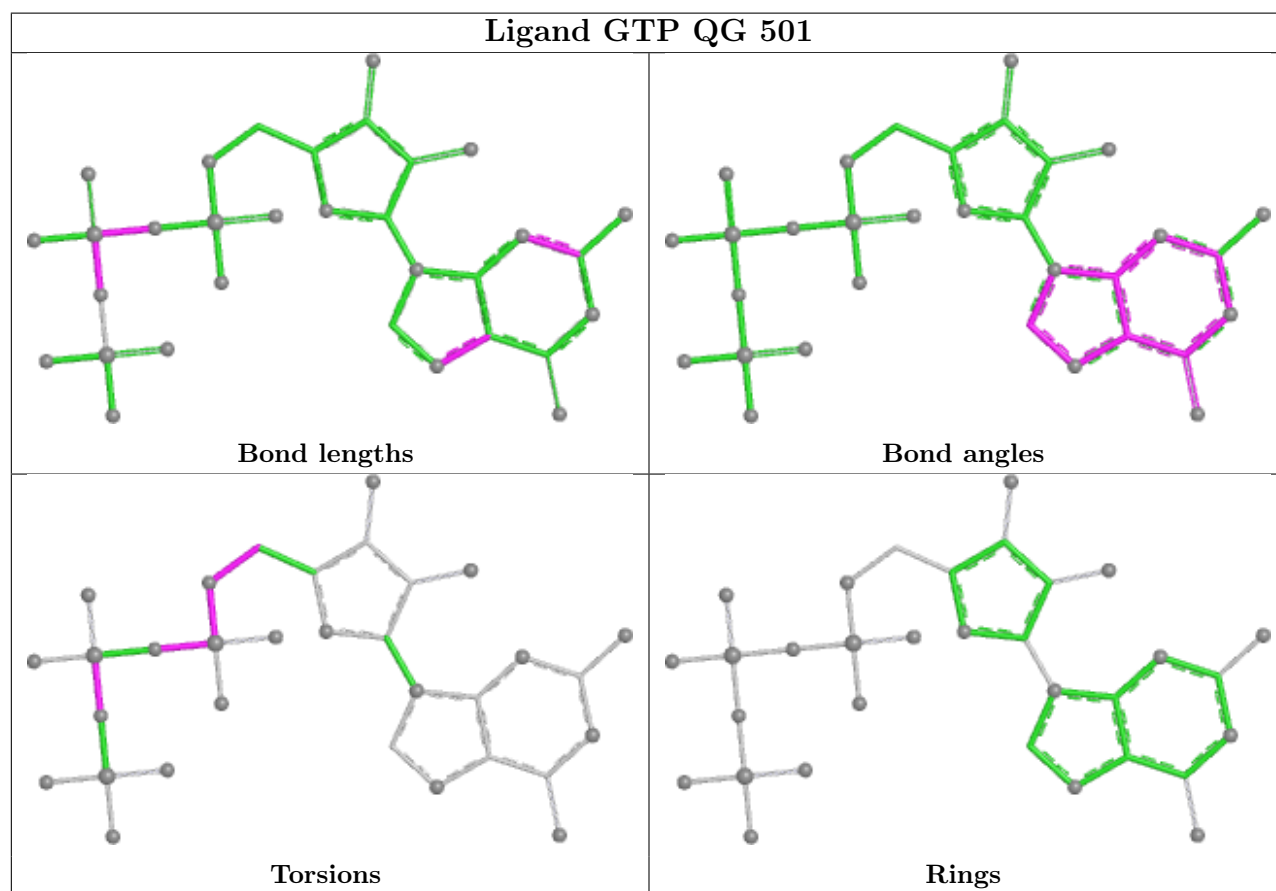
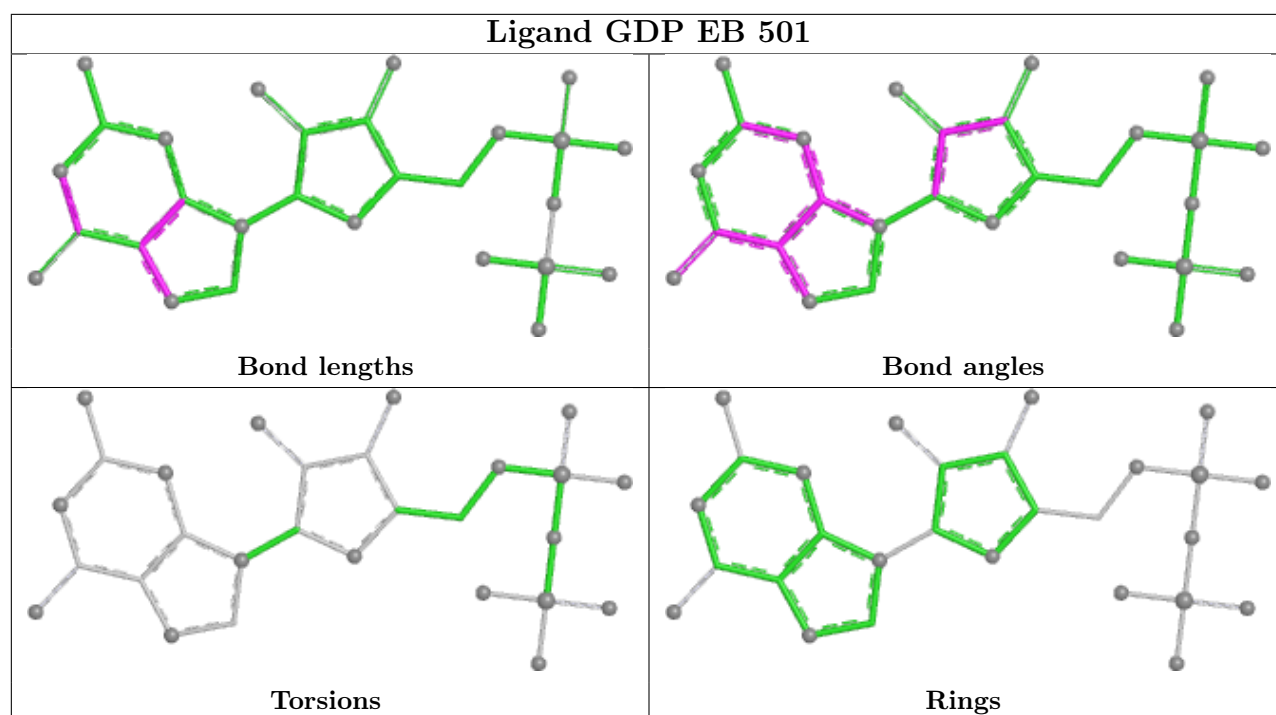


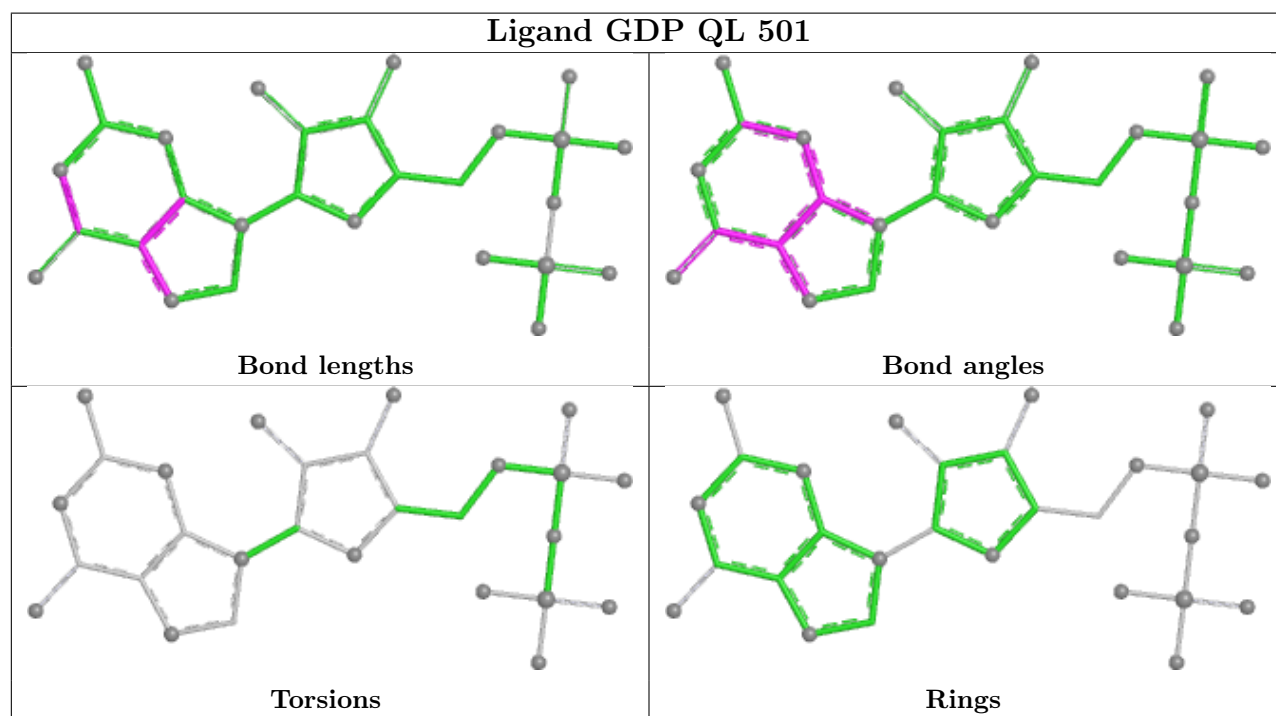
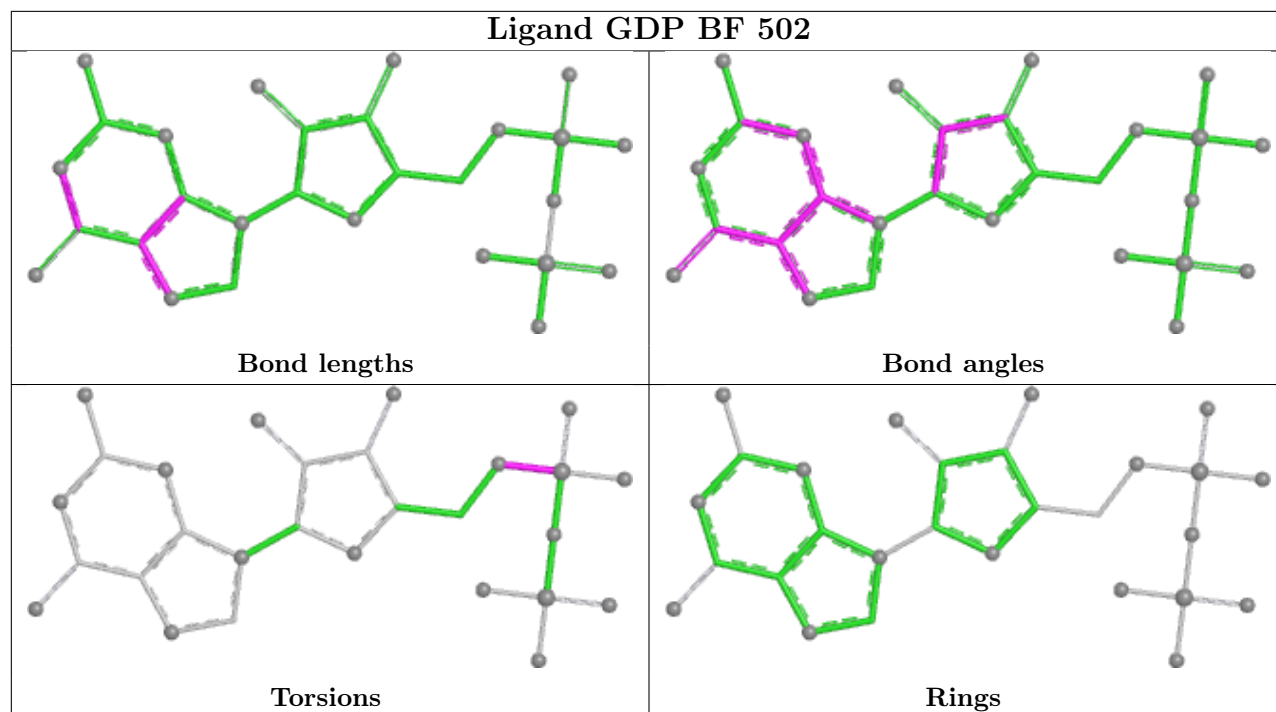
Ligand GTP NI 501

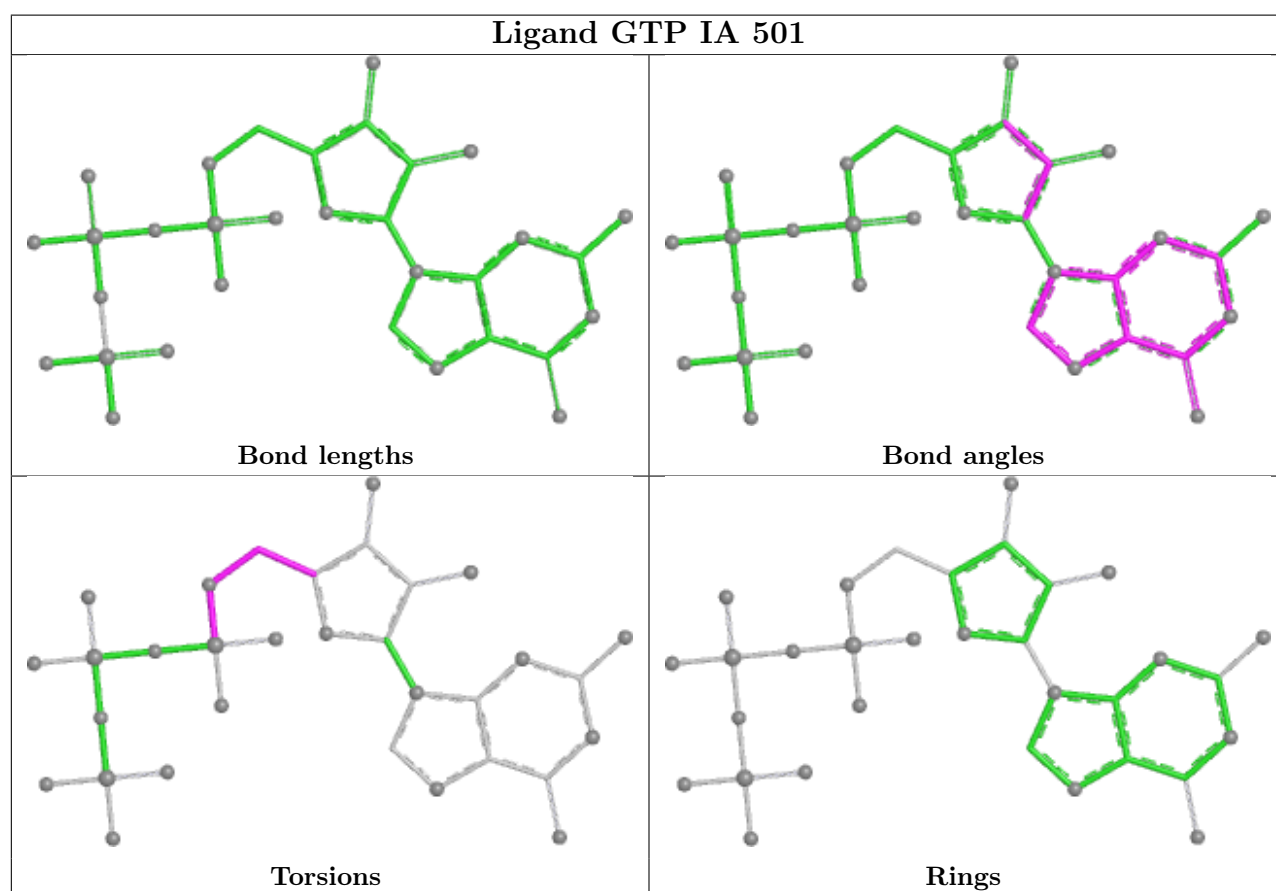
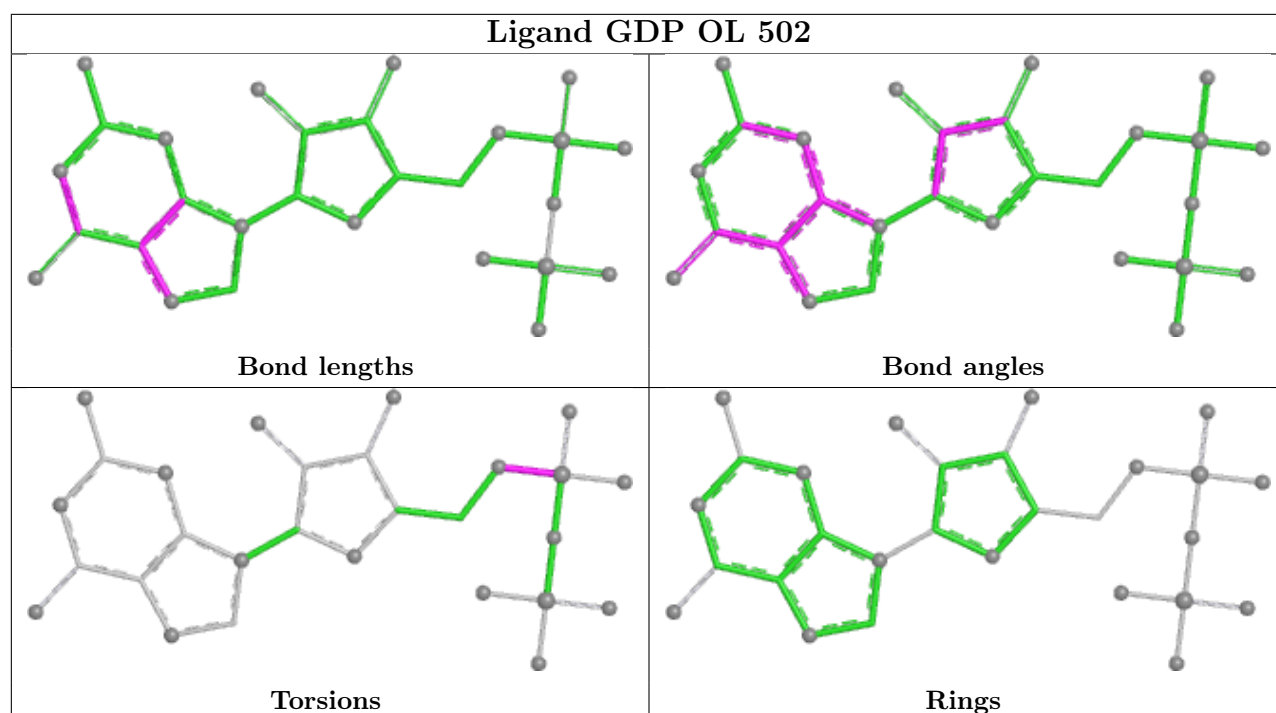


Ligand GTP SG 501

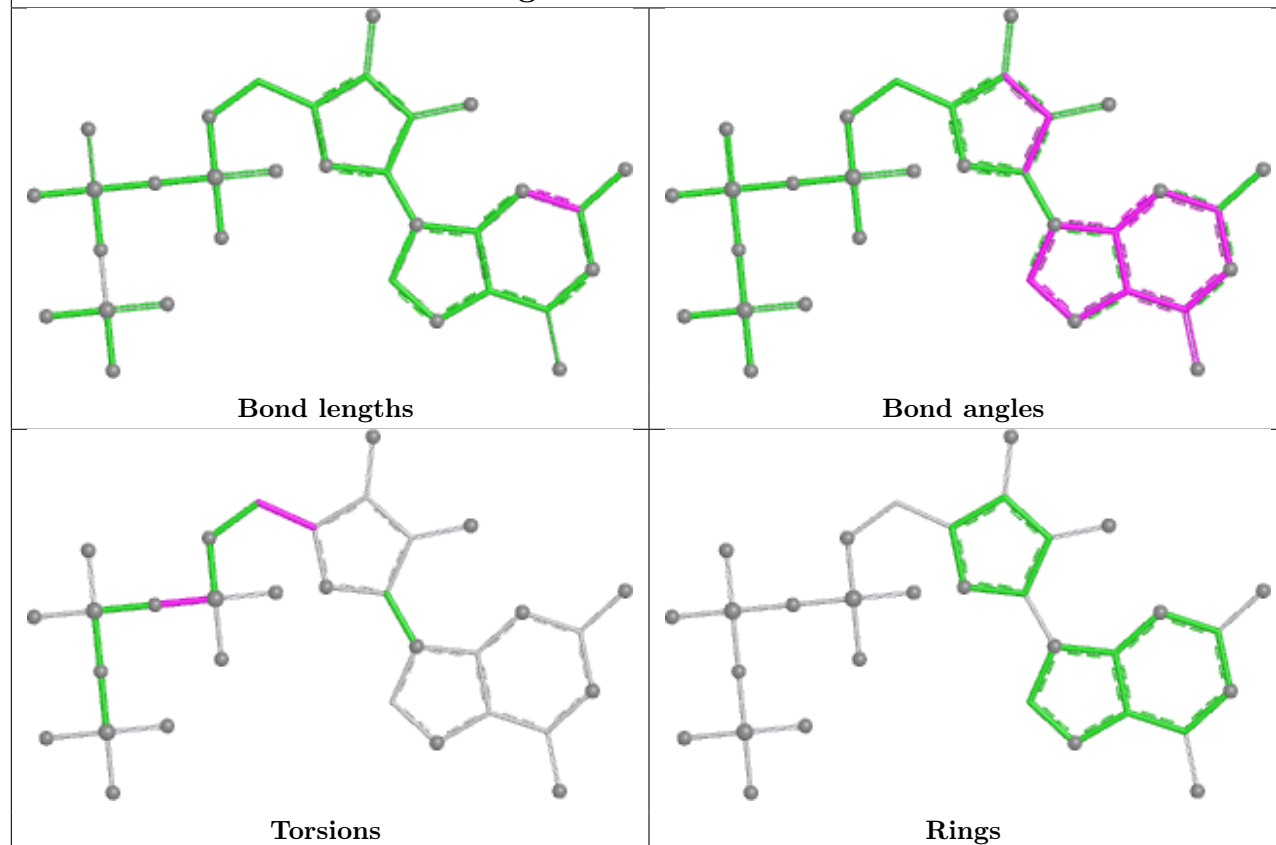




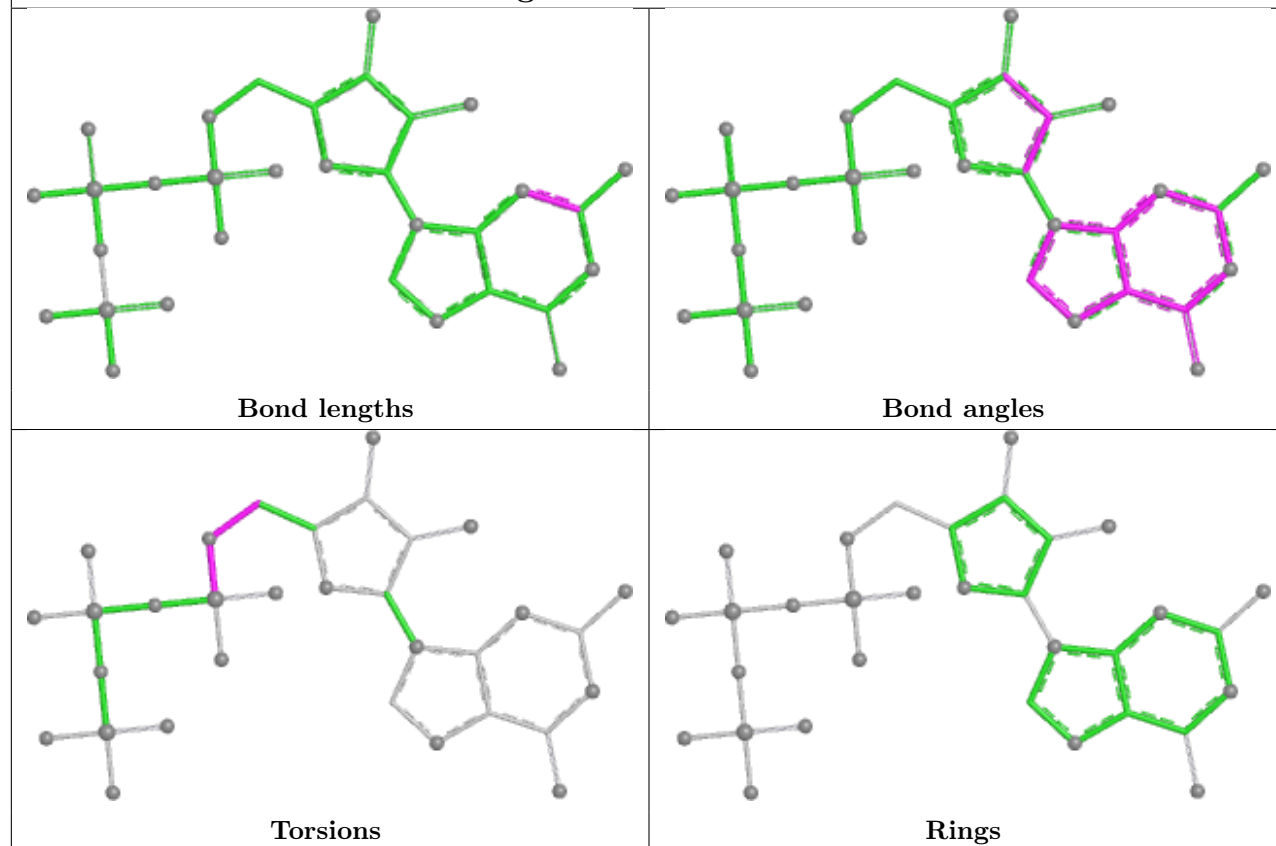




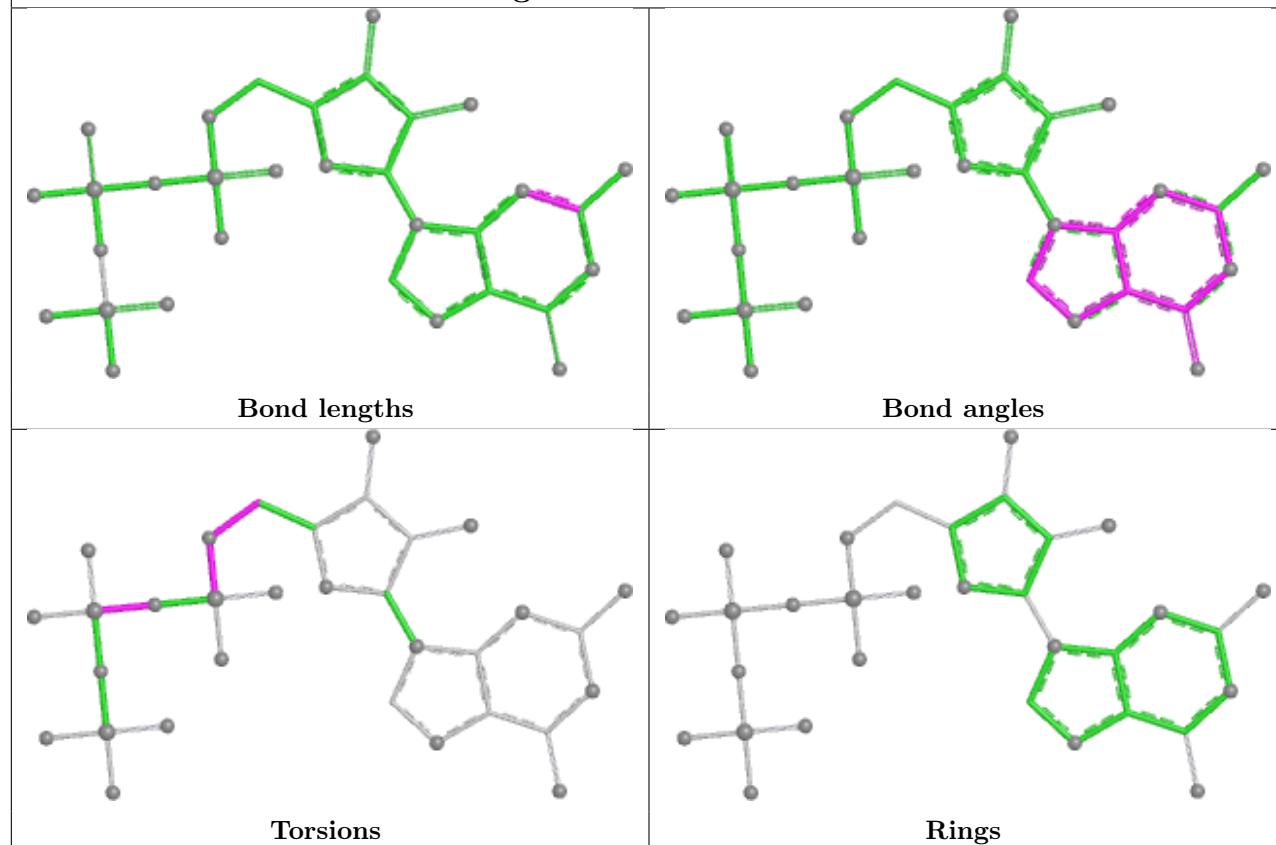
Ligand GTP OE 501



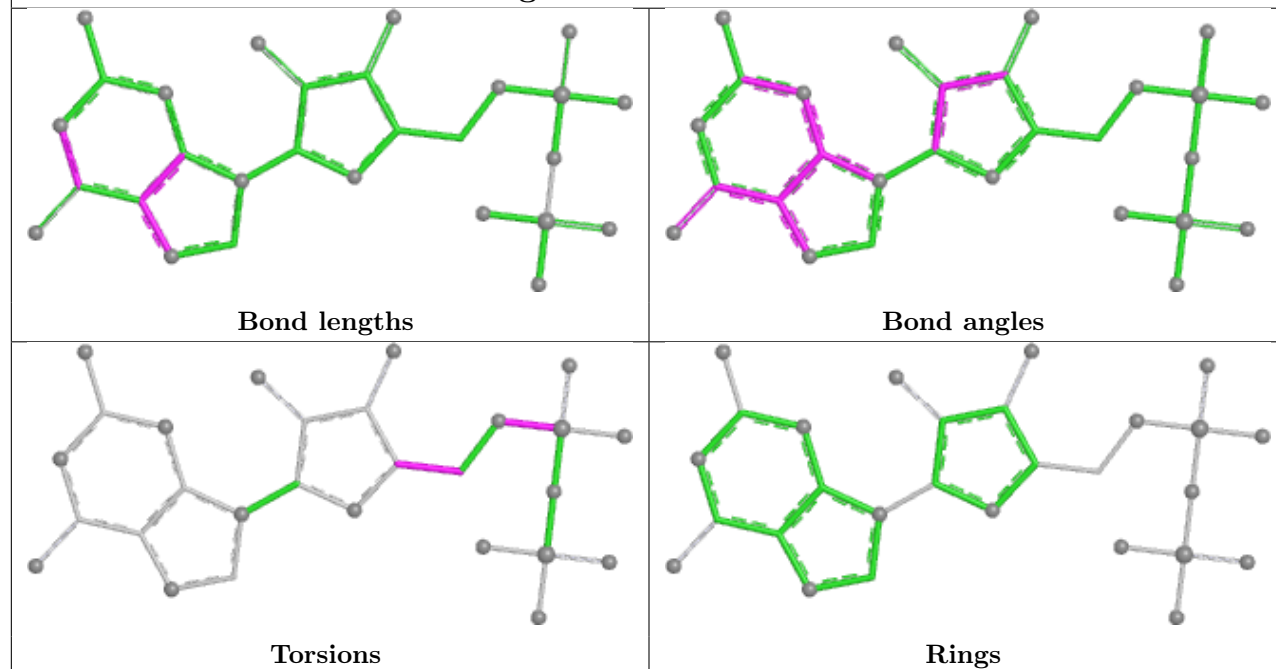
Ligand GTP CA 501

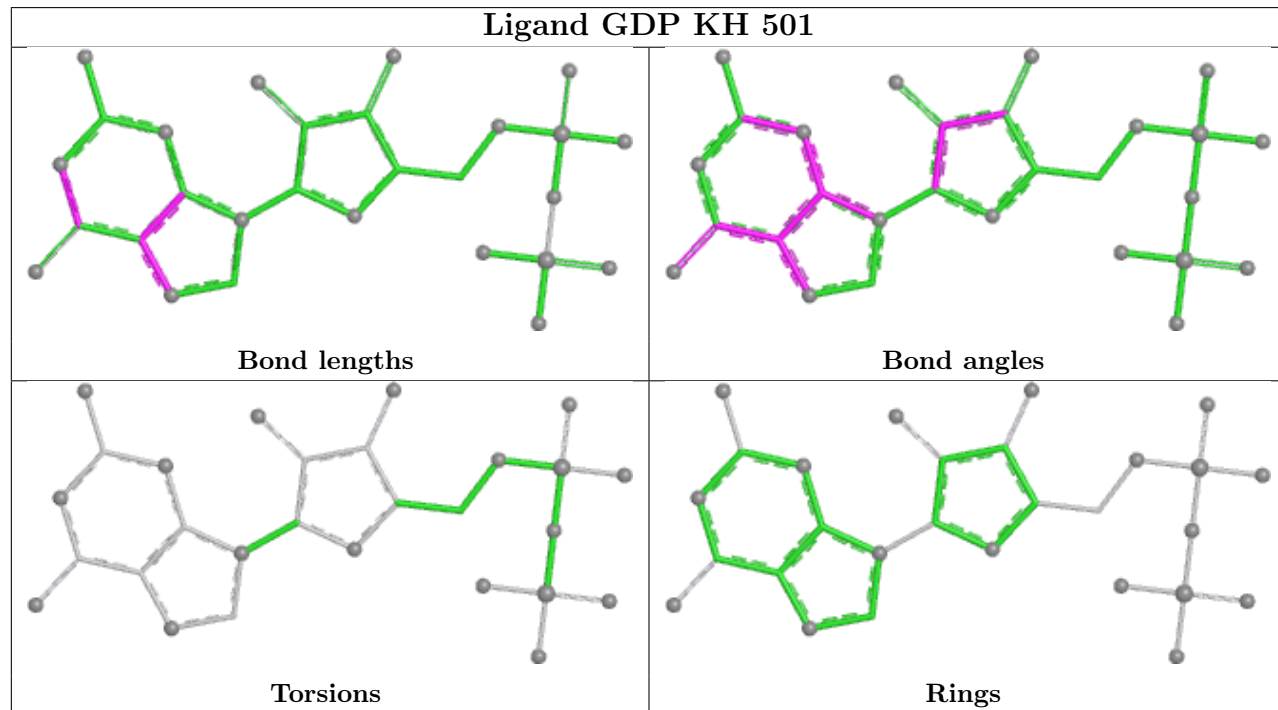
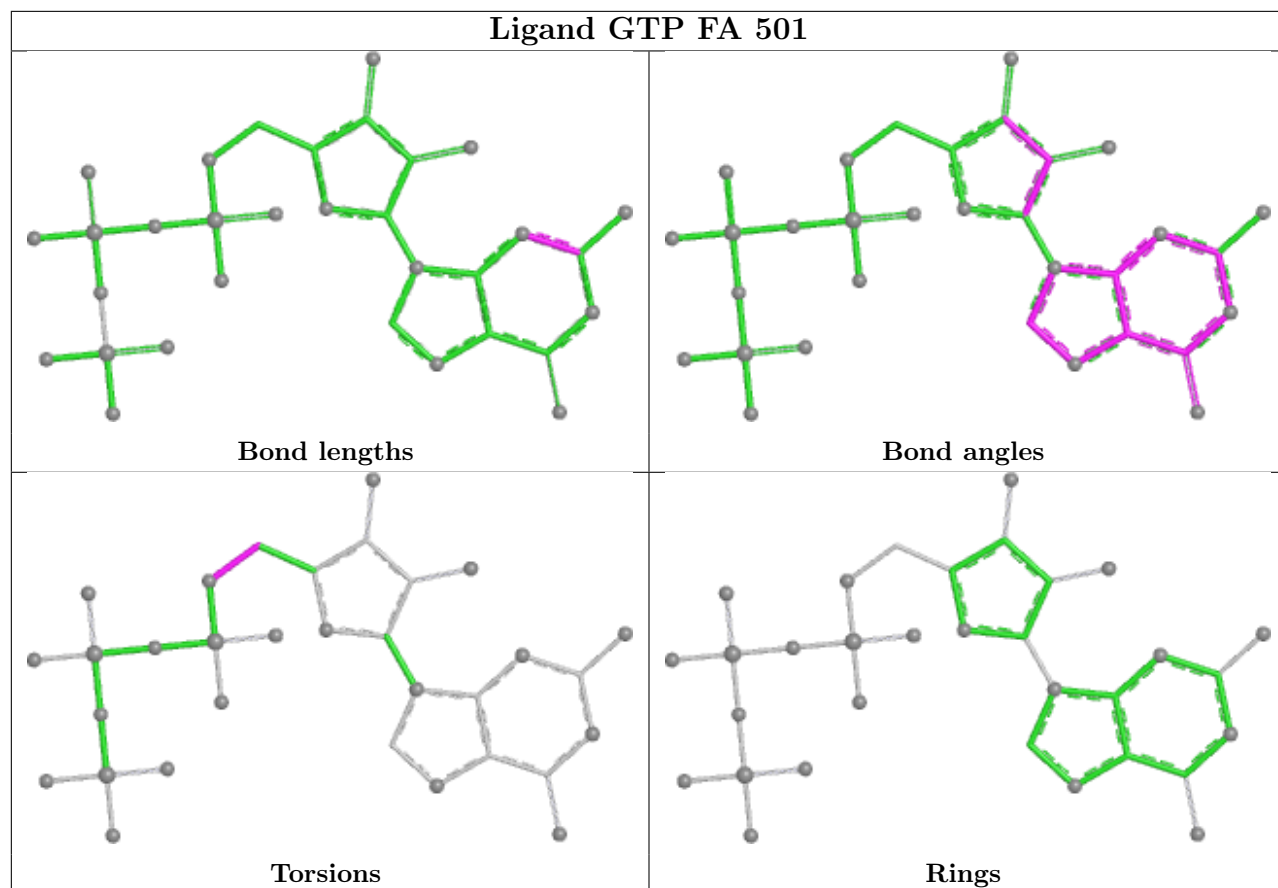


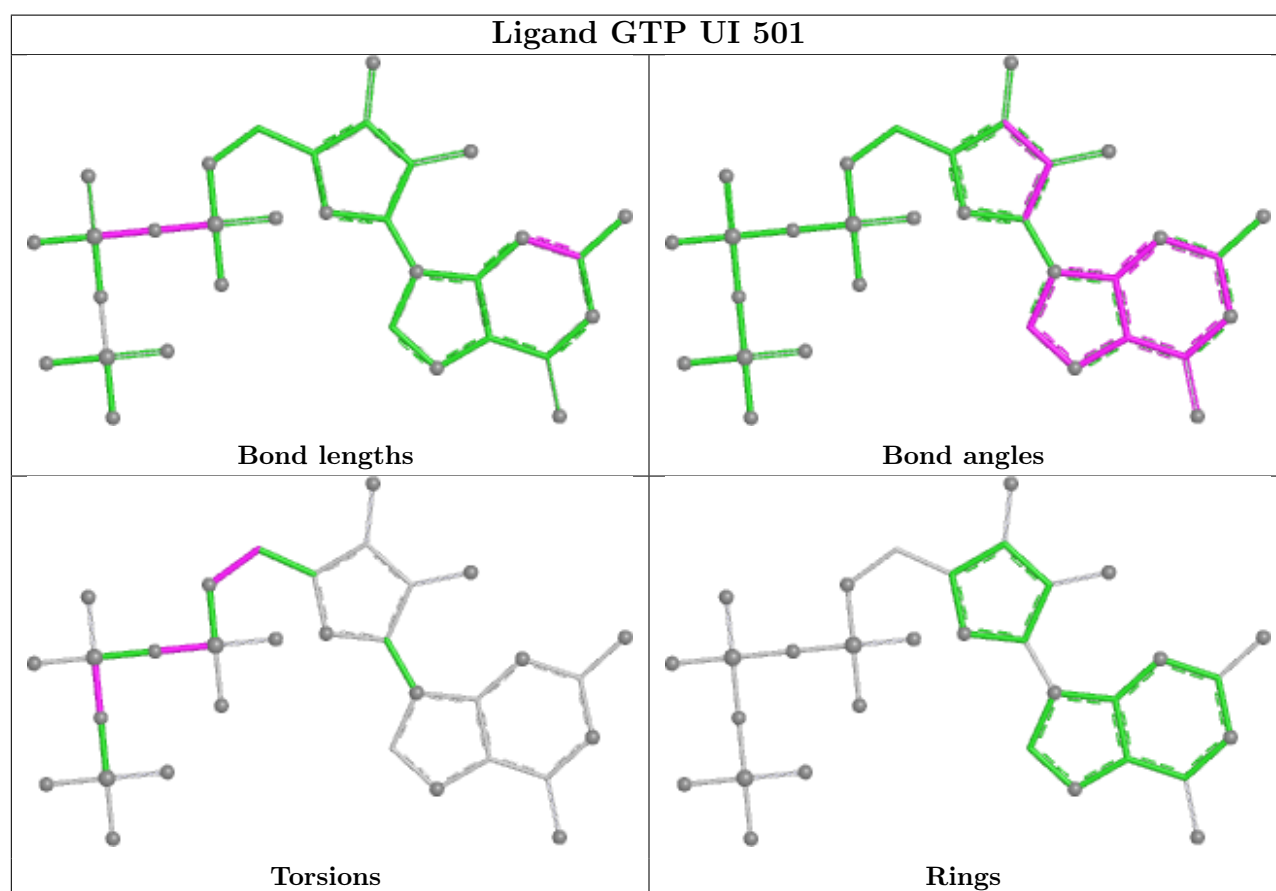
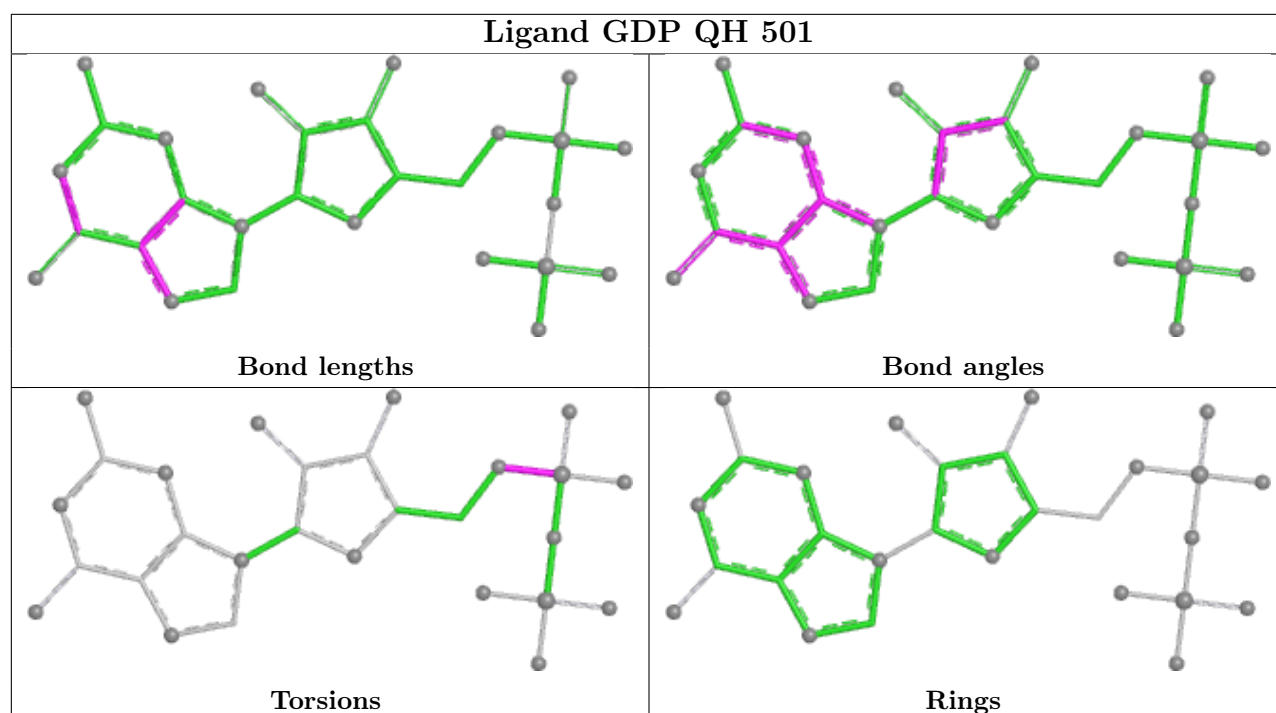
Ligand GTP DM 501



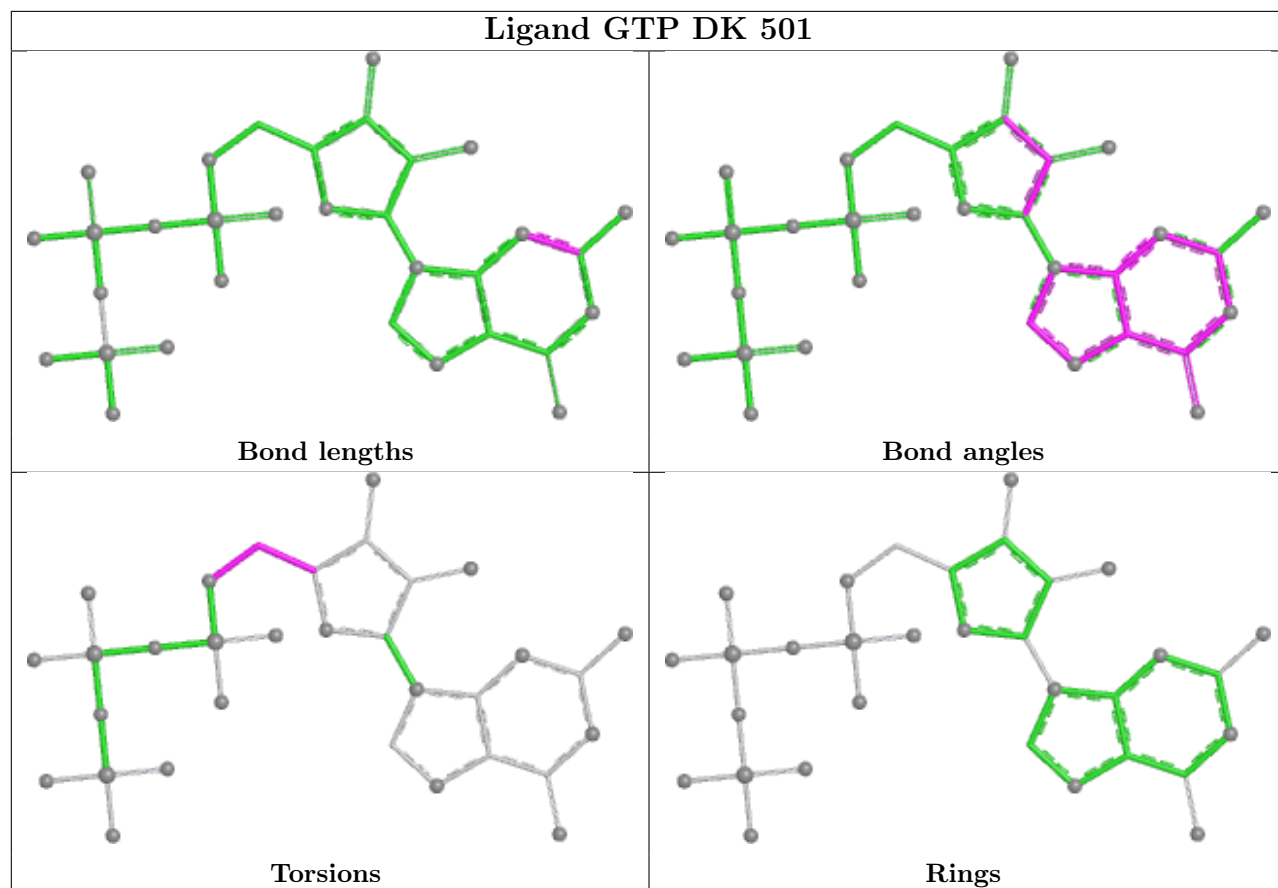
Ligand GDP JN 501



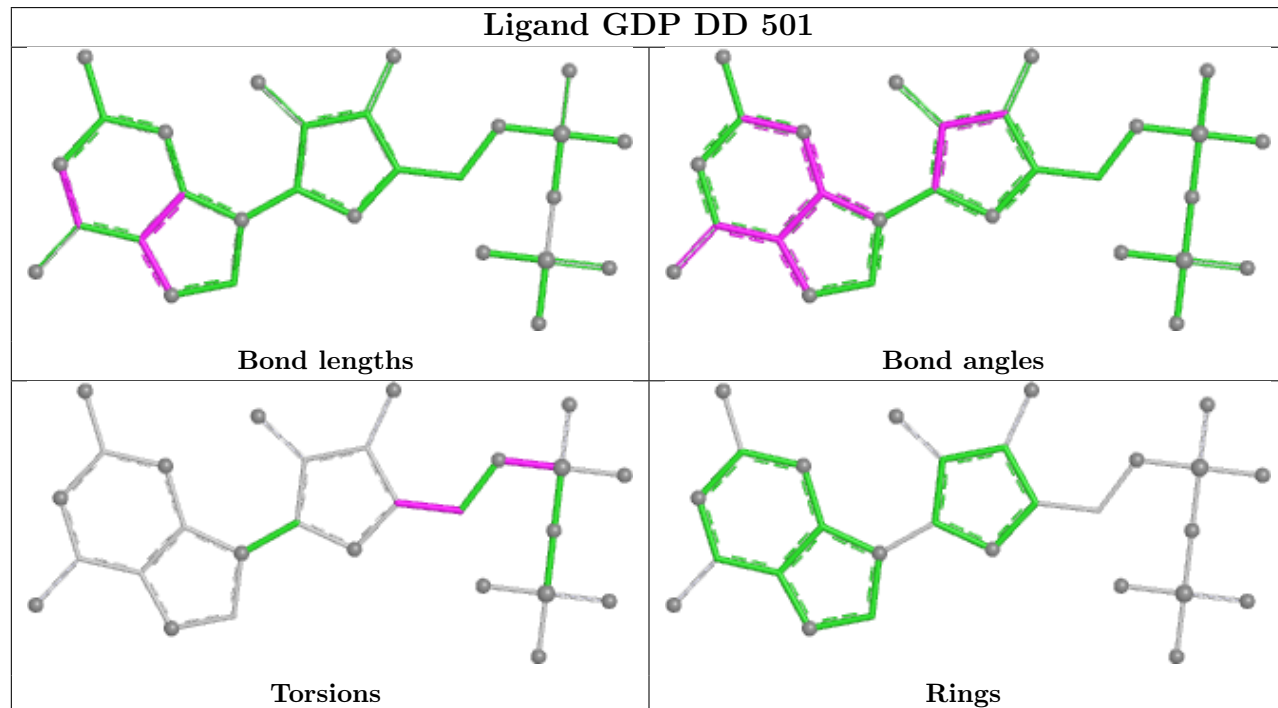




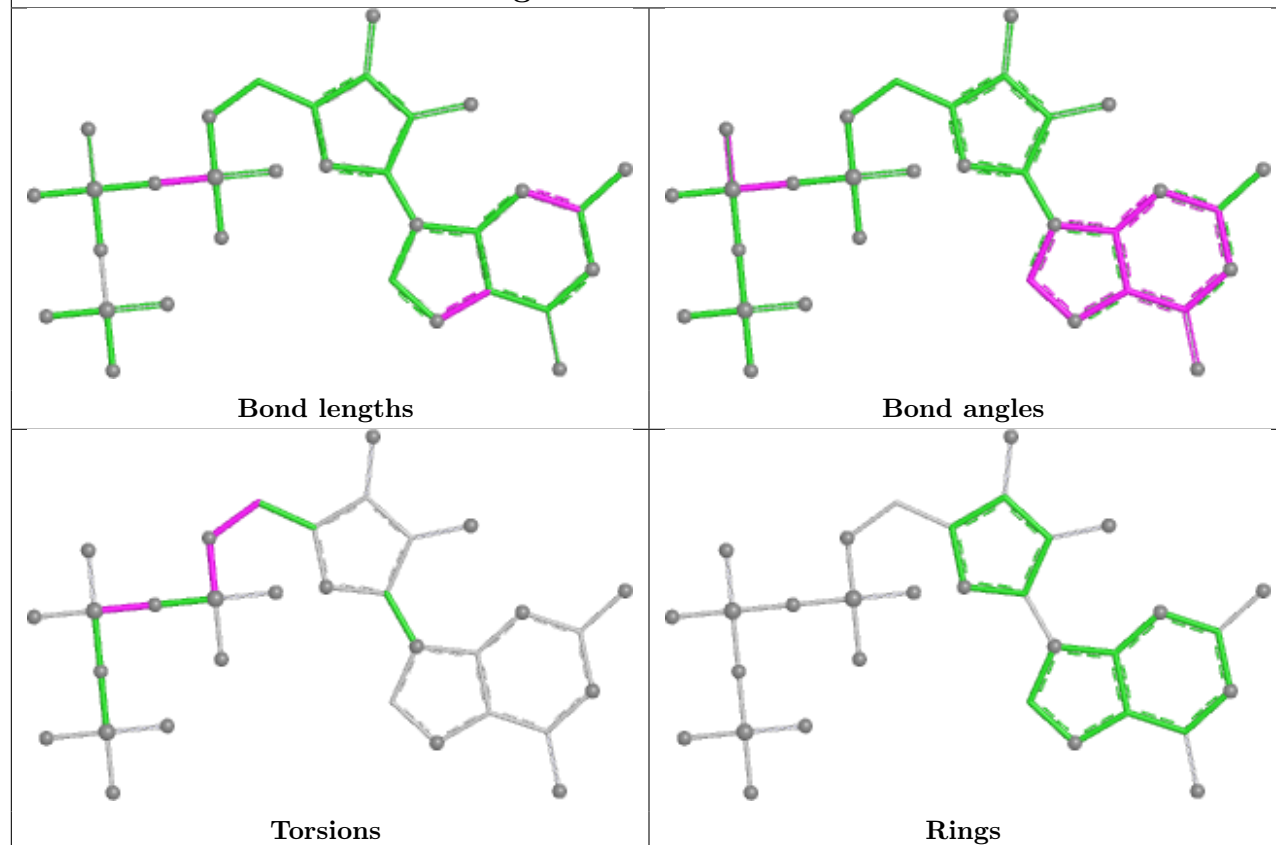
Ligand GTP DK 501



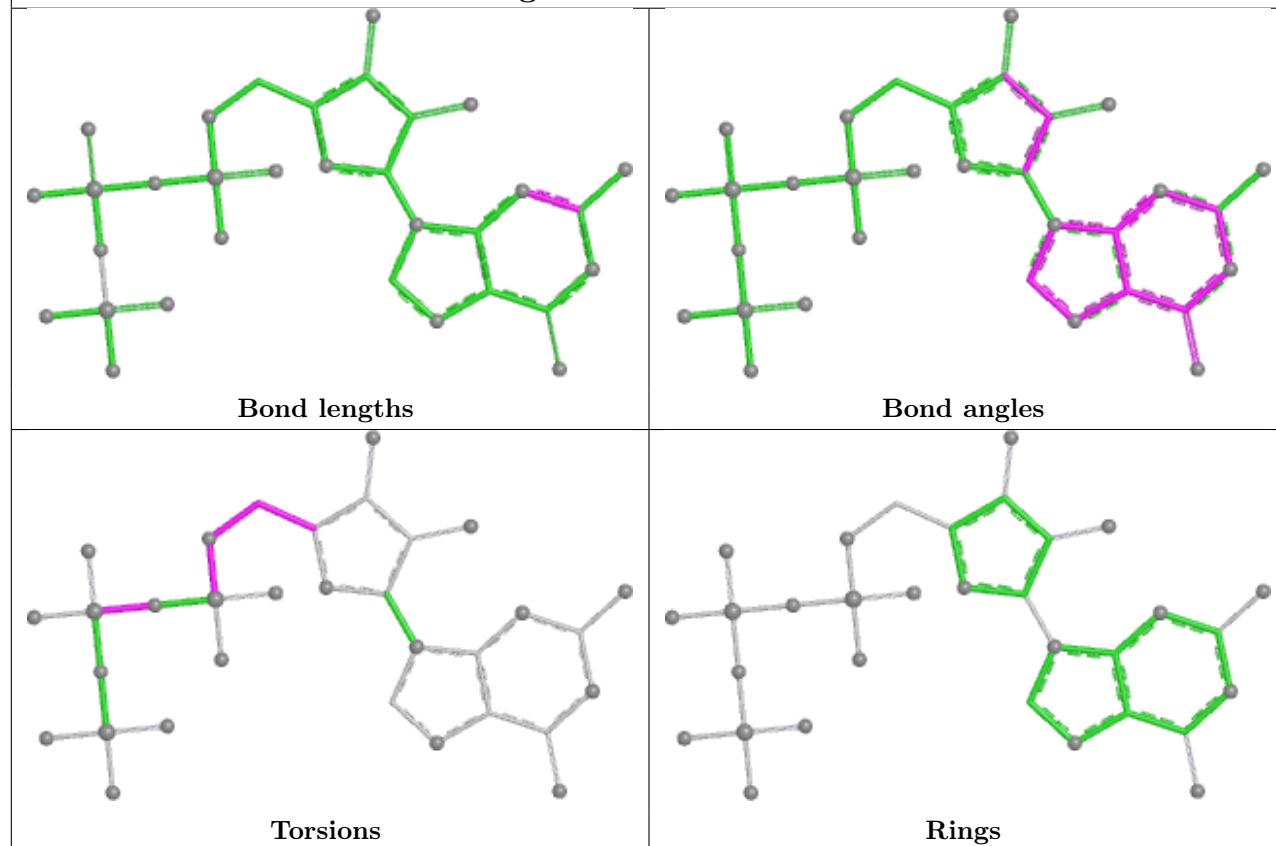
Ligand GDP DD 501

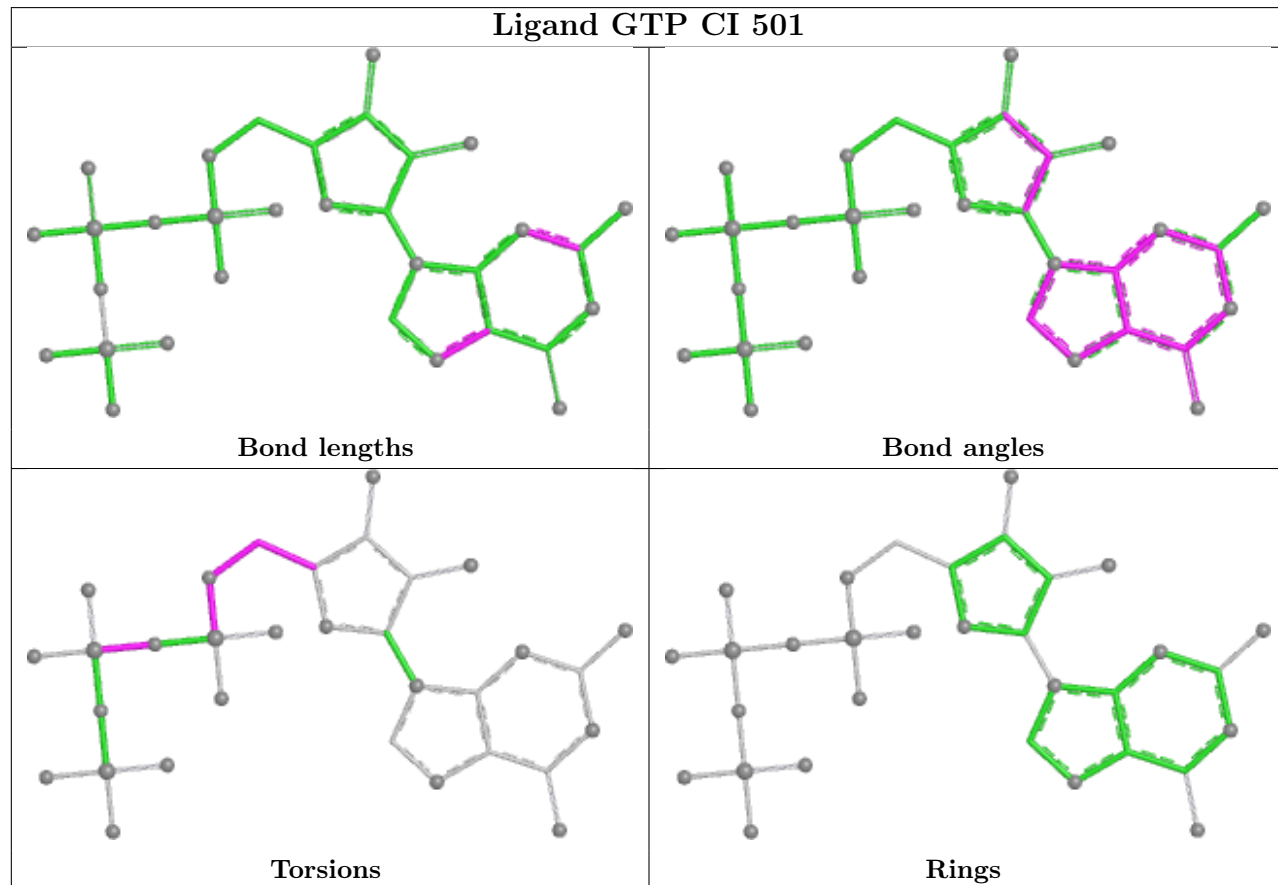
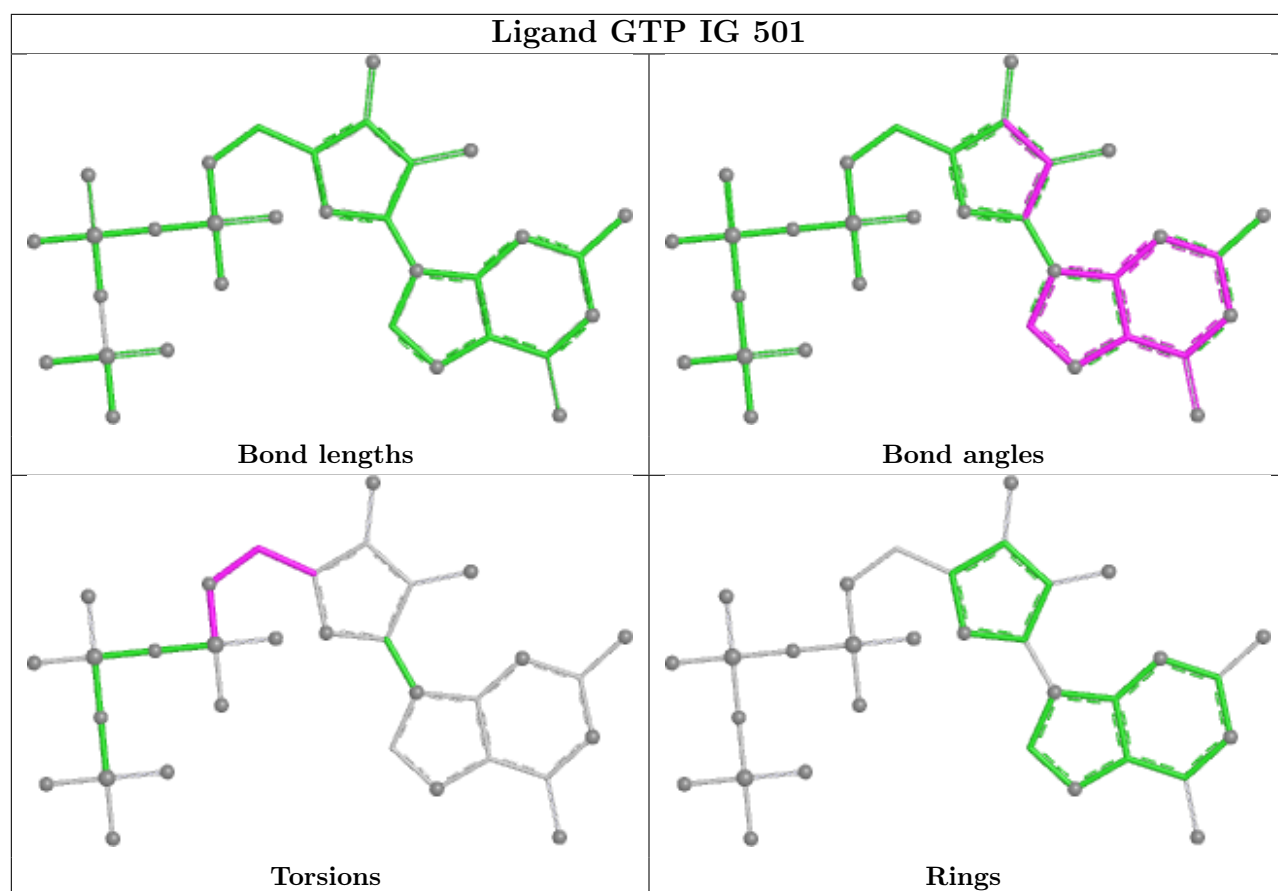


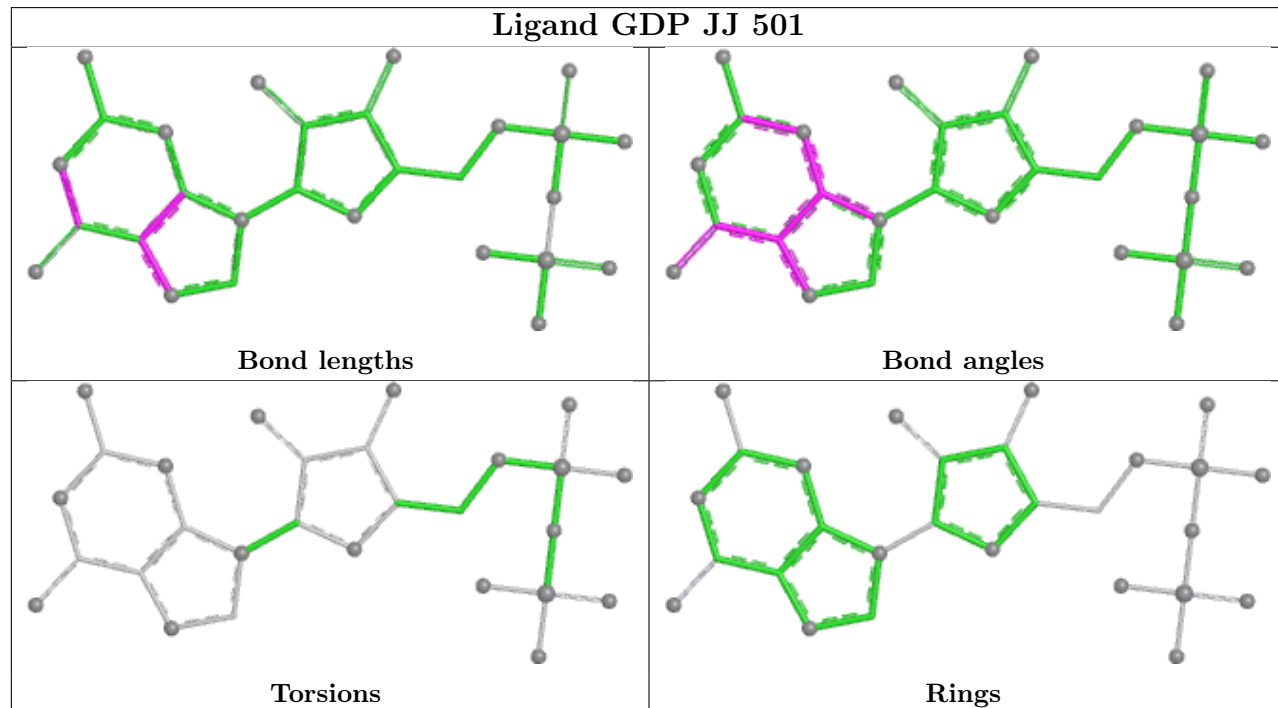
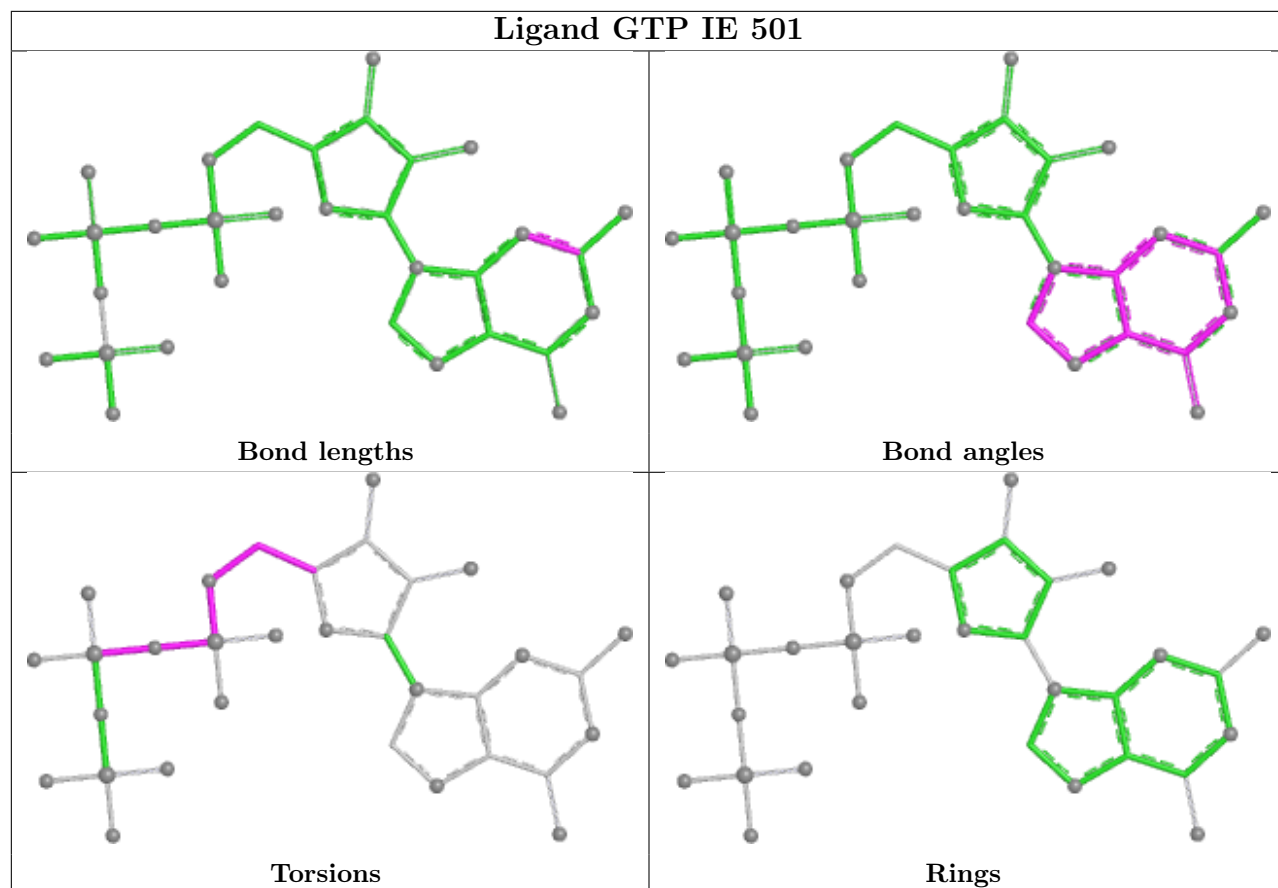
Ligand GTP RM 501



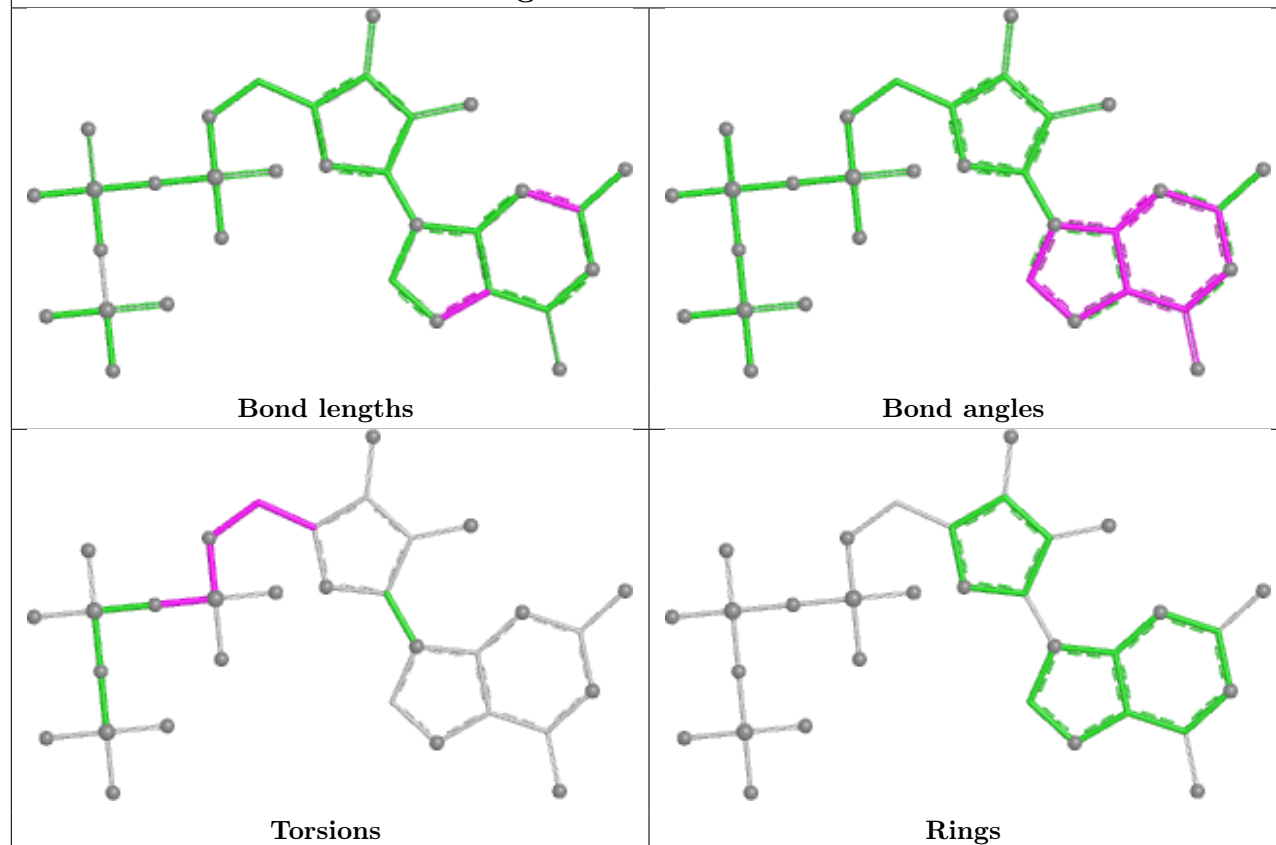
Ligand GTP BE 501



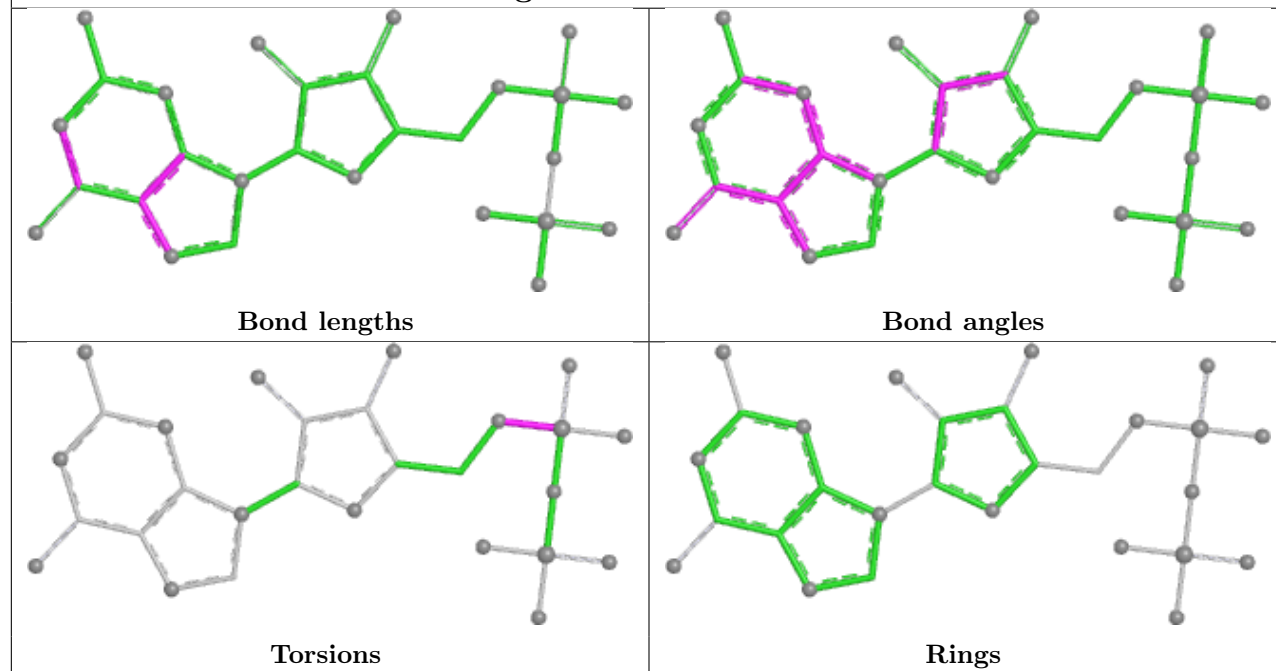


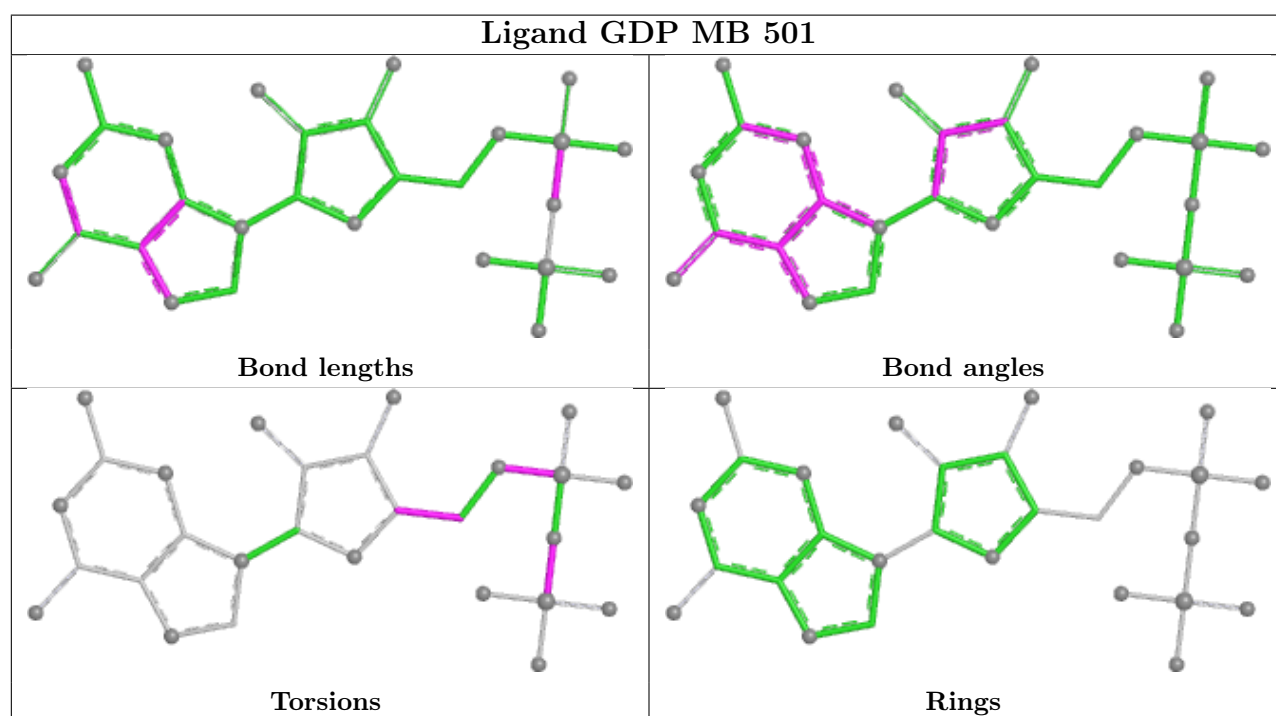
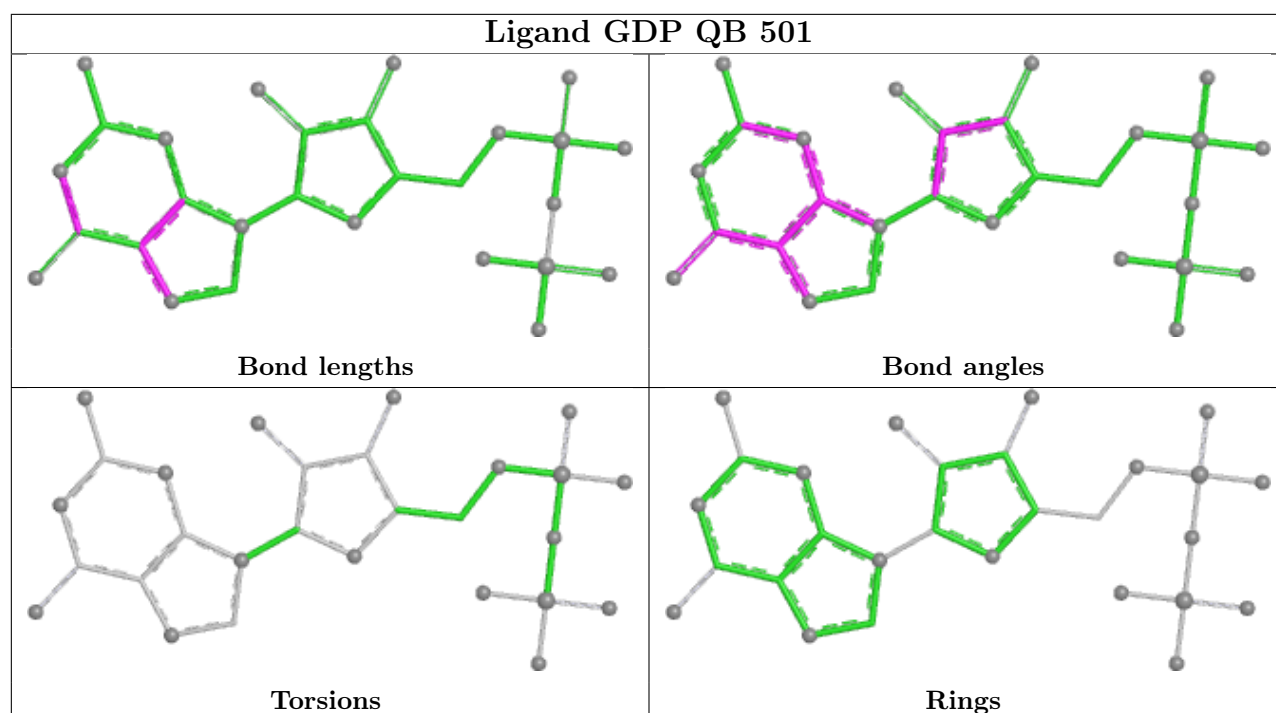


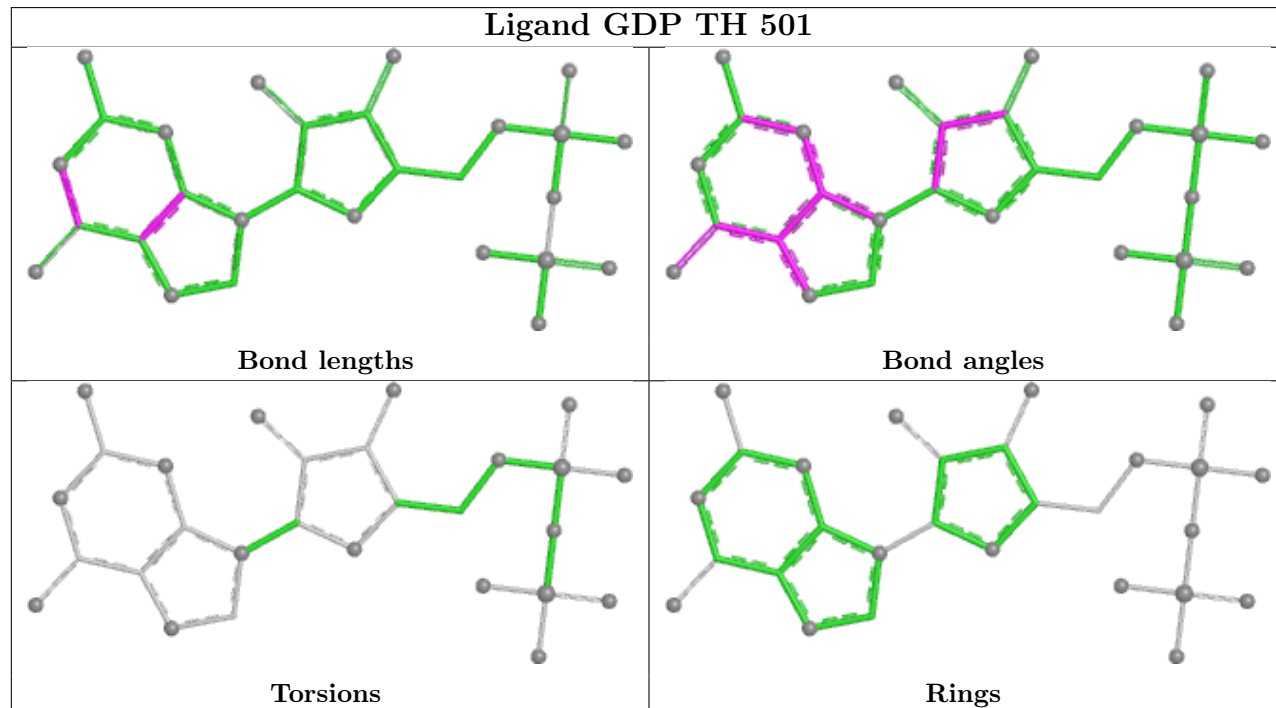
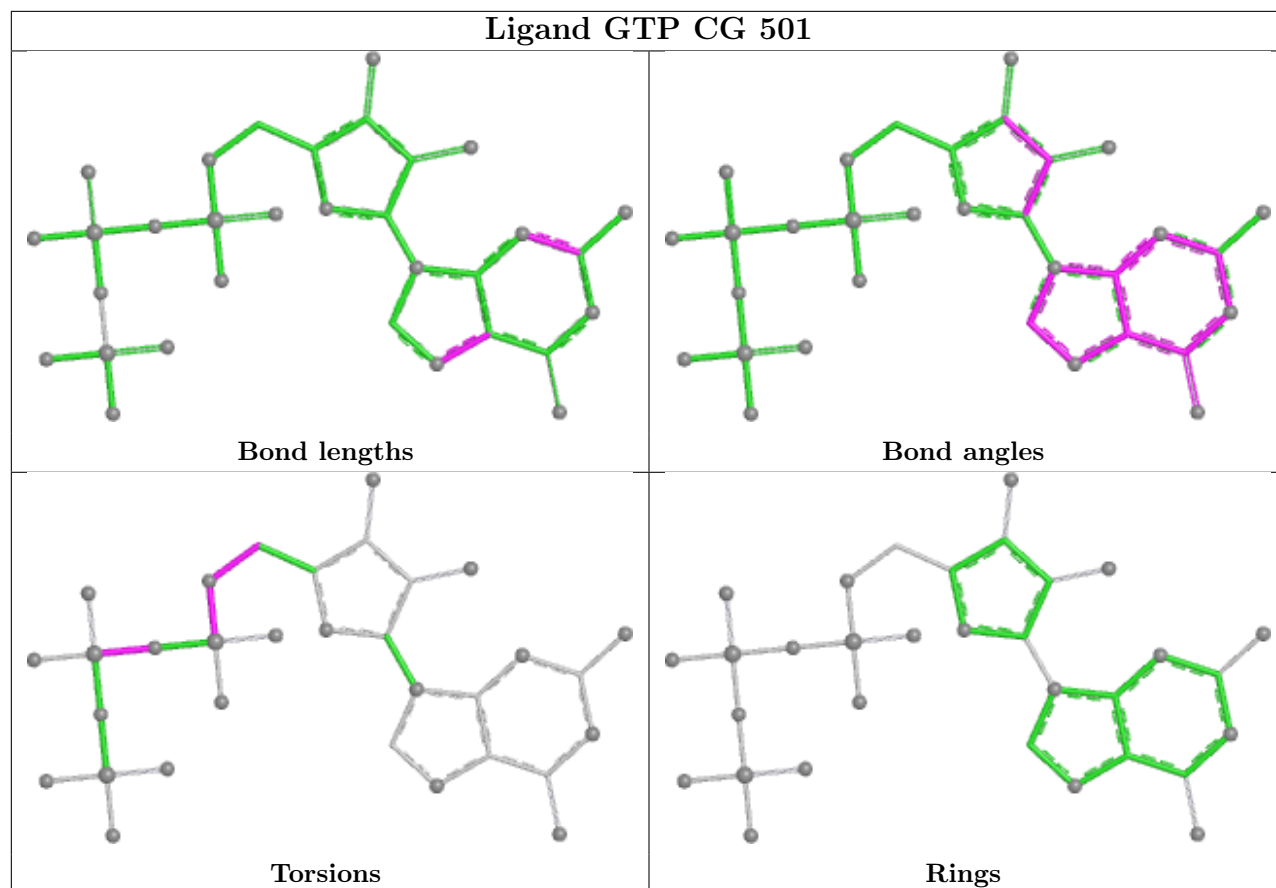
Ligand GTP TG 501

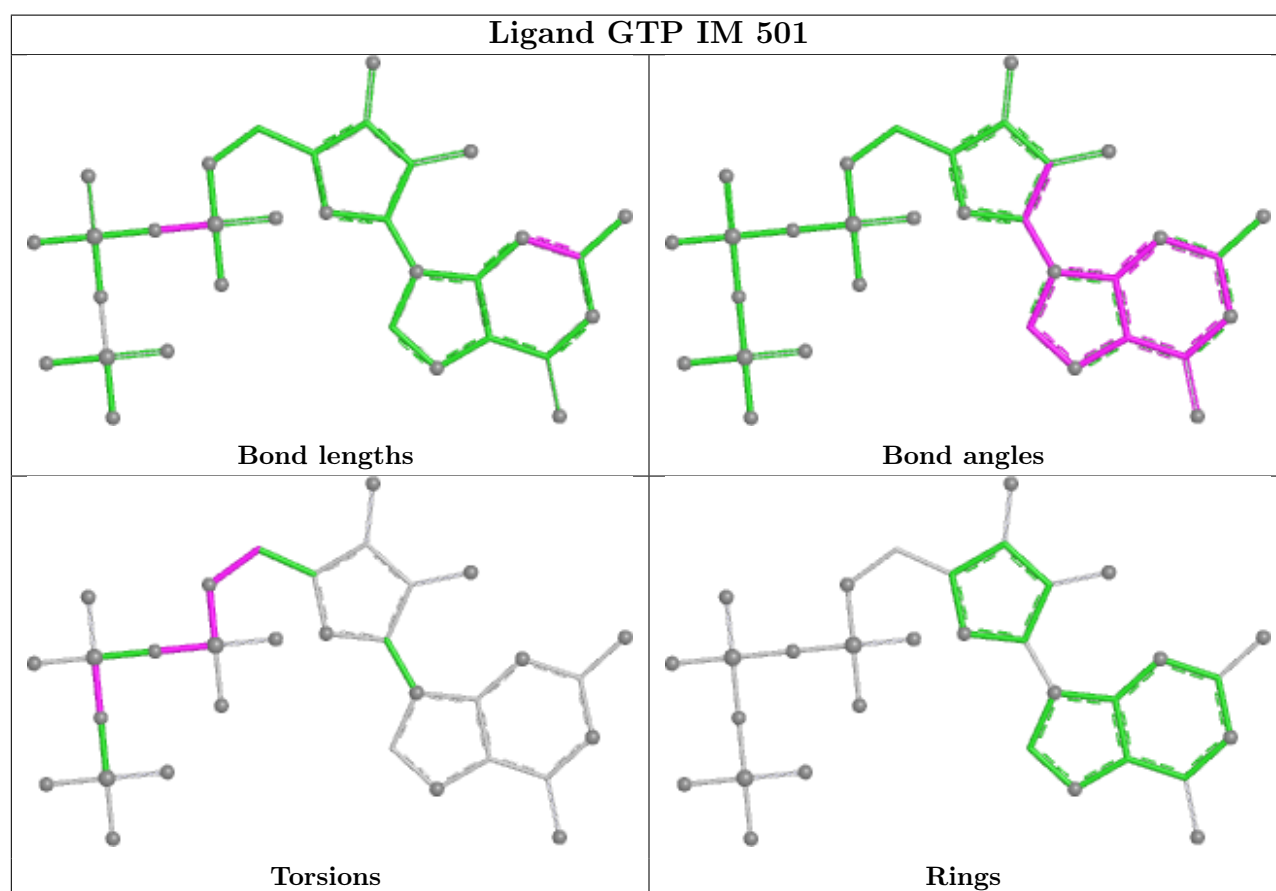
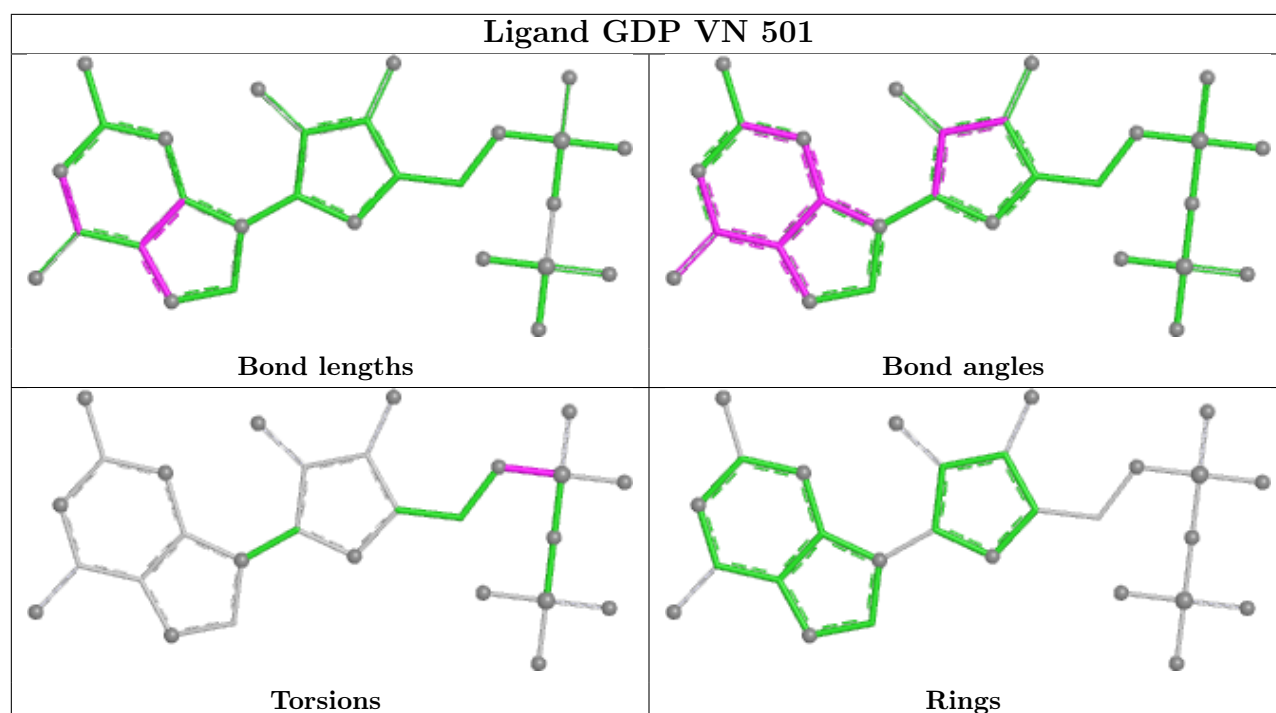


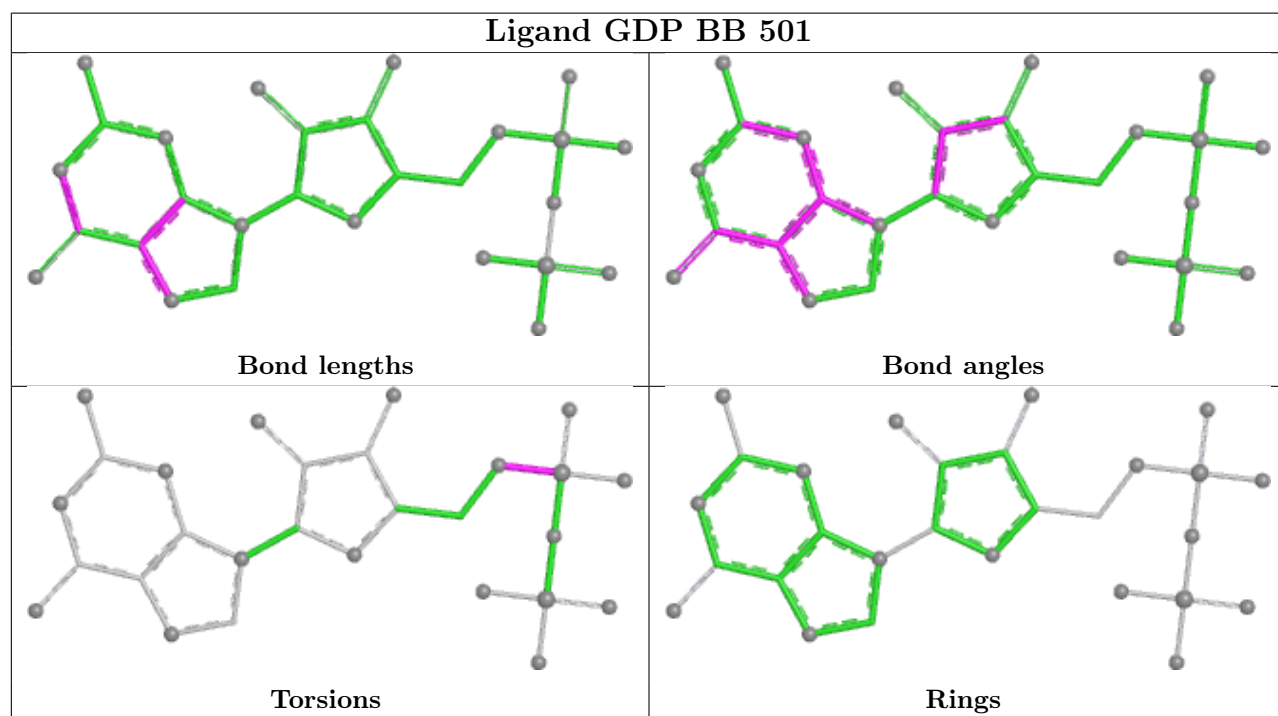
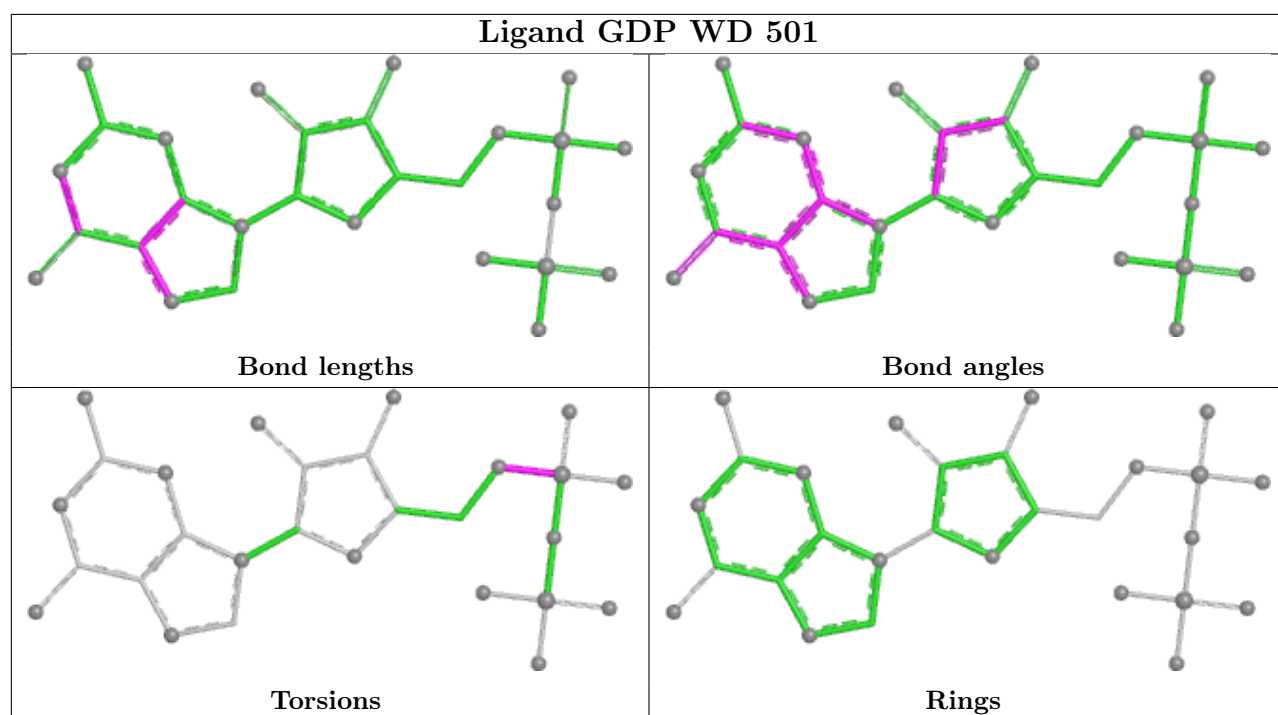
Ligand GDP OH 501

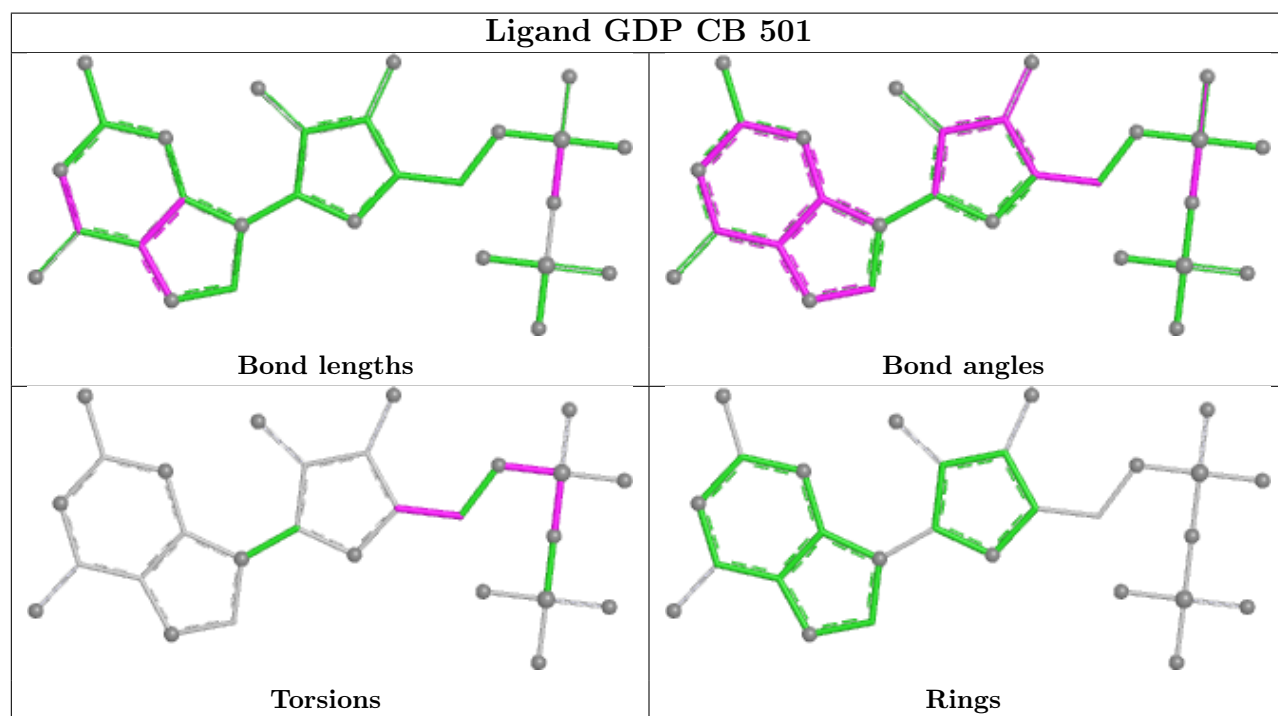
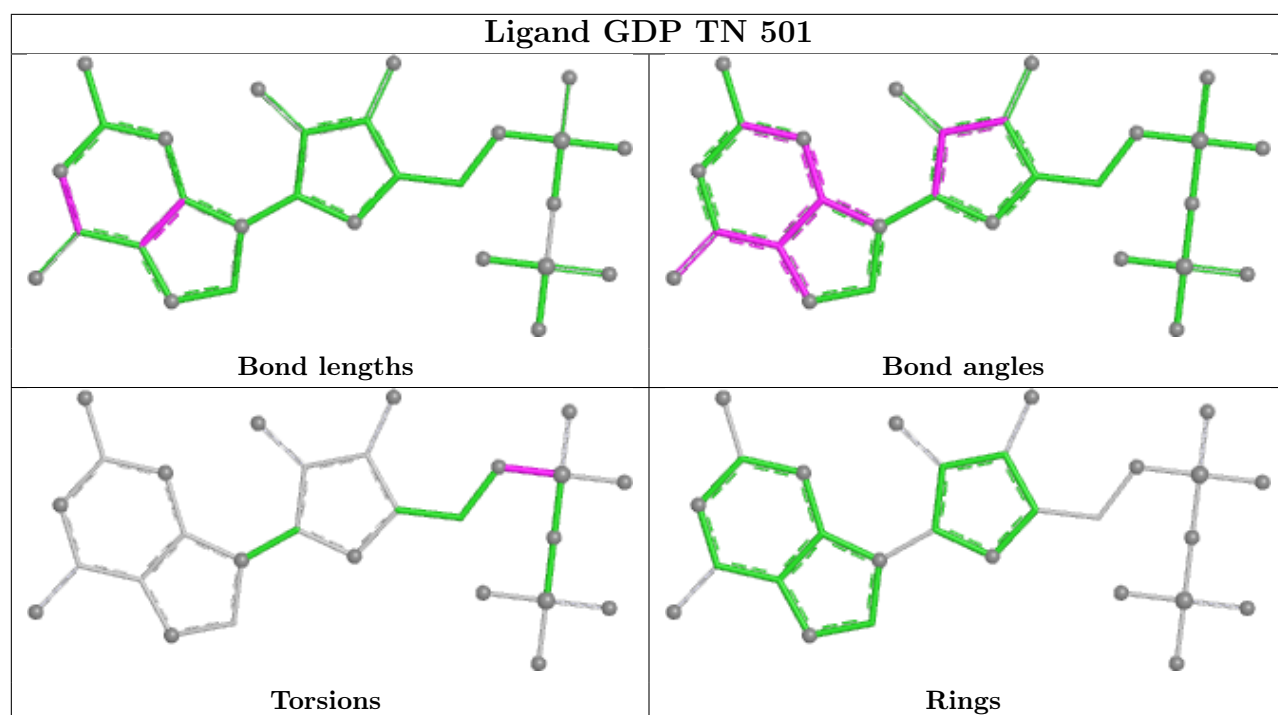


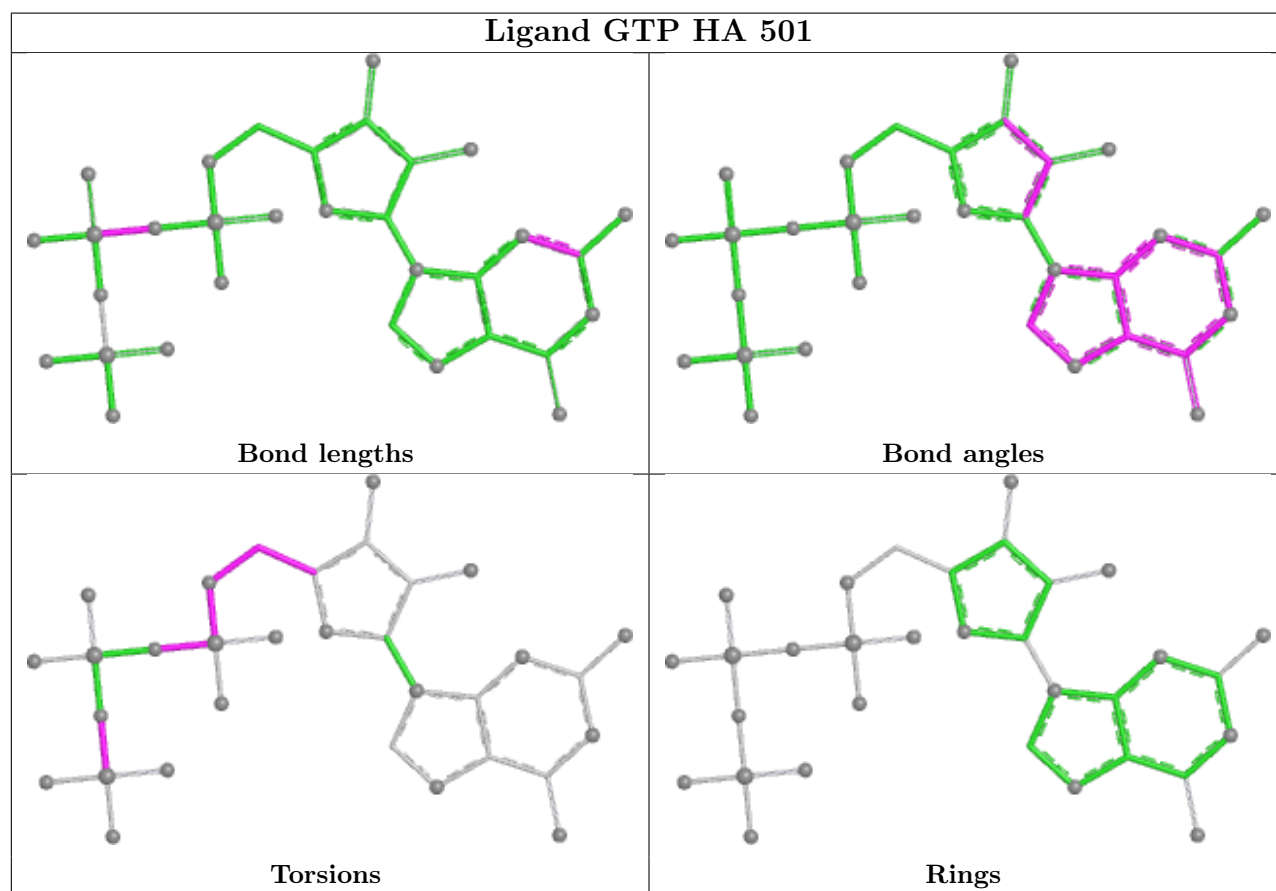
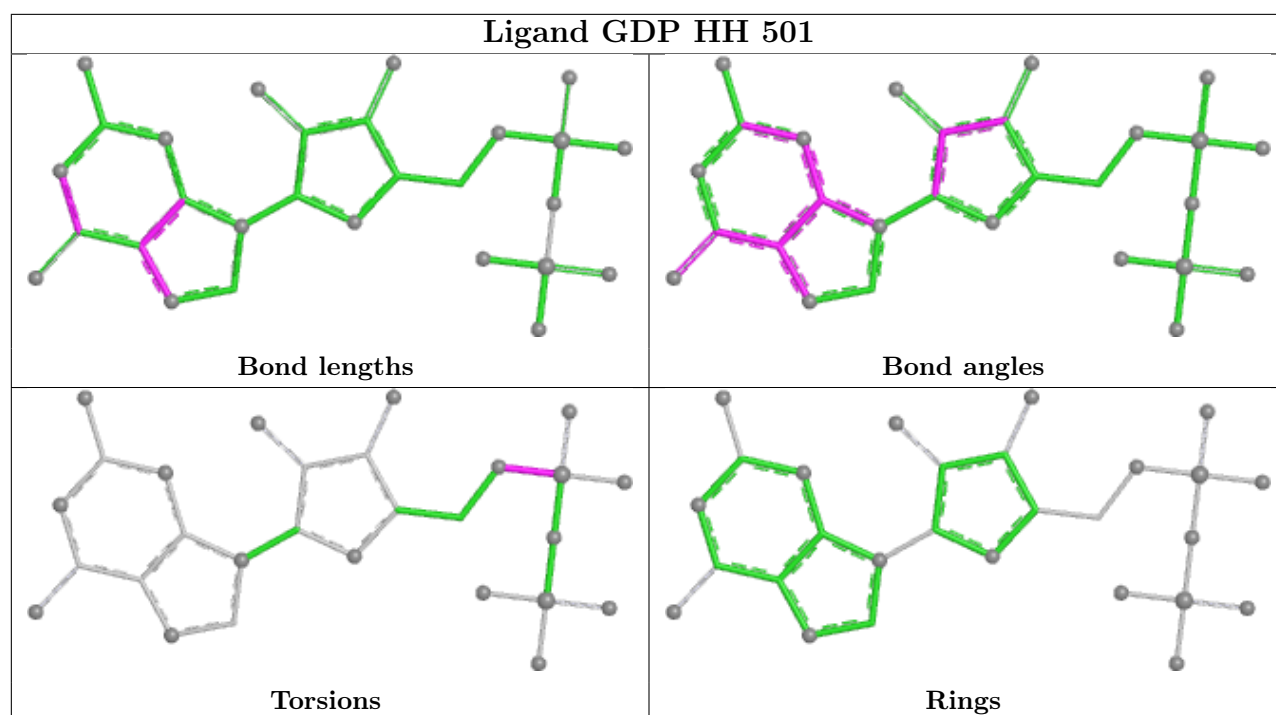


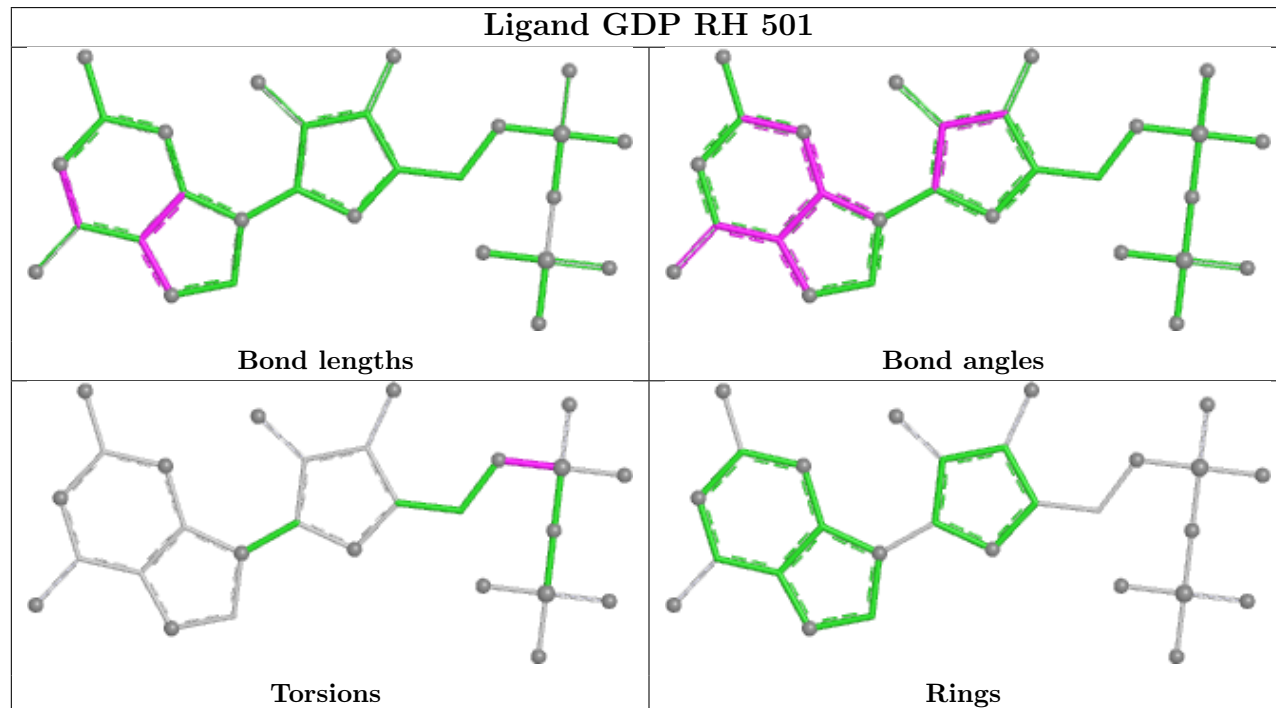
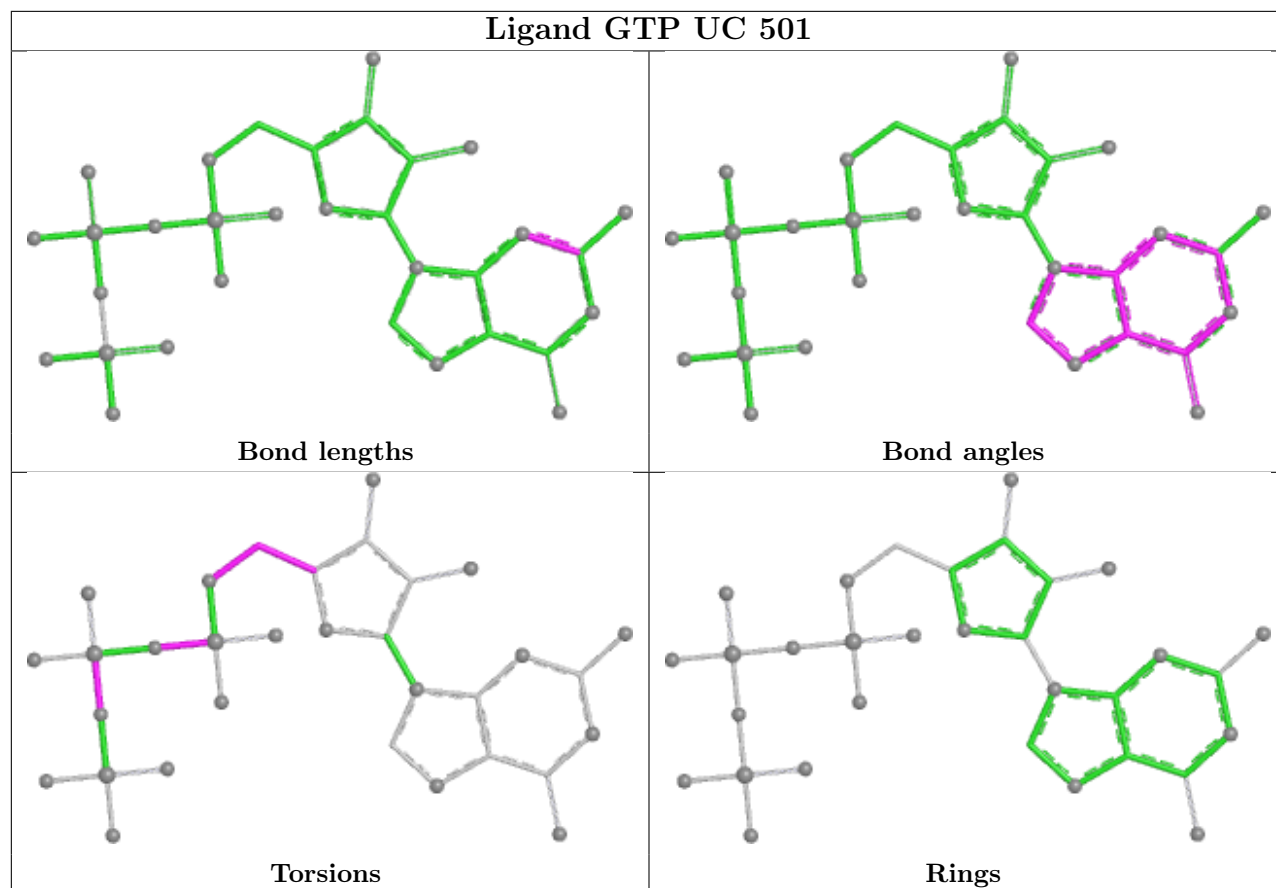




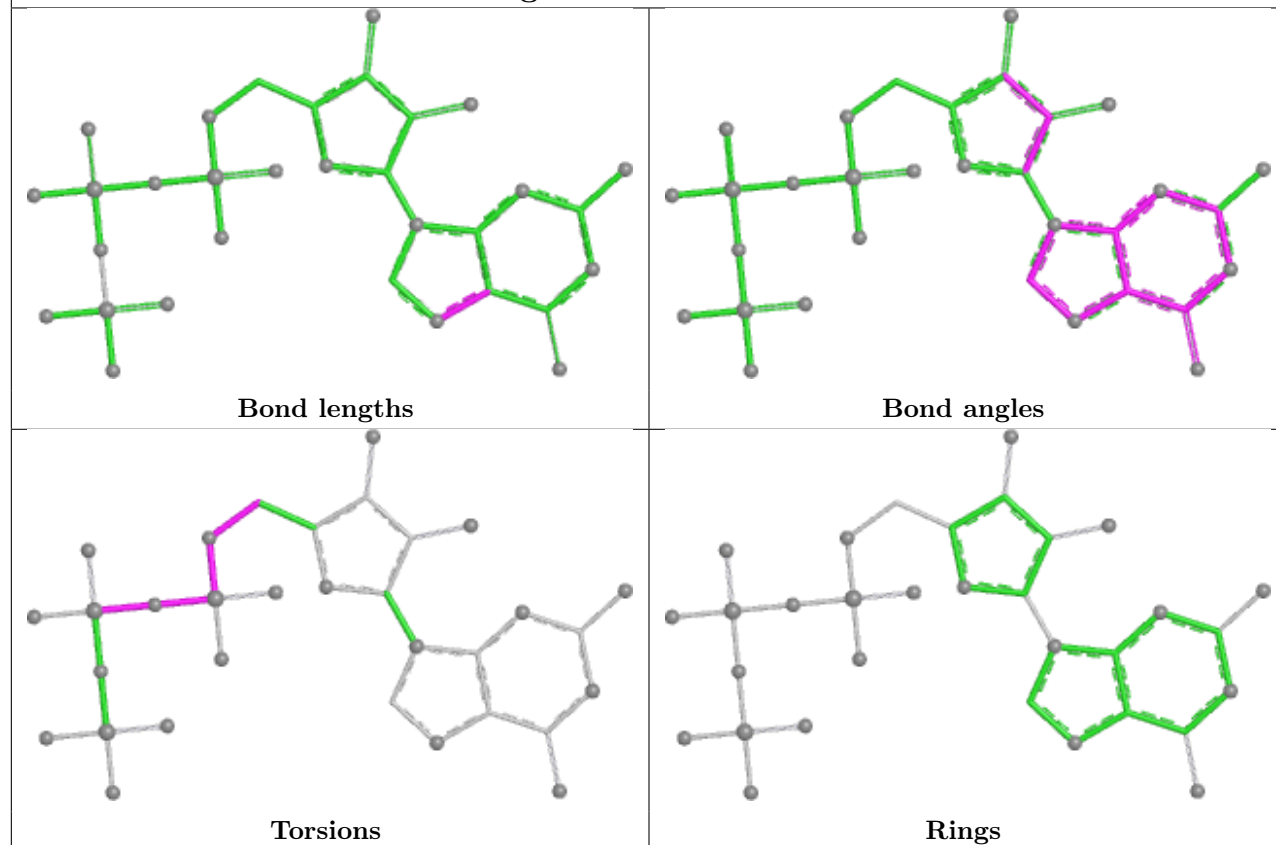




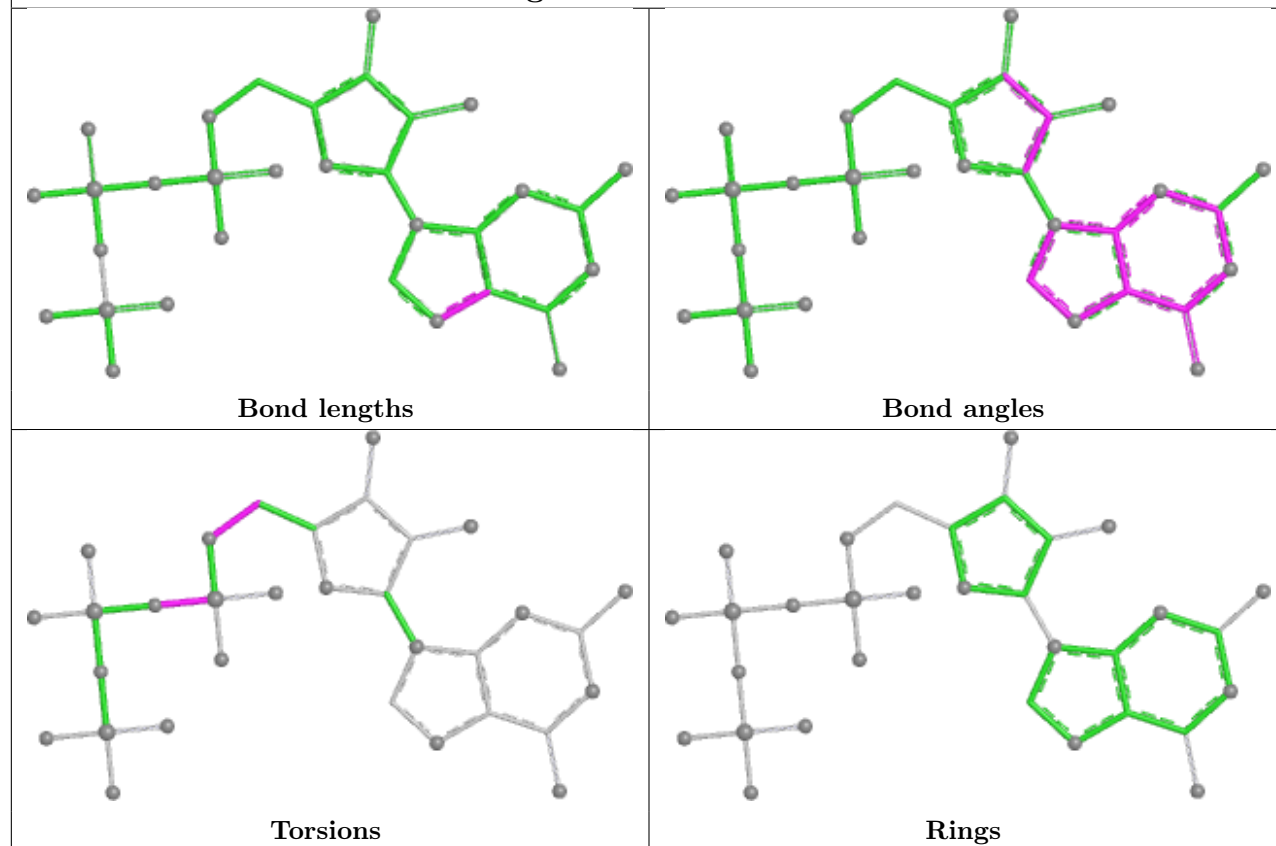


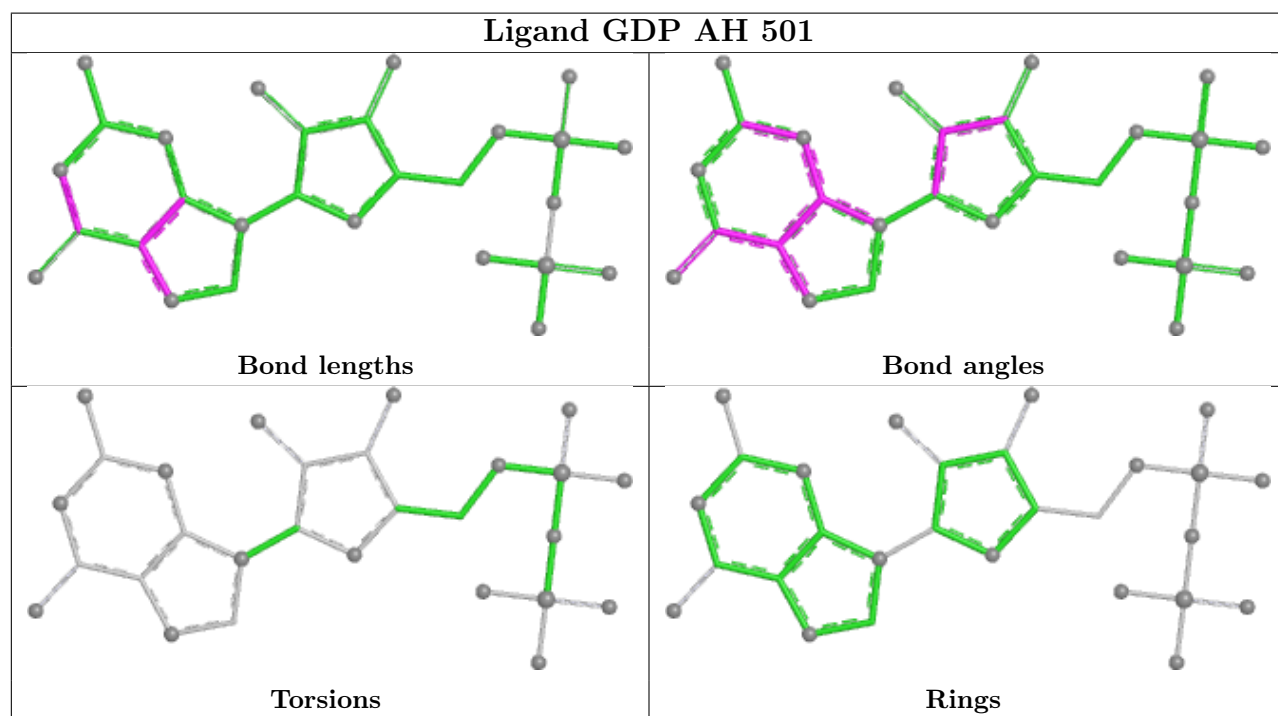
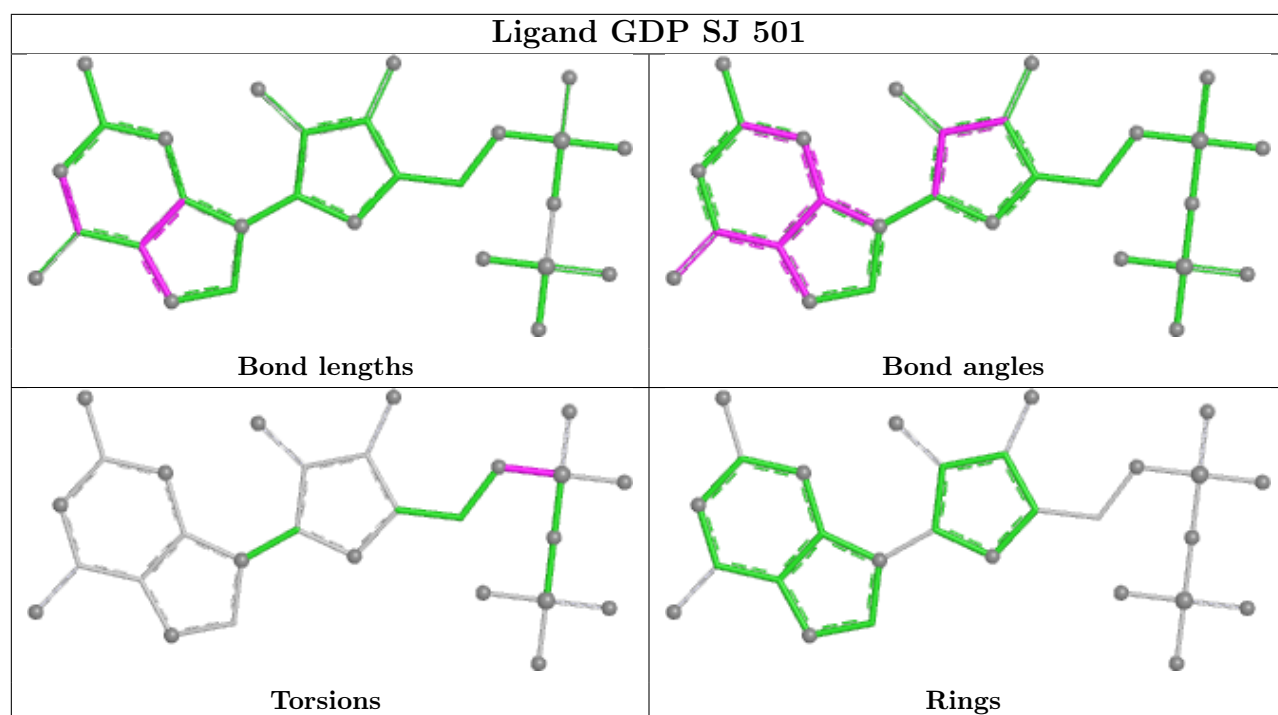


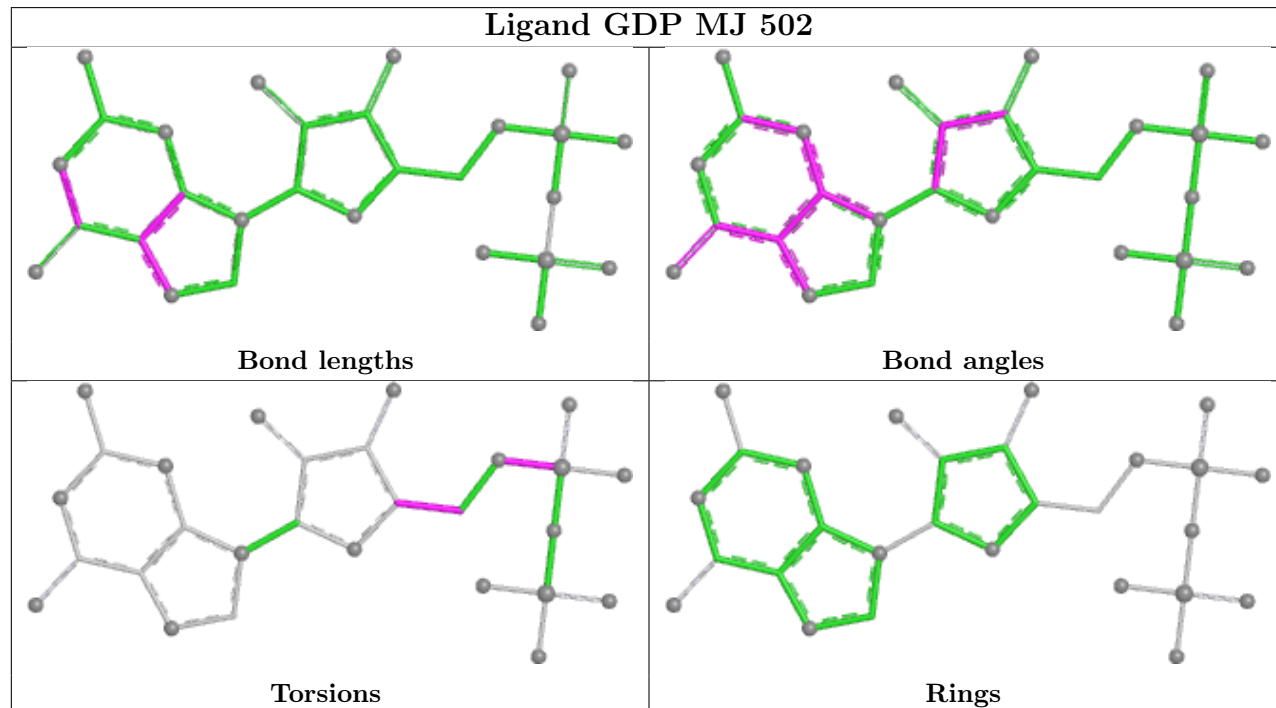
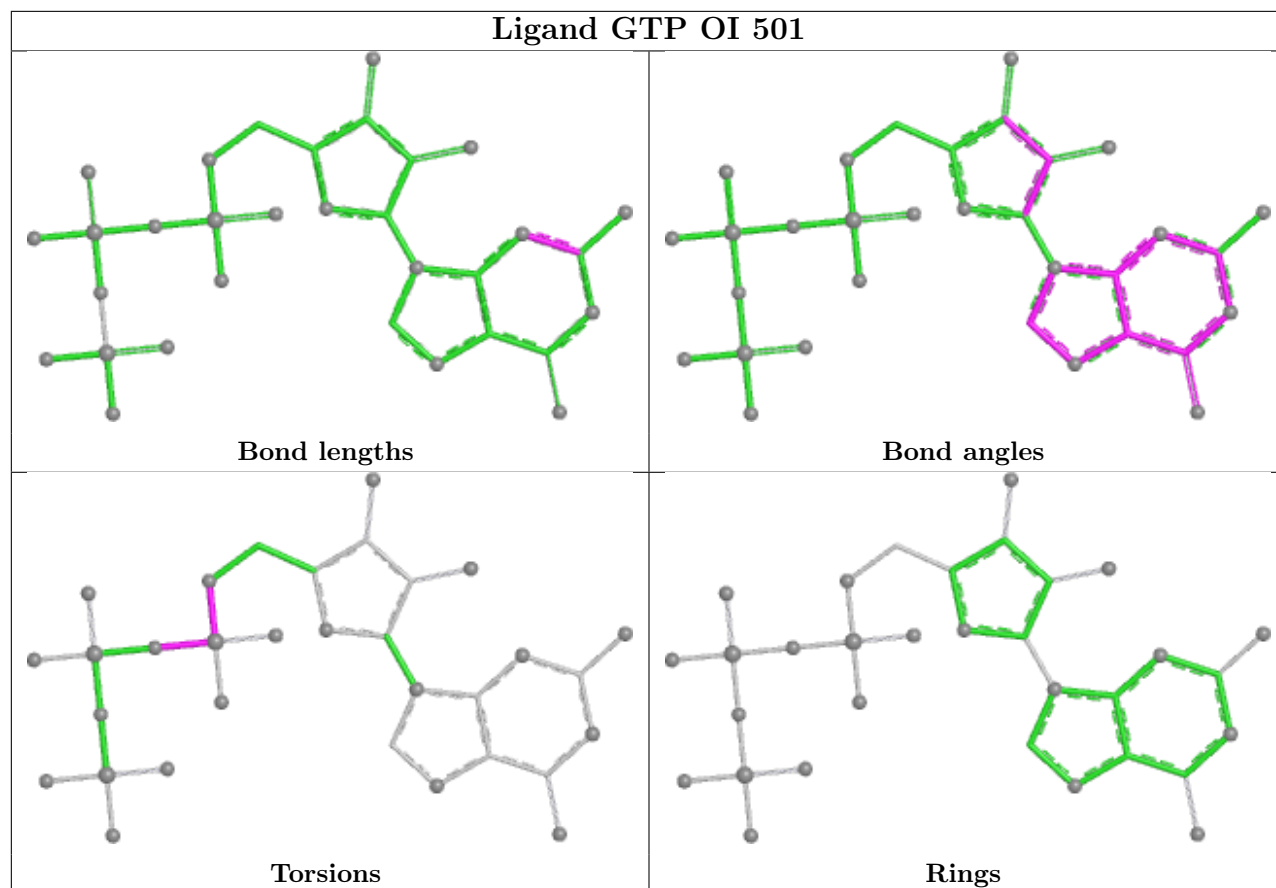
Ligand GTP KJ 501



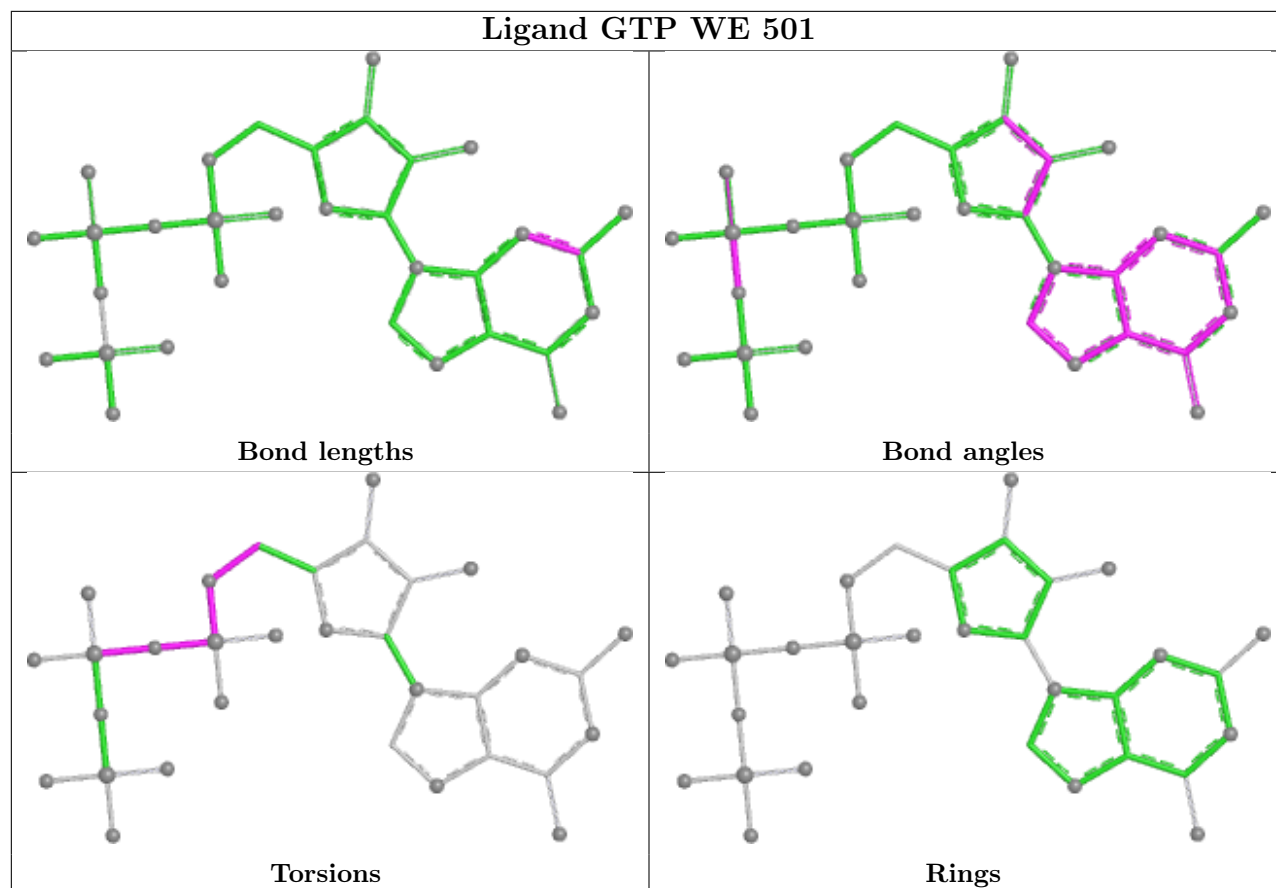
Ligand GTP LI 501



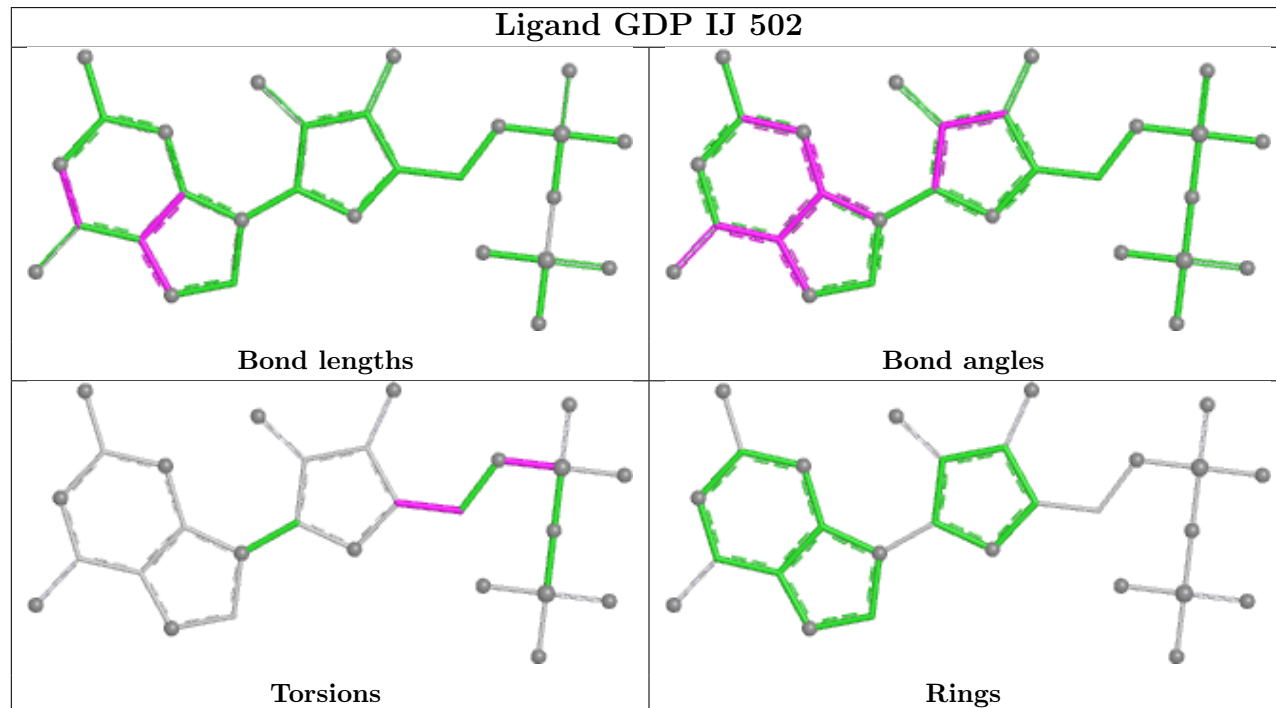




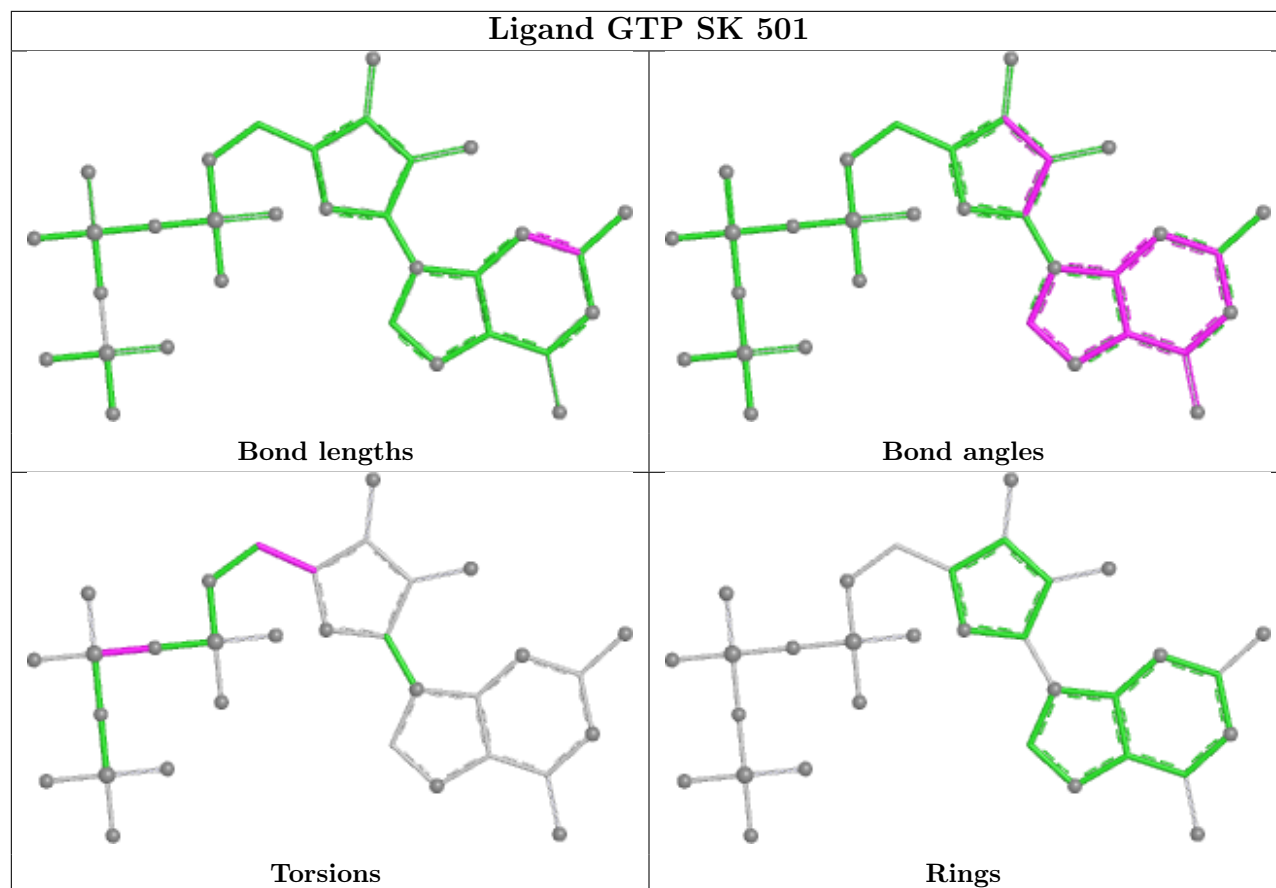
Ligand GTP WE 501



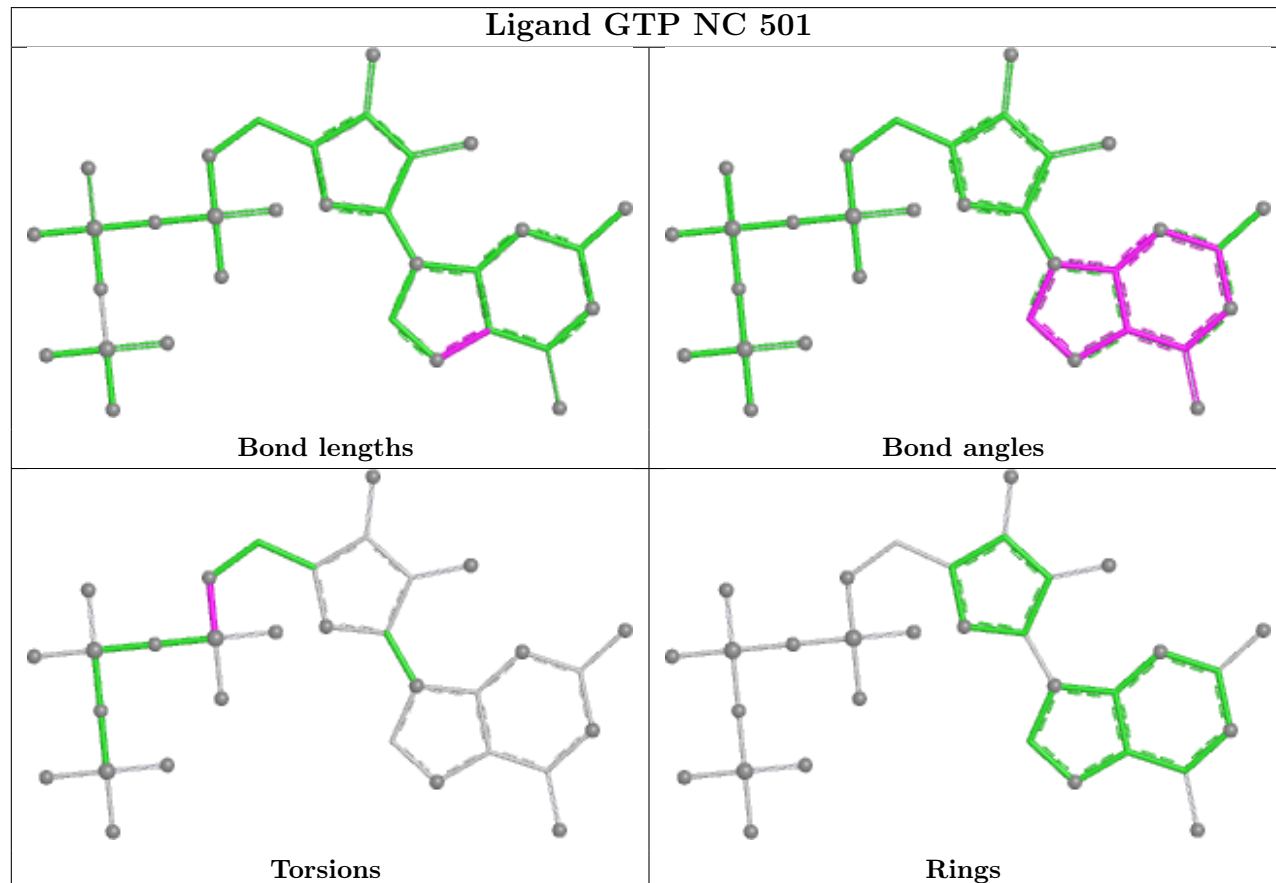
Ligand GDP IJ 502



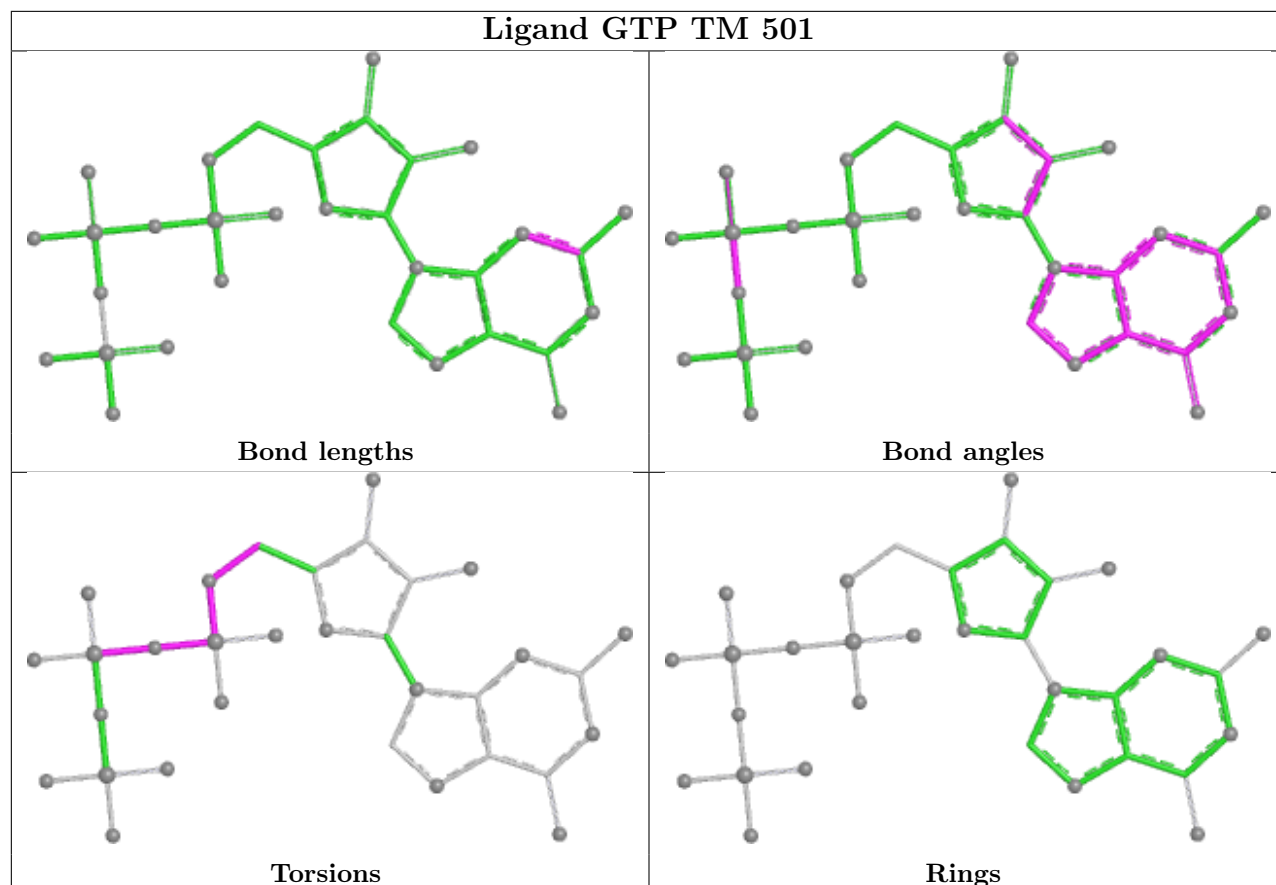
Ligand GTP SK 501



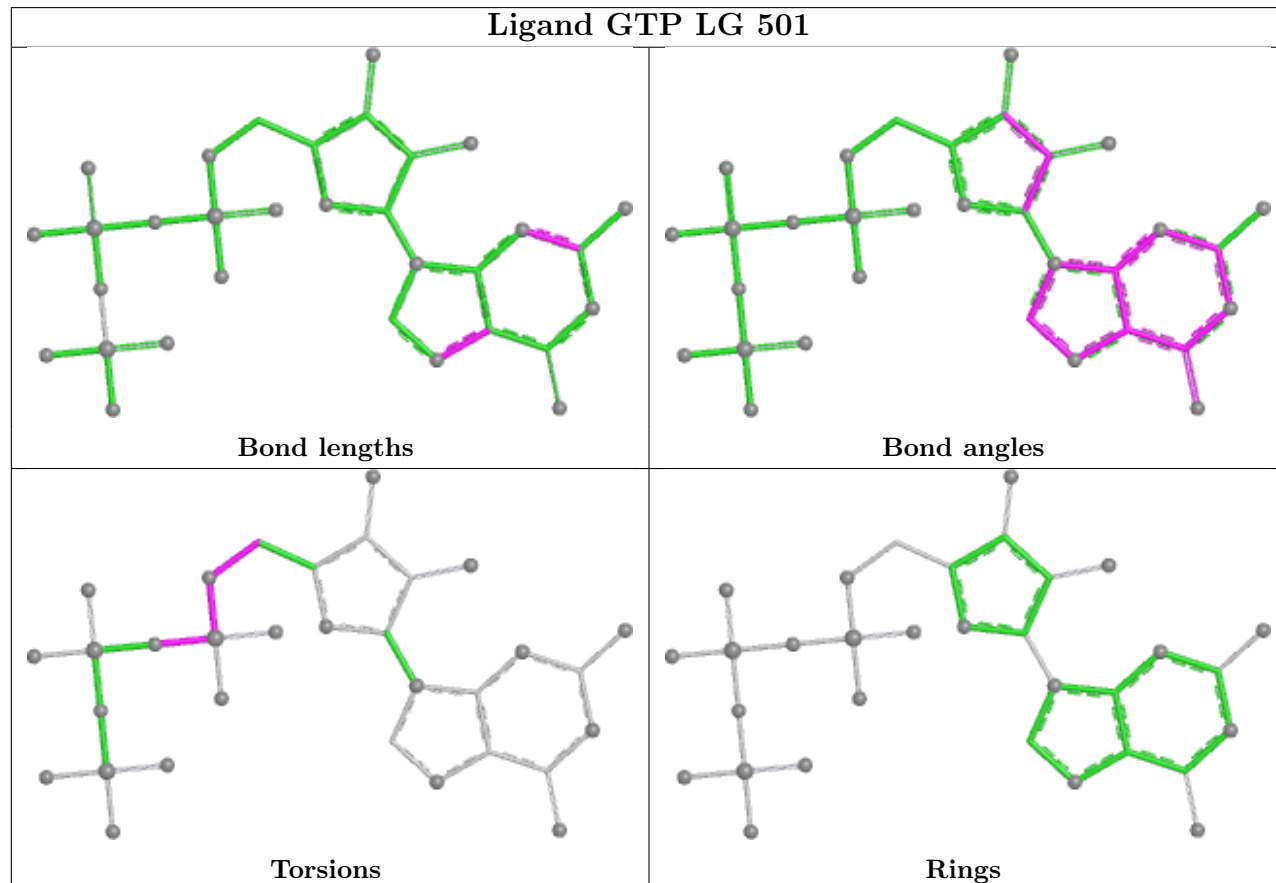
Ligand GTP NC 501



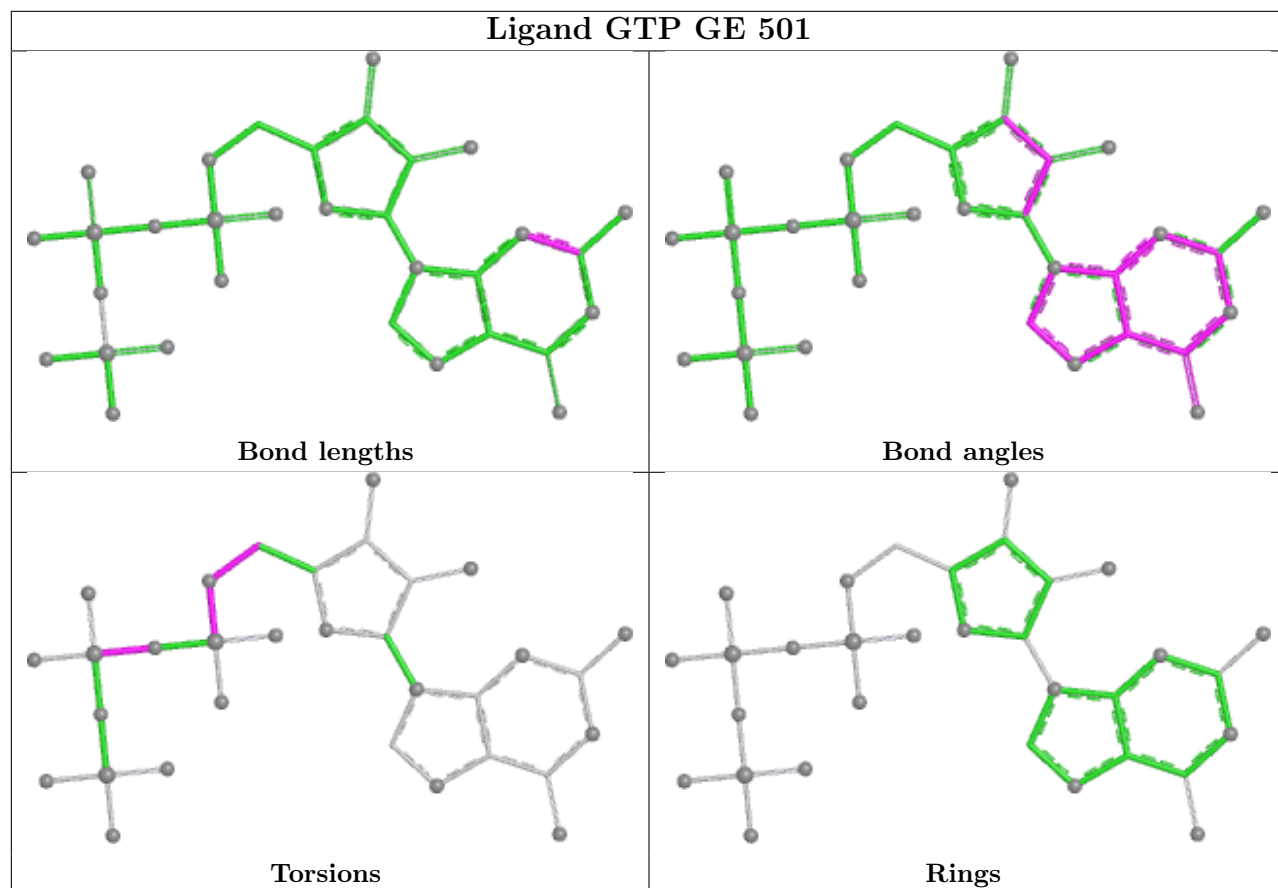
Ligand GTP TM 501



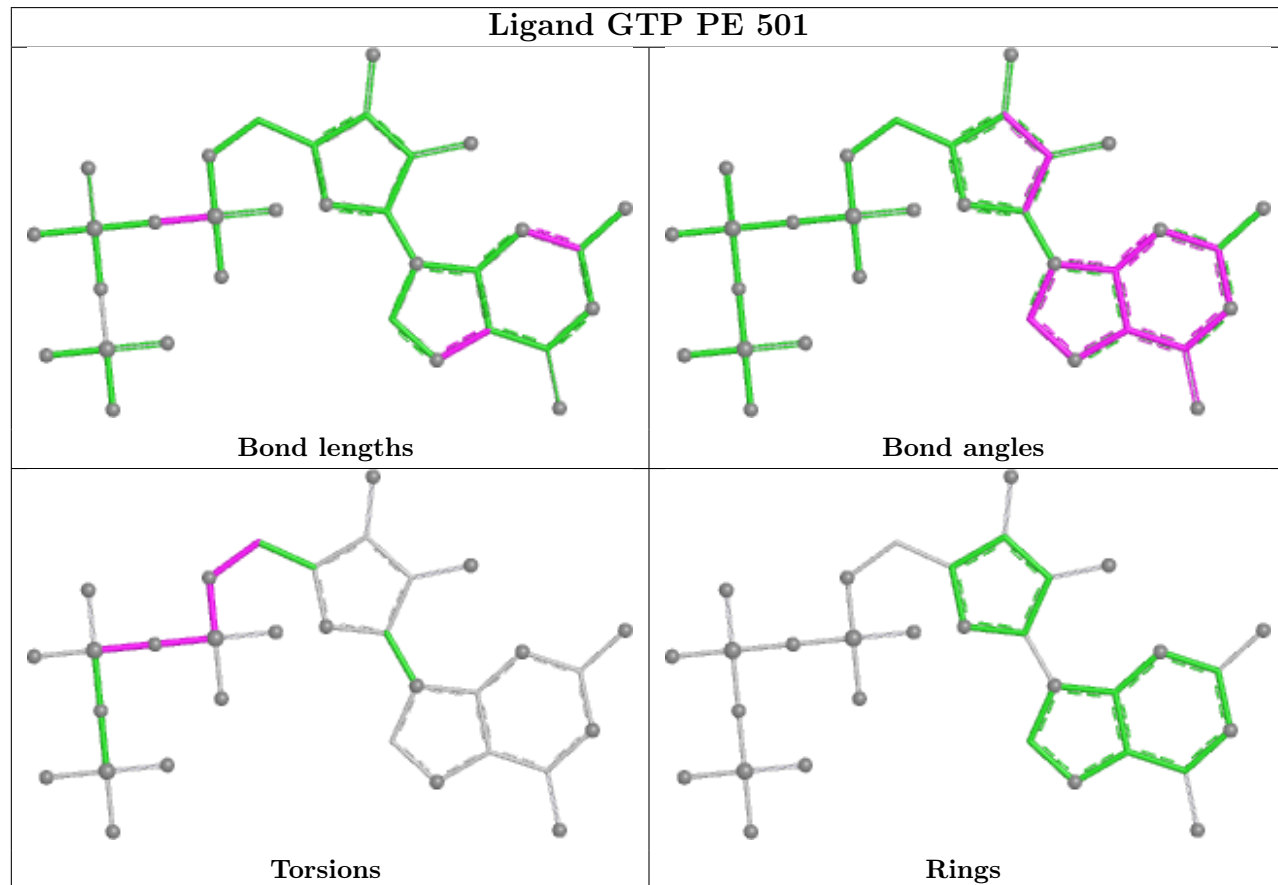
Ligand GTP LG 501

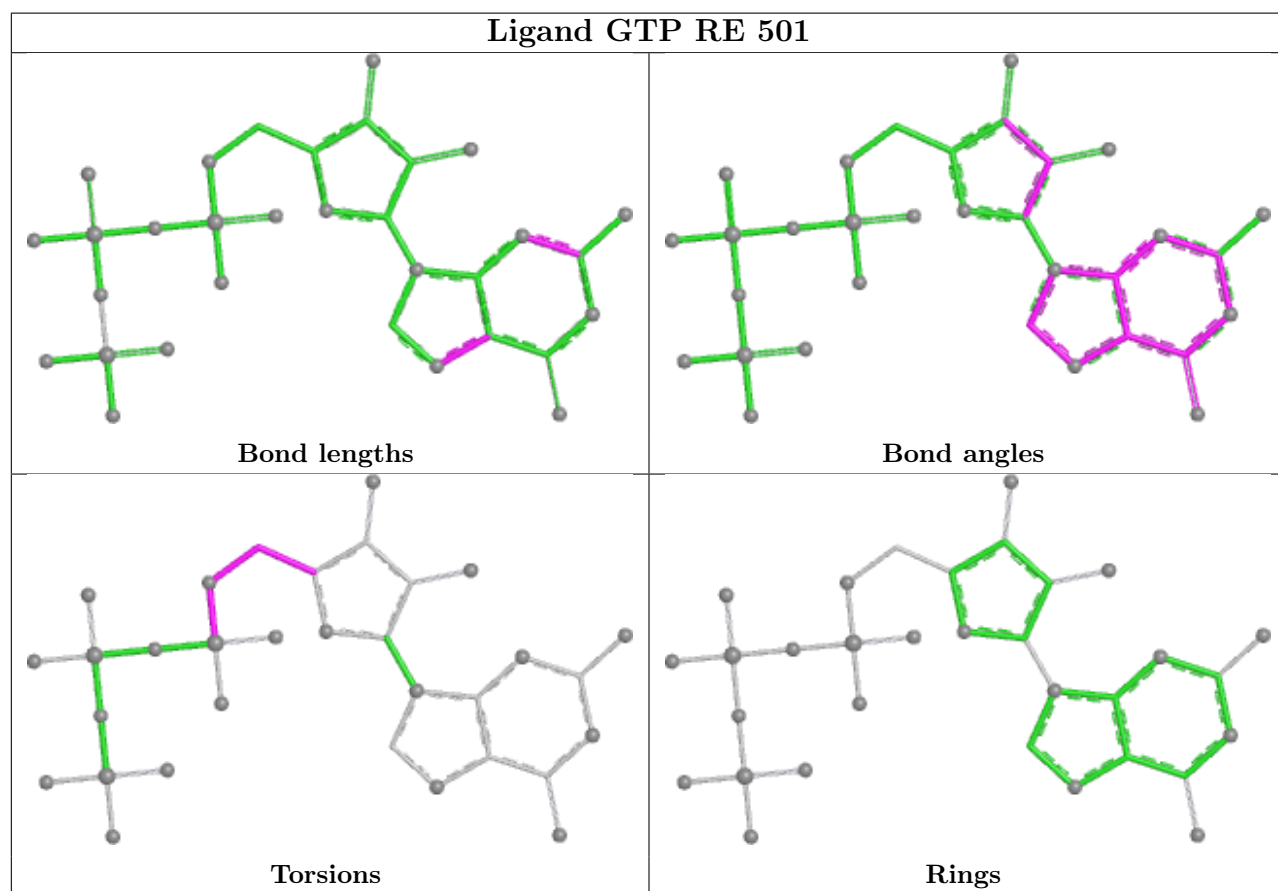
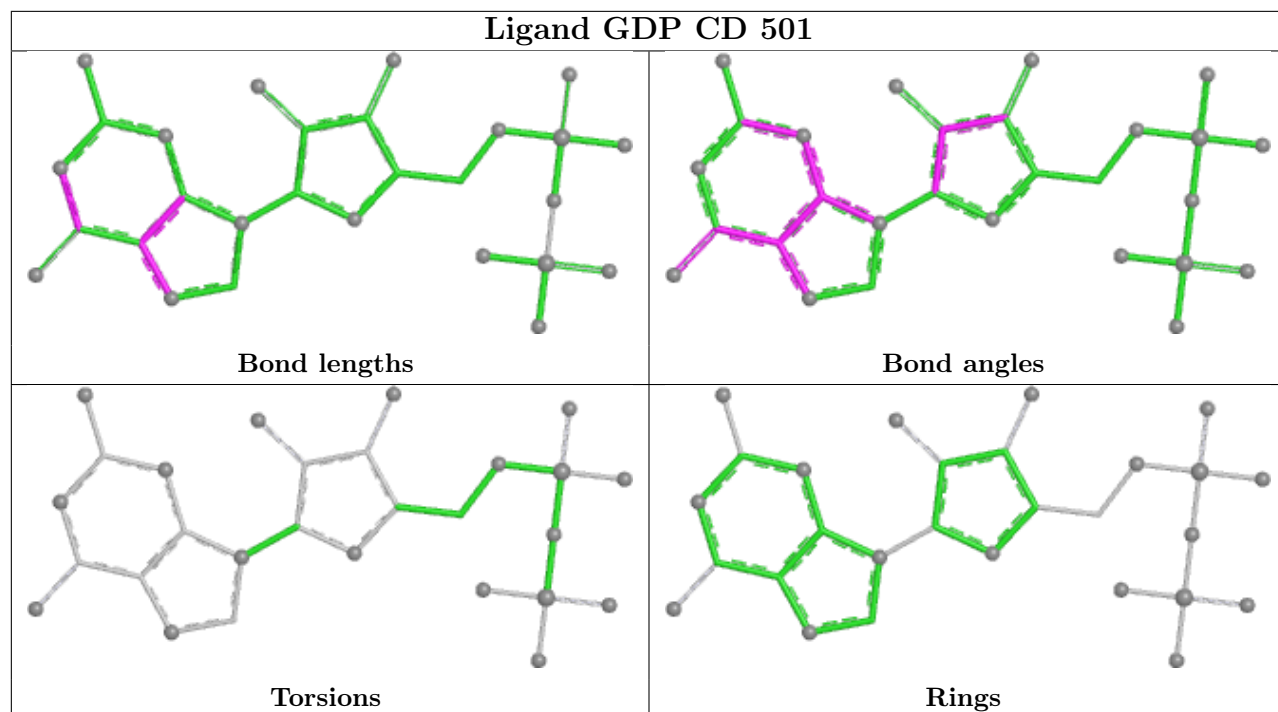


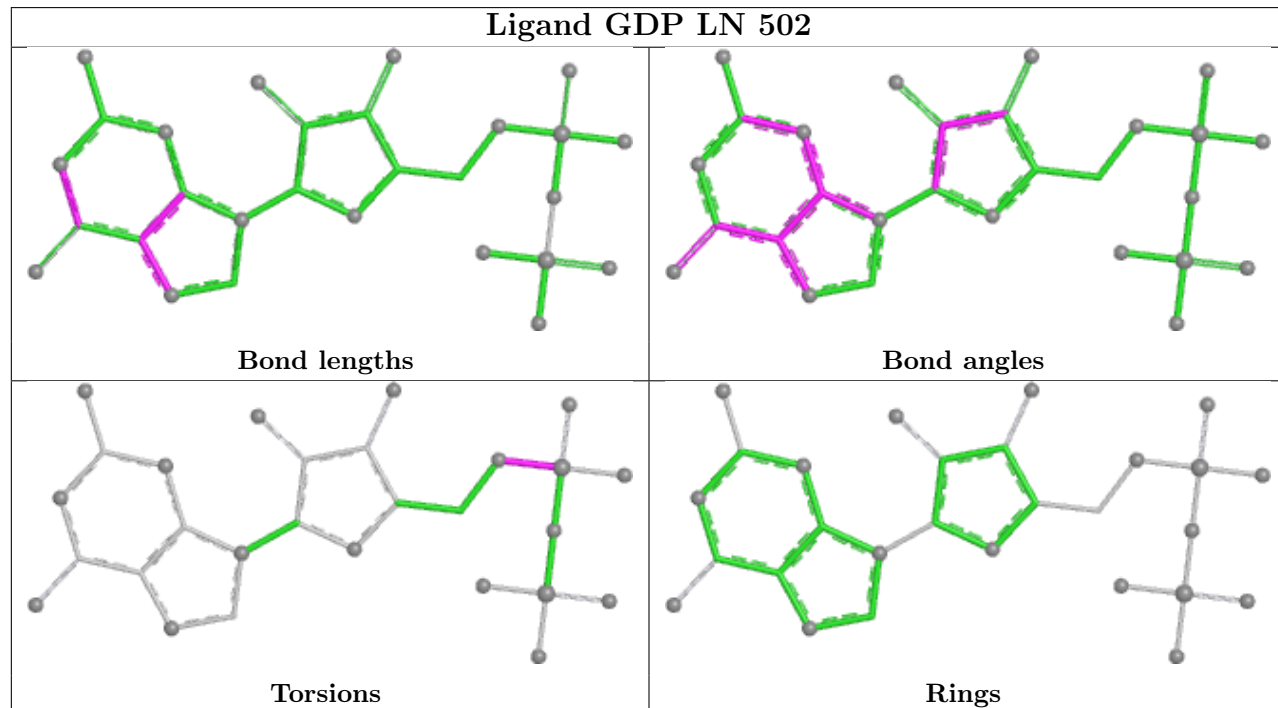
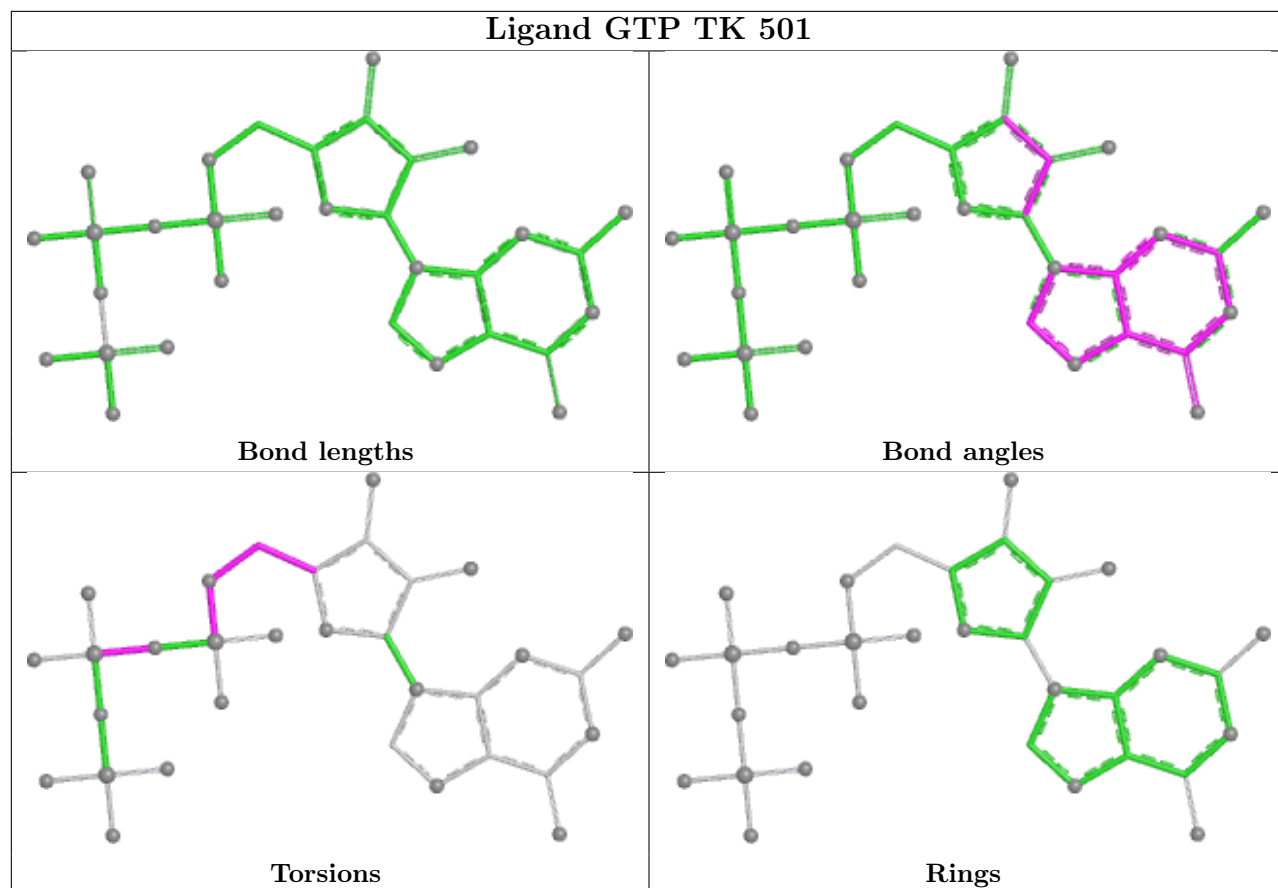
Ligand GTP GE 501



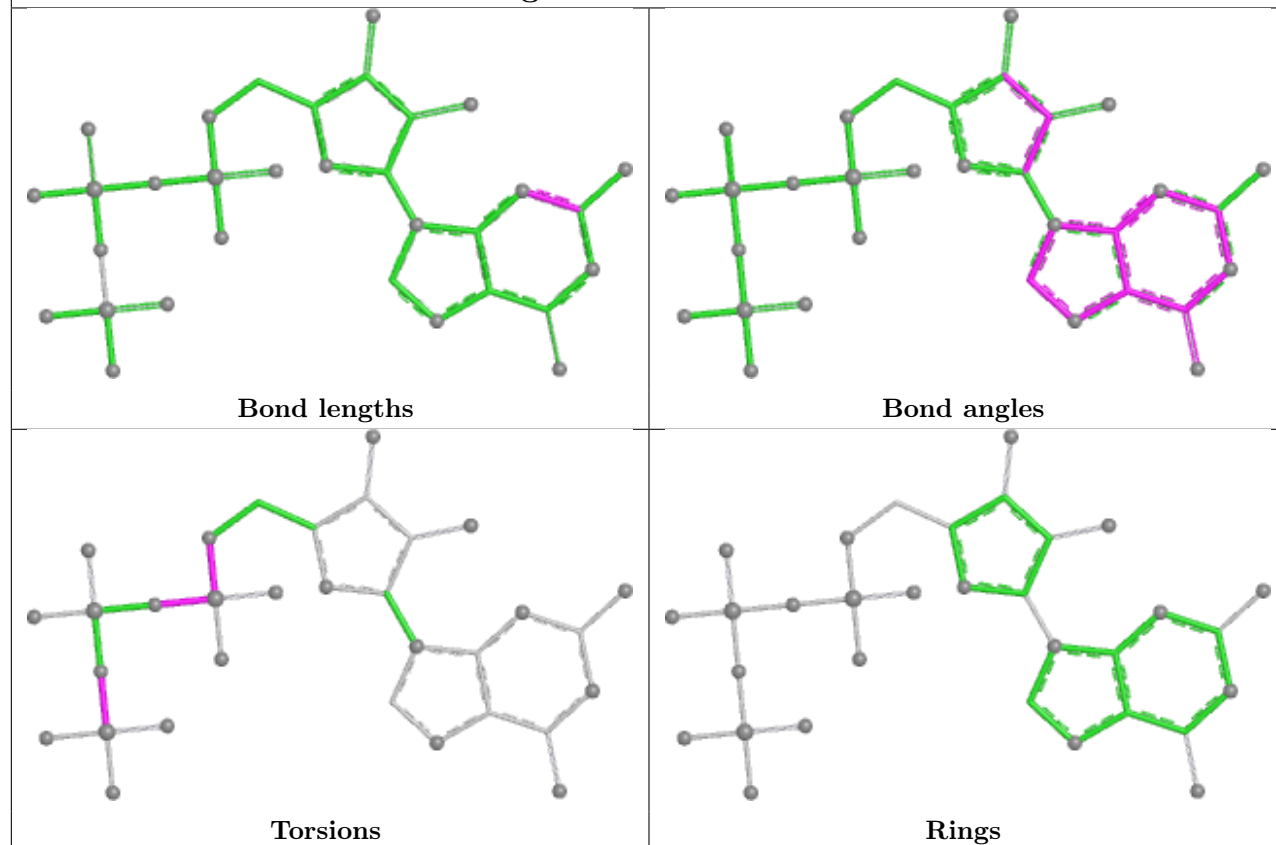
Ligand GTP PE 501



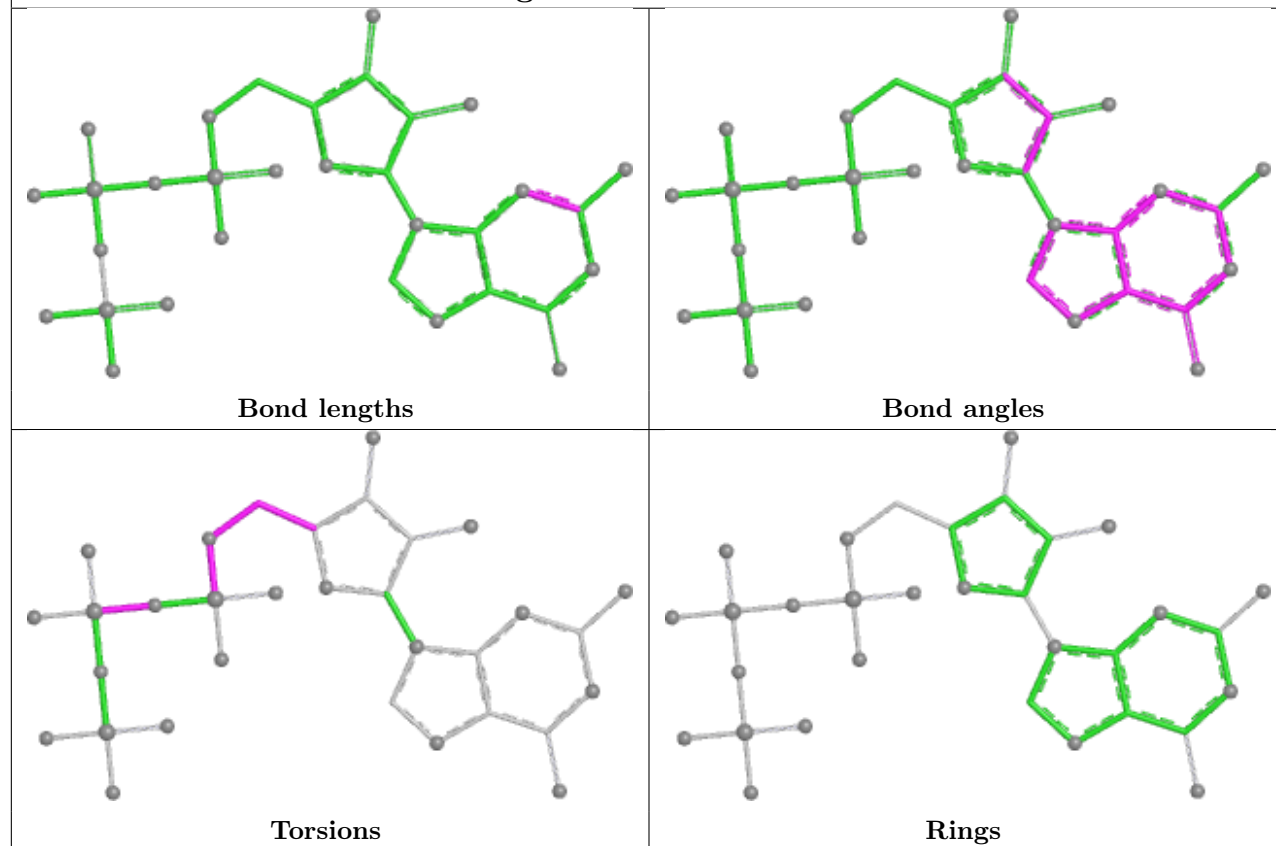


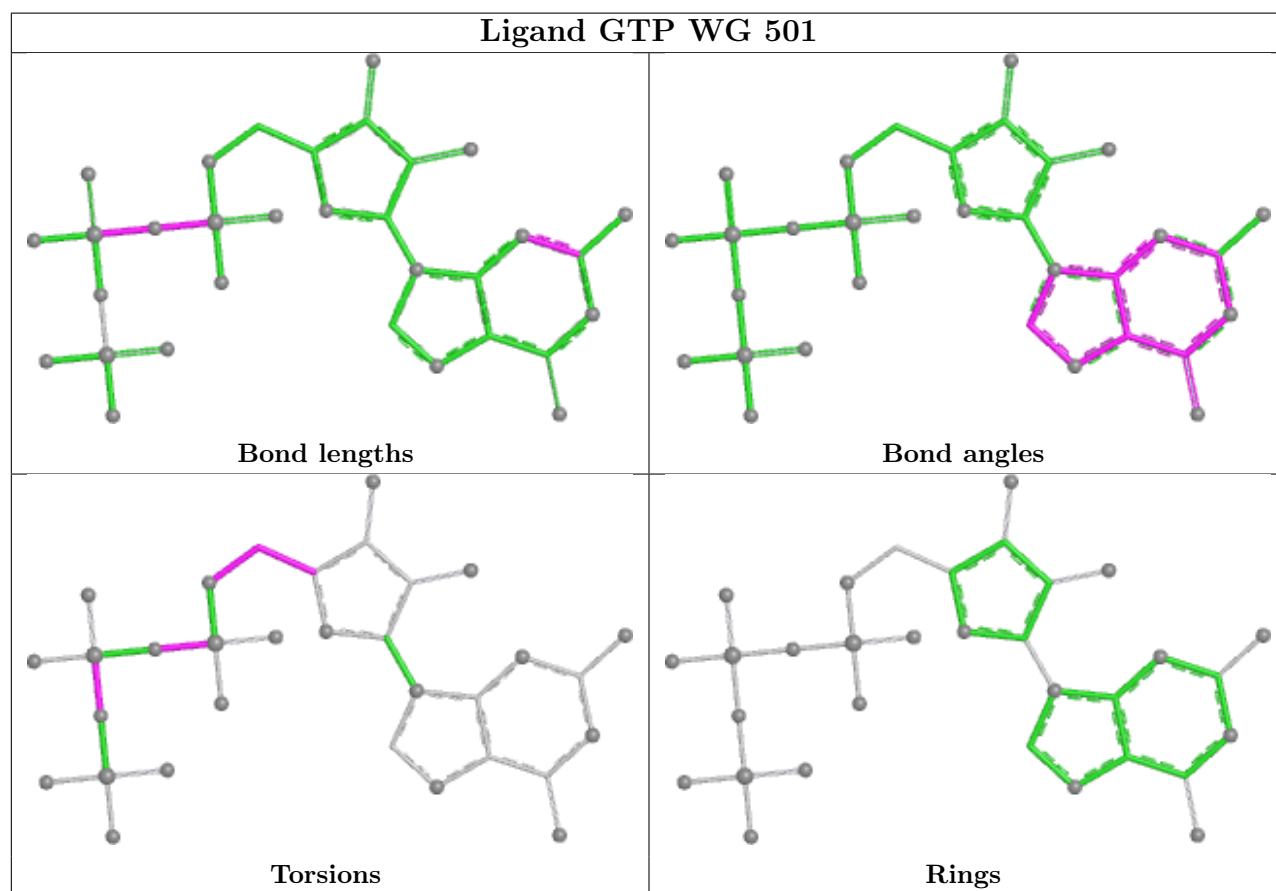
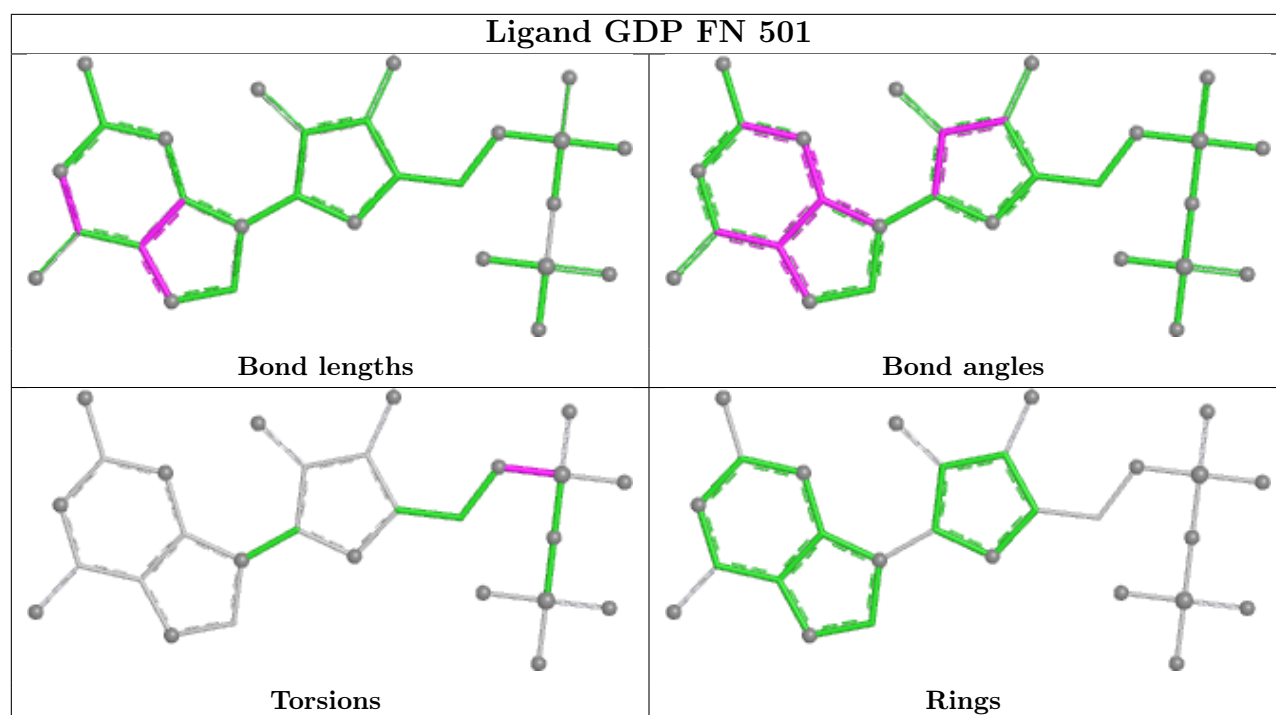


Ligand GTP JC 501

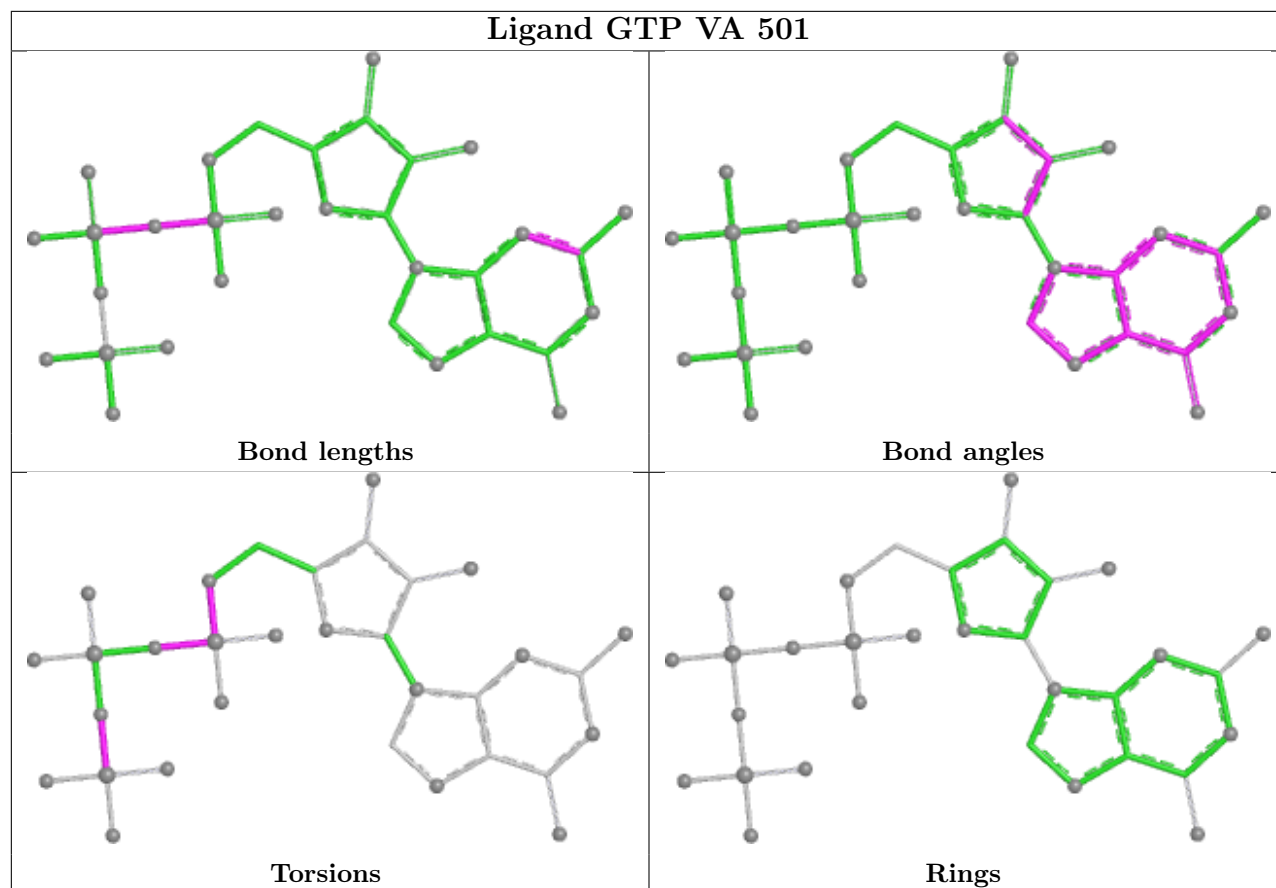


Ligand GTP KA 501

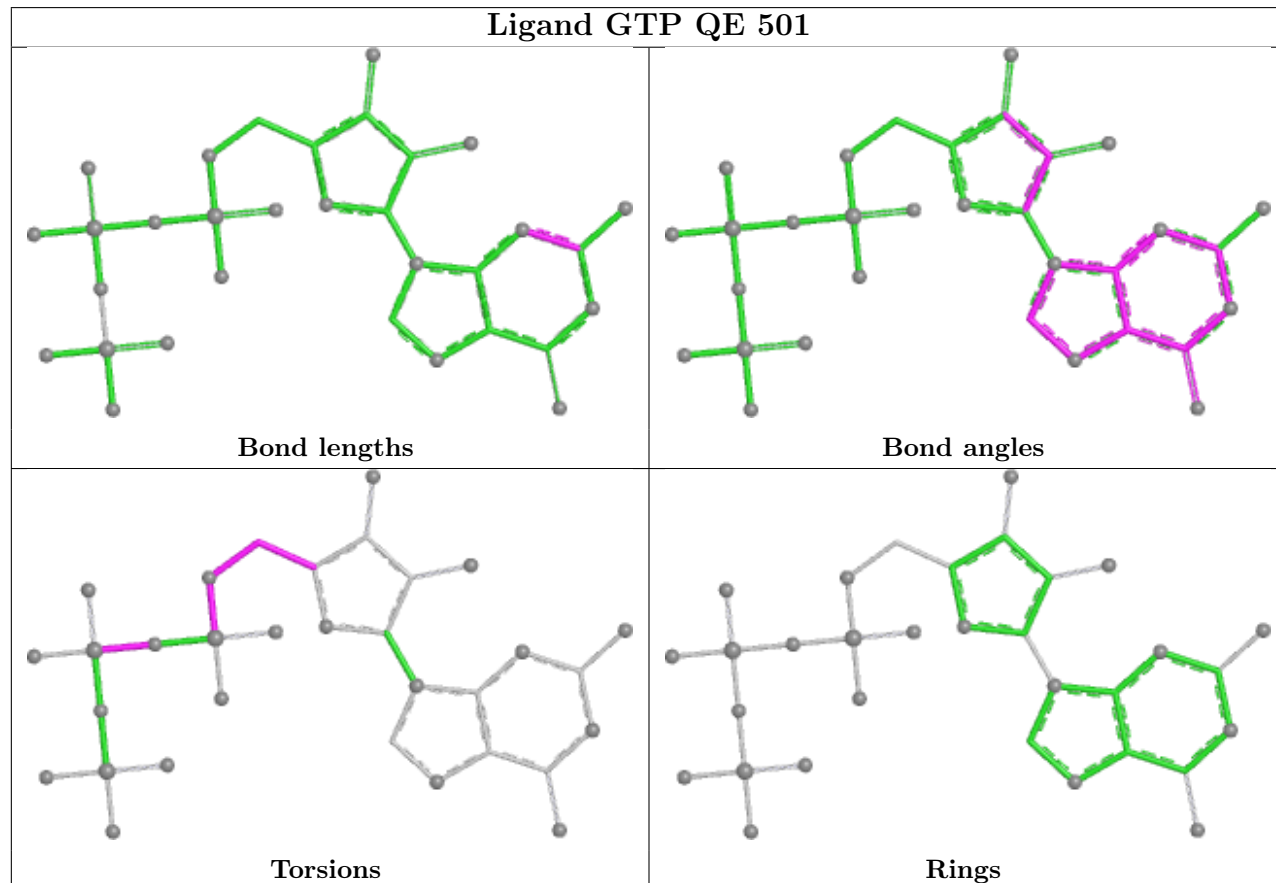


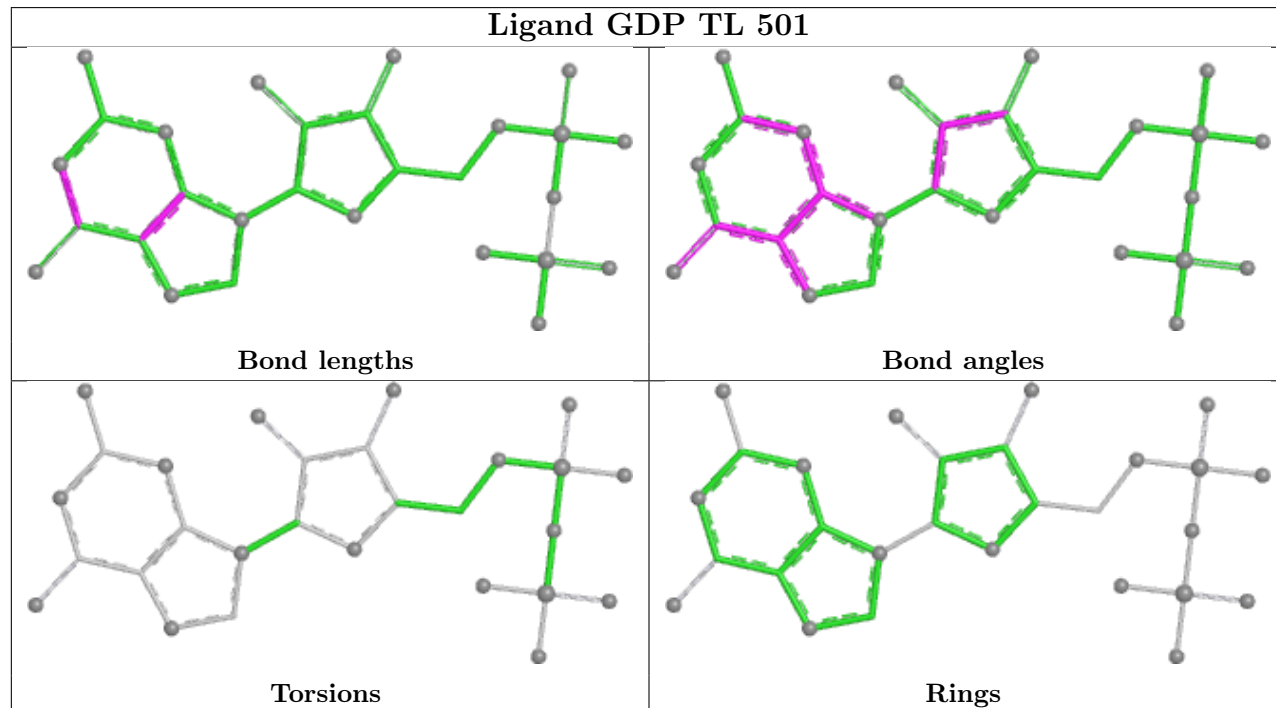
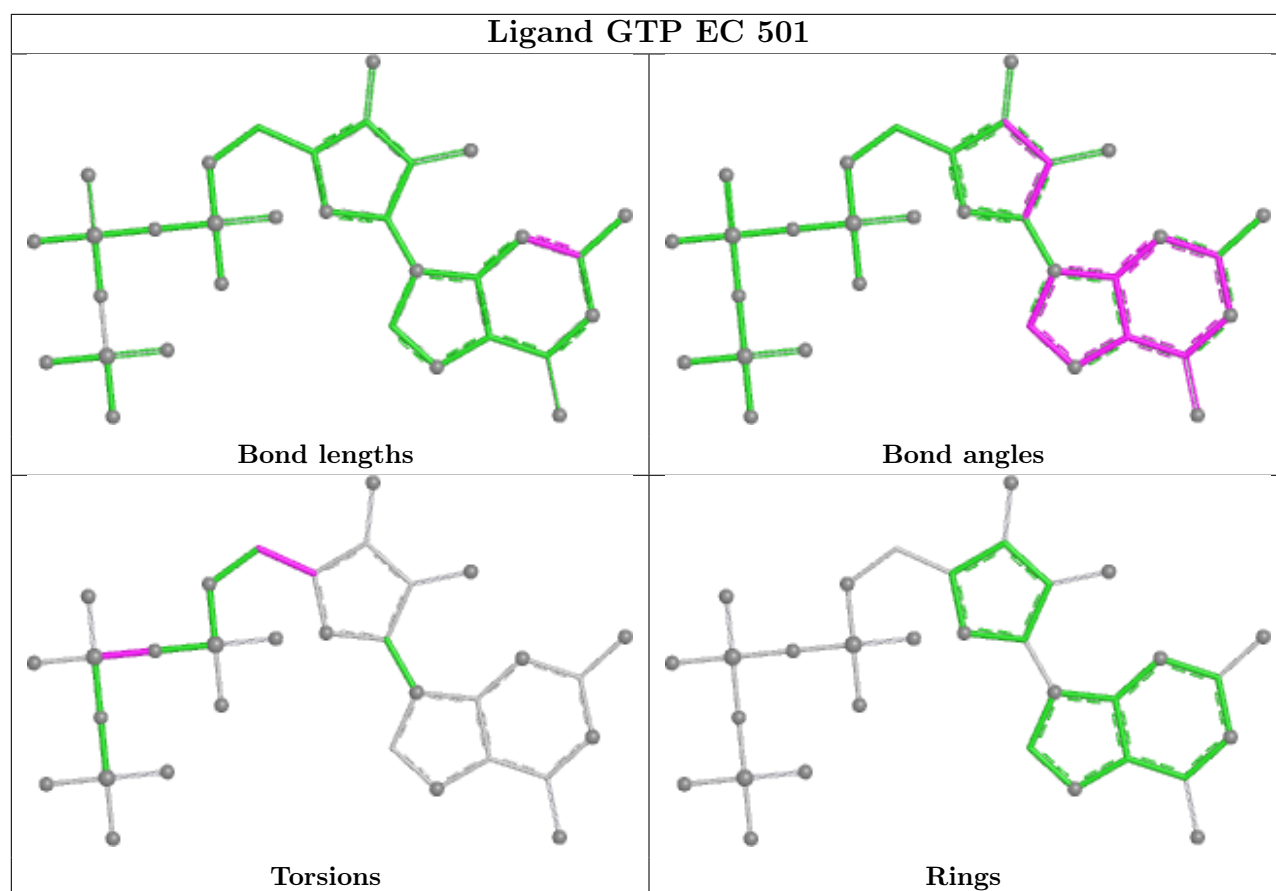


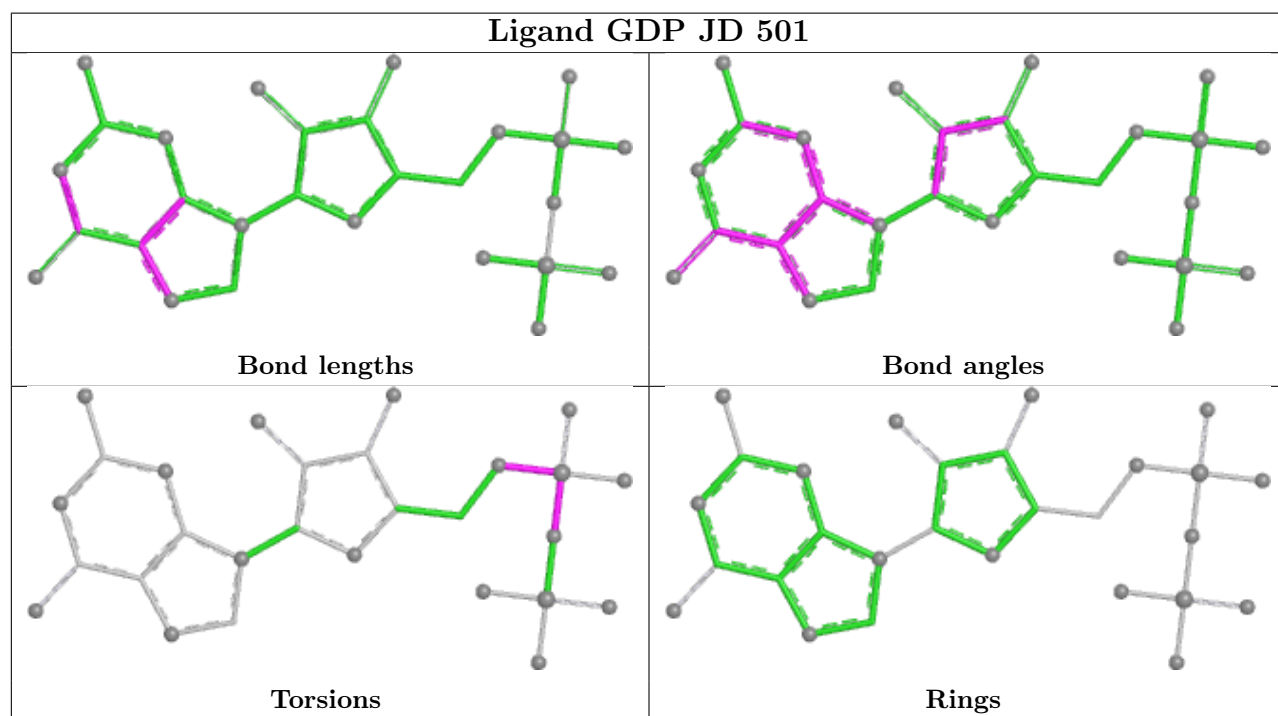
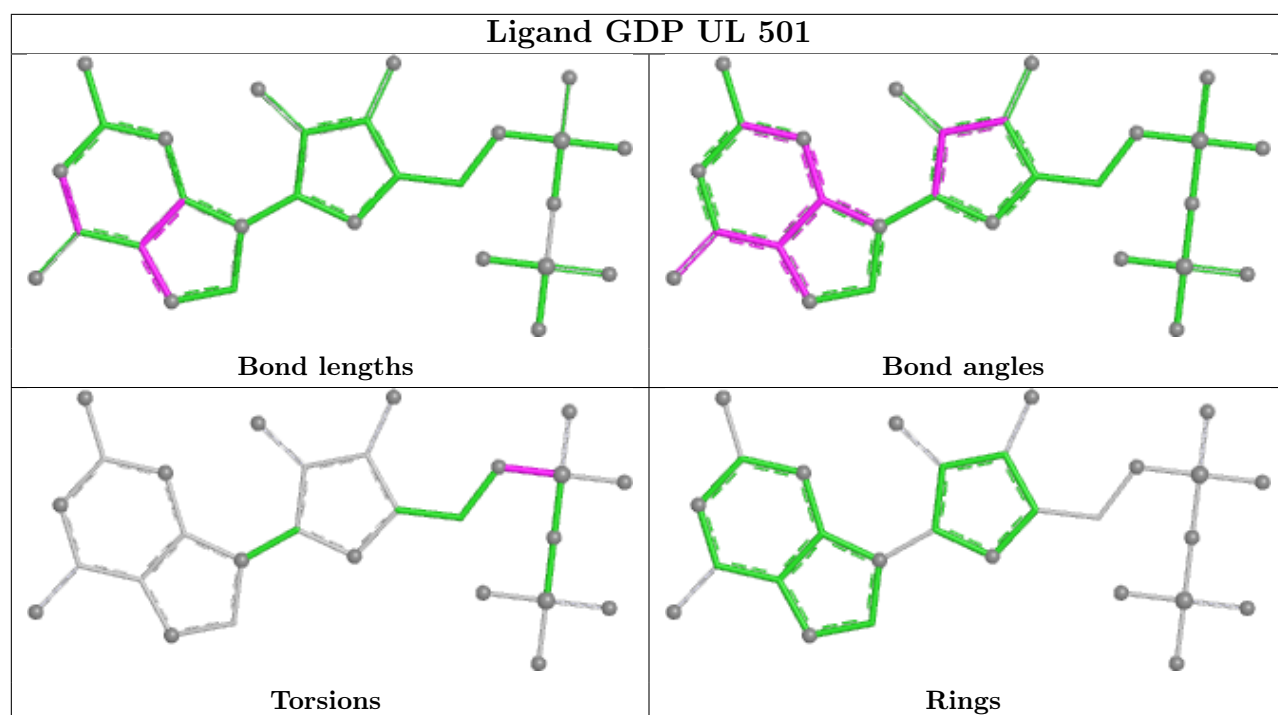
Ligand GTP VA 501

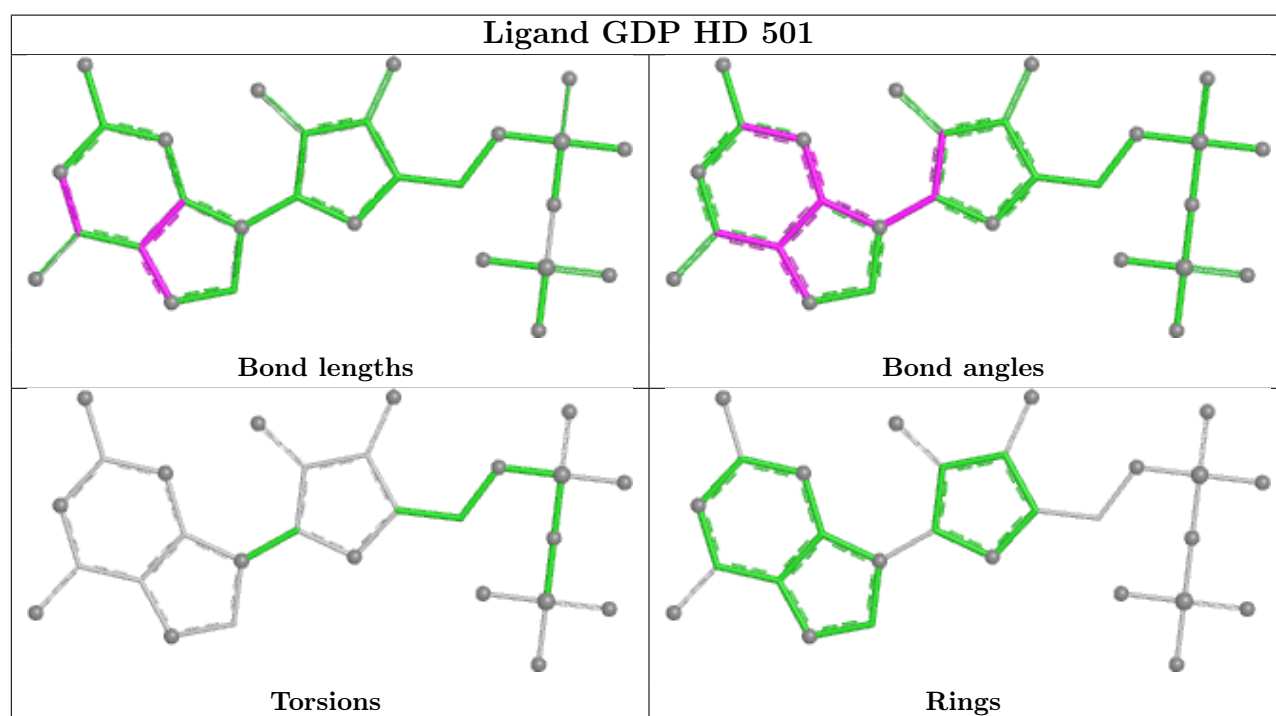
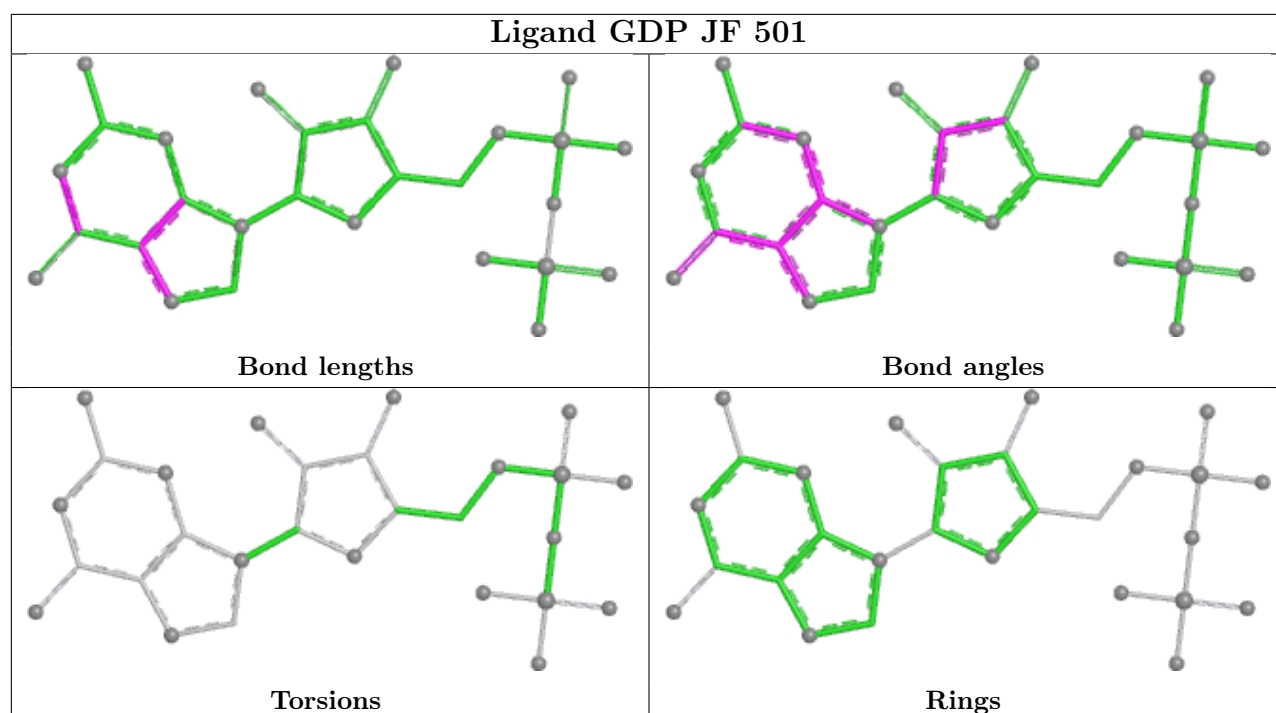


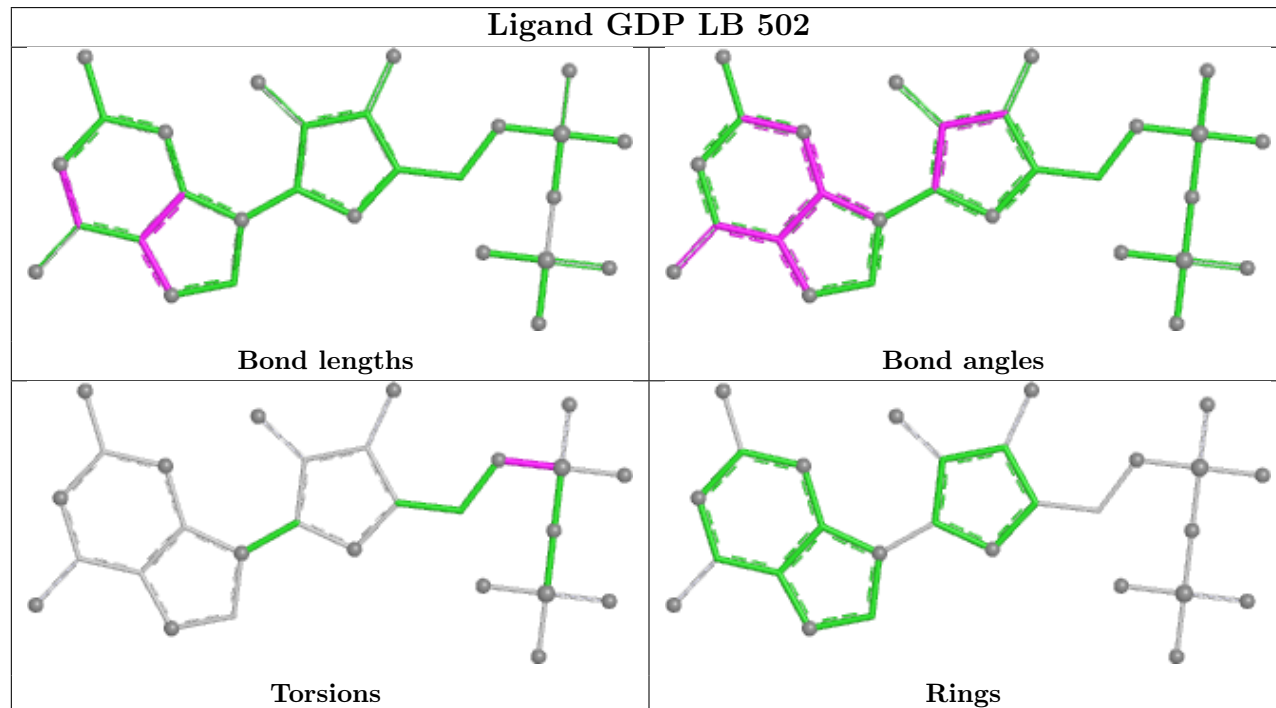
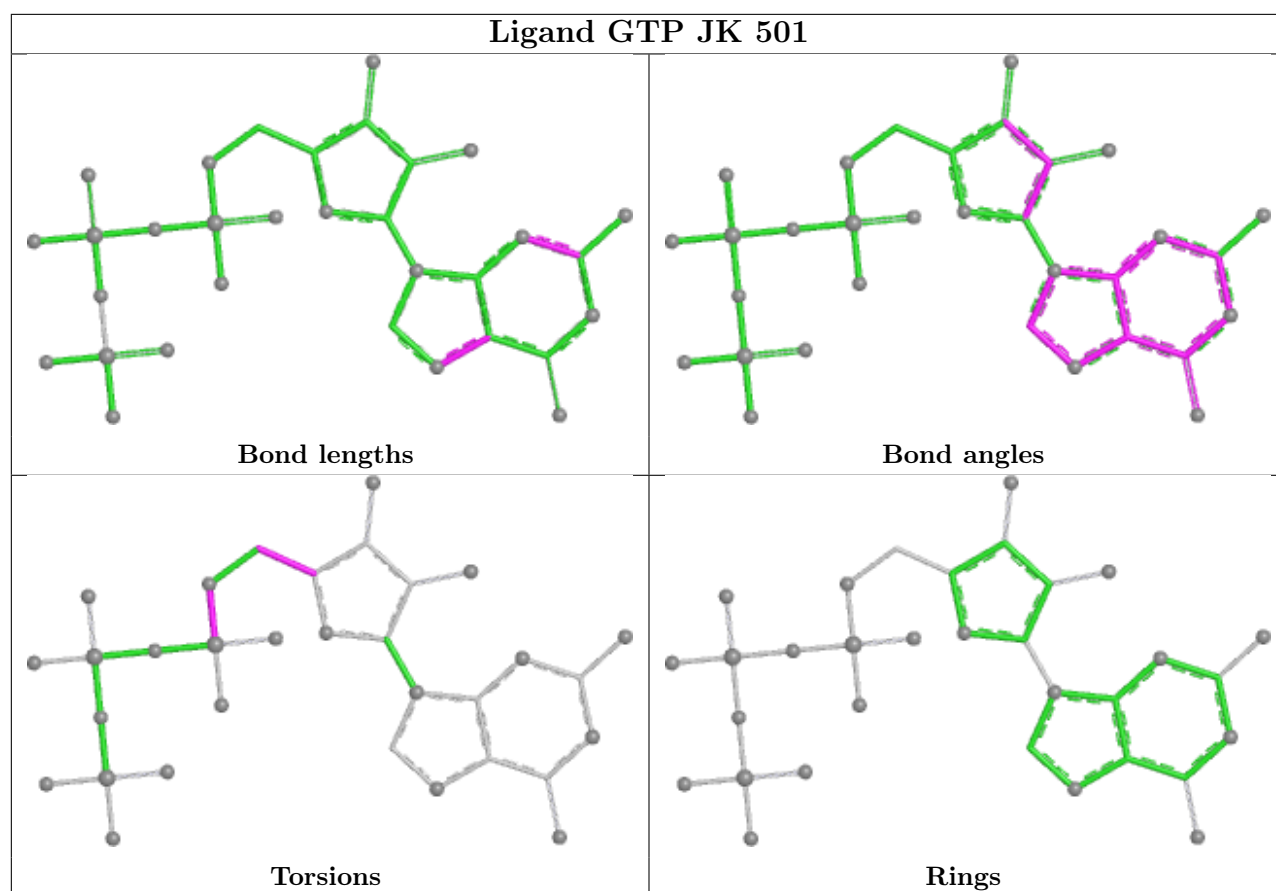
Ligand GTP QE 501

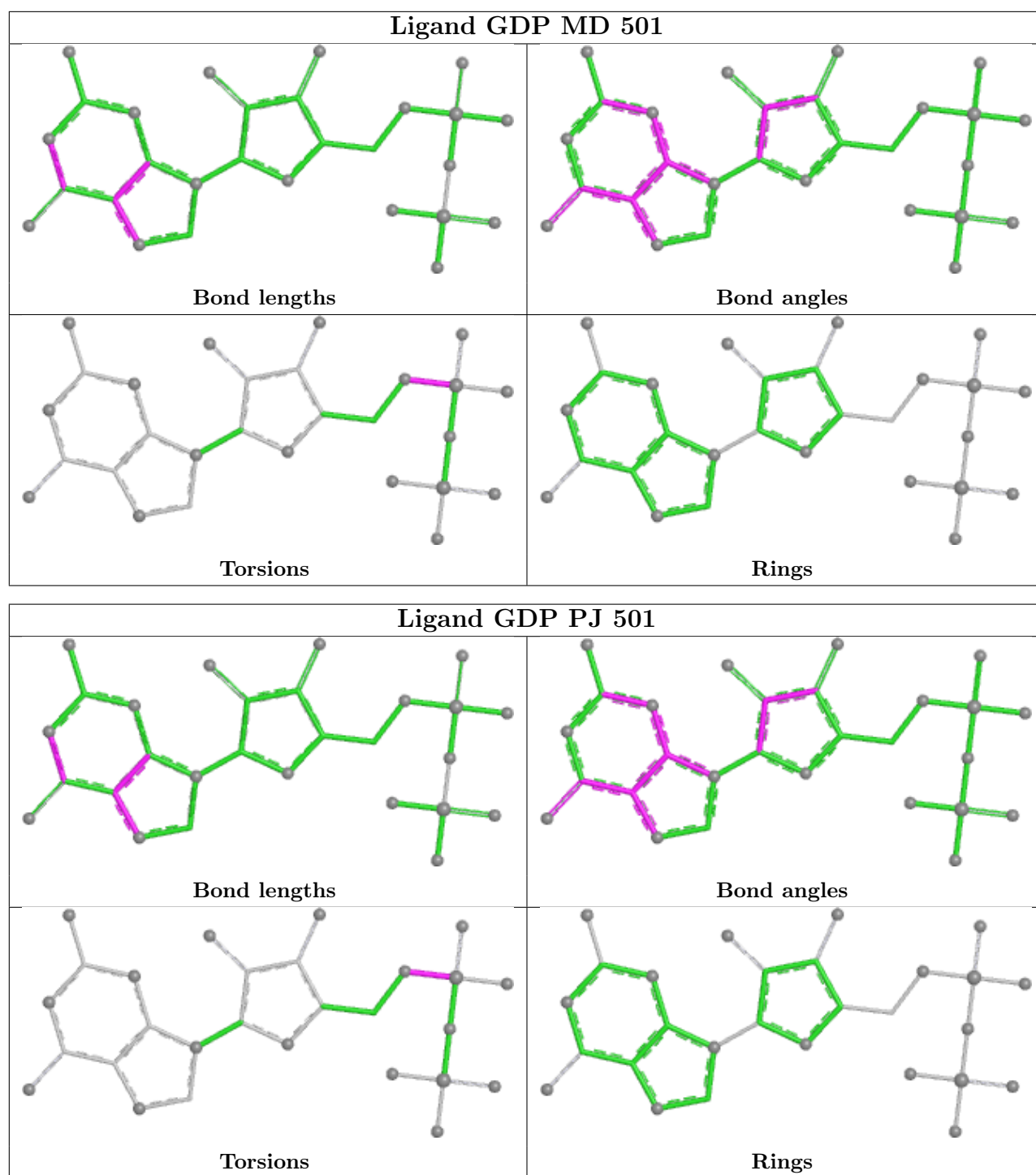




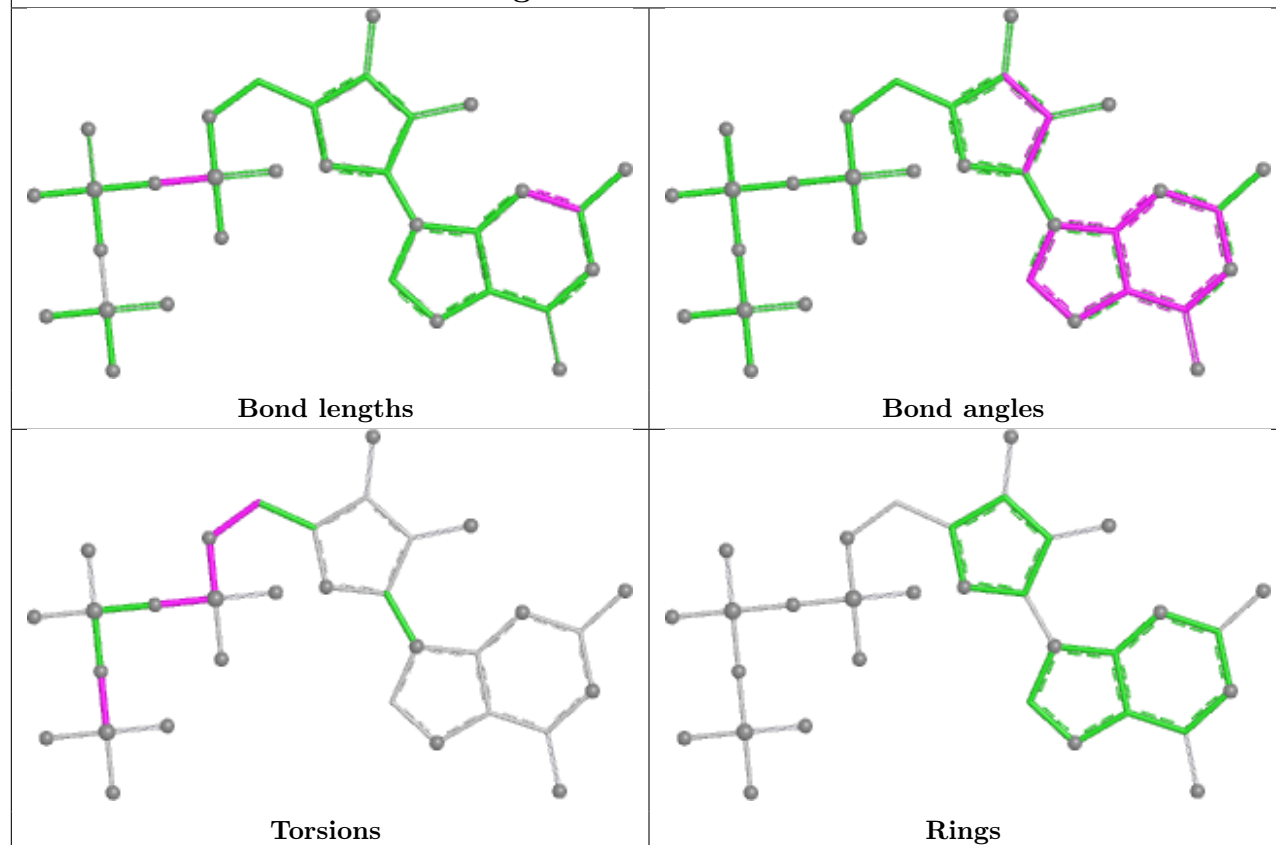




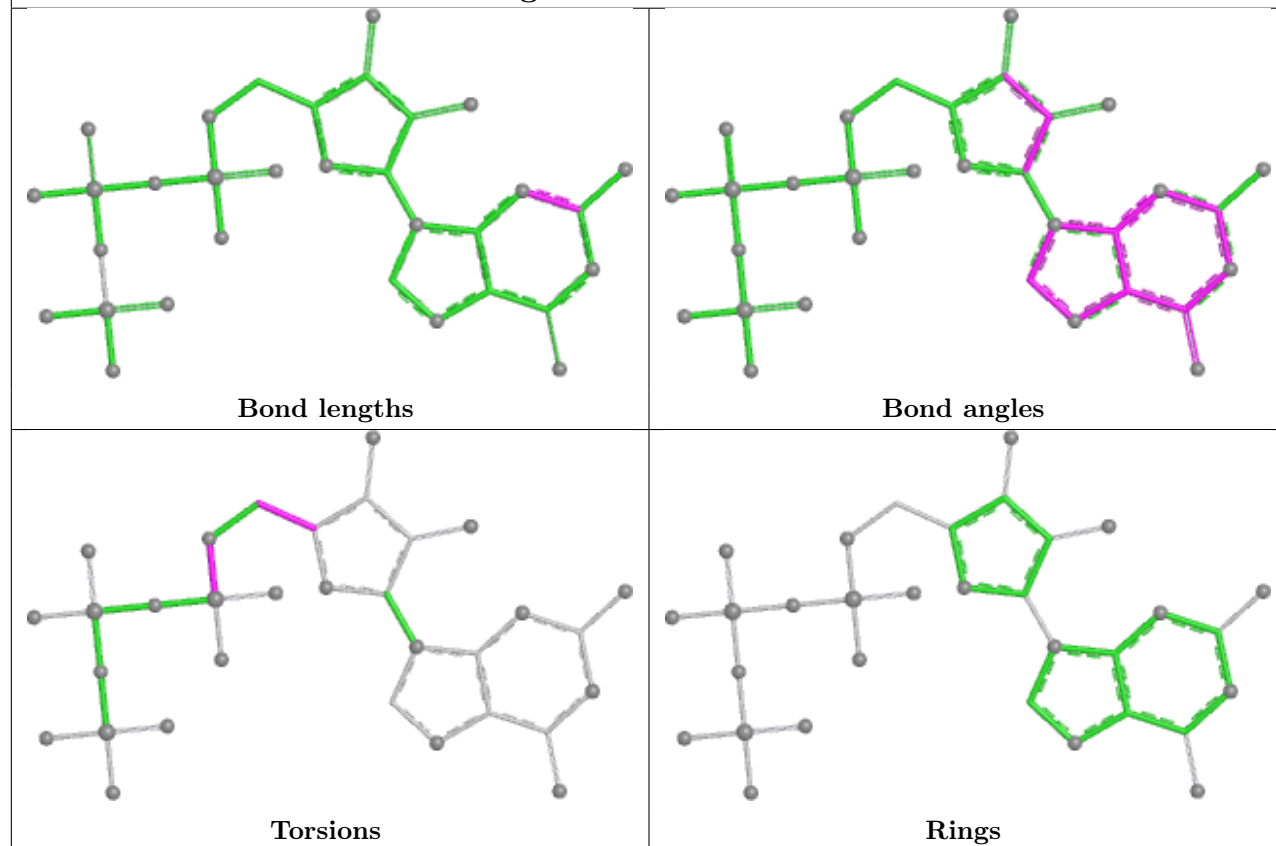


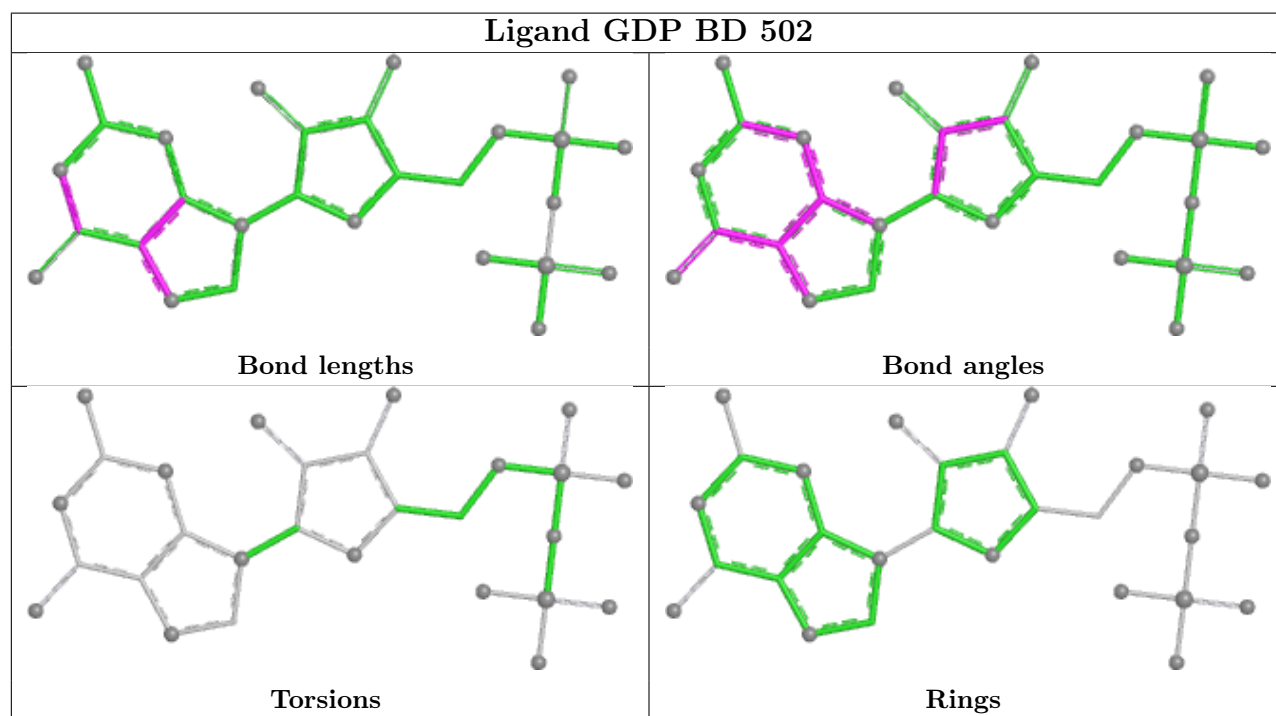
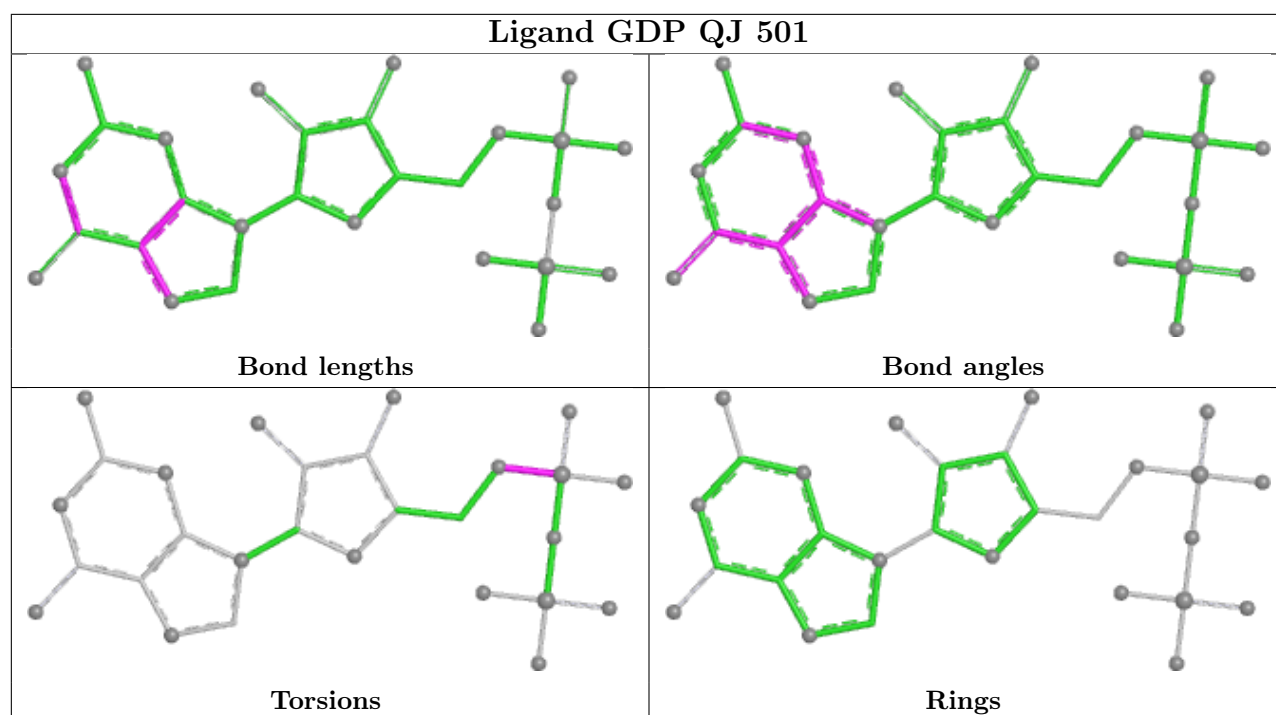


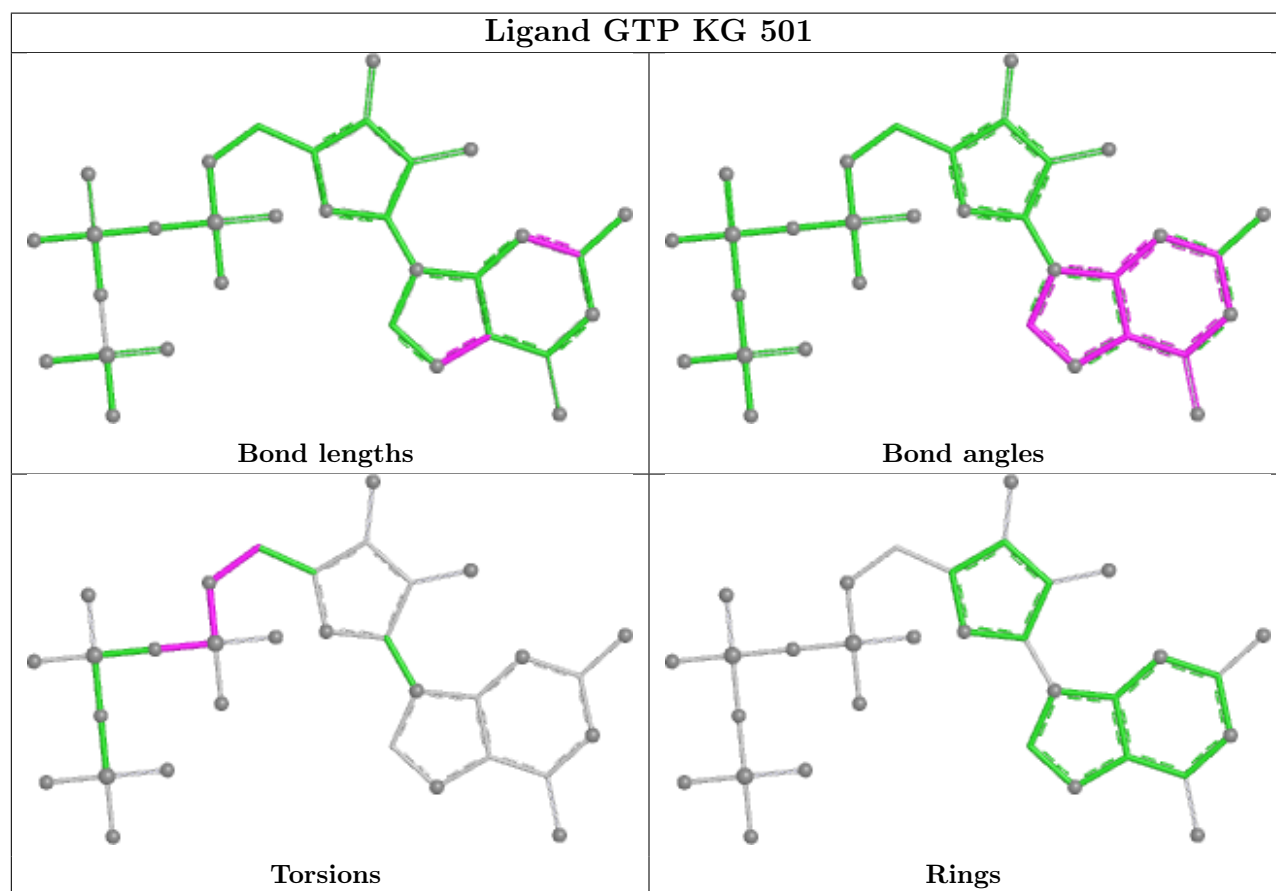
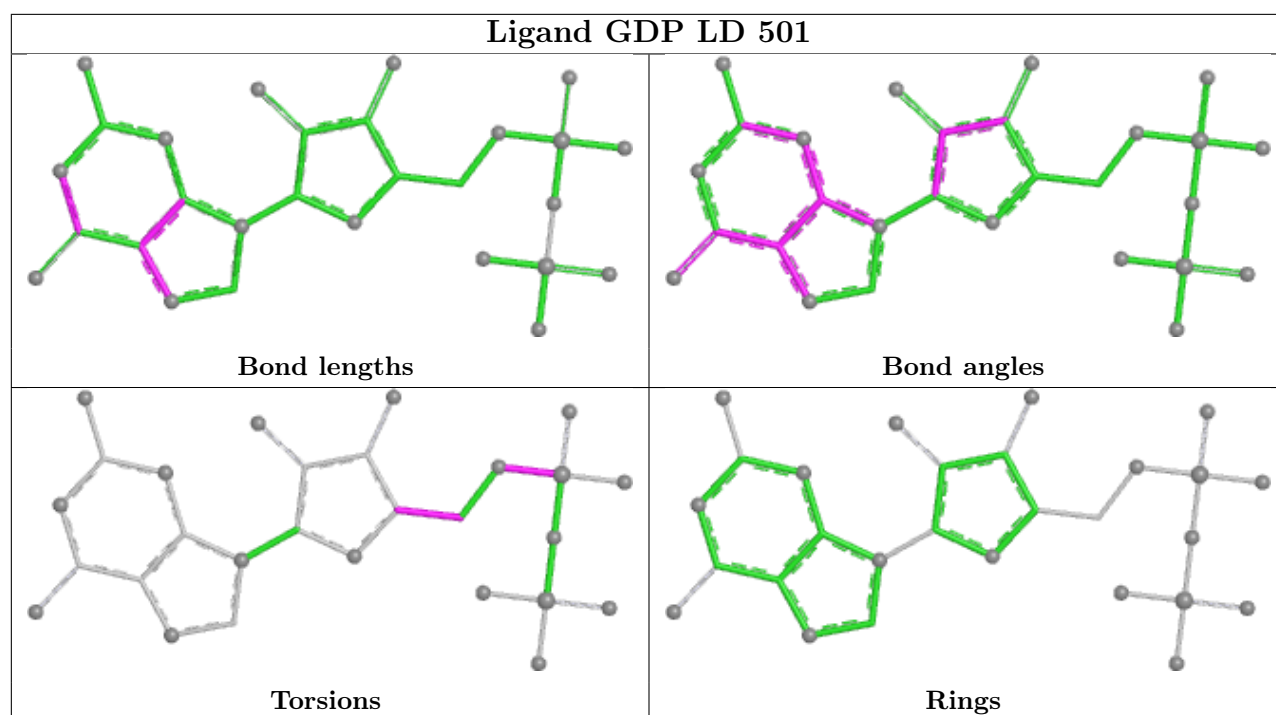
Ligand GTP VM 501

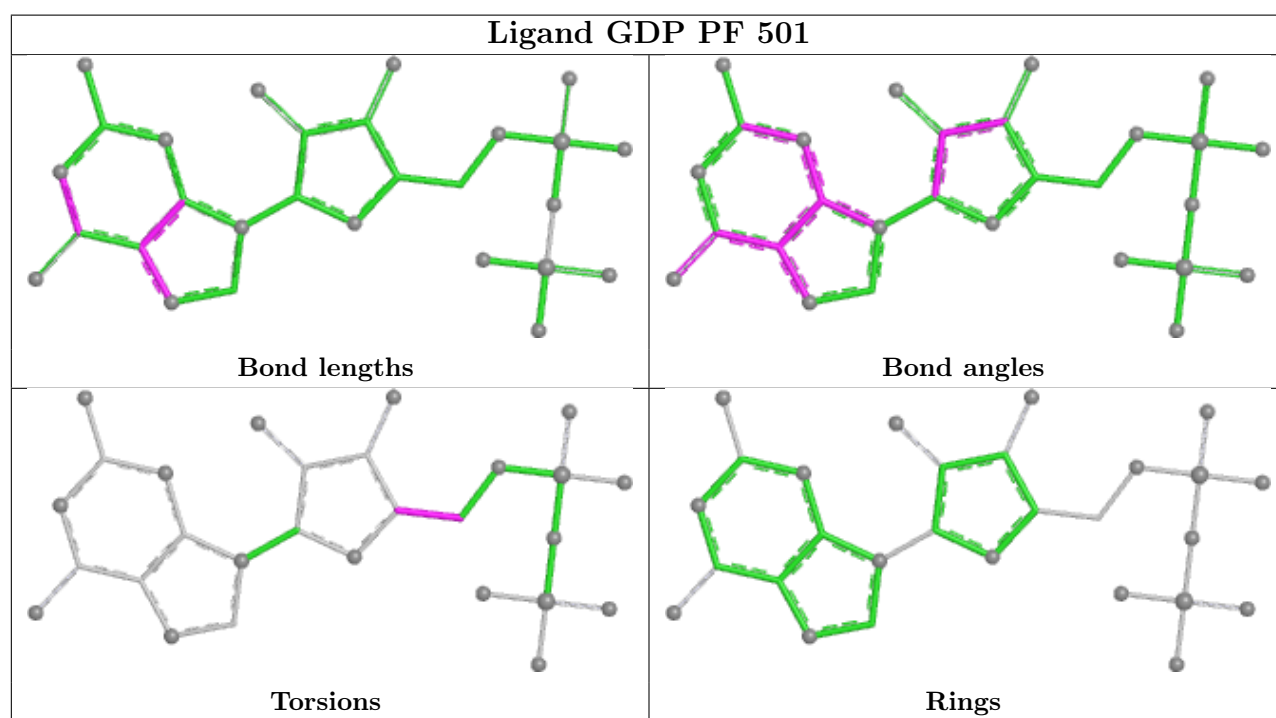
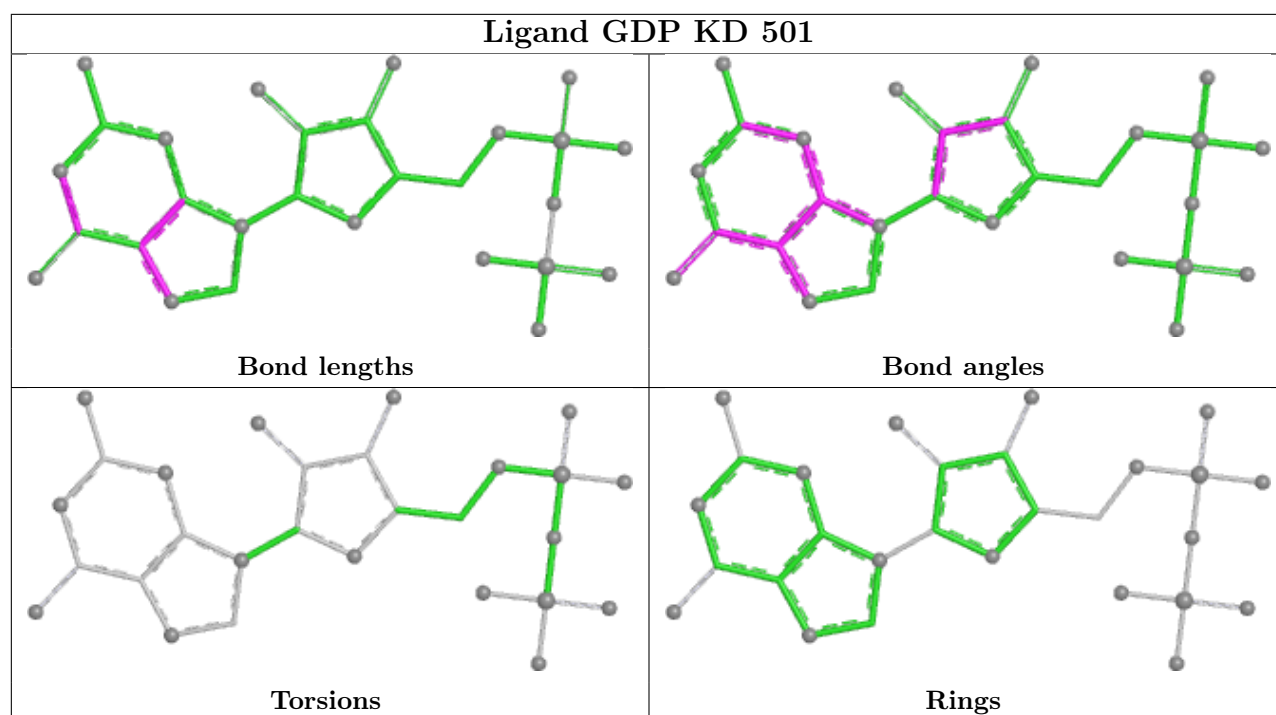


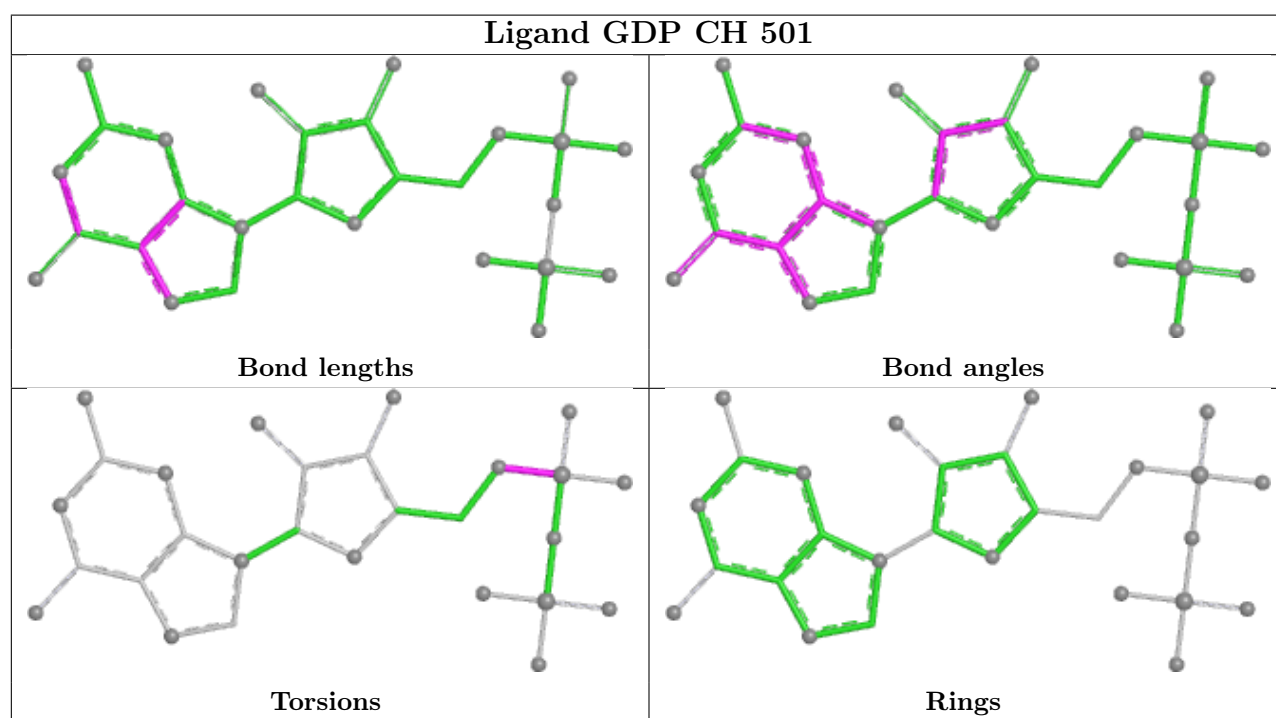
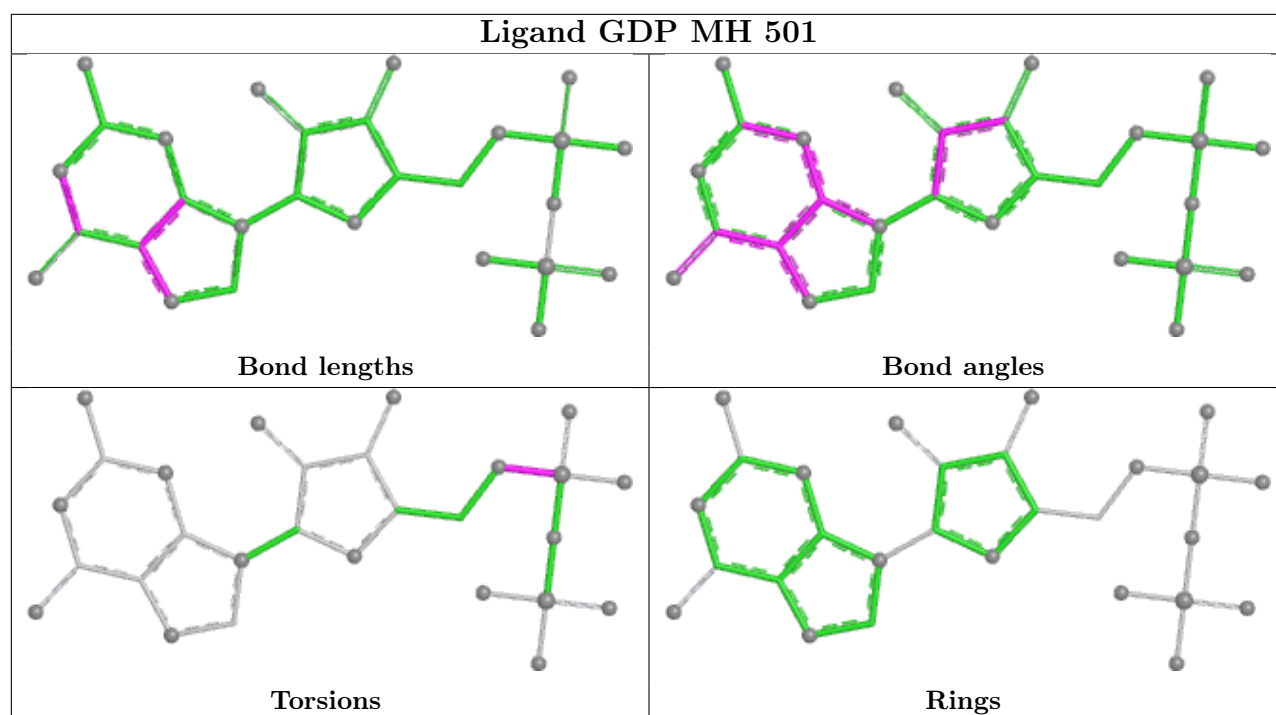
Ligand GTP LC 501

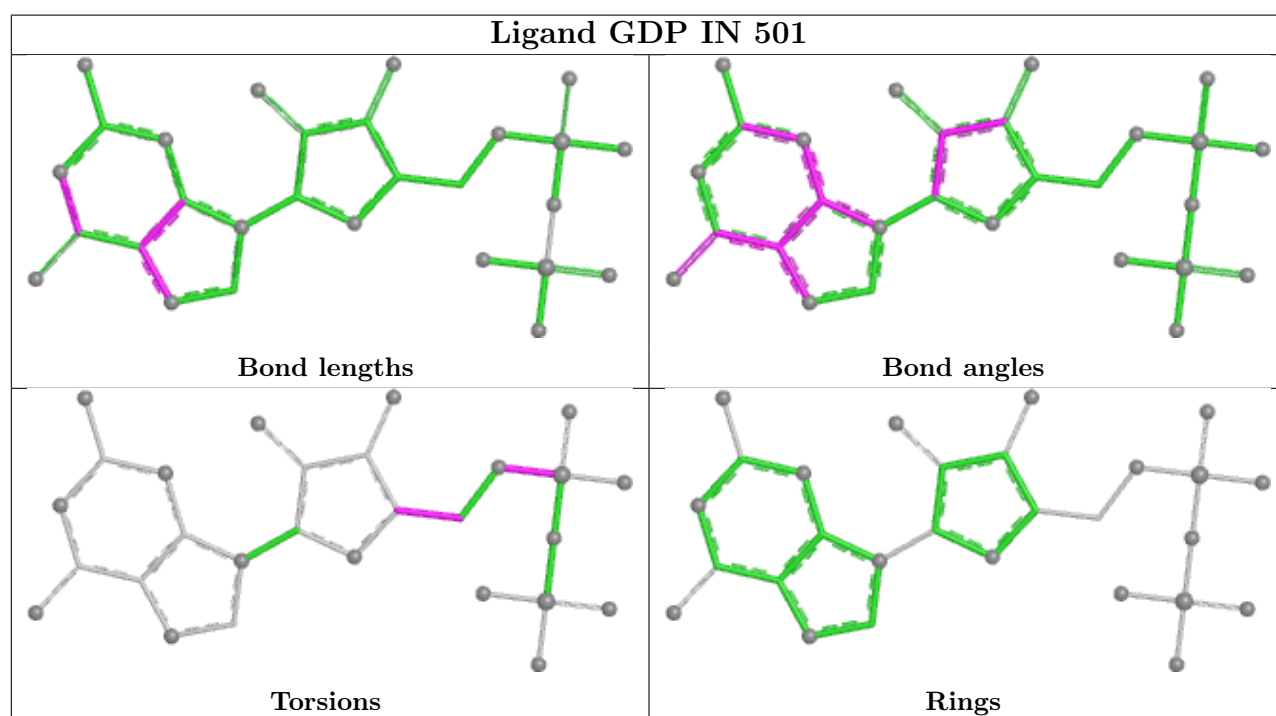
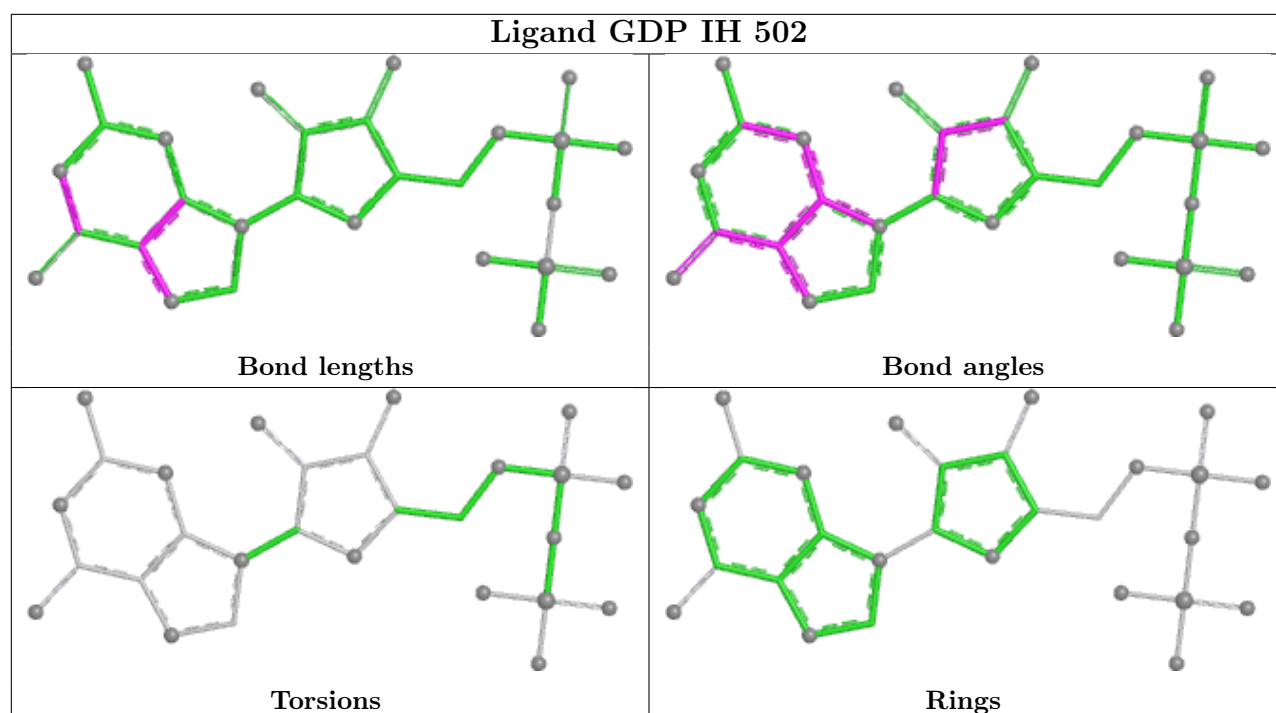




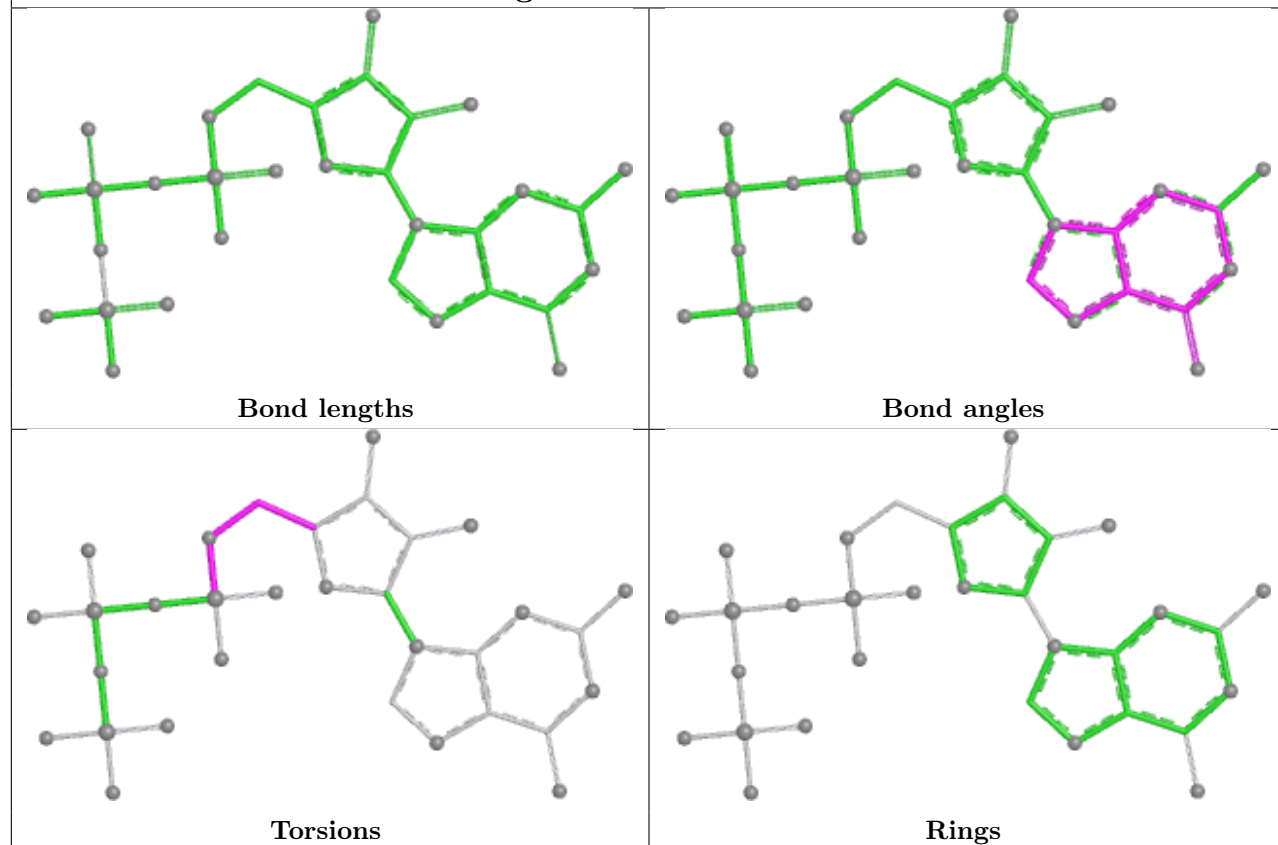




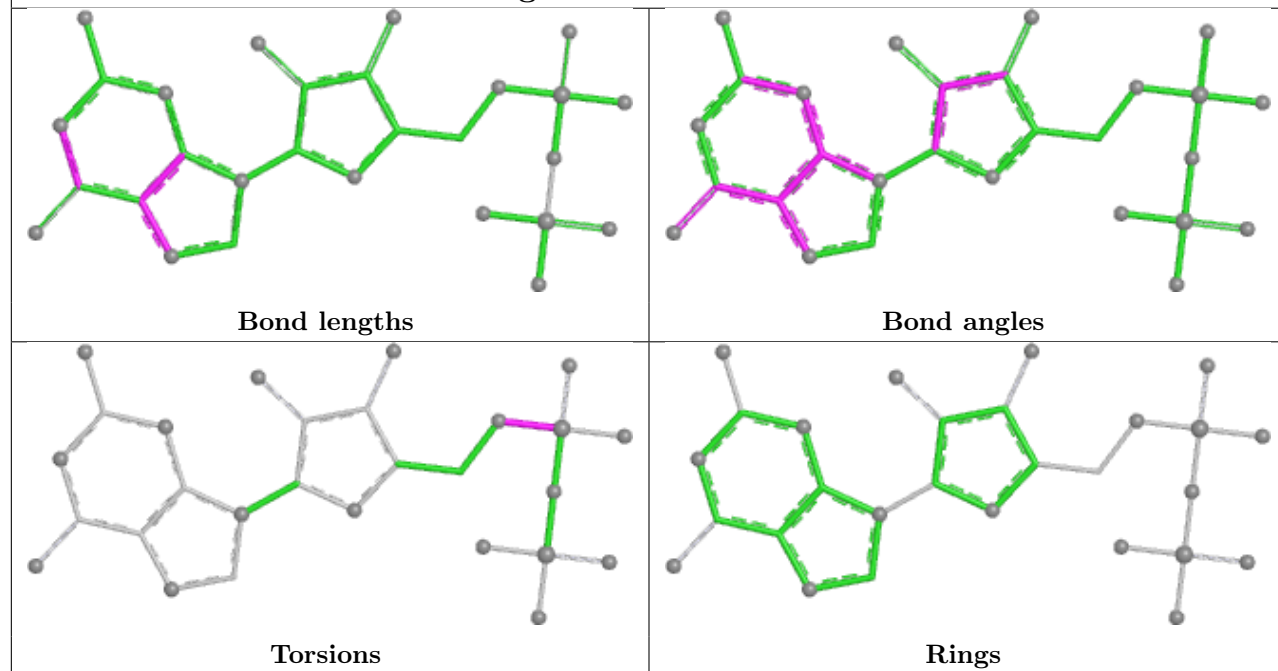




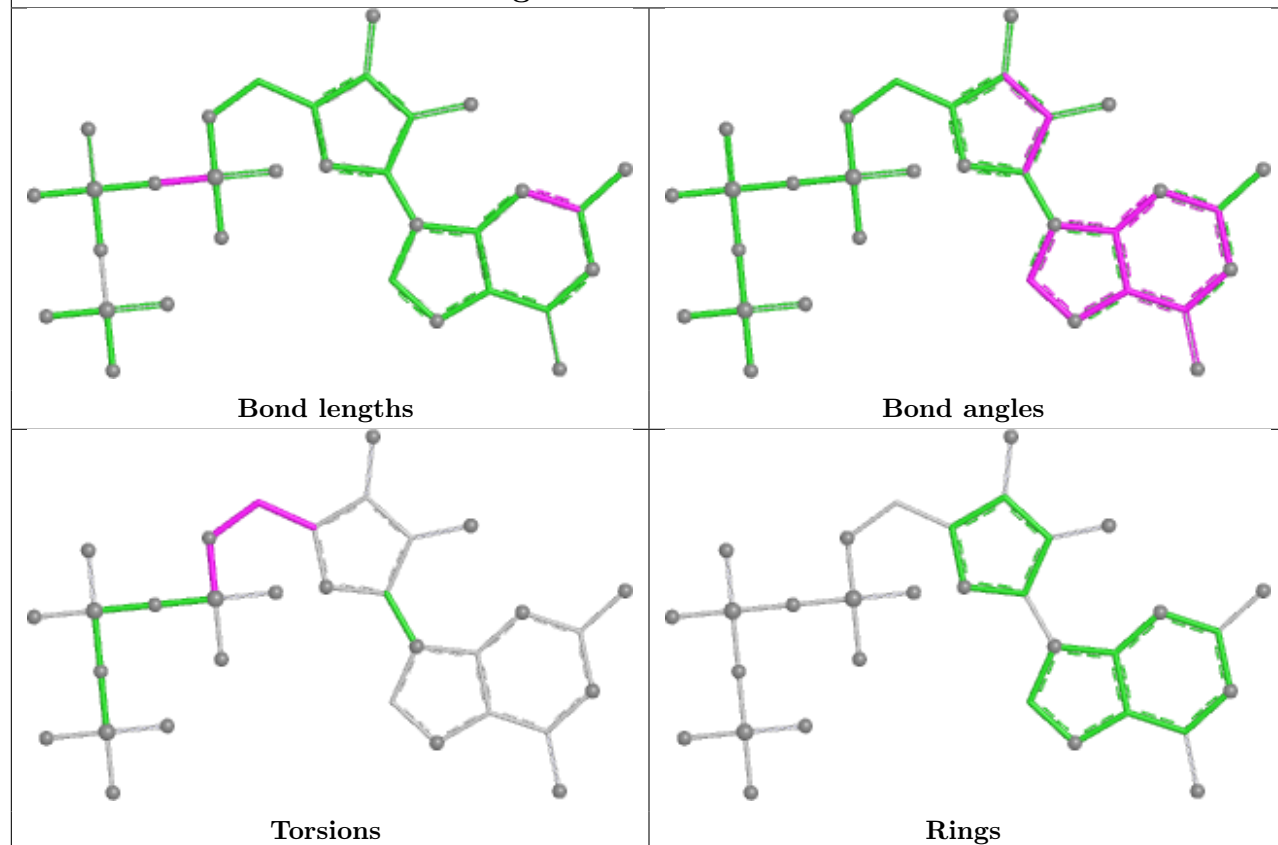
Ligand GTP NG 501



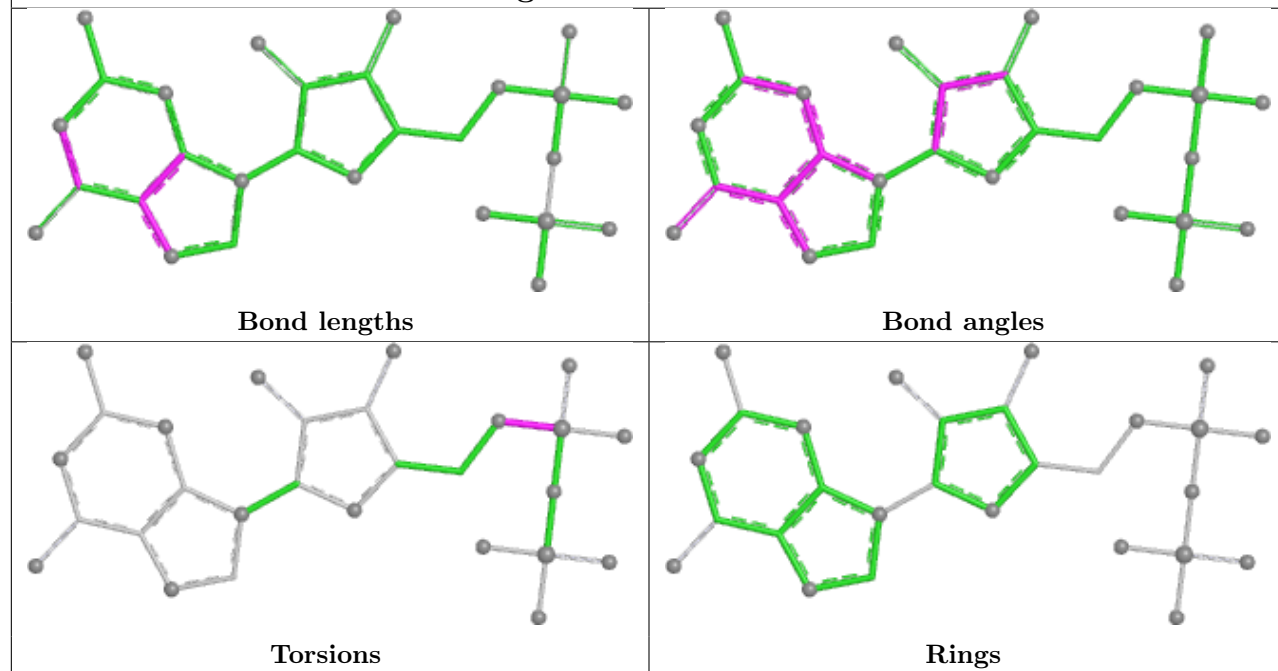
Ligand GDP SD 501



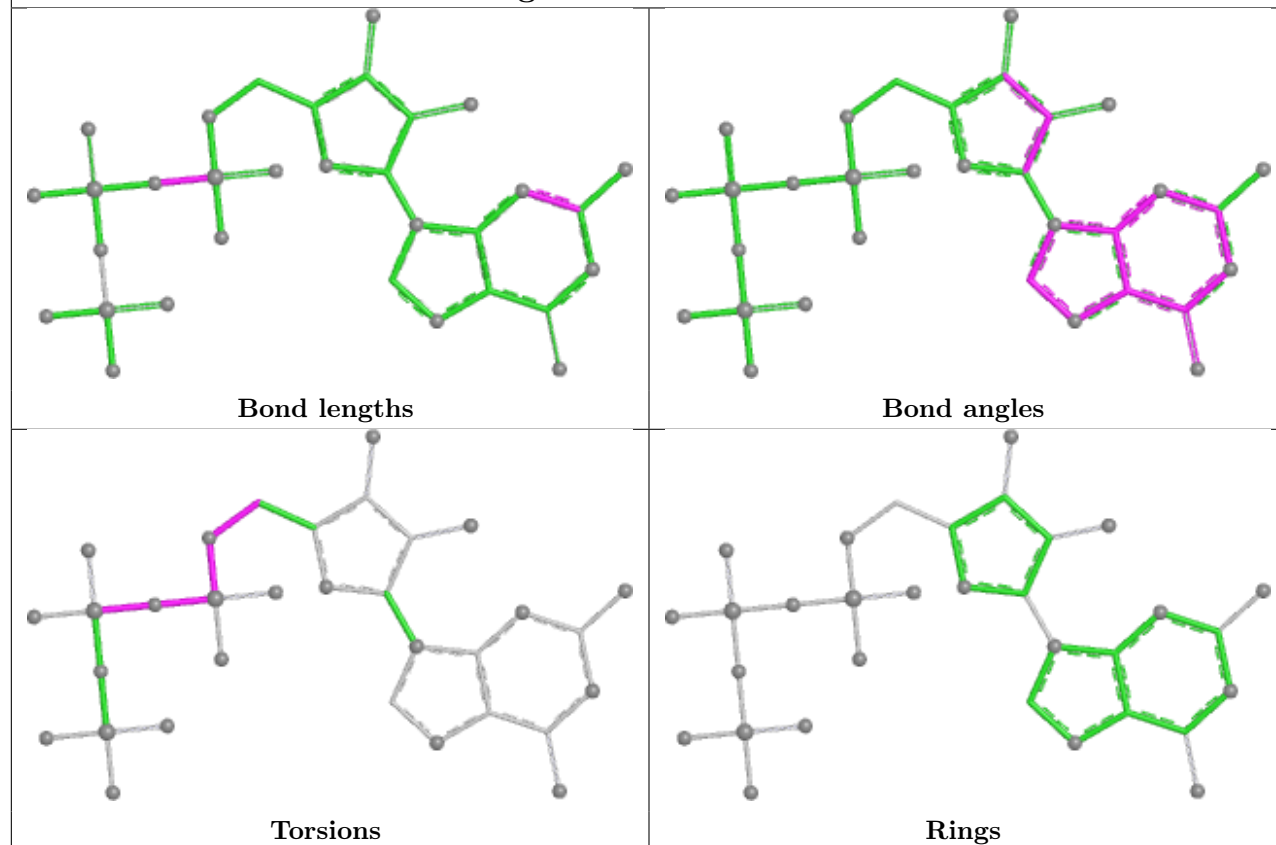
Ligand GTP WC 501



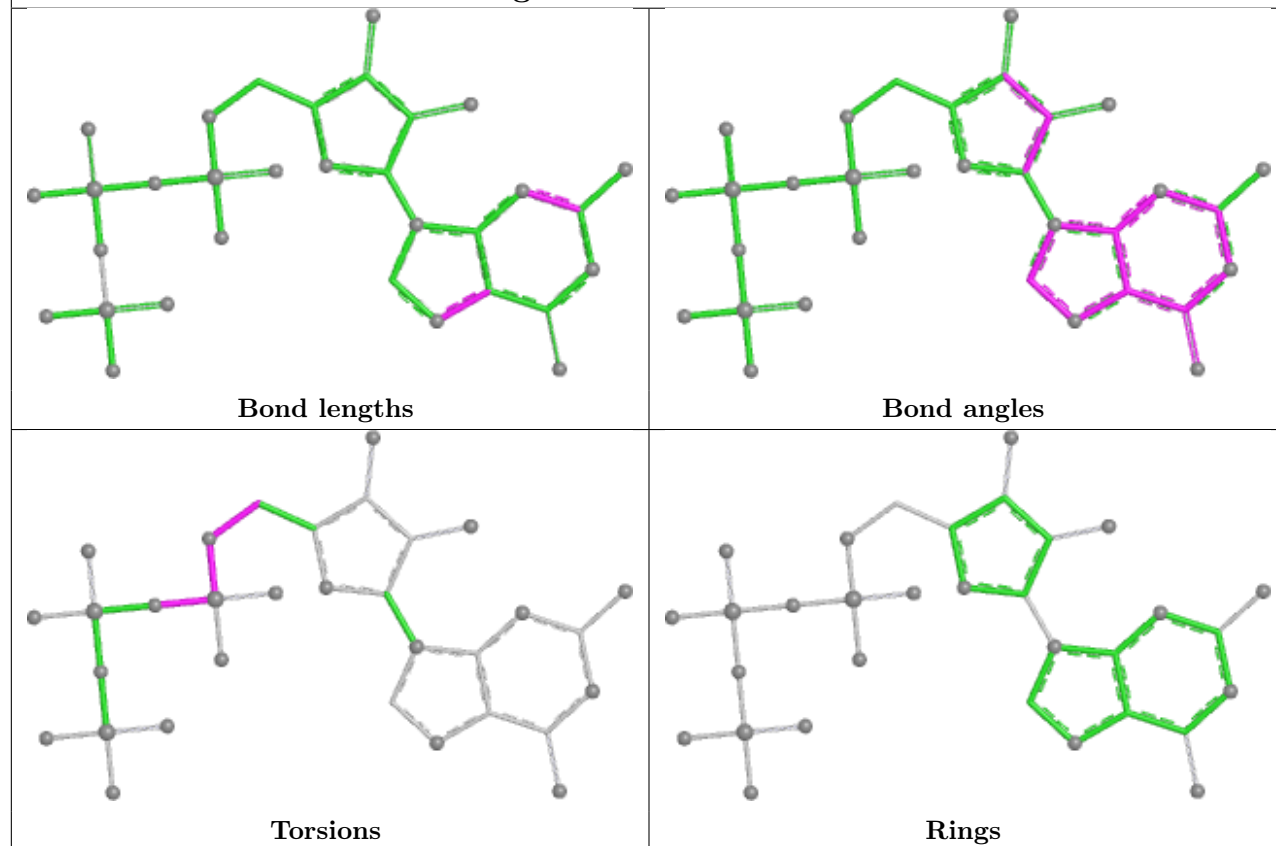
Ligand GDP FH 501



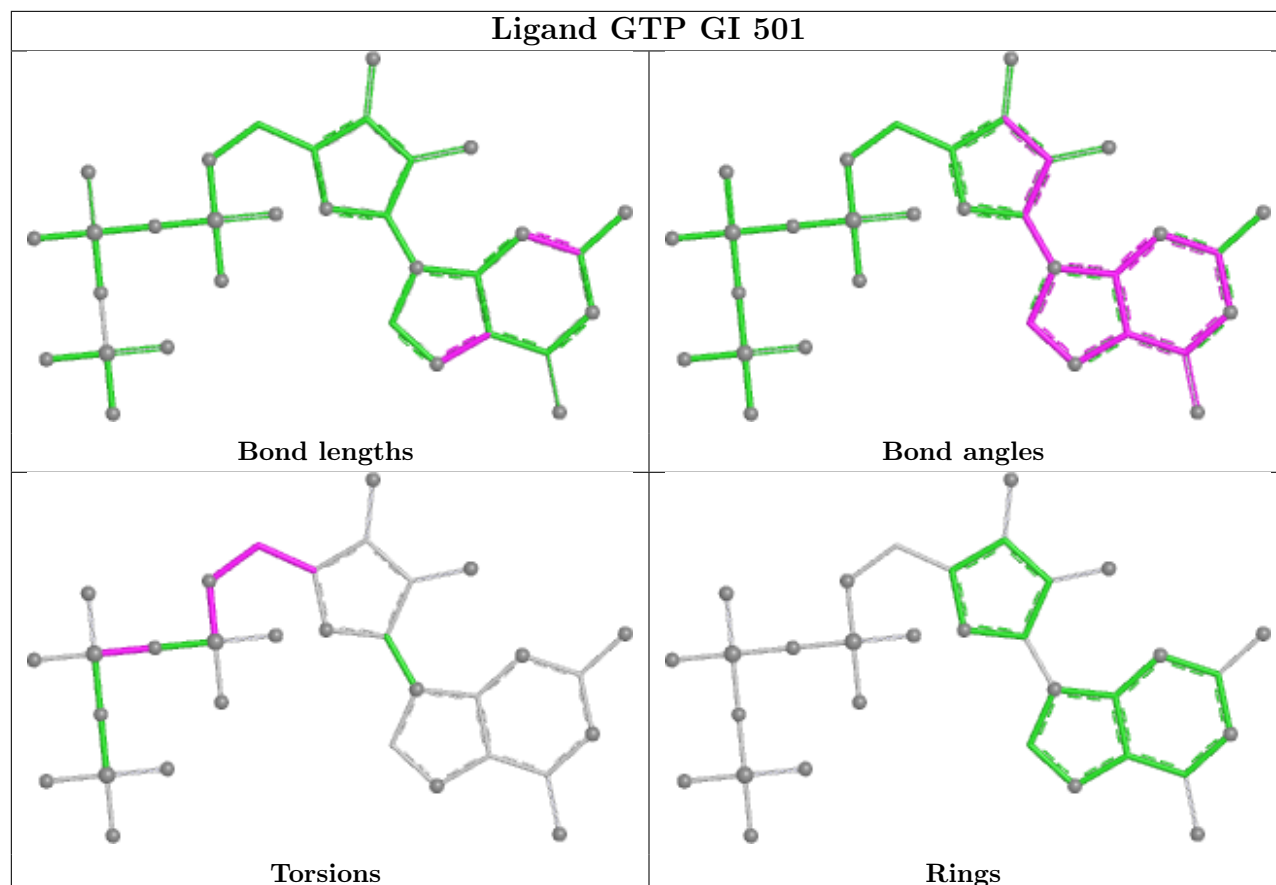
Ligand GTP UE 501



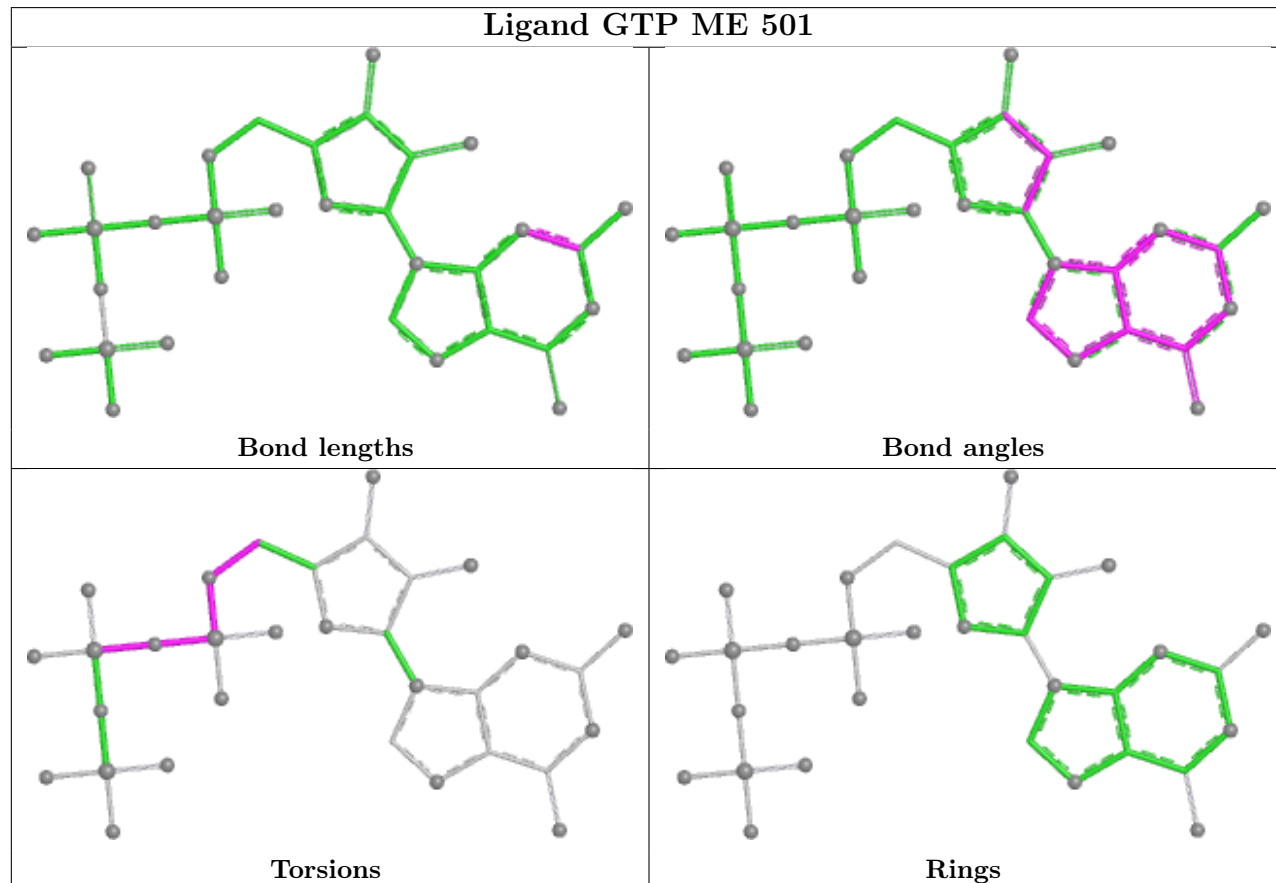
Ligand GTP UM 501

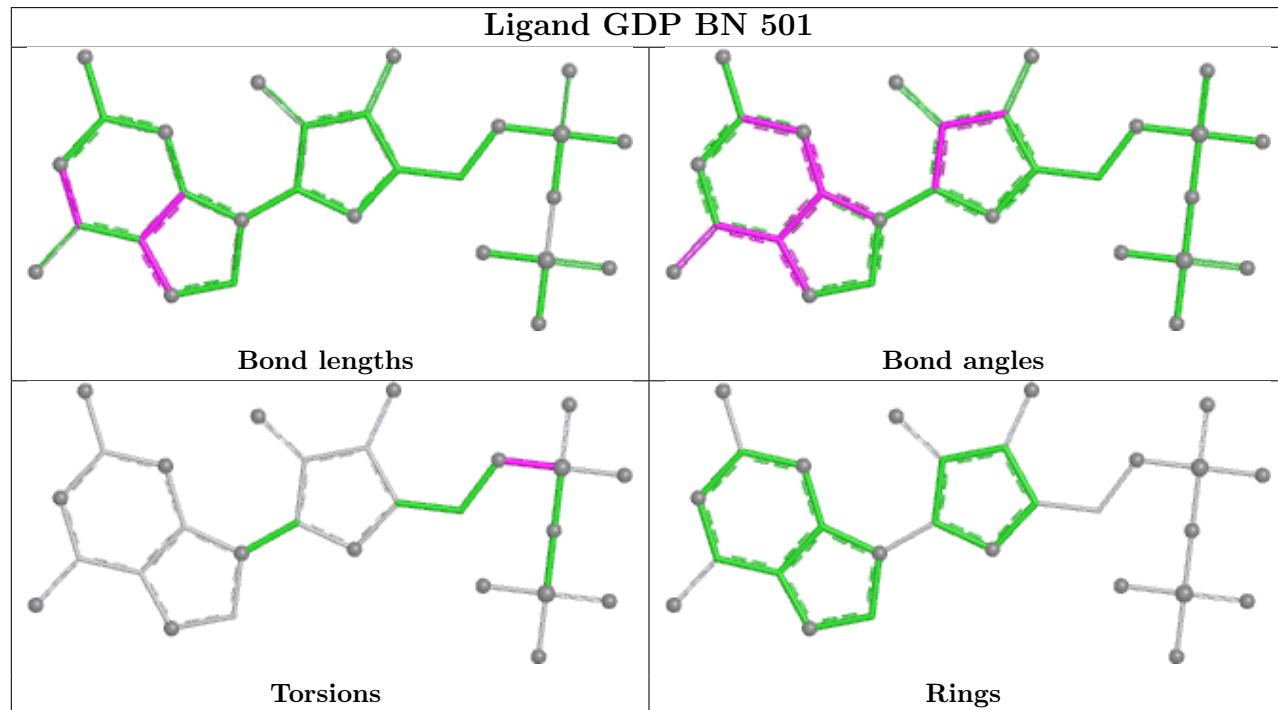
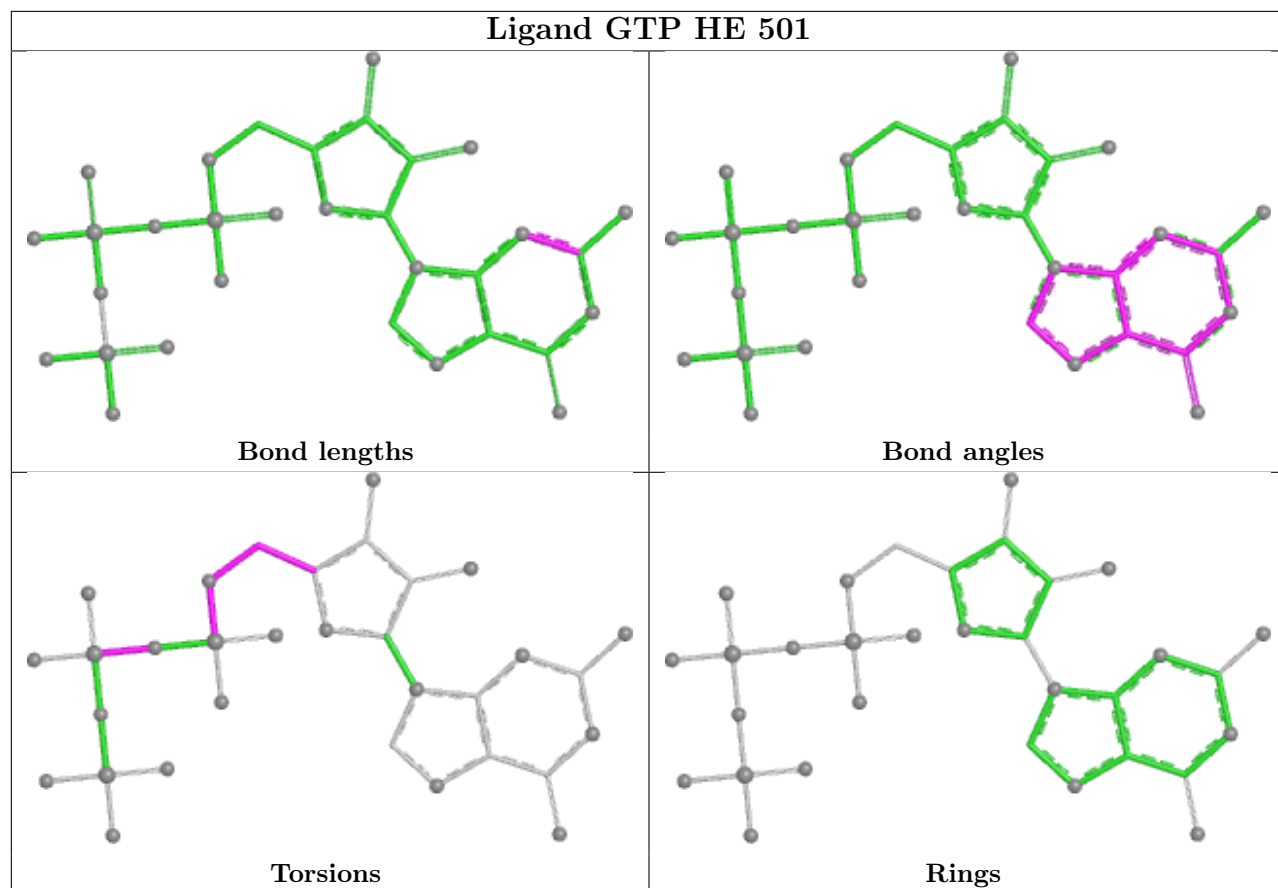


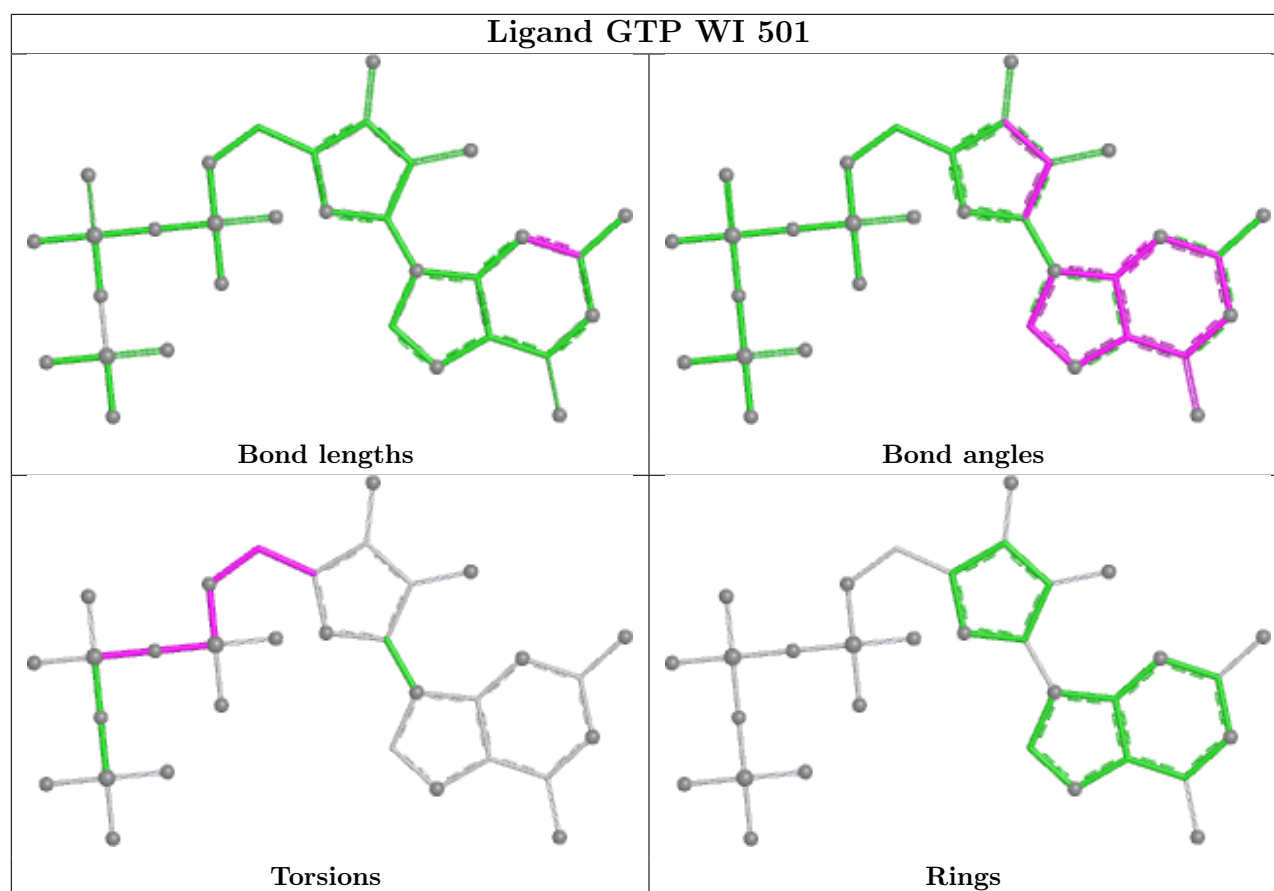
Ligand GTP GI 501



Ligand GTP ME 501







4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	1V	14
15	2V	13
15	3V	11
37	5D	6
35	7R	5
14	1U	5
14	0U	5
35	5R	5
35	4R	4
45	BH	4
44	EM	4

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
44	SM	4
26	1R	4
44	NM	4
44	ME	3
45	DJ	3
45	TN	3
45	QJ	3
45	KN	3
45	PD	3
45	UB	3
13	1T	3
44	DG	3
45	AN	3
44	SC	3
38	5G	3
45	IL	2
44	GK	2
44	MG	2
45	VN	2
45	VF	2
45	SB	2
45	GF	2
45	CL	2
45	NN	2
38	5H	2
44	TG	2
4	1C	2
44	RM	2
44	HI	2
44	VC	2
45	TH	2
45	DF	2
44	WA	2
30	2G	2
44	KK	2
44	SE	2
44	HA	2
23	1M	2
44	TM	2
40	6F	2
45	FH	2
45	AJ	2

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
13	0T	2
44	AA	2
4	0C	2
26	2R	2
45	DB	2
26	3R	2
45	MF	2
44	LE	2
44	EK	2
45	HB	2
44	CK	2
44	AC	2
42	8L	1
44	FG	1
45	CH	1
9	1H	1
45	MB	1
44	PI	1
45	VL	1
6	2E	1
44	EE	1
44	RG	1
45	BJ	1
45	VD	1
45	GH	1
45	JF	1
45	WH	1
45	GN	1
45	JL	1
44	UC	1
38	5F	1
44	AM	1
45	UD	1
44	WC	1
44	OA	1
45	WJ	1
44	WK	1
44	QM	1
44	BG	1
44	GC	1
44	GM	1
13	2T	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
45	JJ	1
45	QF	1
12	2S	1
45	DL	1
44	WG	1
24	3O	1
44	MI	1
44	SG	1
18	1F	1
44	BK	1
44	UK	1
45	ML	1
44	CG	1

The worst 5 of 245 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	8L	213:UNK	C	263:UNK	N	38.22
1	3V	1:MET	C	2:GLU	N	15.78
1	ME	433:GLU	C	434:GLU	N	14.54
1	IL	87:PRO	C	88:ASP	N	14.40
1	DJ	279:GLN	C	280:GLN	N	12.77

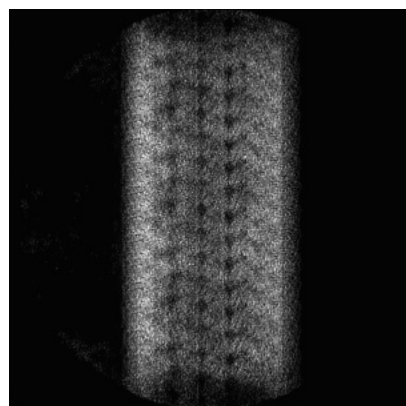
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40436. These allow visual inspection of the internal detail of the map and identification of artifacts.

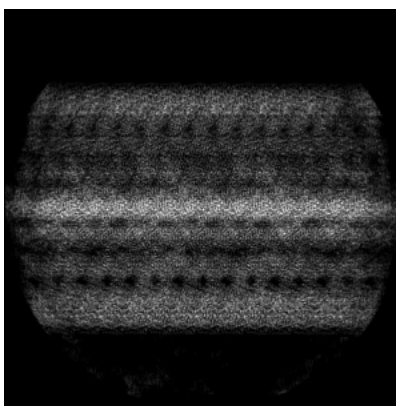
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

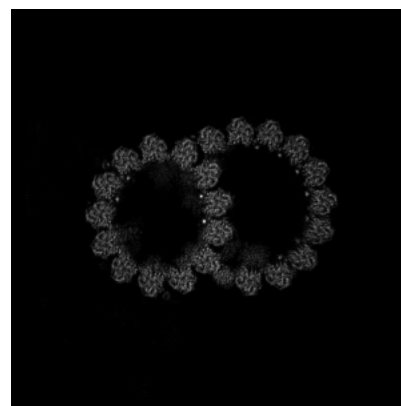
5.1.1 Primary map



X

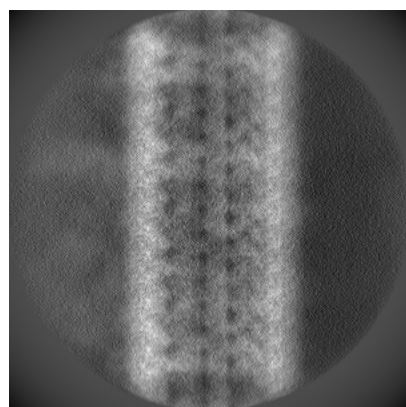


Y

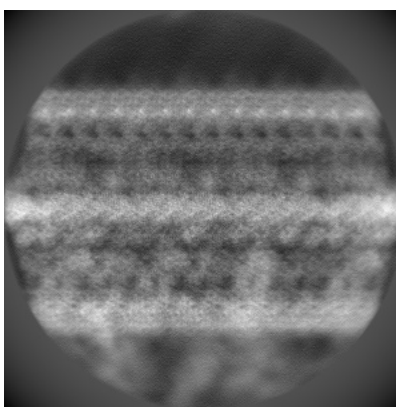


Z

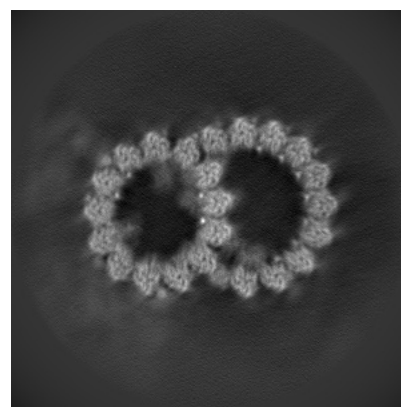
5.1.2 Raw map



X



Y

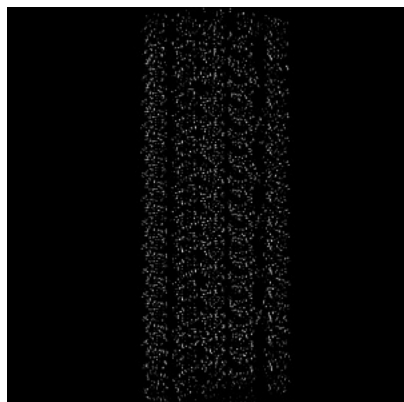


Z

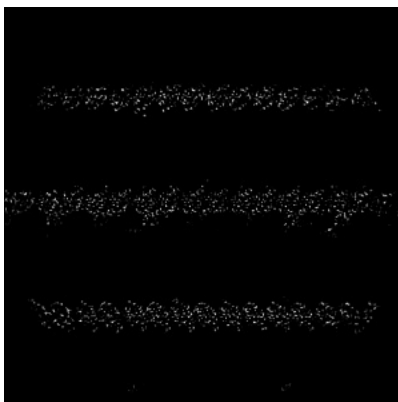
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

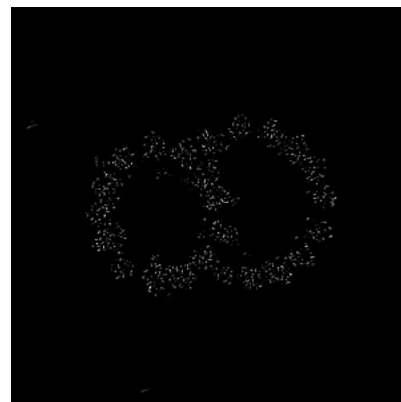
5.2.1 Primary map



X Index: 256

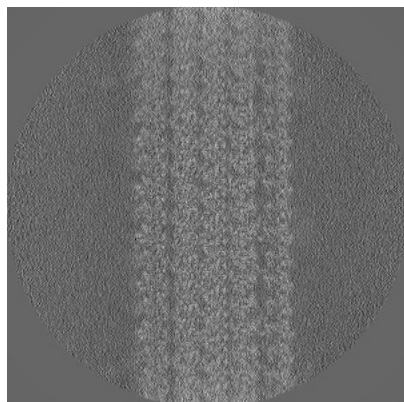


Y Index: 256

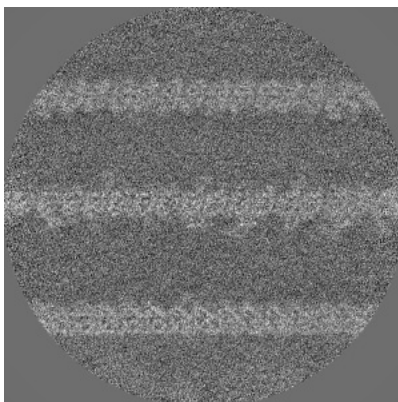


Z Index: 256

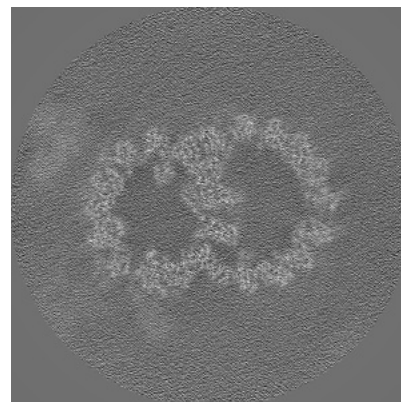
5.2.2 Raw map



X Index: 256



Y Index: 256

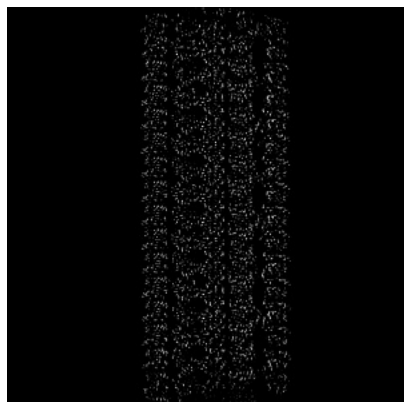


Z Index: 256

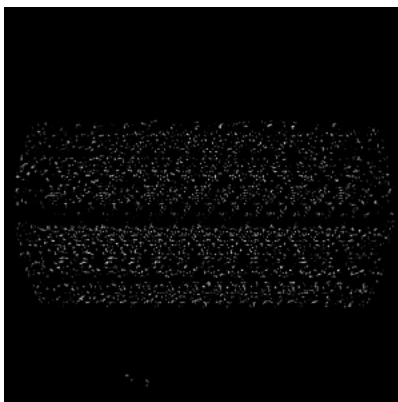
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

5.3.1 Primary map



X Index: 255

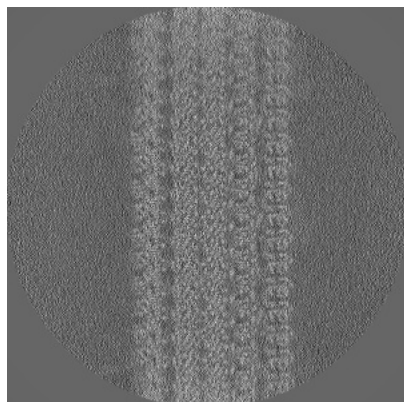


Y Index: 173

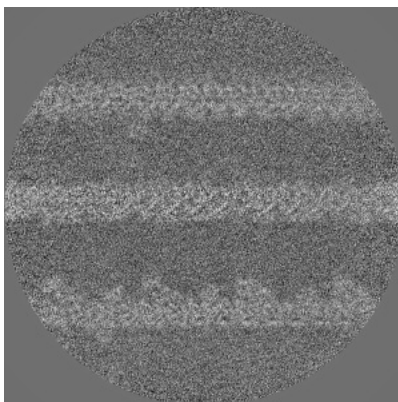


Z Index: 200

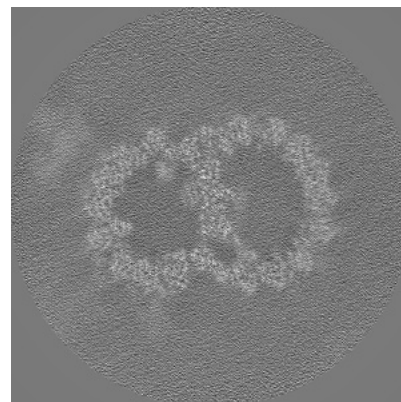
5.3.2 Raw map



X Index: 258



Y Index: 225

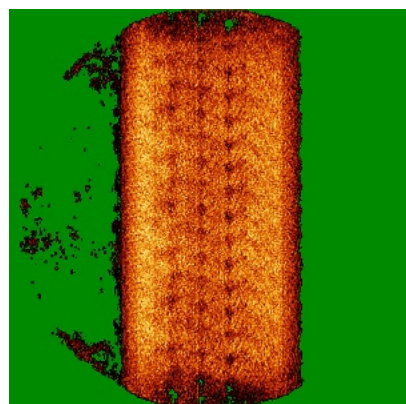


Z Index: 262

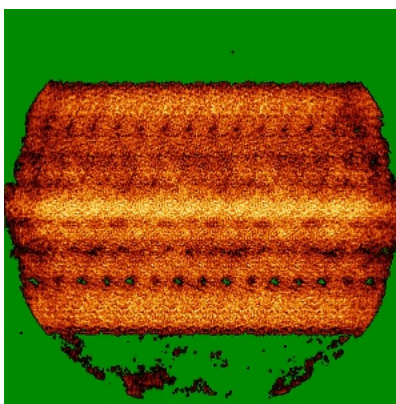
The images above show the largest variance slices of the map in three orthogonal directions.

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

5.4.1 Primary map



X

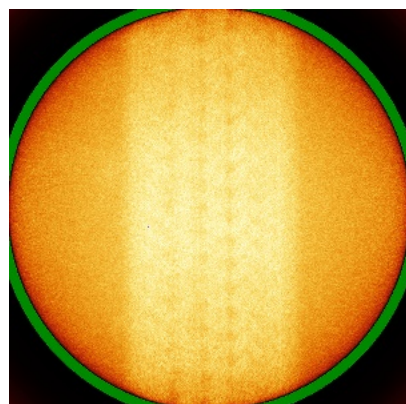


Y

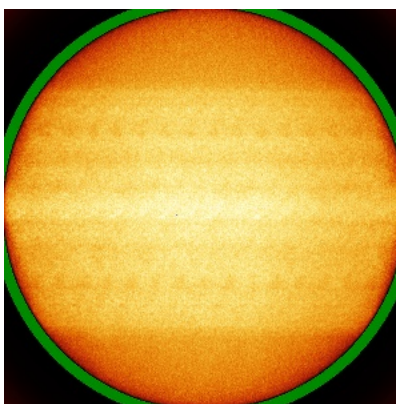


Z

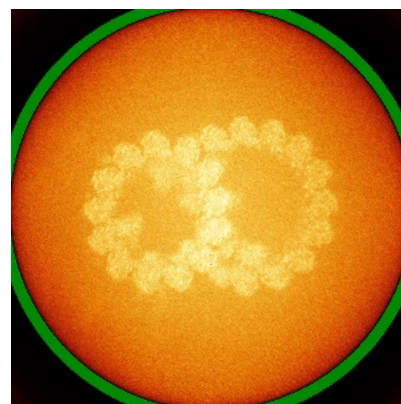
5.4.2 Raw map



X



Y

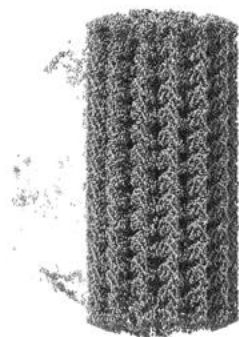


Z

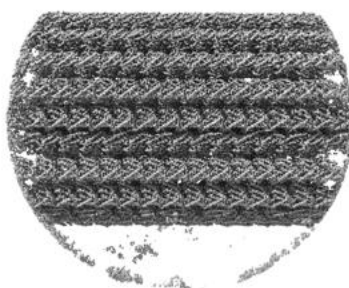
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

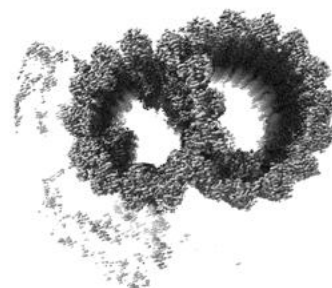
5.5.1 Primary map



X



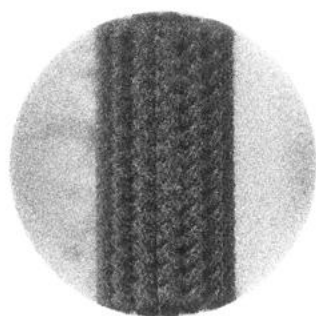
Y



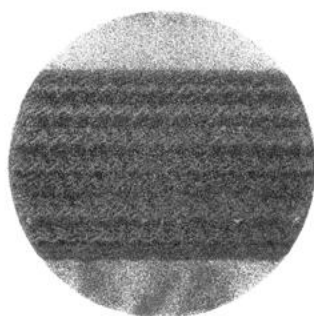
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

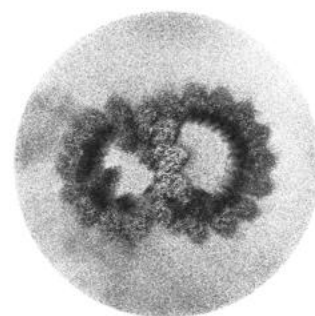
5.5.2 Raw map



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.

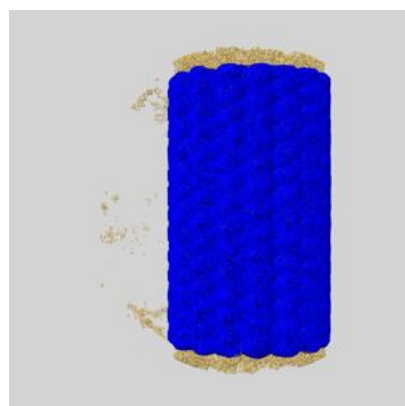
5.6 Mask visualisation [i](#)

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

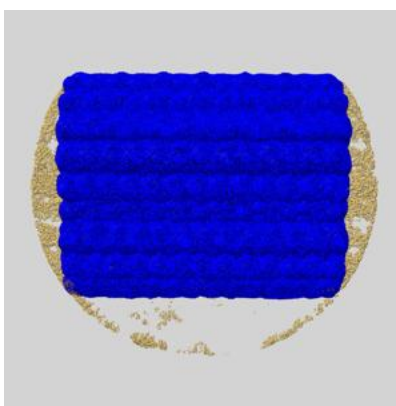
A mask typically either:

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

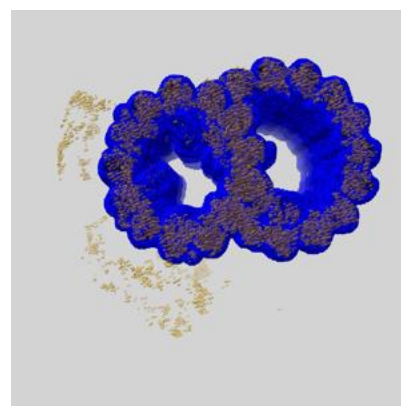
5.6.1 emd_40436_msk_1.map [i](#)



X



Y

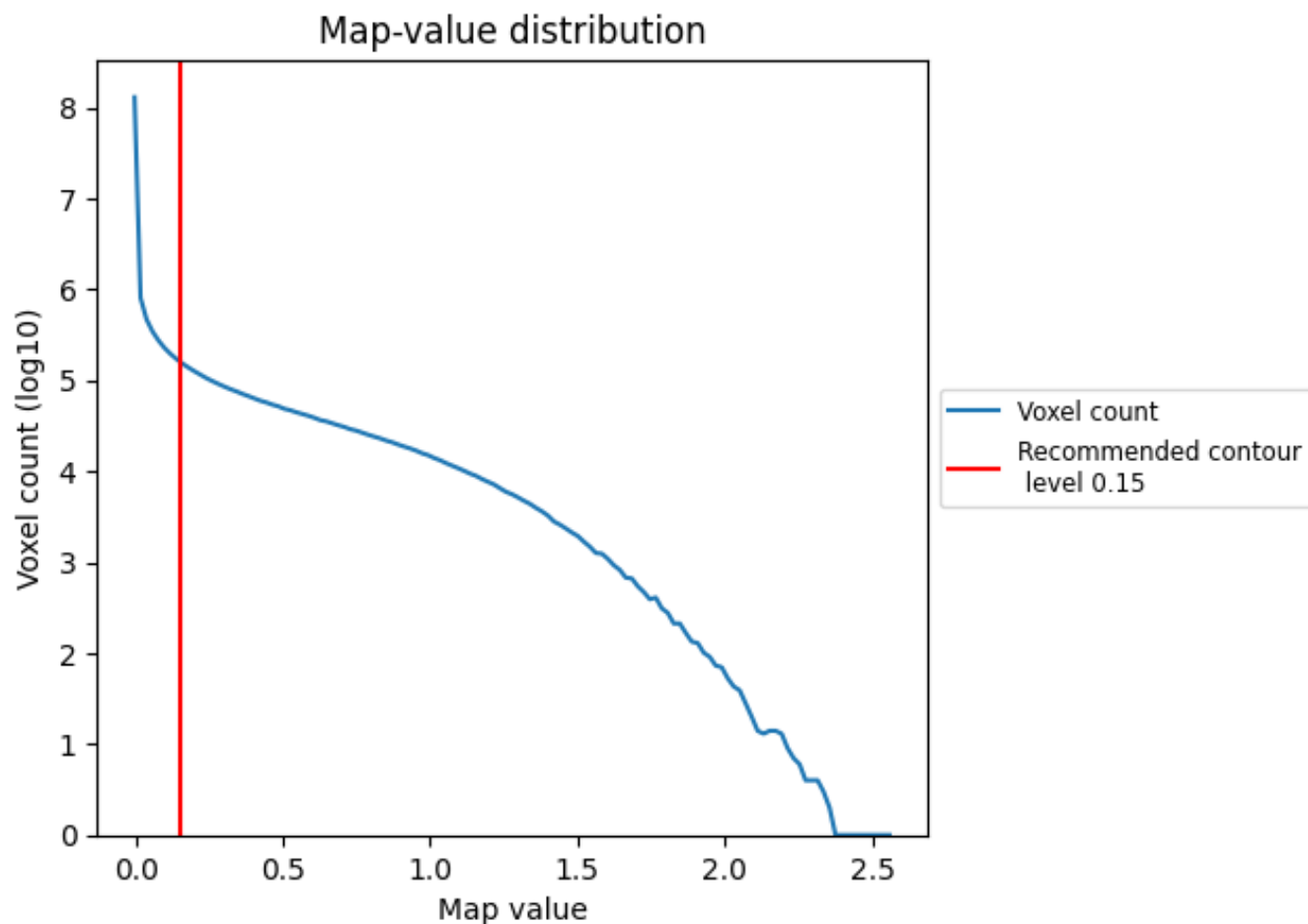


Z

6 Map analysis [i](#)

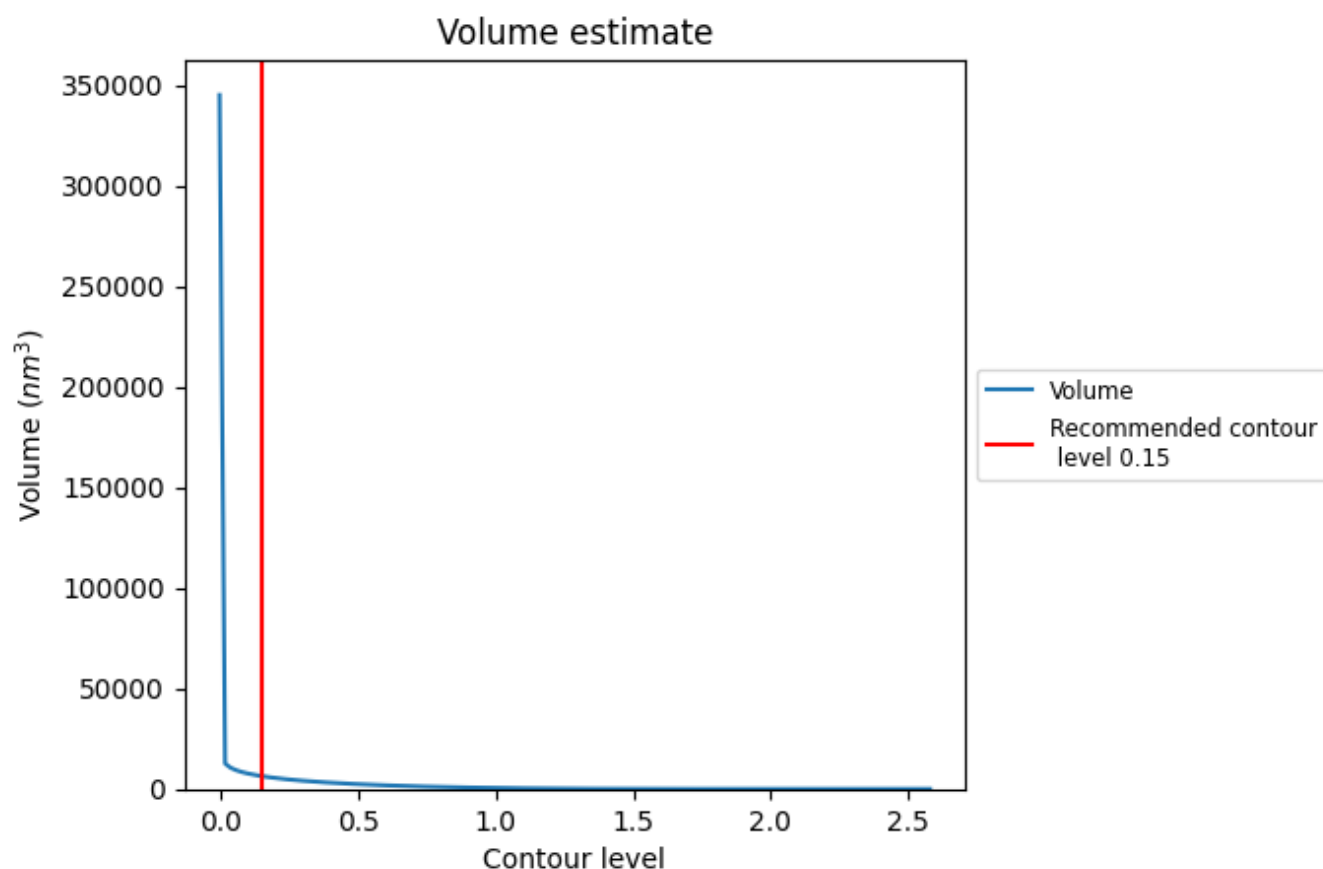
This section contains the results of statistical analysis of the map.

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.

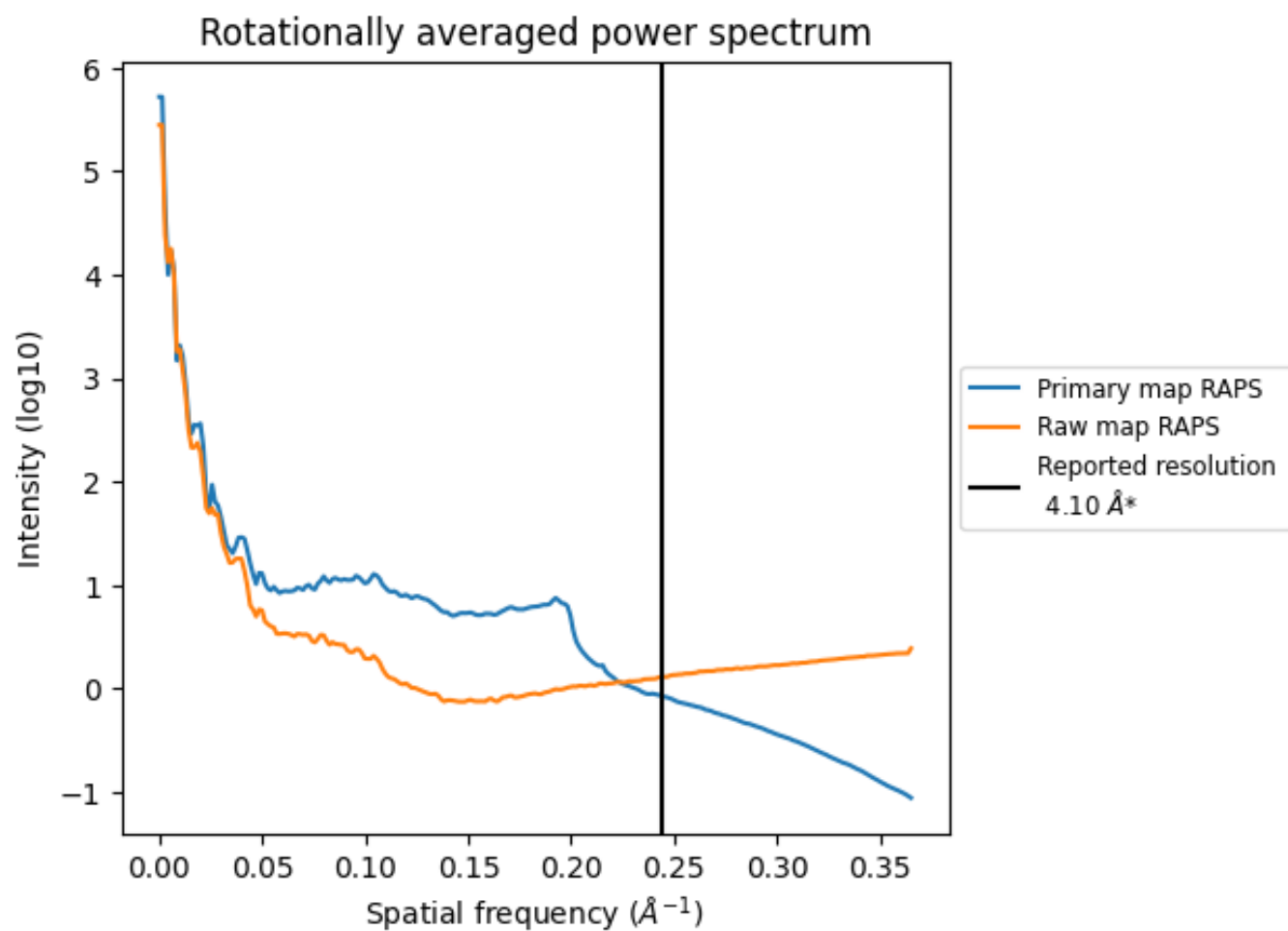
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 6396 nm^3 ; this corresponds to an approximate mass of 5778 kDa.

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

6.3 Rotationally averaged power spectrum ⓘ

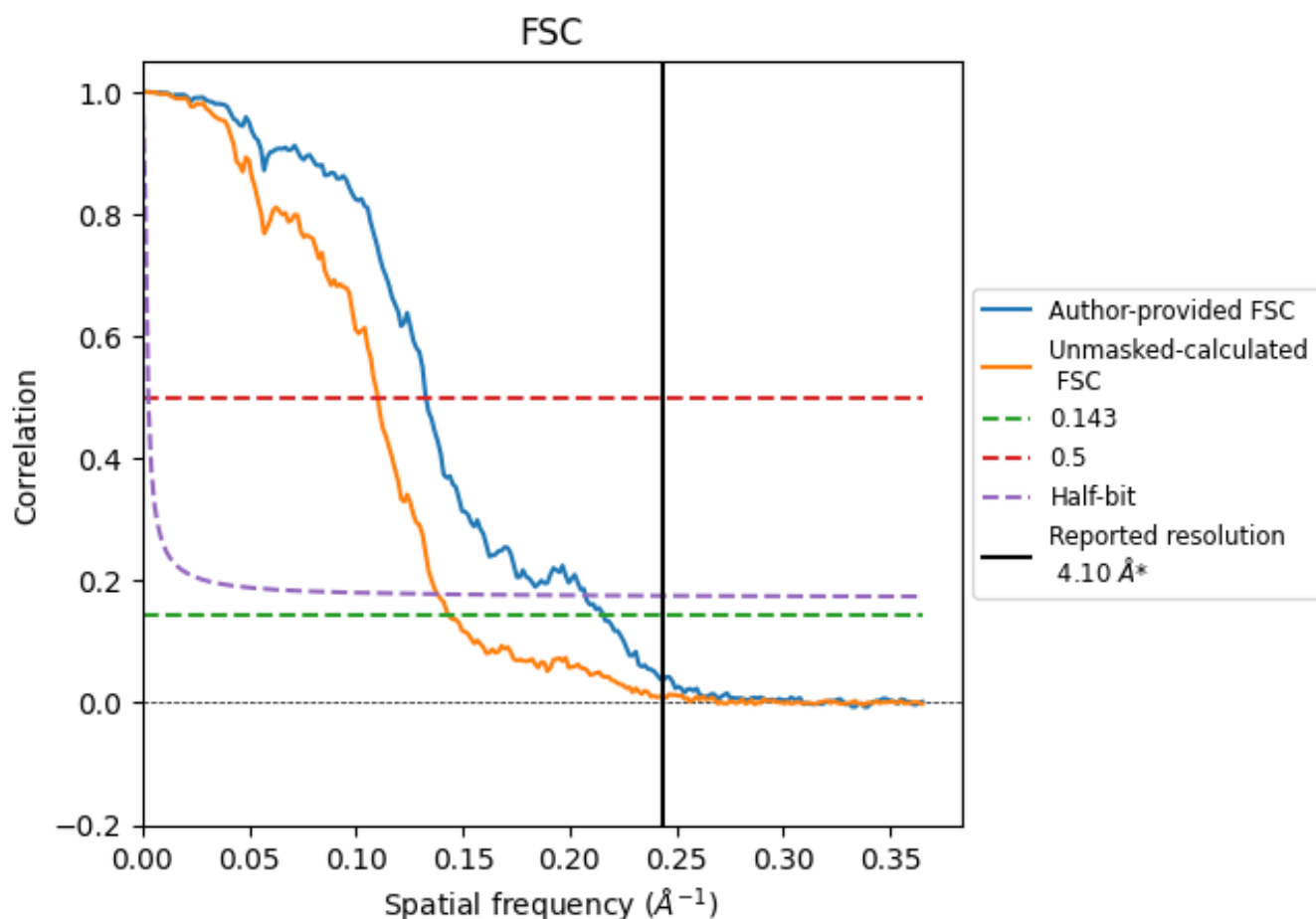


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

7.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.64	7.54	4.82
Unmasked-calculated*	6.97	9.08	7.24

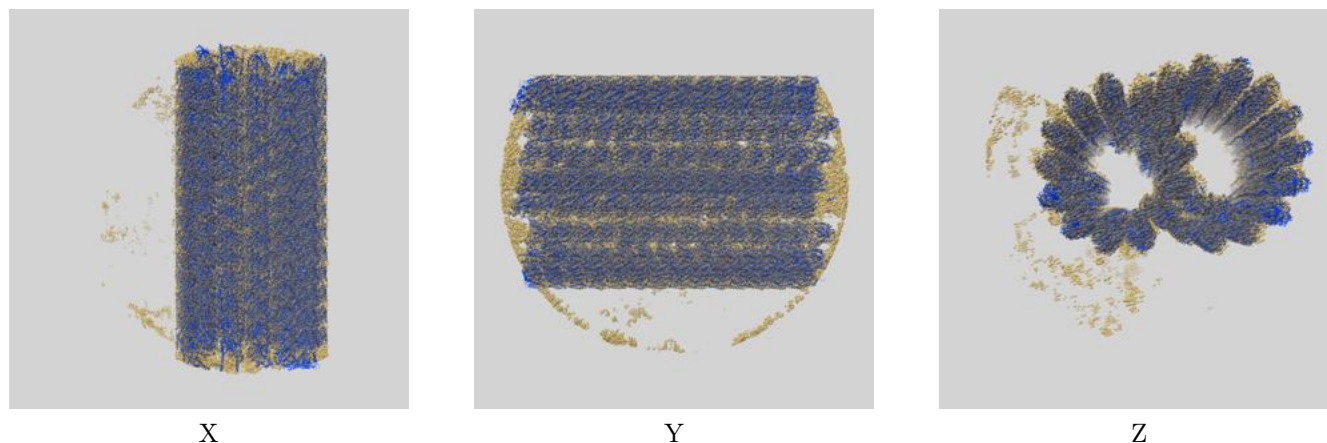
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.64 differs from the reported value 4.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.97 differs from the reported value 4.1 by more than 10 %

8 Map-model fit [i](#)

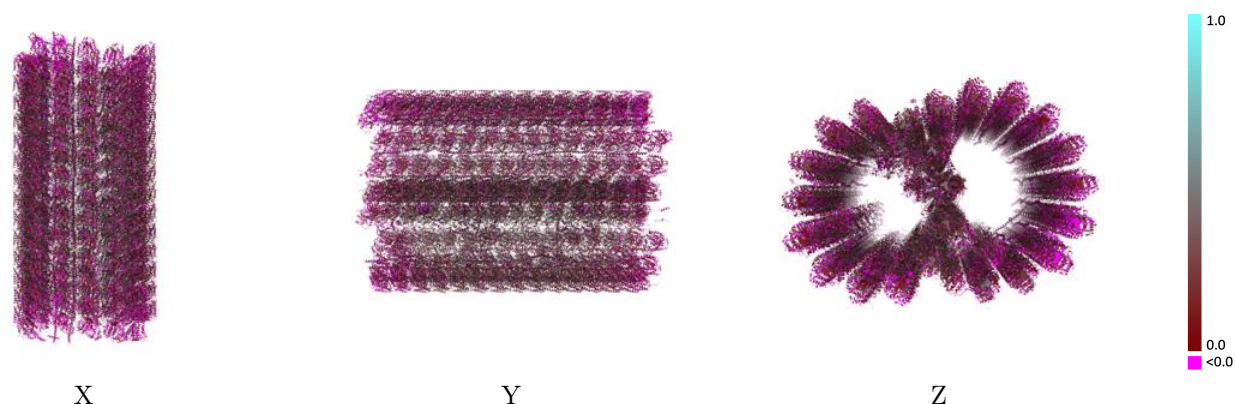
This section contains information regarding the fit between EMDB map EMD-40436 and PDB model 8SF7. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



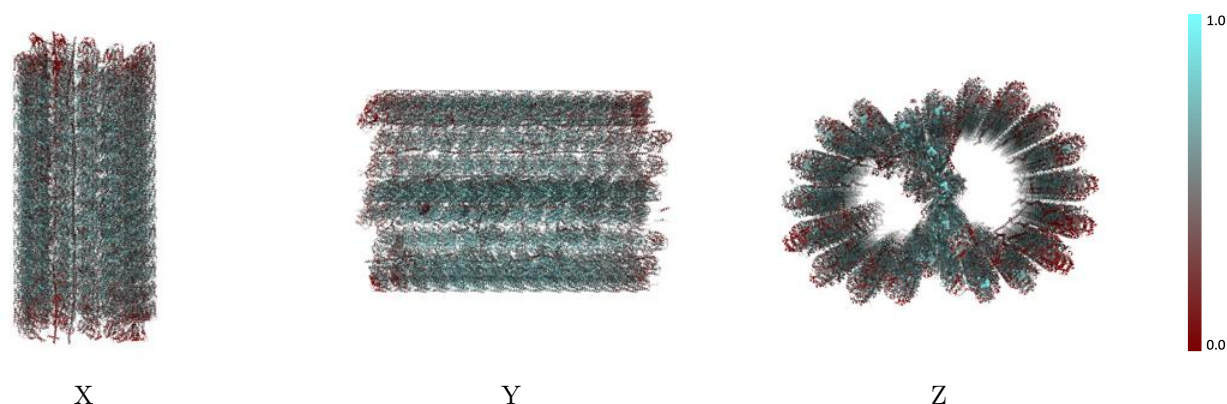
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



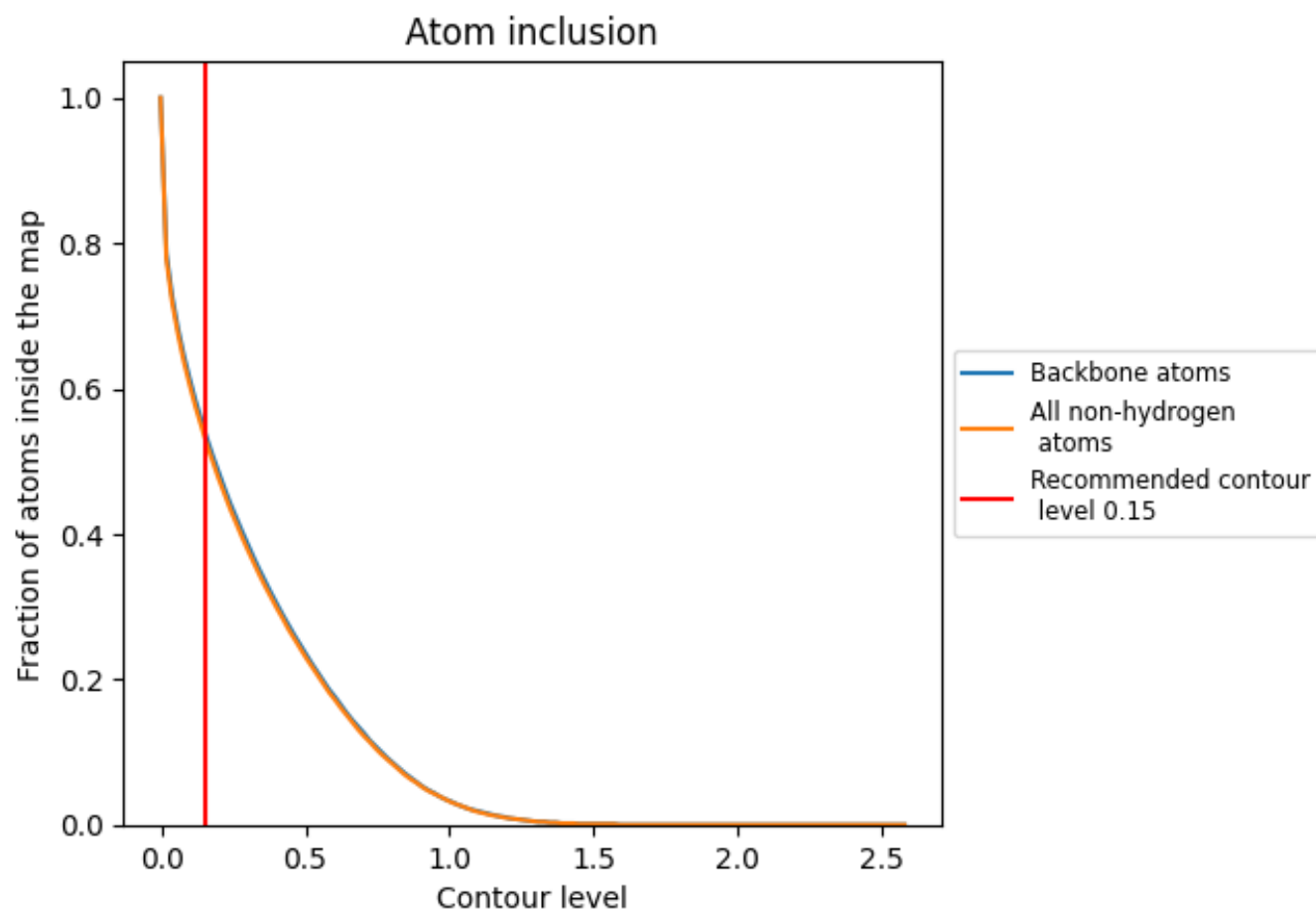
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

8.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 53% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5330	 0.2060
0A	 0.4040	 0.1360
0B	 0.4670	 0.1850
0C	 0.5620	 0.2160
0D	 0.3880	 0.0990
0E	 0.2890	 0.0540
0F	 0.4690	 0.1740
0G	 0.3760	 0.1210
0H	 0.3630	 0.0820
0N	 0.4800	 0.1610
0Q	 0.5790	 0.2580
0S	 0.3570	 0.1000
0T	 0.2560	 0.0500
0U	 0.3920	 0.1050
0V	 0.2830	 0.0920
0X	 0.5220	 0.1570
1A	 0.5330	 0.2140
1B	 0.4630	 0.1570
1C	 0.4970	 0.1550
1D	 0.5210	 0.1870
1E	 0.3880	 0.1330
1F	 0.4910	 0.2020
1G	 0.3840	 0.1280
1H	 0.3380	 0.0600
1I	 0.4430	 0.1830
1J	 0.4270	 0.1400
1K	 0.3820	 0.0860
1L	 0.4960	 0.1960
1M	 0.4990	 0.1940
1N	 0.5240	 0.2060
1O	 0.1270	 -0.0060
1P	 0.2600	 0.0410
1Q	 0.6680	 0.3120
1R	 0.5800	 0.2470
1S	 0.5740	 0.2280



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
1T	 0.5490	 0.2140
1U	 0.5680	 0.2310
1V	 0.3950	 0.1400
1W	 0.5250	 0.1760
1X	 0.5950	 0.2260
2A	 0.5970	 0.2370
2B	 0.0540	 -0.0040
2C	 0.4140	 0.1080
2D	 0.4710	 0.1660
2E	 0.4540	 0.1430
2F	 0.4180	 0.1480
2G	 0.4700	 0.1630
2H	 0.4430	 0.1830
2I	 0.4490	 0.1750
2K	 0.3830	 0.0780
2L	 0.3940	 0.1240
2M	 0.5530	 0.2100
2N	 0.4100	 0.1350
2O	 0.2770	 0.0200
2P	 0.3180	 0.0700
2Q	 0.6590	 0.3080
2R	 0.5980	 0.2630
2S	 0.6060	 0.2490
2T	 0.5600	 0.2150
2U	 0.5740	 0.2320
2V	 0.3920	 0.1370
2W	 0.3830	 0.0920
2X	 0.6020	 0.2240
3A	 0.4980	 0.1750
3B	 0.2170	 0.0330
3C	 0.4980	 0.1590
3D	 0.2900	 0.0970
3E	 0.2580	 0.0450
3H	 0.4640	 0.2140
3I	 0.4680	 0.2030
3L	 0.3240	 0.0810
3O	 0.2550	 0.0260
3Q	 0.6510	 0.3090
3R	 0.5420	 0.2200
3S	 0.5410	 0.2090
3T	 0.5300	 0.1920
3U	 0.4310	 0.1270

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
3V	 0.3650	 0.1140
3X	 0.5330	 0.1680
4C	 0.4030	 0.1090
4F	 0.2910	 0.0920
4H	 0.4190	 0.1910
4Q	 0.6670	 0.3180
4R	 0.6080	 0.2570
4S	 0.5930	 0.2610
4X	 0.5620	 0.2200
5A	 0.2820	 0.0960
5B	 0.3830	 0.1500
5C	 0.3810	 0.1500
5D	 0.1660	 -0.0560
5E	 0.1630	 0.0310
5F	 0.3030	 0.1110
5G	 0.3500	 0.1190
5H	 0.2570	 0.0890
5I	 0.2530	 0.0730
5J	 0.3180	 0.1090
5K	 0.2300	 0.0160
5Q	 0.6790	 0.3320
5R	 0.5950	 0.2450
5S	 0.6140	 0.2800
6F	 0.3770	 0.1480
6G	 0.3200	 0.0760
6H	 0.4660	 0.1320
6Q	 0.5710	 0.2630
6R	 0.3680	 0.0620
7R	 0.4340	 0.1410
8L	 0.5290	 0.1590
8N	 0.4450	 0.1210
8P	 0.4320	 0.1340
8R	 0.3940	 0.1160
AA	 0.6480	 0.2940
AB	 0.4940	 0.1750
AC	 0.7150	 0.3500
AD	 0.7060	 0.3450
AE	 0.7320	 0.3690
AF	 0.6960	 0.3410
AG	 0.7220	 0.3650
AH	 0.7140	 0.3570
AI	 0.7250	 0.3750

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
AJ	 0.7020	 0.3500
AK	 0.7360	 0.3730
AL	 0.7360	 0.3700
AM	 0.6540	 0.3030
AN	 0.6890	 0.3210
BA	 0.5230	 0.1950
BB	 0.3140	 0.0080
BC	 0.6890	 0.3360
BD	 0.6440	 0.2890
BE	 0.7000	 0.3410
BF	 0.6810	 0.3360
BG	 0.7010	 0.3410
BH	 0.6810	 0.3290
BI	 0.7010	 0.3470
BJ	 0.7000	 0.3450
BK	 0.7000	 0.3430
BL	 0.7070	 0.3490
BM	 0.6380	 0.2740
BN	 0.6830	 0.3160
CA	 0.3950	 0.0940
CB	 0.5070	 0.1690
CC	 0.5650	 0.2230
CD	 0.6100	 0.2610
CE	 0.6240	 0.2780
CF	 0.6040	 0.2480
CG	 0.6060	 0.2620
CH	 0.6300	 0.2660
CI	 0.6490	 0.3020
CJ	 0.6290	 0.2740
CK	 0.6300	 0.2790
CL	 0.5880	 0.2260
CM	 0.4980	 0.1710
CN	 0.4090	 0.0960
DA	 0.3310	 0.0530
DB	 0.4620	 0.1290
DC	 0.4980	 0.1620
DD	 0.5580	 0.2070
DE	 0.5840	 0.2450
DF	 0.5880	 0.2440
DG	 0.5800	 0.2250
DH	 0.5930	 0.2420
DI	 0.6200	 0.2620

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
DJ	 0.6070	 0.2390
DK	 0.6060	 0.2590
DL	 0.5370	 0.1930
DM	 0.4710	 0.1260
DN	 0.3500	 0.0640
EA	 0.2840	 0.0600
EB	 0.4650	 0.1090
EC	 0.4860	 0.1430
ED	 0.5570	 0.2020
EE	 0.5760	 0.2160
EF	 0.6030	 0.2300
EG	 0.6230	 0.2560
EH	 0.6090	 0.2380
EI	 0.6200	 0.2520
EJ	 0.5940	 0.2290
EK	 0.5970	 0.2300
EL	 0.5210	 0.1680
EM	 0.4790	 0.1420
EN	 0.3530	 0.0610
FA	 0.5100	 0.1650
FB	 0.4400	 0.1110
FC	 0.6050	 0.2400
FD	 0.5790	 0.2120
FE	 0.6370	 0.2680
FF	 0.6230	 0.2500
FG	 0.6370	 0.2650
FH	 0.6250	 0.2560
FI	 0.6520	 0.2800
FJ	 0.6450	 0.2820
FK	 0.5500	 0.1850
FL	 0.6010	 0.2330
FM	 0.2090	 0.0340
FN	 0.4240	 0.0950
GA	 0.4970	 0.1550
GB	 0.4210	 0.0980
GC	 0.6260	 0.2500
GD	 0.5950	 0.2190
GE	 0.6580	 0.2880
GF	 0.6500	 0.2750
GG	 0.6600	 0.2880
GH	 0.6520	 0.2800
GI	 0.6660	 0.2950

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
GJ	 0.6640	 0.2920
GK	 0.5580	 0.2030
GL	 0.5980	 0.2390
GM	 0.3580	 0.0720
GN	 0.4070	 0.0890
HA	 0.4840	 0.1540
HB	 0.3760	 0.0830
HC	 0.6240	 0.2680
HD	 0.5690	 0.2220
HE	 0.6600	 0.3000
HF	 0.6490	 0.2950
HG	 0.6470	 0.2830
HH	 0.6440	 0.2750
HI	 0.6640	 0.3010
HJ	 0.6410	 0.2880
HK	 0.5910	 0.2310
HL	 0.6280	 0.2730
HM	 0.3940	 0.0860
HN	 0.4980	 0.1520
IA	 0.5150	 0.1830
IB	 0.3950	 0.0910
IC	 0.6350	 0.2770
ID	 0.6130	 0.2650
IE	 0.6700	 0.3110
IF	 0.6490	 0.2920
IG	 0.6500	 0.3010
IH	 0.6450	 0.2810
II	 0.6770	 0.3180
IJ	 0.6460	 0.2980
IK	 0.6500	 0.2970
IL	 0.6620	 0.3110
IM	 0.4520	 0.1320
IN	 0.5620	 0.2140
JA	 0.6370	 0.2780
JB	 0.5760	 0.2190
JC	 0.6730	 0.3060
JD	 0.6580	 0.2880
JE	 0.6990	 0.3300
JF	 0.7070	 0.3460
JG	 0.6760	 0.3120
JH	 0.6920	 0.3250
JI	 0.6920	 0.3260

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
JJ	 0.6780	 0.3090
JK	 0.6510	 0.2960
JL	 0.6780	 0.3140
JM	 0.3660	 0.0890
JN	 0.5450	 0.1970
KA	 0.6360	 0.2650
KB	 0.5890	 0.2270
KC	 0.6940	 0.3410
KD	 0.6780	 0.3170
KE	 0.7120	 0.3430
KF	 0.7000	 0.3360
KG	 0.6950	 0.3270
KH	 0.7010	 0.3370
KI	 0.7050	 0.3350
KJ	 0.6950	 0.3200
KK	 0.6750	 0.3140
KL	 0.7180	 0.3450
KM	 0.5530	 0.2140
KN	 0.6260	 0.2490
LA	 0.6330	 0.2710
LB	 0.5800	 0.2180
LC	 0.6600	 0.3120
LD	 0.6630	 0.3050
LE	 0.6830	 0.3220
LF	 0.6750	 0.3060
LG	 0.6590	 0.3000
LH	 0.6820	 0.3230
LI	 0.6760	 0.3140
LJ	 0.6760	 0.3040
LK	 0.6370	 0.2480
LL	 0.6890	 0.3260
LM	 0.5970	 0.2400
LN	 0.6450	 0.2850
MA	 0.6550	 0.2930
MB	 0.5840	 0.2330
MC	 0.6770	 0.3240
MD	 0.7130	 0.3550
ME	 0.6810	 0.3250
MF	 0.6720	 0.3120
MG	 0.6750	 0.3150
MH	 0.6950	 0.3530
MI	 0.6860	 0.3350

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
MJ	 0.6720	 0.2980
MK	 0.6880	 0.3260
ML	 0.7020	 0.3530
MM	 0.6150	 0.2620
MN	 0.6370	 0.2690
NA	 0.5040	 0.1820
NB	 0.4420	 0.1320
NC	 0.6010	 0.2440
ND	 0.5530	 0.2160
NE	 0.6210	 0.2700
NF	 0.6240	 0.2690
NG	 0.6130	 0.2630
NH	 0.6020	 0.2410
NI	 0.6150	 0.2620
NJ	 0.6180	 0.2590
NK	 0.5990	 0.2470
NL	 0.5910	 0.2470
NM	 0.4080	 0.1130
NN	 0.5310	 0.2000
OA	 0.4540	 0.1380
OB	 0.3730	 0.0980
OC	 0.5480	 0.2100
OD	 0.5110	 0.1750
OE	 0.5880	 0.2340
OF	 0.5730	 0.2210
OG	 0.5940	 0.2420
OH	 0.5880	 0.2300
OI	 0.5880	 0.2410
OJ	 0.5610	 0.2220
OK	 0.5280	 0.2030
OL	 0.5820	 0.2200
OM	 0.3810	 0.1030
ON	 0.4900	 0.1600
PA	 0.4020	 0.1010
PB	 0.2990	 0.0500
PC	 0.5250	 0.1810
PD	 0.4620	 0.1320
PE	 0.5700	 0.2190
PF	 0.5450	 0.2000
PG	 0.5810	 0.2270
PH	 0.5610	 0.2200
PI	 0.5710	 0.2230

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
PJ	 0.5550	 0.2070
PK	 0.5470	 0.2010
PL	 0.5370	 0.1960
PM	 0.3630	 0.0910
PN	 0.4640	 0.1350
QA	 0.2900	 0.0500
QB	 0.4390	 0.1170
QC	 0.4850	 0.1390
QD	 0.4870	 0.1590
QE	 0.5240	 0.1880
QF	 0.5470	 0.1990
QG	 0.5670	 0.2170
QH	 0.5520	 0.2000
QI	 0.5500	 0.2020
QJ	 0.5030	 0.1660
QK	 0.5280	 0.1780
QL	 0.4470	 0.1280
QM	 0.3790	 0.0880
QN	 0.2280	 0.0360
RA	 0.2520	 0.0270
RB	 0.3800	 0.0910
RC	 0.4690	 0.1350
RD	 0.5110	 0.1580
RE	 0.5260	 0.1770
RF	 0.5330	 0.1940
RG	 0.5510	 0.1910
RH	 0.5630	 0.2080
RI	 0.5530	 0.2040
RJ	 0.5290	 0.1710
RK	 0.5440	 0.1840
RL	 0.4300	 0.1270
RM	 0.4000	 0.0950
RN	 0.2240	 0.0240
SA	 0.3110	 0.0500
SB	 0.4020	 0.0910
SC	 0.4770	 0.1420
SD	 0.5050	 0.1620
SE	 0.5260	 0.1820
SF	 0.5360	 0.1950
SG	 0.5750	 0.2130
SH	 0.5460	 0.1950
SI	 0.5760	 0.2150

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SJ	 0.5410	 0.1900
SK	 0.5410	 0.1890
SL	 0.4890	 0.1480
SM	 0.3890	 0.0930
SN	 0.3100	 0.0500
TA	 0.2420	 0.0260
TB	 0.2480	 0.0350
TC	 0.3930	 0.1030
TD	 0.4750	 0.1410
TE	 0.4970	 0.1570
TF	 0.4820	 0.1500
TG	 0.5390	 0.1870
TH	 0.5200	 0.1700
TI	 0.5330	 0.1900
TJ	 0.5120	 0.1640
TK	 0.4830	 0.1530
TL	 0.4400	 0.1250
TM	 0.3830	 0.0880
TN	 0.2970	 0.0480
UA	 0.2100	 -0.0040
UB	 0.2710	 0.0520
UC	 0.4320	 0.1230
UD	 0.4770	 0.1490
UE	 0.5080	 0.1710
UF	 0.5010	 0.1540
UG	 0.5040	 0.1720
UH	 0.4990	 0.1630
UI	 0.5220	 0.1740
UJ	 0.5190	 0.1700
UK	 0.5140	 0.1630
UL	 0.4550	 0.1250
UM	 0.4260	 0.1170
UN	 0.3080	 0.0430
VA	 0.4720	 0.1590
VB	 0.3730	 0.0890
VC	 0.5560	 0.2050
VD	 0.5360	 0.1910
VE	 0.5800	 0.2250
VF	 0.5740	 0.2240
VG	 0.5810	 0.2290
VH	 0.5700	 0.2210
VI	 0.5690	 0.2180

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
VJ	 0.5560	 0.2210
VK	 0.5160	 0.1720
VL	 0.5410	 0.1960
VM	 0.3240	 0.0640
VN	 0.4000	 0.1130
WA	 0.5190	 0.1770
WB	 0.4230	 0.1160
WC	 0.5820	 0.2320
WD	 0.5730	 0.2240
WE	 0.5930	 0.2400
WF	 0.5690	 0.2190
WG	 0.5960	 0.2460
WH	 0.5920	 0.2360
WI	 0.6030	 0.2510
WJ	 0.5710	 0.2300
WK	 0.5830	 0.2170
WL	 0.5890	 0.2370
WM	 0.3880	 0.0850
WN	 0.4660	 0.1430