



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 03:22 AM UTC

PDB ID : 9D5N / pdb_00009d5n
EMDB ID : EMD-46580
Title : 48-nm doublet microtubule from *Trichomonas vaginalis* strain G3
Authors : Stevens, A.; Zhou, H.Z.; Kashyap, S.; Crofut, E.J.
Deposited on : 2024-08-13
Resolution : 4.20 Å (reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

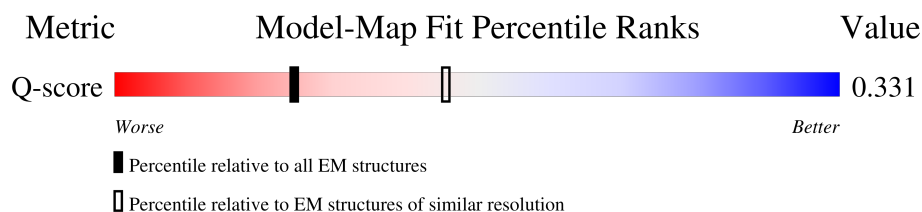
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	5410 (3.70 - 4.70)

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

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 1449349 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 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	F1	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fm	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fn	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fo	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fp	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fq	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fr	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fs	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	A0	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Ft	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fu	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fv	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fw	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fx	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fy	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	Fz	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	GH	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	GU	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	GV	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	GW	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	GX	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	GY	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	GZ	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ga	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Gb	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Gc	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Gd	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ge	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Gf	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Gg	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Gh	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Gi	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Gj	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Gk	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Gm	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	O	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	P	427	Total 3369	C 2127	N 577	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	X	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	A3	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	m	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	n	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	r	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AA	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AB	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AC	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AD	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AE	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AF	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AG	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AH	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AL	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AM	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AN	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AO	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AP	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AQ	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AR	427	Total 3369	C 2127	N 577	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AS	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AT	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AU	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AV	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AW	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AX	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AY	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	AZ	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Aa	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ab	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ac	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ad	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ae	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Af	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ag	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ah	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ai	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Am	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	An	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ao	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ap	427	Total 3369	C 2127	N 577	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aq	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ar	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	As	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	At	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Au	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Av	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Az	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	BA	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	BB	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	BC	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	BD	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	BE	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	BF	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	BG	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	BH	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	BW	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	BZ	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ba	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bb	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Be	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bf	427	Total 3369	C 2127	N 577	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bg	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bh	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bi	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bj	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bk	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bl	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bm	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bn	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bo	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bp	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bq	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Br	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bs	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Bt	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DL	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DM	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DN	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DO	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DP	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DQ	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DR	427	Total 3369	C 2127	N 577	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DS	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DT	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DU	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DV	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DW	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DX	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DY	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	DZ	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Da	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Db	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dc	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dd	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	De	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Df	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dg	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dh	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Di	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dj	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dk	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dq	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dr	427	Total 3369	C 2127	N 577	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ds	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dt	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Du	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dv	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dw	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Dx	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	E0	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	E9	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EL	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EM	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EN	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EO	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EP	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EQ	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	ER	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	ES	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	ET	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EU	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EV	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EW	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EX	427	Total 3369	C 2127	N 577	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	EY	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	EZ	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ea	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Eb	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ec	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ed	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ef	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	7	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	Ev	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	F1	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	F2	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	8	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	F4	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	FA	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	FB	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	FC	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	FD	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	FE	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	FF	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	FG	427	Total 3369	C 2127	N 577	O 644	S 21	0	0
1	FH	427	Total 3369	C 2127	N 577	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FI	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	FJ	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	FK	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	FL	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	FN	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		
1	9	427	Total	C	N	O	S	0	0
			3369	2127	577	644	21		

- Molecule 2 is a protein called FAP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	55	Total	C	N	O	S	0	0
			451	280	83	86	2		

- Molecule 3 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Fi	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	Fj	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	Fk	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	G1	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	G2	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	G3	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	G4	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	G5	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	G6	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	GA	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	GB	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GC	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GD	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GE	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	A1	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GF	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GG	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GI	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GJ	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GK	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GL	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GM	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GN	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GO	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GP	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GQ	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GR	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GS	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	GT	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	A2	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gl	430	Total 3365	C 2140	N 570	O 635	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Gn	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Go	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gp	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gq	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gr	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gs	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gt	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gu	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gv	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gw	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gx	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gy	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Gz	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Q	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	R	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	S	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	T	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	V	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	W	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Y	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Z	430	Total 3365	C 2140	N 570	O 635	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	b	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	c	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	d	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	e	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	f	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	g	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	h	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	i	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	j	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	k	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	l	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	o	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	p	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	A4	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	q	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	s	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	t	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	u	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	v	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	w	430	Total 3365	C 2140	N 570	O 635	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	x	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	y	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	z	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	A5	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	A6	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	A7	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	A8	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	A9	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	AI	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	AJ	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	AK	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	1	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Aj	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ak	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Al	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	2	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Aw	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ax	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ay	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	B0	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	B1	430	Total 3365	C 2140	N 570	O 635	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	B2	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	B3	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	B4	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	B5	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	B6	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	B7	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	B8	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	B9	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BI	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BJ	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BK	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BL	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BM	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BN	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BO	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	3	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BP	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BQ	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BR	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BS	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BT	430	Total 3365	C 2140	N 570	O 635	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	BU	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BV	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BX	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	BY	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Bc	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Bd	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Bu	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	4	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Bv	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Bw	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Bx	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	By	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Bz	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	CA	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	CB	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	5	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	E1	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	E2	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	E3	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	6	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	E4	430	Total 3365	C 2140	N 570	O 635	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	E5	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	E6	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	E7	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	E8	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ee	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Eg	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Eh	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ei	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ej	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ek	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	El	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Em	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	En	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Eo	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ep	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Eq	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Er	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Es	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Et	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Eu	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ew	430	Total 3365	C 2140	N 570	O 635	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ex	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ey	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	Ez	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	F0	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	F3	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	F5	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	F6	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	F7	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	F8	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	F9	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FM	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FO	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FP	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FQ	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FR	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FS	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FT	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FU	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FV	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FW	430	Total 3365	C 2140	N 570	O 635	S 20	0	0
3	FX	430	Total 3365	C 2140	N 570	O 635	S 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	FY	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	FZ	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	Fa	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	Fb	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	Fc	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	Fd	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	Fe	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	Ff	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	Fg	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		
3	Fh	430	Total	C	N	O	S	0	0
			3365	2140	570	635	20		

- Molecule 4 is a protein called IQ calmodulin-binding motif family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	291	Total	C	N	O	S	0	0
			2367	1461	450	451	5		
4	CD	291	Total	C	N	O	S	0	0
			2367	1461	450	451	5		
4	Ca	291	Total	C	N	O	S	0	0
			2367	1461	450	451	5		
4	Cb	291	Total	C	N	O	S	0	0
			2367	1461	450	451	5		

- Molecule 5 is a protein called Flagellar protofilament ribbon protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G0	319	Total	C	N	O	S	0	0
			2691	1629	514	538	10		
5	G7	151	Total	C	N	O	S	0	0
			1252	740	252	256	4		
5	G8	287	Total	C	N	O	S	0	0
			2415	1452	469	486	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	G9	181	Total	C	N	O	S	0	0
			1544	947	292	300	5		

- Molecule 6 is a protein called TvFAP40.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	377	Total	C	N	O	S	0	0
			3065	1888	582	581	14		
6	CE	377	Total	C	N	O	S	0	0
			3065	1888	582	581	14		
6	Cm	377	Total	C	N	O	S	0	0
			3065	1888	582	581	14		
6	Cn	377	Total	C	N	O	S	0	0
			3065	1888	582	581	14		

- Molecule 7 is a protein called Parkin co-regulated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	HA	208	Total	C	N	O	S	0	0
			1704	1093	302	303	6		
7	HB	208	Total	C	N	O	S	0	0
			1704	1093	302	303	6		
7	HC	208	Total	C	N	O	S	0	0
			1704	1093	302	303	6		
7	HD	208	Total	C	N	O	S	0	0
			1704	1093	302	303	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	302	Total	C	N	O	S	0	0
			2520	1522	488	497	13		
8	CJ	136	Total	C	N	O	S	0	0
			1128	696	209	216	7		
8	CK	358	Total	C	N	O	S	0	0
			2981	1807	575	584	15		
8	CL	154	Total	C	N	O	S	0	0
			1289	783	248	255	3		

- Molecule 9 is a protein called Cilia- and flagella-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	184	Total	C	N	O	S	0	0
			1547	1001	265	273	8		
9	C1	184	Total	C	N	O	S	0	0
			1547	1001	265	273	8		
9	CI	184	Total	C	N	O	S	0	0
			1547	1001	265	273	8		
9	Cu	184	Total	C	N	O	S	0	0
			1547	1001	265	273	8		
9	Cv	184	Total	C	N	O	S	0	0
			1547	1001	265	273	8		
9	Cw	184	Total	C	N	O	S	0	0
			1547	1001	265	273	8		
9	Cx	184	Total	C	N	O	S	0	0
			1547	1001	265	273	8		
9	Cy	184	Total	C	N	O	S	0	0
			1547	1001	265	273	8		

- Molecule 10 is a protein called Cilia- and flagella-associated protein 53.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	95	Total	C	N	O	S	0	0
			809	486	164	157	2		
10	CV	226	Total	C	N	O	S	0	0
			1881	1136	360	379	6		
10	CX	221	Total	C	N	O	S	0	0
			1871	1128	373	365	5		

- Molecule 11 is a protein called Trichohyalin-plectin-homology domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	243	Total	C	N	O	S	0	0
			2042	1240	397	399	6		
11	C	181	Total	C	N	O	S	0	0
			1531	928	288	310	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C2	192	Total	C	N	O	S	0	0
			1589	1032	262	290	5		
12	C3	192	Total	C	N	O	S	0	0
			1589	1032	262	290	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	Cz	192	Total	C	N	O	S	0	0
			1589	1032	262	290	5		

- Molecule 13 is a protein called Enkurin.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CC	239	Total	C	N	O	S	0	0
			1971	1249	341	375	6		
13	CY	239	Total	C	N	O	S	0	0
			1971	1249	341	375	6		
13	CZ	239	Total	C	N	O	S	0	0
			1971	1249	341	375	6		
13	F	239	Total	C	N	O	S	0	0
			1971	1249	341	375	6		

- Molecule 14 is a protein called FAP77.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CF	213	Total	C	N	O	S	0	0
			1691	1048	319	317	7		
14	Cc	213	Total	C	N	O	S	0	0
			1691	1048	319	317	7		
14	Cf	213	Total	C	N	O	S	0	0
			1691	1048	319	317	7		
14	Cg	213	Total	C	N	O	S	0	0
			1691	1048	319	317	7		

- Molecule 15 is a protein called EF hand family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CG	193	Total	C	N	O	S	0	0
			1607	1034	264	302	7		
15	Ch	193	Total	C	N	O	S	0	0
			1607	1034	264	302	7		
15	Ci	193	Total	C	N	O	S	0	0
			1607	1034	264	302	7		
15	Cj	193	Total	C	N	O	S	0	0
			1607	1034	264	302	7		
15	Ck	193	Total	C	N	O	S	0	0
			1607	1034	264	302	7		
15	Cl	193	Total	C	N	O	S	0	0
			1607	1034	264	302	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	193	Total	C	N	O	S	0	0
			1607	1034	264	302	7		

- Molecule 16 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CH	605	Total	C	N	O	S	0	0
			4612	2889	812	884	27		
16	Cd	605	Total	C	N	O	S	0	0
			4612	2889	812	884	27		
16	Ce	605	Total	C	N	O	S	0	0
			4612	2889	812	884	27		
16	D	605	Total	C	N	O	S	0	0
			4612	2889	812	884	27		

- Molecule 17 is a protein called Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CM	375	Total	C	N	O	S	0	0
			2975	1899	495	571	10		
17	CO	375	Total	C	N	O	S	0	0
			2975	1899	495	571	10		
17	CP	375	Total	C	N	O	S	0	0
			2975	1899	495	571	10		

- Molecule 18 is a protein called FAP161.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CN	232	Total	C	N	O	S	0	0
			1836	1148	315	358	15		
18	CQ	232	Total	C	N	O	S	0	0
			1836	1148	315	358	15		

- Molecule 19 is a protein called RIIa domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CR	48	Total	C	N	O	S	0	0
			407	257	72	76	2		

- Molecule 20 is a protein called FAP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CS	97	Total	C	N	O	S	0	0
			780	477	153	148	2		

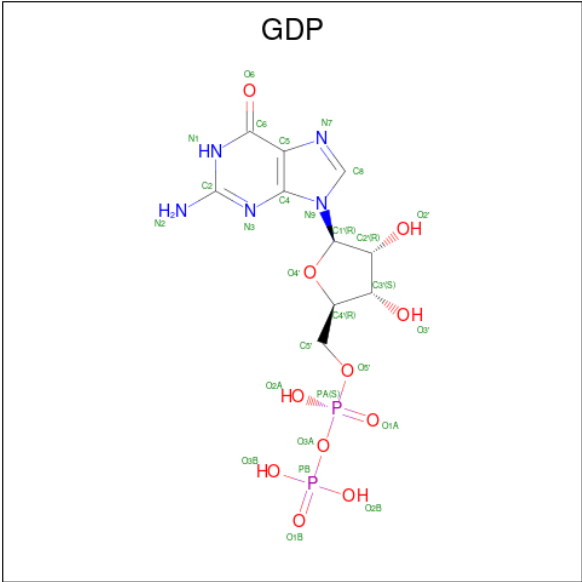
- Molecule 21 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CT	400	Total	C	N	O	S	0	0
			3402	2038	675	672	17		
21	CU	163	Total	C	N	O	S	0	0
			1382	850	263	263	6		

- Molecule 22 is a protein called MGC84469 protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CW	500	Total	C	N	O	S	0	0
			4099	2602	713	772	12		
22	Co	500	Total	C	N	O	S	0	0
			4099	2602	713	772	12		
22	Cp	500	Total	C	N	O	S	0	0
			4099	2602	713	772	12		
22	Cq	500	Total	C	N	O	S	0	0
			4099	2602	713	772	12		
22	Cr	500	Total	C	N	O	S	0	0
			4099	2602	713	772	12		
22	Cs	500	Total	C	N	O	S	0	0
			4099	2602	713	772	12		
22	Ct	500	Total	C	N	O	S	0	0
			4099	2602	713	772	12		

- Molecule 23 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
23	0	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fl	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fm	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fn	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fo	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fp	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fq	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fr	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fs	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	A0	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Ft	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fu	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fv	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Fw	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
23	Fx	1	Total 28	C 10	N 5	O 11	P 2	0
23	Fy	1	Total 28	C 10	N 5	O 11	P 2	0
23	Fz	1	Total 28	C 10	N 5	O 11	P 2	0
23	GH	1	Total 28	C 10	N 5	O 11	P 2	0
23	GU	1	Total 28	C 10	N 5	O 11	P 2	0
23	GV	1	Total 28	C 10	N 5	O 11	P 2	0
23	GW	1	Total 28	C 10	N 5	O 11	P 2	0
23	GX	1	Total 28	C 10	N 5	O 11	P 2	0
23	GY	1	Total 28	C 10	N 5	O 11	P 2	0
23	GZ	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ga	1	Total 28	C 10	N 5	O 11	P 2	0
23	Gb	1	Total 28	C 10	N 5	O 11	P 2	0
23	Gc	1	Total 28	C 10	N 5	O 11	P 2	0
23	Gd	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ge	1	Total 28	C 10	N 5	O 11	P 2	0
23	Gf	1	Total 28	C 10	N 5	O 11	P 2	0
23	Gg	1	Total 28	C 10	N 5	O 11	P 2	0
23	Gh	1	Total 28	C 10	N 5	O 11	P 2	0
23	Gi	1	Total 28	C 10	N 5	O 11	P 2	0
23	Gj	1	Total 28	C 10	N 5	O 11	P 2	0
23	Gk	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
23	Gm	1	Total 28	C 10	N 5	O 11	P 2	0
23	O	1	Total 28	C 10	N 5	O 11	P 2	0
23	P	1	Total 28	C 10	N 5	O 11	P 2	0
23	U	1	Total 28	C 10	N 5	O 11	P 2	0
23	X	1	Total 28	C 10	N 5	O 11	P 2	0
23	A3	1	Total 28	C 10	N 5	O 11	P 2	0
23	m	1	Total 28	C 10	N 5	O 11	P 2	0
23	n	1	Total 28	C 10	N 5	O 11	P 2	0
23	r	1	Total 28	C 10	N 5	O 11	P 2	0
23	AA	1	Total 28	C 10	N 5	O 11	P 2	0
23	AB	1	Total 28	C 10	N 5	O 11	P 2	0
23	AC	1	Total 28	C 10	N 5	O 11	P 2	0
23	AD	1	Total 28	C 10	N 5	O 11	P 2	0
23	AE	1	Total 28	C 10	N 5	O 11	P 2	0
23	AF	1	Total 28	C 10	N 5	O 11	P 2	0
23	AG	1	Total 28	C 10	N 5	O 11	P 2	0
23	AH	1	Total 28	C 10	N 5	O 11	P 2	0
23	AL	1	Total 28	C 10	N 5	O 11	P 2	0
23	AM	1	Total 28	C 10	N 5	O 11	P 2	0
23	AN	1	Total 28	C 10	N 5	O 11	P 2	0
23	AO	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
23	AP	1	Total 28	C 10	N 5	O 11	P 2	0
23	AQ	1	Total 28	C 10	N 5	O 11	P 2	0
23	AR	1	Total 28	C 10	N 5	O 11	P 2	0
23	AS	1	Total 28	C 10	N 5	O 11	P 2	0
23	AT	1	Total 28	C 10	N 5	O 11	P 2	0
23	AU	1	Total 28	C 10	N 5	O 11	P 2	0
23	AV	1	Total 28	C 10	N 5	O 11	P 2	0
23	AW	1	Total 28	C 10	N 5	O 11	P 2	0
23	AX	1	Total 28	C 10	N 5	O 11	P 2	0
23	AY	1	Total 28	C 10	N 5	O 11	P 2	0
23	AZ	1	Total 28	C 10	N 5	O 11	P 2	0
23	Aa	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ab	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ac	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ad	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ae	1	Total 28	C 10	N 5	O 11	P 2	0
23	Af	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ag	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ah	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ai	1	Total 28	C 10	N 5	O 11	P 2	0
23	Am	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
23	An	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ao	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ap	1	Total 28	C 10	N 5	O 11	P 2	0
23	Aq	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ar	1	Total 28	C 10	N 5	O 11	P 2	0
23	As	1	Total 28	C 10	N 5	O 11	P 2	0
23	At	1	Total 28	C 10	N 5	O 11	P 2	0
23	Au	1	Total 28	C 10	N 5	O 11	P 2	0
23	Av	1	Total 28	C 10	N 5	O 11	P 2	0
23	Az	1	Total 28	C 10	N 5	O 11	P 2	0
23	BA	1	Total 28	C 10	N 5	O 11	P 2	0
23	BB	1	Total 28	C 10	N 5	O 11	P 2	0
23	BC	1	Total 28	C 10	N 5	O 11	P 2	0
23	BD	1	Total 28	C 10	N 5	O 11	P 2	0
23	BE	1	Total 28	C 10	N 5	O 11	P 2	0
23	BF	1	Total 28	C 10	N 5	O 11	P 2	0
23	BG	1	Total 28	C 10	N 5	O 11	P 2	0
23	BH	1	Total 28	C 10	N 5	O 11	P 2	0
23	BW	1	Total 28	C 10	N 5	O 11	P 2	0
23	BZ	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ba	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
23	Bb	1	Total 28	C 10	N 5	O 11	P 2	0
23	Be	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bf	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bg	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bh	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bi	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bj	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bk	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bl	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bm	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bn	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bo	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bp	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bq	1	Total 28	C 10	N 5	O 11	P 2	0
23	Br	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bs	1	Total 28	C 10	N 5	O 11	P 2	0
23	Bt	1	Total 28	C 10	N 5	O 11	P 2	0
23	DL	1	Total 28	C 10	N 5	O 11	P 2	0
23	DM	1	Total 28	C 10	N 5	O 11	P 2	0
23	DN	1	Total 28	C 10	N 5	O 11	P 2	0
23	DO	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
23	DP	1	Total 28	C 10	N 5	O 11	P 2	0
23	DQ	1	Total 28	C 10	N 5	O 11	P 2	0
23	DR	1	Total 28	C 10	N 5	O 11	P 2	0
23	DS	1	Total 28	C 10	N 5	O 11	P 2	0
23	DT	1	Total 28	C 10	N 5	O 11	P 2	0
23	DU	1	Total 28	C 10	N 5	O 11	P 2	0
23	DV	1	Total 28	C 10	N 5	O 11	P 2	0
23	DW	1	Total 28	C 10	N 5	O 11	P 2	0
23	DX	1	Total 28	C 10	N 5	O 11	P 2	0
23	DY	1	Total 28	C 10	N 5	O 11	P 2	0
23	DZ	1	Total 28	C 10	N 5	O 11	P 2	0
23	Da	1	Total 28	C 10	N 5	O 11	P 2	0
23	Db	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dc	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dd	1	Total 28	C 10	N 5	O 11	P 2	0
23	De	1	Total 28	C 10	N 5	O 11	P 2	0
23	Df	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dg	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dh	1	Total 28	C 10	N 5	O 11	P 2	0
23	Di	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dj	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
23	Dk	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dq	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dr	1	Total 28	C 10	N 5	O 11	P 2	0
23	Ds	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dt	1	Total 28	C 10	N 5	O 11	P 2	0
23	Du	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dv	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dw	1	Total 28	C 10	N 5	O 11	P 2	0
23	Dx	1	Total 28	C 10	N 5	O 11	P 2	0
23	E0	1	Total 28	C 10	N 5	O 11	P 2	0
23	E9	1	Total 28	C 10	N 5	O 11	P 2	0
23	EL	1	Total 28	C 10	N 5	O 11	P 2	0
23	EM	1	Total 28	C 10	N 5	O 11	P 2	0
23	EN	1	Total 28	C 10	N 5	O 11	P 2	0
23	EO	1	Total 28	C 10	N 5	O 11	P 2	0
23	EP	1	Total 28	C 10	N 5	O 11	P 2	0
23	EQ	1	Total 28	C 10	N 5	O 11	P 2	0
23	ER	1	Total 28	C 10	N 5	O 11	P 2	0
23	ES	1	Total 28	C 10	N 5	O 11	P 2	0
23	ET	1	Total 28	C 10	N 5	O 11	P 2	0
23	EU	1	Total 28	C 10	N 5	O 11	P 2	0

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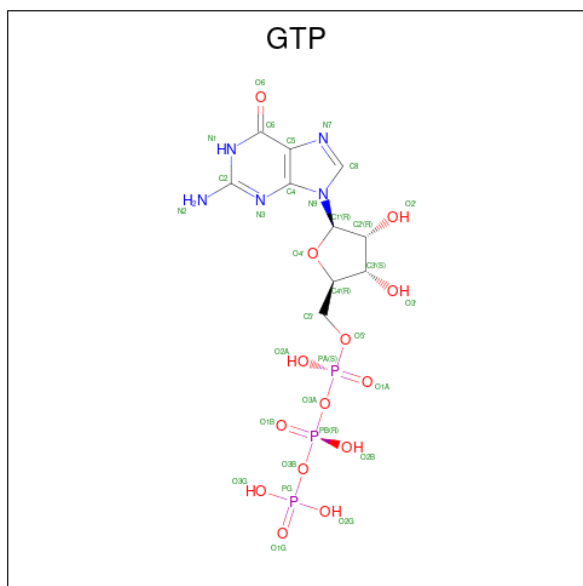
Mol	Chain	Residues	Atoms					AltConf
23	EV	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	EW	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	EX	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	EY	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	EZ	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Ea	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Eb	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Ec	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Ed	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Ef	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	7	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	Ev	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	F1	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	F2	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	8	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	F4	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FA	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FB	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FC	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FD	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FE	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
23	FF	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FG	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FH	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FI	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FJ	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FK	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FL	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	FN	1	Total	C	N	O	P	0
			28	10	5	11	2	
23	9	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 24 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
24	Fi	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Fj	1	Total	C	N	O	P	0
			32	10	5	14	3	

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Mol	Chain	Residues	Atoms					AltConf
24	Fk	1	Total 32	C 10	N 5	O 14	P 3	0
24	G1	1	Total 32	C 10	N 5	O 14	P 3	0
24	G2	1	Total 32	C 10	N 5	O 14	P 3	0
24	G3	1	Total 32	C 10	N 5	O 14	P 3	0
24	G4	1	Total 32	C 10	N 5	O 14	P 3	0
24	G5	1	Total 32	C 10	N 5	O 14	P 3	0
24	G6	1	Total 32	C 10	N 5	O 14	P 3	0
24	GA	1	Total 32	C 10	N 5	O 14	P 3	0
24	GB	1	Total 32	C 10	N 5	O 14	P 3	0
24	GC	1	Total 32	C 10	N 5	O 14	P 3	0
24	GD	1	Total 32	C 10	N 5	O 14	P 3	0
24	GE	1	Total 32	C 10	N 5	O 14	P 3	0
24	A1	1	Total 32	C 10	N 5	O 14	P 3	0
24	GF	1	Total 32	C 10	N 5	O 14	P 3	0
24	GG	1	Total 32	C 10	N 5	O 14	P 3	0
24	GI	1	Total 32	C 10	N 5	O 14	P 3	0
24	GJ	1	Total 32	C 10	N 5	O 14	P 3	0
24	GK	1	Total 32	C 10	N 5	O 14	P 3	0
24	GL	1	Total 32	C 10	N 5	O 14	P 3	0
24	GM	1	Total 32	C 10	N 5	O 14	P 3	0
24	GN	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
24	GO	1	Total 32	C 10	N 5	O 14	P 3	0
24	GP	1	Total 32	C 10	N 5	O 14	P 3	0
24	GQ	1	Total 32	C 10	N 5	O 14	P 3	0
24	GR	1	Total 32	C 10	N 5	O 14	P 3	0
24	GS	1	Total 32	C 10	N 5	O 14	P 3	0
24	GT	1	Total 32	C 10	N 5	O 14	P 3	0
24	A2	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gl	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gn	1	Total 32	C 10	N 5	O 14	P 3	0
24	Go	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gp	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gq	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gr	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gs	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gt	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gu	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gv	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gw	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gx	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gy	1	Total 32	C 10	N 5	O 14	P 3	0
24	Gz	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
24	Q	1	Total 32	C 10	N 5	O 14	P 3	0
24	S	1	Total 32	C 10	N 5	O 14	P 3	0
24	T	1	Total 32	C 10	N 5	O 14	P 3	0
24	V	1	Total 32	C 10	N 5	O 14	P 3	0
24	W	1	Total 32	C 10	N 5	O 14	P 3	0
24	Y	1	Total 32	C 10	N 5	O 14	P 3	0
24	Z	1	Total 32	C 10	N 5	O 14	P 3	0
24	a	1	Total 32	C 10	N 5	O 14	P 3	0
24	b	1	Total 32	C 10	N 5	O 14	P 3	0
24	c	1	Total 32	C 10	N 5	O 14	P 3	0
24	d	1	Total 32	C 10	N 5	O 14	P 3	0
24	e	1	Total 32	C 10	N 5	O 14	P 3	0
24	f	1	Total 32	C 10	N 5	O 14	P 3	0
24	g	1	Total 32	C 10	N 5	O 14	P 3	0
24	h	1	Total 32	C 10	N 5	O 14	P 3	0
24	i	1	Total 32	C 10	N 5	O 14	P 3	0
24	j	1	Total 32	C 10	N 5	O 14	P 3	0
24	k	1	Total 32	C 10	N 5	O 14	P 3	0
24	l	1	Total 32	C 10	N 5	O 14	P 3	0
24	o	1	Total 32	C 10	N 5	O 14	P 3	0
24	p	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
24	A4	1	Total 32	C 10	N 5	O 14	P 3	0
24	q	1	Total 32	C 10	N 5	O 14	P 3	0
24	s	1	Total 32	C 10	N 5	O 14	P 3	0
24	t	1	Total 32	C 10	N 5	O 14	P 3	0
24	u	1	Total 32	C 10	N 5	O 14	P 3	0
24	v	1	Total 32	C 10	N 5	O 14	P 3	0
24	w	1	Total 32	C 10	N 5	O 14	P 3	0
24	x	1	Total 32	C 10	N 5	O 14	P 3	0
24	y	1	Total 32	C 10	N 5	O 14	P 3	0
24	z	1	Total 32	C 10	N 5	O 14	P 3	0
24	A5	1	Total 32	C 10	N 5	O 14	P 3	0
24	A6	1	Total 32	C 10	N 5	O 14	P 3	0
24	A7	1	Total 32	C 10	N 5	O 14	P 3	0
24	A8	1	Total 32	C 10	N 5	O 14	P 3	0
24	A9	1	Total 32	C 10	N 5	O 14	P 3	0
24	AI	1	Total 32	C 10	N 5	O 14	P 3	0
24	AJ	1	Total 32	C 10	N 5	O 14	P 3	0
24	AK	1	Total 32	C 10	N 5	O 14	P 3	0
24	1	1	Total 32	C 10	N 5	O 14	P 3	0
24	AS	1	Total 32	C 10	N 5	O 14	P 3	0
24	Aj	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
24	Ak	1	Total 32	C 10	N 5	O 14	P 3	0
24	Al	1	Total 32	C 10	N 5	O 14	P 3	0
24	2	1	Total 32	C 10	N 5	O 14	P 3	0
24	Aw	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ax	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ay	1	Total 32	C 10	N 5	O 14	P 3	0
24	B0	1	Total 32	C 10	N 5	O 14	P 3	0
24	B1	1	Total 32	C 10	N 5	O 14	P 3	0
24	B2	1	Total 32	C 10	N 5	O 14	P 3	0
24	B3	1	Total 32	C 10	N 5	O 14	P 3	0
24	B4	1	Total 32	C 10	N 5	O 14	P 3	0
24	B5	1	Total 32	C 10	N 5	O 14	P 3	0
24	B6	1	Total 32	C 10	N 5	O 14	P 3	0
24	B7	1	Total 32	C 10	N 5	O 14	P 3	0
24	B8	1	Total 32	C 10	N 5	O 14	P 3	0
24	B9	1	Total 32	C 10	N 5	O 14	P 3	0
24	BI	1	Total 32	C 10	N 5	O 14	P 3	0
24	BJ	1	Total 32	C 10	N 5	O 14	P 3	0
24	BK	1	Total 32	C 10	N 5	O 14	P 3	0
24	BL	1	Total 32	C 10	N 5	O 14	P 3	0
24	BM	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
24	BN	1	Total 32	C 10	N 5	O 14	P 3	0
24	BO	1	Total 32	C 10	N 5	O 14	P 3	0
24	3	1	Total 32	C 10	N 5	O 14	P 3	0
24	BP	1	Total 32	C 10	N 5	O 14	P 3	0
24	BQ	1	Total 32	C 10	N 5	O 14	P 3	0
24	BR	1	Total 32	C 10	N 5	O 14	P 3	0
24	BS	1	Total 32	C 10	N 5	O 14	P 3	0
24	BT	1	Total 32	C 10	N 5	O 14	P 3	0
24	BU	1	Total 32	C 10	N 5	O 14	P 3	0
24	BV	1	Total 32	C 10	N 5	O 14	P 3	0
24	BX	1	Total 32	C 10	N 5	O 14	P 3	0
24	BY	1	Total 32	C 10	N 5	O 14	P 3	0
24	Bc	1	Total 32	C 10	N 5	O 14	P 3	0
24	Bd	1	Total 32	C 10	N 5	O 14	P 3	0
24	Bu	1	Total 32	C 10	N 5	O 14	P 3	0
24	4	1	Total 32	C 10	N 5	O 14	P 3	0
24	Bv	1	Total 32	C 10	N 5	O 14	P 3	0
24	Bw	1	Total 32	C 10	N 5	O 14	P 3	0
24	Bx	1	Total 32	C 10	N 5	O 14	P 3	0
24	By	1	Total 32	C 10	N 5	O 14	P 3	0
24	Bz	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
24	CA	1	Total 32	C 10	N 5	O 14	P 3	0
24	CB	1	Total 32	C 10	N 5	O 14	P 3	0
24	5	1	Total 32	C 10	N 5	O 14	P 3	0
24	E1	1	Total 32	C 10	N 5	O 14	P 3	0
24	E2	1	Total 32	C 10	N 5	O 14	P 3	0
24	E3	1	Total 32	C 10	N 5	O 14	P 3	0
24	6	1	Total 32	C 10	N 5	O 14	P 3	0
24	E4	1	Total 32	C 10	N 5	O 14	P 3	0
24	E5	1	Total 32	C 10	N 5	O 14	P 3	0
24	E6	1	Total 32	C 10	N 5	O 14	P 3	0
24	E7	1	Total 32	C 10	N 5	O 14	P 3	0
24	E8	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ee	1	Total 32	C 10	N 5	O 14	P 3	0
24	Eg	1	Total 32	C 10	N 5	O 14	P 3	0
24	Eh	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ei	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ej	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ek	1	Total 32	C 10	N 5	O 14	P 3	0
24	El	1	Total 32	C 10	N 5	O 14	P 3	0
24	Em	1	Total 32	C 10	N 5	O 14	P 3	0
24	En	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
24	Eo	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ep	1	Total 32	C 10	N 5	O 14	P 3	0
24	Eq	1	Total 32	C 10	N 5	O 14	P 3	0
24	Er	1	Total 32	C 10	N 5	O 14	P 3	0
24	Es	1	Total 32	C 10	N 5	O 14	P 3	0
24	Et	1	Total 32	C 10	N 5	O 14	P 3	0
24	Eu	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ew	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ex	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ey	1	Total 32	C 10	N 5	O 14	P 3	0
24	Ez	1	Total 32	C 10	N 5	O 14	P 3	0
24	F0	1	Total 32	C 10	N 5	O 14	P 3	0
24	F3	1	Total 32	C 10	N 5	O 14	P 3	0
24	F5	1	Total 32	C 10	N 5	O 14	P 3	0
24	F6	1	Total 32	C 10	N 5	O 14	P 3	0
24	F7	1	Total 32	C 10	N 5	O 14	P 3	0
24	F8	1	Total 32	C 10	N 5	O 14	P 3	0
24	F9	1	Total 32	C 10	N 5	O 14	P 3	0
24	FM	1	Total 32	C 10	N 5	O 14	P 3	0
24	FO	1	Total 32	C 10	N 5	O 14	P 3	0
24	FP	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
24	FQ	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FR	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FS	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FT	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FU	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FV	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FW	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FX	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FY	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	FZ	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Fa	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Fb	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Fc	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Fd	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Fe	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Ff	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Fg	1	Total	C	N	O	P	0
			32	10	5	14	3	
24	Fh	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	Fi	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
25	Fj	1	Total 1	Mg 1	0
25	Fk	1	Total 1	Mg 1	0
25	G1	1	Total 1	Mg 1	0
25	G2	1	Total 1	Mg 1	0
25	G3	1	Total 1	Mg 1	0
25	G4	1	Total 1	Mg 1	0
25	G5	1	Total 1	Mg 1	0
25	G6	1	Total 1	Mg 1	0
25	GA	1	Total 1	Mg 1	0
25	GB	1	Total 1	Mg 1	0
25	GC	1	Total 1	Mg 1	0
25	GD	1	Total 1	Mg 1	0
25	GE	1	Total 1	Mg 1	0
25	A1	1	Total 1	Mg 1	0
25	GF	1	Total 1	Mg 1	0
25	GG	1	Total 1	Mg 1	0
25	GI	1	Total 1	Mg 1	0
25	GJ	1	Total 1	Mg 1	0
25	GK	1	Total 1	Mg 1	0
25	GL	1	Total 1	Mg 1	0
25	GM	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
25	GN	1	Total 1	Mg 1	0
25	GO	1	Total 1	Mg 1	0
25	GP	1	Total 1	Mg 1	0
25	GQ	1	Total 1	Mg 1	0
25	GR	1	Total 1	Mg 1	0
25	GS	1	Total 1	Mg 1	0
25	GT	1	Total 1	Mg 1	0
25	A2	1	Total 1	Mg 1	0
25	Gl	1	Total 1	Mg 1	0
25	Gn	1	Total 1	Mg 1	0
25	Go	1	Total 1	Mg 1	0
25	Gp	1	Total 1	Mg 1	0
25	Gq	1	Total 1	Mg 1	0
25	Gr	1	Total 1	Mg 1	0
25	Gs	1	Total 1	Mg 1	0
25	Gt	1	Total 1	Mg 1	0
25	Gu	1	Total 1	Mg 1	0
25	Gv	1	Total 1	Mg 1	0
25	Gw	1	Total 1	Mg 1	0
25	Gx	1	Total 1	Mg 1	0
25	Gy	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
25	Gz	1	Total 1	Mg 1	0
25	Q	1	Total 1	Mg 1	0
25	R	1	Total 1	Mg 1	0
25	S	1	Total 1	Mg 1	0
25	T	1	Total 1	Mg 1	0
25	V	1	Total 1	Mg 1	0
25	W	1	Total 1	Mg 1	0
25	Y	1	Total 1	Mg 1	0
25	Z	1	Total 1	Mg 1	0
25	a	1	Total 1	Mg 1	0
25	b	1	Total 1	Mg 1	0
25	c	1	Total 1	Mg 1	0
25	d	1	Total 1	Mg 1	0
25	e	1	Total 1	Mg 1	0
25	f	1	Total 1	Mg 1	0
25	g	1	Total 1	Mg 1	0
25	h	1	Total 1	Mg 1	0
25	i	1	Total 1	Mg 1	0
25	j	1	Total 1	Mg 1	0
25	k	1	Total 1	Mg 1	0
25	l	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
25	o	1	Total 1	Mg 1	0
25	p	1	Total 1	Mg 1	0
25	A4	1	Total 1	Mg 1	0
25	q	1	Total 1	Mg 1	0
25	s	1	Total 1	Mg 1	0
25	t	1	Total 1	Mg 1	0
25	v	1	Total 1	Mg 1	0
25	w	1	Total 1	Mg 1	0
25	y	1	Total 1	Mg 1	0
25	z	1	Total 1	Mg 1	0
25	A5	1	Total 1	Mg 1	0
25	A6	1	Total 1	Mg 1	0
25	A7	1	Total 1	Mg 1	0
25	A8	1	Total 1	Mg 1	0
25	A9	1	Total 1	Mg 1	0
25	AJ	1	Total 1	Mg 1	0
25	AK	1	Total 1	Mg 1	0
25	1	1	Total 1	Mg 1	0
25	AQ	1	Total 1	Mg 1	0
25	AV	1	Total 1	Mg 1	0
25	Ac	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
25	Ah	1	Total 1	Mg 1	0
25	Ak	1	Total 1	Mg 1	0
25	Al	1	Total 1	Mg 1	0
25	Au	1	Total 1	Mg 1	0
25	2	1	Total 1	Mg 1	0
25	Aw	1	Total 1	Mg 1	0
25	Ax	1	Total 1	Mg 1	0
25	Ay	1	Total 1	Mg 1	0
25	B1	1	Total 1	Mg 1	0
25	B2	1	Total 1	Mg 1	0
25	B3	1	Total 1	Mg 1	0
25	B4	1	Total 1	Mg 1	0
25	B5	1	Total 1	Mg 1	0
25	B6	1	Total 1	Mg 1	0
25	B8	1	Total 1	Mg 1	0
25	B9	1	Total 1	Mg 1	0
25	BG	1	Total 1	Mg 1	0
25	BI	1	Total 1	Mg 1	0
25	BJ	1	Total 1	Mg 1	0
25	BK	1	Total 1	Mg 1	0
25	BL	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
25	BM	1	Total 1	Mg 1	0
25	BN	1	Total 1	Mg 1	0
25	BO	1	Total 1	Mg 1	0
25	3	1	Total 1	Mg 1	0
25	BP	1	Total 1	Mg 1	0
25	BQ	1	Total 1	Mg 1	0
25	BS	1	Total 1	Mg 1	0
25	BU	1	Total 1	Mg 1	0
25	BV	1	Total 1	Mg 1	0
25	BX	1	Total 1	Mg 1	0
25	BY	1	Total 1	Mg 1	0
25	Bc	1	Total 1	Mg 1	0
25	Bd	1	Total 1	Mg 1	0
25	Bl	1	Total 1	Mg 1	0
25	Bq	1	Total 1	Mg 1	0
25	Bu	1	Total 1	Mg 1	0
25	4	1	Total 1	Mg 1	0
25	Bv	1	Total 1	Mg 1	0
25	Bw	1	Total 1	Mg 1	0
25	Bx	1	Total 1	Mg 1	0
25	By	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
25	Bz	1	Total 1	Mg 1	0
25	CA	1	Total 1	Mg 1	0
25	CB	1	Total 1	Mg 1	0
25	5	1	Total 1	Mg 1	0
25	E1	1	Total 1	Mg 1	0
25	E2	1	Total 1	Mg 1	0
25	E3	1	Total 1	Mg 1	0
25	6	1	Total 1	Mg 1	0
25	E4	1	Total 1	Mg 1	0
25	E5	1	Total 1	Mg 1	0
25	E6	1	Total 1	Mg 1	0
25	E7	1	Total 1	Mg 1	0
25	E8	1	Total 1	Mg 1	0
25	Ee	1	Total 1	Mg 1	0
25	Eg	1	Total 1	Mg 1	0
25	Eh	1	Total 1	Mg 1	0
25	Ei	1	Total 1	Mg 1	0
25	Ej	1	Total 1	Mg 1	0
25	Ek	1	Total 1	Mg 1	0
25	El	1	Total 1	Mg 1	0
25	Em	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
25	En	1	Total 1	Mg 1	0
25	Eo	1	Total 1	Mg 1	0
25	Ep	1	Total 1	Mg 1	0
25	Eq	1	Total 1	Mg 1	0
25	Er	1	Total 1	Mg 1	0
25	Es	1	Total 1	Mg 1	0
25	Et	1	Total 1	Mg 1	0
25	Eu	1	Total 1	Mg 1	0
25	Ew	1	Total 1	Mg 1	0
25	Ex	1	Total 1	Mg 1	0
25	Ey	1	Total 1	Mg 1	0
25	Ez	1	Total 1	Mg 1	0
25	F0	1	Total 1	Mg 1	0
25	F3	1	Total 1	Mg 1	0
25	F5	1	Total 1	Mg 1	0
25	F6	1	Total 1	Mg 1	0
25	F7	1	Total 1	Mg 1	0
25	F8	1	Total 1	Mg 1	0
25	F9	1	Total 1	Mg 1	0
25	FM	1	Total 1	Mg 1	0
25	FO	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
25	FP	1	Total 1	Mg 1	0
25	FQ	1	Total 1	Mg 1	0
25	FR	1	Total 1	Mg 1	0
25	FS	1	Total 1	Mg 1	0
25	FT	1	Total 1	Mg 1	0
25	FU	1	Total 1	Mg 1	0
25	FV	1	Total 1	Mg 1	0
25	FW	1	Total 1	Mg 1	0
25	FX	1	Total 1	Mg 1	0
25	FY	1	Total 1	Mg 1	0
25	FZ	1	Total 1	Mg 1	0
25	Fa	1	Total 1	Mg 1	0
25	Fb	1	Total 1	Mg 1	0
25	Fc	1	Total 1	Mg 1	0
25	Fd	1	Total 1	Mg 1	0
25	Fe	1	Total 1	Mg 1	0
25	Ff	1	Total 1	Mg 1	0
25	Fg	1	Total 1	Mg 1	0
25	Fh	1	Total 1	Mg 1	0

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

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	409692	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.899	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.128	Depositor
Map size (Å)	717.2, 731.5, 1054.9	wwPDB
Map dimensions	652, 665, 959	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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 567 ligands modelled in this entry, 188 are monoatomic - leaving 379 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
23	GDP	EL	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
24	GTP	Eh	501	25	33,34,34	1.01	2 (6%)	50,54,54	1.58	9 (18%)
23	GDP	Av	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
23	GDP	A0	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
24	GTP	Eq	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.59	9 (18%)
23	GDP	O	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
23	GDP	AB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
24	GTP	GK	501	25	33,34,34	1.04	3 (9%)	50,54,54	1.58	9 (18%)
24	GTP	BL	602	25	33,34,34	1.01	3 (9%)	50,54,54	1.57	9 (18%)
23	GDP	9	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	5 (11%)
23	GDP	AY	501	-	29,30,30	1.18	4 (13%)	45,47,47	1.77	7 (15%)
23	GDP	Fp	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.76	6 (13%)
23	GDP	AZ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	Ex	501	25	33,34,34	1.08	3 (9%)	50,54,54	1.58	8 (16%)
23	GDP	Db	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
23	GDP	Dr	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	5 (11%)
24	GTP	B0	501	25	33,34,34	1.00	3 (9%)	50,54,54	1.59	8 (16%)
23	GDP	GV	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
24	GTP	GQ	602	25	33,34,34	1.04	3 (9%)	50,54,54	1.65	9 (18%)
24	GTP	q	602	25	33,34,34	0.99	3 (9%)	50,54,54	1.60	9 (18%)
23	GDP	BE	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
24	GTP	Gn	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.56	8 (16%)
24	GTP	BI	602	25	33,34,34	0.96	1 (3%)	50,54,54	1.58	8 (16%)
23	GDP	GX	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	5 (11%)
23	GDP	X	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
23	GDP	Dt	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	5 (11%)
24	GTP	u	501	25	33,34,34	1.00	3 (9%)	50,54,54	1.58	8 (16%)
23	GDP	Ac	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	5 (11%)
24	GTP	BK	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.58	8 (16%)
23	GDP	Dd	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.73	7 (15%)
23	GDP	Gj	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	8 (17%)
23	GDP	Fy	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	GDP	Fo	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
23	GDP	E9	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
23	GDP	AE	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
23	GDP	Ft	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.74	6 (13%)
23	GDP	De	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.75	7 (15%)
24	GTP	A1	602	25	33,34,34	0.93	1 (3%)	50,54,54	1.57	9 (18%)
24	GTP	Fa	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.56	8 (16%)
23	GDP	Af	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	7 (15%)
23	GDP	F4	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
24	GTP	1	602	25	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
24	GTP	Ep	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.56	9 (18%)
24	GTP	Gt	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.55	9 (18%)
23	GDP	EM	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
23	GDP	AL	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
23	GDP	FL	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	7 (15%)
24	GTP	GR	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.61	8 (16%)
24	GTP	5	602	25	33,34,34	0.98	2 (6%)	50,54,54	1.59	9 (18%)
23	GDP	F1	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
23	GDP	Ef	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
24	GTP	GT	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.54	8 (16%)
24	GTP	Bd	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.55	9 (18%)
23	GDP	AO	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
23	GDP	FC	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
23	GDP	E0	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.76	6 (13%)
24	GTP	v	602	25	33,34,34	0.98	3 (9%)	50,54,54	1.57	9 (18%)
23	GDP	Dx	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	5 (11%)
24	GTP	Fc	501	25	33,34,34	1.01	2 (6%)	50,54,54	1.60	8 (16%)
23	GDP	Be	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
24	GTP	GG	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.57	9 (18%)
23	GDP	Fu	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	5 (11%)
24	GTP	BR	501	25	33,34,34	1.00	4 (12%)	50,54,54	1.59	8 (16%)
23	GDP	8	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
23	GDP	Dv	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	Gl	501	25	33,34,34	0.97	2 (6%)	50,54,54	1.56	9 (18%)
23	GDP	Fr	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	GTP	F5	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.59	9 (18%)
23	GDP	Fs	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	7 (15%)
23	GDP	DX	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
24	GTP	FT	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.57	9 (18%)
24	GTP	s	602	25	33,34,34	1.00	2 (6%)	50,54,54	1.60	9 (18%)
24	GTP	En	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.58	9 (18%)
24	GTP	A2	602	25	33,34,34	0.93	1 (3%)	50,54,54	1.55	8 (16%)
23	GDP	AQ	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
24	GTP	Bw	602	25	33,34,34	0.98	3 (9%)	50,54,54	1.57	8 (16%)
23	GDP	Ba	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
23	GDP	Bg	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
23	GDP	ET	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
23	GDP	AR	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.73	5 (11%)
24	GTP	B6	602	25	33,34,34	0.99	2 (6%)	50,54,54	1.59	9 (18%)
23	GDP	Fz	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
23	GDP	Gk	501	-	29,30,30	1.25	4 (13%)	45,47,47	1.77	7 (15%)
24	GTP	Es	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	DQ	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.75	7 (15%)
24	GTP	GL	501	25	33,34,34	1.03	3 (9%)	50,54,54	1.59	9 (18%)
24	GTP	t	602	25	33,34,34	0.99	2 (6%)	50,54,54	1.61	9 (18%)
24	GTP	Aw	602	25	33,34,34	0.99	2 (6%)	50,54,54	1.57	9 (18%)
23	GDP	FH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)
23	GDP	Bt	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.74	7 (15%)
24	GTP	j	602	25	33,34,34	1.01	3 (9%)	50,54,54	1.58	8 (16%)
23	GDP	Fl	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
23	GDP	AF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.70	5 (11%)
24	GTP	Fk	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.57	8 (16%)
24	GTP	FW	501	25	33,34,34	0.98	2 (6%)	50,54,54	1.55	8 (16%)
24	GTP	G5	501	25	33,34,34	0.97	3 (9%)	50,54,54	1.63	8 (16%)
24	GTP	CA	602	25	33,34,34	0.98	2 (6%)	50,54,54	1.58	8 (16%)
24	GTP	B2	602	25	33,34,34	1.01	3 (9%)	50,54,54	1.58	8 (16%)
24	GTP	AS	501	25	33,34,34	1.01	2 (6%)	50,54,54	1.61	9 (18%)
23	GDP	Ed	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	7 (15%)
24	GTP	A8	501	25	33,34,34	1.01	2 (6%)	50,54,54	1.57	9 (18%)
23	GDP	Gh	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	GDP	FF	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	5 (11%)
23	GDP	FI	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	5 (11%)
24	GTP	w	602	25	33,34,34	0.97	2 (6%)	50,54,54	1.57	9 (18%)
24	GTP	Ee	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.56	9 (18%)
24	GTP	Gu	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	Bk	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	5 (11%)
24	GTP	Fg	501	25	33,34,34	0.98	2 (6%)	50,54,54	1.57	8 (16%)
23	GDP	AU	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)
24	GTP	GO	602	25	33,34,34	1.00	2 (6%)	50,54,54	1.59	9 (18%)
24	GTP	A9	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	Dj	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
24	GTP	BM	602	25	33,34,34	1.03	3 (9%)	50,54,54	1.59	8 (16%)
24	GTP	h	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.57	9 (18%)
24	GTP	Fi	501	25	33,34,34	1.06	3 (9%)	50,54,54	1.59	8 (16%)
23	GDP	r	501	-	29,30,30	1.28	3 (10%)	45,47,47	1.79	7 (15%)
23	GDP	FD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
23	GDP	EV	501	-	29,30,30	1.27	3 (10%)	45,47,47	1.82	7 (15%)
23	GDP	Bm	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.74	5 (11%)
24	GTP	GE	501	25	33,34,34	1.06	3 (9%)	50,54,54	1.59	8 (16%)
24	GTP	Ez	501	25	33,34,34	1.02	4 (12%)	50,54,54	1.57	8 (16%)
24	GTP	BV	602	25	33,34,34	1.01	2 (6%)	50,54,54	1.58	9 (18%)
23	GDP	Ga	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.77	6 (13%)
23	GDP	DW	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	6 (13%)
24	GTP	FR	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.56	9 (18%)
23	GDP	n	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	By	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.60	9 (18%)
23	GDP	AG	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
24	GTP	FY	501	25	33,34,34	0.98	2 (6%)	50,54,54	1.59	9 (18%)
24	GTP	FM	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.58	9 (18%)
24	GTP	FZ	501	25	33,34,34	0.99	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	GU	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
24	GTP	GS	501	25	33,34,34	0.96	1 (3%)	50,54,54	1.60	8 (16%)
24	GTP	GC	501	25	33,34,34	1.00	3 (9%)	50,54,54	1.59	8 (16%)
24	GTP	AK	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	Bj	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.71	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	GDP	DO	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
23	GDP	Ge	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	6 (13%)
24	GTP	Bu	602	25	33,34,34	0.96	2 (6%)	50,54,54	1.56	8 (16%)
23	GDP	FB	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.73	6 (13%)
23	GDP	Bq	602	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
24	GTP	Aj	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.57	8 (16%)
24	GTP	G2	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.60	8 (16%)
24	GTP	k	602	25	33,34,34	0.99	2 (6%)	50,54,54	1.57	9 (18%)
24	GTP	E1	501	25	33,34,34	1.06	4 (12%)	50,54,54	1.66	9 (18%)
23	GDP	Ae	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	8 (17%)
24	GTP	Ay	602	25	33,34,34	0.98	3 (9%)	50,54,54	1.57	9 (18%)
23	GDP	EW	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)
23	GDP	Dw	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)
23	GDP	DM	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	6 (13%)
23	GDP	DL	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	d	602	25	33,34,34	0.98	2 (6%)	50,54,54	1.59	8 (16%)
23	GDP	GW	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.76	6 (13%)
24	GTP	GP	501	25	33,34,34	1.06	4 (12%)	50,54,54	1.58	8 (16%)
23	GDP	At	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.75	5 (11%)
24	GTP	Ek	501	25	33,34,34	1.01	2 (6%)	50,54,54	1.57	9 (18%)
23	GDP	DN	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
23	GDP	DR	501	-	29,30,30	1.24	4 (13%)	45,47,47	1.80	7 (15%)
24	GTP	B1	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.57	8 (16%)
23	GDP	AM	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	7 (15%)
23	GDP	BB	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	6 (13%)
24	GTP	GI	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.57	9 (18%)
23	GDP	m	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	A7	501	25	33,34,34	1.01	2 (6%)	50,54,54	1.56	9 (18%)
23	GDP	FG	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
24	GTP	Et	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.59	9 (18%)
23	GDP	Bn	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.78	8 (17%)
24	GTP	F9	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.58	9 (18%)
24	GTP	3	602	25	33,34,34	0.91	1 (3%)	50,54,54	1.56	8 (16%)
24	GTP	F8	501	25	33,34,34	1.04	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	Ad	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	GTP	BJ	602	25	33,34,34	0.98	2 (6%)	50,54,54	1.59	8 (16%)
24	GTP	Gx	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.60	9 (18%)
24	GTP	GB	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.58	8 (16%)
24	GTP	G6	501	25	33,34,34	0.97	1 (3%)	50,54,54	1.56	9 (18%)
23	GDP	GY	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
24	GTP	A6	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.57	9 (18%)
23	GDP	AN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
24	GTP	GJ	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.56	8 (16%)
23	GDP	F2	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
24	GTP	Ey	602	25	33,34,34	1.04	3 (9%)	50,54,54	1.67	8 (16%)
23	GDP	Gd	501	-	29,30,30	1.25	4 (13%)	45,47,47	1.80	8 (17%)
24	GTP	B5	602	25	33,34,34	0.98	2 (6%)	50,54,54	1.59	9 (18%)
24	GTP	Ew	501	25	33,34,34	1.07	4 (12%)	50,54,54	1.61	8 (16%)
23	GDP	Ap	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
23	GDP	BA	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	5 (11%)
24	GTP	GM	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.59	8 (16%)
23	GDP	Ab	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	5 (11%)
23	GDP	FA	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
24	GTP	GA	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.57	9 (18%)
23	GDP	DP	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	7 (15%)
24	GTP	BY	602	25	33,34,34	0.92	1 (3%)	50,54,54	1.58	9 (18%)
24	GTP	Go	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.57	9 (18%)
24	GTP	BS	602	25	33,34,34	0.94	1 (3%)	50,54,54	1.56	8 (16%)
24	GTP	G4	602	25	33,34,34	1.05	3 (9%)	50,54,54	1.58	8 (16%)
24	GTP	Gq	501	25	33,34,34	1.00	3 (9%)	50,54,54	1.56	8 (16%)
24	GTP	AI	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.59	8 (16%)
23	GDP	BH	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	7 (15%)
24	GTP	G3	602	25	33,34,34	1.09	4 (12%)	50,54,54	1.61	8 (16%)
24	GTP	E6	602	25	33,34,34	1.03	3 (9%)	50,54,54	1.59	8 (16%)
24	GTP	Q	602	25	33,34,34	0.98	2 (6%)	50,54,54	1.55	8 (16%)
24	GTP	E2	501	25	33,34,34	1.04	3 (9%)	50,54,54	1.58	8 (16%)
23	GDP	EX	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
23	GDP	FN	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.74	6 (13%)
23	GDP	DY	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	F0	501	25	33,34,34	1.00	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
23	GDP	U	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
23	GDP	DT	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	7 (15%)
24	GTP	Er	501	25	33,34,34	0.97	2 (6%)	50,54,54	1.58	9 (18%)
24	GTP	F6	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.55	8 (16%)
23	GDP	Gi	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.75	6 (13%)
24	GTP	A4	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.57	8 (16%)
24	GTP	Gz	501	25	33,34,34	0.98	2 (6%)	50,54,54	1.57	9 (18%)
23	GDP	Bp	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
24	GTP	2	602	25	33,34,34	0.93	1 (3%)	50,54,54	1.57	8 (16%)
23	GDP	7	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.76	6 (13%)
24	GTP	BP	602	25	33,34,34	1.04	4 (12%)	50,54,54	1.61	8 (16%)
23	GDP	Ah	602	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
24	GTP	l	602	25	33,34,34	1.03	3 (9%)	50,54,54	1.54	8 (16%)
24	GTP	W	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	Gb	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	7 (15%)
24	GTP	e	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.57	9 (18%)
23	GDP	EP	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
24	GTP	b	602	25	33,34,34	1.01	3 (9%)	50,54,54	1.60	8 (16%)
24	GTP	BU	602	25	33,34,34	0.95	1 (3%)	50,54,54	1.58	8 (16%)
24	GTP	BQ	602	25	33,34,34	0.98	2 (6%)	50,54,54	1.58	9 (18%)
24	GTP	A5	501	25	33,34,34	1.02	2 (6%)	50,54,54	1.57	9 (18%)
23	GDP	Ag	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)
23	GDP	Am	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.73	6 (13%)
23	GDP	EQ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	E8	501	25	33,34,34	0.98	2 (6%)	50,54,54	1.57	9 (18%)
24	GTP	FS	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.58	9 (18%)
24	GTP	E7	501	25	33,34,34	1.00	3 (9%)	50,54,54	1.64	8 (16%)
23	GDP	Ao	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.71	6 (13%)
24	GTP	6	602	25	33,34,34	0.99	2 (6%)	50,54,54	1.60	9 (18%)
24	GTP	E4	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.55	9 (18%)
23	GDP	Bf	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.71	6 (13%)
24	GTP	B7	501	25	33,34,34	1.00	3 (9%)	50,54,54	1.59	9 (18%)
24	GTP	z	602	25	33,34,34	1.00	2 (6%)	50,54,54	1.58	9 (18%)
24	GTP	i	602	25	33,34,34	0.98	3 (9%)	50,54,54	1.58	8 (16%)
24	GTP	FU	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.57	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	GTP	Gw	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	AA	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
23	GDP	Gm	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	5 (11%)
23	GDP	Df	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
24	GTP	Eu	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.59	8 (16%)
23	GDP	Bb	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.71	6 (13%)
23	GDP	BC	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.75	5 (11%)
23	GDP	GH	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
23	GDP	ER	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.78	7 (15%)
24	GTP	Bc	501	25	33,34,34	1.01	2 (6%)	50,54,54	1.56	9 (18%)
24	GTP	S	602	25	33,34,34	0.97	1 (3%)	50,54,54	1.56	8 (16%)
23	GDP	Bs	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
24	GTP	F7	501	25	33,34,34	1.03	4 (12%)	50,54,54	1.59	9 (18%)
23	GDP	BD	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	8 (17%)
24	GTP	BX	602	25	33,34,34	0.94	1 (3%)	50,54,54	1.56	8 (16%)
24	GTP	FQ	501	25	33,34,34	1.02	2 (6%)	50,54,54	1.57	8 (16%)
24	GTP	o	501	25	33,34,34	0.99	3 (9%)	50,54,54	1.57	8 (16%)
24	GTP	Gr	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.56	9 (18%)
24	GTP	GN	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.60	9 (18%)
24	GTP	B4	602	25	33,34,34	0.99	2 (6%)	50,54,54	1.59	8 (16%)
23	GDP	DS	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
23	GDP	FE	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	x	501	25	33,34,34	0.99	1 (3%)	50,54,54	1.62	8 (16%)
23	GDP	BZ	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
23	GDP	Di	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
24	GTP	Al	602	25	33,34,34	1.01	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	Fv	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	6 (13%)
24	GTP	GD	501	25	33,34,34	1.08	4 (12%)	50,54,54	1.60	8 (16%)
23	GDP	GZ	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.76	6 (13%)
24	GTP	Eg	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.56	8 (16%)
23	GDP	EZ	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	5 (11%)
24	GTP	GF	501	25	33,34,34	1.09	4 (12%)	50,54,54	1.60	8 (16%)
23	GDP	Bl	602	-	29,30,30	1.18	3 (10%)	45,47,47	1.63	5 (11%)
24	GTP	Eo	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.58	9 (18%)
24	GTP	FV	602	25	33,34,34	1.01	2 (6%)	50,54,54	1.57	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	GDP	Gc	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
23	GDP	Dk	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)
23	GDP	BG	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
24	GTP	Fb	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.57	8 (16%)
23	GDP	Fq	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	6 (13%)
23	GDP	AD	501	-	29,30,30	1.14	2 (6%)	45,47,47	1.76	6 (13%)
24	GTP	Gs	501	25	33,34,34	1.00	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	AT	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
24	GTP	CB	602	25	33,34,34	1.01	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	Bi	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
24	GTP	FX	501	25	33,34,34	1.03	3 (9%)	50,54,54	1.58	9 (18%)
24	GTP	Ei	501	25	33,34,34	1.04	4 (12%)	50,54,54	1.61	8 (16%)
23	GDP	Bo	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
24	GTP	BO	602	25	33,34,34	1.00	2 (6%)	50,54,54	1.58	9 (18%)
24	GTP	E3	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.66	8 (16%)
23	GDP	FJ	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	5 (11%)
23	GDP	Au	602	-	29,30,30	1.15	2 (6%)	45,47,47	1.73	6 (13%)
23	GDP	Ea	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.75	7 (15%)
23	GDP	EU	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	G1	501	25	33,34,34	1.03	3 (9%)	50,54,54	1.57	8 (16%)
23	GDP	DU	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
24	GTP	T	602	25	33,34,34	0.99	2 (6%)	50,54,54	1.61	9 (18%)
23	GDP	Du	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
24	GTP	Bx	602	25	33,34,34	1.02	3 (9%)	50,54,54	1.62	9 (18%)
24	GTP	BT	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.57	8 (16%)
24	GTP	FP	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.57	9 (18%)
24	GTP	Ax	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.58	8 (16%)
24	GTP	B8	602	25	33,34,34	0.98	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	Da	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	F3	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.60	9 (18%)
24	GTP	p	602	25	33,34,34	0.98	1 (3%)	50,54,54	1.60	9 (18%)
24	GTP	Gy	501	25	33,34,34	0.99	3 (9%)	50,54,54	1.59	9 (18%)
24	GTP	E5	501	25	33,34,34	1.07	4 (12%)	50,54,54	1.65	10 (20%)
23	GDP	EY	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
23	GDP	Ds	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.75	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	GDP	Br	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.80	6 (13%)
24	GTP	y	602	25	33,34,34	0.99	3 (9%)	50,54,54	1.58	9 (18%)
23	GDP	Fw	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
24	GTP	AJ	602	25	33,34,34	0.94	1 (3%)	50,54,54	1.57	8 (16%)
23	GDP	BF	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
23	GDP	AH	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.70	6 (13%)
23	GDP	EN	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	7 (15%)
24	GTP	a	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.58	8 (16%)
24	GTP	Bv	602	25	33,34,34	0.95	1 (3%)	50,54,54	1.60	8 (16%)
23	GDP	Fx	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	5 (11%)
23	GDP	Gg	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
23	GDP	Dc	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.76	7 (15%)
23	GDP	AS	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	8 (17%)
24	GTP	El	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.58	9 (18%)
24	GTP	Y	602	25	33,34,34	0.96	2 (6%)	50,54,54	1.56	8 (16%)
24	GTP	Ff	501	25	33,34,34	1.02	2 (6%)	50,54,54	1.63	8 (16%)
23	GDP	Fn	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	6 (13%)
23	GDP	AX	501	-	29,30,30	1.14	2 (6%)	45,47,47	1.76	6 (13%)
23	GDP	Ec	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.79	7 (15%)
24	GTP	g	602	25	33,34,34	0.98	2 (6%)	50,54,54	1.60	8 (16%)
24	GTP	Ak	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.59	9 (18%)
23	GDP	Aa	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.72	6 (13%)
23	GDP	Az	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	6 (13%)
23	GDP	AP	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	5 (11%)
23	GDP	AW	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	6 (13%)
23	GDP	Ar	501	-	29,30,30	1.18	4 (13%)	45,47,47	1.77	7 (15%)
23	GDP	DV	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.73	7 (15%)
23	GDP	An	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
24	GTP	Em	501	25	33,34,34	1.01	3 (9%)	50,54,54	1.56	9 (18%)
24	GTP	f	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.56	8 (16%)
24	GTP	B9	602	25	33,34,34	0.99	3 (9%)	50,54,54	1.59	9 (18%)
24	GTP	4	602	25	33,34,34	0.93	1 (3%)	50,54,54	1.56	8 (16%)
23	GDP	A3	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
24	GTP	BN	602	25	33,34,34	1.00	3 (9%)	50,54,54	1.58	8 (16%)
23	GDP	Ai	501	-	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
24	GTP	Bz	602	25	33,34,34	1.01	4 (12%)	50,54,54	1.57	9 (18%)
23	GDP	AV	602	-	29,30,30	1.27	4 (13%)	45,47,47	1.76	6 (13%)
24	GTP	Z	602	25	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
24	GTP	B3	602	25	33,34,34	1.00	2 (6%)	50,54,54	1.55	9 (18%)
24	GTP	V	602	25	33,34,34	0.99	3 (9%)	50,54,54	1.60	8 (16%)
23	GDP	Dq	501	-	29,30,30	1.14	2 (6%)	45,47,47	1.76	5 (11%)
23	GDP	AC	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.77	7 (15%)
23	GDP	Aq	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.75	5 (11%)
23	GDP	FK	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.74	7 (15%)
23	GDP	DZ	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.75	7 (15%)
24	GTP	Fh	501	25	33,34,34	1.08	4 (12%)	50,54,54	1.66	9 (18%)
23	GDP	Eb	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	5 (11%)
24	GTP	Fd	602	25	33,34,34	1.08	4 (12%)	50,54,54	1.59	8 (16%)
23	GDP	As	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	7 (15%)
23	GDP	BW	501	-	29,30,30	1.13	2 (6%)	45,47,47	1.75	7 (15%)
23	GDP	ES	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	6 (13%)
24	GTP	c	602	25	33,34,34	0.99	4 (12%)	50,54,54	1.58	8 (16%)
24	GTP	Fj	501	25	33,34,34	1.13	4 (12%)	50,54,54	1.66	8 (16%)
24	GTP	Gv	501	25	33,34,34	1.03	2 (6%)	50,54,54	1.57	8 (16%)
24	GTP	Fe	501	25	33,34,34	1.04	3 (9%)	50,54,54	1.57	8 (16%)
23	GDP	EO	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
24	GTP	Ej	501	25	33,34,34	0.99	2 (6%)	50,54,54	1.58	9 (18%)
23	GDP	Fm	501	-	29,30,30	1.16	2 (6%)	45,47,47	1.76	7 (15%)
24	GTP	Gp	501	25	33,34,34	1.02	3 (9%)	50,54,54	1.59	9 (18%)
23	GDP	Bh	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.77	7 (15%)
23	GDP	Ev	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.77	7 (15%)
23	GDP	Gf	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
24	GTP	FO	501	25	33,34,34	1.00	2 (6%)	50,54,54	1.56	8 (16%)
23	GDP	Dg	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
23	GDP	P	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.77	7 (15%)
23	GDP	Dh	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
23	GDP	0	501	-	29,30,30	1.13	2 (6%)	45,47,47	1.71	6 (13%)

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
23	GDP	EL	501	-	-	5/16/32/32	0/3/3/3
24	GTP	Eh	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Av	501	-	-	5/16/32/32	0/3/3/3
23	GDP	A0	501	-	-	3/16/32/32	0/3/3/3
24	GTP	Eq	501	25	-	4/22/38/38	0/3/3/3
23	GDP	O	501	-	-	2/16/32/32	0/3/3/3
23	GDP	AB	501	-	-	1/16/32/32	0/3/3/3
24	GTP	GK	501	25	-	4/22/38/38	0/3/3/3
24	GTP	BL	602	25	-	7/22/38/38	0/3/3/3
23	GDP	9	501	-	-	3/16/32/32	0/3/3/3
23	GDP	AY	501	-	-	3/16/32/32	0/3/3/3
23	GDP	Fp	501	-	-	5/16/32/32	0/3/3/3
23	GDP	AZ	501	-	-	4/16/32/32	0/3/3/3
24	GTP	Ex	501	25	-	7/22/38/38	0/3/3/3
23	GDP	Db	501	-	-	8/16/32/32	0/3/3/3
23	GDP	Dr	501	-	-	4/16/32/32	0/3/3/3
24	GTP	B0	501	25	-	4/22/38/38	0/3/3/3
23	GDP	GV	501	-	-	5/16/32/32	0/3/3/3
24	GTP	GQ	602	25	-	6/22/38/38	0/3/3/3
24	GTP	q	602	25	-	4/22/38/38	0/3/3/3
23	GDP	BE	501	-	-	3/16/32/32	0/3/3/3
24	GTP	Gn	501	25	-	4/22/38/38	0/3/3/3
24	GTP	BI	602	25	-	11/22/38/38	0/3/3/3
23	GDP	GX	501	-	-	3/16/32/32	0/3/3/3
23	GDP	X	501	-	-	2/16/32/32	0/3/3/3
23	GDP	Dt	501	-	-	0/16/32/32	0/3/3/3
24	GTP	u	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Ac	501	-	-	1/16/32/32	0/3/3/3
24	GTP	BK	602	25	-	3/22/38/38	0/3/3/3
23	GDP	Dd	501	-	-	8/16/32/32	0/3/3/3
23	GDP	Gj	501	-	-	6/16/32/32	0/3/3/3
23	GDP	Fy	501	-	-	8/16/32/32	0/3/3/3
23	GDP	Fo	501	-	-	3/16/32/32	0/3/3/3
23	GDP	E9	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	AE	501	-	-	3/16/32/32	0/3/3/3
23	GDP	Ft	501	-	-	6/16/32/32	0/3/3/3
23	GDP	De	501	-	-	3/16/32/32	0/3/3/3
24	GTP	A1	602	25	-	3/22/38/38	0/3/3/3
24	GTP	Fa	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Af	501	-	-	3/16/32/32	0/3/3/3
23	GDP	F4	501	-	-	8/16/32/32	0/3/3/3
24	GTP	1	602	25	-	3/22/38/38	0/3/3/3
24	GTP	Ep	501	25	-	4/22/38/38	0/3/3/3
24	GTP	Gt	501	25	-	7/22/38/38	0/3/3/3
23	GDP	EM	501	-	-	5/16/32/32	0/3/3/3
23	GDP	AL	501	-	-	5/16/32/32	0/3/3/3
23	GDP	FL	501	-	-	8/16/32/32	0/3/3/3
24	GTP	GR	501	25	-	7/22/38/38	0/3/3/3
24	GTP	5	602	25	-	3/22/38/38	0/3/3/3
23	GDP	F1	501	-	-	7/16/32/32	0/3/3/3
23	GDP	Ef	501	-	-	6/16/32/32	0/3/3/3
24	GTP	GT	501	25	-	4/22/38/38	0/3/3/3
24	GTP	Bd	501	25	-	5/22/38/38	0/3/3/3
23	GDP	AO	501	-	-	6/16/32/32	0/3/3/3
23	GDP	FC	501	-	-	1/16/32/32	0/3/3/3
23	GDP	E0	501	-	-	5/16/32/32	0/3/3/3
24	GTP	v	602	25	-	5/22/38/38	0/3/3/3
23	GDP	Dx	501	-	-	3/16/32/32	0/3/3/3
24	GTP	Fc	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Be	501	-	-	4/16/32/32	0/3/3/3
24	GTP	GG	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Fu	501	-	-	1/16/32/32	0/3/3/3
24	GTP	BR	501	25	-	5/22/38/38	0/3/3/3
23	GDP	8	501	-	-	3/16/32/32	0/3/3/3
23	GDP	Dv	501	-	-	1/16/32/32	0/3/3/3
24	GTP	Gl	501	25	-	3/22/38/38	0/3/3/3
23	GDP	Fr	501	-	-	2/16/32/32	0/3/3/3
24	GTP	F5	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Fs	501	-	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	DX	501	-	-	4/16/32/32	0/3/3/3
24	GTP	FT	501	25	-	4/22/38/38	0/3/3/3
24	GTP	s	602	25	-	3/22/38/38	0/3/3/3
24	GTP	En	501	25	-	4/22/38/38	0/3/3/3
24	GTP	A2	602	25	-	3/22/38/38	0/3/3/3
23	GDP	AQ	501	-	-	2/16/32/32	0/3/3/3
24	GTP	Bw	602	25	-	11/22/38/38	0/3/3/3
23	GDP	Ba	501	-	-	2/16/32/32	0/3/3/3
23	GDP	Bg	501	-	-	5/16/32/32	0/3/3/3
23	GDP	ET	501	-	-	6/16/32/32	0/3/3/3
23	GDP	AR	501	-	-	7/16/32/32	0/3/3/3
24	GTP	B6	602	25	-	5/22/38/38	0/3/3/3
23	GDP	Fz	501	-	-	6/16/32/32	0/3/3/3
23	GDP	Gk	501	-	-	1/16/32/32	0/3/3/3
24	GTP	Es	501	25	-	4/22/38/38	0/3/3/3
23	GDP	DQ	501	-	-	6/16/32/32	0/3/3/3
24	GTP	GL	501	25	-	3/22/38/38	0/3/3/3
24	GTP	t	602	25	-	3/22/38/38	0/3/3/3
24	GTP	Aw	602	25	-	5/22/38/38	0/3/3/3
23	GDP	FH	501	-	-	6/16/32/32	0/3/3/3
23	GDP	Bt	501	-	-	2/16/32/32	0/3/3/3
24	GTP	j	602	25	-	5/22/38/38	0/3/3/3
23	GDP	Fl	501	-	-	6/16/32/32	0/3/3/3
23	GDP	AF	501	-	-	4/16/32/32	0/3/3/3
24	GTP	Fk	501	25	-	3/22/38/38	0/3/3/3
24	GTP	FW	501	25	-	5/22/38/38	0/3/3/3
24	GTP	G5	501	25	-	3/22/38/38	0/3/3/3
24	GTP	CA	602	25	-	5/22/38/38	0/3/3/3
24	GTP	B2	602	25	-	5/22/38/38	0/3/3/3
24	GTP	AS	501	25	-	2/22/38/38	0/3/3/3
23	GDP	Ed	501	-	-	6/16/32/32	0/3/3/3
24	GTP	A8	501	25	-	5/22/38/38	0/3/3/3
23	GDP	Gh	501	-	-	8/16/32/32	0/3/3/3
23	GDP	FF	501	-	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	FI	501	-	-	6/16/32/32	0/3/3/3
24	GTP	w	602	25	-	4/22/38/38	0/3/3/3
24	GTP	Ee	501	25	-	5/22/38/38	0/3/3/3
24	GTP	Gu	501	25	-	6/22/38/38	0/3/3/3
23	GDP	Bk	501	-	-	6/16/32/32	0/3/3/3
24	GTP	Fg	501	25	-	3/22/38/38	0/3/3/3
23	GDP	AU	501	-	-	2/16/32/32	0/3/3/3
24	GTP	GO	602	25	-	4/22/38/38	0/3/3/3
24	GTP	A9	501	25	-	5/22/38/38	0/3/3/3
23	GDP	Dj	501	-	-	6/16/32/32	0/3/3/3
24	GTP	BM	602	25	-	6/22/38/38	0/3/3/3
24	GTP	h	602	25	-	6/22/38/38	0/3/3/3
24	GTP	Fi	501	25	-	6/22/38/38	0/3/3/3
23	GDP	r	501	-	-	2/16/32/32	0/3/3/3
23	GDP	FD	501	-	-	6/16/32/32	0/3/3/3
23	GDP	EV	501	-	-	3/16/32/32	0/3/3/3
23	GDP	Bm	501	-	-	4/16/32/32	0/3/3/3
24	GTP	GE	501	25	-	7/22/38/38	0/3/3/3
24	GTP	Ez	501	25	-	7/22/38/38	0/3/3/3
24	GTP	BV	602	25	-	5/22/38/38	0/3/3/3
23	GDP	Ga	501	-	-	2/16/32/32	0/3/3/3
23	GDP	DW	501	-	-	6/16/32/32	0/3/3/3
24	GTP	FR	501	25	-	5/22/38/38	0/3/3/3
23	GDP	n	501	-	-	2/16/32/32	0/3/3/3
24	GTP	By	602	25	-	3/22/38/38	0/3/3/3
23	GDP	AG	501	-	-	3/16/32/32	0/3/3/3
24	GTP	FY	501	25	-	4/22/38/38	0/3/3/3
24	GTP	FM	501	25	-	4/22/38/38	0/3/3/3
24	GTP	FZ	501	25	-	5/22/38/38	0/3/3/3
23	GDP	GU	501	-	-	3/16/32/32	0/3/3/3
24	GTP	GS	501	25	-	4/22/38/38	0/3/3/3
24	GTP	GC	501	25	-	4/22/38/38	0/3/3/3
24	GTP	AK	602	25	-	4/22/38/38	0/3/3/3
23	GDP	Bj	501	-	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	DO	501	-	-	6/16/32/32	0/3/3/3
23	GDP	Ge	501	-	-	2/16/32/32	0/3/3/3
24	GTP	Bu	602	25	-	6/22/38/38	0/3/3/3
23	GDP	FB	501	-	-	2/16/32/32	0/3/3/3
23	GDP	Bq	602	-	-	2/16/32/32	0/3/3/3
24	GTP	Aj	501	25	-	3/22/38/38	0/3/3/3
24	GTP	G2	501	25	-	5/22/38/38	0/3/3/3
24	GTP	k	602	25	-	4/22/38/38	0/3/3/3
24	GTP	E1	501	25	-	7/22/38/38	0/3/3/3
23	GDP	Ae	501	-	-	4/16/32/32	0/3/3/3
24	GTP	Ay	602	25	-	4/22/38/38	0/3/3/3
23	GDP	EW	501	-	-	6/16/32/32	0/3/3/3
23	GDP	Dw	501	-	-	0/16/32/32	0/3/3/3
23	GDP	DM	501	-	-	6/16/32/32	0/3/3/3
23	GDP	DL	501	-	-	8/16/32/32	0/3/3/3
24	GTP	d	602	25	-	2/22/38/38	0/3/3/3
23	GDP	GW	501	-	-	3/16/32/32	0/3/3/3
24	GTP	GP	501	25	-	9/22/38/38	0/3/3/3
23	GDP	At	501	-	-	5/16/32/32	0/3/3/3
24	GTP	Ek	501	25	-	3/22/38/38	0/3/3/3
23	GDP	DN	501	-	-	8/16/32/32	0/3/3/3
23	GDP	DR	501	-	-	1/16/32/32	0/3/3/3
24	GTP	B1	602	25	-	5/22/38/38	0/3/3/3
23	GDP	AM	501	-	-	5/16/32/32	0/3/3/3
23	GDP	BB	501	-	-	7/16/32/32	0/3/3/3
24	GTP	GI	501	25	-	4/22/38/38	0/3/3/3
23	GDP	m	501	-	-	2/16/32/32	0/3/3/3
24	GTP	A7	501	25	-	4/22/38/38	0/3/3/3
23	GDP	FG	501	-	-	5/16/32/32	0/3/3/3
24	GTP	Et	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Bn	501	-	-	5/16/32/32	0/3/3/3
24	GTP	F9	501	25	-	5/22/38/38	0/3/3/3
24	GTP	3	602	25	-	3/22/38/38	0/3/3/3
24	GTP	F8	501	25	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	Ad	501	-	-	7/16/32/32	0/3/3/3
24	GTP	BJ	602	25	-	2/22/38/38	0/3/3/3
24	GTP	Gx	501	25	-	5/22/38/38	0/3/3/3
24	GTP	GB	501	25	-	4/22/38/38	0/3/3/3
24	GTP	G6	501	25	-	3/22/38/38	0/3/3/3
23	GDP	GY	501	-	-	3/16/32/32	0/3/3/3
24	GTP	A6	501	25	-	4/22/38/38	0/3/3/3
23	GDP	AN	501	-	-	4/16/32/32	0/3/3/3
24	GTP	GJ	501	25	-	5/22/38/38	0/3/3/3
23	GDP	F2	501	-	-	6/16/32/32	0/3/3/3
24	GTP	Ey	602	25	-	7/22/38/38	0/3/3/3
23	GDP	Gd	501	-	-	3/16/32/32	0/3/3/3
24	GTP	B5	602	25	-	3/22/38/38	0/3/3/3
24	GTP	Ew	501	25	-	6/22/38/38	0/3/3/3
23	GDP	Ap	501	-	-	4/16/32/32	0/3/3/3
23	GDP	BA	501	-	-	5/16/32/32	0/3/3/3
24	GTP	GM	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Ab	501	-	-	6/16/32/32	0/3/3/3
23	GDP	FA	501	-	-	4/16/32/32	0/3/3/3
24	GTP	GA	501	25	-	3/22/38/38	0/3/3/3
23	GDP	DP	501	-	-	5/16/32/32	0/3/3/3
24	GTP	BY	602	25	-	3/22/38/38	0/3/3/3
24	GTP	Go	501	25	-	3/22/38/38	0/3/3/3
24	GTP	BS	602	25	-	6/22/38/38	0/3/3/3
24	GTP	G4	602	25	-	10/22/38/38	0/3/3/3
24	GTP	Gq	501	25	-	4/22/38/38	0/3/3/3
24	GTP	AI	501	25	-	4/22/38/38	0/3/3/3
23	GDP	BH	501	-	-	6/16/32/32	0/3/3/3
24	GTP	G3	602	25	-	6/22/38/38	0/3/3/3
24	GTP	E6	602	25	-	5/22/38/38	0/3/3/3
24	GTP	Q	602	25	-	7/22/38/38	0/3/3/3
24	GTP	E2	501	25	-	6/22/38/38	0/3/3/3
23	GDP	EX	501	-	-	5/16/32/32	0/3/3/3
23	GDP	FN	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	DY	501	-	-	6/16/32/32	0/3/3/3
24	GTP	F0	501	25	-	5/22/38/38	0/3/3/3
23	GDP	U	501	-	-	2/16/32/32	0/3/3/3
23	GDP	DT	501	-	-	7/16/32/32	0/3/3/3
24	GTP	Er	501	25	-	4/22/38/38	0/3/3/3
24	GTP	F6	501	25	-	5/22/38/38	0/3/3/3
23	GDP	Gi	501	-	-	6/16/32/32	0/3/3/3
24	GTP	A4	501	25	-	4/22/38/38	0/3/3/3
24	GTP	Gz	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Bp	501	-	-	3/16/32/32	0/3/3/3
24	GTP	2	602	25	-	3/22/38/38	0/3/3/3
23	GDP	7	501	-	-	0/16/32/32	0/3/3/3
24	GTP	BP	602	25	-	4/22/38/38	0/3/3/3
23	GDP	Ah	602	-	-	2/16/32/32	0/3/3/3
24	GTP	l	602	25	-	4/22/38/38	0/3/3/3
24	GTP	W	602	25	-	6/22/38/38	0/3/3/3
23	GDP	Gb	501	-	-	7/16/32/32	0/3/3/3
24	GTP	e	602	25	-	4/22/38/38	0/3/3/3
23	GDP	EP	501	-	-	4/16/32/32	0/3/3/3
24	GTP	b	602	25	-	6/22/38/38	0/3/3/3
24	GTP	BU	602	25	-	6/22/38/38	0/3/3/3
24	GTP	BQ	602	25	-	3/22/38/38	0/3/3/3
24	GTP	A5	501	25	-	5/22/38/38	0/3/3/3
23	GDP	Ag	501	-	-	5/16/32/32	0/3/3/3
23	GDP	Am	501	-	-	1/16/32/32	0/3/3/3
23	GDP	EQ	501	-	-	5/16/32/32	0/3/3/3
24	GTP	E8	501	25	-	4/22/38/38	0/3/3/3
24	GTP	FS	501	25	-	3/22/38/38	0/3/3/3
24	GTP	E7	501	25	-	1/22/38/38	0/3/3/3
23	GDP	Ao	501	-	-	3/16/32/32	0/3/3/3
24	GTP	6	602	25	-	3/22/38/38	0/3/3/3
24	GTP	E4	501	25	-	5/22/38/38	0/3/3/3
23	GDP	Bf	501	-	-	3/16/32/32	0/3/3/3
24	GTP	B7	501	25	-	3/22/38/38	0/3/3/3
24	GTP	z	602	25	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	GTP	i	602	25	-	6/22/38/38	0/3/3/3
24	GTP	FU	501	25	-	5/22/38/38	0/3/3/3
24	GTP	Gw	501	25	-	4/22/38/38	0/3/3/3
23	GDP	AA	501	-	-	2/16/32/32	0/3/3/3
23	GDP	Gm	501	-	-	4/16/32/32	0/3/3/3
23	GDP	Df	501	-	-	7/16/32/32	0/3/3/3
24	GTP	Eu	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Bb	501	-	-	3/16/32/32	0/3/3/3
23	GDP	BC	501	-	-	4/16/32/32	0/3/3/3
23	GDP	GH	501	-	-	4/16/32/32	0/3/3/3
23	GDP	ER	501	-	-	4/16/32/32	0/3/3/3
24	GTP	Bc	501	25	-	4/22/38/38	0/3/3/3
24	GTP	S	602	25	-	9/22/38/38	0/3/3/3
23	GDP	Bs	501	-	-	4/16/32/32	0/3/3/3
24	GTP	F7	501	25	-	5/22/38/38	0/3/3/3
23	GDP	BD	501	-	-	6/16/32/32	0/3/3/3
24	GTP	BX	602	25	-	3/22/38/38	0/3/3/3
24	GTP	FQ	501	25	-	5/22/38/38	0/3/3/3
24	GTP	o	501	25	-	10/22/38/38	0/3/3/3
24	GTP	Gr	501	25	-	4/22/38/38	0/3/3/3
24	GTP	GN	501	25	-	6/22/38/38	0/3/3/3
24	GTP	B4	602	25	-	3/22/38/38	0/3/3/3
23	GDP	DS	501	-	-	6/16/32/32	0/3/3/3
23	GDP	FE	501	-	-	3/16/32/32	0/3/3/3
24	GTP	x	501	25	-	3/22/38/38	0/3/3/3
23	GDP	BZ	501	-	-	2/16/32/32	0/3/3/3
23	GDP	Di	501	-	-	6/16/32/32	0/3/3/3
24	GTP	Al	602	25	-	6/22/38/38	0/3/3/3
23	GDP	Fv	501	-	-	4/16/32/32	0/3/3/3
24	GTP	GD	501	25	-	6/22/38/38	0/3/3/3
23	GDP	GZ	501	-	-	5/16/32/32	0/3/3/3
24	GTP	Eg	501	25	-	5/22/38/38	0/3/3/3
23	GDP	EZ	501	-	-	6/16/32/32	0/3/3/3
24	GTP	GF	501	25	-	10/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	Bl	602	-	-	4/16/32/32	0/3/3/3
24	GTP	Eo	501	25	-	4/22/38/38	0/3/3/3
24	GTP	FV	602	25	-	4/22/38/38	0/3/3/3
23	GDP	Gc	501	-	-	6/16/32/32	0/3/3/3
23	GDP	Dk	501	-	-	6/16/32/32	0/3/3/3
23	GDP	BG	501	-	-	2/16/32/32	0/3/3/3
24	GTP	Fb	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Fq	501	-	-	4/16/32/32	0/3/3/3
23	GDP	AD	501	-	-	1/16/32/32	0/3/3/3
24	GTP	Gs	501	25	-	3/22/38/38	0/3/3/3
23	GDP	AT	501	-	-	4/16/32/32	0/3/3/3
24	GTP	CB	602	25	-	5/22/38/38	0/3/3/3
23	GDP	Bi	501	-	-	4/16/32/32	0/3/3/3
24	GTP	FX	501	25	-	4/22/38/38	0/3/3/3
24	GTP	Ei	501	25	-	7/22/38/38	0/3/3/3
23	GDP	Bo	501	-	-	3/16/32/32	0/3/3/3
24	GTP	BO	602	25	-	4/22/38/38	0/3/3/3
24	GTP	E3	501	25	-	4/22/38/38	0/3/3/3
23	GDP	FJ	501	-	-	6/16/32/32	0/3/3/3
23	GDP	Au	602	-	-	0/16/32/32	0/3/3/3
23	GDP	Ea	501	-	-	8/16/32/32	0/3/3/3
23	GDP	EU	501	-	-	6/16/32/32	0/3/3/3
24	GTP	G1	501	25	-	4/22/38/38	0/3/3/3
23	GDP	DU	501	-	-	2/16/32/32	0/3/3/3
24	GTP	T	602	25	-	2/22/38/38	0/3/3/3
23	GDP	Du	501	-	-	0/16/32/32	0/3/3/3
24	GTP	Bx	602	25	-	4/22/38/38	0/3/3/3
24	GTP	BT	501	25	-	3/22/38/38	0/3/3/3
24	GTP	FP	501	25	-	4/22/38/38	0/3/3/3
24	GTP	Ax	602	25	-	4/22/38/38	0/3/3/3
24	GTP	B8	602	25	-	5/22/38/38	0/3/3/3
23	GDP	Da	501	-	-	8/16/32/32	0/3/3/3
24	GTP	F3	501	25	-	4/22/38/38	0/3/3/3
24	GTP	p	602	25	-	2/22/38/38	0/3/3/3
24	GTP	Gy	501	25	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	GTP	E5	501	25	-	7/22/38/38	0/3/3/3
23	GDP	EY	501	-	-	8/16/32/32	0/3/3/3
23	GDP	Ds	501	-	-	0/16/32/32	0/3/3/3
23	GDP	Br	501	-	-	5/16/32/32	0/3/3/3
24	GTP	y	602	25	-	5/22/38/38	0/3/3/3
23	GDP	Fw	501	-	-	6/16/32/32	0/3/3/3
24	GTP	AJ	602	25	-	5/22/38/38	0/3/3/3
23	GDP	BF	501	-	-	6/16/32/32	0/3/3/3
23	GDP	AH	501	-	-	4/16/32/32	0/3/3/3
23	GDP	EN	501	-	-	3/16/32/32	0/3/3/3
24	GTP	a	602	25	-	5/22/38/38	0/3/3/3
24	GTP	Bv	602	25	-	2/22/38/38	0/3/3/3
23	GDP	Fx	501	-	-	6/16/32/32	0/3/3/3
23	GDP	Gg	501	-	-	6/16/32/32	0/3/3/3
23	GDP	Dc	501	-	-	5/16/32/32	0/3/3/3
23	GDP	AS	502	-	-	5/16/32/32	0/3/3/3
24	GTP	El	501	25	-	5/22/38/38	0/3/3/3
24	GTP	Y	602	25	-	8/22/38/38	0/3/3/3
24	GTP	Ff	501	25	-	7/22/38/38	0/3/3/3
23	GDP	Fn	501	-	-	5/16/32/32	0/3/3/3
23	GDP	AX	501	-	-	4/16/32/32	0/3/3/3
23	GDP	Ec	501	-	-	3/16/32/32	0/3/3/3
24	GTP	g	602	25	-	3/22/38/38	0/3/3/3
24	GTP	Ak	602	25	-	6/22/38/38	0/3/3/3
23	GDP	Aa	501	-	-	7/16/32/32	0/3/3/3
23	GDP	Az	501	-	-	3/16/32/32	0/3/3/3
23	GDP	AP	501	-	-	6/16/32/32	0/3/3/3
23	GDP	AW	501	-	-	6/16/32/32	0/3/3/3
23	GDP	Ar	501	-	-	5/16/32/32	0/3/3/3
23	GDP	DV	501	-	-	8/16/32/32	0/3/3/3
23	GDP	An	501	-	-	3/16/32/32	0/3/3/3
24	GTP	Em	501	25	-	7/22/38/38	0/3/3/3
24	GTP	f	602	25	-	3/22/38/38	0/3/3/3
24	GTP	B9	602	25	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	GTP	4	602	25	-	3/22/38/38	0/3/3/3
23	GDP	A3	501	-	-	1/16/32/32	0/3/3/3
24	GTP	BN	602	25	-	6/22/38/38	0/3/3/3
23	GDP	Ai	501	-	-	5/16/32/32	0/3/3/3
24	GTP	Bz	602	25	-	5/22/38/38	0/3/3/3
23	GDP	AV	602	-	-	1/16/32/32	0/3/3/3
24	GTP	Z	602	25	-	2/22/38/38	0/3/3/3
24	GTP	B3	602	25	-	4/22/38/38	0/3/3/3
24	GTP	V	602	25	-	3/22/38/38	0/3/3/3
23	GDP	Dq	501	-	-	1/16/32/32	0/3/3/3
23	GDP	AC	501	-	-	3/16/32/32	0/3/3/3
23	GDP	Aq	501	-	-	4/16/32/32	0/3/3/3
23	GDP	FK	501	-	-	7/16/32/32	0/3/3/3
23	GDP	DZ	501	-	-	5/16/32/32	0/3/3/3
24	GTP	Fh	501	25	-	6/22/38/38	0/3/3/3
23	GDP	Eb	501	-	-	6/16/32/32	0/3/3/3
24	GTP	Fd	602	25	-	6/22/38/38	0/3/3/3
23	GDP	As	501	-	-	4/16/32/32	0/3/3/3
23	GDP	BW	501	-	-	1/16/32/32	0/3/3/3
23	GDP	ES	501	-	-	3/16/32/32	0/3/3/3
24	GTP	c	602	25	-	11/22/38/38	0/3/3/3
24	GTP	Fj	501	25	-	6/22/38/38	0/3/3/3
24	GTP	Gv	501	25	-	4/22/38/38	0/3/3/3
24	GTP	Fe	501	25	-	9/22/38/38	0/3/3/3
23	GDP	EO	501	-	-	3/16/32/32	0/3/3/3
24	GTP	Ej	501	25	-	5/22/38/38	0/3/3/3
23	GDP	Fm	501	-	-	4/16/32/32	0/3/3/3
24	GTP	Gp	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Bh	501	-	-	5/16/32/32	0/3/3/3
23	GDP	Ev	501	-	-	2/16/32/32	0/3/3/3
23	GDP	Gf	501	-	-	2/16/32/32	0/3/3/3
24	GTP	FO	501	25	-	4/22/38/38	0/3/3/3
23	GDP	Dg	501	-	-	3/16/32/32	0/3/3/3
23	GDP	P	501	-	-	2/16/32/32	0/3/3/3
23	GDP	Dh	501	-	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	GDP	0	501	-	-	7/16/32/32	0/3/3/3

The worst 5 of 1033 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	501	GDP	C5-C4	3.52	1.48	1.38
23	AV	602	GDP	C5-C4	3.45	1.48	1.38
23	EV	501	GDP	C5-C4	3.45	1.48	1.38
23	DR	501	GDP	C5-C4	3.43	1.48	1.38
23	Gd	501	GDP	C5-C4	3.34	1.47	1.38

The worst 5 of 2807 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AM	501	GDP	C5-C4-N3	-6.34	118.31	128.39
23	Bh	501	GDP	C5-C4-N3	-6.26	118.43	128.39
23	r	501	GDP	C5-C4-N3	-6.25	118.44	128.39
23	X	501	GDP	C5-C4-N3	-6.25	118.45	128.39
23	O	501	GDP	C5-C4-N3	-6.24	118.45	128.39

There are no chirality outliers.

5 of 1688 torsion outliers are listed below:

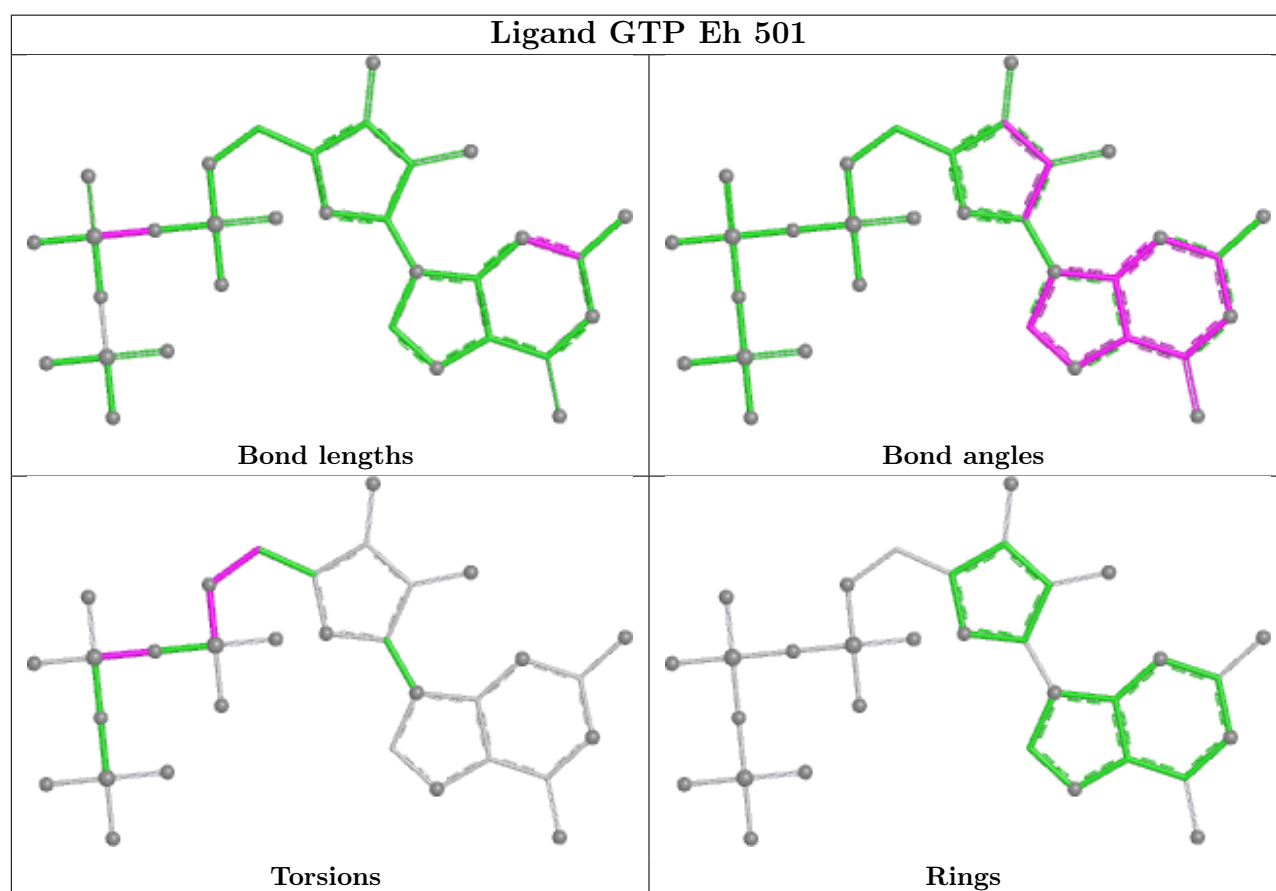
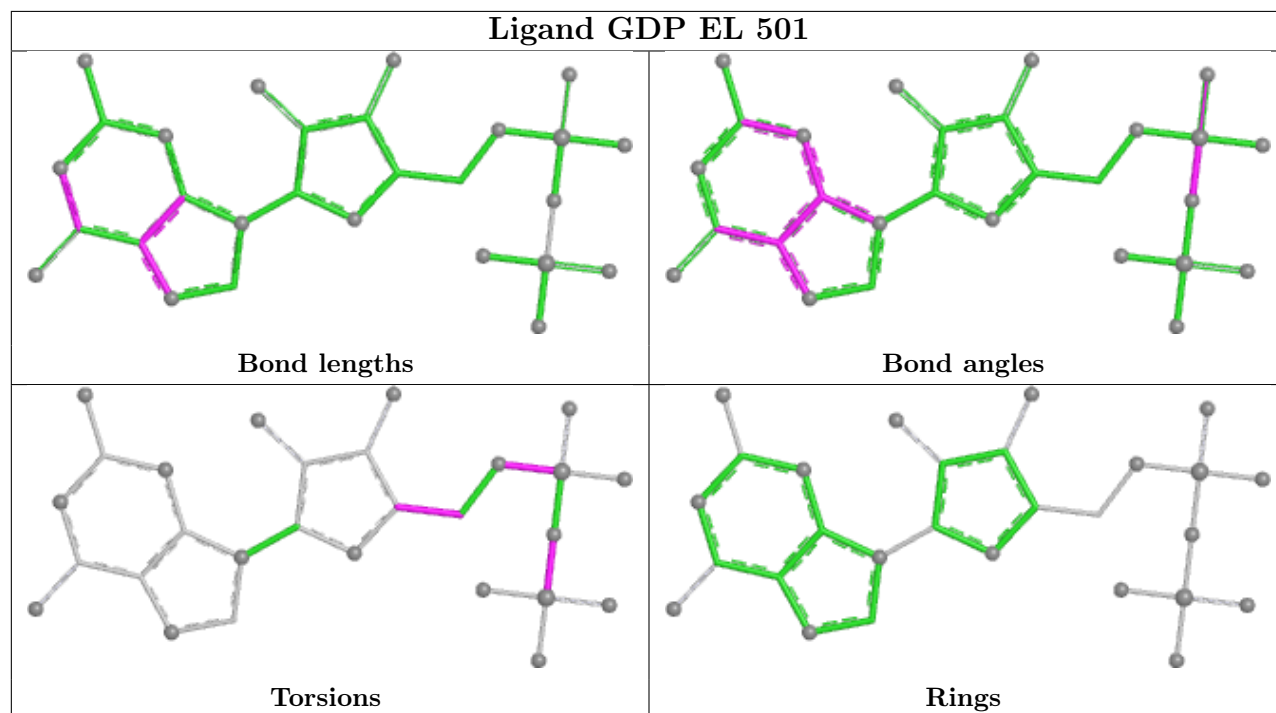
Mol	Chain	Res	Type	Atoms
23	0	501	GDP	PA-O3A-PB-O2B
23	0	501	GDP	C5'-O5'-PA-O3A
23	0	501	GDP	C5'-O5'-PA-O1A
23	0	501	GDP	C5'-O5'-PA-O2A
23	Fo	501	GDP	PA-O3A-PB-O3B

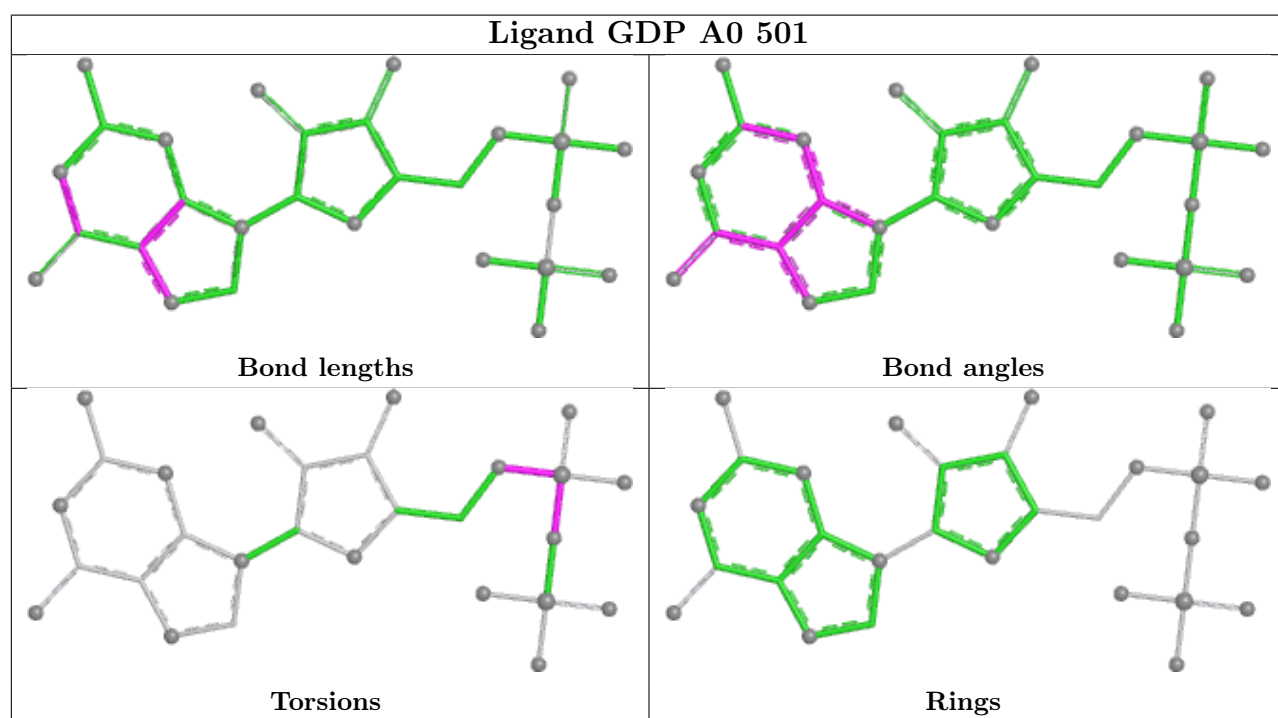
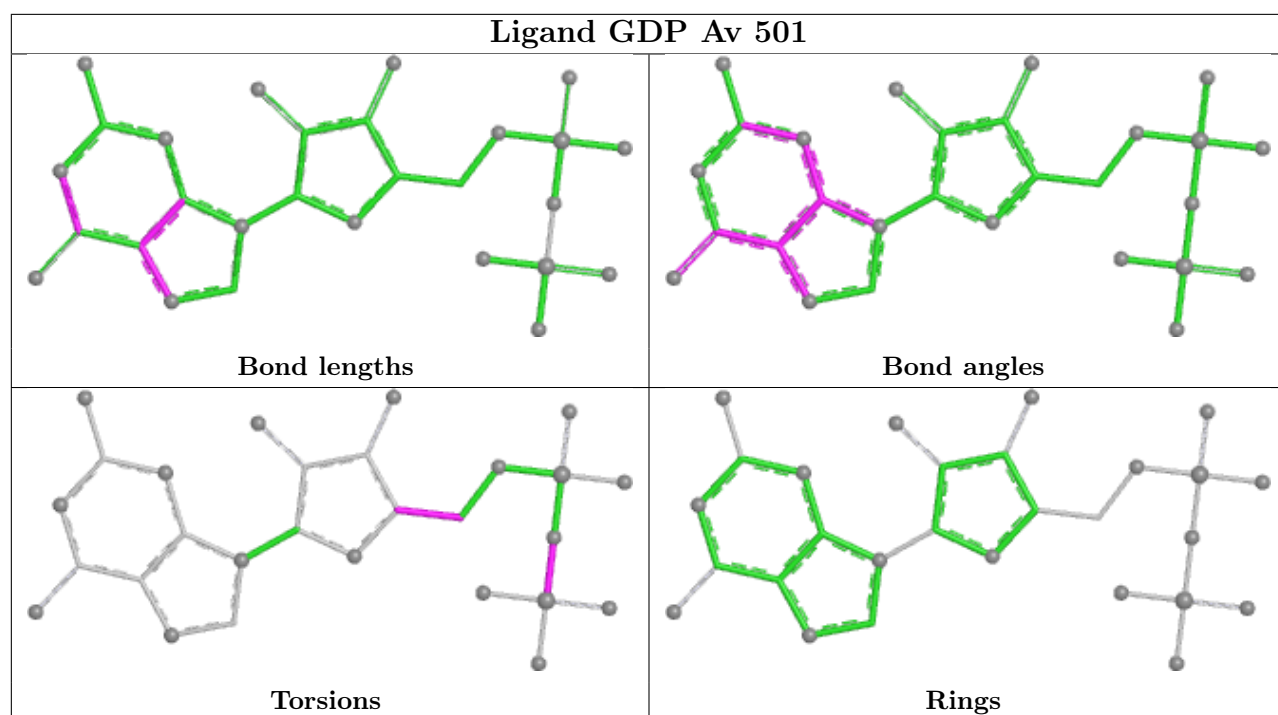
There are no ring outliers.

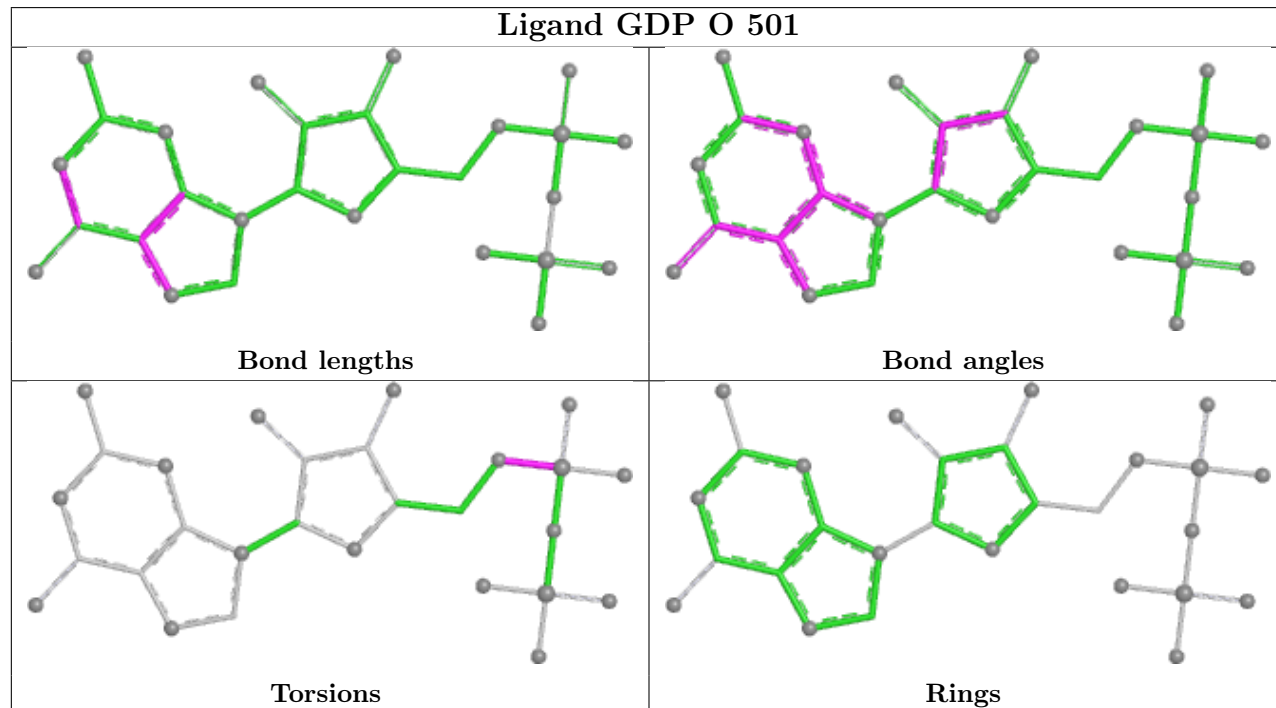
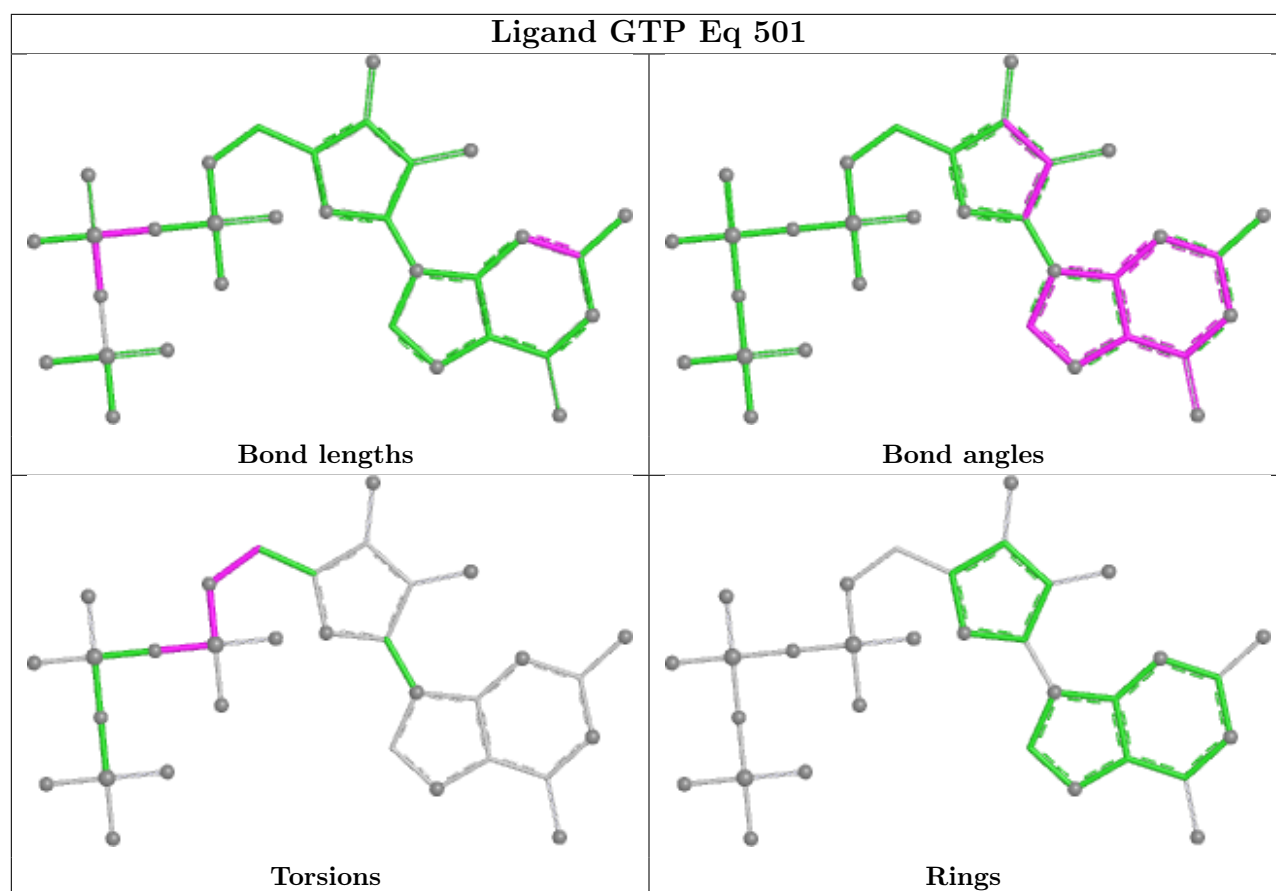
No monomer is involved in short contacts.

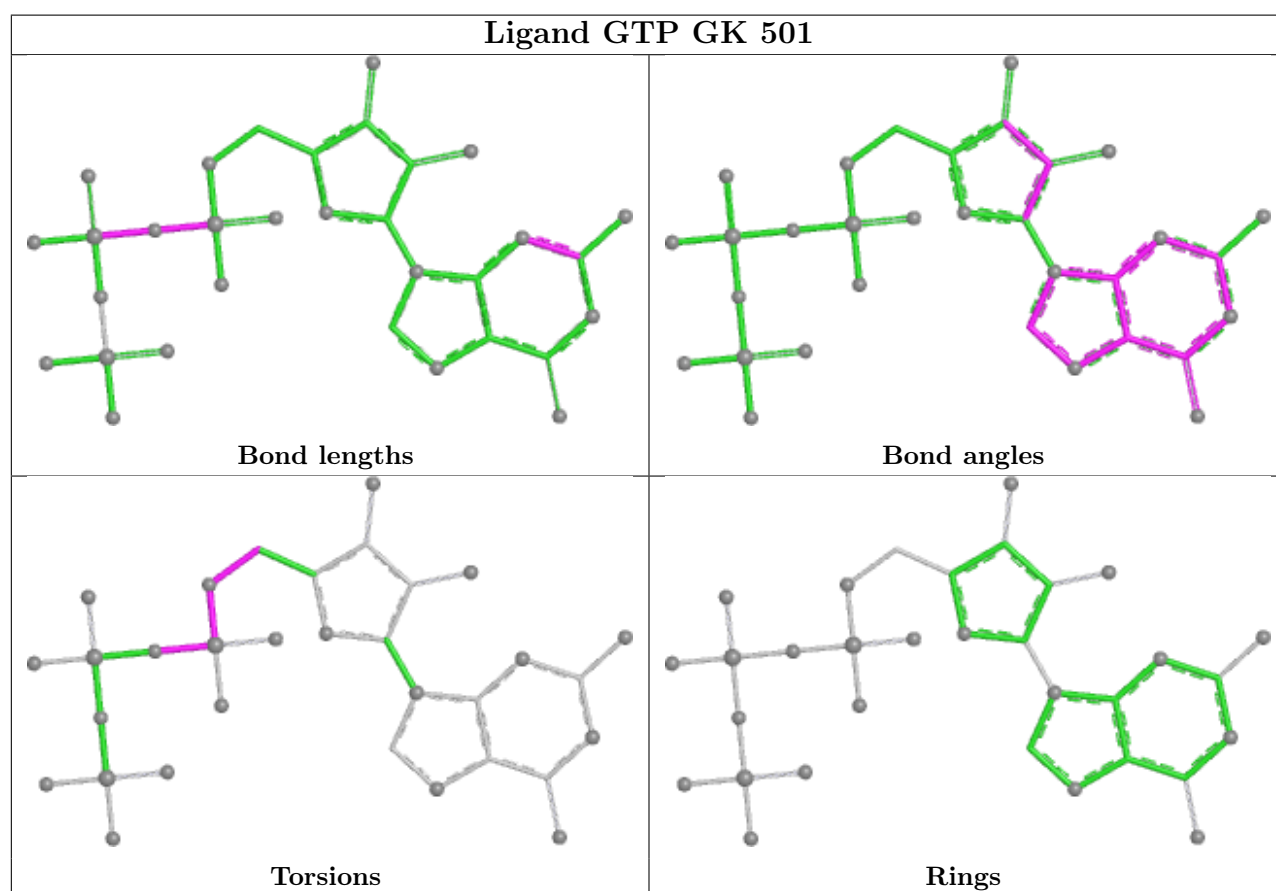
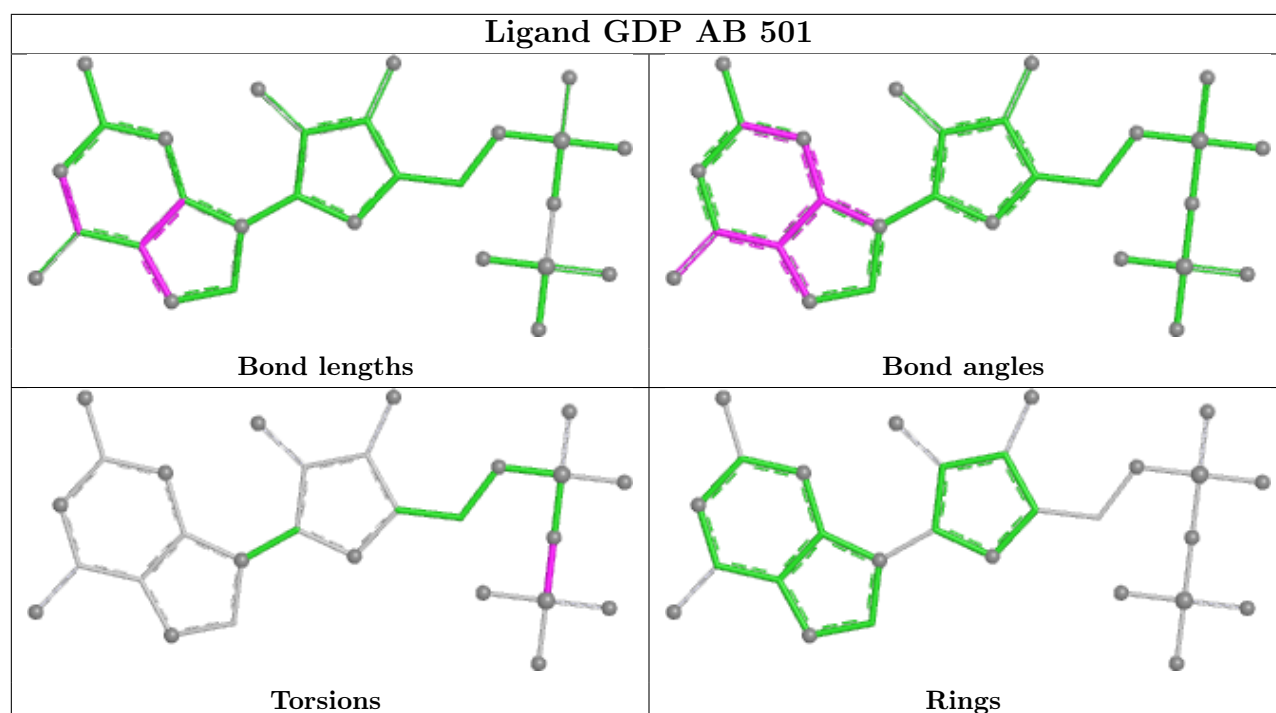
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

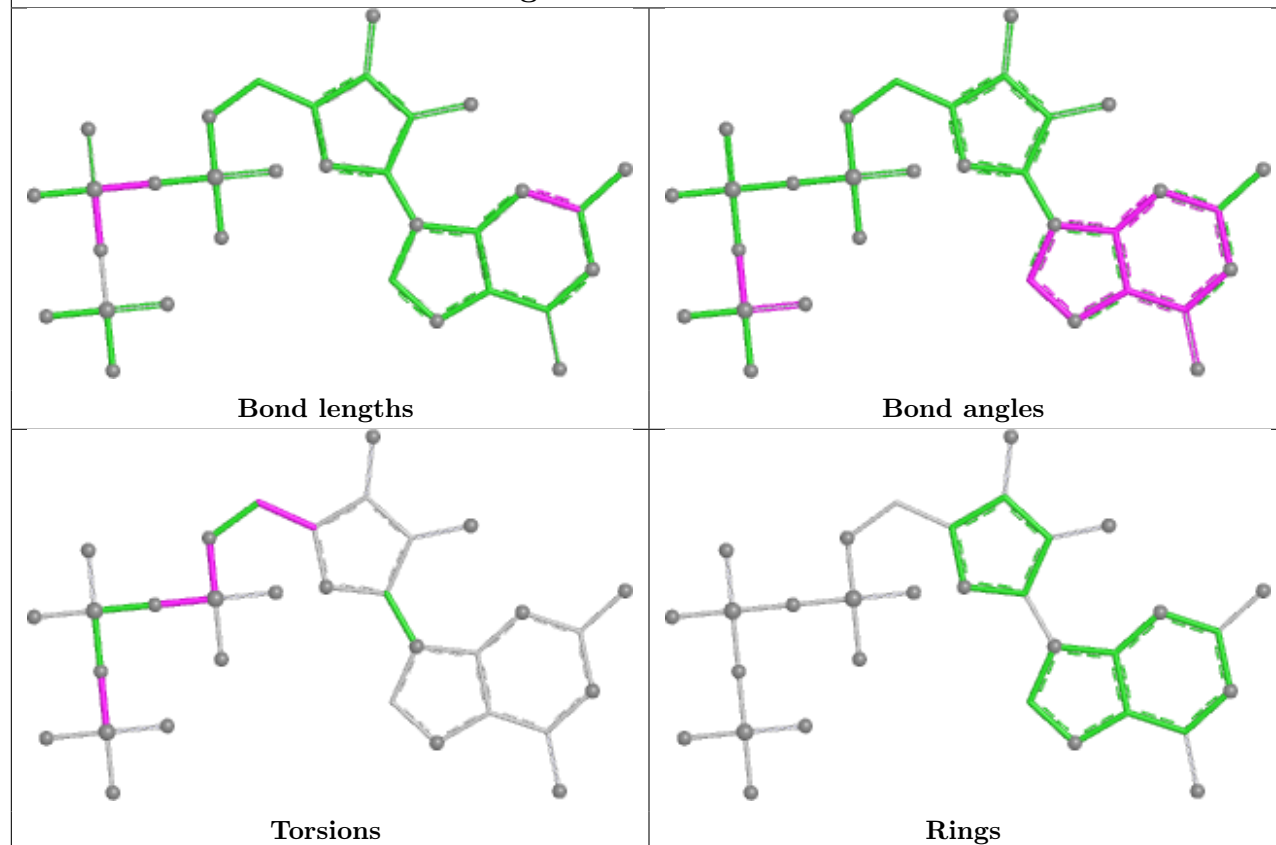




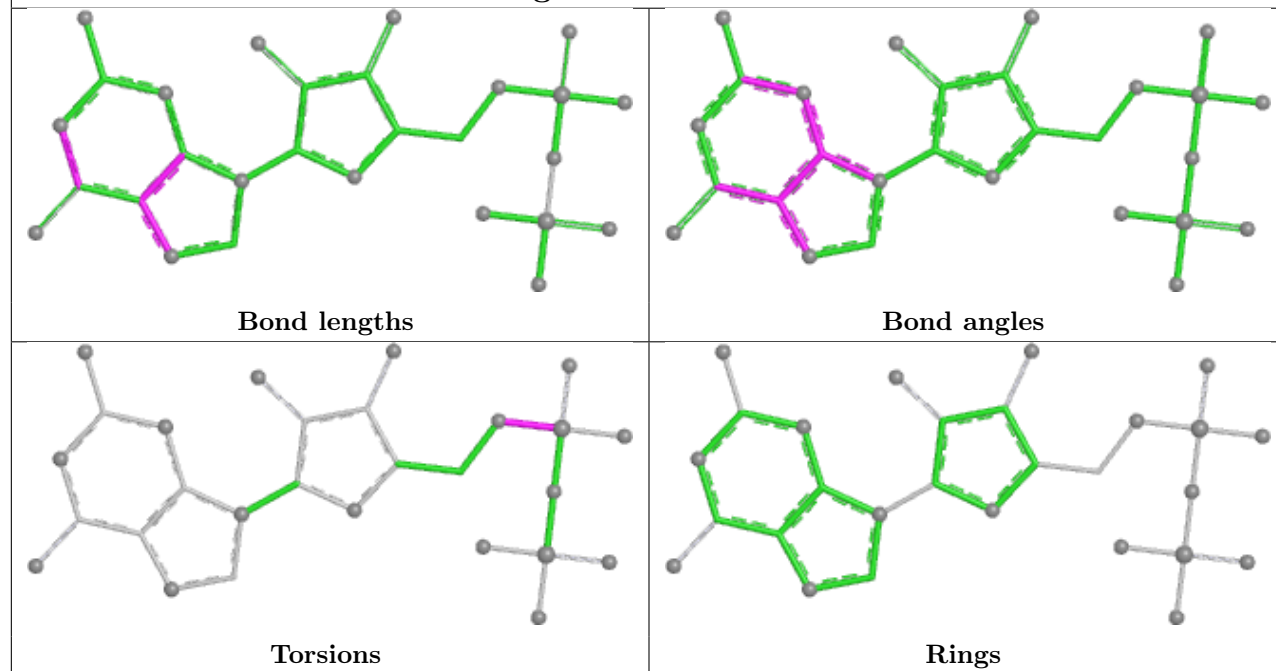


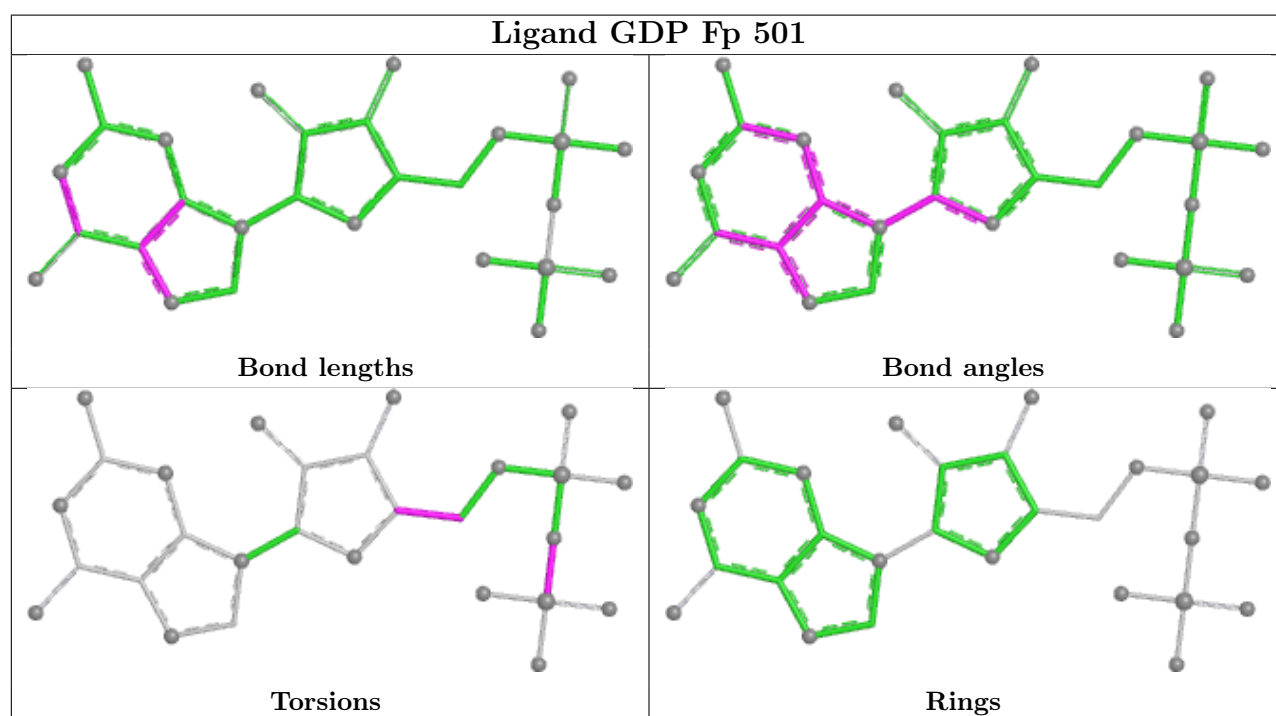
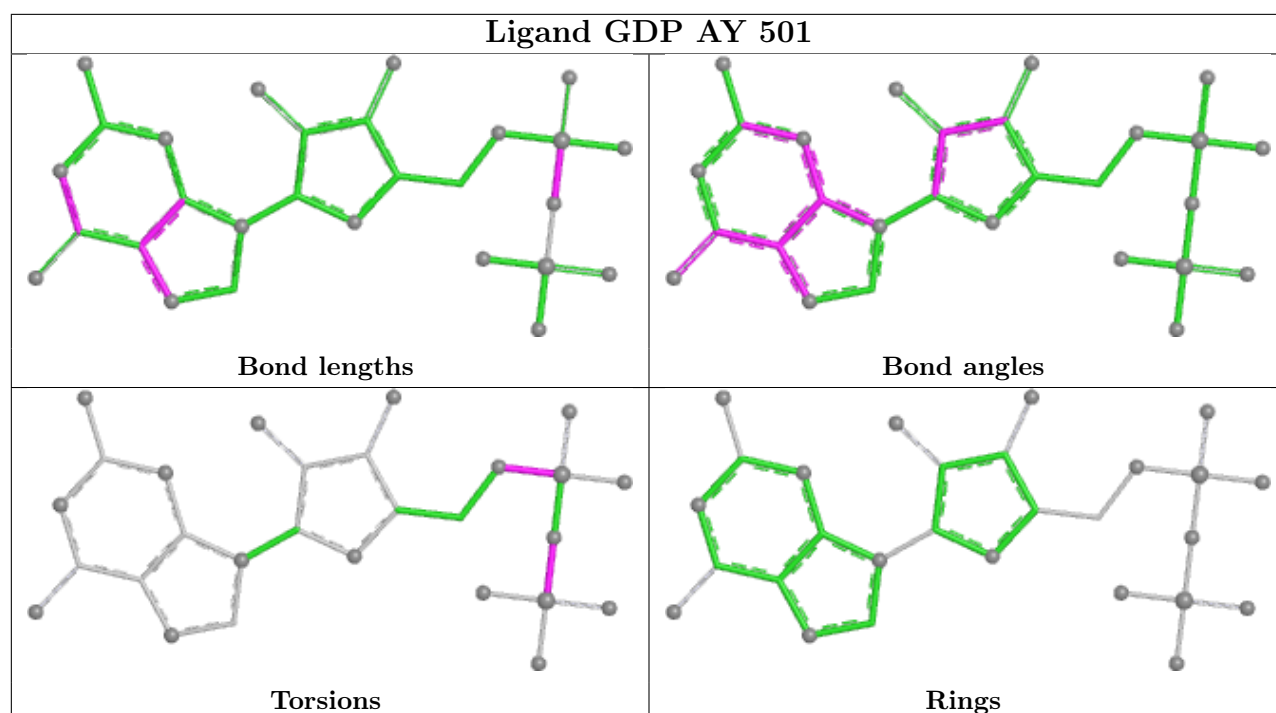


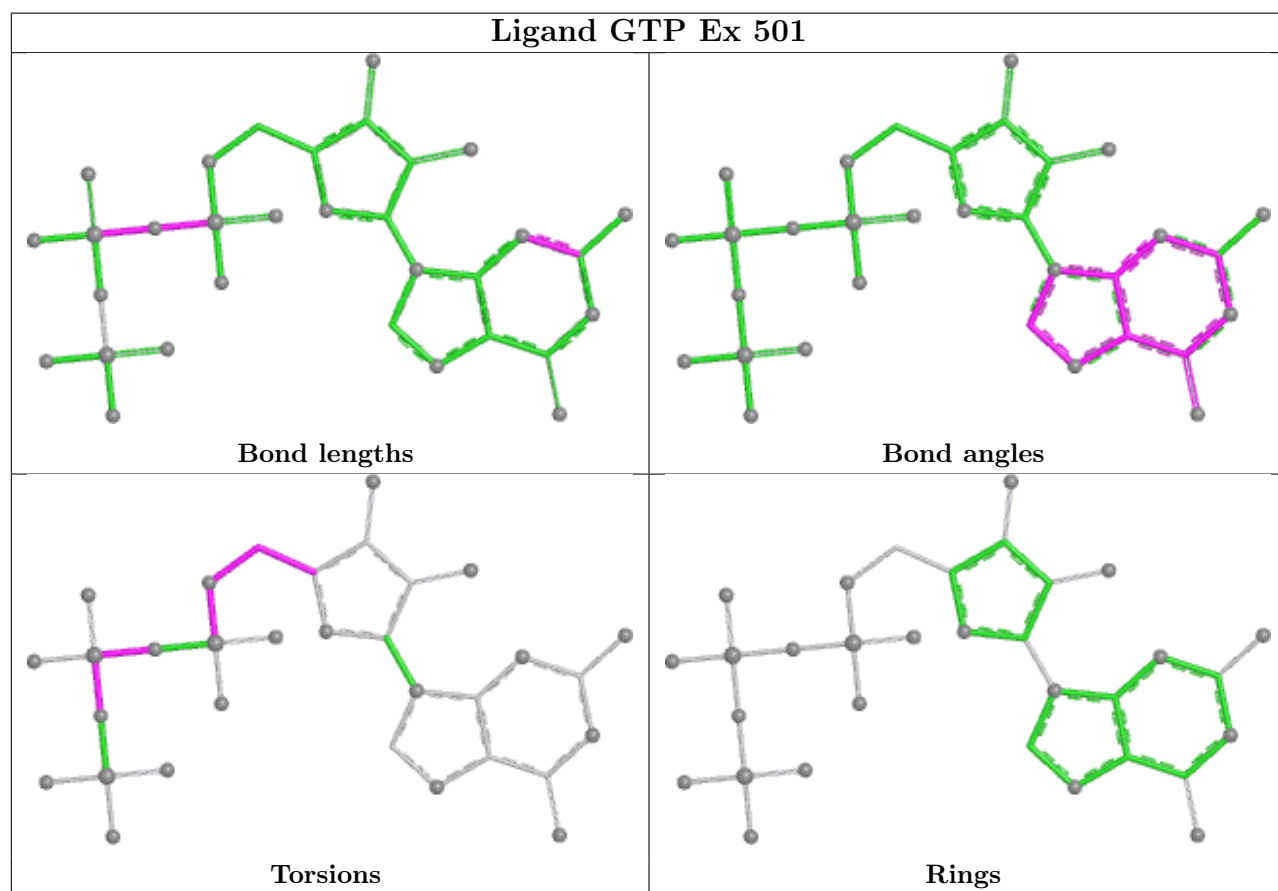
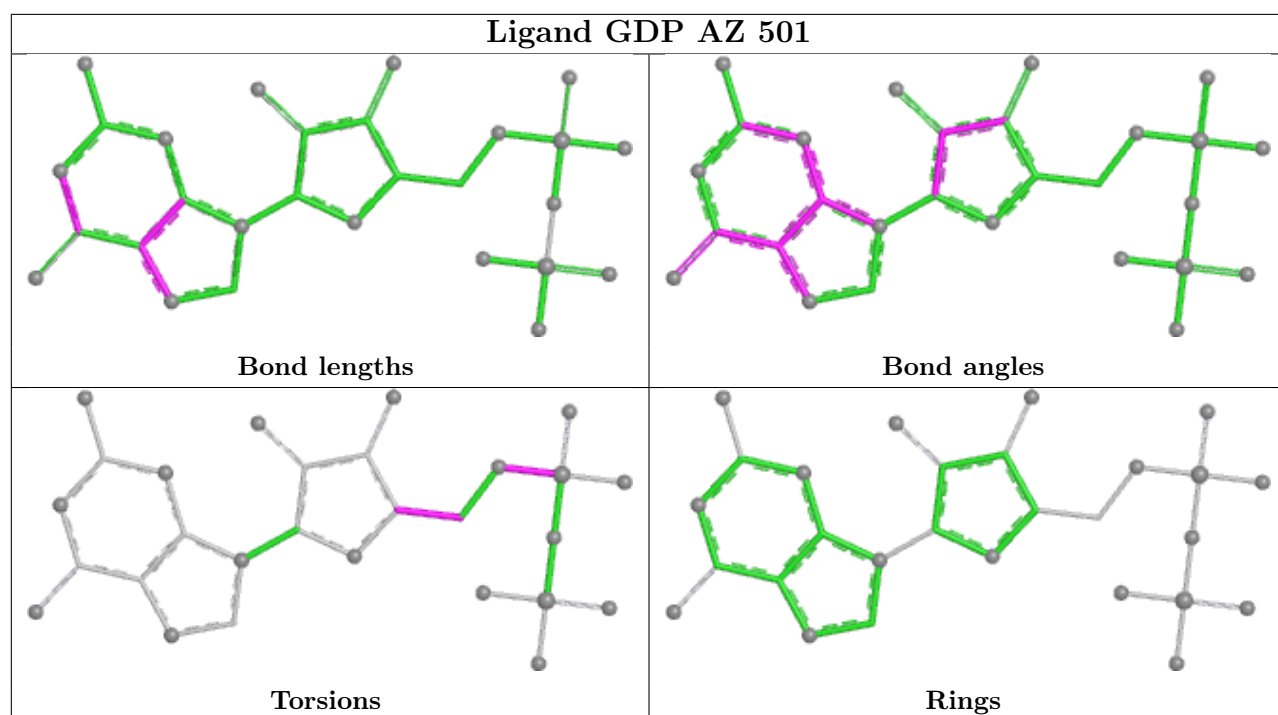
Ligand GTP BL 602

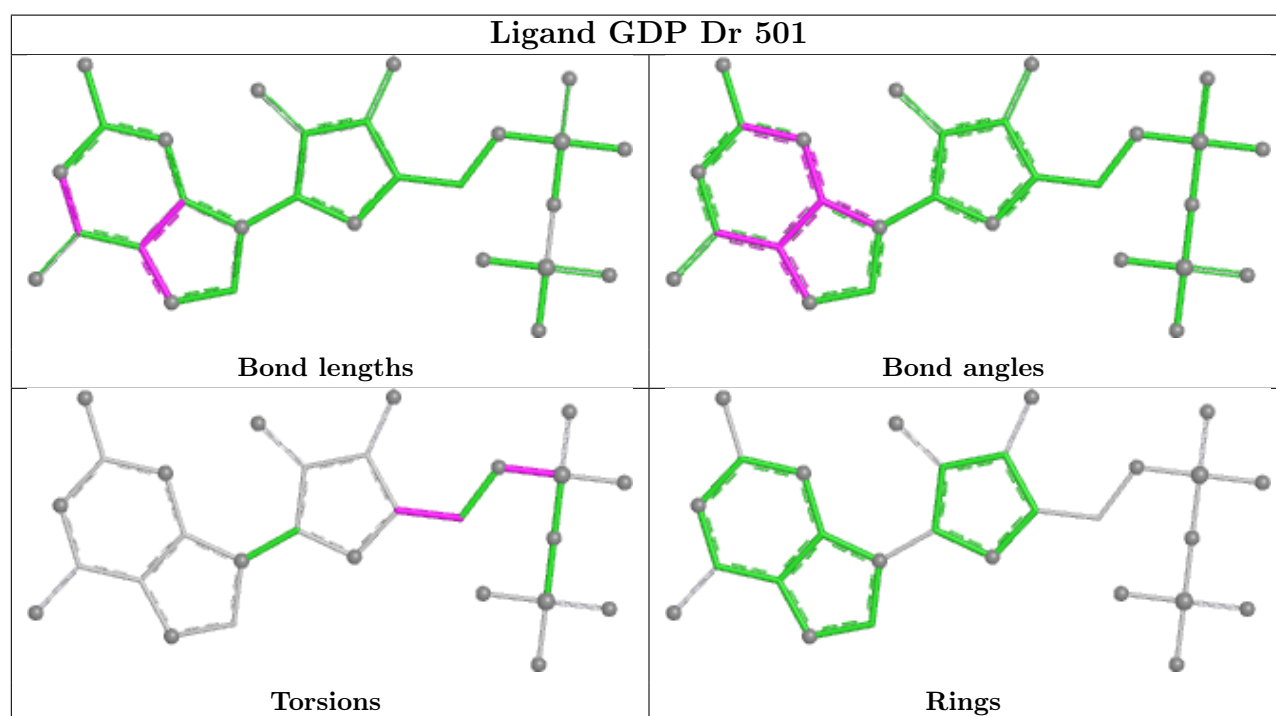
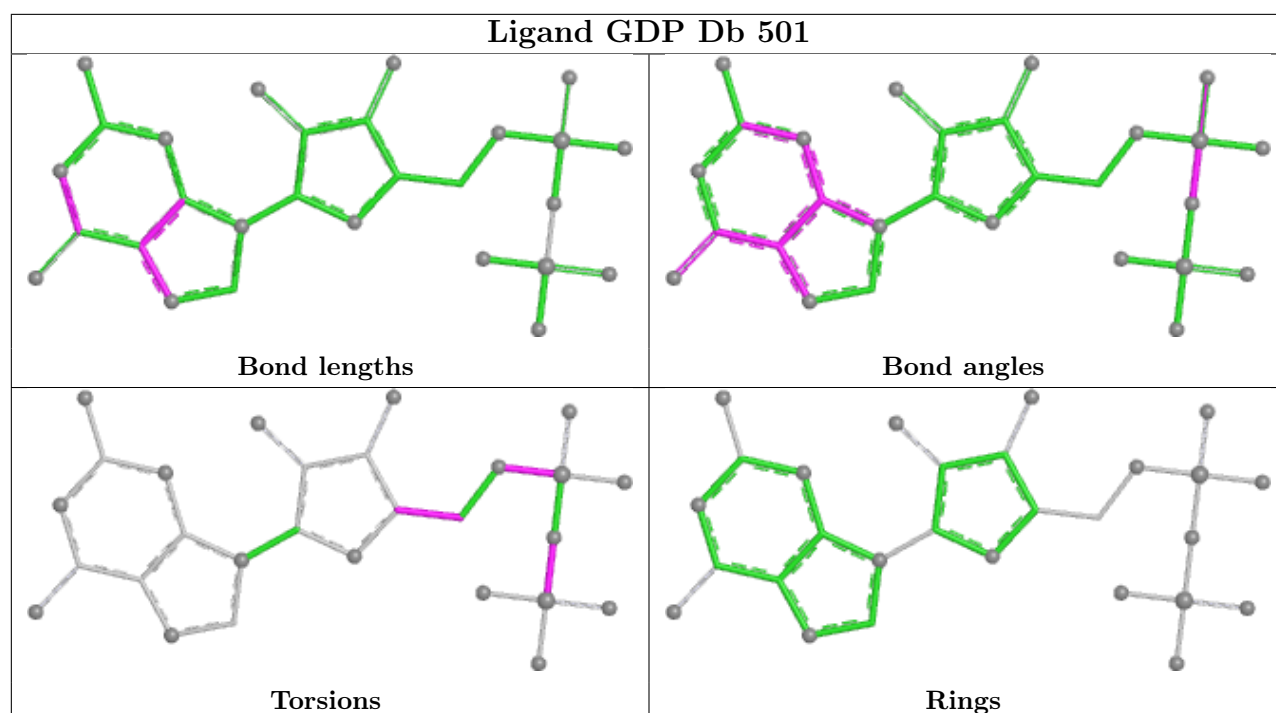


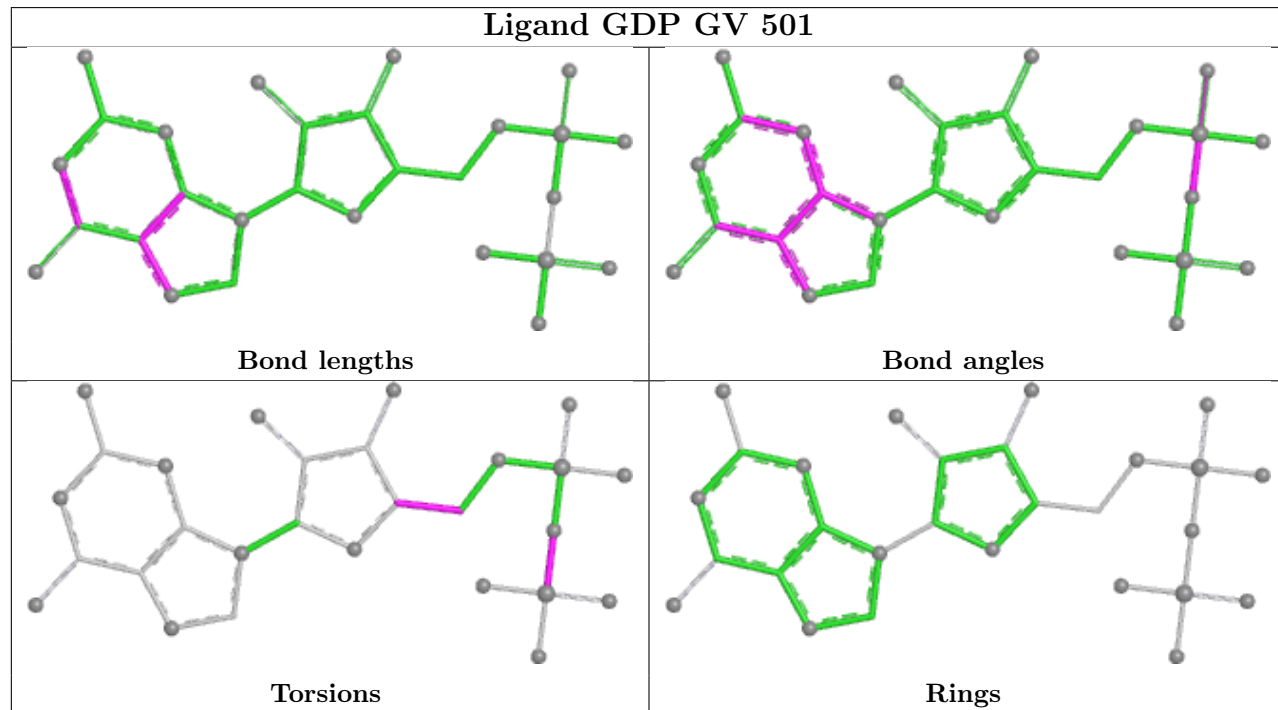
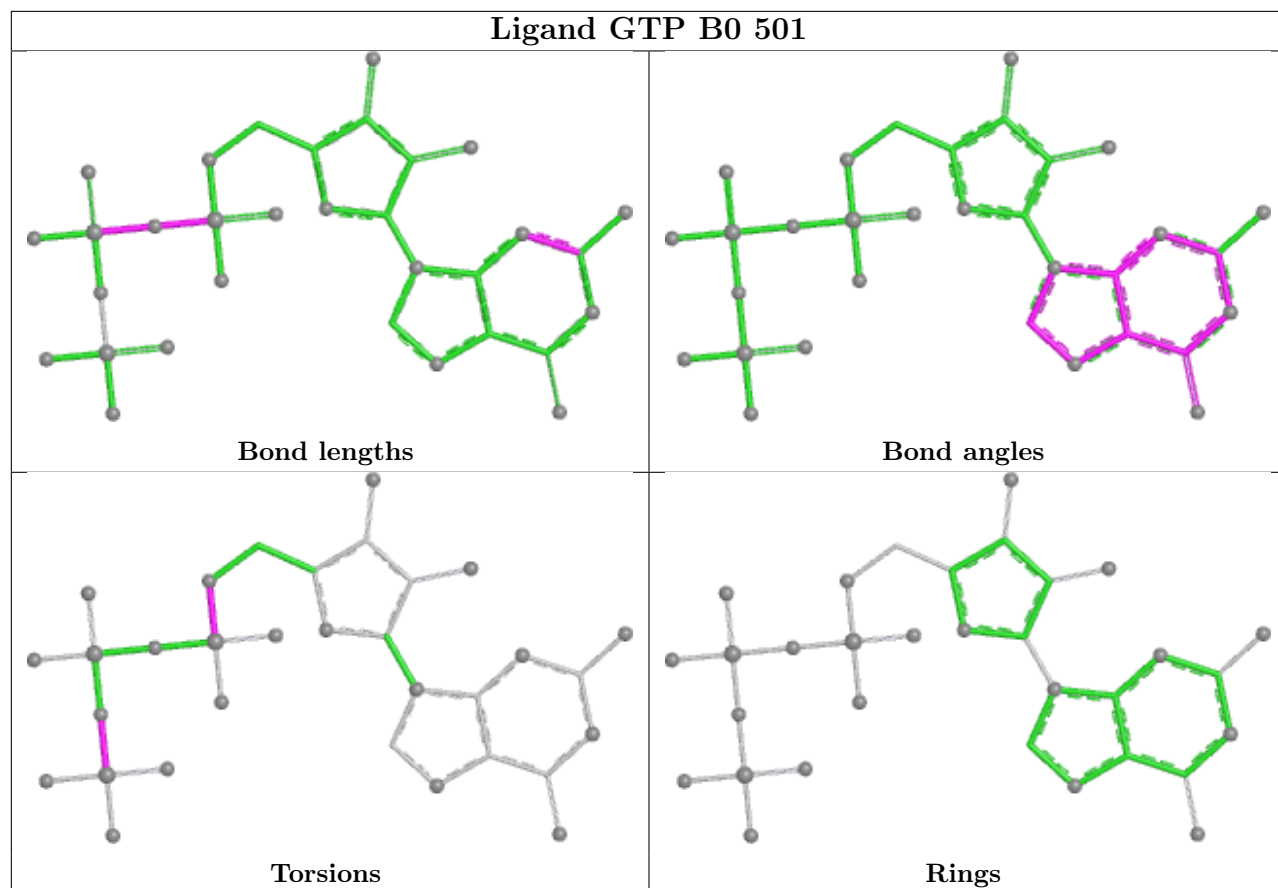
Ligand GDP 9 501



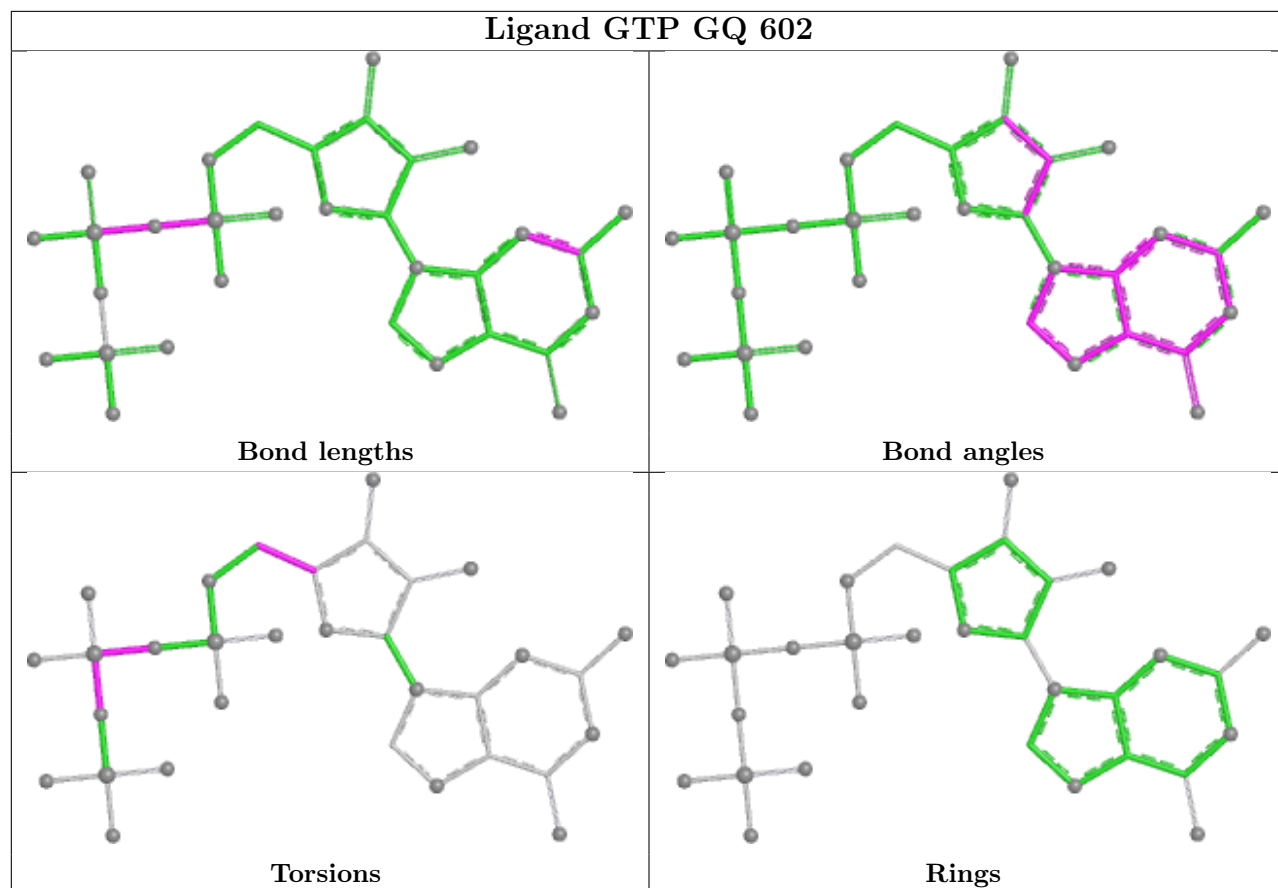




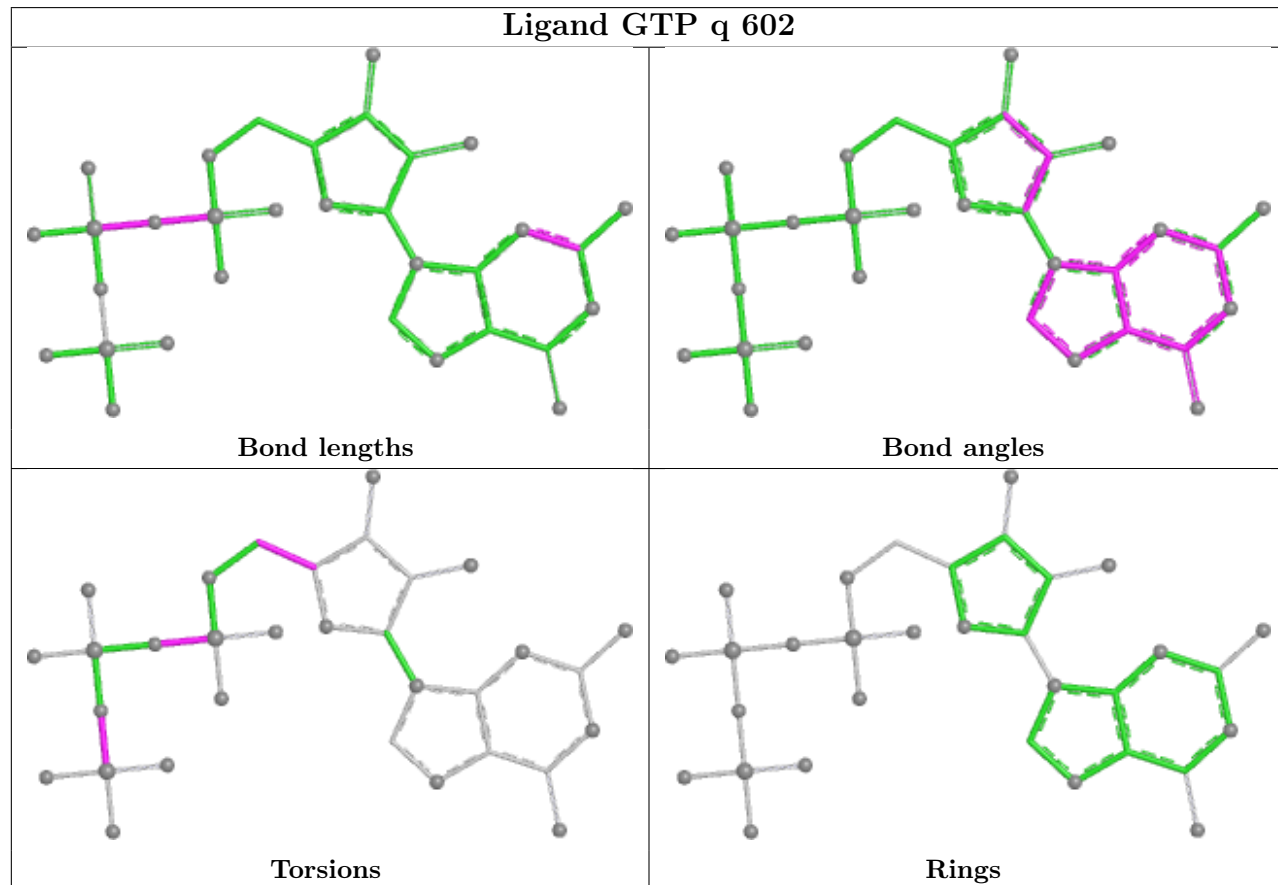


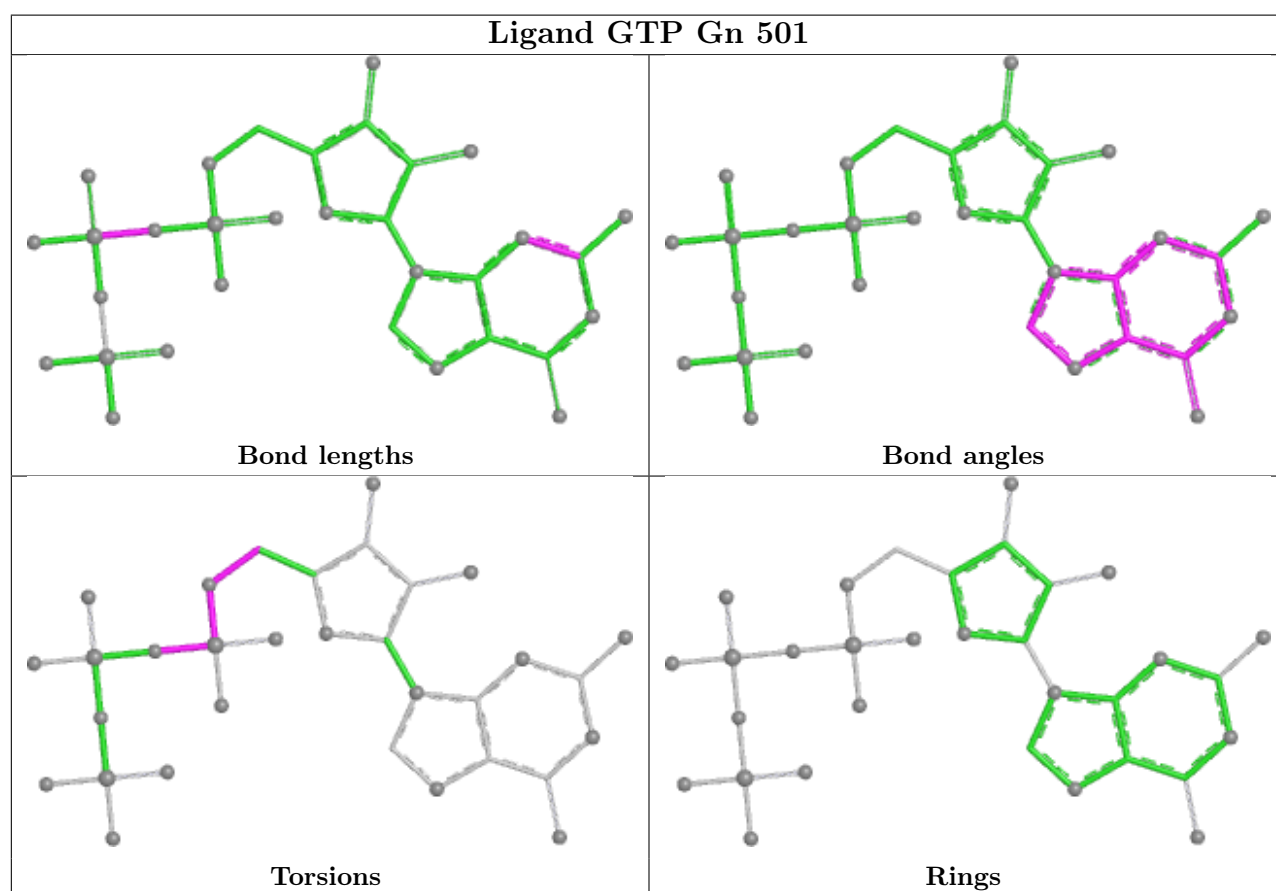
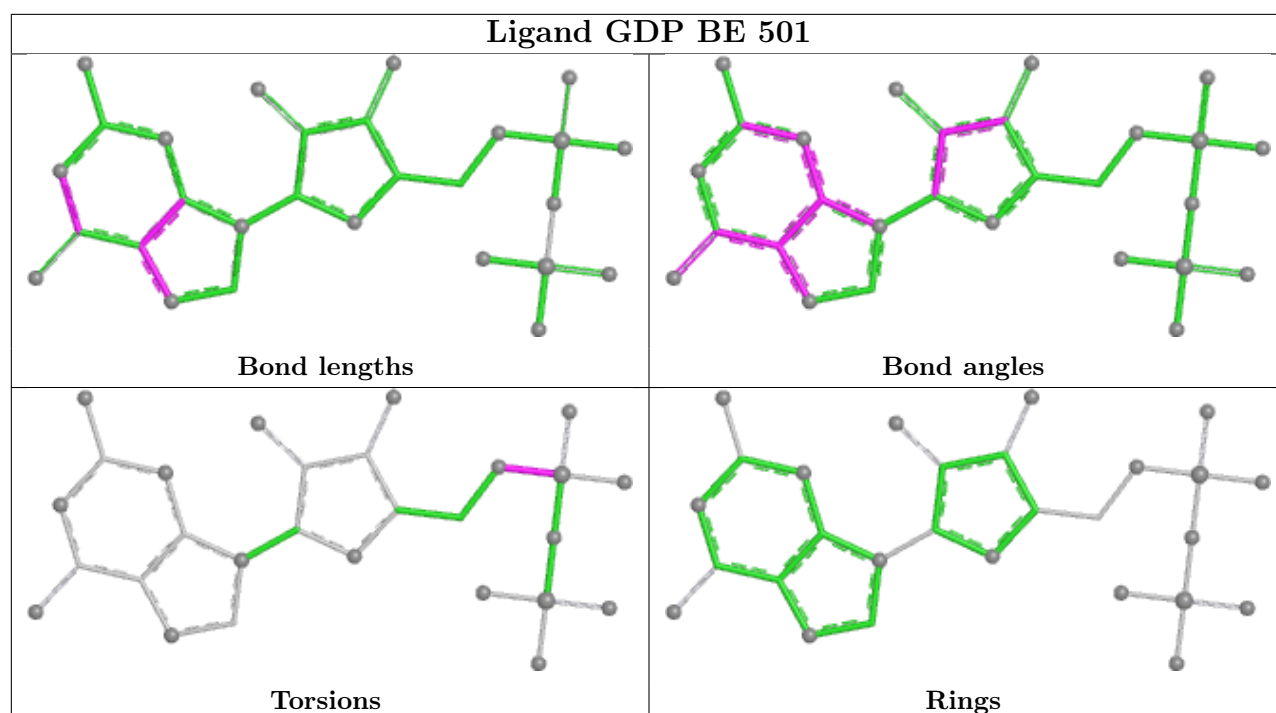


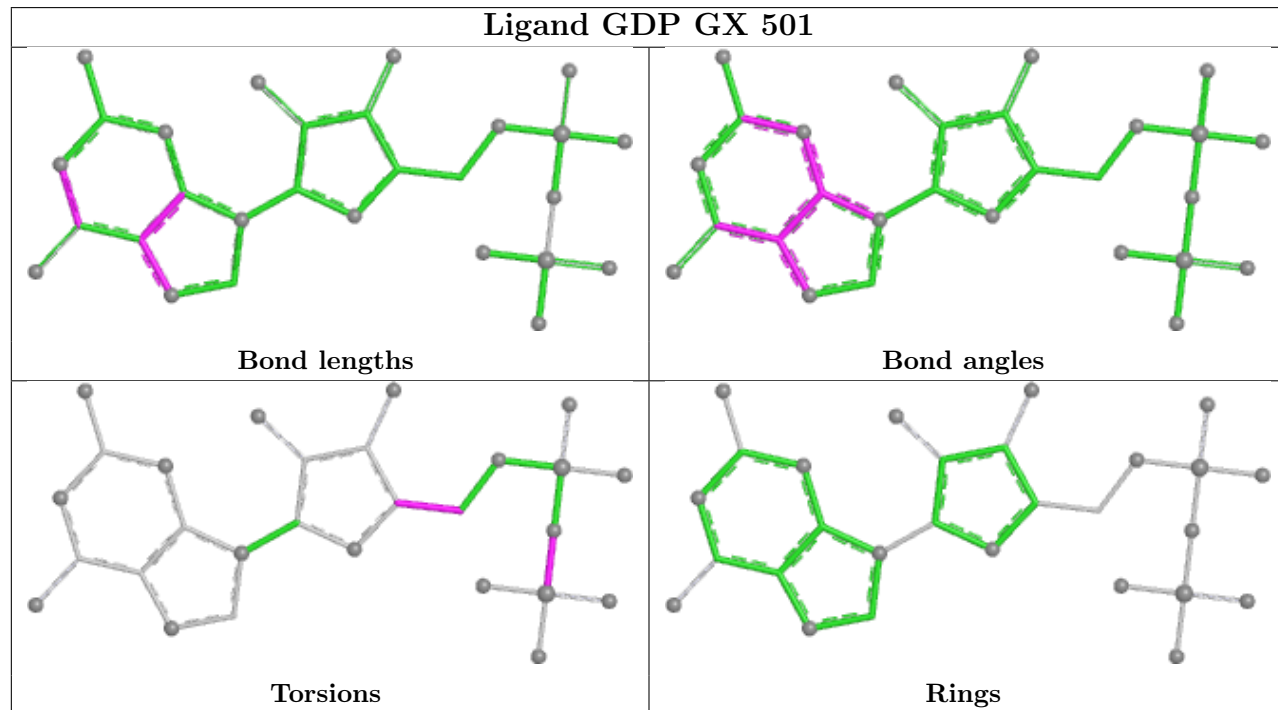
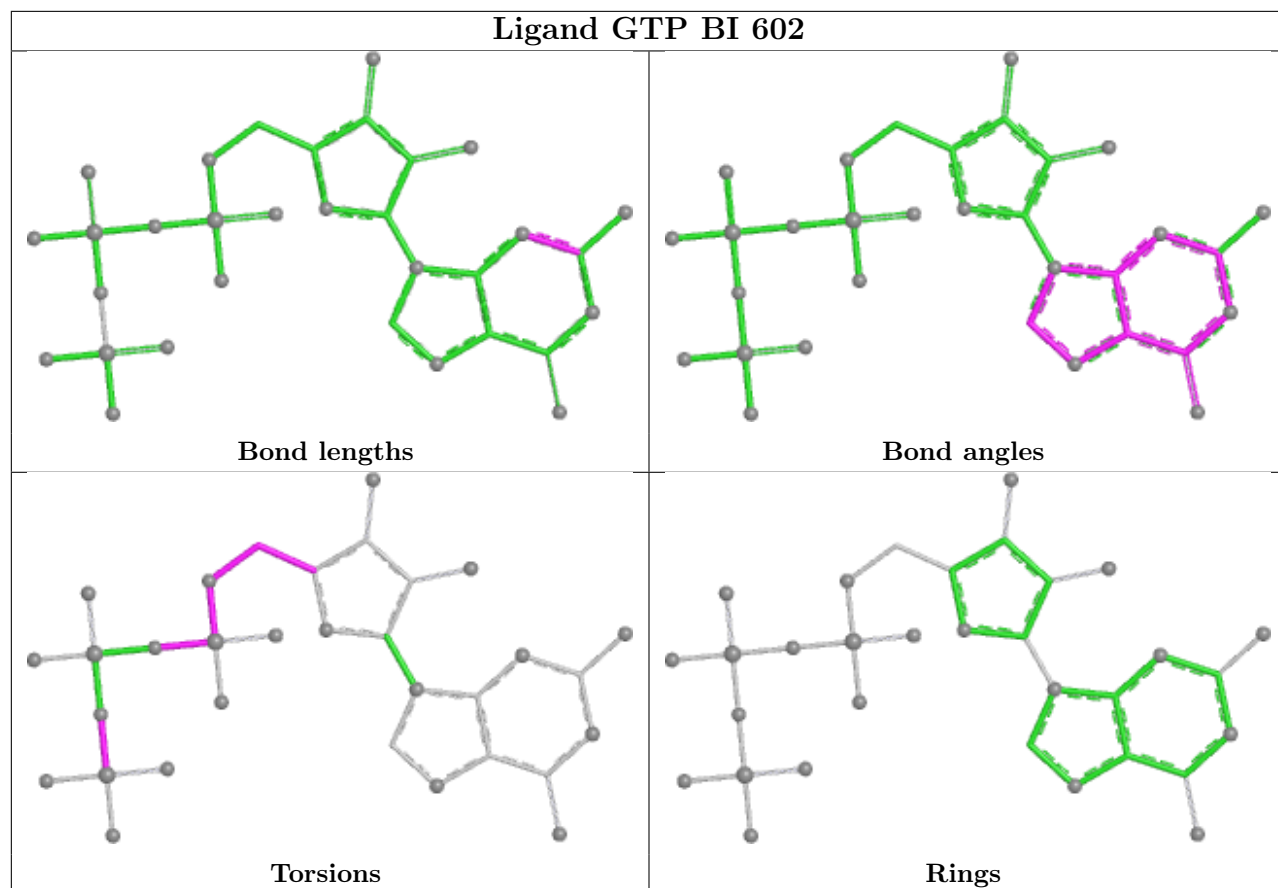
Ligand GTP GQ 602

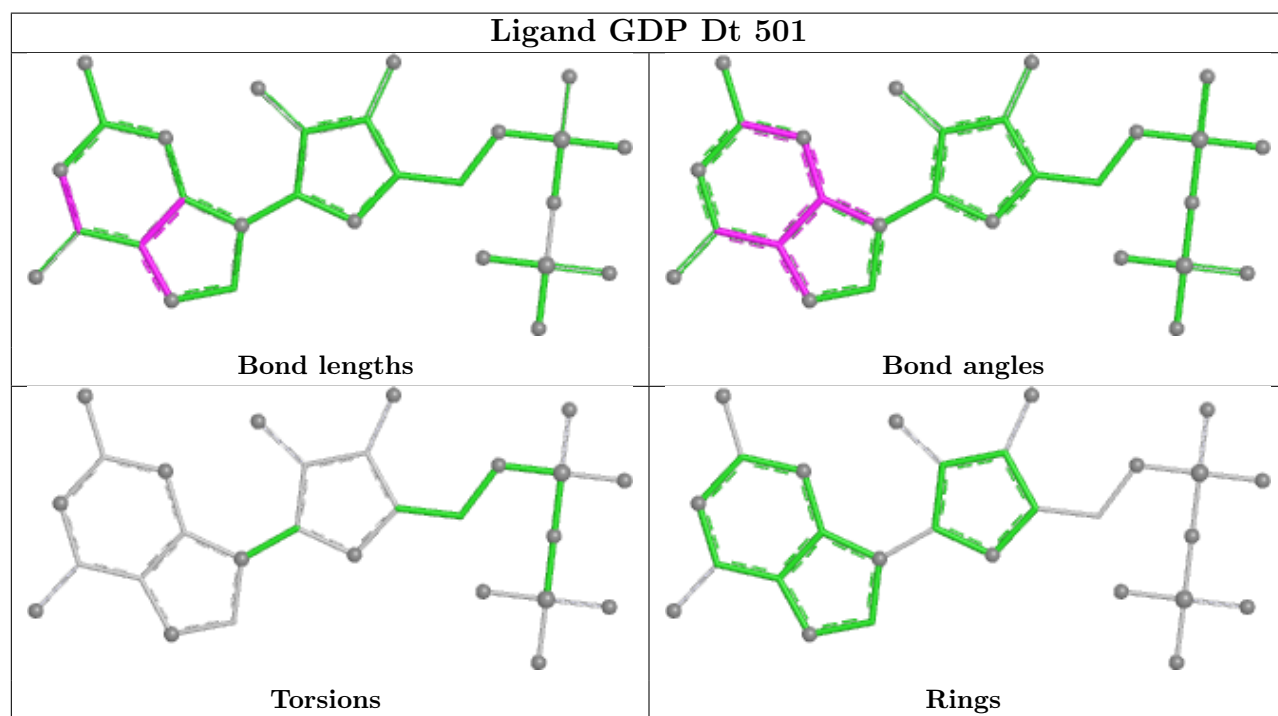
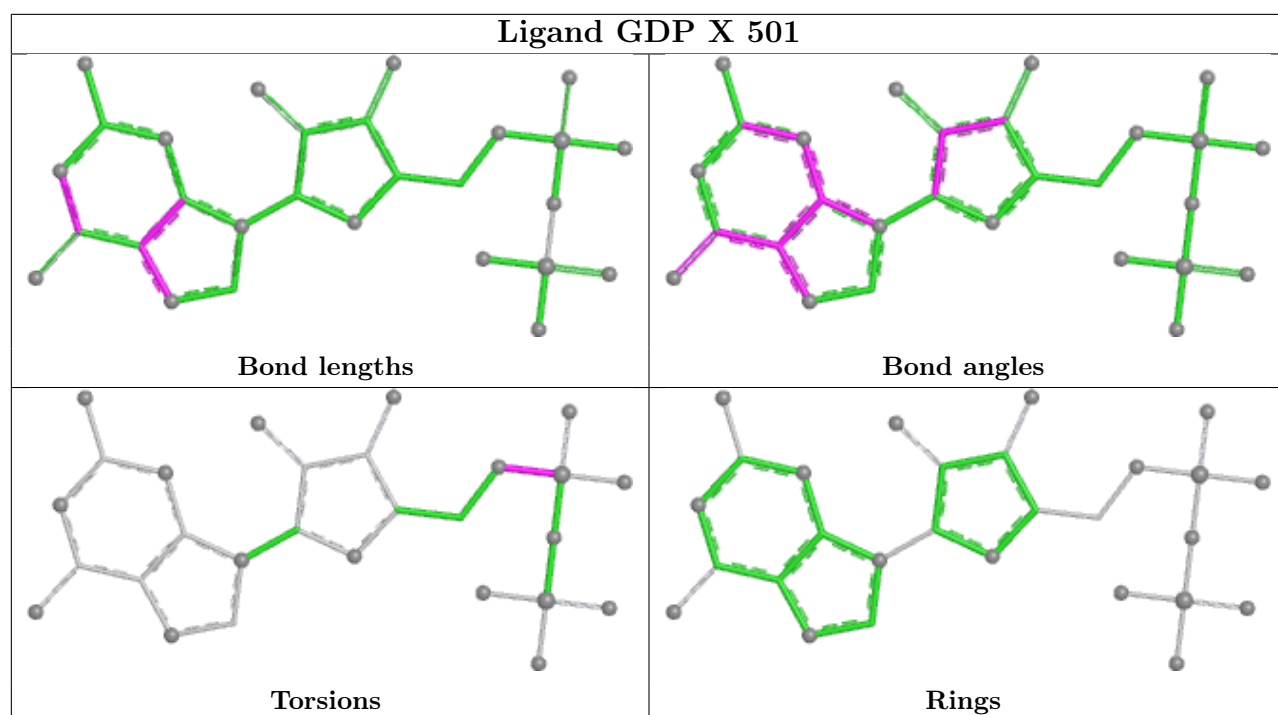


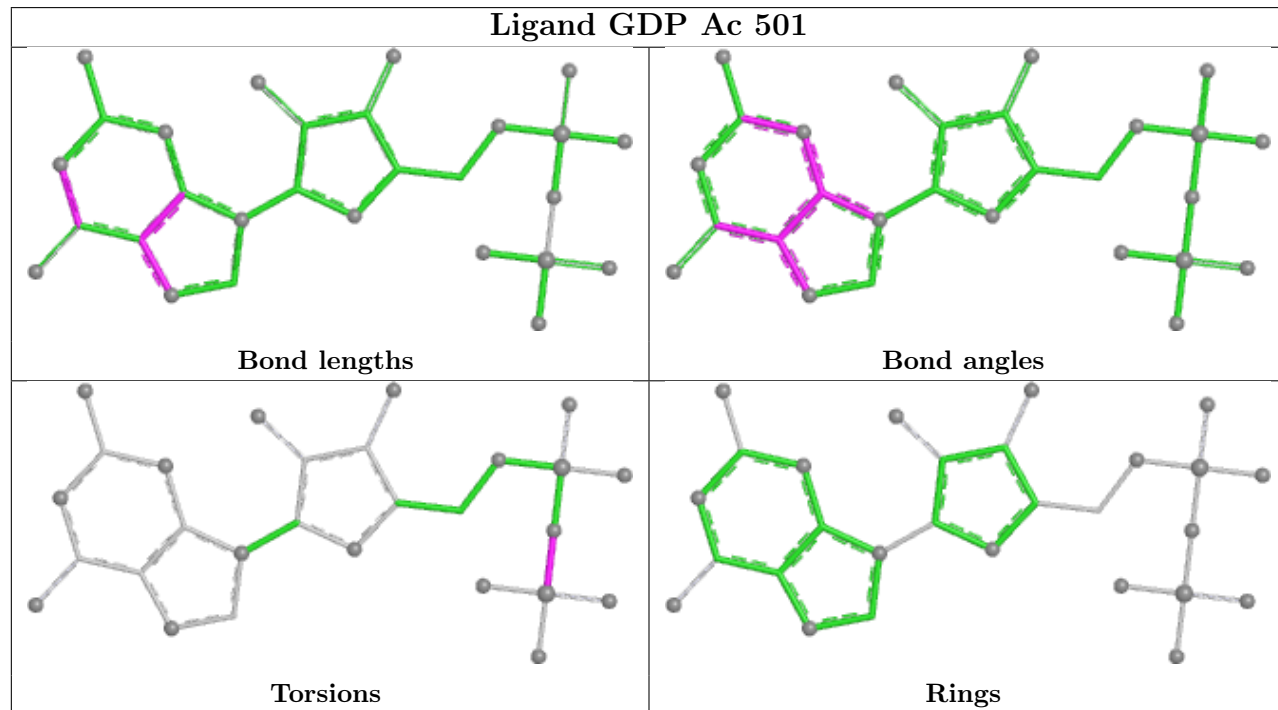
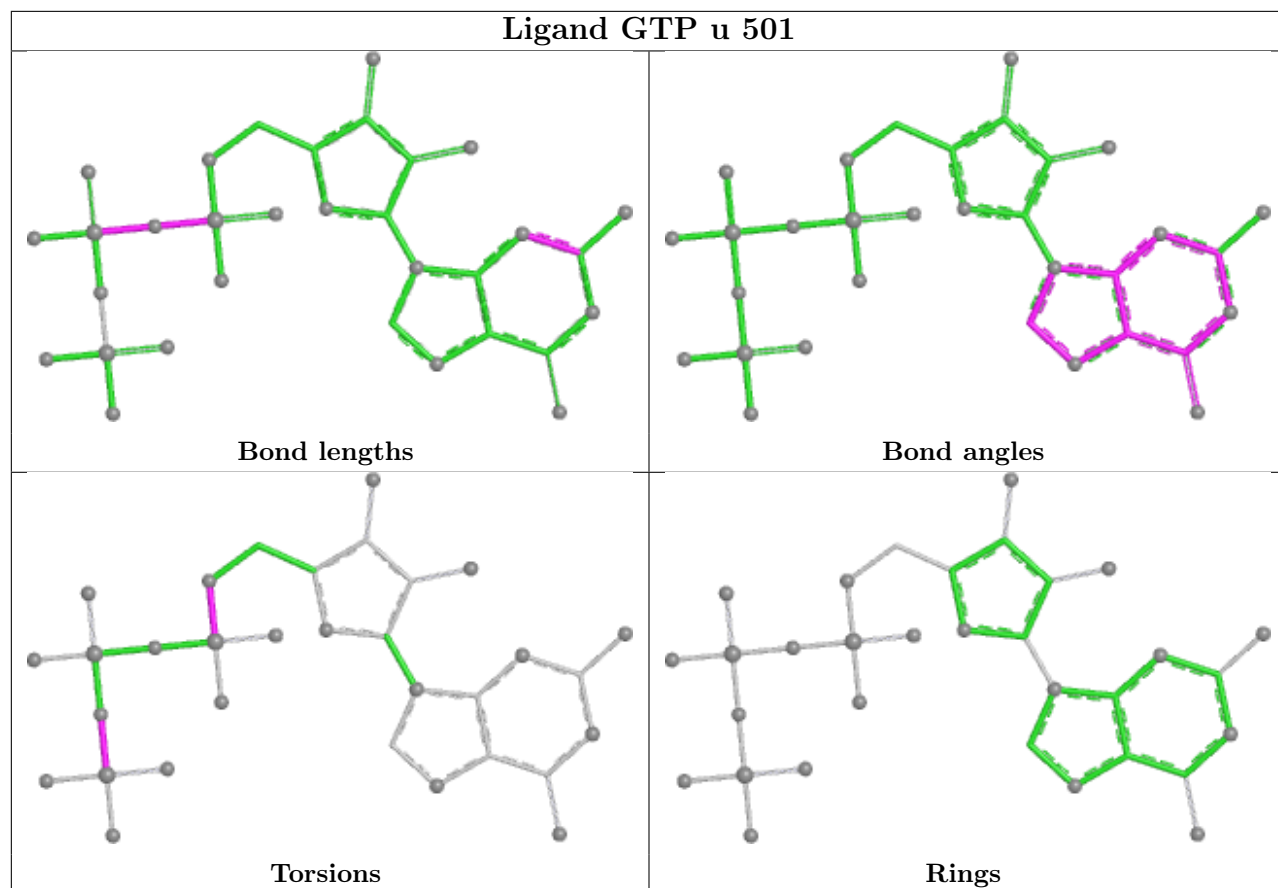
Ligand GTP q 602



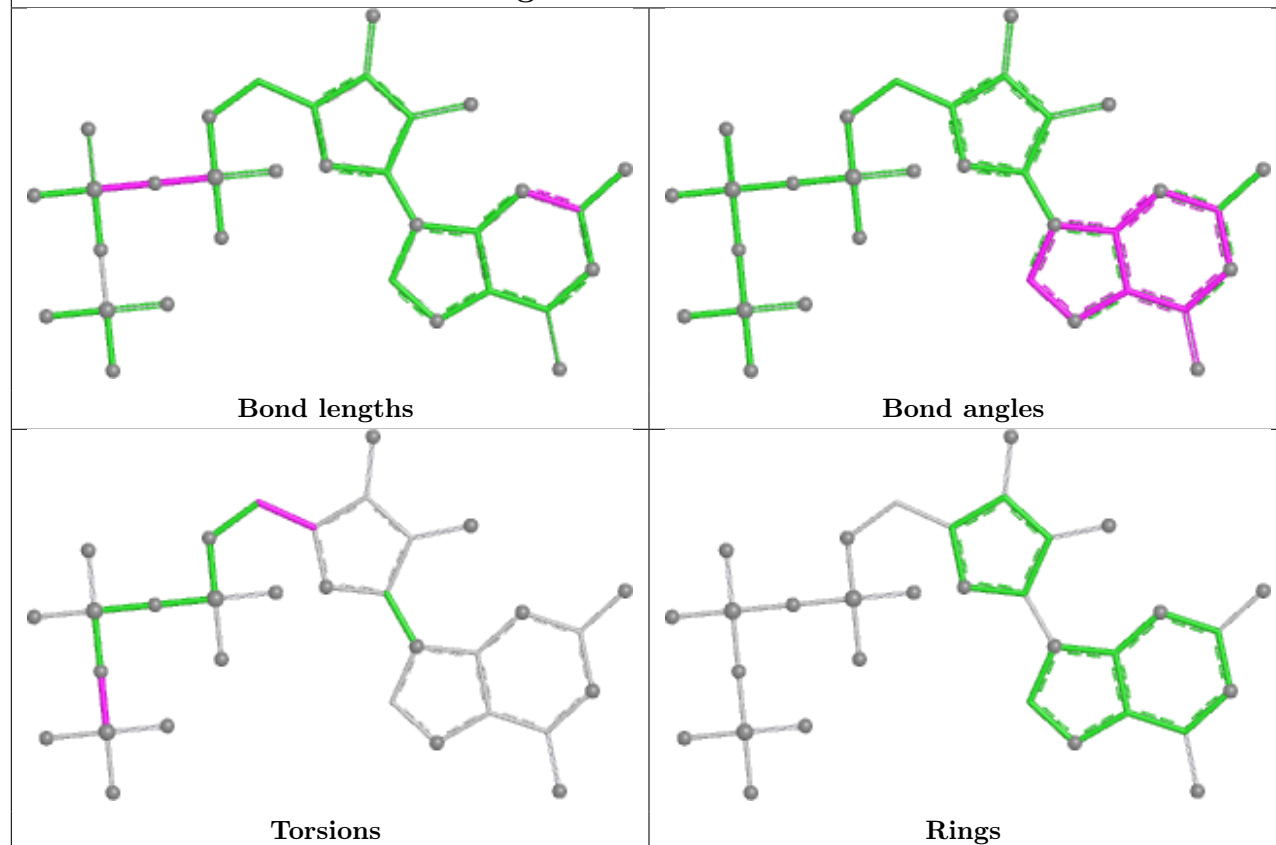




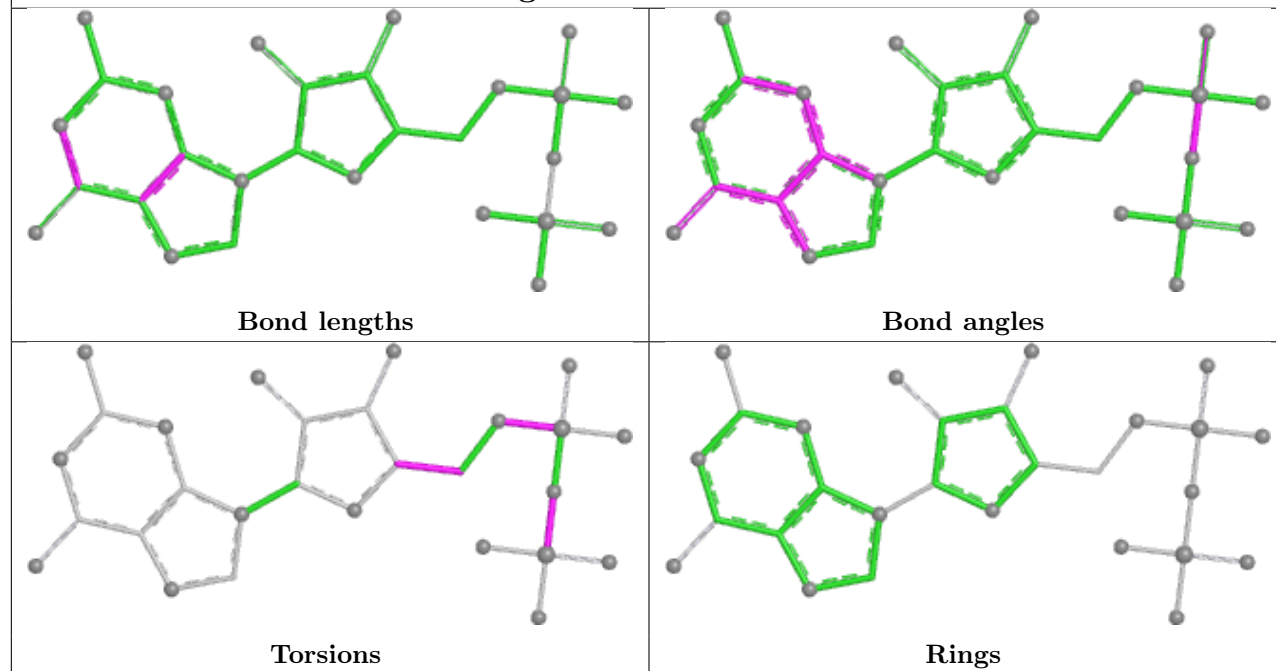


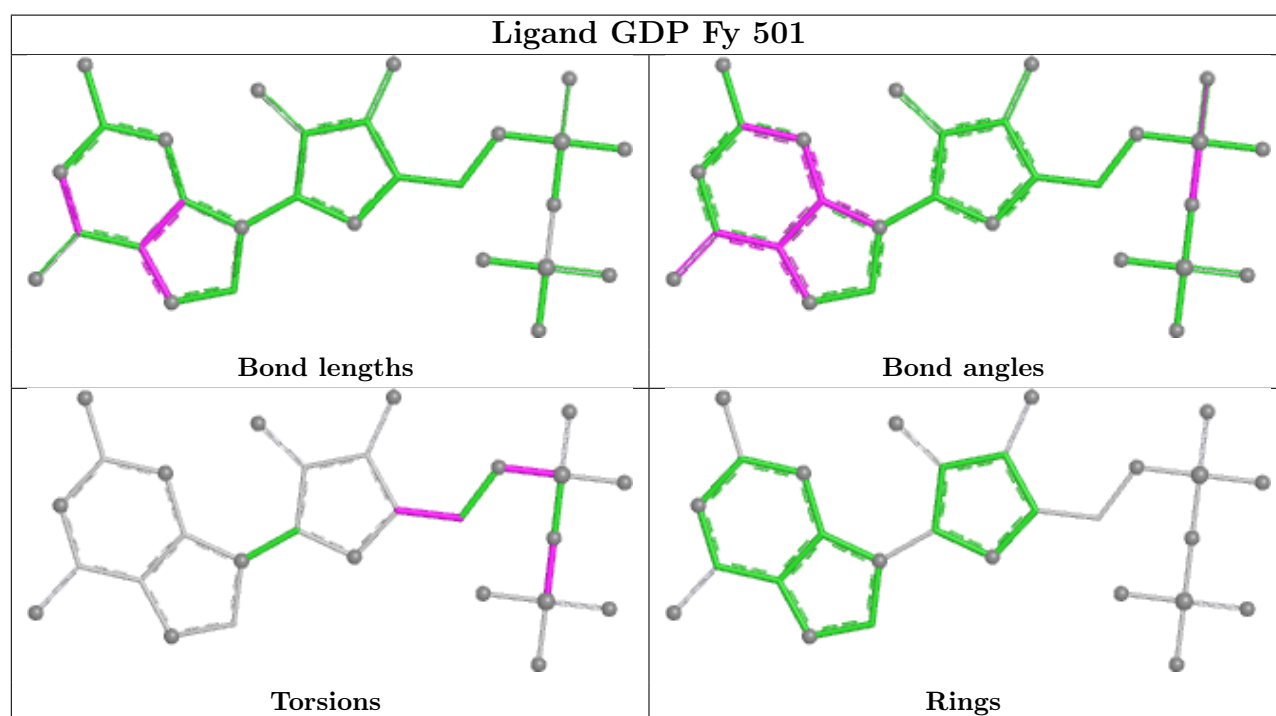
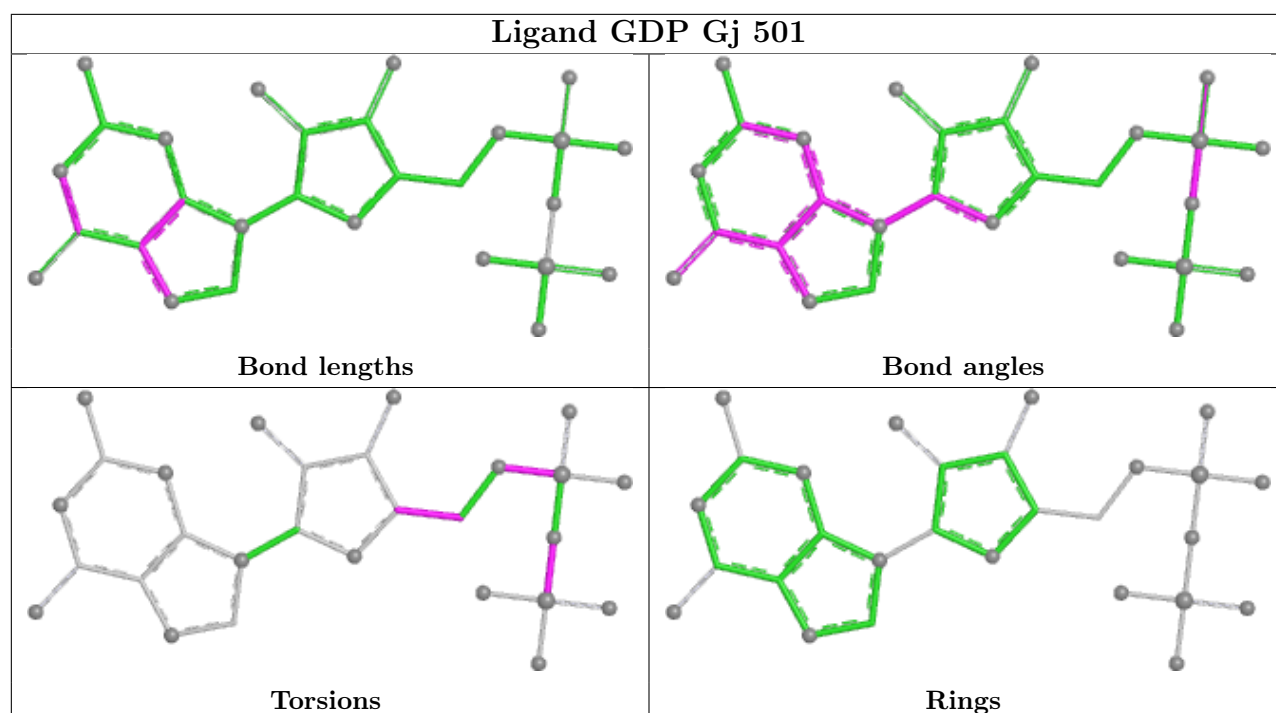


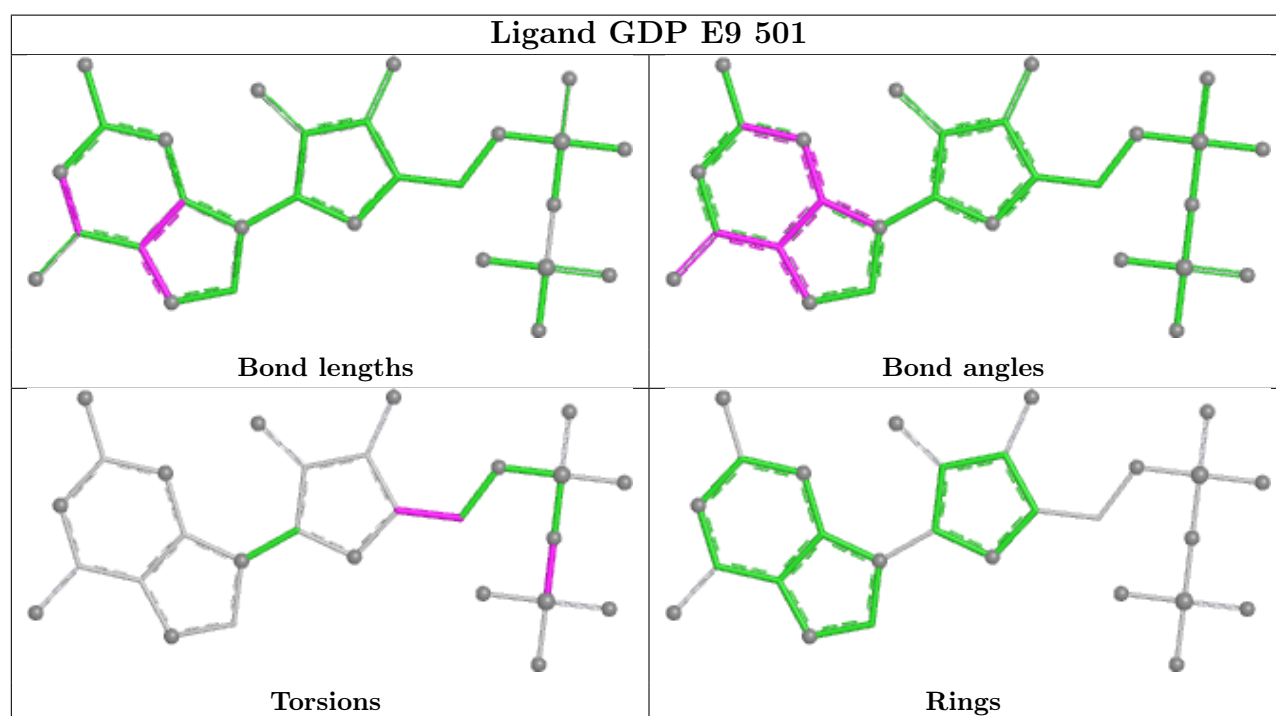
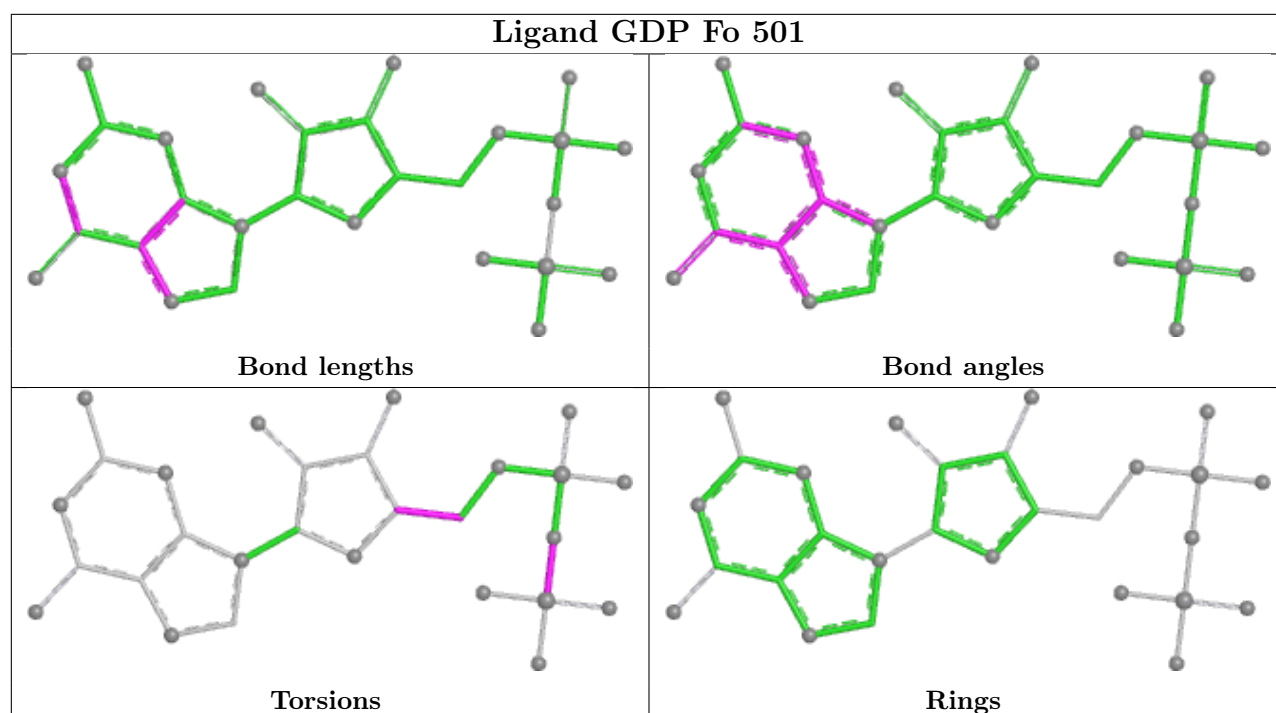
Ligand GTP BK 602

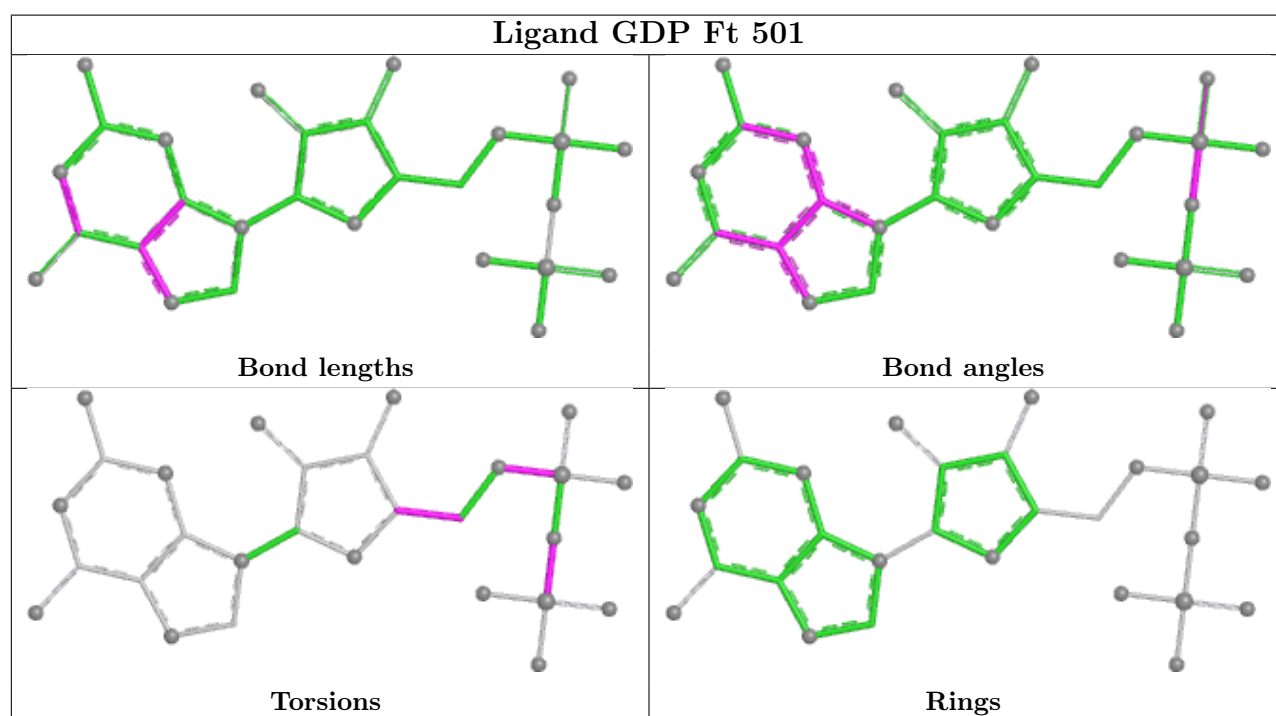
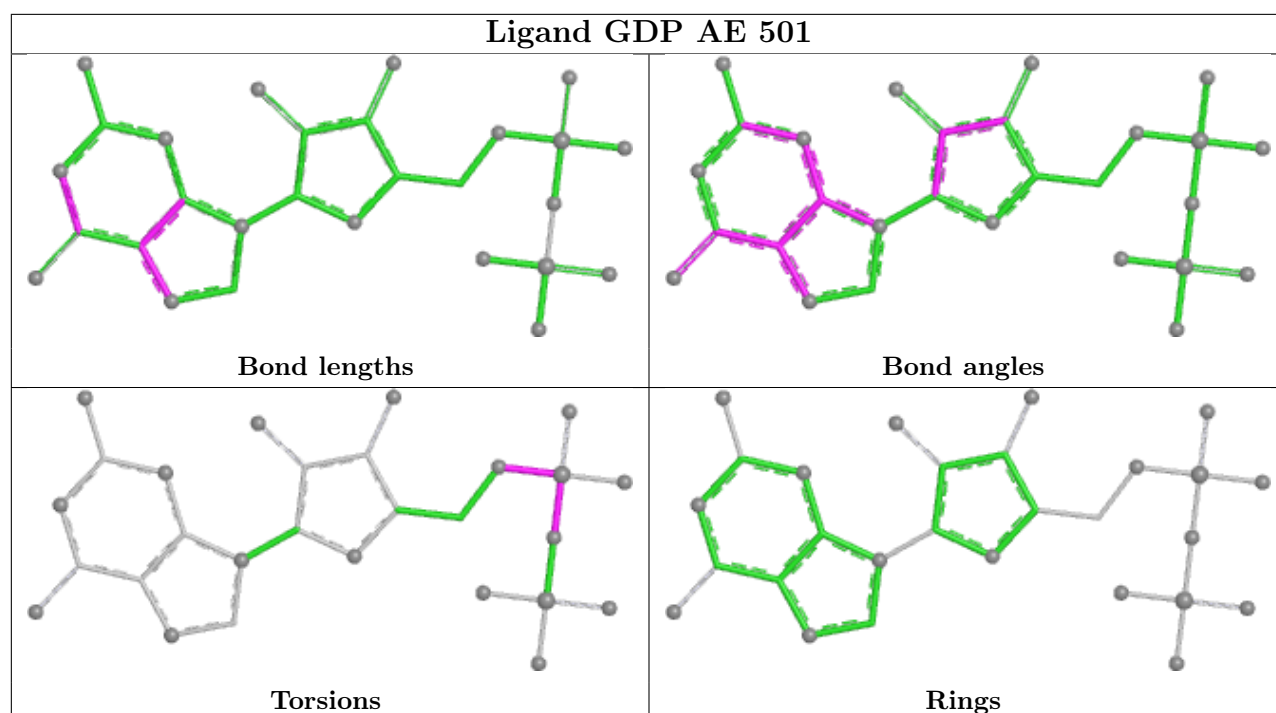


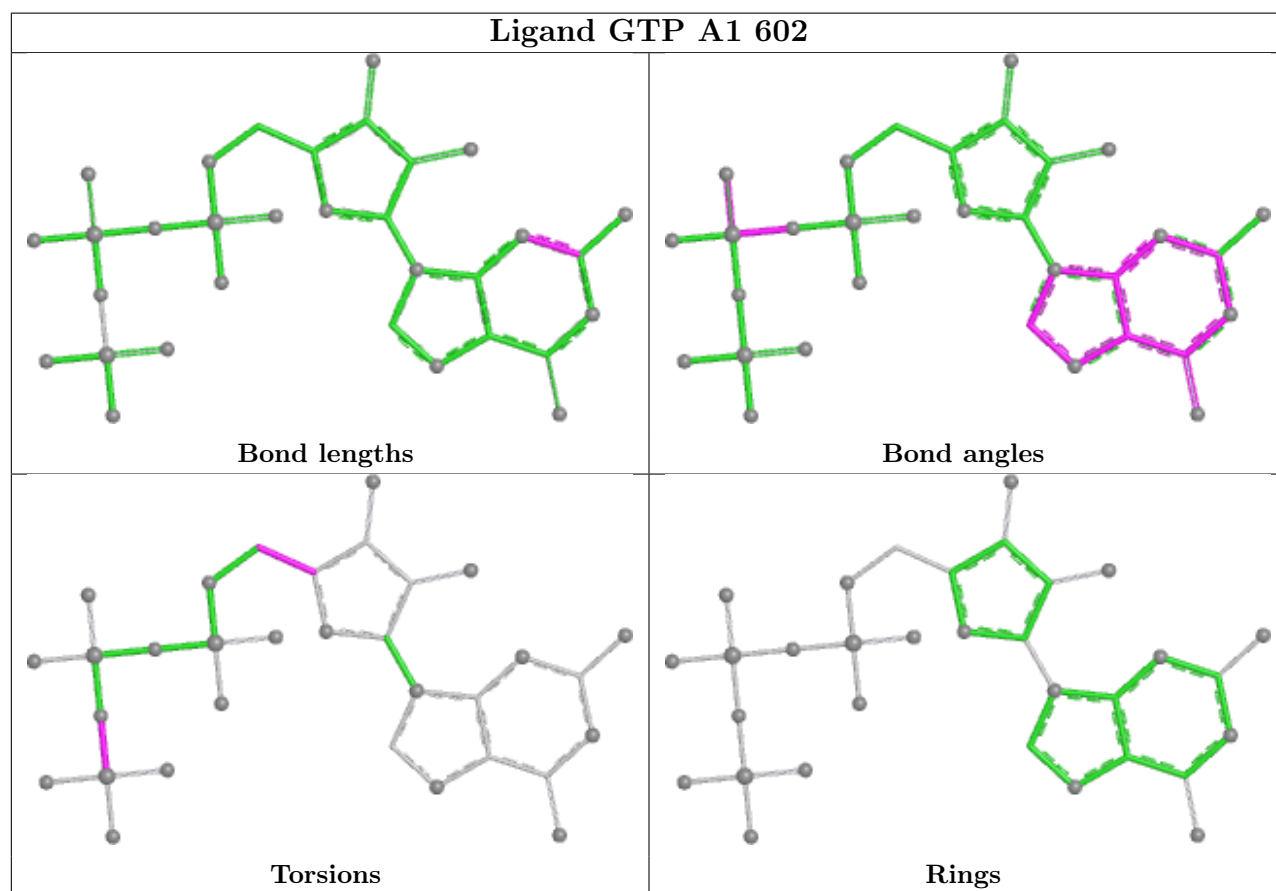
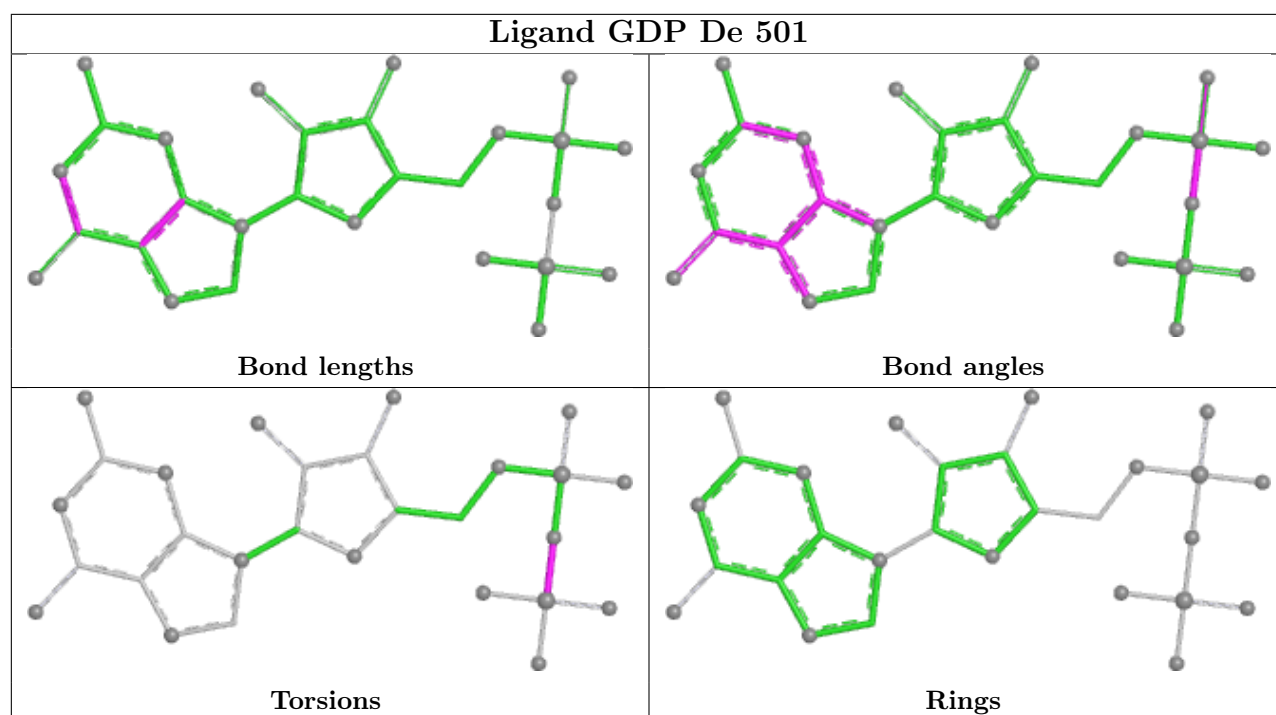
Ligand GDP Dd 501

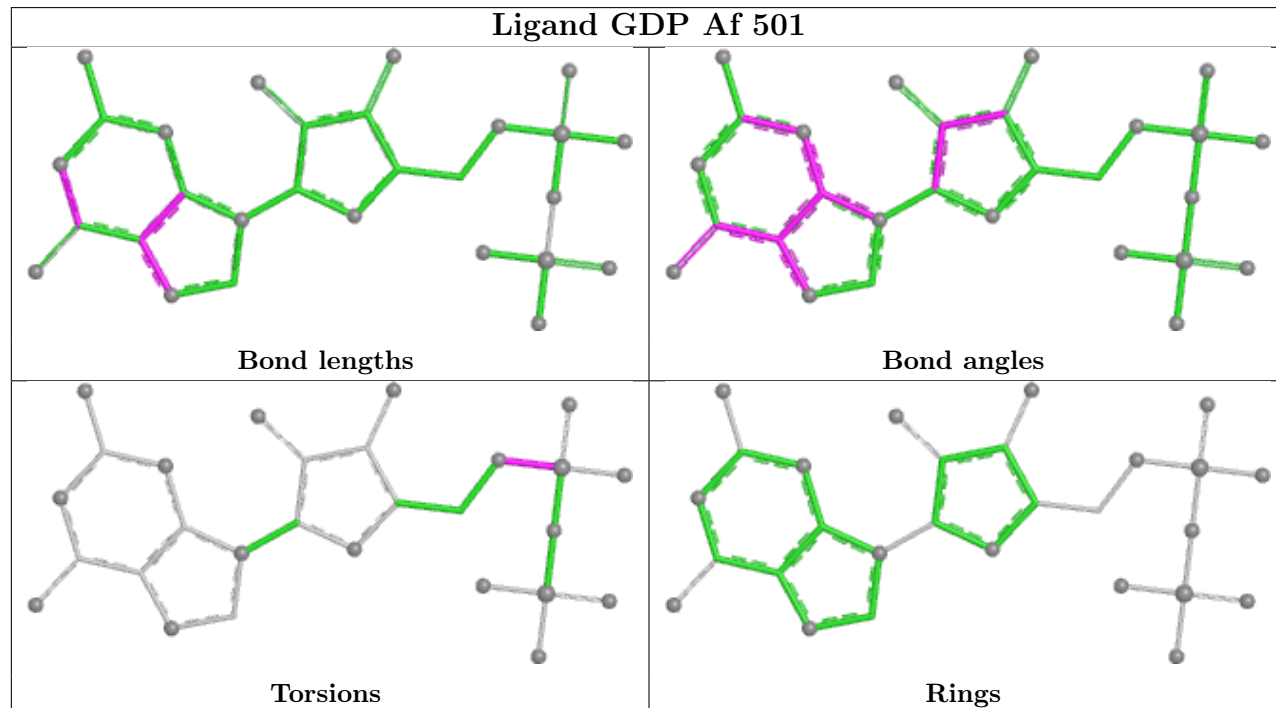
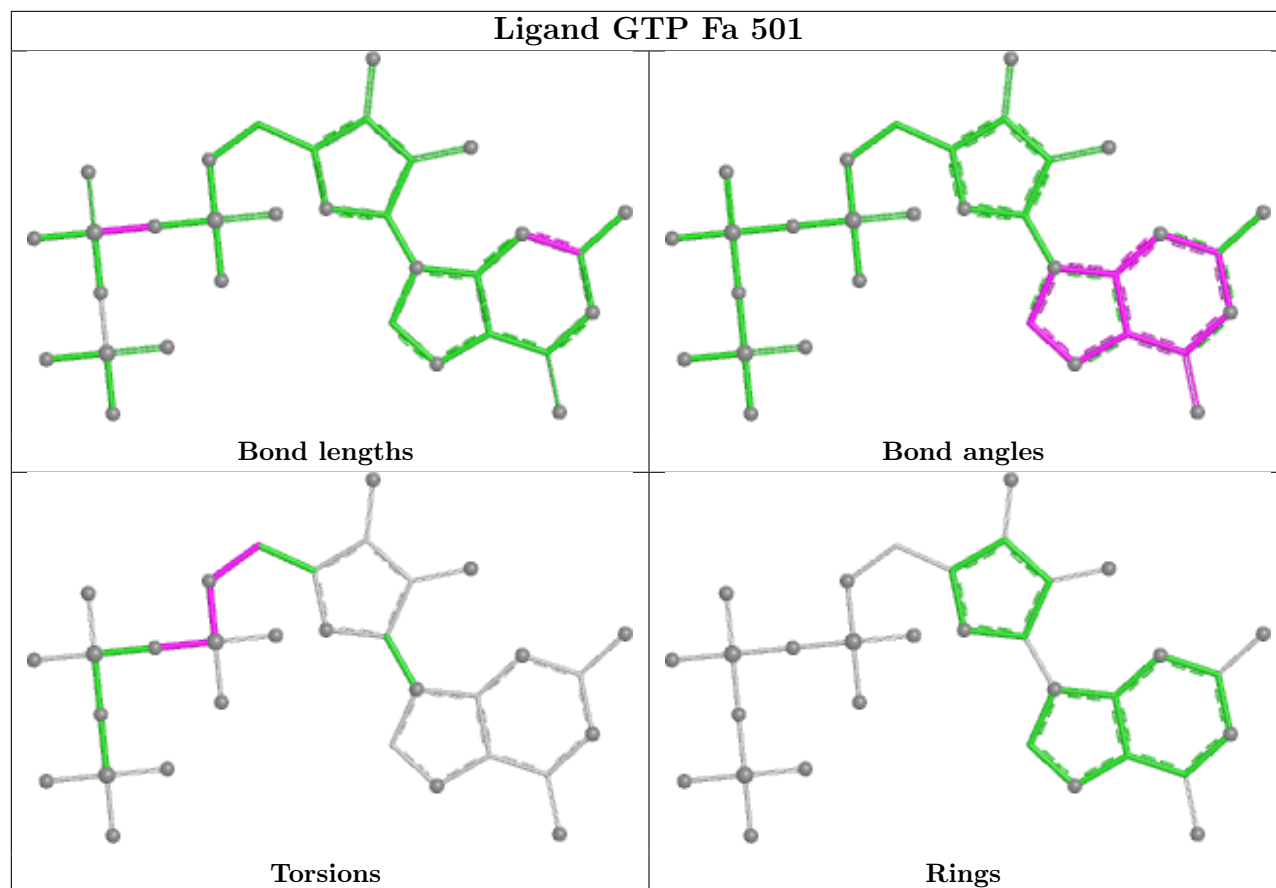


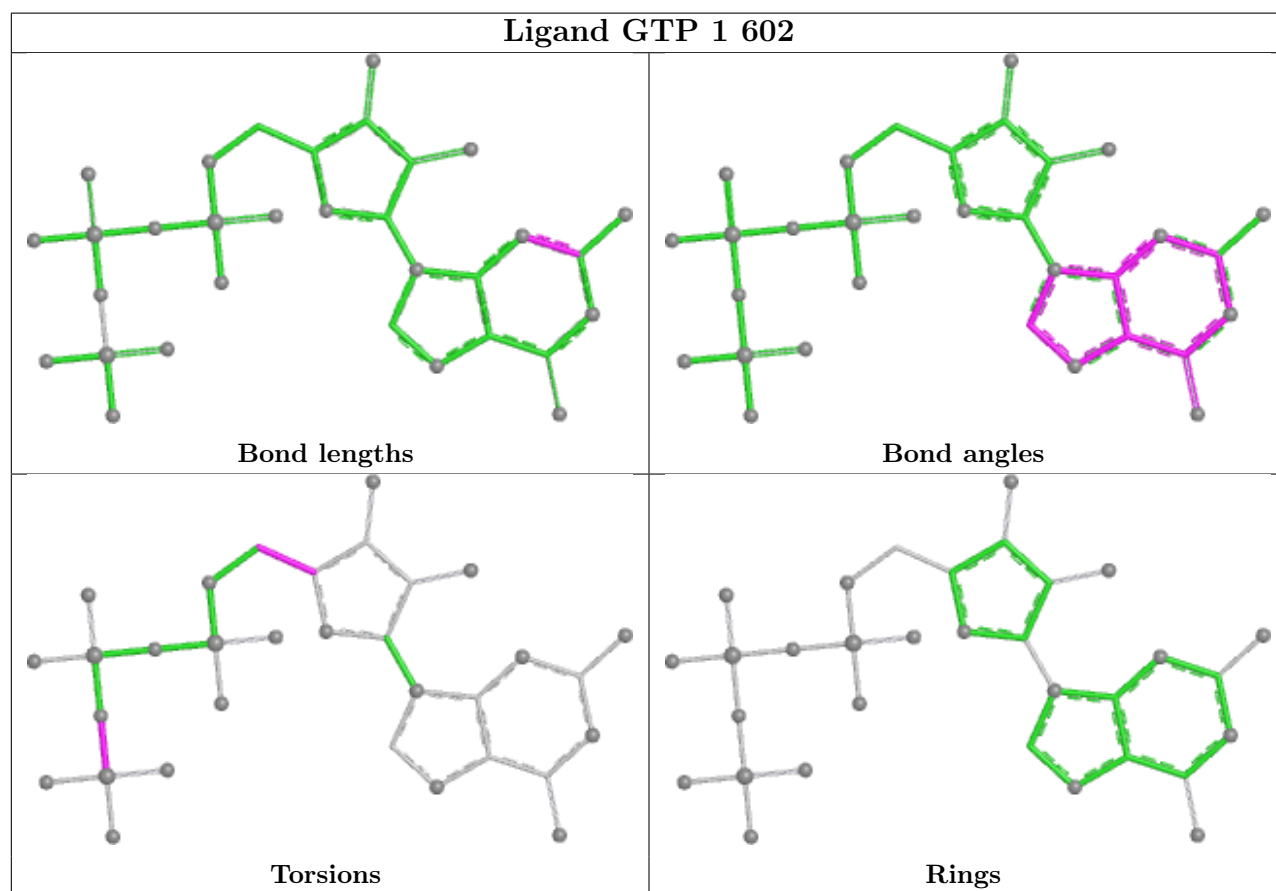
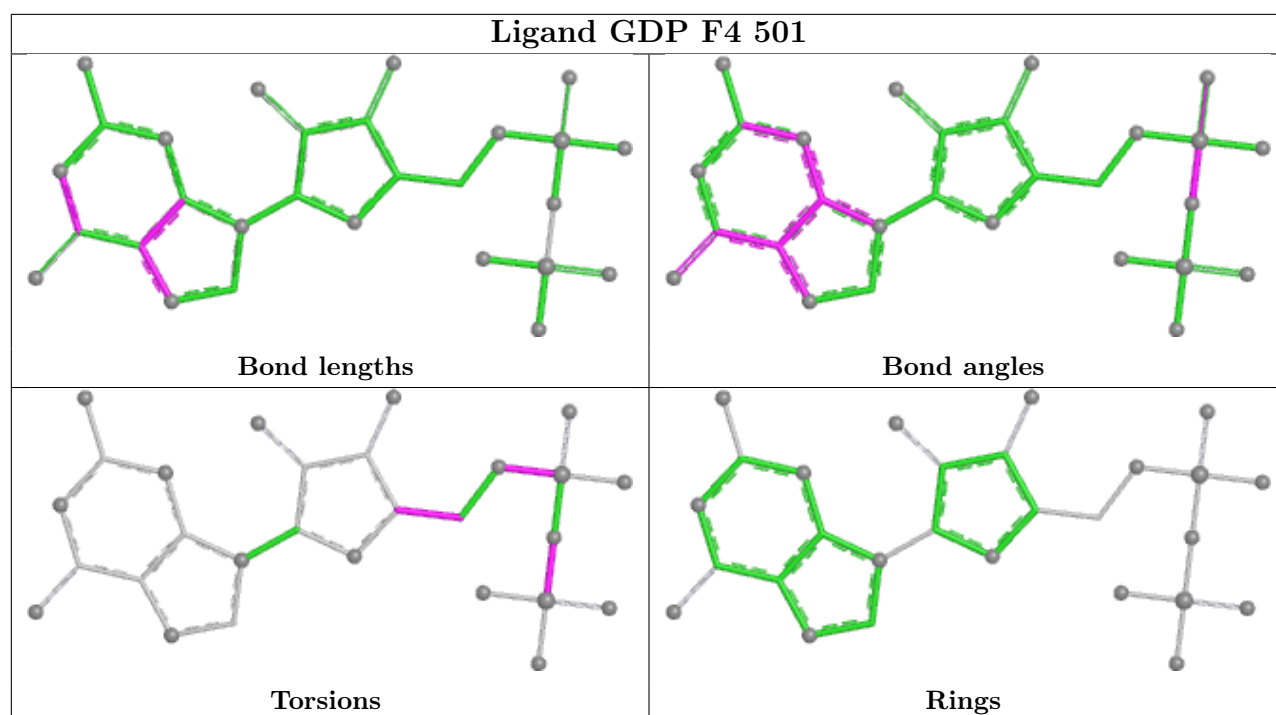


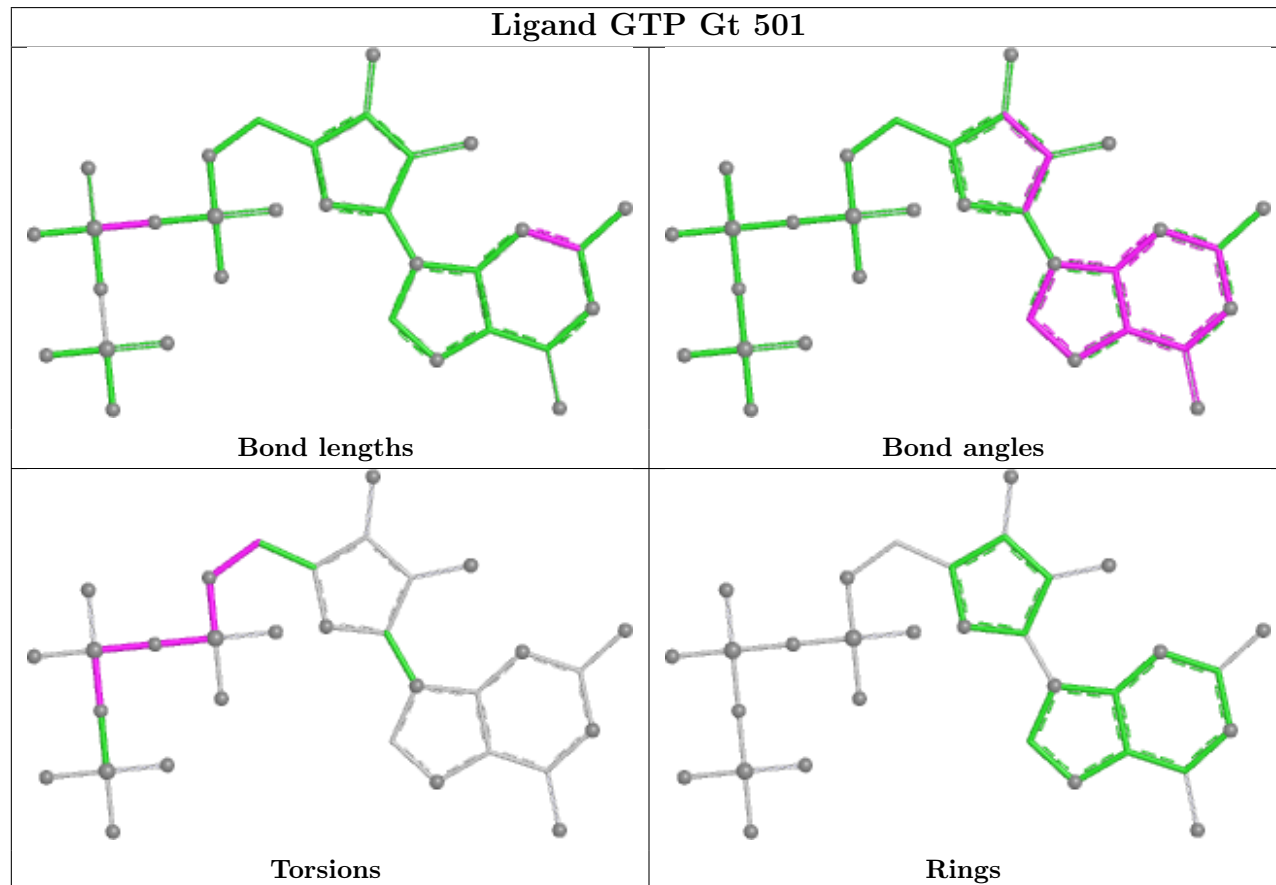
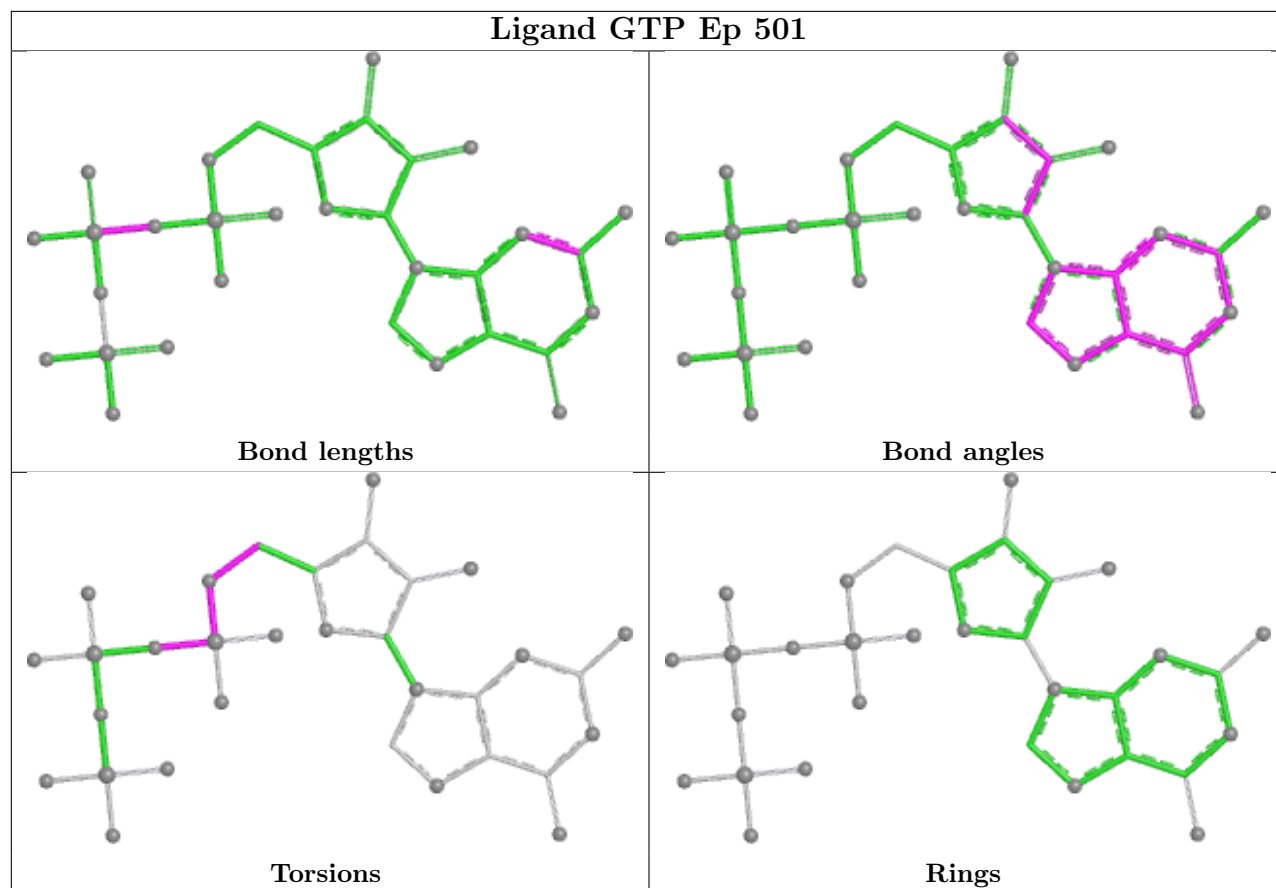


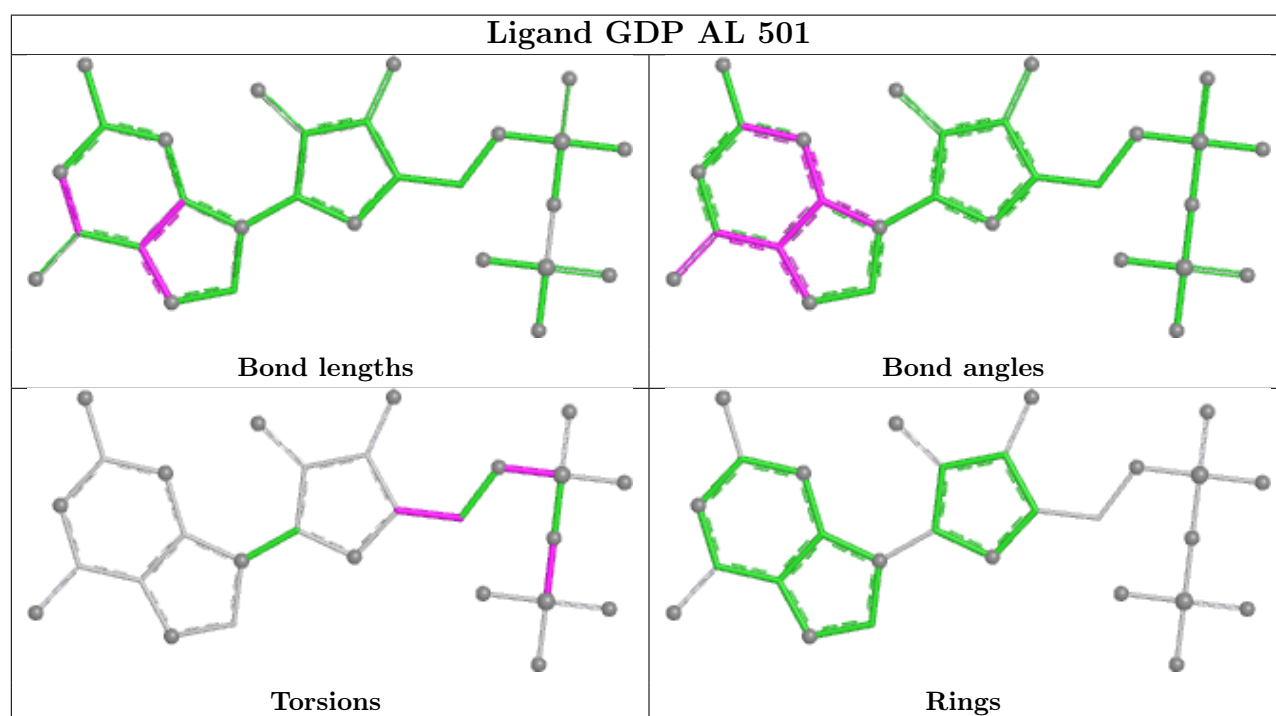
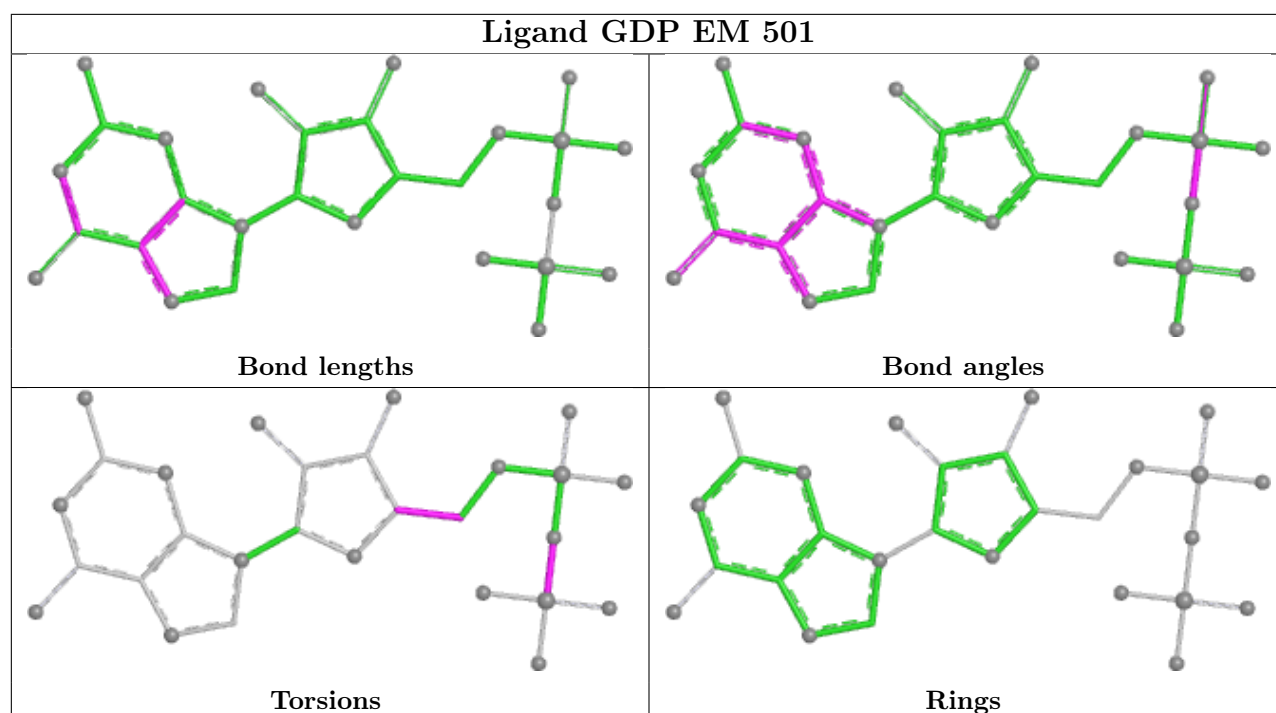


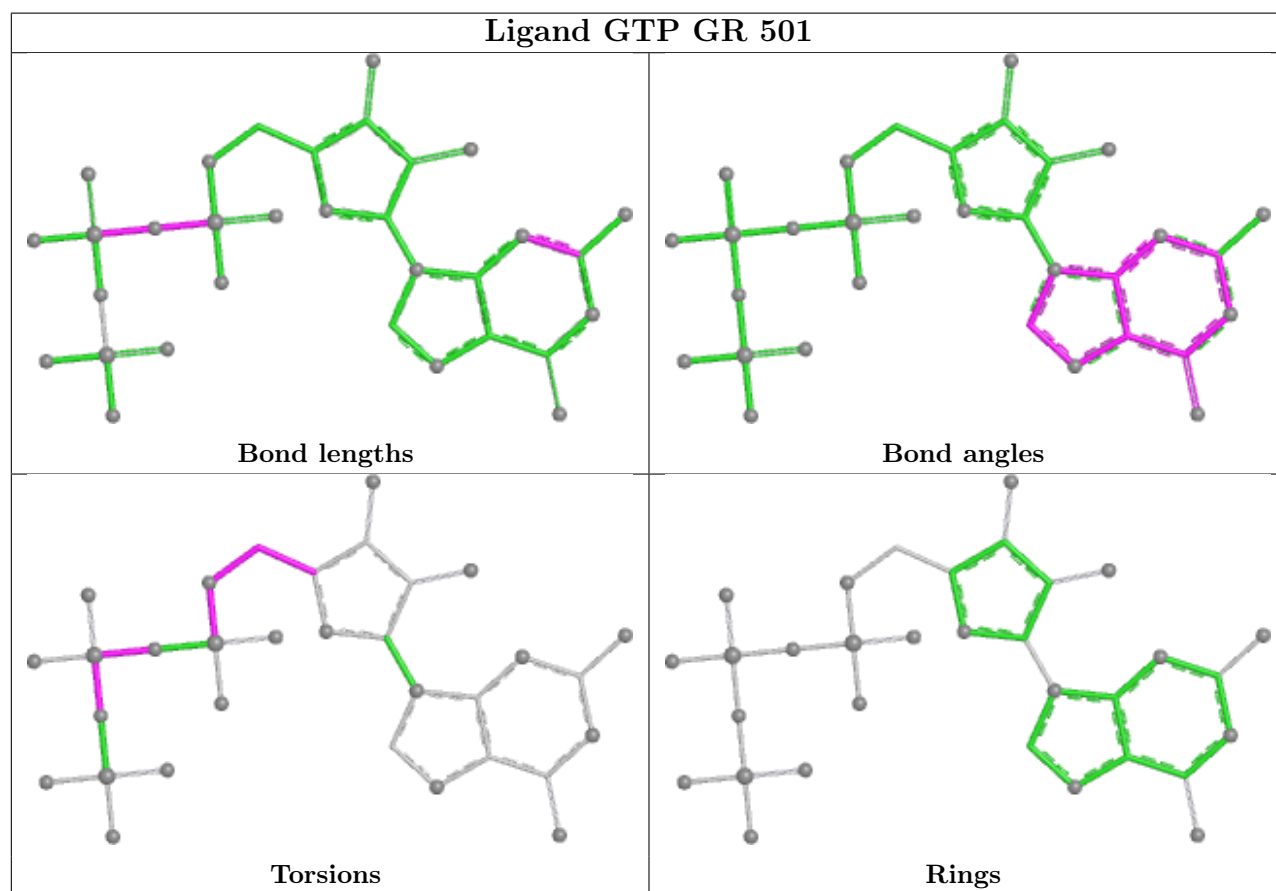
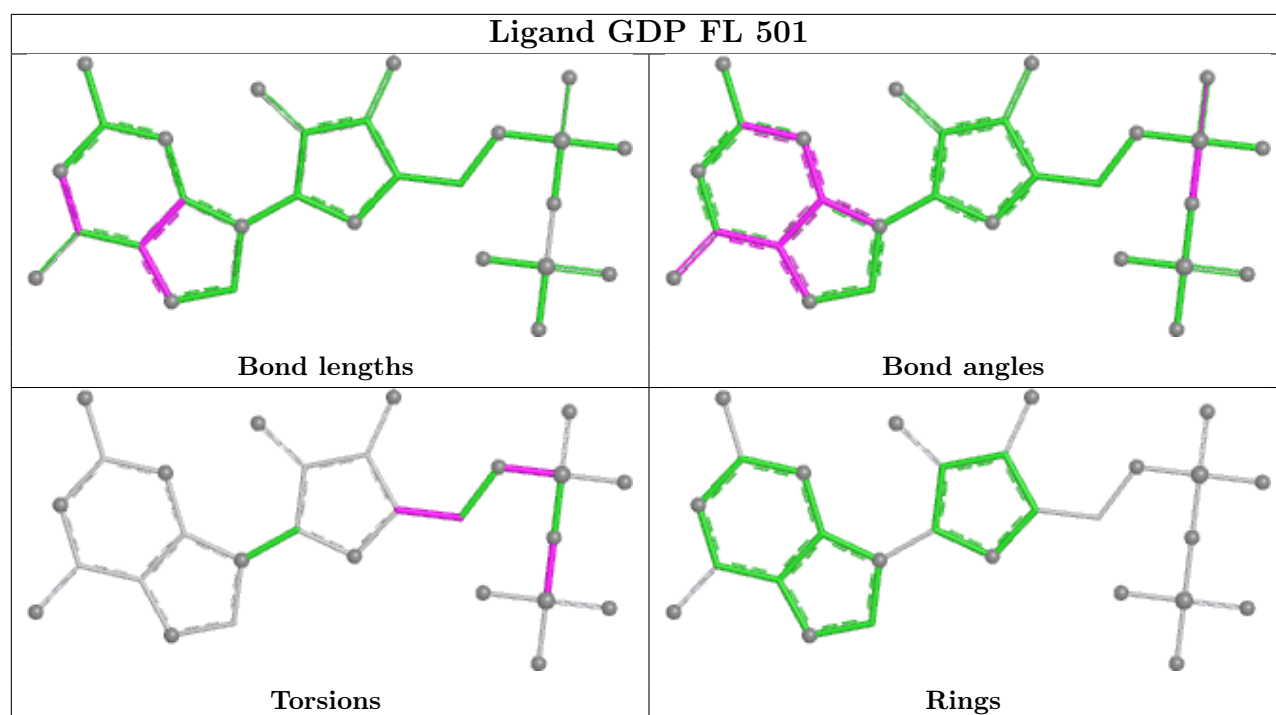




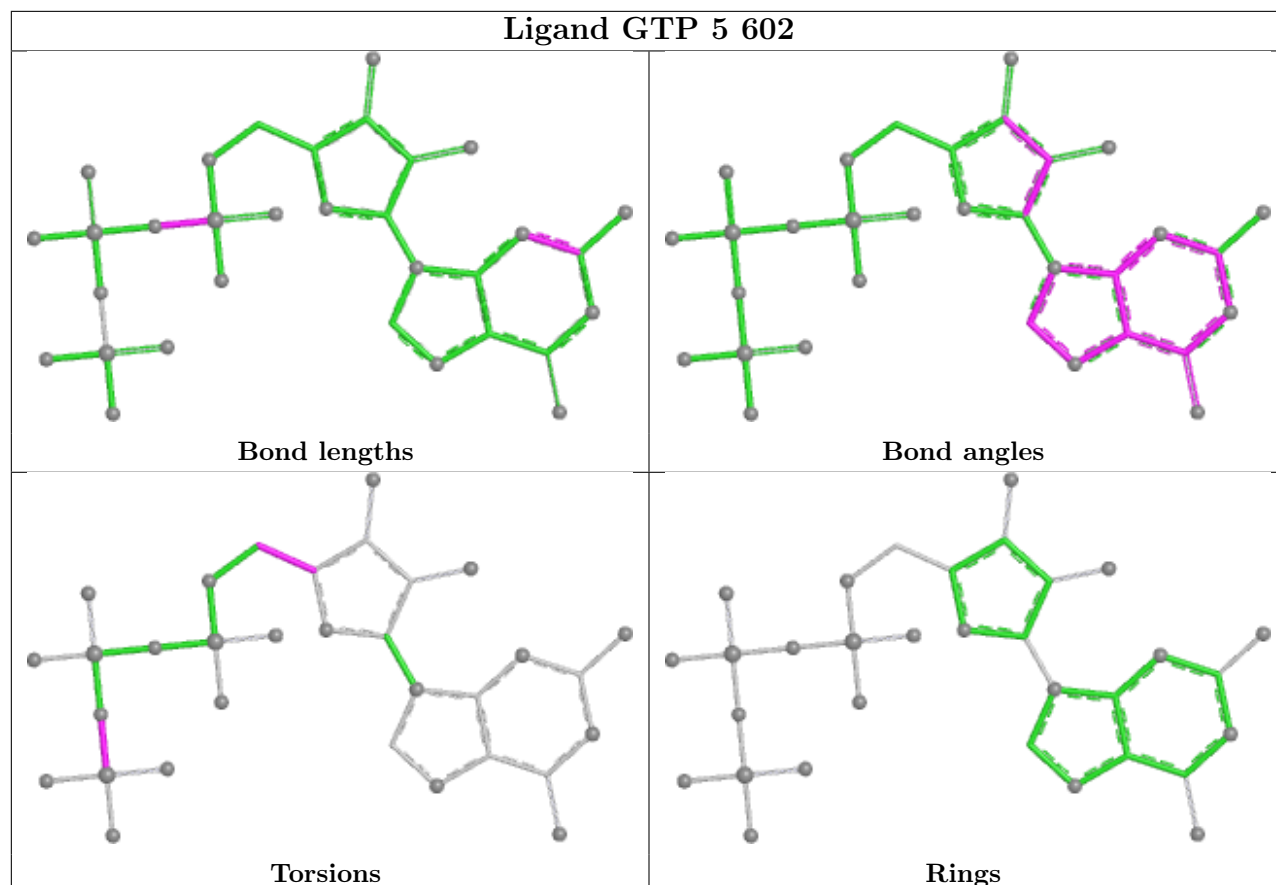




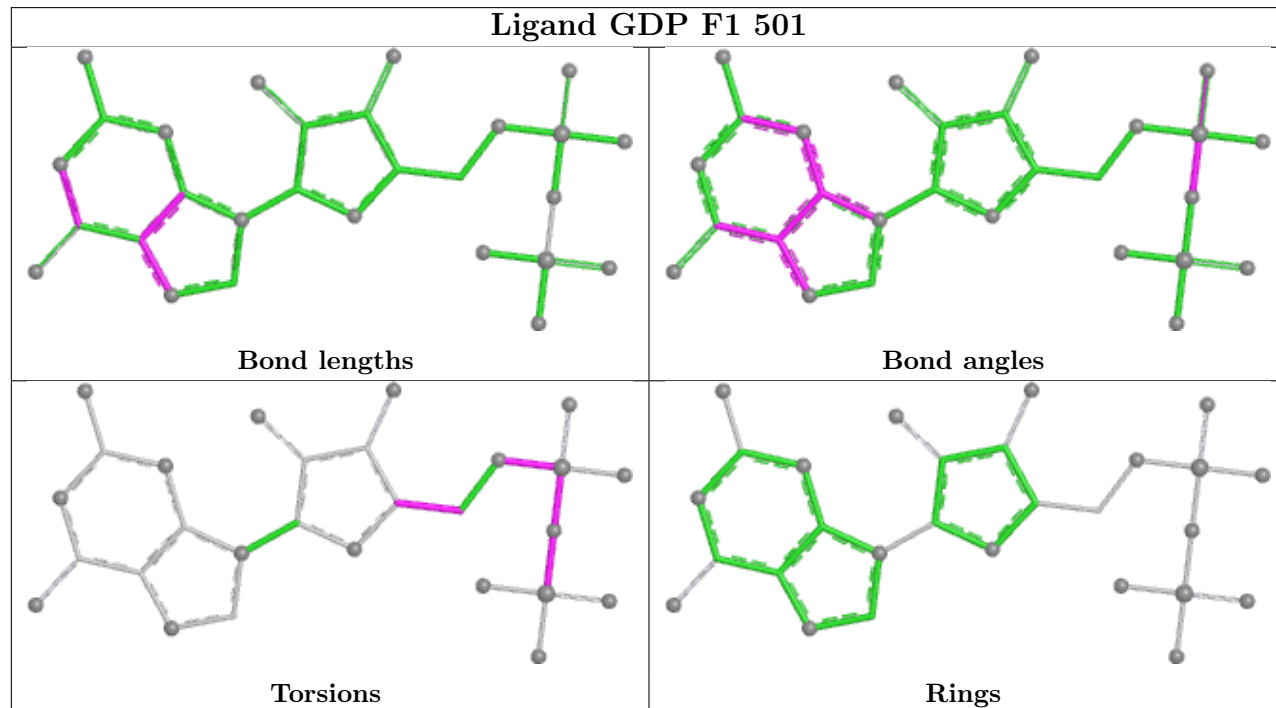


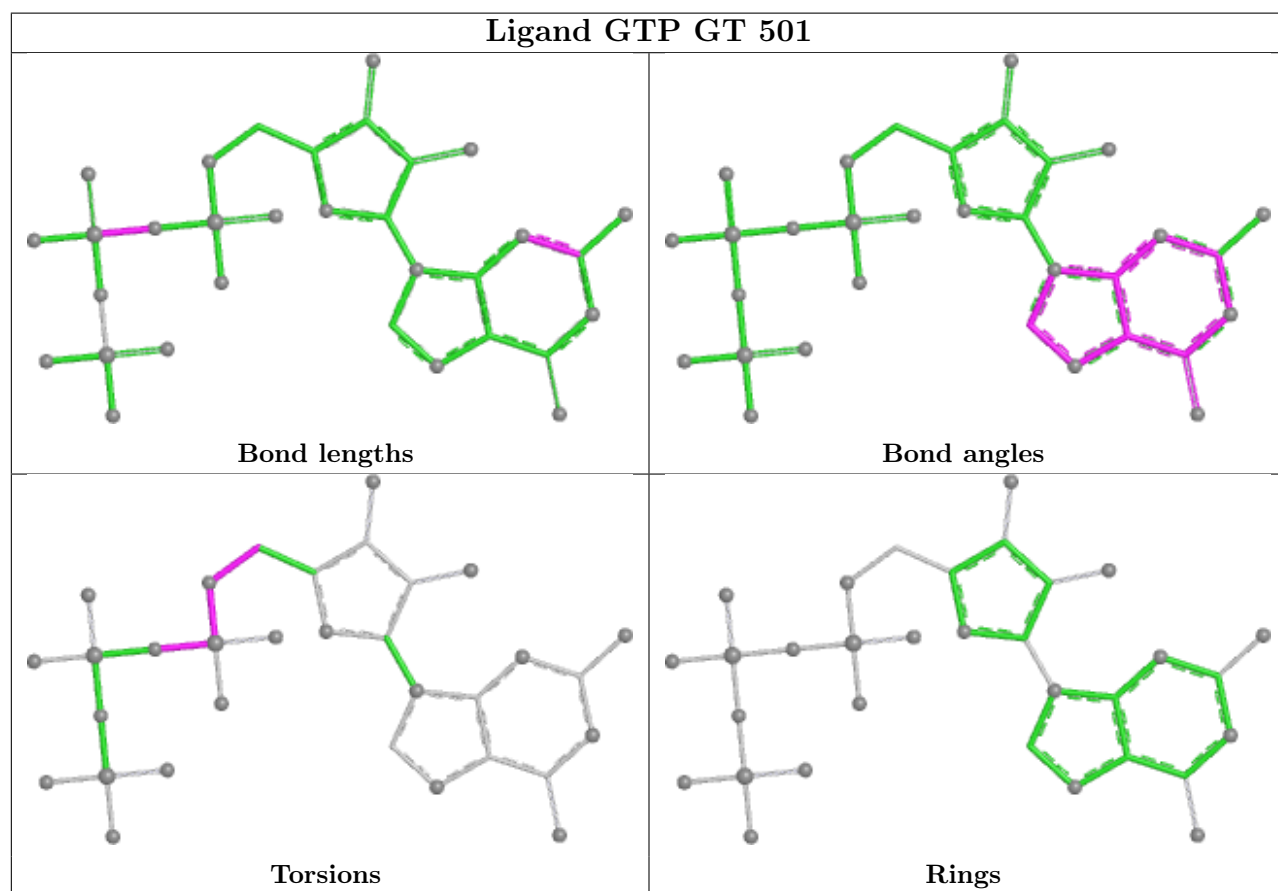
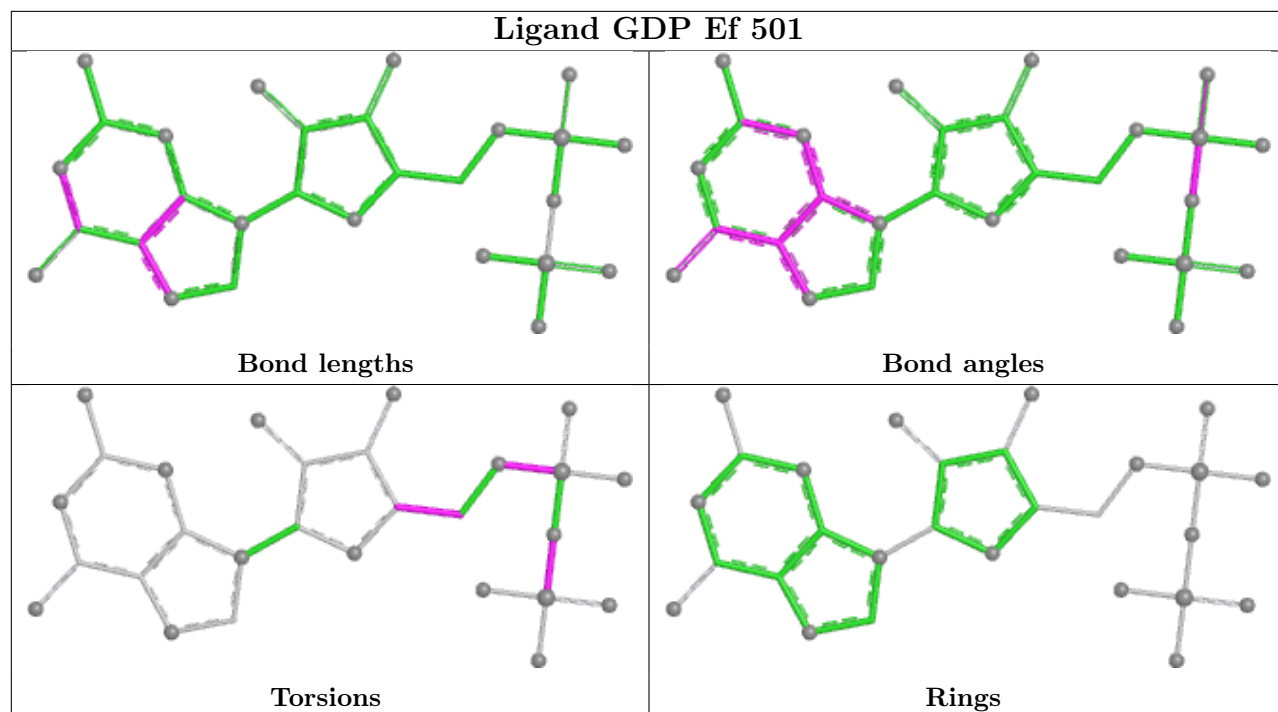


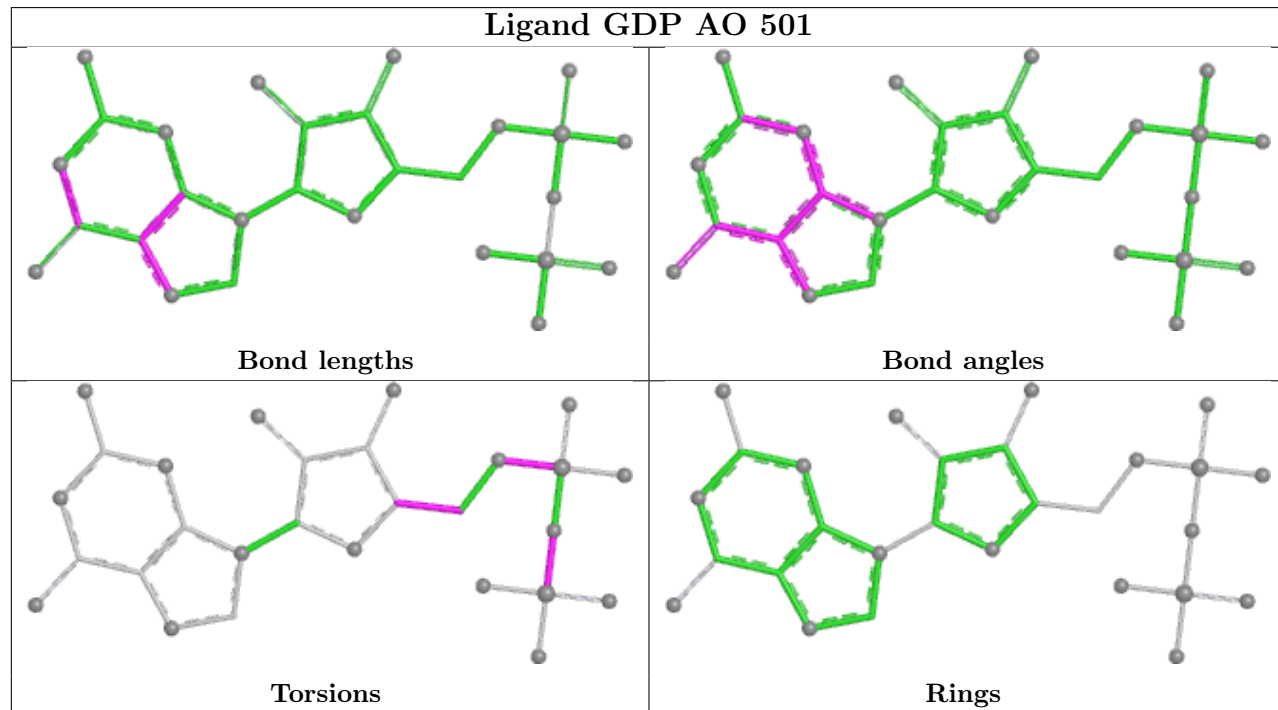
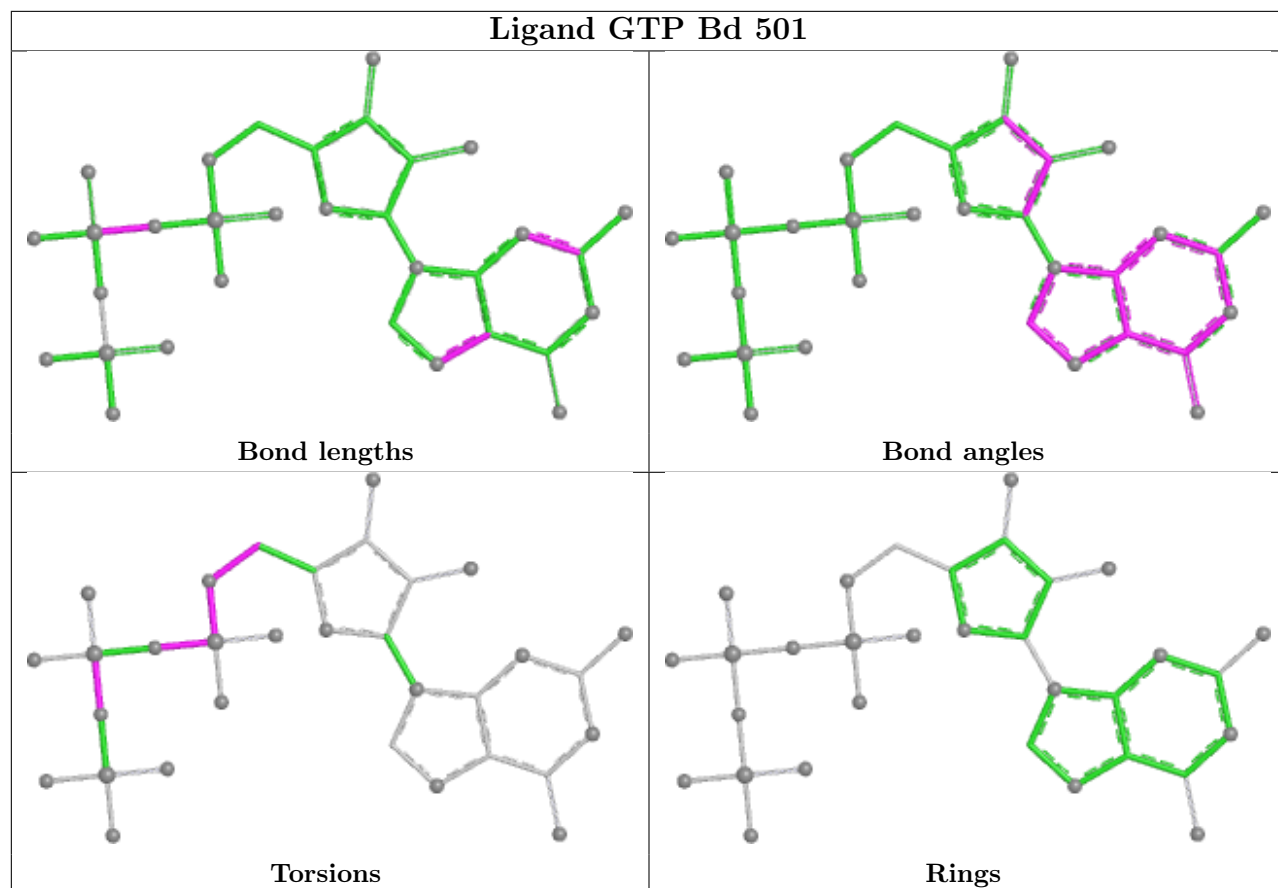
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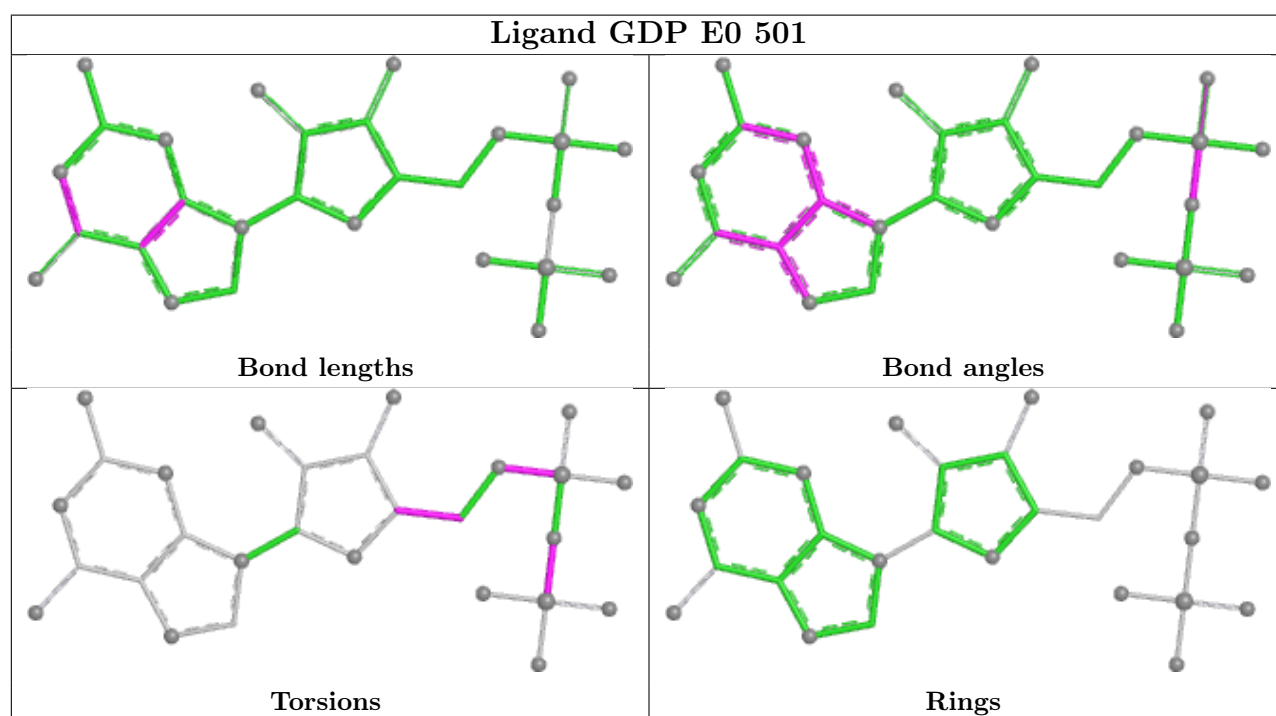
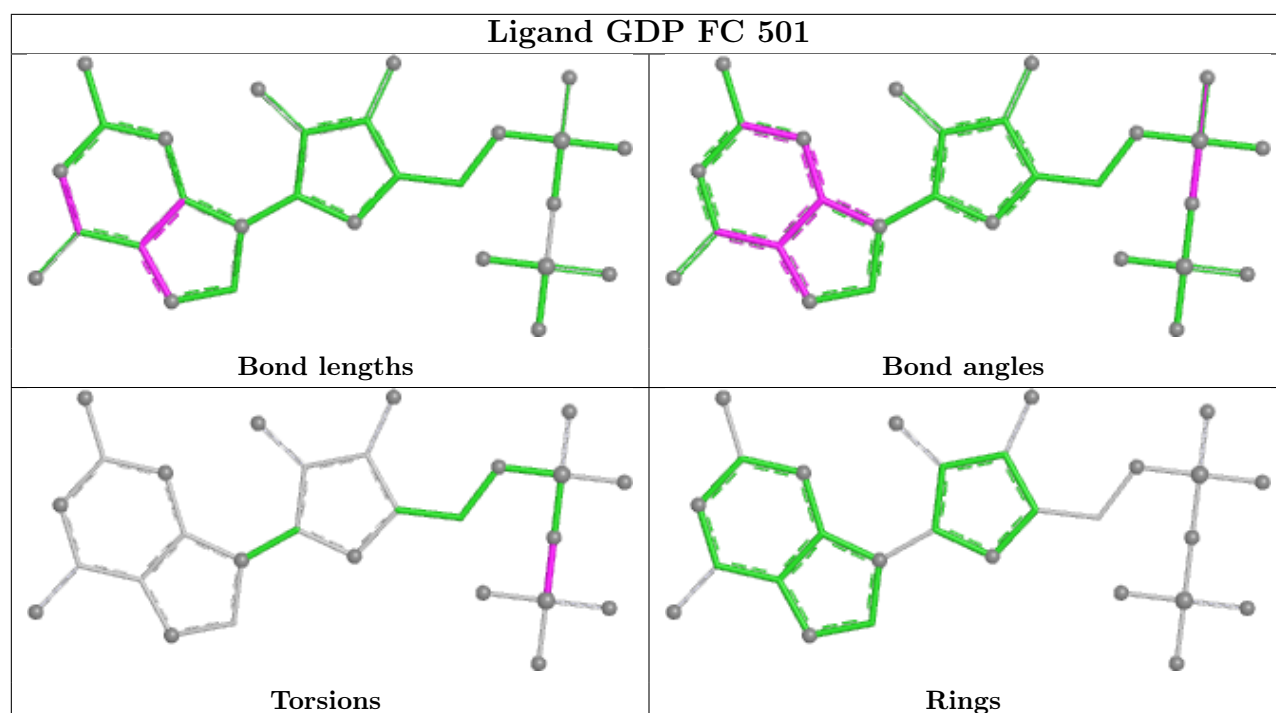


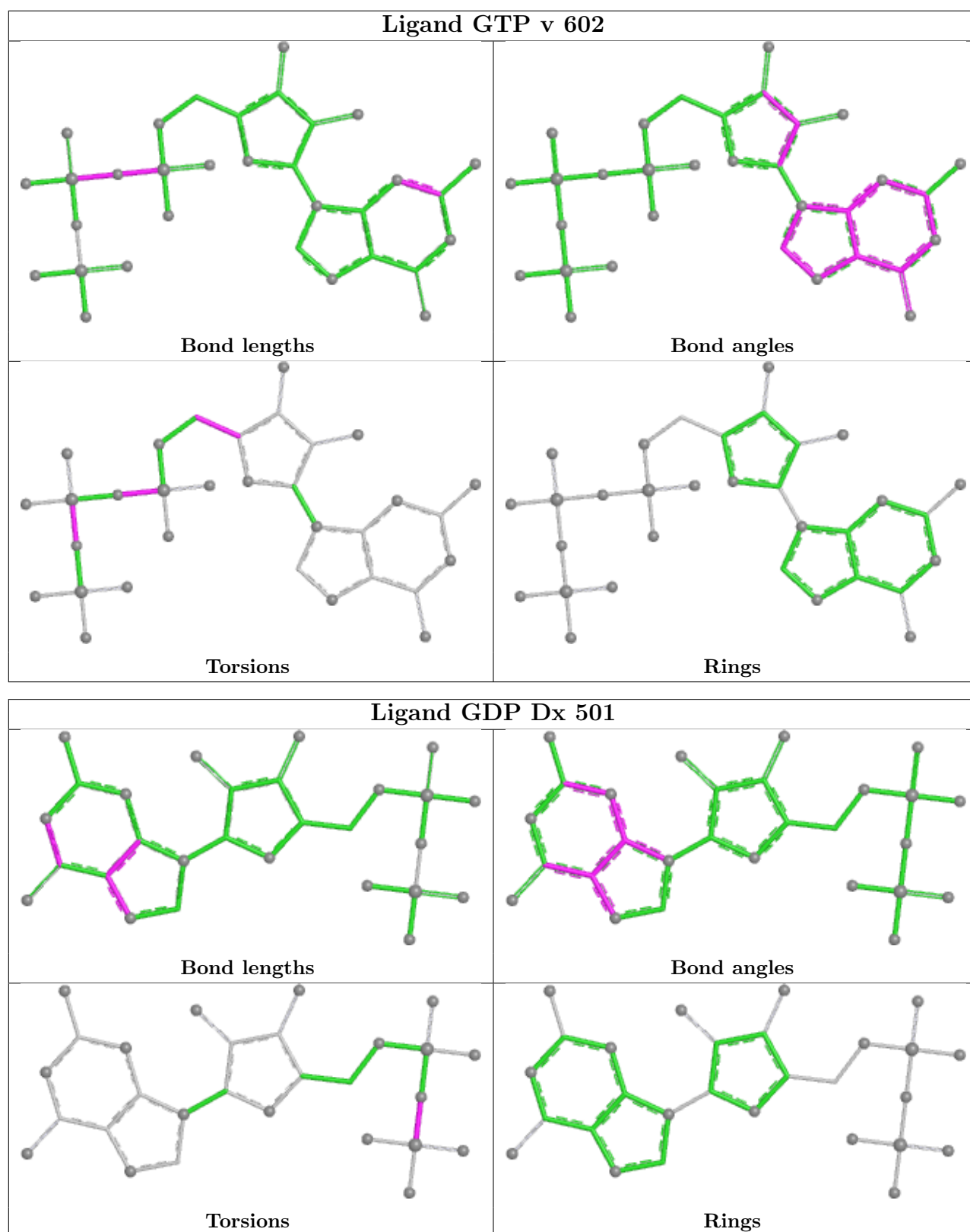
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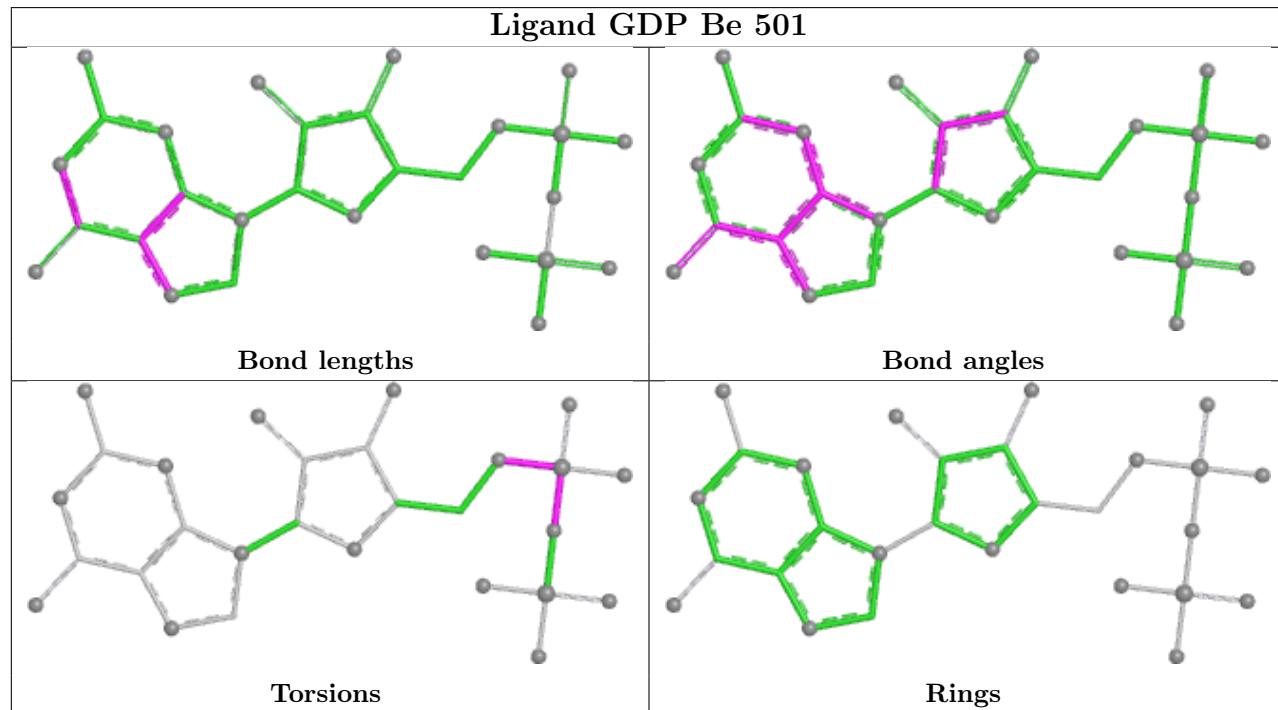
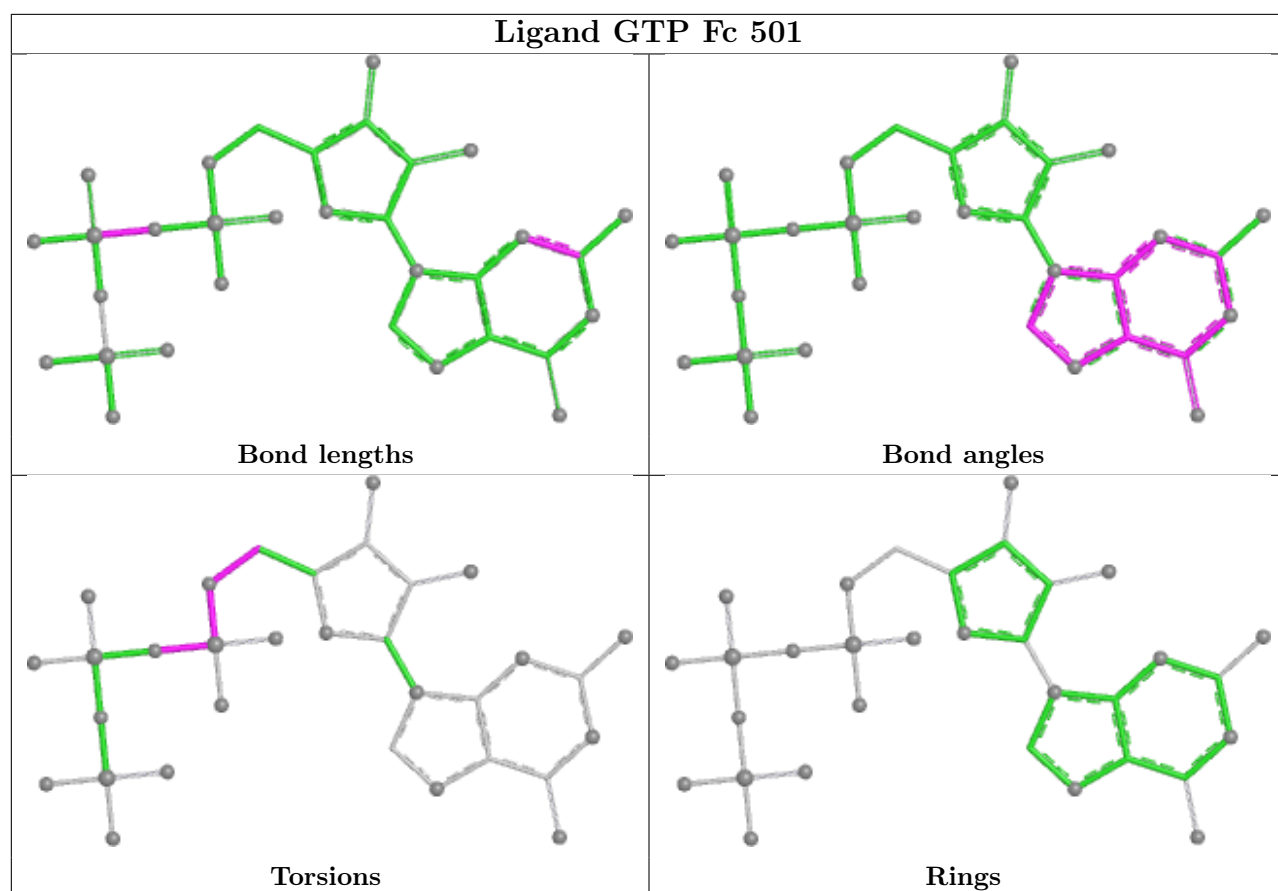




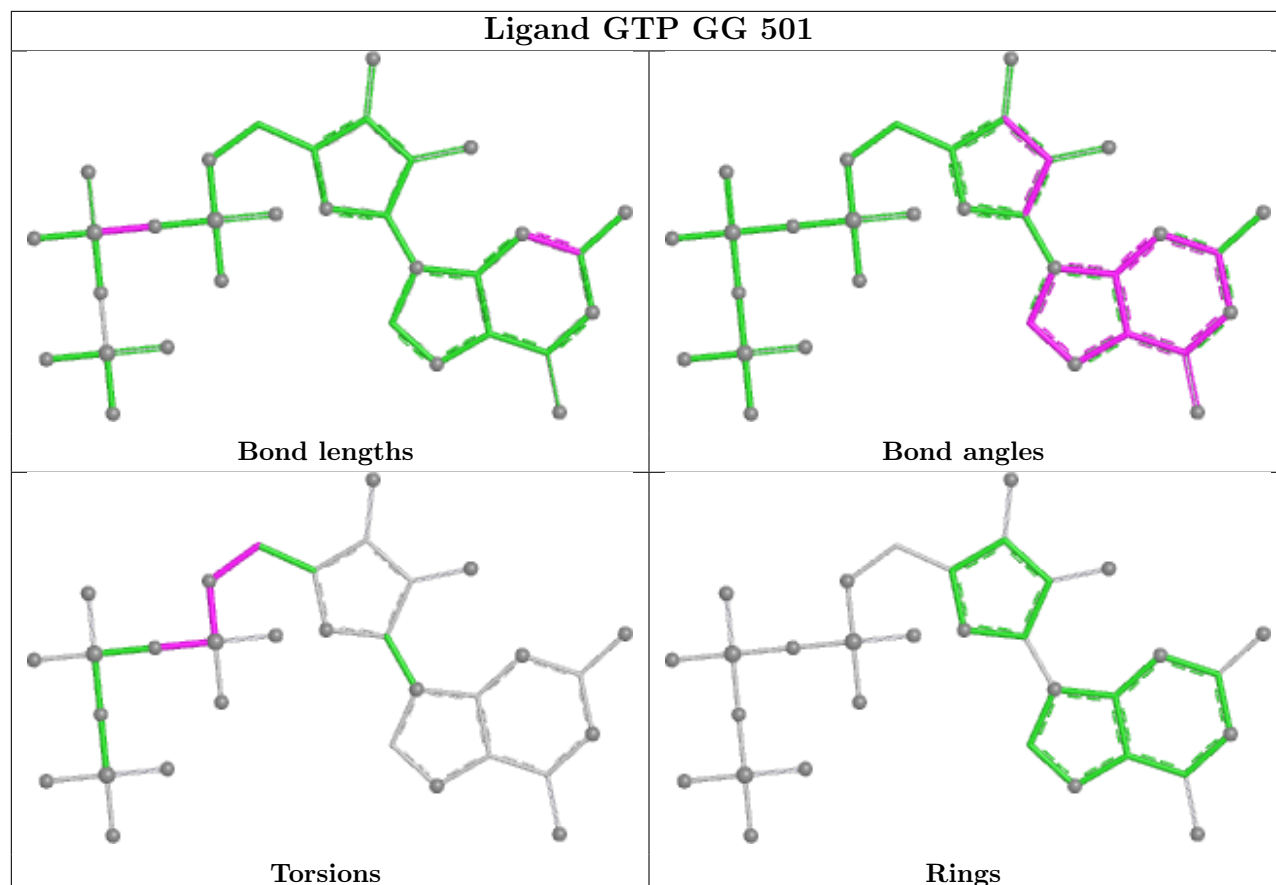




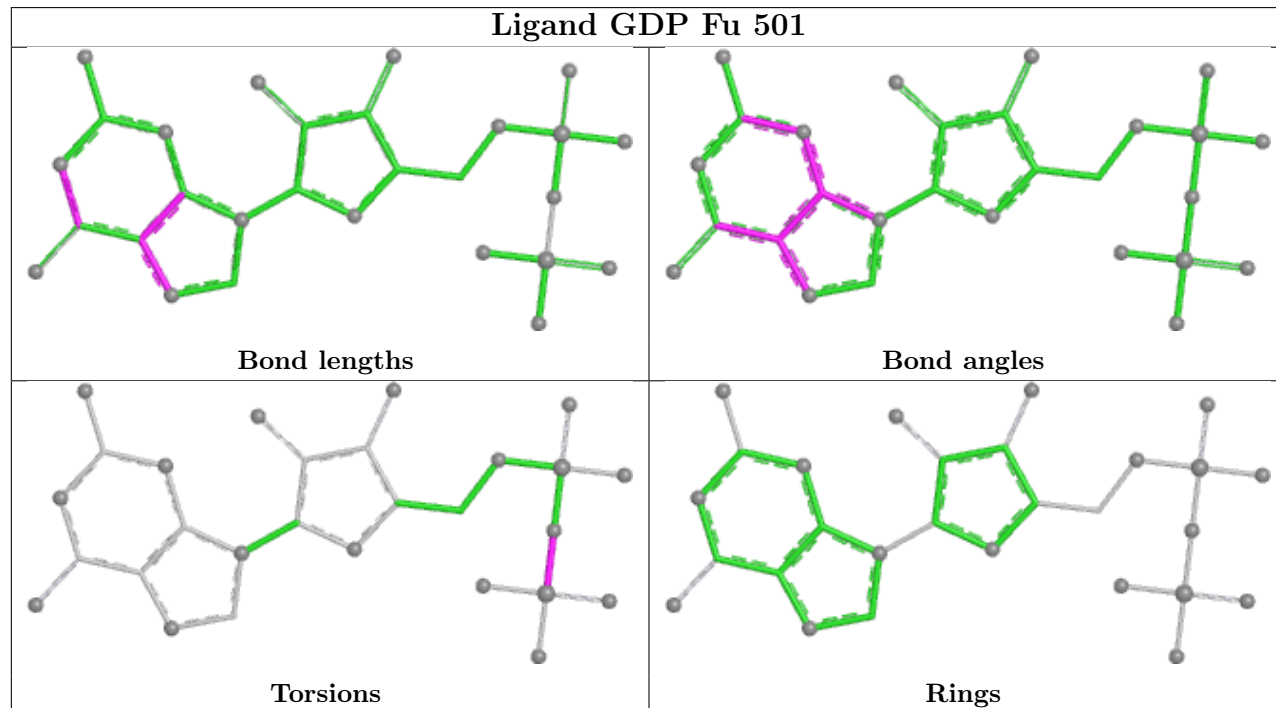




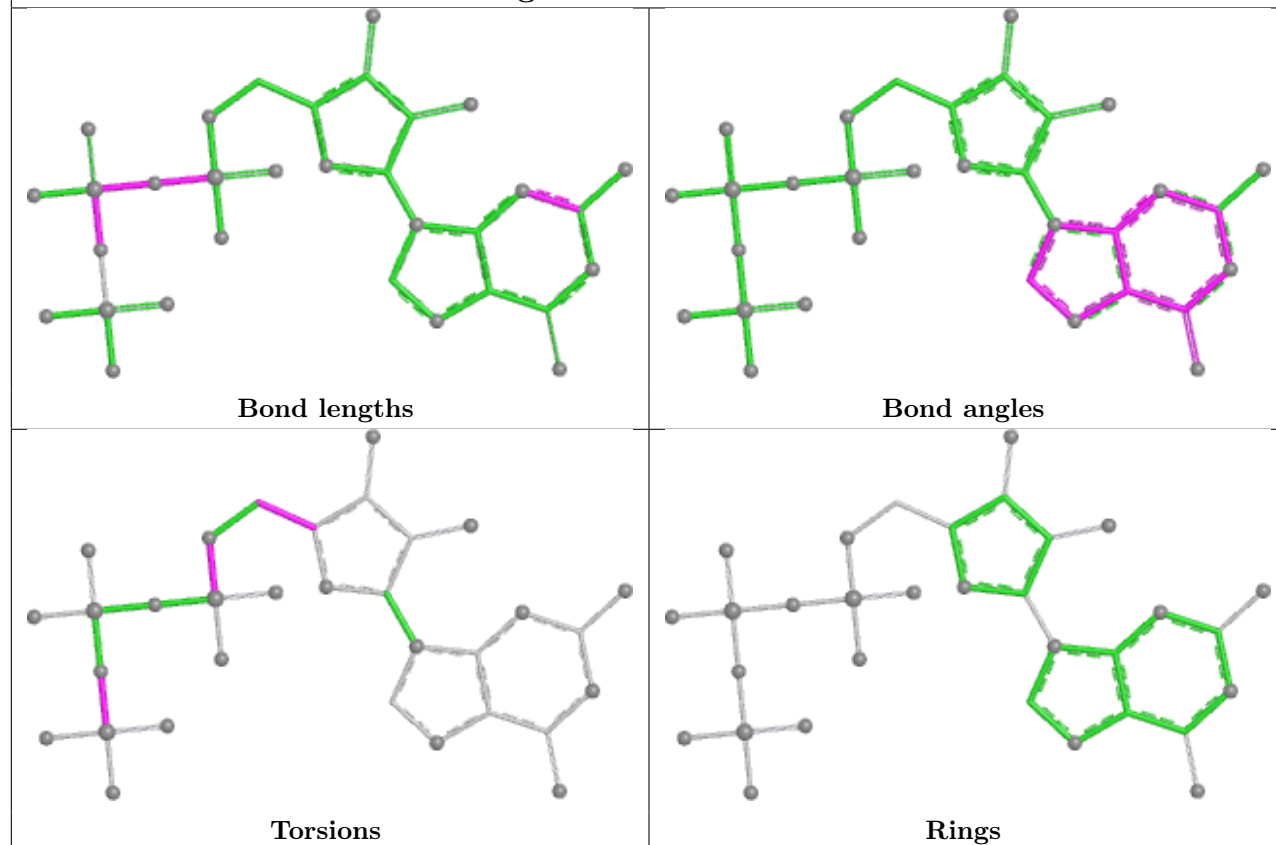
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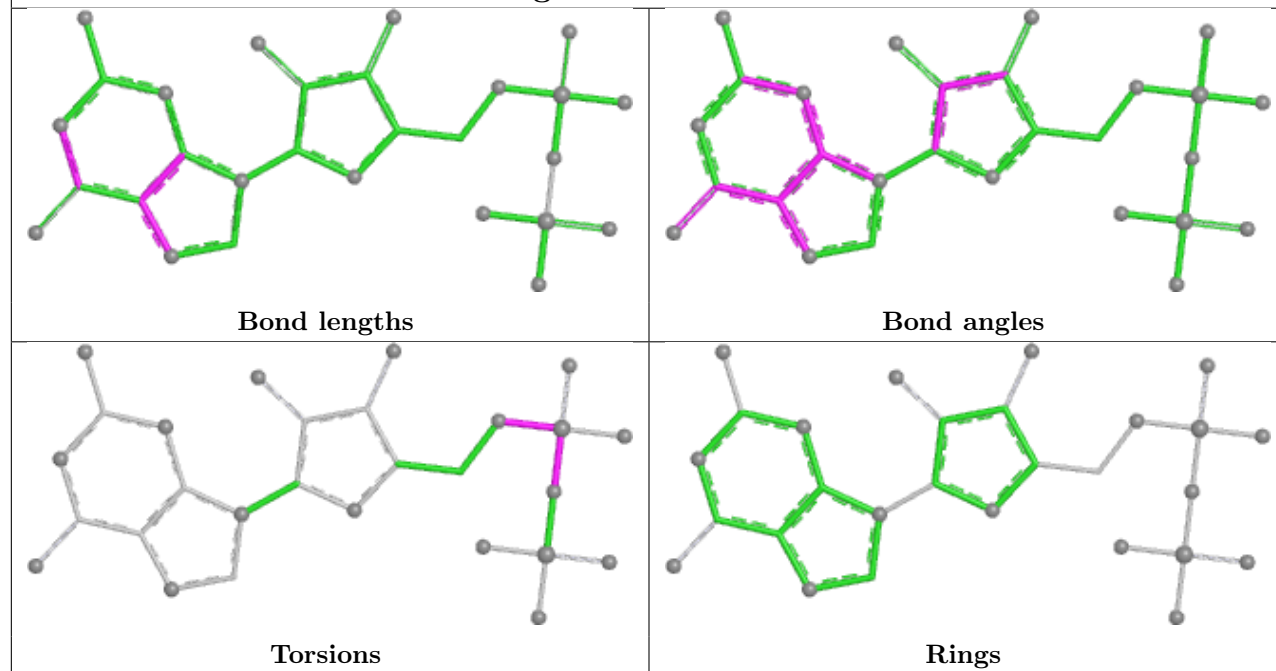
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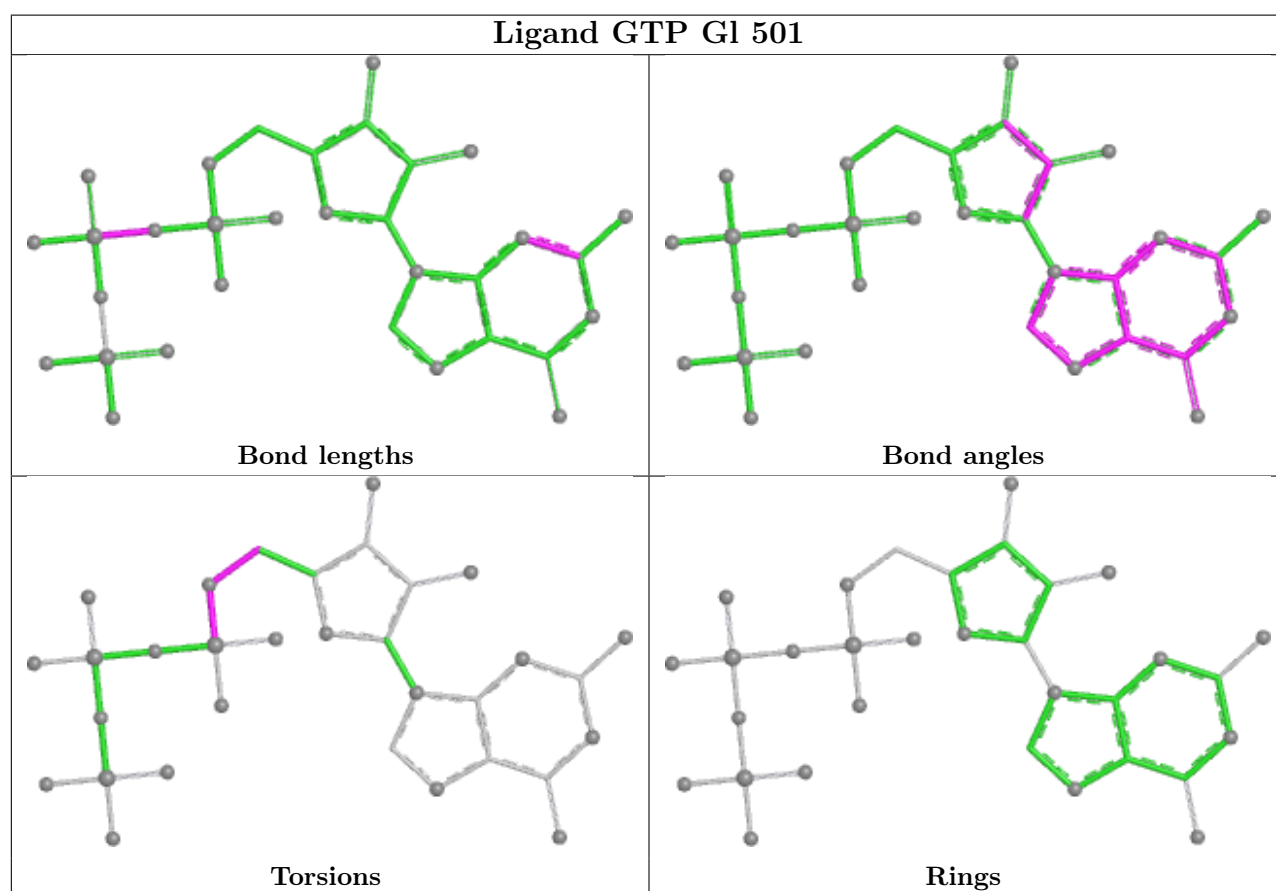
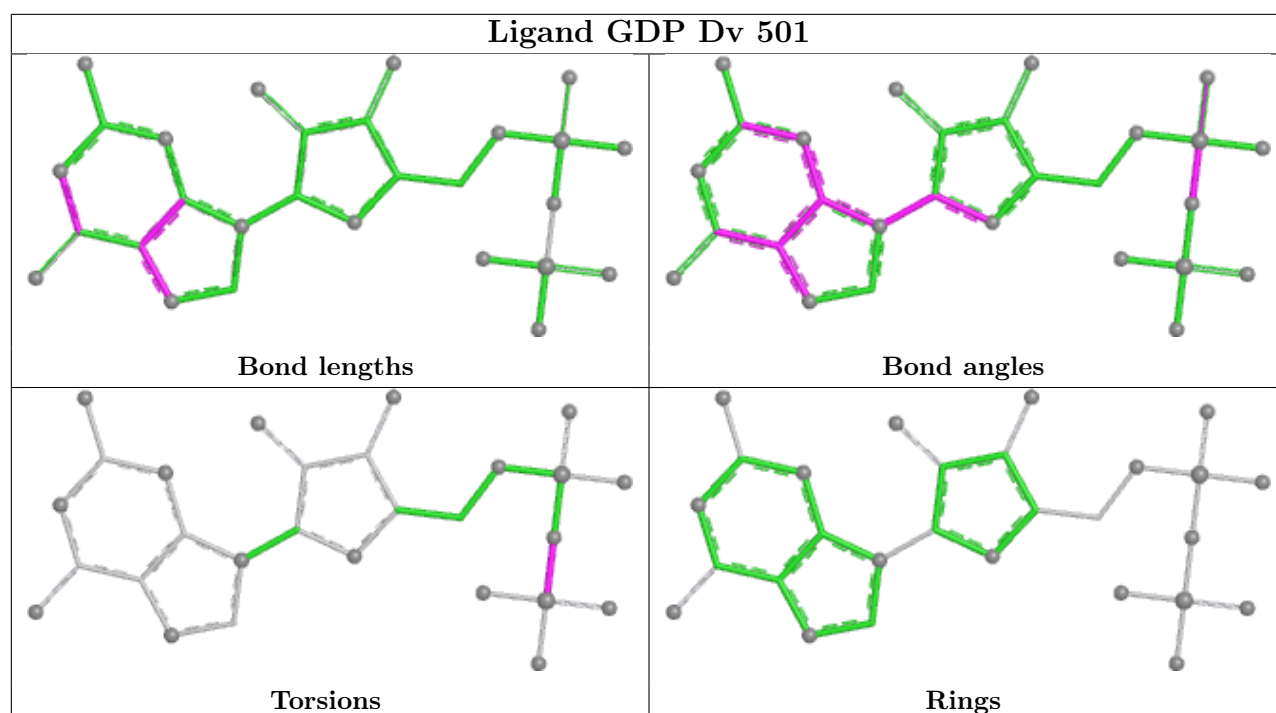


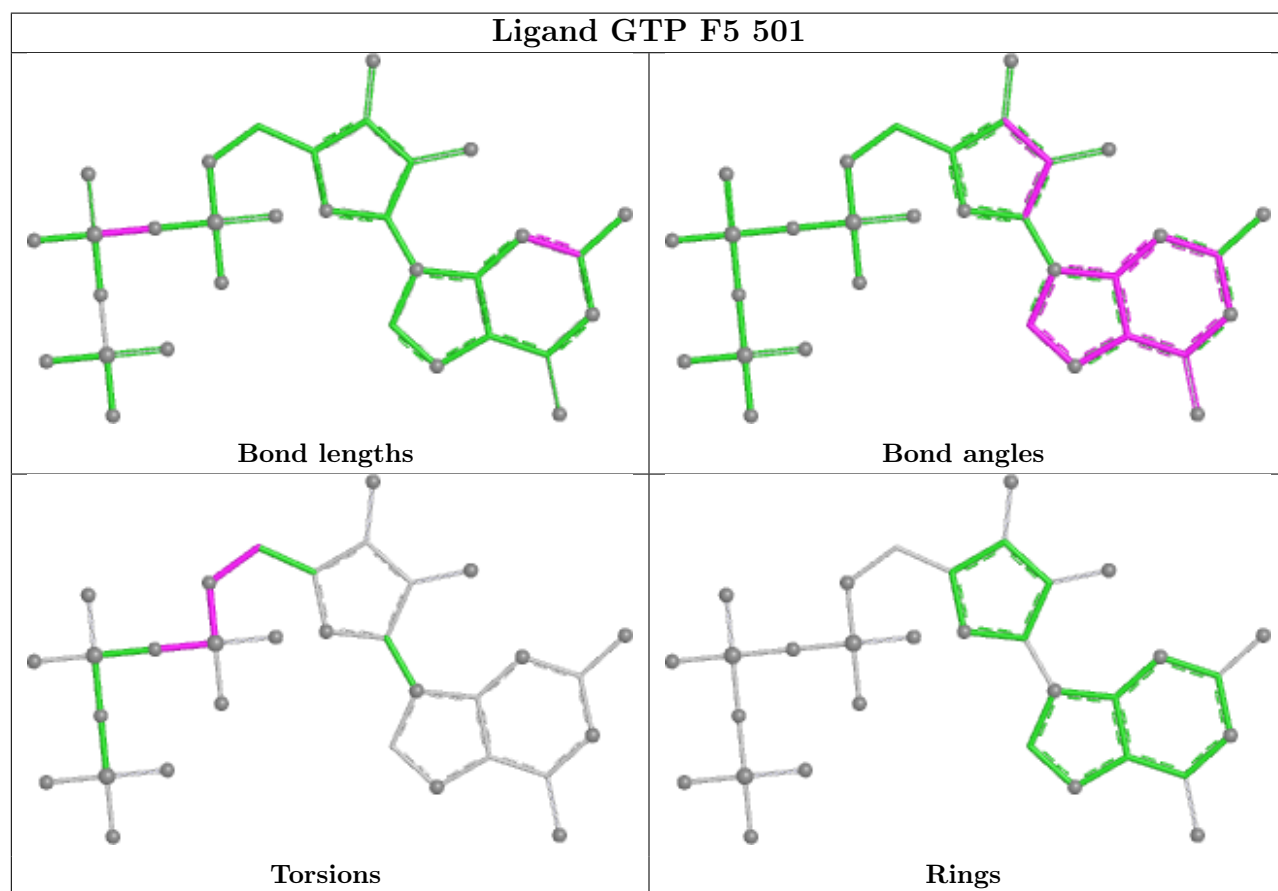
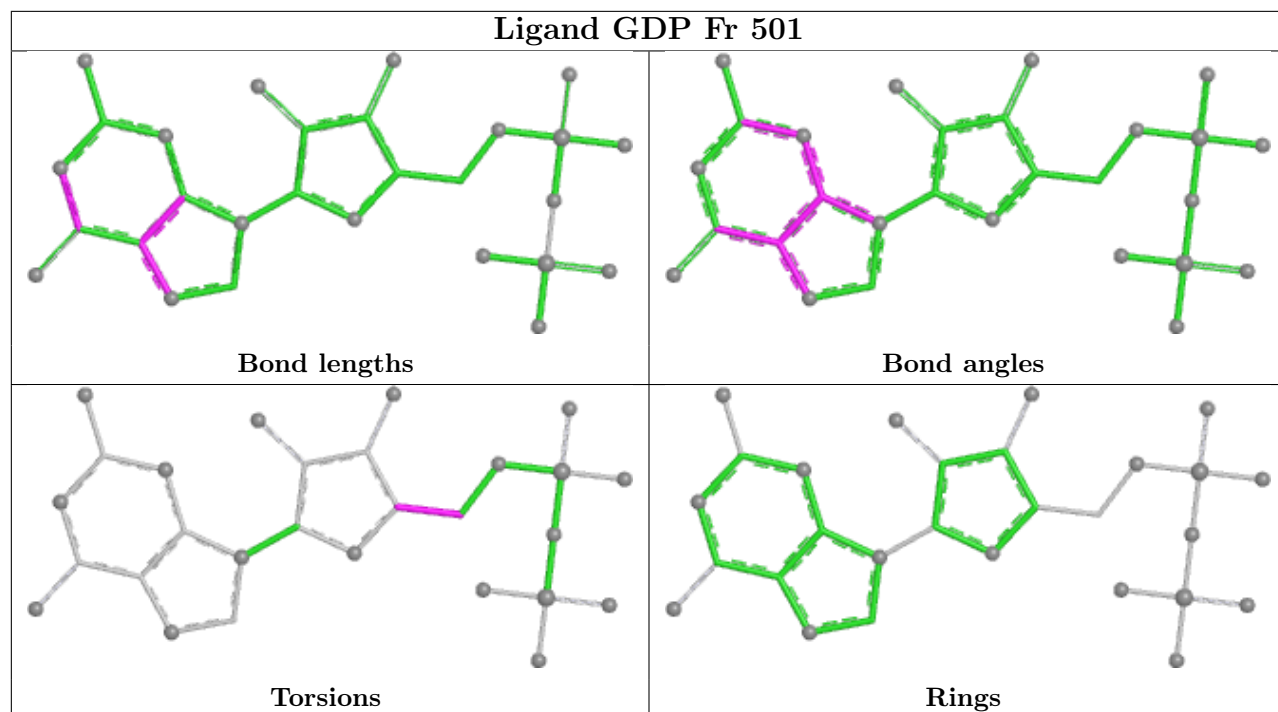
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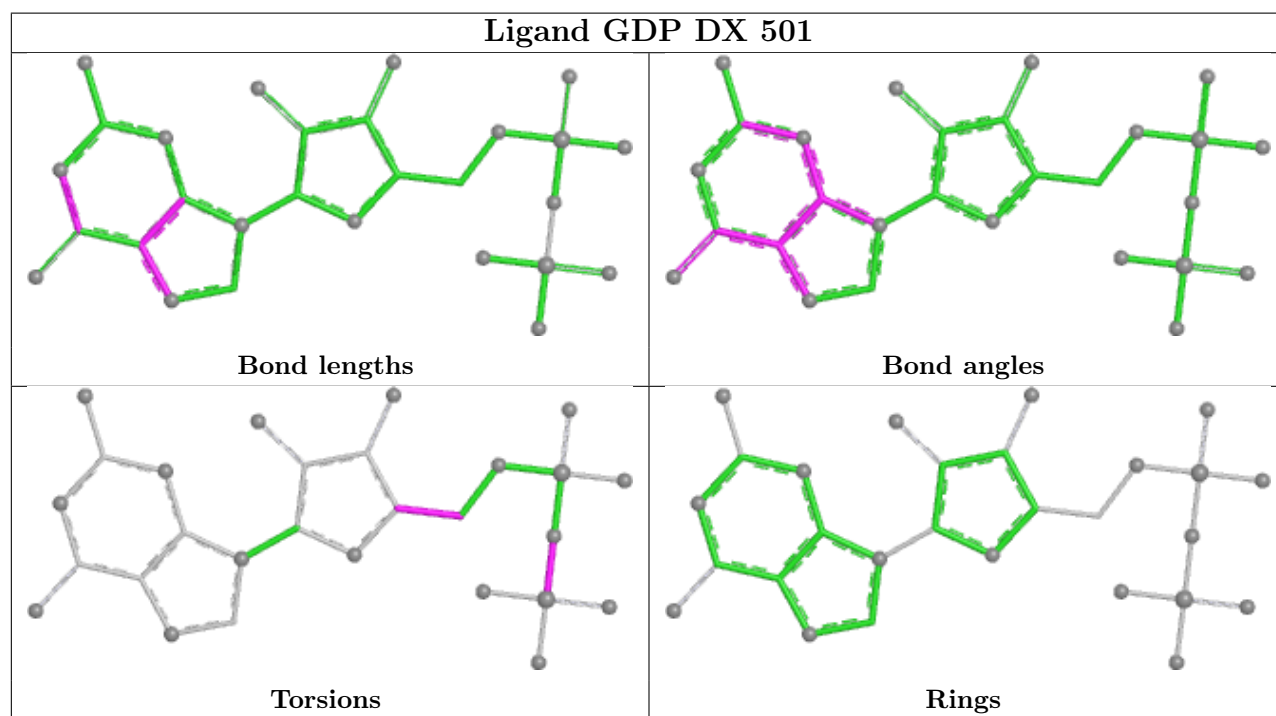
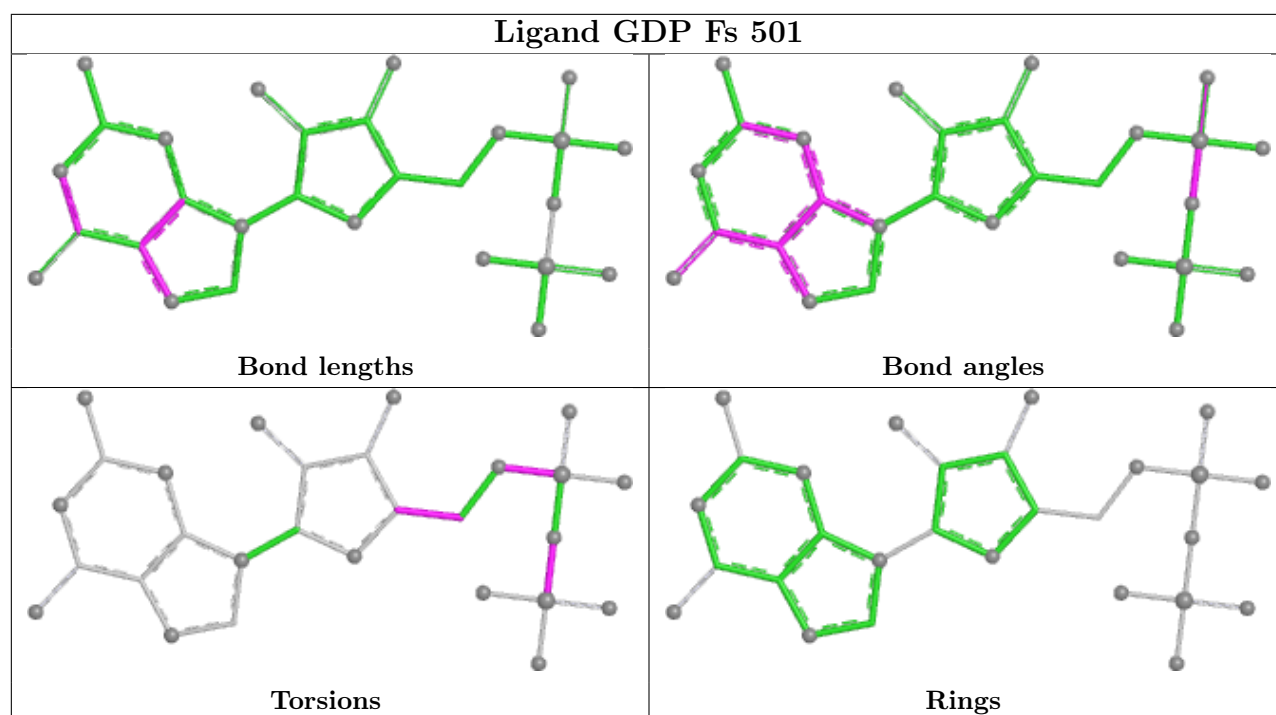


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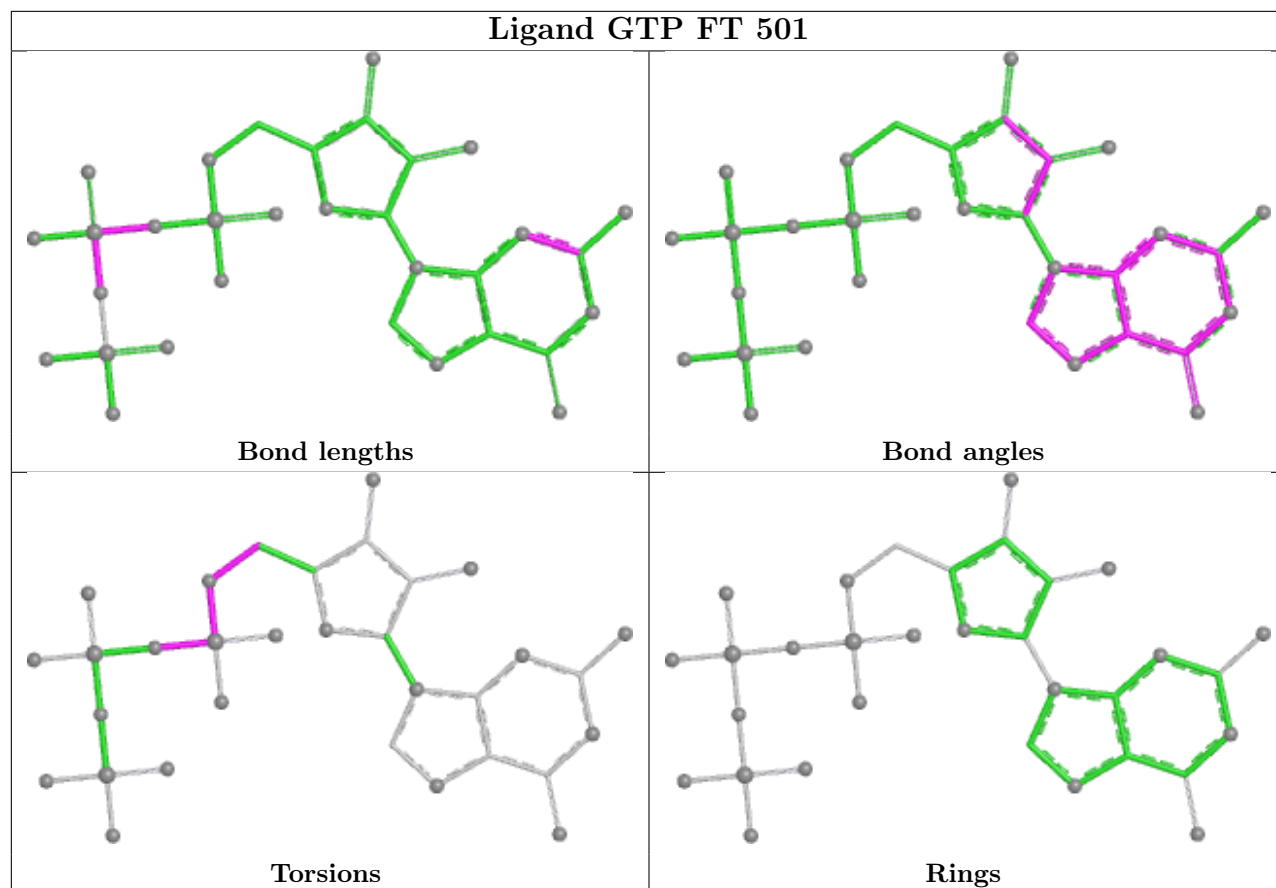




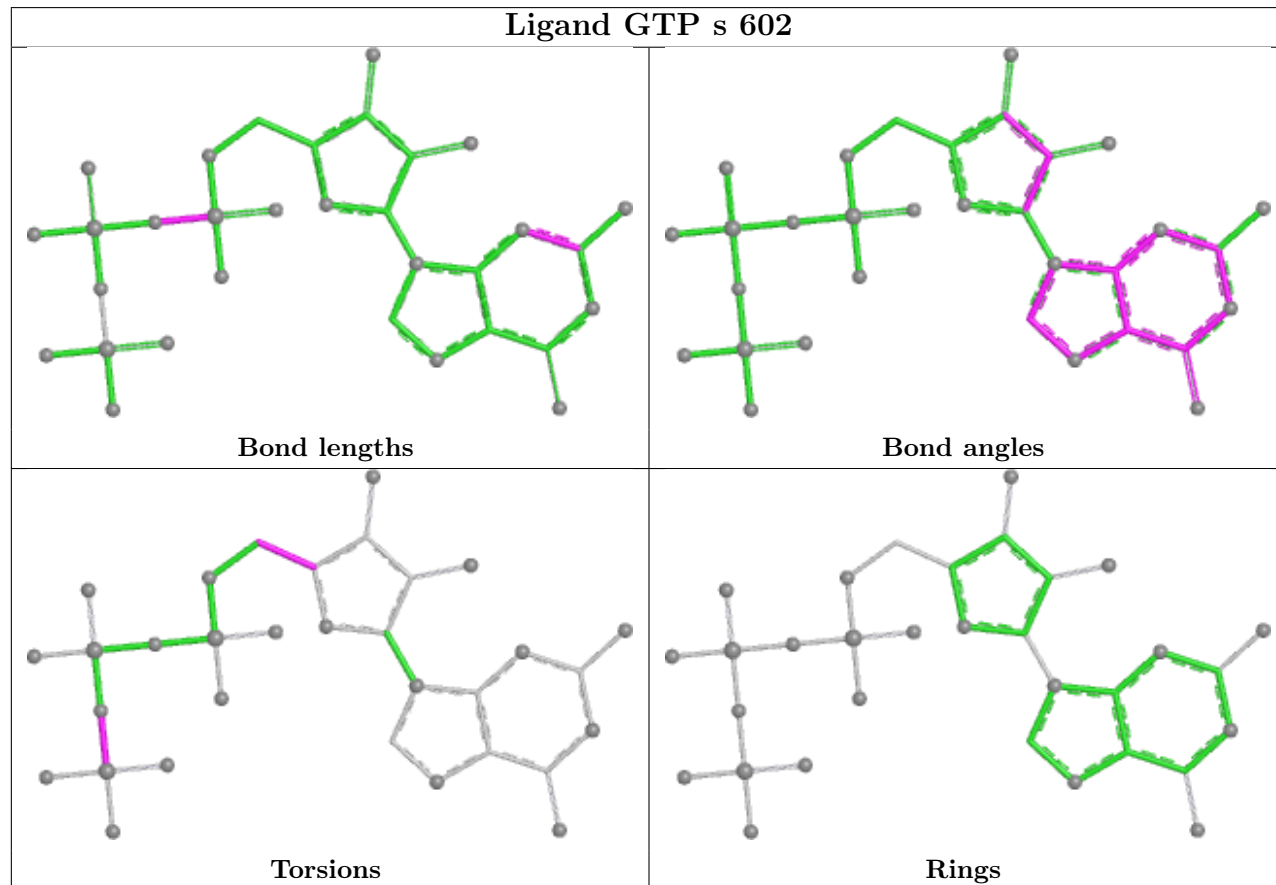




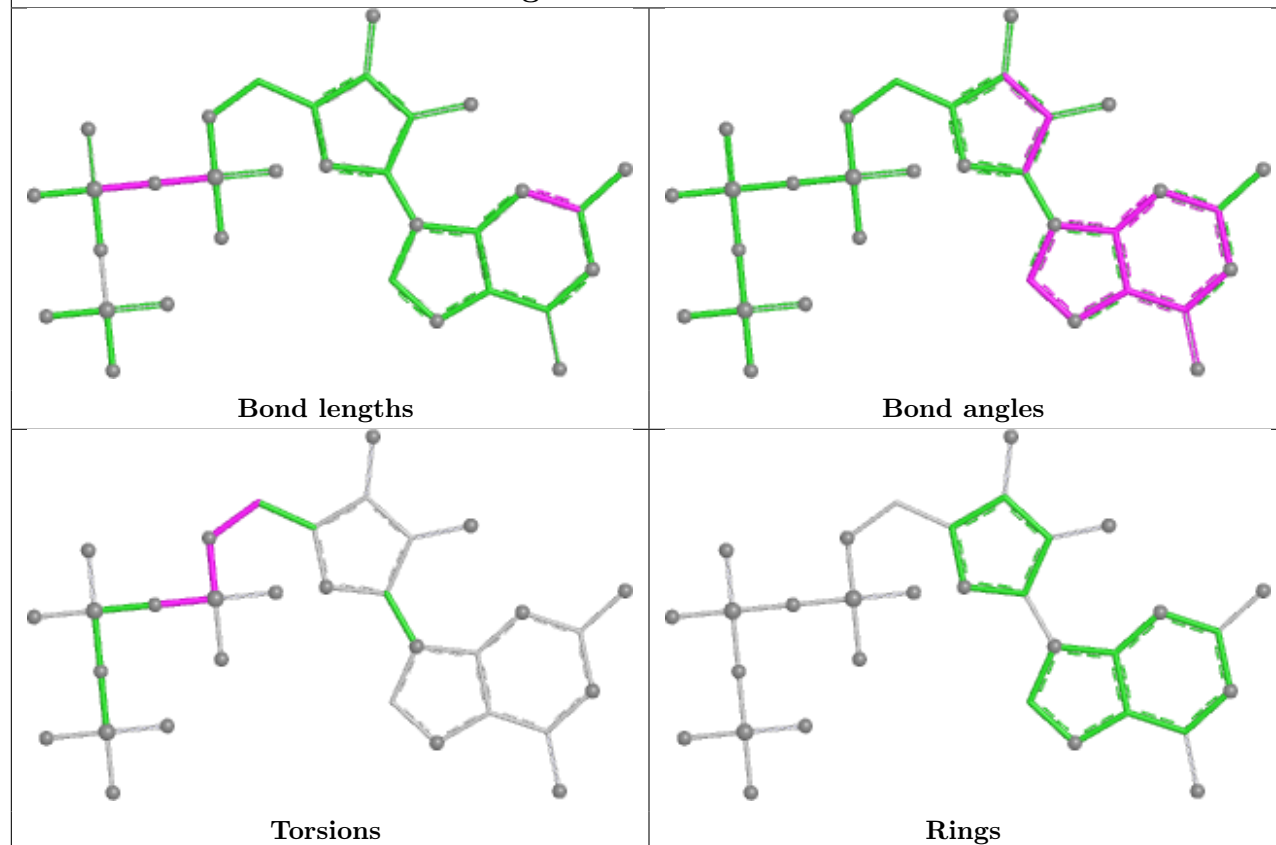
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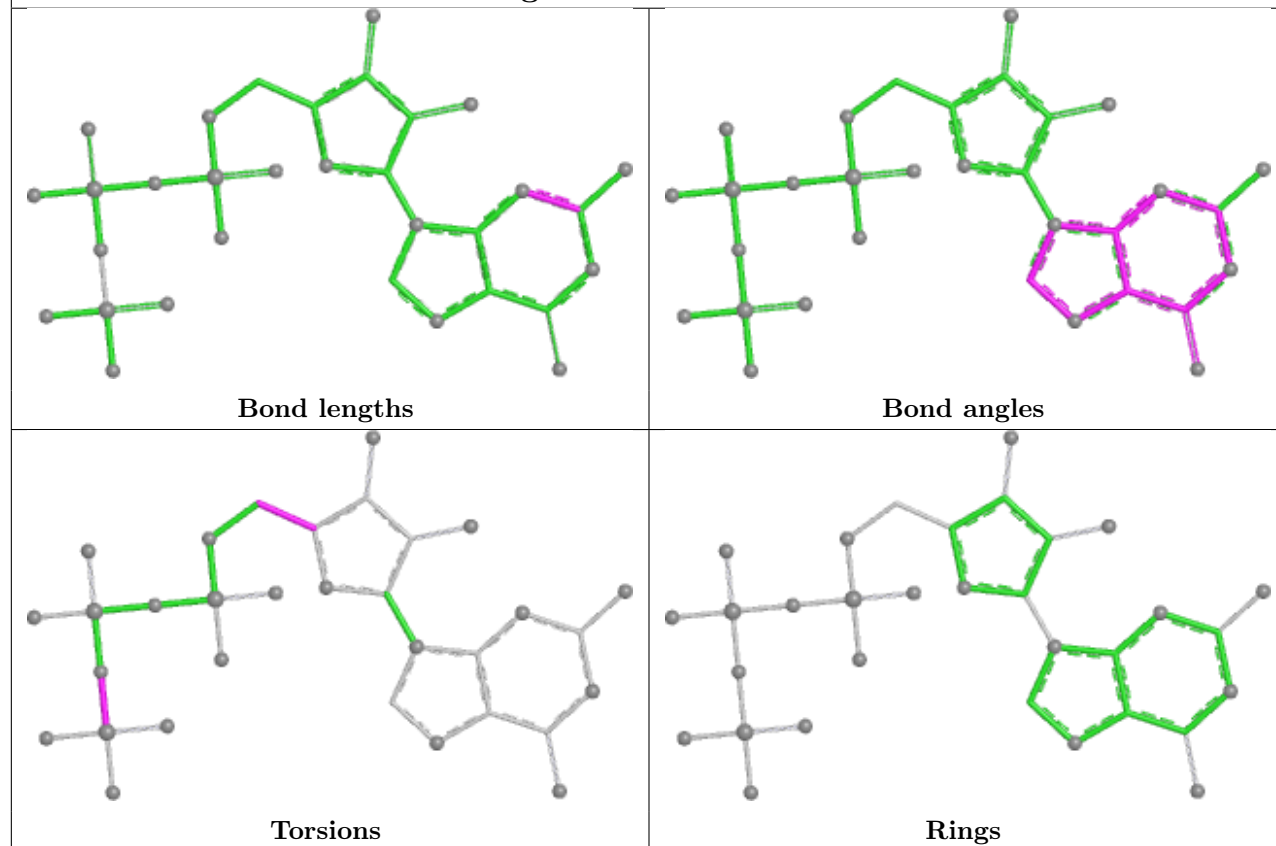
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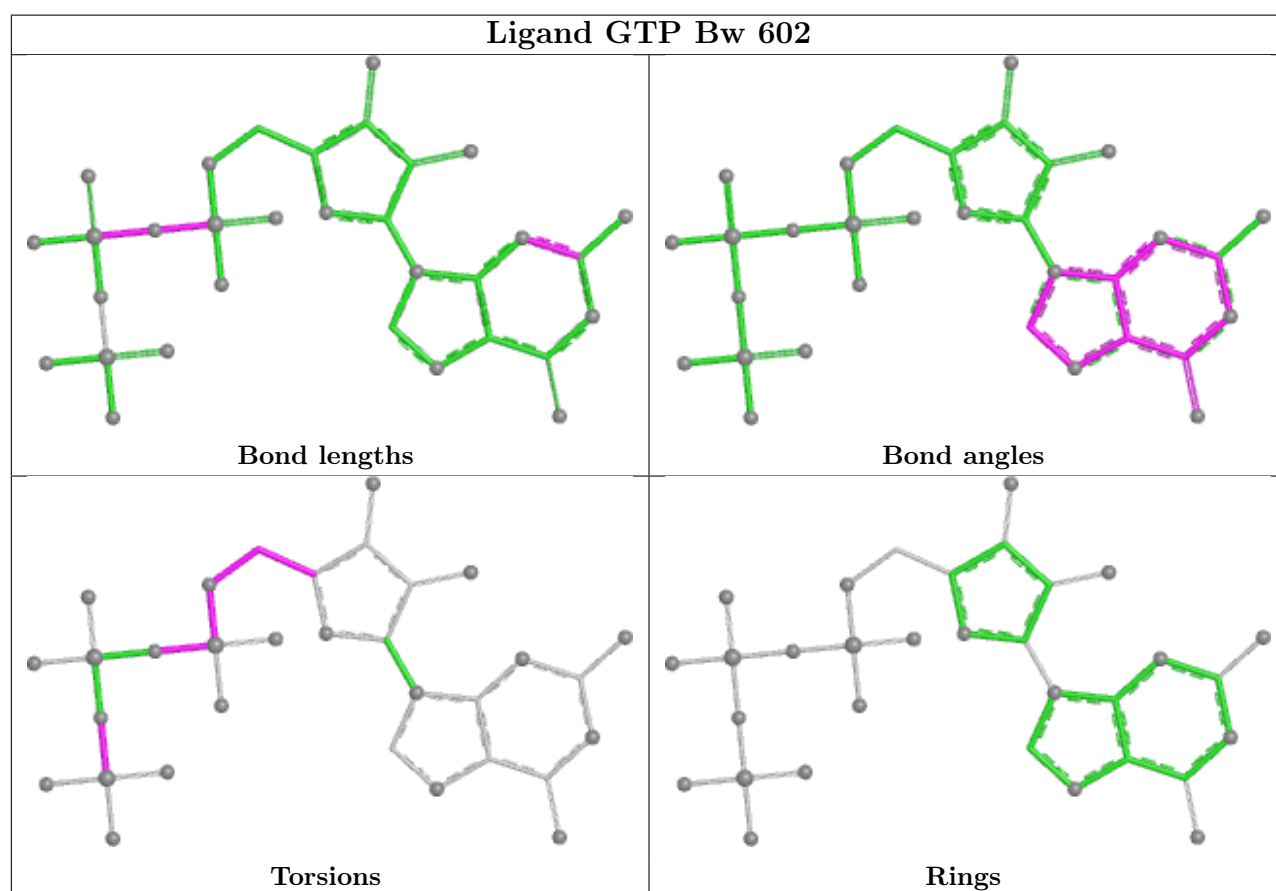
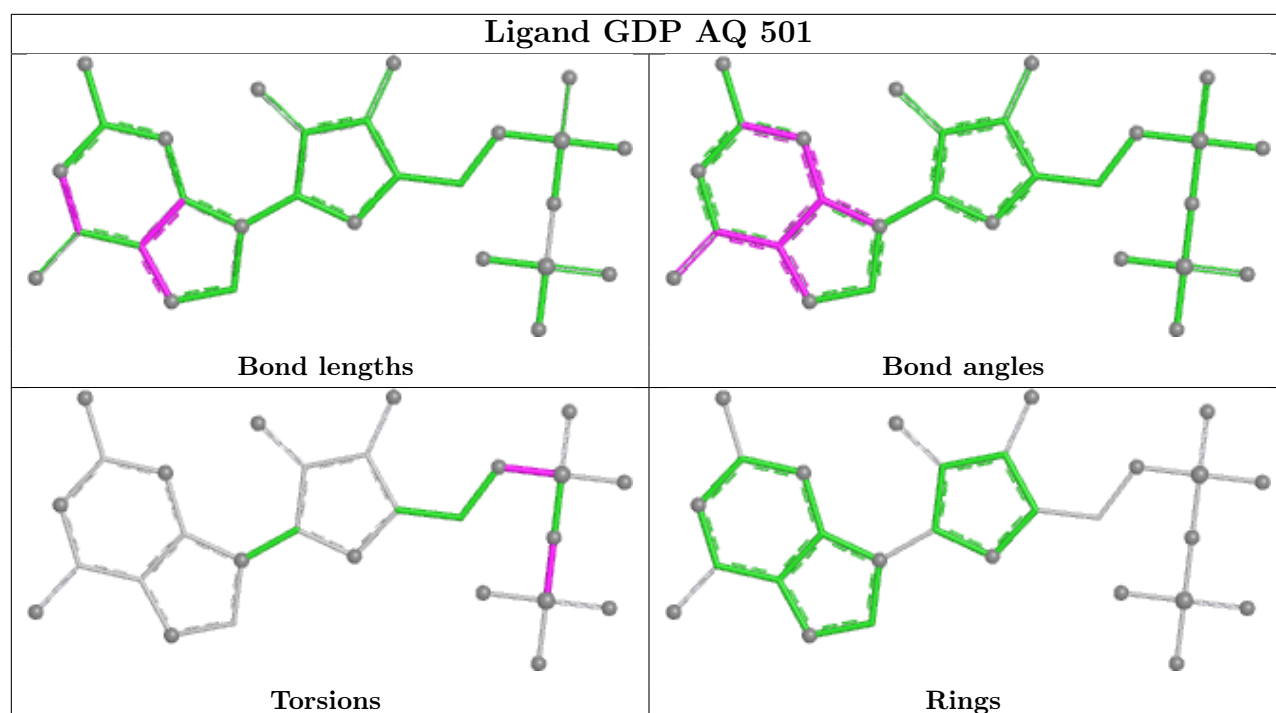


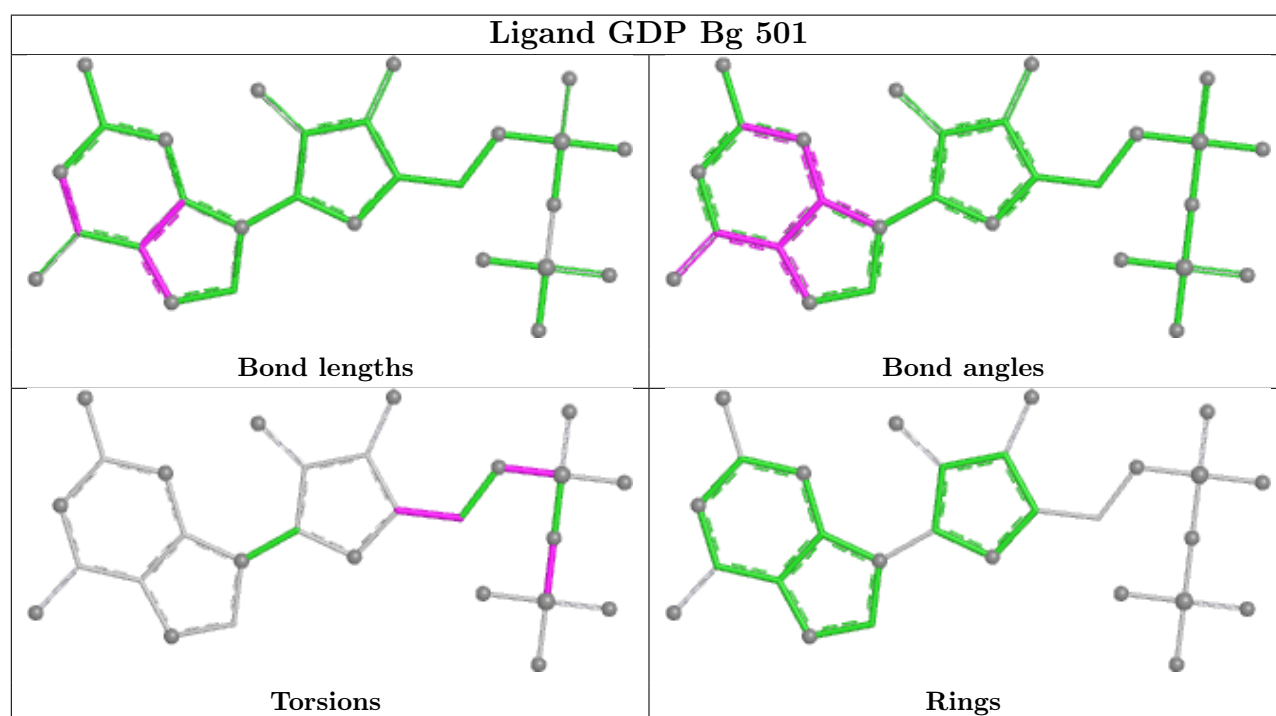
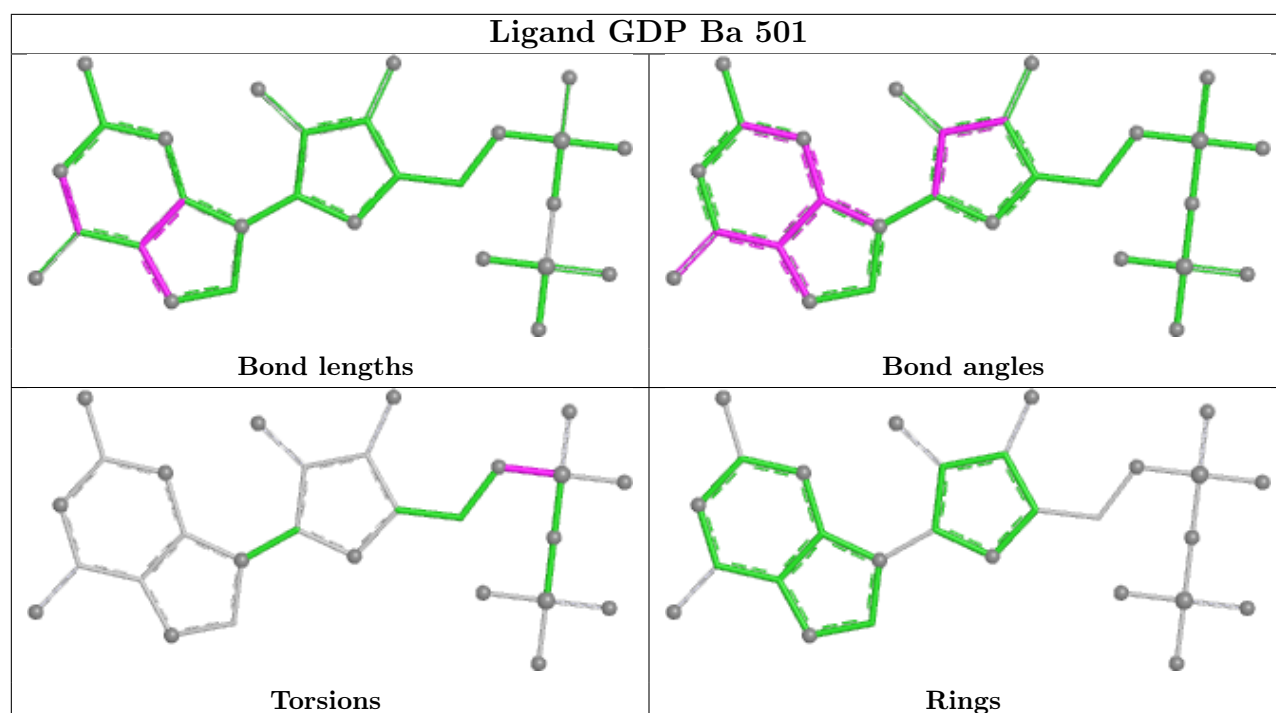
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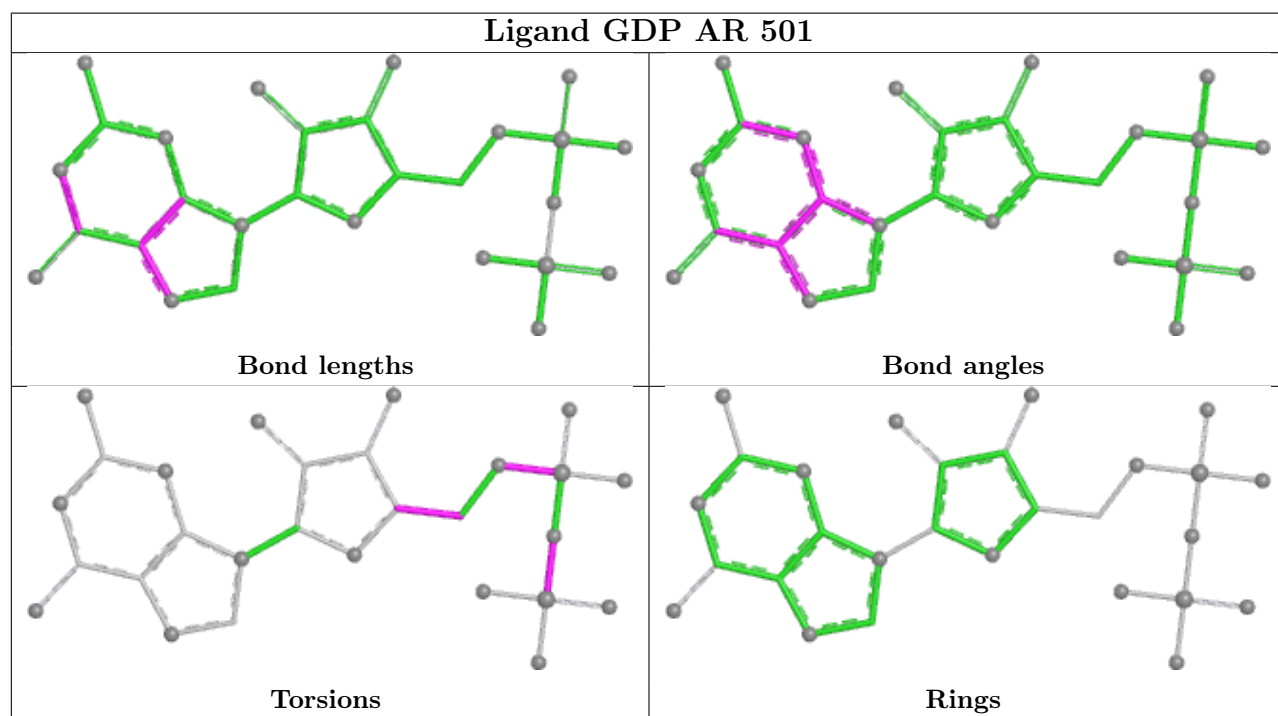
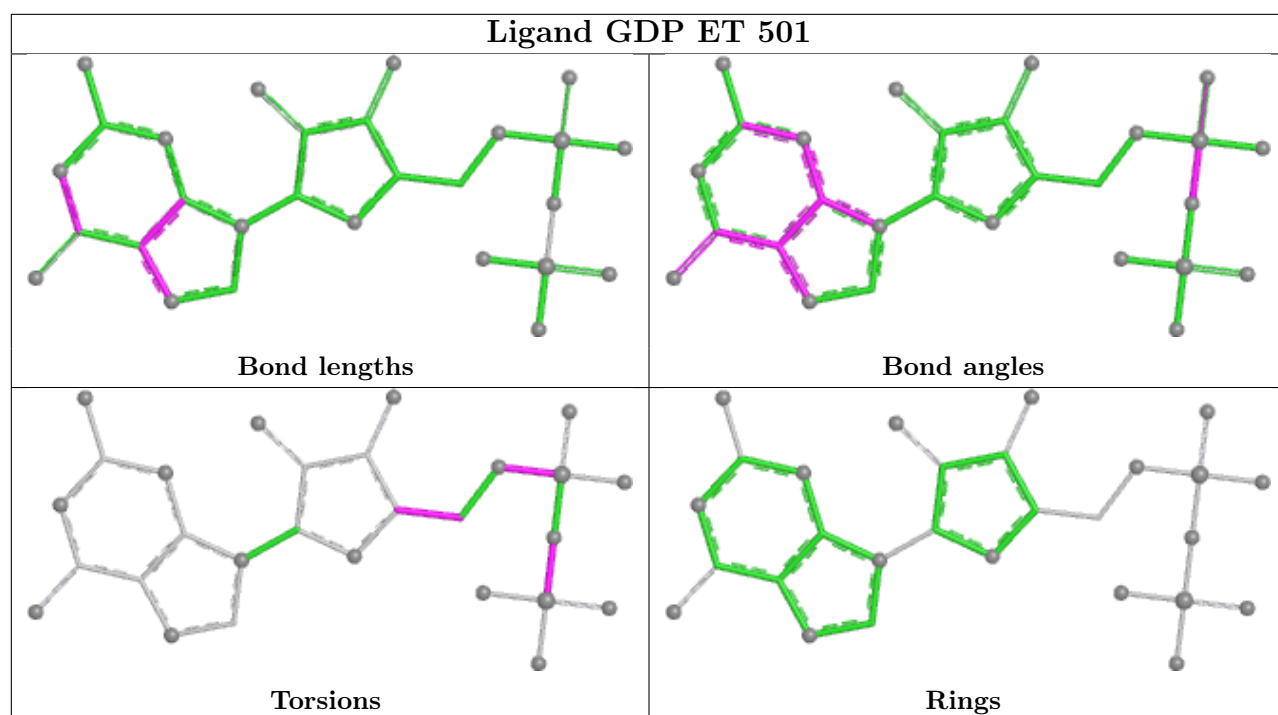


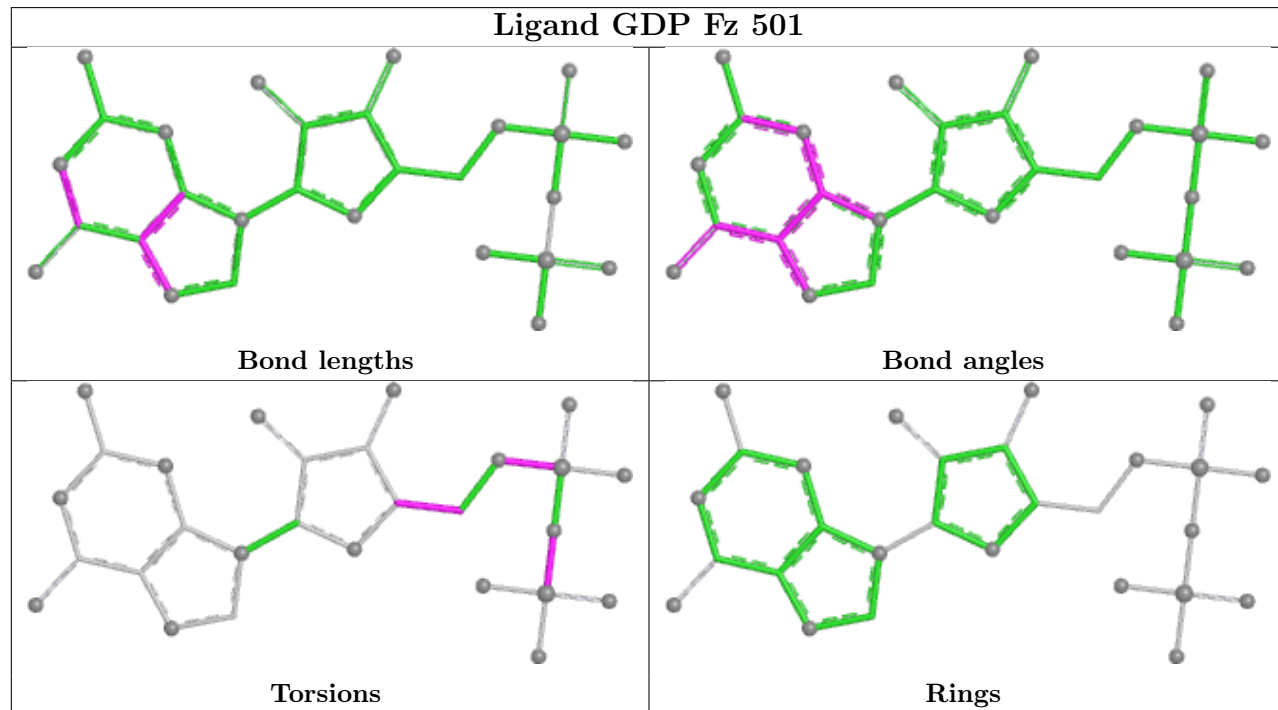
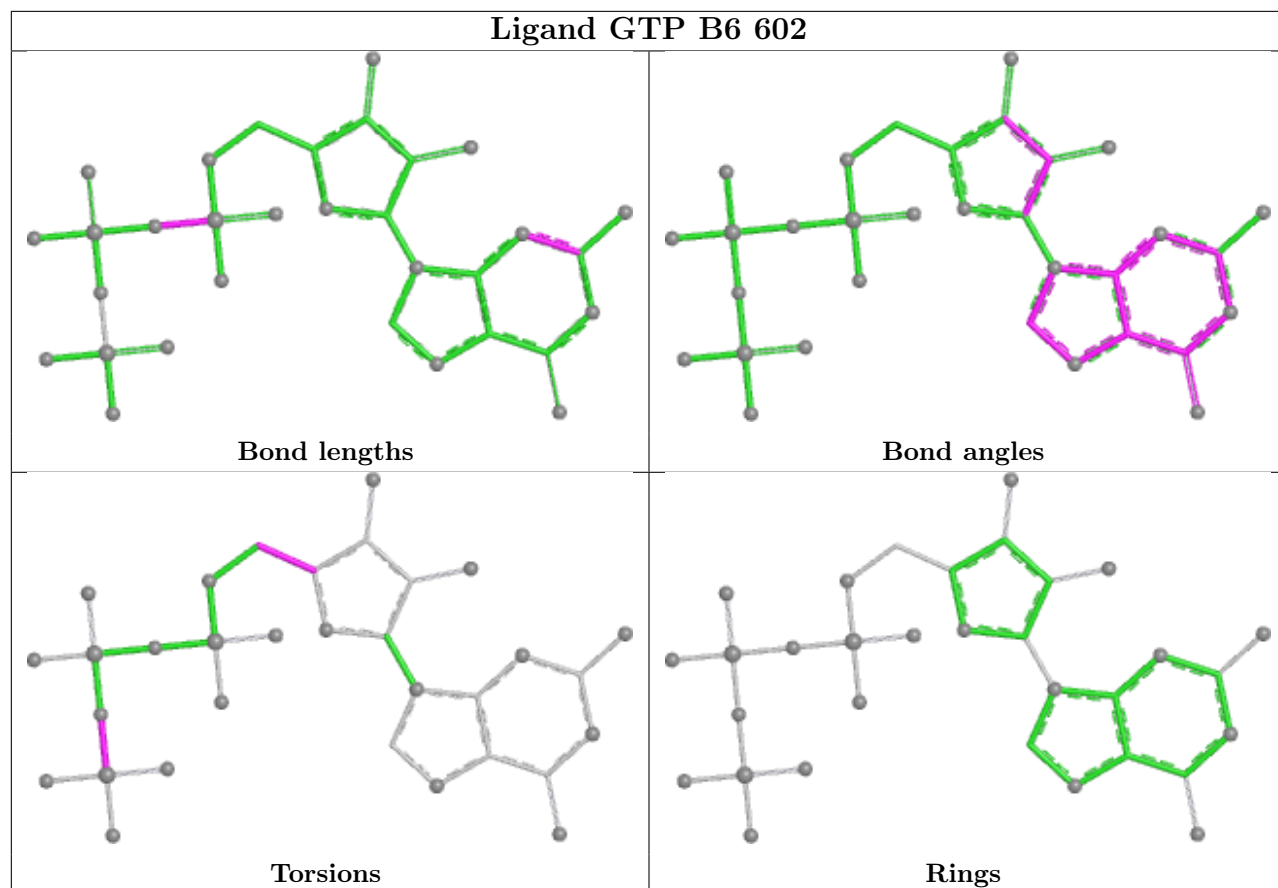
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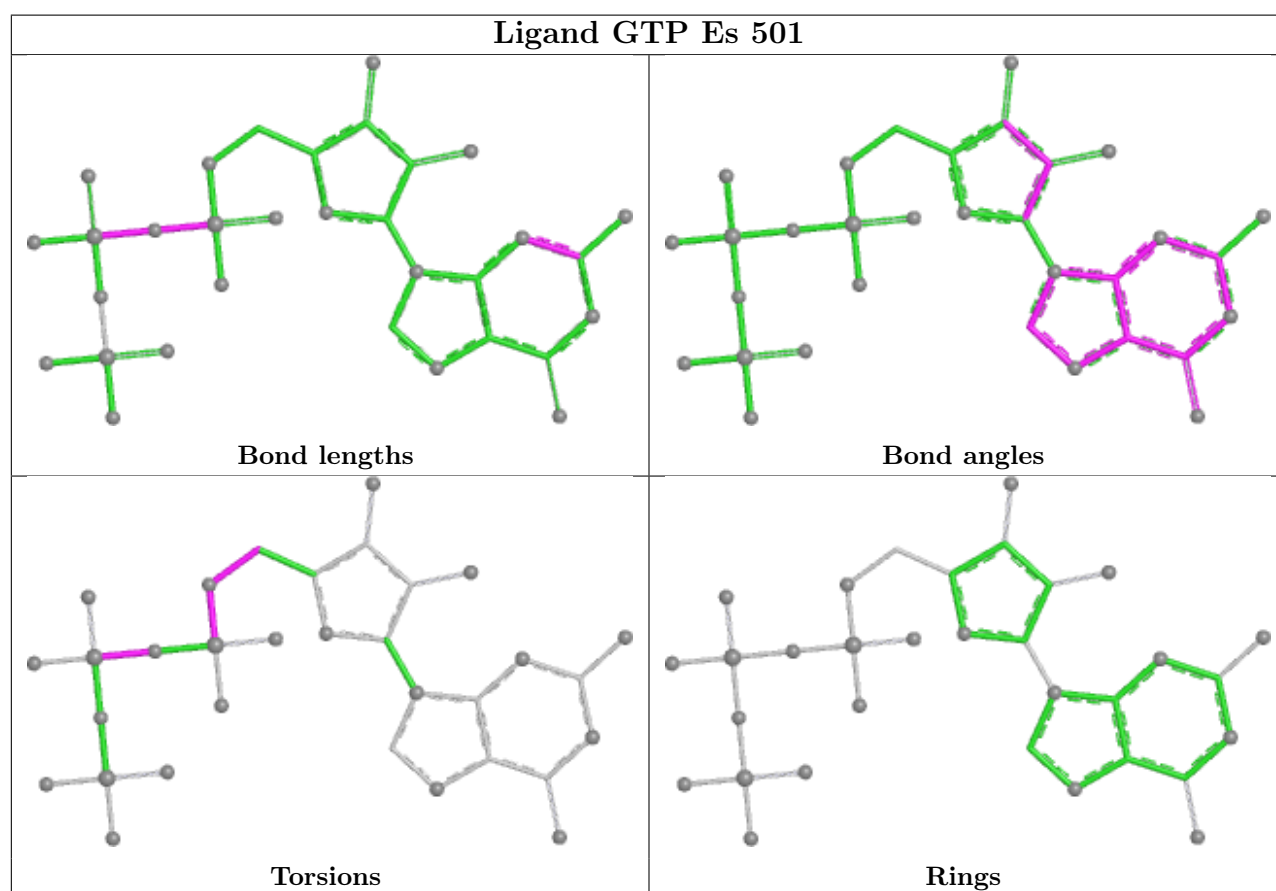
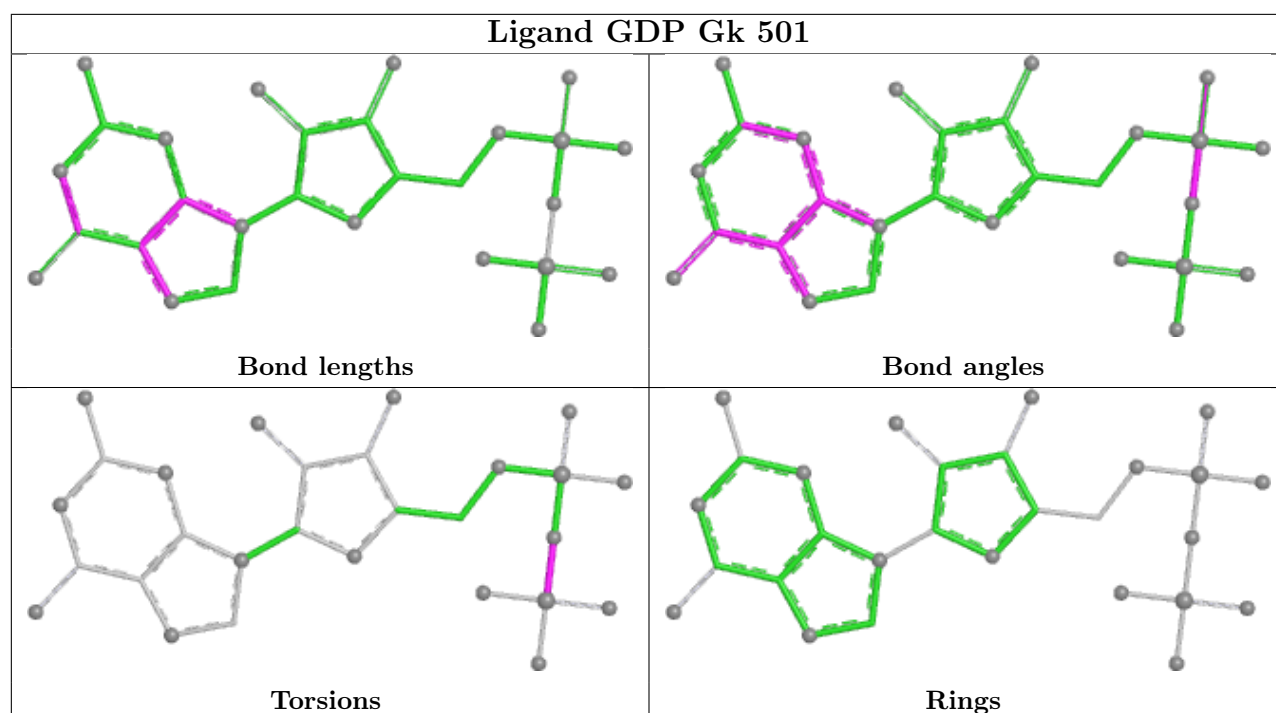


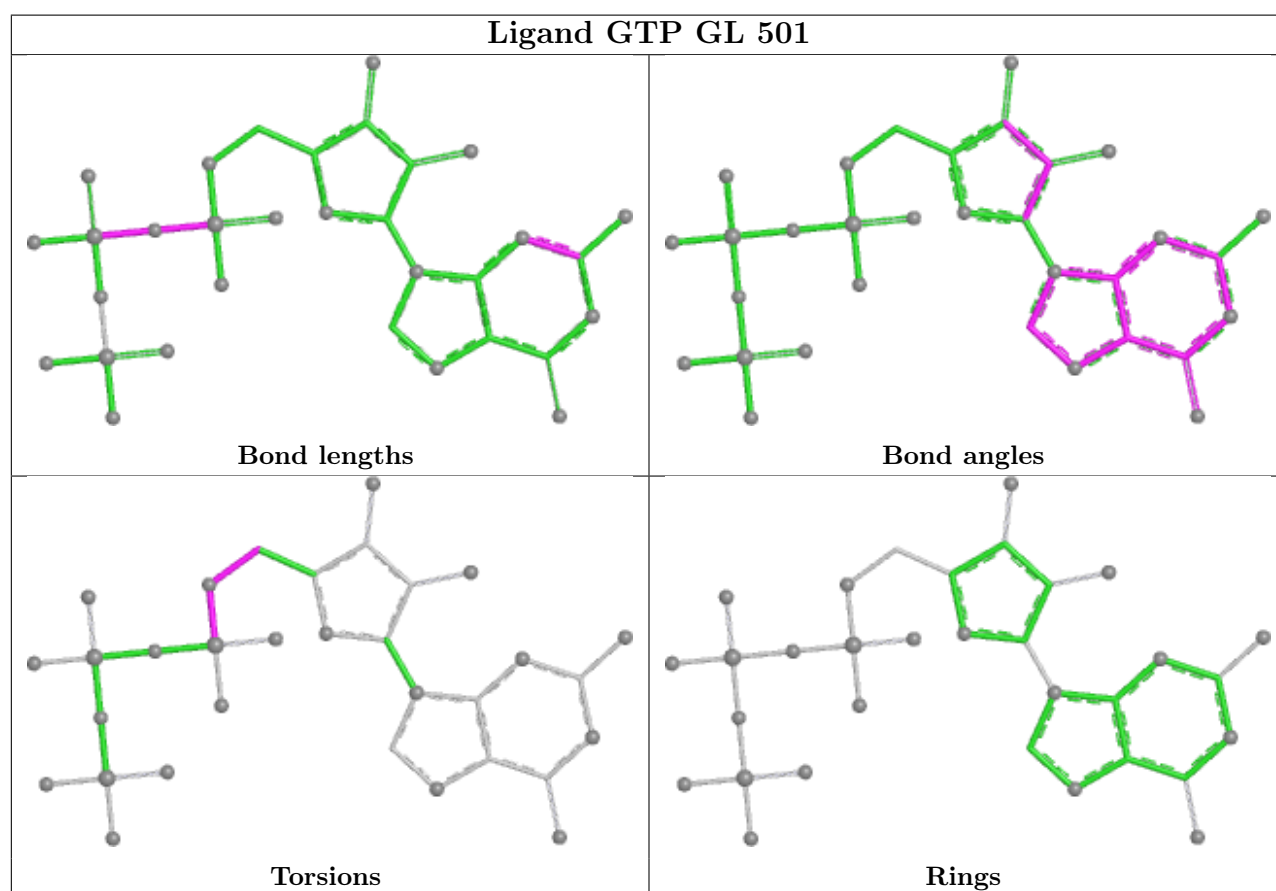
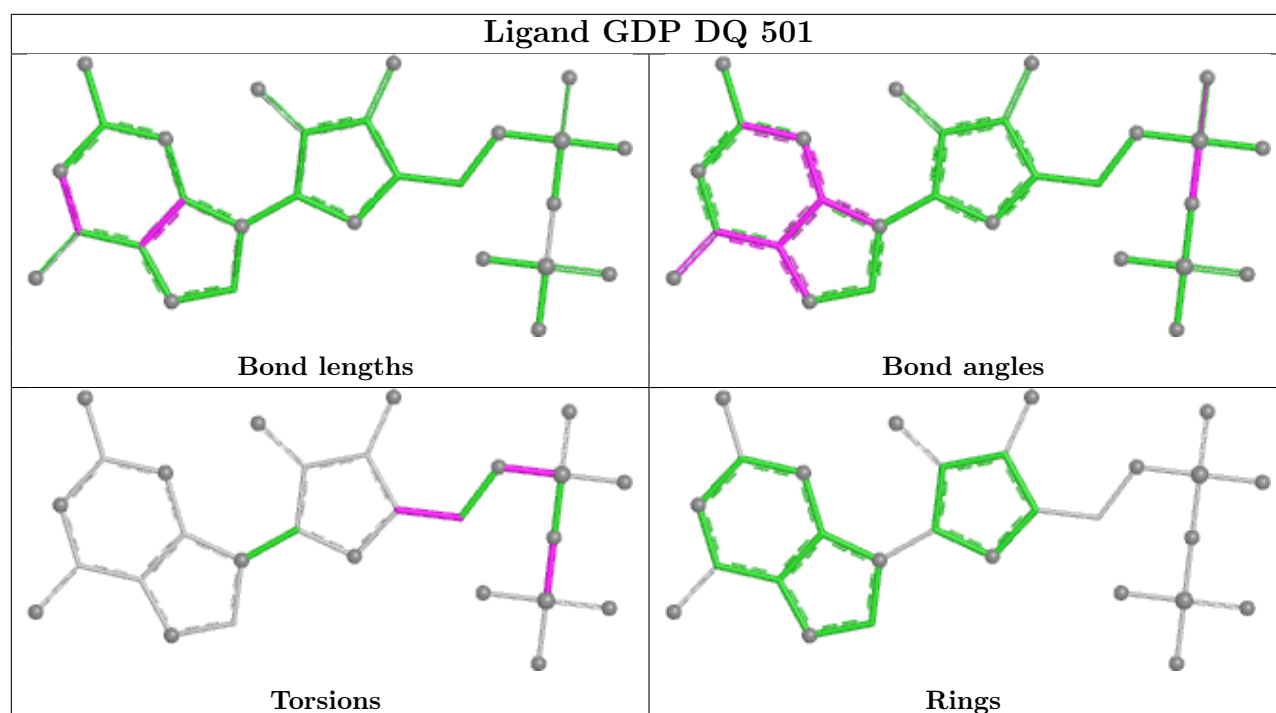




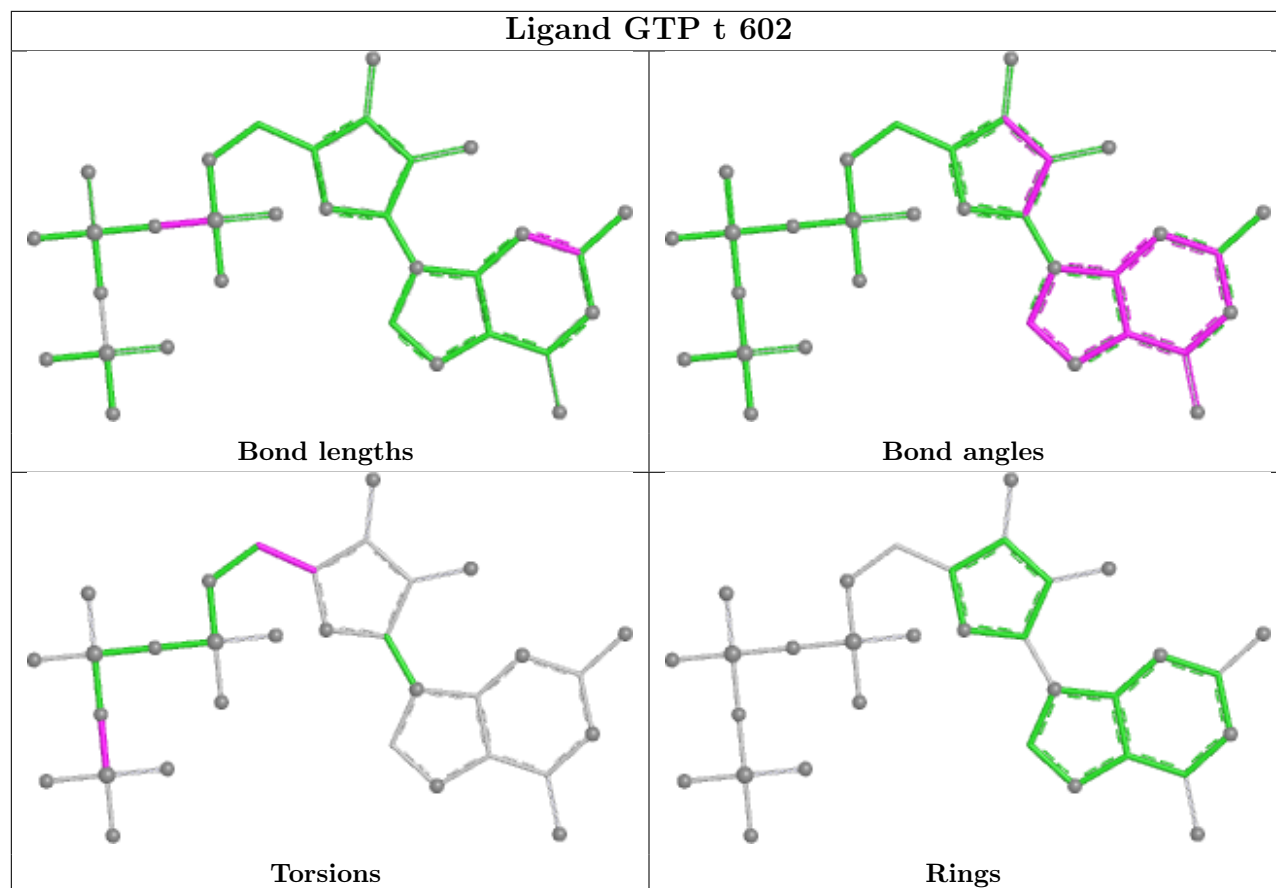




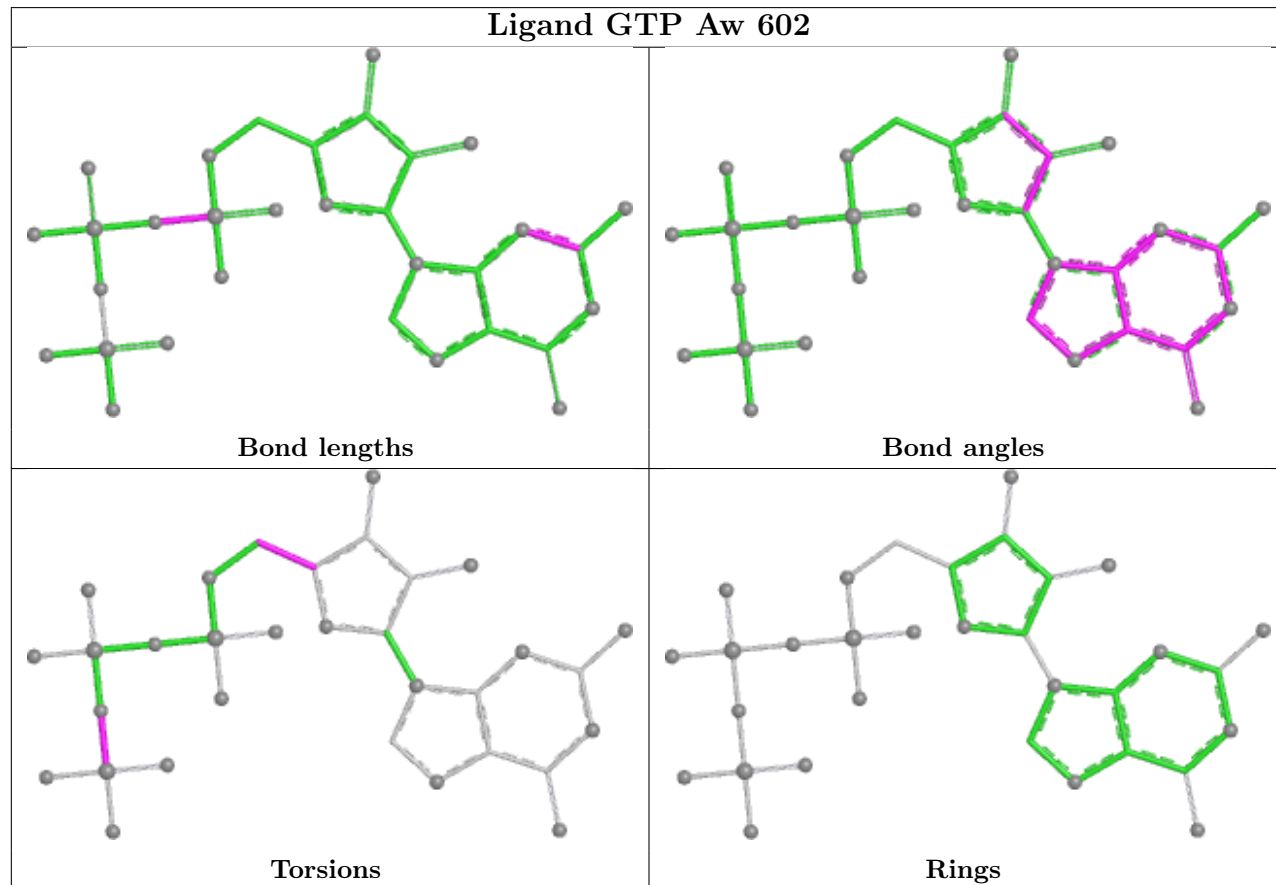


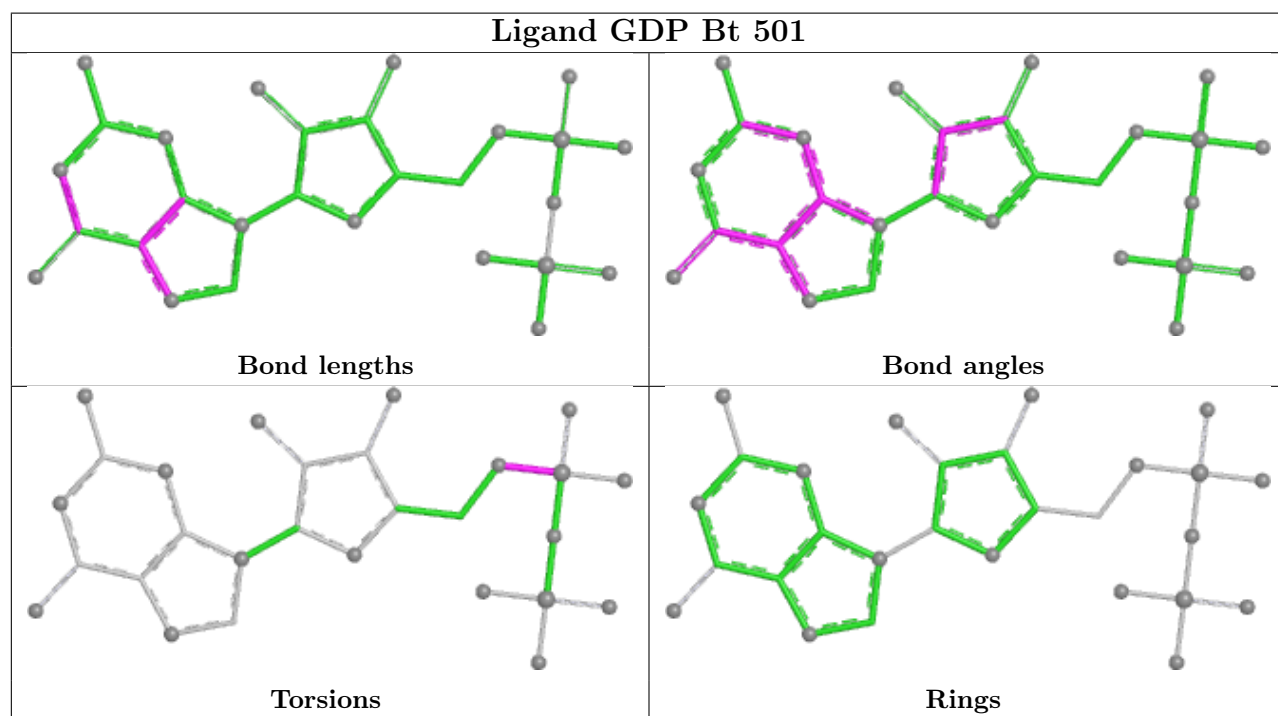
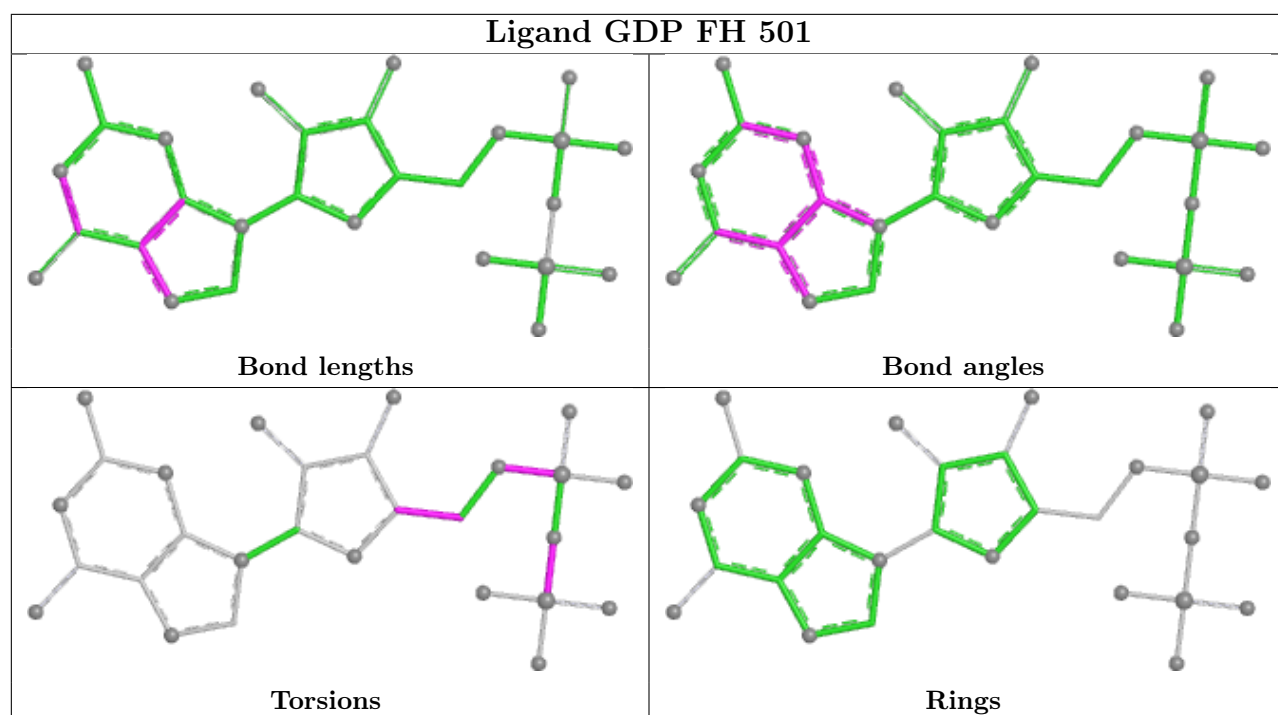


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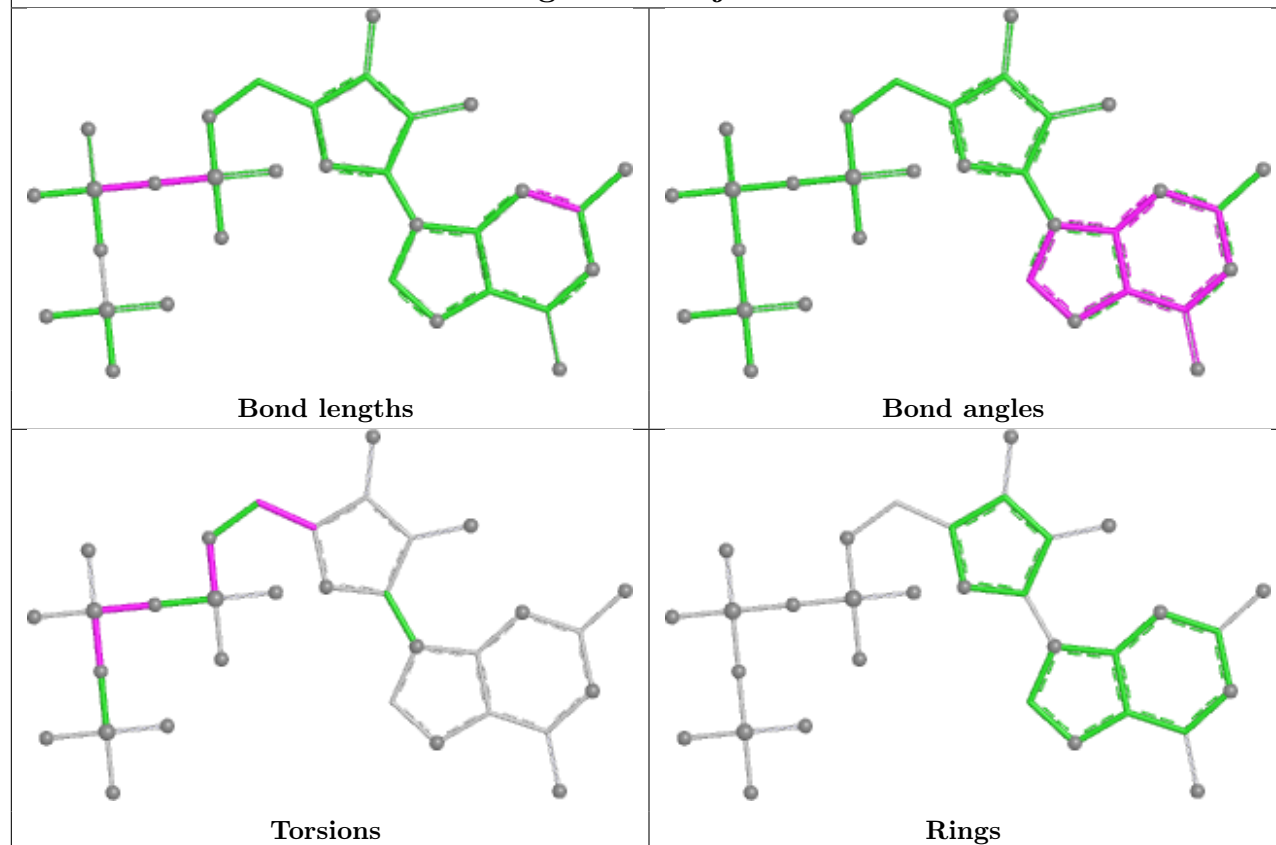


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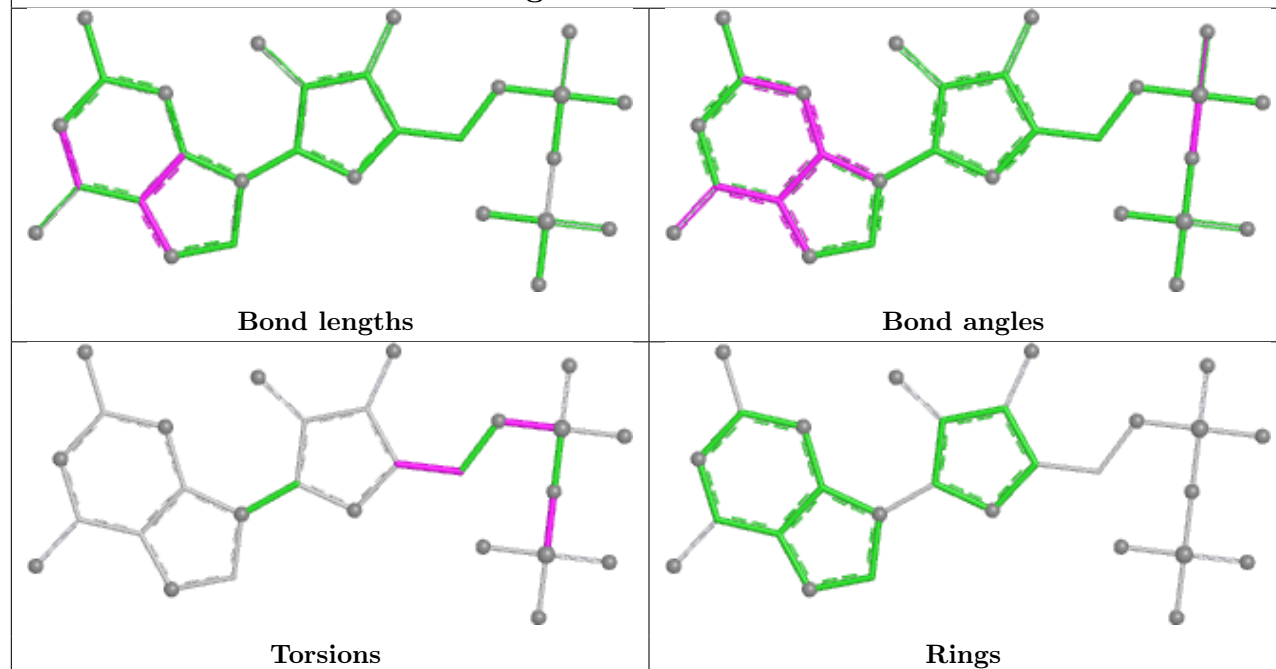


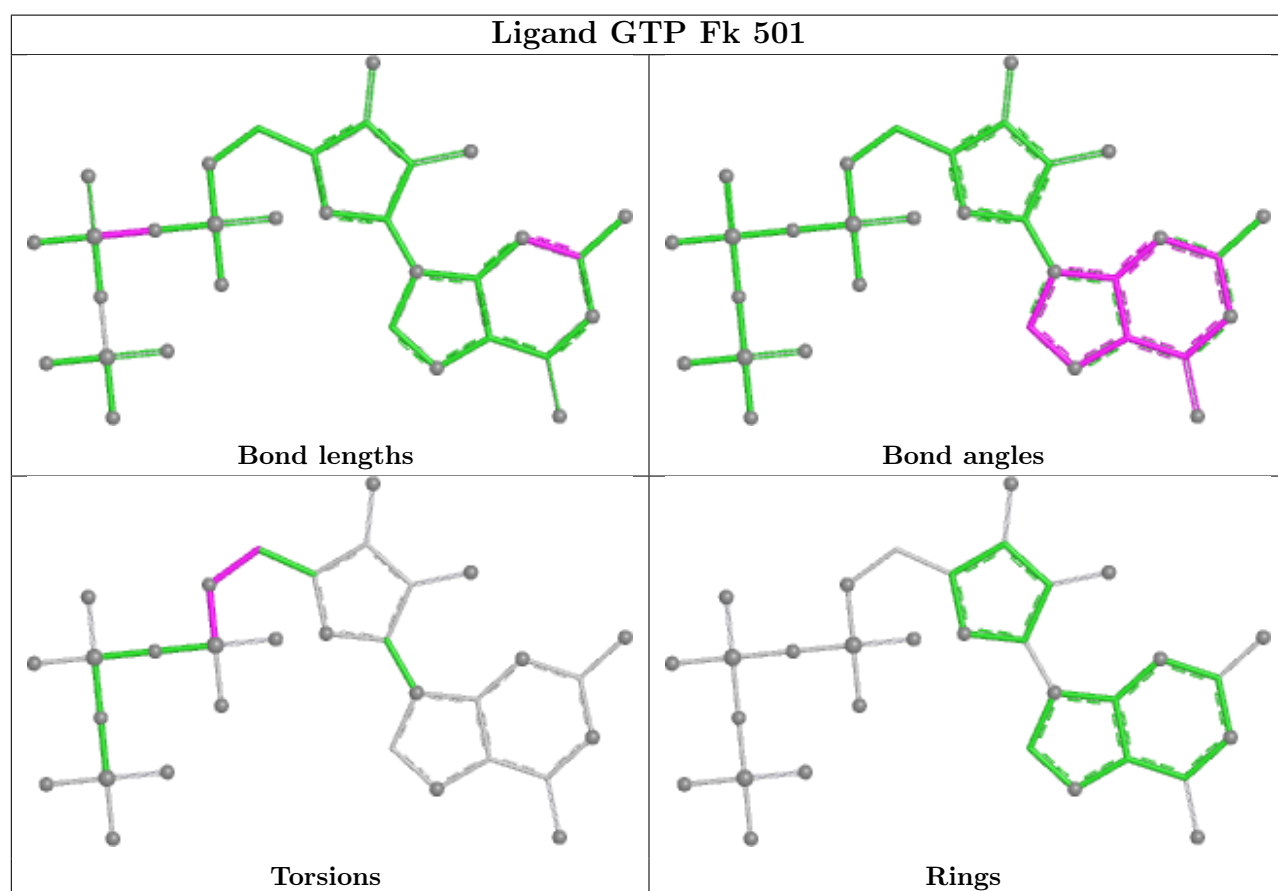
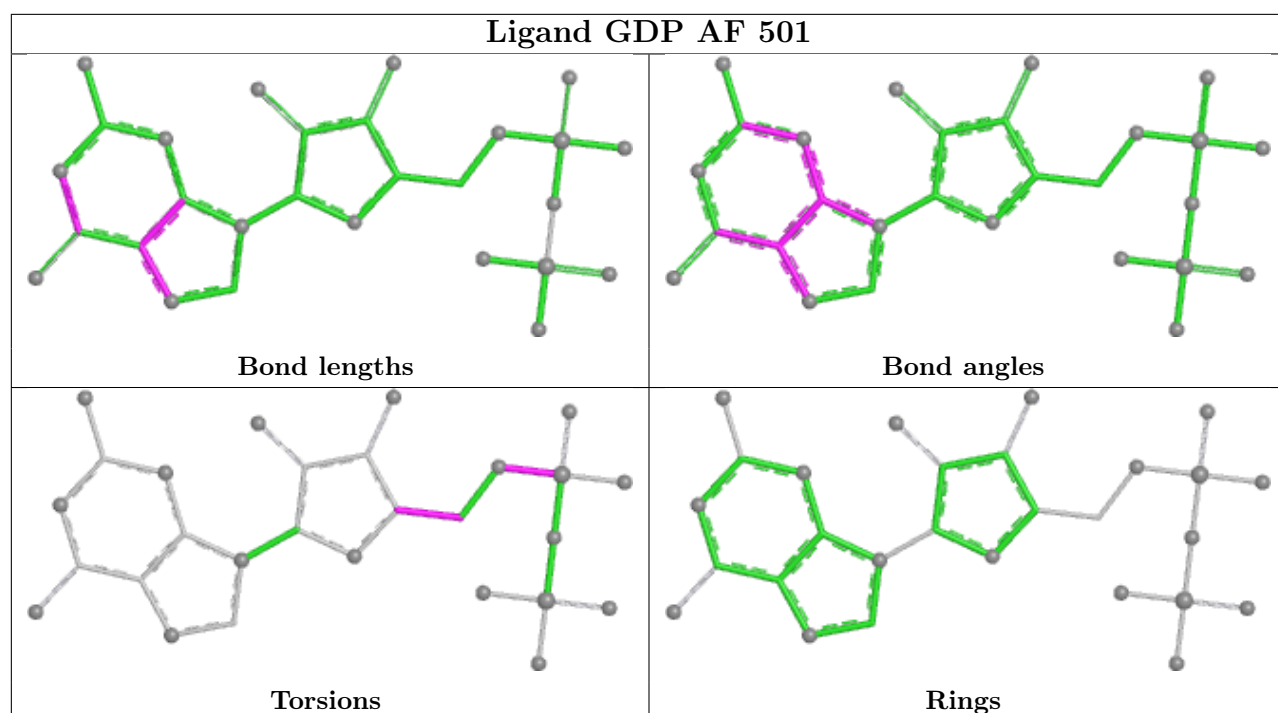


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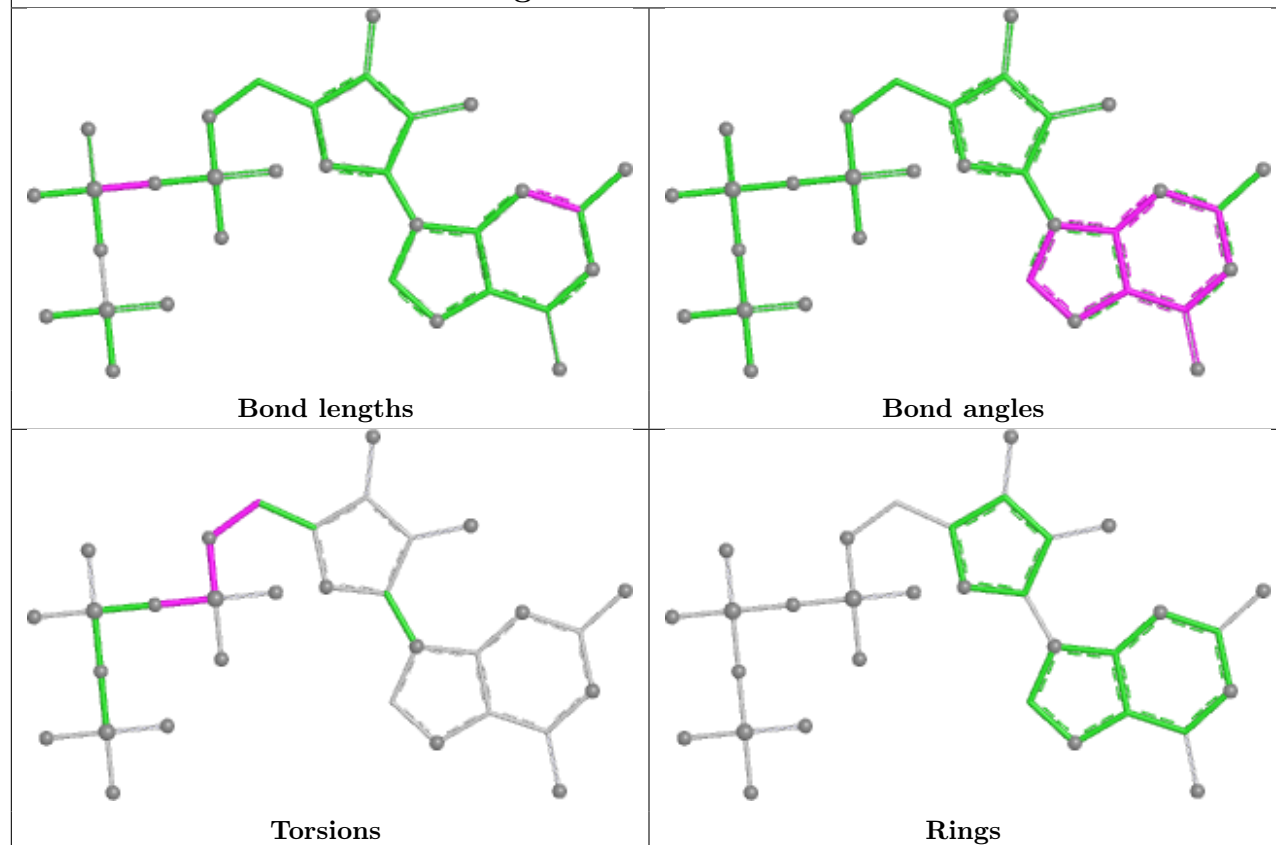


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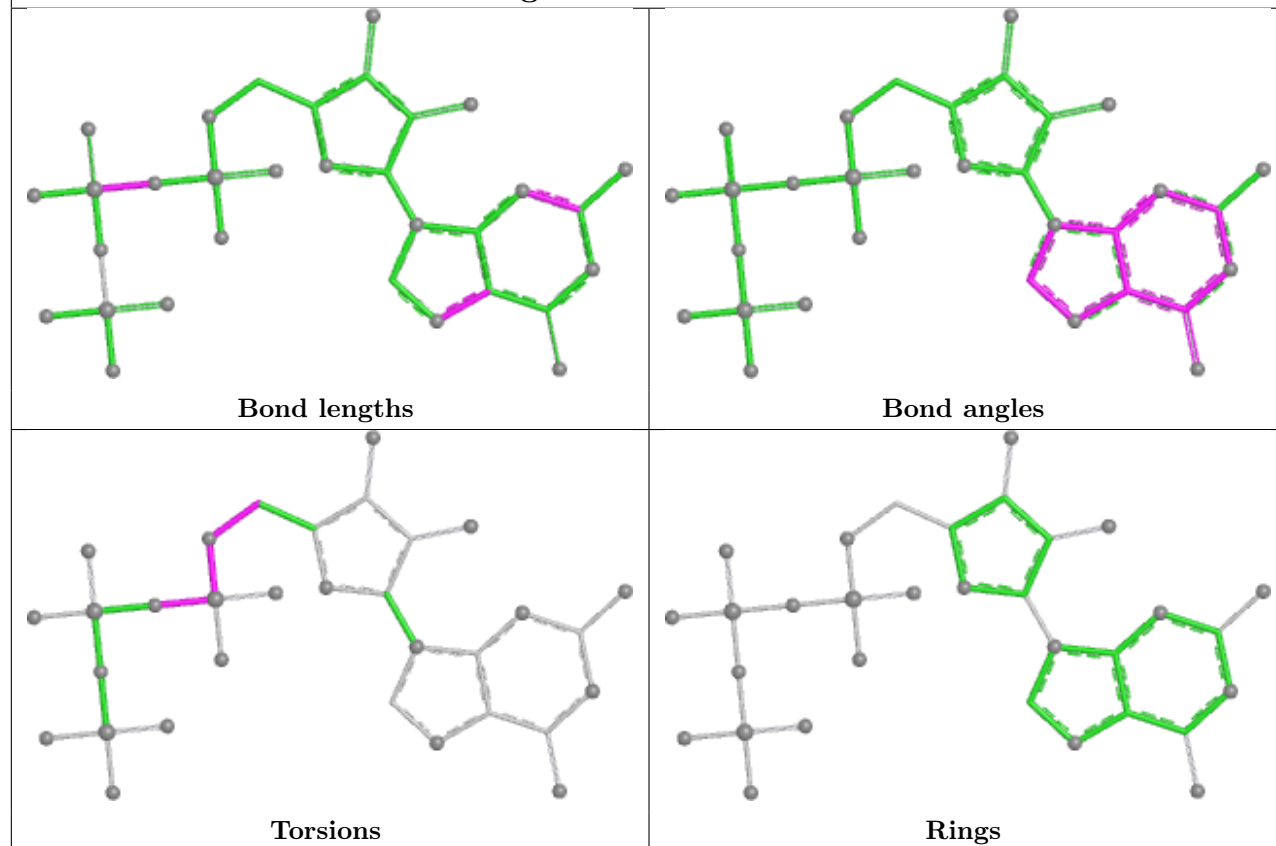




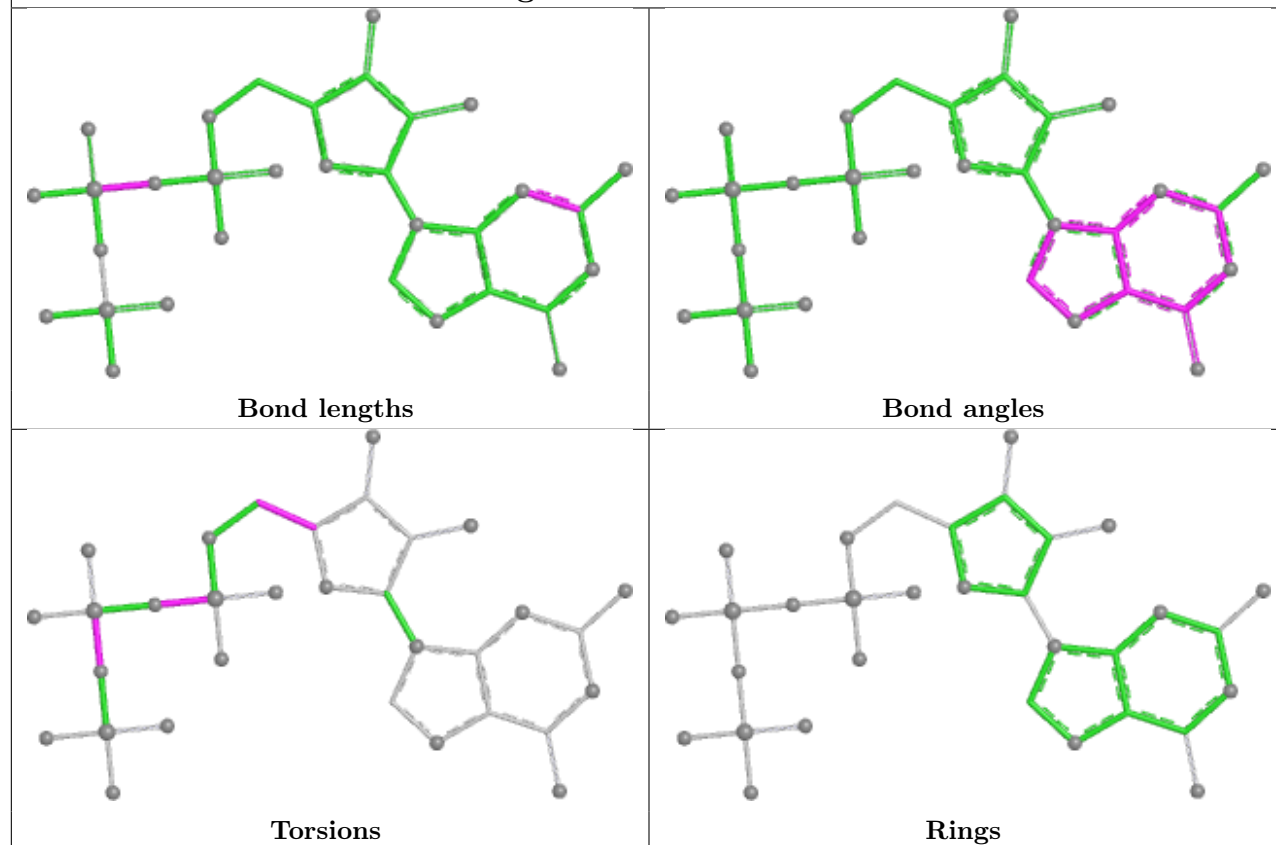
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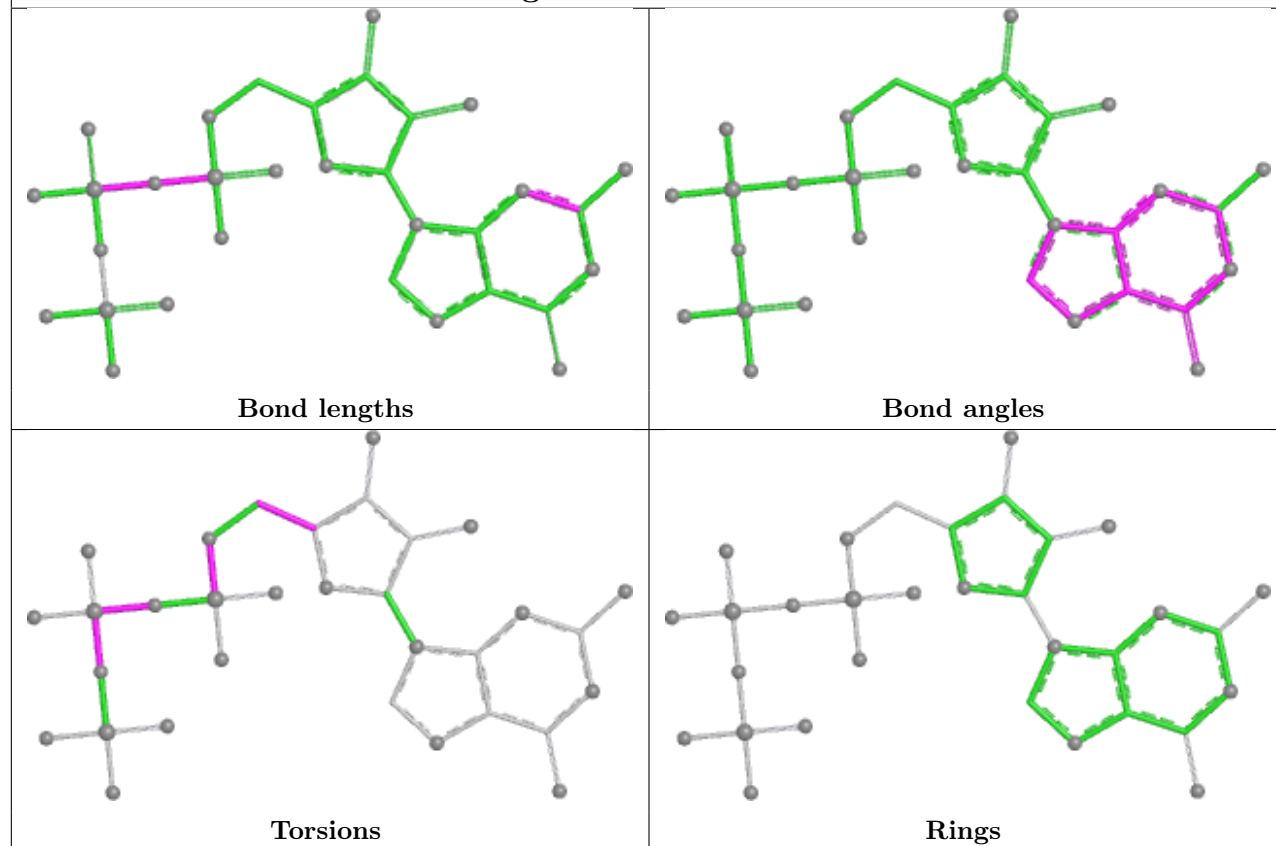
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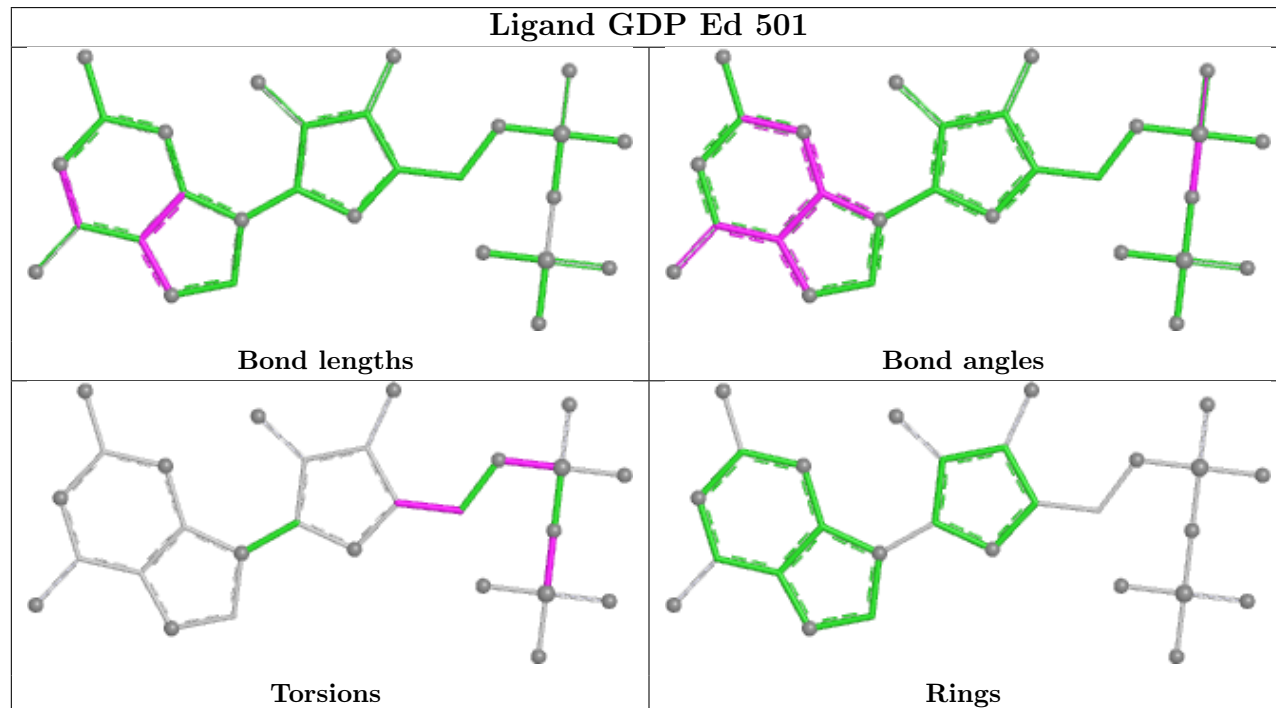
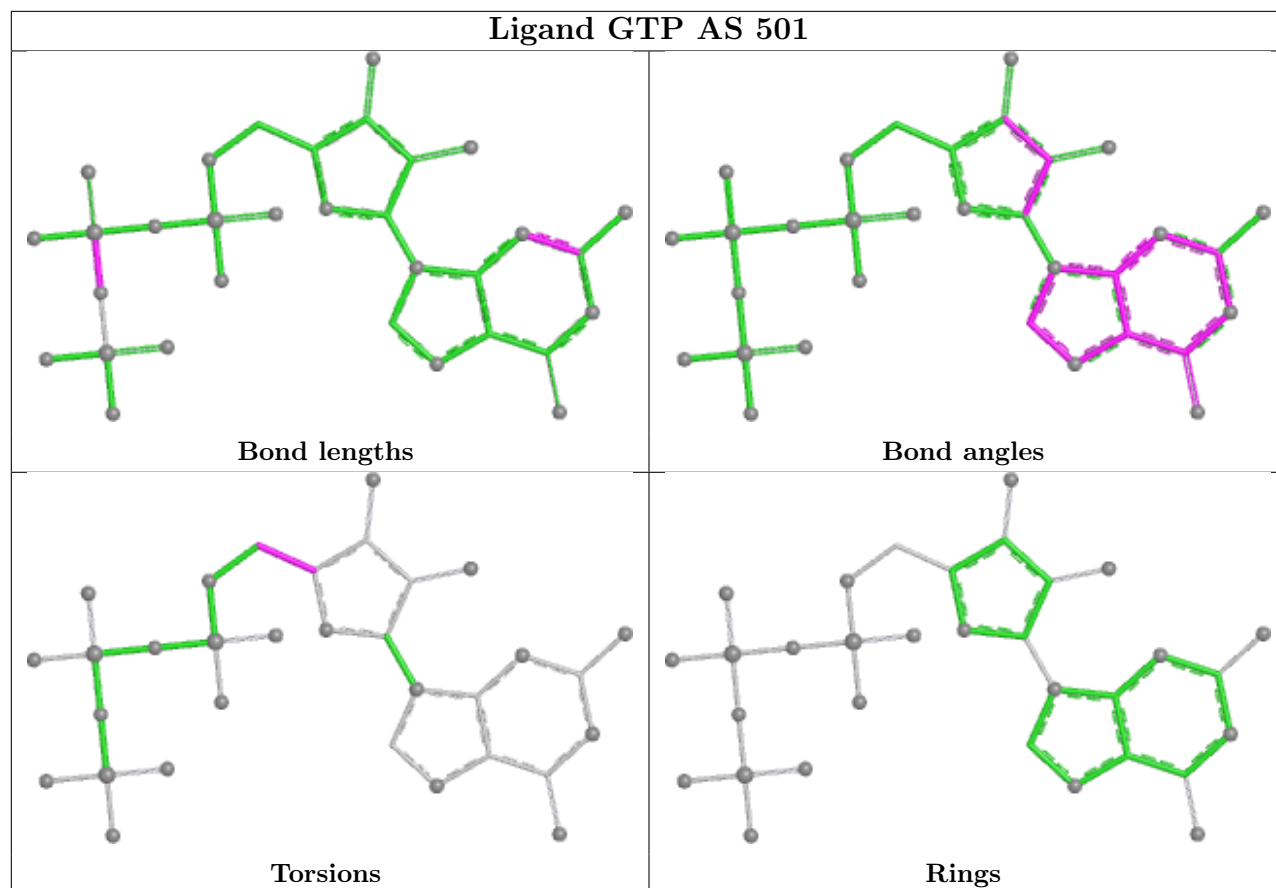


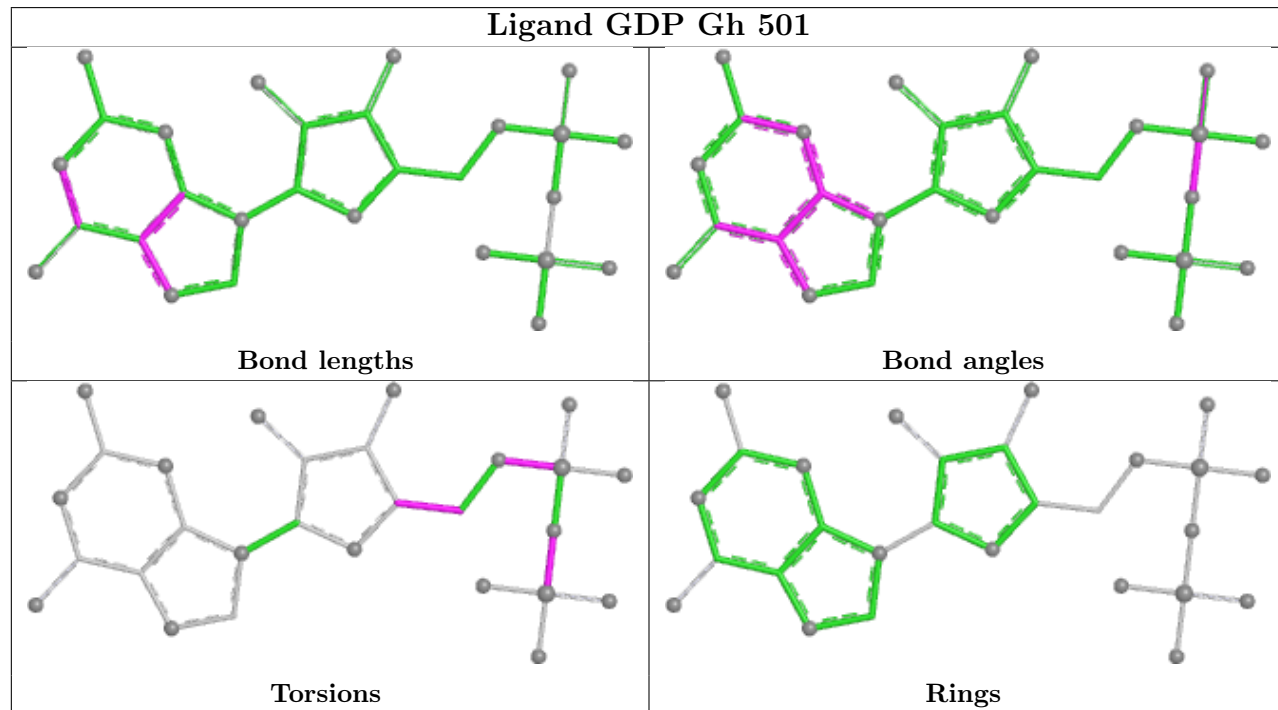
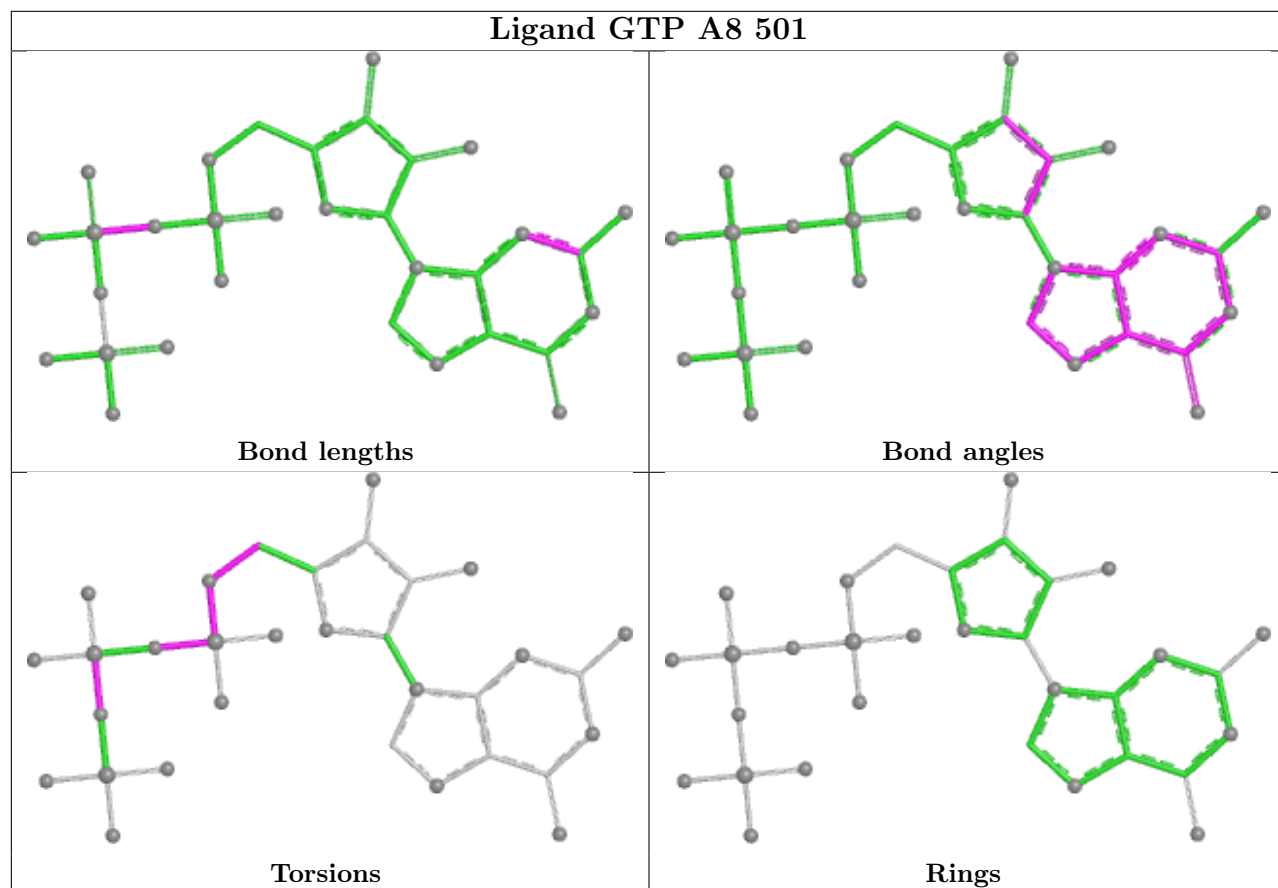
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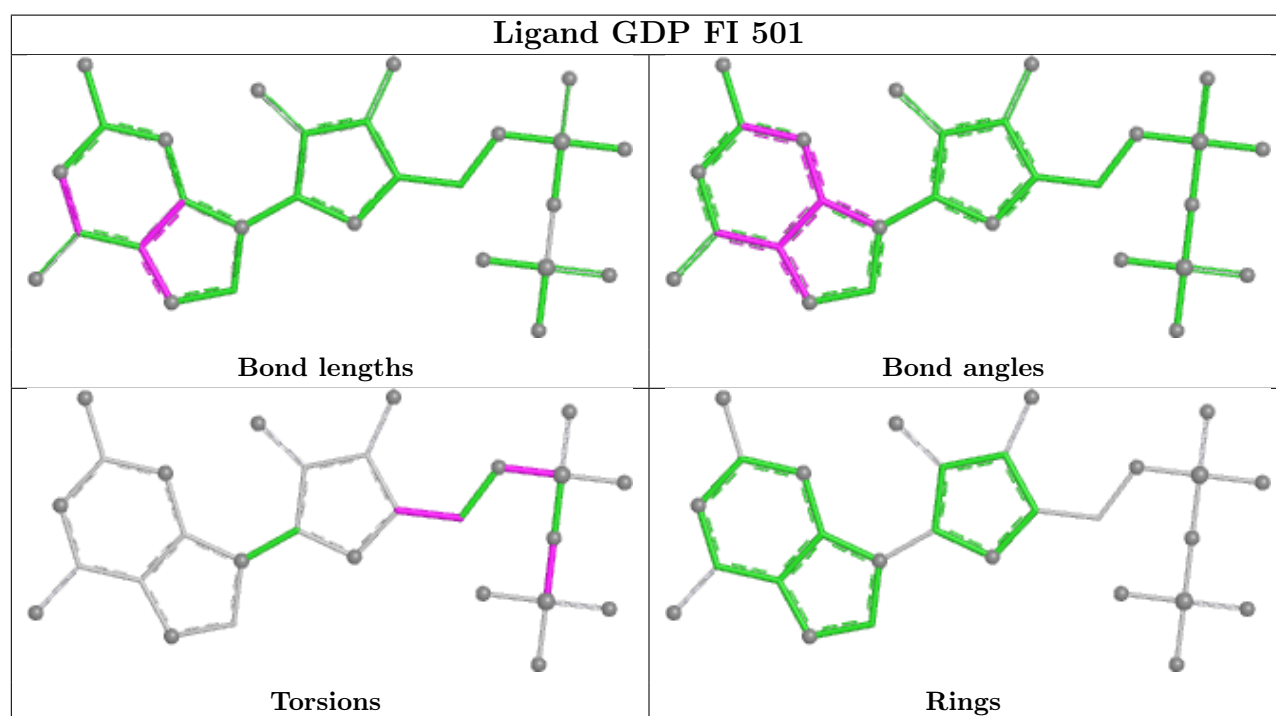
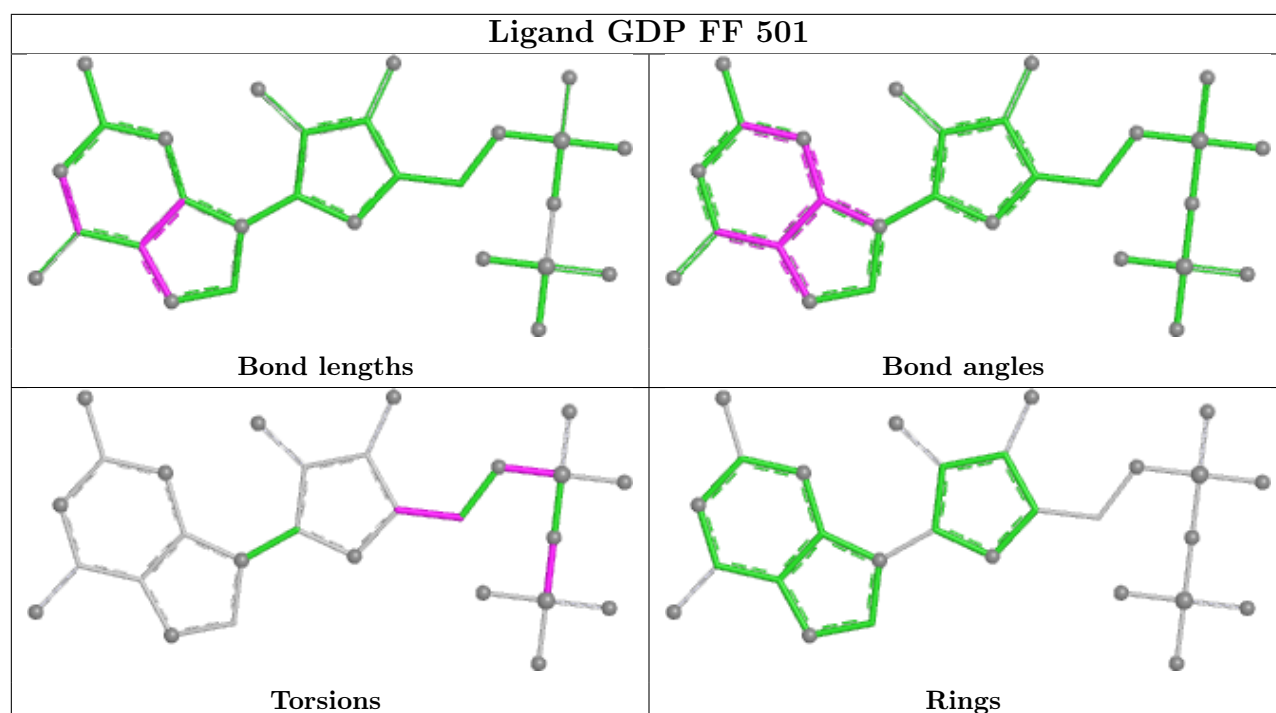


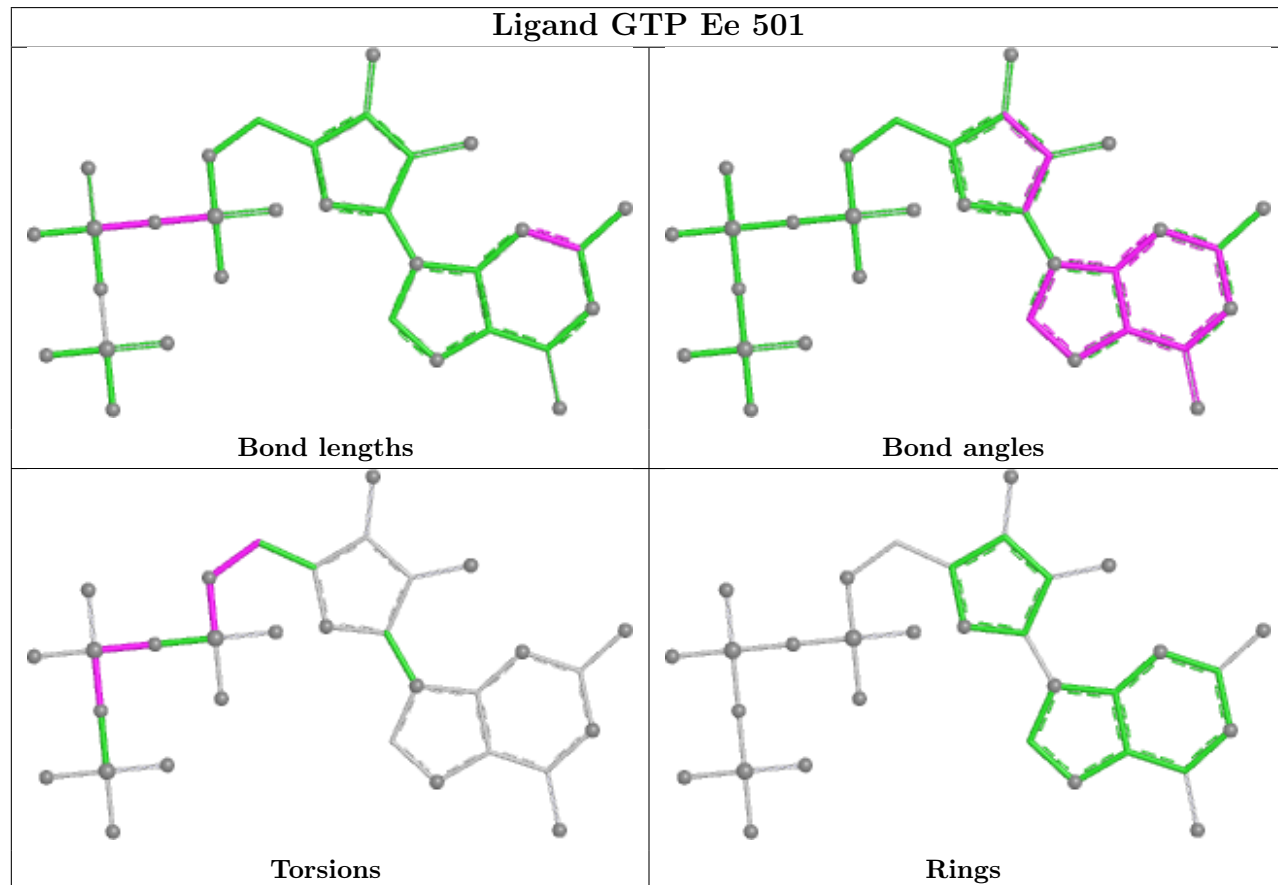
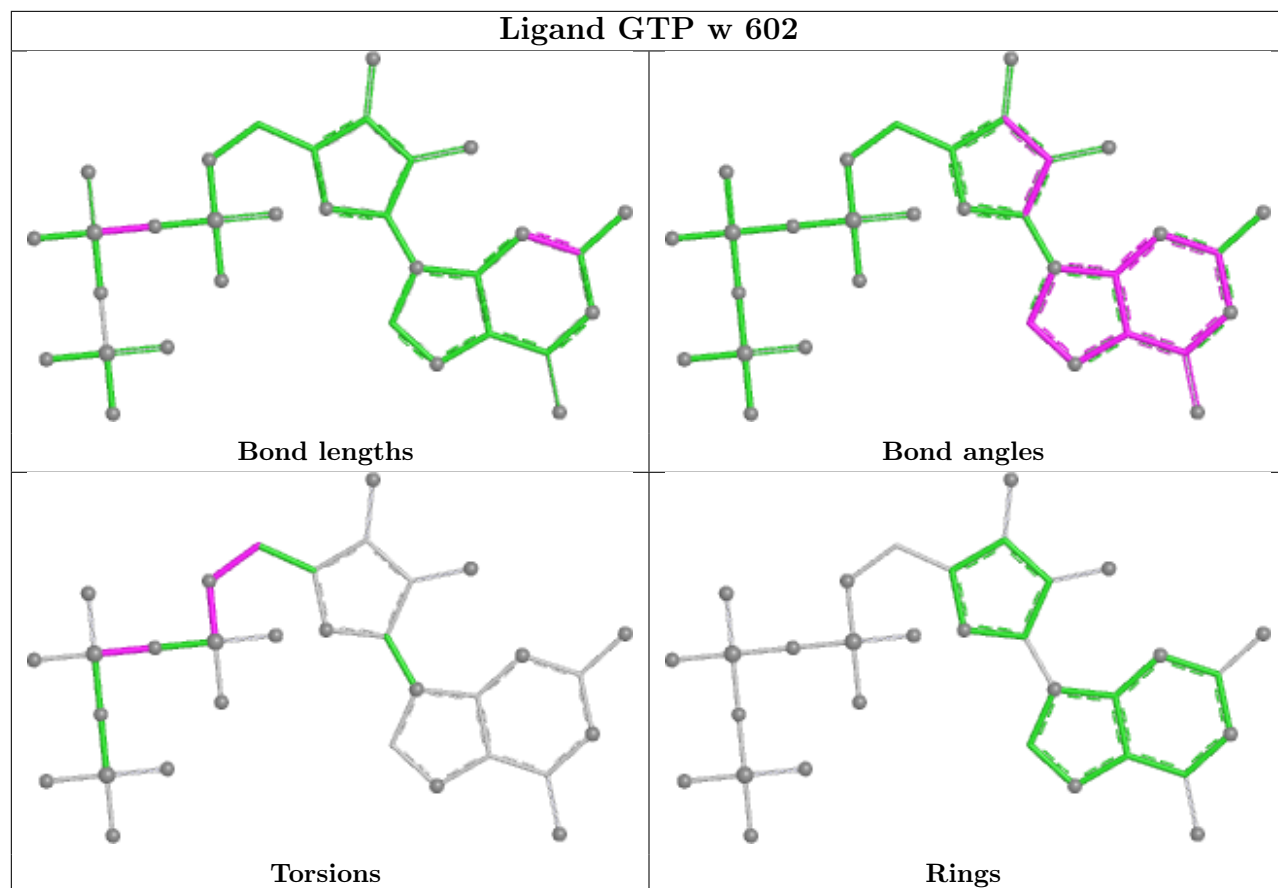
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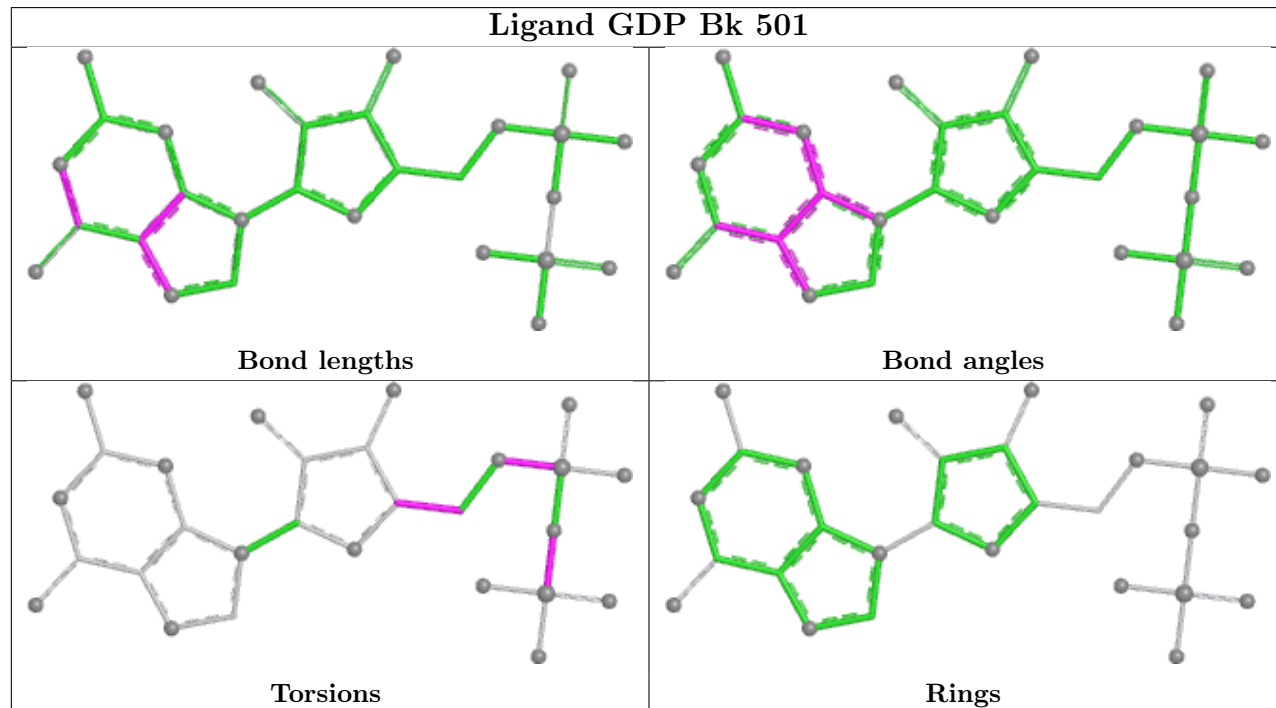
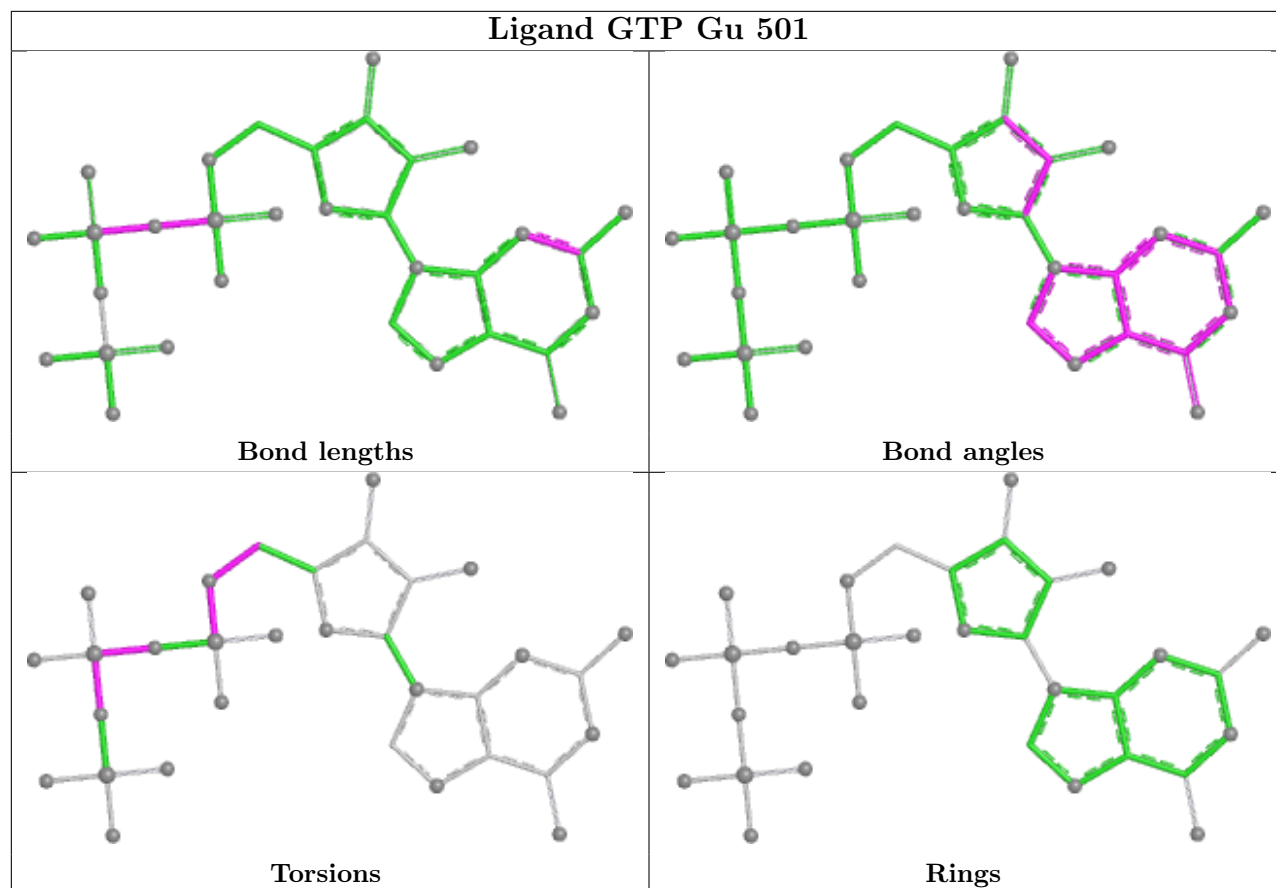


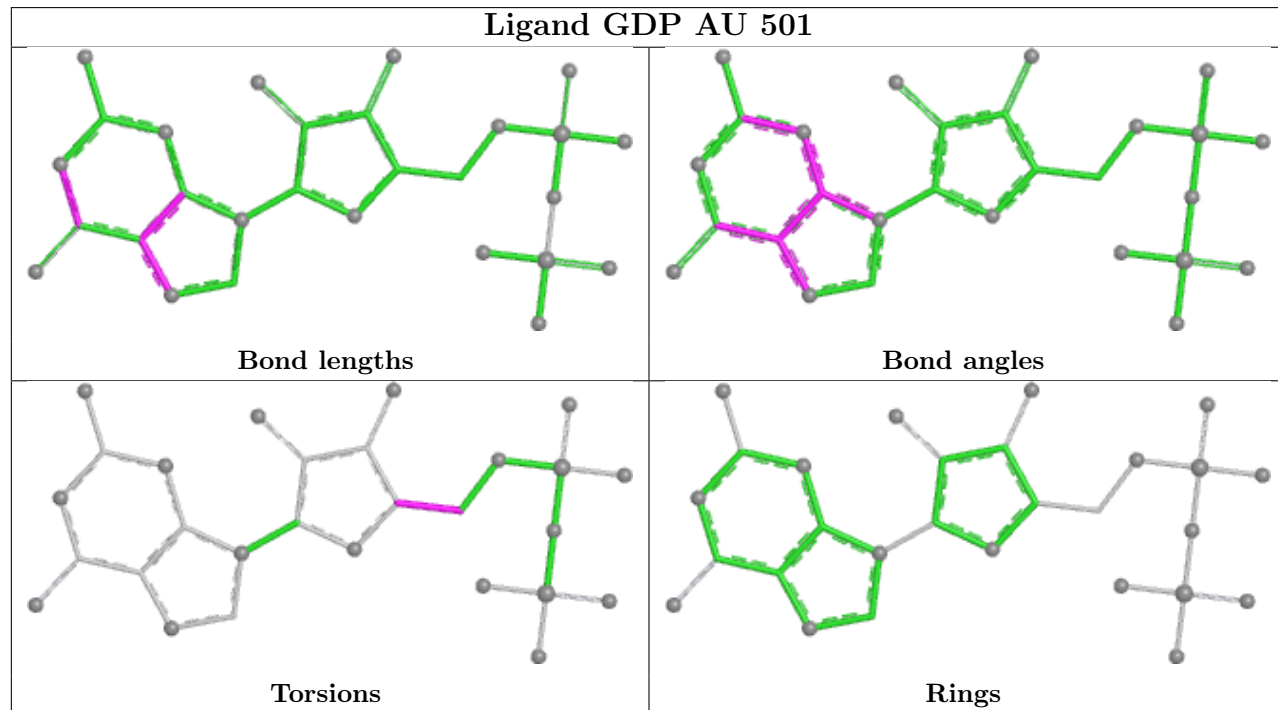
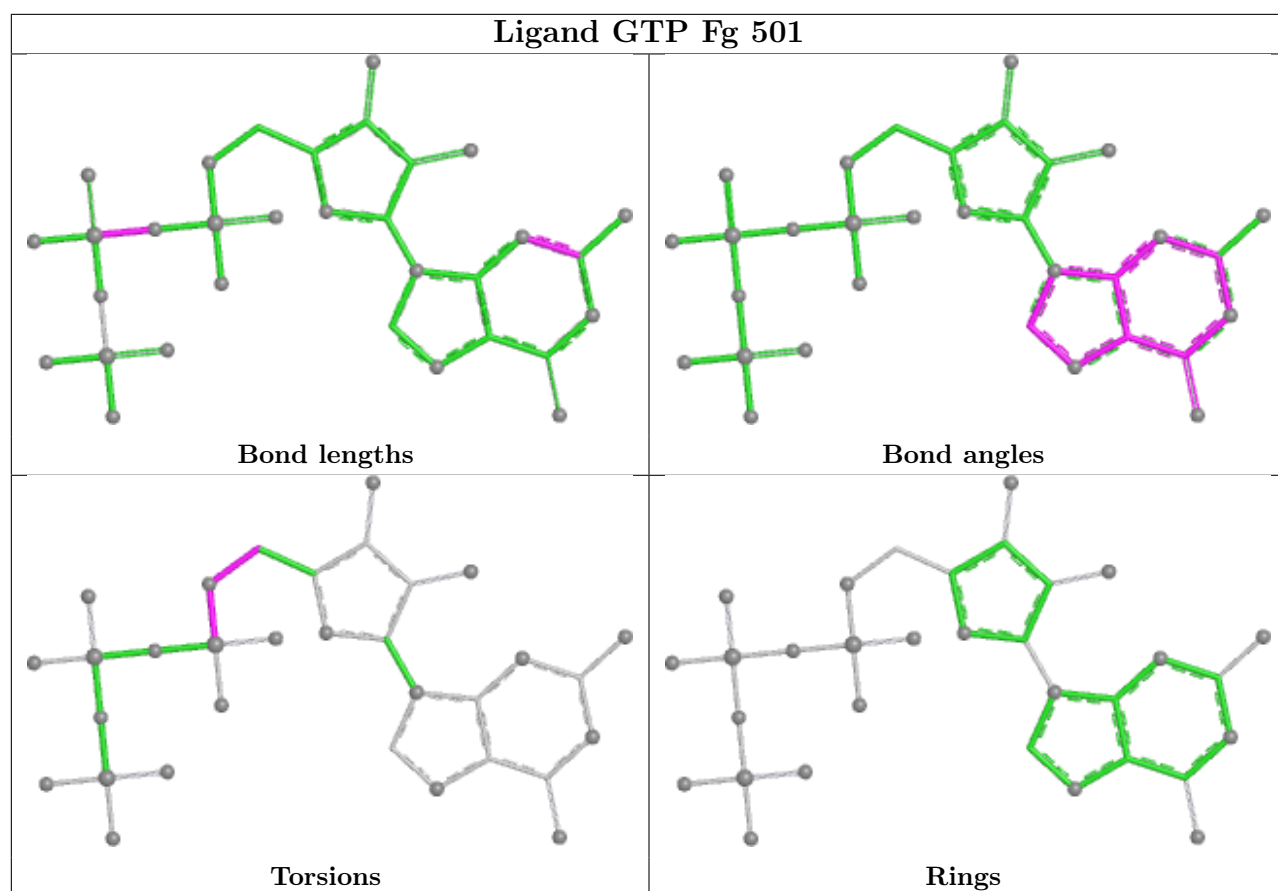




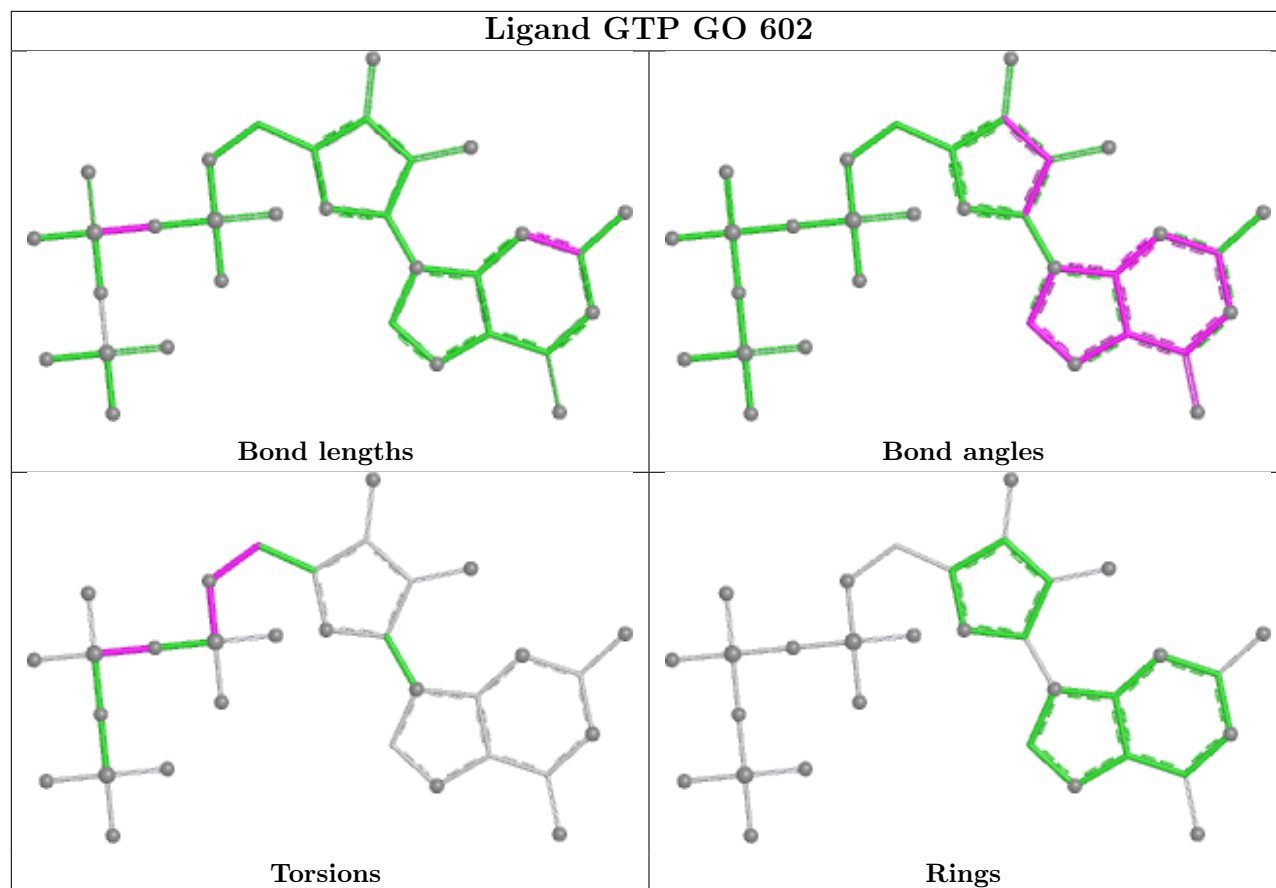




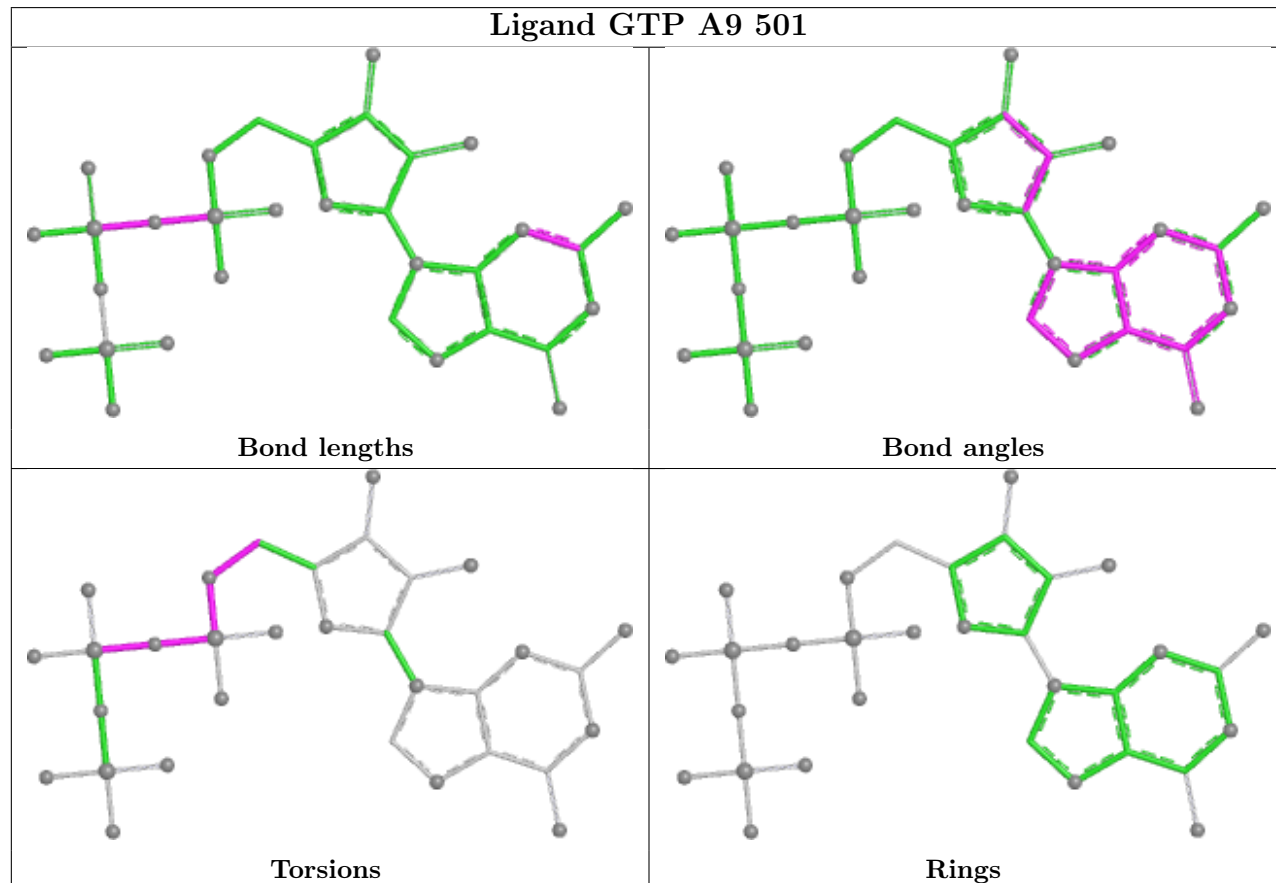


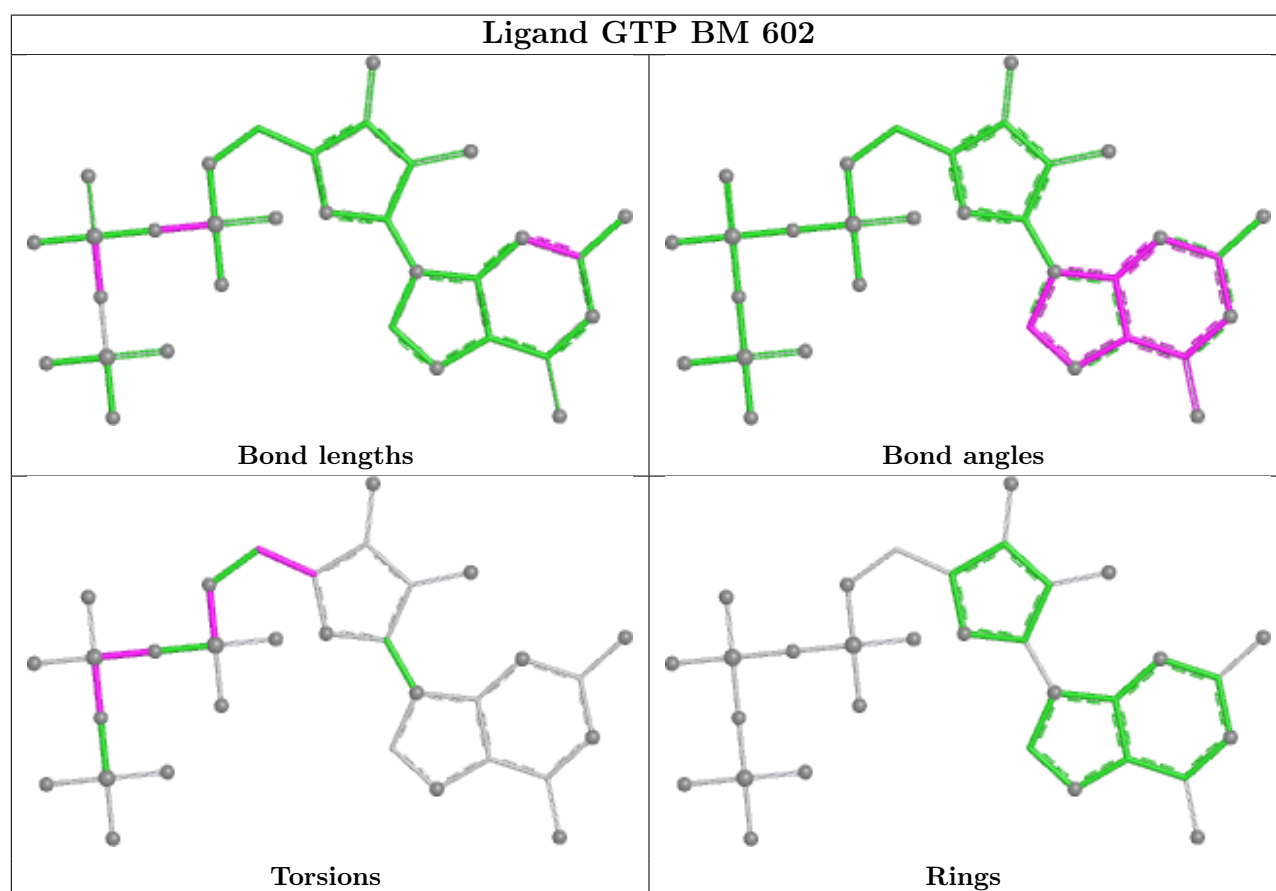
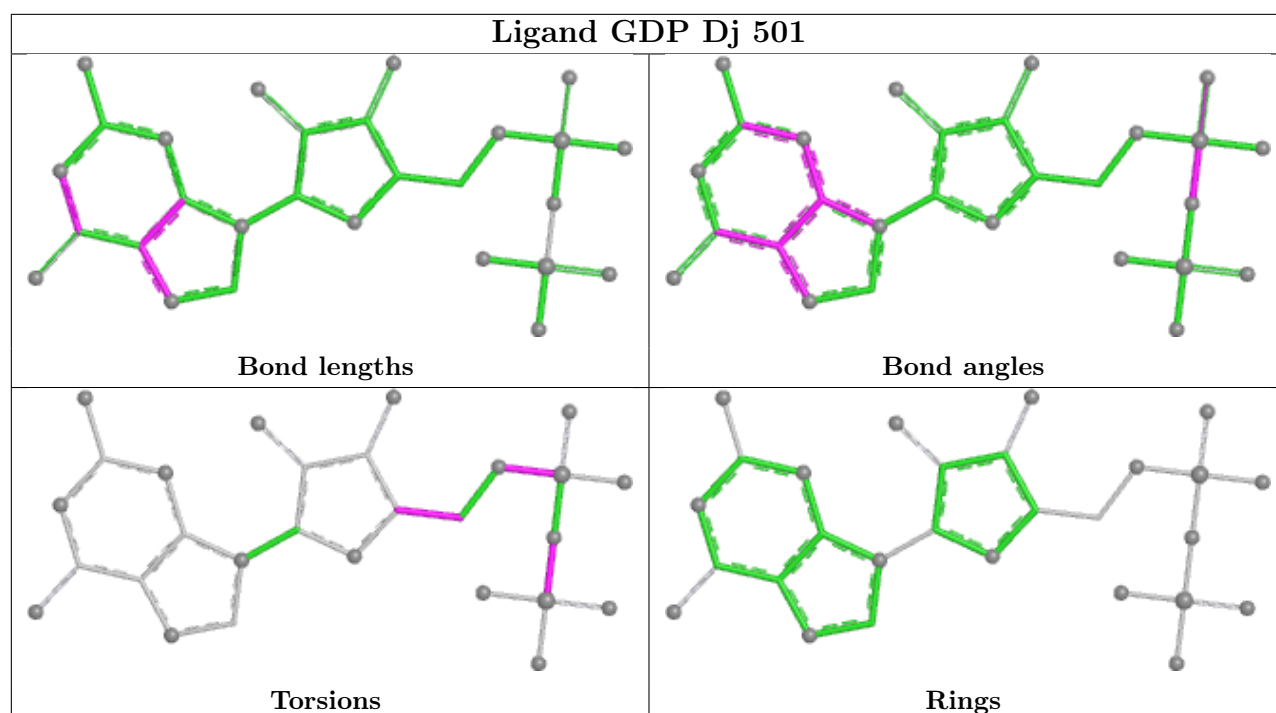


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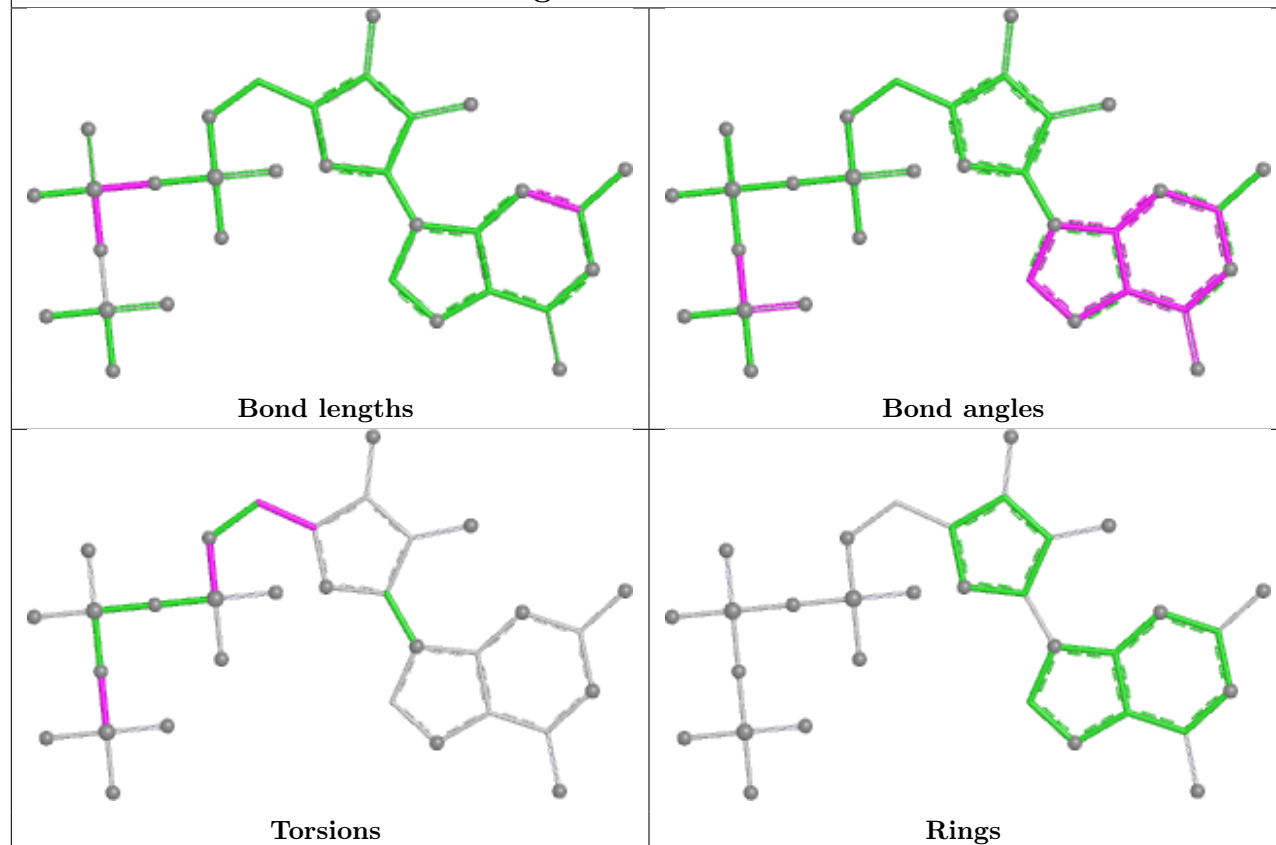


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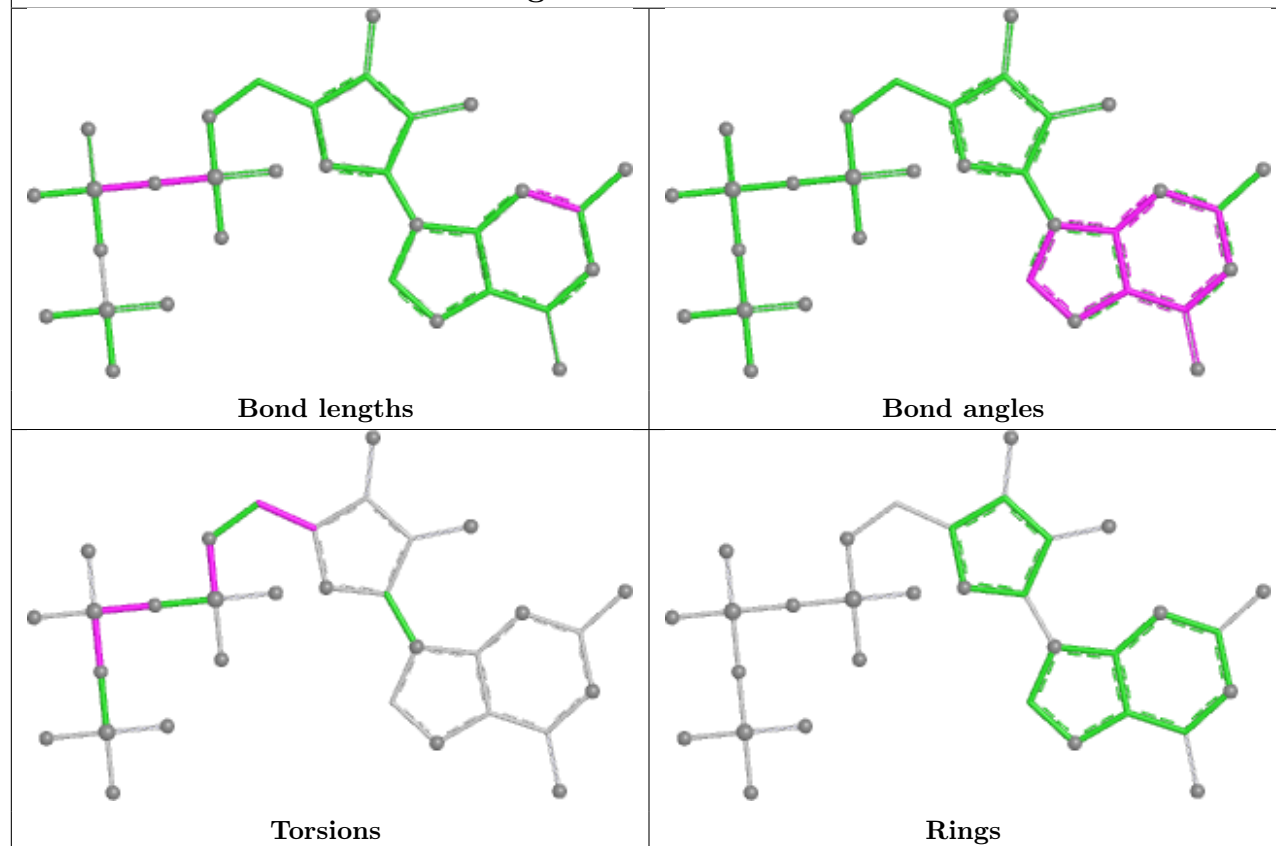


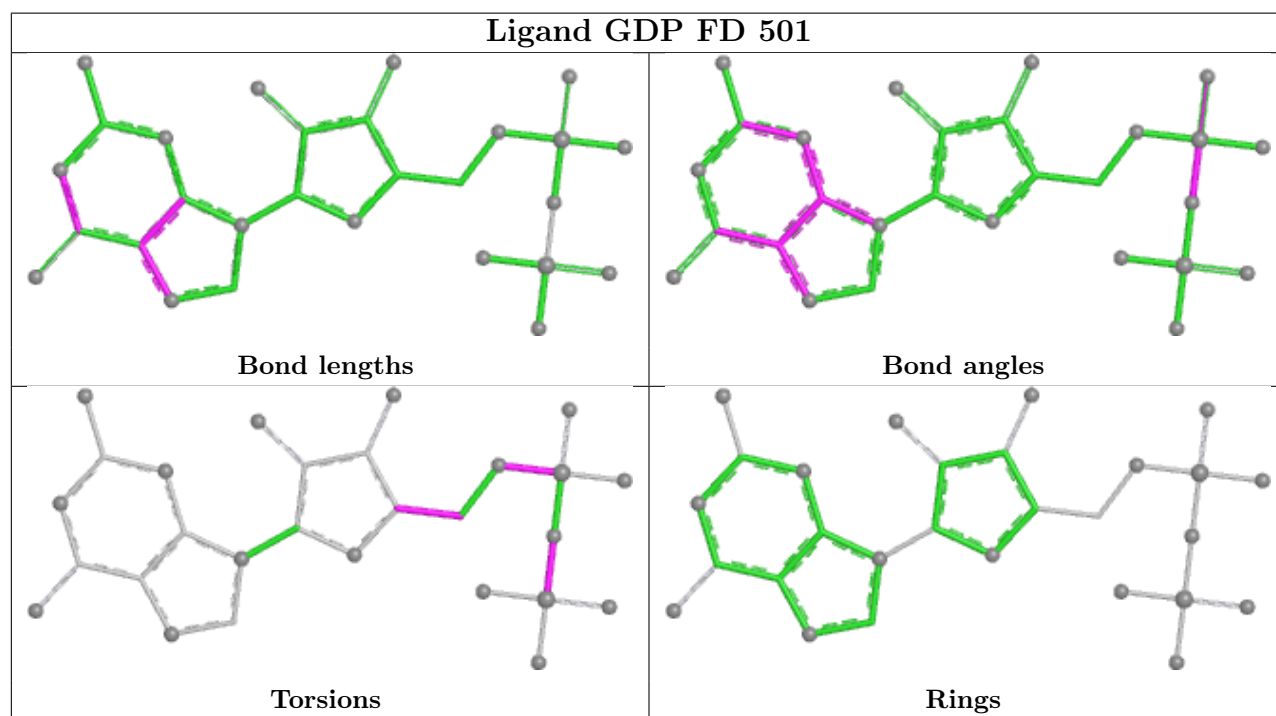
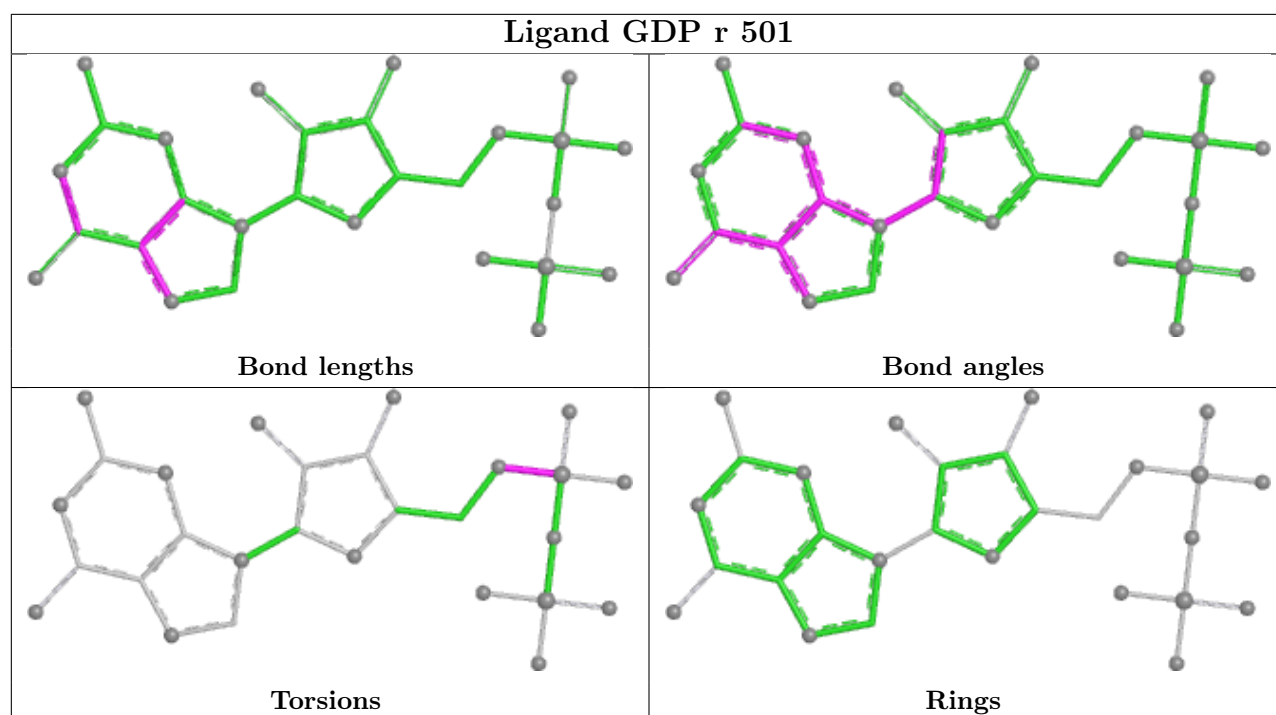


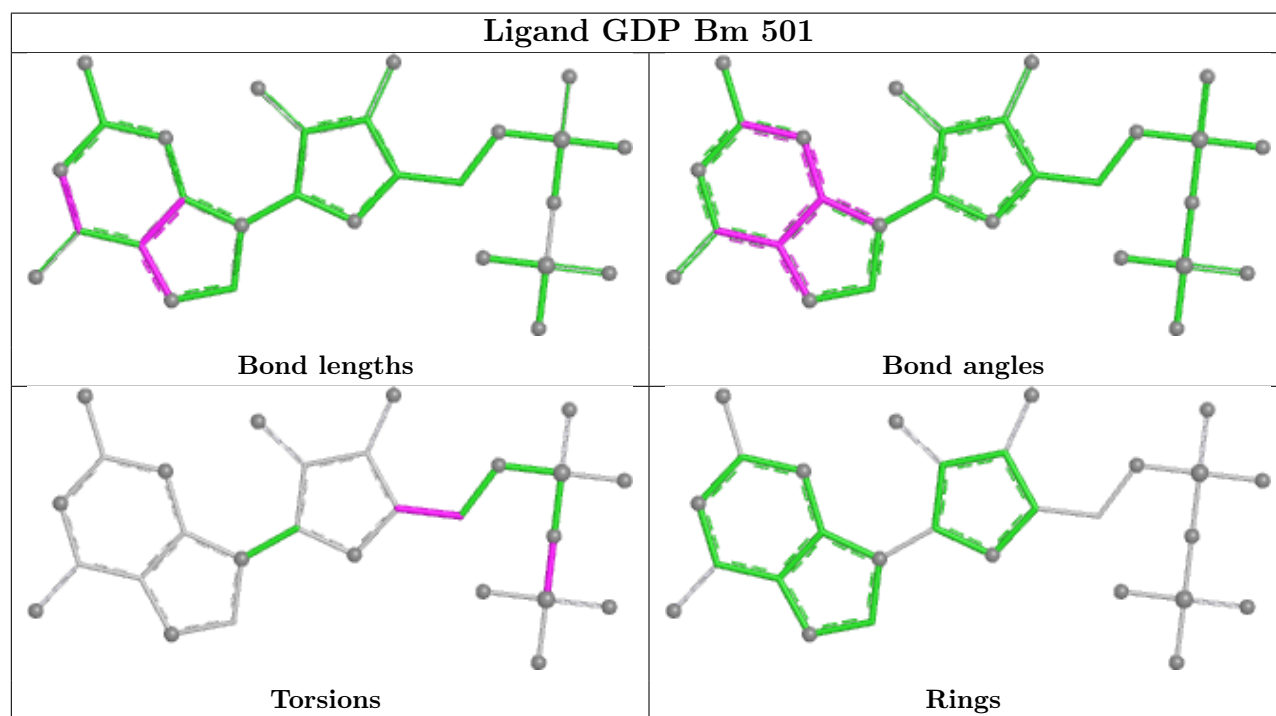
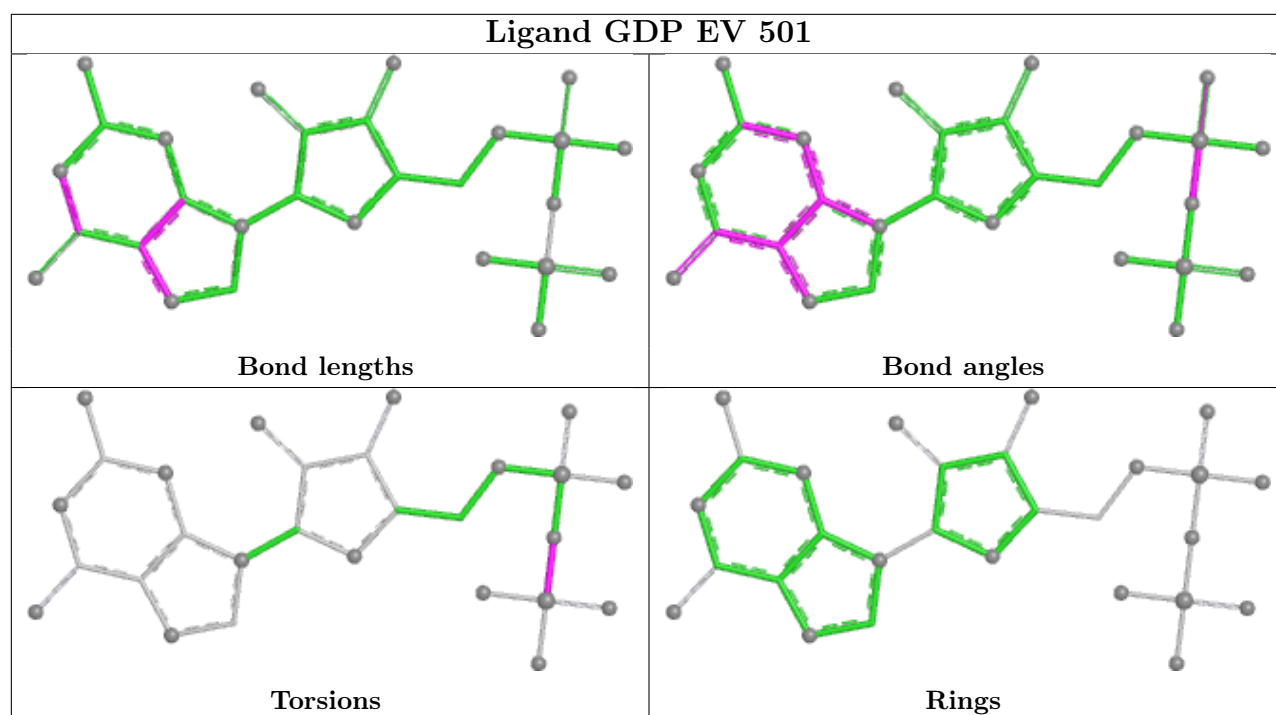
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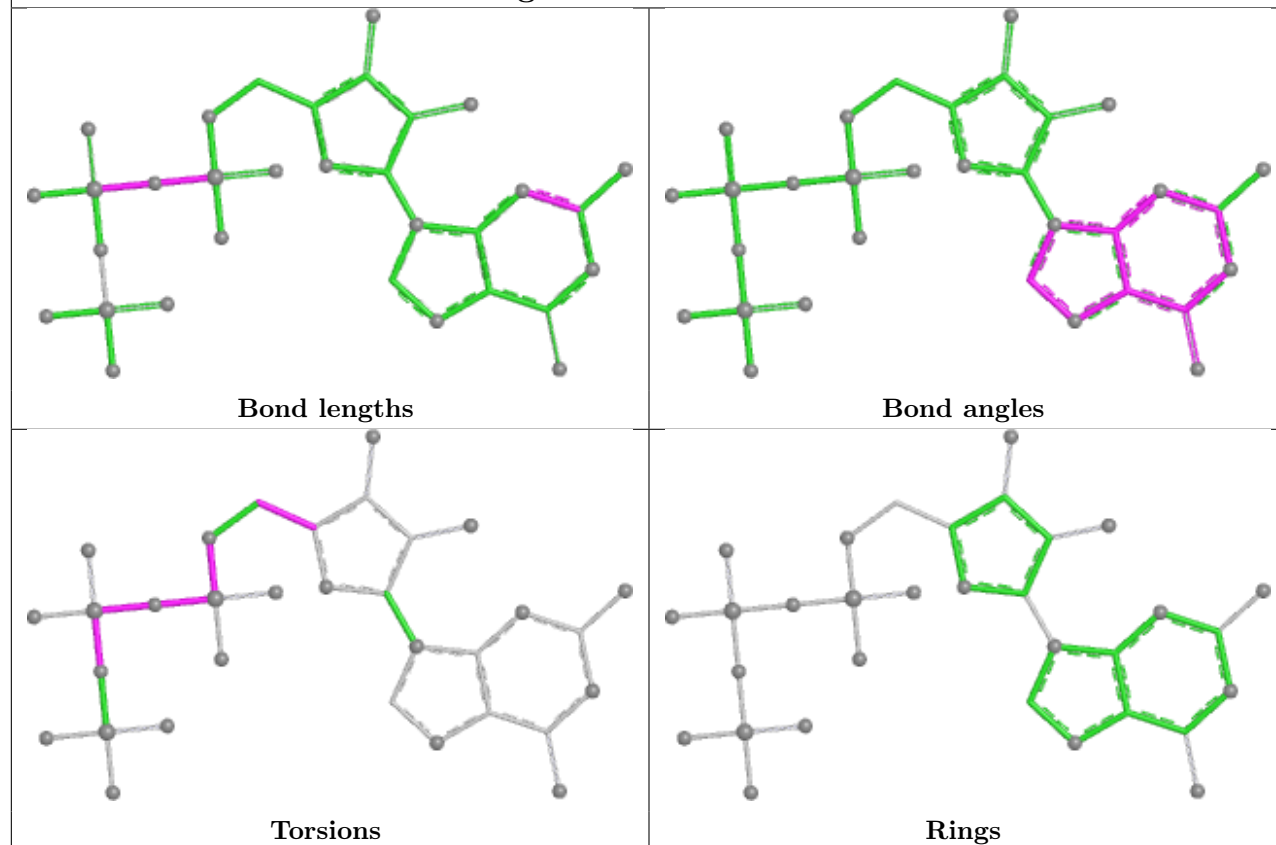
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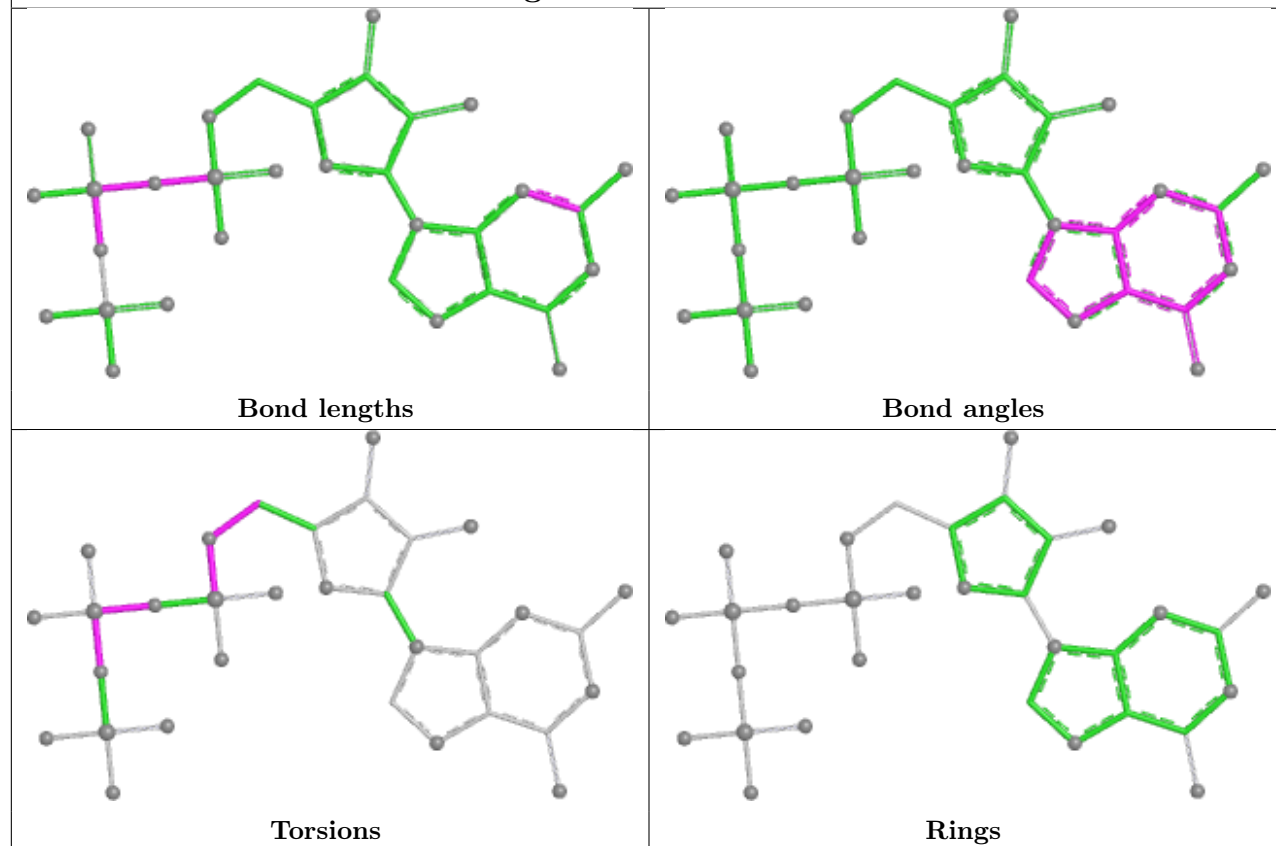




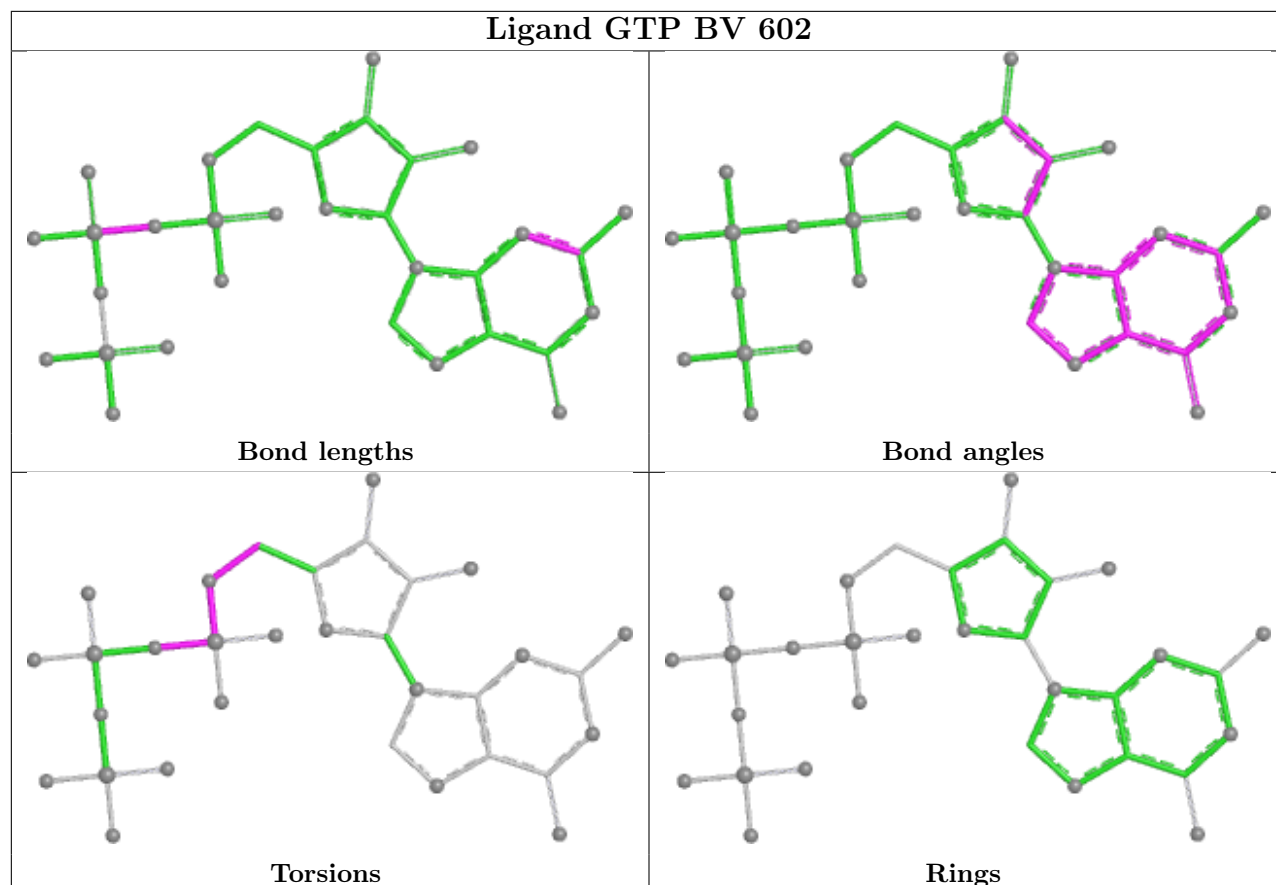
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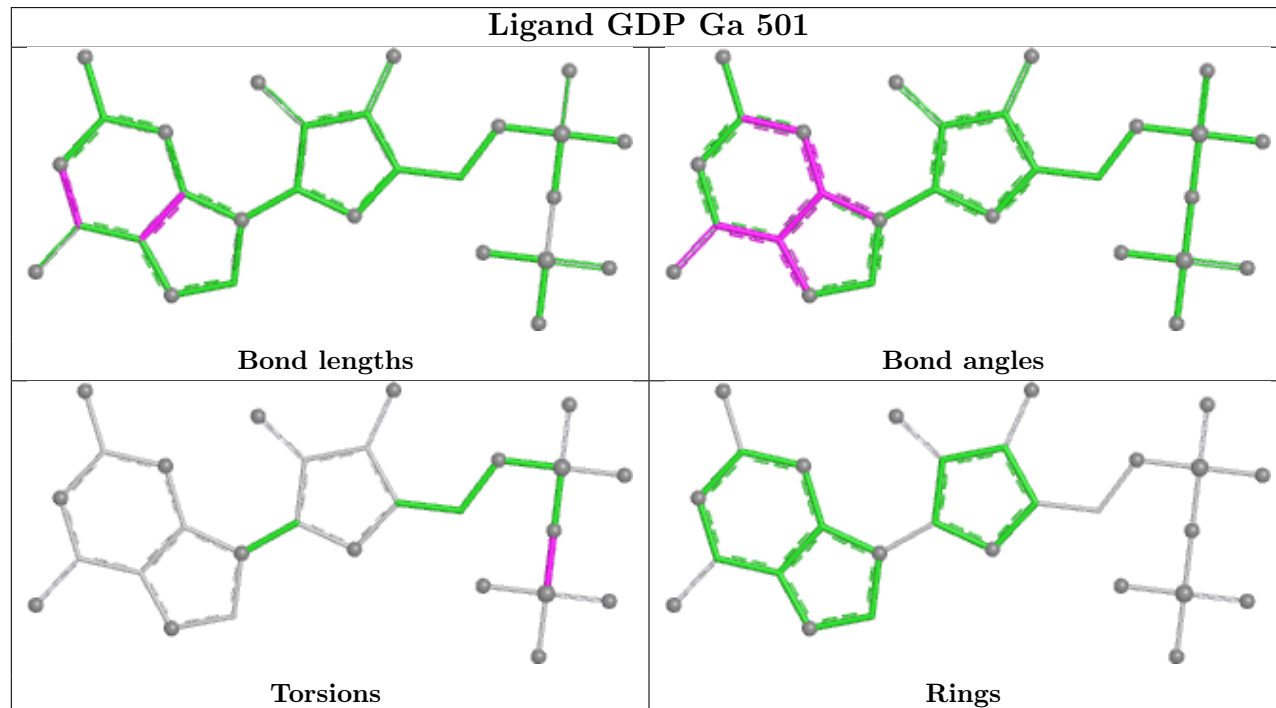
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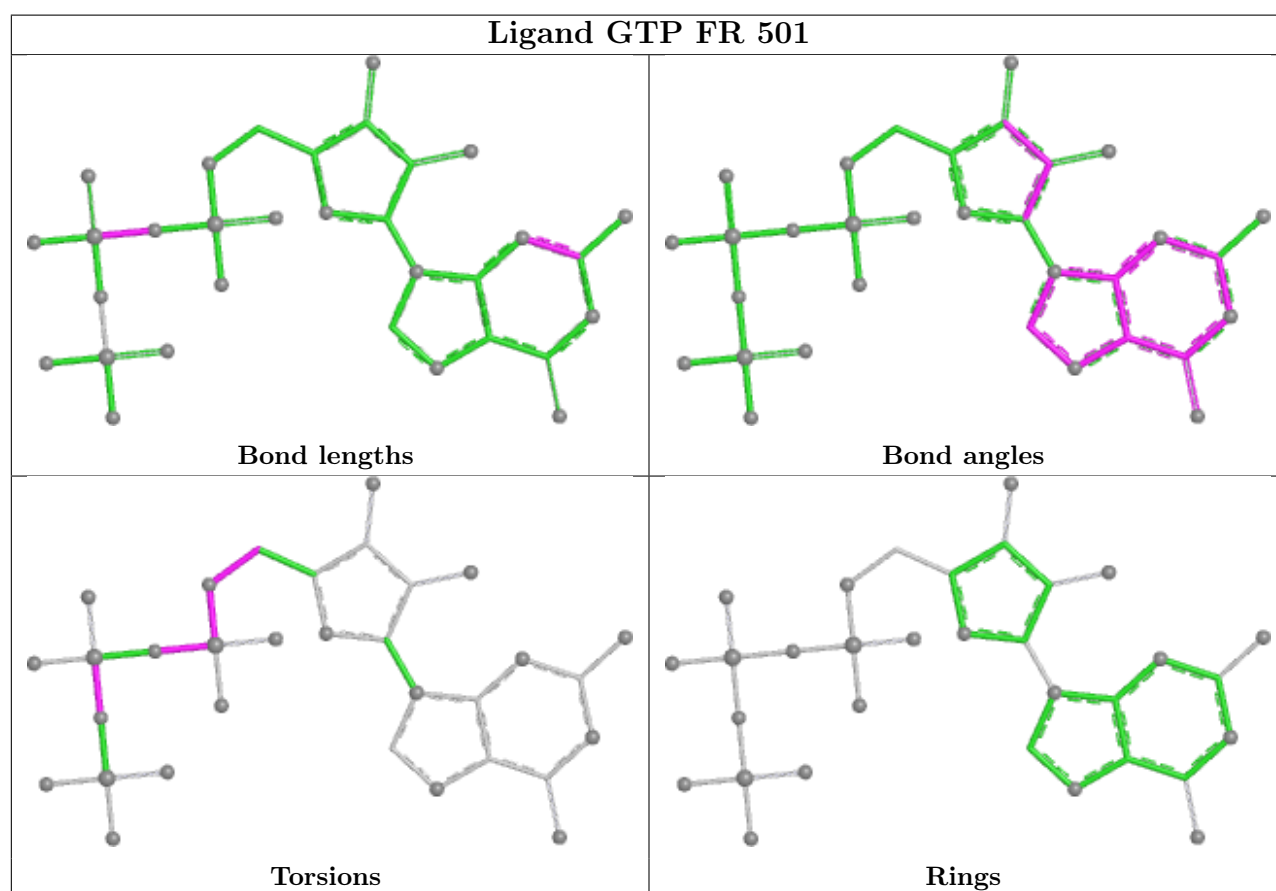
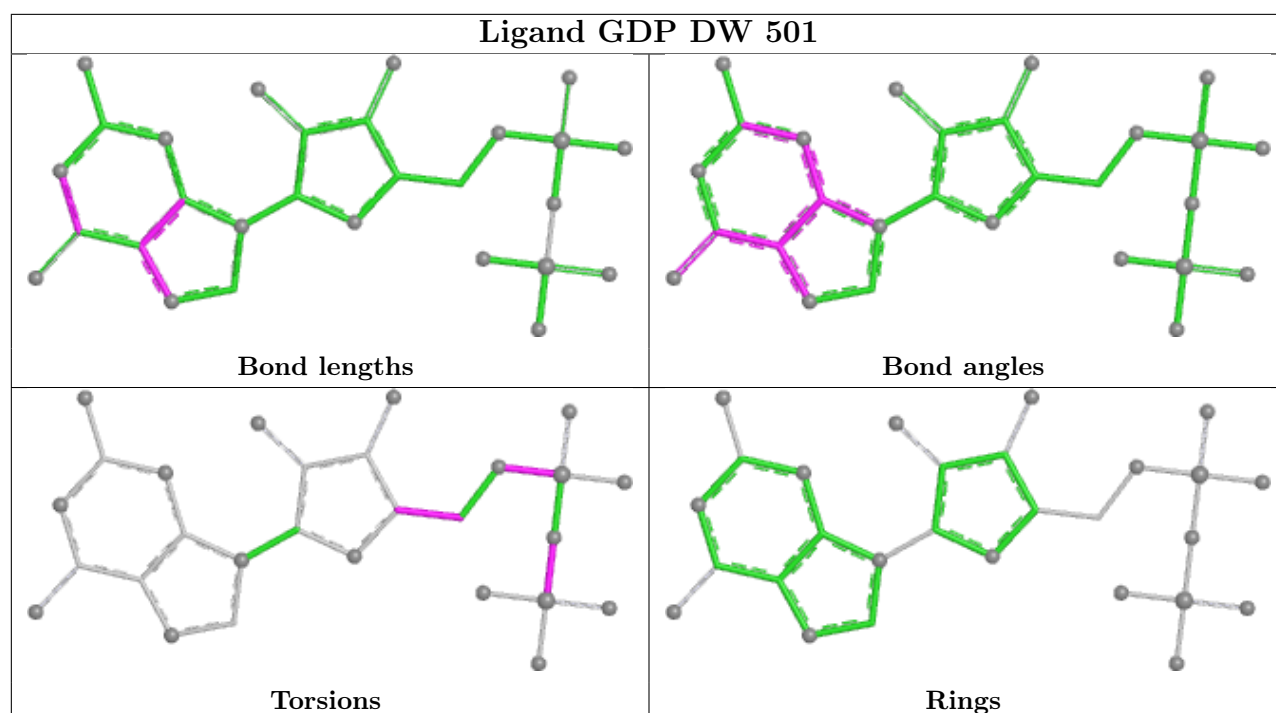


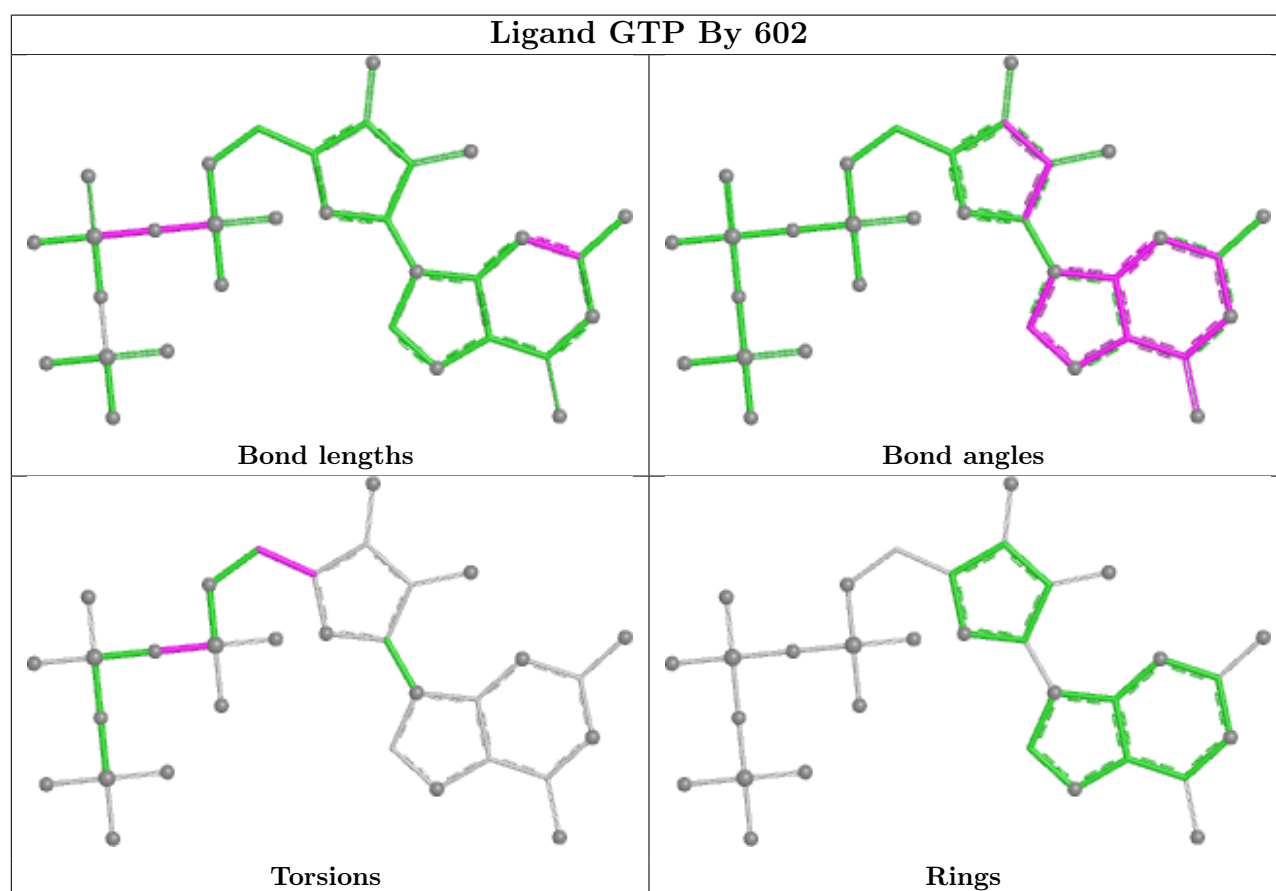
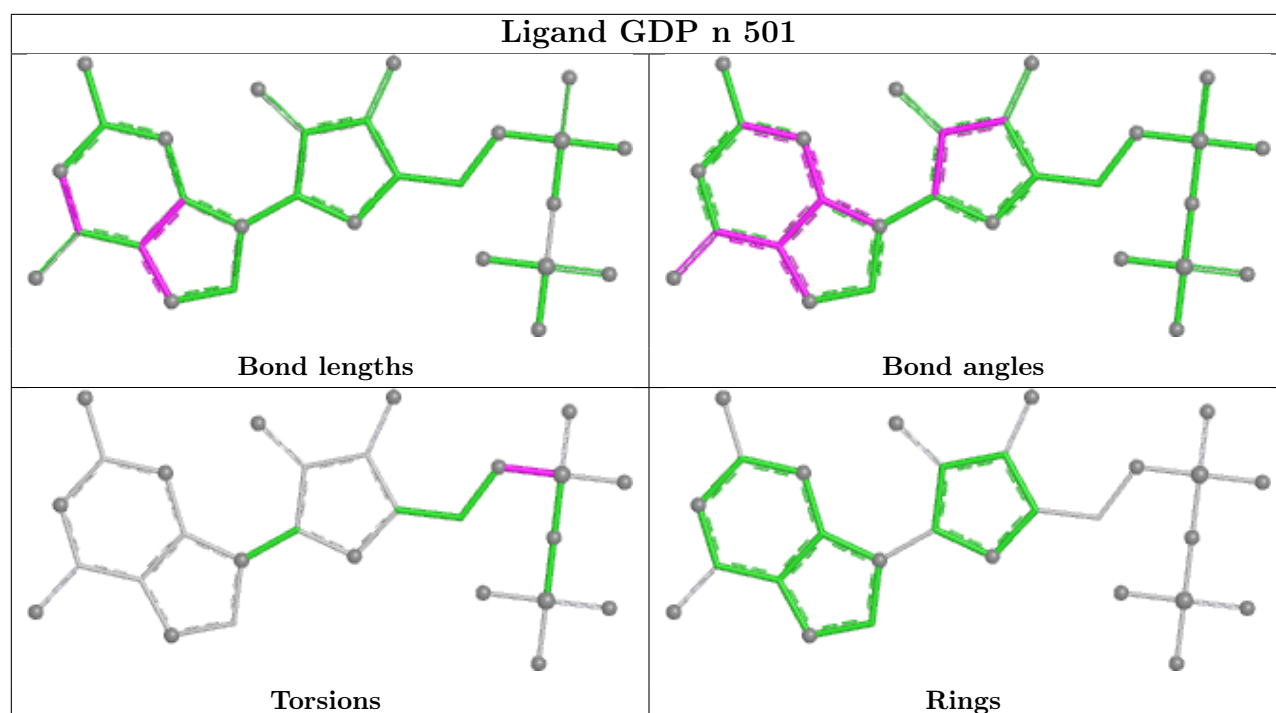
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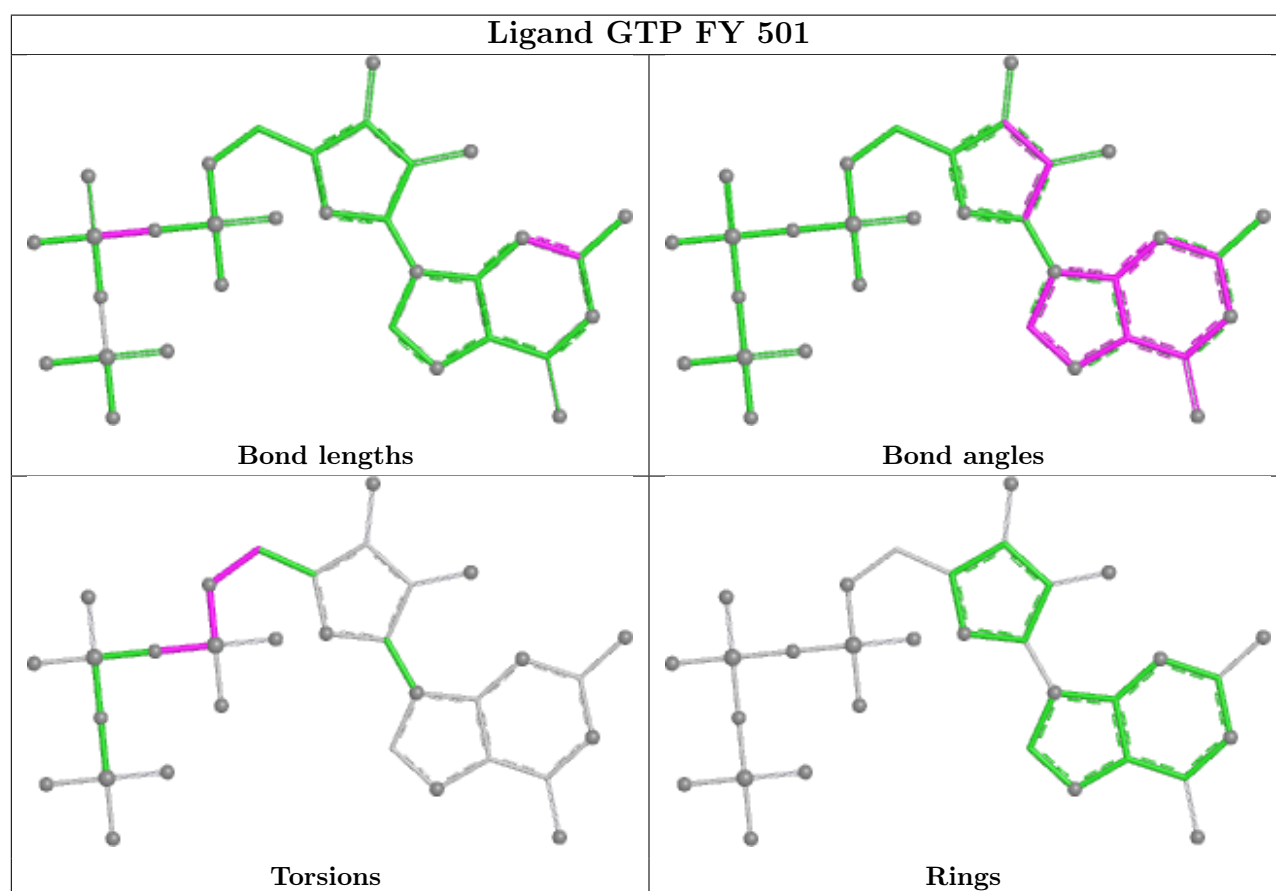
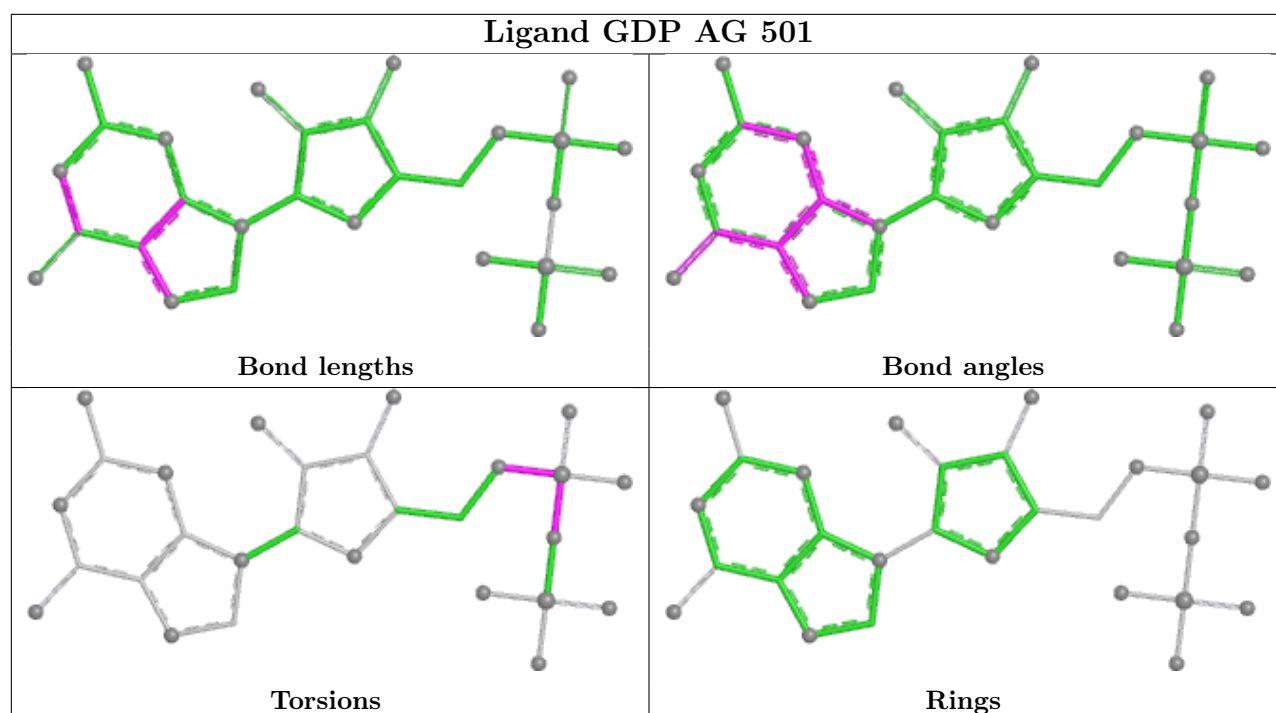


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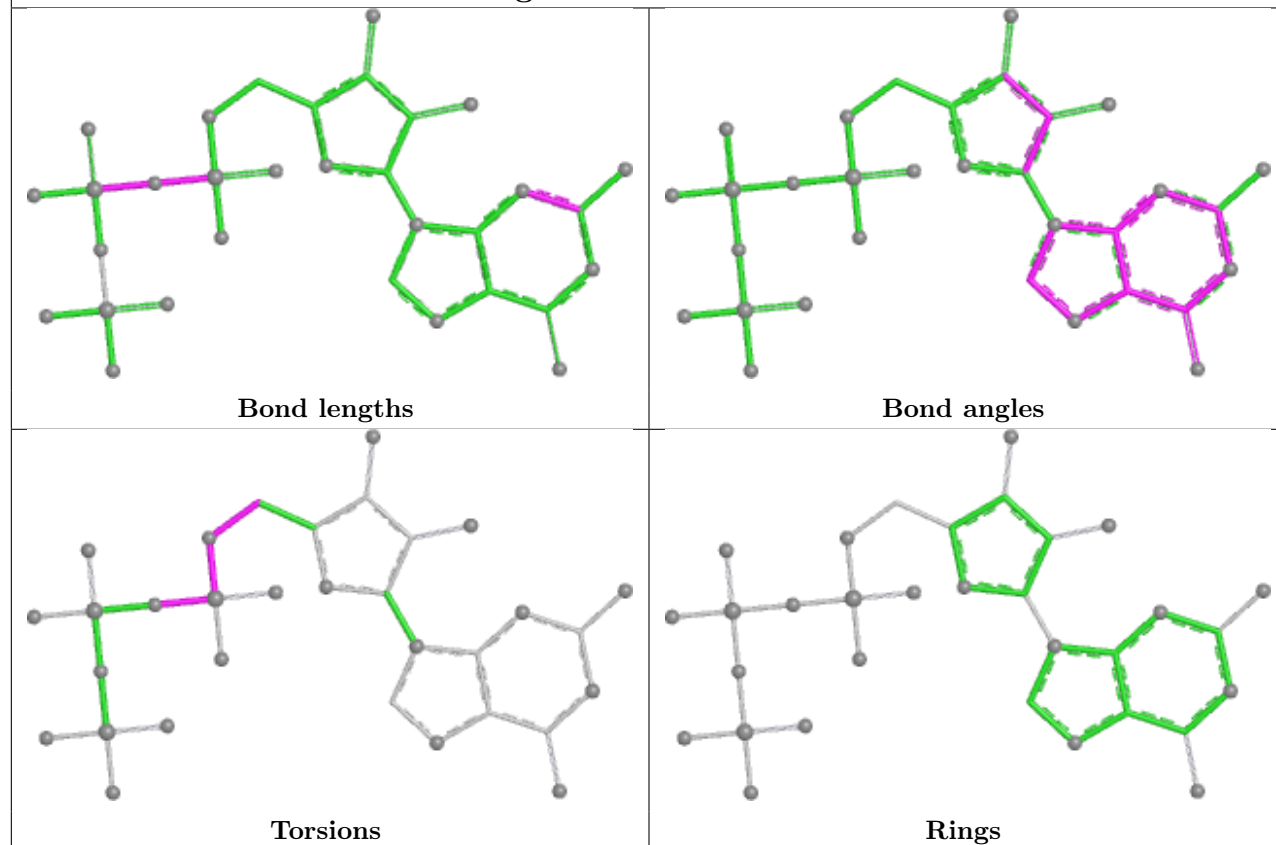




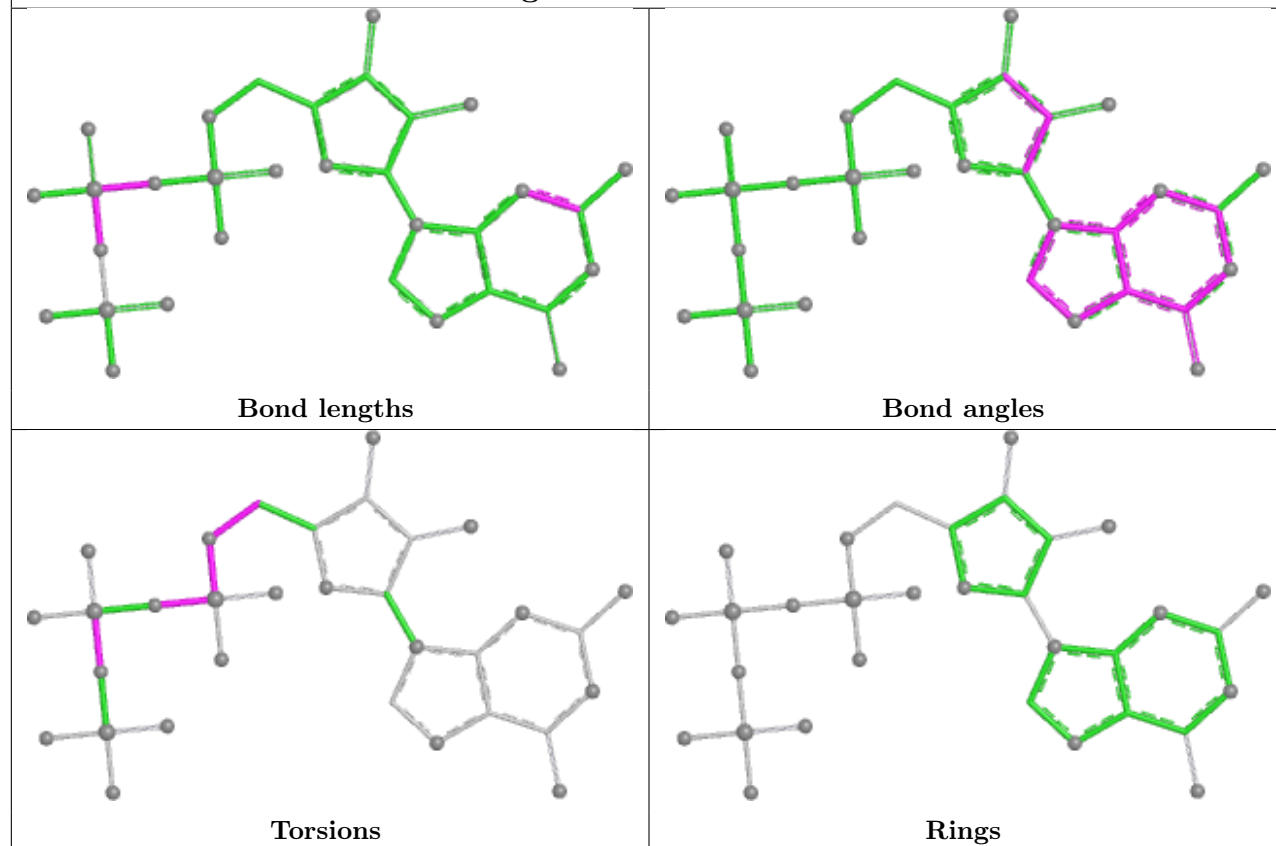


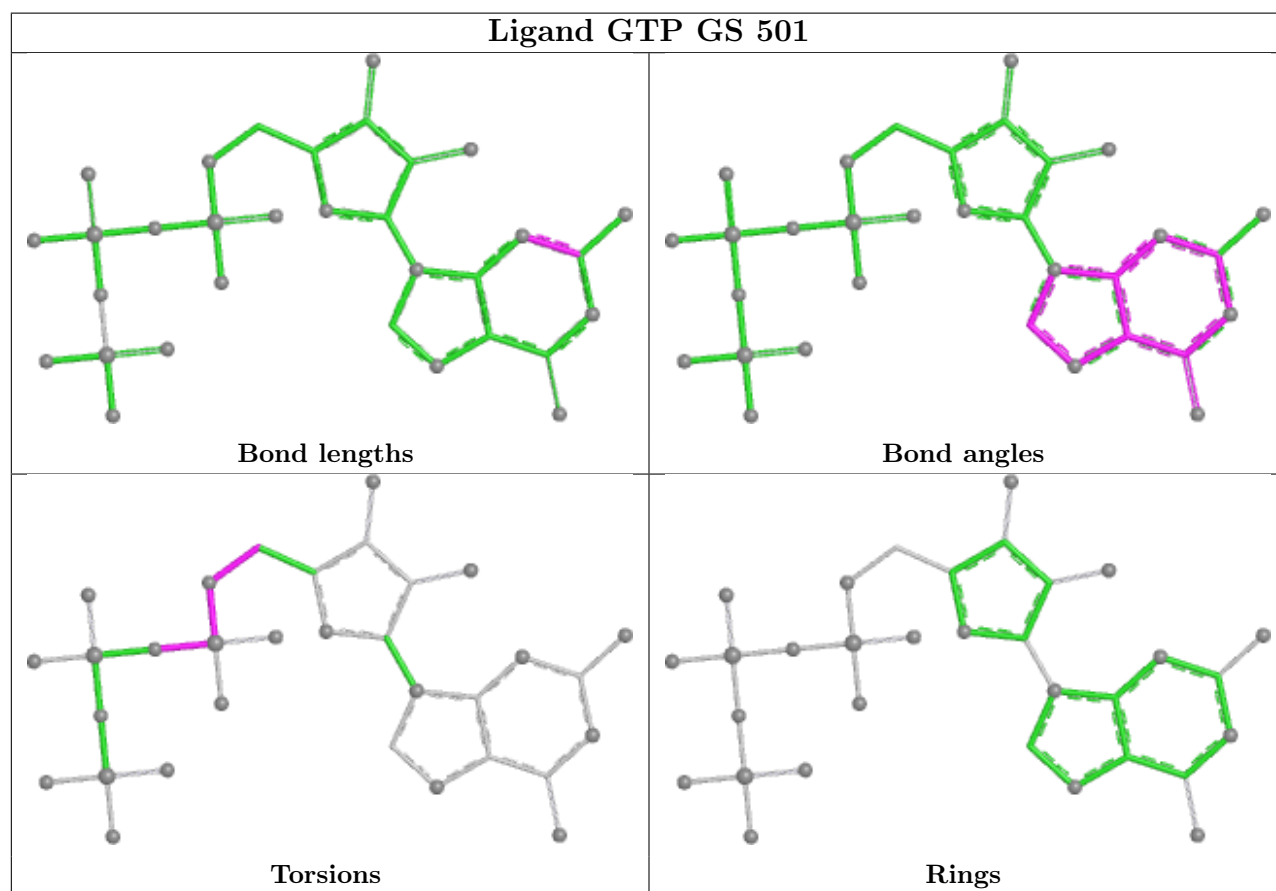
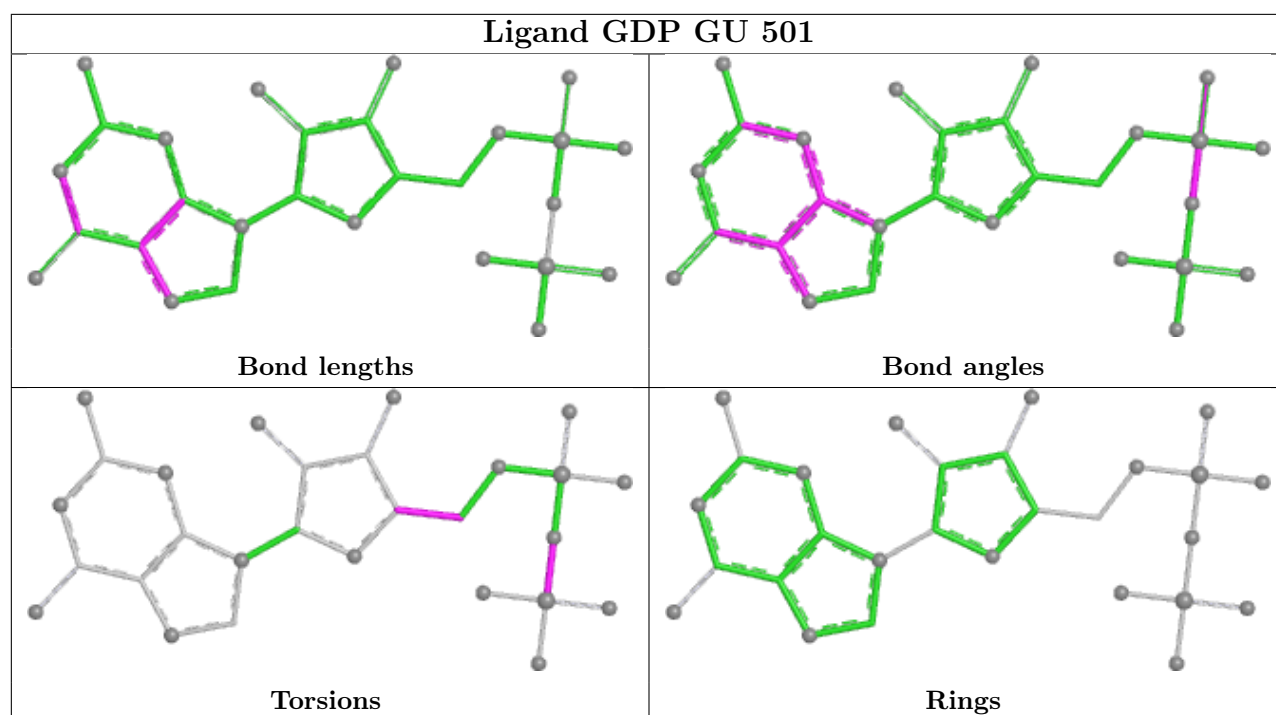


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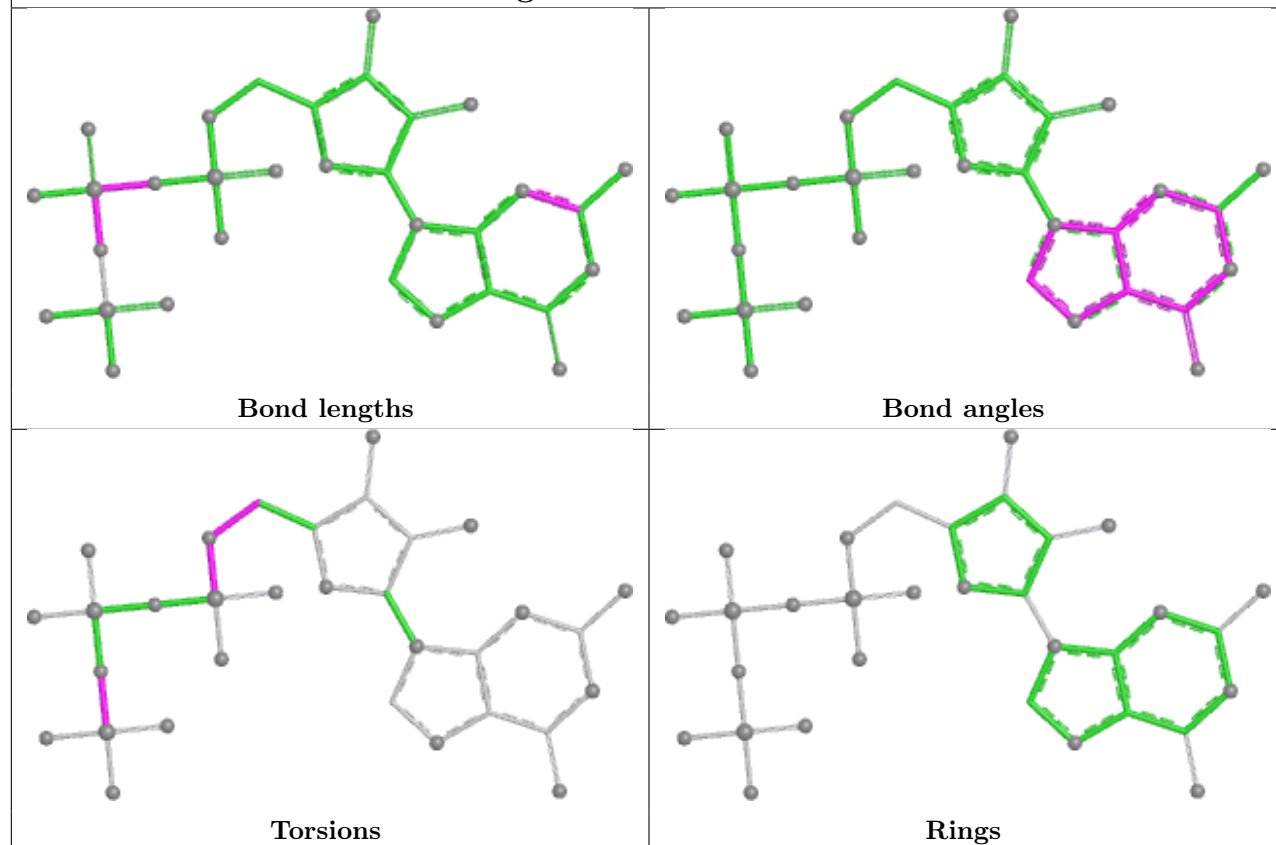


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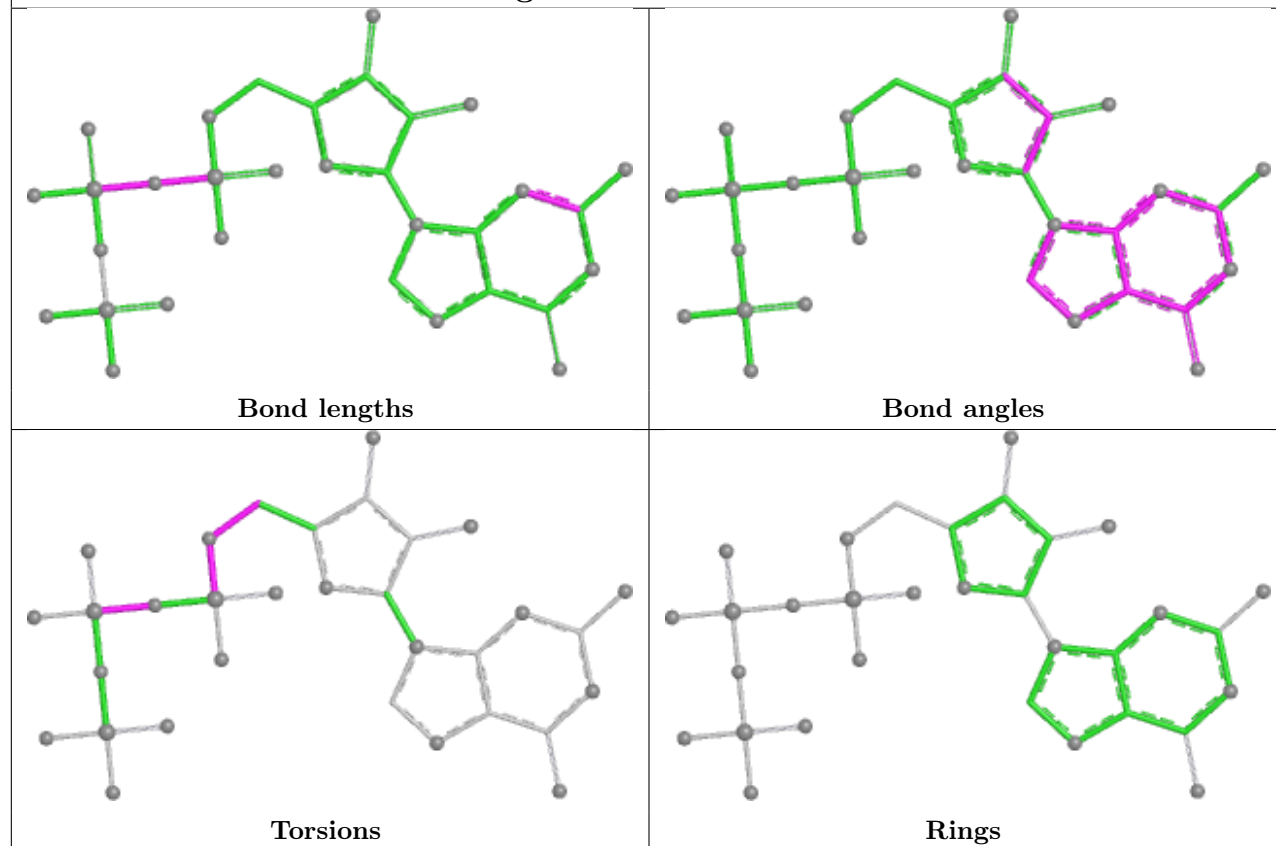


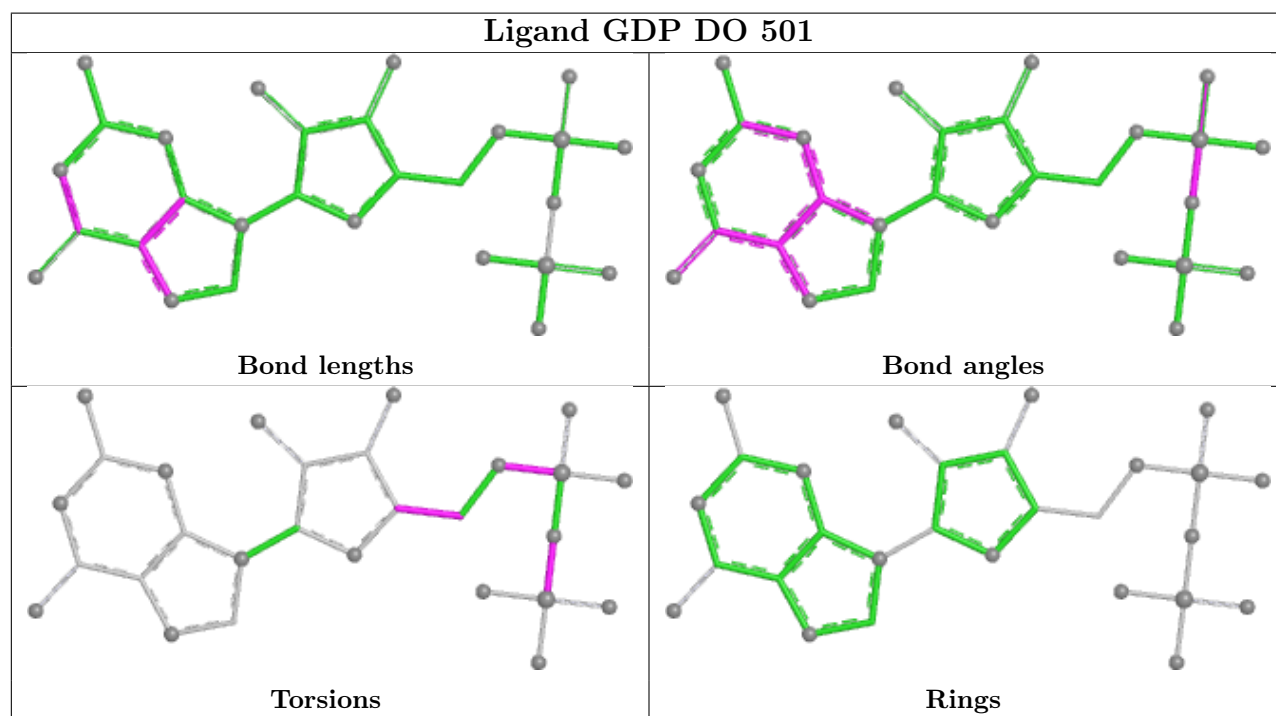
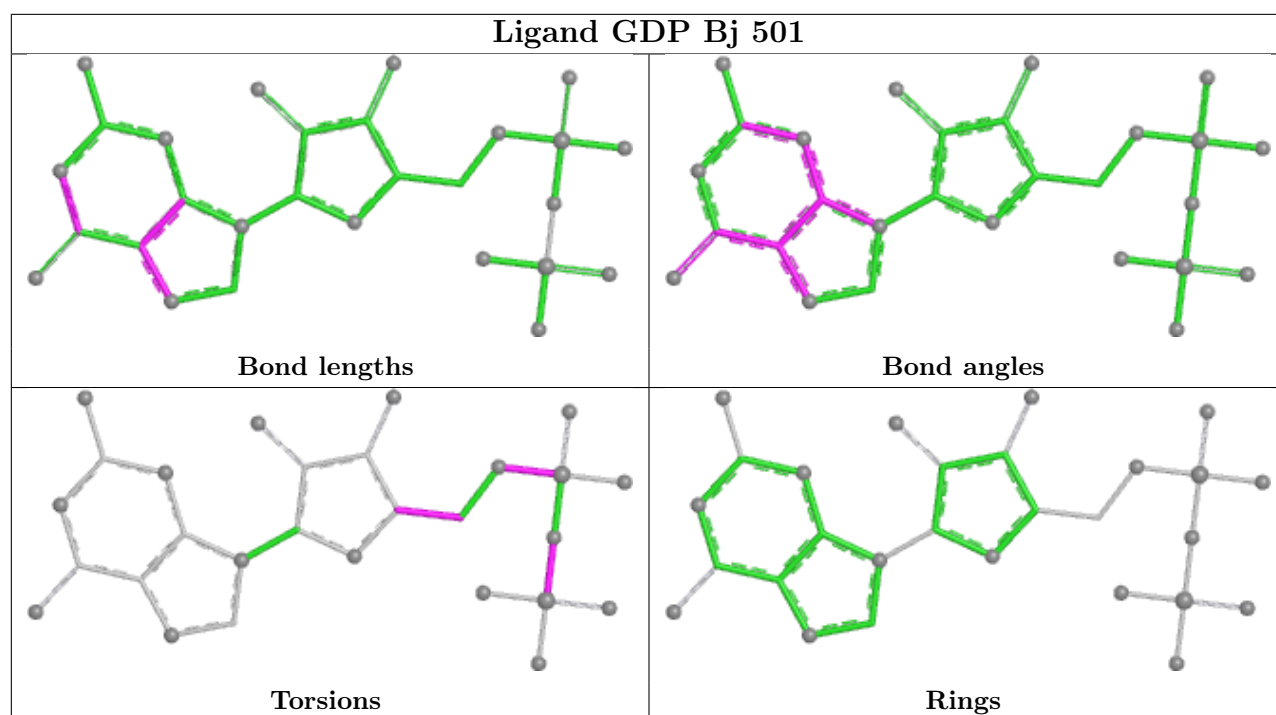


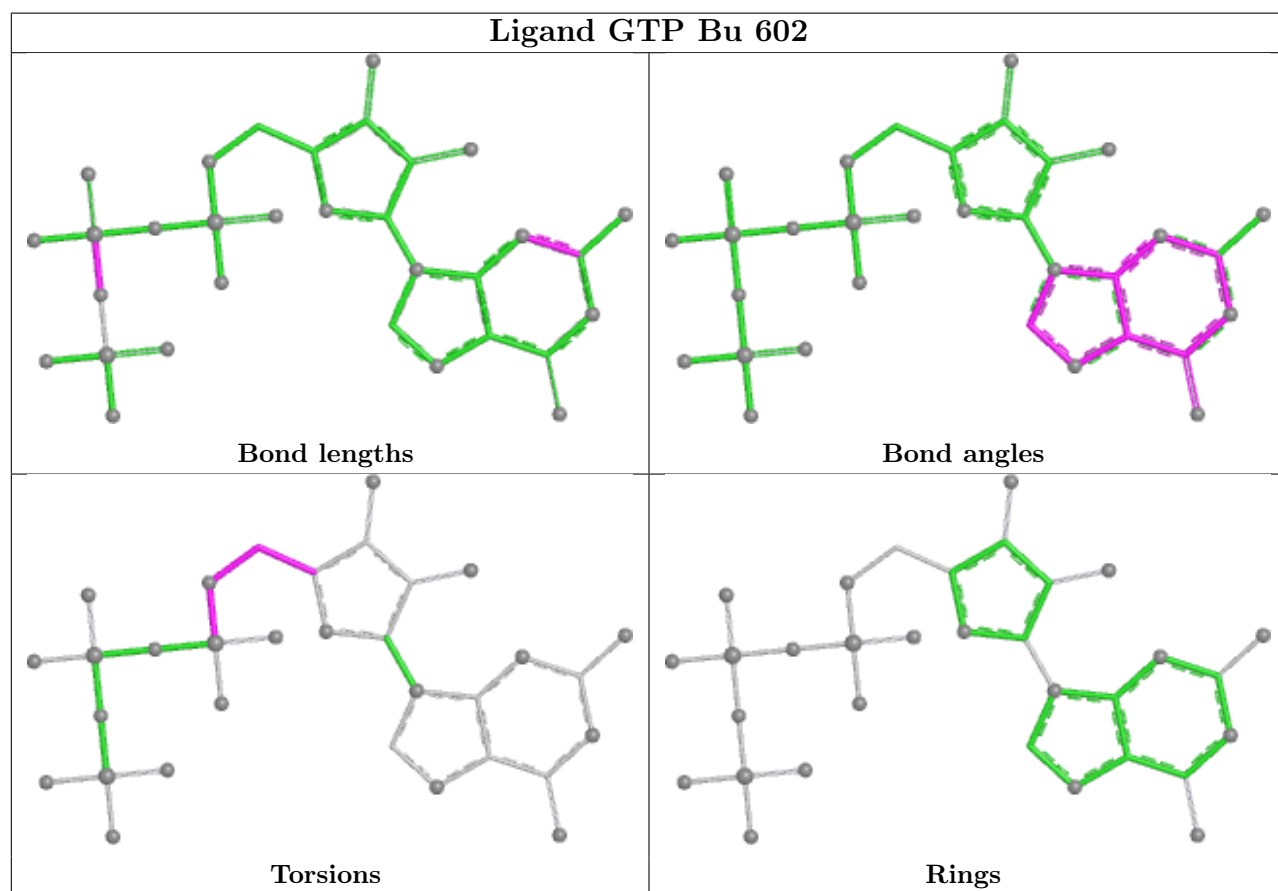
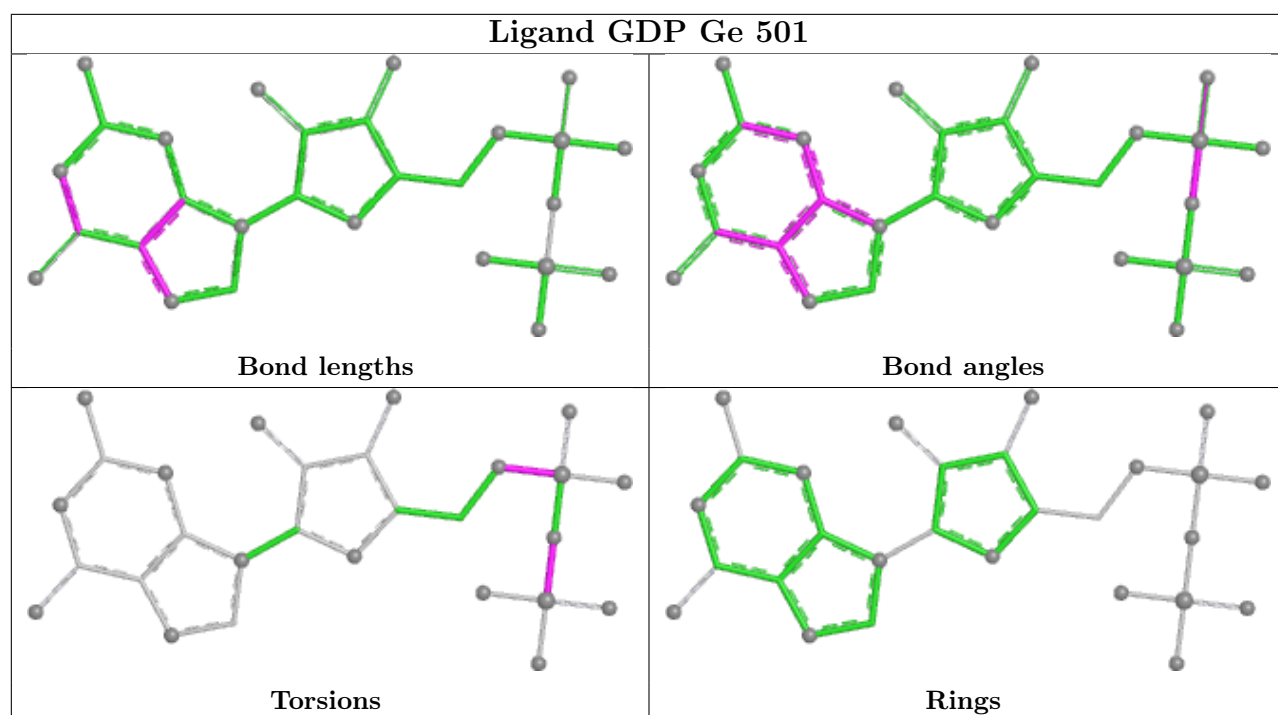
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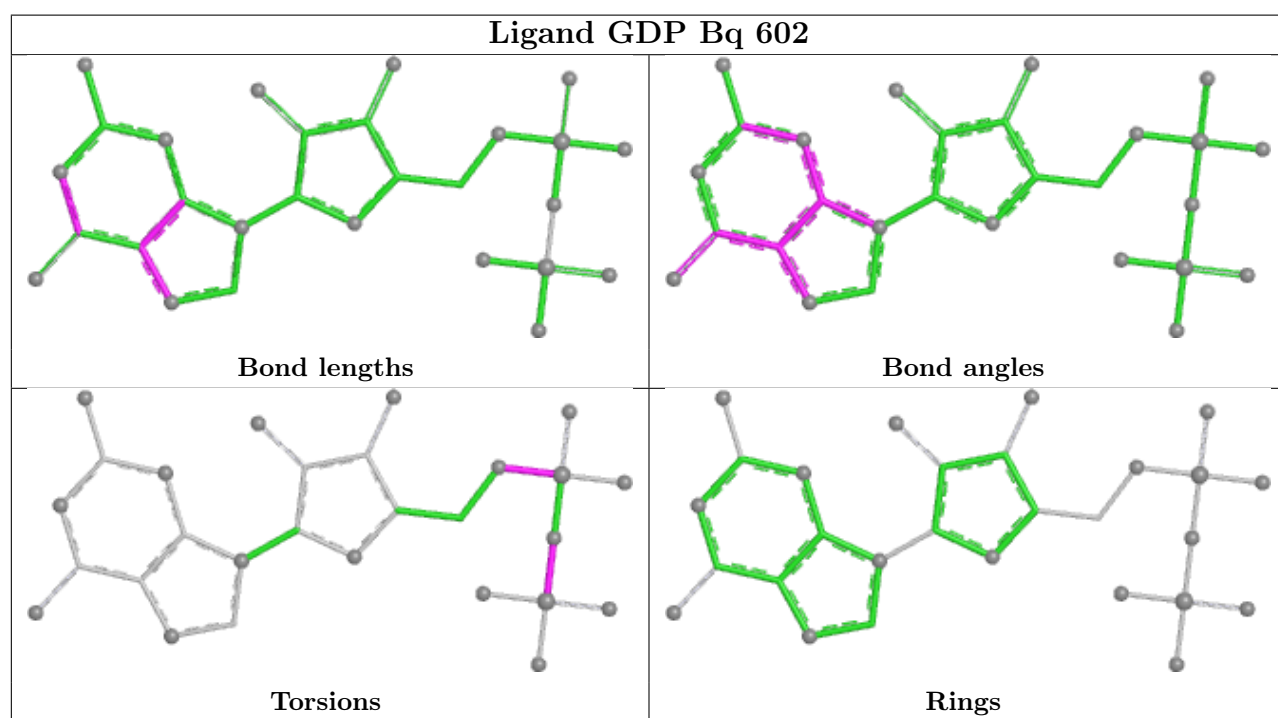
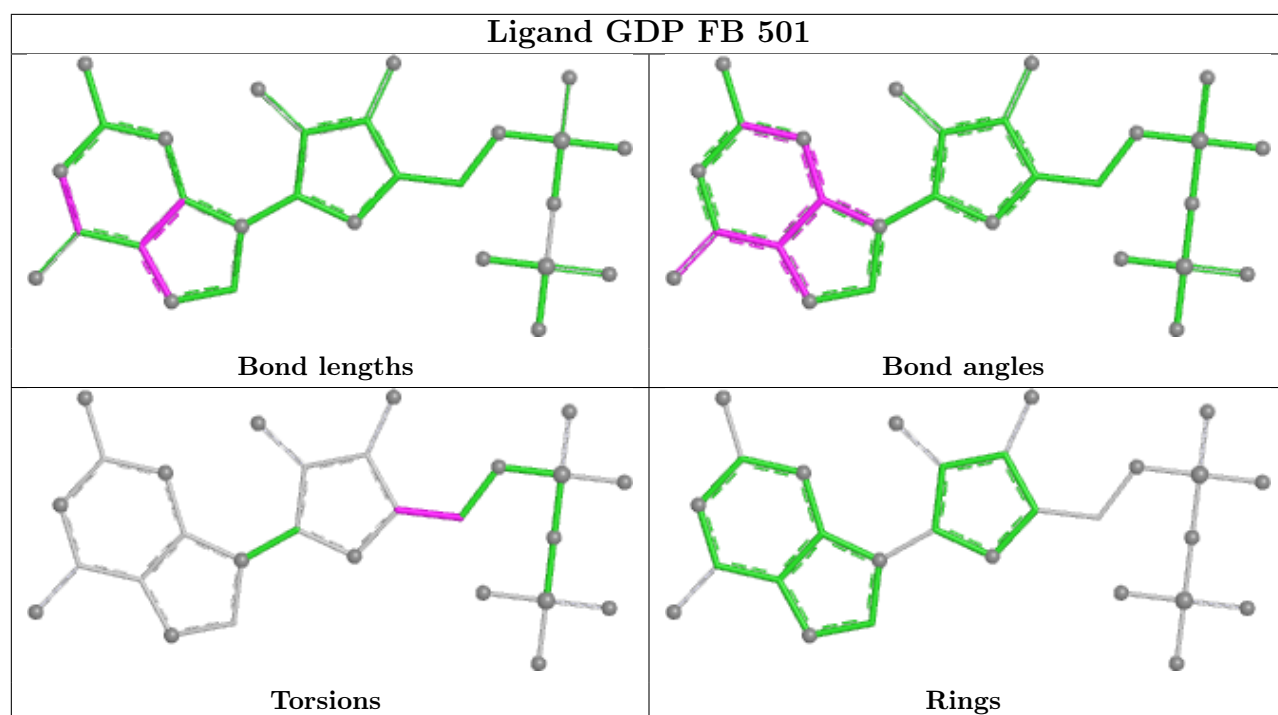


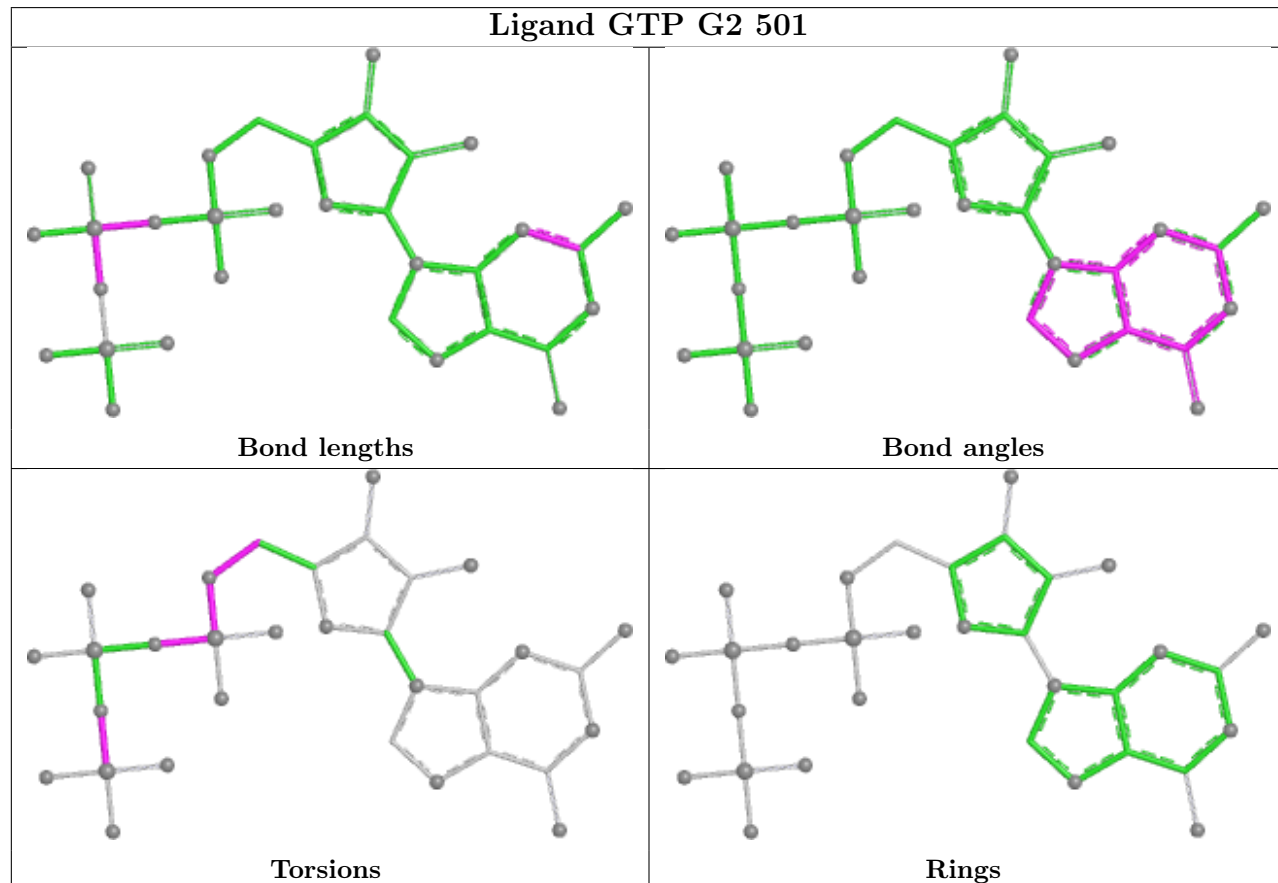
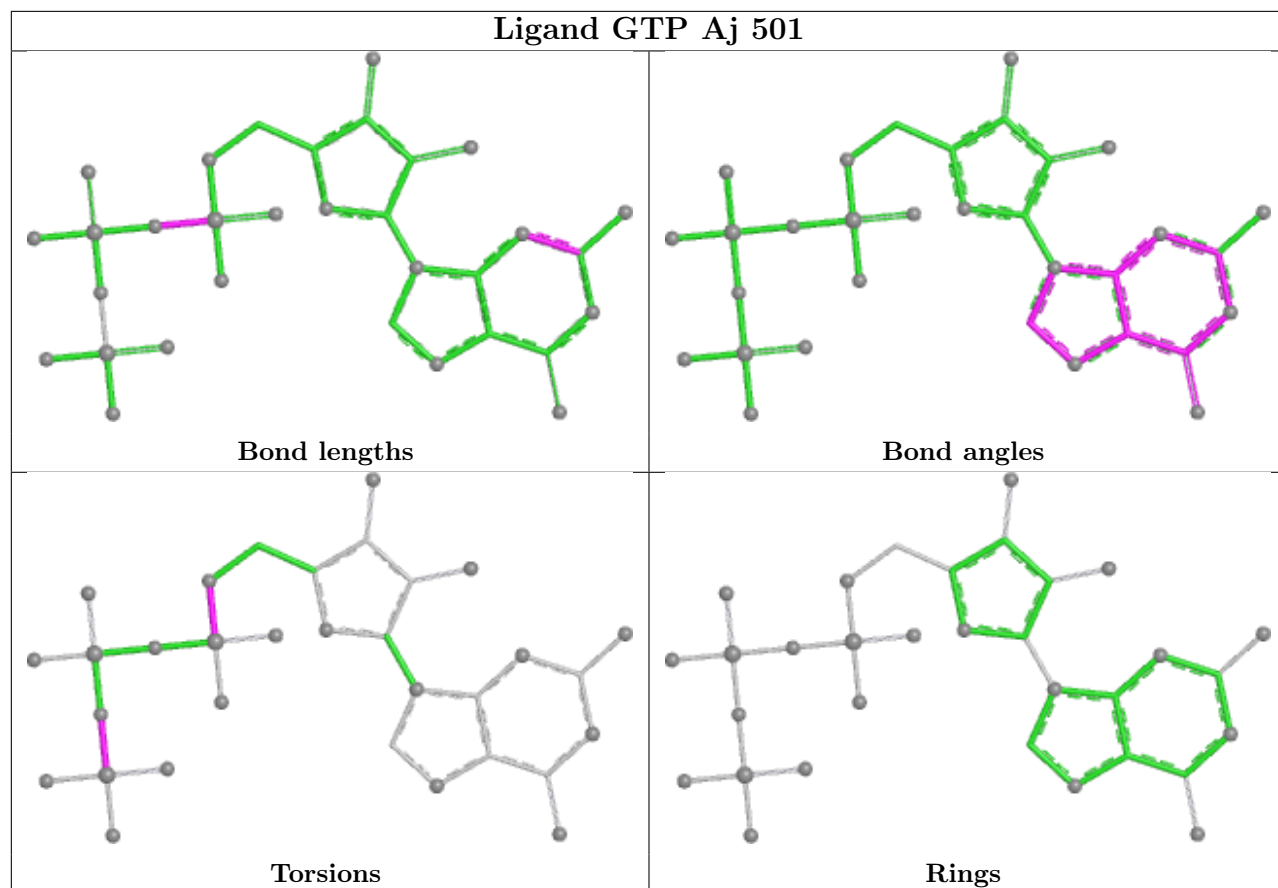
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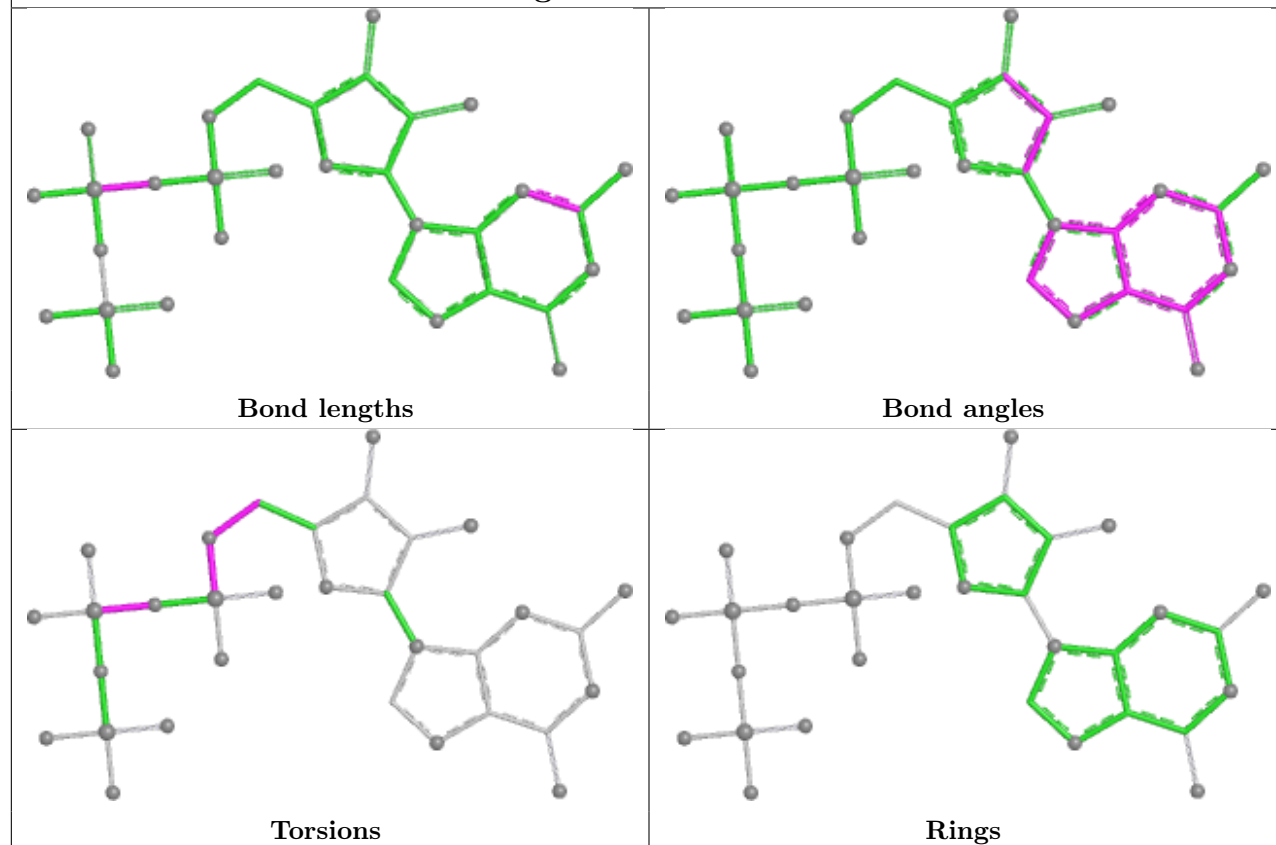




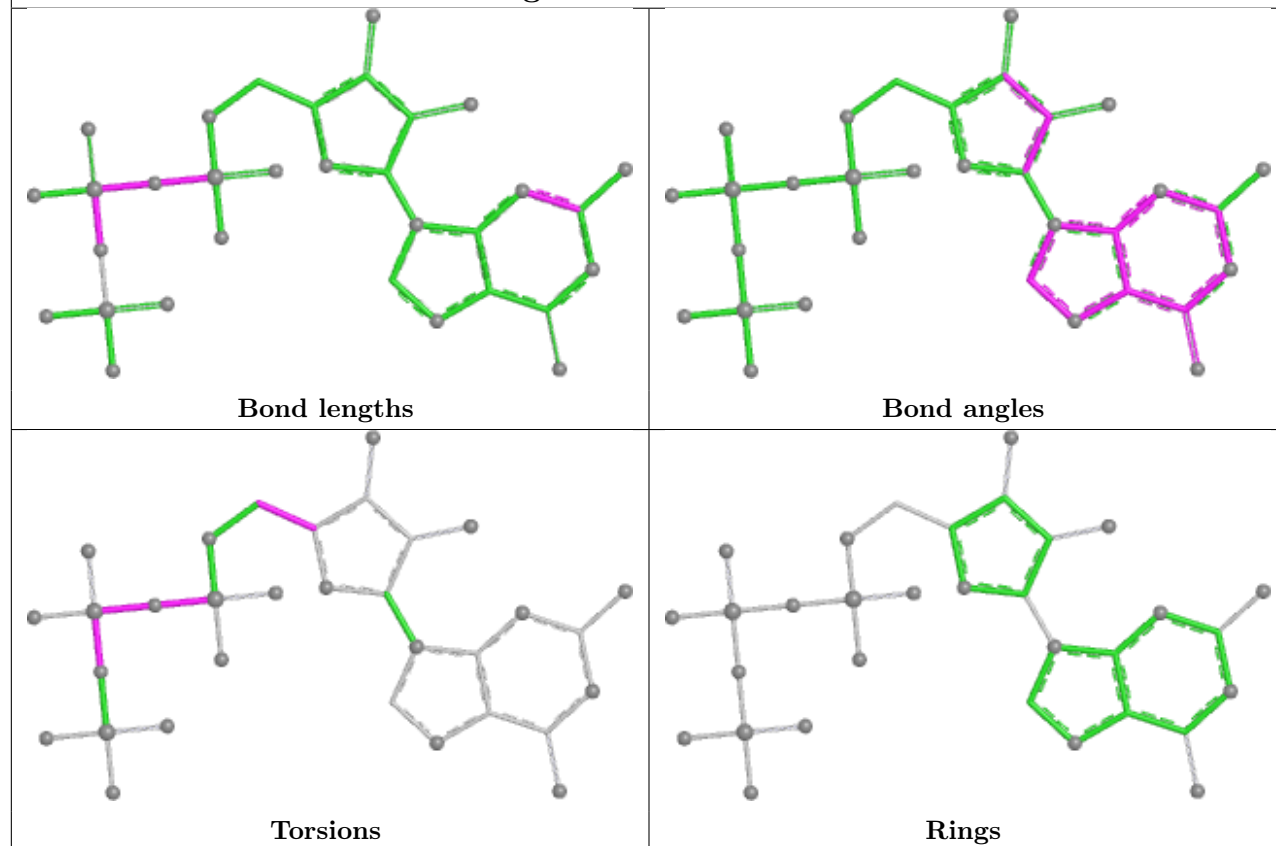


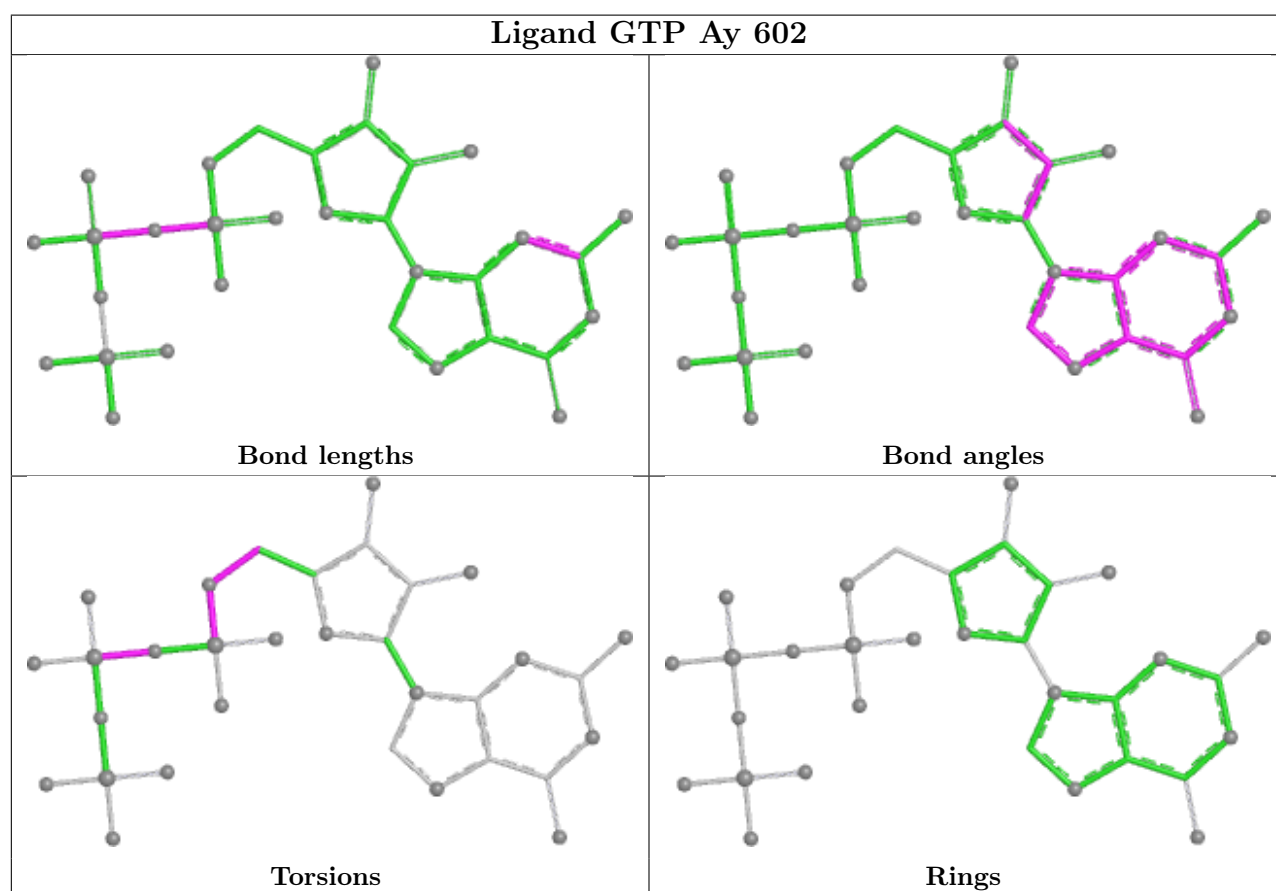
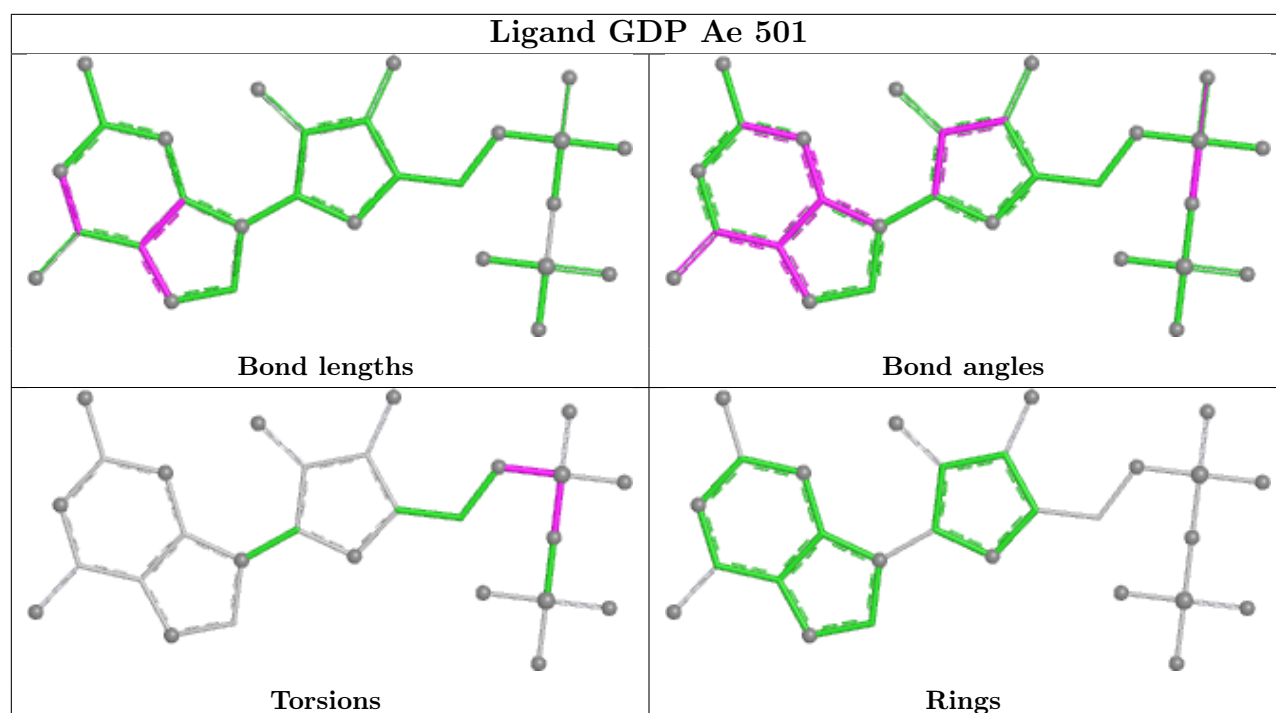


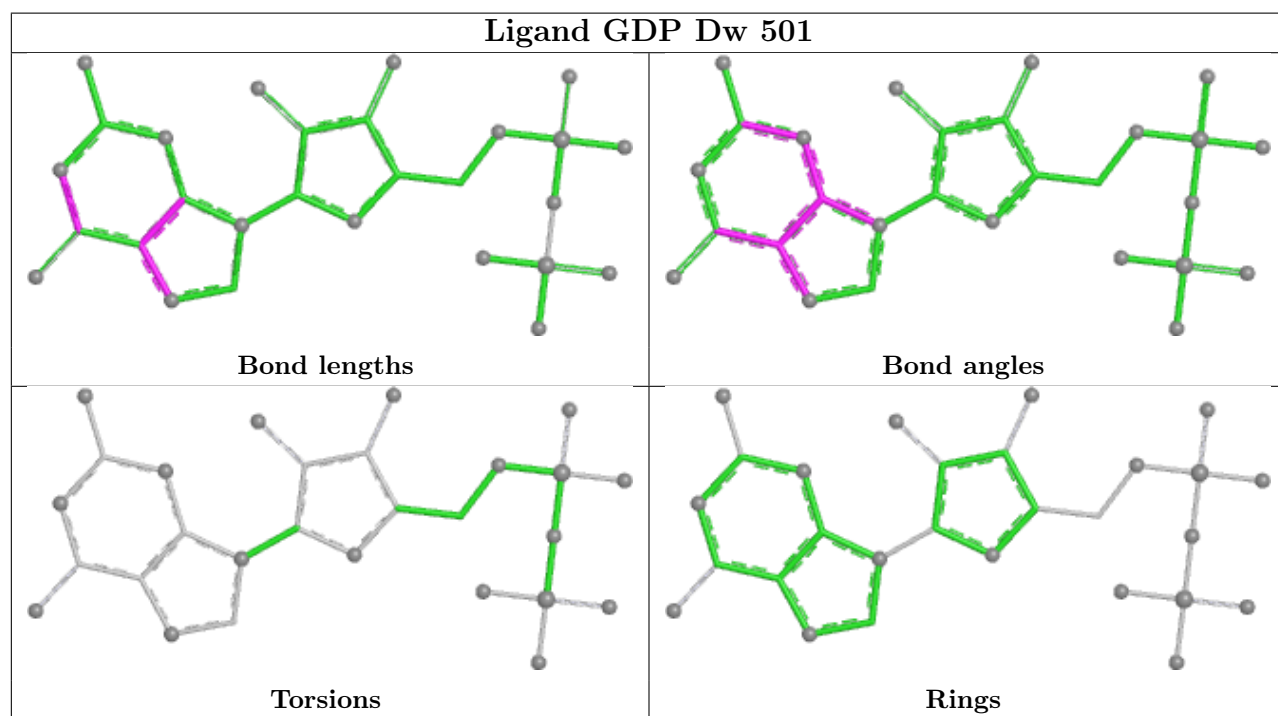
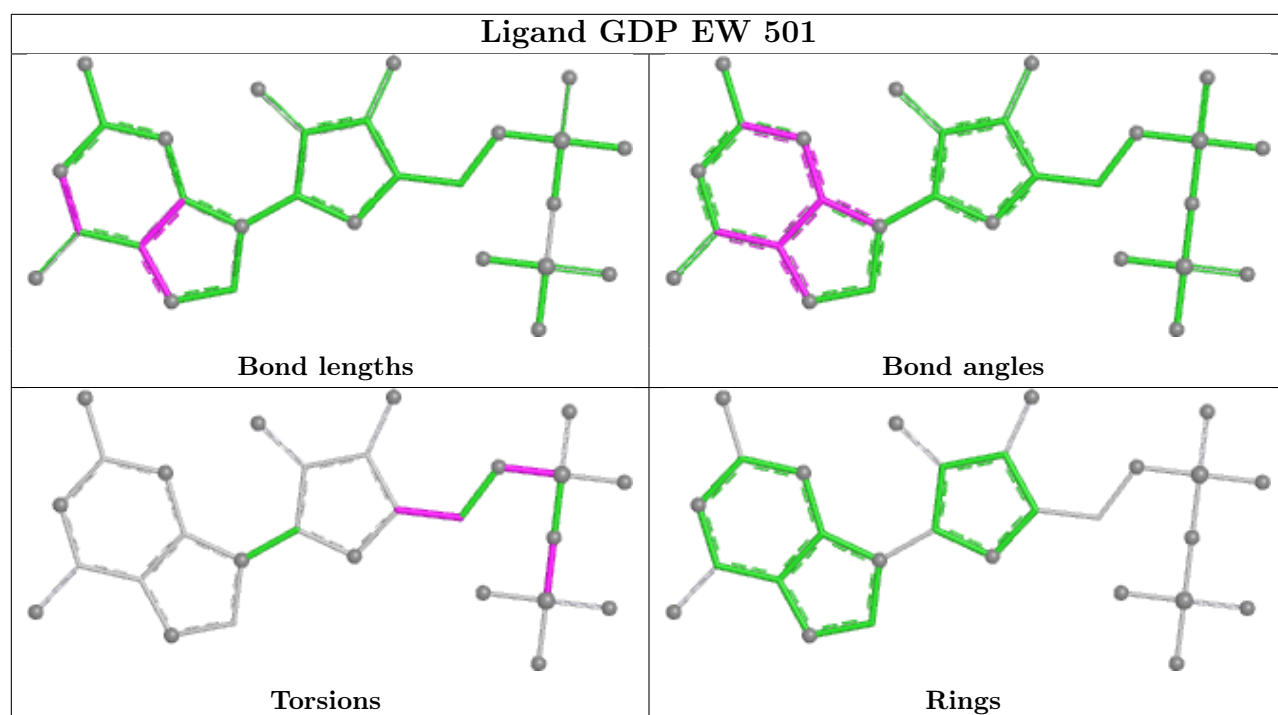
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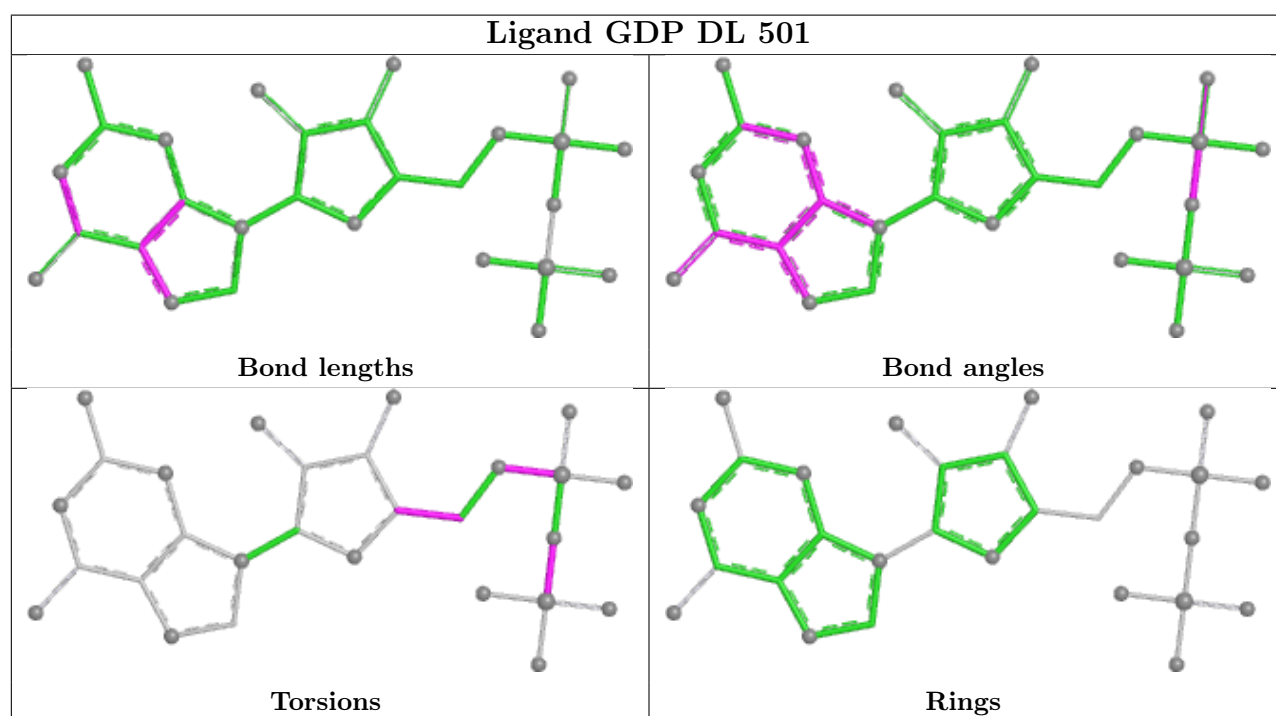
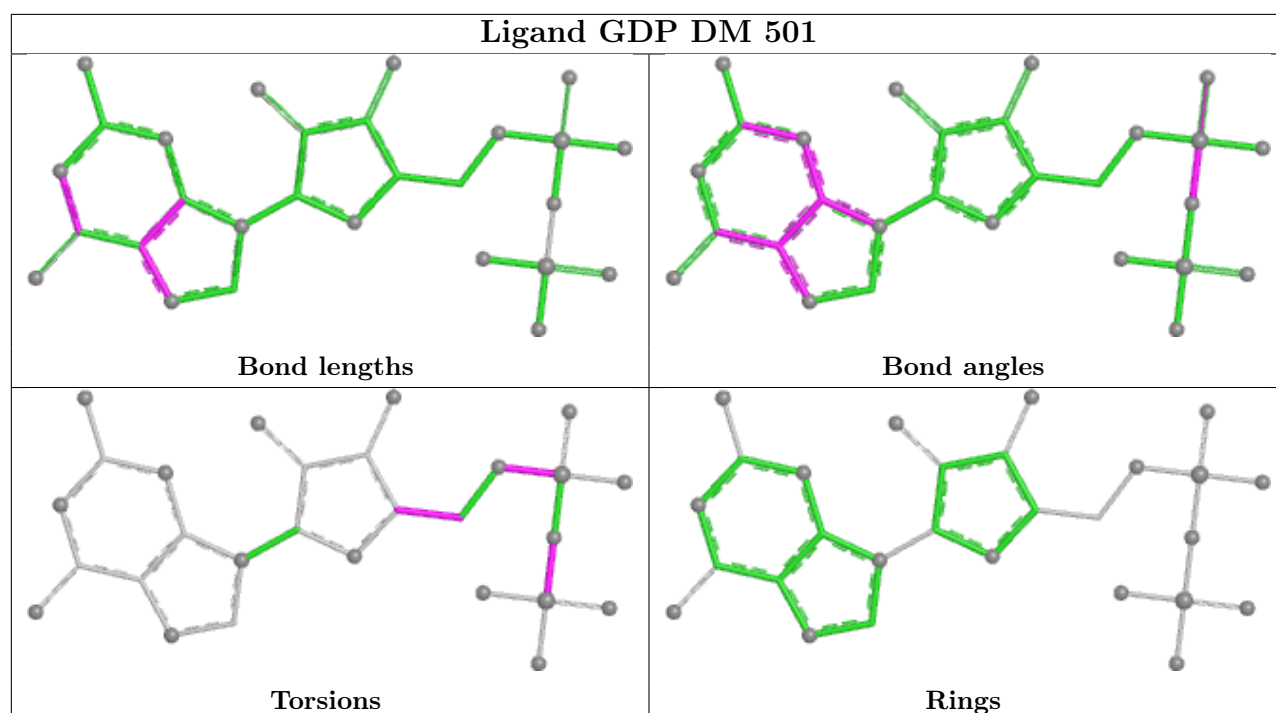


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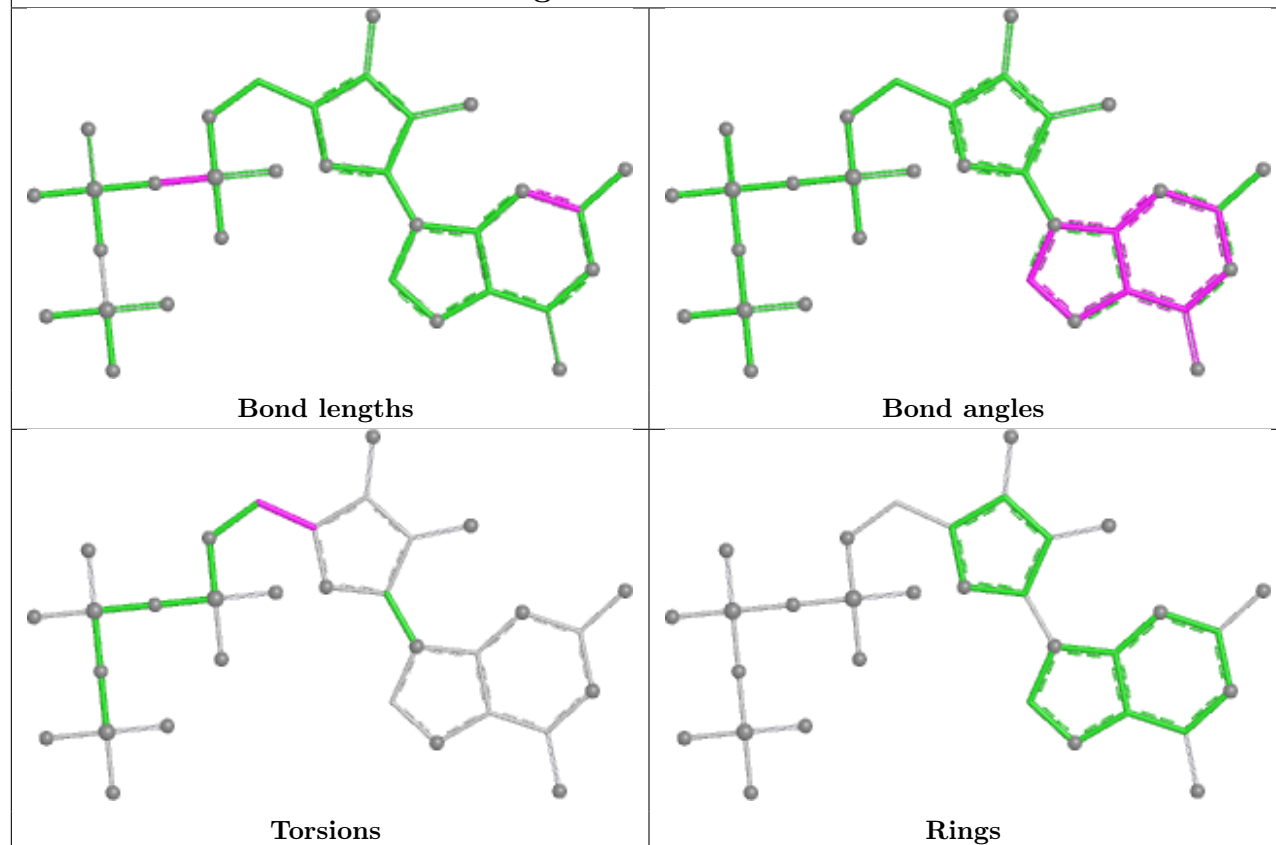




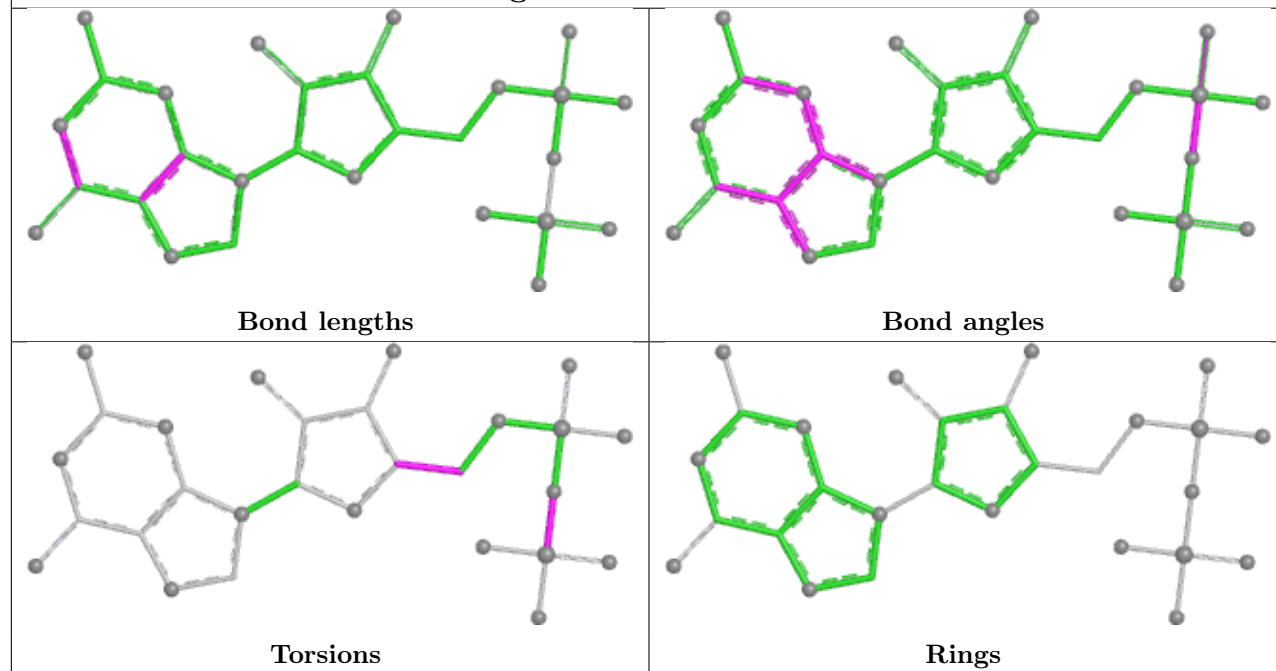




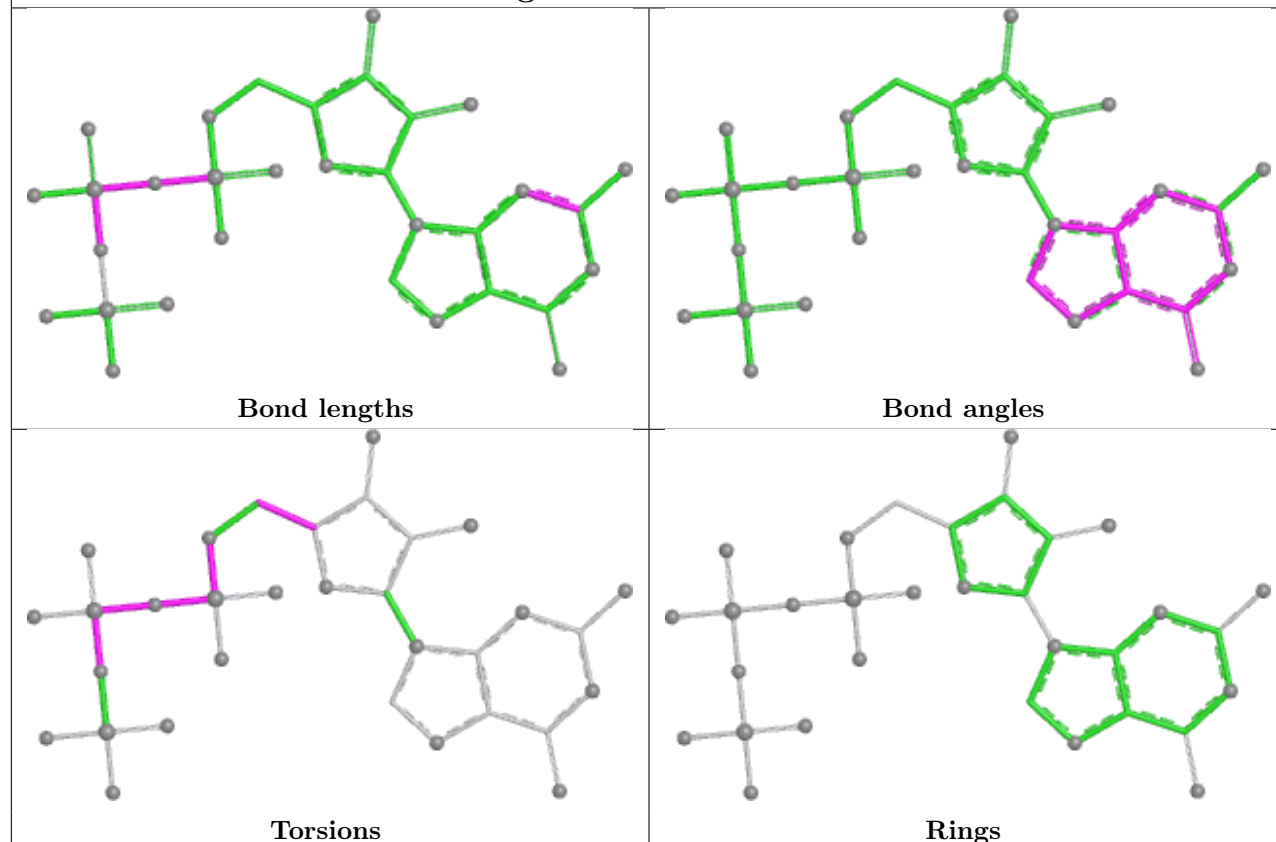
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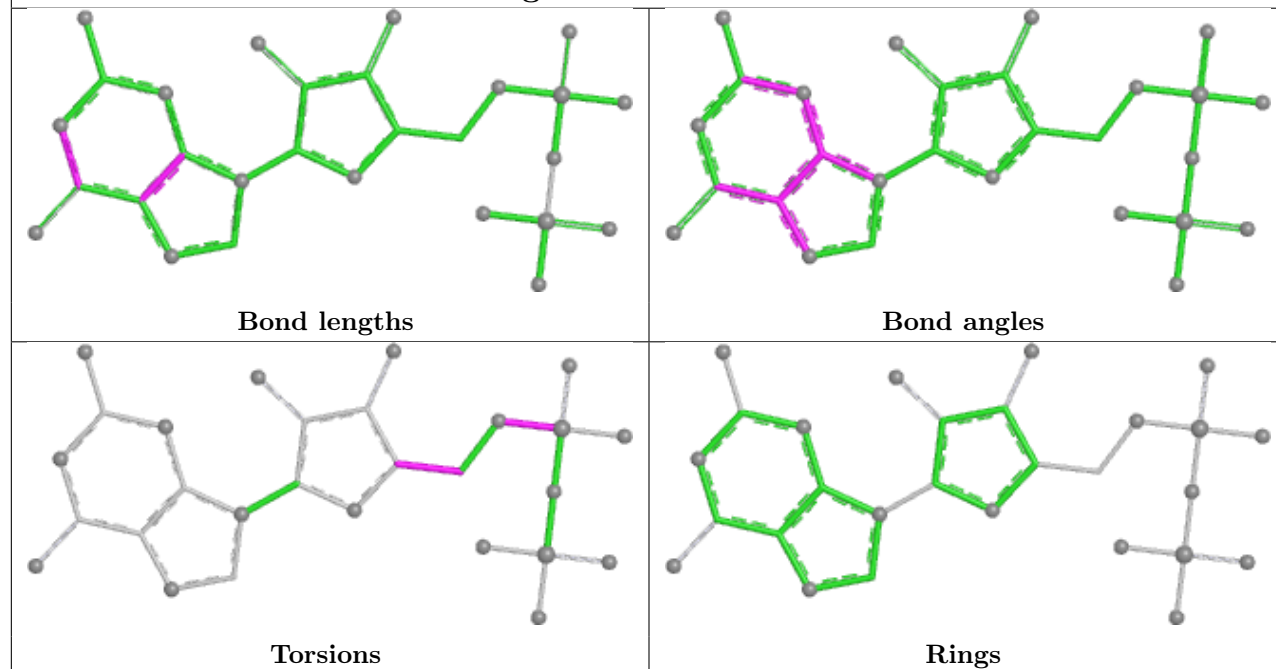
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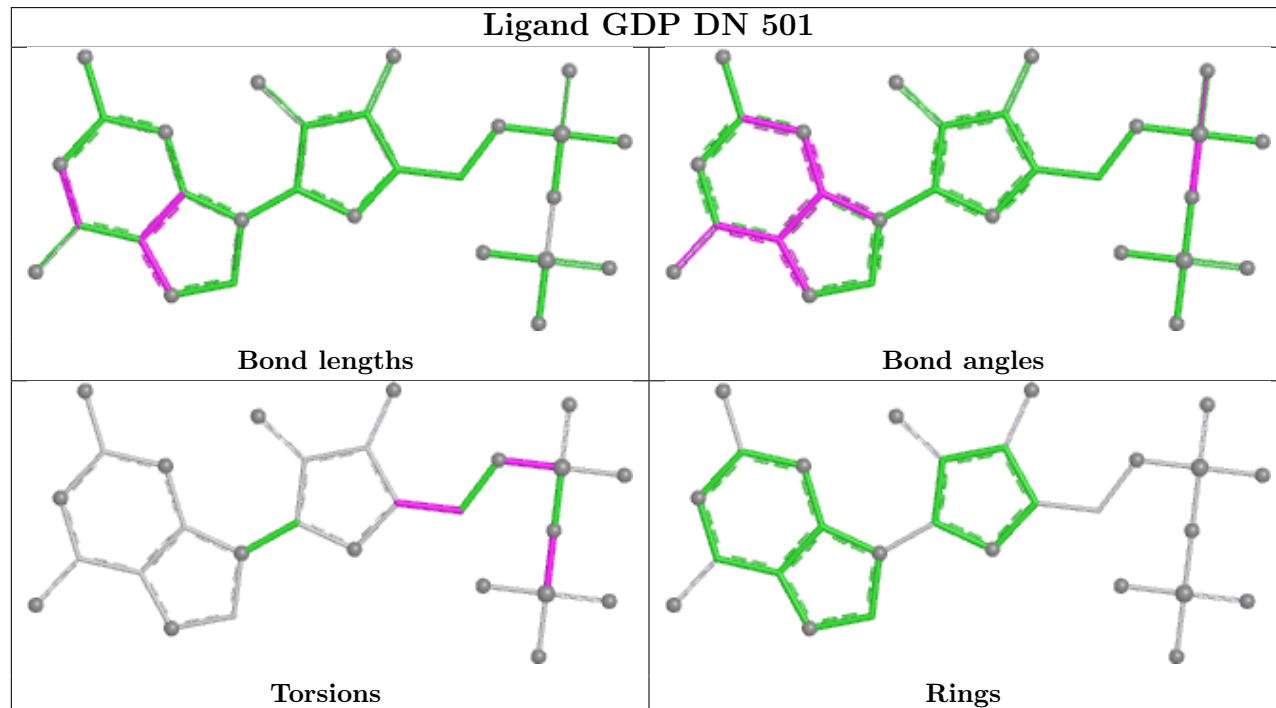
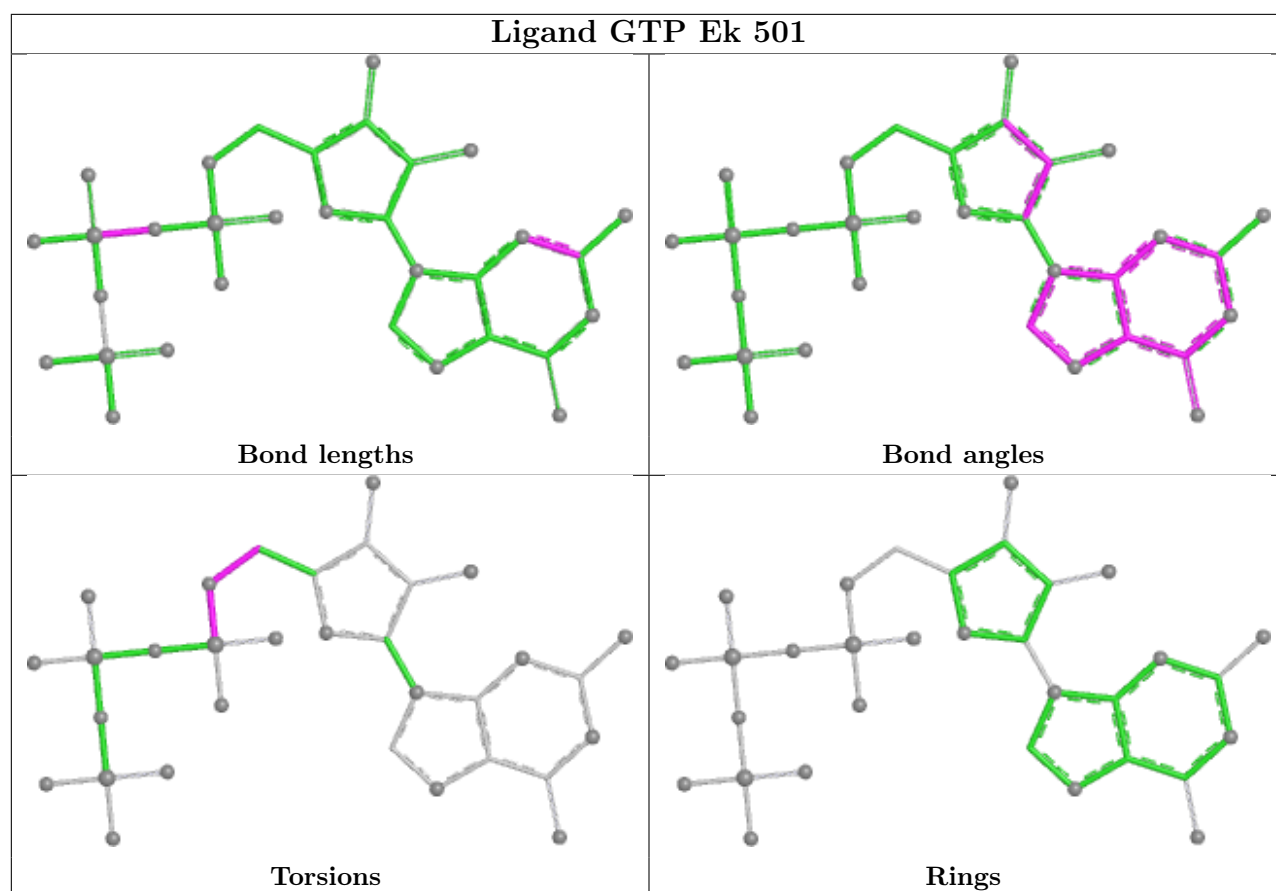


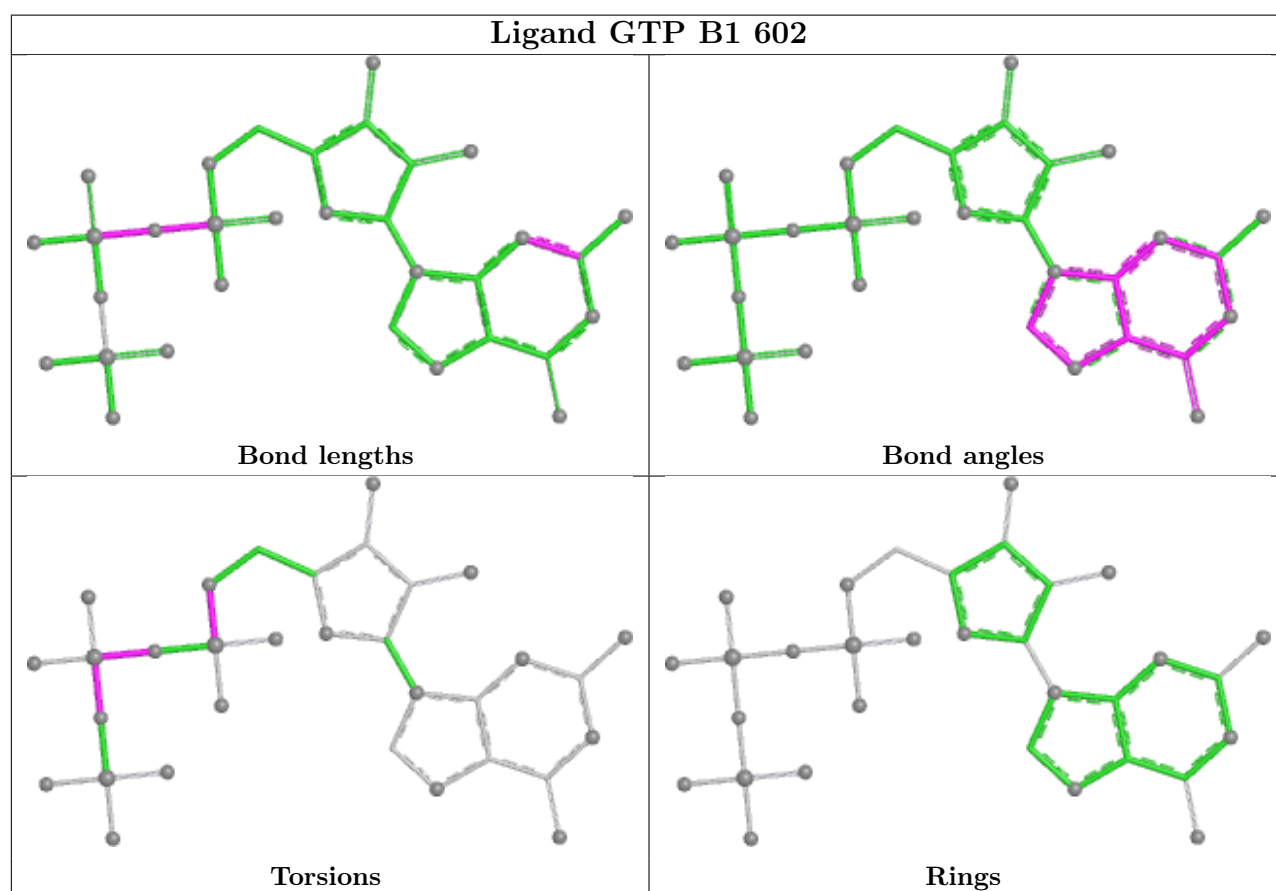
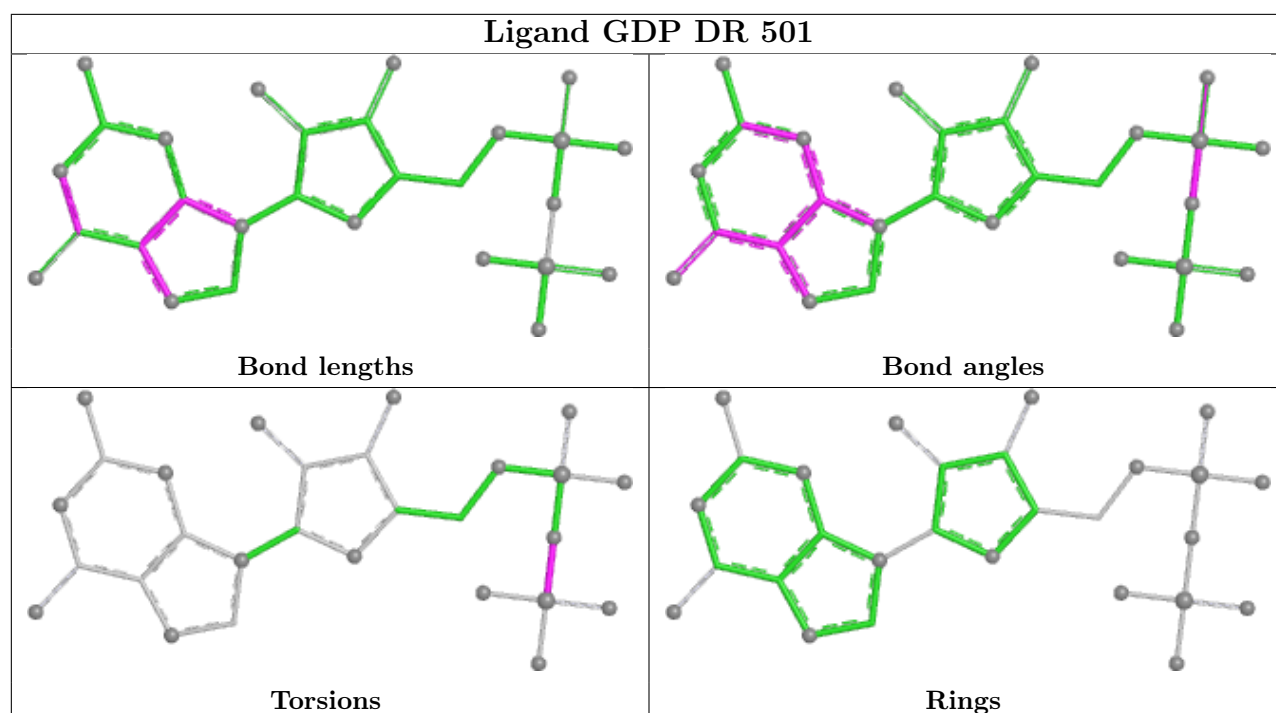
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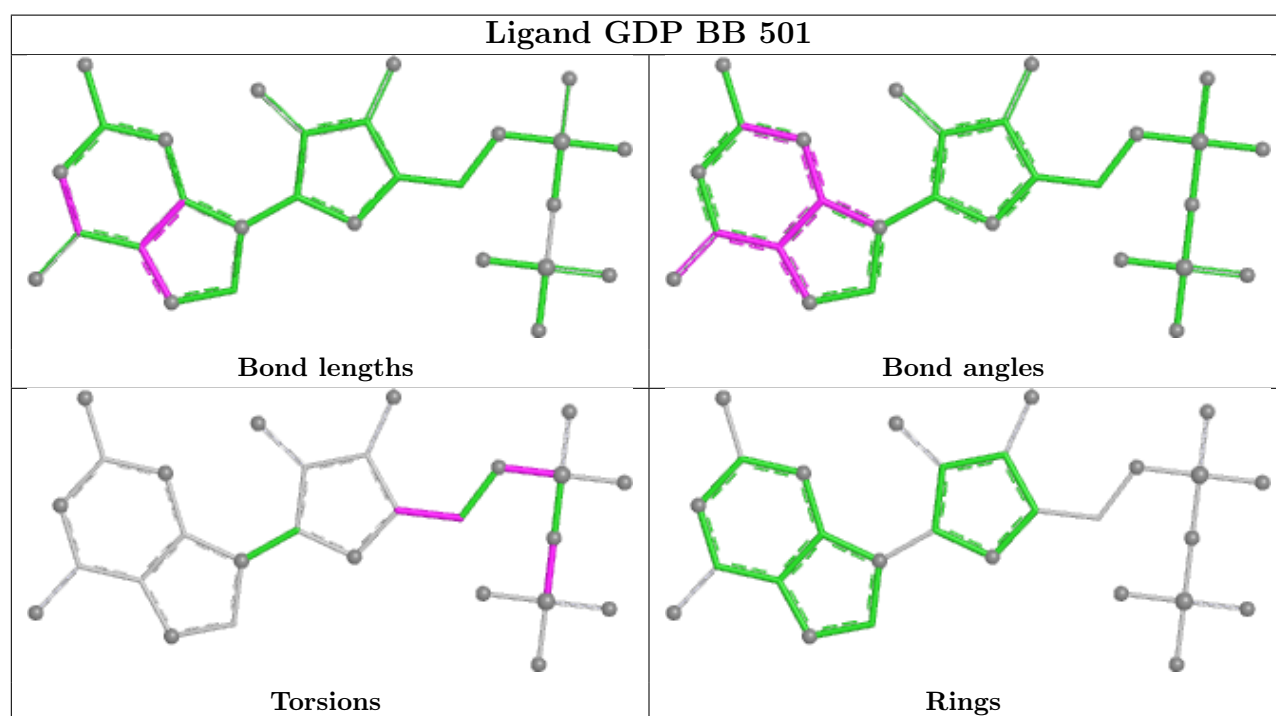
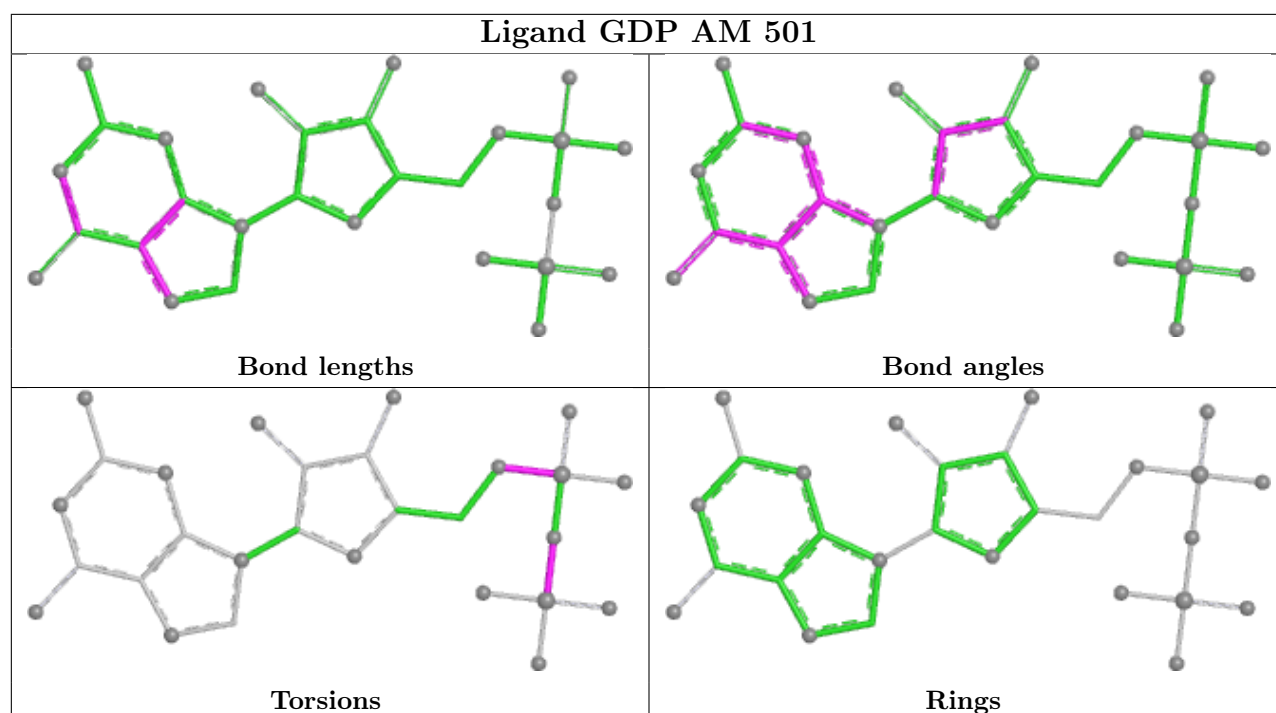


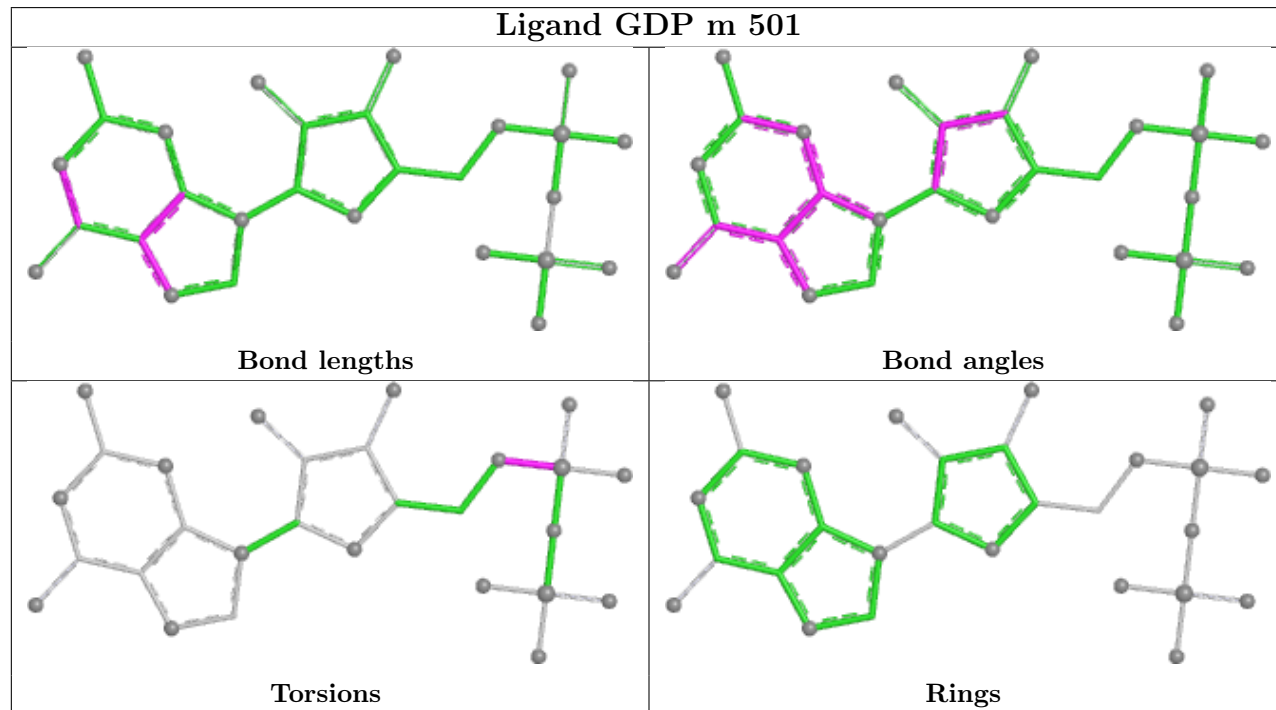
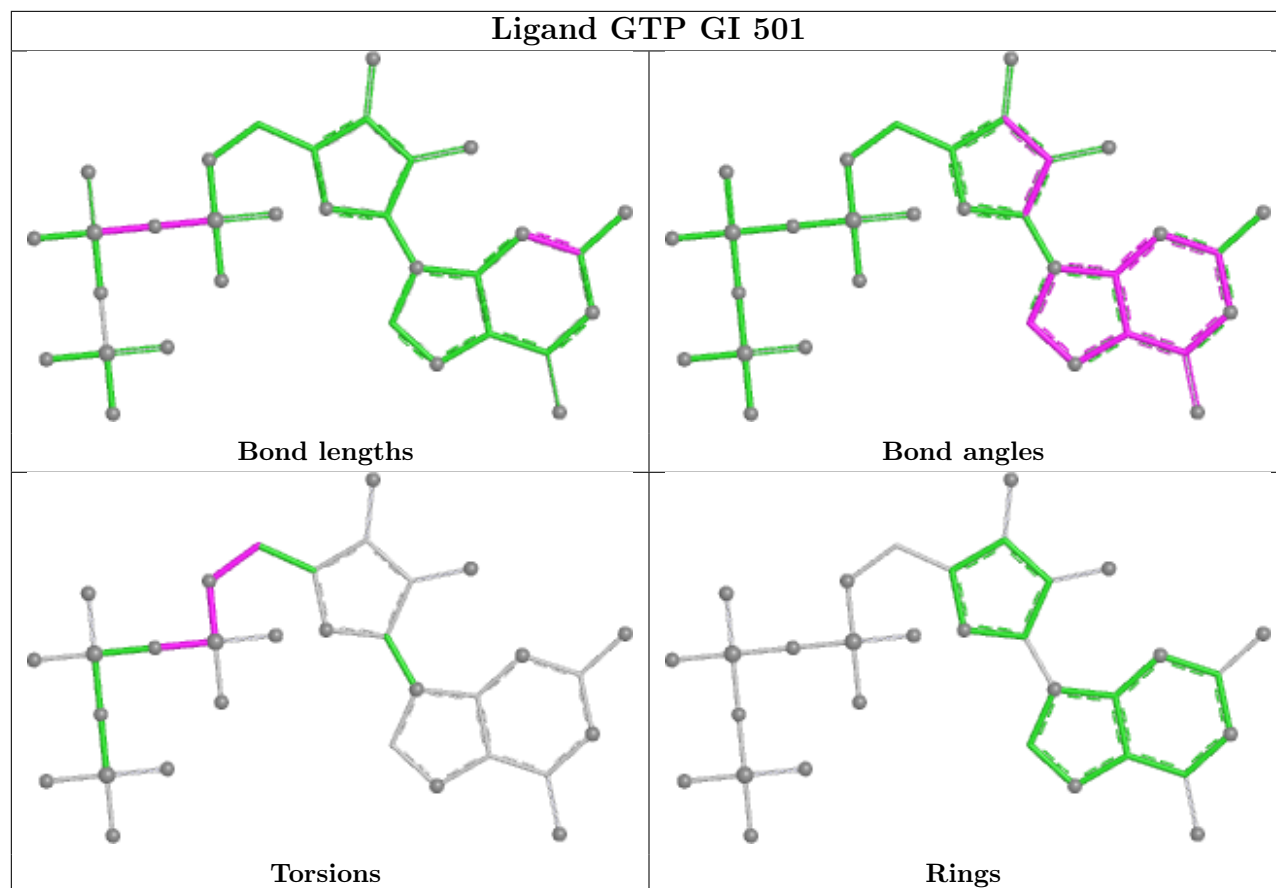
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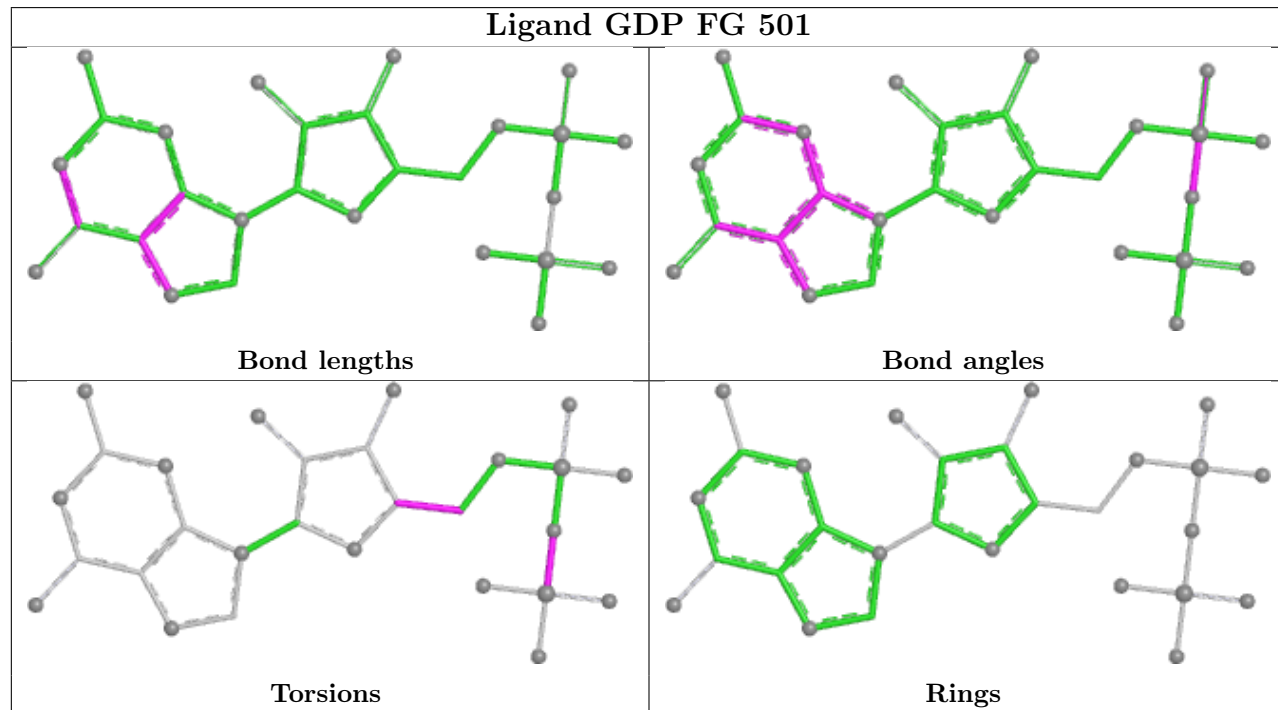
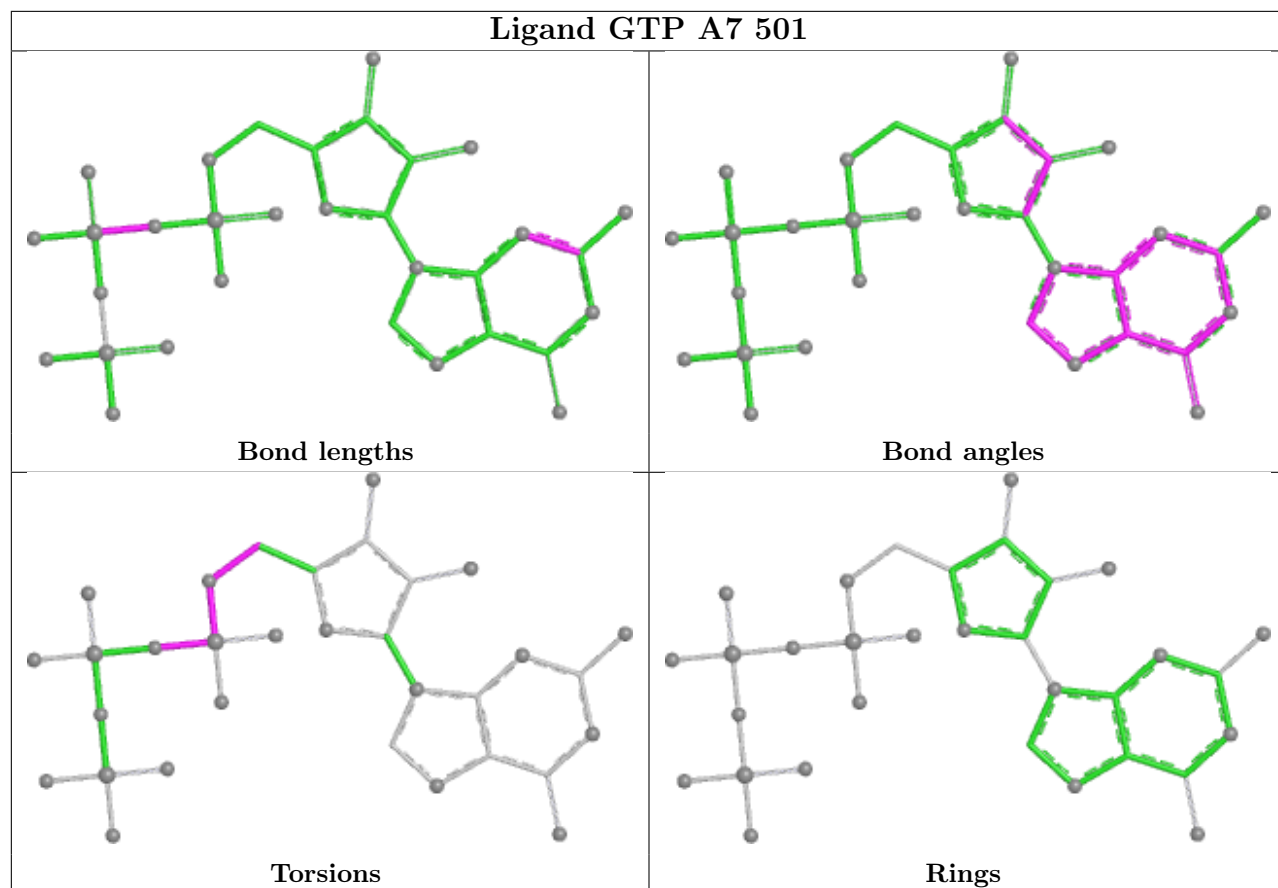


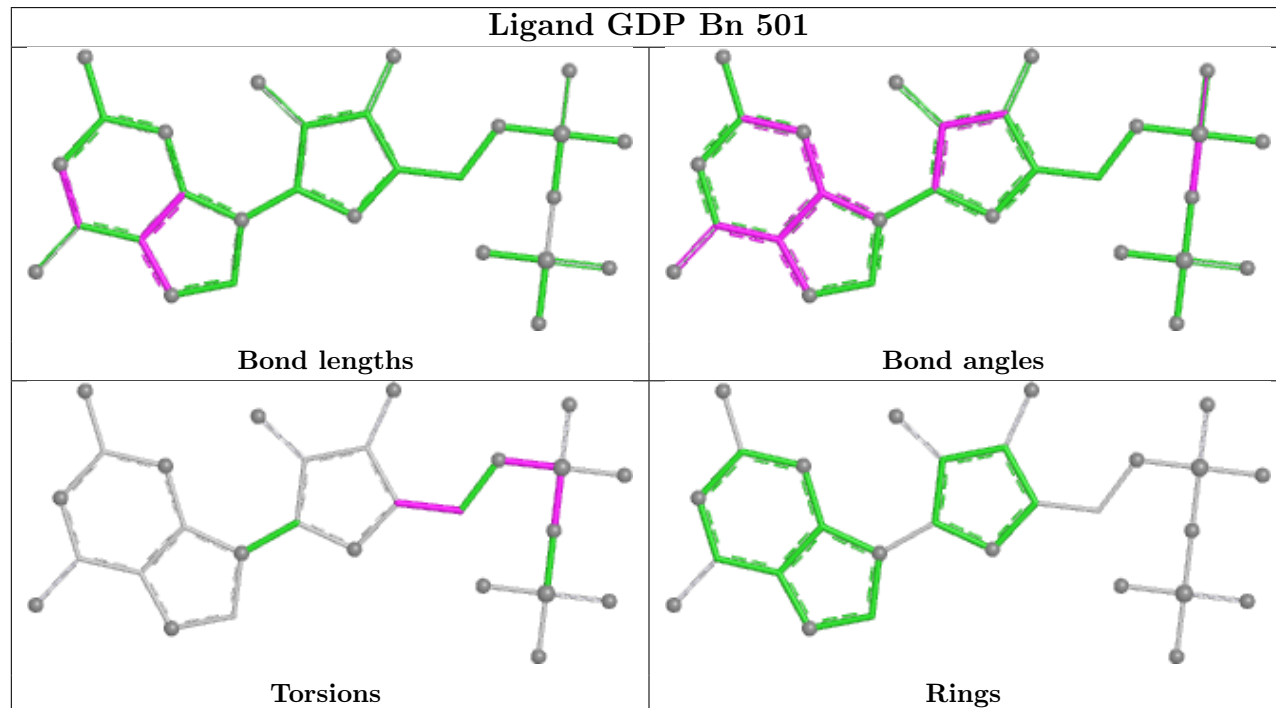
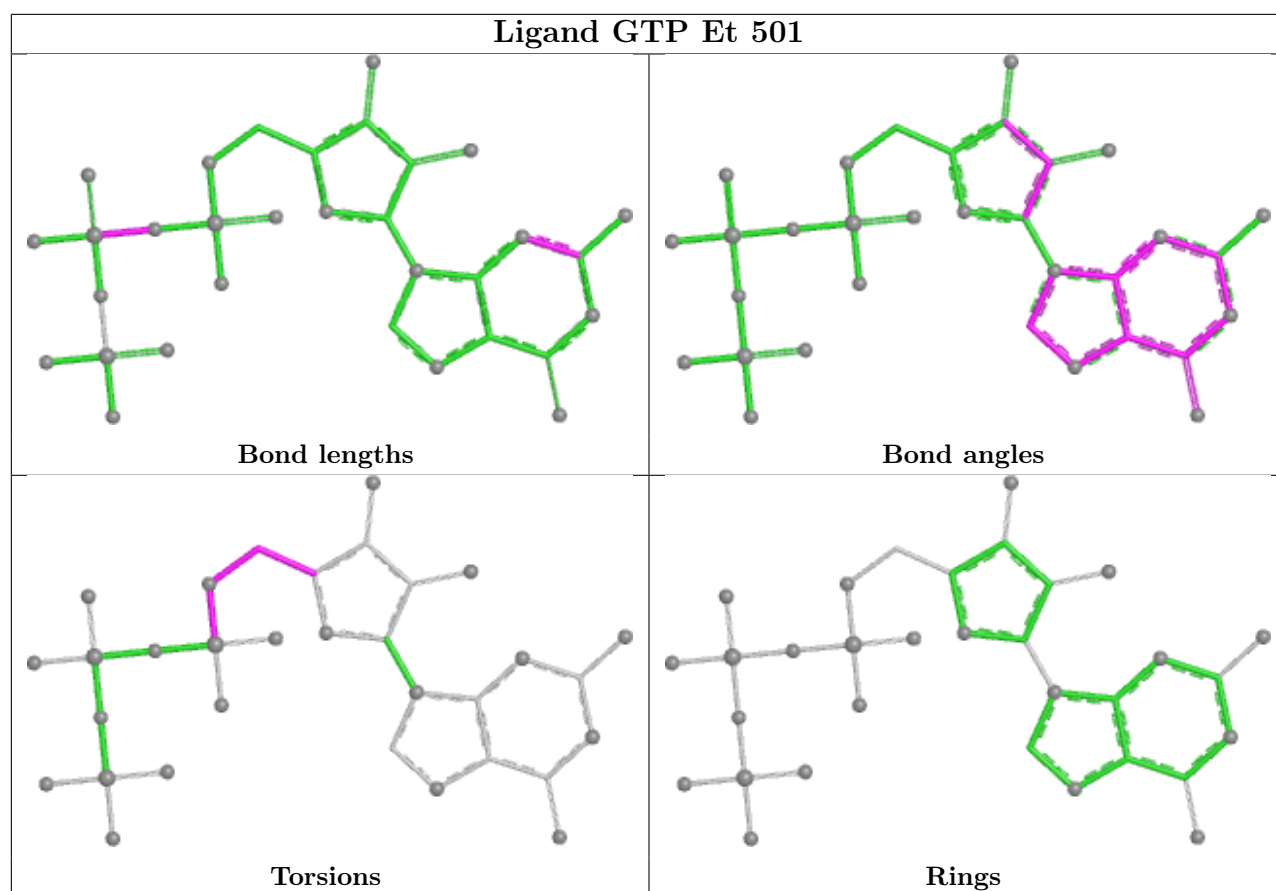




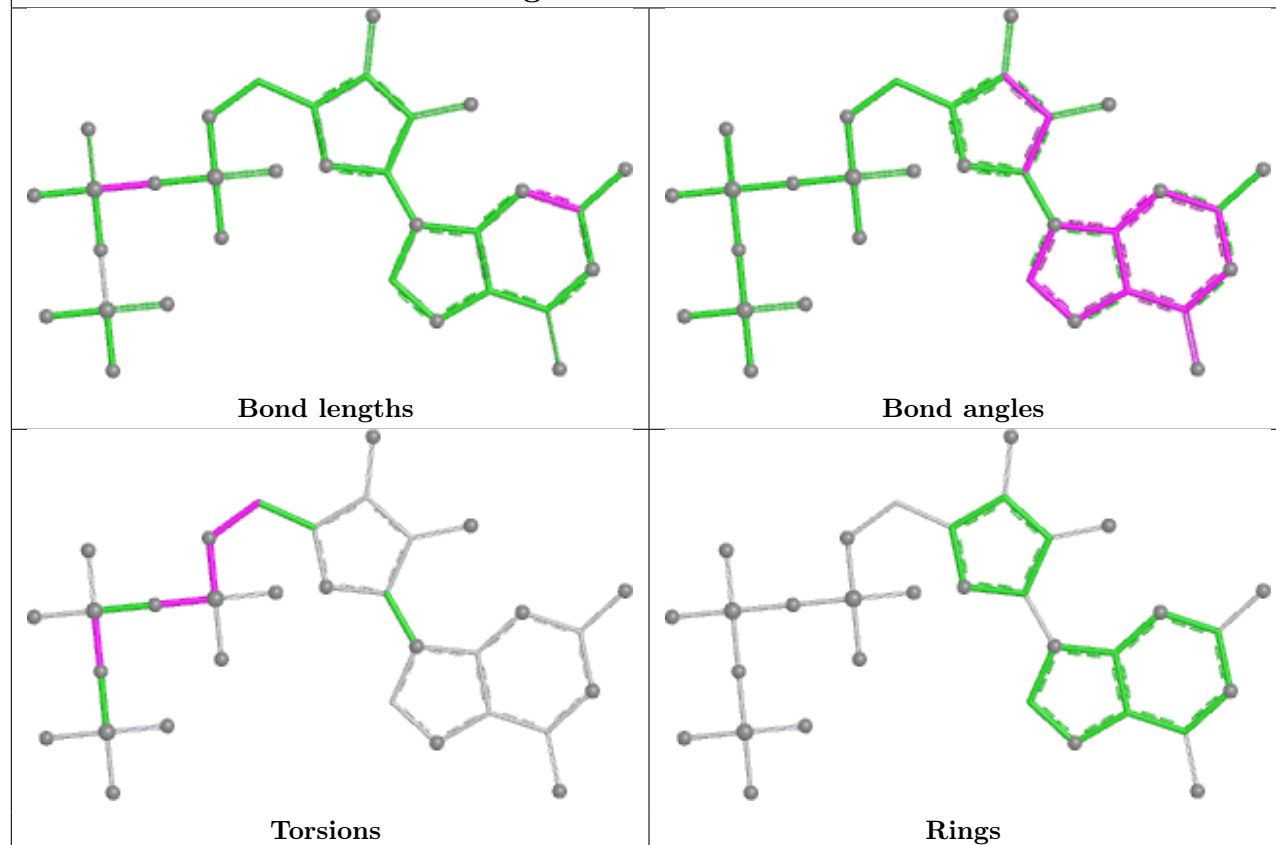




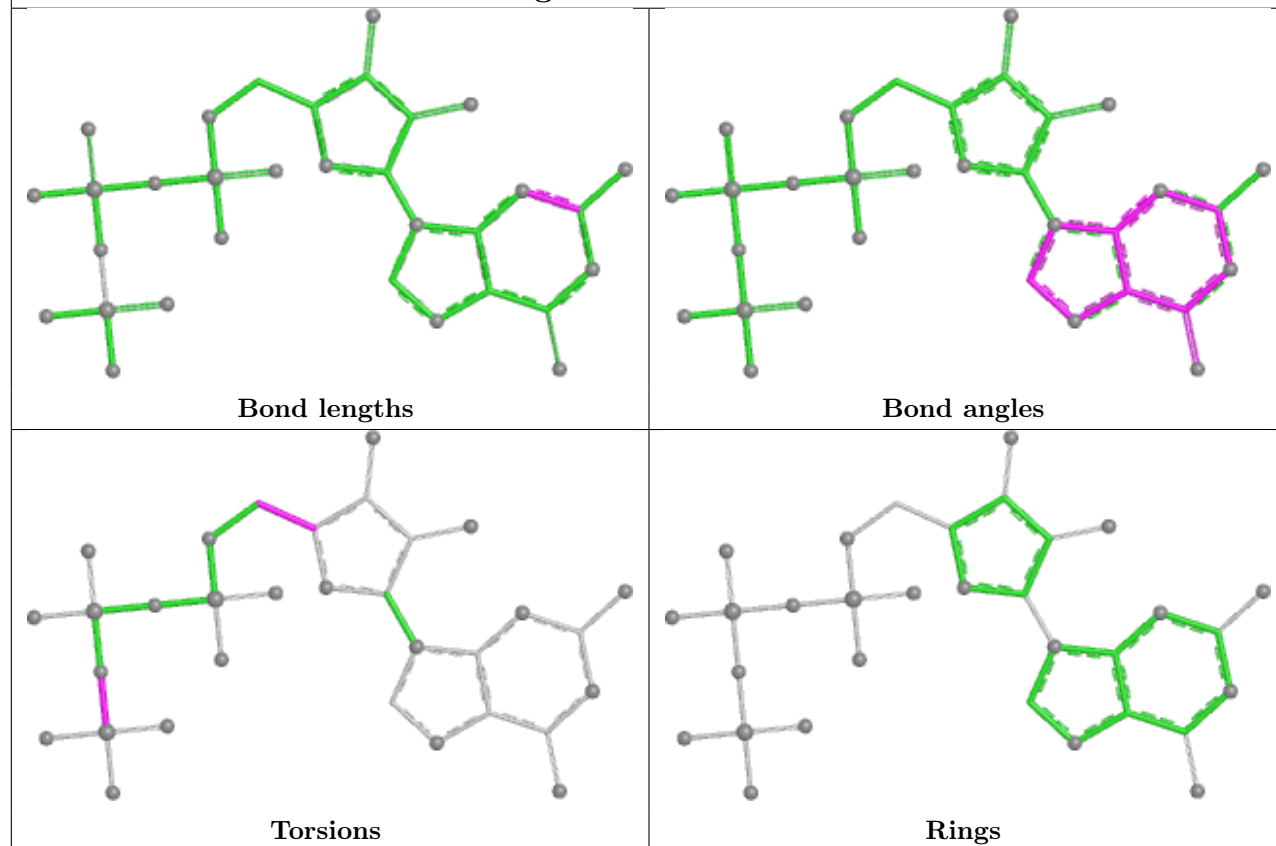


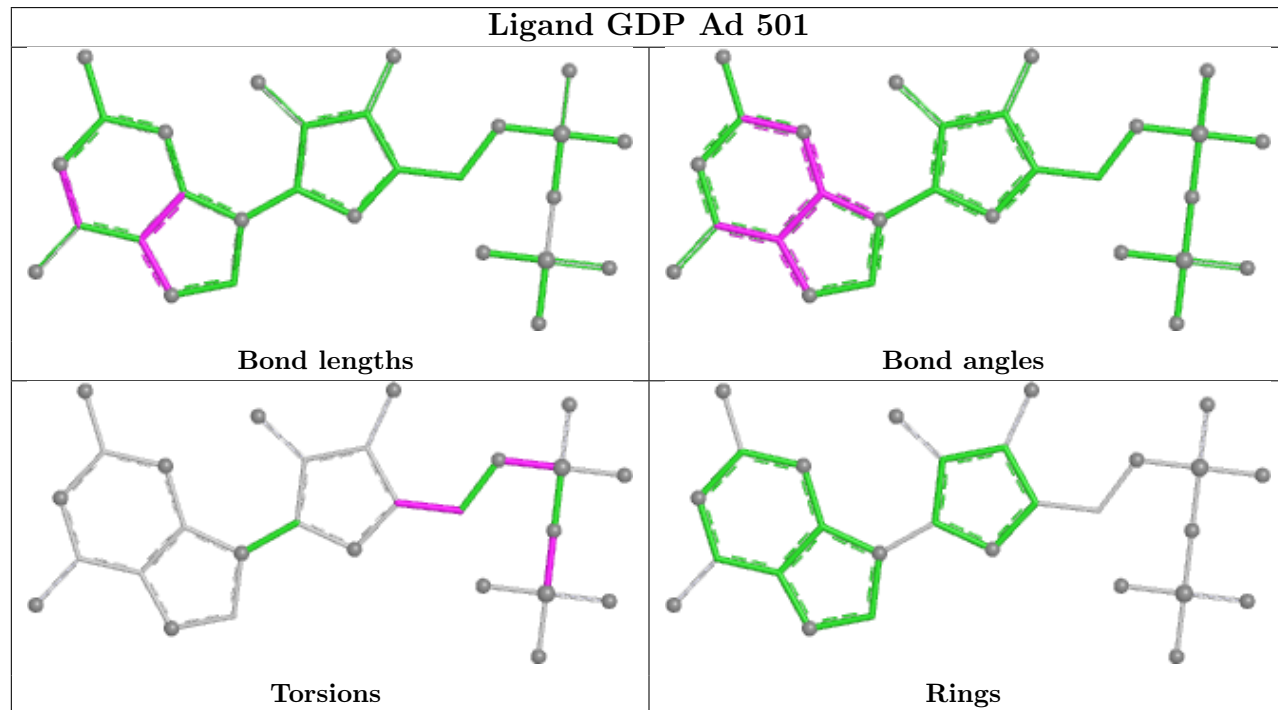
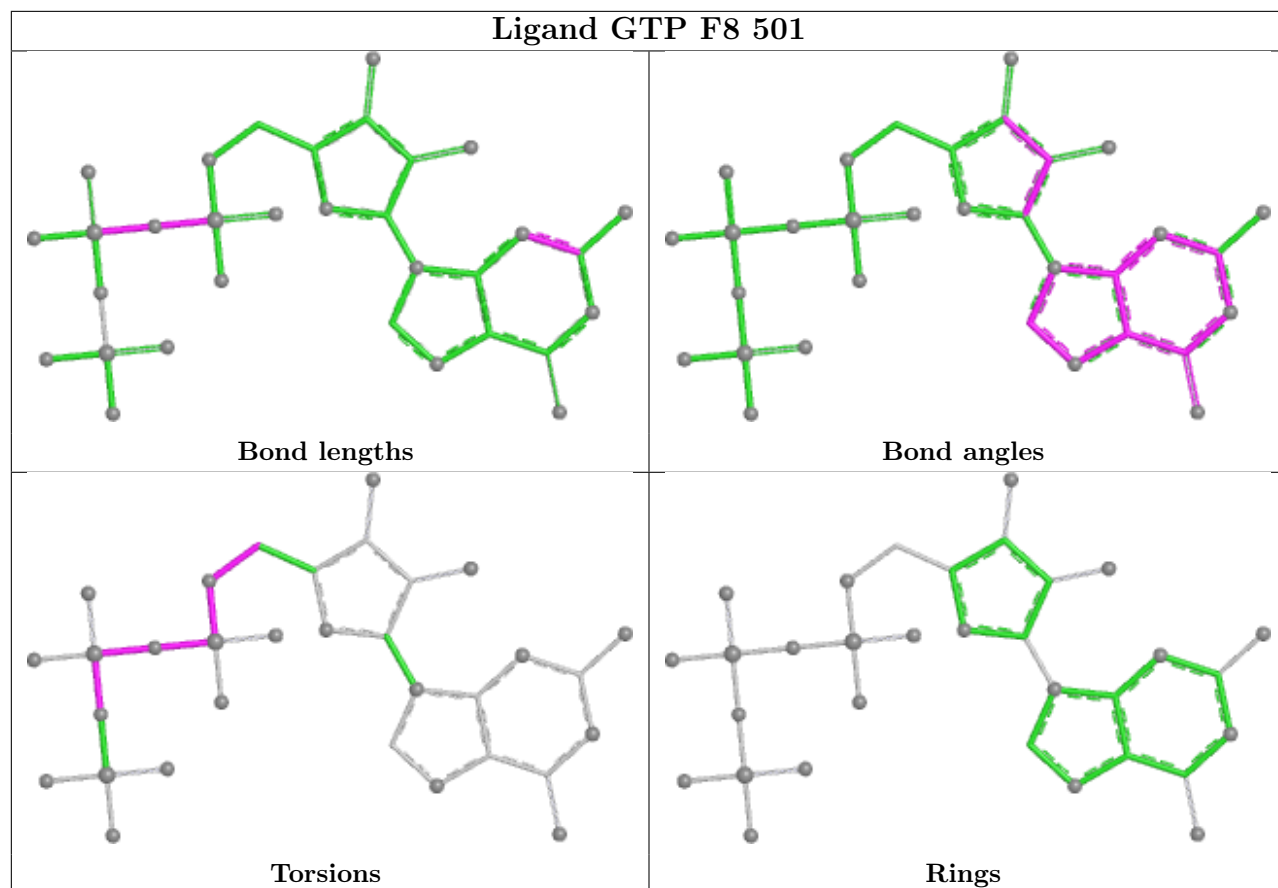


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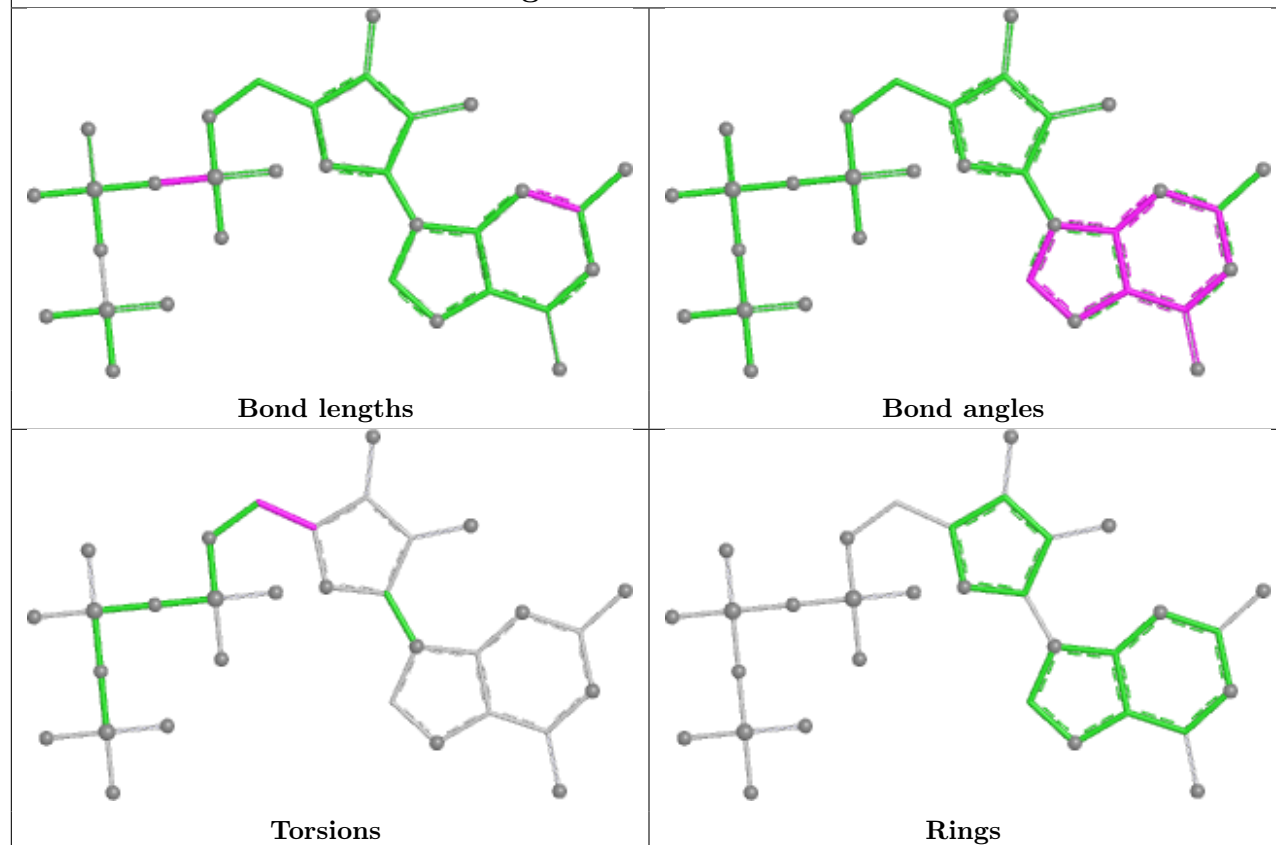


Ligand GTP 3 602

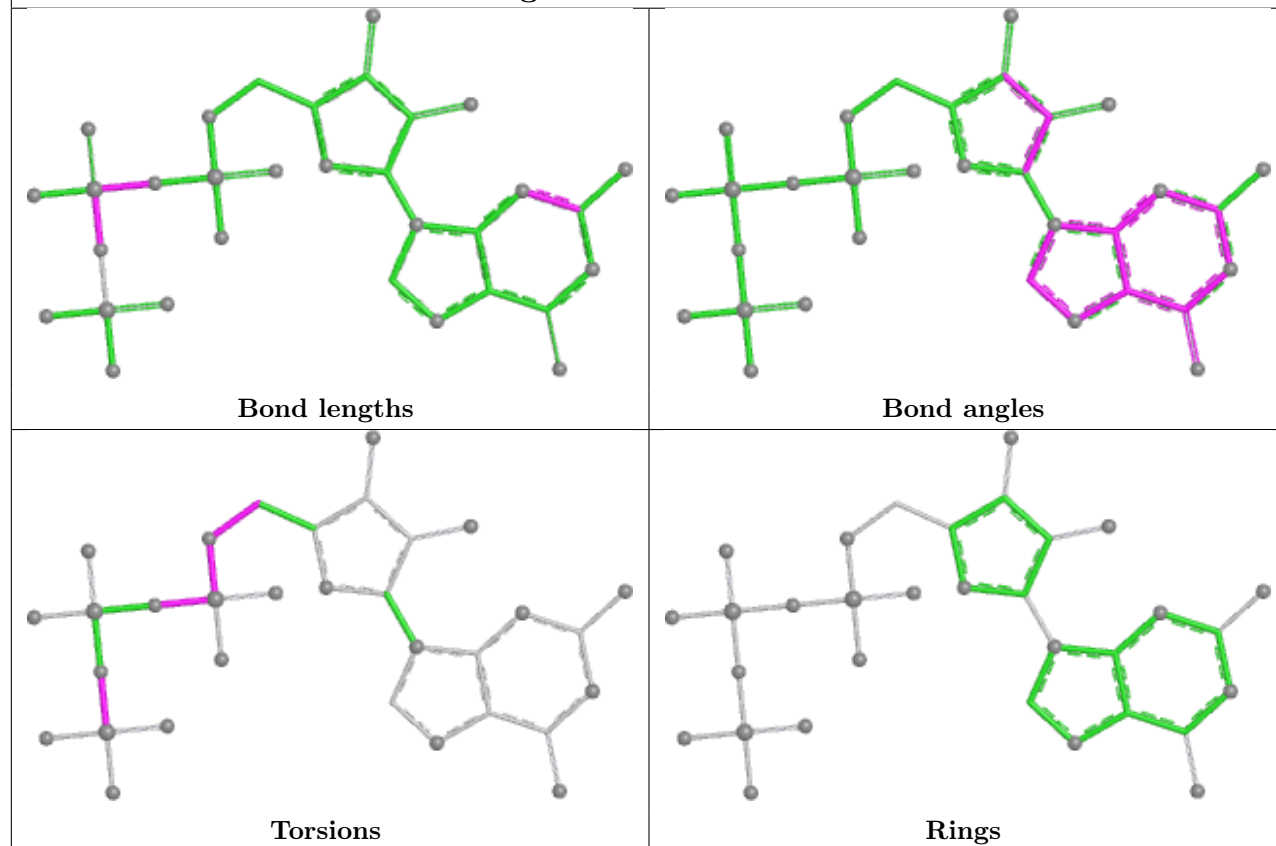




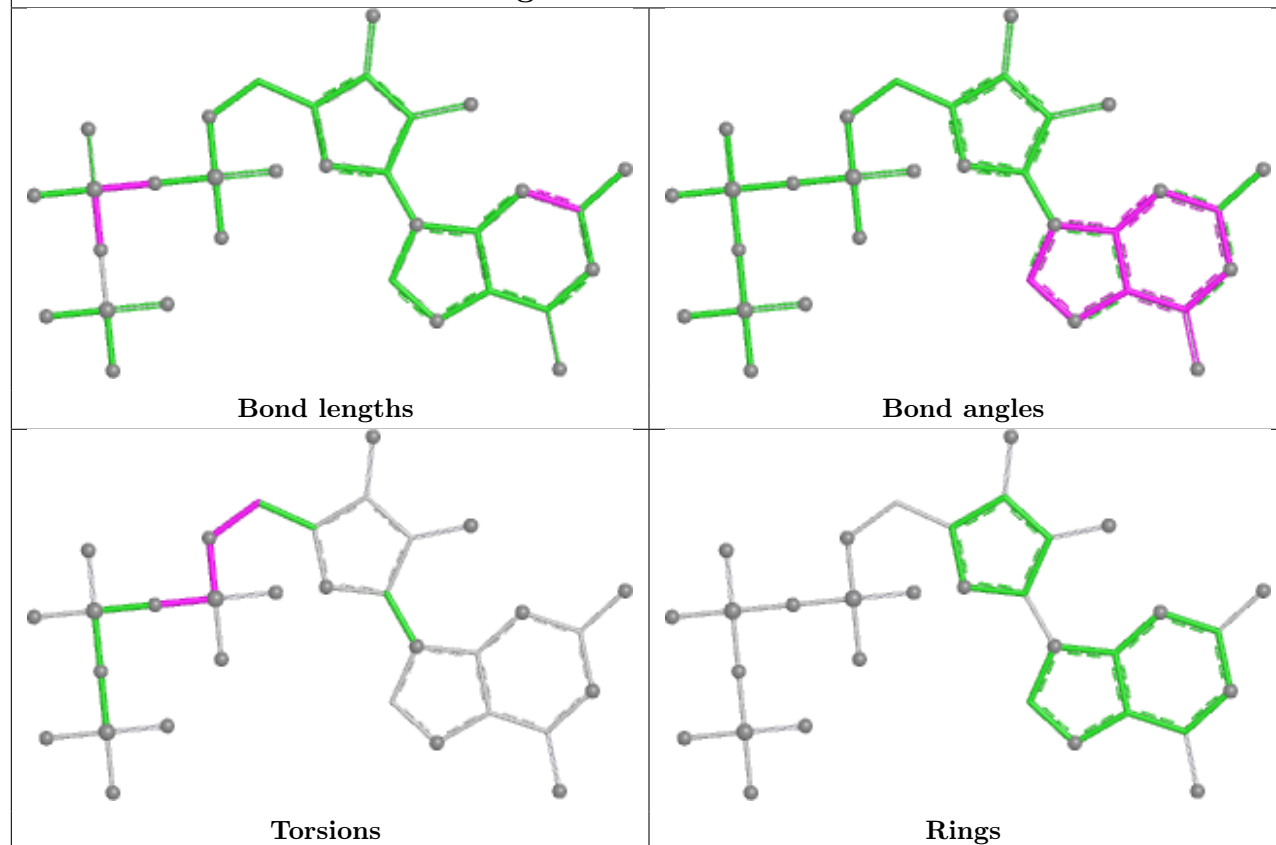
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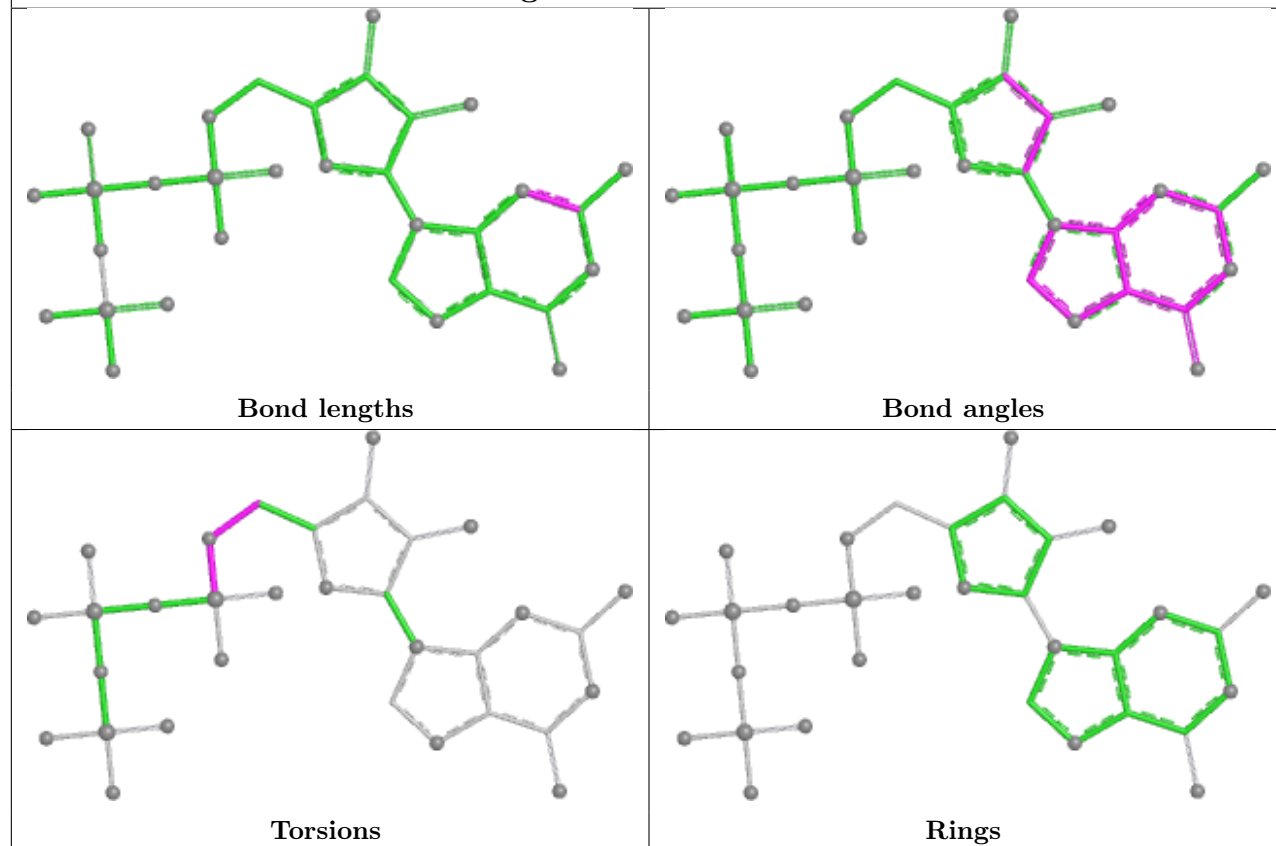
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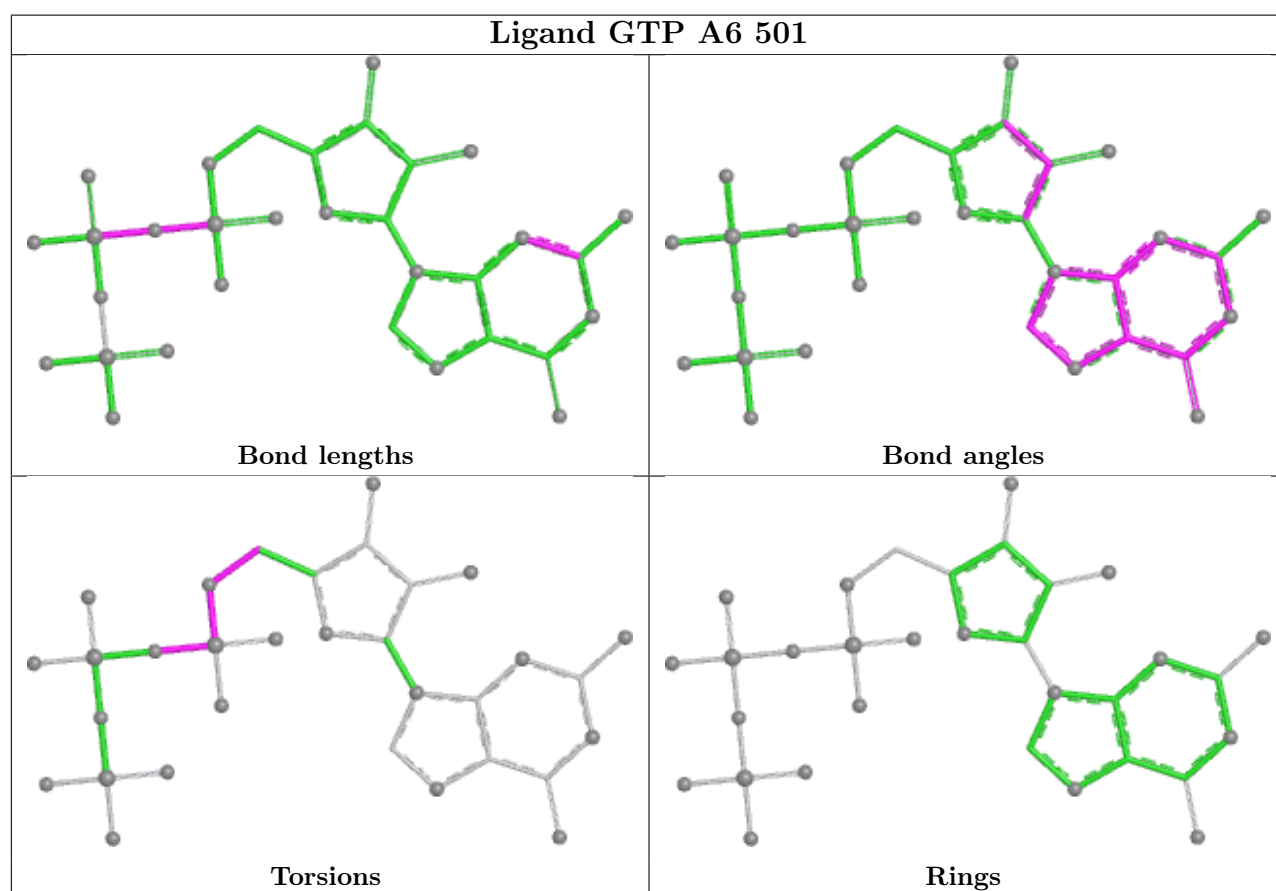
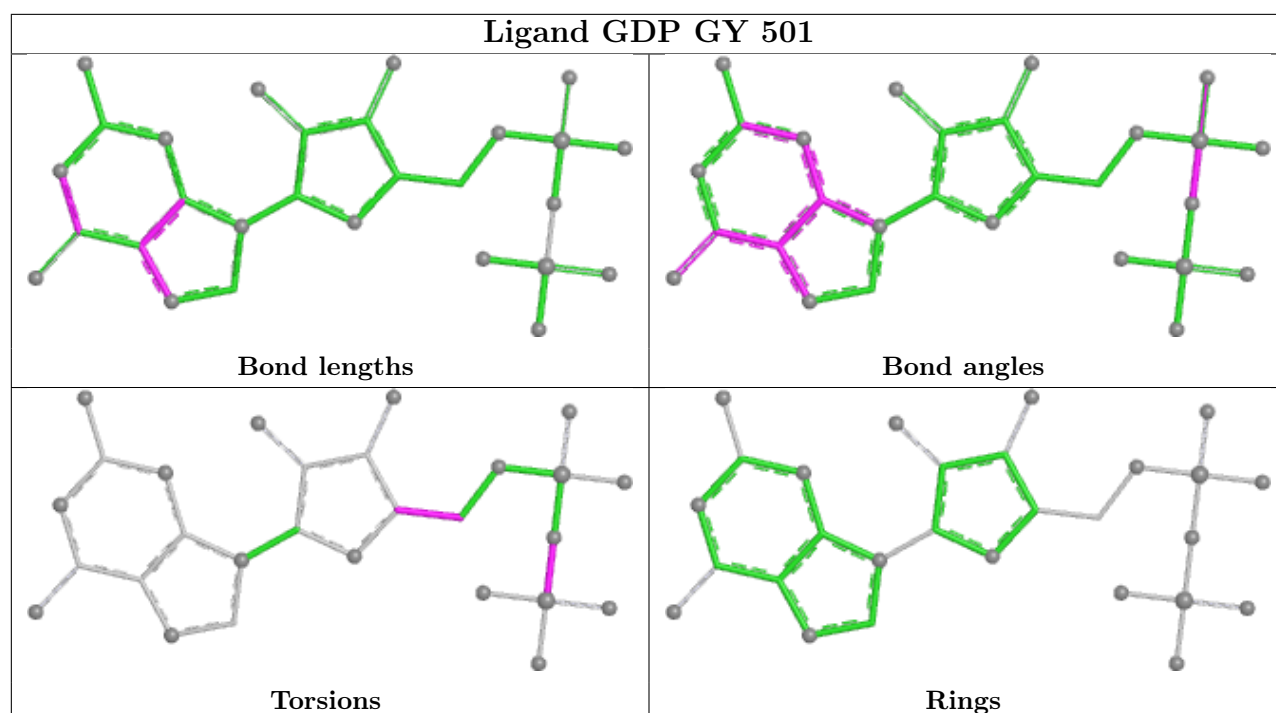


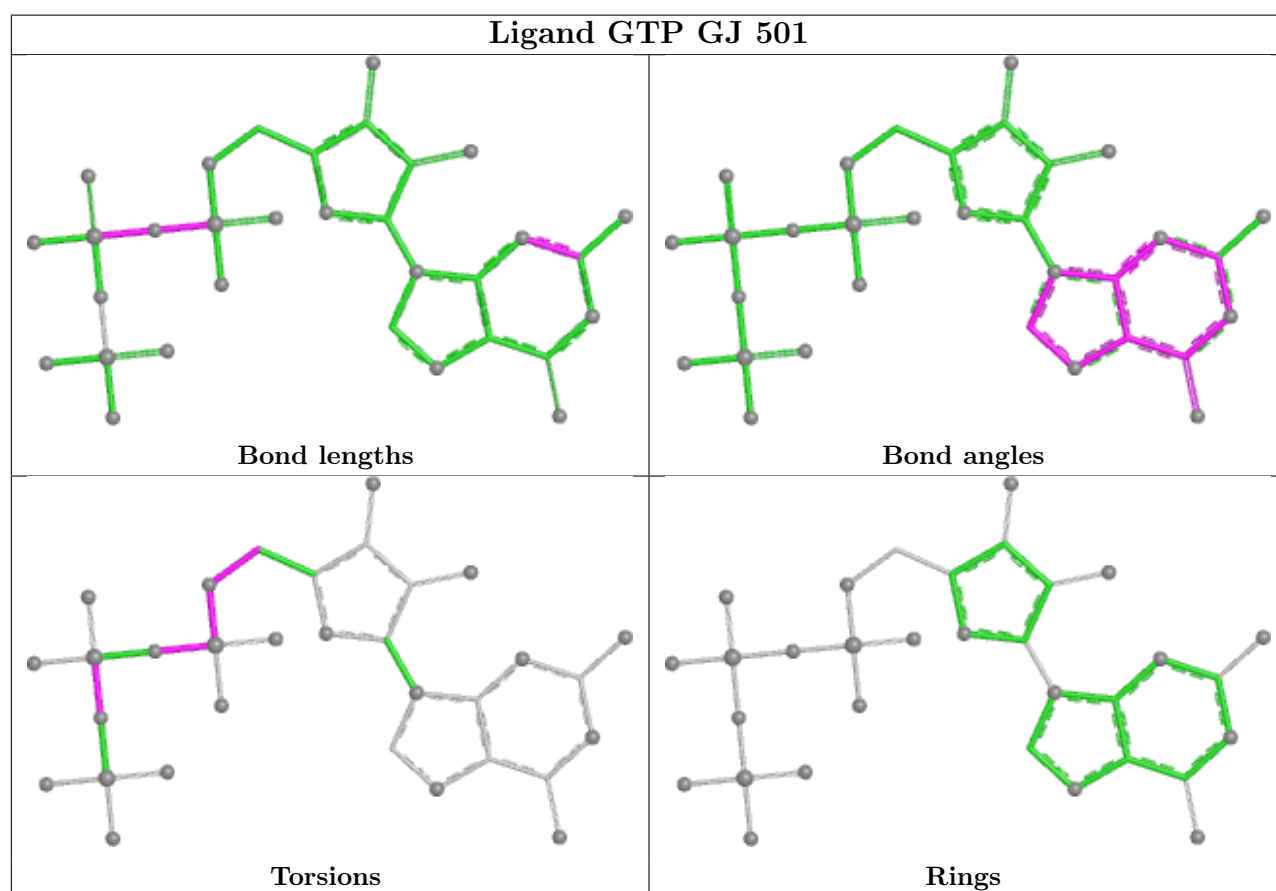
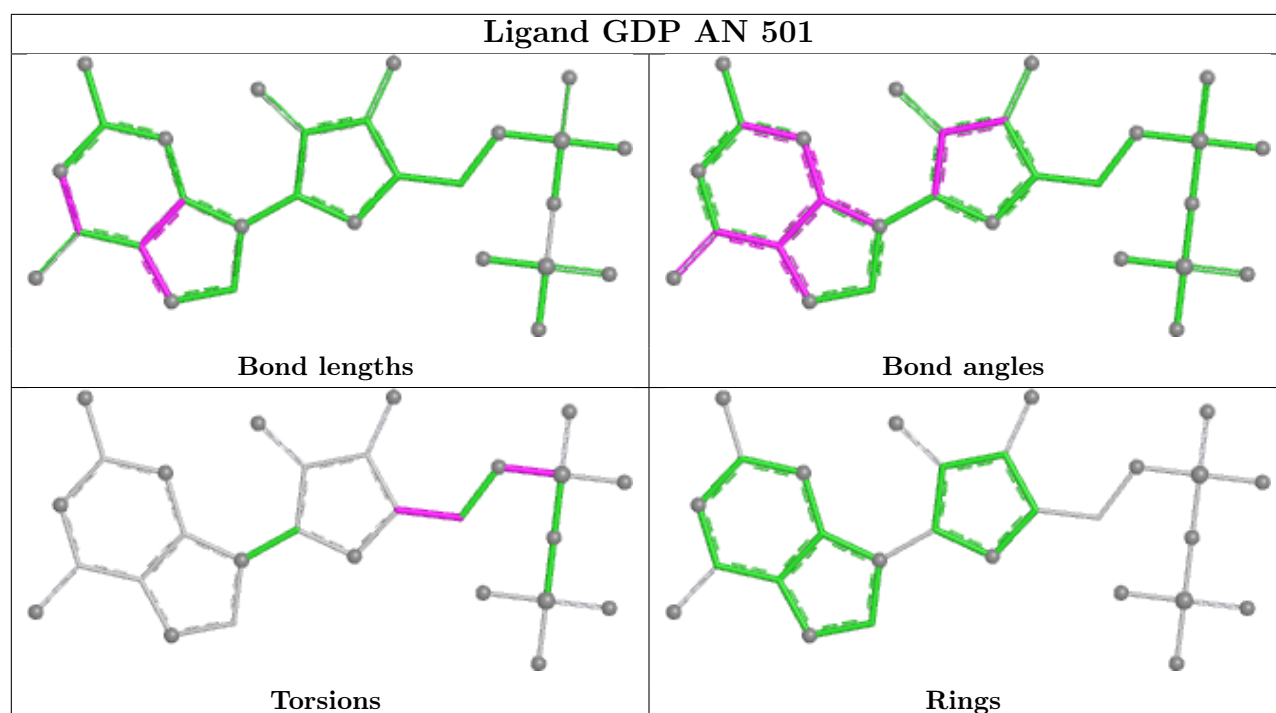
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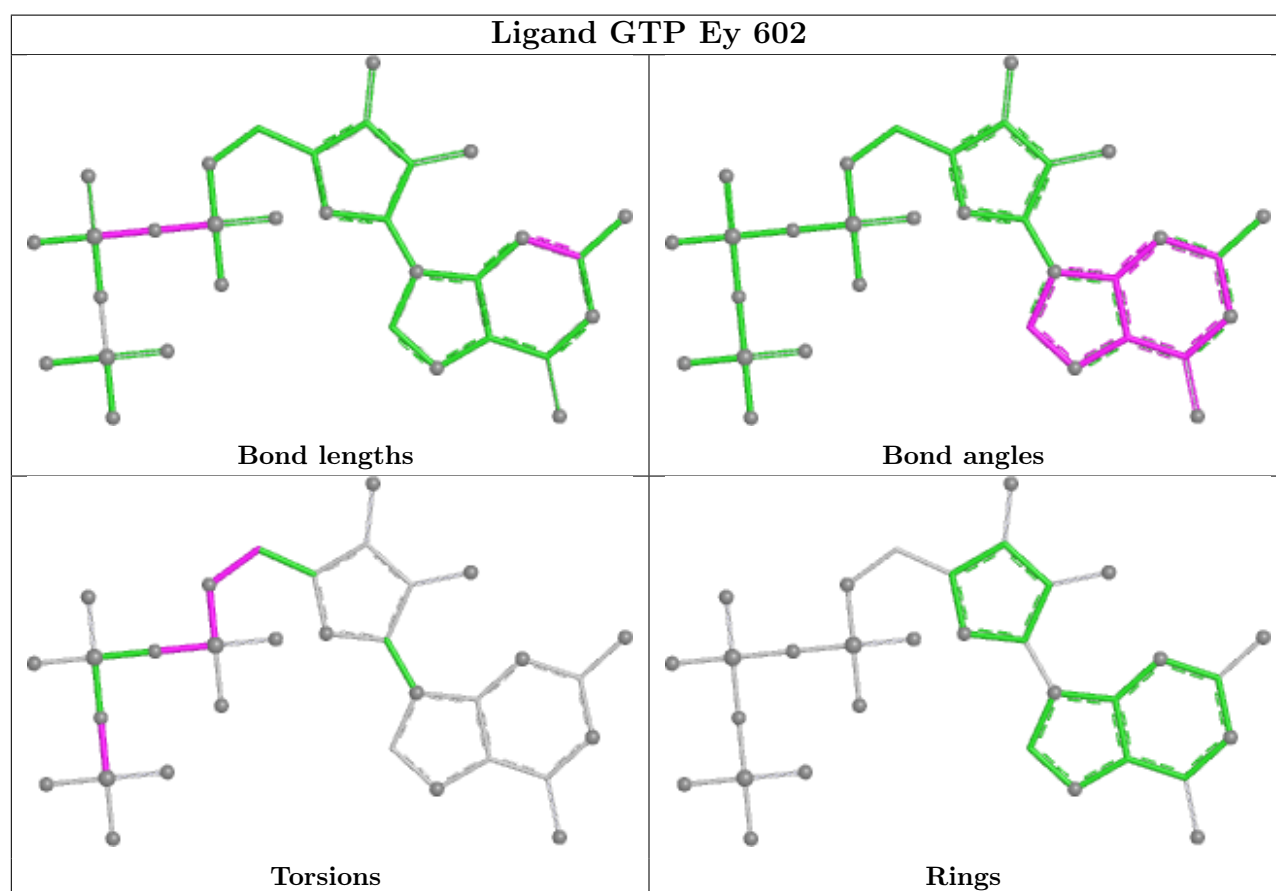
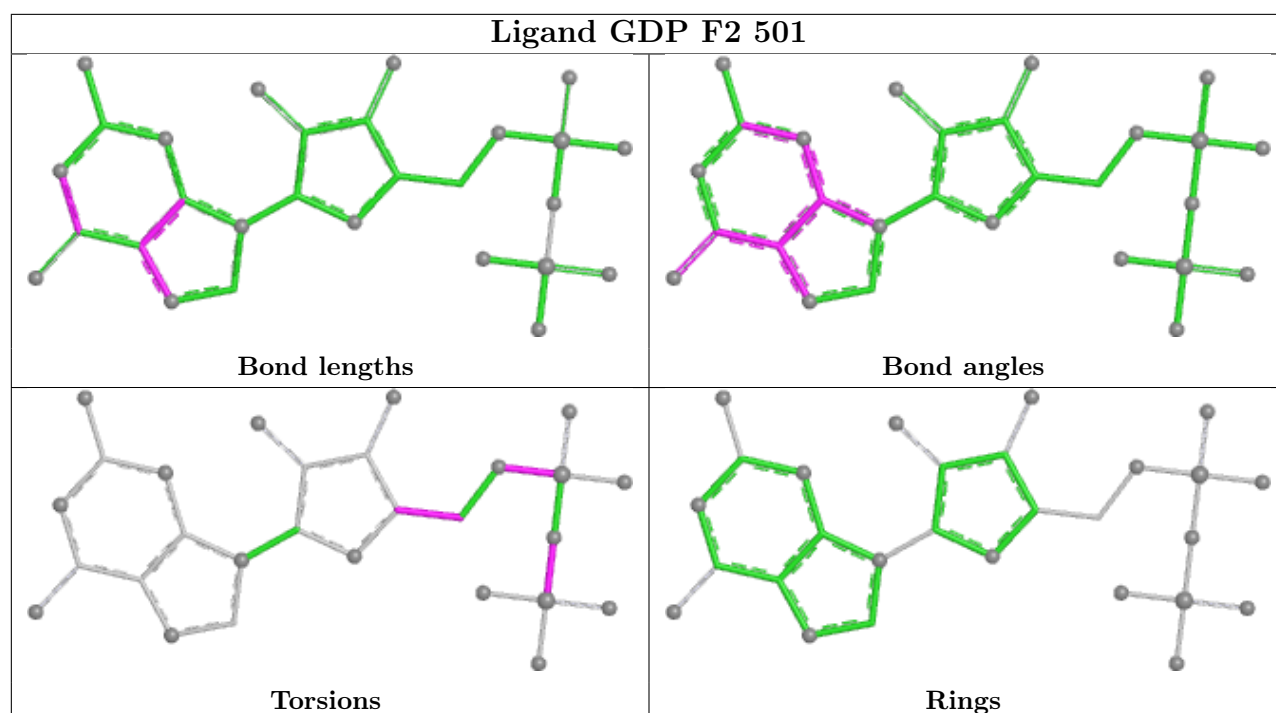


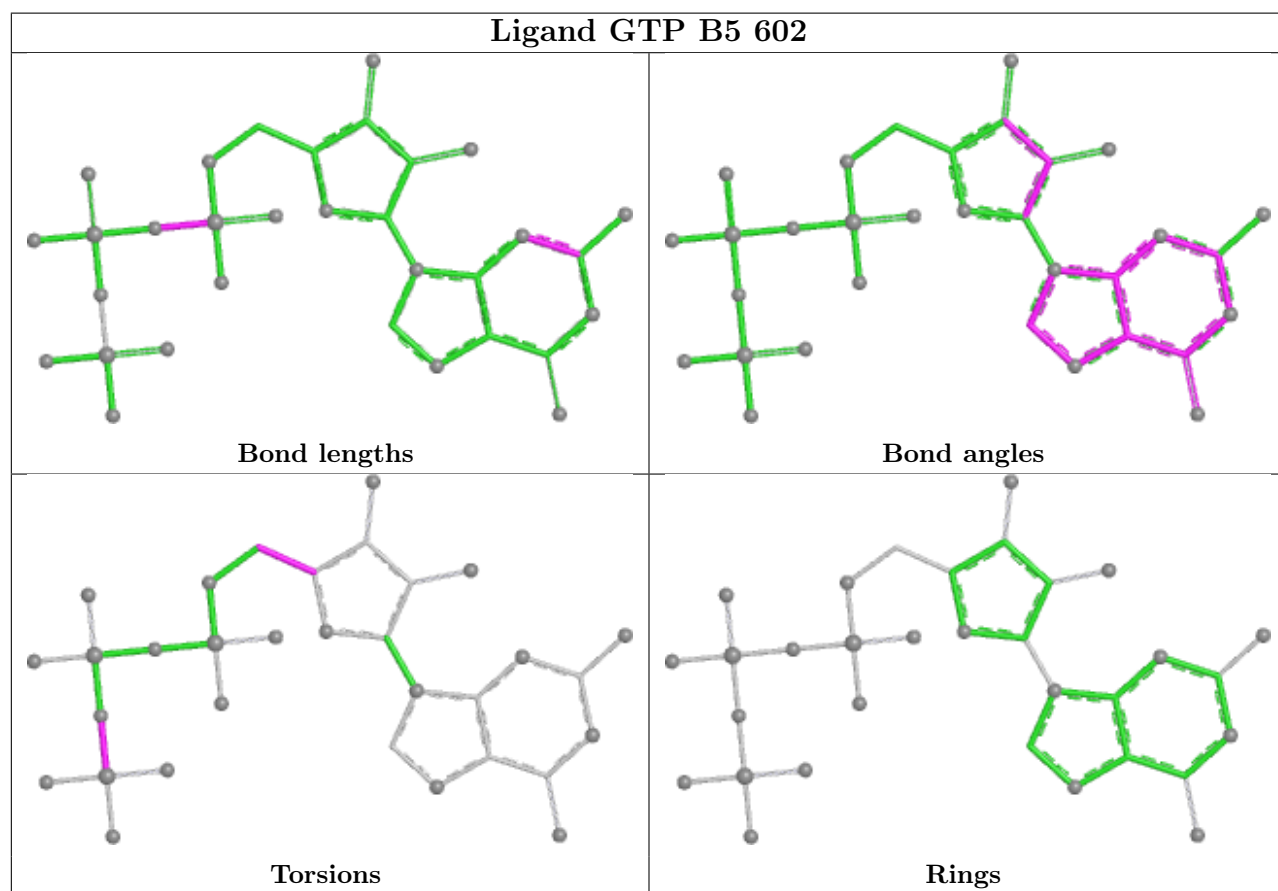
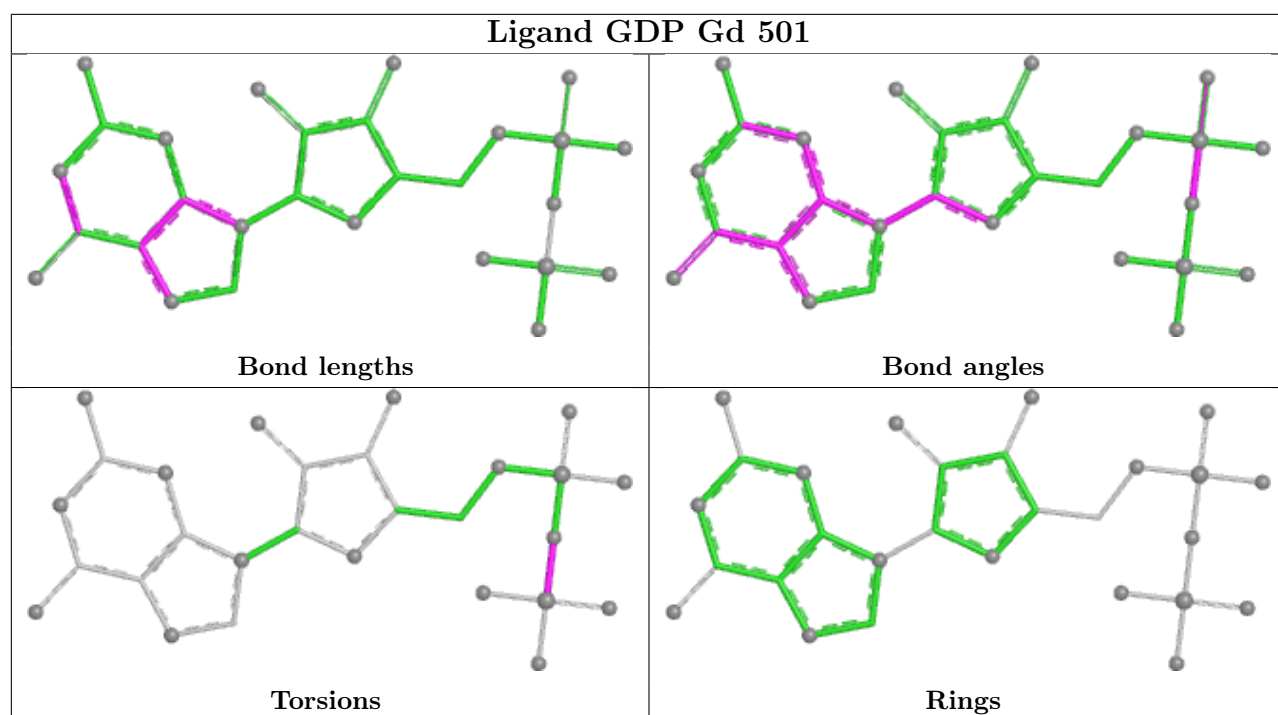
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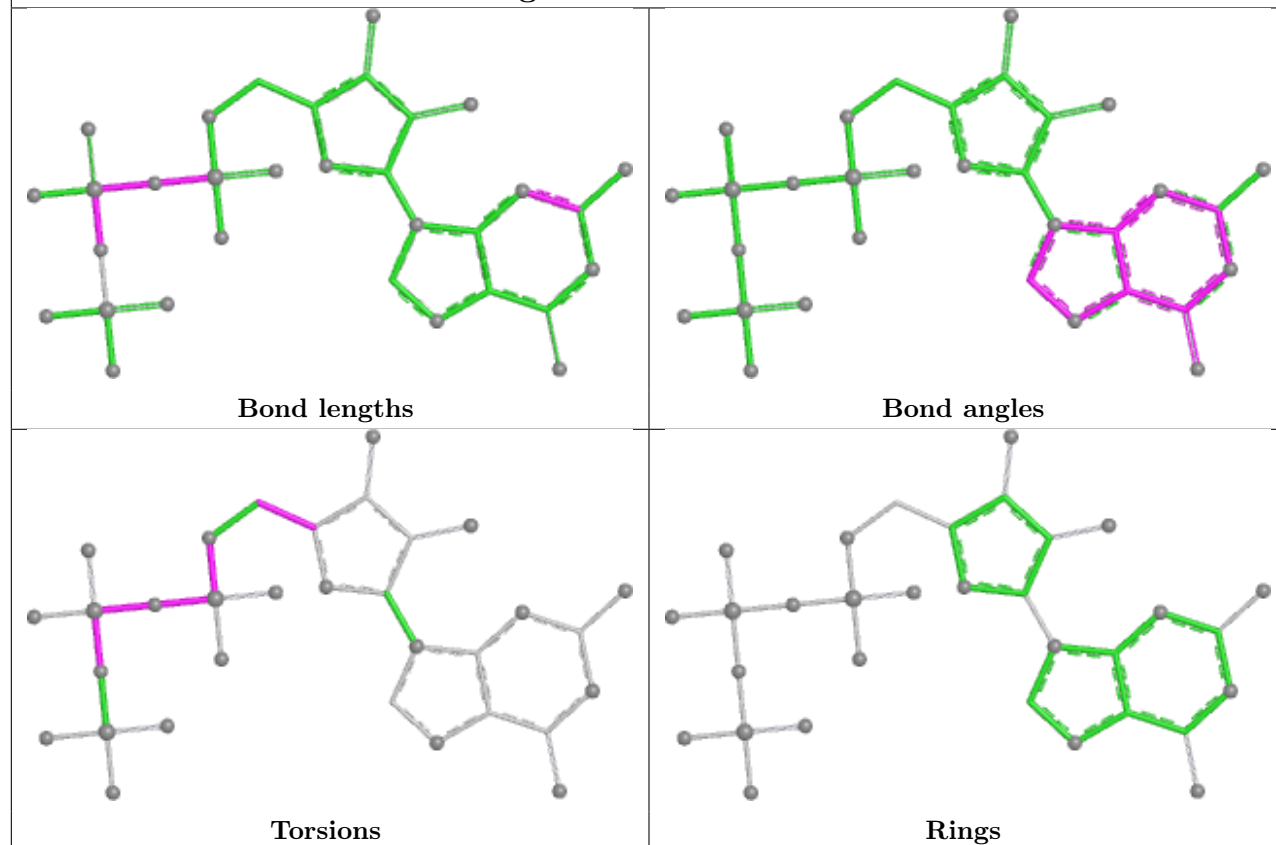




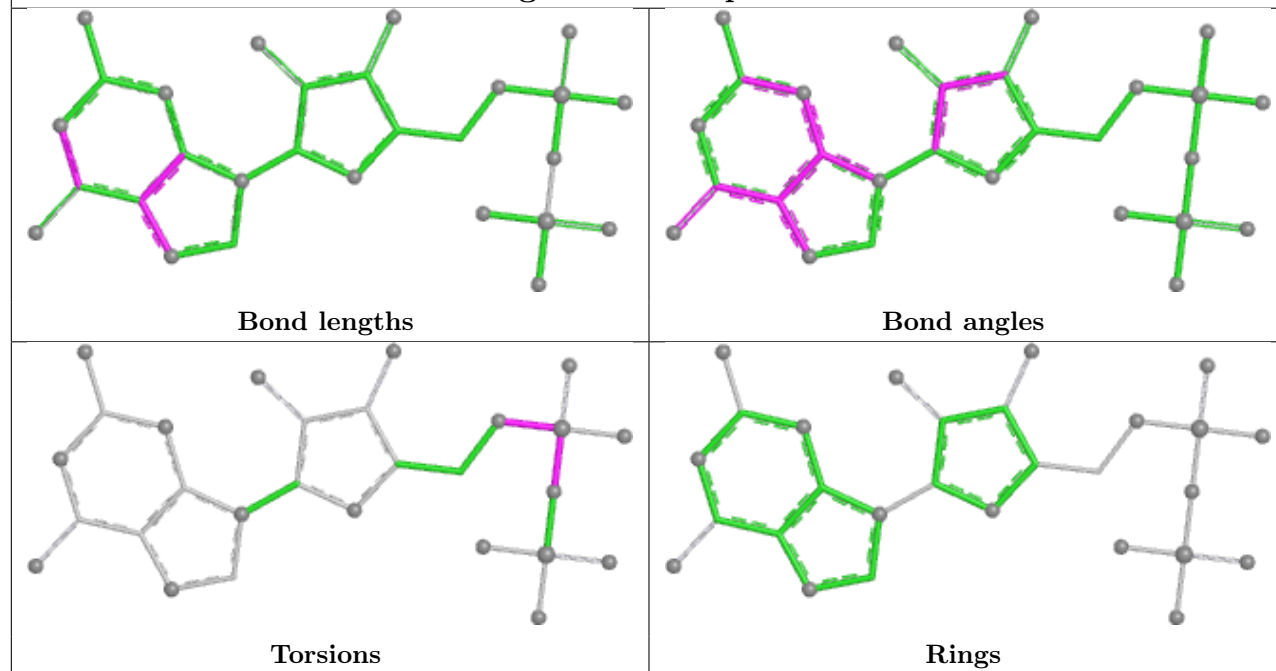


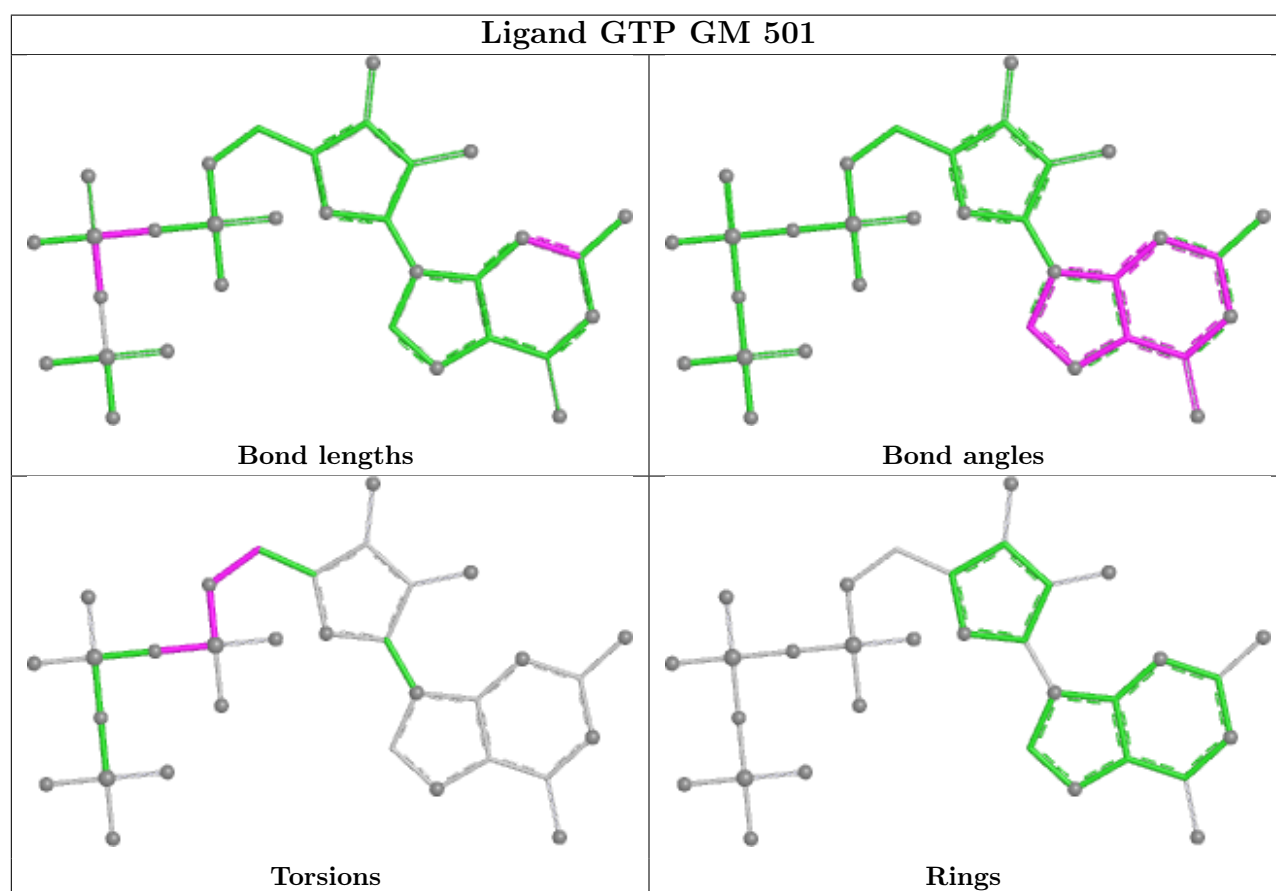
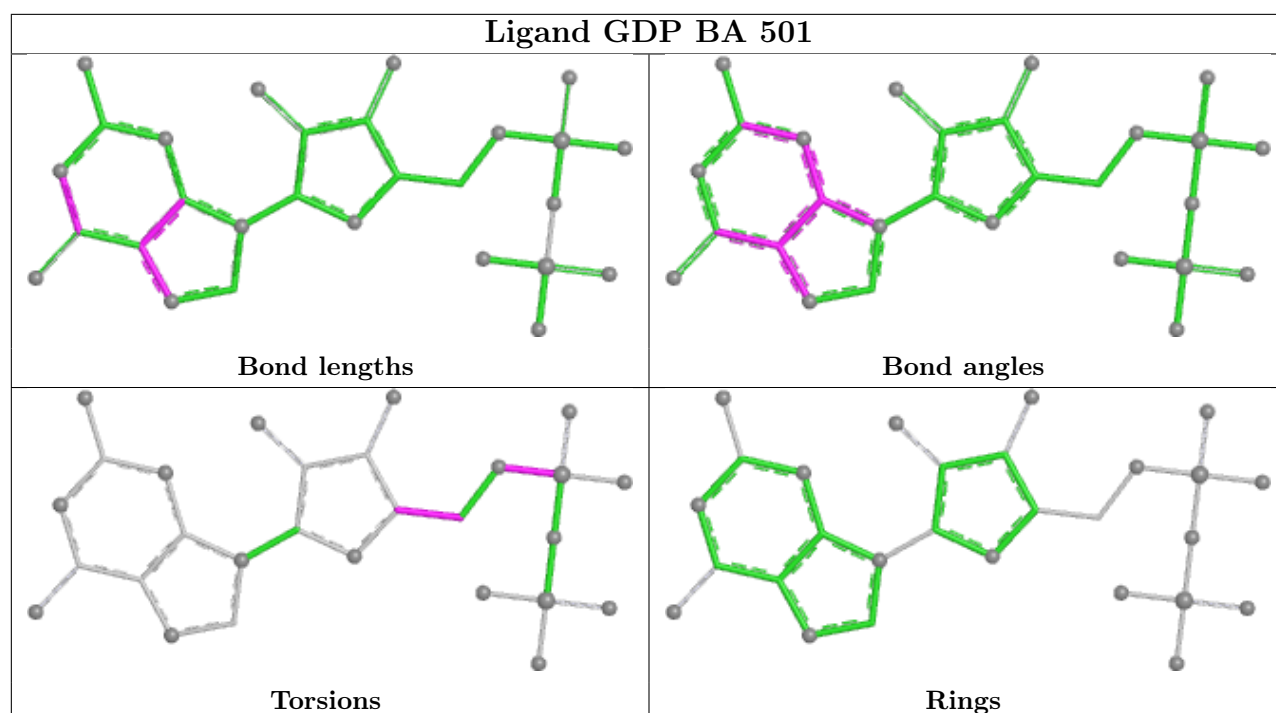


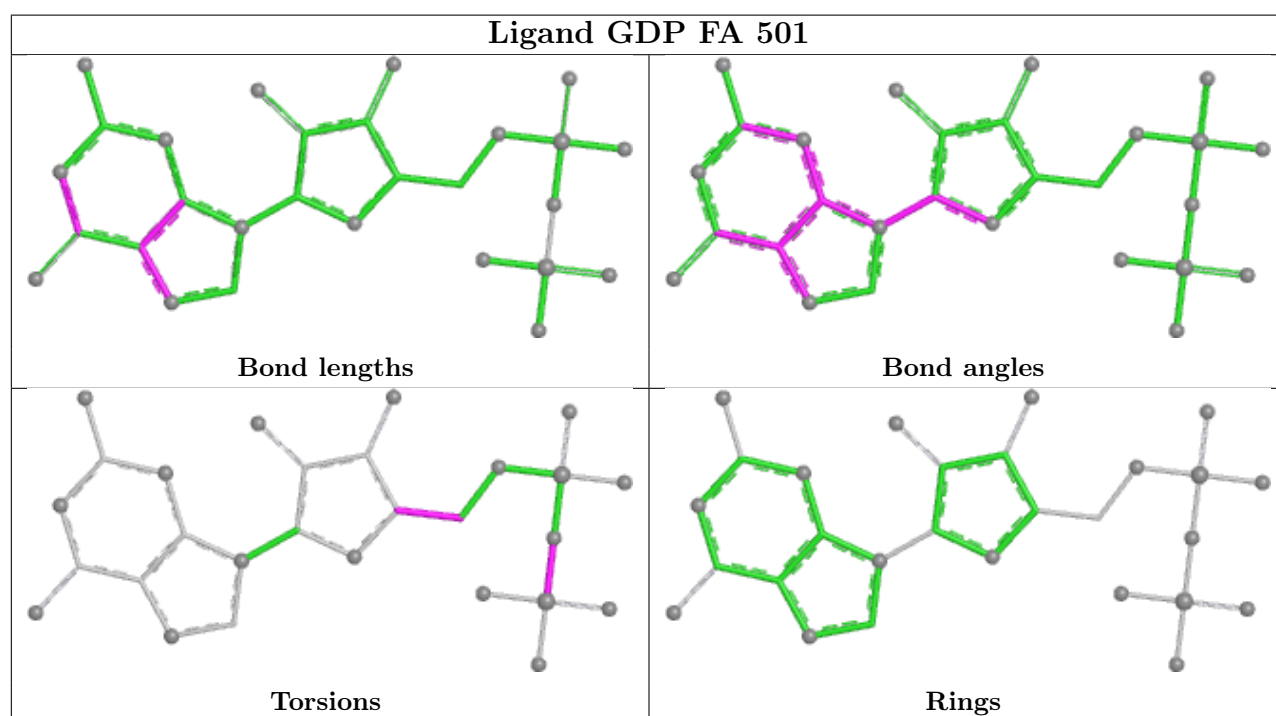
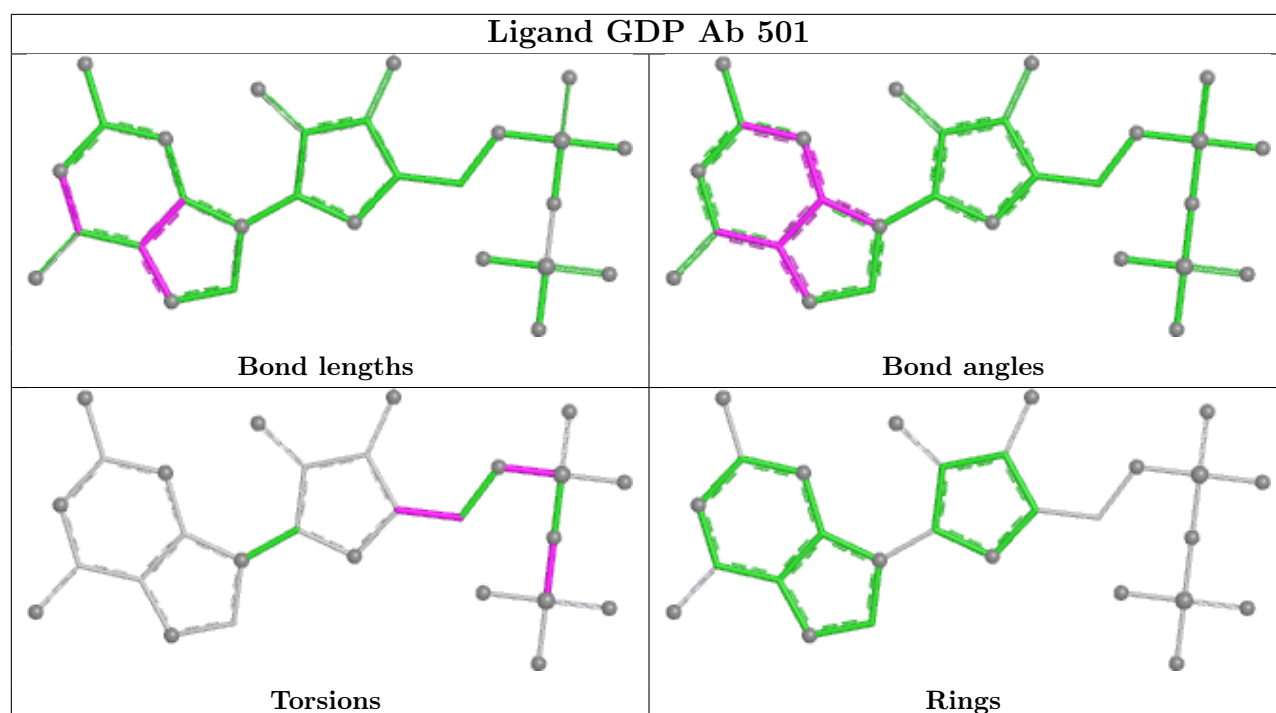
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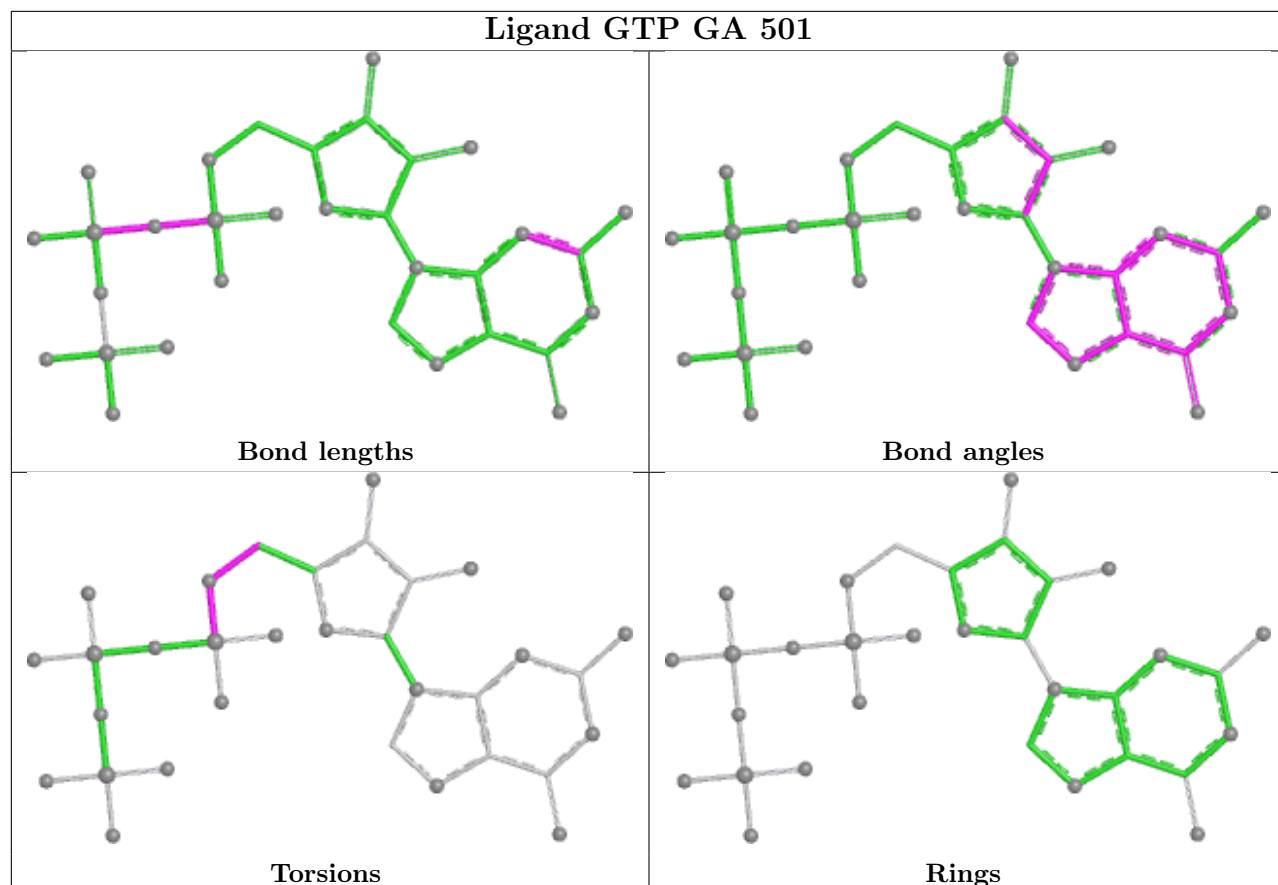
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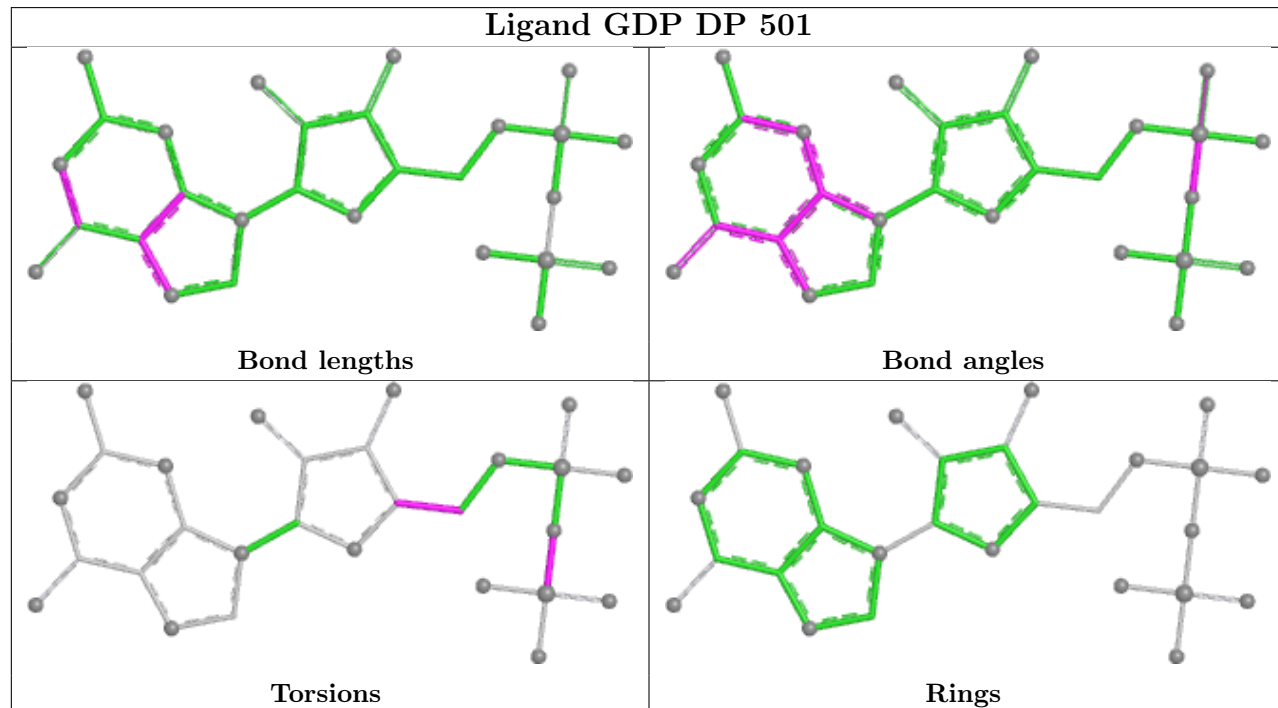




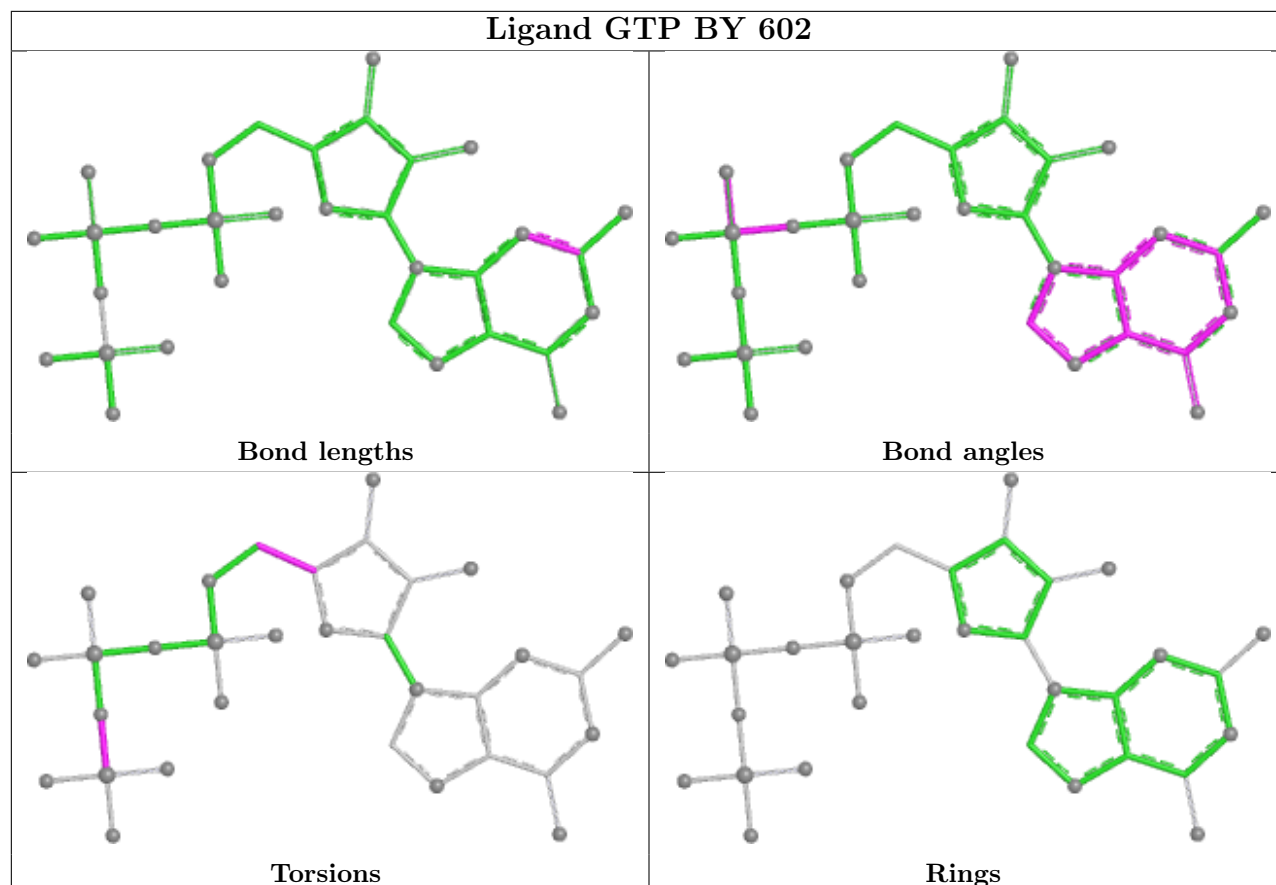
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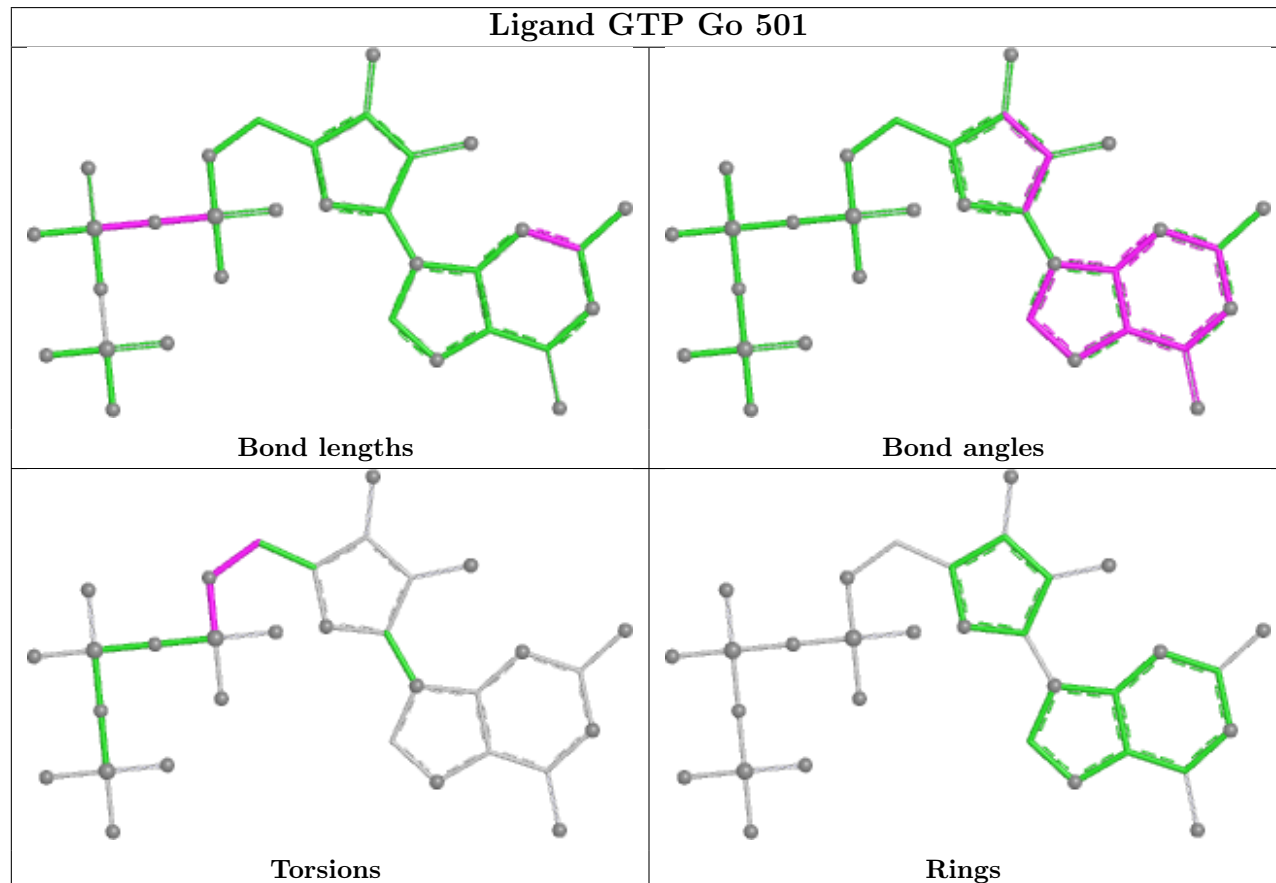
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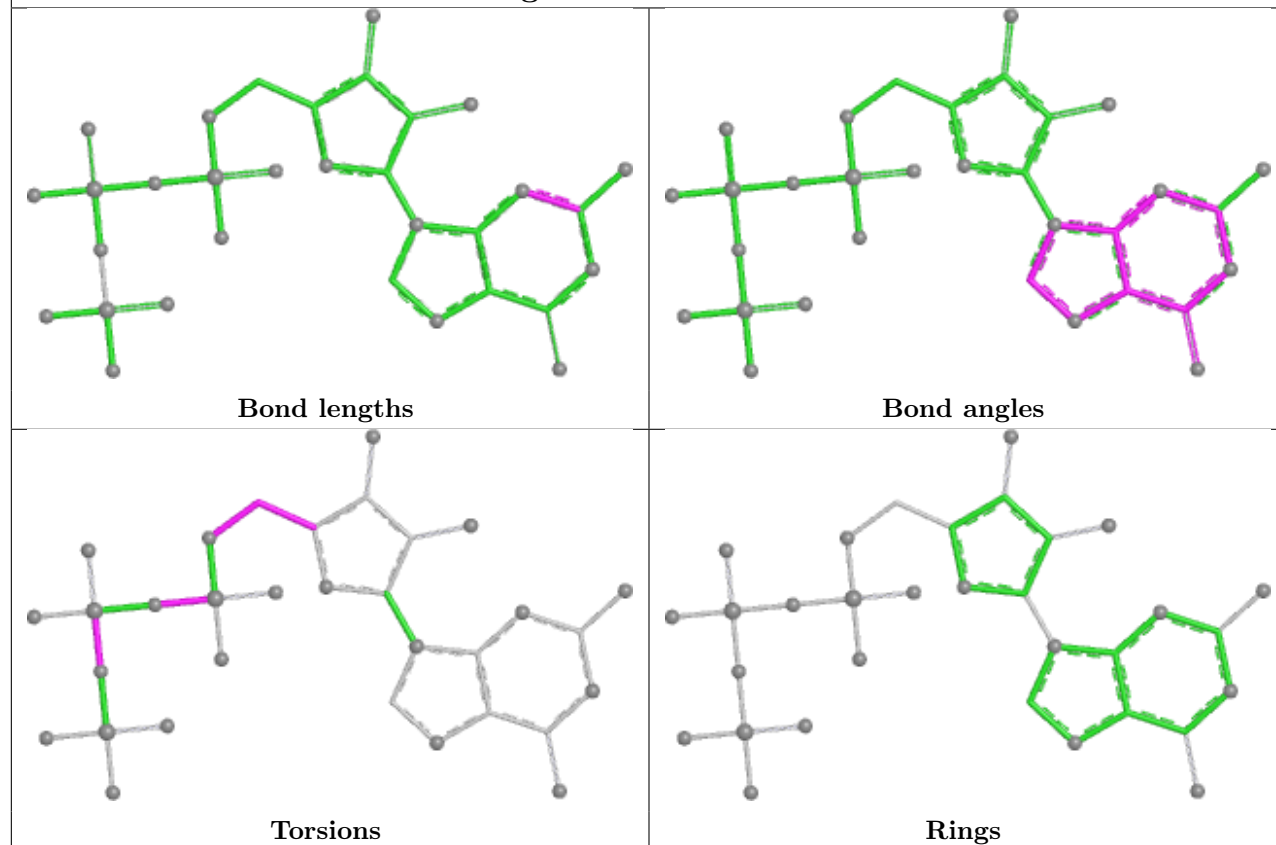
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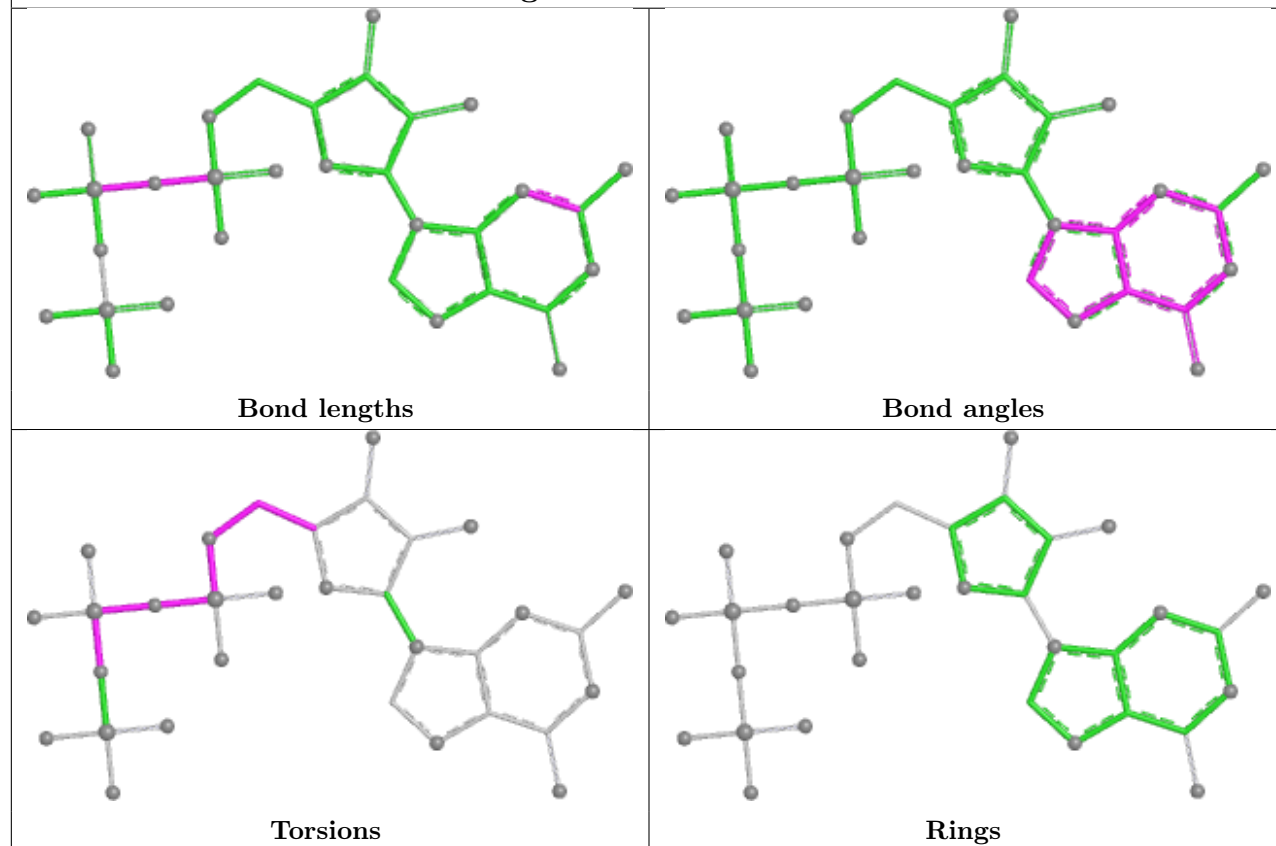
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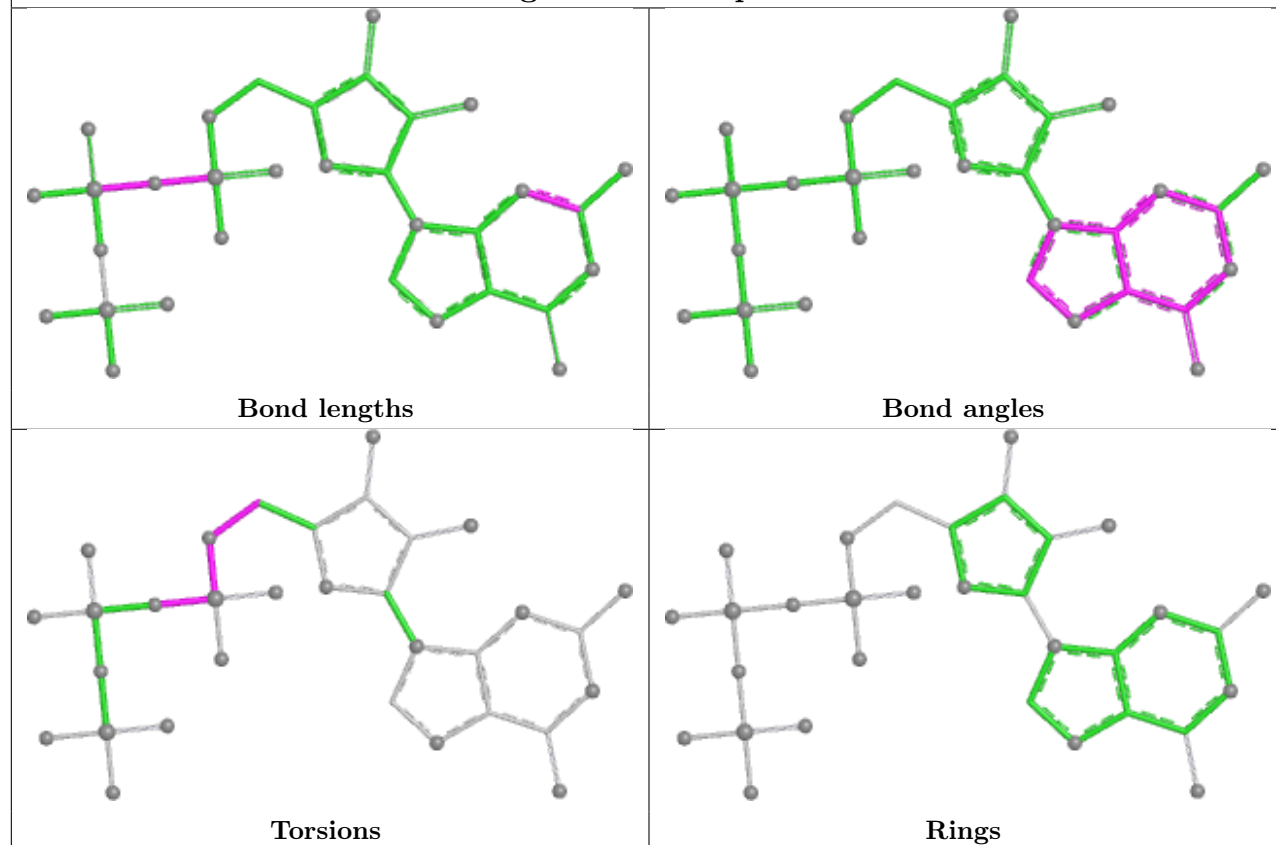
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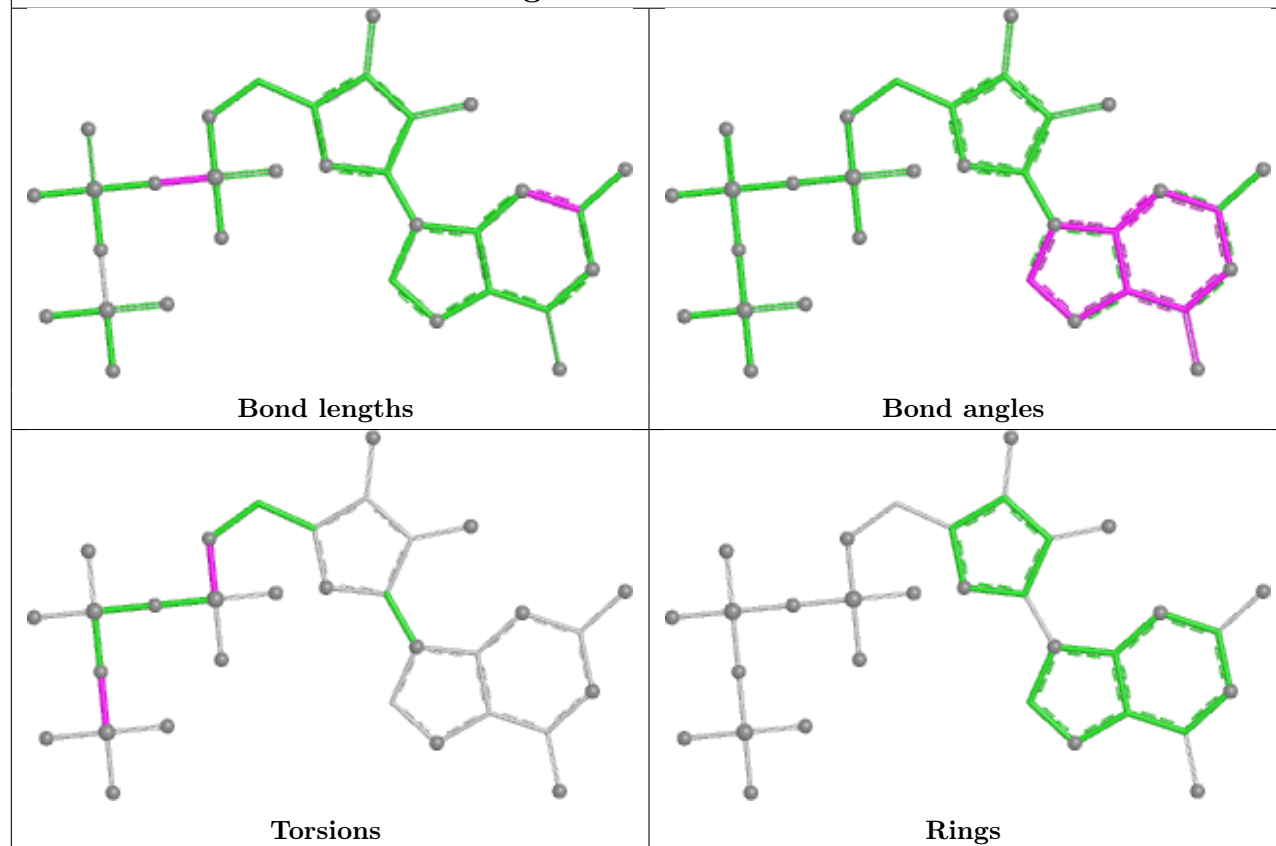
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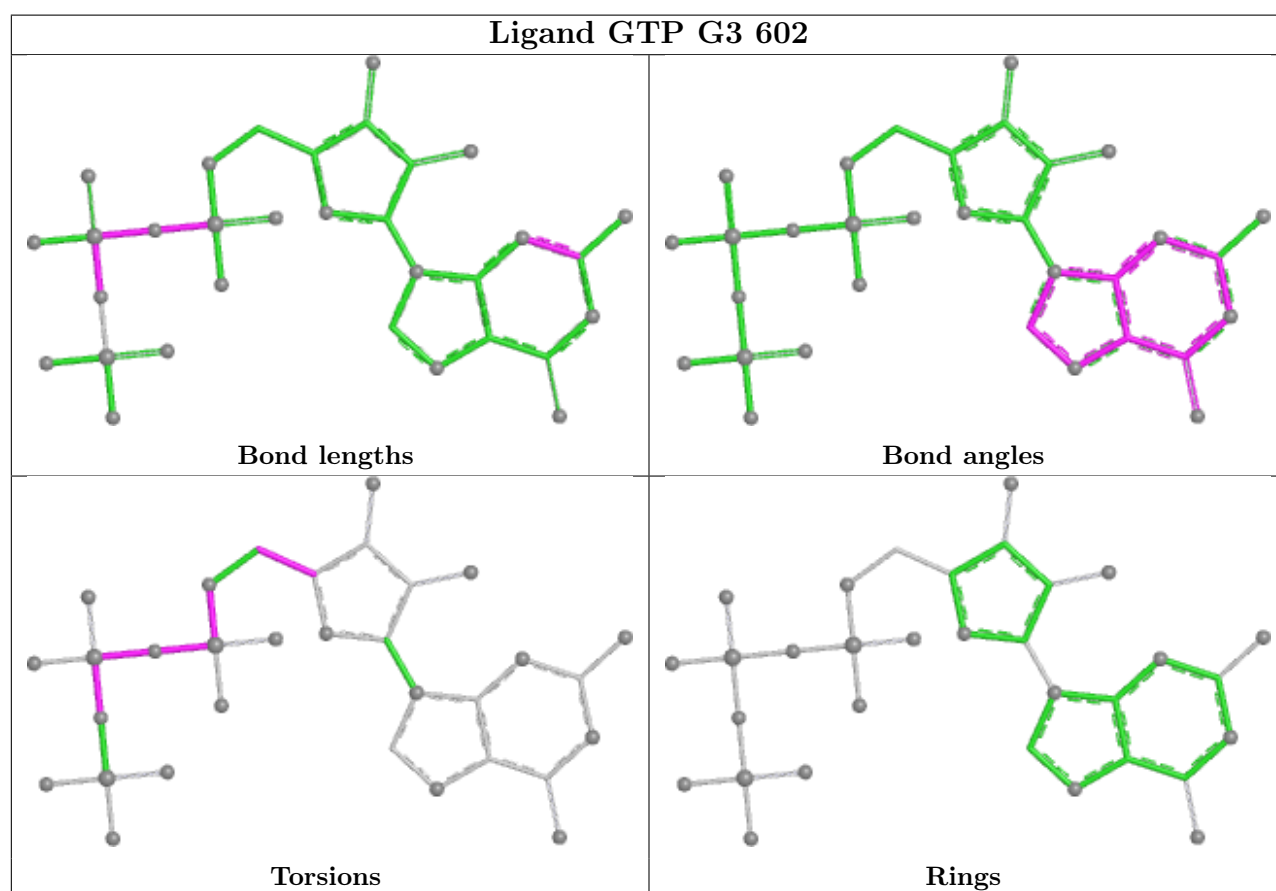
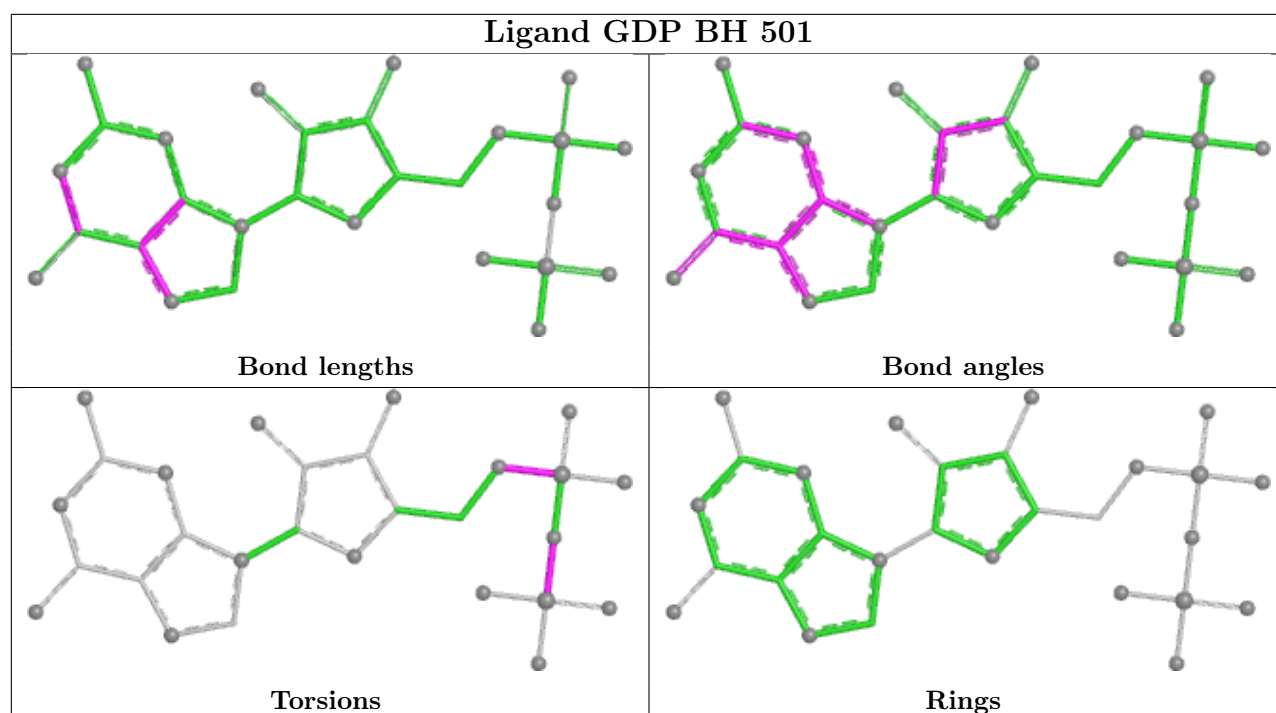


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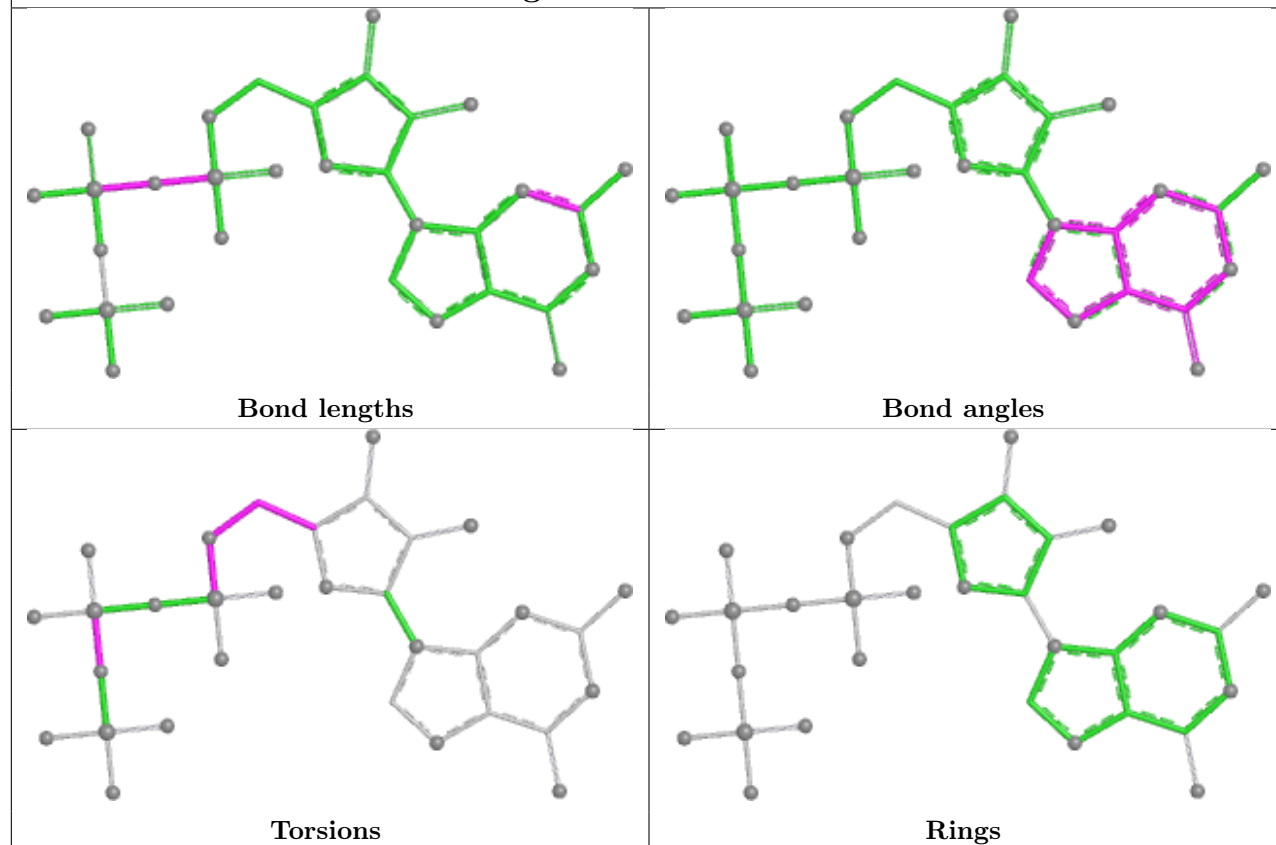


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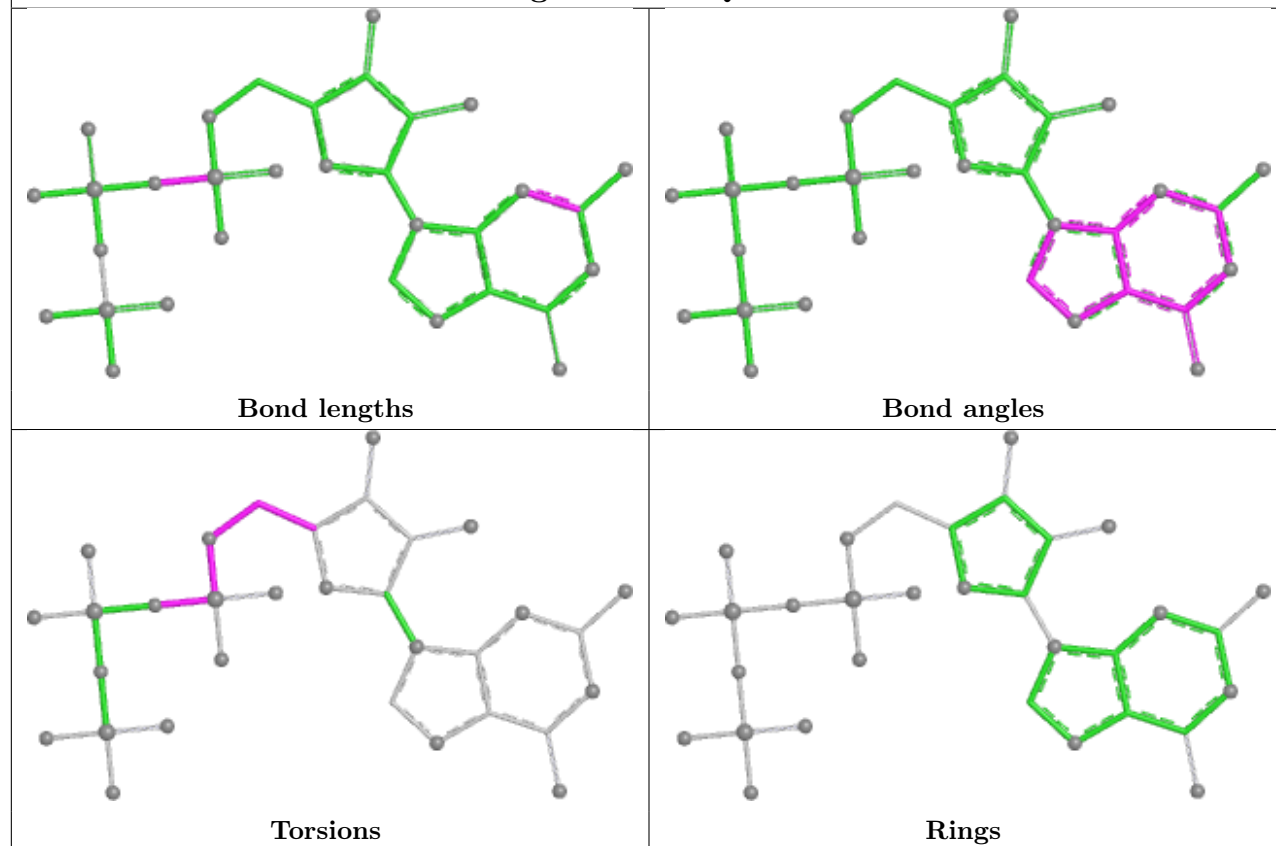


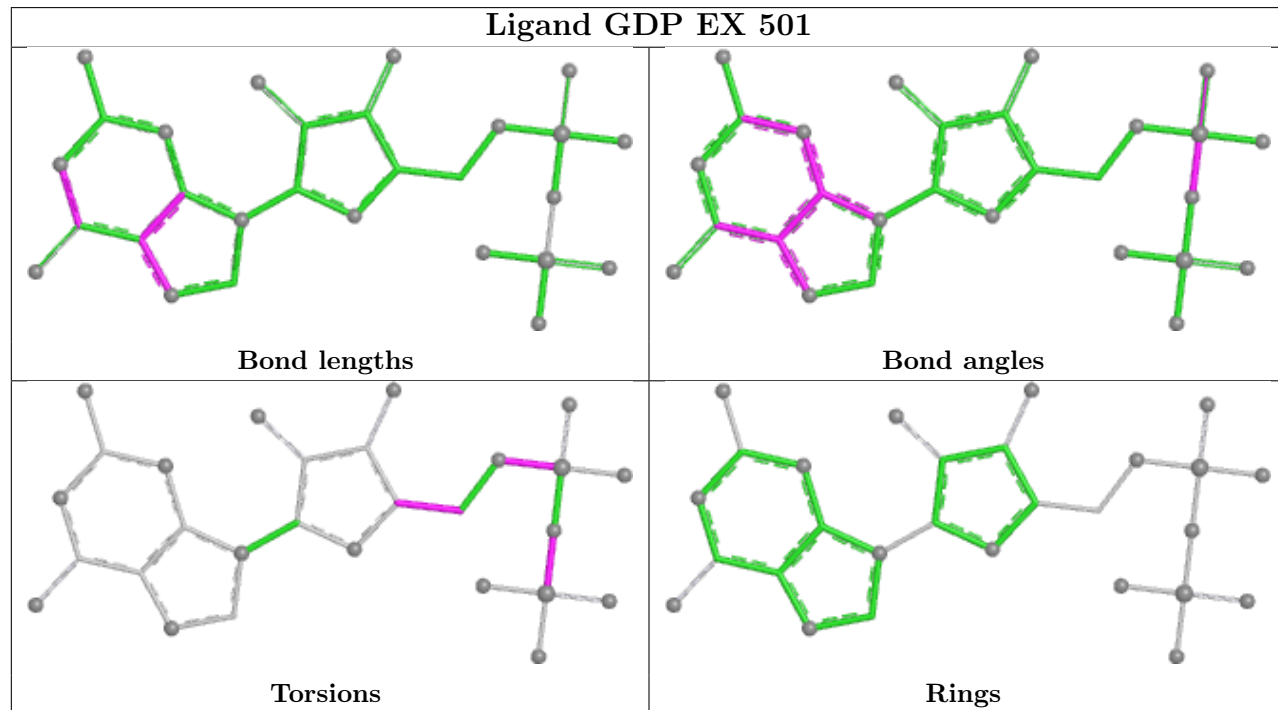
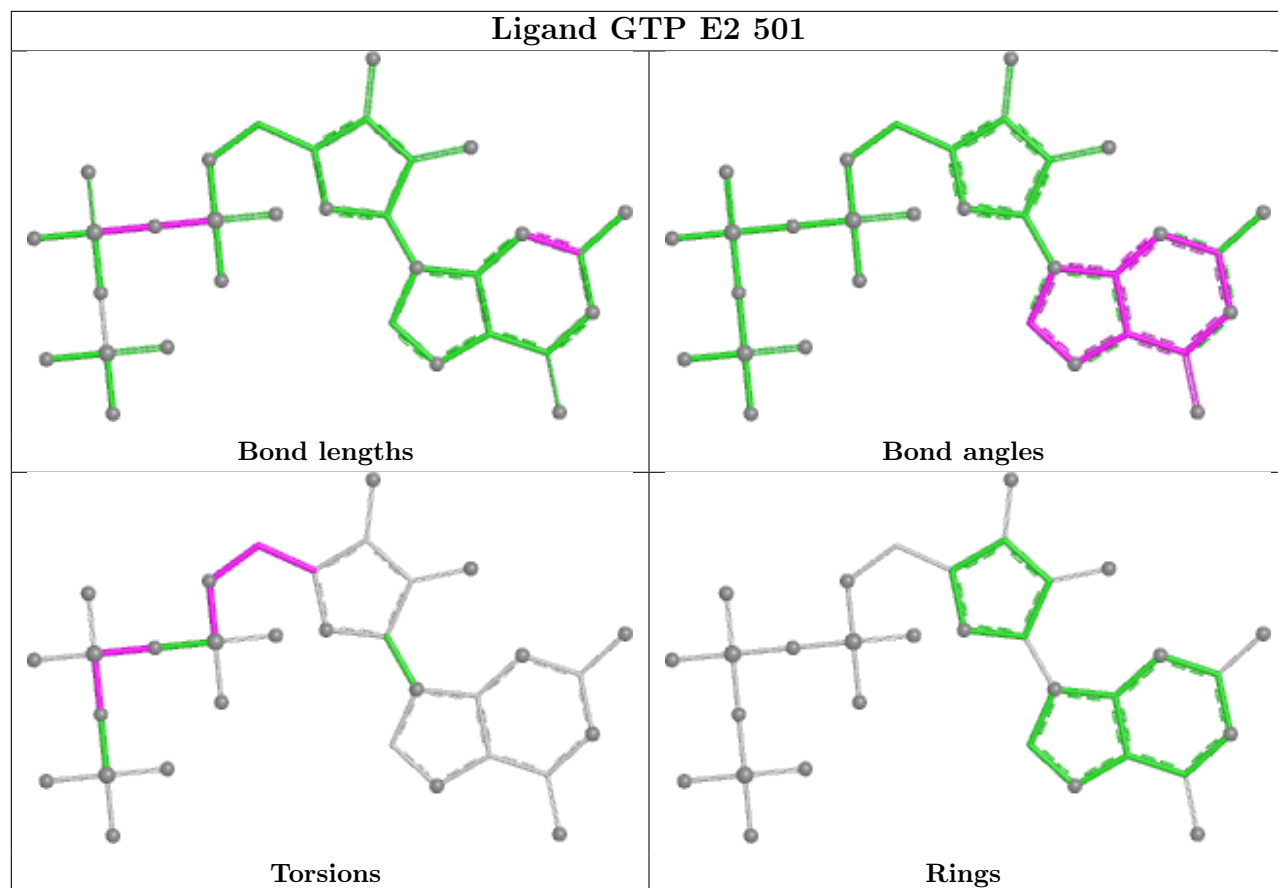


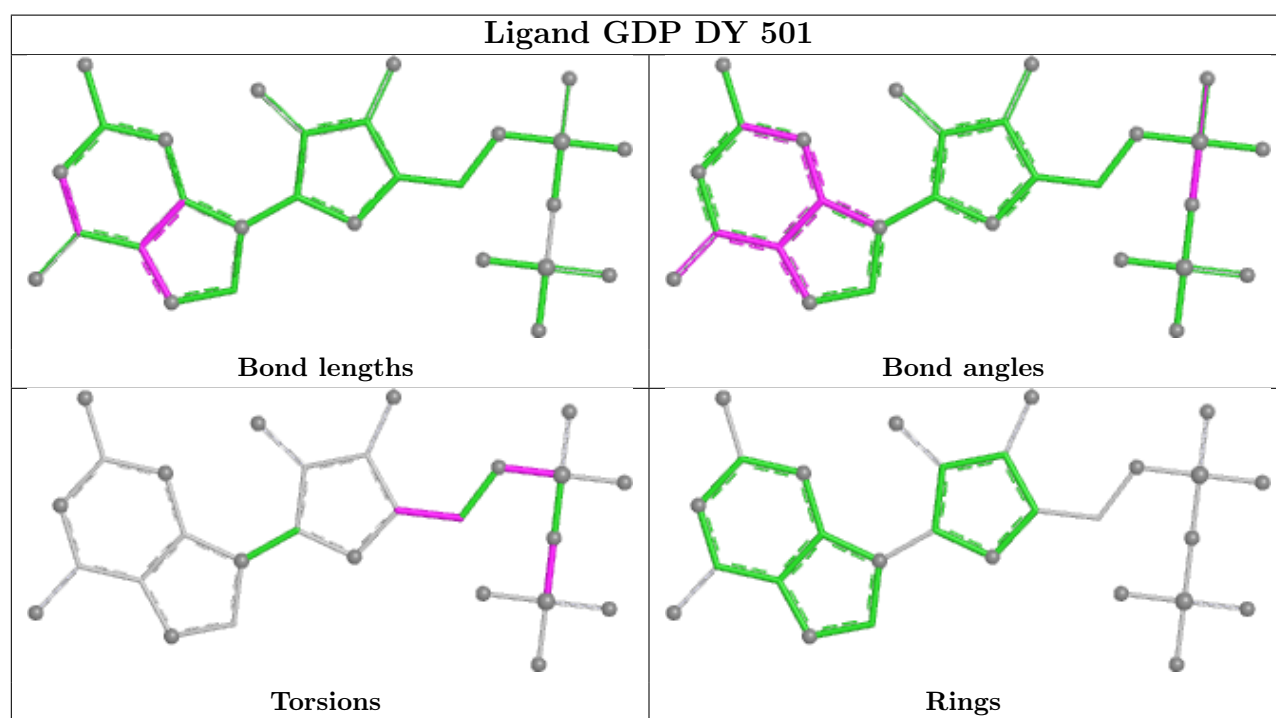
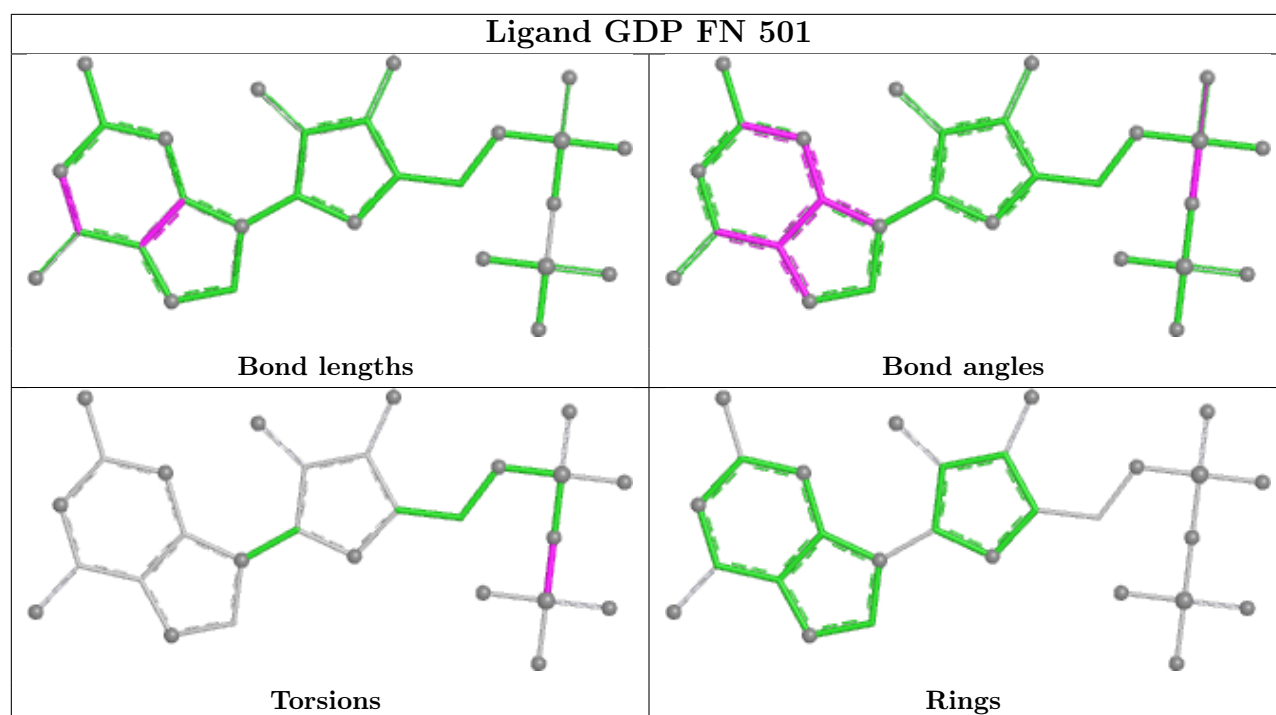
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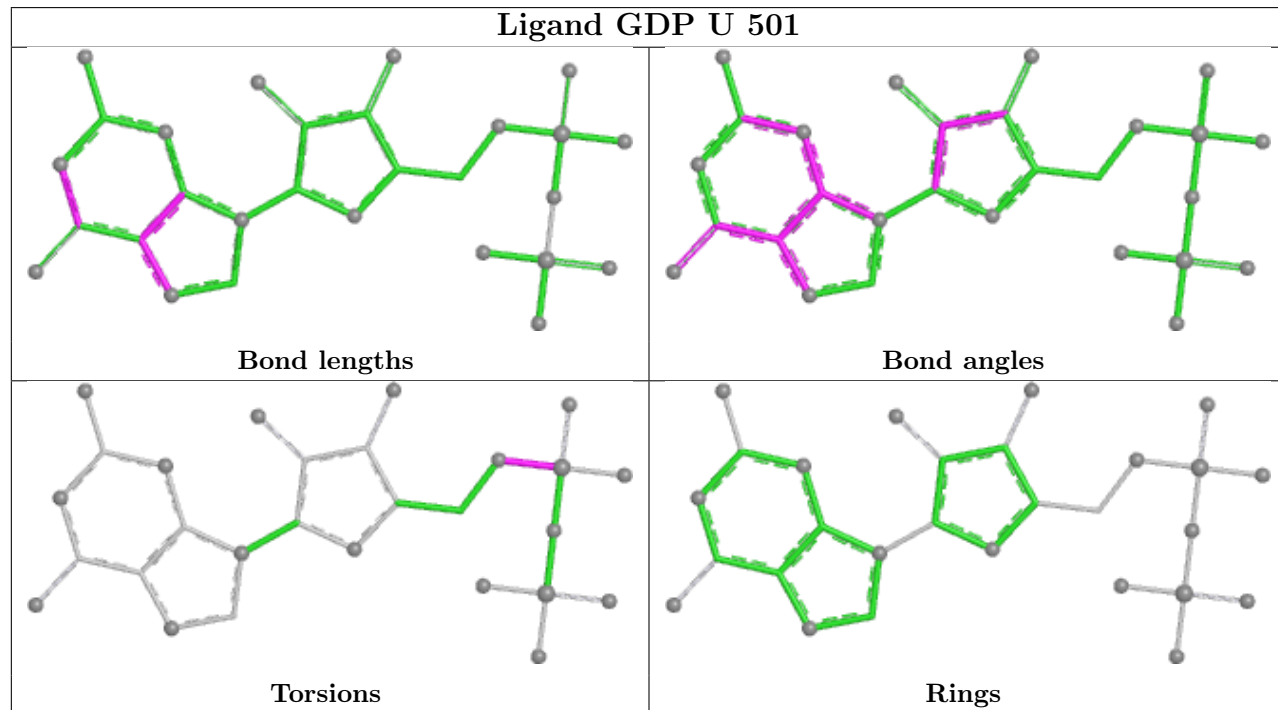
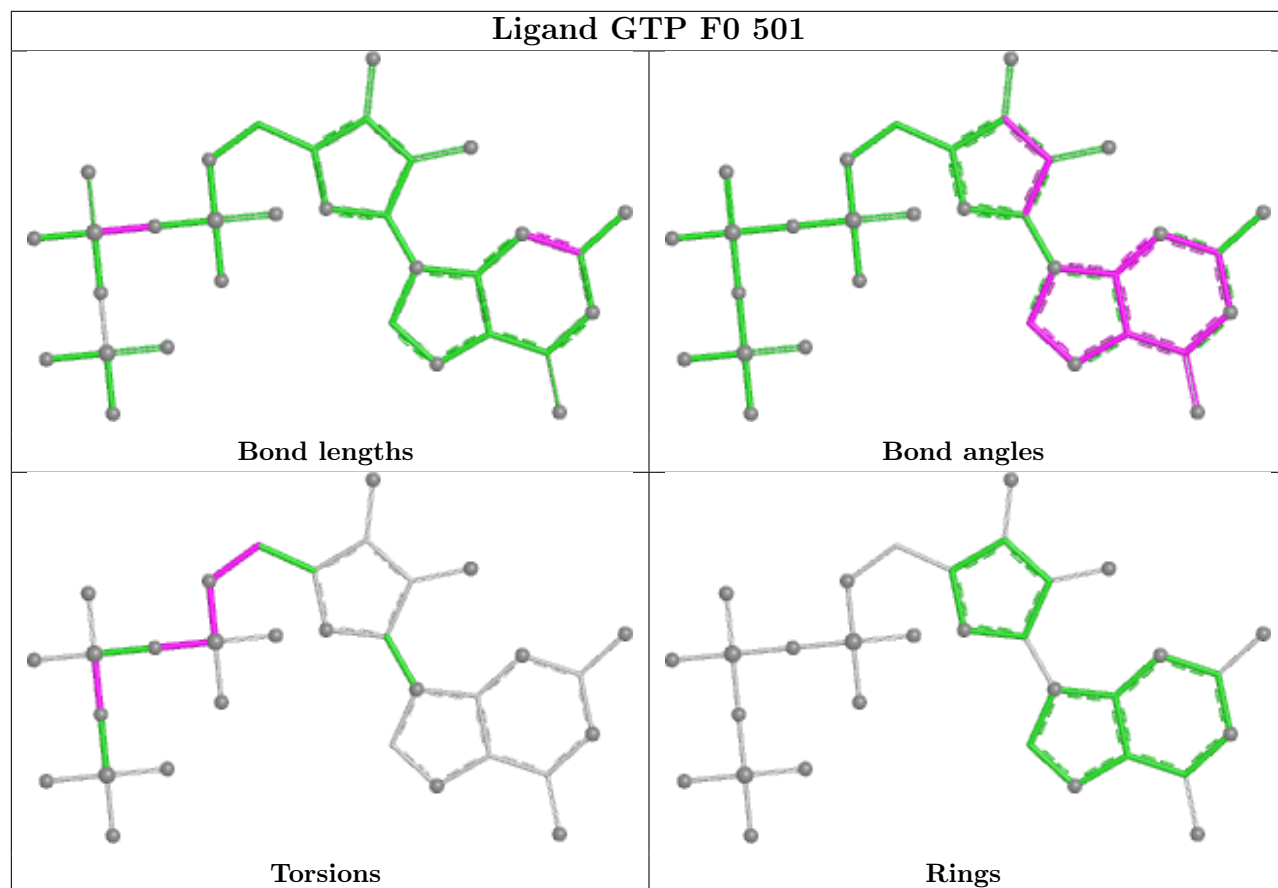


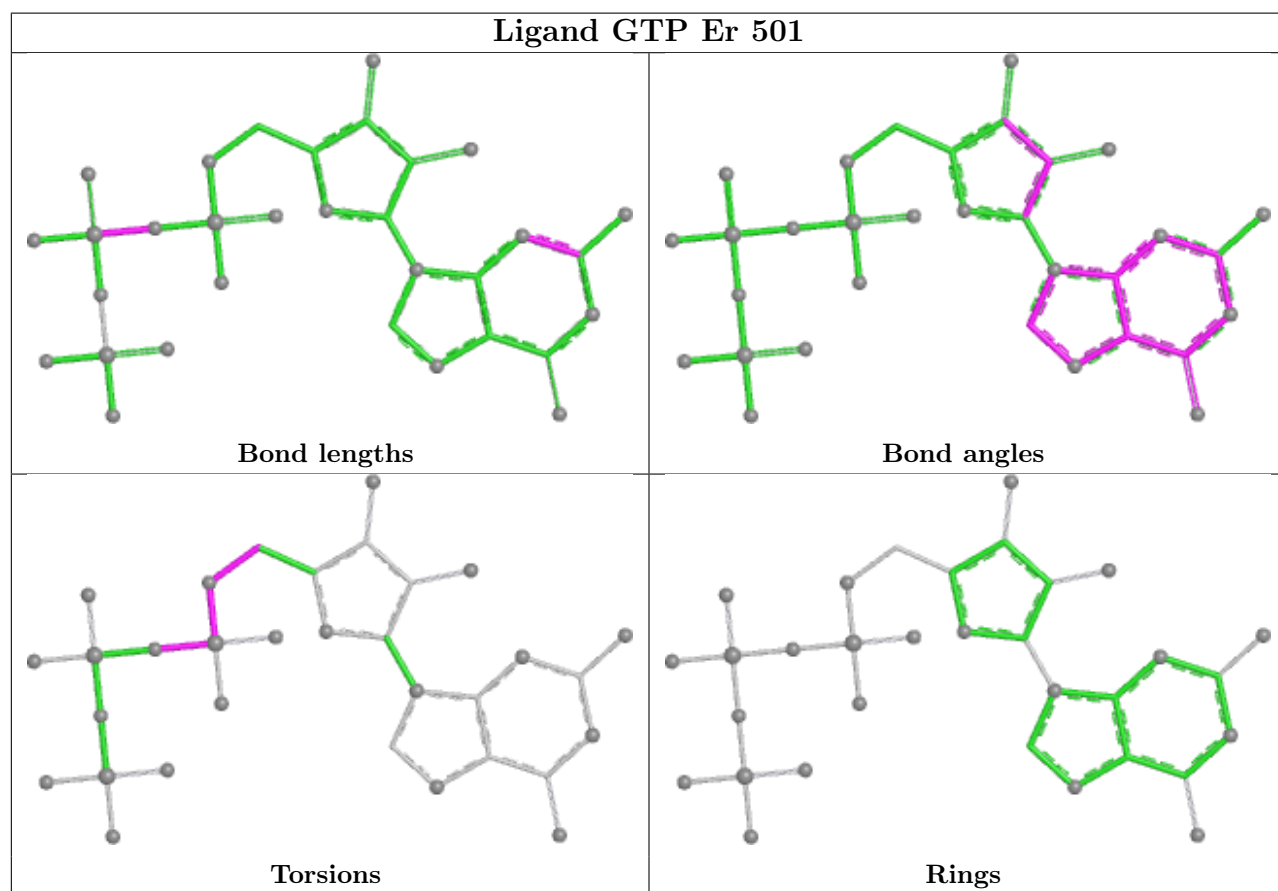
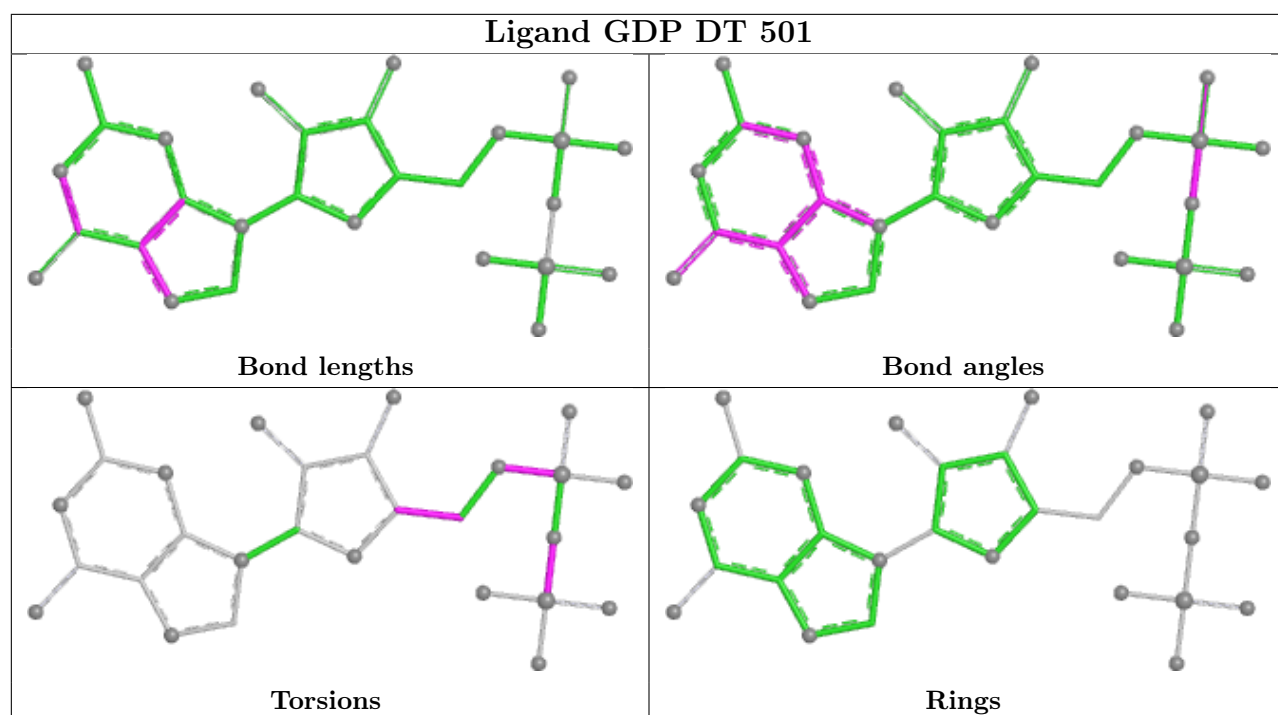
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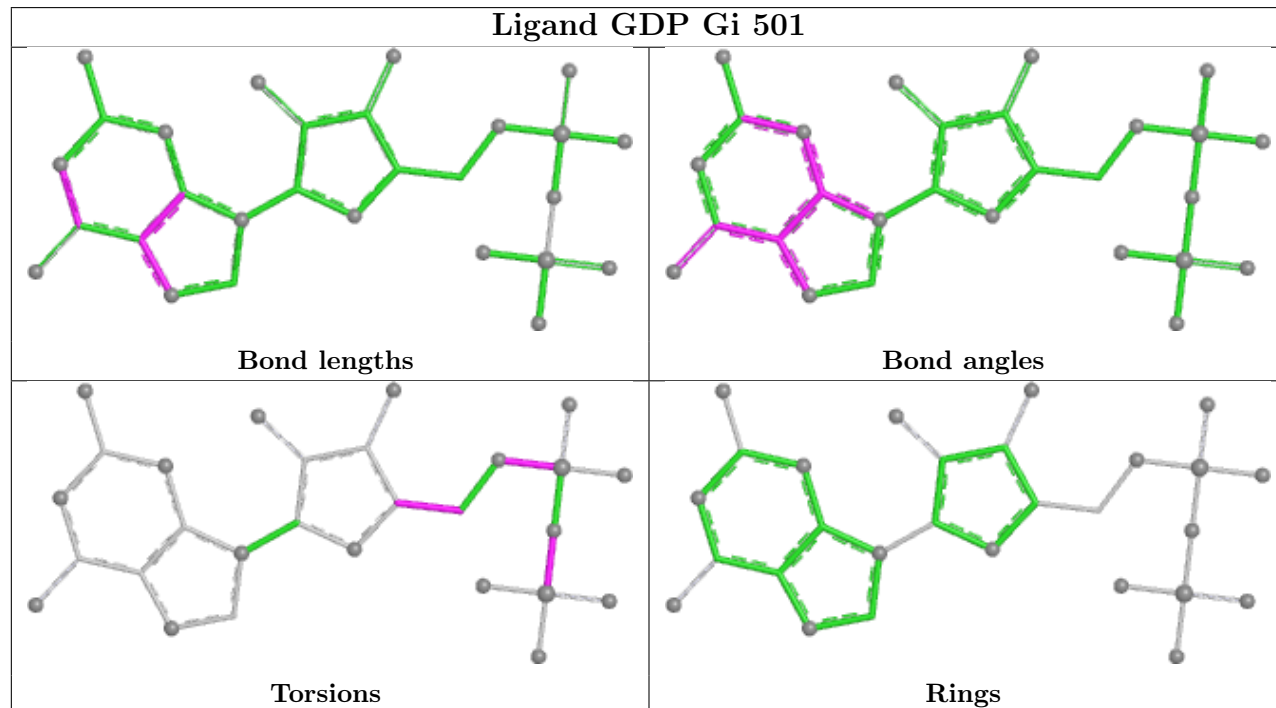
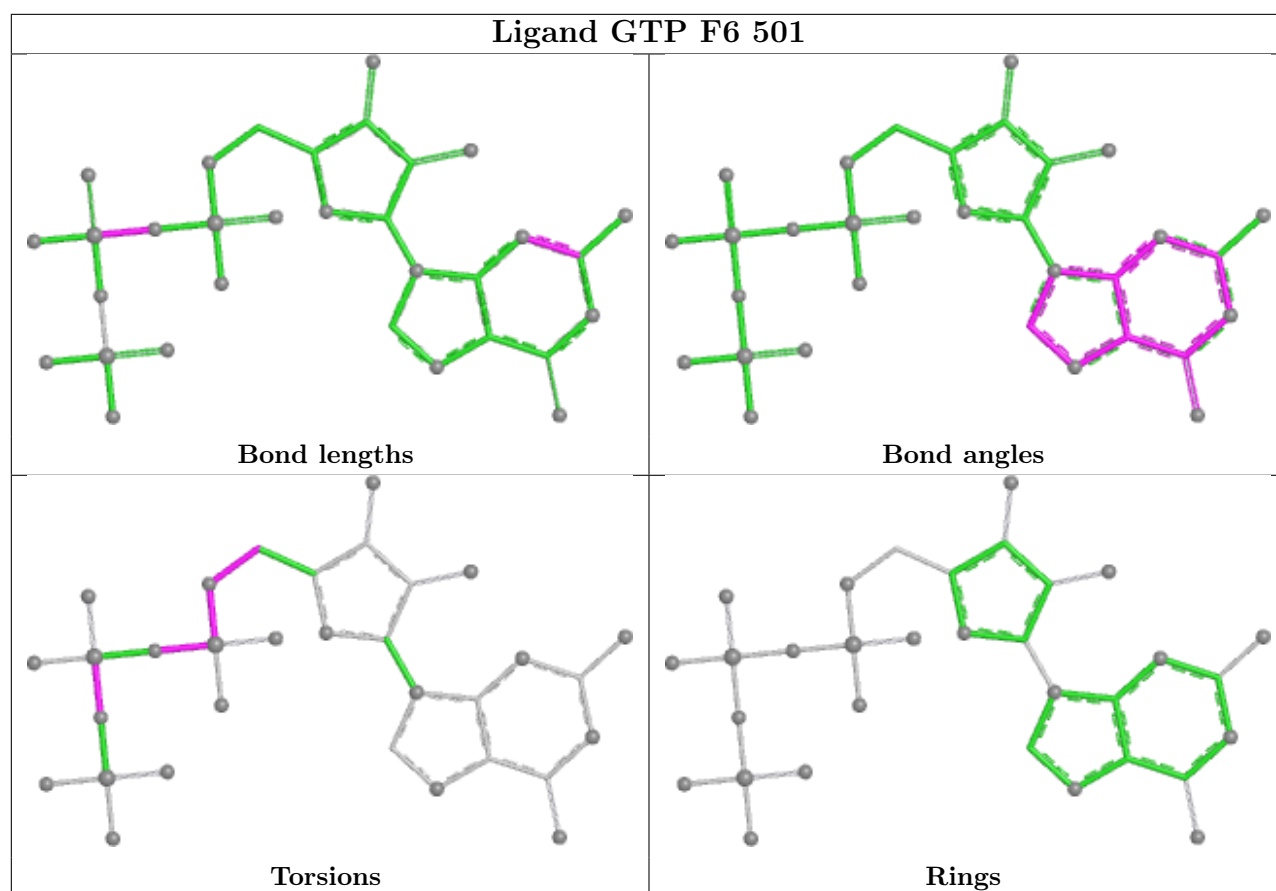




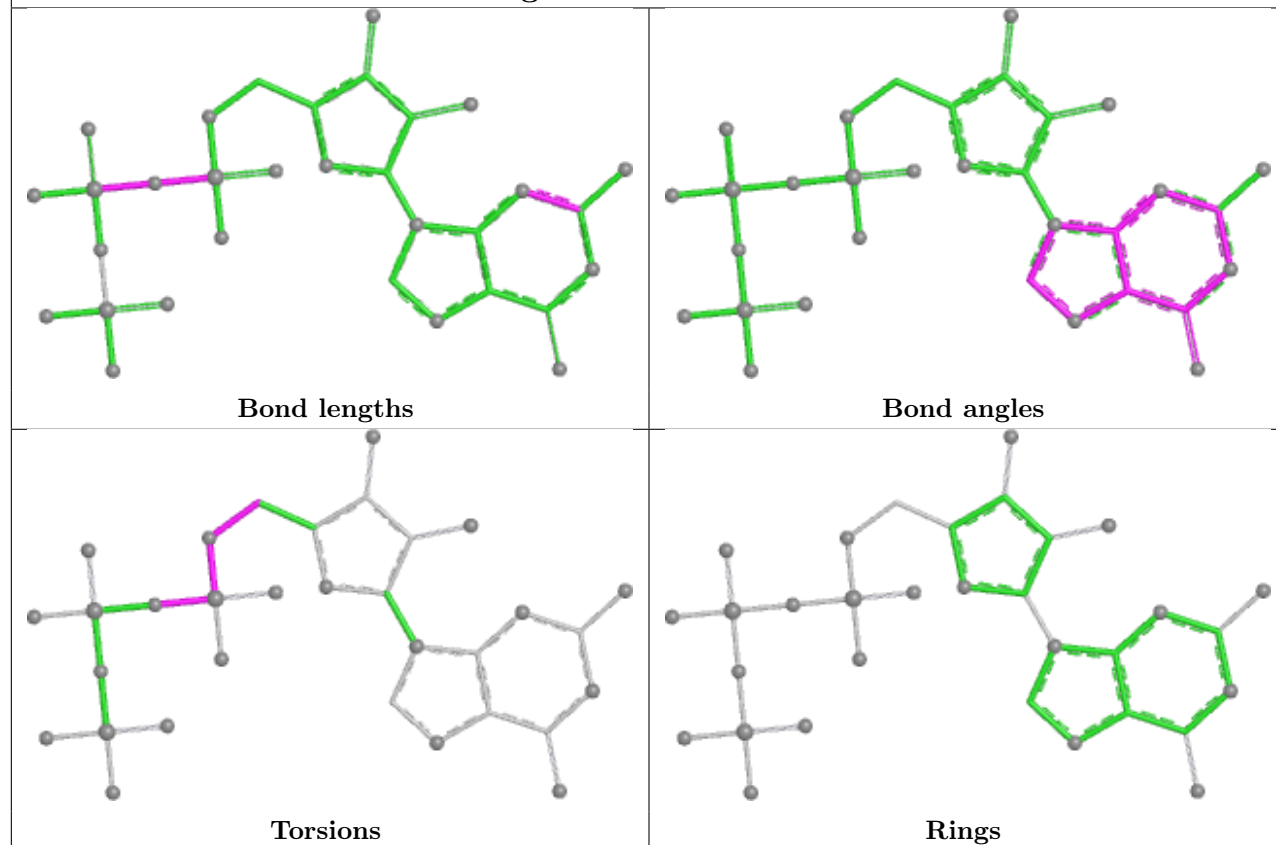




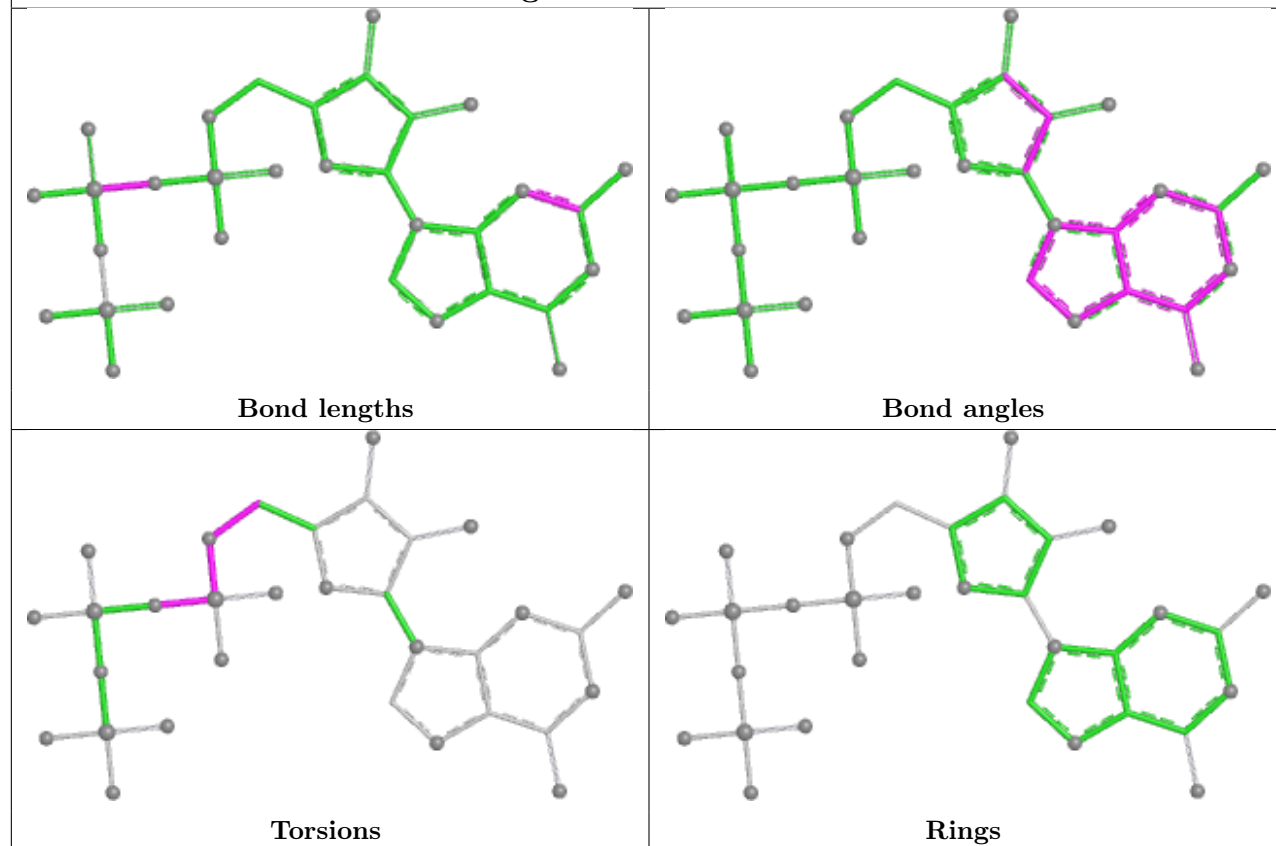


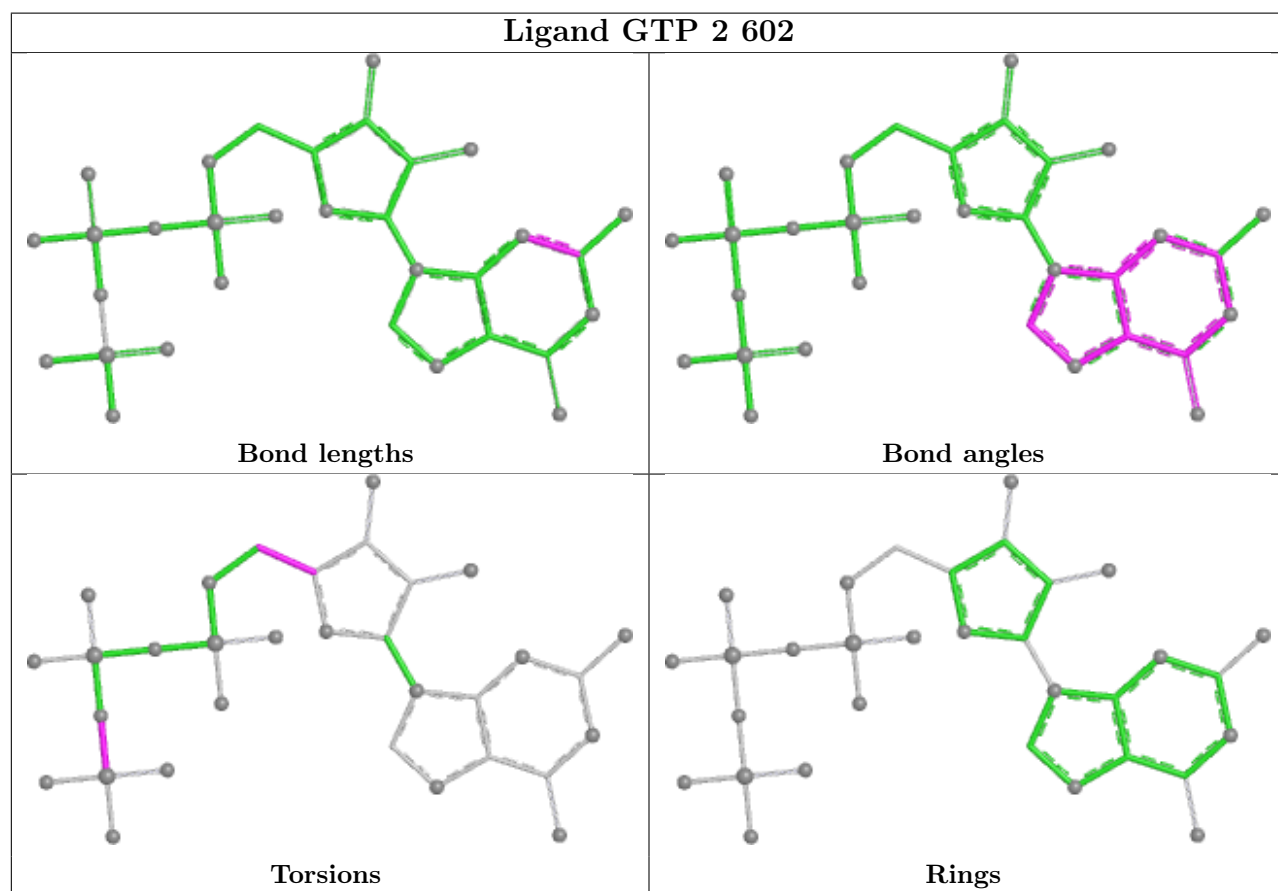
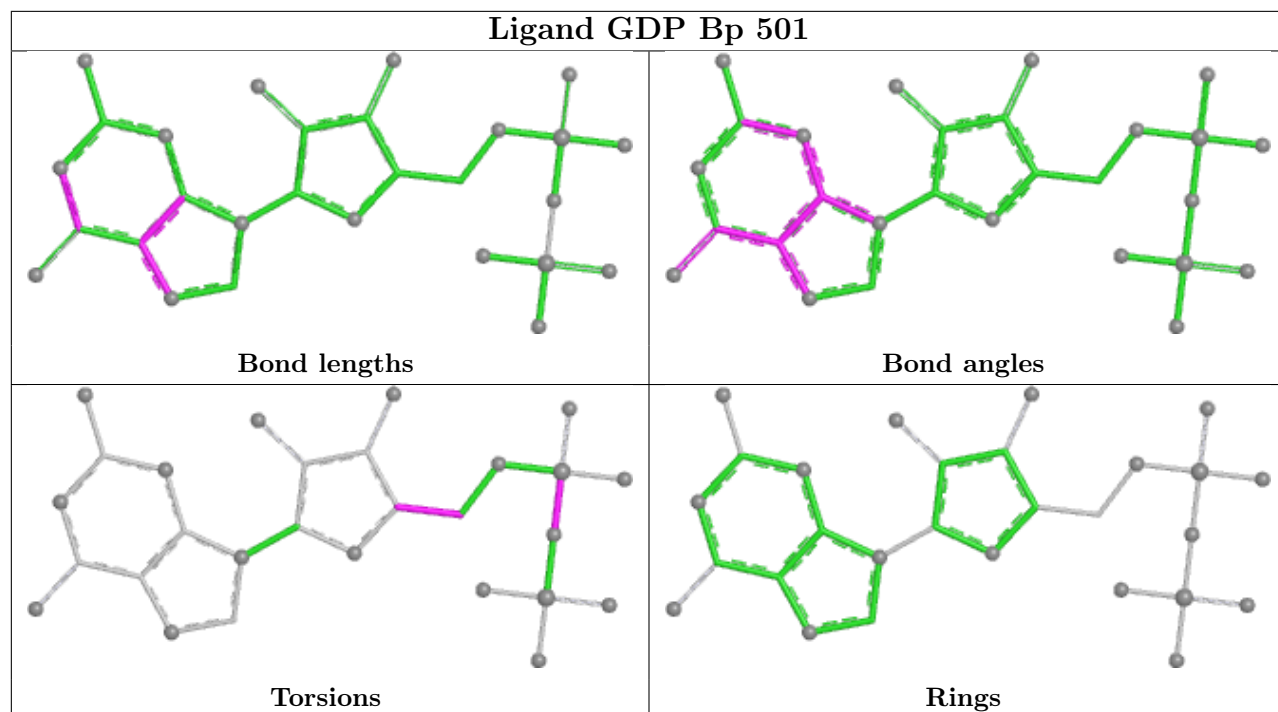


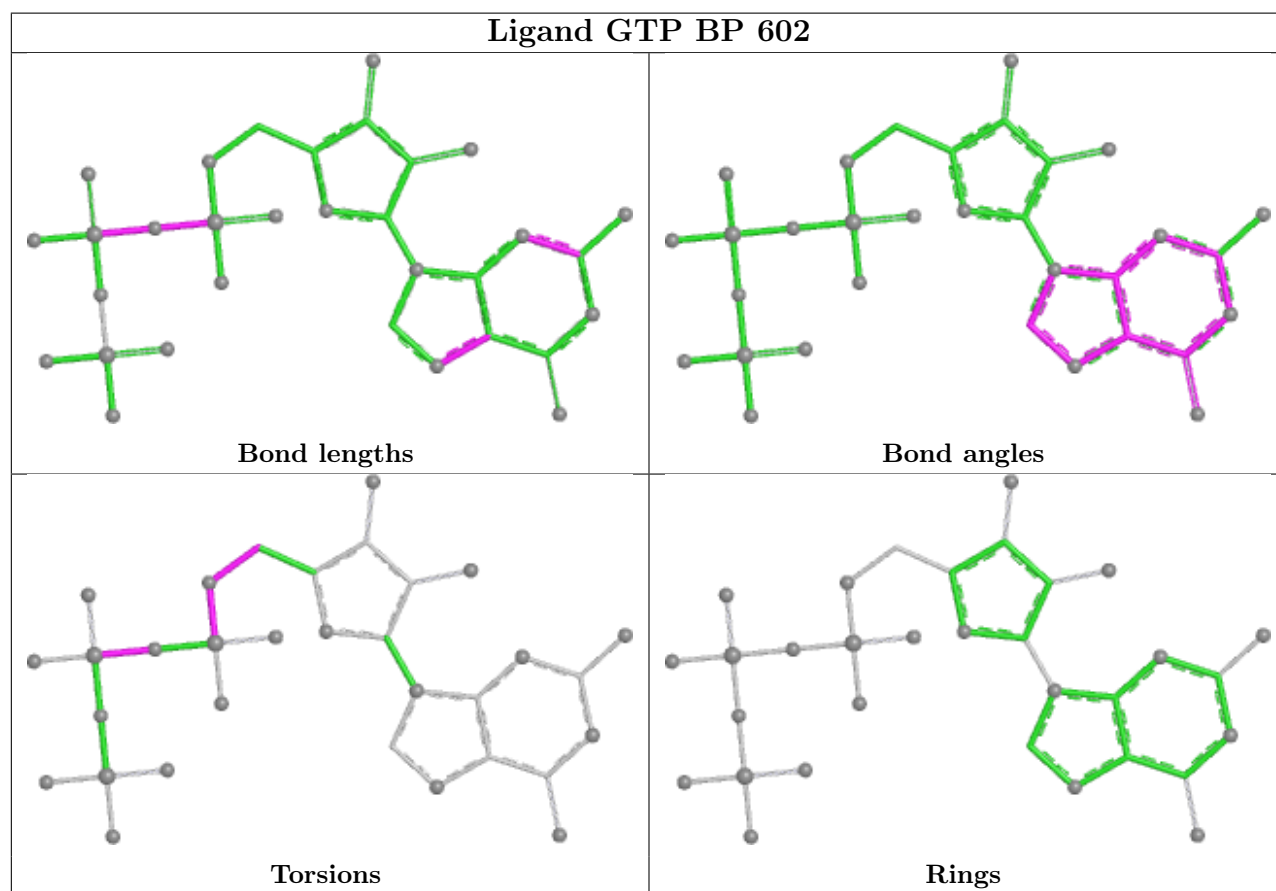
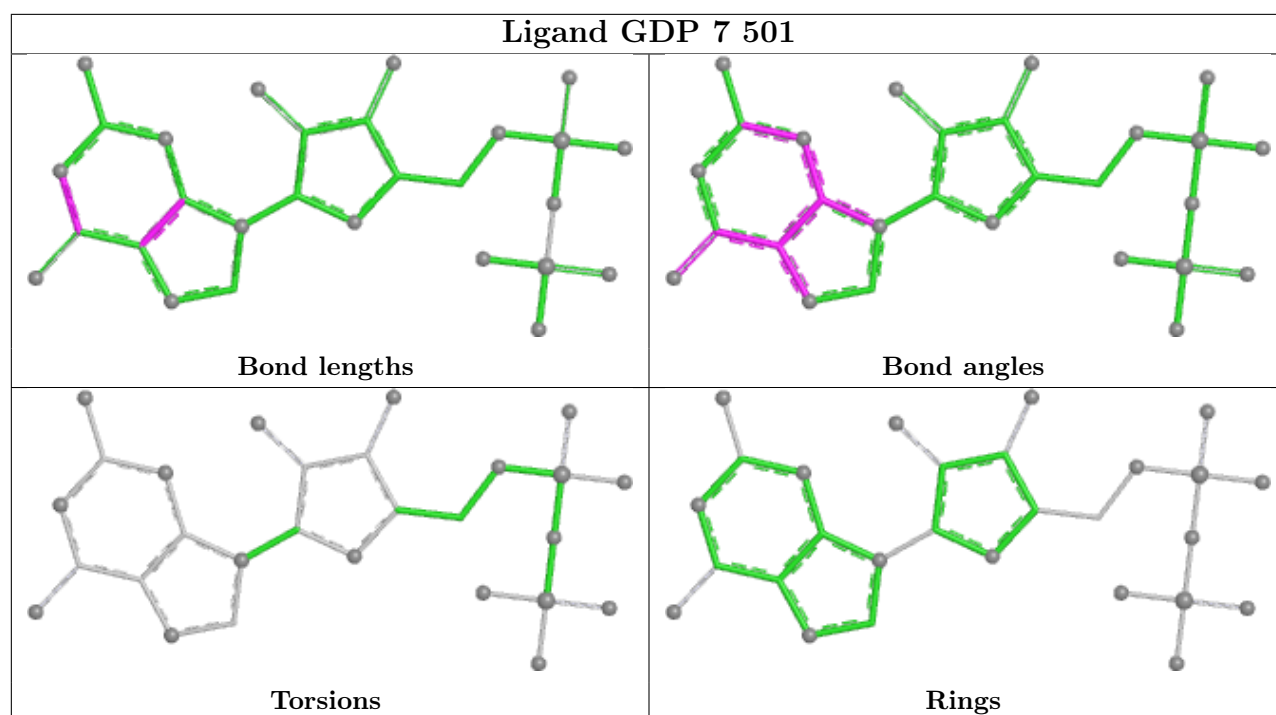
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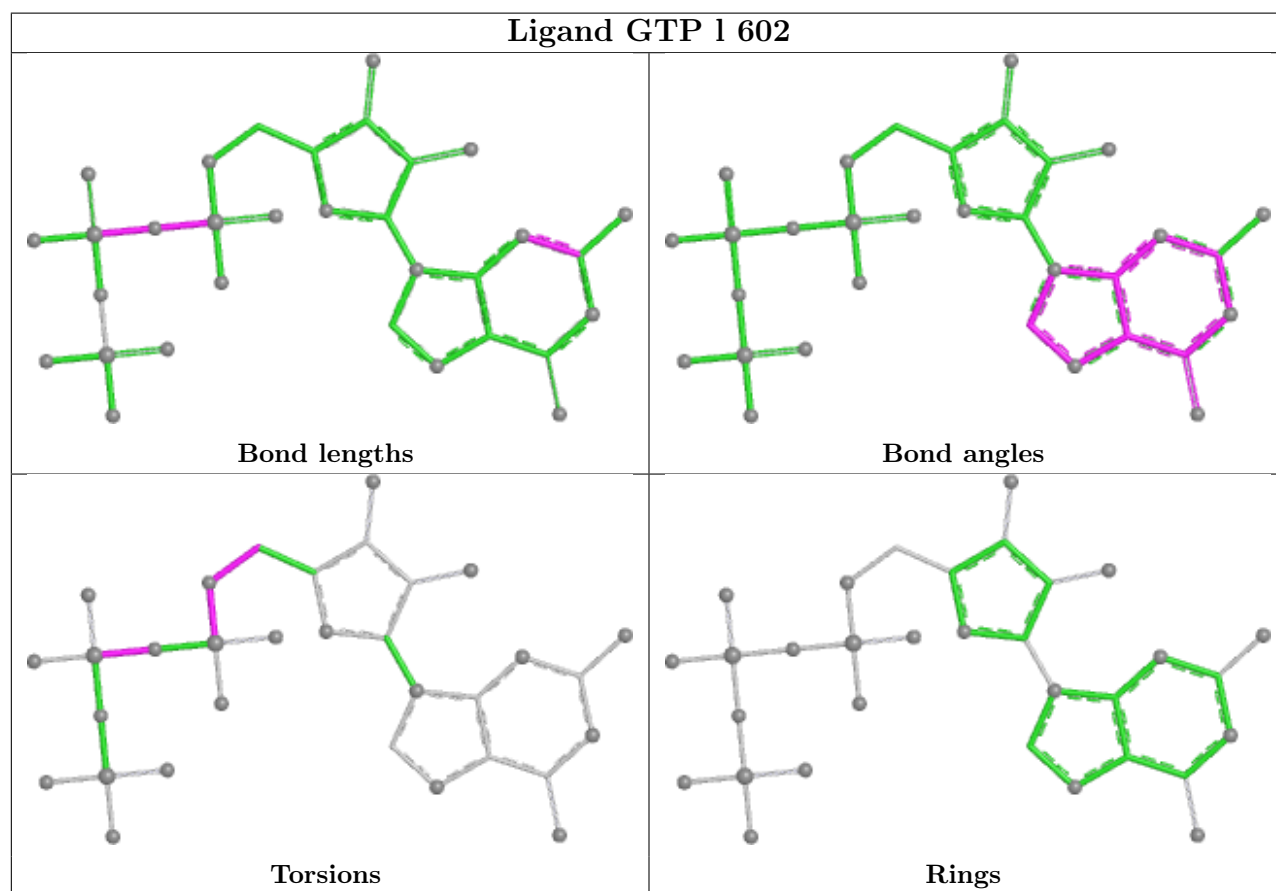
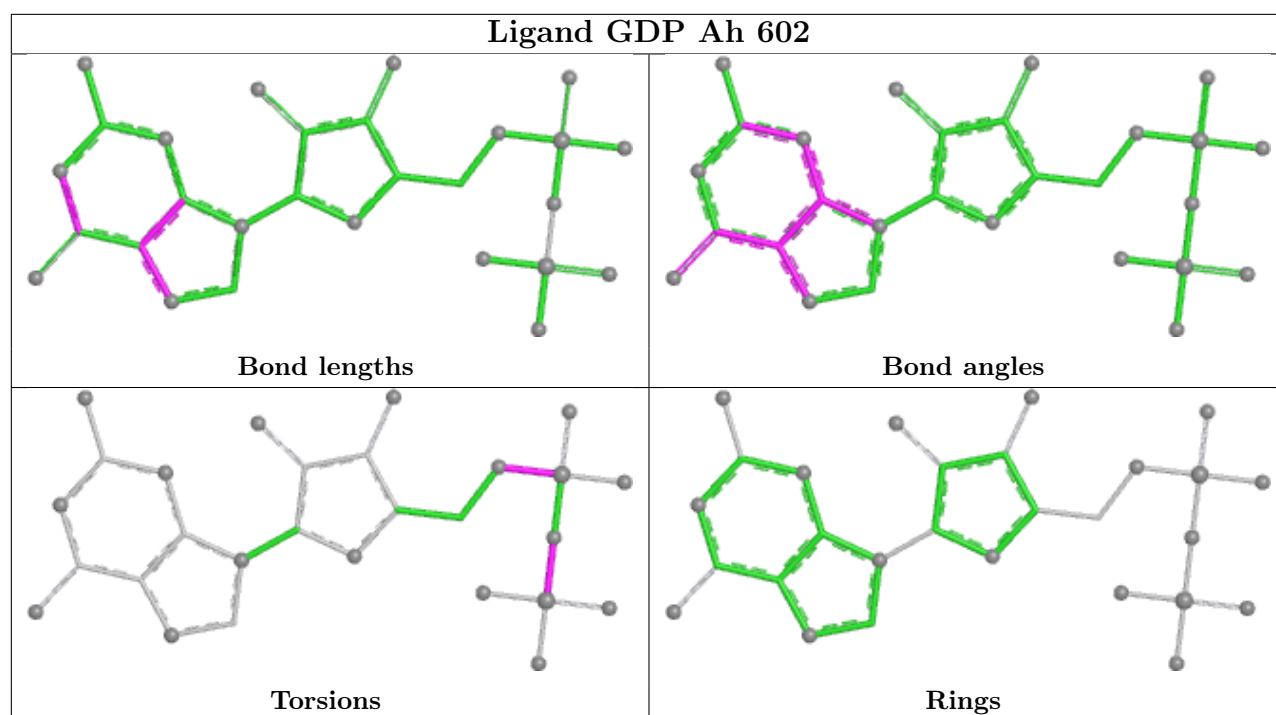


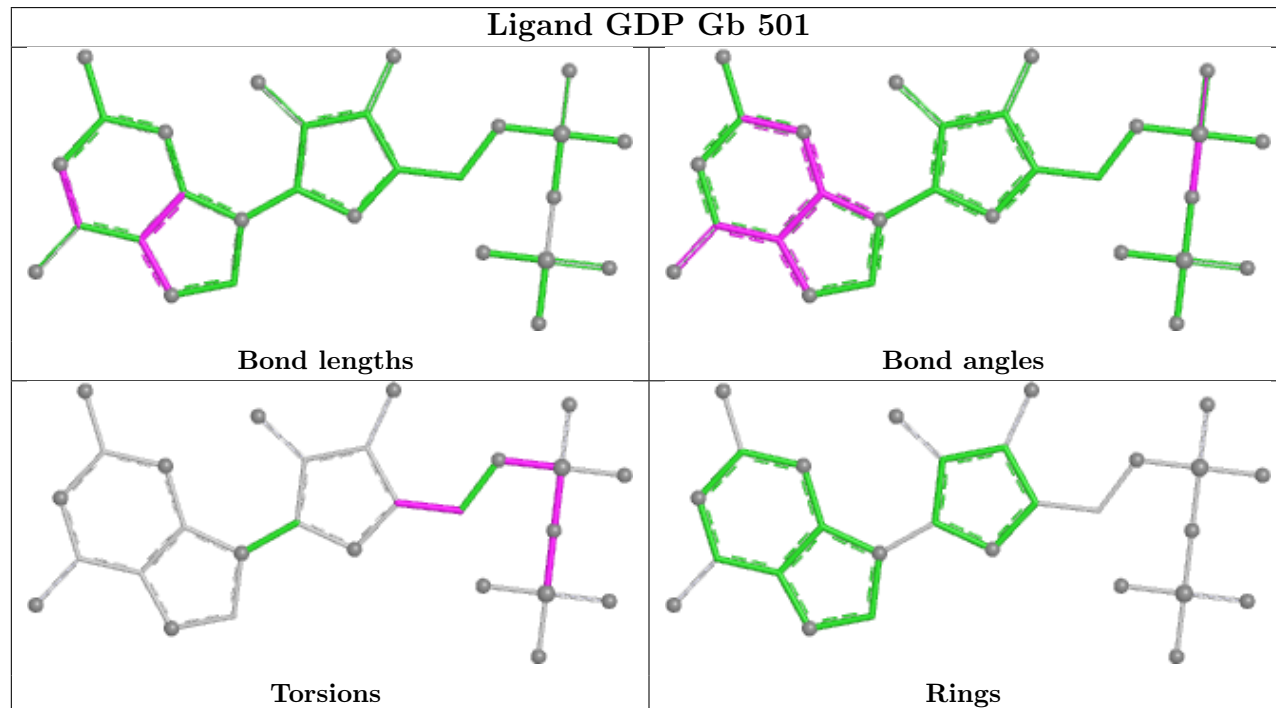
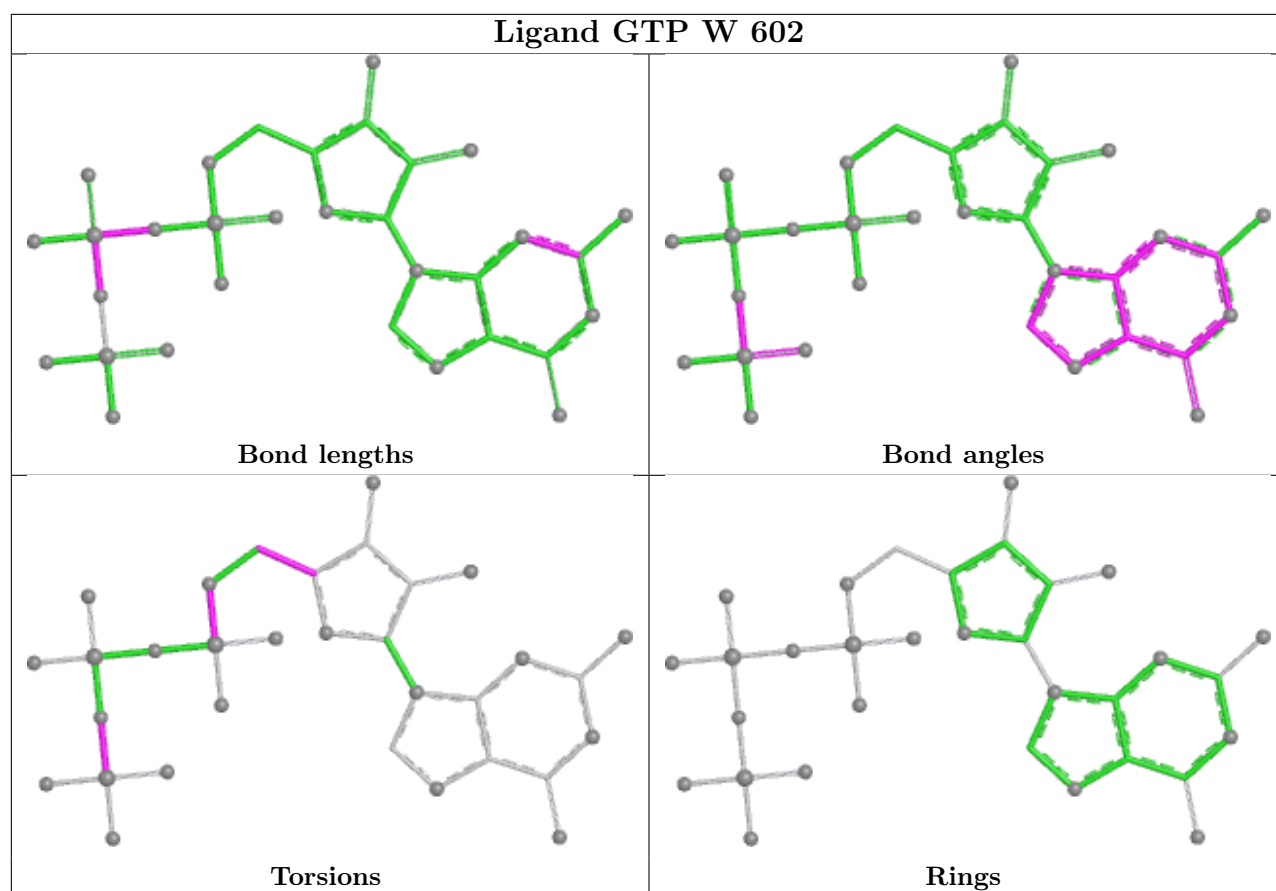
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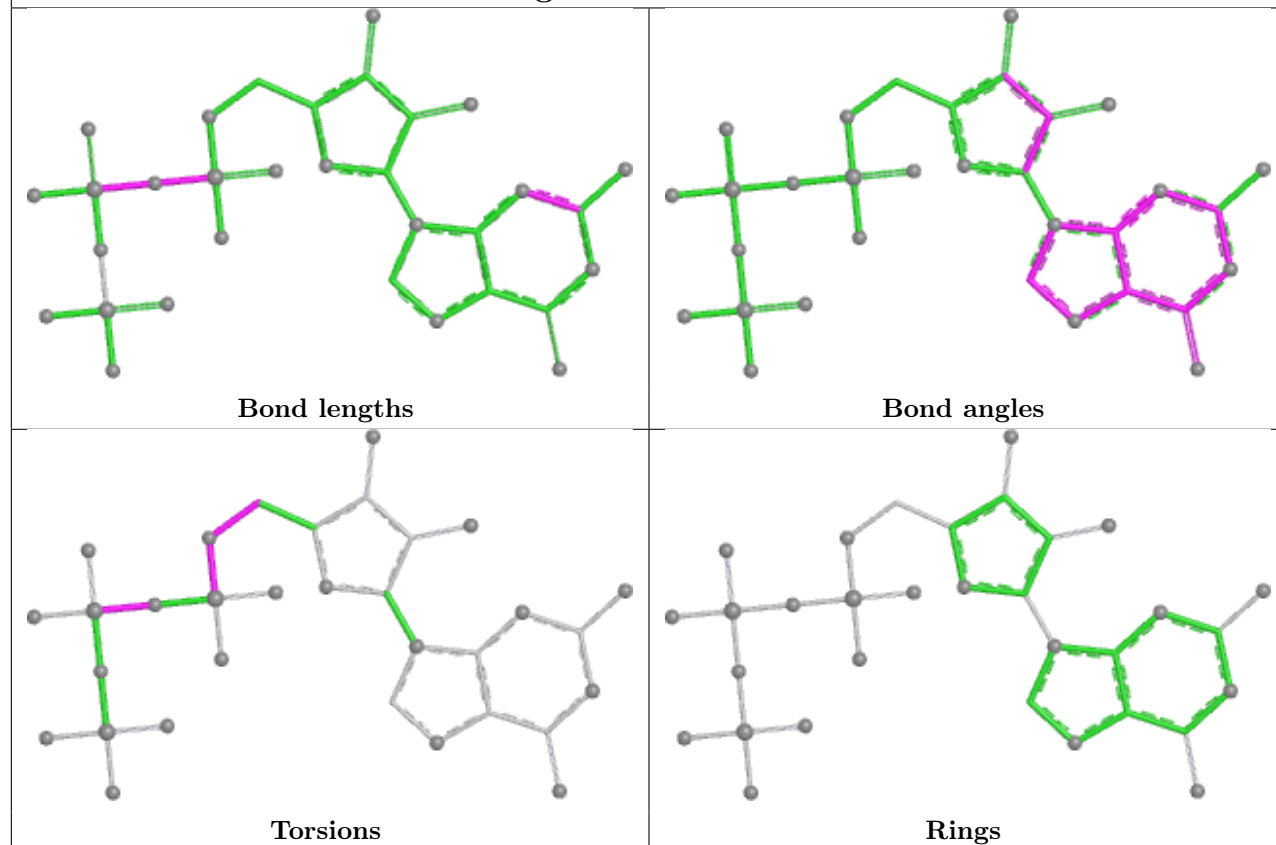




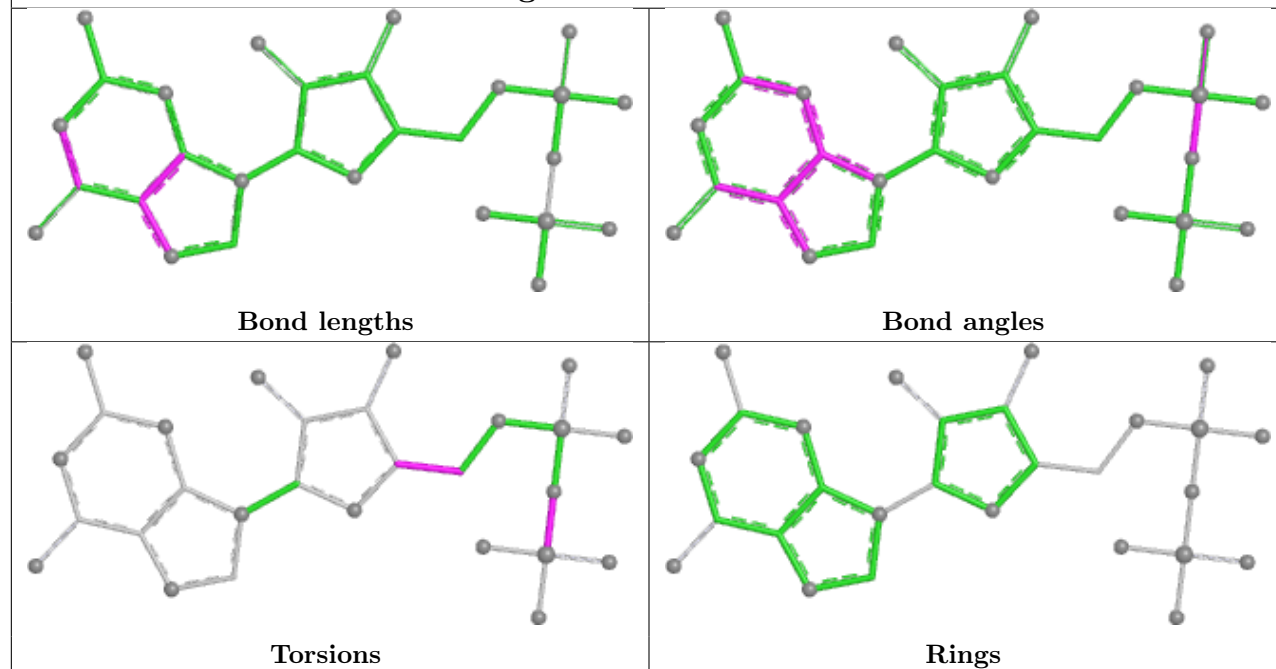




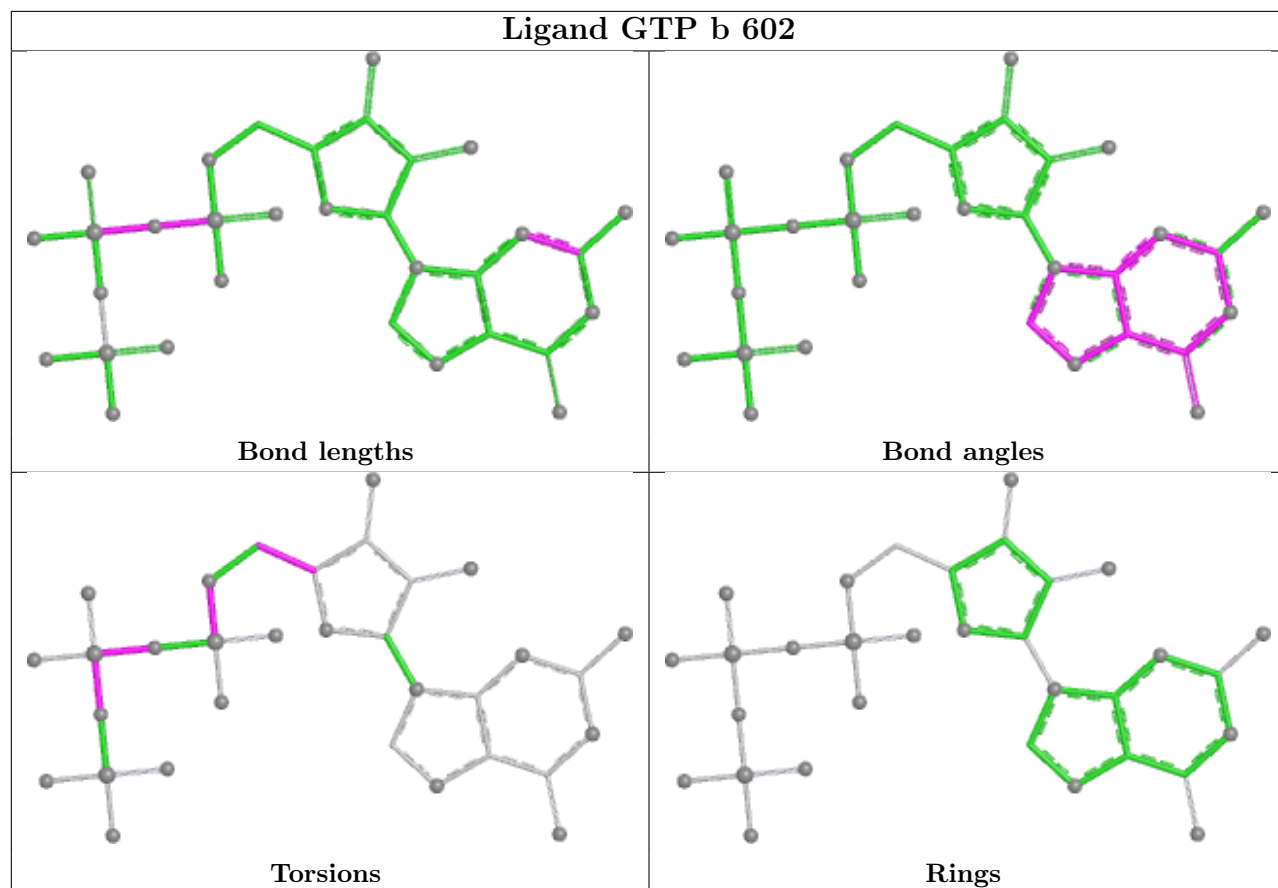
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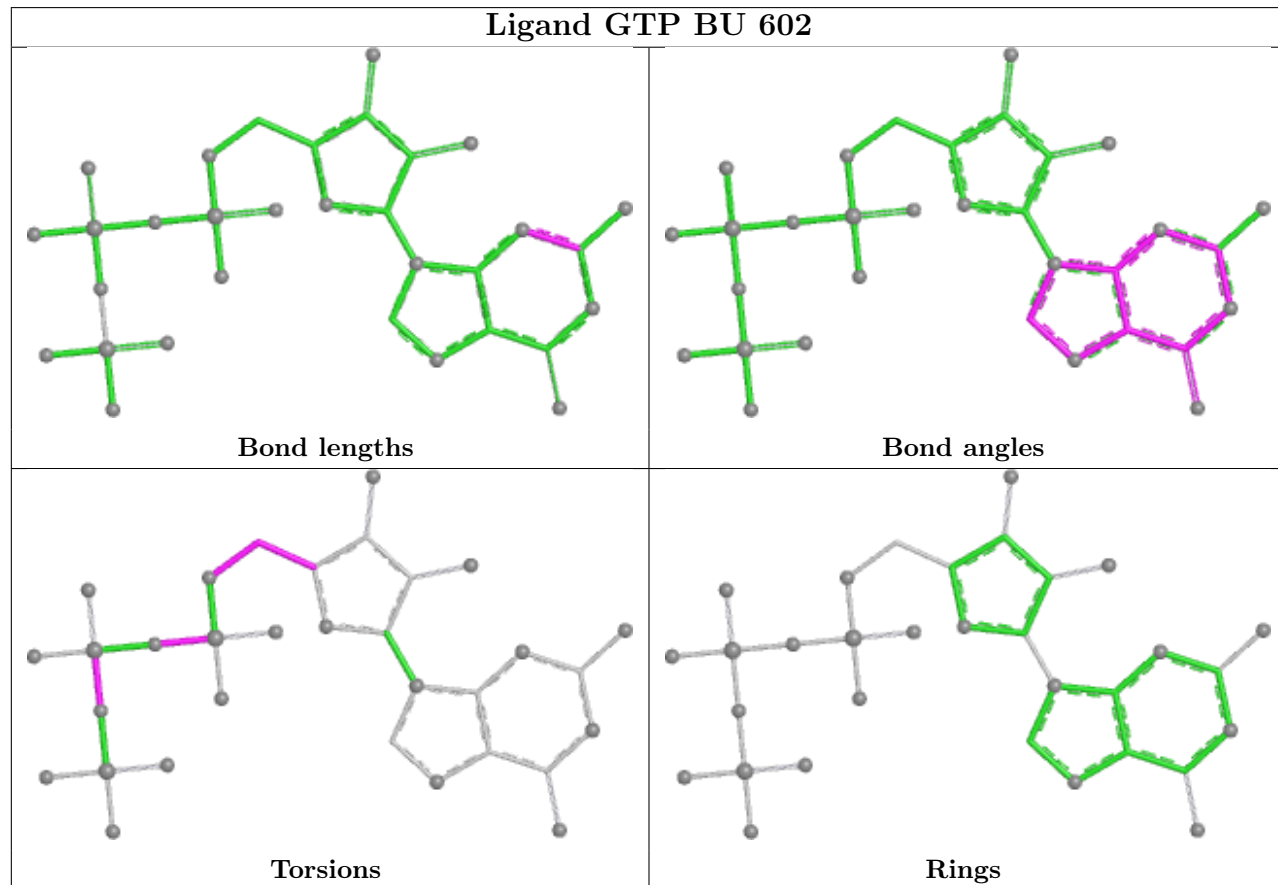
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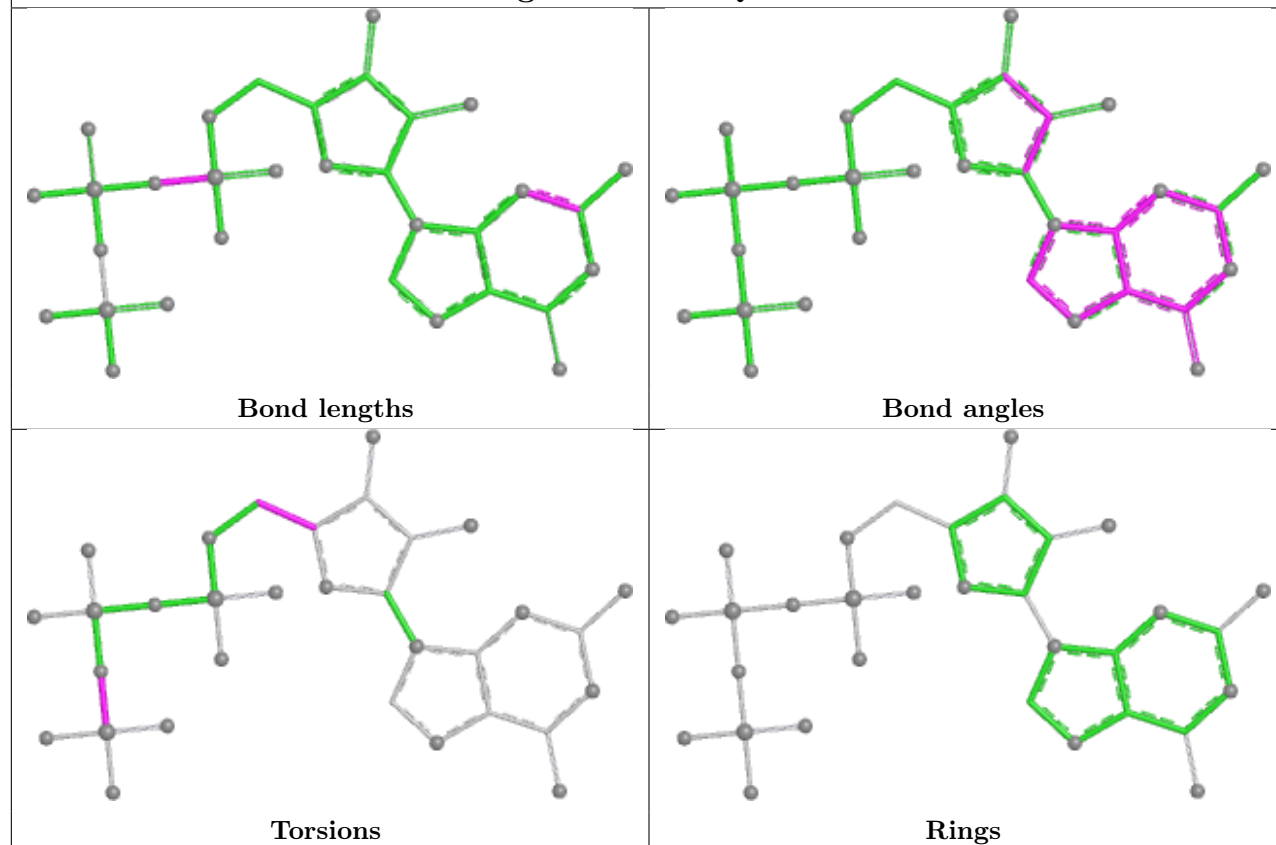
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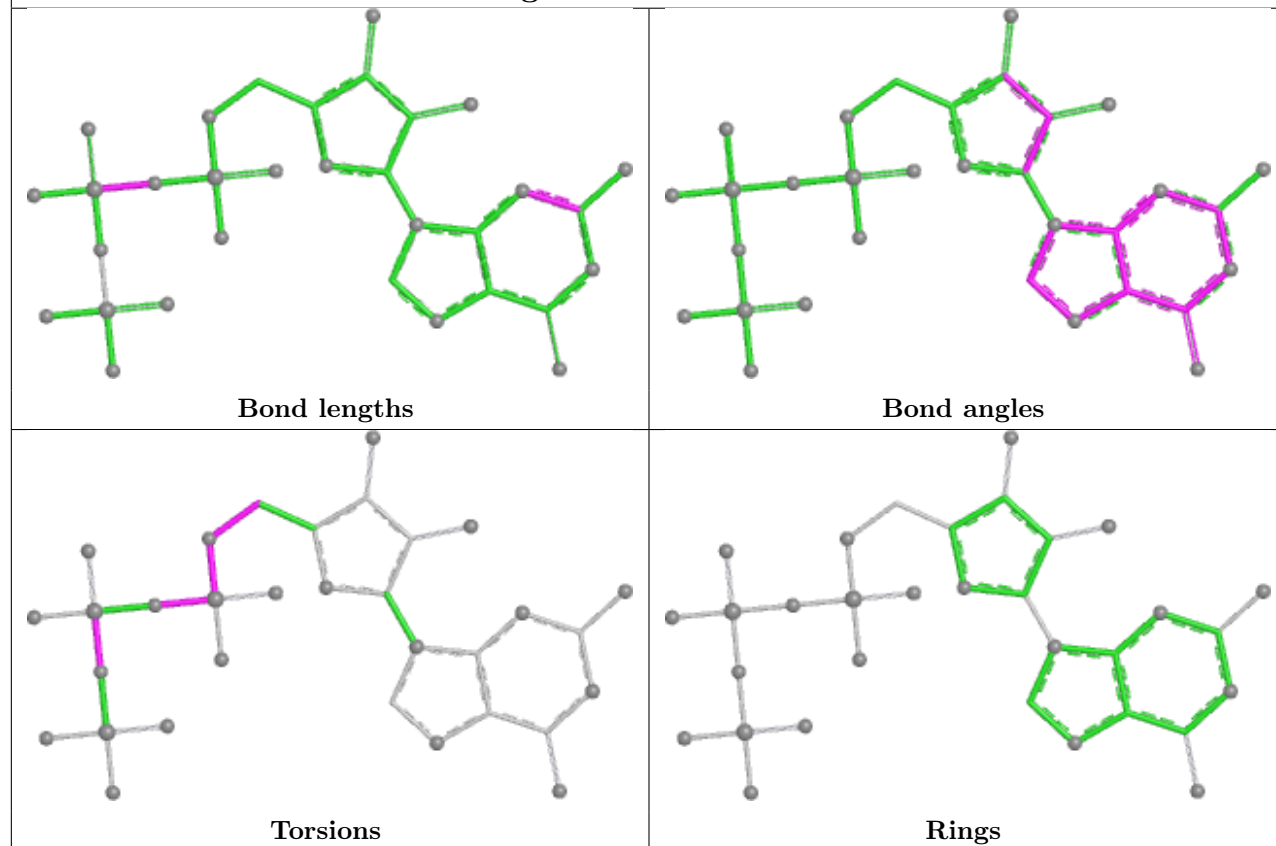
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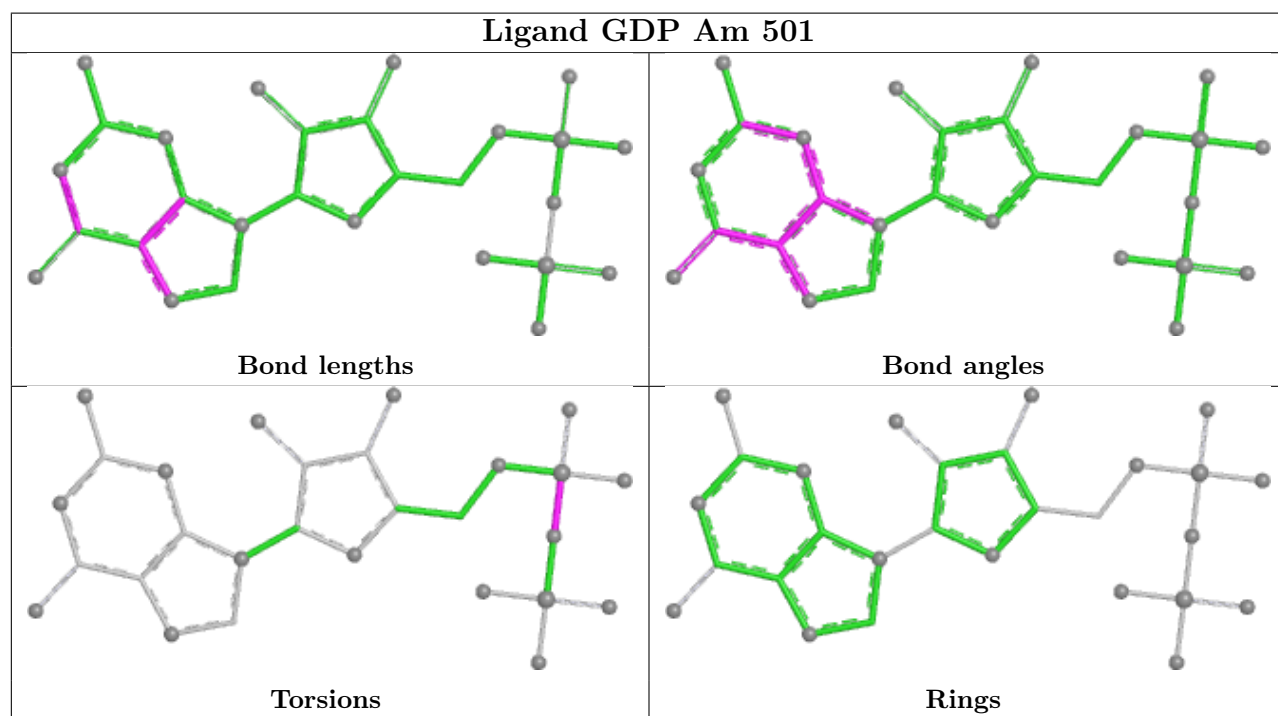
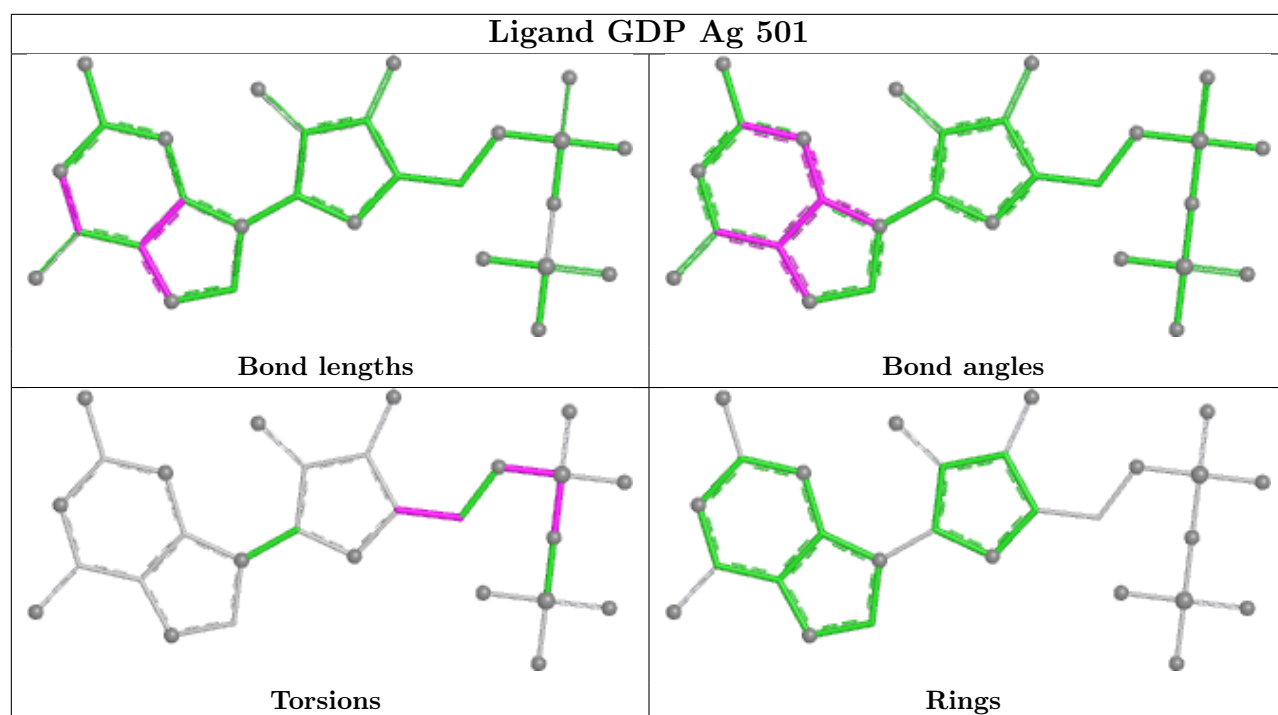


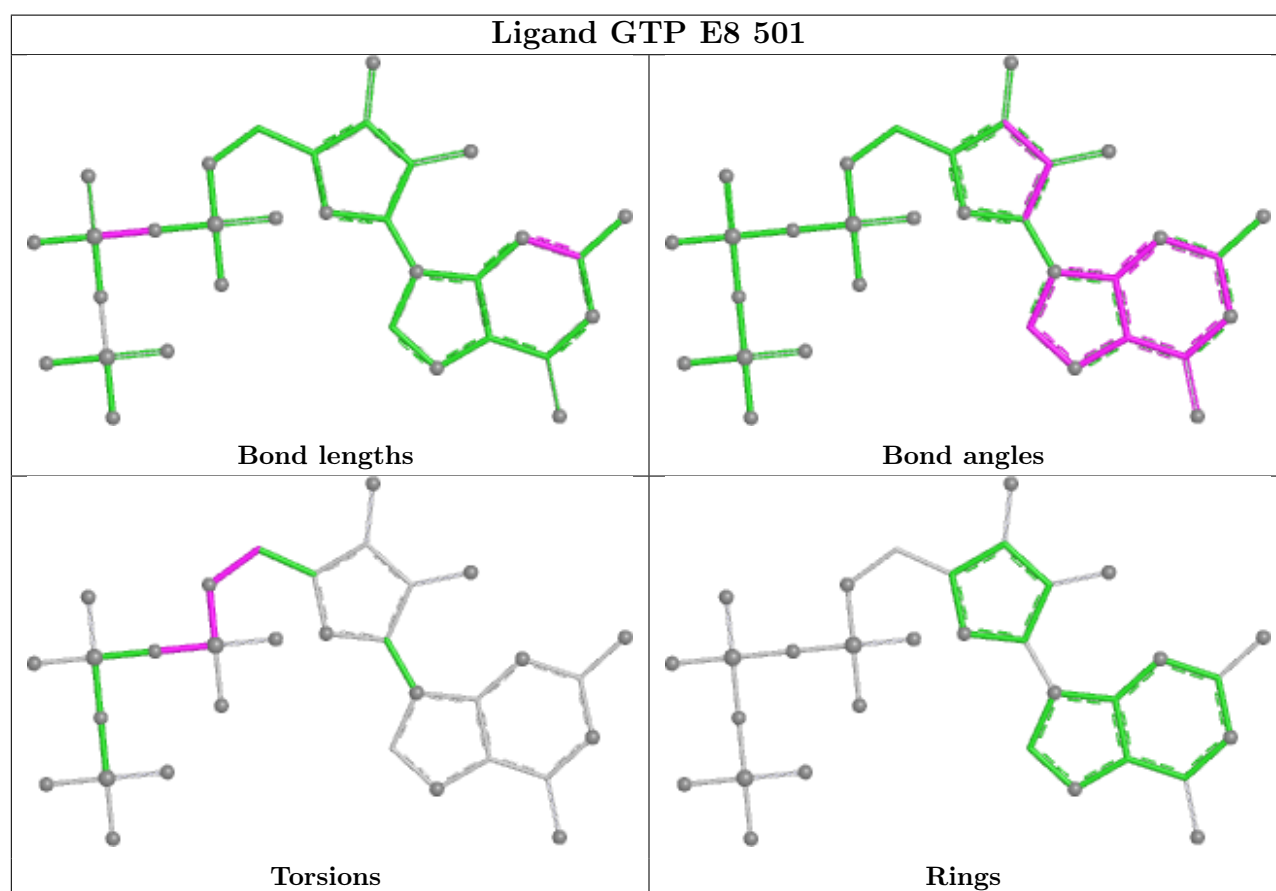
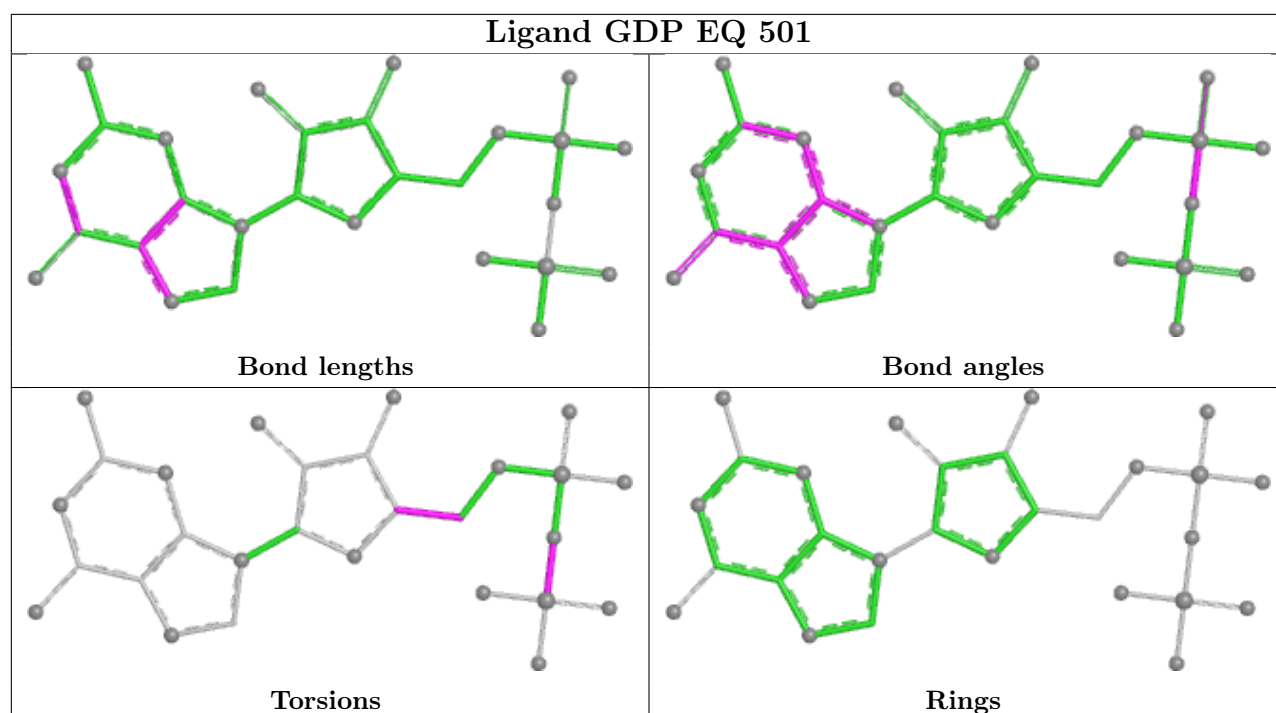
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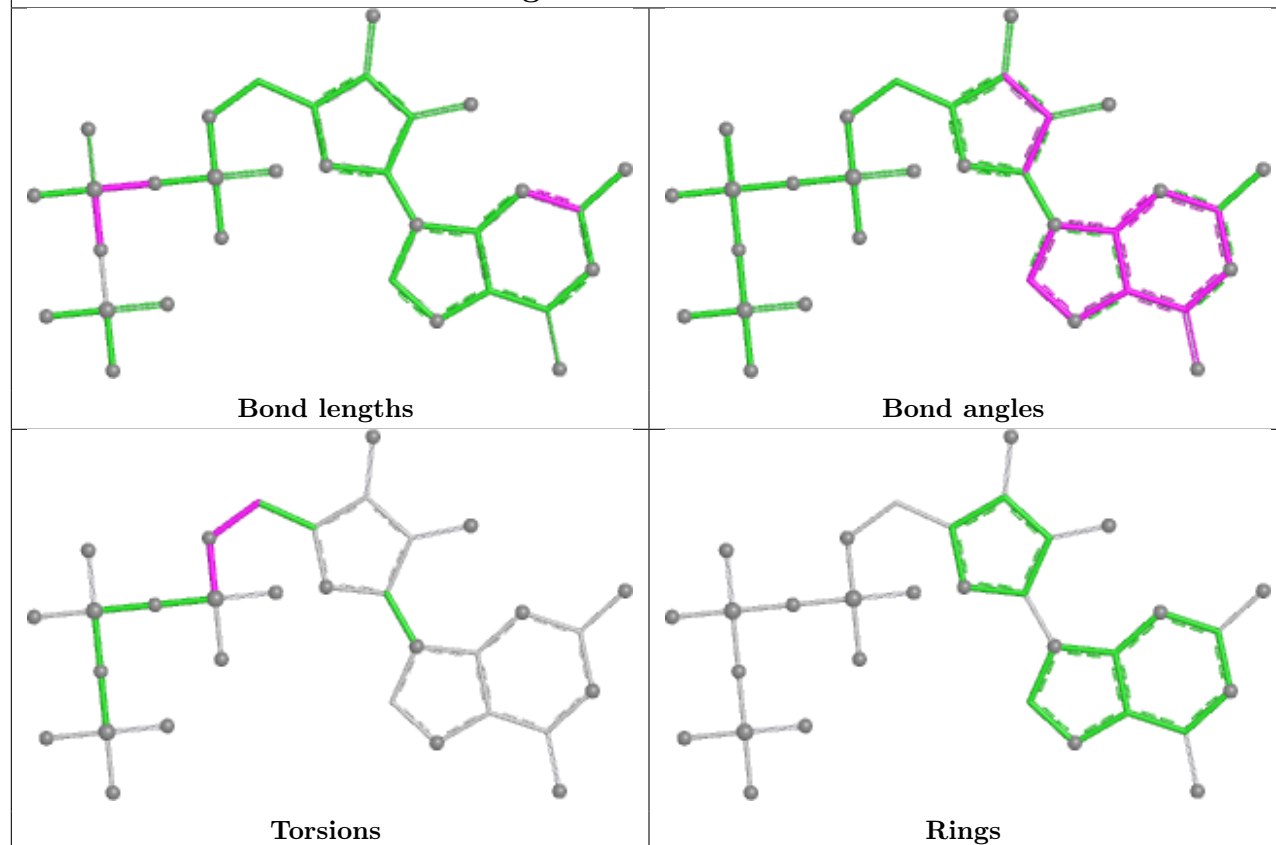
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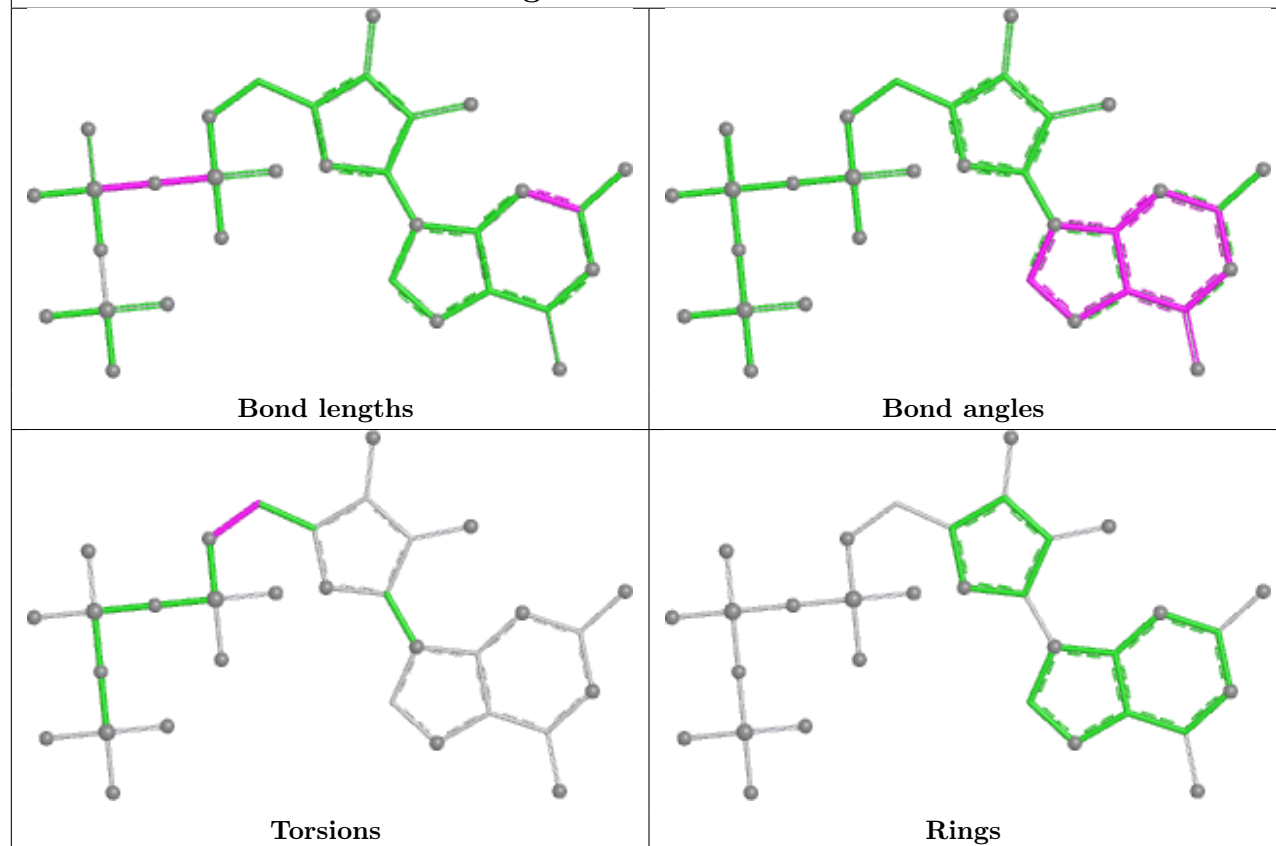


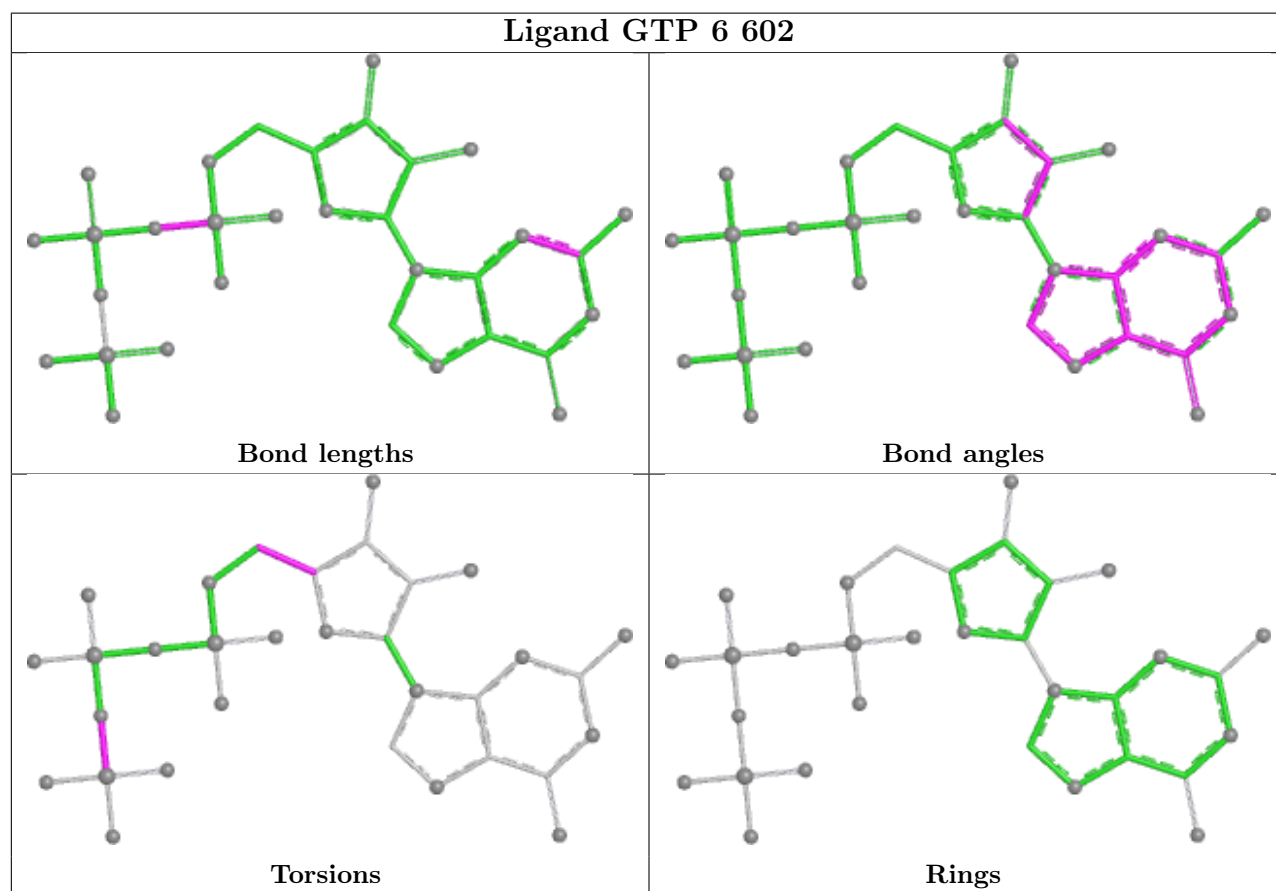
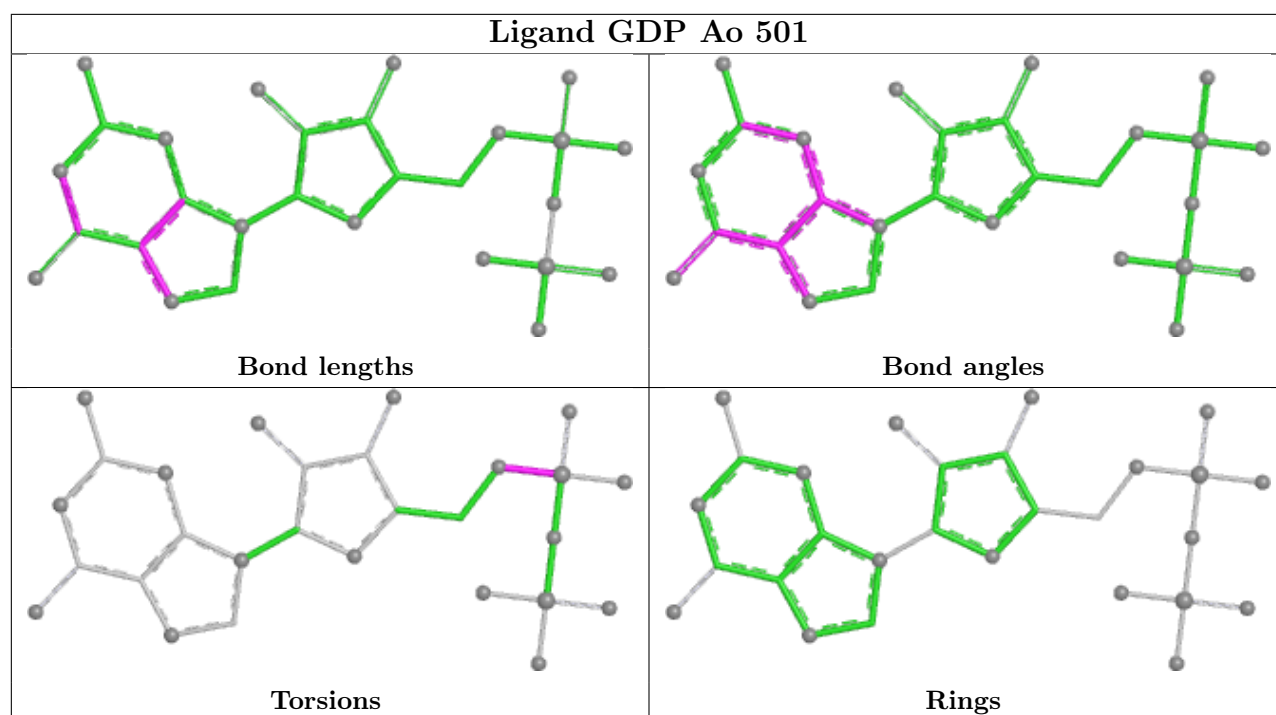


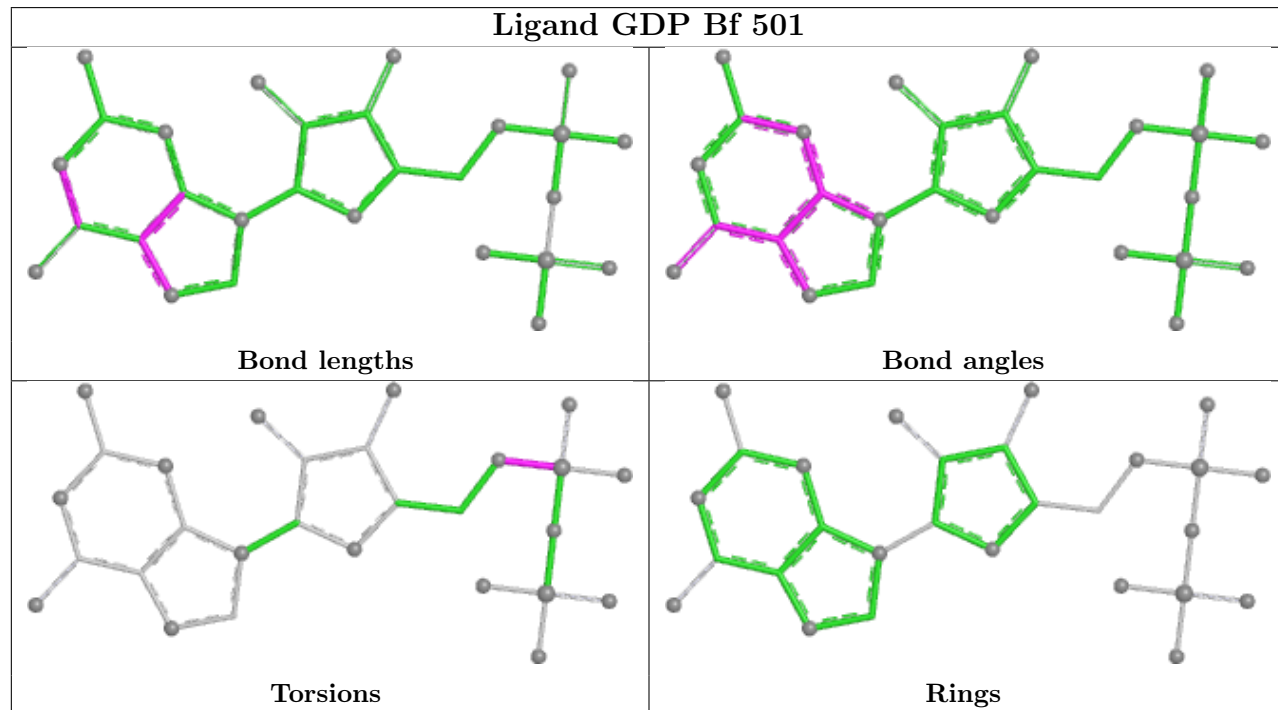
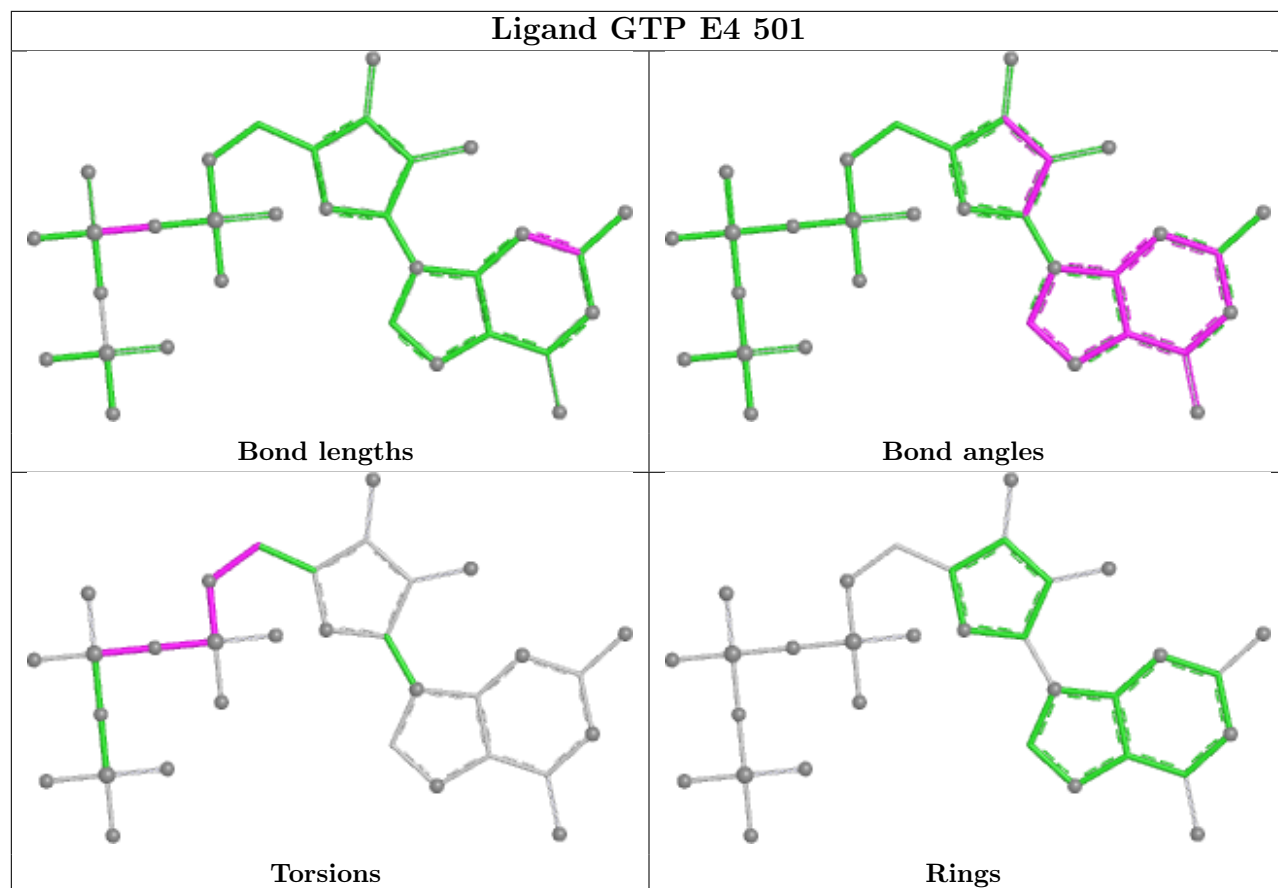
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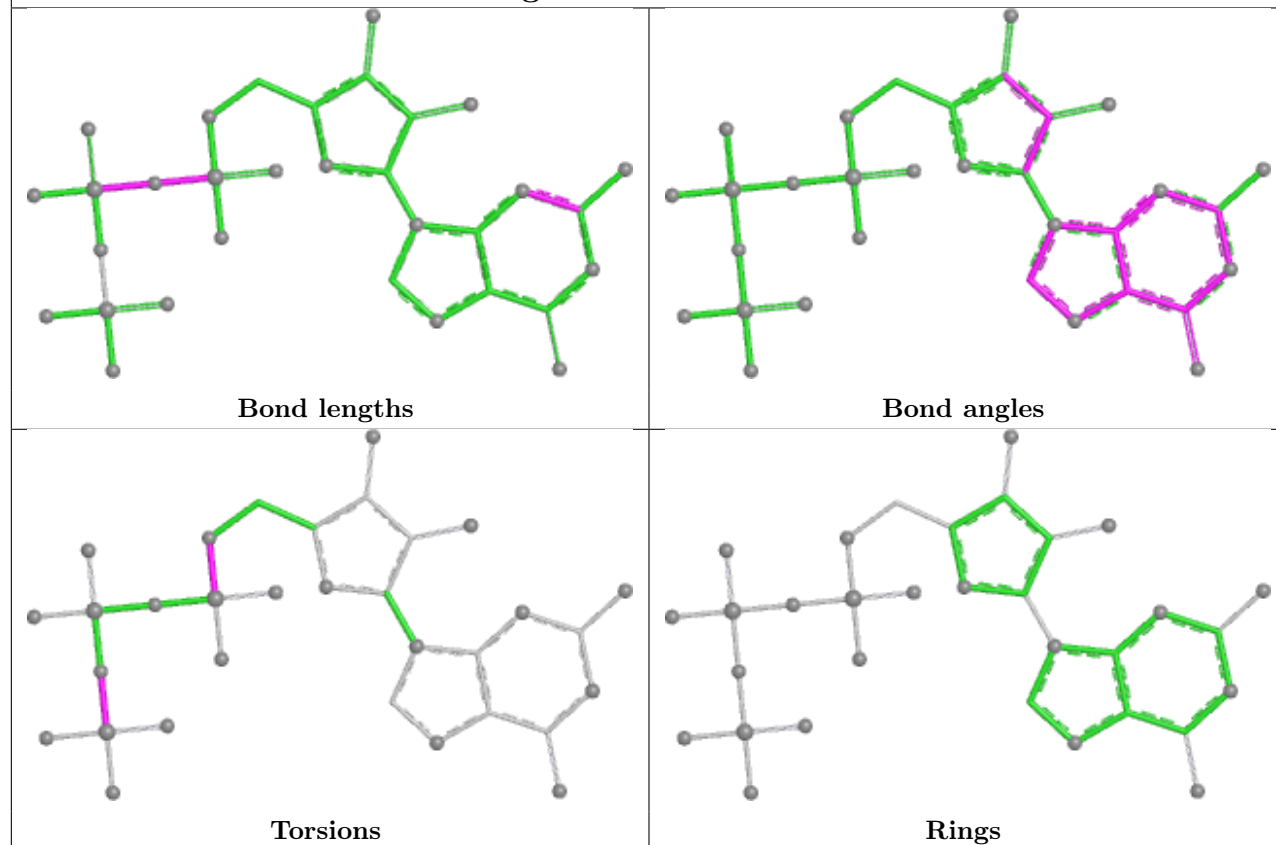
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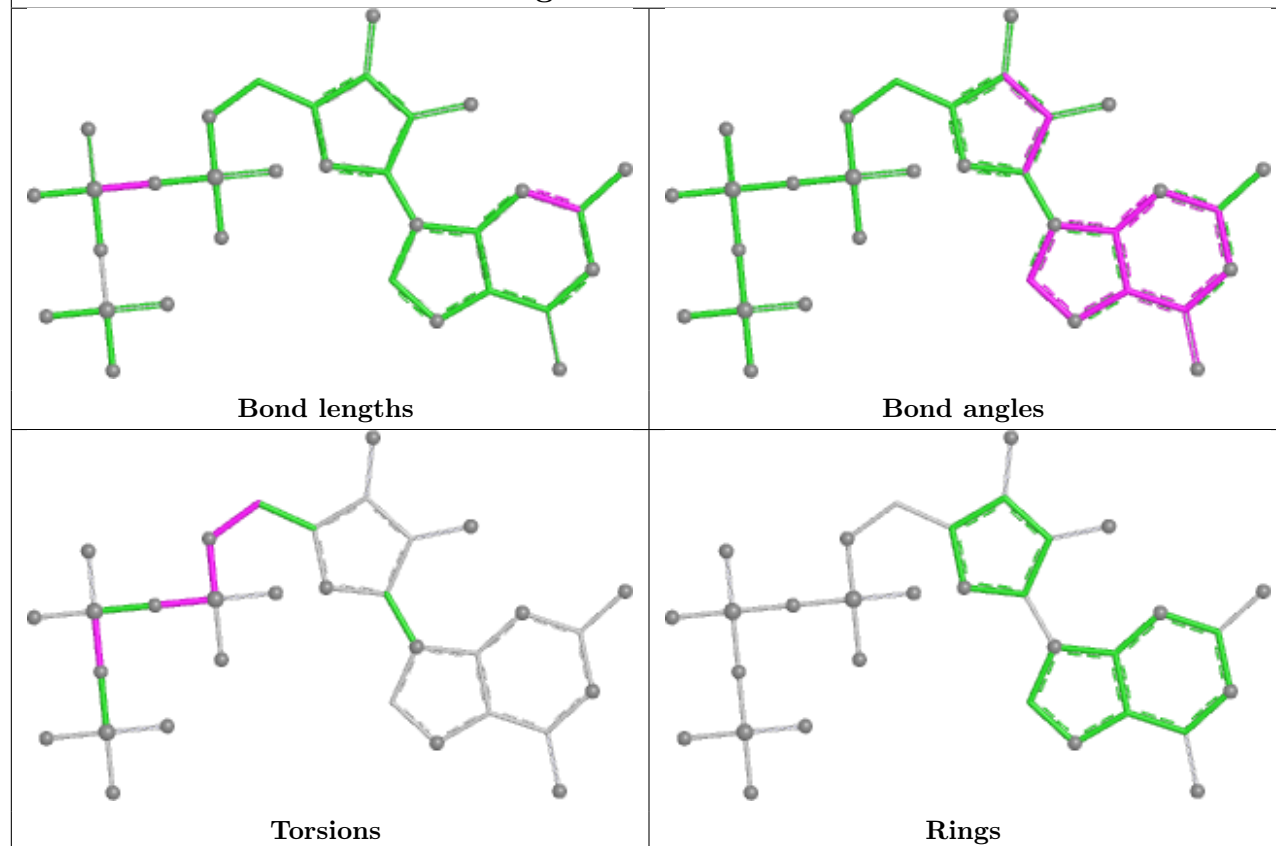




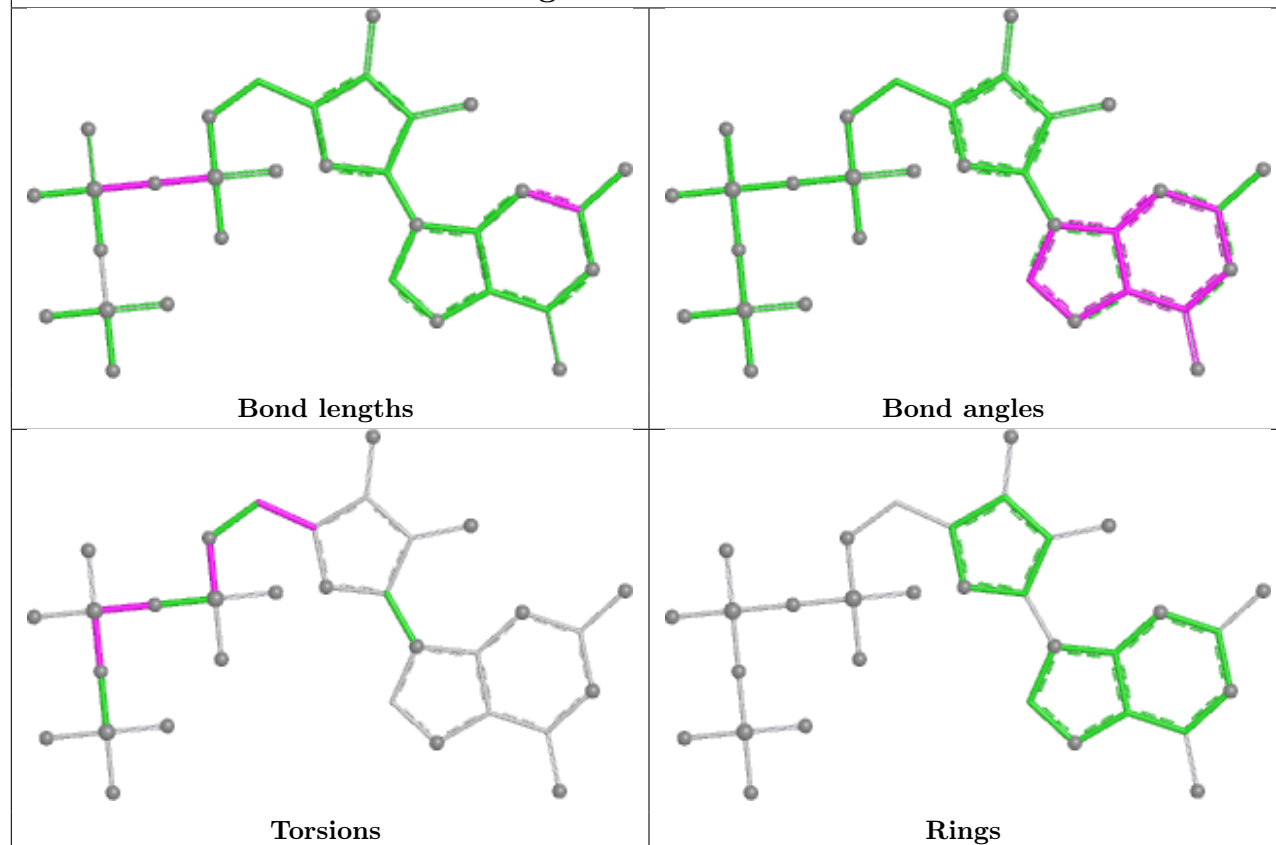
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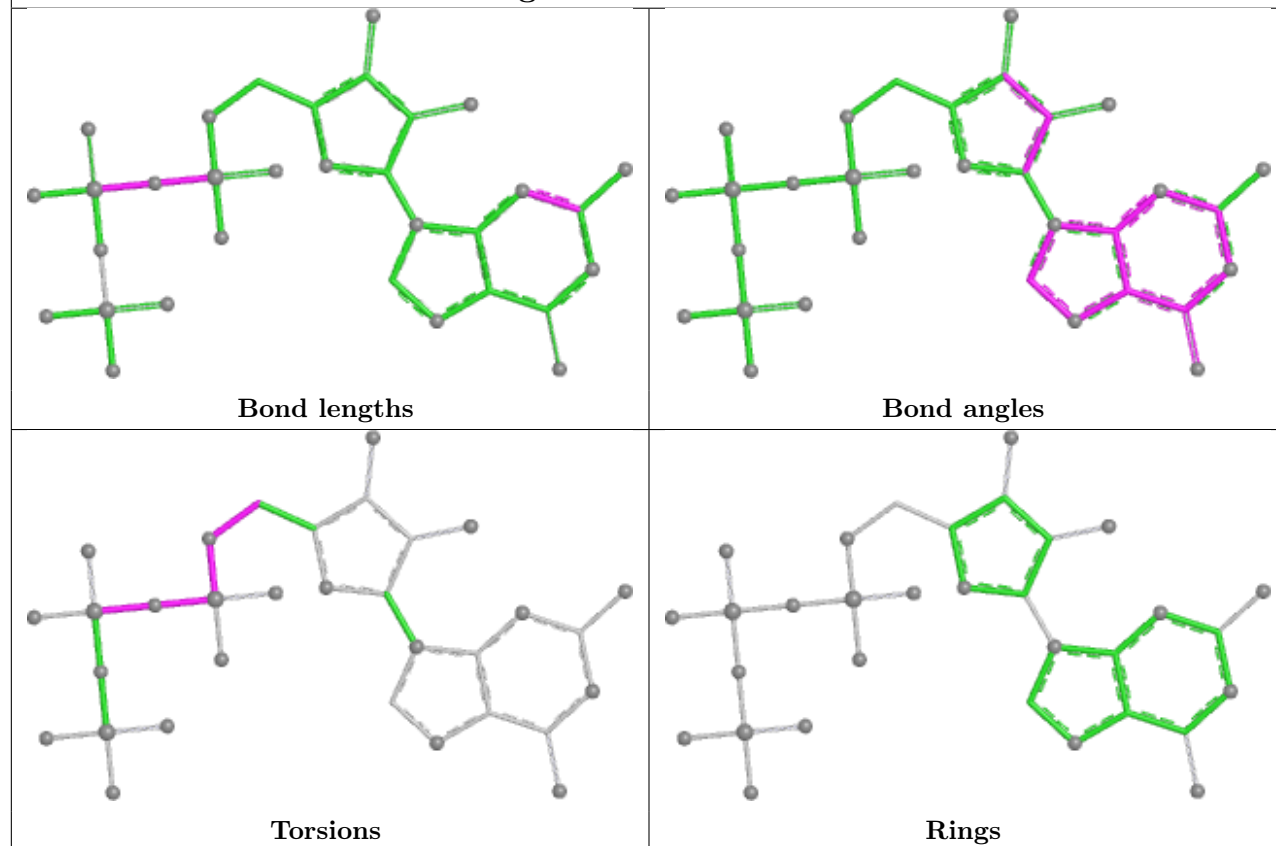
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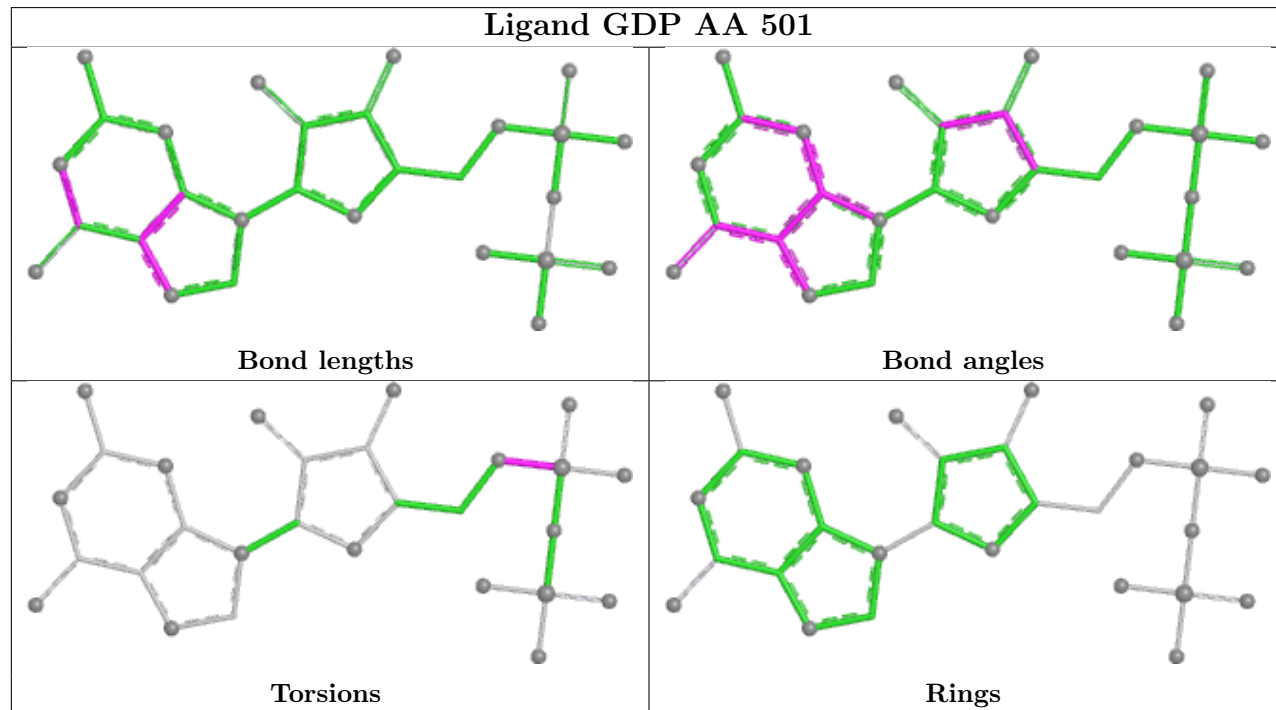
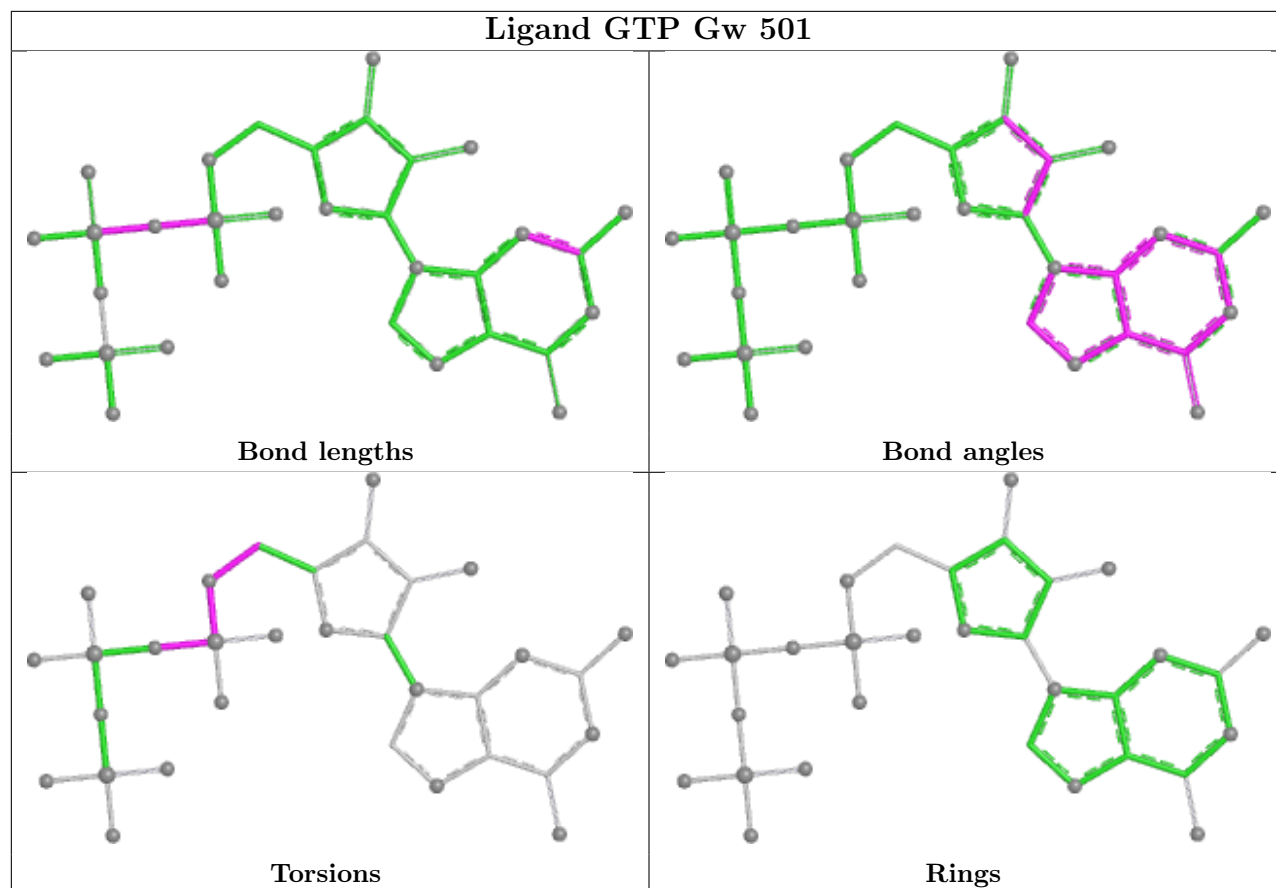


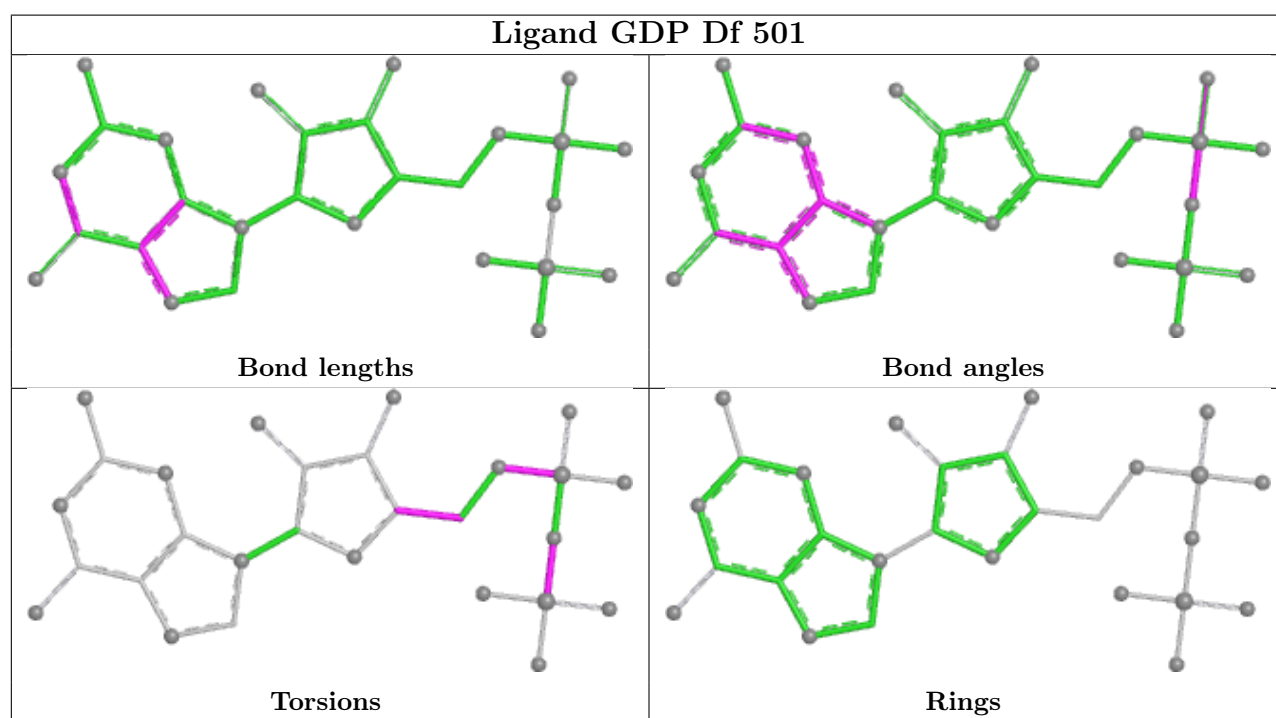
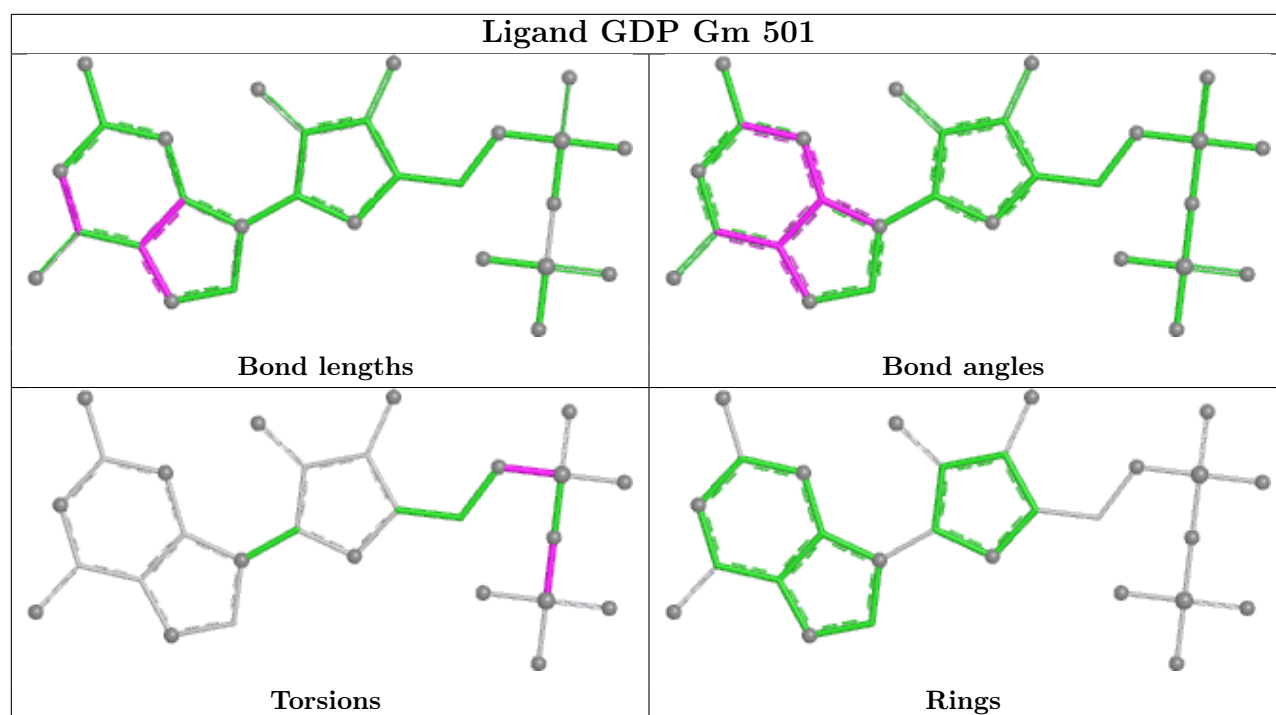
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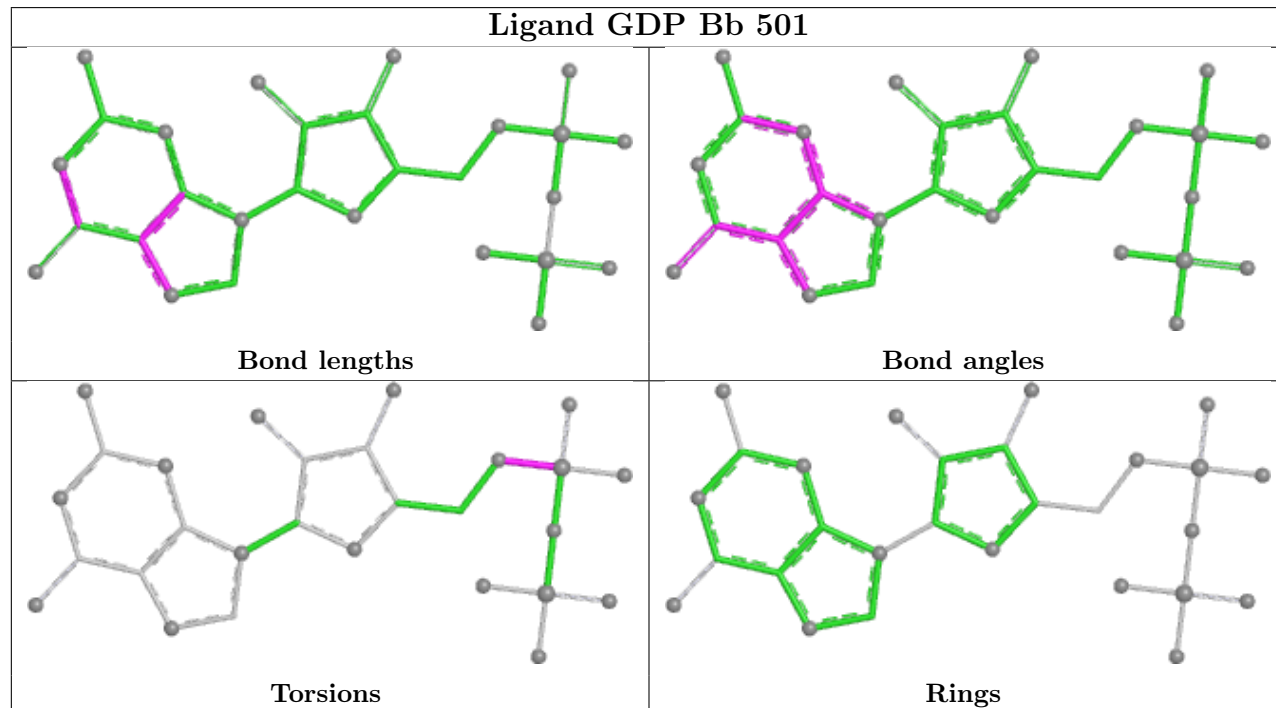
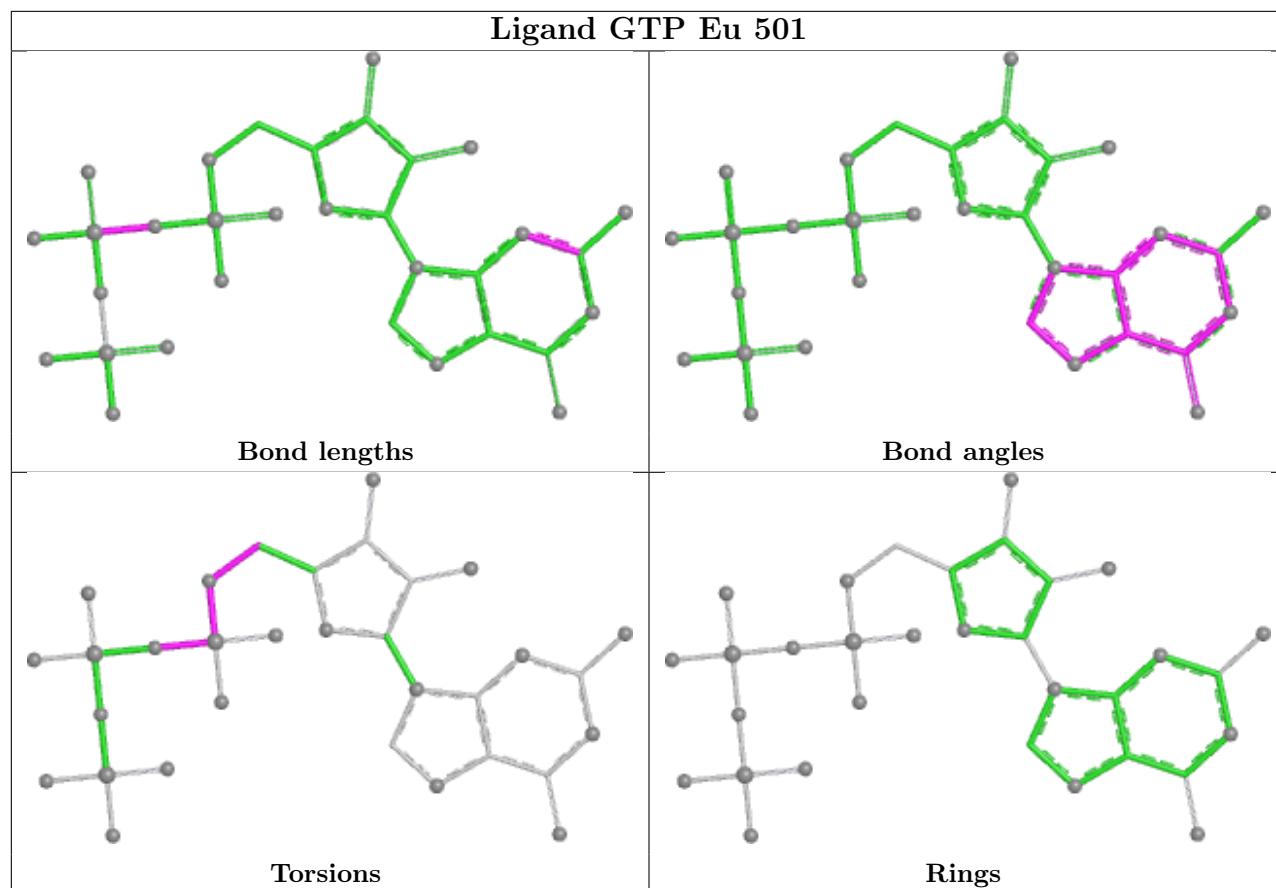


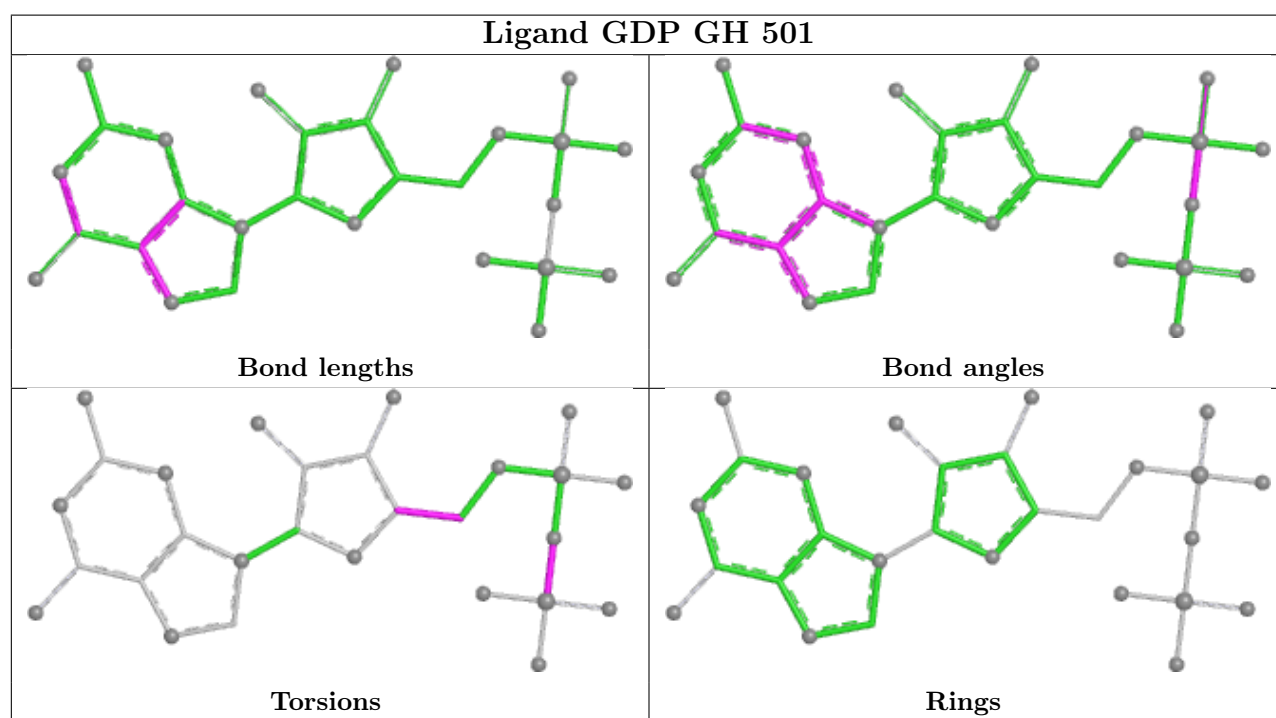
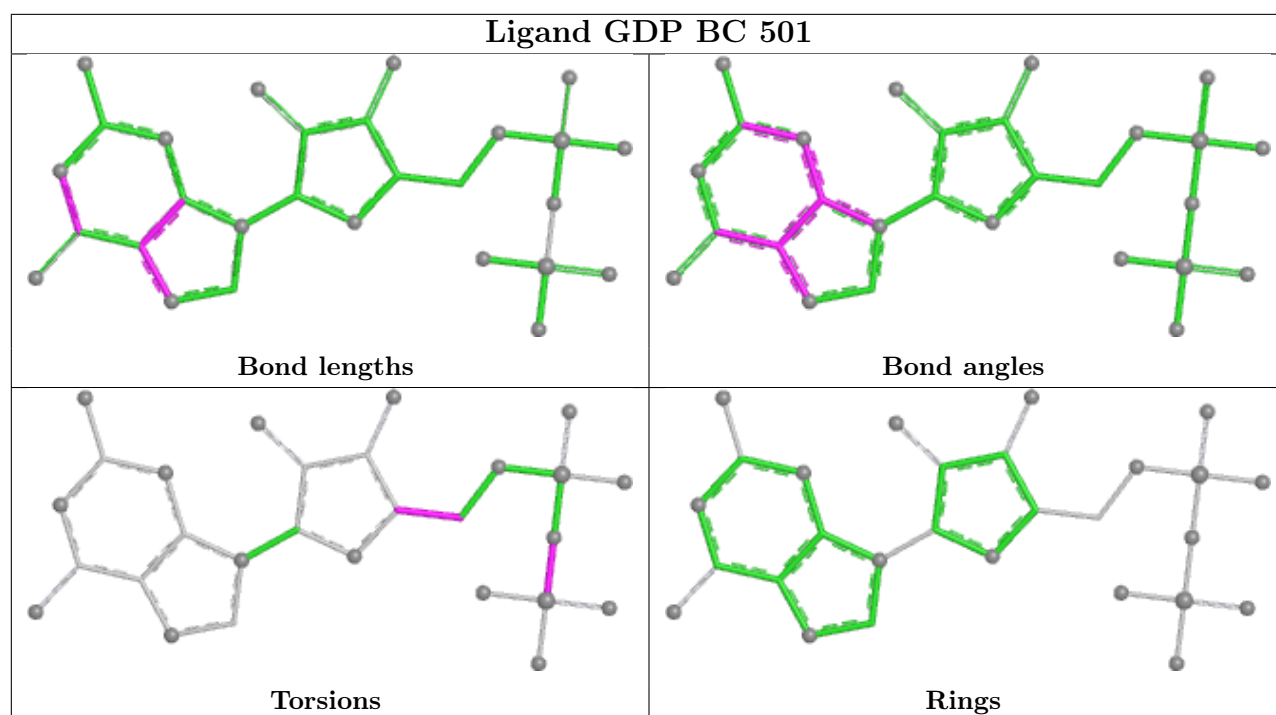
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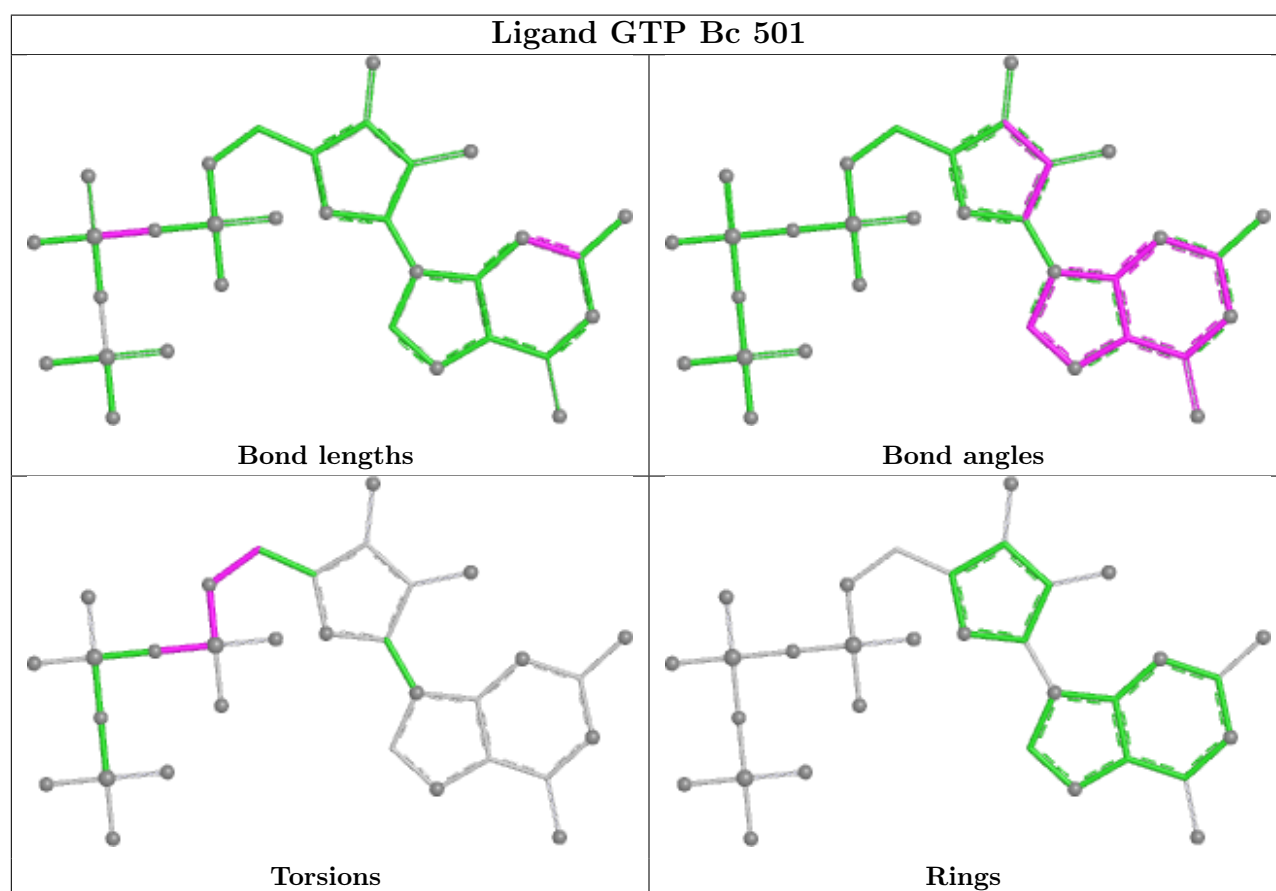
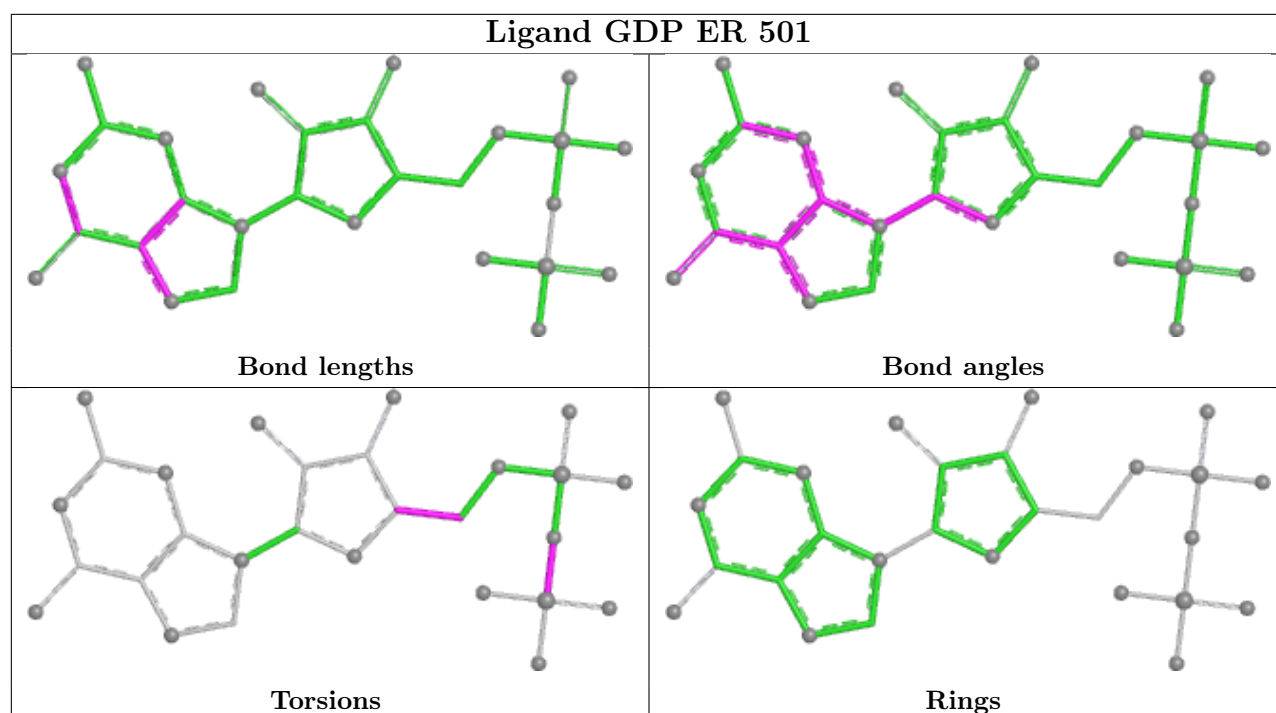




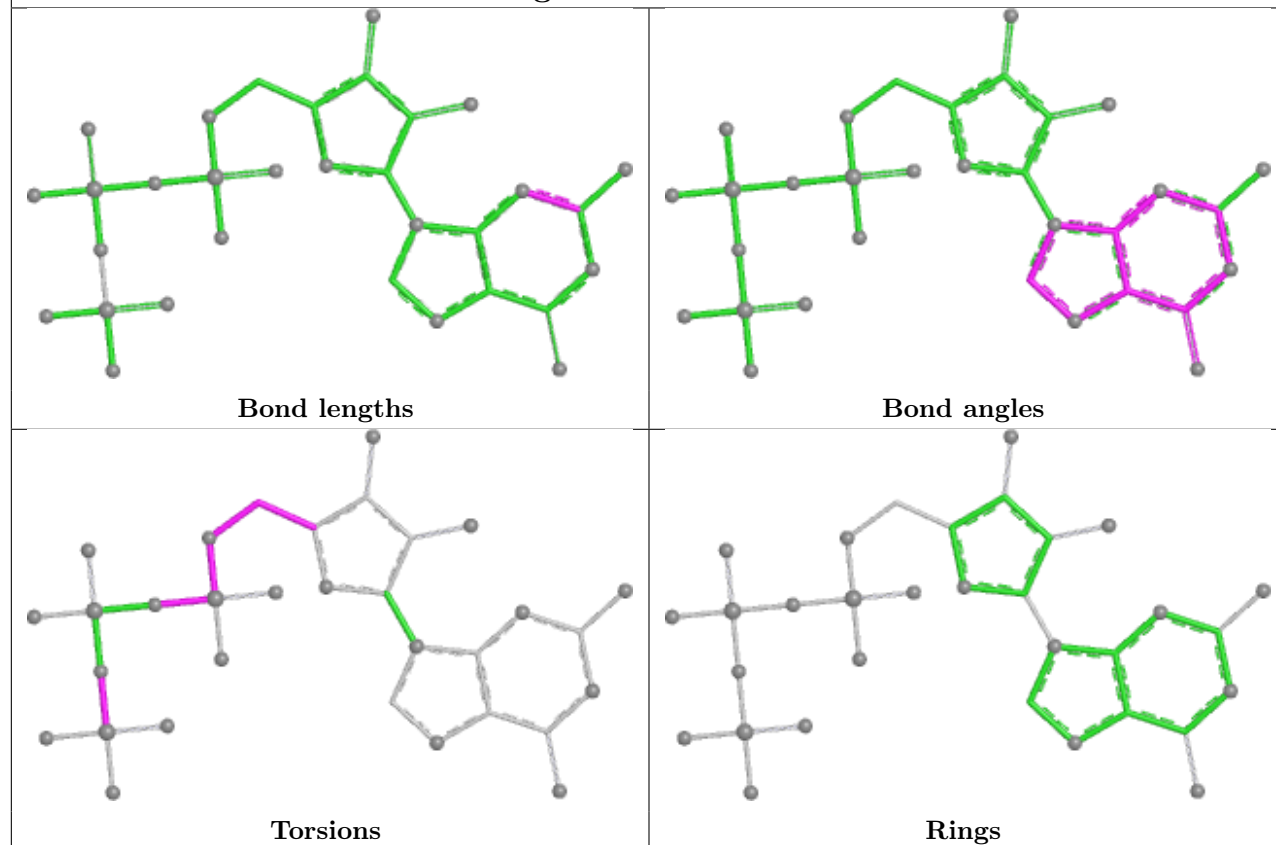




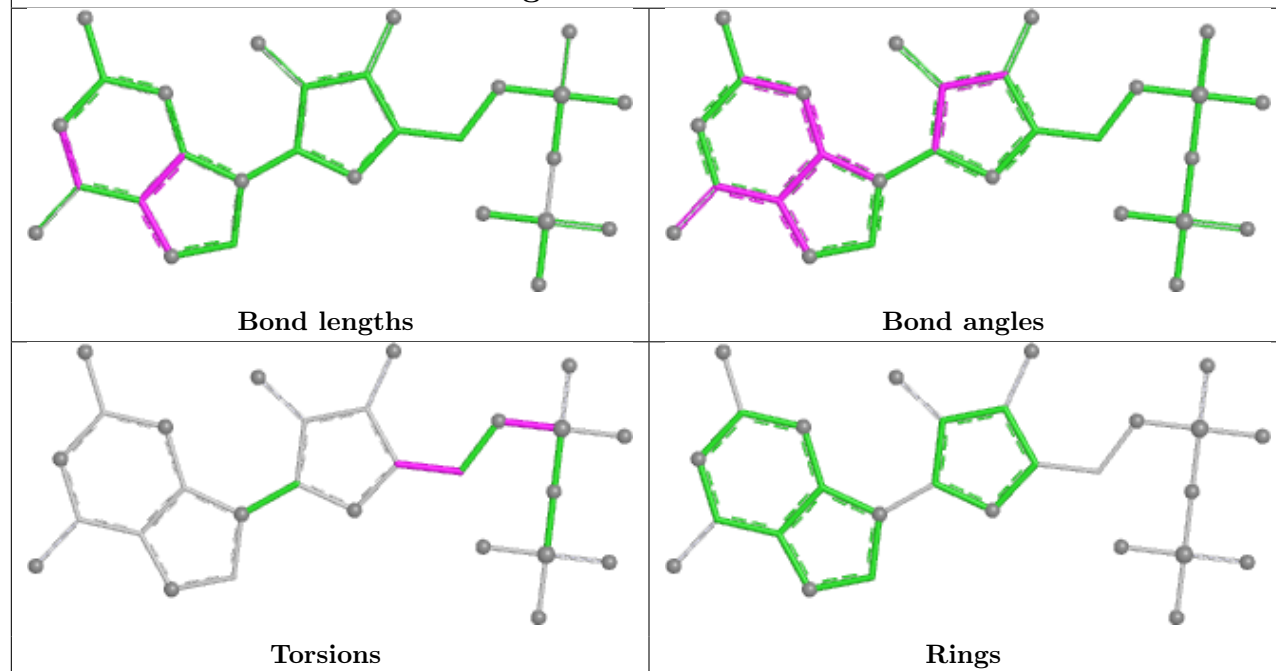


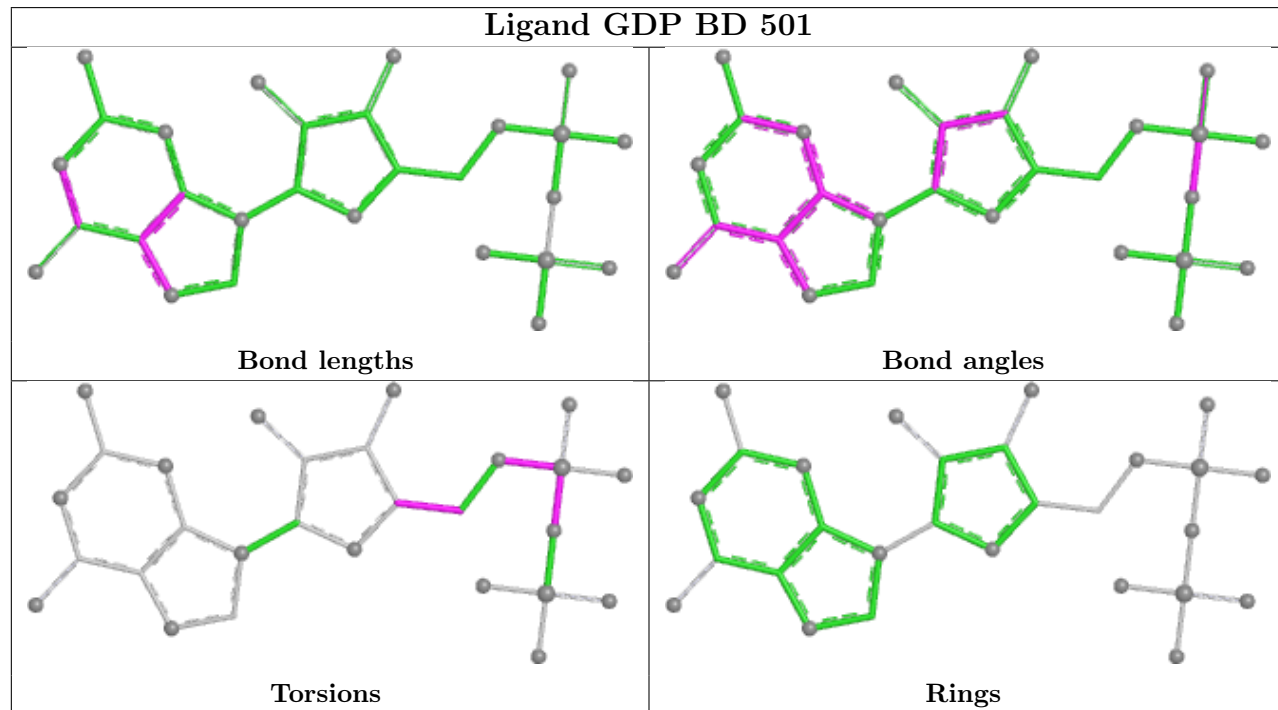
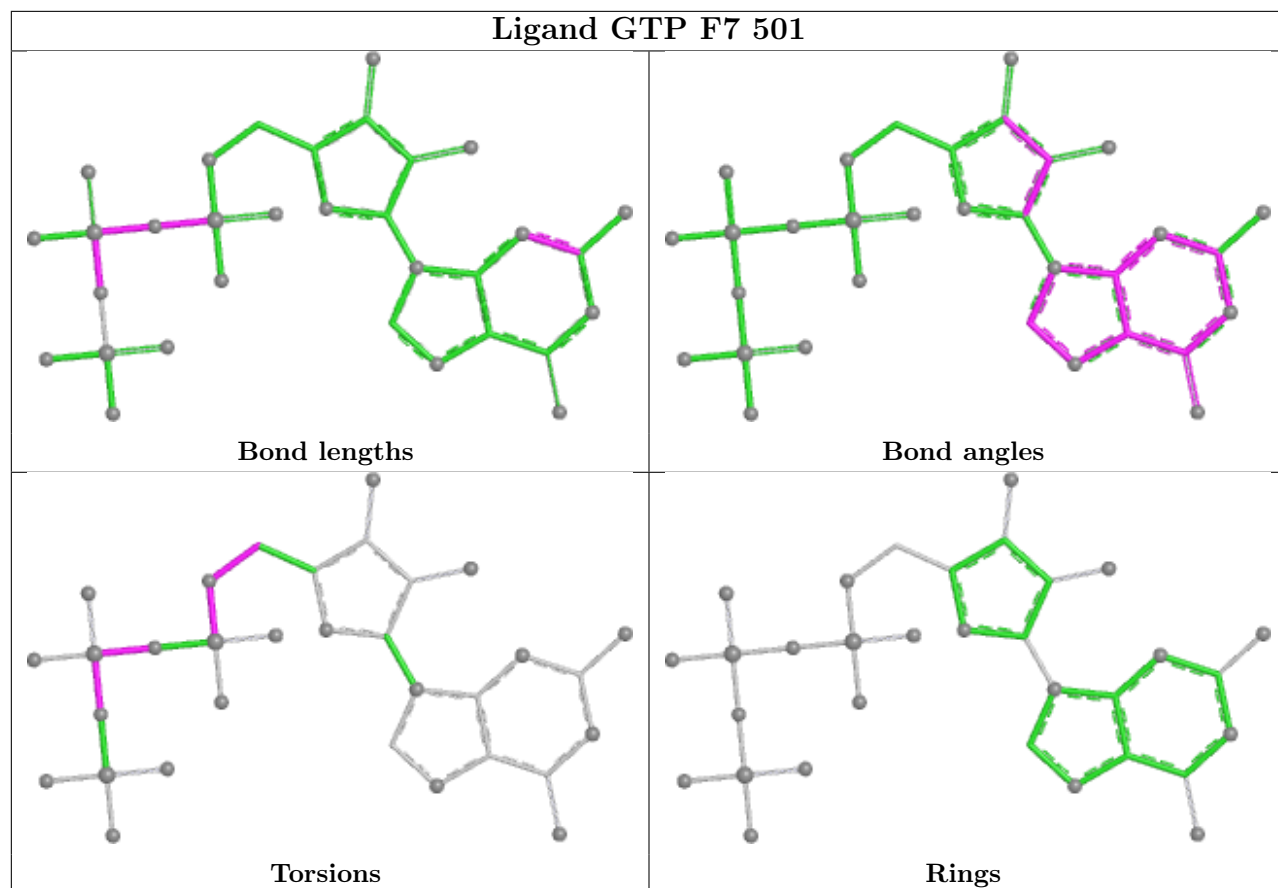


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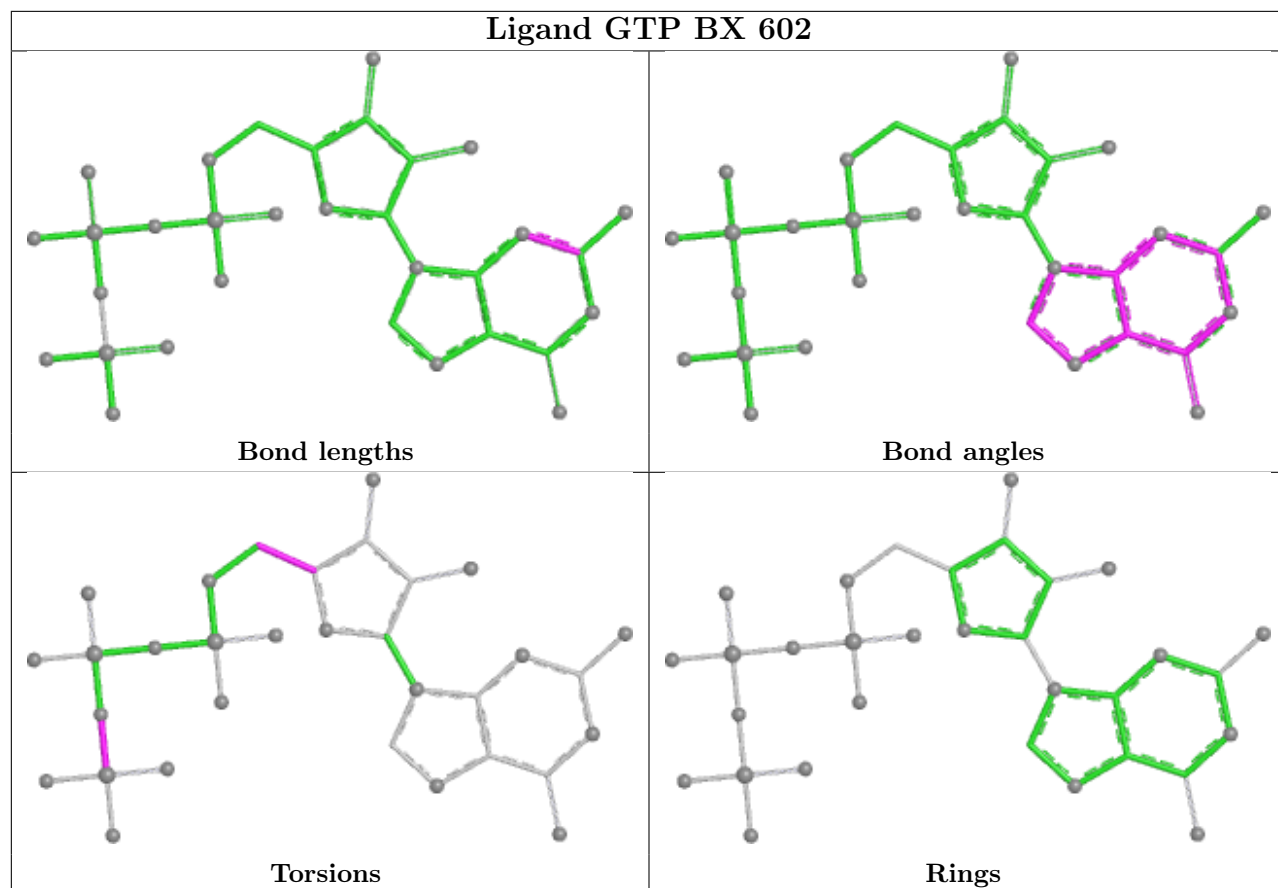


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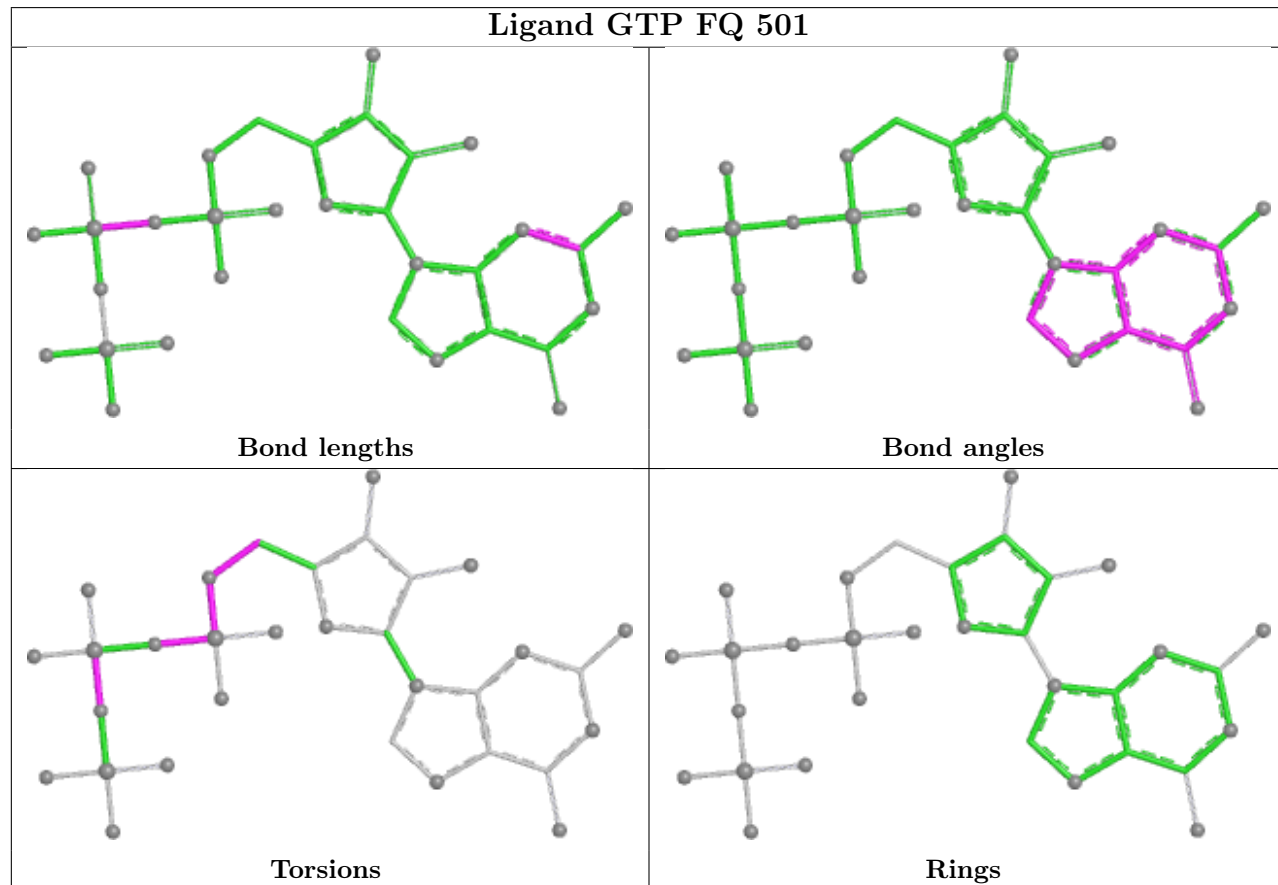




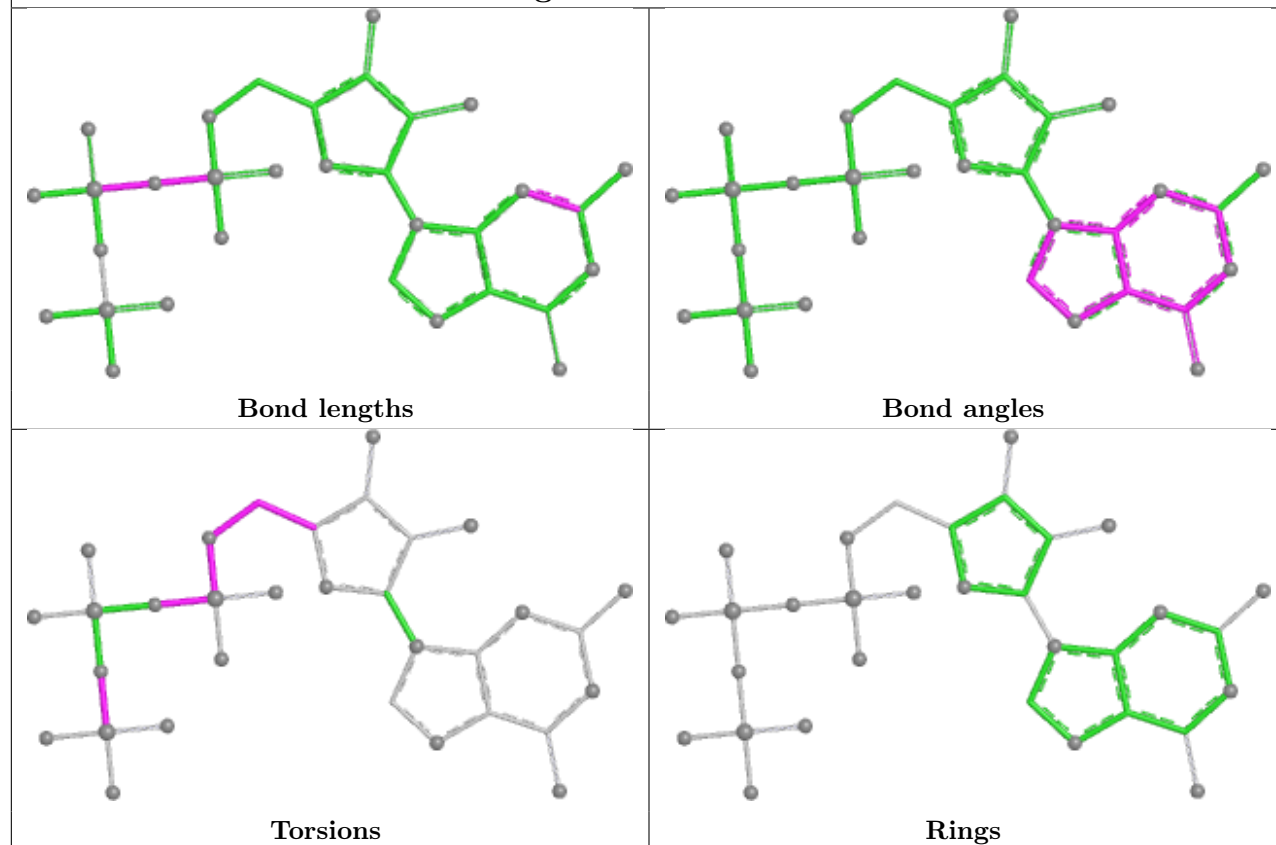
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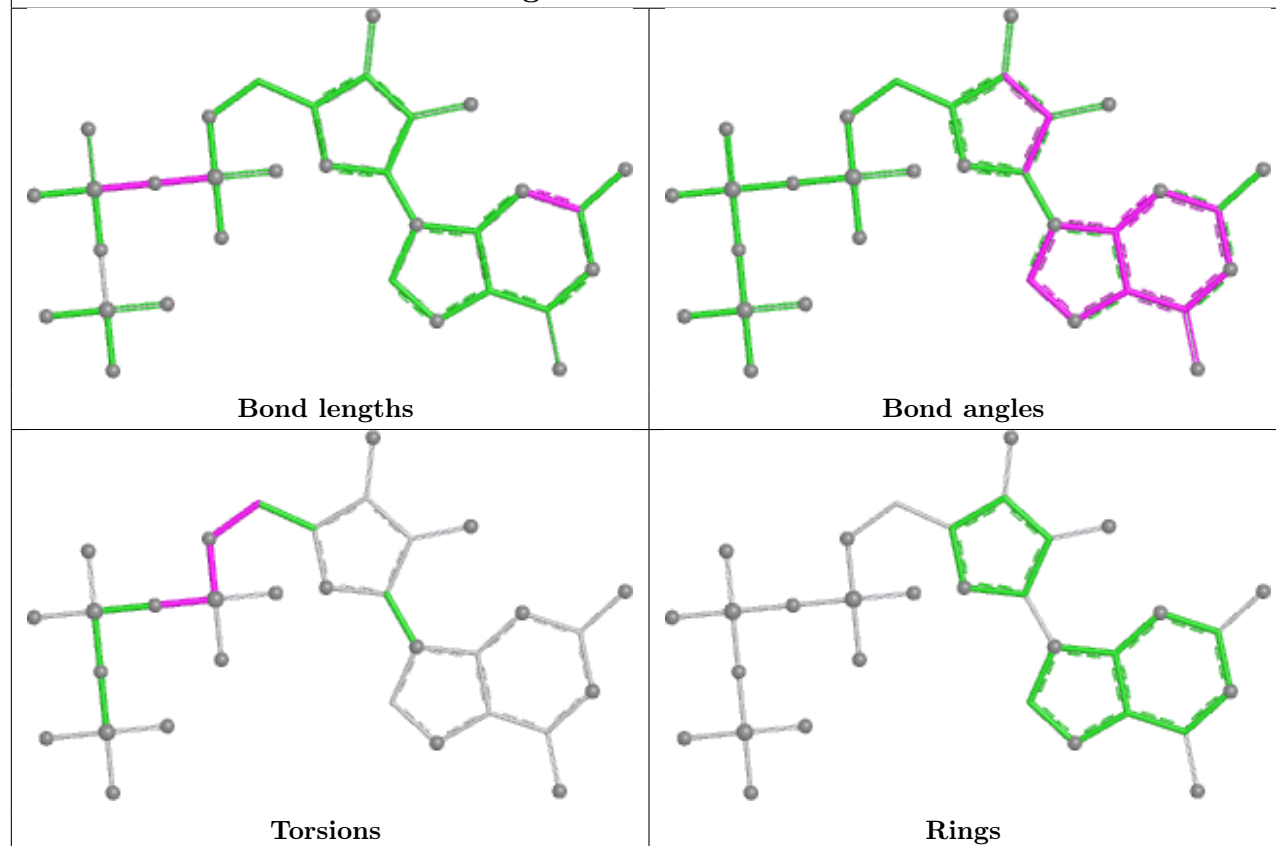
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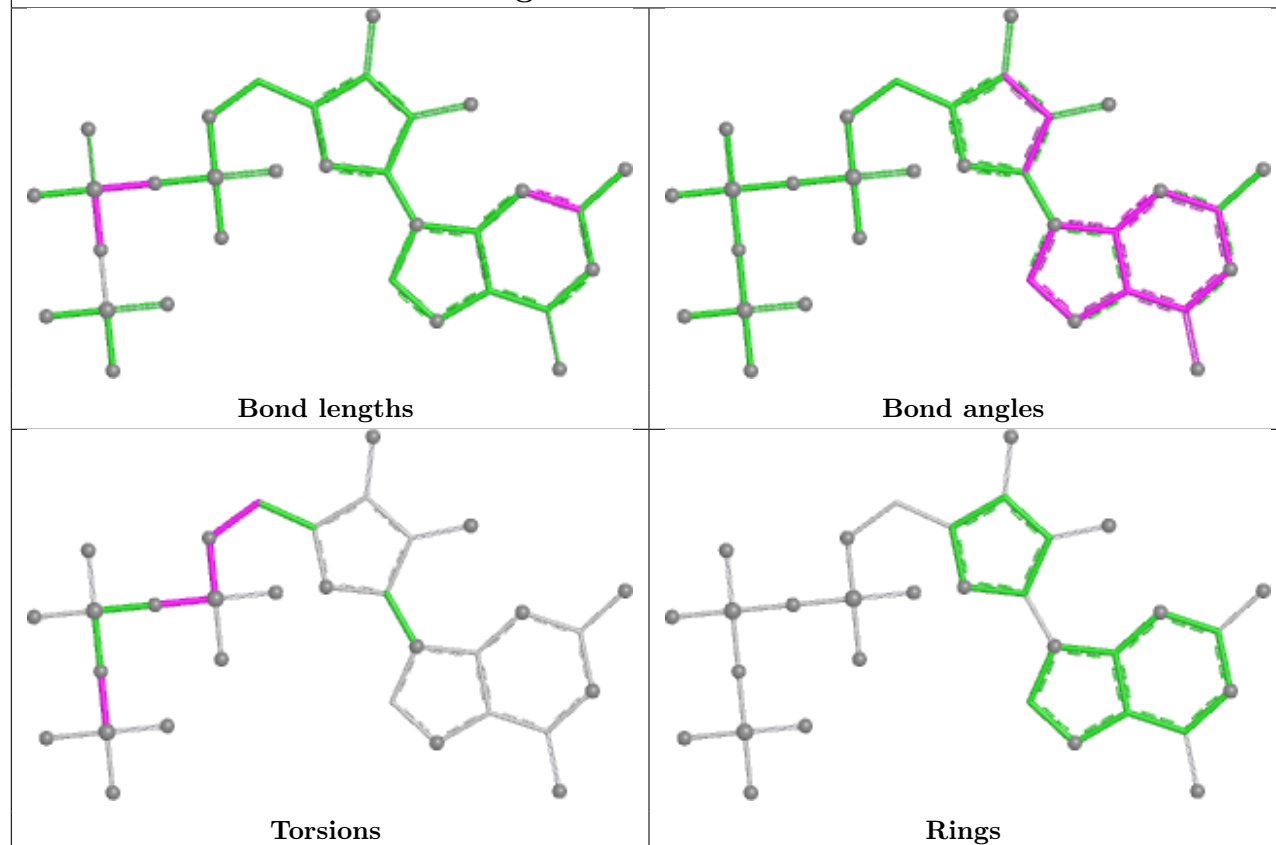
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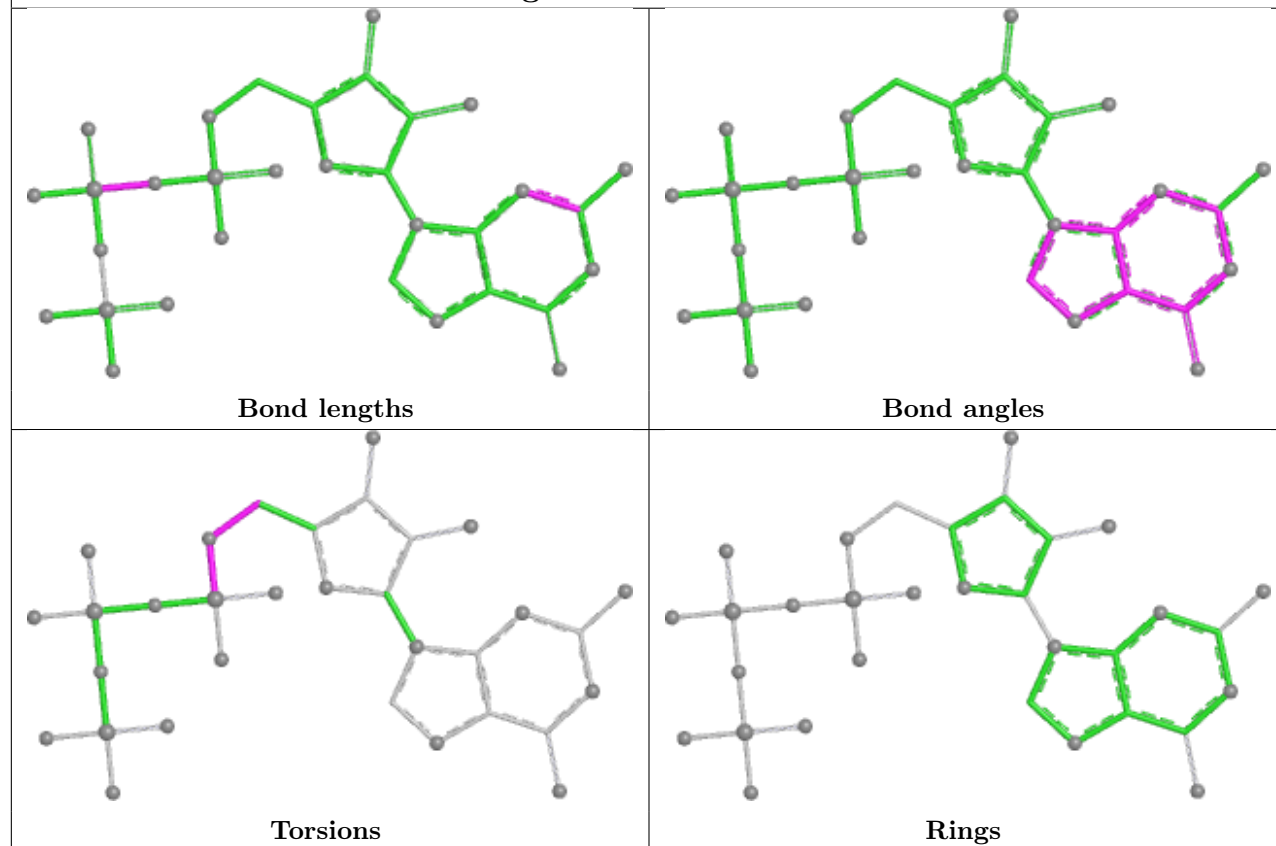
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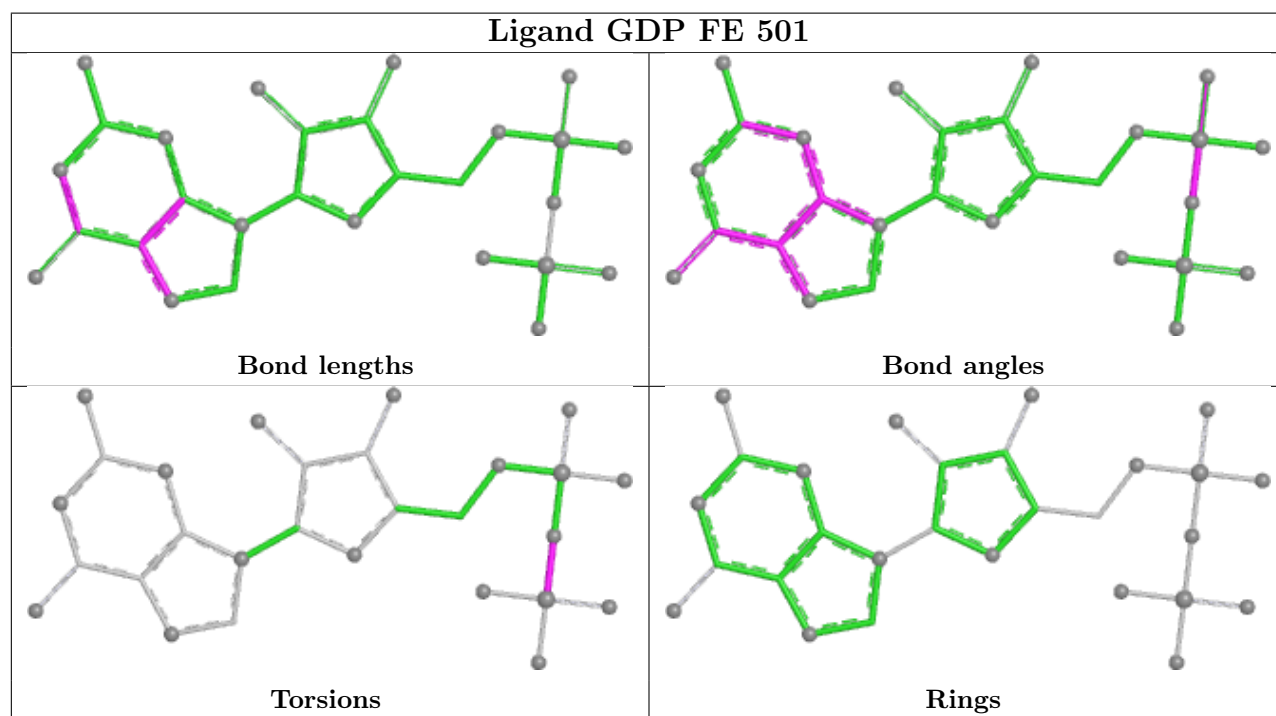
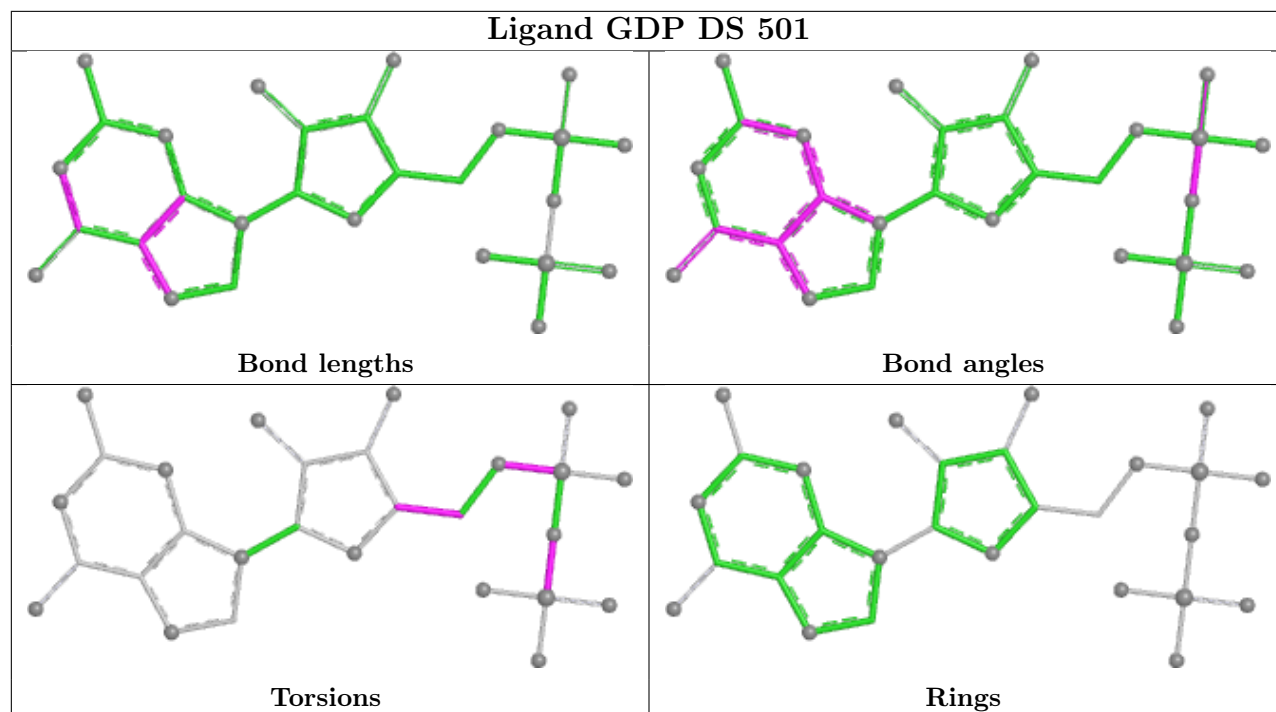


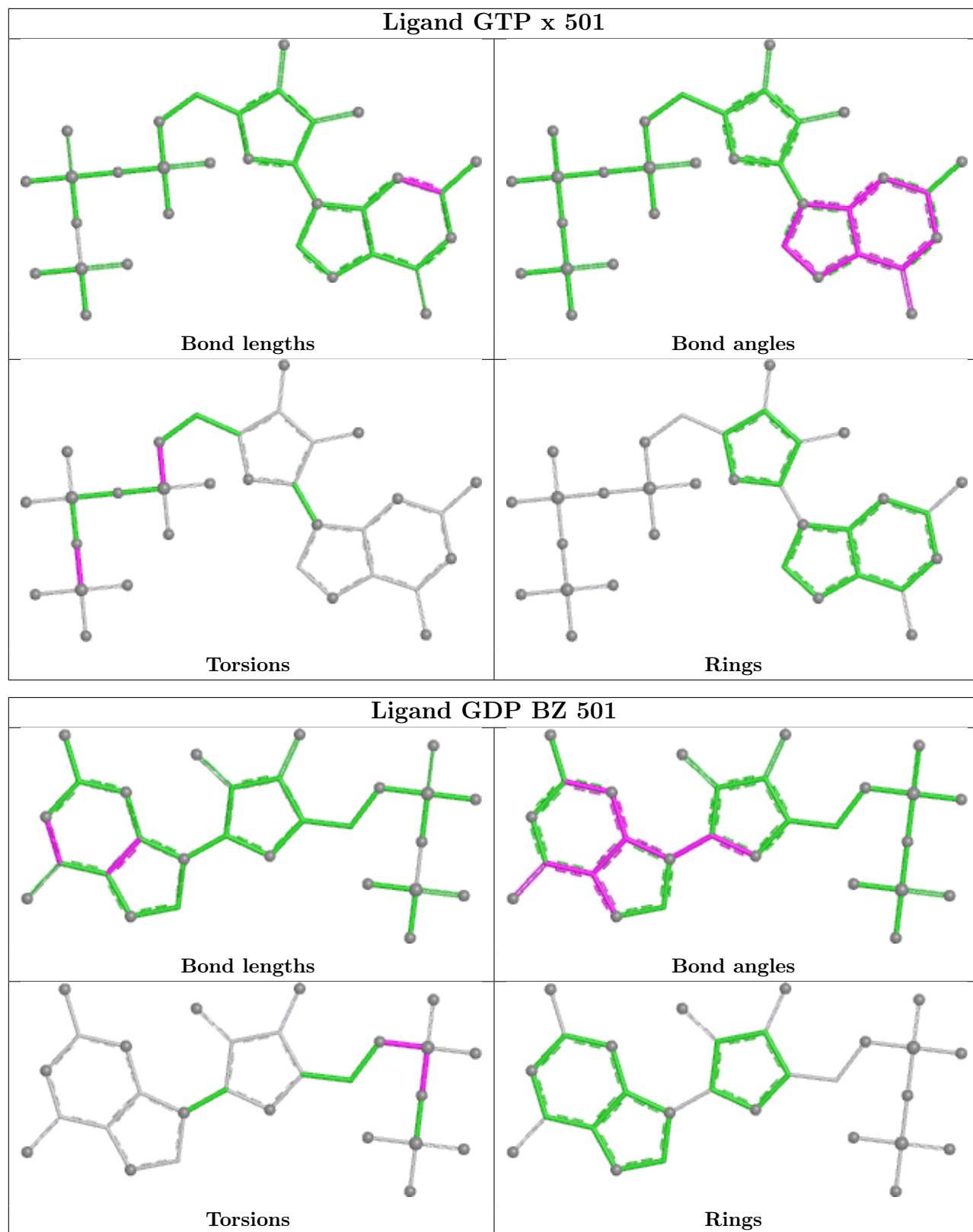
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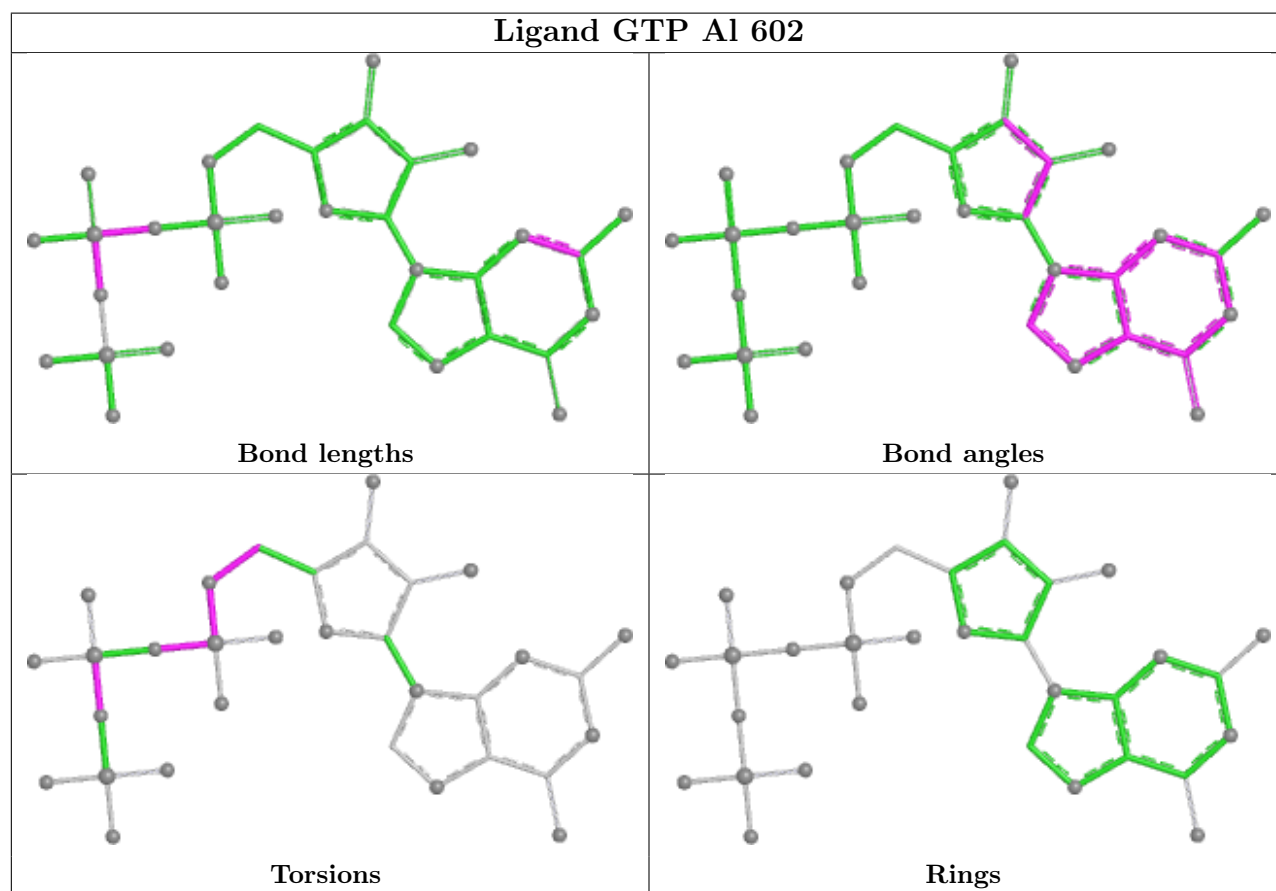
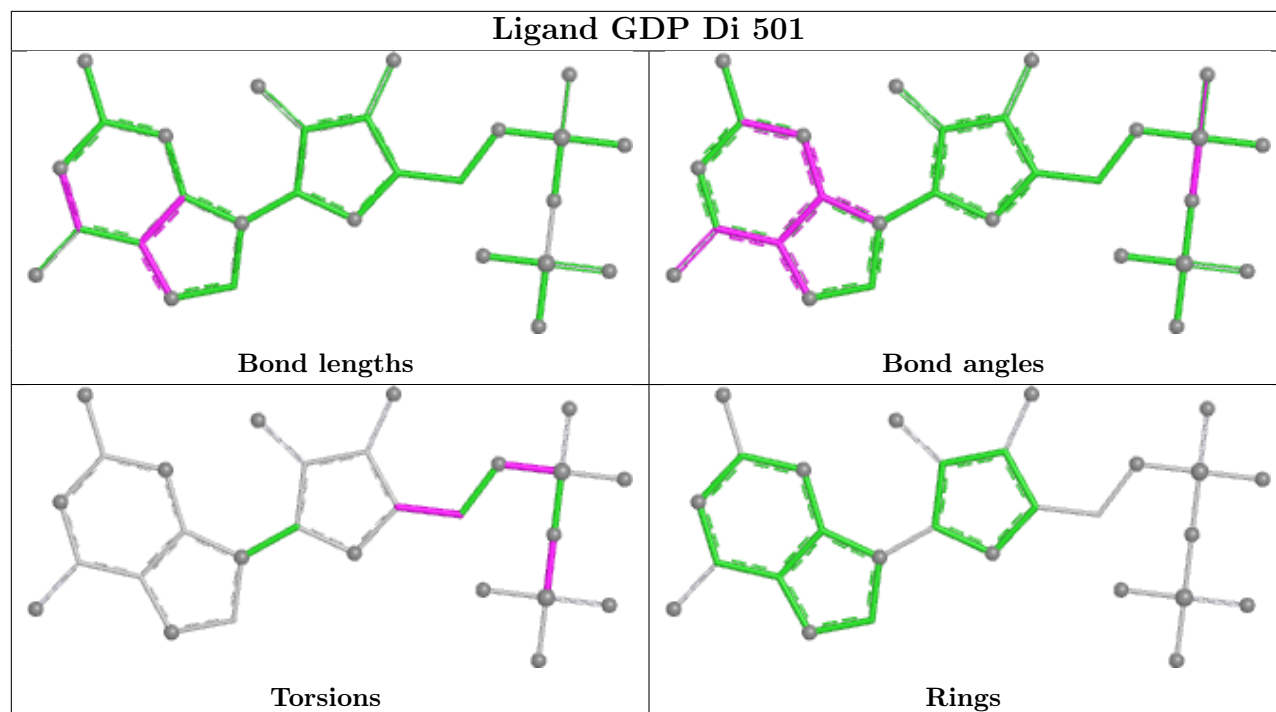


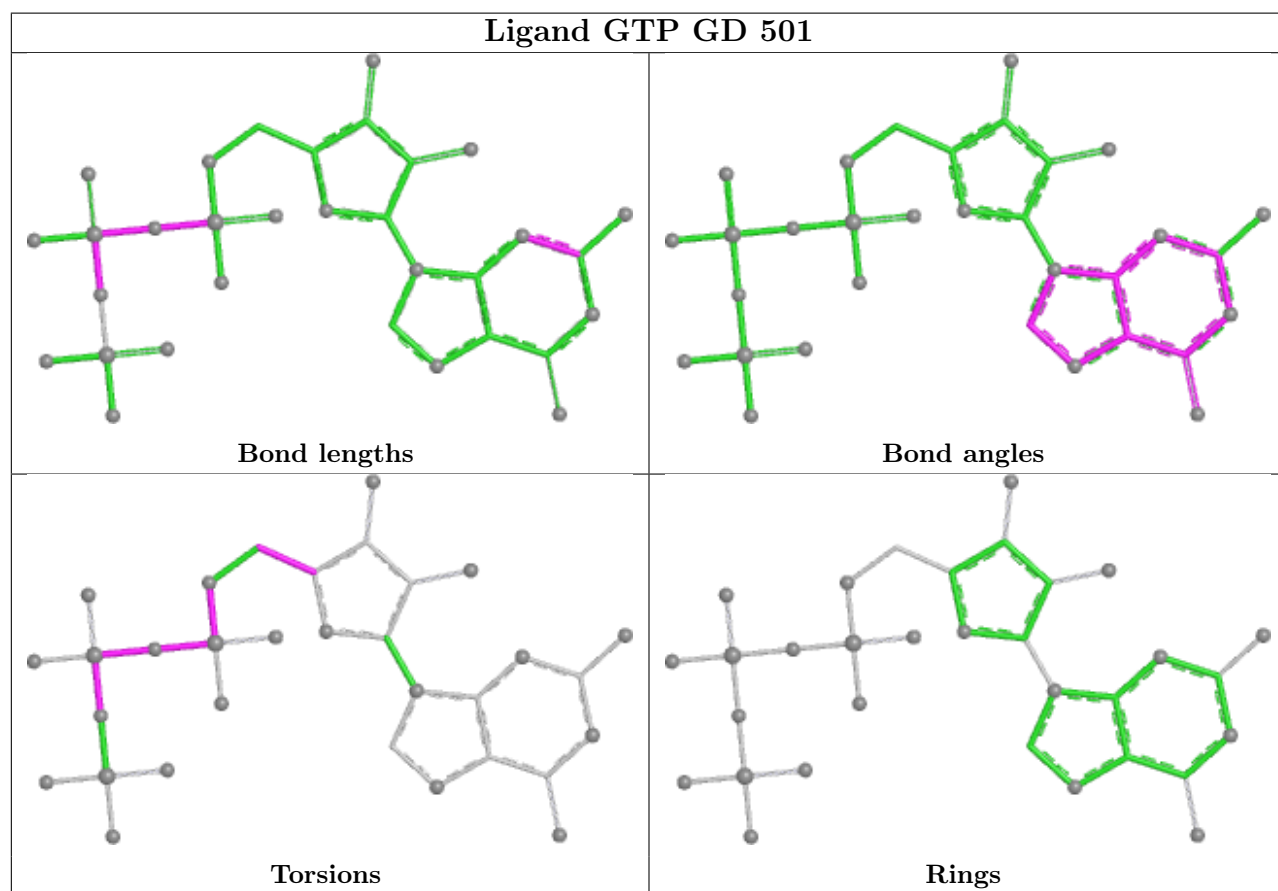
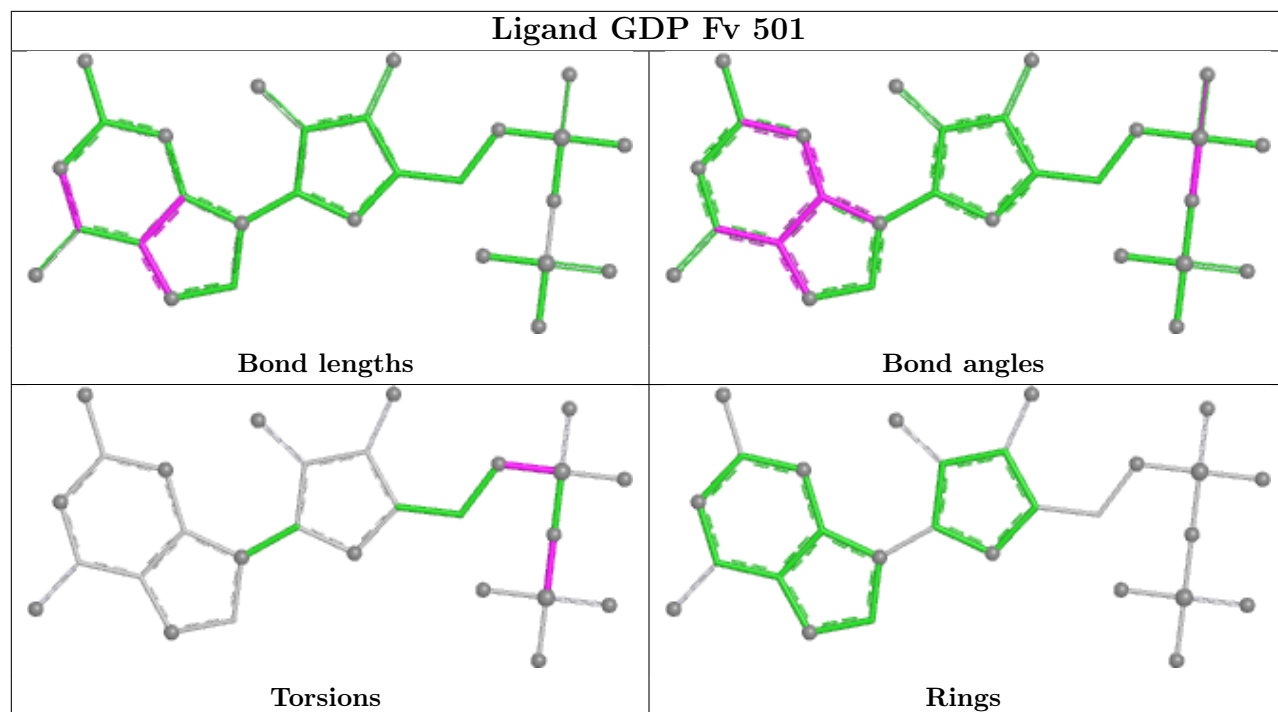
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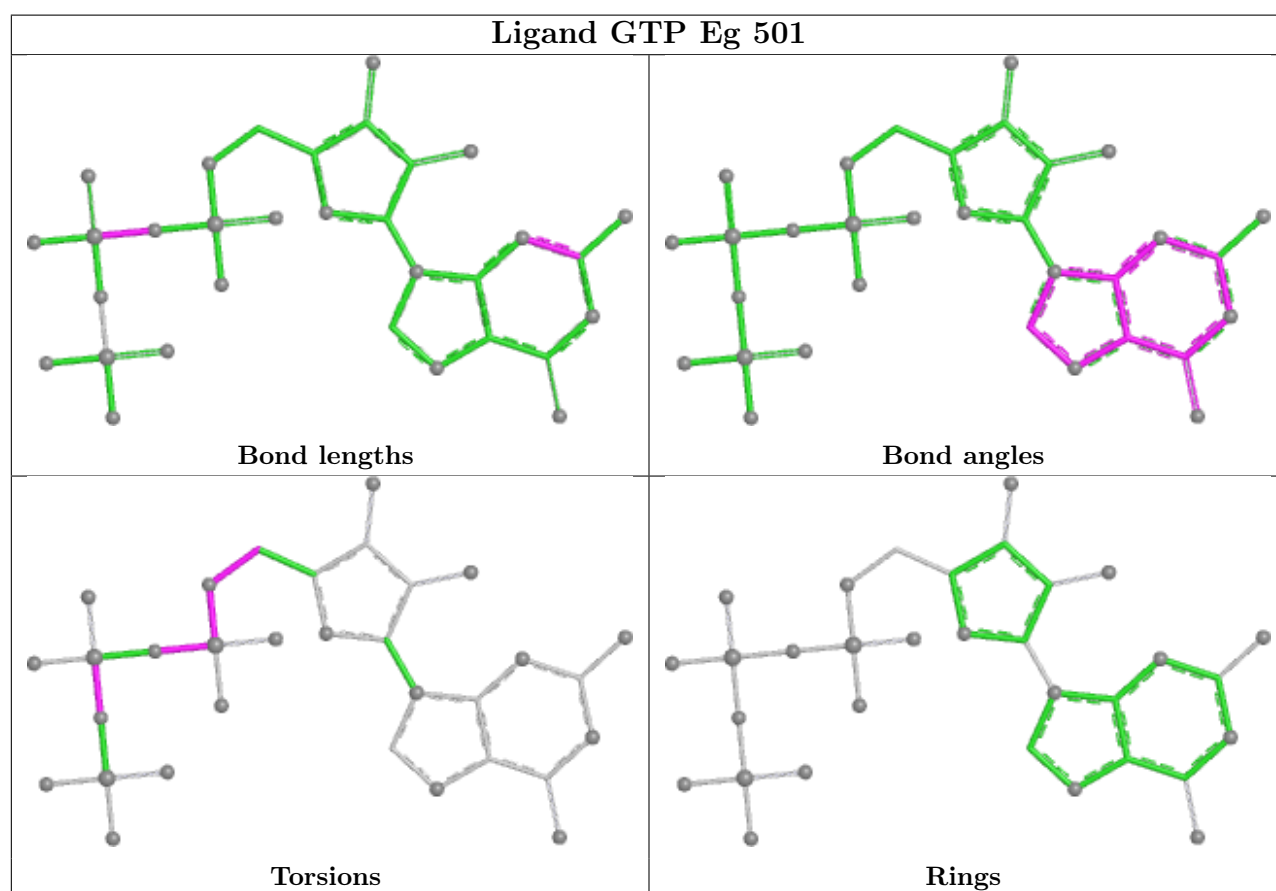
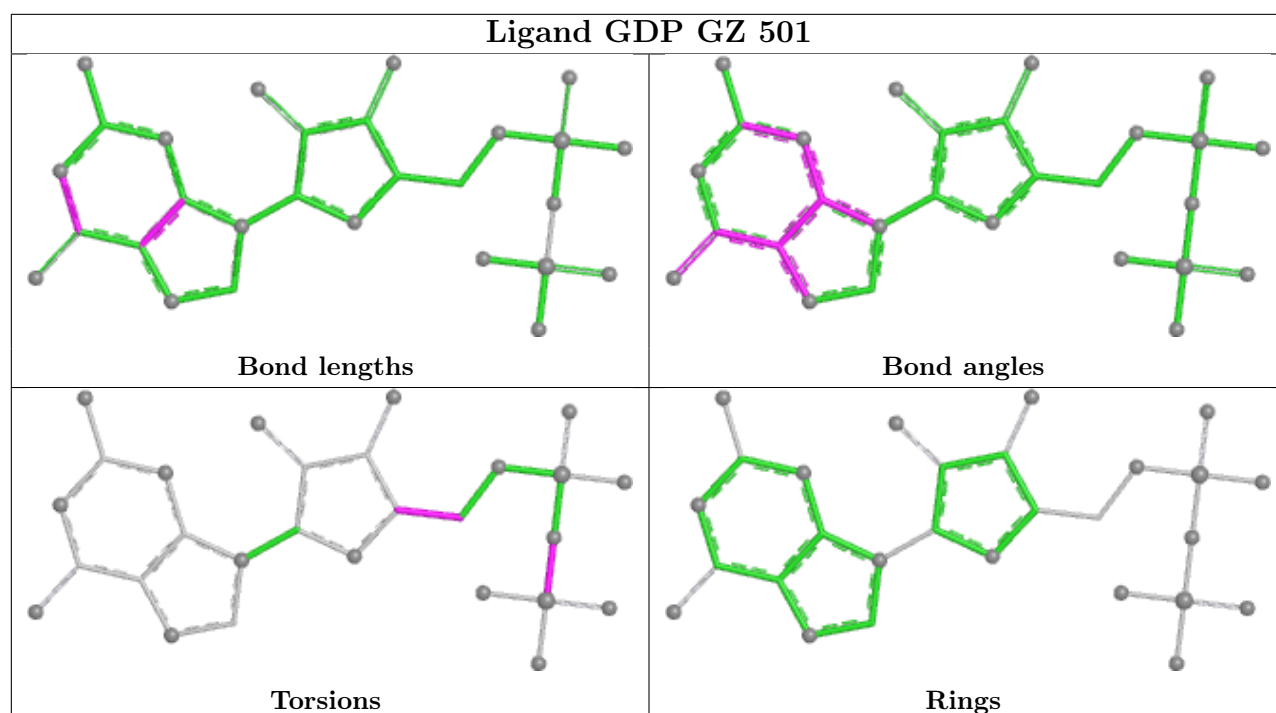


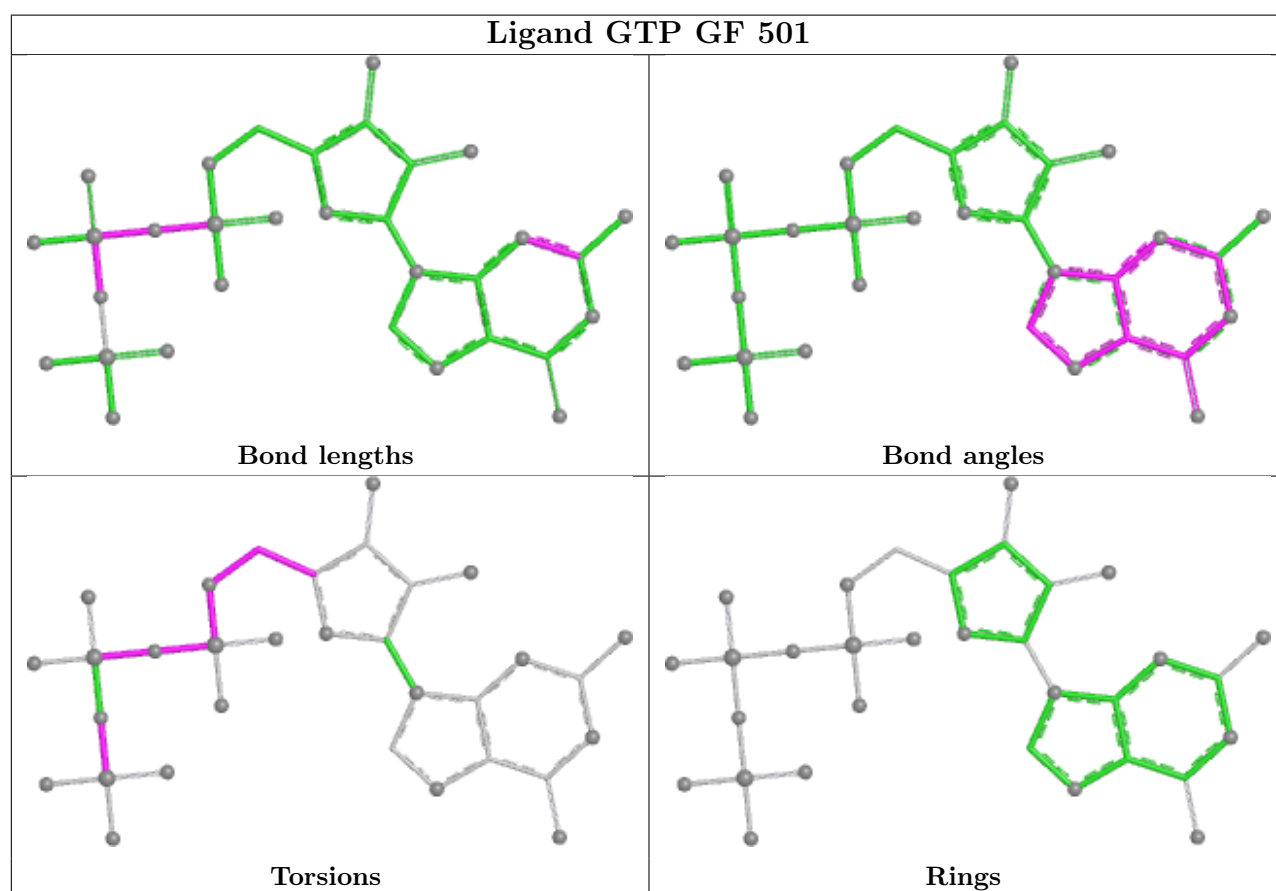
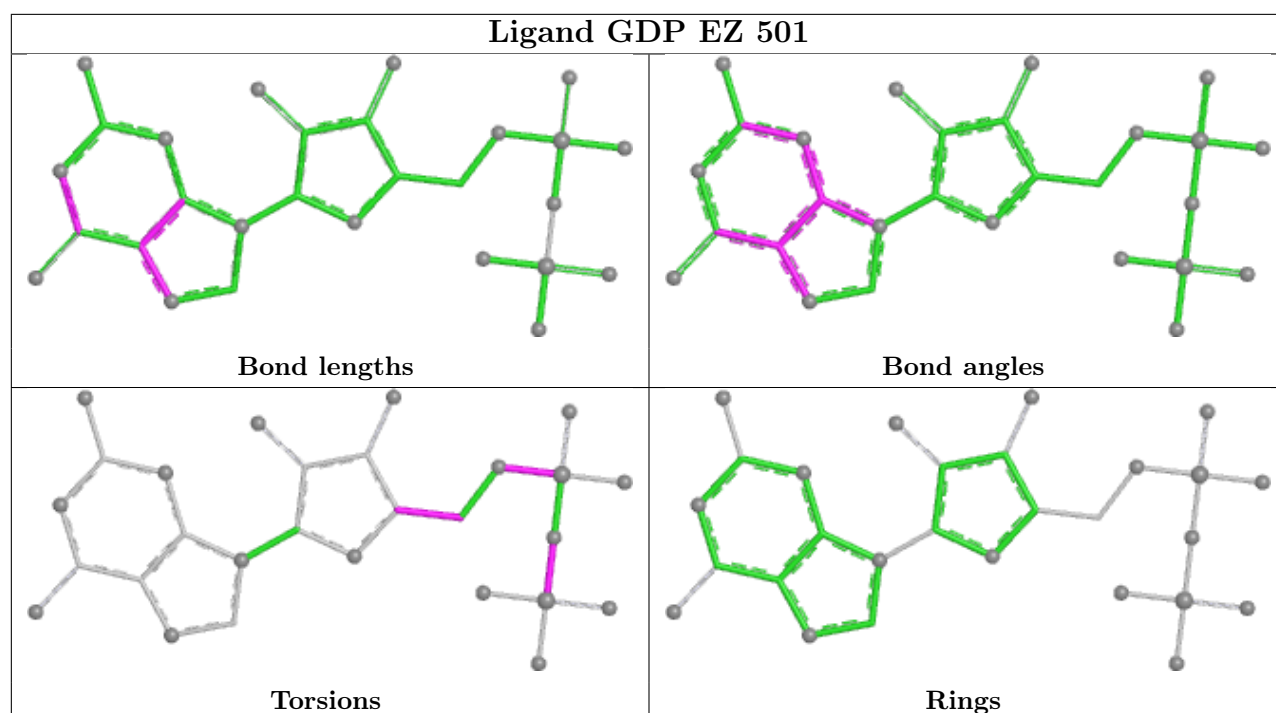


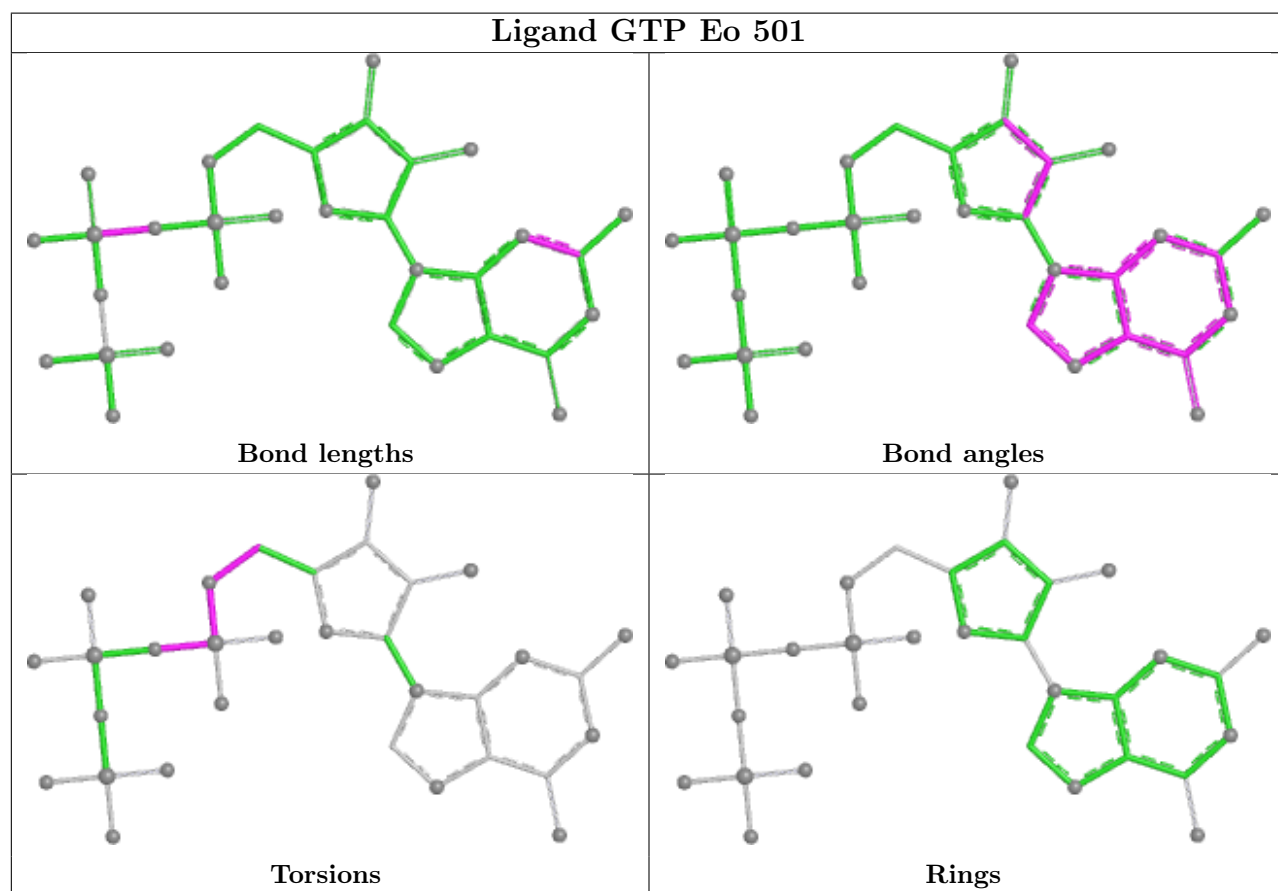
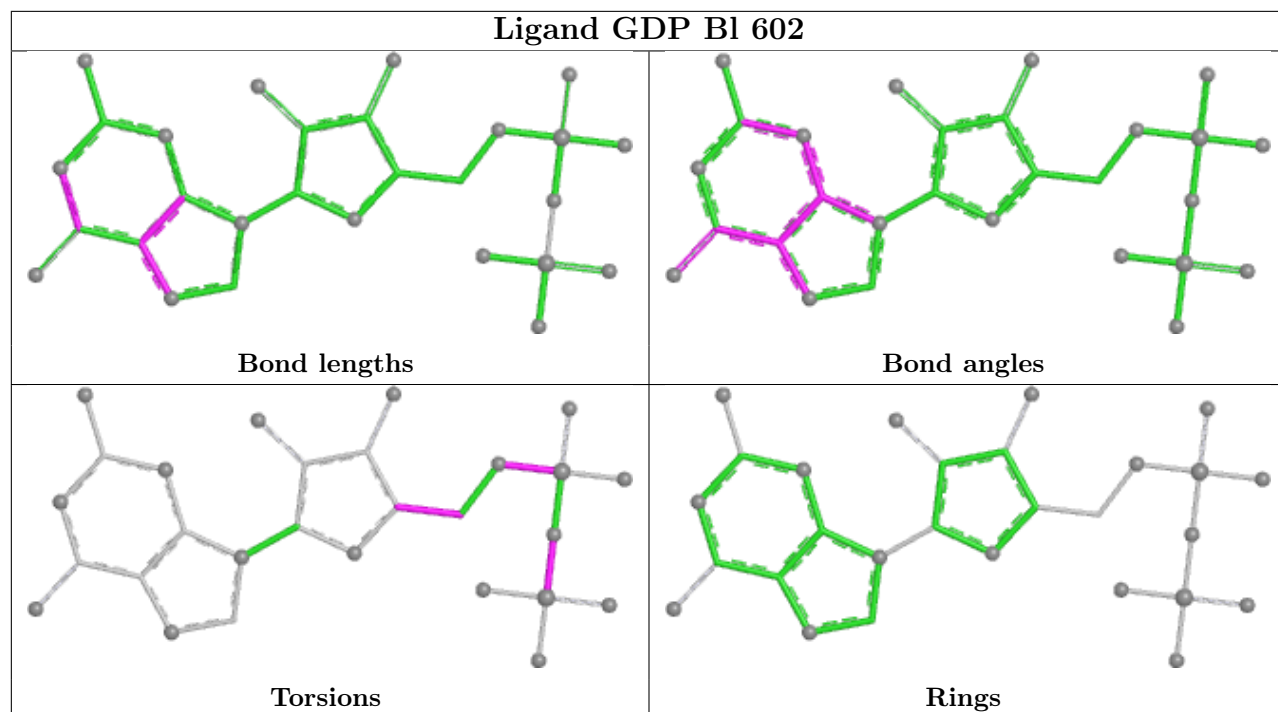




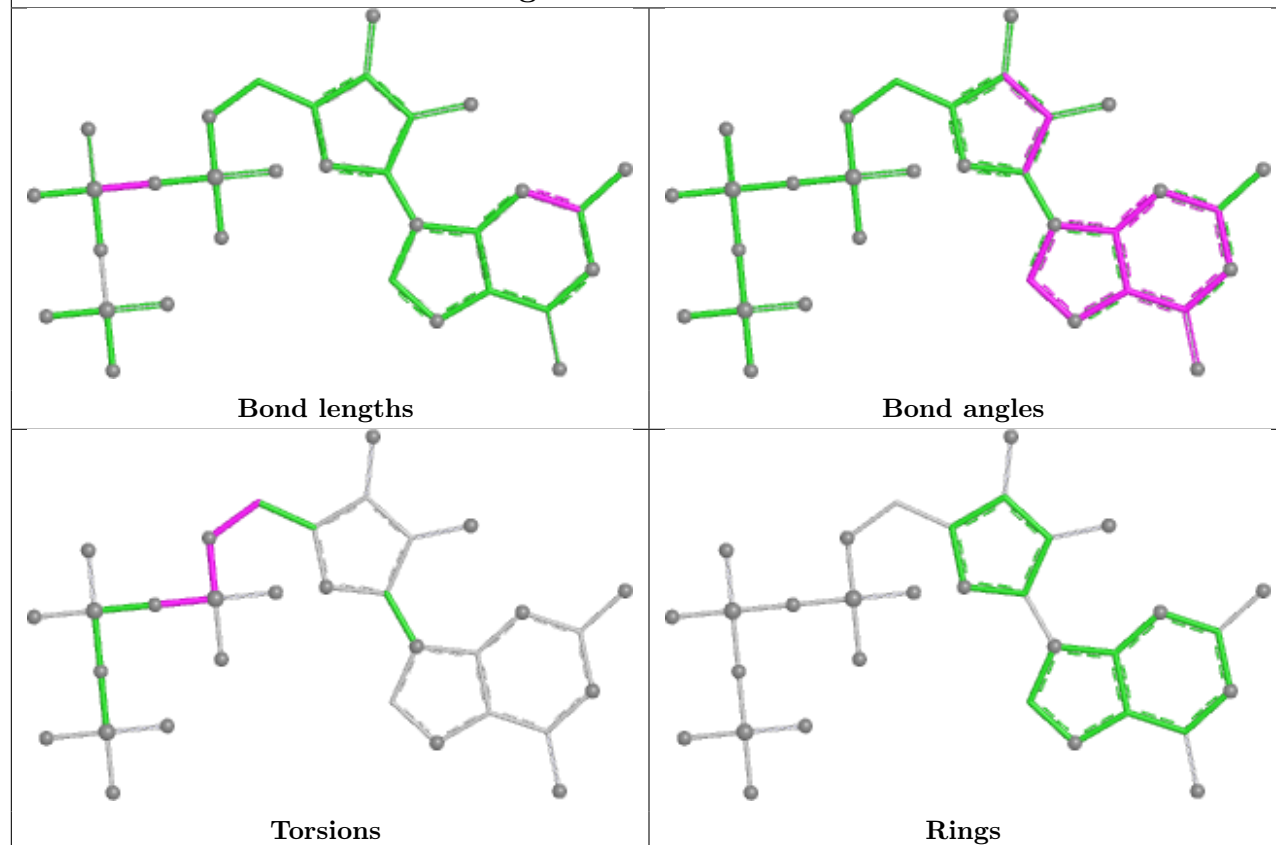




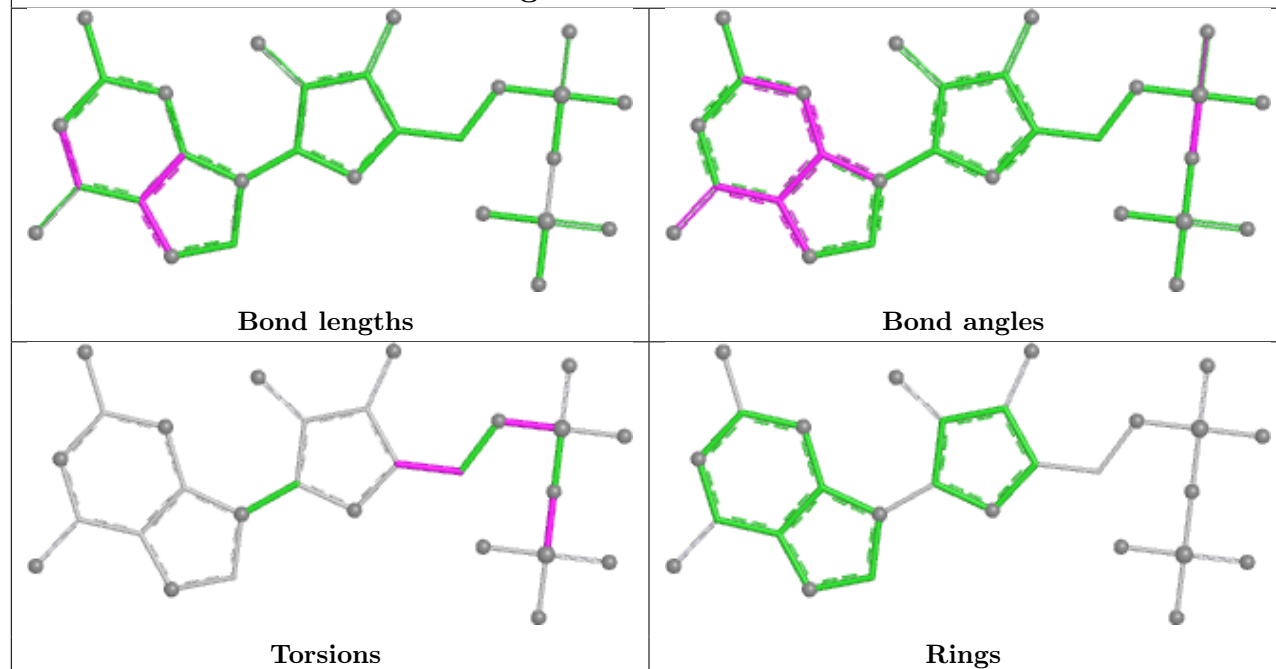


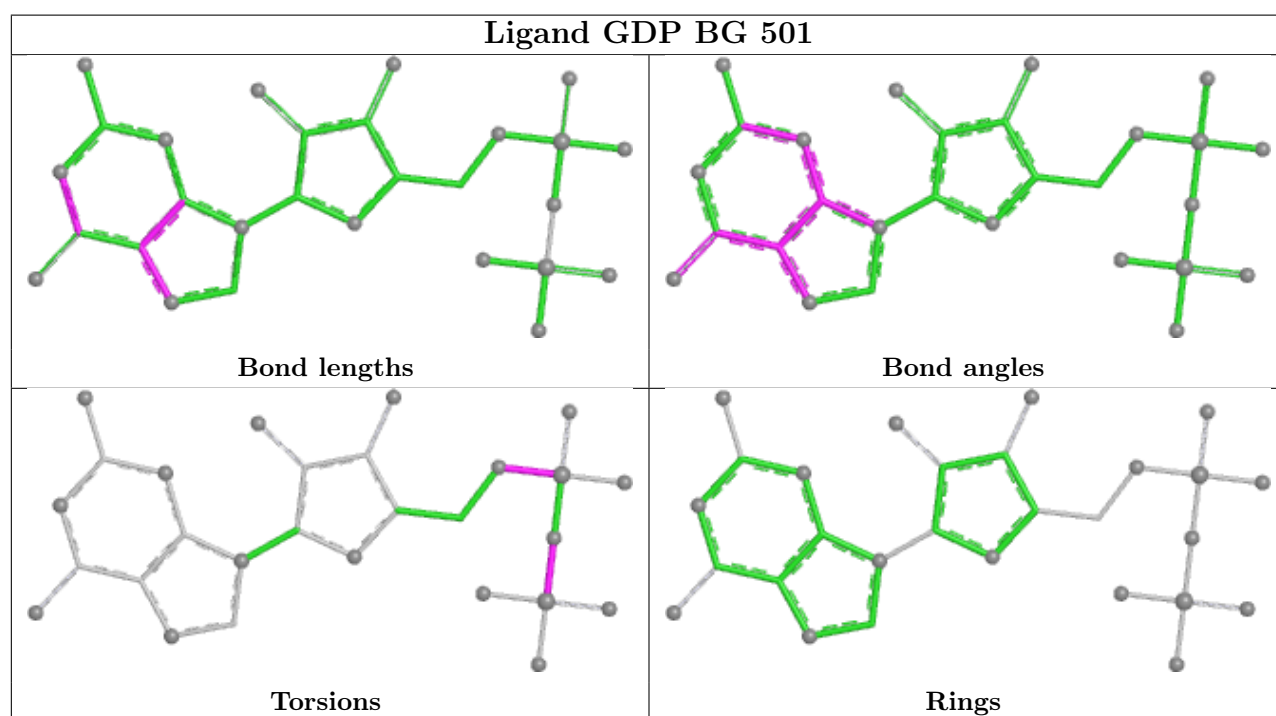
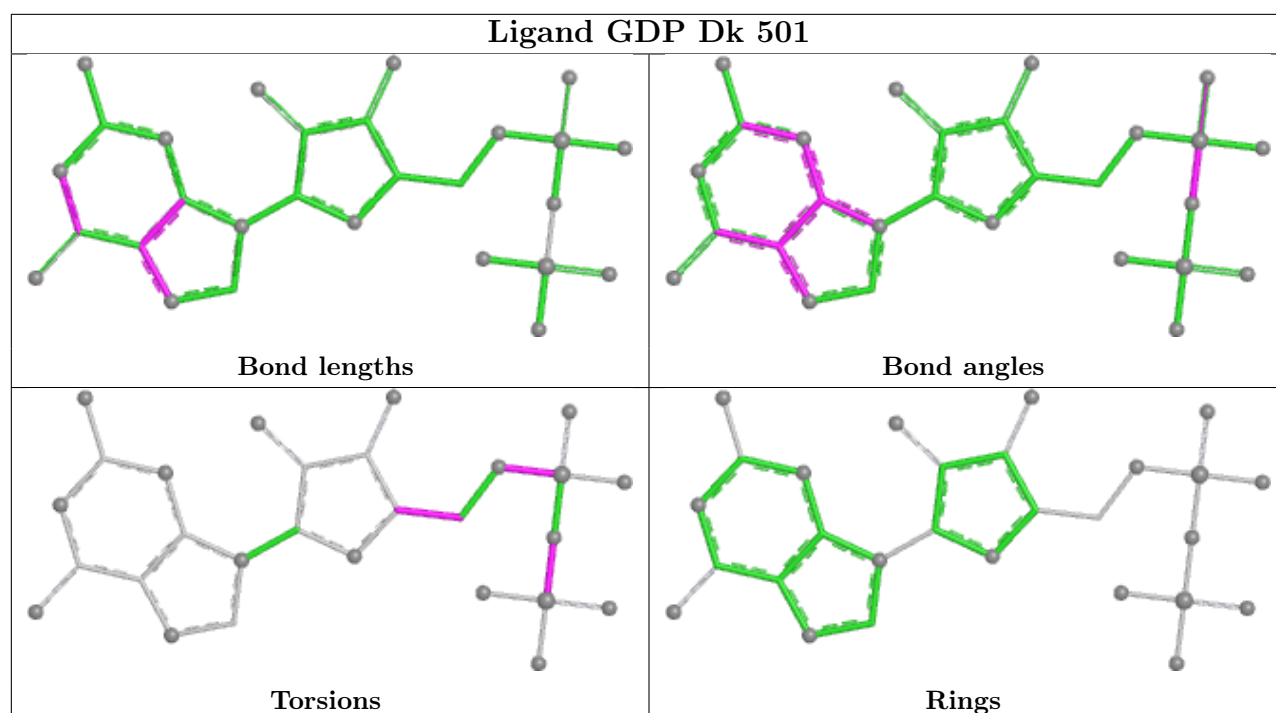


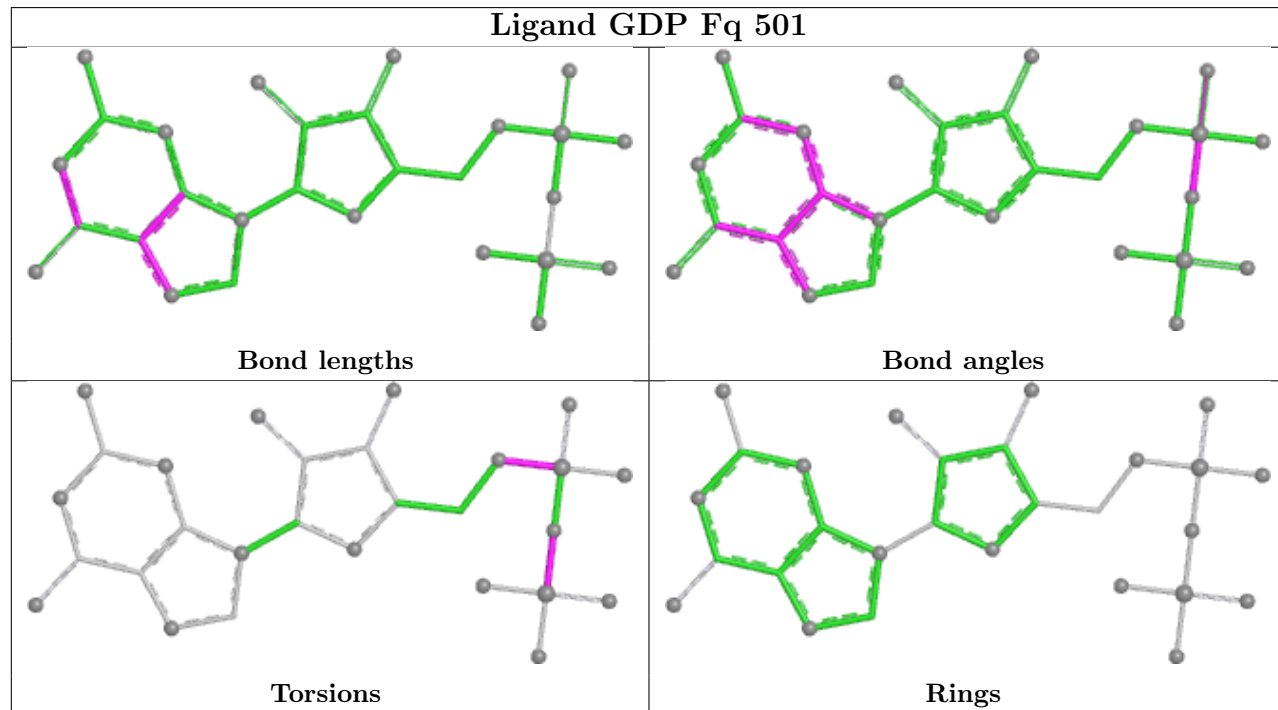
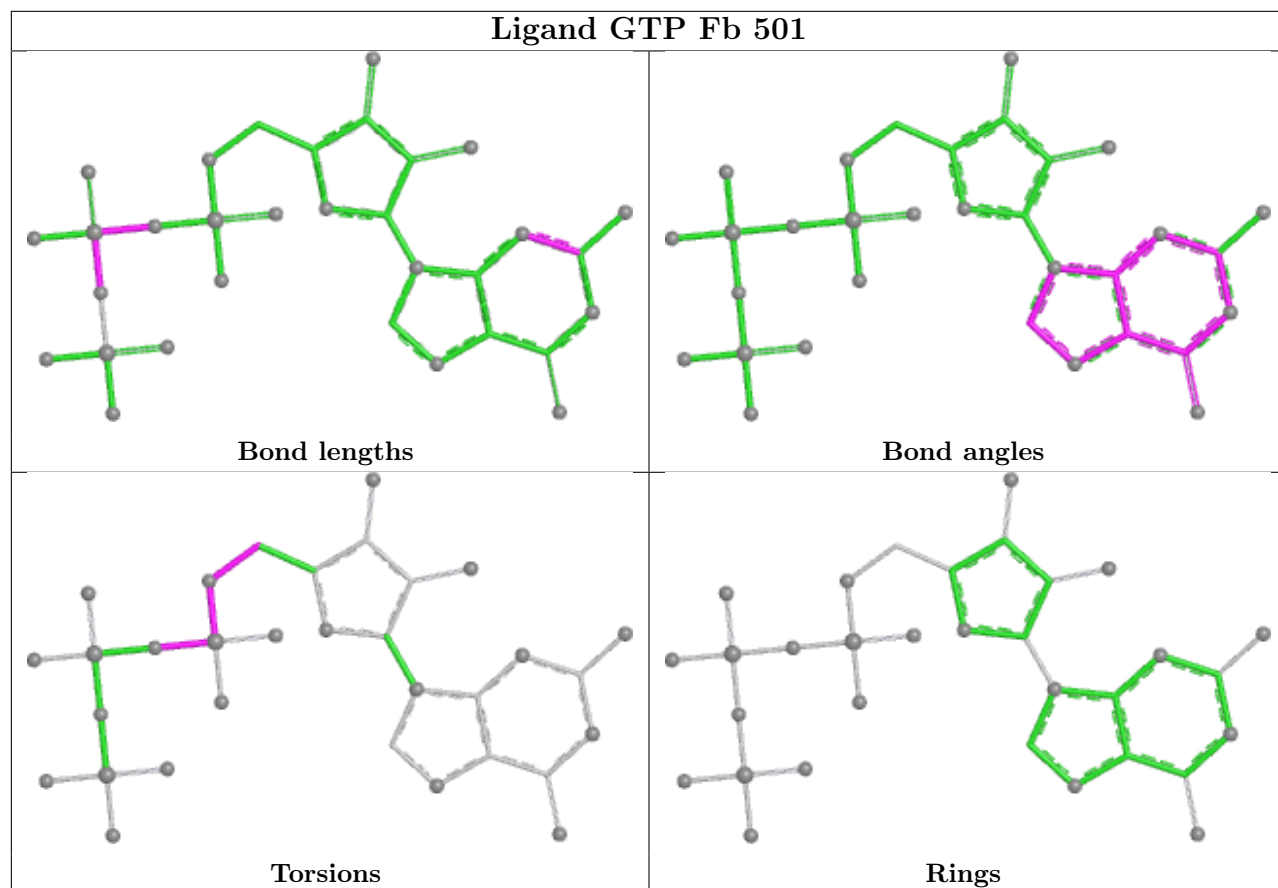
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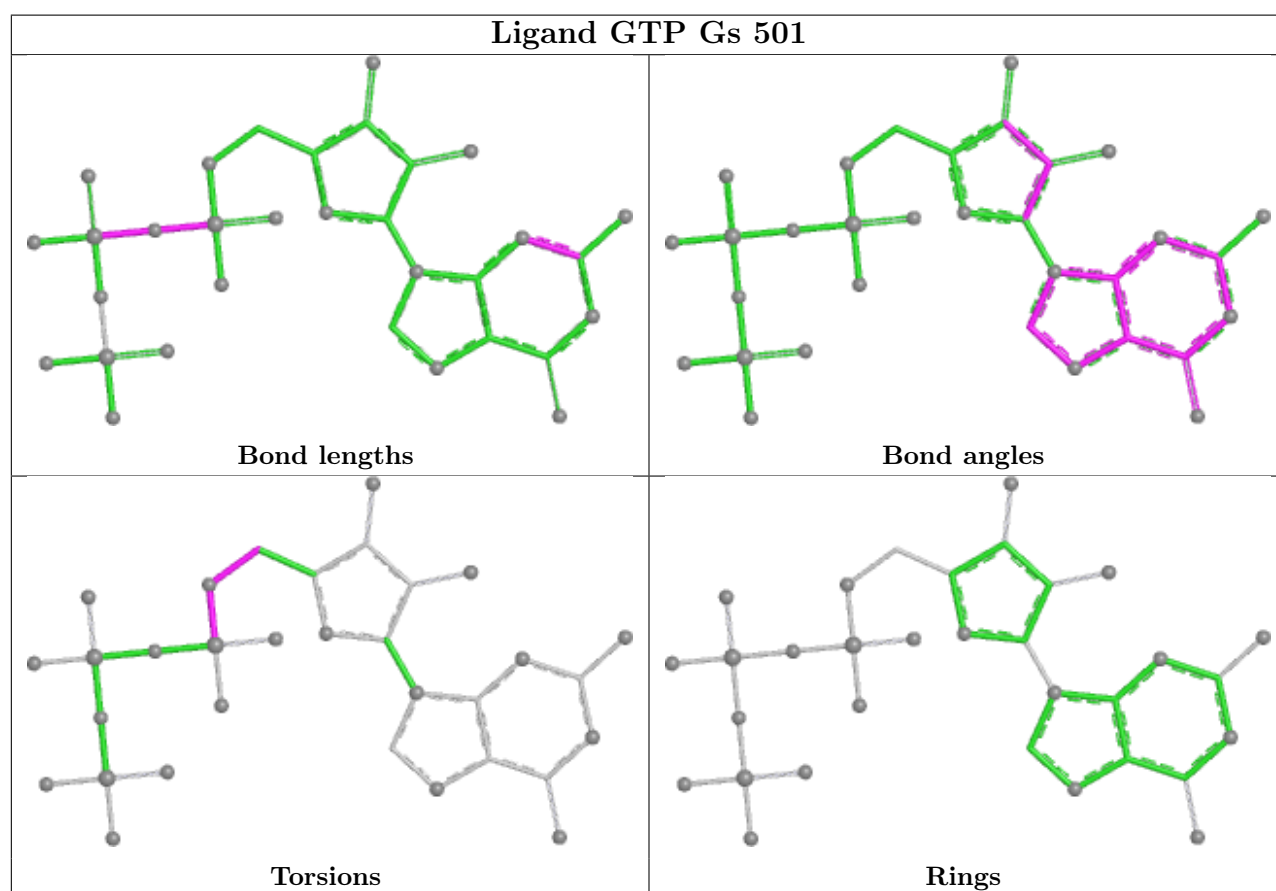
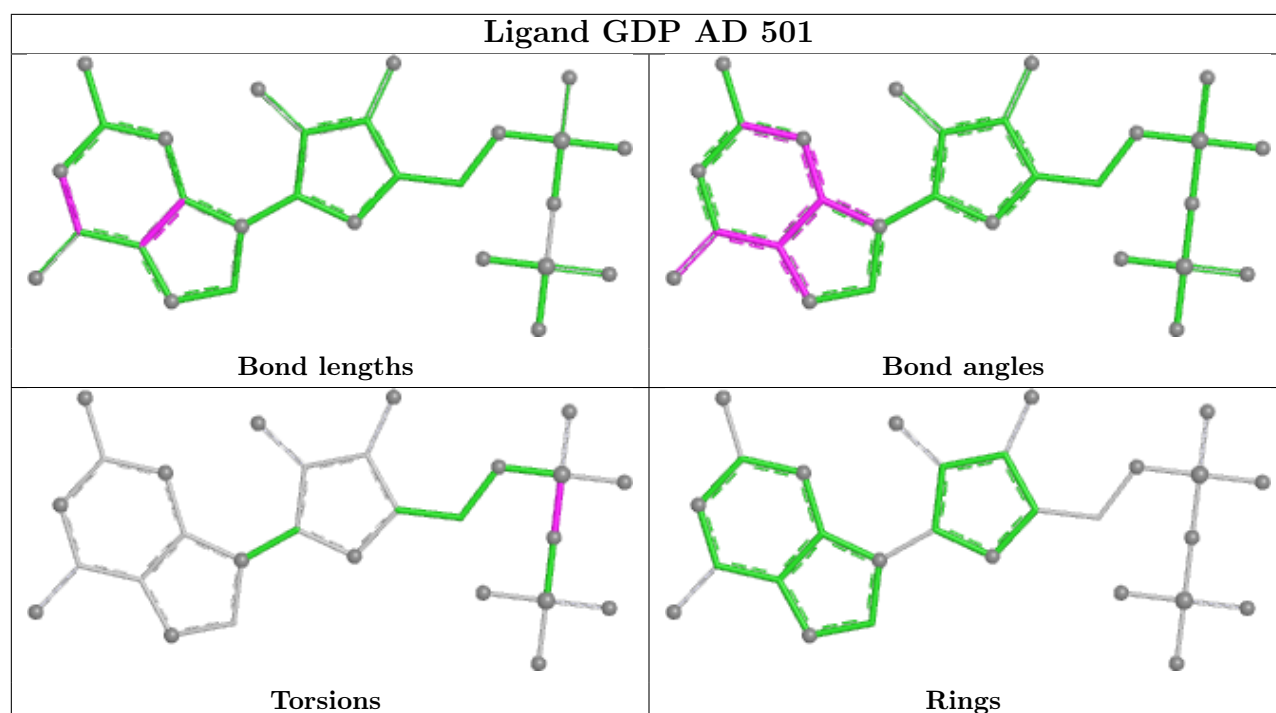


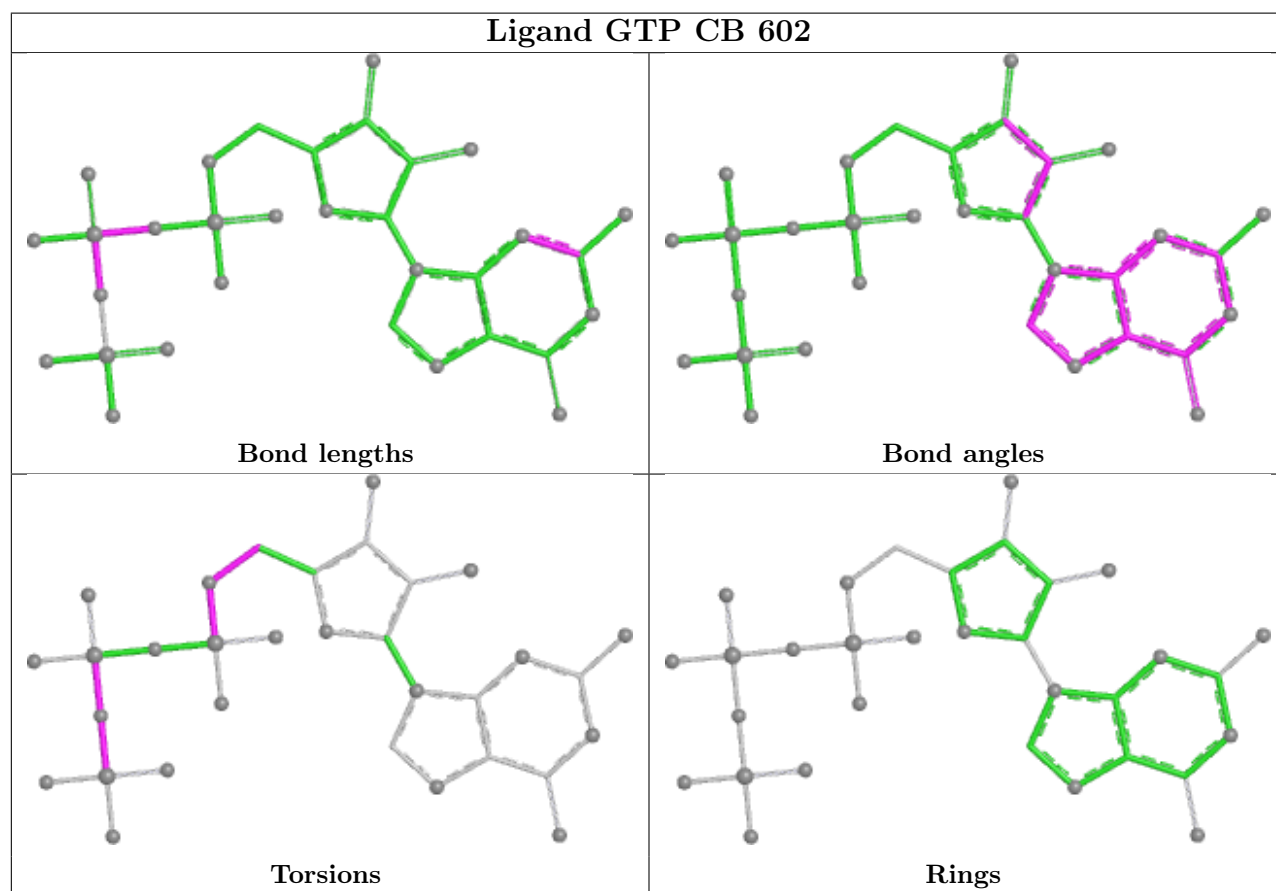
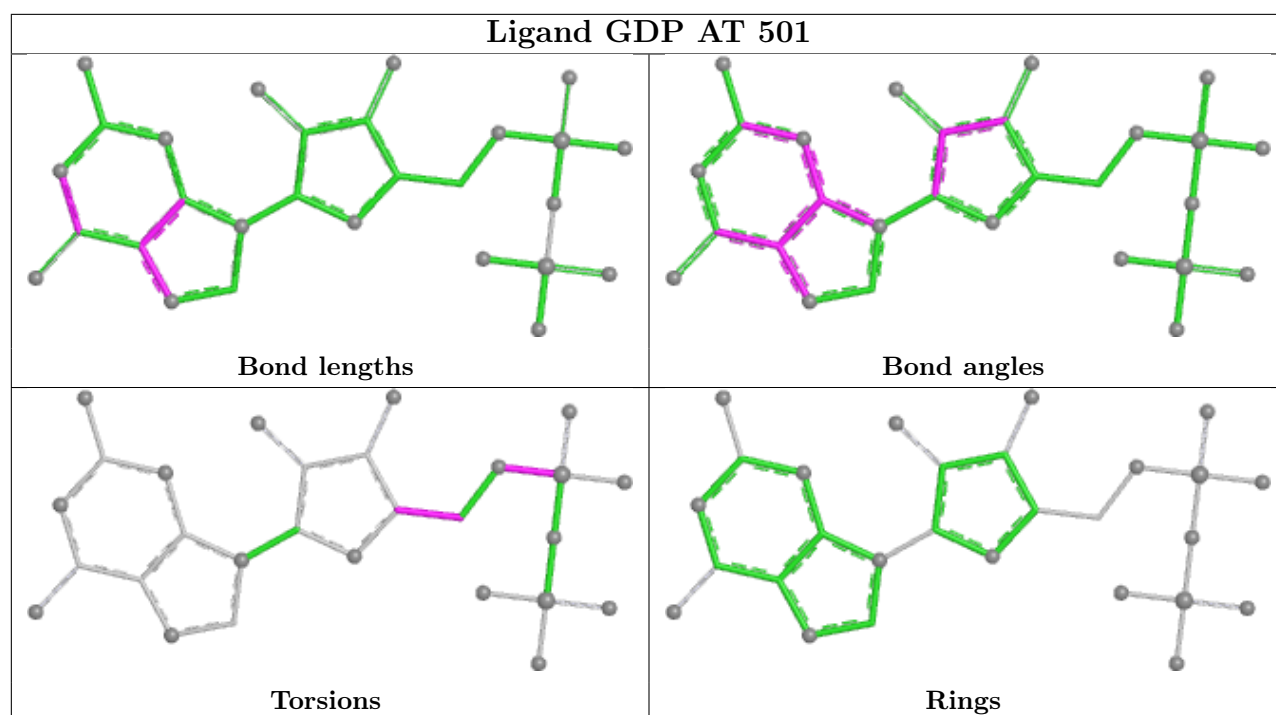
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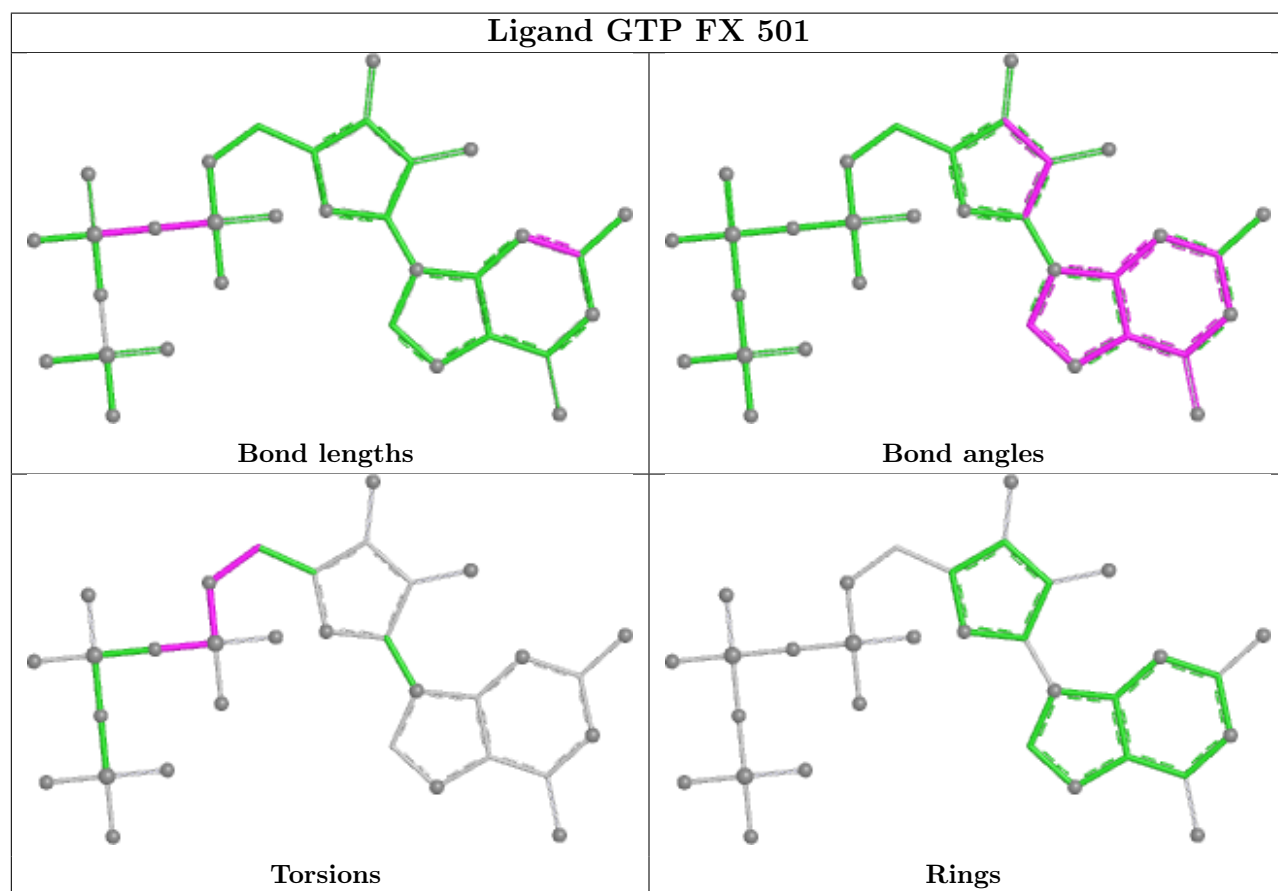
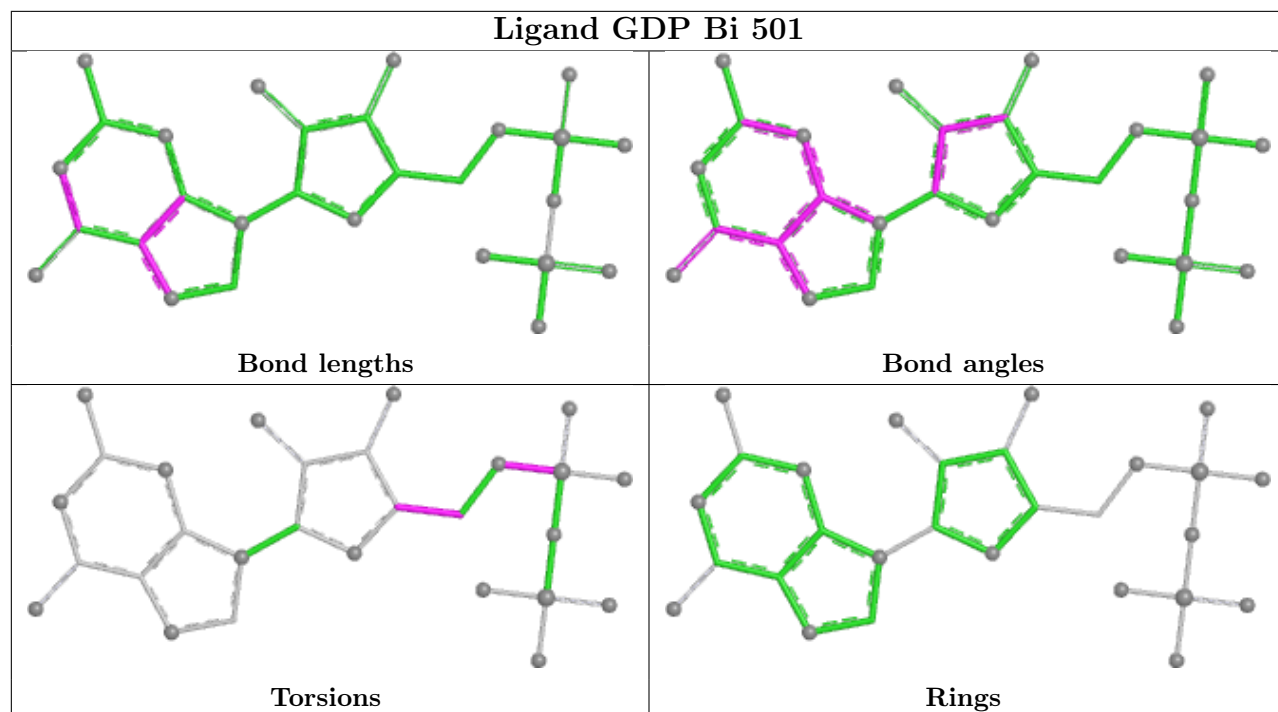


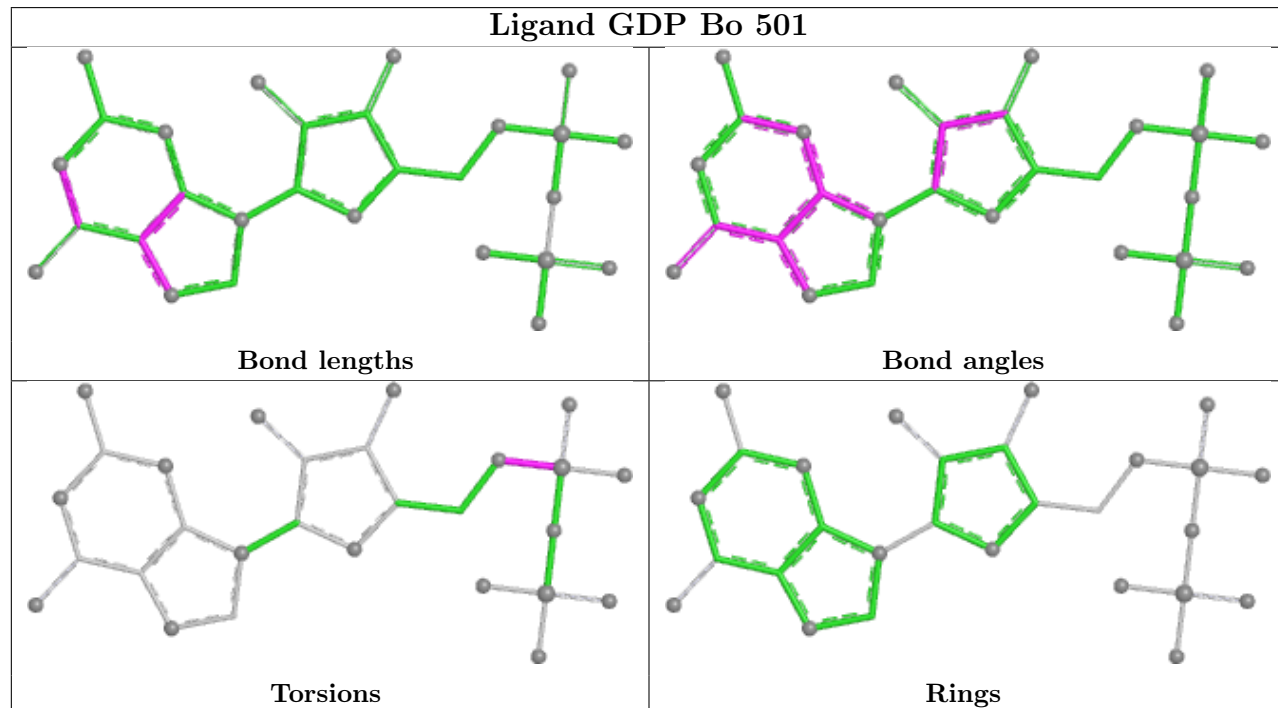
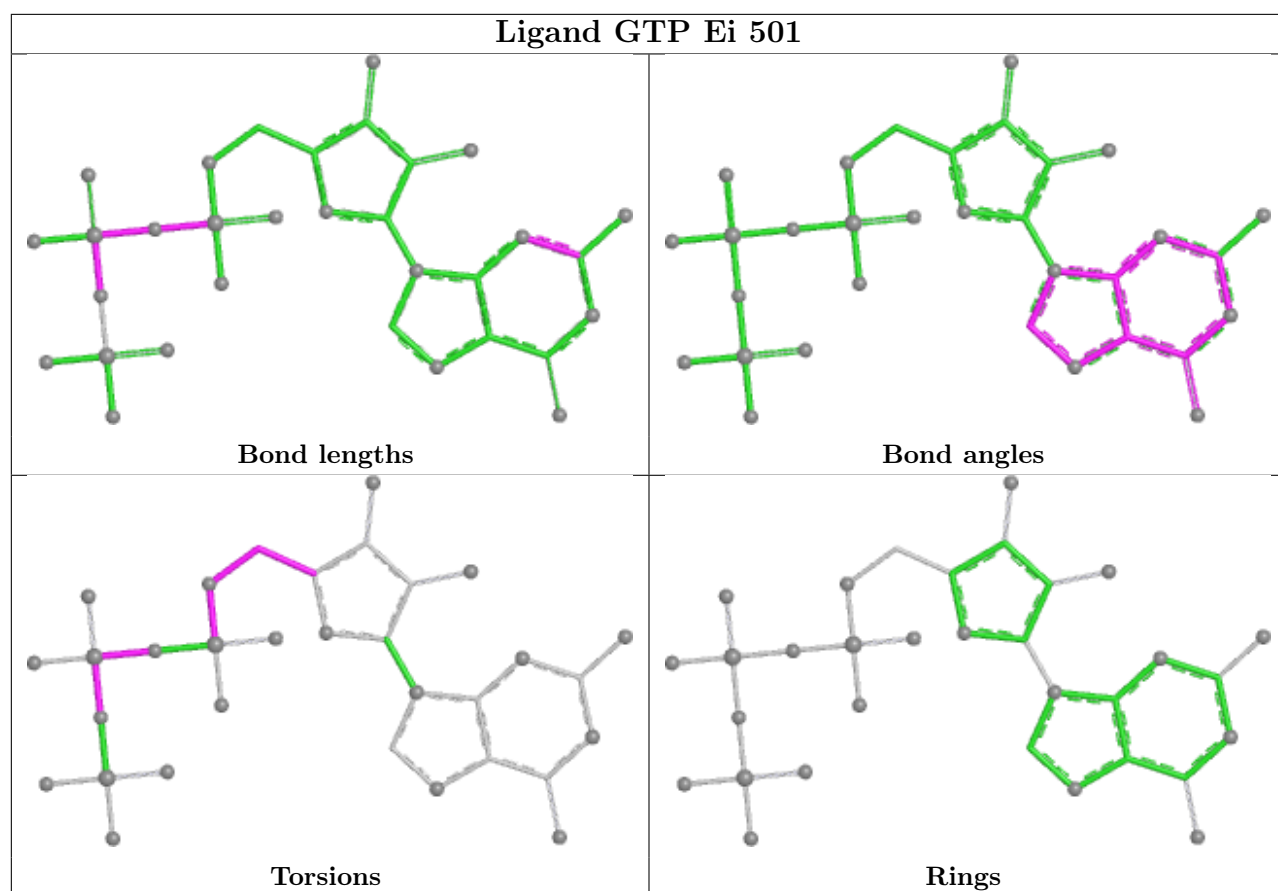




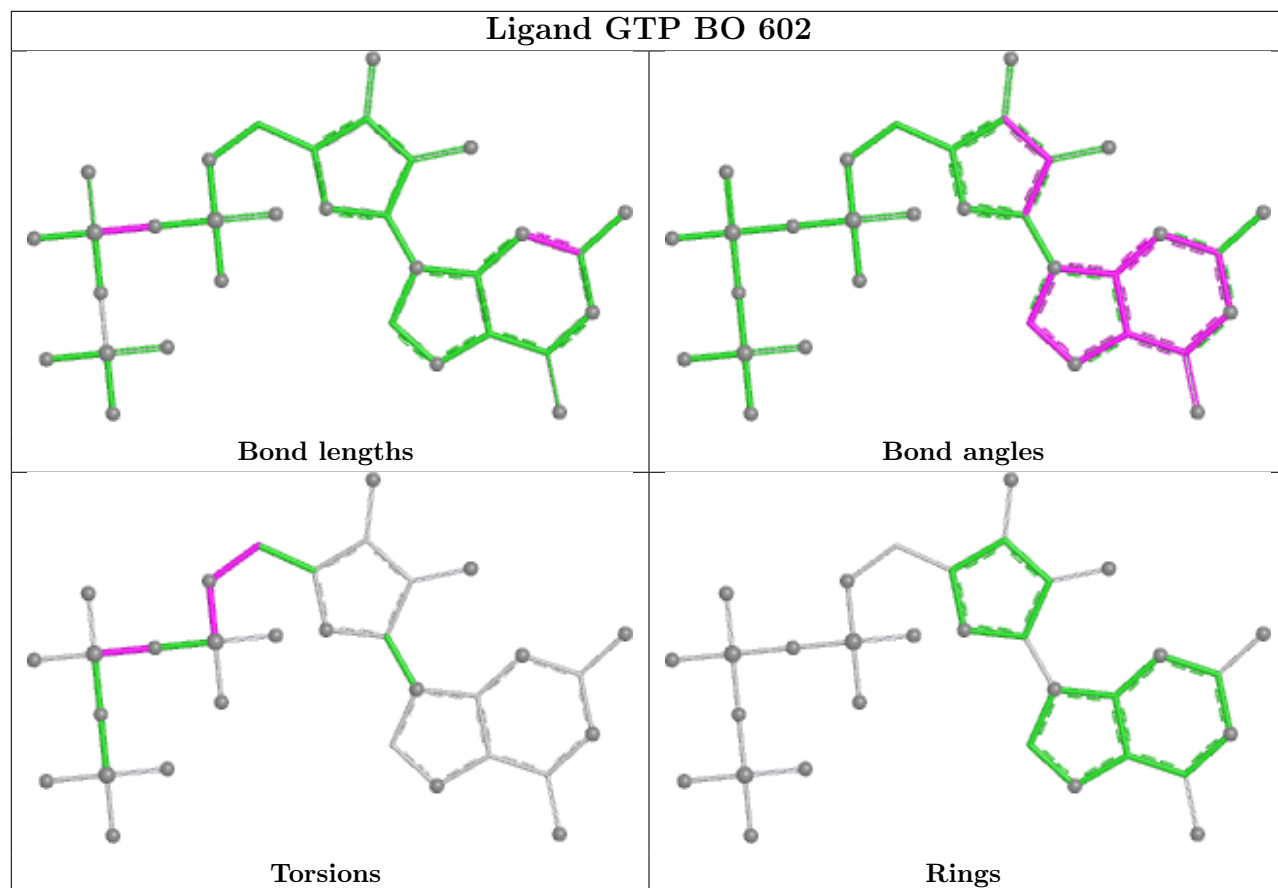




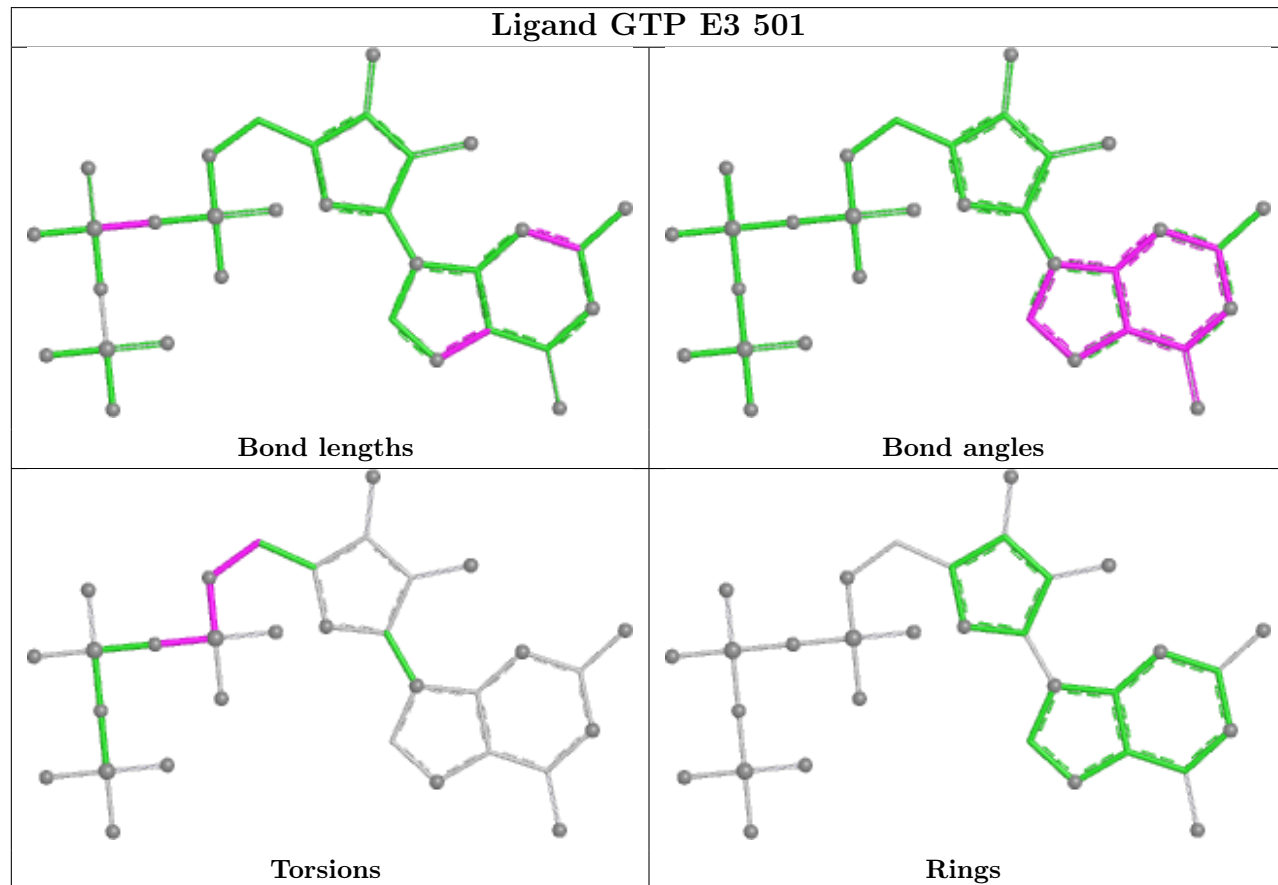


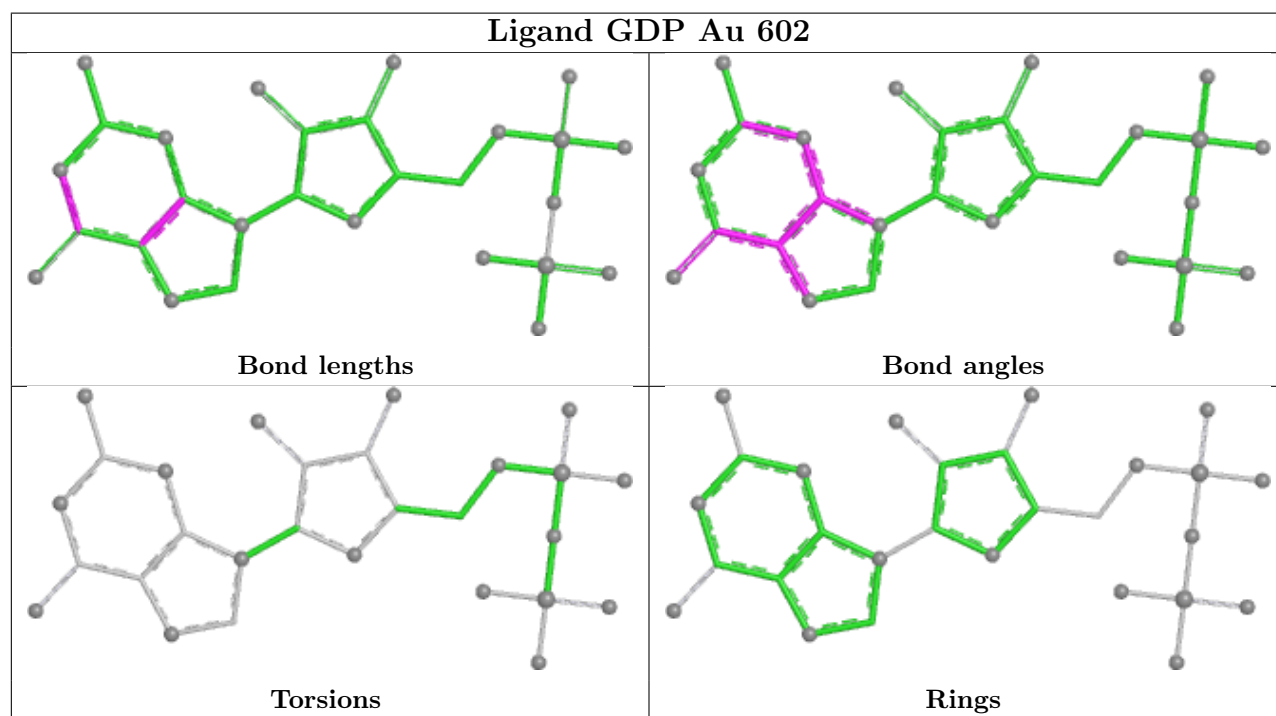
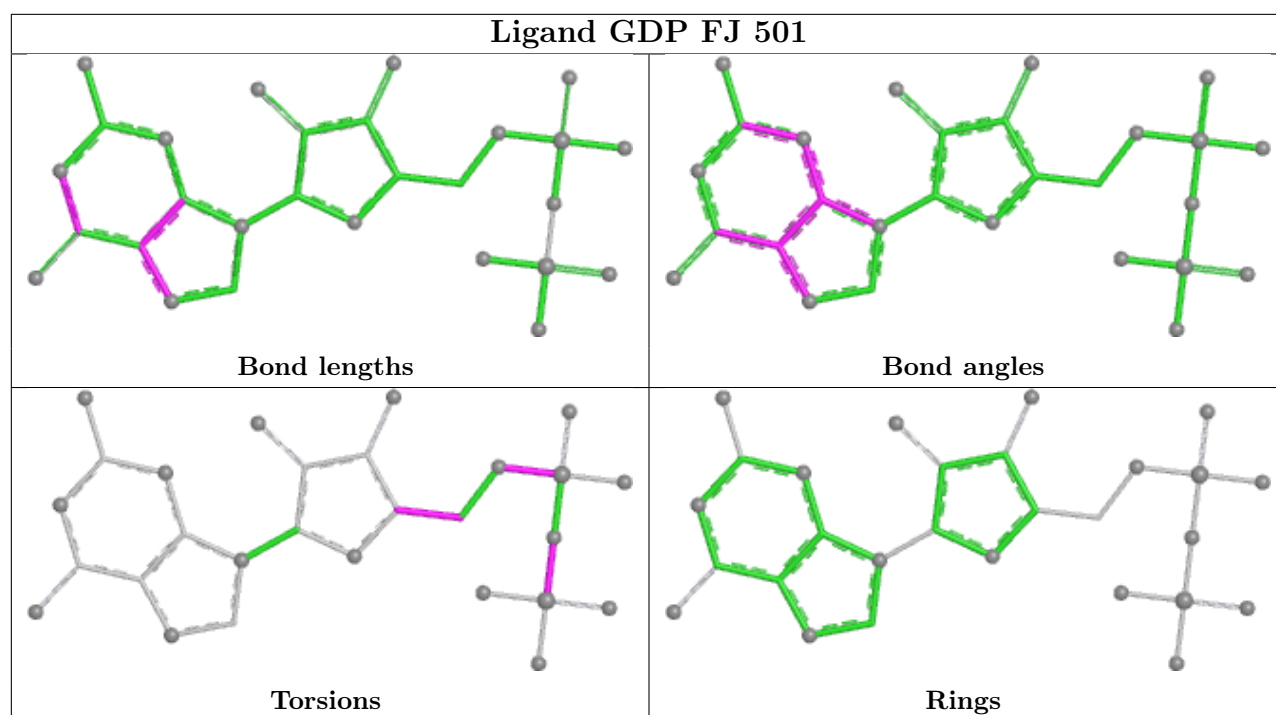


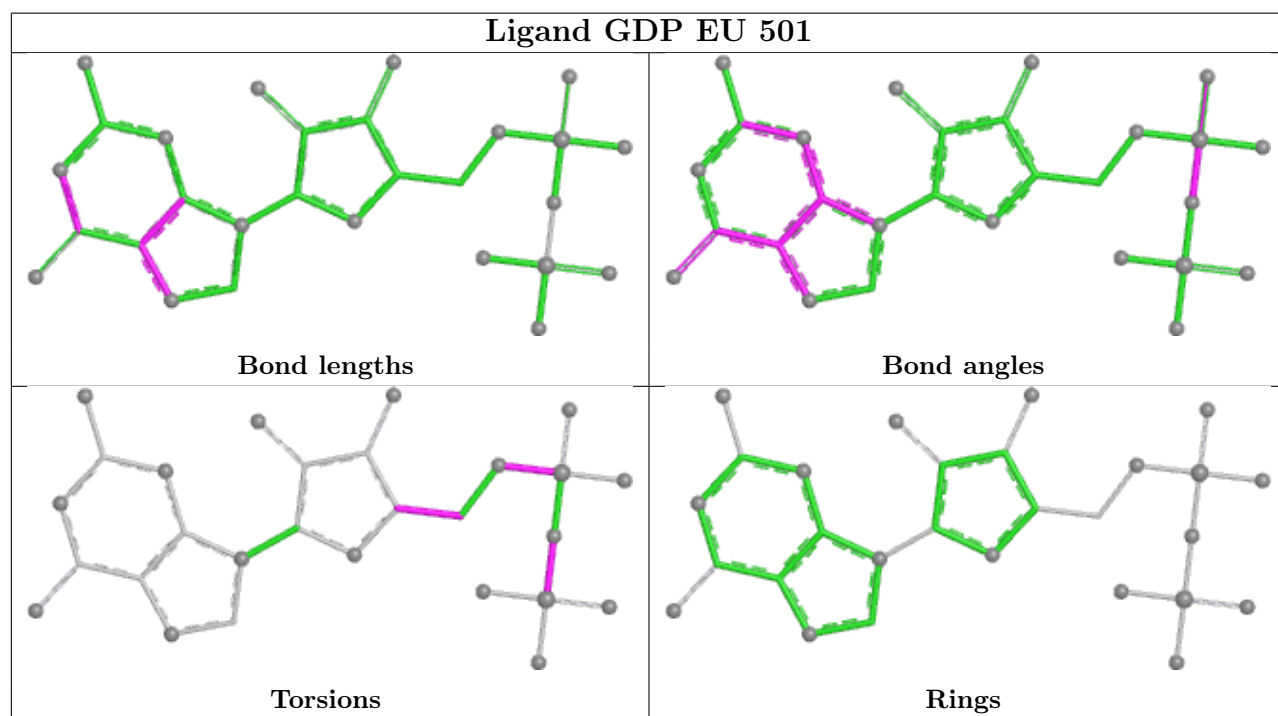
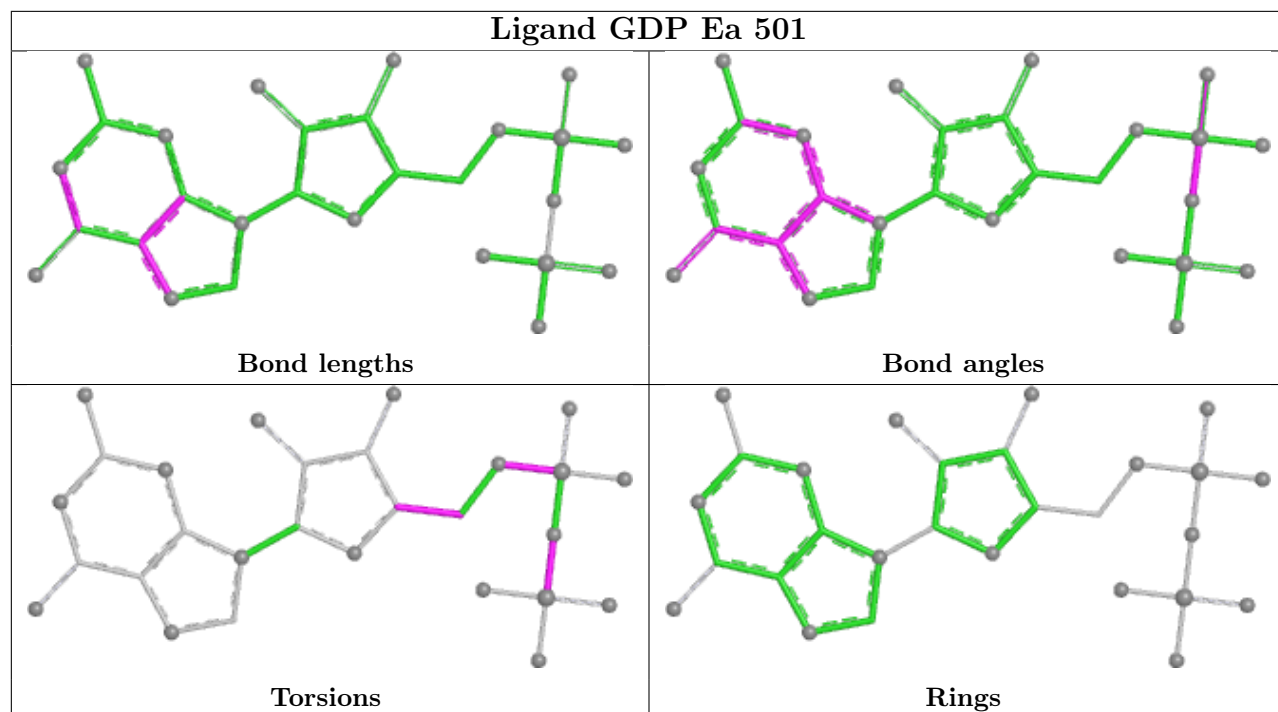
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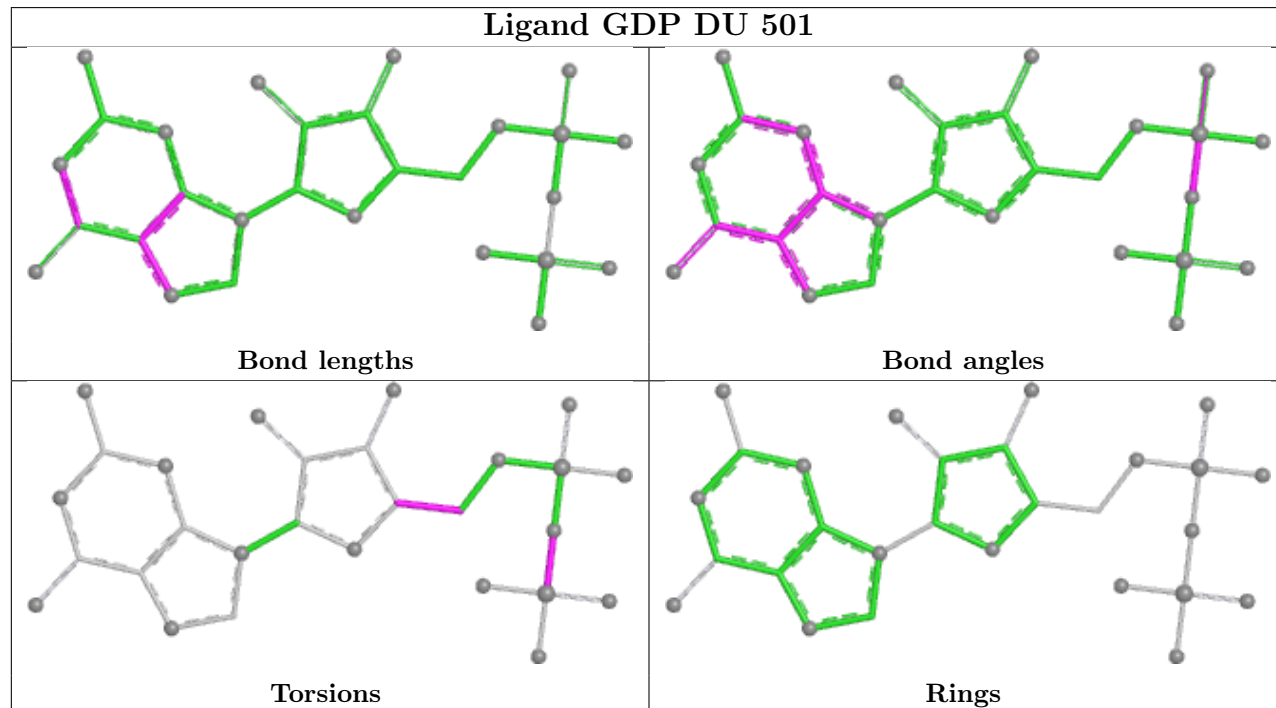
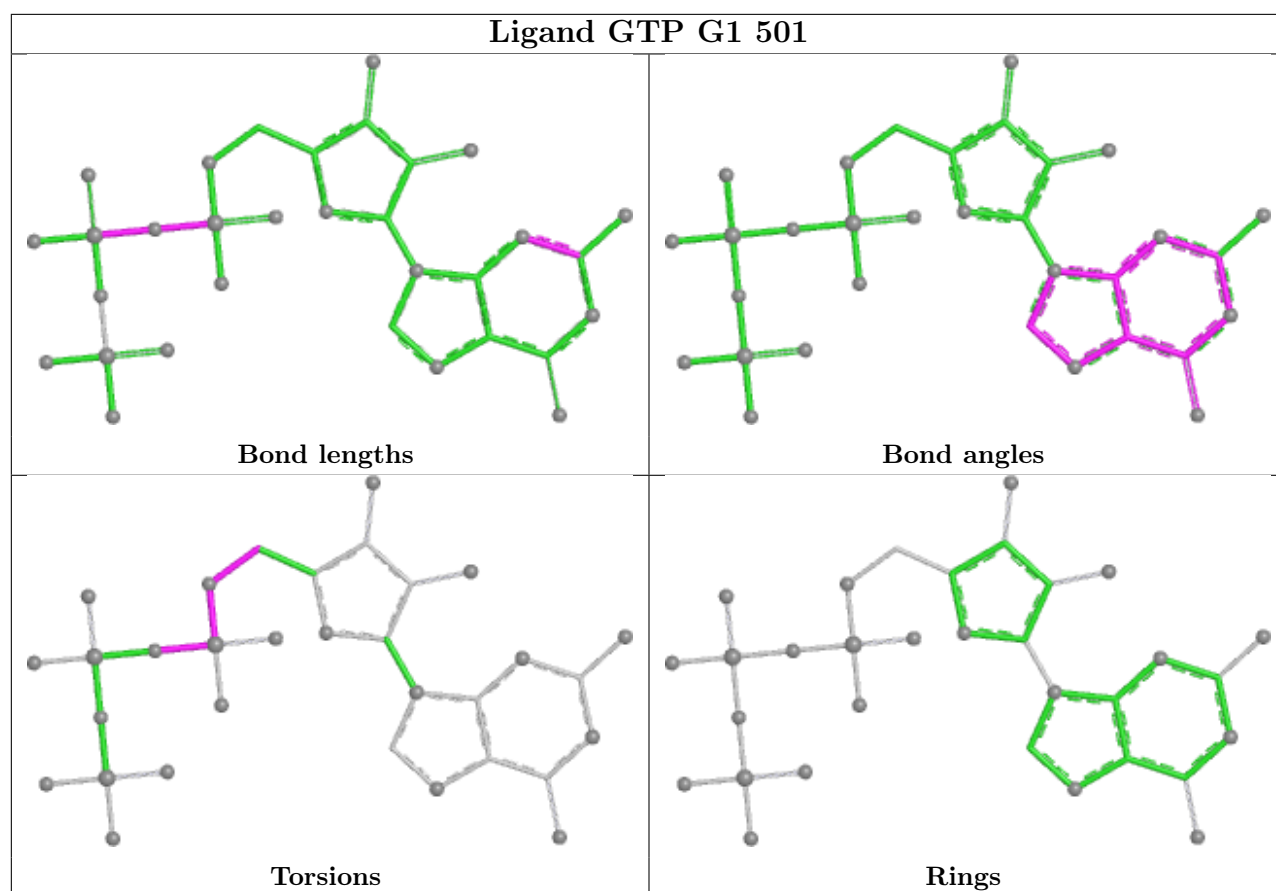


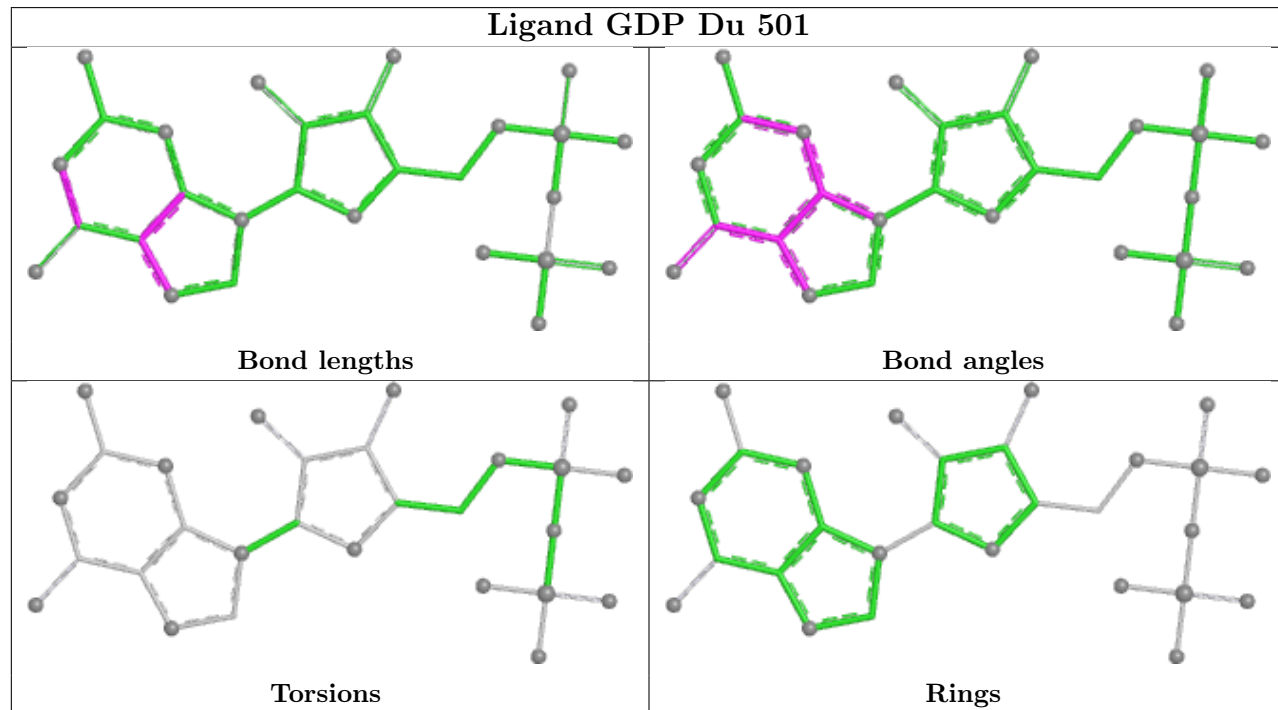
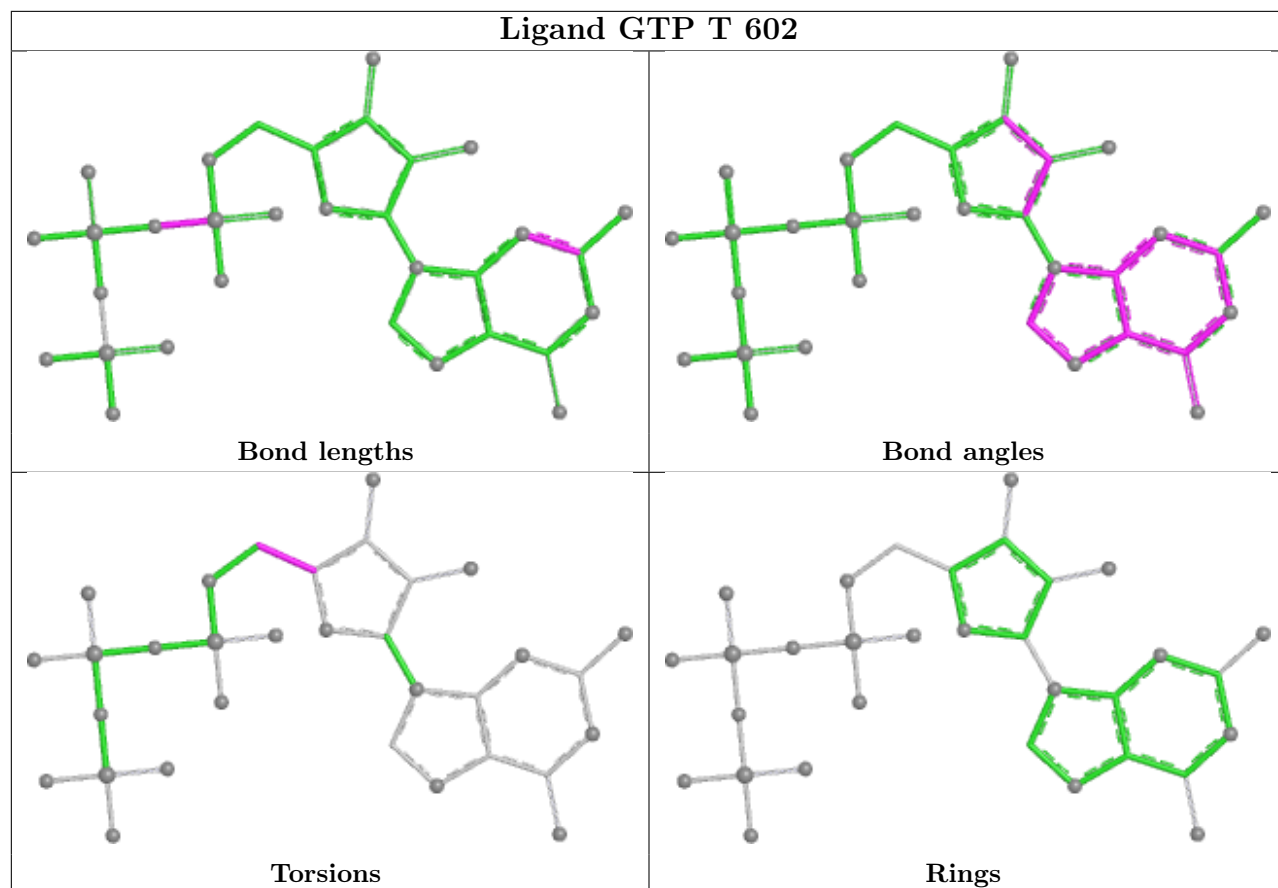
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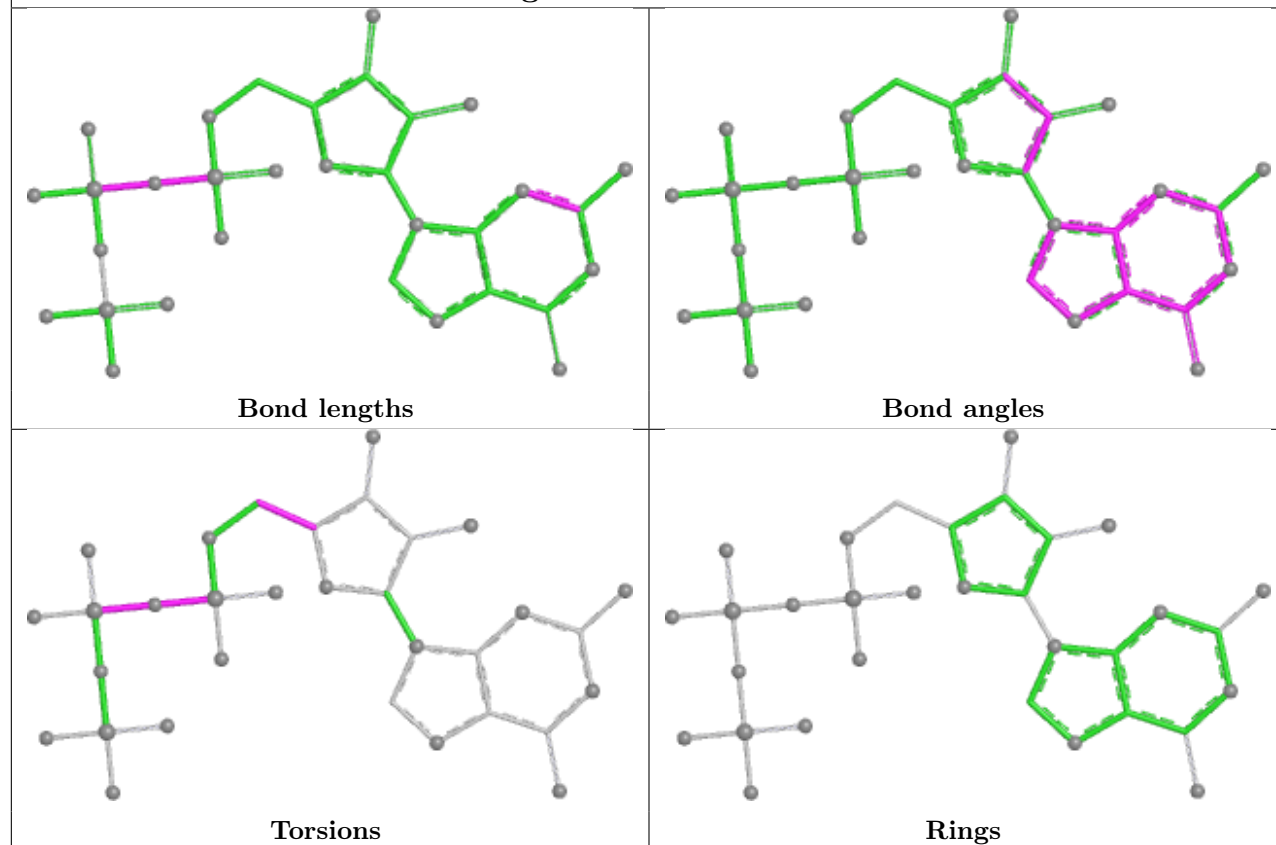




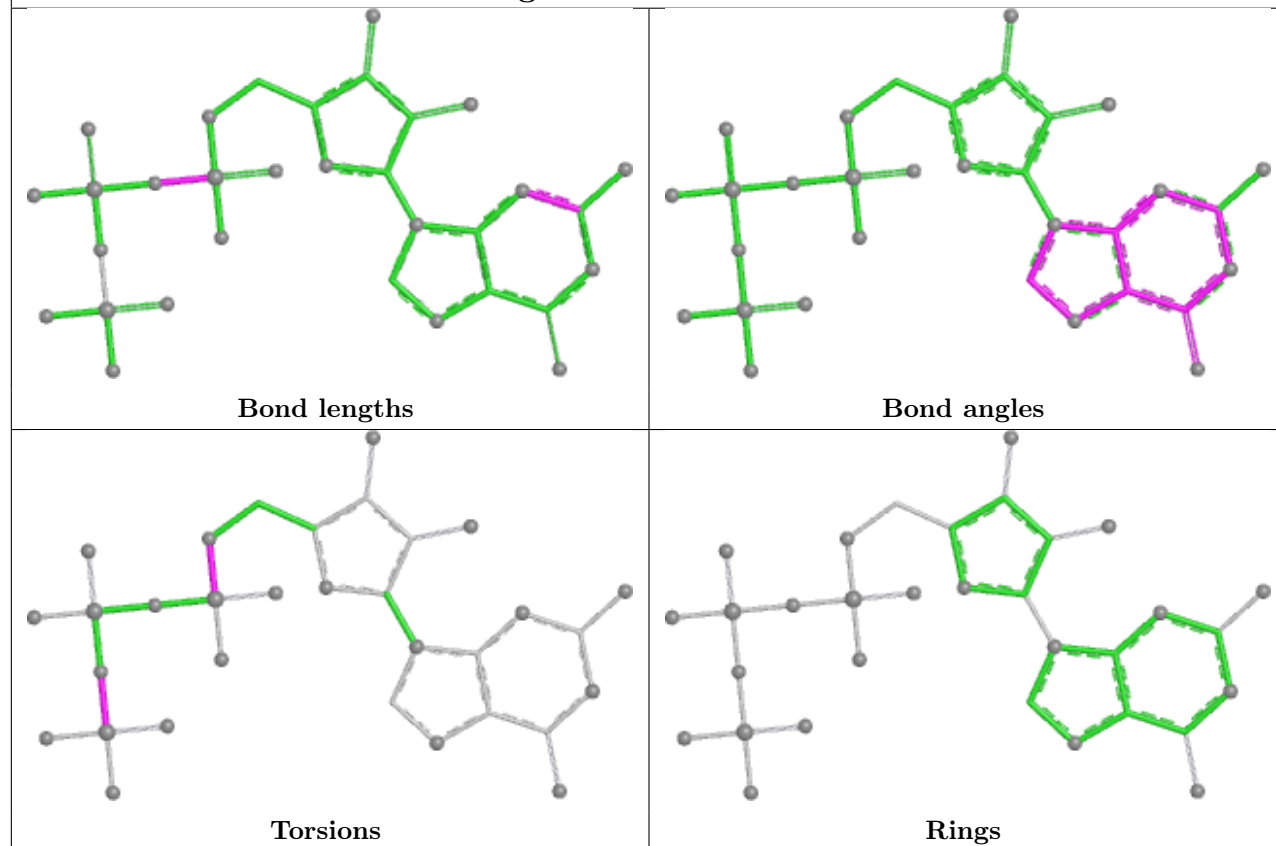


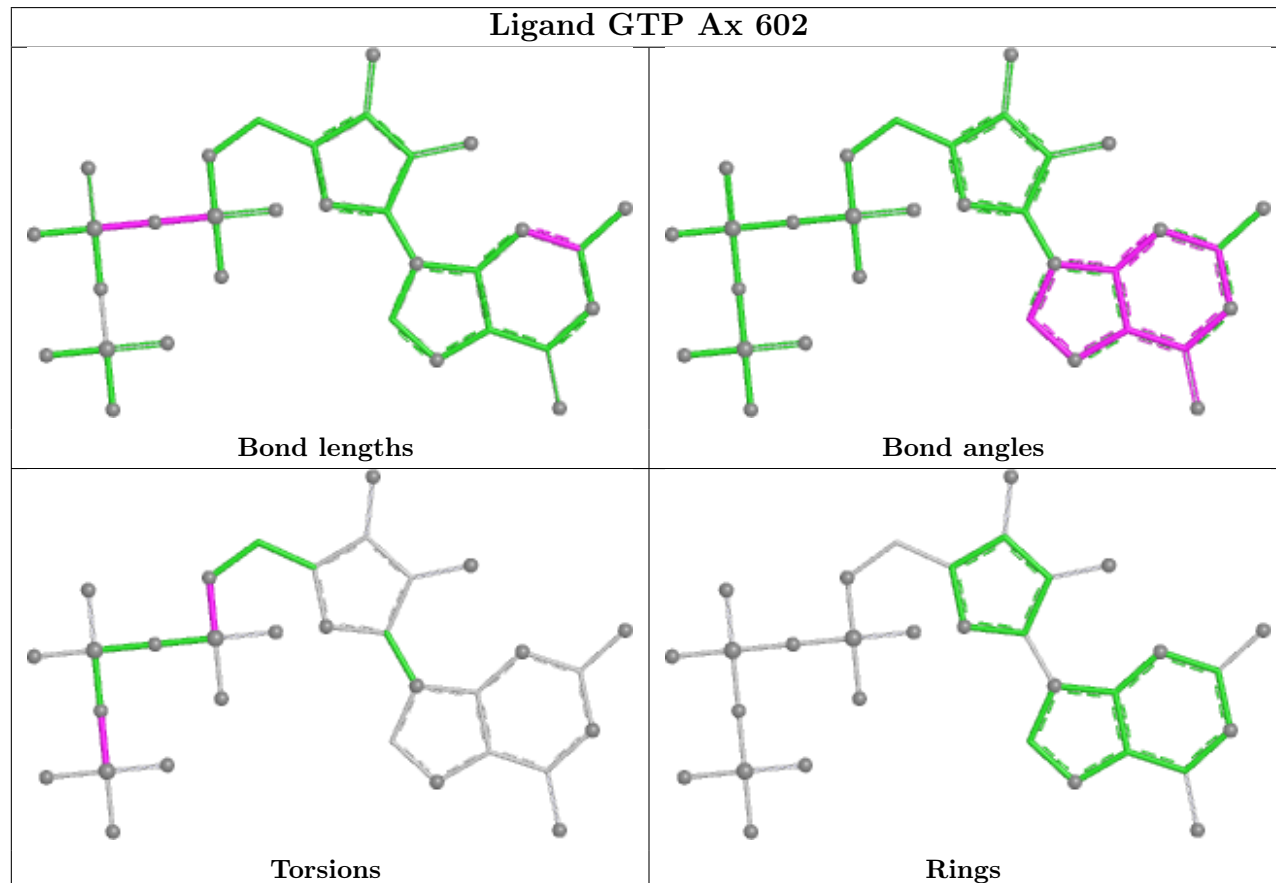
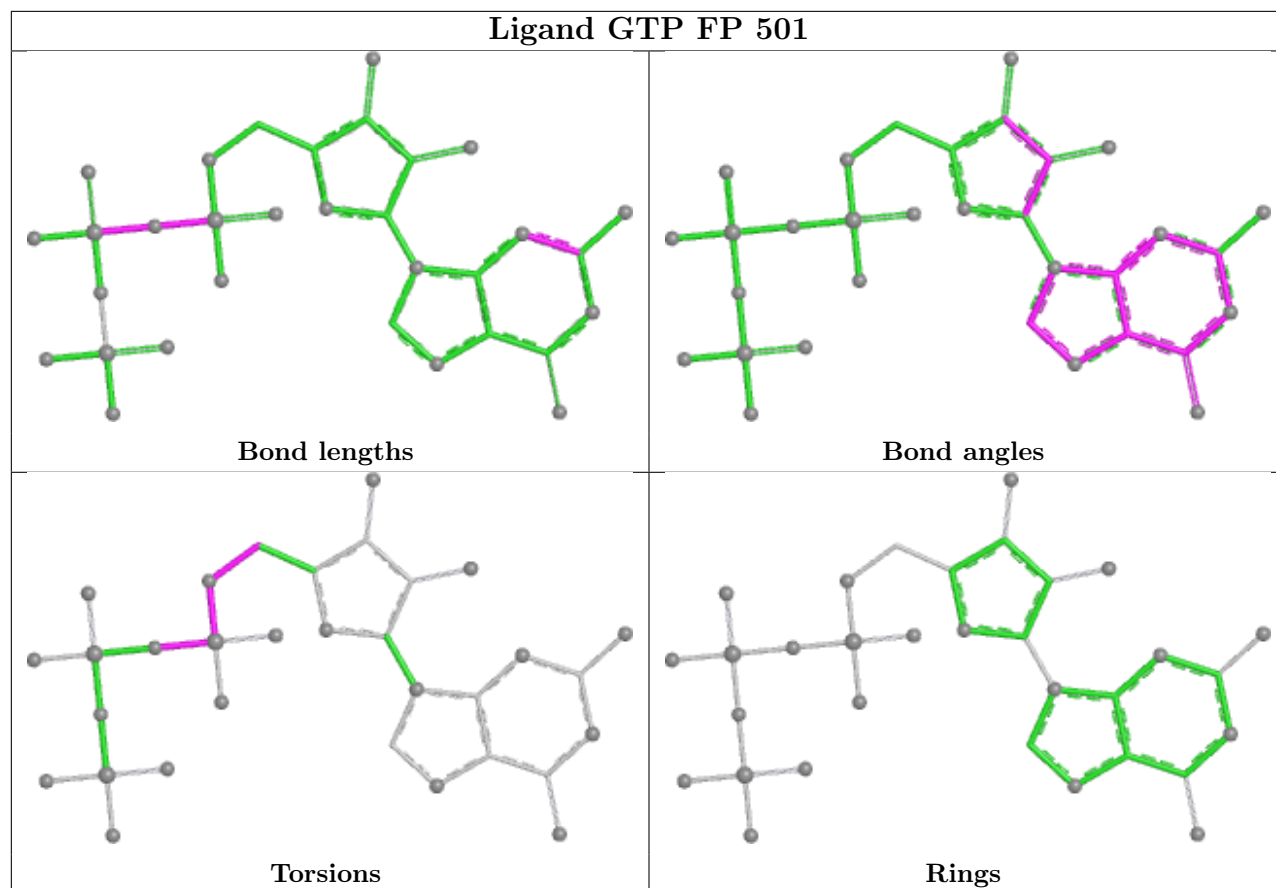


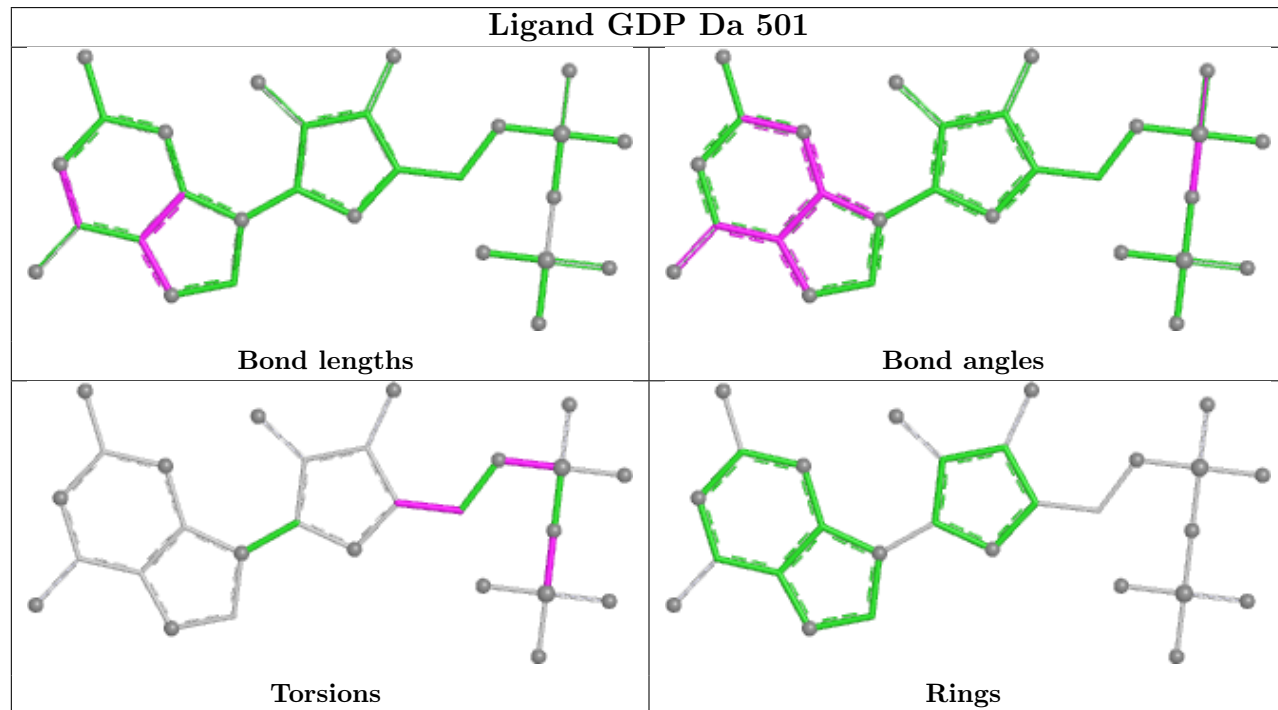
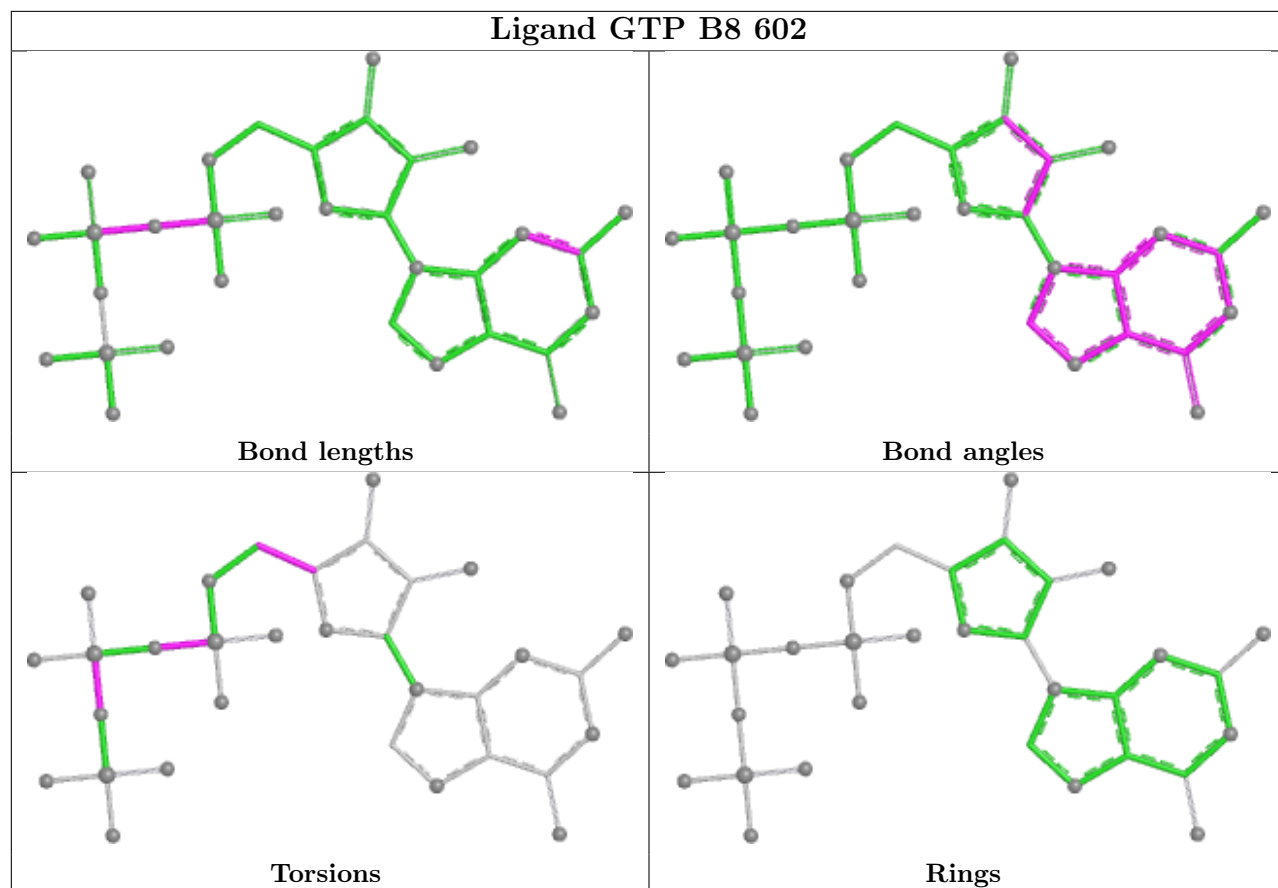
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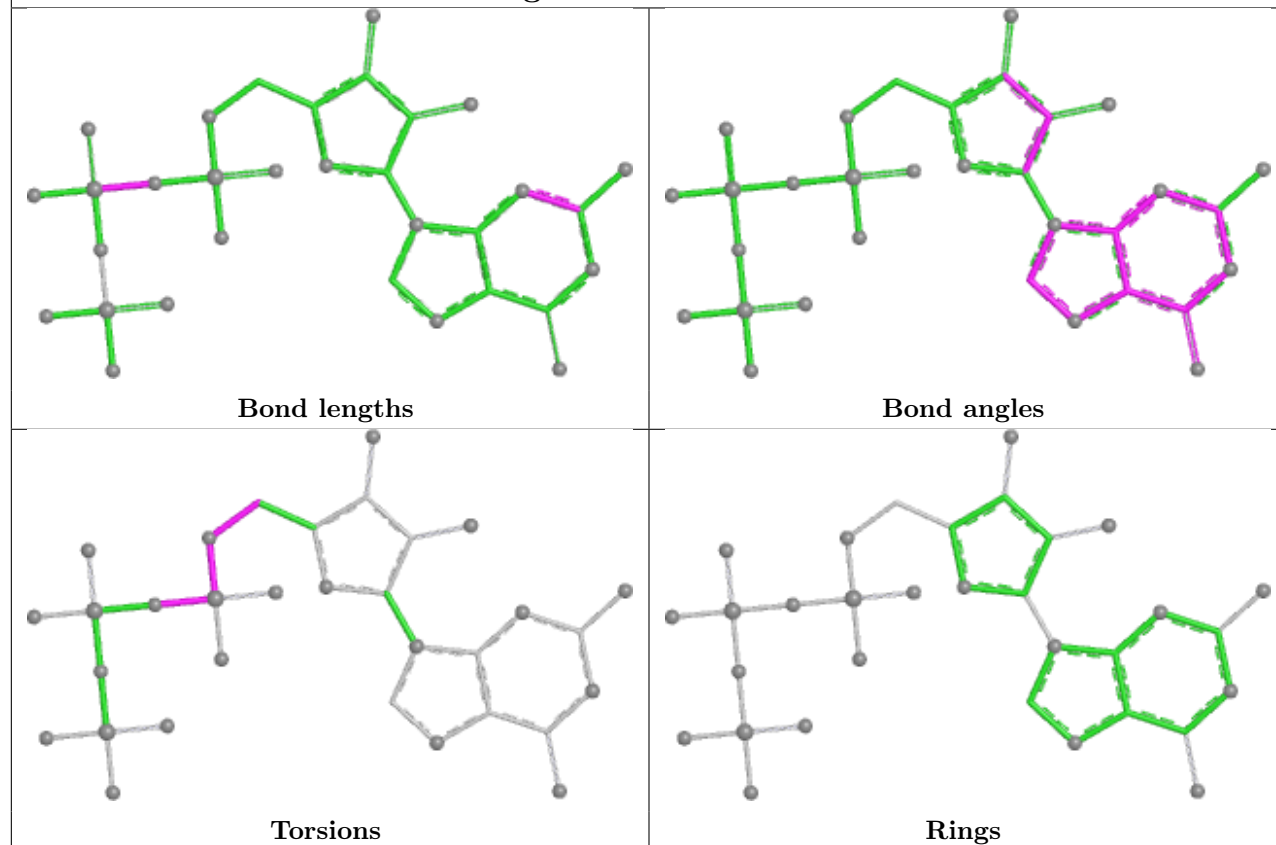
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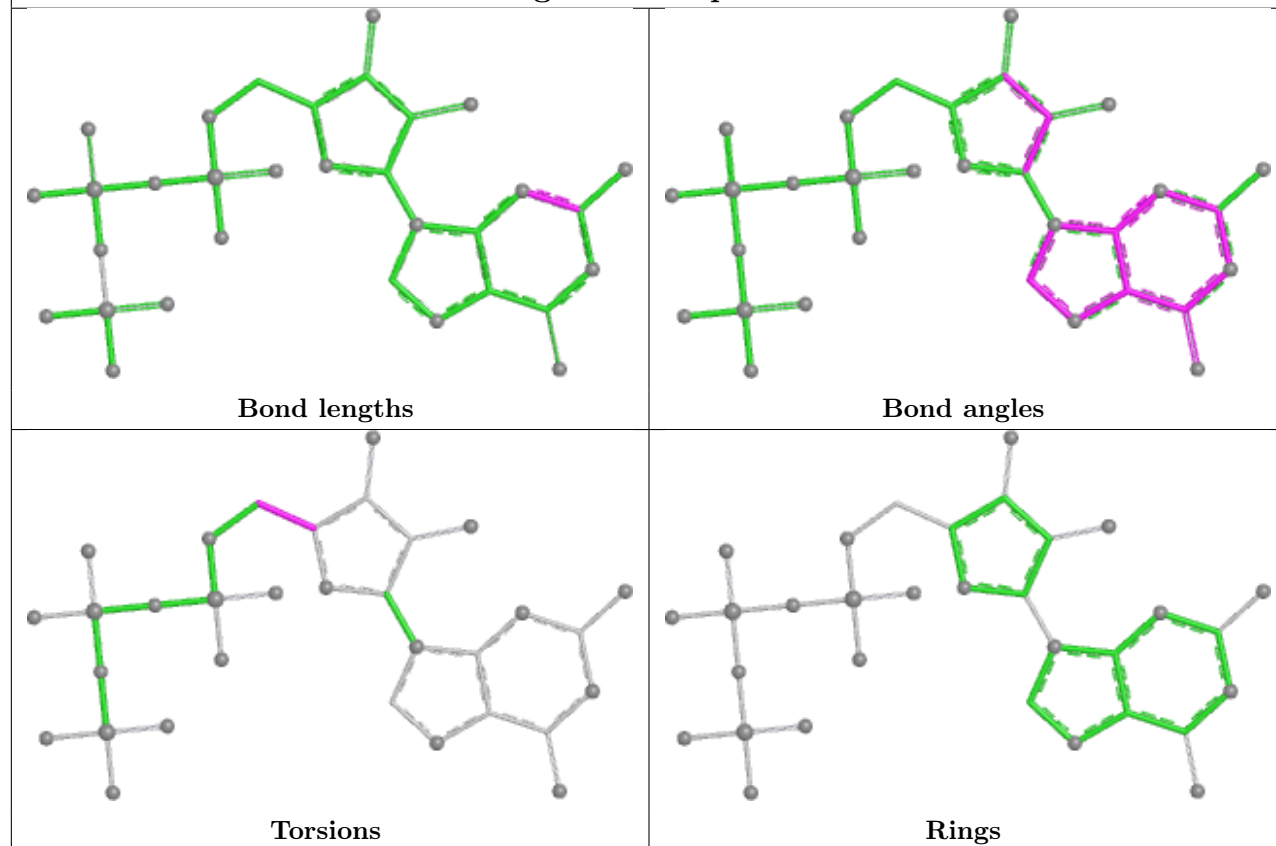




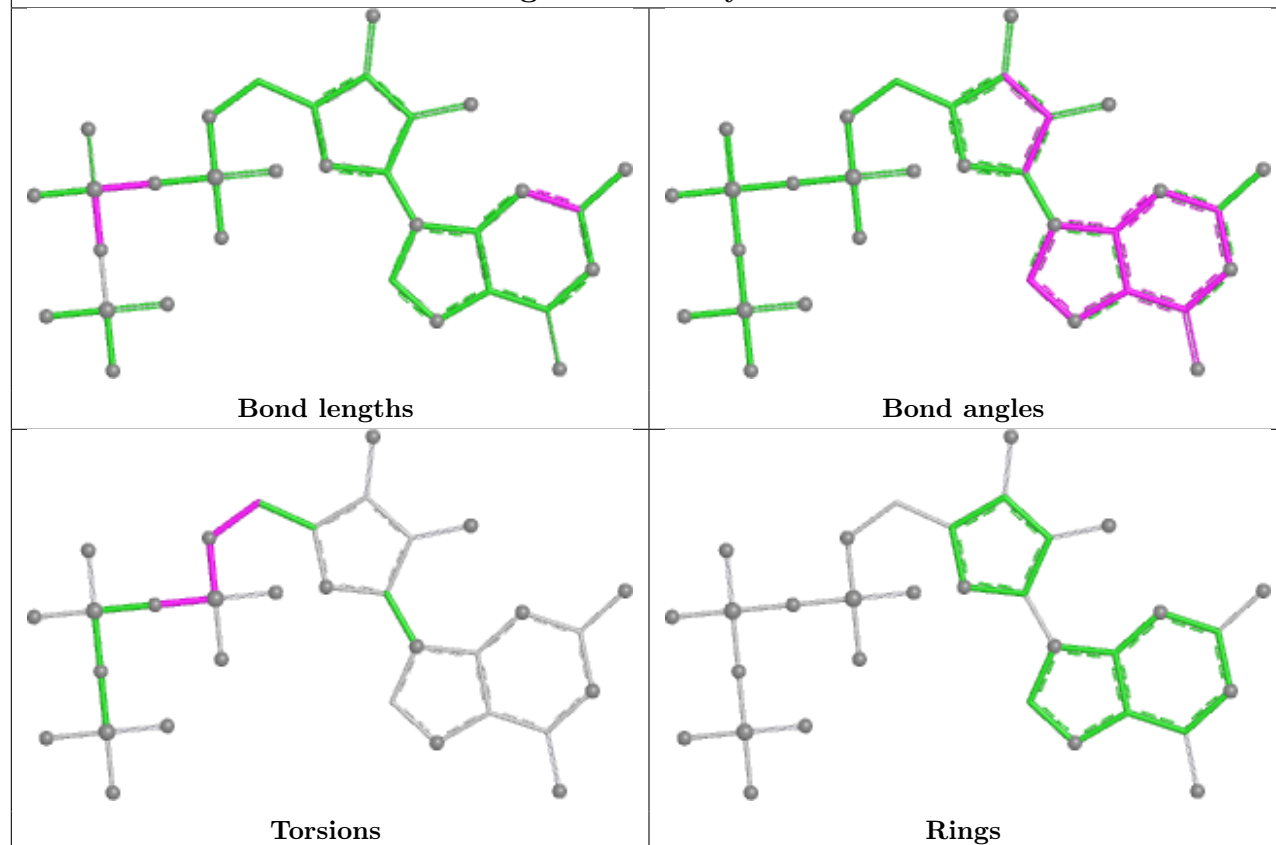
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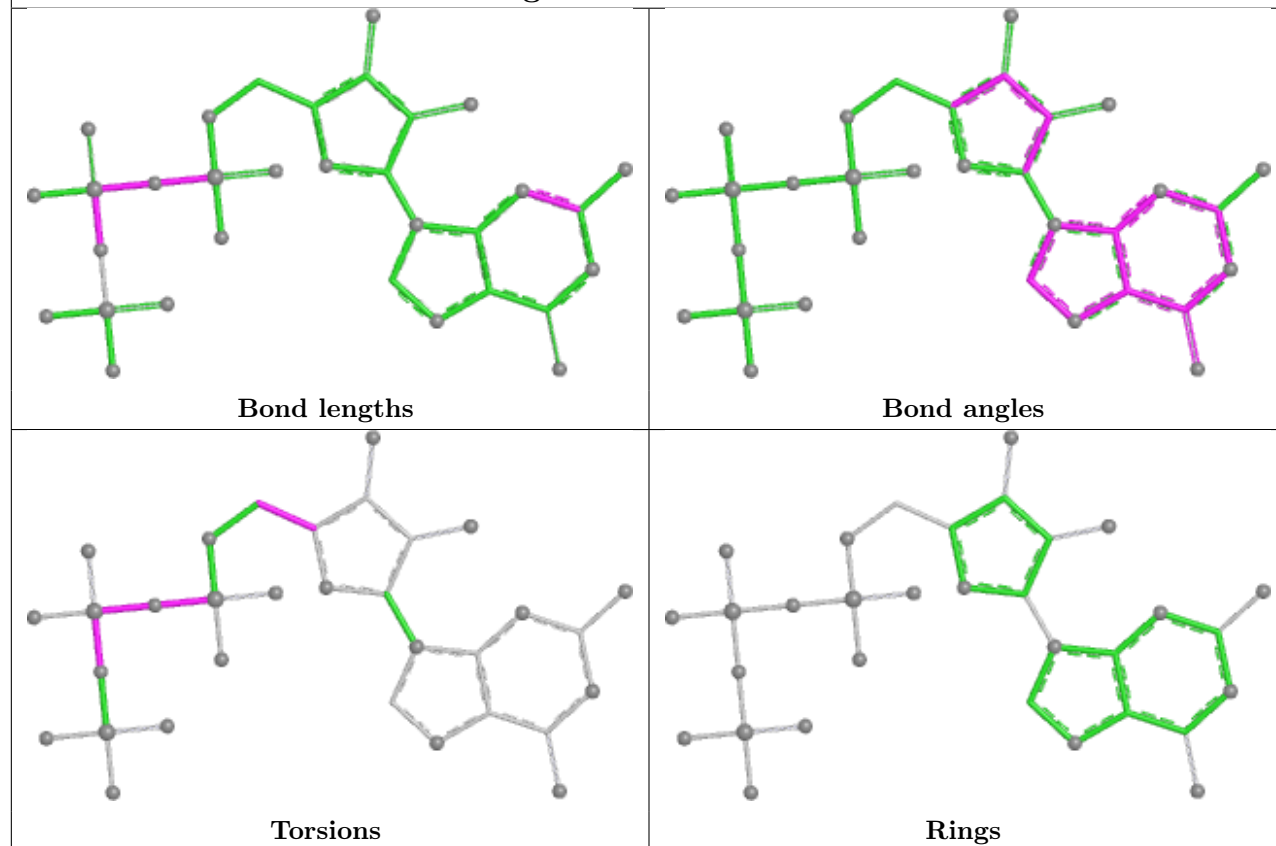
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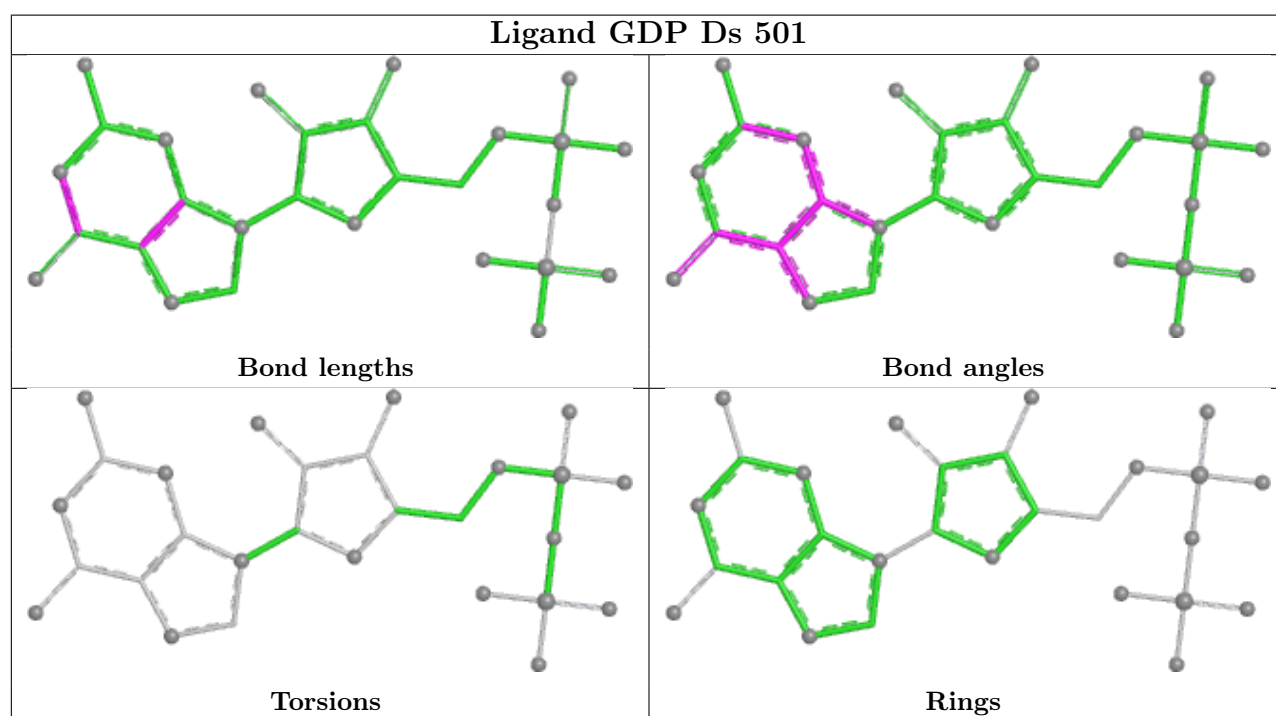
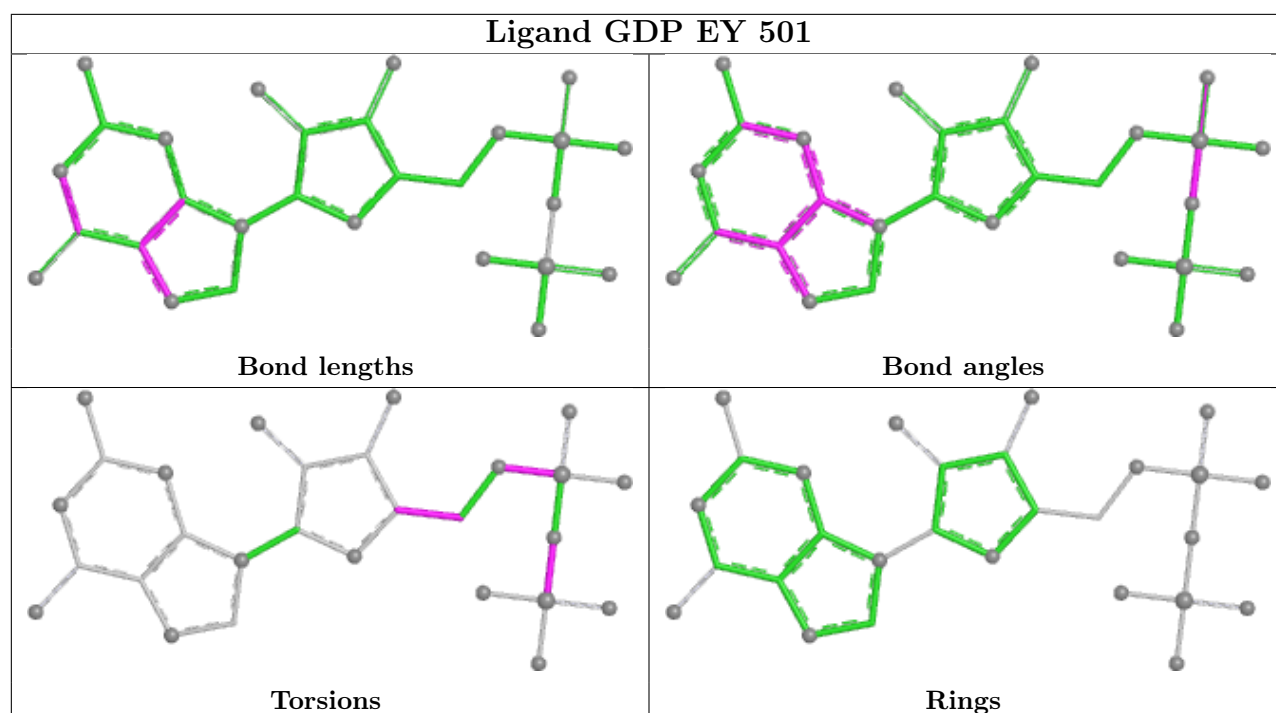


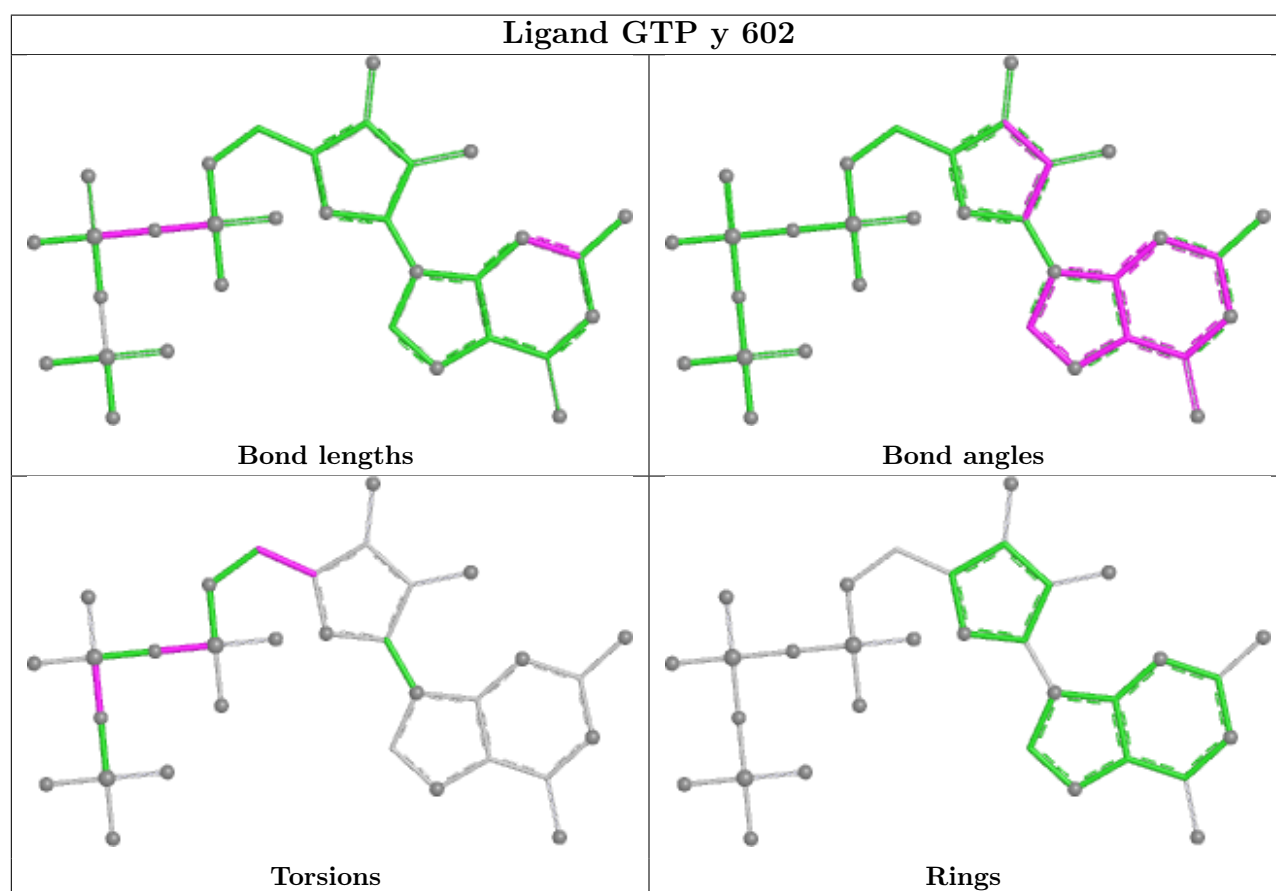
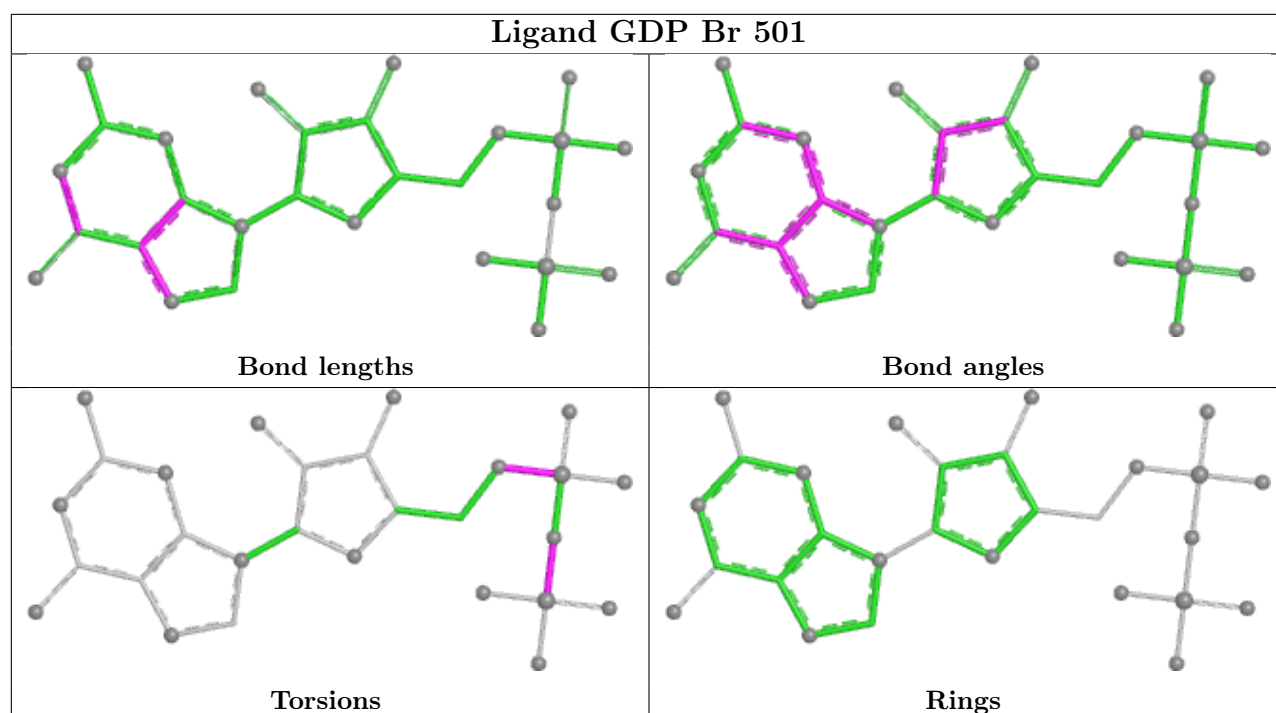
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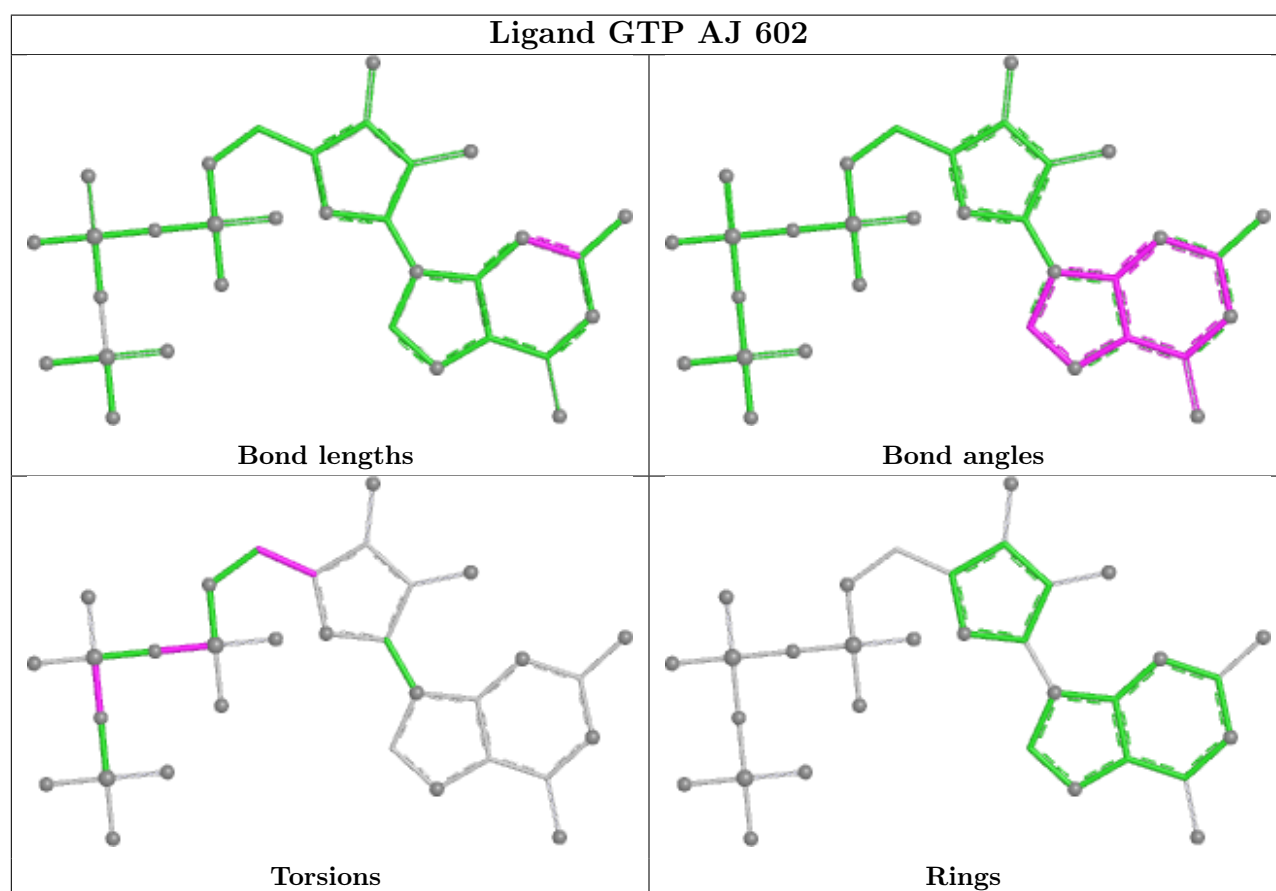
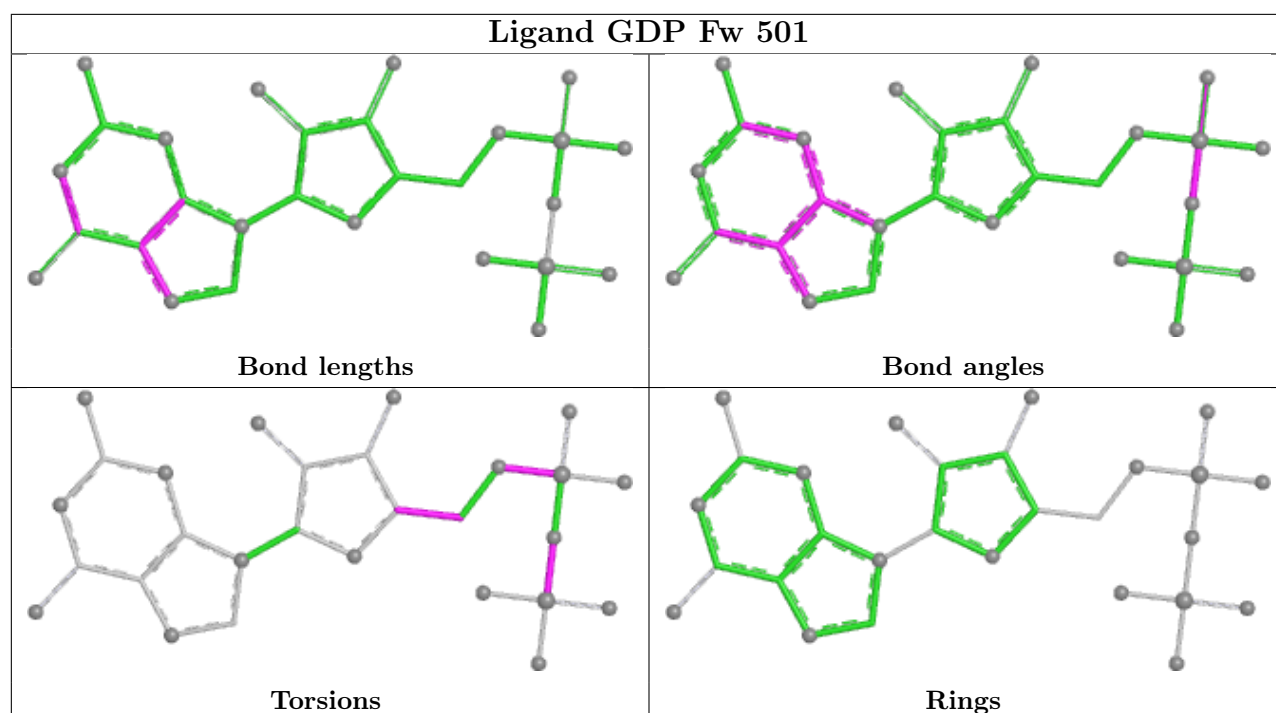


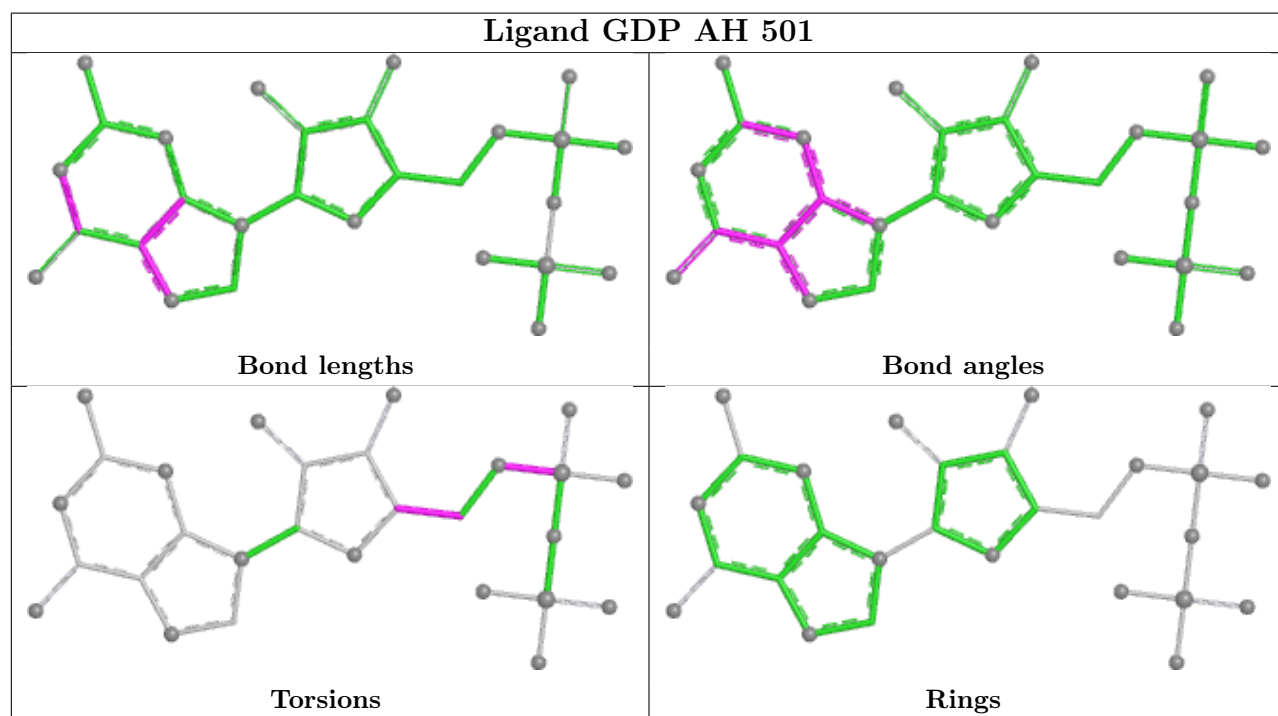
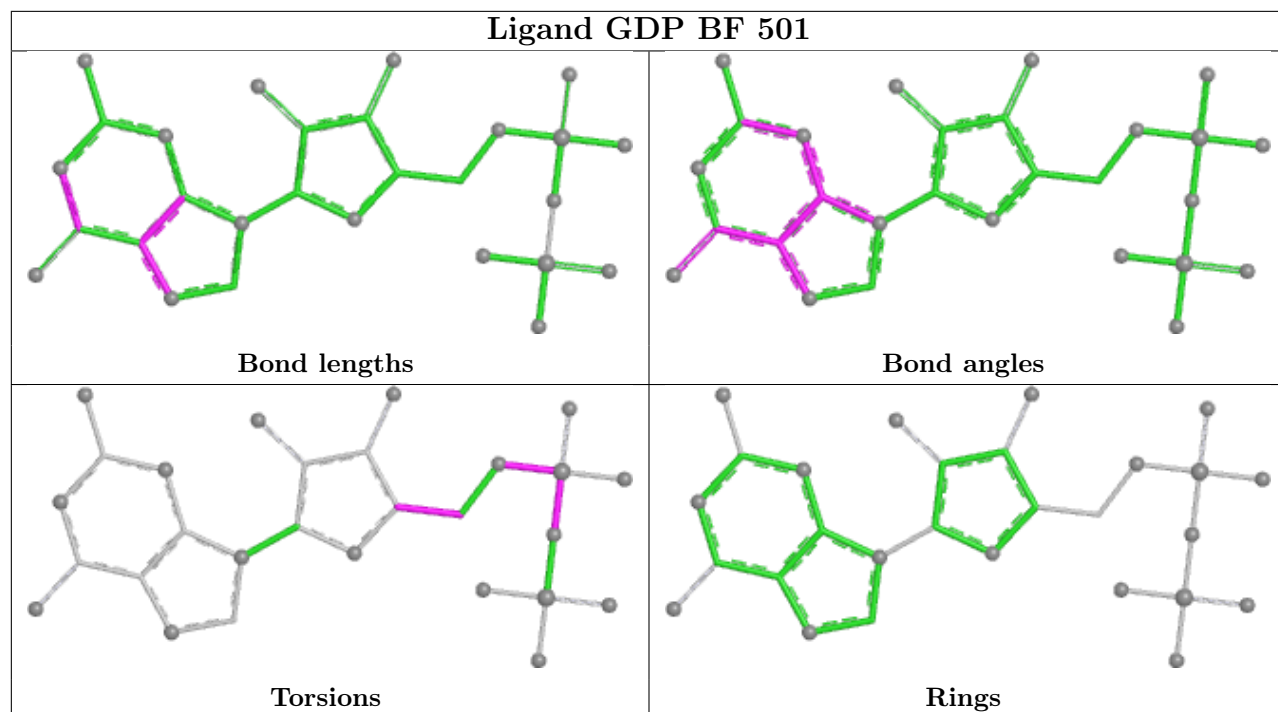
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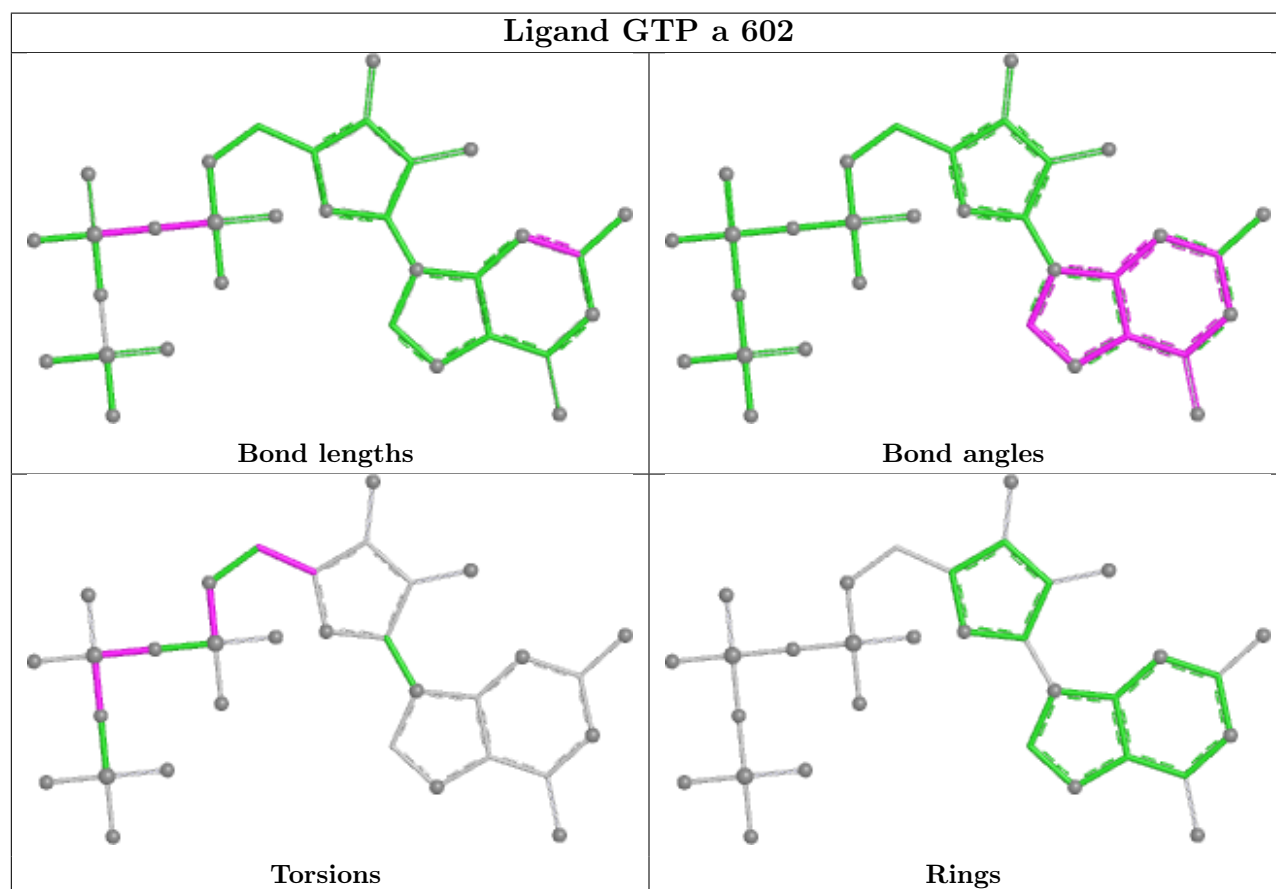
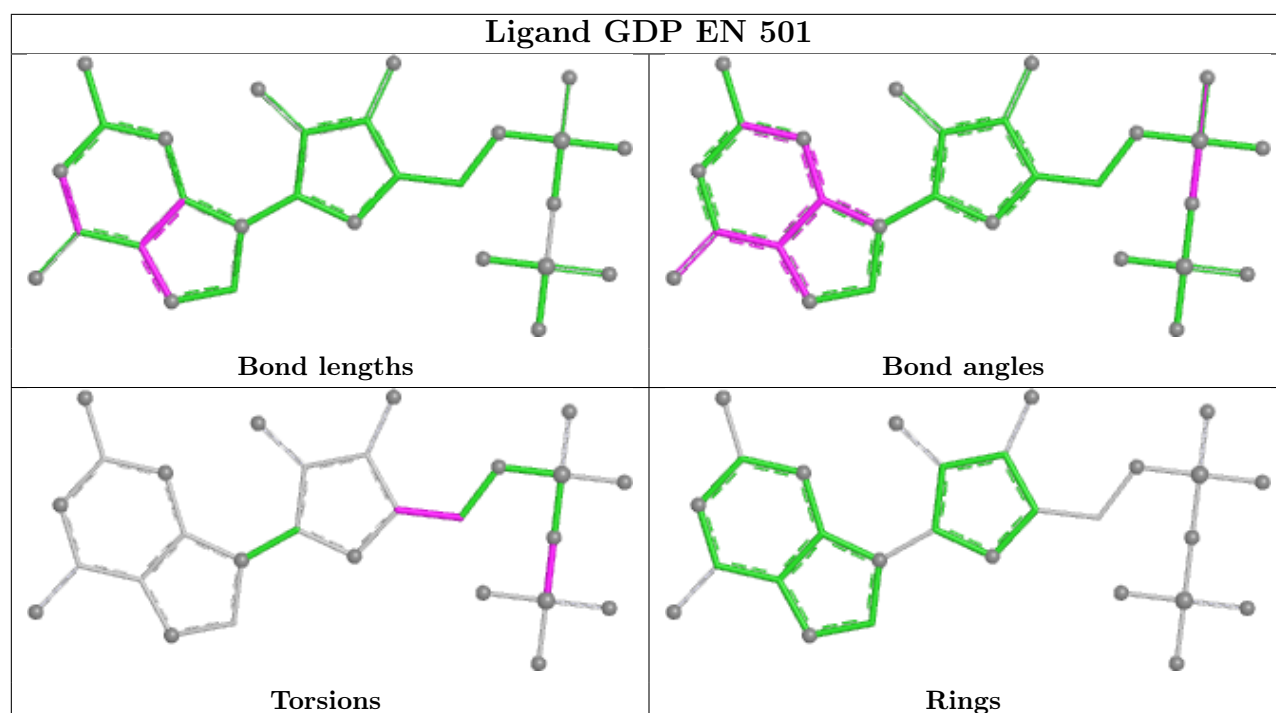


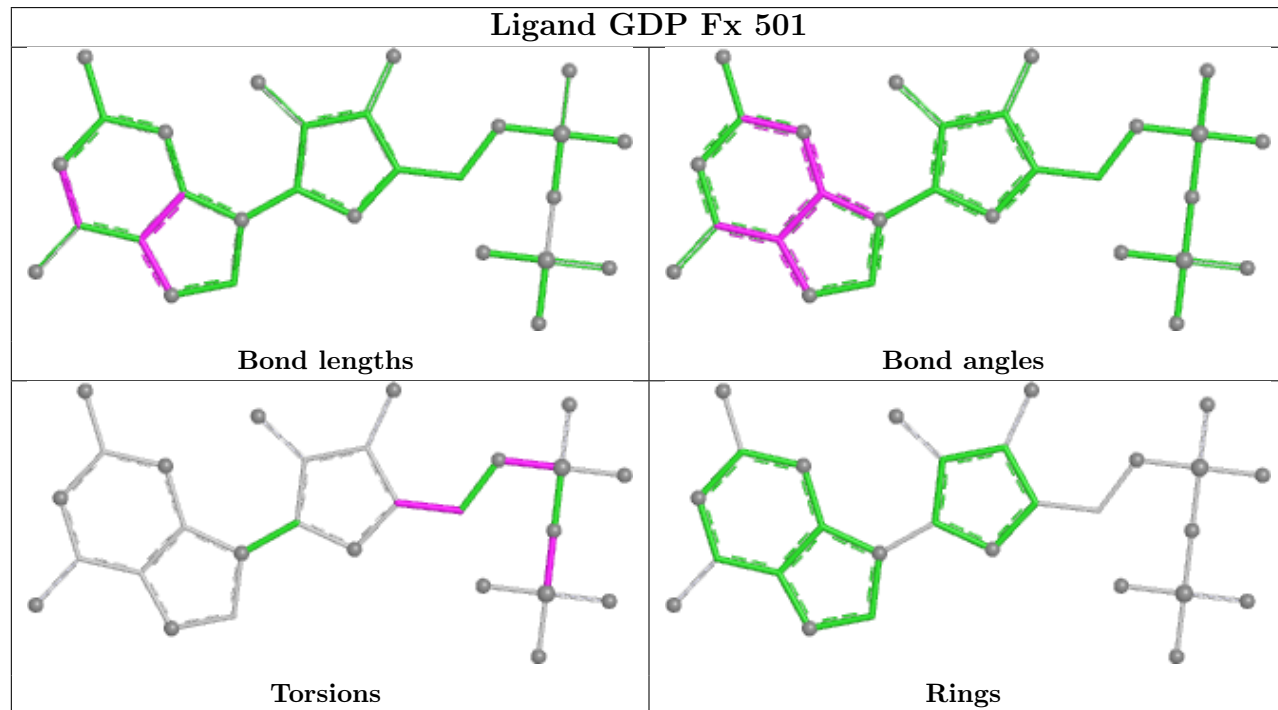
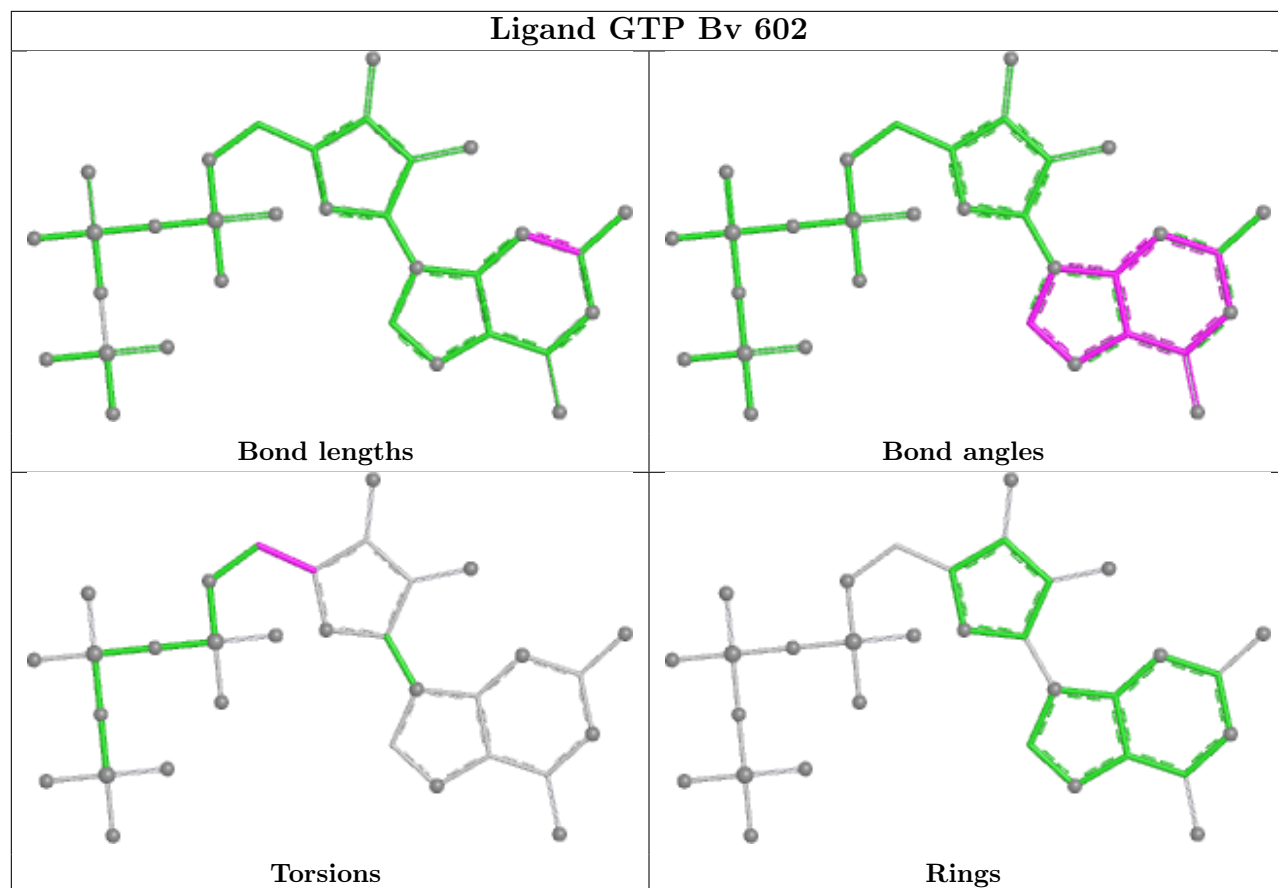


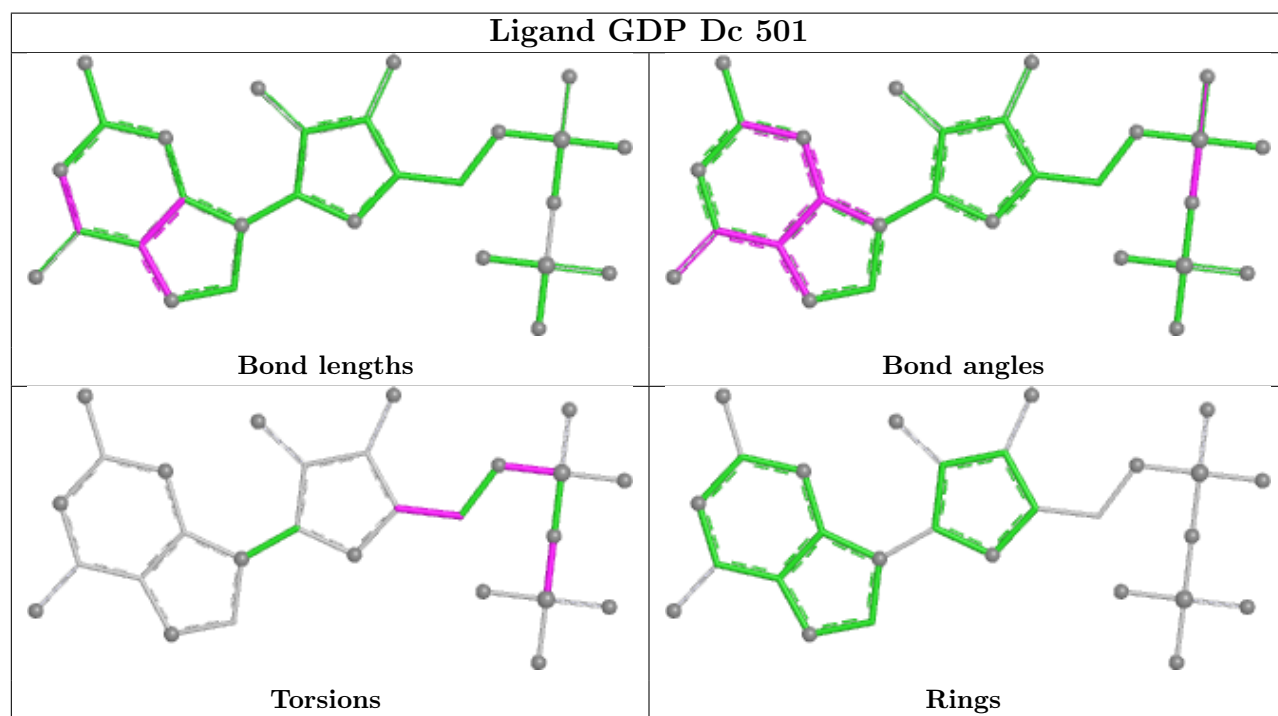
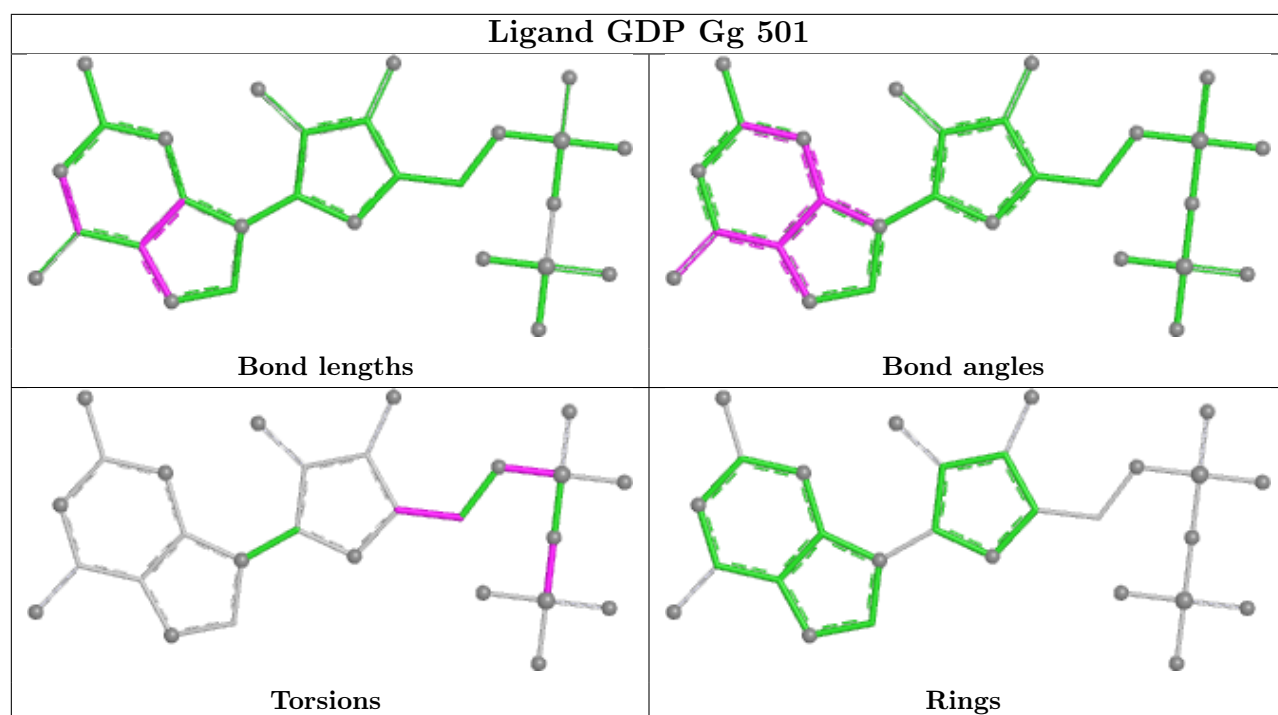


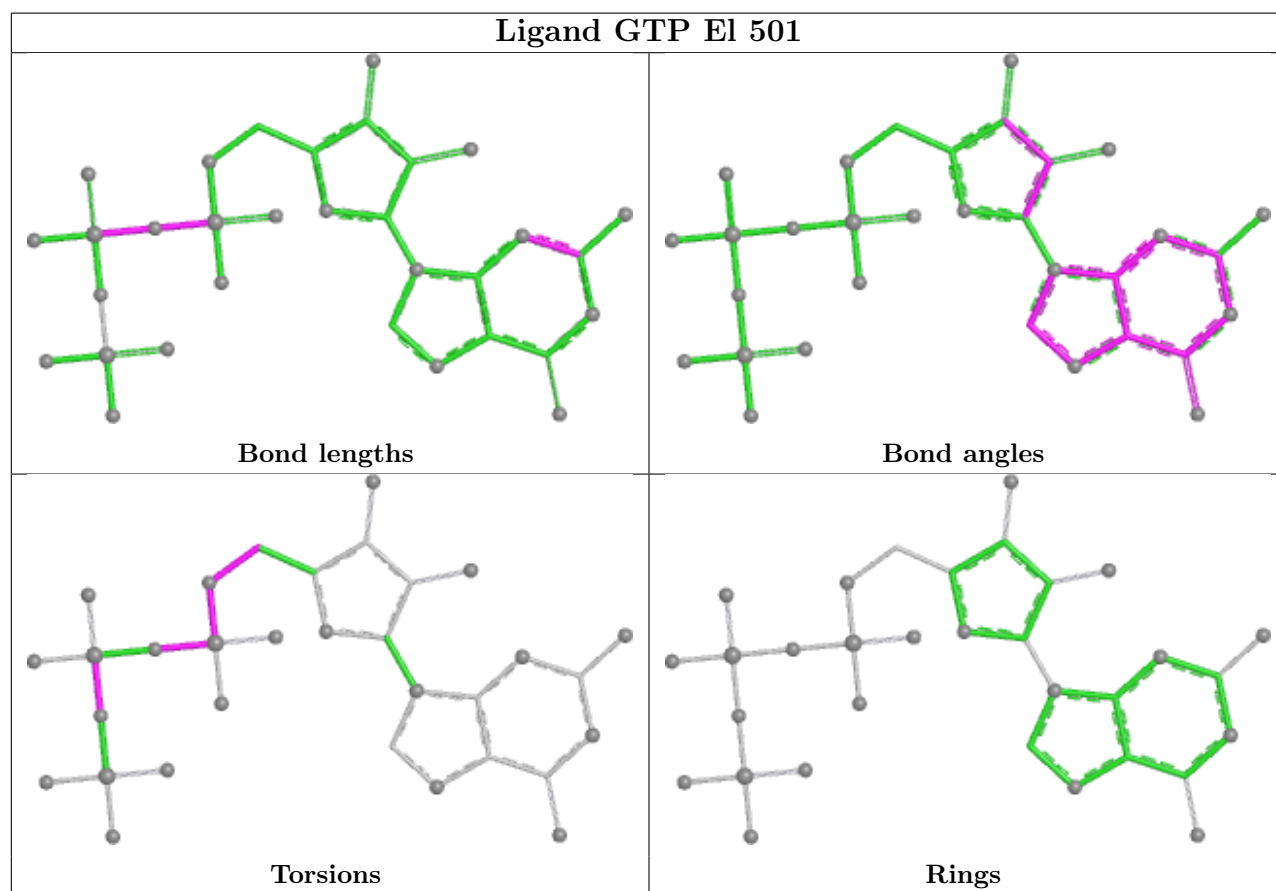
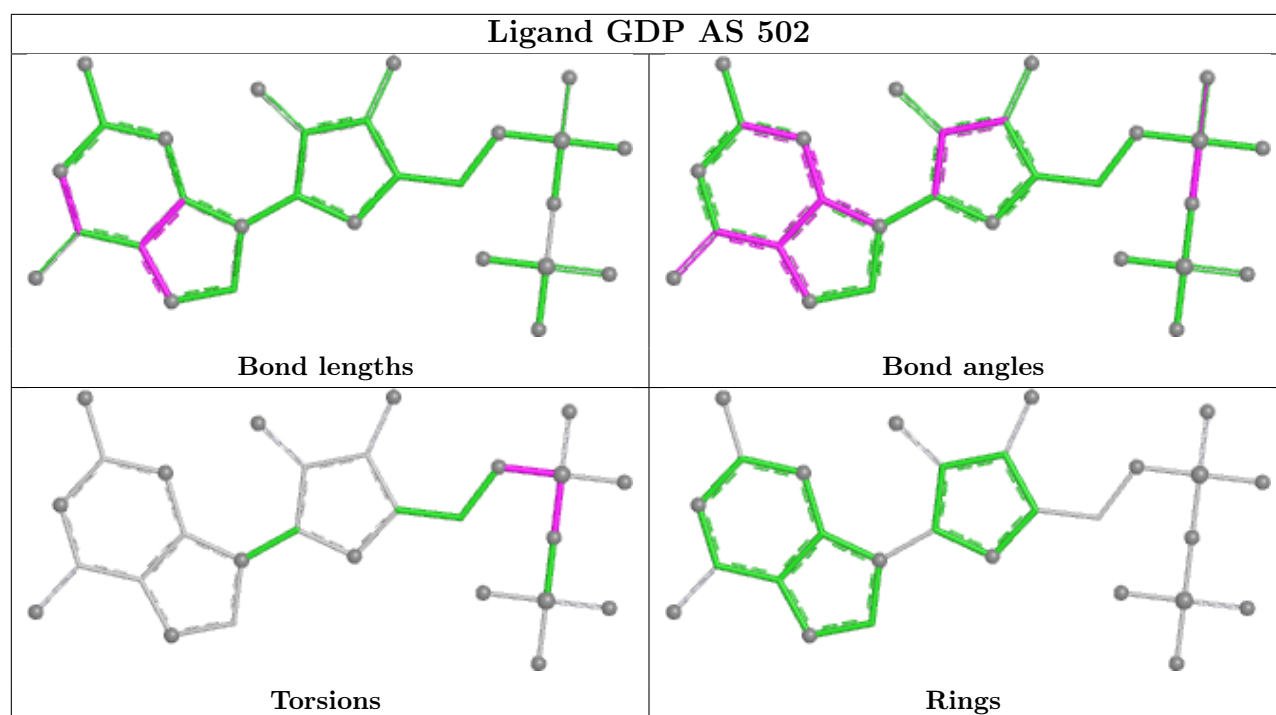


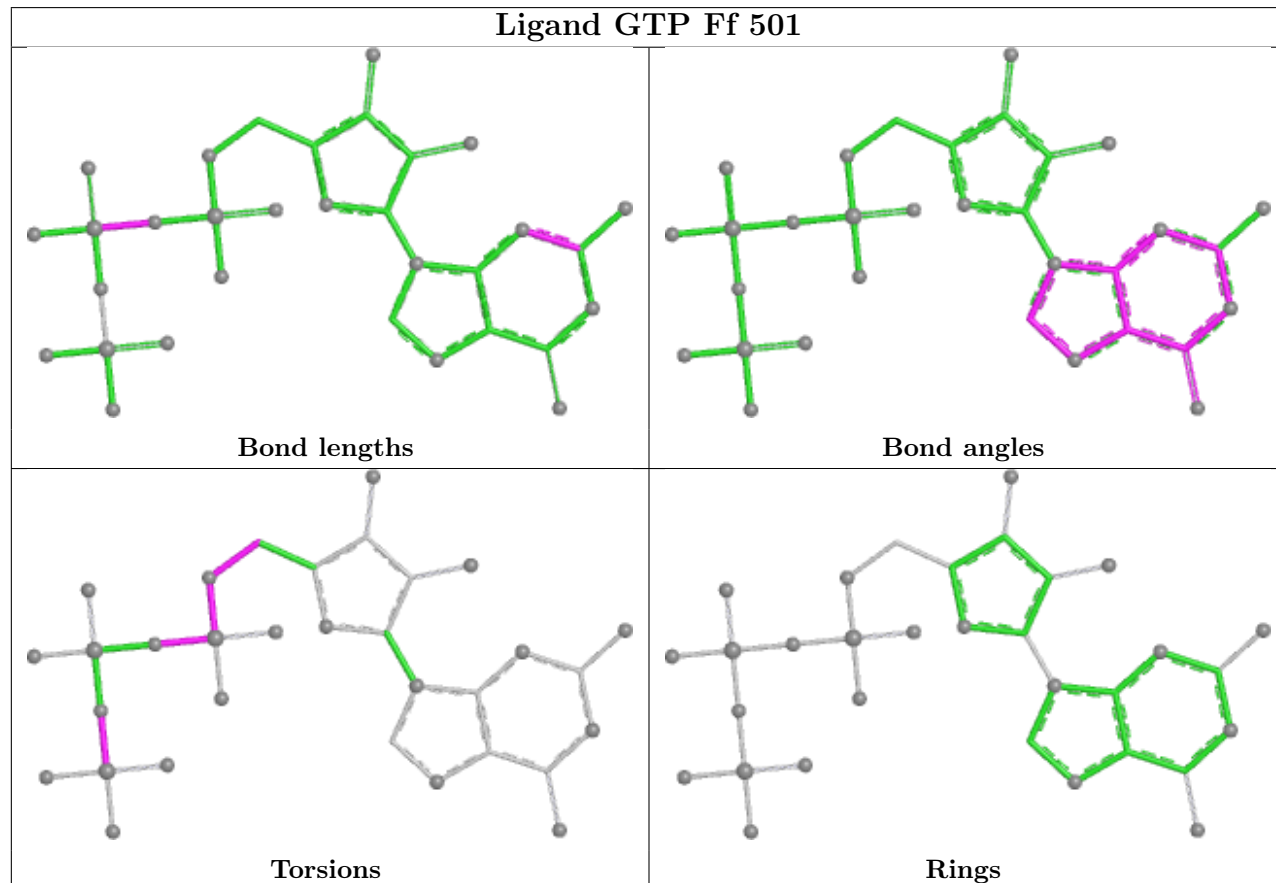
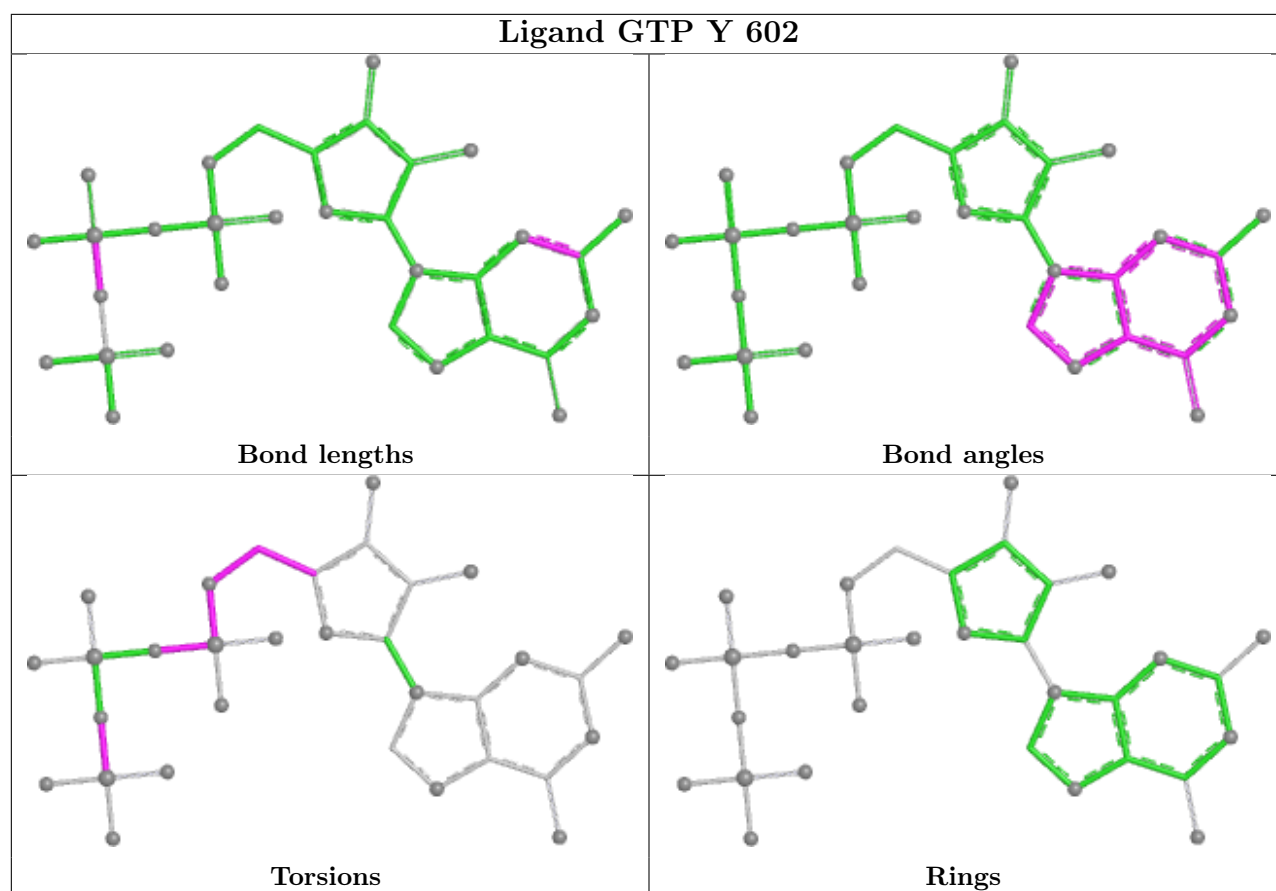


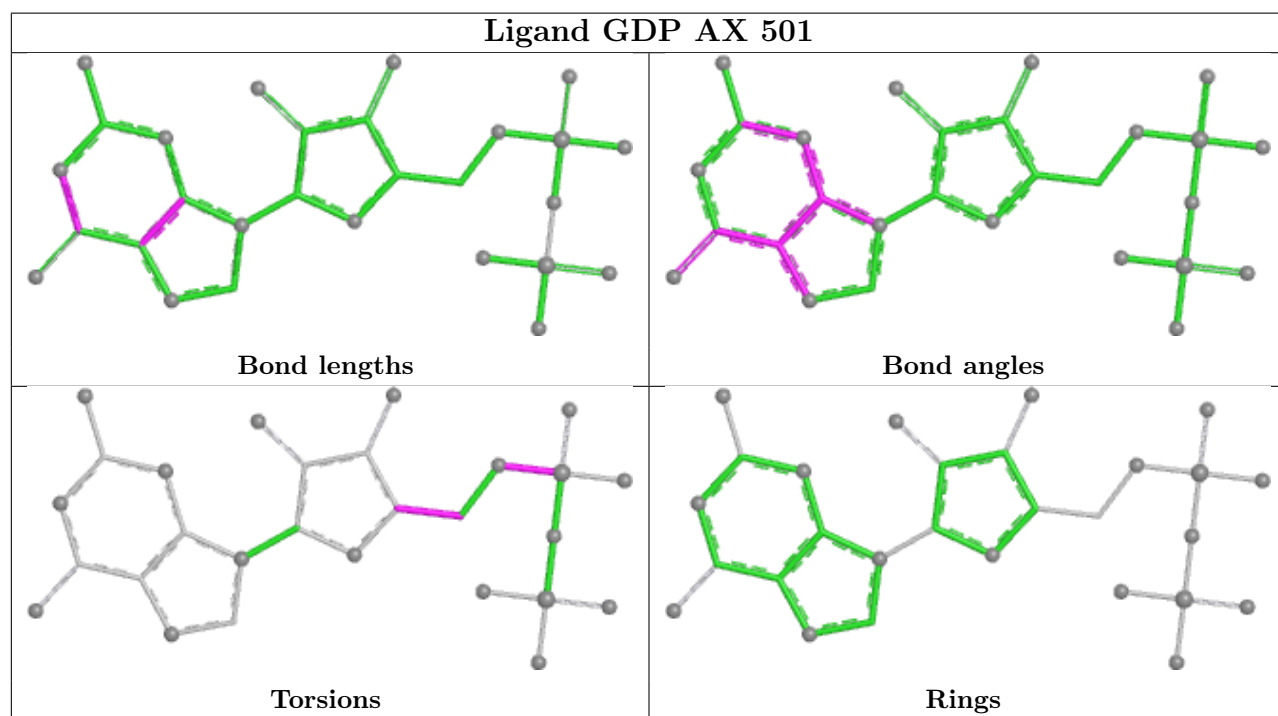
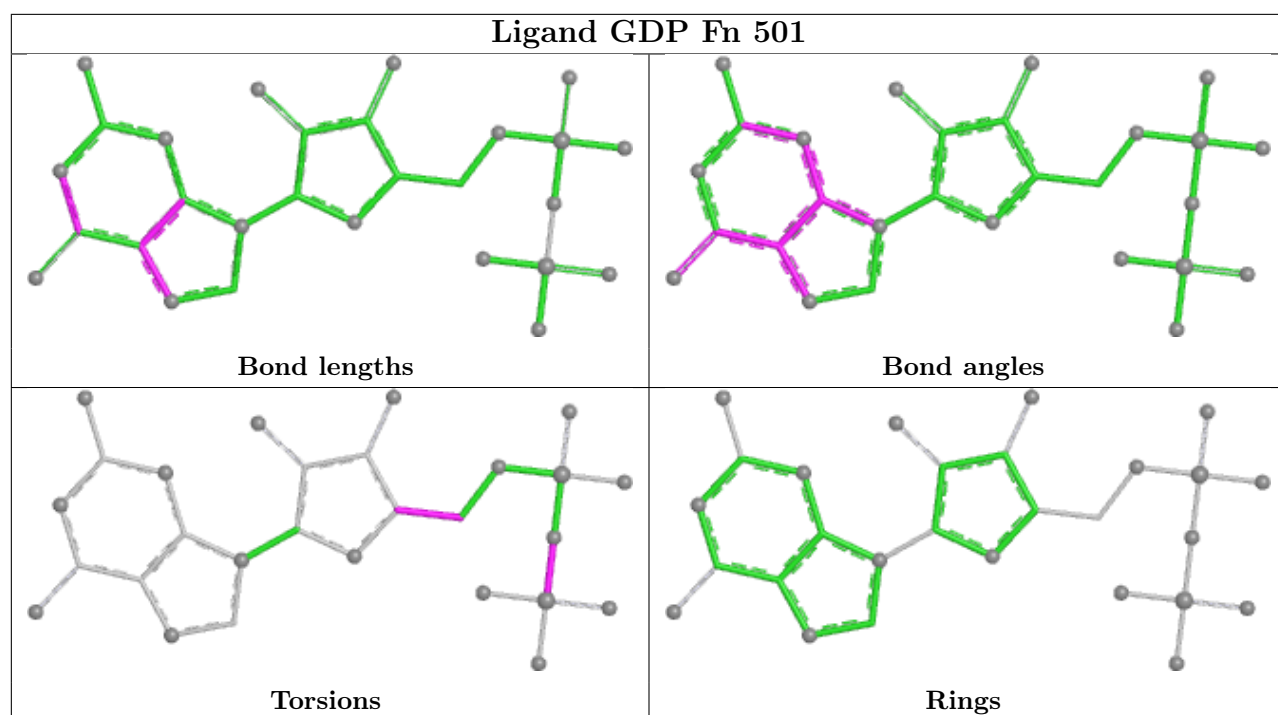


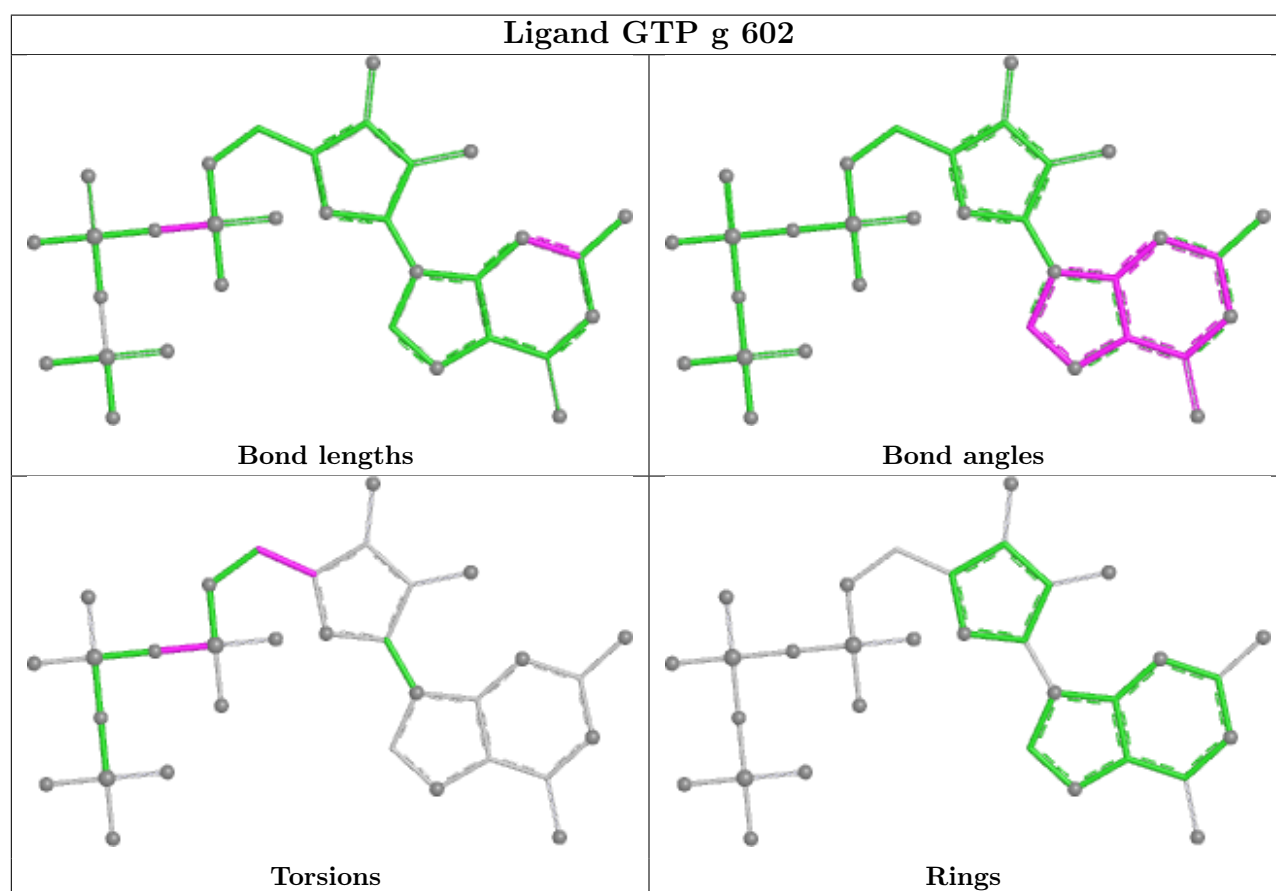
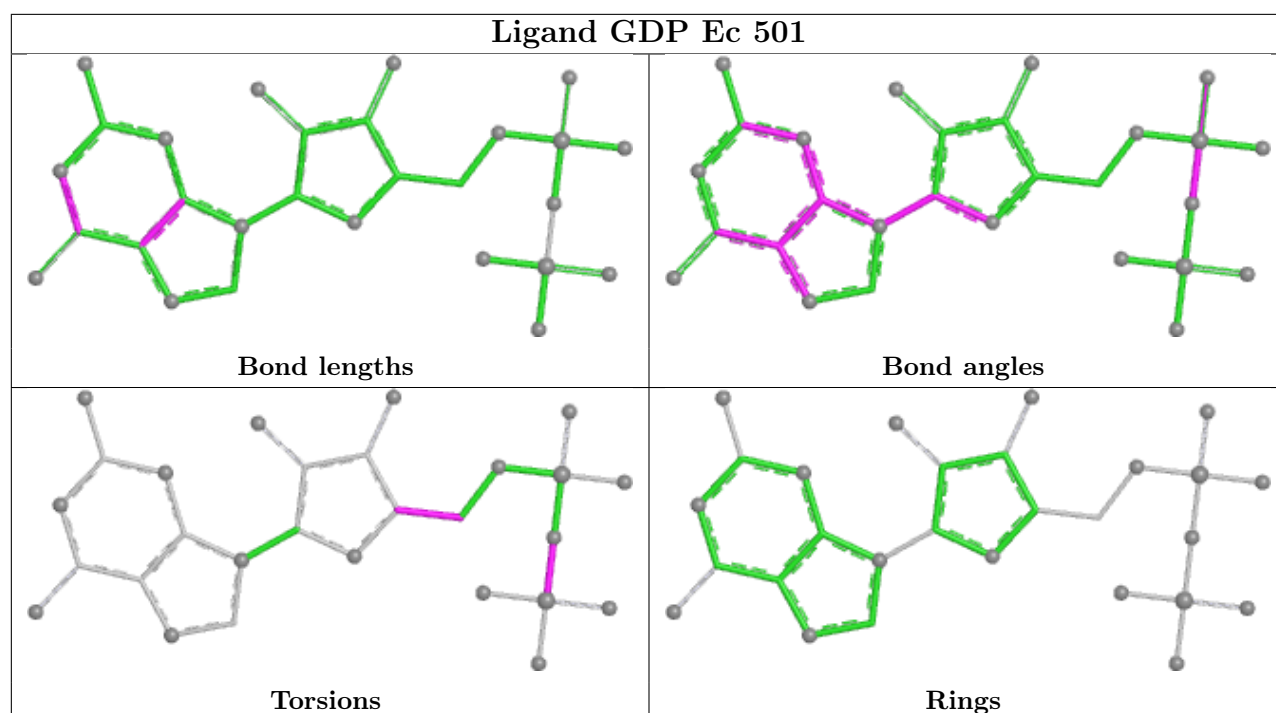




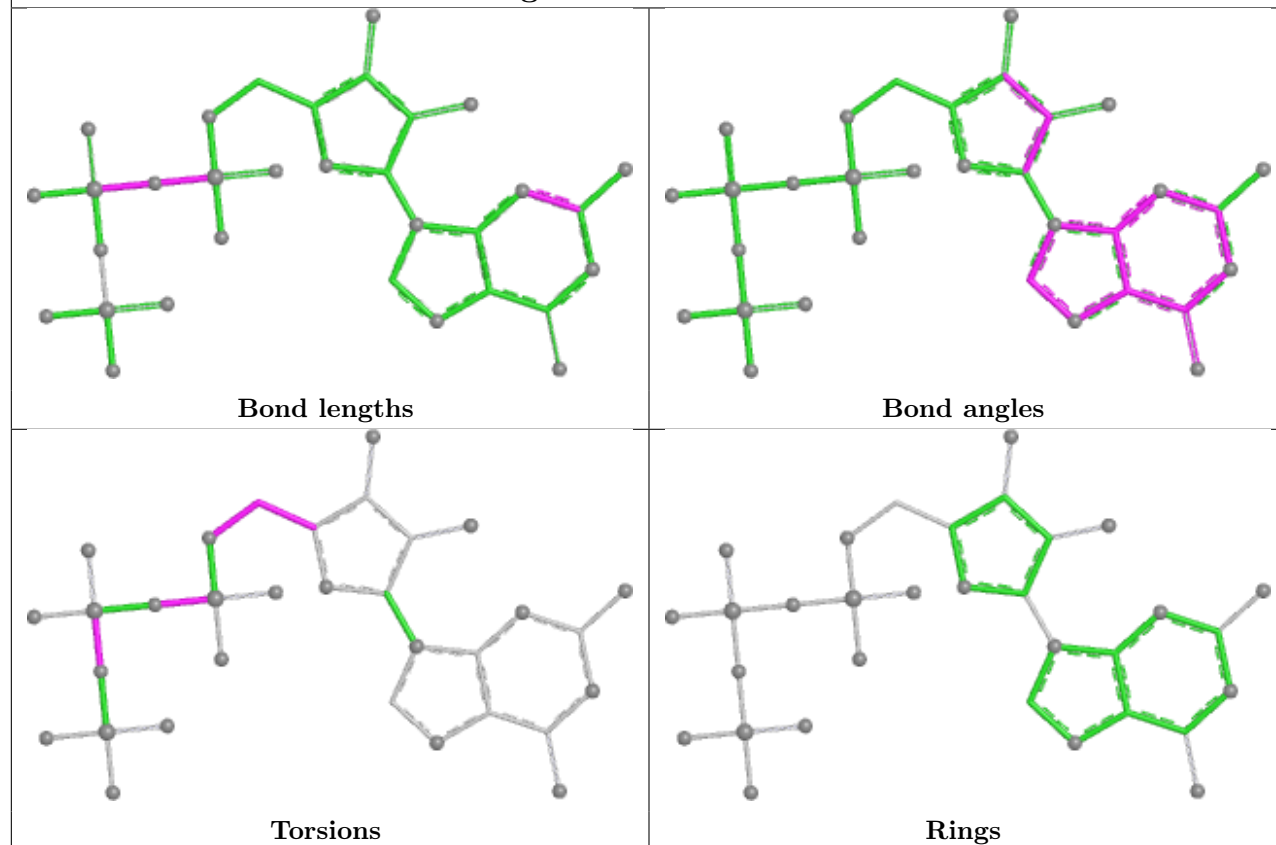




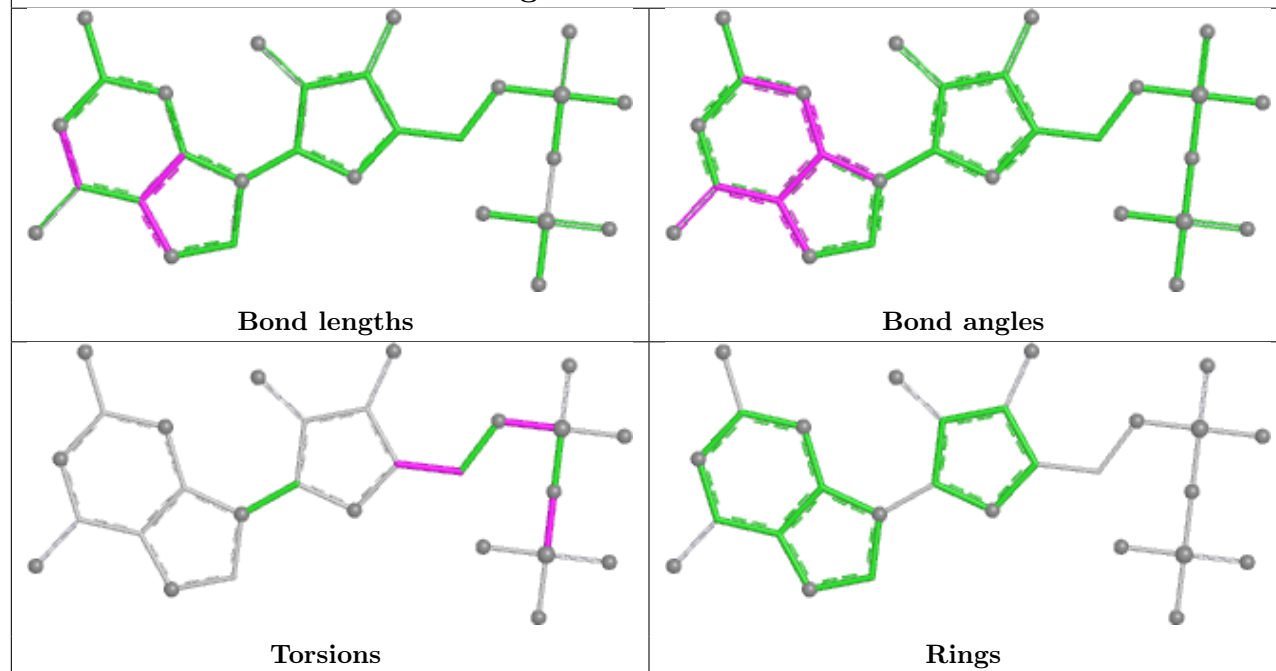


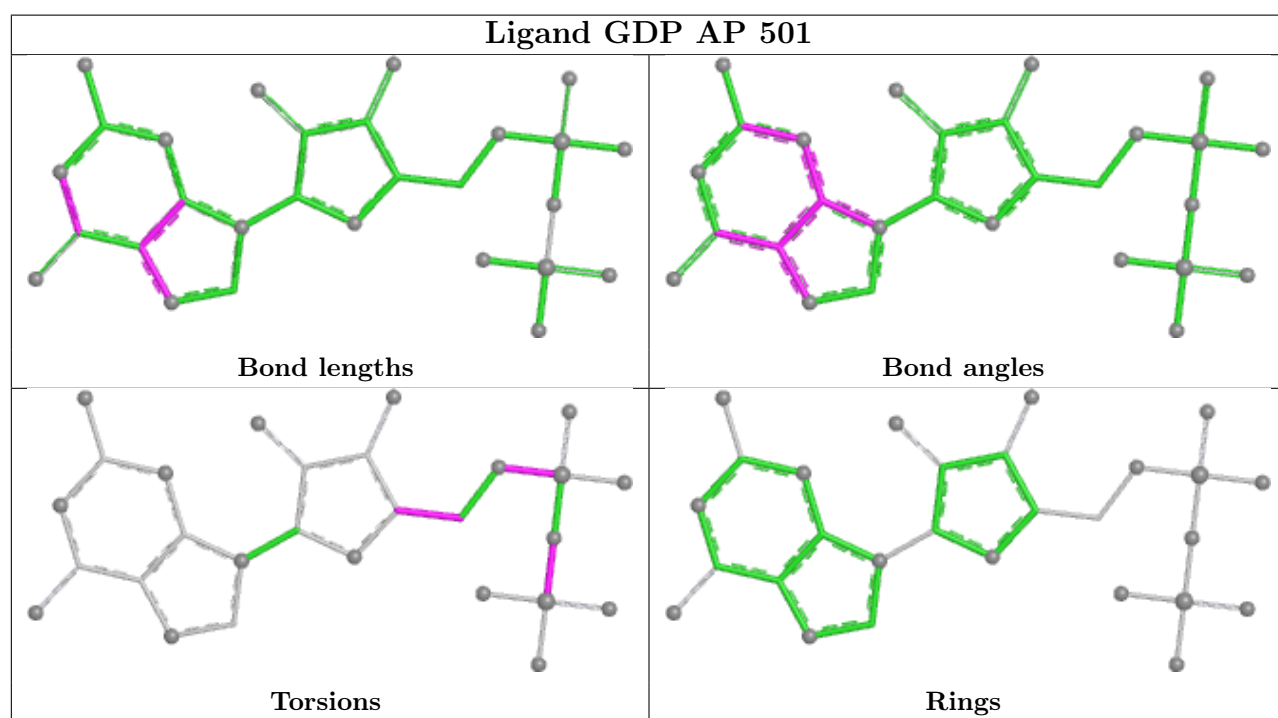
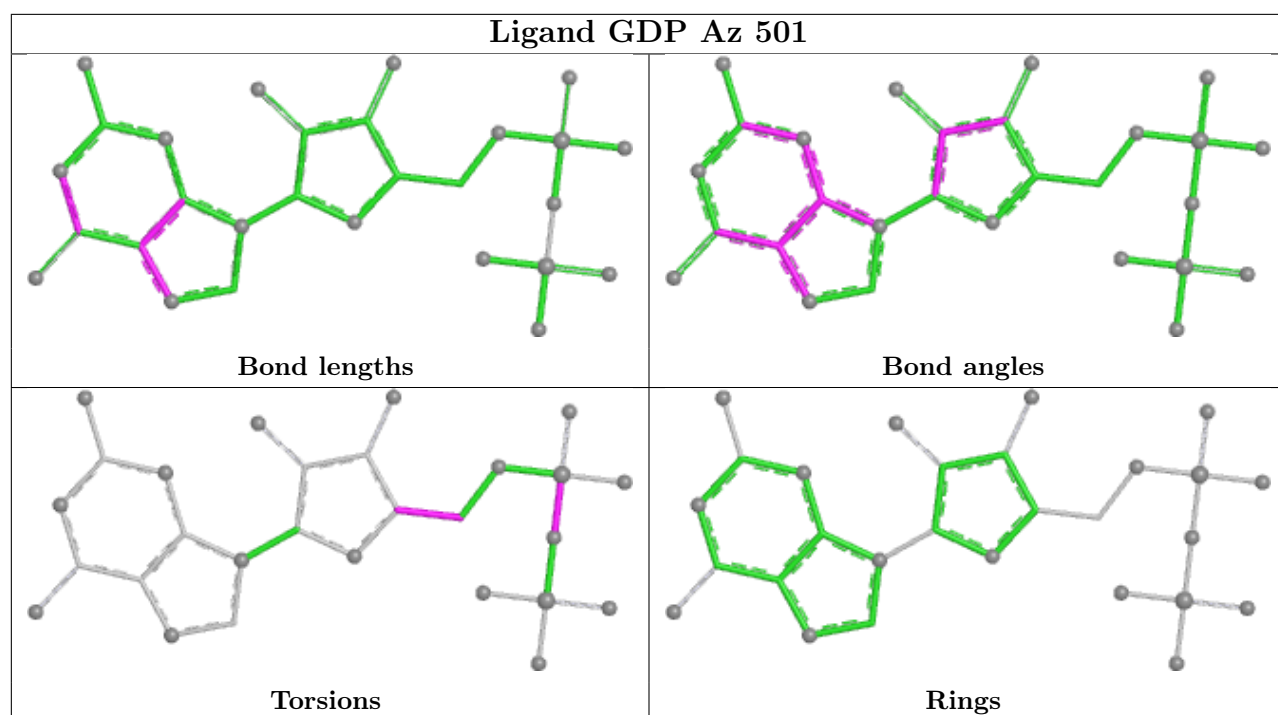


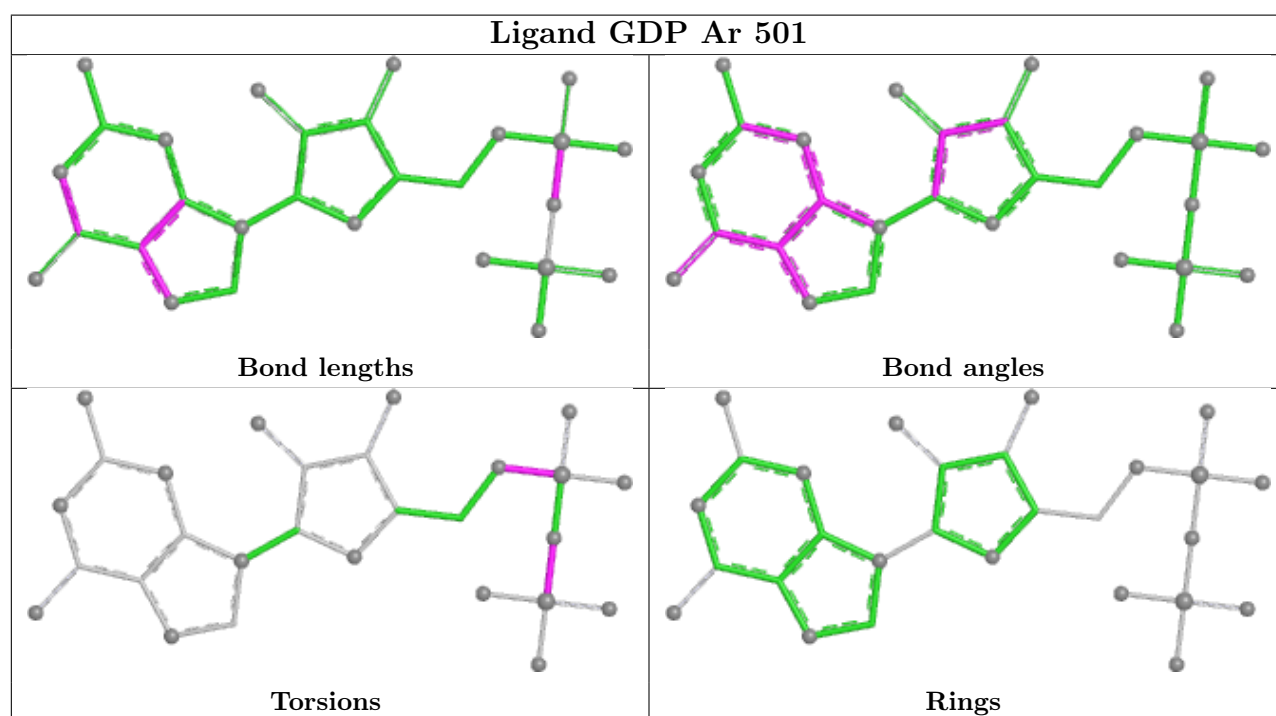
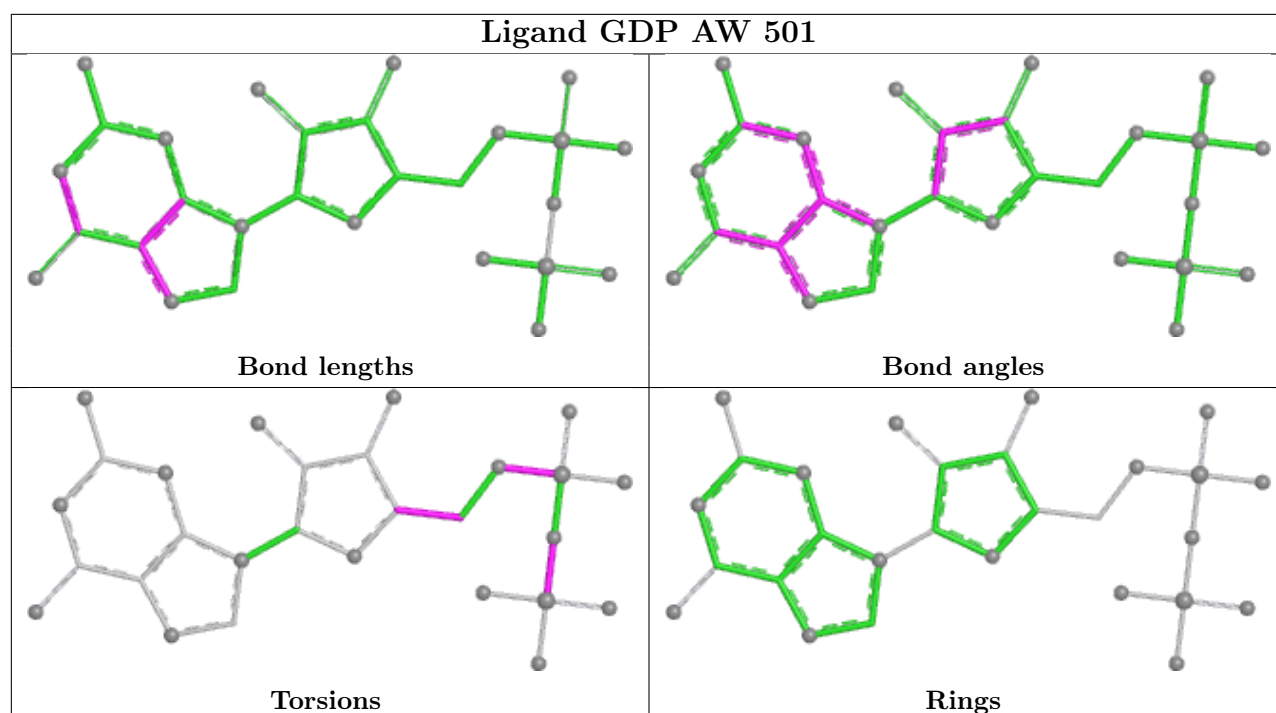
Ligand GTP Ak 602

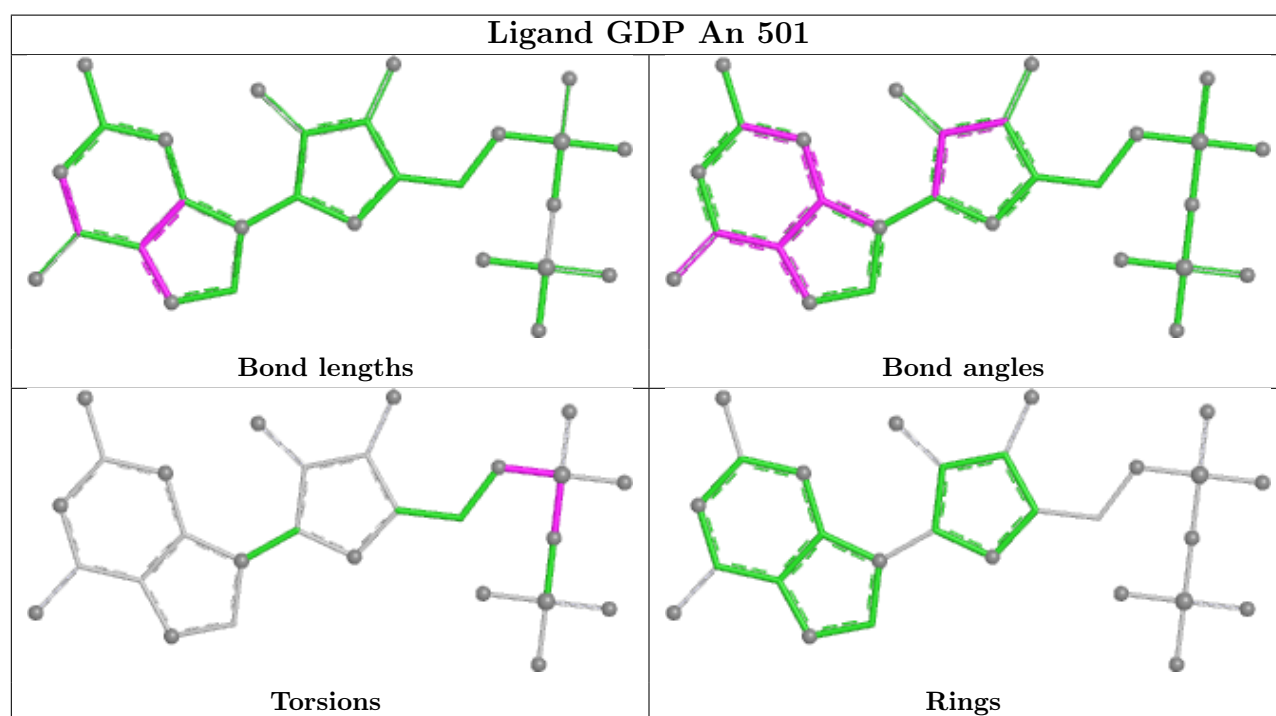
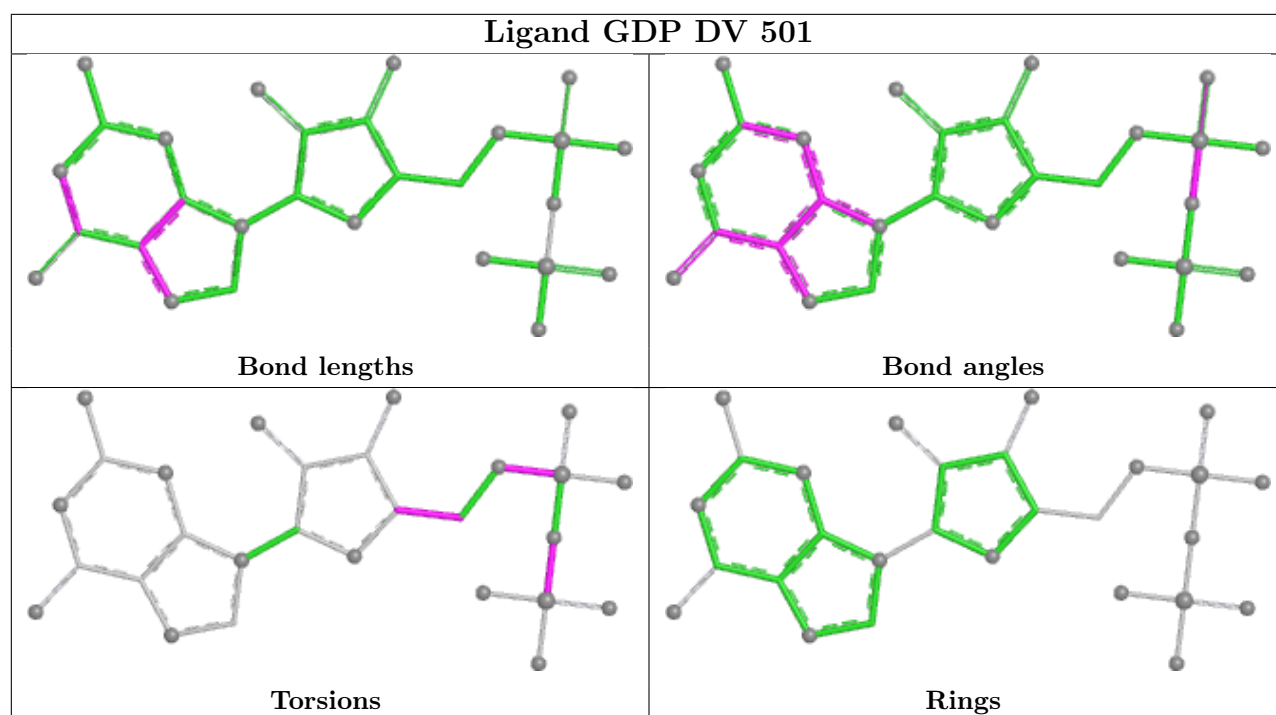


Ligand GDP Aa 501

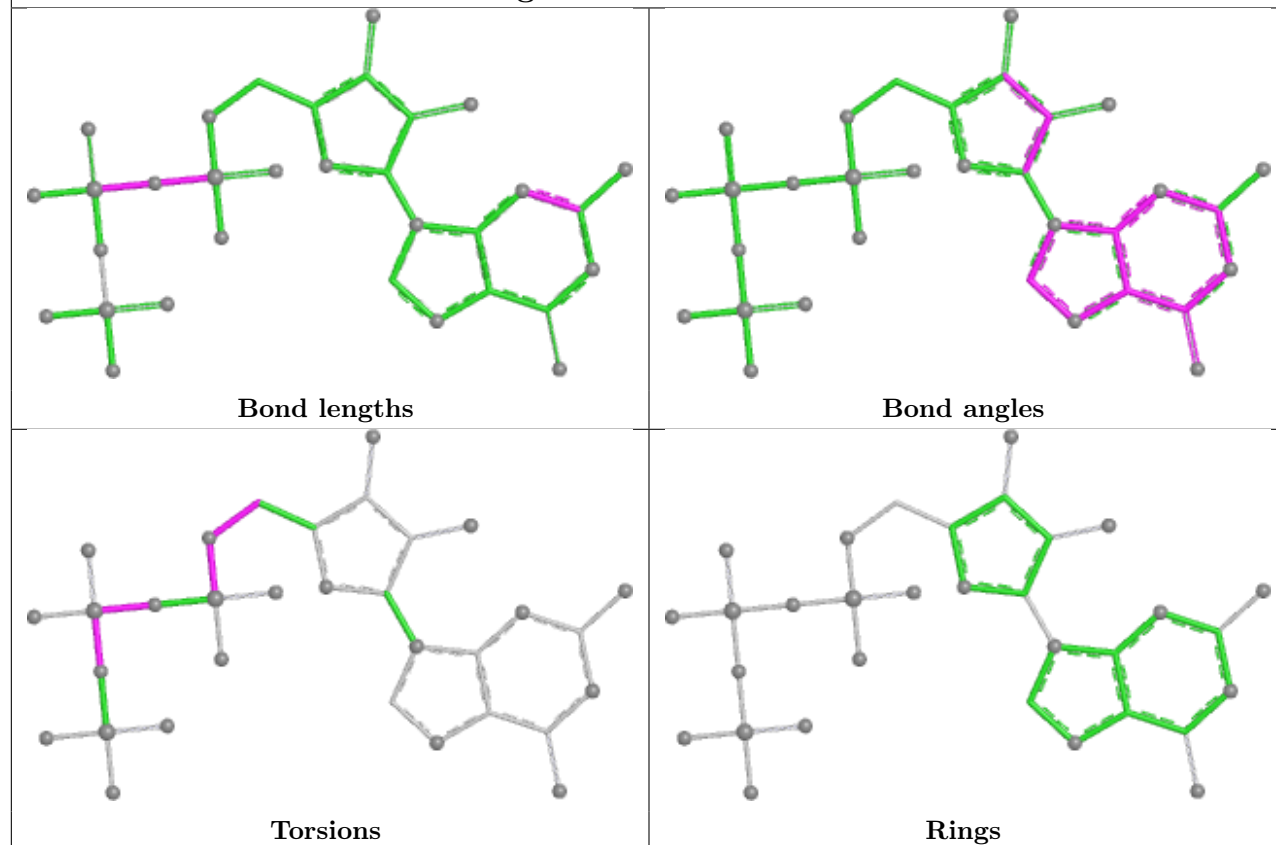




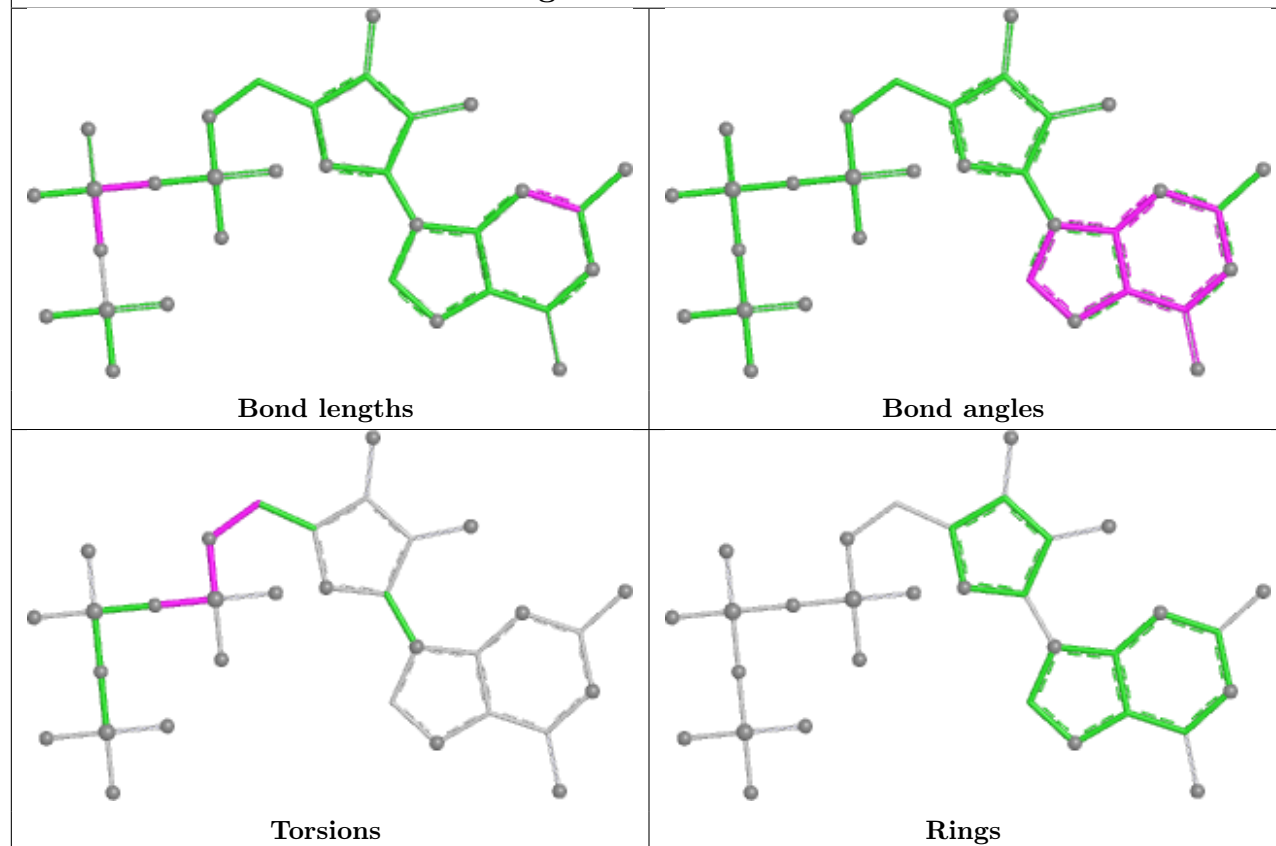




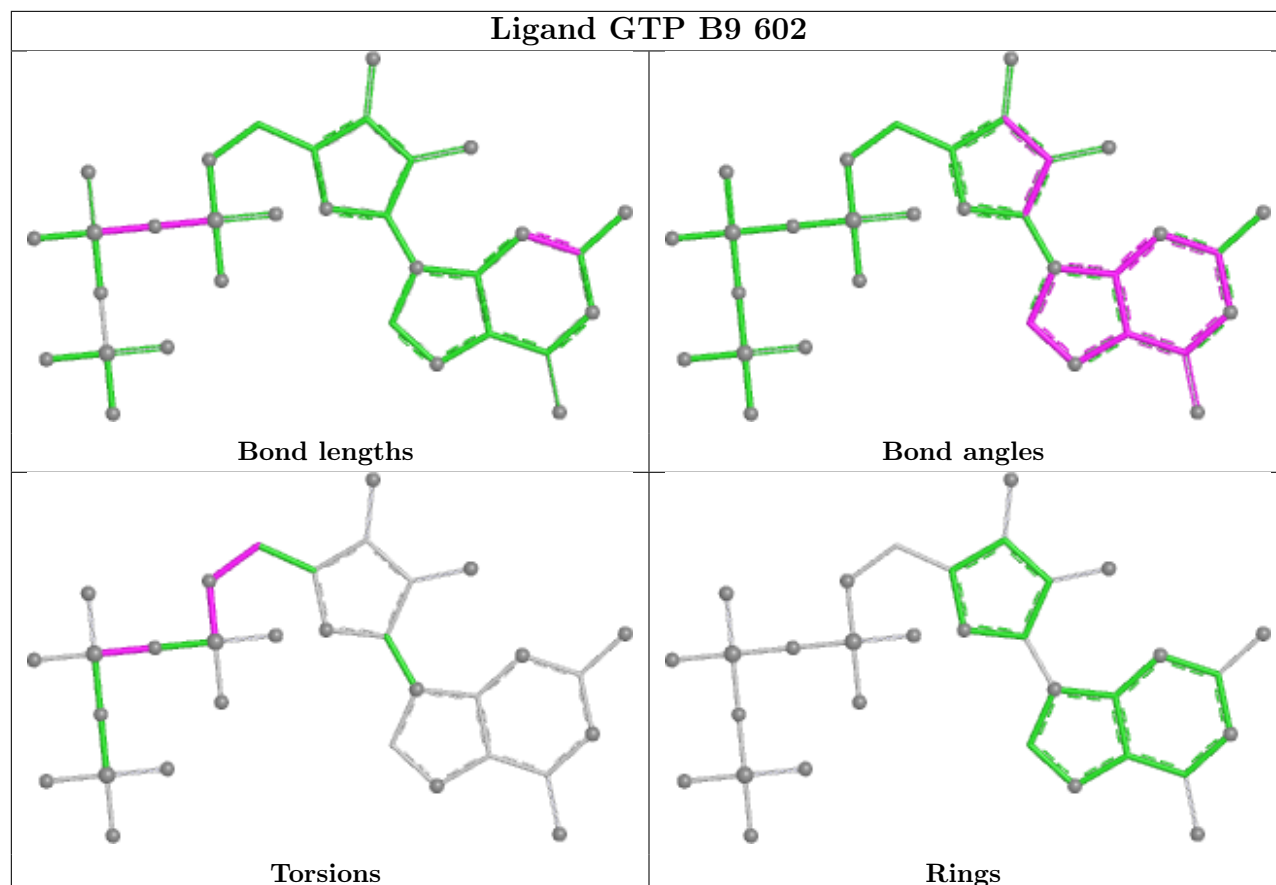
Ligand GTP Em 501



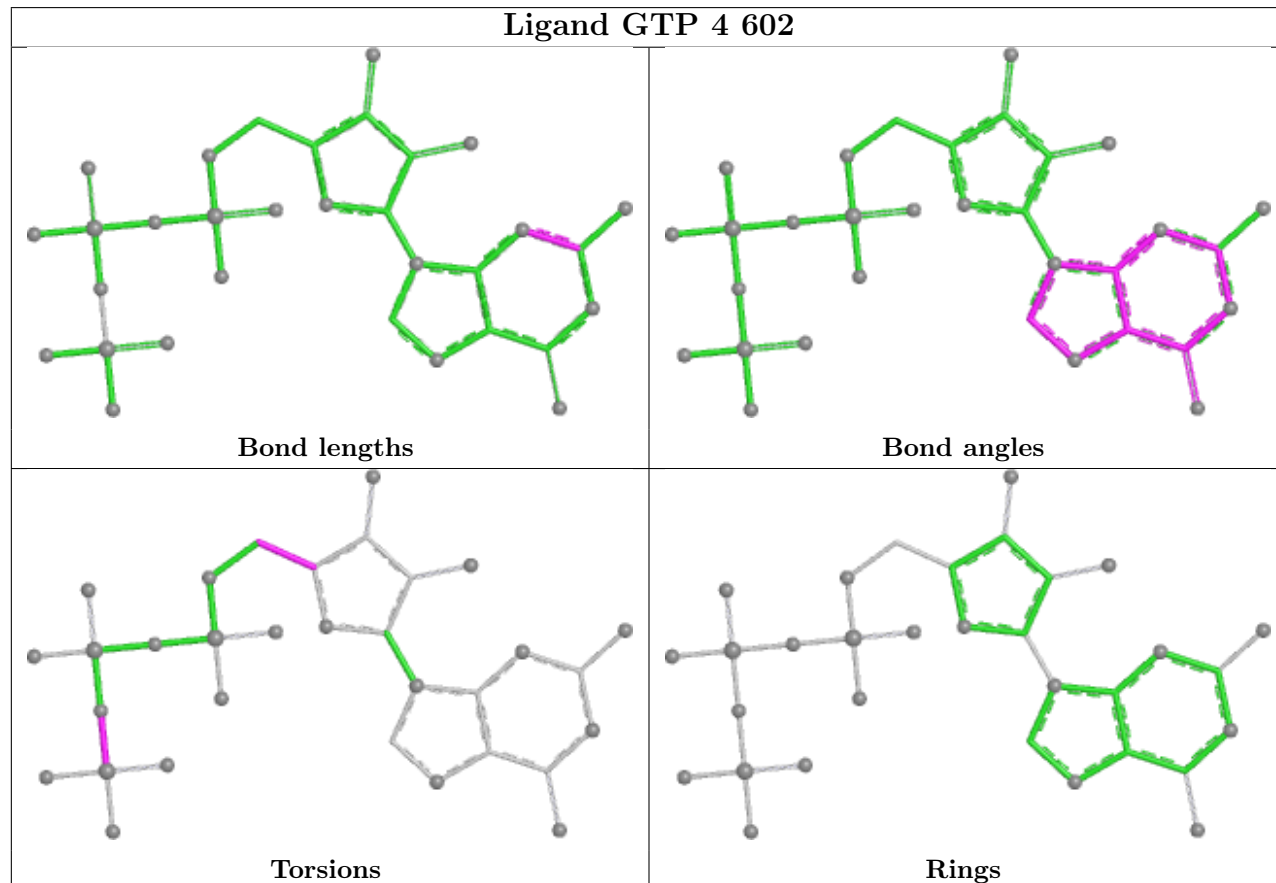
Ligand GTP f 602

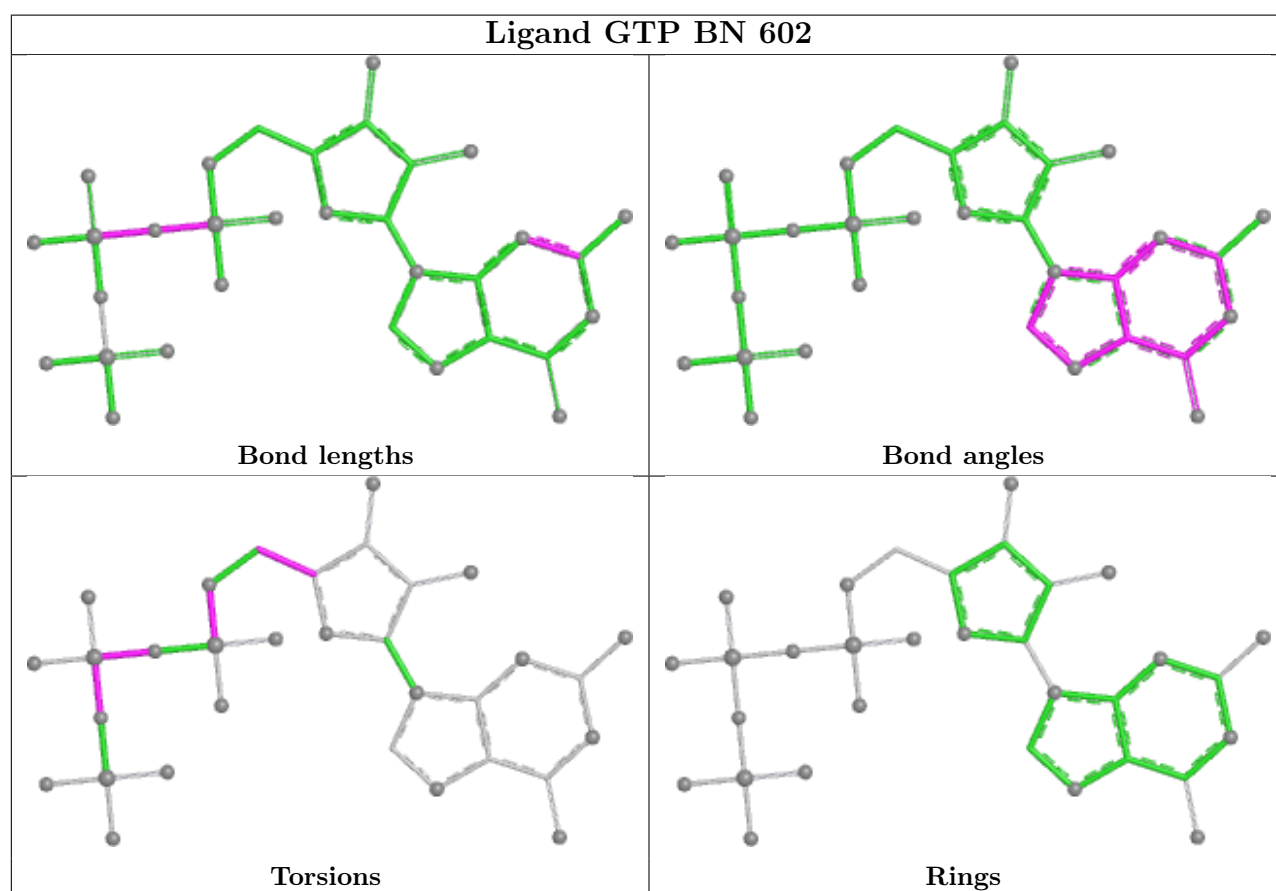
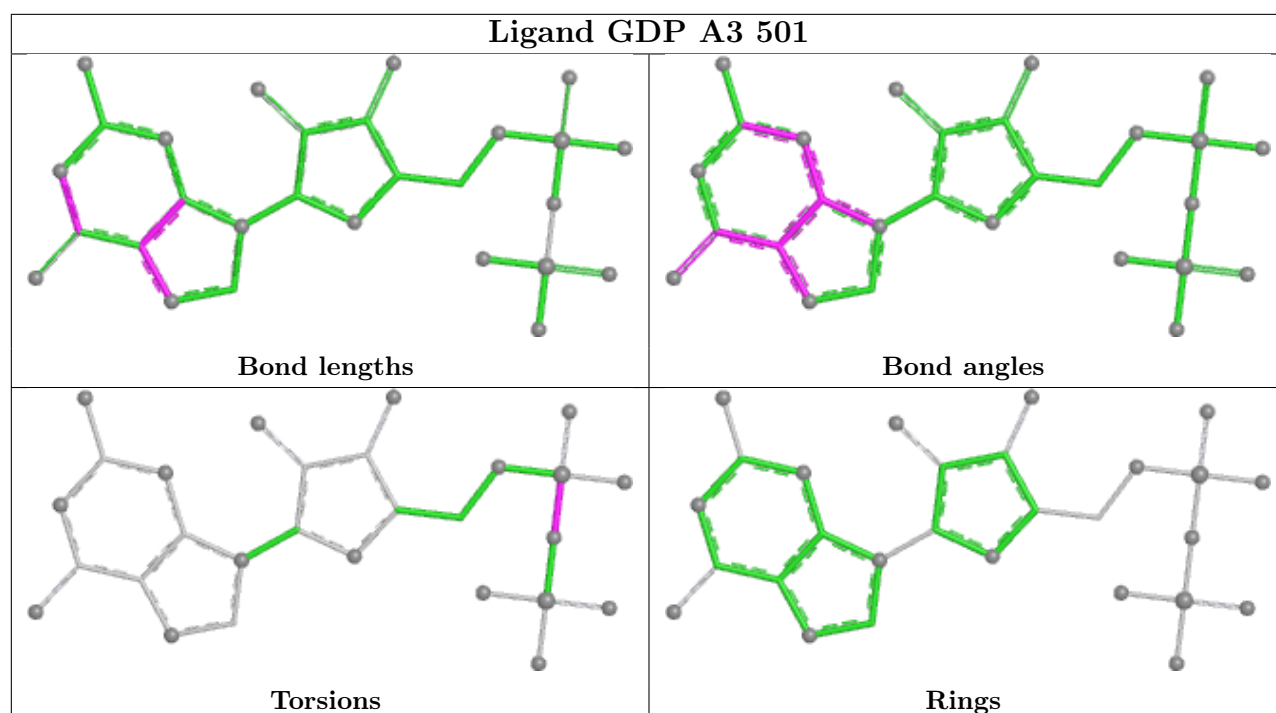


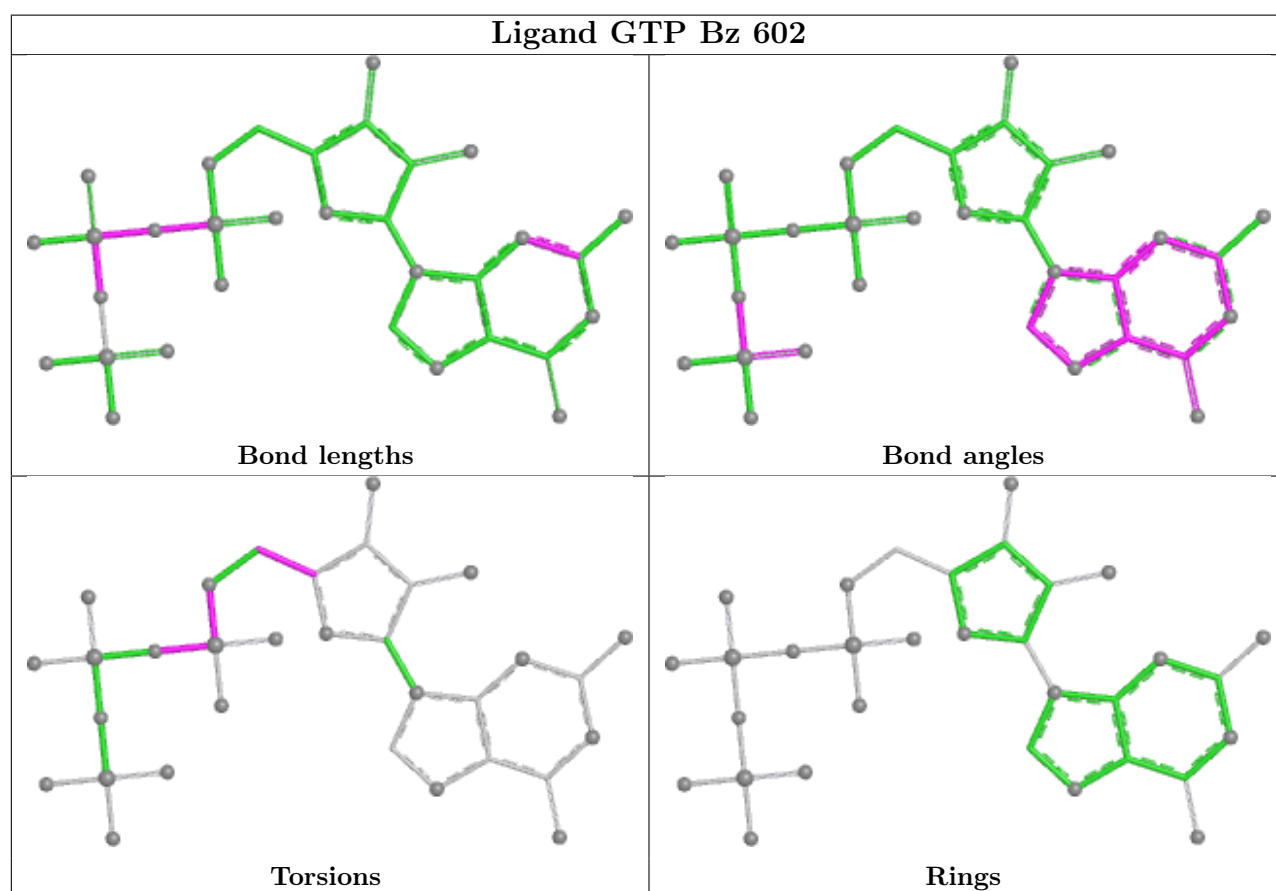
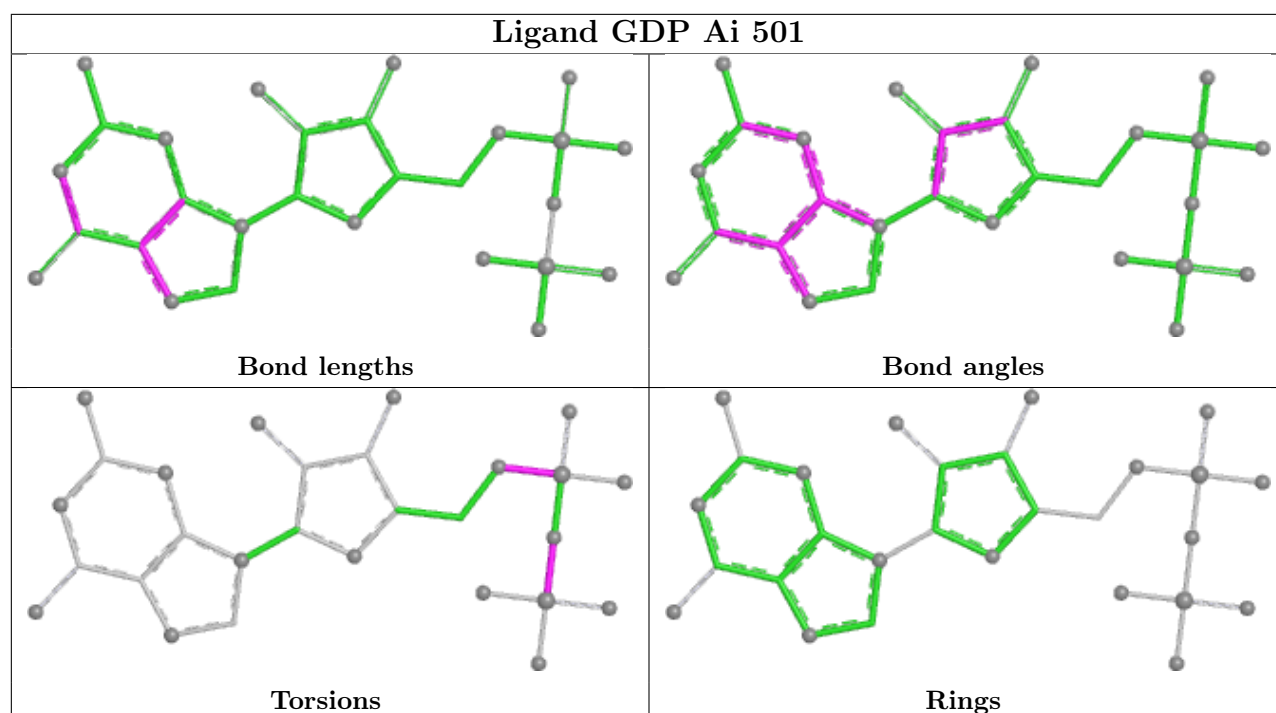
Ligand GTP B9 602

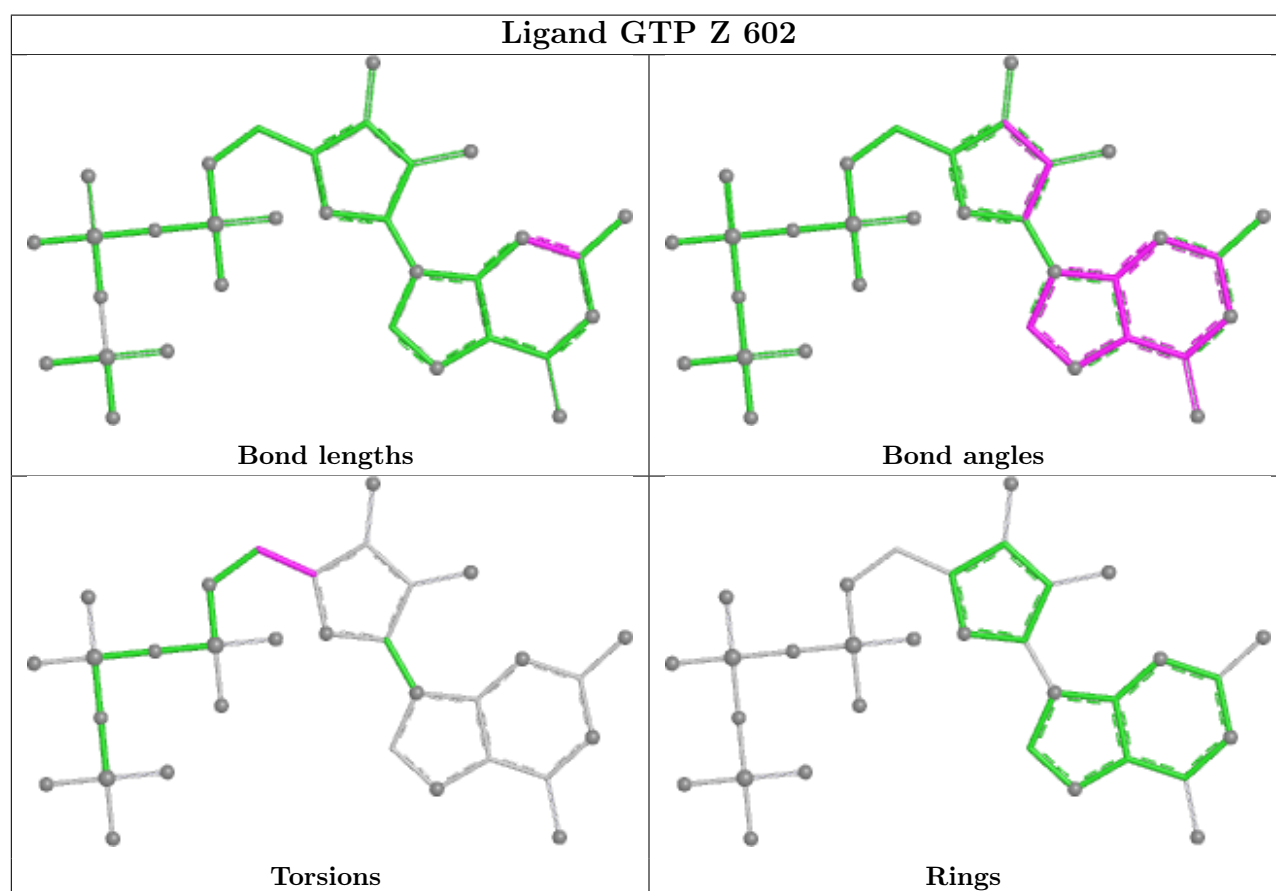
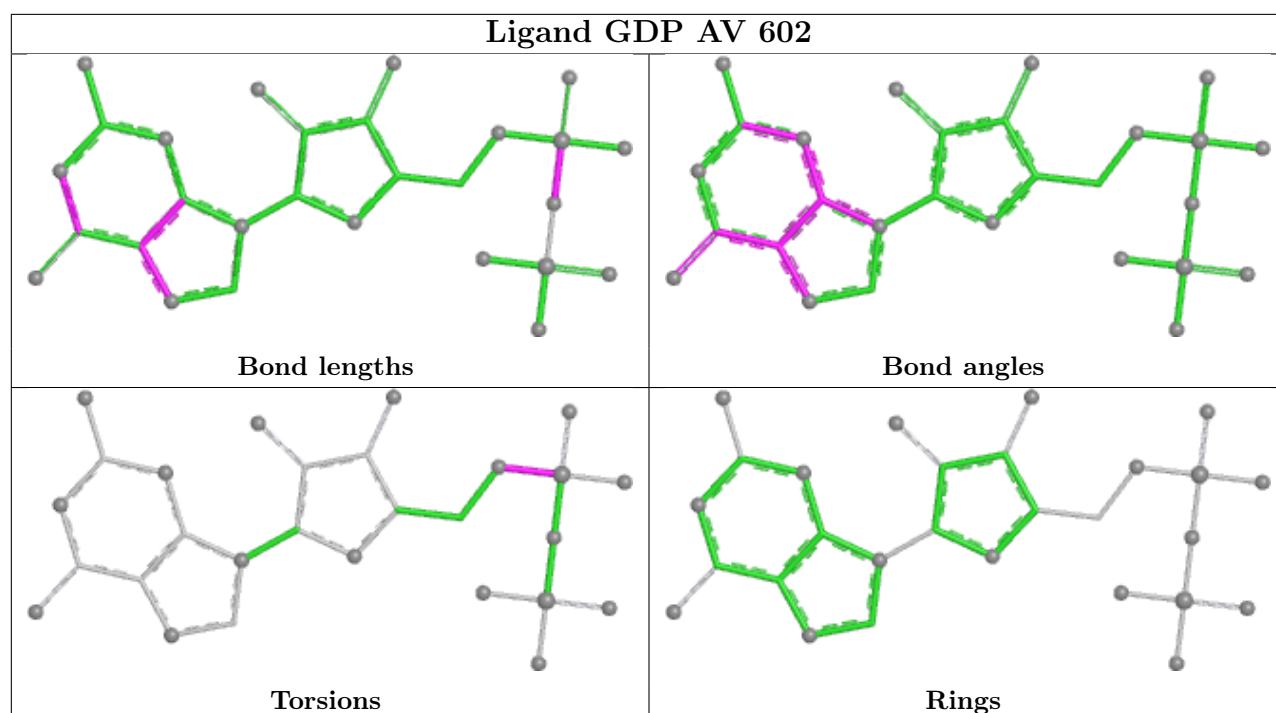


Ligand GTP 4 602

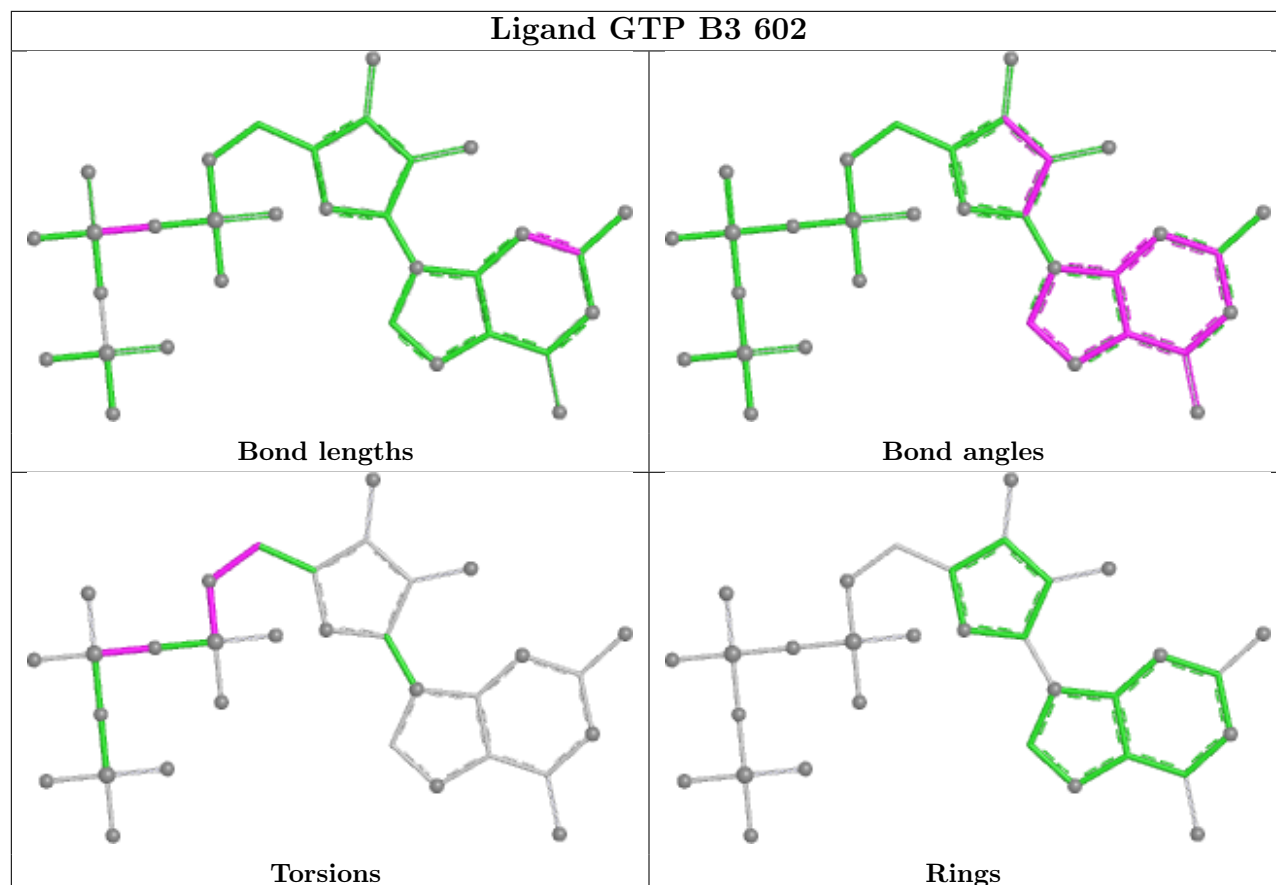




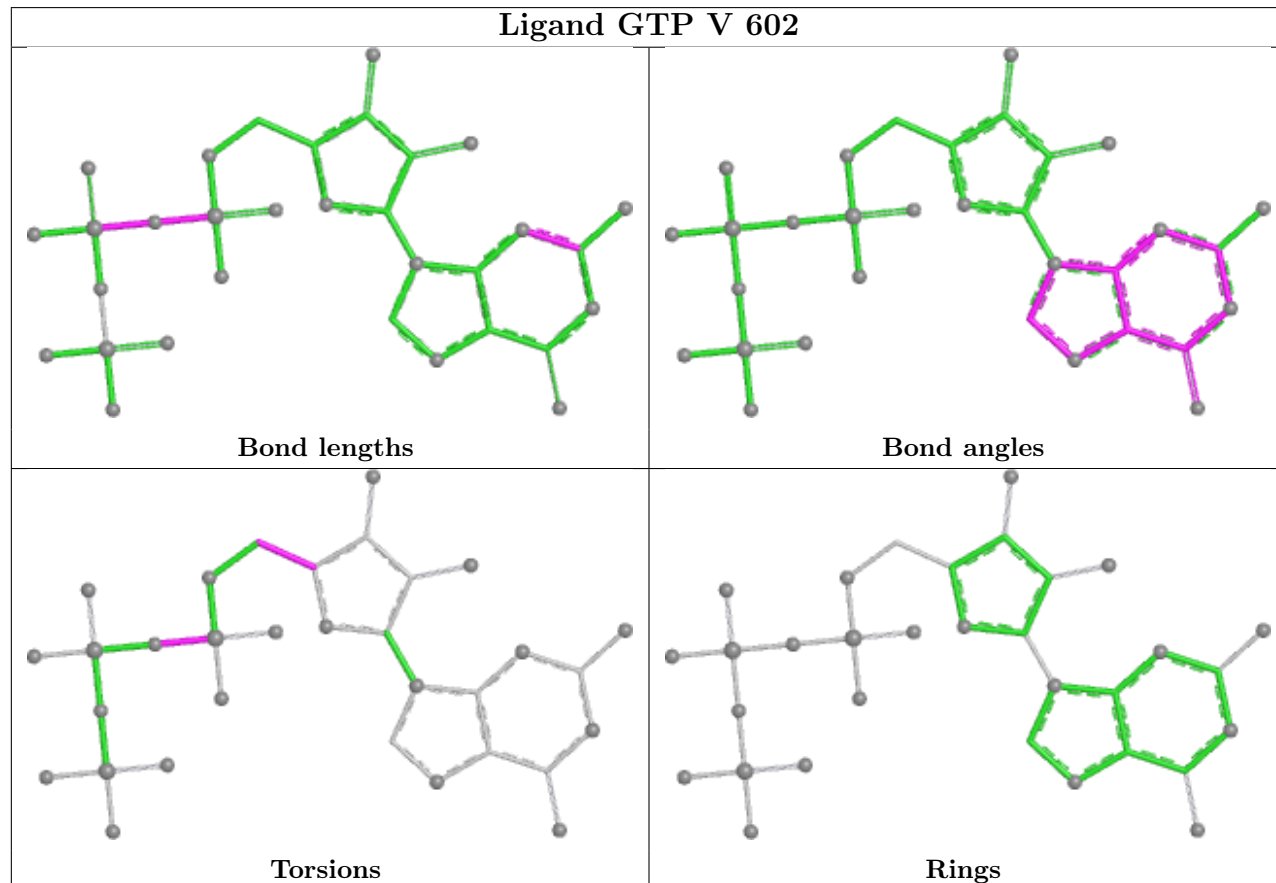


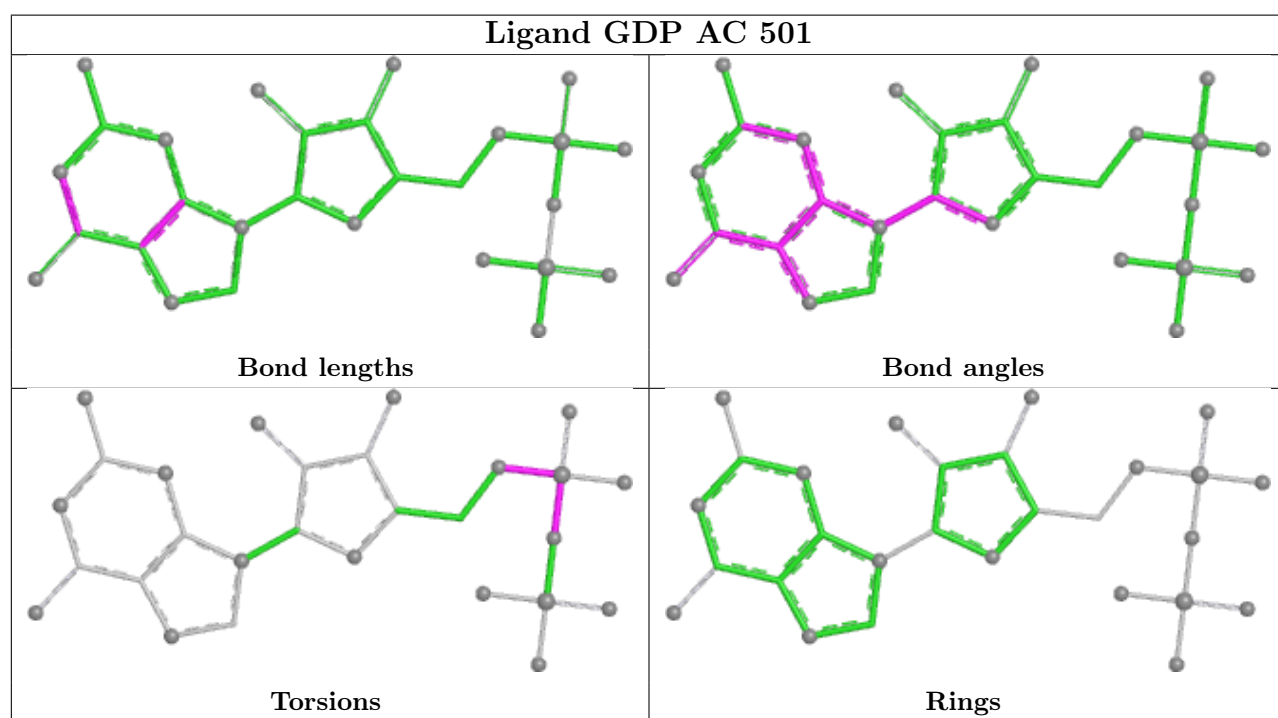
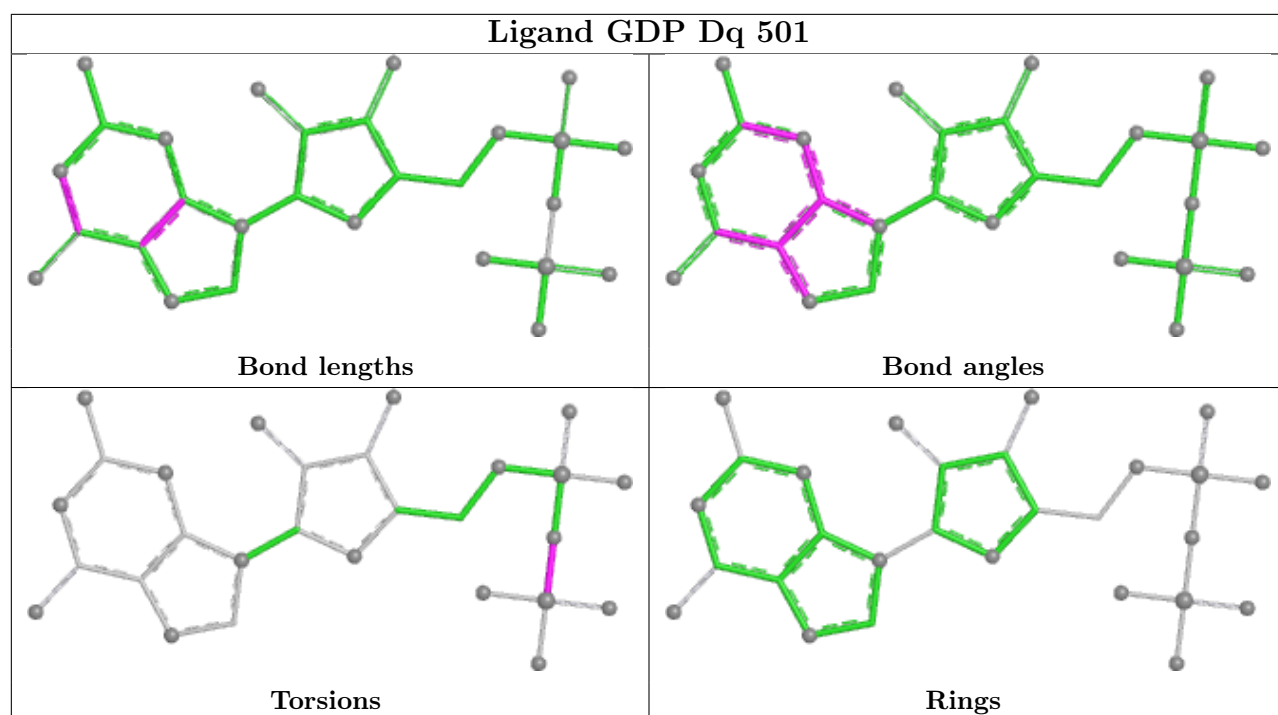


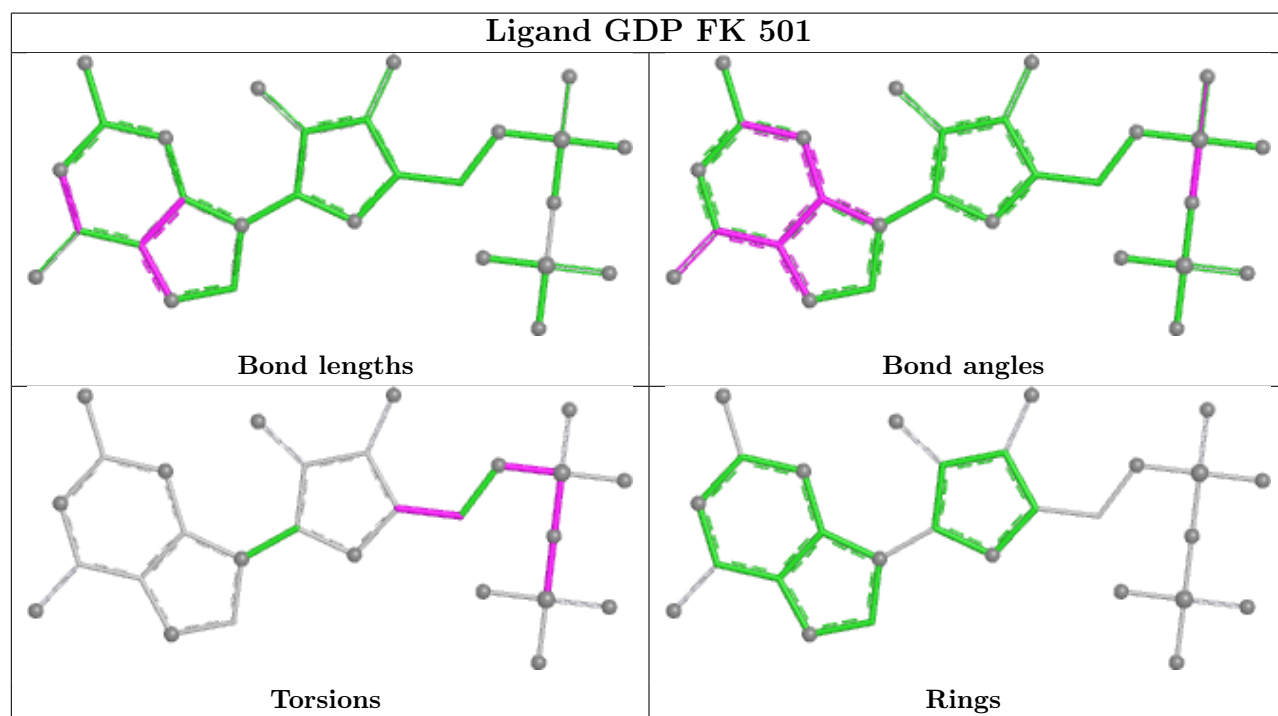
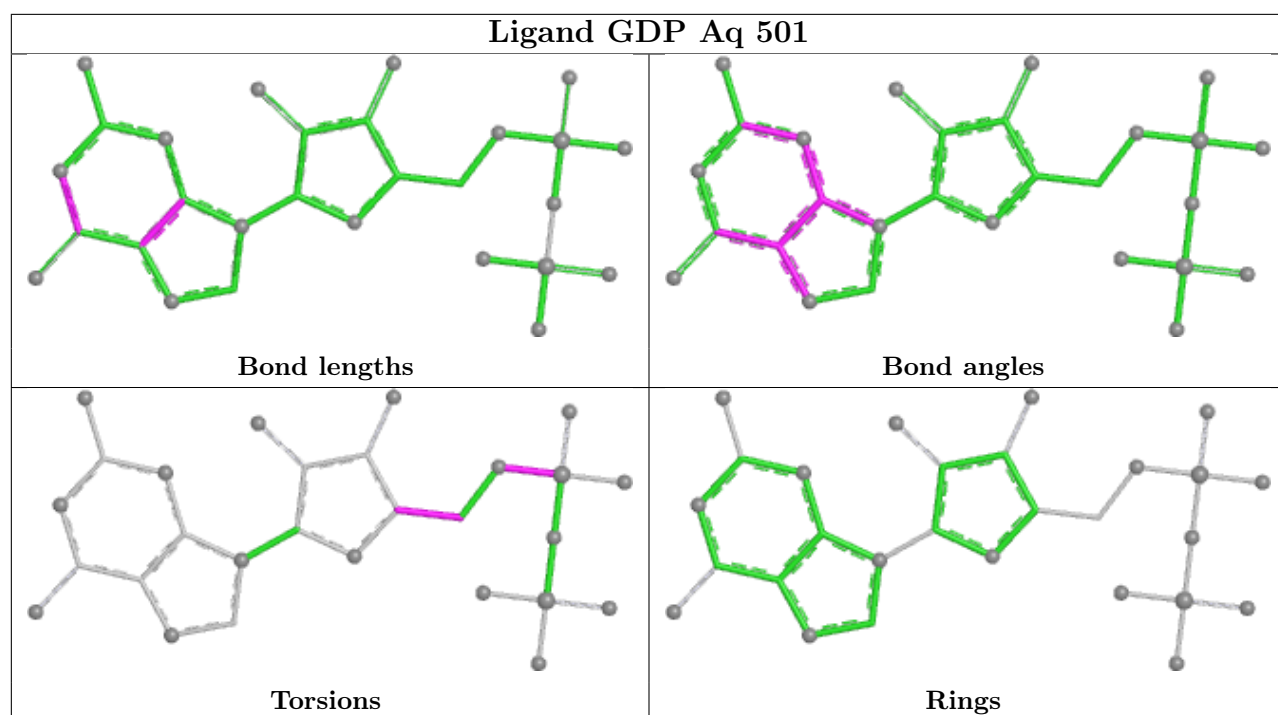
Ligand GTP B3 602

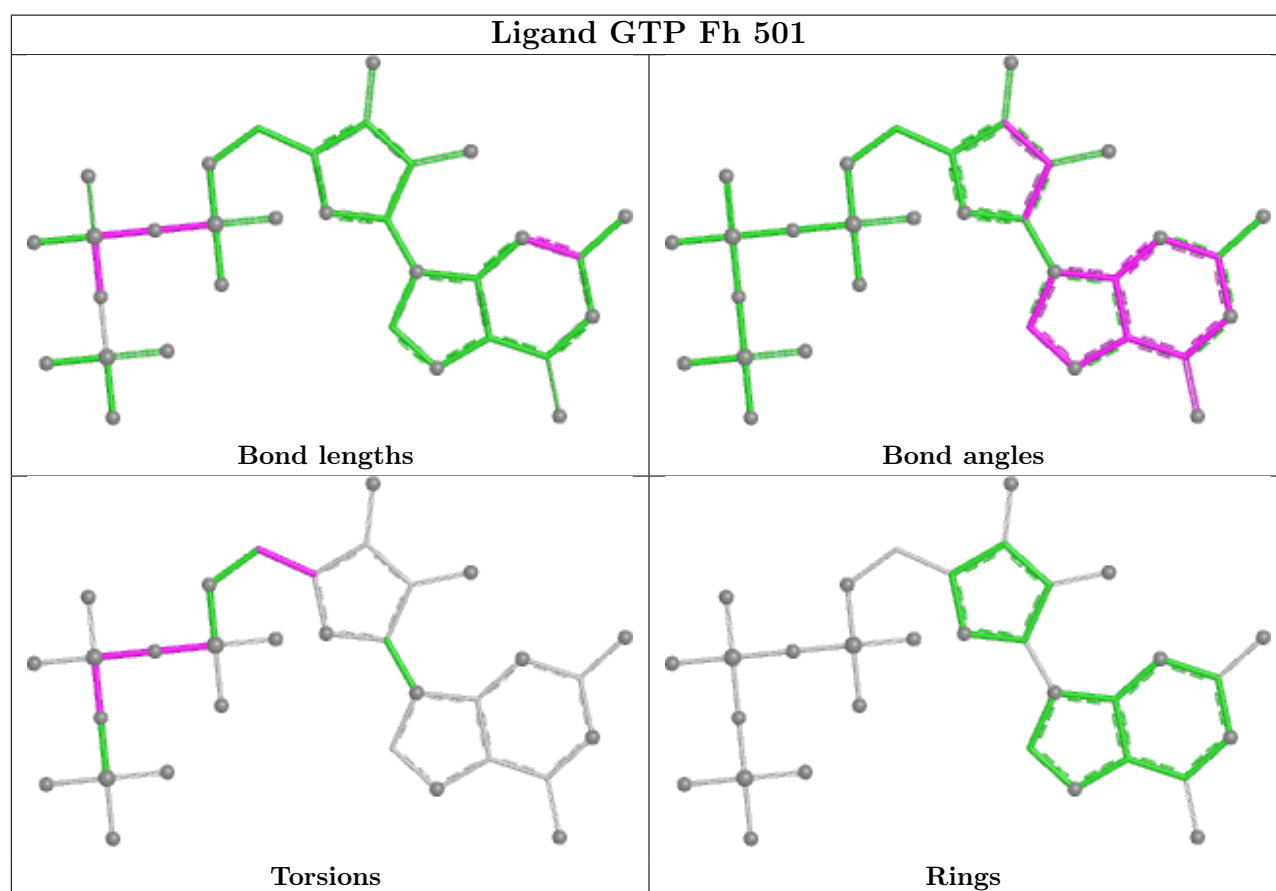
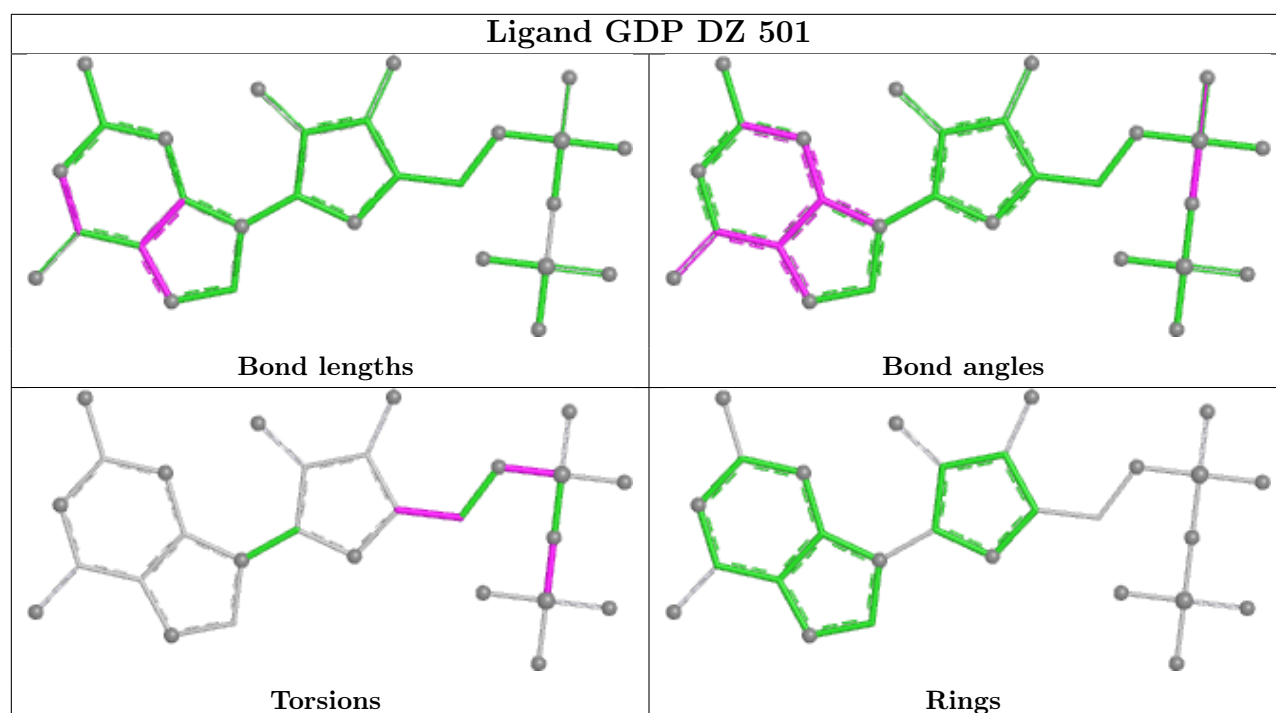


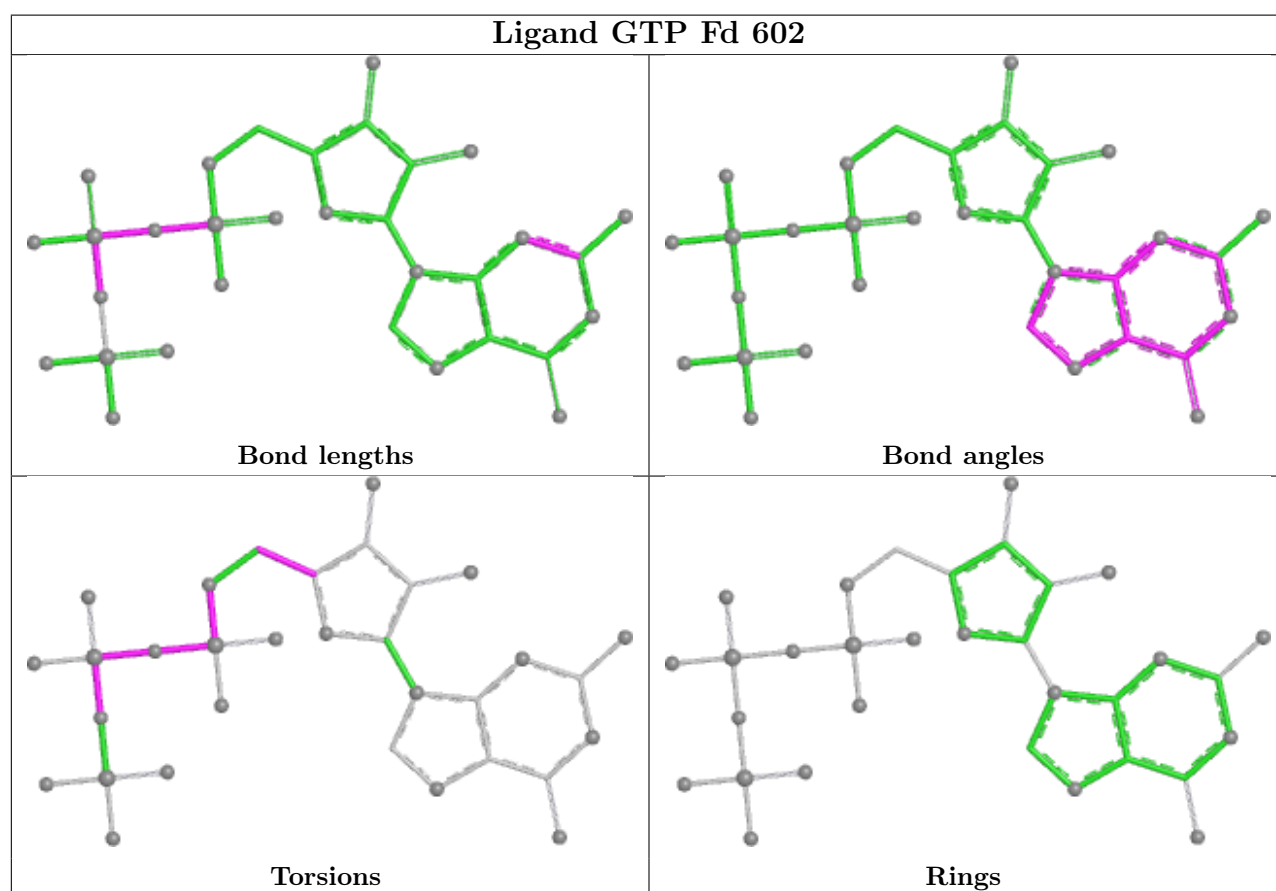
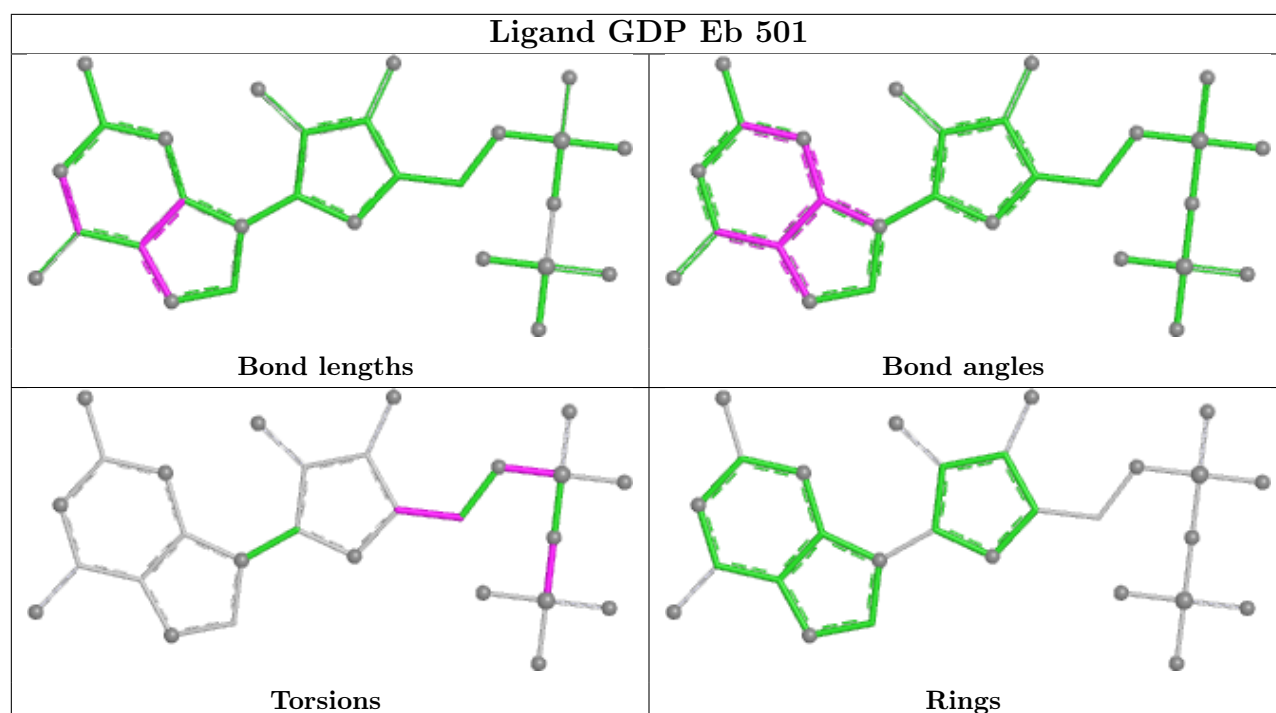
Ligand GTP V 602

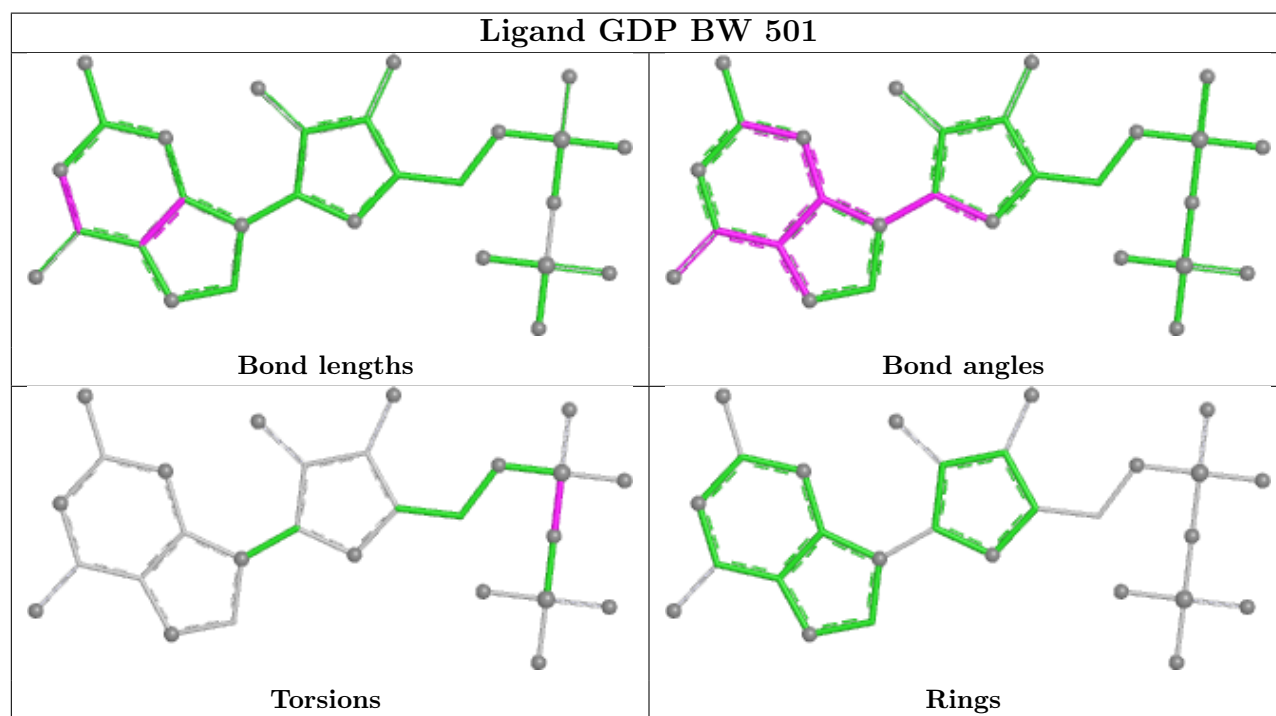
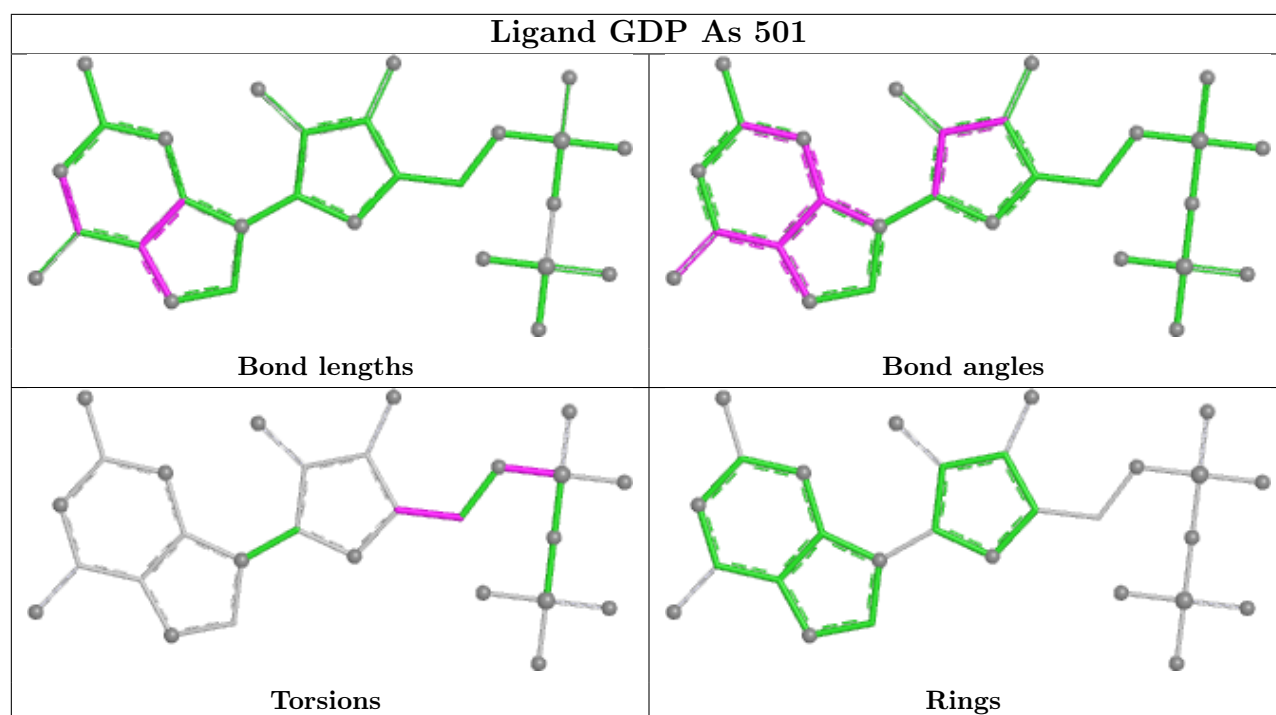


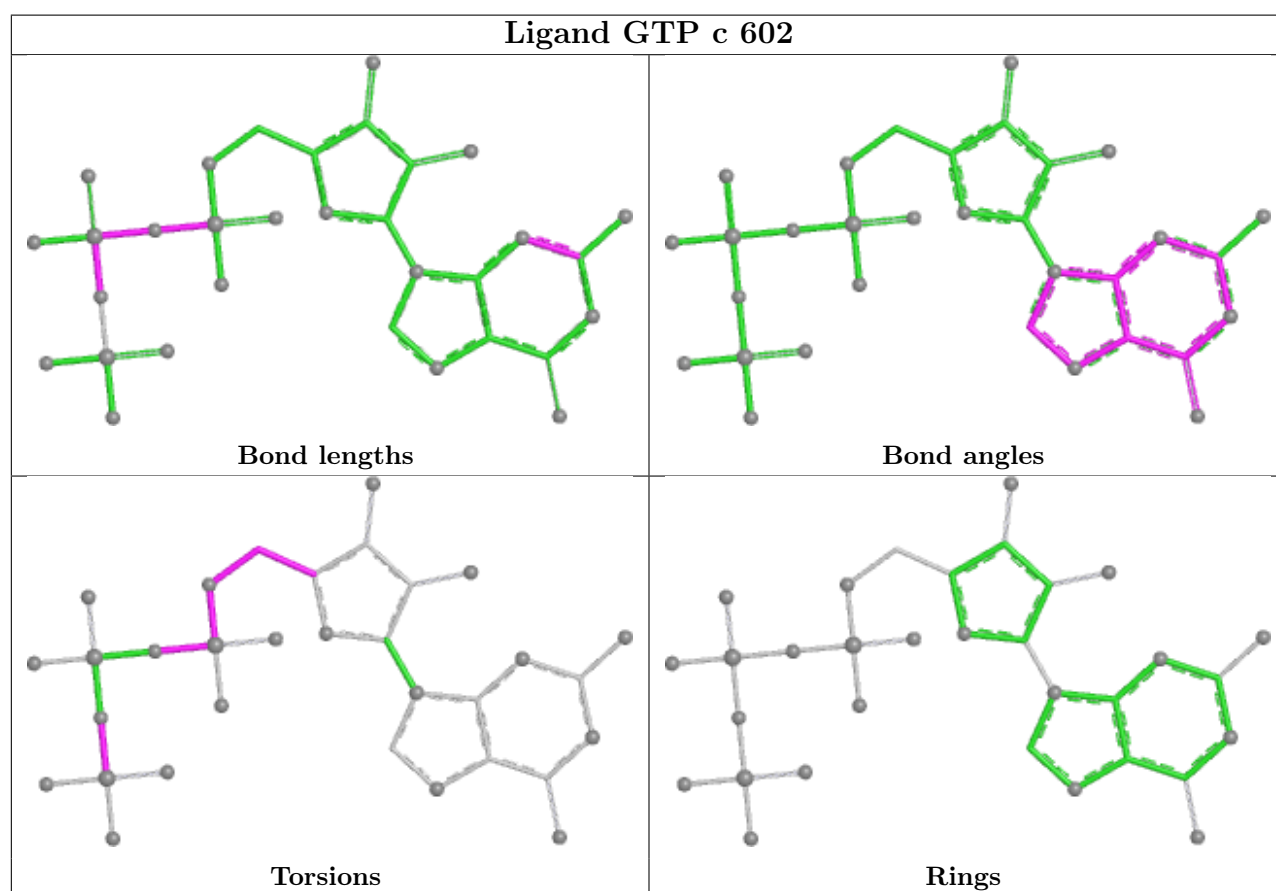
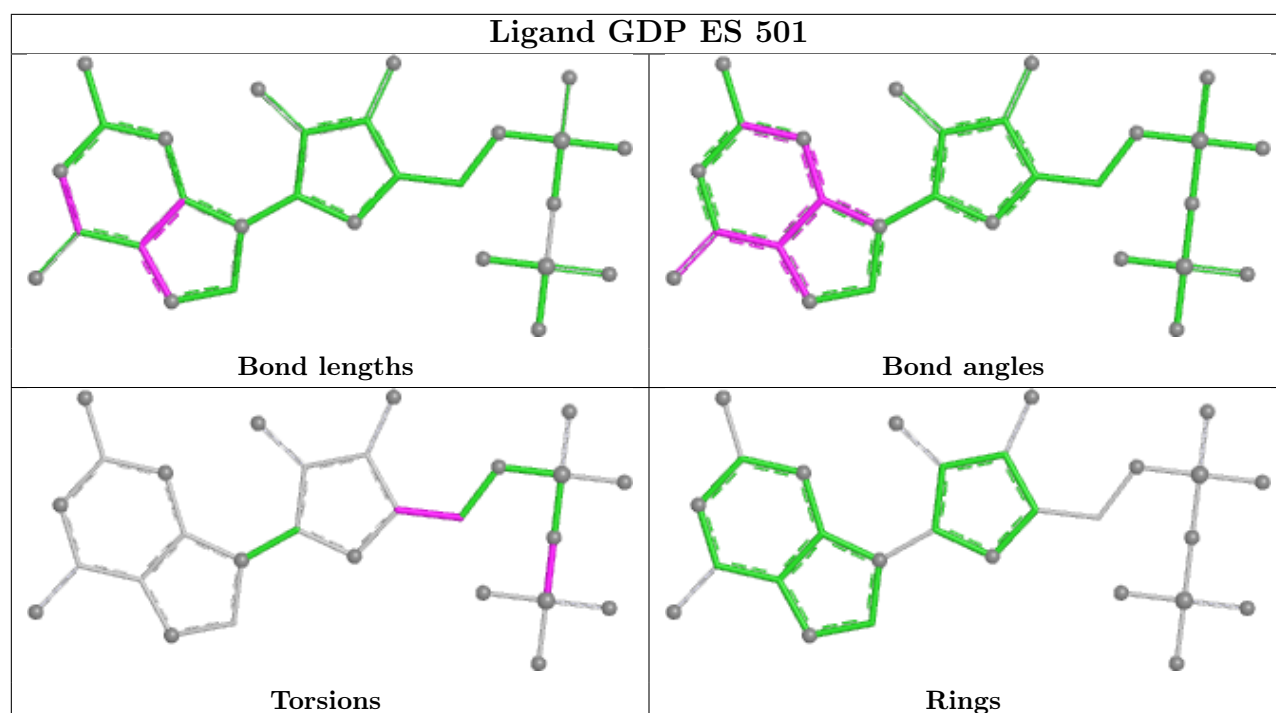


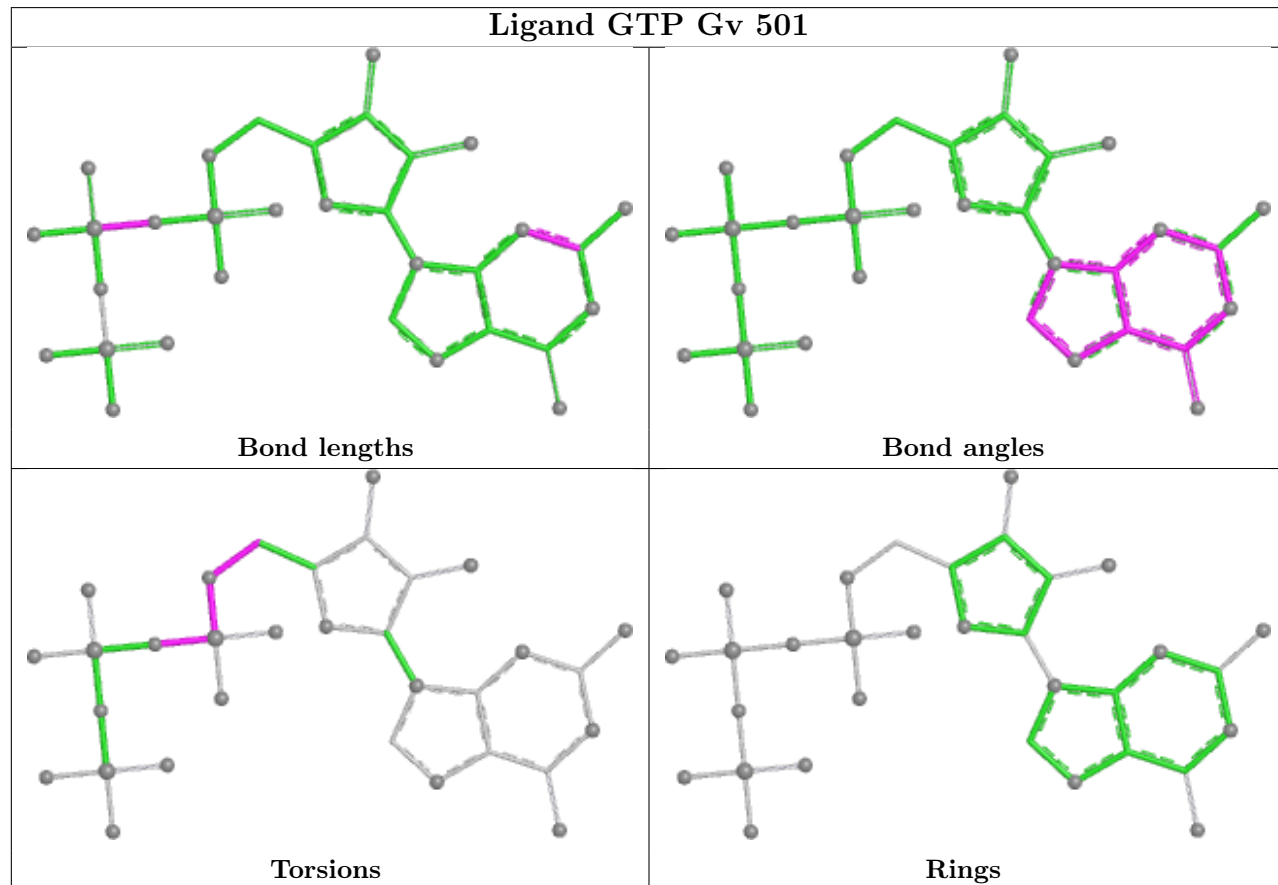
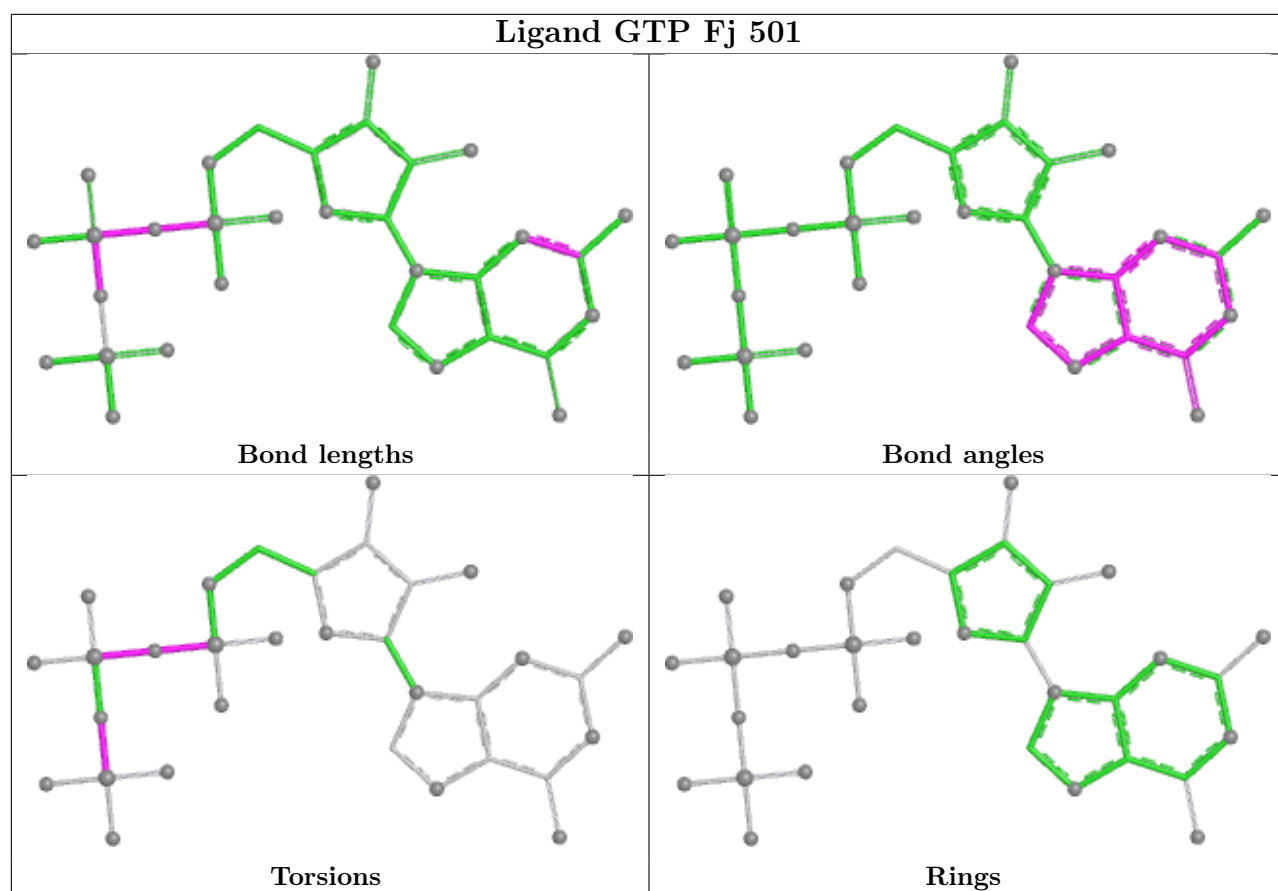


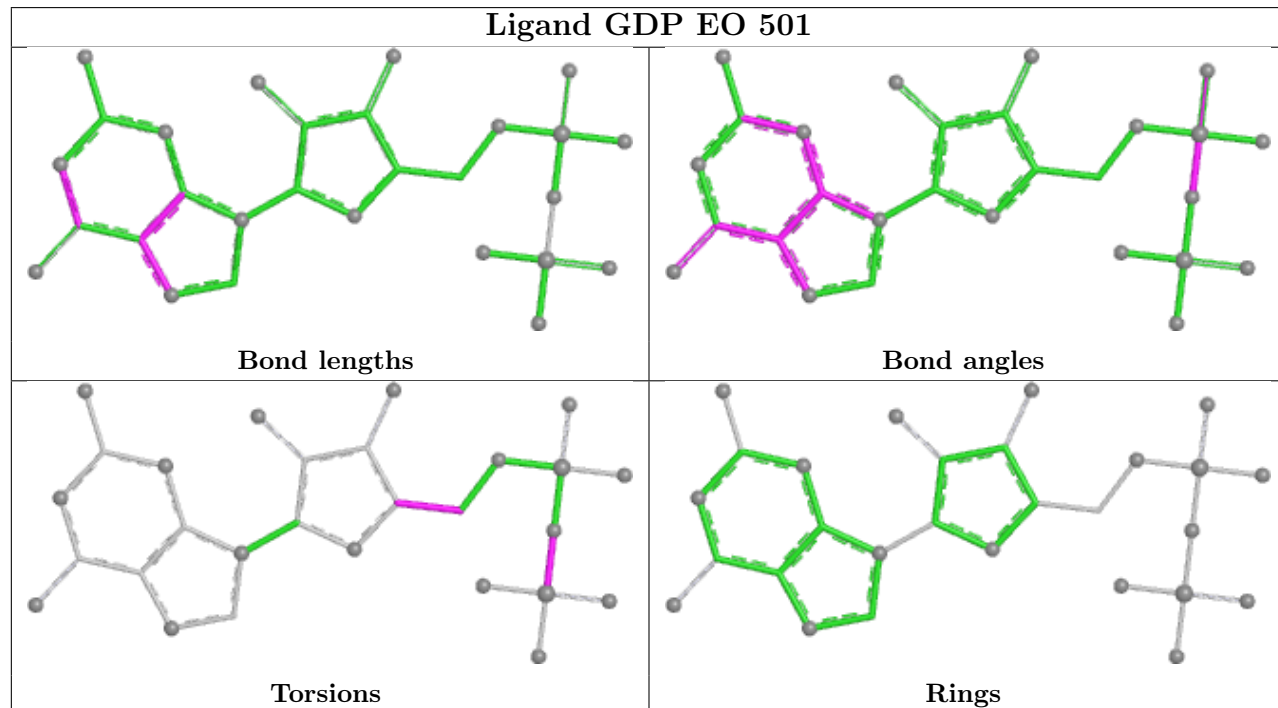
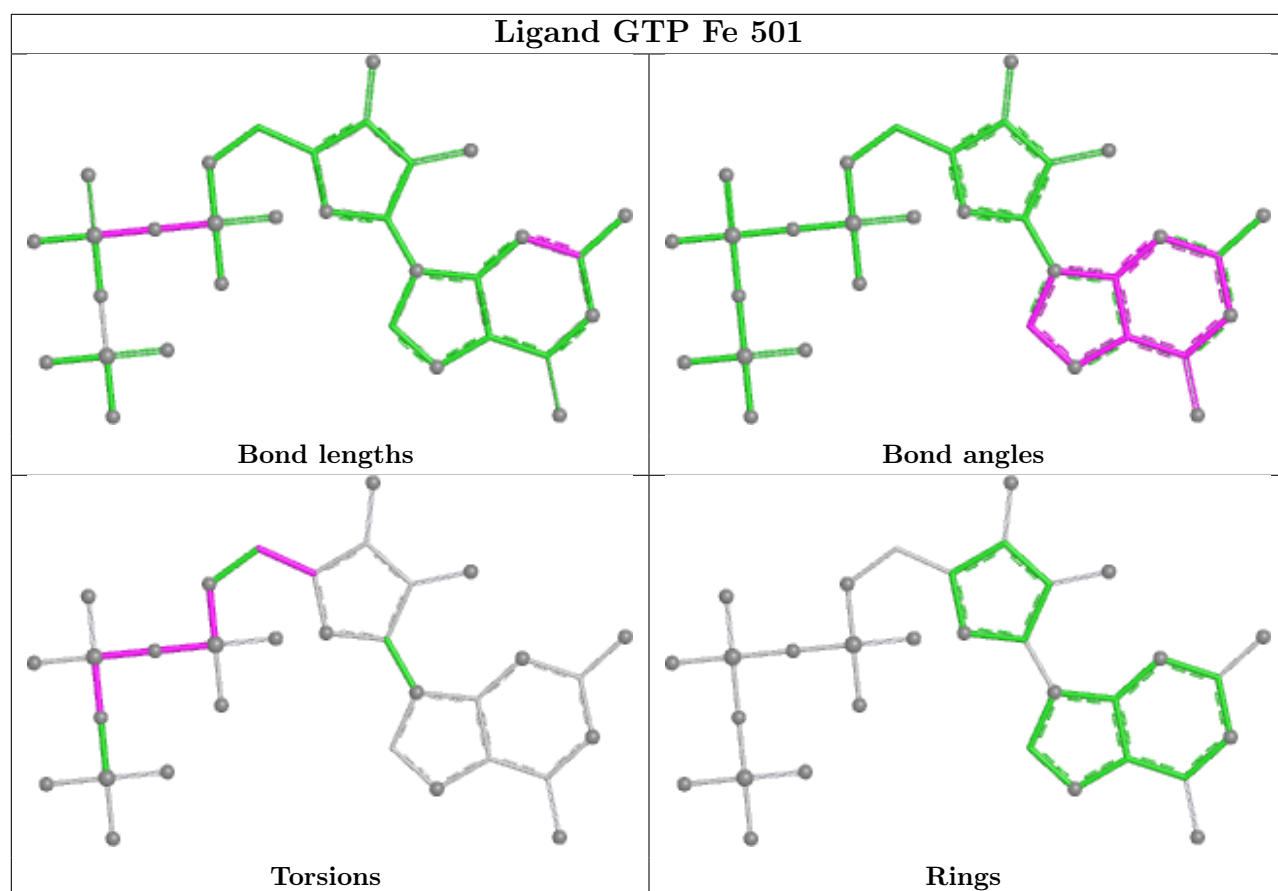


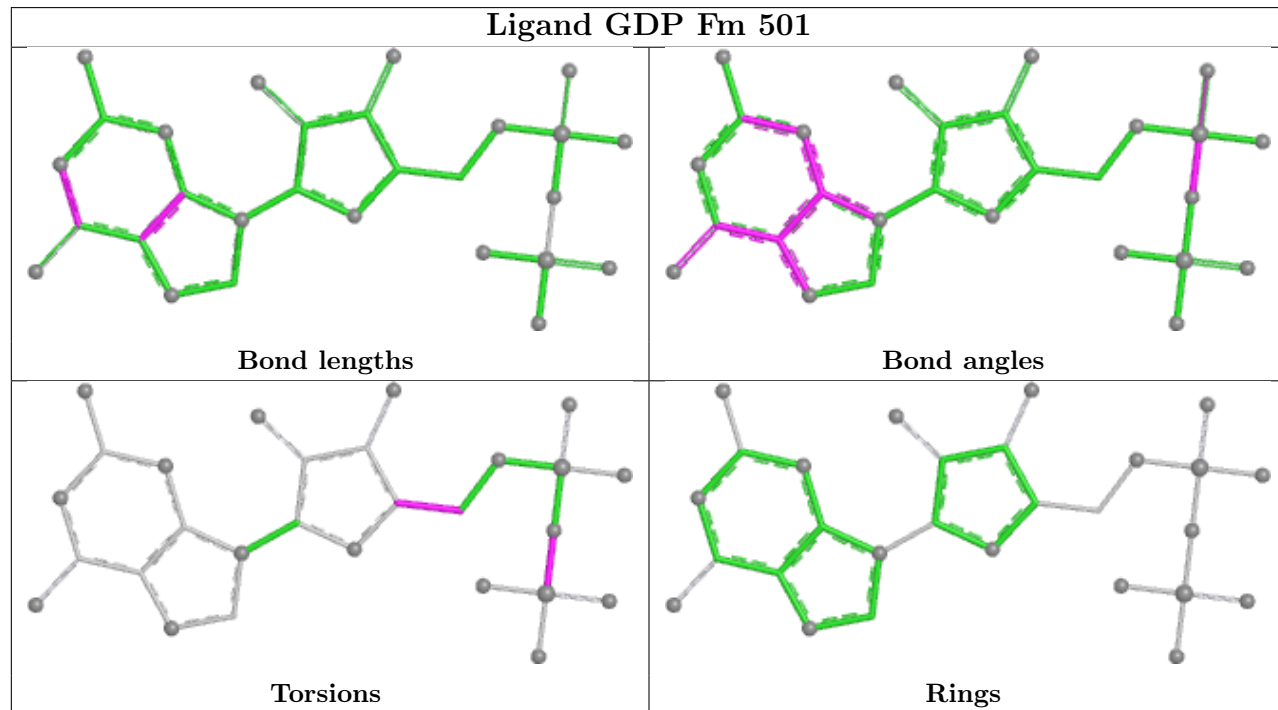
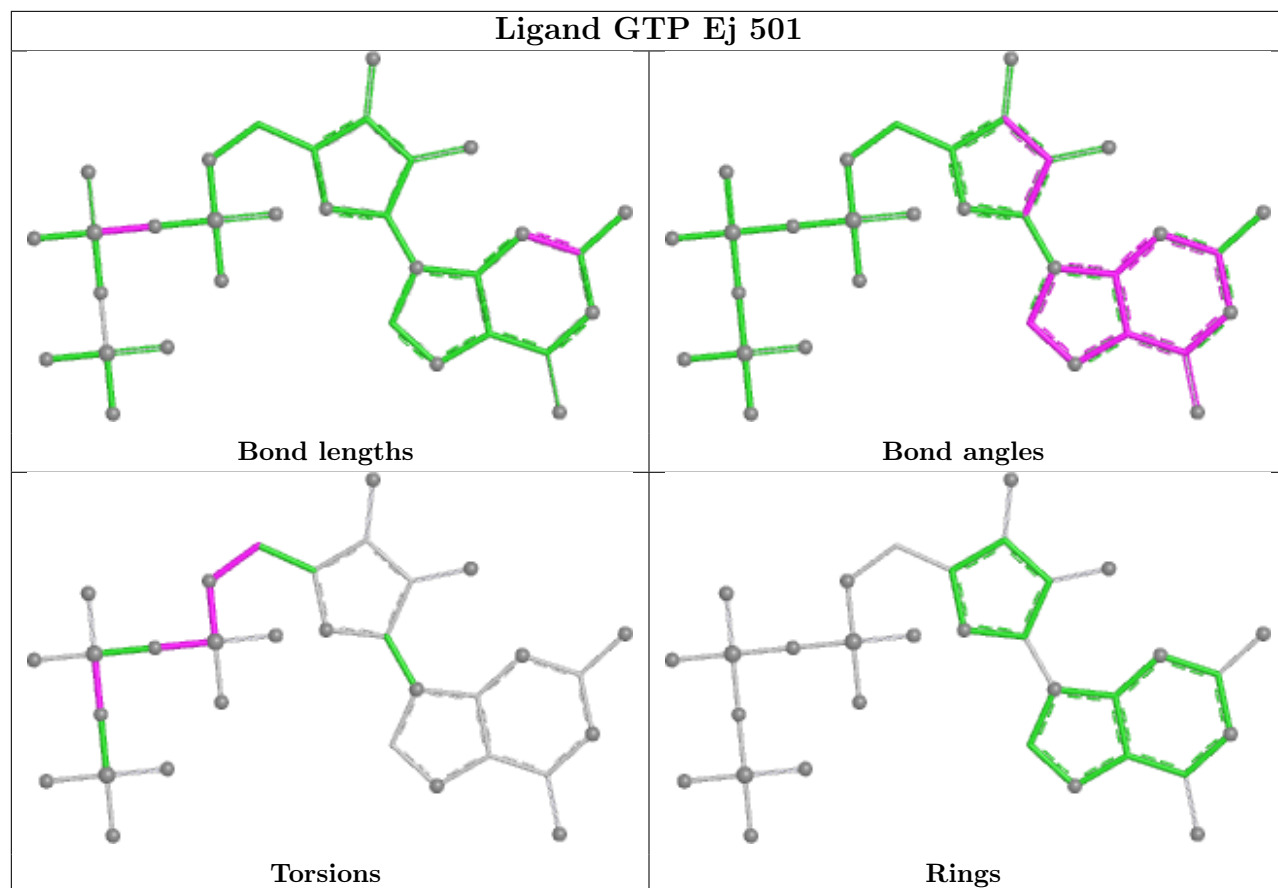




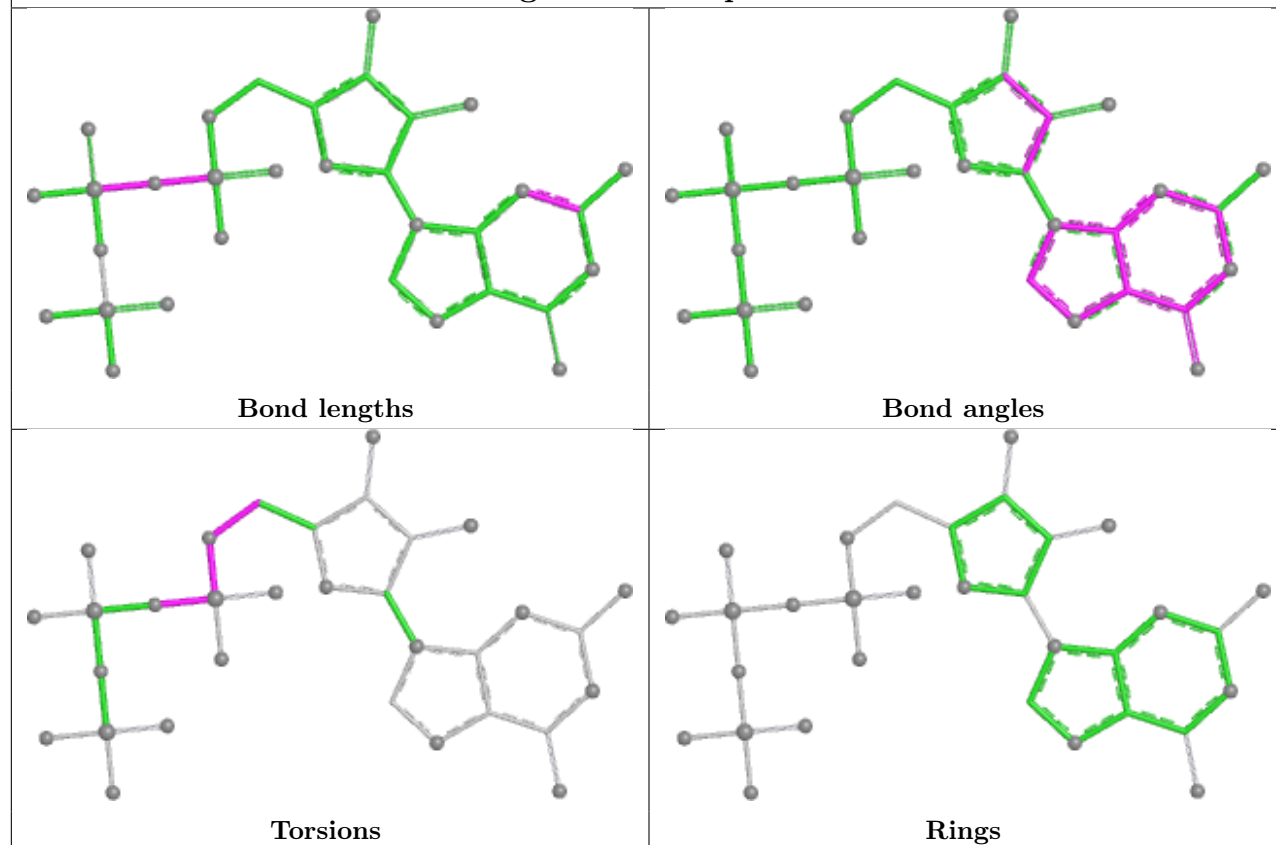




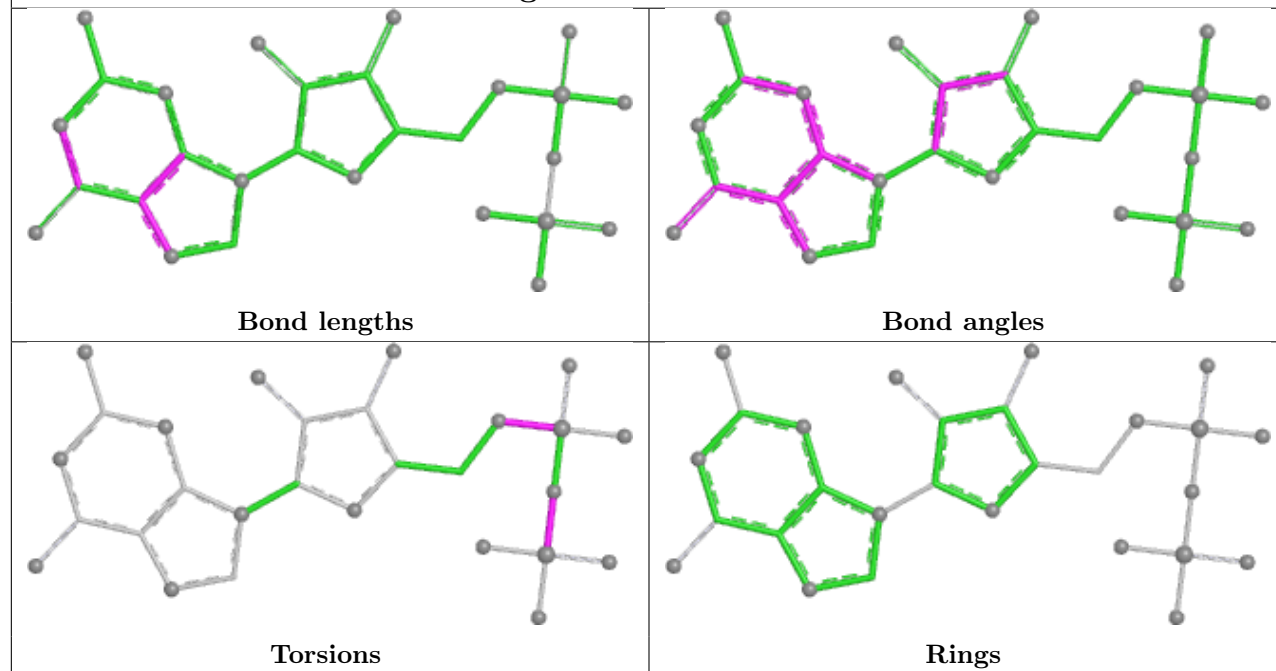


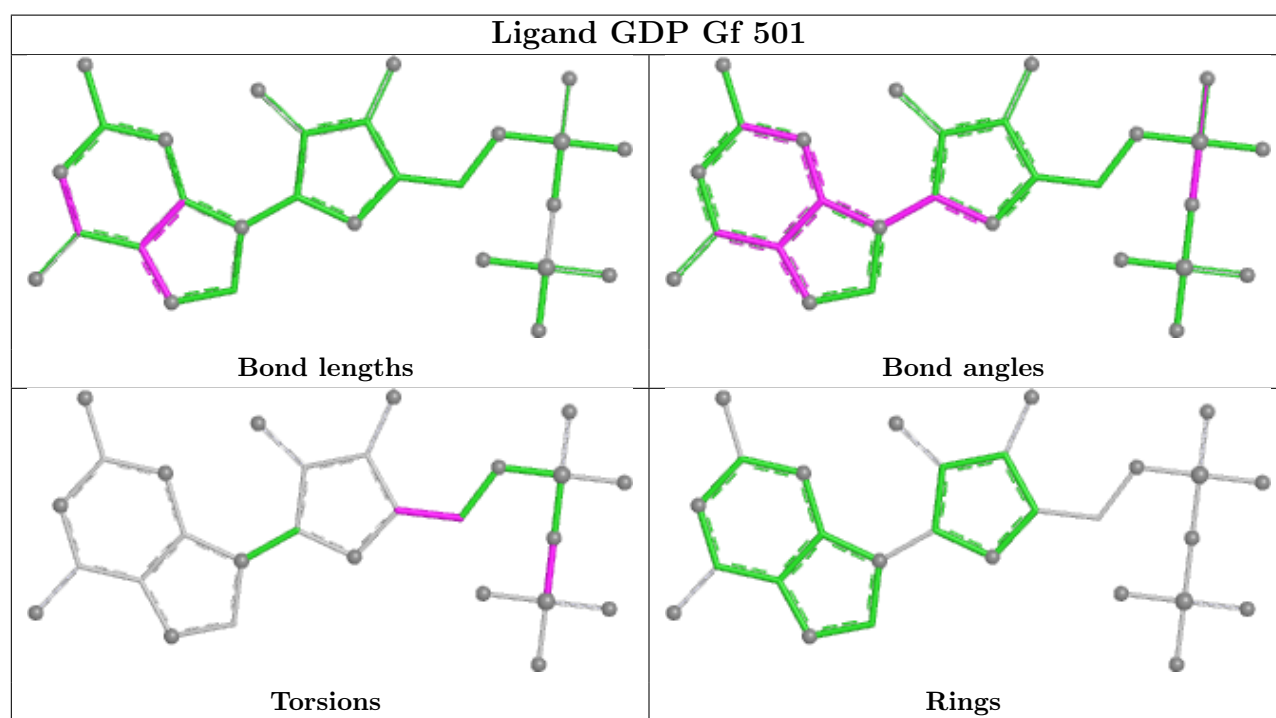
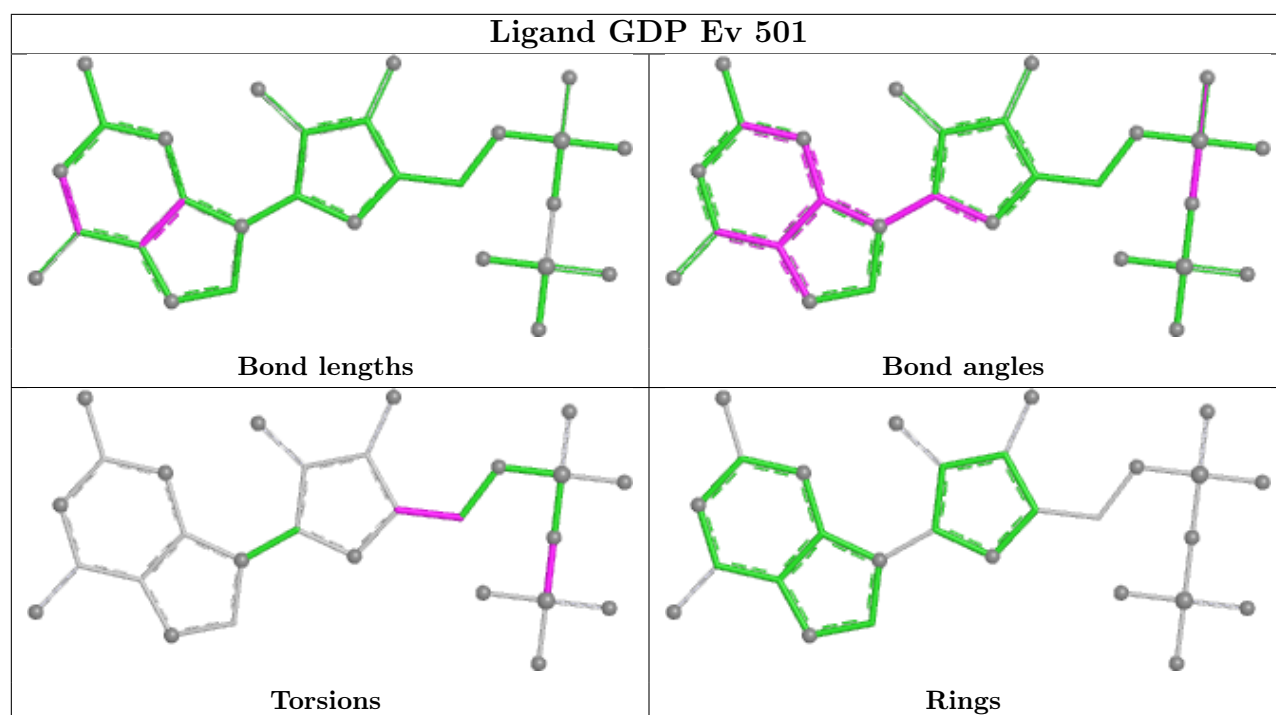


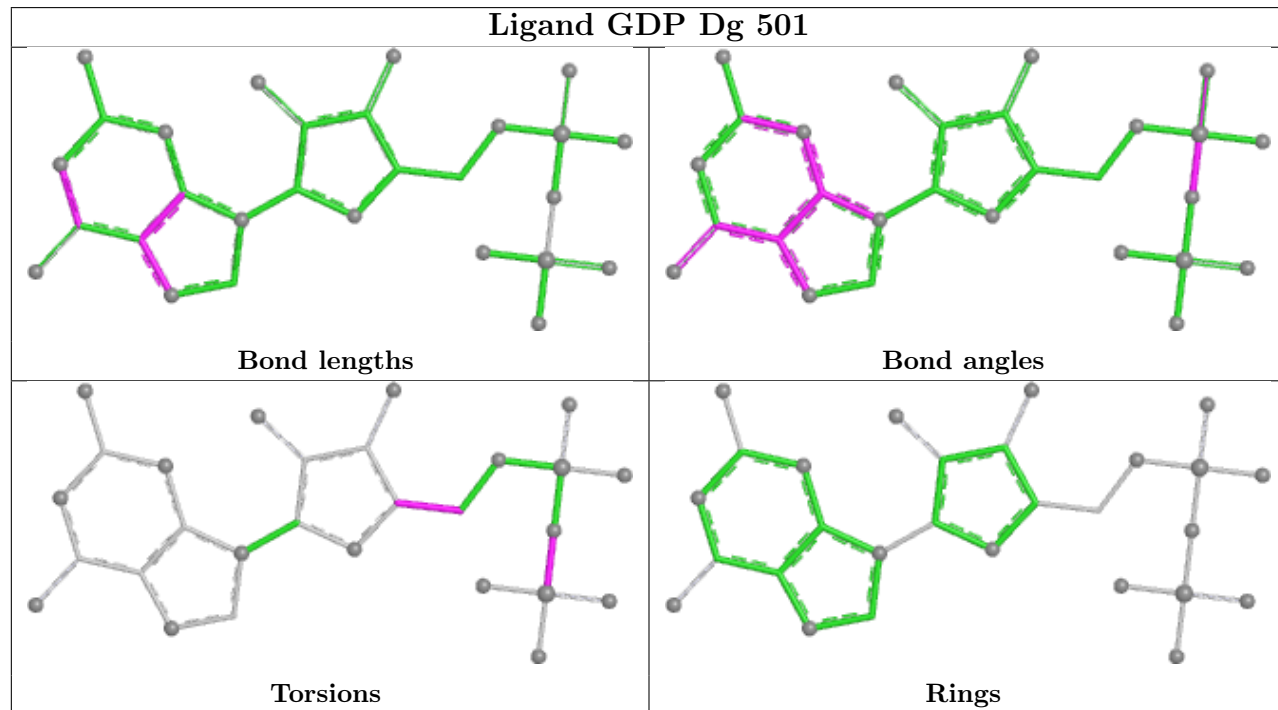
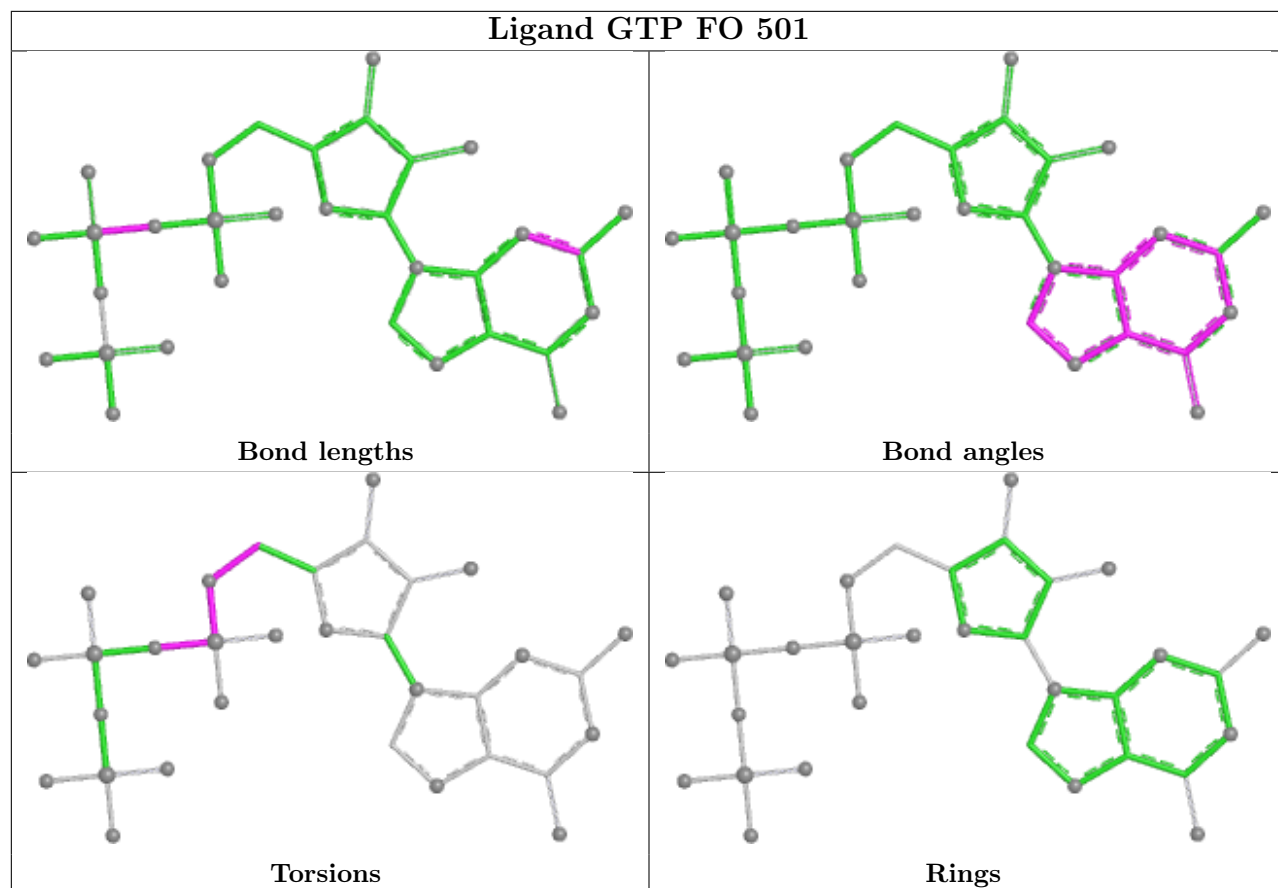
Ligand GTP Gp 501

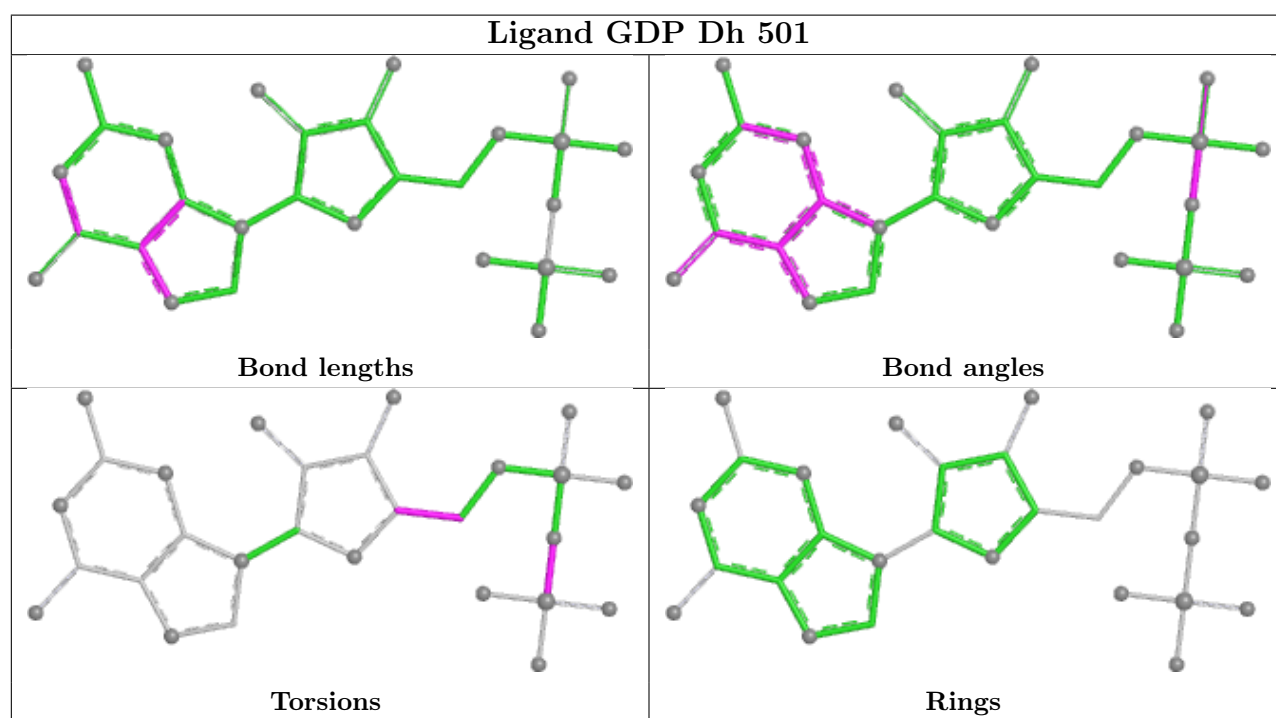
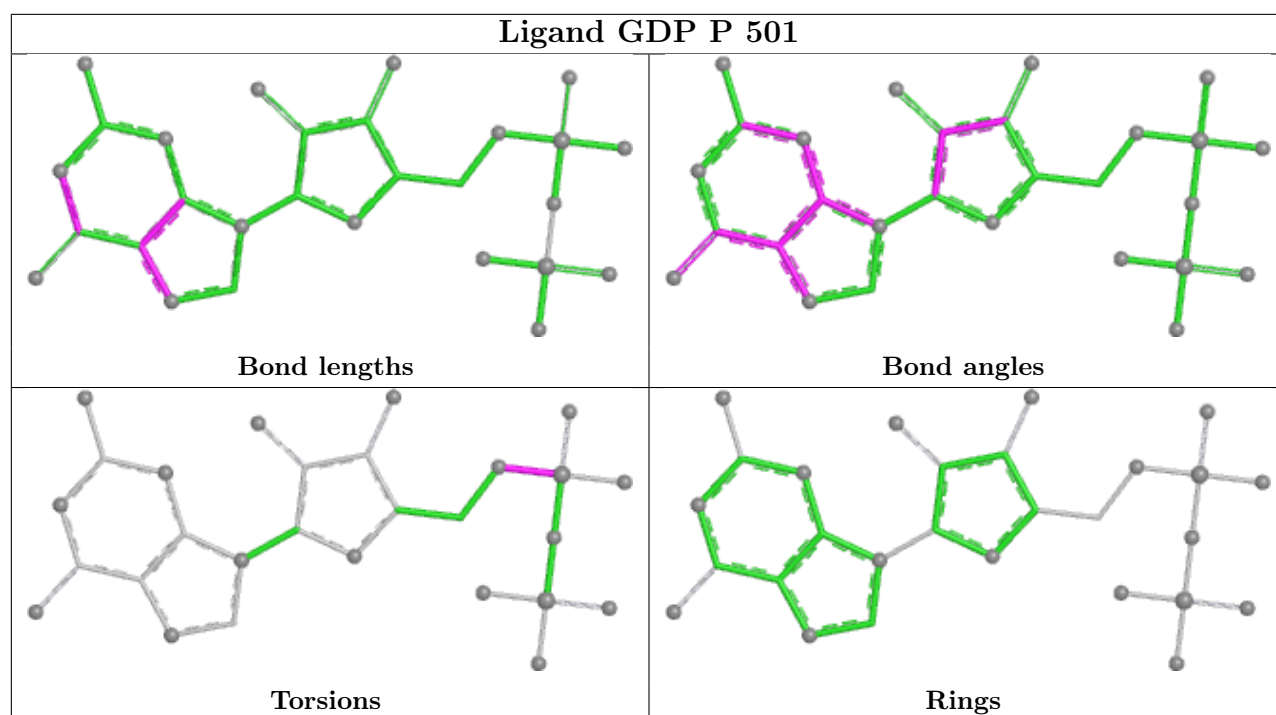


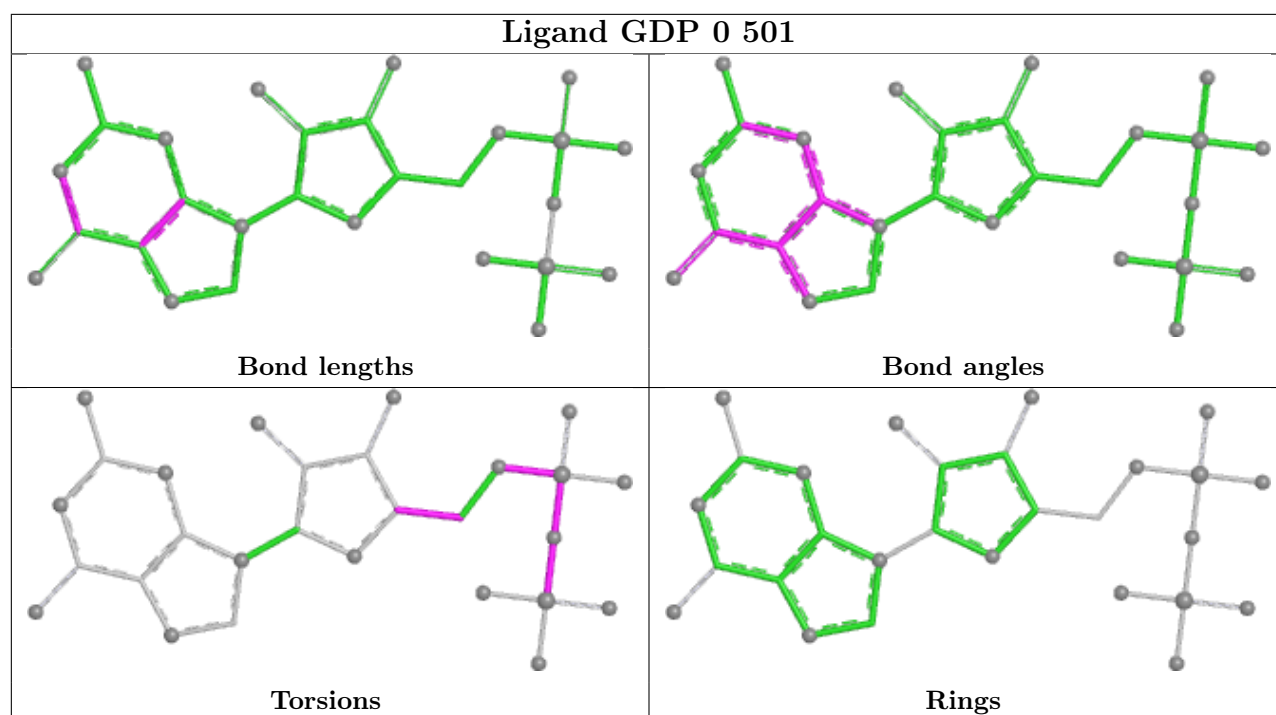
Ligand GDP Bh 501











4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

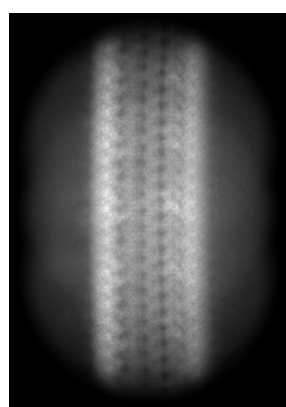
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46580. These allow visual inspection of the internal detail of the map and identification of artifacts.

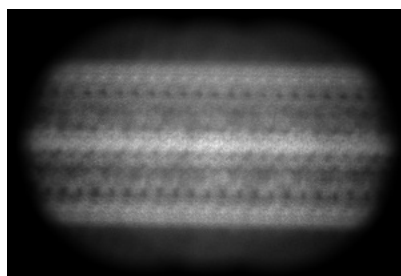
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

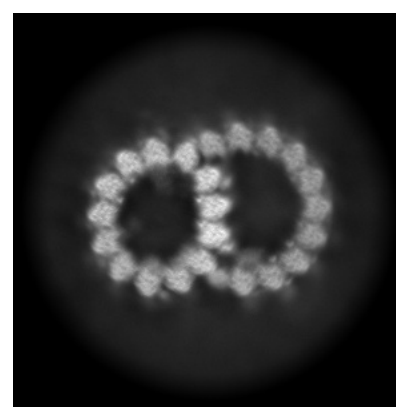
5.1.1 Primary map



X



Y

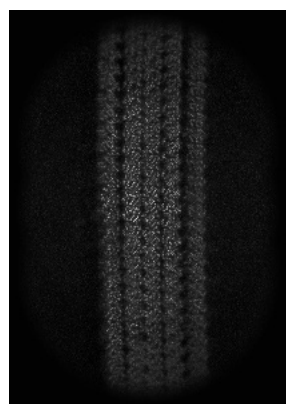


Z

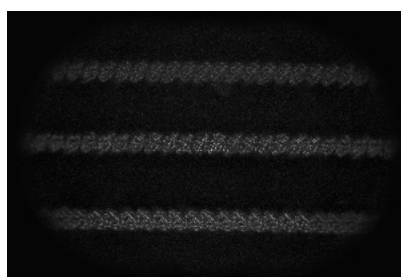
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

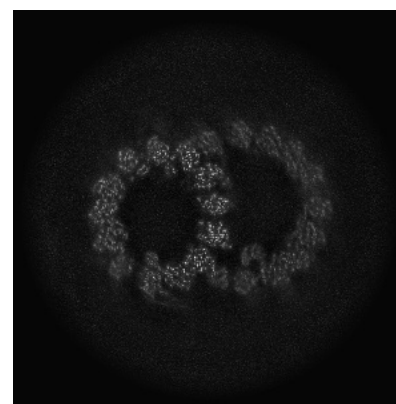
5.2.1 Primary map



X Index: 326



Y Index: 332

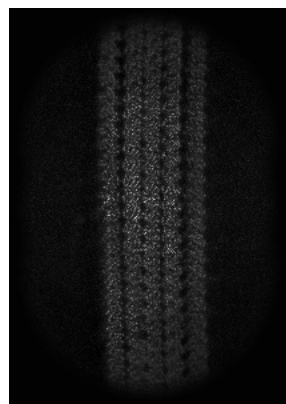


Z Index: 479

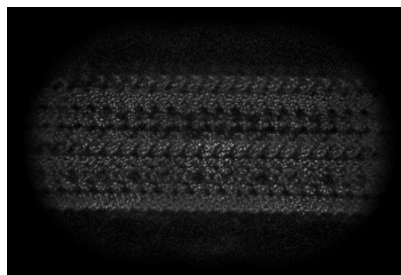
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

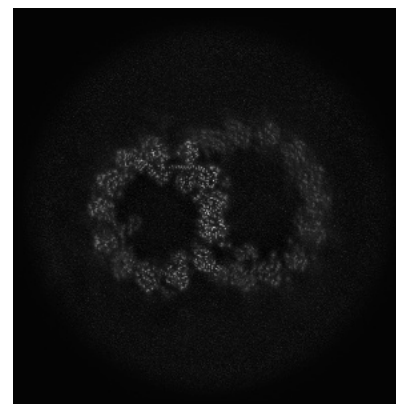
5.3.1 Primary map



X Index: 325



Y Index: 234

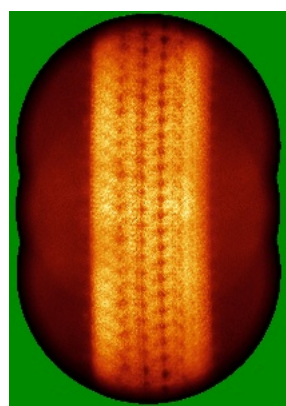


Z Index: 494

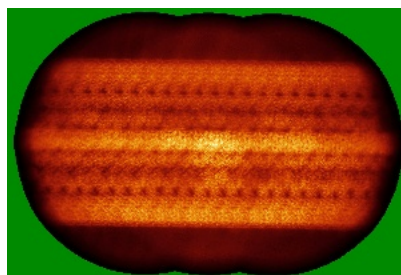
The images above show the largest variance slices of the map in three orthogonal directions.

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

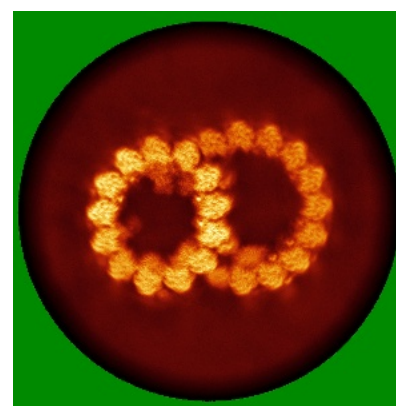
5.4.1 Primary map



X



Y



Z

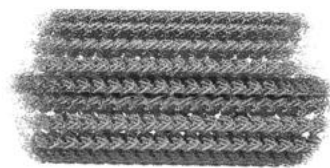
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

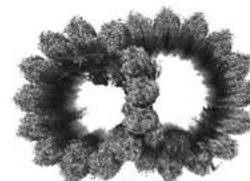
5.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.128. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

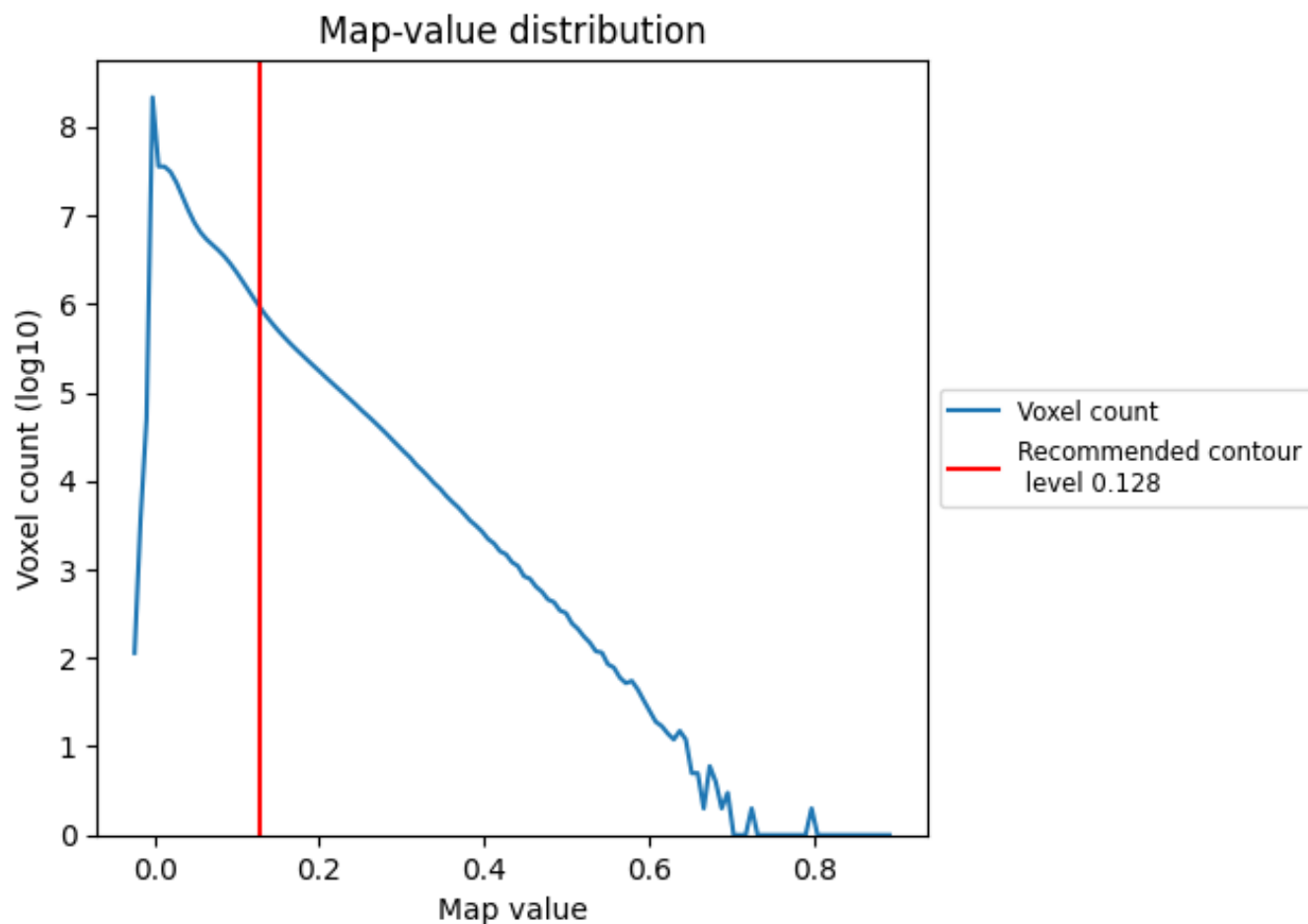
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

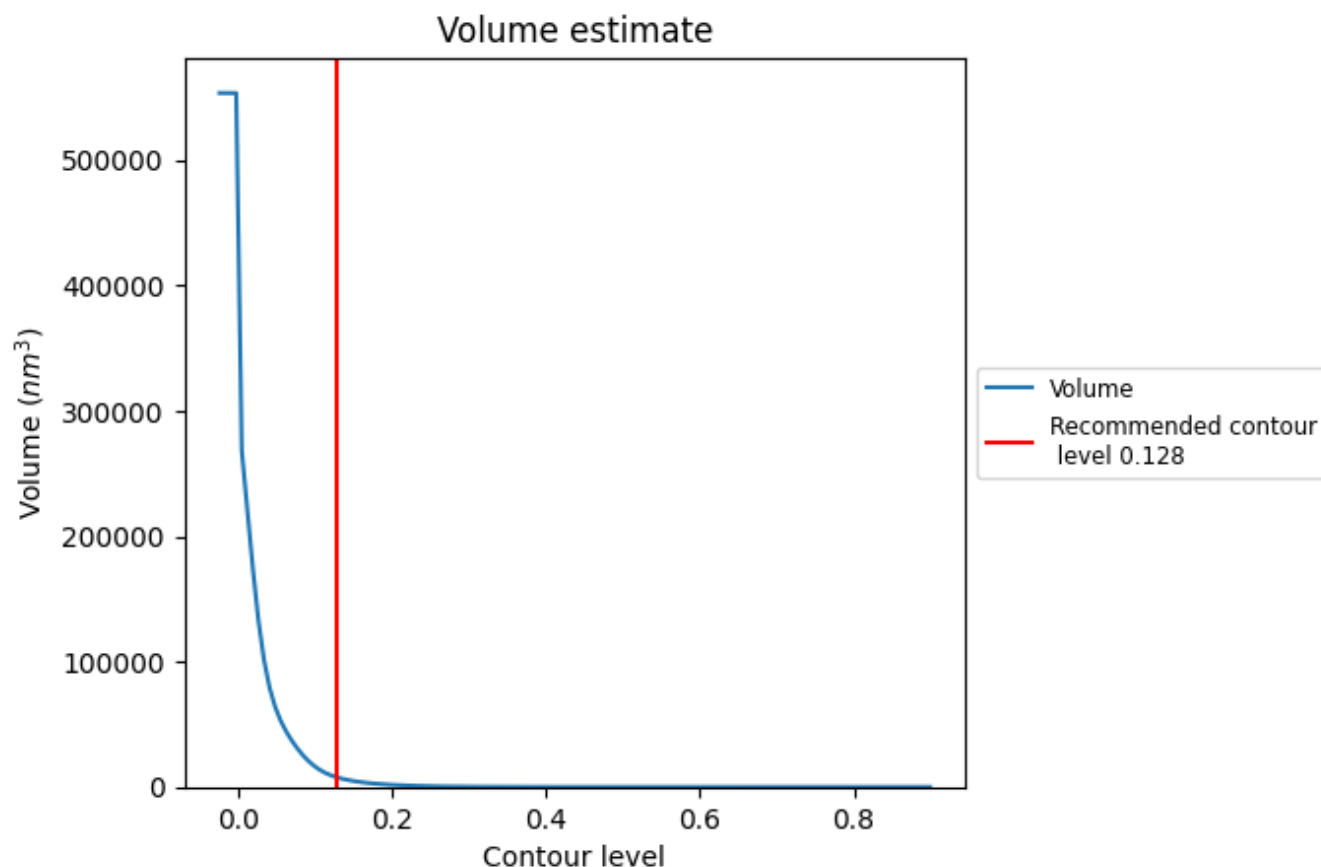
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution [i](#)



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

6.2 Volume estimate [i](#)



The volume at the recommended contour level is 7740 nm³; this corresponds to an approximate mass of 6992 kDa.

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

6.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

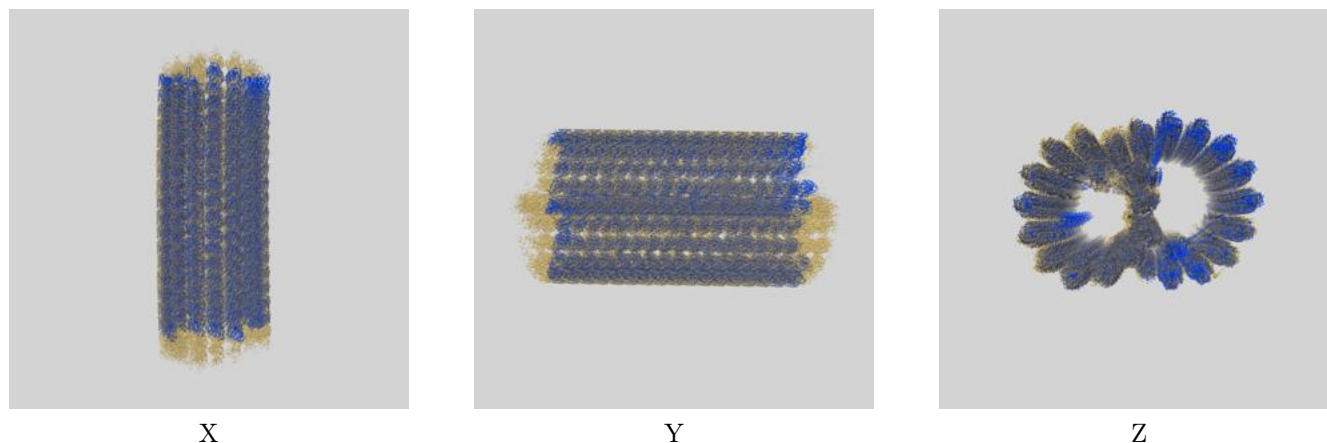
7 Fourier-Shell correlation ⓘ

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

8 Map-model fit [i](#)

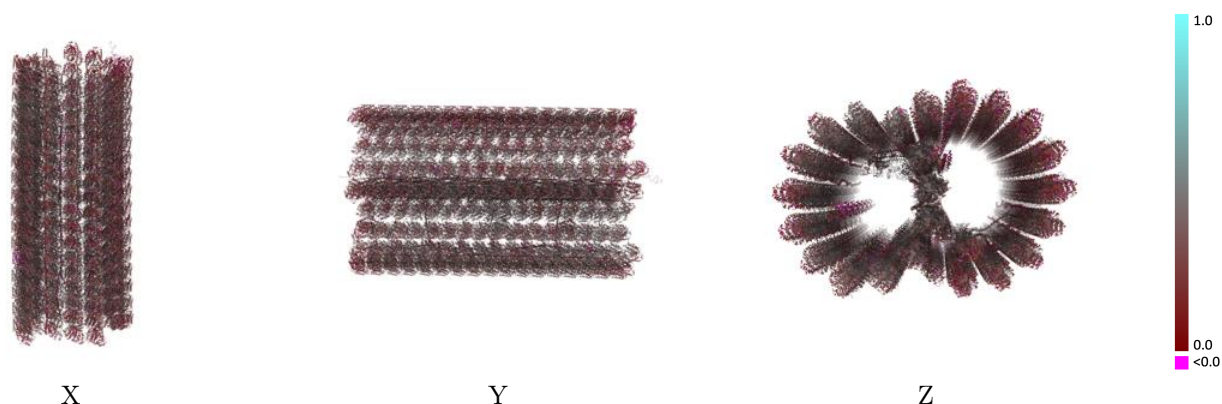
This section contains information regarding the fit between EMDB map EMD-46580 and PDB model 9D5N. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



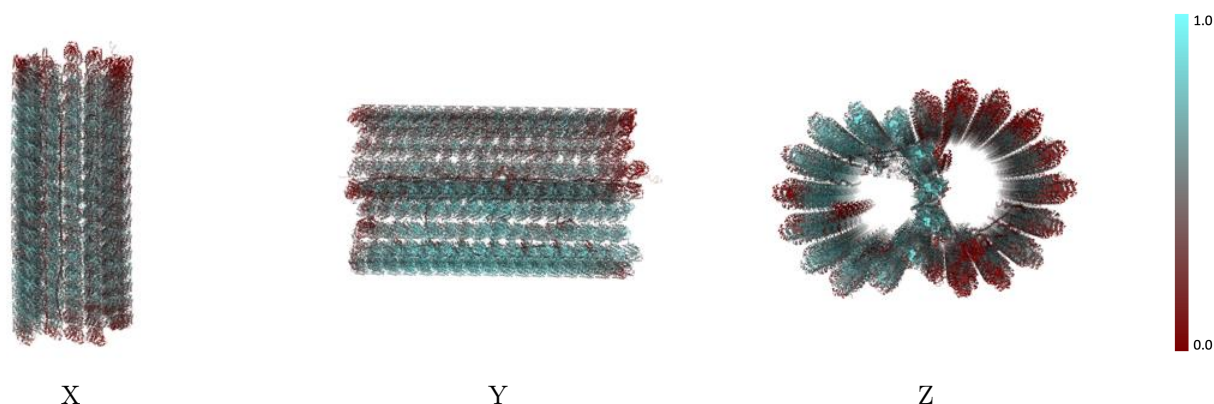
The images above show the 3D surface view of the map at the recommended contour level 0.128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



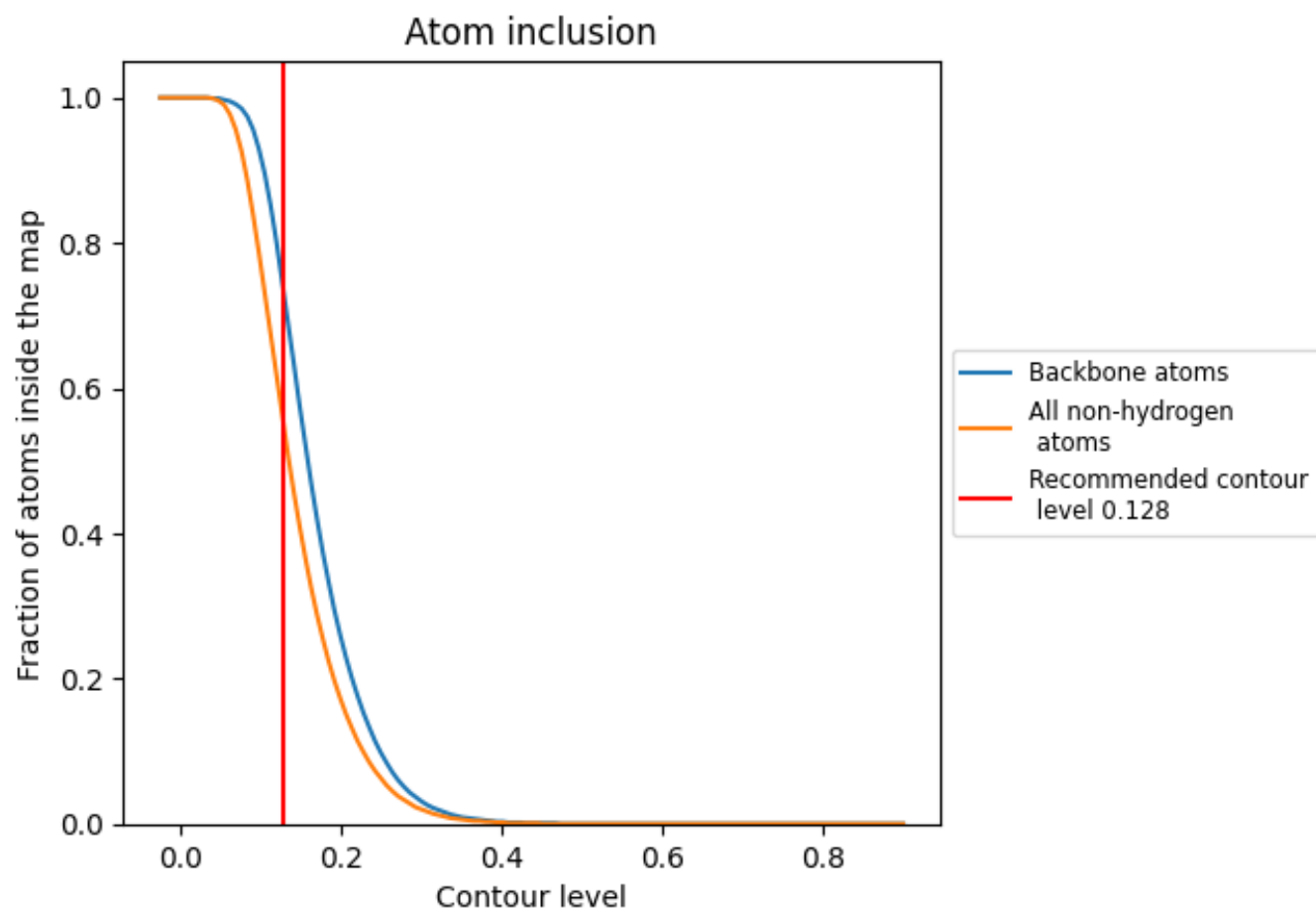
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.128).

8.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5560	 0.3310
0	 0.4340	 0.2860
1	 0.4530	 0.3020
2	 0.4420	 0.2960
3	 0.5040	 0.3310
4	 0.3290	 0.3010
5	 0.4640	 0.3170
6	 0.4580	 0.3190
7	 0.1970	 0.0050
8	 0.3830	 0.2850
9	 0.5300	 0.3180
A	 0.3480	 0.2660
A0	 0.1420	 0.2460
A1	 0.2540	 0.2580
A2	 0.5190	 0.3300
A3	 0.4130	 0.3060
A4	 0.5900	 0.3050
A5	 0.7260	 0.3540
A6	 0.6090	 0.3110
A7	 0.6150	 0.3250
A8	 0.6670	 0.3710
A9	 0.2970	 0.2630
AA	 0.5140	 0.3220
AB	 0.4410	 0.2870
AC	 0.4460	 0.3360
AD	 0.6560	 0.3670
AE	 0.4410	 0.2940
AF	 0.5170	 0.3170
AG	 0.4980	 0.3200
AH	 0.4390	 0.3300
AI	 0.4900	 0.3090
AJ	 0.6270	 0.3750
AK	 0.4550	 0.3190
AL	 0.5110	 0.3230
AM	 0.4310	 0.3150



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Chain	Atom inclusion	Q-score
AN	0.5030	0.3100
AO	0.4860	0.2970
AP	0.6090	0.3460
AQ	0.5020	0.3060
AR	0.6210	0.3510
AS	0.4460	0.3100
AT	0.4670	0.2720
AU	0.5180	0.3160
AV	0.4480	0.2620
AW	0.5410	0.3260
AX	0.5040	0.3060
AY	0.3800	0.2860
AZ	0.4600	0.2880
Aa	0.4590	0.3160
Ab	0.5760	0.3510
Ac	0.4560	0.2900
Ad	0.5830	0.3620
Ae	0.4120	0.3220
Af	0.5040	0.3160
Ag	0.5370	0.3560
Ah	0.4730	0.3150
Ai	0.5600	0.3680
Aj	0.4010	0.3100
Ak	0.2070	0.2820
Al	0.4870	0.3140
Am	0.1100	0.2350
An	0.4130	0.3140
Ao	0.2580	0.2880
Ap	0.2300	0.2840
Aq	0.2390	0.2710
Ar	0.2480	0.2920
As	0.3540	0.2920
At	0.3320	0.2970
Au	0.3200	0.2850
Av	0.1530	0.2710
Aw	0.2120	0.2570
Ax	0.1370	0.2200
Ay	0.3210	0.3050
Az	0.6200	0.3510
B	0.1360	0.1820
B0	0.4720	0.2870
B1	0.5180	0.3380

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Chain	Atom inclusion	Q-score
B2	 0.5950	 0.3480
B3	 0.5520	 0.3450
B4	 0.6030	 0.3630
B5	 0.4740	 0.2920
B6	 0.3640	 0.2700
B7	 0.4960	 0.2580
B8	 0.5130	 0.3280
B9	 0.5350	 0.3410
BA	 0.4420	 0.2990
BB	 0.3430	 0.2810
BC	 0.3480	 0.2710
BD	 0.2800	 0.2860
BE	 0.3700	 0.2690
BF	 0.5300	 0.3320
BG	 0.3430	 0.2710
BH	 0.5810	 0.3440
BI	 0.4820	 0.3230
BJ	 0.3740	 0.3230
BK	 0.1470	 0.2140
BL	 0.4880	 0.3100
BM	 0.4570	 0.2950
BN	 0.6070	 0.3550
BO	 0.5380	 0.3450
BP	 0.6300	 0.3670
BQ	 0.4260	 0.3160
BR	 0.1840	 0.2330
BS	 0.6010	 0.3670
BT	 0.4620	 0.3170
BU	 0.6300	 0.3590
BV	 0.3160	 0.2890
BW	 0.5200	 0.3180
BX	 0.4710	 0.3050
BY	 0.5030	 0.3060
BZ	 0.4680	 0.2950
Ba	 0.5340	 0.3350
Bb	 0.4680	 0.2930
Bc	 0.7630	 0.3870
Bd	 0.8090	 0.4020
Be	 0.4680	 0.3130
Bf	 0.4580	 0.2940
Bg	 0.4330	 0.2680
Bh	 0.4410	 0.2850

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Chain	Atom inclusion	Q-score
Bi	 0.4230	 0.2580
Bj	 0.4470	 0.2850
Bk	 0.5280	 0.3300
Bl	 0.4730	 0.2440
Bm	 0.5370	 0.3400
Bn	 0.4160	 0.2750
Bo	 0.4940	 0.2820
Bp	 0.5440	 0.3250
Bq	 0.4880	 0.2770
Br	 0.5620	 0.3300
Bs	 0.4760	 0.3130
Bt	 0.4020	 0.2660
Bu	 0.4160	 0.2780
Bv	 0.4390	 0.2890
Bw	 0.4800	 0.2940
Bx	 0.3820	 0.2760
By	 0.4550	 0.2690
Bz	 0.4970	 0.2900
C	 0.1080	 0.1580
C1	 0.4590	 0.3760
C2	 0.4110	 0.3200
C3	 0.4910	 0.3420
CA	 0.6330	 0.3660
CB	 0.3750	 0.2920
CC	 0.3330	 0.3060
CD	 0.1450	 0.2080
CE	 0.4930	 0.3340
CF	 0.1610	 0.2140
CG	 0.3700	 0.2540
CH	 0.0420	 0.2570
CI	 0.1940	 0.3090
CJ	 0.2940	 0.2170
CK	 0.2000	 0.1920
CL	 0.1990	 0.2300
CM	 0.7220	 0.4110
CN	 0.6110	 0.4130
CO	 0.3730	 0.2910
CP	 0.0710	 0.2340
CQ	 0.4400	 0.3610
CR	 0.4640	 0.3290
CS	 0.6320	 0.3960
CT	 0.3560	 0.1970

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Chain	Atom inclusion	Q-score
CU	 0.3020	 0.2220
CV	 0.4600	 0.2370
CW	 0.4860	 0.2990
CX	 0.3350	 0.2360
CY	 0.4500	 0.3290
CZ	 0.4350	 0.3260
Ca	 0.3100	 0.2550
Cb	 0.2050	 0.2220
Cc	 0.2550	 0.2490
Cd	 0.5270	 0.3820
Ce	 0.4610	 0.3560
Cf	 0.2210	 0.2360
Cg	 0.1870	 0.2470
Ch	 0.3960	 0.2410
Ci	 0.3920	 0.2960
Cj	 0.3500	 0.2130
Ck	 0.3700	 0.2930
Cl	 0.3250	 0.2280
Cm	 0.6610	 0.3840
Cn	 0.5700	 0.3670
Co	 0.3600	 0.2860
Cp	 0.3860	 0.2830
Cq	 0.3770	 0.3160
Cr	 0.4180	 0.2880
Cs	 0.4190	 0.2750
Ct	 0.4540	 0.3380
Cu	 0.4760	 0.3460
Cv	 0.5150	 0.3580
Cw	 0.6290	 0.4170
Cx	 0.5590	 0.3750
Cy	 0.5720	 0.3700
Cz	 0.6080	 0.3820
D	 0.3930	 0.3240
DL	 0.7150	 0.3520
DM	 0.7840	 0.3610
DN	 0.7860	 0.3460
DO	 0.7320	 0.3620
DP	 0.6680	 0.3560
DQ	 0.5880	 0.3140
DR	 0.7310	 0.3490
DS	 0.7120	 0.3450
DT	 0.7970	 0.3560

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Chain	Atom inclusion	Q-score
DU	 0.5800	 0.3030
DV	 0.6500	 0.3380
DW	 0.7300	 0.3310
DX	 0.7610	 0.3660
DY	 0.4540	 0.3040
DZ	 0.6680	 0.3870
Da	 0.6730	 0.3740
Db	 0.5690	 0.3410
Dc	 0.4600	 0.2540
Dd	 0.2700	 0.2370
De	 0.3860	 0.2420
Df	 0.8110	 0.3510
Dg	 0.8050	 0.3610
Dh	 0.6530	 0.3180
Di	 0.7850	 0.3730
Dj	 0.7820	 0.3360
Dk	 0.8000	 0.3520
Dq	 0.4020	 0.2720
Dr	 0.6730	 0.3420
Ds	 0.7400	 0.3610
Dt	 0.6110	 0.3090
Du	 0.6810	 0.3680
Dv	 0.6380	 0.3750
Dw	 0.7440	 0.3600
Dx	 0.8380	 0.4150
E	 0.5650	 0.3690
E0	 0.5670	 0.2770
E1	 0.7290	 0.3860
E2	 0.7730	 0.3910
E3	 0.7560	 0.3890
E4	 0.6710	 0.3510
E5	 0.7210	 0.3740
E6	 0.8060	 0.4140
E7	 0.7940	 0.4150
E8	 0.7480	 0.3770
E9	 0.7630	 0.3800
EL	 0.7070	 0.3550
EM	 0.7850	 0.3720
EN	 0.5010	 0.3160
EO	 0.7150	 0.3530
EP	 0.7980	 0.3620
EQ	 0.5730	 0.3330

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Chain	Atom inclusion	Q-score
ER	 0.6100	 0.3260
ES	 0.6050	 0.3770
ET	 0.6740	 0.3760
EU	 0.6070	 0.3850
EV	 0.6810	 0.3820
EW	 0.7730	 0.3910
EX	 0.6500	 0.3920
EY	 0.7010	 0.3820
EZ	 0.6510	 0.3850
Ea	 0.4740	 0.3260
Eb	 0.7560	 0.3860
Ec	 0.2940	 0.2820
Ed	 0.7160	 0.3780
Ee	 0.7210	 0.3500
Ef	 0.6300	 0.3560
Eg	 0.7780	 0.3560
Eh	 0.6830	 0.3230
Ei	 0.7650	 0.3650
Ej	 0.7840	 0.3400
Ek	 0.7590	 0.3830
El	 0.7850	 0.3460
Em	 0.6350	 0.3520
En	 0.7880	 0.3610
Eo	 0.7290	 0.3500
Ep	 0.6220	 0.3380
Eq	 0.5190	 0.2560
Er	 0.6340	 0.3800
Es	 0.5470	 0.3020
Et	 0.6440	 0.3880
Eu	 0.6350	 0.3630
Ev	 0.6250	 0.3100
Ew	 0.6690	 0.3870
Ex	 0.7360	 0.3920
Ey	 0.6550	 0.3640
Ez	 0.4350	 0.3210
F	 0.5010	 0.3440
F0	 0.6500	 0.3940
F1	 0.7670	 0.3890
F2	 0.7630	 0.3980
F3	 0.6420	 0.3780
F4	 0.7280	 0.3850
F5	 0.6360	 0.3650

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Chain	Atom inclusion	Q-score
F6	 0.5710	 0.3340
F7	 0.3790	 0.2800
F8	 0.5710	 0.3320
F9	 0.6200	 0.3510
FA	 0.6900	 0.3500
FB	 0.7410	 0.3820
FC	 0.6630	 0.3590
FD	 0.7800	 0.4130
FE	 0.6100	 0.3560
FF	 0.8140	 0.4100
FG	 0.6760	 0.3650
FH	 0.8870	 0.4470
FI	 0.8740	 0.4430
FJ	 0.8230	 0.4120
FK	 0.8630	 0.4470
FL	 0.8140	 0.4120
FM	 0.5770	 0.3090
FN	 0.7920	 0.3940
FO	 0.7650	 0.3680
FP	 0.6970	 0.3780
FQ	 0.7670	 0.3590
FR	 0.7310	 0.3710
FS	 0.7770	 0.3860
FT	 0.6850	 0.3480
FU	 0.6760	 0.3580
FV	 0.7070	 0.3770
FW	 0.7500	 0.3950
FX	 0.5480	 0.2830
FY	 0.7040	 0.3690
FZ	 0.6180	 0.3390
Fa	 0.7000	 0.3850
Fb	 0.7210	 0.3790
Fc	 0.6940	 0.3860
Fd	 0.7940	 0.4090
Fe	 0.8570	 0.4350
Ff	 0.8360	 0.4250
Fg	 0.8370	 0.4300
Fh	 0.4690	 0.3460
Fi	 0.5830	 0.3710
Fj	 0.6160	 0.3750
Fk	 0.6120	 0.3570
Fl	 0.6730	 0.3700

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Chain	Atom inclusion	Q-score
Fm	 0.1910	 0.2280
Fn	 0.6900	 0.3870
Fo	 0.3900	 0.2770
Fp	 0.6910	 0.3830
Fq	 0.5520	 0.3170
Fr	 0.6990	 0.3960
Fs	 0.6310	 0.3750
Ft	 0.7100	 0.4090
Fu	 0.6520	 0.3960
Fv	 0.7240	 0.3740
Fw	 0.5850	 0.3650
Fx	 0.8260	 0.4220
Fy	 0.7850	 0.4100
Fz	 0.7480	 0.3930
G	 0.3330	 0.2490
G0	 0.6690	 0.3530
G1	 0.5840	 0.3410
G2	 0.7780	 0.4000
G3	 0.7040	 0.3790
G4	 0.8620	 0.4310
G5	 0.8400	 0.4330
G6	 0.8020	 0.4210
G7	 0.5440	 0.2570
G8	 0.7370	 0.3540
G9	 0.6680	 0.3670
GA	 0.4370	 0.2950
GB	 0.6750	 0.4040
GC	 0.4770	 0.3360
GD	 0.6980	 0.3850
GE	 0.8110	 0.4140
GF	 0.7910	 0.4080
GG	 0.7430	 0.3780
GH	 0.3670	 0.2460
GI	 0.4370	 0.2980
GJ	 0.6010	 0.3240
GK	 0.6530	 0.3310
GL	 0.5980	 0.3070
GM	 0.3620	 0.2820
GN	 0.5430	 0.3230
GO	 0.5340	 0.3480
GP	 0.5620	 0.3660
GQ	 0.8490	 0.4210

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Chain	Atom inclusion	Q-score
GR	 0.8800	 0.4370
GS	 0.8360	 0.4340
GT	 0.8340	 0.4250
GU	 0.8210	 0.3630
GV	 0.8220	 0.3770
GW	 0.6380	 0.3090
GX	 0.7540	 0.3590
GY	 0.4710	 0.2390
GZ	 0.5540	 0.2700
Ga	 0.4610	 0.2660
Gb	 0.7170	 0.3580
Gc	 0.5410	 0.3240
Gd	 0.7340	 0.3850
Ge	 0.6970	 0.3890
Gf	 0.7350	 0.3800
Gg	 0.7910	 0.4150
Gh	 0.7910	 0.4190
Gi	 0.8540	 0.4220
Gj	 0.7450	 0.4030
Gk	 0.8460	 0.4370
Gl	 0.7510	 0.3570
Gm	 0.8390	 0.4360
Gn	 0.8140	 0.3670
Go	 0.7020	 0.3370
Gp	 0.8150	 0.3670
Gq	 0.7550	 0.3240
Gr	 0.8100	 0.3690
Gs	 0.7710	 0.3380
Gt	 0.7010	 0.3370
Gu	 0.7830	 0.3590
Gv	 0.7240	 0.3530
Gw	 0.5140	 0.2480
Gx	 0.6120	 0.2870
Gy	 0.5130	 0.2900
Gz	 0.7280	 0.3740
H	 0.6910	 0.3860
HA	 0.4550	 0.3160
HB	 0.2310	 0.2990
HC	 0.0370	 0.2370
HD	 0.4920	 0.3310
I	 0.2770	 0.1940
M	 0.6290	 0.3880

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Chain	Atom inclusion	Q-score
N	 0.5230	 0.2380
O	 0.4340	 0.3050
P	 0.4870	 0.3160
Q	 0.4970	 0.3110
R	 0.4680	 0.3200
S	 0.4610	 0.2760
T	 0.4190	 0.3040
U	 0.3850	 0.2710
V	 0.4800	 0.2950
W	 0.4330	 0.2350
X	 0.4780	 0.3260
Y	 0.5040	 0.3200
Z	 0.4200	 0.3110
a	 0.5760	 0.3310
b	 0.5430	 0.3300
c	 0.3110	 0.2920
d	 0.3600	 0.3090
e	 0.5680	 0.3380
f	 0.5560	 0.3400
g	 0.4800	 0.2940
h	 0.4340	 0.3080
i	 0.5810	 0.3670
j	 0.4400	 0.3370
k	 0.5830	 0.3750
l	 0.3600	 0.3230
m	 0.3860	 0.3060
n	 0.0390	 0.2080
o	 0.0330	 0.1930
p	 0.0810	 0.2180
q	 0.1210	 0.2110
r	 0.3620	 0.2830
s	 0.5240	 0.3240
t	 0.4590	 0.3200
u	 0.4970	 0.2920
v	 0.4580	 0.3060
w	 0.4440	 0.3110
x	 0.4550	 0.2350
y	 0.4170	 0.3010
z	 0.5240	 0.3480