



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 10:32 AM UTC

PDB ID : 6U42 / pdb_00006u42
EMDB ID : EMD-20631
Title : Natively decorated ciliary doublet microtubule
Authors : Ma, M.; Stoyanova, M.; Rademacher, G.; Dutcher, S.K.; Brown, A.; Zhang, R.
Deposited on : 2019-08-22
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 1358547 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	138	Total	C	N	O	S	0	0
			1120	701	192	214	13		
1	3	433	Total	C	N	O	S	0	0
			3397	2131	581	655	30		
1	5	436	Total	C	N	O	S	0	0
			3421	2147	584	660	30		
1	7	437	Total	C	N	O	S	0	0
			3430	2152	585	663	30		
1	9	436	Total	C	N	O	S	0	0
			3421	2147	584	660	30		
1	A1	432	Total	C	N	O	S	0	0
			3388	2126	580	652	30		
1	A3	435	Total	C	N	O	S	0	0
			3410	2138	583	659	30		
1	A5	430	Total	C	N	O	S	0	0
			3370	2116	578	646	30		
1	A7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A9	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B1	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B3	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B8	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	C0	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	C2	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	C4	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	C6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	C8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	D0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	D2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	D4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	D6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	D8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	E0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	E2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	E4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	E6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	E8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	F0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	F2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	F6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	F8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	G0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	G2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	G4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	G6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	G8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	H2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	H4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	H6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	H8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	I0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	I2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	I4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	I8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	J0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	J2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	J4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	J6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	J8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	K0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	K4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	K6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	K8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	L0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	L2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	L4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	L6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	M0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	M2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	M4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	M6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	M8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	N0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	N2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	N6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	N8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	O0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	O2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	O4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	O6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	O8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	P4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	P6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	P8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Q0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Q2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Q4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Q6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q8	420	Total	C	N	O	S	0	0
			3293	2070	563	631	29		
1	R0	434	Total	C	N	O	S	0	0
			3401	2133	582	656	30		
1	R2	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	R4	430	Total	C	N	O	S	0	0
			3370	2116	578	646	30		
1	R6	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	R8	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	S0	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	S2	431	Total	C	N	O	S	0	0
			3379	2121	579	649	30		
1	S4	427	Total	C	N	O	S	0	0
			3354	2107	575	642	30		
1	S6	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	S8	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	T0	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	T2	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	T4	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	T6	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	T8	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	U2	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	U4	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	U6	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	U8	430	Total	C	N	O	S	0	0
			3370	2116	578	646	30		
1	V0	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	V2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	V4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	V6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	V8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	W0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	W2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	W4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	W6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	W8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	X0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	X2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	X4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	X6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	X8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Y0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Y2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Y4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Y6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Y8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Z0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Z2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Z4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Z6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Z8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0A	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0C	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0E	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0G	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0I	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0K	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0M	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0O	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0Q	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0S	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0U	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0W	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	0Y	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	1A	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	1C	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	1E	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	1G	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	1K	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	1M	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	1O	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	1Q	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	1S	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	1U	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	1W	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2A	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2C	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2E	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2G	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2I	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2K	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2M	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2Q	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2S	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2U	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2W	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	2Y	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	3A	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	3C	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	3G	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3I	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	3K	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	3M	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	3O	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	3Q	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	3S	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

- Molecule 2 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	4	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	6	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	8	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	A0	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	A2	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	A4	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	A8	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	B0	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	B2	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	B4	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	B7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	B9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	C1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	C5	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	C7	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	C9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	D1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	D3	428	Total	C	N	O	S	0	0
			3324	2106	566	631	21		
2	D5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	D7	428	Total	C	N	O	S	0	0
			3324	2106	566	631	21		
2	E1	428	Total	C	N	O	S	0	0
			3324	2106	566	631	21		
2	E3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	E5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	E7	428	Total	C	N	O	S	0	0
			3324	2106	566	631	21		
2	E9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	F1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	F3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	F5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	F7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	F9	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	G1	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	G3	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	G5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	G9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	H1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	H3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	H5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	H7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	H9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	I1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	I3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	I5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	I7	429	Total	C	N	O	S	0	0
			3332	2110	567	634	21		
2	I9	428	Total	C	N	O	S	0	0
			3324	2106	566	631	21		
2	J1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	J3	428	Total	C	N	O	S	0	0
			3326	2107	566	632	21		
2	J5	437	Total	C	N	O	S	0	0
			3385	2141	576	647	21		
2	J7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	J9	437	Total	C	N	O	S	0	0
			3385	2141	576	647	21		
2	K1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	K3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	K5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	K7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	K9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	L1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	L3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	L5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	L7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	L9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	M1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	M3	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	M5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	M7	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	M9	437	Total	C	N	O	S	0	0
			3385	2141	576	647	21		
2	N1	428	Total	C	N	O	S	0	0
			3324	2106	566	631	21		
2	N3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	N5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	N7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	N9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	O1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	O3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	O5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	O7	431	Total	C	N	O	S	0	0
			3340	2114	569	636	21		
2	O9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	P5	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	P7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	P9	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	Q1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Q3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Q5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Q9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	R1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	R3	428	Total	C	N	O	S	0	0
			3327	2108	566	632	21		
2	R5	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	R7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	R9	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	S1	429	Total	C	N	O	S	0	0
			3333	2111	567	634	21		
2	S5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	S7	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	S9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	T1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	T3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	T5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	T7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	U1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	U3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	U5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	U7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	U9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	V1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	V3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	V7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	V9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	W1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	W3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	W5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	W7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	W9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	X3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	X5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	X7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	X9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Y1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Y3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Y5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Z1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Z3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Z5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Z7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Z9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0B	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0F	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0H	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0J	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0L	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0N	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0P	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0R	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0V	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0X	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0Z	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1B	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1D	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1F	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1H	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	1L	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1N	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1P	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1R	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1T	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1V	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1X	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	1Z	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2B	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2D	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2F	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2H	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2J	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2L	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2N	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2P	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2R	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2T	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2V	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2X	437	Total	C	N	O	S	0	0
			3385	2141	576	647	21		
2	2Z	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	3B	437	Total	C	N	O	S	0	0
			3383	2140	576	646	21		
2	3D	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3F	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3H	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3J	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3L	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3N	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3P	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3R	437	Total	C	N	O	S	0	0
			3385	2141	576	647	21		
2	3T	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

- Molecule 3 is a protein called PACRG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3V	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	3X	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	3Z	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	4B	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	4D	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	4F	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	4H	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	4J	204	Total	C	N	O	S	0	0
			1643	1060	281	296	6		

- Molecule 4 is a protein called FAP20.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3W	184	Total	C	N	O	S	0	0
			1515	971	264	273	7		
4	3Y	184	Total	C	N	O	S	0	0
			1515	971	264	273	7		
4	4A	184	Total	C	N	O	S	0	0
			1515	971	264	273	7		
4	4C	184	Total	C	N	O	S	0	0
			1515	971	264	273	7		
4	4E	184	Total	C	N	O	S	0	0
			1515	971	264	273	7		
4	4G	184	Total	C	N	O	S	0	0
			1515	971	264	273	7		
4	4I	184	Total	C	N	O	S	0	0
			1515	971	264	273	7		

- Molecule 5 is a protein called FAP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4L	238	Total	C	N	O	S	0	0
			1921	1164	366	381	10		
5	4M	316	Total	C	N	O	S	0	0
			2622	1589	514	503	16		

- Molecule 6 is a protein called FAP127.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4N	52	Total	C	N	O	S	0	0
			422	260	76	85	1		
6	4O	478	Total	C	N	O	S	0	0
			3995	2407	778	791	19		
6	4P	194	Total	C	N	O	S	0	0
			1588	956	313	315	4		

- Molecule 7 is a protein called RIB43a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4Q	63	Total	C	N	O	S	0	0
			525	324	101	98	2		
7	4R	366	Total	C	N	O	S	0	0
			2982	1819	561	589	13		
7	4S	45	Total	C	N	O		0	0
			371	228	71	72			

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	4T	194	Total	C	N	O	S	0	0
			1574	961	295	307	11		
7	4U	283	Total	C	N	O	S	0	0
			2285	1392	423	461	9		

- Molecule 8 is a protein called FAP112.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4V	83	Total	C	N	O	S	0	0
			653	396	129	124	4		
8	4W	353	Total	C	N	O	S	0	0
			2750	1649	552	538	11		
8	4X	59	Total	C	N	O	S	0	0
			462	284	85	90	3		

- Molecule 9 is a protein called FAP210.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4Y	126	Total	C	N	O	S	0	0
			1004	625	187	189	3		
9	4Z	389	Total	C	N	O	S	0	0
			3158	1908	627	615	8		

- Molecule 10 is a protein called FAP45.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5A	228	Total	C	N	O	S	0	0
			1902	1154	367	372	9		
10	5B	249	Total	C	N	O	S	0	0
			2074	1257	391	410	16		
10	5C	370	Total	C	N	O	S	0	0
			3103	1881	597	604	21		
10	5D	106	Total	C	N	O	S	0	0
			901	542	176	174	9		

- Molecule 11 is a protein called RIB30.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5E	258	Total	C	N	O	S	0	0
			1981	1245	352	380	4		

- Molecule 12 is a protein called FAP363.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	5F	381	Total	C	N	O	S	0	0
			3020	1921	520	569	10		
12	5G	141	Total	C	N	O	S	0	0
			1123	711	203	206	3		
12	7B	97	Total	C	N	O	S	0	0
			753	476	125	148	4		

- Molecule 13 is a protein called FAP126.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	5H	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		
13	5I	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		
13	5J	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		
13	5K	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		

- Molecule 14 is a protein called FAP52.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	5L	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		
14	5M	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		
14	5N	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		

- Molecule 15 is a protein called FAP67.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5O	376	Total	C	N	O	S	0	0
			2927	1862	503	547	15		
15	5P	376	Total	C	N	O	S	0	0
			2927	1862	503	547	15		

- Molecule 16 is a protein called FAP85.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	5Q	191	Total	C	N	O	S	0	0
			1523	961	267	293	2		

- Molecule 17 is a protein called FAP106.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5R	22	Total	C	N	O	S	0	0
			162	100	33	28	1		
17	5S	199	Total	C	N	O	S	0	0
			1572	989	291	288	4		
17	5T	198	Total	C	N	O	S	0	0
			1563	984	290	285	4		
17	5U	199	Total	C	N	O	S	0	0
			1572	989	291	288	4		
17	5V	109	Total	C	N	O	S	0	0
			879	551	164	162	2		

- Molecule 18 is a protein called FAP115.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5X	221	Total	C	N	O	S	0	0
			1793	1153	302	330	8		
18	5Y	221	Total	C	N	O	S	0	0
			1793	1153	302	330	8		
18	5Z	221	Total	C	N	O	S	0	0
			1793	1153	302	330	8		
18	6A	221	Total	C	N	O	S	0	0
			1793	1153	302	330	8		
18	6B	221	Total	C	N	O	S	0	0
			1793	1153	302	330	8		
18	6C	221	Total	C	N	O	S	0	0
			1793	1153	302	330	8		
18	6D	221	Total	C	N	O	S	0	0
			1793	1153	302	330	8		

- Molecule 19 is a protein called FAP143.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6E	255	Total	C	N	O	S	0	0
			1952	1208	345	390	9		

- Molecule 20 is a protein called FAP161.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	6F	394	Total	C	N	O	S	0	0
			2950	1852	518	566	14		

- Molecule 21 is a protein called FAP166.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	6G	183	Total	C	N	O	S	0	0
			1420	891	251	269	9		
21	6H	193	Total	C	N	O	S	0	0
			1493	937	265	282	9		

- Molecule 22 is a protein called FAP252.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6I	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
22	6J	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
22	6K	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
22	6L	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
22	6M	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
22	6N	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
22	6O	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
22	6P	297	Total	C	N	O	S	0	0
			2366	1499	399	454	14		

- Molecule 23 is a protein called FAP276.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	6Q	85	Total	C	N	O	S	0	0
			694	434	130	127	3		
23	6R	85	Total	C	N	O	S	0	0
			694	434	130	127	3		
23	6S	85	Total	C	N	O	S	0	0
			694	434	130	127	3		

- Molecule 24 is a protein called RIB72.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	6T	564	Total	C	N	O	S	0	0
			4590	2928	792	854	16		
24	6U	569	Total	C	N	O	S	0	0
			4623	2949	798	860	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	6V	561	Total	C	N	O	S	0	0
			4569	2915	789	849	16		
24	6W	566	Total	C	N	O	S	0	0
			4606	2938	795	857	16		
24	6X	569	Total	C	N	O	S	0	0
			4631	2954	799	862	16		
24	6Y	562	Total	C	N	O	S	0	0
			4579	2923	791	849	16		
24	6Z	563	Total	C	N	O	S	0	0
			4585	2925	791	853	16		
24	7A	189	Total	C	N	O	S	0	0
			1518	962	267	284	5		

- Molecule 25 is a protein called FAP141.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	7C	98	Total	C	N	O	S	0	0
			794	486	157	149	2		

- Molecule 26 is a protein called FAP222.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7D	132	Total	C	N	O	S	0	0
			1016	637	183	189	7		
26	7E	132	Total	C	N	O	S	0	0
			1016	637	183	189	7		
26	7F	132	Total	C	N	O	S	0	0
			1016	637	183	189	7		

- Molecule 27 is a protein called FAP95.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	7G	224	Total	C	N	O	S	0	0
			1728	1083	305	336	4		

- Molecule 28 is a protein called FAP182.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	7H	138	Total	C	N	O	S	0	0
			1046	651	194	196	5		
28	7X	138	Total	C	N	O	S	0	0
			1046	651	194	196	5		

- Molecule 29 is a protein called FAP129.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7I	228	Total	C	N	O	S	0	0
			1716	1065	311	334	6		
29	7J	362	Total	C	N	O	S	0	0
			2741	1691	505	535	10		

- Molecule 30 is a protein called FAP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7K	423	Total	C	N	O	S	0	0
			3276	2026	620	625	5		
30	7L	176	Total	C	N	O	S	0	0
			1333	819	254	257	3		

- Molecule 31 is a protein called FAP273.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7M	85	Total	C	N	O	S	0	0
			662	411	123	125	3		
31	7N	126	Total	C	N	O	S	0	0
			977	607	179	186	5		

- Molecule 32 is a protein called FAP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7O	59	Total	C	N	O		0	0
			443	270	81	92			
32	7P	182	Total	C	N	O	S	0	0
			1398	865	257	273	3		

- Molecule 33 is a protein called RIB21.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	7Q	71	Total	C	N	O	0	0
			567	352	98	117		

- Molecule 34 is a protein called DC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7R	195	Total	C	N	O	S	0	0
			1619	988	308	317	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
34	7S	160	Total	C	N	O	S	0	0
			1347	818	260	263	6		

- Molecule 35 is a protein called DC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	7T	213	Total	C	N	O	S	0	0
			1738	1068	326	335	9		
35	7U	181	Total	C	N	O	S	0	0
			1476	904	278	285	9		

- Molecule 36 is a protein called DC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	7V	89	Total	C	N	O	S	0	0
			735	457	123	150	5		
36	7W	89	Total	C	N	O	S	0	0
			735	457	123	150	5		

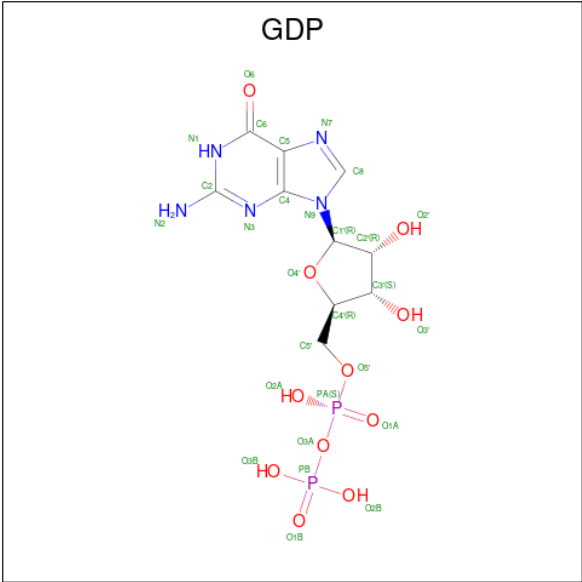
- Molecule 37 is a protein called FAP68.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	7Y	247	Total	C	N	O	S	0	0
			1971	1221	372	370	8		

- Molecule 38 is a protein called FAP90.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	7Z	39	Total	C	N	O	S	0	0
			298	184	50	62	2		
38	8A	207	Total	C	N	O	S	0	0
			1691	1058	305	322	6		
38	8B	213	Total	C	N	O	S	0	0
			1728	1078	311	332	7		
38	8C	213	Total	C	N	O	S	0	0
			1728	1078	311	332	7		
38	8D	157	Total	C	N	O	S	0	0
			1311	820	236	250	5		

- Molecule 39 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
39	2	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	3	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	5	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	7	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	9	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	A9	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	B1	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	B8	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
39	C0	1	Total 28	C 10	N 5	O 11	P 2	0
39	C2	1	Total 28	C 10	N 5	O 11	P 2	0
39	C4	1	Total 28	C 10	N 5	O 11	P 2	0
39	C6	1	Total 28	C 10	N 5	O 11	P 2	0
39	C8	1	Total 28	C 10	N 5	O 11	P 2	0
39	D0	1	Total 28	C 10	N 5	O 11	P 2	0
39	D2	1	Total 28	C 10	N 5	O 11	P 2	0
39	D4	1	Total 28	C 10	N 5	O 11	P 2	0
39	D6	1	Total 28	C 10	N 5	O 11	P 2	0
39	D8	1	Total 28	C 10	N 5	O 11	P 2	0
39	E0	1	Total 28	C 10	N 5	O 11	P 2	0
39	E2	1	Total 28	C 10	N 5	O 11	P 2	0
39	E4	1	Total 28	C 10	N 5	O 11	P 2	0
39	E6	1	Total 28	C 10	N 5	O 11	P 2	0
39	E8	1	Total 28	C 10	N 5	O 11	P 2	0
39	F0	1	Total 28	C 10	N 5	O 11	P 2	0
39	F2	1	Total 28	C 10	N 5	O 11	P 2	0
39	F6	1	Total 28	C 10	N 5	O 11	P 2	0
39	F8	1	Total 28	C 10	N 5	O 11	P 2	0
39	G0	1	Total 28	C 10	N 5	O 11	P 2	0
39	G2	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
39	G4	1	Total 28	C 10	N 5	O 11	P 2	0
39	G6	1	Total 28	C 10	N 5	O 11	P 2	0
39	G8	1	Total 28	C 10	N 5	O 11	P 2	0
39	H2	1	Total 28	C 10	N 5	O 11	P 2	0
39	H4	1	Total 28	C 10	N 5	O 11	P 2	0
39	H6	1	Total 28	C 10	N 5	O 11	P 2	0
39	H8	1	Total 28	C 10	N 5	O 11	P 2	0
39	I0	1	Total 28	C 10	N 5	O 11	P 2	0
39	I2	1	Total 28	C 10	N 5	O 11	P 2	0
39	I4	1	Total 28	C 10	N 5	O 11	P 2	0
39	I8	1	Total 28	C 10	N 5	O 11	P 2	0
39	J0	1	Total 28	C 10	N 5	O 11	P 2	0
39	J2	1	Total 28	C 10	N 5	O 11	P 2	0
39	J4	1	Total 28	C 10	N 5	O 11	P 2	0
39	J6	1	Total 28	C 10	N 5	O 11	P 2	0
39	J8	1	Total 28	C 10	N 5	O 11	P 2	0
39	K0	1	Total 28	C 10	N 5	O 11	P 2	0
39	K4	1	Total 28	C 10	N 5	O 11	P 2	0
39	K6	1	Total 28	C 10	N 5	O 11	P 2	0
39	K8	1	Total 28	C 10	N 5	O 11	P 2	0
39	L0	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
39	L2	1	Total 28	C 10	N 5	O 11	P 2	0
39	L4	1	Total 28	C 10	N 5	O 11	P 2	0
39	L6	1	Total 28	C 10	N 5	O 11	P 2	0
39	M0	1	Total 28	C 10	N 5	O 11	P 2	0
39	M2	1	Total 28	C 10	N 5	O 11	P 2	0
39	M4	1	Total 28	C 10	N 5	O 11	P 2	0
39	M6	1	Total 28	C 10	N 5	O 11	P 2	0
39	M8	1	Total 28	C 10	N 5	O 11	P 2	0
39	N0	1	Total 28	C 10	N 5	O 11	P 2	0
39	N2	1	Total 28	C 10	N 5	O 11	P 2	0
39	N6	1	Total 28	C 10	N 5	O 11	P 2	0
39	N8	1	Total 28	C 10	N 5	O 11	P 2	0
39	O0	1	Total 28	C 10	N 5	O 11	P 2	0
39	O2	1	Total 28	C 10	N 5	O 11	P 2	0
39	O4	1	Total 28	C 10	N 5	O 11	P 2	0
39	O6	1	Total 28	C 10	N 5	O 11	P 2	0
39	O8	1	Total 28	C 10	N 5	O 11	P 2	0
39	P4	1	Total 28	C 10	N 5	O 11	P 2	0
39	P6	1	Total 28	C 10	N 5	O 11	P 2	0
39	P8	1	Total 28	C 10	N 5	O 11	P 2	0
39	Q0	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
39	Q2	1	Total 28	C 10	N 5	O 11	P 2	0
39	Q4	1	Total 28	C 10	N 5	O 11	P 2	0
39	Q6	1	Total 28	C 10	N 5	O 11	P 2	0
39	Q8	1	Total 28	C 10	N 5	O 11	P 2	0
39	R0	1	Total 28	C 10	N 5	O 11	P 2	0
39	R2	1	Total 28	C 10	N 5	O 11	P 2	0
39	R4	1	Total 28	C 10	N 5	O 11	P 2	0
39	R6	1	Total 28	C 10	N 5	O 11	P 2	0
39	R8	1	Total 28	C 10	N 5	O 11	P 2	0
39	S0	1	Total 28	C 10	N 5	O 11	P 2	0
39	S2	1	Total 28	C 10	N 5	O 11	P 2	0
39	S4	1	Total 28	C 10	N 5	O 11	P 2	0
39	S6	1	Total 28	C 10	N 5	O 11	P 2	0
39	S8	1	Total 28	C 10	N 5	O 11	P 2	0
39	T0	1	Total 28	C 10	N 5	O 11	P 2	0
39	T2	1	Total 28	C 10	N 5	O 11	P 2	0
39	T4	1	Total 28	C 10	N 5	O 11	P 2	0
39	T6	1	Total 28	C 10	N 5	O 11	P 2	0
39	T8	1	Total 28	C 10	N 5	O 11	P 2	0
39	U2	1	Total 28	C 10	N 5	O 11	P 2	0
39	U4	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
39	U6	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	U8	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	V0	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	V2	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	V4	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	V6	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	V8	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	W0	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	W2	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	W4	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	W6	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	W8	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	X0	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	X2	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	X4	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	X6	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	X8	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	Y0	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	Y2	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	Y4	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	Y6	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
39	Y8	1	Total 28	C 10	N 5	O 11	P 2	0
39	Z0	1	Total 28	C 10	N 5	O 11	P 2	0
39	Z2	1	Total 28	C 10	N 5	O 11	P 2	0
39	Z4	1	Total 28	C 10	N 5	O 11	P 2	0
39	Z6	1	Total 28	C 10	N 5	O 11	P 2	0
39	Z8	1	Total 28	C 10	N 5	O 11	P 2	0
39	0A	1	Total 28	C 10	N 5	O 11	P 2	0
39	0C	1	Total 28	C 10	N 5	O 11	P 2	0
39	0E	1	Total 28	C 10	N 5	O 11	P 2	0
39	0G	1	Total 28	C 10	N 5	O 11	P 2	0
39	0I	1	Total 28	C 10	N 5	O 11	P 2	0
39	0K	1	Total 28	C 10	N 5	O 11	P 2	0
39	0M	1	Total 28	C 10	N 5	O 11	P 2	0
39	0O	1	Total 28	C 10	N 5	O 11	P 2	0
39	0Q	1	Total 28	C 10	N 5	O 11	P 2	0
39	0S	1	Total 28	C 10	N 5	O 11	P 2	0
39	0U	1	Total 28	C 10	N 5	O 11	P 2	0
39	0W	1	Total 28	C 10	N 5	O 11	P 2	0
39	0Y	1	Total 28	C 10	N 5	O 11	P 2	0
39	1A	1	Total 28	C 10	N 5	O 11	P 2	0
39	1C	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
39	1E	1	Total 28	C 10	N 5	O 11	P 2	0
39	1G	1	Total 28	C 10	N 5	O 11	P 2	0
39	1K	1	Total 28	C 10	N 5	O 11	P 2	0
39	1M	1	Total 28	C 10	N 5	O 11	P 2	0
39	1O	1	Total 28	C 10	N 5	O 11	P 2	0
39	1Q	1	Total 28	C 10	N 5	O 11	P 2	0
39	1S	1	Total 28	C 10	N 5	O 11	P 2	0
39	1U	1	Total 28	C 10	N 5	O 11	P 2	0
39	1W	1	Total 28	C 10	N 5	O 11	P 2	0
39	2A	1	Total 28	C 10	N 5	O 11	P 2	0
39	2C	1	Total 28	C 10	N 5	O 11	P 2	0
39	2E	1	Total 28	C 10	N 5	O 11	P 2	0
39	2G	1	Total 28	C 10	N 5	O 11	P 2	0
39	2I	1	Total 28	C 10	N 5	O 11	P 2	0
39	2K	1	Total 28	C 10	N 5	O 11	P 2	0
39	2M	1	Total 28	C 10	N 5	O 11	P 2	0
39	2Q	1	Total 28	C 10	N 5	O 11	P 2	0
39	2S	1	Total 28	C 10	N 5	O 11	P 2	0
39	2U	1	Total 28	C 10	N 5	O 11	P 2	0
39	2W	1	Total 28	C 10	N 5	O 11	P 2	0
39	2Y	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
39	3A	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	3C	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	3G	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	3I	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	3K	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	3M	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	3O	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	3Q	1	Total	C	N	O	P	0
			28	10	5	11	2	
39	3S	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
40	2	1	Total	Mg	0
			1	1	
40	4	1	Total	Mg	0
			1	1	
40	6	1	Total	Mg	0
			1	1	
40	8	1	Total	Mg	0
			1	1	
40	A0	1	Total	Mg	0
			1	1	
40	A2	1	Total	Mg	0
			1	1	
40	A4	1	Total	Mg	0
			1	1	
40	A8	1	Total	Mg	0
			1	1	
40	B0	1	Total	Mg	0
			1	1	
40	B2	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
40	B4	1	Total 1	Mg 1	0
40	B7	1	Total 1	Mg 1	0
40	B9	1	Total 1	Mg 1	0
40	C1	1	Total 1	Mg 1	0
40	C5	1	Total 1	Mg 1	0
40	C7	1	Total 1	Mg 1	0
40	C9	1	Total 1	Mg 1	0
40	D1	1	Total 1	Mg 1	0
40	D3	1	Total 1	Mg 1	0
40	D5	1	Total 1	Mg 1	0
40	D7	1	Total 1	Mg 1	0
40	E1	1	Total 1	Mg 1	0
40	E3	1	Total 1	Mg 1	0
40	E5	1	Total 1	Mg 1	0
40	E7	1	Total 1	Mg 1	0
40	E9	1	Total 1	Mg 1	0
40	F1	1	Total 1	Mg 1	0
40	F3	1	Total 1	Mg 1	0
40	F5	1	Total 1	Mg 1	0
40	F7	1	Total 1	Mg 1	0
40	F9	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	G1	1	1	1	0
40	G3	1	1	1	0
40	G5	1	1	1	0
40	G7	1	1	1	0
40	G9	1	1	1	0
40	H2	1	1	1	0
40	H3	1	1	1	0
40	H5	1	1	1	0
40	H8	1	1	1	0
40	H9	1	1	1	0
40	I1	1	1	1	0
40	I3	1	1	1	0
40	I5	1	1	1	0
40	I7	1	1	1	0
40	I9	1	1	1	0
40	J1	1	1	1	0
40	J4	1	1	1	0
40	J5	1	1	1	0
40	J7	1	1	1	0
40	J9	1	1	1	0
40	K1	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
40	K3	1	Total 1	Mg 1	0
40	K5	1	Total 1	Mg 1	0
40	K7	1	Total 1	Mg 1	0
40	K9	1	Total 1	Mg 1	0
40	L1	1	Total 1	Mg 1	0
40	L3	1	Total 1	Mg 1	0
40	L5	1	Total 1	Mg 1	0
40	L7	1	Total 1	Mg 1	0
40	L9	1	Total 1	Mg 1	0
40	M1	1	Total 1	Mg 1	0
40	M3	1	Total 1	Mg 1	0
40	M5	1	Total 1	Mg 1	0
40	M7	1	Total 1	Mg 1	0
40	M9	1	Total 1	Mg 1	0
40	N1	1	Total 1	Mg 1	0
40	N3	1	Total 1	Mg 1	0
40	N6	1	Total 1	Mg 1	0
40	N7	1	Total 1	Mg 1	0
40	O0	1	Total 1	Mg 1	0
40	O1	1	Total 1	Mg 1	0
40	O3	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
40	O5	1	Total 1	Mg 1	0
40	O8	1	Total 1	Mg 1	0
40	O9	1	Total 1	Mg 1	0
40	P4	1	Total 1	Mg 1	0
40	P6	1	Total 1	Mg 1	0
40	P7	1	Total 1	Mg 1	0
40	P9	1	Total 1	Mg 1	0
40	Q1	1	Total 1	Mg 1	0
40	Q3	1	Total 1	Mg 1	0
40	Q5	1	Total 1	Mg 1	0
40	Q9	1	Total 1	Mg 1	0
40	R1	1	Total 1	Mg 1	0
40	R3	1	Total 1	Mg 1	0
40	R6	1	Total 1	Mg 1	0
40	R7	1	Total 1	Mg 1	0
40	R9	1	Total 1	Mg 1	0
40	S1	1	Total 1	Mg 1	0
40	S5	1	Total 1	Mg 1	0
40	S7	1	Total 1	Mg 1	0
40	S9	1	Total 1	Mg 1	0
40	T1	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	T3	1	1	1	0
40	T5	1	1	1	0
40	T7	1	1	1	0
40	U1	1	1	1	0
40	U3	1	1	1	0
40	U5	1	1	1	0
40	U7	1	1	1	0
40	U9	1	1	1	0
40	V2	1	1	1	0
40	V3	1	1	1	0
40	V7	1	1	1	0
40	V9	1	1	1	0
40	W2	1	1	1	0
40	W3	1	1	1	0
40	W5	1	1	1	0
40	W8	1	1	1	0
40	W9	1	1	1	0
40	X3	1	1	1	0
40	X5	1	1	1	0
40	X7	1	1	1	0
40	X9	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
40	Y1	1	Total 1	Mg 1	0
40	Y3	1	Total 1	Mg 1	0
40	Y5	1	Total 1	Mg 1	0
40	Y9	1	Total 1	Mg 1	0
40	Z2	1	Total 1	Mg 1	0
40	Z3	1	Total 1	Mg 1	0
40	Z5	1	Total 1	Mg 1	0
40	Z7	1	Total 1	Mg 1	0
40	0A	1	Total 1	Mg 1	0
40	0B	1	Total 1	Mg 1	0
40	0F	1	Total 1	Mg 1	0
40	0H	1	Total 1	Mg 1	0
40	0J	1	Total 1	Mg 1	0
40	0L	1	Total 1	Mg 1	0
40	0N	1	Total 1	Mg 1	0
40	0P	1	Total 1	Mg 1	0
40	0R	1	Total 1	Mg 1	0
40	0W	1	Total 1	Mg 1	0
40	0X	1	Total 1	Mg 1	0
40	1A	1	Total 1	Mg 1	0
40	1B	1	Total 1	Mg 1	0

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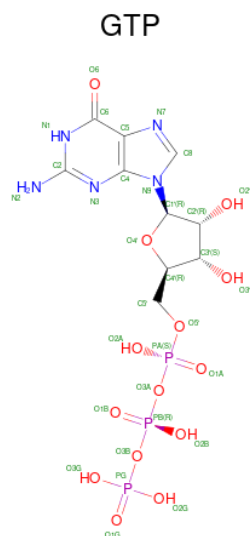
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
40	1D	1	1	1	0
40	1F	1	1	1	0
40	1H	1	1	1	0
40	1L	1	1	1	0
40	1N	1	1	1	0
40	1P	1	1	1	0
40	1R	1	1	1	0
40	1T	1	1	1	0
40	1V	1	1	1	0
40	1X	1	1	1	0
40	1Z	1	1	1	0
40	2B	1	1	1	0
40	2D	1	1	1	0
40	2F	1	1	1	0
40	2H	1	1	1	0
40	2J	1	1	1	0
40	2L	1	1	1	0
40	2N	1	1	1	0
40	2P	1	1	1	0
40	2R	1	1	1	0
40	2T	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
40	2V	1	Total 1	Mg 1	0
40	2X	1	Total 1	Mg 1	0
40	2Z	1	Total 1	Mg 1	0
40	3B	1	Total 1	Mg 1	0
40	3D	1	Total 1	Mg 1	0
40	3F	1	Total 1	Mg 1	0
40	3H	1	Total 1	Mg 1	0
40	3K	1	Total 1	Mg 1	0
40	3L	1	Total 1	Mg 1	0
40	3N	1	Total 1	Mg 1	0
40	3P	1	Total 1	Mg 1	0
40	3R	1	Total 1	Mg 1	0
40	3T	1	Total 1	Mg 1	0

- Molecule 41 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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Mol	Chain	Residues	Atoms					AltConf
41	C5	1	Total 32	C 10	N 5	O 14	P 3	0
41	C8	1	Total 32	C 10	N 5	O 14	P 3	0
41	C9	1	Total 32	C 10	N 5	O 14	P 3	0
41	D1	1	Total 32	C 10	N 5	O 14	P 3	0
41	D3	1	Total 32	C 10	N 5	O 14	P 3	0
41	D5	1	Total 32	C 10	N 5	O 14	P 3	0
41	D7	1	Total 32	C 10	N 5	O 14	P 3	0
41	E1	1	Total 32	C 10	N 5	O 14	P 3	0
41	E4	1	Total 32	C 10	N 5	O 14	P 3	0
41	E6	1	Total 32	C 10	N 5	O 14	P 3	0
41	E8	1	Total 32	C 10	N 5	O 14	P 3	0
41	F0	1	Total 32	C 10	N 5	O 14	P 3	0
41	F1	1	Total 32	C 10	N 5	O 14	P 3	0
41	F3	1	Total 32	C 10	N 5	O 14	P 3	0
41	F5	1	Total 32	C 10	N 5	O 14	P 3	0
41	F8	1	Total 32	C 10	N 5	O 14	P 3	0
41	G0	1	Total 32	C 10	N 5	O 14	P 3	0
41	G1	1	Total 32	C 10	N 5	O 14	P 3	0
41	G4	1	Total 32	C 10	N 5	O 14	P 3	0
41	G5	1	Total 32	C 10	N 5	O 14	P 3	0
41	G7	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
41	G9	1	Total 32	C 10	N 5	O 14	P 3	0
41	H2	1	Total 32	C 10	N 5	O 14	P 3	0
41	H3	1	Total 32	C 10	N 5	O 14	P 3	0
41	H6	1	Total 32	C 10	N 5	O 14	P 3	0
41	H8	1	Total 32	C 10	N 5	O 14	P 3	0
41	I0	1	Total 32	C 10	N 5	O 14	P 3	0
41	I1	1	Total 32	C 10	N 5	O 14	P 3	0
41	I4	1	Total 32	C 10	N 5	O 14	P 3	0
41	I5	1	Total 32	C 10	N 5	O 14	P 3	0
41	I8	1	Total 32	C 10	N 5	O 14	P 3	0
41	J0	1	Total 32	C 10	N 5	O 14	P 3	0
41	J2	1	Total 32	C 10	N 5	O 14	P 3	0
41	J4	1	Total 32	C 10	N 5	O 14	P 3	0
41	J6	1	Total 32	C 10	N 5	O 14	P 3	0
41	J8	1	Total 32	C 10	N 5	O 14	P 3	0
41	K0	1	Total 32	C 10	N 5	O 14	P 3	0
41	K1	1	Total 32	C 10	N 5	O 14	P 3	0
41	K4	1	Total 32	C 10	N 5	O 14	P 3	0
41	K6	1	Total 32	C 10	N 5	O 14	P 3	0
41	K7	1	Total 32	C 10	N 5	O 14	P 3	0
41	K9	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
41	L2	1	Total 32	C 10	N 5	O 14	P 3	0
41	L4	1	Total 32	C 10	N 5	O 14	P 3	0
41	L6	1	Total 32	C 10	N 5	O 14	P 3	0
41	L7	1	Total 32	C 10	N 5	O 14	P 3	0
41	M0	1	Total 32	C 10	N 5	O 14	P 3	0
41	M2	1	Total 32	C 10	N 5	O 14	P 3	0
41	M4	1	Total 32	C 10	N 5	O 14	P 3	0
41	M6	1	Total 32	C 10	N 5	O 14	P 3	0
41	M7	1	Total 32	C 10	N 5	O 14	P 3	0
41	N0	1	Total 32	C 10	N 5	O 14	P 3	0
41	N1	1	Total 32	C 10	N 5	O 14	P 3	0
41	N3	1	Total 32	C 10	N 5	O 14	P 3	0
41	N6	1	Total 32	C 10	N 5	O 14	P 3	0
41	N8	1	Total 32	C 10	N 5	O 14	P 3	0
41	O0	1	Total 32	C 10	N 5	O 14	P 3	0
41	O2	1	Total 32	C 10	N 5	O 14	P 3	0
41	O4	1	Total 32	C 10	N 5	O 14	P 3	0
41	O6	1	Total 32	C 10	N 5	O 14	P 3	0
41	O8	1	Total 32	C 10	N 5	O 14	P 3	0
41	O9	1	Total 32	C 10	N 5	O 14	P 3	0
41	P4	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
41	P6	1	Total 32	C 10	N 5	O 14	P 3	0
41	P8	1	Total 32	C 10	N 5	O 14	P 3	0
41	P9	1	Total 32	C 10	N 5	O 14	P 3	0
41	Q2	1	Total 32	C 10	N 5	O 14	P 3	0
41	Q4	1	Total 32	C 10	N 5	O 14	P 3	0
41	Q6	1	Total 32	C 10	N 5	O 14	P 3	0
41	R0	1	Total 32	C 10	N 5	O 14	P 3	0
41	R2	1	Total 32	C 10	N 5	O 14	P 3	0
41	R4	1	Total 32	C 10	N 5	O 14	P 3	0
41	R6	1	Total 32	C 10	N 5	O 14	P 3	0
41	R8	1	Total 32	C 10	N 5	O 14	P 3	0
41	S0	1	Total 32	C 10	N 5	O 14	P 3	0
41	S2	1	Total 32	C 10	N 5	O 14	P 3	0
41	S5	1	Total 32	C 10	N 5	O 14	P 3	0
41	S8	1	Total 32	C 10	N 5	O 14	P 3	0
41	S9	1	Total 32	C 10	N 5	O 14	P 3	0
41	T2	1	Total 32	C 10	N 5	O 14	P 3	0
41	T4	1	Total 32	C 10	N 5	O 14	P 3	0
41	T6	1	Total 32	C 10	N 5	O 14	P 3	0
41	T8	1	Total 32	C 10	N 5	O 14	P 3	0
41	U2	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
41	U4	1	Total 32	C 10	N 5	O 14	P 3	0
41	U6	1	Total 32	C 10	N 5	O 14	P 3	0
41	U7	1	Total 32	C 10	N 5	O 14	P 3	0
41	U9	1	Total 32	C 10	N 5	O 14	P 3	0
41	V2	1	Total 32	C 10	N 5	O 14	P 3	0
41	V3	1	Total 32	C 10	N 5	O 14	P 3	0
41	V8	1	Total 32	C 10	N 5	O 14	P 3	0
41	W0	1	Total 32	C 10	N 5	O 14	P 3	0
41	W2	1	Total 32	C 10	N 5	O 14	P 3	0
41	W4	1	Total 32	C 10	N 5	O 14	P 3	0
41	W5	1	Total 32	C 10	N 5	O 14	P 3	0
41	W8	1	Total 32	C 10	N 5	O 14	P 3	0
41	X0	1	Total 32	C 10	N 5	O 14	P 3	0
41	X4	1	Total 32	C 10	N 5	O 14	P 3	0
41	X6	1	Total 32	C 10	N 5	O 14	P 3	0
41	X7	1	Total 32	C 10	N 5	O 14	P 3	0
41	Y0	1	Total 32	C 10	N 5	O 14	P 3	0
41	Y1	1	Total 32	C 10	N 5	O 14	P 3	0
41	Y4	1	Total 32	C 10	N 5	O 14	P 3	0
41	Y6	1	Total 32	C 10	N 5	O 14	P 3	0
41	Z0	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
41	Z2	1	Total 32	C 10	N 5	O 14	P 3	0
41	Z3	1	Total 32	C 10	N 5	O 14	P 3	0
41	Z6	1	Total 32	C 10	N 5	O 14	P 3	0
41	Z7	1	Total 32	C 10	N 5	O 14	P 3	0
41	0A	1	Total 32	C 10	N 5	O 14	P 3	0
41	0C	1	Total 32	C 10	N 5	O 14	P 3	0
41	0F	1	Total 32	C 10	N 5	O 14	P 3	0
41	0I	1	Total 32	C 10	N 5	O 14	P 3	0
41	0K	1	Total 32	C 10	N 5	O 14	P 3	0
41	0M	1	Total 32	C 10	N 5	O 14	P 3	0
41	0O	1	Total 32	C 10	N 5	O 14	P 3	0
41	0Q	1	Total 32	C 10	N 5	O 14	P 3	0
41	0S	1	Total 32	C 10	N 5	O 14	P 3	0
41	0V	1	Total 32	C 10	N 5	O 14	P 3	0
41	0Y	1	Total 32	C 10	N 5	O 14	P 3	0
41	1A	1	Total 32	C 10	N 5	O 14	P 3	0
41	1C	1	Total 32	C 10	N 5	O 14	P 3	0
41	1D	1	Total 32	C 10	N 5	O 14	P 3	0
41	1G	1	Total 32	C 10	N 5	O 14	P 3	0
41	1H	1	Total 32	C 10	N 5	O 14	P 3	0
41	1L	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
41	1N	1	Total 32	C 10	N 5	O 14	P 3	0
41	1Q	1	Total 32	C 10	N 5	O 14	P 3	0
41	1S	1	Total 32	C 10	N 5	O 14	P 3	0
41	1T	1	Total 32	C 10	N 5	O 14	P 3	0
41	1W	1	Total 32	C 10	N 5	O 14	P 3	0
41	1X	1	Total 32	C 10	N 5	O 14	P 3	0
41	2A	1	Total 32	C 10	N 5	O 14	P 3	0
41	2C	1	Total 32	C 10	N 5	O 14	P 3	0
41	2E	1	Total 32	C 10	N 5	O 14	P 3	0
41	2G	1	Total 32	C 10	N 5	O 14	P 3	0
41	2I	1	Total 32	C 10	N 5	O 14	P 3	0
41	2K	1	Total 32	C 10	N 5	O 14	P 3	0
41	2L	1	Total 32	C 10	N 5	O 14	P 3	0
41	2N	1	Total 32	C 10	N 5	O 14	P 3	0
41	2Q	1	Total 32	C 10	N 5	O 14	P 3	0
41	2S	1	Total 32	C 10	N 5	O 14	P 3	0
41	2U	1	Total 32	C 10	N 5	O 14	P 3	0
41	2W	1	Total 32	C 10	N 5	O 14	P 3	0
41	2Y	1	Total 32	C 10	N 5	O 14	P 3	0
41	3A	1	Total 32	C 10	N 5	O 14	P 3	0
41	3C	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
41	3D	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	3G	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	3I	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	3K	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	3M	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	3O	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	3P	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	3S	1	Total	C	N	O	P	0
			32	10	5	14	3	
41	3T	1	Total	C	N	O	P	0
			32	10	5	14	3	

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, C1	Depositor
Number of particles used	143765	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 510 ligands modelled in this entry, 170 are monoatomic - leaving 340 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
39	GDP	C6	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.76	6 (13%)
41	GTP	1C	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.53	8 (16%)
39	GDP	K4	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.77	7 (15%)
41	GTP	N8	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
41	GTP	E6	501	40	33,34,34	0.88	0	50,54,54	1.54	8 (16%)
41	GTP	2G	501	40	33,34,34	0.88	2 (6%)	50,54,54	1.57	8 (16%)
39	GDP	V0	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.80	7 (15%)
39	GDP	R2	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.78	7 (15%)
39	GDP	3S	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.74	6 (13%)
41	GTP	3T	501	40	33,34,34	0.96	2 (6%)	50,54,54	1.60	9 (18%)
41	GTP	Z2	501	40	33,34,34	0.90	0	50,54,54	1.54	8 (16%)
41	GTP	C9	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.64	8 (16%)
39	GDP	G8	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
41	GTP	R8	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
41	GTP	O4	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.61	9 (18%)
39	GDP	3M	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.75	6 (13%)
39	GDP	M0	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.77	8 (17%)
39	GDP	I2	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.75	6 (13%)
39	GDP	3C	502	-	29,30,30	1.18	4 (13%)	45,47,47	1.79	9 (20%)
41	GTP	M7	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
41	GTP	4	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.60	8 (16%)
39	GDP	O8	503	-	29,30,30	1.16	4 (13%)	45,47,47	1.77	5 (11%)
41	GTP	I5	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.57	9 (18%)
41	GTP	K0	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.61	8 (16%)
41	GTP	C5	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.59	8 (16%)
41	GTP	V3	501	40	33,34,34	0.89	2 (6%)	50,54,54	1.62	8 (16%)
41	GTP	S2	501	40	33,34,34	0.92	1 (3%)	50,54,54	1.54	8 (16%)
39	GDP	2K	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	6 (13%)
41	GTP	N3	501	40	33,34,34	0.97	2 (6%)	50,54,54	1.56	9 (18%)
39	GDP	Y4	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.74	6 (13%)
39	GDP	T0	501	-	29,30,30	1.17	4 (13%)	45,47,47	1.77	7 (15%)
39	GDP	Z4	501	-	29,30,30	1.17	4 (13%)	45,47,47	1.69	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	GDP	P4	503	-	29,30,30	1.17	4 (13%)	45,47,47	1.75	7 (15%)
41	GTP	1D	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.56	9 (18%)
41	GTP	1G	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.54	8 (16%)
39	GDP	0O	502	-	29,30,30	1.19	4 (13%)	45,47,47	1.80	9 (20%)
39	GDP	Z2	503	-	29,30,30	1.17	4 (13%)	45,47,47	1.72	6 (13%)
39	GDP	D4	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.71	6 (13%)
41	GTP	S8	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.60	8 (16%)
41	GTP	0I	501	40	33,34,34	0.88	0	50,54,54	1.54	8 (16%)
41	GTP	R0	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
39	GDP	0U	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.82	9 (20%)
39	GDP	B5	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.75	5 (11%)
39	GDP	3Q	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.77	7 (15%)
39	GDP	H6	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.75	7 (15%)
39	GDP	1O	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
39	GDP	1K	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.81	8 (17%)
39	GDP	K6	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.80	7 (15%)
41	GTP	Y0	501	40	33,34,34	0.86	0	50,54,54	1.59	8 (16%)
39	GDP	P8	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	7 (15%)
41	GTP	V2	501	40	33,34,34	0.86	2 (6%)	50,54,54	1.57	8 (16%)
39	GDP	3I	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.85	9 (20%)
41	GTP	C8	501	40	33,34,34	0.93	1 (3%)	50,54,54	1.59	8 (16%)
41	GTP	2Q	501	40	33,34,34	0.91	2 (6%)	50,54,54	1.64	8 (16%)
41	GTP	0M	501	40	33,34,34	0.90	0	50,54,54	1.54	8 (16%)
41	GTP	0K	501	40	33,34,34	0.89	0	50,54,54	1.53	8 (16%)
41	GTP	O2	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.62	8 (16%)
41	GTP	1S	501	40	33,34,34	0.90	2 (6%)	50,54,54	1.59	8 (16%)
39	GDP	J0	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.76	7 (15%)
41	GTP	G9	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.53	9 (18%)
41	GTP	1W	501	40	33,34,34	0.91	2 (6%)	50,54,54	1.57	9 (18%)
41	GTP	3M	501	40	33,34,34	0.91	2 (6%)	50,54,54	1.66	8 (16%)
39	GDP	C2	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	8 (17%)
41	GTP	F3	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.59	8 (16%)
39	GDP	U8	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
41	GTP	O0	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.56	8 (16%)
39	GDP	H2	503	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	GDP	Z8	501	-	29,30,30	1.17	4 (13%)	45,47,47	1.70	6 (13%)
41	GTP	S5	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.60	8 (16%)
41	GTP	D5	501	40	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)
39	GDP	E6	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.76	6 (13%)
39	GDP	7	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.79	7 (15%)
39	GDP	U4	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	8 (17%)
39	GDP	Y6	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	7 (15%)
41	GTP	Q6	501	40	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
39	GDP	A9	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.74	6 (13%)
39	GDP	S0	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.77	8 (17%)
41	GTP	I8	501	40	33,34,34	0.87	2 (6%)	50,54,54	1.59	9 (18%)
41	GTP	L4	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
41	GTP	2E	501	40	33,34,34	0.87	1 (3%)	50,54,54	1.57	8 (16%)
39	GDP	A7	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
39	GDP	0Y	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.83	7 (15%)
41	GTP	Y6	501	40	33,34,34	0.85	0	50,54,54	1.57	8 (16%)
39	GDP	I0	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
39	GDP	Y8	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
41	GTP	K9	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.54	8 (16%)
39	GDP	F8	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
41	GTP	0Y	501	40	33,34,34	0.87	2 (6%)	50,54,54	1.55	8 (16%)
39	GDP	C0	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
39	GDP	V8	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.78	8 (17%)
39	GDP	K0	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	8 (17%)
39	GDP	2W	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.82	9 (20%)
39	GDP	A5	501	-	29,30,30	1.14	4 (13%)	45,47,47	1.73	7 (15%)
39	GDP	A1	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.75	6 (13%)
39	GDP	G0	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
39	GDP	L2	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.75	5 (11%)
39	GDP	W2	503	-	29,30,30	1.17	3 (10%)	45,47,47	1.82	8 (17%)
39	GDP	Q2	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.77	6 (13%)
41	GTP	2C	501	40	33,34,34	0.87	0	50,54,54	1.59	8 (16%)
41	GTP	3I	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.62	8 (16%)
41	GTP	A4	501	40	33,34,34	0.87	1 (3%)	50,54,54	1.53	8 (16%)
41	GTP	3O	501	40	33,34,34	0.93	2 (6%)	50,54,54	1.63	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	GTP	H2	501	40	33,34,34	0.92	2 (6%)	50,54,54	1.55	8 (16%)
41	GTP	T6	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.60	8 (16%)
41	GTP	J4	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.58	8 (16%)
39	GDP	W8	503	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
41	GTP	G7	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.55	8 (16%)
41	GTP	X6	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.59	8 (16%)
39	GDP	B1	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.77	7 (15%)
39	GDP	O4	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.76	6 (13%)
39	GDP	R6	503	-	29,30,30	1.17	4 (13%)	45,47,47	1.78	9 (20%)
39	GDP	Q8	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.75	6 (13%)
39	GDP	2I	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.78	7 (15%)
39	GDP	1A	503	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	8 (17%)
39	GDP	D8	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
39	GDP	D2	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.71	6 (13%)
39	GDP	1Q	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.76	7 (15%)
39	GDP	G6	501	-	29,30,30	1.17	4 (13%)	45,47,47	1.75	6 (13%)
39	GDP	Y2	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.76	6 (13%)
39	GDP	1C	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	6 (13%)
39	GDP	N2	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.77	7 (15%)
41	GTP	1X	501	40	33,34,34	0.94	1 (3%)	50,54,54	1.61	9 (18%)
41	GTP	U6	501	40	33,34,34	0.89	2 (6%)	50,54,54	1.57	9 (18%)
39	GDP	X4	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
39	GDP	L6	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	8 (17%)
39	GDP	T8	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.74	6 (13%)
39	GDP	S4	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.77	7 (15%)
41	GTP	I1	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
41	GTP	8	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.60	9 (18%)
41	GTP	N1	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.57	8 (16%)
39	GDP	T2	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.77	6 (13%)
41	GTP	3G	501	40	33,34,34	0.90	2 (6%)	50,54,54	1.63	8 (16%)
41	GTP	I0	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.55	8 (16%)
39	GDP	3A	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.82	9 (20%)
39	GDP	N0	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.77	7 (15%)
39	GDP	2Y	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.79	7 (15%)
41	GTP	O9	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.62	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	GDP	V2	503	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	8 (17%)
41	GTP	2N	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.59	9 (18%)
39	GDP	9	501	-	29,30,30	1.18	4 (13%)	45,47,47	1.77	6 (13%)
39	GDP	0E	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	8 (17%)
41	GTP	D1	501	40	33,34,34	0.92	1 (3%)	50,54,54	1.62	8 (16%)
39	GDP	2A	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.81	8 (17%)
41	GTP	1N	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
39	GDP	0S	502	-	29,30,30	1.19	3 (10%)	45,47,47	1.81	8 (17%)
39	GDP	2C	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.82	6 (13%)
39	GDP	F0	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
41	GTP	G0	501	40	33,34,34	0.89	0	50,54,54	1.55	8 (16%)
39	GDP	A3	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.84	9 (20%)
41	GTP	0V	501	40	33,34,34	0.88	2 (6%)	50,54,54	1.53	8 (16%)
39	GDP	J8	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
41	GTP	R2	501	40	33,34,34	0.92	2 (6%)	50,54,54	1.59	8 (16%)
39	GDP	H8	503	-	29,30,30	1.17	4 (13%)	45,47,47	1.77	6 (13%)
39	GDP	3	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.78	7 (15%)
41	GTP	F8	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.55	8 (16%)
39	GDP	O0	503	-	29,30,30	1.16	4 (13%)	45,47,47	1.76	6 (13%)
41	GTP	J6	501	40	33,34,34	0.88	2 (6%)	50,54,54	1.60	8 (16%)
41	GTP	H3	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.54	8 (16%)
41	GTP	1A	501	40	33,34,34	0.90	2 (6%)	50,54,54	1.53	8 (16%)
39	GDP	N8	502	-	29,30,30	1.18	4 (13%)	45,47,47	1.73	6 (13%)
39	GDP	G4	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.73	6 (13%)
39	GDP	Z6	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.68	6 (13%)
41	GTP	3K	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.61	8 (16%)
41	GTP	3A	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.62	8 (16%)
41	GTP	2W	501	40	33,34,34	0.93	1 (3%)	50,54,54	1.63	8 (16%)
41	GTP	Z3	501	40	33,34,34	0.89	0	50,54,54	1.54	8 (16%)
41	GTP	J2	501	40	33,34,34	0.87	1 (3%)	50,54,54	1.60	8 (16%)
39	GDP	V4	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.82	8 (17%)
39	GDP	M2	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.74	7 (15%)
41	GTP	K7	501	40	33,34,34	0.87	2 (6%)	50,54,54	1.60	8 (16%)
41	GTP	Q2	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
39	GDP	R0	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	GTP	F1	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.55	8 (16%)
39	GDP	3O	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.77	6 (13%)
41	GTP	0A	501	40	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
39	GDP	Z0	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.72	7 (15%)
39	GDP	2E	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.78	6 (13%)
41	GTP	F5	501	40	33,34,34	0.87	0	50,54,54	1.53	9 (18%)
41	GTP	B0	501	40	33,34,34	0.88	2 (6%)	50,54,54	1.61	9 (18%)
39	GDP	0C	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
41	GTP	O6	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.60	9 (18%)
41	GTP	H6	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.55	9 (18%)
41	GTP	S9	501	40	33,34,34	0.56	0	50,54,54	0.72	0
39	GDP	K8	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.77	6 (13%)
39	GDP	U2	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.74	7 (15%)
41	GTP	W4	501	40	33,34,34	0.86	2 (6%)	50,54,54	1.61	9 (18%)
39	GDP	T4	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
39	GDP	C4	501	-	29,30,30	1.17	4 (13%)	45,47,47	1.73	5 (11%)
39	GDP	X2	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.75	5 (11%)
41	GTP	A9	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.63	9 (18%)
41	GTP	C1	501	40	33,34,34	0.85	2 (6%)	50,54,54	1.62	9 (18%)
41	GTP	N6	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.55	8 (16%)
41	GTP	3P	501	40	33,34,34	0.93	1 (3%)	50,54,54	1.65	8 (16%)
41	GTP	P6	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.55	8 (16%)
41	GTP	D7	501	40	33,34,34	0.92	1 (3%)	50,54,54	1.61	10 (20%)
41	GTP	J0	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.63	9 (18%)
39	GDP	2S	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.80	9 (20%)
41	GTP	G1	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
41	GTP	T2	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.62	8 (16%)
41	GTP	U9	501	40	33,34,34	0.89	2 (6%)	50,54,54	1.56	8 (16%)
41	GTP	M0	501	40	33,34,34	0.86	1 (3%)	50,54,54	1.58	9 (18%)
41	GTP	J8	501	40	33,34,34	0.87	2 (6%)	50,54,54	1.64	9 (18%)
41	GTP	U4	501	40	33,34,34	0.88	2 (6%)	50,54,54	1.59	9 (18%)
41	GTP	2I	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.60	8 (16%)
41	GTP	N0	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.57	8 (16%)
41	GTP	2Y	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.61	8 (16%)
39	GDP	3K	503	-	29,30,30	1.16	4 (13%)	45,47,47	1.79	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	GTP	1T	501	40	33,34,34	0.93	2 (6%)	50,54,54	1.61	9 (18%)
41	GTP	0S	501	40	33,34,34	0.93	1 (3%)	50,54,54	1.59	8 (16%)
39	GDP	W0	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
41	GTP	Y1	501	40	33,34,34	0.86	0	50,54,54	1.57	8 (16%)
41	GTP	B2	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.56	8 (16%)
39	GDP	M6	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.80	9 (20%)
41	GTP	3C	501	40	33,34,34	0.91	2 (6%)	50,54,54	1.65	8 (16%)
39	GDP	F2	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
39	GDP	X0	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
41	GTP	2A	501	40	33,34,34	0.86	0	50,54,54	1.58	8 (16%)
39	GDP	W6	501	-	29,30,30	1.14	4 (13%)	45,47,47	1.78	7 (15%)
39	GDP	J4	503	-	29,30,30	1.15	4 (13%)	45,47,47	1.76	7 (15%)
39	GDP	0Q	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)
39	GDP	0K	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
41	GTP	K4	501	40	33,34,34	0.87	1 (3%)	50,54,54	1.54	9 (18%)
41	GTP	W5	501	40	33,34,34	0.86	2 (6%)	50,54,54	1.61	8 (16%)
41	GTP	X7	501	40	33,34,34	0.91	0	50,54,54	1.60	8 (16%)
39	GDP	E0	501	-	29,30,30	1.17	4 (13%)	45,47,47	1.70	7 (15%)
41	GTP	G5	501	40	33,34,34	0.88	1 (3%)	50,54,54	1.53	8 (16%)
41	GTP	D3	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.59	8 (16%)
39	GDP	1W	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	7 (15%)
41	GTP	0C	501	40	33,34,34	0.94	0	50,54,54	1.56	8 (16%)
39	GDP	D6	501	-	29,30,30	1.17	4 (13%)	45,47,47	1.72	6 (13%)
39	GDP	I4	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
39	GDP	1E	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.82	7 (15%)
41	GTP	2U	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.60	8 (16%)
41	GTP	3D	501	40	33,34,34	0.92	2 (6%)	50,54,54	1.66	9 (18%)
41	GTP	A1	501	40	33,34,34	0.87	1 (3%)	50,54,54	1.60	9 (18%)
39	GDP	O2	502	-	29,30,30	1.19	4 (13%)	45,47,47	1.79	5 (11%)
41	GTP	A2	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.67	9 (18%)
41	GTP	L2	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.56	8 (16%)
41	GTP	U2	501	40	33,34,34	0.89	2 (6%)	50,54,54	1.56	8 (16%)
41	GTP	P4	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.56	8 (16%)
39	GDP	Q4	502	-	29,30,30	1.18	4 (13%)	45,47,47	1.73	6 (13%)
41	GTP	K1	501	40	33,34,34	0.99	2 (6%)	50,54,54	1.59	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	GTP	Z0	501	40	33,34,34	0.93	1 (3%)	50,54,54	1.52	8 (16%)
41	GTP	R6	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
39	GDP	E4	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.73	6 (13%)
39	GDP	D0	501	-	29,30,30	1.18	4 (13%)	45,47,47	1.73	6 (13%)
41	GTP	B5	501	40	33,34,34	0.87	1 (3%)	50,54,54	1.57	8 (16%)
39	GDP	Q0	501	-	29,30,30	1.17	4 (13%)	45,47,47	1.75	9 (20%)
41	GTP	7	501	40	33,34,34	0.92	1 (3%)	50,54,54	1.59	9 (18%)
39	GDP	V6	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	7 (15%)
41	GTP	O8	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
41	GTP	3S	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.60	8 (16%)
41	GTP	P9	501	40	33,34,34	0.92	1 (3%)	50,54,54	1.58	8 (16%)
39	GDP	2U	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.83	10 (22%)
39	GDP	B3	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.75	7 (15%)
39	GDP	0G	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.75	7 (15%)
39	GDP	O6	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.78	5 (11%)
41	GTP	Y4	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.58	8 (16%)
39	GDP	1U	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.82	7 (15%)
39	GDP	C8	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.71	6 (13%)
39	GDP	E8	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.71	6 (13%)
39	GDP	2G	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.77	5 (11%)
41	GTP	U7	501	40	33,34,34	0.89	2 (6%)	50,54,54	1.57	8 (16%)
41	GTP	T4	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.58	8 (16%)
39	GDP	W4	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.82	9 (20%)
39	GDP	X8	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.73	6 (13%)
39	GDP	L4	502	-	29,30,30	1.18	4 (13%)	45,47,47	1.76	7 (15%)
39	GDP	R8	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.84	10 (22%)
41	GTP	X4	501	40	33,34,34	0.94	1 (3%)	50,54,54	1.61	8 (16%)
41	GTP	1L	501	40	33,34,34	0.91	2 (6%)	50,54,54	1.56	8 (16%)
39	GDP	0A	503	-	29,30,30	1.18	3 (10%)	45,47,47	1.75	6 (13%)
39	GDP	S8	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.78	6 (13%)
39	GDP	F6	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.75	7 (15%)
41	GTP	2K	501	40	33,34,34	0.87	1 (3%)	50,54,54	1.59	8 (16%)
39	GDP	E2	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.73	6 (13%)
39	GDP	2M	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.81	7 (15%)
41	GTP	S0	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.54	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	GTP	Z7	501	40	33,34,34	0.91	0	50,54,54	1.55	8 (16%)
39	GDP	M8	501	-	29,30,30	1.14	4 (13%)	45,47,47	1.75	6 (13%)
39	GDP	S2	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.74	7 (15%)
41	GTP	1H	501	40	33,34,34	0.86	1 (3%)	50,54,54	1.57	9 (18%)
41	GTP	M4	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.58	9 (18%)
41	GTP	M6	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.62	8 (16%)
39	GDP	H4	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.81	7 (15%)
39	GDP	G2	501	-	29,30,30	1.17	4 (13%)	45,47,47	1.75	6 (13%)
41	GTP	R4	501	40	33,34,34	0.92	2 (6%)	50,54,54	1.60	8 (16%)
39	GDP	2Q	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.81	9 (20%)
41	GTP	2L	501	40	33,34,34	0.89	2 (6%)	50,54,54	1.58	8 (16%)
41	GTP	E4	501	40	33,34,34	0.87	0	50,54,54	1.55	8 (16%)
41	GTP	H8	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.55	8 (16%)
39	GDP	1G	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.82	7 (15%)
41	GTP	C0	501	40	33,34,34	0.86	2 (6%)	50,54,54	1.61	9 (18%)
39	GDP	S6	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.75	7 (15%)
41	GTP	0O	501	40	33,34,34	0.91	1 (3%)	50,54,54	1.57	8 (16%)
39	GDP	T6	502	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	7 (15%)
39	GDP	J2	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.78	7 (15%)
39	GDP	M4	502	-	29,30,30	1.14	4 (13%)	45,47,47	1.72	6 (13%)
39	GDP	1S	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.79	7 (15%)
41	GTP	F0	501	40	33,34,34	0.88	0	50,54,54	1.54	8 (16%)
41	GTP	2S	501	40	33,34,34	0.93	1 (3%)	50,54,54	1.62	8 (16%)
41	GTP	E1	501	40	33,34,34	0.90	2 (6%)	50,54,54	1.58	8 (16%)
39	GDP	2	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.73	6 (13%)
41	GTP	0Q	501	40	33,34,34	0.92	0	50,54,54	1.57	8 (16%)
39	GDP	U6	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	7 (15%)
39	GDP	X6	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
41	GTP	3	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.59	8 (16%)
41	GTP	K6	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.57	8 (16%)
41	GTP	V8	501	40	33,34,34	0.87	1 (3%)	50,54,54	1.59	8 (16%)
39	GDP	5	501	-	29,30,30	1.16	4 (13%)	45,47,47	1.77	6 (13%)
39	GDP	B8	501	-	29,30,30	1.15	4 (13%)	45,47,47	1.77	6 (13%)
39	GDP	1M	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.82	8 (17%)
41	GTP	P8	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.54	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	GTP	B7	501	40	33,34,34	0.86	1 (3%)	50,54,54	1.57	8 (16%)
41	GTP	I4	501	40	33,34,34	0.92	2 (6%)	50,54,54	1.57	8 (16%)
39	GDP	3G	502	-	29,30,30	1.16	4 (13%)	45,47,47	1.78	7 (15%)
41	GTP	G4	501	40	33,34,34	0.89	0	50,54,54	1.52	8 (16%)
39	GDP	Q6	502	-	29,30,30	1.17	4 (13%)	45,47,47	1.76	7 (15%)
39	GDP	0W	502	-	29,30,30	1.15	3 (10%)	45,47,47	1.84	7 (15%)
39	GDP	N6	503	-	29,30,30	1.16	4 (13%)	45,47,47	1.73	6 (13%)
41	GTP	L6	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.60	8 (16%)
41	GTP	Z6	501	40	33,34,34	0.92	1 (3%)	50,54,54	1.55	8 (16%)
41	GTP	1Q	501	40	33,34,34	0.91	2 (6%)	50,54,54	1.63	8 (16%)
39	GDP	P6	503	-	29,30,30	1.18	4 (13%)	45,47,47	1.76	6 (13%)
41	GTP	W0	501	40	33,34,34	0.88	2 (6%)	50,54,54	1.64	9 (18%)
39	GDP	0M	502	-	29,30,30	1.19	3 (10%)	45,47,47	1.80	7 (15%)
41	GTP	E8	501	40	33,34,34	0.88	0	50,54,54	1.55	8 (16%)
39	GDP	I8	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.77	7 (15%)
41	GTP	M2	501	40	33,34,34	0.90	1 (3%)	50,54,54	1.60	8 (16%)
39	GDP	0I	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
39	GDP	L0	501	-	29,30,30	1.17	4 (13%)	45,47,47	1.80	7 (15%)
41	GTP	X0	501	40	33,34,34	0.89	2 (6%)	50,54,54	1.59	9 (18%)
41	GTP	W2	501	40	33,34,34	0.87	2 (6%)	50,54,54	1.58	8 (16%)
41	GTP	T8	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.59	8 (16%)
41	GTP	L7	501	40	33,34,34	0.99	2 (6%)	50,54,54	1.65	9 (18%)
39	GDP	J6	502	-	29,30,30	1.15	4 (13%)	45,47,47	1.79	8 (17%)
41	GTP	0F	501	40	33,34,34	0.89	0	50,54,54	1.54	8 (16%)
41	GTP	Q4	501	40	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
41	GTP	W8	501	40	33,34,34	0.89	1 (3%)	50,54,54	1.60	8 (16%)
39	GDP	Y0	502	-	29,30,30	1.14	4 (13%)	45,47,47	1.76	7 (15%)
39	GDP	R4	502	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	C6	501	-	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	1C	501	40	-	8/22/38/38	0/3/3/3
39	GDP	K4	502	-	-	1/16/32/32	0/3/3/3
41	GTP	N8	501	40	-	8/22/38/38	0/3/3/3
41	GTP	E6	501	40	-	8/22/38/38	0/3/3/3
41	GTP	2G	501	40	-	7/22/38/38	0/3/3/3
39	GDP	V0	501	-	-	1/16/32/32	0/3/3/3
39	GDP	R2	502	-	-	1/16/32/32	0/3/3/3
39	GDP	3S	502	-	-	4/16/32/32	0/3/3/3
41	GTP	3T	501	40	-	8/22/38/38	0/3/3/3
41	GTP	Z2	501	40	-	9/22/38/38	0/3/3/3
41	GTP	C9	501	40	-	5/22/38/38	0/3/3/3
39	GDP	G8	501	-	-	1/16/32/32	0/3/3/3
41	GTP	R8	501	40	-	6/22/38/38	0/3/3/3
41	GTP	O4	501	40	-	8/22/38/38	0/3/3/3
39	GDP	3M	502	-	-	7/16/32/32	0/3/3/3
39	GDP	M0	502	-	-	3/16/32/32	0/3/3/3
39	GDP	I2	501	-	-	1/16/32/32	0/3/3/3
39	GDP	3C	502	-	-	3/16/32/32	0/3/3/3
41	GTP	M7	501	40	-	8/22/38/38	0/3/3/3
41	GTP	4	501	40	-	6/22/38/38	0/3/3/3
39	GDP	O8	503	-	-	1/16/32/32	0/3/3/3
41	GTP	I5	501	40	-	9/22/38/38	0/3/3/3
41	GTP	K0	501	40	-	8/22/38/38	0/3/3/3
41	GTP	C5	501	40	-	7/22/38/38	0/3/3/3
41	GTP	V3	501	40	-	7/22/38/38	0/3/3/3
41	GTP	S2	501	40	-	6/22/38/38	0/3/3/3
39	GDP	2K	502	-	-	1/16/32/32	0/3/3/3
41	GTP	N3	501	40	-	9/22/38/38	0/3/3/3
39	GDP	Y4	502	-	-	6/16/32/32	0/3/3/3
39	GDP	T0	501	-	-	4/16/32/32	0/3/3/3
39	GDP	Z4	501	-	-	1/16/32/32	0/3/3/3
39	GDP	P4	503	-	-	4/16/32/32	0/3/3/3
41	GTP	1D	501	40	-	7/22/38/38	0/3/3/3
41	GTP	1G	501	40	-	9/22/38/38	0/3/3/3
39	GDP	0O	502	-	-	1/16/32/32	0/3/3/3
39	GDP	Z2	503	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	D4	501	-	-	6/16/32/32	0/3/3/3
41	GTP	S8	501	40	-	7/22/38/38	0/3/3/3
41	GTP	0I	501	40	-	9/22/38/38	0/3/3/3
41	GTP	R0	501	40	-	8/22/38/38	0/3/3/3
39	GDP	0U	501	-	-	6/16/32/32	0/3/3/3
39	GDP	B5	502	-	-	4/16/32/32	0/3/3/3
39	GDP	3Q	501	-	-	3/16/32/32	0/3/3/3
39	GDP	H6	502	-	-	1/16/32/32	0/3/3/3
39	GDP	1O	501	-	-	1/16/32/32	0/3/3/3
39	GDP	1K	501	-	-	4/16/32/32	0/3/3/3
39	GDP	K6	502	-	-	2/16/32/32	0/3/3/3
41	GTP	Y0	501	40	-	8/22/38/38	0/3/3/3
39	GDP	P8	502	-	-	3/16/32/32	0/3/3/3
41	GTP	V2	501	40	-	6/22/38/38	0/3/3/3
39	GDP	3I	502	-	-	4/16/32/32	0/3/3/3
41	GTP	C8	501	40	-	2/22/38/38	0/3/3/3
41	GTP	2Q	501	40	-	8/22/38/38	0/3/3/3
41	GTP	0M	501	40	-	7/22/38/38	0/3/3/3
41	GTP	0K	501	40	-	8/22/38/38	0/3/3/3
41	GTP	O2	501	40	-	9/22/38/38	0/3/3/3
41	GTP	1S	501	40	-	5/22/38/38	0/3/3/3
39	GDP	J0	502	-	-	1/16/32/32	0/3/3/3
41	GTP	G9	501	40	-	9/22/38/38	0/3/3/3
41	GTP	1W	501	40	-	7/22/38/38	0/3/3/3
41	GTP	3M	501	40	-	6/22/38/38	0/3/3/3
39	GDP	C2	501	-	-	2/16/32/32	0/3/3/3
41	GTP	F3	501	40	-	5/22/38/38	0/3/3/3
39	GDP	U8	501	-	-	3/16/32/32	0/3/3/3
41	GTP	O0	501	40	-	8/22/38/38	0/3/3/3
39	GDP	H2	503	-	-	0/16/32/32	0/3/3/3
39	GDP	Z8	501	-	-	1/16/32/32	0/3/3/3
41	GTP	S5	501	40	-	4/22/38/38	0/3/3/3
41	GTP	D5	501	40	-	4/22/38/38	0/3/3/3
39	GDP	E6	502	-	-	6/16/32/32	0/3/3/3
39	GDP	7	502	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	U4	502	-	-	6/16/32/32	0/3/3/3
39	GDP	Y6	502	-	-	6/16/32/32	0/3/3/3
41	GTP	Q6	501	40	-	6/22/38/38	0/3/3/3
39	GDP	A9	502	-	-	3/16/32/32	0/3/3/3
39	GDP	S0	502	-	-	4/16/32/32	0/3/3/3
41	GTP	I8	501	40	-	7/22/38/38	0/3/3/3
41	GTP	L4	501	40	-	7/22/38/38	0/3/3/3
41	GTP	2E	501	40	-	9/22/38/38	0/3/3/3
39	GDP	A7	501	-	-	5/16/32/32	0/3/3/3
39	GDP	0Y	502	-	-	1/16/32/32	0/3/3/3
41	GTP	Y6	501	40	-	8/22/38/38	0/3/3/3
39	GDP	I0	502	-	-	1/16/32/32	0/3/3/3
39	GDP	Y8	501	-	-	3/16/32/32	0/3/3/3
41	GTP	K9	501	40	-	6/22/38/38	0/3/3/3
39	GDP	F8	502	-	-	1/16/32/32	0/3/3/3
41	GTP	0Y	501	40	-	9/22/38/38	0/3/3/3
39	GDP	C0	502	-	-	3/16/32/32	0/3/3/3
39	GDP	V8	502	-	-	3/16/32/32	0/3/3/3
39	GDP	K0	502	-	-	4/16/32/32	0/3/3/3
39	GDP	2W	502	-	-	5/16/32/32	0/3/3/3
39	GDP	A5	501	-	-	0/16/32/32	0/3/3/3
39	GDP	A1	502	-	-	6/16/32/32	0/3/3/3
39	GDP	G0	502	-	-	1/16/32/32	0/3/3/3
39	GDP	L2	502	-	-	3/16/32/32	0/3/3/3
39	GDP	W2	503	-	-	1/16/32/32	0/3/3/3
39	GDP	Q2	502	-	-	3/16/32/32	0/3/3/3
41	GTP	2C	501	40	-	9/22/38/38	0/3/3/3
41	GTP	3I	501	40	-	8/22/38/38	0/3/3/3
41	GTP	A4	501	40	-	6/22/38/38	0/3/3/3
41	GTP	3O	501	40	-	6/22/38/38	0/3/3/3
41	GTP	H2	501	40	-	8/22/38/38	0/3/3/3
41	GTP	T6	501	40	-	5/22/38/38	0/3/3/3
41	GTP	J4	501	40	-	6/22/38/38	0/3/3/3
39	GDP	W8	503	-	-	2/16/32/32	0/3/3/3
41	GTP	G7	501	40	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	X6	501	40	-	7/22/38/38	0/3/3/3
39	GDP	B1	501	-	-	2/16/32/32	0/3/3/3
39	GDP	O4	502	-	-	6/16/32/32	0/3/3/3
39	GDP	R6	503	-	-	3/16/32/32	0/3/3/3
39	GDP	Q8	501	-	-	3/16/32/32	0/3/3/3
39	GDP	2I	502	-	-	5/16/32/32	0/3/3/3
39	GDP	1A	503	-	-	3/16/32/32	0/3/3/3
39	GDP	D8	501	-	-	2/16/32/32	0/3/3/3
39	GDP	D2	501	-	-	4/16/32/32	0/3/3/3
39	GDP	1Q	502	-	-	1/16/32/32	0/3/3/3
39	GDP	G6	501	-	-	5/16/32/32	0/3/3/3
39	GDP	Y2	501	-	-	2/16/32/32	0/3/3/3
39	GDP	1C	502	-	-	2/16/32/32	0/3/3/3
39	GDP	N2	501	-	-	3/16/32/32	0/3/3/3
41	GTP	1X	501	40	-	7/22/38/38	0/3/3/3
41	GTP	U6	501	40	-	8/22/38/38	0/3/3/3
39	GDP	X4	502	-	-	4/16/32/32	0/3/3/3
39	GDP	L6	502	-	-	6/16/32/32	0/3/3/3
39	GDP	T8	502	-	-	3/16/32/32	0/3/3/3
39	GDP	S4	501	-	-	1/16/32/32	0/3/3/3
41	GTP	I1	501	40	-	9/22/38/38	0/3/3/3
41	GTP	8	501	40	-	5/22/38/38	0/3/3/3
41	GTP	N1	501	40	-	7/22/38/38	0/3/3/3
39	GDP	T2	502	-	-	4/16/32/32	0/3/3/3
41	GTP	3G	501	40	-	8/22/38/38	0/3/3/3
41	GTP	I0	501	40	-	7/22/38/38	0/3/3/3
39	GDP	3A	502	-	-	4/16/32/32	0/3/3/3
39	GDP	N0	502	-	-	1/16/32/32	0/3/3/3
39	GDP	2Y	502	-	-	7/16/32/32	0/3/3/3
41	GTP	O9	501	40	-	6/22/38/38	0/3/3/3
39	GDP	V2	503	-	-	3/16/32/32	0/3/3/3
41	GTP	2N	501	40	-	8/22/38/38	0/3/3/3
39	GDP	9	501	-	-	0/16/32/32	0/3/3/3
39	GDP	0E	501	-	-	2/16/32/32	0/3/3/3
41	GTP	D1	501	40	-	5/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	2A	502	-	-	0/16/32/32	0/3/3/3
41	GTP	1N	501	40	-	8/22/38/38	0/3/3/3
39	GDP	0S	502	-	-	2/16/32/32	0/3/3/3
39	GDP	2C	502	-	-	1/16/32/32	0/3/3/3
39	GDP	F0	502	-	-	3/16/32/32	0/3/3/3
41	GTP	G0	501	40	-	9/22/38/38	0/3/3/3
39	GDP	A3	501	-	-	5/16/32/32	0/3/3/3
41	GTP	0V	501	40	-	9/22/38/38	0/3/3/3
39	GDP	J8	502	-	-	2/16/32/32	0/3/3/3
41	GTP	R2	501	40	-	6/22/38/38	0/3/3/3
39	GDP	H8	503	-	-	4/16/32/32	0/3/3/3
39	GDP	3	502	-	-	3/16/32/32	0/3/3/3
41	GTP	F8	501	40	-	8/22/38/38	0/3/3/3
39	GDP	O0	503	-	-	3/16/32/32	0/3/3/3
41	GTP	J6	501	40	-	8/22/38/38	0/3/3/3
41	GTP	H3	501	40	-	8/22/38/38	0/3/3/3
41	GTP	1A	501	40	-	9/22/38/38	0/3/3/3
39	GDP	N8	502	-	-	7/16/32/32	0/3/3/3
39	GDP	G4	502	-	-	1/16/32/32	0/3/3/3
39	GDP	Z6	502	-	-	1/16/32/32	0/3/3/3
41	GTP	3K	501	40	-	4/22/38/38	0/3/3/3
41	GTP	3A	501	40	-	6/22/38/38	0/3/3/3
41	GTP	2W	501	40	-	8/22/38/38	0/3/3/3
41	GTP	Z3	501	40	-	8/22/38/38	0/3/3/3
41	GTP	J2	501	40	-	8/22/38/38	0/3/3/3
39	GDP	V4	501	-	-	4/16/32/32	0/3/3/3
39	GDP	M2	502	-	-	1/16/32/32	0/3/3/3
41	GTP	K7	501	40	-	9/22/38/38	0/3/3/3
41	GTP	Q2	501	40	-	6/22/38/38	0/3/3/3
39	GDP	R0	502	-	-	4/16/32/32	0/3/3/3
41	GTP	F1	501	40	-	7/22/38/38	0/3/3/3
39	GDP	3O	502	-	-	5/16/32/32	0/3/3/3
41	GTP	0A	501	40	-	9/22/38/38	0/3/3/3
39	GDP	Z0	502	-	-	4/16/32/32	0/3/3/3
39	GDP	2E	502	-	-	1/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	F5	501	40	-	7/22/38/38	0/3/3/3
41	GTP	B0	501	40	-	8/22/38/38	0/3/3/3
39	GDP	0C	502	-	-	3/16/32/32	0/3/3/3
41	GTP	O6	501	40	-	7/22/38/38	0/3/3/3
41	GTP	H6	501	40	-	9/22/38/38	0/3/3/3
41	GTP	S9	501	40	-	3/22/38/38	0/3/3/3
39	GDP	K8	501	-	-	5/16/32/32	0/3/3/3
39	GDP	U2	502	-	-	4/16/32/32	0/3/3/3
41	GTP	W4	501	40	-	7/22/38/38	0/3/3/3
39	GDP	T4	502	-	-	4/16/32/32	0/3/3/3
39	GDP	C4	501	-	-	2/16/32/32	0/3/3/3
39	GDP	X2	501	-	-	4/16/32/32	0/3/3/3
41	GTP	A9	501	40	-	9/22/38/38	0/3/3/3
41	GTP	C1	501	40	-	7/22/38/38	0/3/3/3
41	GTP	N6	501	40	-	7/22/38/38	0/3/3/3
41	GTP	3P	501	40	-	9/22/38/38	0/3/3/3
41	GTP	P6	501	40	-	8/22/38/38	0/3/3/3
41	GTP	D7	501	40	-	4/22/38/38	0/3/3/3
41	GTP	J0	501	40	-	8/22/38/38	0/3/3/3
39	GDP	2S	502	-	-	4/16/32/32	0/3/3/3
41	GTP	G1	501	40	-	9/22/38/38	0/3/3/3
41	GTP	T2	501	40	-	6/22/38/38	0/3/3/3
41	GTP	U9	501	40	-	8/22/38/38	0/3/3/3
41	GTP	M0	501	40	-	8/22/38/38	0/3/3/3
41	GTP	J8	501	40	-	6/22/38/38	0/3/3/3
41	GTP	U4	501	40	-	7/22/38/38	0/3/3/3
41	GTP	2I	501	40	-	7/22/38/38	0/3/3/3
41	GTP	N0	501	40	-	9/22/38/38	0/3/3/3
41	GTP	2Y	501	40	-	8/22/38/38	0/3/3/3
39	GDP	3K	503	-	-	4/16/32/32	0/3/3/3
41	GTP	1T	501	40	-	7/22/38/38	0/3/3/3
41	GTP	0S	501	40	-	8/22/38/38	0/3/3/3
39	GDP	W0	502	-	-	5/16/32/32	0/3/3/3
41	GTP	Y1	501	40	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	B2	501	40	-	4/22/38/38	0/3/3/3
39	GDP	M6	502	-	-	5/16/32/32	0/3/3/3
41	GTP	3C	501	40	-	6/22/38/38	0/3/3/3
39	GDP	F2	501	-	-	3/16/32/32	0/3/3/3
39	GDP	X0	502	-	-	1/16/32/32	0/3/3/3
41	GTP	2A	501	40	-	8/22/38/38	0/3/3/3
39	GDP	W6	501	-	-	0/16/32/32	0/3/3/3
39	GDP	J4	503	-	-	4/16/32/32	0/3/3/3
39	GDP	0Q	502	-	-	4/16/32/32	0/3/3/3
39	GDP	0K	502	-	-	2/16/32/32	0/3/3/3
41	GTP	K4	501	40	-	8/22/38/38	0/3/3/3
41	GTP	W5	501	40	-	6/22/38/38	0/3/3/3
41	GTP	X7	501	40	-	9/22/38/38	0/3/3/3
39	GDP	E0	501	-	-	3/16/32/32	0/3/3/3
41	GTP	G5	501	40	-	7/22/38/38	0/3/3/3
41	GTP	D3	501	40	-	6/22/38/38	0/3/3/3
39	GDP	1W	502	-	-	1/16/32/32	0/3/3/3
41	GTP	0C	501	40	-	8/22/38/38	0/3/3/3
39	GDP	D6	501	-	-	6/16/32/32	0/3/3/3
39	GDP	I4	502	-	-	1/16/32/32	0/3/3/3
39	GDP	1E	501	-	-	1/16/32/32	0/3/3/3
41	GTP	2U	501	40	-	8/22/38/38	0/3/3/3
41	GTP	3D	501	40	-	8/22/38/38	0/3/3/3
41	GTP	A1	501	40	-	9/22/38/38	0/3/3/3
39	GDP	O2	502	-	-	5/16/32/32	0/3/3/3
41	GTP	A2	501	40	-	2/22/38/38	0/3/3/3
41	GTP	L2	501	40	-	7/22/38/38	0/3/3/3
41	GTP	U2	501	40	-	7/22/38/38	0/3/3/3
41	GTP	P4	501	40	-	8/22/38/38	0/3/3/3
39	GDP	Q4	502	-	-	6/16/32/32	0/3/3/3
41	GTP	K1	501	40	-	7/22/38/38	0/3/3/3
41	GTP	Z0	501	40	-	8/22/38/38	0/3/3/3
41	GTP	R6	501	40	-	6/22/38/38	0/3/3/3
39	GDP	E4	502	-	-	5/16/32/32	0/3/3/3
39	GDP	D0	501	-	-	8/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	B5	501	40	-	7/22/38/38	0/3/3/3
39	GDP	Q0	501	-	-	4/16/32/32	0/3/3/3
41	GTP	7	501	40	-	8/22/38/38	0/3/3/3
39	GDP	V6	501	-	-	4/16/32/32	0/3/3/3
41	GTP	O8	501	40	-	8/22/38/38	0/3/3/3
41	GTP	3S	501	40	-	7/22/38/38	0/3/3/3
41	GTP	P9	501	40	-	8/22/38/38	0/3/3/3
39	GDP	2U	502	-	-	5/16/32/32	0/3/3/3
39	GDP	B3	501	-	-	4/16/32/32	0/3/3/3
39	GDP	0G	501	-	-	2/16/32/32	0/3/3/3
39	GDP	O6	502	-	-	4/16/32/32	0/3/3/3
41	GTP	Y4	501	40	-	9/22/38/38	0/3/3/3
39	GDP	1U	501	-	-	4/16/32/32	0/3/3/3
39	GDP	C8	502	-	-	3/16/32/32	0/3/3/3
39	GDP	E8	502	-	-	4/16/32/32	0/3/3/3
39	GDP	2G	502	-	-	4/16/32/32	0/3/3/3
41	GTP	U7	501	40	-	8/22/38/38	0/3/3/3
41	GTP	T4	501	40	-	5/22/38/38	0/3/3/3
39	GDP	W4	502	-	-	4/16/32/32	0/3/3/3
39	GDP	X8	501	-	-	3/16/32/32	0/3/3/3
39	GDP	L4	502	-	-	1/16/32/32	0/3/3/3
39	GDP	R8	502	-	-	3/16/32/32	0/3/3/3
41	GTP	X4	501	40	-	8/22/38/38	0/3/3/3
41	GTP	1L	501	40	-	6/22/38/38	0/3/3/3
39	GDP	0A	503	-	-	1/16/32/32	0/3/3/3
39	GDP	S8	502	-	-	4/16/32/32	0/3/3/3
39	GDP	F6	501	-	-	4/16/32/32	0/3/3/3
41	GTP	2K	501	40	-	8/22/38/38	0/3/3/3
39	GDP	E2	501	-	-	5/16/32/32	0/3/3/3
39	GDP	2M	501	-	-	1/16/32/32	0/3/3/3
41	GTP	S0	501	40	-	8/22/38/38	0/3/3/3
41	GTP	Z7	501	40	-	7/22/38/38	0/3/3/3
39	GDP	M8	501	-	-	4/16/32/32	0/3/3/3
39	GDP	S2	502	-	-	5/16/32/32	0/3/3/3
41	GTP	1H	501	40	-	9/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	GTP	M4	501	40	-	8/22/38/38	0/3/3/3
41	GTP	M6	501	40	-	8/22/38/38	0/3/3/3
39	GDP	H4	501	-	-	4/16/32/32	0/3/3/3
39	GDP	G2	501	-	-	3/16/32/32	0/3/3/3
41	GTP	R4	501	40	-	8/22/38/38	0/3/3/3
39	GDP	2Q	502	-	-	2/16/32/32	0/3/3/3
41	GTP	2L	501	40	-	8/22/38/38	0/3/3/3
41	GTP	E4	501	40	-	6/22/38/38	0/3/3/3
41	GTP	H8	501	40	-	9/22/38/38	0/3/3/3
39	GDP	1G	502	-	-	0/16/32/32	0/3/3/3
41	GTP	C0	501	40	-	8/22/38/38	0/3/3/3
39	GDP	S6	501	-	-	7/16/32/32	0/3/3/3
41	GTP	0O	501	40	-	9/22/38/38	0/3/3/3
39	GDP	T6	502	-	-	7/16/32/32	0/3/3/3
39	GDP	J2	502	-	-	7/16/32/32	0/3/3/3
39	GDP	M4	502	-	-	4/16/32/32	0/3/3/3
39	GDP	1S	502	-	-	1/16/32/32	0/3/3/3
41	GTP	F0	501	40	-	6/22/38/38	0/3/3/3
41	GTP	2S	501	40	-	8/22/38/38	0/3/3/3
41	GTP	E1	501	40	-	6/22/38/38	0/3/3/3
39	GDP	2	501	-	-	6/16/32/32	0/3/3/3
41	GTP	0Q	501	40	-	8/22/38/38	0/3/3/3
39	GDP	U6	502	-	-	2/16/32/32	0/3/3/3
39	GDP	X6	502	-	-	4/16/32/32	0/3/3/3
41	GTP	3	501	40	-	5/22/38/38	0/3/3/3
41	GTP	K6	501	40	-	6/22/38/38	0/3/3/3
41	GTP	V8	501	40	-	7/22/38/38	0/3/3/3
39	GDP	5	501	-	-	2/16/32/32	0/3/3/3
39	GDP	B8	501	-	-	6/16/32/32	0/3/3/3
39	GDP	1M	501	-	-	1/16/32/32	0/3/3/3
41	GTP	P8	501	40	-	7/22/38/38	0/3/3/3
41	GTP	B7	501	40	-	8/22/38/38	0/3/3/3
41	GTP	I4	501	40	-	8/22/38/38	0/3/3/3
39	GDP	3G	502	-	-	3/16/32/32	0/3/3/3
41	GTP	G4	501	40	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	GDP	Q6	502	-	-	6/16/32/32	0/3/3/3
39	GDP	0W	502	-	-	2/16/32/32	0/3/3/3
39	GDP	N6	503	-	-	6/16/32/32	0/3/3/3
41	GTP	L6	501	40	-	6/22/38/38	0/3/3/3
41	GTP	Z6	501	40	-	9/22/38/38	0/3/3/3
41	GTP	1Q	501	40	-	6/22/38/38	0/3/3/3
39	GDP	P6	503	-	-	4/16/32/32	0/3/3/3
41	GTP	W0	501	40	-	8/22/38/38	0/3/3/3
39	GDP	0M	502	-	-	2/16/32/32	0/3/3/3
41	GTP	E8	501	40	-	5/22/38/38	0/3/3/3
39	GDP	I8	502	-	-	1/16/32/32	0/3/3/3
41	GTP	M2	501	40	-	8/22/38/38	0/3/3/3
39	GDP	0I	502	-	-	1/16/32/32	0/3/3/3
39	GDP	L0	501	-	-	2/16/32/32	0/3/3/3
41	GTP	X0	501	40	-	6/22/38/38	0/3/3/3
41	GTP	W2	501	40	-	7/22/38/38	0/3/3/3
41	GTP	T8	501	40	-	8/22/38/38	0/3/3/3
41	GTP	L7	501	40	-	8/22/38/38	0/3/3/3
39	GDP	J6	502	-	-	1/16/32/32	0/3/3/3
41	GTP	0F	501	40	-	9/22/38/38	0/3/3/3
41	GTP	Q4	501	40	-	8/22/38/38	0/3/3/3
41	GTP	W8	501	40	-	7/22/38/38	0/3/3/3
39	GDP	Y0	502	-	-	5/16/32/32	0/3/3/3
39	GDP	R4	502	-	-	7/16/32/32	0/3/3/3

The worst 5 of 803 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	0S	502	GDP	C5-C4	3.21	1.47	1.38
39	1E	501	GDP	C5-C4	3.05	1.47	1.38
39	O2	502	GDP	C6-N1	-3.00	1.33	1.38
39	0C	502	GDP	C5-C4	3.00	1.47	1.38
39	0E	501	GDP	C5-C4	2.99	1.47	1.38

The worst 5 of 2553 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	0S	502	GDP	C5-C4-N3	-6.42	118.17	128.39
39	1E	501	GDP	C5-C4-N3	-6.36	118.26	128.39
39	3I	502	GDP	C5-C4-N3	-6.32	118.33	128.39
39	W0	502	GDP	C5-C4-N3	-6.31	118.34	128.39
39	V6	501	GDP	C5-C4-N3	-6.29	118.39	128.39

There are no chirality outliers.

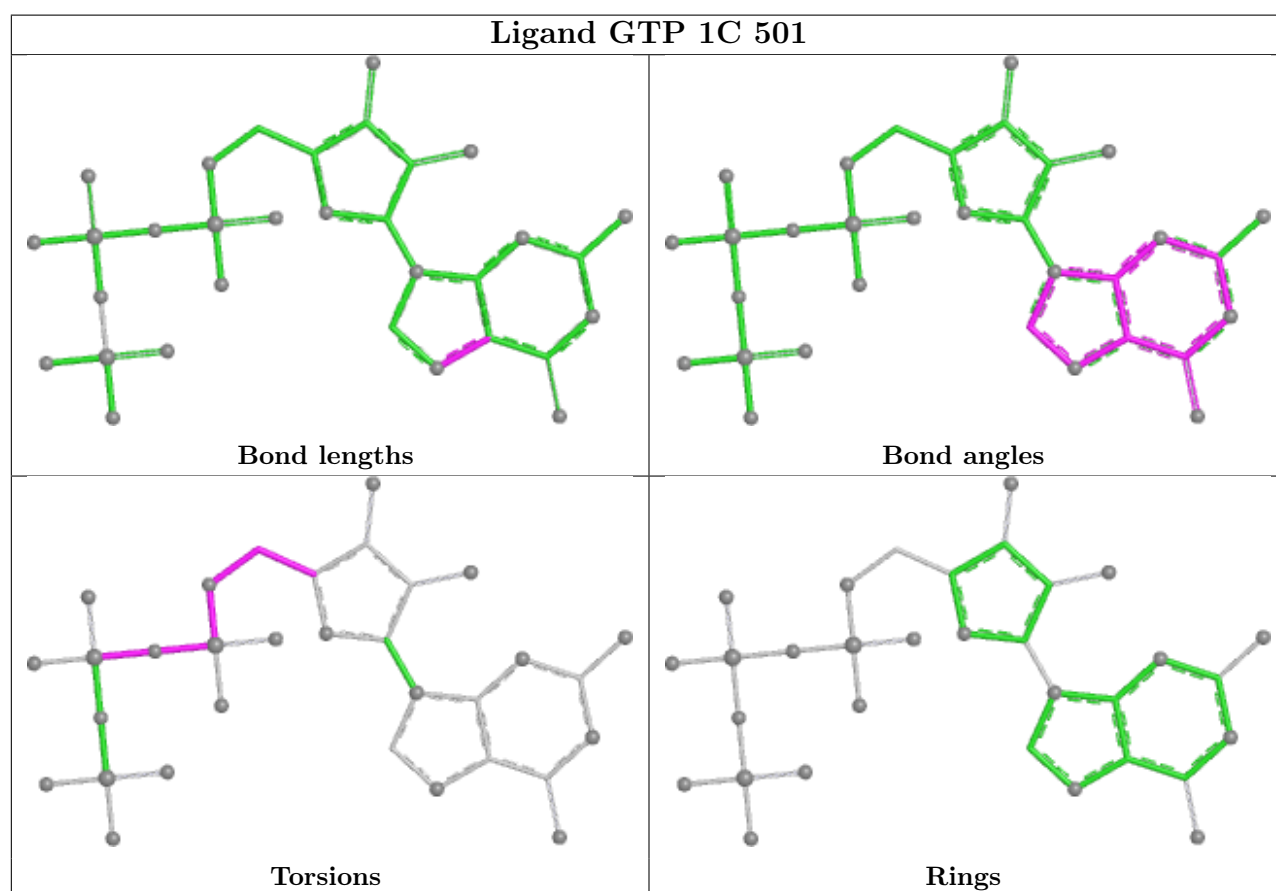
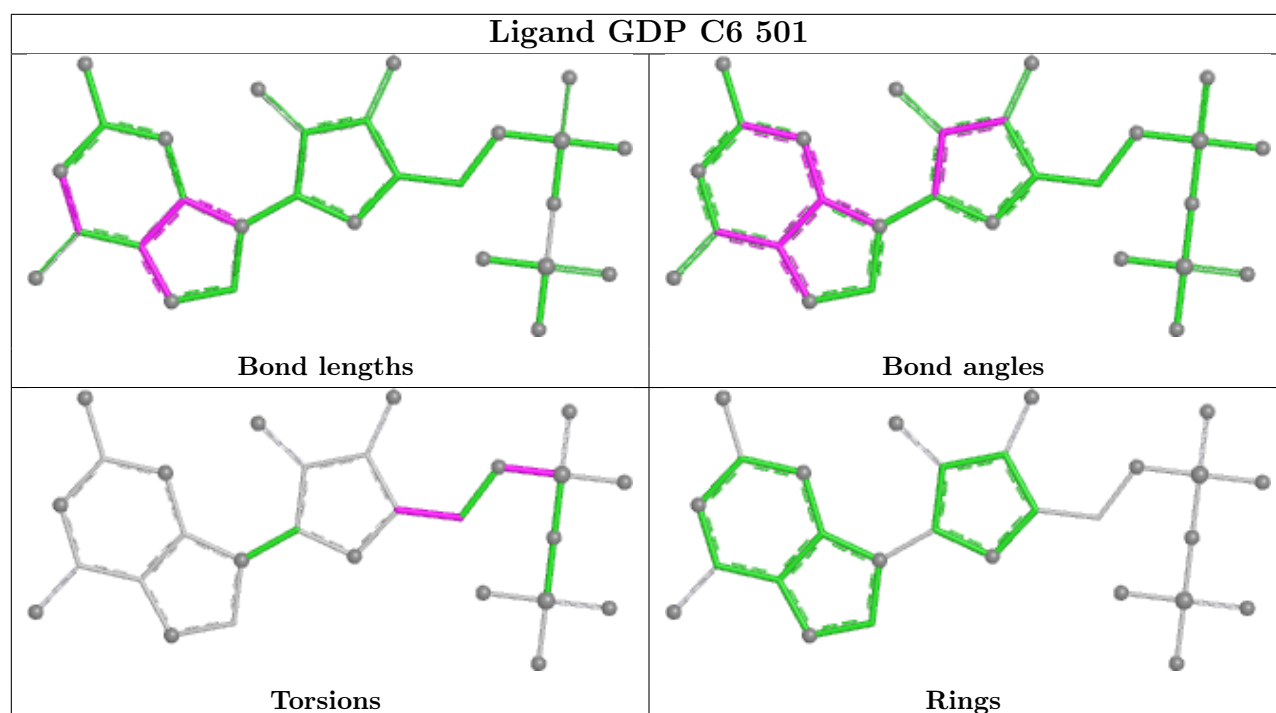
5 of 1774 torsion outliers are listed below:

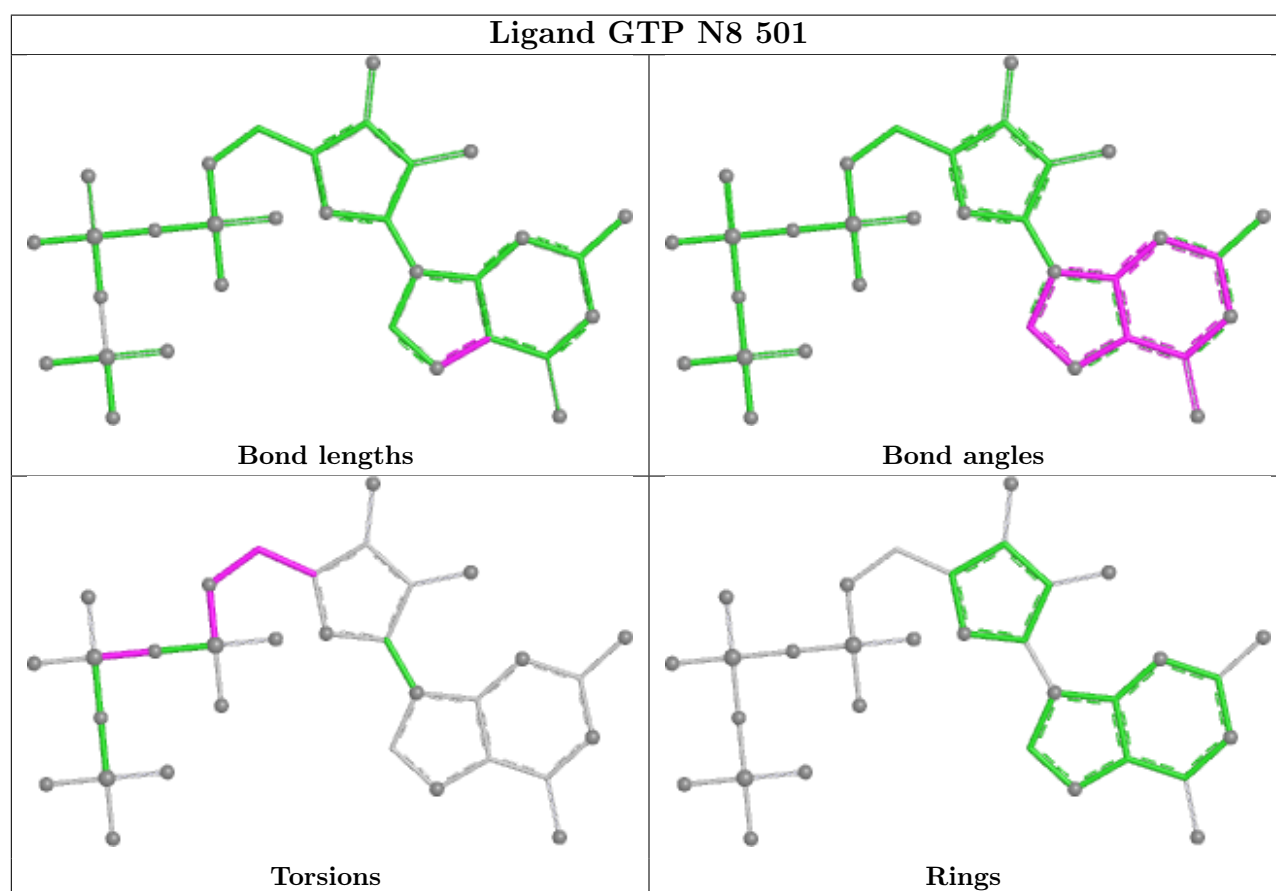
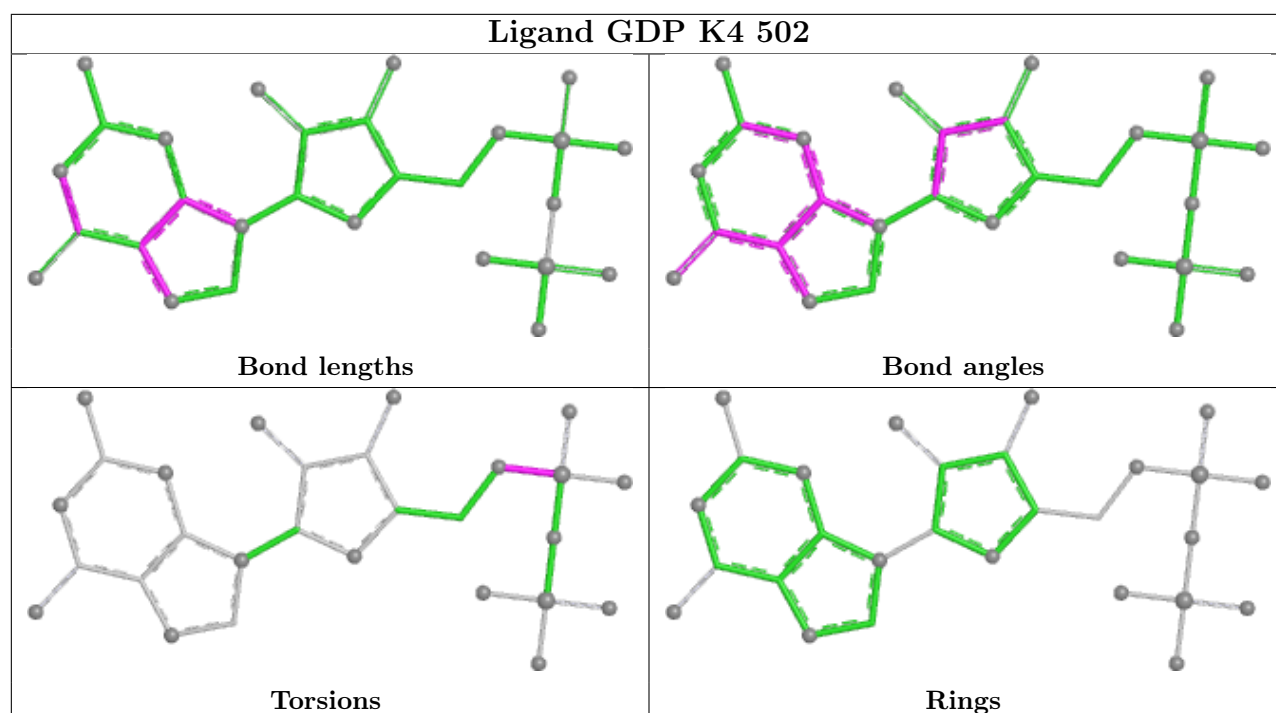
Mol	Chain	Res	Type	Atoms
39	2	501	GDP	PA-O3A-PB-O3B
39	2	501	GDP	C5'-O5'-PA-O3A
39	2	501	GDP	C5'-O5'-PA-O1A
39	3	502	GDP	C5'-O5'-PA-O3A
39	3	502	GDP	C5'-O5'-PA-O2A

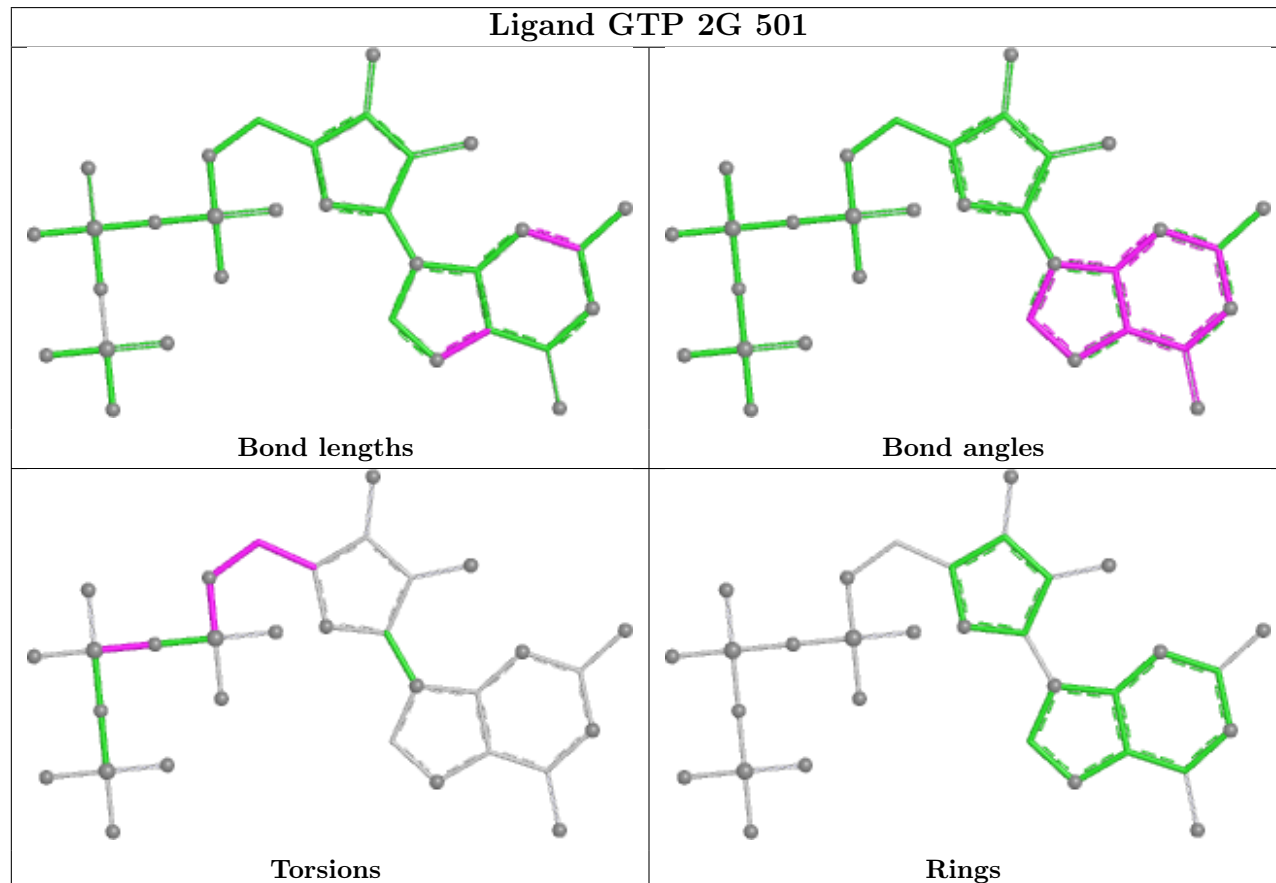
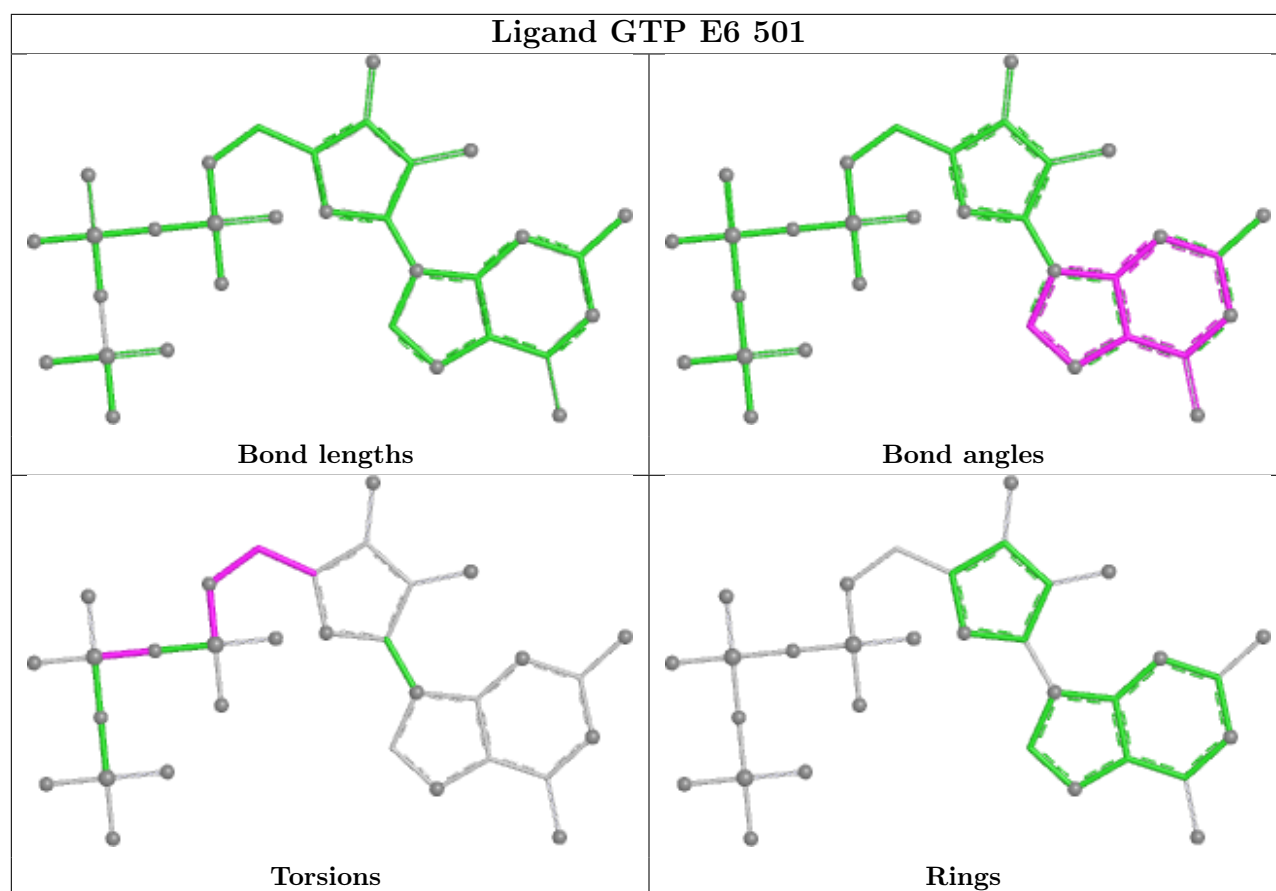
There are no ring outliers.

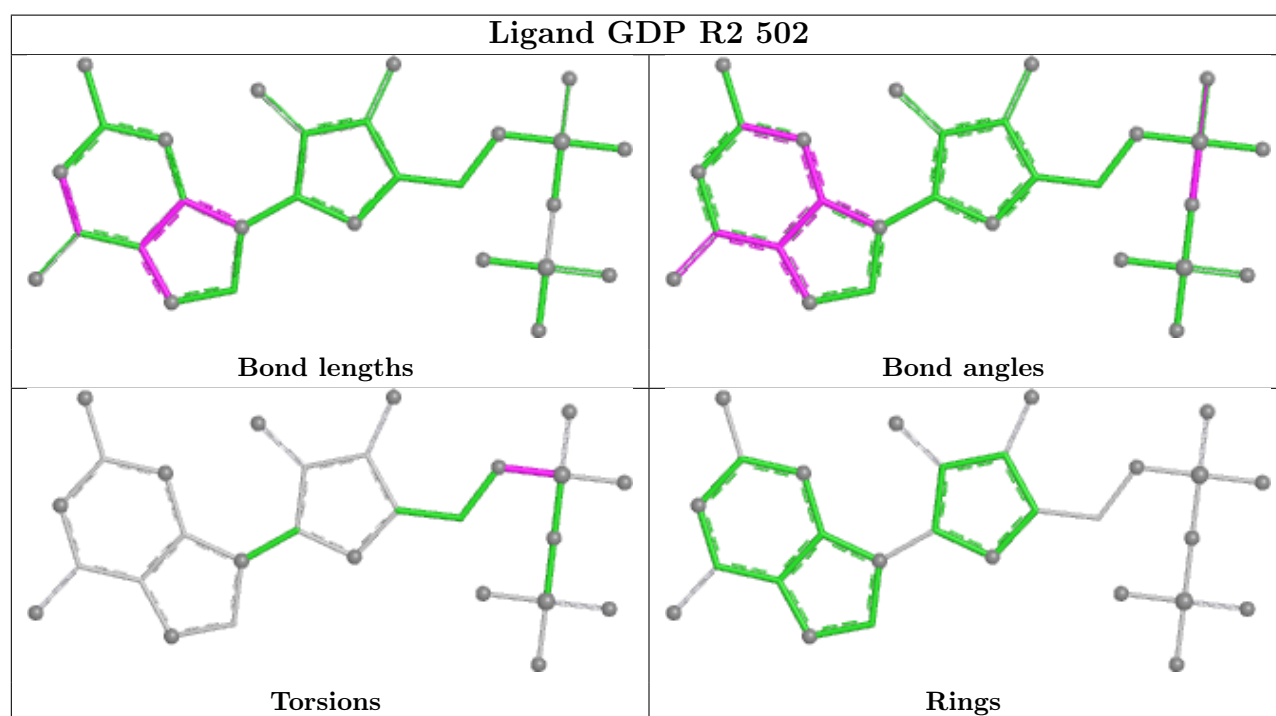
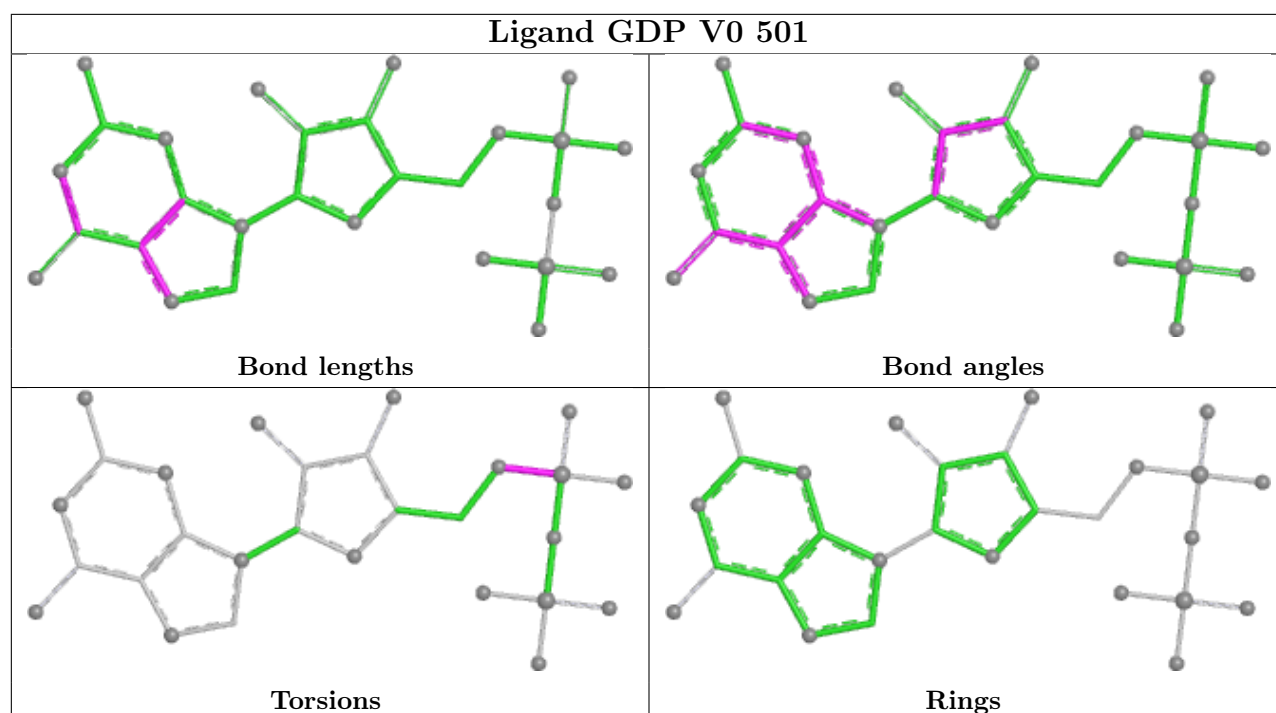
No monomer is involved in short contacts.

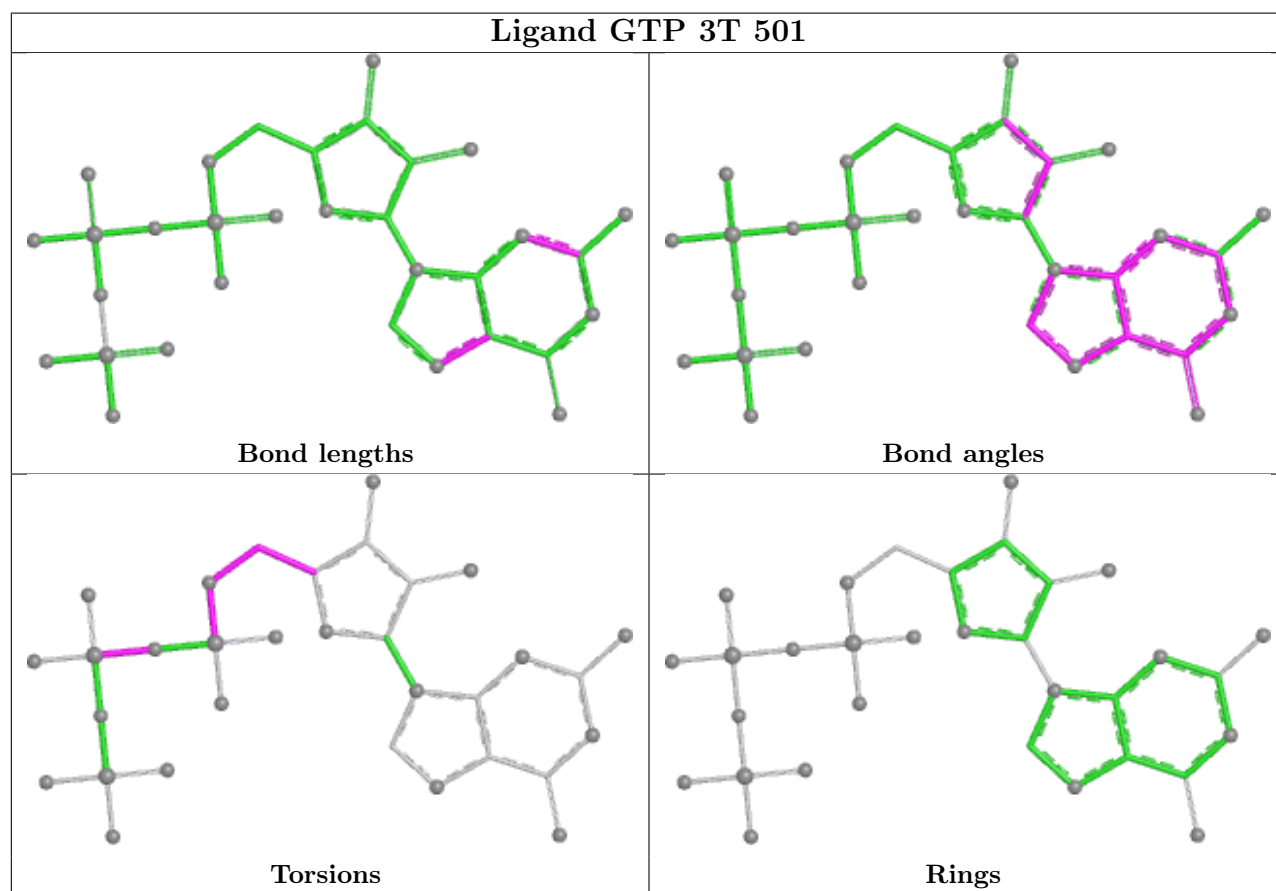
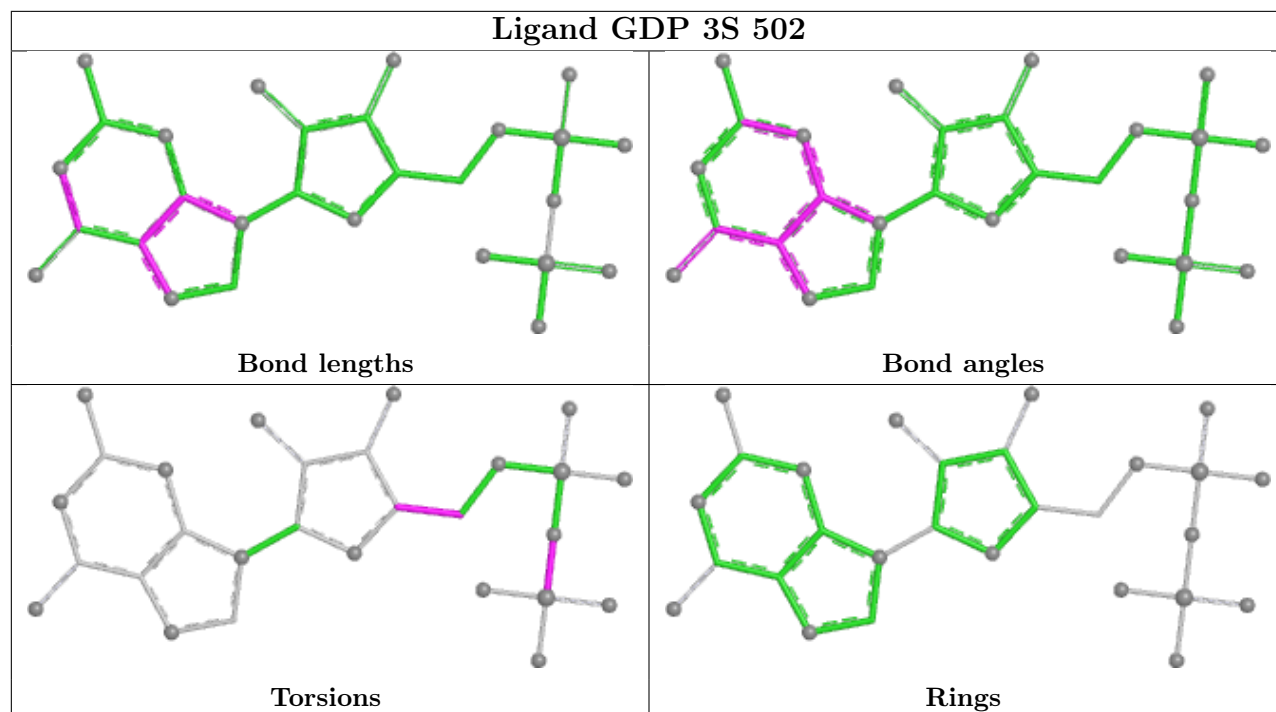
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

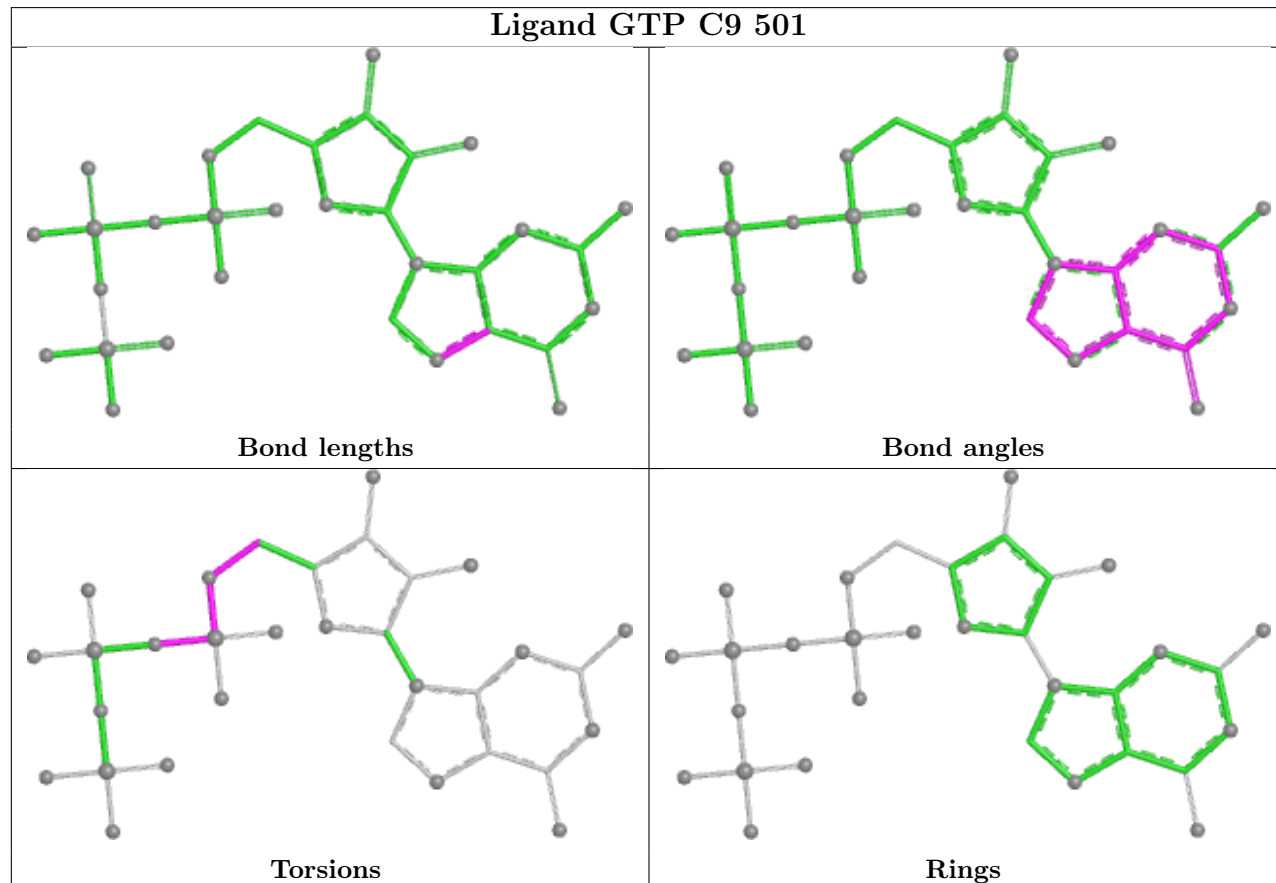
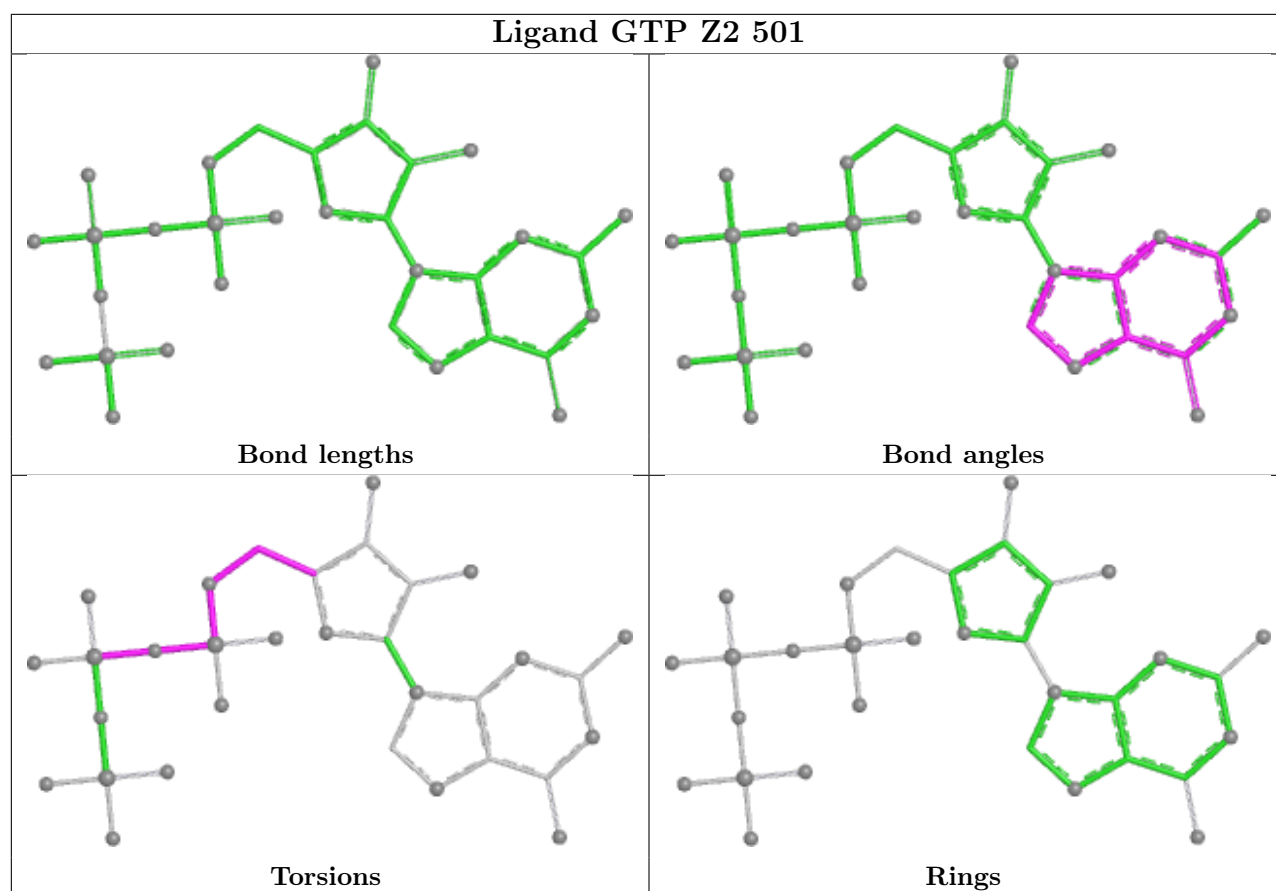


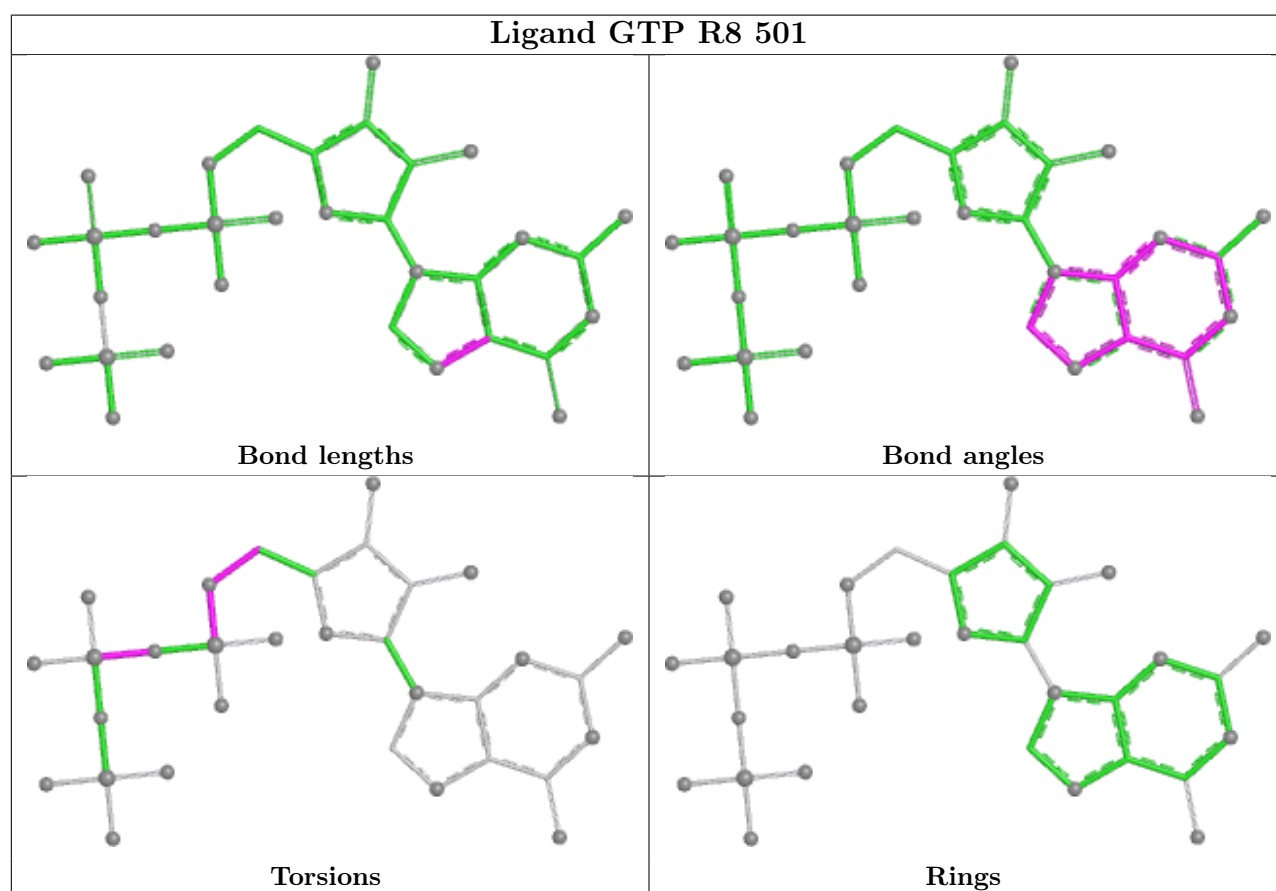
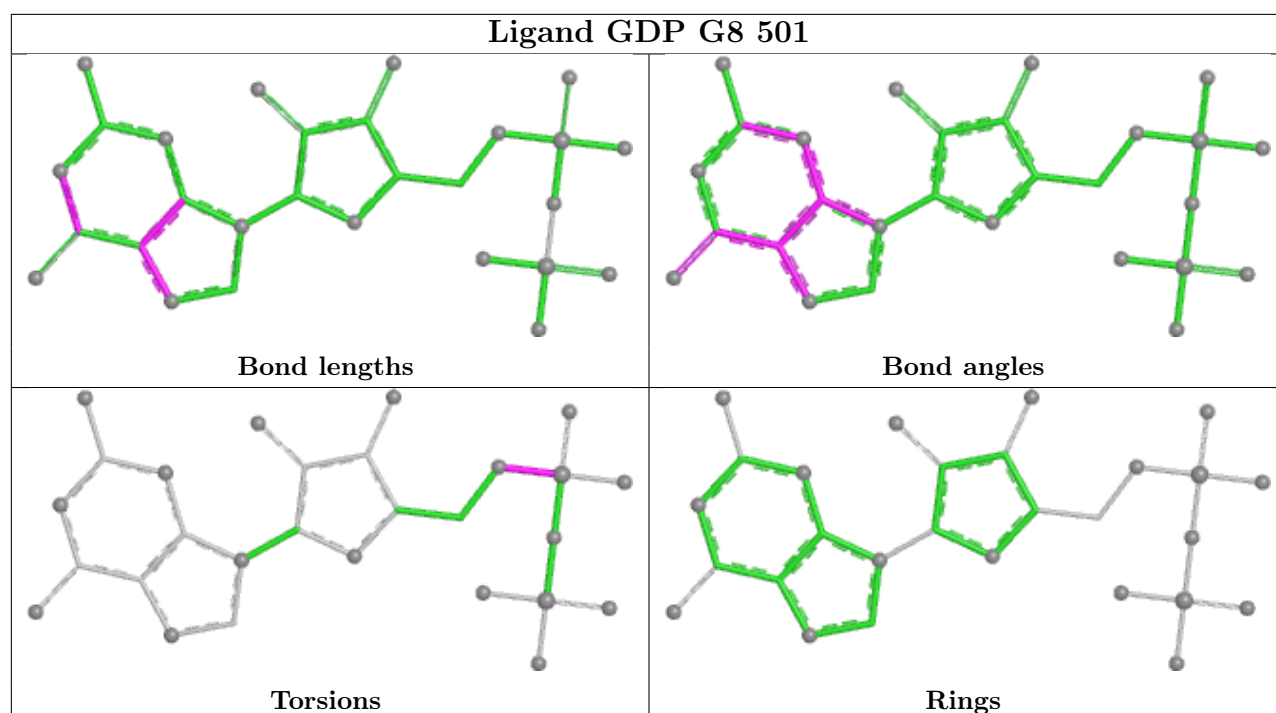


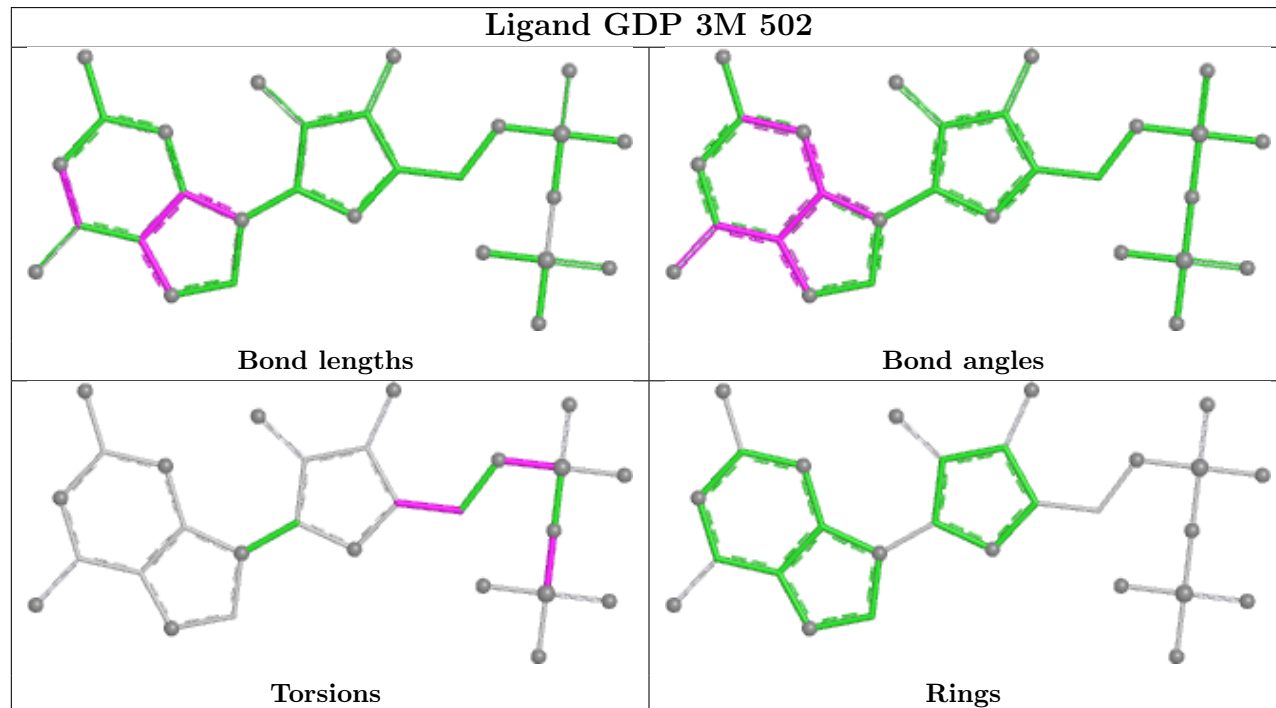
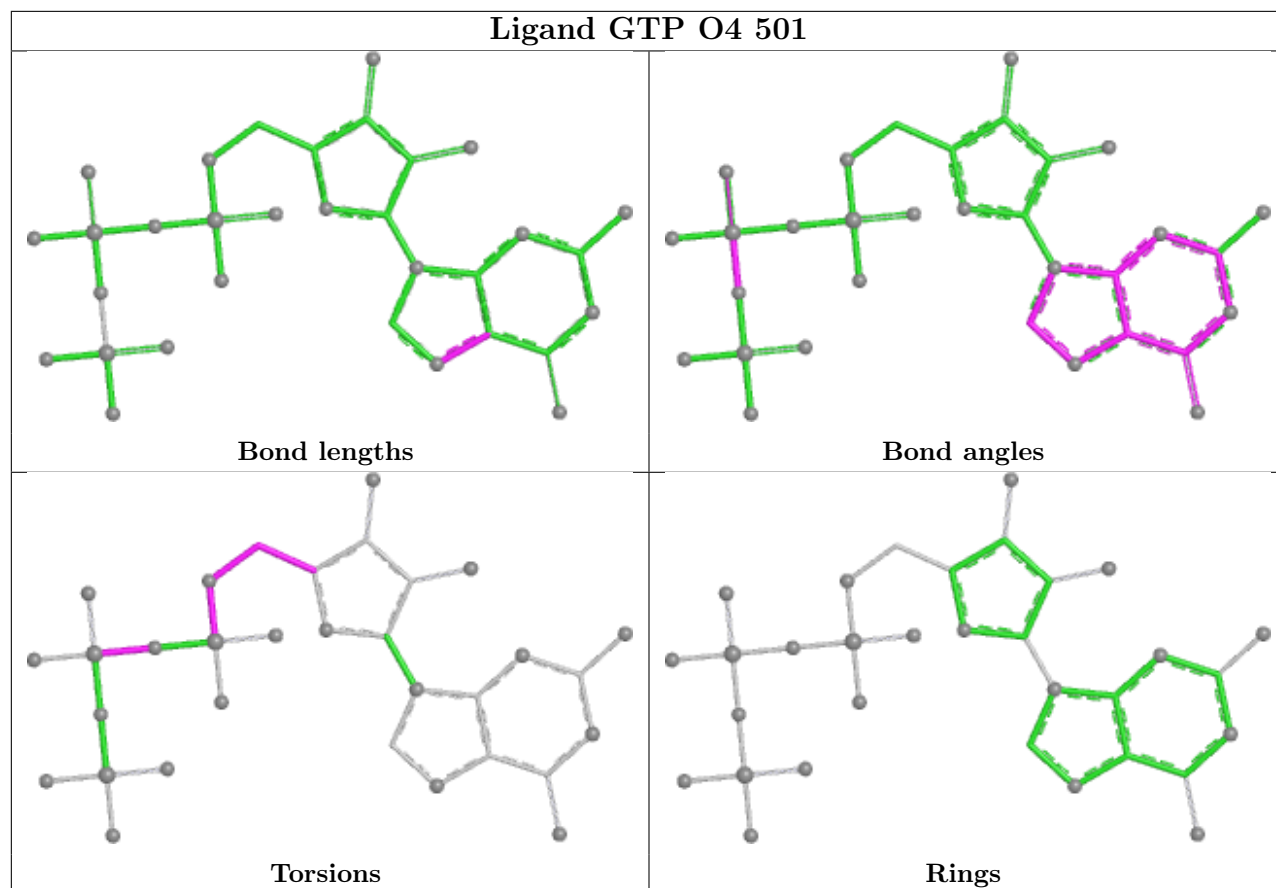


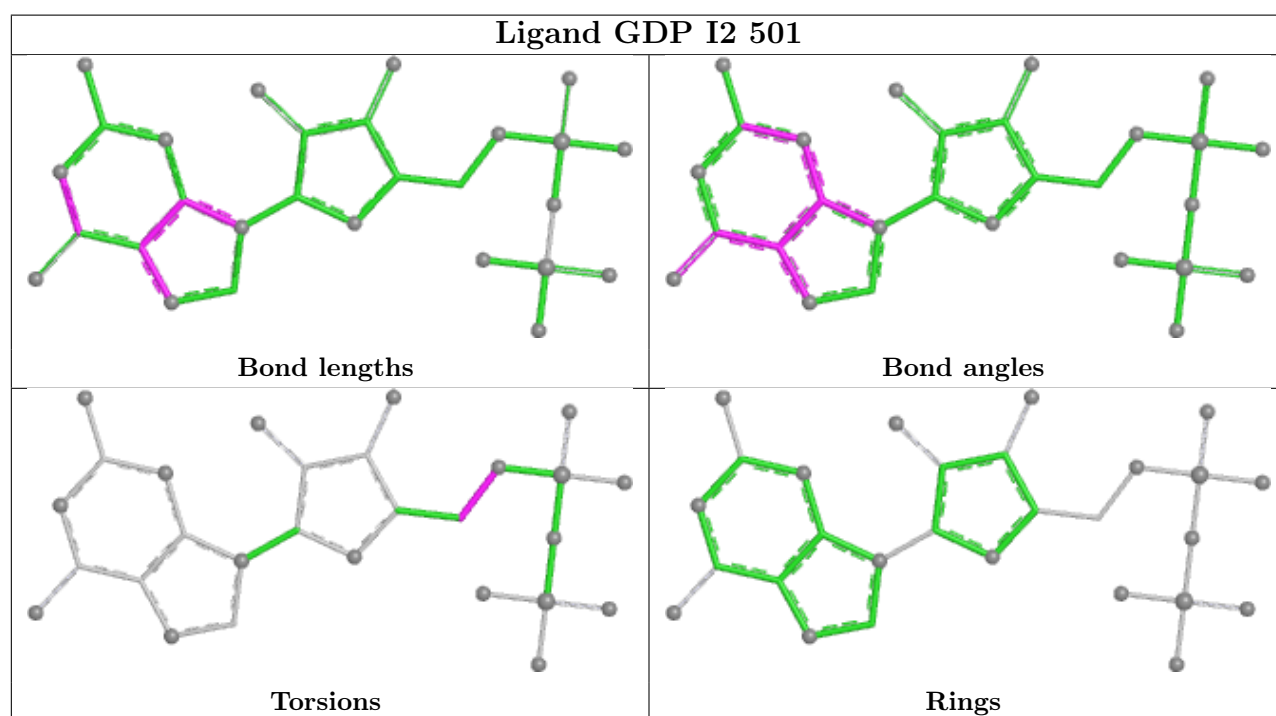
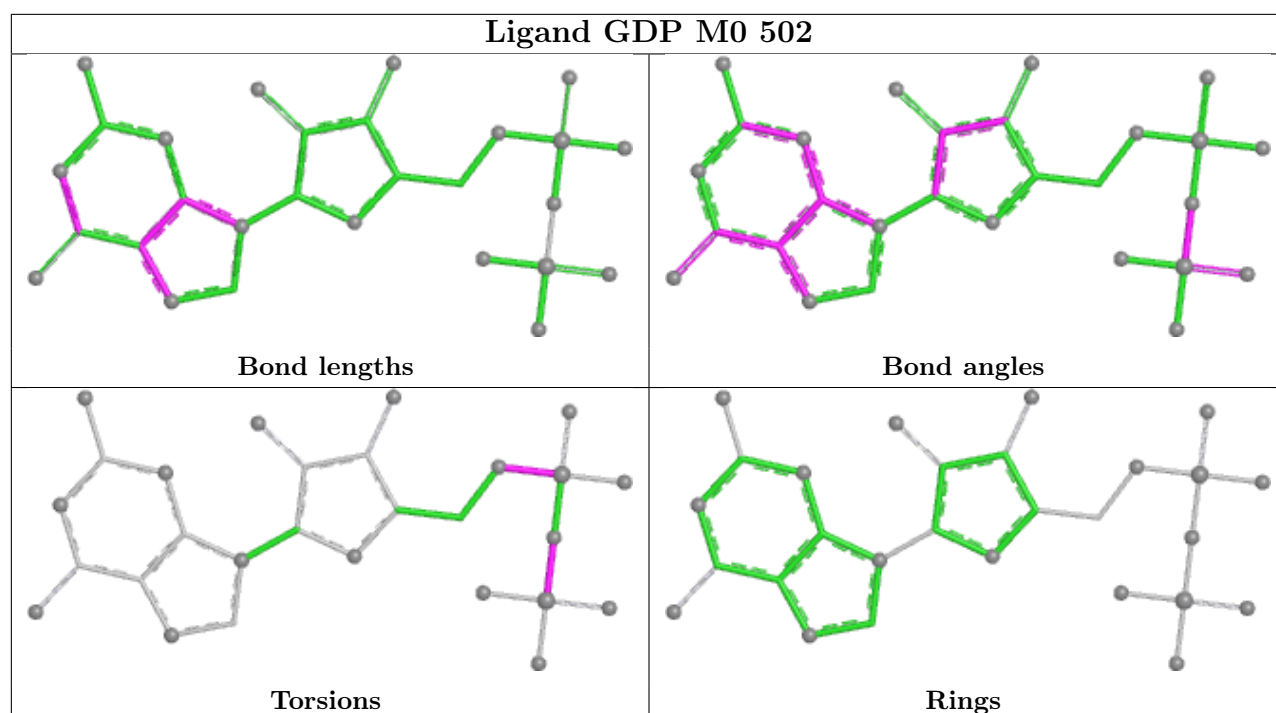


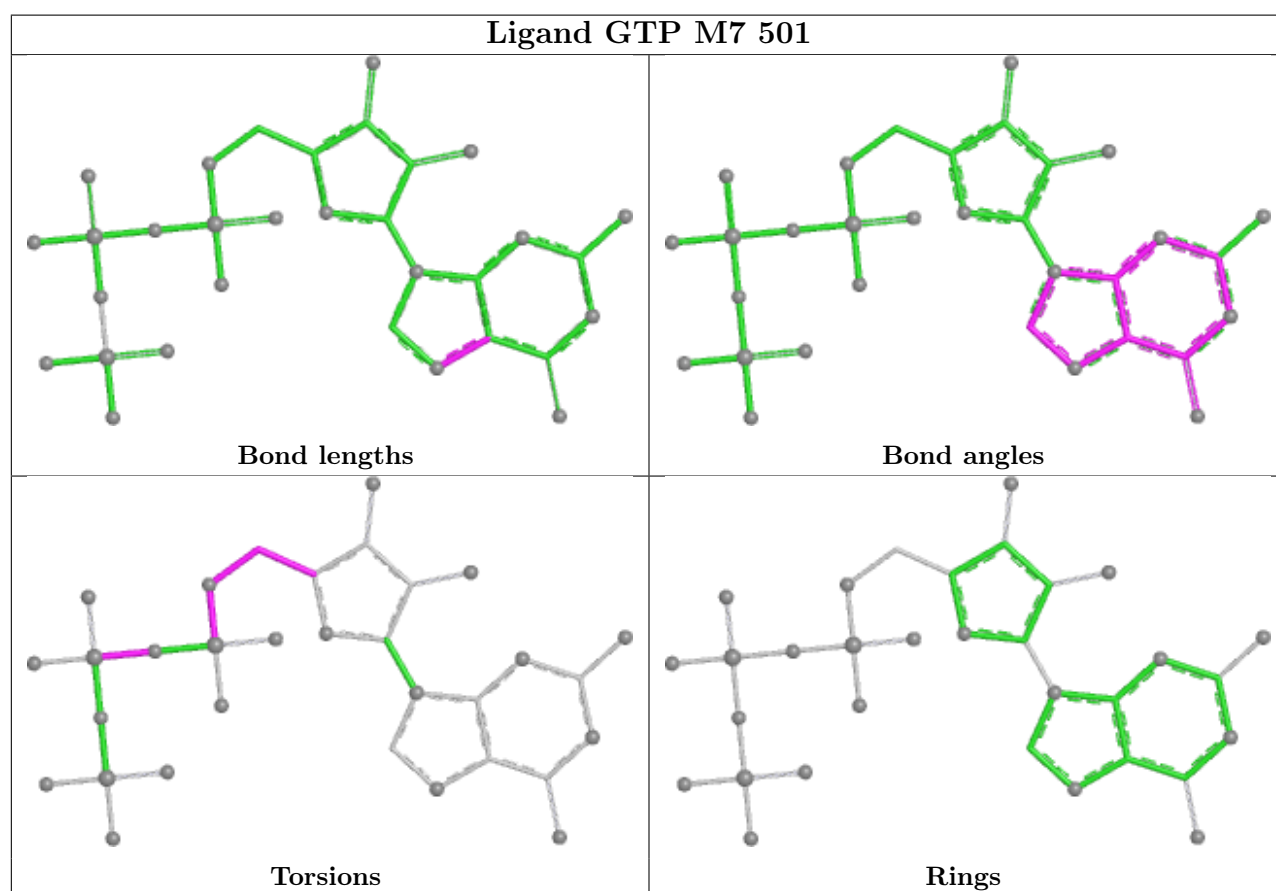
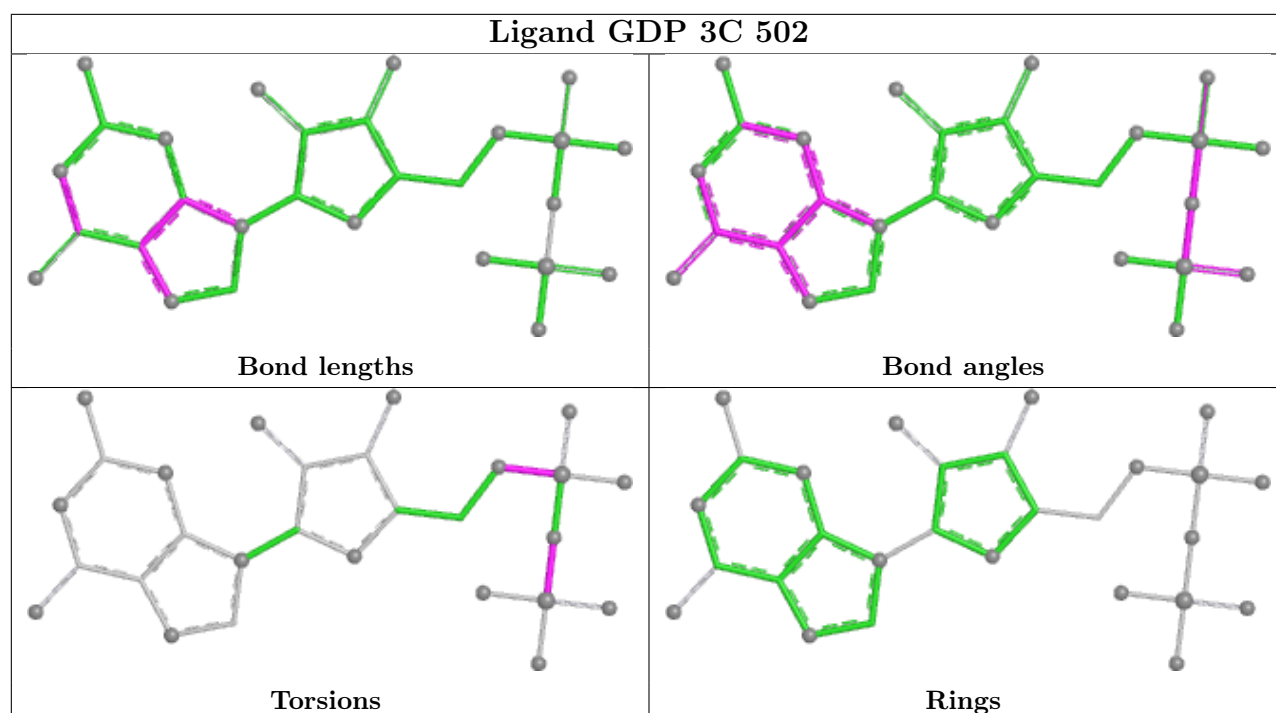


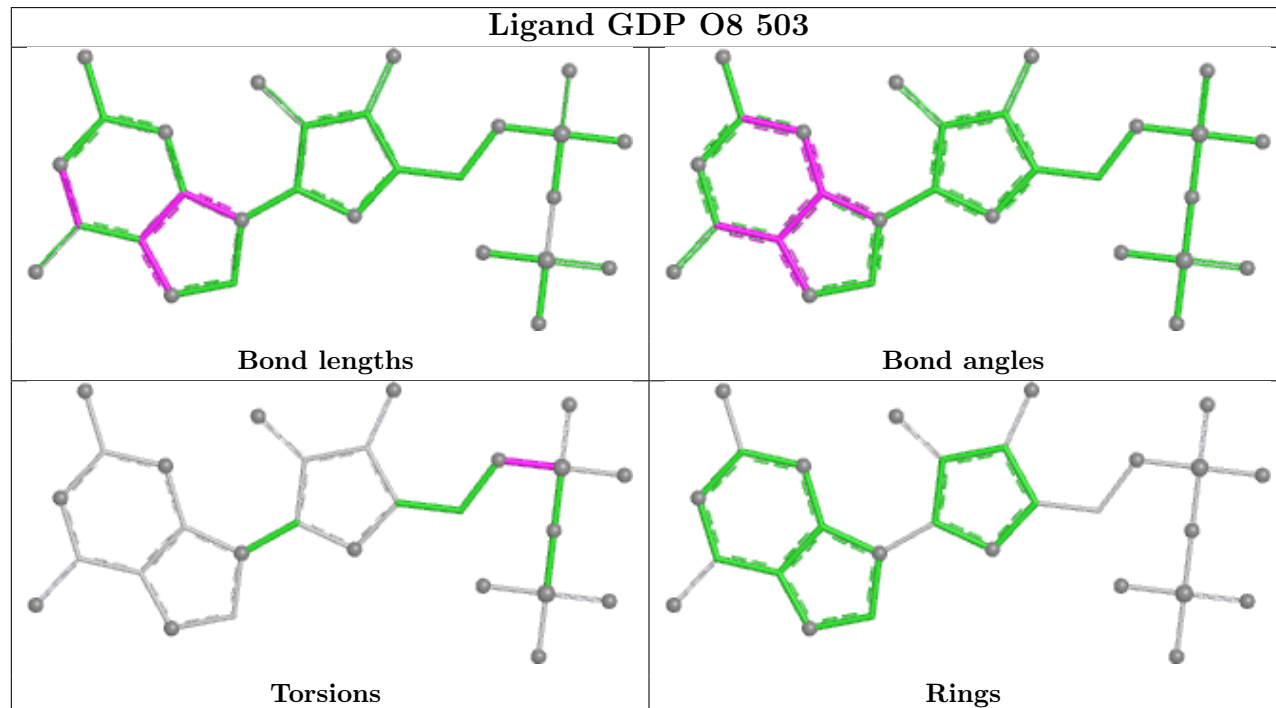
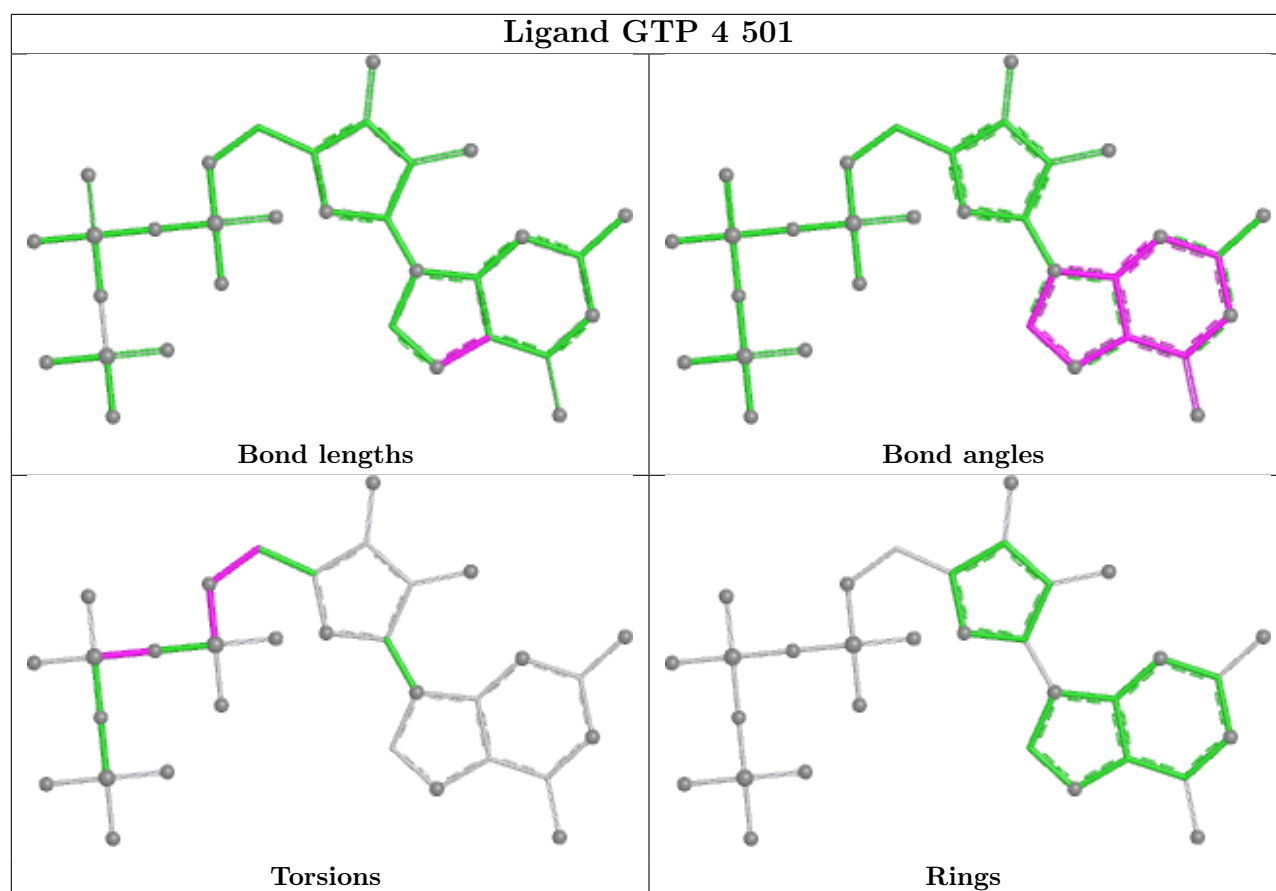


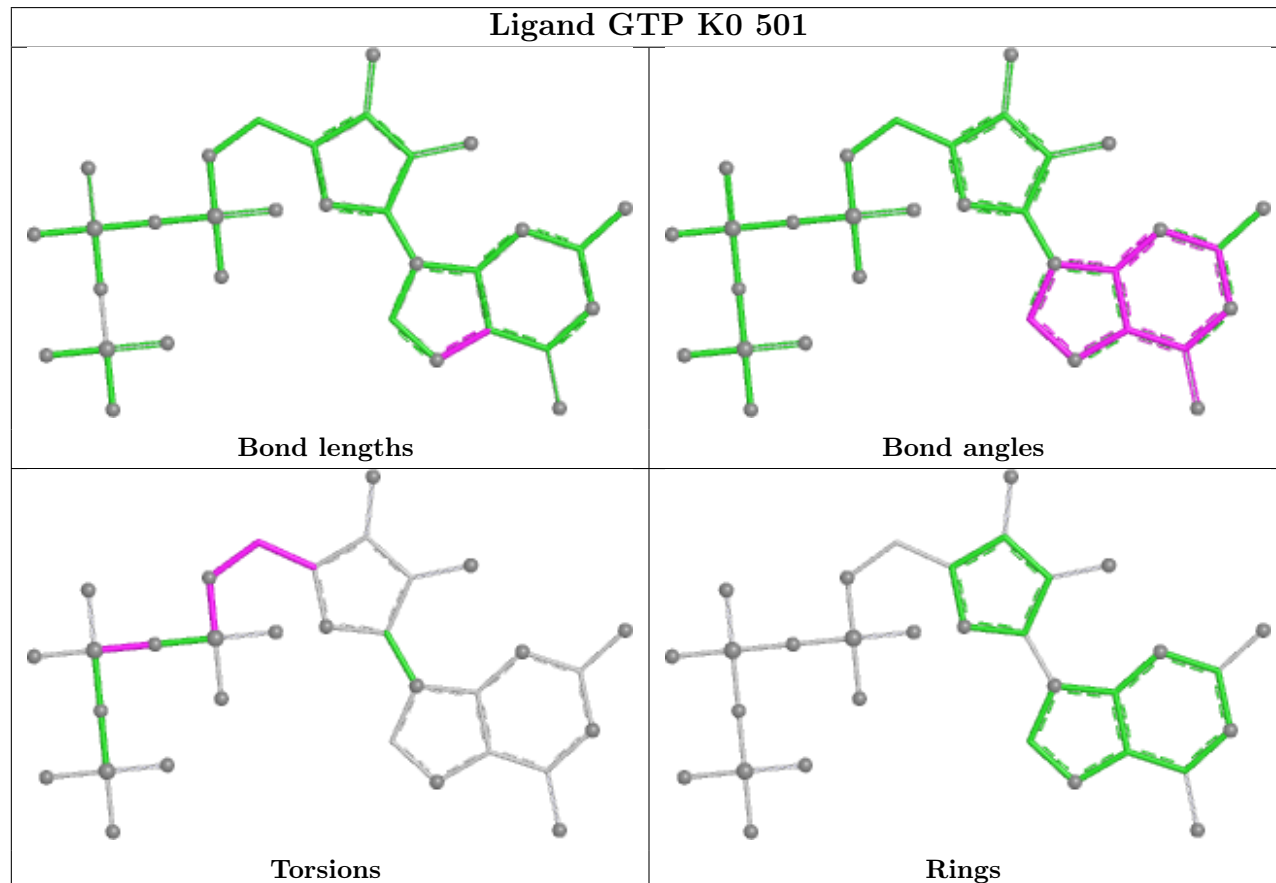
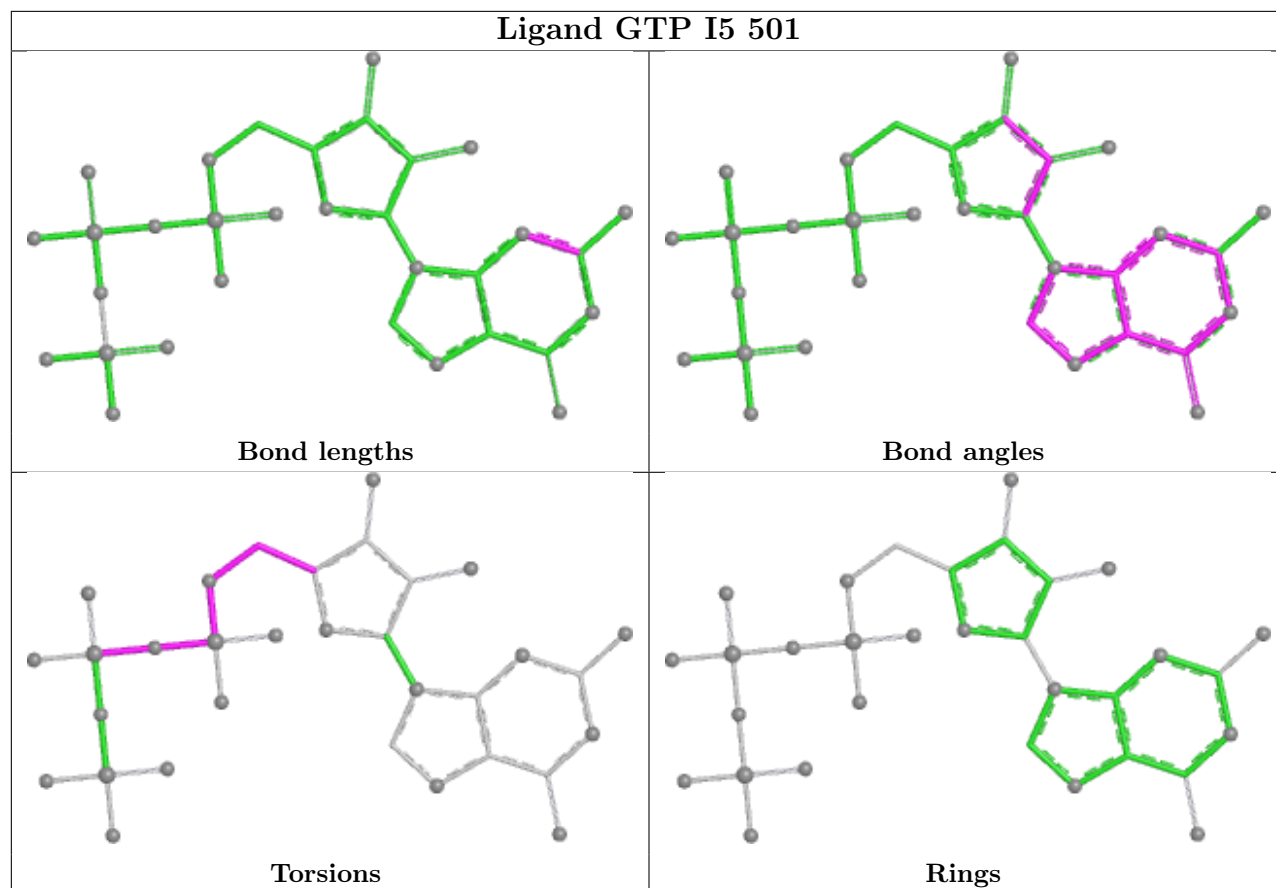




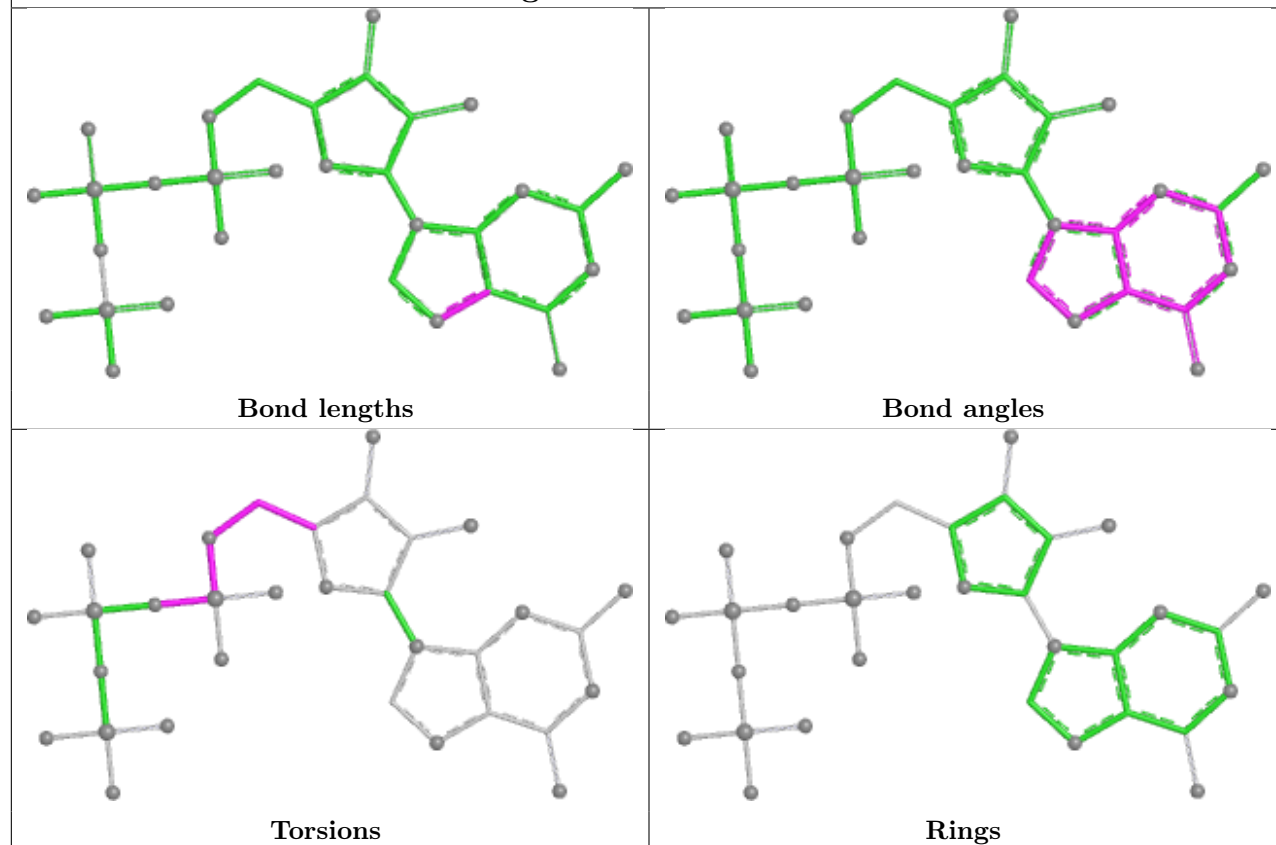




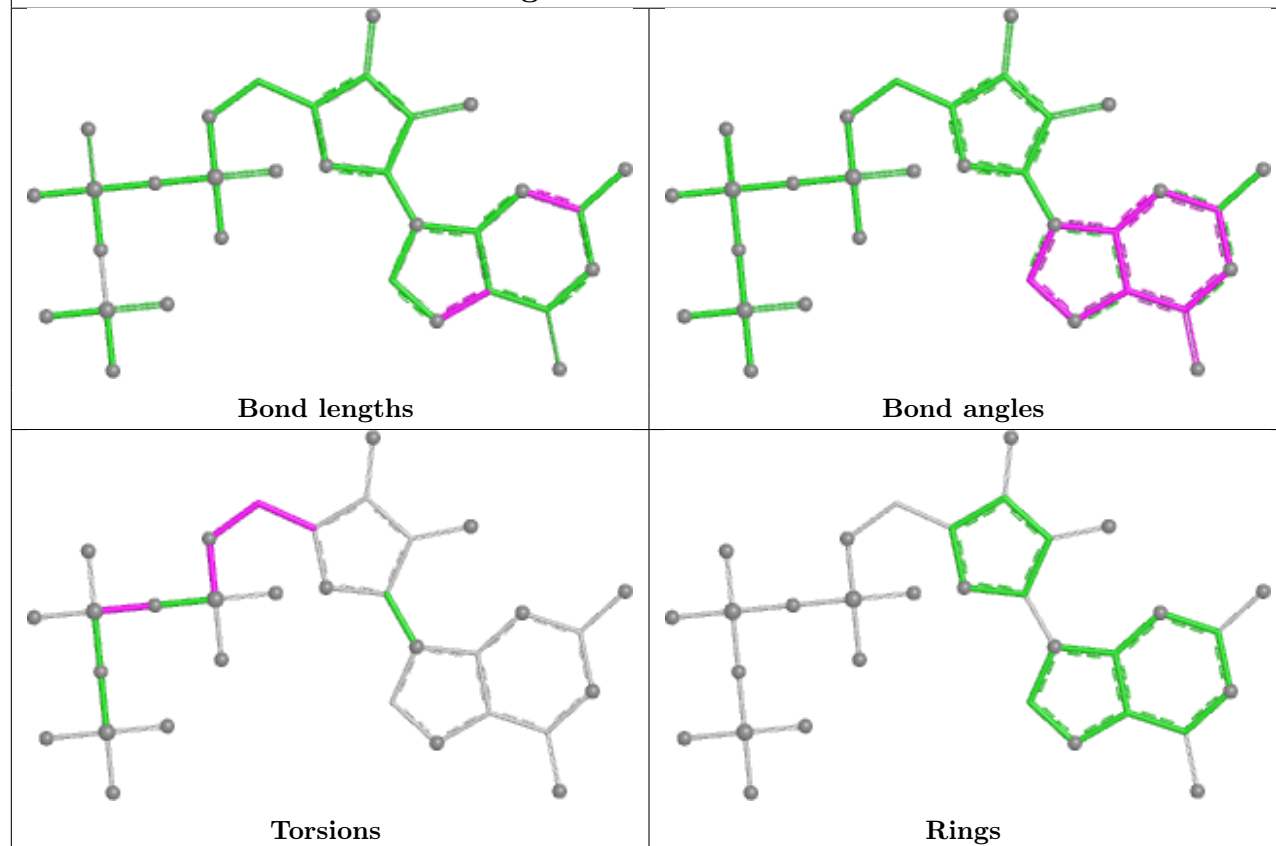


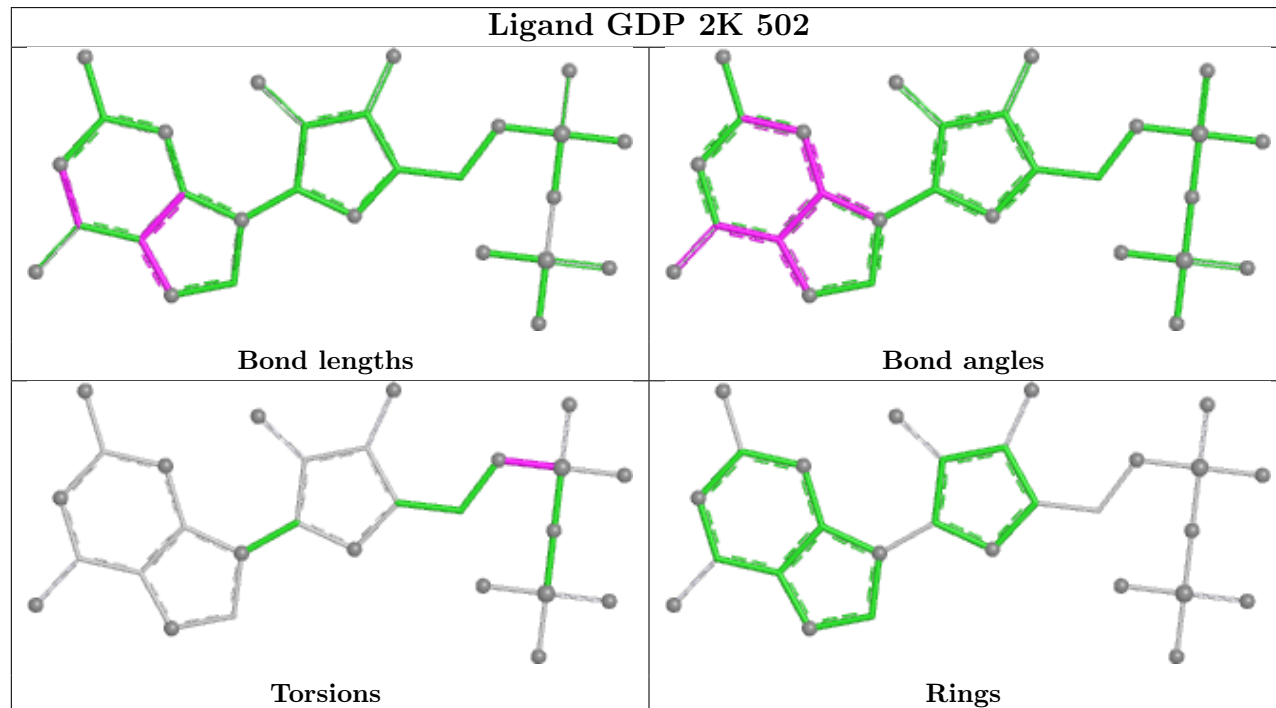
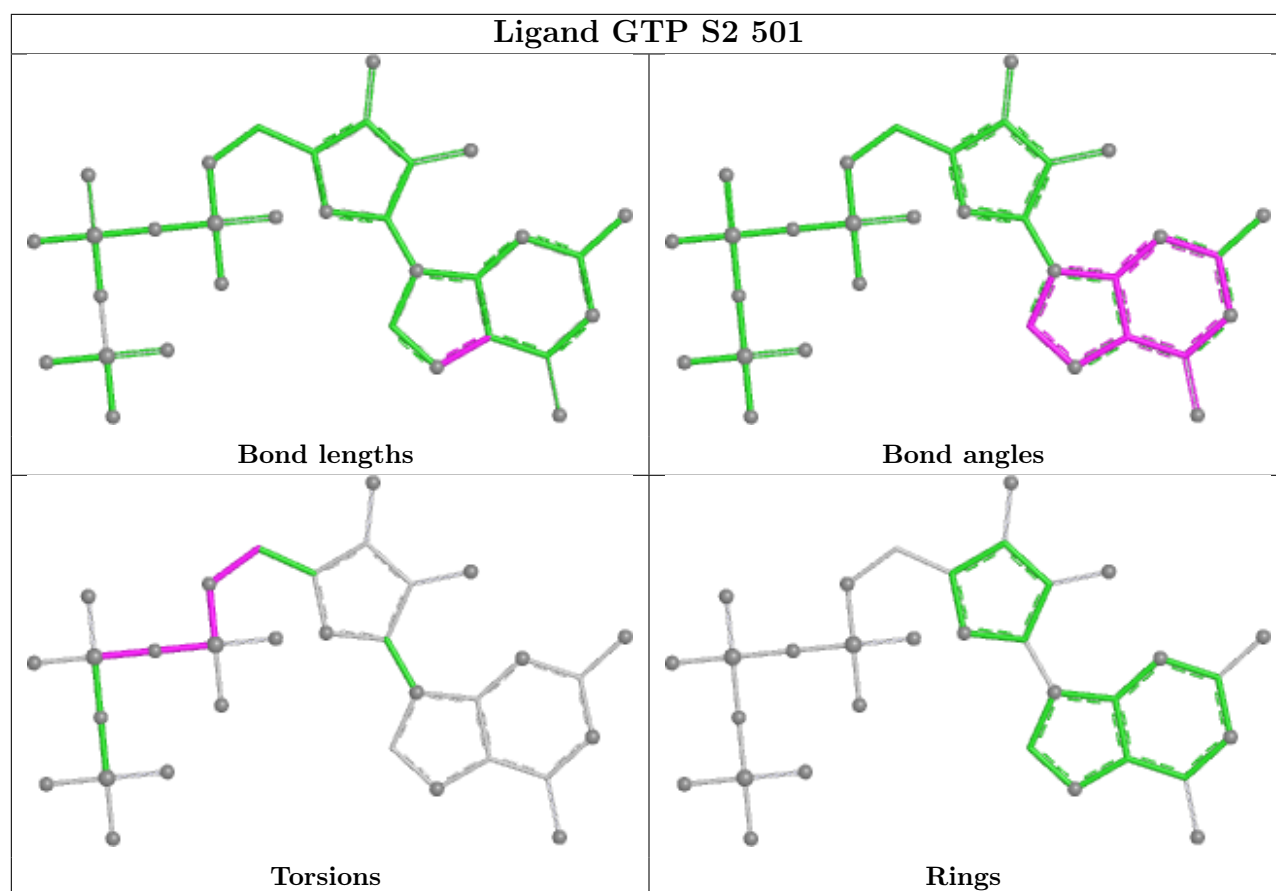


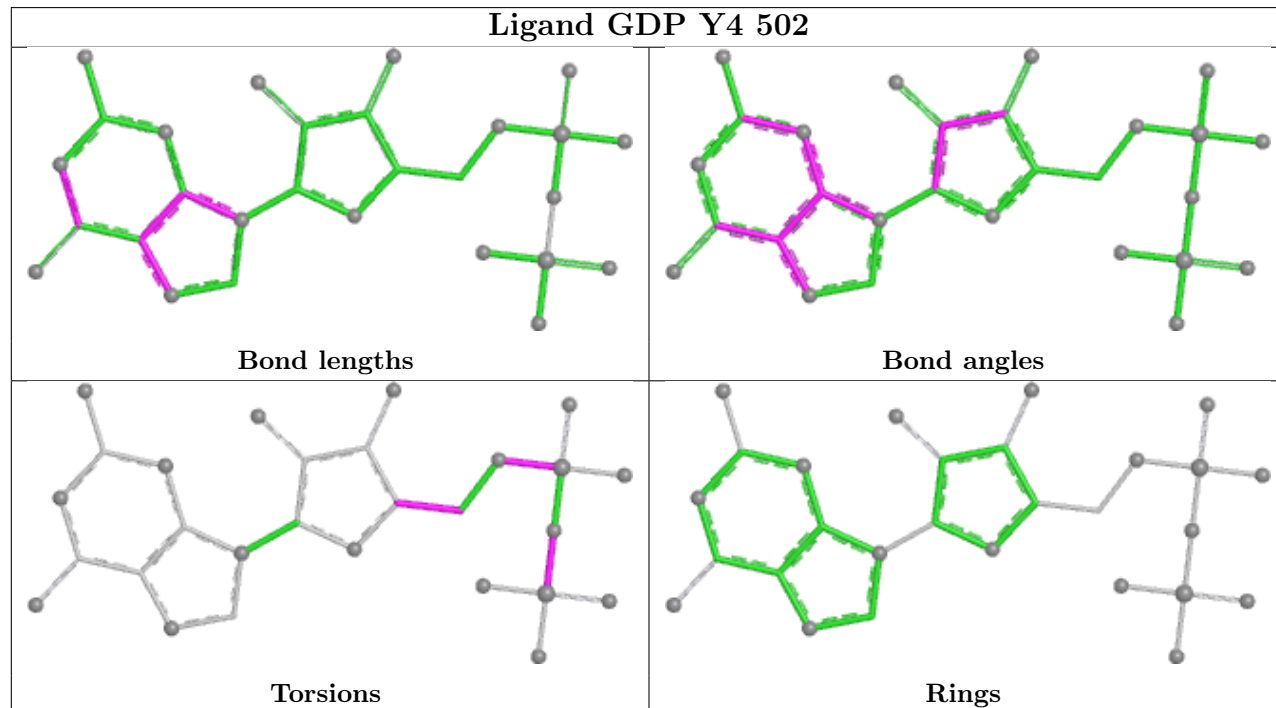
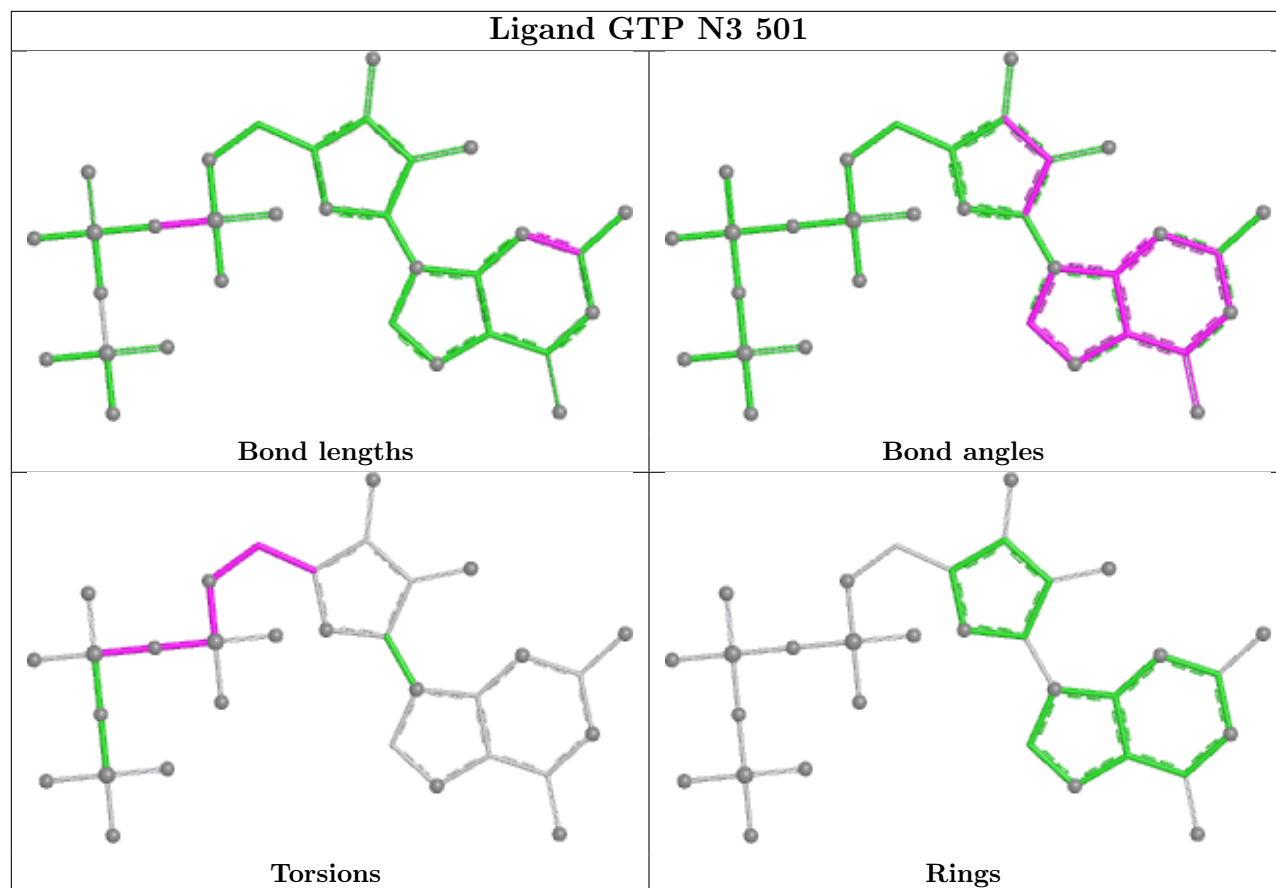
Ligand GTP C5 501

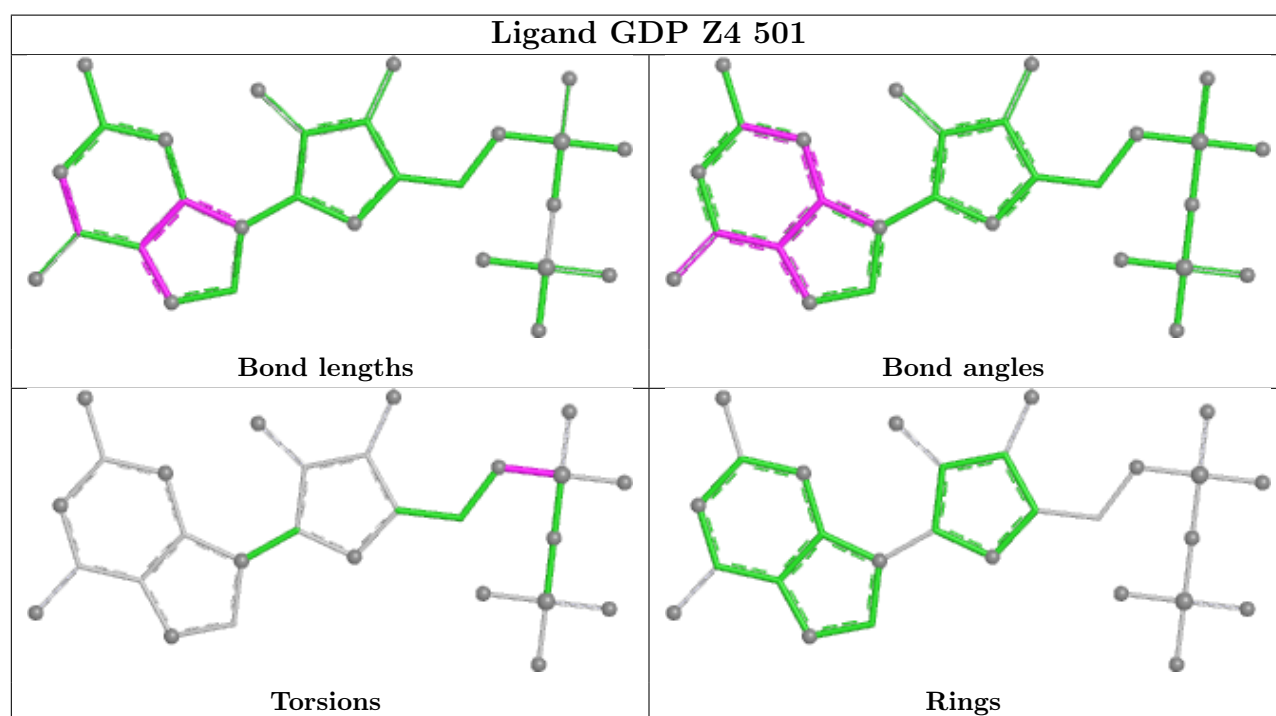
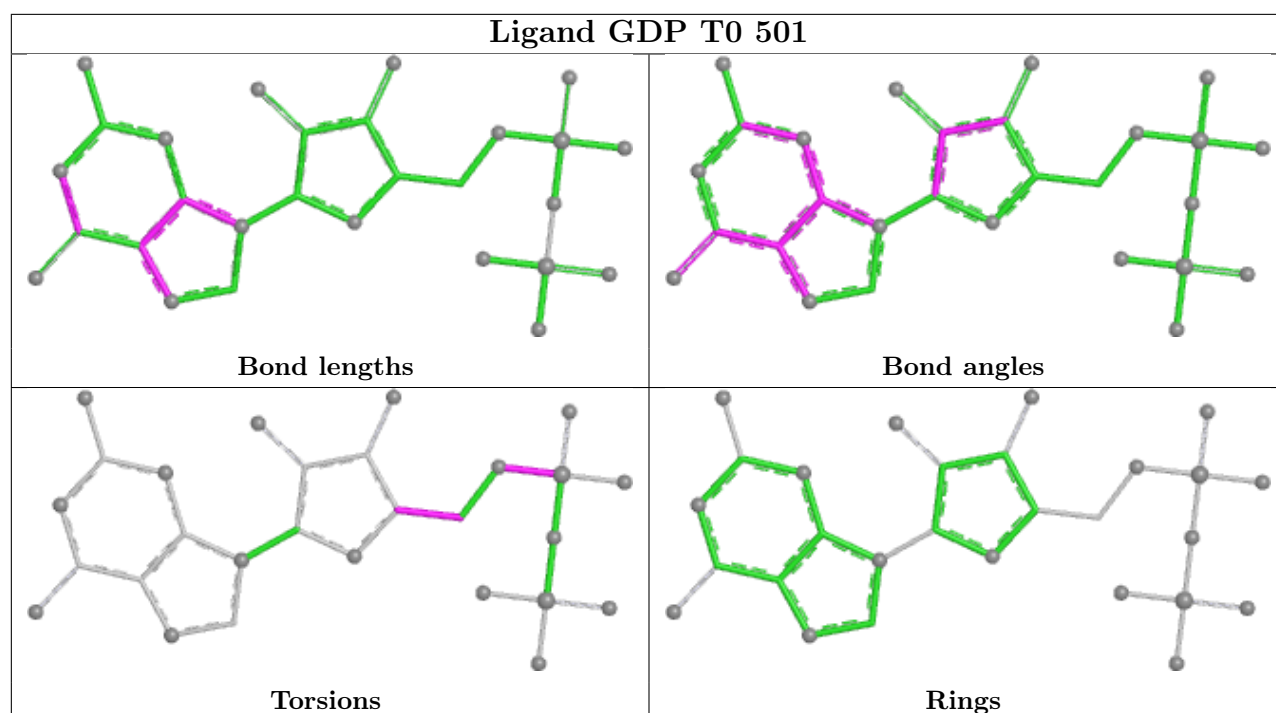


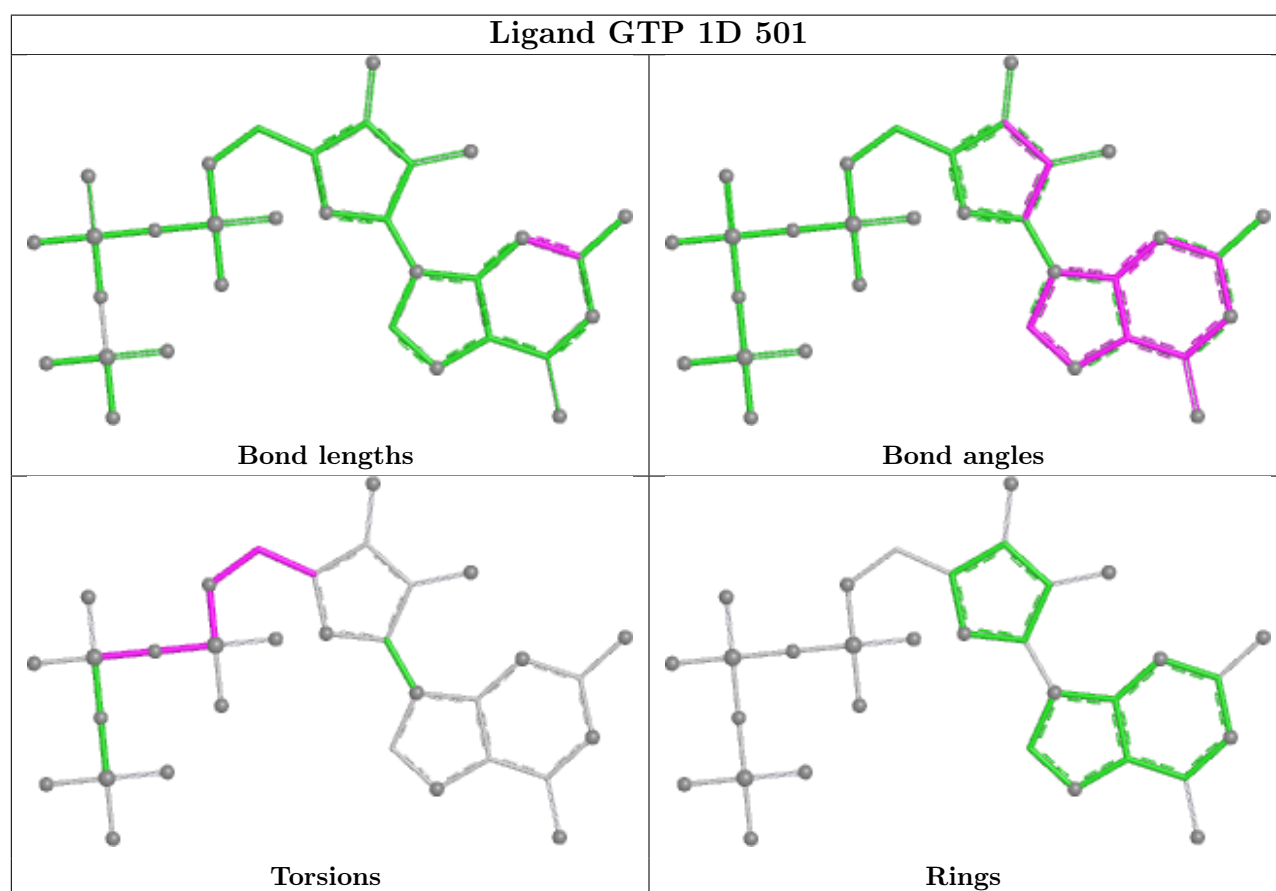
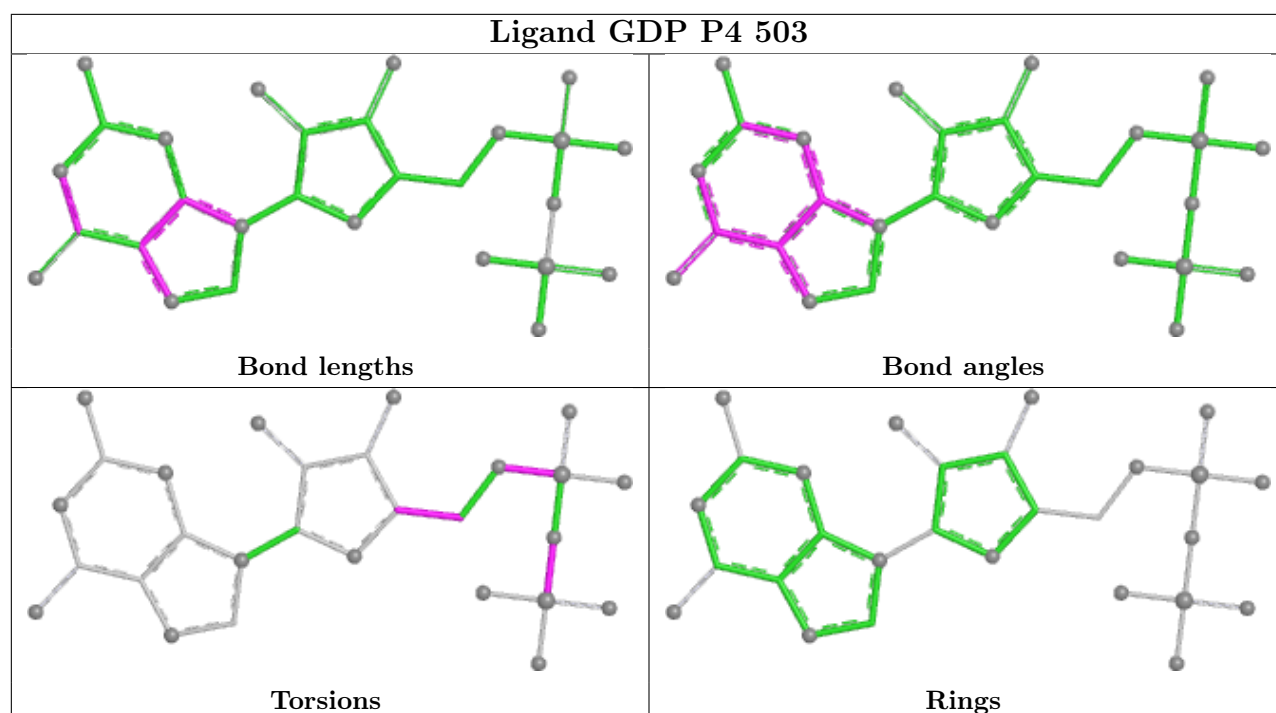
Ligand GTP V3 501

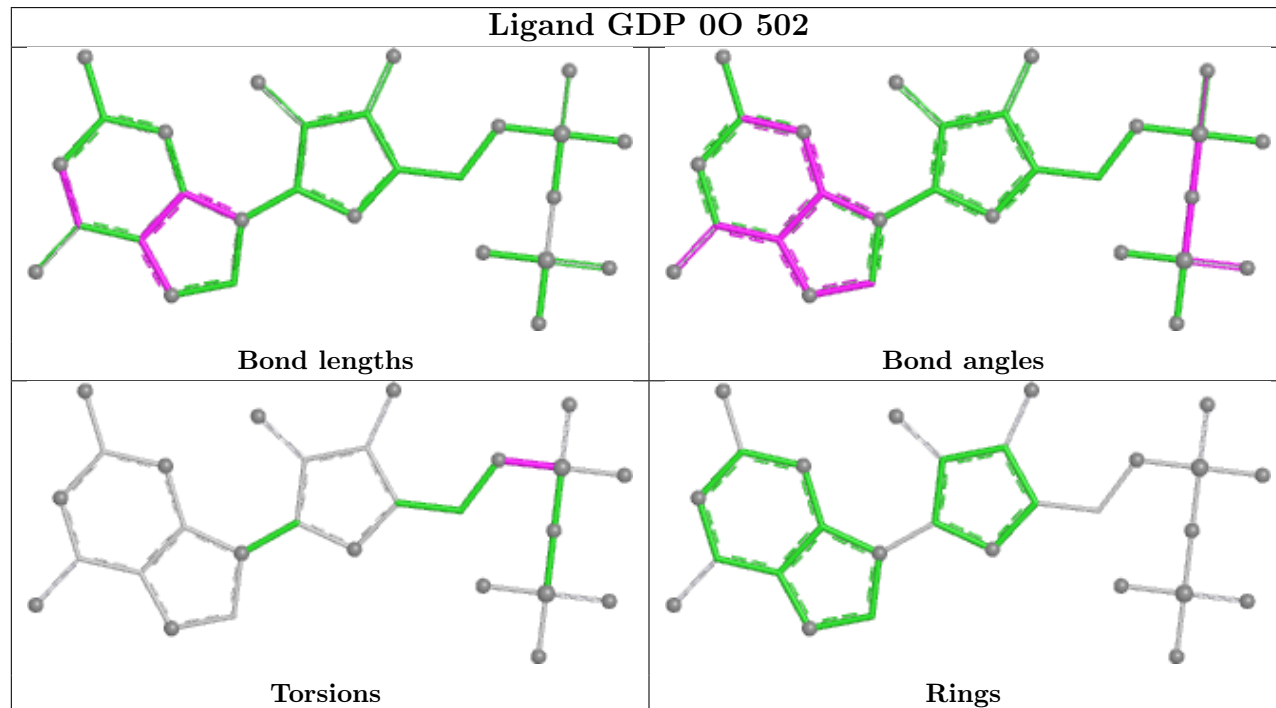
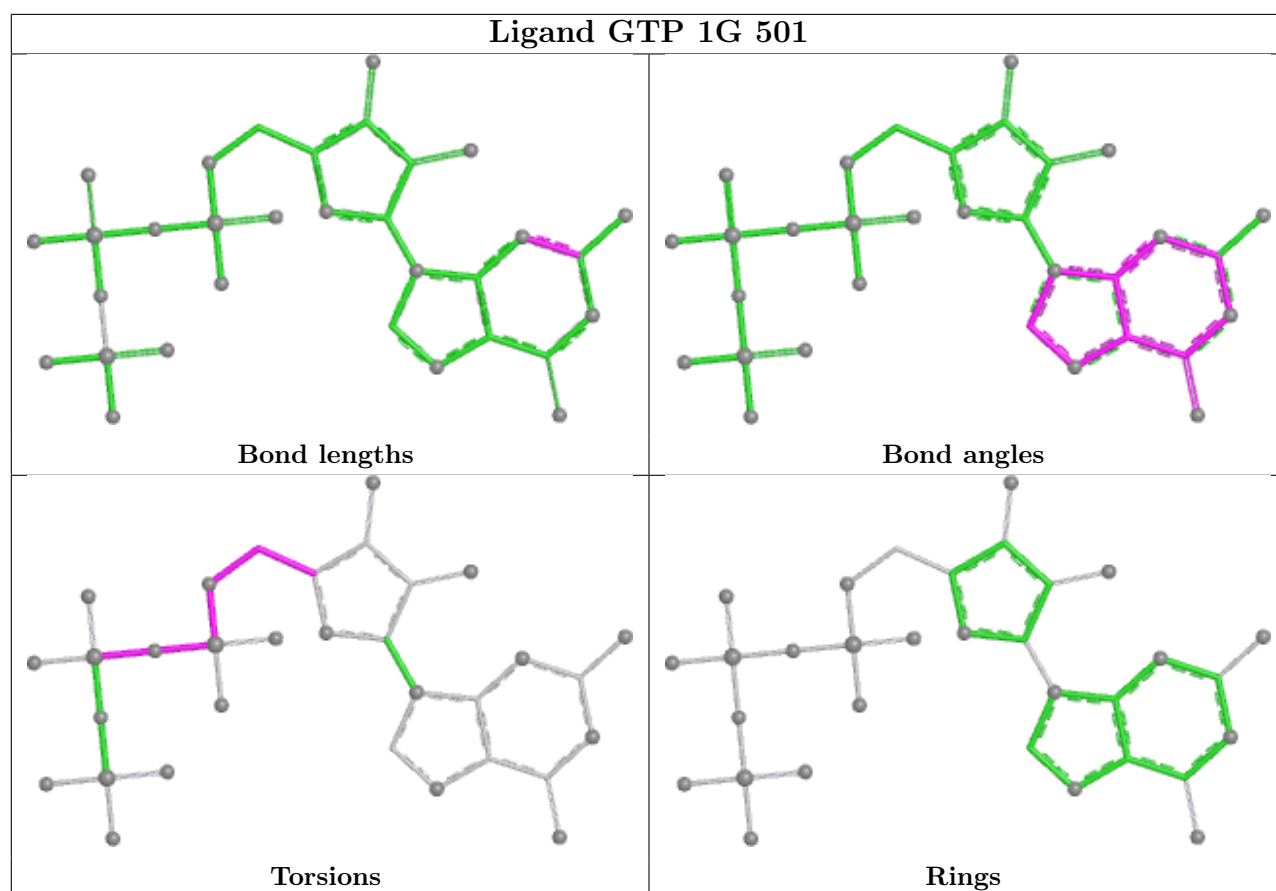


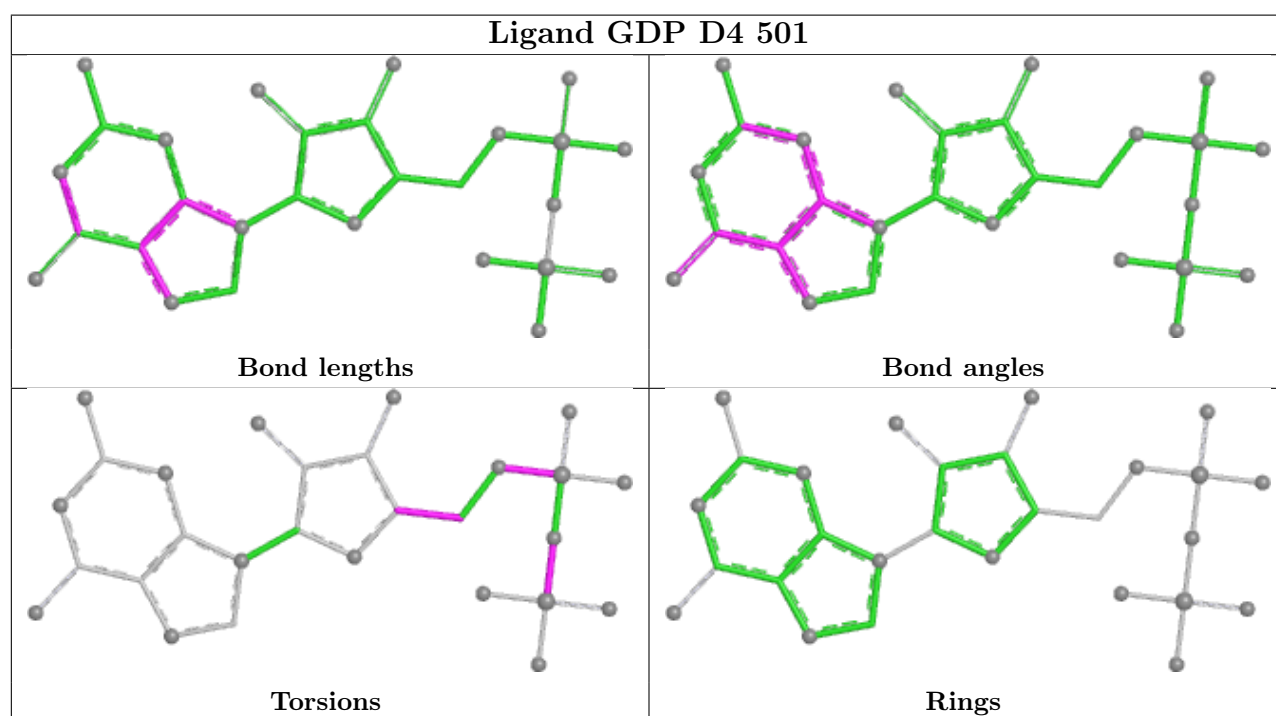
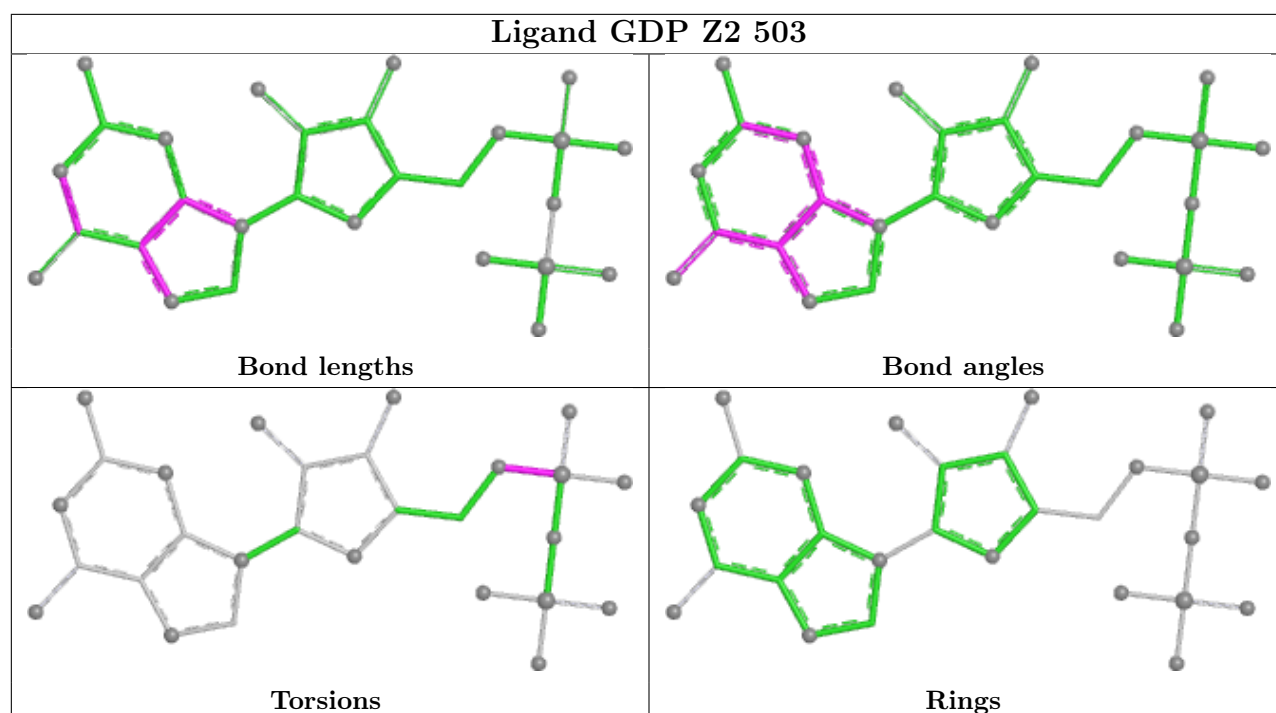


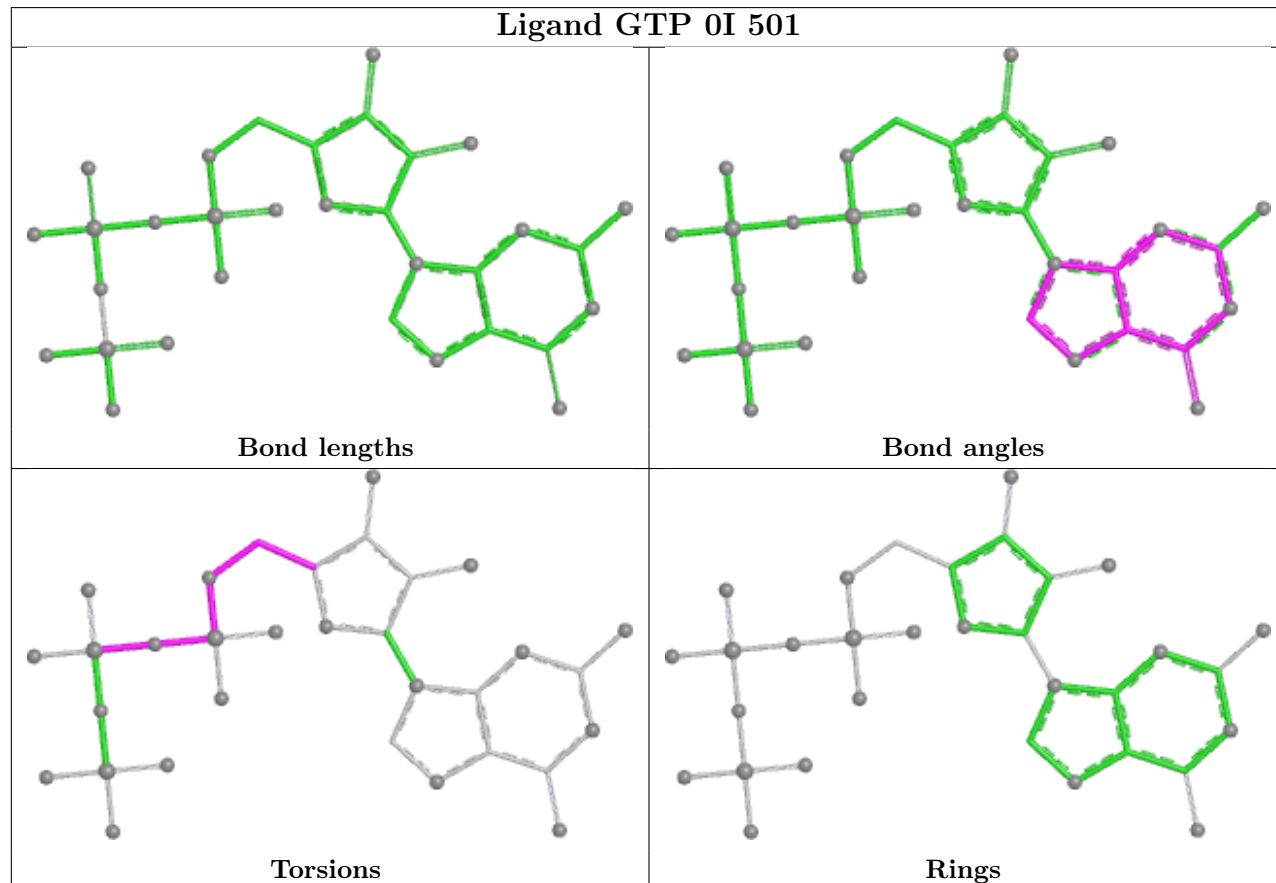
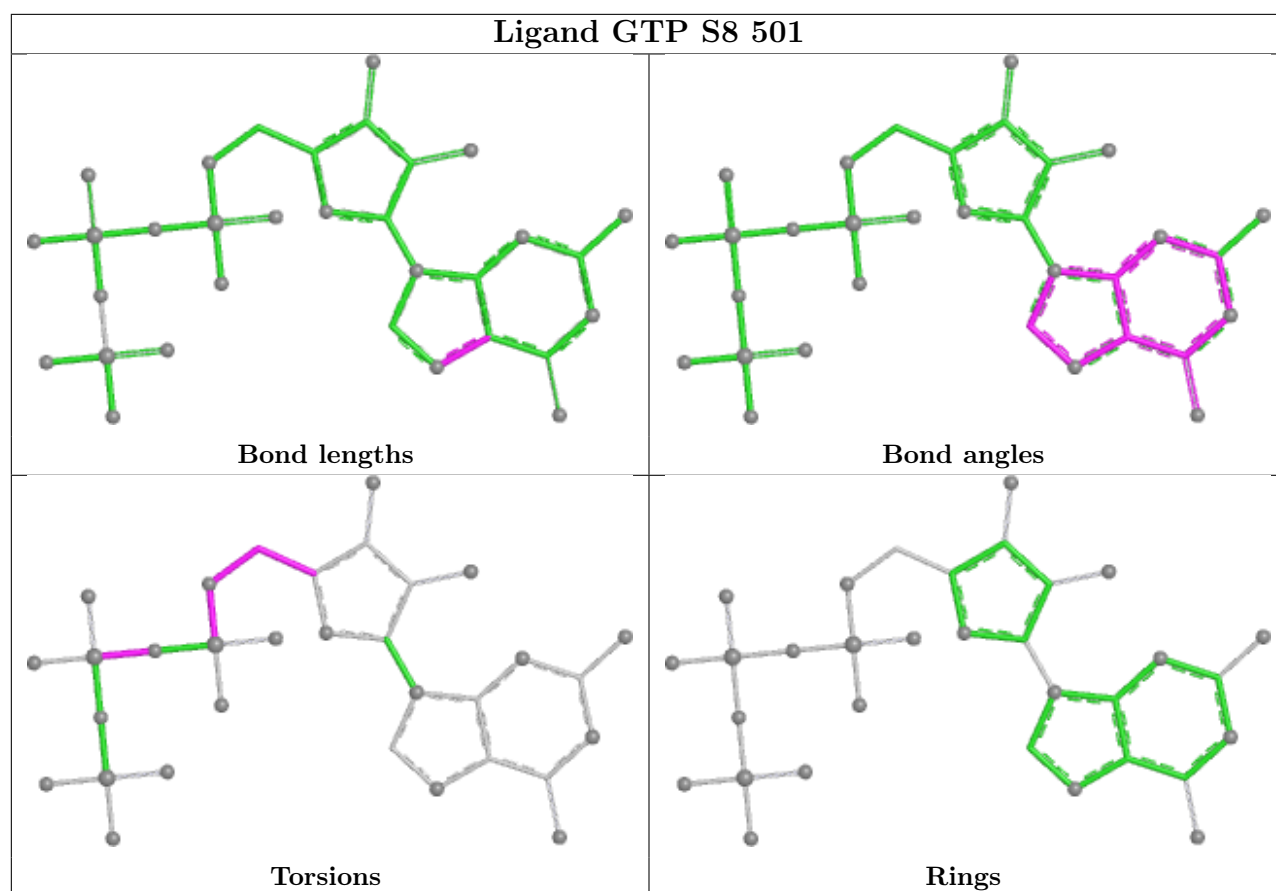


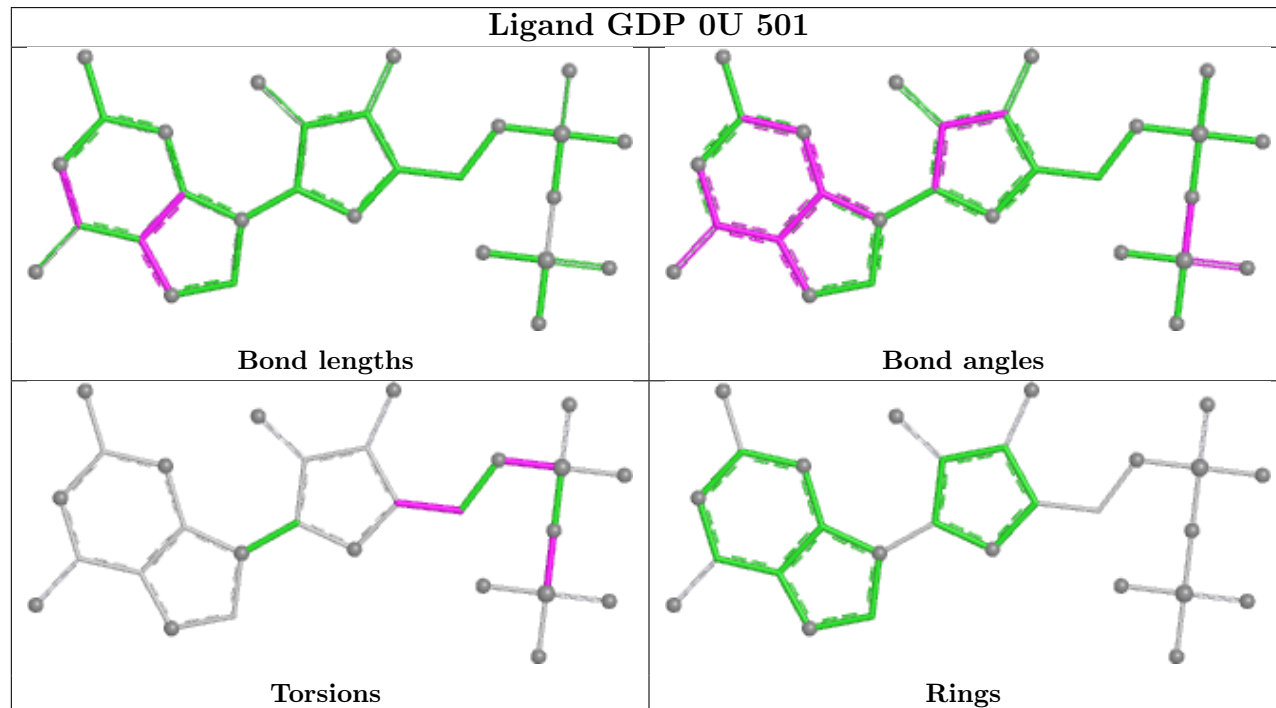
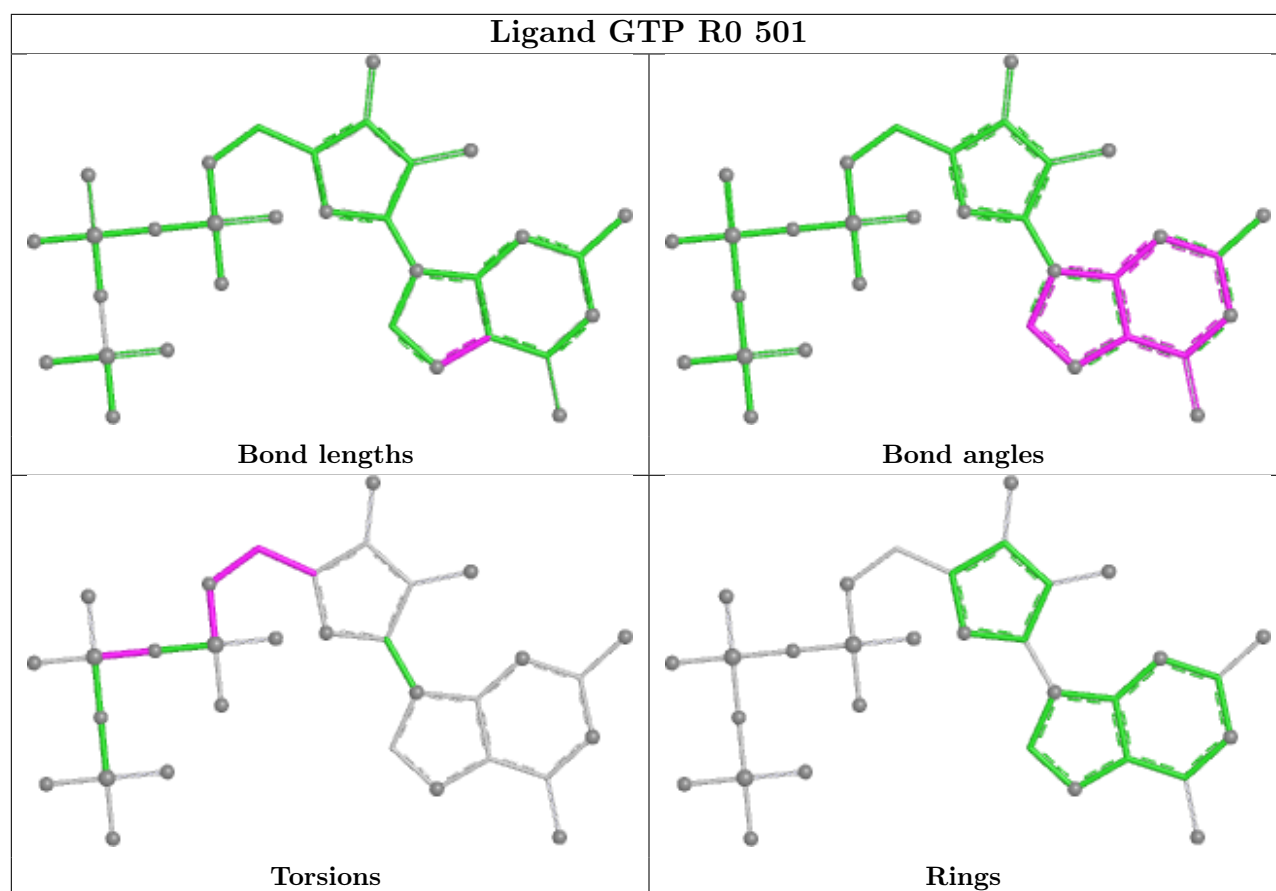


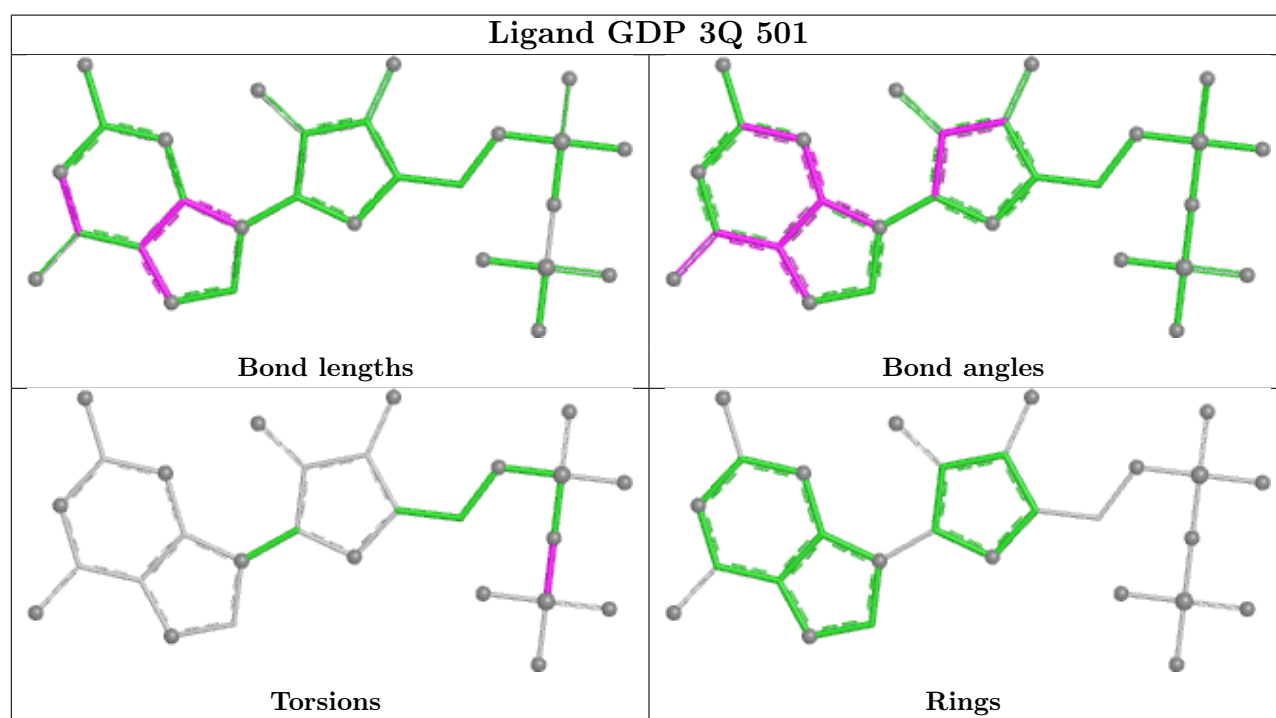
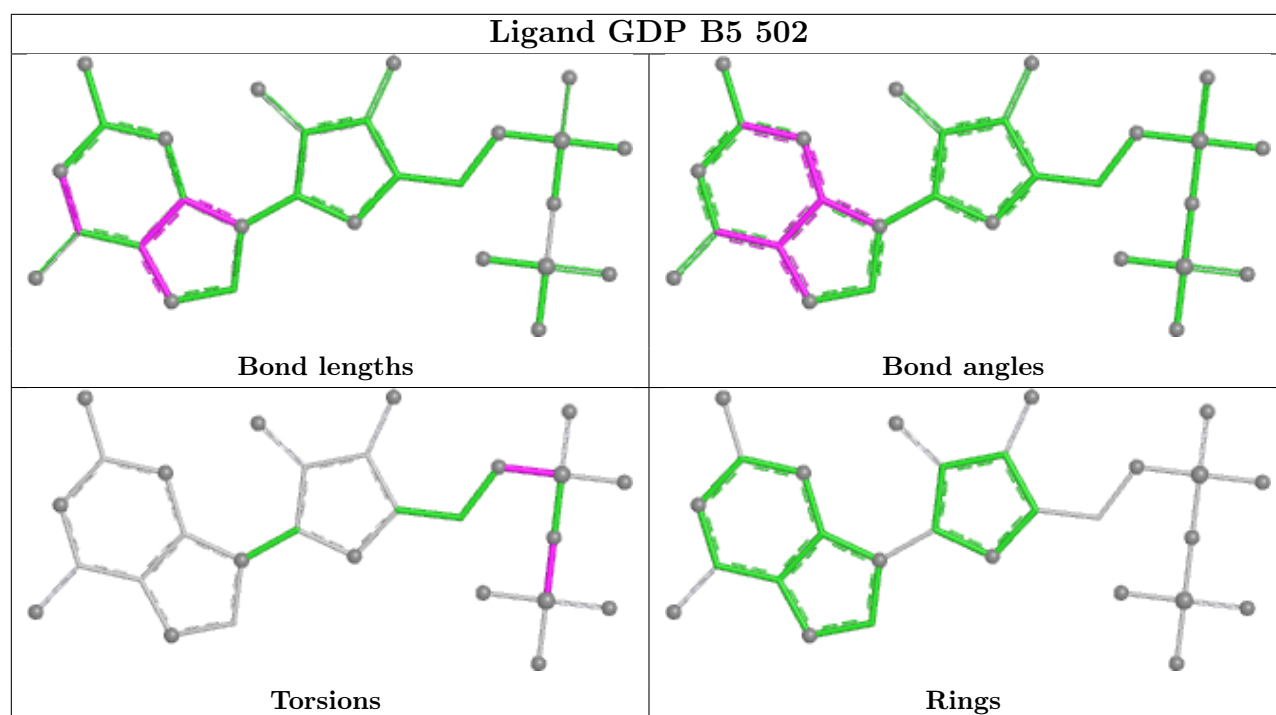


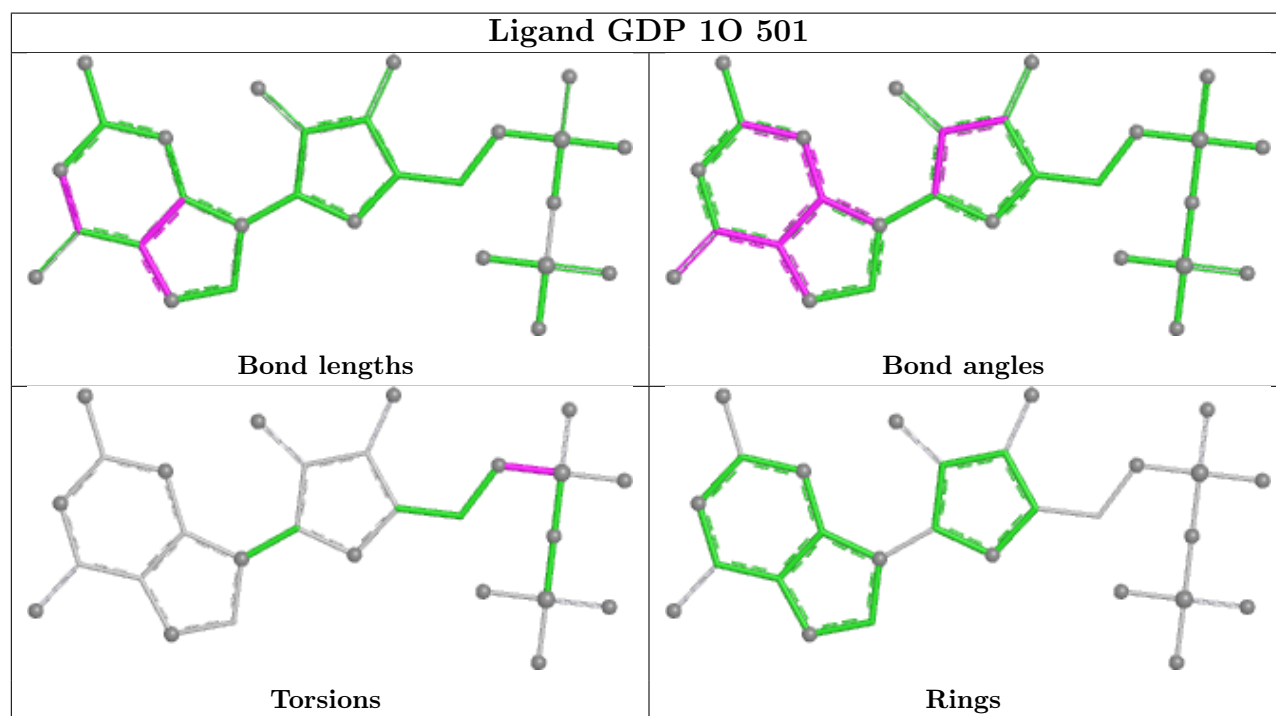
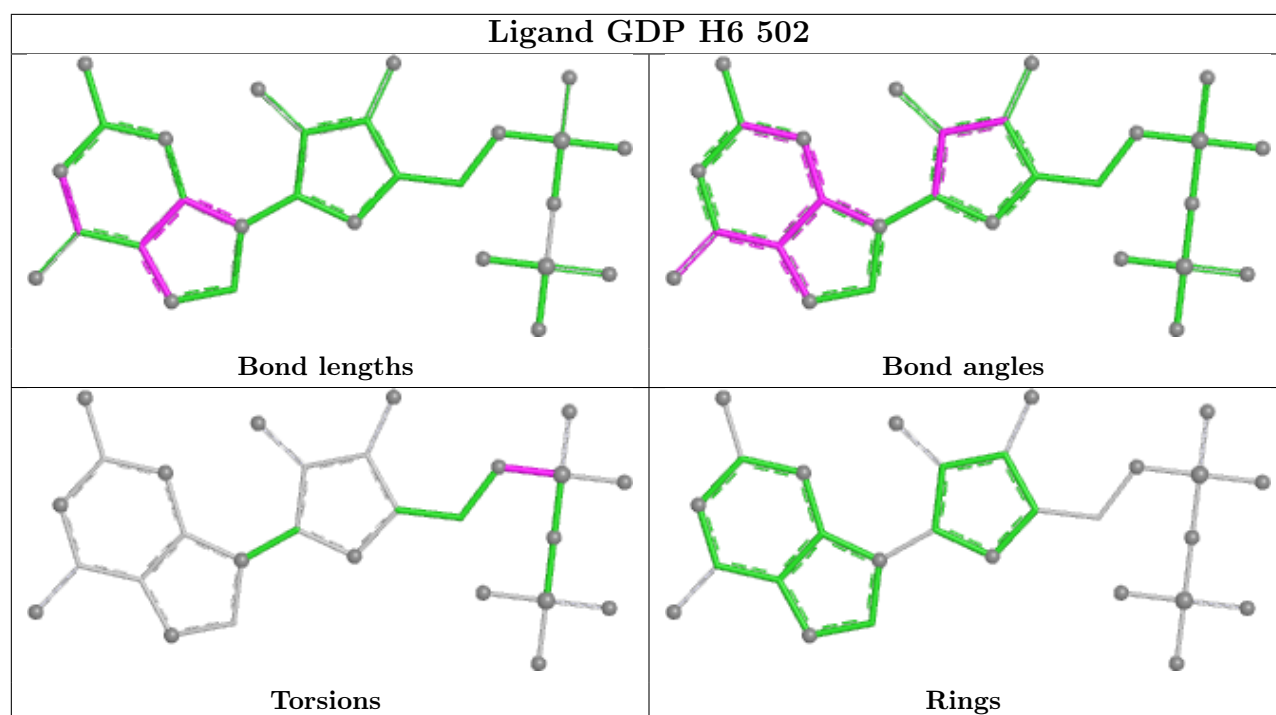


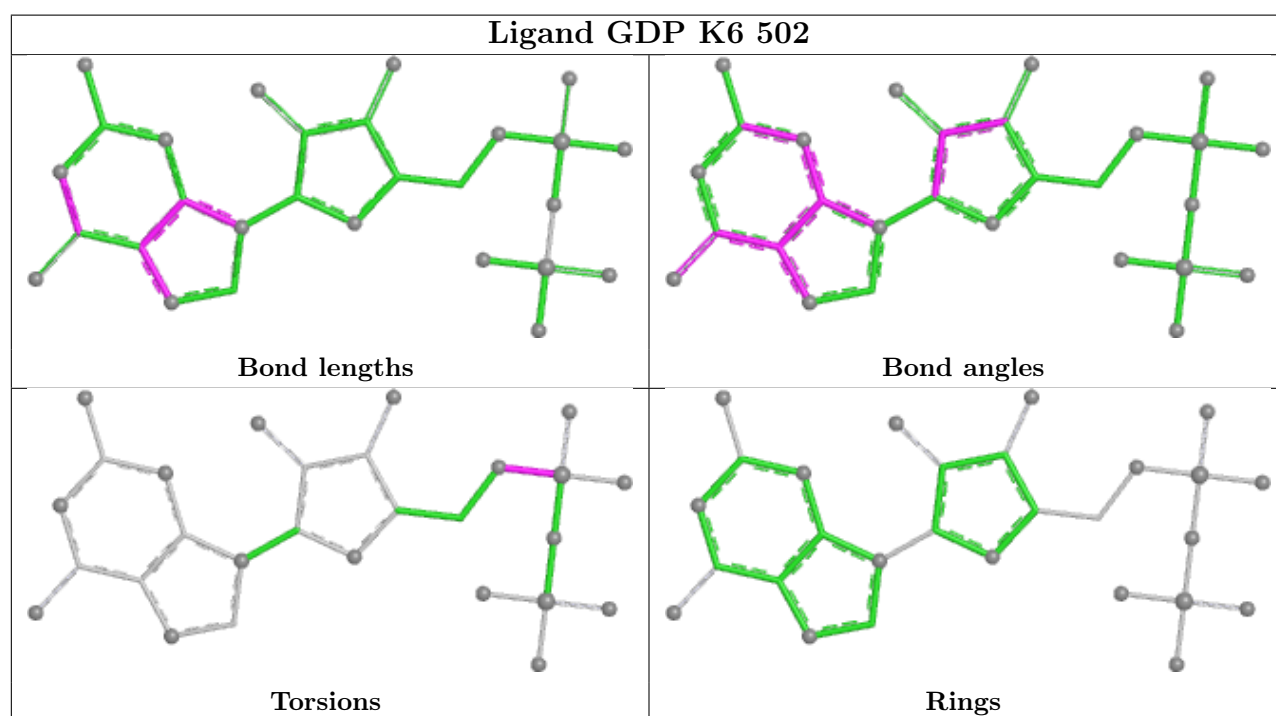
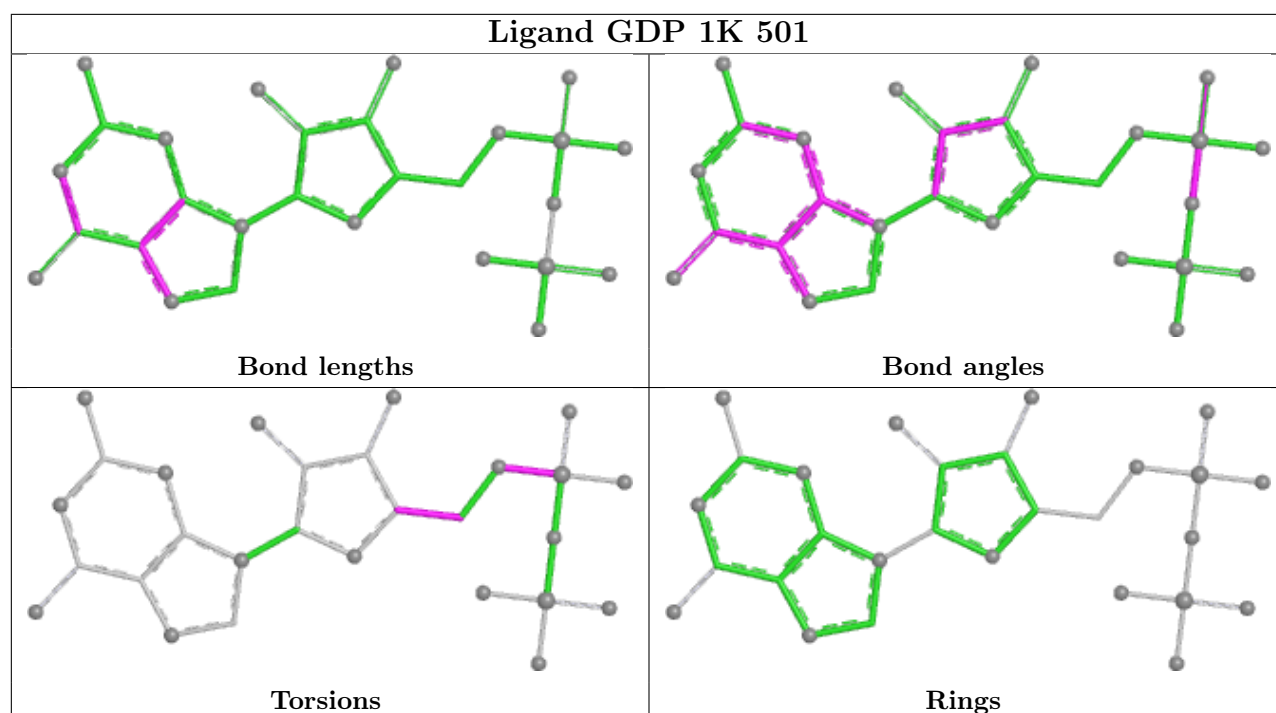


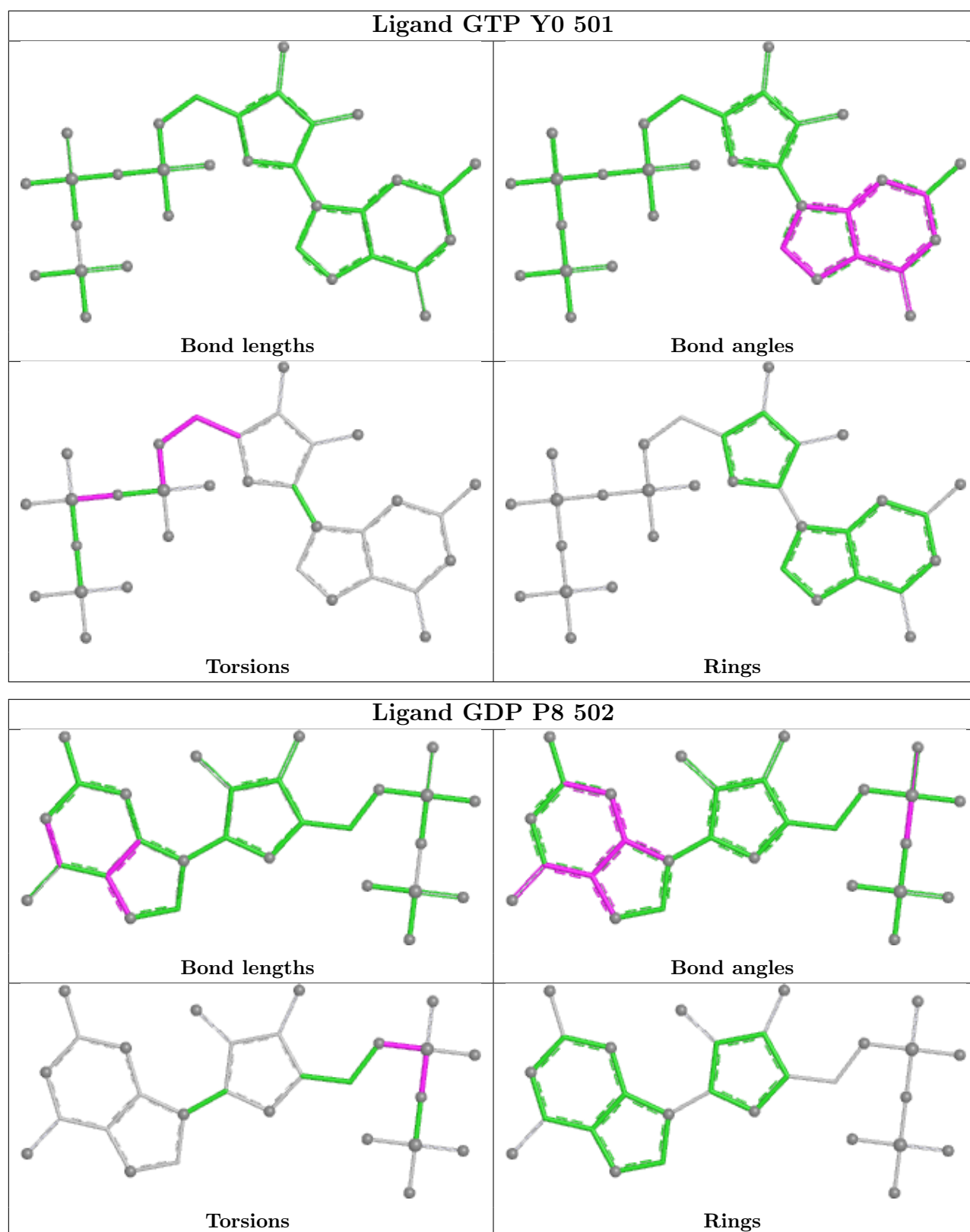


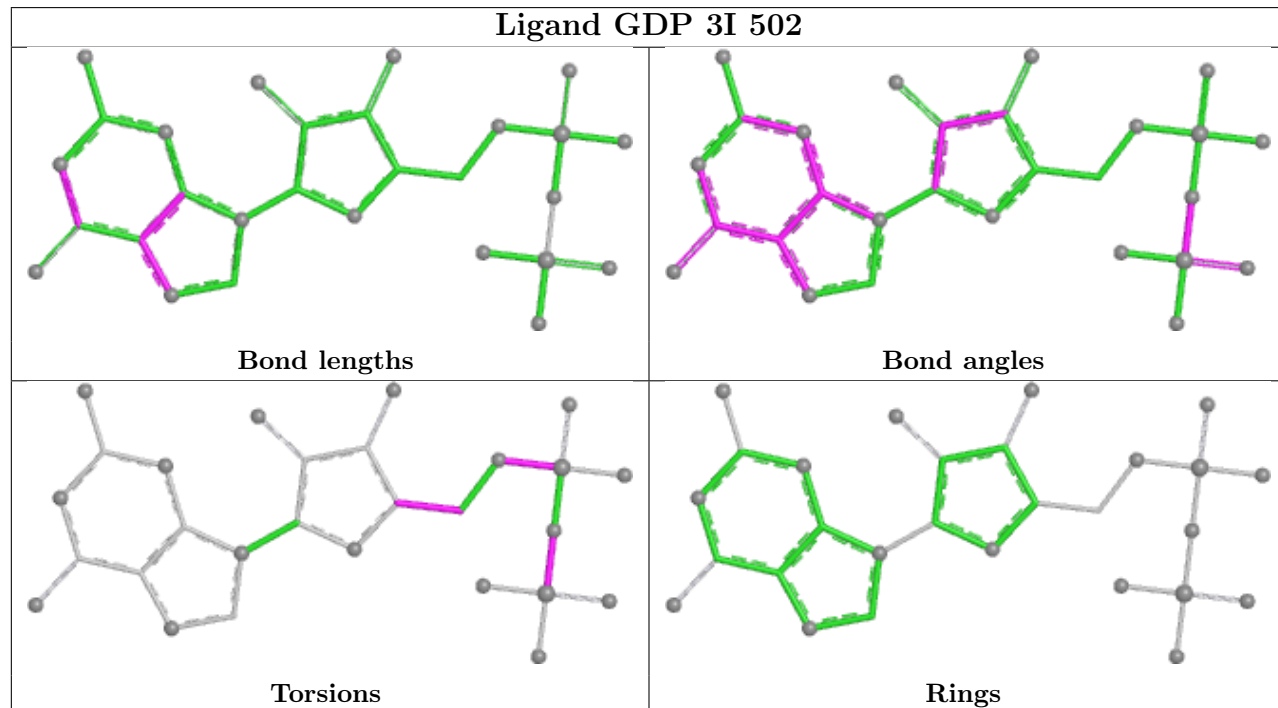
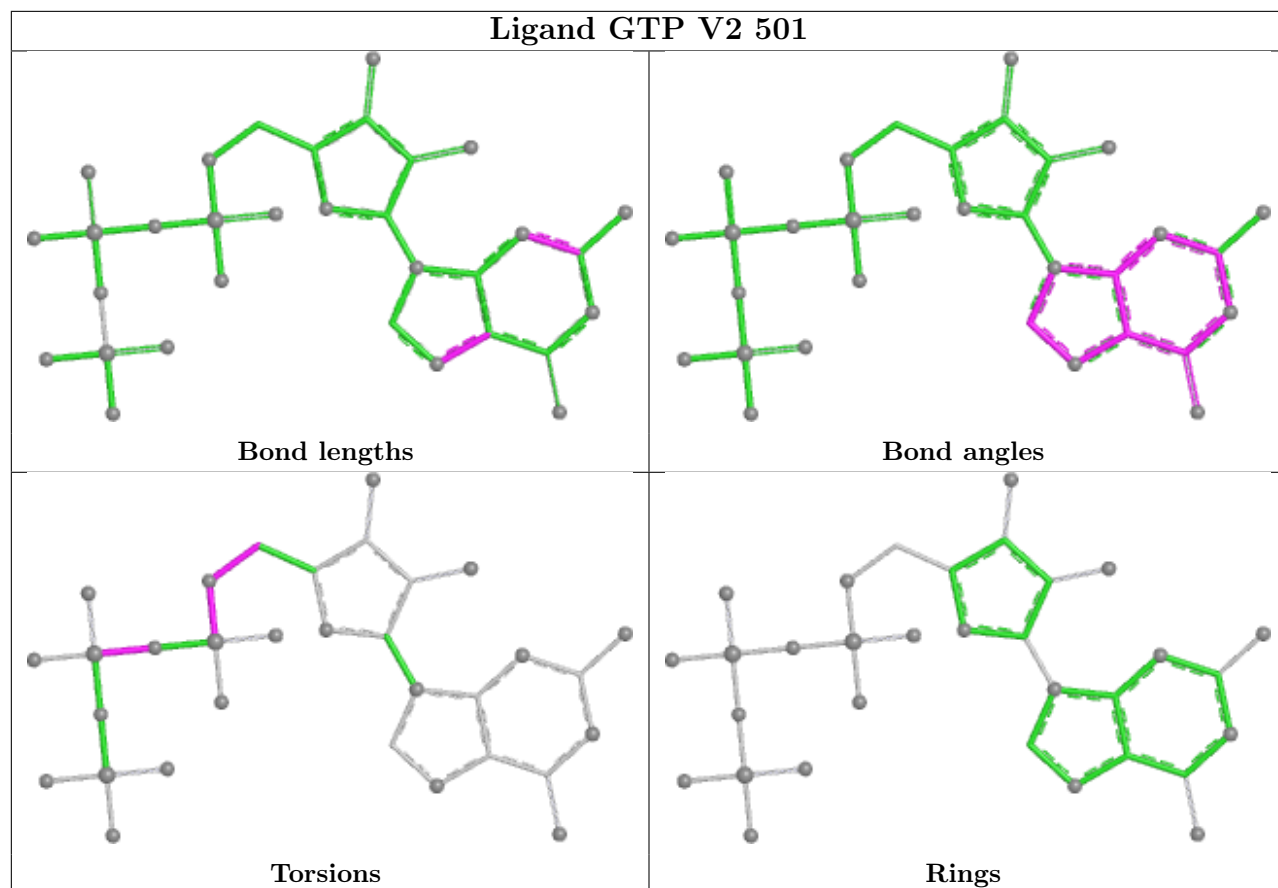




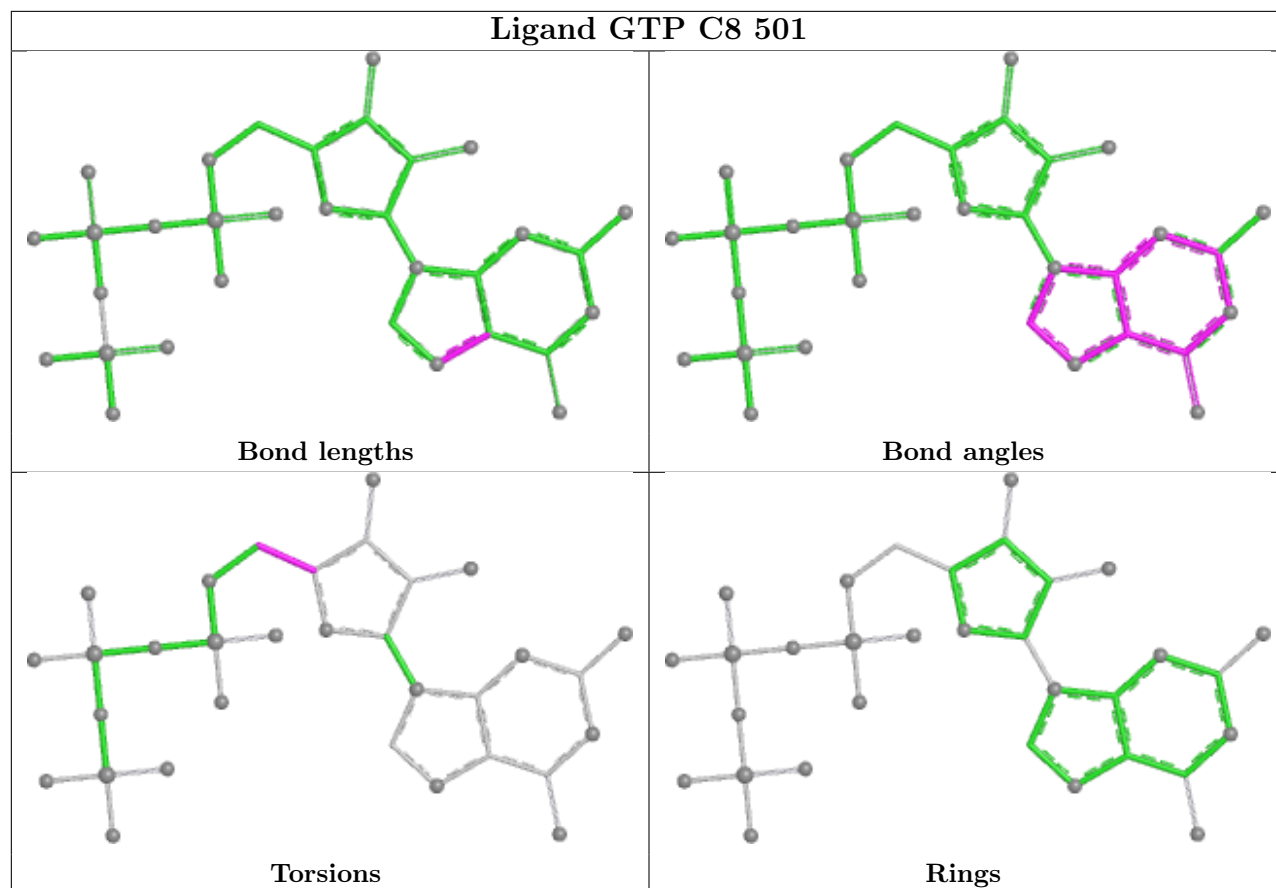




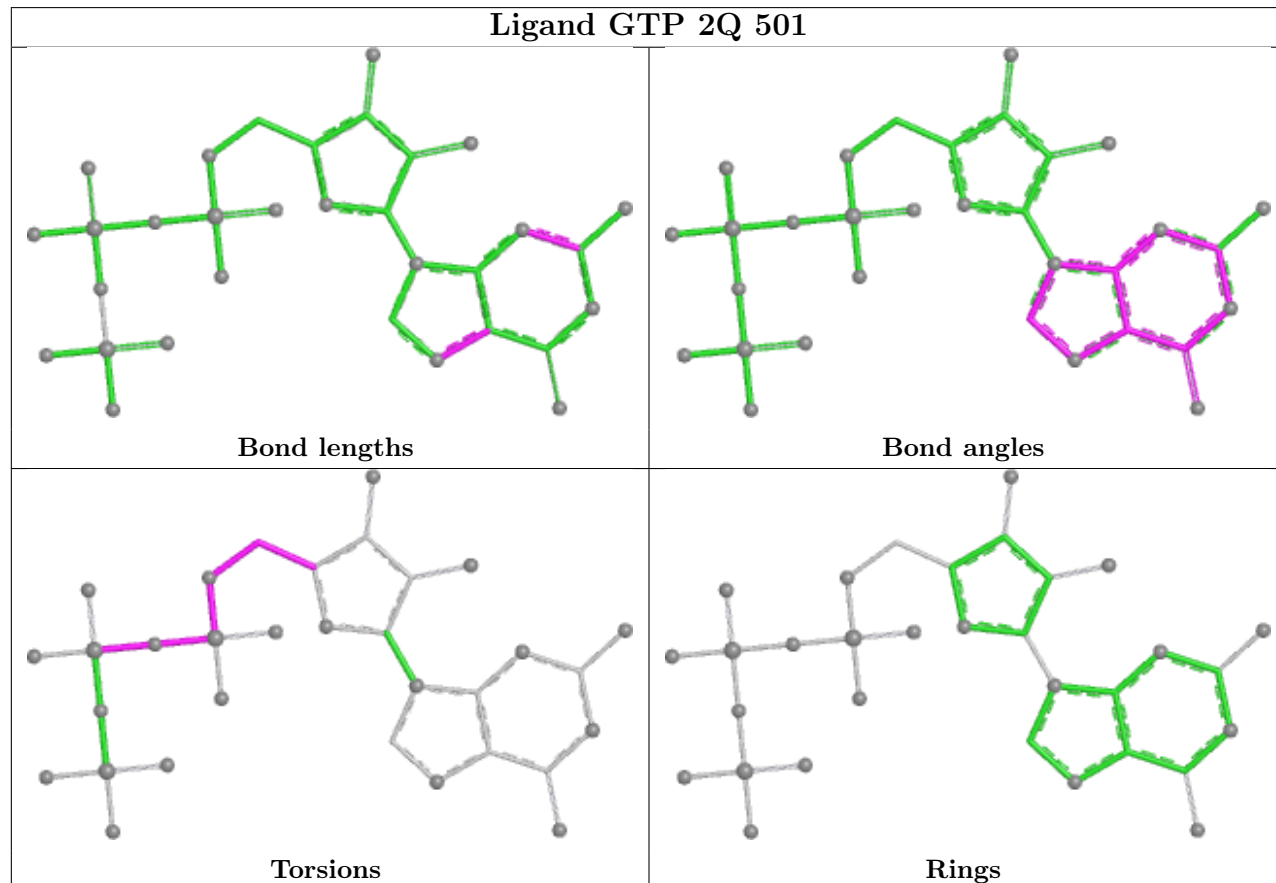


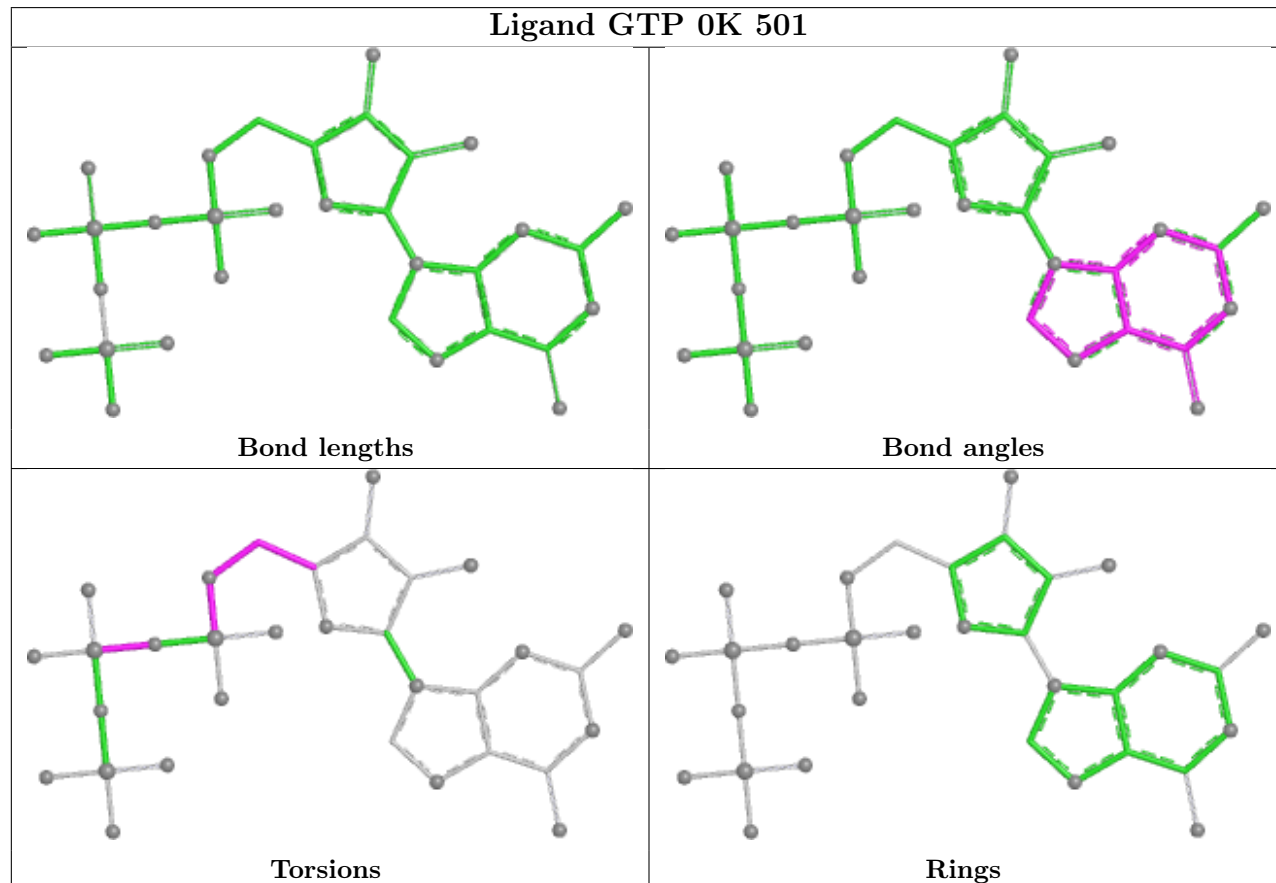
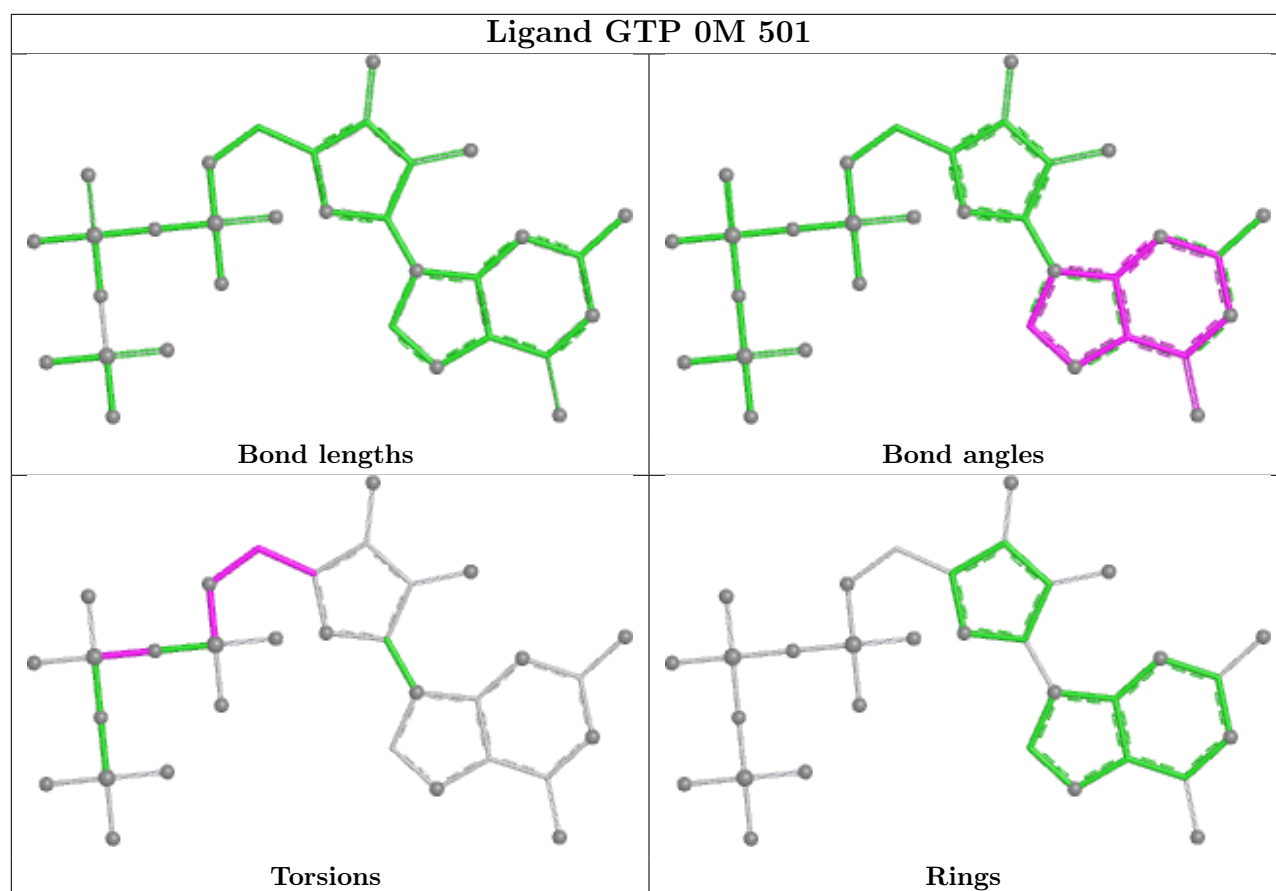


Ligand GTP C8 501

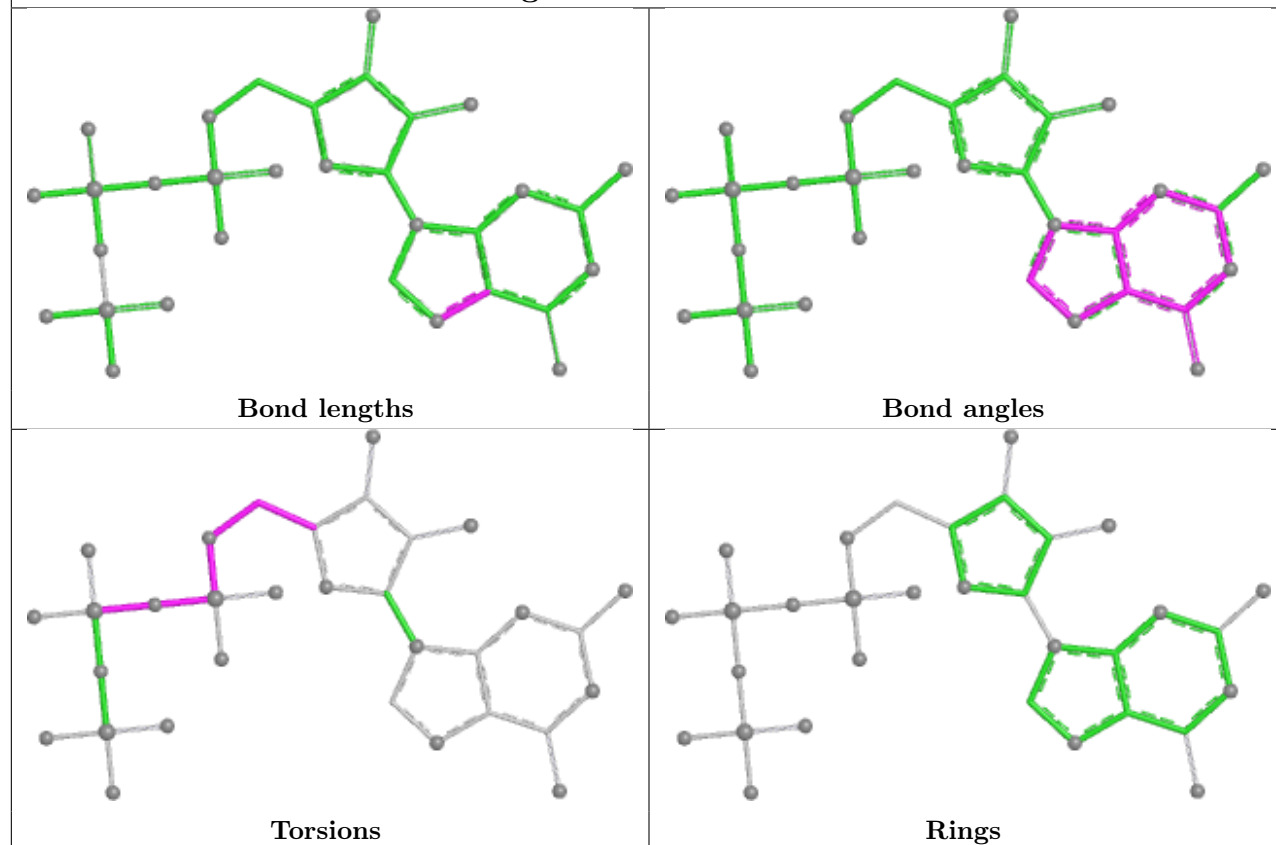


Ligand GTP 2Q 501

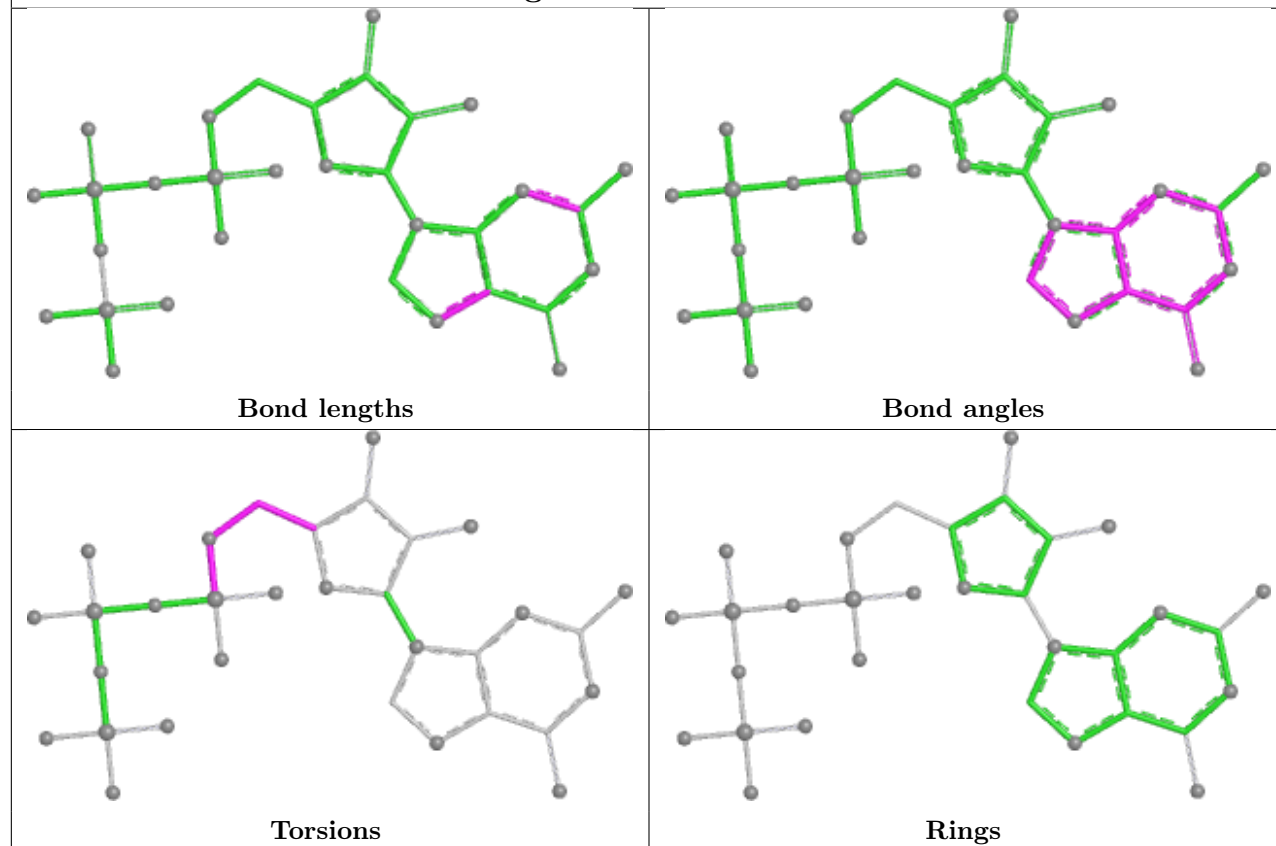


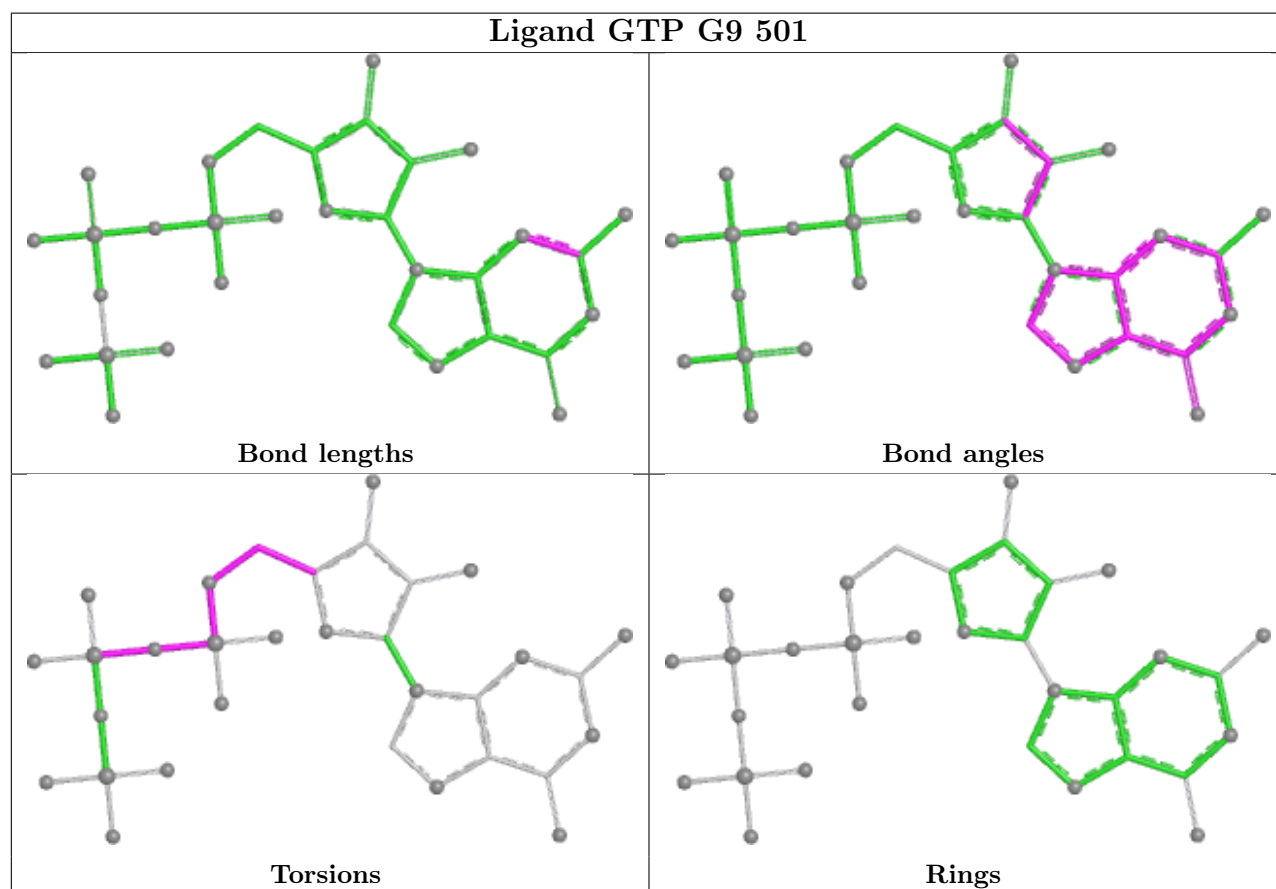
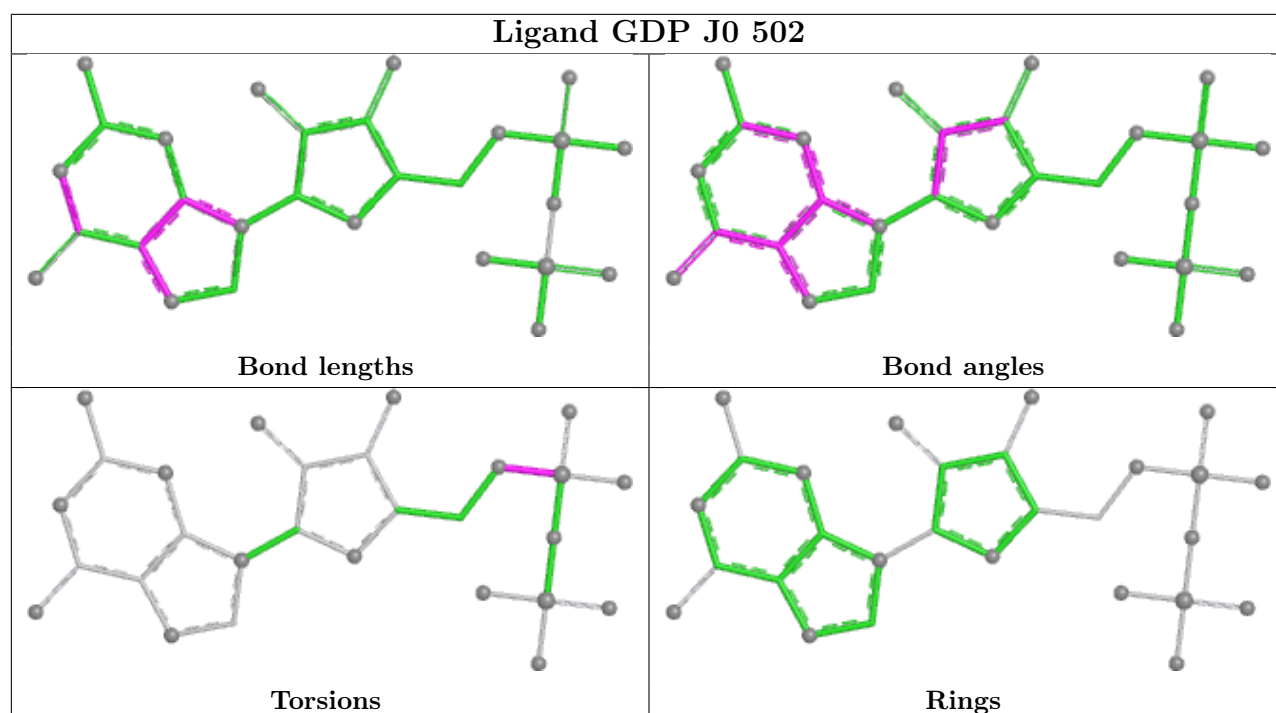


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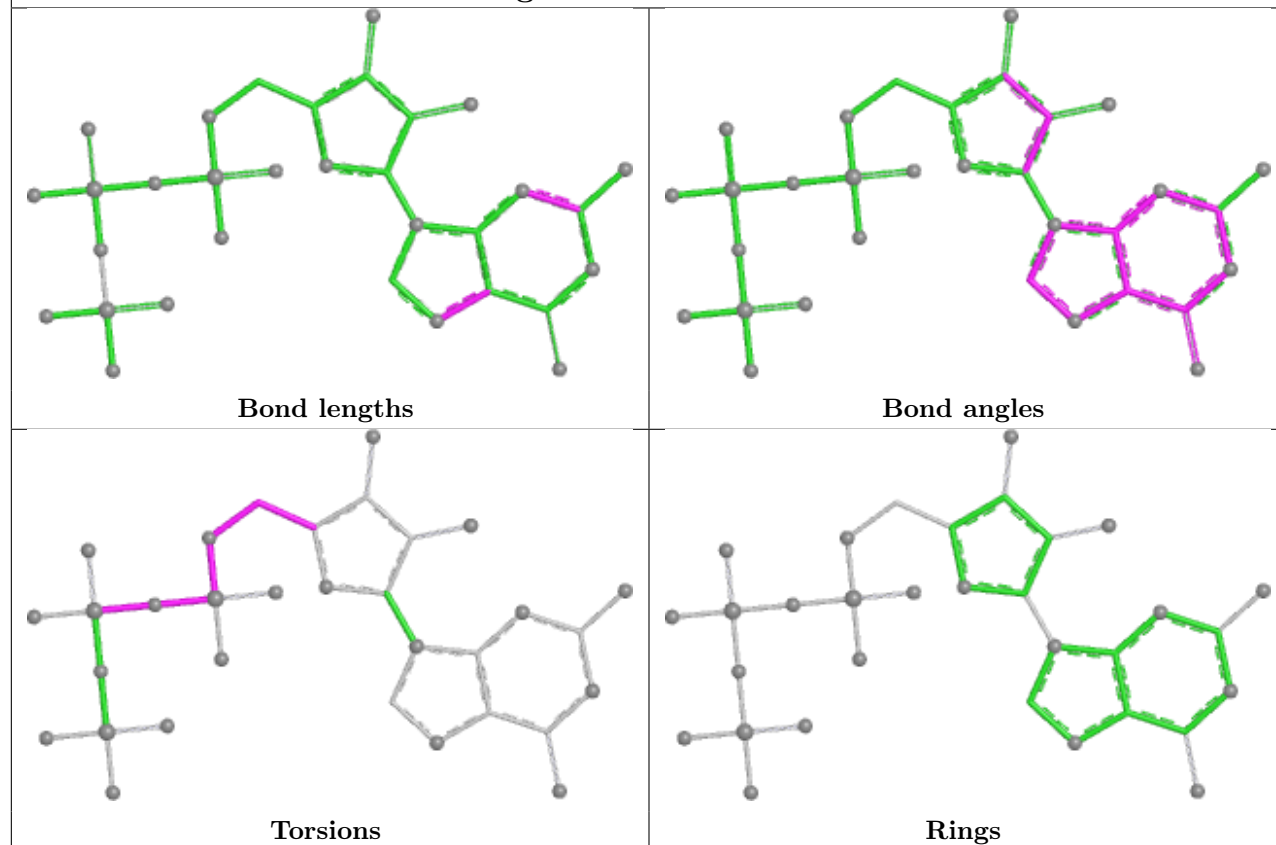


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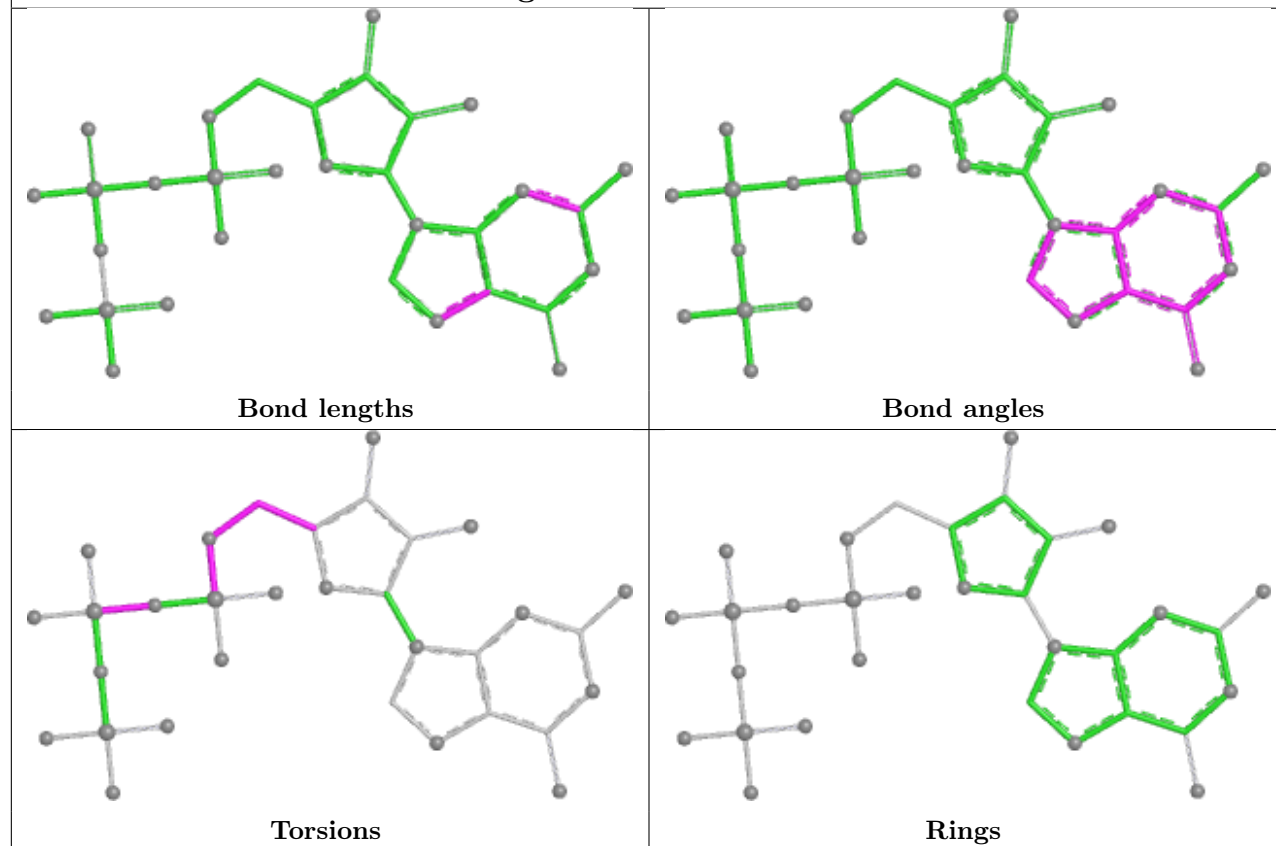


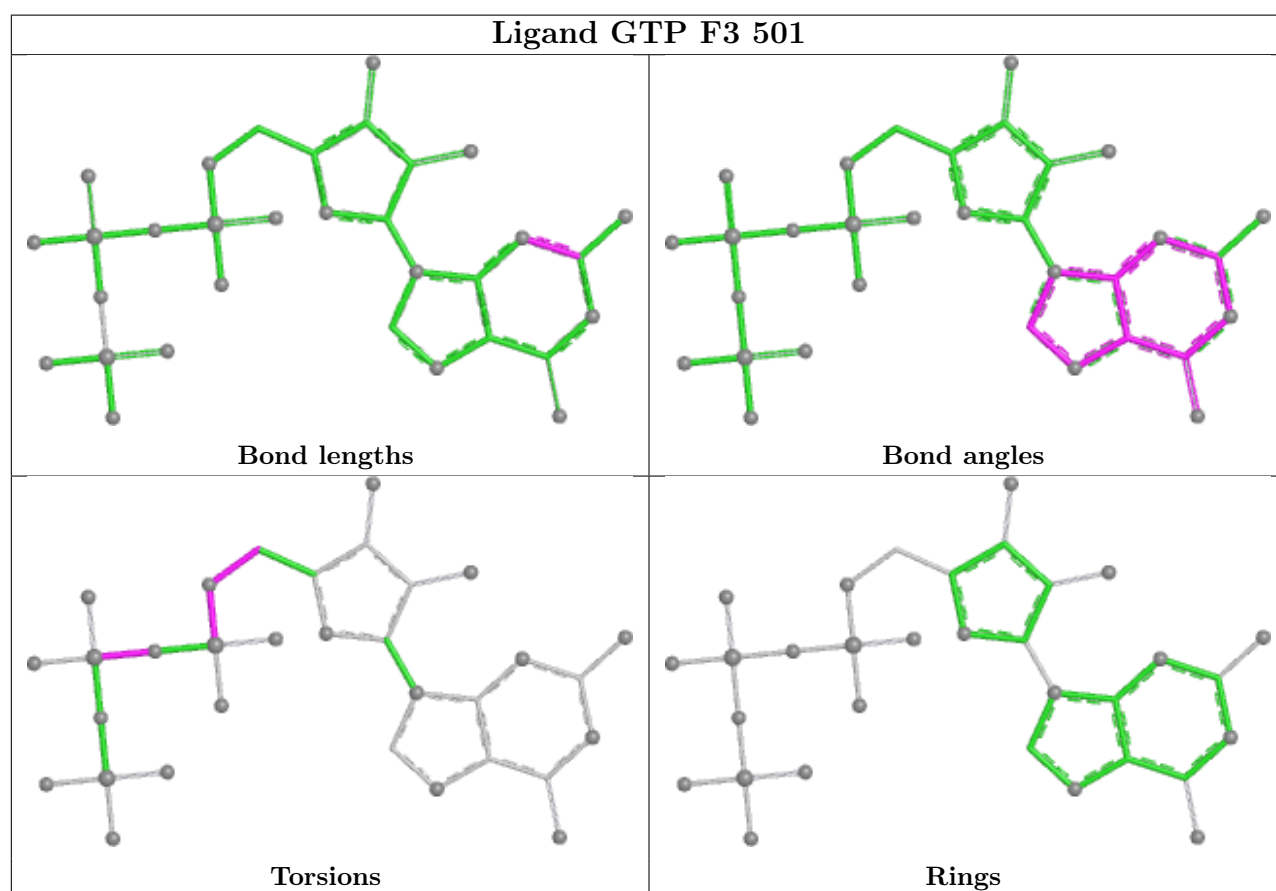
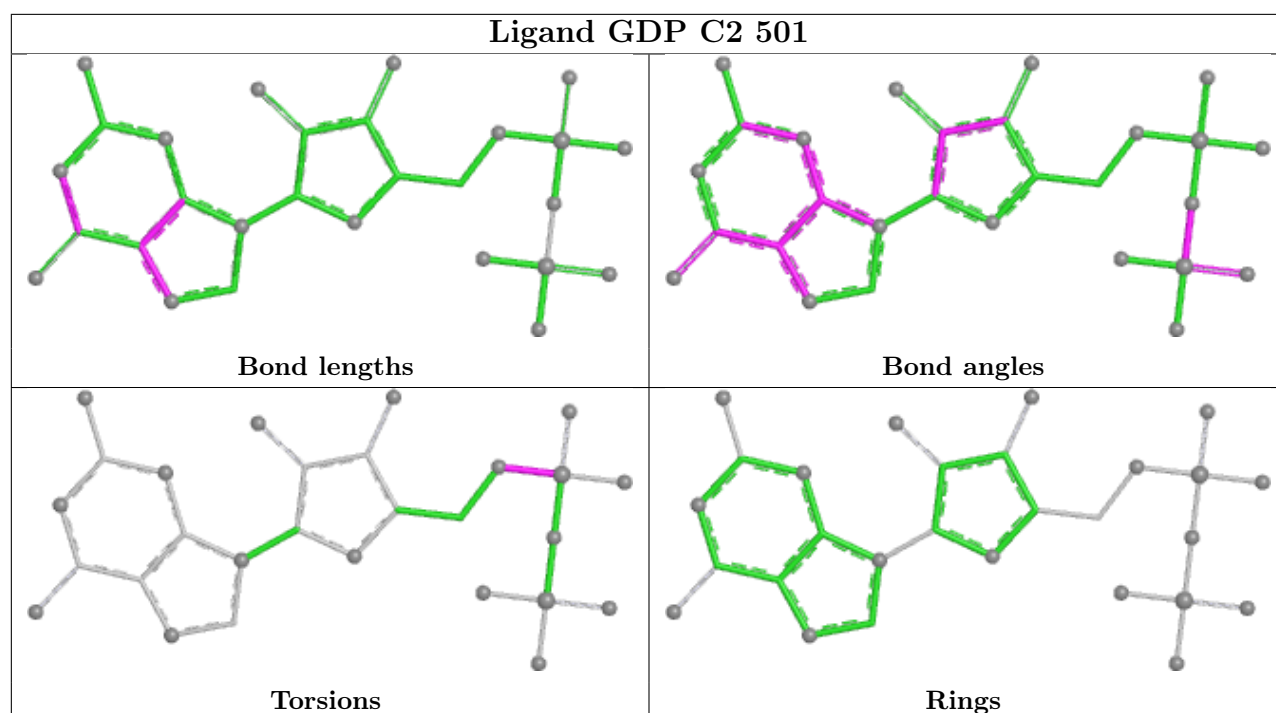


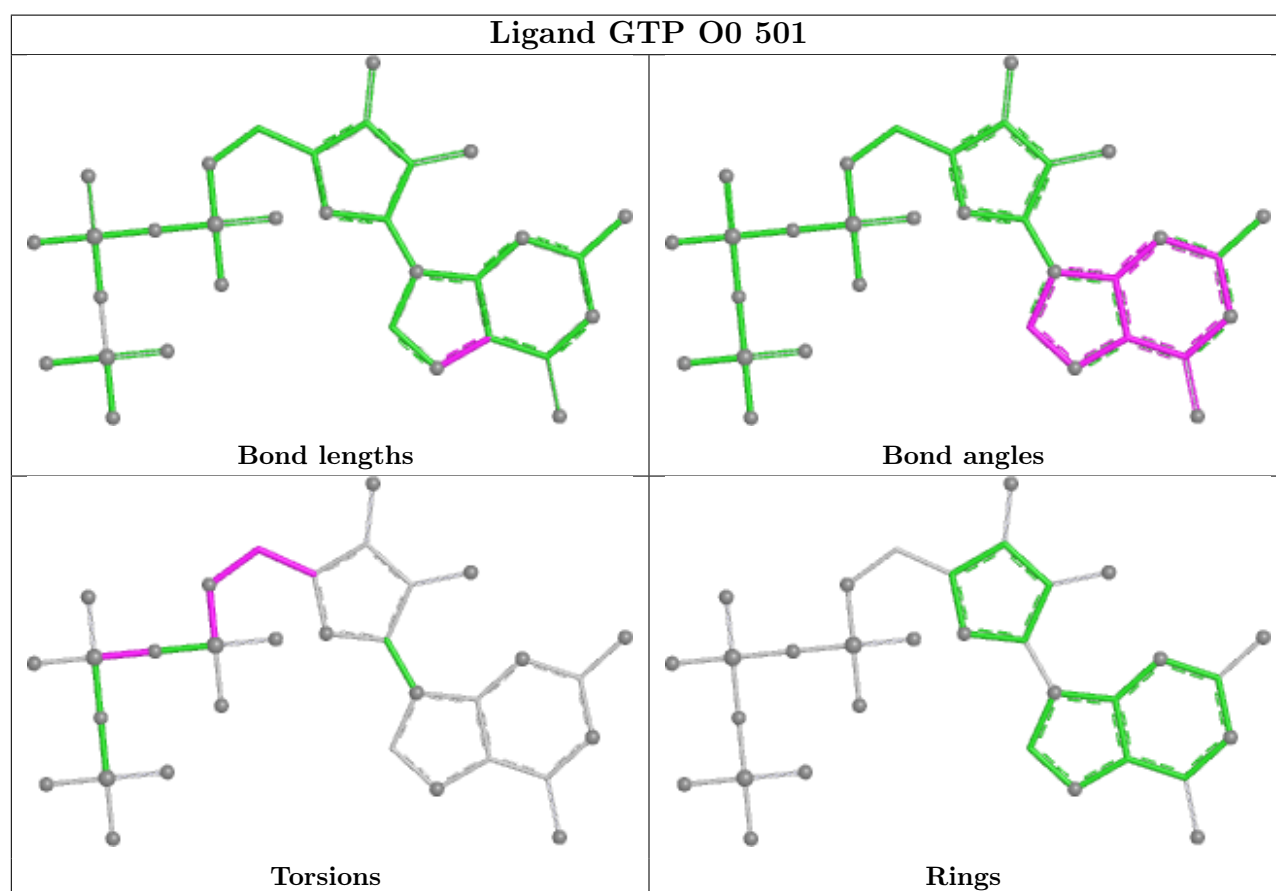
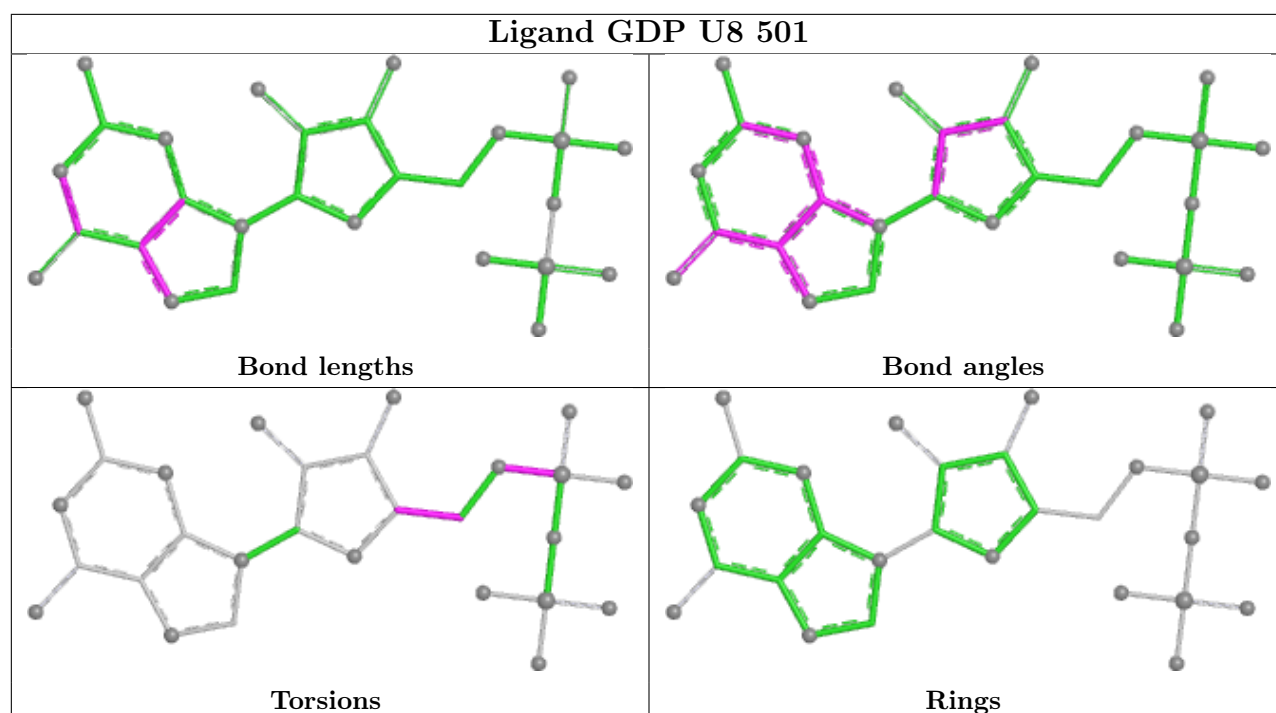
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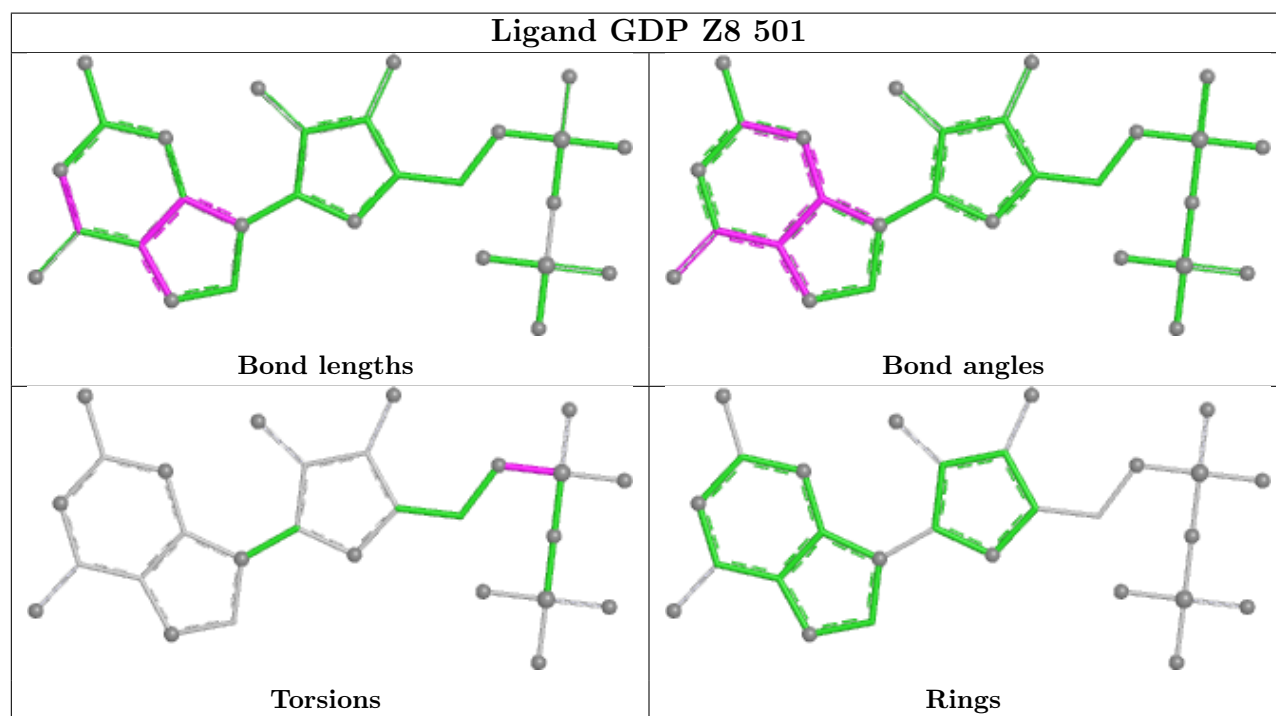
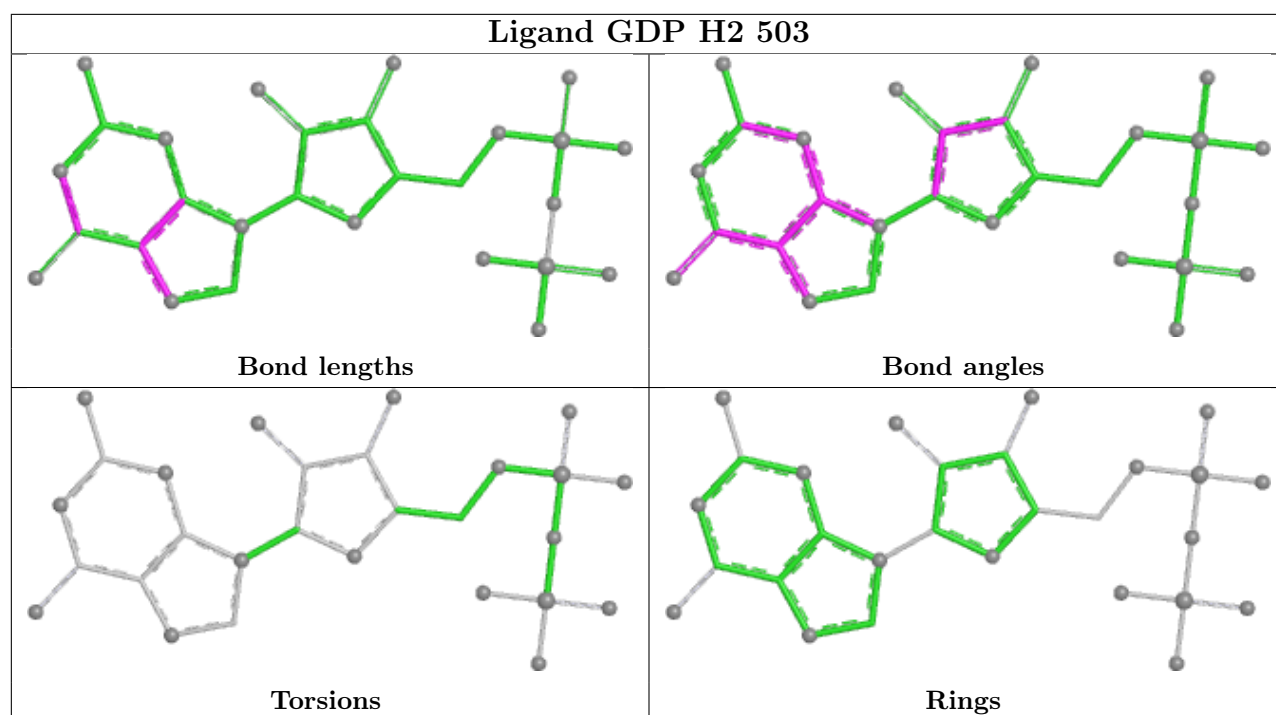


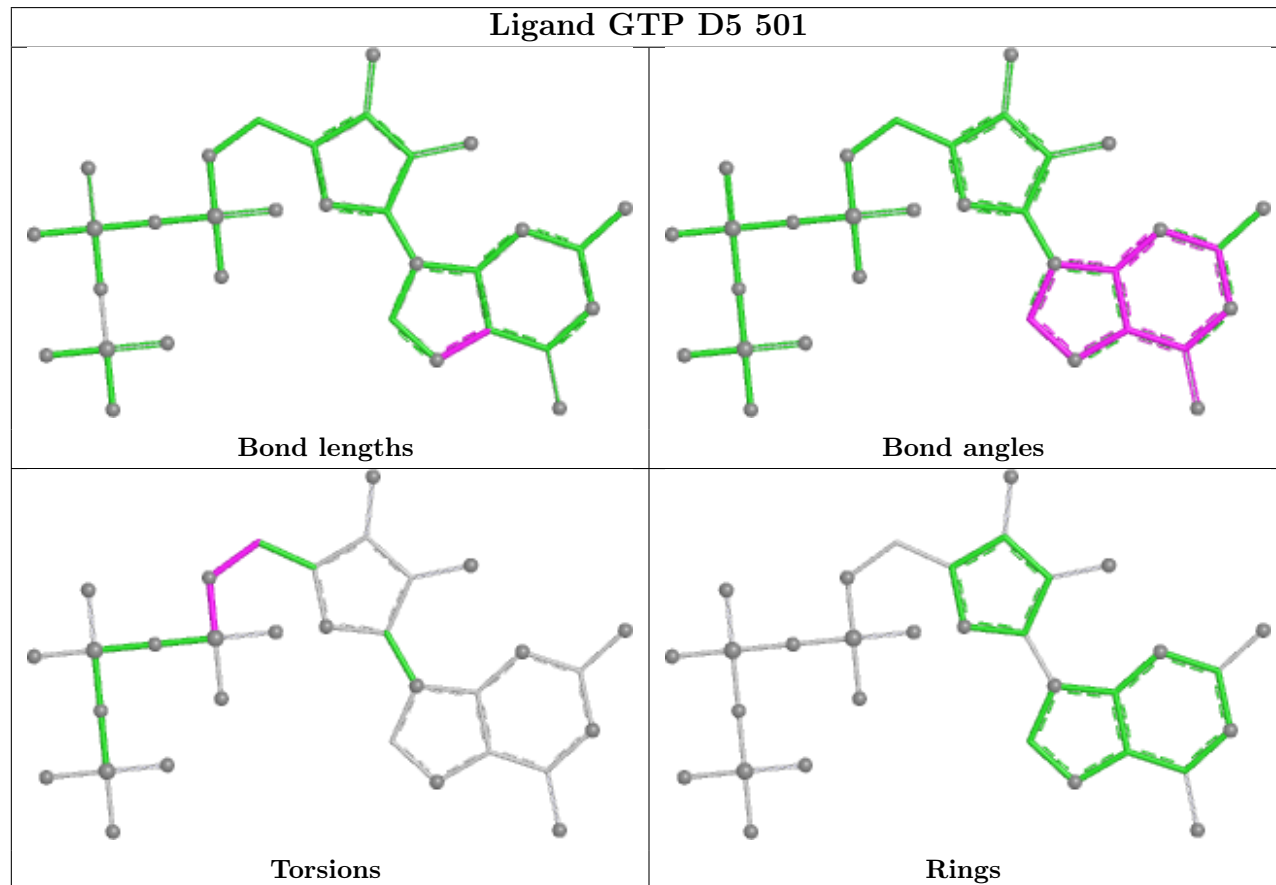
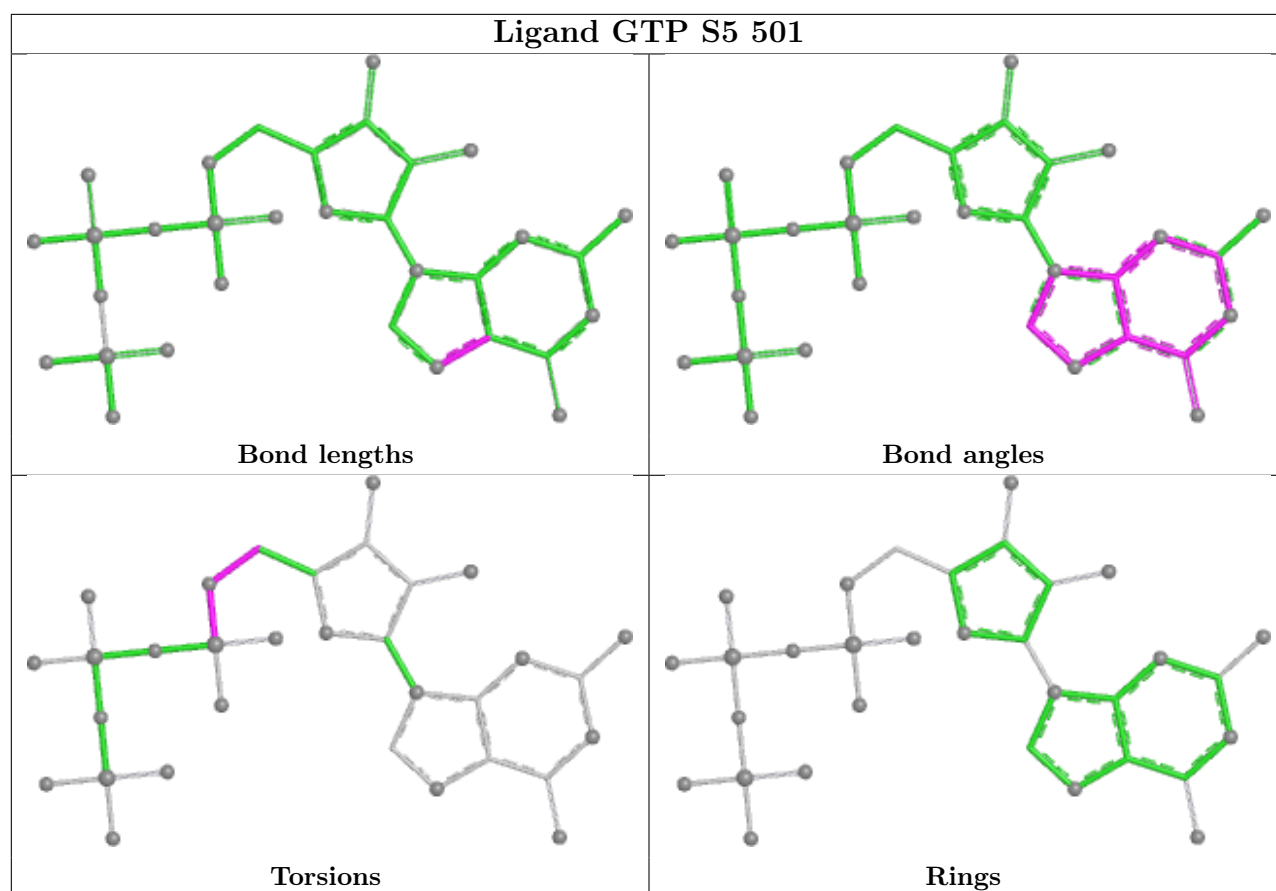
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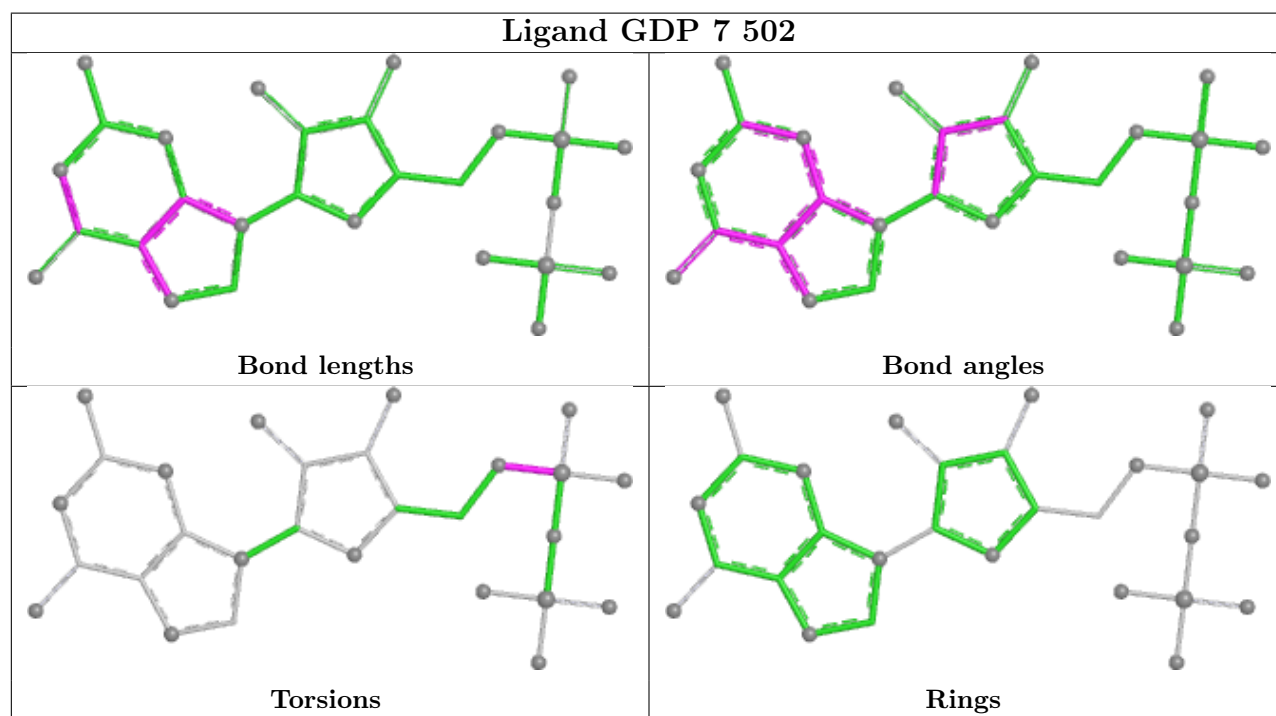
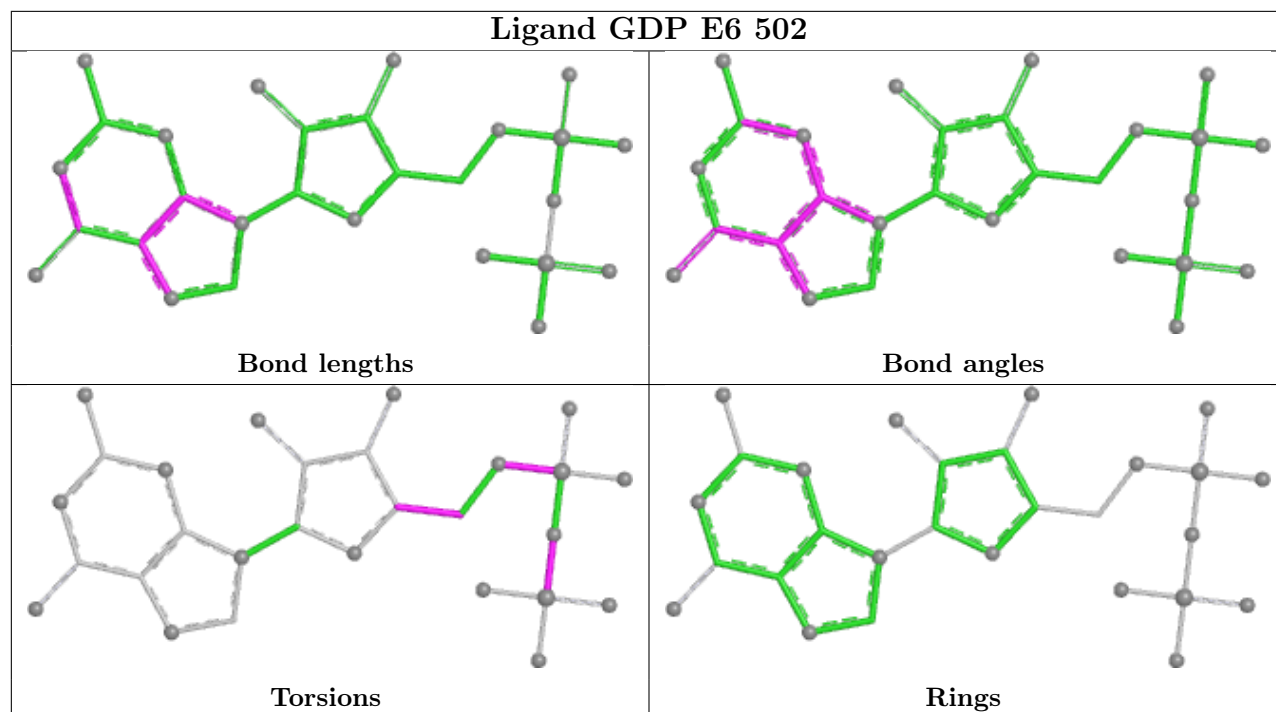


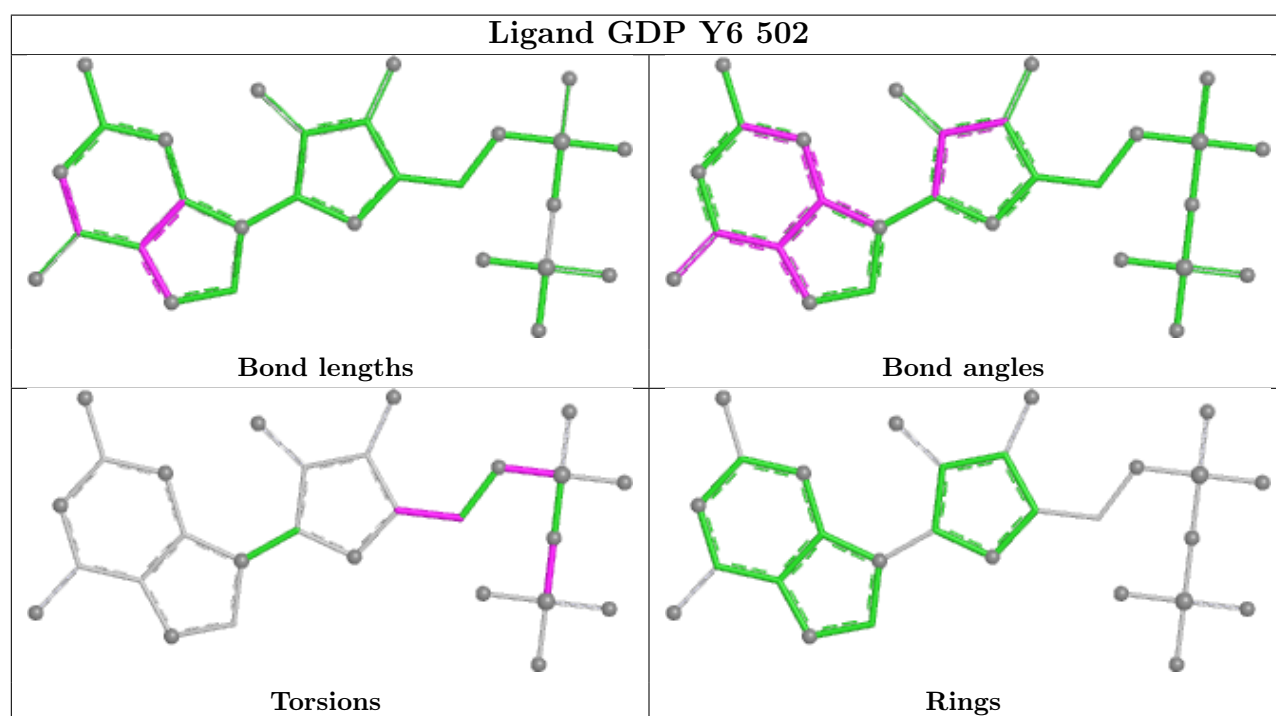
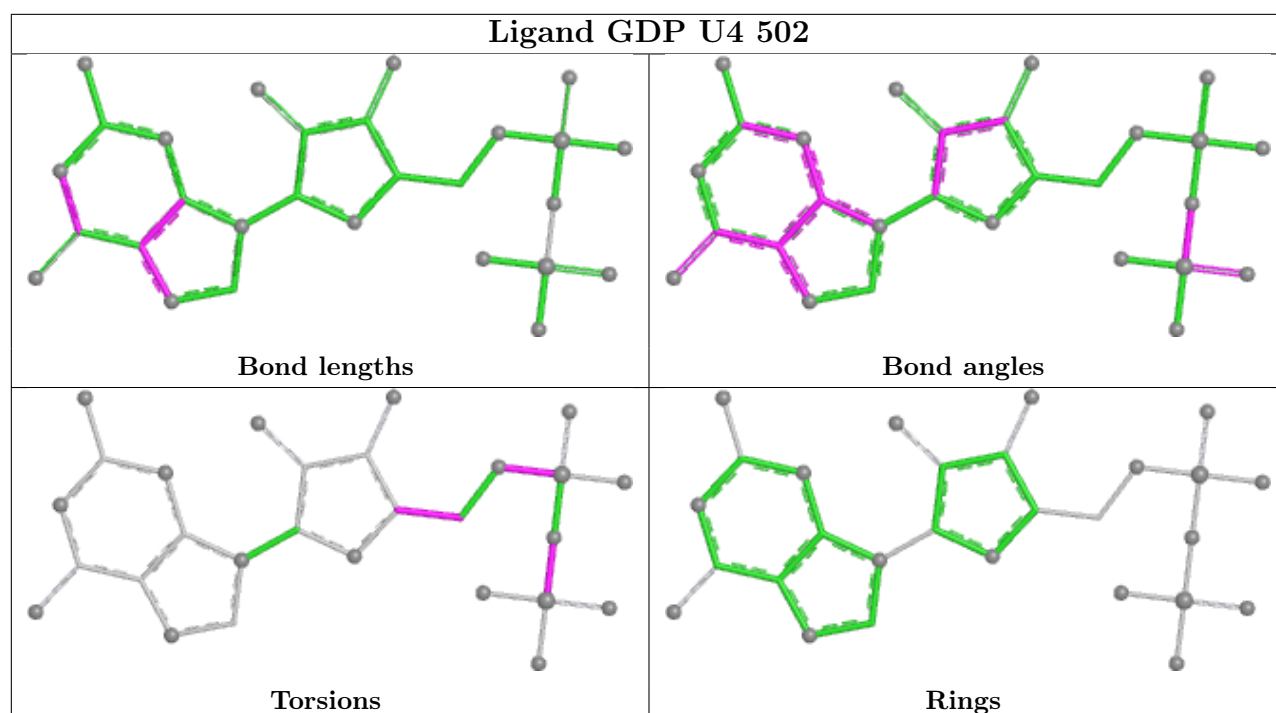


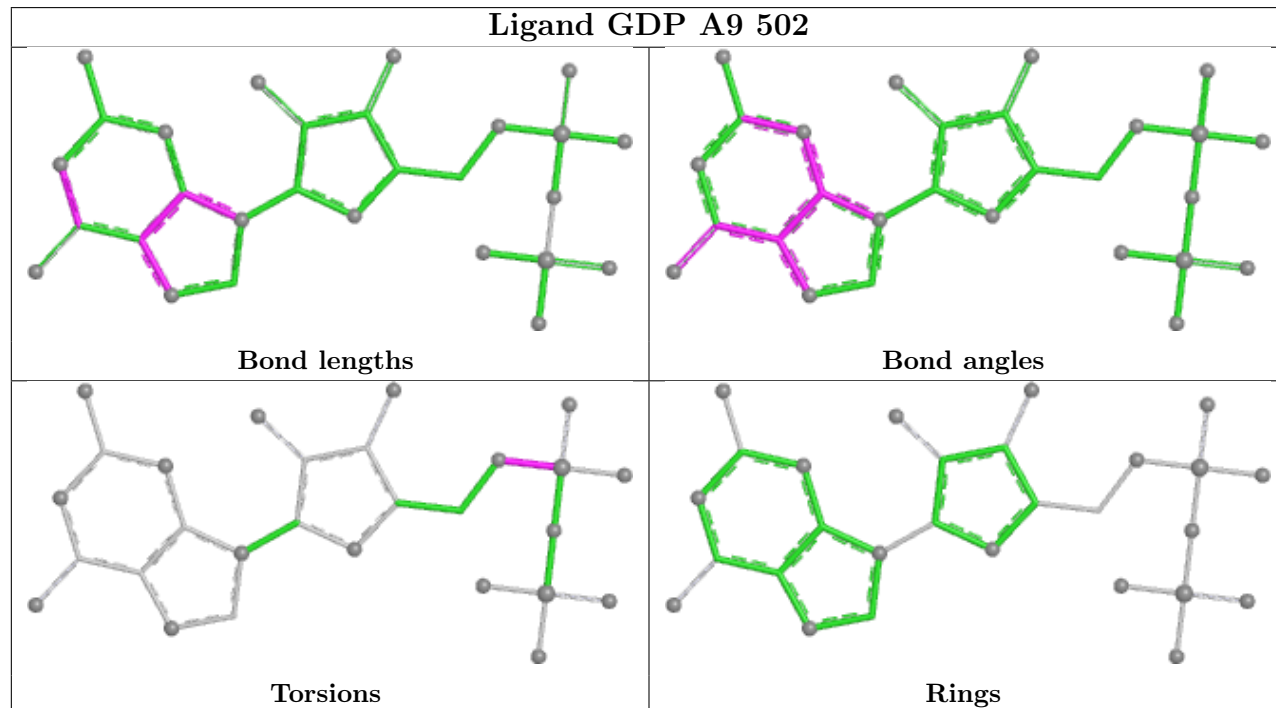
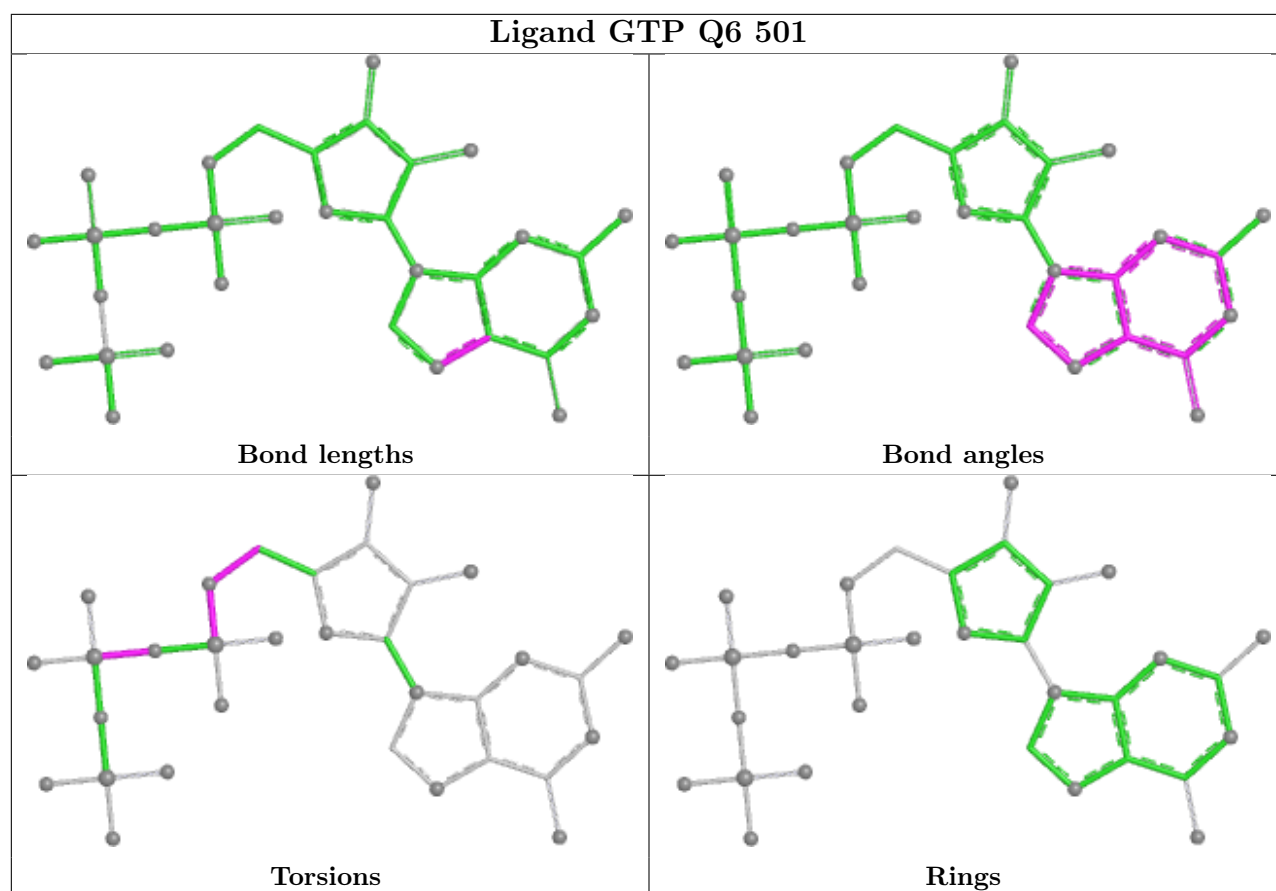


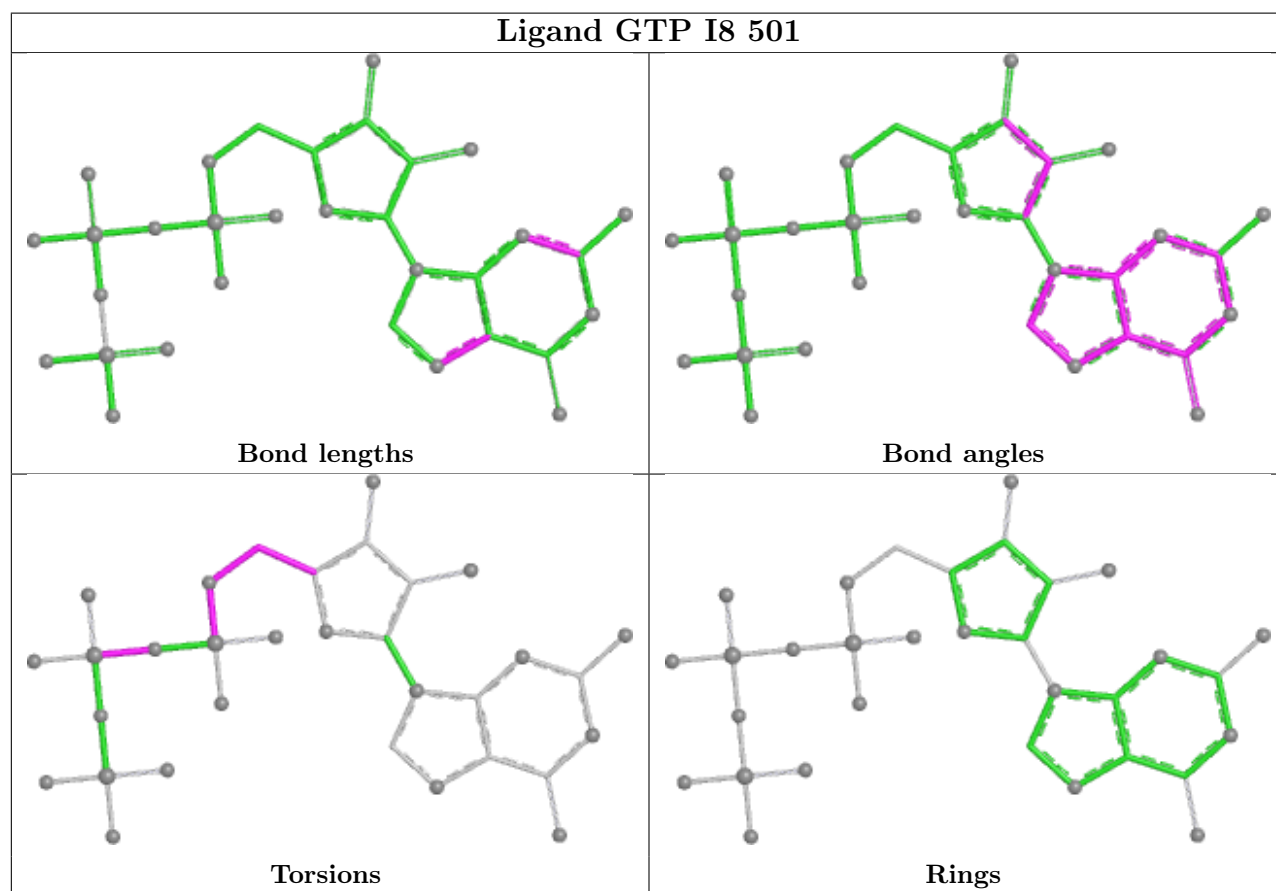
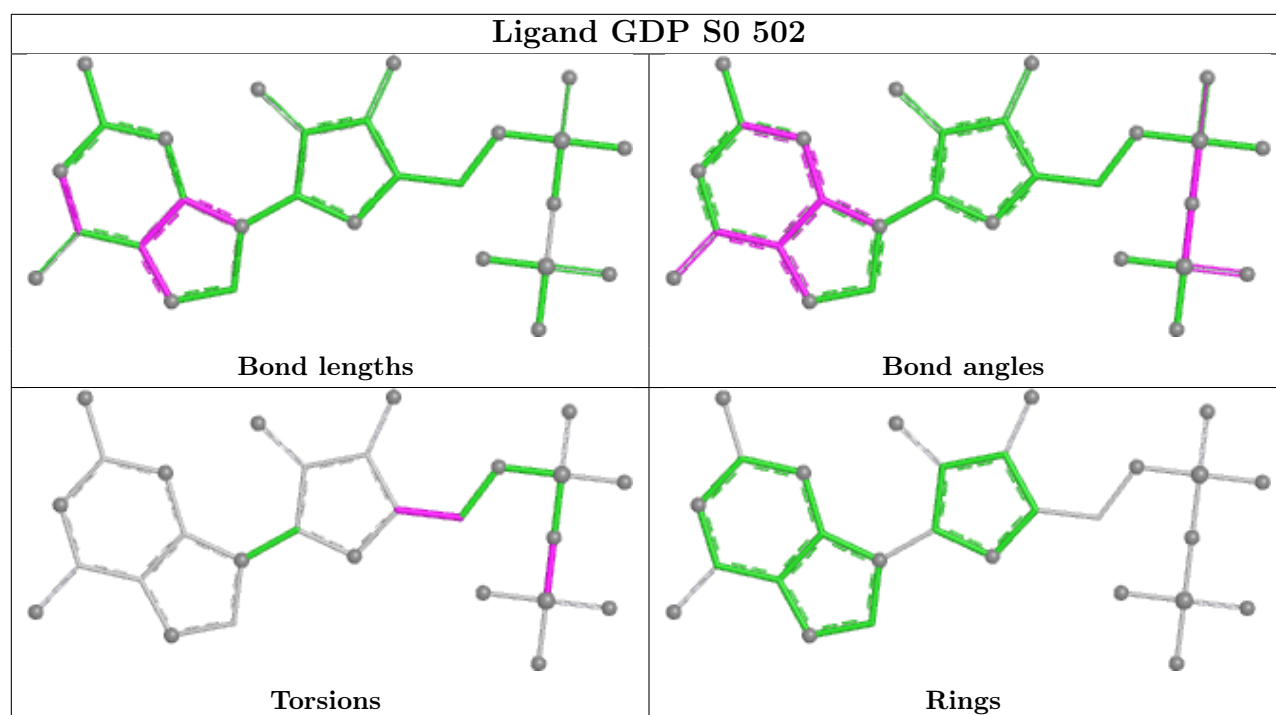


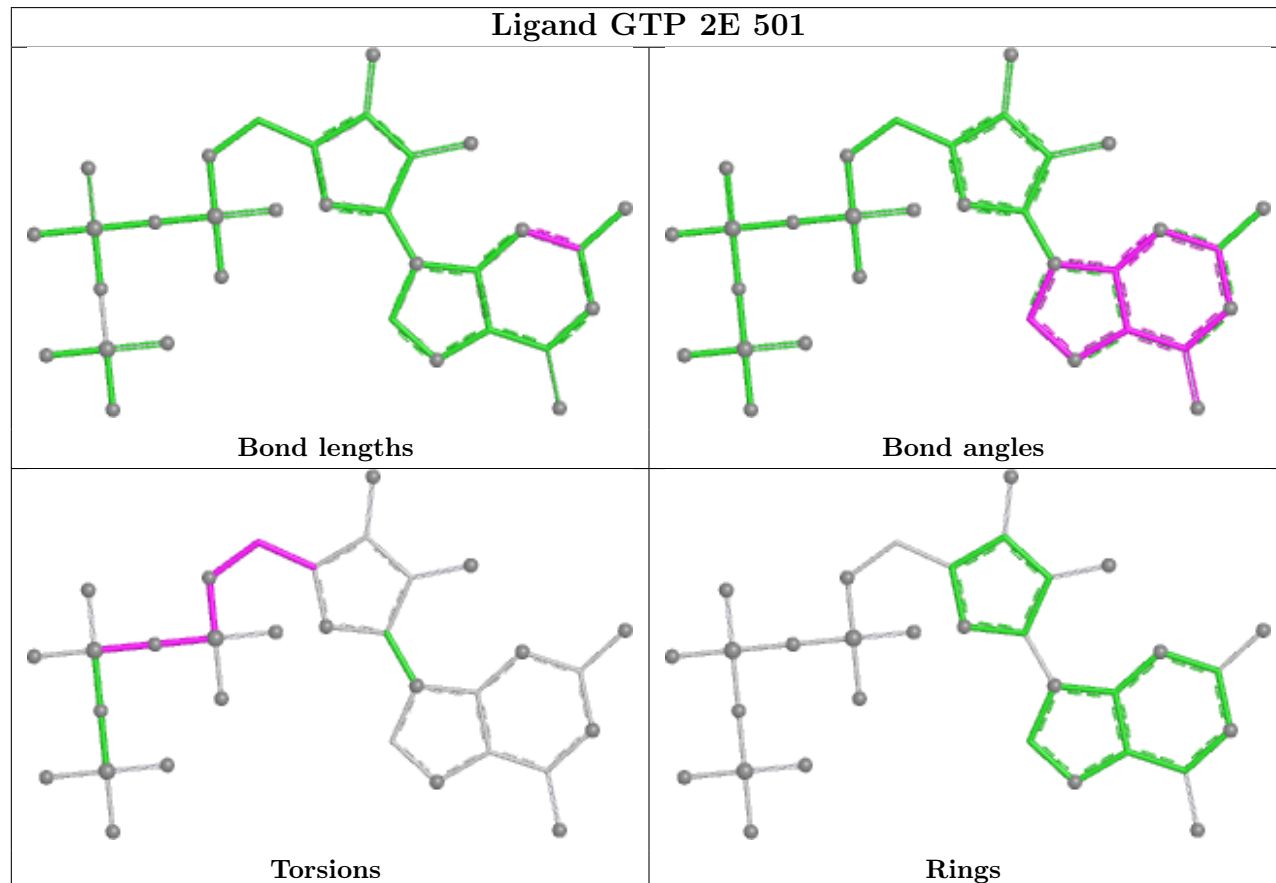
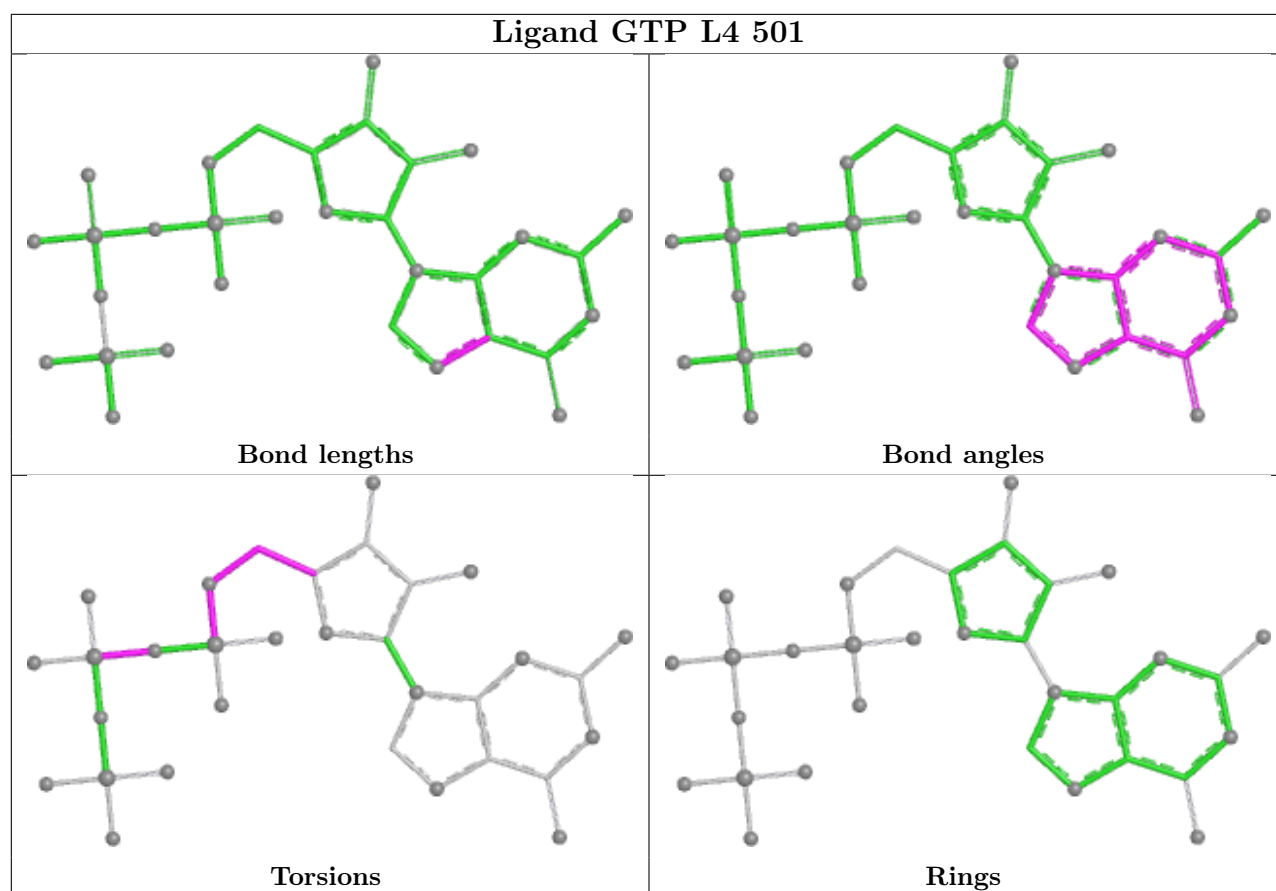


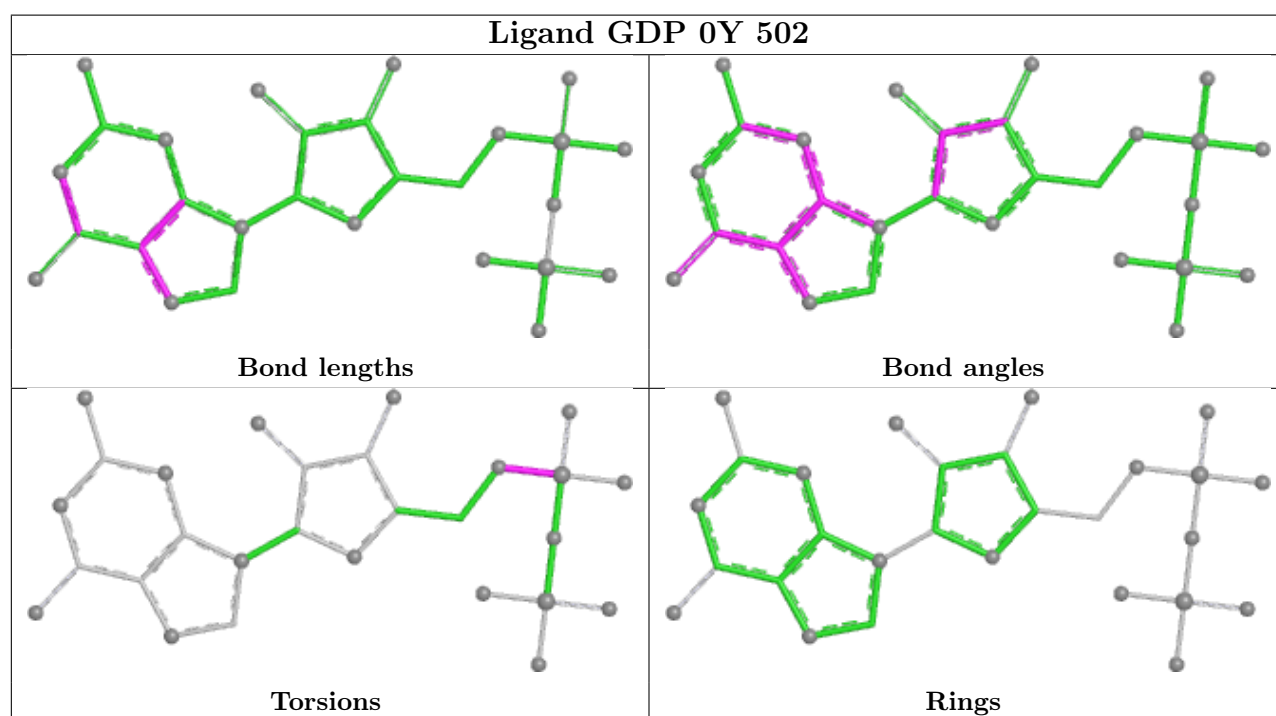
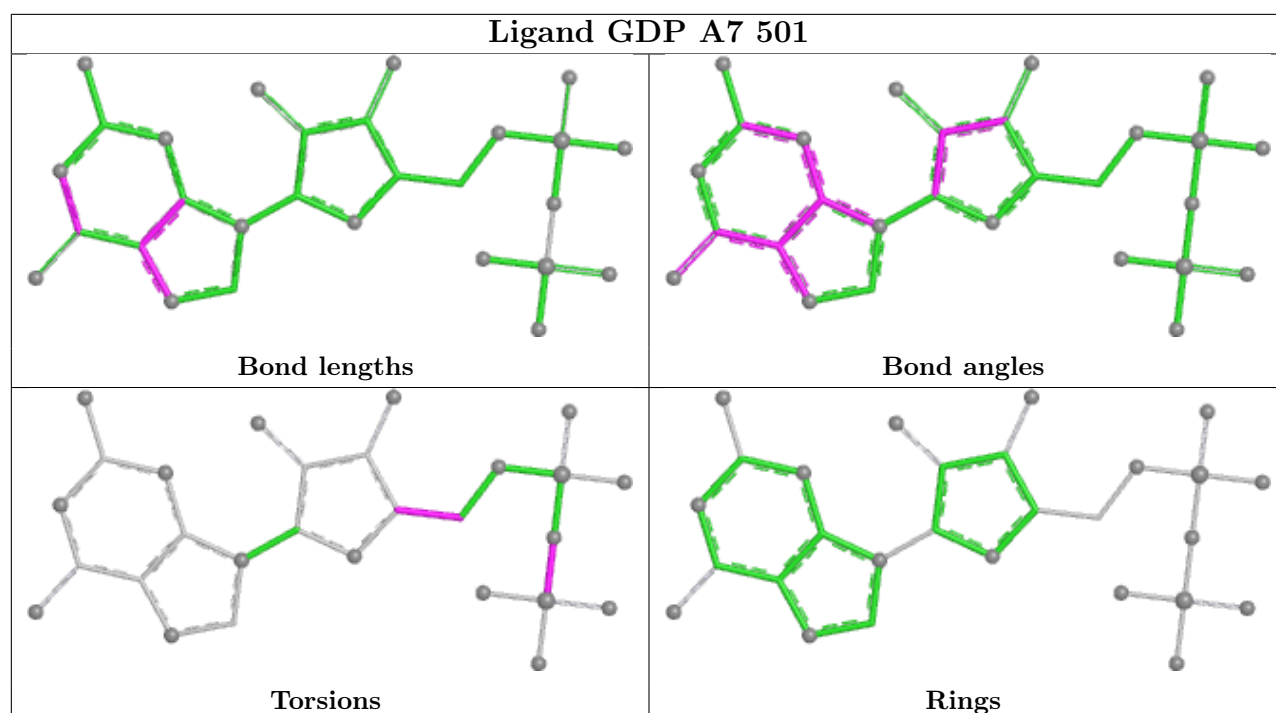


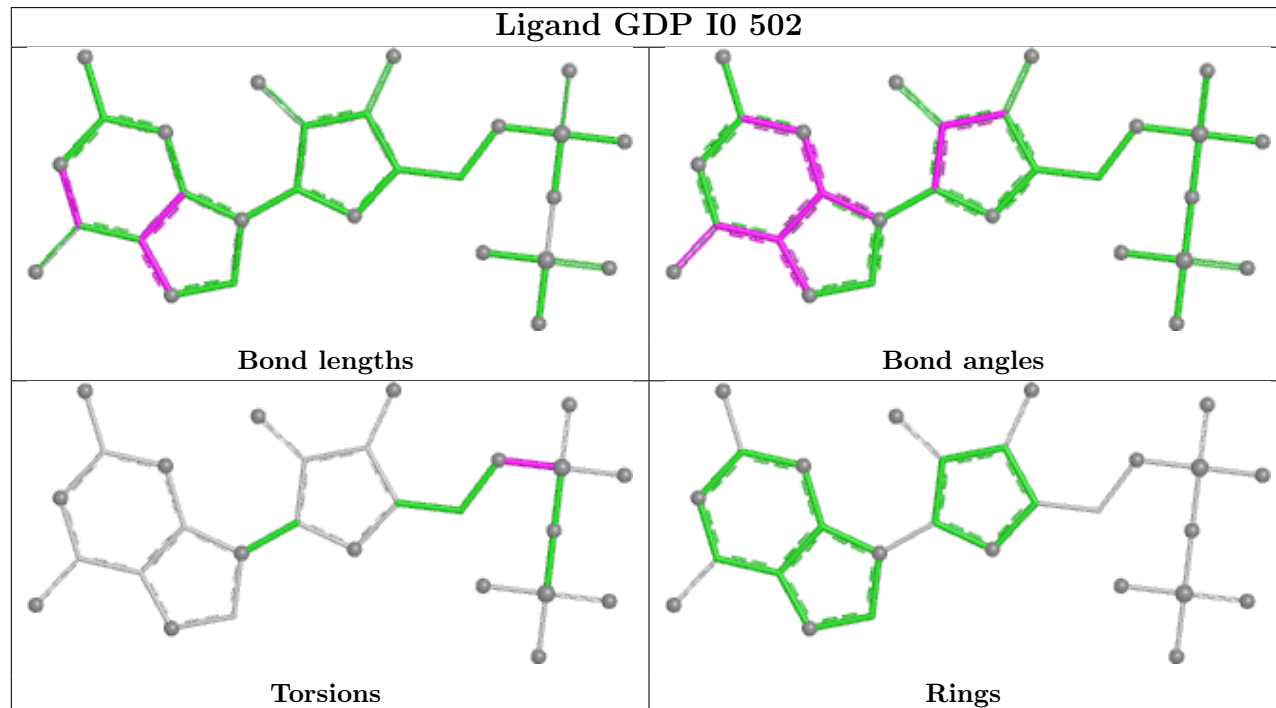
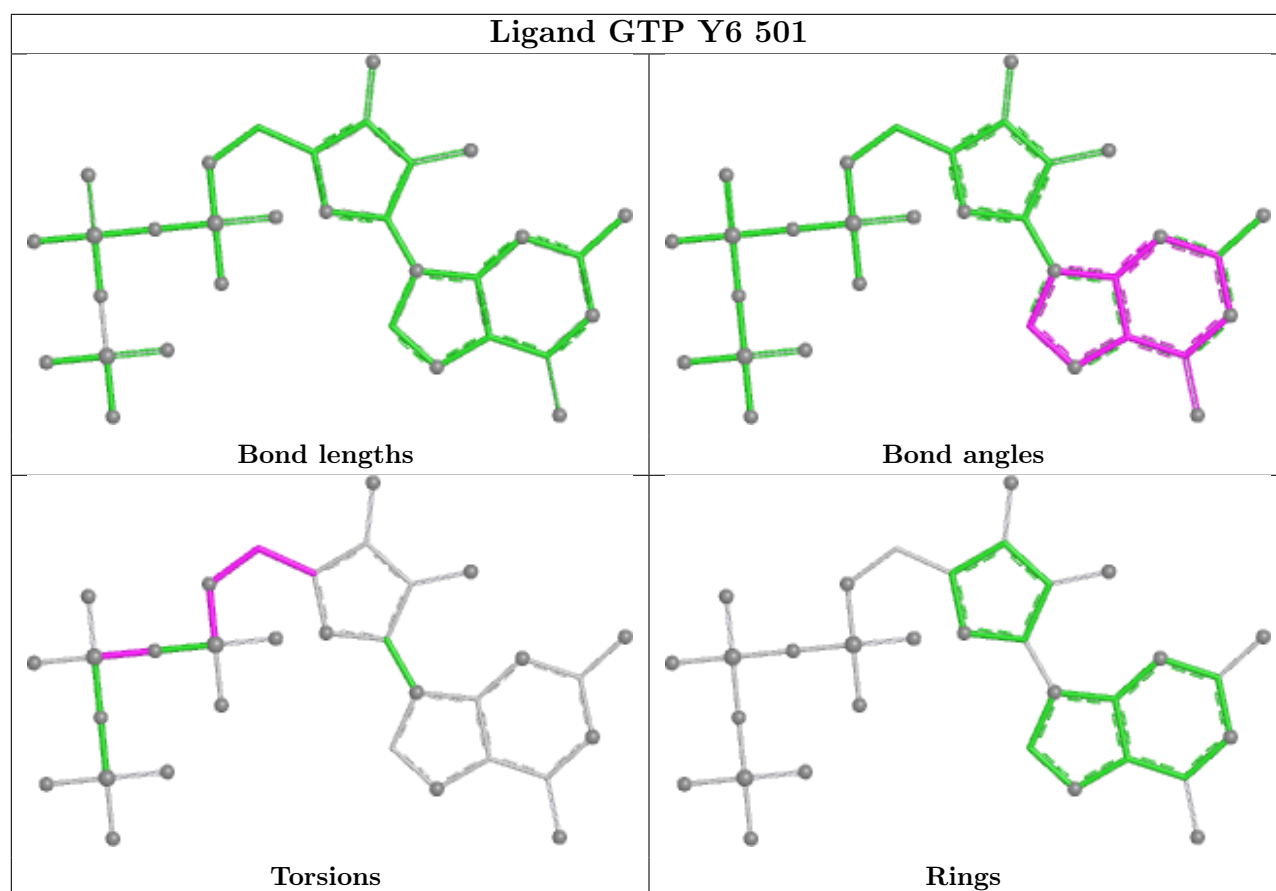


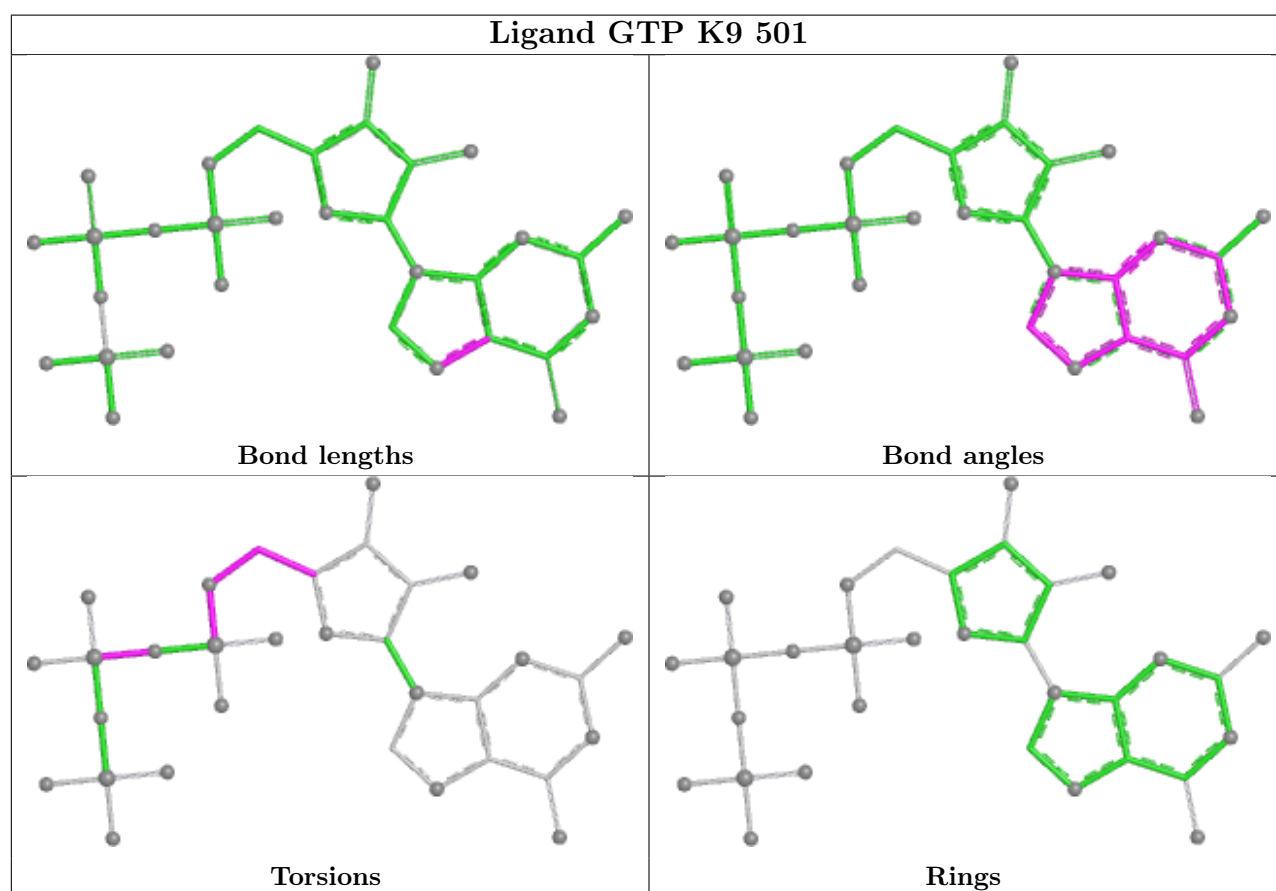
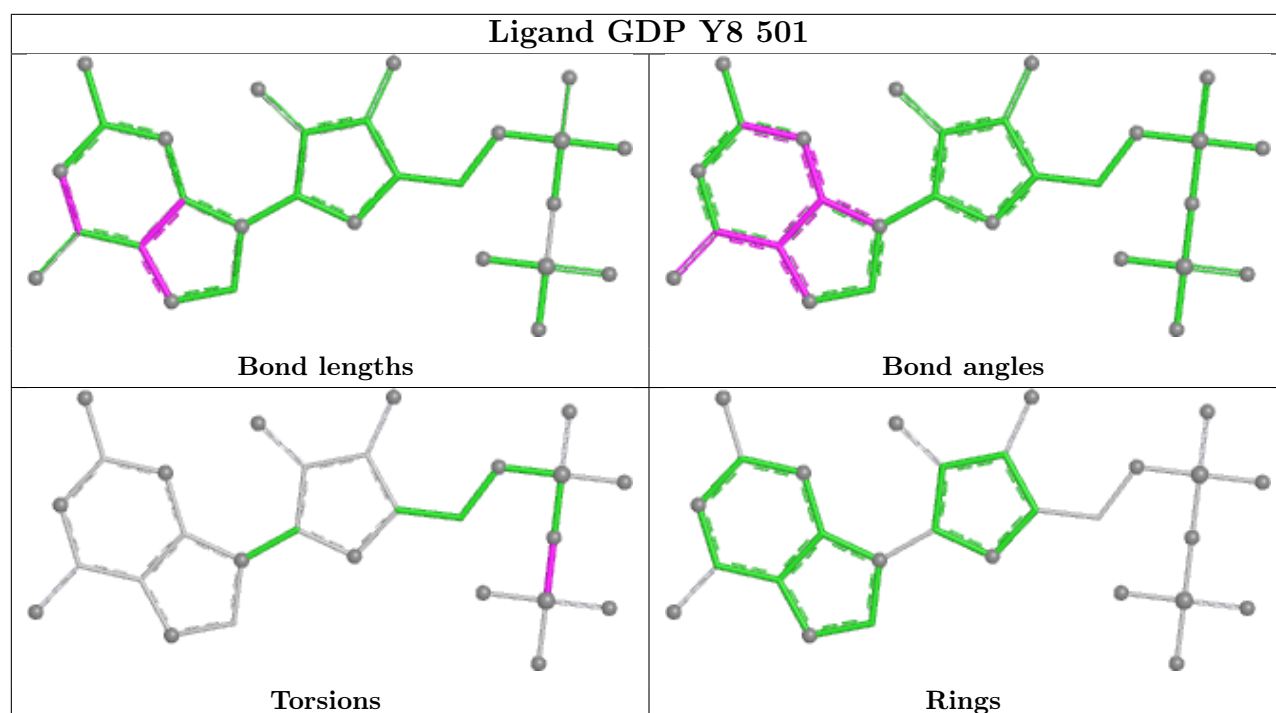


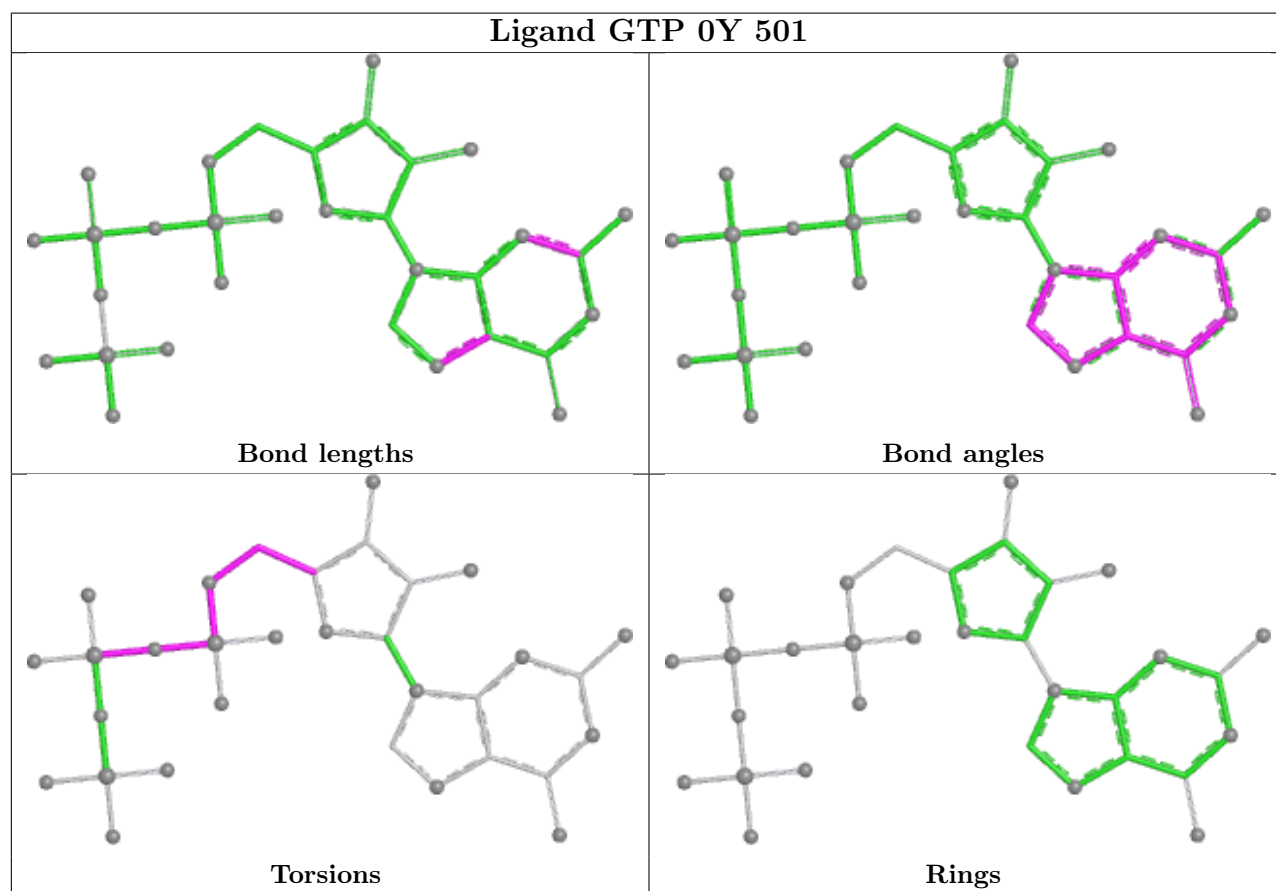
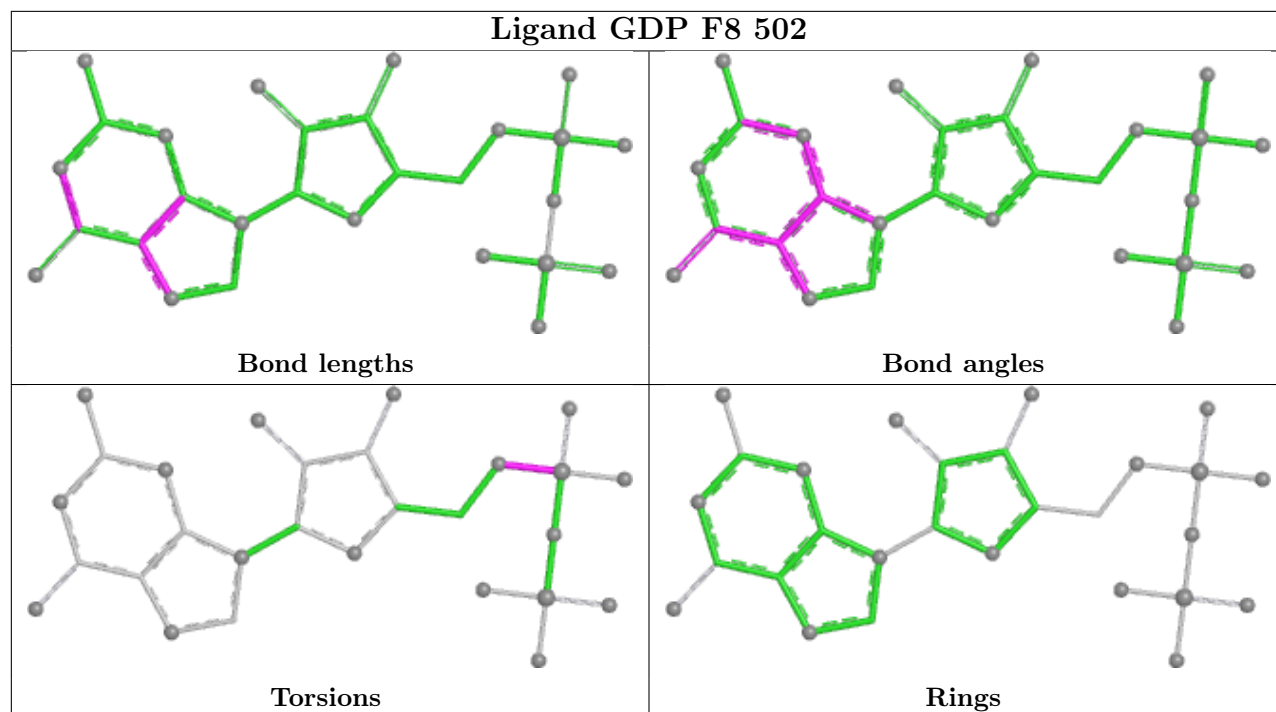


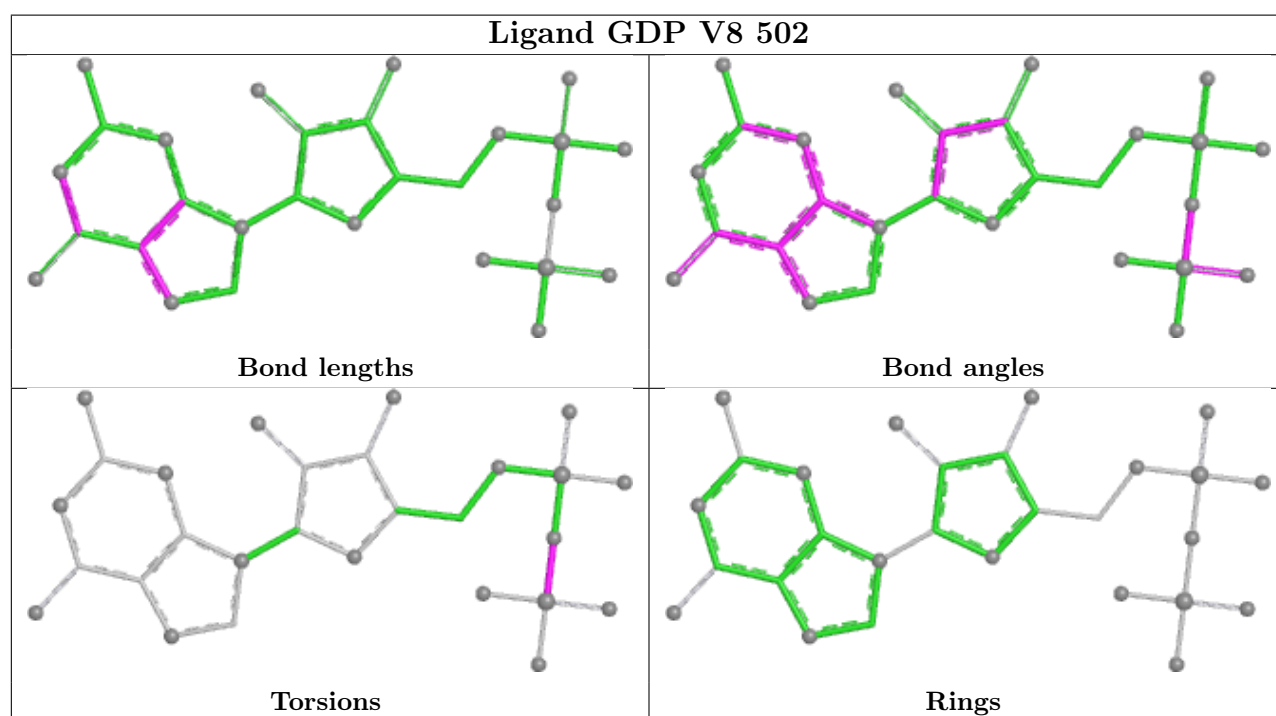
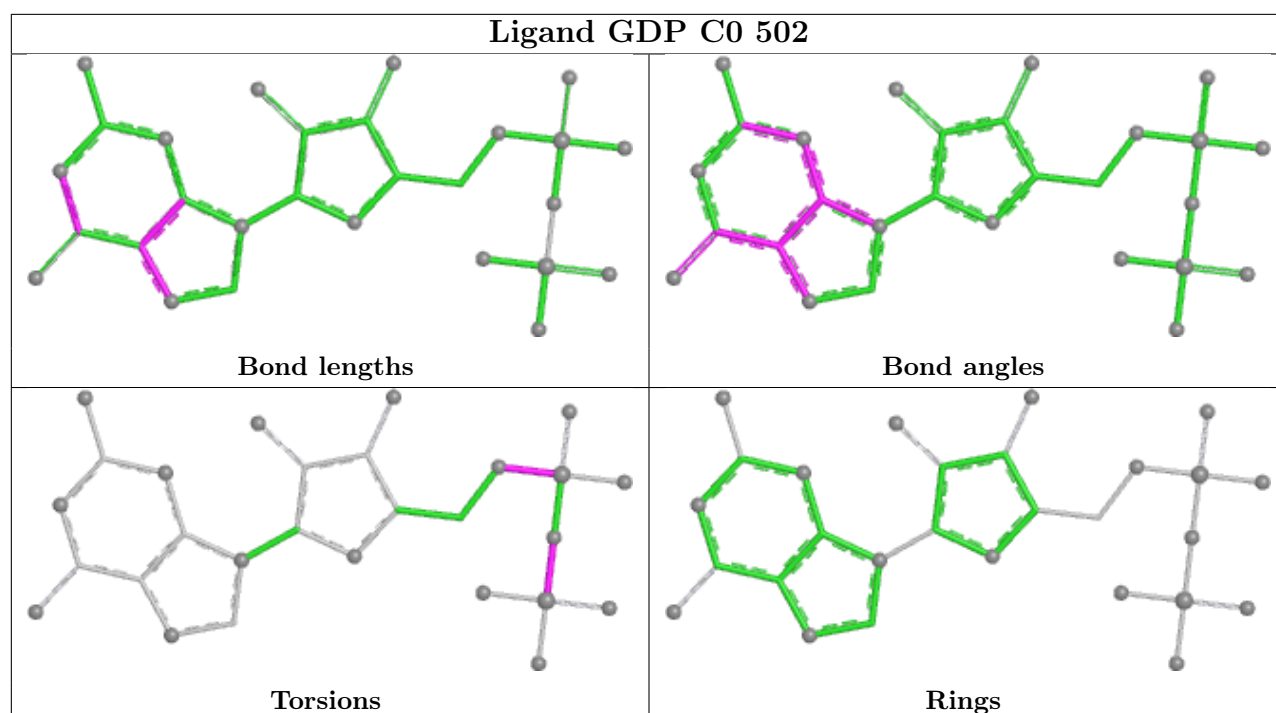


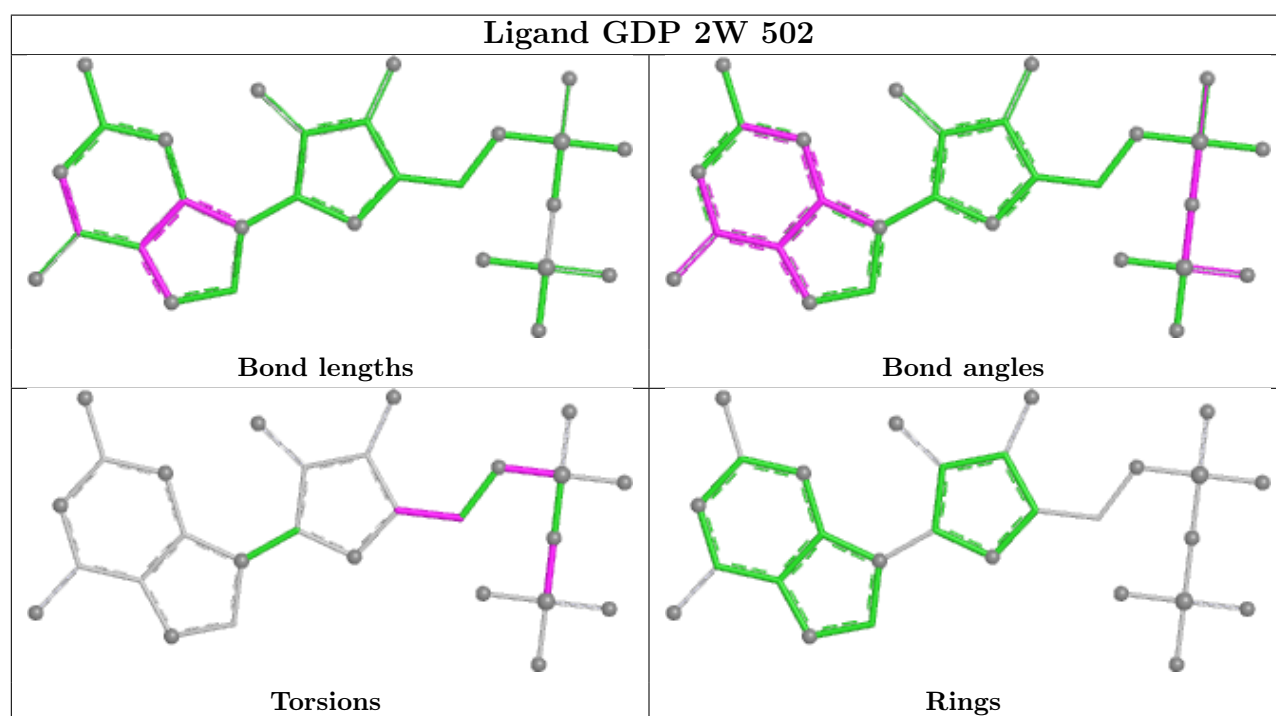
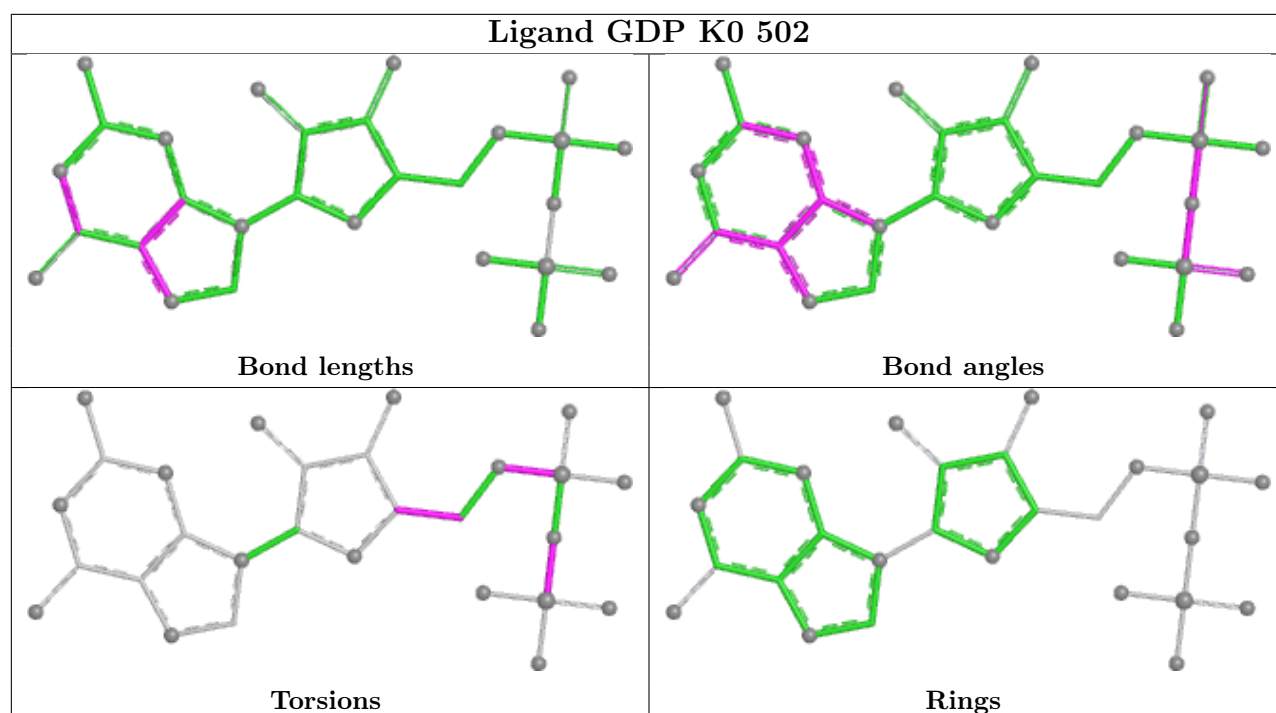


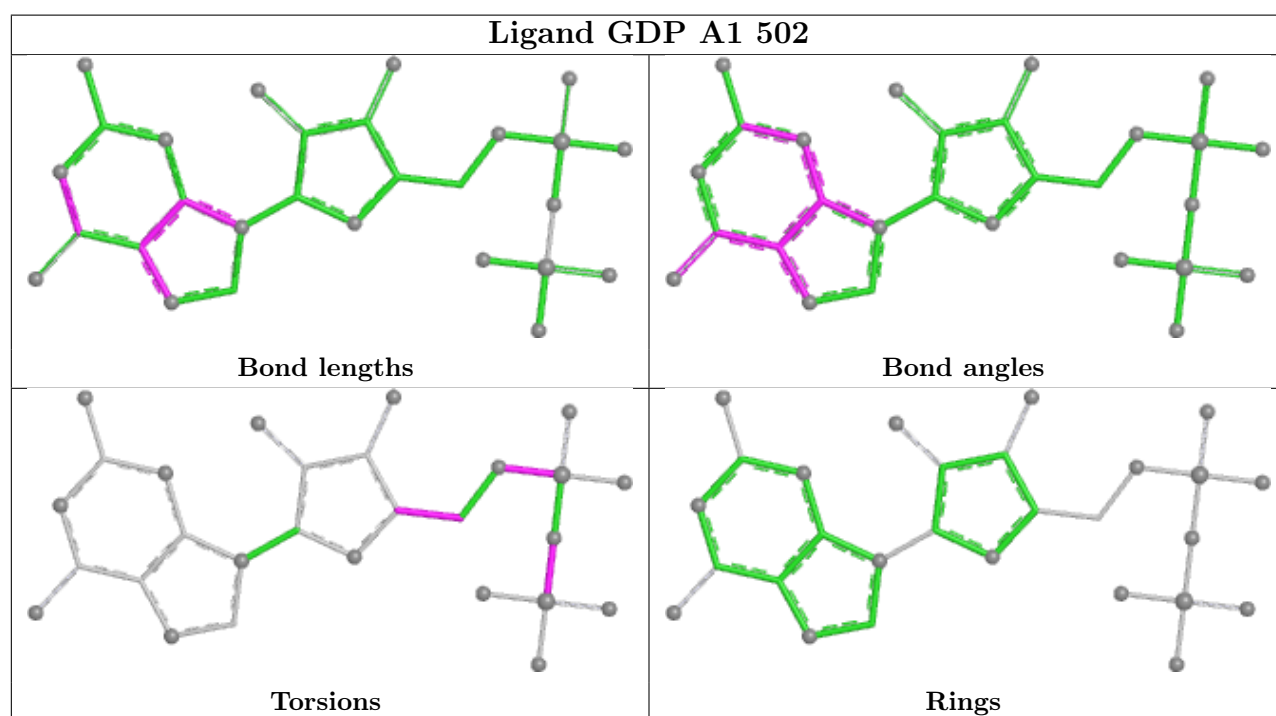
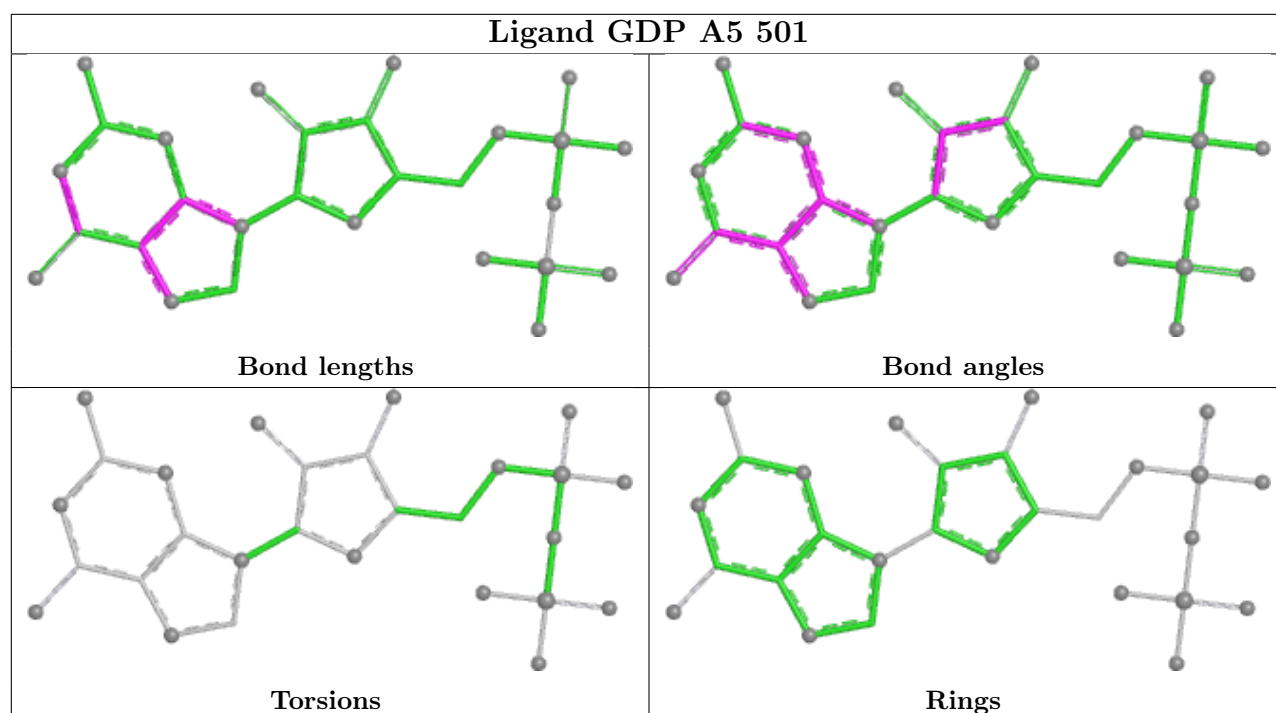


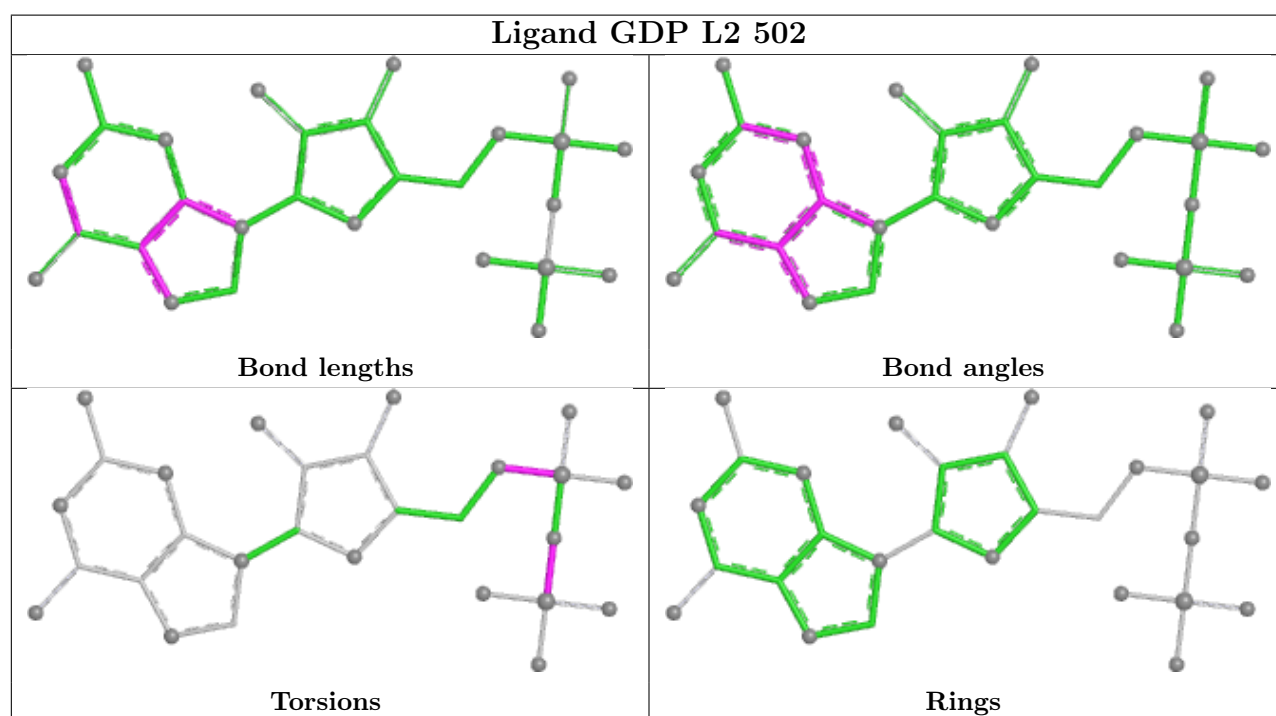
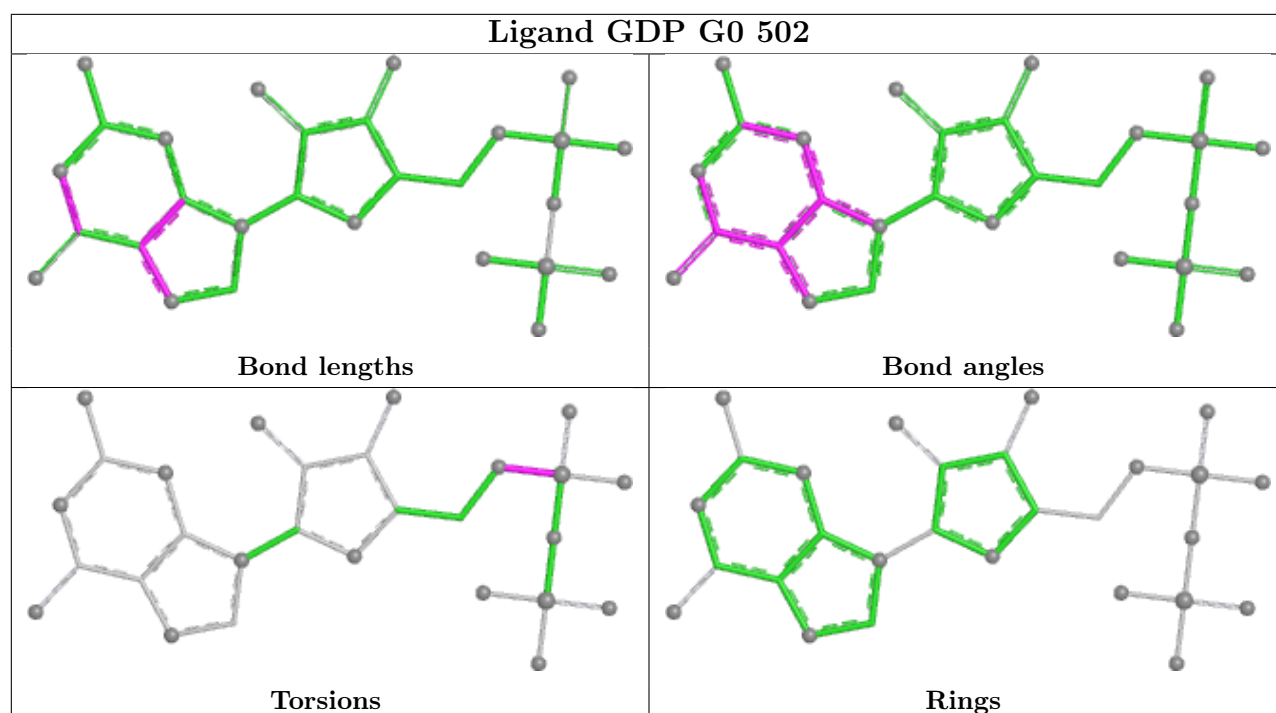


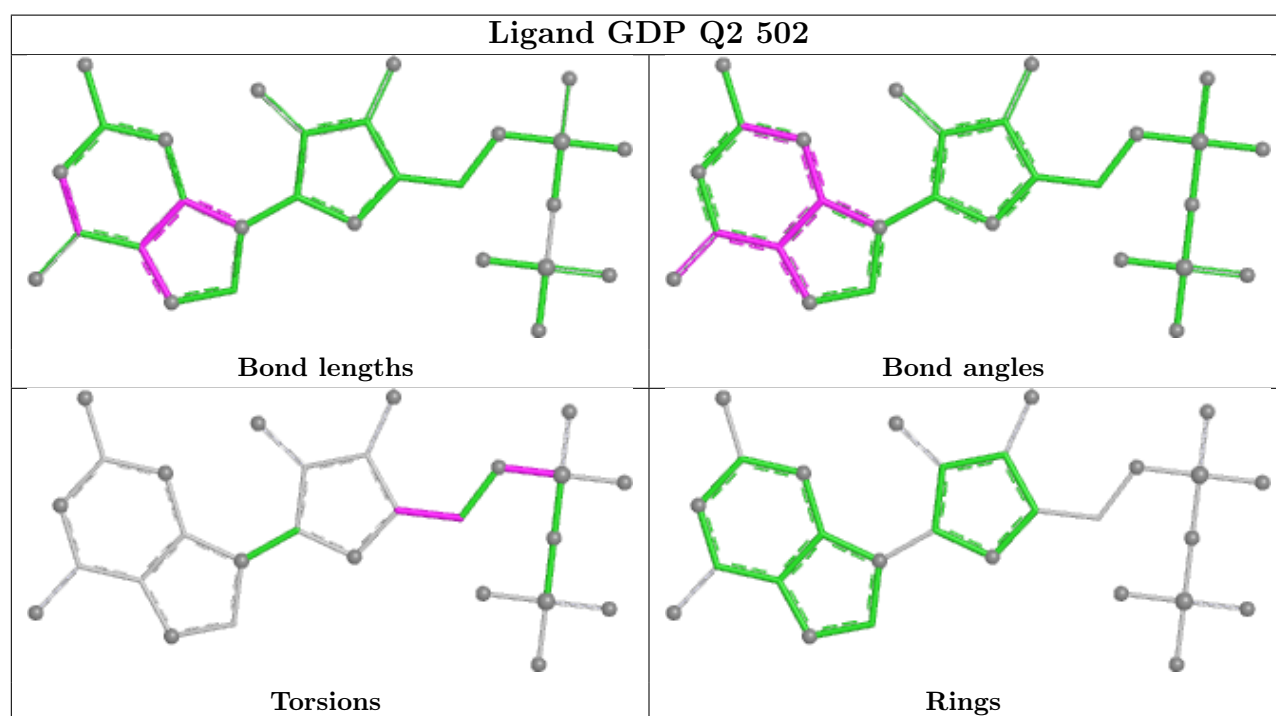
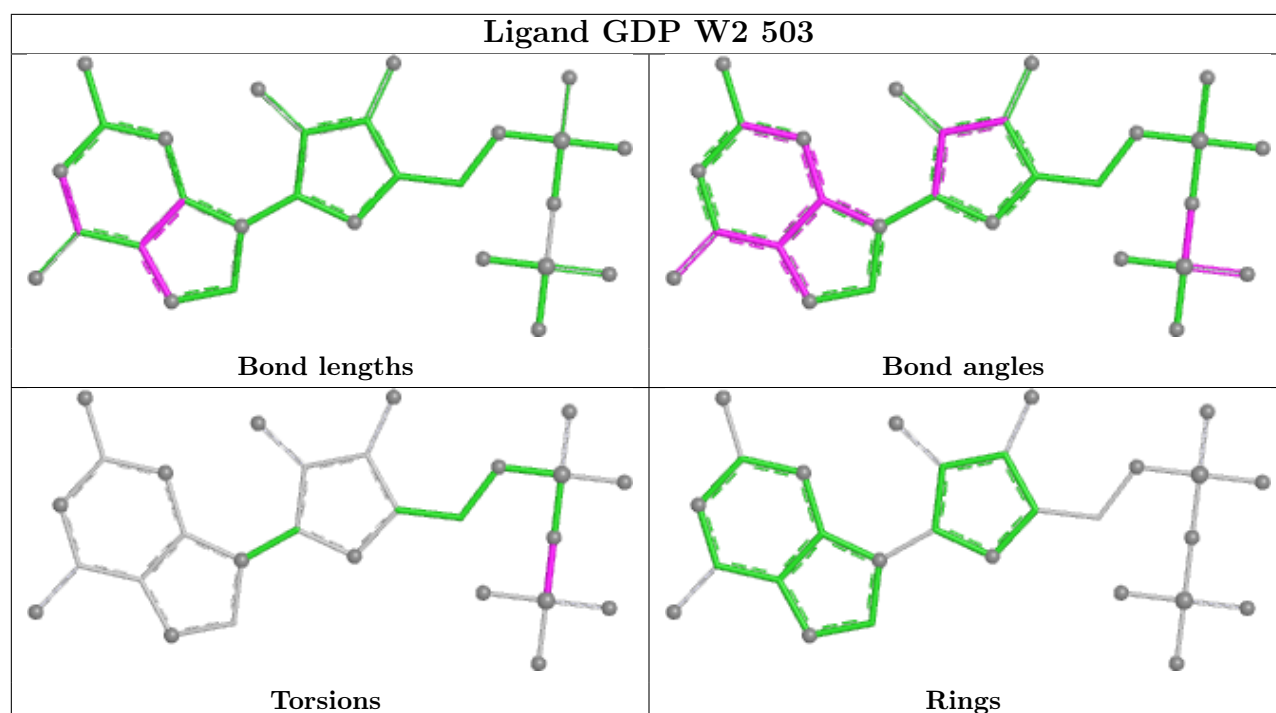




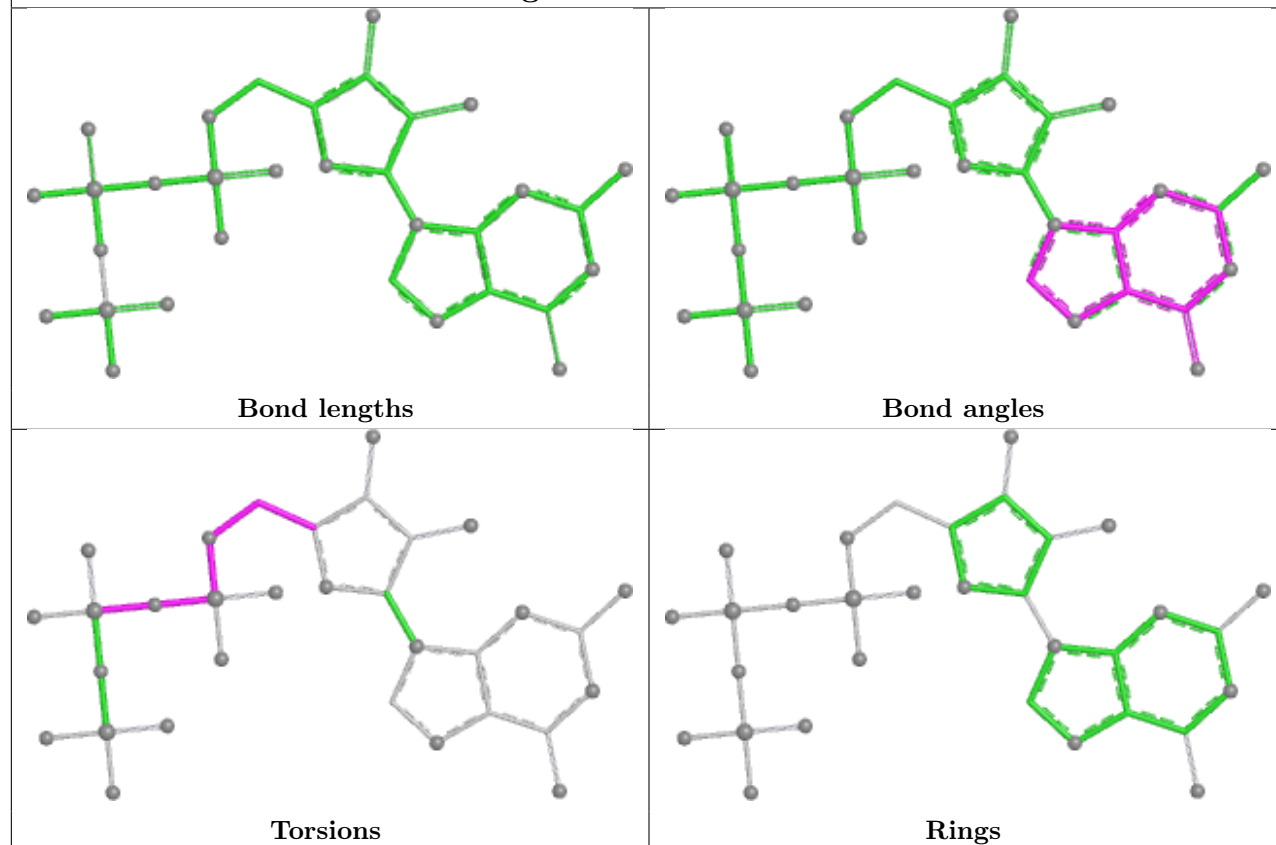




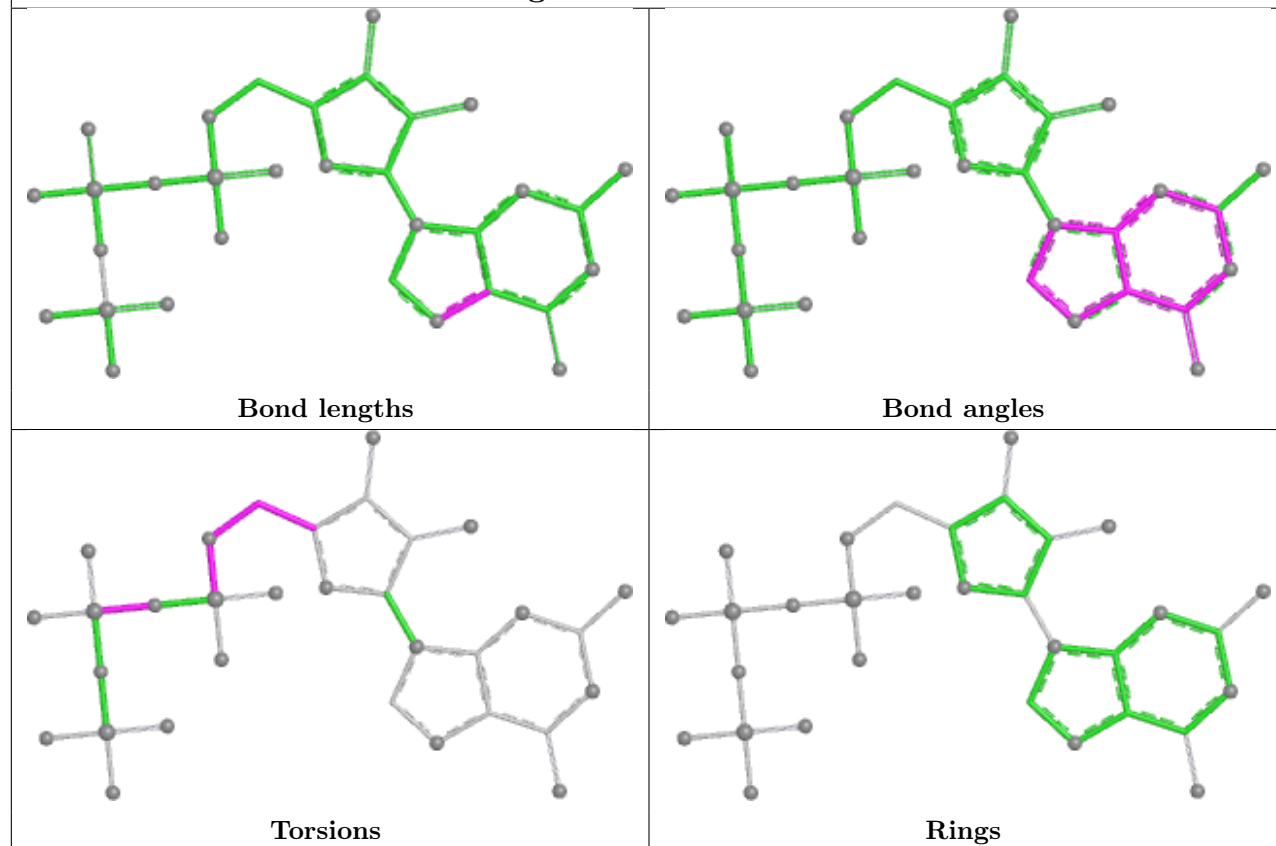




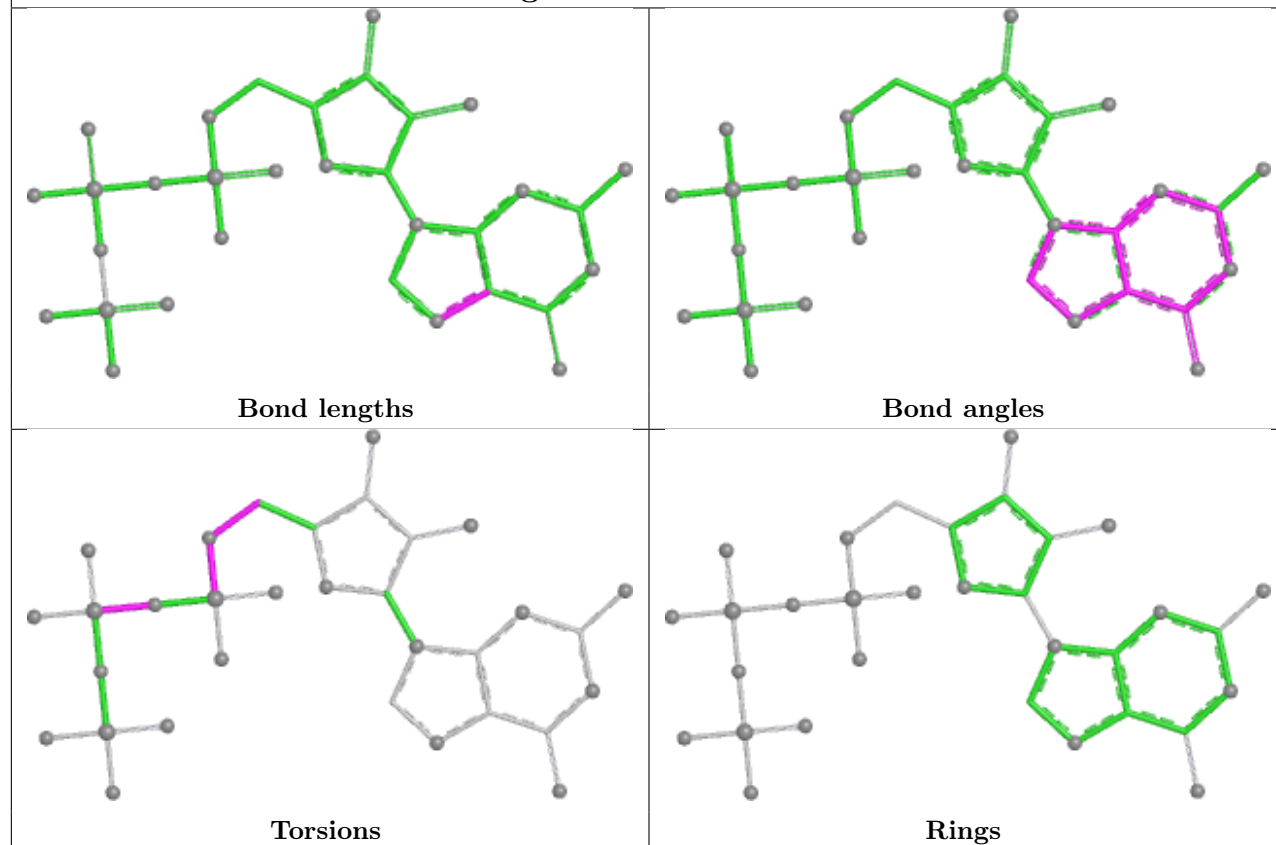
Ligand GTP 2C 501



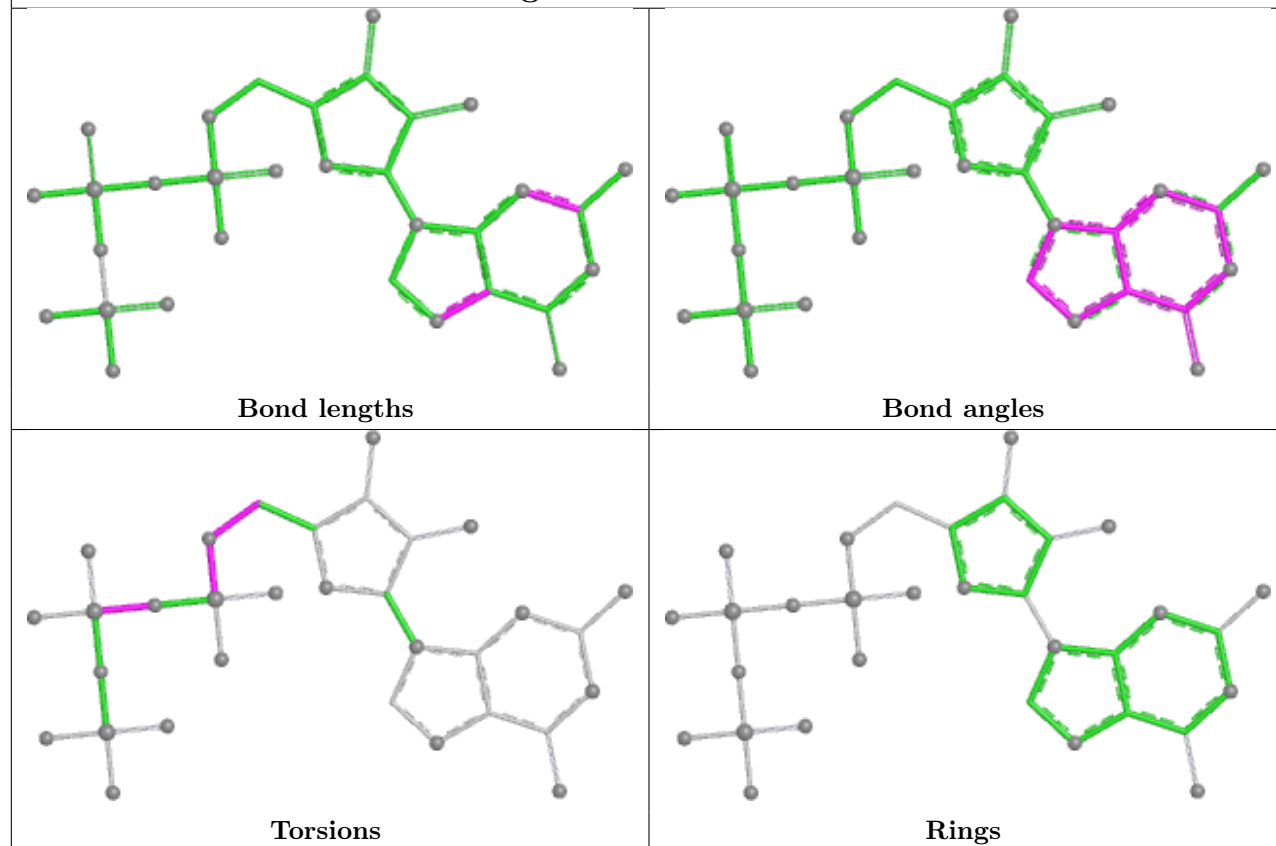
Ligand GTP 3I 501



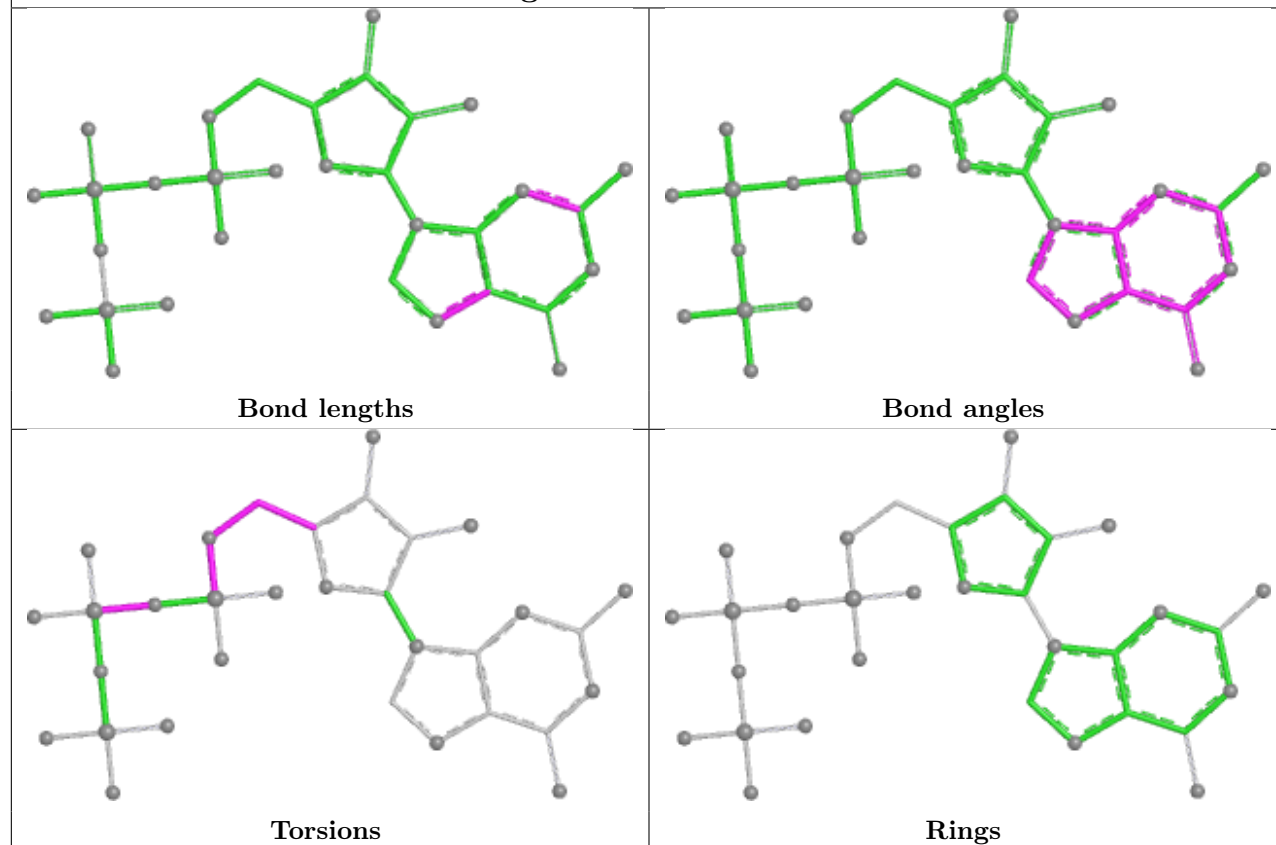
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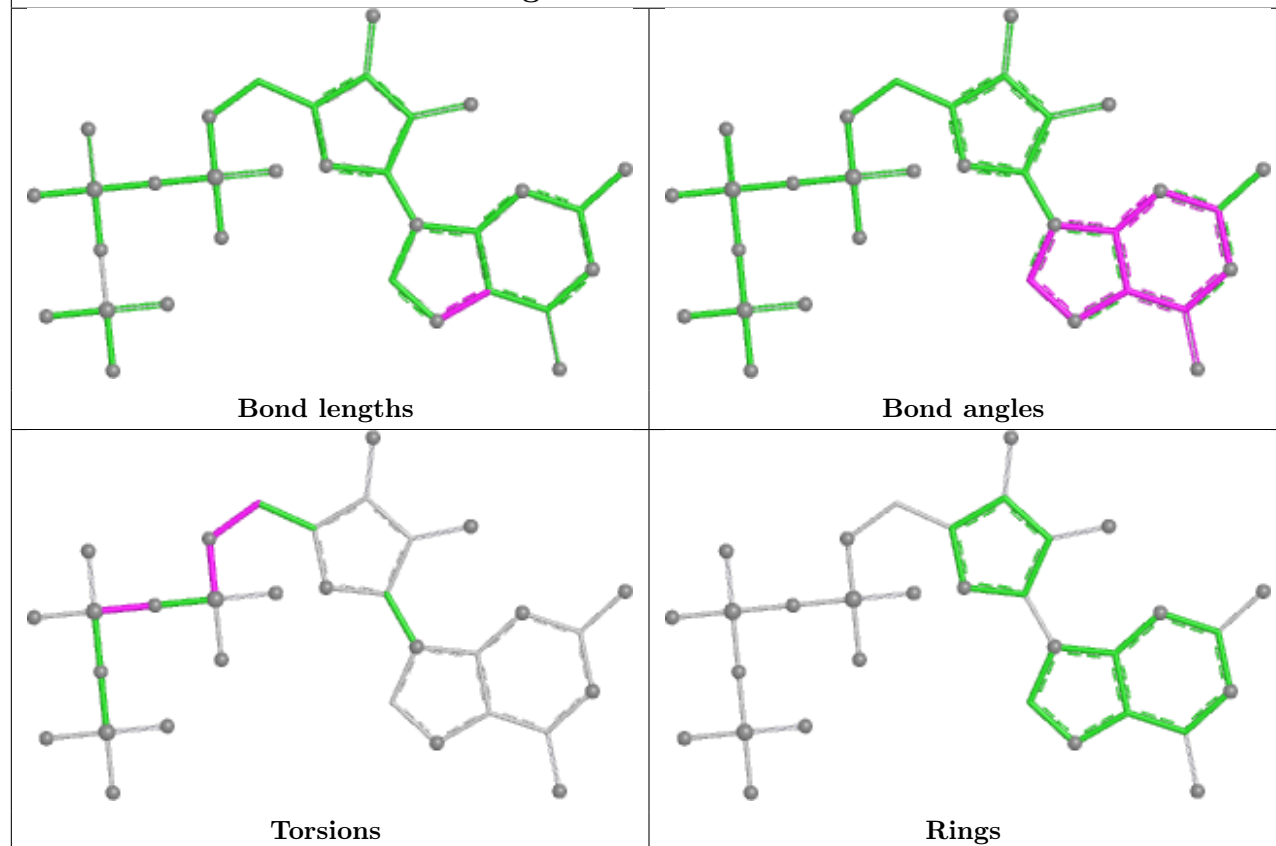
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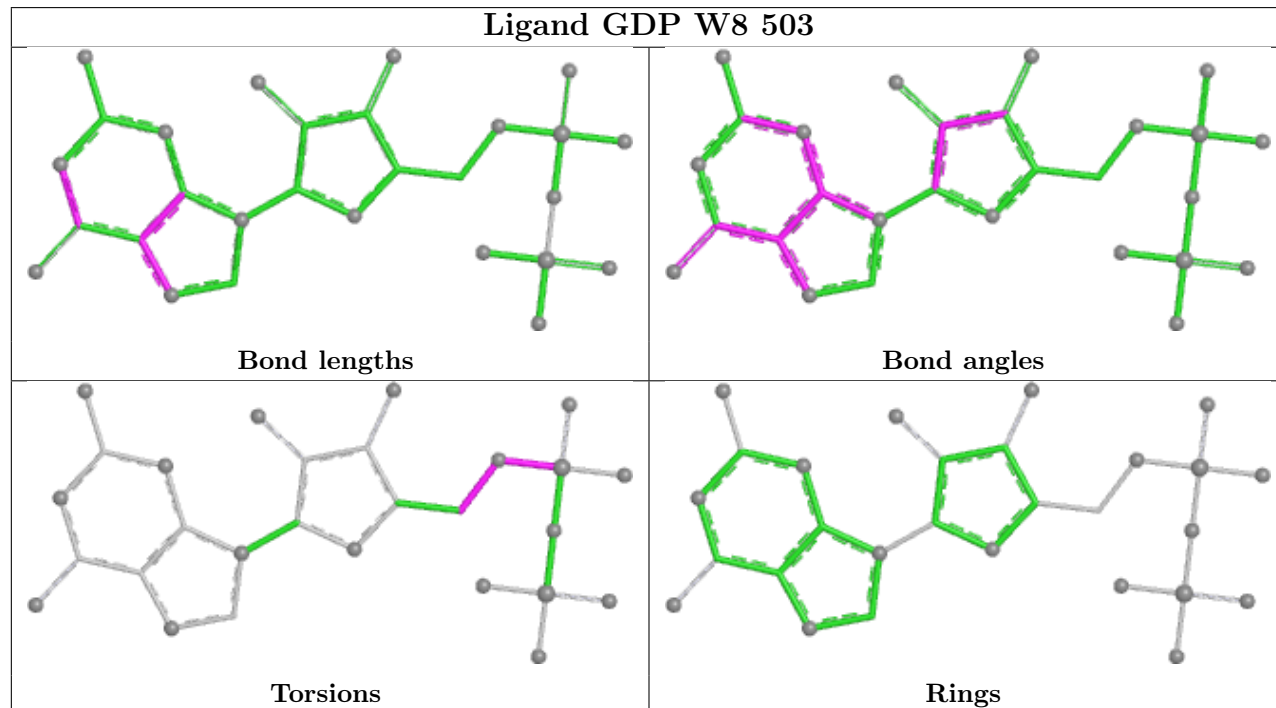
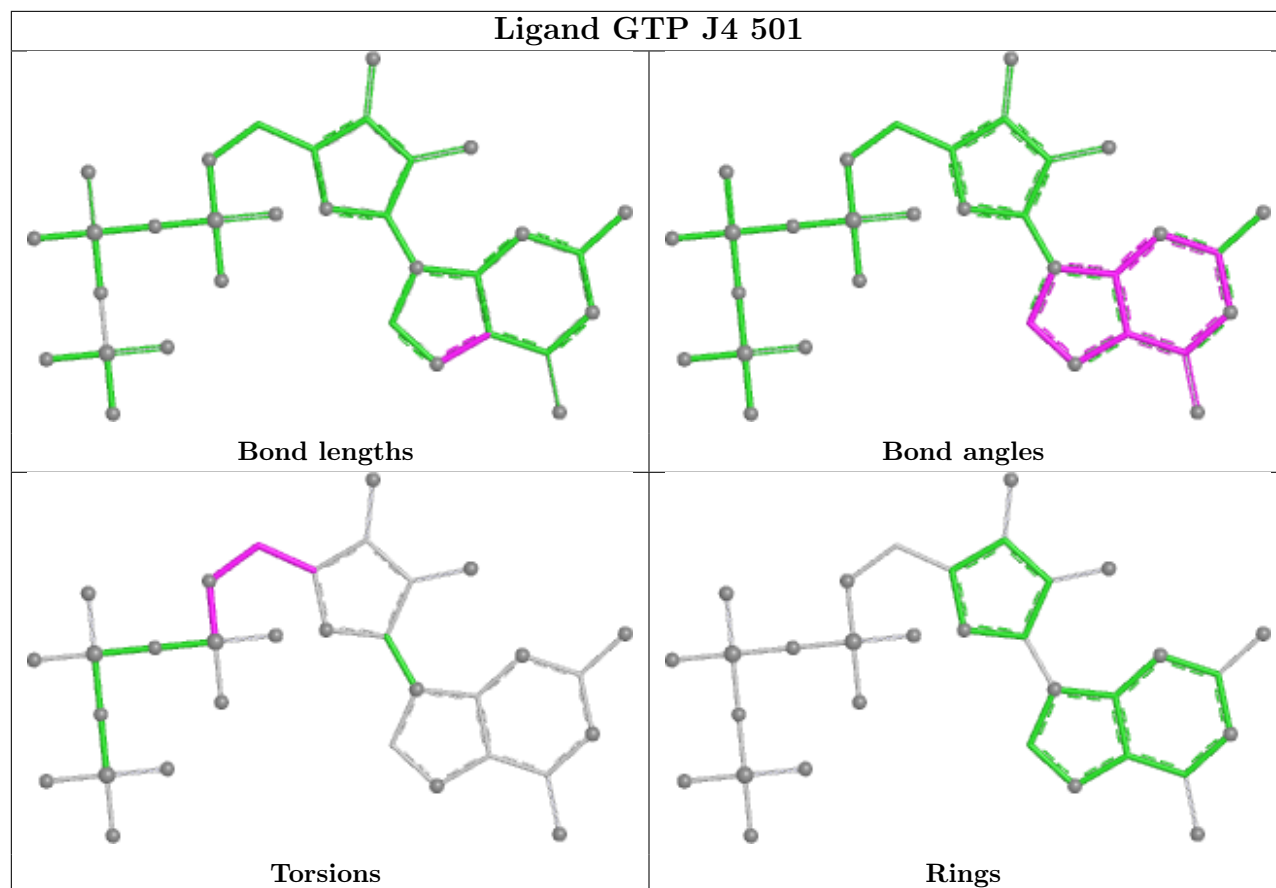


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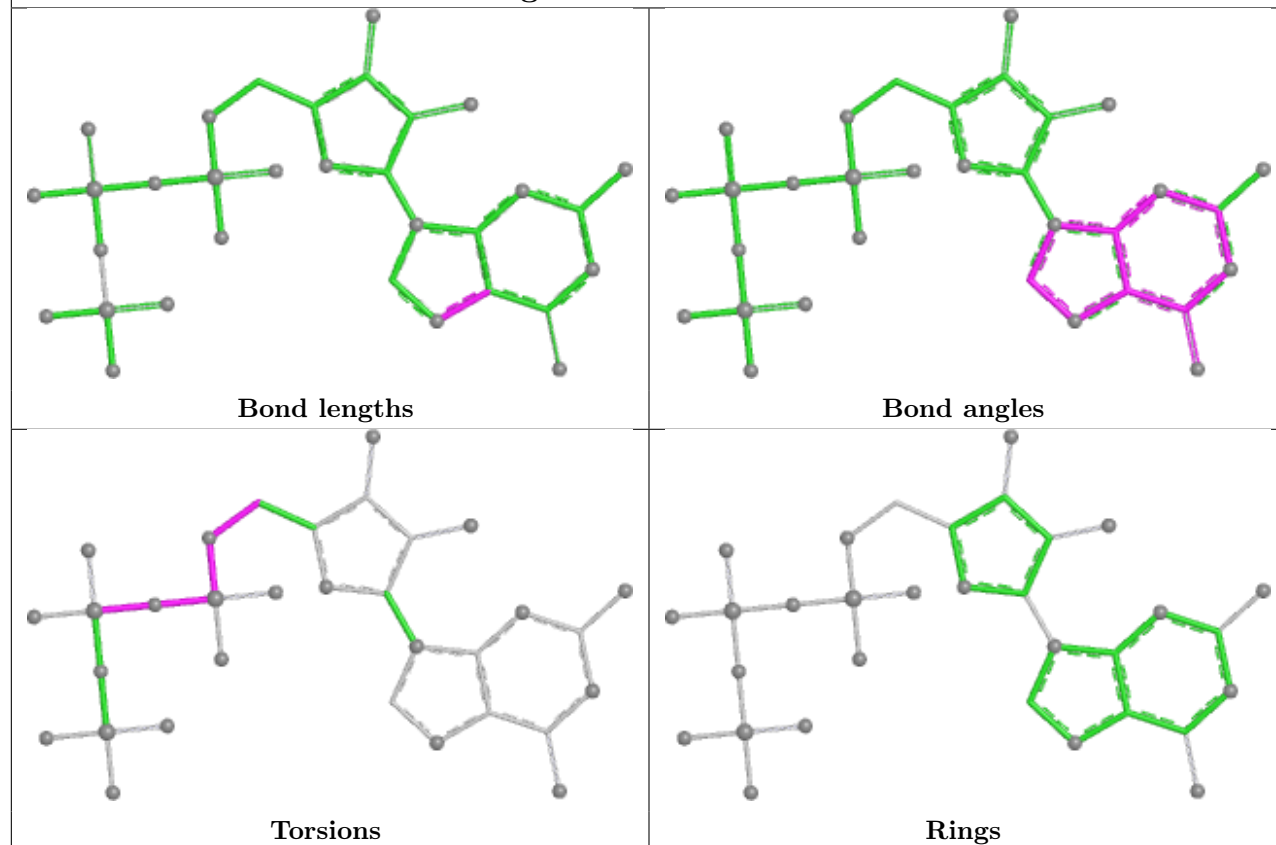


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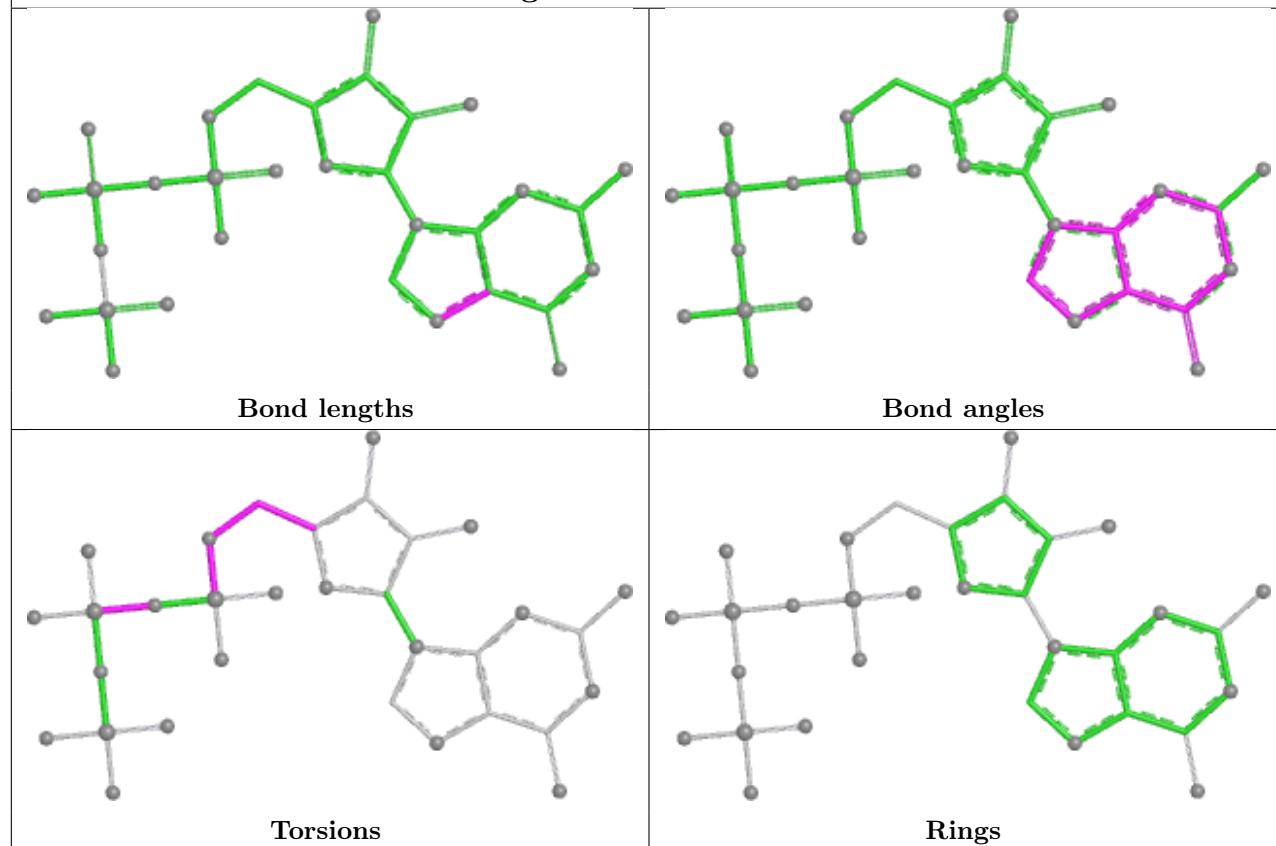


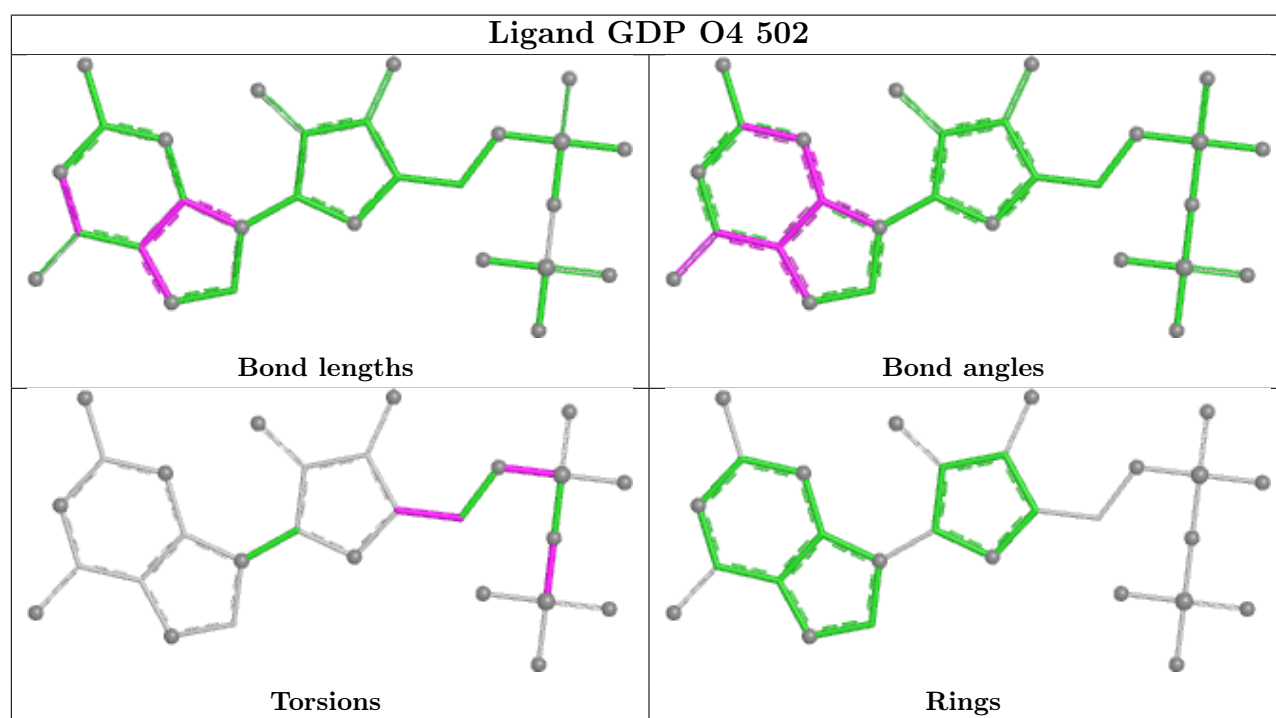
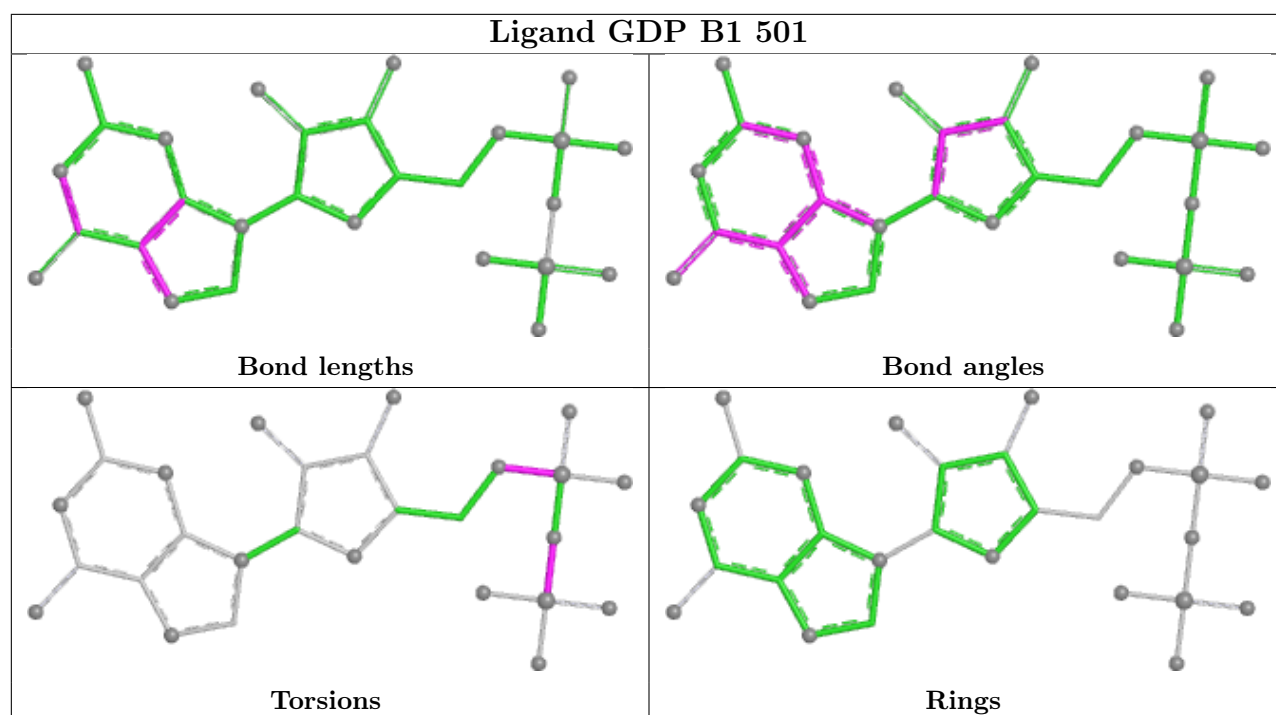


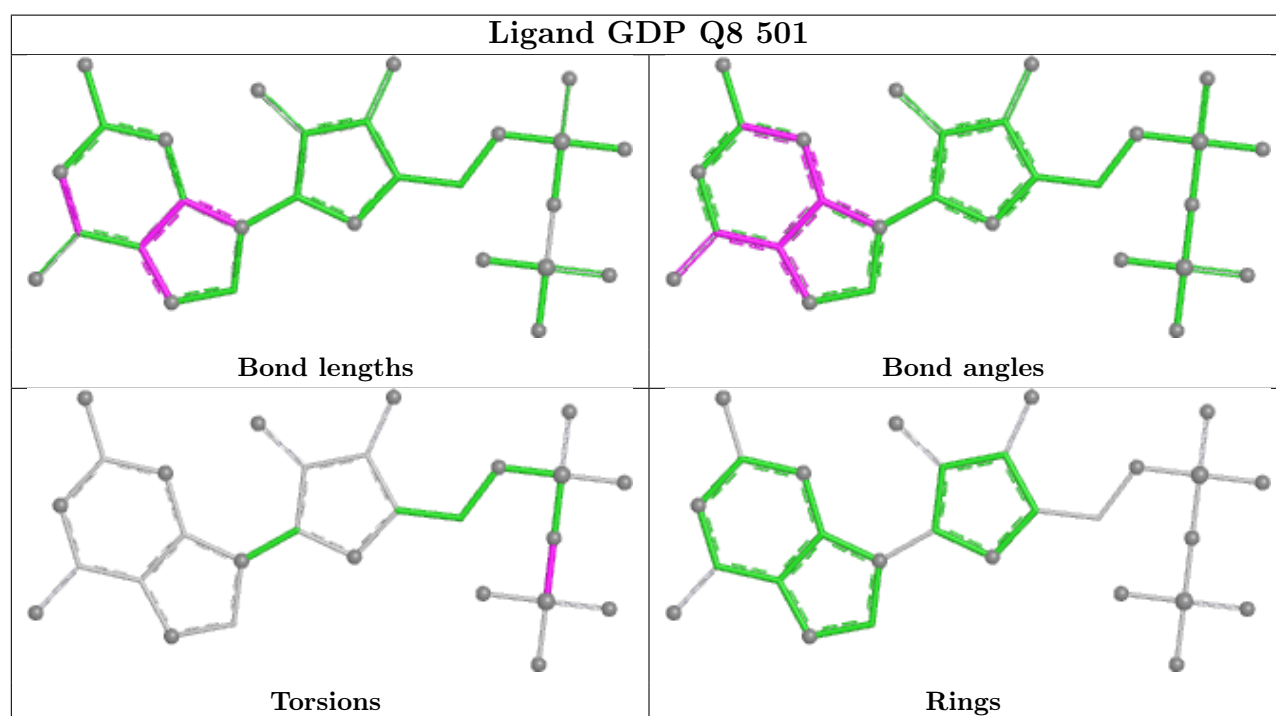
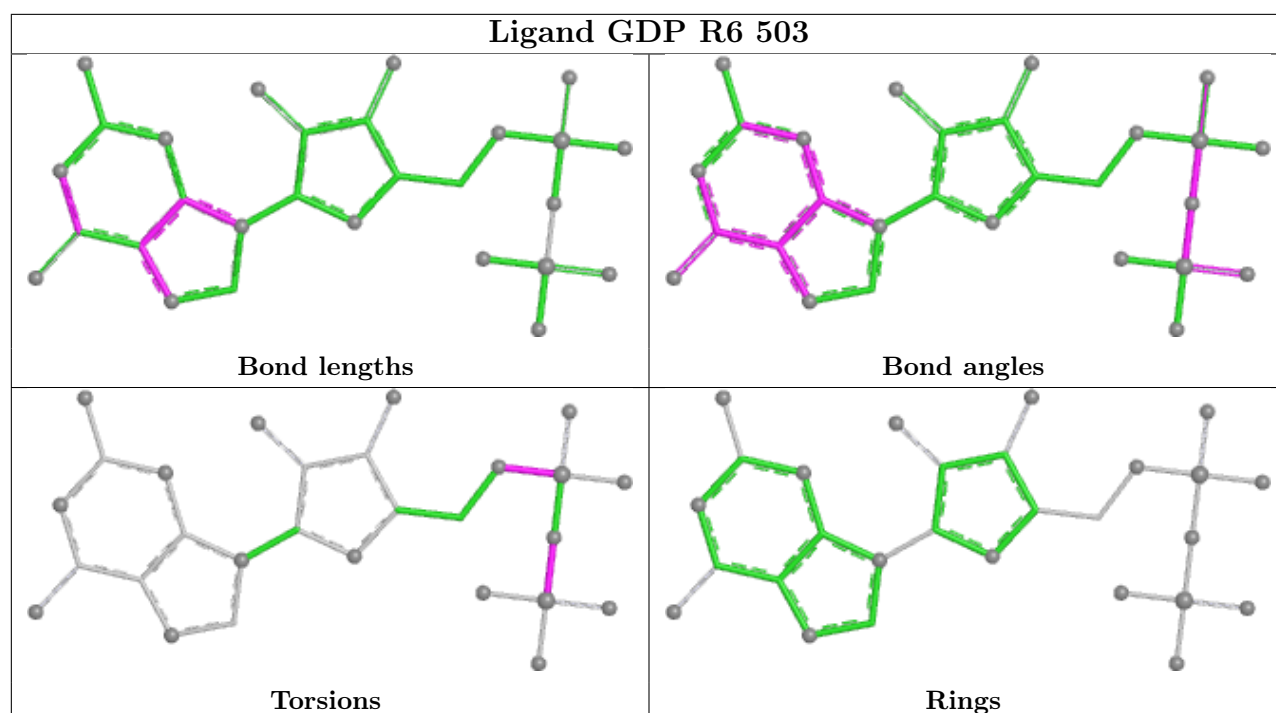
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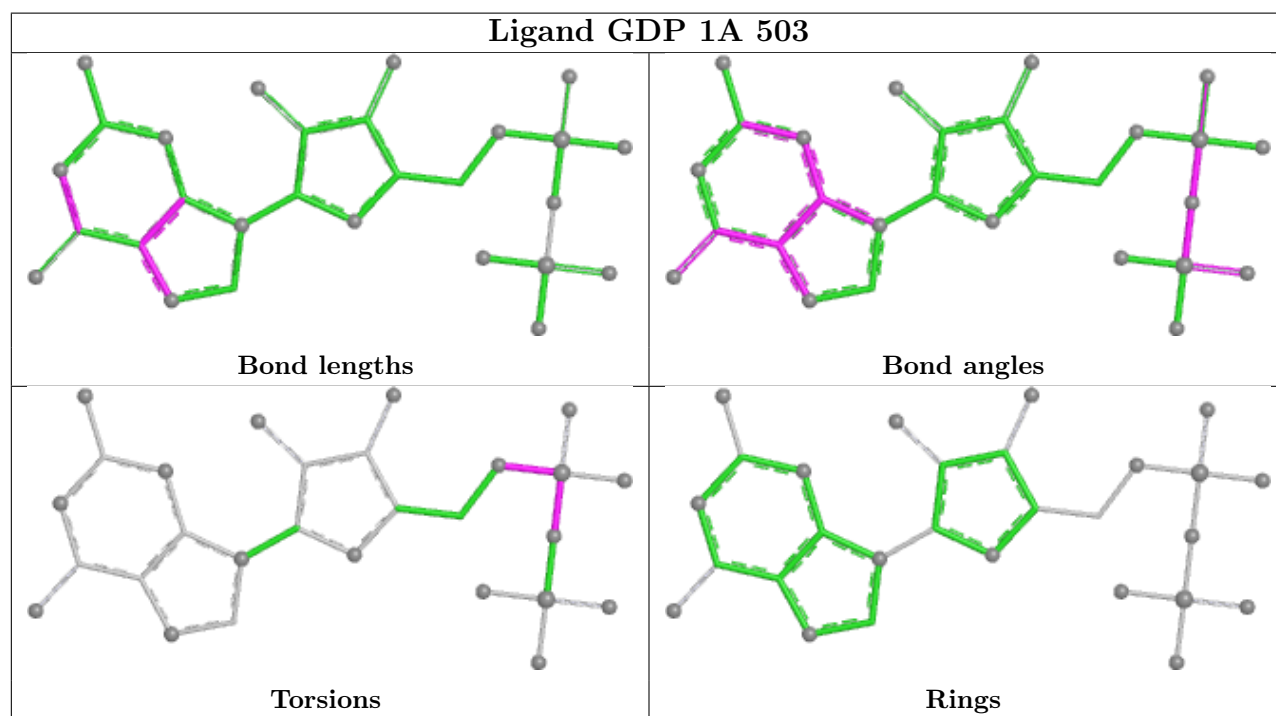
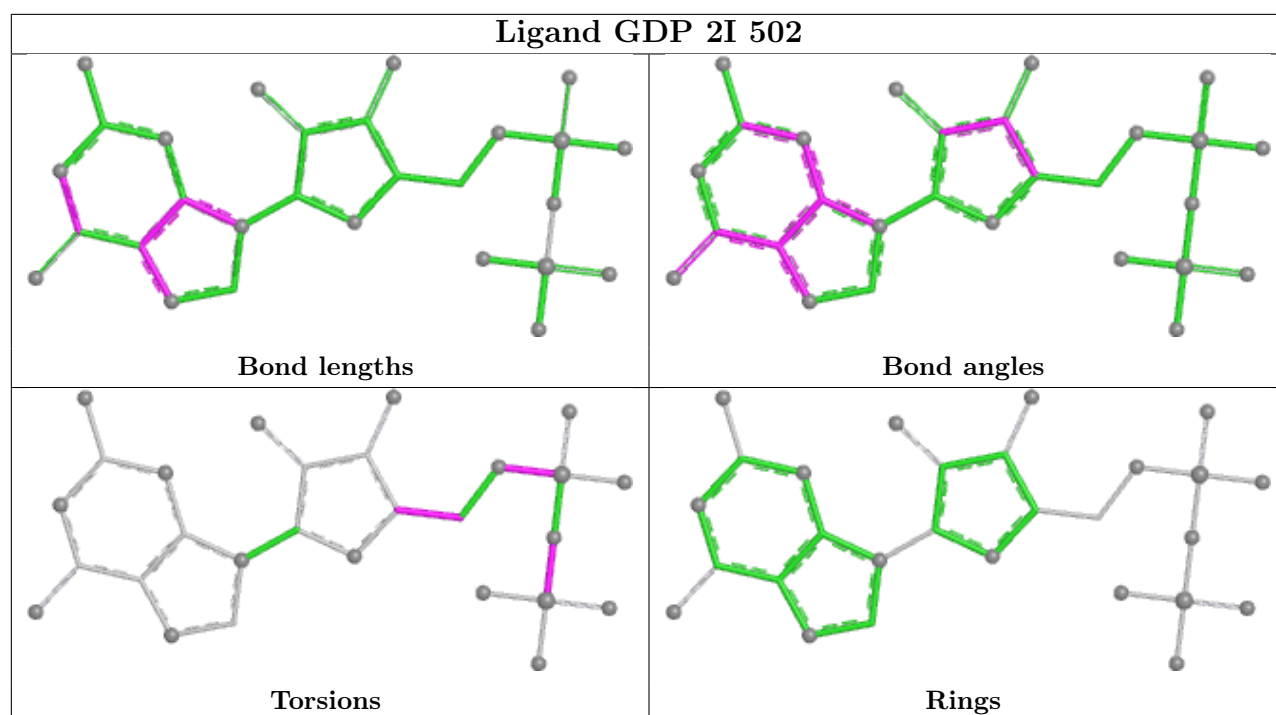


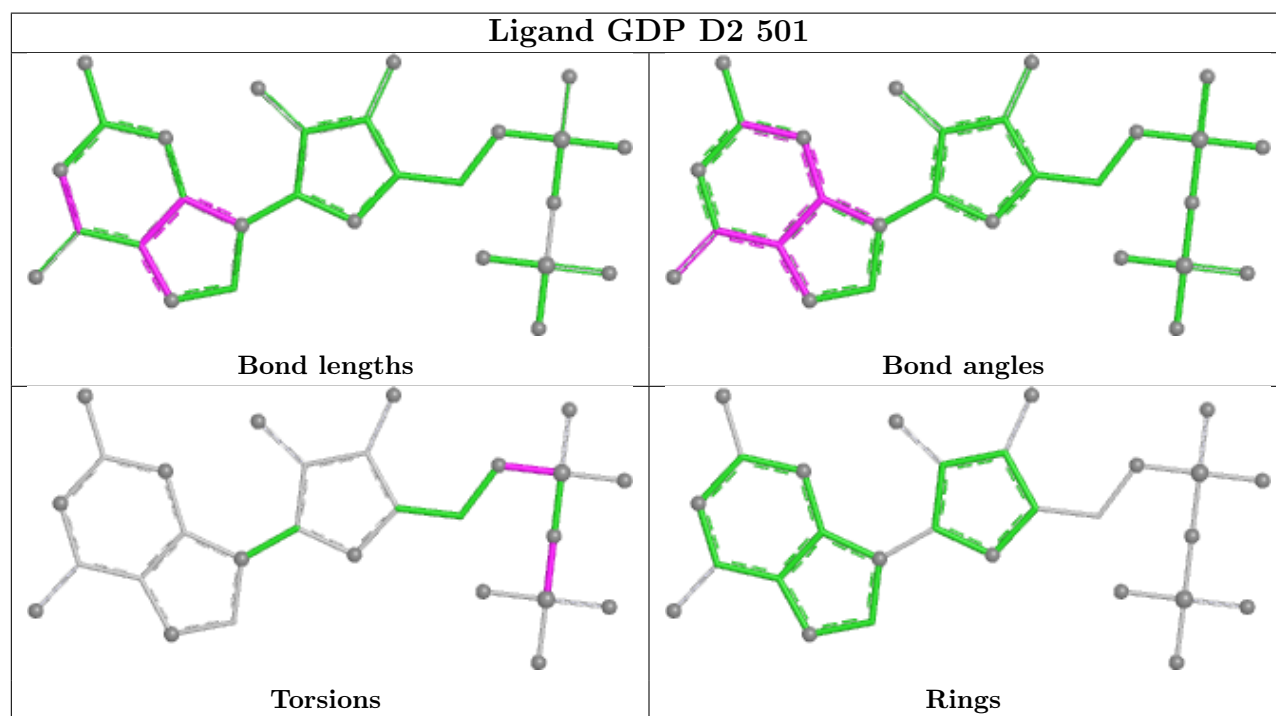
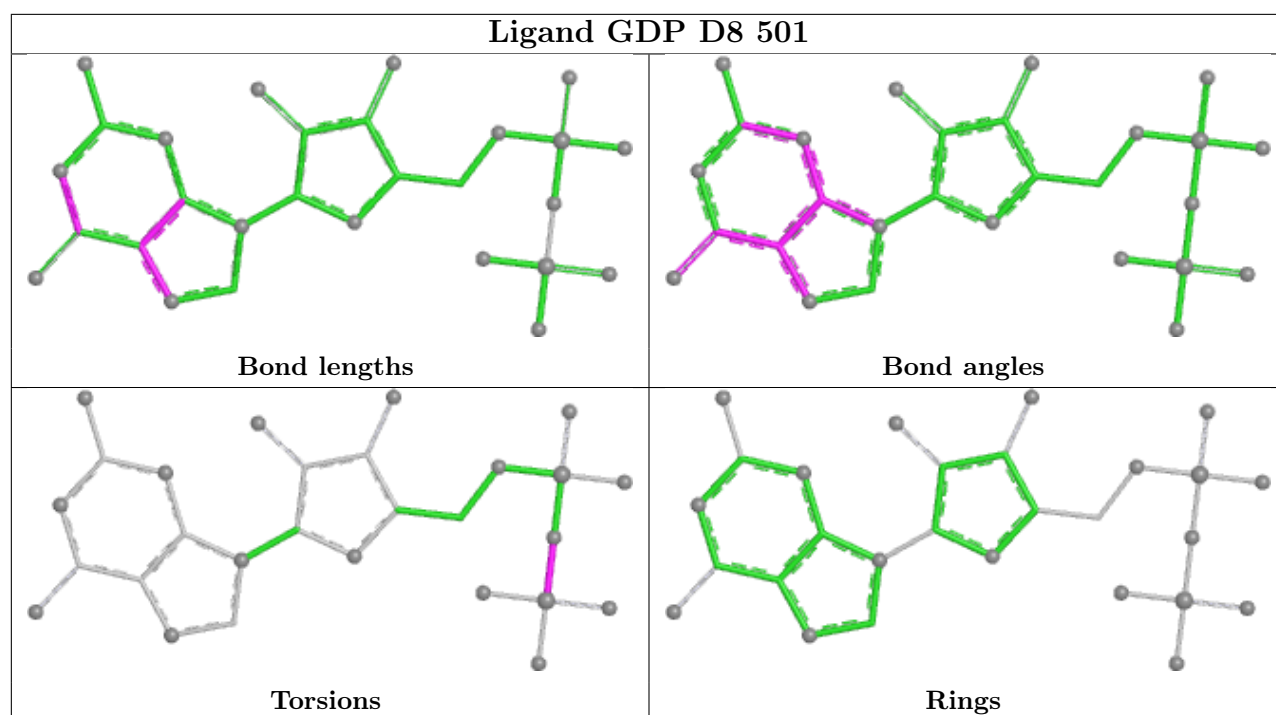
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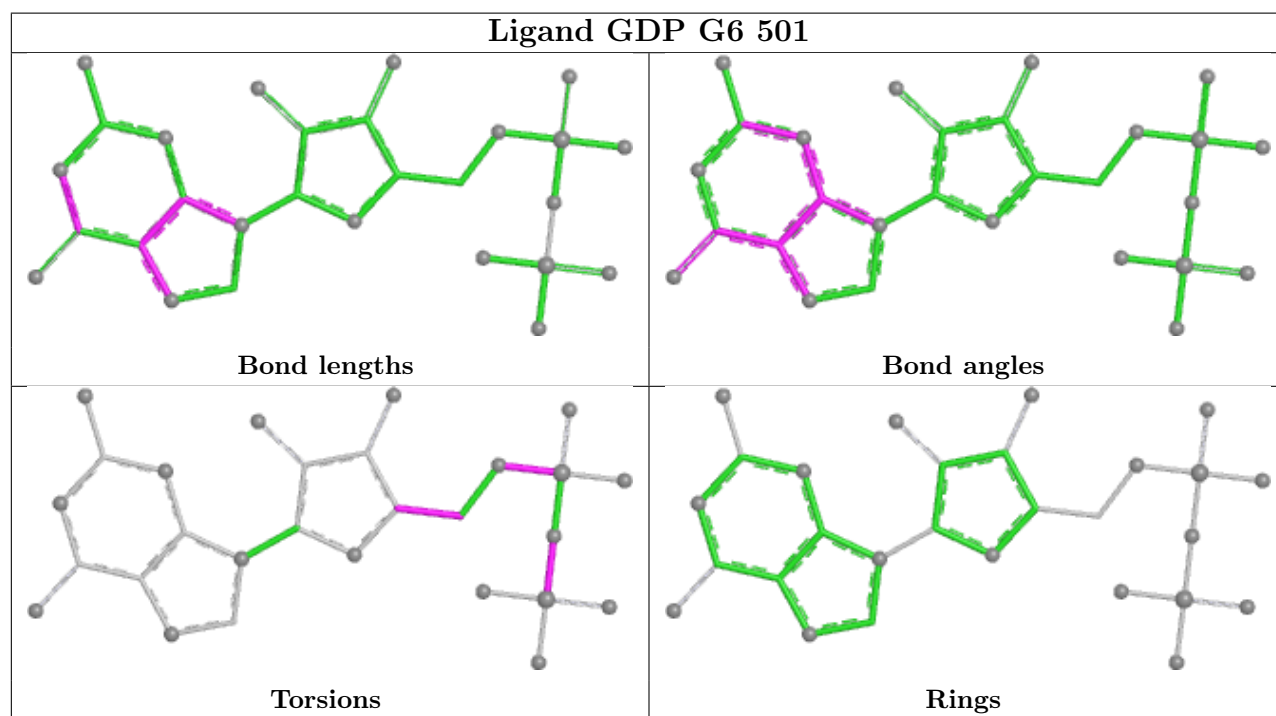
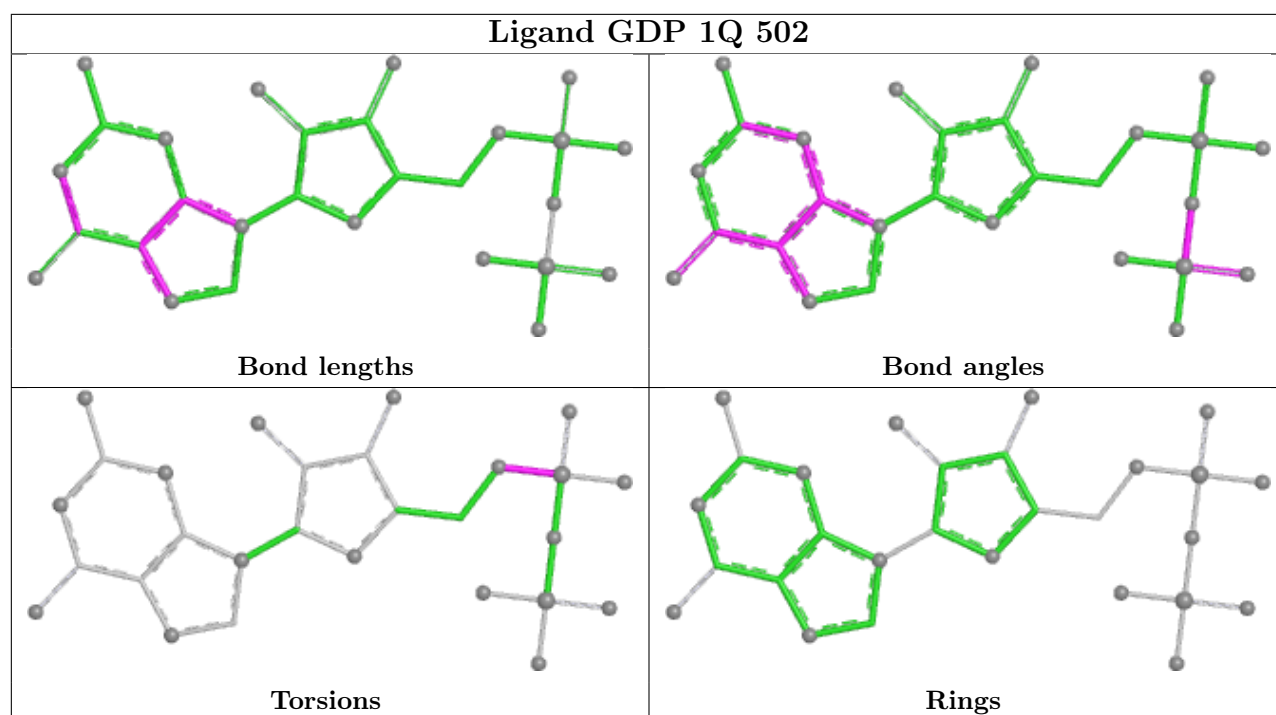


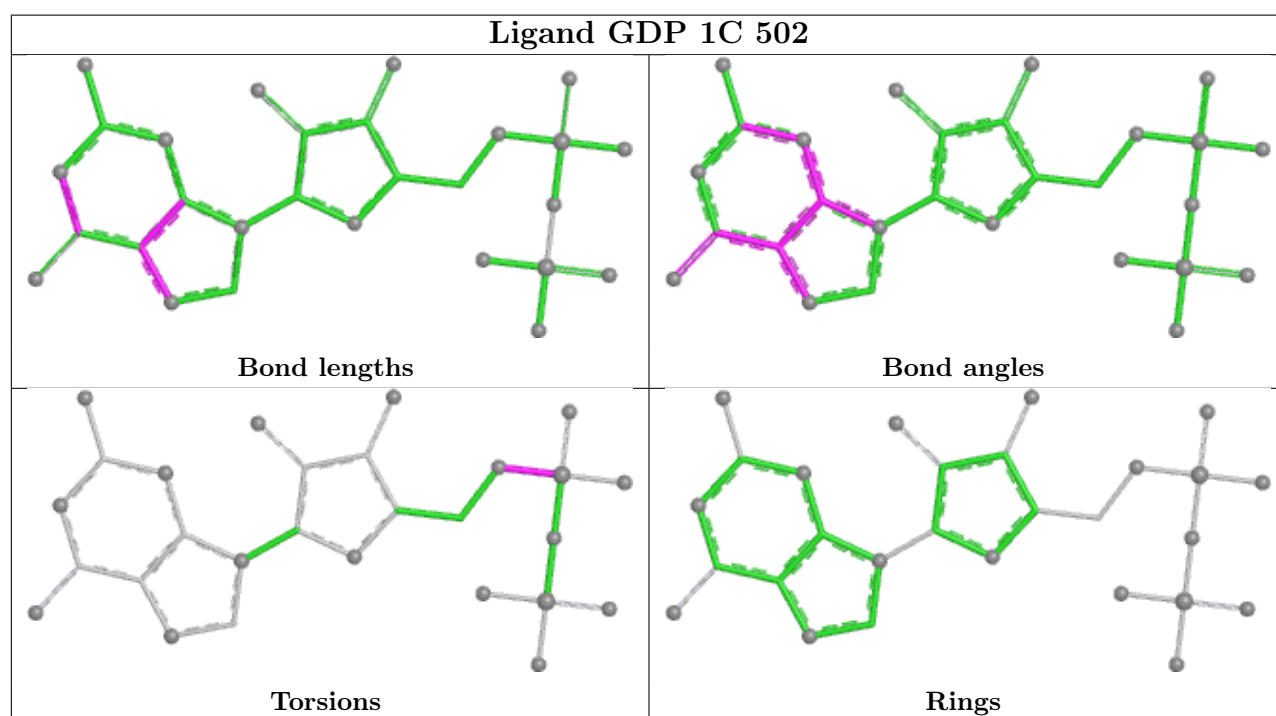
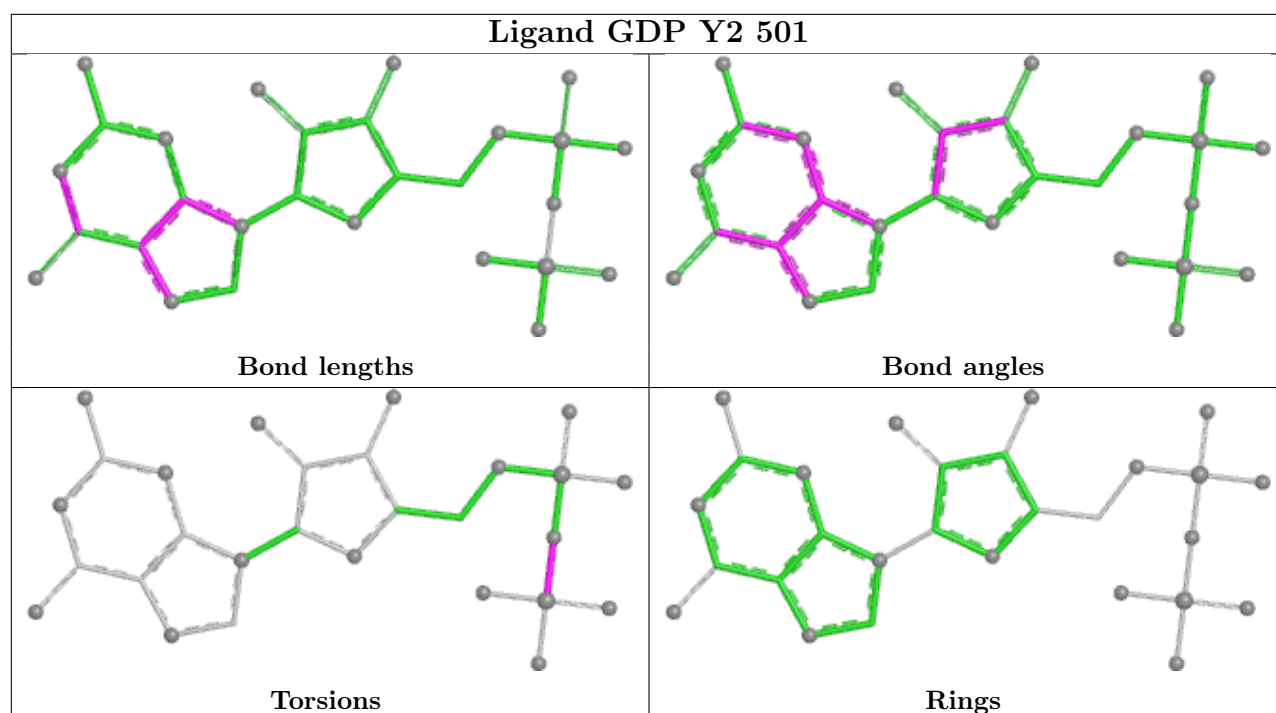


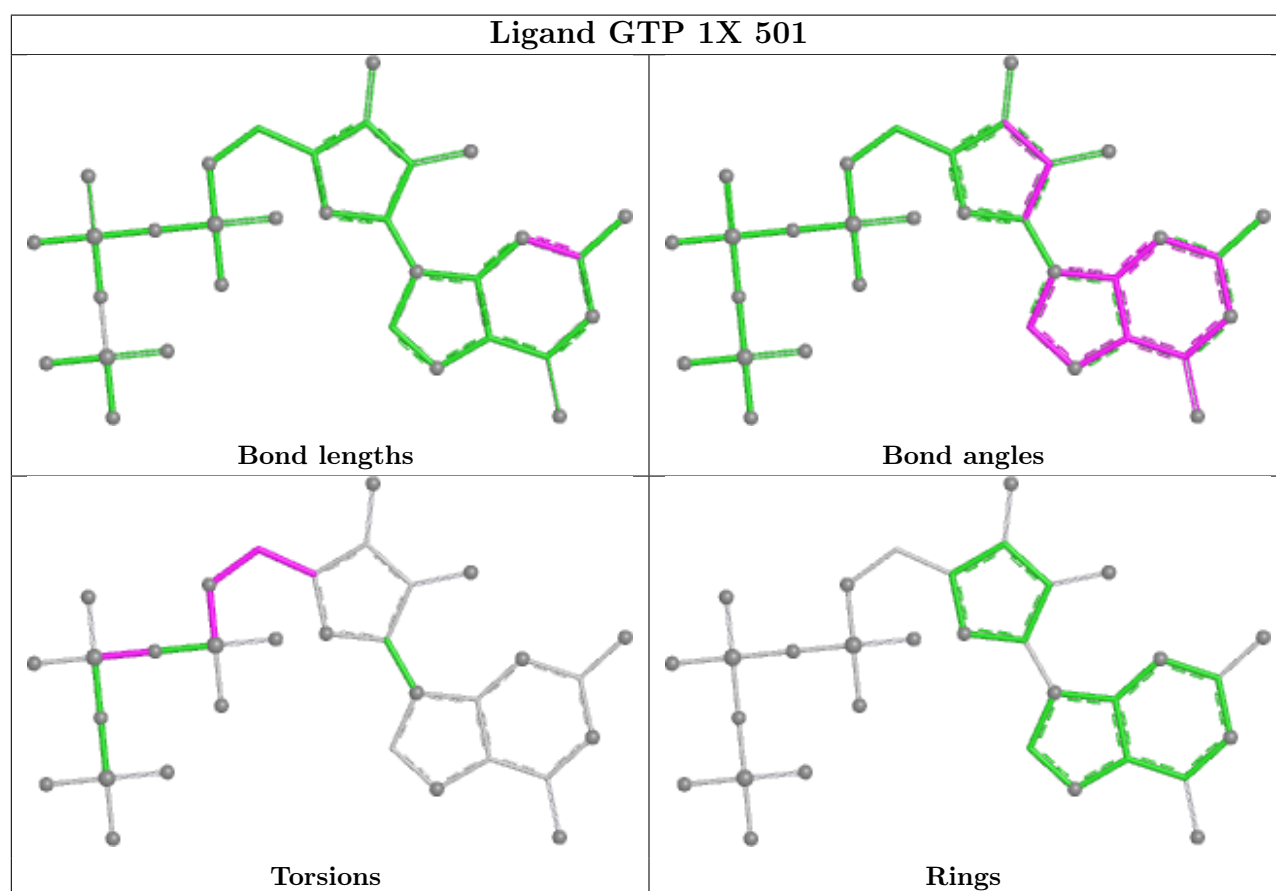
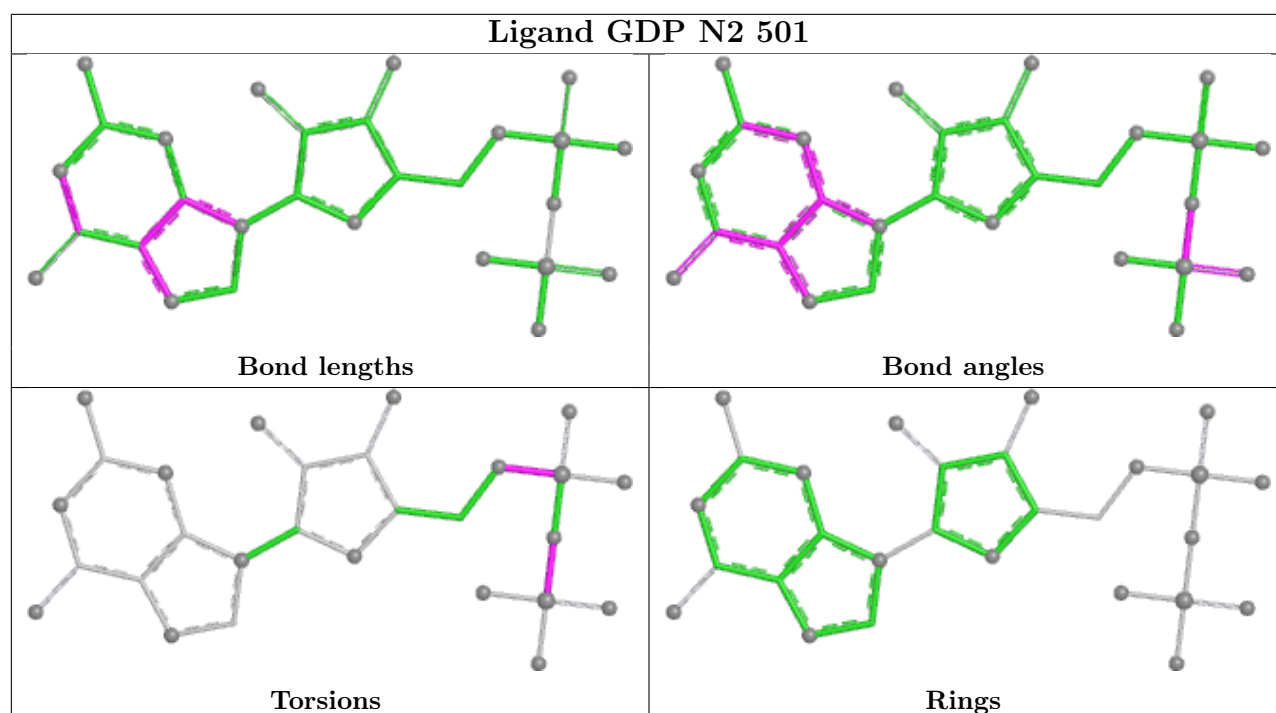


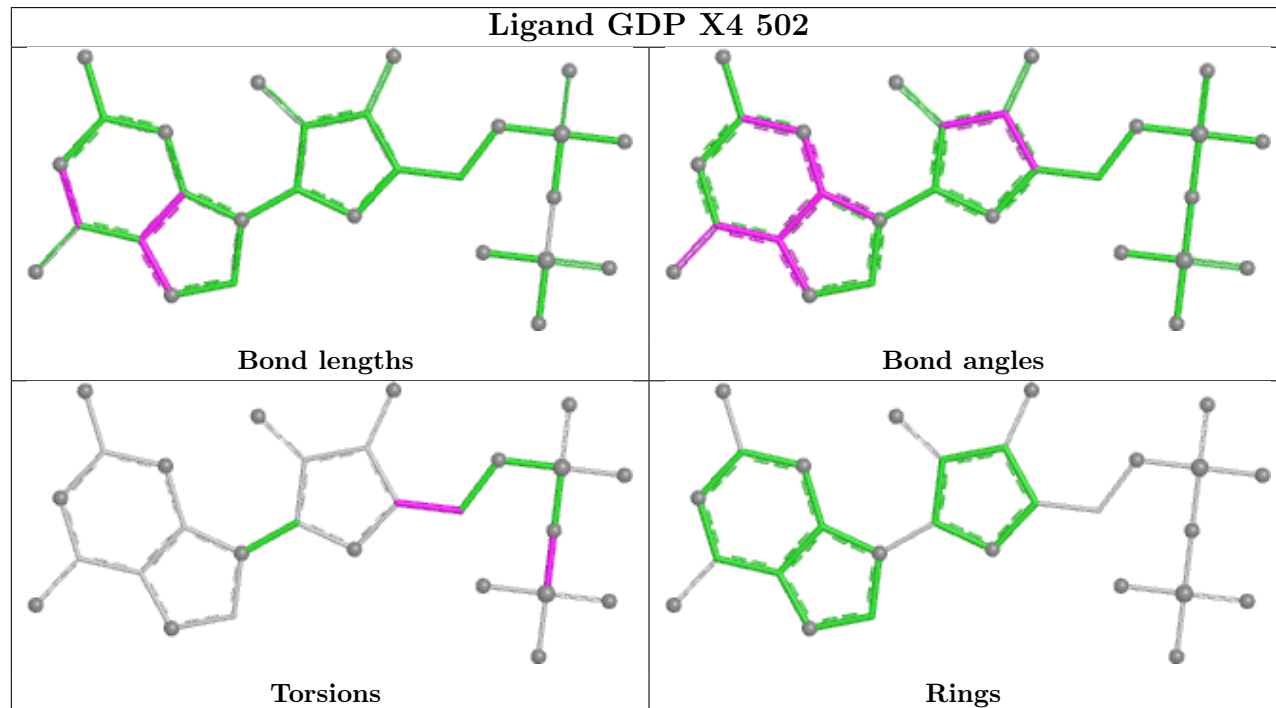
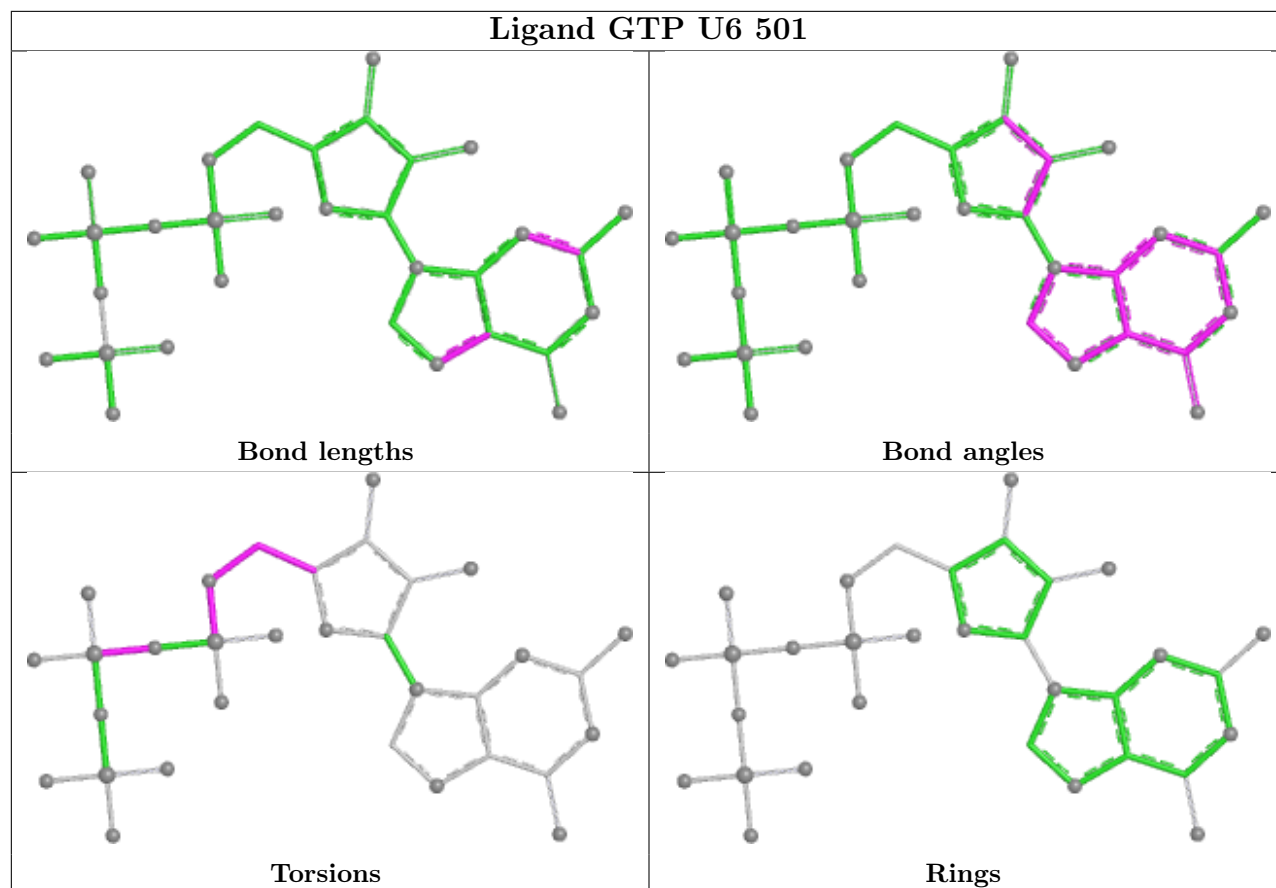


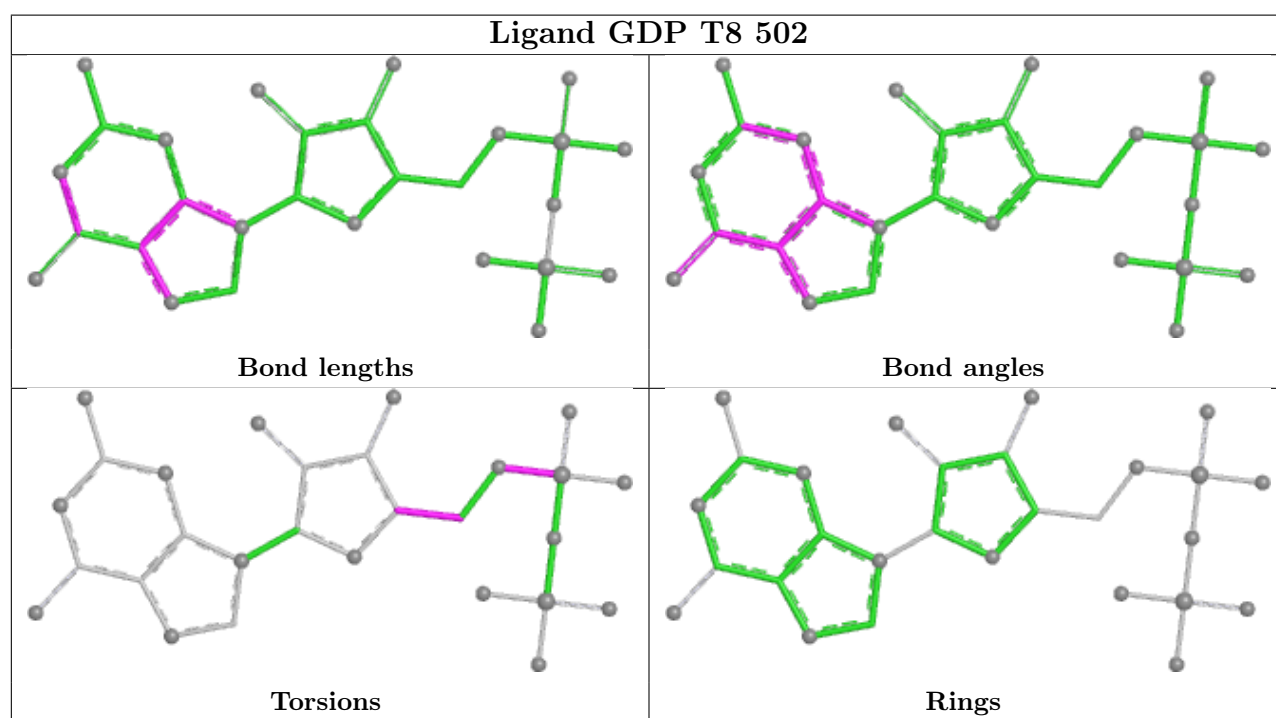
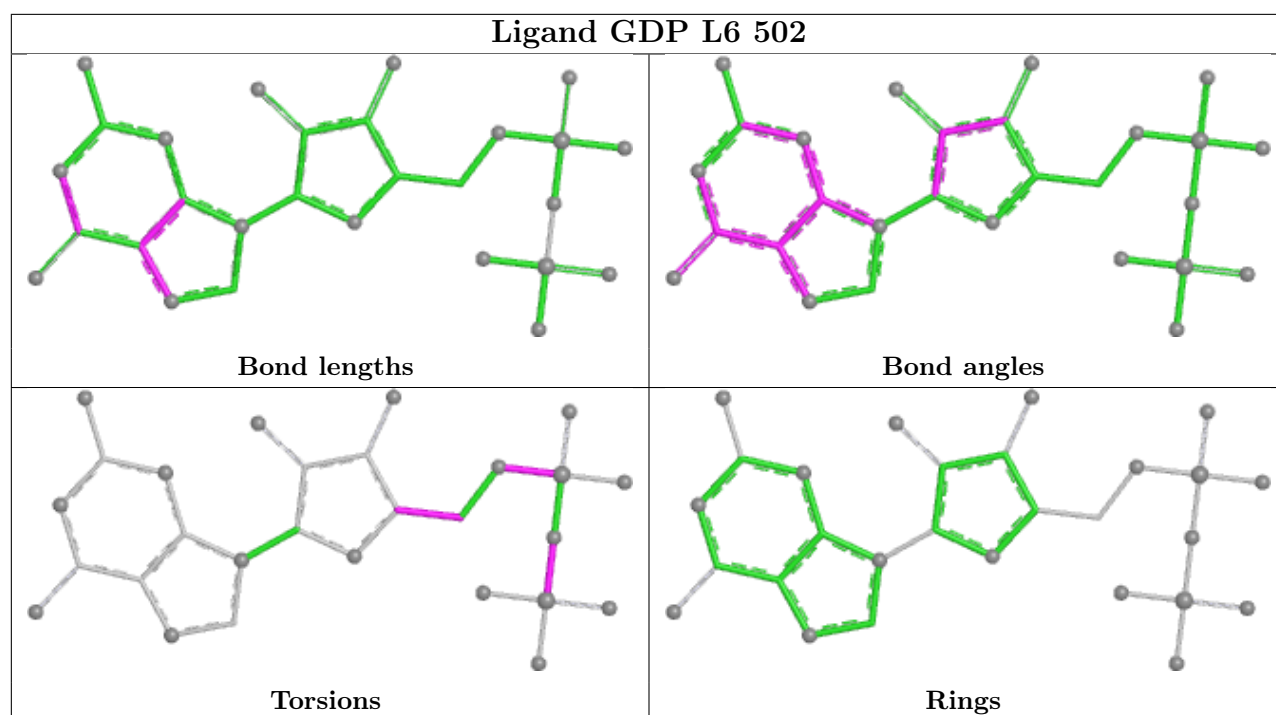


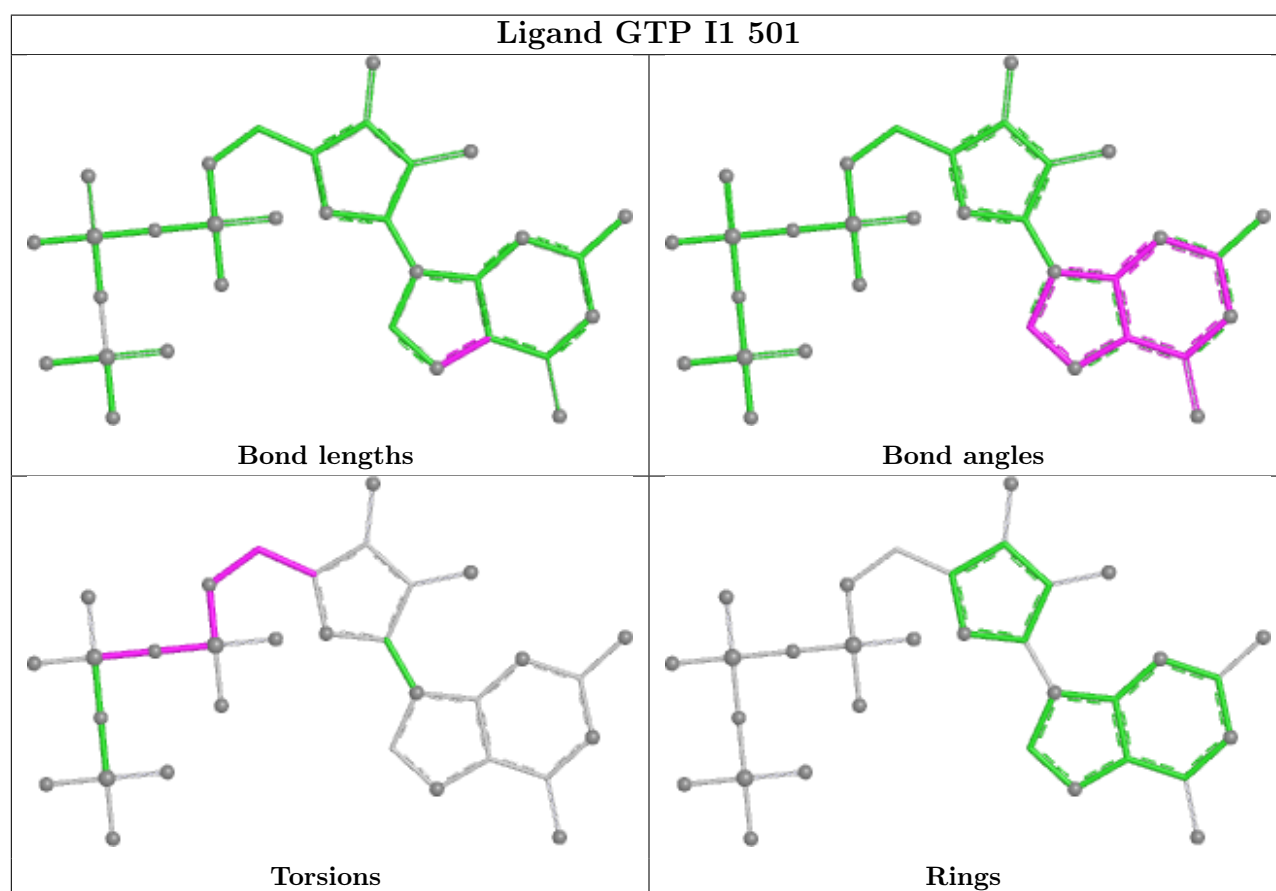
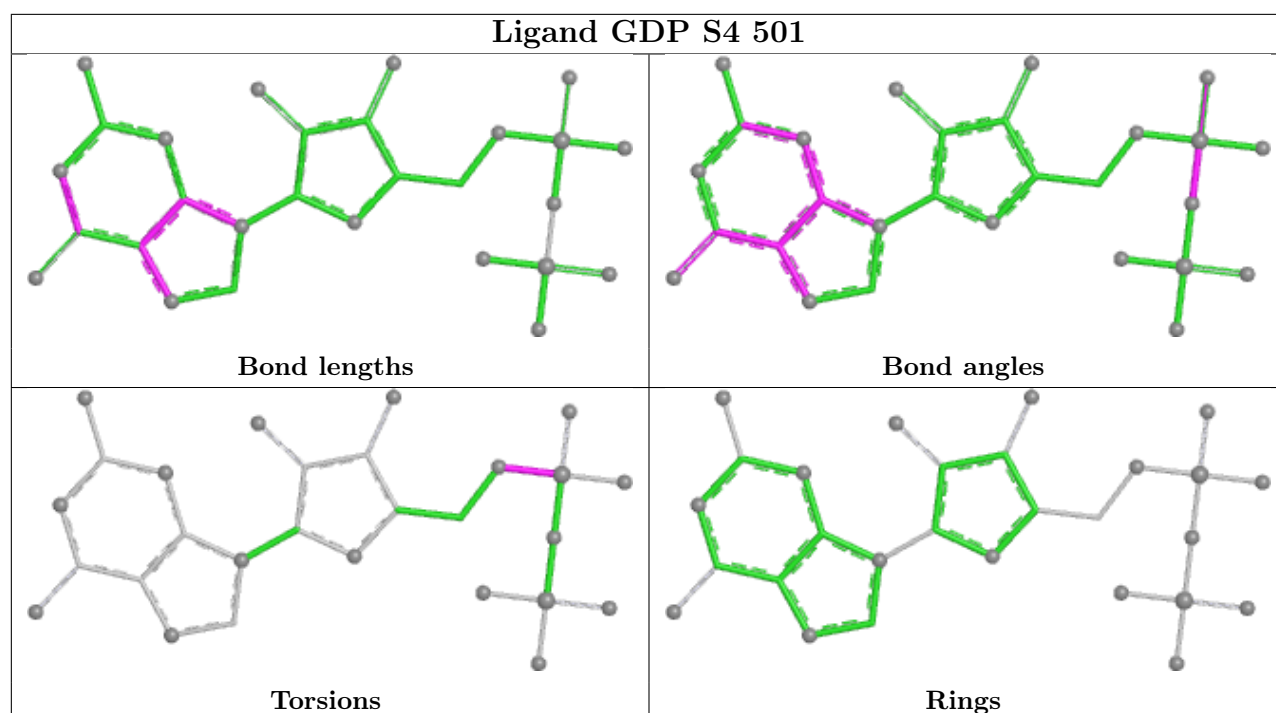




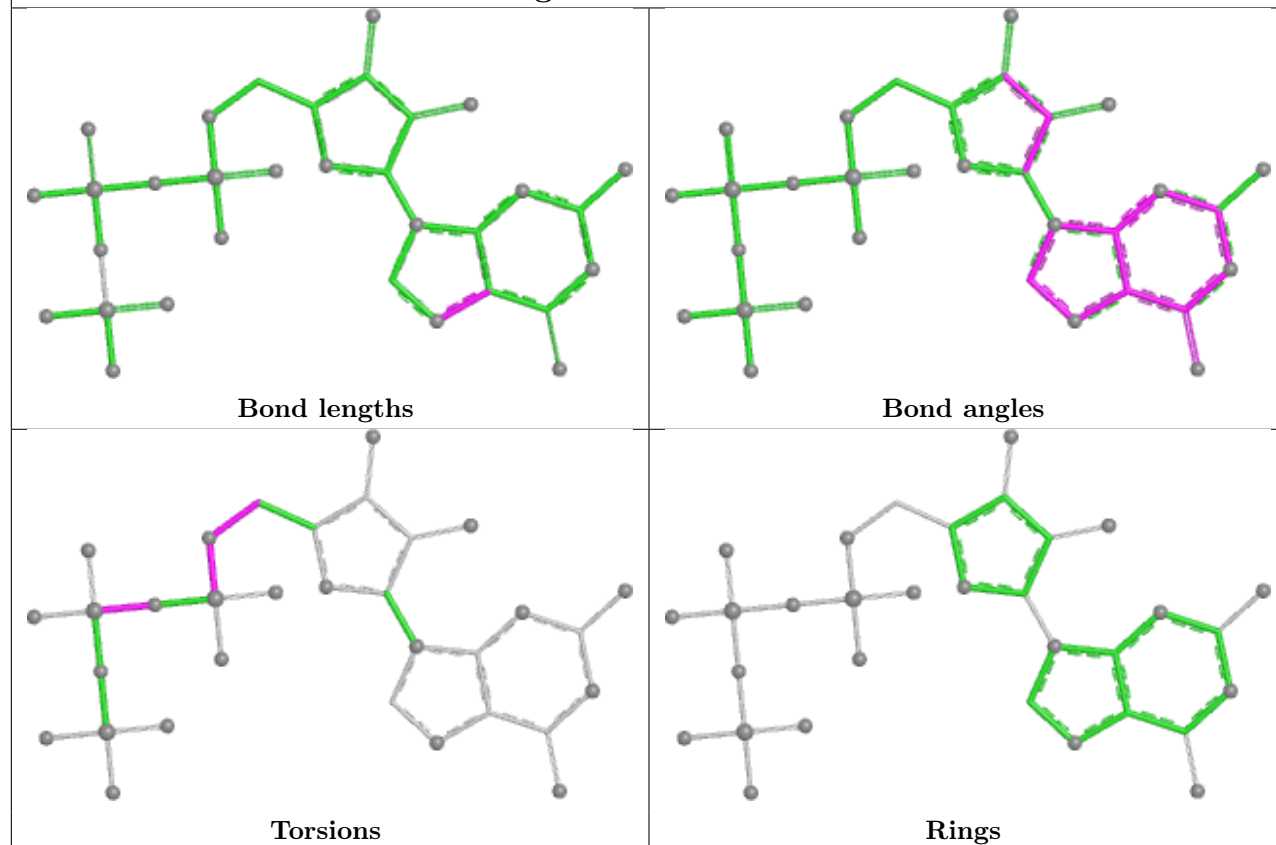




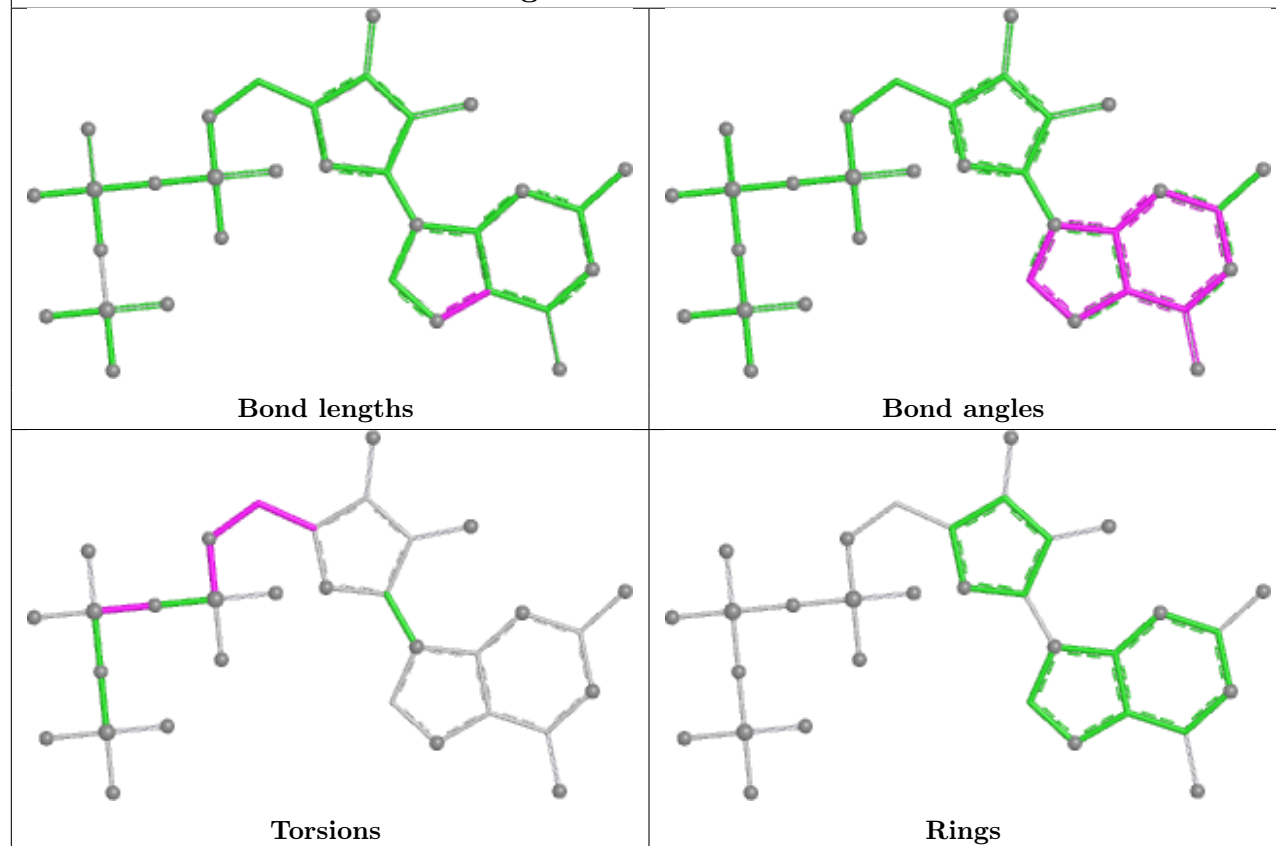


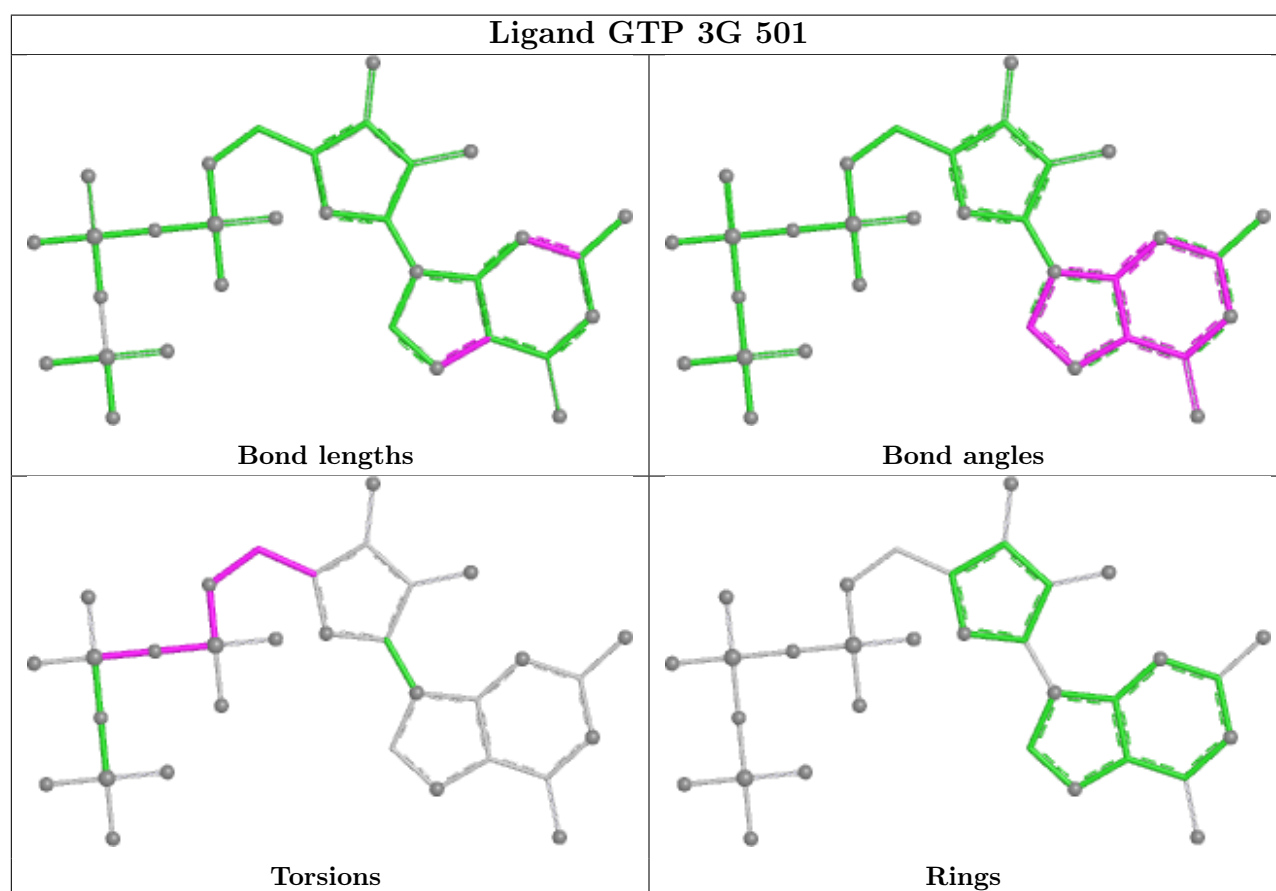
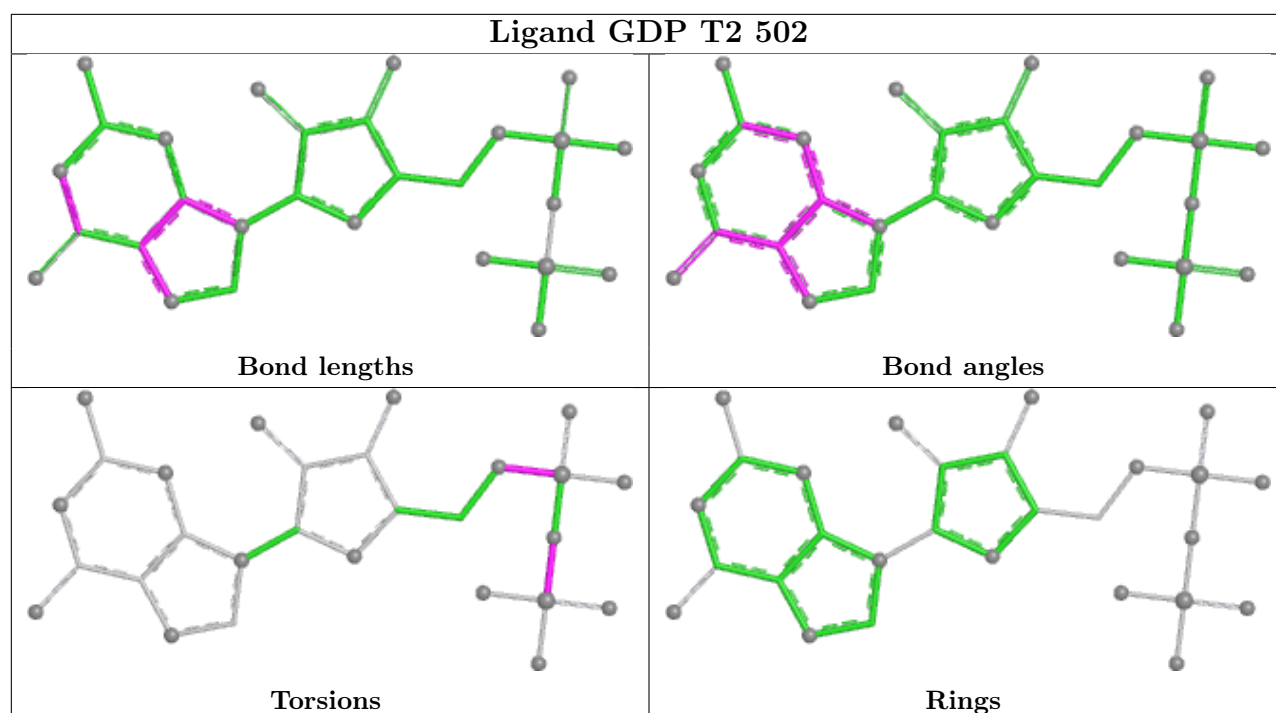


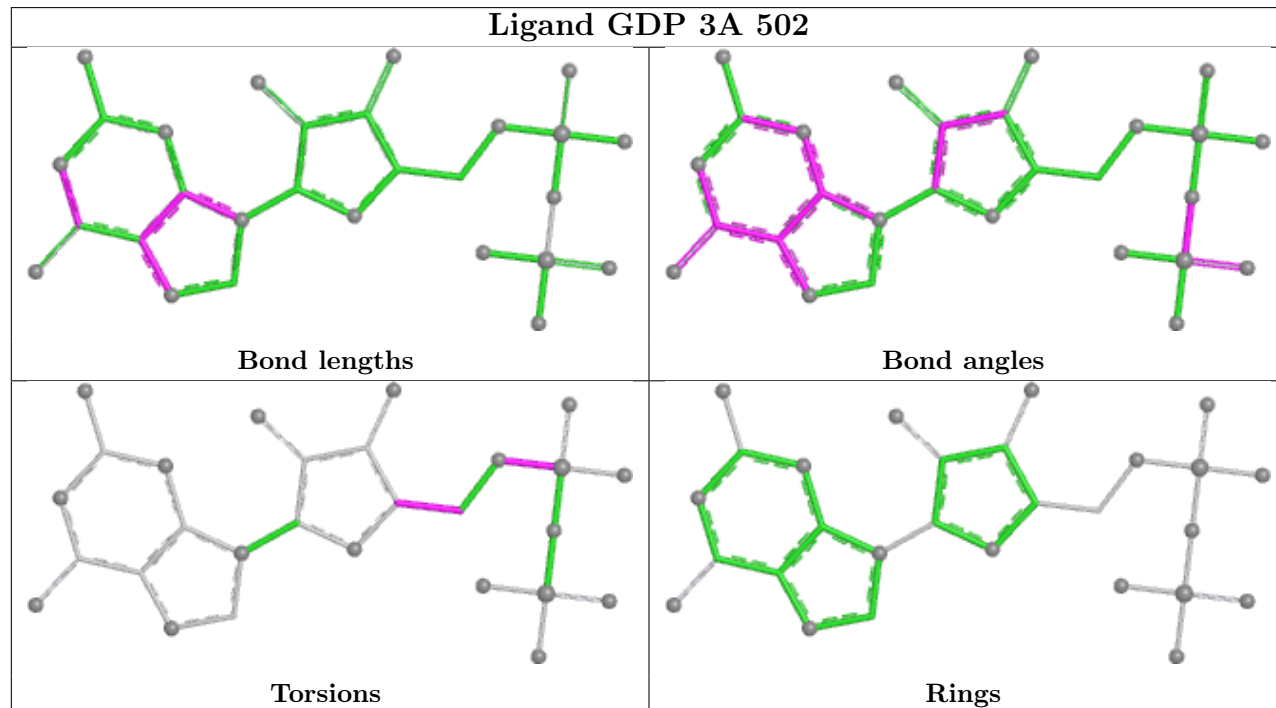
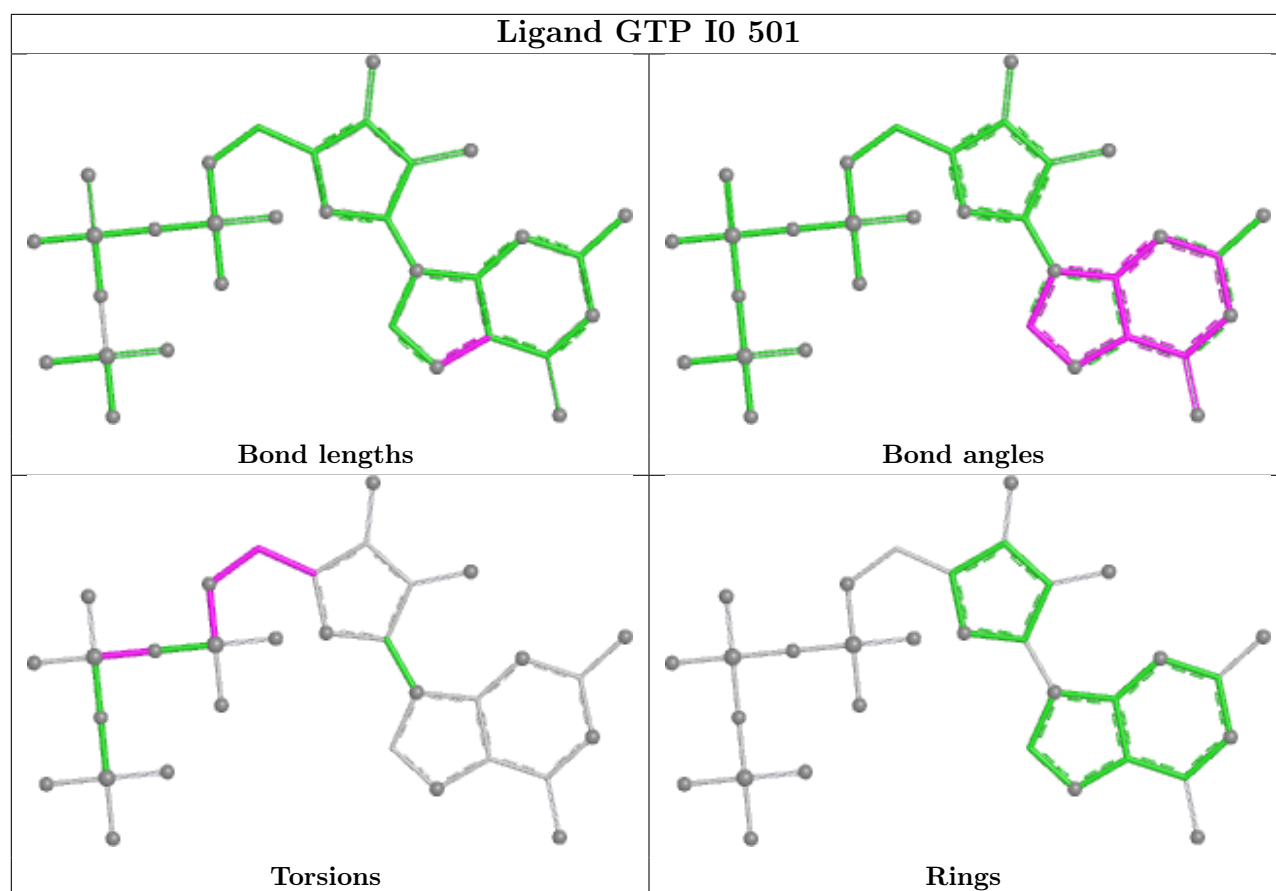
Ligand GTP 8 501

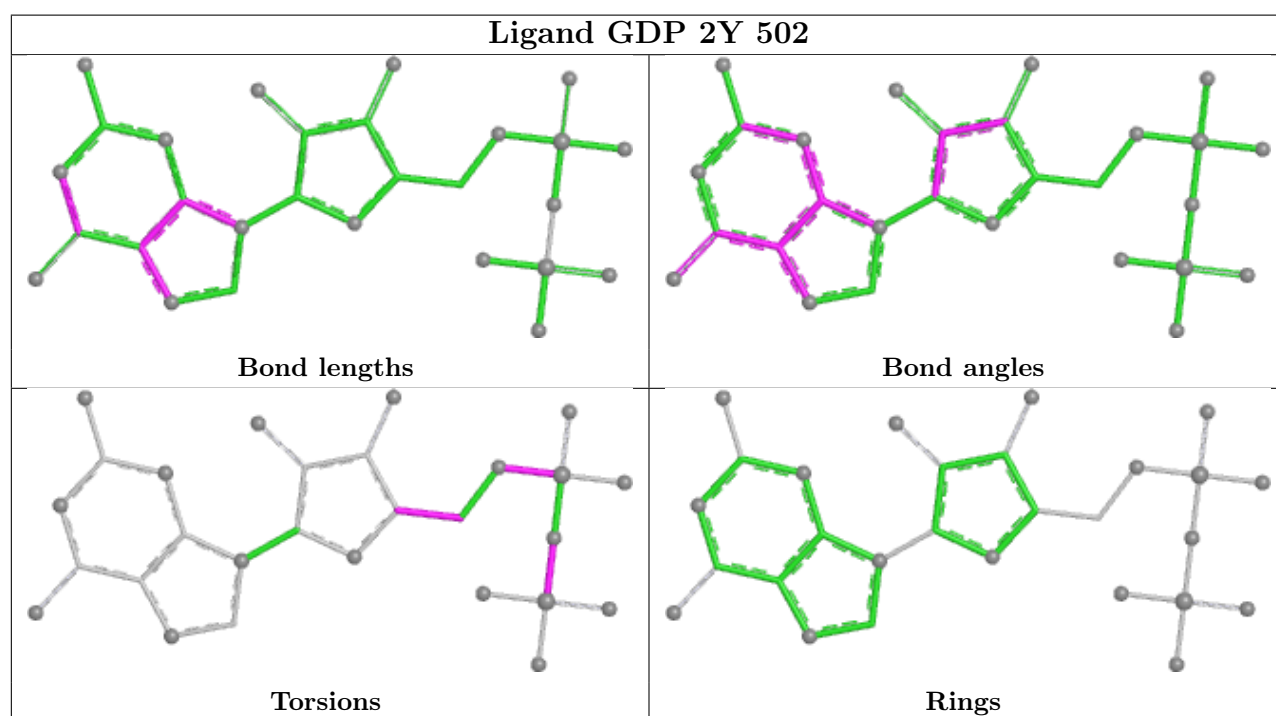
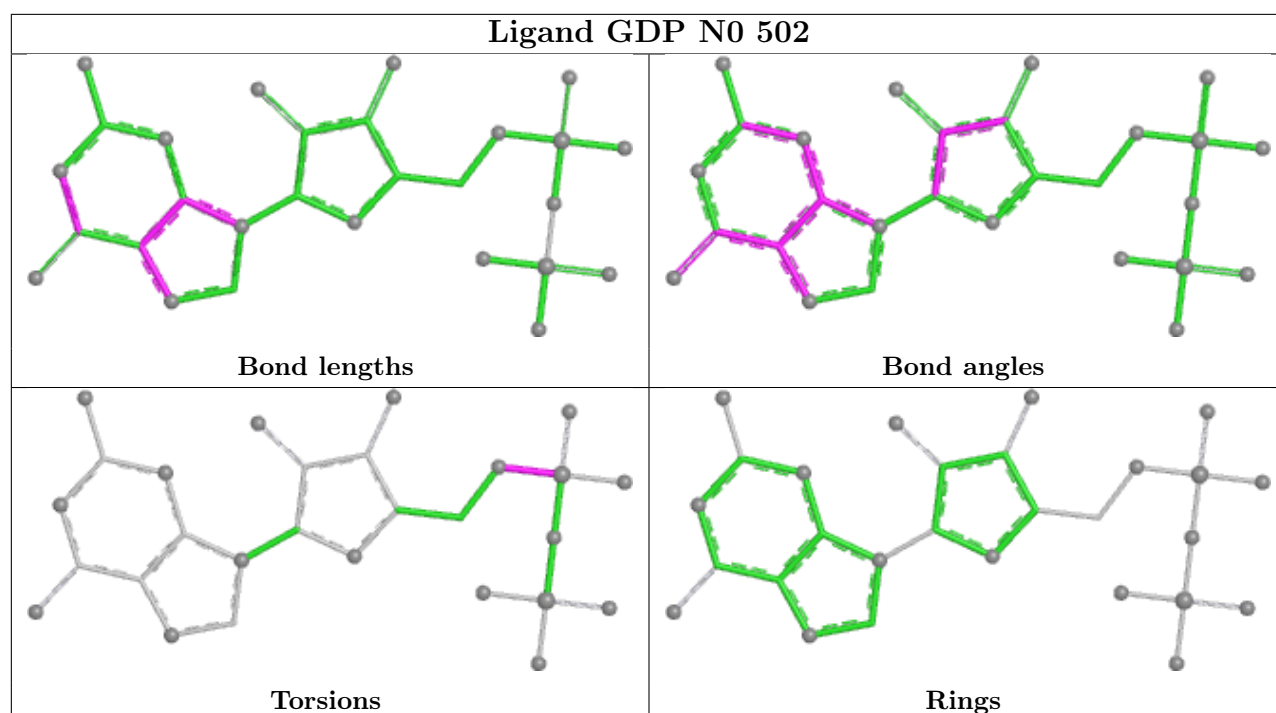


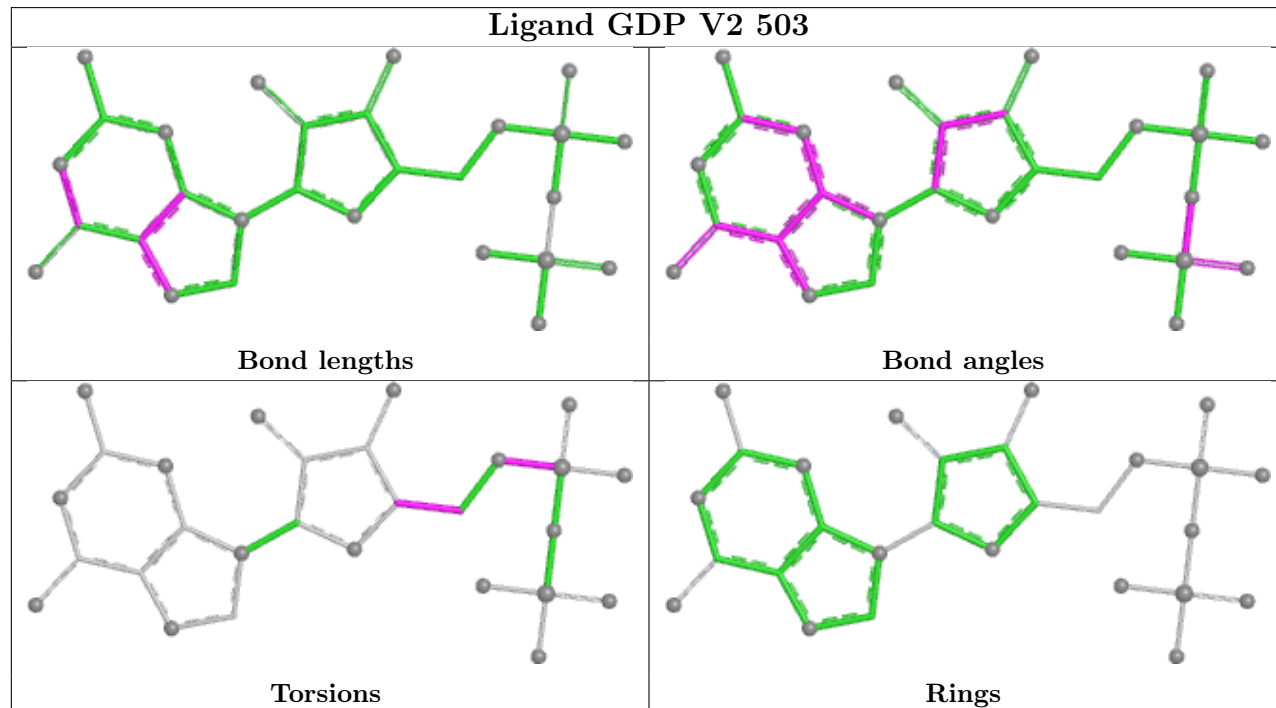
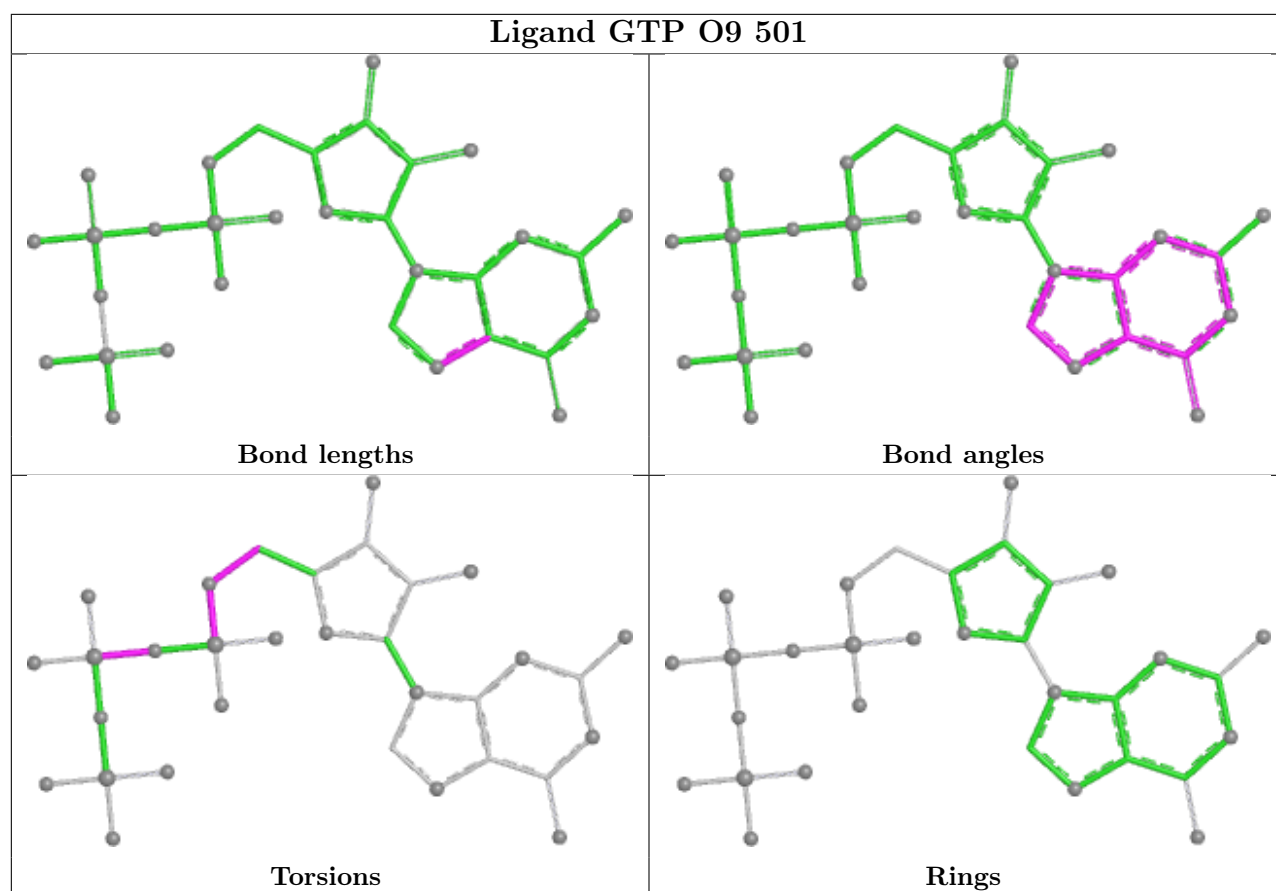
Ligand GTP N1 501

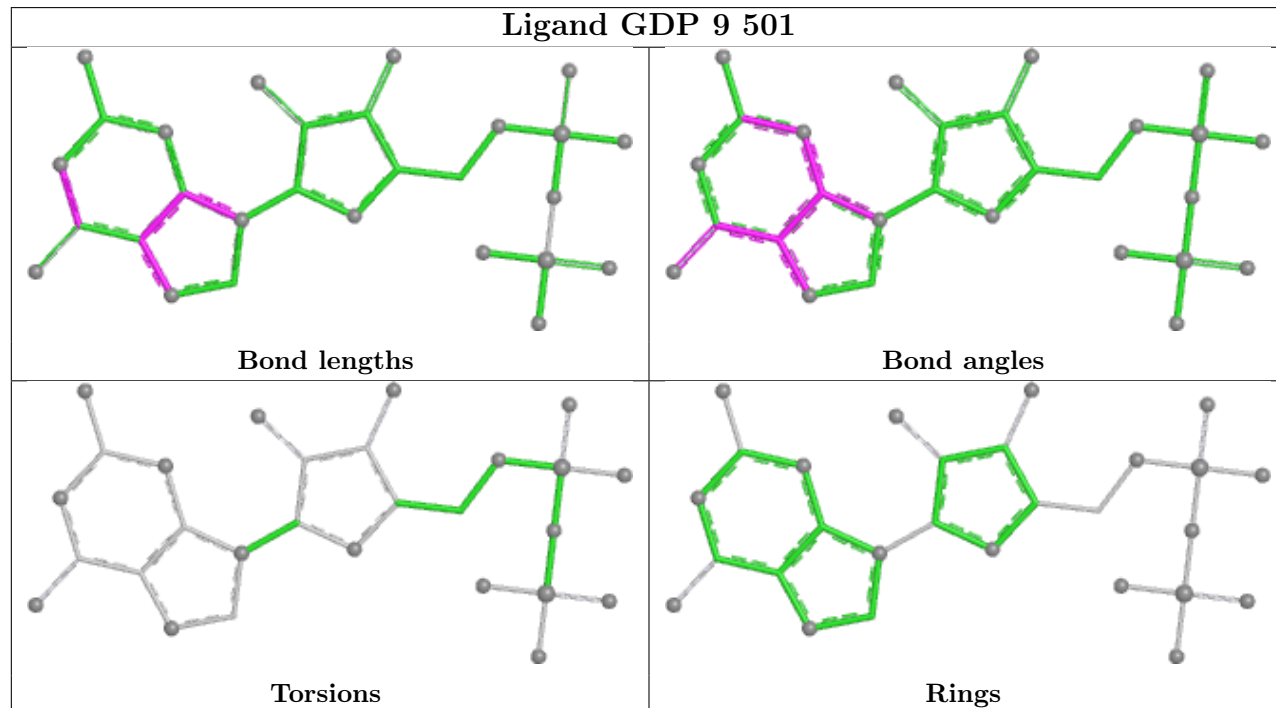
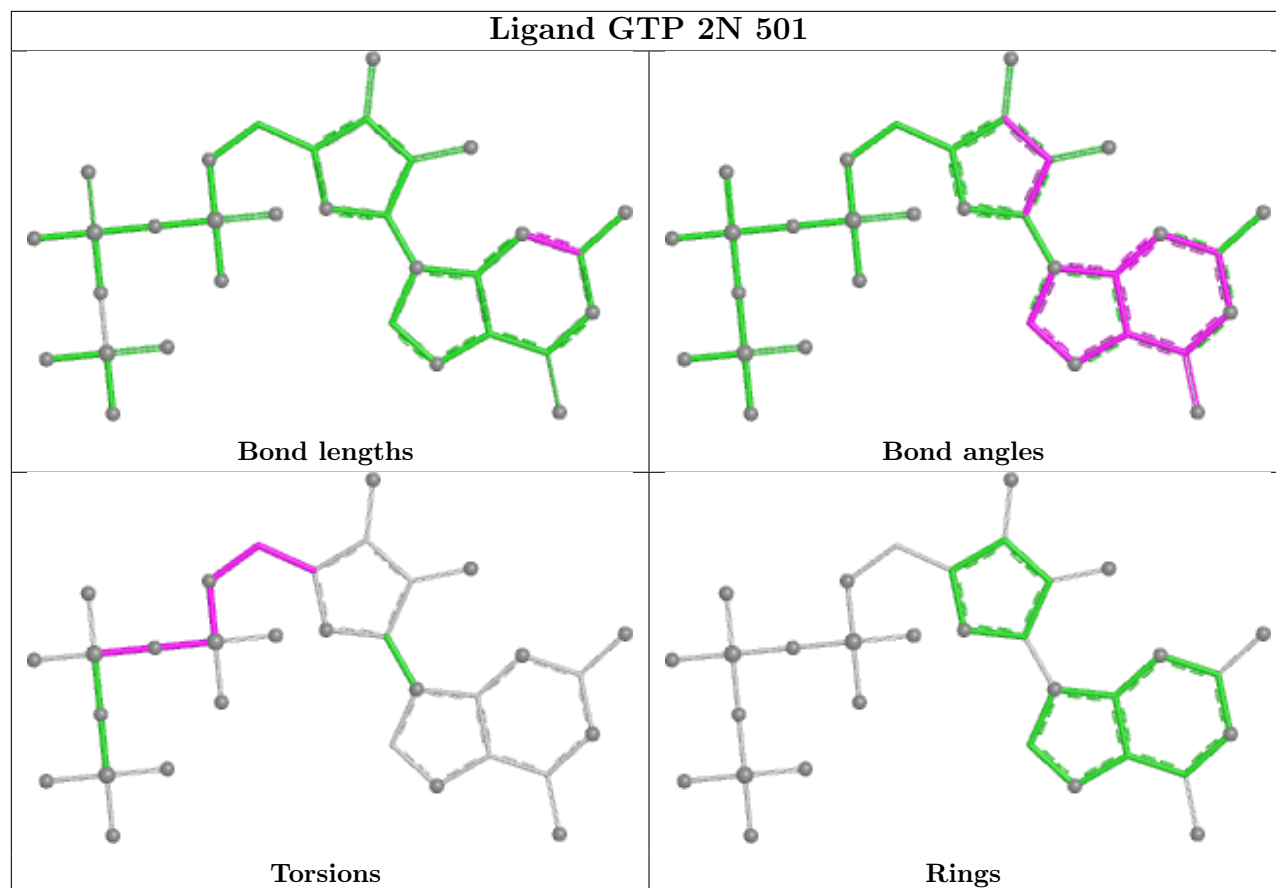


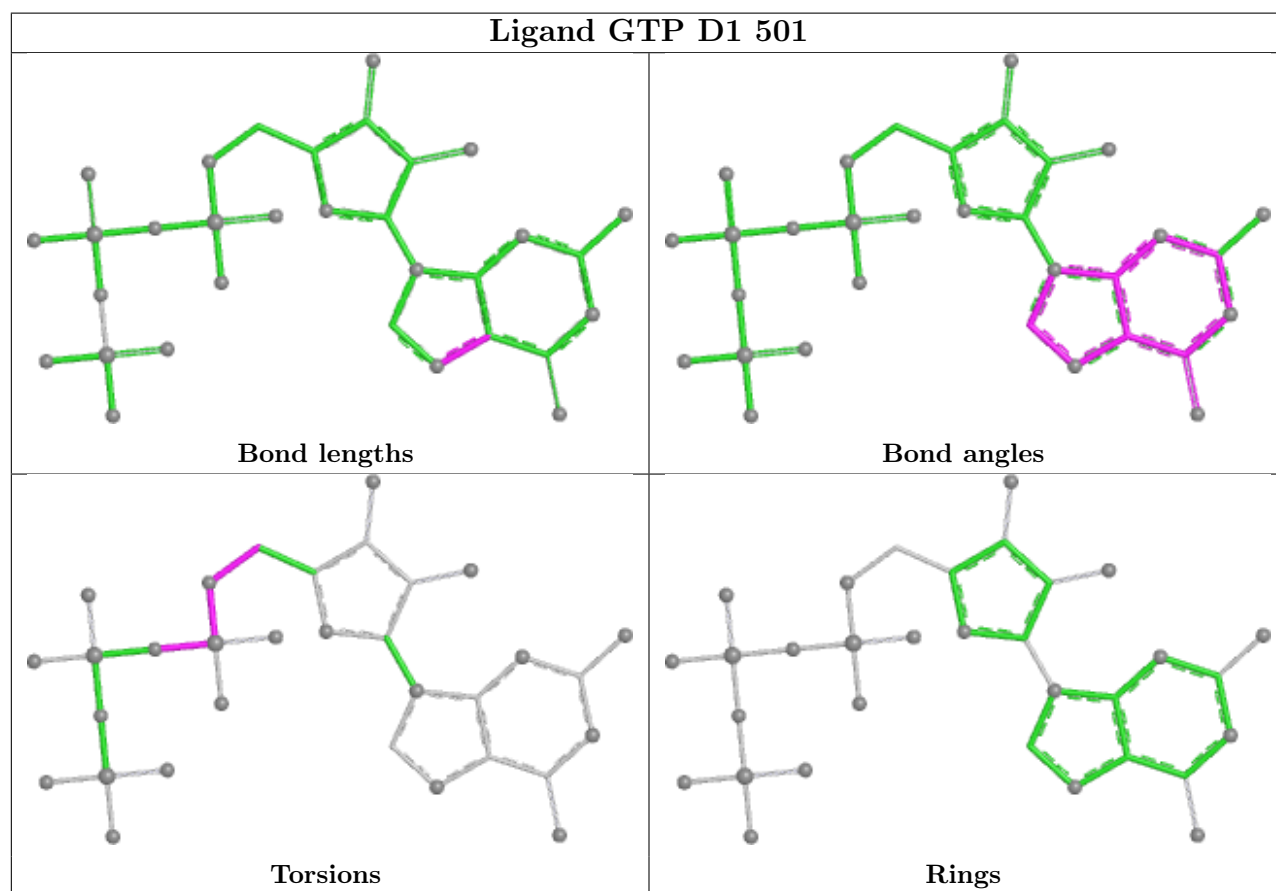
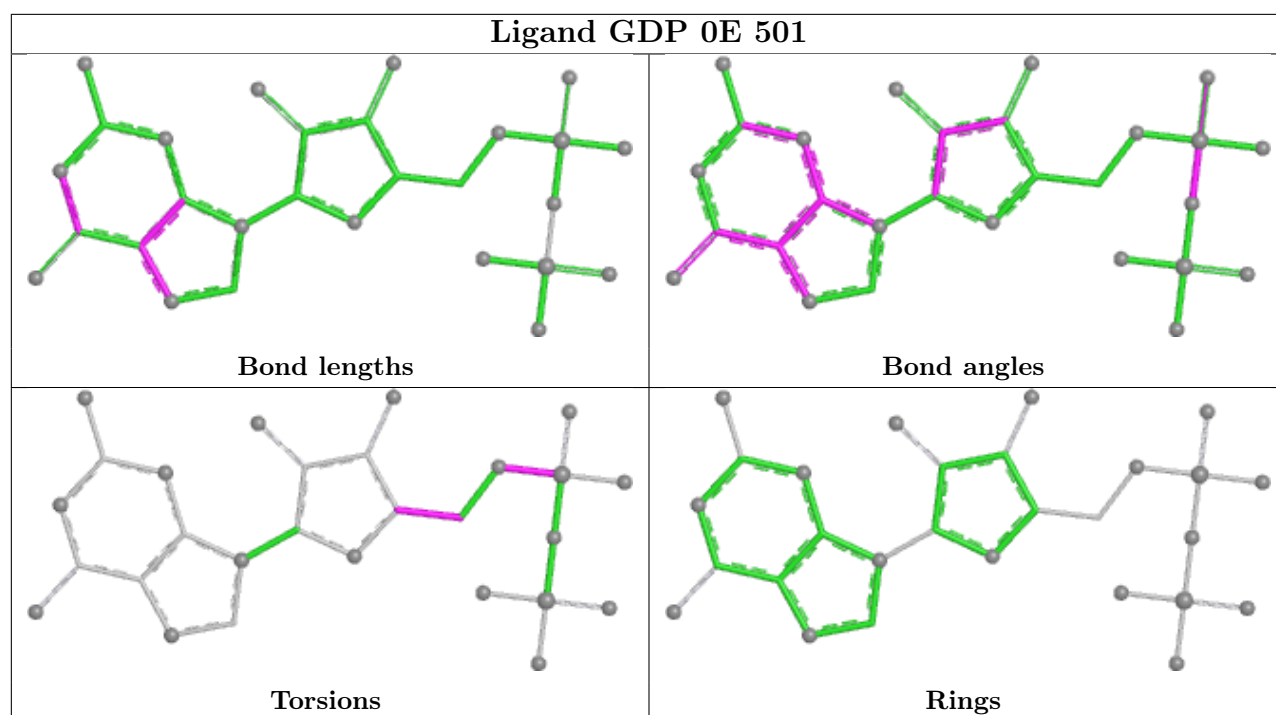


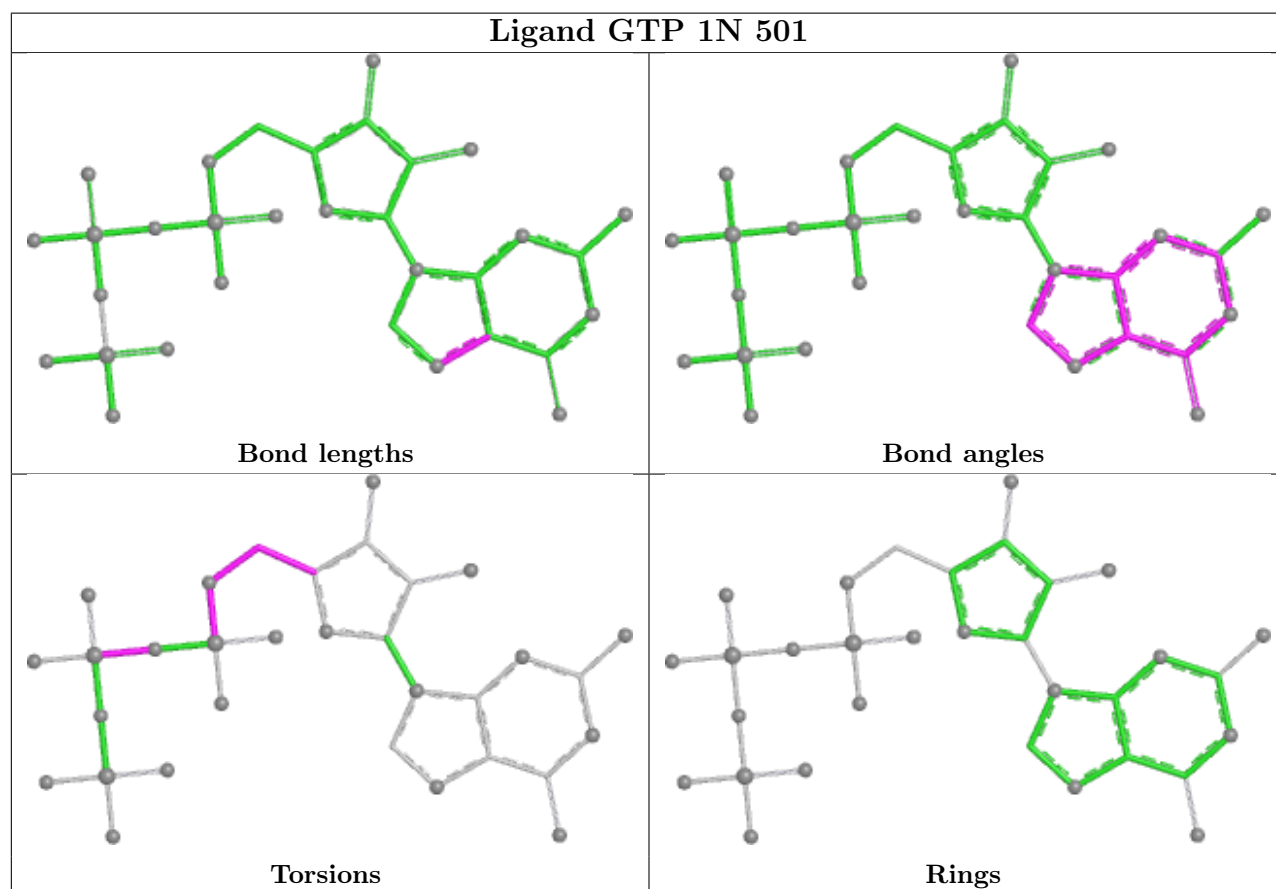
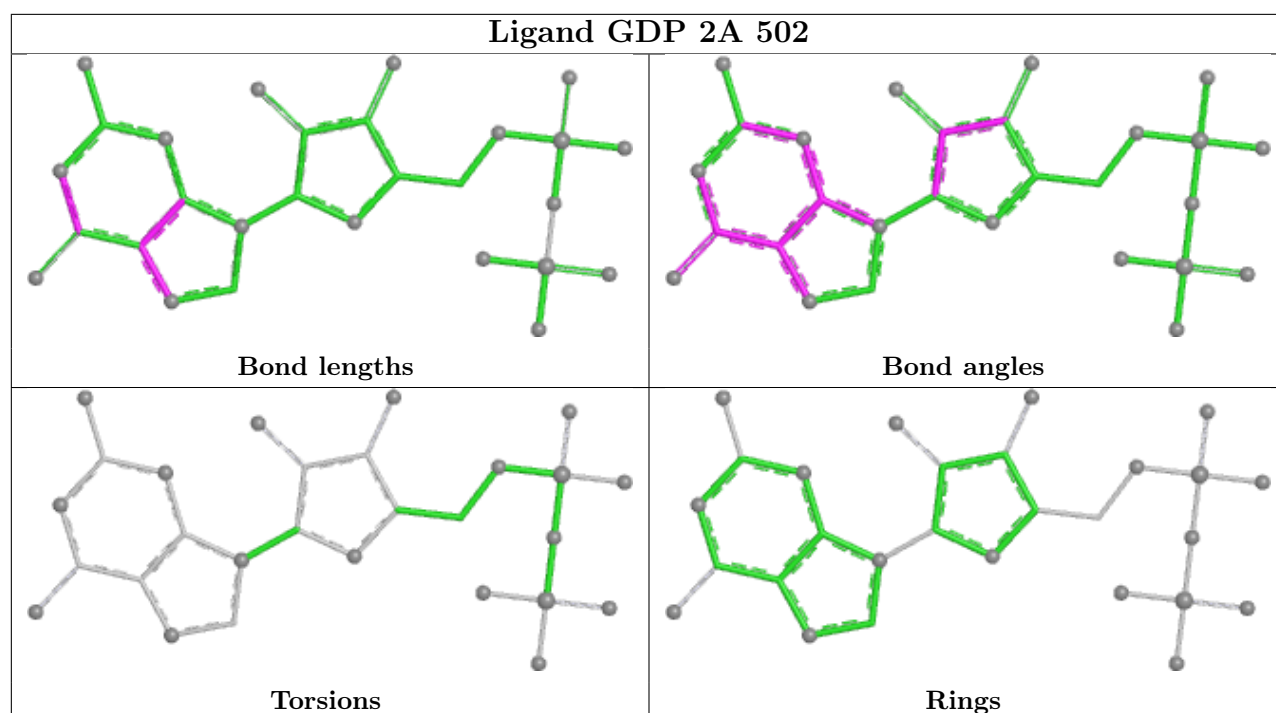


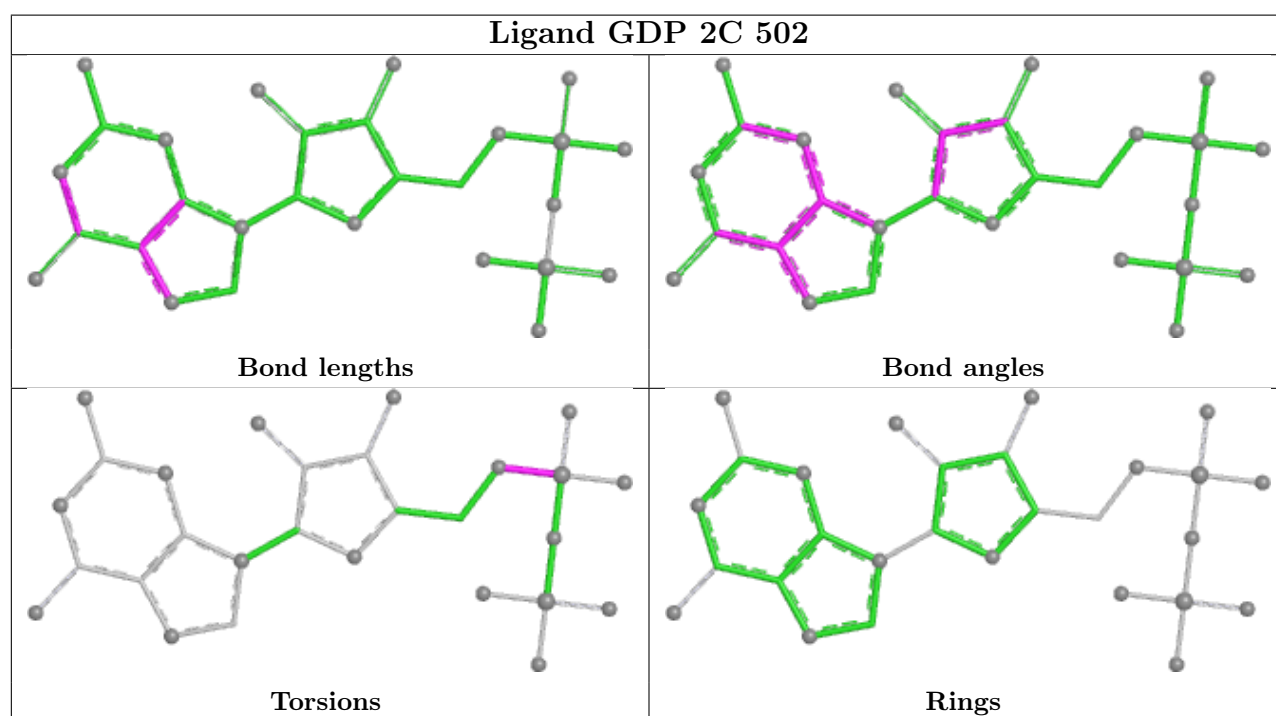
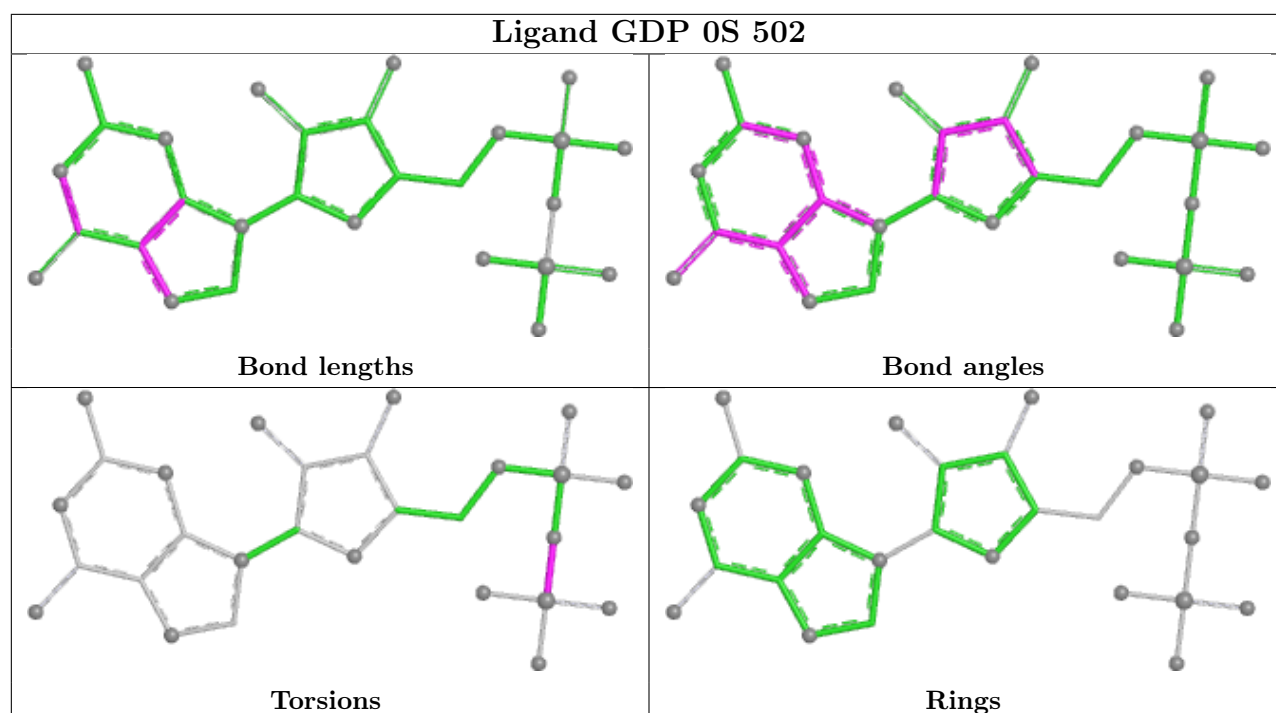


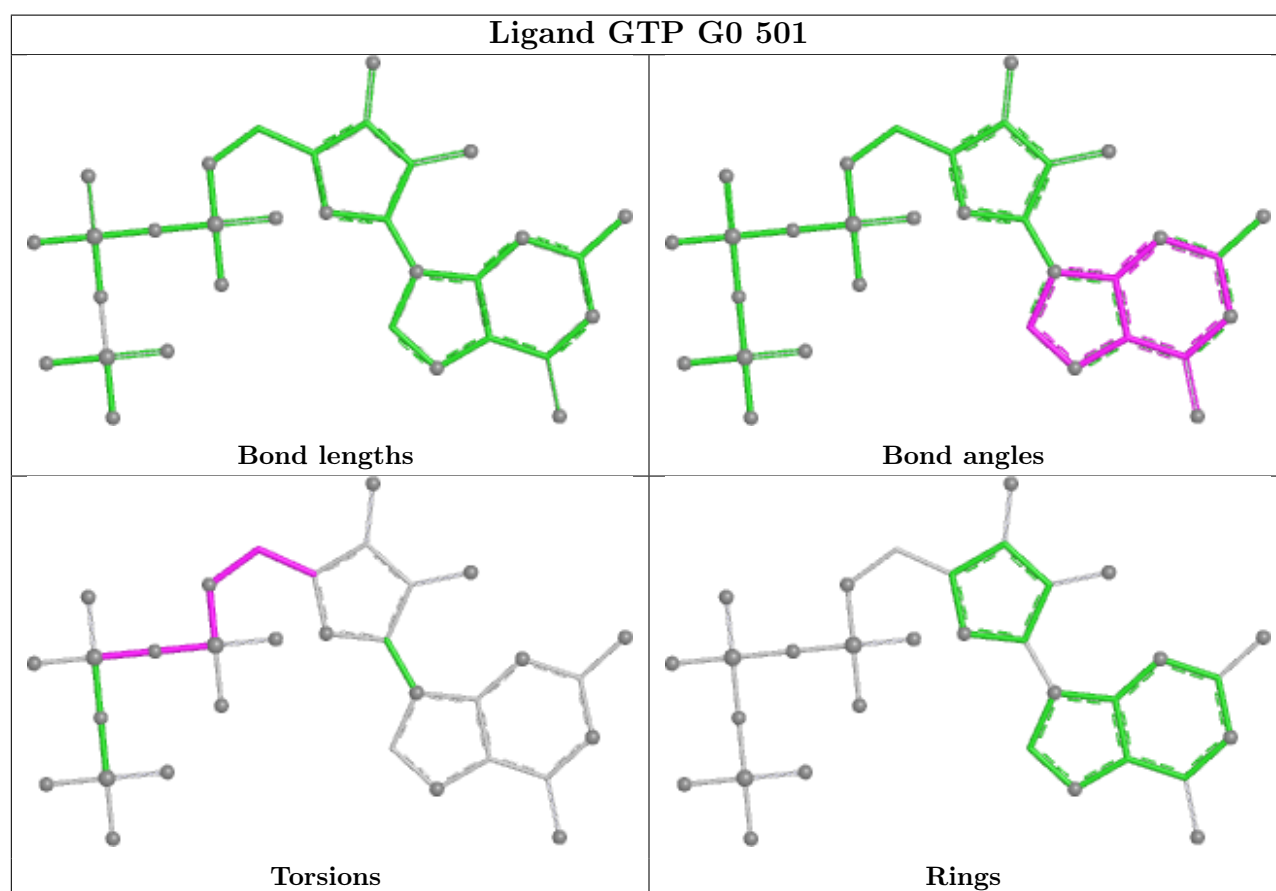
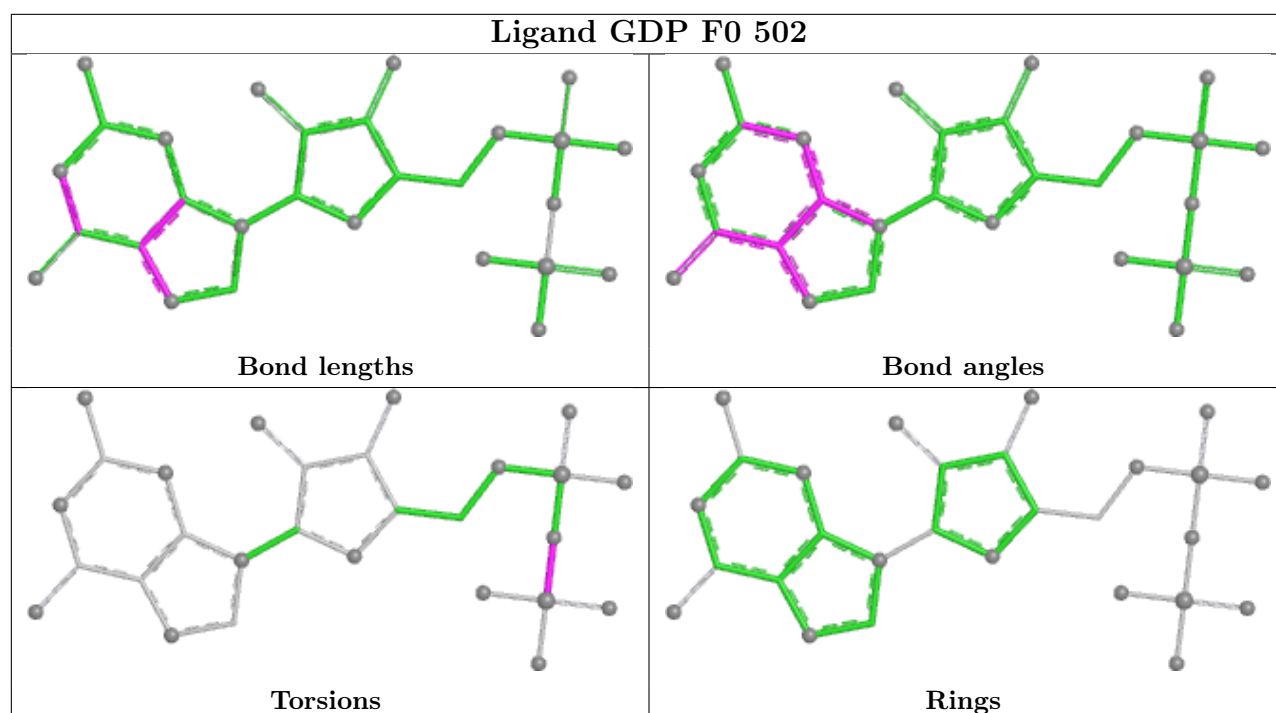


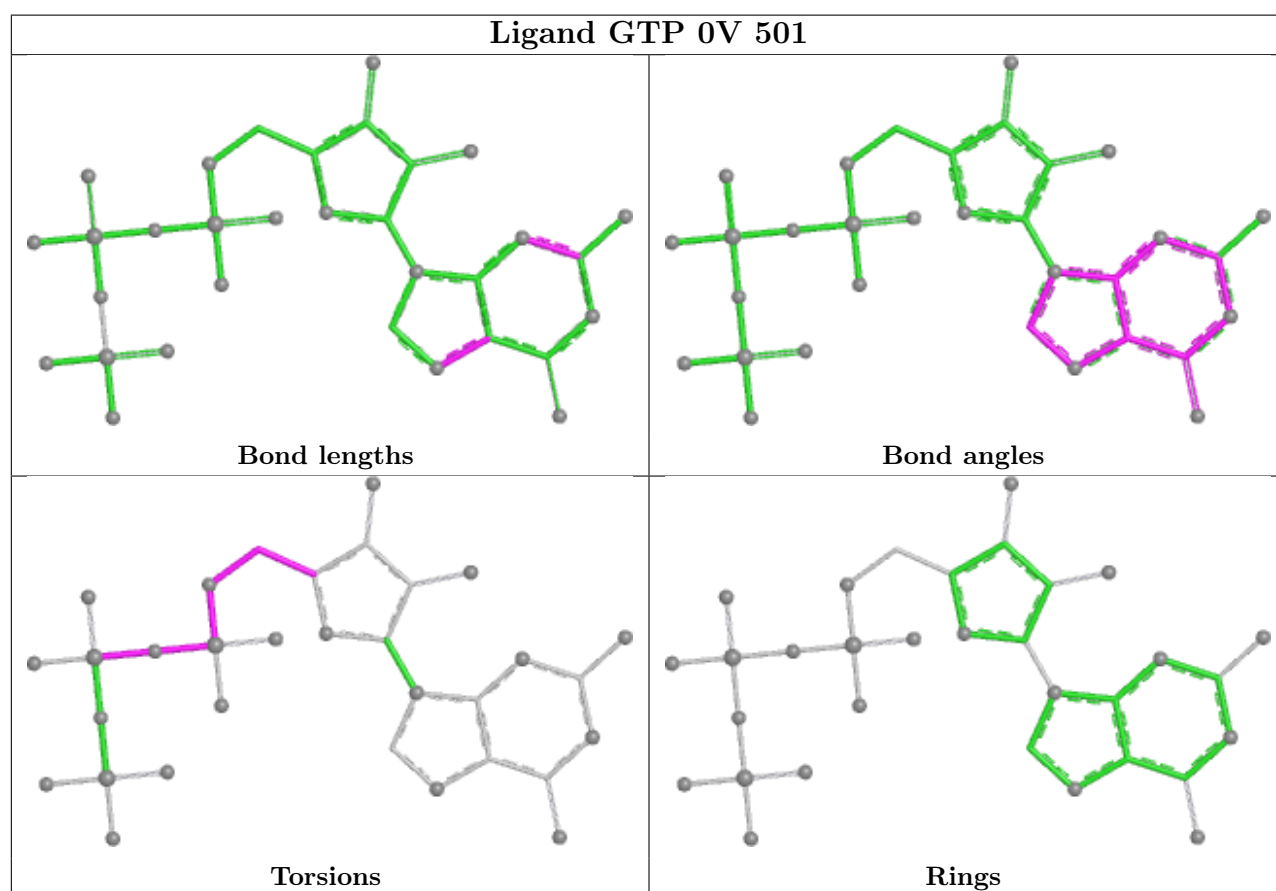
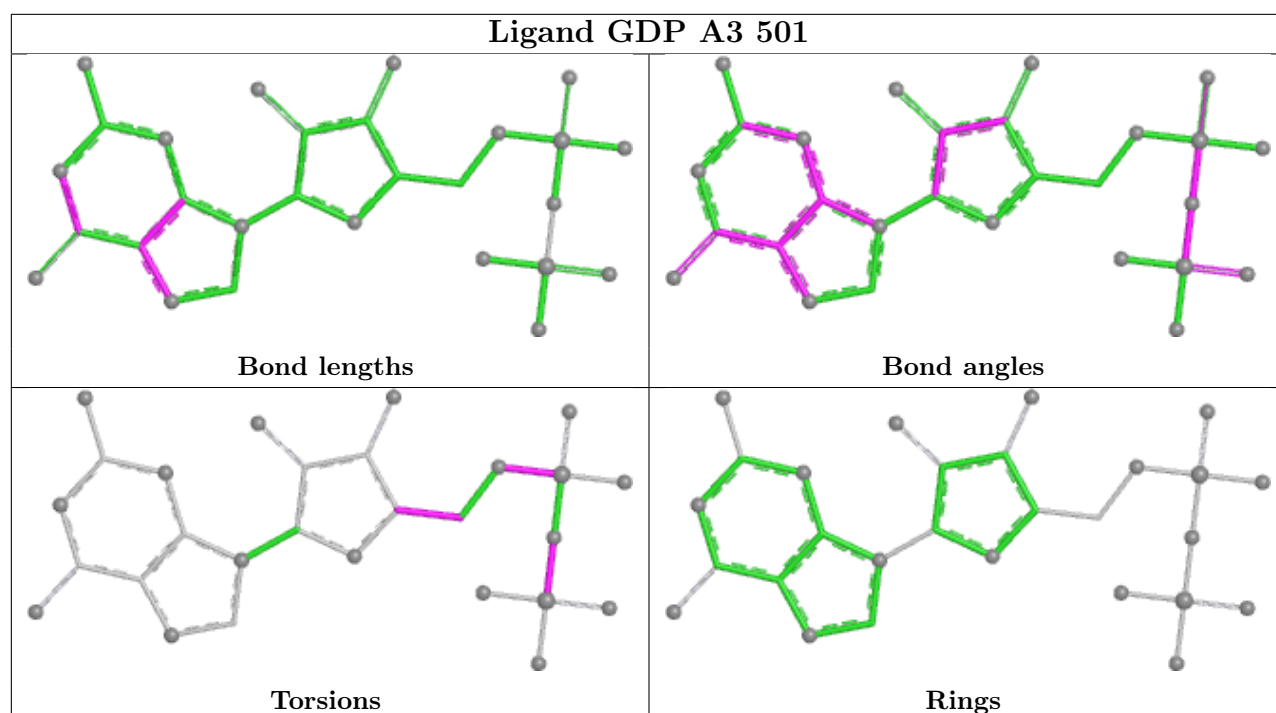


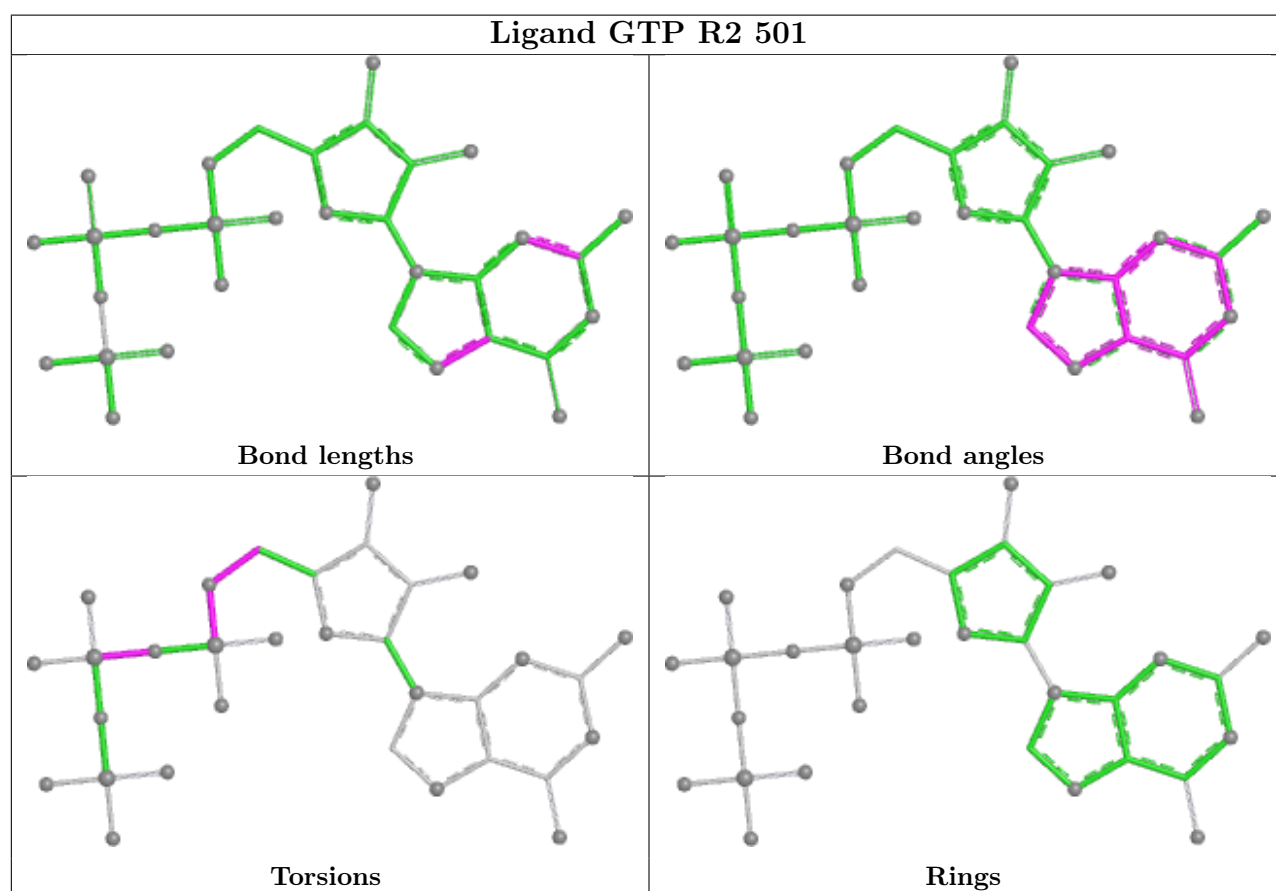
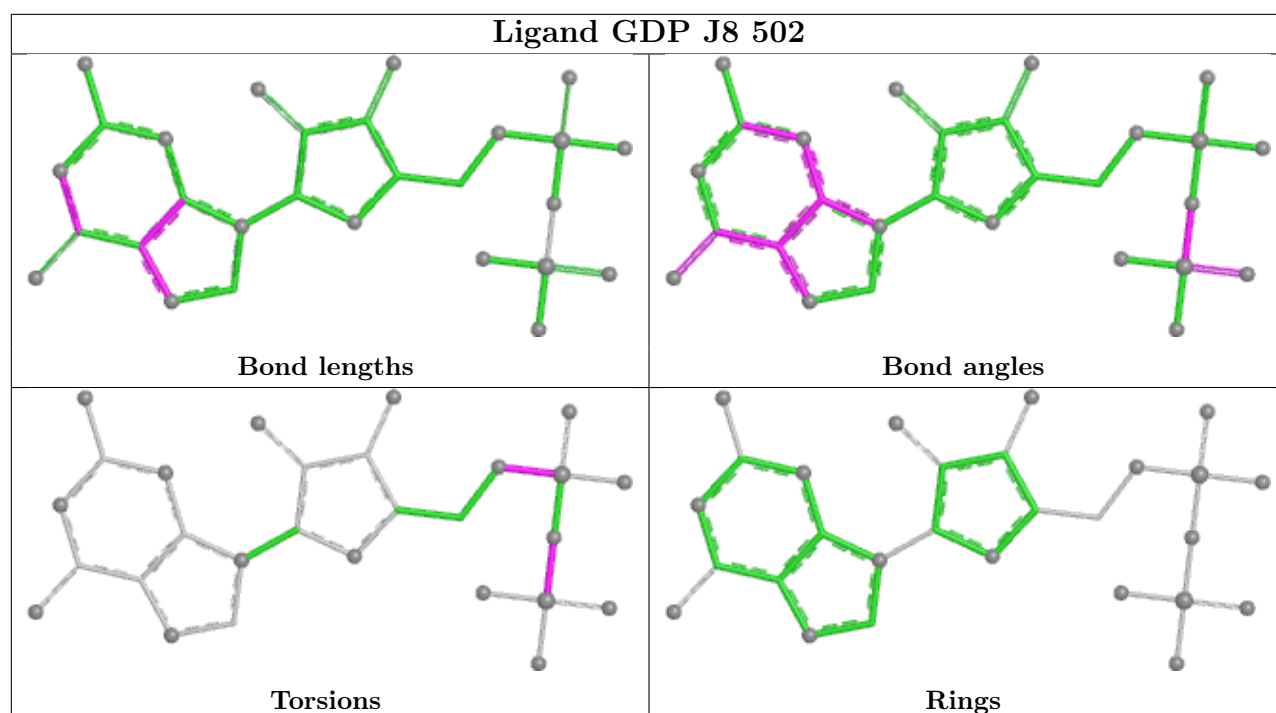


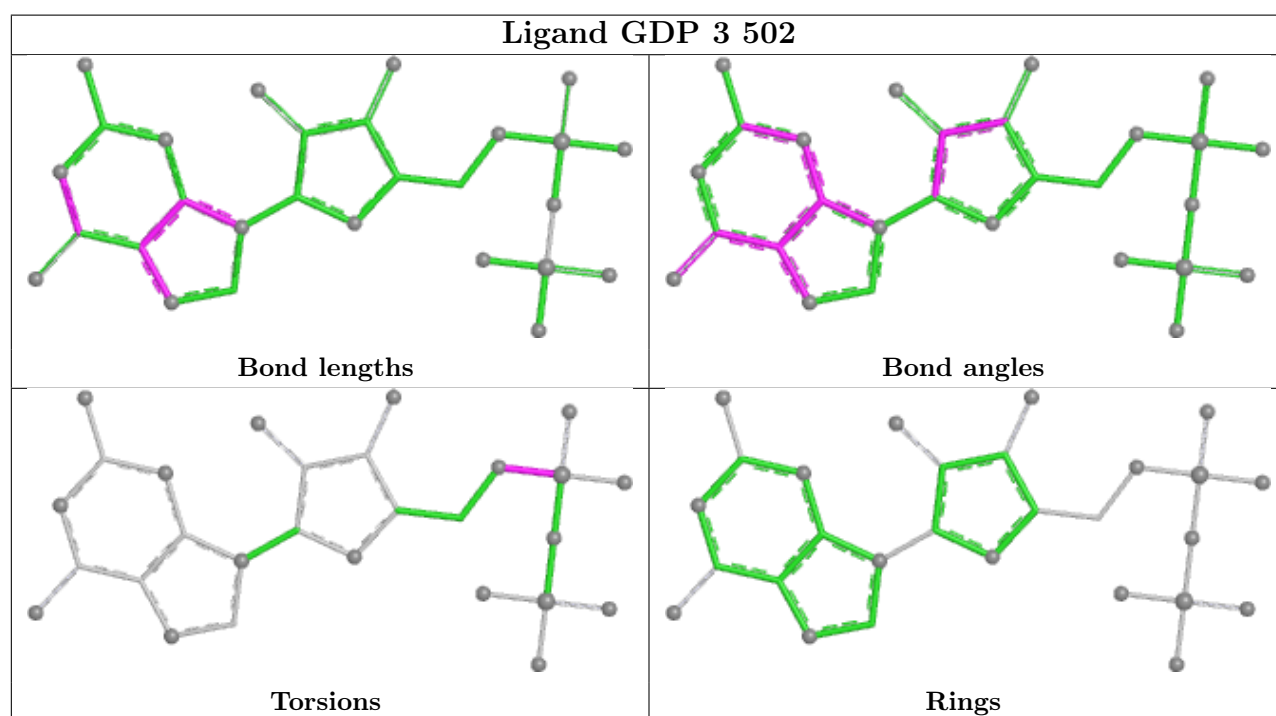
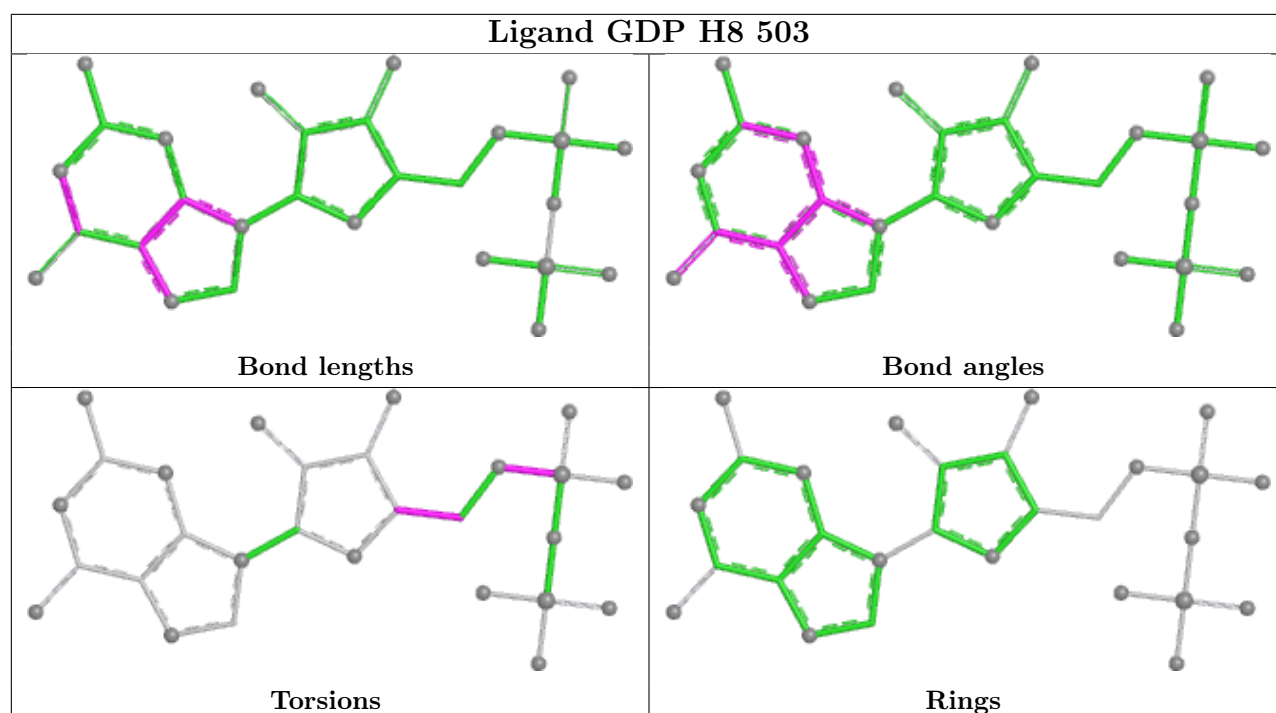


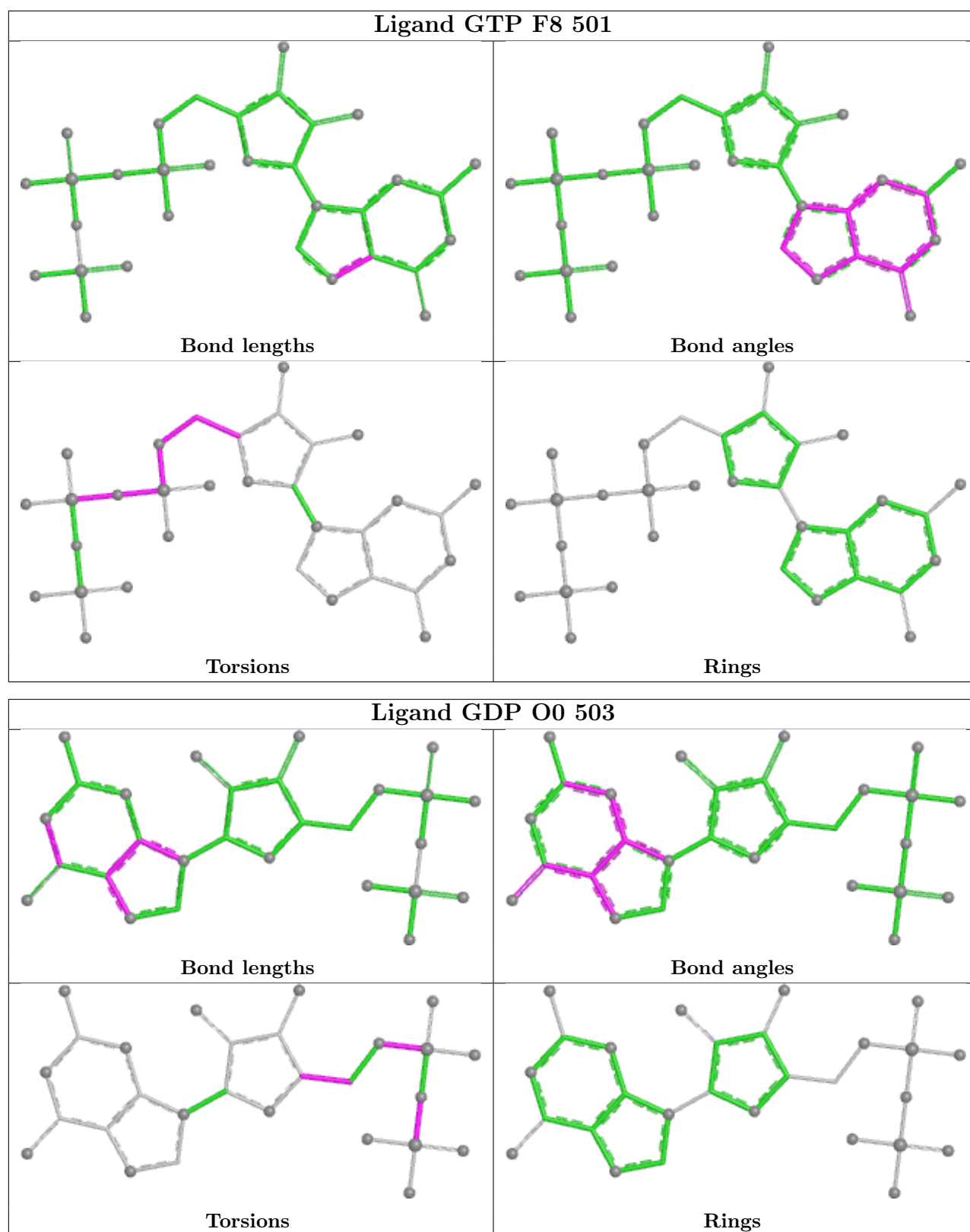


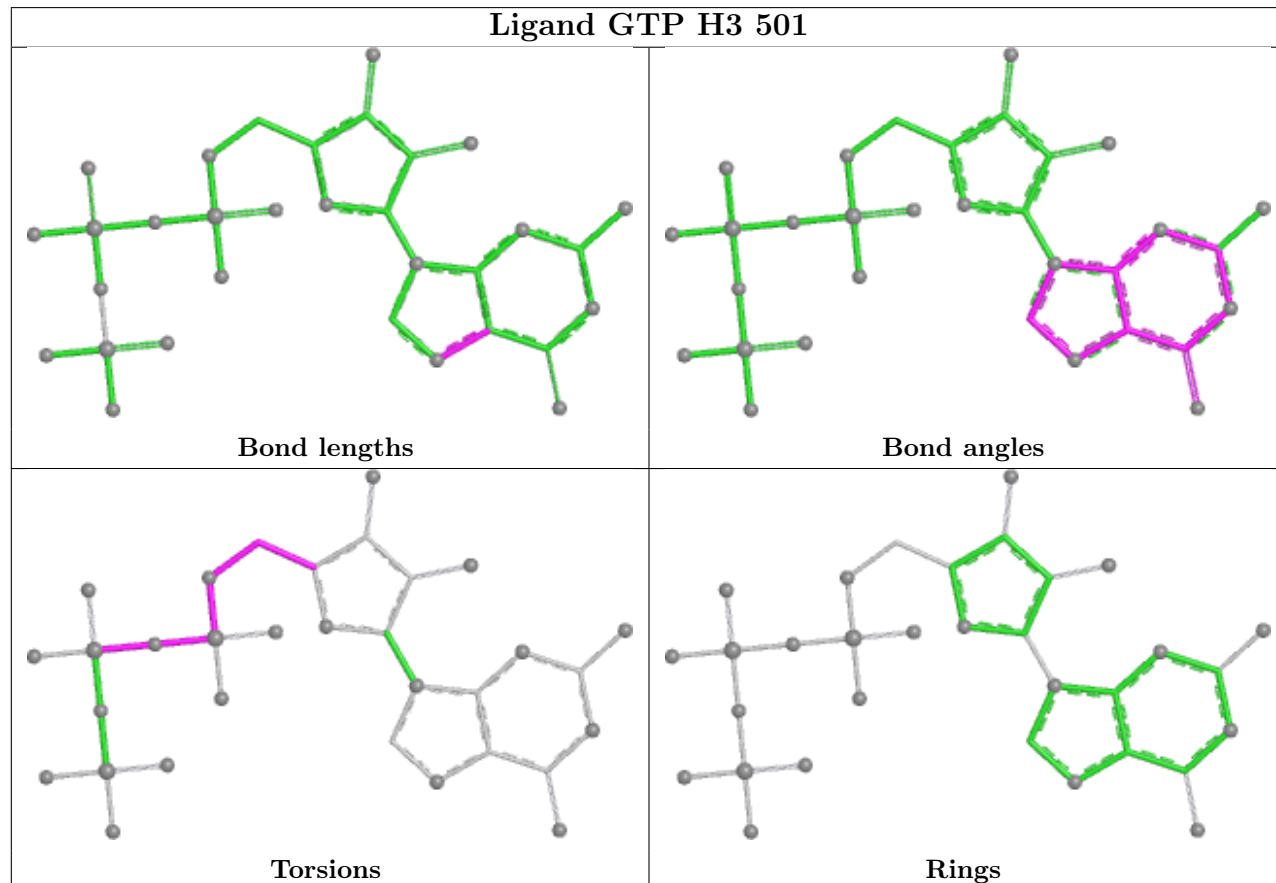
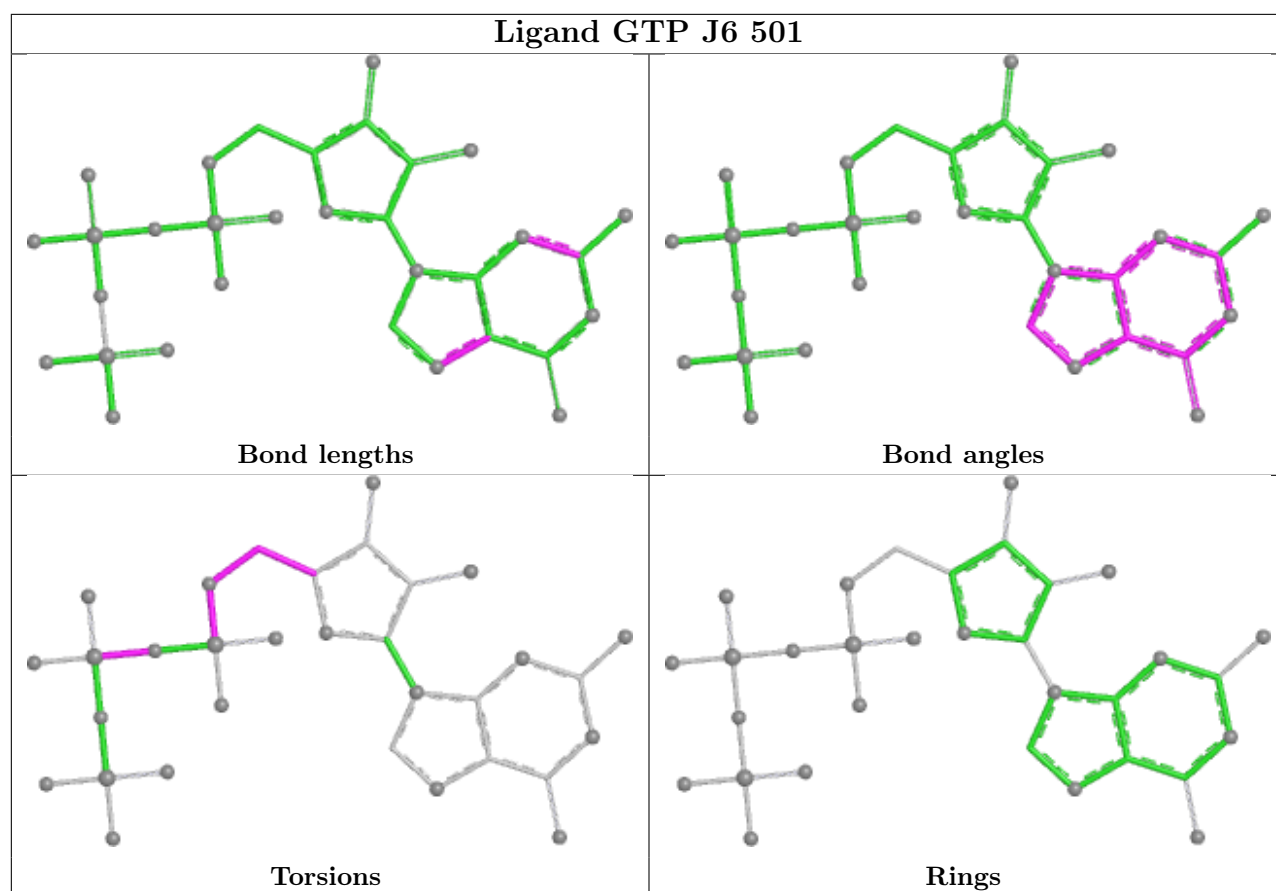


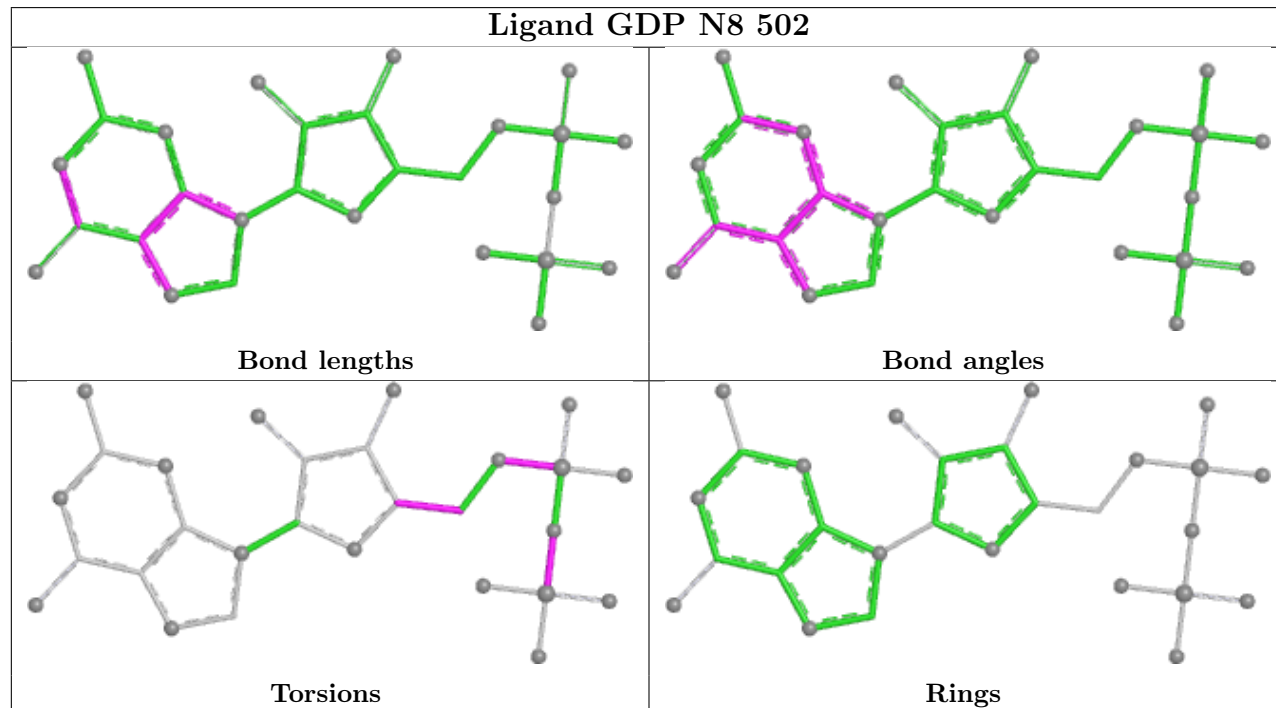
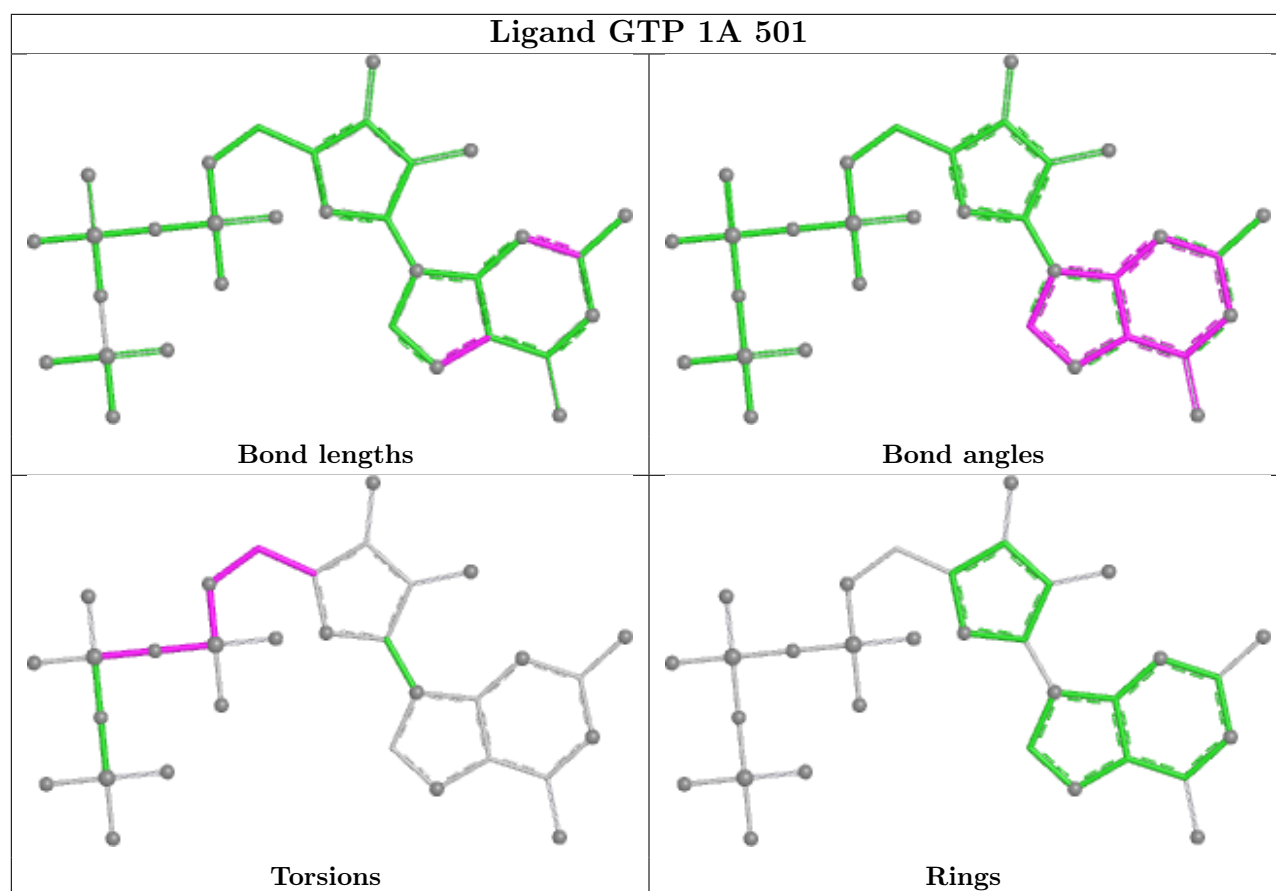


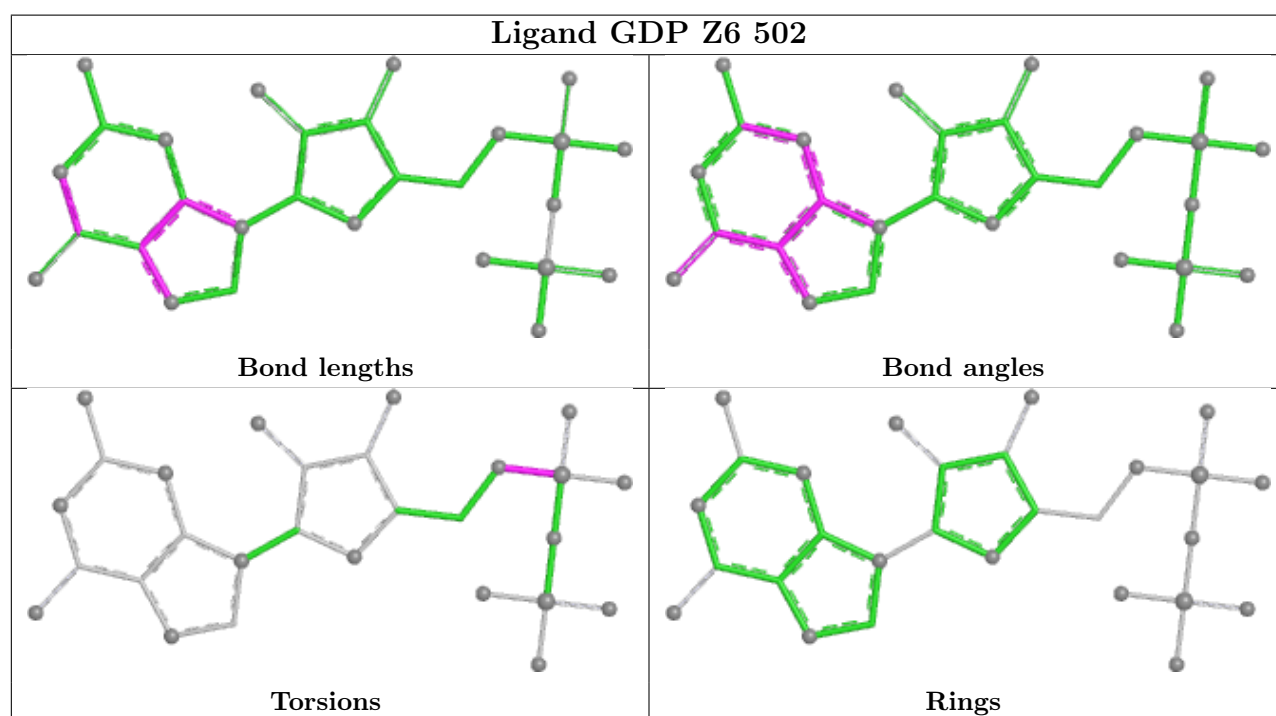
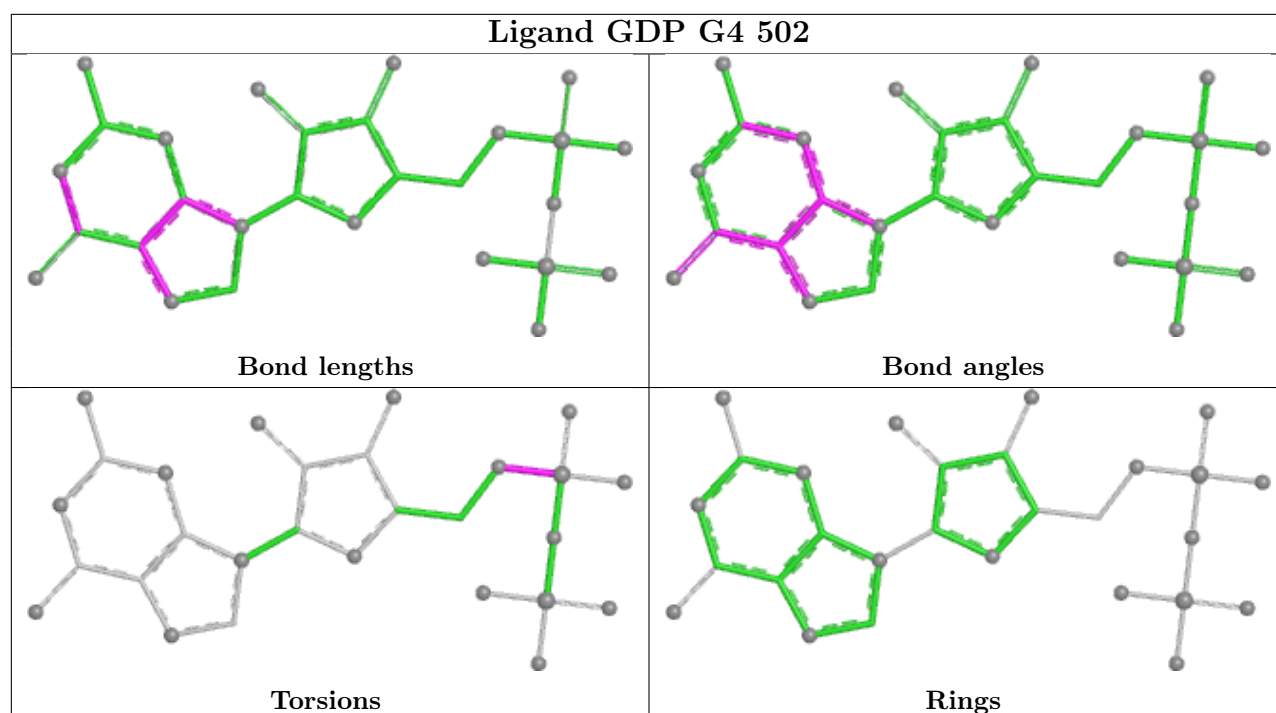




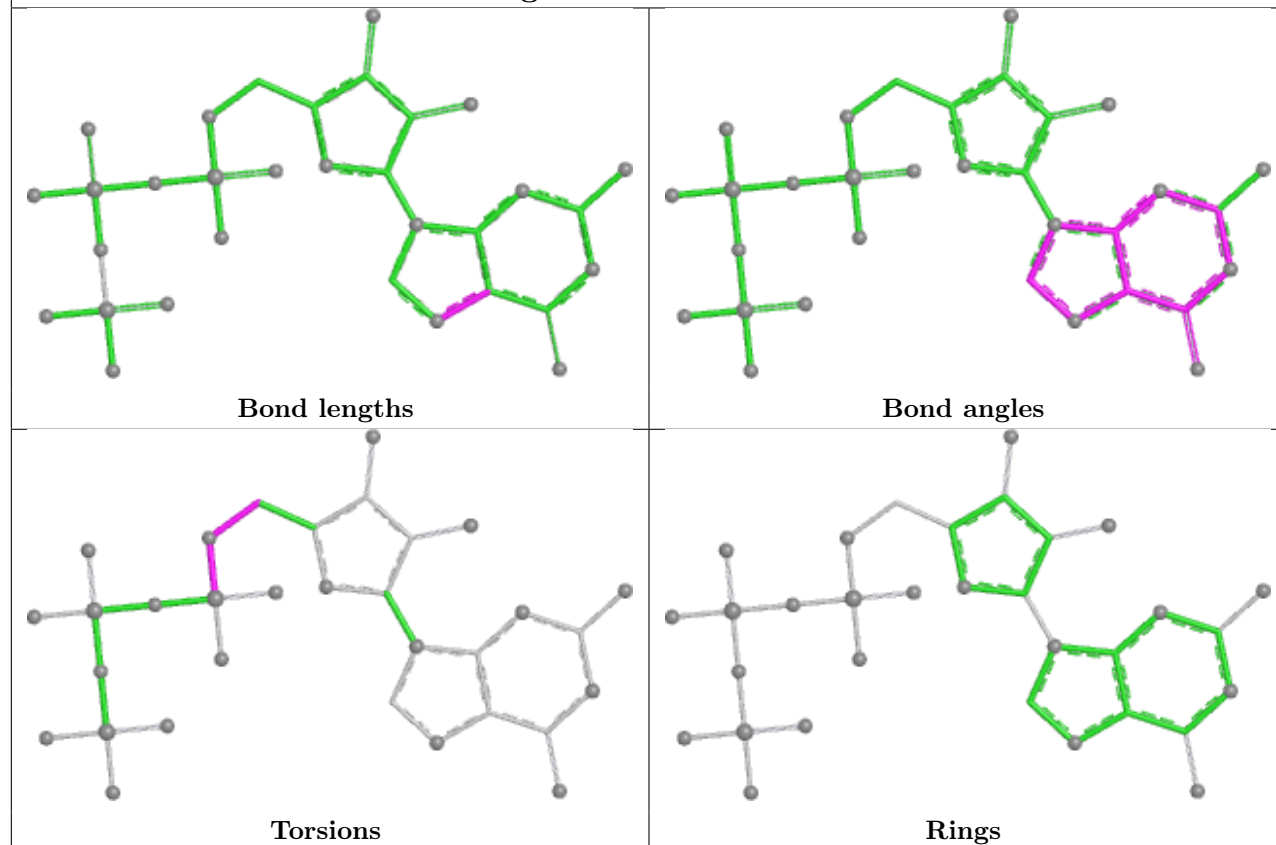




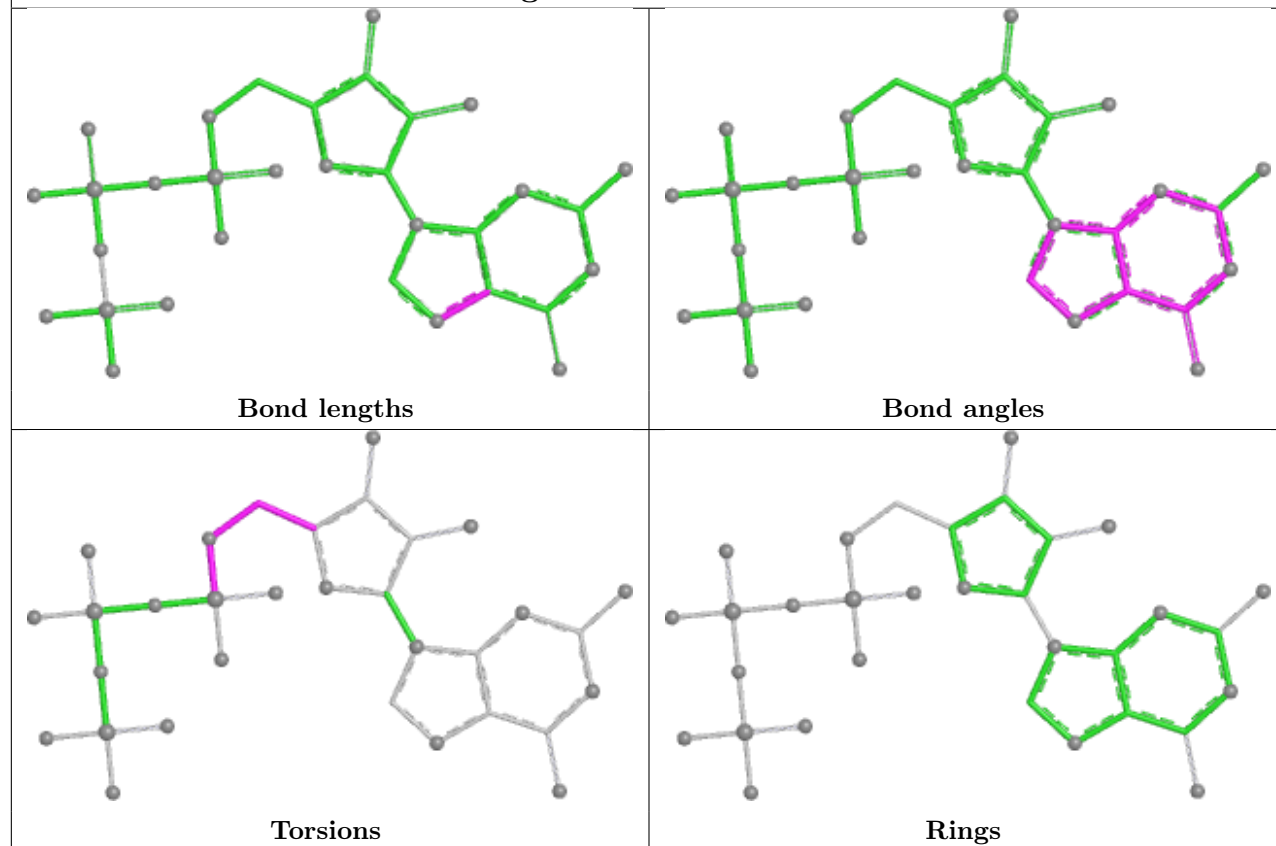




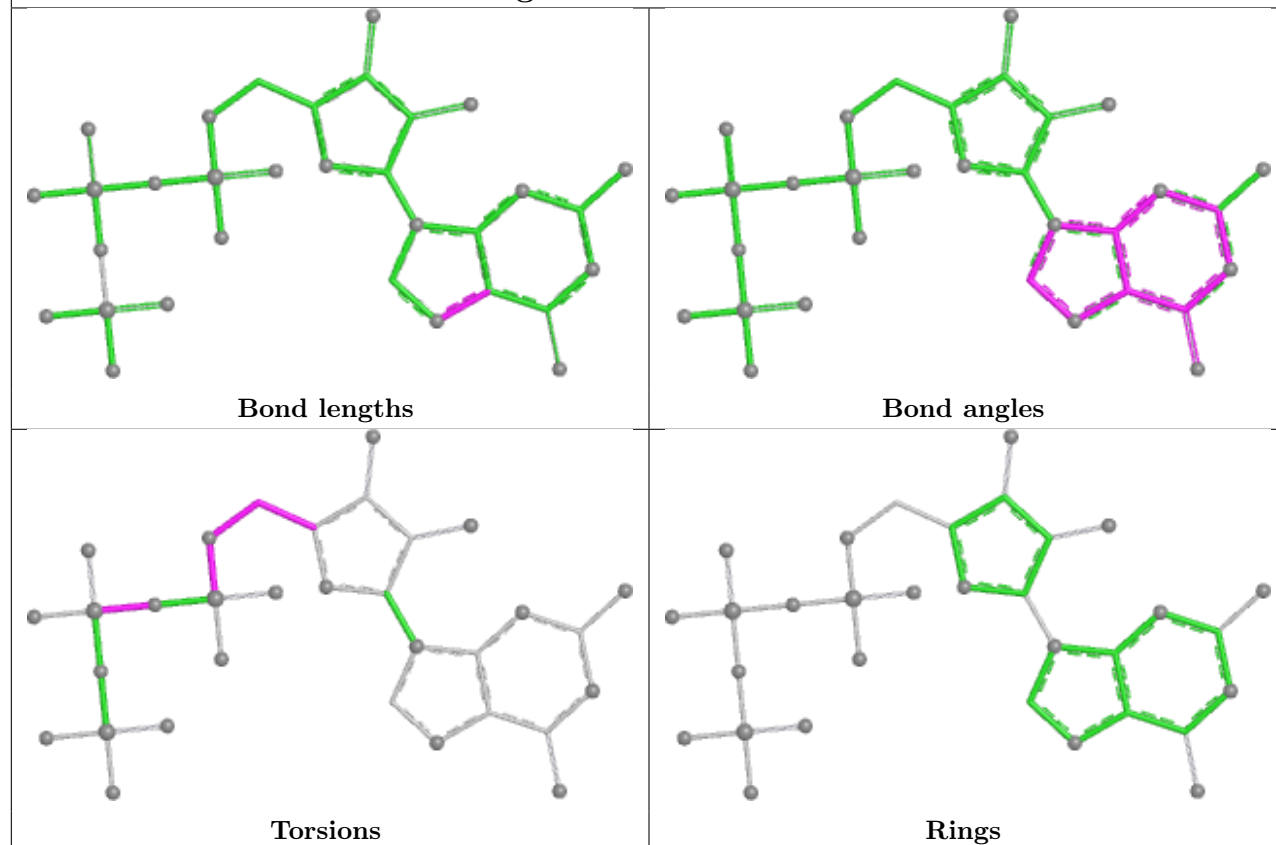
Ligand GTP 3K 501



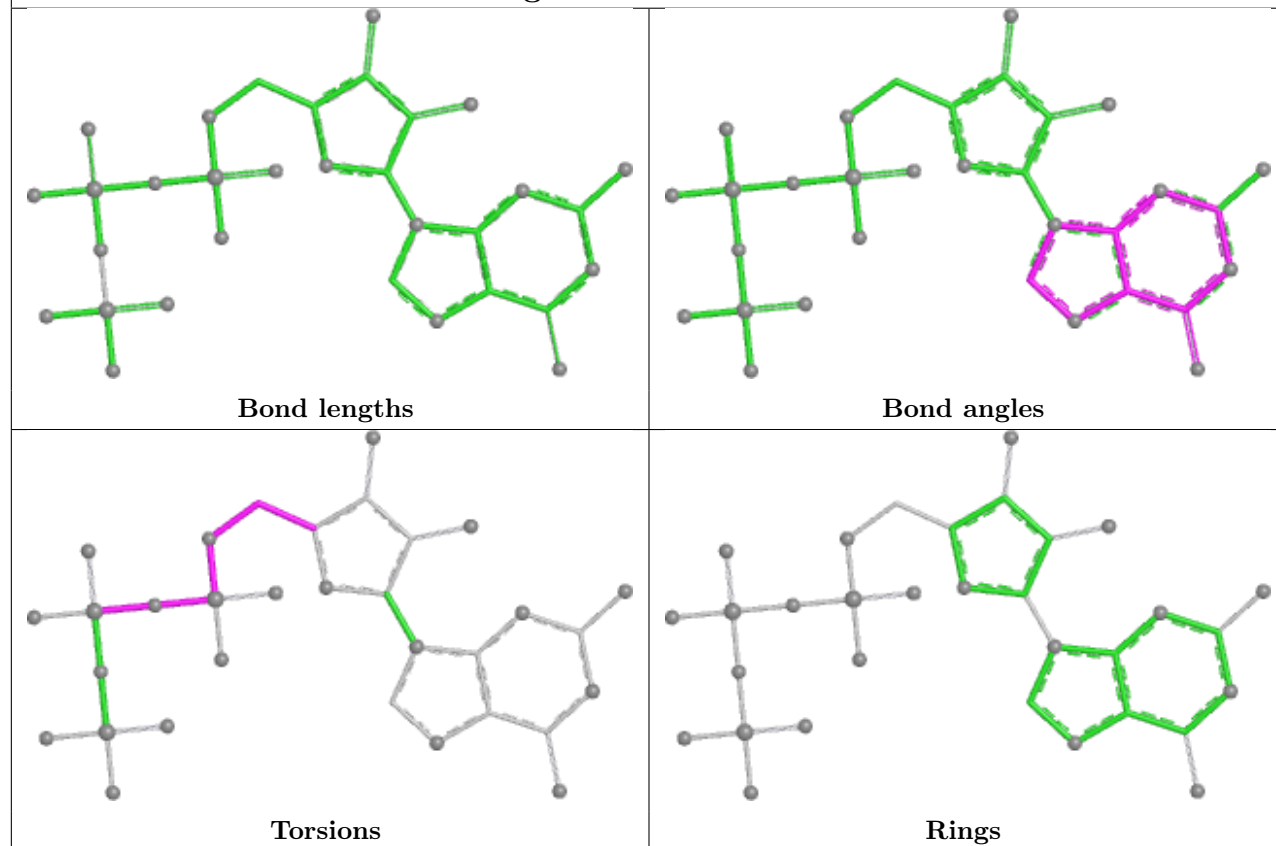
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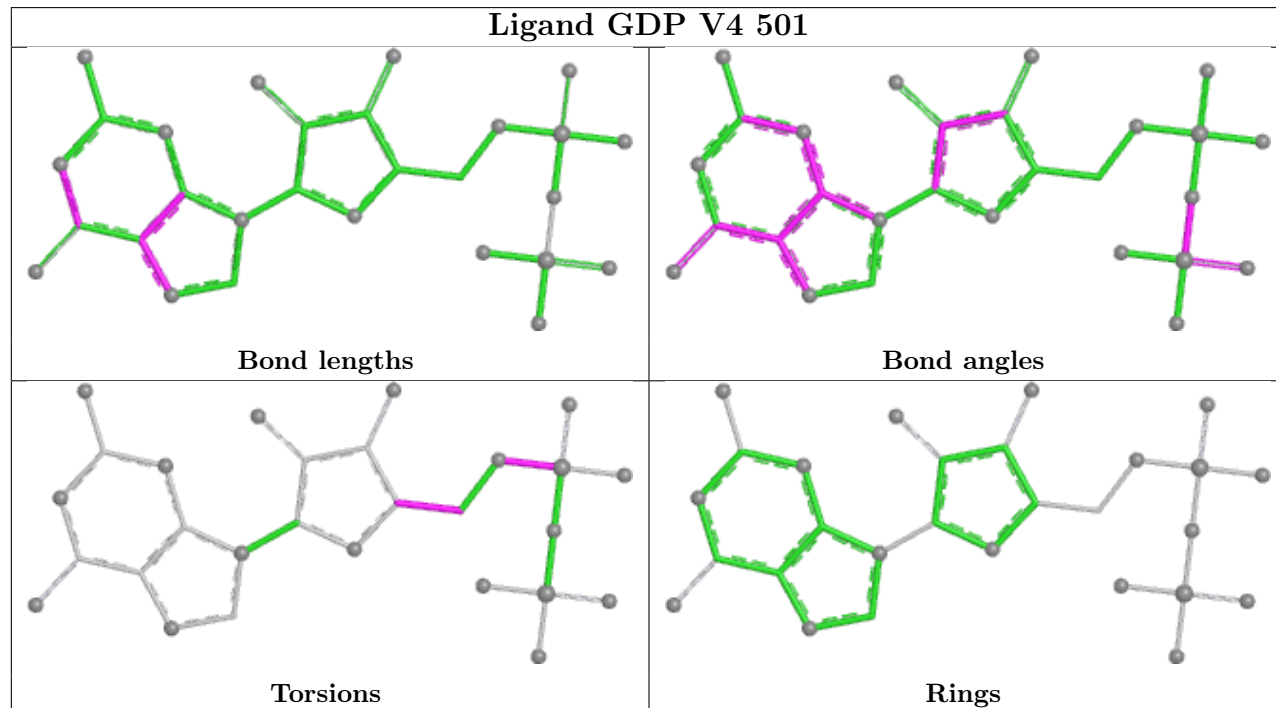
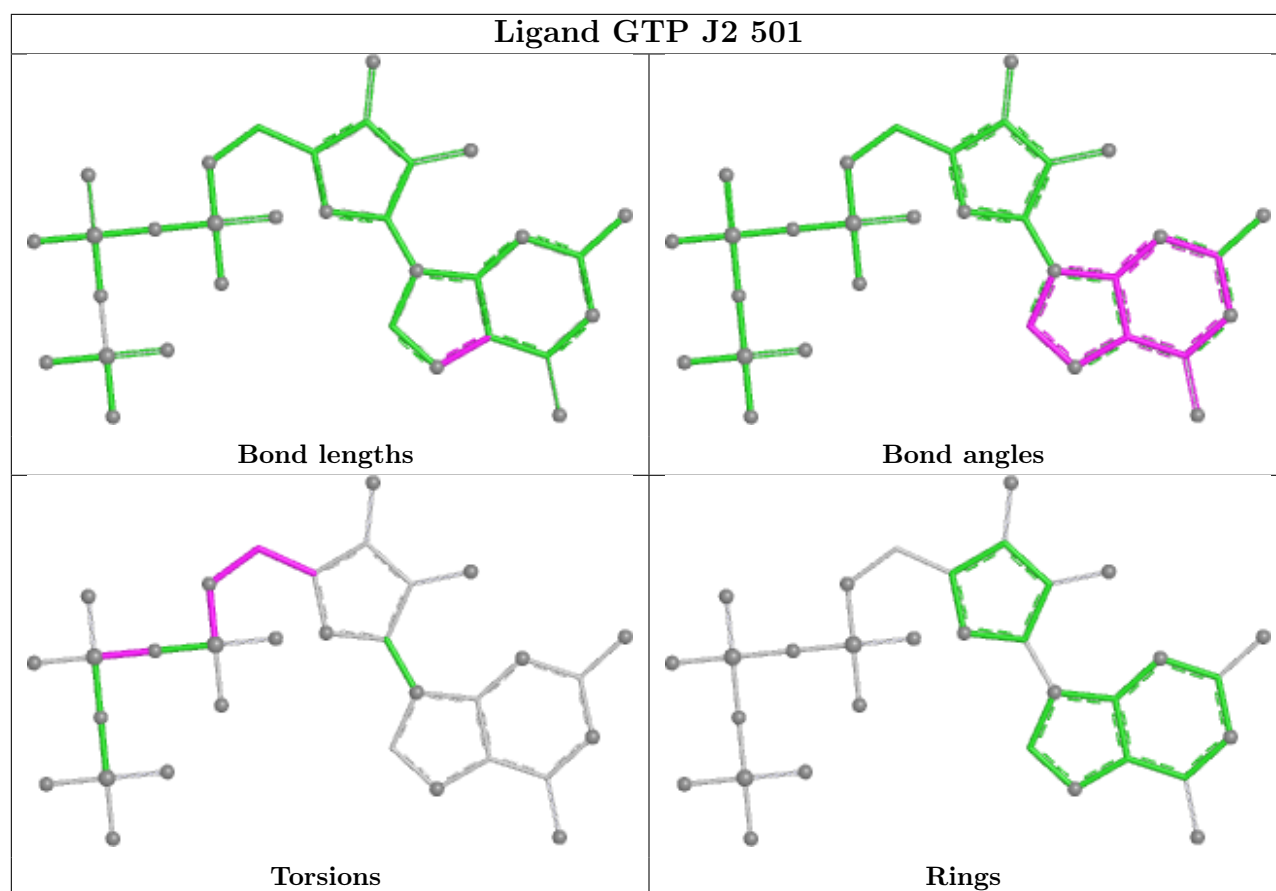


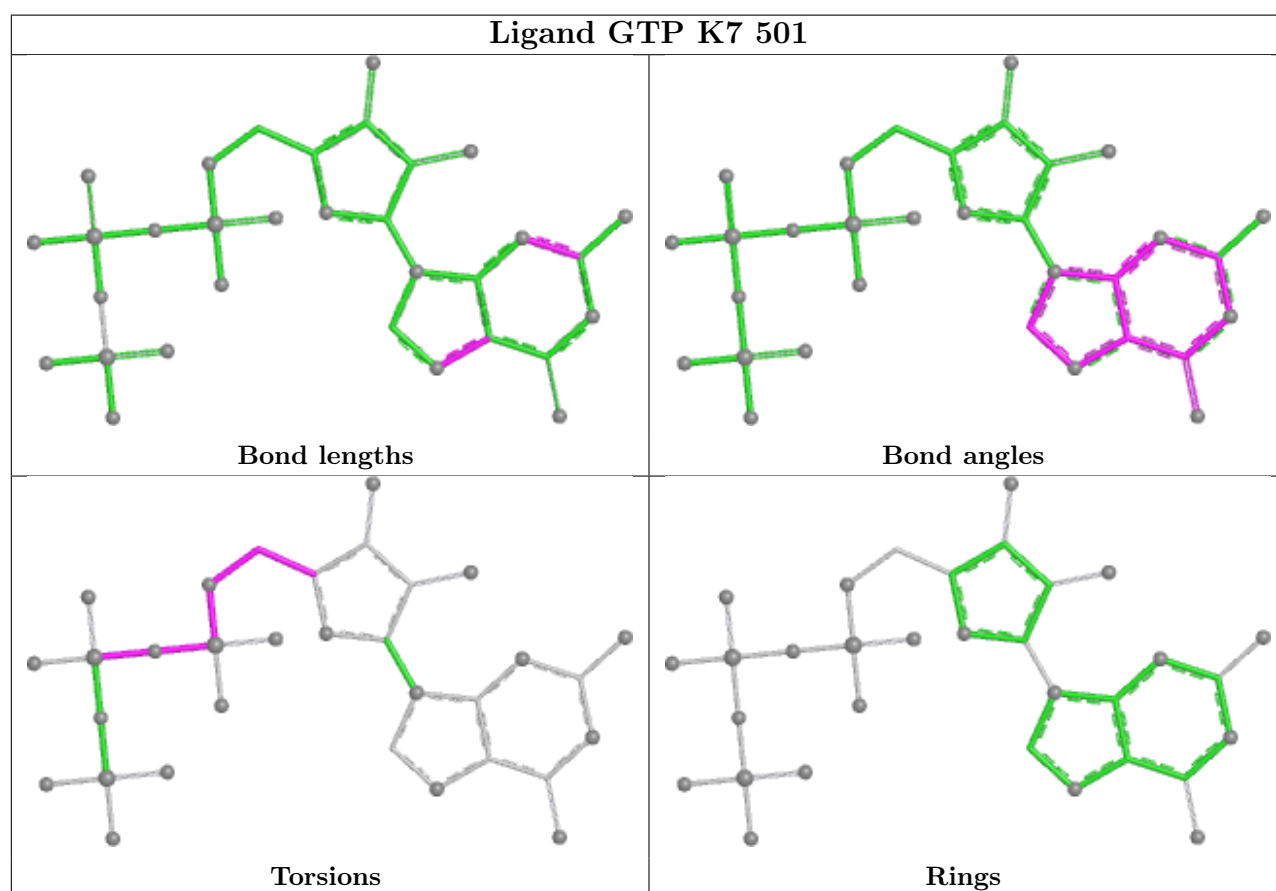
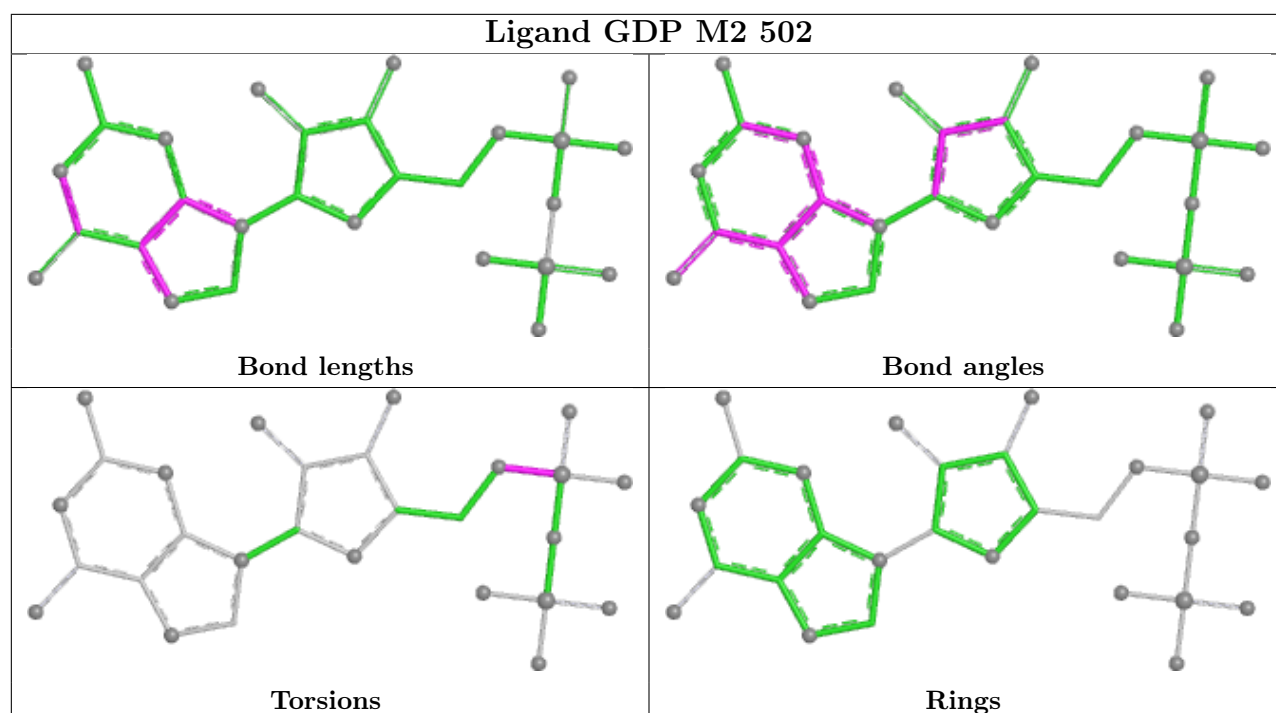
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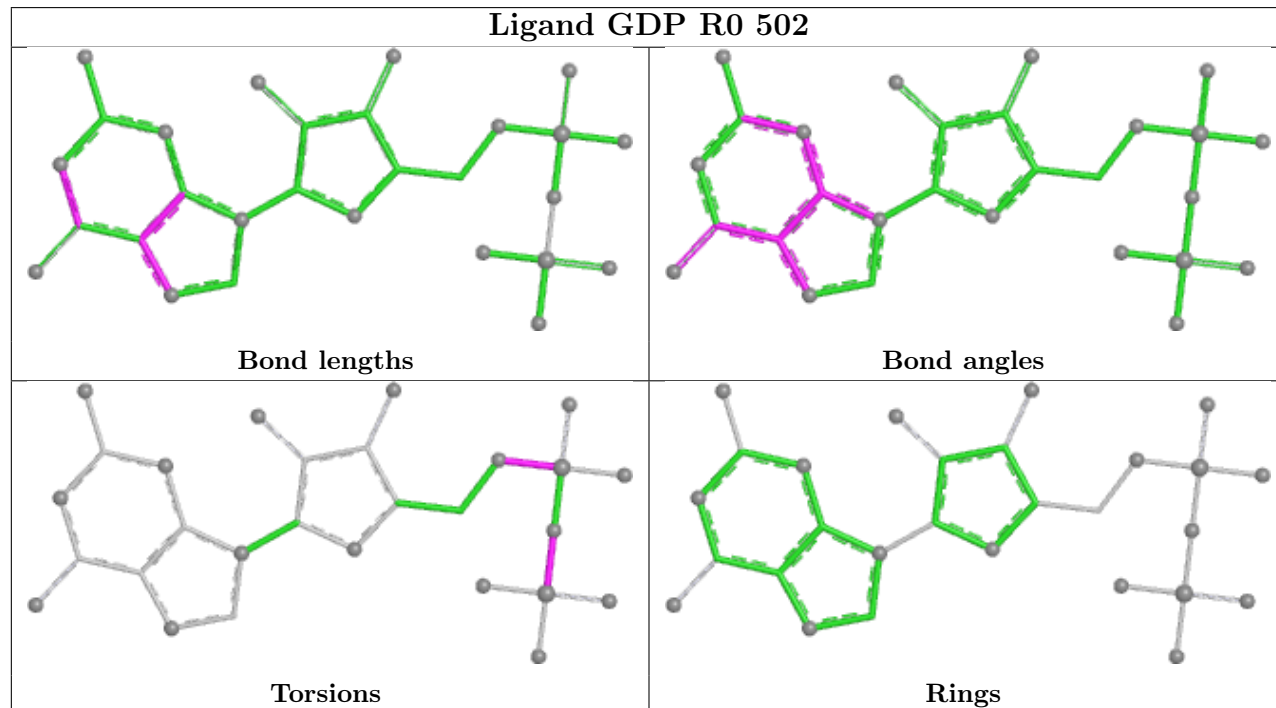
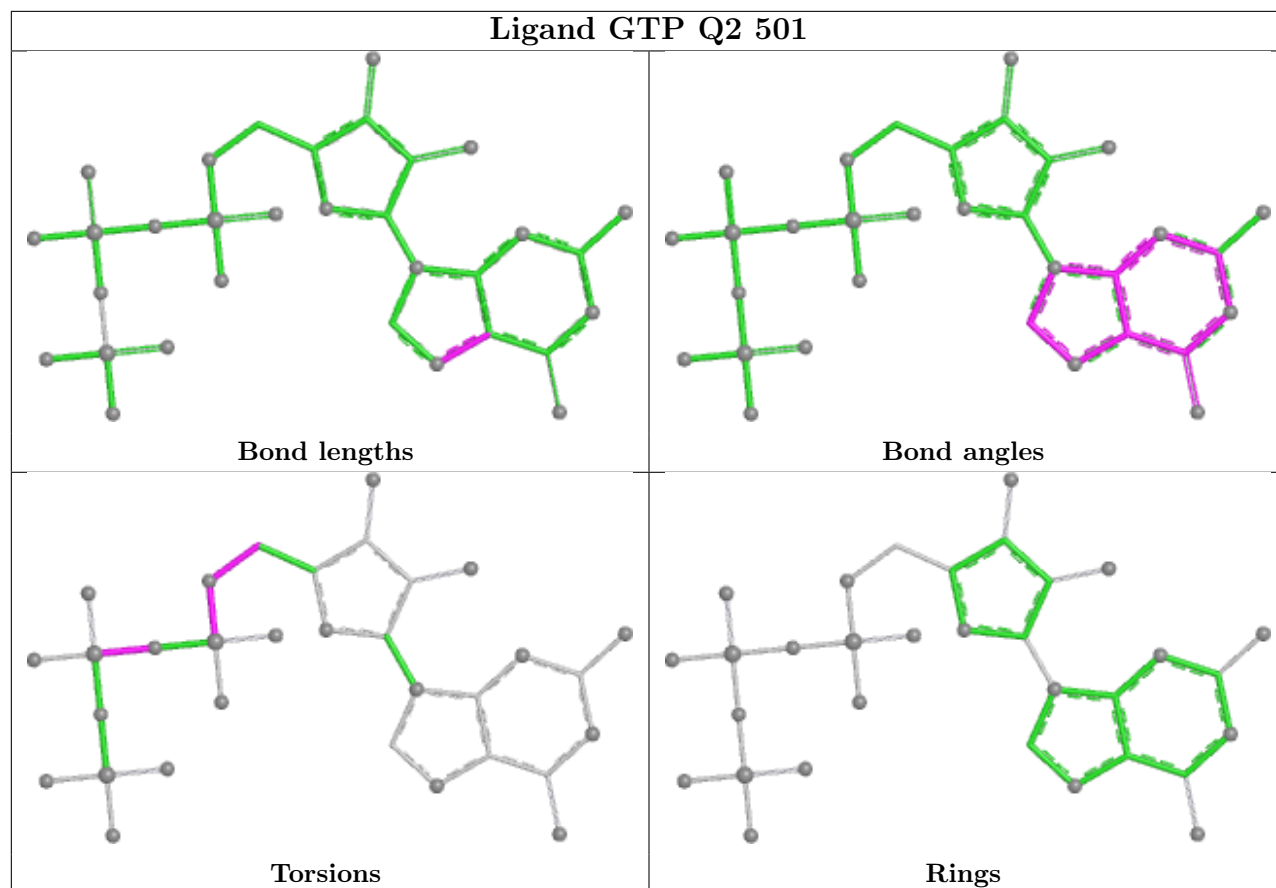


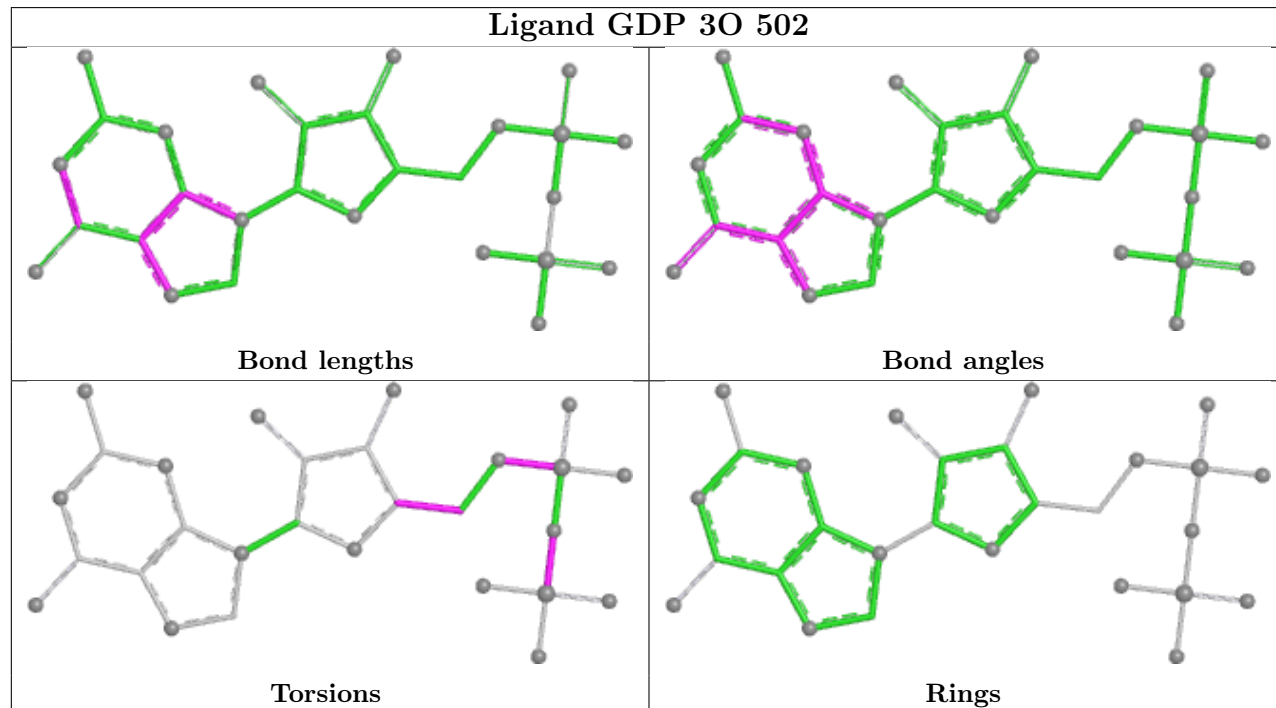
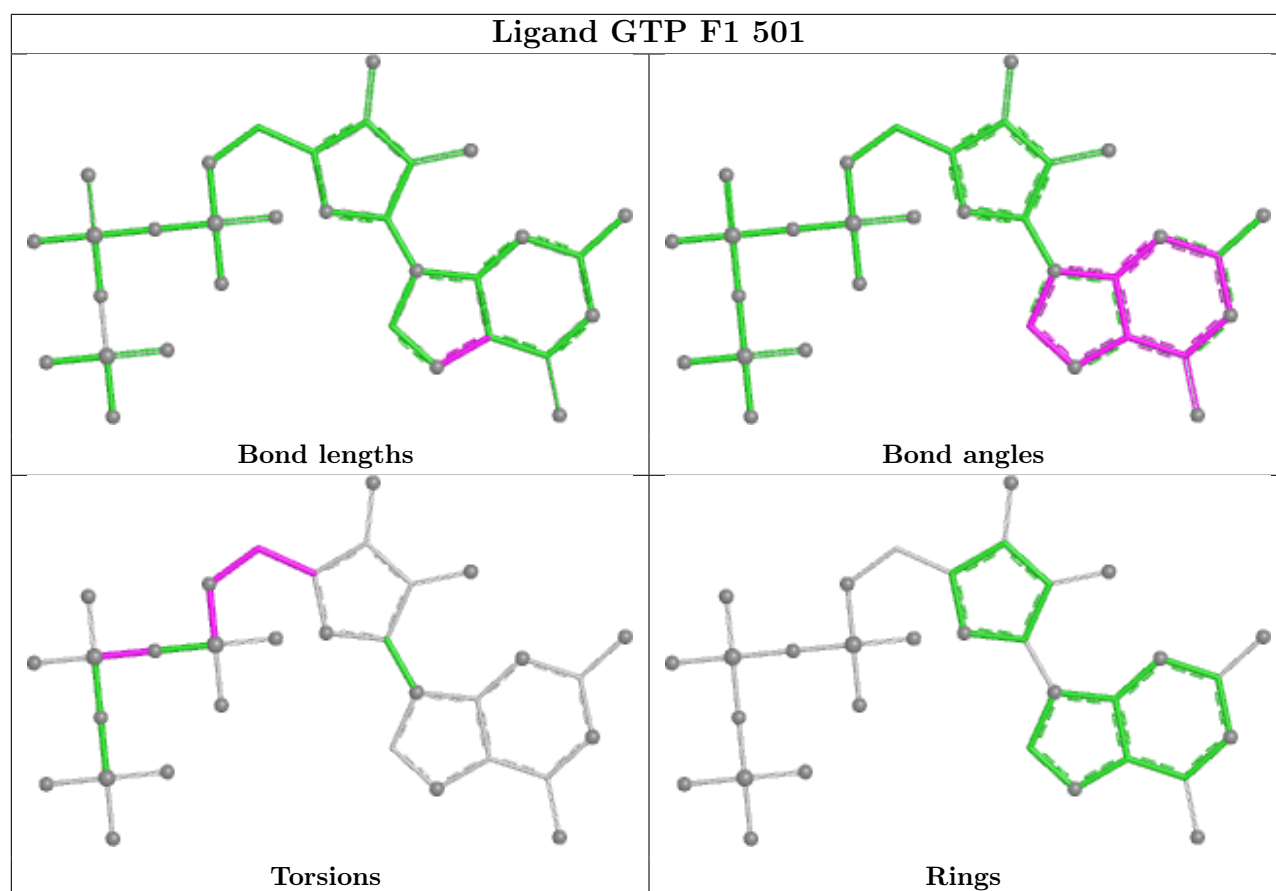
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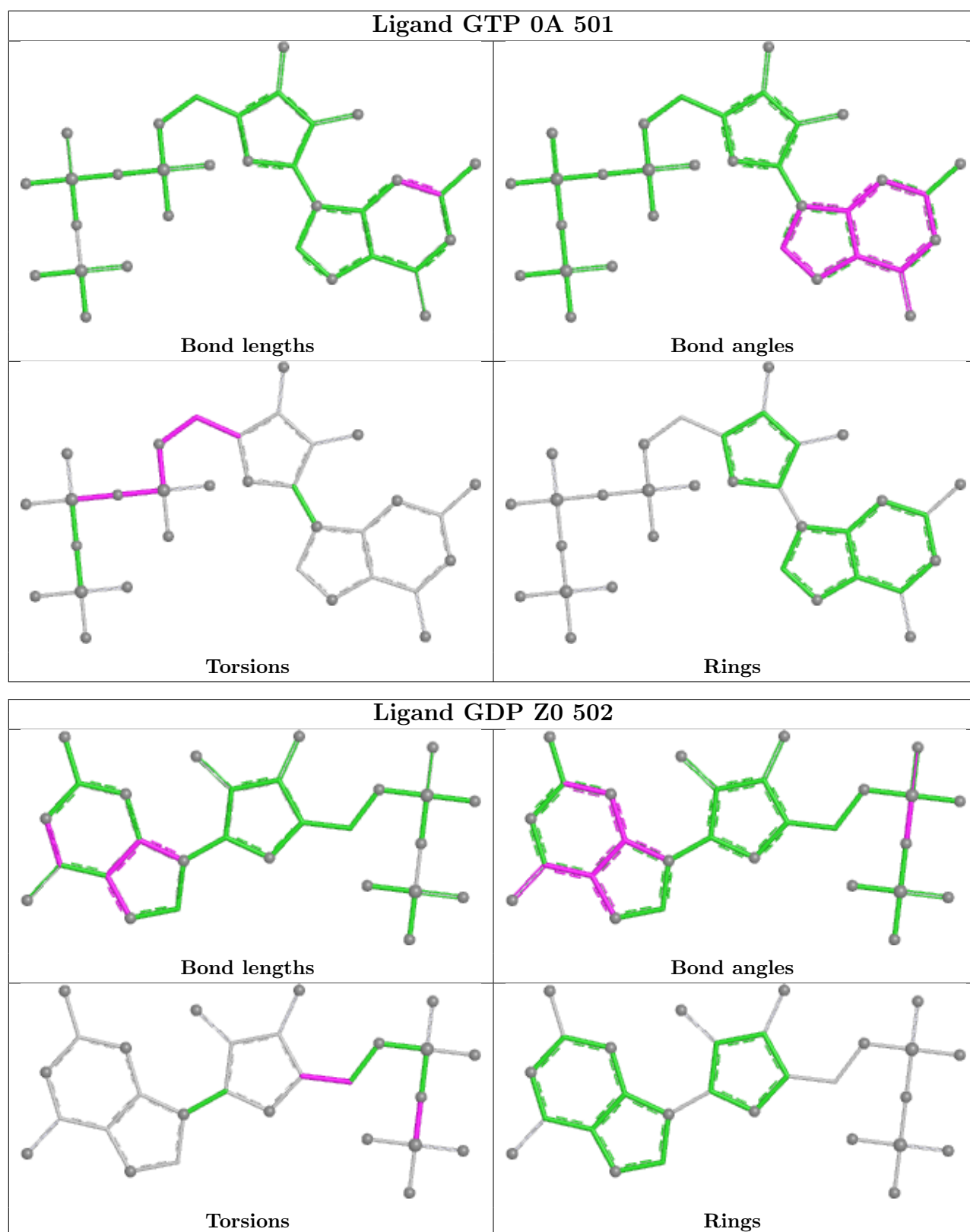


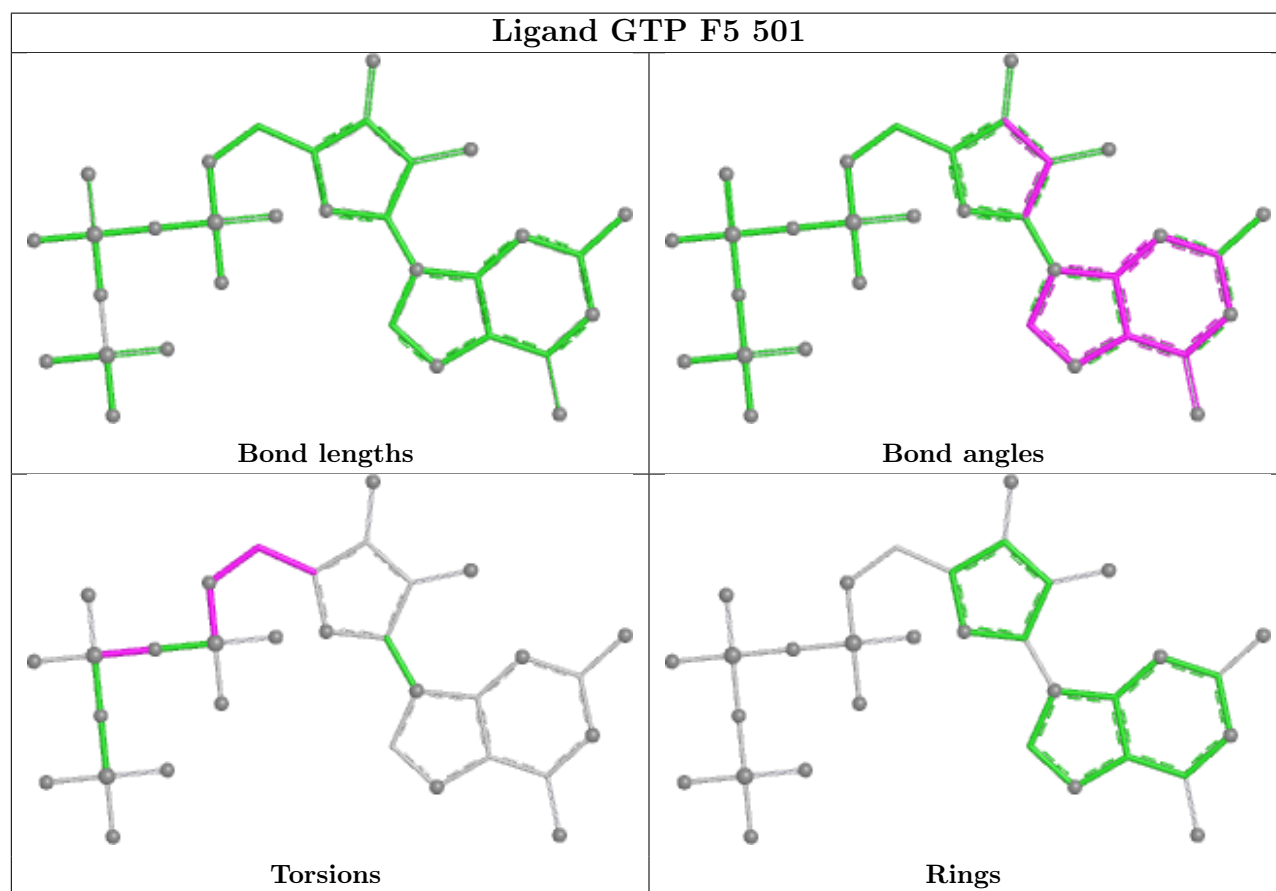
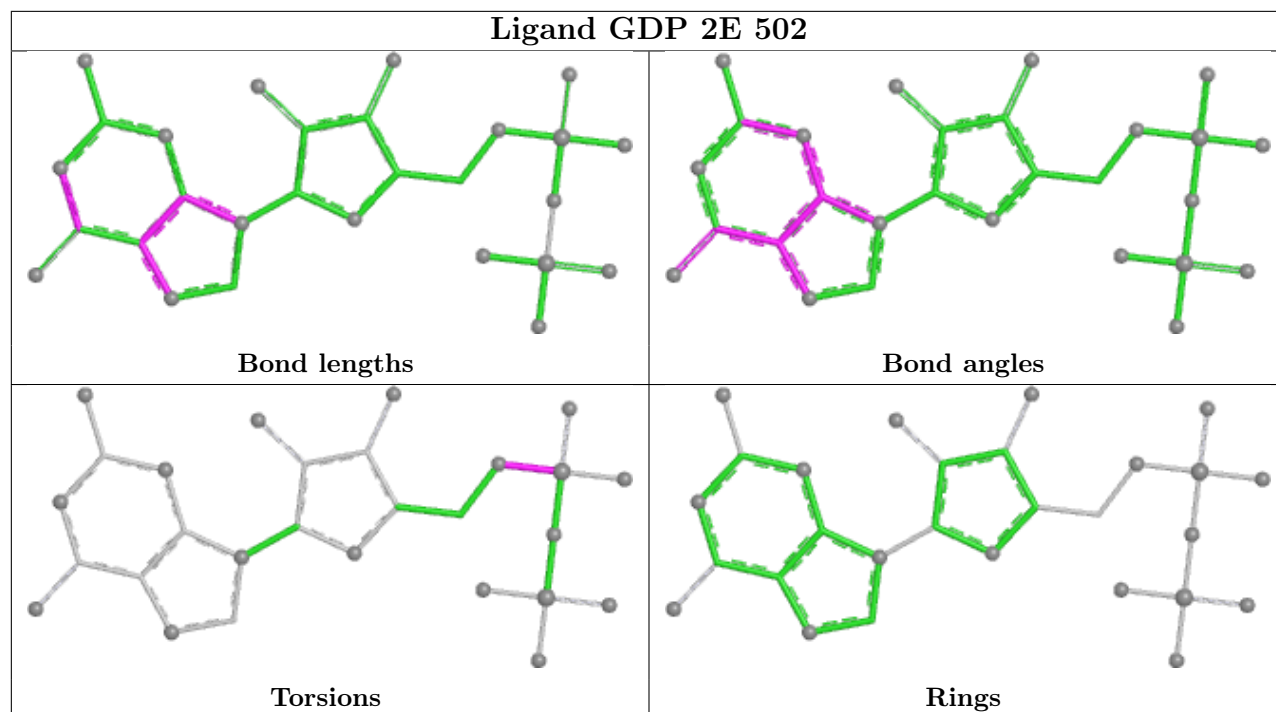


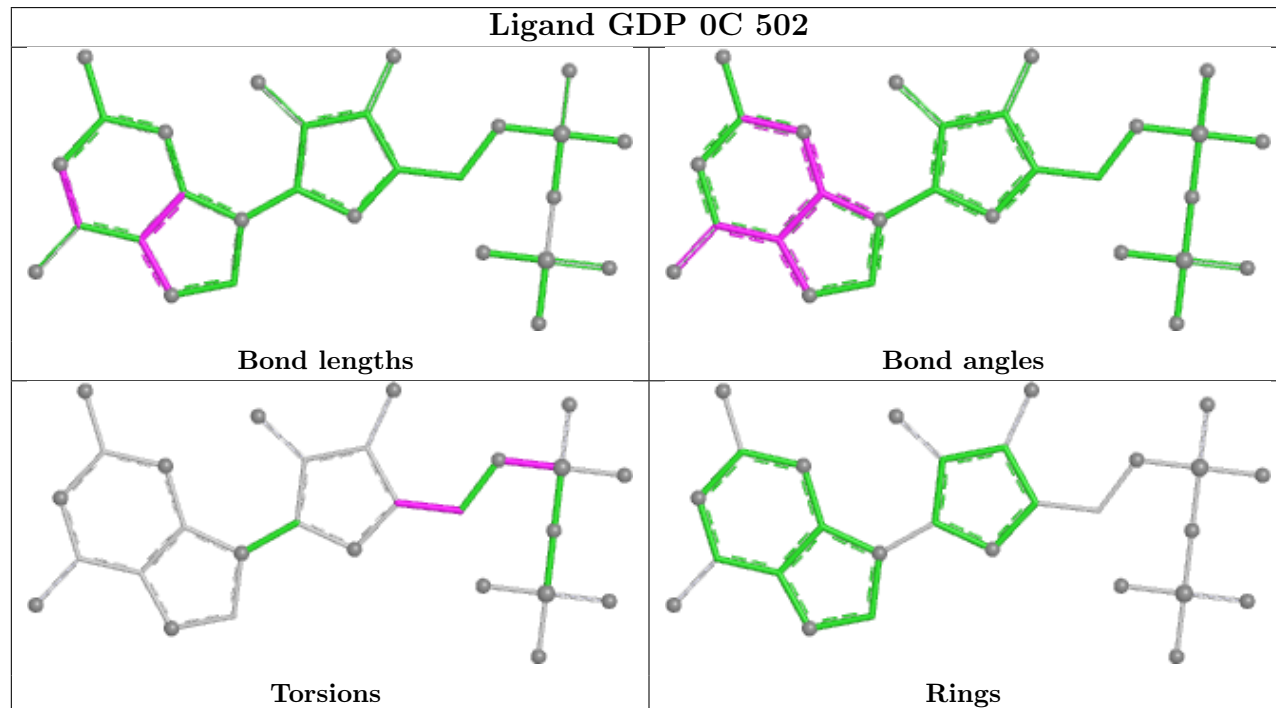
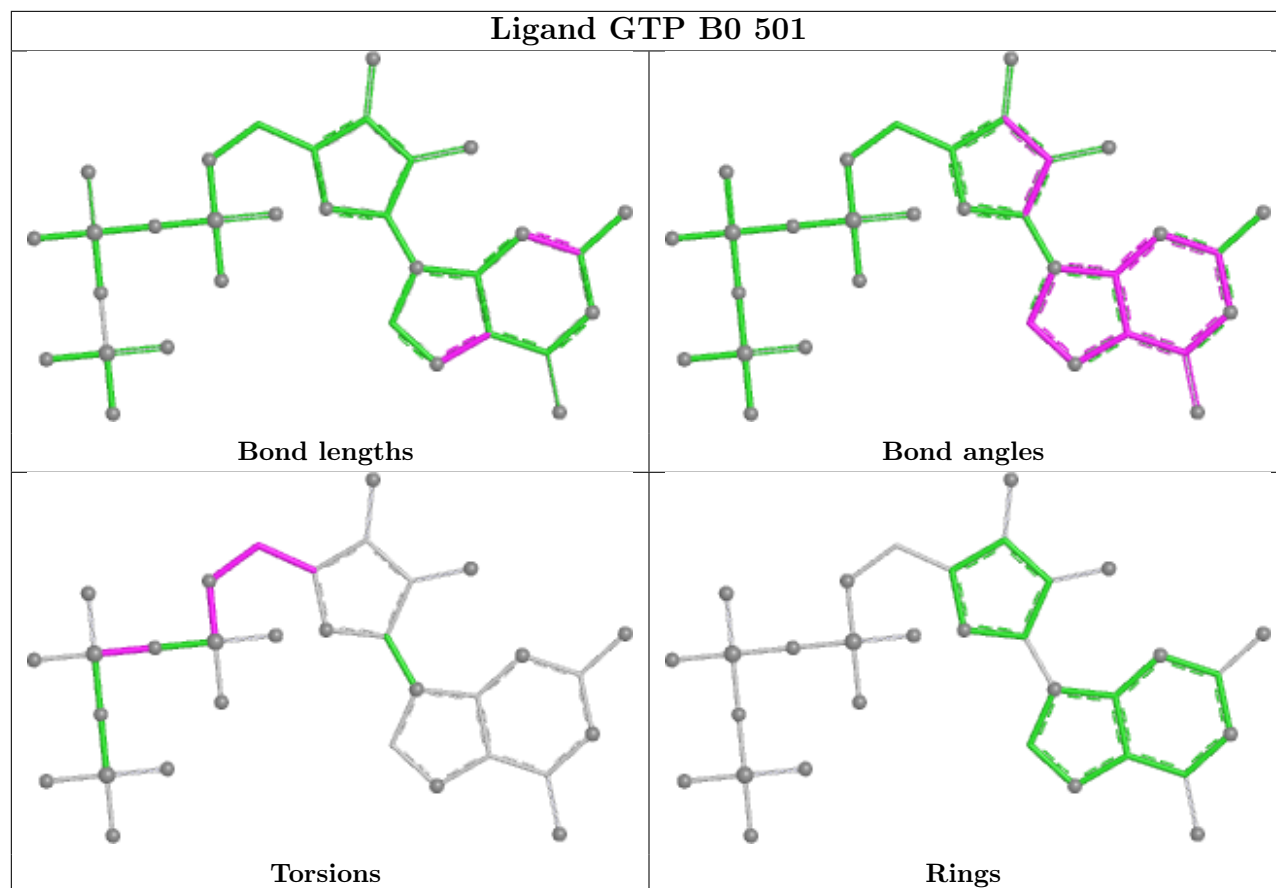




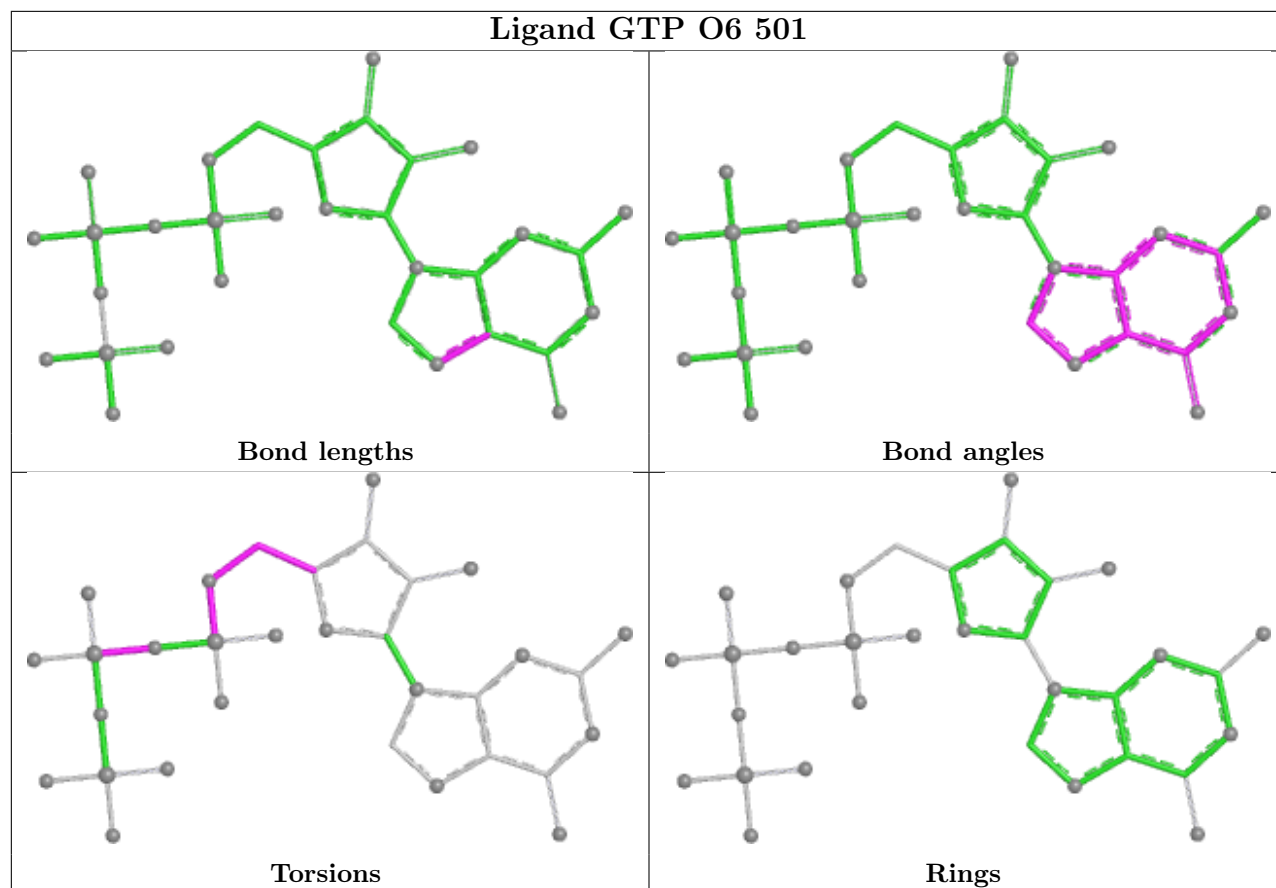




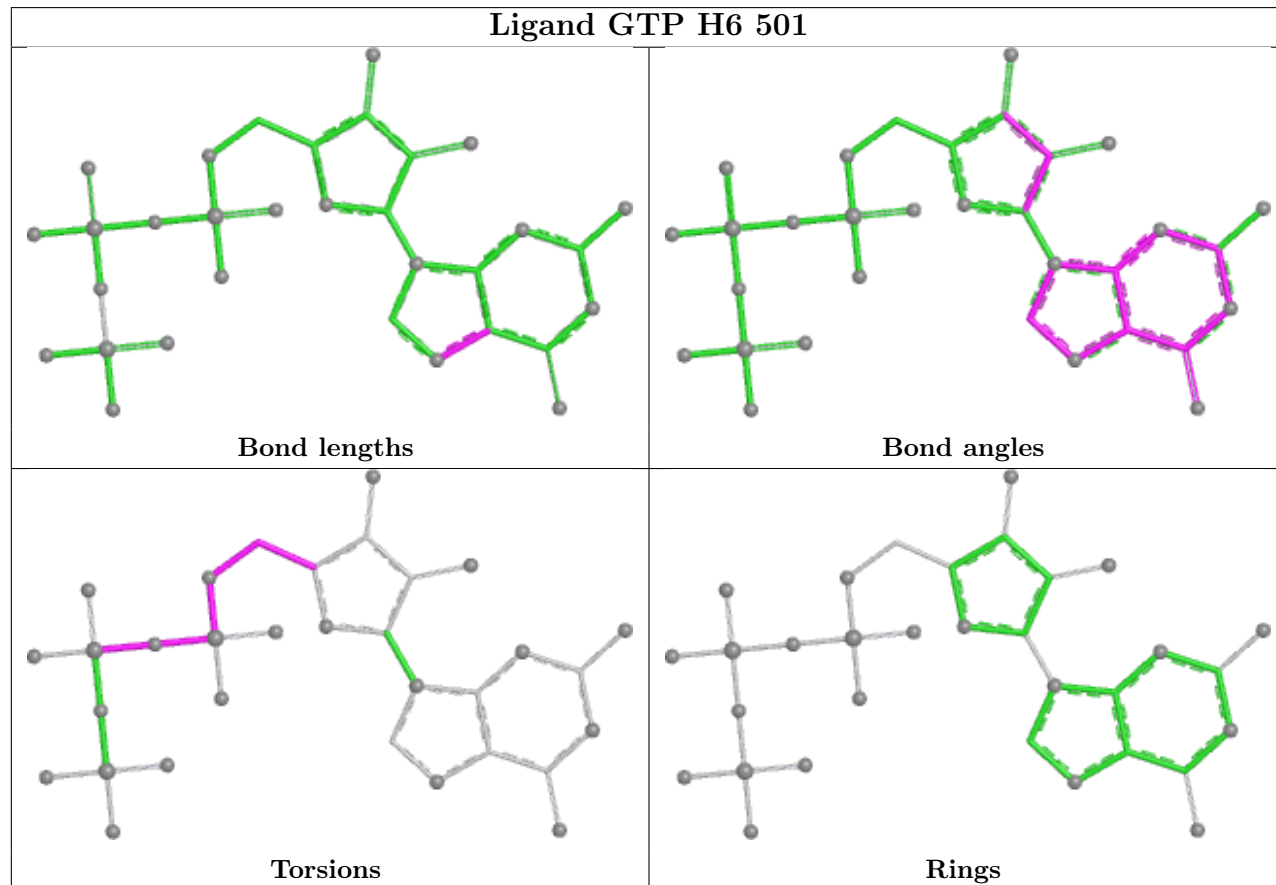


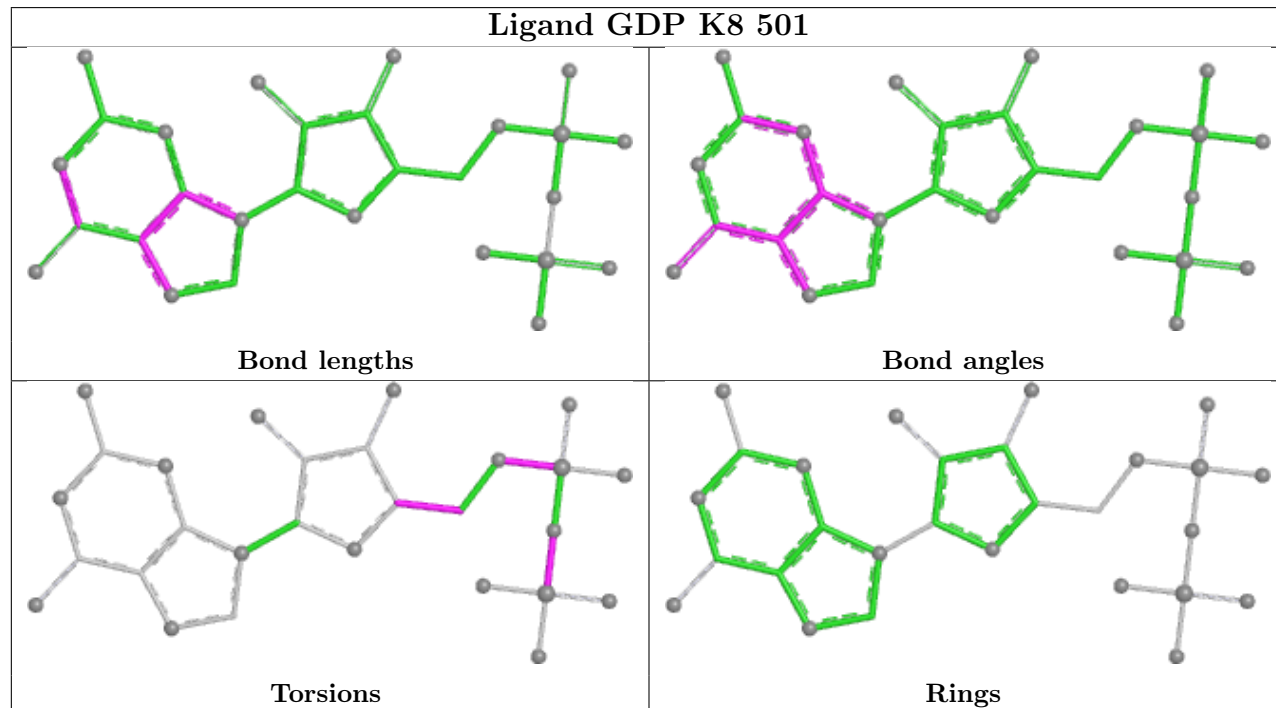
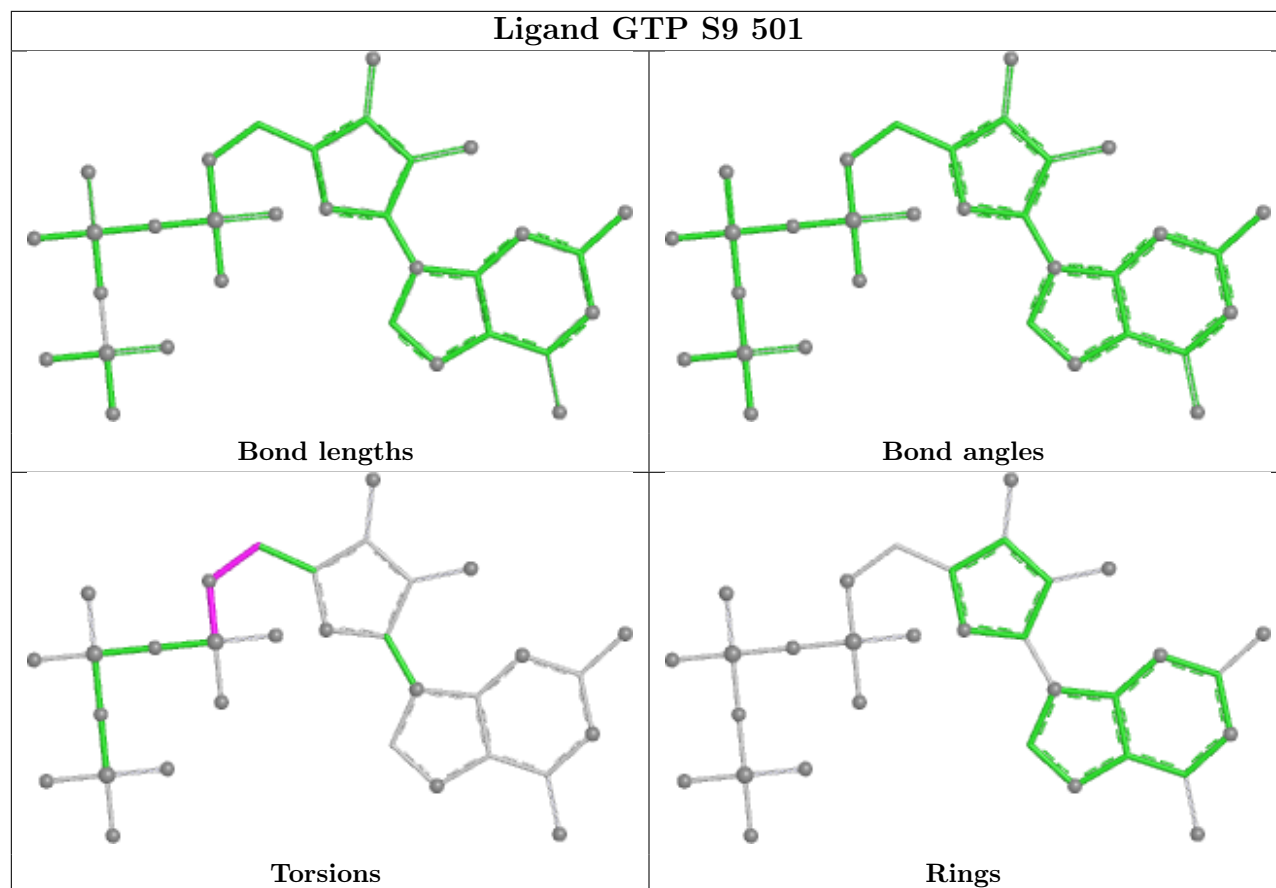


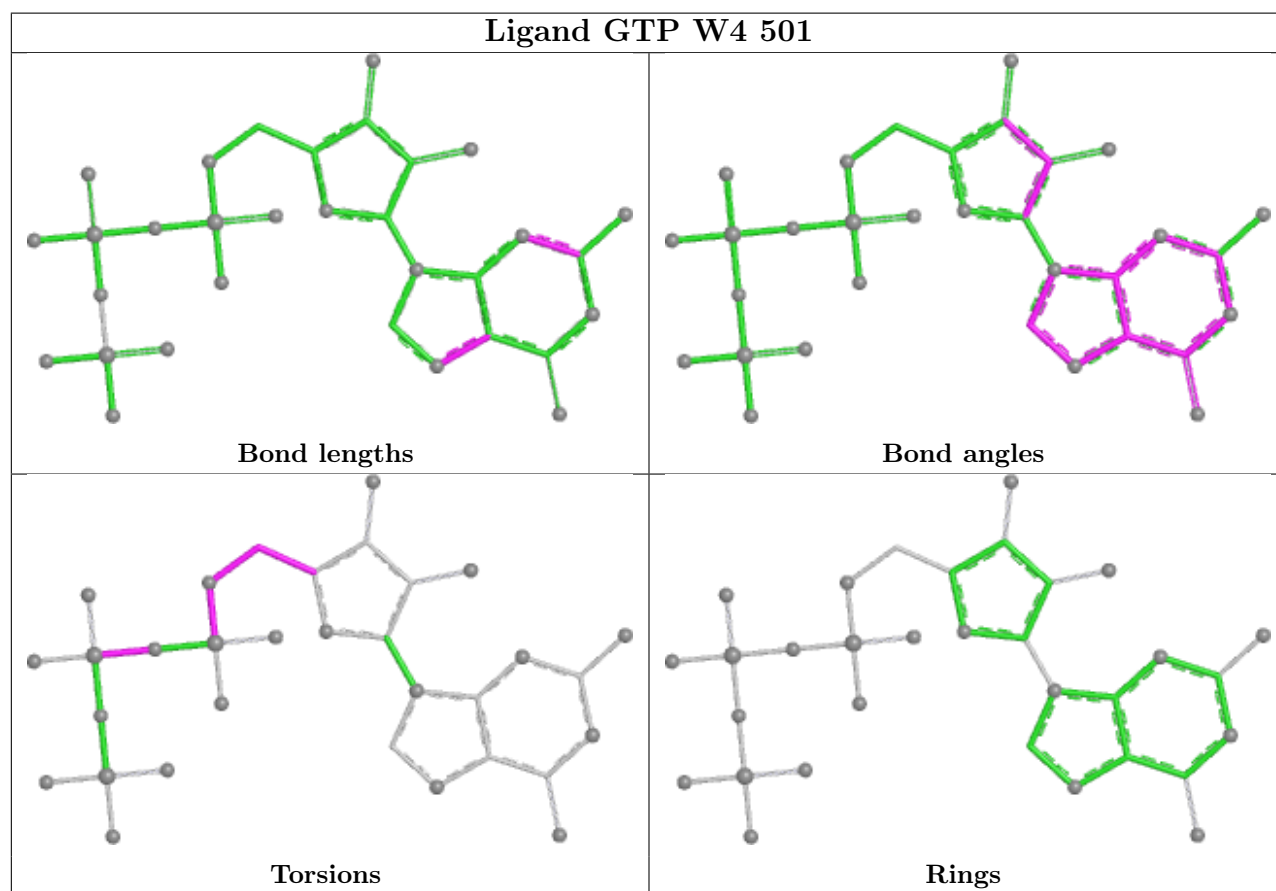
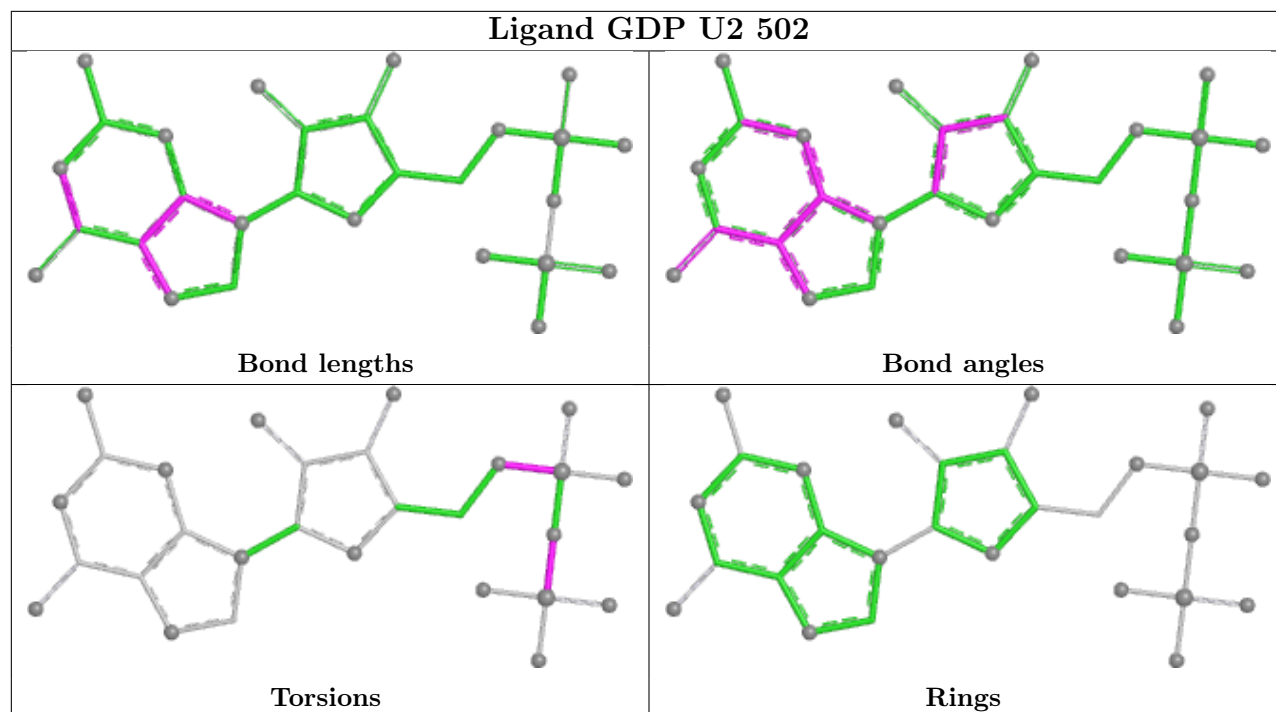
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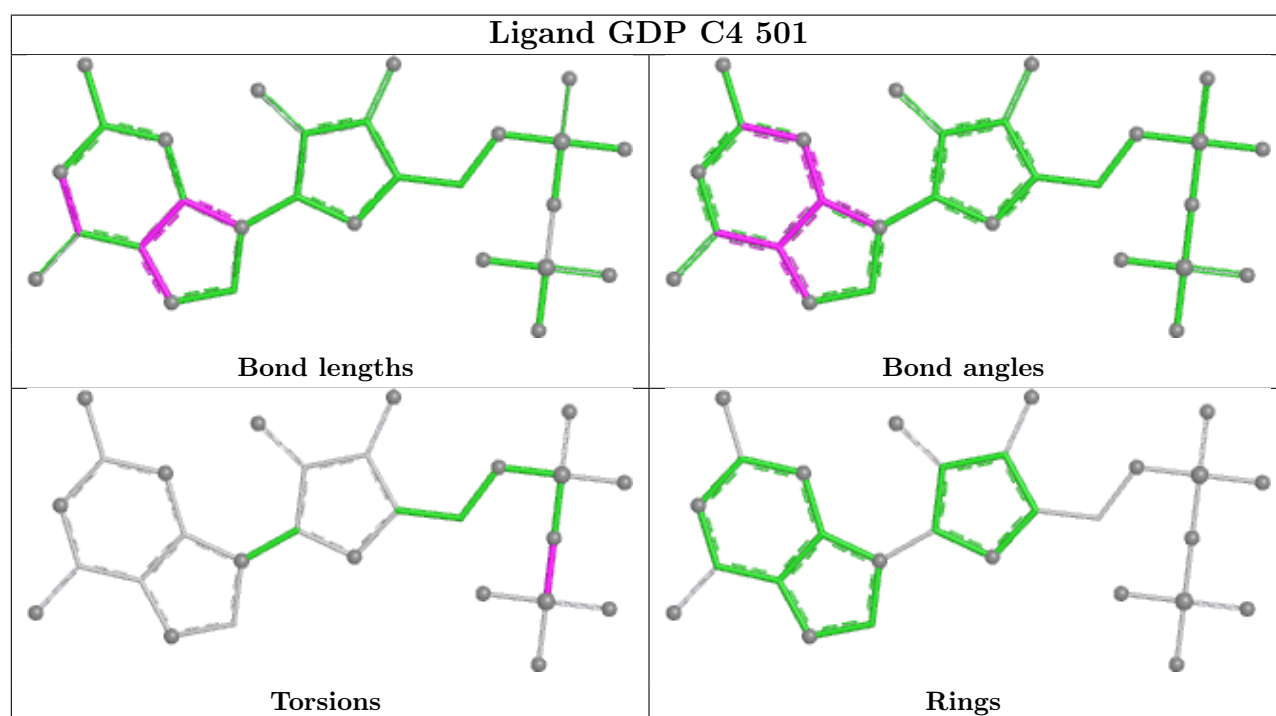
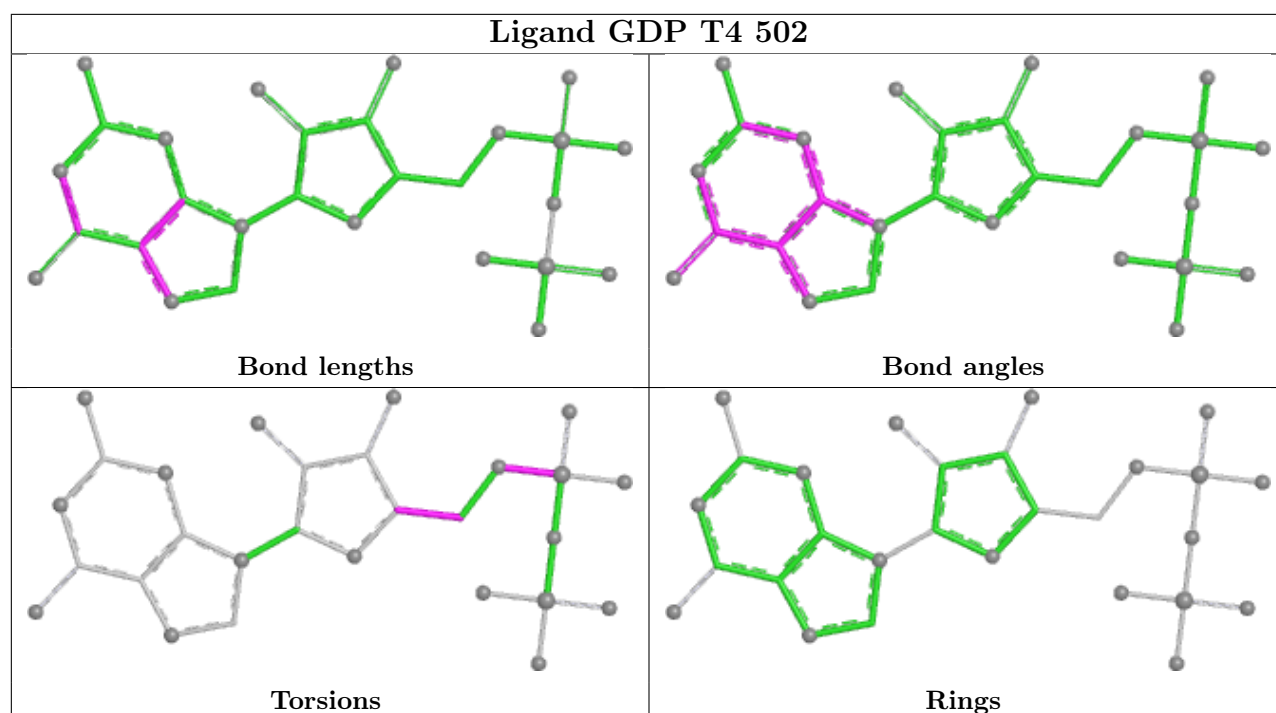


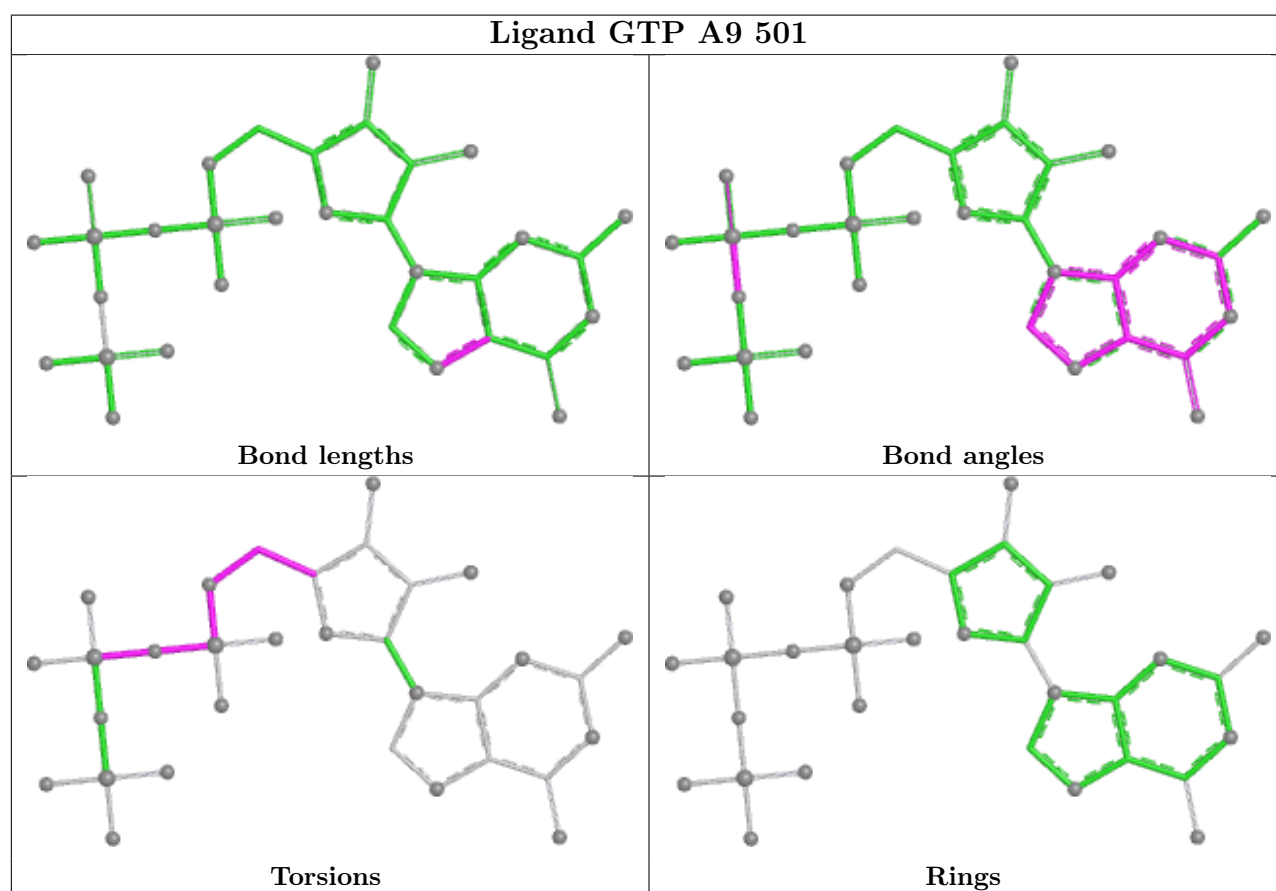
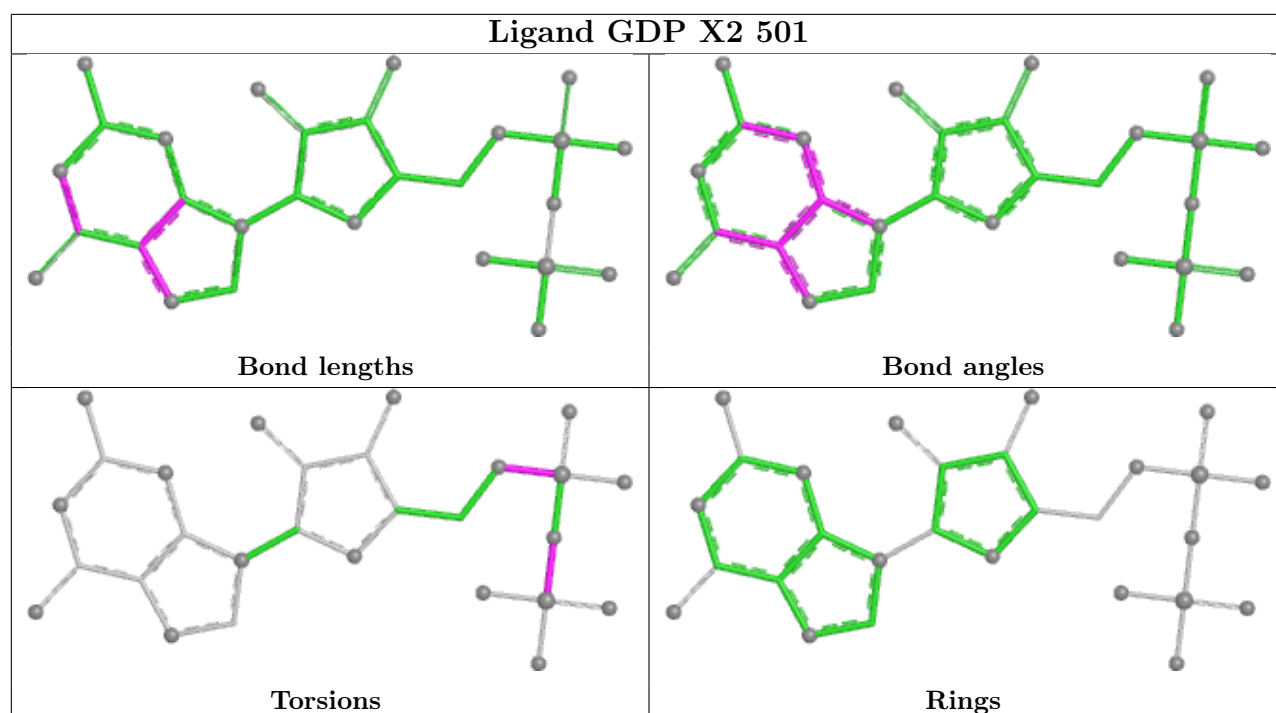
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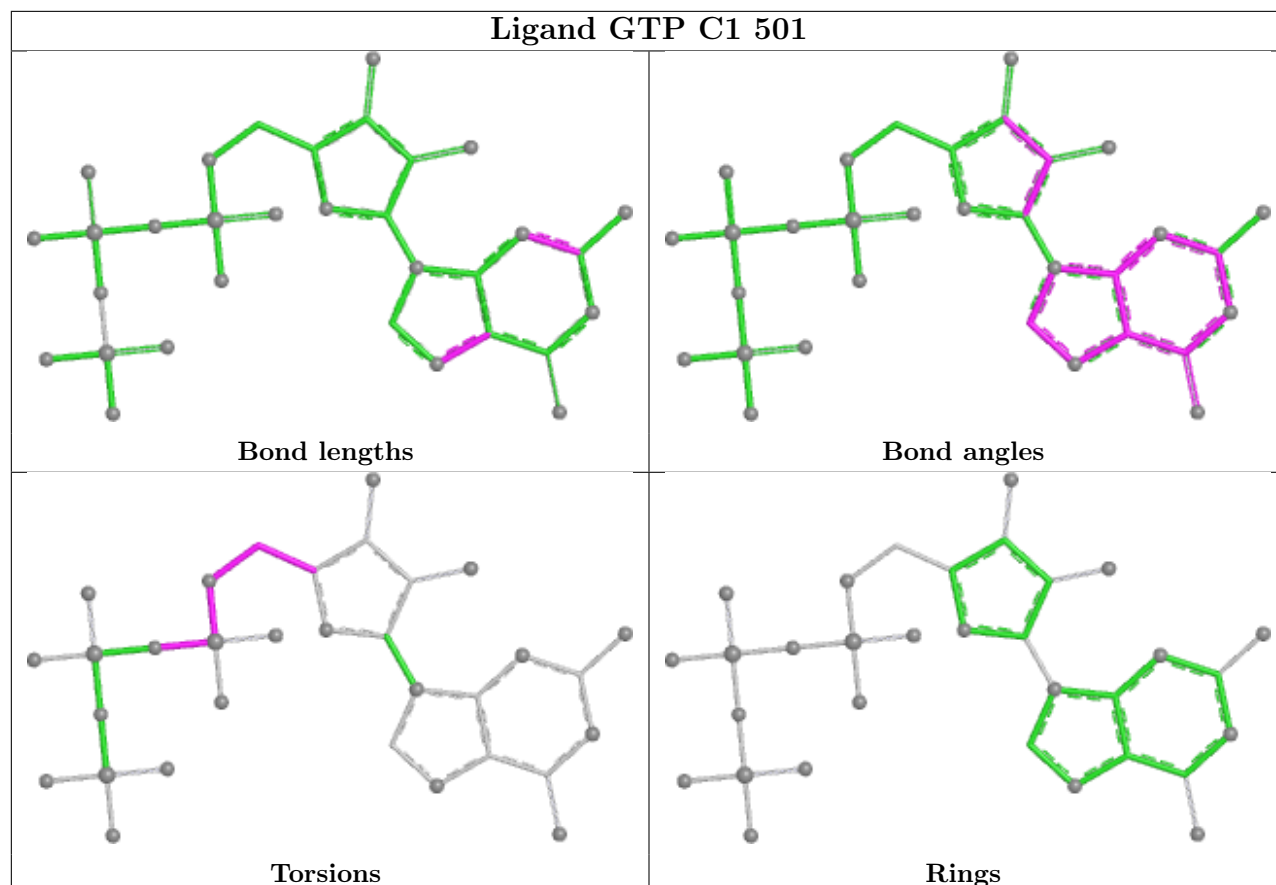




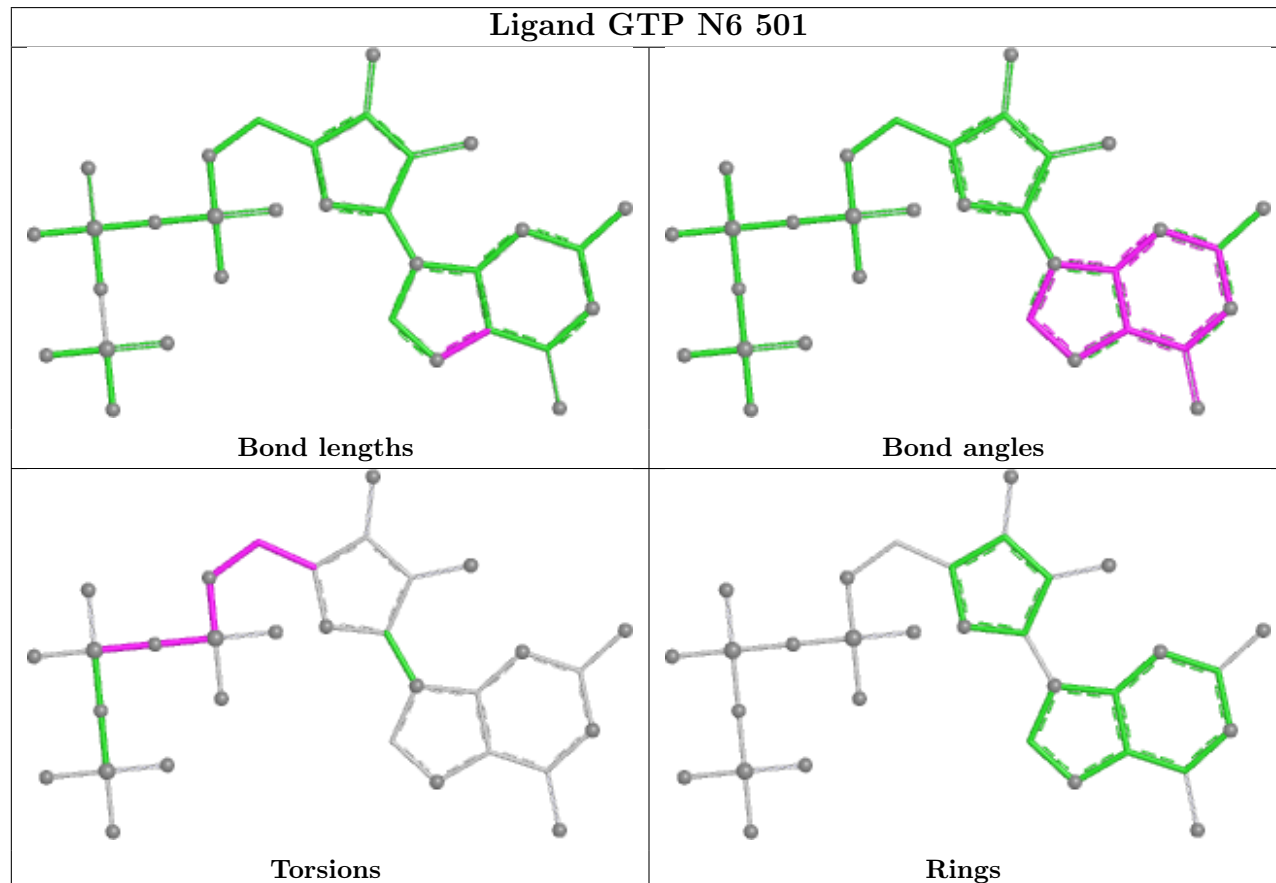




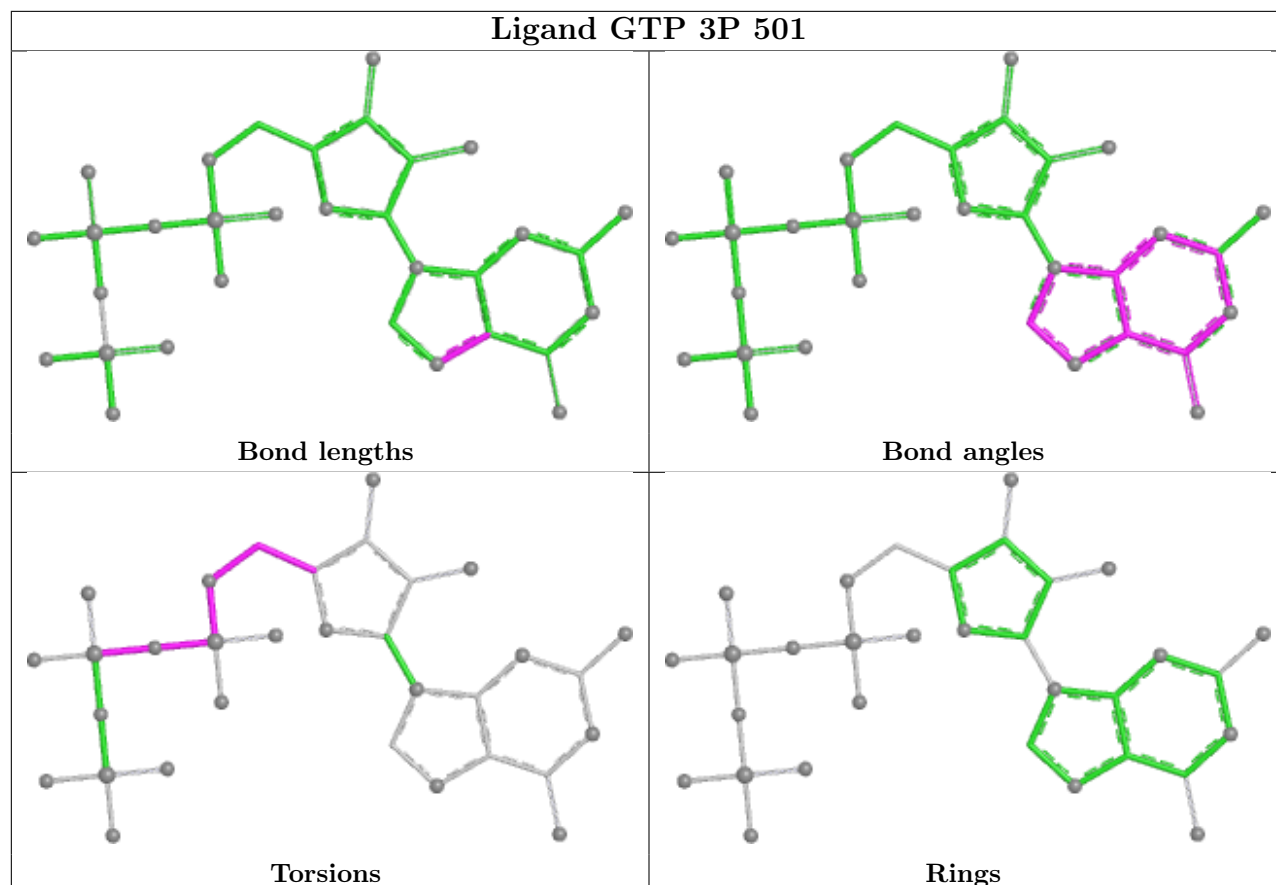
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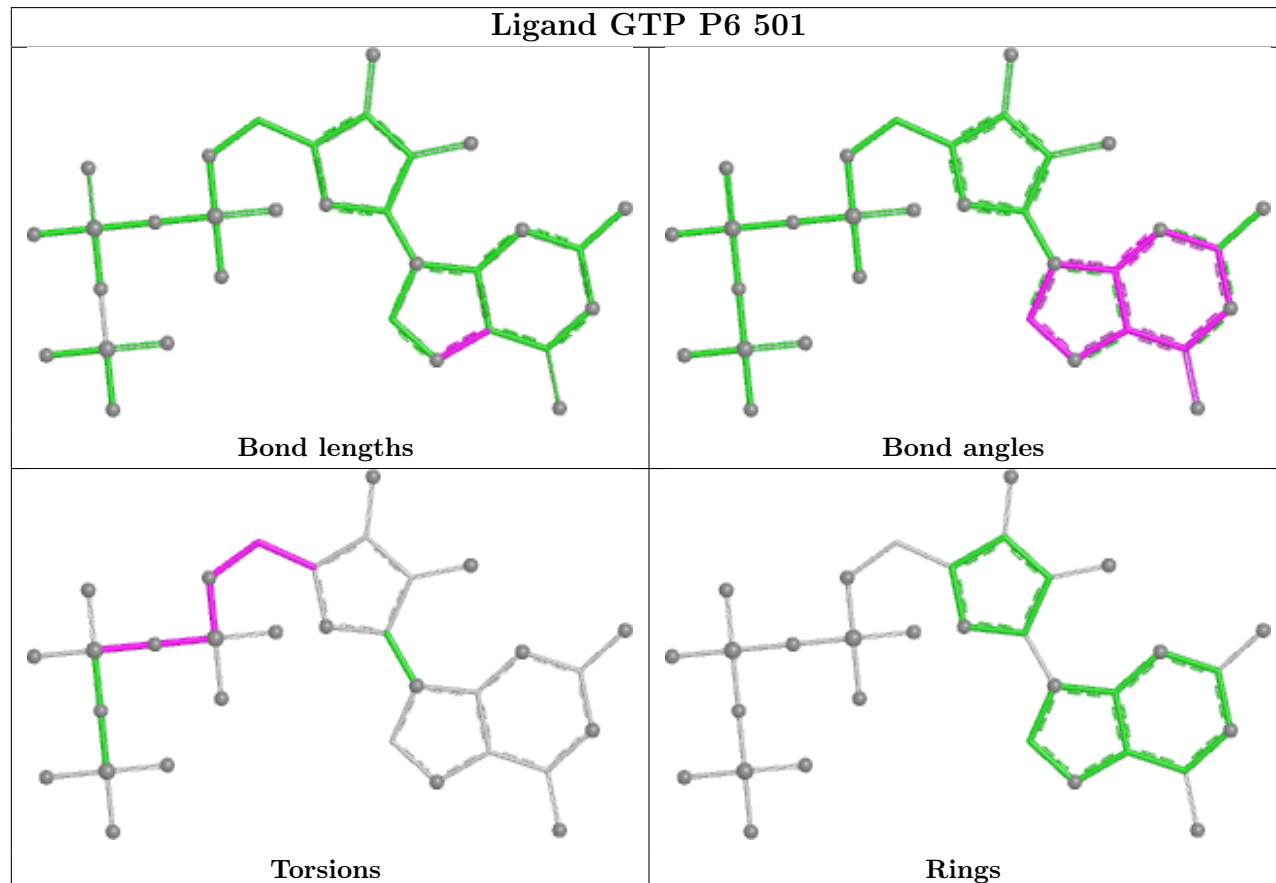
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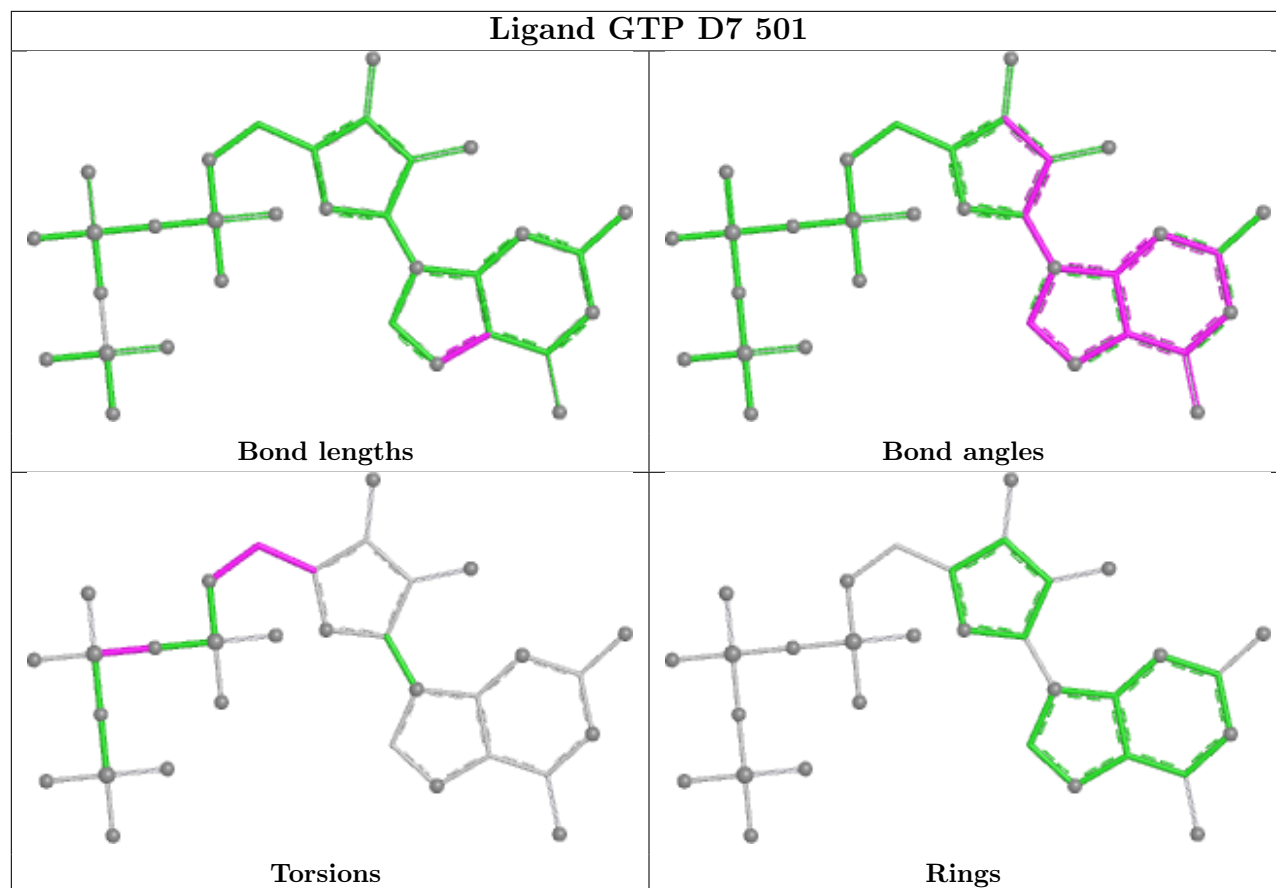
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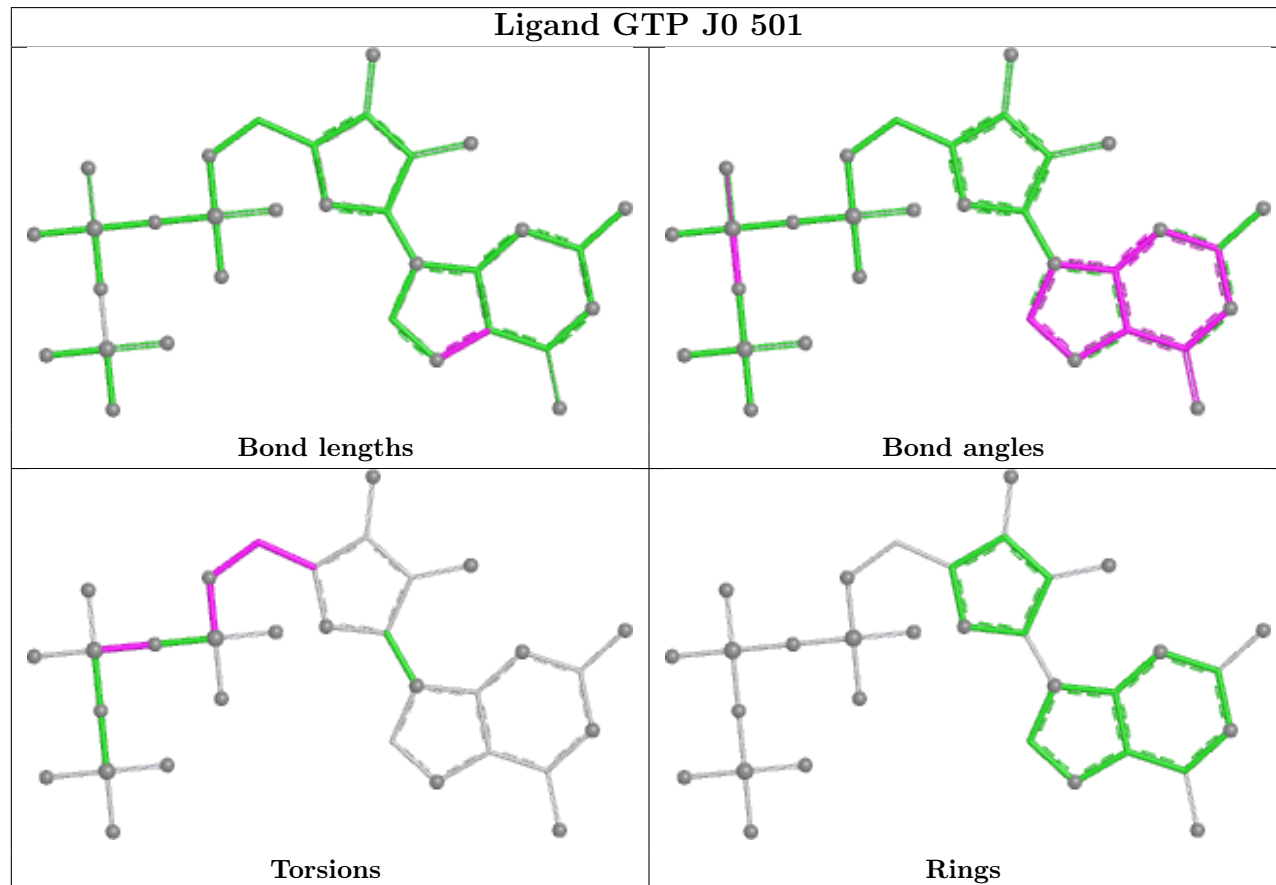
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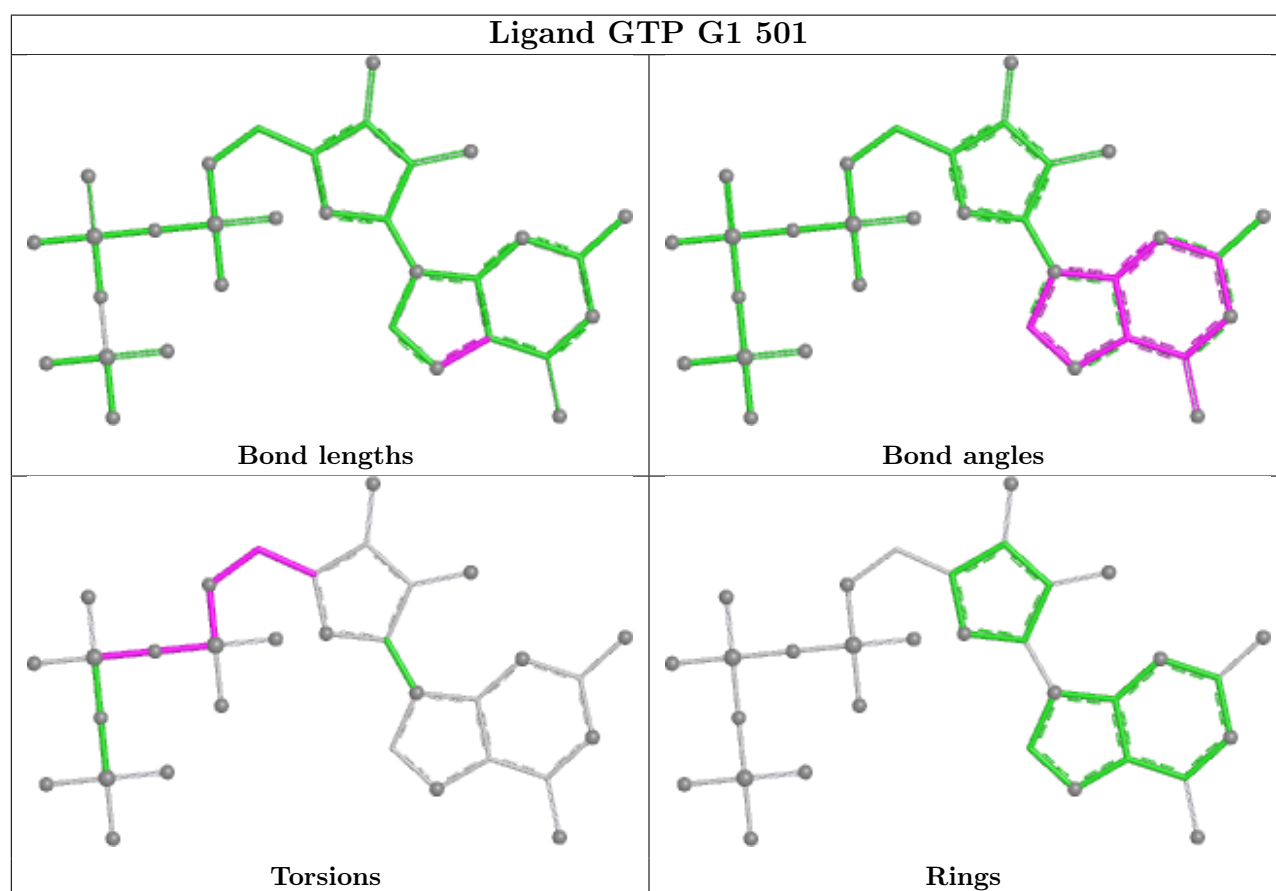
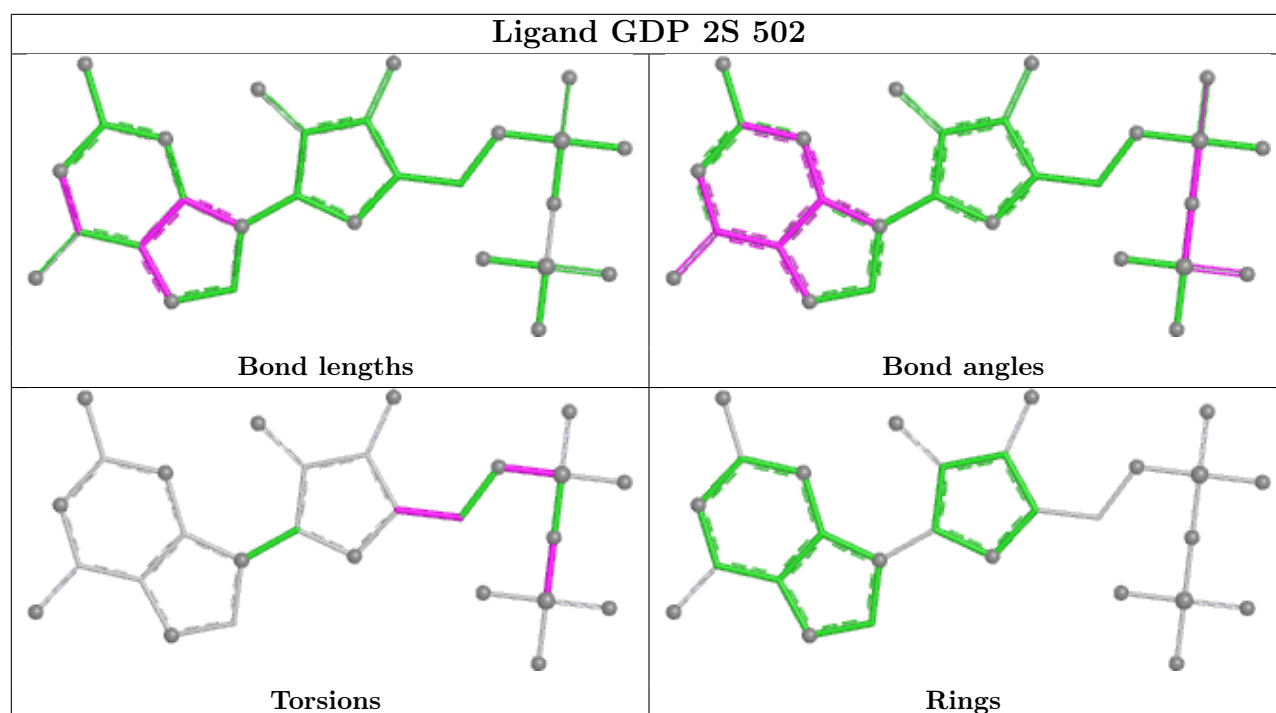


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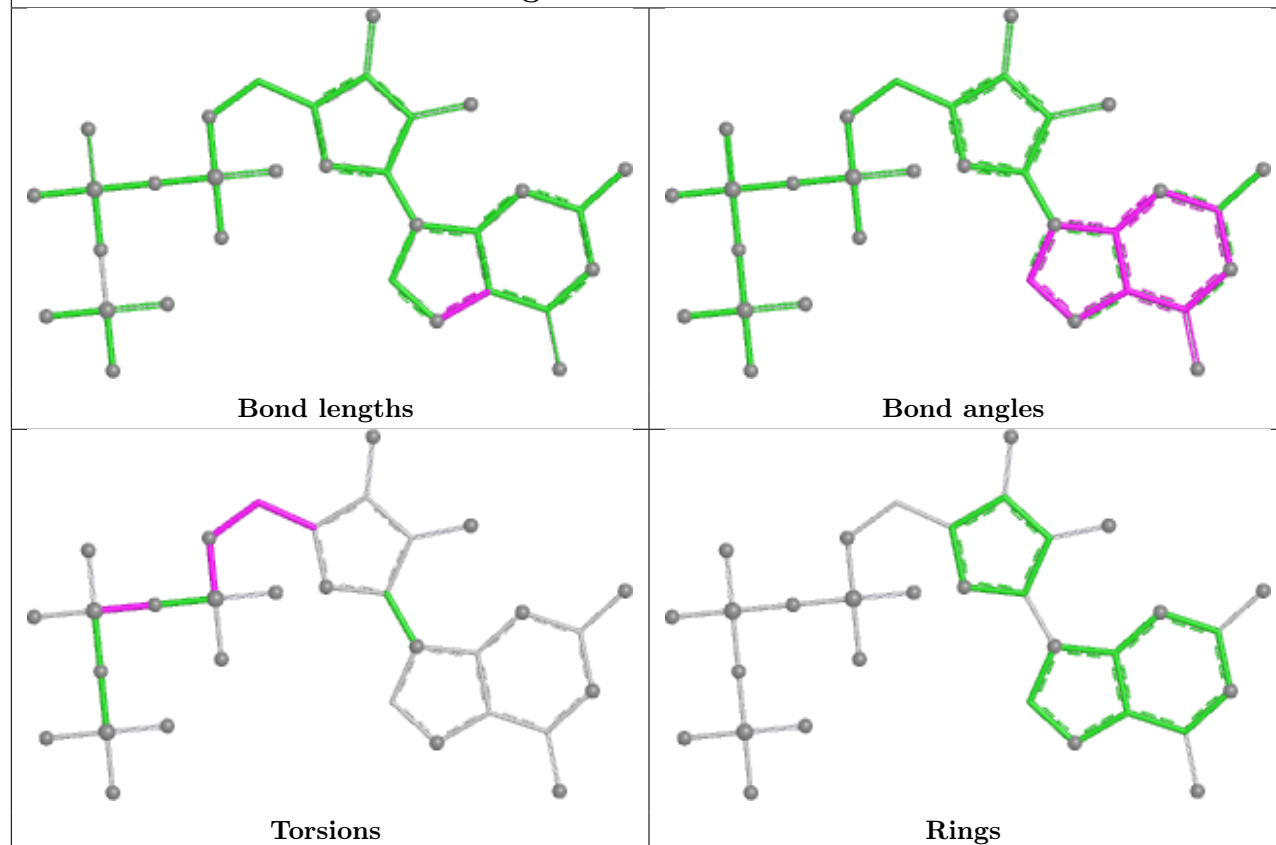


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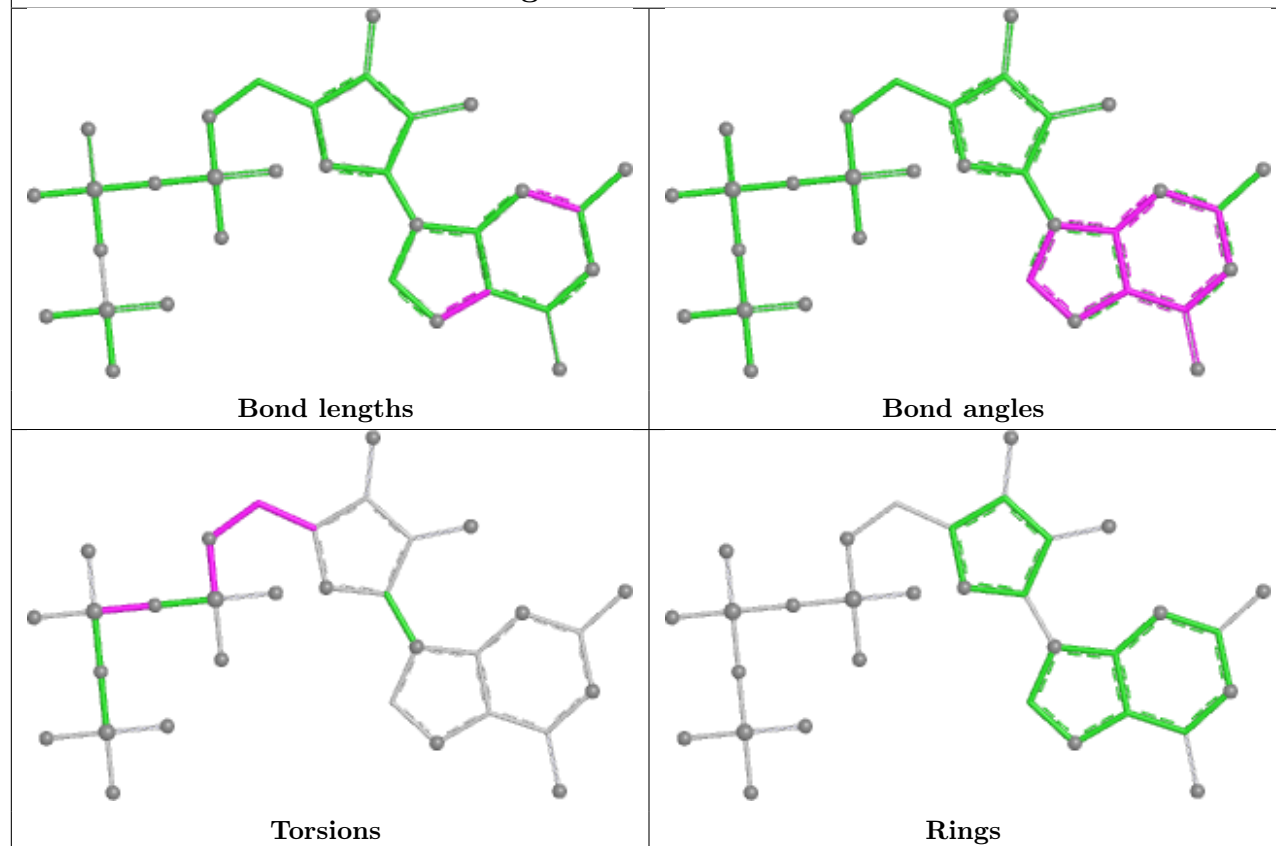




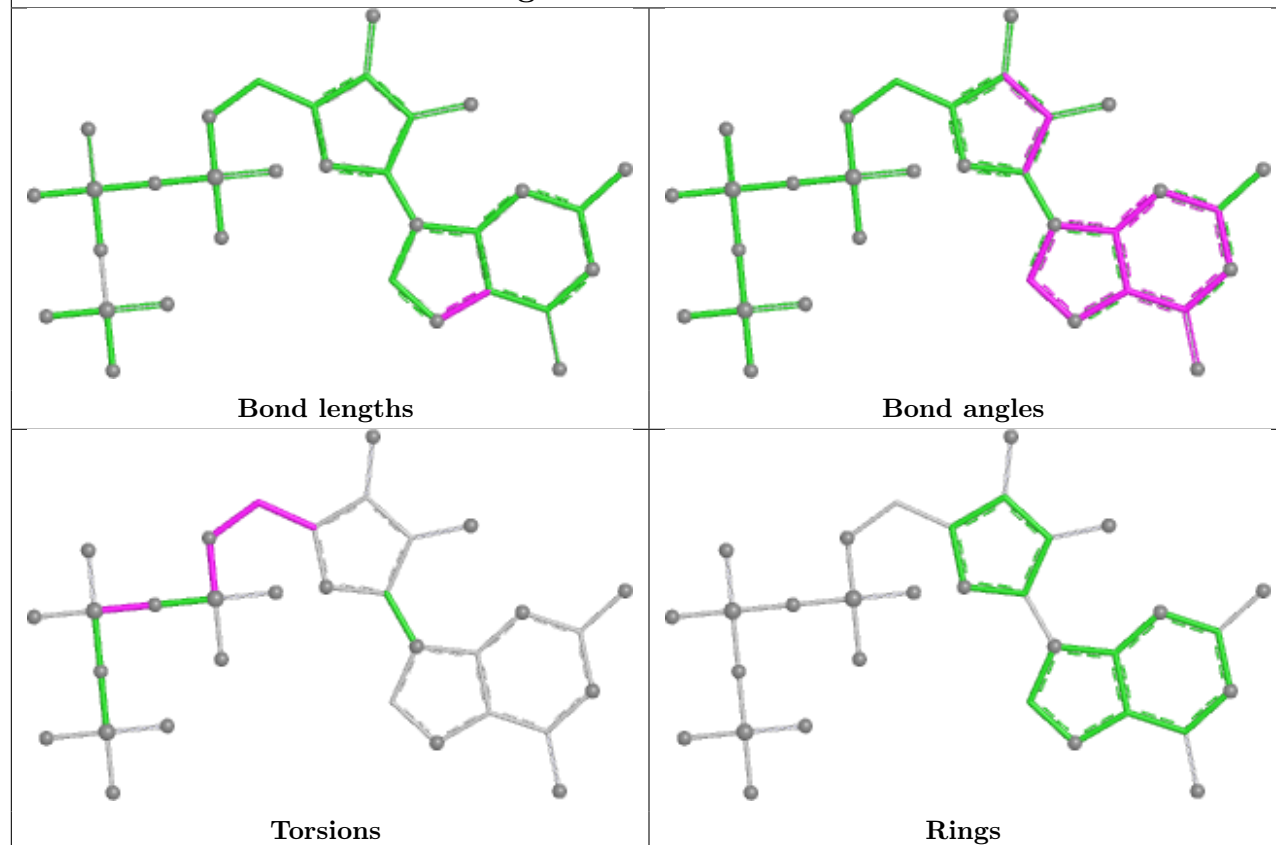
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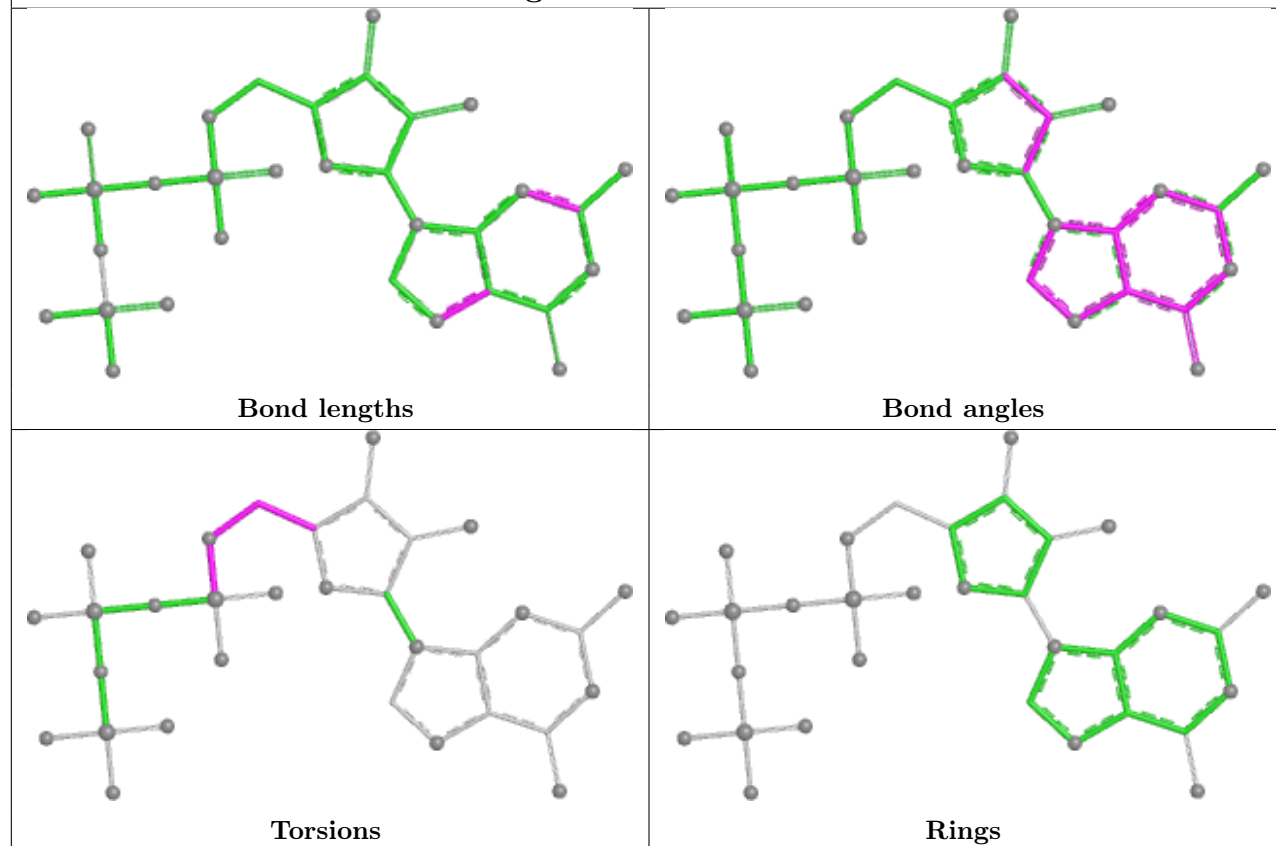
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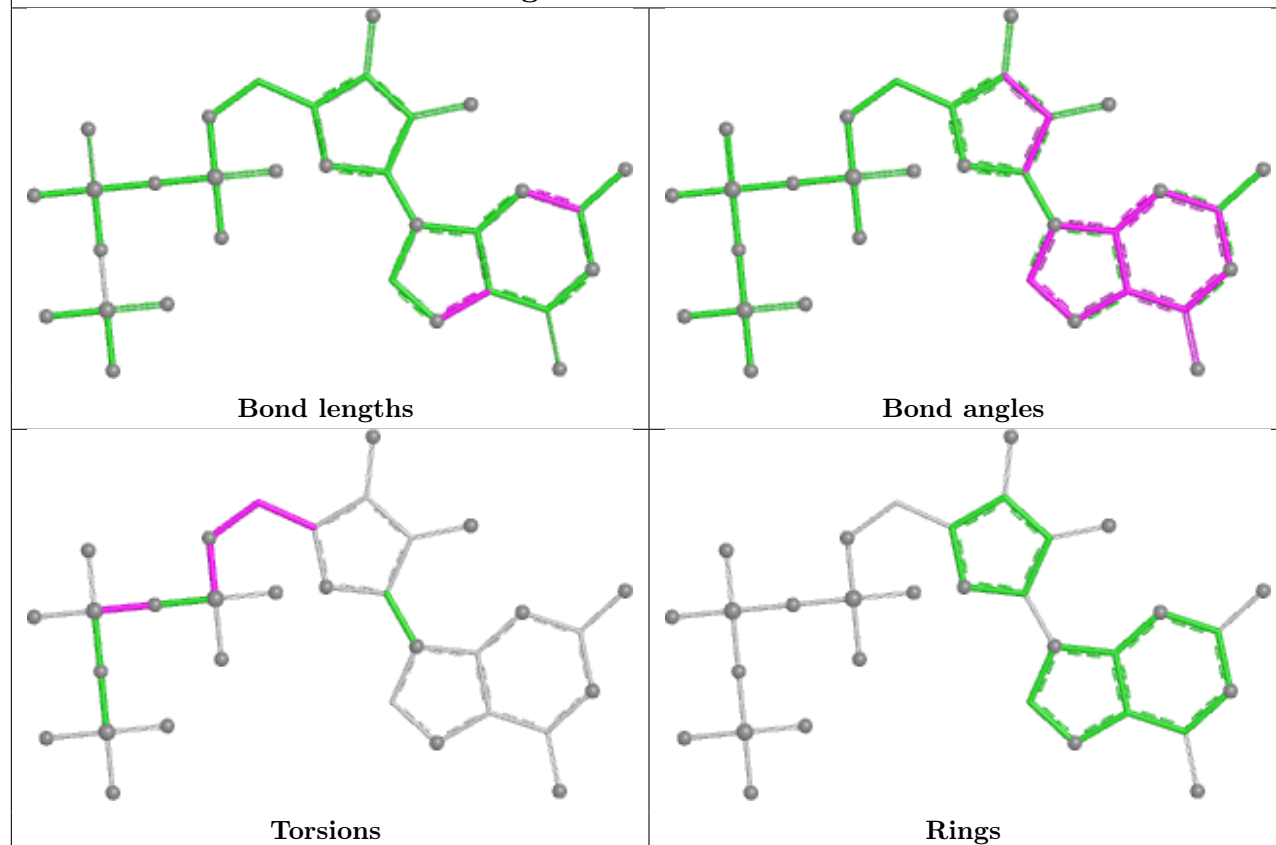
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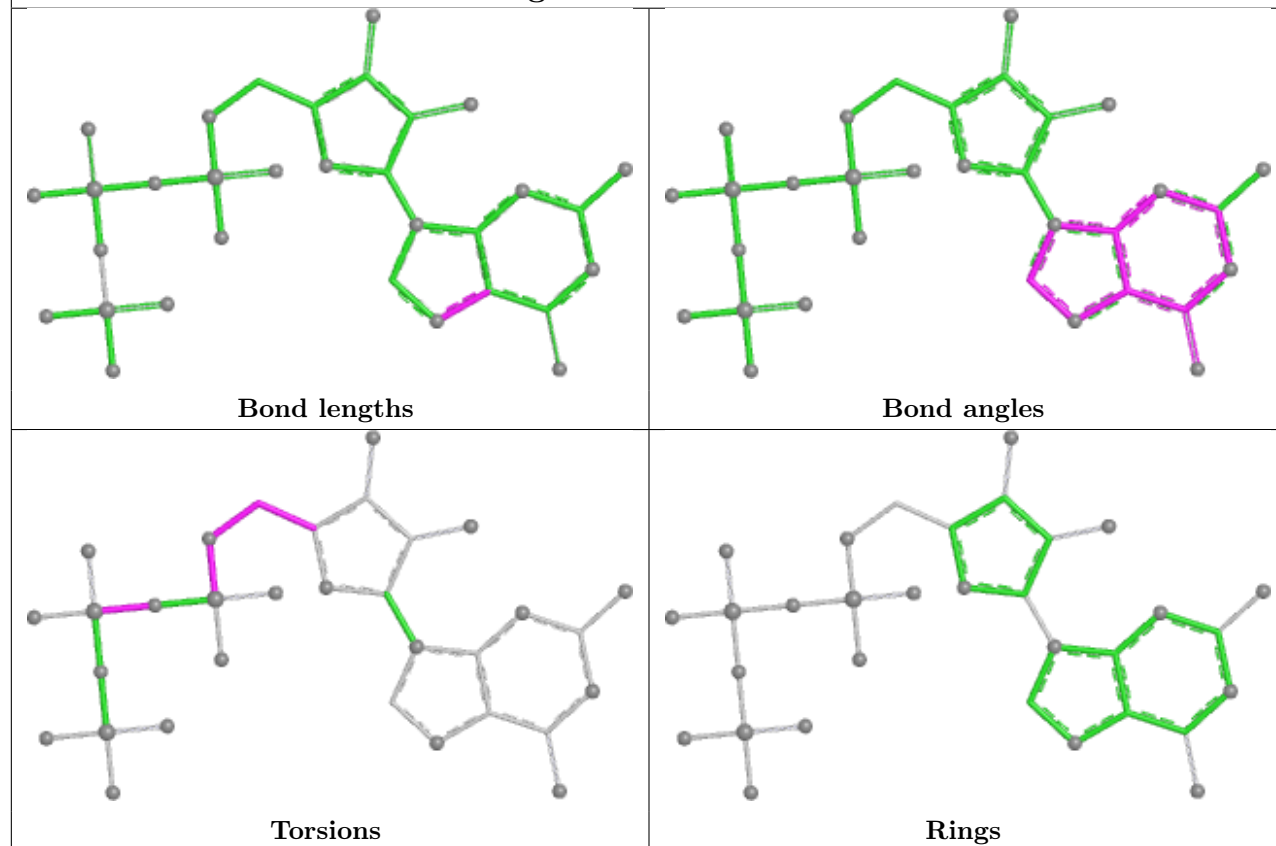
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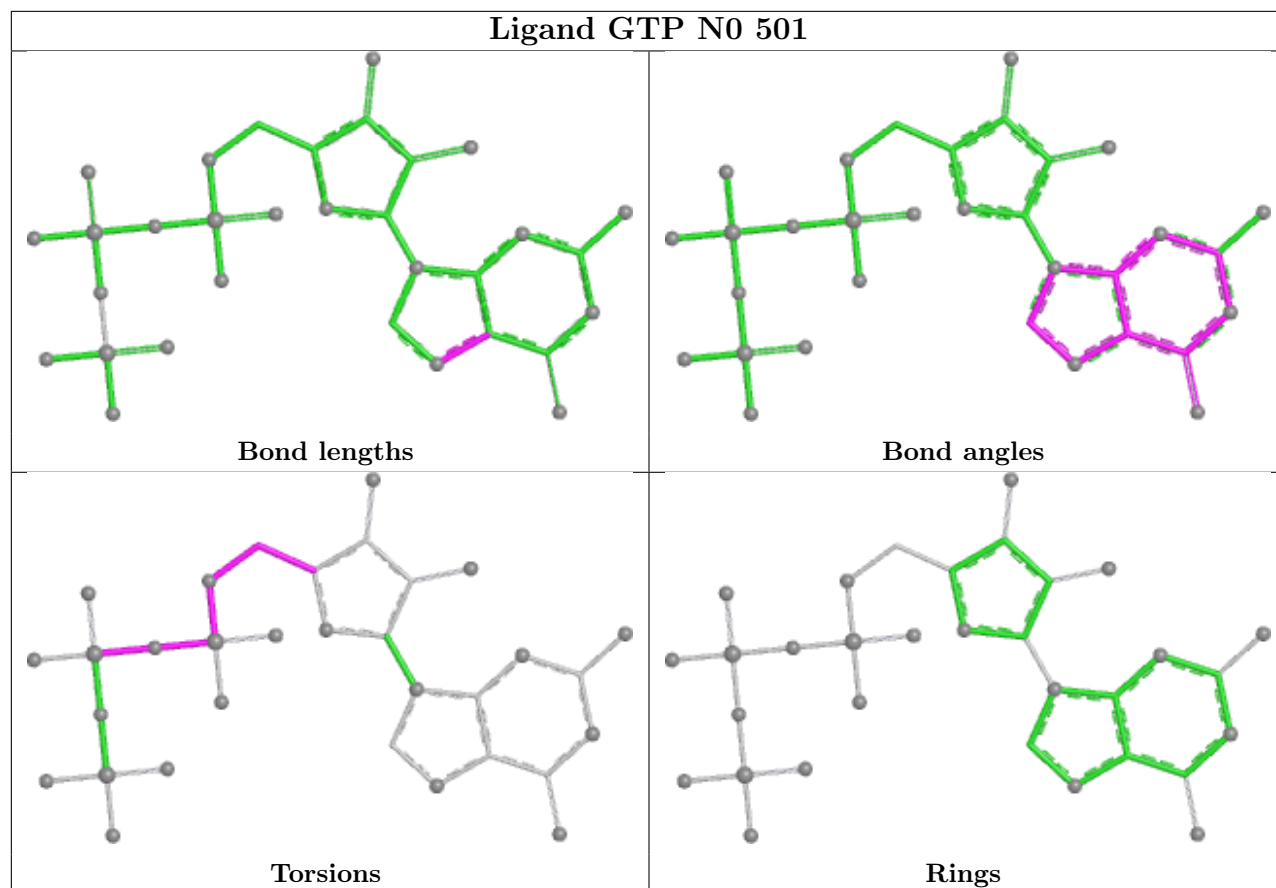
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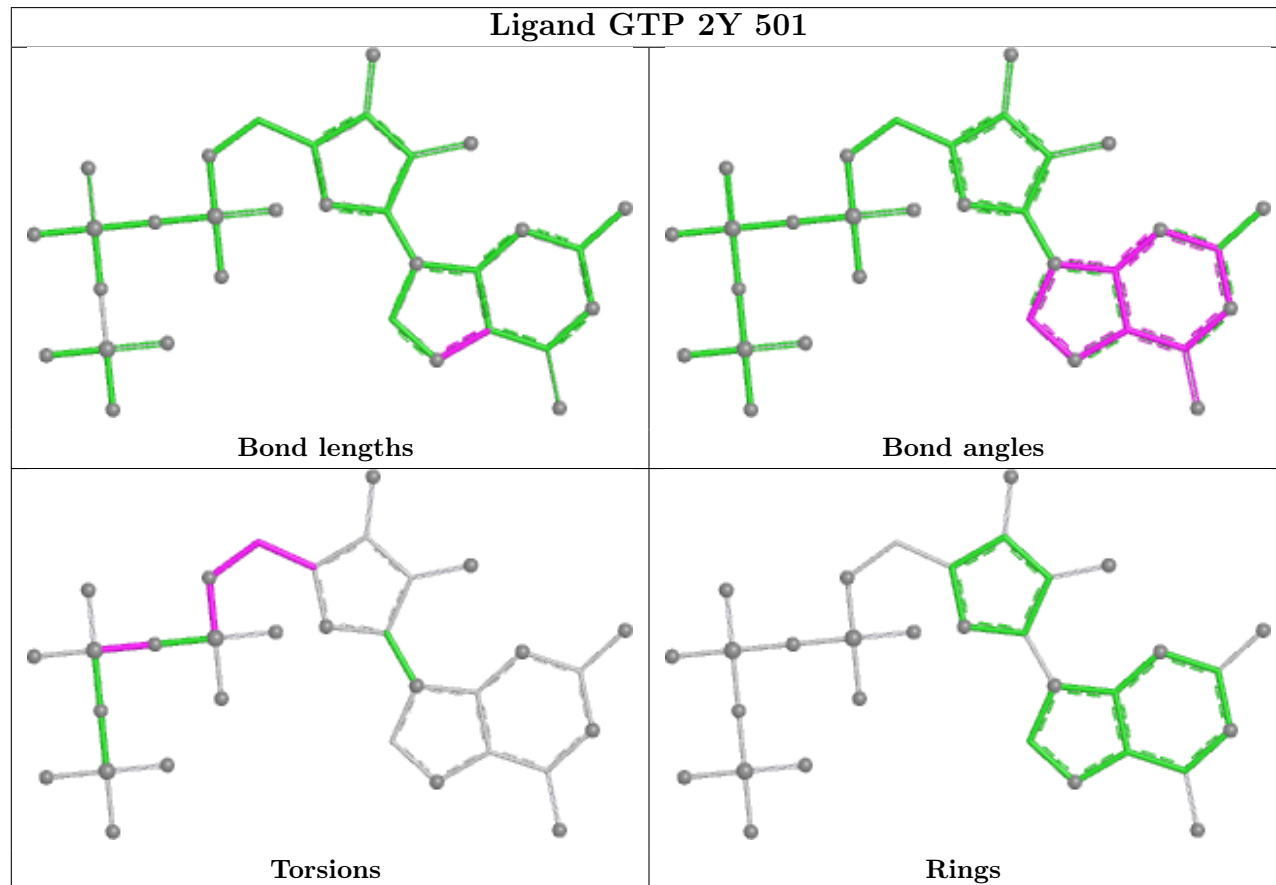
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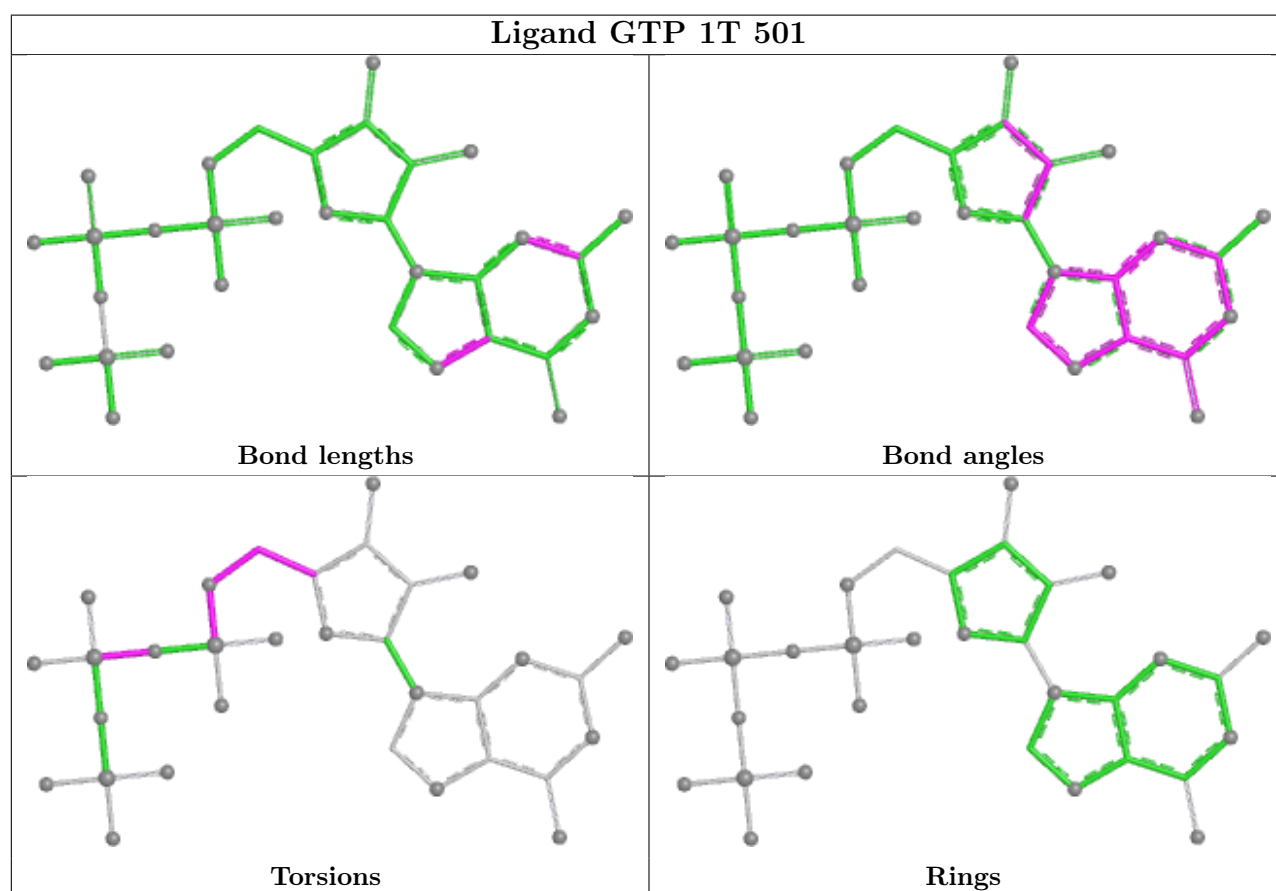
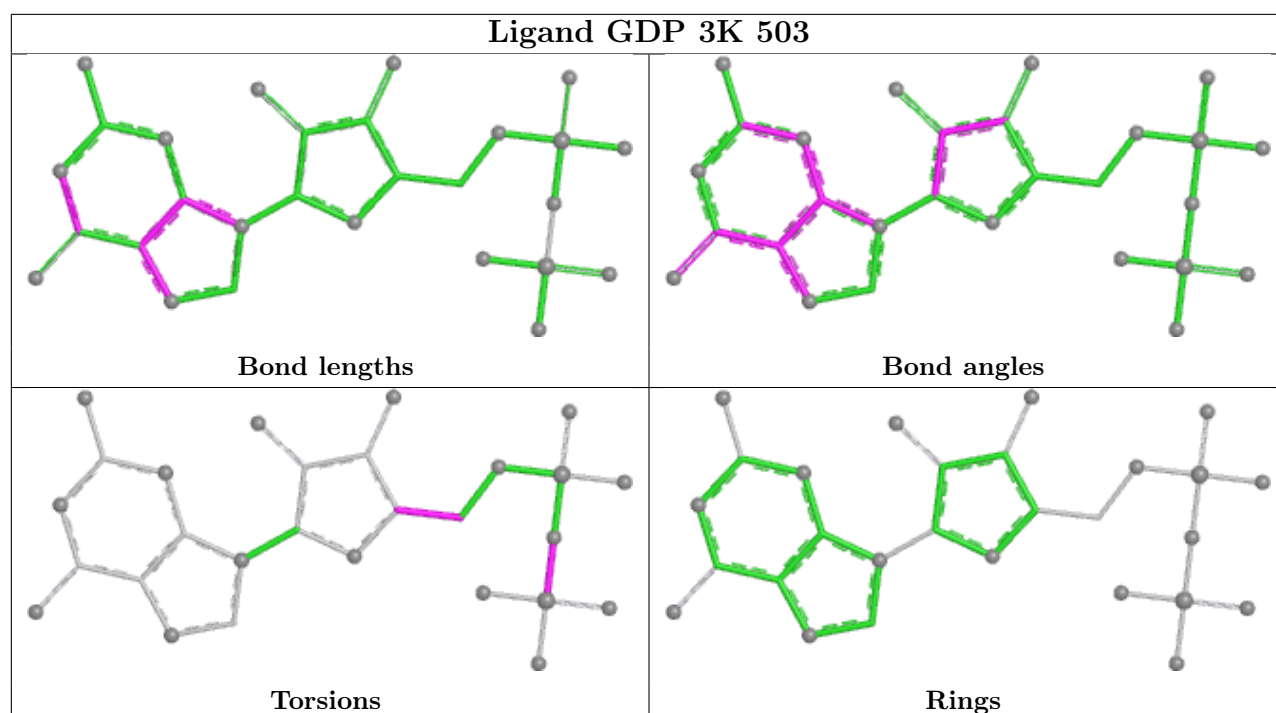


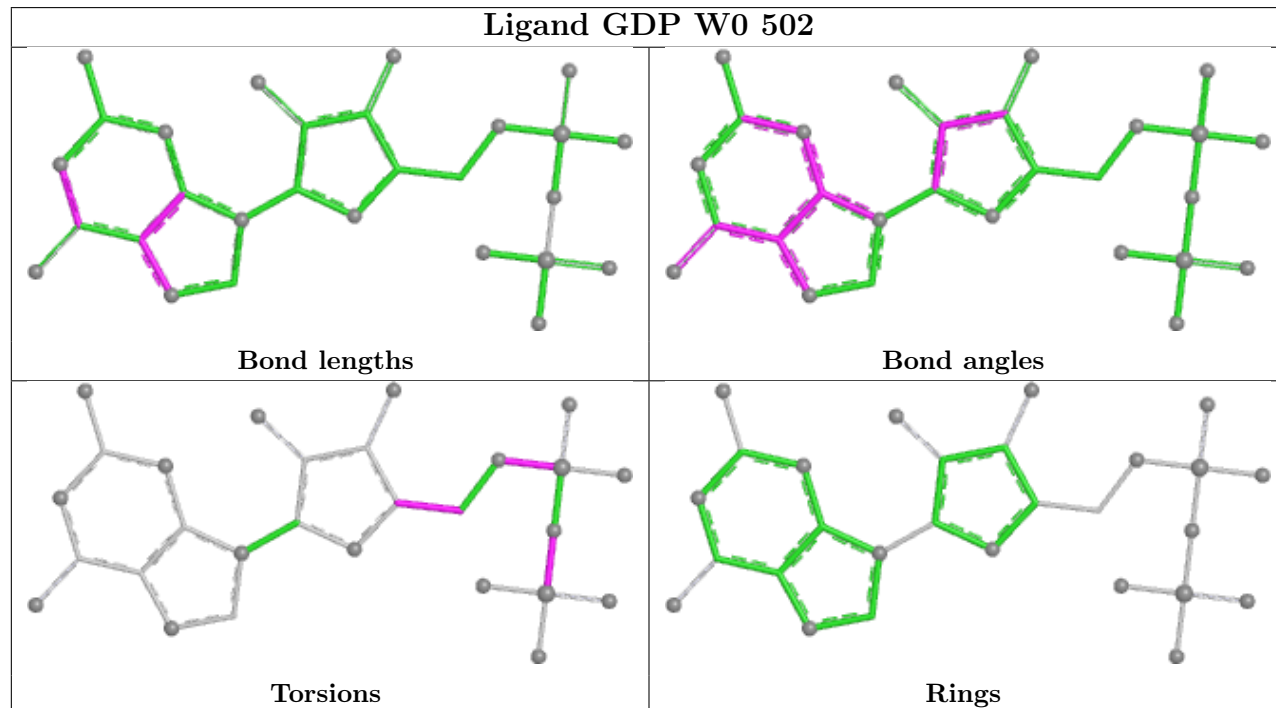
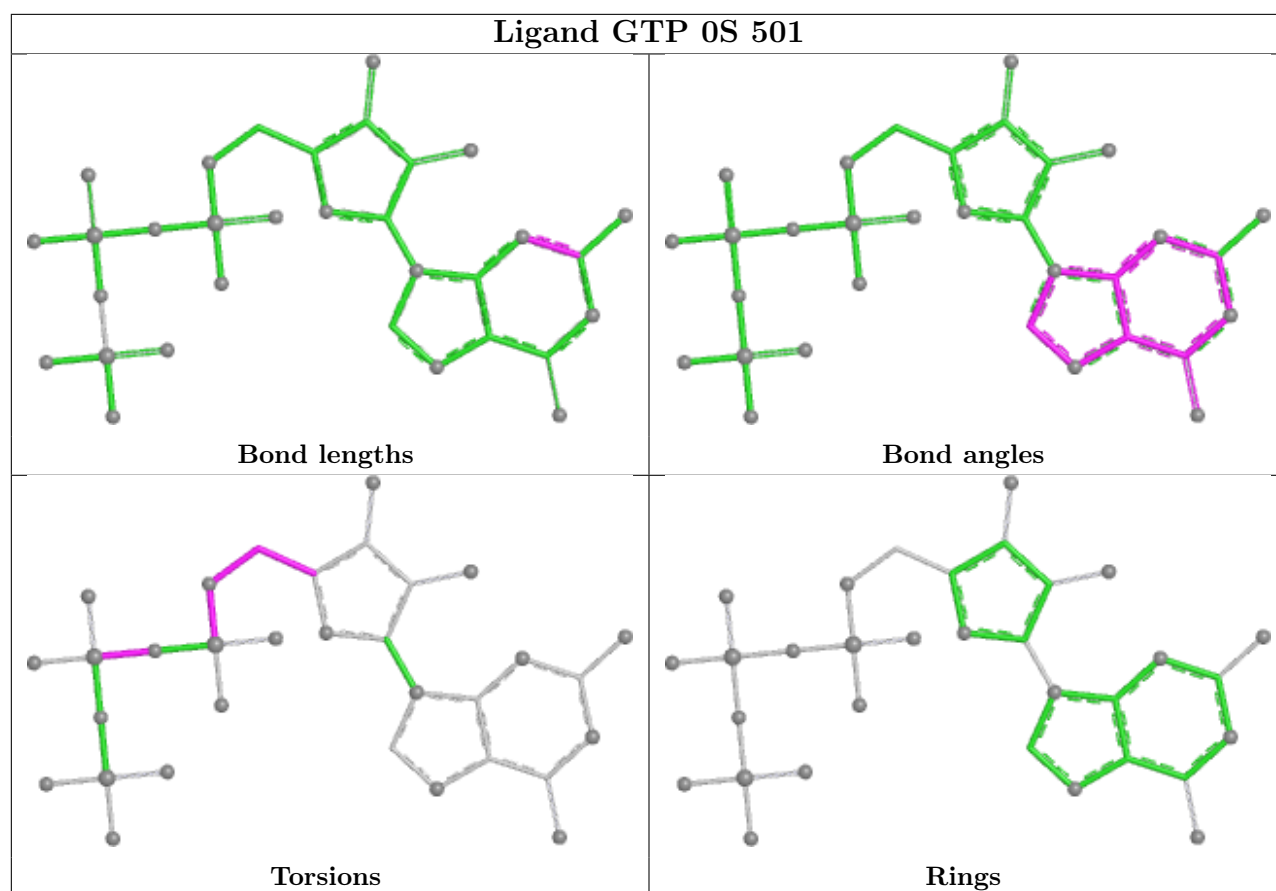
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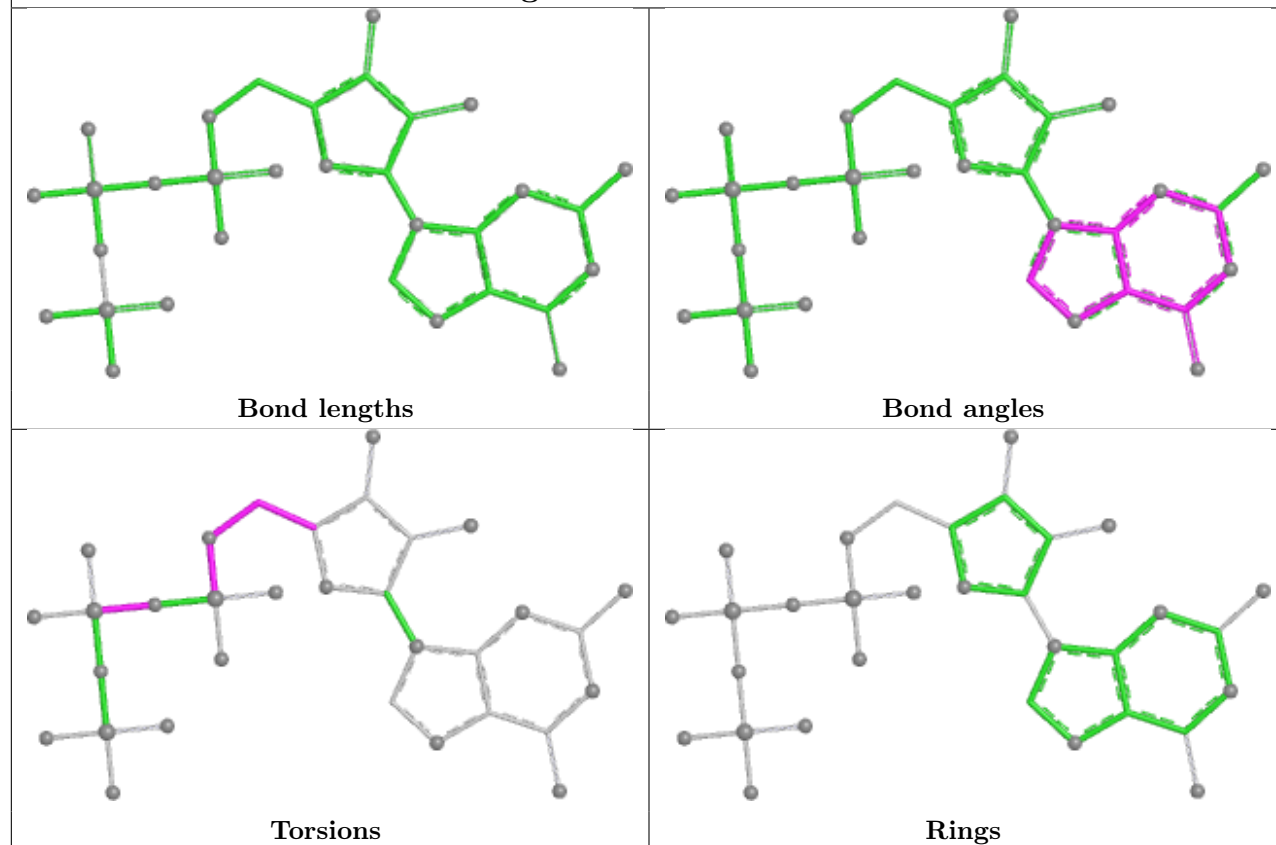
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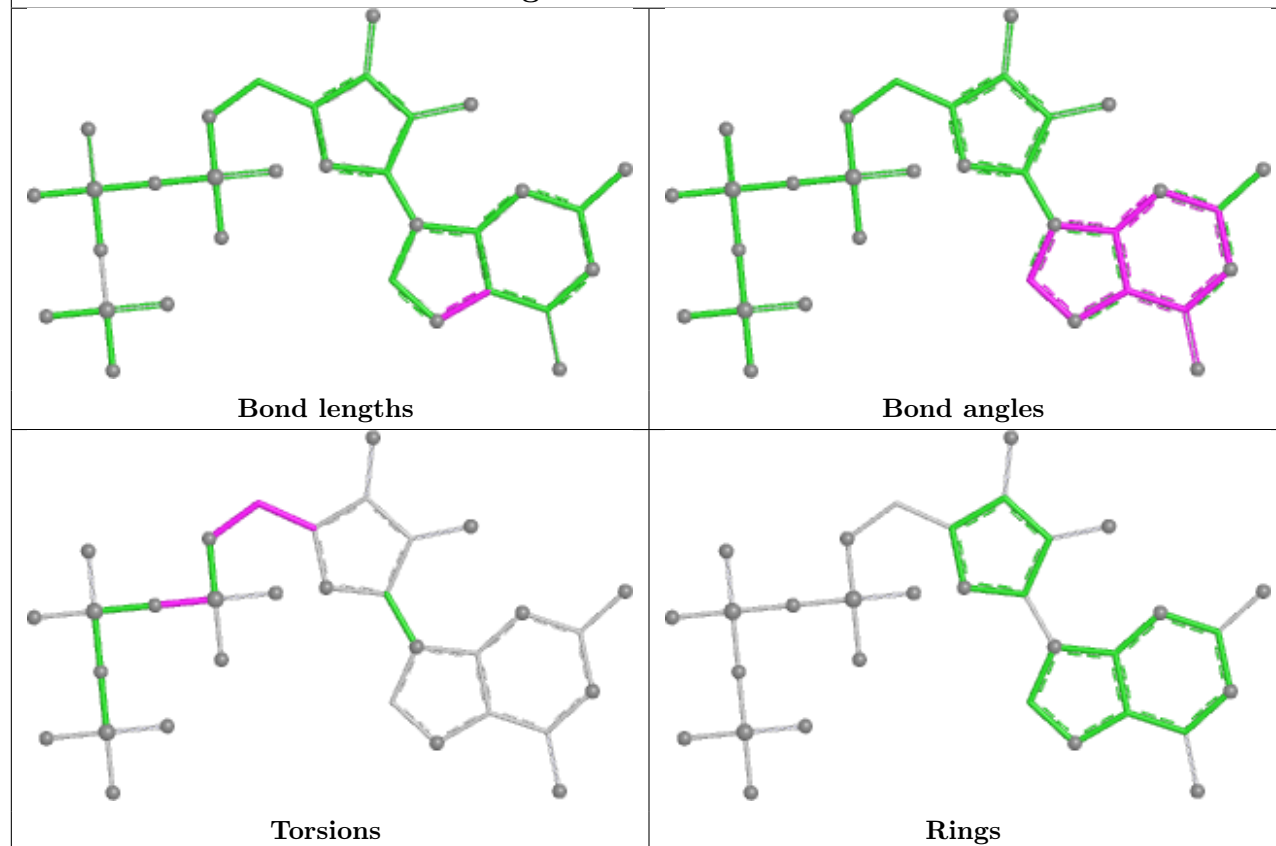


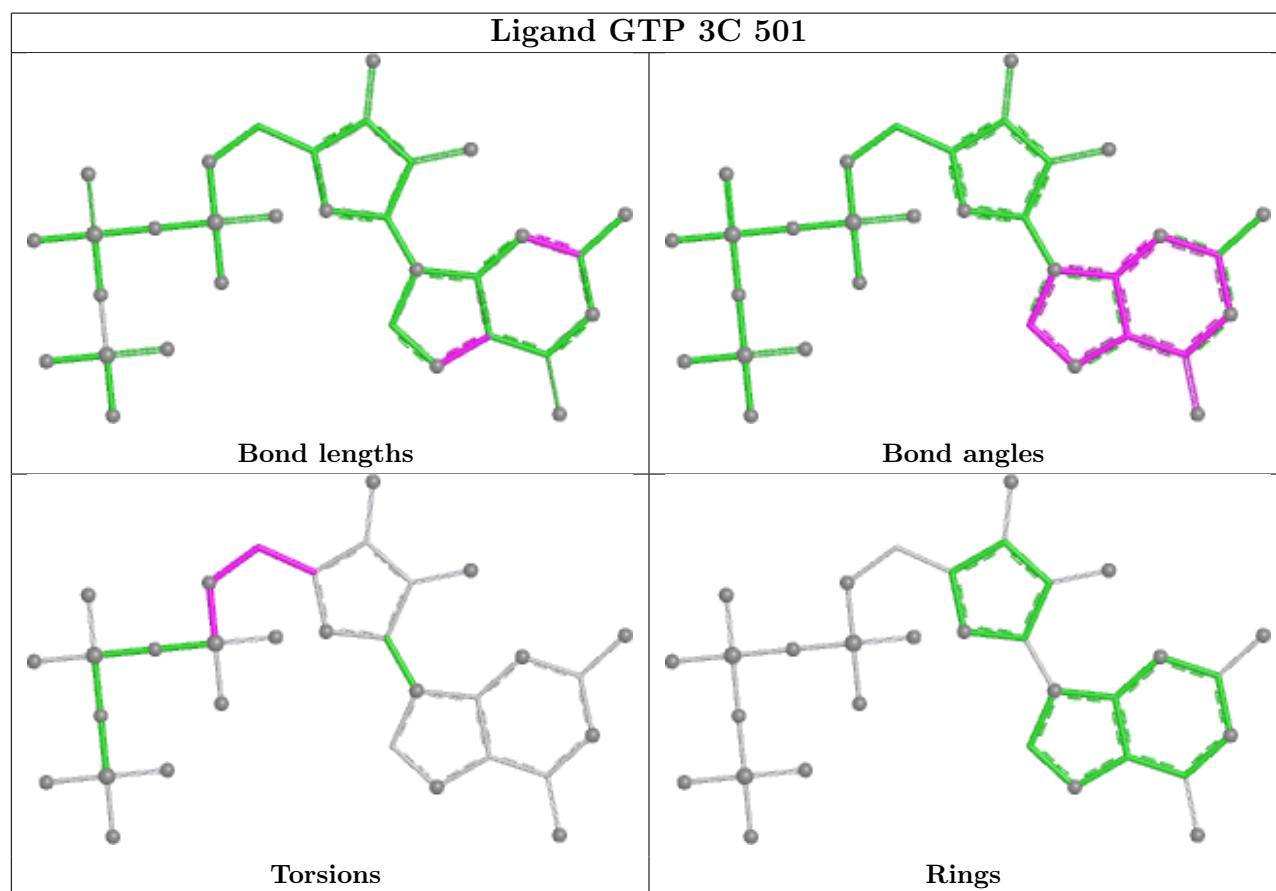
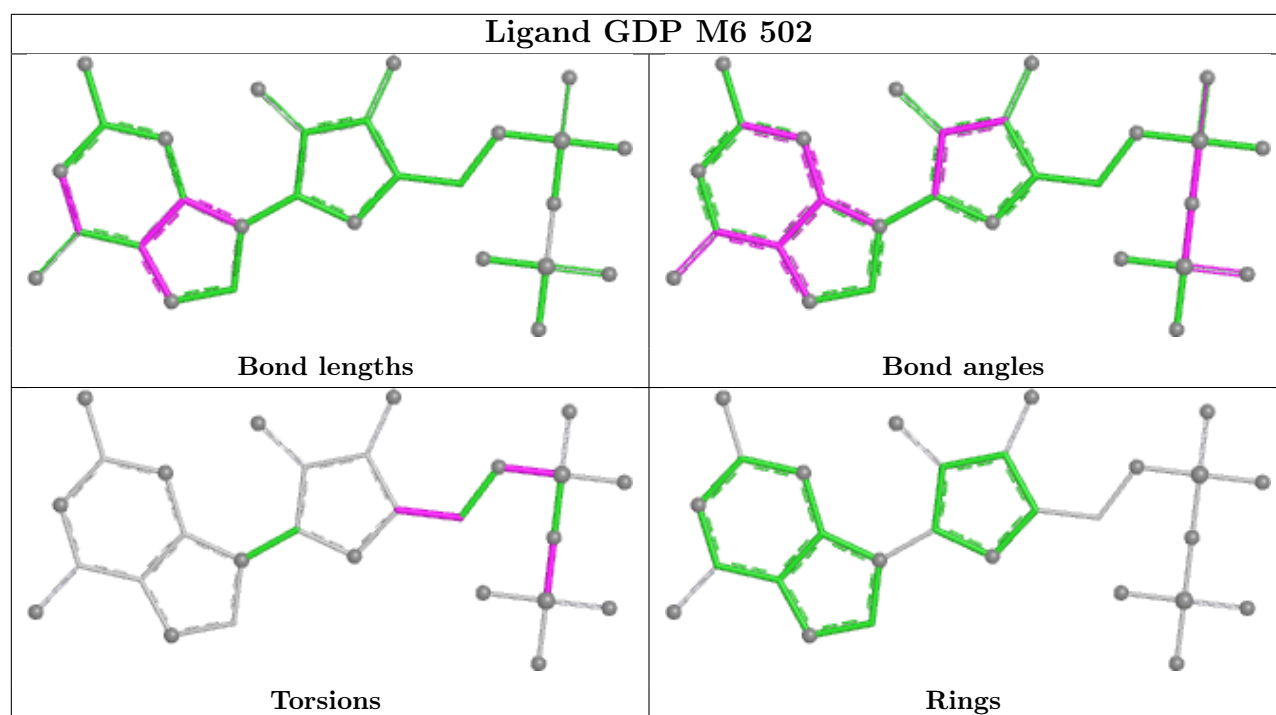


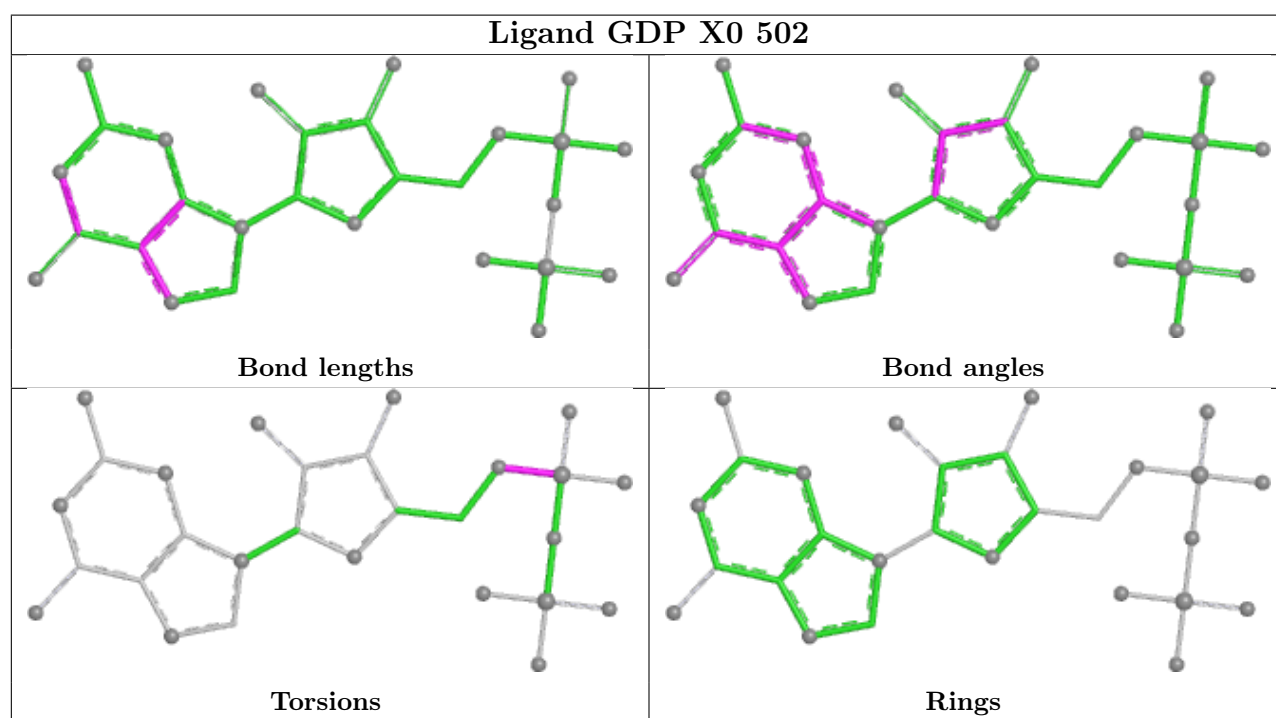
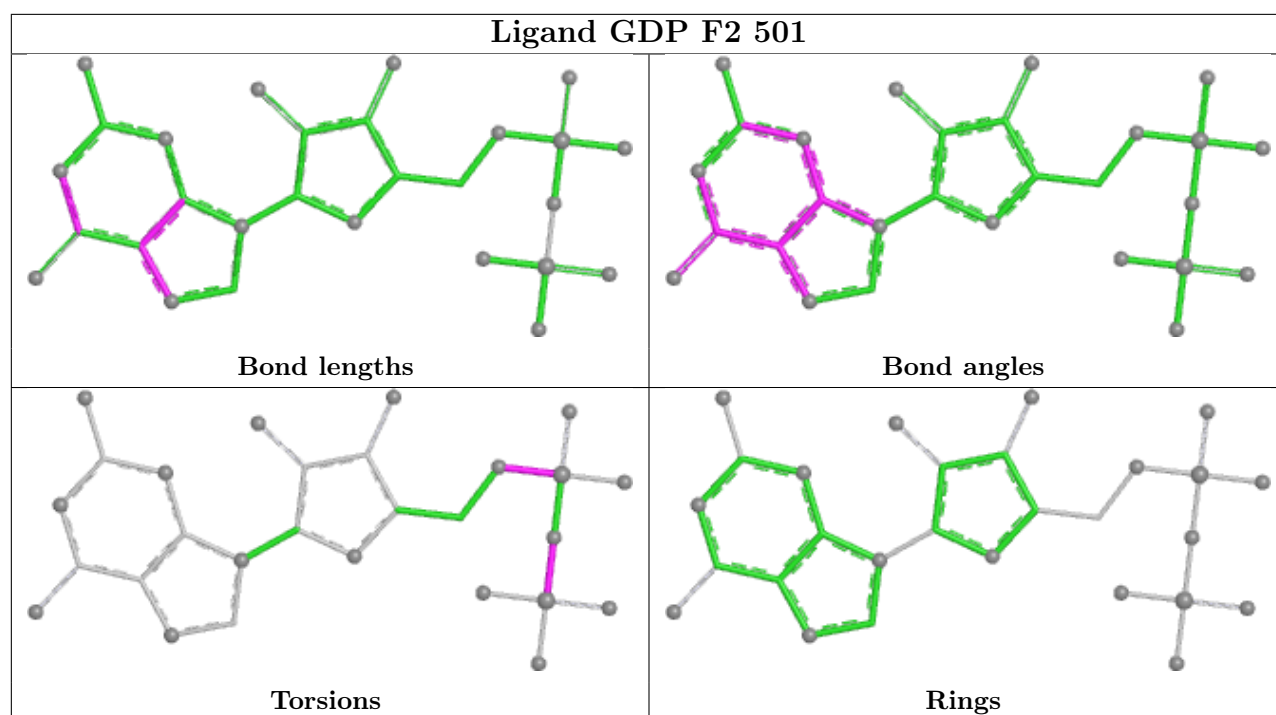
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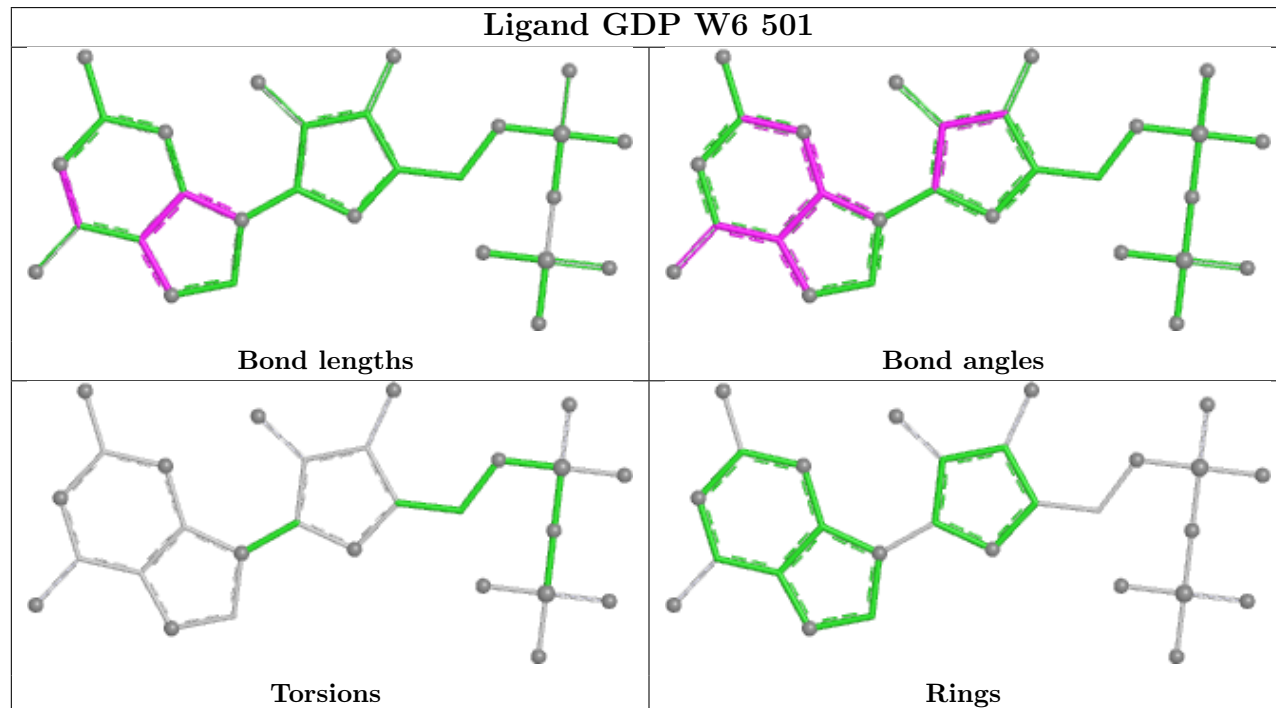
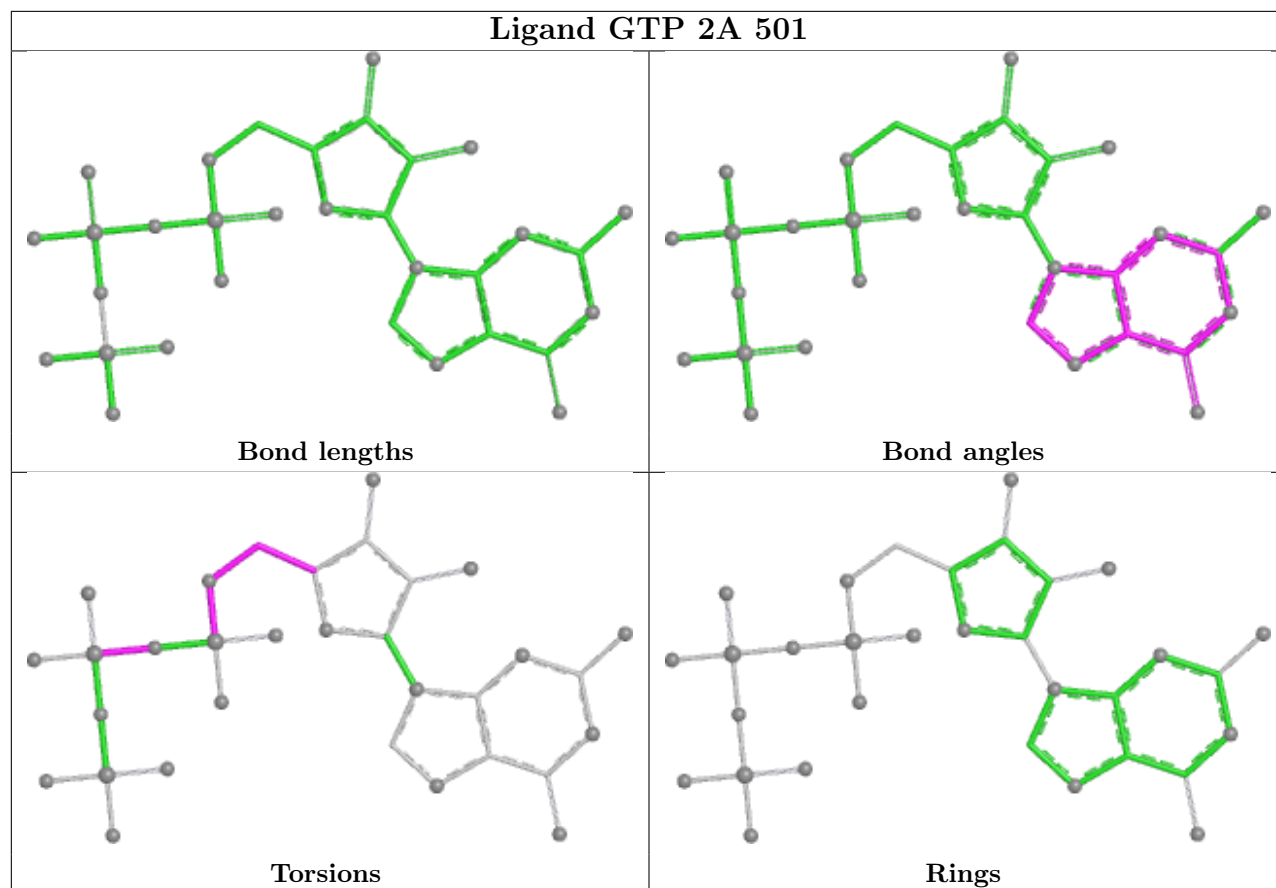


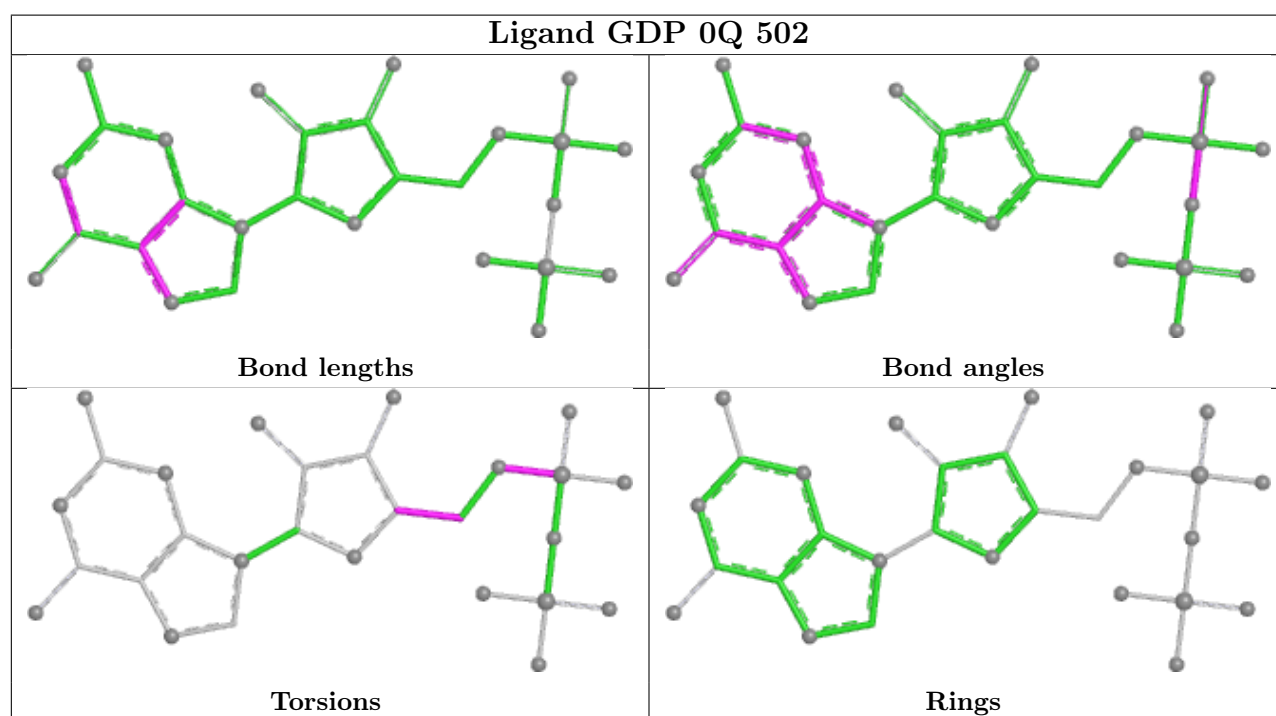
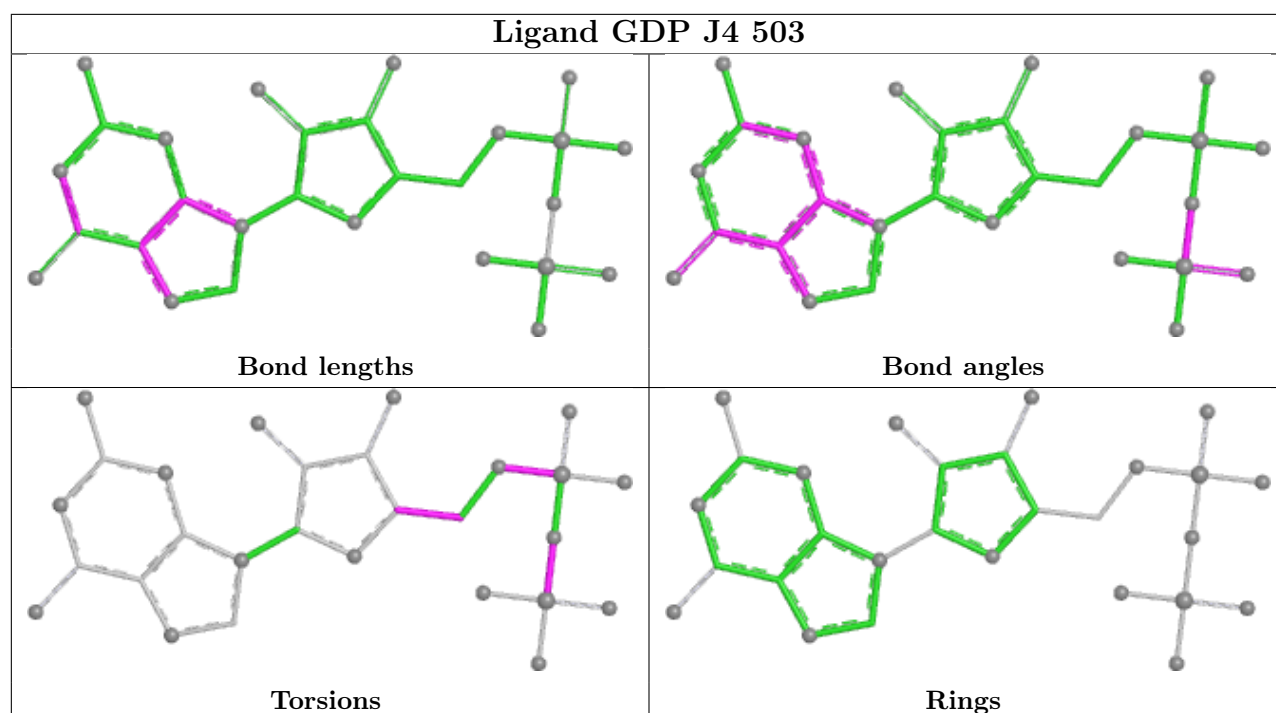
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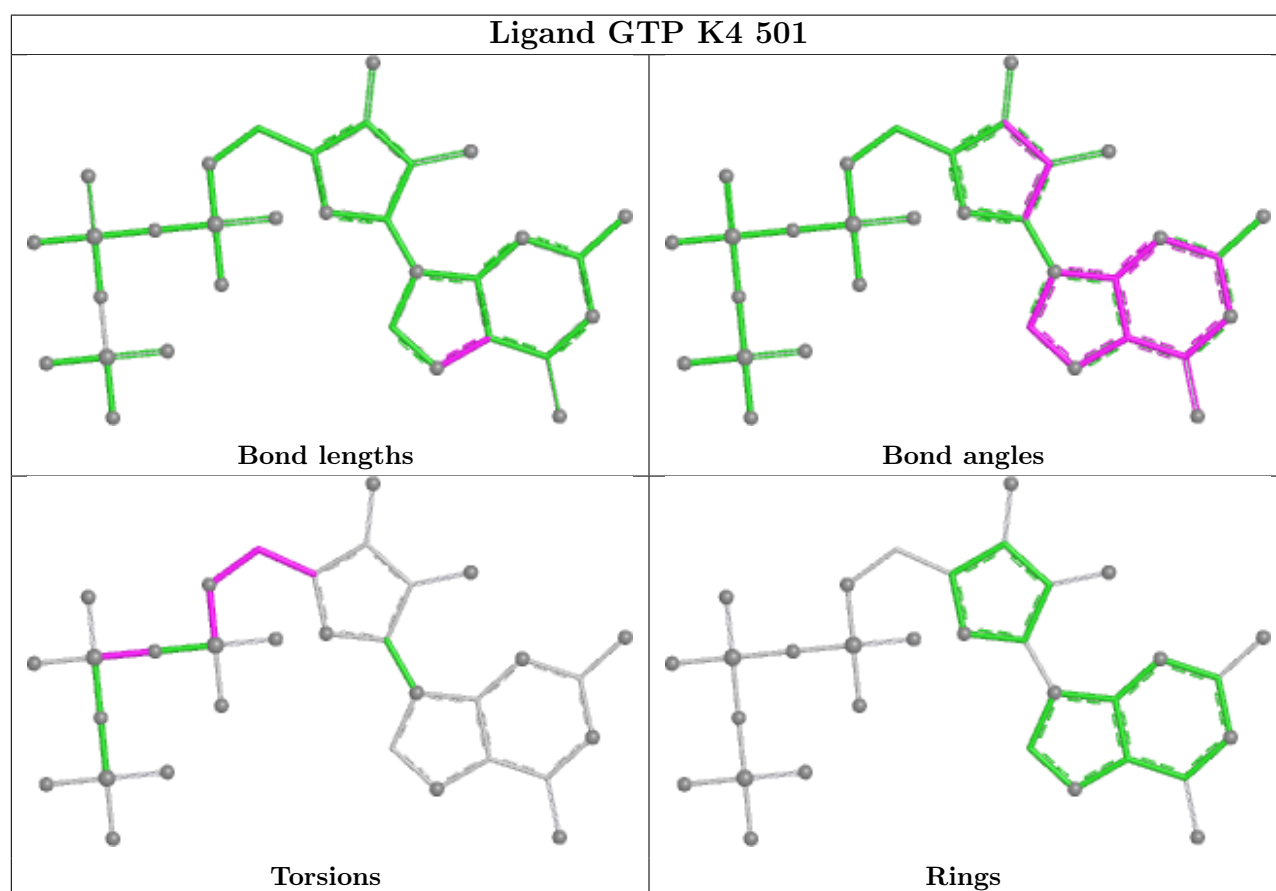
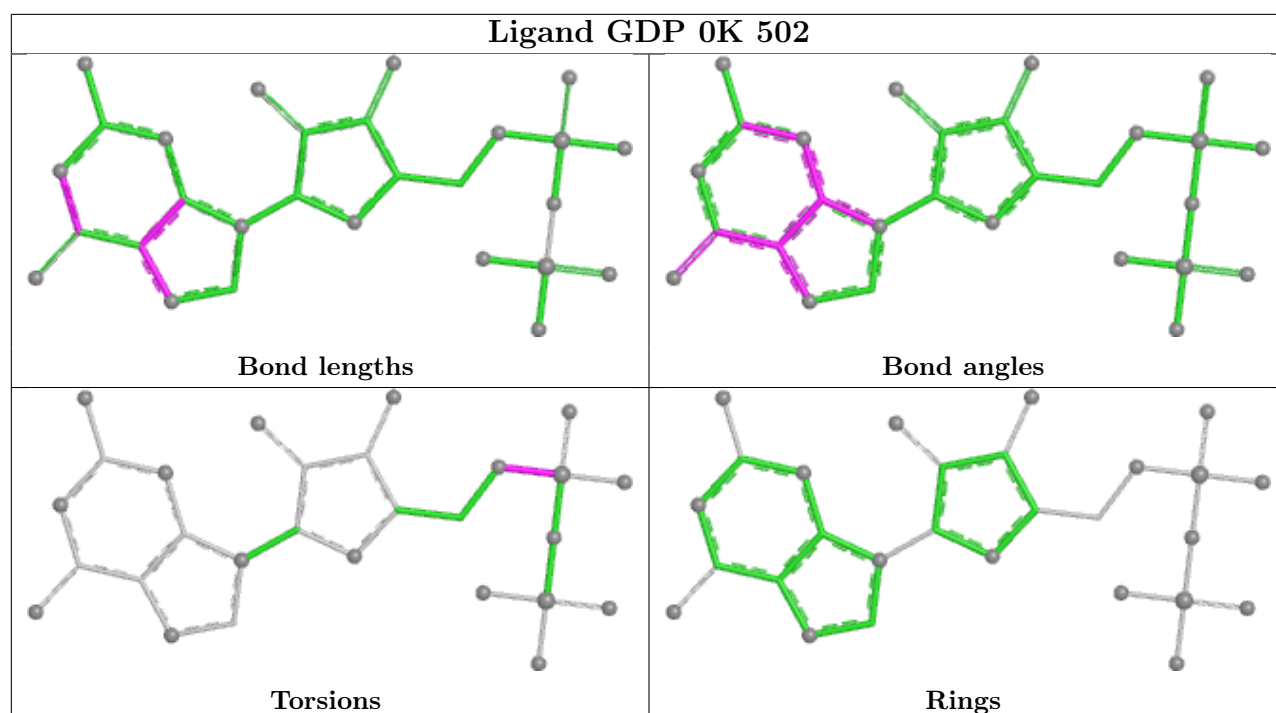




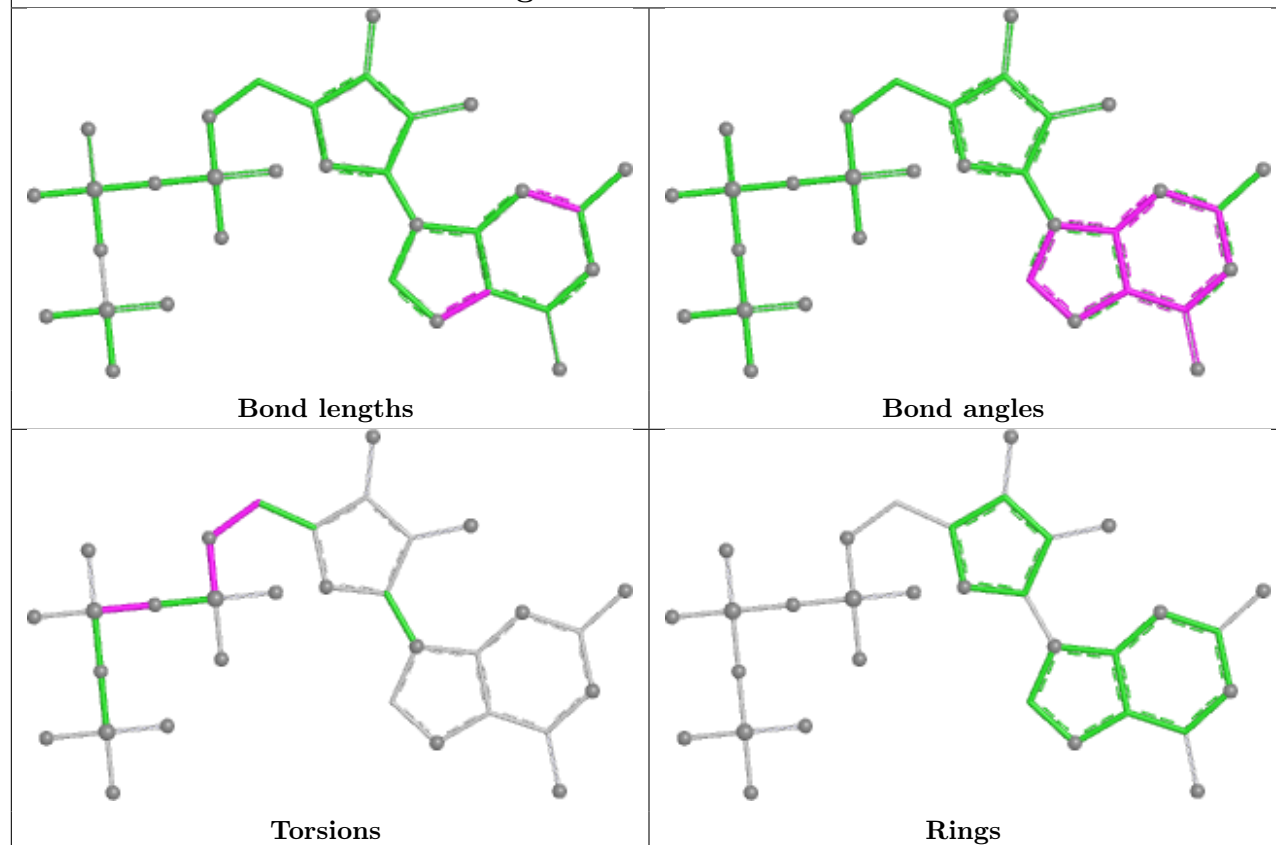




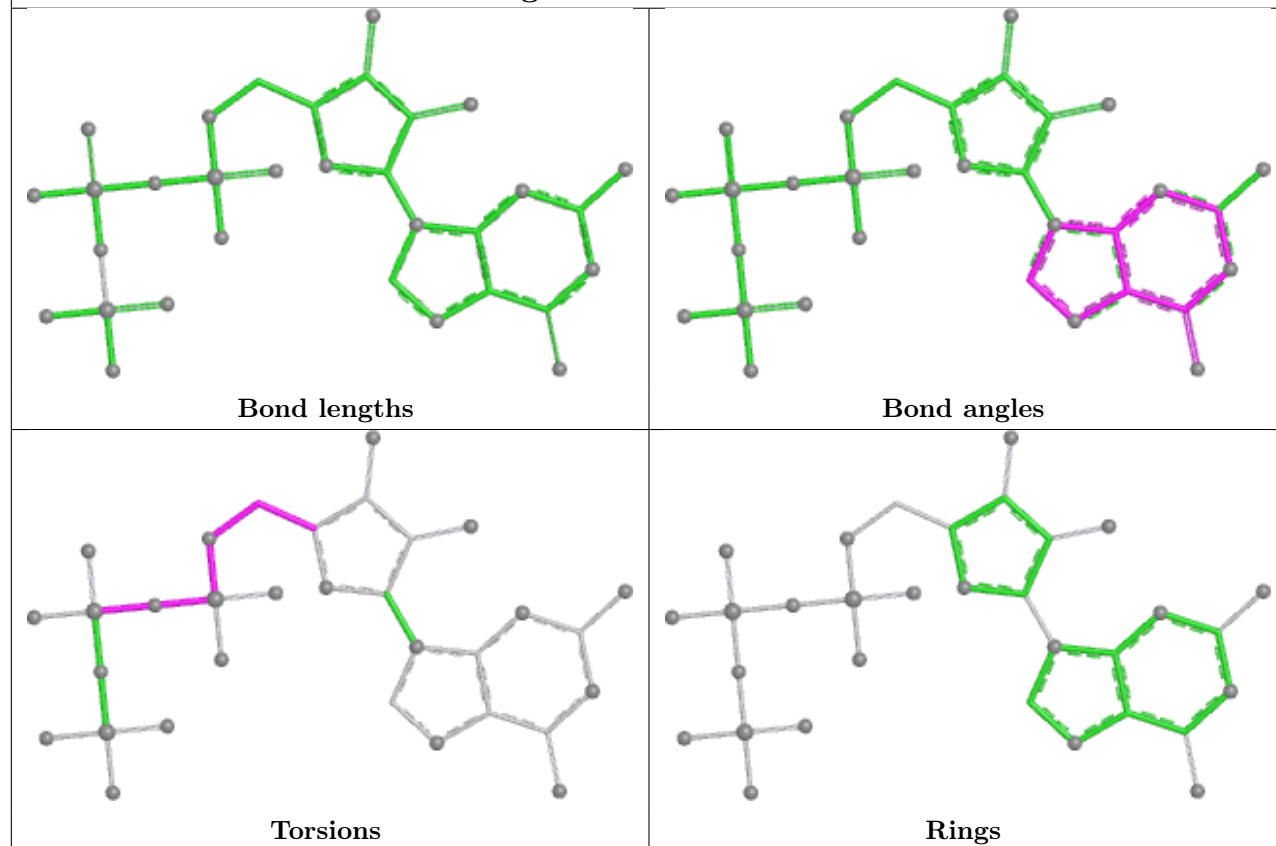


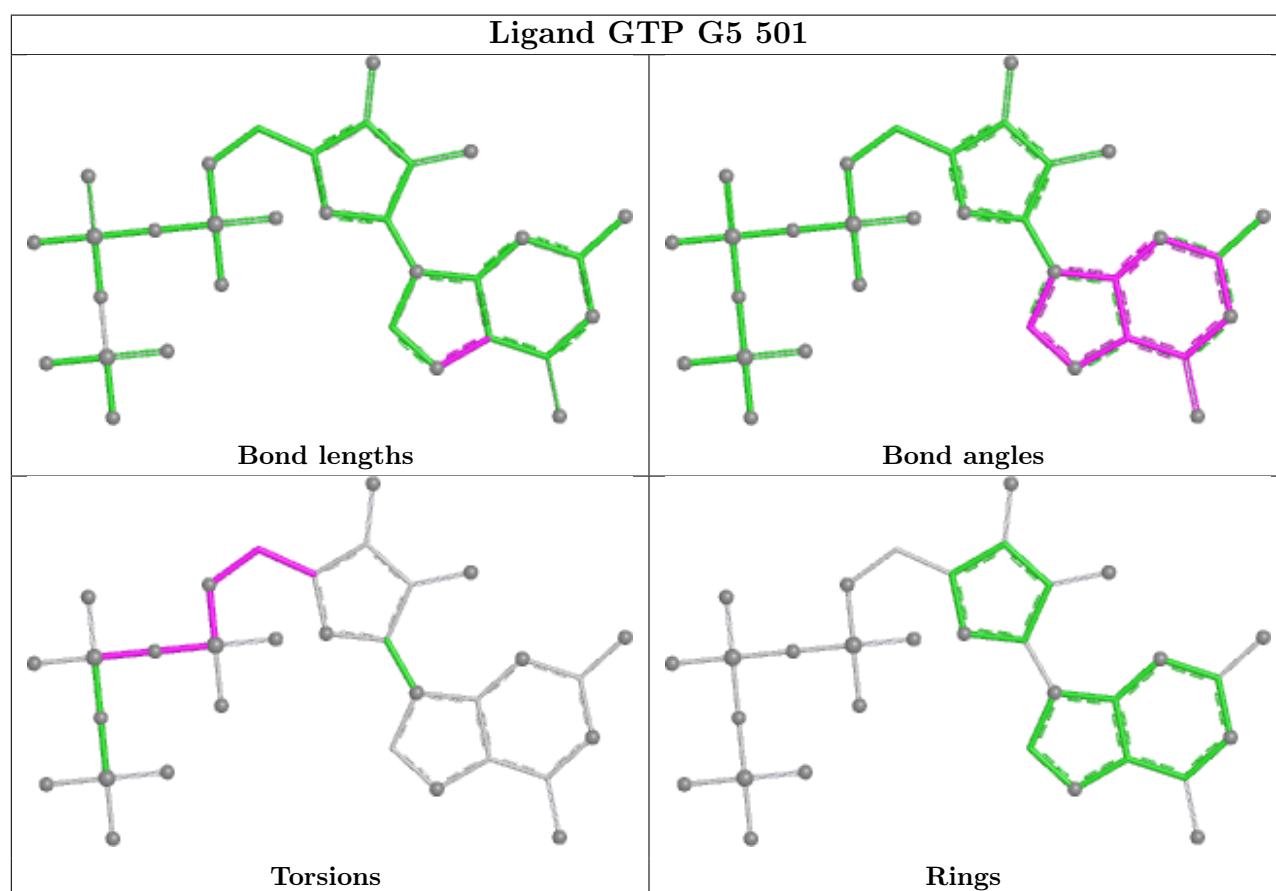
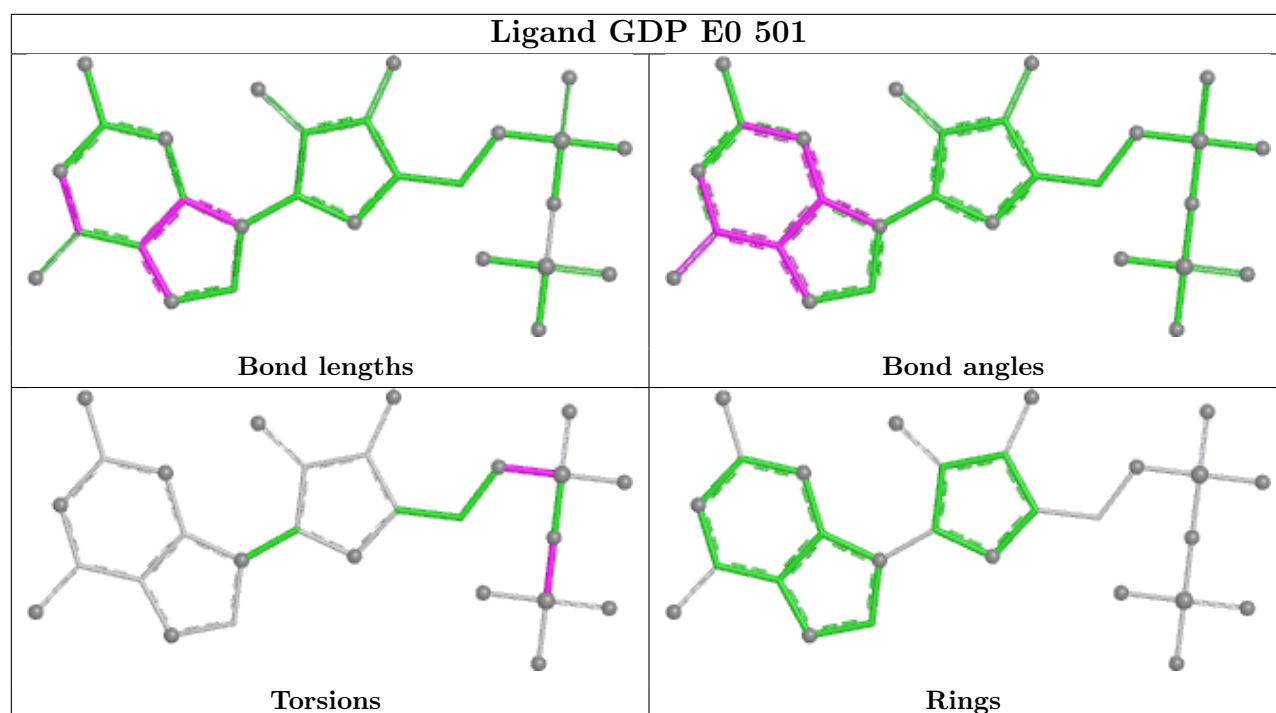


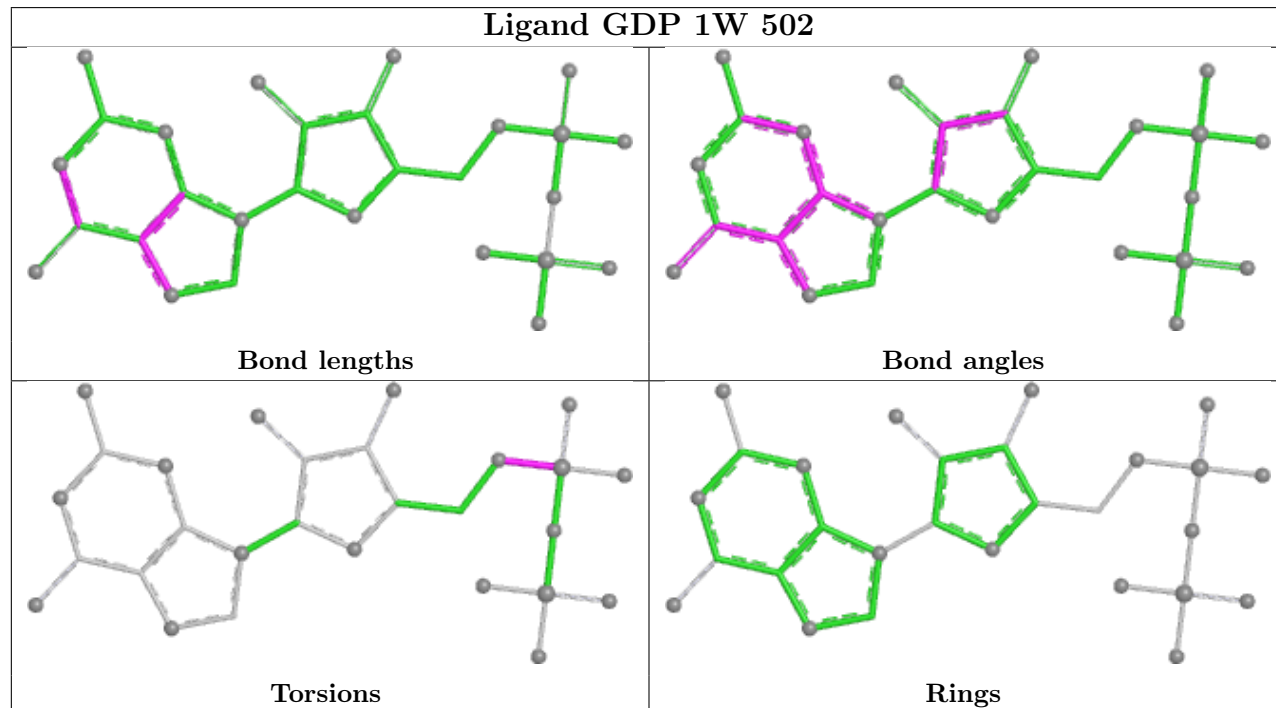
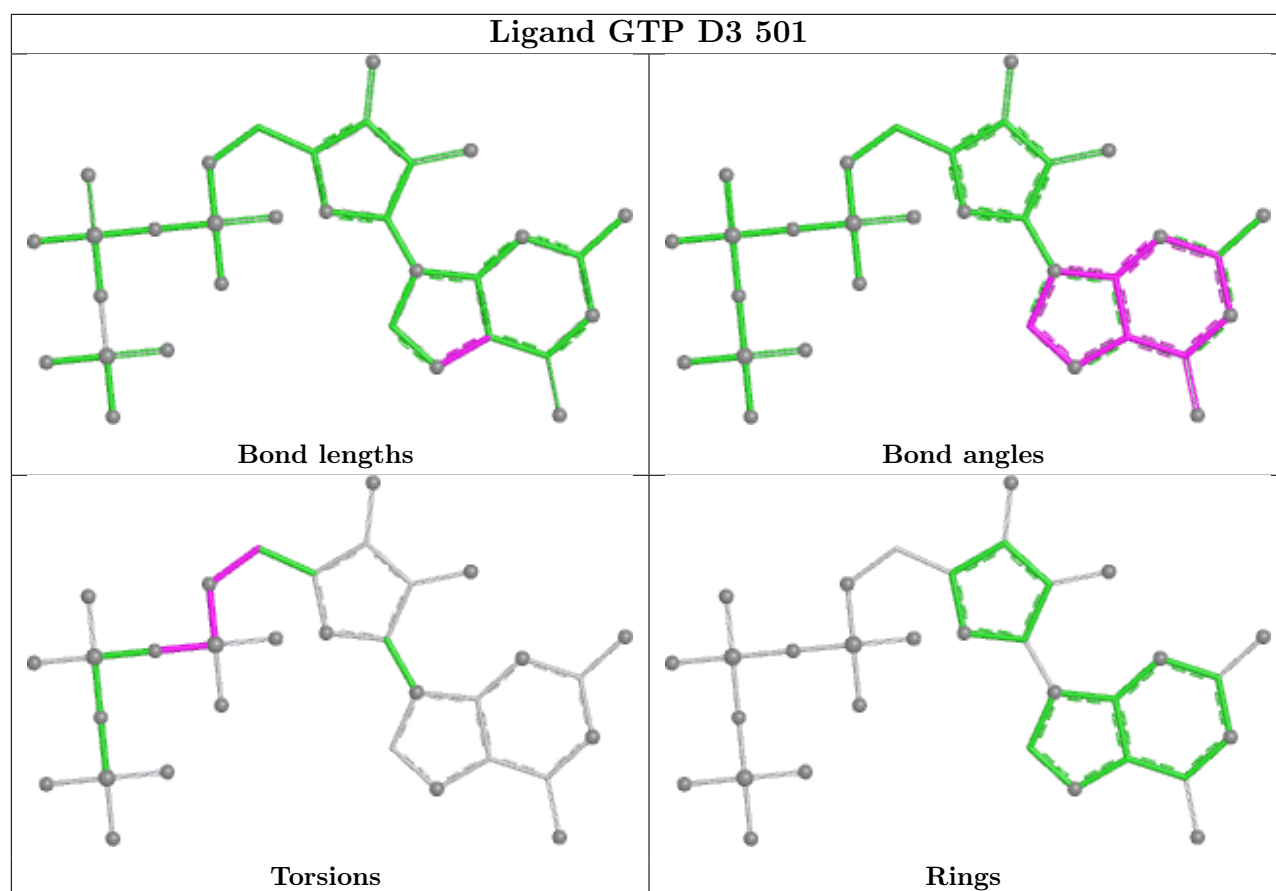
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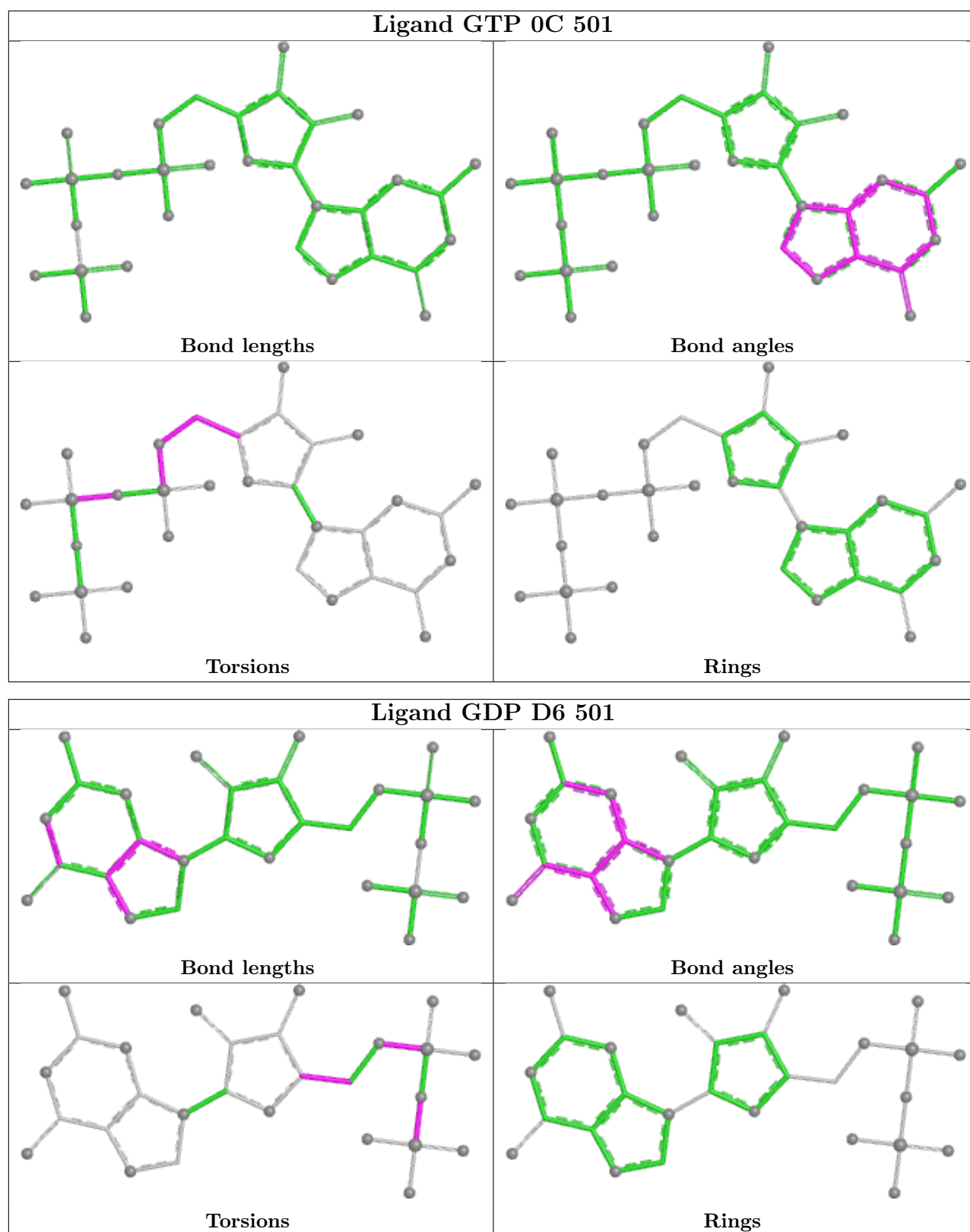


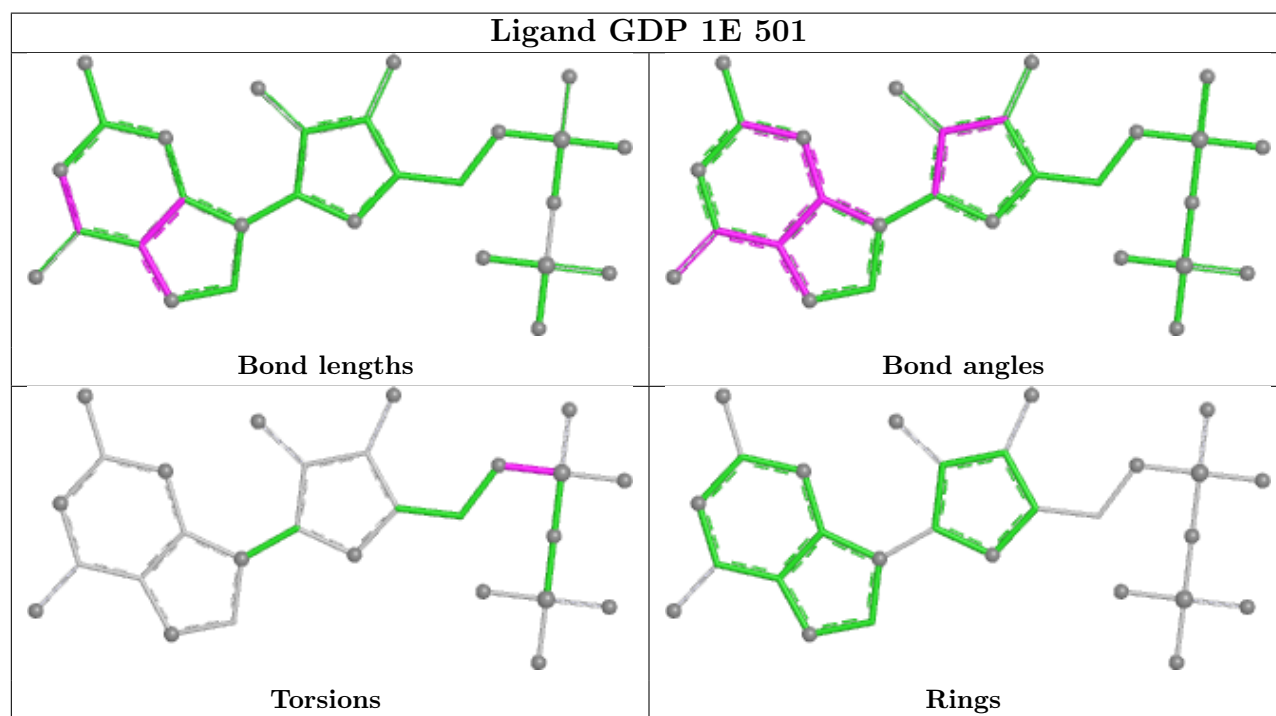
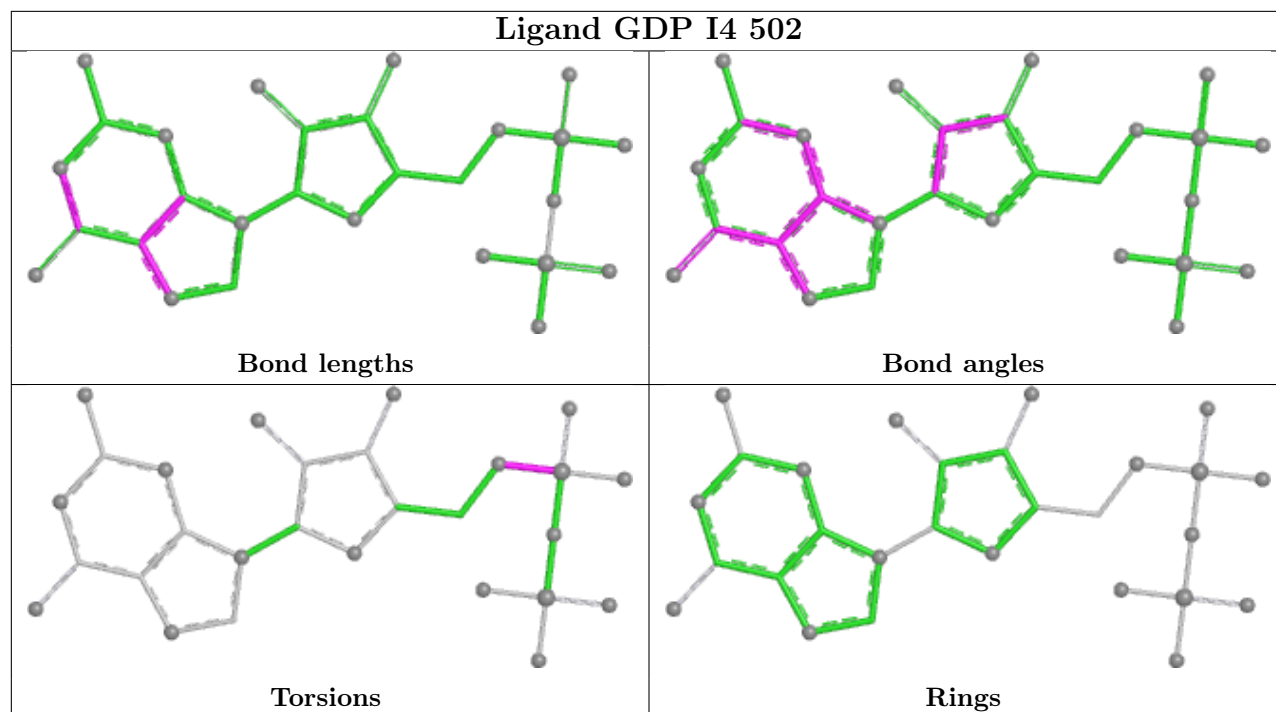
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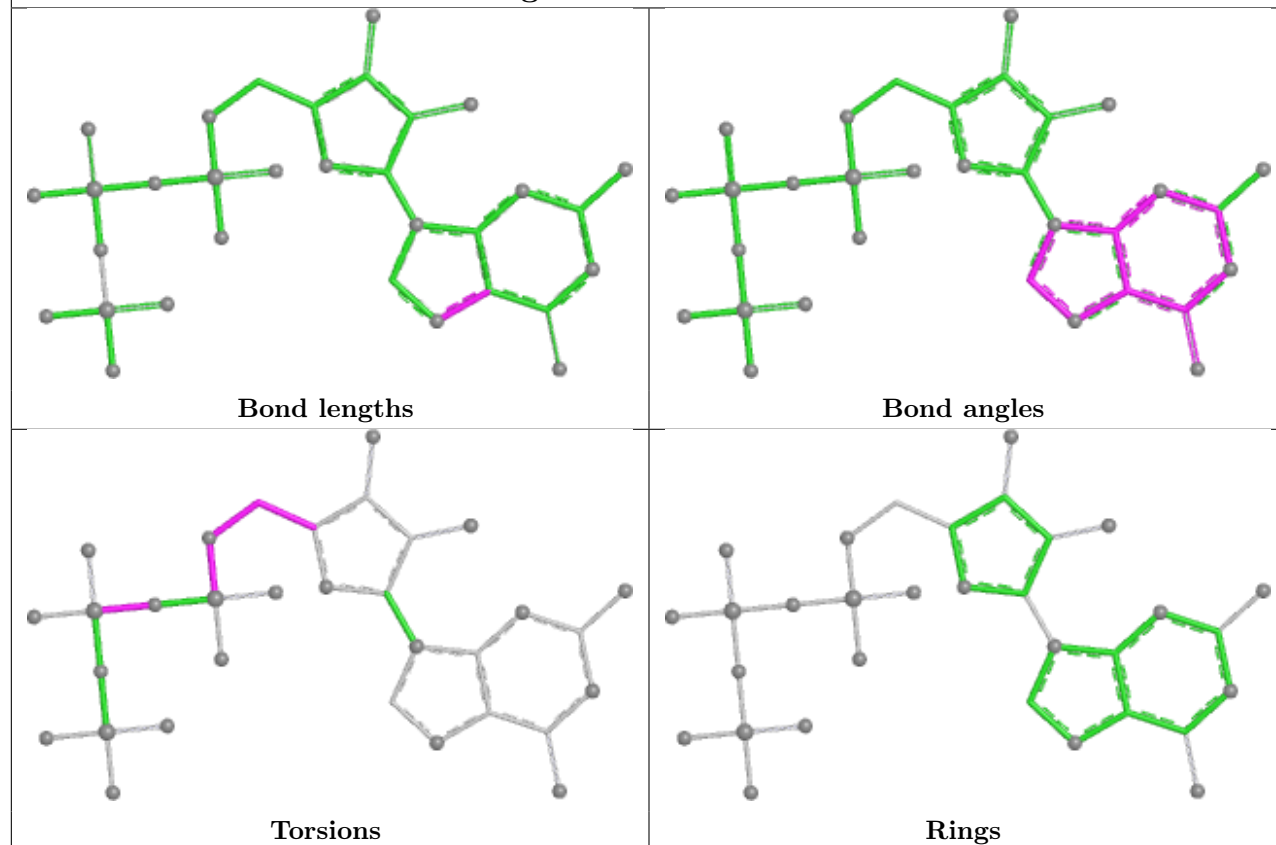




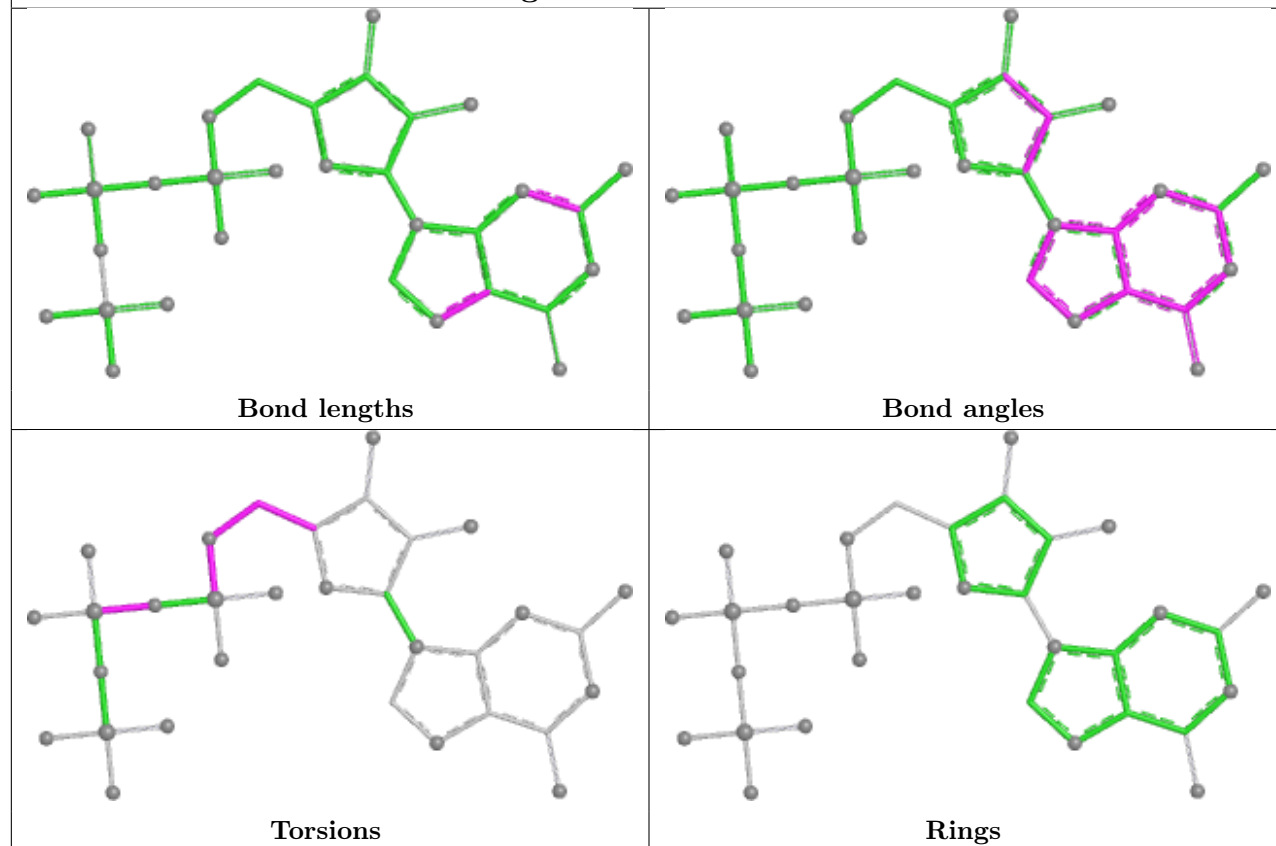


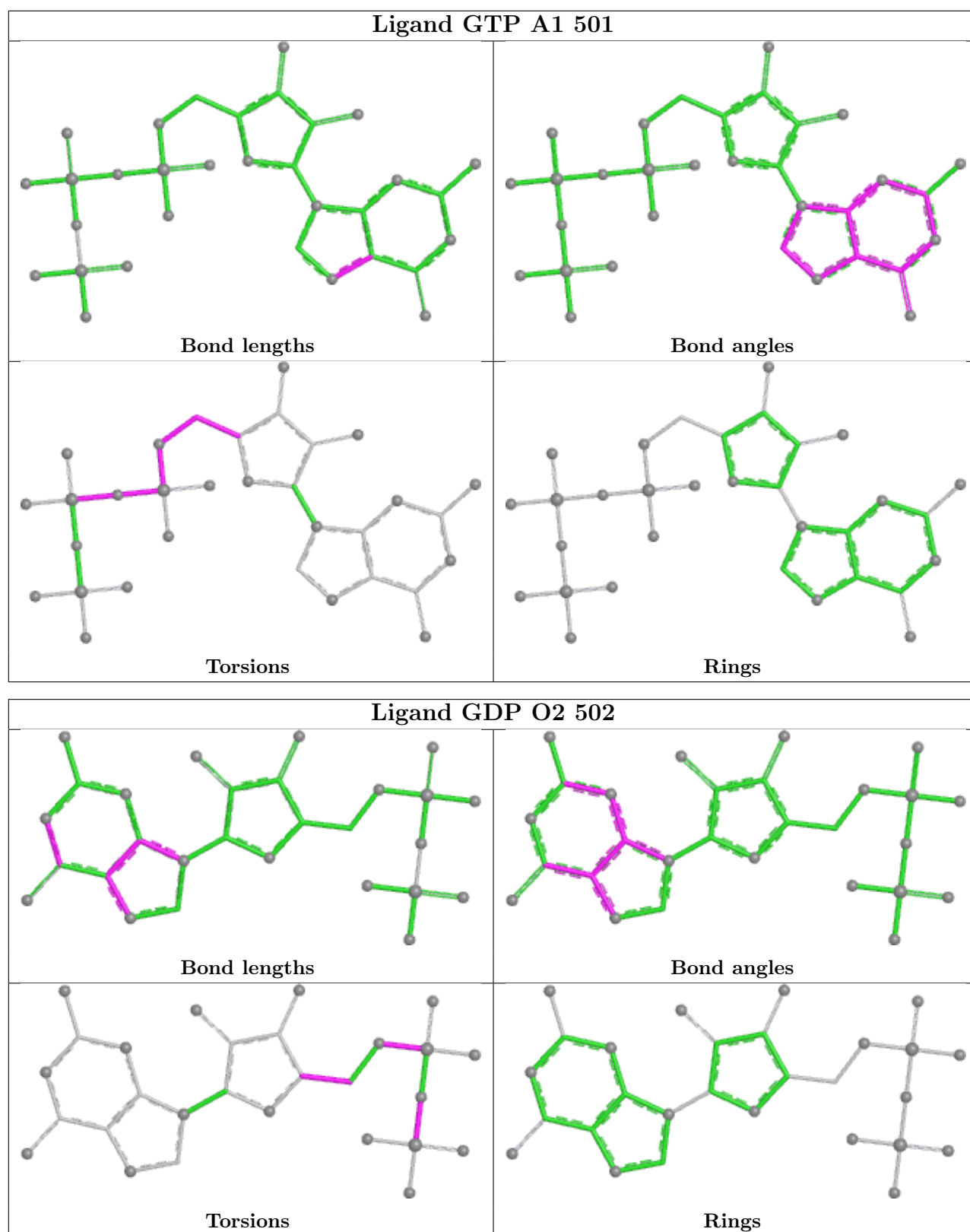


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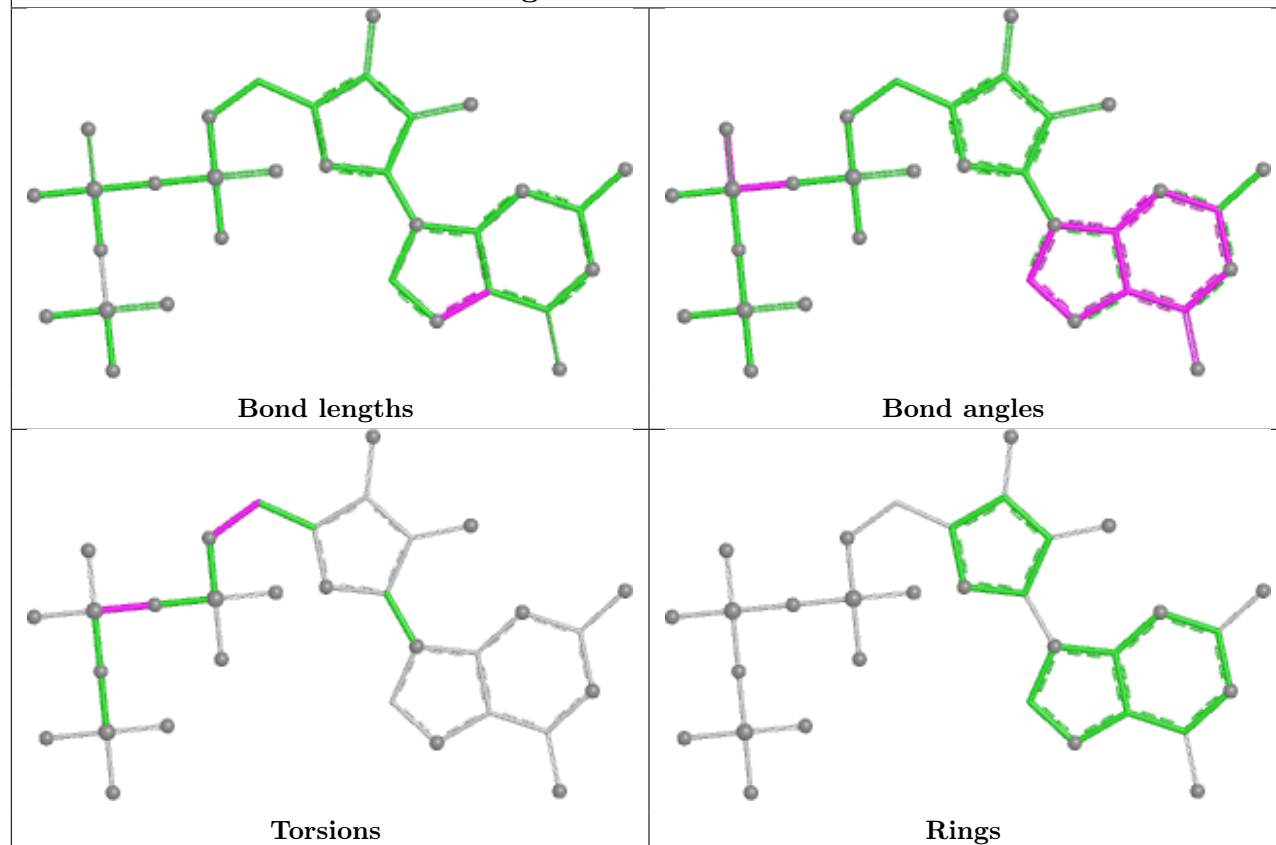


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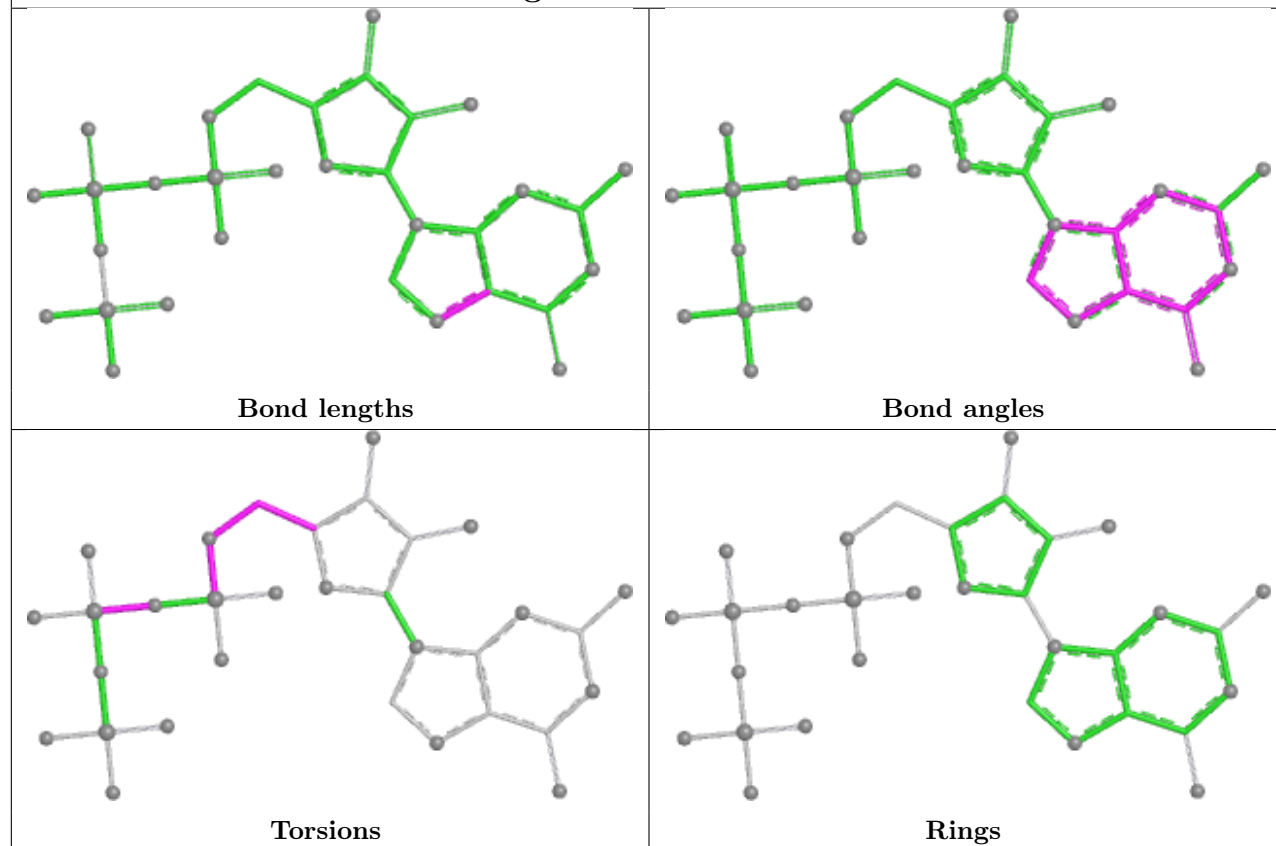




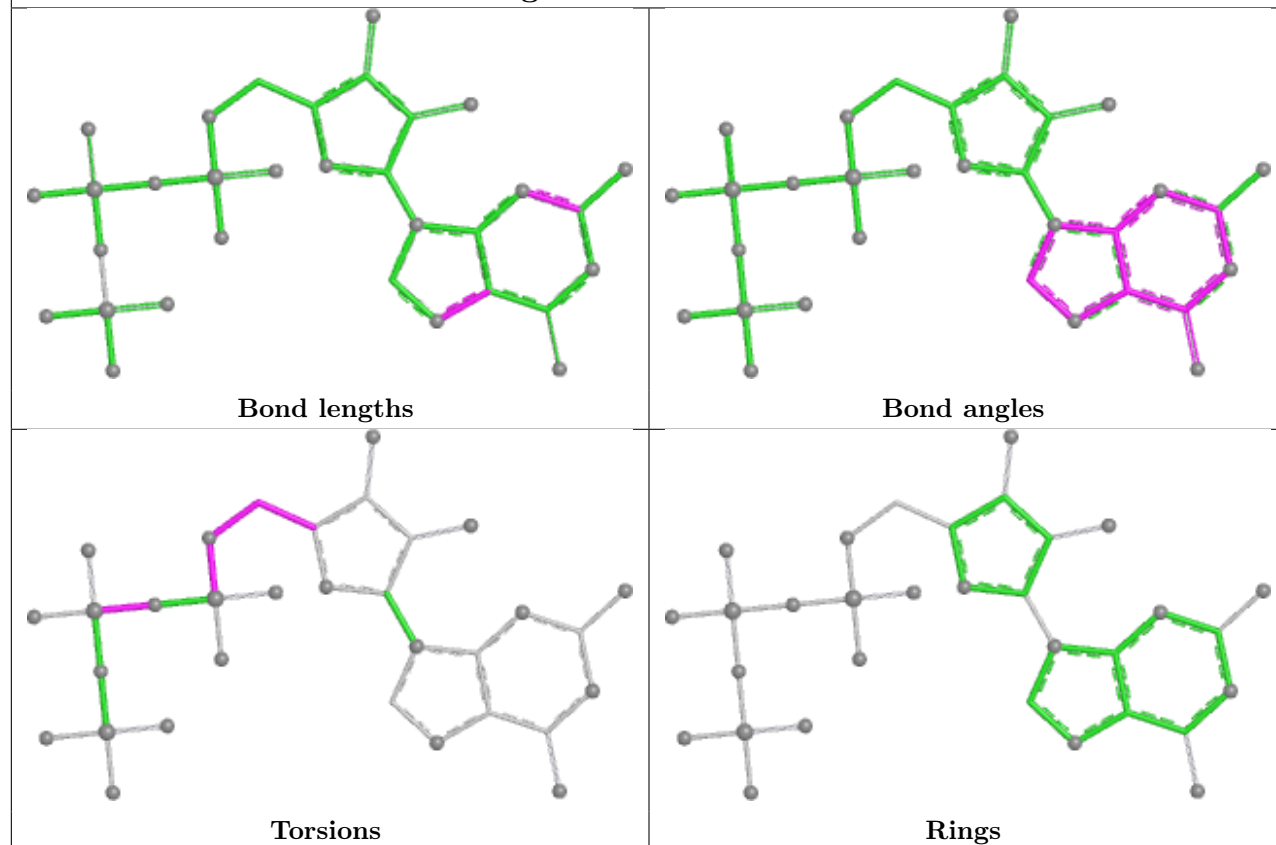
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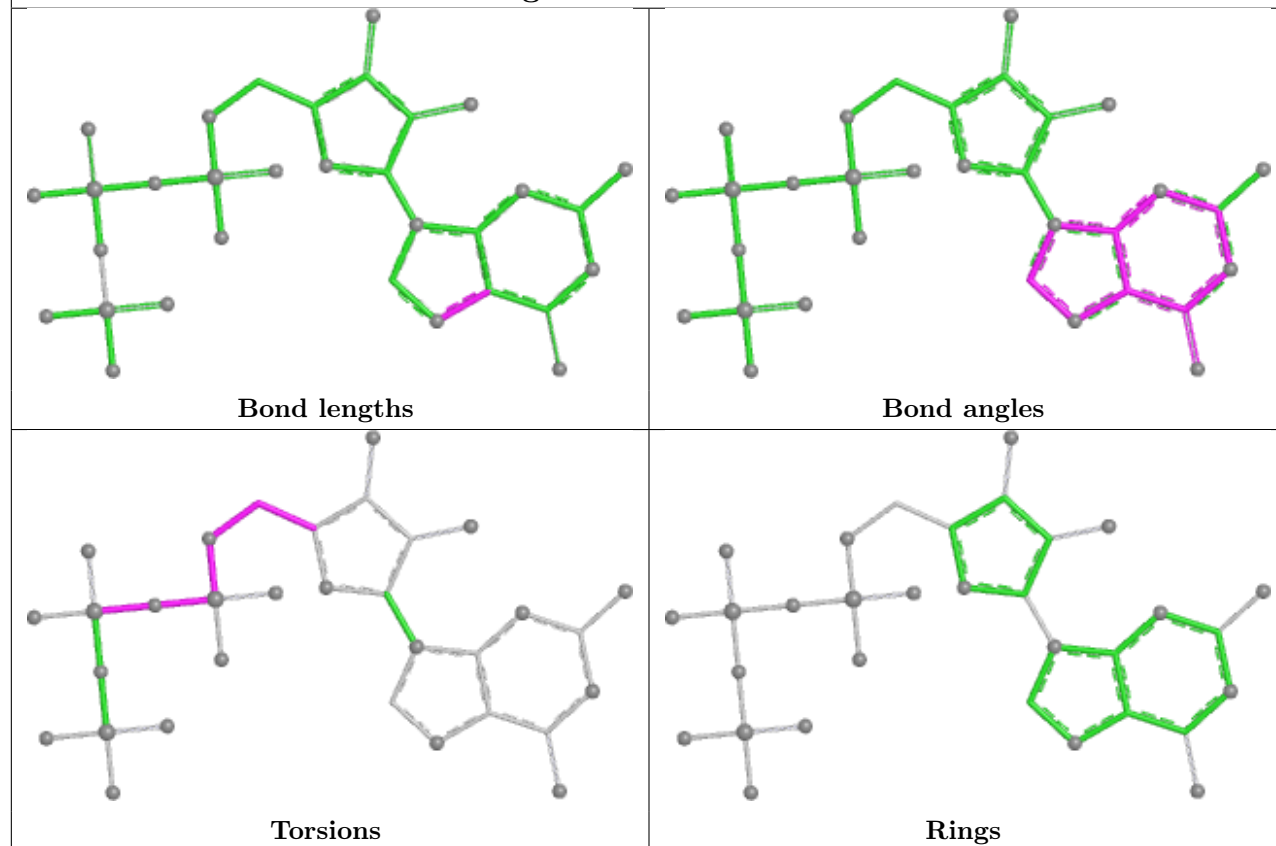
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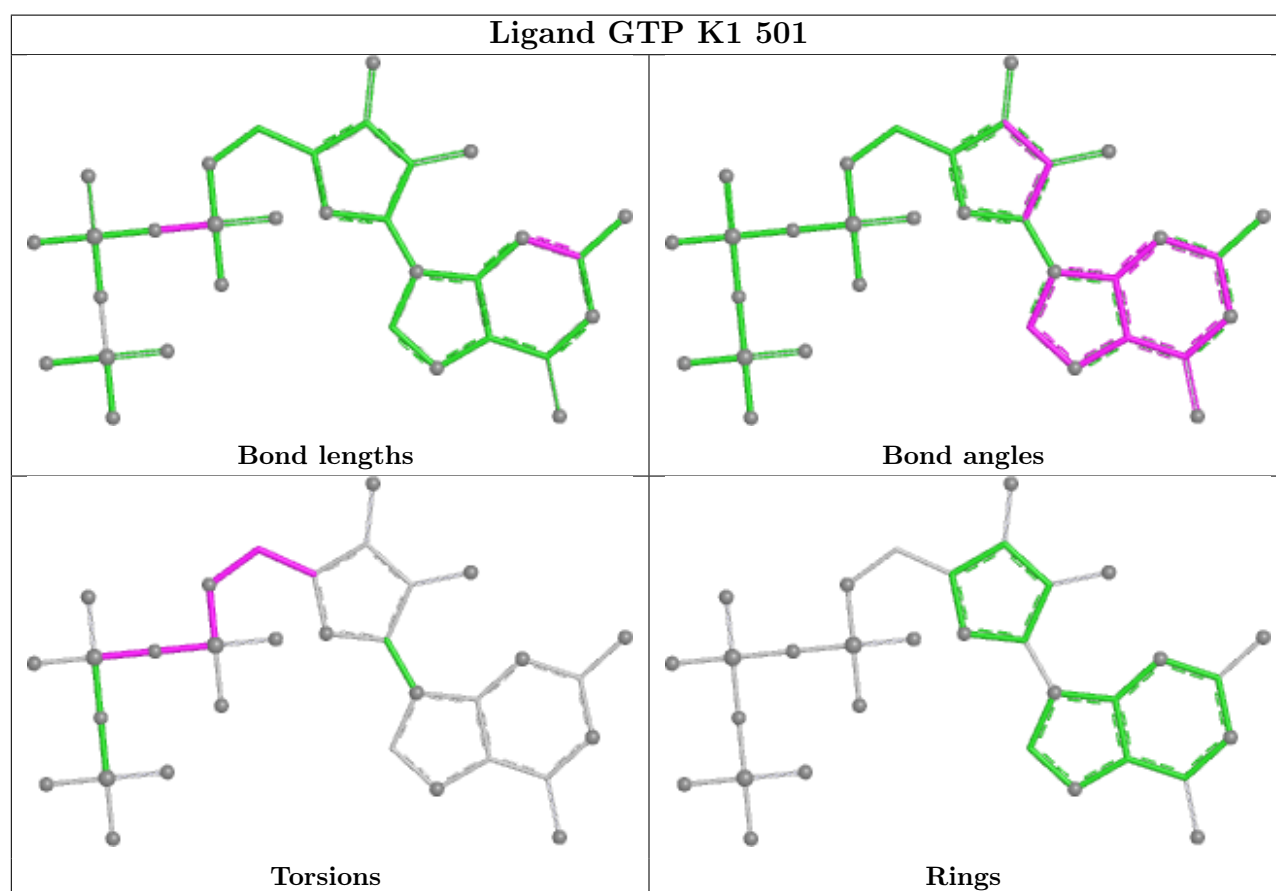
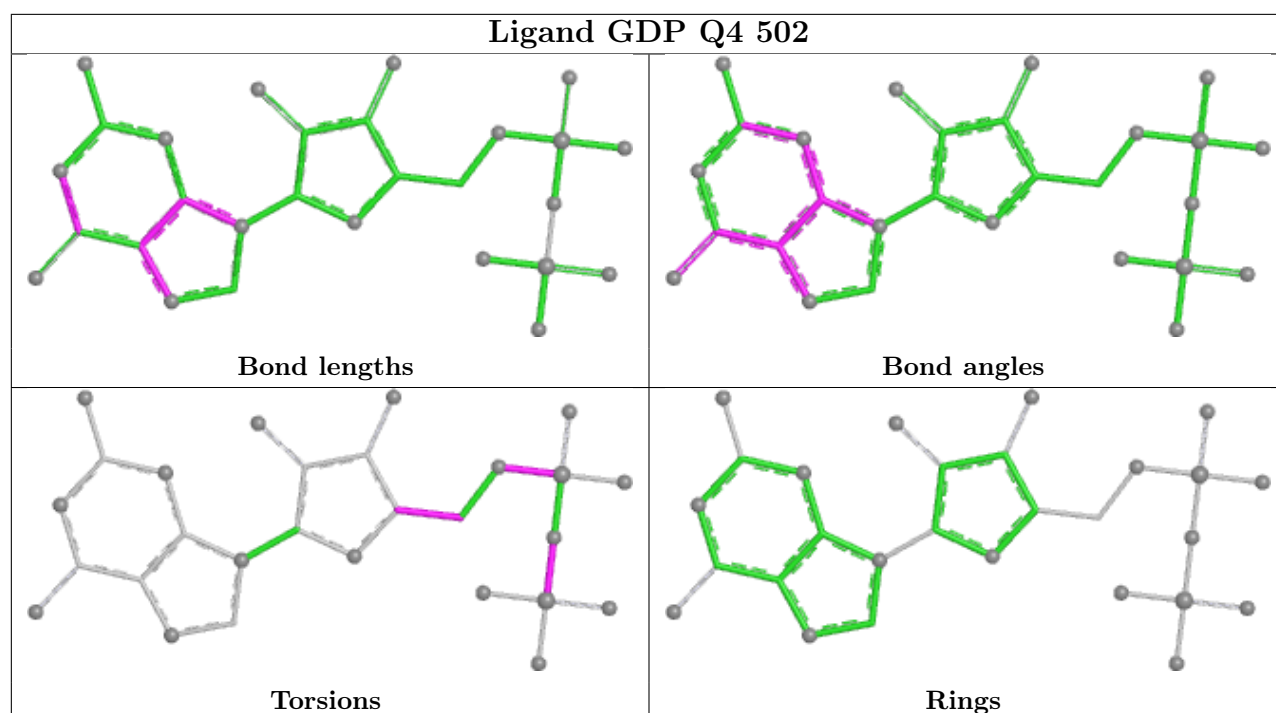


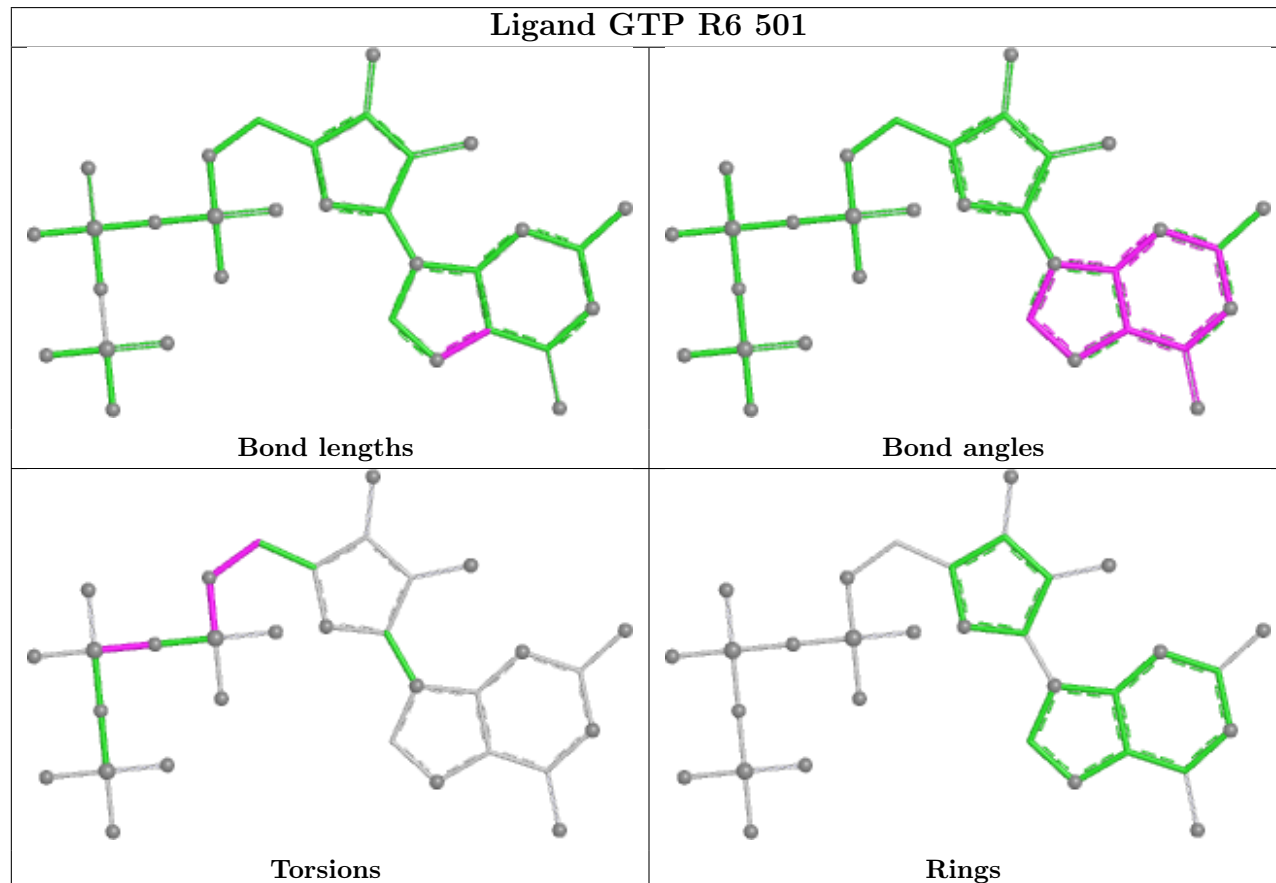
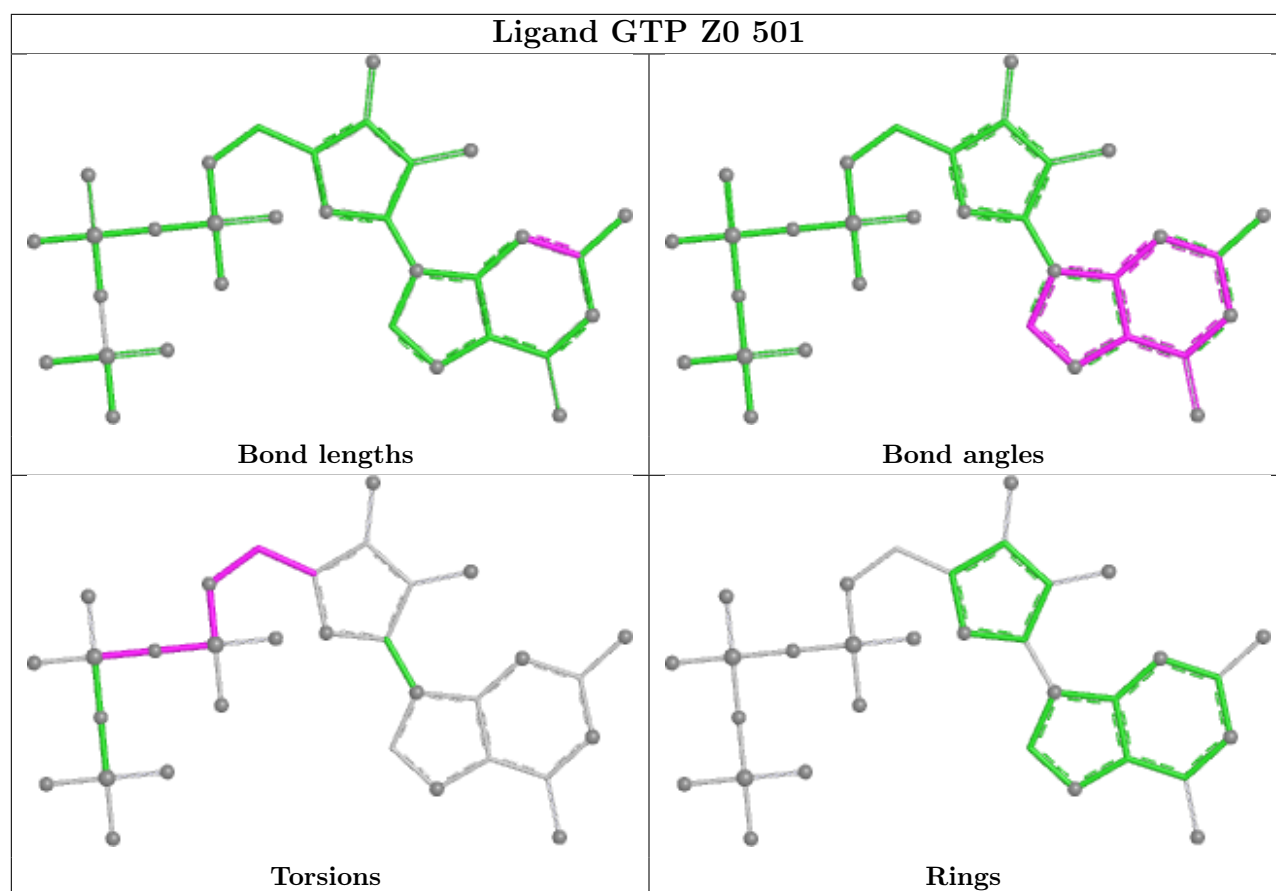
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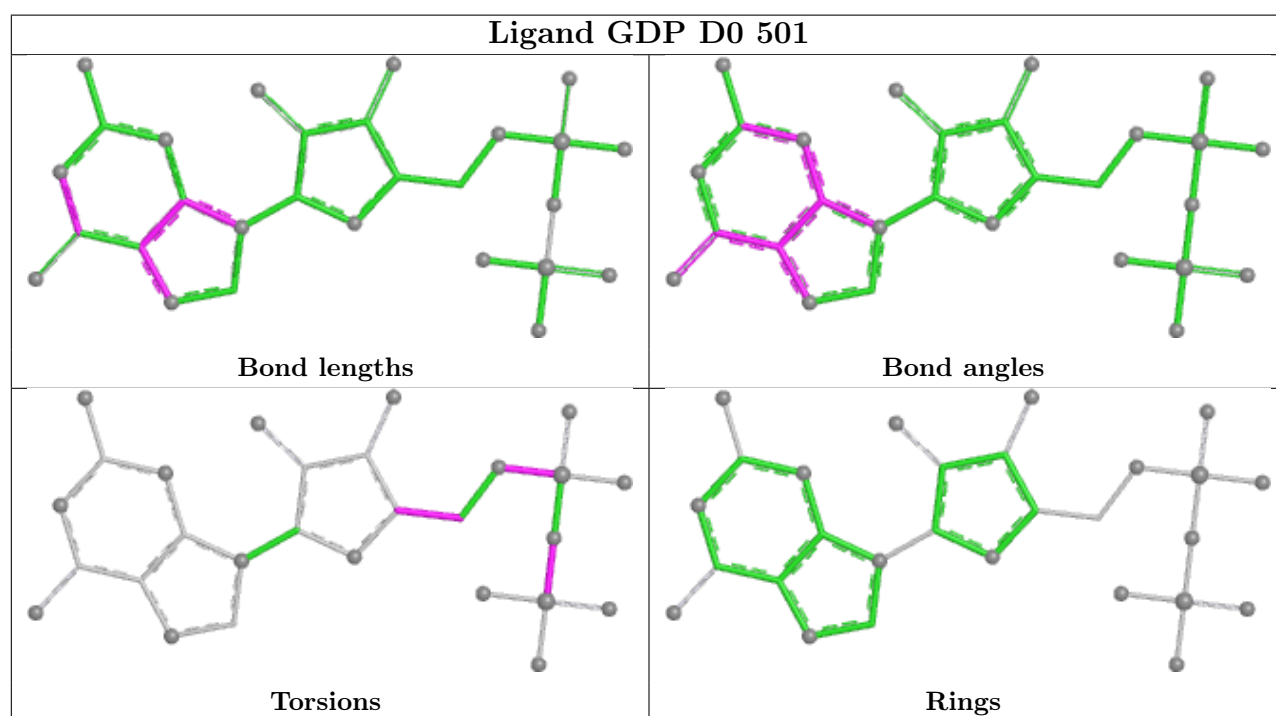
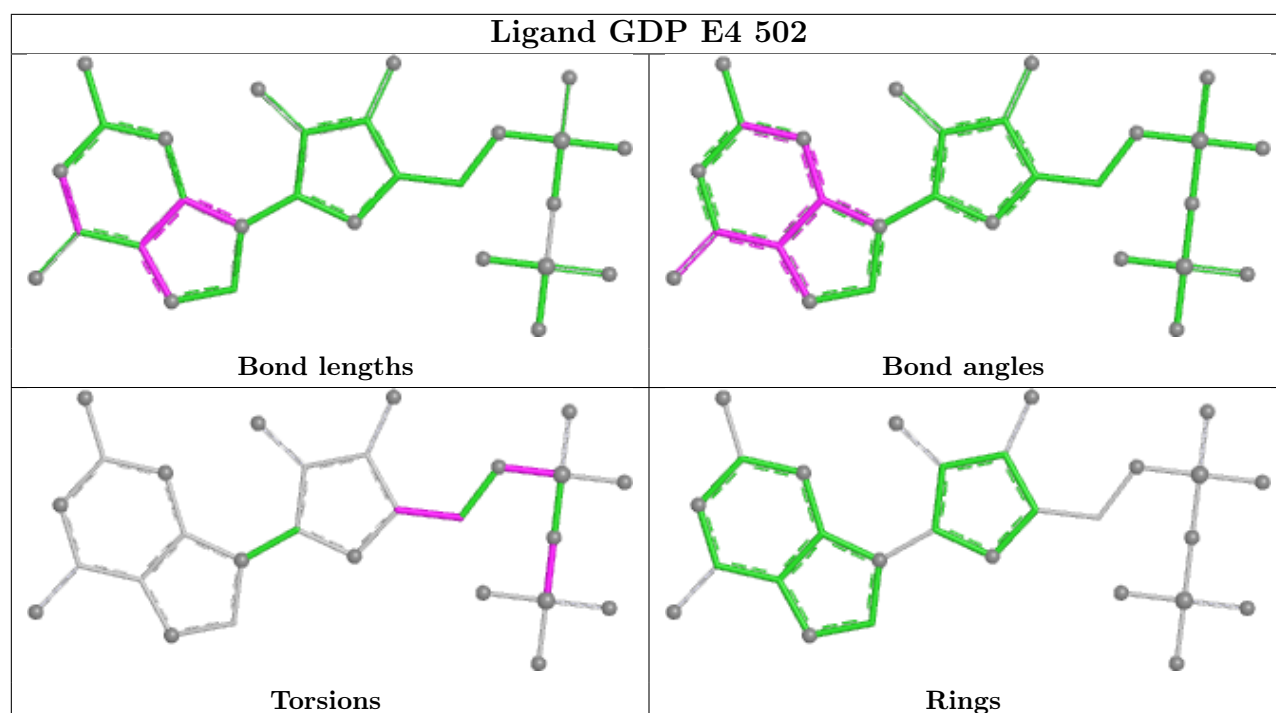


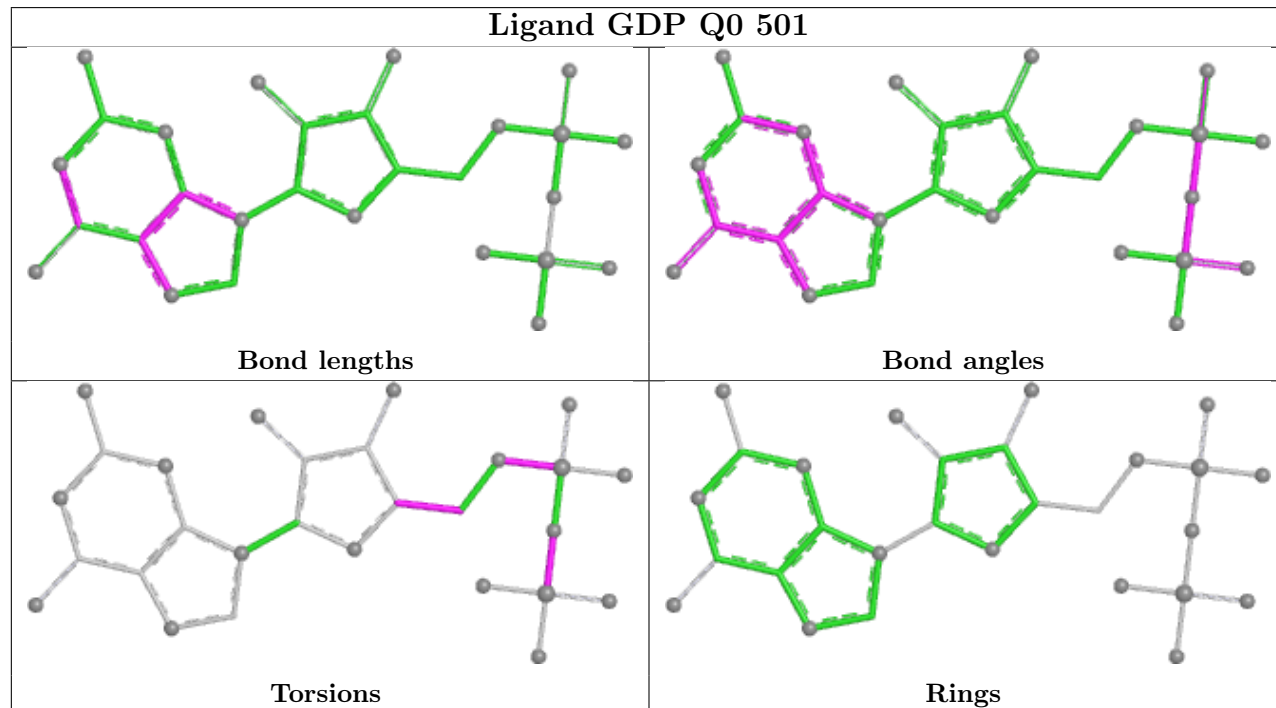
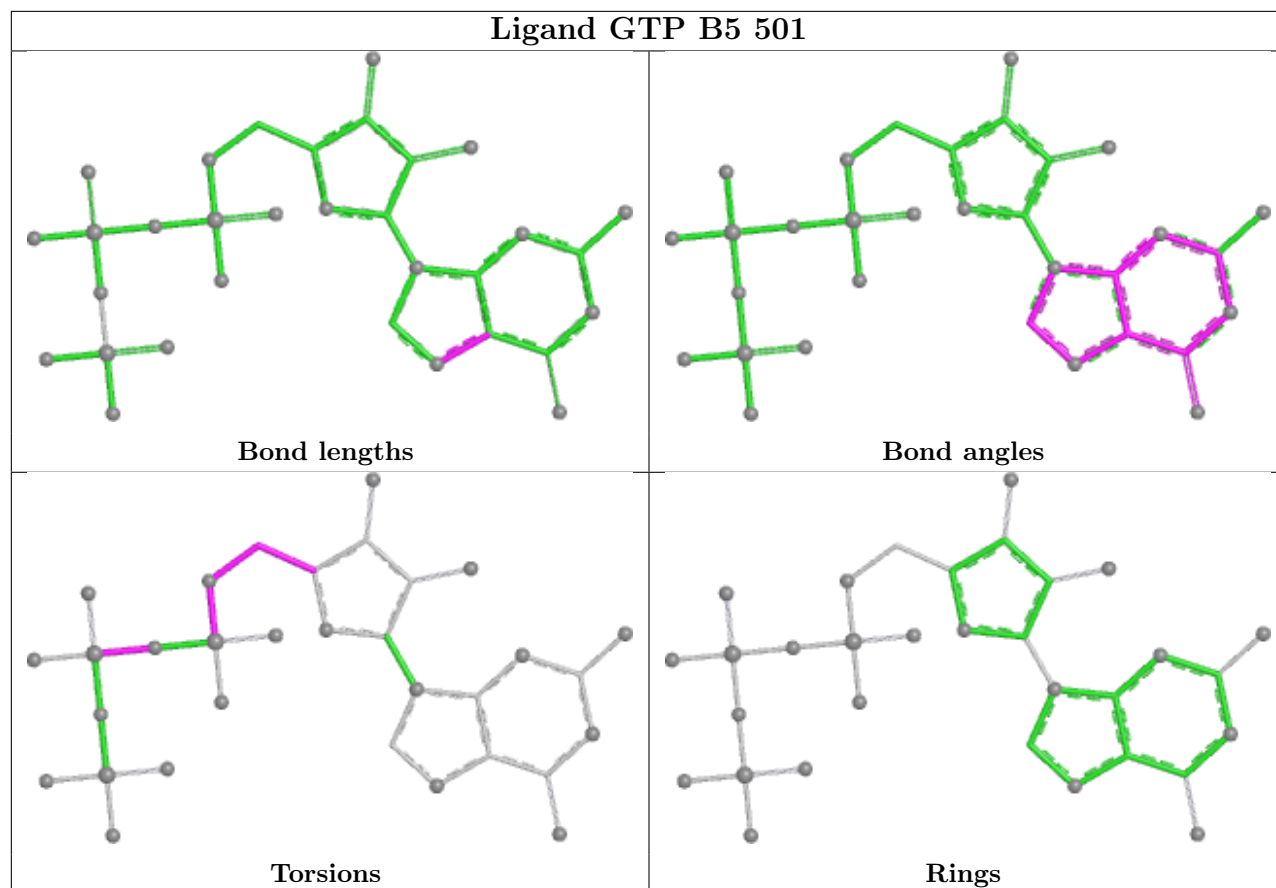
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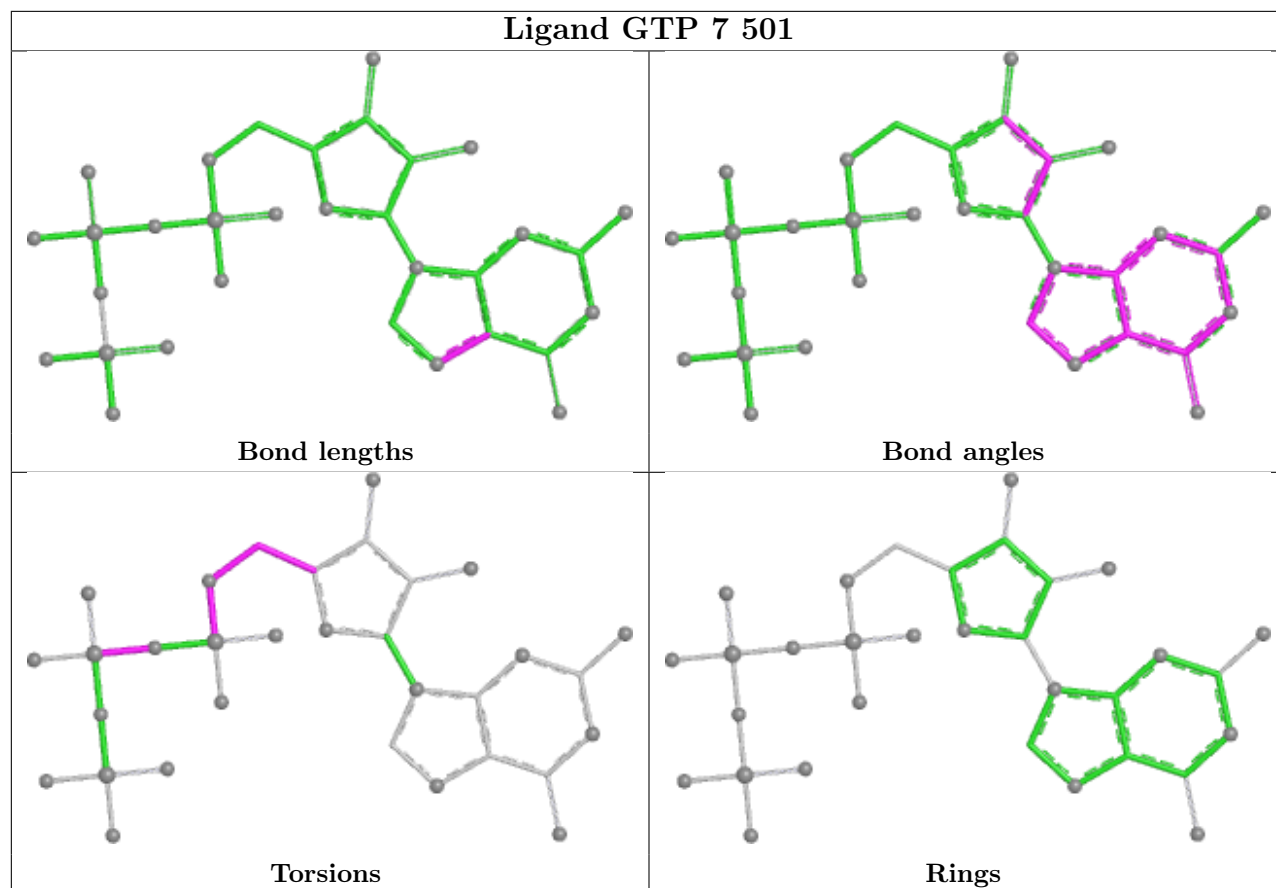




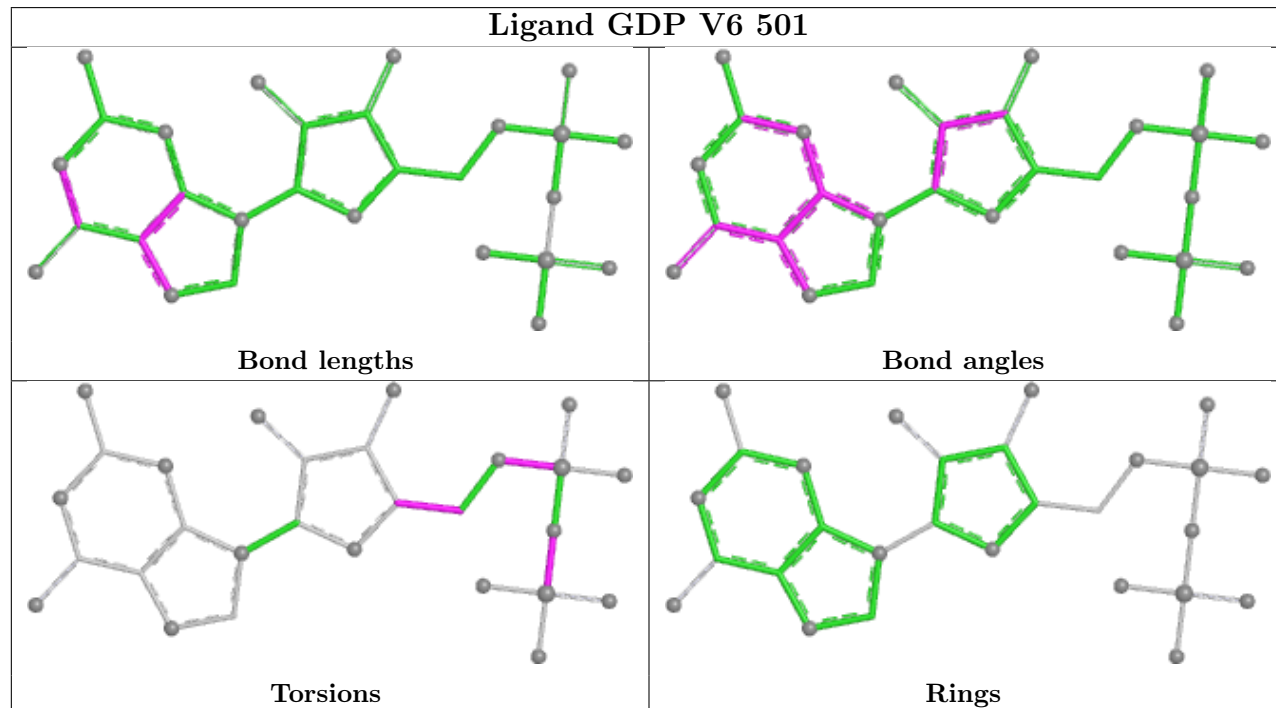




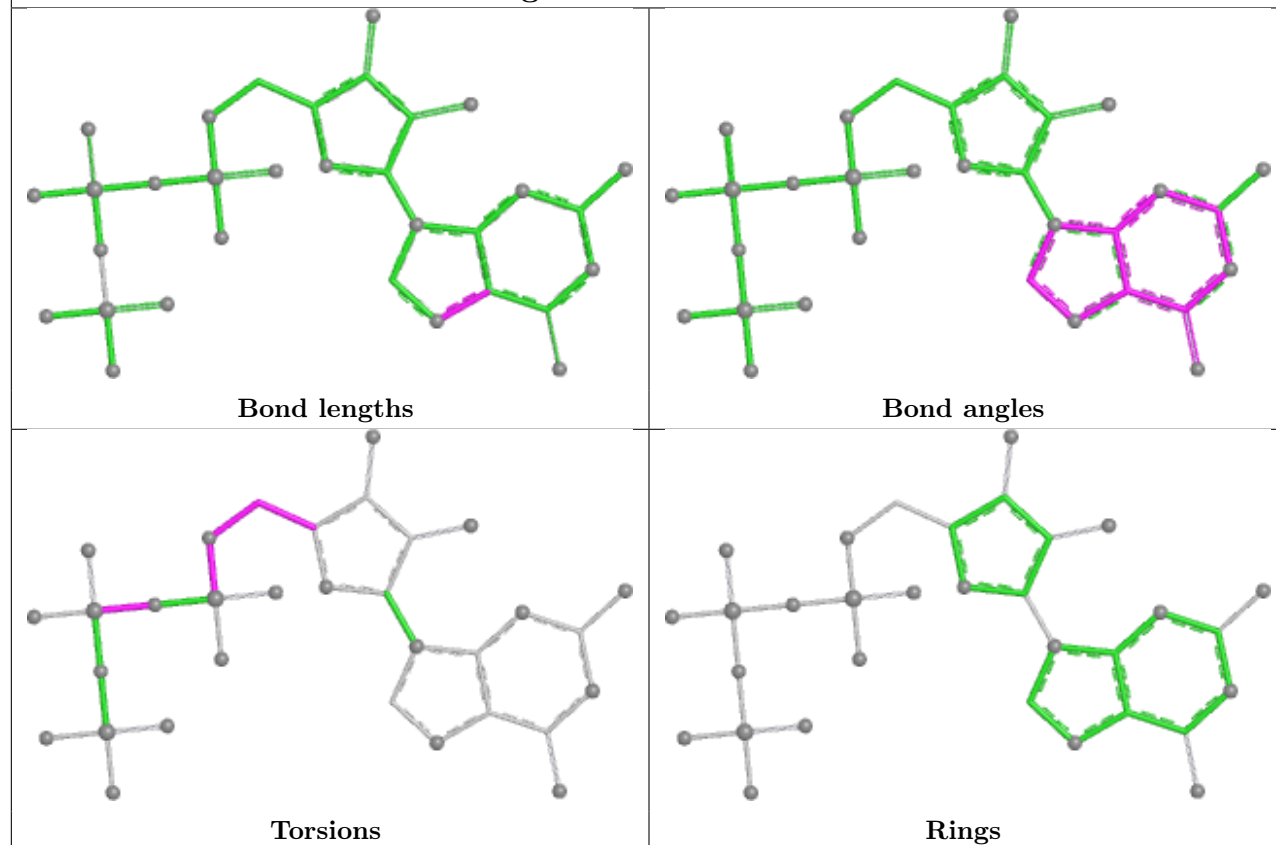
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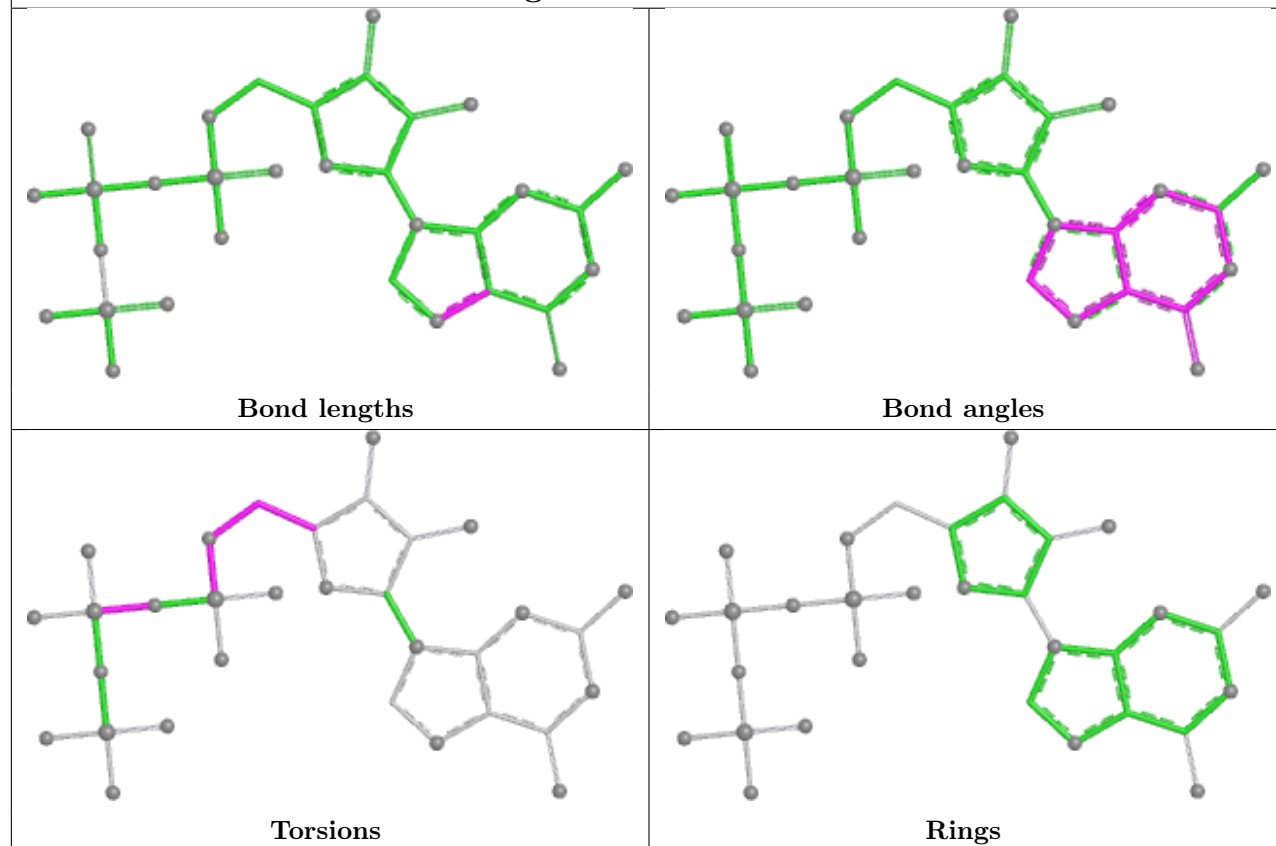
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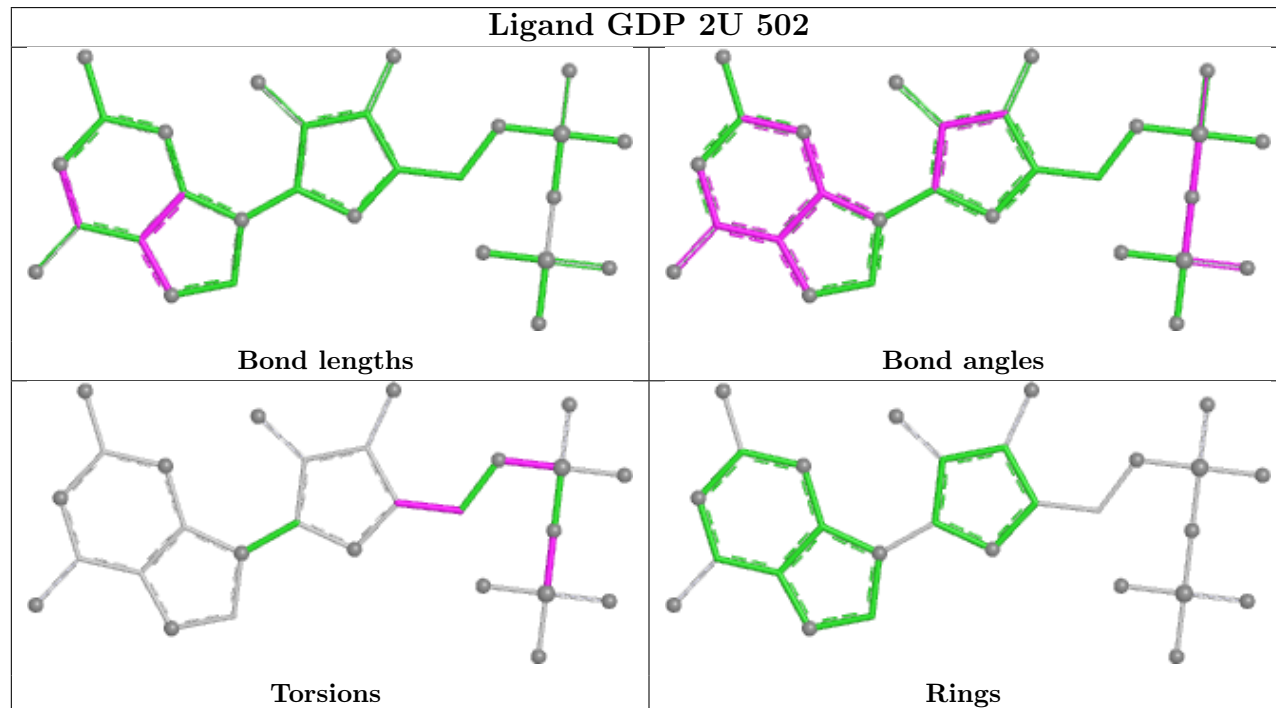
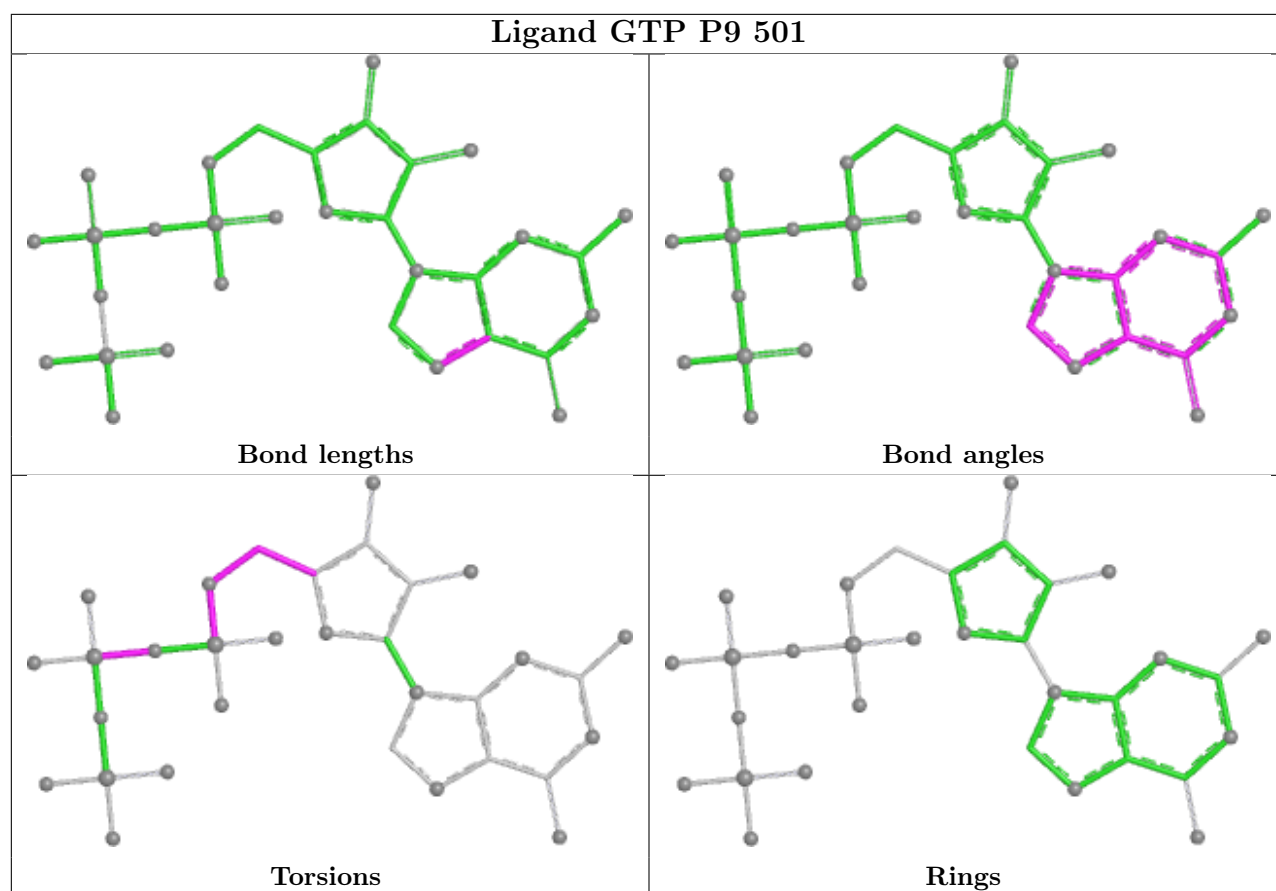


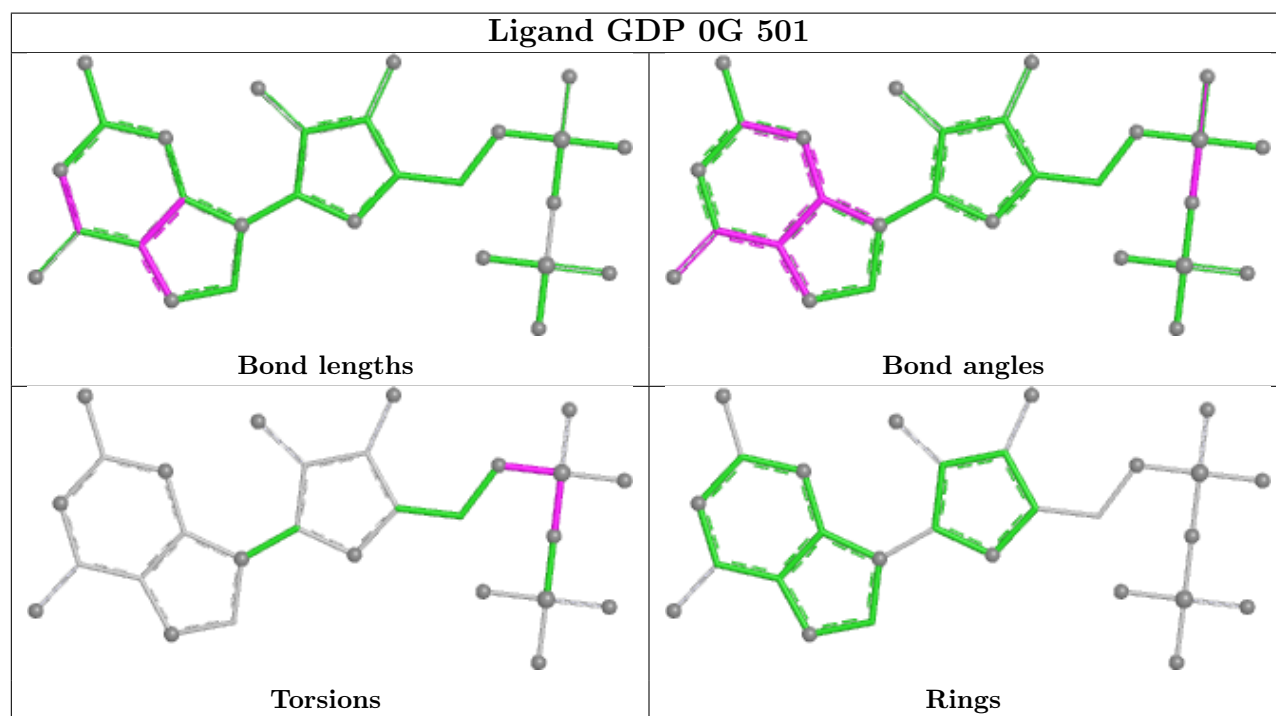
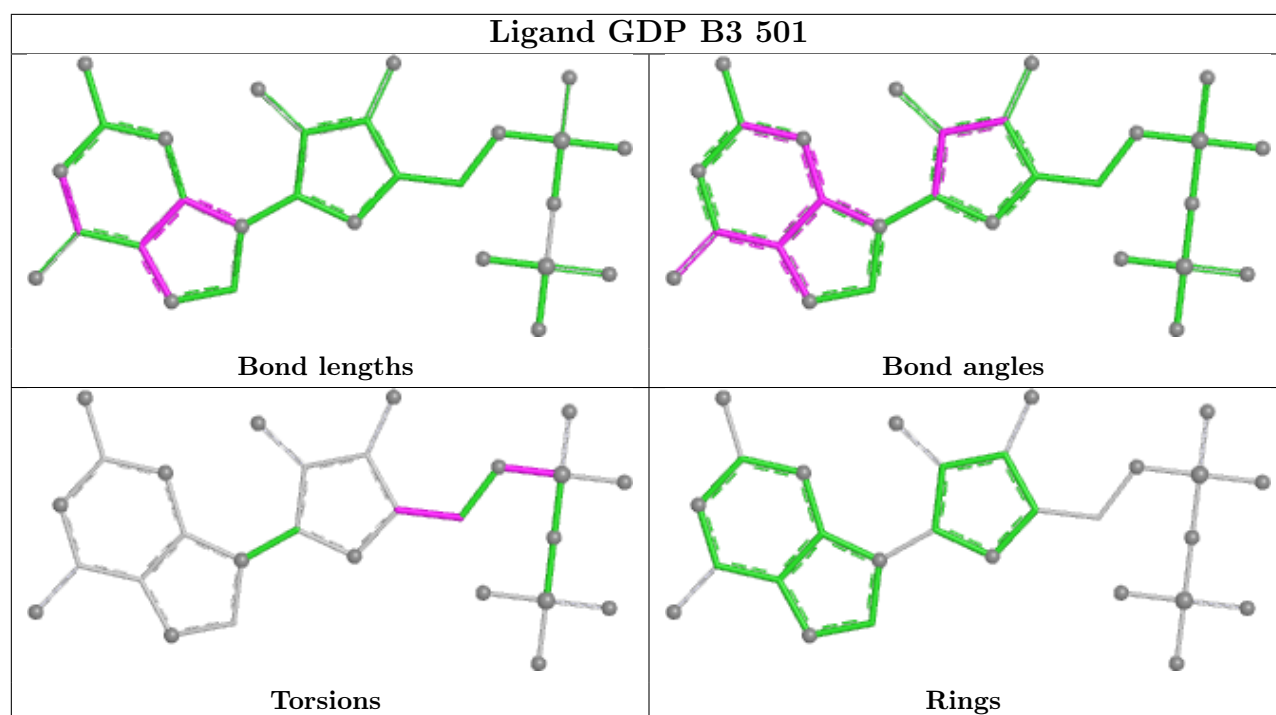
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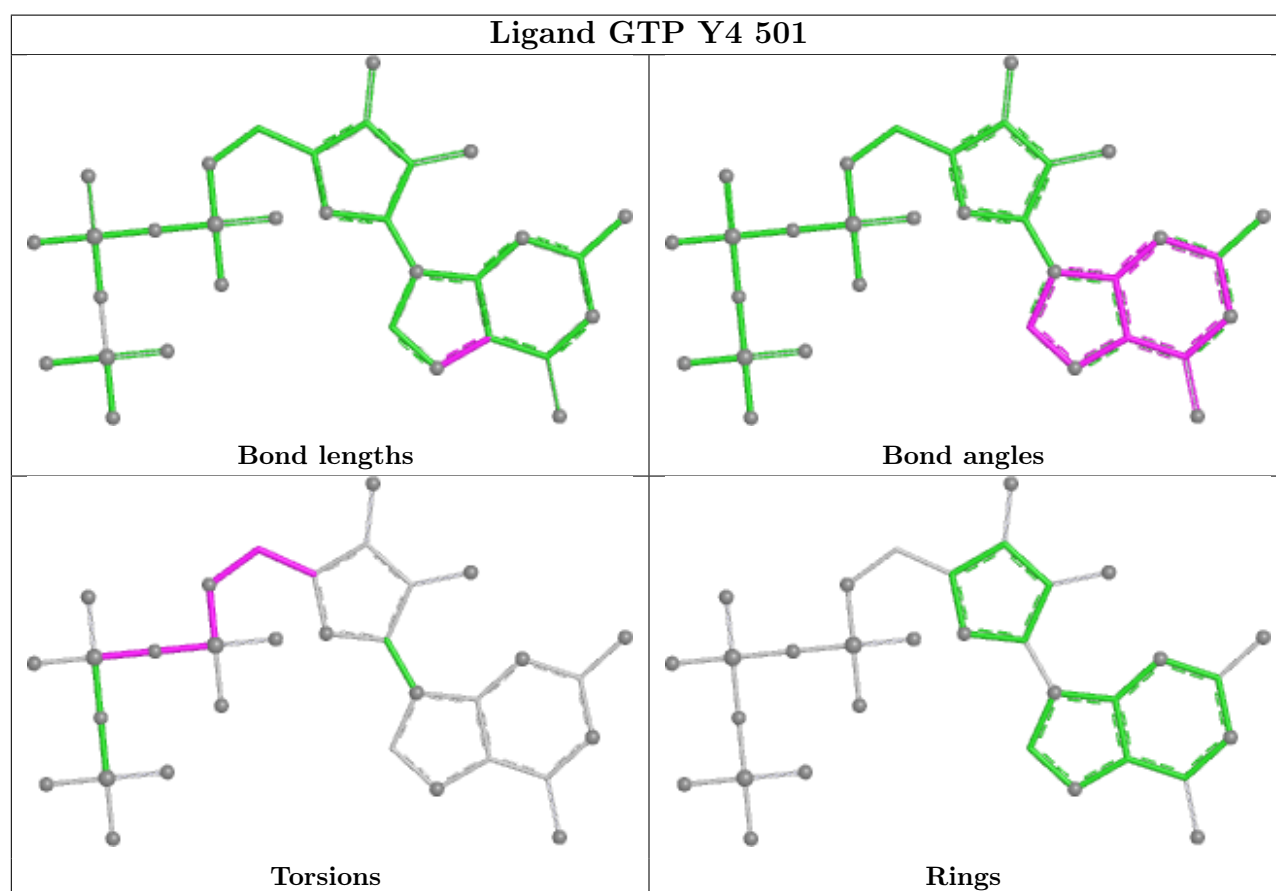
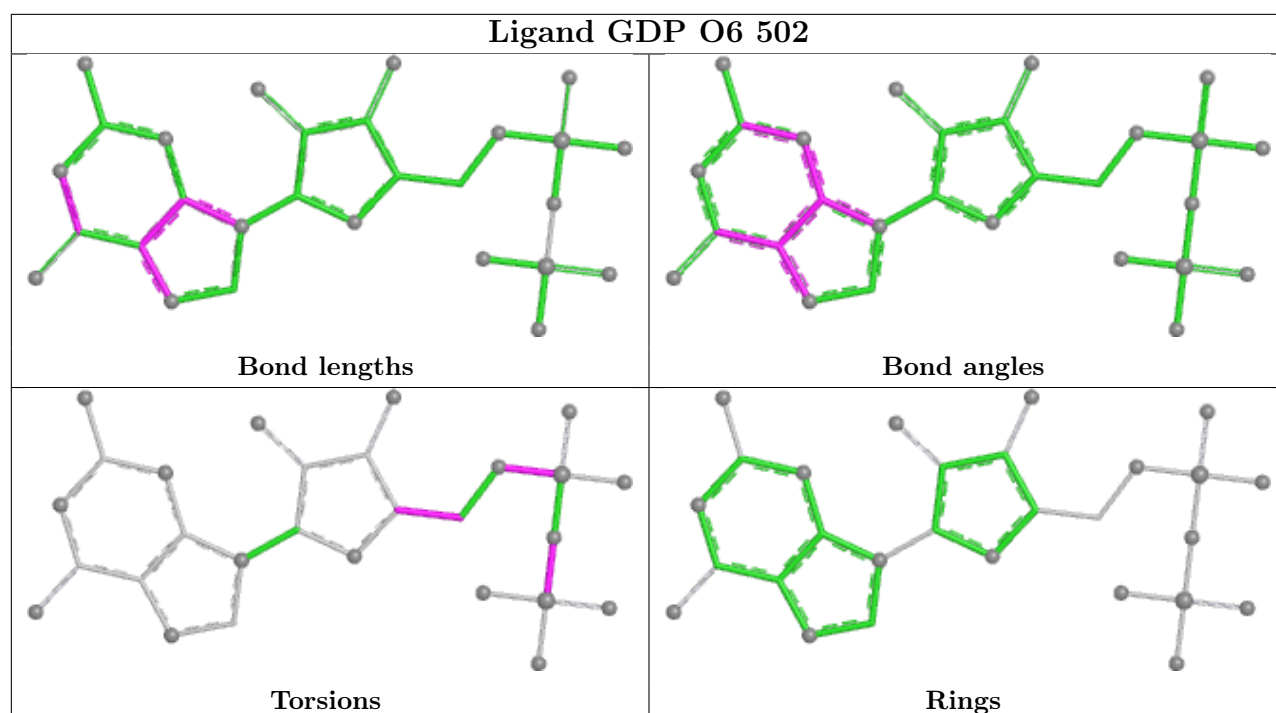


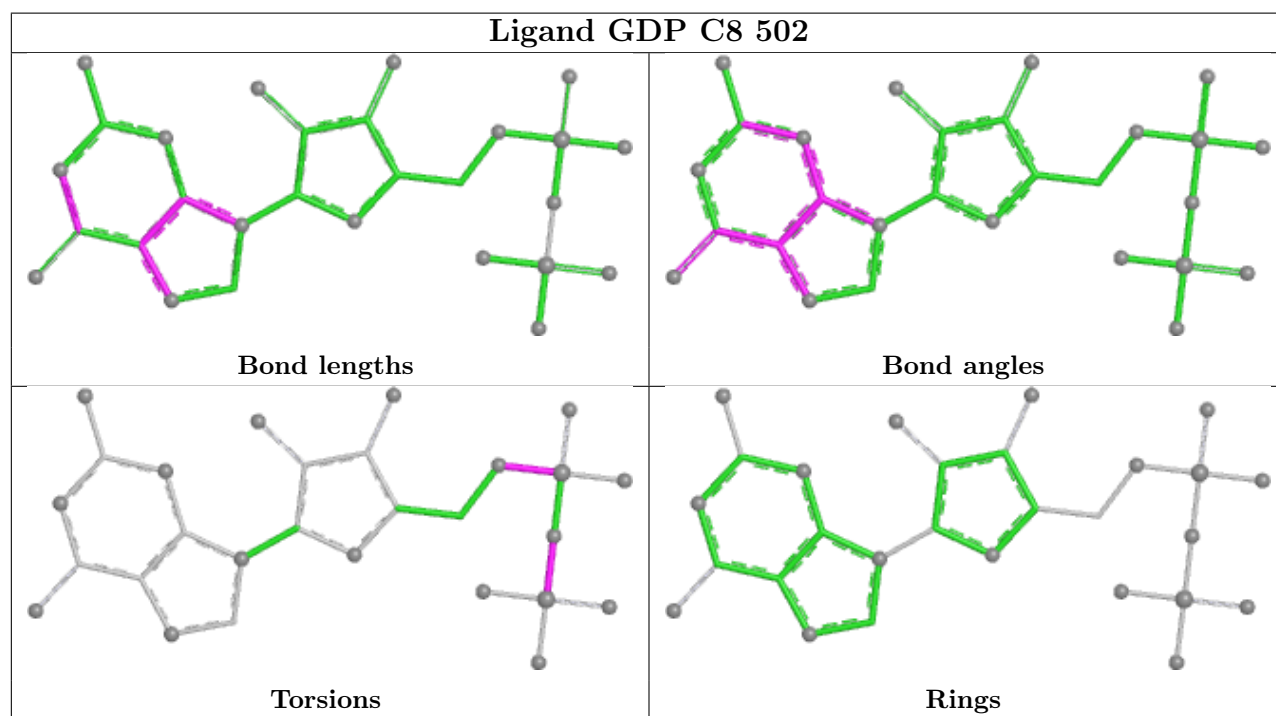
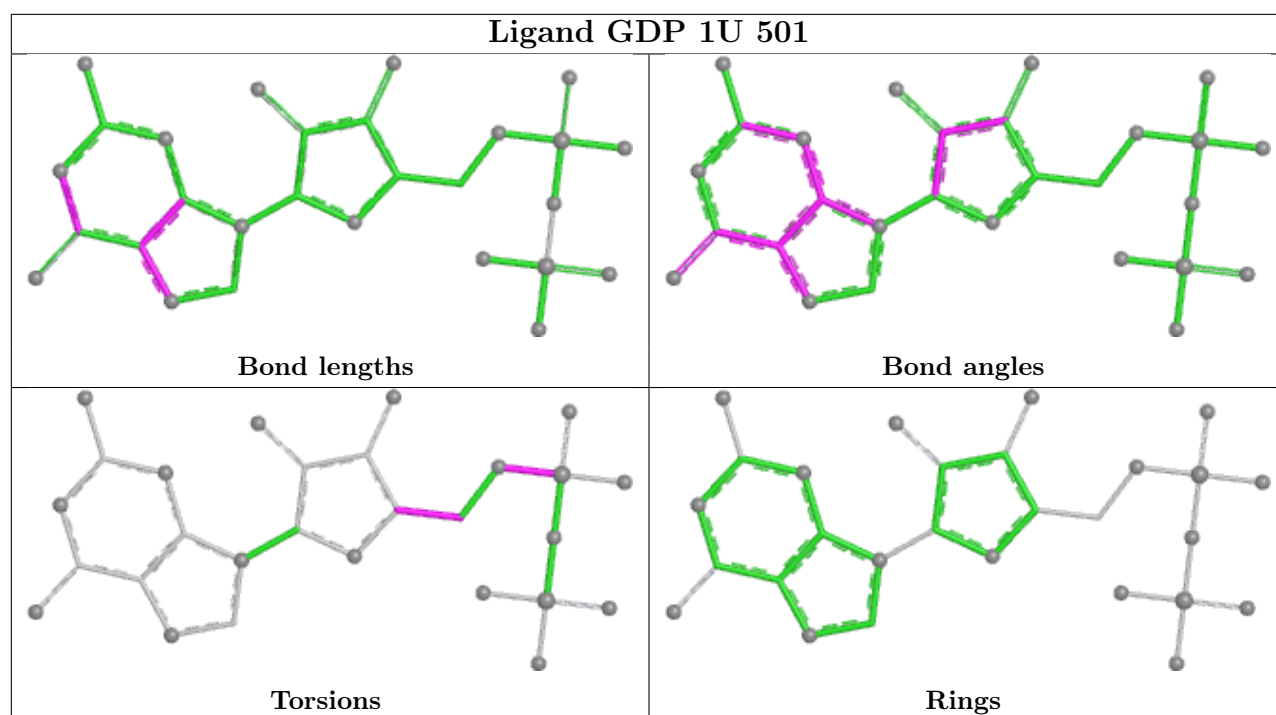
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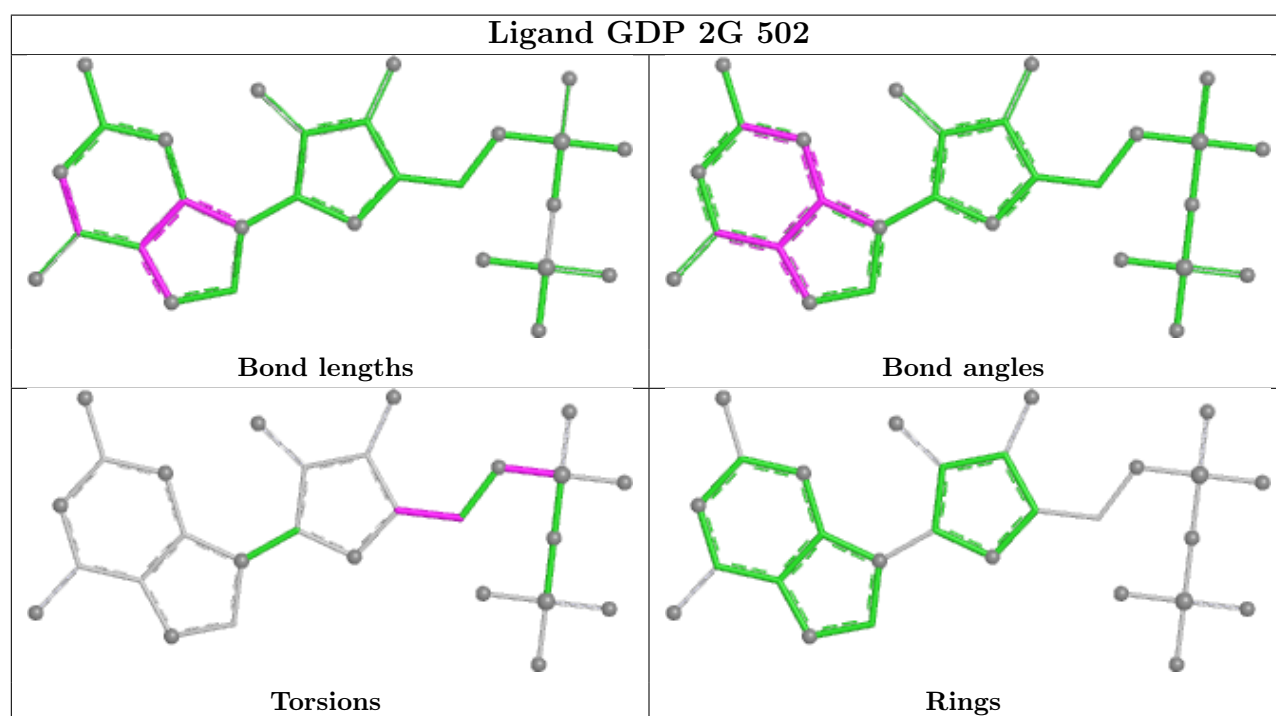
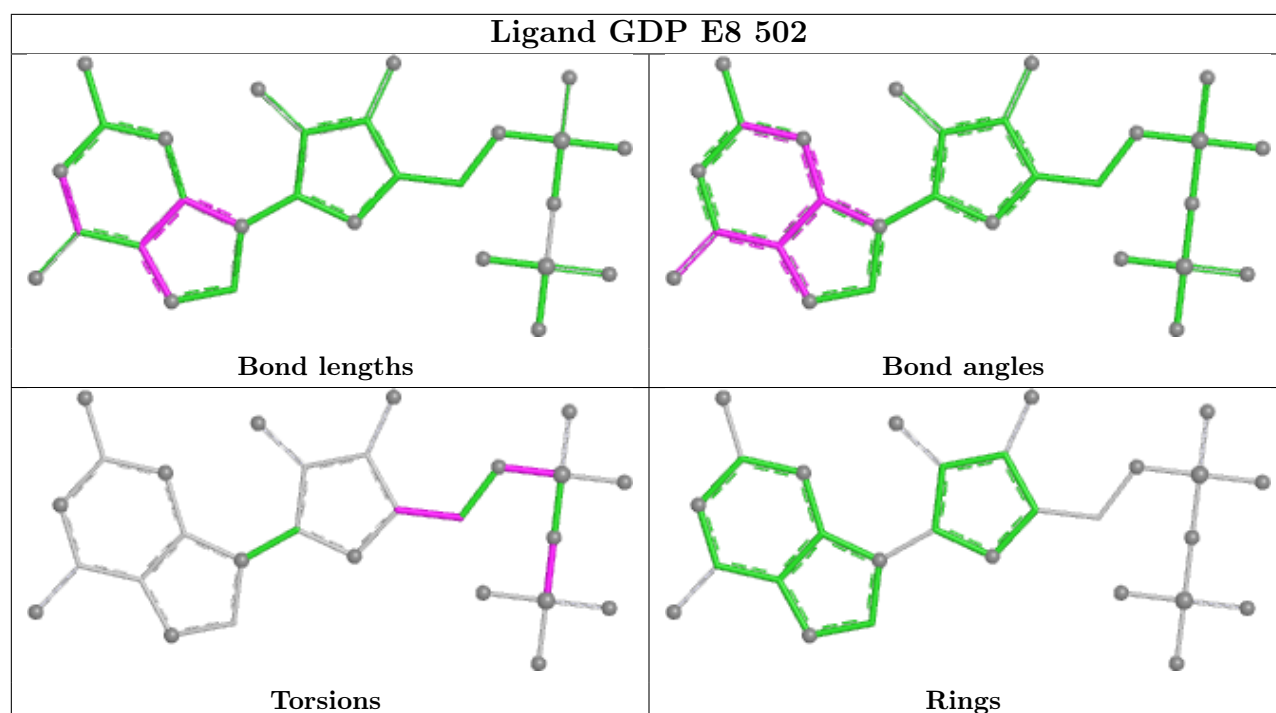




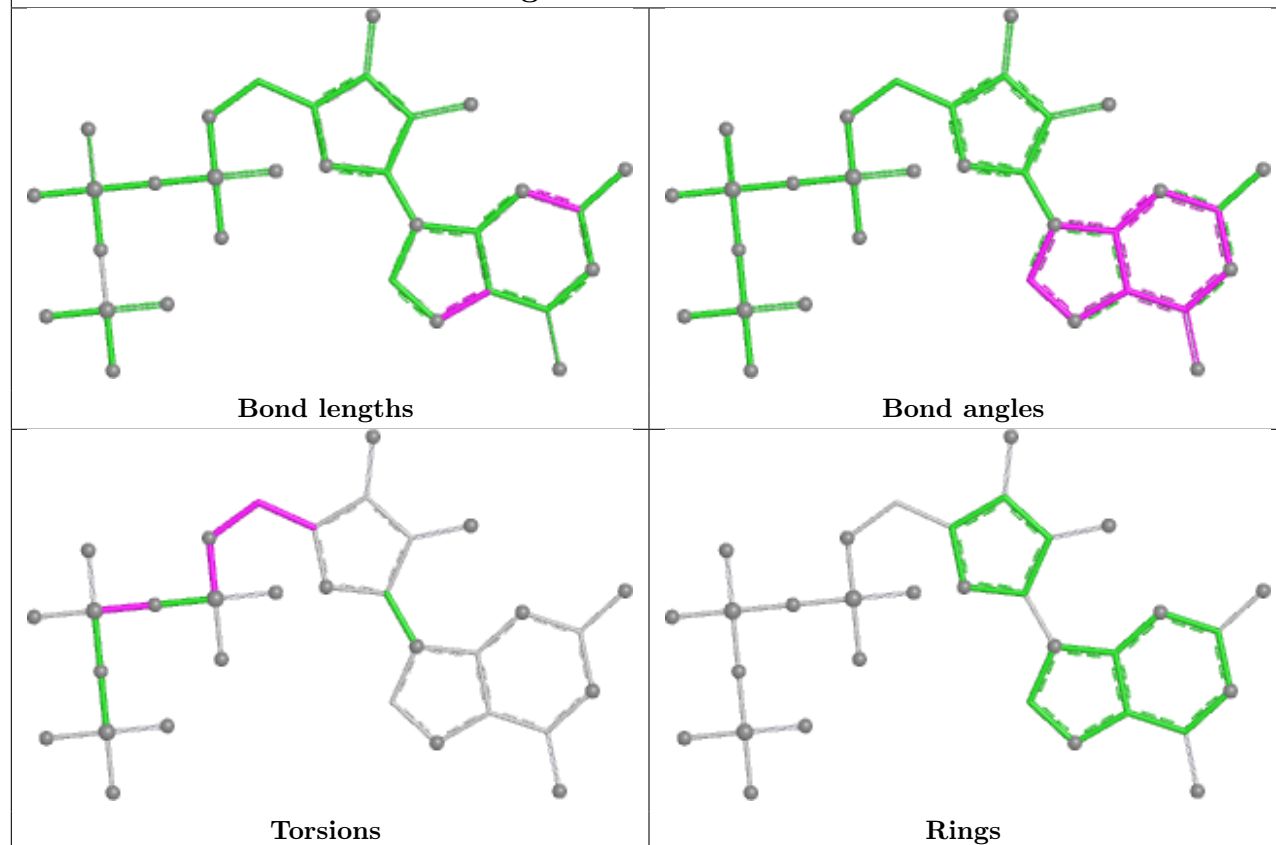




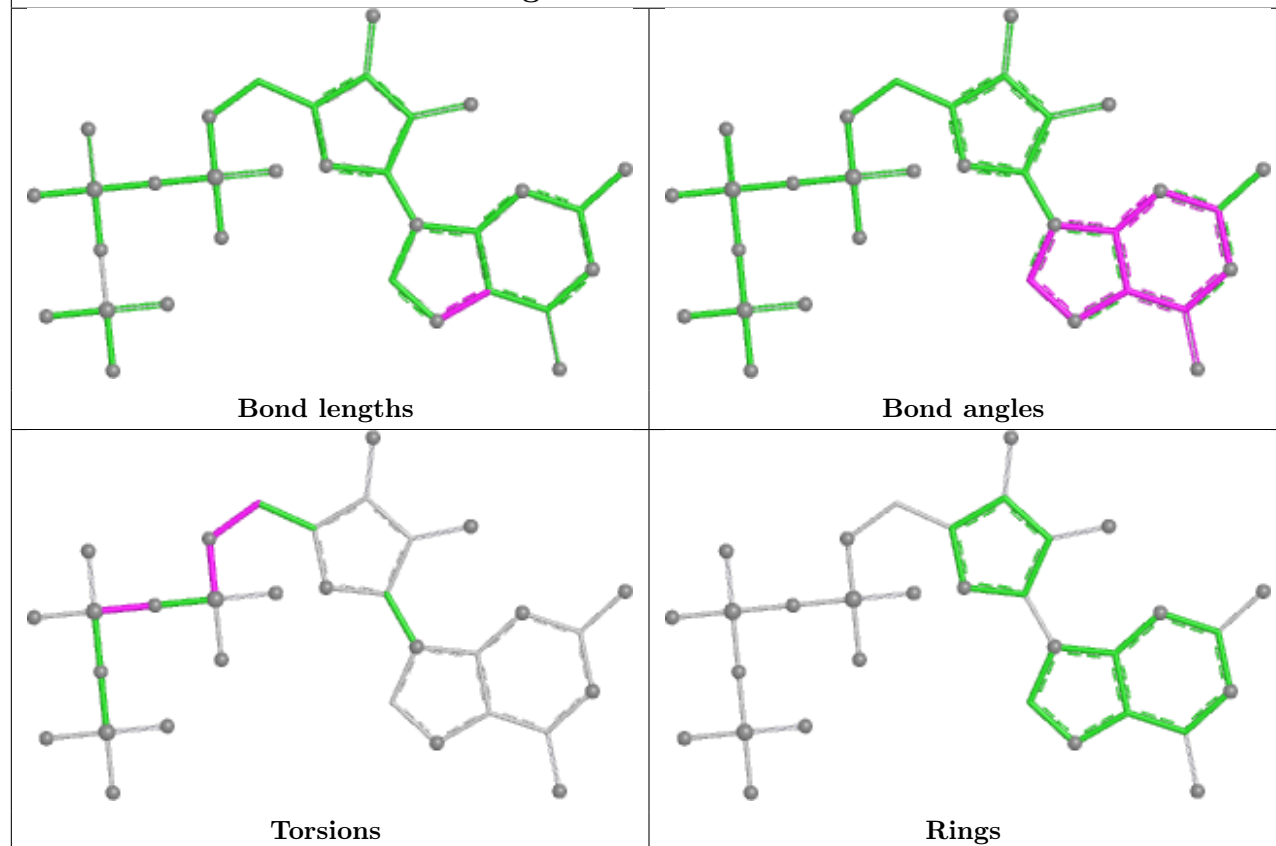


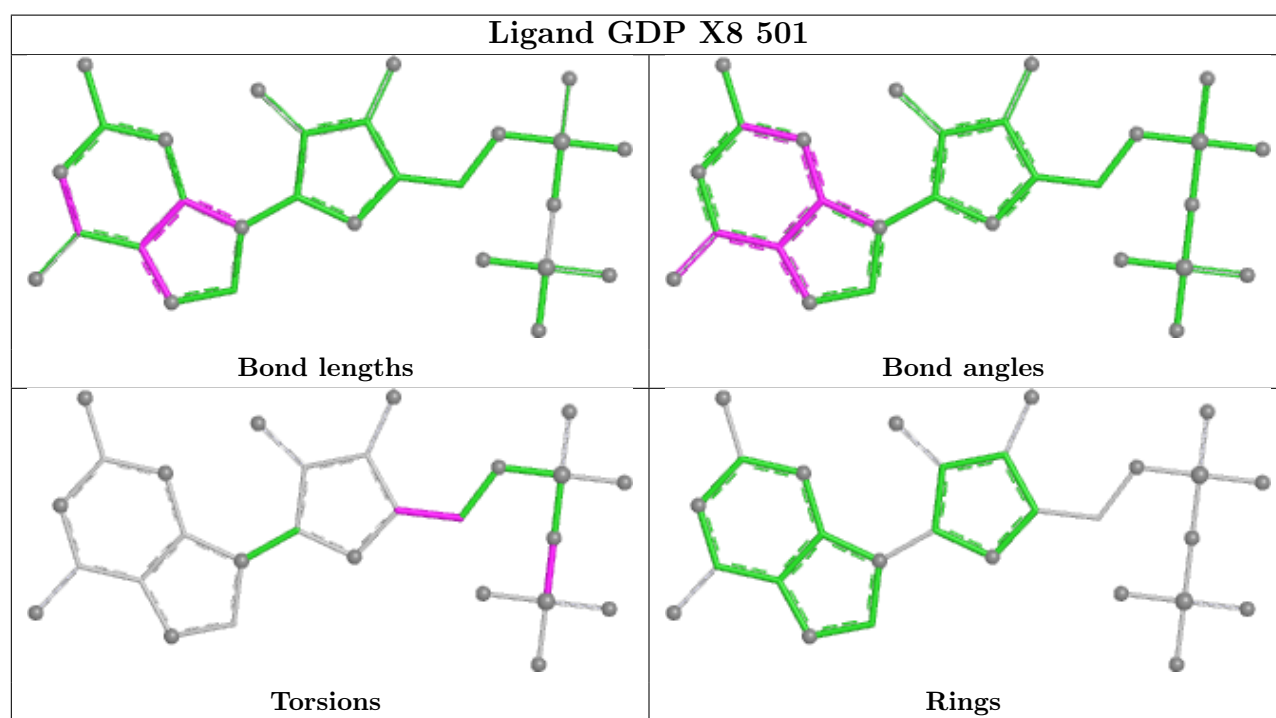
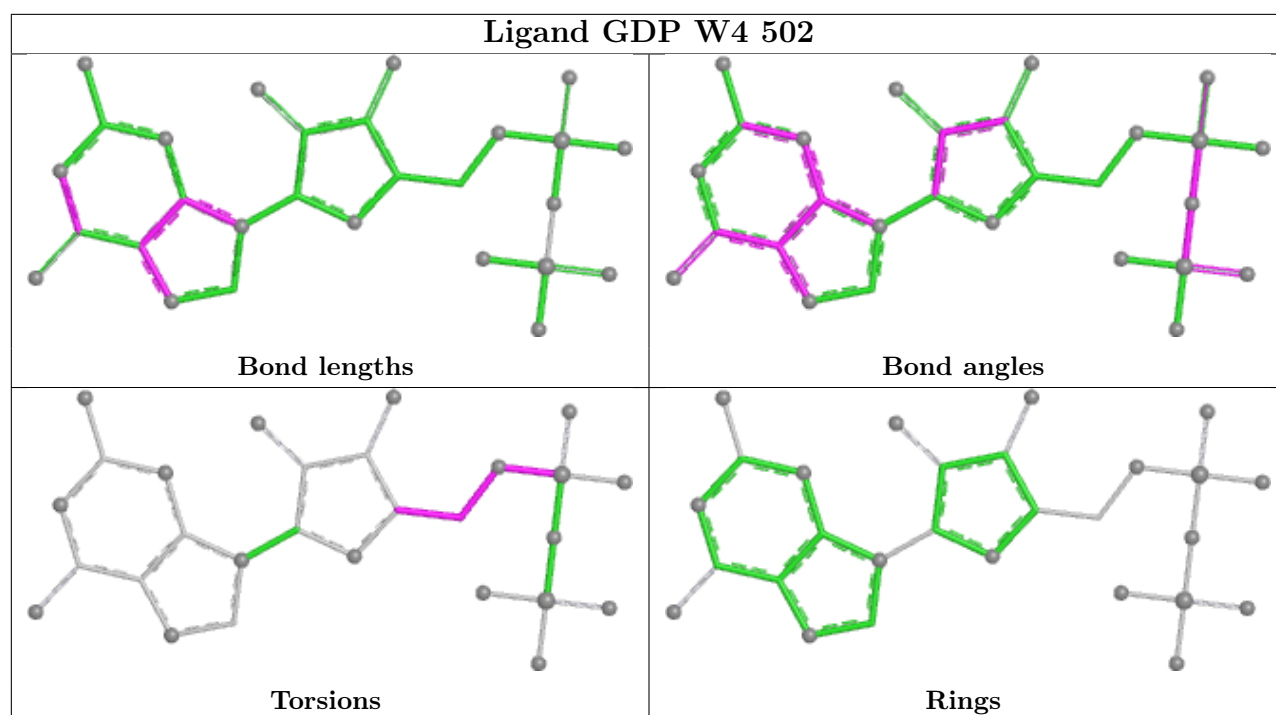


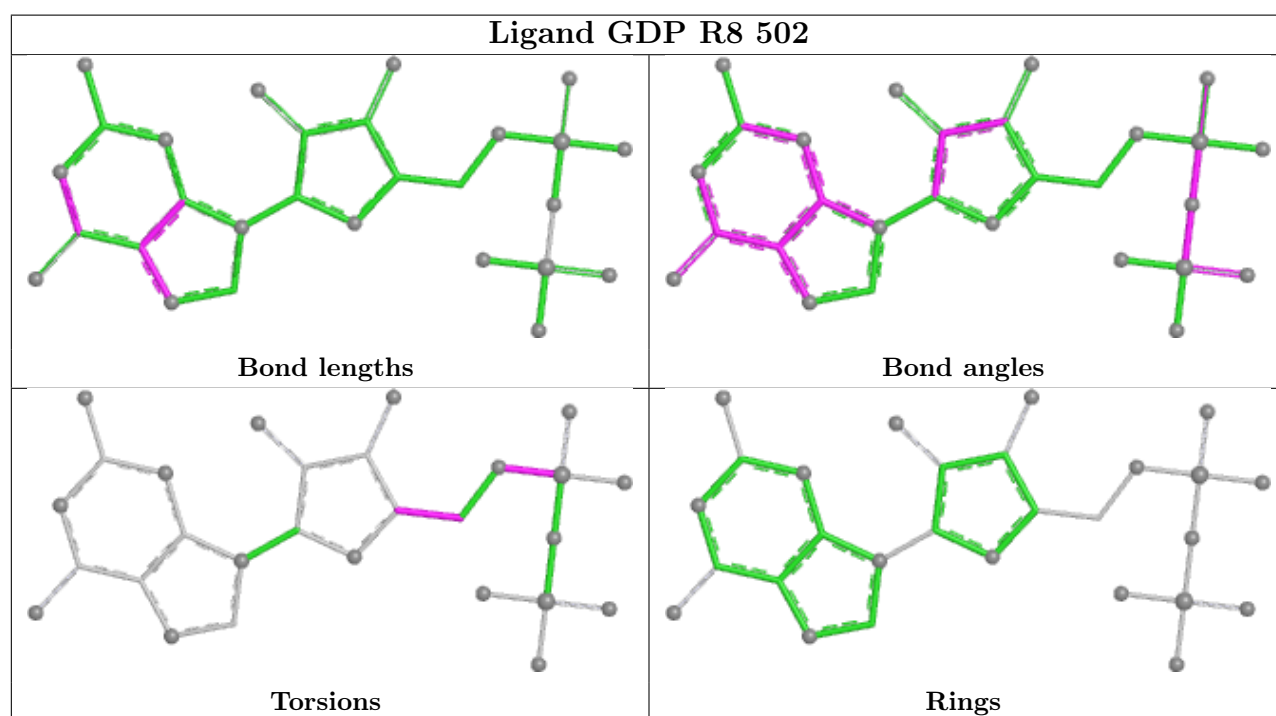
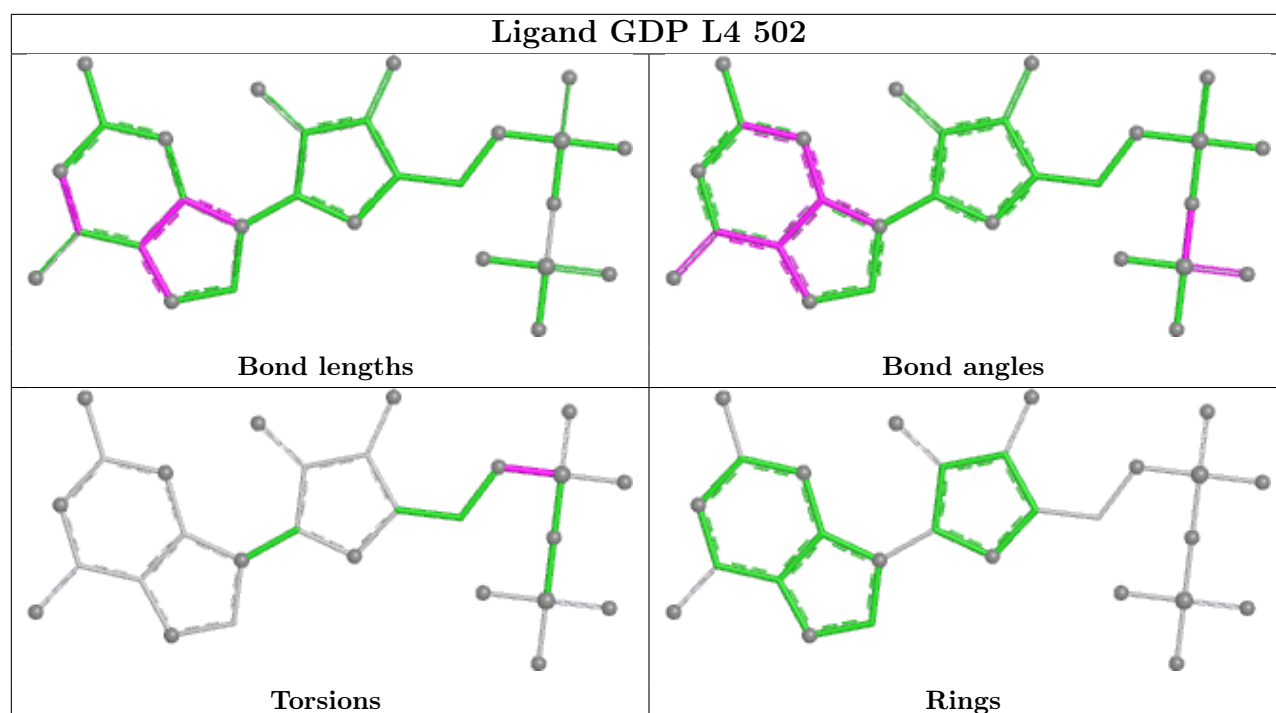
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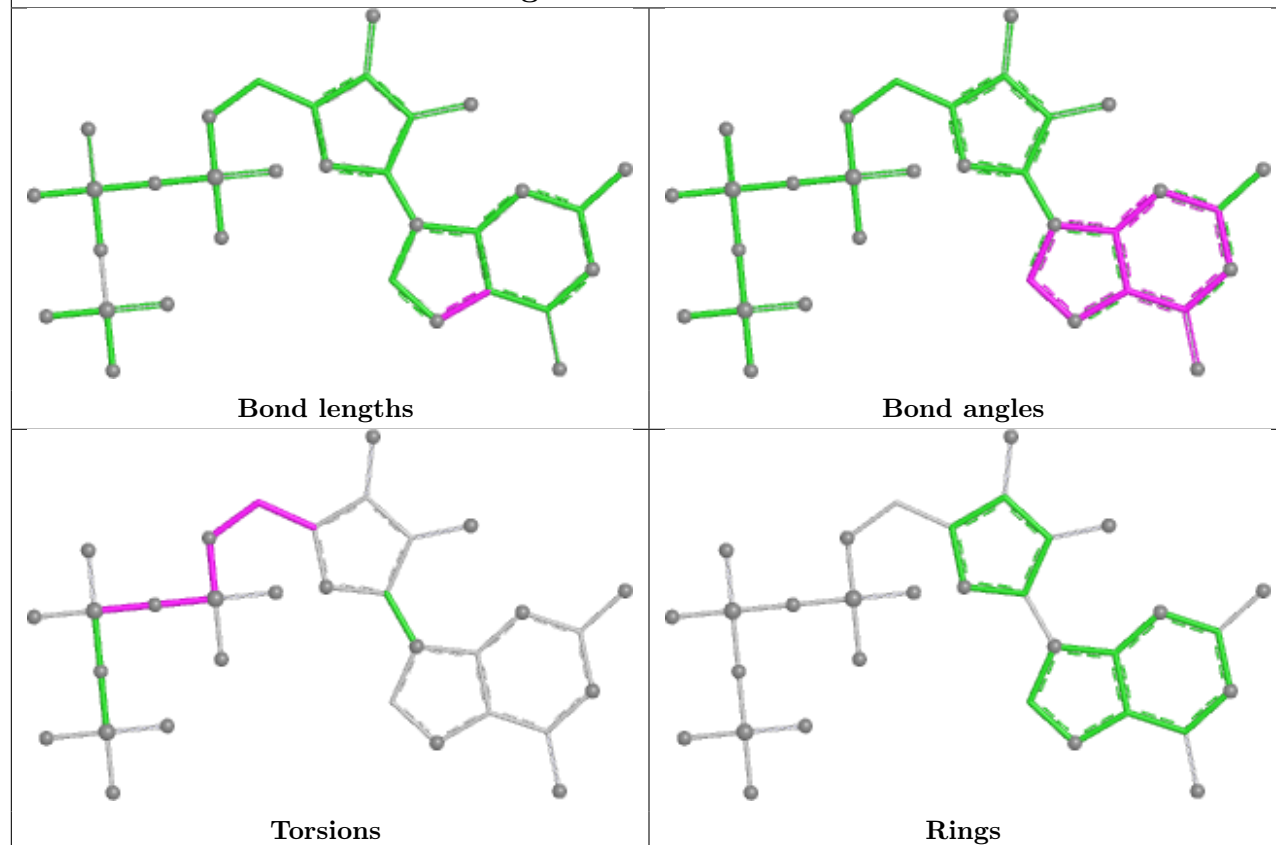
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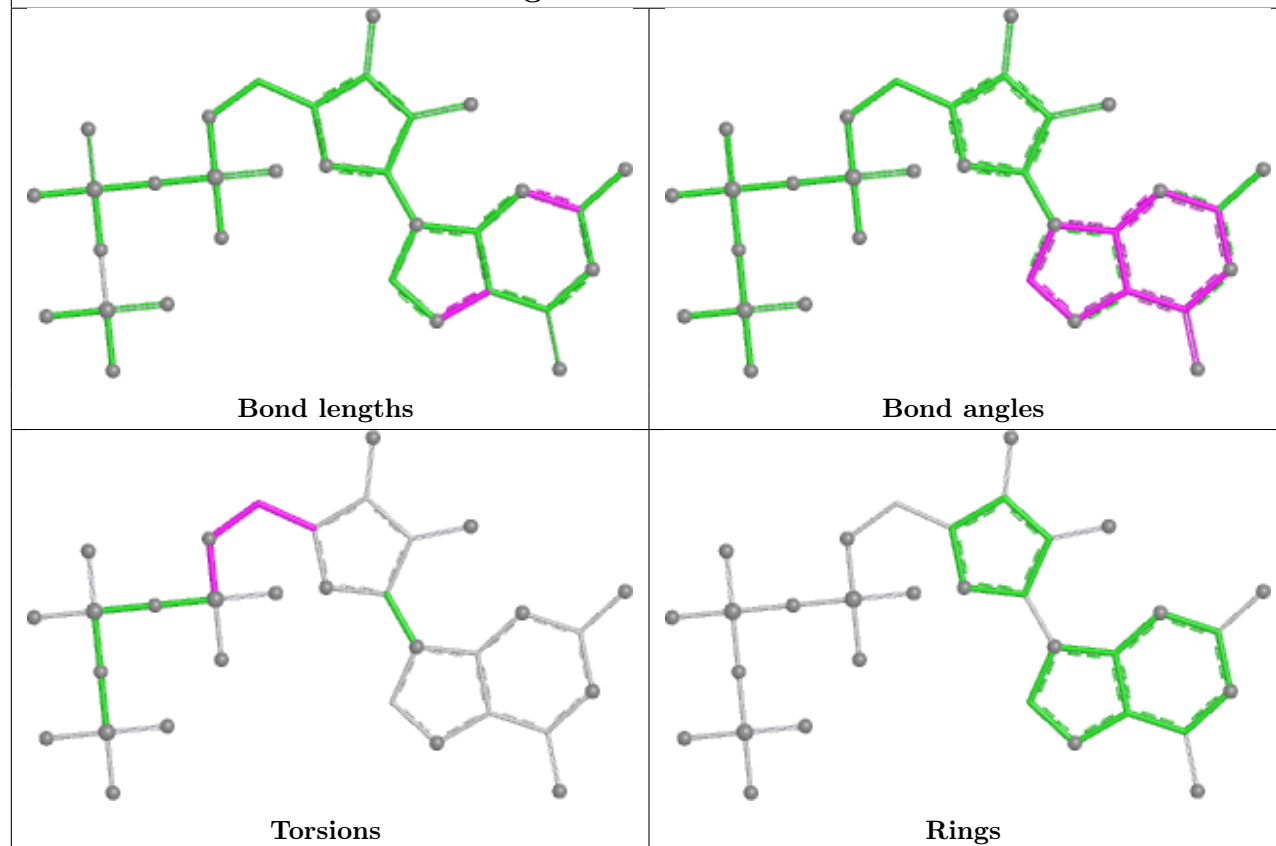


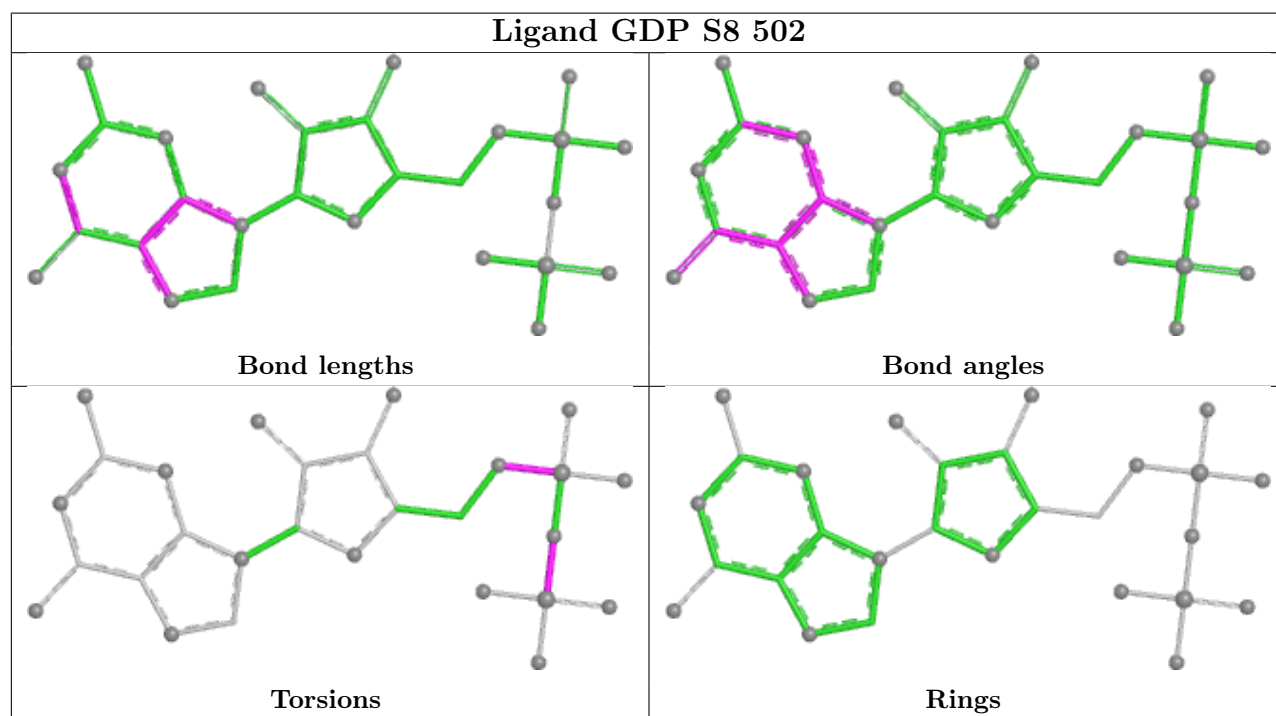
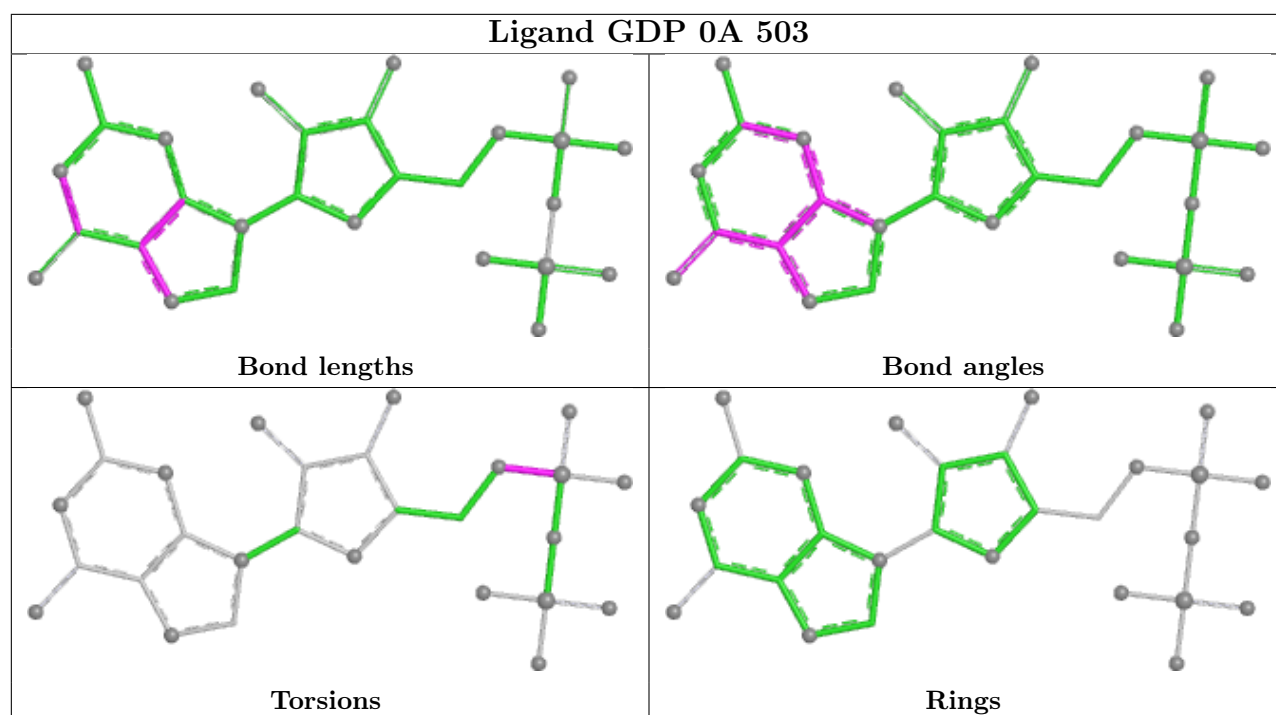


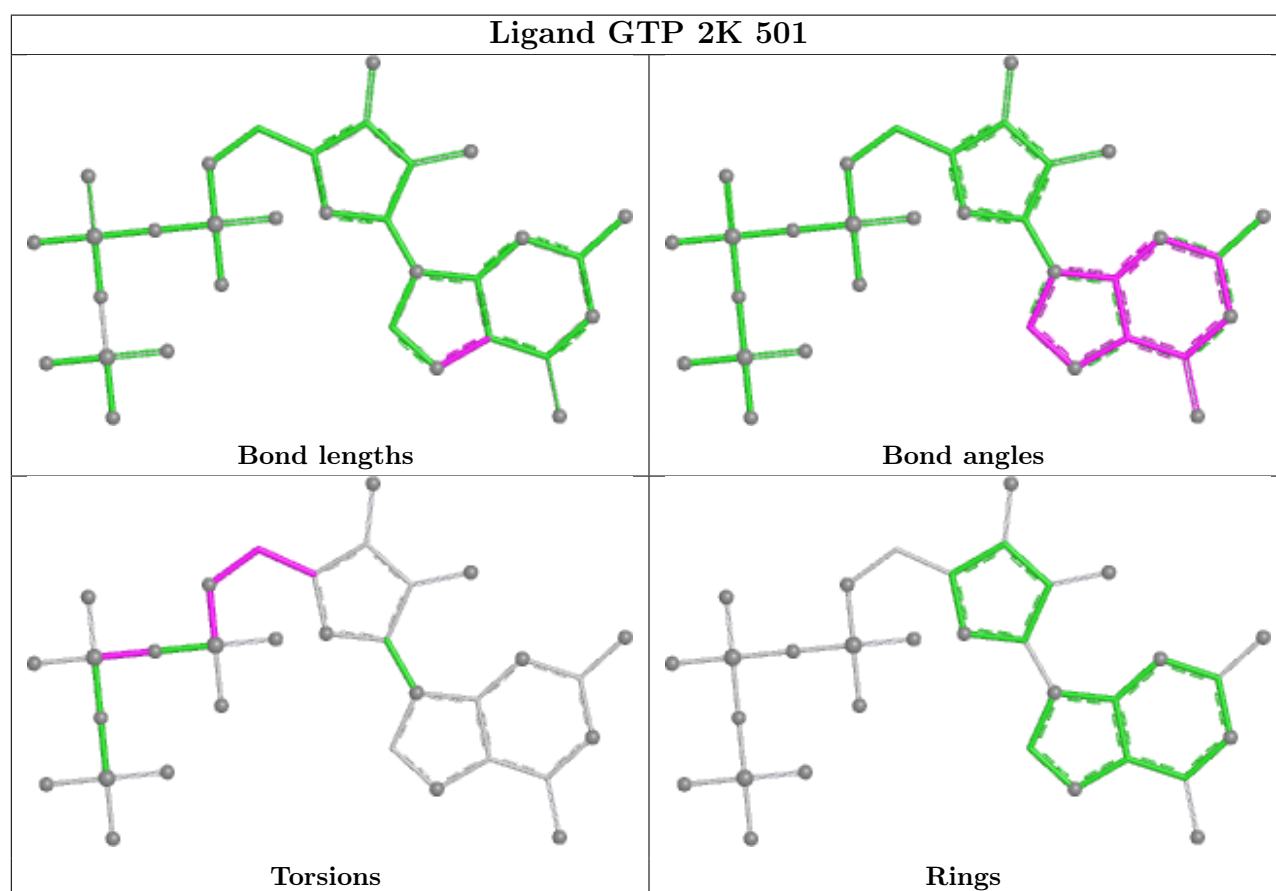
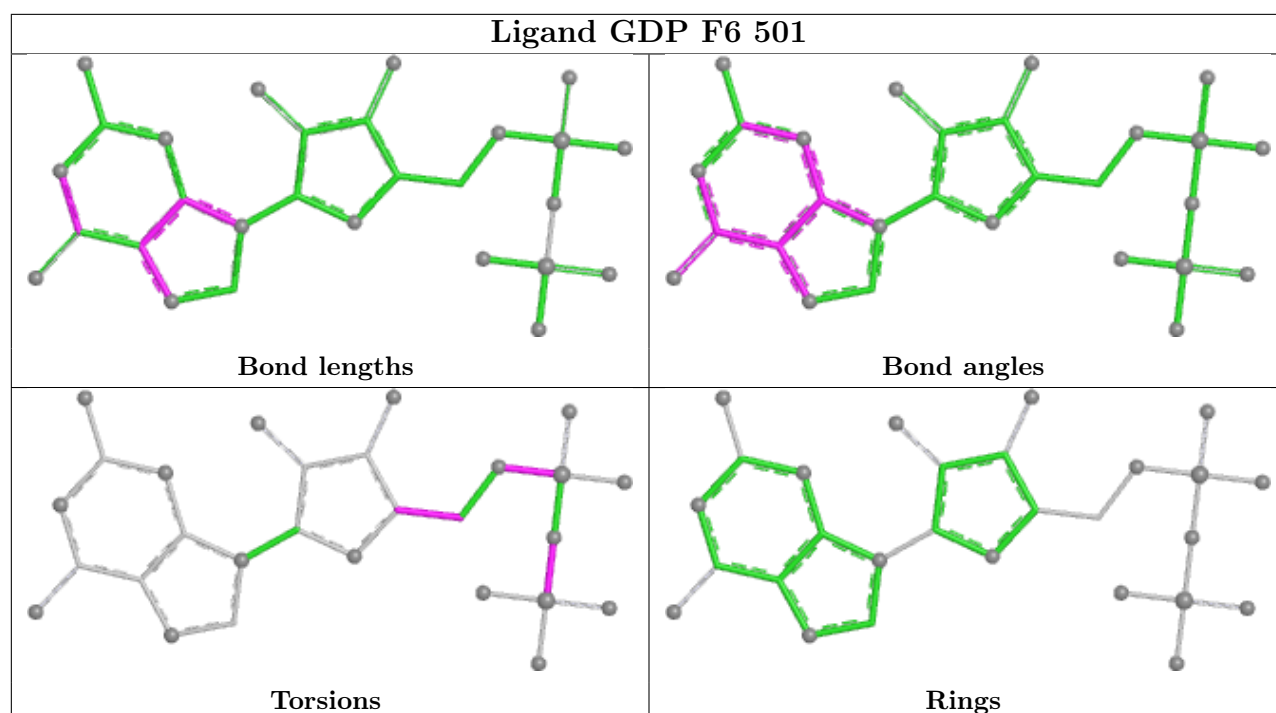
Ligand GTP X4 501

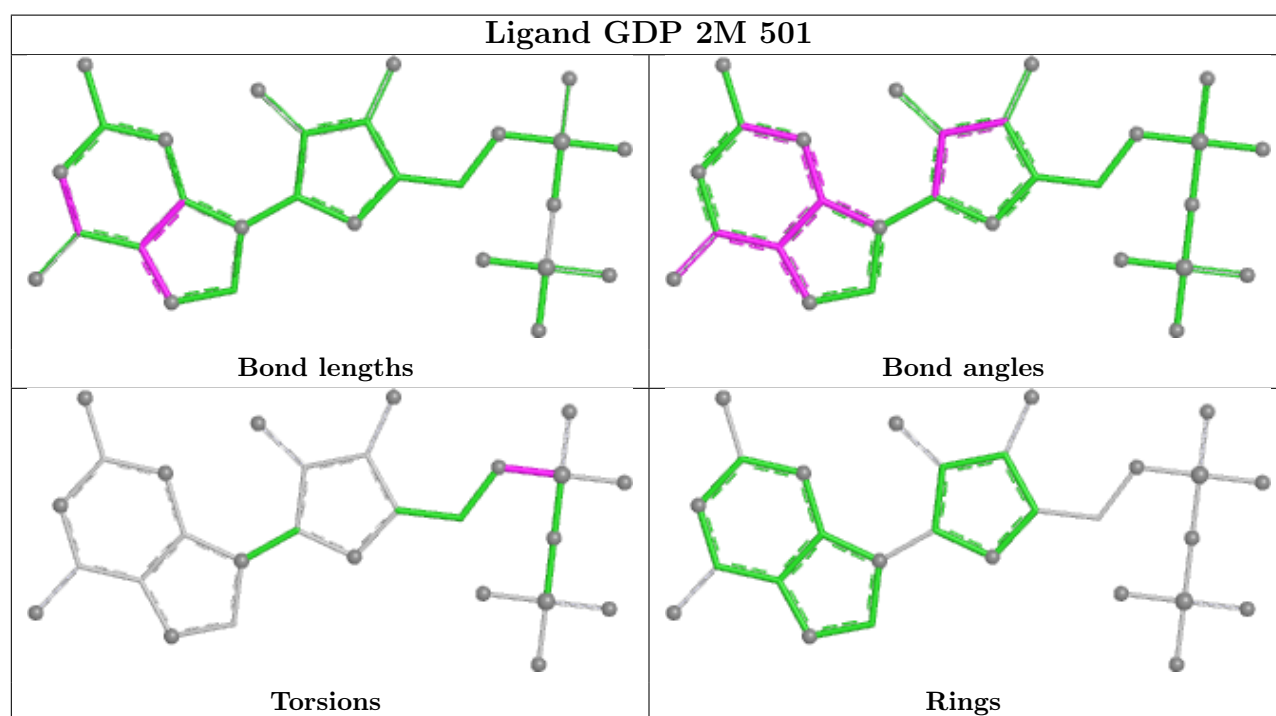
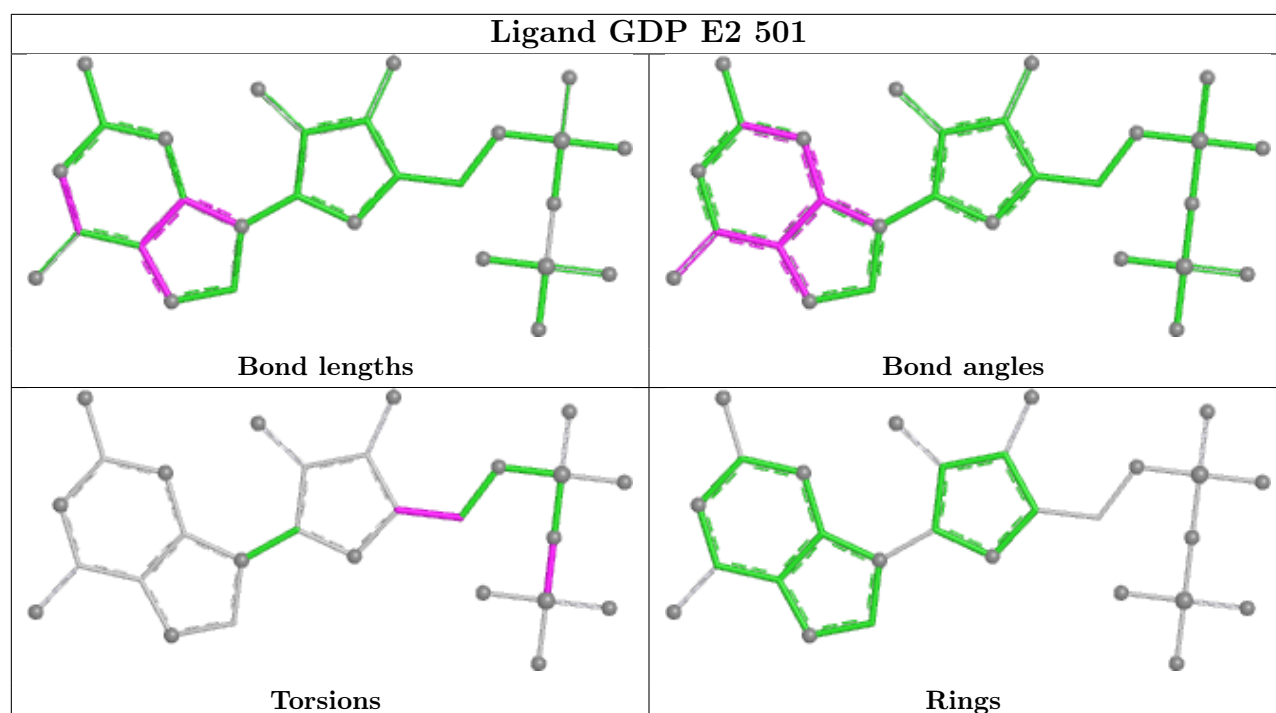


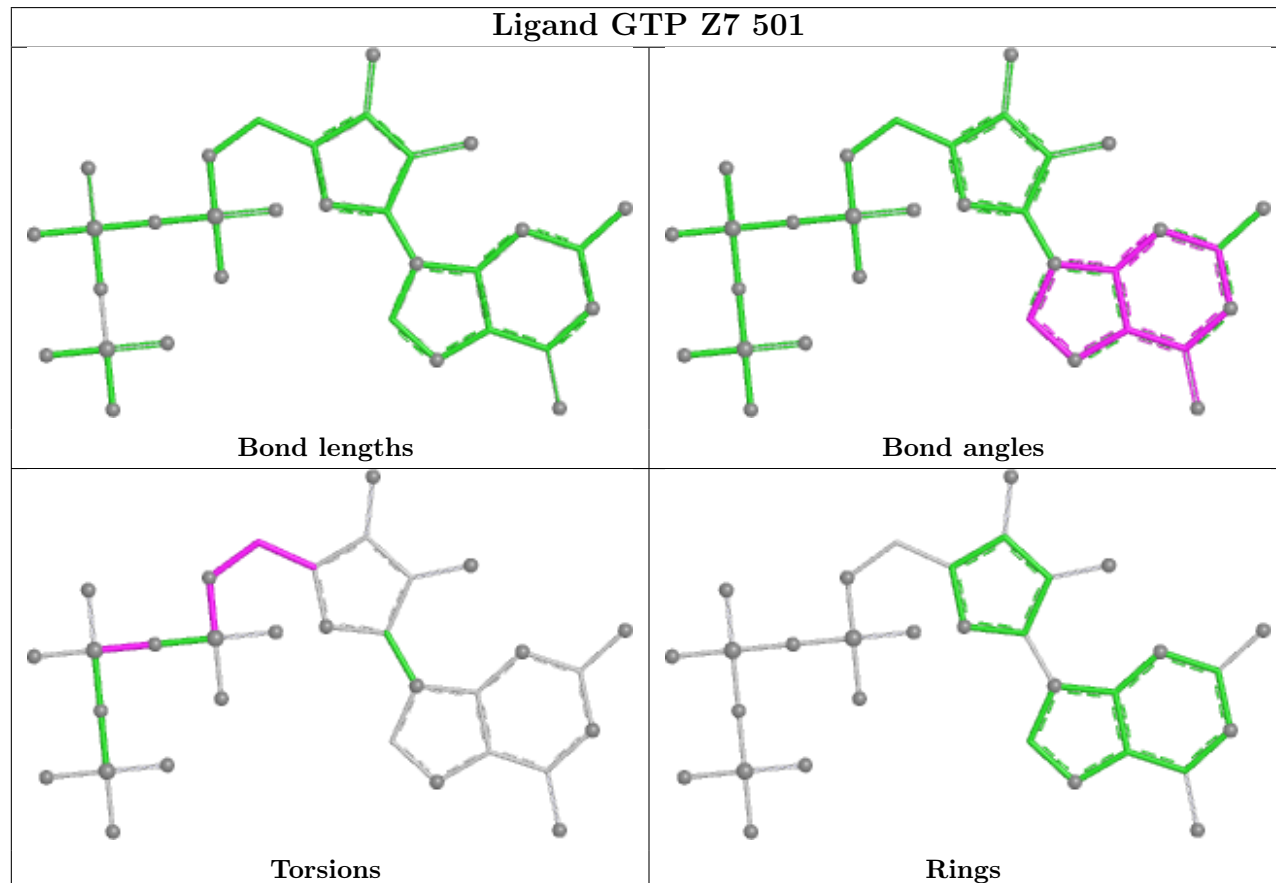
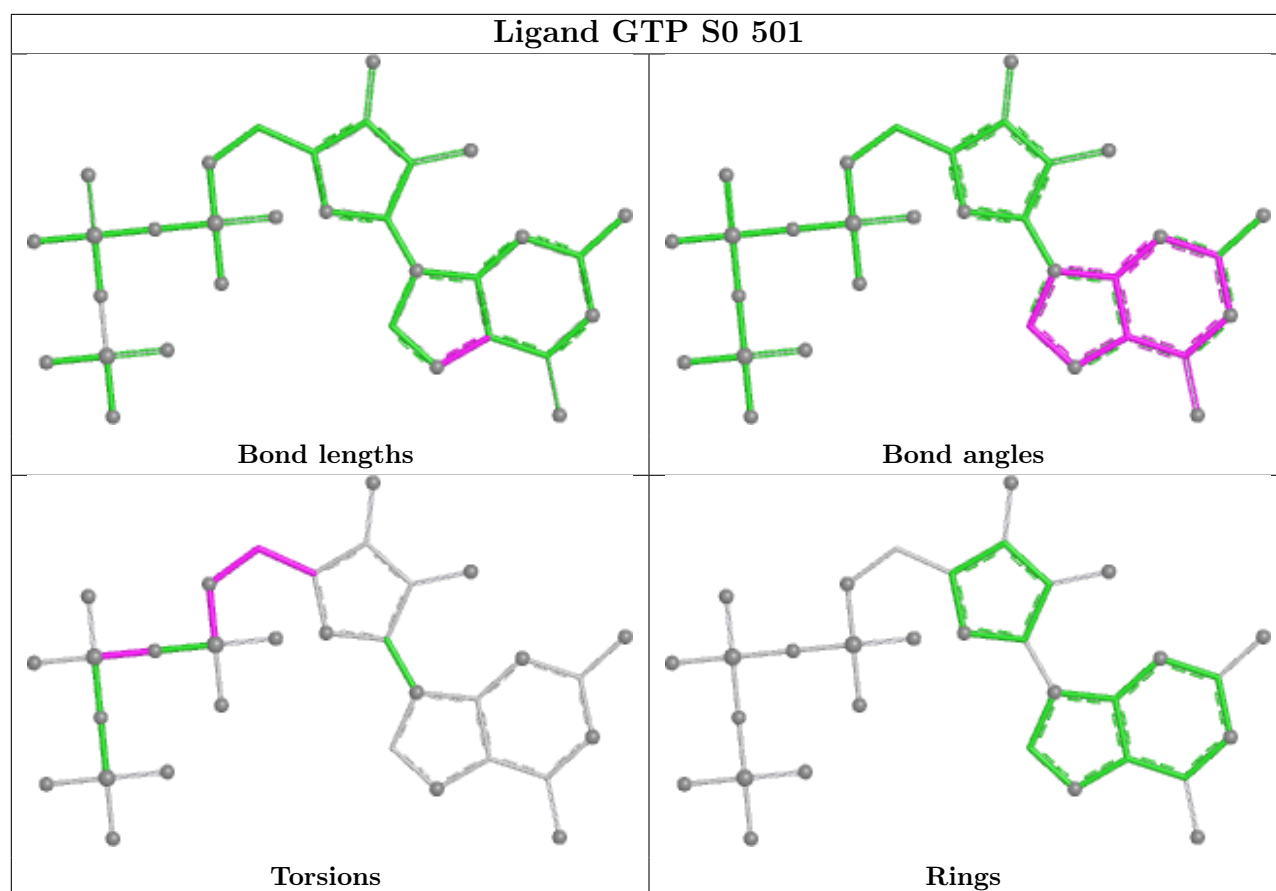
Ligand GTP 1L 501

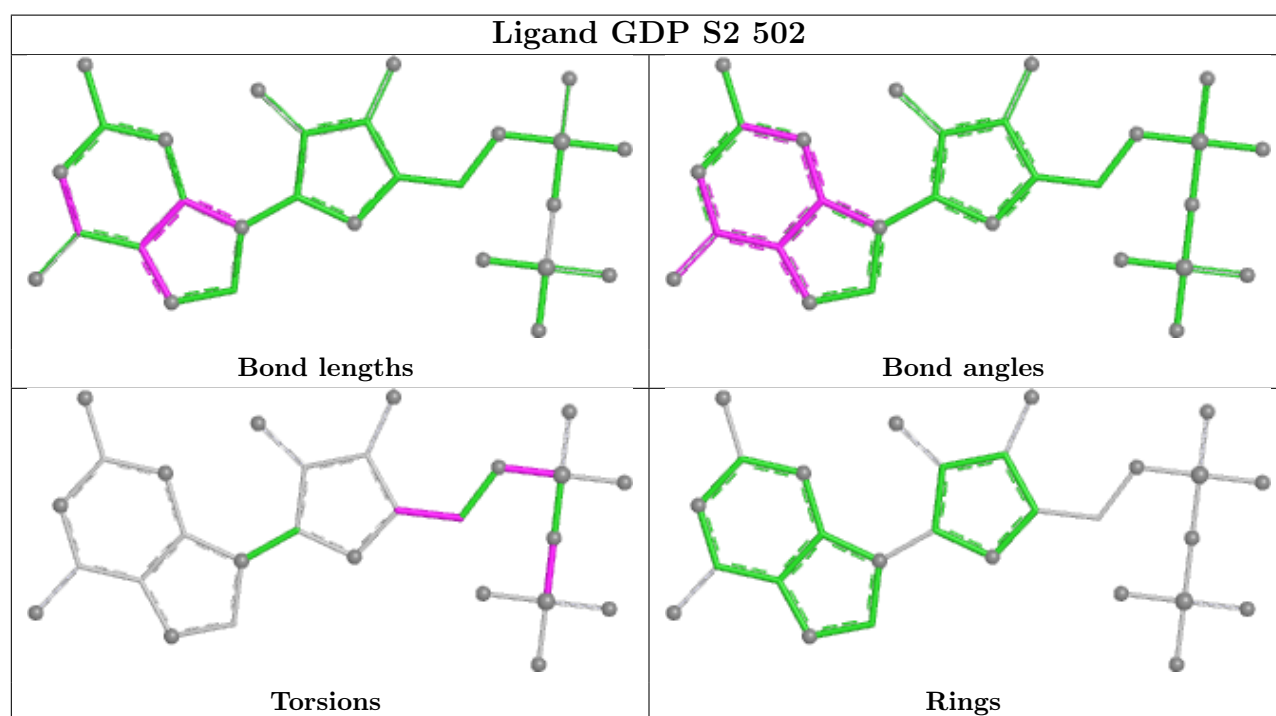
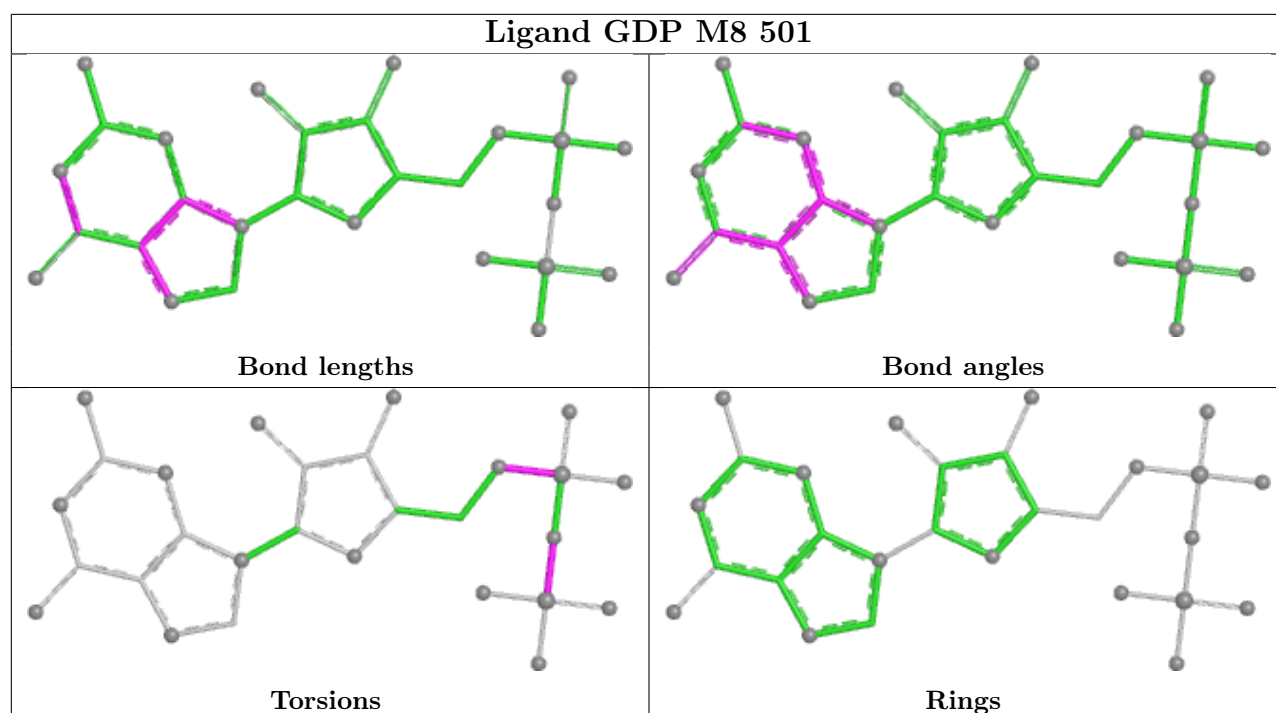




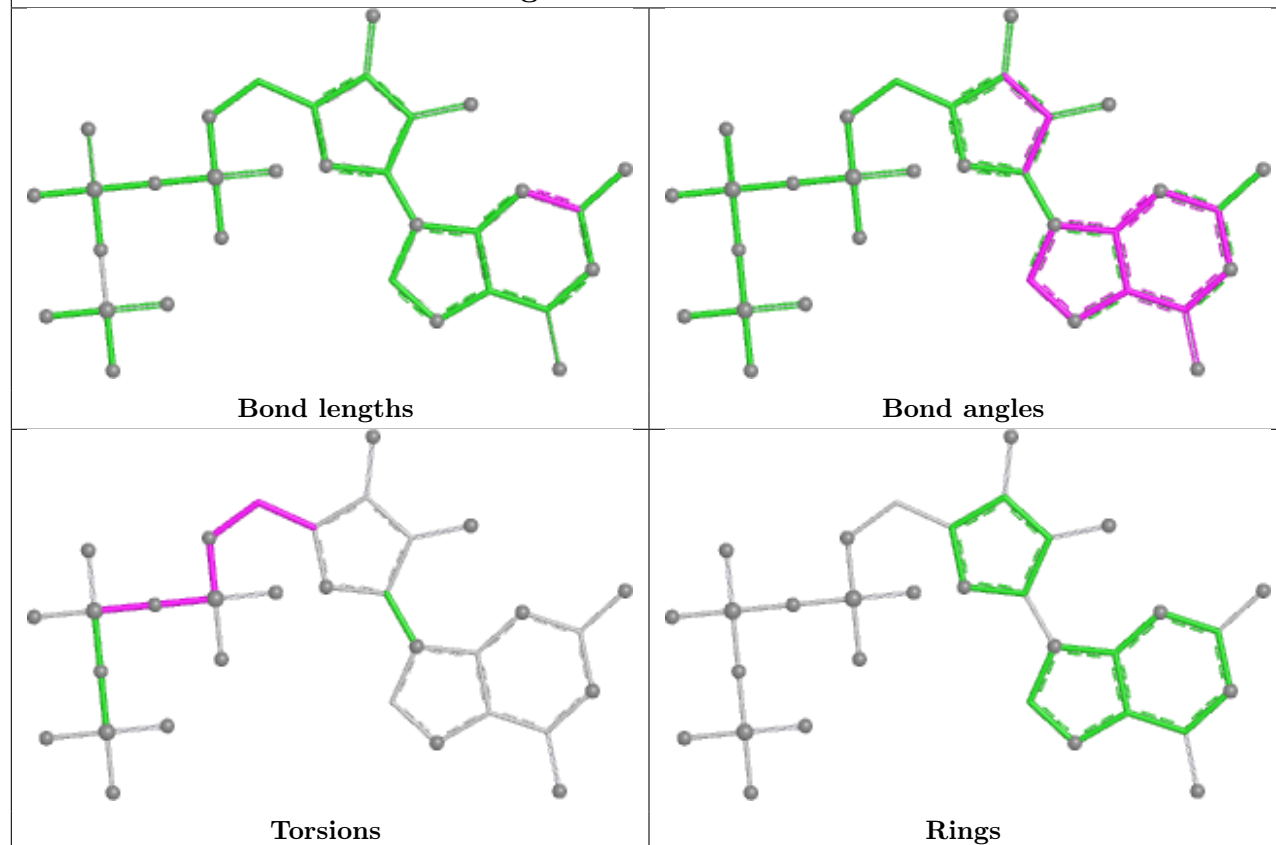




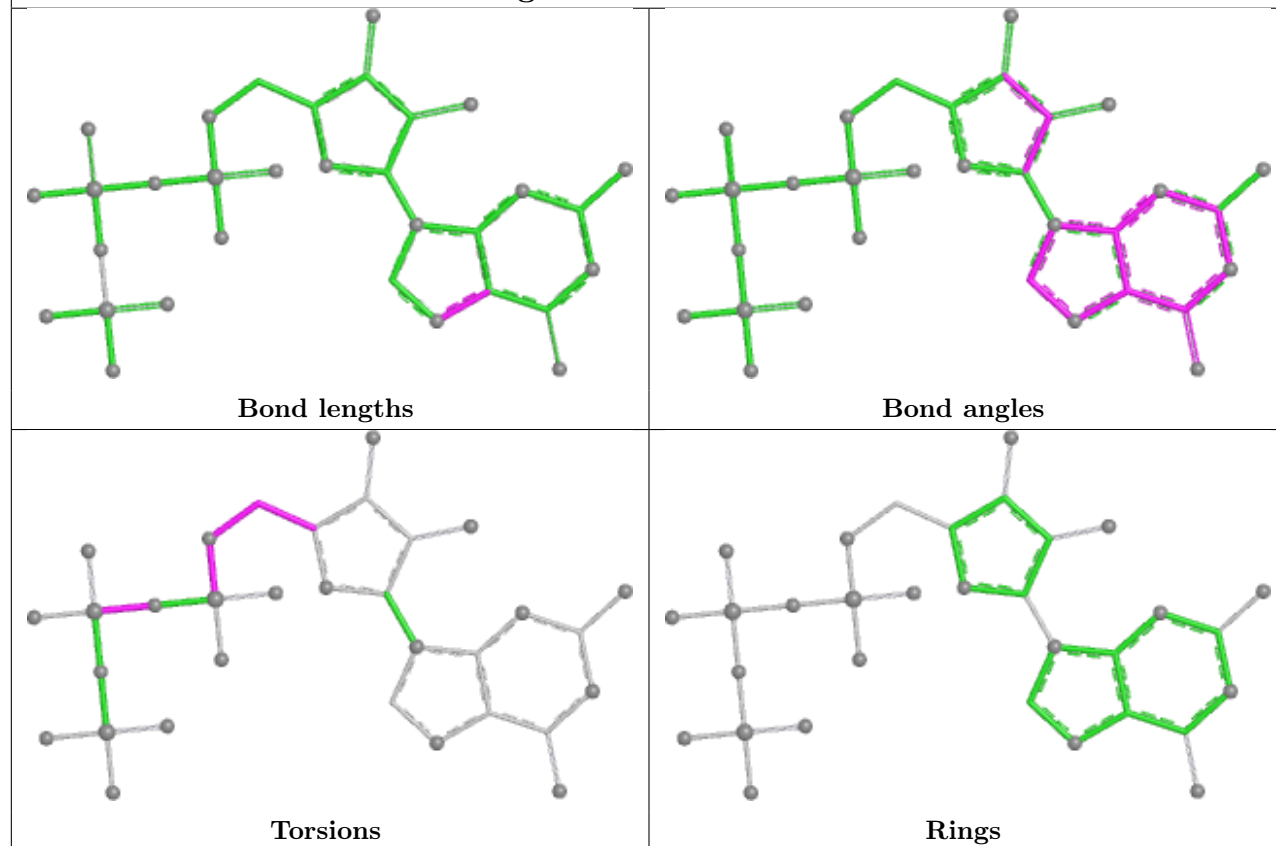


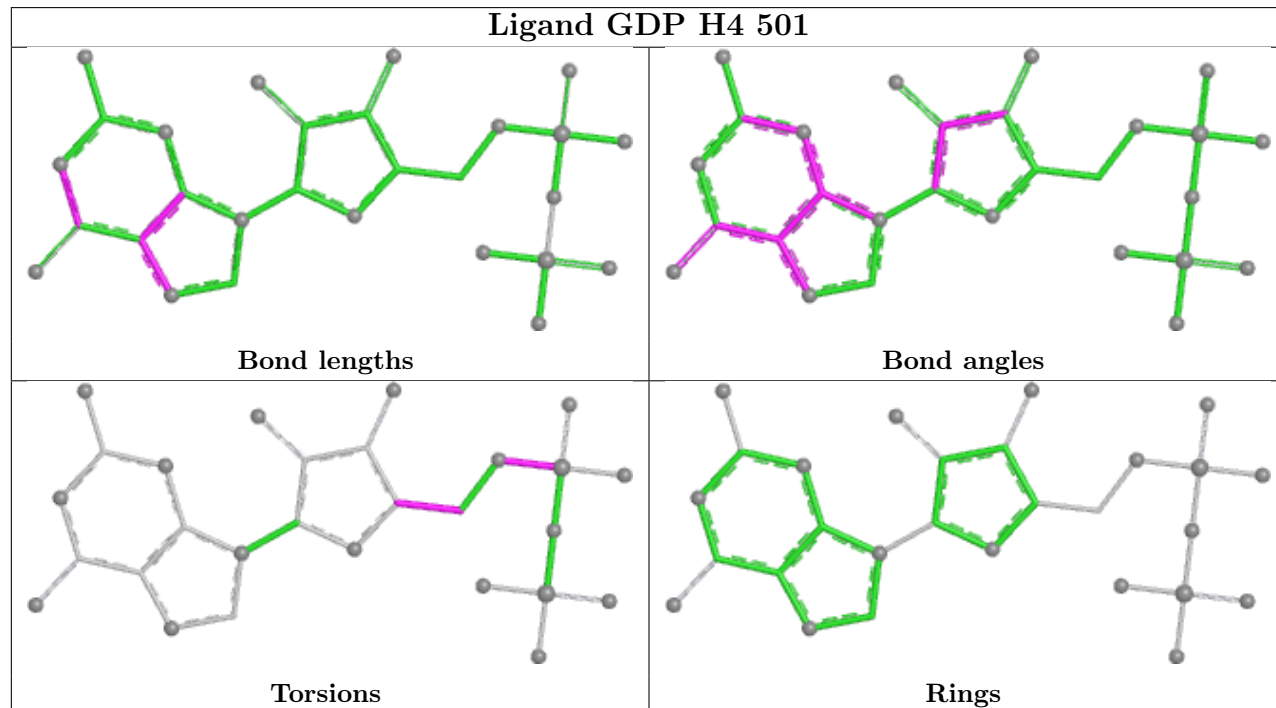
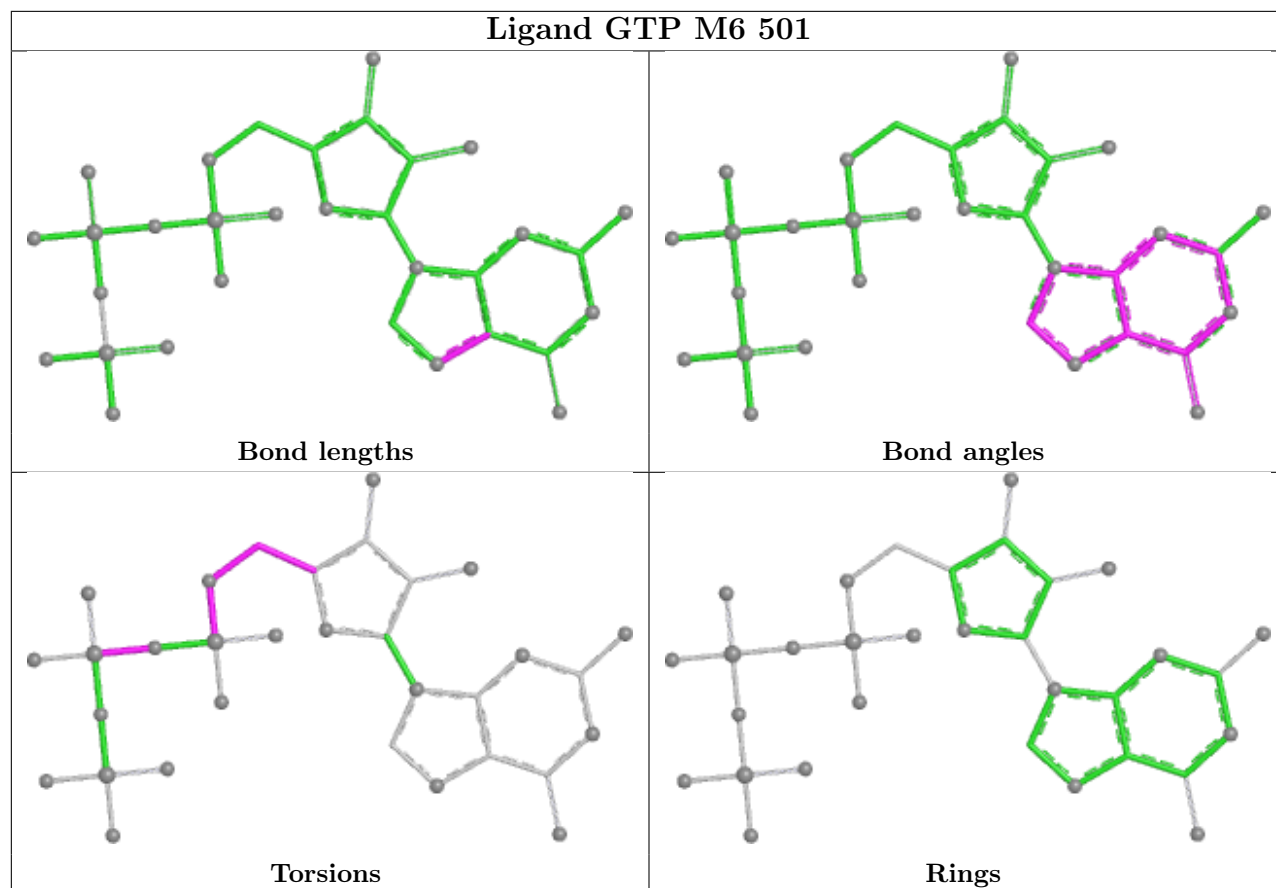


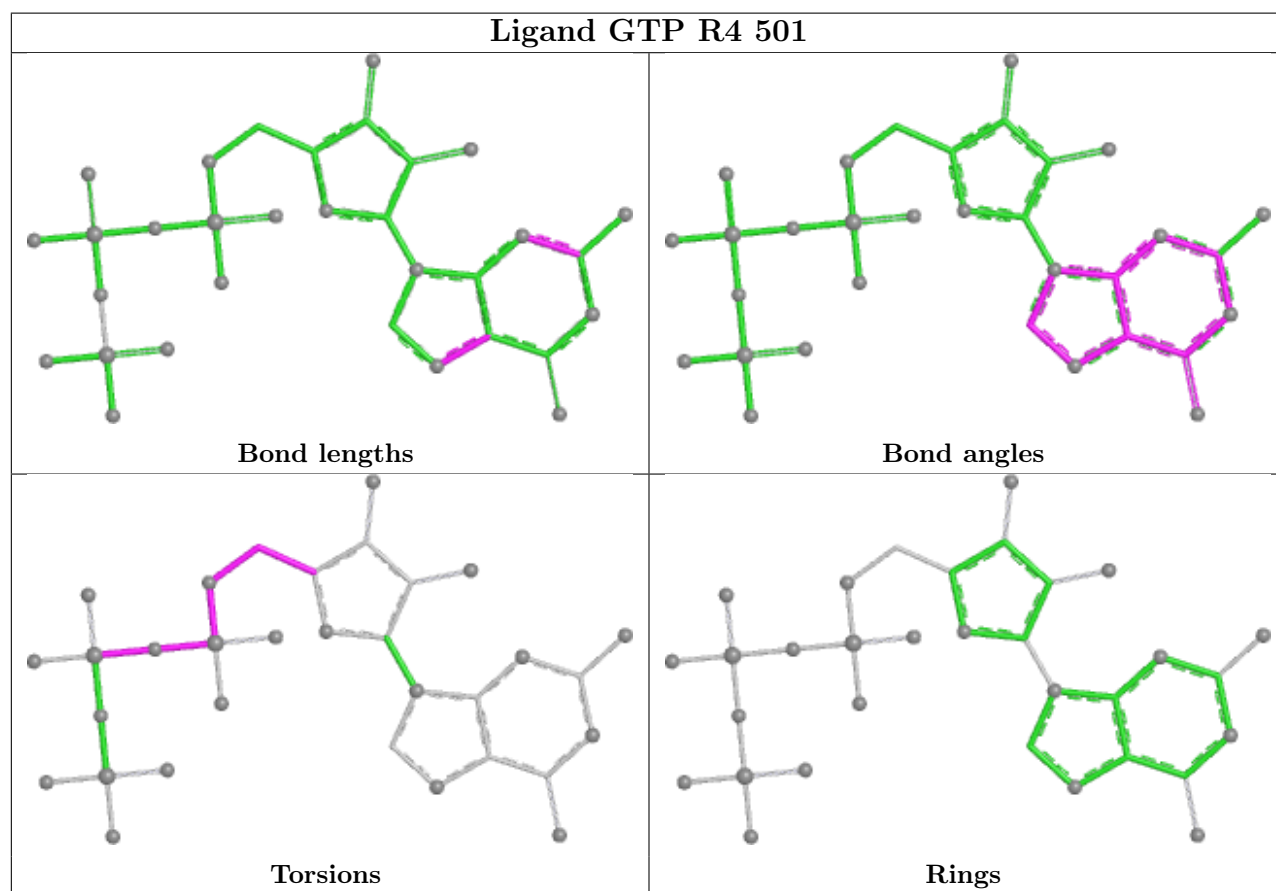
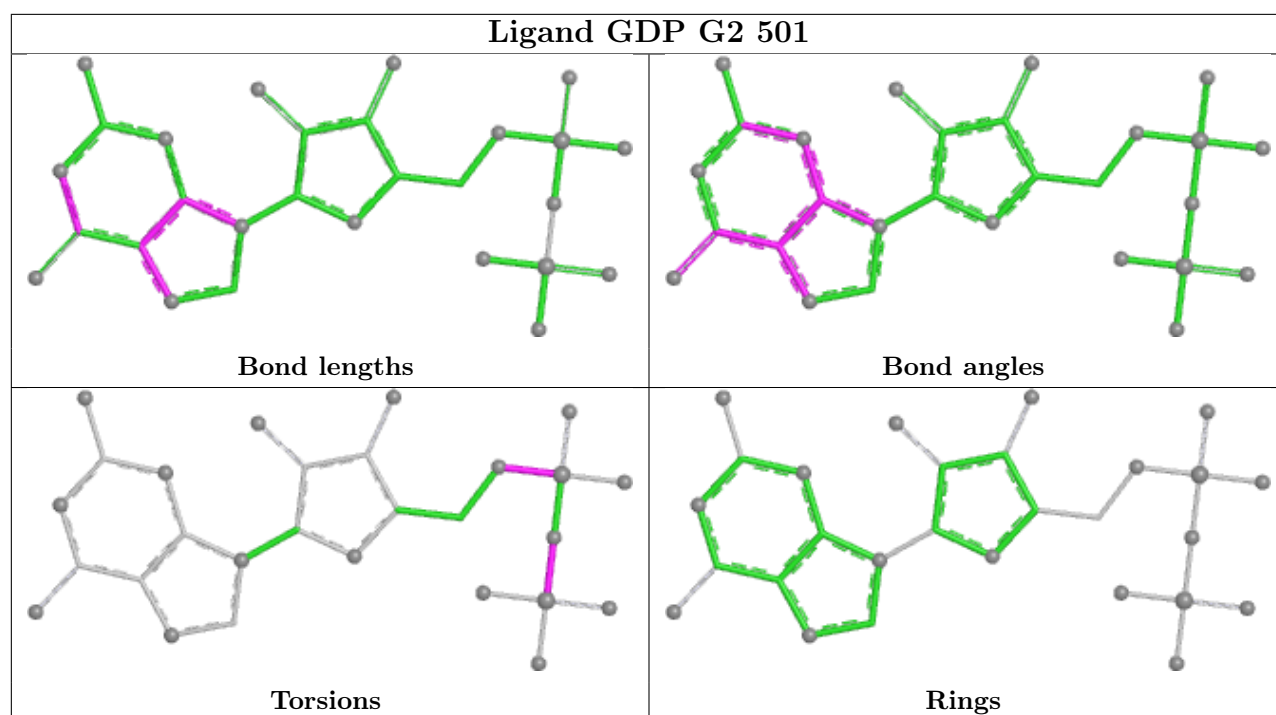
Ligand GTP 1H 501

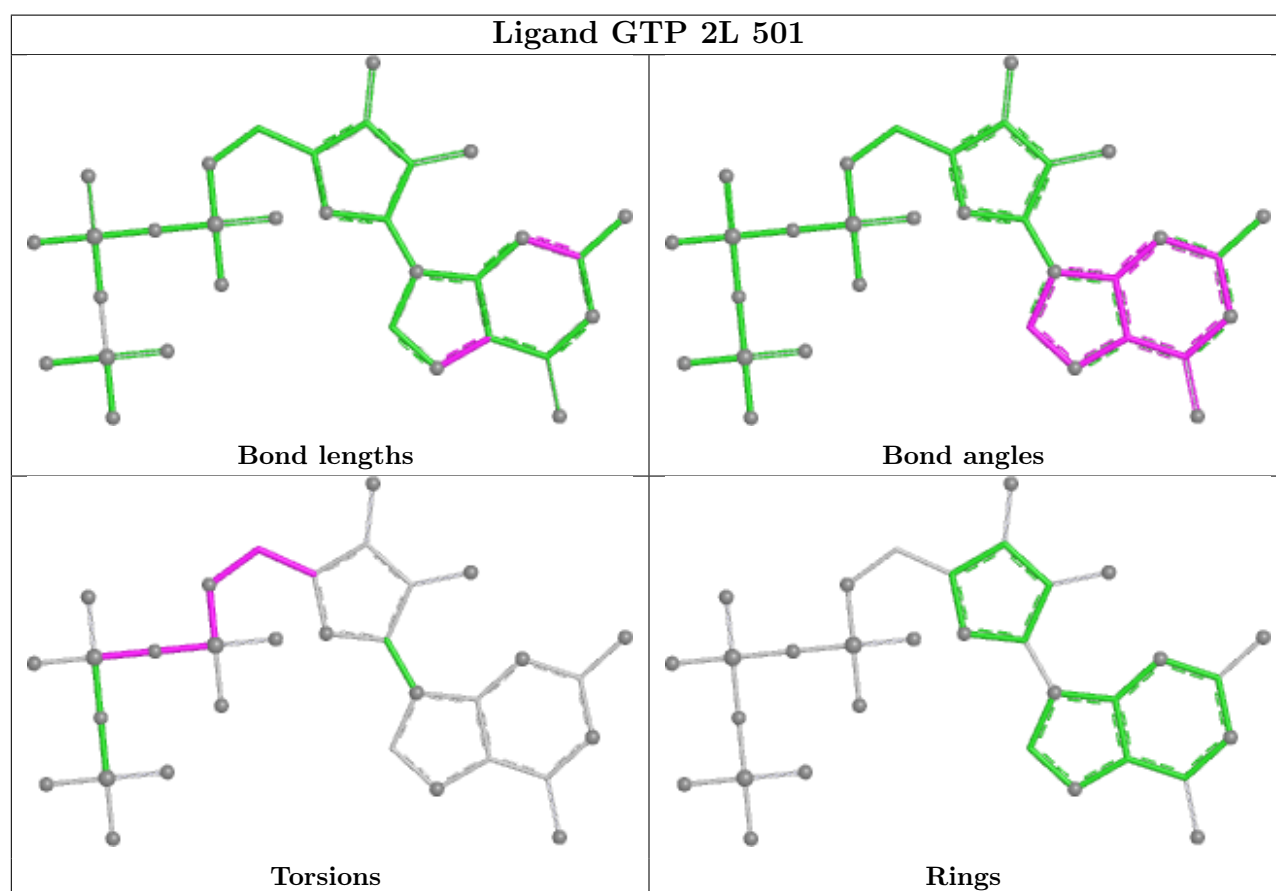
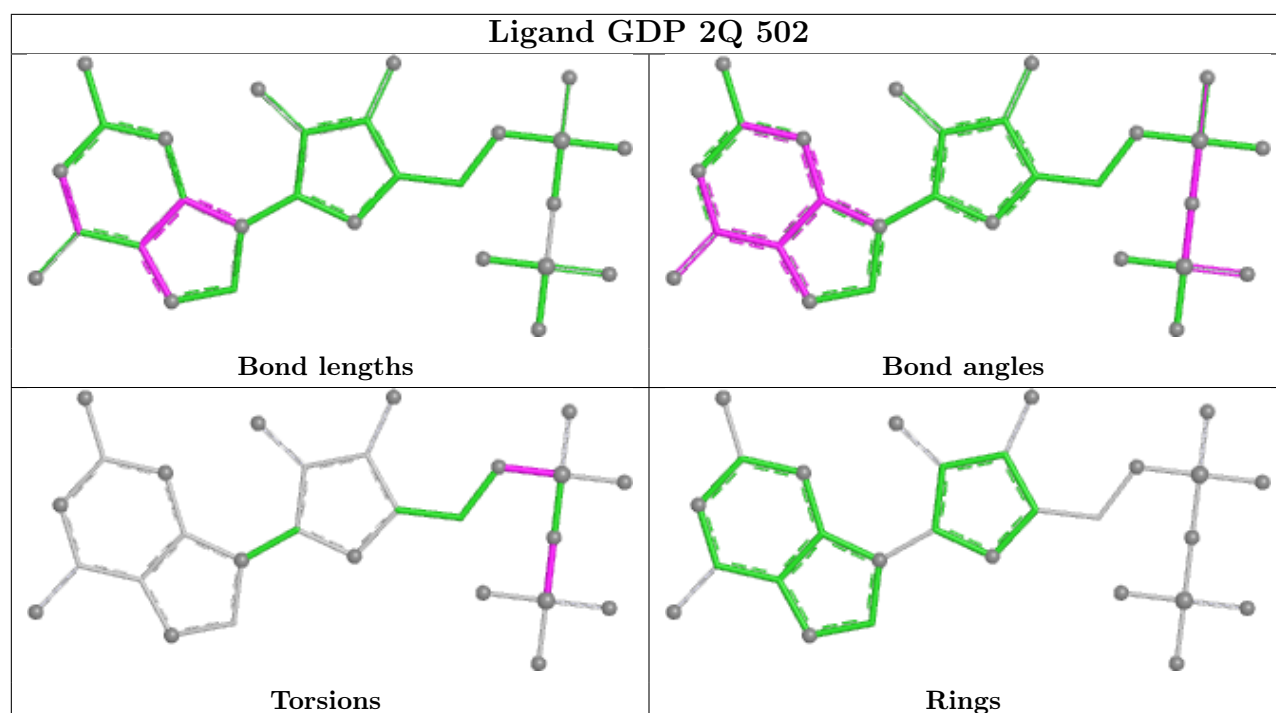


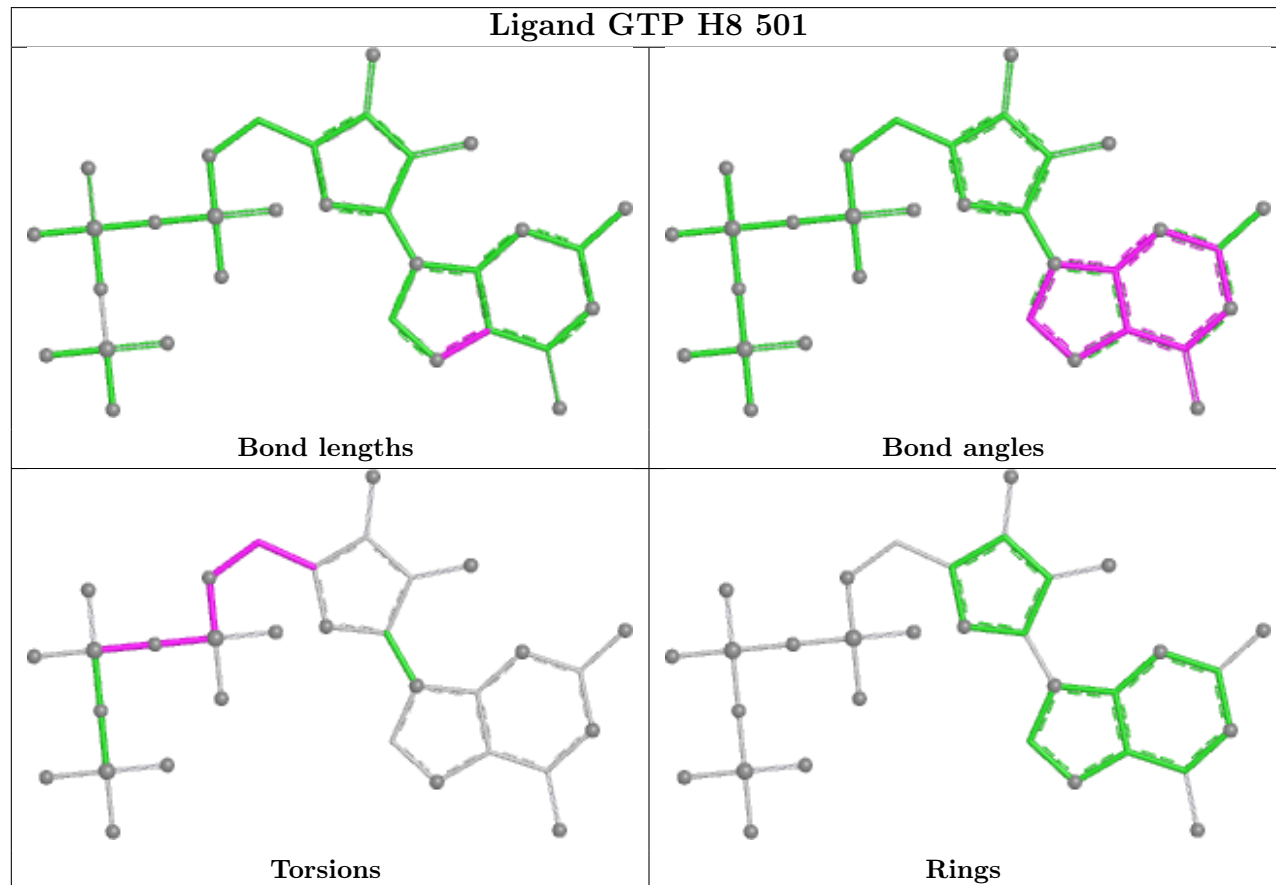
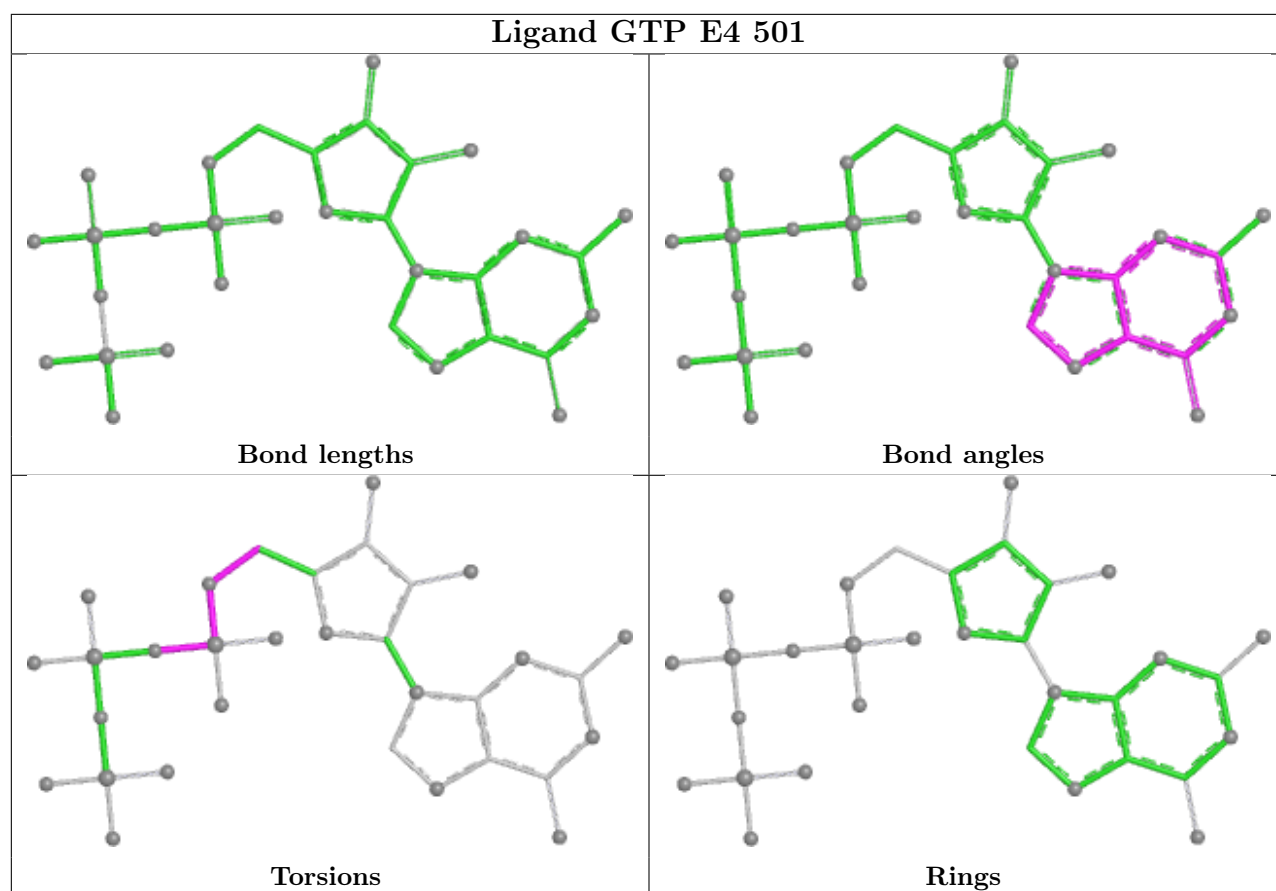
Ligand GTP M4 501

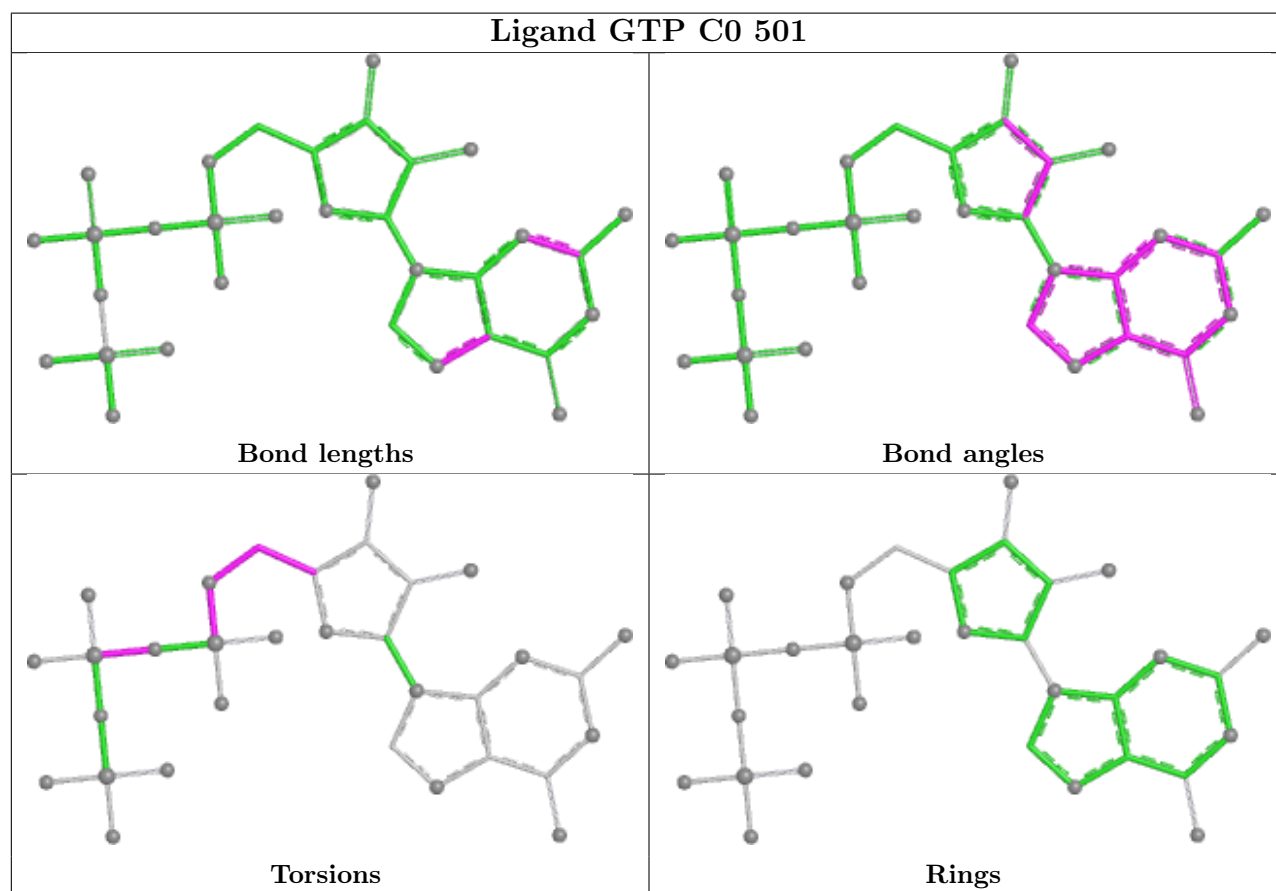
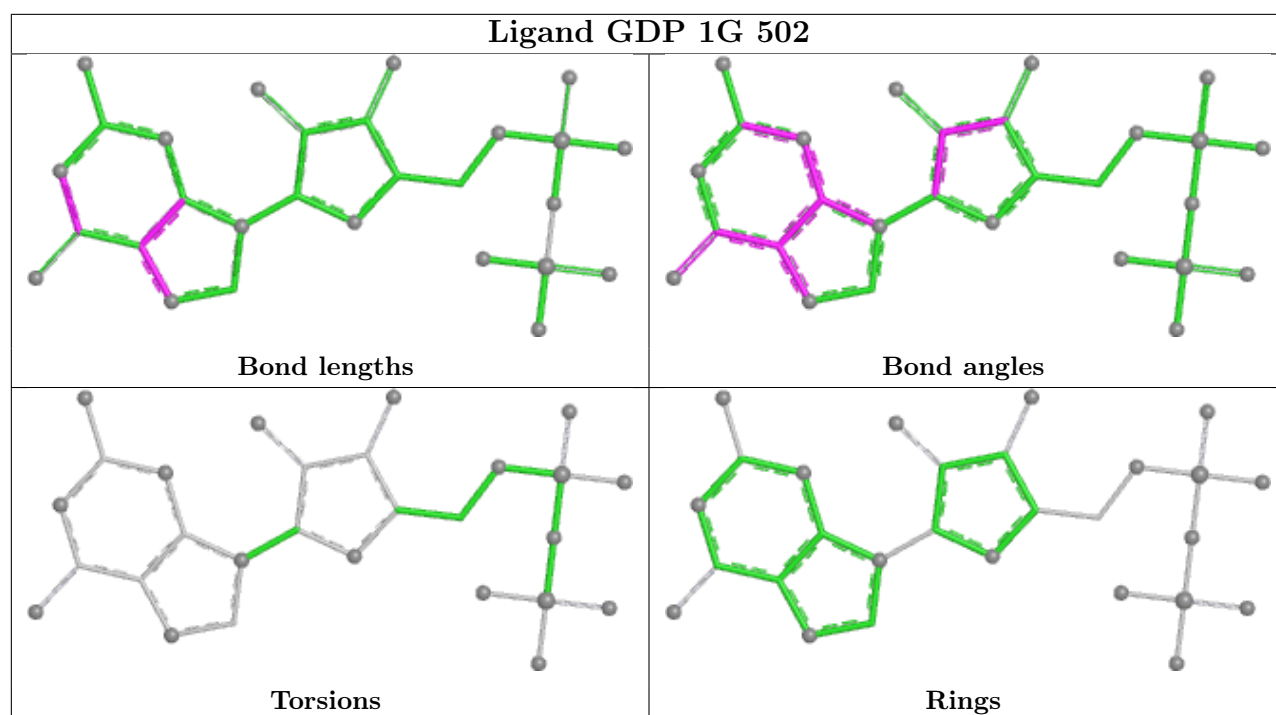


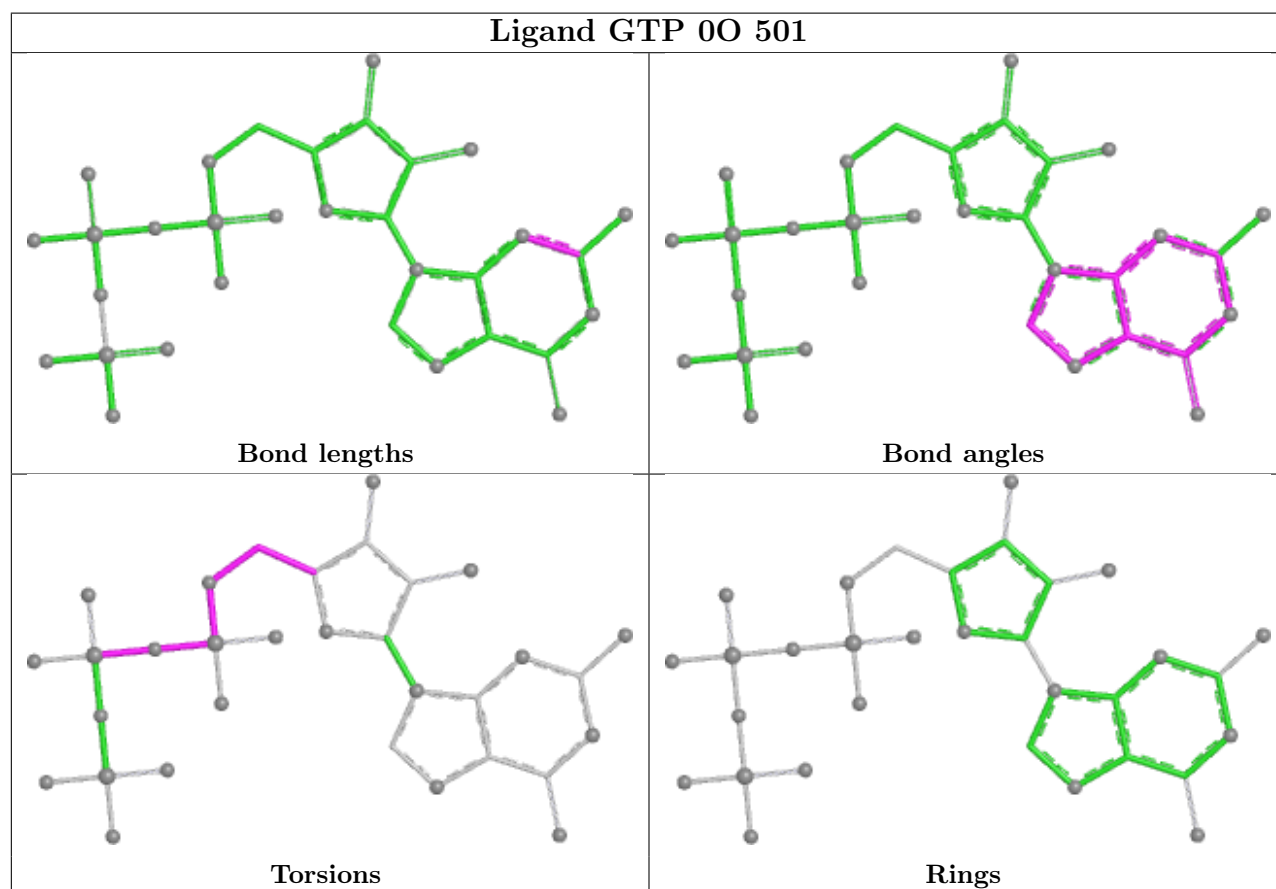
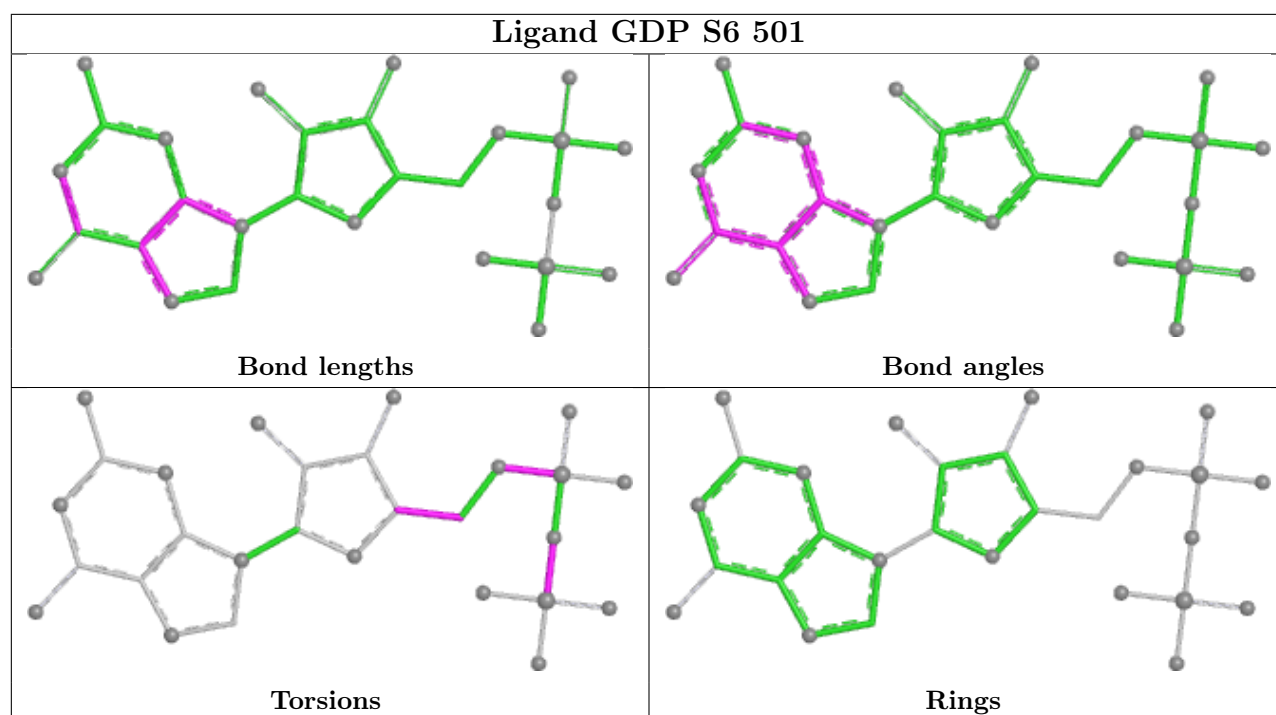


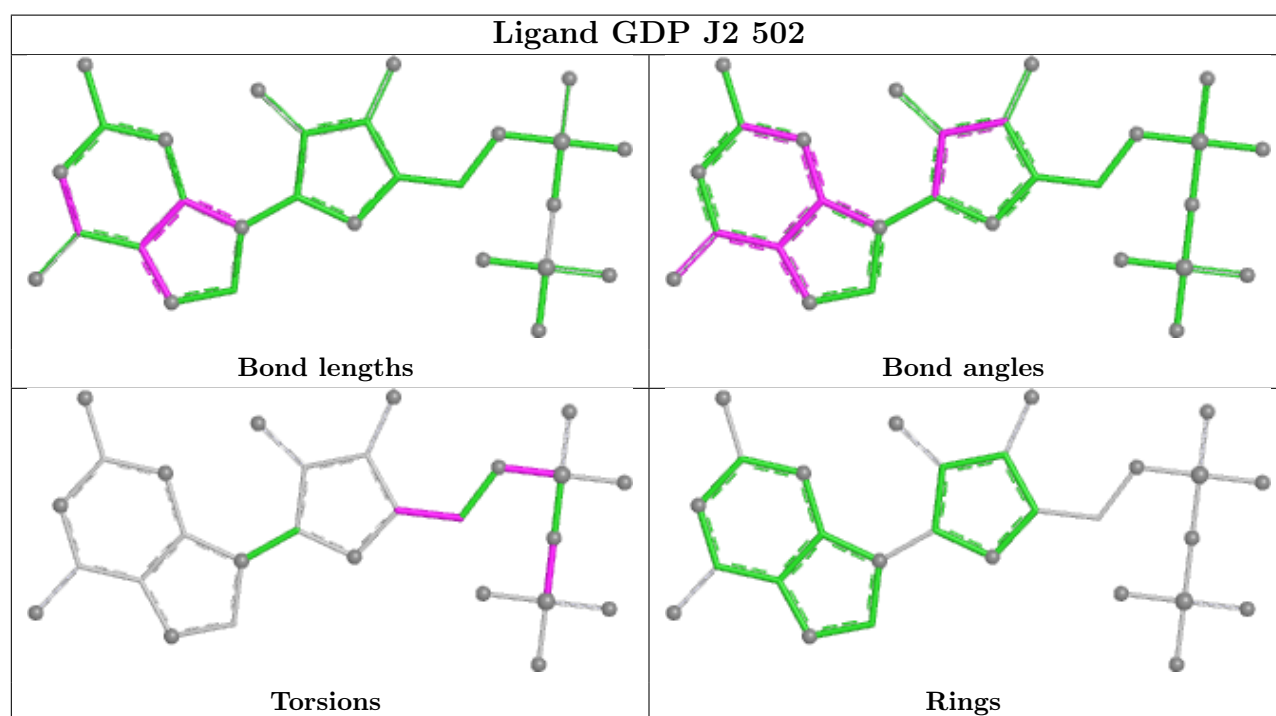
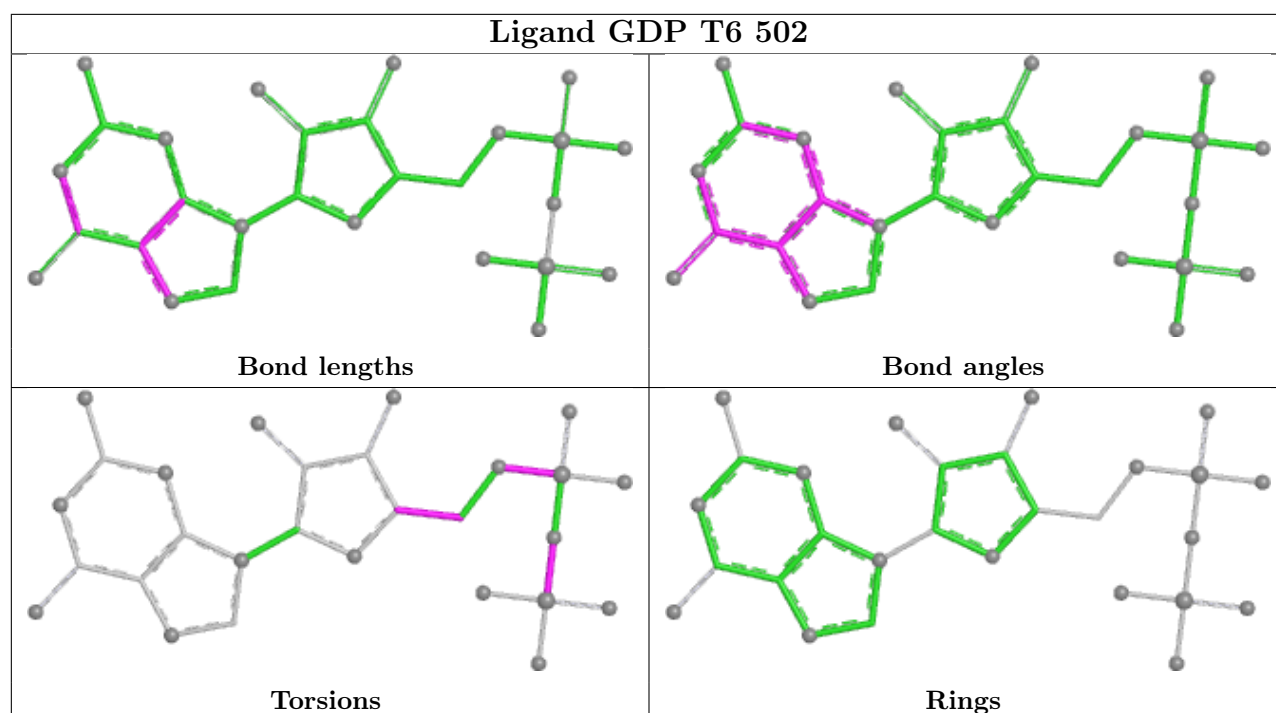


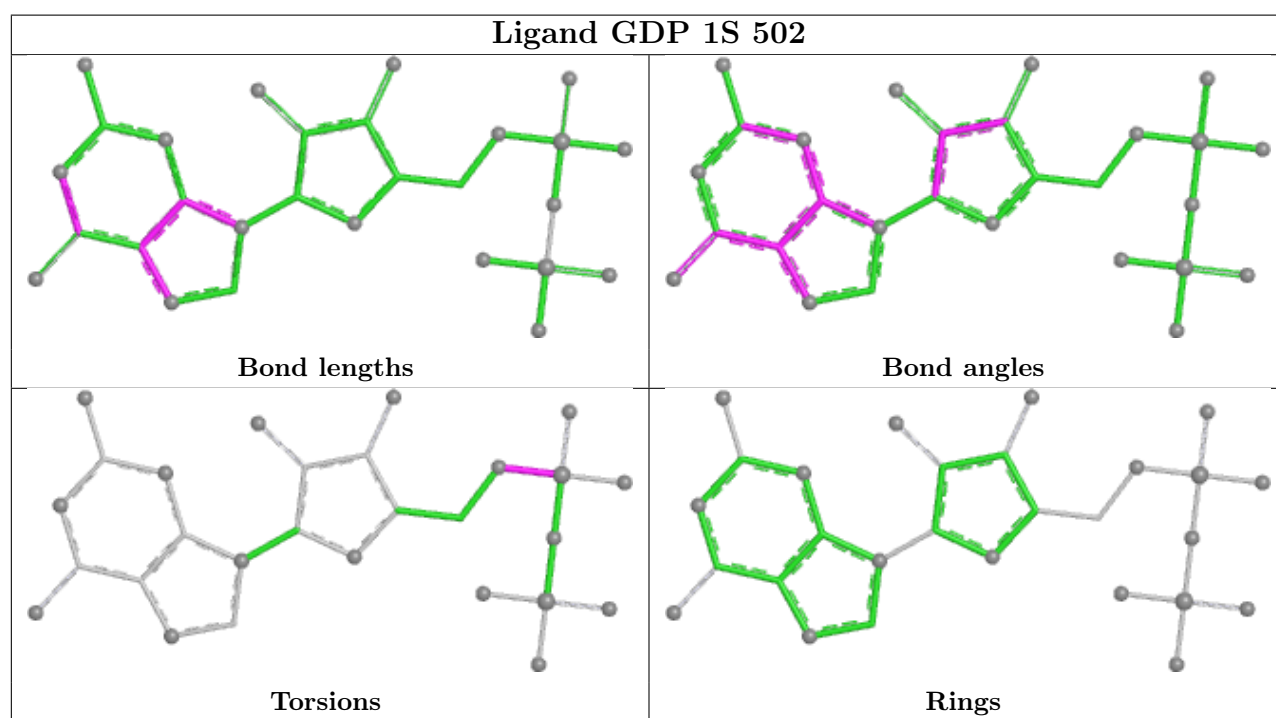
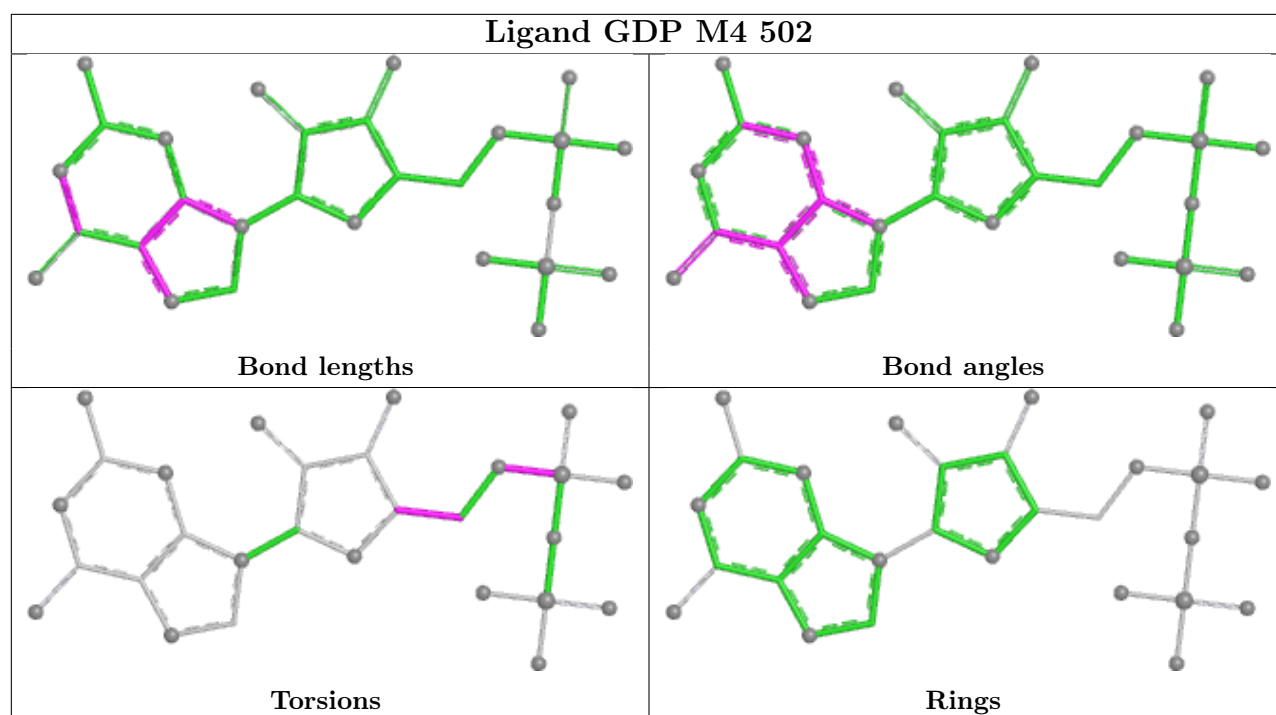


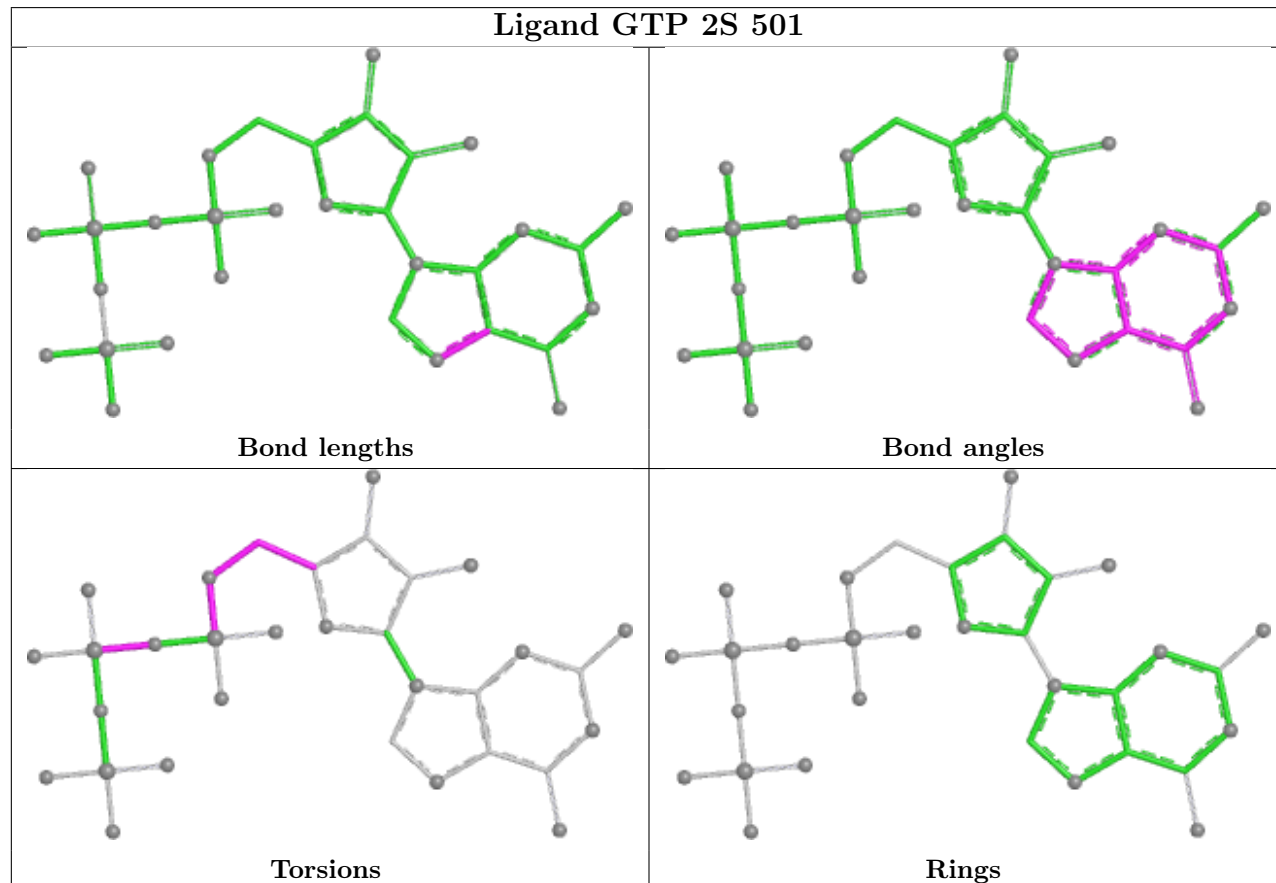
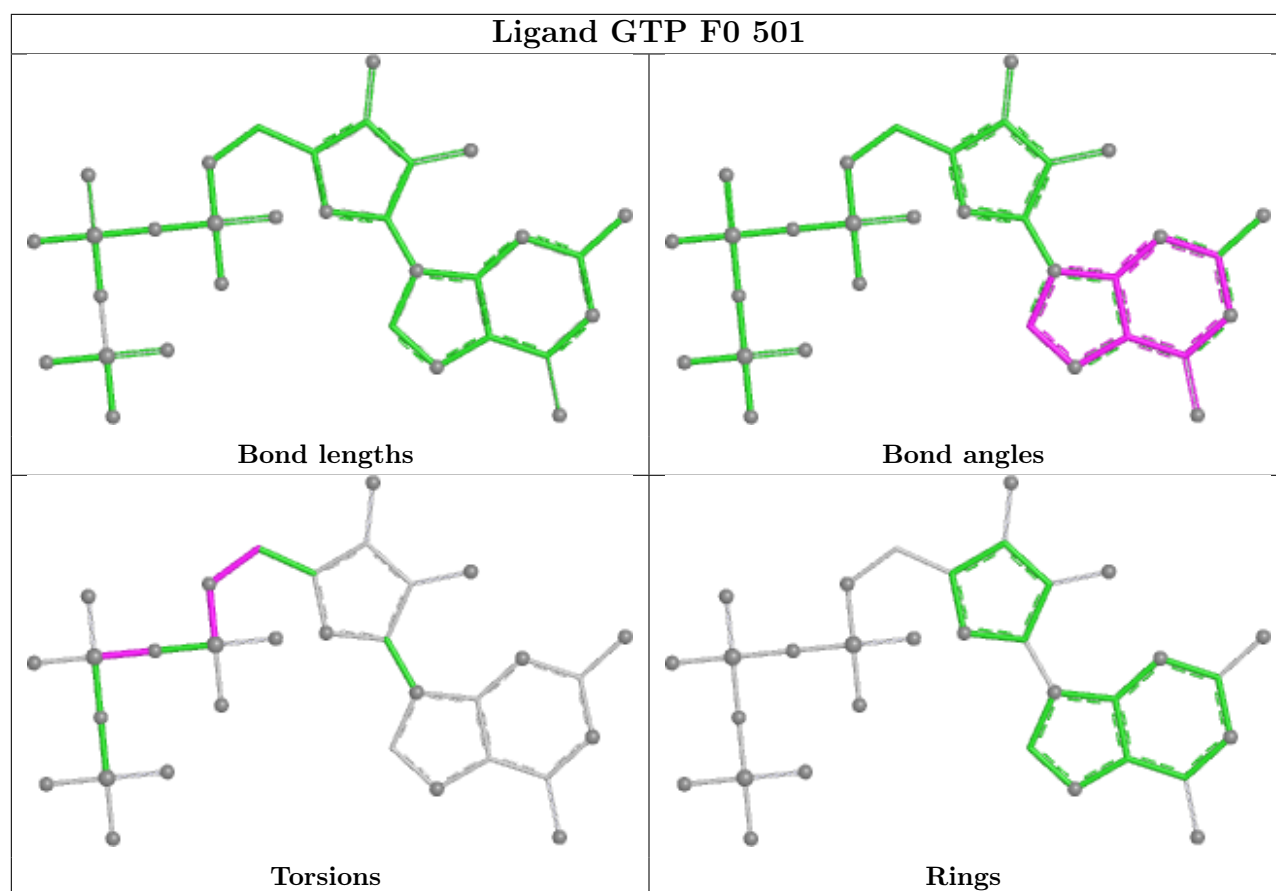


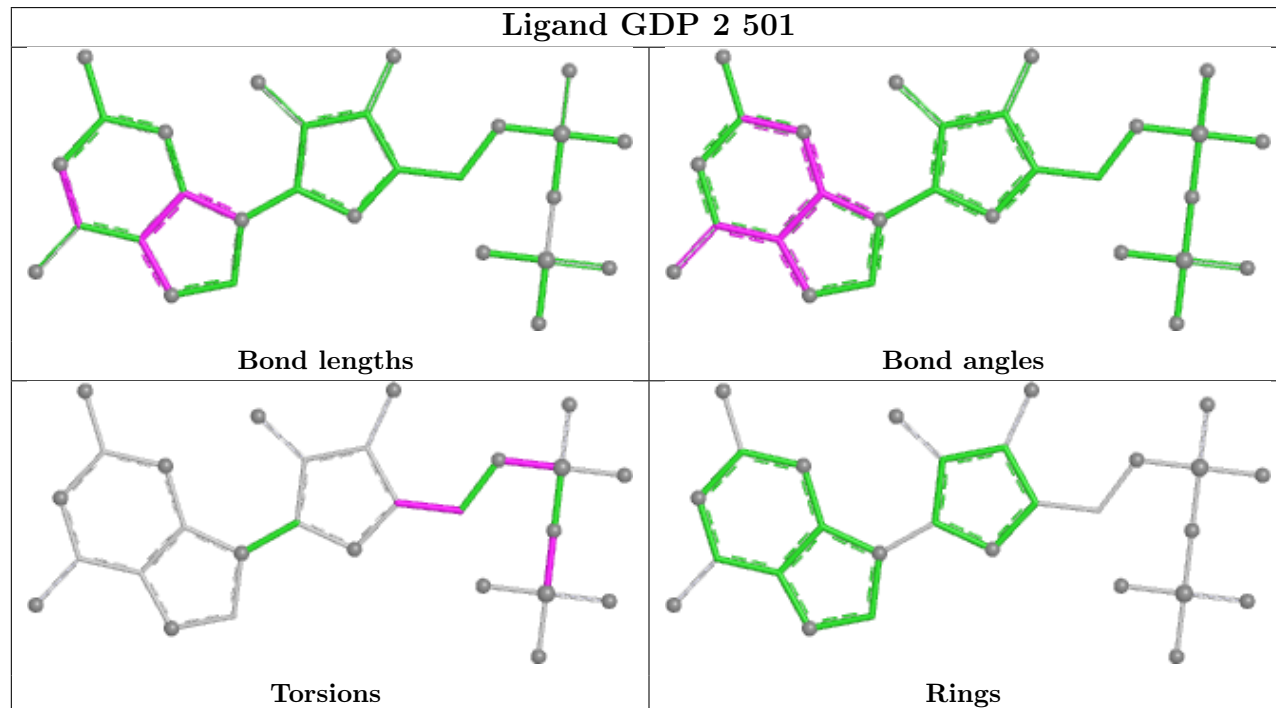
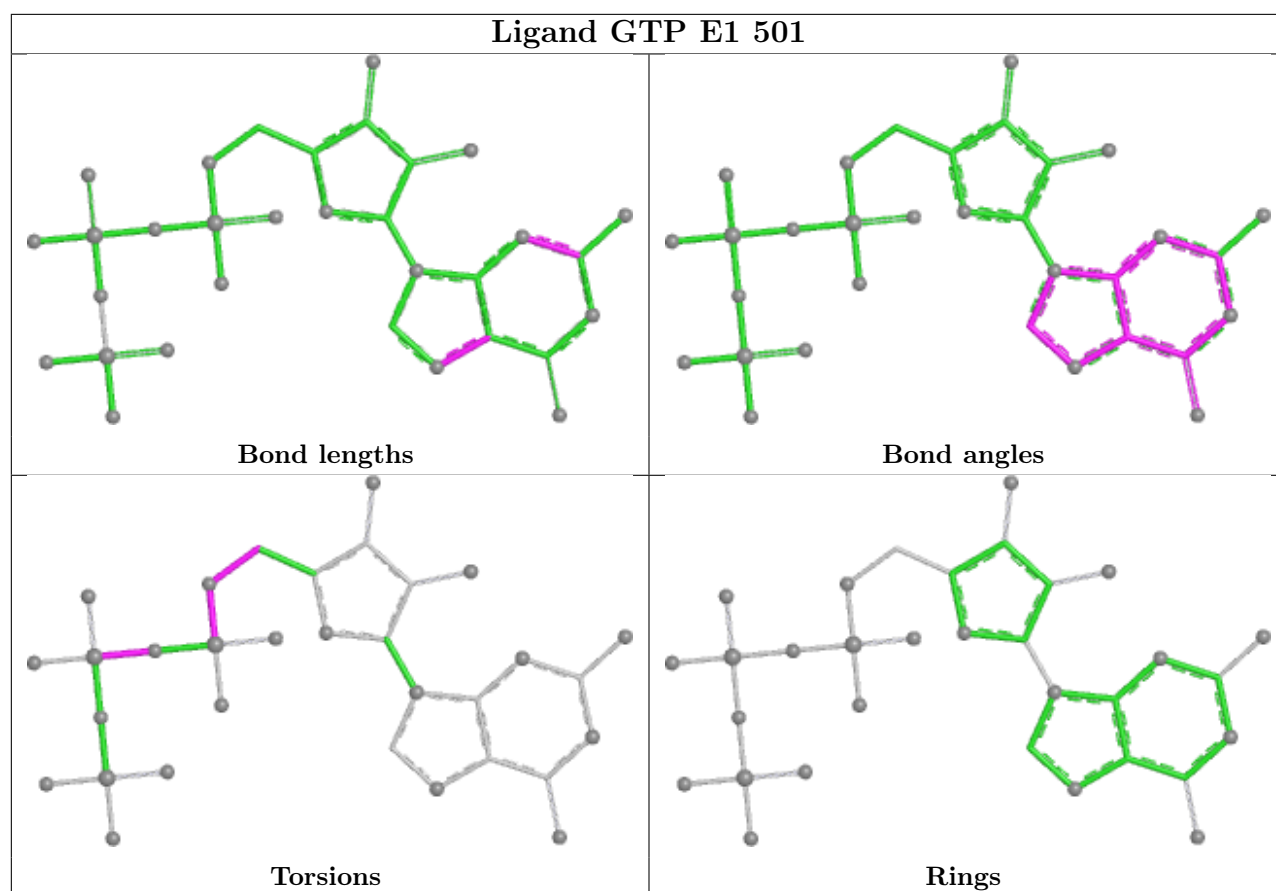


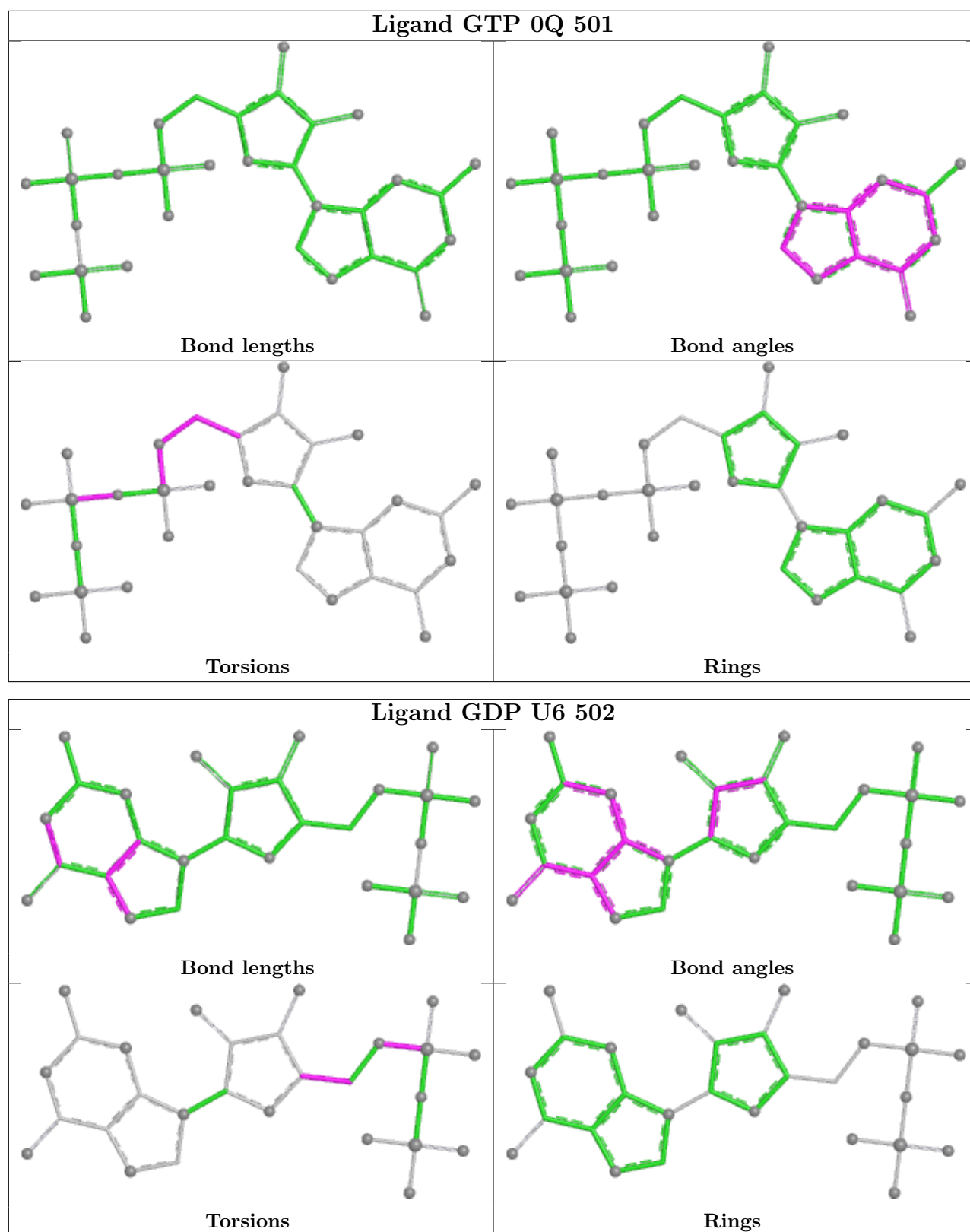


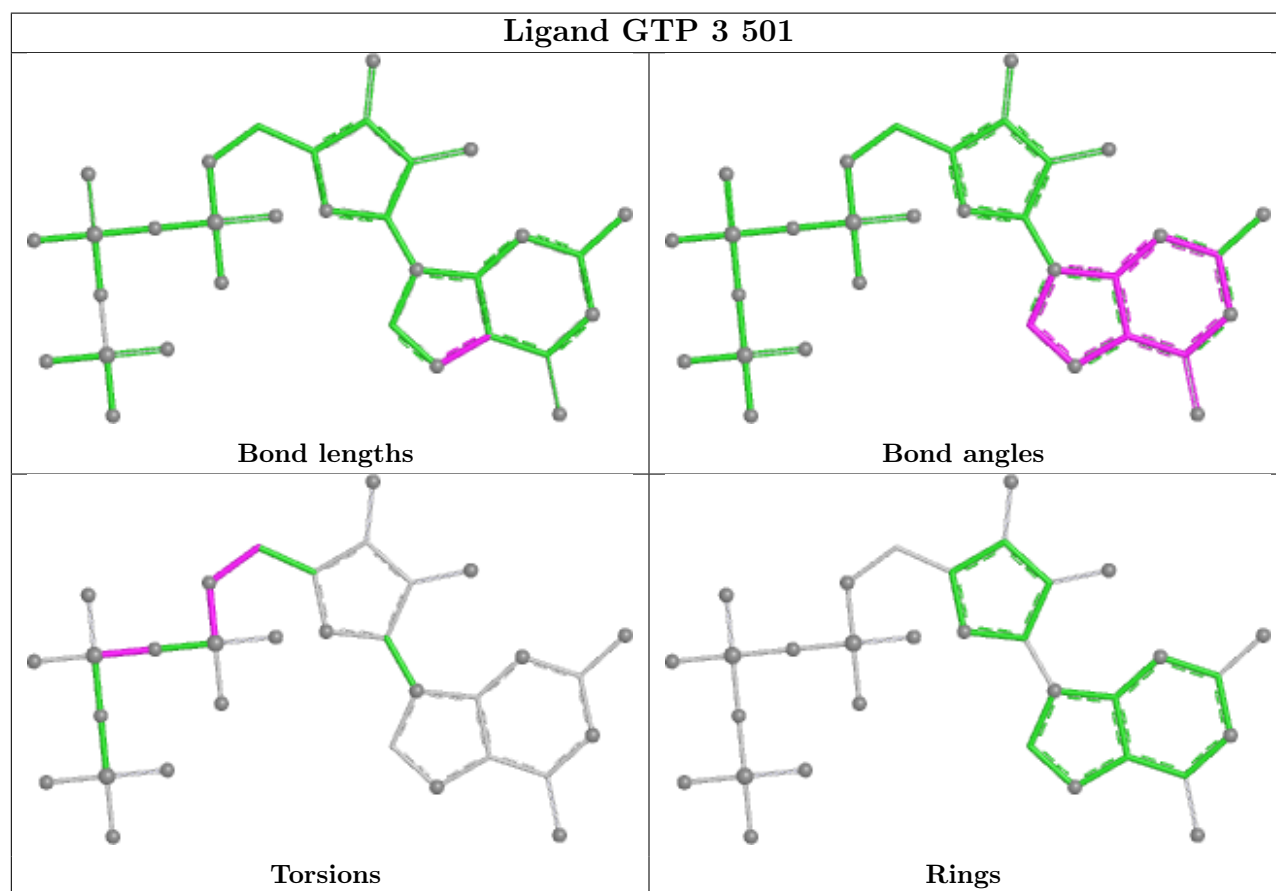
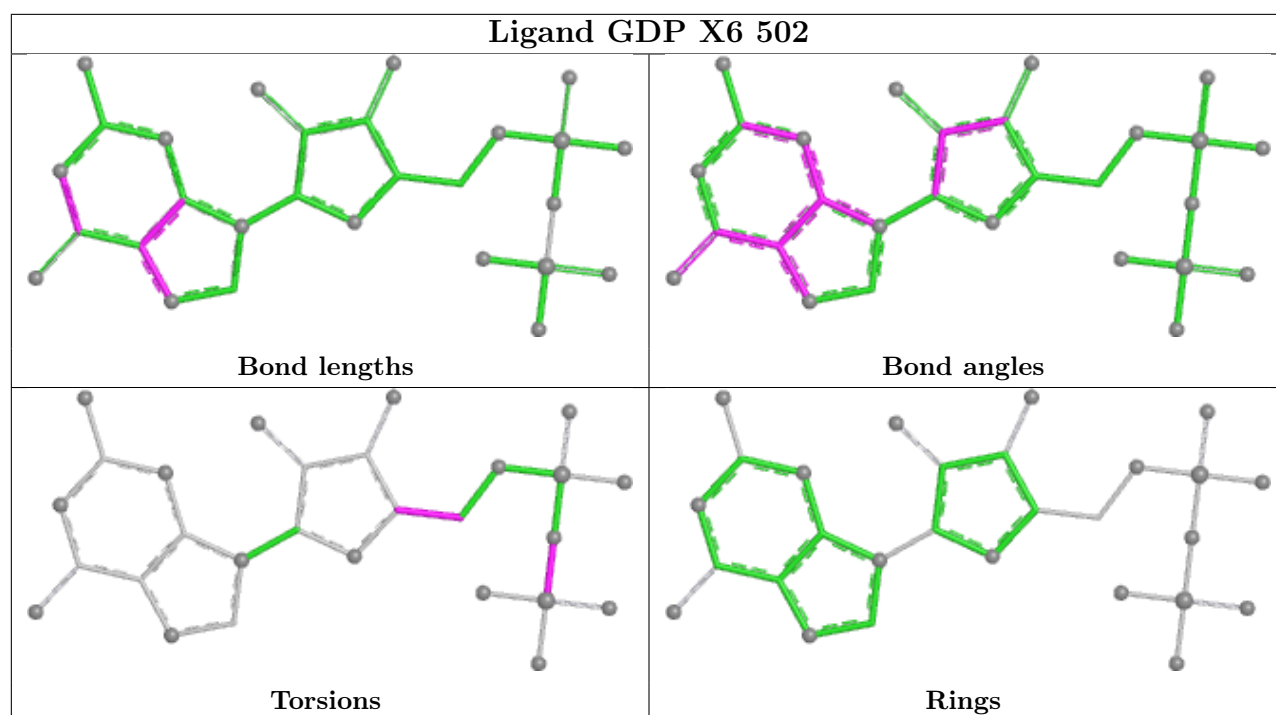




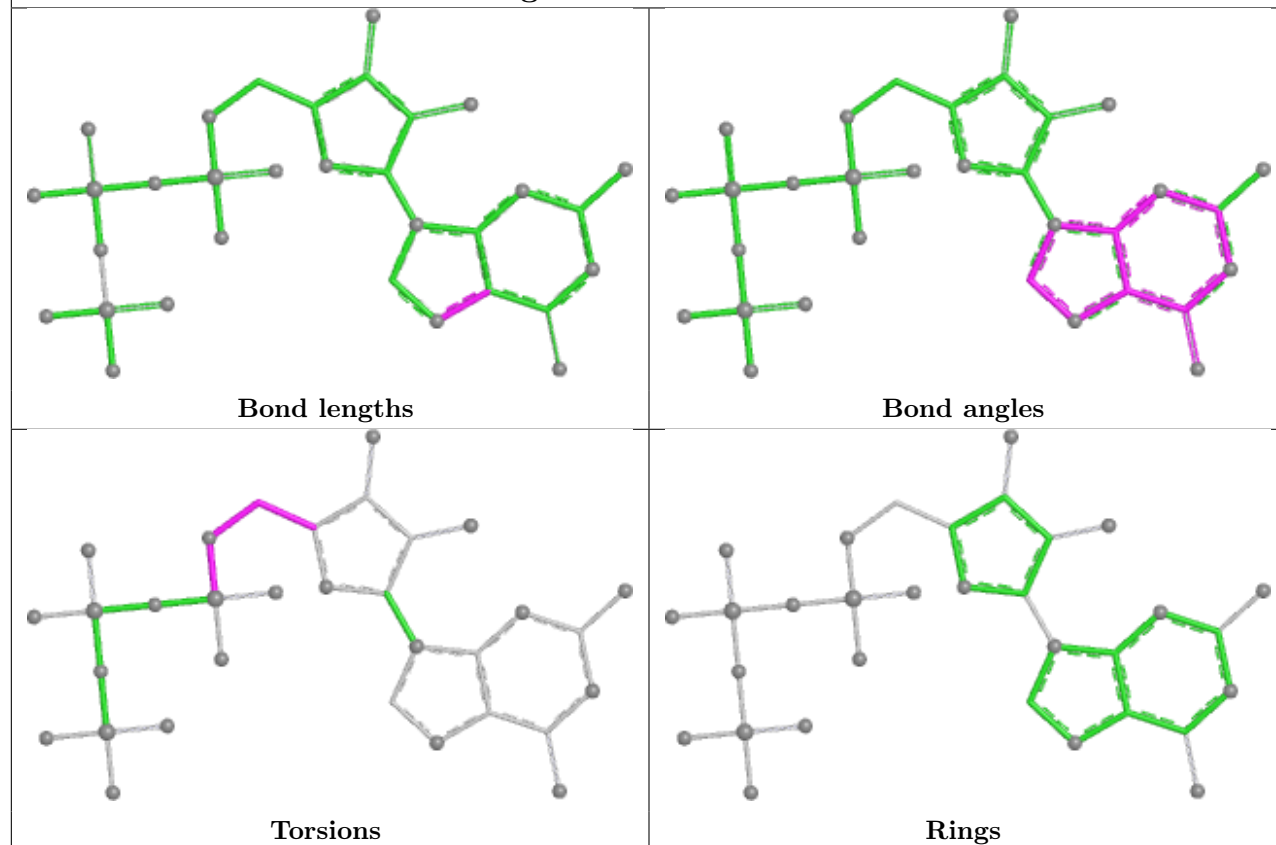




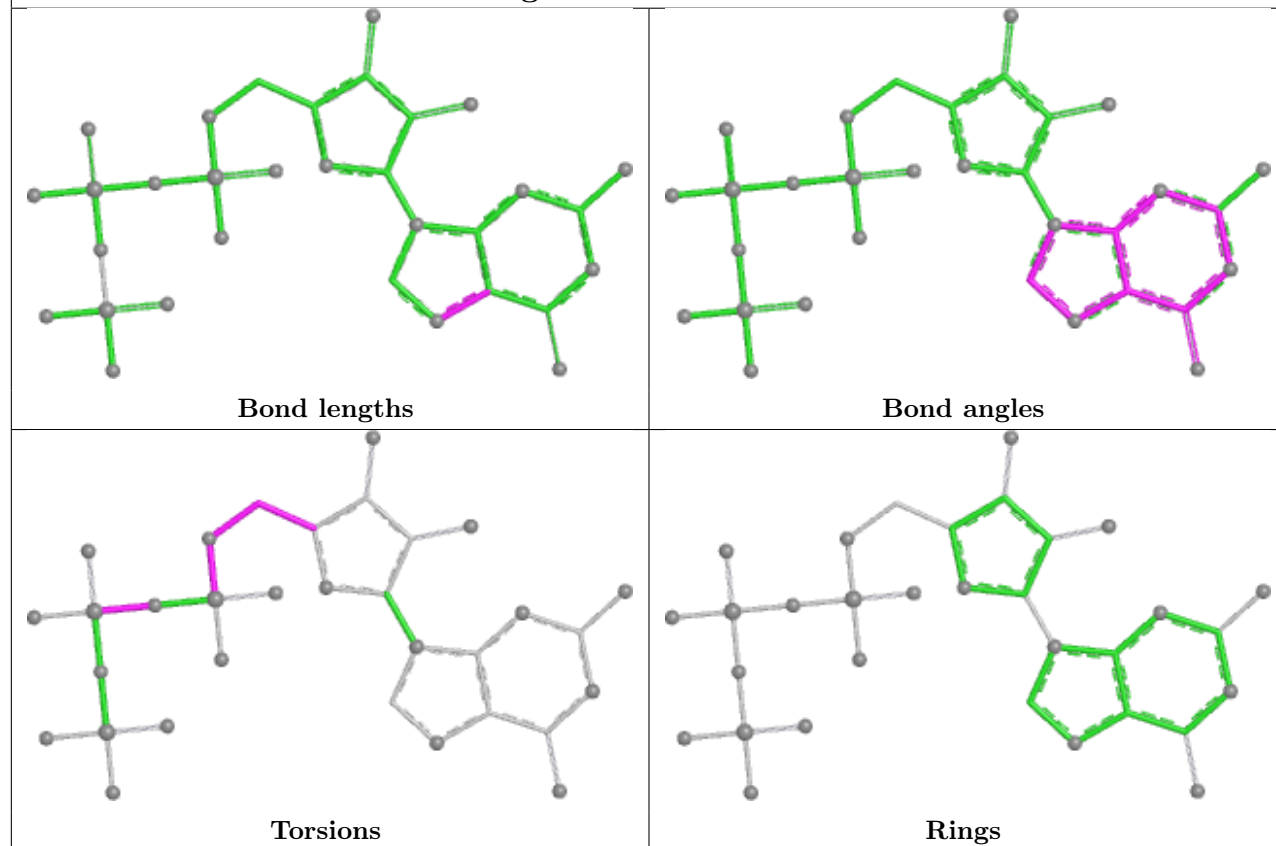


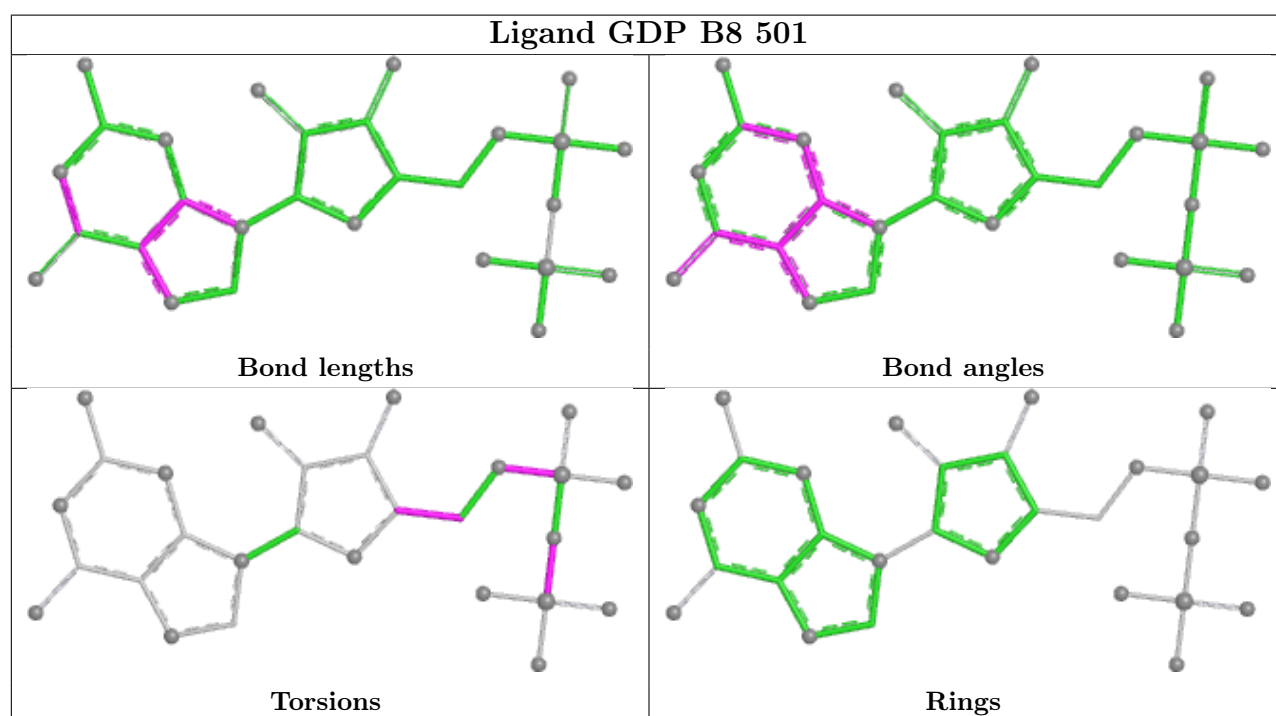
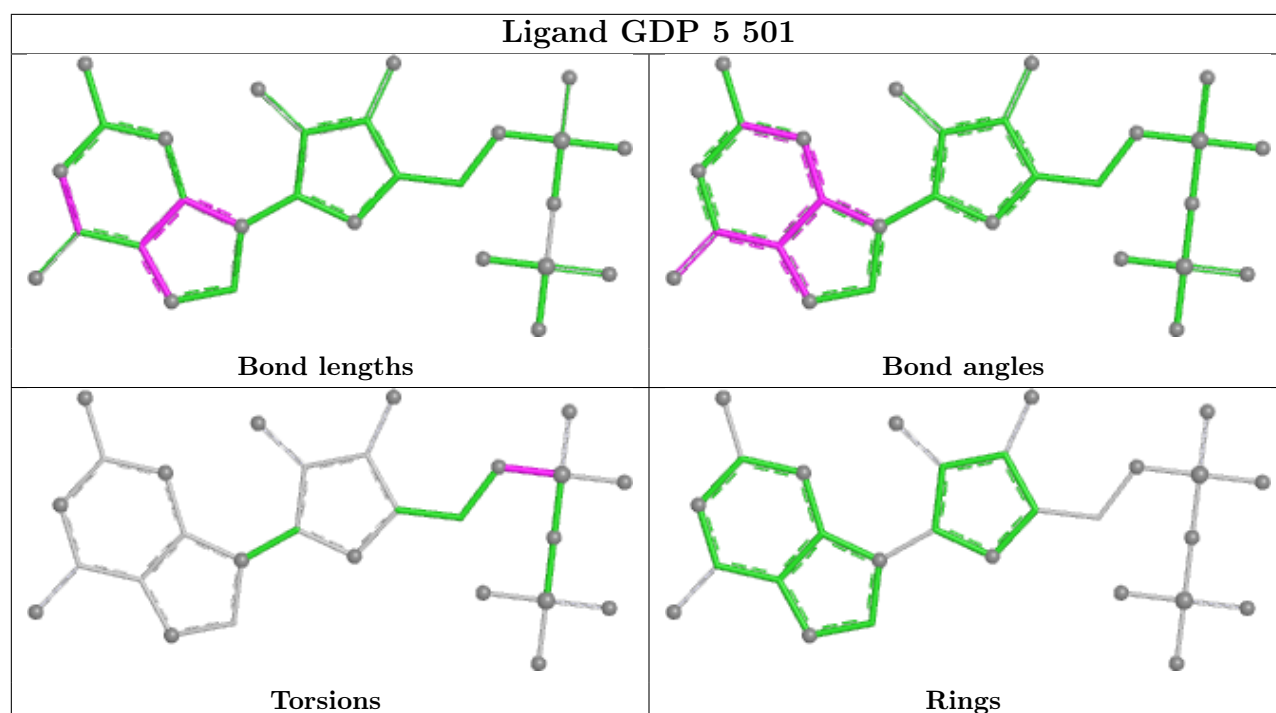


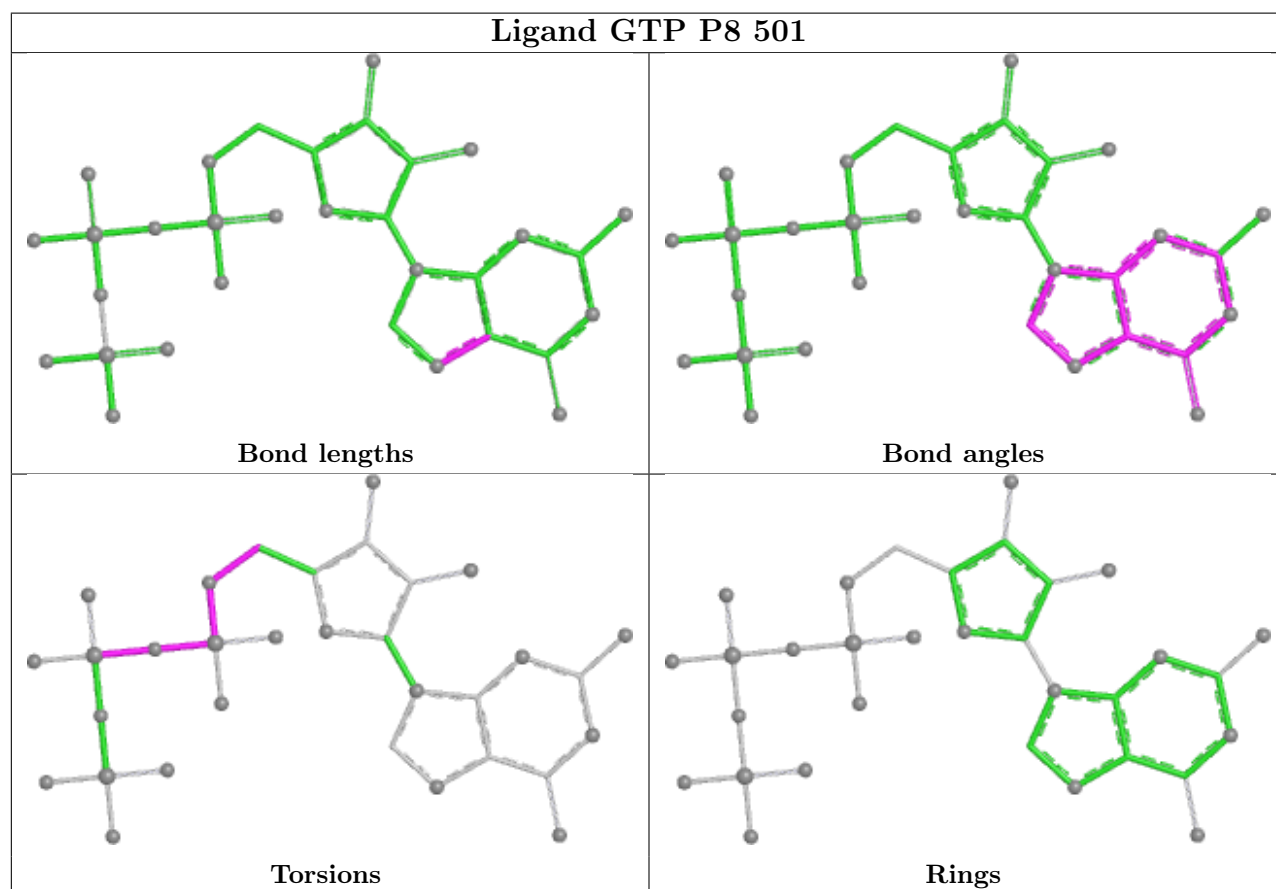
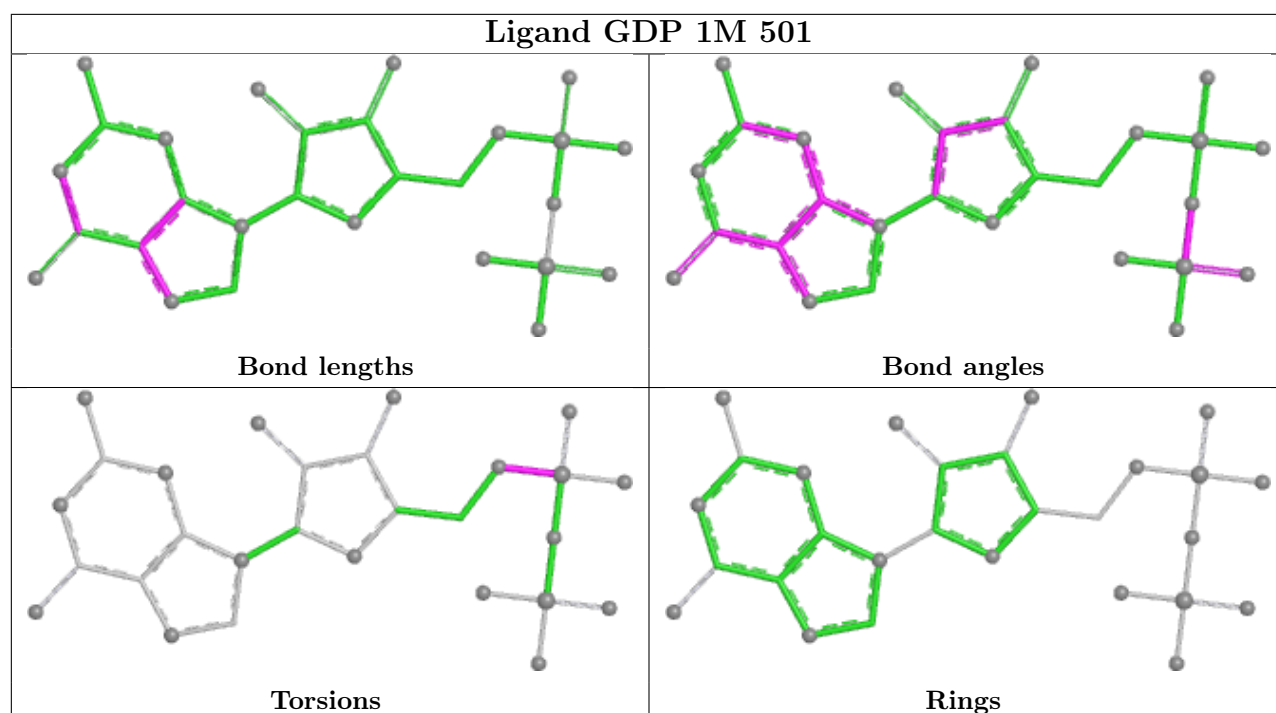
Ligand GTP K6 501



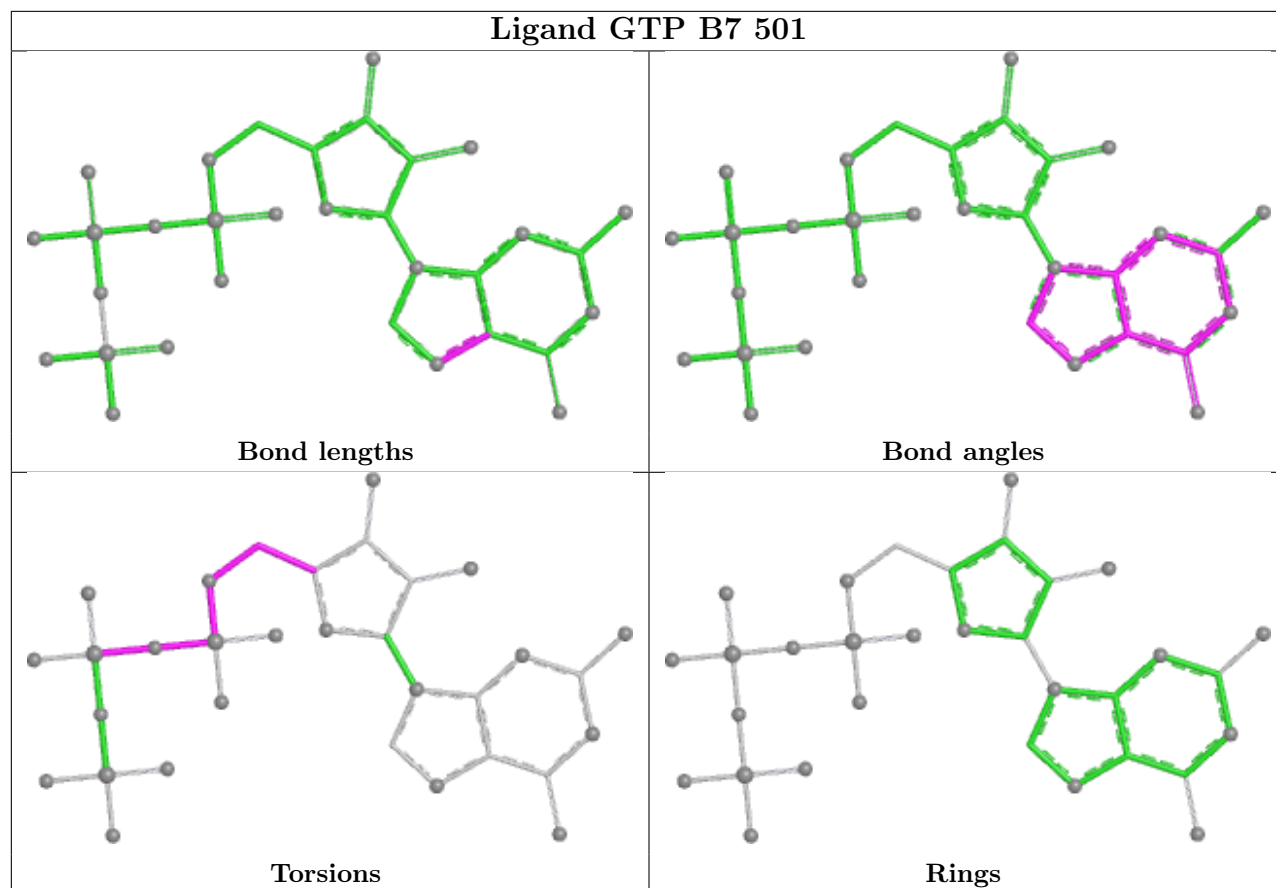
Ligand GTP V8 501



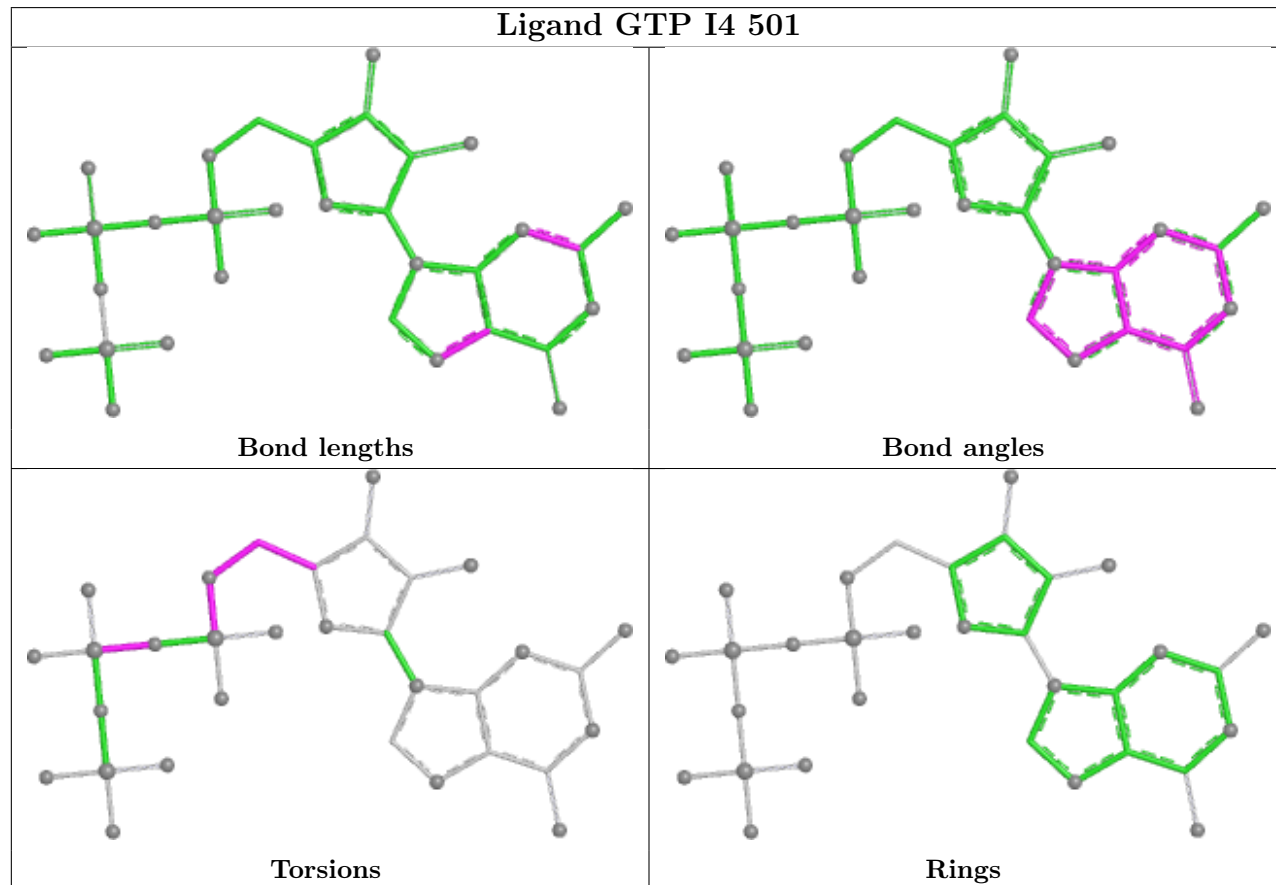


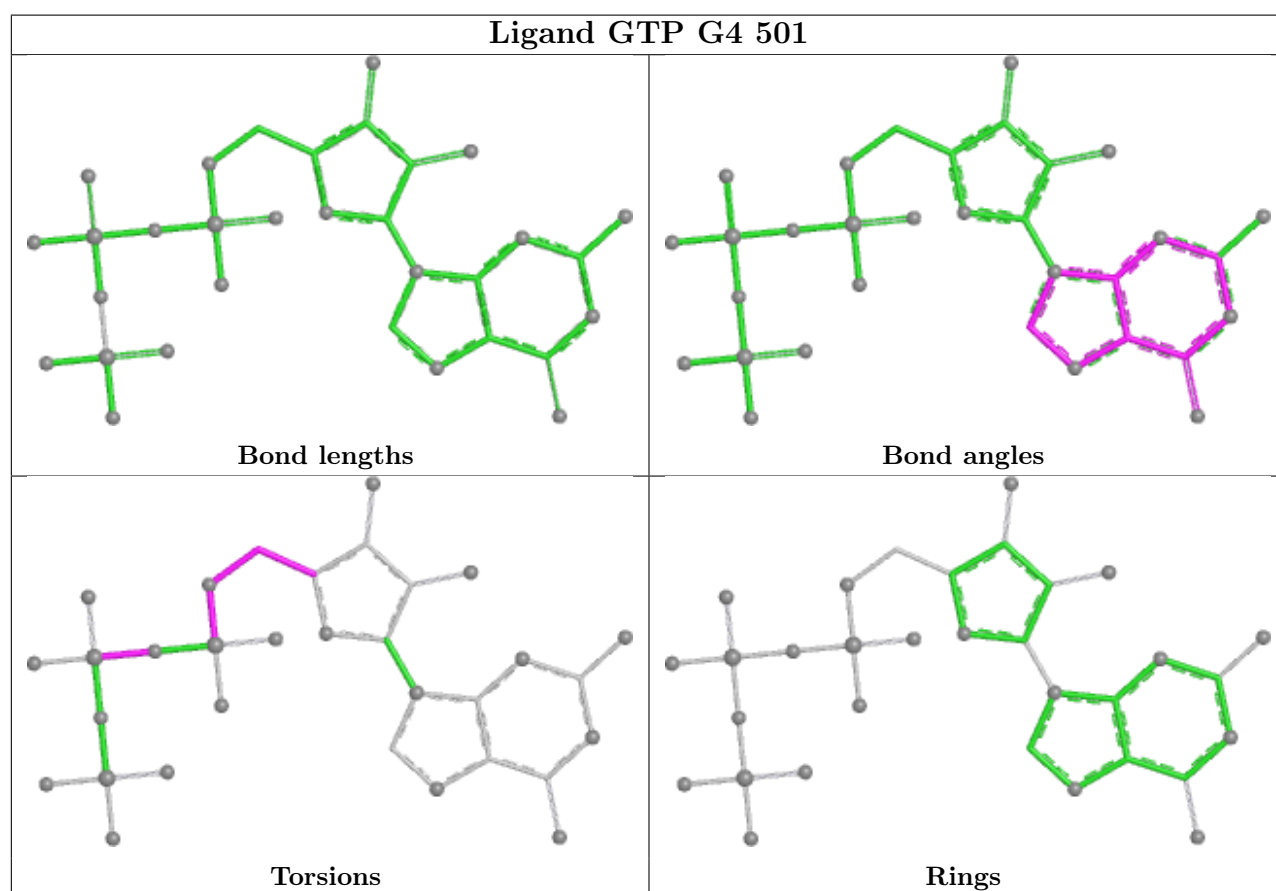
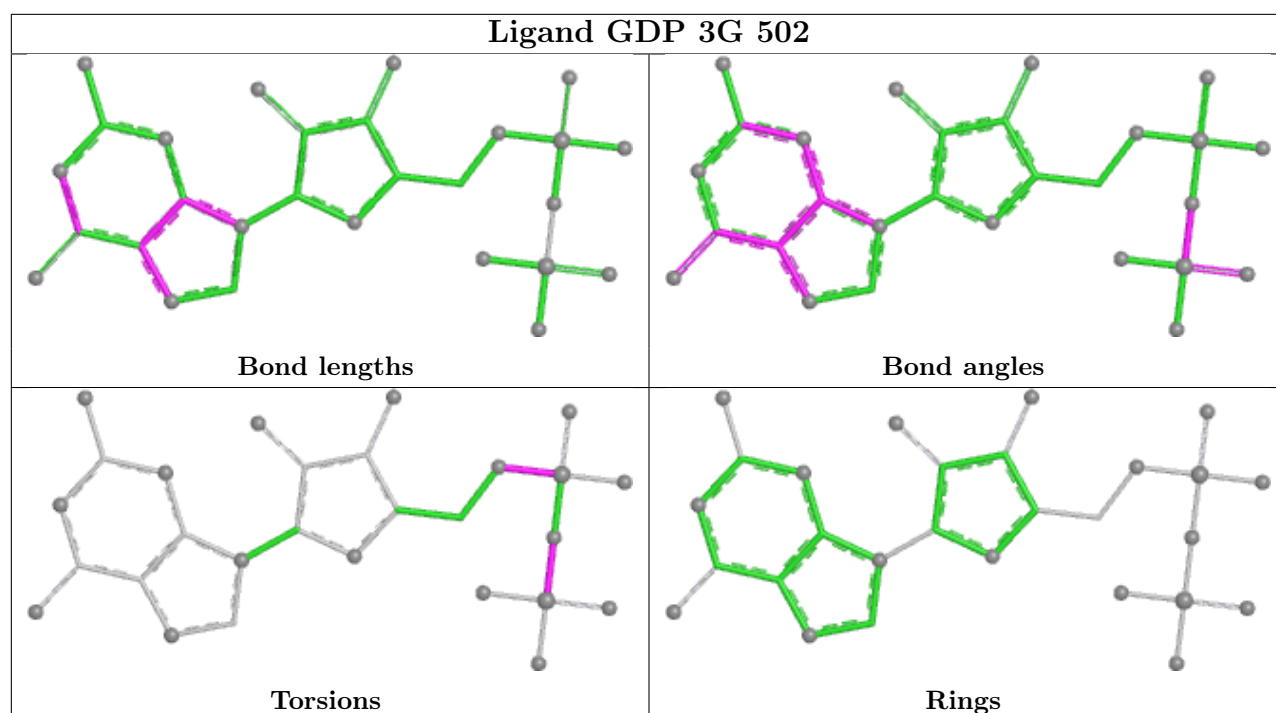


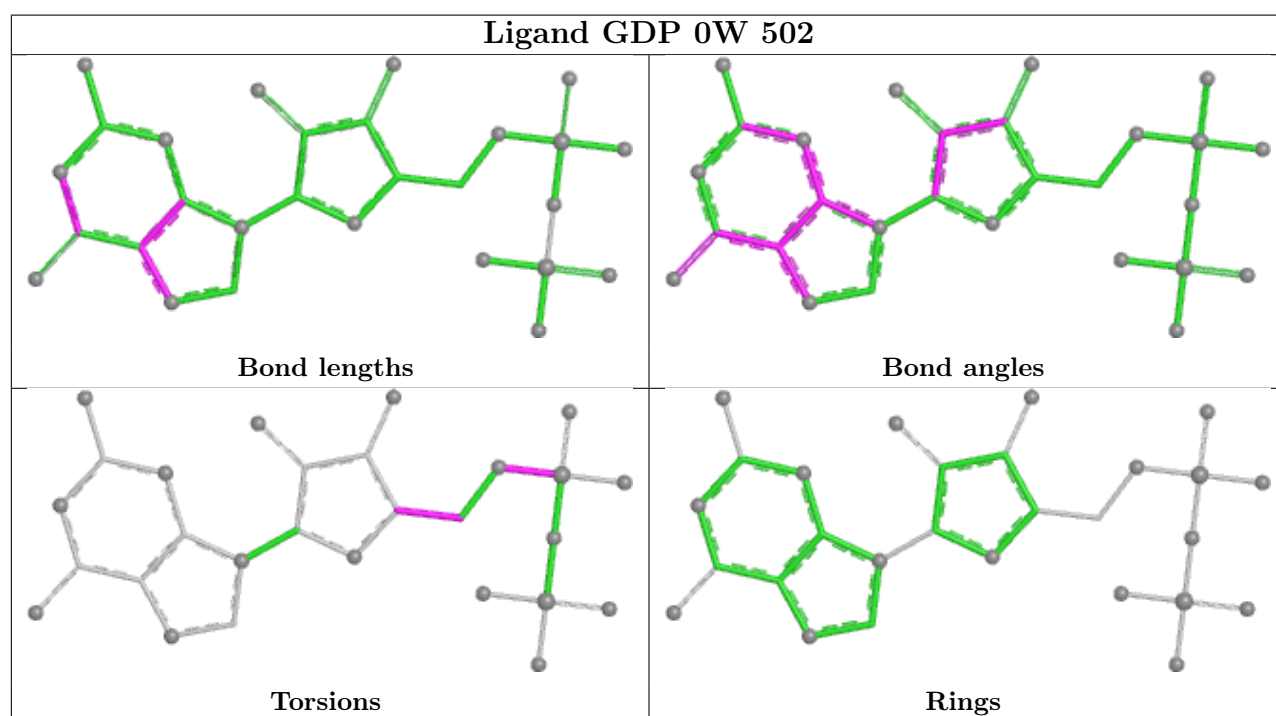
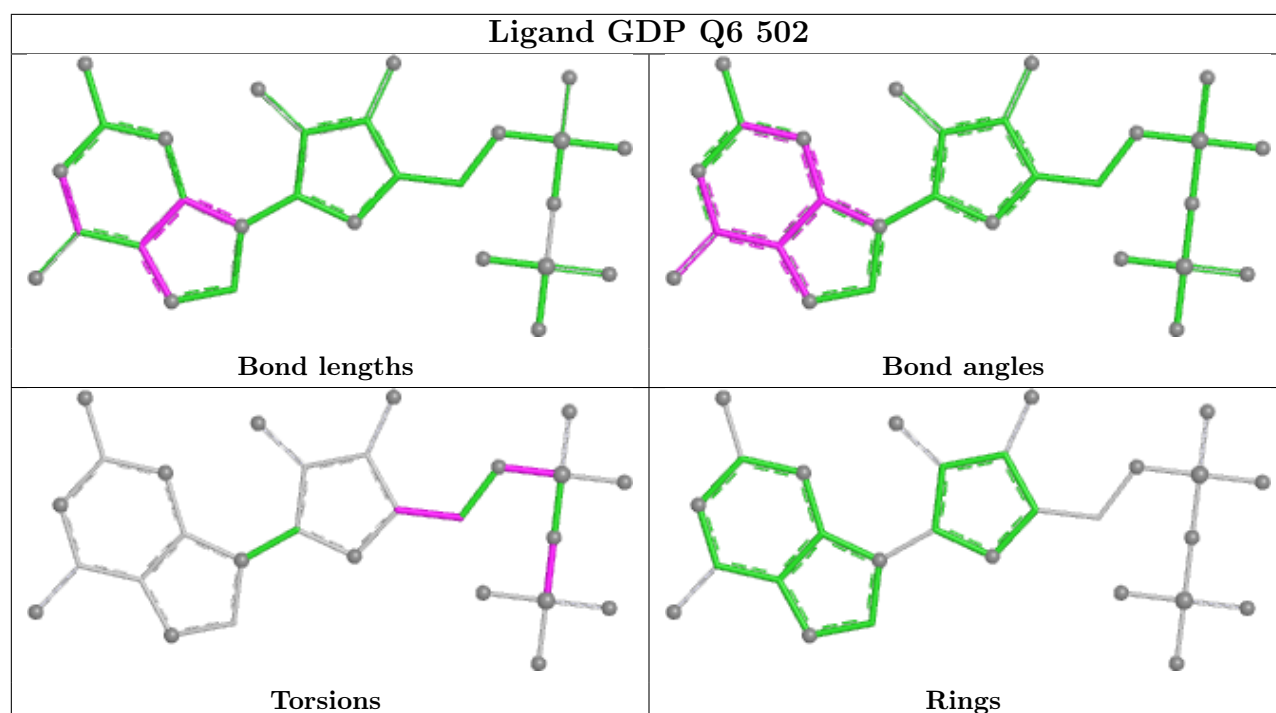
Ligand GTP B7 501

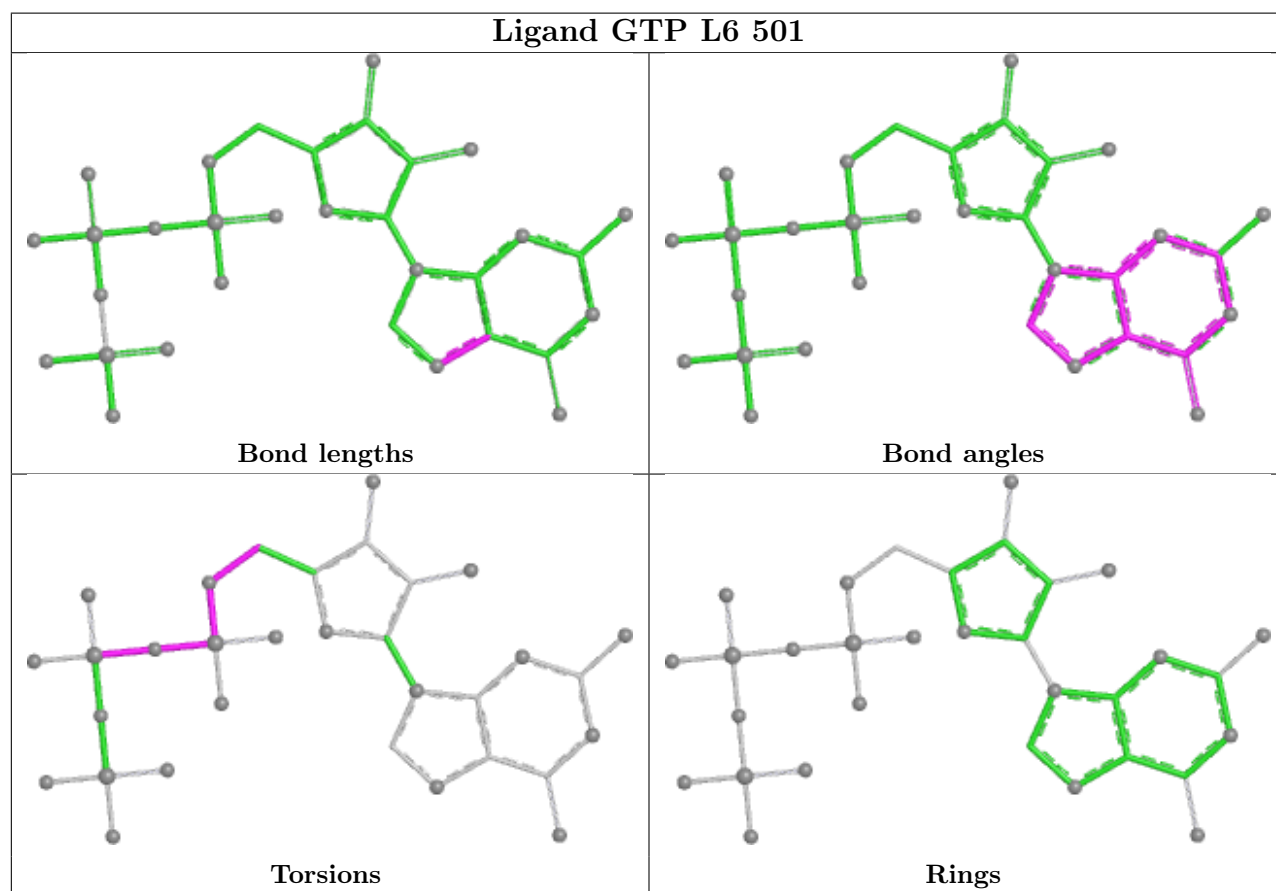
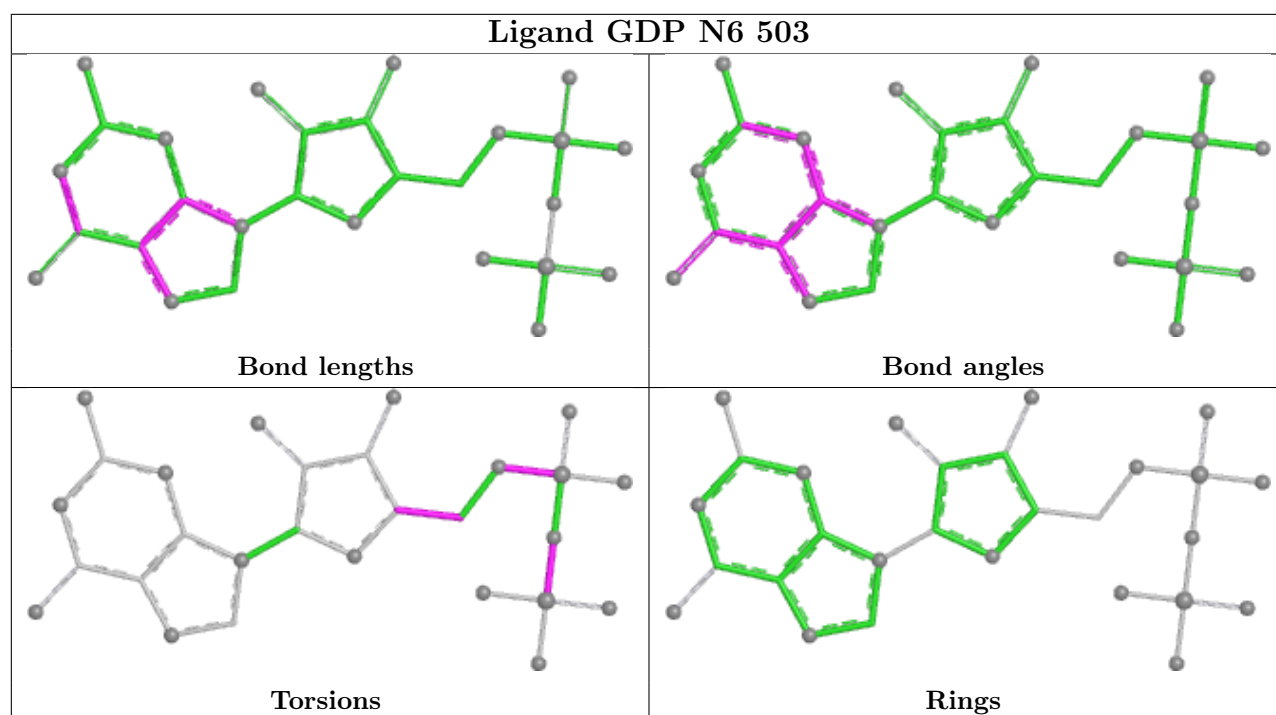


Ligand GTP I4 501

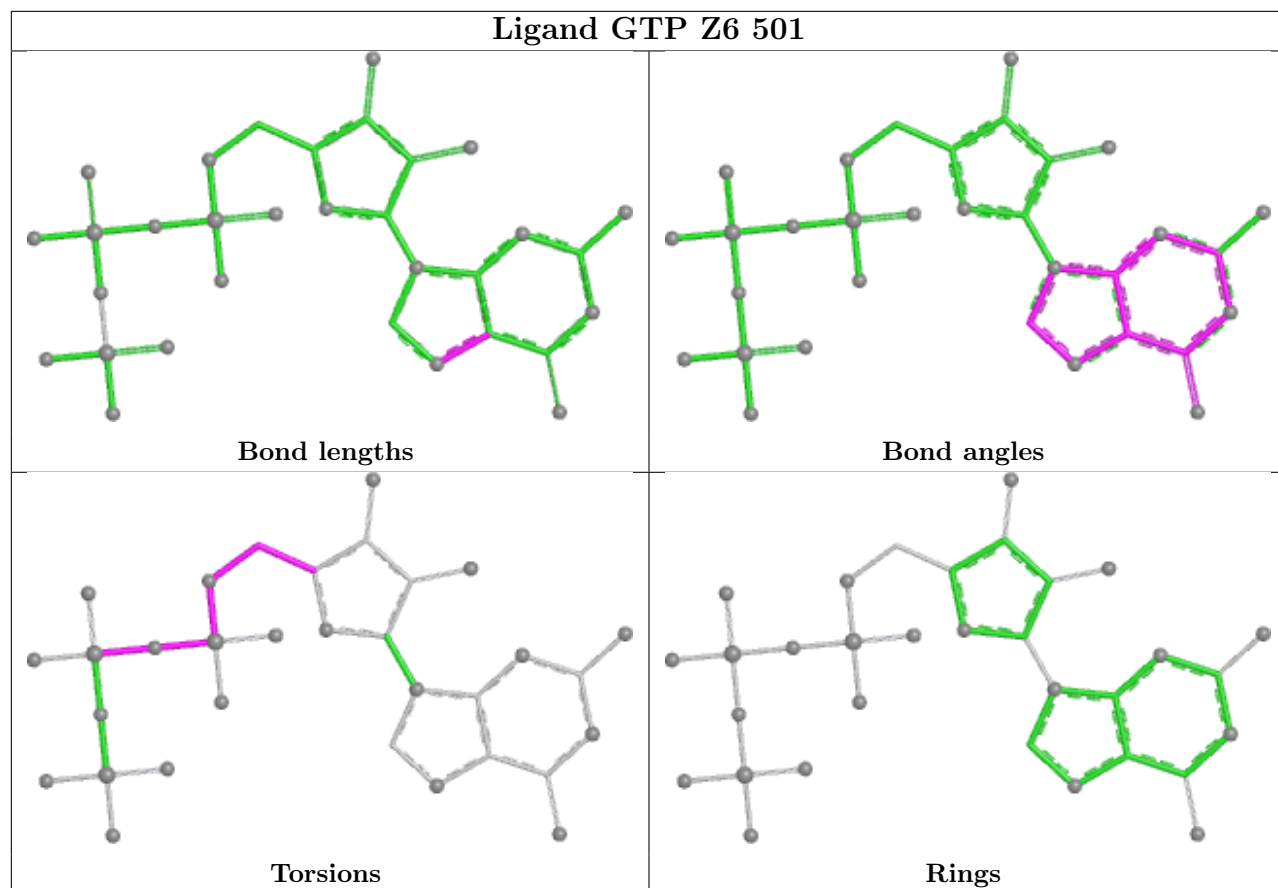




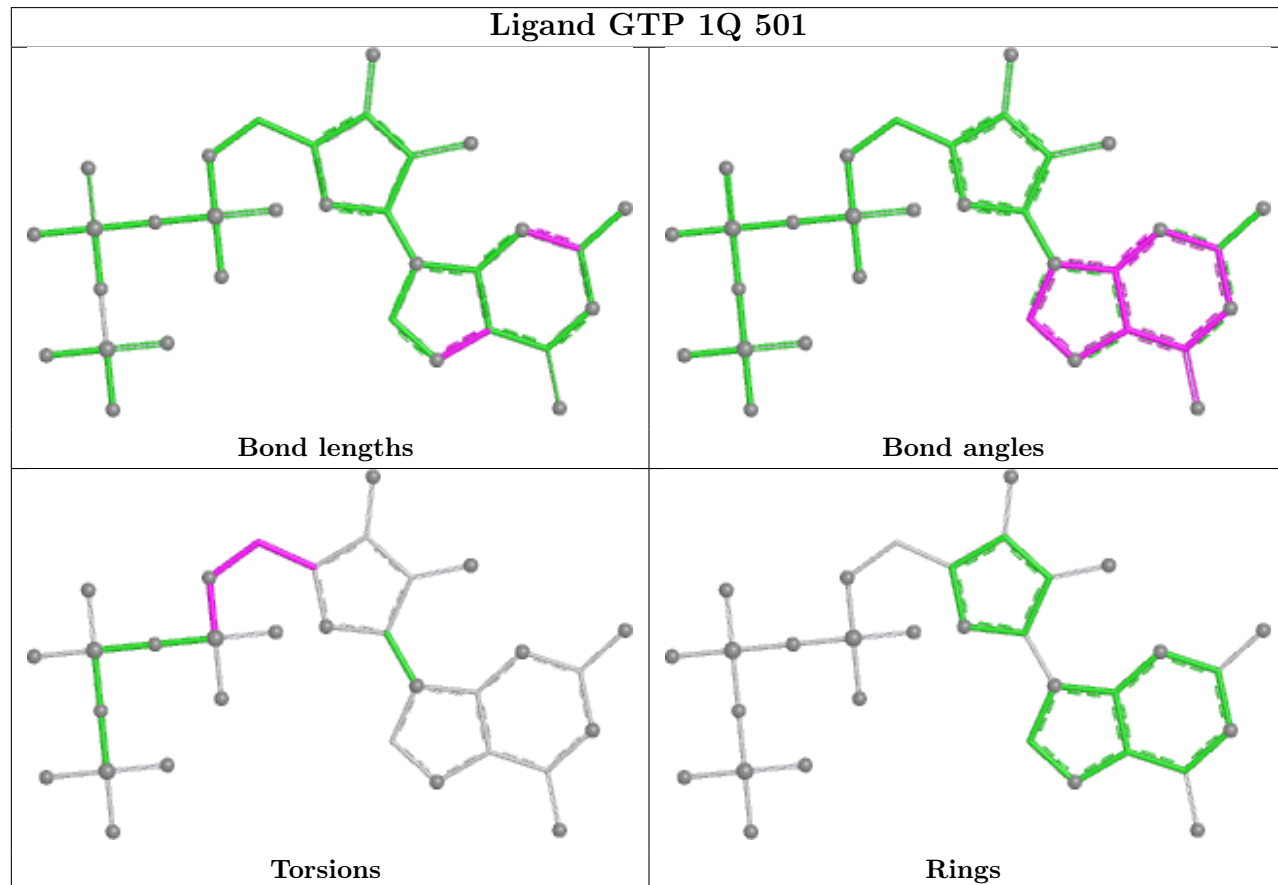


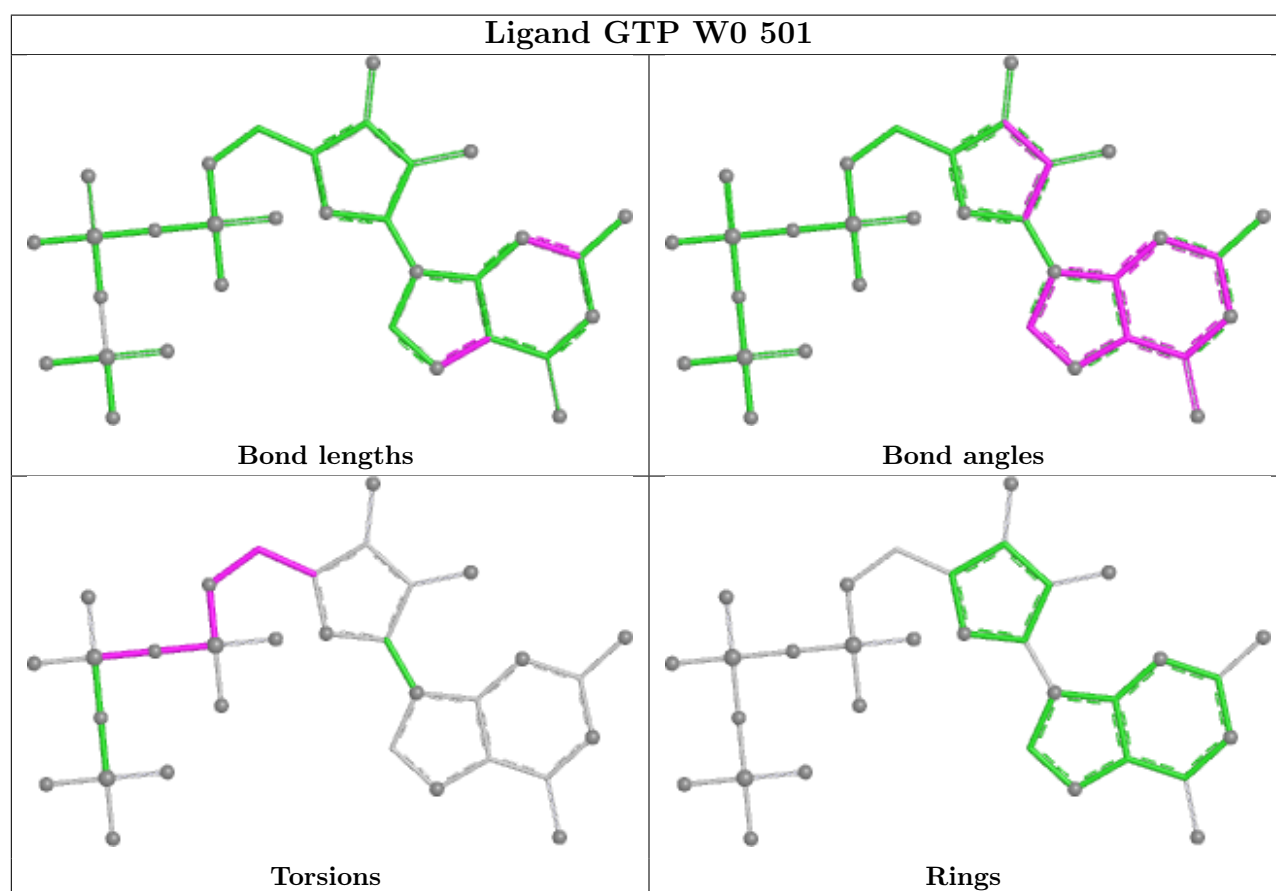
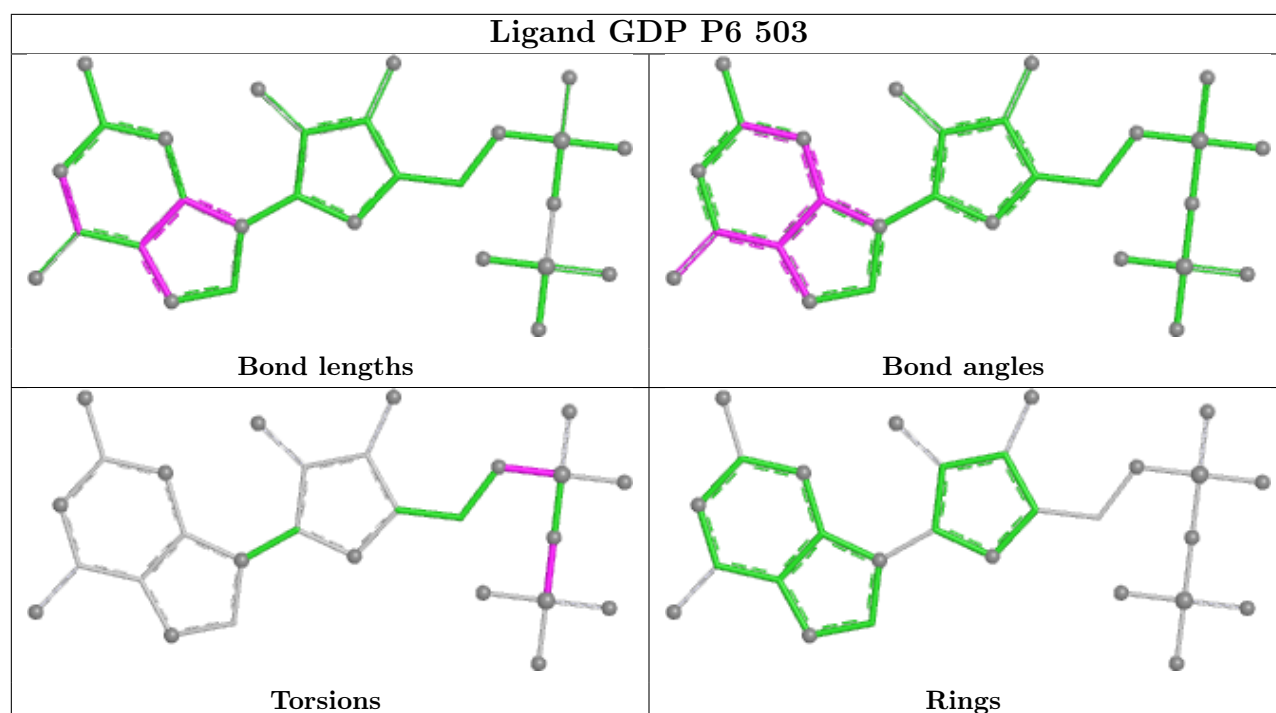


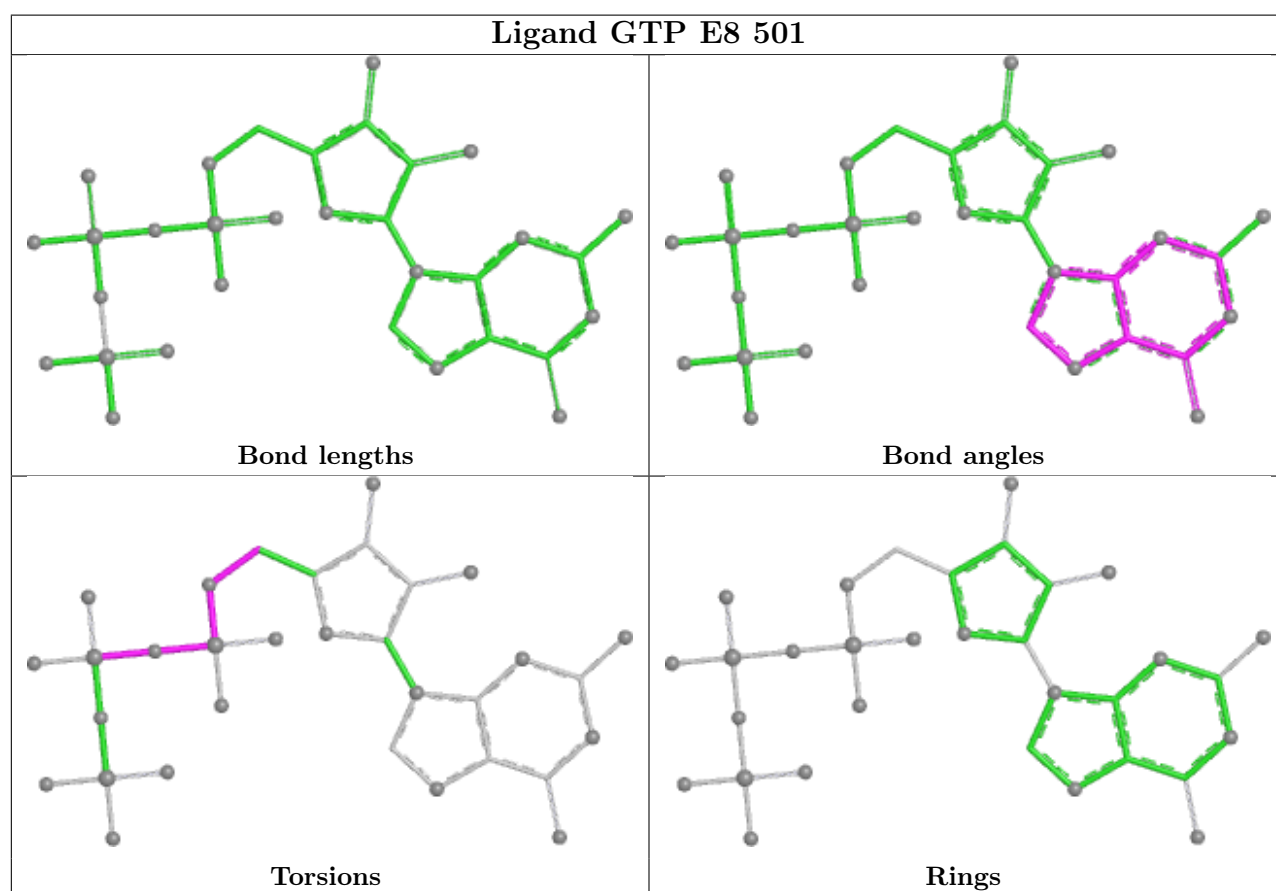
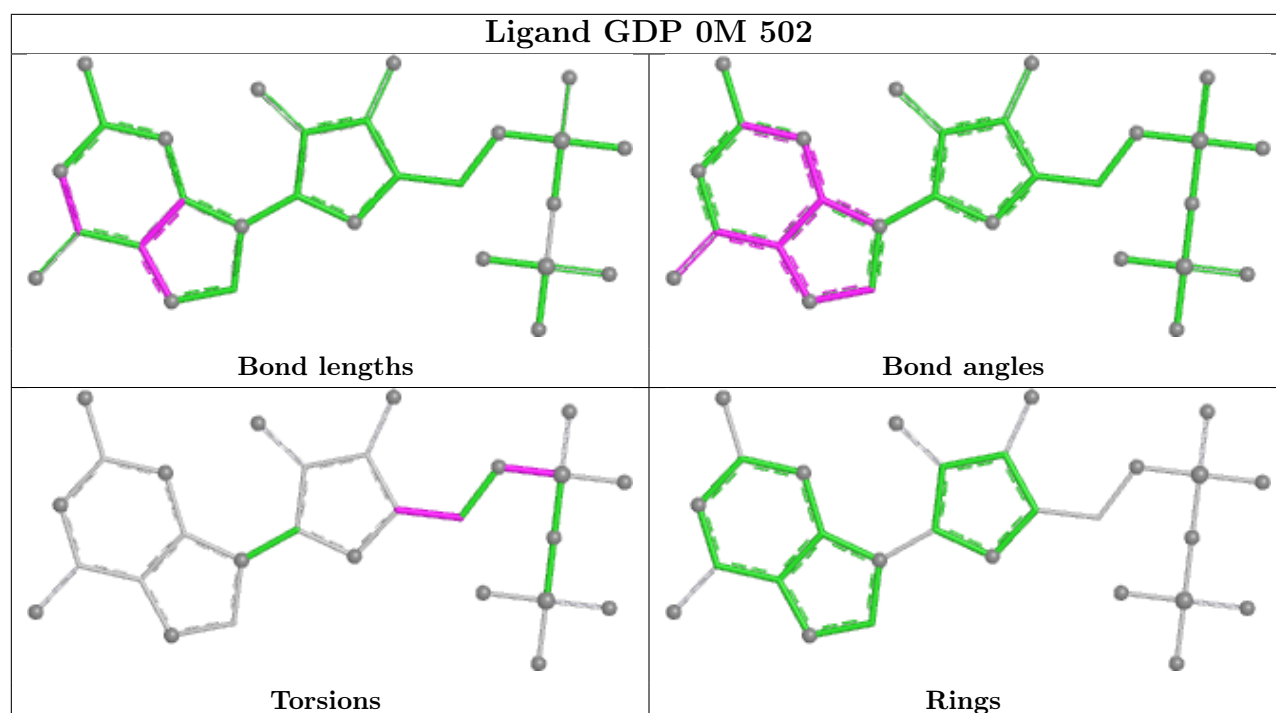
Ligand GTP Z6 501

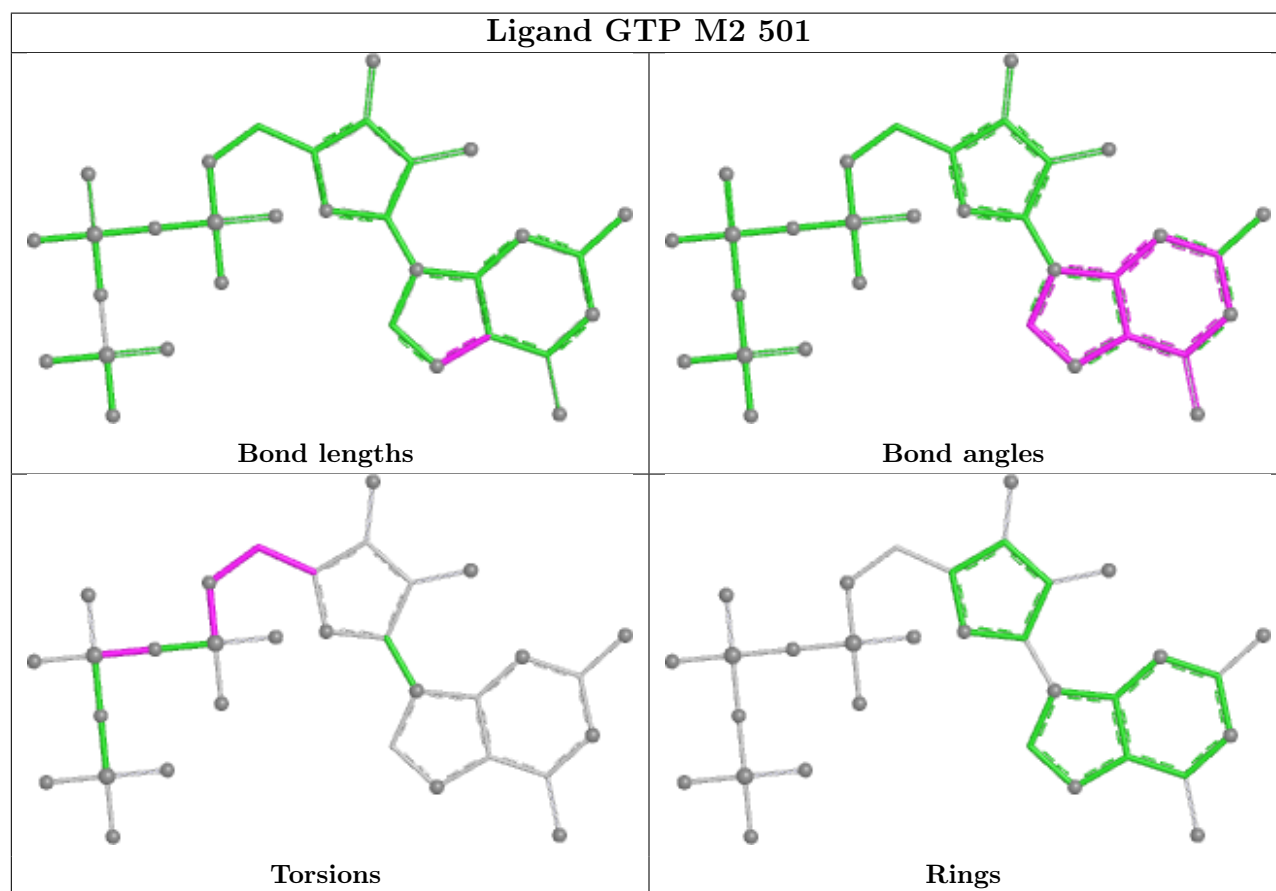
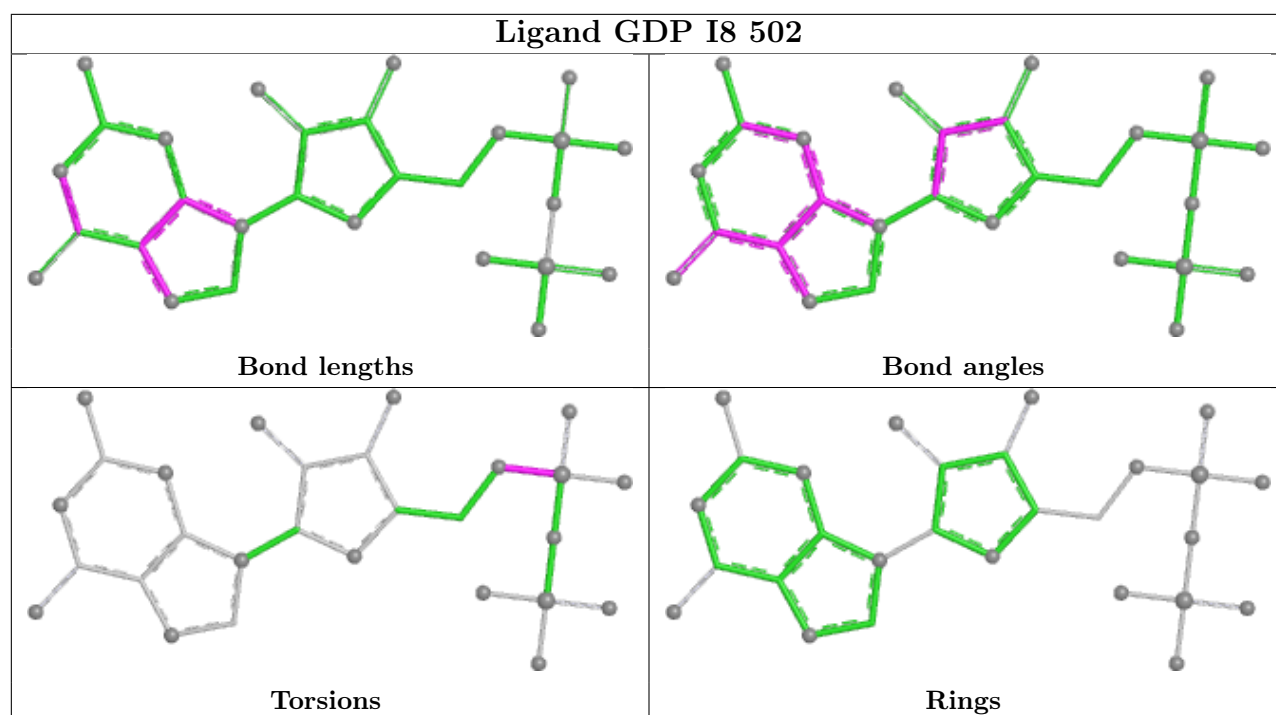


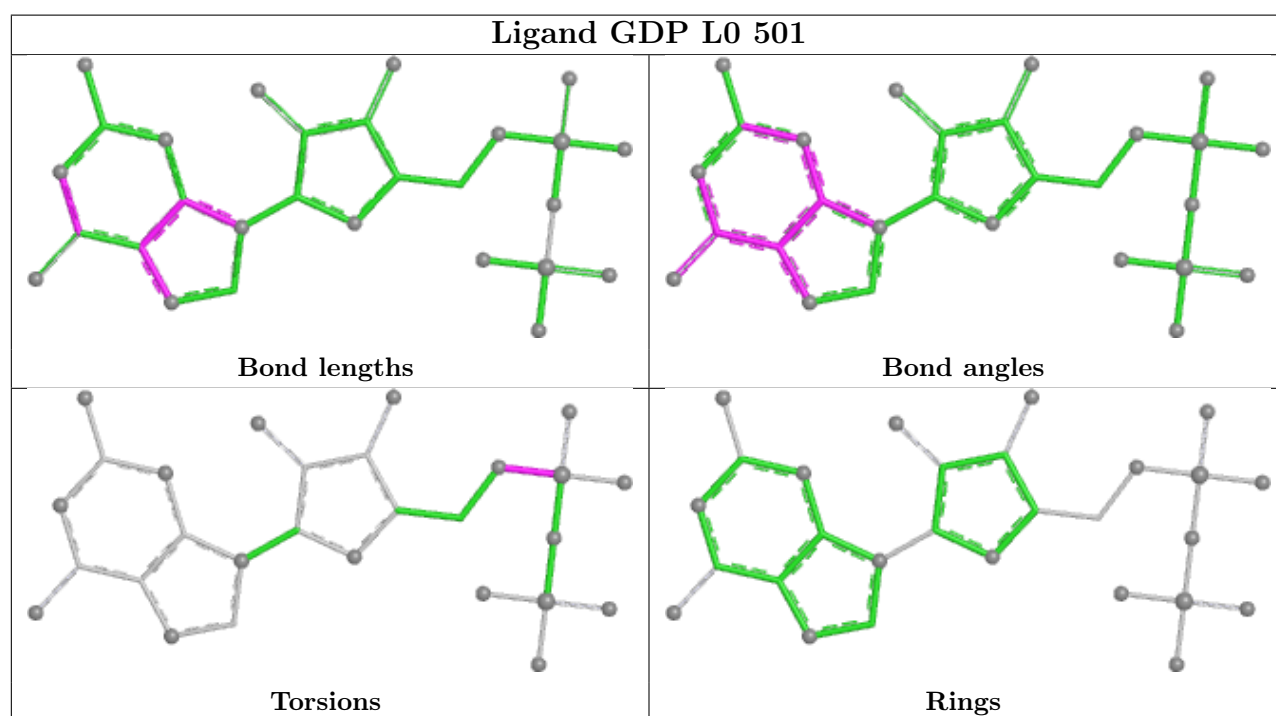
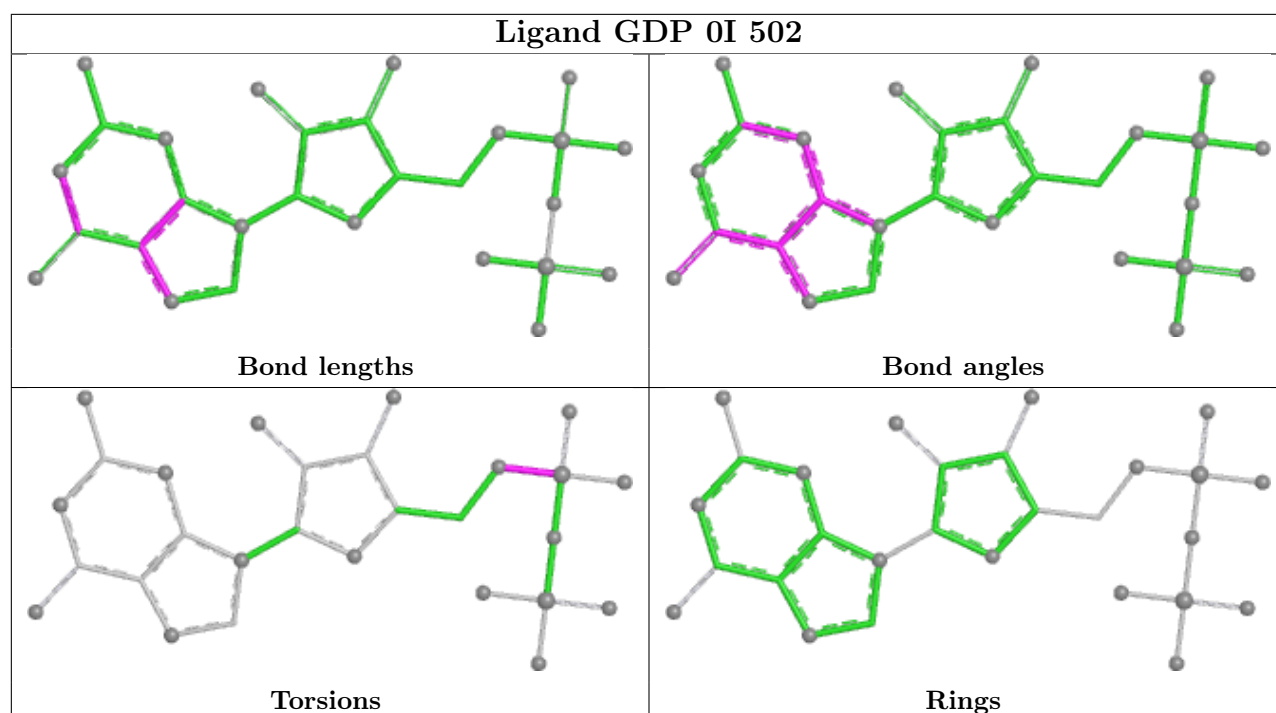
Ligand GTP 1Q 501



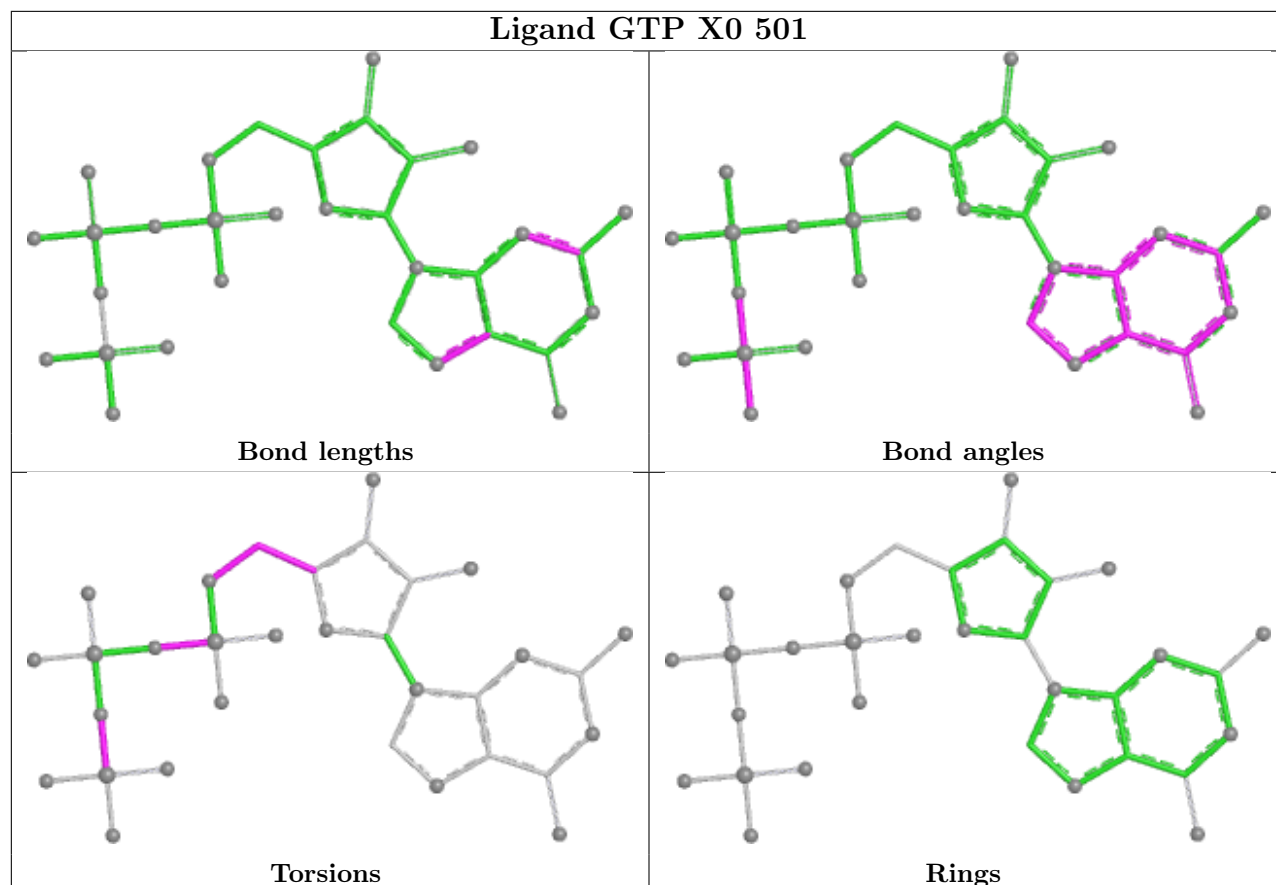




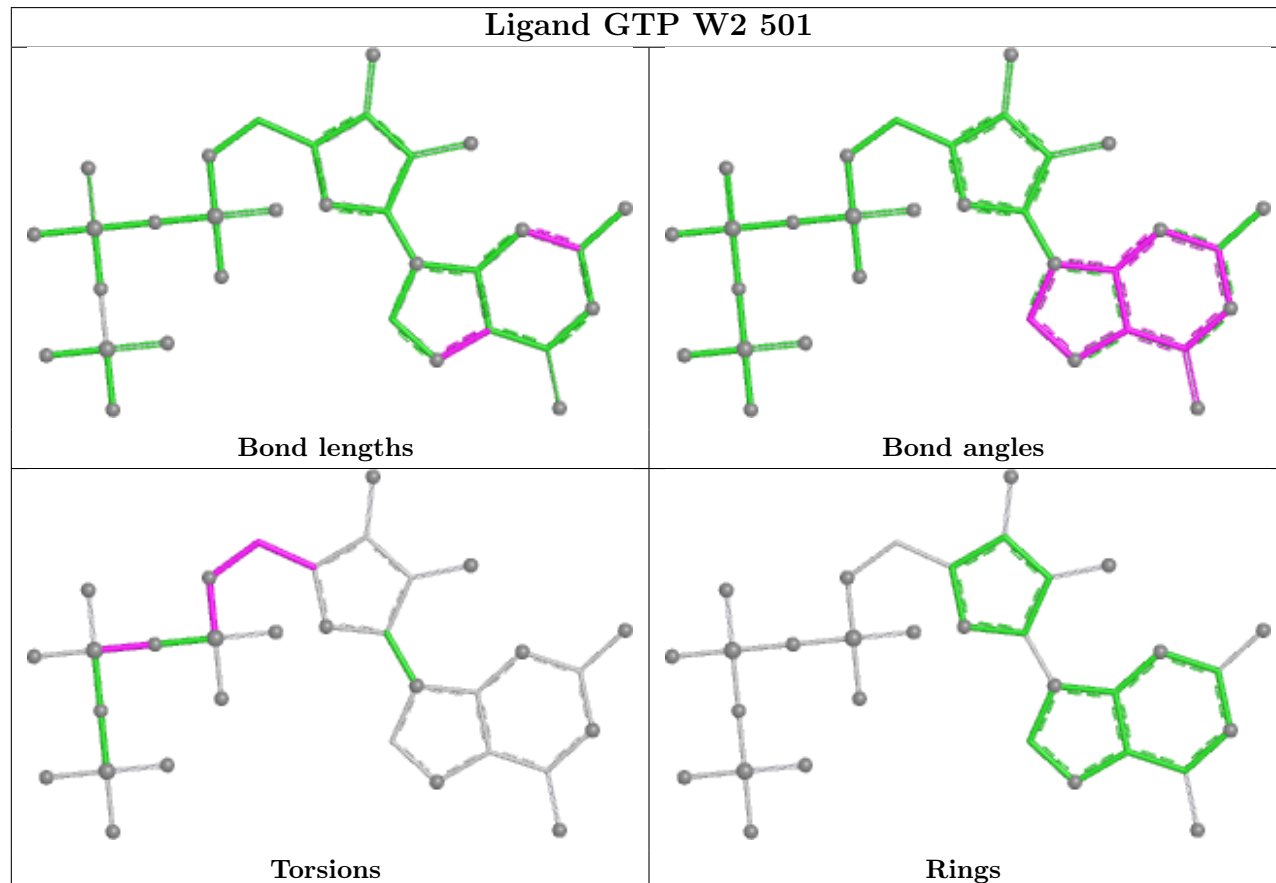




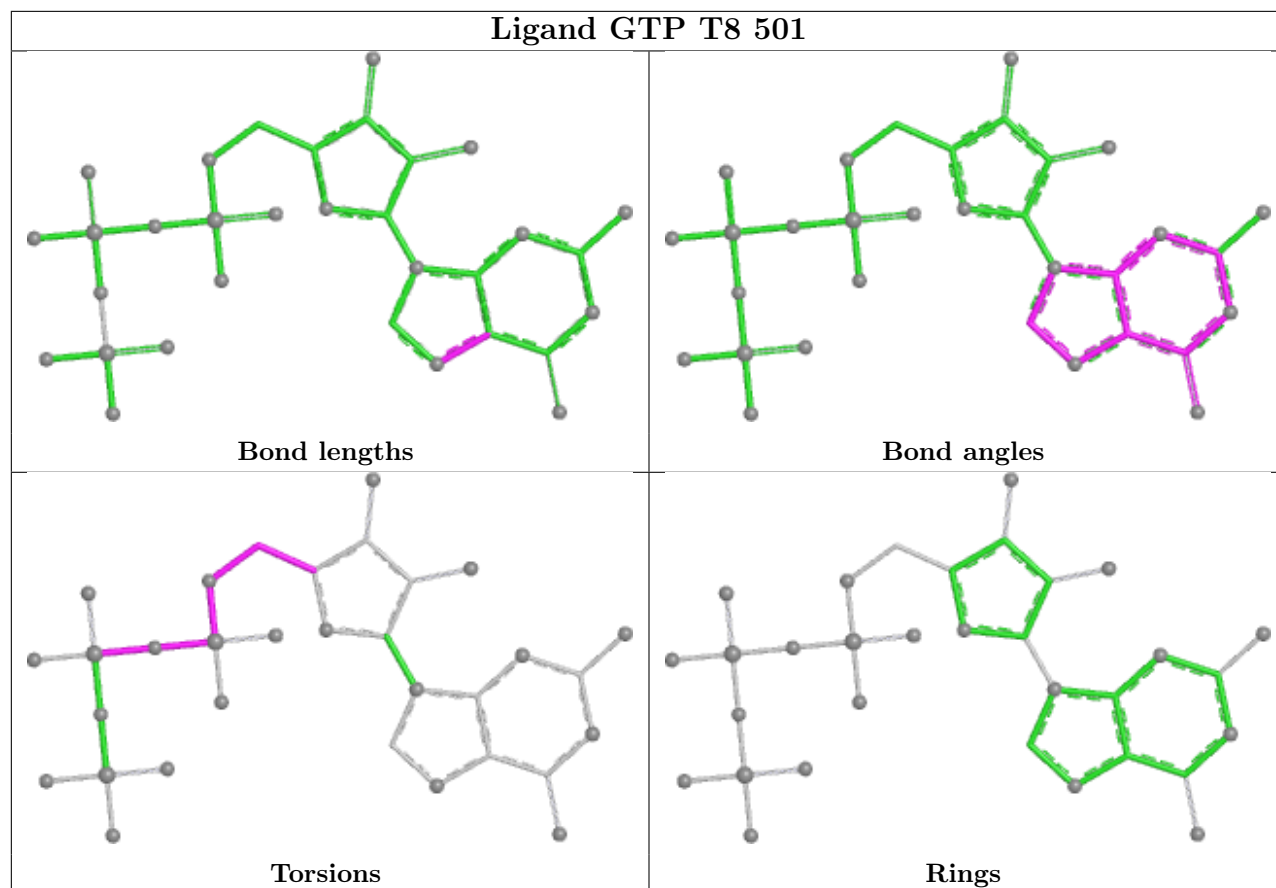
Ligand GTP X0 501



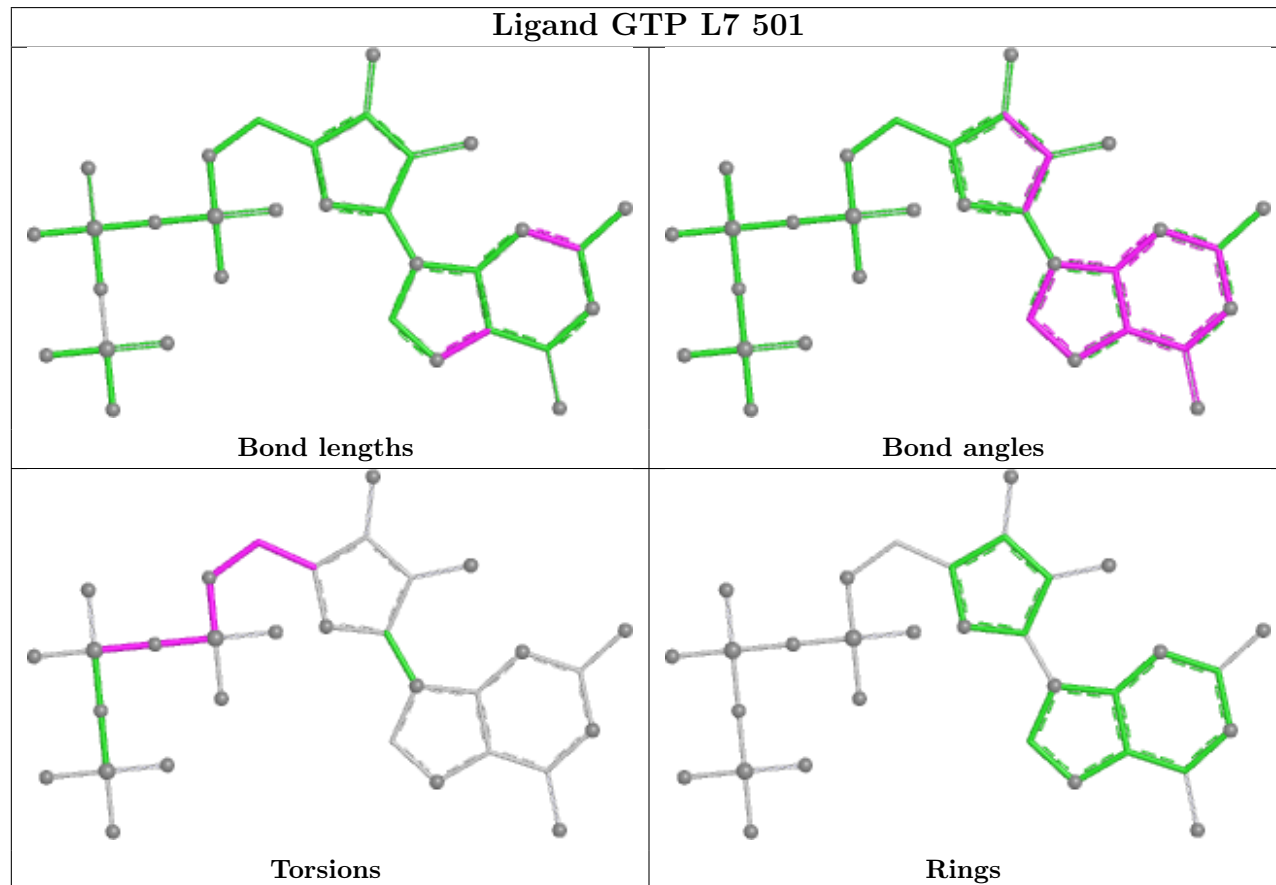
Ligand GTP W2 501

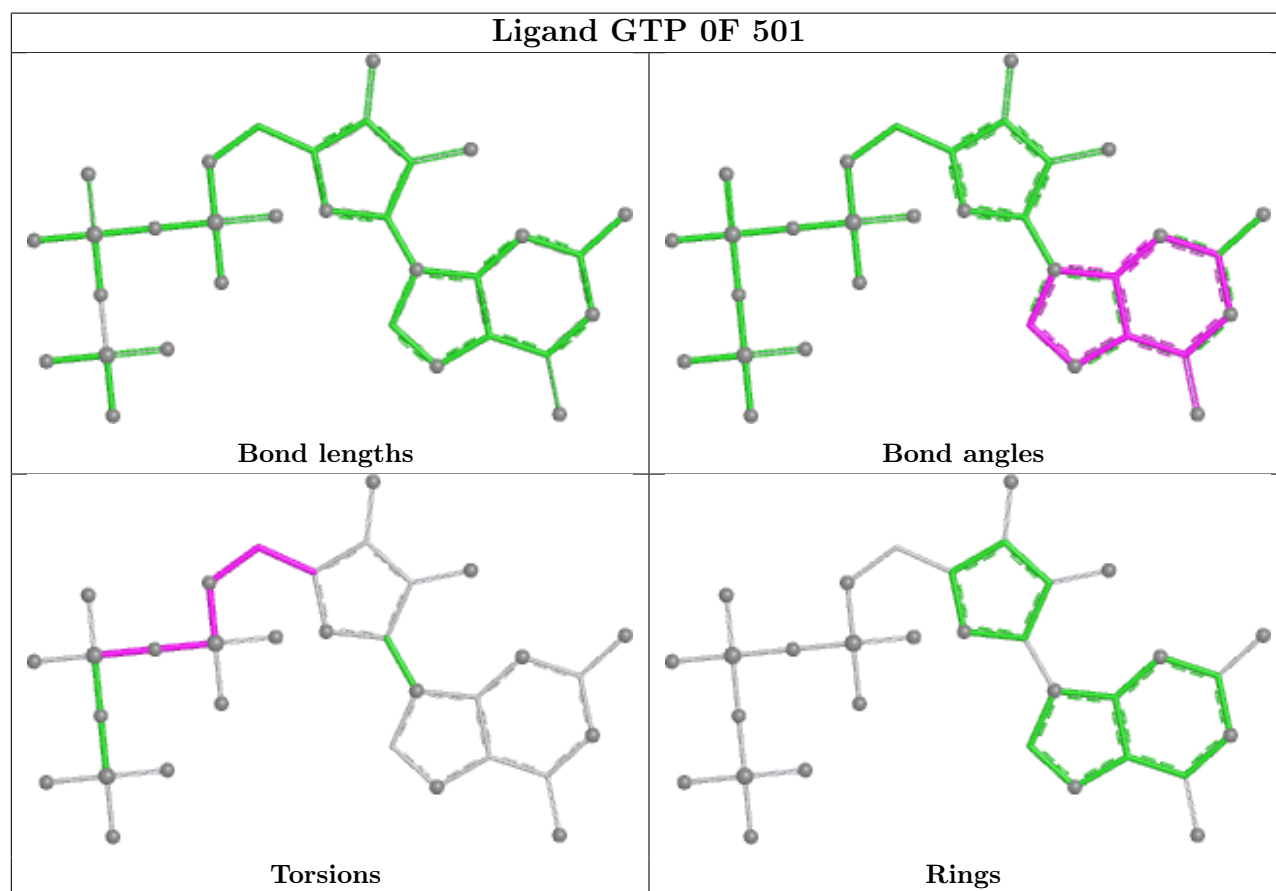
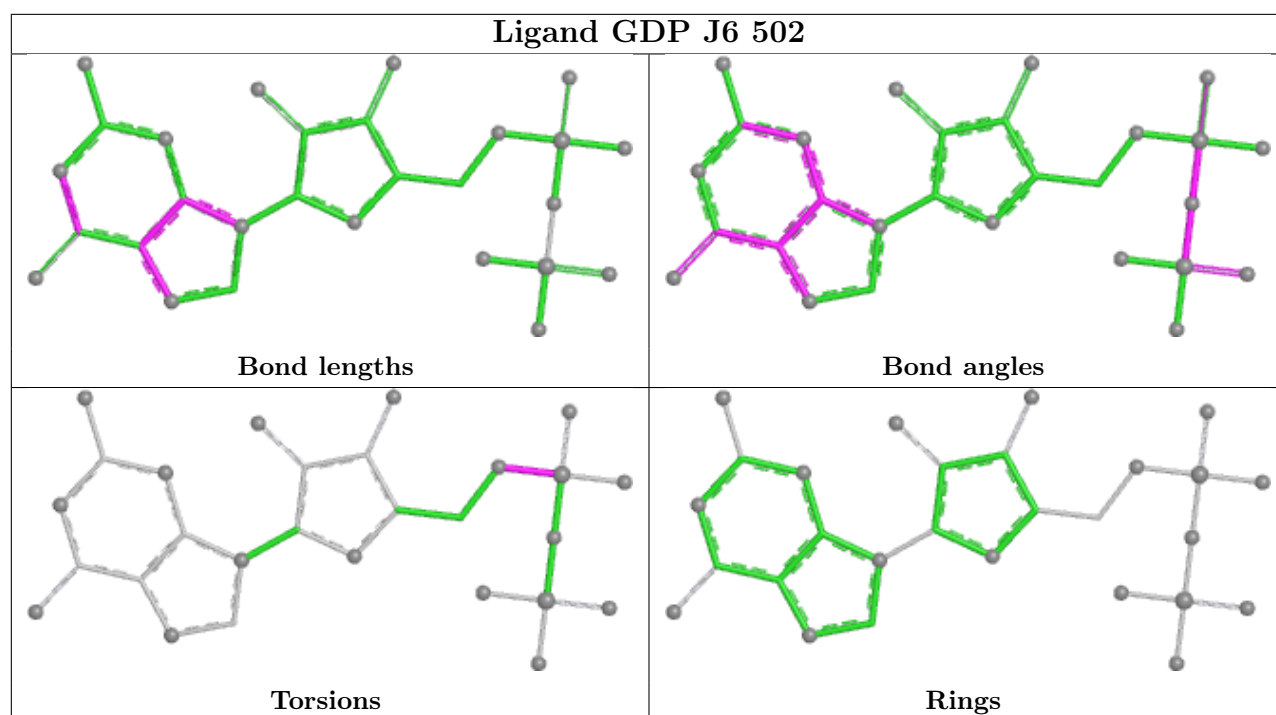


Ligand GTP T8 501

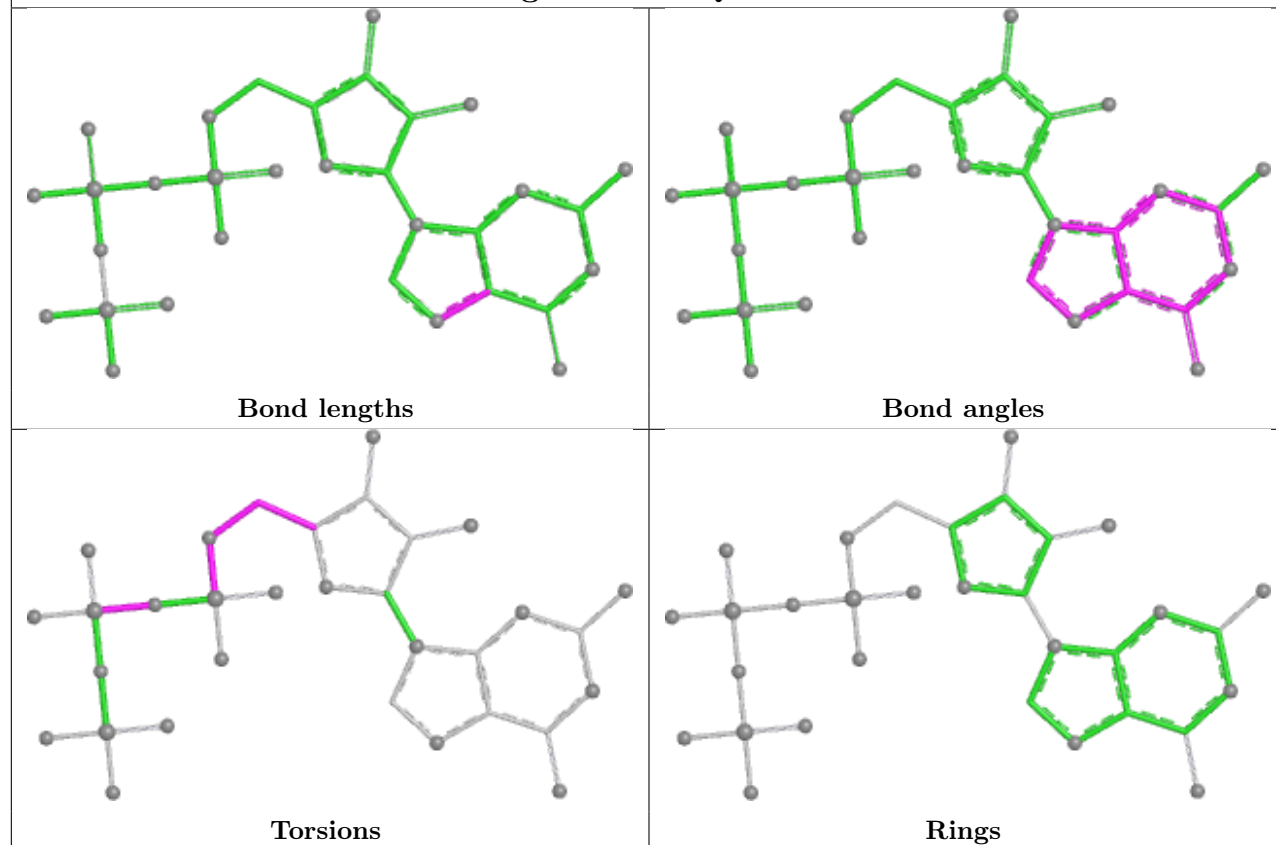


Ligand GTP L7 501

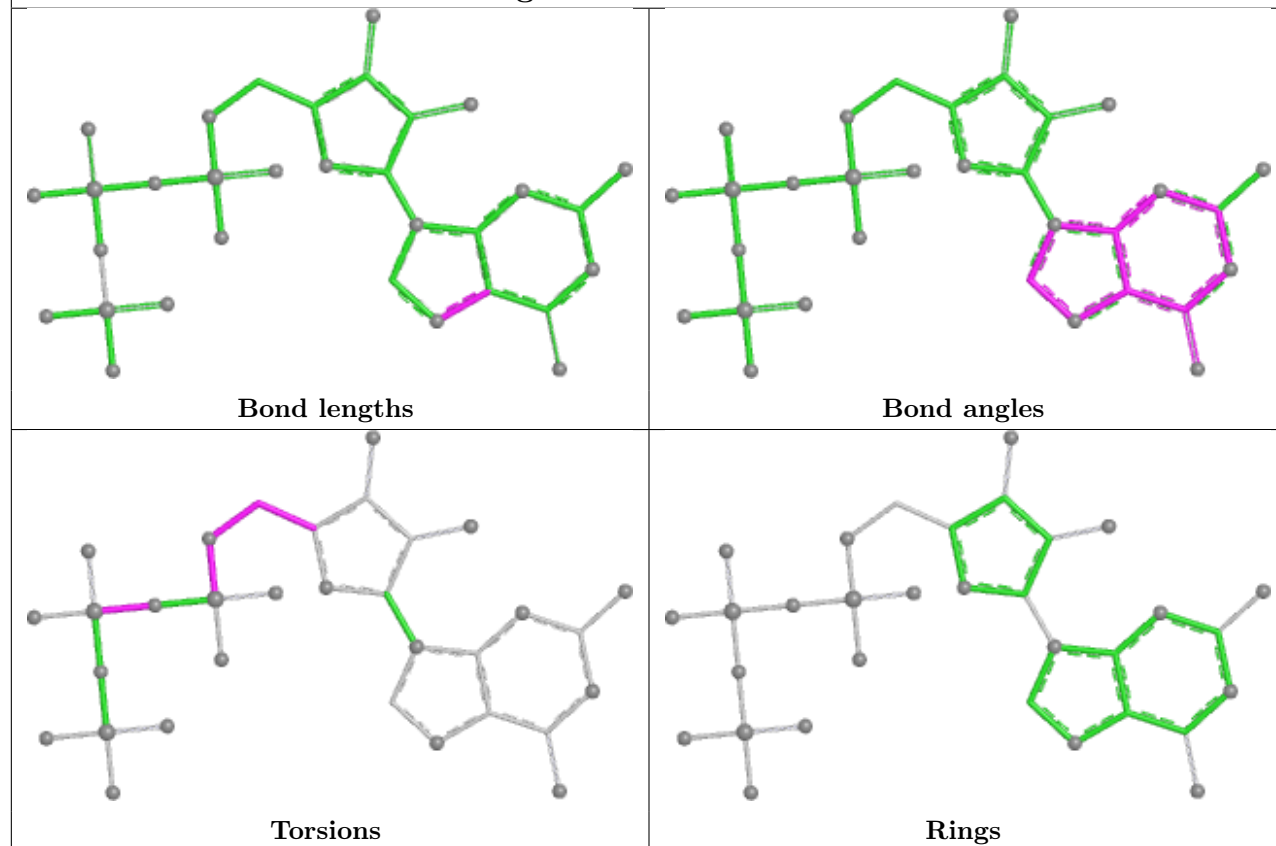


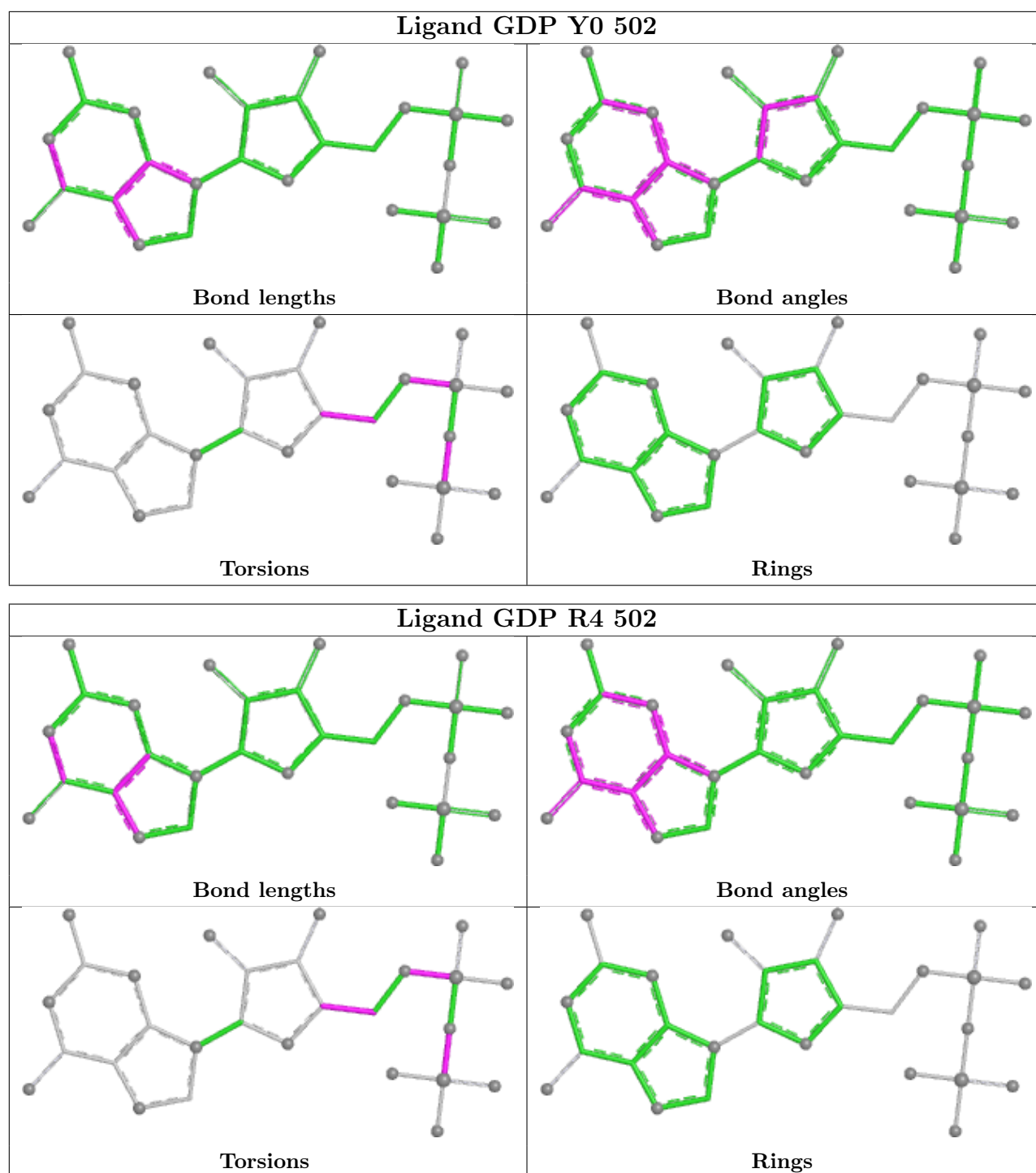


Ligand GTP Q4 501



Ligand GTP W8 501





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-20631. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

5.1 Orthogonal projections

This section was not generated.

5.2 Central slices

This section was not generated.

5.3 Largest variance slices

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

5.5 Orthogonal surface views

This section was not generated.

5.6 Mask visualisation

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

6 Map analysis ⓘ

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

6.1 Map-value distribution ⓘ

This section was not generated.

6.2 Volume estimate versus contour level ⓘ

This section was not generated.

6.3 Rotationally averaged power spectrum ⓘ

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

7 Fourier-Shell correlation

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

8 Map-model fit

This section was not generated.