



# wwPDB EM Validation Summary Report ⓘ

Apr 10, 2026 – 02:25 PM UTC

PDB ID : 8GLV / pdb\_00008glv  
EMDB ID : EMD-40220  
Title : 96-nm repeat unit of doublet microtubules from *Chlamydomonas reinhardtii* flagella  
Authors : Walton, T.; Brown, A.  
Deposited on : 2023-03-23  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.48.1

## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

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

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

## 2 Entry composition [i](#)

There are 130 unique types of molecules in this entry. The entry contains 3968189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin beta.

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	3G	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	3I	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	3K	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	3M	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	3O	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	3Q	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	3S	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	8H	433	Total 3397	C 2131	N 581	O 655	S 30	0	0
1	8J	436	Total 3421	C 2147	N 584	O 660	S 30	0	0
1	8L	437	Total 3430	C 2152	N 585	O 663	S 30	0	0
1	8N	436	Total 3421	C 2147	N 584	O 660	S 30	0	0
1	A1	432	Total 3388	C 2126	N 580	O 652	S 30	0	0
1	A3	435	Total 3410	C 2138	N 583	O 659	S 30	0	0
1	A5	430	Total 3370	C 2116	N 578	O 646	S 30	0	0
1	A6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	A7	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	A9	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	AJ	436	Total 3421	C 2147	N 584	O 660	S 30	0	0
1	Ah	436	Total 3421	C 2147	N 584	O 660	S 30	0	0
1	Aj	437	Total 3430	C 2152	N 585	O 663	S 30	0	0
1	Al	436	Total 3421	C 2147	N 584	O 660	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	An	432	Total 3388	C 2126	N 580	O 652	S 30	0	0
1	Ap	435	Total 3410	C 2138	N 583	O 659	S 30	0	0
1	Au	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Aw	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Ay	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	B1	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	B3	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	B5	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	B6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	B8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	BB	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	BG	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	BI	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	BK	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	BM	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	BO	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	BS	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	BU	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	BW	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	BY	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Ba	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bf	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Bh	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Bj	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Bl	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Bn	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Bs	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Bu	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Bw	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	By	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	C0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	C2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	C4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	C6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	C8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	CE	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	CG	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	CI	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	CK	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	CM	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	CR	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	CT	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	CV	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	CX	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	CZ	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Ce	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Cg	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Ci	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Ck	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Cm	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Cr	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Ct	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Cv	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Cx	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Cz	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	D0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	D2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	D4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	D6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	D8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	DE	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	DG	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	DI	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	DK	426	3346	2103	574	639	30	0	0
1	DM	426	3346	2103	574	639	30	0	0
1	DR	426	3346	2103	574	639	30	0	0
1	DT	430	3370	2116	578	646	30	0	0
1	DV	426	3346	2103	574	639	30	0	0
1	DX	431	3379	2121	579	649	30	0	0
1	DZ	426	3346	2103	574	639	30	0	0
1	De	426	3346	2103	574	639	30	0	0
1	Dg	426	3346	2103	574	639	30	0	0
1	Di	426	3346	2103	574	639	30	0	0
1	Dk	426	3346	2103	574	639	30	0	0
1	Dm	426	3346	2103	574	639	30	0	0
1	Dr	426	3346	2103	574	639	30	0	0
1	Dt	426	3346	2103	574	639	30	0	0
1	Dv	430	3370	2116	578	646	30	0	0
1	Dx	426	3346	2103	574	639	30	0	0
1	Dz	426	3346	2103	574	639	30	0	0
1	E0	426	3346	2103	574	639	30	0	0
1	E2	426	3346	2103	574	639	30	0	0
1	E4	426	3346	2103	574	639	30	0	0
1	E6	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E8	426	3346	2103	574	639	30	0	0
1	ED	426	3346	2103	574	639	30	0	0
1	EF	426	3346	2103	574	639	30	0	0
1	EH	426	3346	2103	574	639	30	0	0
1	EJ	426	3346	2103	574	639	30	0	0
1	EL	426	3346	2103	574	639	30	0	0
1	EQ	426	3346	2103	574	639	30	0	0
1	ES	426	3346	2103	574	639	30	0	0
1	EU	426	3346	2103	574	639	30	0	0
1	EW	426	3346	2103	574	639	30	0	0
1	EY	426	3346	2103	574	639	30	0	0
1	Ed	426	3346	2103	574	639	30	0	0
1	Ef	426	3346	2103	574	639	30	0	0
1	Eh	426	3346	2103	574	639	30	0	0
1	Ej	426	3346	2103	574	639	30	0	0
1	El	426	3346	2103	574	639	30	0	0
1	Eq	426	3346	2103	574	639	30	0	0
1	Es	426	3346	2103	574	639	30	0	0
1	Eu	426	3346	2103	574	639	30	0	0
1	Ew	426	3346	2103	574	639	30	0	0
1	F0	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	F2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	F6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	F8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	FC	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	FE	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	FG	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	FI	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	FK	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	FP	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	FR	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	FT	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	FV	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	FX	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Fc	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Fe	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Fg	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Fi	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Fk	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Fp	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Fr	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Ft	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Fv	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Fx	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	G0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	G2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	G4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	G6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	G8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	GB	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	GD	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	GF	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	GH	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	GJ	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	H2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	H4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	H6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	H8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	I0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	I2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	I4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	I8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	IK	432	Total 3388	C 2126	N 580	O 652	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IM	435	Total 3410	C 2138	N 583	O 659	S 30	0	0
1	IW	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	IY	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Ij	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Il	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Iw	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Iy	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	J0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	J2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	J4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	J6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	J8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	JJ	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	JL	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	JU	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	JW	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	JY	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Jh	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Jj	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Jl	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Ju	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Jw	426	3346	2103	574	639	30	0	0
1	Jy	426	3346	2103	574	639	30	0	0
1	K0	426	3346	2103	574	639	30	0	0
1	K4	426	3346	2103	574	639	30	0	0
1	K6	426	3346	2103	574	639	30	0	0
1	K8	426	3346	2103	574	639	30	0	0
1	KH	426	3346	2103	574	639	30	0	0
1	KJ	426	3346	2103	574	639	30	0	0
1	KL	426	3346	2103	574	639	30	0	0
1	KU	426	3346	2103	574	639	30	0	0
1	KW	426	3346	2103	574	639	30	0	0
1	KY	426	3346	2103	574	639	30	0	0
1	Kh	426	3346	2103	574	639	30	0	0
1	Kj	426	3346	2103	574	639	30	0	0
1	Kl	426	3346	2103	574	639	30	0	0
1	Kv	426	3346	2103	574	639	30	0	0
1	Kx	431	3379	2121	579	649	30	0	0
1	L0	426	3346	2103	574	639	30	0	0
1	L2	426	3346	2103	574	639	30	0	0
1	L4	426	3346	2103	574	639	30	0	0
1	L6	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	LH	426	3346	2103	574	639	30	0	0
1	LJ	426	3346	2103	574	639	30	0	0
1	LT	430	3370	2116	578	646	30	0	0
1	LV	426	3346	2103	574	639	30	0	0
1	LX	426	3346	2103	574	639	30	0	0
1	Lh	426	3346	2103	574	639	30	0	0
1	Lj	426	3346	2103	574	639	30	0	0
1	Lu	426	3346	2103	574	639	30	0	0
1	Lw	426	3346	2103	574	639	30	0	0
1	M0	426	3346	2103	574	639	30	0	0
1	M2	426	3346	2103	574	639	30	0	0
1	M4	426	3346	2103	574	639	30	0	0
1	M6	426	3346	2103	574	639	30	0	0
1	M8	426	3346	2103	574	639	30	0	0
1	MG	426	3346	2103	574	639	30	0	0
1	MI	426	3346	2103	574	639	30	0	0
1	MT	426	3346	2103	574	639	30	0	0
1	MV	426	3346	2103	574	639	30	0	0
1	Mg	426	3346	2103	574	639	30	0	0
1	Mi	426	3346	2103	574	639	30	0	0
1	Mt	426	3346	2103	574	639	30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Mv	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	N0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	N2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	N6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	N8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	NF	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	NH	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	NJ	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	NS	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	NU	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	NW	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Nf	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Nh	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Nj	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	O0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	O2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	O4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	O6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	O8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	P4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	P6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	P8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Q0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Q2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Q4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Q6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Q8	420	Total 3293	C 2070	N 563	O 631	S 29	0	0
1	R0	434	Total 3401	C 2133	N 582	O 656	S 30	0	0
1	R2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	R4	430	Total 3370	C 2116	N 578	O 646	S 30	0	0
1	R6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	R8	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
1	S0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	S2	431	Total 3379	C 2121	N 579	O 649	S 30	0	0
1	S4	427	Total 3354	C 2107	N 575	O 642	S 30	0	0
1	S6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	S8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	T0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	T2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	T4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	T6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	T8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	U2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	U4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	U6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	U8	430	Total 3370	C 2116	N 578	O 646	S 30	0	0
1	V0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	V2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	V4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	V6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	V8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	W0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	W2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	W4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	W6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	W8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	X0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	X2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	X4	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	X6	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	X8	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Y0	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
1	Y2	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y4	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	Y6	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	Y8	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	Z0	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	Z2	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	Z4	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	Z6	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	Z8	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

- Molecule 2 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0B	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0F	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0H	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0J	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0L	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0N	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0P	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0R	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0V	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0X	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	0Z	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	2T	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2V	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	2X	437	Total	C	N	O	S	0	0
			3385	2141	576	647	21		
2	2Z	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3B	437	Total	C	N	O	S	0	0
			3383	2140	576	646	21		
2	3D	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3F	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3H	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3J	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3L	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3N	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3P	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	3R	437	Total	C	N	O	S	0	0
			3385	2141	576	647	21		
2	3T	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	8F	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	8I	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	8K	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	8M	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	A0	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	A2	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	A4	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A8	427	3318	2103	565	629	21	0	0
2	AT	436	3376	2136	575	644	21	0	0
2	Ag	436	3376	2136	575	644	21	0	0
2	Ai	436	3376	2136	575	644	21	0	0
2	Ak	436	3376	2136	575	644	21	0	0
2	Am	436	3376	2136	575	644	21	0	0
2	Ao	436	3376	2136	575	644	21	0	0
2	At	427	3318	2103	565	629	21	0	0
2	Av	427	3318	2103	565	629	21	0	0
2	Ax	427	3318	2103	565	629	21	0	0
2	Az	427	3318	2103	565	629	21	0	0
2	B0	427	3318	2103	565	629	21	0	0
2	B2	427	3318	2103	565	629	21	0	0
2	B4	427	3318	2103	565	629	21	0	0
2	B7	427	3318	2103	565	629	21	0	0
2	B9	427	3318	2103	565	629	21	0	0
2	BA	427	3318	2103	565	629	21	0	0
2	BF	436	3376	2136	575	644	21	0	0
2	BH	427	3318	2103	565	629	21	0	0
2	BJ	427	3318	2103	565	629	21	0	0
2	BL	428	3324	2106	566	631	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BN	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	BT	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	BV	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	BX	428	Total 3324	C 2106	N 566	O 631	S 21	0	0
2	BZ	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Bb	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Bg	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	Bi	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	Bk	443	Total 3418	C 2159	N 582	O 656	S 21	0	0
2	Bm	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Bo	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Bt	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Bv	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Bx	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Bz	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	C1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	C3	431	Total 3340	C 2114	N 569	O 636	S 21	0	0
2	C5	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	C7	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	C9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	CA	427	Total 3318	C 2103	N 565	O 629	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	CF	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	CH	428	Total 3326	C 2107	N 566	O 632	S 21	0	0
2	CJ	437	Total 3385	C 2141	N 576	O 647	S 21	0	0
2	CL	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	CN	437	Total 3385	C 2141	N 576	O 647	S 21	0	0
2	CS	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	CU	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	CW	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	CY	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Cf	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	Ch	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Cj	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	Cl	437	Total 3385	C 2141	N 576	O 647	S 21	0	0
2	Cs	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Cu	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Cw	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Cy	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	D1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	D3	428	Total 3324	C 2106	N 566	O 631	S 21	0	0
2	D5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	D7	428	Total 3324	C 2106	N 566	O 631	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	DD	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	DF	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	DH	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	DJ	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	DL	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	DN	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	DQ	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	DS	428	Total 3327	C 2108	N 566	O 632	S 21	0	0
2	DU	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	DW	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	DY	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	Da	429	Total 3333	C 2111	N 567	O 634	S 21	0	0
2	Dd	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	Df	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Dh	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Dj	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Di	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Dq	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Ds	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Du	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Dw	427	Total 3318	C 2103	N 565	O 629	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Dy	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	E1	428	Total 3324	C 2106	N 566	O 631	S 21	0	0
2	E3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	E5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	E7	428	Total 3324	C 2106	N 566	O 631	S 21	0	0
2	E9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	EC	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	EE	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	EG	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	EI	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	EK	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	EP	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	ER	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	ET	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	EV	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	EX	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Ec	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Ee	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Eg	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Ei	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Ek	427	Total 3318	C 2103	N 565	O 629	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Ep	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Er	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Et	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Ev	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Ex	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	F1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	F3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	F5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	F7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	F9	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	FD	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	FF	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	FH	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	FJ	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	FL	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	FQ	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	FS	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	FU	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	FW	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	FY	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Fd	427	Total 3318	C 2103	N 565	O 629	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Ff	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Fh	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Fj	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Fl	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Fq	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Fs	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Fu	437	Total 3385	C 2141	N 576	O 647	S 21	0	0
2	Fw	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	G1	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	G3	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	G5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	G7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	G9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	GC	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	GE	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	GG	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	GI	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	H1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	H3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	H5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	H7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H9	427	3318	2103	565	629	21	0	0
2	Hu	436	3376	2136	575	644	21	0	0
2	I1	427	3318	2103	565	629	21	0	0
2	I3	427	3318	2103	565	629	21	0	0
2	I5	427	3318	2103	565	629	21	0	0
2	I7	429	3332	2110	567	634	21	0	0
2	I9	428	3324	2106	566	631	21	0	0
2	IL	436	3376	2136	575	644	21	0	0
2	IV	427	3318	2103	565	629	21	0	0
2	IX	427	3318	2103	565	629	21	0	0
2	IZ	427	3318	2103	565	629	21	0	0
2	Ii	427	3318	2103	565	629	21	0	0
2	Ik	428	3324	2106	566	631	21	0	0
2	Im	427	3318	2103	565	629	21	0	0
2	Iv	428	3324	2106	566	631	21	0	0
2	Ix	427	3318	2103	565	629	21	0	0
2	Iz	427	3318	2103	565	629	21	0	0
2	J1	427	3318	2103	565	629	21	0	0
2	J3	428	3326	2107	566	632	21	0	0
2	J5	437	3385	2141	576	647	21	0	0
2	J7	427	3318	2103	565	629	21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	J9	437	Total	C	N	O	S	0	0
			3385	2141	576	647	21		
2	JI	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	JK	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	JV	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	JX	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Ji	437	Total	C	N	O	S	0	0
			3385	2141	576	647	21		
2	Jk	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Jv	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Jx	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	K1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	K3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	K5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	K7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	K9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	KI	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
2	KK	437	Total	C	N	O	S	0	0
			3385	2141	576	647	21		
2	KV	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	KX	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Ki	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Kk	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Kw	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Ky	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	L1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	L3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	L5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	L7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	L9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	LI	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	LK	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	LU	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	LW	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Li	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Lk	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Lv	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Lx	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	M1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	M3	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	M5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	M7	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	M9	437	Total 3385	C 2141	N 576	O 647	S 21	0	0
2	MF	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	MH	427	Total 3318	C 2103	N 565	O 629	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	MJ	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	MS	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	MU	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	MW	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Mf	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Mh	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Mj	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Ms	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Mu	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Mw	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	N1	428	Total 3324	C 2106	N 566	O 631	S 21	0	0
2	N3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	N5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	N7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	N9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	NG	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	NI	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	NT	437	Total 3385	C 2141	N 576	O 647	S 21	0	0
2	NV	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Ng	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Ni	427	Total 3318	C 2103	N 565	O 629	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	O1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	O3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	O5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	O7	431	Total 3340	C 2114	N 569	O 636	S 21	0	0
2	O9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	P3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	P5	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	P7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	P9	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	Q1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Q3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Q5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	Q9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	R1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	R3	428	Total 3327	C 2108	N 566	O 632	S 21	0	0
2	R5	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	R7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	R9	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
2	S1	429	Total 3333	C 2111	N 567	O 634	S 21	0	0
2	S5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	S7	436	Total 3376	C 2136	N 575	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	T1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	T3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	T5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	T7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	U1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	U3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	U5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	U7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	U9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	V1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	V3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	V7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	V9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	W1	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	W3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	W5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	W7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	W9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	X3	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
2	X5	427	Total 3318	C 2103	N 565	O 629	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	X7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	X9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Y1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Y3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Y5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Y9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Z1	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Z3	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Z5	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Z7	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	Z9	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

- Molecule 3 is a protein called PACRG.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	GP	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	GR	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	GT	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	GV	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	GX	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	Nt	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		
3	Nv	297	Total	C	N	O	S	0	0
			2329	1491	401	428	9		

- Molecule 4 is a protein called Cilia- and flagella-associated protein 20.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ns	184	Total	C	N	O	S	0	0
			1515	971	264	273	7		
4	Nu	184	Total	C	N	O	S	0	0
			1515	971	264	273	7		
4	Nw	184	Total	C	N	O	S	0	0
			1515	971	264	273	7		

- Molecule 5 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4O	478	Total	C	N	O	S	0	0
			3995	2407	778	791	19		
5	5D	478	Total	C	N	O	S	0	0
			3995	2407	778	791	19		
5	Gd	120	Total	C	N	O	S	0	0
			992	599	196	195	2		
5	OA	167	Total	C	N	O	S	0	0
			1403	847	273	275	8		

- Molecule 6 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4Q	171	Total	C	N	O	S	0	0
			1349	806	273	264	6		
6	4W	385	Total	C	N	O	S	0	0
			2989	1794	600	581	14		
6	Nz	324	Total	C	N	O	S	0	0
			2511	1500	508	493	10		

- Molecule 7 is a protein called Coiled-coil protein associated with protofilament ribbons.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4R	366	Total	C	N	O	S	0	0
			2982	1819	561	589	13		
7	Ga	366	Total	C	N	O	S	0	0
			2982	1819	561	589	13		
7	Gf	349	Total	C	N	O	S	0	0
			2838	1728	533	565	12		
7	Gi	205	Total	C	N	O	S	0	0
			1672	1020	315	335	2		
7	Gj	337	Total	C	N	O	S	0	0
			2748	1673	515	547	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	OG	199	Total	C	N	O	S	0	0
			1609	981	300	317	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4X	376	Total	C	N	O	S	0	0
			3157	1918	605	614	20		
8	5C	370	Total	C	N	O	S	0	0
			3103	1881	597	604	21		
8	Go	210	Total	C	N	O	S	0	0
			1743	1054	332	343	14		
8	Gp	376	Total	C	N	O	S	0	0
			3157	1918	605	614	20		
8	Gq	29	Total	C	N	O	S	0	0
			238	145	45	43	5		
8	OD	370	Total	C	N	O	S	0	0
			3103	1881	597	604	21		
8	OO	161	Total	C	N	O	S	0	0
			1346	820	261	260	5		

- Molecule 9 is a protein called FAP34.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	5E	258	Total	C	N	O	S	0	0
			1981	1245	352	380	4		
9	Gr	258	Total	C	N	O	S	0	0
			1981	1245	352	380	4		
9	OQ	103	Total	C	N	O	S	0	0
			783	493	143	146	1		

- Molecule 10 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5F	381	Total	C	N	O	S	0	0
			3020	1921	520	569	10		
10	7B	174	Total	C	N	O	S	0	0
			1382	875	235	265	7		
10	Gs	311	Total	C	N	O	S	0	0
			2466	1576	425	459	6		

- Molecule 11 is a protein called Protein Flattop homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5H	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		
11	5I	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		
11	5J	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		
11	5K	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		
11	Gv	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		
11	Gw	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		
11	Gx	96	Total	C	N	O	S	0	0
			764	481	138	144	1		
11	OV	135	Total	C	N	O	S	0	0
			1069	674	190	202	3		

- Molecule 12 is a protein called FAP52.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	5L	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		
12	5M	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		
12	5N	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		
12	Ad	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		
12	Ae	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		
12	Af	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		
12	Eo	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		
12	HG	626	Total	C	N	O	S	0	0
			4757	2992	827	912	26		

- Molecule 13 is a protein called Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	5O	376	Total	C	N	O	S	0	0
			2927	1862	503	547	15		
13	5P	376	Total	C	N	O	S	0	0
			2927	1862	503	547	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	Gy	376	Total	C	N	O	S	0	0
			2927	1862	503	547	15		
13	Gz	376	Total	C	N	O	S	0	0
			2927	1862	503	547	15		
13	OY	376	Total	C	N	O	S	0	0
			2927	1862	503	547	15		

- Molecule 14 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	5Q	191	Total	C	N	O	S	0	0
			1523	961	267	293	2		
14	HA	191	Total	C	N	O	S	0	0
			1523	961	267	293	2		
14	OZ	17	Total	C	N	O		0	0
			135	89	22	24			

- Molecule 15 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5S	199	Total	C	N	O	S	0	0
			1572	989	291	288	4		
15	5T	198	Total	C	N	O	S	0	0
			1563	984	290	285	4		
15	5U	199	Total	C	N	O	S	0	0
			1572	989	291	288	4		
15	5V	198	Total	C	N	O	S	0	0
			1563	984	290	285	4		
15	HD	198	Total	C	N	O	S	0	0
			1563	984	290	285	4		
15	HE	199	Total	C	N	O	S	0	0
			1572	989	291	288	4		
15	Oc	65	Total	C	N	O	S	0	0
			504	316	93	93	2		
15	Od	199	Total	C	N	O	S	0	0
			1572	989	291	288	4		

- Molecule 16 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	5X	221	Total	C	N	O	S	0	0
			1793	1153	302	330	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	5Y	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	5Z	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	6A	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	6B	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	6C	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	6D	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	HH	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	HI	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	HJ	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	HK	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	HL	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	Oi	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	Oj	221	Total 1793	C 1153	N 302	O 330	S 8	0	0
16	Ok	221	Total 1793	C 1153	N 302	O 330	S 8	0	0

- Molecule 17 is a protein called FAP143.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6E	255	Total 1952	C 1208	N 345	O 390	S 9	0	0
17	HN	255	Total 1952	C 1208	N 345	O 390	S 9	0	0
17	Om	134	Total 1036	C 638	N 187	O 208	S 3	0	0

- Molecule 18 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6F	394	Total	C	N	O	S	0	0
			2950	1852	518	566	14		
18	HO	394	Total	C	N	O	S	0	0
			2950	1852	518	566	14		
18	On	394	Total	C	N	O	S	0	0
			2950	1852	518	566	14		
18	zp	394	Total	C	N	O	S	0	0
			2950	1852	518	566	14		
18	zq	394	Total	C	N	O	S	0	0
			2950	1852	518	566	14		

- Molecule 19 is a protein called FAP166.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6G	183	Total	C	N	O	S	0	0
			1420	891	251	269	9		
19	6H	193	Total	C	N	O	S	0	0
			1493	937	265	282	9		
19	HP	183	Total	C	N	O	S	0	0
			1420	891	251	269	9		
19	HQ	193	Total	C	N	O	S	0	0
			1493	937	265	282	9		
19	Op	193	Total	C	N	O	S	0	0
			1493	937	265	282	9		

- Molecule 20 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	6I	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	6J	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	6K	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	6L	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	6M	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	6N	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	6O	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	6P	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
20	HS	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	HT	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	HU	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	HV	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	HW	222	Total	C	N	O	S	0	0
			1800	1138	304	347	11		
20	Ot	99	Total	C	N	O	S	0	0
			754	482	130	139	3		
20	Ou	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		
20	Ov	329	Total	C	N	O	S	0	0
			2617	1660	442	501	14		

- Molecule 21 is a protein called FAP339.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	6Q	85	Total	C	N	O	S	0	0
			694	434	130	127	3		
21	6R	85	Total	C	N	O	S	0	0
			694	434	130	127	3		
21	6S	85	Total	C	N	O	S	0	0
			694	434	130	127	3		
21	HY	85	Total	C	N	O	S	0	0
			694	434	130	127	3		
21	HZ	85	Total	C	N	O	S	0	0
			694	434	130	127	3		
21	Ha	85	Total	C	N	O	S	0	0
			694	434	130	127	3		
21	Oy	85	Total	C	N	O	S	0	0
			694	434	130	127	3		
21	Oz	85	Total	C	N	O	S	0	0
			694	434	130	127	3		

- Molecule 22 is a protein called Protofilament ribbon protein of flagellar microtubules.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6T	583	Total	C	N	O	S	0	0
			4708	2999	813	880	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
22	6U	581	Total	C	N	O	S	0	0
			4710	3004	812	876	18		
22	6V	565	Total	C	N	O	S	0	0
			4598	2934	794	854	16		
22	6W	575	Total	C	N	O	S	0	0
			4673	2979	806	870	18		
22	6X	565	Total	C	N	O	S	0	0
			4598	2934	794	854	16		
22	6Y	560	Total	C	N	O	S	0	0
			4563	2913	788	846	16		
22	6Z	583	Total	C	N	O	S	0	0
			4708	2999	813	880	16		
22	Hb	581	Total	C	N	O	S	0	0
			4710	3004	812	876	18		
22	Hc	565	Total	C	N	O	S	0	0
			4598	2934	794	854	16		
22	Hd	575	Total	C	N	O	S	0	0
			4673	2979	806	870	18		
22	He	565	Total	C	N	O	S	0	0
			4598	2934	794	854	16		
22	Hf	560	Total	C	N	O	S	0	0
			4563	2913	788	846	16		
22	Hg	45	Total	C	N	O	S	0	0
			341	219	57	64	1		
22	PD	425	Total	C	N	O	S	0	0
			3453	2210	589	642	12		
22	PE	565	Total	C	N	O	S	0	0
			4598	2934	794	854	16		
22	PF	560	Total	C	N	O	S	0	0
			4563	2913	788	846	16		

- Molecule 23 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	7C	83	Total	C	N	O	S	0	0
			692	427	138	125	2		
23	Hj	83	Total	C	N	O	S	0	0
			692	427	138	125	2		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7C	17	MET	LEU	conflict	UNP A0A835TDA6

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Chain	Residue	Modelled	Actual	Comment	Reference
7C	22	GLN	GLU	conflict	UNP A0A835TDA6
7C	36	GLN	LYS	conflict	UNP A0A835TDA6
7C	38	THR	SER	conflict	UNP A0A835TDA6
7C	39	GLU	ASP	conflict	UNP A0A835TDA6
7C	40	ARG	LYS	conflict	UNP A0A835TDA6
7C	46	PRO	GLN	conflict	UNP A0A835TDA6
7C	74	GLN	GLU	conflict	UNP A0A835TDA6
7C	94	MET	ALA	conflict	UNP A0A835TDA6
Hj	17	MET	LEU	conflict	UNP A0A835TDA6
Hj	22	GLN	GLU	conflict	UNP A0A835TDA6
Hj	36	GLN	LYS	conflict	UNP A0A835TDA6
Hj	38	THR	SER	conflict	UNP A0A835TDA6
Hj	39	GLU	ASP	conflict	UNP A0A835TDA6
Hj	40	ARG	LYS	conflict	UNP A0A835TDA6
Hj	46	PRO	GLN	conflict	UNP A0A835TDA6
Hj	74	GLN	GLU	conflict	UNP A0A835TDA6
Hj	94	MET	ALA	conflict	UNP A0A835TDA6

- Molecule 24 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	7D	132	Total	C	N	O	S	0	0
			1016	637	183	189	7		
24	7E	132	Total	C	N	O	S	0	0
			1016	637	183	189	7		
24	Hk	132	Total	C	N	O	S	0	0
			1016	637	183	189	7		
24	Hl	132	Total	C	N	O	S	0	0
			1016	637	183	189	7		
24	PK	132	Total	C	N	O	S	0	0
			1016	637	183	189	7		

- Molecule 25 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	7G	224	Total	C	N	O	S	0	0
			1728	1083	305	336	4		
25	Hn	224	Total	C	N	O	S	0	0
			1728	1083	305	336	4		

- Molecule 26 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	7H	438	3224	2026	570	614	14	0	0
26	7X	438	3224	2026	570	614	14	0	0

- Molecule 27 is a protein called FAP129.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	7I	440	3329	2062	610	646	11	0	0
27	7J	362	2741	1691	505	535	10	0	0
27	Hp	231	1760	1088	327	337	8	0	0

- Molecule 28 is a protein called FAP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	7K	423	3276	2026	620	625	5	0	0
28	Hq	423	3276	2026	620	625	5	0	0
28	Hr	106	807	499	152	154	2	0	0
28	PQ	110	873	544	157	171	1	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7K	1	MET	-	initiating methionine	UNP A0A2K3CNK8
7K	2	SER	-	expression tag	UNP A0A2K3CNK8
7K	3	LEU	-	expression tag	UNP A0A2K3CNK8
7K	4	THR	-	expression tag	UNP A0A2K3CNK8
7K	5	THR	-	expression tag	UNP A0A2K3CNK8
7K	6	GLN	-	expression tag	UNP A0A2K3CNK8
7K	7	SER	-	expression tag	UNP A0A2K3CNK8
7K	8	LEU	-	expression tag	UNP A0A2K3CNK8
7K	9	ARG	-	expression tag	UNP A0A2K3CNK8
7K	10	ARG	-	expression tag	UNP A0A2K3CNK8
7K	11	THR	-	expression tag	UNP A0A2K3CNK8
7K	12	ASN	-	expression tag	UNP A0A2K3CNK8
7K	13	TYR	-	expression tag	UNP A0A2K3CNK8

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Chain	Residue	Modelled	Actual	Comment	Reference
7K	14	GLU	-	expression tag	UNP A0A2K3CNK8
7K	15	ALA	-	expression tag	UNP A0A2K3CNK8
7K	16	GLU	-	expression tag	UNP A0A2K3CNK8
Hq	1	MET	-	initiating methionine	UNP A0A2K3CNK8
Hq	2	SER	-	expression tag	UNP A0A2K3CNK8
Hq	3	LEU	-	expression tag	UNP A0A2K3CNK8
Hq	4	THR	-	expression tag	UNP A0A2K3CNK8
Hq	5	THR	-	expression tag	UNP A0A2K3CNK8
Hq	6	GLN	-	expression tag	UNP A0A2K3CNK8
Hq	7	SER	-	expression tag	UNP A0A2K3CNK8
Hq	8	LEU	-	expression tag	UNP A0A2K3CNK8
Hq	9	ARG	-	expression tag	UNP A0A2K3CNK8
Hq	10	ARG	-	expression tag	UNP A0A2K3CNK8
Hq	11	THR	-	expression tag	UNP A0A2K3CNK8
Hq	12	ASN	-	expression tag	UNP A0A2K3CNK8
Hq	13	TYR	-	expression tag	UNP A0A2K3CNK8
Hq	14	GLU	-	expression tag	UNP A0A2K3CNK8
Hq	15	ALA	-	expression tag	UNP A0A2K3CNK8
Hq	16	GLU	-	expression tag	UNP A0A2K3CNK8
Hr	1	MET	-	initiating methionine	UNP A0A2K3CNK8
Hr	2	SER	-	expression tag	UNP A0A2K3CNK8
Hr	3	LEU	-	expression tag	UNP A0A2K3CNK8
Hr	4	THR	-	expression tag	UNP A0A2K3CNK8
Hr	5	THR	-	expression tag	UNP A0A2K3CNK8
Hr	6	GLN	-	expression tag	UNP A0A2K3CNK8
Hr	7	SER	-	expression tag	UNP A0A2K3CNK8
Hr	8	LEU	-	expression tag	UNP A0A2K3CNK8
Hr	9	ARG	-	expression tag	UNP A0A2K3CNK8
Hr	10	ARG	-	expression tag	UNP A0A2K3CNK8
Hr	11	THR	-	expression tag	UNP A0A2K3CNK8
Hr	12	ASN	-	expression tag	UNP A0A2K3CNK8
Hr	13	TYR	-	expression tag	UNP A0A2K3CNK8
Hr	14	GLU	-	expression tag	UNP A0A2K3CNK8
Hr	15	ALA	-	expression tag	UNP A0A2K3CNK8
Hr	16	GLU	-	expression tag	UNP A0A2K3CNK8
PQ	1	MET	-	initiating methionine	UNP A0A2K3CNK8
PQ	2	SER	-	expression tag	UNP A0A2K3CNK8
PQ	3	LEU	-	expression tag	UNP A0A2K3CNK8
PQ	4	THR	-	expression tag	UNP A0A2K3CNK8
PQ	5	THR	-	expression tag	UNP A0A2K3CNK8
PQ	6	GLN	-	expression tag	UNP A0A2K3CNK8
PQ	7	SER	-	expression tag	UNP A0A2K3CNK8

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Chain	Residue	Modelled	Actual	Comment	Reference
PQ	8	LEU	-	expression tag	UNP A0A2K3CNK8
PQ	9	ARG	-	expression tag	UNP A0A2K3CNK8
PQ	10	ARG	-	expression tag	UNP A0A2K3CNK8
PQ	11	THR	-	expression tag	UNP A0A2K3CNK8
PQ	12	ASN	-	expression tag	UNP A0A2K3CNK8
PQ	13	TYR	-	expression tag	UNP A0A2K3CNK8
PQ	14	GLU	-	expression tag	UNP A0A2K3CNK8
PQ	15	ALA	-	expression tag	UNP A0A2K3CNK8
PQ	16	GLU	-	expression tag	UNP A0A2K3CNK8

- Molecule 29 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	7M	126	Total 977	C 607	N 179	O 186	S 5	0	0
29	7N	126	Total 977	C 607	N 179	O 186	S 5	0	0
29	Ht	76	Total 583	C 360	N 111	O 109	S 3	0	0

- Molecule 30 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	7P	197	Total 1520	C 939	N 283	O 295	S 3	0	0
30	Hv	172	Total 1336	C 825	N 249	O 259	S 3	0	0
30	PV	197	Total 1520	C 939	N 283	O 295	S 3	0	0

- Molecule 31 is a protein called FAP306.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	7Q	71	Total 567	C 352	N 98	O 117	0	0
31	Hw	71	Total 567	C 352	N 98	O 117	0	0
31	PW	71	Total 567	C 352	N 98	O 117	0	0
31	zn	42	Total 341	C 217	N 53	O 71	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
31	zo	42	Total	C	N	O	0	0
			341	217	53	71		

- Molecule 32 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7Y	247	Total	C	N	O	S	0	0
			1971	1221	372	370	8		
32	ID	247	Total	C	N	O	S	0	0
			1971	1221	372	370	8		
32	Pe	208	Total	C	N	O	S	0	0
			1663	1029	312	315	7		

- Molecule 33 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	8B	213	Total	C	N	O	S	0	0
			1728	1078	311	332	7		
33	8C	213	Total	C	N	O	S	0	0
			1728	1078	311	332	7		
33	IG	213	Total	C	N	O	S	0	0
			1728	1078	311	332	7		
33	IH	213	Total	C	N	O	S	0	0
			1728	1078	311	332	7		
33	Pi	213	Total	C	N	O	S	0	0
			1728	1078	311	332	7		

- Molecule 34 is a protein called Dynein axonemal light chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AA	195	Total	C	N	O	S	4	0
			1554	981	264	302	7		
34	Cb	195	Total	C	N	O	S	4	0
			1554	981	264	302	7		
34	Gg	195	Total	C	N	O	S	4	0
			1554	981	264	302	7		
34	Ll	195	Total	C	N	O	S	4	0
			1554	981	264	302	7		

- Molecule 35 is a protein called Outer dynein arm-docking complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AB	404	Total	C	N	O	S	0	0
			3309	2024	618	652	15		
35	AY	404	Total	C	N	O	S	0	0
			3309	2024	618	652	15		
35	Fb	332	Total	C	N	O	S	0	0
			2724	1663	507	539	15		
35	MM	158	Total	C	N	O	S	0	0
			1239	764	218	251	6		
35	MR	404	Total	C	N	O	S	0	0
			3309	2024	618	652	15		
35	MY	202	Total	C	N	O	S	0	0
			1681	1027	320	328	6		
35	Ma	58	Total	C	N	O		0	0
			463	287	85	91			

- Molecule 36 is a protein called Outer dynein arm-docking complex protein DC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AC	170	Total	C	N	O	S	0	0
			1384	863	242	270	9		
36	AZ	170	Total	C	N	O	S	0	0
			1384	863	242	270	9		
36	Fn	170	Total	C	N	O	S	0	0
			1384	863	242	270	9		
36	LN	170	Total	C	N	O	S	0	0
			1384	863	242	270	9		
36	MO	170	Total	C	N	O	S	0	0
			1384	863	242	270	9		

- Molecule 37 is a protein called Dynein gamma chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AD	4484	Total	C	N	O	S	0	0
			36045	22979	6151	6707	208		
37	AX	4484	Total	C	N	O	S	0	0
			36045	22979	6151	6707	208		
37	Fa	4484	Total	C	N	O	S	0	0
			36045	22979	6151	6707	208		
37	Ks	1170	Total	C	N	O	S	0	0
			9491	6012	1642	1785	52		
37	Lo	4484	Total	C	N	O	S	0	0
			36045	22979	6151	6707	208		

- Molecule 38 is a protein called IC97/Casc1 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	AE	633	4866	3070	883	896	17	0	0

- Molecule 39 is a protein called Axonemal inner arm I1 intermediate chain dynein IC138.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	AF	540	4240	2684	719	813	24	0	0

- Molecule 40 is a protein called IC140.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	AG	732	5632	3523	1015	1073	21	0	0

- Molecule 41 is a protein called Axonemal inner arm dynein I1/f subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	AH	182	1313	811	238	263	1	0	0

- Molecule 42 is a protein called Dynein light chain roadblock LC7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	AI	100	780	488	140	149	3	0	0
42	Bc	94	741	466	133	140	2	0	0
42	Bd	94	741	466	133	140	2	0	0
42	GY	94	741	466	133	140	2	0	0
42	LC	94	741	466	133	140	2	0	0
42	MA	94	741	466	133	140	2	0	0

- Molecule 43 is a protein called Dynein light chain roadblock LC7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	AK	105	840	533	150	155	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
43	BQ	103	Total	C	N	O	S	0	0
			827	525	148	153	1		
43	BR	103	Total	C	N	O	S	0	0
			827	525	148	153	1		
43	GN	103	Total	C	N	O	S	0	0
			827	525	148	153	1		
43	L8	103	Total	C	N	O	S	0	0
			827	525	148	153	1		
43	LB	103	Total	C	N	O	S	0	0
			827	525	148	153	1		

- Molecule 44 is a protein called Dynein 8 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AL	91	Total	C	N	O	S	0	0
			725	463	122	135	5		
44	AM	86	Total	C	N	O	S	0	0
			696	447	117	128	4		
44	AN	91	Total	C	N	O	S	0	0
			726	463	122	136	5		
44	AO	91	Total	C	N	O	S	0	0
			726	463	122	136	5		
44	AP	91	Total	C	N	O	S	0	0
			726	463	122	136	5		
44	AQ	91	Total	C	N	O	S	0	0
			726	463	122	136	5		
44	Be	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
44	Bp	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
44	Bq	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
44	Br	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
44	CB	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
44	CC	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
44	CD	85	Total	C	N	O	S	0	0
			691	444	116	127	4		
44	CO	85	Total	C	N	O	S	0	0
			691	444	116	127	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
44	FA	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
44	FB	85	Total	C	N	O	S	0	0
			691	444	116	127	4		
44	GZ	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
44	Ge	82	Total	C	N	O	S	0	0
			671	433	112	122	4		
44	I6	84	Total	C	N	O		0	0
			417	249	84	84			
44	Io	84	Total	C	N	O		0	0
			417	249	84	84			
44	Ip	84	Total	C	N	O		0	0
			417	249	84	84			
44	Iq	84	Total	C	N	O		0	0
			417	249	84	84			
44	Ir	84	Total	C	N	O		0	0
			417	249	84	84			
44	Is	84	Total	C	N	O		0	0
			417	249	84	84			
44	It	84	Total	C	N	O		0	0
			417	249	84	84			
44	Iu	84	Total	C	N	O		0	0
			417	249	84	84			
44	KM	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
44	KN	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
44	KO	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
44	KP	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
44	KQ	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
44	KR	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
44	KS	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
44	KT	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
44	Kc	84	Total	C	N	O	S	0	0
			686	442	115	125	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Kd	84	Total 686	C 442	N 115	O 125	S 4	0	0
44	Ke	84	Total 686	C 442	N 115	O 125	S 4	0	0
44	Kf	84	Total 686	C 442	N 115	O 125	S 4	0	0
44	LD	82	Total 671	C 433	N 112	O 122	S 4	0	0
44	LE	82	Total 671	C 433	N 112	O 122	S 4	0	0
44	LF	82	Total 671	C 433	N 112	O 122	S 4	0	0
44	LG	85	Total 691	C 444	N 116	O 127	S 4	0	0
44	MB	82	Total 671	C 433	N 112	O 122	S 4	0	0
44	MC	82	Total 671	C 433	N 112	O 122	S 4	0	0
44	MD	82	Total 671	C 433	N 112	O 122	S 4	0	0
44	ME	85	Total 691	C 444	N 116	O 127	S 4	0	0

- Molecule 45 is a protein called Dynein light chain Tctex1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	AR	114	Total 885	C 556	N 148	O 172	S 9	0	0

- Molecule 46 is a protein called Inner arm dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	AS	120	Total 969	C 618	N 166	O 182	S 3	0	0

- Molecule 47 is a protein called Dynein light chain 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	AU	98	Total 805	C 523	N 128	O 146	S 8	0	0
47	Ca	98	Total 805	C 523	N 128	O 146	S 8	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
47	FN	98	Total	C	N	O	S	0	0
			805	523	128	146	8		
47	LM	98	Total	C	N	O	S	0	0
			805	523	128	146	8		
47	ML	98	Total	C	N	O	S	0	0
			805	523	128	146	8		

- Molecule 48 is a protein called Cilia- and flagella-associated protein 73.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AV	273	Total	C	N	O	S	0	0
			2224	1380	395	444	5		

- Molecule 49 is a protein called Cilia- and flagella-associated protein 100.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AW	410	Total	C	N	O	S	0	0
			3290	2022	593	661	14		

- Molecule 50 is a protein called Dynein, 78 kDa intermediate chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Aa	587	Total	C	N	O	S	0	0
			4676	2956	803	887	30		
50	Ab	587	Total	C	N	O	S	0	0
			4676	2956	803	887	30		
50	Fo	587	Total	C	N	O	S	0	0
			4676	2956	803	887	30		
50	Kt	587	Total	C	N	O	S	0	0
			4676	2956	803	887	30		
50	Lp	587	Total	C	N	O	S	0	0
			4676	2956	803	887	30		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	474	PRO	ALA	conflict	UNP Q39578
Ab	474	PRO	ALA	conflict	UNP Q39578
Fo	474	PRO	ALA	conflict	UNP Q39578
Kt	474	PRO	ALA	conflict	UNP Q39578
Lp	474	PRO	ALA	conflict	UNP Q39578

- Molecule 51 is a protein called WD\_REPEATS\_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ac	533	Total	C	N	O	S	0	0
			4184	2639	707	817	21		
51	Aq	533	Total	C	N	O	S	0	0
			4184	2639	707	817	21		
51	Fz	533	Total	C	N	O	S	0	0
			4184	2639	707	817	21		
51	Ku	533	Total	C	N	O	S	0	0
			4184	2639	707	817	21		
51	Lq	533	Total	C	N	O	S	0	0
			4184	2639	707	817	21		

- Molecule 52 is a protein called Flagellar outer dynein arm light chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Ar	125	Total	C	N	O	S	0	0
			1035	657	175	198	5		
52	As	125	Total	C	N	O	S	0	0
			1035	657	175	198	5		
52	GA	125	Total	C	N	O	S	0	0
			1035	657	175	198	5		
52	Kz	125	Total	C	N	O	S	0	0
			1035	657	175	198	5		
52	Lr	125	Total	C	N	O	S	0	0
			1035	657	175	198	5		

- Molecule 53 is a protein called Dynein 18 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BC	138	Total	C	N	O	S	0	0
			1089	677	183	220	9		
53	BD	138	Total	C	N	O	S	0	0
			1089	677	183	220	9		
53	GL	138	Total	C	N	O	S	0	0
			1089	677	183	220	9		
53	K2	138	Total	C	N	O	S	0	0
			1089	677	183	220	9		
53	Lt	138	Total	C	N	O	S	0	0
			1089	677	183	220	9		

- Molecule 54 is a protein called Dynein 11 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BE	107	Total	C	N	O	S	0	0
			875	567	144	161	3		
54	BP	107	Total	C	N	O	S	0	0
			875	567	144	161	3		
54	GM	107	Total	C	N	O	S	0	0
			875	567	144	161	3		
54	LA	107	Total	C	N	O	S	0	0
			875	567	144	161	3		
54	Lz	107	Total	C	N	O	S	0	0
			875	567	144	161	3		

- Molecule 55 is a protein called Dynein light chain 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	CP	117	Total	C	N	O	S	0	0
			909	568	153	181	7		
55	CQ	117	Total	C	N	O	S	0	0
			909	568	153	181	7		
55	FM	117	Total	C	N	O	S	0	0
			909	568	153	181	7		
55	LL	117	Total	C	N	O	S	0	0
			909	568	153	181	7		
55	MK	117	Total	C	N	O	S	0	0
			909	568	153	181	7		

- Molecule 56 is a protein called Outer dynein arm protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Cc	402	Total	C	N	O	S	0	0
			3238	1993	585	646	14		
56	Cd	402	Total	C	N	O	S	0	0
			3238	1993	585	646	14		
56	Gk	332	Total	C	N	O	S	0	0
			2668	1637	482	539	10		
56	MN	190	Total	C	N	O	S	0	0
			1509	931	261	312	5		
56	MX	403	Total	C	N	O	S	0	0
			3247	1999	587	647	14		
56	MZ	213	Total	C	N	O	S	0	0
			1738	1068	326	335	9		
56	Mb	56	Total	C	N	O	S	0	0
			453	285	82	85	1		

- Molecule 57 is a protein called AAA+ ATPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	Cn	4500	35901	22840	6137	6740	184	0	0

- Molecule 58 is a protein called Dynein-1-beta heavy chain, flagellar inner arm I1 complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	Co	4499	35837	22826	6150	6688	173	0	0

- Molecule 59 is a protein called WD\_REPEATS\_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	Cp	1075	8547	5343	1495	1665	44	0	0
59	Cq	1076	8553	5346	1496	1666	45	0	0

- Molecule 60 is a protein called Inner-arm dynein f/I1 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	D9	238	1843	1163	315	358	7	0	0

- Molecule 61 is a protein called Heavy chain alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	DA	4407	34821	22130	5926	6559	206	0	0
61	DP	4407	34821	22130	5926	6559	206	0	0
61	Gl	4407	34821	22130	5926	6559	206	0	0
61	Lm	4407	34821	22130	5926	6559	206	0	0

- Molecule 62 is a protein called Flagellar outer dynein arm heavy chain beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	DB	4520	36194	23030	6145	6804	215	0	0
62	Db	4520	36194	23030	6145	6804	215	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
62	Gt	4520	Total	C	N	O	S	0	0
			36194	23030	6145	6804	215		
62	Kr	765	Total	C	N	O	S	0	0
			6182	3945	1040	1160	37		
62	Ln	4520	Total	C	N	O	S	0	0
			36194	23030	6145	6804	215		

- Molecule 63 is a protein called Dynein 14 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	DC	129	Total	C	N	O	S	0	0
			999	647	163	185	4		
63	Dc	129	Total	C	N	O	S	0	0
			999	647	163	185	4		
63	HB	129	Total	C	N	O	S	0	0
			999	647	163	185	4		
63	Ly	129	Total	C	N	O	S	0	0
			999	647	163	185	4		

- Molecule 64 is a protein called Dynein 16 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	DO	156	Total	C	N	O	S	0	0
			1217	763	215	232	7		
64	Dn	156	Total	C	N	O	S	0	0
			1217	763	215	232	7		
64	Gu	156	Total	C	N	O	S	0	0
			1217	763	215	232	7		
64	Ls	156	Total	C	N	O	S	0	0
			1217	763	215	232	7		

- Molecule 65 is a protein called FAP44.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Do	1542	Total	C	N	O	S	0	0
			11463	7132	2104	2195	32		
65	MP	94	Total	C	N	O	S	0	0
			749	456	143	148	2		

- Molecule 66 is a protein called FAP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Dp	1611	Total	C	N	O	S	0	0
			11683	7241	2168	2226	48		
66	MQ	116	Total	C	N	O	S	0	0
			939	576	189	171	3		

- Molecule 67 is a protein called Dynein regulatory complex protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	EA	585	Total	C	N	O	S	0	0
			4819	2976	891	937	15		

- Molecule 68 is a protein called Dynein regulatory complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	EB	459	Total	C	N	O	S	0	0
			3783	2333	708	726	16		

- Molecule 69 is a protein called Dynein regulatory complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	EM	208	Total	C	N	O	S	0	0
			1608	1011	280	307	10		

- Molecule 70 is a protein called Dynein regulatory complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	EN	447	Total	C	N	O	S	0	0
			3721	2320	667	723	11		
70	EO	466	Total	C	N	O	S	0	0
			3839	2390	688	750	11		

- Molecule 71 is a protein called Dynein regulatory complex protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	EZ	166	Total	C	N	O	S	0	0
			1312	823	230	253	6		
71	HF	166	Total	C	N	O	S	0	0
			1311	823	230	252	6		
71	HM	166	Total	C	N	O	S	0	0
			1311	823	230	252	6		

- Molecule 72 is a protein called ATPase AAA-type core domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	Ea	836	6655	4204	1201	1217	33	0	0

- Molecule 73 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	Eb	1355	10789	6774	1945	2027	43	0	0

- Molecule 74 is a protein called Dynein regulatory complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	Em	524	4240	2641	731	850	18	0	0

- Molecule 75 is a protein called Dynein regulatory complex protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	En	406	3244	2003	604	619	18	0	0

- Molecule 76 is a protein called Dynein regulatory complex protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	Ey	356	2879	1768	540	568	3	0	0

- Molecule 77 is a protein called DRC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	Ez	390	3047	1900	556	572	19	0	0

- Molecule 78 is a protein called DUF4201 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	F4	347	2762	1710	503	539	10	0	0

- Molecule 79 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	FO	163	Total	C	N	O	S	0	0
			1277	782	210	275	10		
79	JC	143	Total	C	N	O	S	0	0
			737	443	144	148	2		

- Molecule 80 is a protein called Caltractin.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	FZ	169	Total	C	N	O	S	0	0
			1360	839	231	282	8		
80	Md	169	Total	C	N	O	S	0	0
			1360	839	231	282	8		
80	MI	151	Total	C	N	O	S	0	0
			1218	752	202	257	7		

- Molecule 81 is a protein called AAA+ ATPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Fm	3953	Total	C	N	O	S	0	0
			31358	19922	5377	5890	169		

- Molecule 82 is a protein called DUF4201 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Fy	317	Total	C	N	O	S	0	0
			2600	1593	492	510	5		

- Molecule 83 is a protein called Cilia- and flagella-associated protein 299.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	GK	237	Total	C	N	O	S	0	0
			1933	1200	346	383	4		

- Molecule 84 is a protein called Cilia- and flagella-associated protein 53.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Gb	270	Total	C	N	O	S	0	0
			2234	1353	440	428	13		
84	Ny	32	Total	C	N	O		0	0
			258	159	51	48			
84	OL	470	Total	C	N	O	S	0	0
			3848	2333	750	744	21		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	ON	470	3848	2333	750	744	21	0	0

- Molecule 85 is a protein called FAP210.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Gc	429	3494	2120	687	677	10	0	0
85	Gm	320	2618	1573	527	511	7	0	0
85	Gn	239	1907	1165	371	364	7	0	0

- Molecule 86 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	Gh	377	2931	1857	494	556	24	0	0
86	JD	377	2930	1857	494	555	24	0	0
86	Km	370	2880	1828	487	542	23	0	0
86	Ld	377	2930	1857	494	555	24	0	0
86	Mc	377	2931	1857	494	556	24	0	0
86	Mk	377	2931	1857	494	556	24	0	0

- Molecule 87 is a protein called Flagellar radial spoke protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
87	H0	483	3644	2330	623	679	12	0	0
87	HZ	483	3644	2330	623	679	12	0	0
87	JT	483	3644	2330	623	679	12	0	0
87	JZ	483	3644	2330	623	679	12	0	0

- Molecule 88 is a protein called Flagellar radial spoke protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
88	HX	749	Total	C	N	O	S	0	0
			5698	3611	962	1111	14		
88	Hh	749	Total	C	N	O	S	0	0
			5698	3611	962	1111	14		
88	JH	749	Total	C	N	O	S	0	0
			5698	3611	962	1111	14		
88	JM	749	Total	C	N	O	S	0	0
			5698	3611	962	1111	14		

- Molecule 89 is a protein called Flagellar radial spoke protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
89	Hi	427	Total	C	N	O	S	0	0
			3248	2048	577	614	9		
89	Hm	427	Total	C	N	O	S	0	0
			3248	2048	577	614	9		
89	JN	427	Total	C	N	O	S	0	0
			3248	2048	577	614	9		
89	JO	427	Total	C	N	O	S	0	0
			3248	2048	577	614	9		

- Molecule 90 is a protein called Radial spoke protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
90	Ho	290	Total	C	N	O	S	0	0
			2170	1342	402	417	9		
90	Hs	287	Total	C	N	O	S	0	0
			2163	1337	399	418	9		
90	JP	310	Total	C	N	O	S	0	0
			2418	1506	430	473	9		
90	JQ	331	Total	C	N	O	S	0	0
			2583	1607	457	510	9		

- Molecule 91 is a protein called Radial spoke protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
91	Hx	421	Total	C	N	O	S	0	0
			3207	2043	535	621	8		
91	Hy	421	Total	C	N	O	S	0	0
			3207	2043	535	621	8		
91	JR	421	Total	C	N	O	S	0	0
			3207	2043	535	621	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
91	JS	421	Total	C	N	O	S	0	0
			3207	2043	535	621	8		

- Molecule 92 is a protein called Flagellar radial spoke protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
92	IA	428	Total	C	N	O	S	0	0
			3214	2043	544	614	13		
92	IB	428	Total	C	N	O	S	0	0
			3214	2043	544	614	13		
92	Ja	428	Total	C	N	O	S	0	0
			3214	2043	544	614	13		
92	Jb	428	Total	C	N	O	S	0	0
			3214	2043	544	614	13		

- Molecule 93 is a protein called Radial spoke protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
93	IC	47	Total	C	N	O	S	0	0
			373	243	62	67	1		
93	IE	40	Total	C	N	O		0	0
			316	208	53	55			
93	KD	44	Total	C	N	O		0	0
			353	232	59	62			
93	KE	40	Total	C	N	O		0	0
			316	208	53	55			

- Molecule 94 is a protein called Radial spoke protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
94	IF	249	Total	C	N	O	S	0	0
			1930	1233	327	365	5		
94	II	249	Total	C	N	O	S	0	0
			1930	1233	327	365	5		
94	IJ	249	Total	C	N	O	S	0	0
			1930	1233	327	365	5		
94	IN	249	Total	C	N	O	S	0	0
			1930	1233	327	365	5		
94	Jc	249	Total	C	N	O	S	0	0
			1930	1233	327	365	5		
94	Jd	249	Total	C	N	O	S	0	0
			1930	1233	327	365	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
94	Je	249	Total	C	N	O	S	0	0
			1930	1233	327	365	5		
94	Jf	249	Total	C	N	O	S	0	0
			1930	1233	327	365	5		

- Molecule 95 is a protein called Radial spoke protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
95	IO	199	Total	C	N	O	S	0	0
			1530	977	257	287	9		
95	IP	199	Total	C	N	O	S	0	0
			1530	977	257	287	9		
95	Jg	199	Total	C	N	O	S	0	0
			1530	977	257	287	9		
95	Jm	199	Total	C	N	O	S	0	0
			1530	977	257	287	9		

- Molecule 96 is a protein called Radial spoke protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
96	IQ	48	Total	C	N	O	S	0	0
			382	250	64	67	1		
96	IR	182	Total	C	N	O	S	0	0
			1055	649	198	206	2		
96	KF	49	Total	C	N	O	S	0	0
			391	255	65	70	1		
96	KG	160	Total	C	N	O		0	0
			891	544	172	175			

- Molecule 97 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
97	IS	163	Total	C	N	O	S	0	0
			1241	796	210	231	4		
97	Jn	163	Total	C	N	O	S	0	0
			1241	796	210	231	4		

- Molecule 98 is a protein called Radial spoke protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
98	IT	379	Total	C	N	O	S	0	0
			2787	1753	506	518	10		

- Molecule 99 is a protein called Radial spoke protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
99	IU	213	Total	C	N	O	S	0	0
			1693	1092	296	301	4		
99	Ia	213	Total	C	N	O	S	0	0
			1693	1092	296	301	4		
99	Ih	64	Total	C	N	O	S	0	0
			528	335	90	100	3		
99	In	64	Total	C	N	O	S	0	0
			528	335	90	100	3		
99	Jo	213	Total	C	N	O	S	0	0
			1693	1092	296	301	4		
99	Jp	213	Total	C	N	O	S	0	0
			1693	1092	296	301	4		
99	KA	64	Total	C	N	O	S	0	0
			528	335	90	100	3		
99	KB	64	Total	C	N	O	S	0	0
			528	335	90	100	3		

- Molecule 100 is a protein called UNKNOWN.

Mol	Chain	Residues	Atoms				AltConf	Trace
100	Ib	34	Total	C	N	O	0	0
			170	102	34	34		

- Molecule 101 is a protein called Nucleoside diphosphate kinase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
101	Ic	201	Total	C	N	O	S	0	0
			1558	1010	267	276	5		
101	Id	201	Total	C	N	O	S	0	0
			1558	1010	267	276	5		
101	Jq	201	Total	C	N	O	S	0	0
			1558	1010	267	276	5		
101	Jr	201	Total	C	N	O	S	0	0
			1558	1010	267	276	5		

- Molecule 102 is a protein called Cytochrome b5 heme-binding domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
102	Ie	213	Total	C	N	O	S	0	0
			1756	1130	299	320	7		
102	Js	213	Total	C	N	O	S	0	0
			1756	1130	299	320	7		

- Molecule 103 is a protein called FAP385.

Mol	Chain	Residues	Atoms					AltConf	Trace
103	If	50	Total	C	N	O	S	0	0
			427	273	73	78	3		
103	Ig	50	Total	C	N	O	S	0	0
			427	273	73	78	3		
103	Jt	50	Total	C	N	O	S	0	0
			427	273	73	78	3		
103	Jz	50	Total	C	N	O	S	0	0
			427	273	73	78	3		

- Molecule 104 is a protein called FAP207.

Mol	Chain	Residues	Atoms					AltConf	Trace
104	JA	184	Total	C	N	O		0	0
			887	519	184	184			
104	Ka	204	Total	C	N	O	S	0	0
			1639	1029	294	310	6		

- Molecule 105 is a protein called FAP253.

Mol	Chain	Residues	Atoms				AltConf	Trace
105	JB	290	Total	C	N	O	0	0
			1441	861	290	290		

- Molecule 106 is a protein called 28 kDa inner dynein arm light chain, axonemal.

Mol	Chain	Residues	Atoms					AltConf	Trace
106	JE	204	Total	C	N	O	S	0	0
			1663	1037	292	327	7		
106	JF	202	Total	C	N	O	S	0	0
			1656	1033	291	325	7		
106	Kn	202	Total	C	N	O	S	0	0
			1665	1037	295	327	6		
106	Ko	202	Total	C	N	O	S	0	0
			1666	1043	294	323	6		
106	La	212	Total	C	N	O	S	0	0
			1741	1090	305	339	7		
106	Lb	212	Total	C	N	O	S	0	0
			1741	1090	305	339	7		

- Molecule 107 is a protein called AAA+ ATPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
107	JG	4016	31543	20072	5418	5886	167	0	0

- Molecule 108 is a protein called UNKNOWN.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
108	KC	72	360	216	72	72	0	0

- Molecule 109 is a protein called Radial spoke protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
109	KZ	327	2438	1529	434	465	10	0	0

- Molecule 110 is a protein called Radial spike protein 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
110	Kb	307	1516	902	307	307	0	0

- Molecule 111 is a protein called DHC\_N2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
111	Kg	3950	31252	19918	5344	5825	165	0	0

- Molecule 112 is a protein called Flagellar-associated protein 59.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
112	Kp	410	3379	2066	639	662	12	0	0
112	LR	416	3346	2054	639	645	8	0	0

- Molecule 113 is a protein called Flagellar-associated protein 172.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
113	Kq	426	3398	2082	627	682	7	0	0
113	LS	420	3329	2034	625	659	11	0	0

- Molecule 114 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
114	LO	1132	8687	5486	1540	1599	62	0	0

- Molecule 115 is a protein called Cilia- and flagella-associated protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
115	LP	543	4527	2813	818	882	14	0	0
115	LQ	537	4478	2785	808	872	13	0	0

- Molecule 116 is a protein called FAP251.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
116	LY	906	6866	4326	1202	1313	25	0	0

- Molecule 117 is a protein called Cilia- and flagella-associated protein 61.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
117	LZ	1099	8237	5184	1431	1580	42	0	0

- Molecule 118 is a protein called DHC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
118	Lc	4049	32022	20394	5454	5998	176	0	0

- Molecule 119 is a protein called Subunit of axonemal inner dynein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
119	Le	380	2873	1821	494	542	16	0	0

- Molecule 120 is a protein called Subunit of axonemal inner dynein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
120	Lf	396	3032	1885	542	588	17	0	0

- Molecule 121 is a protein called CFAP91 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
121	Lg	349	2760	1707	524	523	6	0	0

- Molecule 122 is a protein called AAA+ ATPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
122	Me	3936	30885	19642	5311	5753	179	0	0

- Molecule 123 is a protein called AAA+ ATPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
123	Mm	3942	31070	19760	5327	5794	189	0	0

- Molecule 124 is a protein called Cilia- and flagella-associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
124	za	106	809	513	145	147	4	0	0
124	zb	205	1586	1009	281	289	7	0	0
124	zc	205	1586	1009	281	289	7	0	0
124	zd	205	1586	1009	281	289	7	0	0
124	ze	205	1586	1009	281	289	7	0	0
124	zf	205	1586	1009	281	289	7	0	0
124	zg	205	1586	1009	281	289	7	0	0
124	zh	205	1586	1009	281	289	7	0	0
124	zi	20	169	109	28	31	1	0	0

- Molecule 125 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
125	zj	170	Total	C	N	O	0	0
			1360	861	241	258		
125	zk	54	Total	C	N	O	0	0
			440	276	82	82		
125	zl	170	Total	C	N	O	0	0
			1360	861	241	258		

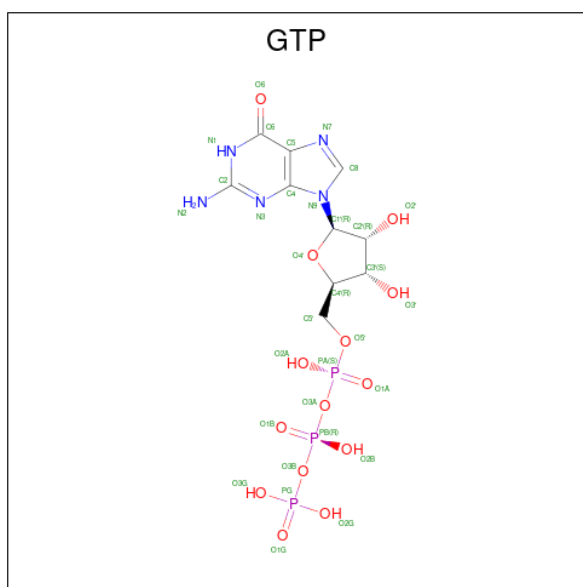
- Molecule 126 is a protein called Flagellar associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
126	zr	119	Total	C	N	O	S	0	0
			951	596	168	182	5		
126	zs	119	Total	C	N	O	S	0	0
			951	596	168	182	5		

- Molecule 127 is a protein called FAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
127	zt	194	Total	C	N	O	S	0	0
			1509	942	278	281	8		
127	zu	194	Total	C	N	O	S	0	0
			1509	942	278	281	8		
127	zv	194	Total	C	N	O	S	0	0
			1509	942	278	281	8		
127	zw	194	Total	C	N	O	S	0	0
			1509	942	278	281	8		
127	zx	194	Total	C	N	O	S	0	0
			1509	942	278	281	8		
127	zy	194	Total	C	N	O	S	0	0
			1509	942	278	281	8		
127	zz	194	Total	C	N	O	S	0	0
			1509	942	278	281	8		

- Molecule 128 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	0A	1	Total 32	C 10	N 5	O 14	P 3	0
128	0C	1	Total 32	C 10	N 5	O 14	P 3	0
128	0F	1	Total 32	C 10	N 5	O 14	P 3	0
128	0I	1	Total 32	C 10	N 5	O 14	P 3	0
128	0K	1	Total 32	C 10	N 5	O 14	P 3	0
128	0M	1	Total 32	C 10	N 5	O 14	P 3	0
128	0O	1	Total 32	C 10	N 5	O 14	P 3	0
128	0Q	1	Total 32	C 10	N 5	O 14	P 3	0
128	0R	1	Total 32	C 10	N 5	O 14	P 3	0
128	0V	1	Total 32	C 10	N 5	O 14	P 3	0
128	0Y	1	Total 32	C 10	N 5	O 14	P 3	0
128	1A	1	Total 32	C 10	N 5	O 14	P 3	0
128	1C	1	Total 32	C 10	N 5	O 14	P 3	0
128	1D	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	1G	1	Total 32	C 10	N 5	O 14	P 3	0
128	1H	1	Total 32	C 10	N 5	O 14	P 3	0
128	1L	1	Total 32	C 10	N 5	O 14	P 3	0
128	1N	1	Total 32	C 10	N 5	O 14	P 3	0
128	1Q	1	Total 32	C 10	N 5	O 14	P 3	0
128	1S	1	Total 32	C 10	N 5	O 14	P 3	0
128	1T	1	Total 32	C 10	N 5	O 14	P 3	0
128	1W	1	Total 32	C 10	N 5	O 14	P 3	0
128	1X	1	Total 32	C 10	N 5	O 14	P 3	0
128	2A	1	Total 32	C 10	N 5	O 14	P 3	0
128	2C	1	Total 32	C 10	N 5	O 14	P 3	0
128	2E	1	Total 32	C 10	N 5	O 14	P 3	0
128	2G	1	Total 32	C 10	N 5	O 14	P 3	0
128	2I	1	Total 32	C 10	N 5	O 14	P 3	0
128	2K	1	Total 32	C 10	N 5	O 14	P 3	0
128	2L	1	Total 32	C 10	N 5	O 14	P 3	0
128	2Q	1	Total 32	C 10	N 5	O 14	P 3	0
128	2S	1	Total 32	C 10	N 5	O 14	P 3	0
128	2U	1	Total 32	C 10	N 5	O 14	P 3	0
128	2W	1	Total 32	C 10	N 5	O 14	P 3	0
128	2Y	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	3A	1	Total 32	C 10	N 5	O 14	P 3	0
128	3C	1	Total 32	C 10	N 5	O 14	P 3	0
128	3G	1	Total 32	C 10	N 5	O 14	P 3	0
128	3I	1	Total 32	C 10	N 5	O 14	P 3	0
128	3K	1	Total 32	C 10	N 5	O 14	P 3	0
128	3M	1	Total 32	C 10	N 5	O 14	P 3	0
128	3O	1	Total 32	C 10	N 5	O 14	P 3	0
128	3P	1	Total 32	C 10	N 5	O 14	P 3	0
128	3S	1	Total 32	C 10	N 5	O 14	P 3	0
128	8H	1	Total 32	C 10	N 5	O 14	P 3	0
128	8I	1	Total 32	C 10	N 5	O 14	P 3	0
128	8L	1	Total 32	C 10	N 5	O 14	P 3	0
128	8M	1	Total 32	C 10	N 5	O 14	P 3	0
128	A1	1	Total 32	C 10	N 5	O 14	P 3	0
128	A2	1	Total 32	C 10	N 5	O 14	P 3	0
128	A4	1	Total 32	C 10	N 5	O 14	P 3	0
128	A9	1	Total 32	C 10	N 5	O 14	P 3	0
128	AT	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ag	1	Total 32	C 10	N 5	O 14	P 3	0
128	Aj	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ak	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	An	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ao	1	Total 32	C 10	N 5	O 14	P 3	0
128	At	1	Total 32	C 10	N 5	O 14	P 3	0
128	Av	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ay	1	Total 32	C 10	N 5	O 14	P 3	0
128	Az	1	Total 32	C 10	N 5	O 14	P 3	0
128	B0	1	Total 32	C 10	N 5	O 14	P 3	0
128	B2	1	Total 32	C 10	N 5	O 14	P 3	0
128	B5	1	Total 32	C 10	N 5	O 14	P 3	0
128	B7	1	Total 32	C 10	N 5	O 14	P 3	0
128	BB	1	Total 32	C 10	N 5	O 14	P 3	0
128	BG	1	Total 32	C 10	N 5	O 14	P 3	0
128	BH	1	Total 32	C 10	N 5	O 14	P 3	0
128	BJ	1	Total 32	C 10	N 5	O 14	P 3	0
128	BL	1	Total 32	C 10	N 5	O 14	P 3	0
128	BN	1	Total 32	C 10	N 5	O 14	P 3	0
128	BU	1	Total 32	C 10	N 5	O 14	P 3	0
128	BW	1	Total 32	C 10	N 5	O 14	P 3	0
128	BY	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ba	1	Total 32	C 10	N 5	O 14	P 3	0
128	Bb	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	Bf	1	Total 32	C 10	N 5	O 14	P 3	0
128	Bh	1	Total 32	C 10	N 5	O 14	P 3	0
128	Bi	1	Total 32	C 10	N 5	O 14	P 3	0
128	Bl	1	Total 32	C 10	N 5	O 14	P 3	0
128	Bm	1	Total 32	C 10	N 5	O 14	P 3	0
128	Bo	1	Total 32	C 10	N 5	O 14	P 3	0
128	Bu	1	Total 32	C 10	N 5	O 14	P 3	0
128	Bw	1	Total 32	C 10	N 5	O 14	P 3	0
128	By	1	Total 32	C 10	N 5	O 14	P 3	0
128	Bz	1	Total 32	C 10	N 5	O 14	P 3	0
128	C0	1	Total 32	C 10	N 5	O 14	P 3	0
128	C1	1	Total 32	C 10	N 5	O 14	P 3	0
128	C4	1	Total 32	C 10	N 5	O 14	P 3	0
128	C5	1	Total 32	C 10	N 5	O 14	P 3	0
128	C8	1	Total 32	C 10	N 5	O 14	P 3	0
128	C9	1	Total 32	C 10	N 5	O 14	P 3	0
128	CE	1	Total 32	C 10	N 5	O 14	P 3	0
128	CG	1	Total 32	C 10	N 5	O 14	P 3	0
128	CI	1	Total 32	C 10	N 5	O 14	P 3	0
128	CK	1	Total 32	C 10	N 5	O 14	P 3	0
128	CM	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	CR	1	Total 32	C 10	N 5	O 14	P 3	0
128	CS	1	Total 32	C 10	N 5	O 14	P 3	0
128	CU	1	Total 32	C 10	N 5	O 14	P 3	0
128	CX	1	Total 32	C 10	N 5	O 14	P 3	0
128	CZ	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ce	1	Total 32	C 10	N 5	O 14	P 3	0
128	Cg	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ci	1	Total 32	C 10	N 5	O 14	P 3	0
128	Cj	1	Total 32	C 10	N 5	O 14	P 3	0
128	Cm	1	Total 32	C 10	N 5	O 14	P 3	0
128	Cr	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ct	1	Total 32	C 10	N 5	O 14	P 3	0
128	Cv	1	Total 32	C 10	N 5	O 14	P 3	0
128	Cx	1	Total 32	C 10	N 5	O 14	P 3	0
128	Cz	1	Total 32	C 10	N 5	O 14	P 3	0
128	D1	1	Total 32	C 10	N 5	O 14	P 3	0
128	D3	1	Total 32	C 10	N 5	O 14	P 3	0
128	D5	1	Total 32	C 10	N 5	O 14	P 3	0
128	D7	1	Total 32	C 10	N 5	O 14	P 3	0
128	DE	1	Total 32	C 10	N 5	O 14	P 3	0
128	DG	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	DH	1	32	10	5	14	3	0
128	DK	1	32	10	5	14	3	0
128	DM	1	32	10	5	14	3	0
128	DR	1	32	10	5	14	3	0
128	DT	1	32	10	5	14	3	0
128	DV	1	32	10	5	14	3	0
128	DX	1	32	10	5	14	3	0
128	DZ	1	32	10	5	14	3	0
128	De	1	32	10	5	14	3	0
128	Df	1	32	10	5	14	3	0
128	Di	1	32	10	5	14	3	0
128	Dk	1	32	10	5	14	3	0
128	Dm	1	32	10	5	14	3	0
128	Dr	1	32	10	5	14	3	0
128	Dt	1	32	10	5	14	3	0
128	Du	1	32	10	5	14	3	0
128	Dw	1	32	10	5	14	3	0
128	Dz	1	32	10	5	14	3	0
128	E0	1	32	10	5	14	3	0
128	E1	1	32	10	5	14	3	0
128	E4	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	E6	1	Total 32	C 10	N 5	O 14	P 3	0
128	E8	1	Total 32	C 10	N 5	O 14	P 3	0
128	ED	1	Total 32	C 10	N 5	O 14	P 3	0
128	EF	1	Total 32	C 10	N 5	O 14	P 3	0
128	EH	1	Total 32	C 10	N 5	O 14	P 3	0
128	EI	1	Total 32	C 10	N 5	O 14	P 3	0
128	EL	1	Total 32	C 10	N 5	O 14	P 3	0
128	EQ	1	Total 32	C 10	N 5	O 14	P 3	0
128	ER	1	Total 32	C 10	N 5	O 14	P 3	0
128	EU	1	Total 32	C 10	N 5	O 14	P 3	0
128	EV	1	Total 32	C 10	N 5	O 14	P 3	0
128	EY	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ed	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ee	1	Total 32	C 10	N 5	O 14	P 3	0
128	Eh	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ei	1	Total 32	C 10	N 5	O 14	P 3	0
128	El	1	Total 32	C 10	N 5	O 14	P 3	0
128	Eq	1	Total 32	C 10	N 5	O 14	P 3	0
128	Es	1	Total 32	C 10	N 5	O 14	P 3	0
128	Eu	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ew	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	F0	1	Total 32	C 10	N 5	O 14	P 3	0
128	F1	1	Total 32	C 10	N 5	O 14	P 3	0
128	F3	1	Total 32	C 10	N 5	O 14	P 3	0
128	F5	1	Total 32	C 10	N 5	O 14	P 3	0
128	F8	1	Total 32	C 10	N 5	O 14	P 3	0
128	FE	1	Total 32	C 10	N 5	O 14	P 3	0
128	FG	1	Total 32	C 10	N 5	O 14	P 3	0
128	FI	1	Total 32	C 10	N 5	O 14	P 3	0
128	FJ	1	Total 32	C 10	N 5	O 14	P 3	0
128	FQ	1	Total 32	C 10	N 5	O 14	P 3	0
128	FT	1	Total 32	C 10	N 5	O 14	P 3	0
128	FV	1	Total 32	C 10	N 5	O 14	P 3	0
128	FW	1	Total 32	C 10	N 5	O 14	P 3	0
128	Fc	1	Total 32	C 10	N 5	O 14	P 3	0
128	Fe	1	Total 32	C 10	N 5	O 14	P 3	0
128	Fg	1	Total 32	C 10	N 5	O 14	P 3	0
128	Fi	1	Total 32	C 10	N 5	O 14	P 3	0
128	Fk	1	Total 32	C 10	N 5	O 14	P 3	0
128	Fl	1	Total 32	C 10	N 5	O 14	P 3	0
128	Fp	1	Total 32	C 10	N 5	O 14	P 3	0
128	Fr	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	Ft	1	Total 32	C 10	N 5	O 14	P 3	0
128	Fv	1	Total 32	C 10	N 5	O 14	P 3	0
128	Fx	1	Total 32	C 10	N 5	O 14	P 3	0
128	G0	1	Total 32	C 10	N 5	O 14	P 3	0
128	G1	1	Total 32	C 10	N 5	O 14	P 3	0
128	G3	1	Total 32	C 10	N 5	O 14	P 3	0
128	G5	1	Total 32	C 10	N 5	O 14	P 3	0
128	G7	1	Total 32	C 10	N 5	O 14	P 3	0
128	GB	1	Total 32	C 10	N 5	O 14	P 3	0
128	GD	1	Total 32	C 10	N 5	O 14	P 3	0
128	GF	1	Total 32	C 10	N 5	O 14	P 3	0
128	GH	1	Total 32	C 10	N 5	O 14	P 3	0
128	GI	1	Total 32	C 10	N 5	O 14	P 3	0
128	H2	1	Total 32	C 10	N 5	O 14	P 3	0
128	H3	1	Total 32	C 10	N 5	O 14	P 3	0
128	H6	1	Total 32	C 10	N 5	O 14	P 3	0
128	H8	1	Total 32	C 10	N 5	O 14	P 3	0
128	I0	1	Total 32	C 10	N 5	O 14	P 3	0
128	I1	1	Total 32	C 10	N 5	O 14	P 3	0
128	I4	1	Total 32	C 10	N 5	O 14	P 3	0
128	I5	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	I8	1	Total 32	C 10	N 5	O 14	P 3	0
128	IK	1	Total 32	C 10	N 5	O 14	P 3	0
128	IL	1	Total 32	C 10	N 5	O 14	P 3	0
128	IW	1	Total 32	C 10	N 5	O 14	P 3	0
128	IX	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ii	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ik	1	Total 32	C 10	N 5	O 14	P 3	0
128	Iw	1	Total 32	C 10	N 5	O 14	P 3	0
128	Iy	1	Total 32	C 10	N 5	O 14	P 3	0
128	J0	1	Total 32	C 10	N 5	O 14	P 3	0
128	J2	1	Total 32	C 10	N 5	O 14	P 3	0
128	J4	1	Total 32	C 10	N 5	O 14	P 3	0
128	J6	1	Total 32	C 10	N 5	O 14	P 3	0
128	J8	1	Total 32	C 10	N 5	O 14	P 3	0
128	JI	1	Total 32	C 10	N 5	O 14	P 3	0
128	JK	1	Total 32	C 10	N 5	O 14	P 3	0
128	JU	1	Total 32	C 10	N 5	O 14	P 3	0
128	JW	1	Total 32	C 10	N 5	O 14	P 3	0
128	JX	1	Total 32	C 10	N 5	O 14	P 3	0
128	Jh	1	Total 32	C 10	N 5	O 14	P 3	0
128	Jj	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	Jl	1	Total 32	C 10	N 5	O 14	P 3	0
128	Jw	1	Total 32	C 10	N 5	O 14	P 3	0
128	Jy	1	Total 32	C 10	N 5	O 14	P 3	0
128	K0	1	Total 32	C 10	N 5	O 14	P 3	0
128	K4	1	Total 32	C 10	N 5	O 14	P 3	0
128	K6	1	Total 32	C 10	N 5	O 14	P 3	0
128	K7	1	Total 32	C 10	N 5	O 14	P 3	0
128	K9	1	Total 32	C 10	N 5	O 14	P 3	0
128	KH	1	Total 32	C 10	N 5	O 14	P 3	0
128	KI	1	Total 32	C 10	N 5	O 14	P 3	0
128	KL	1	Total 32	C 10	N 5	O 14	P 3	0
128	KU	1	Total 32	C 10	N 5	O 14	P 3	0
128	KW	1	Total 32	C 10	N 5	O 14	P 3	0
128	KY	1	Total 32	C 10	N 5	O 14	P 3	0
128	Kj	1	Total 32	C 10	N 5	O 14	P 3	0
128	Kl	1	Total 32	C 10	N 5	O 14	P 3	0
128	Kv	1	Total 32	C 10	N 5	O 14	P 3	0
128	Kx	1	Total 32	C 10	N 5	O 14	P 3	0
128	L2	1	Total 32	C 10	N 5	O 14	P 3	0
128	L4	1	Total 32	C 10	N 5	O 14	P 3	0
128	L6	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	LH	1	Total 32	C 10	N 5	O 14	P 3	0
128	LJ	1	Total 32	C 10	N 5	O 14	P 3	0
128	LU	1	Total 32	C 10	N 5	O 14	P 3	0
128	LX	1	Total 32	C 10	N 5	O 14	P 3	0
128	Lh	1	Total 32	C 10	N 5	O 14	P 3	0
128	Li	1	Total 32	C 10	N 5	O 14	P 3	0
128	Lu	1	Total 32	C 10	N 5	O 14	P 3	0
128	Lv	1	Total 32	C 10	N 5	O 14	P 3	0
128	M0	1	Total 32	C 10	N 5	O 14	P 3	0
128	M2	1	Total 32	C 10	N 5	O 14	P 3	0
128	M4	1	Total 32	C 10	N 5	O 14	P 3	0
128	M6	1	Total 32	C 10	N 5	O 14	P 3	0
128	M7	1	Total 32	C 10	N 5	O 14	P 3	0
128	MG	1	Total 32	C 10	N 5	O 14	P 3	0
128	MH	1	Total 32	C 10	N 5	O 14	P 3	0
128	MT	1	Total 32	C 10	N 5	O 14	P 3	0
128	MV	1	Total 32	C 10	N 5	O 14	P 3	0
128	Mg	1	Total 32	C 10	N 5	O 14	P 3	0
128	Mh	1	Total 32	C 10	N 5	O 14	P 3	0
128	Mt	1	Total 32	C 10	N 5	O 14	P 3	0
128	Mu	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	N0	1	Total 32	C 10	N 5	O 14	P 3	0
128	N1	1	Total 32	C 10	N 5	O 14	P 3	0
128	N6	1	Total 32	C 10	N 5	O 14	P 3	0
128	N8	1	Total 32	C 10	N 5	O 14	P 3	0
128	NF	1	Total 32	C 10	N 5	O 14	P 3	0
128	NH	1	Total 32	C 10	N 5	O 14	P 3	0
128	NJ	1	Total 32	C 10	N 5	O 14	P 3	0
128	NS	1	Total 32	C 10	N 5	O 14	P 3	0
128	NU	1	Total 32	C 10	N 5	O 14	P 3	0
128	NW	1	Total 32	C 10	N 5	O 14	P 3	0
128	Nf	1	Total 32	C 10	N 5	O 14	P 3	0
128	Nh	1	Total 32	C 10	N 5	O 14	P 3	0
128	Ni	1	Total 32	C 10	N 5	O 14	P 3	0
128	O0	1	Total 32	C 10	N 5	O 14	P 3	0
128	O2	1	Total 32	C 10	N 5	O 14	P 3	0
128	O4	1	Total 32	C 10	N 5	O 14	P 3	0
128	O6	1	Total 32	C 10	N 5	O 14	P 3	0
128	O8	1	Total 32	C 10	N 5	O 14	P 3	0
128	P4	1	Total 32	C 10	N 5	O 14	P 3	0
128	P6	1	Total 32	C 10	N 5	O 14	P 3	0
128	P8	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
128	P9	1	Total 32	C 10	N 5	O 14	P 3	0
128	Q2	1	Total 32	C 10	N 5	O 14	P 3	0
128	Q4	1	Total 32	C 10	N 5	O 14	P 3	0
128	Q6	1	Total 32	C 10	N 5	O 14	P 3	0
128	R0	1	Total 32	C 10	N 5	O 14	P 3	0
128	R2	1	Total 32	C 10	N 5	O 14	P 3	0
128	R4	1	Total 32	C 10	N 5	O 14	P 3	0
128	R6	1	Total 32	C 10	N 5	O 14	P 3	0
128	R8	1	Total 32	C 10	N 5	O 14	P 3	0
128	S0	1	Total 32	C 10	N 5	O 14	P 3	0
128	S2	1	Total 32	C 10	N 5	O 14	P 3	0
128	S5	1	Total 32	C 10	N 5	O 14	P 3	0
128	S8	1	Total 32	C 10	N 5	O 14	P 3	0
128	S9	1	Total 32	C 10	N 5	O 14	P 3	0
128	T2	1	Total 32	C 10	N 5	O 14	P 3	0
128	T4	1	Total 32	C 10	N 5	O 14	P 3	0
128	T6	1	Total 32	C 10	N 5	O 14	P 3	0
128	T8	1	Total 32	C 10	N 5	O 14	P 3	0
128	U2	1	Total 32	C 10	N 5	O 14	P 3	0
128	U4	1	Total 32	C 10	N 5	O 14	P 3	0
128	U6	1	Total 32	C 10	N 5	O 14	P 3	0

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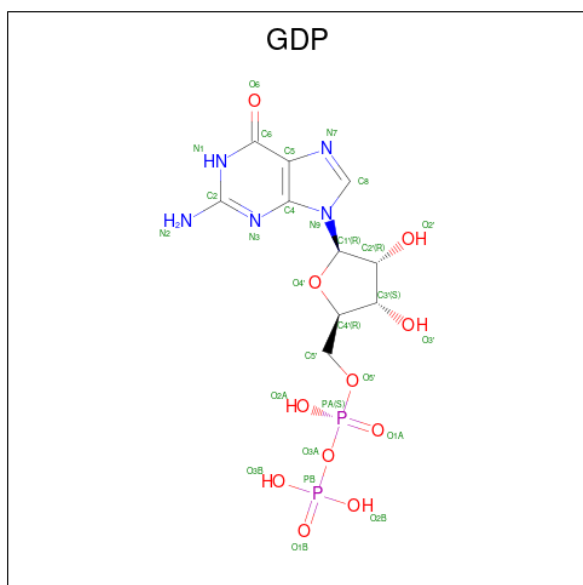
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
128	U7	1	32	10	5	14	3	0
128	U9	1	32	10	5	14	3	0
128	V2	1	32	10	5	14	3	0
128	V3	1	32	10	5	14	3	0
128	V8	1	32	10	5	14	3	0
128	W0	1	32	10	5	14	3	0
128	W2	1	32	10	5	14	3	0
128	W4	1	32	10	5	14	3	0
128	W5	1	32	10	5	14	3	0
128	W8	1	32	10	5	14	3	0
128	X0	1	32	10	5	14	3	0
128	X4	1	32	10	5	14	3	0
128	X6	1	32	10	5	14	3	0
128	X7	1	32	10	5	14	3	0
128	Y0	1	32	10	5	14	3	0
128	Y1	1	32	10	5	14	3	0
128	Y4	1	32	10	5	14	3	0
128	Y6	1	32	10	5	14	3	0
128	Z0	1	32	10	5	14	3	0
128	Z2	1	32	10	5	14	3	0
128	Z3	1	32	10	5	14	3	0

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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
128	Z6	1	Total	C	N	O	P	0
			32	10	5	14	3	
128	Z7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 129 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
129	0A	1	Total	C	N	O	P	0
			28	10	5	11	2	
129	0C	1	Total	C	N	O	P	0
			28	10	5	11	2	
129	0E	1	Total	C	N	O	P	0
			28	10	5	11	2	
129	0G	1	Total	C	N	O	P	0
			28	10	5	11	2	
129	0I	1	Total	C	N	O	P	0
			28	10	5	11	2	
129	0K	1	Total	C	N	O	P	0
			28	10	5	11	2	
129	0M	1	Total	C	N	O	P	0
			28	10	5	11	2	
129	0O	1	Total	C	N	O	P	0
			28	10	5	11	2	
129	0Q	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	0S	1	Total 28	C 10	N 5	O 11	P 2	0
129	0U	1	Total 28	C 10	N 5	O 11	P 2	0
129	0W	1	Total 28	C 10	N 5	O 11	P 2	0
129	0Y	1	Total 28	C 10	N 5	O 11	P 2	0
129	1A	1	Total 28	C 10	N 5	O 11	P 2	0
129	1C	1	Total 28	C 10	N 5	O 11	P 2	0
129	1E	1	Total 28	C 10	N 5	O 11	P 2	0
129	1G	1	Total 28	C 10	N 5	O 11	P 2	0
129	1K	1	Total 28	C 10	N 5	O 11	P 2	0
129	1M	1	Total 28	C 10	N 5	O 11	P 2	0
129	1O	1	Total 28	C 10	N 5	O 11	P 2	0
129	1Q	1	Total 28	C 10	N 5	O 11	P 2	0
129	1S	1	Total 28	C 10	N 5	O 11	P 2	0
129	1U	1	Total 28	C 10	N 5	O 11	P 2	0
129	1W	1	Total 28	C 10	N 5	O 11	P 2	0
129	2A	1	Total 28	C 10	N 5	O 11	P 2	0
129	2C	1	Total 28	C 10	N 5	O 11	P 2	0
129	2E	1	Total 28	C 10	N 5	O 11	P 2	0
129	2G	1	Total 28	C 10	N 5	O 11	P 2	0
129	2I	1	Total 28	C 10	N 5	O 11	P 2	0
129	2K	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	2M	1	Total 28	C 10	N 5	O 11	P 2	0
129	2Q	1	Total 28	C 10	N 5	O 11	P 2	0
129	2S	1	Total 28	C 10	N 5	O 11	P 2	0
129	2U	1	Total 28	C 10	N 5	O 11	P 2	0
129	2W	1	Total 28	C 10	N 5	O 11	P 2	0
129	2Y	1	Total 28	C 10	N 5	O 11	P 2	0
129	3A	1	Total 28	C 10	N 5	O 11	P 2	0
129	3C	1	Total 28	C 10	N 5	O 11	P 2	0
129	3G	1	Total 28	C 10	N 5	O 11	P 2	0
129	3I	1	Total 28	C 10	N 5	O 11	P 2	0
129	3K	1	Total 28	C 10	N 5	O 11	P 2	0
129	3M	1	Total 28	C 10	N 5	O 11	P 2	0
129	3O	1	Total 28	C 10	N 5	O 11	P 2	0
129	3Q	1	Total 28	C 10	N 5	O 11	P 2	0
129	3S	1	Total 28	C 10	N 5	O 11	P 2	0
129	8H	1	Total 28	C 10	N 5	O 11	P 2	0
129	8J	1	Total 28	C 10	N 5	O 11	P 2	0
129	8L	1	Total 28	C 10	N 5	O 11	P 2	0
129	8N	1	Total 28	C 10	N 5	O 11	P 2	0
129	A1	1	Total 28	C 10	N 5	O 11	P 2	0
129	A3	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	A5	1	28	10	5	11	2	0
129	A6	1	28	10	5	11	2	0
129	A7	1	28	10	5	11	2	0
129	A9	1	28	10	5	11	2	0
129	AJ	1	28	10	5	11	2	0
129	Ah	1	28	10	5	11	2	0
129	Aj	1	28	10	5	11	2	0
129	Al	1	28	10	5	11	2	0
129	An	1	28	10	5	11	2	0
129	Ap	1	28	10	5	11	2	0
129	Au	1	28	10	5	11	2	0
129	Aw	1	28	10	5	11	2	0
129	Ay	1	28	10	5	11	2	0
129	B1	1	28	10	5	11	2	0
129	B3	1	28	10	5	11	2	0
129	B5	1	28	10	5	11	2	0
129	B6	1	28	10	5	11	2	0
129	B8	1	28	10	5	11	2	0
129	BB	1	28	10	5	11	2	0
129	BG	1	28	10	5	11	2	0
129	BI	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	BK	1	28	10	5	11	2	0
129	BM	1	28	10	5	11	2	0
129	BO	1	28	10	5	11	2	0
129	BS	1	28	10	5	11	2	0
129	BU	1	28	10	5	11	2	0
129	BW	1	28	10	5	11	2	0
129	BY	1	28	10	5	11	2	0
129	Ba	1	28	10	5	11	2	0
129	Bf	1	28	10	5	11	2	0
129	Bh	1	28	10	5	11	2	0
129	Bj	1	28	10	5	11	2	0
129	Bl	1	28	10	5	11	2	0
129	Bn	1	28	10	5	11	2	0
129	Bs	1	28	10	5	11	2	0
129	Bu	1	28	10	5	11	2	0
129	Bw	1	28	10	5	11	2	0
129	By	1	28	10	5	11	2	0
129	C0	1	28	10	5	11	2	0
129	C2	1	28	10	5	11	2	0
129	C4	1	28	10	5	11	2	0
129	C6	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	C8	1	Total 28	C 10	N 5	O 11	P 2	0
129	CE	1	Total 28	C 10	N 5	O 11	P 2	0
129	CG	1	Total 28	C 10	N 5	O 11	P 2	0
129	CI	1	Total 28	C 10	N 5	O 11	P 2	0
129	CK	1	Total 28	C 10	N 5	O 11	P 2	0
129	CM	1	Total 28	C 10	N 5	O 11	P 2	0
129	CR	1	Total 28	C 10	N 5	O 11	P 2	0
129	CT	1	Total 28	C 10	N 5	O 11	P 2	0
129	CV	1	Total 28	C 10	N 5	O 11	P 2	0
129	CX	1	Total 28	C 10	N 5	O 11	P 2	0
129	CZ	1	Total 28	C 10	N 5	O 11	P 2	0
129	Ce	1	Total 28	C 10	N 5	O 11	P 2	0
129	Cg	1	Total 28	C 10	N 5	O 11	P 2	0
129	Ci	1	Total 28	C 10	N 5	O 11	P 2	0
129	Ck	1	Total 28	C 10	N 5	O 11	P 2	0
129	Cm	1	Total 28	C 10	N 5	O 11	P 2	0
129	Cr	1	Total 28	C 10	N 5	O 11	P 2	0
129	Ct	1	Total 28	C 10	N 5	O 11	P 2	0
129	Cv	1	Total 28	C 10	N 5	O 11	P 2	0
129	Cx	1	Total 28	C 10	N 5	O 11	P 2	0
129	Cz	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	D0	1	28	10	5	11	2	0
129	D2	1	28	10	5	11	2	0
129	D4	1	28	10	5	11	2	0
129	D6	1	28	10	5	11	2	0
129	D8	1	28	10	5	11	2	0
129	DE	1	28	10	5	11	2	0
129	DG	1	28	10	5	11	2	0
129	DI	1	28	10	5	11	2	0
129	DK	1	28	10	5	11	2	0
129	DM	1	28	10	5	11	2	0
129	DR	1	28	10	5	11	2	0
129	DT	1	28	10	5	11	2	0
129	DV	1	28	10	5	11	2	0
129	DX	1	28	10	5	11	2	0
129	DZ	1	28	10	5	11	2	0
129	De	1	28	10	5	11	2	0
129	Dg	1	28	10	5	11	2	0
129	Di	1	28	10	5	11	2	0
129	Dk	1	28	10	5	11	2	0
129	Dm	1	28	10	5	11	2	0
129	Dr	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	Dt	1	Total 28	C 10	N 5	O 11	P 2	0
129	Dv	1	Total 28	C 10	N 5	O 11	P 2	0
129	Dx	1	Total 28	C 10	N 5	O 11	P 2	0
129	Dz	1	Total 28	C 10	N 5	O 11	P 2	0
129	E0	1	Total 28	C 10	N 5	O 11	P 2	0
129	E2	1	Total 28	C 10	N 5	O 11	P 2	0
129	E4	1	Total 28	C 10	N 5	O 11	P 2	0
129	E6	1	Total 28	C 10	N 5	O 11	P 2	0
129	E8	1	Total 28	C 10	N 5	O 11	P 2	0
129	ED	1	Total 28	C 10	N 5	O 11	P 2	0
129	EF	1	Total 28	C 10	N 5	O 11	P 2	0
129	EH	1	Total 28	C 10	N 5	O 11	P 2	0
129	EJ	1	Total 28	C 10	N 5	O 11	P 2	0
129	EL	1	Total 28	C 10	N 5	O 11	P 2	0
129	EQ	1	Total 28	C 10	N 5	O 11	P 2	0
129	ES	1	Total 28	C 10	N 5	O 11	P 2	0
129	EU	1	Total 28	C 10	N 5	O 11	P 2	0
129	EW	1	Total 28	C 10	N 5	O 11	P 2	0
129	EY	1	Total 28	C 10	N 5	O 11	P 2	0
129	Ed	1	Total 28	C 10	N 5	O 11	P 2	0
129	Ef	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	Eh	1	Total 28	C 10	N 5	O 11	P 2	0
129	Ej	1	Total 28	C 10	N 5	O 11	P 2	0
129	El	1	Total 28	C 10	N 5	O 11	P 2	0
129	Eq	1	Total 28	C 10	N 5	O 11	P 2	0
129	Es	1	Total 28	C 10	N 5	O 11	P 2	0
129	Eu	1	Total 28	C 10	N 5	O 11	P 2	0
129	Ew	1	Total 28	C 10	N 5	O 11	P 2	0
129	F0	1	Total 28	C 10	N 5	O 11	P 2	0
129	F2	1	Total 28	C 10	N 5	O 11	P 2	0
129	F6	1	Total 28	C 10	N 5	O 11	P 2	0
129	F8	1	Total 28	C 10	N 5	O 11	P 2	0
129	FC	1	Total 28	C 10	N 5	O 11	P 2	0
129	FE	1	Total 28	C 10	N 5	O 11	P 2	0
129	FG	1	Total 28	C 10	N 5	O 11	P 2	0
129	FI	1	Total 28	C 10	N 5	O 11	P 2	0
129	FK	1	Total 28	C 10	N 5	O 11	P 2	0
129	FP	1	Total 28	C 10	N 5	O 11	P 2	0
129	FR	1	Total 28	C 10	N 5	O 11	P 2	0
129	FT	1	Total 28	C 10	N 5	O 11	P 2	0
129	FV	1	Total 28	C 10	N 5	O 11	P 2	0
129	FX	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	Fc	1	Total 28	C 10	N 5	O 11	P 2	0
129	Fe	1	Total 28	C 10	N 5	O 11	P 2	0
129	Fg	1	Total 28	C 10	N 5	O 11	P 2	0
129	Fi	1	Total 28	C 10	N 5	O 11	P 2	0
129	Fk	1	Total 28	C 10	N 5	O 11	P 2	0
129	Fp	1	Total 28	C 10	N 5	O 11	P 2	0
129	Fr	1	Total 28	C 10	N 5	O 11	P 2	0
129	Ft	1	Total 28	C 10	N 5	O 11	P 2	0
129	Fv	1	Total 28	C 10	N 5	O 11	P 2	0
129	Fx	1	Total 28	C 10	N 5	O 11	P 2	0
129	G0	1	Total 28	C 10	N 5	O 11	P 2	0
129	G2	1	Total 28	C 10	N 5	O 11	P 2	0
129	G4	1	Total 28	C 10	N 5	O 11	P 2	0
129	G6	1	Total 28	C 10	N 5	O 11	P 2	0
129	G8	1	Total 28	C 10	N 5	O 11	P 2	0
129	GB	1	Total 28	C 10	N 5	O 11	P 2	0
129	GD	1	Total 28	C 10	N 5	O 11	P 2	0
129	GF	1	Total 28	C 10	N 5	O 11	P 2	0
129	GH	1	Total 28	C 10	N 5	O 11	P 2	0
129	GJ	1	Total 28	C 10	N 5	O 11	P 2	0
129	H2	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	H4	1	28	10	5	11	2	0
129	H6	1	28	10	5	11	2	0
129	H8	1	28	10	5	11	2	0
129	I0	1	28	10	5	11	2	0
129	I2	1	28	10	5	11	2	0
129	I4	1	28	10	5	11	2	0
129	I8	1	28	10	5	11	2	0
129	IK	1	28	10	5	11	2	0
129	IM	1	28	10	5	11	2	0
129	IW	1	28	10	5	11	2	0
129	IY	1	28	10	5	11	2	0
129	Ij	1	28	10	5	11	2	0
129	Il	1	28	10	5	11	2	0
129	Iw	1	28	10	5	11	2	0
129	Iy	1	28	10	5	11	2	0
129	J0	1	28	10	5	11	2	0
129	J2	1	28	10	5	11	2	0
129	J4	1	28	10	5	11	2	0
129	J6	1	28	10	5	11	2	0
129	J8	1	28	10	5	11	2	0
129	JJ	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	JL	1	28	10	5	11	2	0
129	JU	1	28	10	5	11	2	0
129	JW	1	28	10	5	11	2	0
129	JY	1	28	10	5	11	2	0
129	Jh	1	28	10	5	11	2	0
129	Jj	1	28	10	5	11	2	0
129	Jl	1	28	10	5	11	2	0
129	Ju	1	28	10	5	11	2	0
129	Jw	1	28	10	5	11	2	0
129	Jy	1	28	10	5	11	2	0
129	K0	1	28	10	5	11	2	0
129	K4	1	28	10	5	11	2	0
129	K6	1	28	10	5	11	2	0
129	K8	1	28	10	5	11	2	0
129	KH	1	28	10	5	11	2	0
129	KJ	1	28	10	5	11	2	0
129	KL	1	28	10	5	11	2	0
129	KU	1	28	10	5	11	2	0
129	KW	1	28	10	5	11	2	0
129	KY	1	28	10	5	11	2	0
129	Kh	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	Kj	1	Total 28	C 10	N 5	O 11	P 2	0
129	Kl	1	Total 28	C 10	N 5	O 11	P 2	0
129	Kv	1	Total 28	C 10	N 5	O 11	P 2	0
129	Kx	1	Total 28	C 10	N 5	O 11	P 2	0
129	L0	1	Total 28	C 10	N 5	O 11	P 2	0
129	L2	1	Total 28	C 10	N 5	O 11	P 2	0
129	L4	1	Total 28	C 10	N 5	O 11	P 2	0
129	L6	1	Total 28	C 10	N 5	O 11	P 2	0
129	LH	1	Total 28	C 10	N 5	O 11	P 2	0
129	LJ	1	Total 28	C 10	N 5	O 11	P 2	0
129	LT	1	Total 28	C 10	N 5	O 11	P 2	0
129	LV	1	Total 28	C 10	N 5	O 11	P 2	0
129	LX	1	Total 28	C 10	N 5	O 11	P 2	0
129	Lh	1	Total 28	C 10	N 5	O 11	P 2	0
129	Lj	1	Total 28	C 10	N 5	O 11	P 2	0
129	Lu	1	Total 28	C 10	N 5	O 11	P 2	0
129	Lw	1	Total 28	C 10	N 5	O 11	P 2	0
129	M0	1	Total 28	C 10	N 5	O 11	P 2	0
129	M2	1	Total 28	C 10	N 5	O 11	P 2	0
129	M4	1	Total 28	C 10	N 5	O 11	P 2	0
129	M6	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	M8	1	28	10	5	11	2	0
129	MG	1	28	10	5	11	2	0
129	MI	1	28	10	5	11	2	0
129	MT	1	28	10	5	11	2	0
129	MV	1	28	10	5	11	2	0
129	Mg	1	28	10	5	11	2	0
129	Mi	1	28	10	5	11	2	0
129	Mt	1	28	10	5	11	2	0
129	Mv	1	28	10	5	11	2	0
129	N0	1	28	10	5	11	2	0
129	N2	1	28	10	5	11	2	0
129	N6	1	28	10	5	11	2	0
129	N8	1	28	10	5	11	2	0
129	NF	1	28	10	5	11	2	0
129	NH	1	28	10	5	11	2	0
129	NJ	1	28	10	5	11	2	0
129	NS	1	28	10	5	11	2	0
129	NU	1	28	10	5	11	2	0
129	NW	1	28	10	5	11	2	0
129	Nf	1	28	10	5	11	2	0
129	Nh	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	Nj	1	28	10	5	11	2	0
129	O0	1	28	10	5	11	2	0
129	O2	1	28	10	5	11	2	0
129	O4	1	28	10	5	11	2	0
129	O6	1	28	10	5	11	2	0
129	O8	1	28	10	5	11	2	0
129	P4	1	28	10	5	11	2	0
129	P6	1	28	10	5	11	2	0
129	P8	1	28	10	5	11	2	0
129	Q0	1	28	10	5	11	2	0
129	Q2	1	28	10	5	11	2	0
129	Q4	1	28	10	5	11	2	0
129	Q6	1	28	10	5	11	2	0
129	Q8	1	28	10	5	11	2	0
129	R0	1	28	10	5	11	2	0
129	R2	1	28	10	5	11	2	0
129	R4	1	28	10	5	11	2	0
129	R6	1	28	10	5	11	2	0
129	R8	1	28	10	5	11	2	0
129	S0	1	28	10	5	11	2	0
129	S2	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	S4	1	28	10	5	11	2	0
129	S6	1	28	10	5	11	2	0
129	S8	1	28	10	5	11	2	0
129	T0	1	28	10	5	11	2	0
129	T2	1	28	10	5	11	2	0
129	T4	1	28	10	5	11	2	0
129	T6	1	28	10	5	11	2	0
129	T8	1	28	10	5	11	2	0
129	U2	1	28	10	5	11	2	0
129	U4	1	28	10	5	11	2	0
129	U6	1	28	10	5	11	2	0
129	U8	1	28	10	5	11	2	0
129	V0	1	28	10	5	11	2	0
129	V2	1	28	10	5	11	2	0
129	V4	1	28	10	5	11	2	0
129	V6	1	28	10	5	11	2	0
129	V8	1	28	10	5	11	2	0
129	W0	1	28	10	5	11	2	0
129	W2	1	28	10	5	11	2	0
129	W4	1	28	10	5	11	2	0
129	W6	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
129	W8	1	28	10	5	11	2	0
129	X0	1	28	10	5	11	2	0
129	X2	1	28	10	5	11	2	0
129	X4	1	28	10	5	11	2	0
129	X6	1	28	10	5	11	2	0
129	X8	1	28	10	5	11	2	0
129	Y0	1	28	10	5	11	2	0
129	Y2	1	28	10	5	11	2	0
129	Y4	1	28	10	5	11	2	0
129	Y6	1	28	10	5	11	2	0
129	Y8	1	28	10	5	11	2	0
129	Z0	1	28	10	5	11	2	0
129	Z2	1	28	10	5	11	2	0
129	Z4	1	28	10	5	11	2	0
129	Z6	1	28	10	5	11	2	0
129	Z8	1	28	10	5	11	2	0

- Molecule 130 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	0B	1	1	1	0
130	0F	1	1	1	0
130	0I	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	0J	1	1	1	0
130	0L	1	1	1	0
130	0N	1	1	1	0
130	0Q	1	1	1	0
130	0R	1	1	1	0
130	0V	1	1	1	0
130	0X	1	1	1	0
130	0Z	1	1	1	0
130	1B	1	1	1	0
130	1D	1	1	1	0
130	1F	1	1	1	0
130	1H	2	2	2	0
130	1L	1	1	1	0
130	1N	1	1	1	0
130	1P	1	1	1	0
130	1R	1	1	1	0
130	1T	1	1	1	0
130	1V	1	1	1	0
130	1X	1	1	1	0
130	1Z	1	1	1	0
130	2B	1	1	1	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
130	2D	1	Total 1	Mg 1	0
130	2F	1	Total 1	Mg 1	0
130	2H	1	Total 1	Mg 1	0
130	2J	1	Total 1	Mg 1	0
130	2L	1	Total 1	Mg 1	0
130	2N	1	Total 1	Mg 1	0
130	2P	1	Total 1	Mg 1	0
130	2R	1	Total 1	Mg 1	0
130	2T	1	Total 1	Mg 1	0
130	2V	1	Total 1	Mg 1	0
130	2X	1	Total 1	Mg 1	0
130	2Z	1	Total 1	Mg 1	0
130	3B	1	Total 1	Mg 1	0
130	3D	1	Total 1	Mg 1	0
130	3F	1	Total 1	Mg 1	0
130	3H	1	Total 1	Mg 1	0
130	3J	1	Total 1	Mg 1	0
130	3L	1	Total 1	Mg 1	0
130	3N	1	Total 1	Mg 1	0
130	3P	1	Total 1	Mg 1	0
130	3R	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	3T	1	1	1	0
130	8F	1	1	1	0
130	8I	1	1	1	0
130	8K	1	1	1	0
130	8M	1	1	1	0
130	A0	1	1	1	0
130	A2	1	1	1	0
130	A4	1	1	1	0
130	A8	1	1	1	0
130	AT	1	1	1	0
130	Ag	1	1	1	0
130	Ai	1	1	1	0
130	Ak	1	1	1	0
130	Am	1	1	1	0
130	Ao	1	1	1	0
130	At	1	1	1	0
130	Av	1	1	1	0
130	Ay	1	1	1	0
130	Az	1	1	1	0
130	B0	1	1	1	0
130	B2	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	B4	1	1	1	0
130	B7	1	1	1	0
130	B9	1	1	1	0
130	BA	1	1	1	0
130	BF	1	1	1	0
130	BH	1	1	1	0
130	BJ	1	1	1	0
130	BL	1	1	1	0
130	BN	1	1	1	0
130	BT	1	1	1	0
130	BV	1	1	1	0
130	BX	1	1	1	0
130	BZ	1	1	1	0
130	Bb	1	1	1	0
130	Bg	1	1	1	0
130	Bi	1	1	1	0
130	Bk	1	1	1	0
130	Bm	1	1	1	0
130	Bo	1	1	1	0
130	Bt	1	1	1	0
130	Bw	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	By	1	1	1	0
130	Bz	1	1	1	0
130	C1	1	1	1	0
130	C5	1	1	1	0
130	C7	1	1	1	0
130	C9	1	1	1	0
130	CA	1	1	1	0
130	CE	1	1	1	0
130	CF	1	1	1	0
130	CI	1	1	1	0
130	CJ	1	1	1	0
130	CM	1	1	1	0
130	CN	1	1	1	0
130	CS	1	1	1	0
130	CU	1	1	1	0
130	CW	1	1	1	0
130	CY	1	1	1	0
130	Cf	1	1	1	0
130	Ch	1	1	1	0
130	Cj	1	1	1	0
130	Cl	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	Cs	1	1	1	0
130	Cv	1	1	1	0
130	Cw	1	1	1	0
130	Cy	1	1	1	0
130	D1	1	1	1	0
130	D3	1	1	1	0
130	D5	1	1	1	0
130	D7	1	1	1	0
130	DD	1	1	1	0
130	DF	1	1	1	0
130	DH	1	1	1	0
130	DJ	1	1	1	0
130	DL	1	1	1	0
130	DN	1	1	1	0
130	DQ	1	1	1	0
130	DS	1	1	1	0
130	DU	1	1	1	0
130	DW	1	1	1	0
130	DY	1	1	1	0
130	Da	1	1	1	0
130	Dd	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	Df	1	1	1	0
130	Dh	1	1	1	0
130	Dj	1	1	1	0
130	DI	1	1	1	0
130	Dq	1	1	1	0
130	Ds	1	1	1	0
130	Du	1	1	1	0
130	Dw	1	1	1	0
130	Dy	1	1	1	0
130	E1	1	1	1	0
130	E3	1	1	1	0
130	E5	1	1	1	0
130	E7	1	1	1	0
130	E9	1	1	1	0
130	EC	1	1	1	0
130	EE	1	1	1	0
130	EG	1	1	1	0
130	EI	1	1	1	0
130	EK	1	1	1	0
130	EP	1	1	1	0
130	ER	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	ET	1	1	1	0
130	EV	1	1	1	0
130	EX	1	1	1	0
130	Ec	1	1	1	0
130	Ee	1	1	1	0
130	Eg	1	1	1	0
130	Ei	1	1	1	0
130	Ek	1	1	1	0
130	Ep	1	1	1	0
130	Er	1	1	1	0
130	Et	1	1	1	0
130	Ev	1	1	1	0
130	Ex	1	1	1	0
130	F1	1	1	1	0
130	F3	1	1	1	0
130	F5	1	1	1	0
130	F7	1	1	1	0
130	F9	1	1	1	0
130	FD	1	1	1	0
130	FF	1	1	1	0
130	FH	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	FJ	1	1	1	0
130	FL	1	1	1	0
130	FQ	1	1	1	0
130	FT	1	1	1	0
130	FU	1	1	1	0
130	FW	1	1	1	0
130	FY	1	1	1	0
130	Fd	1	1	1	0
130	Ff	1	1	1	0
130	Fh	1	1	1	0
130	Fj	1	1	1	0
130	Fl	1	1	1	0
130	Fq	1	1	1	0
130	Fs	1	1	1	0
130	Fu	1	1	1	0
130	Fw	1	1	1	0
130	G1	1	1	1	0
130	G3	1	1	1	0
130	G5	1	1	1	0
130	G7	1	1	1	0
130	G9	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	GC	1	1	1	0
130	GE	1	1	1	0
130	GG	1	1	1	0
130	GI	1	1	1	0
130	H1	1	1	1	0
130	H3	1	1	1	0
130	H5	1	1	1	0
130	H8	1	1	1	0
130	H9	1	1	1	0
130	Hu	1	1	1	0
130	I1	1	1	1	0
130	I4	1	1	1	0
130	I5	1	1	1	0
130	I7	1	1	1	0
130	I9	1	1	1	0
130	IL	1	1	1	0
130	IV	1	1	1	0
130	IX	1	1	1	0
130	IZ	1	1	1	0
130	li	1	1	1	0
130	lk	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	Im	1	1	1	0
130	Iv	1	1	1	0
130	Ix	1	1	1	0
130	Iz	1	1	1	0
130	J1	1	1	1	0
130	J3	1	1	1	0
130	J5	1	1	1	0
130	J8	1	1	1	0
130	J9	1	1	1	0
130	JI	1	1	1	0
130	JK	1	1	1	0
130	JU	1	1	1	0
130	JW	1	1	1	0
130	JX	1	1	1	0
130	Jh	1	1	1	0
130	Ji	1	1	1	0
130	Jl	1	1	1	0
130	Jv	1	1	1	0
130	Jx	1	1	1	0
130	K3	1	1	1	0
130	K5	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	K7	1	1	1	0
130	K9	1	1	1	0
130	KI	1	1	1	0
130	KK	1	1	1	0
130	KV	1	1	1	0
130	KX	1	1	1	0
130	Kj	1	1	1	0
130	Kk	1	1	1	0
130	Kv	1	1	1	0
130	Kw	1	1	1	0
130	Ky	1	1	1	0
130	L1	1	1	1	0
130	L3	1	1	1	0
130	L5	1	1	1	0
130	L7	1	1	1	0
130	L9	1	1	1	0
130	LI	1	1	1	0
130	LK	1	1	1	0
130	LU	1	1	1	0
130	LW	1	1	1	0
130	Li	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	Lv	1	1	1	0
130	Lx	1	1	1	0
130	M1	1	1	1	0
130	M3	1	1	1	0
130	M5	1	1	1	0
130	M7	1	1	1	0
130	M9	1	1	1	0
130	MF	1	1	1	0
130	MH	1	1	1	0
130	MS	1	1	1	0
130	MU	1	1	1	0
130	MW	1	1	1	0
130	Mf	1	1	1	0
130	Mh	1	1	1	0
130	Mj	1	1	1	0
130	Ms	1	1	1	0
130	Mu	1	1	1	0
130	Mw	1	1	1	0
130	N1	1	1	1	0
130	N3	1	1	1	0
130	N5	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	N7	1	1	1	0
130	N9	1	1	1	0
130	NG	1	1	1	0
130	NI	1	1	1	0
130	NT	1	1	1	0
130	NV	1	1	1	0
130	Ng	1	1	1	0
130	Ni	1	1	1	0
130	O1	1	1	1	0
130	O4	1	1	1	0
130	O5	1	1	1	0
130	O7	1	1	1	0
130	O9	1	1	1	0
130	P4	1	1	1	0
130	P6	1	1	1	0
130	P7	1	1	1	0
130	P9	1	1	1	0
130	Q1	1	1	1	0
130	Q3	1	1	1	0
130	Q5	1	1	1	0
130	Q9	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	R2	1	1	1	0
130	R3	1	1	1	0
130	R5	1	1	1	0
130	R8	1	1	1	0
130	R9	1	1	1	0
130	S1	1	1	1	0
130	S5	1	1	1	0
130	S7	1	1	1	0
130	S9	1	1	1	0
130	T1	1	1	1	0
130	T3	1	1	1	0
130	T5	1	1	1	0
130	T7	1	1	1	0
130	U1	1	1	1	0
130	U3	1	1	1	0
130	U5	1	1	1	0
130	U8	1	1	1	0
130	U9	1	1	1	0
130	V1	1	1	1	0
130	V3	1	1	1	0
130	V7	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
130	V9	1	1	1	0
130	W1	1	1	1	0
130	W3	1	1	1	0
130	W5	1	1	1	0
130	W7	1	1	1	0
130	W9	1	1	1	0
130	X3	1	1	1	0
130	X5	1	1	1	0
130	X7	1	1	1	0
130	X9	1	1	1	0
130	Y1	1	1	1	0
130	Y3	1	1	1	0
130	Y5	1	1	1	0
130	Y9	1	1	1	0
130	Z1	1	1	1	0
130	Z3	1	1	1	0
130	Z5	1	1	1	0
130	Z7	1	1	1	0
130	Z9	1	1	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, Not provided	
Number of particles used	261585	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	61	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.146	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	772.48, 886.72003, 1296.08	wwPDB
Map dimensions	568, 652, 953	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.3599999	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 1009 ligands modelled in this entry, 338 are monoatomic - leaving 671 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
129	GDP	T4	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	Ij	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	3C	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	2G	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	B3	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Jy	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	E8	501	130	29,34,34	1.37	3 (10%)	35,54,54	1.22	4 (11%)
128	GTP	Ed	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.33	5 (14%)
129	GDP	JJ	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	1G	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
129	GDP	O0	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	2C	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	C5	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	Fp	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	2A	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	W2	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	1A	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.28	4 (11%)
128	GTP	3P	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.36	5 (14%)
128	GTP	Bz	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
128	GTP	DK	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	Cm	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
128	GTP	Cg	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
129	GDP	El	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	L6	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	Bh	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	Fi	501	130	29,34,34	1.26	2 (6%)	35,54,54	1.31	3 (8%)
129	GDP	C4	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	Bb	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.26	3 (8%)
128	GTP	KW	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	BG	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
129	GDP	Cg	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.05	2 (6%)
128	GTP	2C	501	130	29,34,34	1.31	5 (17%)	35,54,54	1.39	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
129	GDP	Dg	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	KJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	Bu	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	G2	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	FT	502	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	CK	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	FW	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
129	GDP	S6	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Fc	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	GJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	L0	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Mg	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.11	2 (6%)
129	GDP	V4	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	1T	501	130	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	1D	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	IW	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
129	GDP	Iw	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.05	2 (6%)
129	GDP	DI	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.11	2 (6%)
129	GDP	D8	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.17	3 (10%)
129	GDP	0K	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	0O	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.39	5 (14%)
129	GDP	Mv	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
128	GTP	Bi	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
129	GDP	E0	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	CG	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
129	GDP	E4	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	1L	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	3S	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
128	GTP	C4	502	130	29,34,34	1.23	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	D6	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.15	3 (10%)
129	GDP	DR	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	FJ	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	A4	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	3M	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.28	3 (8%)
128	GTP	0Q	502	130	29,34,34	1.27	2 (6%)	35,54,54	1.27	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
129	GDP	EL	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Ct	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	CT	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	R6	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	1 (3%)
129	GDP	I4	503	-	25,30,30	0.95	1 (4%)	30,47,47	1.17	2 (6%)
129	GDP	Q0	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	1 (3%)
128	GTP	T4	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	0M	502	-	25,30,30	1.01	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	2U	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	MI	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	U6	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	An	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	E1	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	AT	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	Dt	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	Di	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	EH	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.28	4 (11%)
129	GDP	Kl	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	2 (6%)
128	GTP	X0	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
129	GDP	0Q	503	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
129	GDP	Ce	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	EY	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.25	3 (8%)
128	GTP	J6	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.25	4 (11%)
128	GTP	CX	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	0U	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	LU	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	U2	501	130	29,34,34	1.27	3 (10%)	35,54,54	1.27	4 (11%)
129	GDP	Mi	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	K0	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Z6	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	DG	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	Mt	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.31	4 (11%)
128	GTP	Ik	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	Cz	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	X4	501	130	29,34,34	1.29	3 (10%)	35,54,54	1.31	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
129	GDP	0C	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	D0	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	FT	503	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	De	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	BK	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	N0	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	2 (6%)
128	GTP	CZ	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	2K	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
129	GDP	F2	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	T8	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	EI	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.31	4 (11%)
128	GTP	M6	501	130	29,34,34	1.27	3 (10%)	35,54,54	1.26	4 (11%)
129	GDP	A1	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	G6	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	BY	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.39	7 (20%)
128	GTP	3C	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	1E	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	4 (13%)
129	GDP	Aw	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	CM	503	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	CG	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	K4	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	BW	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.34	4 (11%)
129	GDP	X2	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	3G	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	IX	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	H4	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.14	2 (6%)
129	GDP	H6	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.13	2 (6%)
129	GDP	I2	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	W2	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.28	4 (11%)
129	GDP	JL	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	1X	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.29	3 (8%)
129	GDP	FP	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.16	2 (6%)
128	GTP	Aj	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.27	4 (11%)
128	GTP	FQ	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	Ci	501	130	29,34,34	1.26	2 (6%)	35,54,54	1.28	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	Mu	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
129	GDP	FE	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	1O	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	MV	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	2G	501	130	29,34,34	1.27	3 (10%)	35,54,54	1.25	4 (11%)
129	GDP	MG	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	Dw	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	L4	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	G0	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Ju	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Bm	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	2S	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	O0	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	F3	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	F8	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.25	4 (11%)
129	GDP	X6	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	P8	502	-	25,30,30	1.01	1 (4%)	30,47,47	1.14	3 (10%)
128	GTP	1W	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.31	4 (11%)
128	GTP	D5	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	3 (8%)
128	GTP	BU	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.23	3 (8%)
128	GTP	S5	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.25	4 (11%)
129	GDP	Z8	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	2W	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	Ay	502	130	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
128	GTP	Iy	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.24	4 (11%)
129	GDP	FI	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
128	GTP	C9	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.26	3 (8%)
129	GDP	E6	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	IW	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Bu	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.28	5 (14%)
128	GTP	R4	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	Fv	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	Dr	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	LH	501	-	29,34,34	1.24	2 (6%)	35,54,54	1.24	4 (11%)
128	GTP	Ni	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
129	GDP	Eq	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	R8	503	-	25,30,30	0.97	1 (4%)	30,47,47	1.14	3 (10%)
129	GDP	AJ	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
129	GDP	Dv	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	Bn	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	O8	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	Z2	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	G3	502	130	29,34,34	1.29	4 (13%)	35,54,54	1.36	6 (17%)
128	GTP	NH	501	130	29,34,34	2.89	4 (13%)	35,54,54	2.25	10 (28%)
129	GDP	A6	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	BI	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.12	2 (6%)
129	GDP	JU	503	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	Fi	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	8N	501	-	25,30,30	1.01	2 (8%)	30,47,47	1.11	2 (6%)
128	GTP	I4	502	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	2M	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	JW	502	130	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	2I	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	Jl	502	130	29,34,34	1.23	2 (6%)	35,54,54	1.28	5 (14%)
128	GTP	NW	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.26	4 (11%)
129	GDP	D4	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.15	3 (10%)
128	GTP	Kv	501	130	29,34,34	1.26	4 (13%)	35,54,54	1.26	4 (11%)
128	GTP	FI	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.29	4 (11%)
128	GTP	0C	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.29	4 (11%)
128	GTP	Nh	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.26	4 (11%)
129	GDP	C8	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.05	2 (6%)
128	GTP	F5	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.24	4 (11%)
129	GDP	CI	503	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	MH	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	3G	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.28	4 (11%)
128	GTP	2Y	501	130	29,34,34	1.26	4 (13%)	35,54,54	1.28	4 (11%)
129	GDP	Nj	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	CR	502	130	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	C0	501	130	29,34,34	1.26	2 (6%)	35,54,54	1.29	4 (11%)
128	GTP	EF	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	W4	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	F1	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	CX	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	N2	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Y8	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	LX	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	0S	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	3 (10%)
128	GTP	V2	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	DX	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	H6	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.27	4 (11%)
128	GTP	Jj	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	0O	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	3 (10%)
129	GDP	ES	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	1M	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	Z0	501	130	29,34,34	1.28	4 (13%)	35,54,54	1.27	4 (11%)
128	GTP	S2	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	A9	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.24	4 (11%)
128	GTP	Fe	501	130	29,34,34	1.23	3 (10%)	35,54,54	1.27	4 (11%)
128	GTP	Bo	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	A3	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.15	3 (10%)
128	GTP	NU	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	P4	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	3 (8%)
129	GDP	EJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	1 (3%)
128	GTP	X7	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.37	4 (11%)
129	GDP	KW	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	NJ	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	M4	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.27	4 (11%)
129	GDP	0I	503	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	EQ	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.31	4 (11%)
128	GTP	DR	501	130	29,34,34	1.27	2 (6%)	35,54,54	1.30	4 (11%)
129	GDP	3S	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
128	GTP	IL	501	130	29,34,34	1.26	4 (13%)	35,54,54	1.39	7 (20%)
129	GDP	J6	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	H3	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	3K	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.26	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	Dm	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	T2	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	Fg	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	G8	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	A1	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	1 (3%)
129	GDP	1G	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	2 (6%)
128	GTP	li	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
129	GDP	2A	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
128	GTP	GF	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.33	4 (11%)
128	GTP	1H	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	Lh	501	-	29,34,34	1.26	4 (13%)	35,54,54	1.27	4 (11%)
129	GDP	H8	503	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	IM	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	R6	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	O2	501	130	29,34,34	1.27	3 (10%)	35,54,54	1.30	4 (11%)
128	GTP	Jy	501	130	29,34,34	1.26	4 (13%)	35,54,54	1.27	4 (11%)
129	GDP	EW	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	0Y	501	130	29,34,34	1.22	3 (10%)	35,54,54	1.27	4 (11%)
129	GDP	3K	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	Lu	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	3 (10%)
128	GTP	W0	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.27	3 (8%)
129	GDP	Bl	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
129	GDP	R4	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.13	3 (10%)
129	GDP	0G	501	-	25,30,30	1.12	2 (8%)	30,47,47	1.98	9 (30%)
129	GDP	3A	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	3I	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	K6	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Y6	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
129	GDP	LJ	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	3M	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Q6	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	J4	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	3 (8%)
129	GDP	BG	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	BY	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	3 (10%)
129	GDP	O4	503	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	8M	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.26	4 (11%)
129	GDP	T0	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	F8	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.12	3 (10%)
128	GTP	U6	501	130	29,34,34	1.27	4 (13%)	35,54,54	1.27	4 (11%)
129	GDP	BS	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	NH	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Ew	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	IY	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	Z3	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.39	6 (17%)
128	GTP	Jh	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.25	4 (11%)
129	GDP	Cx	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	DE	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	3O	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.30	3 (8%)
128	GTP	Ft	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
129	GDP	X0	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Dz	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.29	5 (14%)
128	GTP	D1	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	3 (8%)
129	GDP	P6	503	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	NW	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	P6	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	A1	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	Mh	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	2E	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.26	4 (11%)
129	GDP	Es	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	CK	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	M0	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.27	4 (11%)
128	GTP	R8	502	130	29,34,34	1.26	2 (6%)	35,54,54	1.26	5 (14%)
129	GDP	DE	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	1 (3%)
129	GDP	Fx	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	U2	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	3 (10%)
128	GTP	Du	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	1S	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
129	GDP	FC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
129	GDP	H2	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	B5	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	KL	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.29	4 (11%)
128	GTP	Q4	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
129	GDP	DG	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
129	GDP	Ck	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	JW	503	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	L2	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	1W	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
129	GDP	Au	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	0A	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	Cv	503	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	BW	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	CZ	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	DT	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	2Q	501	130	29,34,34	1.27	3 (10%)	35,54,54	1.26	4 (11%)
129	GDP	2U	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Dk	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	Dt	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.05	2 (6%)
129	GDP	EU	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	LJ	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.29	4 (11%)
128	GTP	2I	501	130	29,34,34	1.26	4 (13%)	35,54,54	1.27	4 (11%)
129	GDP	GD	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	Jw	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	Ej	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	H2	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	FV	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	BB	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	D3	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.28	3 (8%)
129	GDP	MT	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
128	GTP	K7	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	CU	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
129	GDP	CE	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
129	GDP	Fr	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	I0	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	MV	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.28	4 (11%)
129	GDP	NU	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.10	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	BJ	501	130	29,34,34	1.20	2 (6%)	35,54,54	1.29	3 (8%)
128	GTP	KI	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
129	GDP	DK	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.13	2 (6%)
129	GDP	Kv	503	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	GF	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	2 (6%)
128	GTP	EV	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.29	3 (8%)
129	GDP	F0	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
128	GTP	JU	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.25	4 (11%)
129	GDP	S0	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	V0	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.05	2 (6%)
129	GDP	B8	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	1C	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.15	2 (6%)
128	GTP	0I	502	130	29,34,34	1.23	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	Bh	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Kx	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
128	GTP	Y4	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.30	4 (11%)
128	GTP	Es	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.29	5 (14%)
128	GTP	Ak	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.32	4 (11%)
128	GTP	El	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.29	5 (14%)
128	GTP	K0	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	H8	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	GB	501	130	29,34,34	1.27	2 (6%)	35,54,54	1.31	5 (14%)
129	GDP	EQ	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.12	2 (6%)
129	GDP	BU	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	NS	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	B0	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	N1	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.30	4 (11%)
128	GTP	Y1	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
129	GDP	W4	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	JK	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	ER	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.39	5 (14%)
128	GTP	B2	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	DX	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	IK	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.24	4 (11%)
128	GTP	0A	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
129	GDP	1K	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	Ci	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	KH	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	P4	503	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	Bw	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	N0	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
128	GTP	BL	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.29	3 (8%)
128	GTP	T8	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.27	4 (11%)
128	GTP	Lv	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.28	4 (11%)
129	GDP	Kj	503	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	2 (6%)
129	GDP	X8	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	Eq	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.29	5 (14%)
128	GTP	Fr	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
129	GDP	G4	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	By	502	130	29,34,34	1.23	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	L6	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	LH	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	V8	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	LV	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	FG	501	130	29,34,34	1.27	3 (10%)	35,54,54	1.28	5 (14%)
128	GTP	1Q	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	An	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	DM	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	U4	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.28	4 (11%)
129	GDP	A7	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
128	GTP	At	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
129	GDP	B6	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.12	3 (10%)
128	GTP	Eh	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	I8	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	3A	501	130	29,34,34	1.20	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	Bs	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.14	2 (6%)
129	GDP	8J	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	Ba	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.28	5 (14%)
129	GDP	BO	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Fg	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
129	GDP	8H	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	G1	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.24	4 (11%)
129	GDP	NF	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	K8	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Ce	502	130	29,34,34	1.25	2 (6%)	35,54,54	1.31	4 (11%)
128	GTP	K9	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.28	4 (11%)
128	GTP	X6	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	Ei	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.24	3 (8%)
128	GTP	V8	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.28	4 (11%)
129	GDP	Fk	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	2 (6%)
128	GTP	O4	502	130	29,34,34	1.23	2 (6%)	35,54,54	1.24	4 (11%)
129	GDP	Nf	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	Z0	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	S2	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	A9	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	Cv	502	130	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
128	GTP	Fx	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	Y6	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	0V	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.23	4 (11%)
128	GTP	K6	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	F1	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.30	4 (11%)
129	GDP	DZ	502	-	25,30,30	0.92	1 (4%)	30,47,47	1.12	2 (6%)
128	GTP	2S	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.25	4 (11%)
129	GDP	Jh	503	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	R0	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Nh	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	D7	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	R2	502	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	DT	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
129	GDP	ED	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.11	3 (10%)
129	GDP	M4	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	U8	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	GH	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	X4	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	Fp	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	I1	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	C0	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	2 (6%)
128	GTP	V3	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	M2	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	EH	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	Li	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.30	4 (11%)
129	GDP	E2	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	V2	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	NF	501	-	29,34,34	1.26	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	Eu	501	130	29,34,34	1.31	3 (10%)	35,54,54	1.25	4 (11%)
128	GTP	N6	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	2W	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	M6	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	Cr	502	130	29,34,34	1.24	3 (10%)	35,54,54	1.25	5 (14%)
129	GDP	1U	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	2 (6%)
129	GDP	Ay	503	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	DV	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	W5	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
129	GDP	0Y	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.16	2 (6%)
128	GTP	Z6	501	130	29,34,34	1.28	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	KY	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.29	4 (11%)
129	GDP	Mt	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	2 (6%)
128	GTP	DH	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	Lw	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	J4	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Ag	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	Bf	502	130	29,34,34	1.26	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	Dk	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	Jw	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.25	4 (11%)
128	GTP	Kj	502	130	29,34,34	1.23	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	Aj	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	G7	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	O6	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	2 (6%)
129	GDP	Z4	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	8H	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	GI	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.33	4 (11%)
128	GTP	U7	501	130	29,34,34	1.26	4 (13%)	35,54,54	1.29	4 (11%)
128	GTP	W8	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	O2	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	Ft	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	KU	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	LT	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	J0	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	0W	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.14	3 (10%)
129	GDP	J2	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	DM	502	-	25,30,30	0.93	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	I0	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
128	GTP	O6	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.35	3 (8%)
129	GDP	S4	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	1 (3%)
129	GDP	F6	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	BM	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	2 (6%)
128	GTP	E0	502	130	29,34,34	1.25	2 (6%)	35,54,54	1.24	4 (11%)
128	GTP	L2	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.27	4 (11%)
129	GDP	S8	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	1S	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.13	2 (6%)
129	GDP	Q2	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.14	3 (10%)
129	GDP	Q4	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.14	2 (6%)
129	GDP	CV	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	B7	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.24	4 (11%)
129	GDP	Bw	503	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	J0	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.11	2 (6%)
129	GDP	C2	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	2Q	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	A2	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.41	6 (17%)
128	GTP	Lu	501	-	29,34,34	1.25	3 (10%)	35,54,54	1.25	4 (11%)
129	GDP	BB	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.06	2 (6%)
128	GTP	Az	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	0K	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
128	GTP	1N	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
129	GDP	Y4	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	S9	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	Bj	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	0R	502	130	29,34,34	1.25	3 (10%)	35,54,54	1.25	4 (11%)
128	GTP	CS	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	W6	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	T6	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	Dm	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	J2	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	S8	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.25	4 (11%)
129	GDP	2E	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	EL	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	JX	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	By	503	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	M8	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	2L	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	M0	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	J8	502	130	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	0M	501	130	29,34,34	1.27	3 (10%)	35,54,54	1.27	4 (11%)
128	GTP	Nf	501	-	29,34,34	1.26	3 (10%)	35,54,54	1.25	4 (11%)
128	GTP	R0	501	130	29,34,34	1.23	3 (10%)	35,54,54	1.30	4 (11%)
129	GDP	Jj	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Lj	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	N8	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
128	GTP	Kx	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	M7	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
129	GDP	V6	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	1 (3%)
128	GTP	E4	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	CI	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
128	GTP	Y0	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.24	4 (11%)
128	GTP	B5	501	130	29,34,34	1.24	3 (10%)	35,54,54	1.29	5 (14%)
129	GDP	J8	503	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Fc	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
129	GDP	FR	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	KU	501	-	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	8I	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
129	GDP	Ed	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	3 (10%)
129	GDP	IK	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	A5	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Eu	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.04	2 (6%)
128	GTP	B1	501	130	29,34,34	1.26	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	W0	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	2Y	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	EF	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	De	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	DZ	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	LX	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	Di	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	DV	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.32	4 (11%)
129	GDP	T2	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	BN	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.27	3 (8%)
128	GTP	1C	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
129	GDP	8L	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	M2	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.27	4 (11%)
129	GDP	Il	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	Ee	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
128	GTP	K4	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	MT	501	130	29,34,34	1.29	4 (13%)	35,54,54	1.31	4 (11%)
129	GDP	0E	501	-	25,30,30	1.00	2 (8%)	30,47,47	1.09	2 (6%)
128	GTP	I8	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	U4	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Ef	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Eh	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	FV	501	130	29,34,34	1.27	3 (10%)	35,54,54	1.29	4 (11%)
128	GTP	E6	501	130	29,34,34	1.22	3 (10%)	35,54,54	1.29	4 (11%)
129	GDP	T6	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	JI	502	130	29,34,34	1.23	2 (6%)	35,54,54	1.24	4 (11%)
128	GTP	I5	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	Ap	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	B1	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	GB	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	Dr	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.30	4 (11%)
128	GTP	F0	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	3I	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	Ao	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.40	6 (17%)
128	GTP	Df	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	FG	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.16	4 (13%)
129	GDP	W8	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.11	2 (6%)
128	GTP	FE	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.27	3 (8%)
129	GDP	R2	503	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Mg	501	130	29,34,34	1.23	3 (10%)	35,54,54	1.25	4 (11%)
129	GDP	Cr	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	C6	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	Z2	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.23	4 (11%)
129	GDP	EY	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	KL	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.13	2 (6%)
128	GTP	MG	501	130	29,34,34	1.20	2 (6%)	35,54,54	1.33	5 (14%)
128	GTP	L4	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	Q6	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	G0	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.26	4 (11%)
129	GDP	N6	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.05	2 (6%)
129	GDP	Dz	502	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	JY	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
129	GDP	Bf	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	BH	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.27	3 (8%)
128	GTP	Fk	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.30	5 (14%)
128	GTP	P8	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	KH	501	-	29,34,34	1.26	3 (10%)	35,54,54	1.24	4 (11%)
129	GDP	CR	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	U9	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	Cx	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.26	3 (8%)
128	GTP	CM	502	130	29,34,34	1.25	2 (6%)	35,54,54	1.35	4 (11%)
128	GTP	GD	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.26	4 (11%)
129	GDP	Lh	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	3Q	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
128	GTP	0F	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.24	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
128	GTP	C8	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
129	GDP	KY	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
129	GDP	Ah	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	Cz	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.29	4 (11%)
129	GDP	Y2	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Iy	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	2 (6%)
128	GTP	Q2	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.25	4 (11%)
129	GDP	FX	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.10	1 (3%)
128	GTP	Av	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.26	4 (11%)
128	GTP	N8	501	130	29,34,34	1.27	3 (10%)	35,54,54	1.26	4 (11%)
128	GTP	Iw	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.28	4 (11%)
128	GTP	Fv	501	130	29,34,34	1.27	3 (10%)	35,54,54	1.30	4 (11%)
129	GDP	Ba	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	D2	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)
128	GTP	G5	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
128	GTP	ED	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.30	5 (14%)
128	GTP	Kl	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	1A	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.15	3 (10%)
128	GTP	NS	501	-	29,34,34	1.27	3 (10%)	35,54,54	1.25	4 (11%)
128	GTP	C1	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	Ct	501	130	29,34,34	1.21	2 (6%)	35,54,54	1.25	3 (8%)
128	GTP	O8	501	130	29,34,34	1.22	2 (6%)	35,54,54	1.28	3 (8%)
129	GDP	GH	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	Jl	503	-	25,30,30	0.99	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	Dx	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	S0	501	130	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
129	GDP	FK	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	2 (6%)
129	GDP	Q8	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
129	GDP	NJ	502	-	25,30,30	1.00	1 (4%)	30,47,47	1.09	2 (6%)
128	GTP	CE	502	130	29,34,34	1.21	2 (6%)	35,54,54	1.27	3 (8%)
128	GTP	Cj	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
129	GDP	3O	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
129	GDP	E8	502	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	1 (3%)
129	GDP	Fe	502	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
129	GDP	Y0	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
129	GDP	Cm	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	3 (10%)
128	GTP	Z7	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
128	GTP	P9	501	130	29,34,34	1.26	3 (10%)	35,54,54	1.28	4 (11%)
128	GTP	2K	501	130	29,34,34	1.23	2 (6%)	35,54,54	1.27	3 (8%)
129	GDP	Ew	502	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	1 (3%)
129	GDP	1Q	502	-	25,30,30	0.99	1 (4%)	30,47,47	1.12	2 (6%)
129	GDP	Kh	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.10	2 (6%)
128	GTP	EU	501	130	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
128	GTP	8L	501	130	29,34,34	1.25	3 (10%)	35,54,54	1.28	4 (11%)

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
129	GDP	T4	502	-	-	5/12/32/32	0/3/3/3
129	GDP	Ij	501	-	-	2/12/32/32	0/3/3/3
129	GDP	3C	502	-	-	3/12/32/32	0/3/3/3
129	GDP	2G	502	-	-	1/12/32/32	0/3/3/3
129	GDP	B3	501	-	-	2/12/32/32	0/3/3/3
129	GDP	Jy	502	-	-	4/12/32/32	0/3/3/3
128	GTP	E8	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Ed	501	130	-	3/18/38/38	0/3/3/3
129	GDP	JJ	501	-	-	3/12/32/32	0/3/3/3
128	GTP	1G	501	130	-	6/18/38/38	0/3/3/3
129	GDP	O0	502	-	-	5/12/32/32	0/3/3/3
129	GDP	2C	502	-	-	3/12/32/32	0/3/3/3
128	GTP	C5	501	130	-	5/18/38/38	0/3/3/3
129	GDP	Fp	502	-	-	4/12/32/32	0/3/3/3
128	GTP	2A	501	130	-	9/18/38/38	0/3/3/3
129	GDP	W2	502	-	-	2/12/32/32	0/3/3/3
128	GTP	1A	501	130	-	6/18/38/38	0/3/3/3
128	GTP	3P	501	130	-	9/18/38/38	0/3/3/3
128	GTP	Bz	501	130	-	9/18/38/38	0/3/3/3
128	GTP	DK	501	130	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	Cm	501	130	-	8/18/38/38	0/3/3/3
128	GTP	Cg	501	130	-	7/18/38/38	0/3/3/3
129	GDP	El	502	-	-	1/12/32/32	0/3/3/3
128	GTP	L6	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Bh	501	130	-	8/18/38/38	0/3/3/3
128	GTP	Fi	501	130	-	7/18/38/38	0/3/3/3
129	GDP	C4	501	-	-	1/12/32/32	0/3/3/3
128	GTP	Bb	501	130	-	5/18/38/38	0/3/3/3
128	GTP	KW	501	130	-	8/18/38/38	0/3/3/3
128	GTP	BG	501	130	-	4/18/38/38	0/3/3/3
129	GDP	Cg	502	-	-	2/12/32/32	0/3/3/3
128	GTP	2C	501	130	-	5/18/38/38	0/3/3/3
129	GDP	Dg	501	-	-	5/12/32/32	0/3/3/3
129	GDP	KJ	501	-	-	2/12/32/32	0/3/3/3
129	GDP	Bu	502	-	-	1/12/32/32	0/3/3/3
129	GDP	G2	501	-	-	4/12/32/32	0/3/3/3
128	GTP	FT	502	130	-	8/18/38/38	0/3/3/3
129	GDP	CK	502	-	-	6/12/32/32	0/3/3/3
128	GTP	FW	501	130	-	8/18/38/38	0/3/3/3
129	GDP	S6	501	-	-	2/12/32/32	0/3/3/3
129	GDP	Fc	502	-	-	3/12/32/32	0/3/3/3
129	GDP	GJ	501	-	-	1/12/32/32	0/3/3/3
129	GDP	L0	501	-	-	2/12/32/32	0/3/3/3
129	GDP	Mg	502	-	-	6/12/32/32	0/3/3/3
129	GDP	V4	501	-	-	3/12/32/32	0/3/3/3
128	GTP	1T	501	130	-	9/18/38/38	0/3/3/3
128	GTP	1D	501	130	-	4/18/38/38	0/3/3/3
128	GTP	IW	501	130	-	11/18/38/38	0/3/3/3
129	GDP	Iw	502	-	-	1/12/32/32	0/3/3/3
129	GDP	DI	501	-	-	1/12/32/32	0/3/3/3
129	GDP	D8	501	-	-	4/12/32/32	0/3/3/3
129	GDP	0K	502	-	-	1/12/32/32	0/3/3/3
128	GTP	0O	501	130	-	7/18/38/38	0/3/3/3
129	GDP	Mv	501	-	-	5/12/32/32	0/3/3/3
128	GTP	Bi	501	130	-	9/18/38/38	0/3/3/3
129	GDP	E0	501	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	CG	501	130	-	9/18/38/38	0/3/3/3
129	GDP	E4	502	-	-	4/12/32/32	0/3/3/3
128	GTP	1L	501	130	-	7/18/38/38	0/3/3/3
128	GTP	3S	501	130	-	7/18/38/38	0/3/3/3
128	GTP	C4	502	130	-	4/18/38/38	0/3/3/3
129	GDP	D6	501	-	-	3/12/32/32	0/3/3/3
129	GDP	DR	502	-	-	1/12/32/32	0/3/3/3
128	GTP	FJ	501	130	-	5/18/38/38	0/3/3/3
128	GTP	A4	501	130	-	7/18/38/38	0/3/3/3
128	GTP	3M	501	130	-	6/18/38/38	0/3/3/3
128	GTP	0Q	502	130	-	6/18/38/38	0/3/3/3
129	GDP	EL	502	-	-	4/12/32/32	0/3/3/3
129	GDP	Ct	502	-	-	2/12/32/32	0/3/3/3
129	GDP	CT	501	-	-	3/12/32/32	0/3/3/3
129	GDP	R6	502	-	-	5/12/32/32	0/3/3/3
129	GDP	I4	503	-	-	2/12/32/32	0/3/3/3
129	GDP	Q0	501	-	-	1/12/32/32	0/3/3/3
128	GTP	T4	501	130	-	10/18/38/38	0/3/3/3
129	GDP	0M	502	-	-	4/12/32/32	0/3/3/3
128	GTP	2U	501	130	-	9/18/38/38	0/3/3/3
129	GDP	MI	501	-	-	1/12/32/32	0/3/3/3
129	GDP	U6	502	-	-	3/12/32/32	0/3/3/3
129	GDP	An	502	-	-	5/12/32/32	0/3/3/3
128	GTP	E1	501	130	-	4/18/38/38	0/3/3/3
128	GTP	AT	501	130	-	9/18/38/38	0/3/3/3
128	GTP	Dt	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Di	501	130	-	6/18/38/38	0/3/3/3
128	GTP	EH	501	130	-	10/18/38/38	0/3/3/3
129	GDP	Kl	502	-	-	4/12/32/32	0/3/3/3
128	GTP	X0	501	130	-	4/18/38/38	0/3/3/3
129	GDP	0Q	503	-	-	4/12/32/32	0/3/3/3
129	GDP	Ce	501	-	-	2/12/32/32	0/3/3/3
128	GTP	EY	501	130	-	6/18/38/38	0/3/3/3
128	GTP	J6	501	130	-	8/18/38/38	0/3/3/3
128	GTP	CX	501	130	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
129	GDP	0U	501	-	-	5/12/32/32	0/3/3/3
128	GTP	LU	501	130	-	9/18/38/38	0/3/3/3
128	GTP	U2	501	130	-	7/18/38/38	0/3/3/3
129	GDP	Mi	501	-	-	4/12/32/32	0/3/3/3
129	GDP	K0	502	-	-	5/12/32/32	0/3/3/3
129	GDP	Z6	502	-	-	1/12/32/32	0/3/3/3
128	GTP	DG	501	130	-	5/18/38/38	0/3/3/3
128	GTP	Mt	501	130	-	9/18/38/38	0/3/3/3
128	GTP	Ik	501	130	-	2/18/38/38	0/3/3/3
129	GDP	Cz	502	-	-	3/12/32/32	0/3/3/3
128	GTP	X4	501	130	-	5/18/38/38	0/3/3/3
129	GDP	0C	502	-	-	2/12/32/32	0/3/3/3
129	GDP	D0	501	-	-	3/12/32/32	0/3/3/3
129	GDP	FT	503	-	-	5/12/32/32	0/3/3/3
129	GDP	De	502	-	-	1/12/32/32	0/3/3/3
129	GDP	BK	501	-	-	2/12/32/32	0/3/3/3
129	GDP	N0	502	-	-	5/12/32/32	0/3/3/3
128	GTP	CZ	501	130	-	8/18/38/38	0/3/3/3
129	GDP	2K	502	-	-	3/12/32/32	0/3/3/3
129	GDP	F2	501	-	-	0/12/32/32	0/3/3/3
129	GDP	T8	502	-	-	1/12/32/32	0/3/3/3
128	GTP	EI	501	130	-	9/18/38/38	0/3/3/3
128	GTP	M6	501	130	-	6/18/38/38	0/3/3/3
129	GDP	A1	501	-	-	5/12/32/32	0/3/3/3
129	GDP	G6	501	-	-	5/12/32/32	0/3/3/3
128	GTP	BY	501	130	-	7/18/38/38	0/3/3/3
128	GTP	3C	501	130	-	8/18/38/38	0/3/3/3
129	GDP	1E	501	-	-	5/12/32/32	0/3/3/3
129	GDP	Aw	501	-	-	2/12/32/32	0/3/3/3
129	GDP	CM	503	-	-	5/12/32/32	0/3/3/3
129	GDP	CG	502	-	-	1/12/32/32	0/3/3/3
129	GDP	K4	502	-	-	4/12/32/32	0/3/3/3
128	GTP	BW	501	130	-	7/18/38/38	0/3/3/3
129	GDP	X2	501	-	-	1/12/32/32	0/3/3/3
129	GDP	3G	502	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	IX	501	130	-	7/18/38/38	0/3/3/3
129	GDP	H4	501	-	-	6/12/32/32	0/3/3/3
129	GDP	H6	502	-	-	5/12/32/32	0/3/3/3
129	GDP	I2	501	-	-	2/12/32/32	0/3/3/3
128	GTP	W2	501	130	-	9/18/38/38	0/3/3/3
129	GDP	JL	501	-	-	4/12/32/32	0/3/3/3
128	GTP	1X	501	130	-	9/18/38/38	0/3/3/3
129	GDP	FP	501	-	-	3/12/32/32	0/3/3/3
128	GTP	Aj	501	130	-	7/18/38/38	0/3/3/3
128	GTP	FQ	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Ci	501	130	-	8/18/38/38	0/3/3/3
128	GTP	Mu	501	130	-	7/18/38/38	0/3/3/3
129	GDP	FE	502	-	-	3/12/32/32	0/3/3/3
129	GDP	1O	501	-	-	1/12/32/32	0/3/3/3
129	GDP	MV	502	-	-	1/12/32/32	0/3/3/3
128	GTP	2G	501	130	-	7/18/38/38	0/3/3/3
129	GDP	MG	502	-	-	1/12/32/32	0/3/3/3
128	GTP	Dw	501	130	-	10/18/38/38	0/3/3/3
129	GDP	L4	502	-	-	3/12/32/32	0/3/3/3
129	GDP	G0	502	-	-	5/12/32/32	0/3/3/3
129	GDP	Ju	501	-	-	3/12/32/32	0/3/3/3
128	GTP	Bm	501	130	-	6/18/38/38	0/3/3/3
129	GDP	2S	502	-	-	3/12/32/32	0/3/3/3
128	GTP	O0	501	130	-	6/18/38/38	0/3/3/3
128	GTP	F3	501	130	-	4/18/38/38	0/3/3/3
128	GTP	F8	501	130	-	6/18/38/38	0/3/3/3
129	GDP	X6	502	-	-	0/12/32/32	0/3/3/3
129	GDP	P8	502	-	-	5/12/32/32	0/3/3/3
128	GTP	1W	501	130	-	5/18/38/38	0/3/3/3
128	GTP	D5	501	130	-	4/18/38/38	0/3/3/3
128	GTP	BU	501	130	-	6/18/38/38	0/3/3/3
128	GTP	S5	501	130	-	8/18/38/38	0/3/3/3
129	GDP	Z8	501	-	-	1/12/32/32	0/3/3/3
129	GDP	2W	502	-	-	4/12/32/32	0/3/3/3
128	GTP	Ay	502	130	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	Iy	501	130	-	8/18/38/38	0/3/3/3
129	GDP	FI	502	-	-	6/12/32/32	0/3/3/3
128	GTP	C9	501	130	-	3/18/38/38	0/3/3/3
129	GDP	E6	502	-	-	1/12/32/32	0/3/3/3
129	GDP	IW	502	-	-	3/12/32/32	0/3/3/3
128	GTP	Bu	501	130	-	9/18/38/38	0/3/3/3
128	GTP	R4	501	130	-	9/18/38/38	0/3/3/3
129	GDP	Fv	502	-	-	2/12/32/32	0/3/3/3
129	GDP	Dr	502	-	-	2/12/32/32	0/3/3/3
128	GTP	LH	501	-	-	8/18/38/38	0/3/3/3
128	GTP	Ni	501	130	-	4/18/38/38	0/3/3/3
129	GDP	Eq	502	-	-	1/12/32/32	0/3/3/3
129	GDP	R8	503	-	-	6/12/32/32	0/3/3/3
129	GDP	AJ	501	-	-	3/12/32/32	0/3/3/3
129	GDP	Dv	501	-	-	5/12/32/32	0/3/3/3
129	GDP	Bn	501	-	-	2/12/32/32	0/3/3/3
129	GDP	O8	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Z2	502	-	-	1/12/32/32	0/3/3/3
128	GTP	G3	502	130	-	5/18/38/38	0/3/3/3
128	GTP	NH	501	130	-	6/18/38/38	0/3/3/3
129	GDP	A6	501	-	-	2/12/32/32	0/3/3/3
129	GDP	BI	501	-	-	4/12/32/32	0/3/3/3
129	GDP	JU	503	-	-	6/12/32/32	0/3/3/3
129	GDP	Fi	502	-	-	3/12/32/32	0/3/3/3
129	GDP	8N	501	-	-	5/12/32/32	0/3/3/3
128	GTP	I4	502	130	-	9/18/38/38	0/3/3/3
129	GDP	2M	501	-	-	4/12/32/32	0/3/3/3
128	GTP	JW	502	130	-	8/18/38/38	0/3/3/3
129	GDP	2I	502	-	-	2/12/32/32	0/3/3/3
128	GTP	Jl	502	130	-	6/18/38/38	0/3/3/3
128	GTP	NW	501	130	-	8/18/38/38	0/3/3/3
129	GDP	D4	501	-	-	4/12/32/32	0/3/3/3
128	GTP	Kv	501	130	-	7/18/38/38	0/3/3/3
128	GTP	FI	501	130	-	6/18/38/38	0/3/3/3
128	GTP	0C	501	130	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	Nh	501	130	-	8/18/38/38	0/3/3/3
129	GDP	C8	502	-	-	1/12/32/32	0/3/3/3
128	GTP	F5	501	130	-	7/18/38/38	0/3/3/3
129	GDP	CI	503	-	-	1/12/32/32	0/3/3/3
128	GTP	MH	501	130	-	6/18/38/38	0/3/3/3
128	GTP	3G	501	130	-	8/18/38/38	0/3/3/3
128	GTP	2Y	501	130	-	7/18/38/38	0/3/3/3
129	GDP	Nj	501	-	-	1/12/32/32	0/3/3/3
128	GTP	CR	502	130	-	6/18/38/38	0/3/3/3
128	GTP	C0	501	130	-	8/18/38/38	0/3/3/3
128	GTP	EF	501	130	-	8/18/38/38	0/3/3/3
128	GTP	W4	501	130	-	7/18/38/38	0/3/3/3
128	GTP	F1	501	130	-	4/18/38/38	0/3/3/3
129	GDP	CX	502	-	-	4/12/32/32	0/3/3/3
129	GDP	N2	501	-	-	4/12/32/32	0/3/3/3
129	GDP	Y8	501	-	-	0/12/32/32	0/3/3/3
128	GTP	LX	501	130	-	7/18/38/38	0/3/3/3
129	GDP	0S	501	-	-	1/12/32/32	0/3/3/3
128	GTP	V2	501	130	-	7/18/38/38	0/3/3/3
129	GDP	DX	502	-	-	6/12/32/32	0/3/3/3
128	GTP	H6	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Jj	501	130	-	7/18/38/38	0/3/3/3
129	GDP	0O	502	-	-	1/12/32/32	0/3/3/3
129	GDP	ES	501	-	-	2/12/32/32	0/3/3/3
129	GDP	1M	501	-	-	4/12/32/32	0/3/3/3
128	GTP	Z0	501	130	-	3/18/38/38	0/3/3/3
128	GTP	S2	501	130	-	8/18/38/38	0/3/3/3
128	GTP	A9	501	130	-	4/18/38/38	0/3/3/3
128	GTP	Fe	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Bo	501	130	-	6/18/38/38	0/3/3/3
129	GDP	A3	501	-	-	5/12/32/32	0/3/3/3
128	GTP	NU	501	130	-	7/18/38/38	0/3/3/3
128	GTP	P4	501	130	-	7/18/38/38	0/3/3/3
129	GDP	EJ	501	-	-	3/12/32/32	0/3/3/3
128	GTP	X7	501	130	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
129	GDP	KW	502	-	-	1/12/32/32	0/3/3/3
128	GTP	NJ	501	130	-	5/18/38/38	0/3/3/3
128	GTP	M4	501	130	-	10/18/38/38	0/3/3/3
129	GDP	0I	503	-	-	5/12/32/32	0/3/3/3
128	GTP	EQ	501	130	-	5/18/38/38	0/3/3/3
128	GTP	DR	501	130	-	10/18/38/38	0/3/3/3
129	GDP	3S	502	-	-	1/12/32/32	0/3/3/3
128	GTP	IL	501	130	-	4/18/38/38	0/3/3/3
129	GDP	J6	502	-	-	2/12/32/32	0/3/3/3
128	GTP	H3	501	130	-	8/18/38/38	0/3/3/3
128	GTP	3K	501	130	-	8/18/38/38	0/3/3/3
128	GTP	Dm	501	130	-	8/18/38/38	0/3/3/3
128	GTP	T2	501	130	-	8/18/38/38	0/3/3/3
129	GDP	Fg	502	-	-	1/12/32/32	0/3/3/3
129	GDP	G8	501	-	-	4/12/32/32	0/3/3/3
129	GDP	A1	502	-	-	3/12/32/32	0/3/3/3
129	GDP	1G	502	-	-	5/12/32/32	0/3/3/3
128	GTP	li	501	130	-	3/18/38/38	0/3/3/3
129	GDP	2A	502	-	-	4/12/32/32	0/3/3/3
128	GTP	GF	501	130	-	9/18/38/38	0/3/3/3
128	GTP	1H	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Lh	501	-	-	6/18/38/38	0/3/3/3
129	GDP	H8	503	-	-	5/12/32/32	0/3/3/3
129	GDP	IM	501	-	-	1/12/32/32	0/3/3/3
128	GTP	R6	501	130	-	6/18/38/38	0/3/3/3
128	GTP	O2	501	130	-	8/18/38/38	0/3/3/3
128	GTP	Jy	501	130	-	8/18/38/38	0/3/3/3
129	GDP	EW	501	-	-	1/12/32/32	0/3/3/3
128	GTP	0Y	501	130	-	7/18/38/38	0/3/3/3
129	GDP	3K	502	-	-	0/12/32/32	0/3/3/3
129	GDP	Lu	502	-	-	2/12/32/32	0/3/3/3
128	GTP	W0	501	130	-	7/18/38/38	0/3/3/3
129	GDP	B1	502	-	-	5/12/32/32	0/3/3/3
129	GDP	R4	502	-	-	3/12/32/32	0/3/3/3
129	GDP	0G	501	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
129	GDP	3A	502	-	-	1/12/32/32	0/3/3/3
129	GDP	3I	502	-	-	4/12/32/32	0/3/3/3
129	GDP	K6	502	-	-	4/12/32/32	0/3/3/3
128	GTP	Y6	501	130	-	9/18/38/38	0/3/3/3
129	GDP	LJ	502	-	-	4/12/32/32	0/3/3/3
129	GDP	3M	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Q6	502	-	-	6/12/32/32	0/3/3/3
128	GTP	J4	501	130	-	9/18/38/38	0/3/3/3
129	GDP	BG	502	-	-	1/12/32/32	0/3/3/3
129	GDP	BY	502	-	-	1/12/32/32	0/3/3/3
129	GDP	O4	503	-	-	0/12/32/32	0/3/3/3
128	GTP	8M	501	130	-	11/18/38/38	0/3/3/3
129	GDP	T0	501	-	-	4/12/32/32	0/3/3/3
129	GDP	F8	502	-	-	2/12/32/32	0/3/3/3
128	GTP	U6	501	130	-	7/18/38/38	0/3/3/3
129	GDP	BS	501	-	-	3/12/32/32	0/3/3/3
129	GDP	NH	502	-	-	3/12/32/32	0/3/3/3
128	GTP	Ew	501	130	-	9/18/38/38	0/3/3/3
129	GDP	IY	501	-	-	2/12/32/32	0/3/3/3
128	GTP	Z3	501	130	-	4/18/38/38	0/3/3/3
128	GTP	Jh	501	130	-	6/18/38/38	0/3/3/3
129	GDP	Cx	502	-	-	1/12/32/32	0/3/3/3
128	GTP	DE	501	130	-	6/18/38/38	0/3/3/3
128	GTP	3O	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Ft	501	130	-	9/18/38/38	0/3/3/3
129	GDP	X0	502	-	-	2/12/32/32	0/3/3/3
128	GTP	Dz	501	130	-	6/18/38/38	0/3/3/3
128	GTP	D1	501	130	-	1/18/38/38	0/3/3/3
129	GDP	P6	503	-	-	0/12/32/32	0/3/3/3
129	GDP	NW	502	-	-	2/12/32/32	0/3/3/3
128	GTP	P6	501	130	-	6/18/38/38	0/3/3/3
128	GTP	A1	501	130	-	8/18/38/38	0/3/3/3
128	GTP	Mh	501	130	-	5/18/38/38	0/3/3/3
128	GTP	2E	501	130	-	5/18/38/38	0/3/3/3
129	GDP	Es	502	-	-	1/12/32/32	0/3/3/3
128	GTP	CK	501	130	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	M0	501	130	-	4/18/38/38	0/3/3/3
128	GTP	R8	502	130	-	9/18/38/38	0/3/3/3
129	GDP	DE	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Fx	502	-	-	2/12/32/32	0/3/3/3
129	GDP	U2	502	-	-	1/12/32/32	0/3/3/3
128	GTP	Du	501	130	-	9/18/38/38	0/3/3/3
128	GTP	1S	501	130	-	9/18/38/38	0/3/3/3
129	GDP	FC	501	-	-	4/12/32/32	0/3/3/3
129	GDP	H2	502	-	-	0/12/32/32	0/3/3/3
129	GDP	B5	502	-	-	2/12/32/32	0/3/3/3
128	GTP	KL	501	130	-	6/18/38/38	0/3/3/3
128	GTP	Q4	501	130	-	6/18/38/38	0/3/3/3
129	GDP	DG	502	-	-	6/12/32/32	0/3/3/3
129	GDP	Ck	501	-	-	2/12/32/32	0/3/3/3
129	GDP	JW	503	-	-	4/12/32/32	0/3/3/3
129	GDP	L2	502	-	-	3/12/32/32	0/3/3/3
129	GDP	1W	502	-	-	5/12/32/32	0/3/3/3
129	GDP	Au	501	-	-	2/12/32/32	0/3/3/3
129	GDP	0A	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Cv	503	-	-	1/12/32/32	0/3/3/3
129	GDP	BW	502	-	-	1/12/32/32	0/3/3/3
129	GDP	CZ	502	-	-	4/12/32/32	0/3/3/3
129	GDP	DT	502	-	-	3/12/32/32	0/3/3/3
128	GTP	2Q	501	130	-	7/18/38/38	0/3/3/3
129	GDP	2U	502	-	-	3/12/32/32	0/3/3/3
129	GDP	Dk	502	-	-	6/12/32/32	0/3/3/3
129	GDP	Dt	502	-	-	3/12/32/32	0/3/3/3
129	GDP	EU	502	-	-	3/12/32/32	0/3/3/3
128	GTP	LJ	501	130	-	9/18/38/38	0/3/3/3
128	GTP	2I	501	130	-	8/18/38/38	0/3/3/3
129	GDP	GD	502	-	-	3/12/32/32	0/3/3/3
129	GDP	Jw	502	-	-	2/12/32/32	0/3/3/3
129	GDP	Ej	501	-	-	1/12/32/32	0/3/3/3
128	GTP	H2	501	130	-	7/18/38/38	0/3/3/3
129	GDP	FV	502	-	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	BB	501	130	-	7/18/38/38	0/3/3/3
128	GTP	D3	501	130	-	3/18/38/38	0/3/3/3
129	GDP	MT	502	-	-	2/12/32/32	0/3/3/3
128	GTP	K7	501	130	-	4/18/38/38	0/3/3/3
128	GTP	CU	501	130	-	5/18/38/38	0/3/3/3
129	GDP	CE	501	-	-	1/12/32/32	0/3/3/3
129	GDP	Fr	502	-	-	4/12/32/32	0/3/3/3
129	GDP	I0	502	-	-	4/12/32/32	0/3/3/3
128	GTP	MV	501	130	-	7/18/38/38	0/3/3/3
129	GDP	NU	502	-	-	2/12/32/32	0/3/3/3
128	GTP	BJ	501	130	-	4/18/38/38	0/3/3/3
128	GTP	KI	501	130	-	8/18/38/38	0/3/3/3
129	GDP	DK	502	-	-	5/12/32/32	0/3/3/3
129	GDP	Kv	503	-	-	4/12/32/32	0/3/3/3
129	GDP	GF	502	-	-	1/12/32/32	0/3/3/3
128	GTP	EV	501	130	-	5/18/38/38	0/3/3/3
129	GDP	F0	502	-	-	1/12/32/32	0/3/3/3
128	GTP	JU	501	130	-	7/18/38/38	0/3/3/3
129	GDP	S0	502	-	-	1/12/32/32	0/3/3/3
129	GDP	V0	501	-	-	2/12/32/32	0/3/3/3
129	GDP	B8	501	-	-	2/12/32/32	0/3/3/3
129	GDP	1C	502	-	-	6/12/32/32	0/3/3/3
128	GTP	0I	502	130	-	8/18/38/38	0/3/3/3
129	GDP	Bh	502	-	-	5/12/32/32	0/3/3/3
129	GDP	Kx	502	-	-	6/12/32/32	0/3/3/3
128	GTP	Y4	501	130	-	5/18/38/38	0/3/3/3
128	GTP	Es	501	130	-	9/18/38/38	0/3/3/3
128	GTP	Ak	501	130	-	7/18/38/38	0/3/3/3
128	GTP	El	501	130	-	7/18/38/38	0/3/3/3
128	GTP	K0	501	130	-	7/18/38/38	0/3/3/3
128	GTP	H8	501	130	-	8/18/38/38	0/3/3/3
128	GTP	GB	501	130	-	9/18/38/38	0/3/3/3
129	GDP	EQ	502	-	-	0/12/32/32	0/3/3/3
129	GDP	BU	502	-	-	2/12/32/32	0/3/3/3
129	GDP	NS	502	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	B0	501	130	-	8/18/38/38	0/3/3/3
128	GTP	N1	501	130	-	8/18/38/38	0/3/3/3
128	GTP	Y1	501	130	-	3/18/38/38	0/3/3/3
129	GDP	W4	502	-	-	2/12/32/32	0/3/3/3
128	GTP	JK	501	130	-	5/18/38/38	0/3/3/3
128	GTP	ER	501	130	-	8/18/38/38	0/3/3/3
128	GTP	B2	501	130	-	8/18/38/38	0/3/3/3
128	GTP	DX	501	130	-	9/18/38/38	0/3/3/3
128	GTP	IK	501	130	-	7/18/38/38	0/3/3/3
128	GTP	0A	501	130	-	7/18/38/38	0/3/3/3
129	GDP	1K	501	-	-	5/12/32/32	0/3/3/3
129	GDP	Ci	502	-	-	4/12/32/32	0/3/3/3
129	GDP	KH	502	-	-	2/12/32/32	0/3/3/3
129	GDP	P4	503	-	-	1/12/32/32	0/3/3/3
128	GTP	Bw	501	130	-	9/18/38/38	0/3/3/3
128	GTP	N0	501	130	-	9/18/38/38	0/3/3/3
128	GTP	BL	501	130	-	3/18/38/38	0/3/3/3
128	GTP	T8	501	130	-	4/18/38/38	0/3/3/3
128	GTP	Lv	501	130	-	7/18/38/38	0/3/3/3
129	GDP	Kj	503	-	-	4/12/32/32	0/3/3/3
129	GDP	X8	501	-	-	1/12/32/32	0/3/3/3
128	GTP	Eq	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Fr	501	130	-	8/18/38/38	0/3/3/3
129	GDP	G4	501	-	-	3/12/32/32	0/3/3/3
128	GTP	By	502	130	-	8/18/38/38	0/3/3/3
129	GDP	L6	502	-	-	3/12/32/32	0/3/3/3
129	GDP	LH	502	-	-	1/12/32/32	0/3/3/3
129	GDP	V8	502	-	-	4/12/32/32	0/3/3/3
129	GDP	LV	501	-	-	1/12/32/32	0/3/3/3
128	GTP	FG	501	130	-	10/18/38/38	0/3/3/3
128	GTP	1Q	501	130	-	9/18/38/38	0/3/3/3
128	GTP	An	501	130	-	9/18/38/38	0/3/3/3
128	GTP	DM	501	130	-	8/18/38/38	0/3/3/3
128	GTP	U4	501	130	-	10/18/38/38	0/3/3/3
129	GDP	A7	501	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	At	501	130	-	8/18/38/38	0/3/3/3
129	GDP	B6	501	-	-	5/12/32/32	0/3/3/3
128	GTP	Eh	501	130	-	8/18/38/38	0/3/3/3
129	GDP	I8	502	-	-	1/12/32/32	0/3/3/3
128	GTP	3A	501	130	-	7/18/38/38	0/3/3/3
129	GDP	Bs	501	-	-	5/12/32/32	0/3/3/3
129	GDP	8J	501	-	-	2/12/32/32	0/3/3/3
128	GTP	Ba	501	130	-	3/18/38/38	0/3/3/3
129	GDP	BO	501	-	-	4/12/32/32	0/3/3/3
128	GTP	Fg	501	130	-	7/18/38/38	0/3/3/3
129	GDP	8H	502	-	-	2/12/32/32	0/3/3/3
128	GTP	G1	501	130	-	7/18/38/38	0/3/3/3
129	GDP	NF	502	-	-	1/12/32/32	0/3/3/3
129	GDP	K8	501	-	-	2/12/32/32	0/3/3/3
128	GTP	Ce	502	130	-	10/18/38/38	0/3/3/3
128	GTP	K9	501	130	-	9/18/38/38	0/3/3/3
128	GTP	X6	501	130	-	8/18/38/38	0/3/3/3
128	GTP	Ei	501	130	-	6/18/38/38	0/3/3/3
128	GTP	V8	501	130	-	8/18/38/38	0/3/3/3
129	GDP	Fk	502	-	-	3/12/32/32	0/3/3/3
128	GTP	O4	502	130	-	8/18/38/38	0/3/3/3
129	GDP	Nf	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Z0	502	-	-	0/12/32/32	0/3/3/3
129	GDP	S2	502	-	-	1/12/32/32	0/3/3/3
129	GDP	A9	502	-	-	4/12/32/32	0/3/3/3
128	GTP	Cv	502	130	-	6/18/38/38	0/3/3/3
128	GTP	Fx	501	130	-	9/18/38/38	0/3/3/3
129	GDP	Y6	502	-	-	0/12/32/32	0/3/3/3
128	GTP	0V	501	130	-	7/18/38/38	0/3/3/3
128	GTP	K6	501	130	-	9/18/38/38	0/3/3/3
128	GTP	F1	501	130	-	6/18/38/38	0/3/3/3
129	GDP	DZ	502	-	-	3/12/32/32	0/3/3/3
128	GTP	2S	501	130	-	6/18/38/38	0/3/3/3
129	GDP	Jh	503	-	-	1/12/32/32	0/3/3/3
129	GDP	R0	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Nh	502	-	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	D7	501	130	-	3/18/38/38	0/3/3/3
128	GTP	R2	502	130	-	9/18/38/38	0/3/3/3
128	GTP	DT	501	130	-	9/18/38/38	0/3/3/3
129	GDP	ED	502	-	-	4/12/32/32	0/3/3/3
129	GDP	M4	502	-	-	2/12/32/32	0/3/3/3
129	GDP	U8	502	-	-	4/12/32/32	0/3/3/3
128	GTP	GH	501	130	-	9/18/38/38	0/3/3/3
129	GDP	X4	502	-	-	0/12/32/32	0/3/3/3
128	GTP	Fp	501	130	-	8/18/38/38	0/3/3/3
128	GTP	I1	501	130	-	9/18/38/38	0/3/3/3
129	GDP	C0	502	-	-	1/12/32/32	0/3/3/3
128	GTP	V3	501	130	-	8/18/38/38	0/3/3/3
129	GDP	M2	502	-	-	3/12/32/32	0/3/3/3
129	GDP	EH	502	-	-	1/12/32/32	0/3/3/3
128	GTP	Li	501	130	-	9/18/38/38	0/3/3/3
129	GDP	E2	501	-	-	2/12/32/32	0/3/3/3
129	GDP	V2	502	-	-	3/12/32/32	0/3/3/3
128	GTP	NF	501	-	-	6/18/38/38	0/3/3/3
128	GTP	Eu	501	130	-	8/18/38/38	0/3/3/3
128	GTP	N6	501	130	-	9/18/38/38	0/3/3/3
128	GTP	2W	501	130	-	8/18/38/38	0/3/3/3
129	GDP	M6	502	-	-	3/12/32/32	0/3/3/3
128	GTP	Cr	502	130	-	5/18/38/38	0/3/3/3
129	GDP	1U	501	-	-	5/12/32/32	0/3/3/3
129	GDP	Ay	503	-	-	3/12/32/32	0/3/3/3
129	GDP	DV	502	-	-	4/12/32/32	0/3/3/3
128	GTP	W5	501	130	-	8/18/38/38	0/3/3/3
129	GDP	0Y	502	-	-	5/12/32/32	0/3/3/3
128	GTP	Z6	501	130	-	5/18/38/38	0/3/3/3
128	GTP	KY	501	130	-	6/18/38/38	0/3/3/3
129	GDP	Mt	502	-	-	6/12/32/32	0/3/3/3
128	GTP	DH	501	130	-	8/18/38/38	0/3/3/3
129	GDP	Lw	501	-	-	1/12/32/32	0/3/3/3
129	GDP	J4	502	-	-	1/12/32/32	0/3/3/3
128	GTP	Ag	501	130	-	10/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	Bf	502	130	-	8/18/38/38	0/3/3/3
128	GTP	Dk	501	130	-	8/18/38/38	0/3/3/3
128	GTP	Jw	501	130	-	5/18/38/38	0/3/3/3
128	GTP	Kj	502	130	-	7/18/38/38	0/3/3/3
129	GDP	Aj	502	-	-	1/12/32/32	0/3/3/3
128	GTP	G7	501	130	-	8/18/38/38	0/3/3/3
129	GDP	O6	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Z4	501	-	-	1/12/32/32	0/3/3/3
128	GTP	8H	501	130	-	9/18/38/38	0/3/3/3
128	GTP	GI	501	130	-	9/18/38/38	0/3/3/3
128	GTP	U7	501	130	-	10/18/38/38	0/3/3/3
128	GTP	W8	501	130	-	7/18/38/38	0/3/3/3
129	GDP	O2	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Ft	502	-	-	4/12/32/32	0/3/3/3
129	GDP	KU	502	-	-	1/12/32/32	0/3/3/3
129	GDP	LT	501	-	-	4/12/32/32	0/3/3/3
128	GTP	J0	501	130	-	8/18/38/38	0/3/3/3
129	GDP	0W	501	-	-	5/12/32/32	0/3/3/3
129	GDP	J2	502	-	-	1/12/32/32	0/3/3/3
129	GDP	DM	502	-	-	4/12/32/32	0/3/3/3
128	GTP	I0	501	130	-	8/18/38/38	0/3/3/3
128	GTP	O6	501	130	-	5/18/38/38	0/3/3/3
129	GDP	S4	501	-	-	1/12/32/32	0/3/3/3
129	GDP	F6	501	-	-	3/12/32/32	0/3/3/3
129	GDP	BM	501	-	-	5/12/32/32	0/3/3/3
128	GTP	E0	502	130	-	6/18/38/38	0/3/3/3
128	GTP	L2	501	130	-	7/18/38/38	0/3/3/3
129	GDP	S8	502	-	-	1/12/32/32	0/3/3/3
129	GDP	1S	502	-	-	5/12/32/32	0/3/3/3
129	GDP	Q2	502	-	-	5/12/32/32	0/3/3/3
129	GDP	Q4	502	-	-	5/12/32/32	0/3/3/3
129	GDP	CV	501	-	-	4/12/32/32	0/3/3/3
128	GTP	B7	501	130	-	4/18/38/38	0/3/3/3
129	GDP	Bw	503	-	-	6/12/32/32	0/3/3/3
129	GDP	J0	502	-	-	3/12/32/32	0/3/3/3
129	GDP	C2	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
129	GDP	2Q	502	-	-	2/12/32/32	0/3/3/3
128	GTP	A2	501	130	-	4/18/38/38	0/3/3/3
128	GTP	Lu	501	-	-	8/18/38/38	0/3/3/3
129	GDP	BB	502	-	-	1/12/32/32	0/3/3/3
128	GTP	Az	501	130	-	7/18/38/38	0/3/3/3
128	GTP	0K	501	130	-	3/18/38/38	0/3/3/3
128	GTP	1N	501	130	-	8/18/38/38	0/3/3/3
129	GDP	Y4	502	-	-	1/12/32/32	0/3/3/3
128	GTP	S9	501	130	-	8/18/38/38	0/3/3/3
129	GDP	Bj	501	-	-	5/12/32/32	0/3/3/3
128	GTP	0R	502	130	-	8/18/38/38	0/3/3/3
128	GTP	CS	501	130	-	4/18/38/38	0/3/3/3
129	GDP	W6	501	-	-	2/12/32/32	0/3/3/3
128	GTP	T6	501	130	-	9/18/38/38	0/3/3/3
129	GDP	Dm	502	-	-	1/12/32/32	0/3/3/3
128	GTP	J2	501	130	-	8/18/38/38	0/3/3/3
128	GTP	S8	501	130	-	7/18/38/38	0/3/3/3
129	GDP	2E	502	-	-	3/12/32/32	0/3/3/3
128	GTP	EL	501	130	-	7/18/38/38	0/3/3/3
128	GTP	JX	501	130	-	9/18/38/38	0/3/3/3
129	GDP	By	503	-	-	4/12/32/32	0/3/3/3
129	GDP	M8	501	-	-	2/12/32/32	0/3/3/3
128	GTP	2L	501	130	-	7/18/38/38	0/3/3/3
129	GDP	M0	502	-	-	1/12/32/32	0/3/3/3
128	GTP	J8	502	130	-	9/18/38/38	0/3/3/3
128	GTP	0M	501	130	-	9/18/38/38	0/3/3/3
128	GTP	Nf	501	-	-	7/18/38/38	0/3/3/3
128	GTP	R0	501	130	-	8/18/38/38	0/3/3/3
129	GDP	Jj	502	-	-	3/12/32/32	0/3/3/3
129	GDP	Lj	501	-	-	6/12/32/32	0/3/3/3
129	GDP	N8	502	-	-	1/12/32/32	0/3/3/3
128	GTP	Kx	501	130	-	8/18/38/38	0/3/3/3
128	GTP	M7	501	130	-	9/18/38/38	0/3/3/3
129	GDP	V6	501	-	-	5/12/32/32	0/3/3/3
128	GTP	E4	501	130	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	CI	501	130	-	9/18/38/38	0/3/3/3
128	GTP	Y0	501	130	-	9/18/38/38	0/3/3/3
128	GTP	B5	501	130	-	6/18/38/38	0/3/3/3
129	GDP	J8	503	-	-	3/12/32/32	0/3/3/3
128	GTP	Fc	501	130	-	7/18/38/38	0/3/3/3
129	GDP	FR	501	-	-	1/12/32/32	0/3/3/3
128	GTP	KU	501	-	-	6/18/38/38	0/3/3/3
128	GTP	8I	501	130	-	9/18/38/38	0/3/3/3
129	GDP	Ed	502	-	-	1/12/32/32	0/3/3/3
129	GDP	IK	502	-	-	3/12/32/32	0/3/3/3
129	GDP	A5	501	-	-	2/12/32/32	0/3/3/3
129	GDP	Eu	502	-	-	2/12/32/32	0/3/3/3
128	GTP	B1	501	130	-	6/18/38/38	0/3/3/3
129	GDP	W0	502	-	-	2/12/32/32	0/3/3/3
129	GDP	2Y	502	-	-	1/12/32/32	0/3/3/3
129	GDP	EF	502	-	-	4/12/32/32	0/3/3/3
128	GTP	De	501	130	-	7/18/38/38	0/3/3/3
128	GTP	DZ	501	130	-	9/18/38/38	0/3/3/3
129	GDP	LX	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Di	502	-	-	1/12/32/32	0/3/3/3
128	GTP	DV	501	130	-	6/18/38/38	0/3/3/3
129	GDP	T2	502	-	-	1/12/32/32	0/3/3/3
128	GTP	BN	501	130	-	5/18/38/38	0/3/3/3
128	GTP	1C	501	130	-	6/18/38/38	0/3/3/3
129	GDP	8L	502	-	-	2/12/32/32	0/3/3/3
128	GTP	M2	501	130	-	9/18/38/38	0/3/3/3
129	GDP	Il	501	-	-	2/12/32/32	0/3/3/3
128	GTP	Ee	501	130	-	6/18/38/38	0/3/3/3
128	GTP	K4	501	130	-	5/18/38/38	0/3/3/3
128	GTP	MT	501	130	-	4/18/38/38	0/3/3/3
129	GDP	0E	501	-	-	3/12/32/32	0/3/3/3
128	GTP	I8	501	130	-	7/18/38/38	0/3/3/3
129	GDP	U4	502	-	-	3/12/32/32	0/3/3/3
129	GDP	Ef	501	-	-	1/12/32/32	0/3/3/3
129	GDP	Eh	502	-	-	1/12/32/32	0/3/3/3
128	GTP	FV	501	130	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	E6	501	130	-	6/18/38/38	0/3/3/3
129	GDP	T6	502	-	-	1/12/32/32	0/3/3/3
128	GTP	JI	502	130	-	6/18/38/38	0/3/3/3
128	GTP	I5	501	130	-	9/18/38/38	0/3/3/3
129	GDP	Ap	501	-	-	5/12/32/32	0/3/3/3
129	GDP	B1	501	-	-	2/12/32/32	0/3/3/3
129	GDP	GB	502	-	-	4/12/32/32	0/3/3/3
128	GTP	Dr	501	130	-	10/18/38/38	0/3/3/3
128	GTP	F0	501	130	-	5/18/38/38	0/3/3/3
128	GTP	3I	501	130	-	6/18/38/38	0/3/3/3
128	GTP	Ao	501	130	-	4/18/38/38	0/3/3/3
128	GTP	Df	501	130	-	9/18/38/38	0/3/3/3
129	GDP	FG	502	-	-	5/12/32/32	0/3/3/3
129	GDP	W8	502	-	-	4/12/32/32	0/3/3/3
128	GTP	FE	501	130	-	7/18/38/38	0/3/3/3
129	GDP	R2	503	-	-	1/12/32/32	0/3/3/3
128	GTP	Mg	501	130	-	7/18/38/38	0/3/3/3
129	GDP	Cr	501	-	-	1/12/32/32	0/3/3/3
129	GDP	C6	501	-	-	2/12/32/32	0/3/3/3
128	GTP	Z2	501	130	-	7/18/38/38	0/3/3/3
129	GDP	EY	502	-	-	2/12/32/32	0/3/3/3
129	GDP	KL	502	-	-	4/12/32/32	0/3/3/3
128	GTP	MG	501	130	-	7/18/38/38	0/3/3/3
128	GTP	L4	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Q6	501	130	-	8/18/38/38	0/3/3/3
128	GTP	G0	501	130	-	6/18/38/38	0/3/3/3
129	GDP	N6	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Dz	502	-	-	2/12/32/32	0/3/3/3
129	GDP	JY	501	-	-	5/12/32/32	0/3/3/3
129	GDP	Bf	501	-	-	5/12/32/32	0/3/3/3
128	GTP	BH	501	130	-	5/18/38/38	0/3/3/3
128	GTP	Fk	501	130	-	5/18/38/38	0/3/3/3
128	GTP	P8	501	130	-	8/18/38/38	0/3/3/3
128	GTP	KH	501	-	-	5/18/38/38	0/3/3/3
129	GDP	CR	501	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	U9	501	130	-	9/18/38/38	0/3/3/3
128	GTP	Cx	501	130	-	6/18/38/38	0/3/3/3
128	GTP	CM	502	130	-	9/18/38/38	0/3/3/3
128	GTP	GD	501	130	-	8/18/38/38	0/3/3/3
129	GDP	Lh	502	-	-	1/12/32/32	0/3/3/3
129	GDP	3Q	501	-	-	1/12/32/32	0/3/3/3
128	GTP	0F	501	130	-	8/18/38/38	0/3/3/3
128	GTP	C8	501	130	-	3/18/38/38	0/3/3/3
129	GDP	KY	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Ah	501	-	-	2/12/32/32	0/3/3/3
128	GTP	Cz	501	130	-	6/18/38/38	0/3/3/3
129	GDP	Y2	501	-	-	1/12/32/32	0/3/3/3
129	GDP	Iy	502	-	-	0/12/32/32	0/3/3/3
128	GTP	Q2	501	130	-	8/18/38/38	0/3/3/3
129	GDP	FX	501	-	-	7/12/32/32	0/3/3/3
128	GTP	Av	501	130	-	8/18/38/38	0/3/3/3
128	GTP	N8	501	130	-	6/18/38/38	0/3/3/3
128	GTP	Iw	501	130	-	5/18/38/38	0/3/3/3
128	GTP	Fv	501	130	-	8/18/38/38	0/3/3/3
129	GDP	Ba	502	-	-	1/12/32/32	0/3/3/3
129	GDP	D2	501	-	-	2/12/32/32	0/3/3/3
128	GTP	G5	501	130	-	4/18/38/38	0/3/3/3
128	GTP	ED	501	130	-	8/18/38/38	0/3/3/3
128	GTP	Kl	501	130	-	7/18/38/38	0/3/3/3
129	GDP	1A	502	-	-	5/12/32/32	0/3/3/3
128	GTP	NS	501	-	-	6/18/38/38	0/3/3/3
128	GTP	C1	501	130	-	7/18/38/38	0/3/3/3
128	GTP	Ct	501	130	-	6/18/38/38	0/3/3/3
128	GTP	O8	501	130	-	6/18/38/38	0/3/3/3
129	GDP	GH	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Jl	503	-	-	5/12/32/32	0/3/3/3
129	GDP	Dx	501	-	-	2/12/32/32	0/3/3/3
128	GTP	S0	501	130	-	9/18/38/38	0/3/3/3
129	GDP	FK	501	-	-	5/12/32/32	0/3/3/3
129	GDP	Q8	501	-	-	1/12/32/32	0/3/3/3
129	GDP	NJ	502	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
128	GTP	CE	502	130	-	8/18/38/38	0/3/3/3
128	GTP	Cj	501	130	-	9/18/38/38	0/3/3/3
129	GDP	3O	502	-	-	1/12/32/32	0/3/3/3
129	GDP	E8	502	-	-	0/12/32/32	0/3/3/3
129	GDP	Fe	502	-	-	4/12/32/32	0/3/3/3
129	GDP	Y0	502	-	-	1/12/32/32	0/3/3/3
129	GDP	Cm	502	-	-	3/12/32/32	0/3/3/3
128	GTP	Z7	501	130	-	3/18/38/38	0/3/3/3
128	GTP	P9	501	130	-	9/18/38/38	0/3/3/3
128	GTP	2K	501	130	-	9/18/38/38	0/3/3/3
129	GDP	Ew	502	-	-	2/12/32/32	0/3/3/3
129	GDP	1Q	502	-	-	5/12/32/32	0/3/3/3
129	GDP	Kh	501	-	-	1/12/32/32	0/3/3/3
128	GTP	EU	501	130	-	6/18/38/38	0/3/3/3
128	GTP	8L	501	130	-	7/18/38/38	0/3/3/3

The worst 5 of 1122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
128	NH	501	GTP	PA-O3A	10.50	1.70	1.59
128	NH	501	GTP	PB-O3A	9.75	1.70	1.59
128	E8	501	GTP	C5-C6	-4.62	1.38	1.47
128	Ak	501	GTP	C5-C6	-4.44	1.38	1.47
128	DM	501	GTP	C5-C6	-4.41	1.38	1.47

The worst 5 of 2040 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
128	NH	501	GTP	O2A-PA-O3A	7.13	126.54	107.27
129	0G	501	GDP	O2A-PA-O3A	5.58	122.36	107.27
128	NH	501	GTP	O5'-PA-O1A	-4.96	89.27	108.94
128	NH	501	GTP	C8-N7-C5	4.33	109.93	102.55
128	NH	501	GTP	C4'-O4'-C1'	3.89	113.49	109.92

There are no chirality outliers.

5 of 3236 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
128	0A	501	GTP	C5'-O5'-PA-O3A

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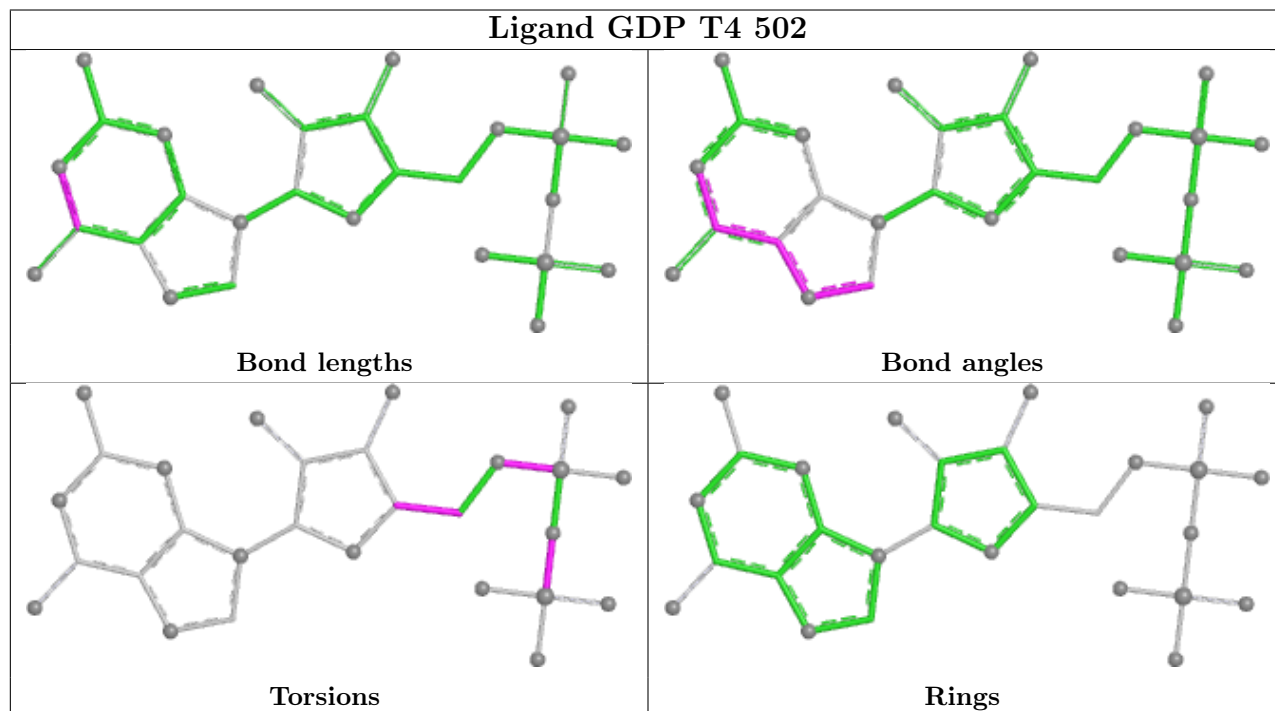
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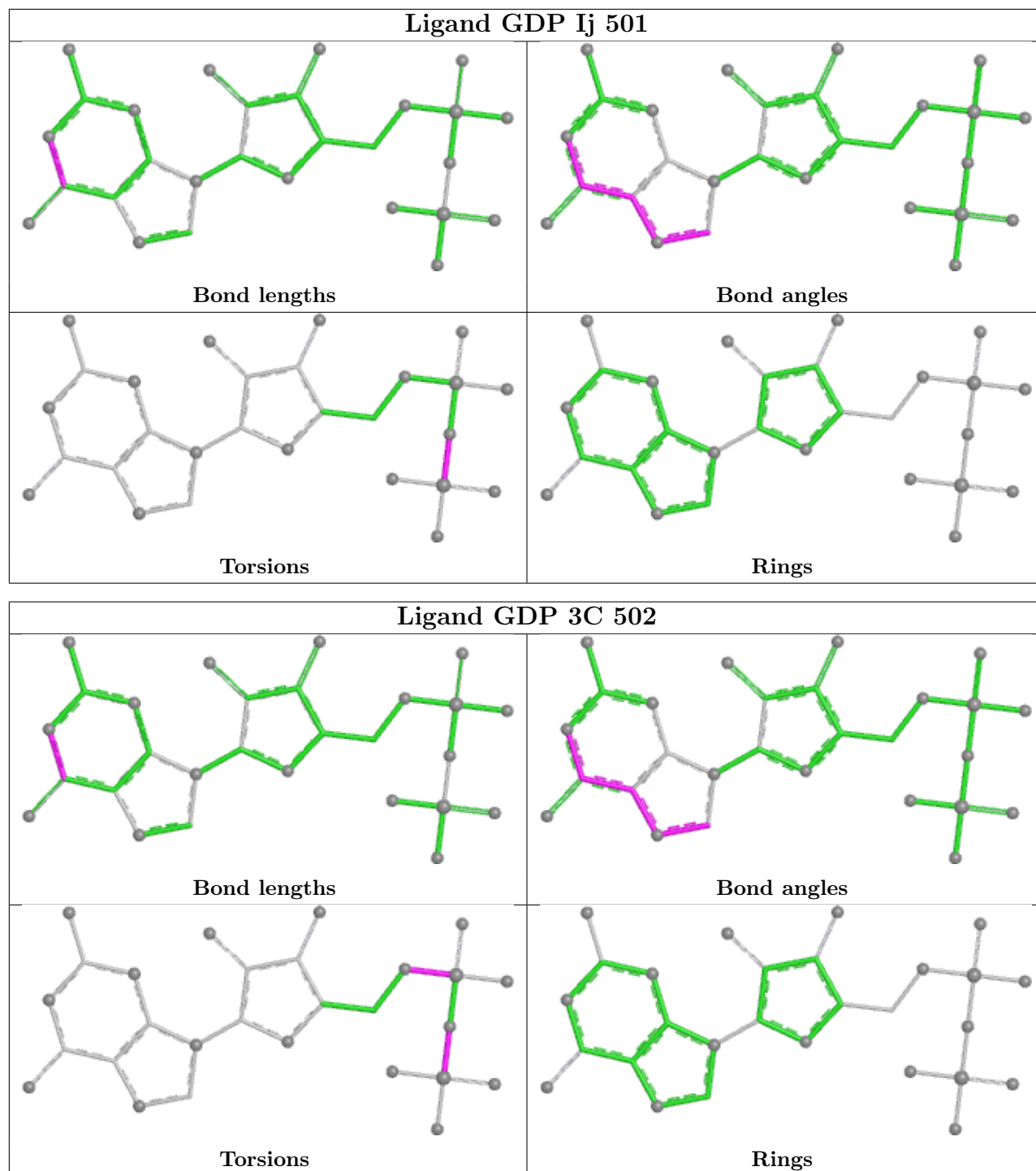
Mol	Chain	Res	Type	Atoms
128	0A	501	GTP	C5'-O5'-PA-O2A
128	0C	501	GTP	C5'-O5'-PA-O3A
128	0C	501	GTP	C5'-O5'-PA-O2A
128	0F	501	GTP	PB-O3A-PA-O5'

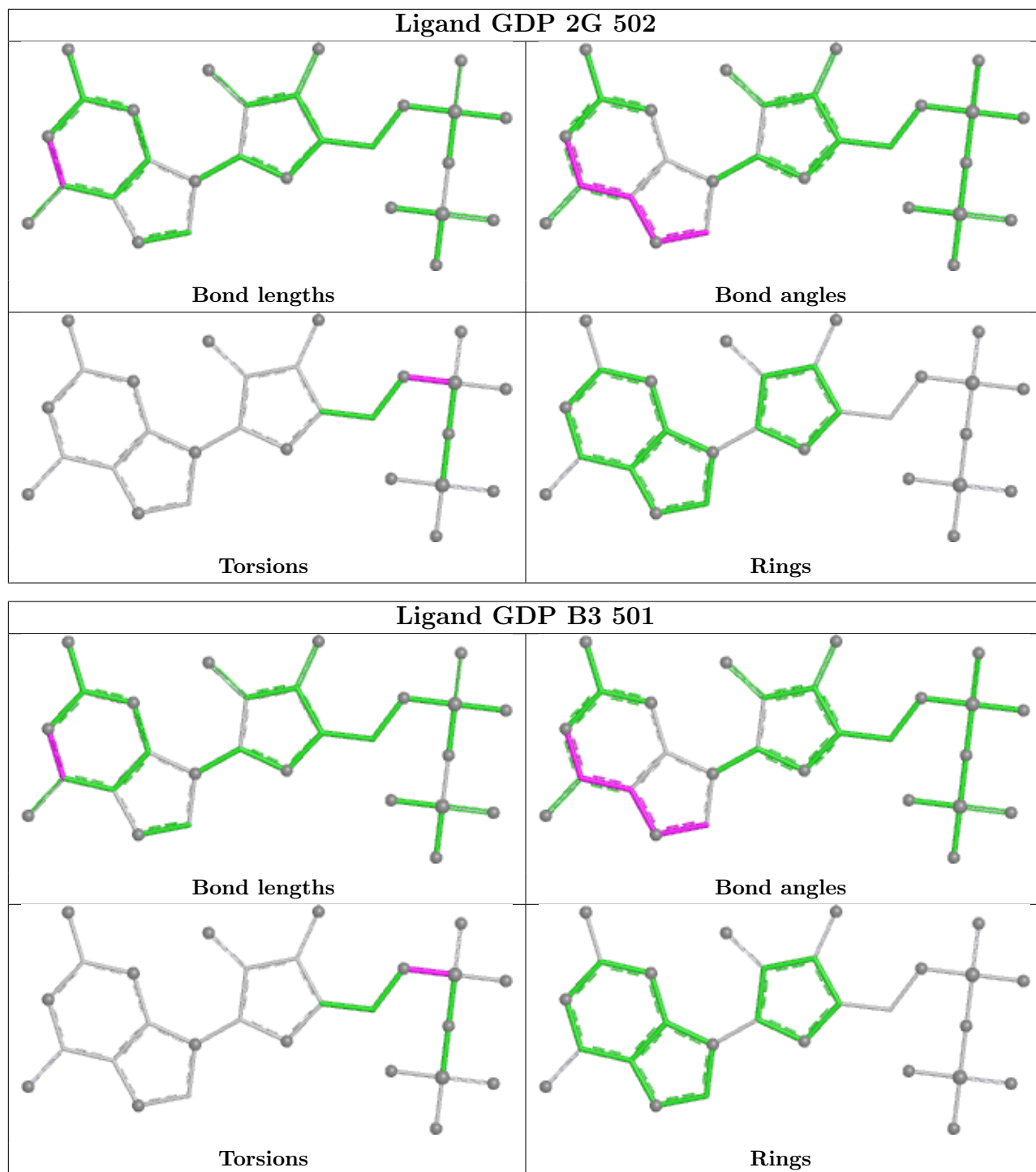
There are no ring outliers.

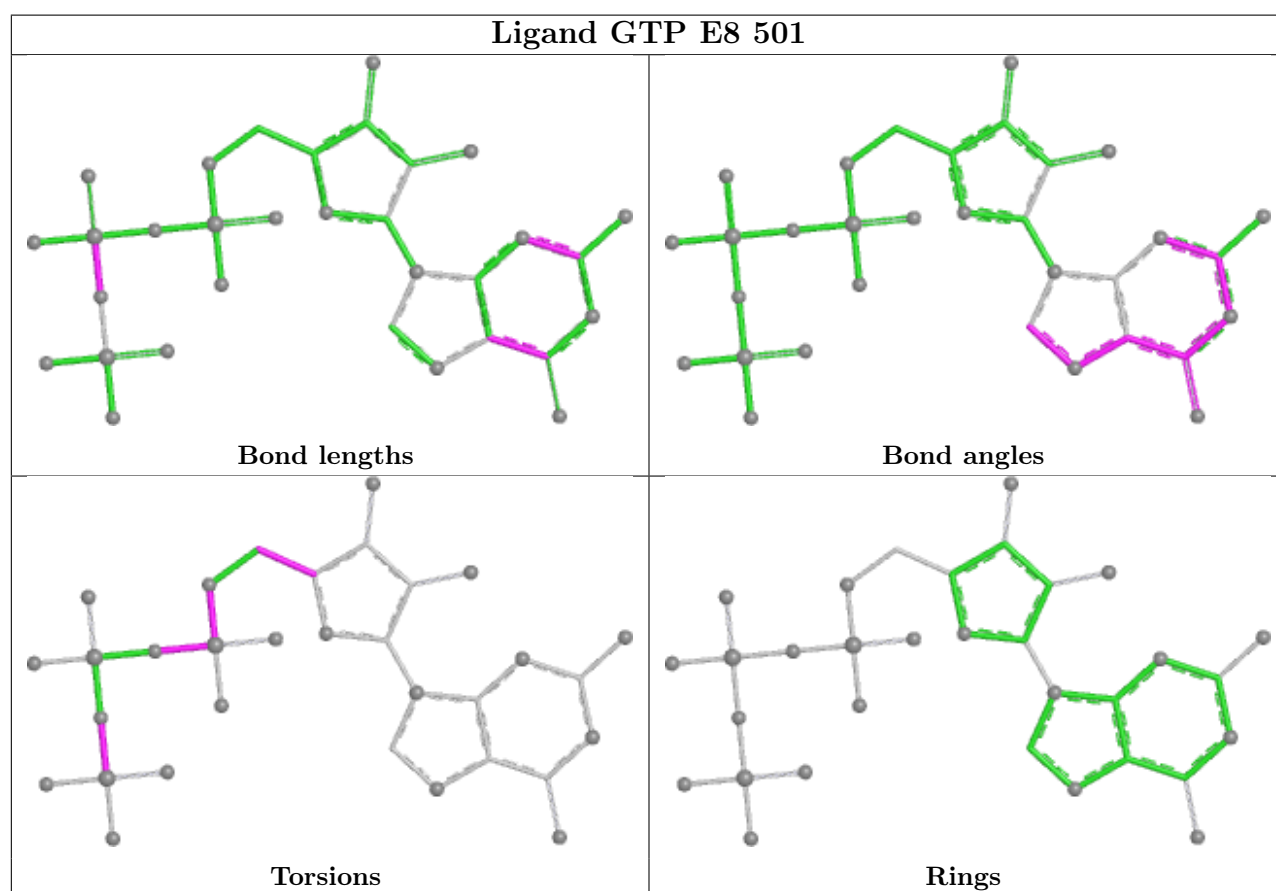
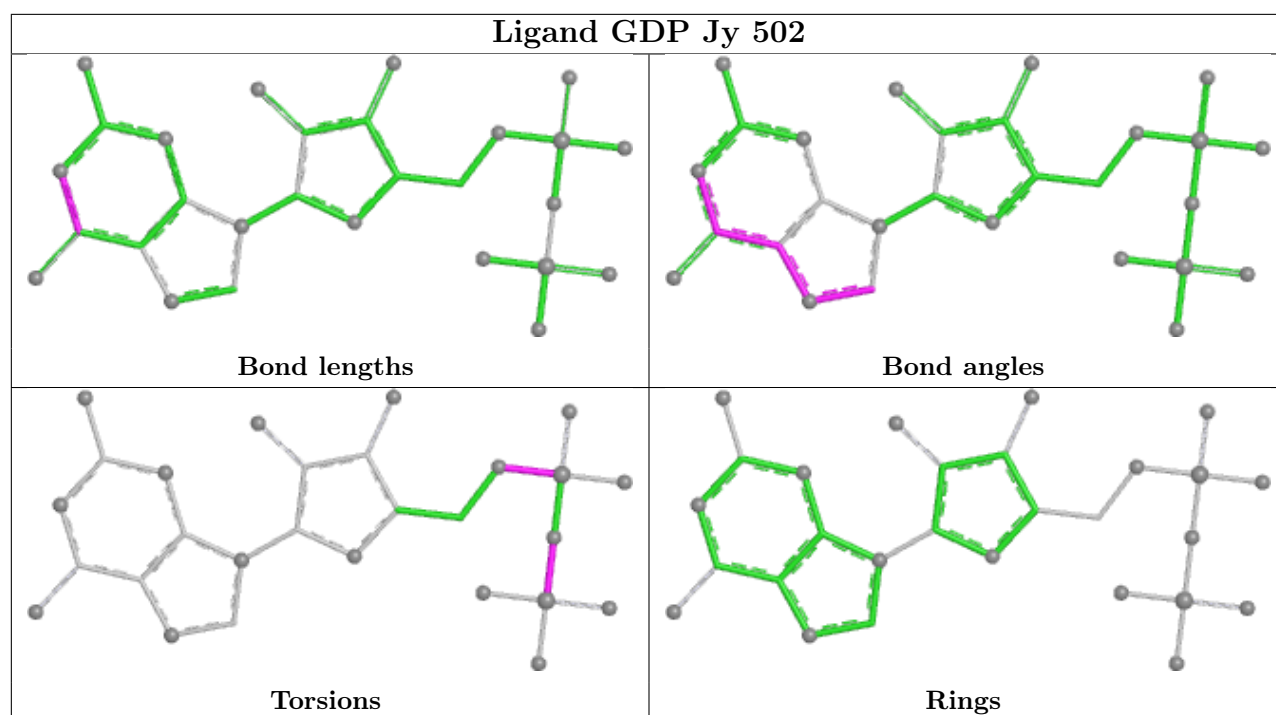
No monomer is involved in short contacts.

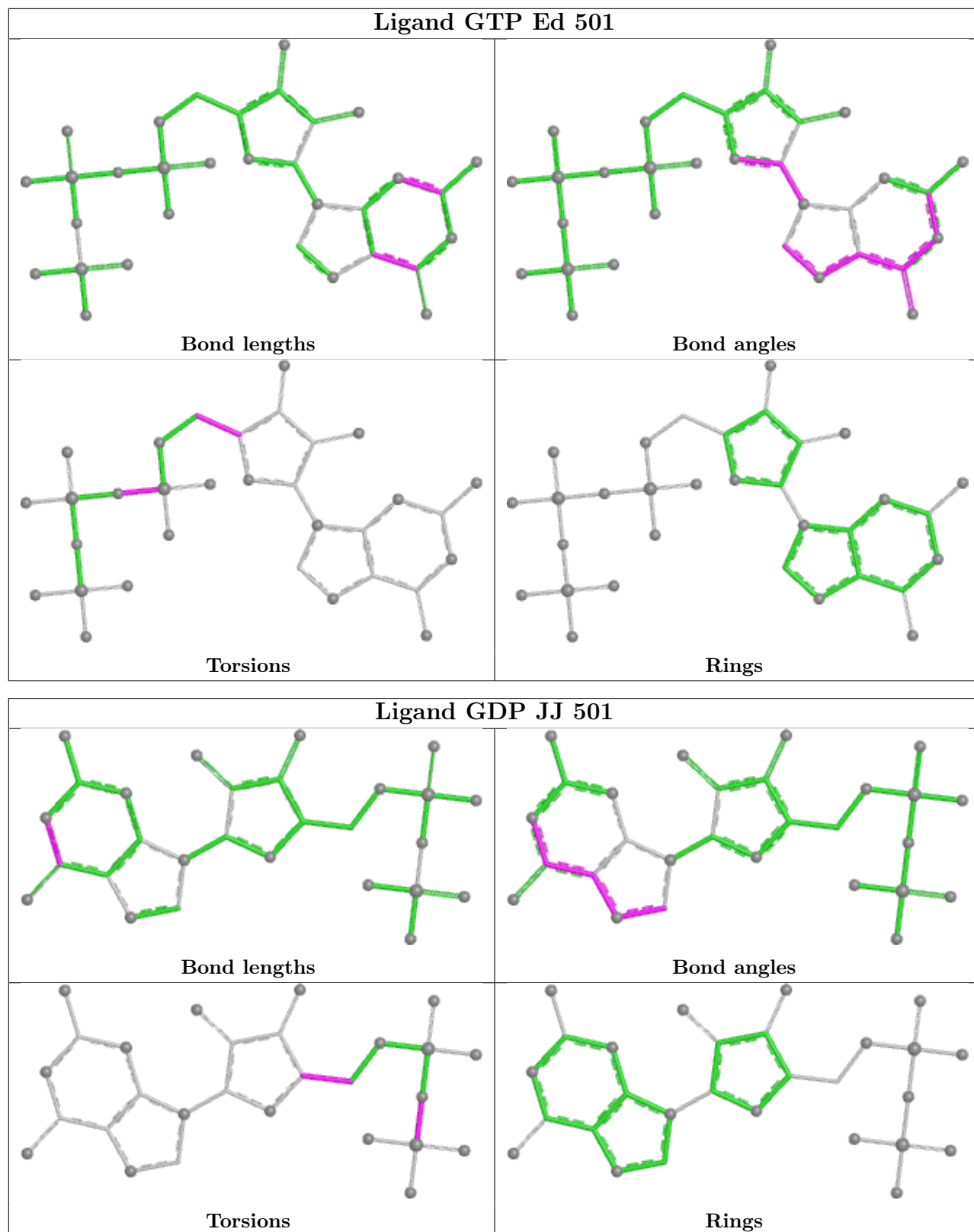
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

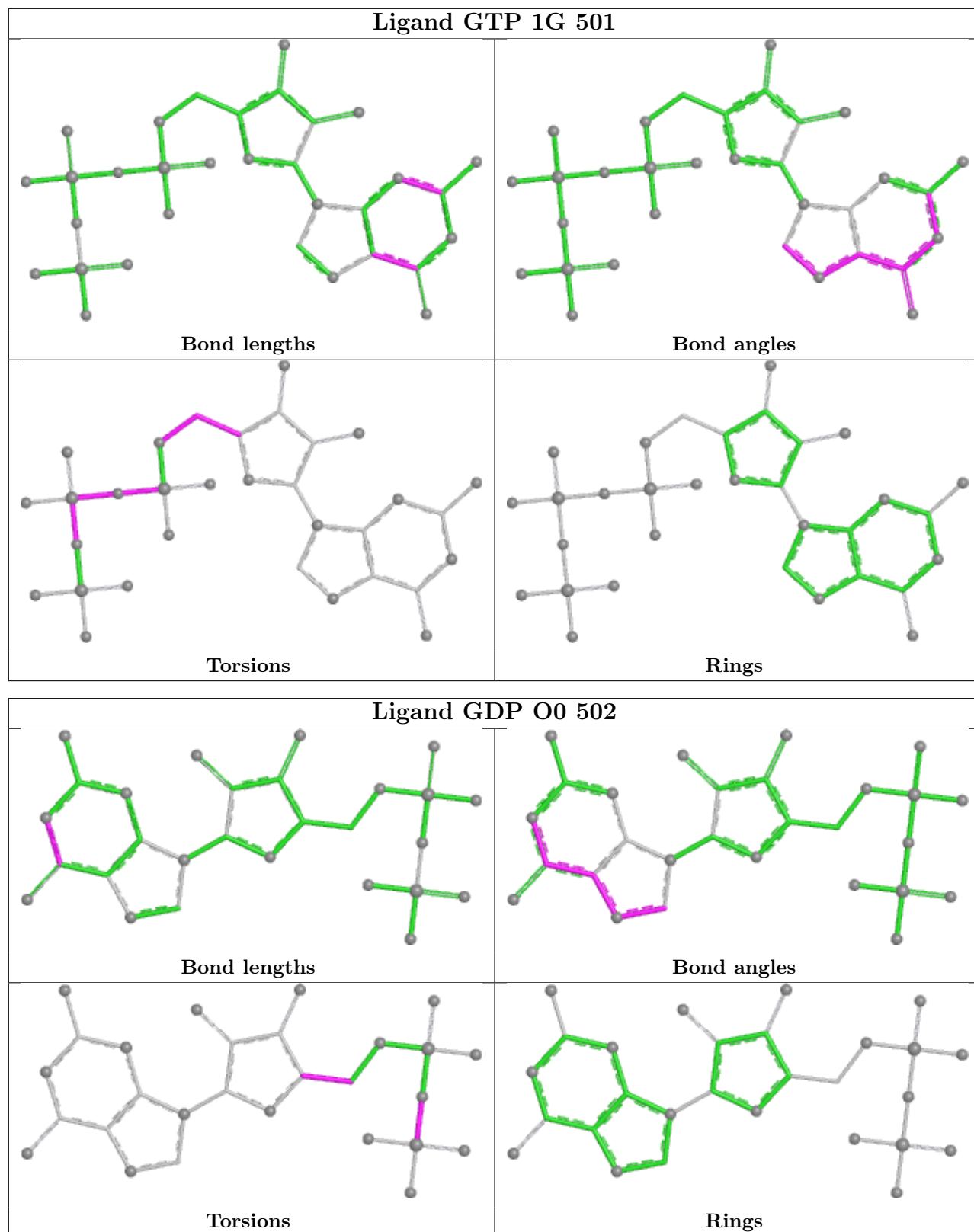


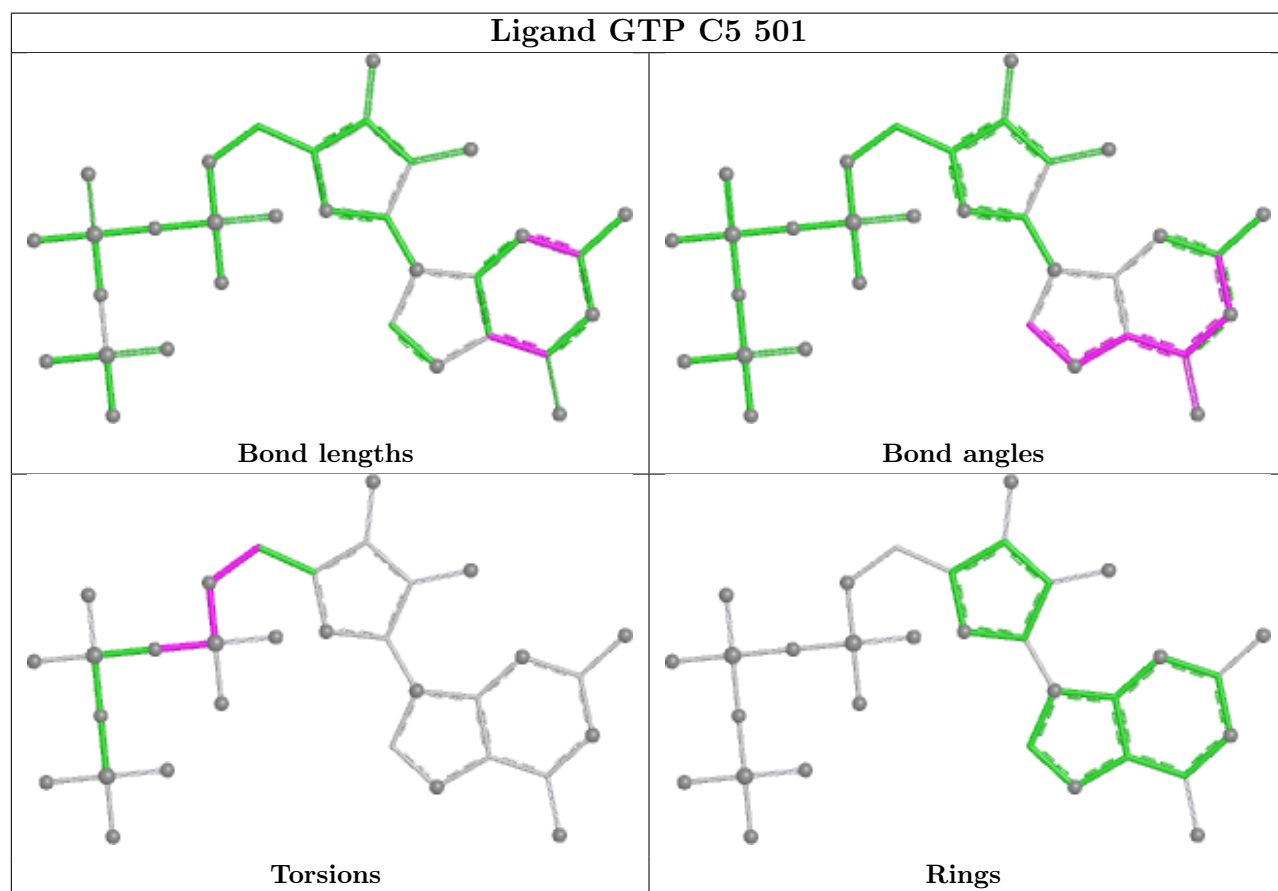
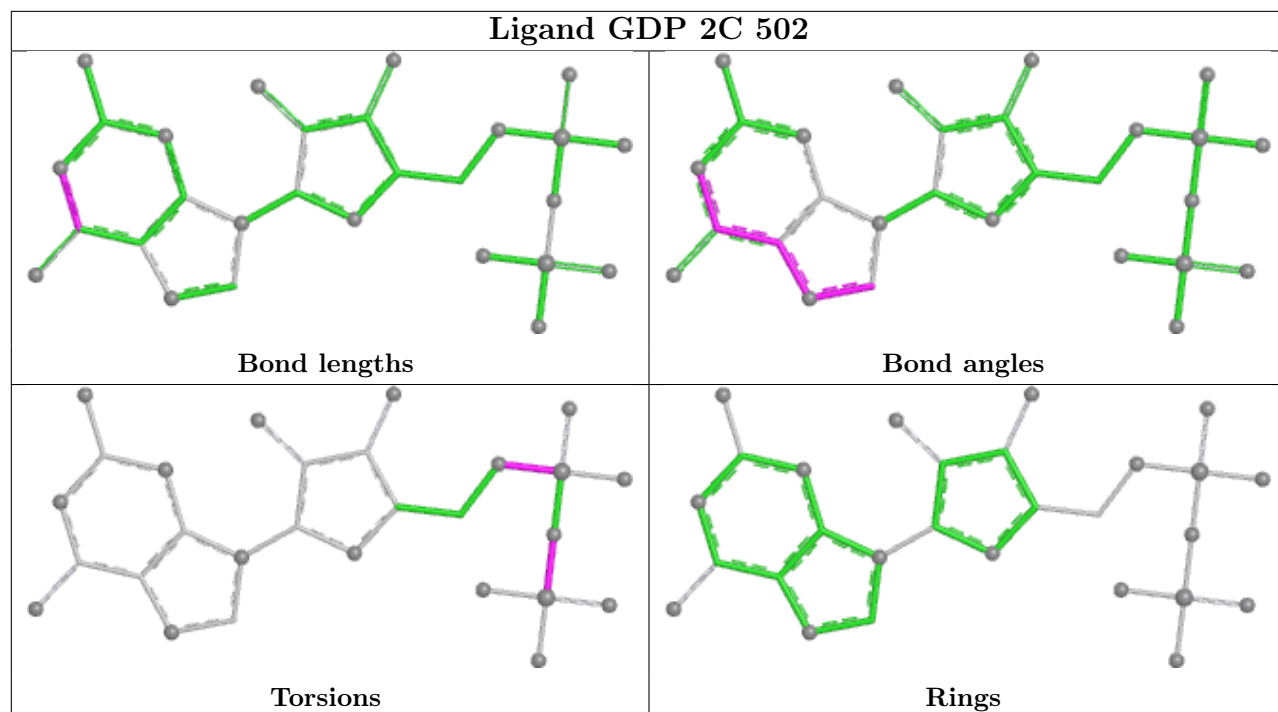


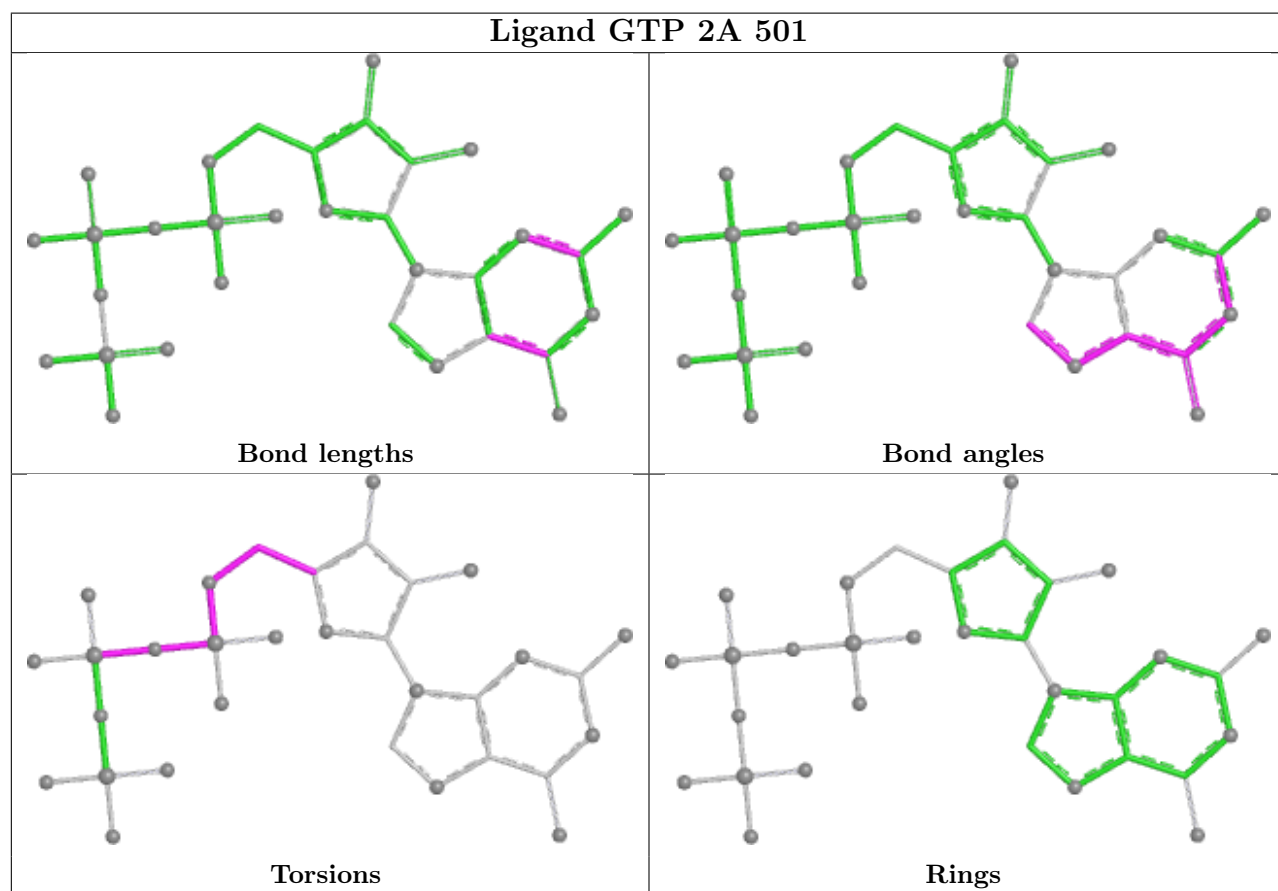
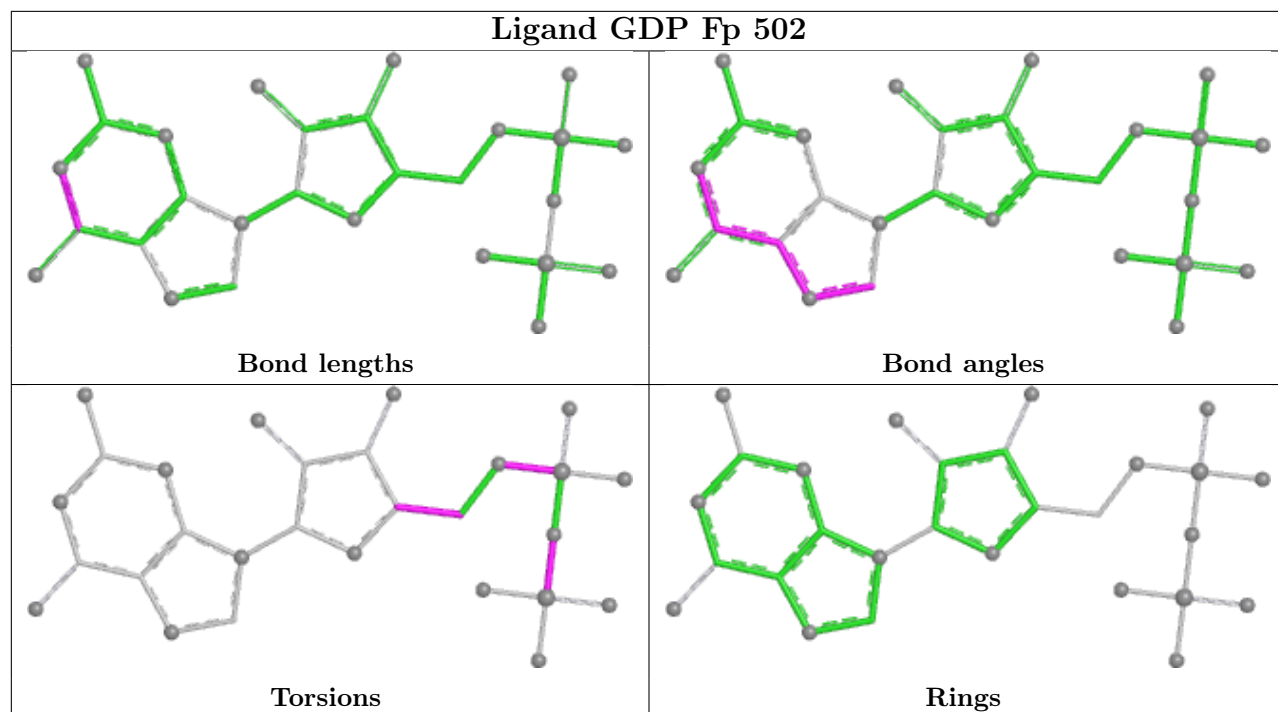


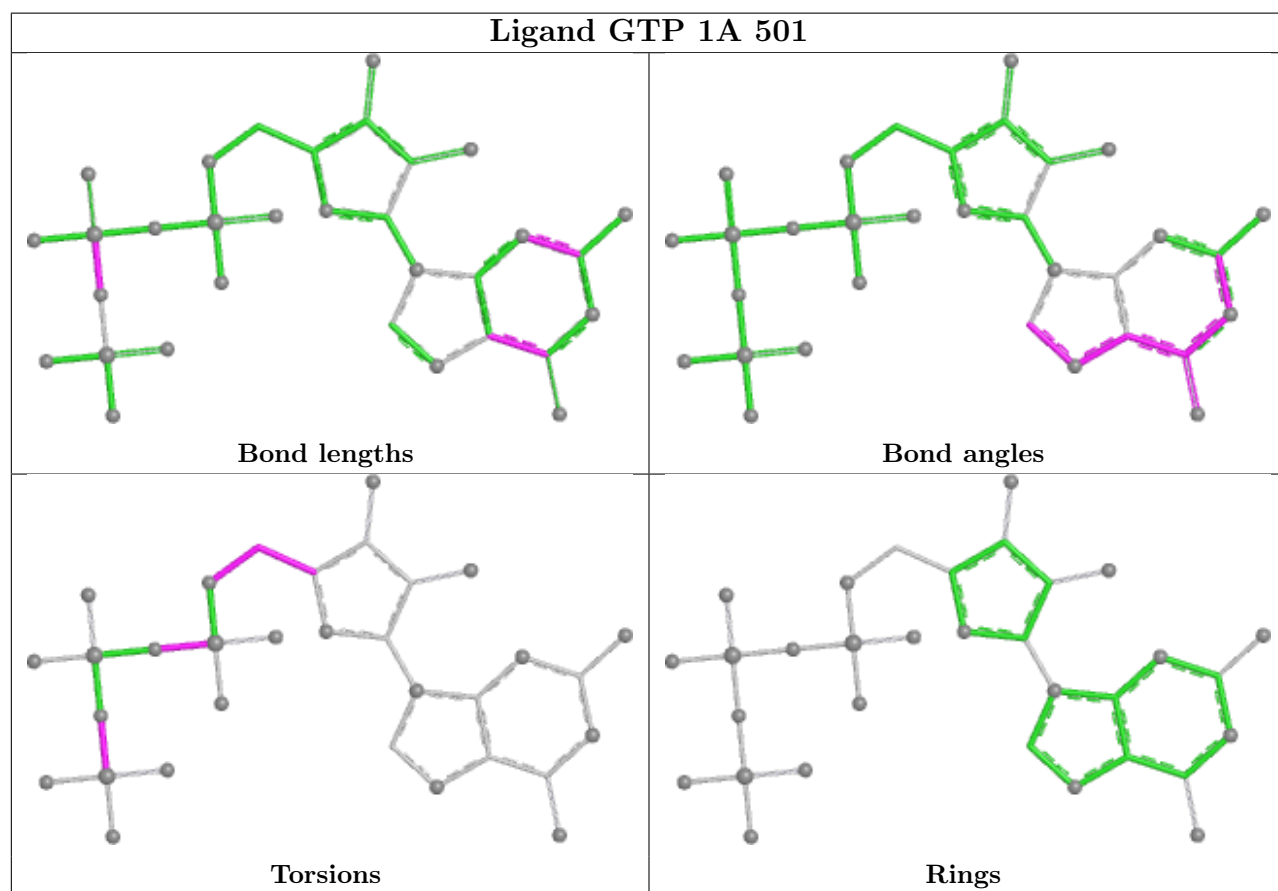
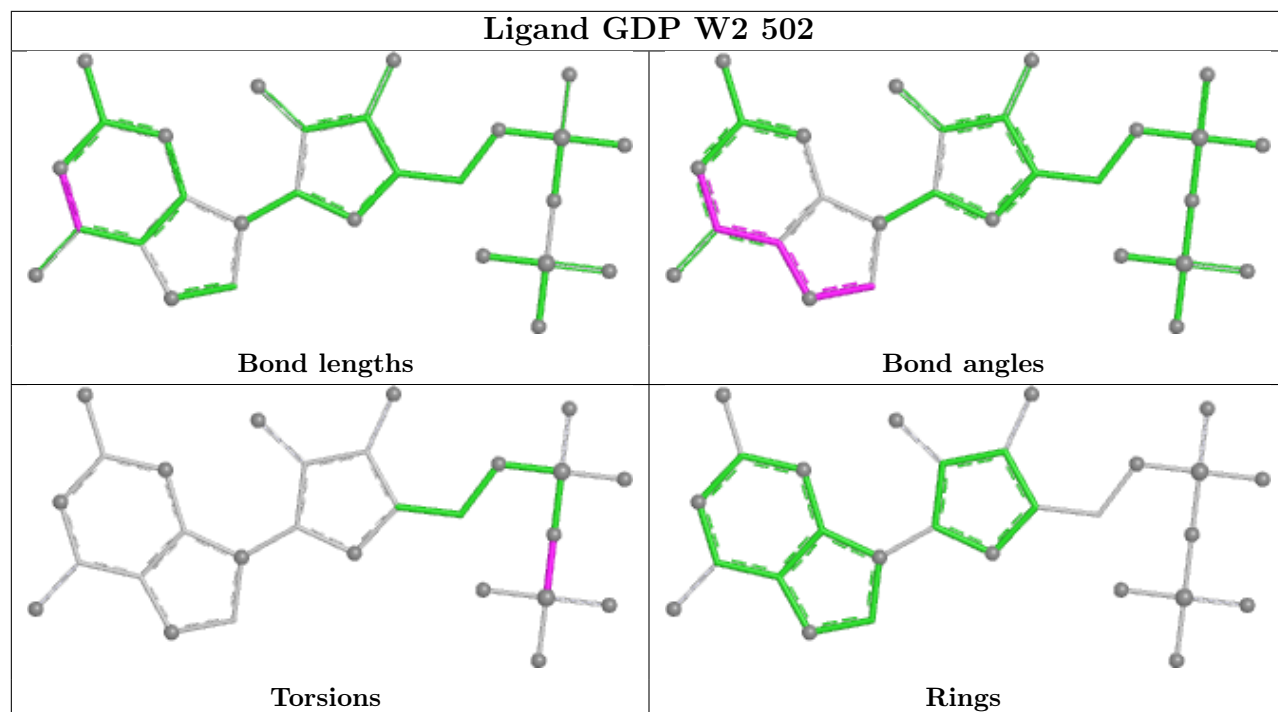


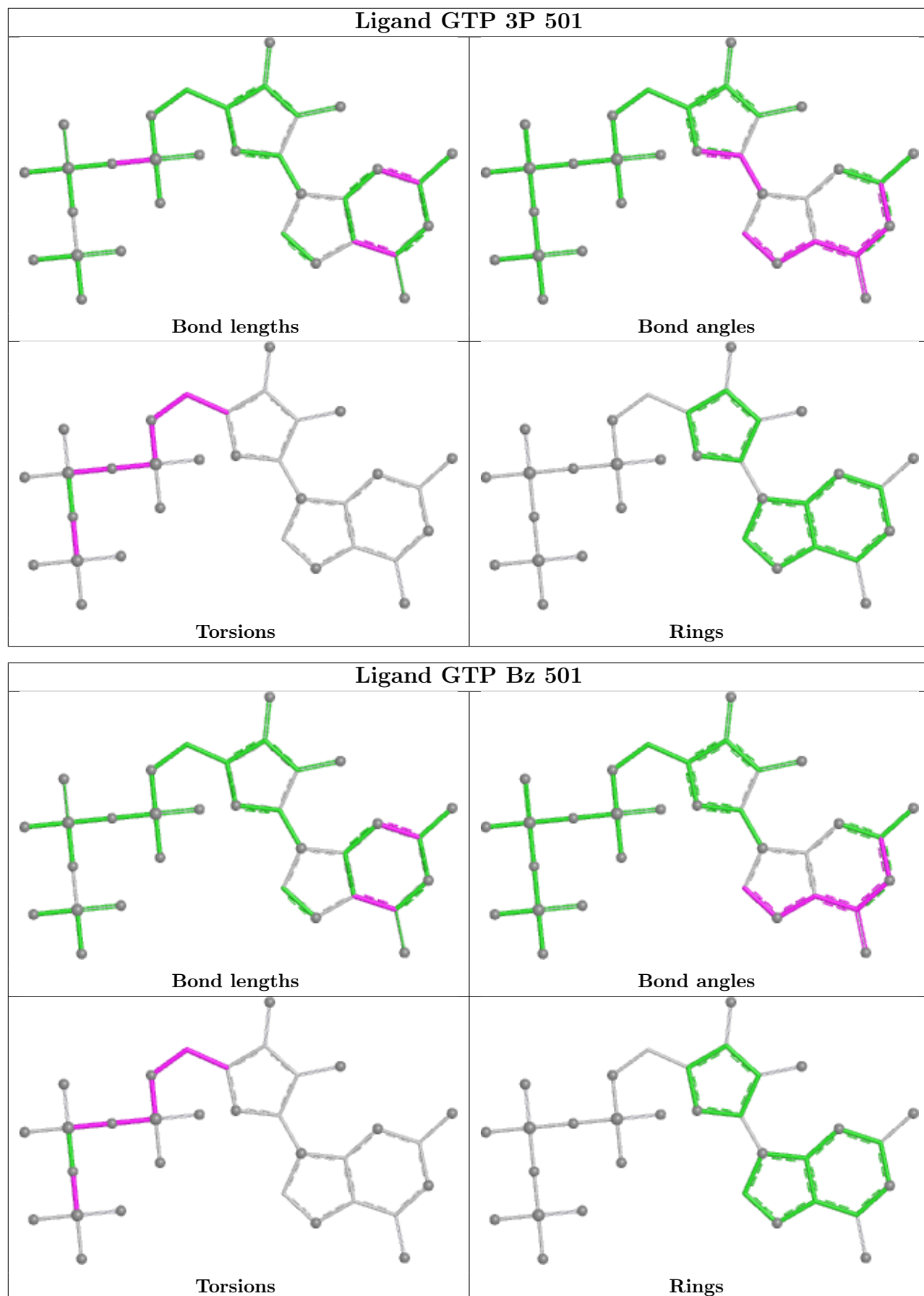


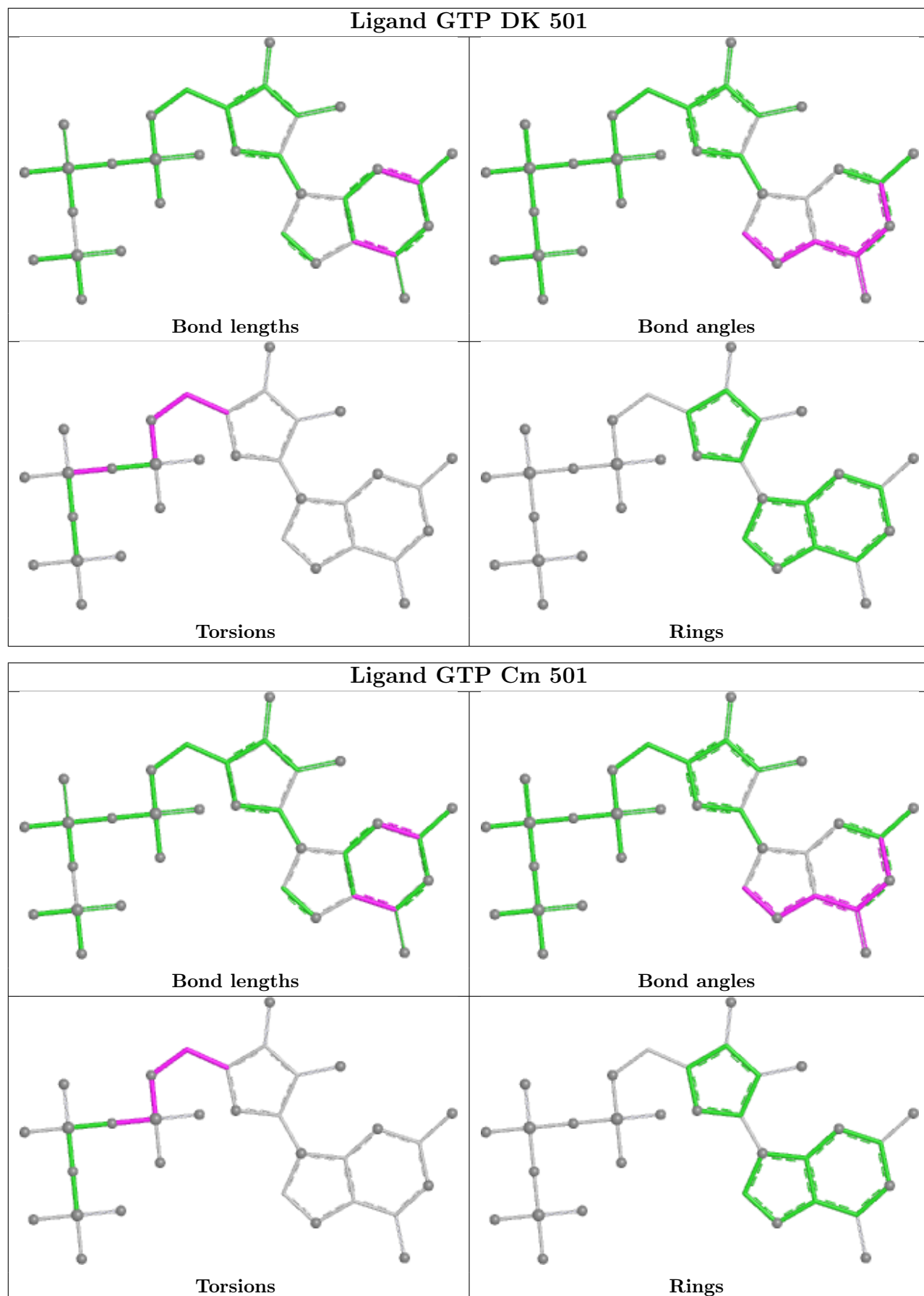


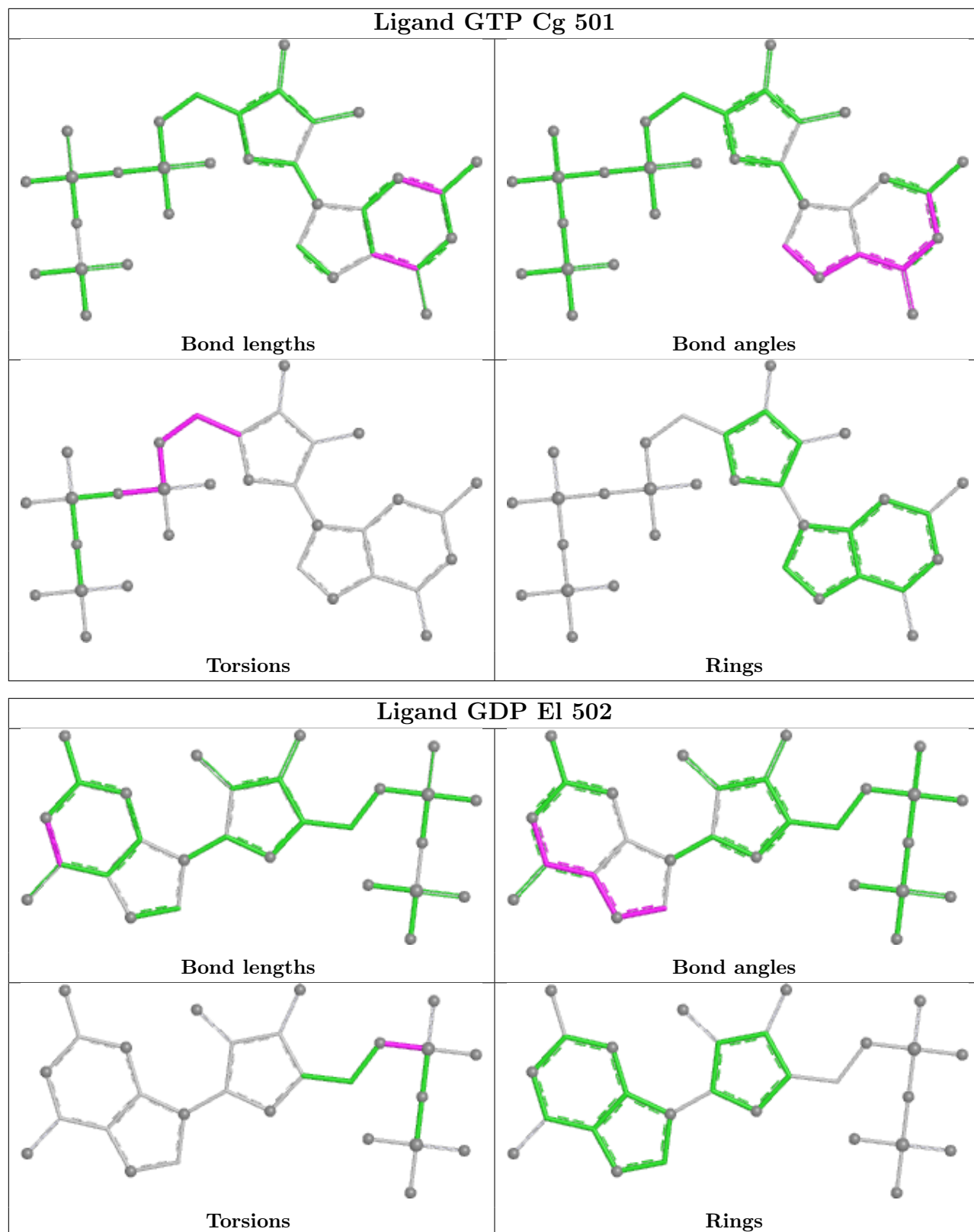


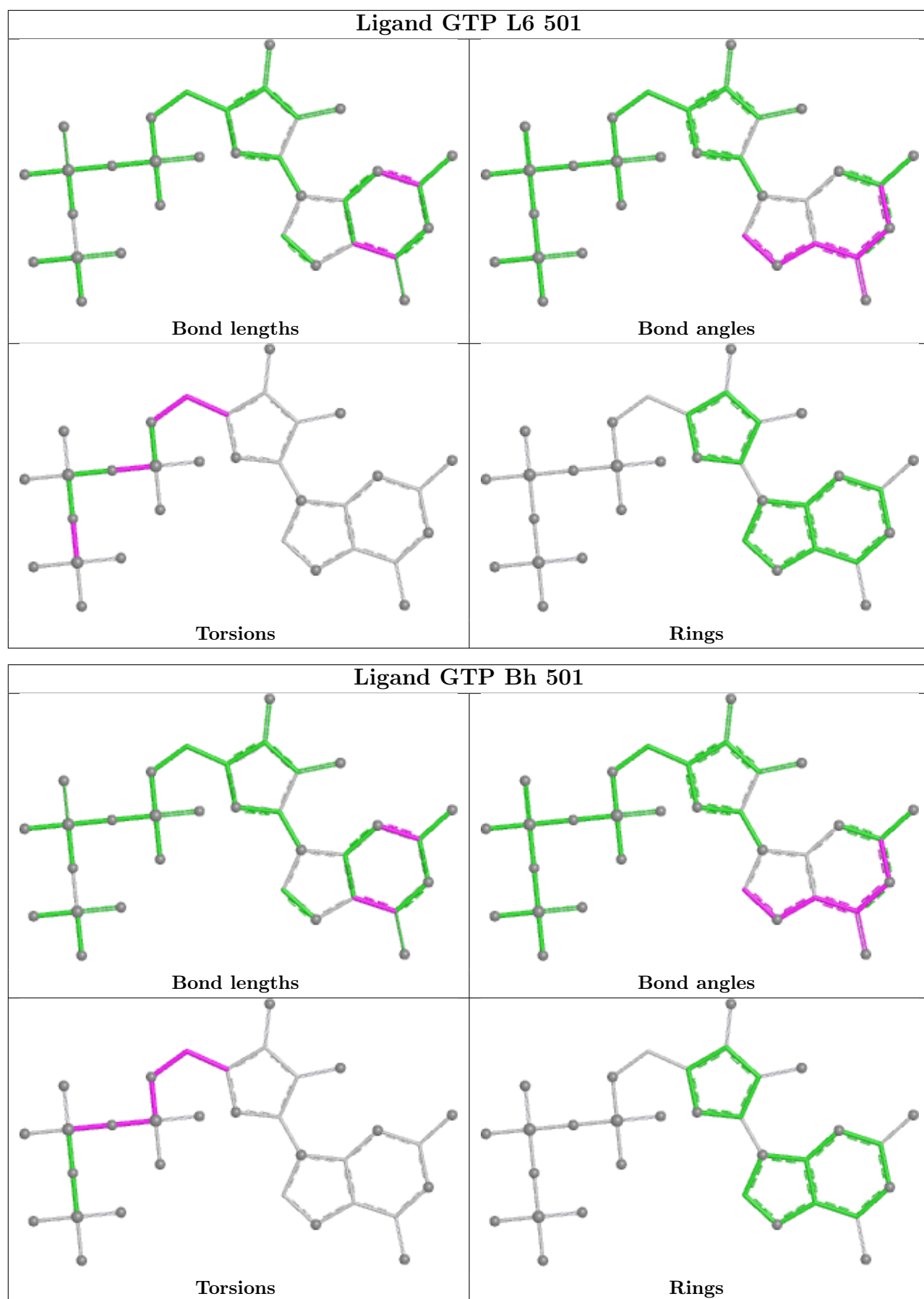


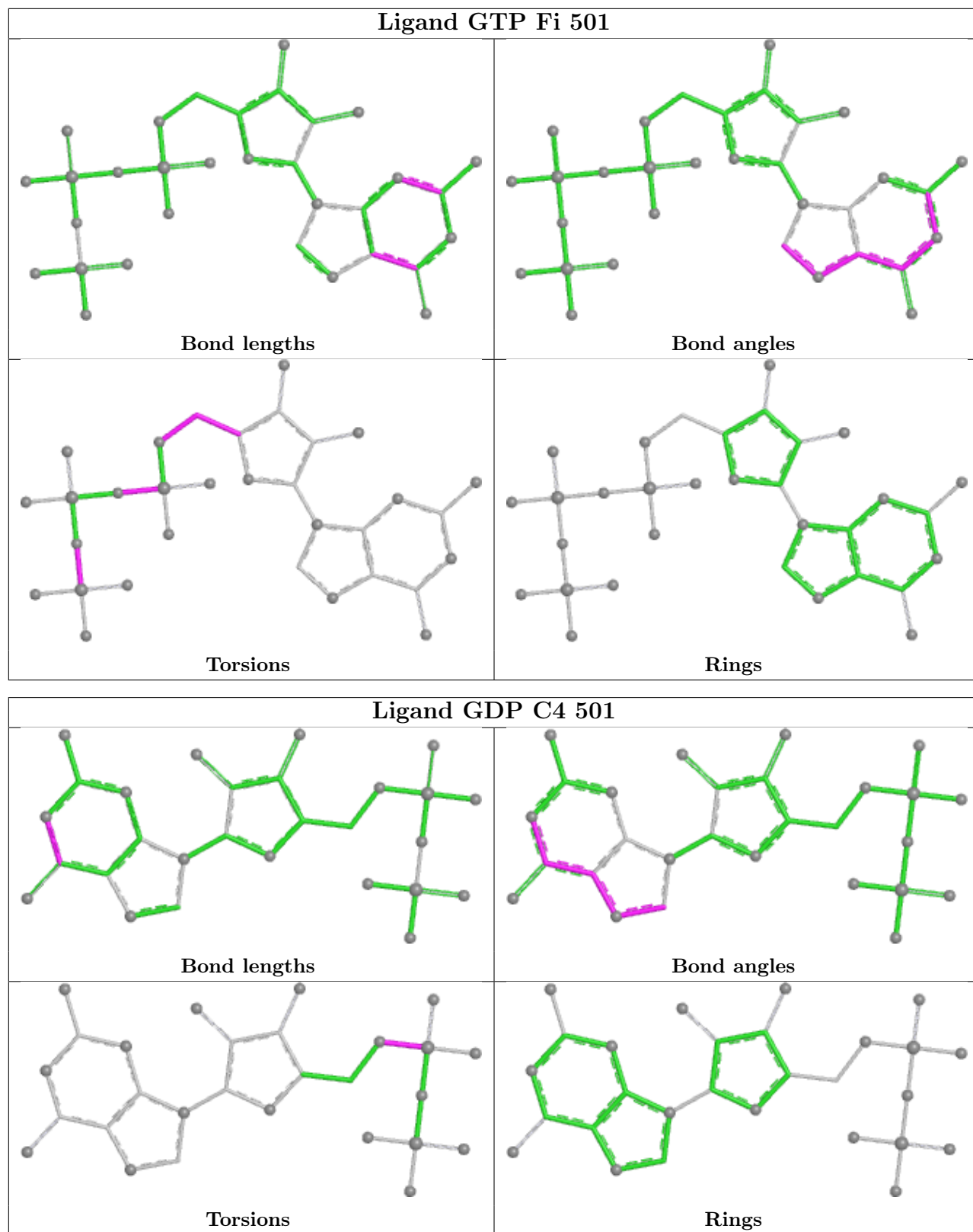


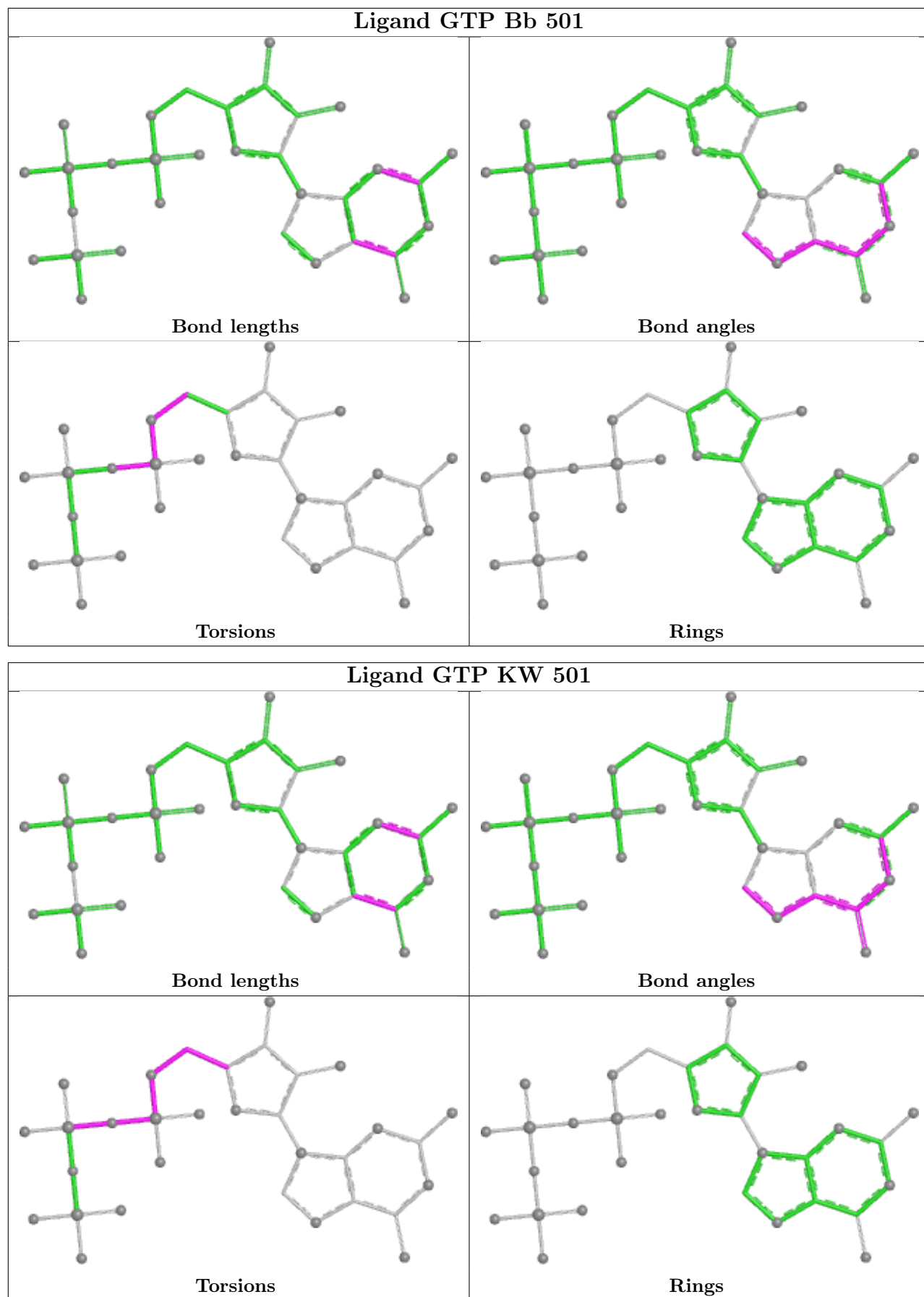


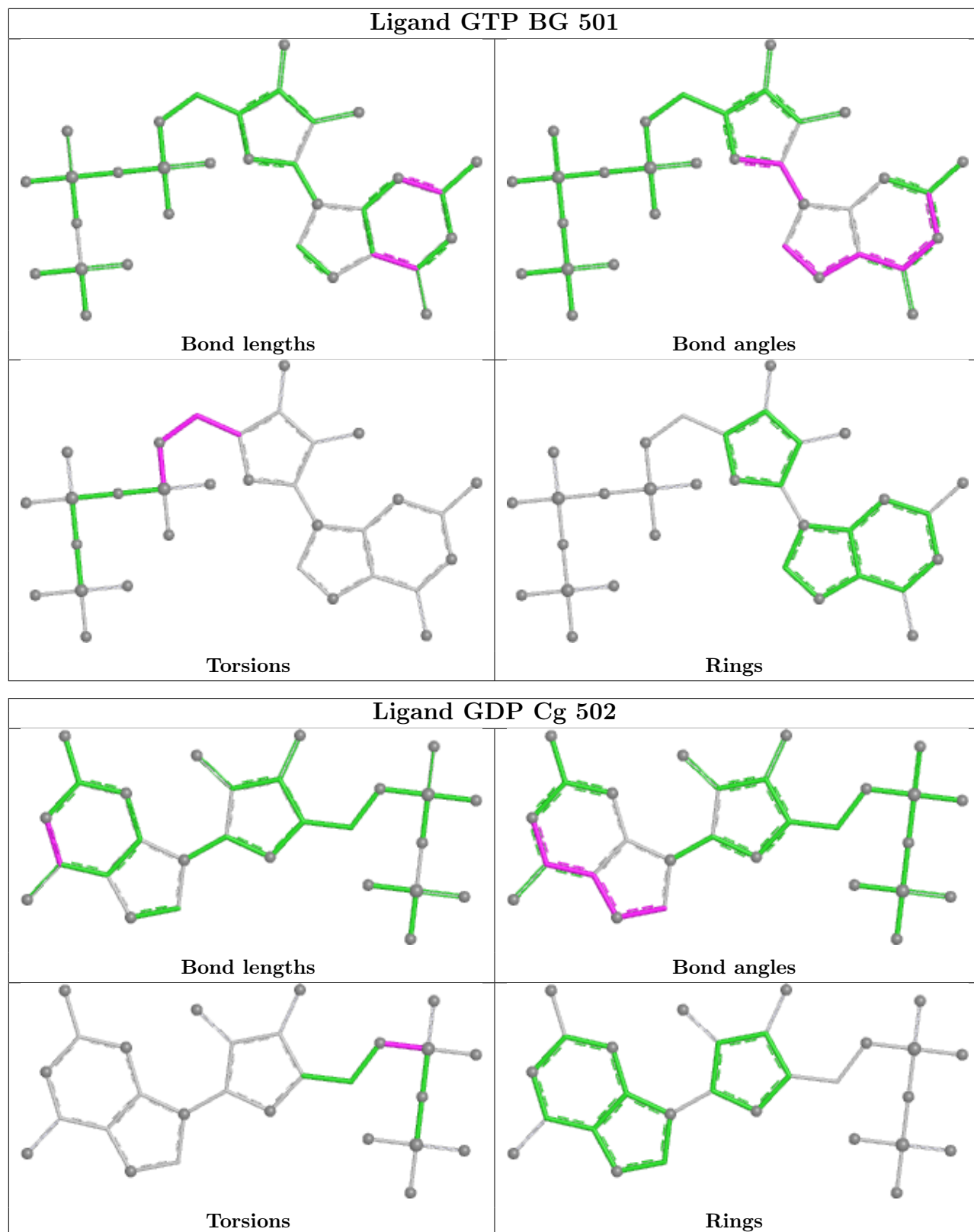


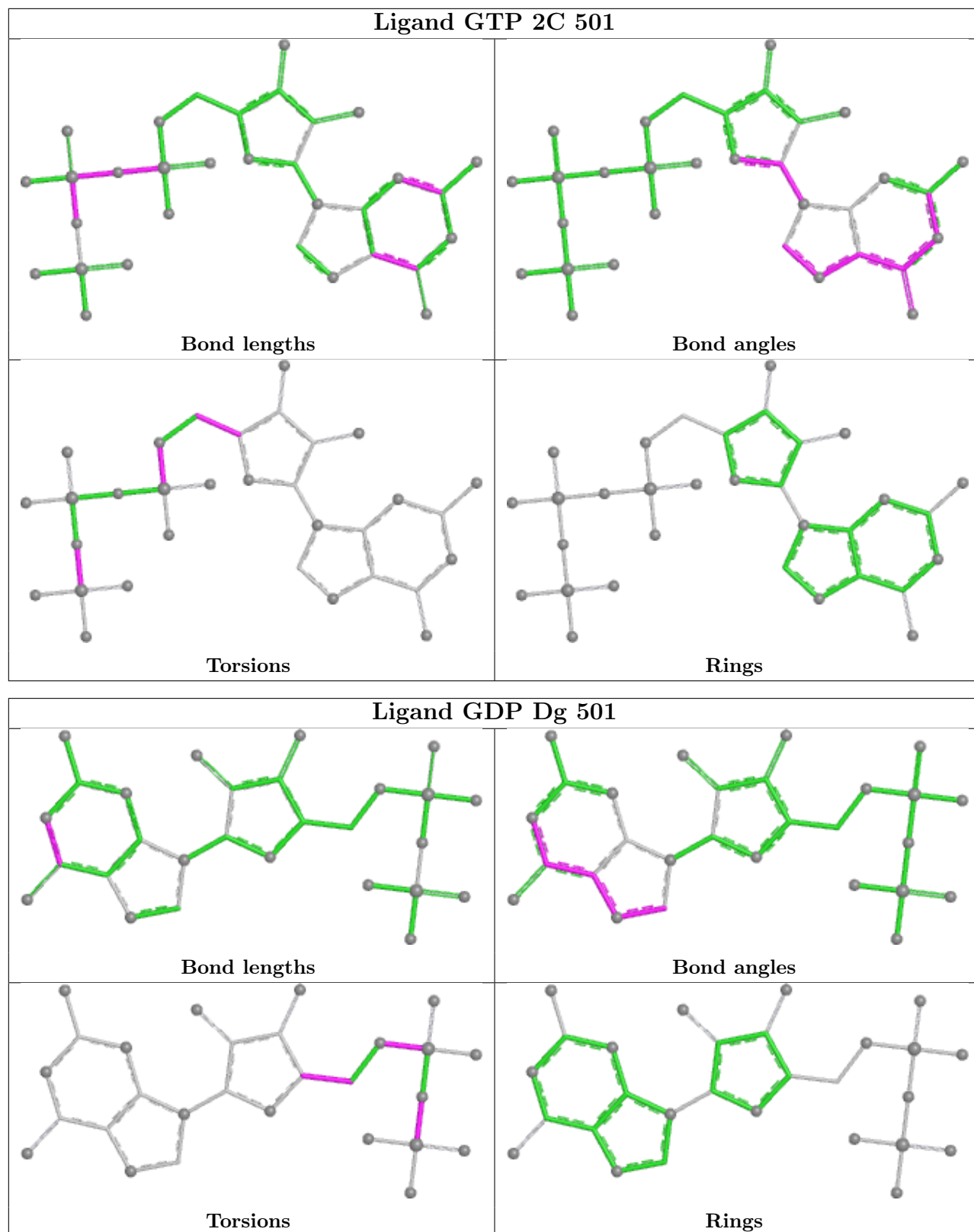


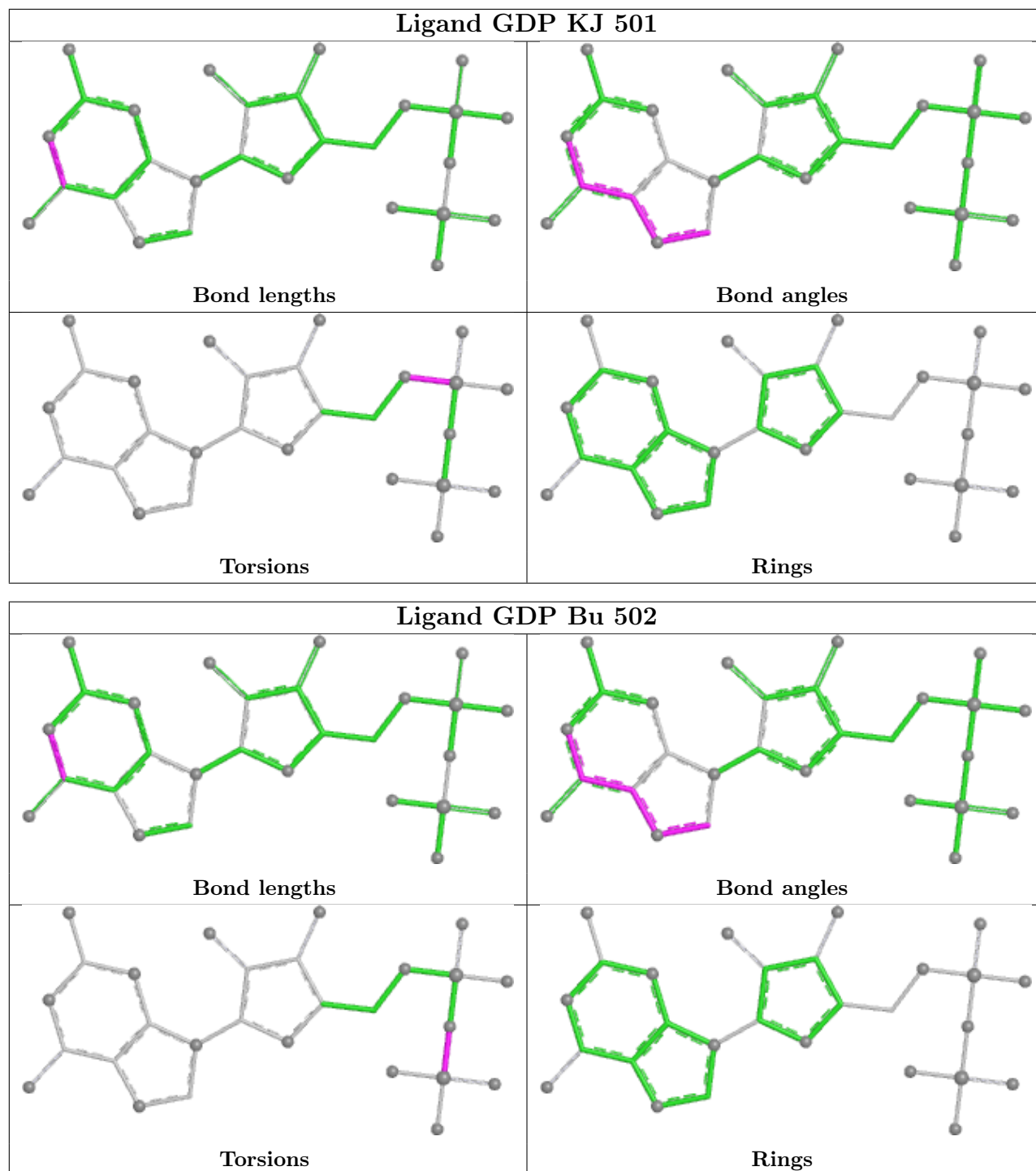


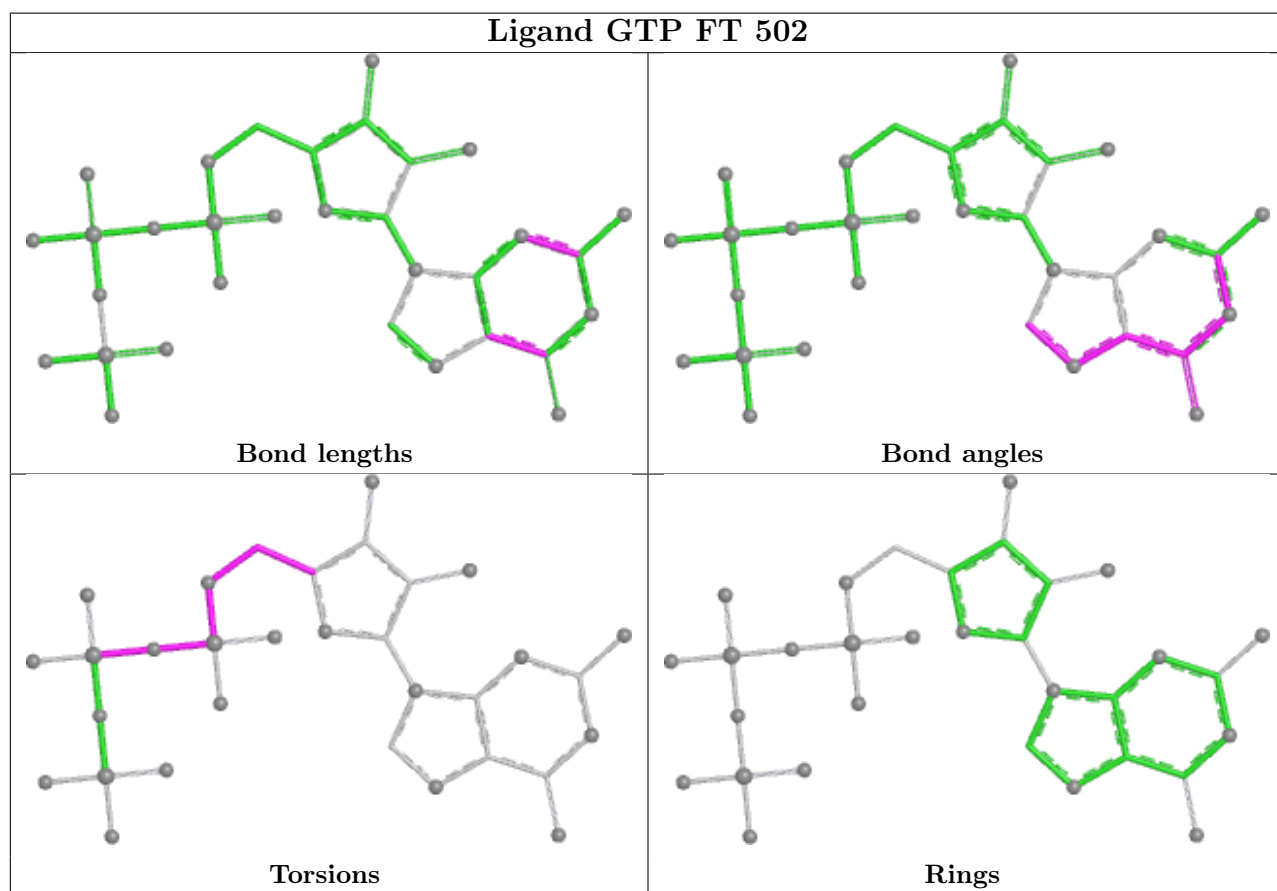
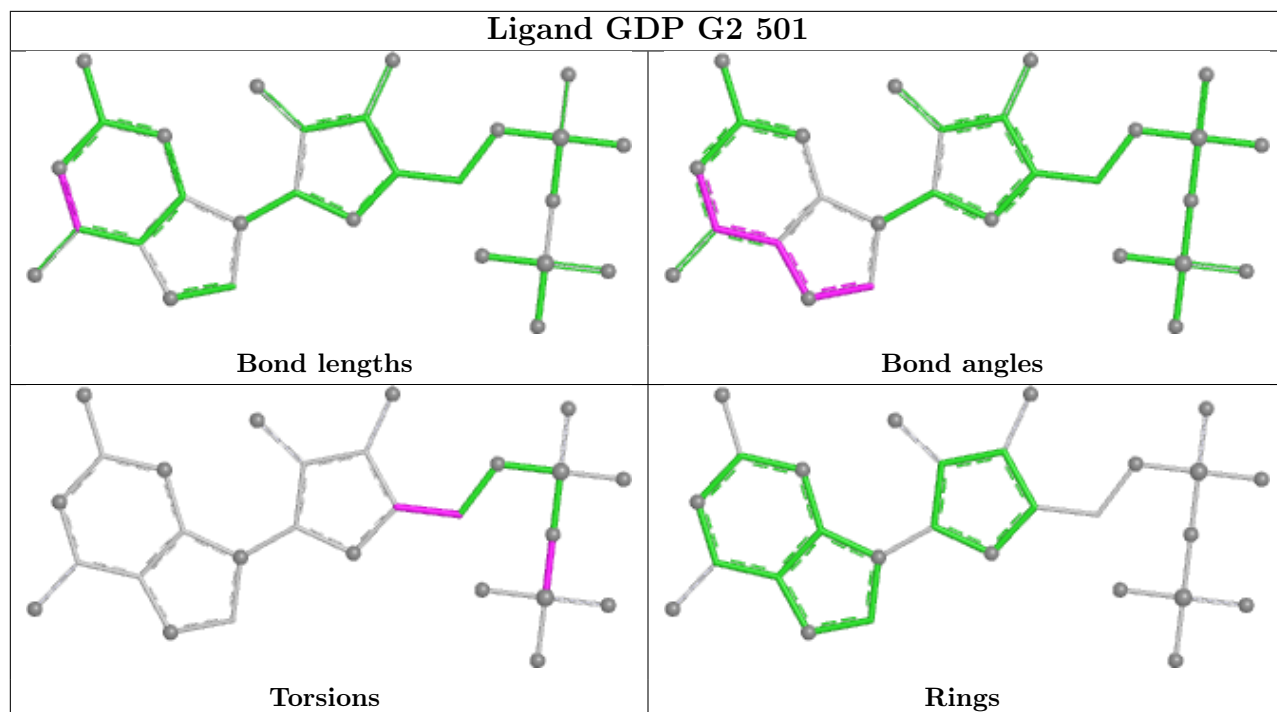


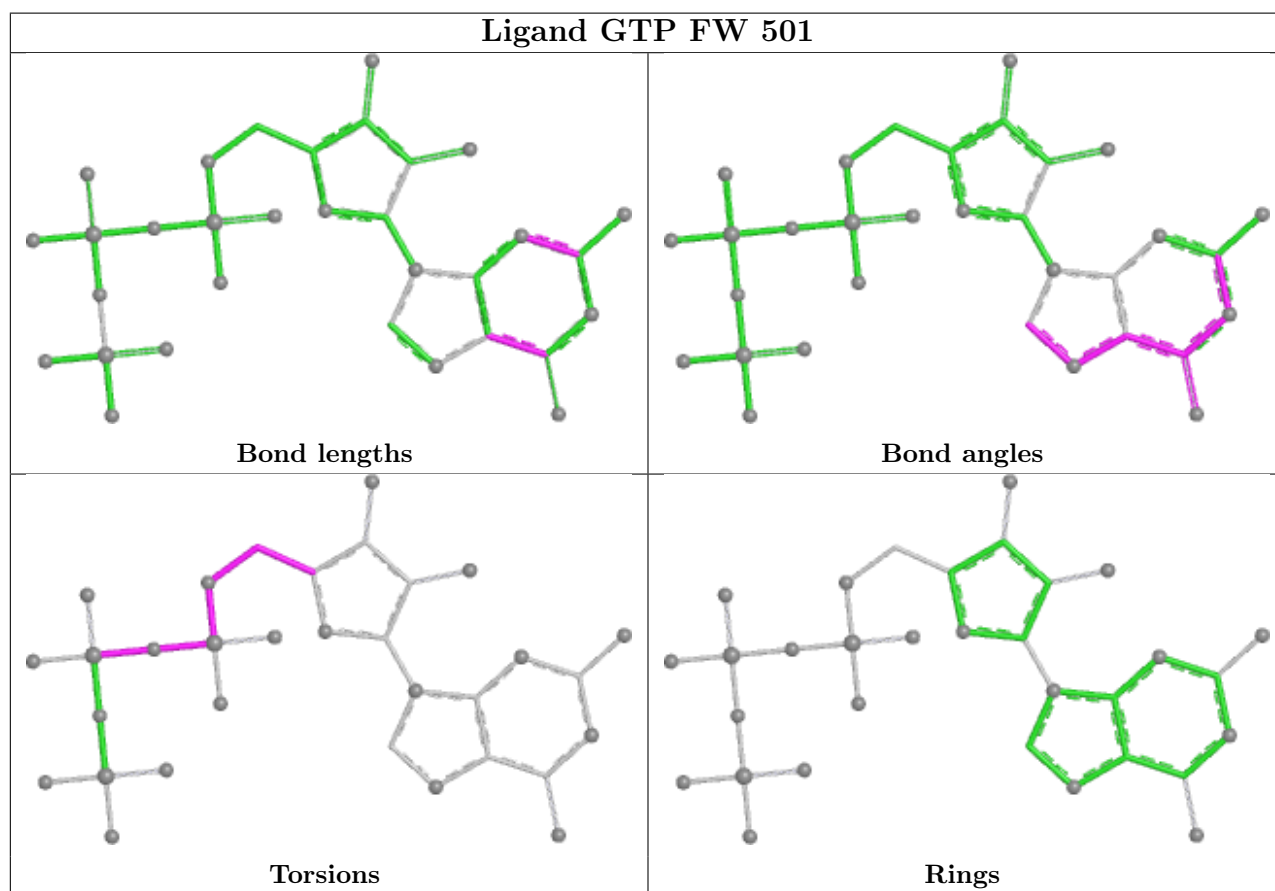
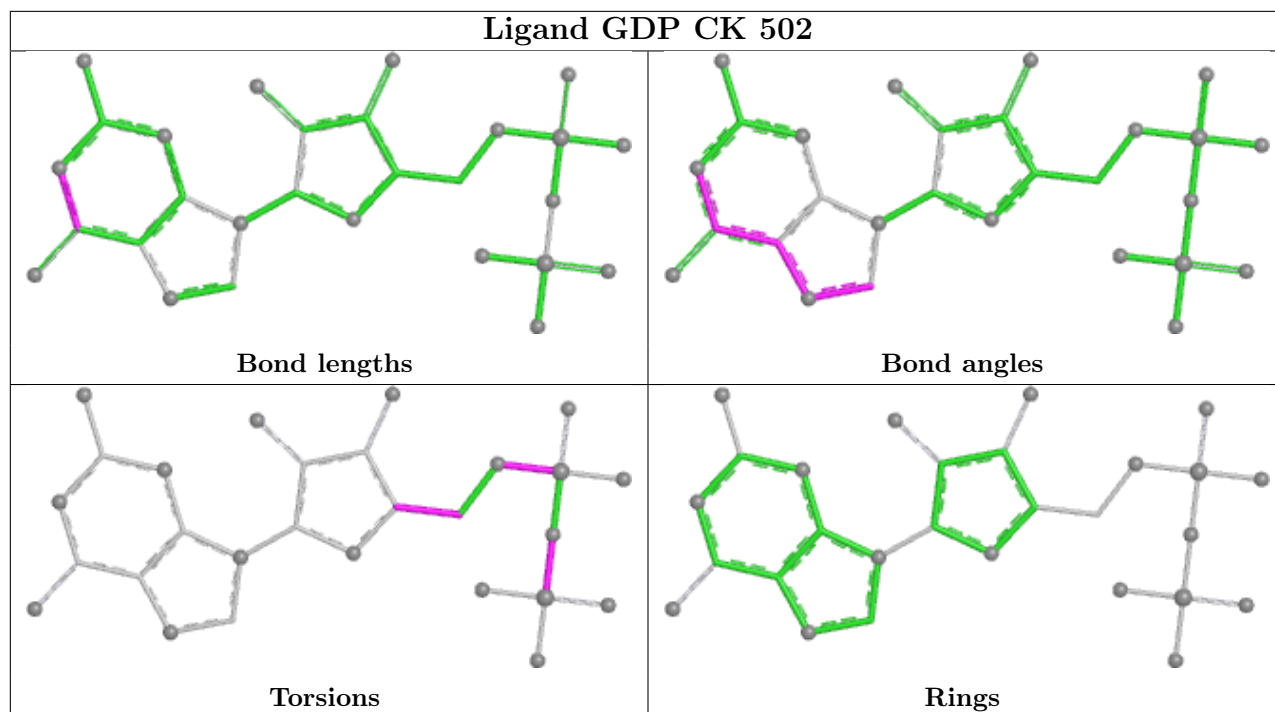


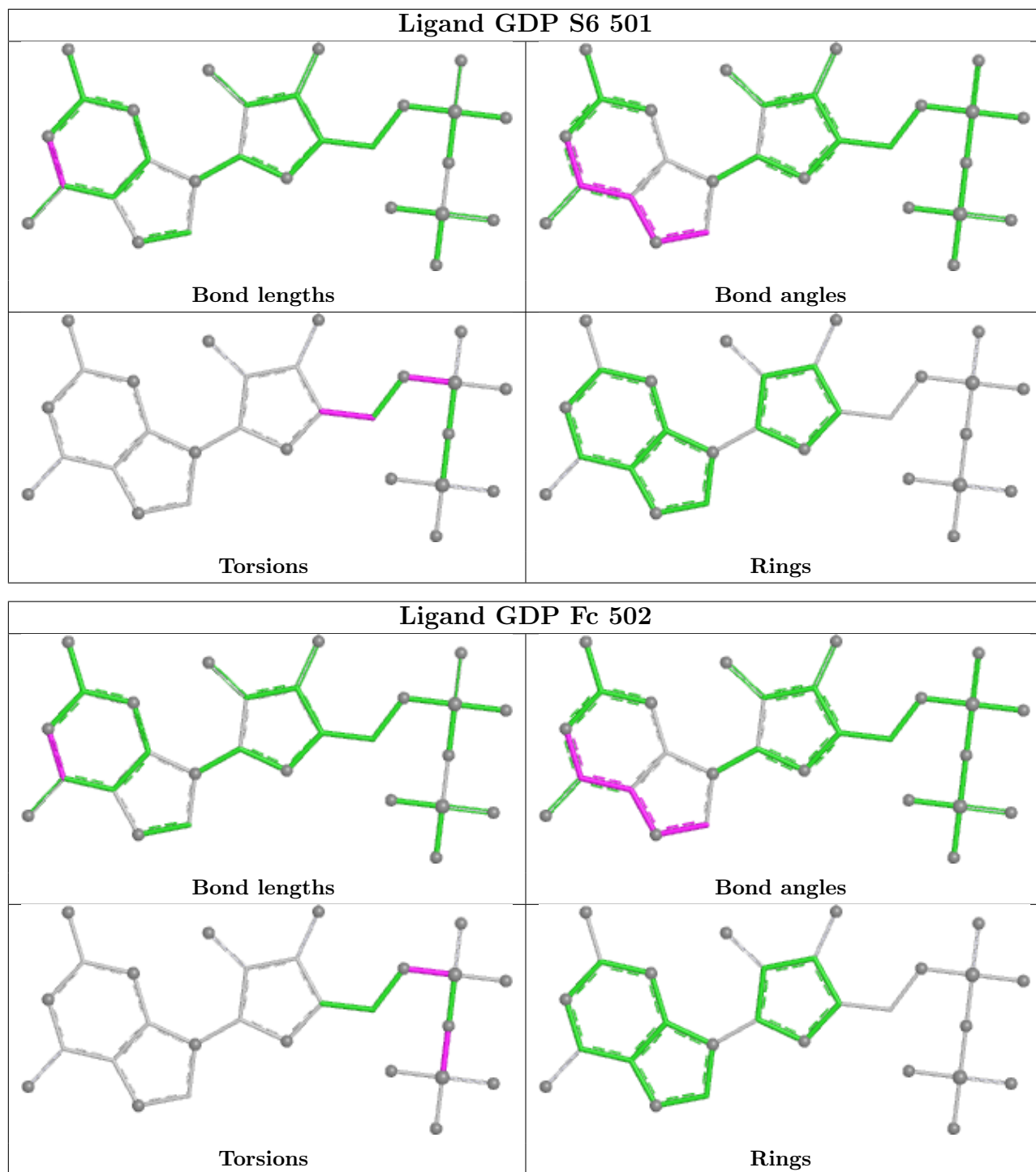


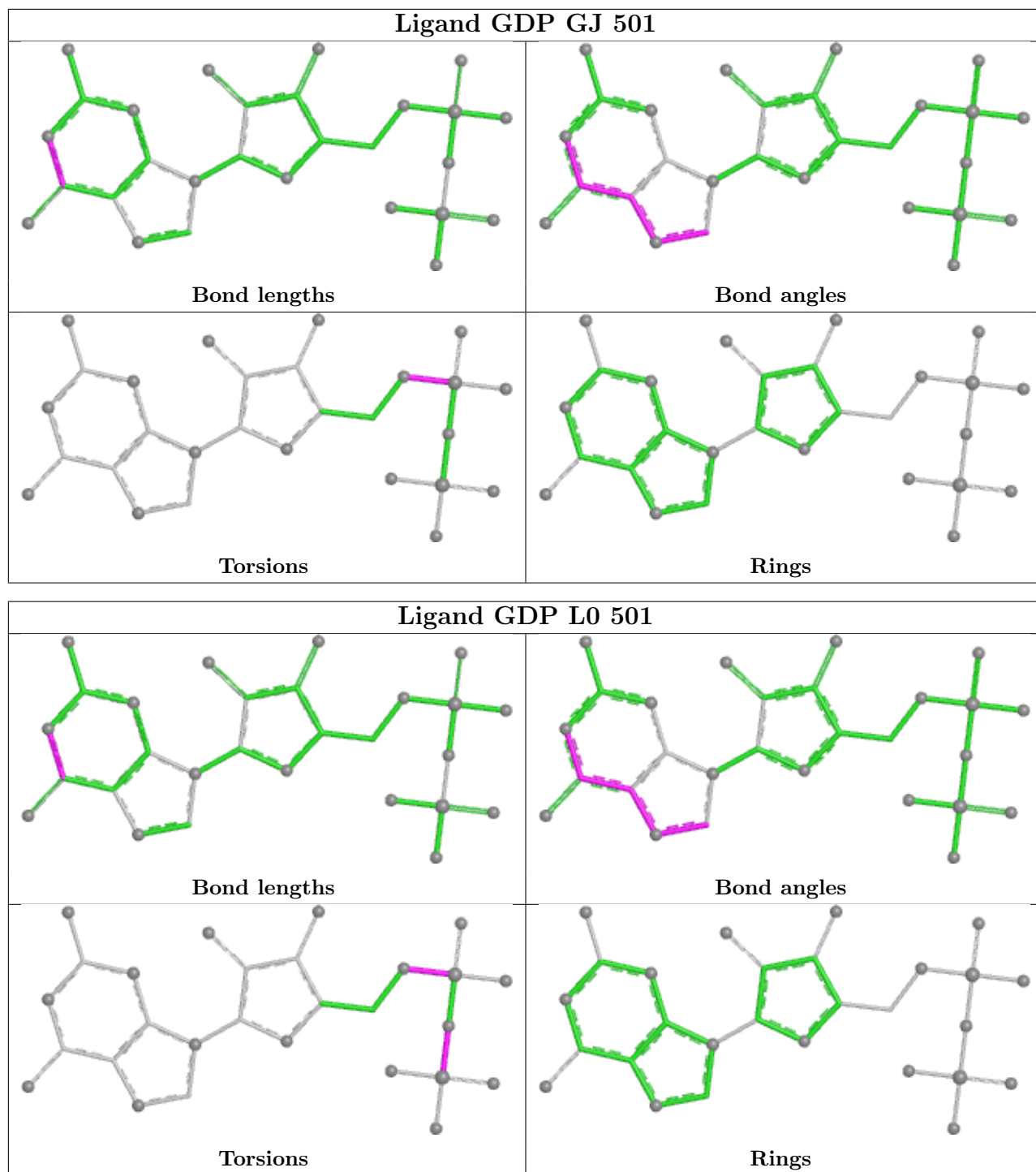


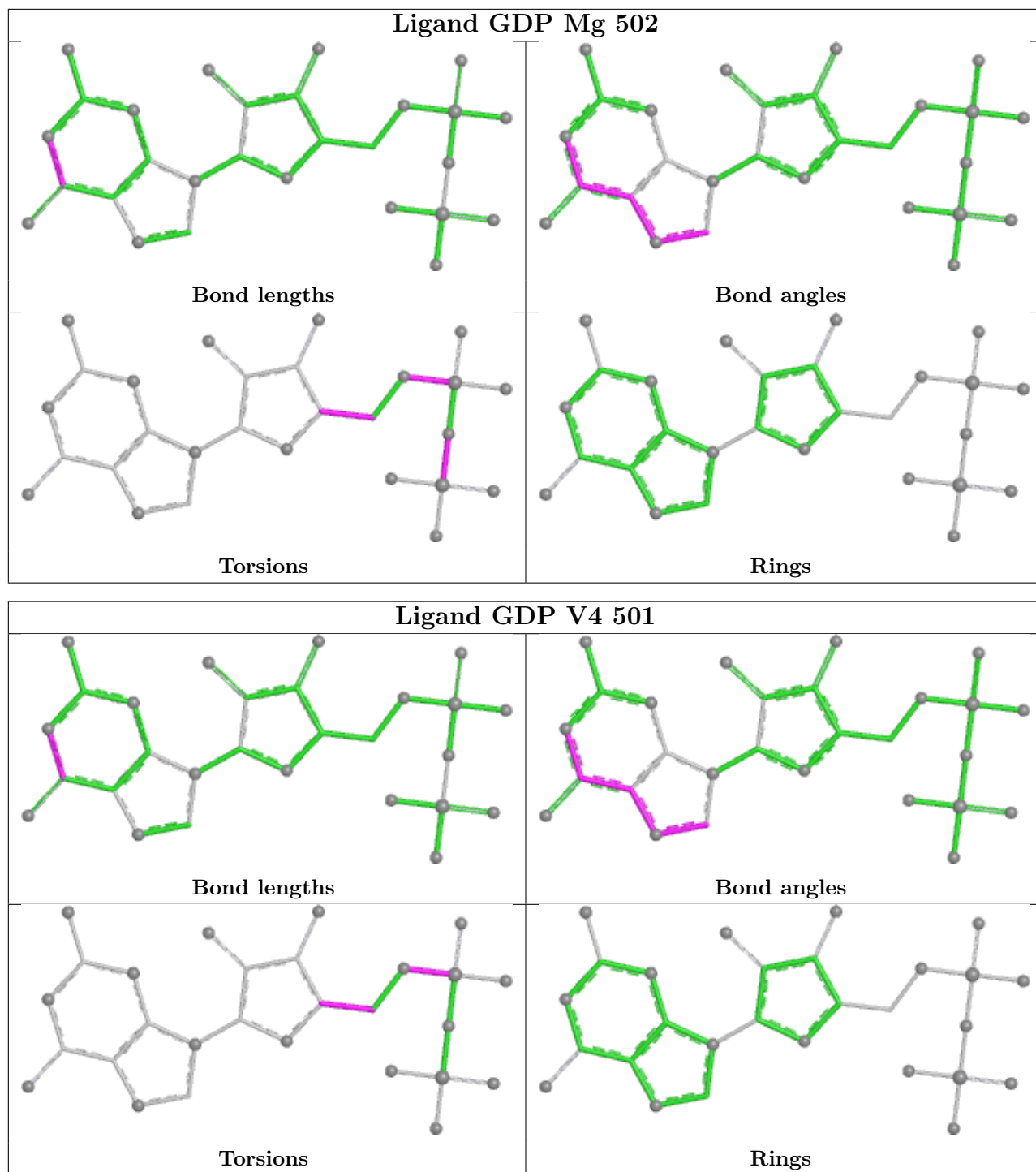


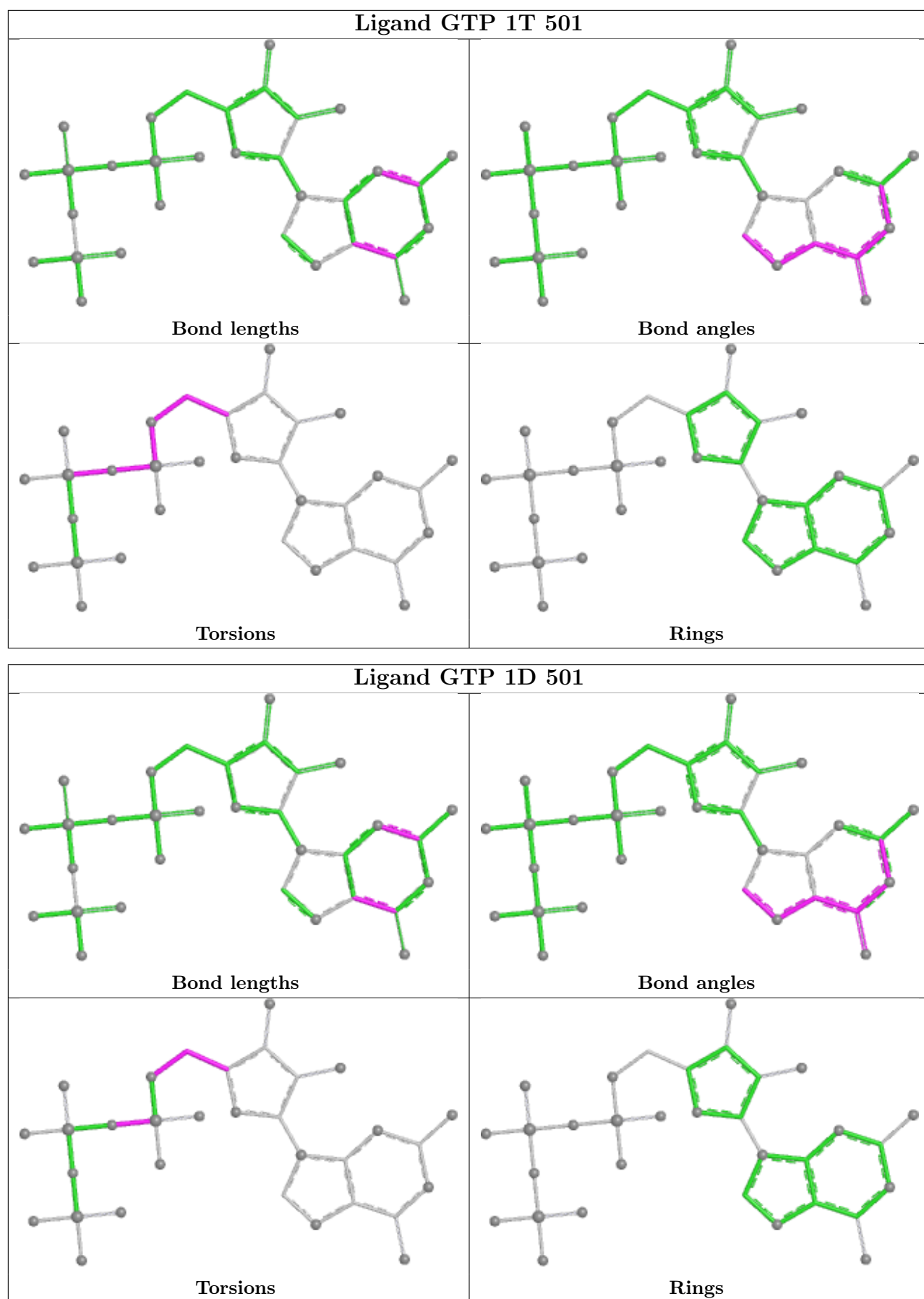


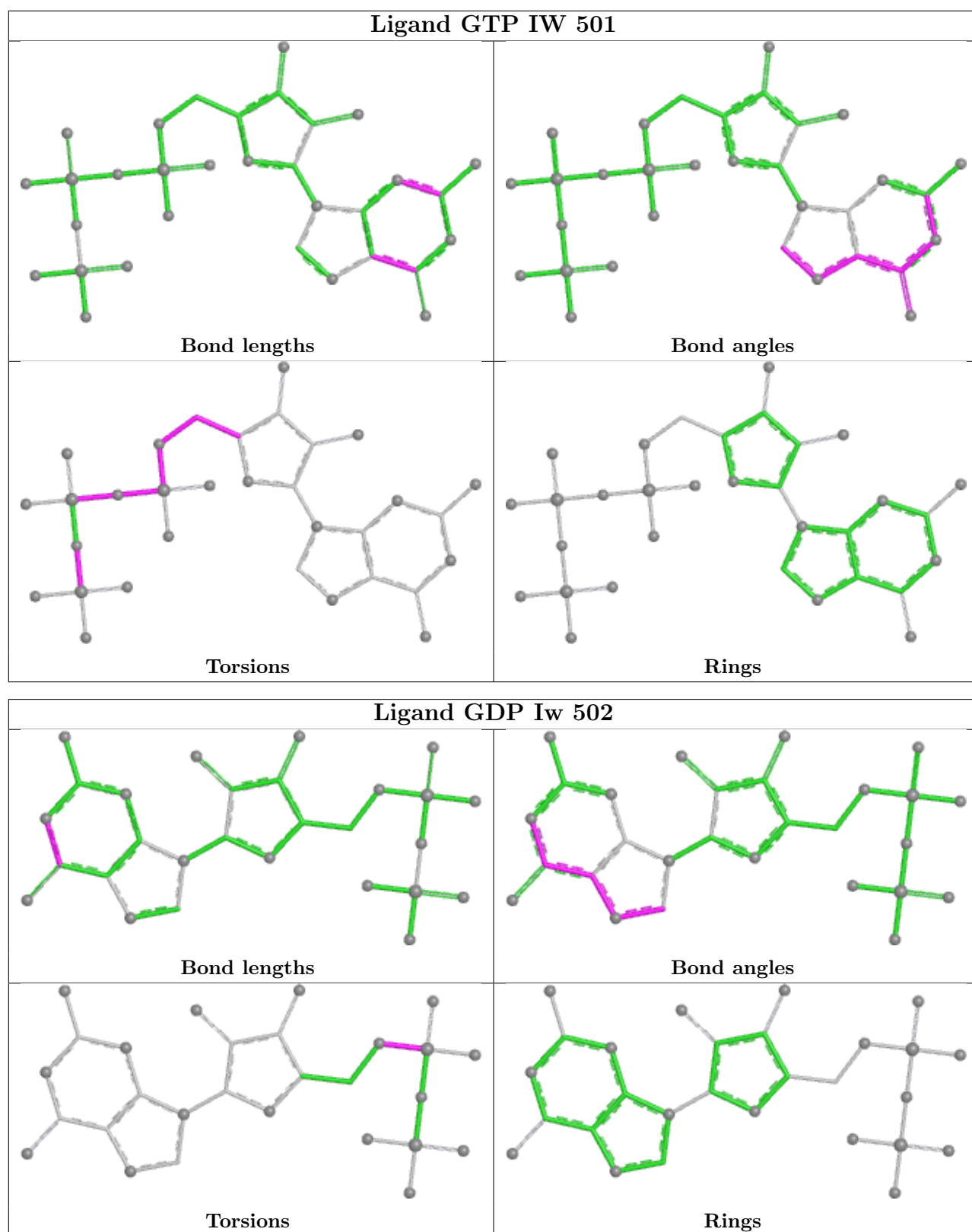


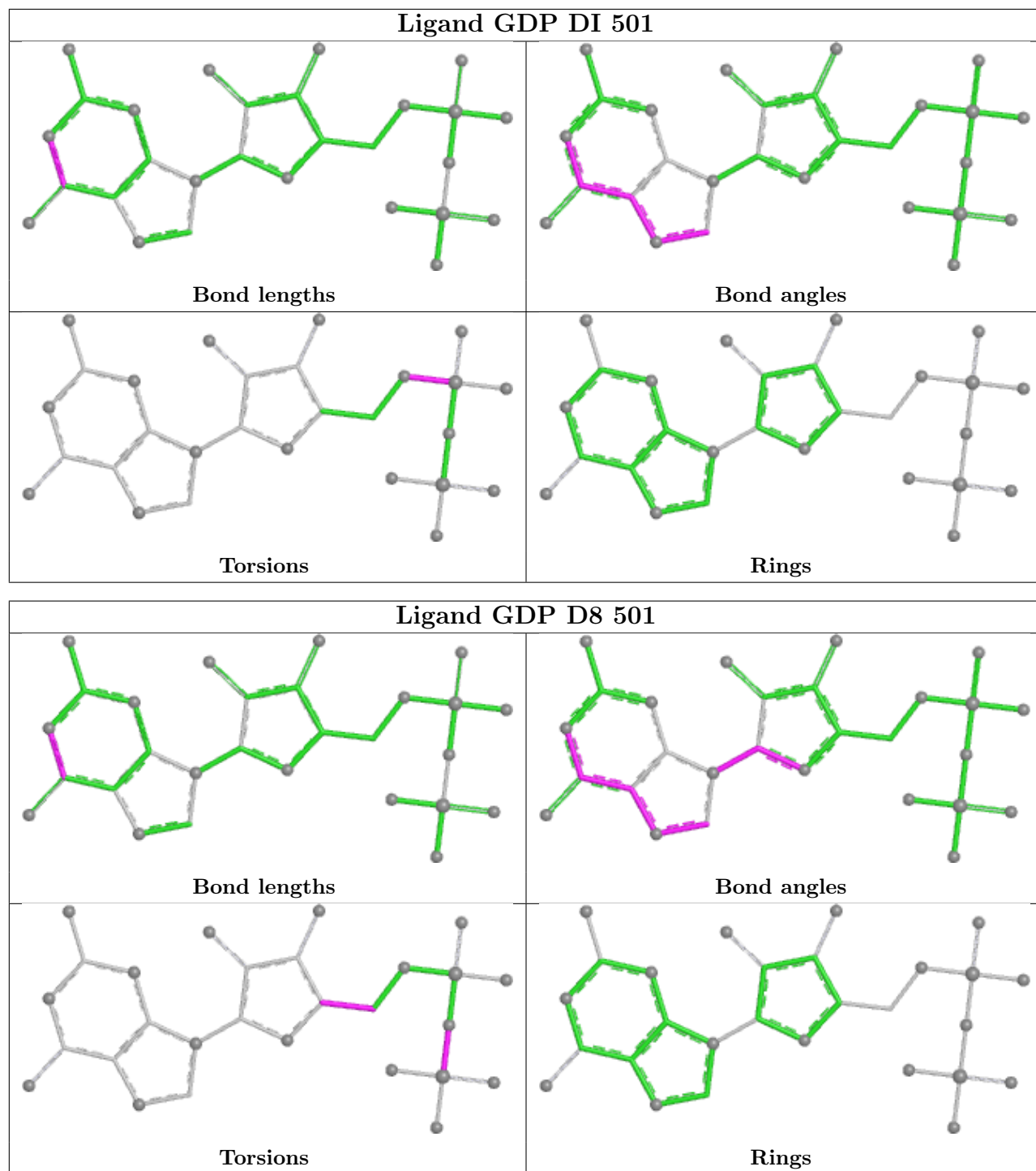


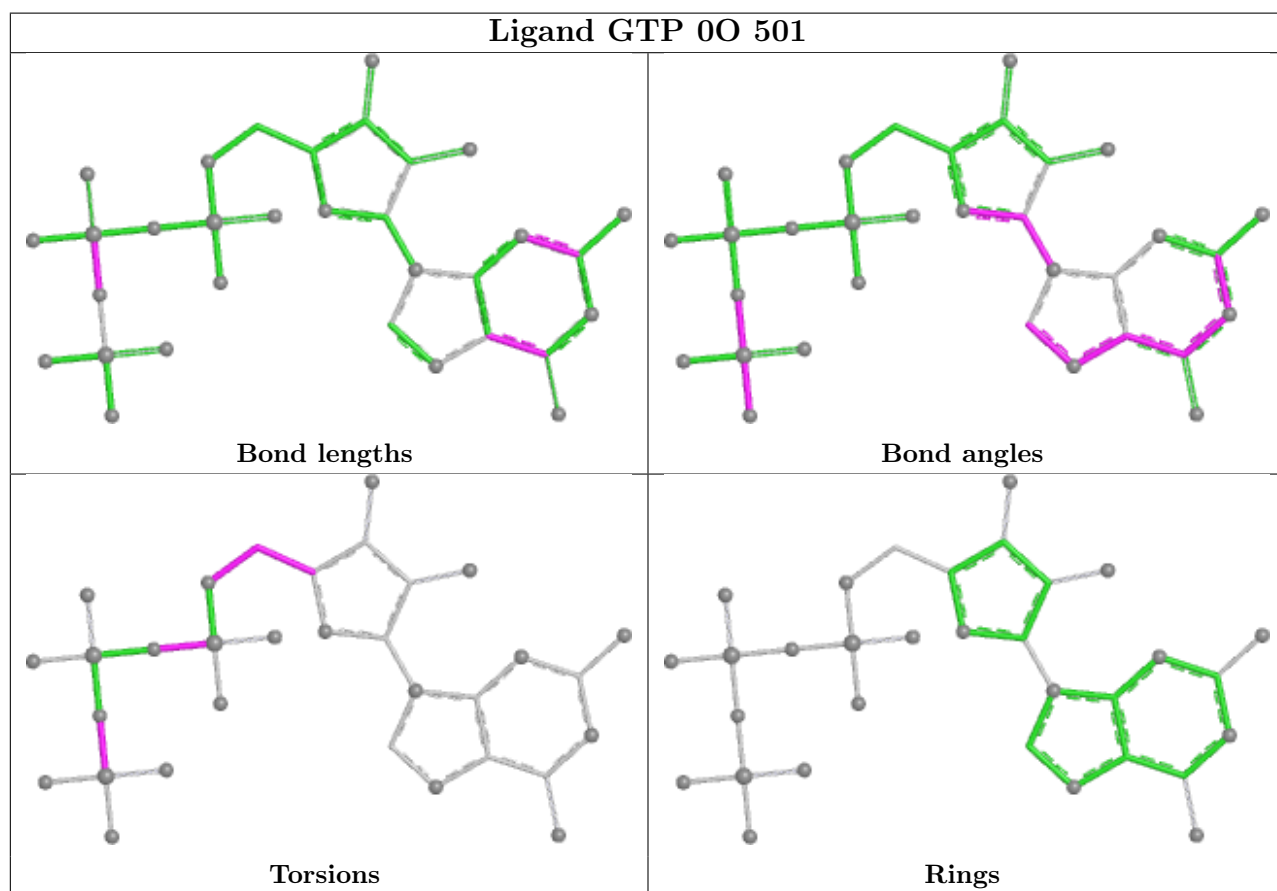
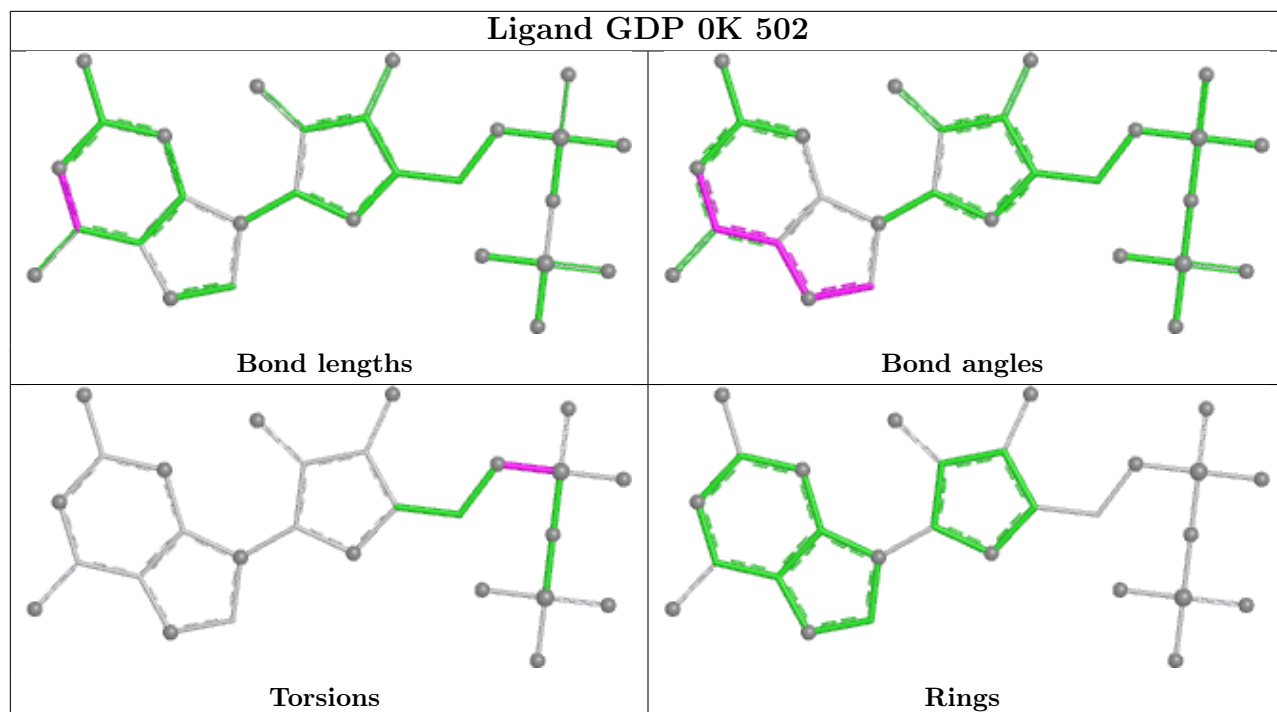


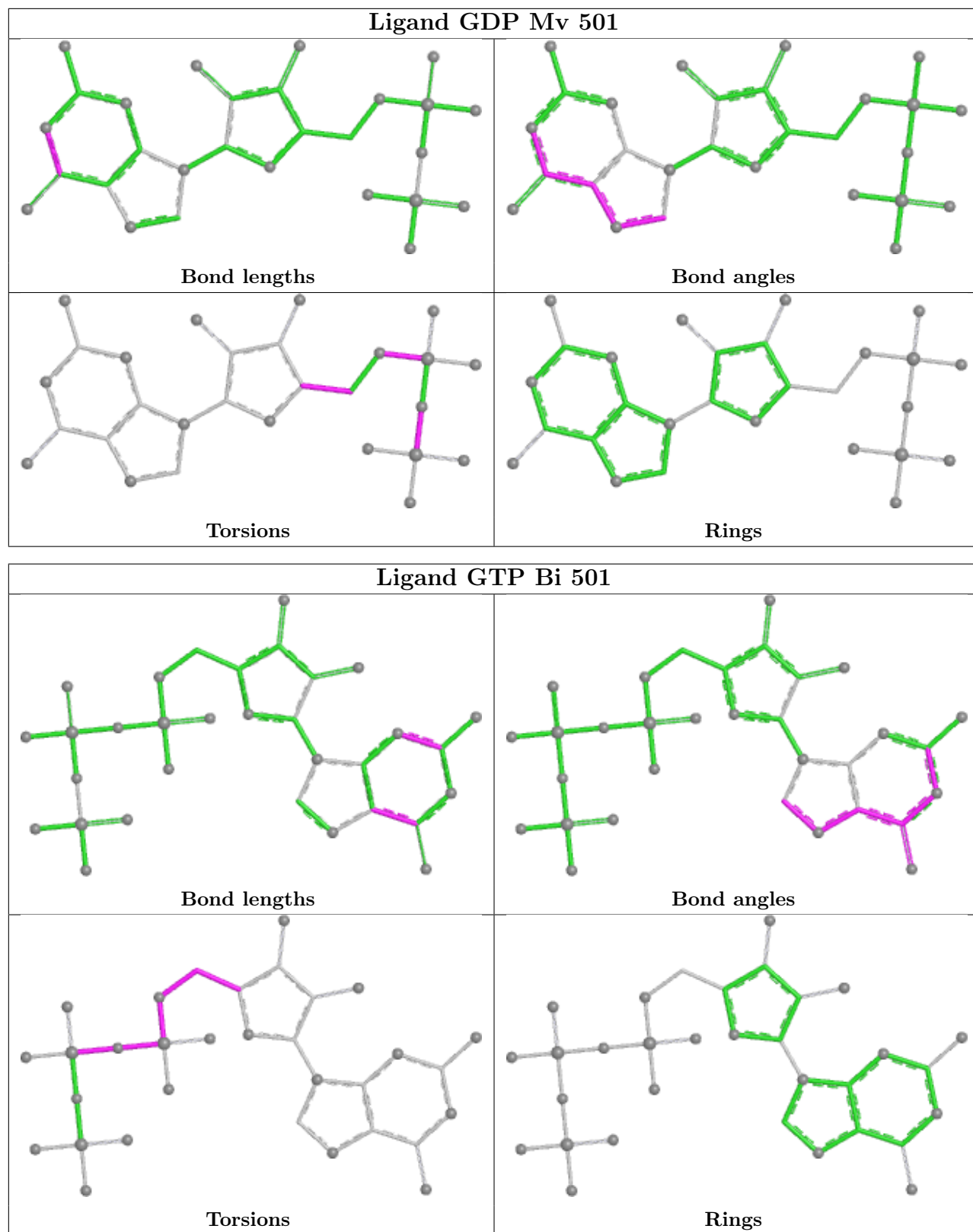


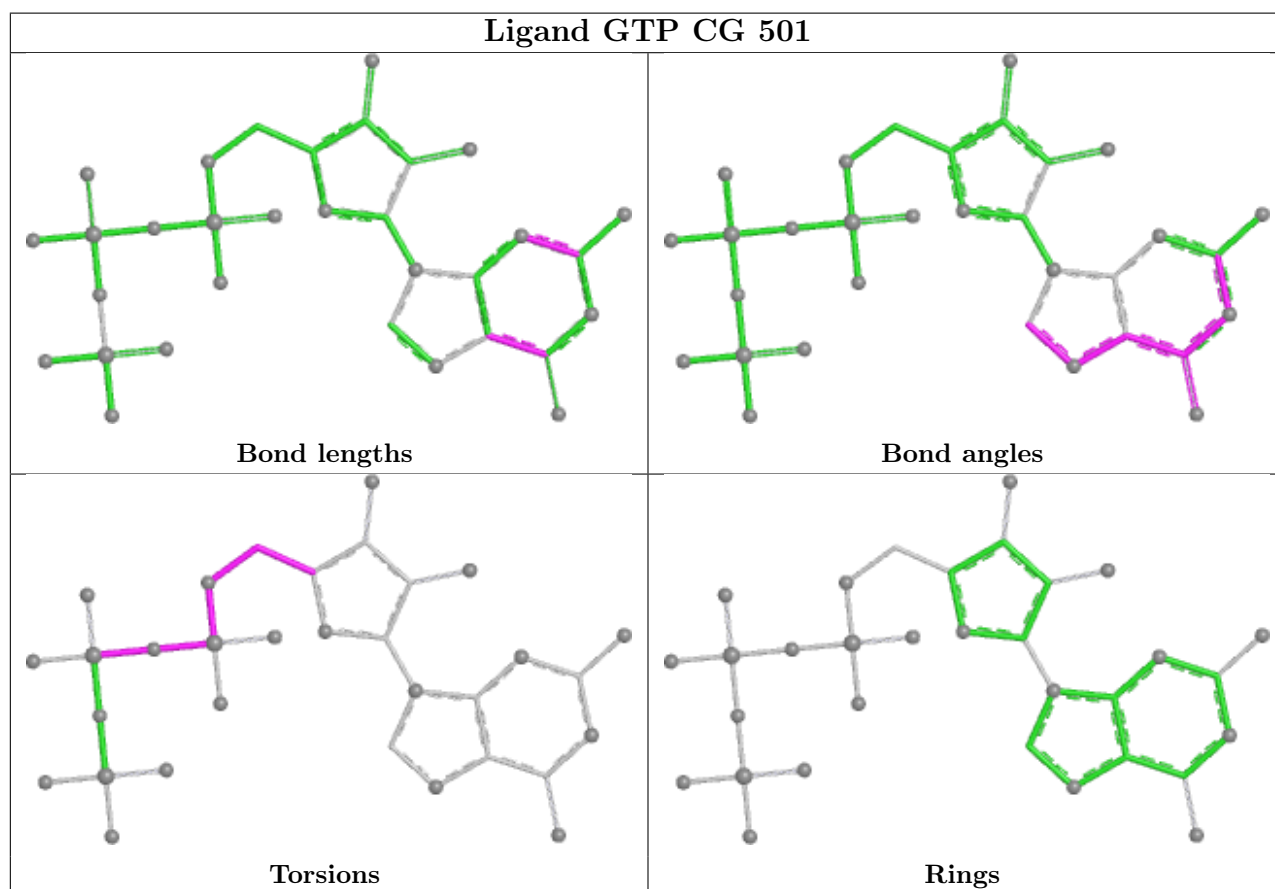
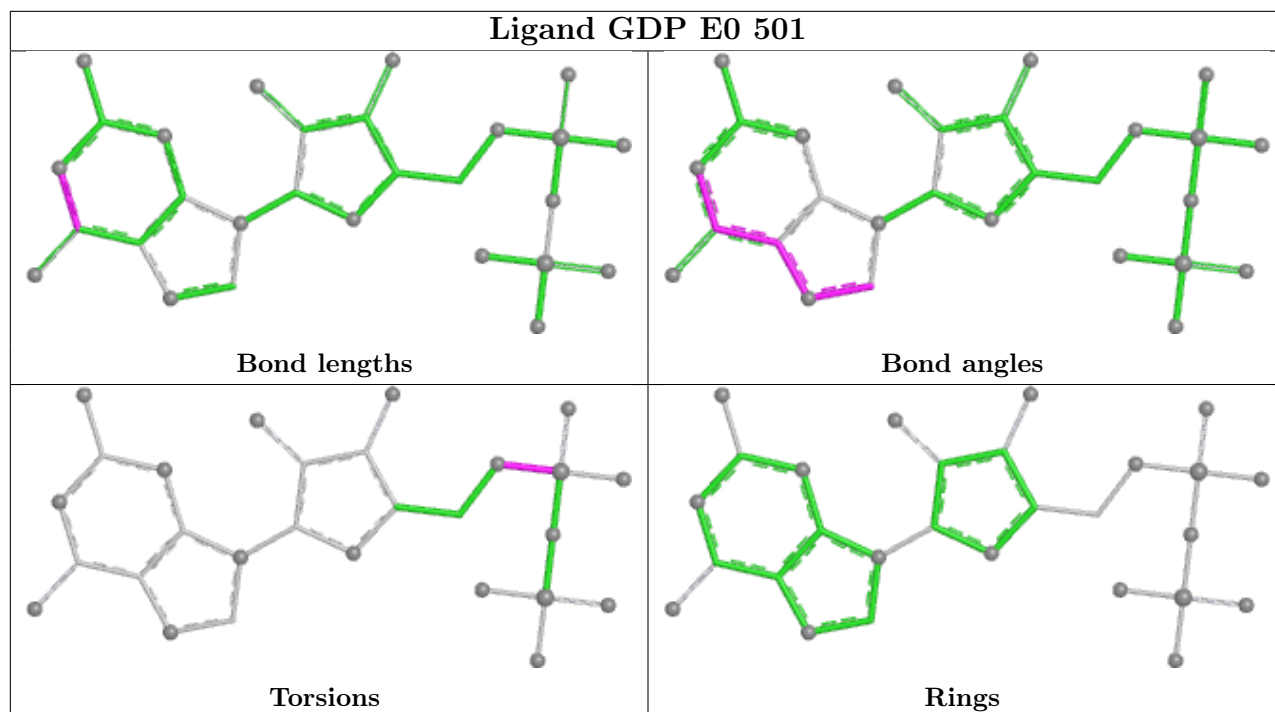


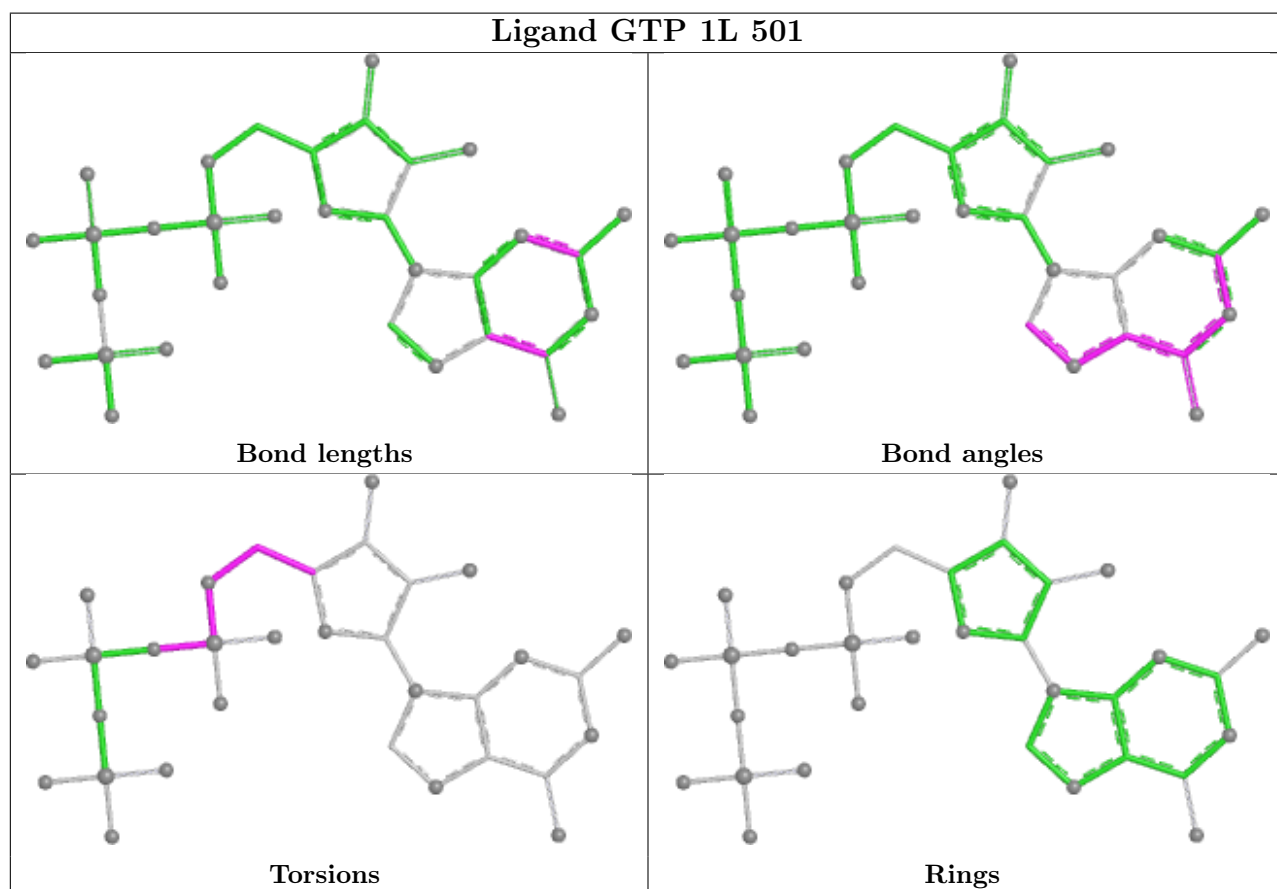
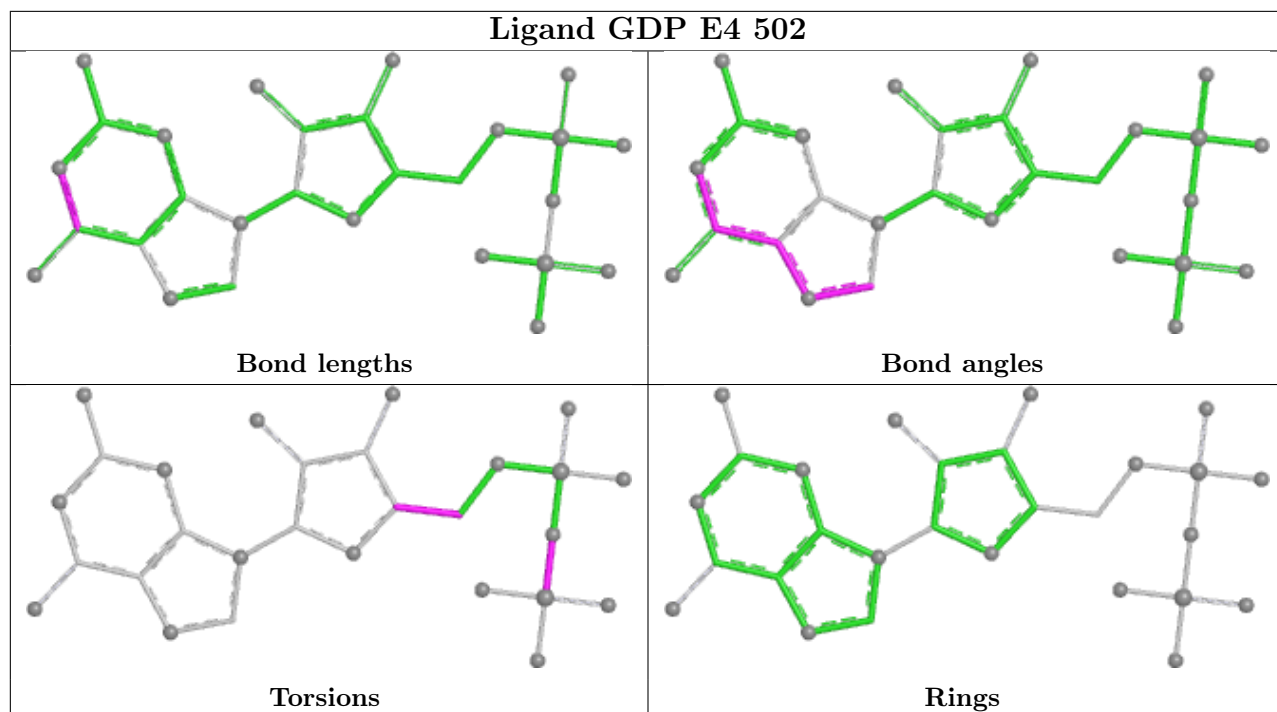


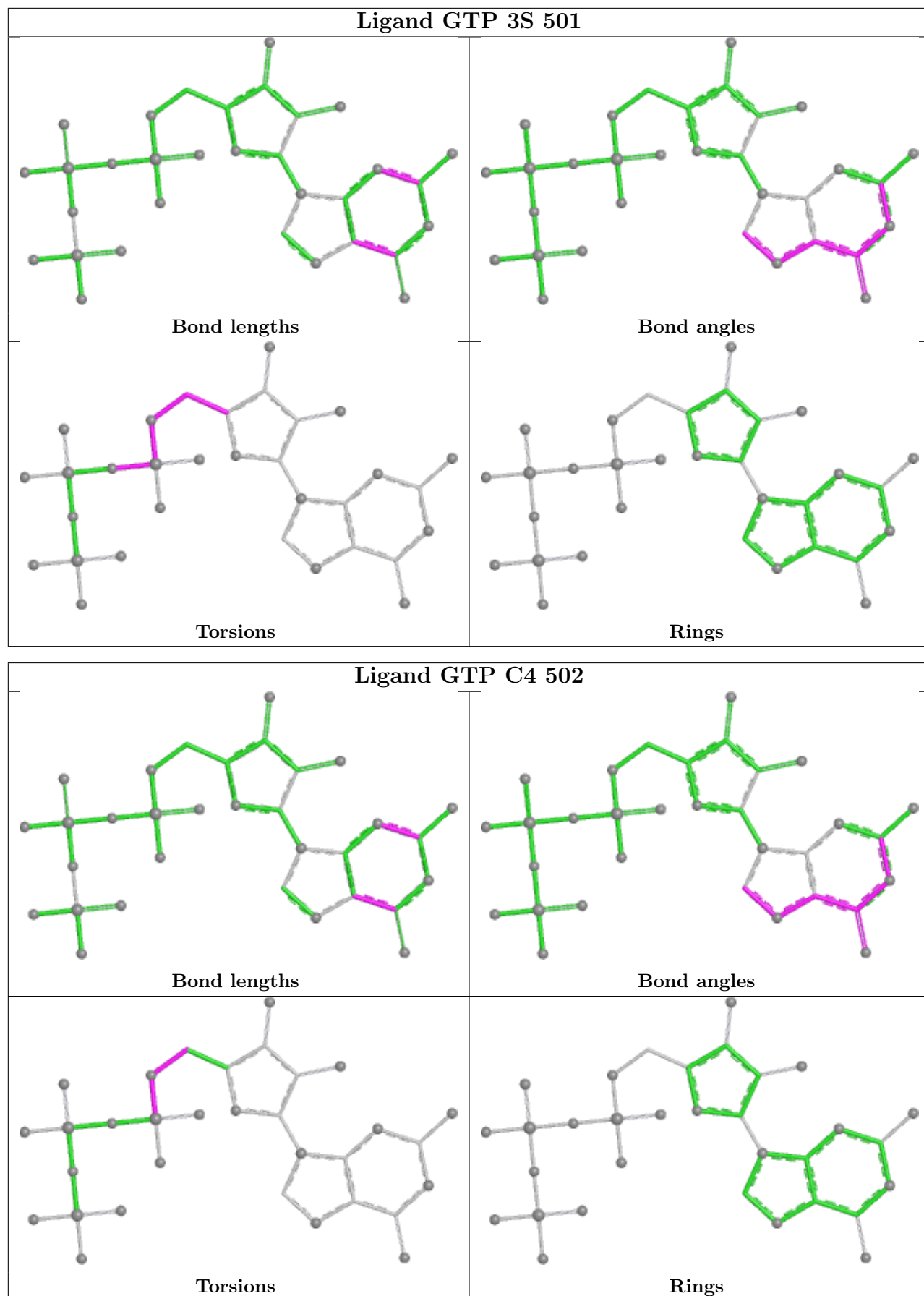


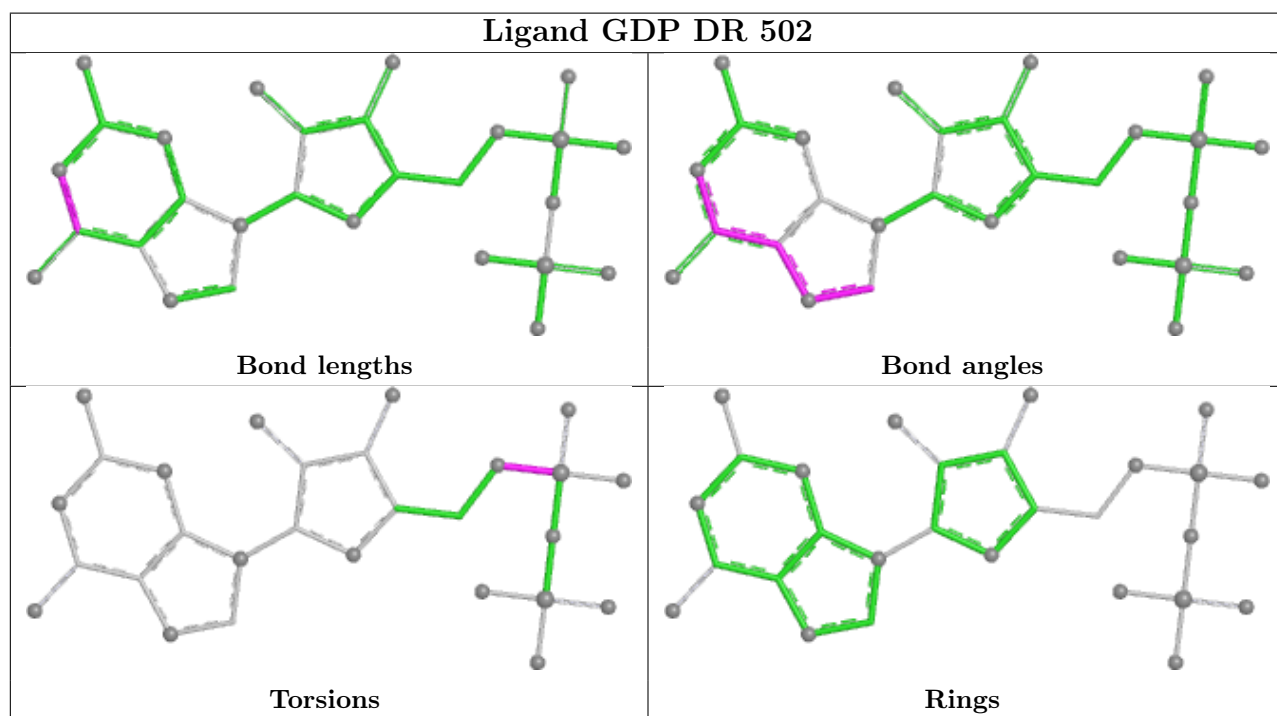
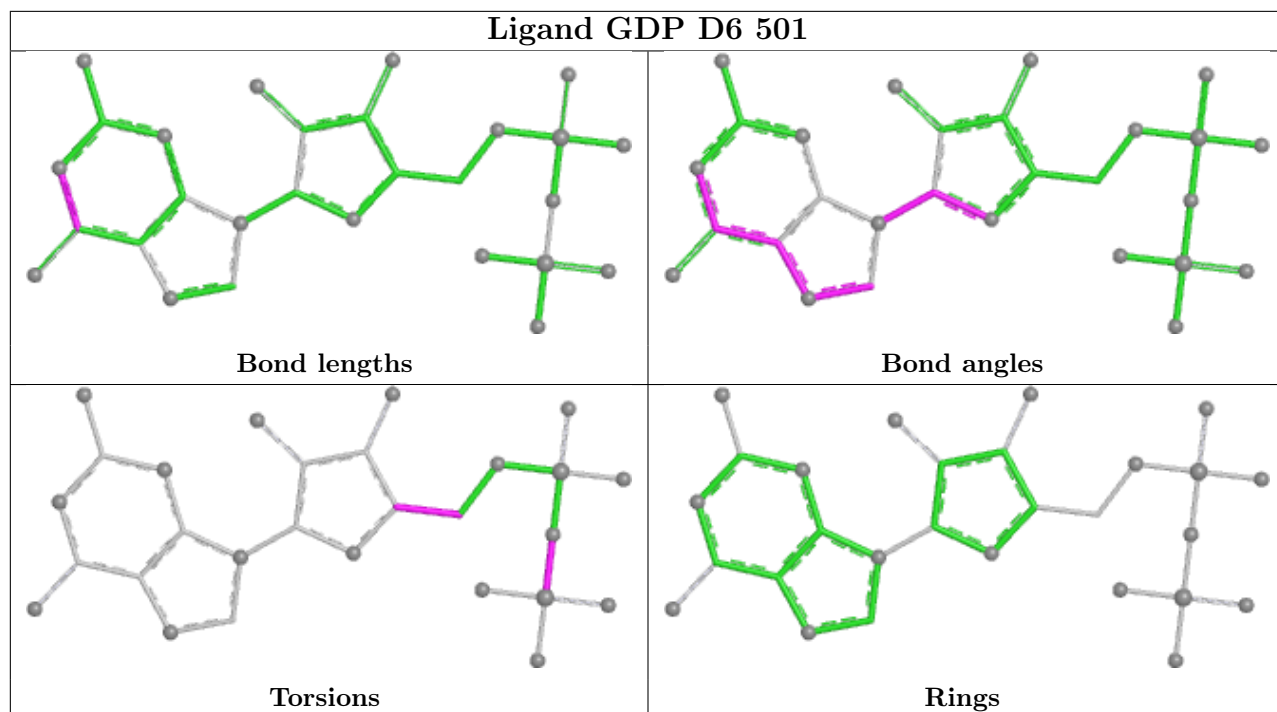


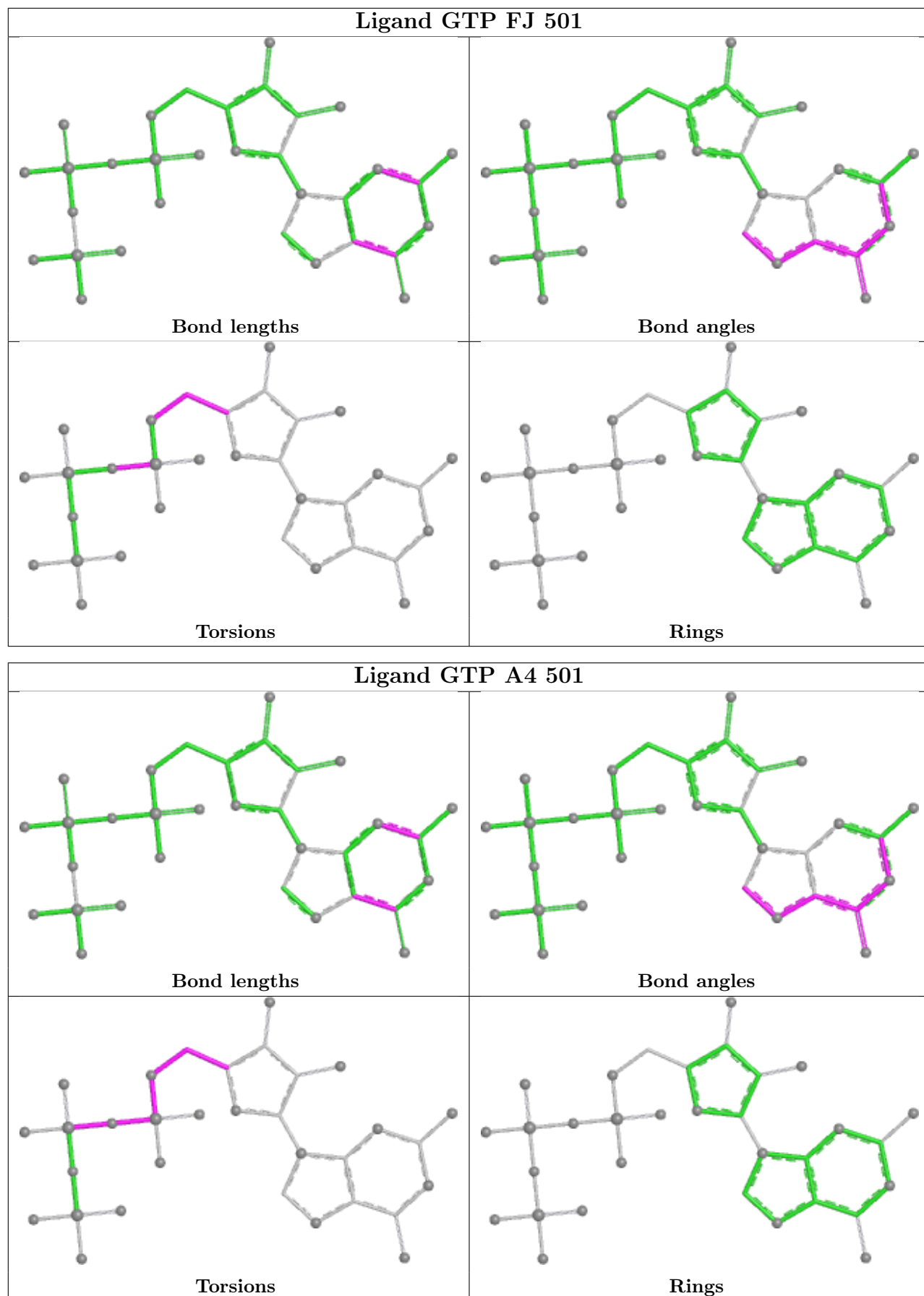


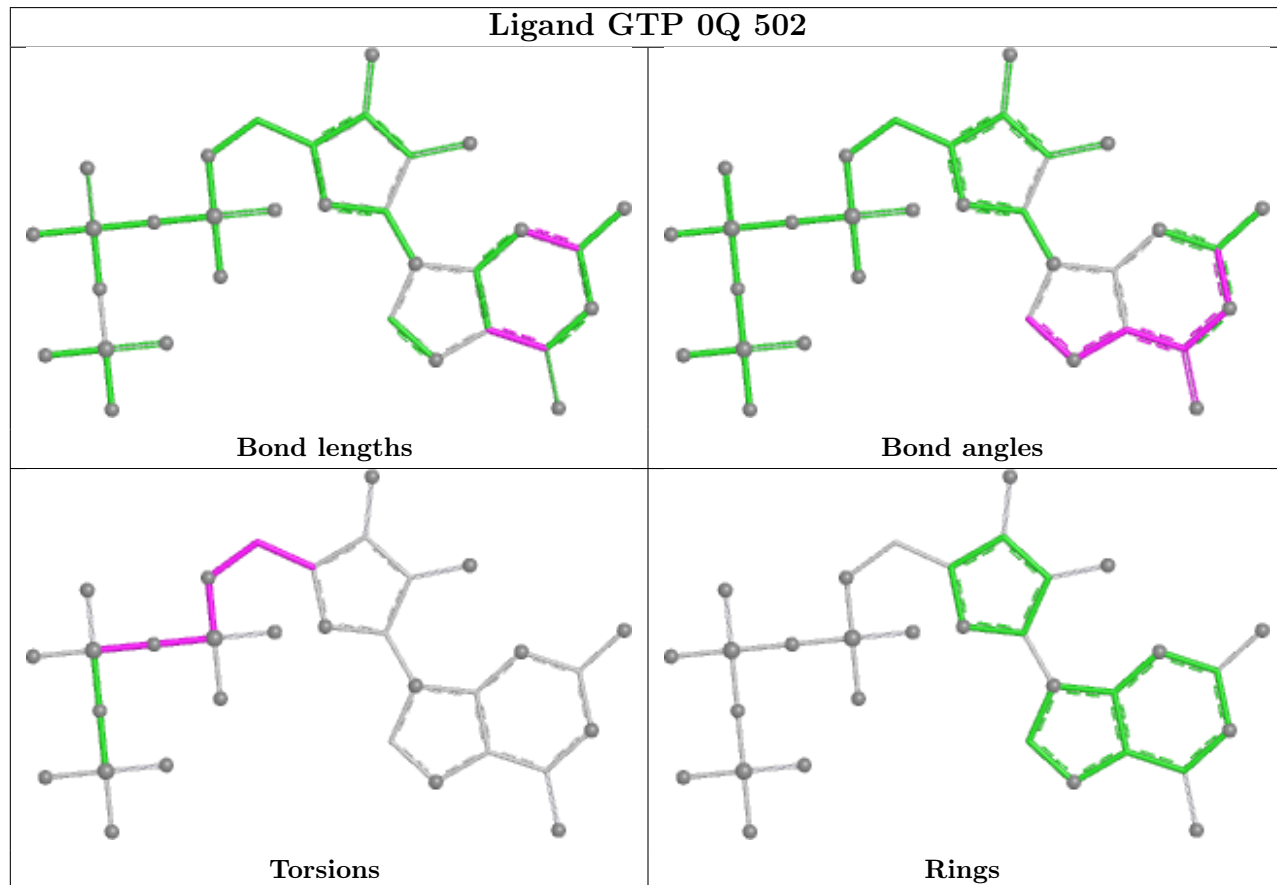
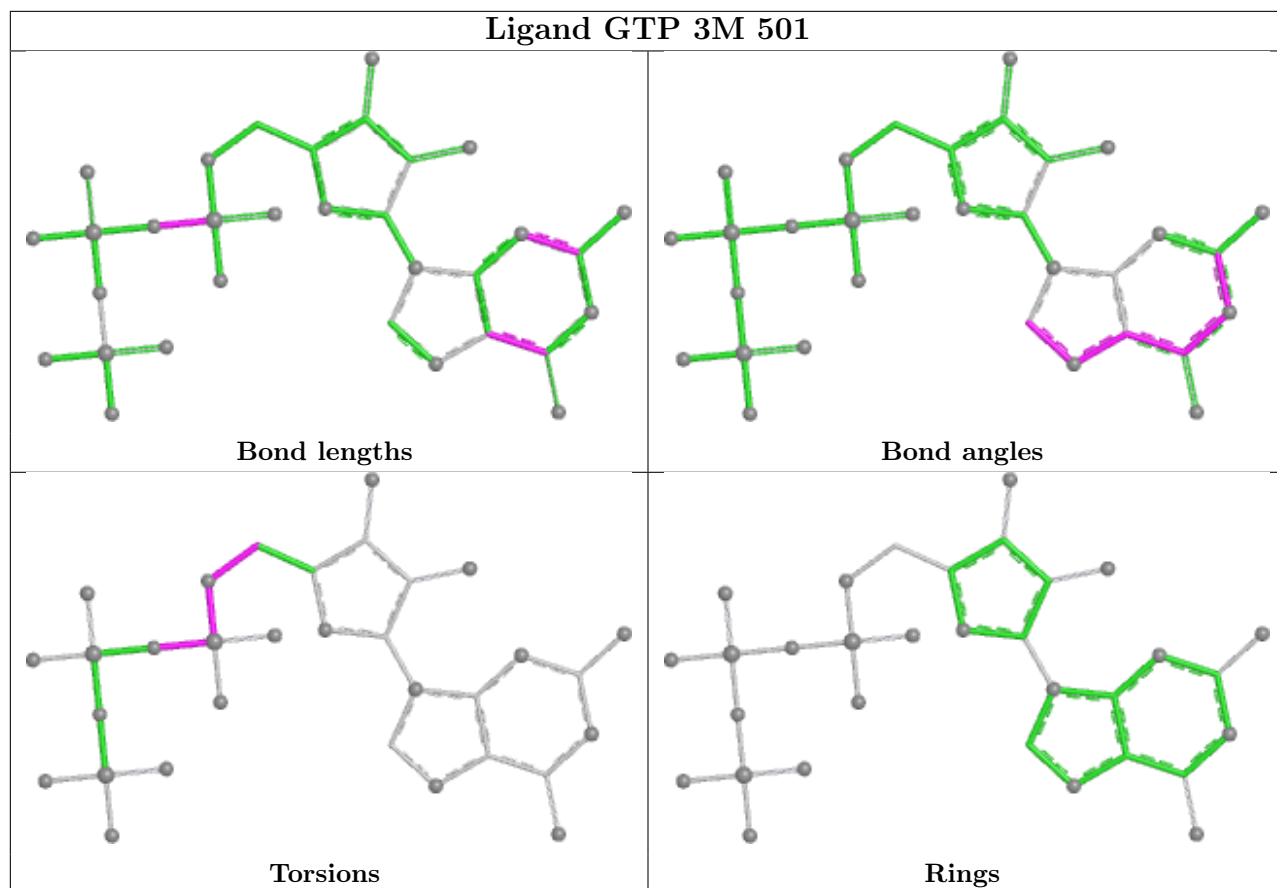


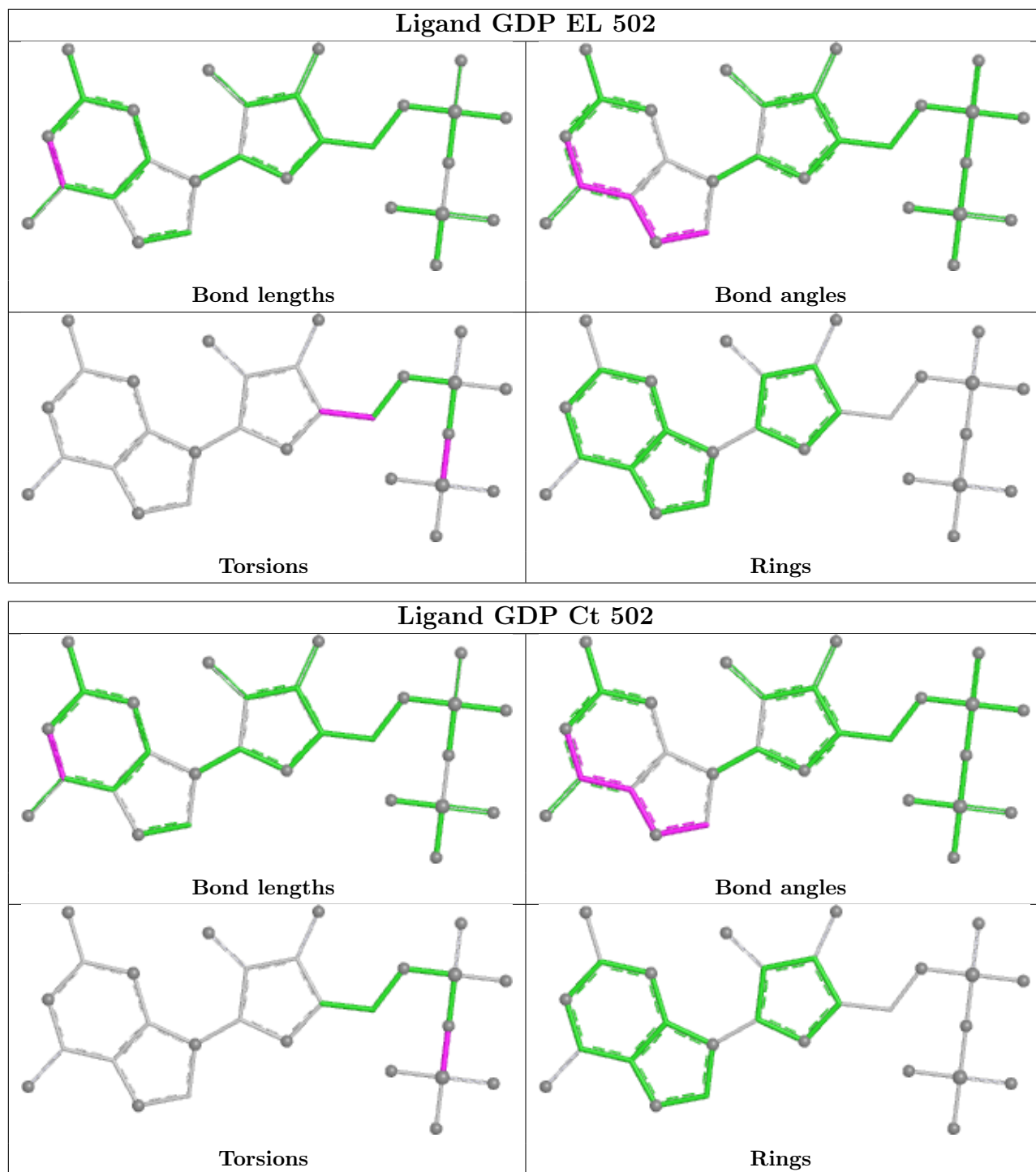


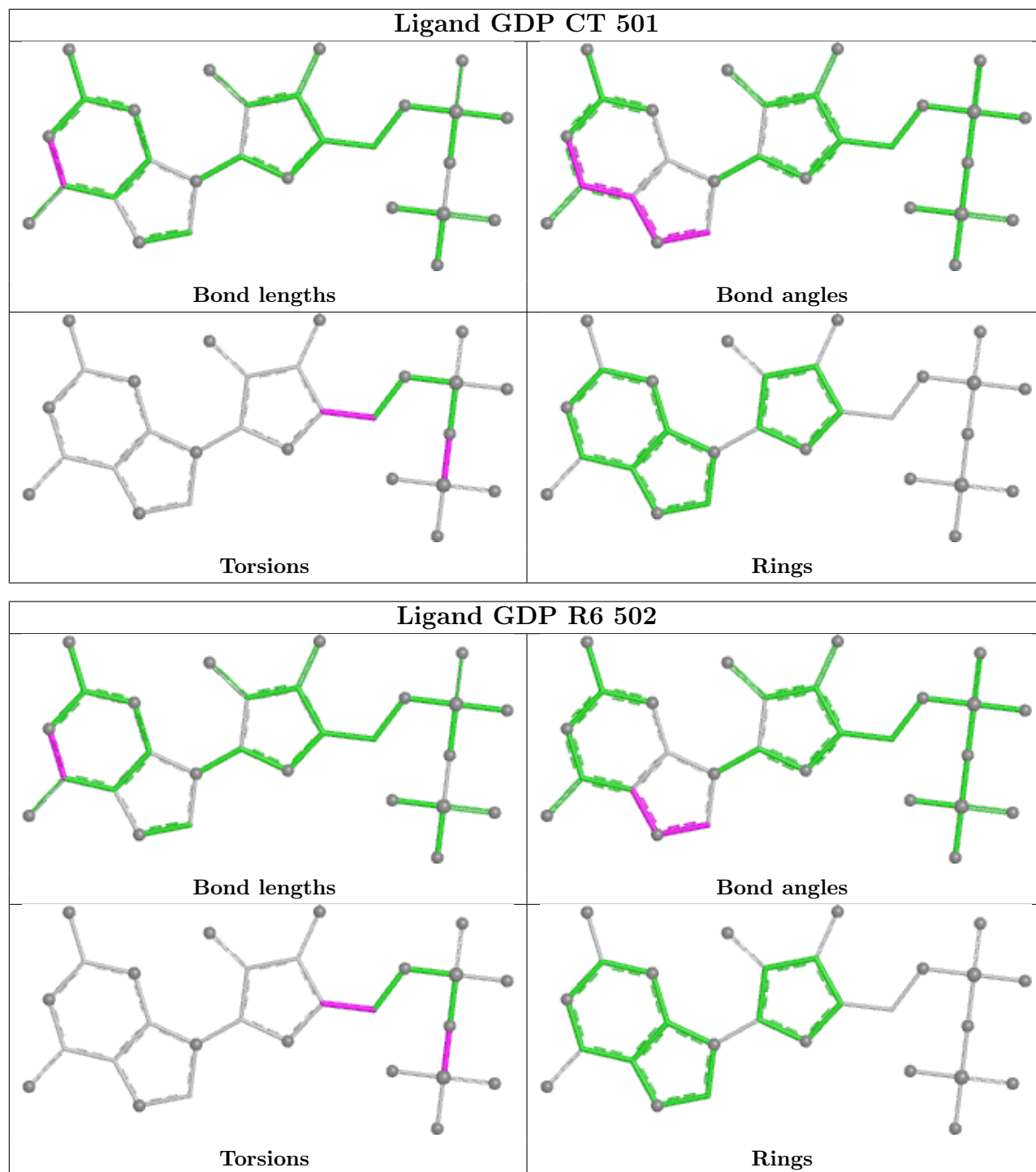


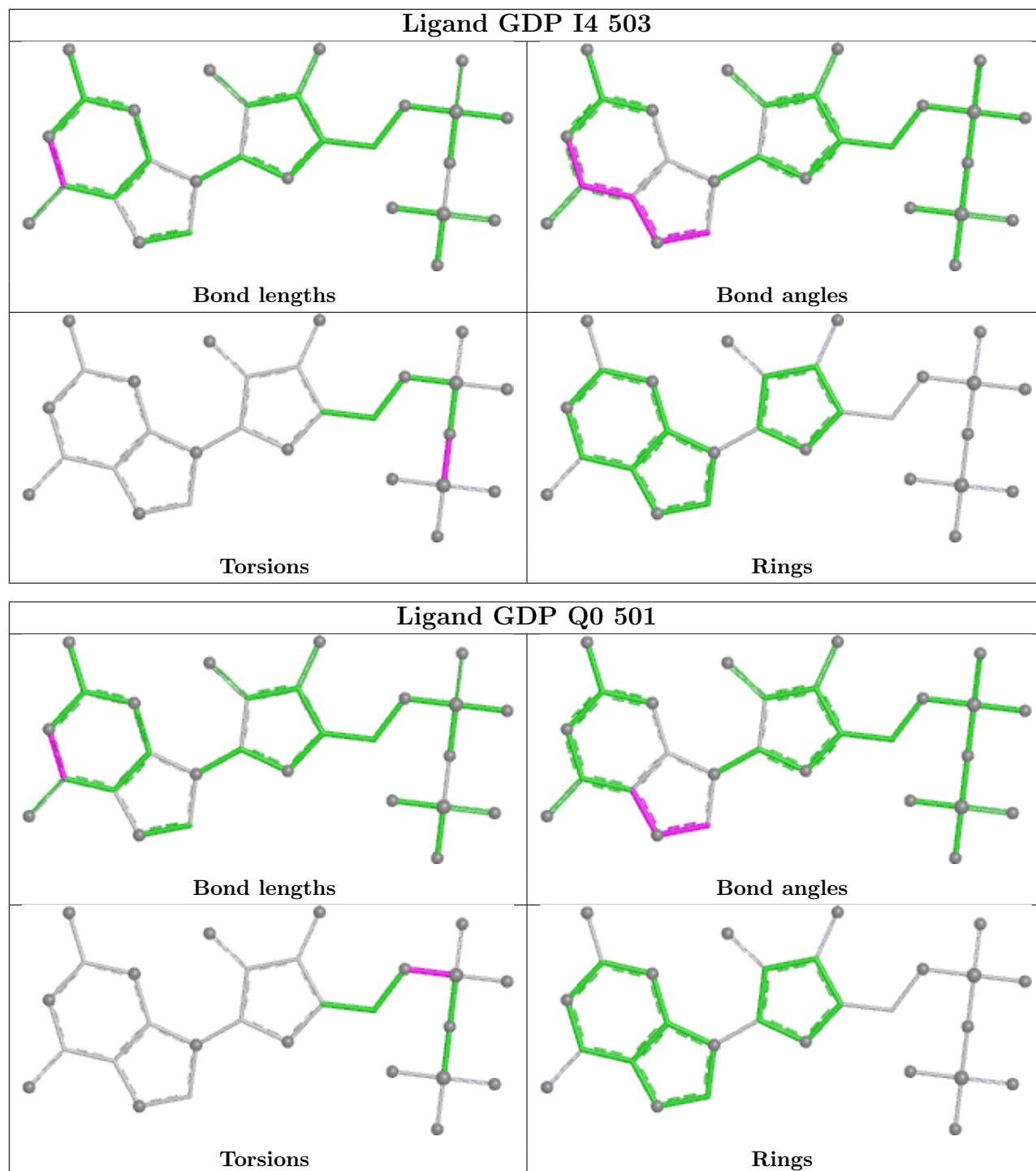


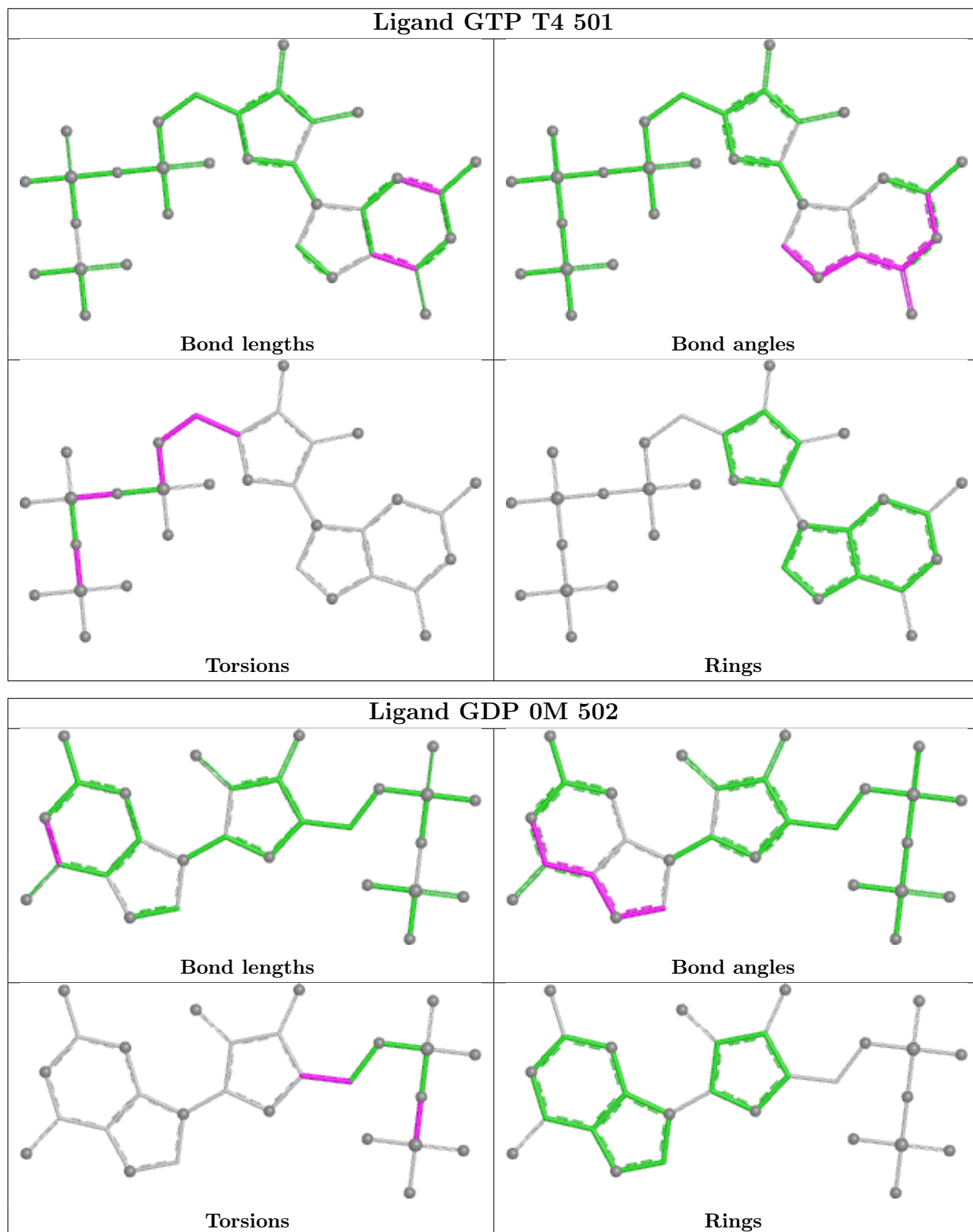


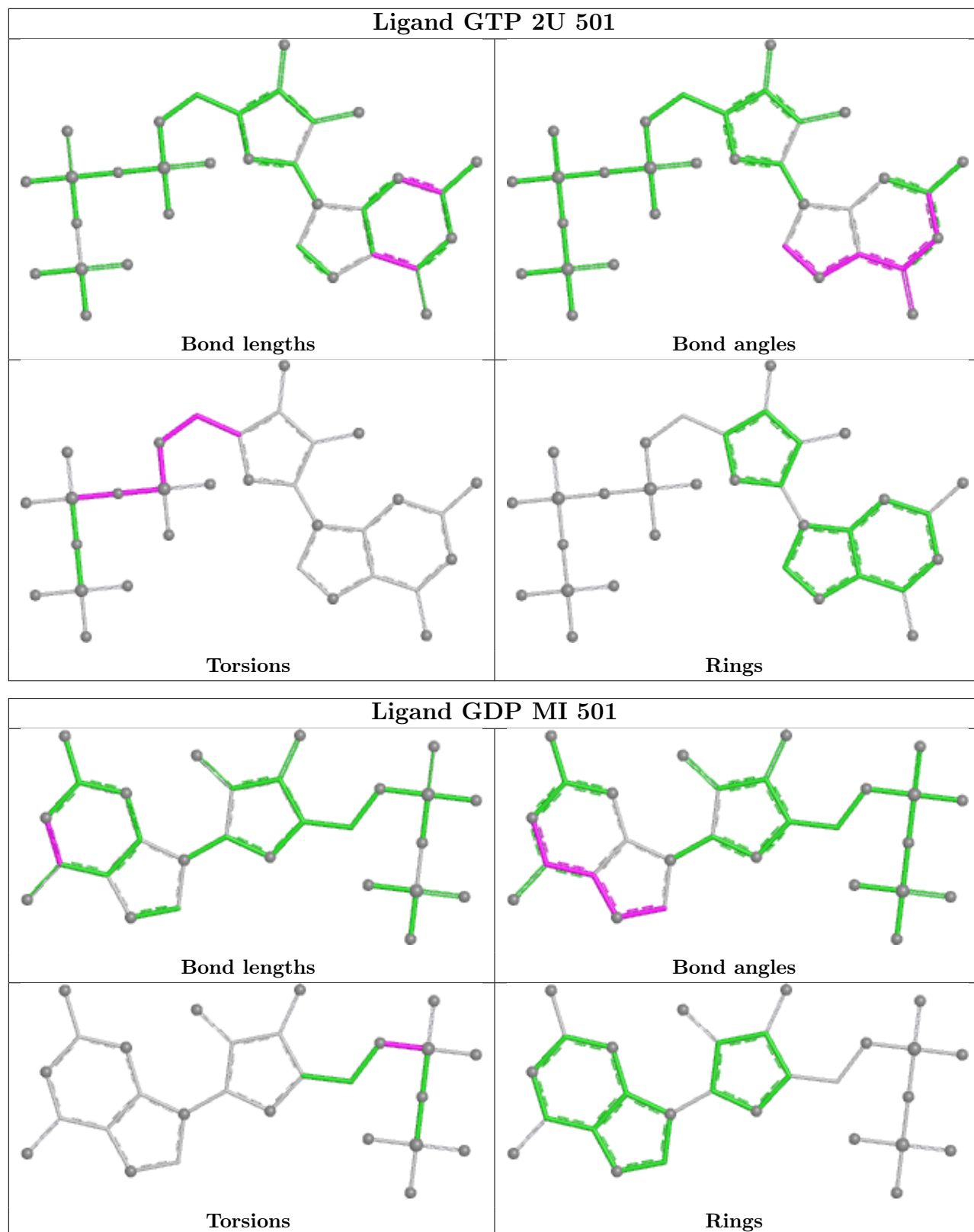


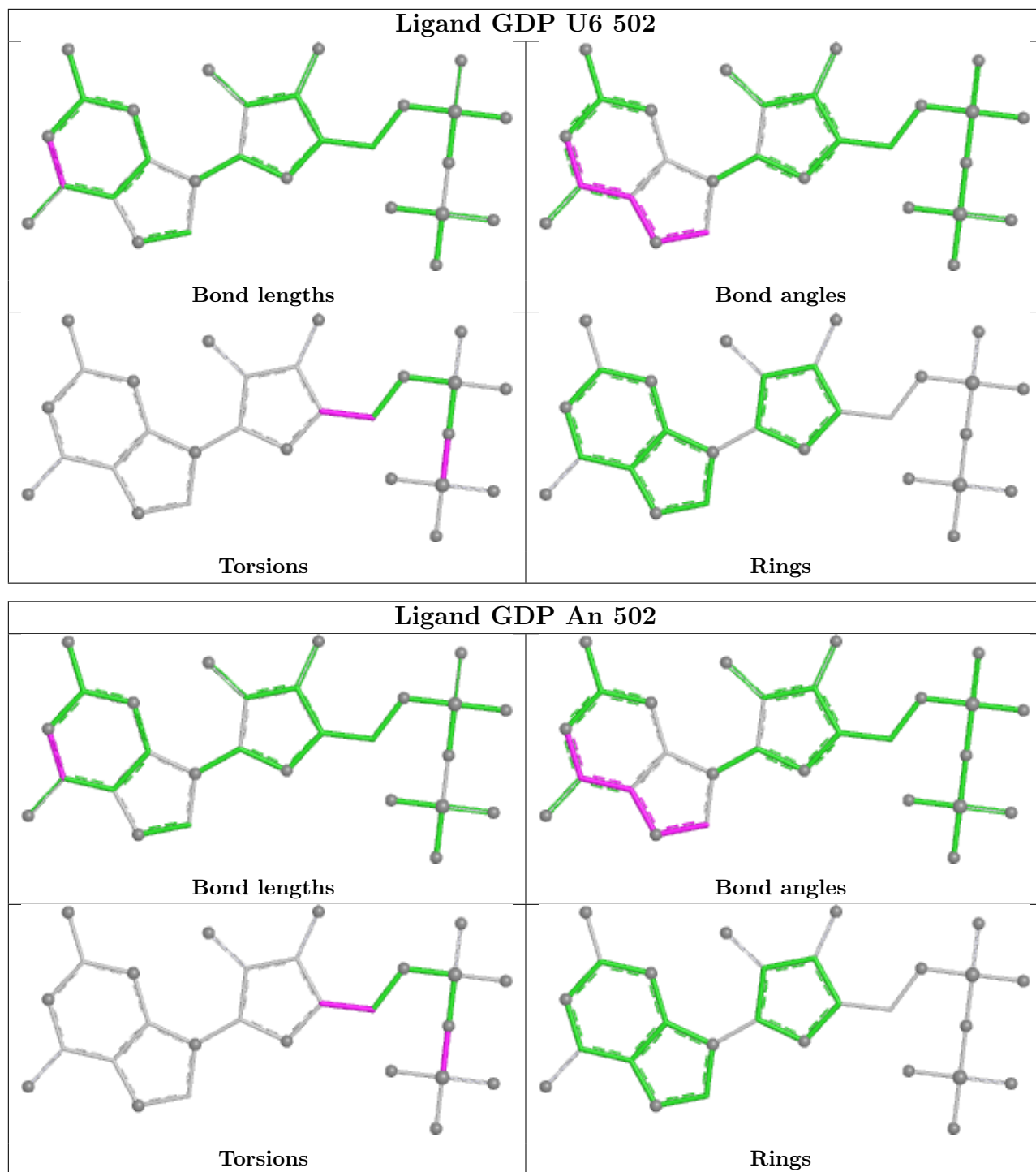


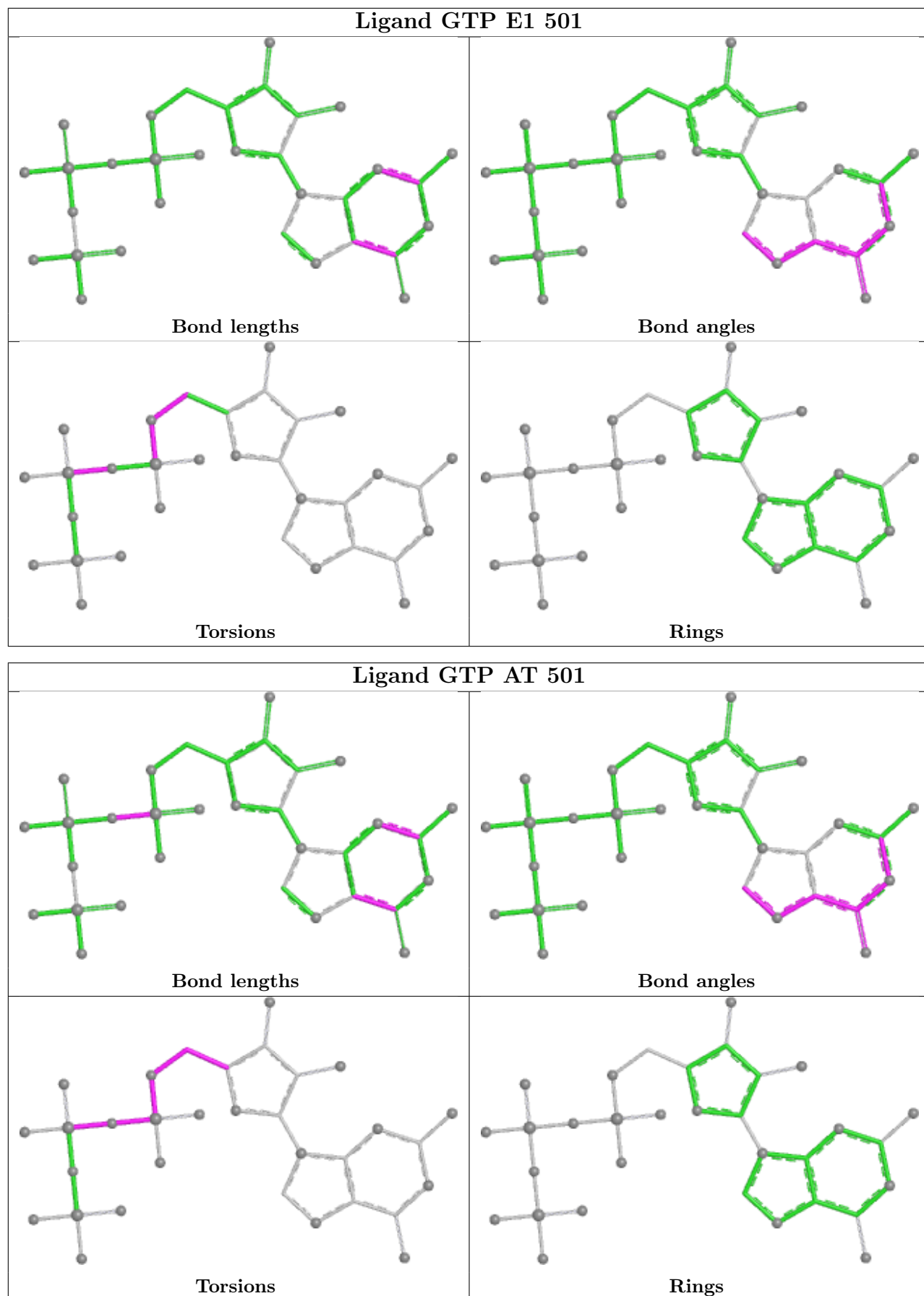


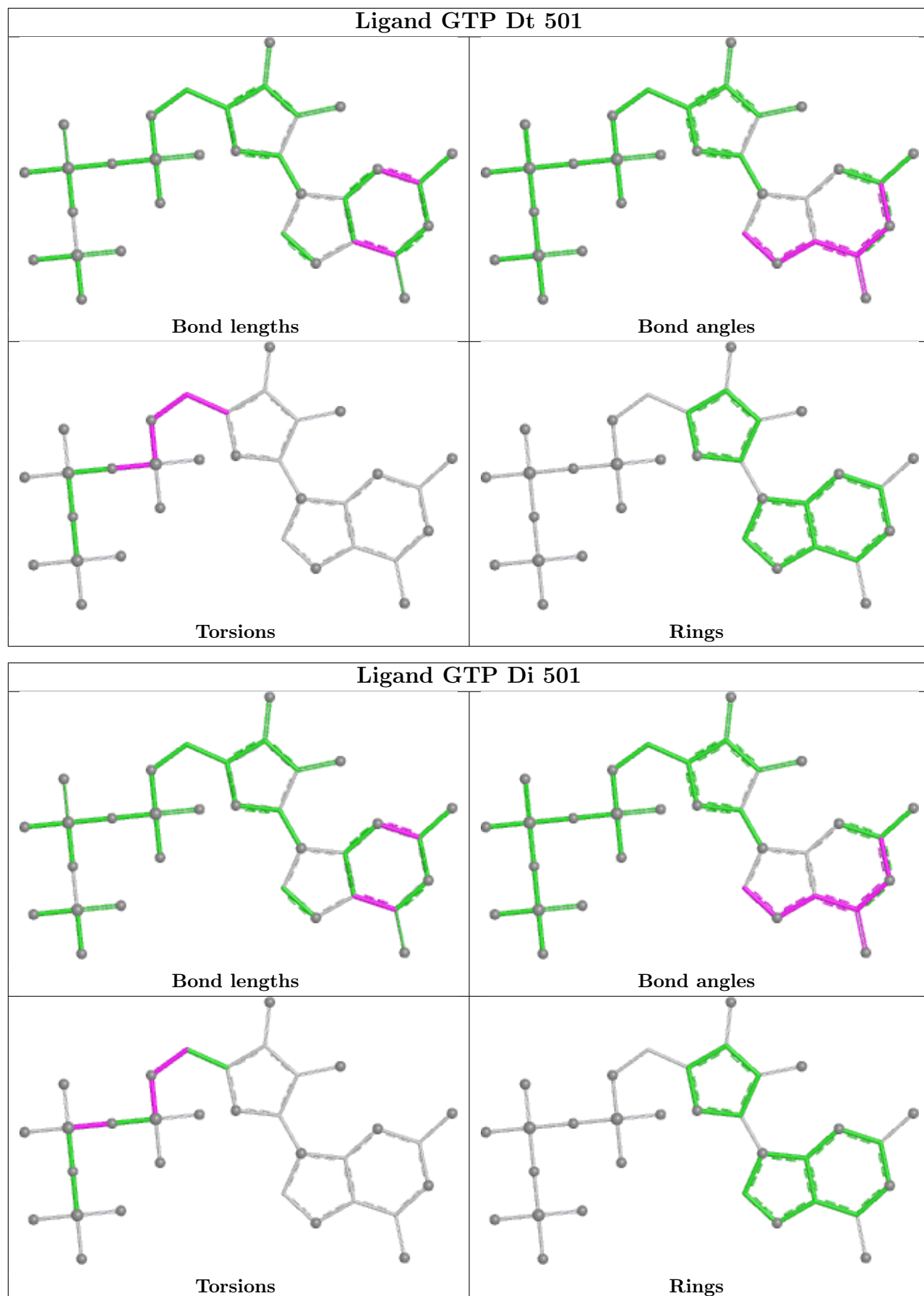


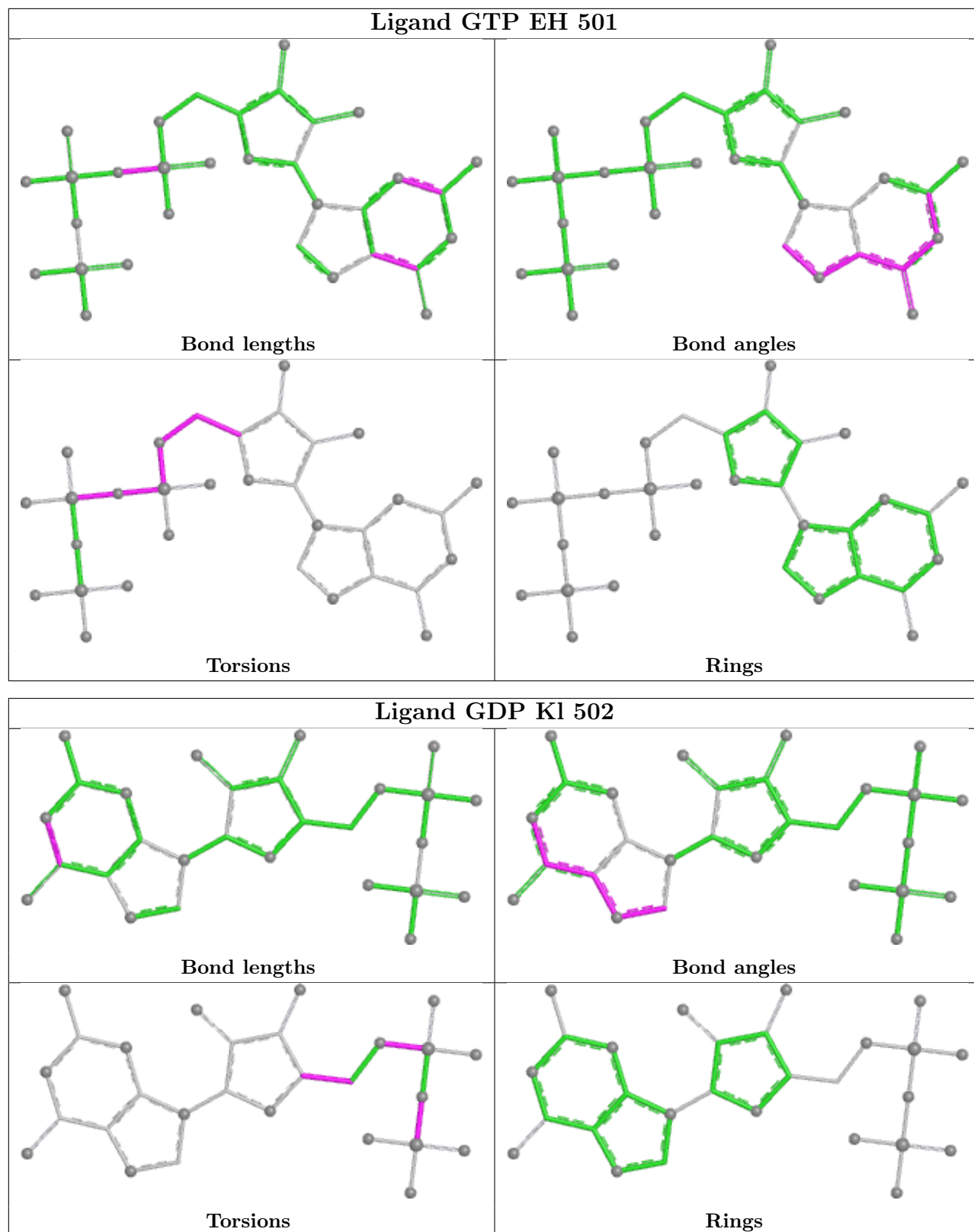


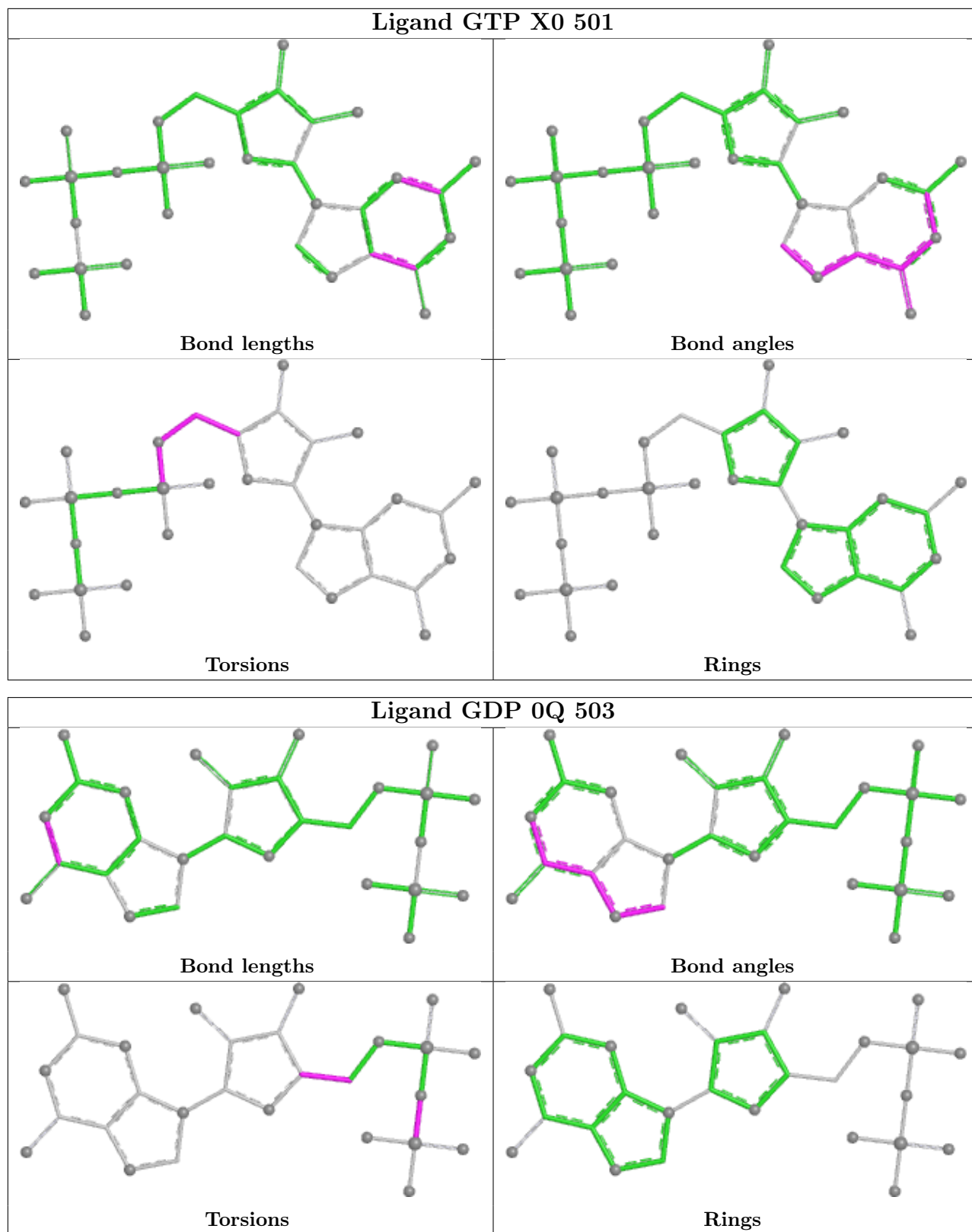


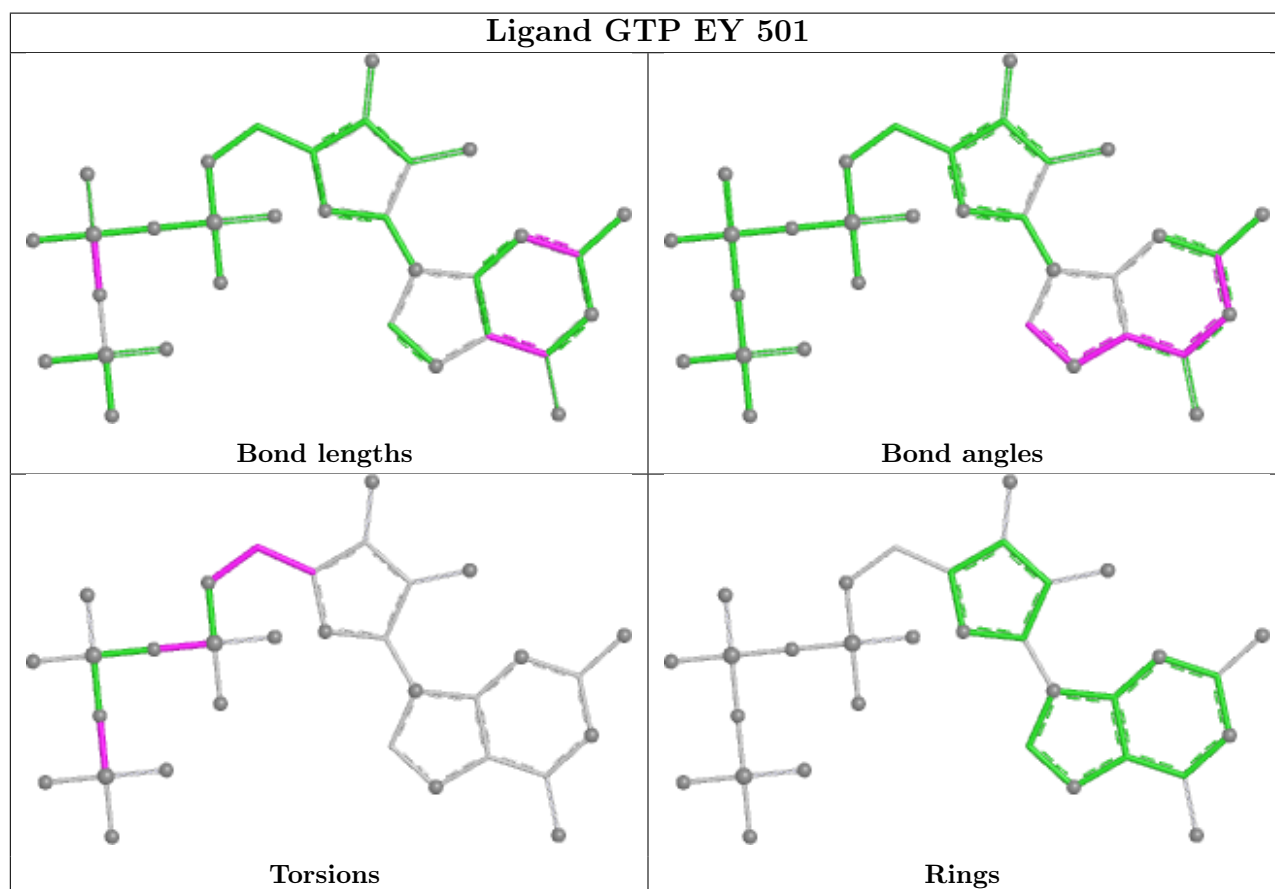
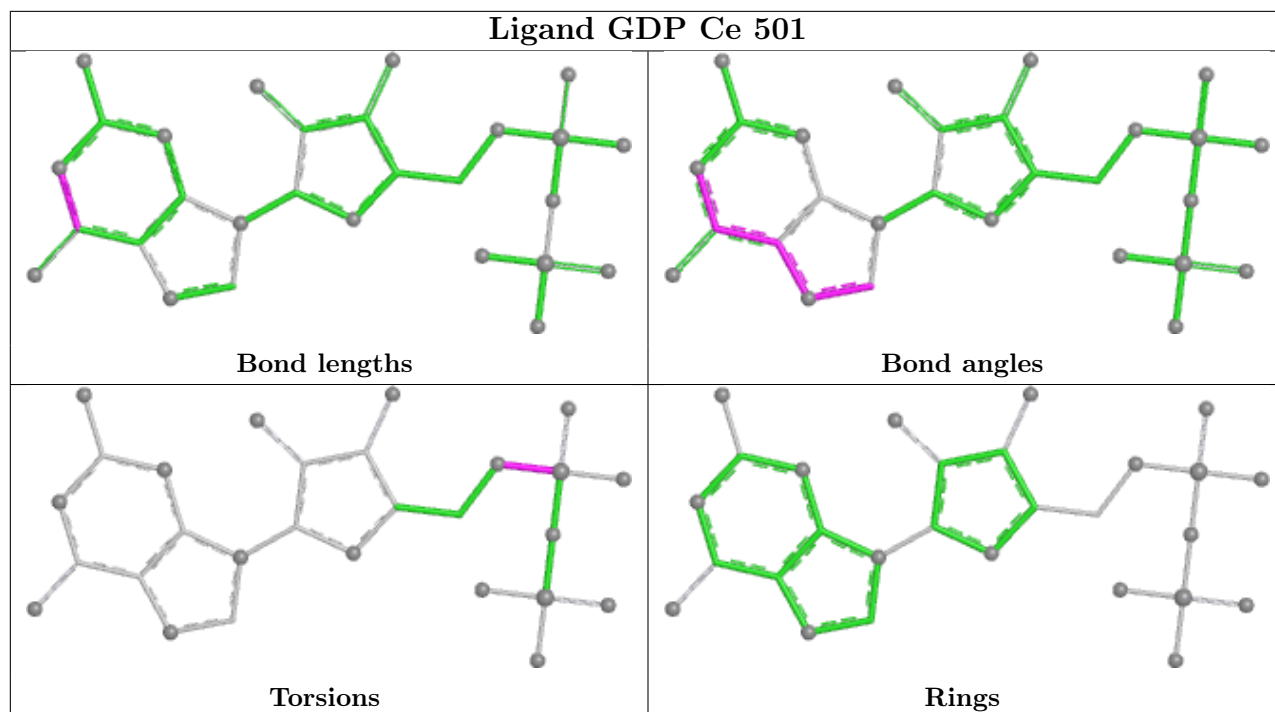


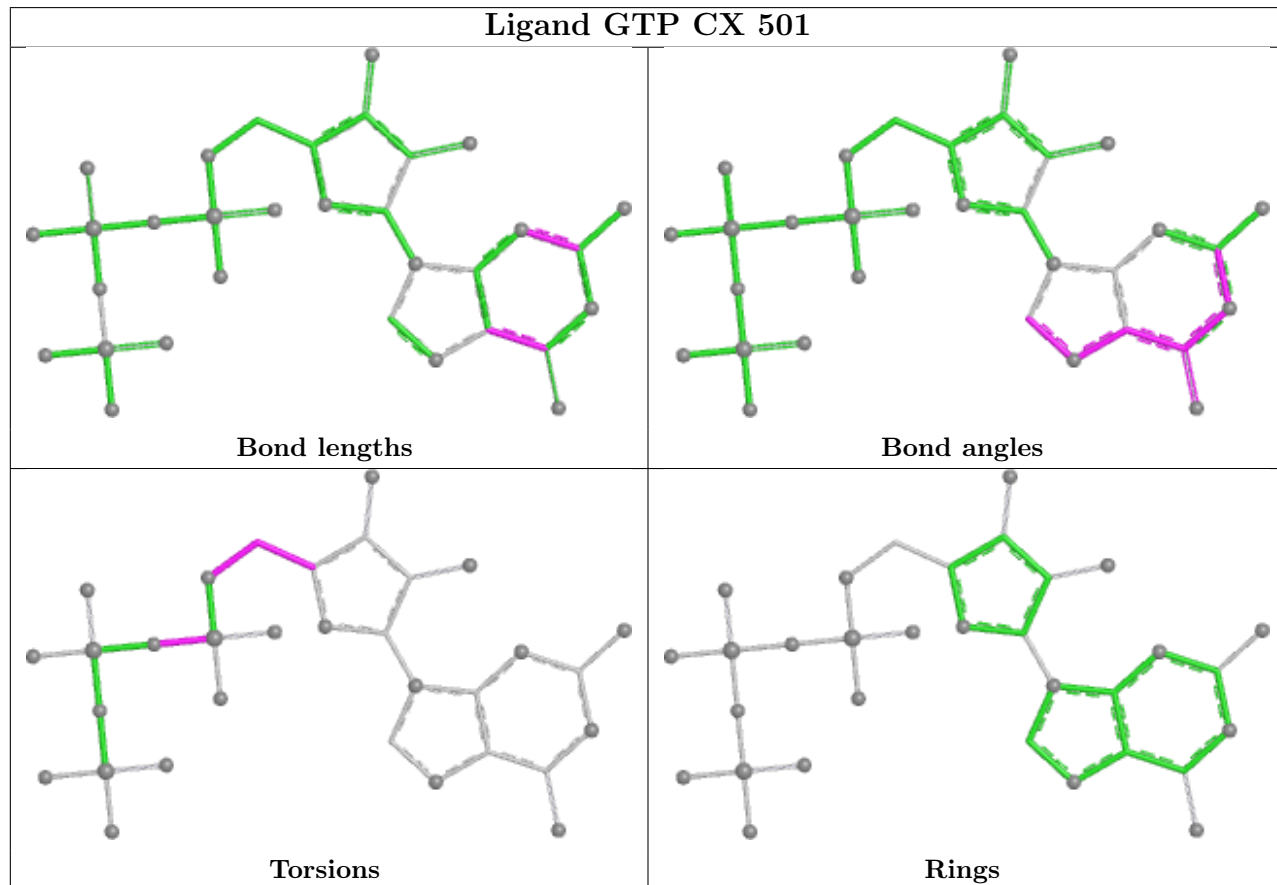
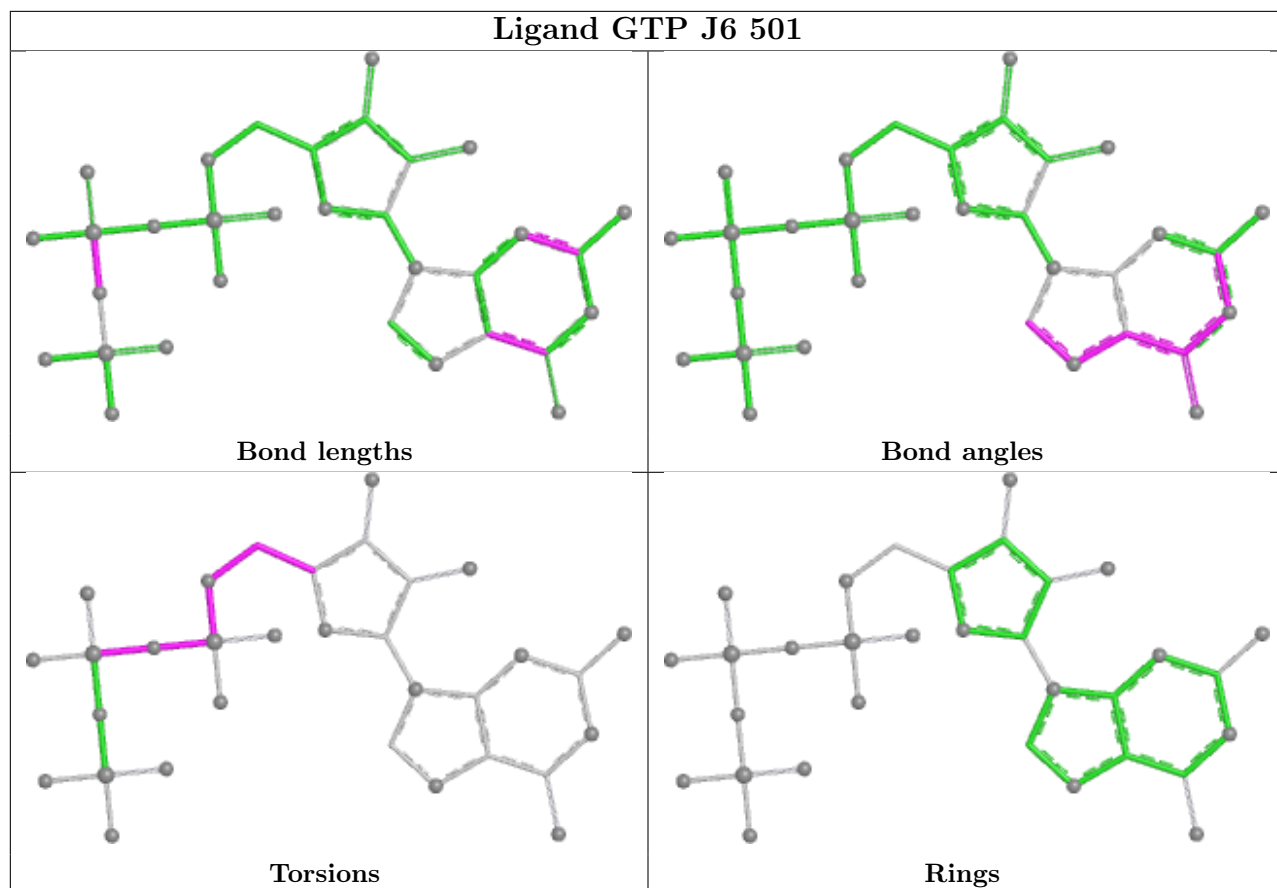


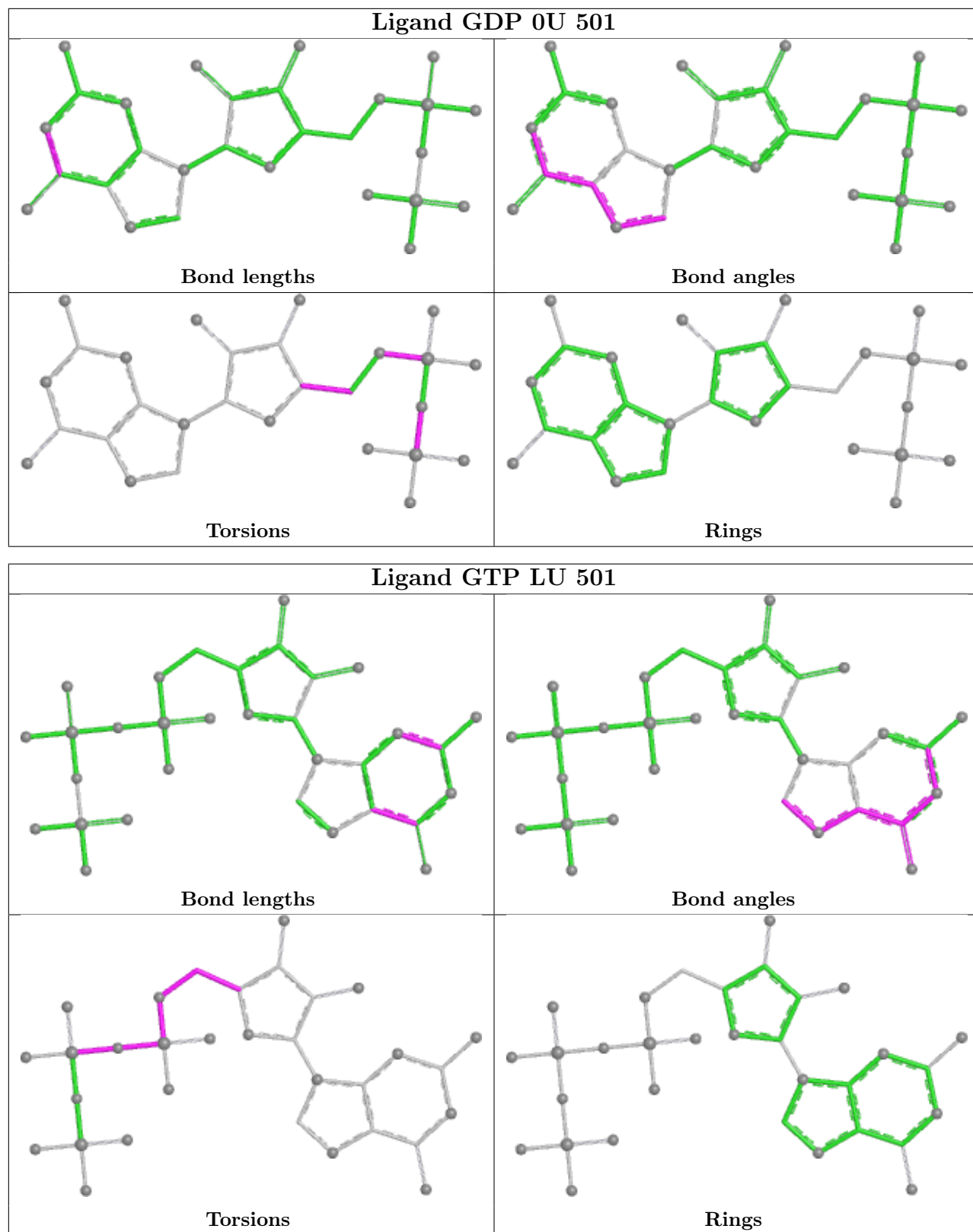


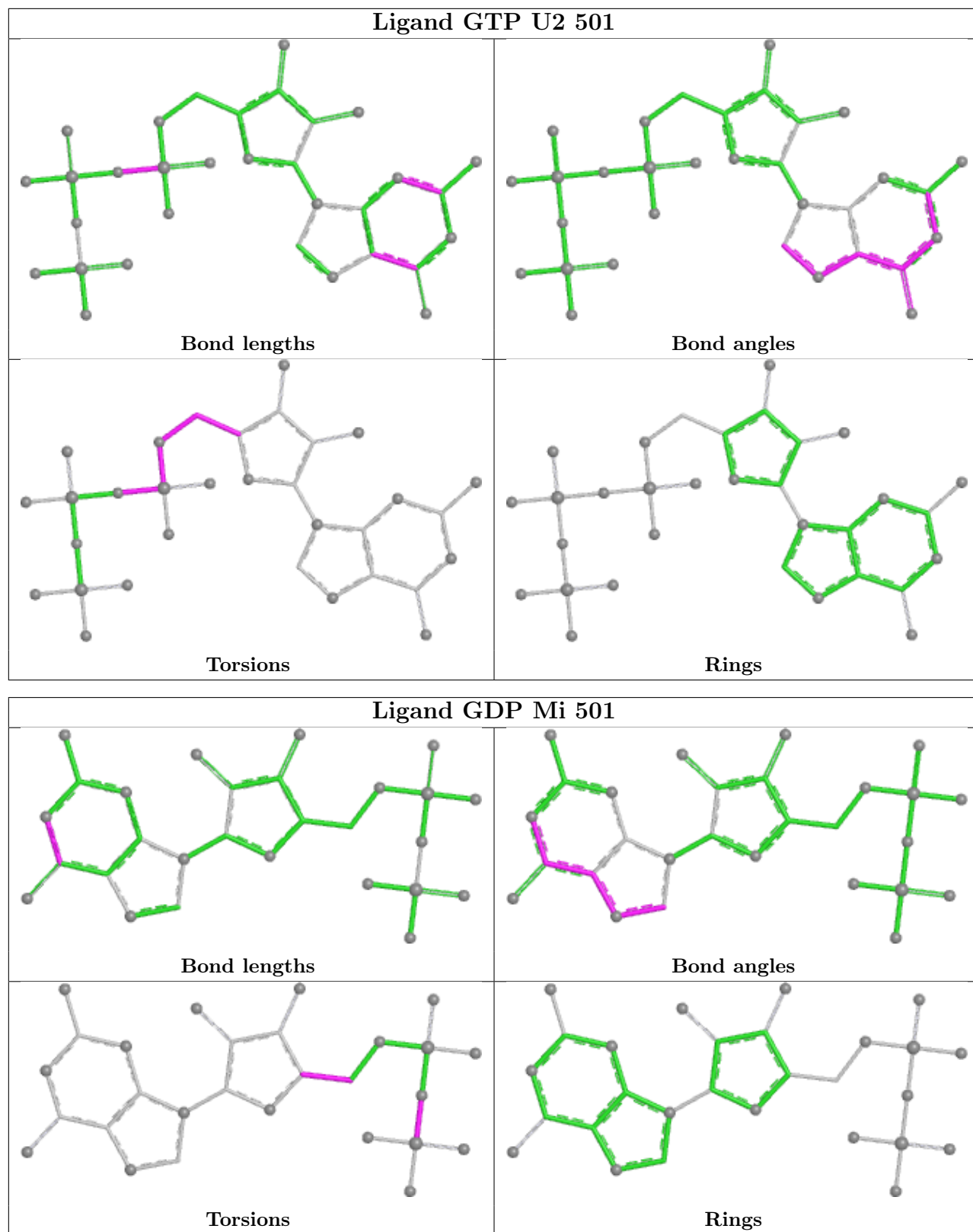


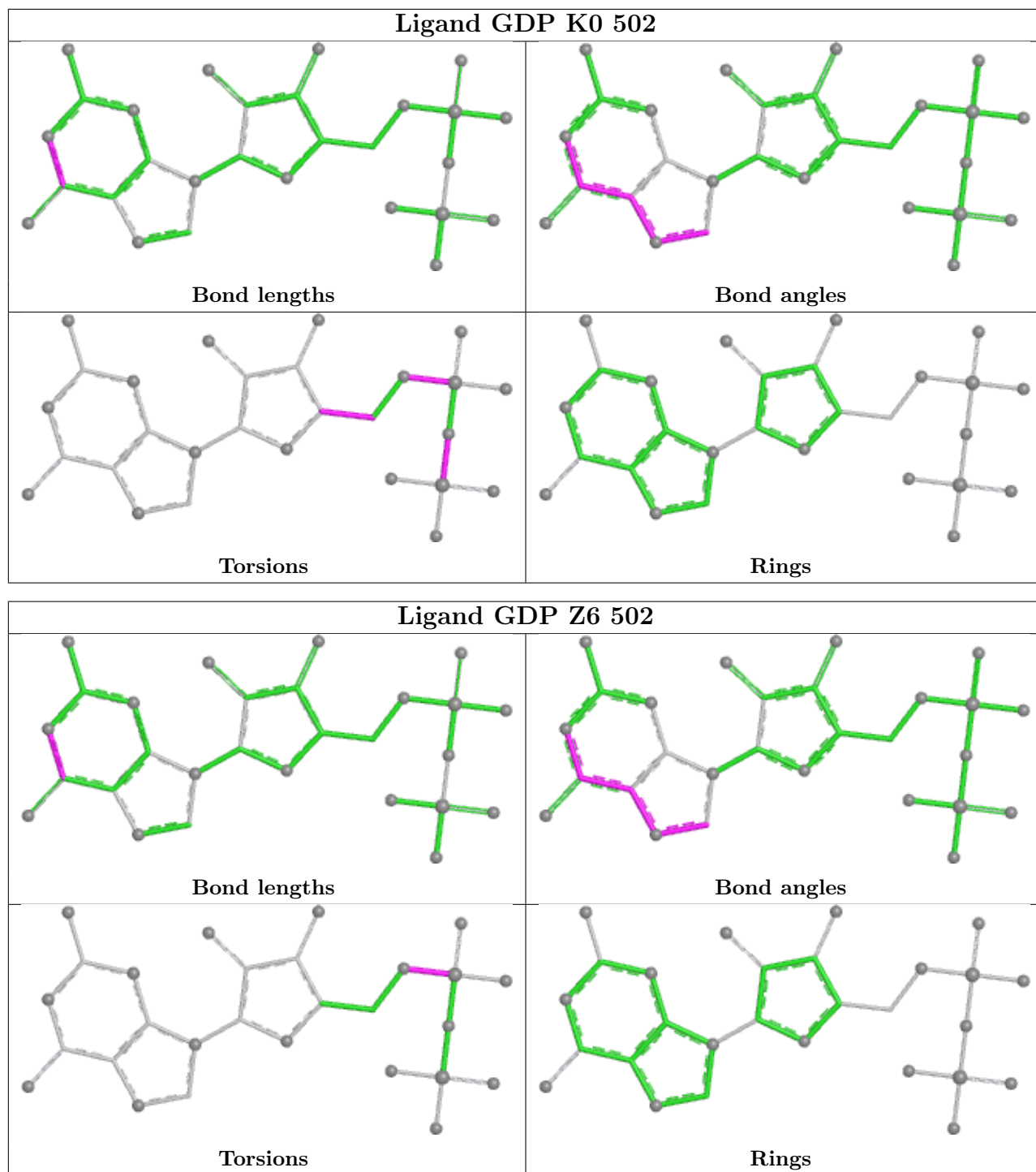


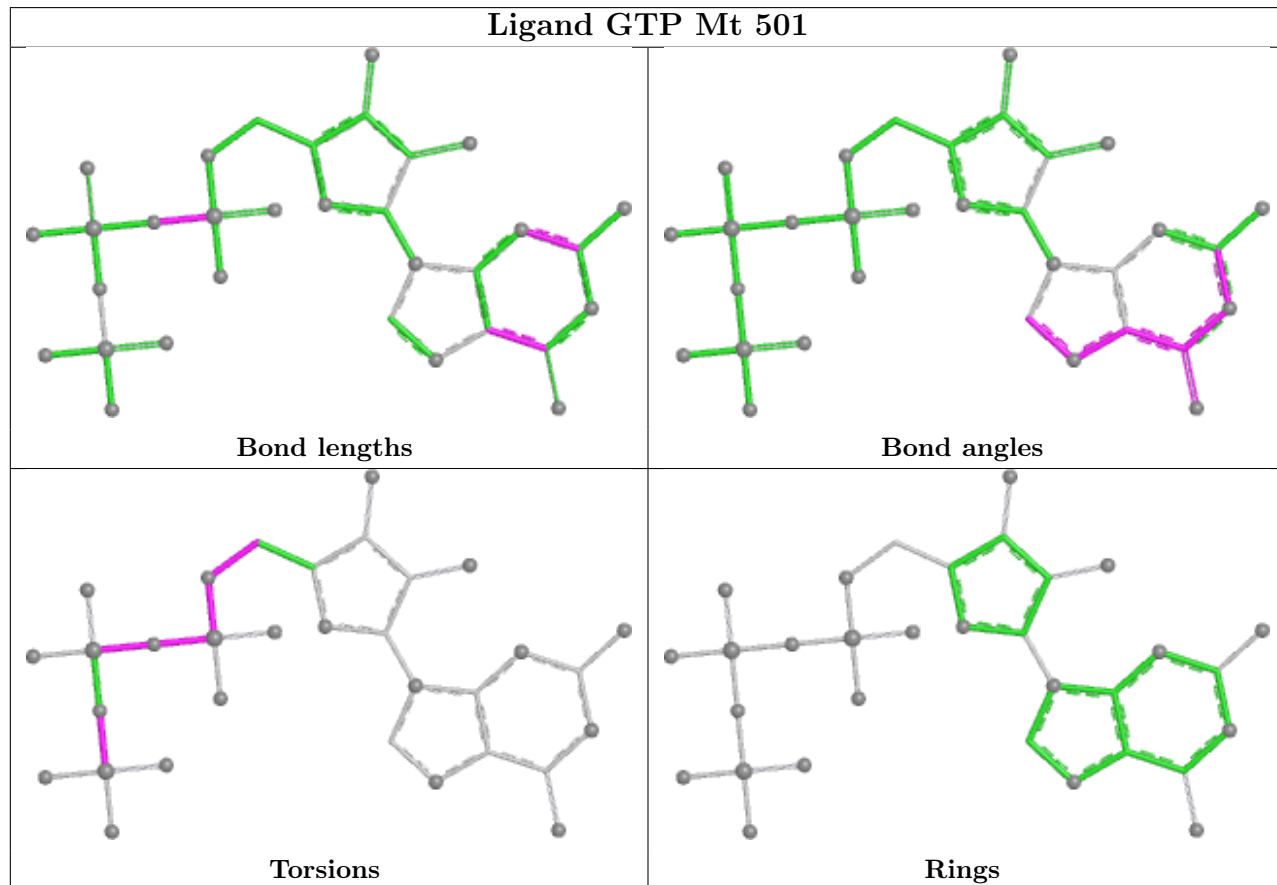
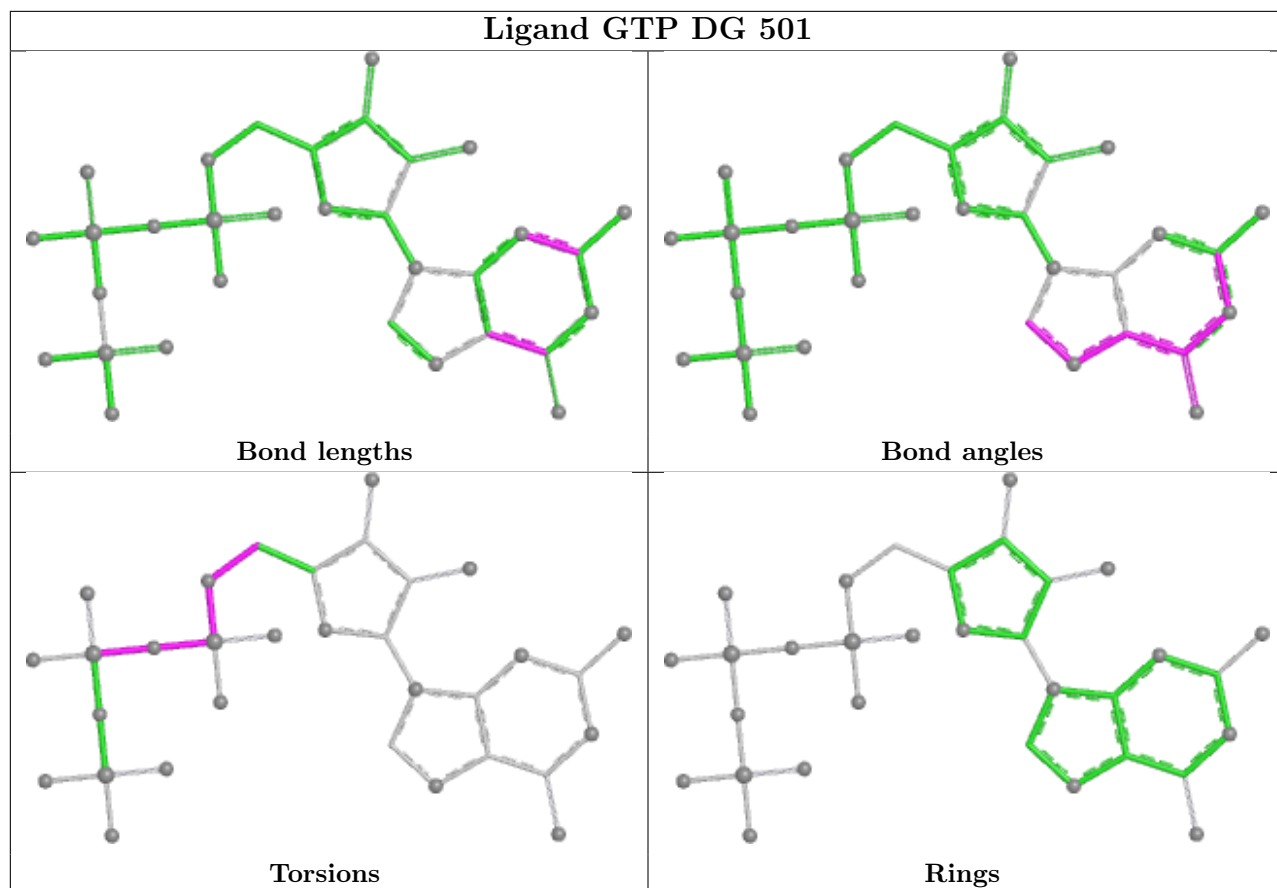


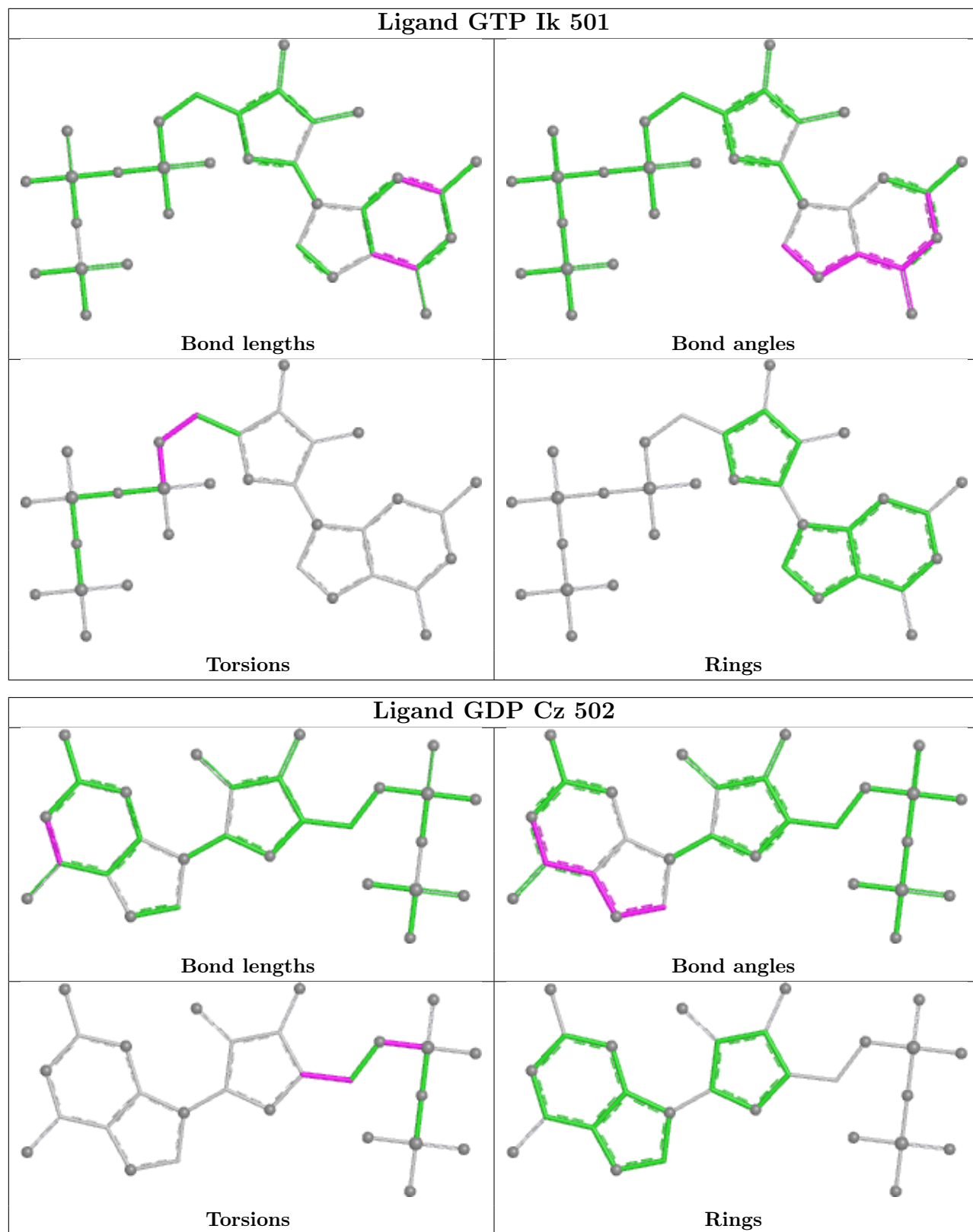


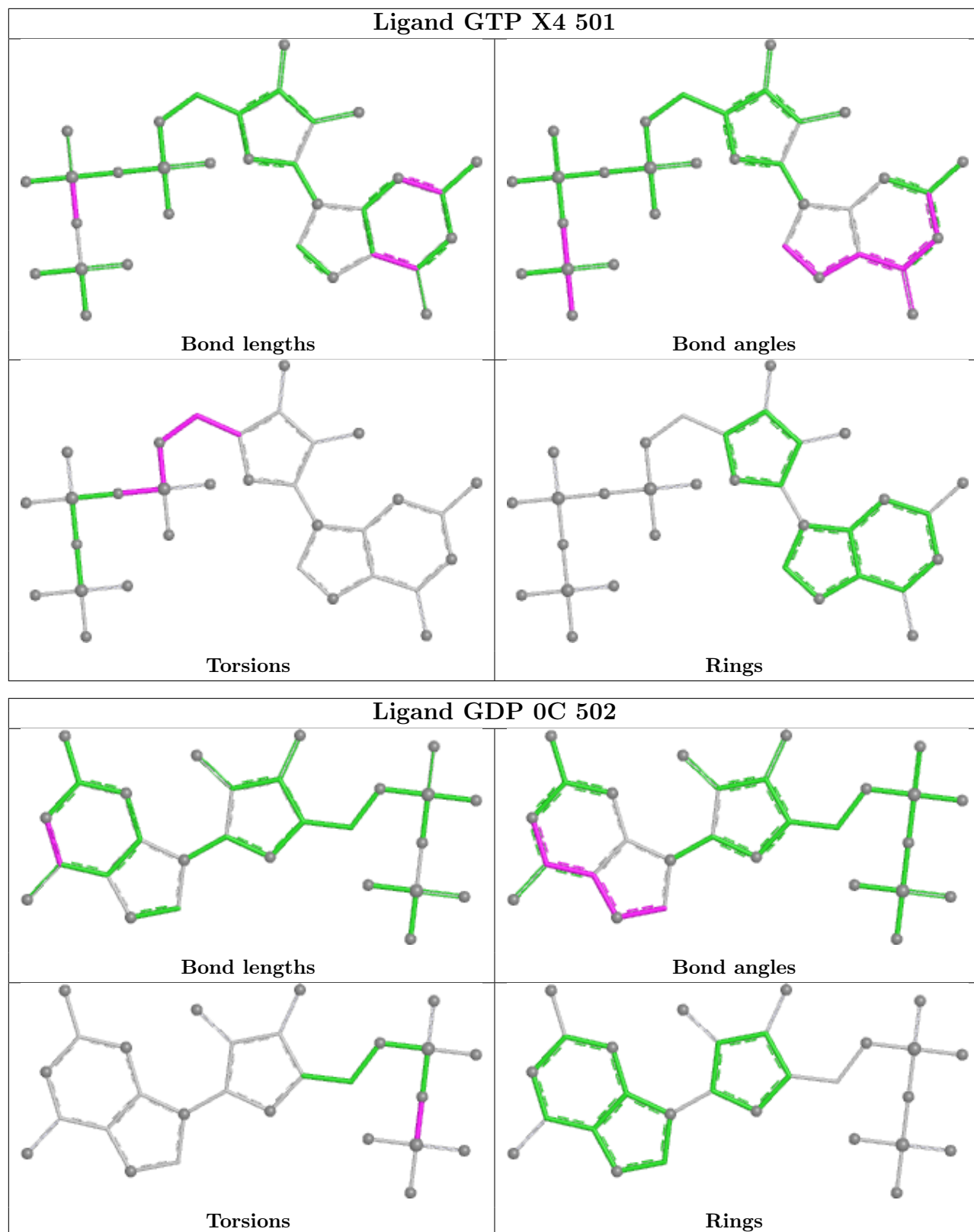


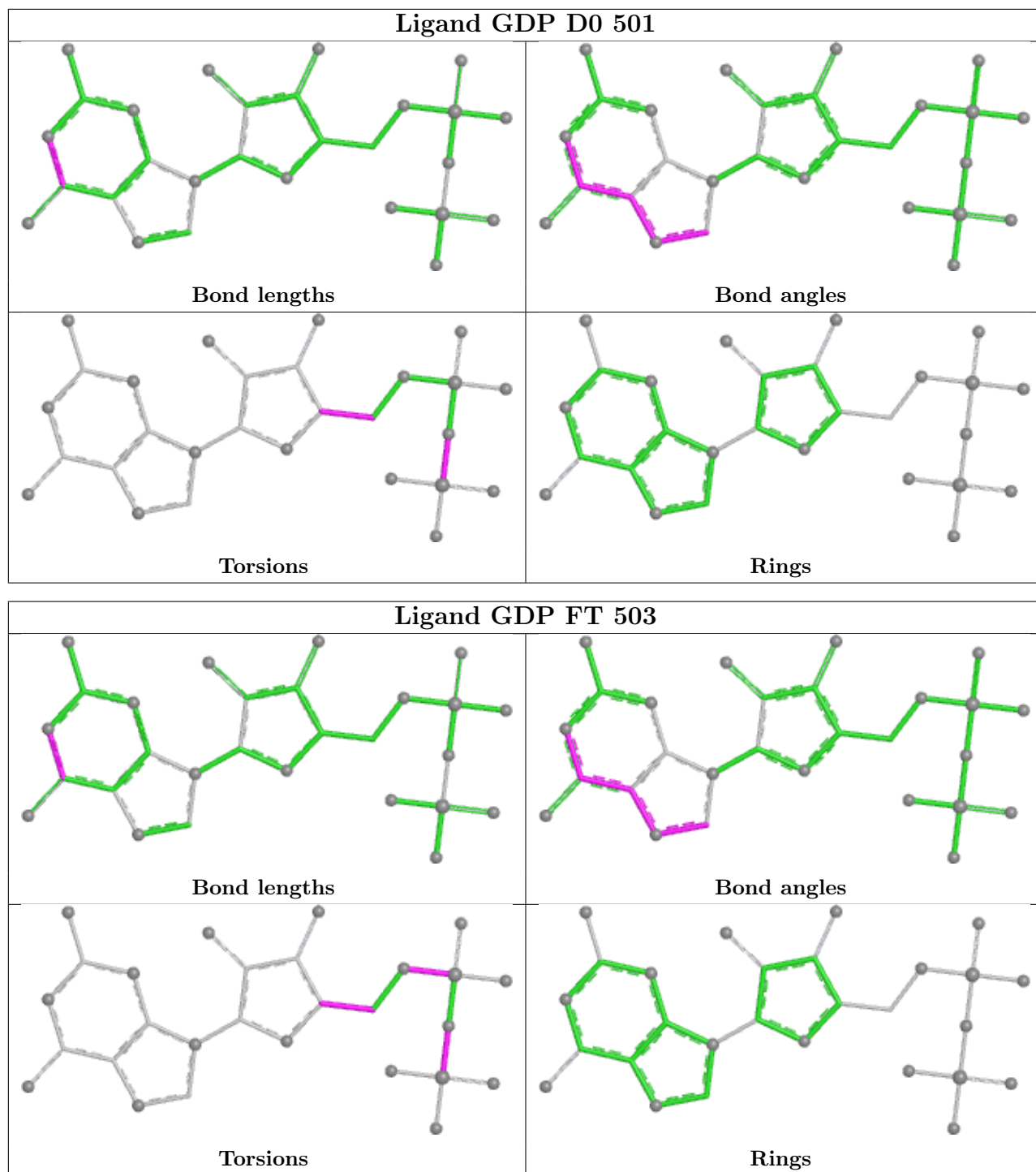


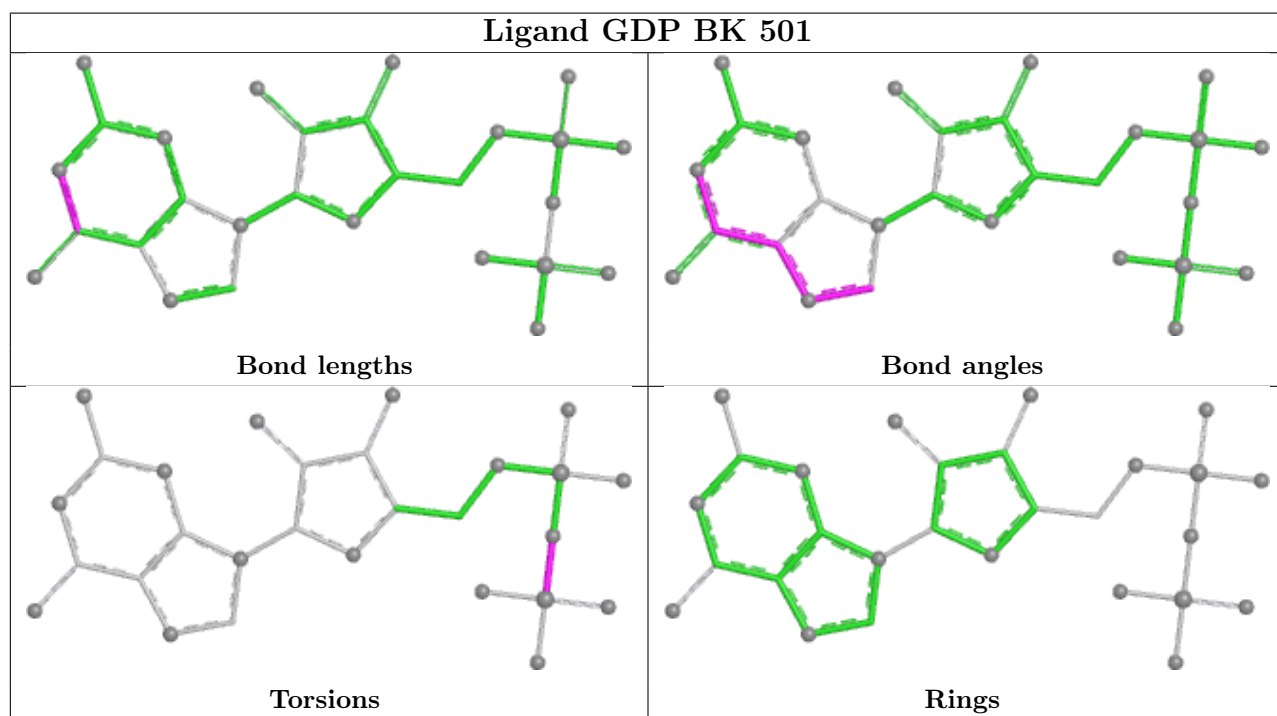
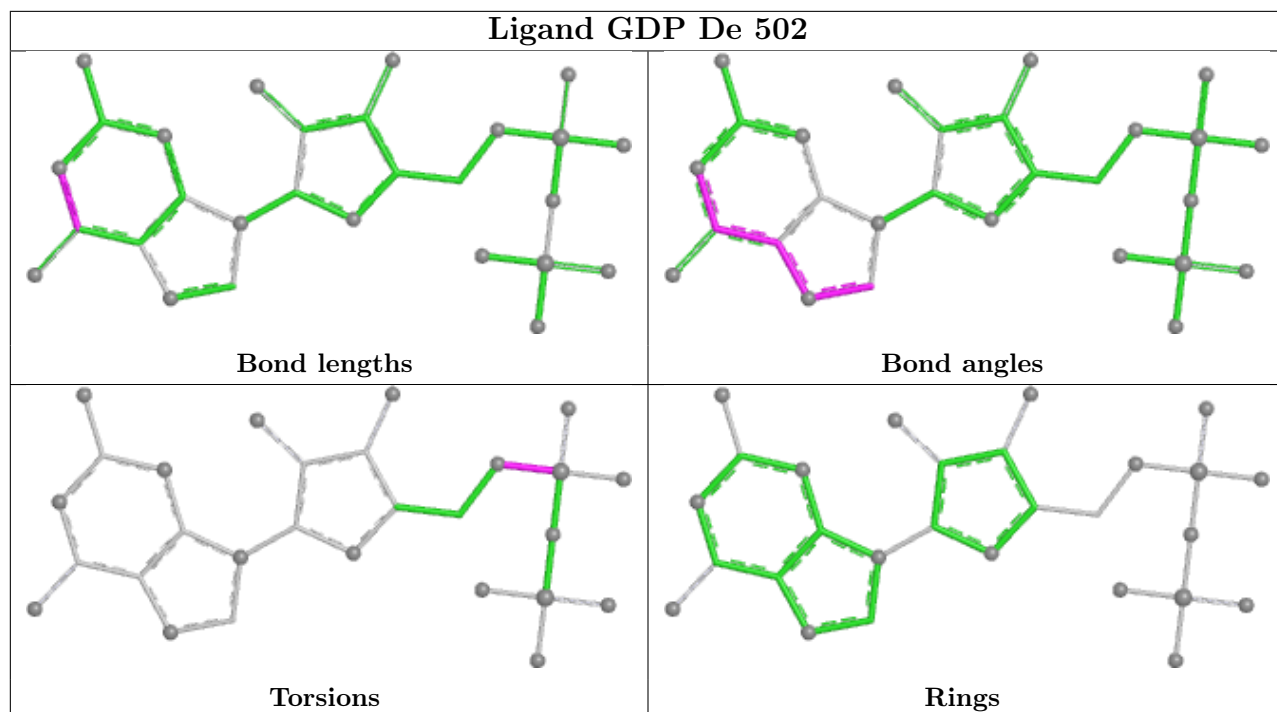


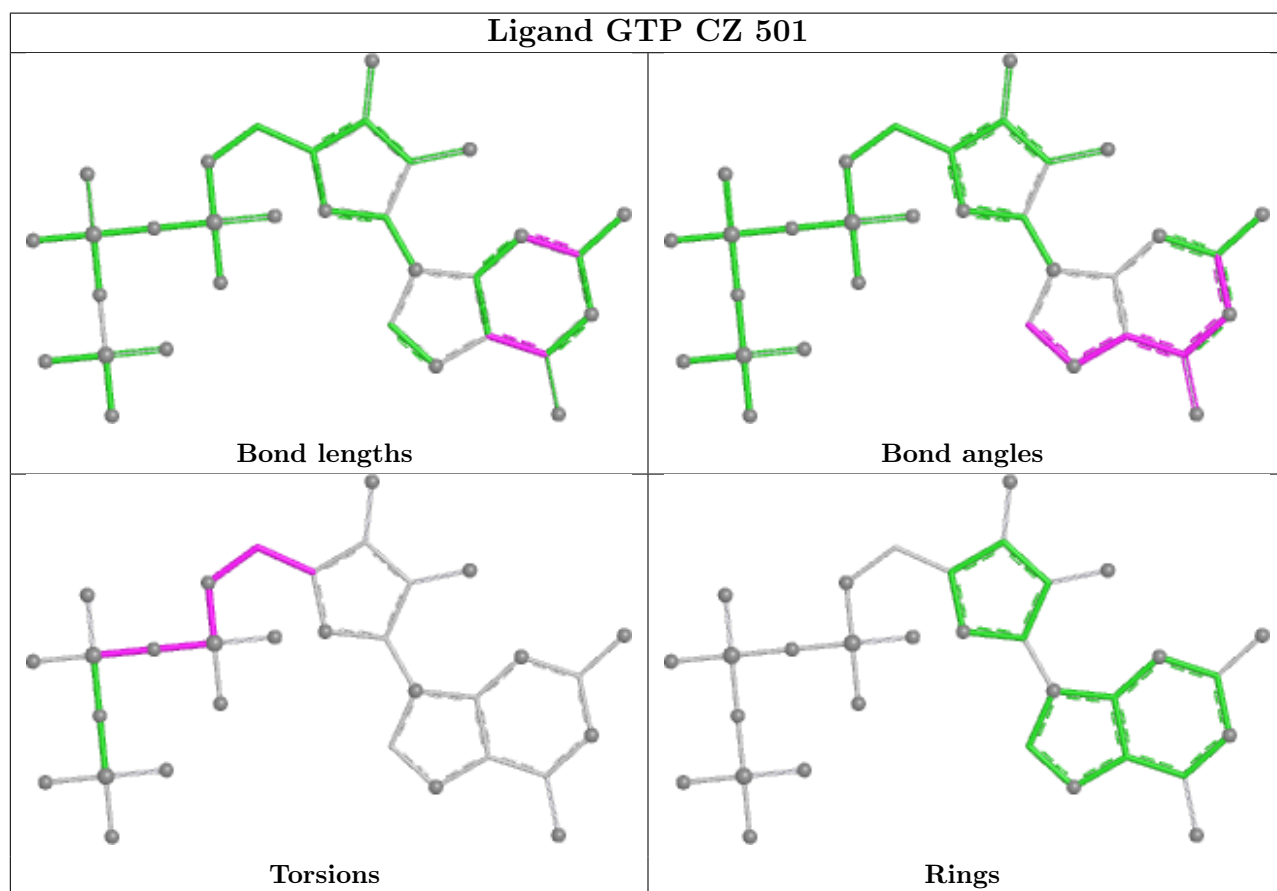
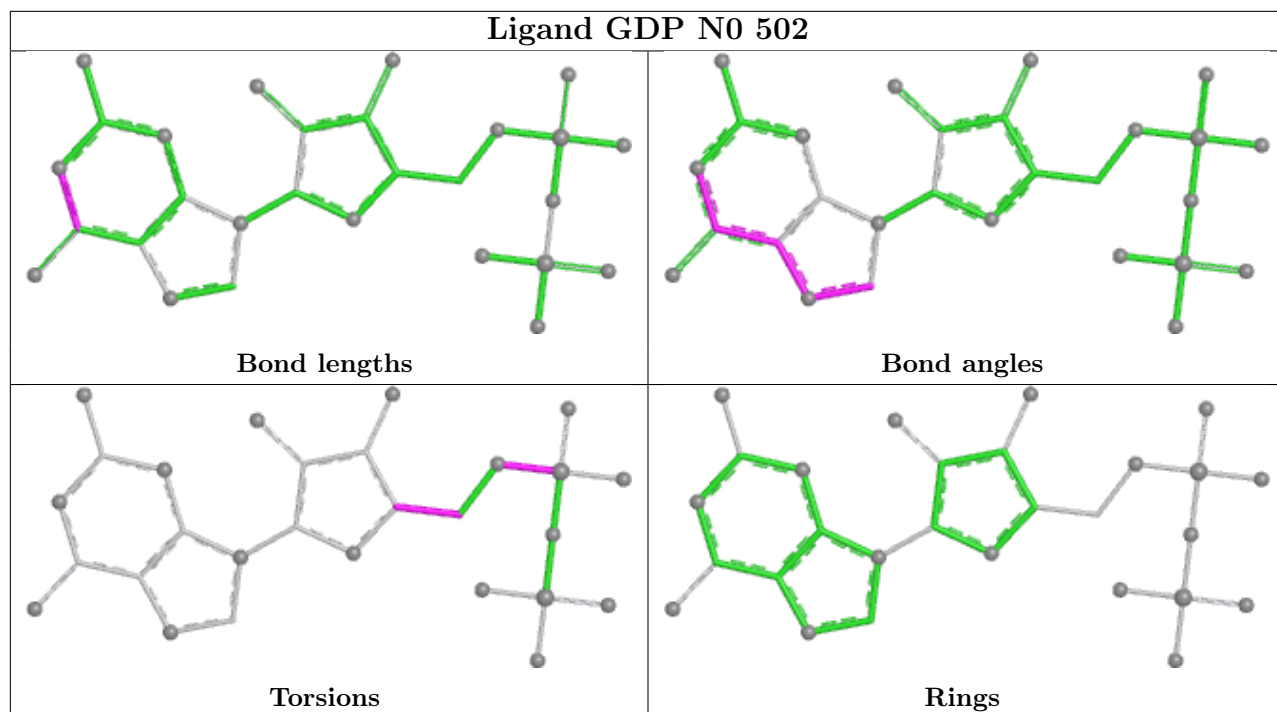


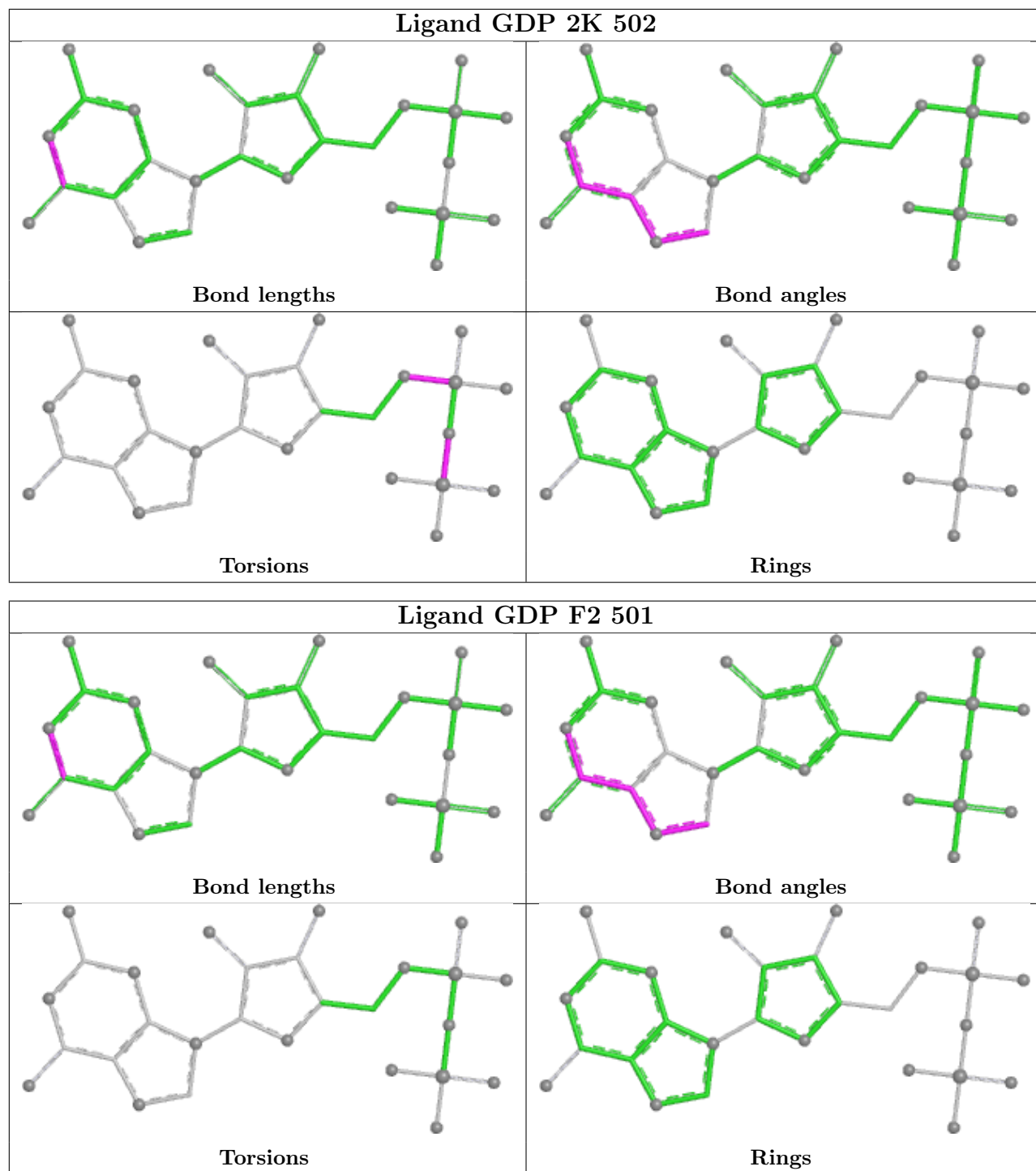


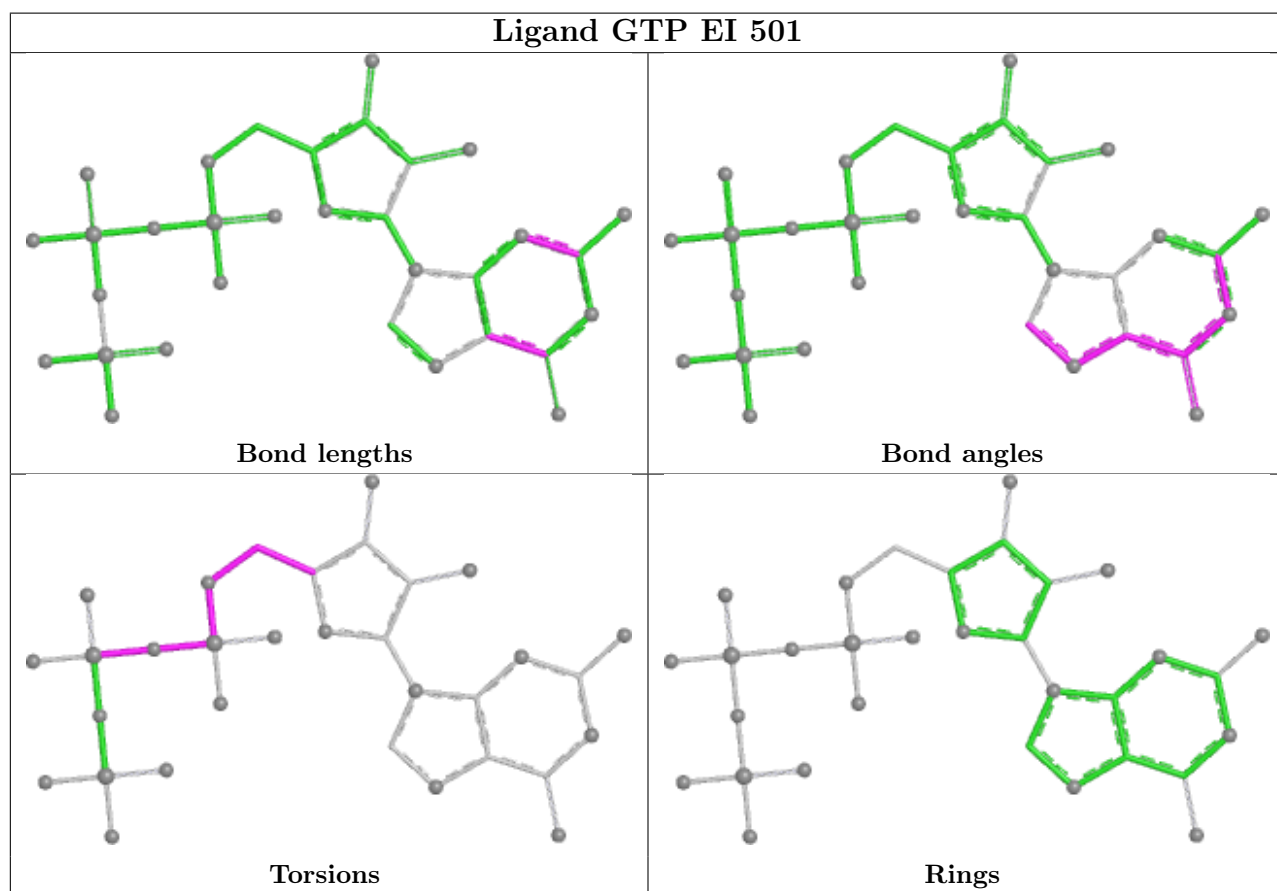
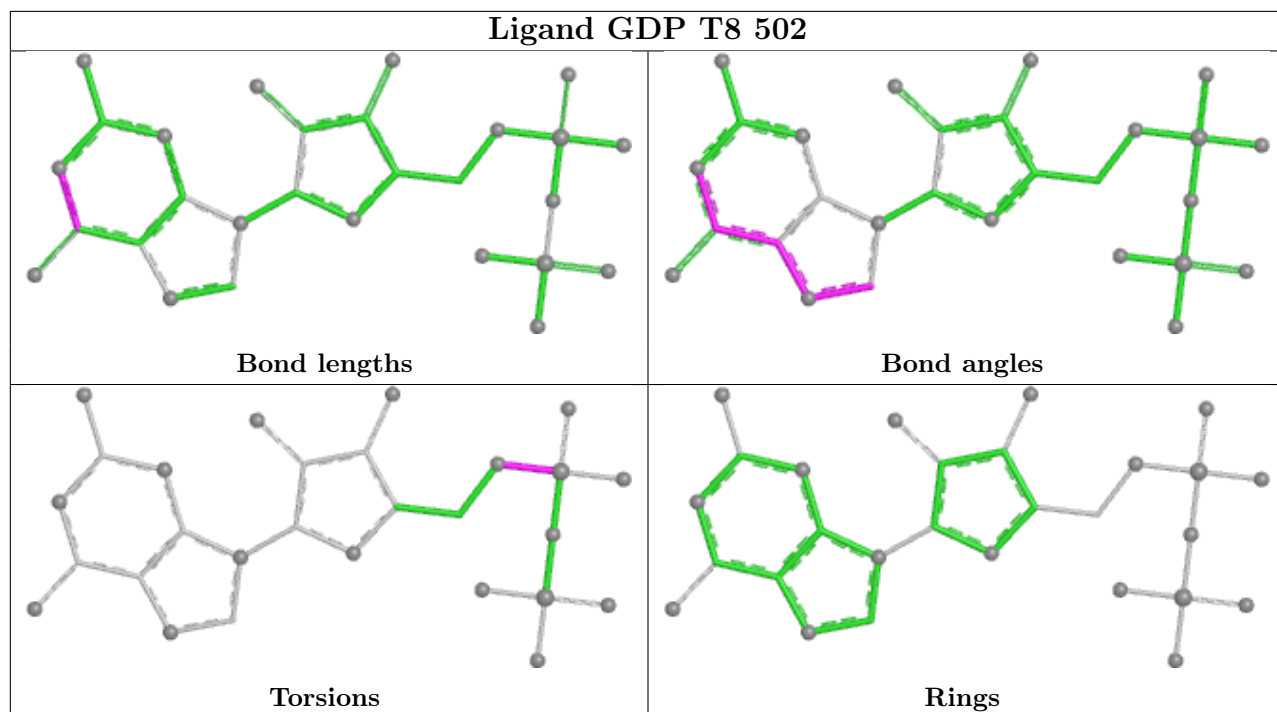


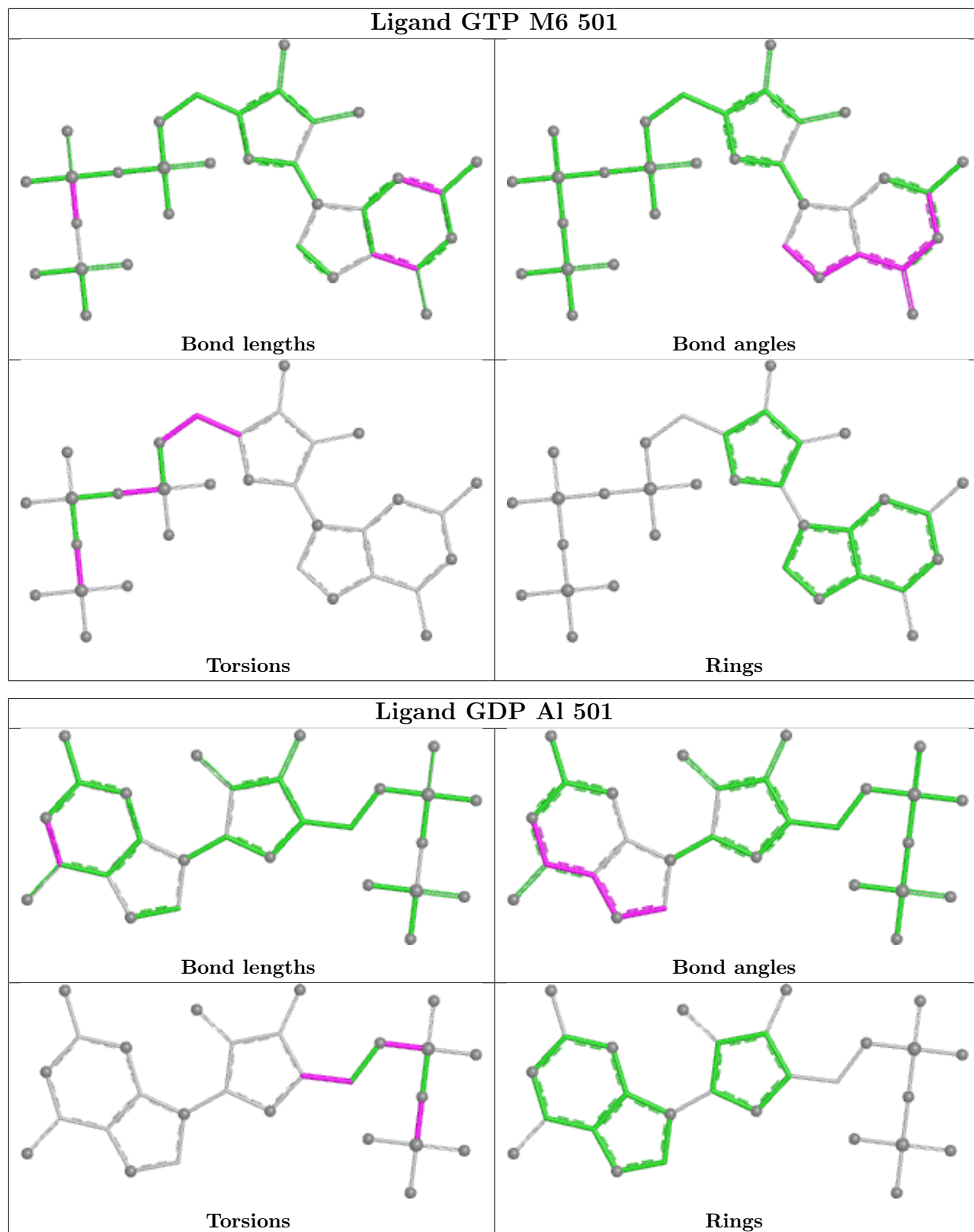


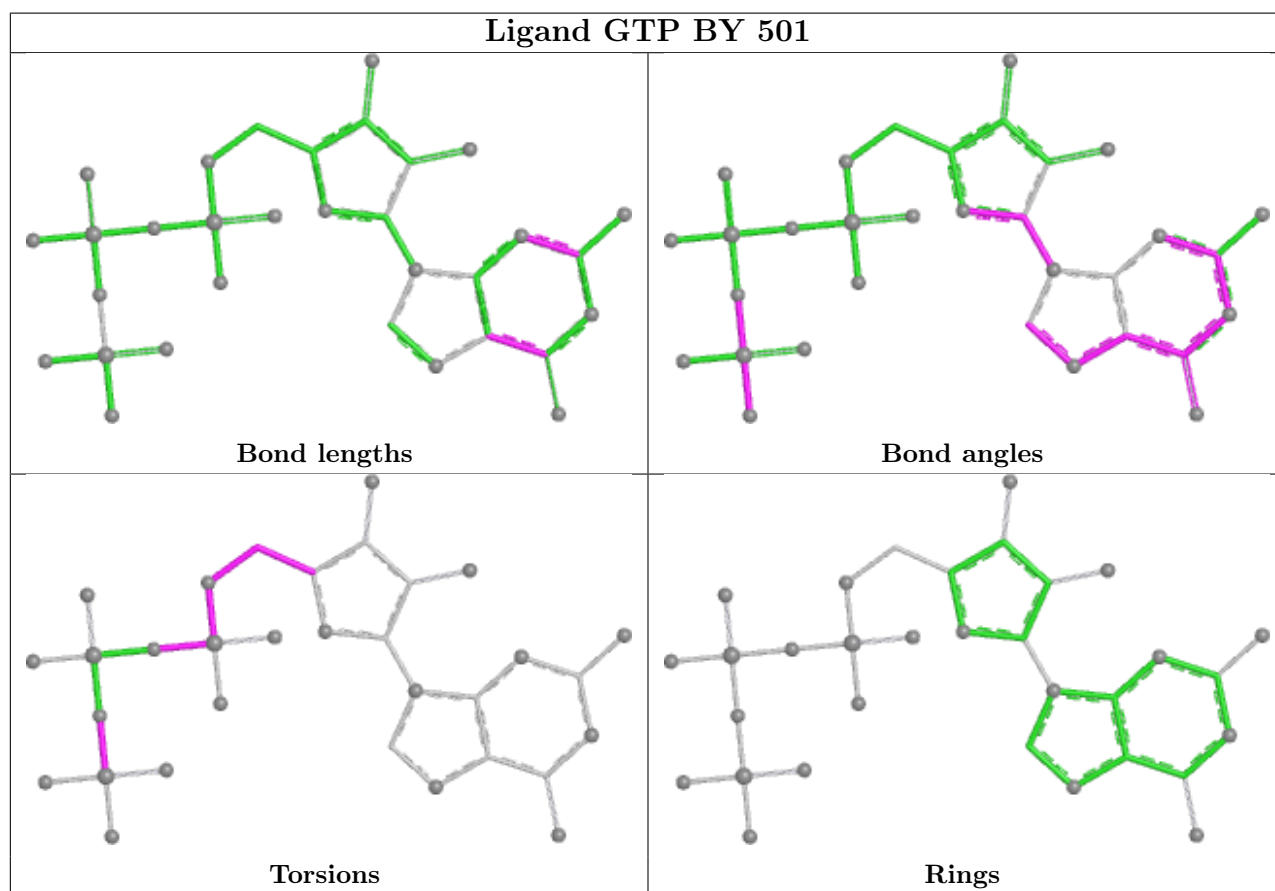
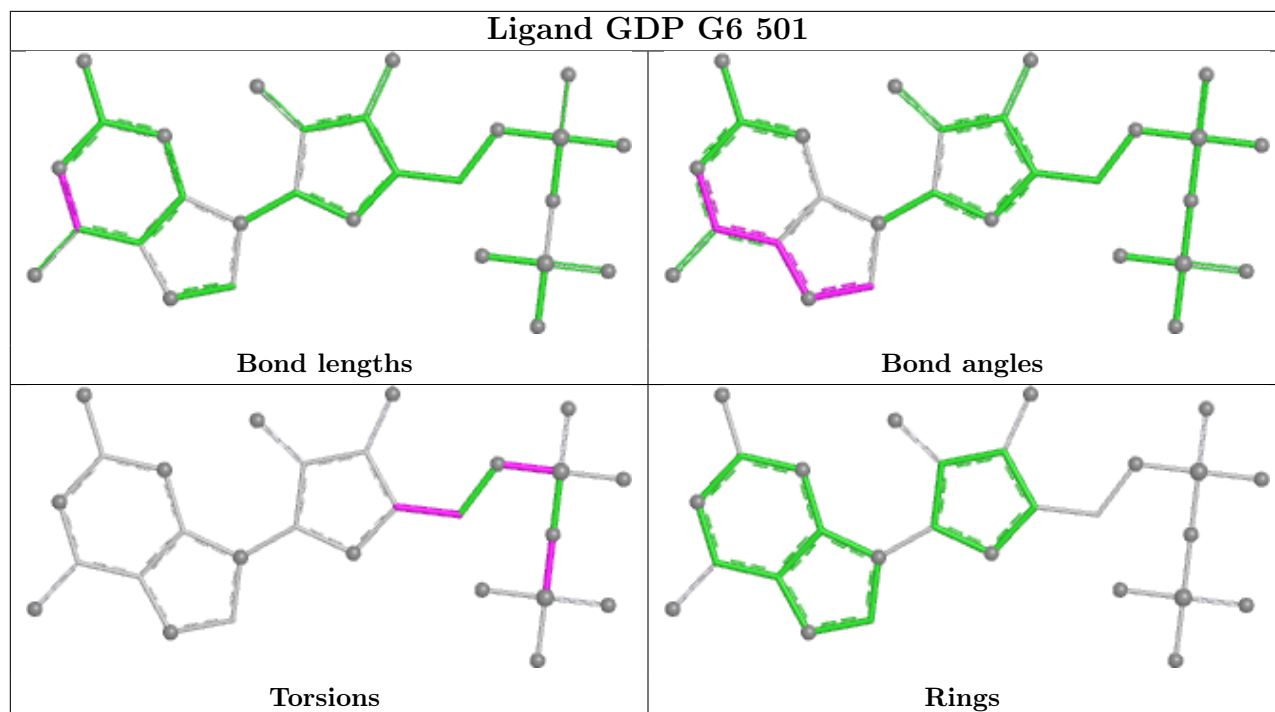


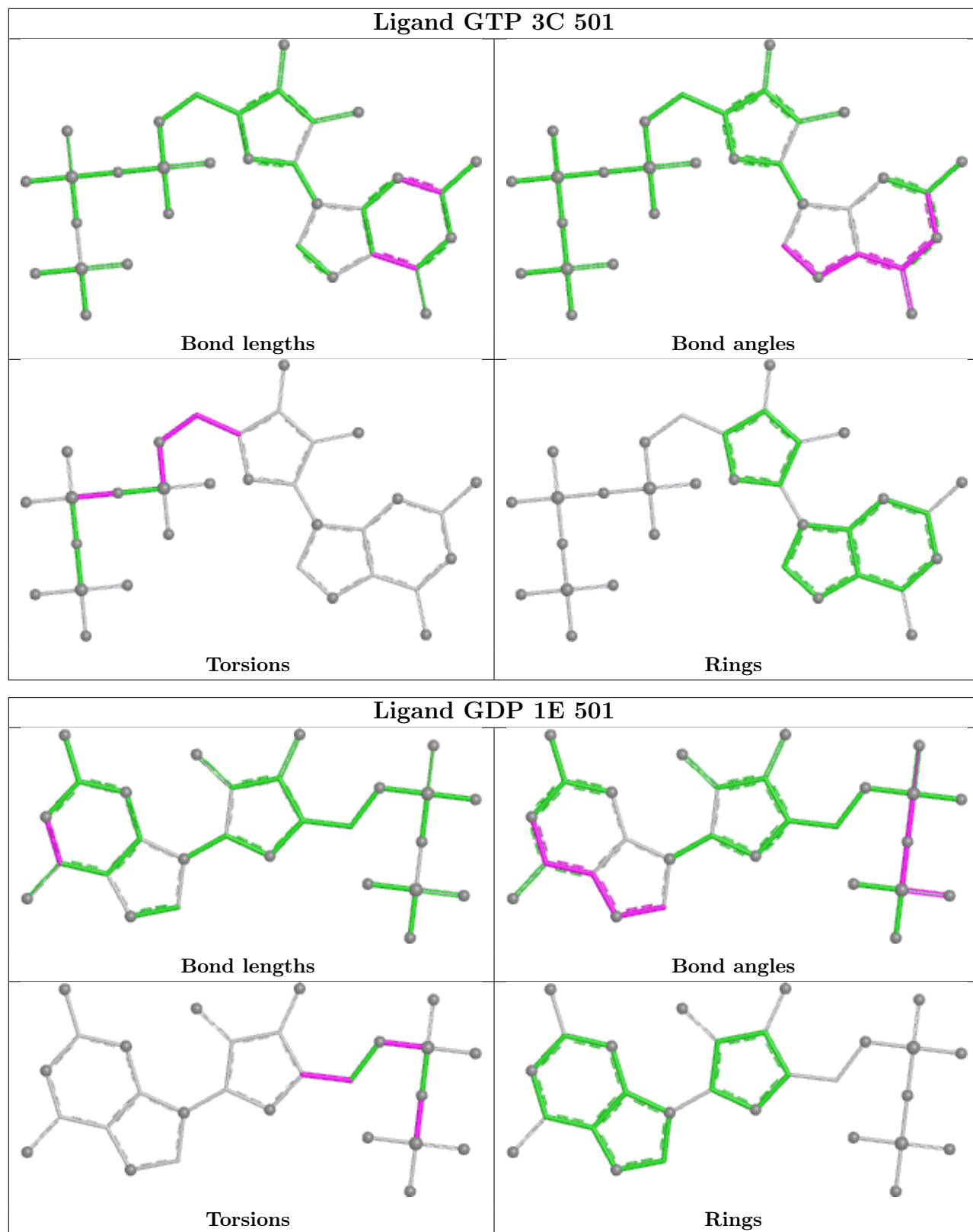


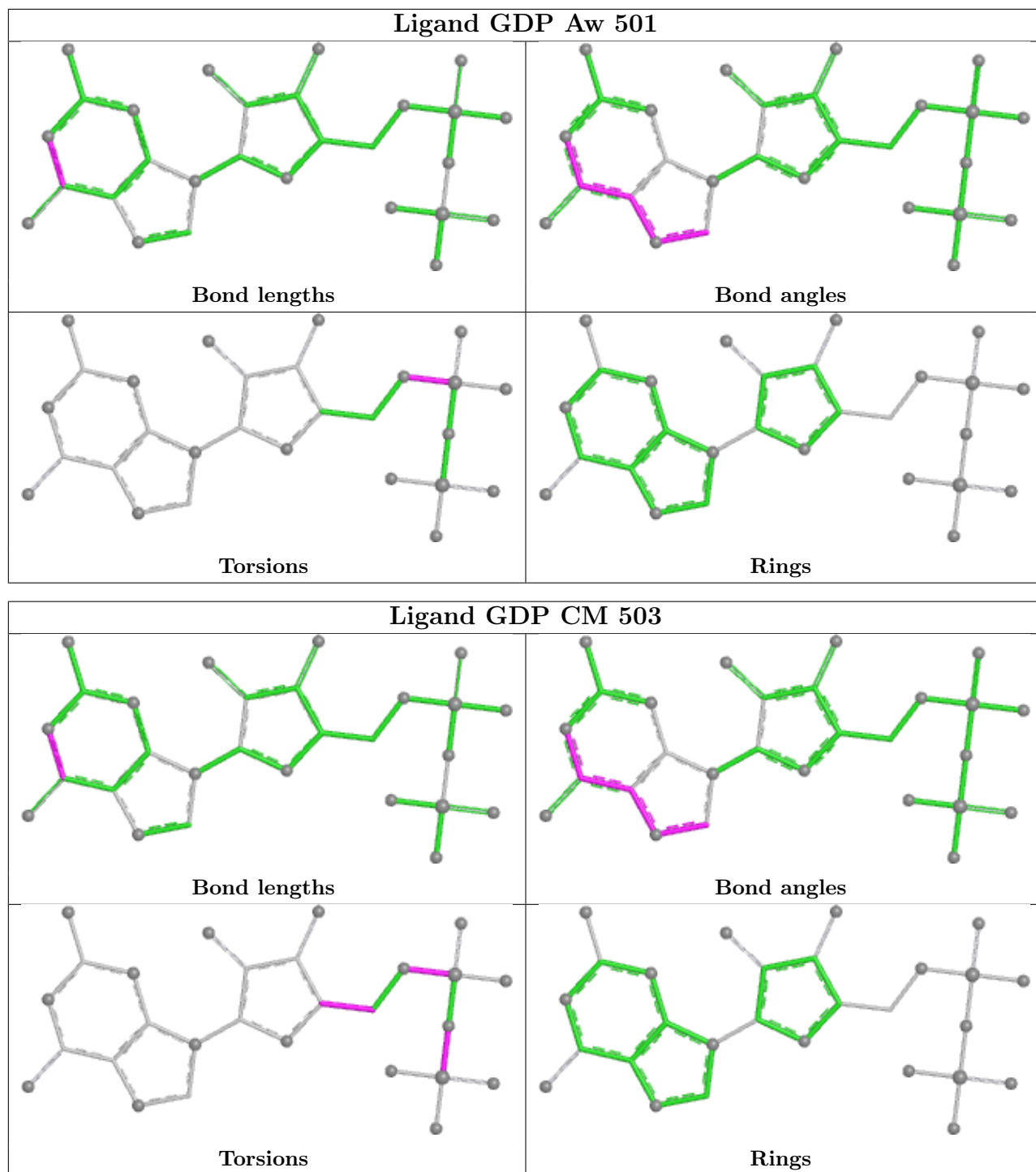


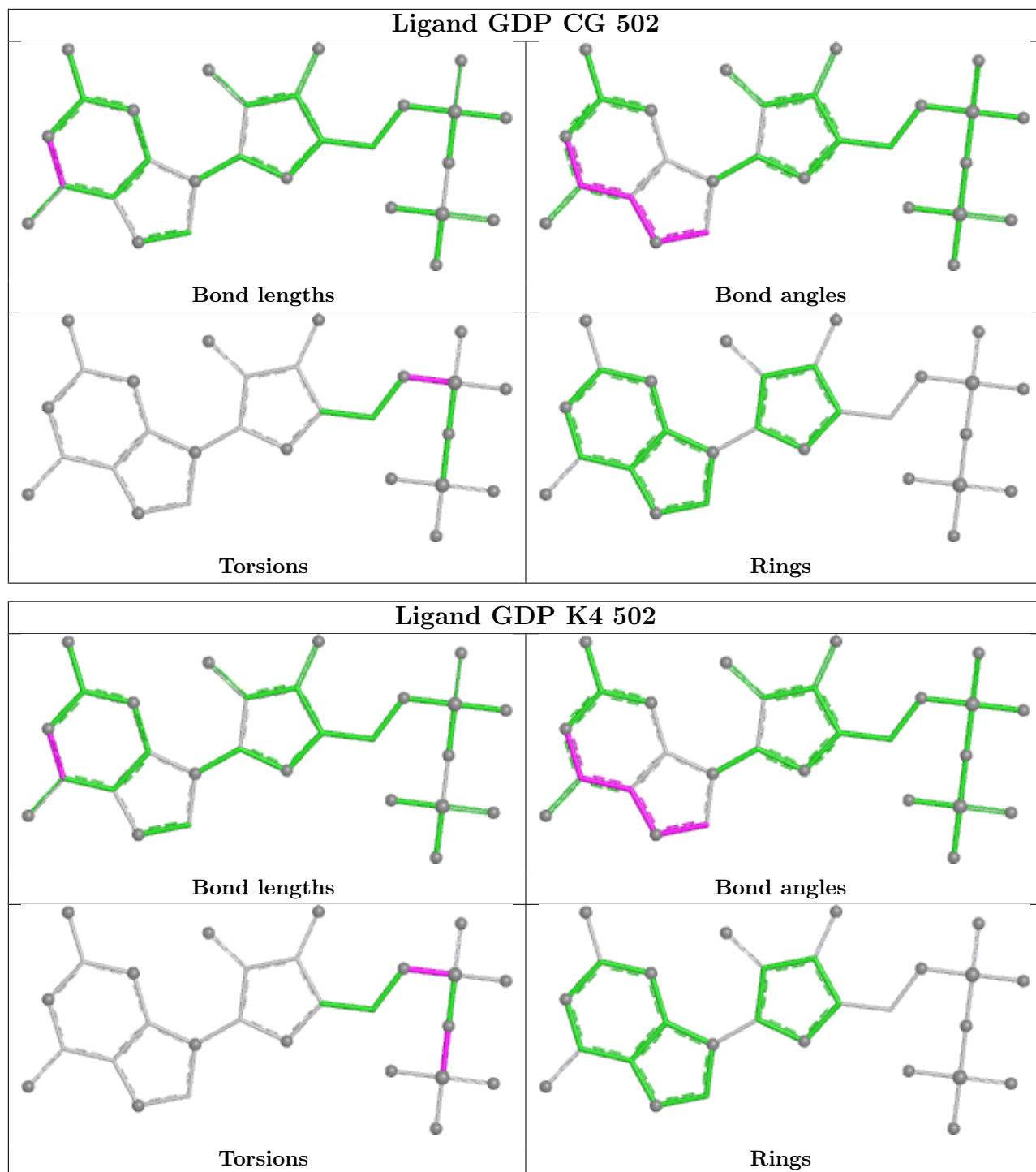


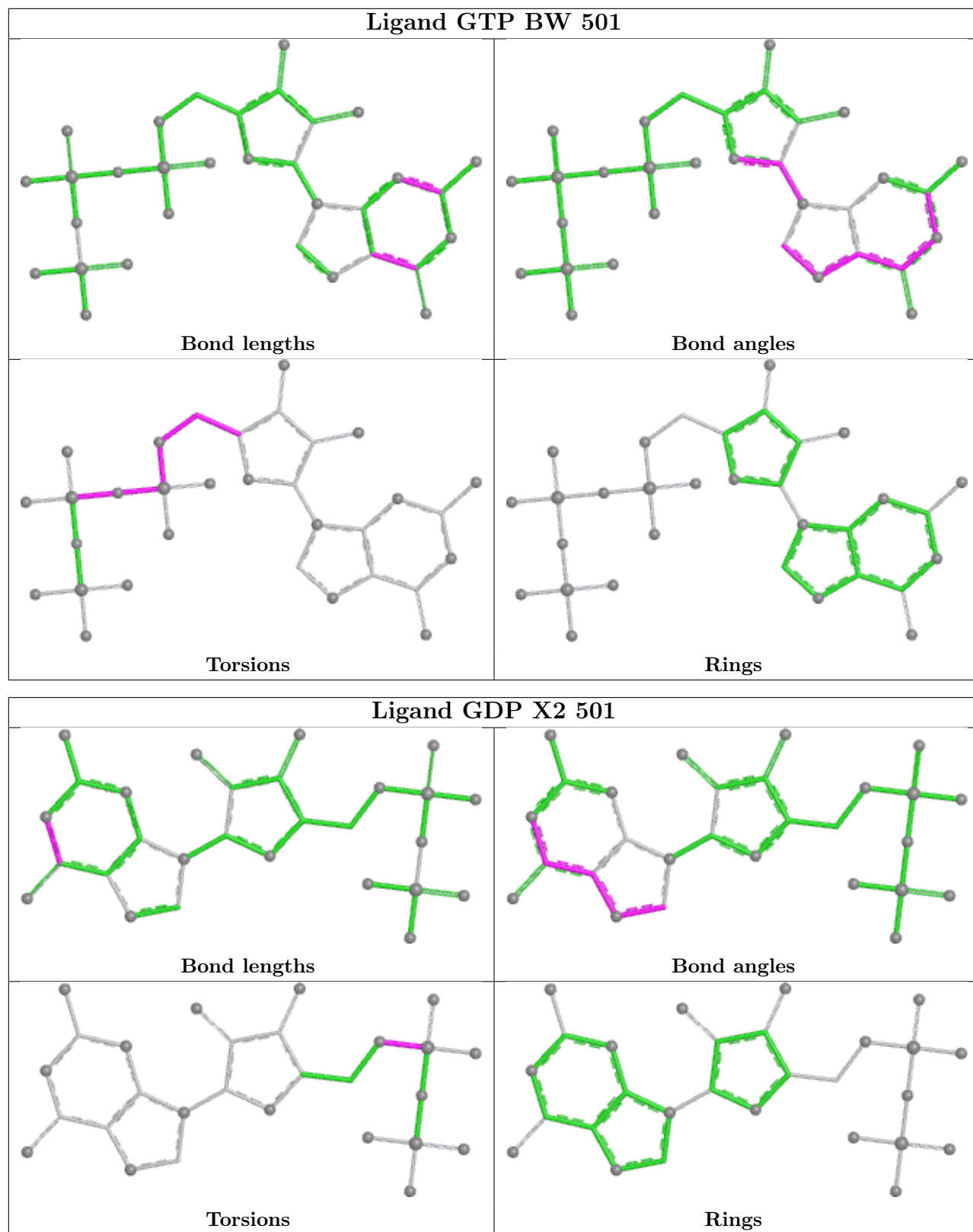


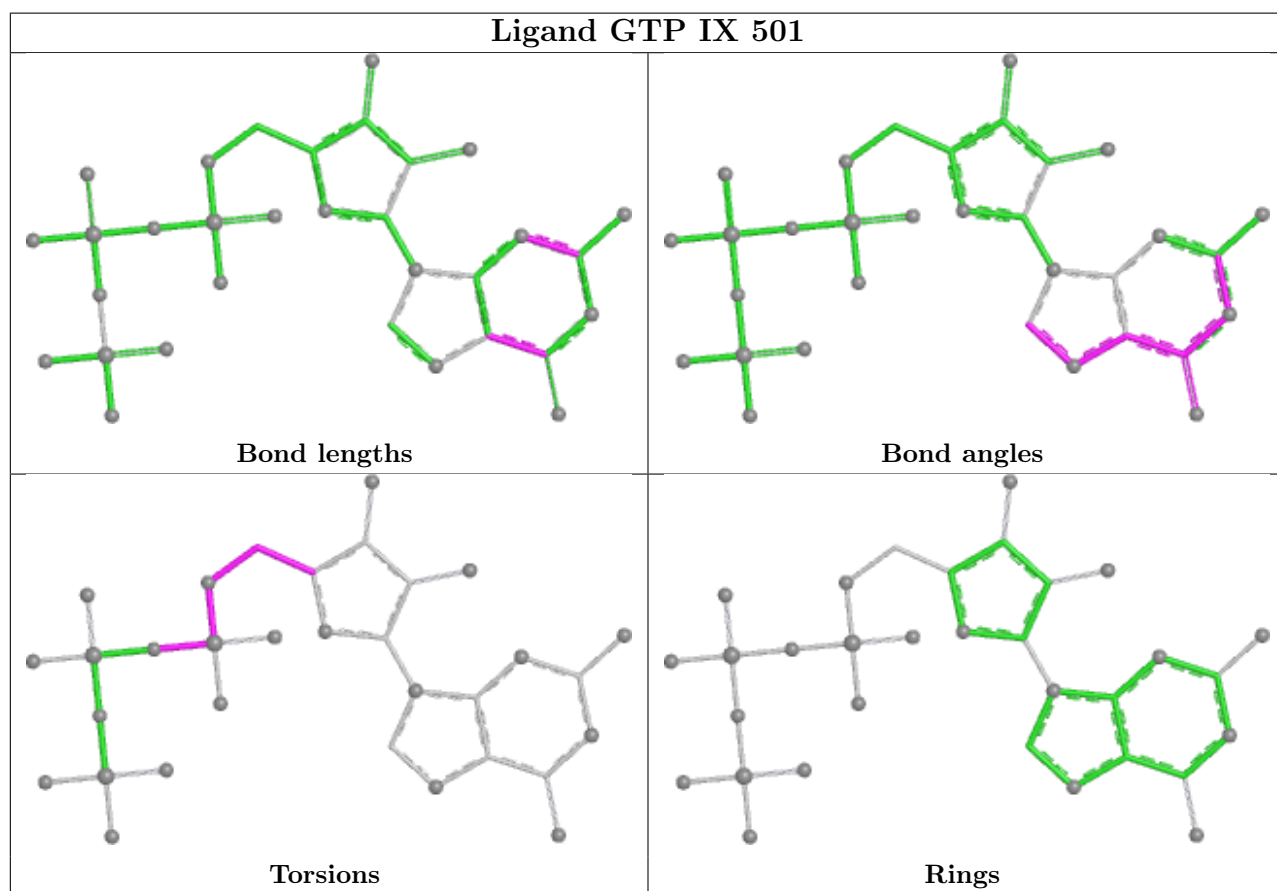
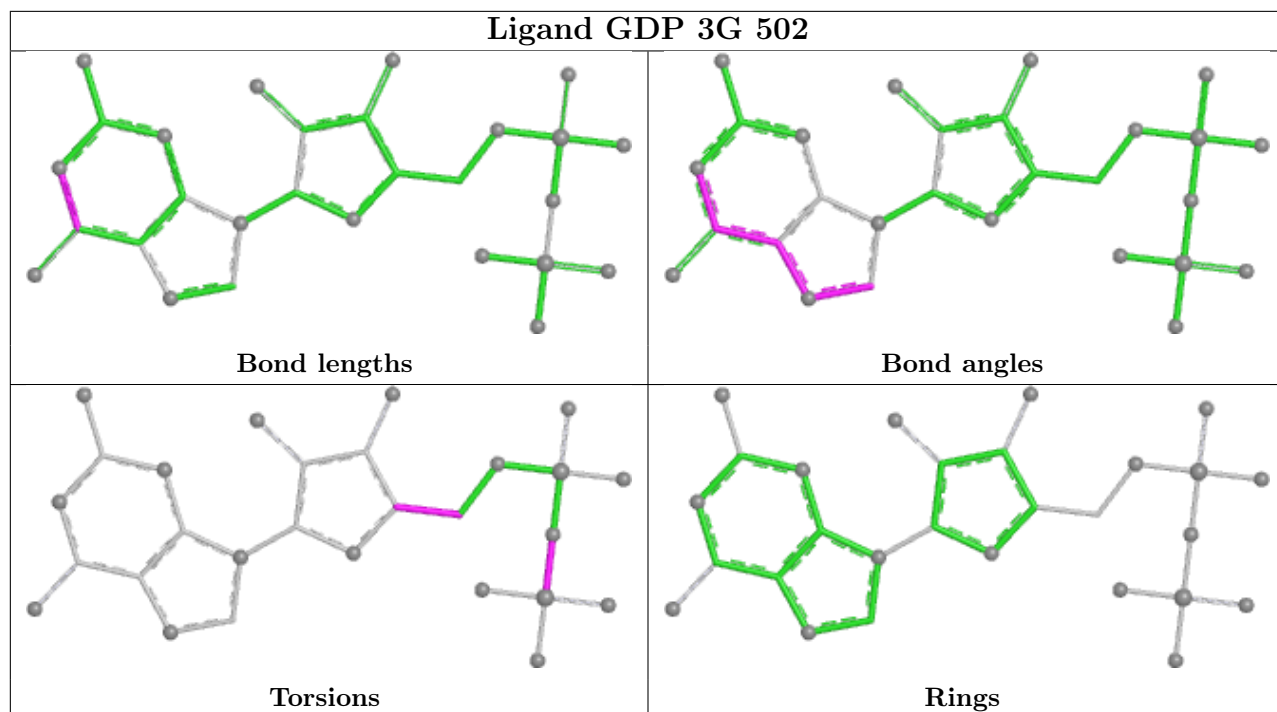


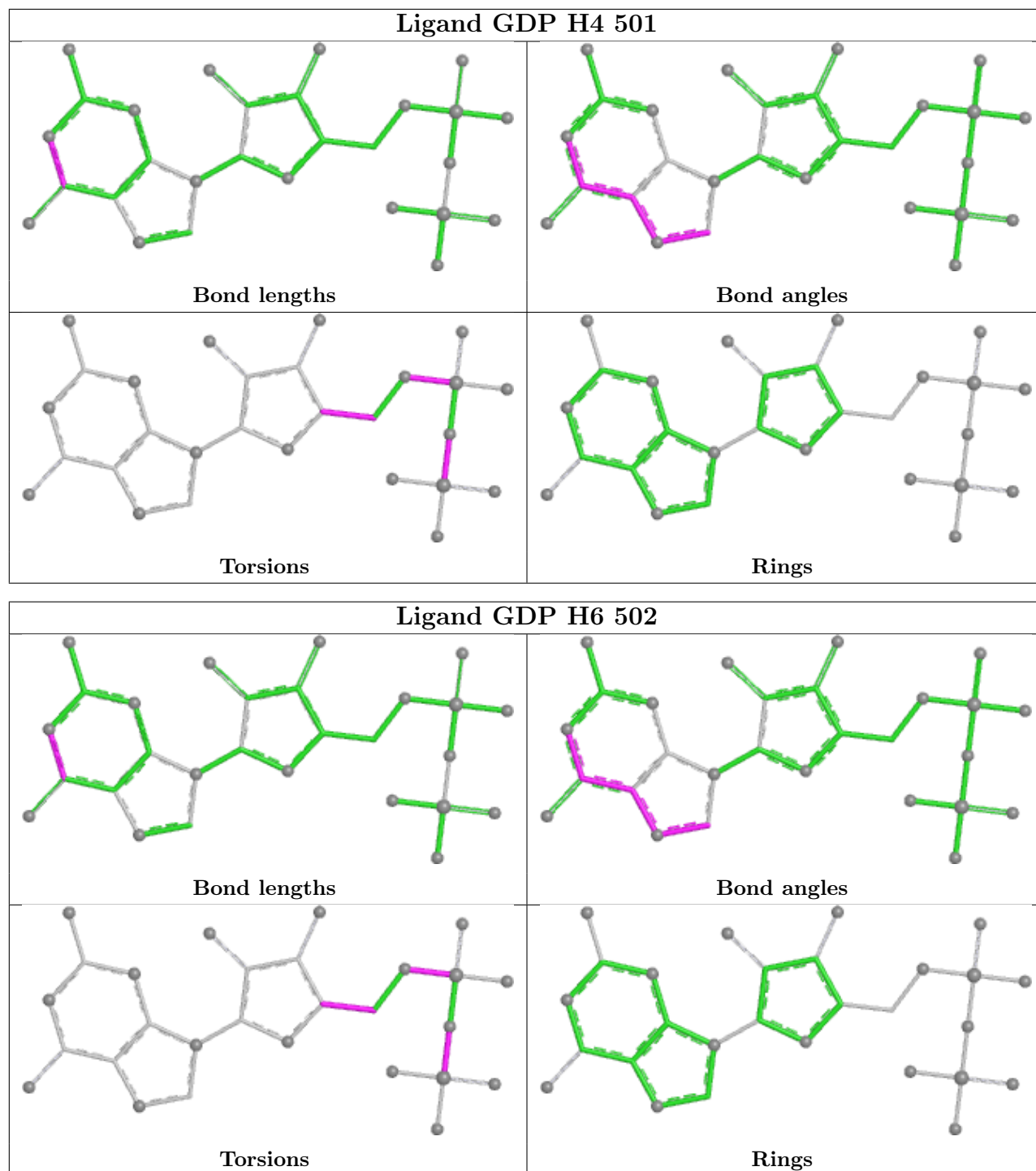


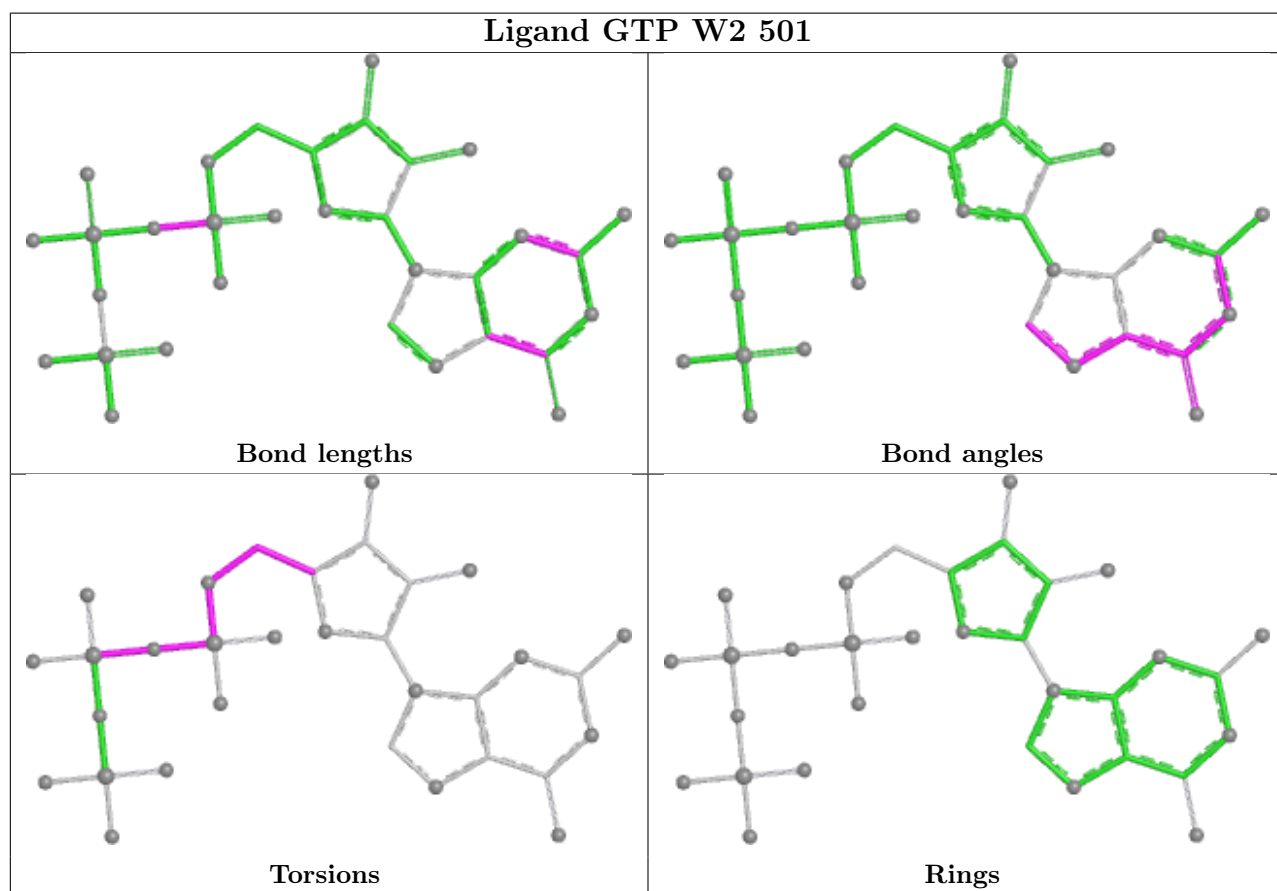
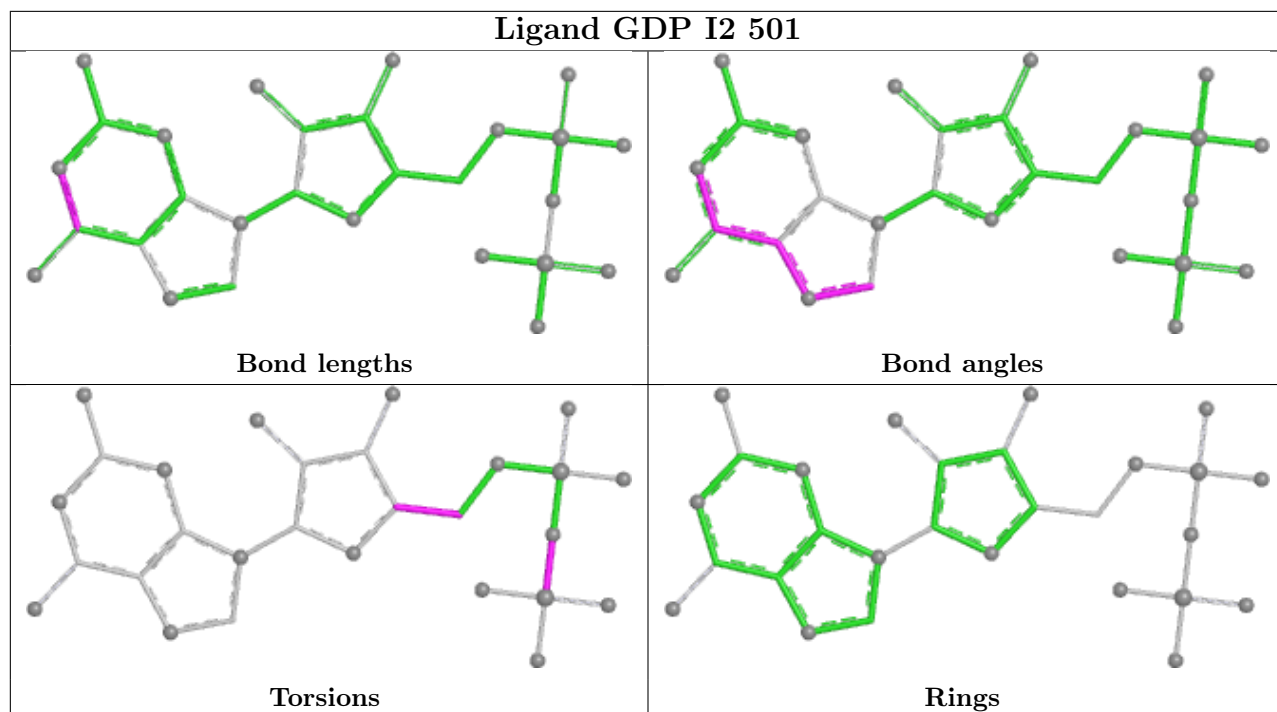


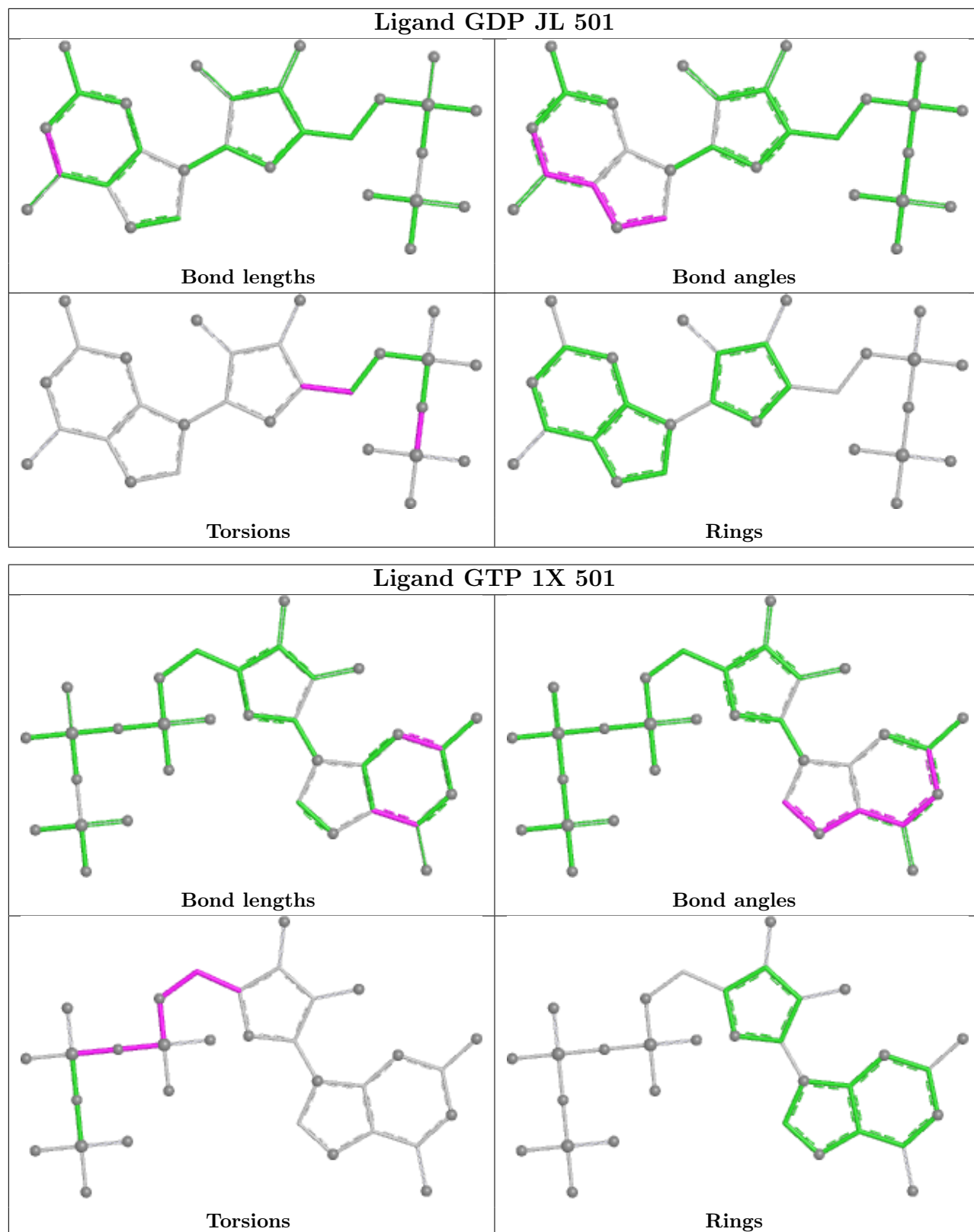


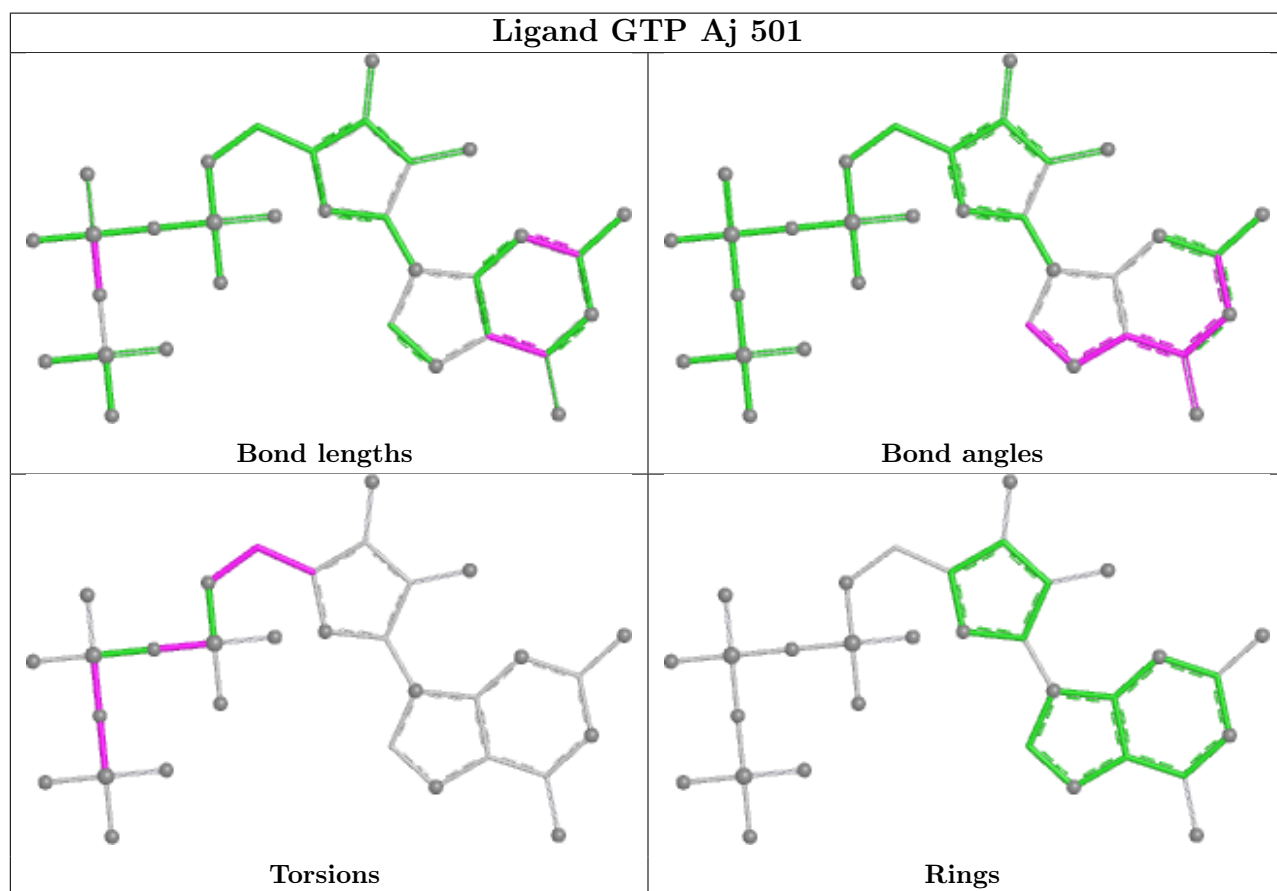
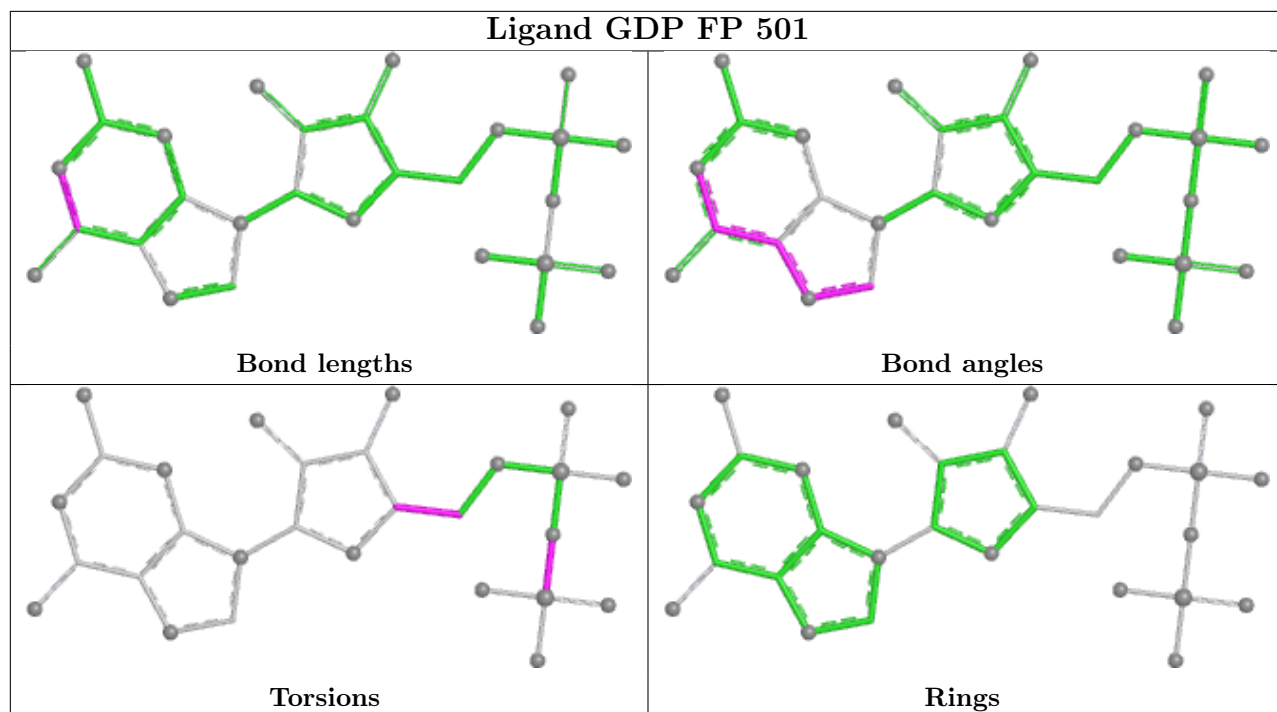


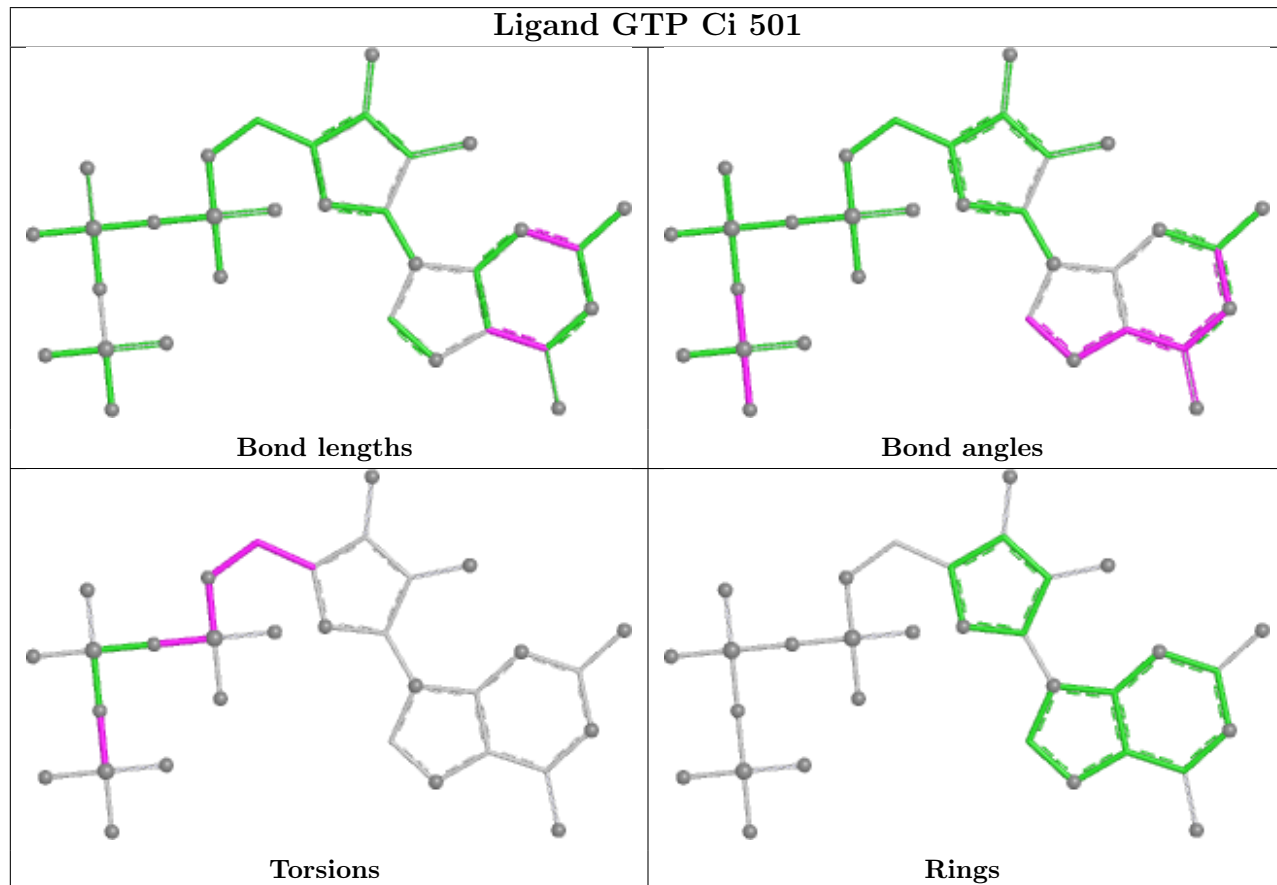
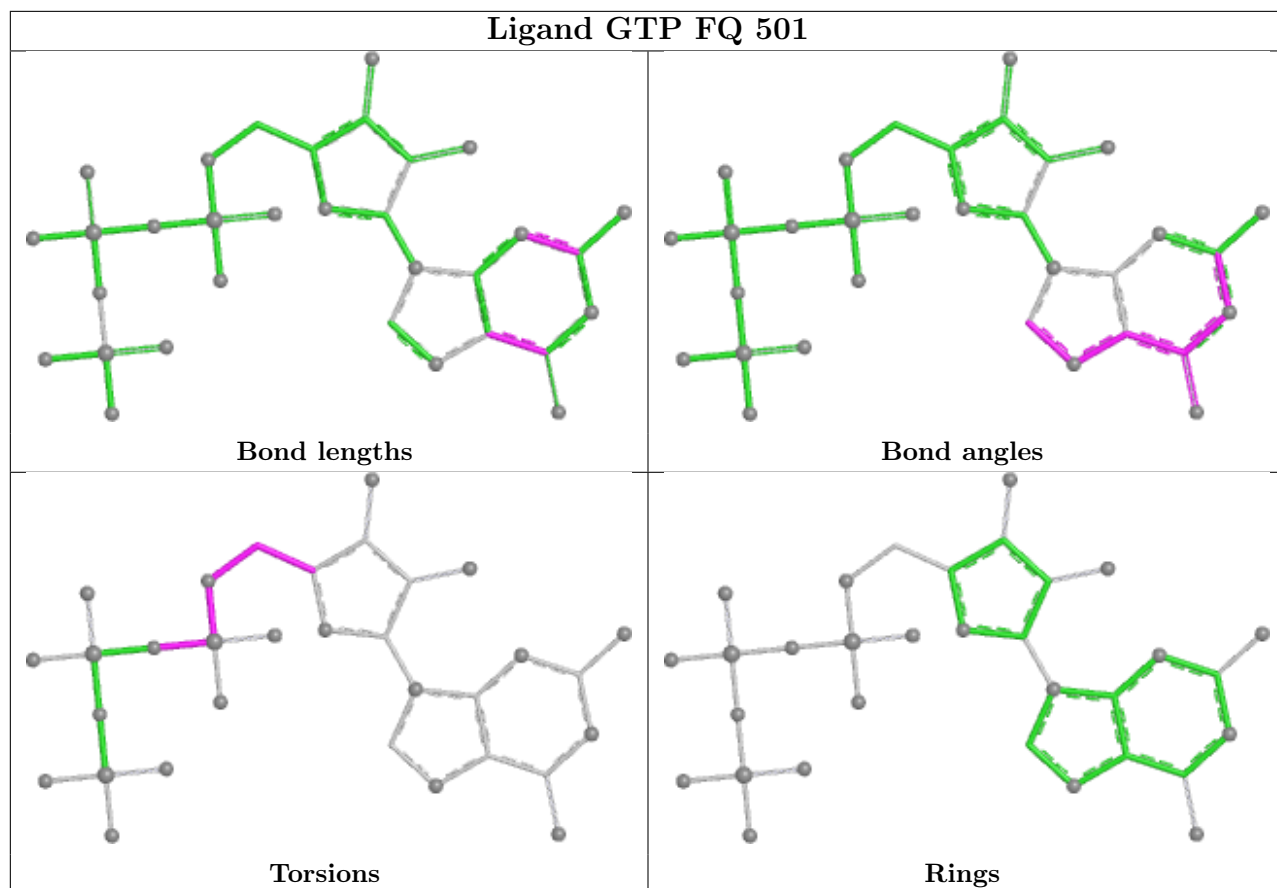


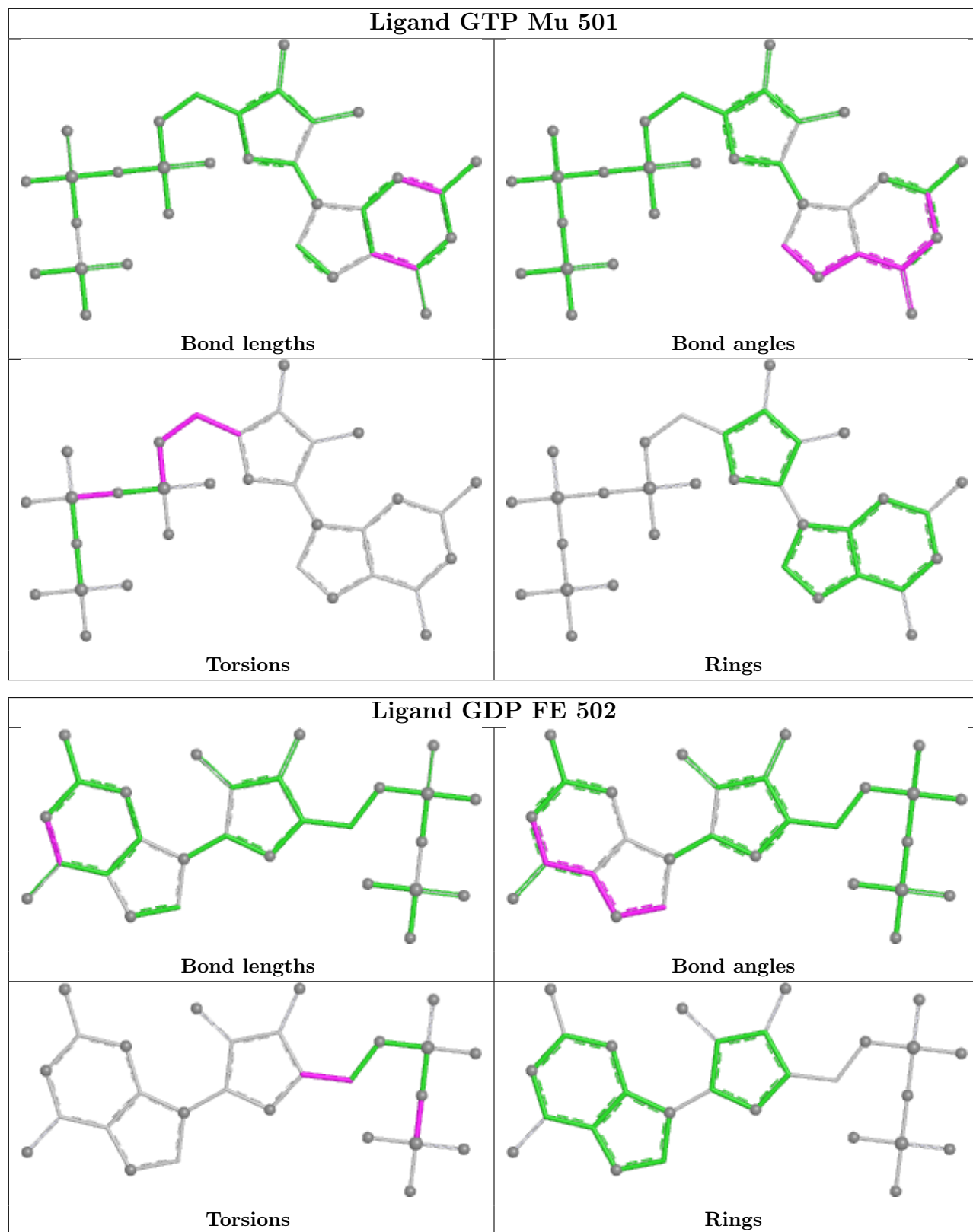


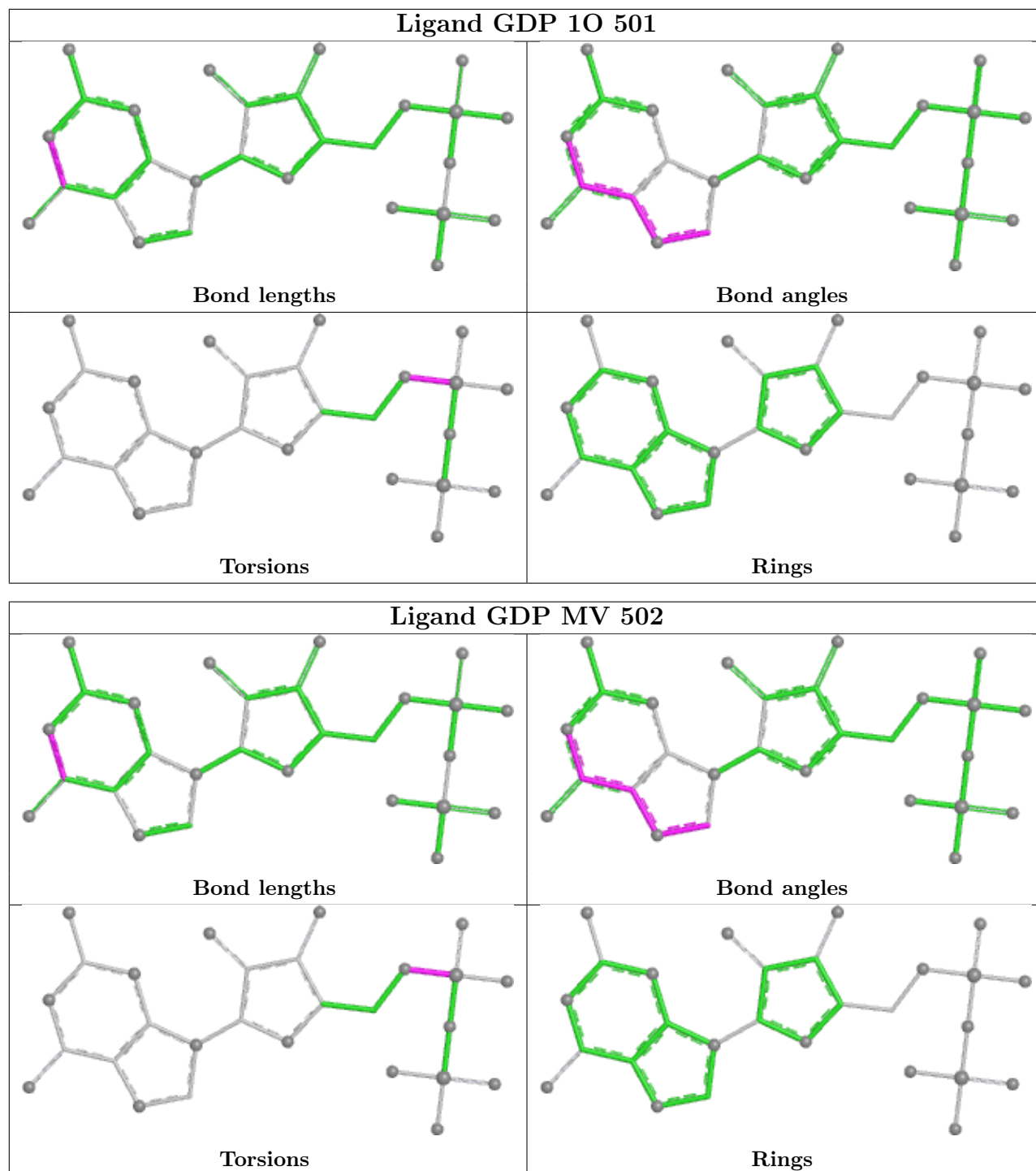


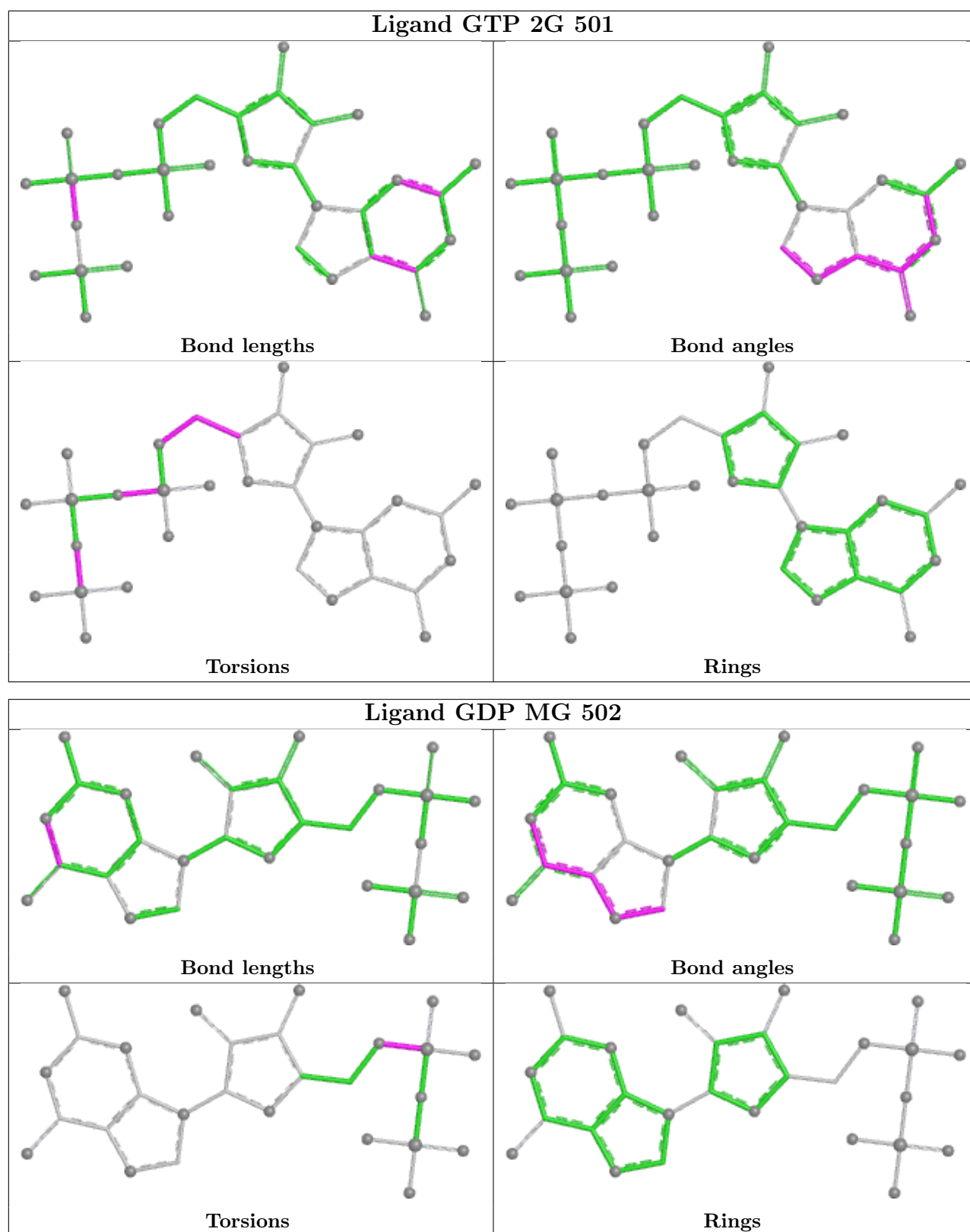


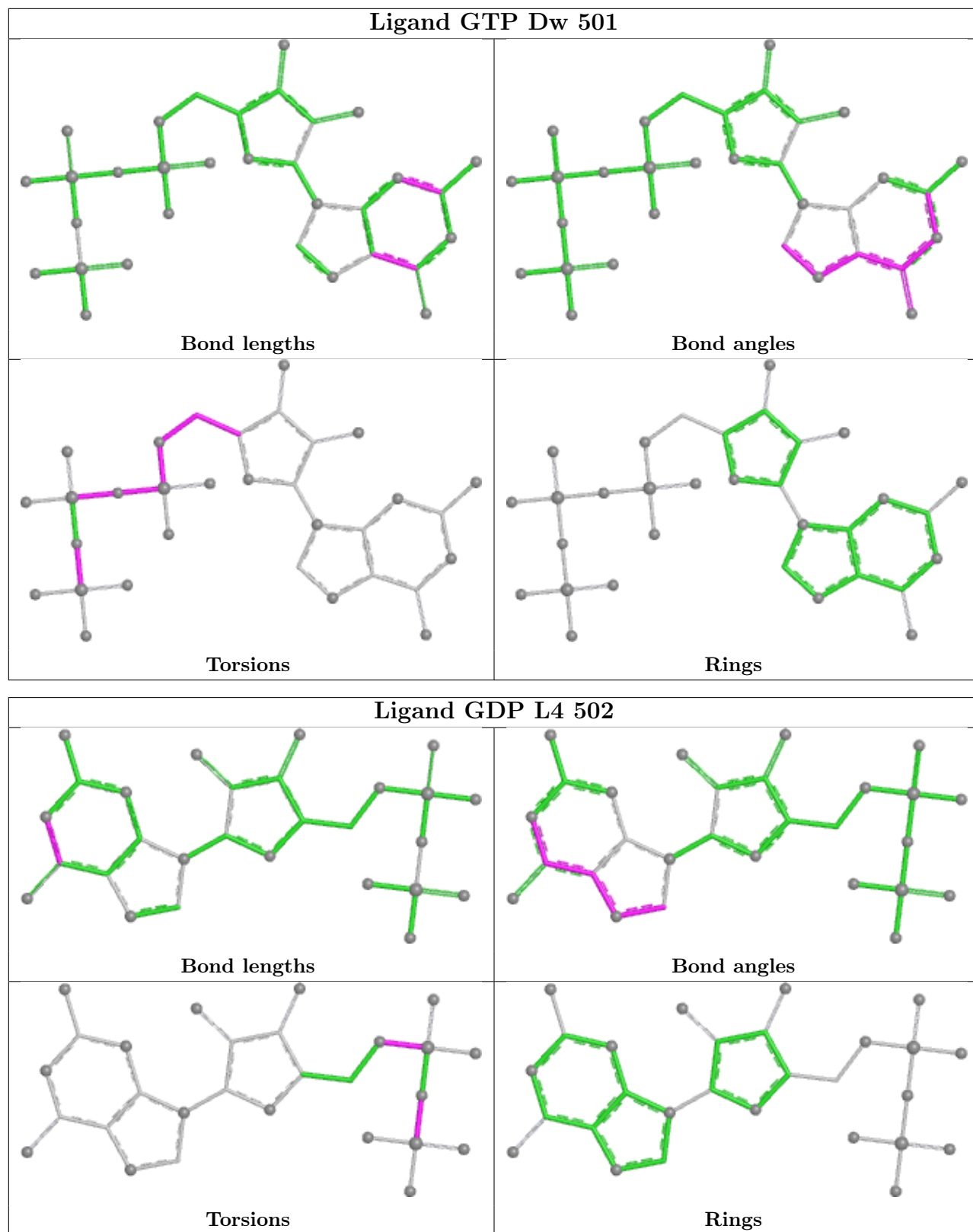


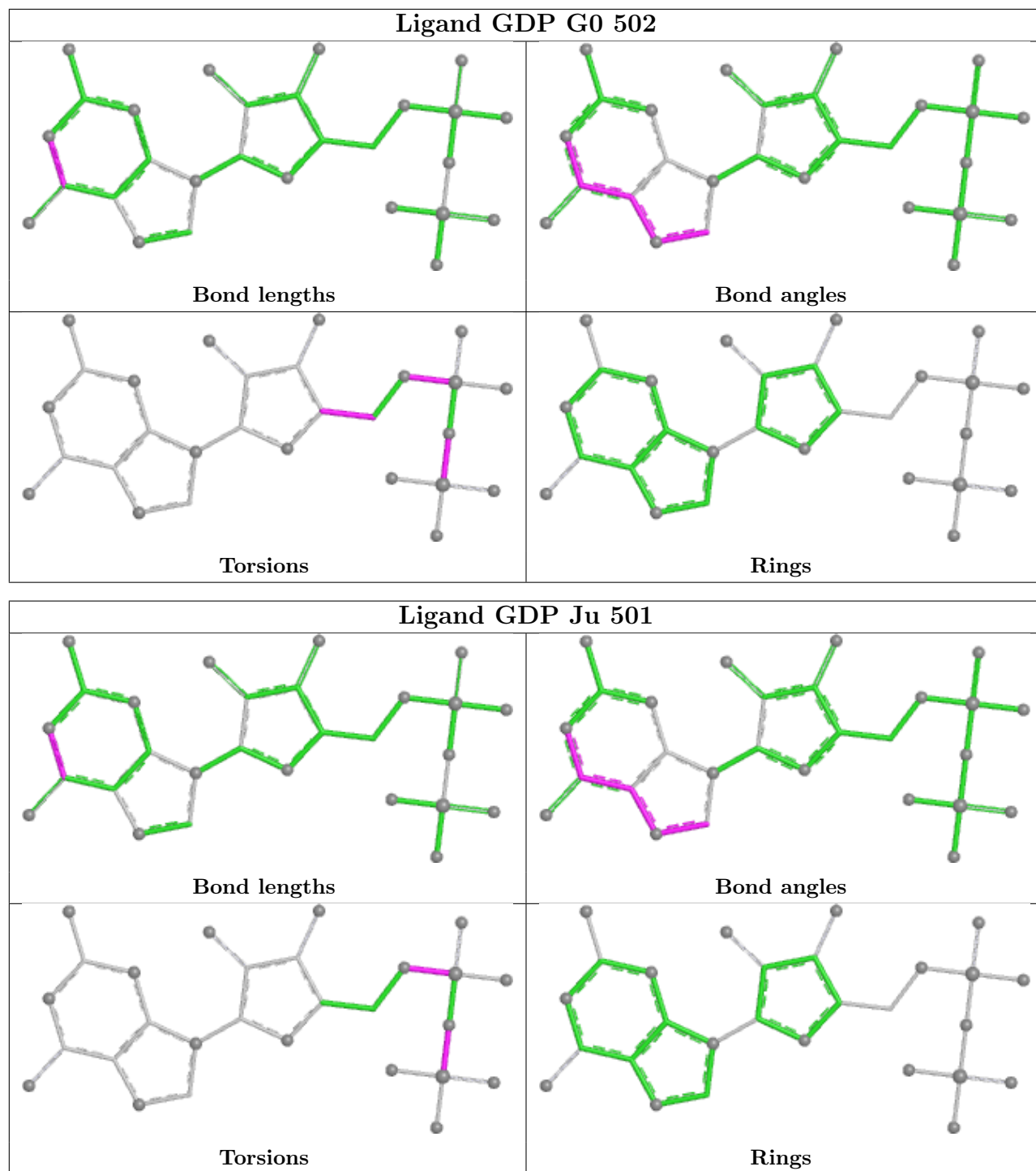


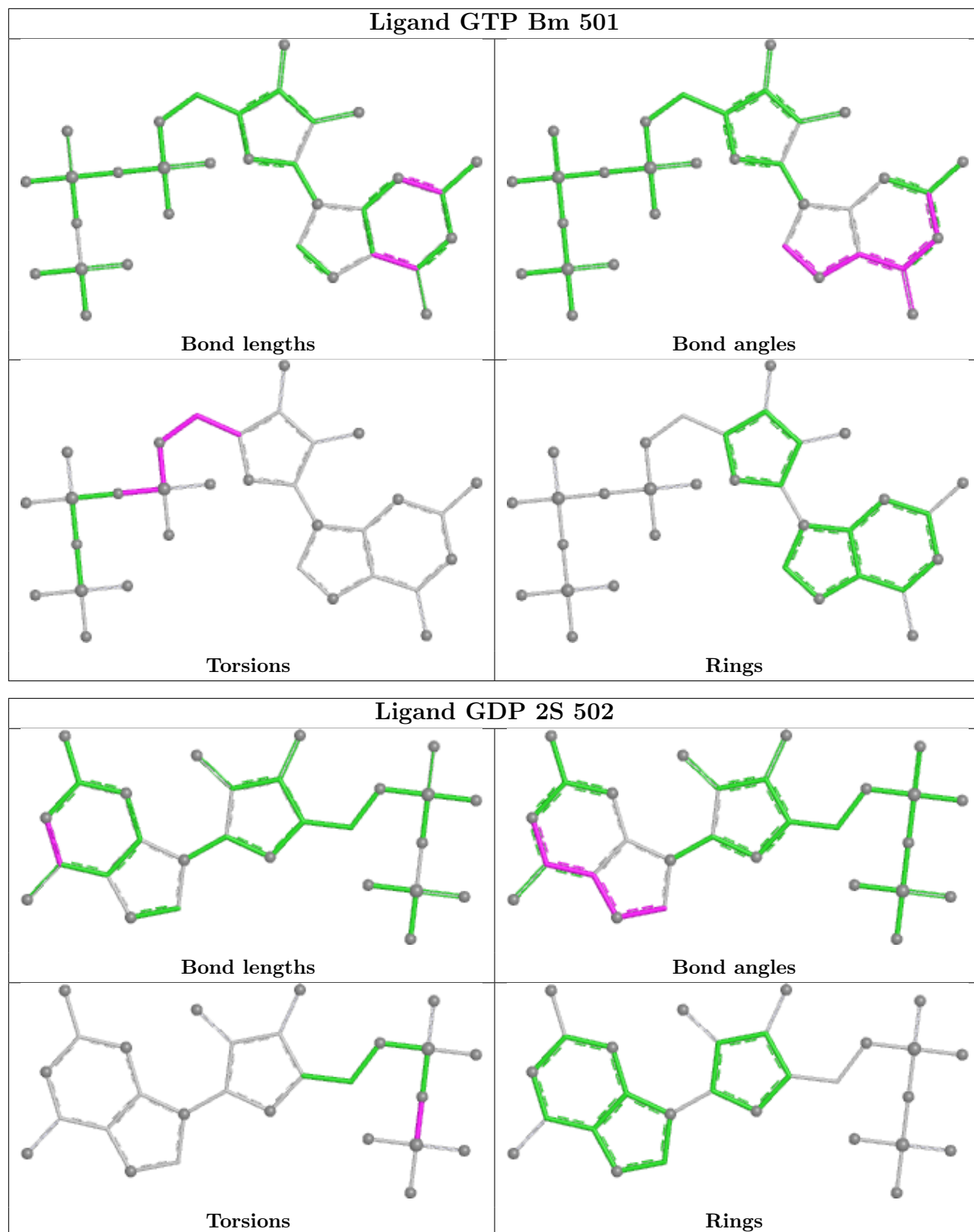


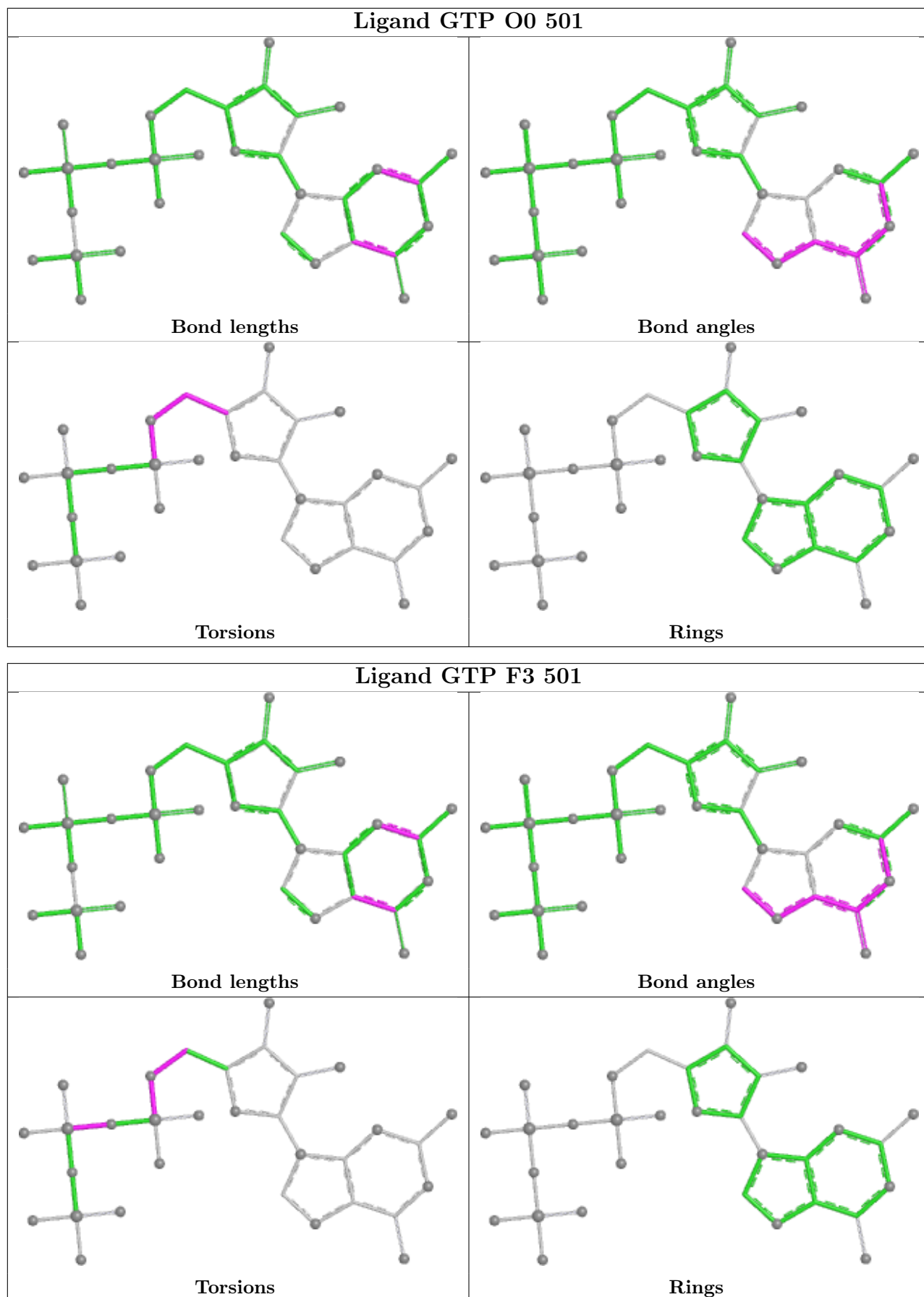


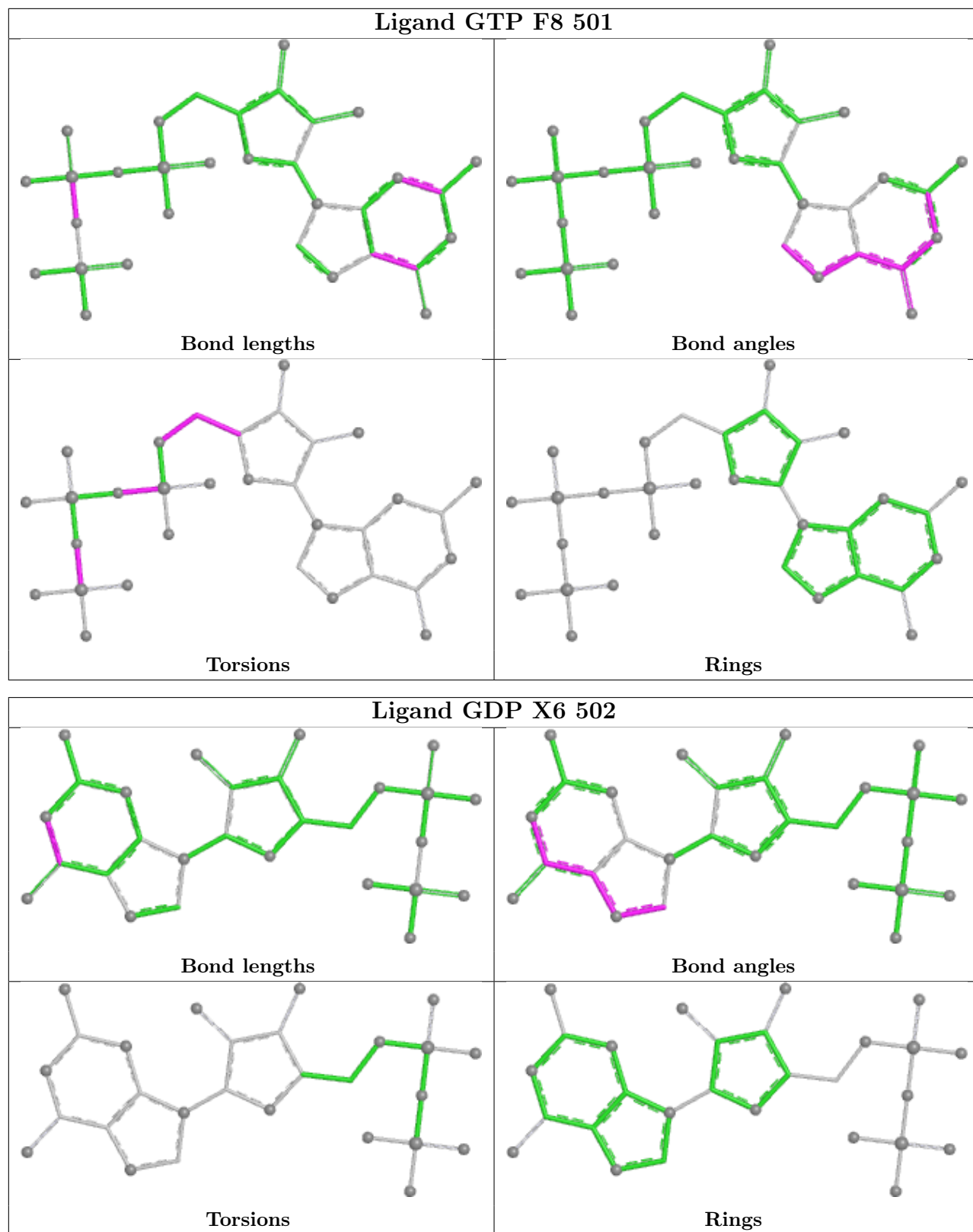


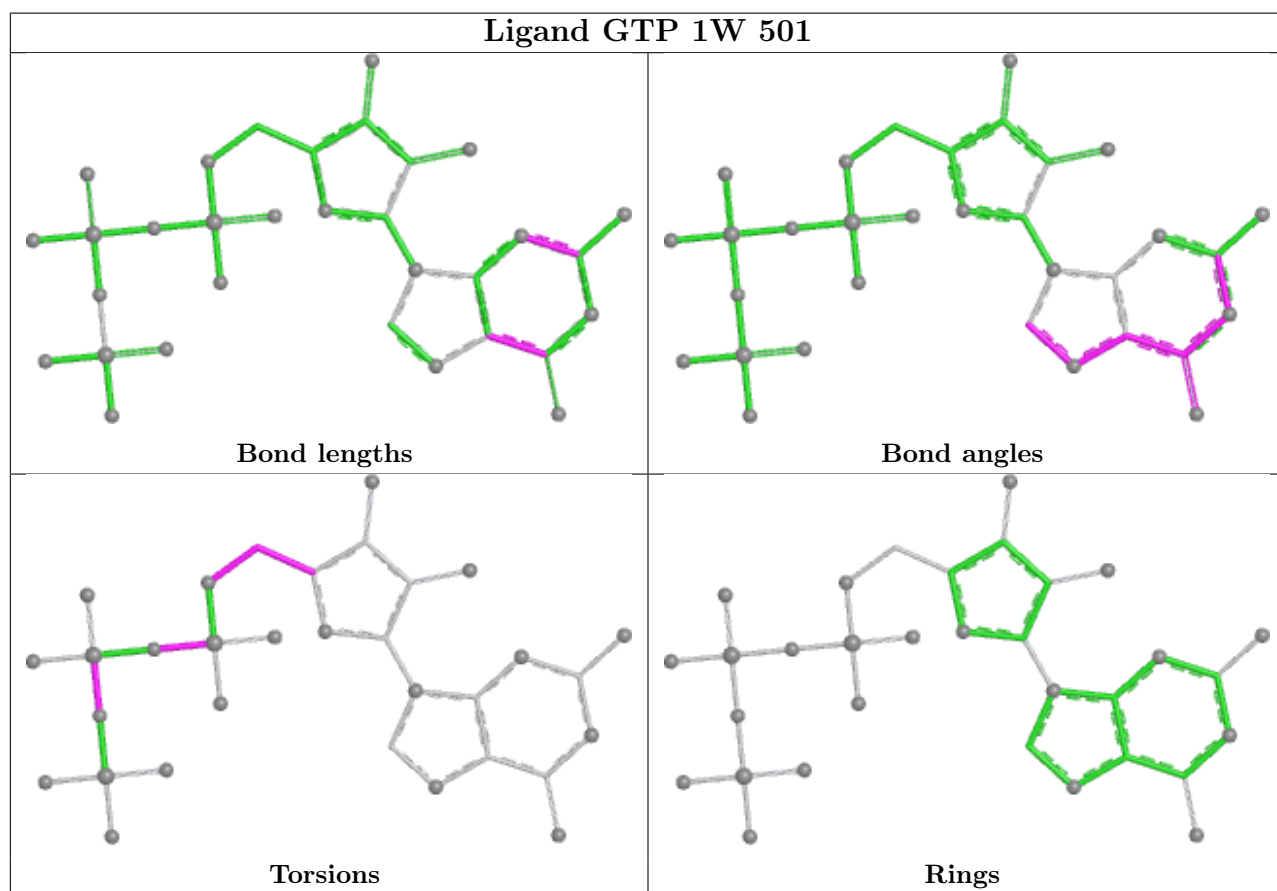
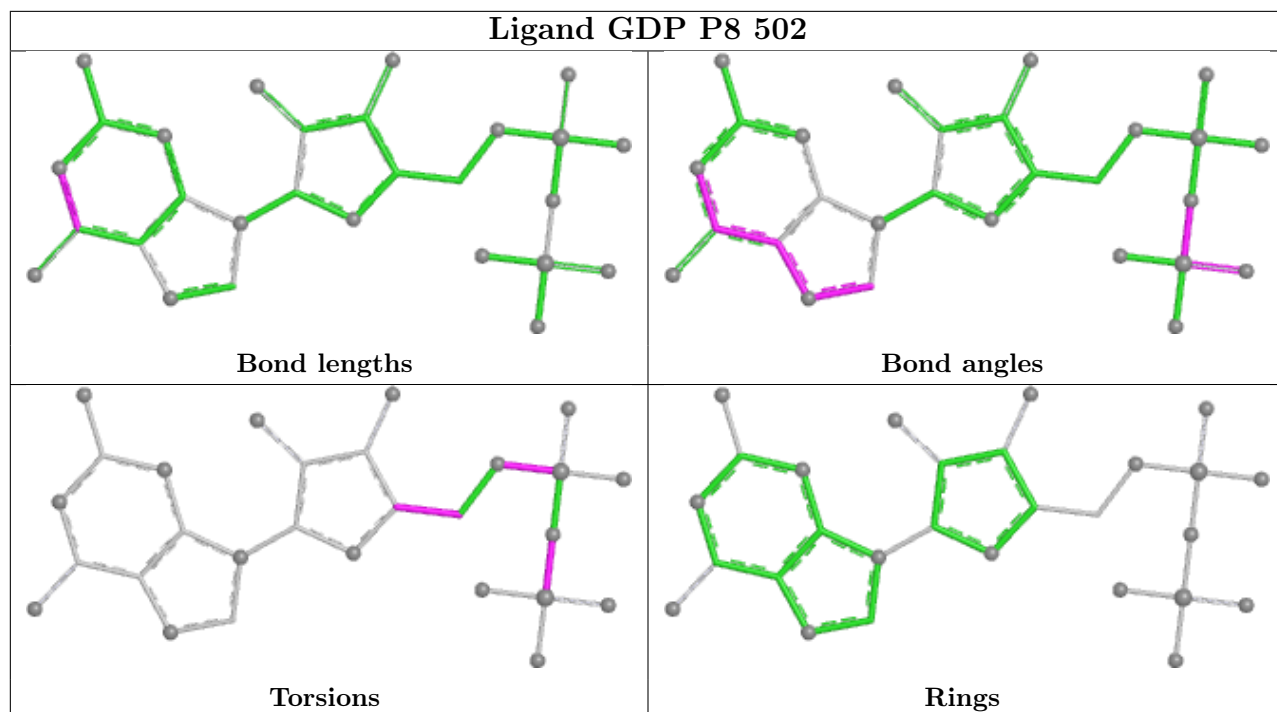


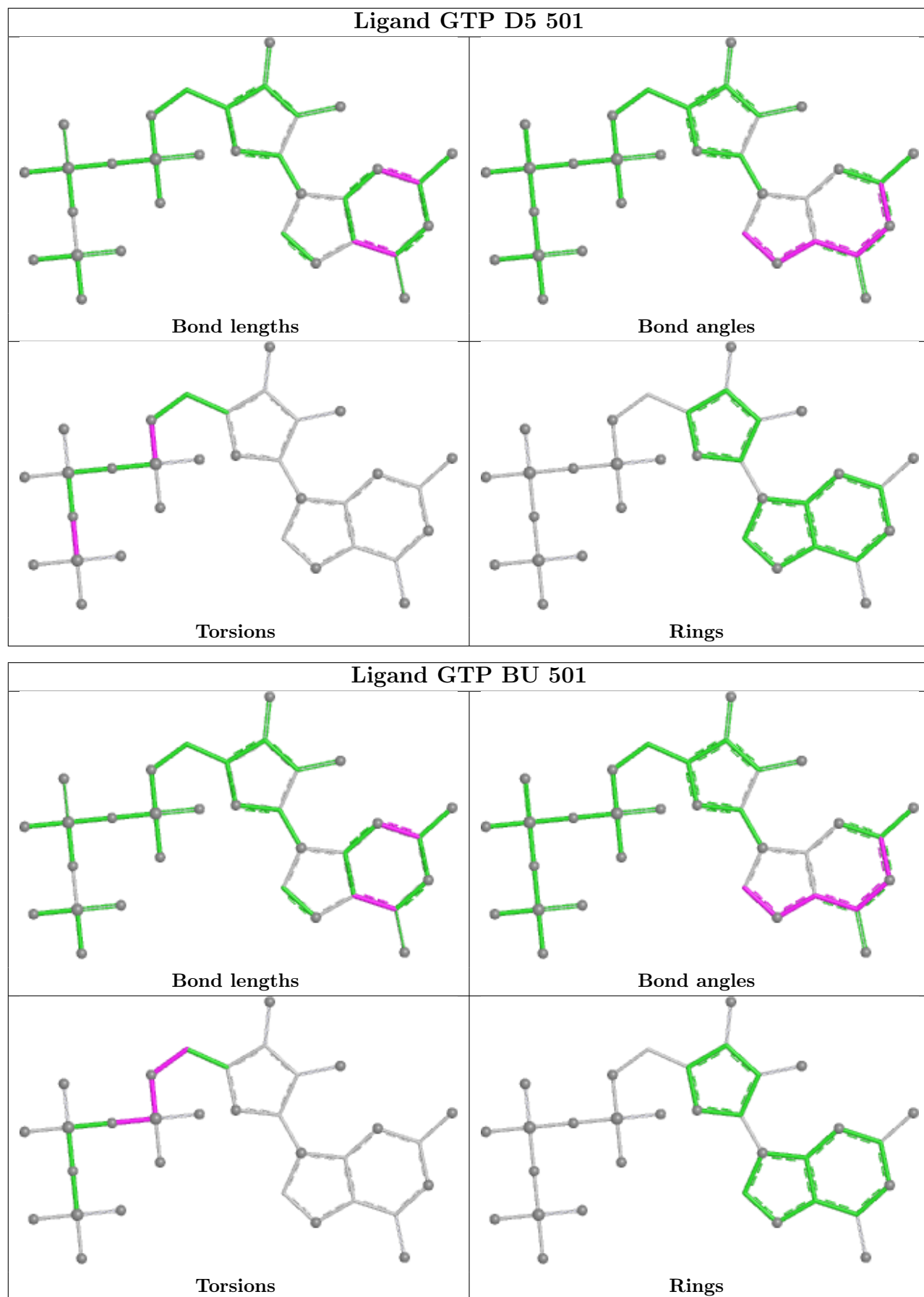


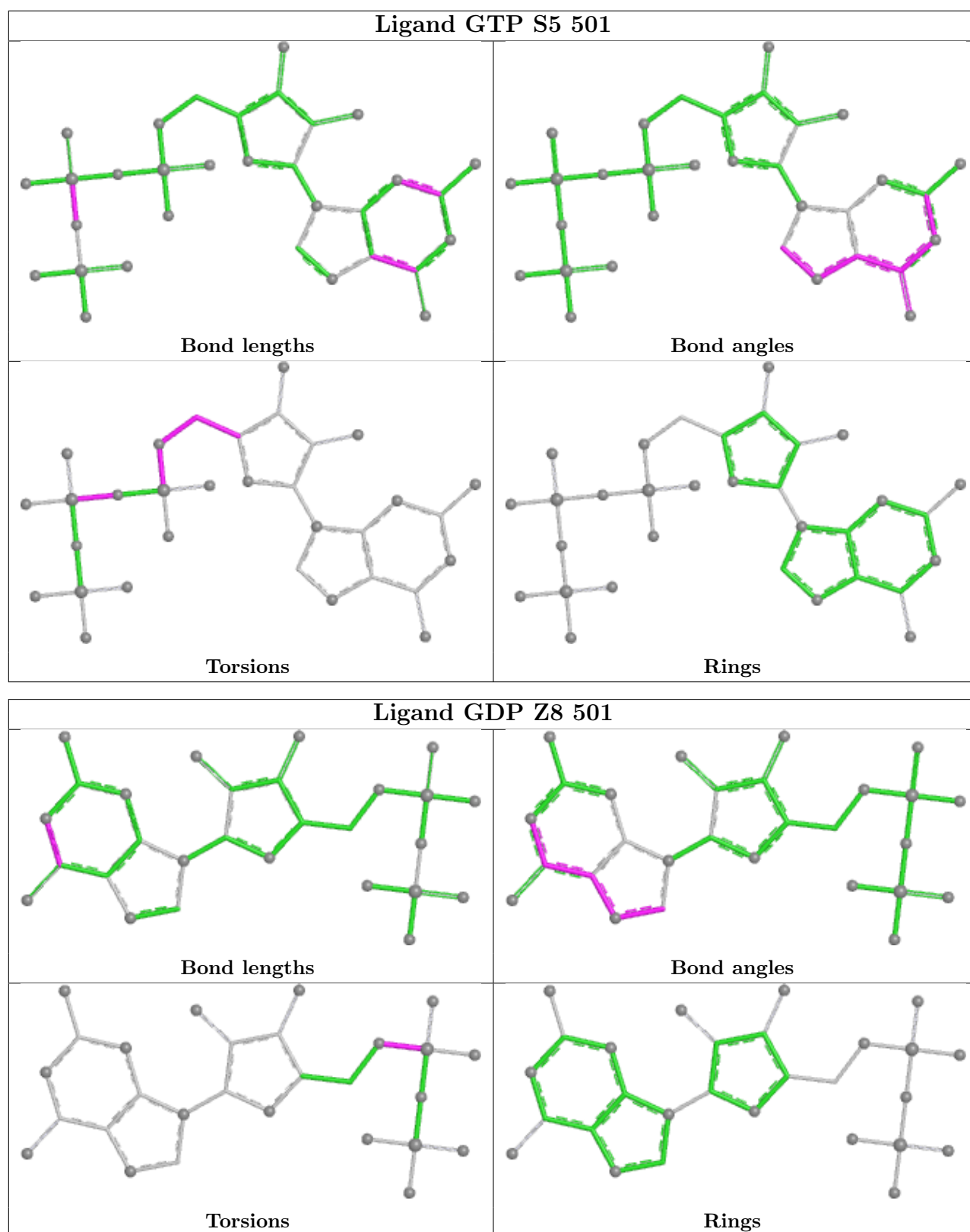


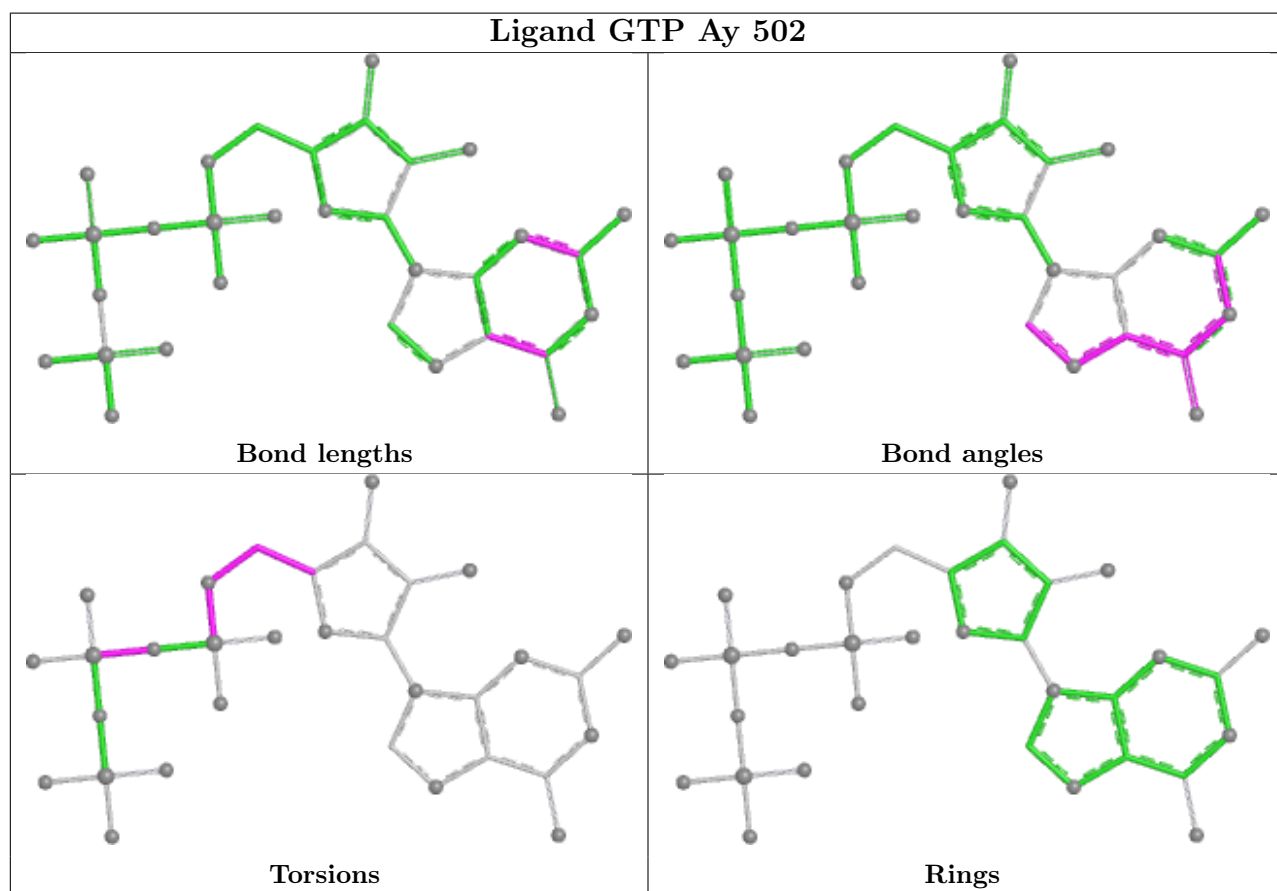
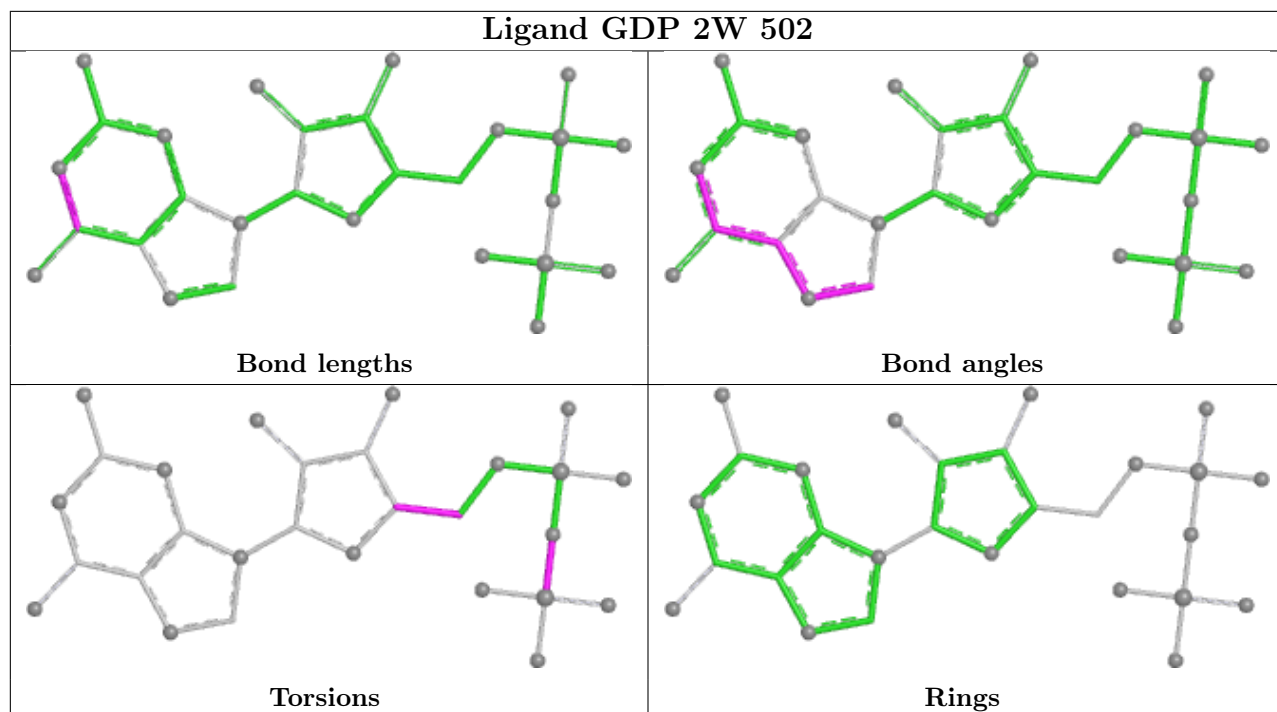


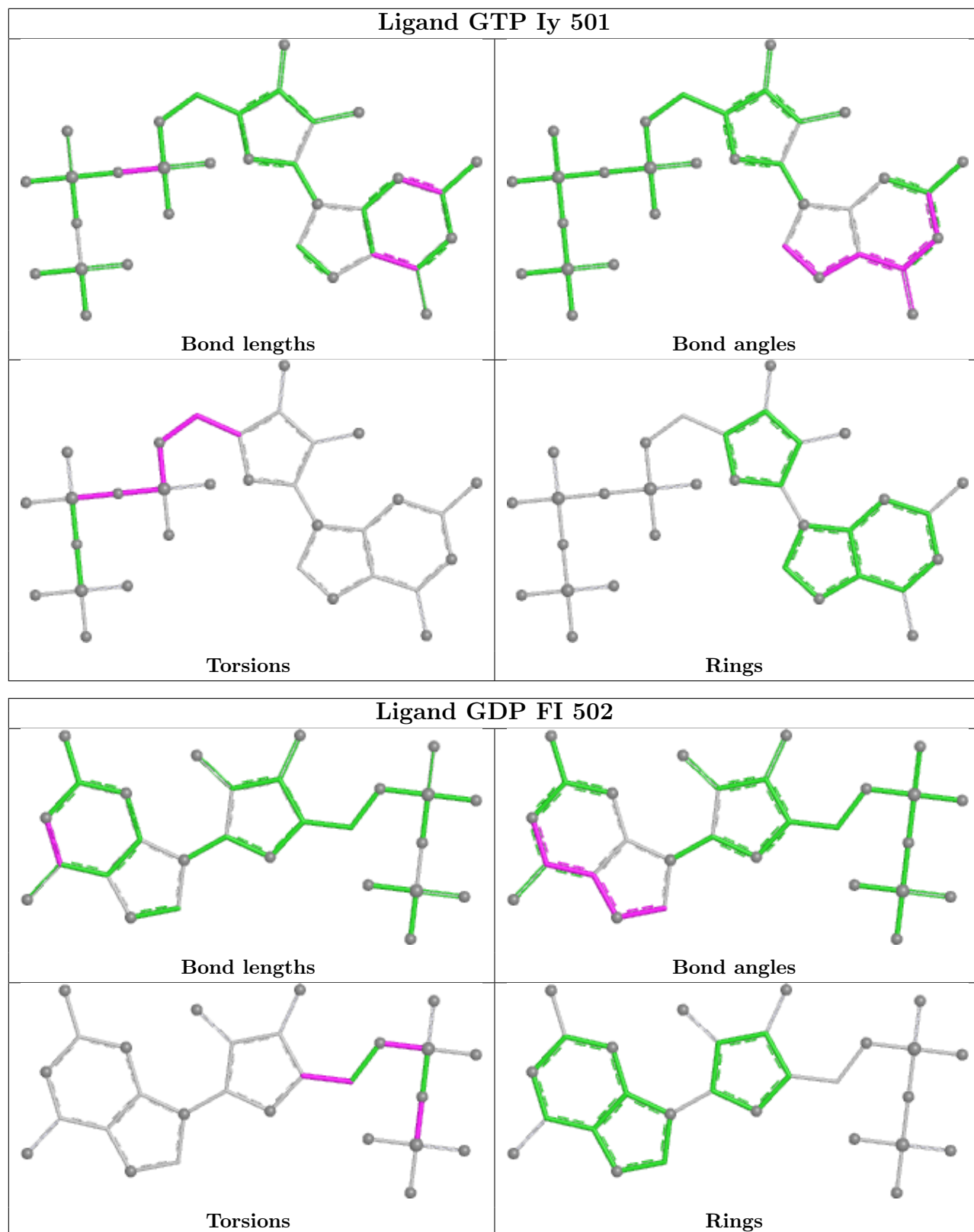


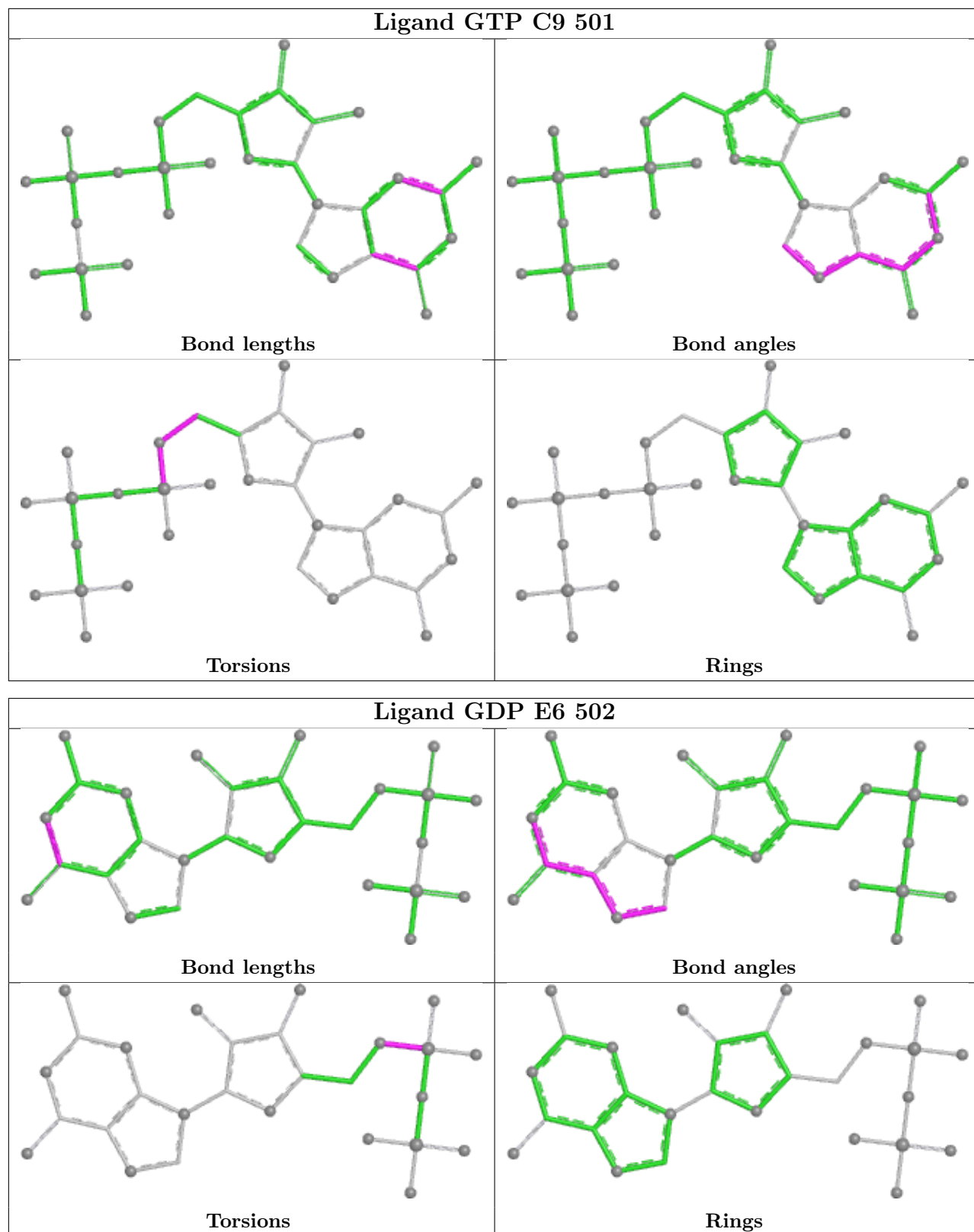


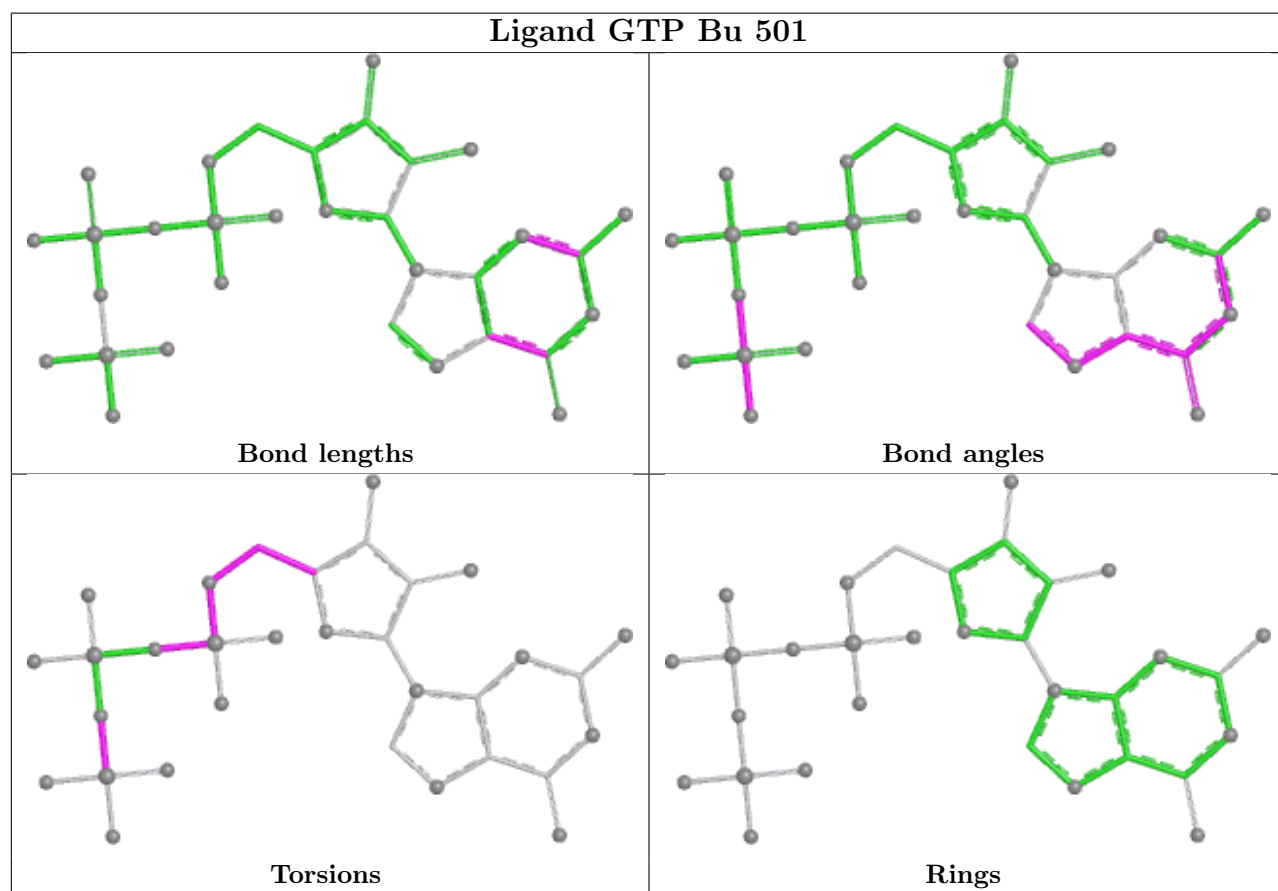
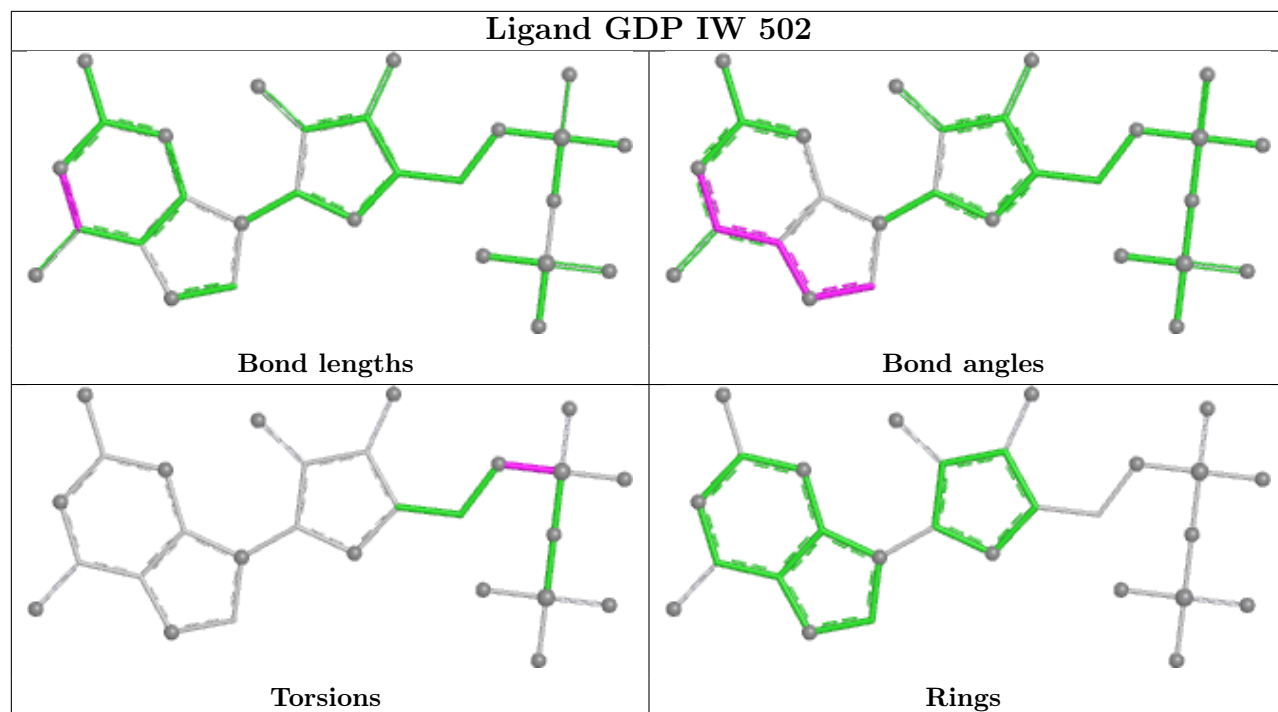


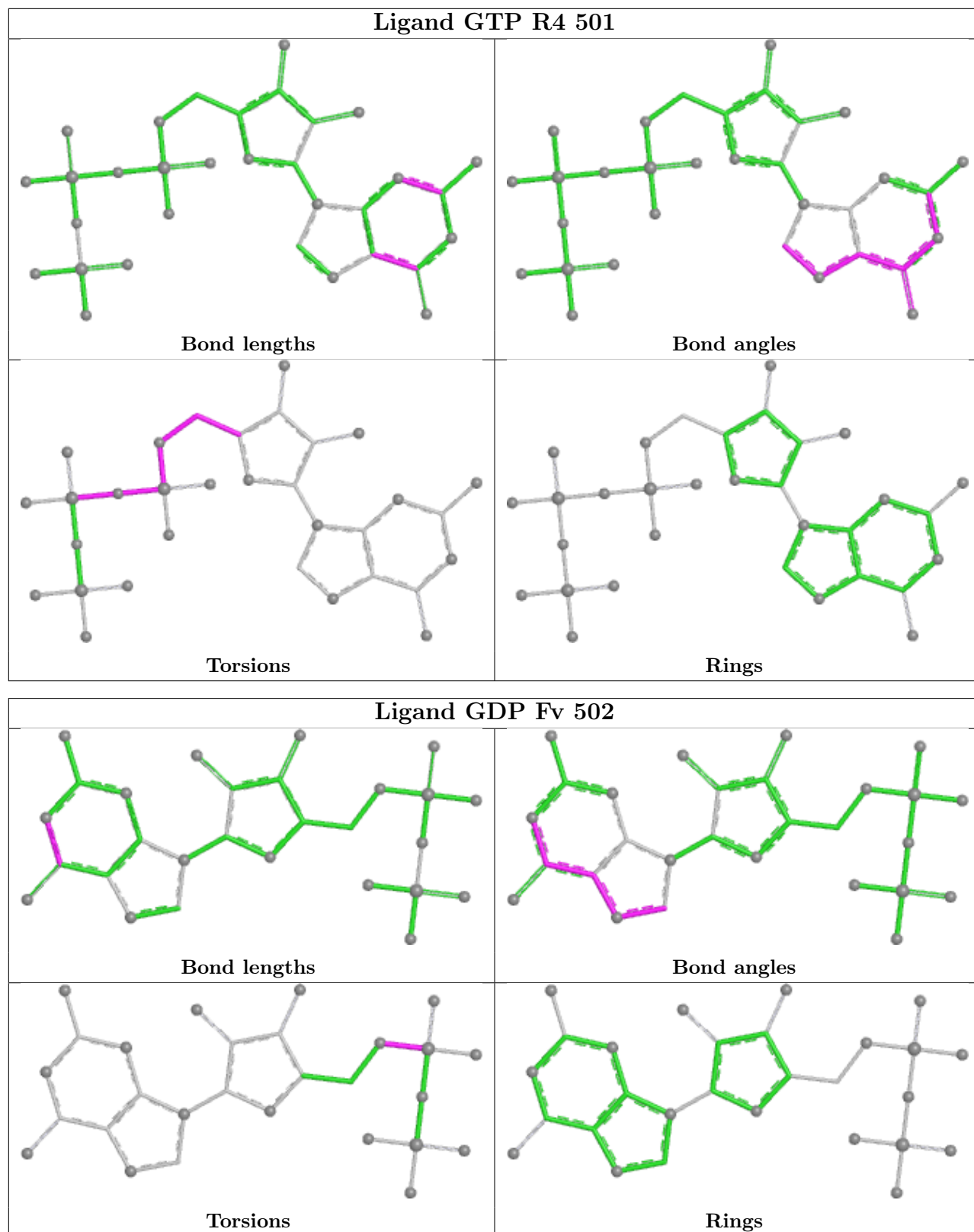


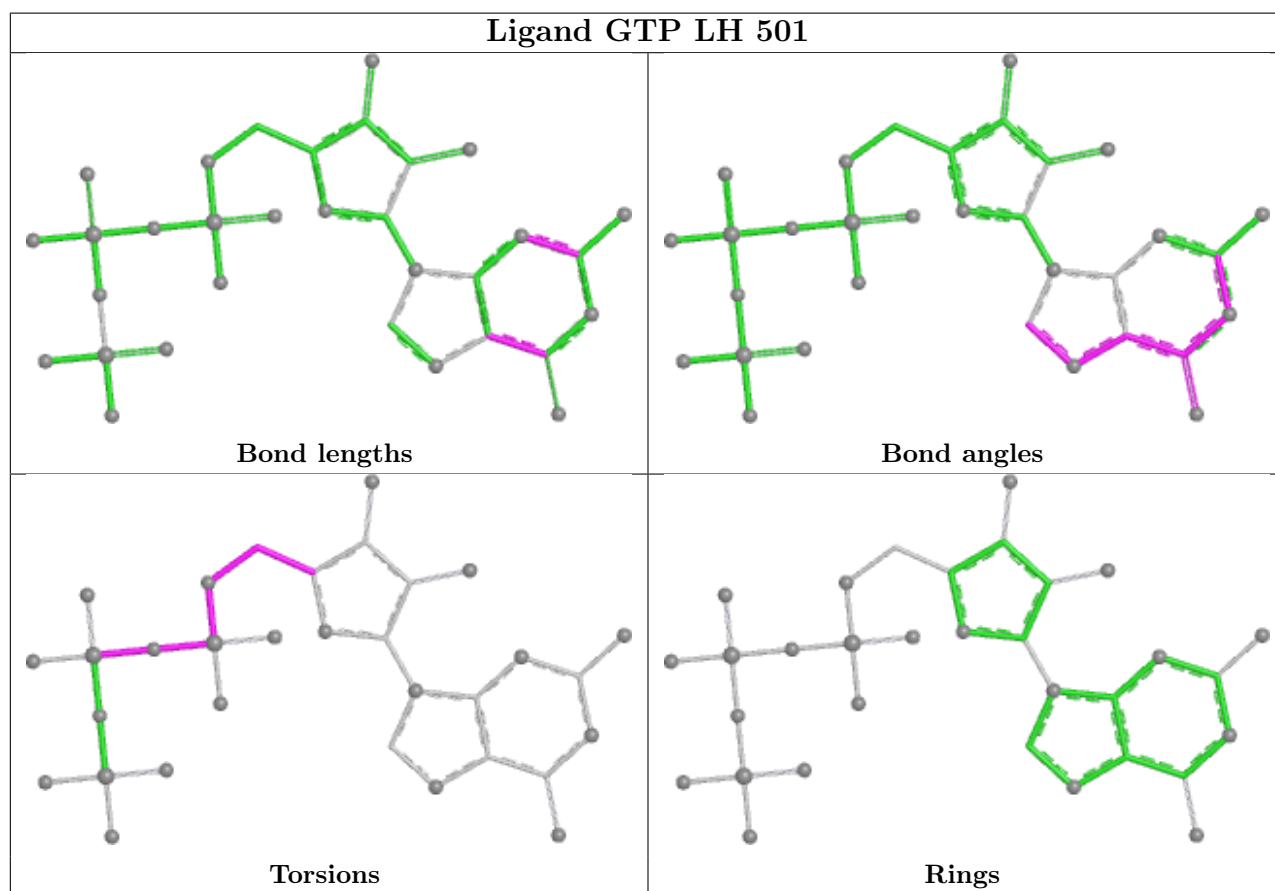
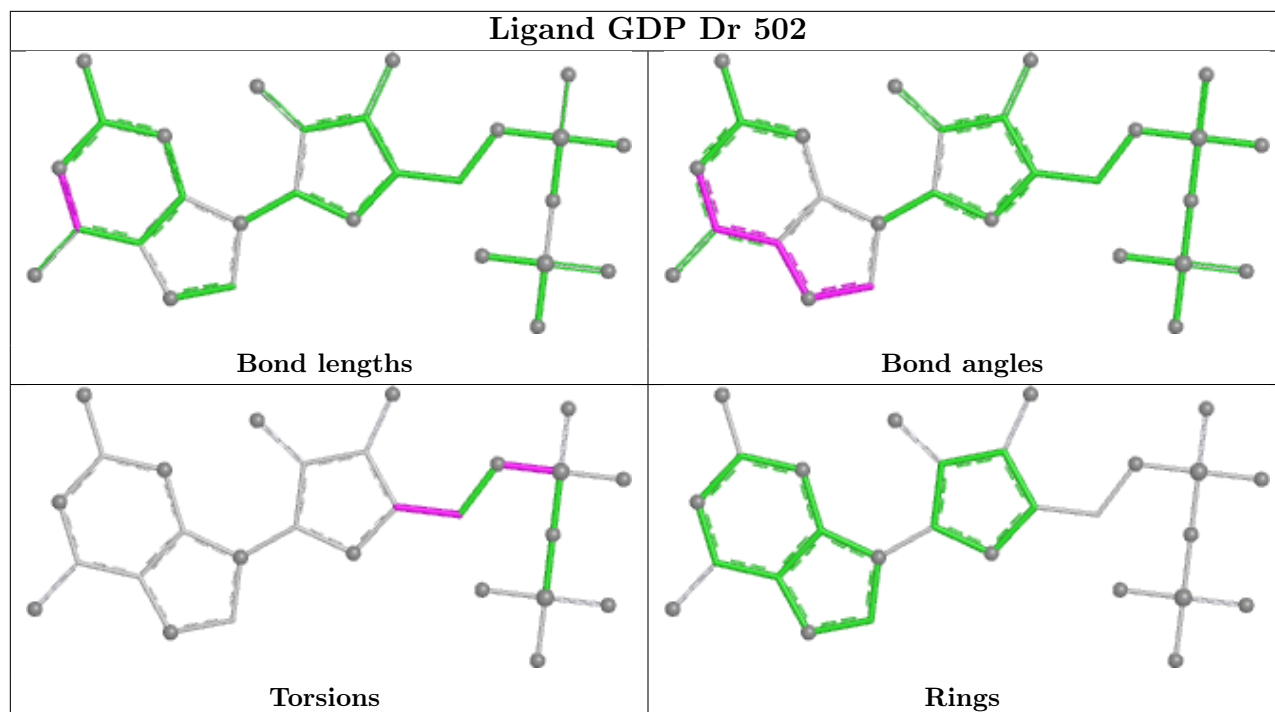


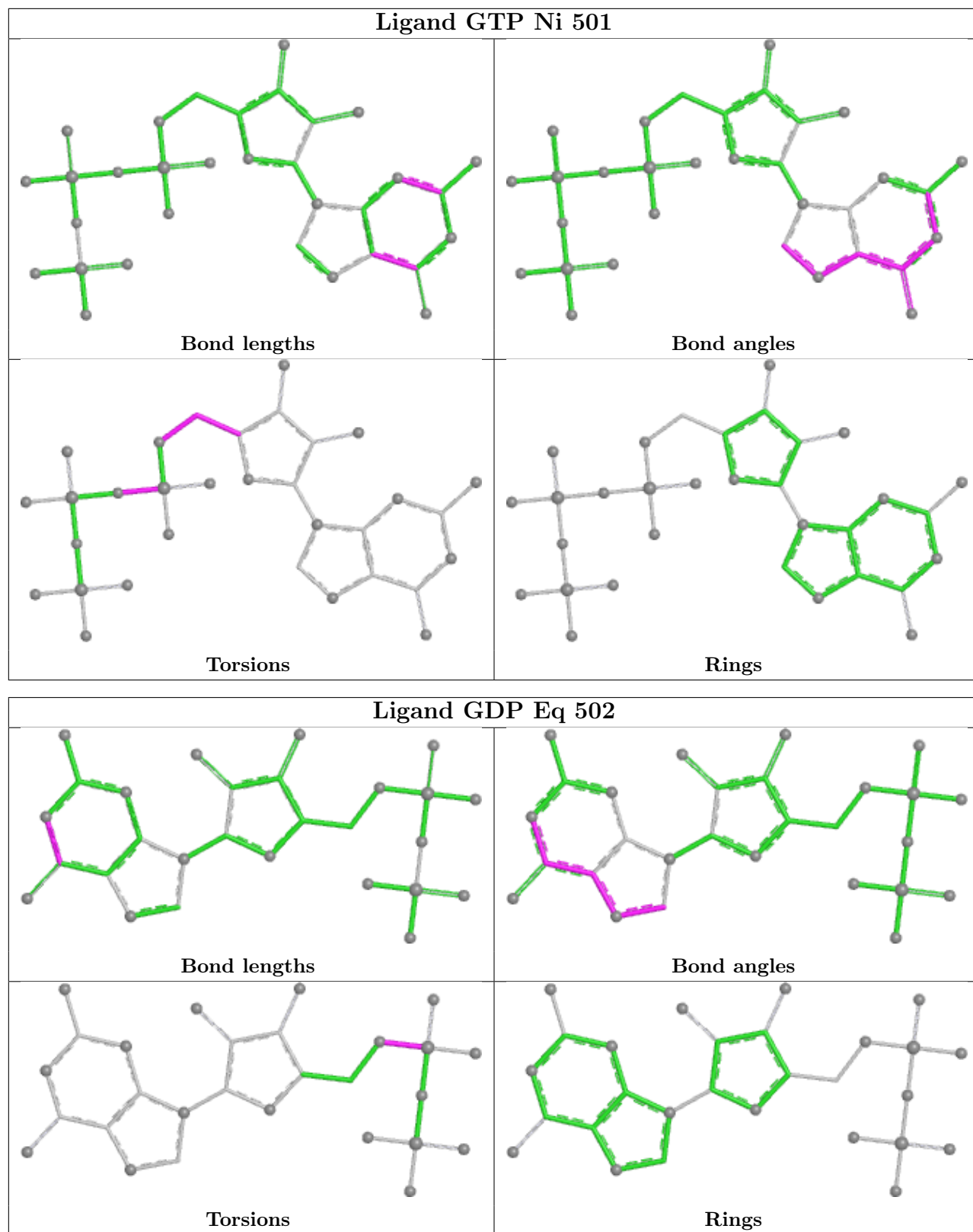


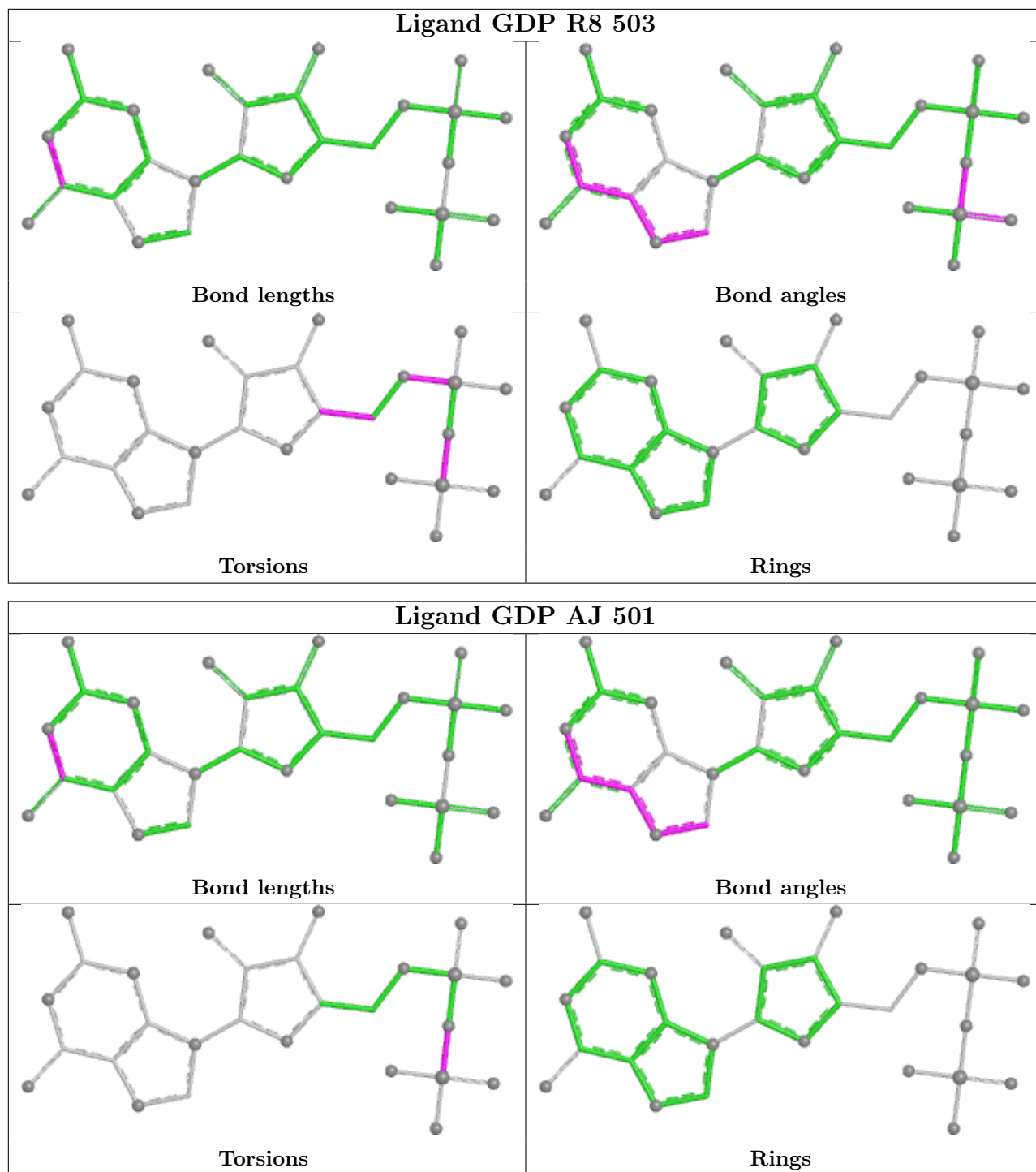


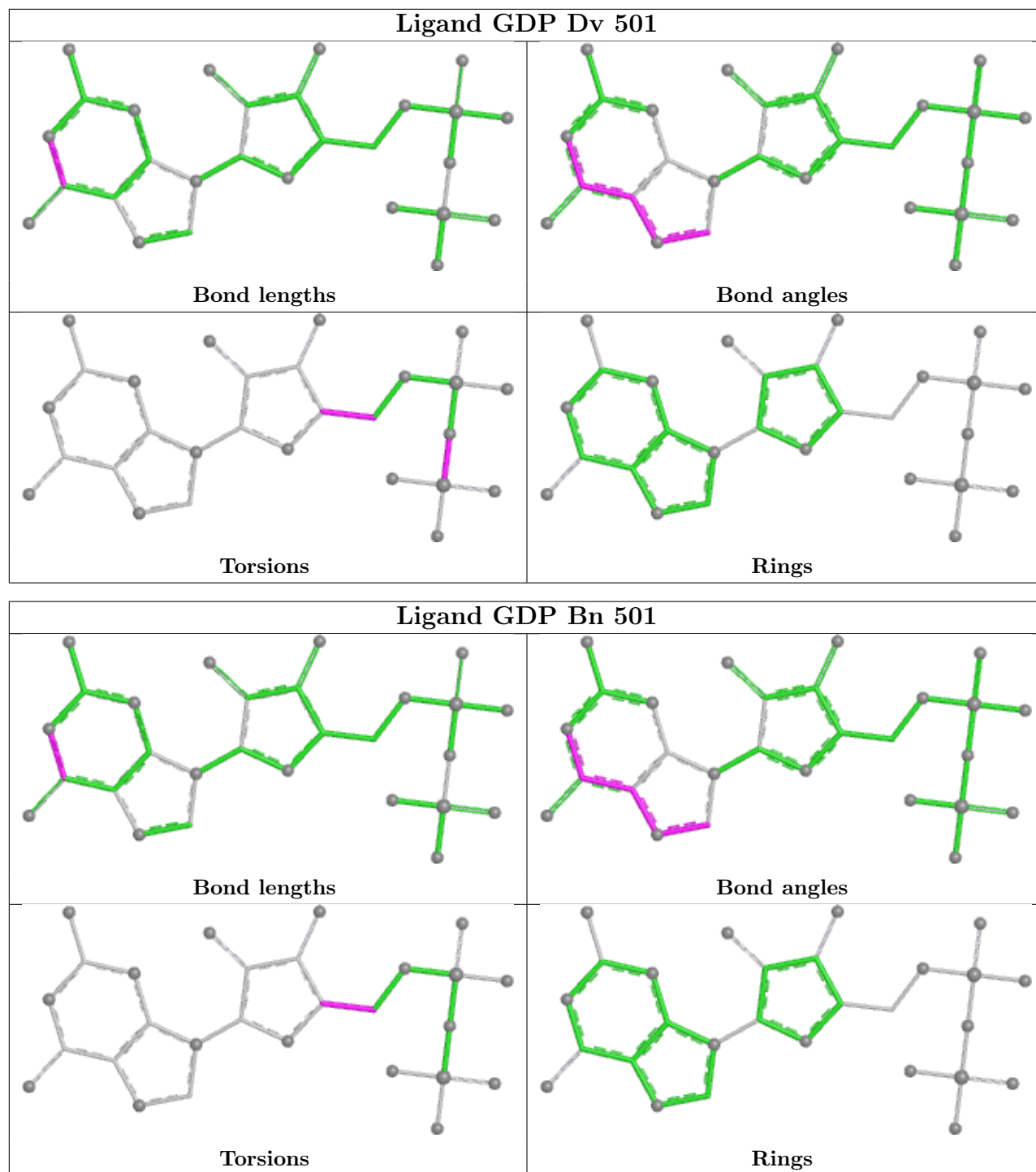


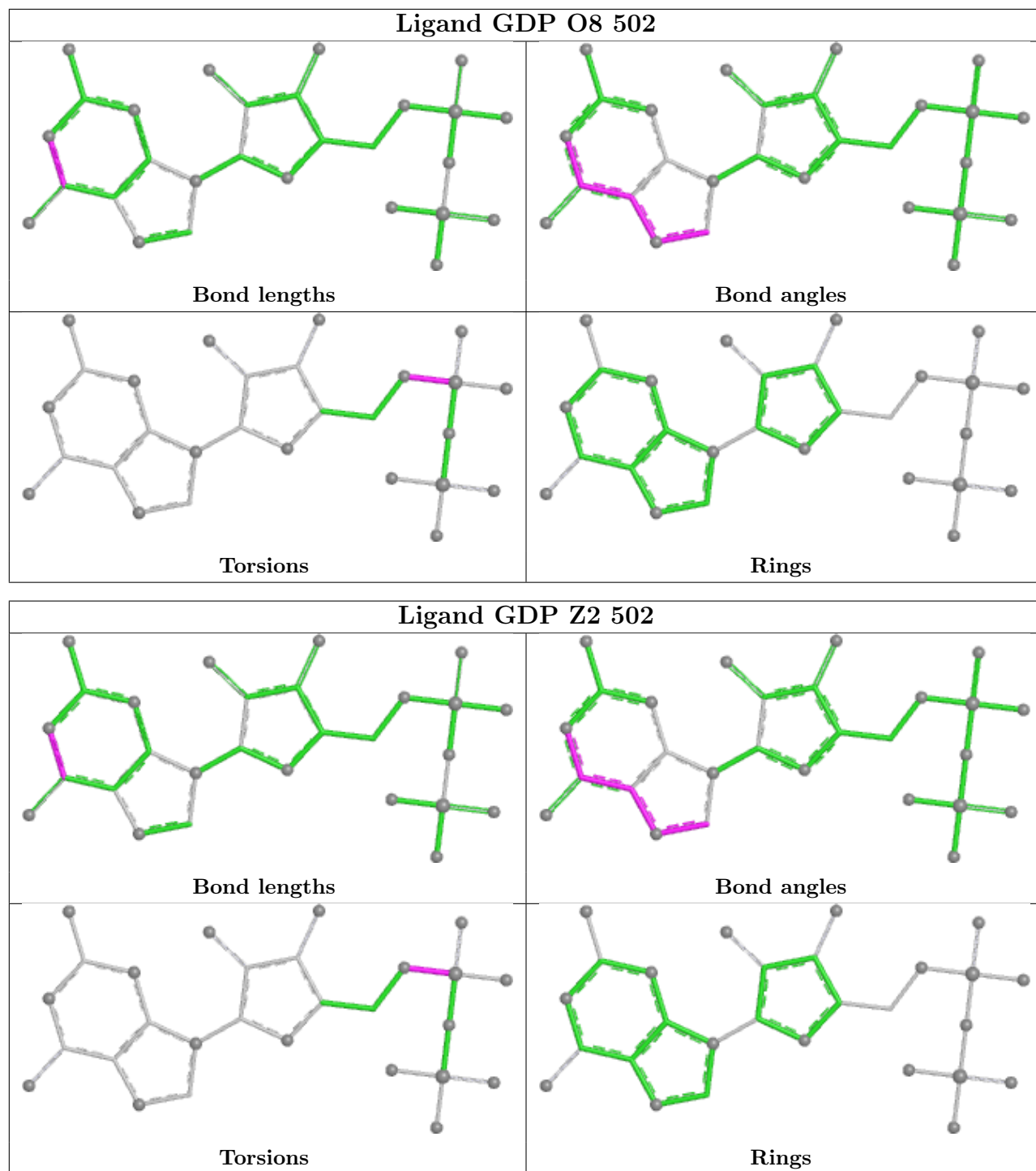


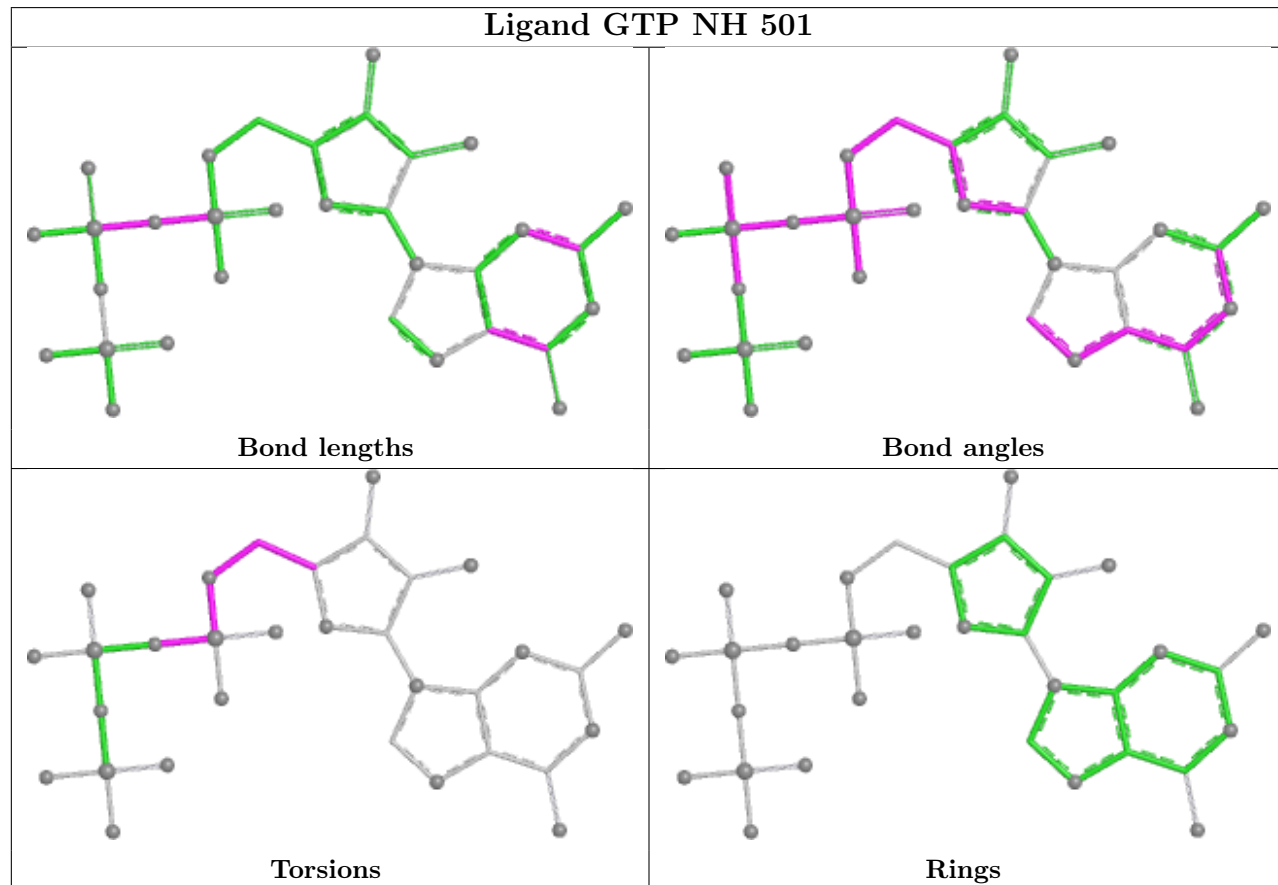
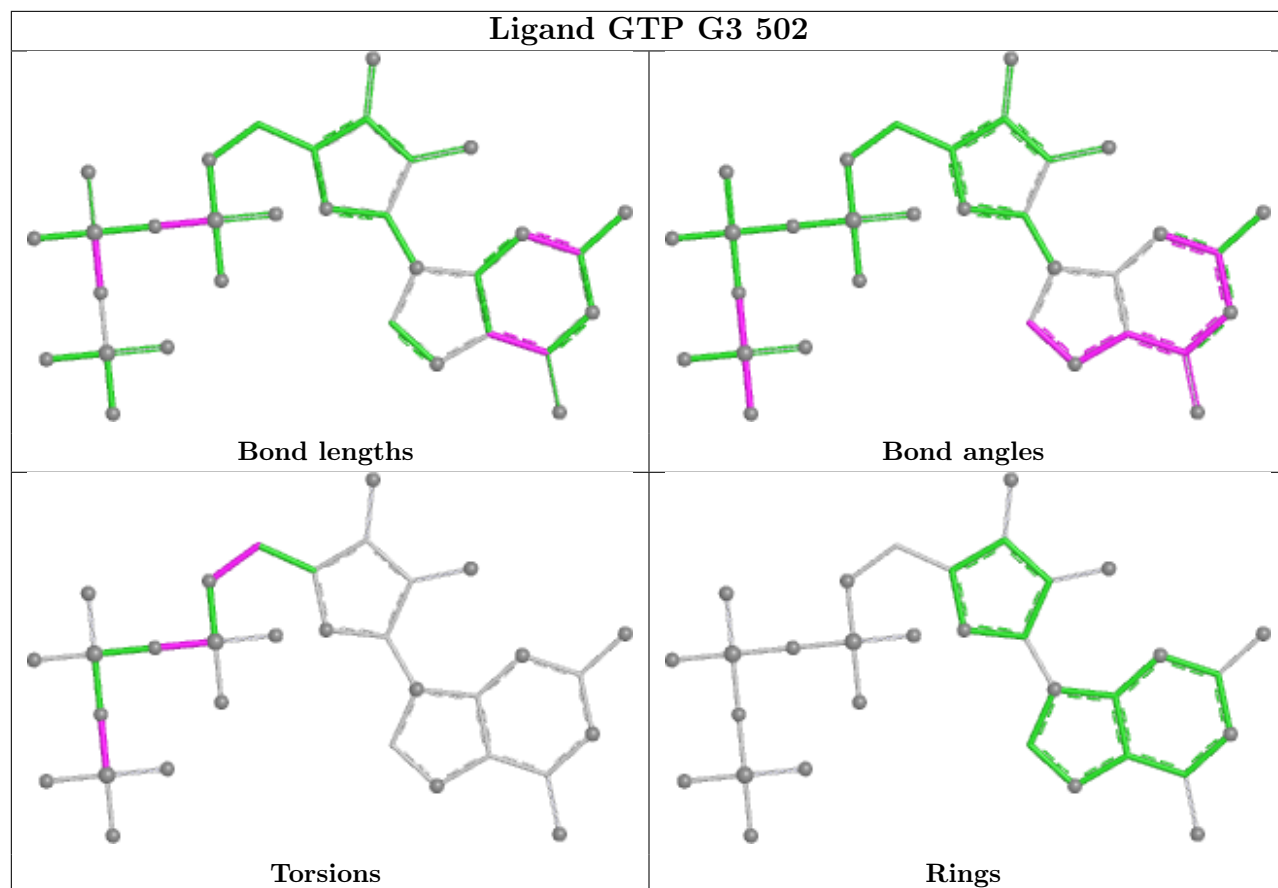


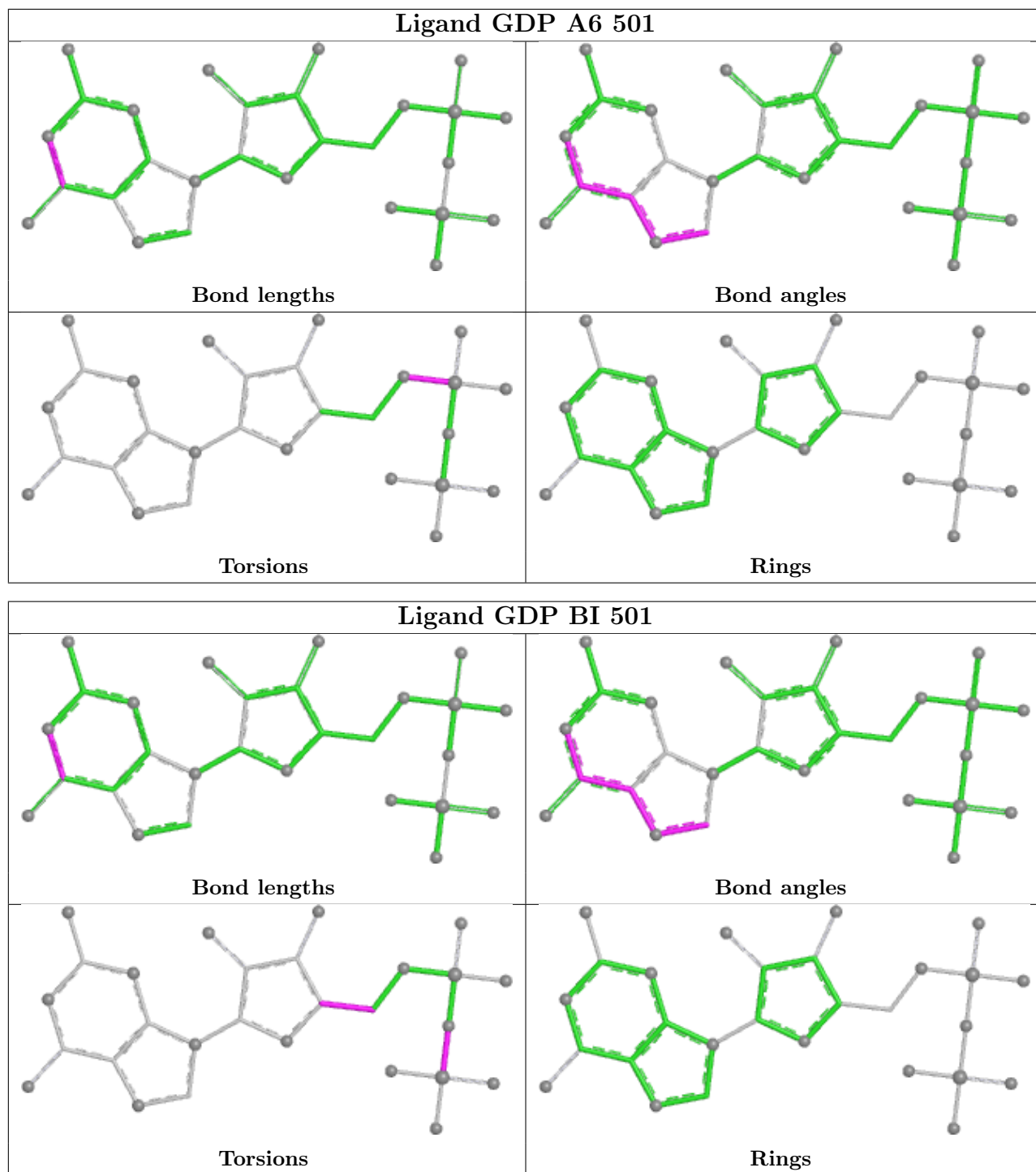


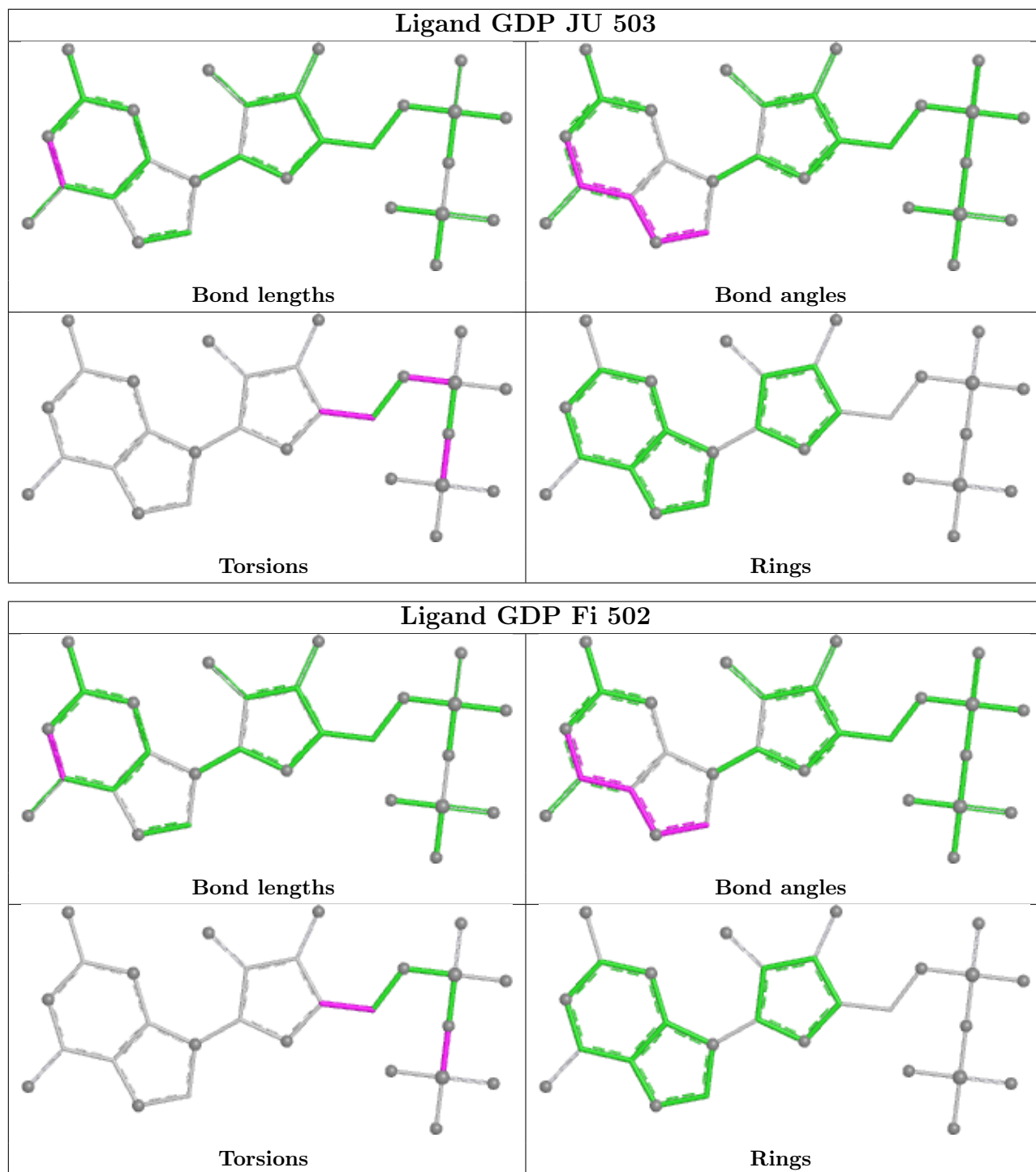


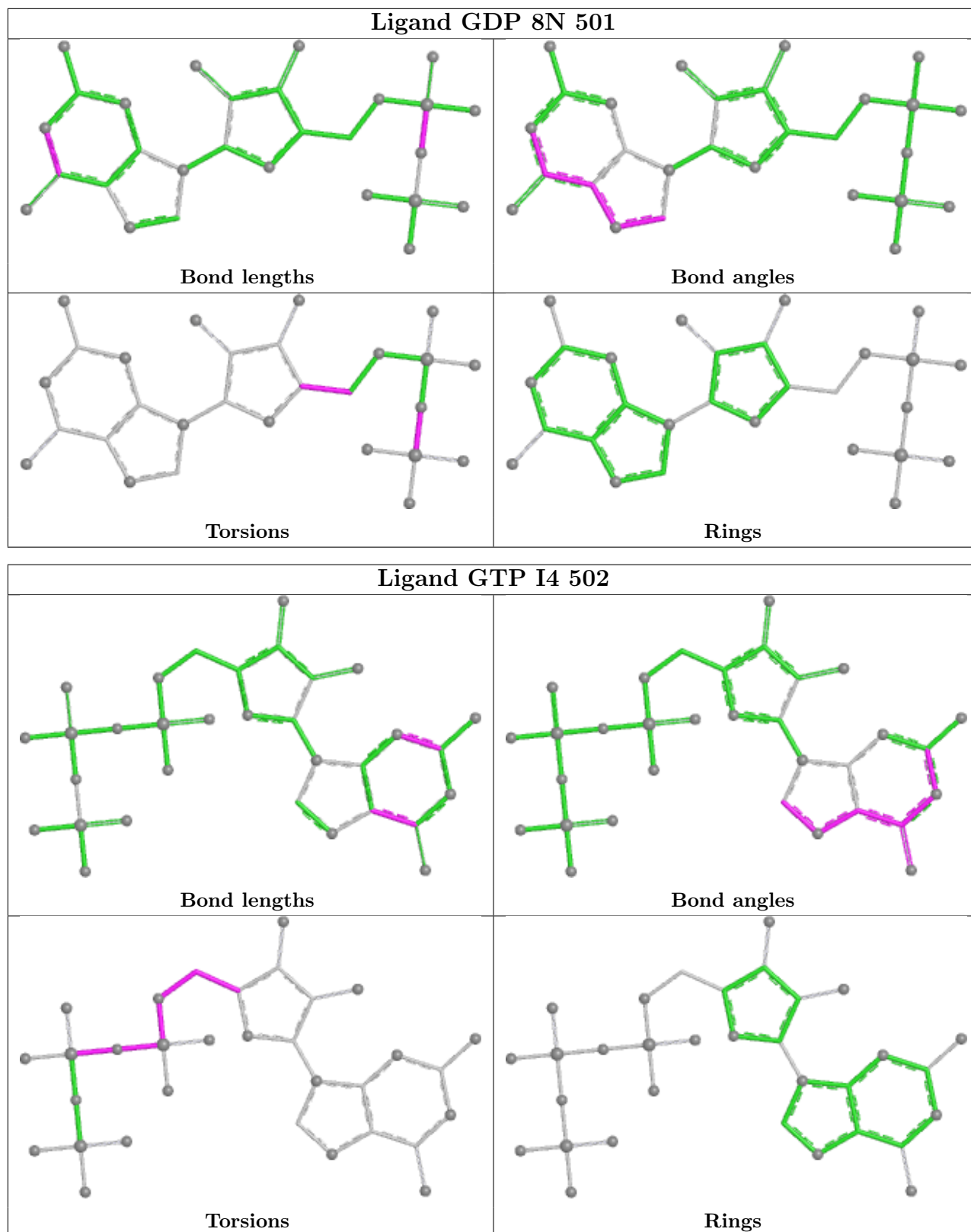


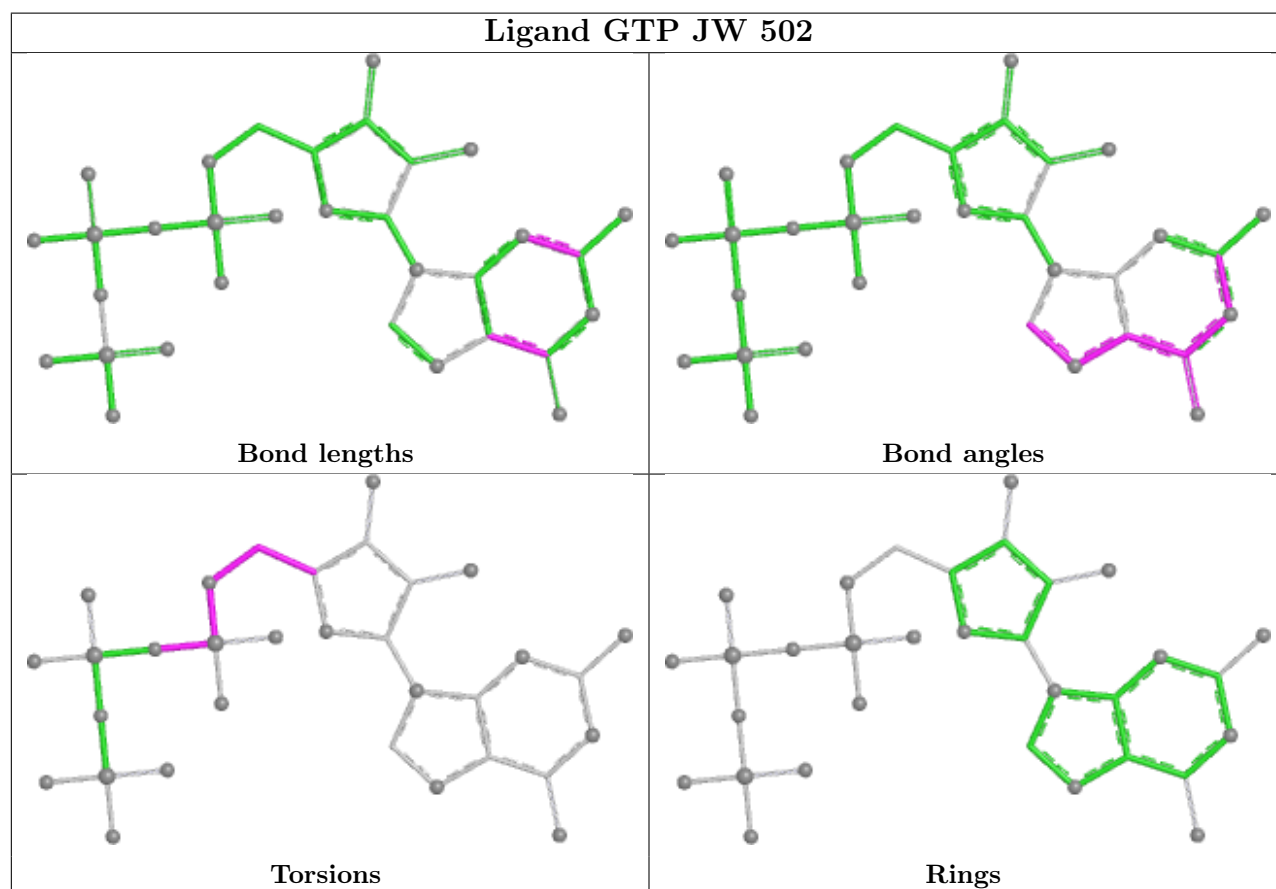
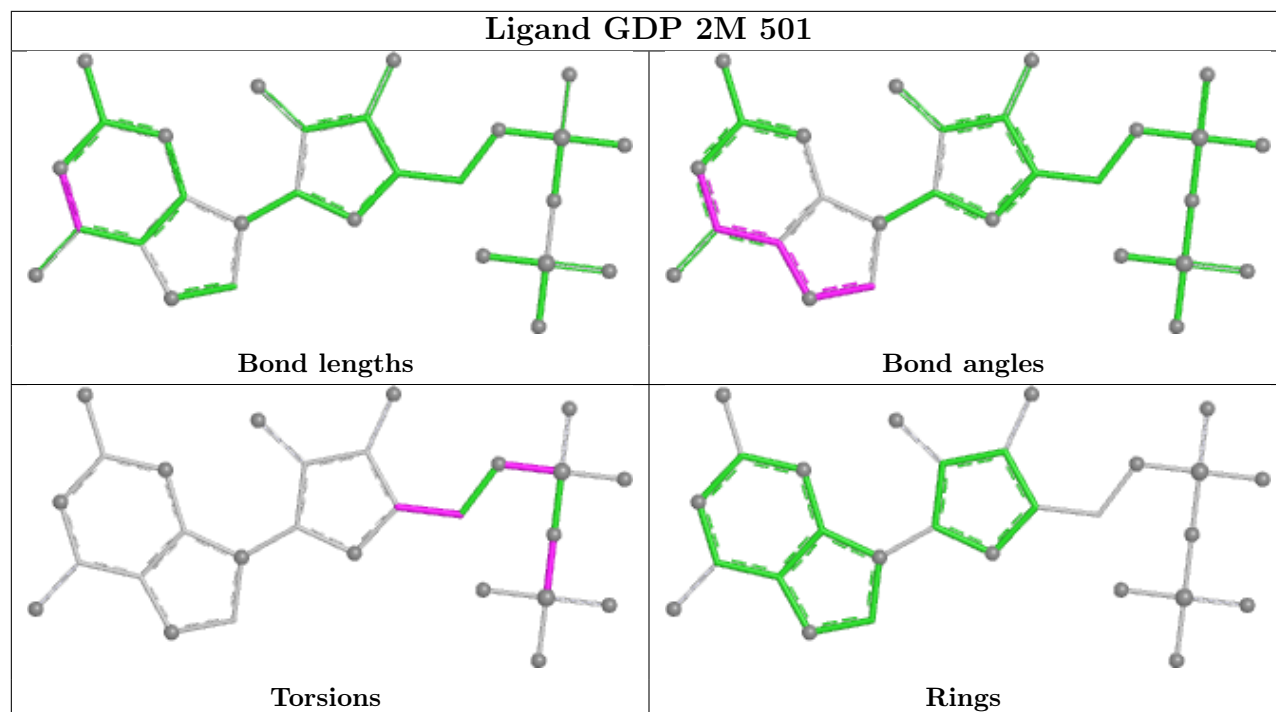


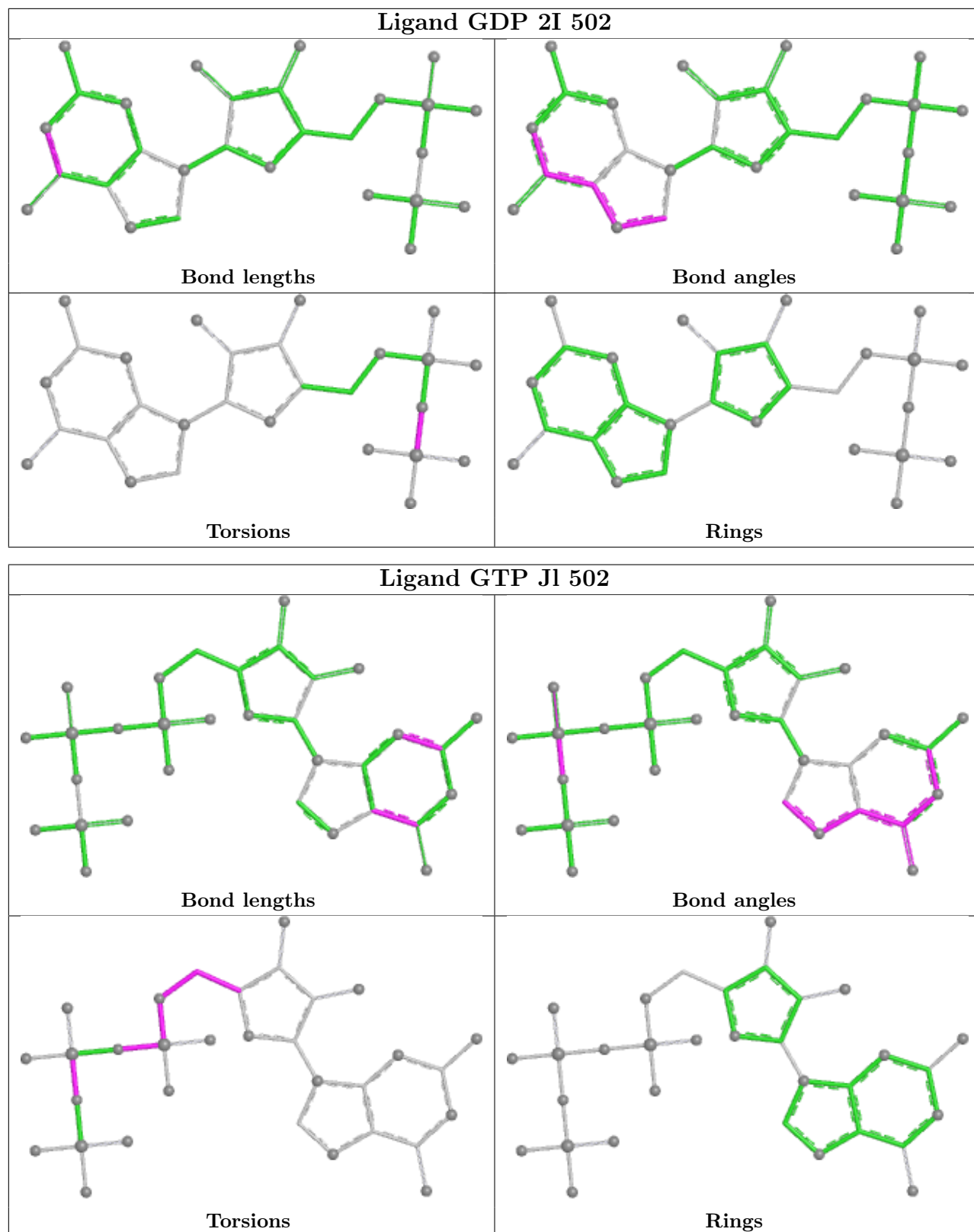


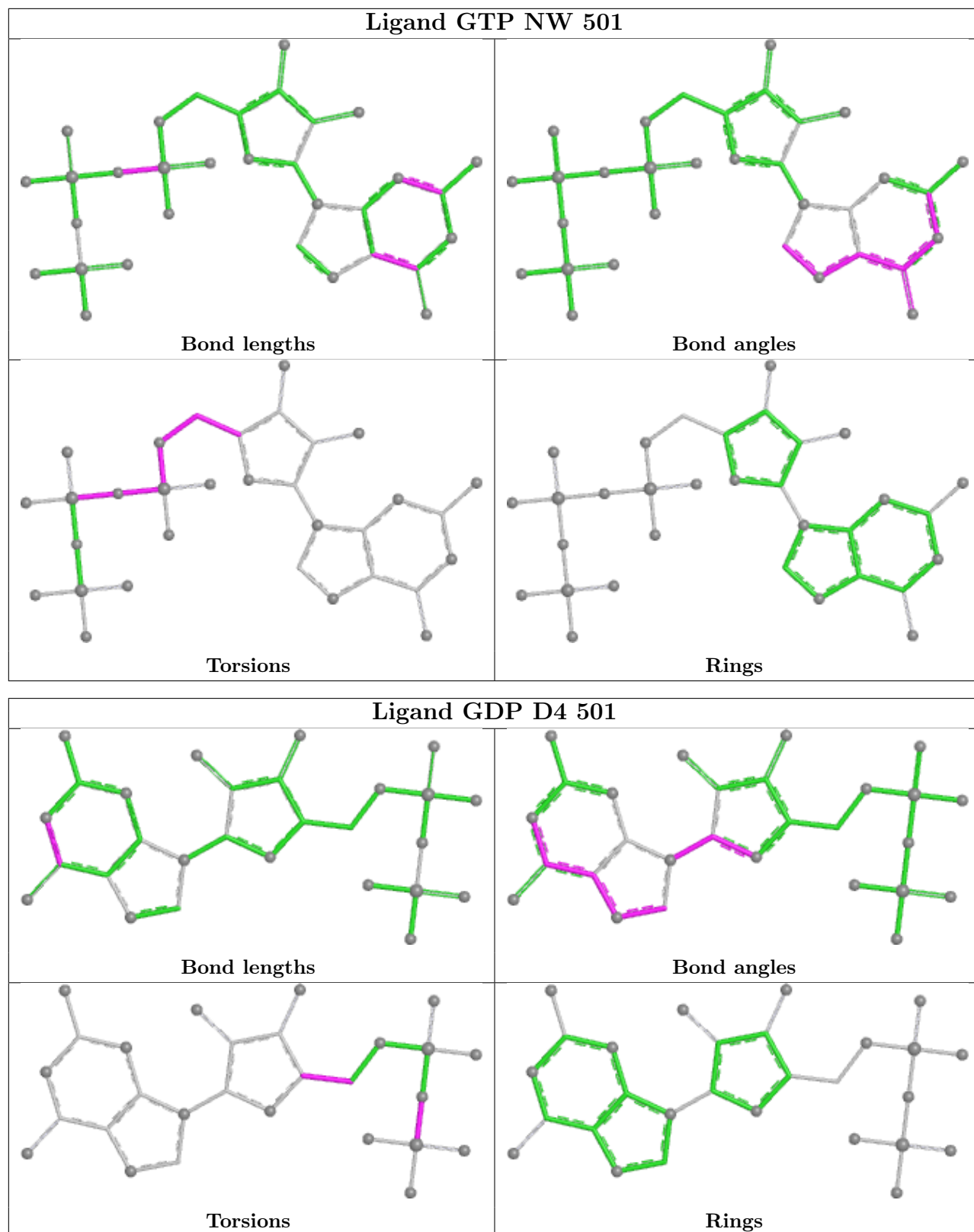


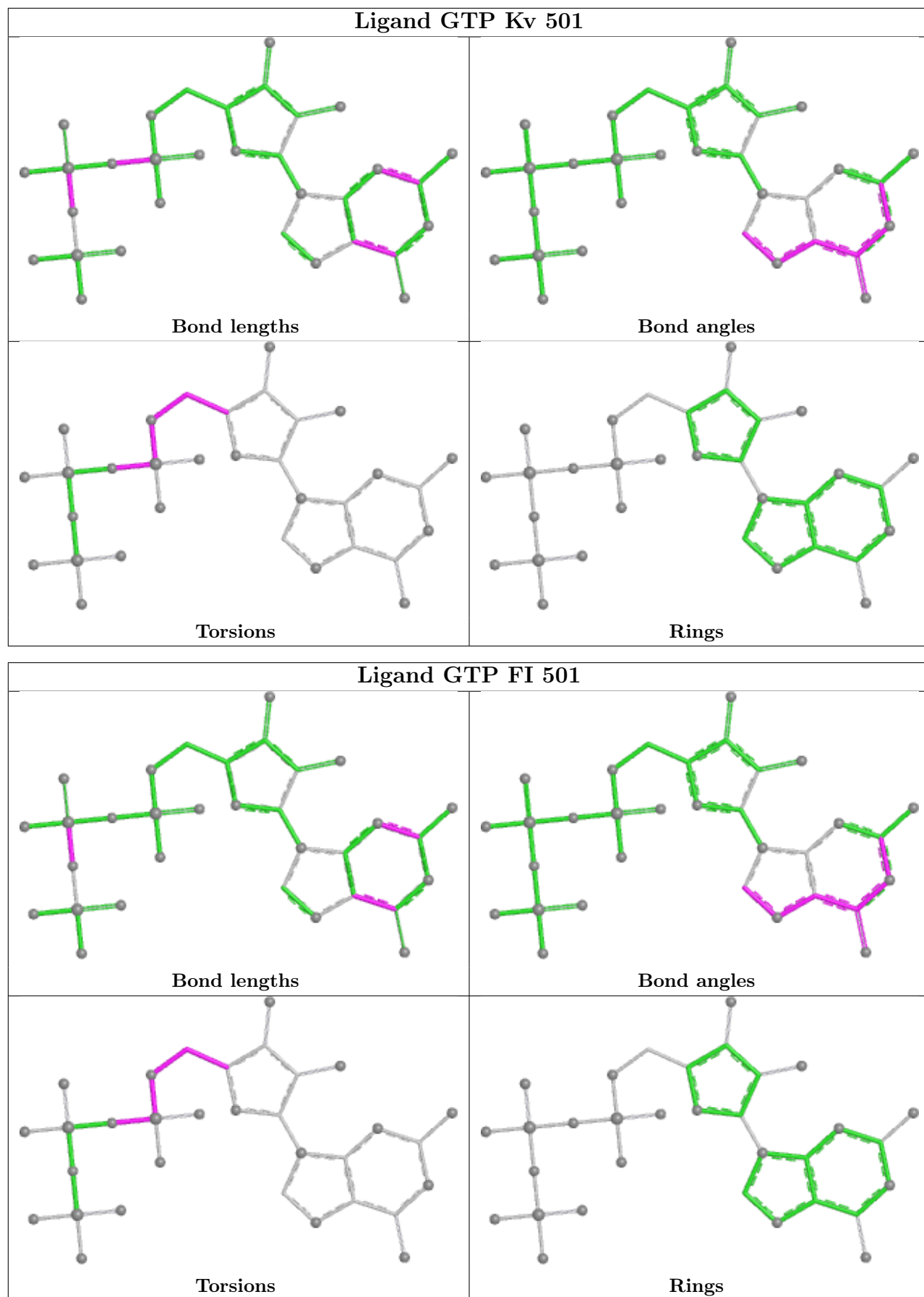


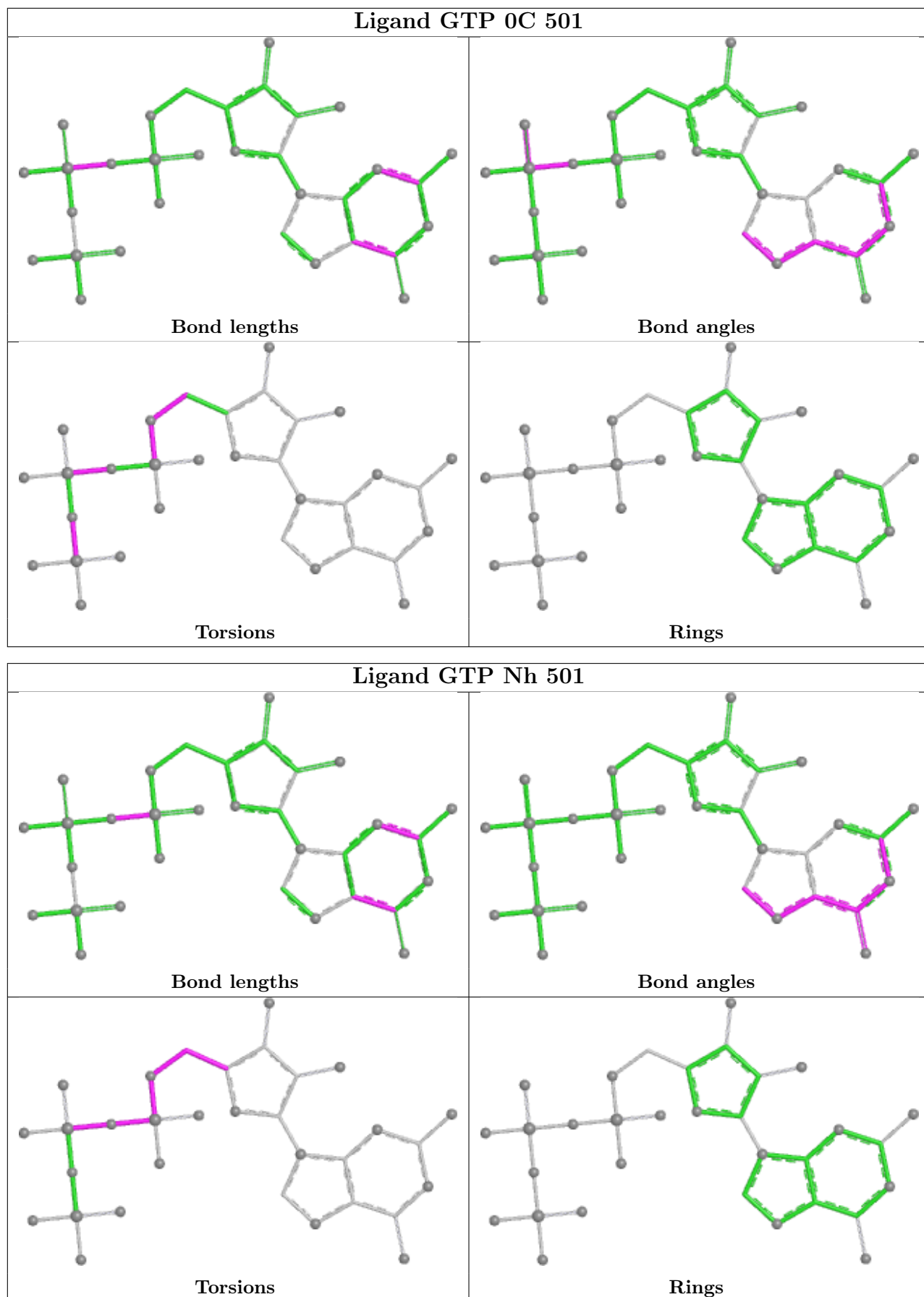


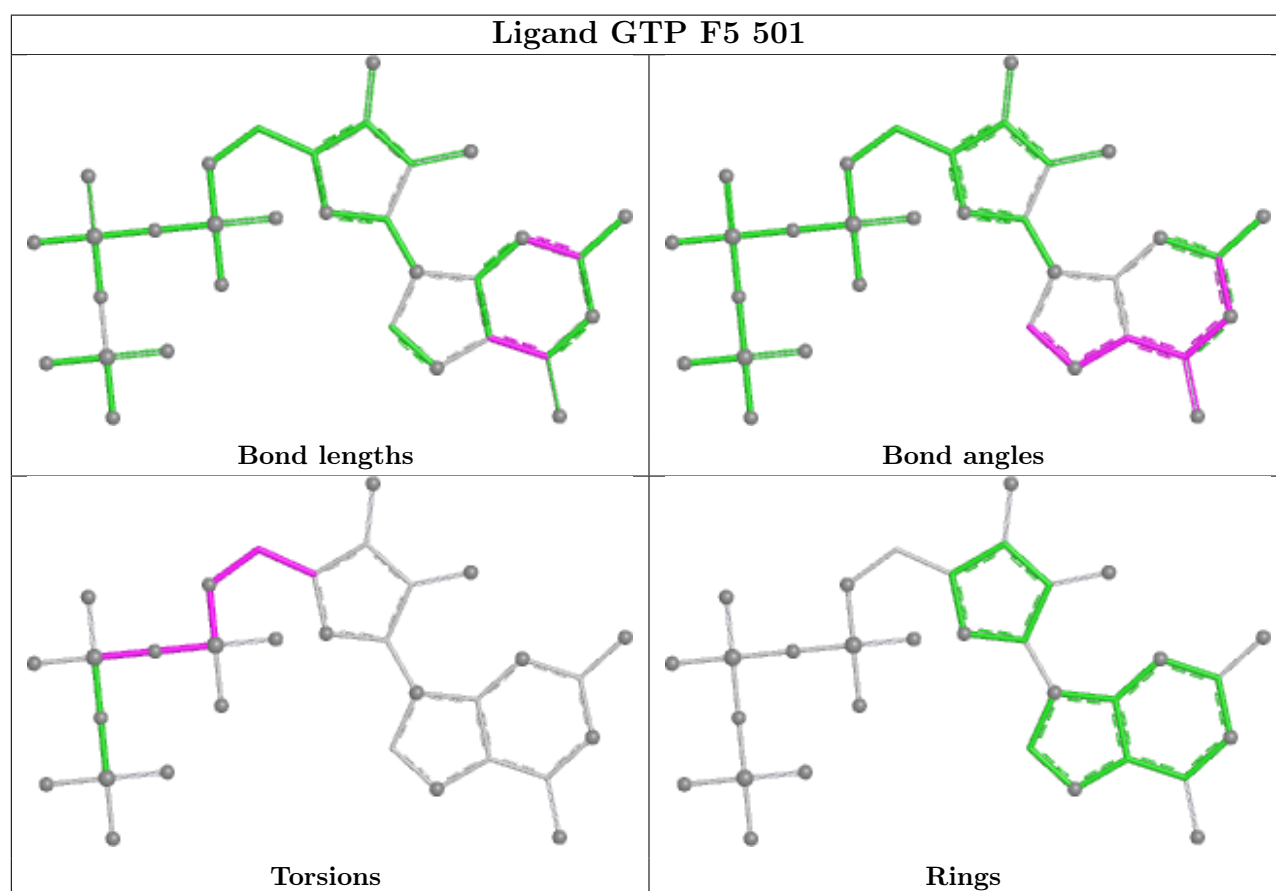
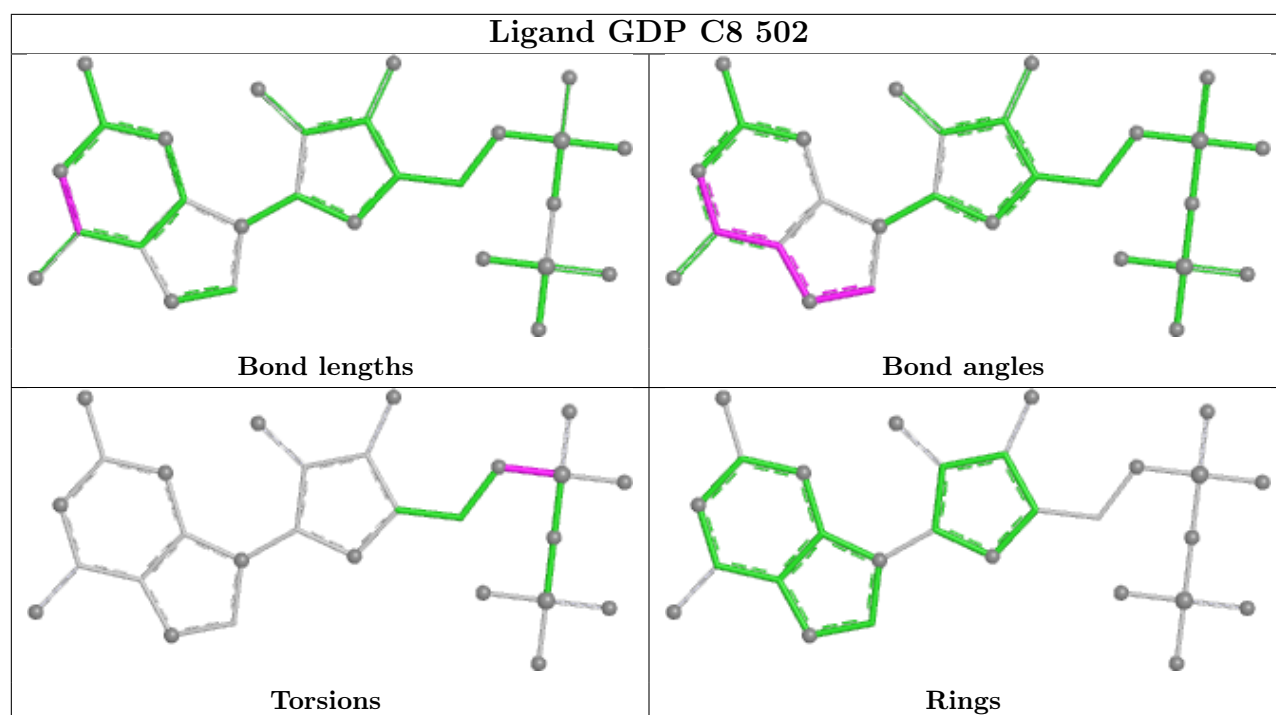


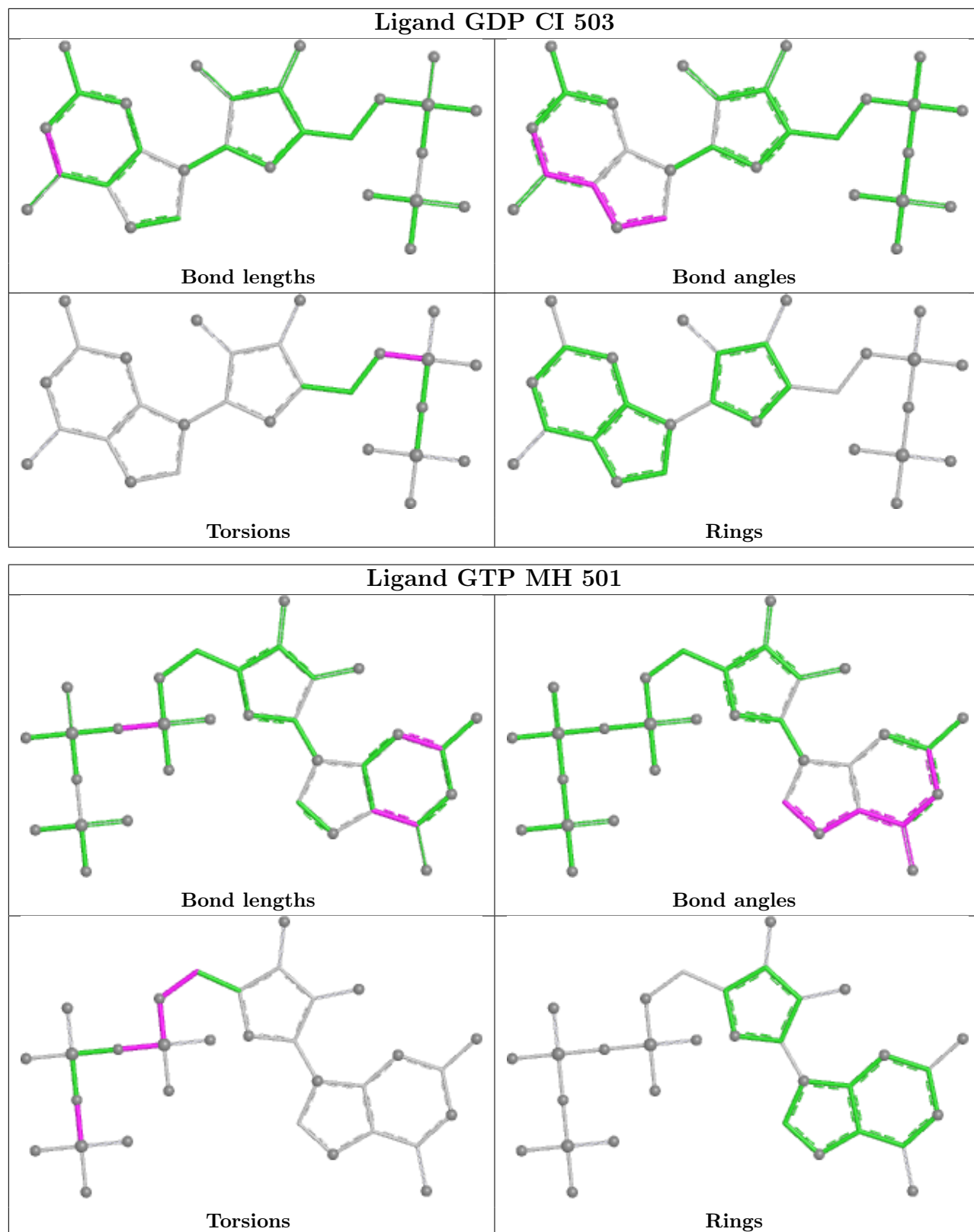


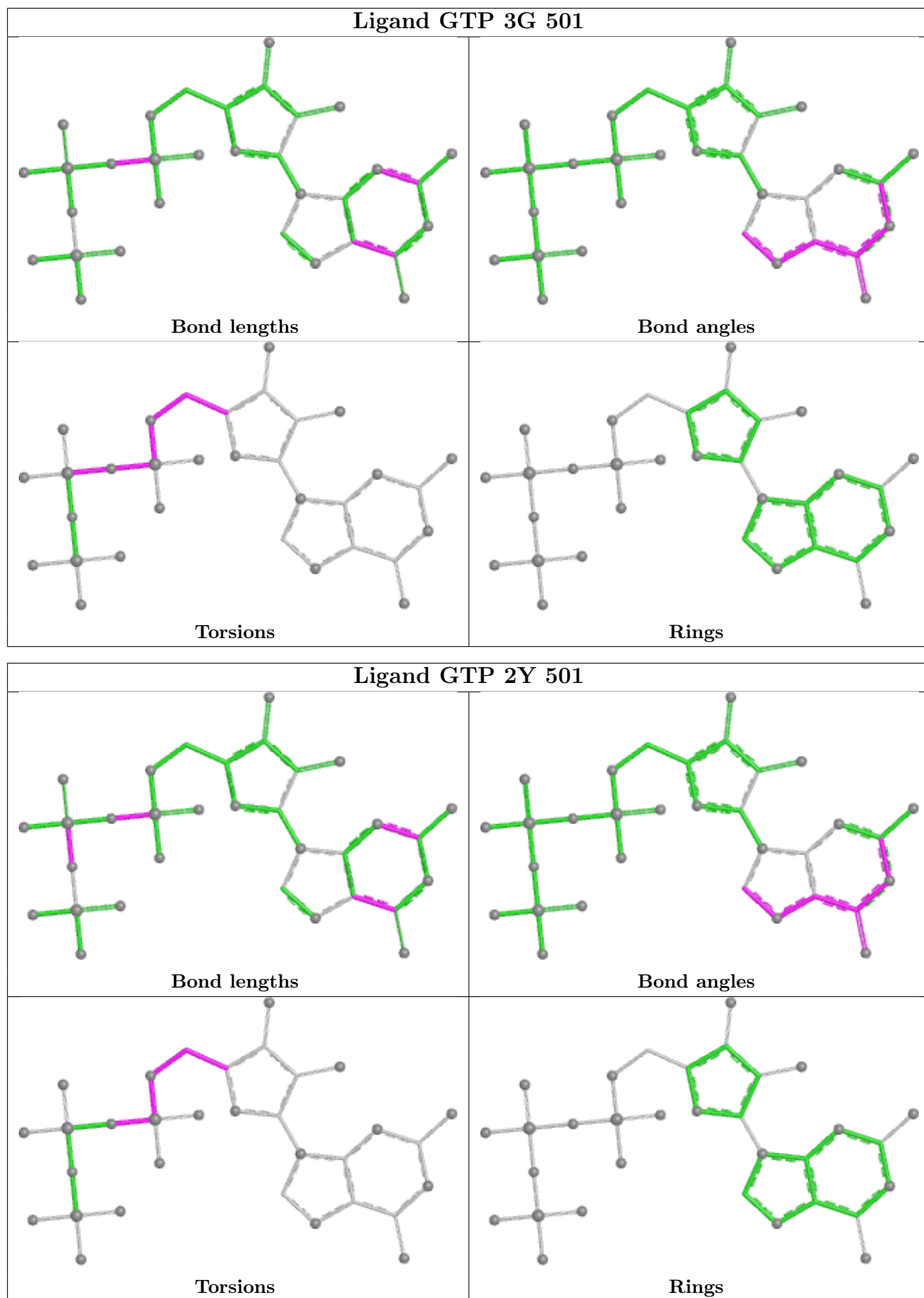


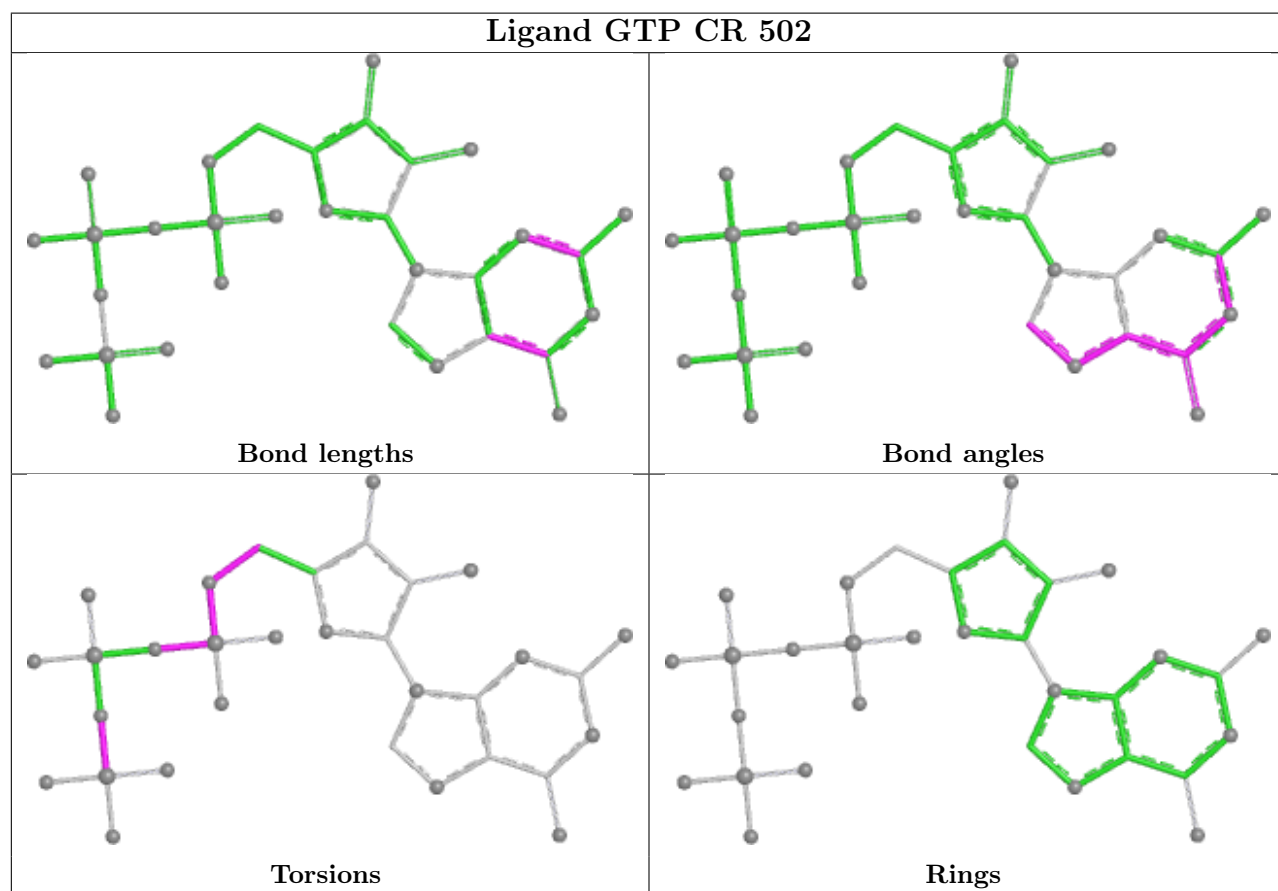
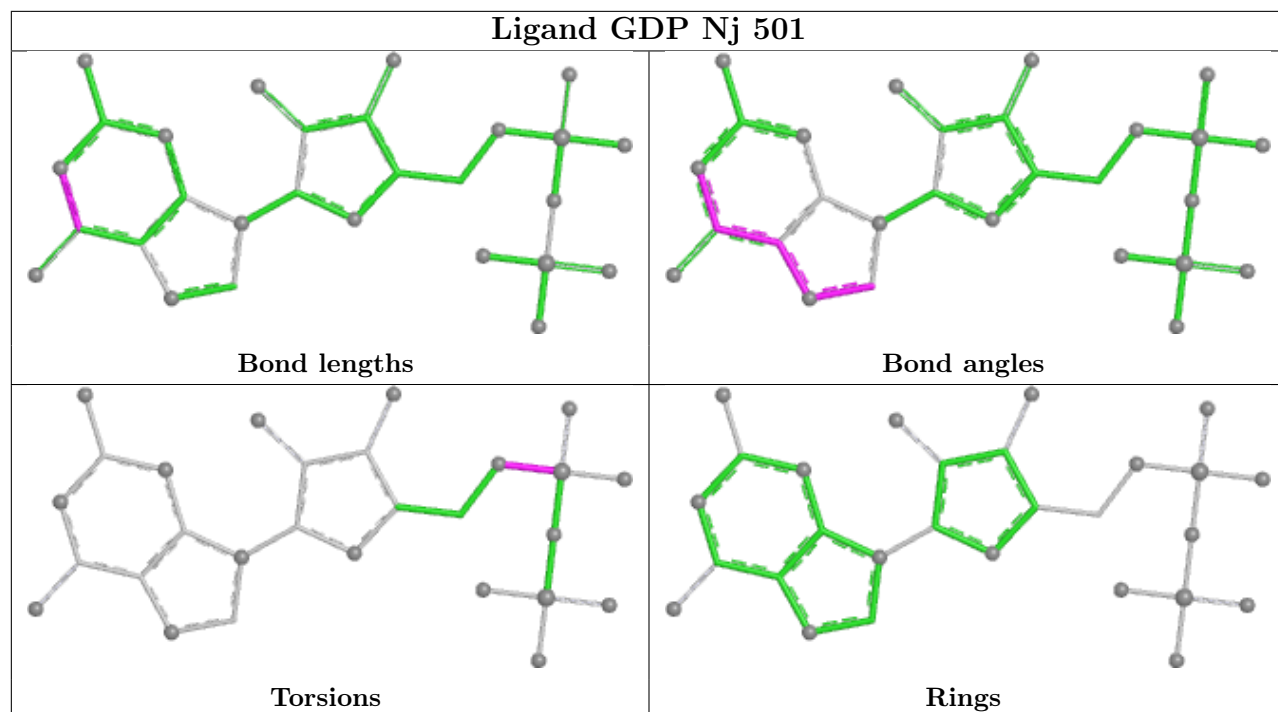


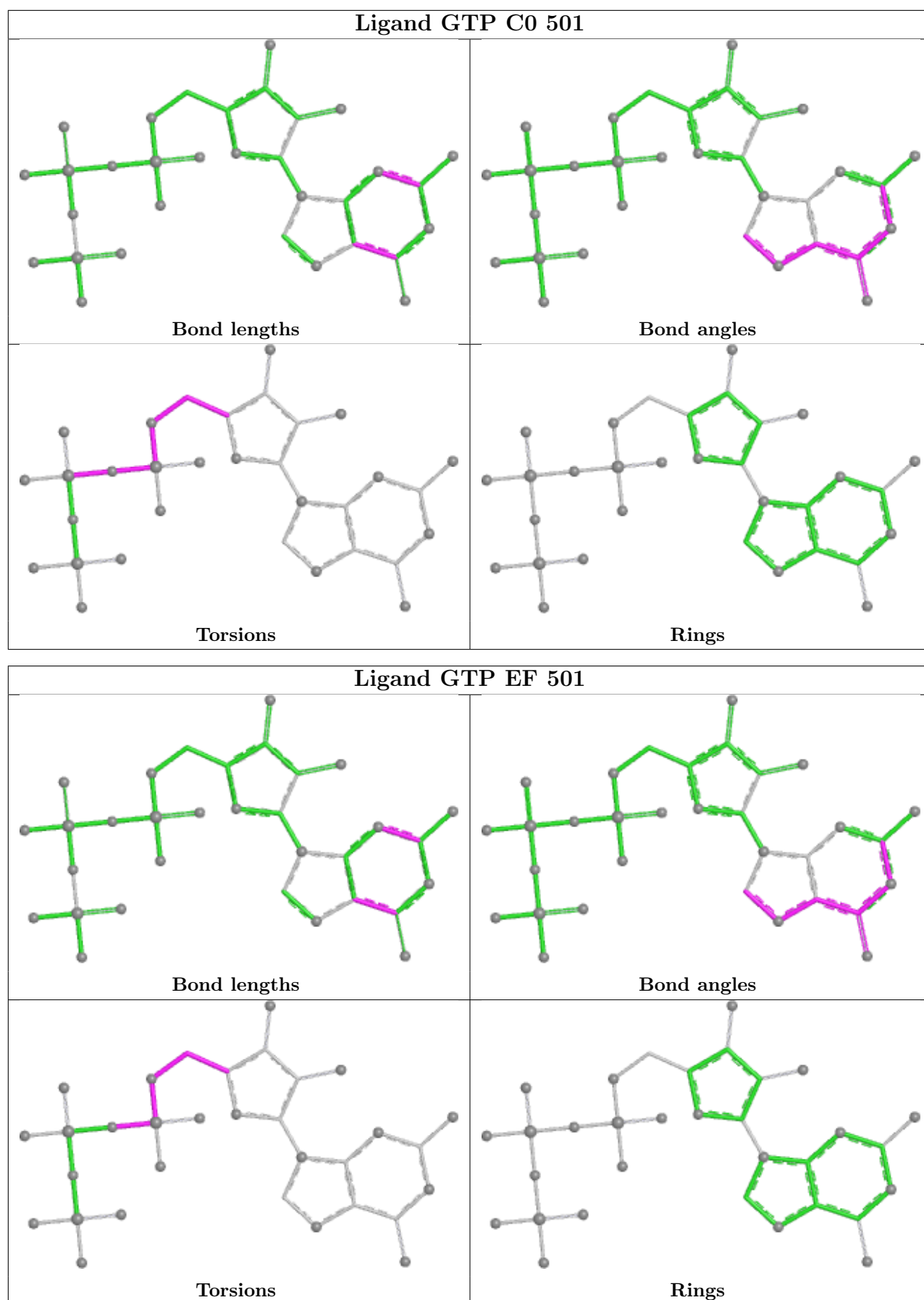


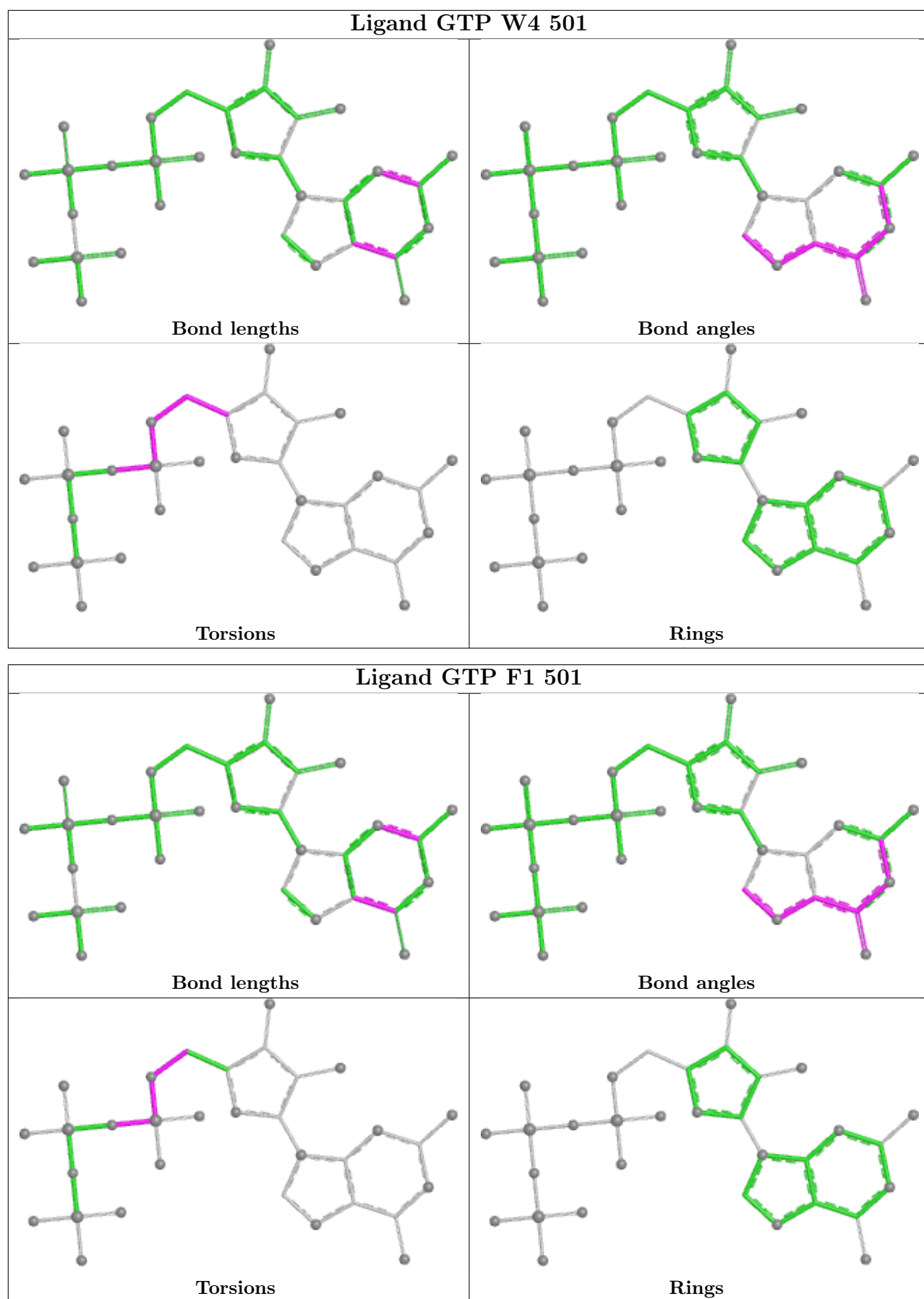


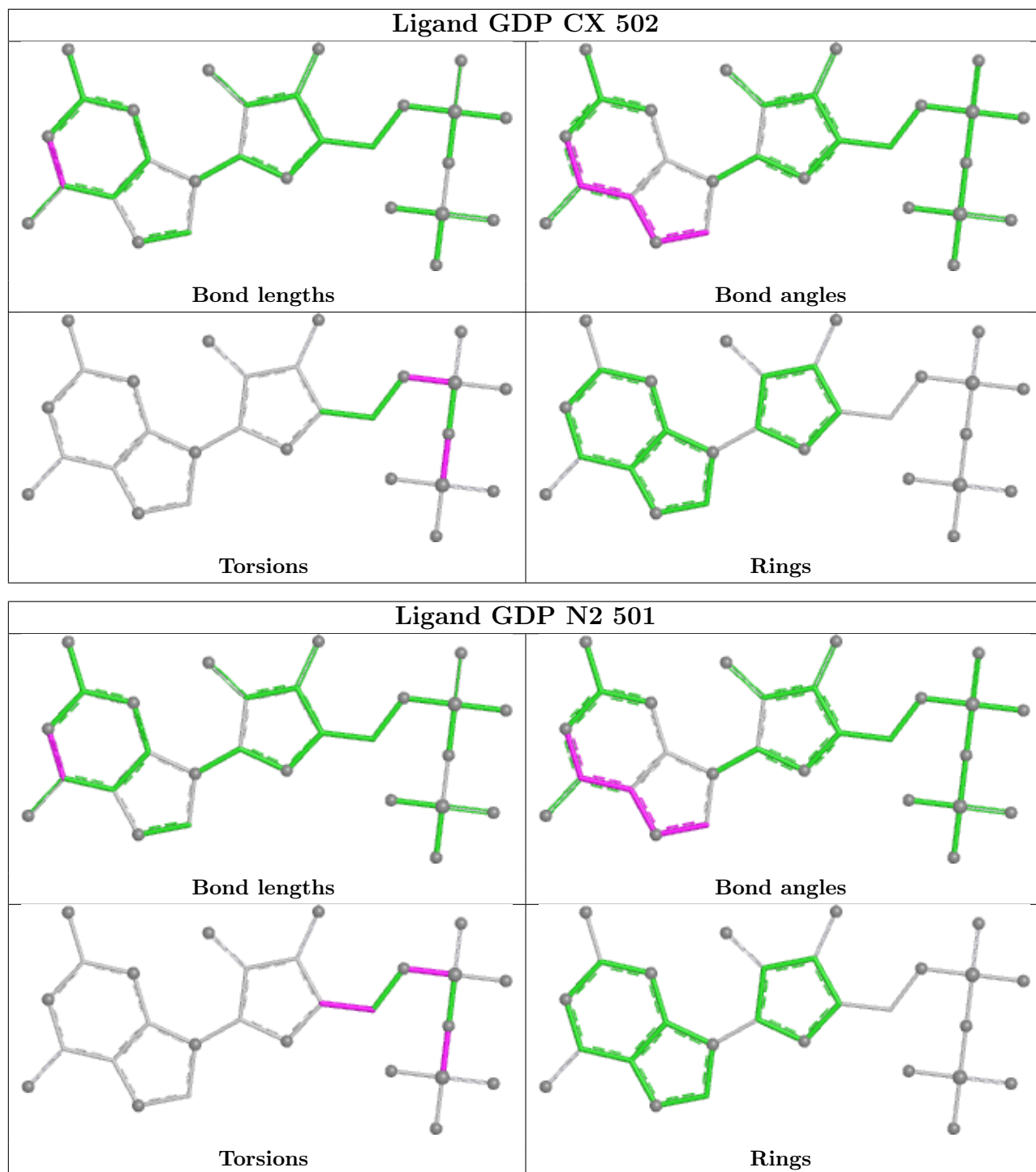


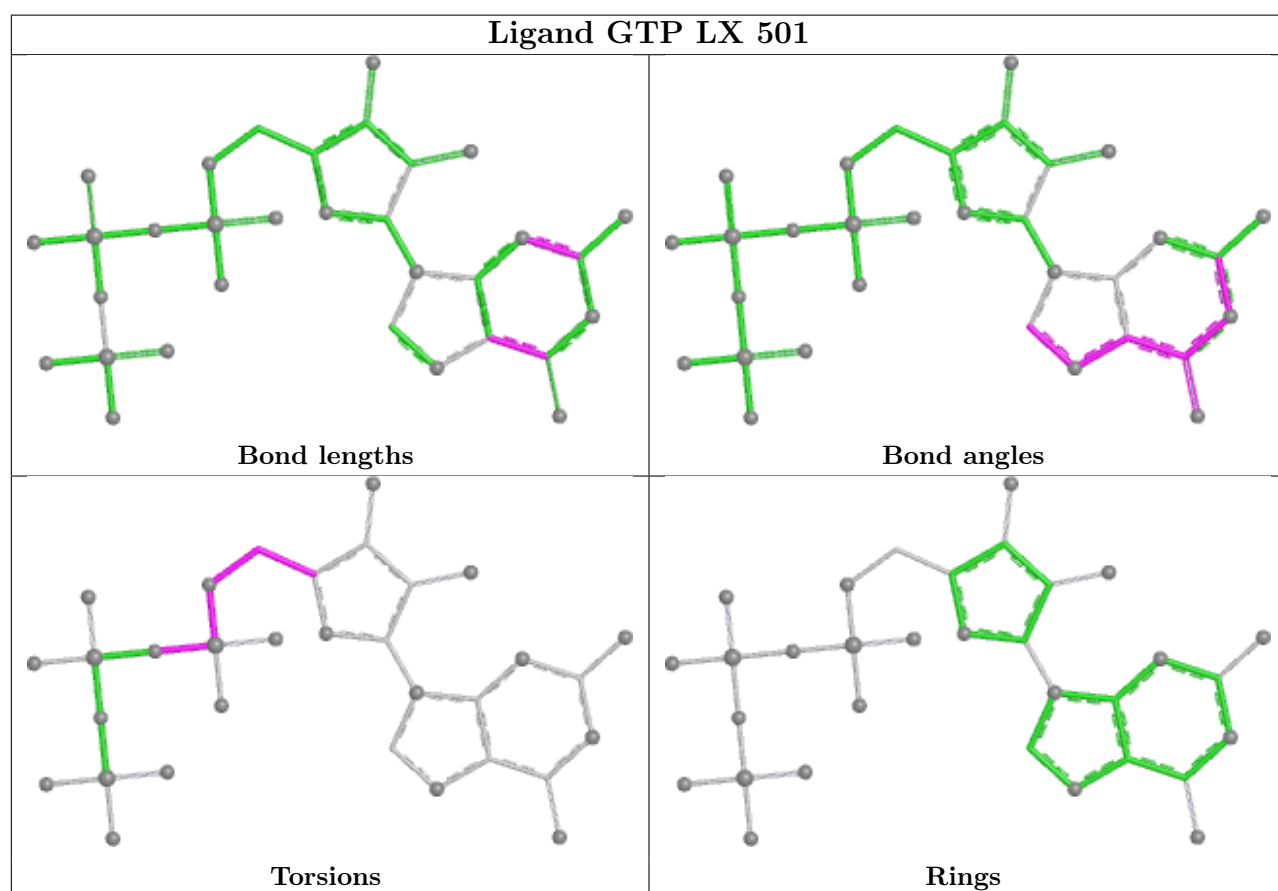
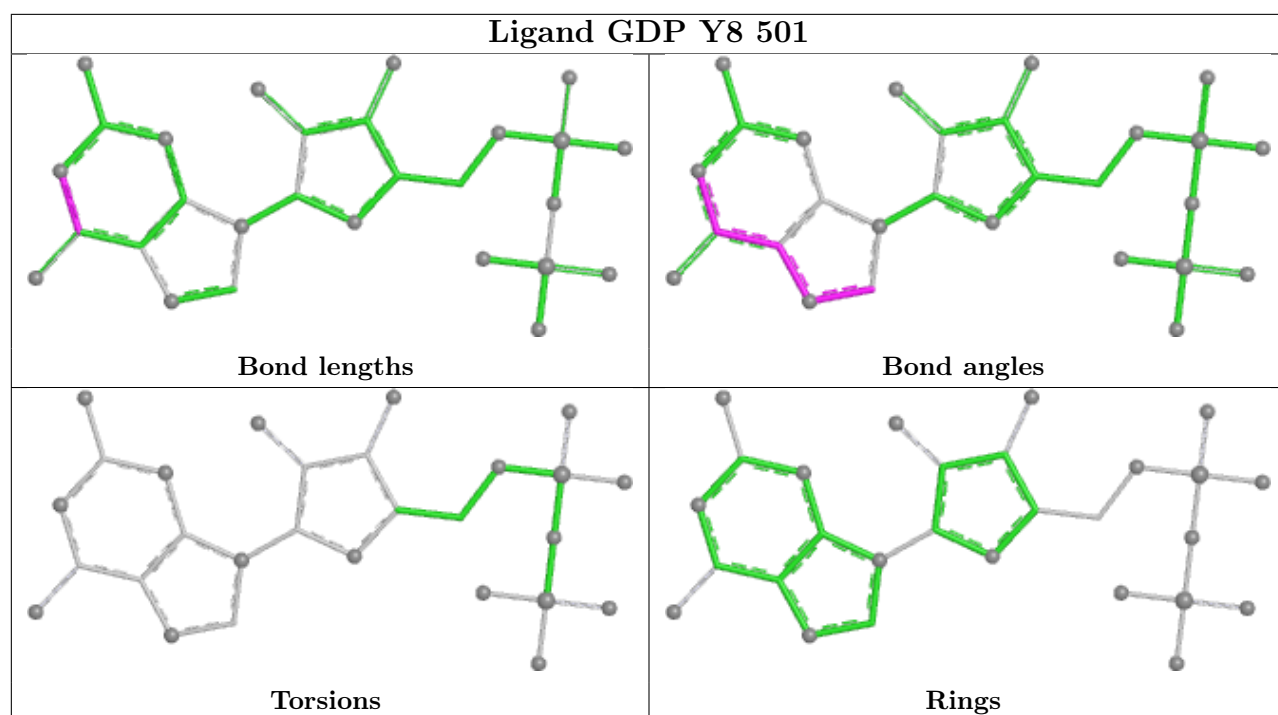


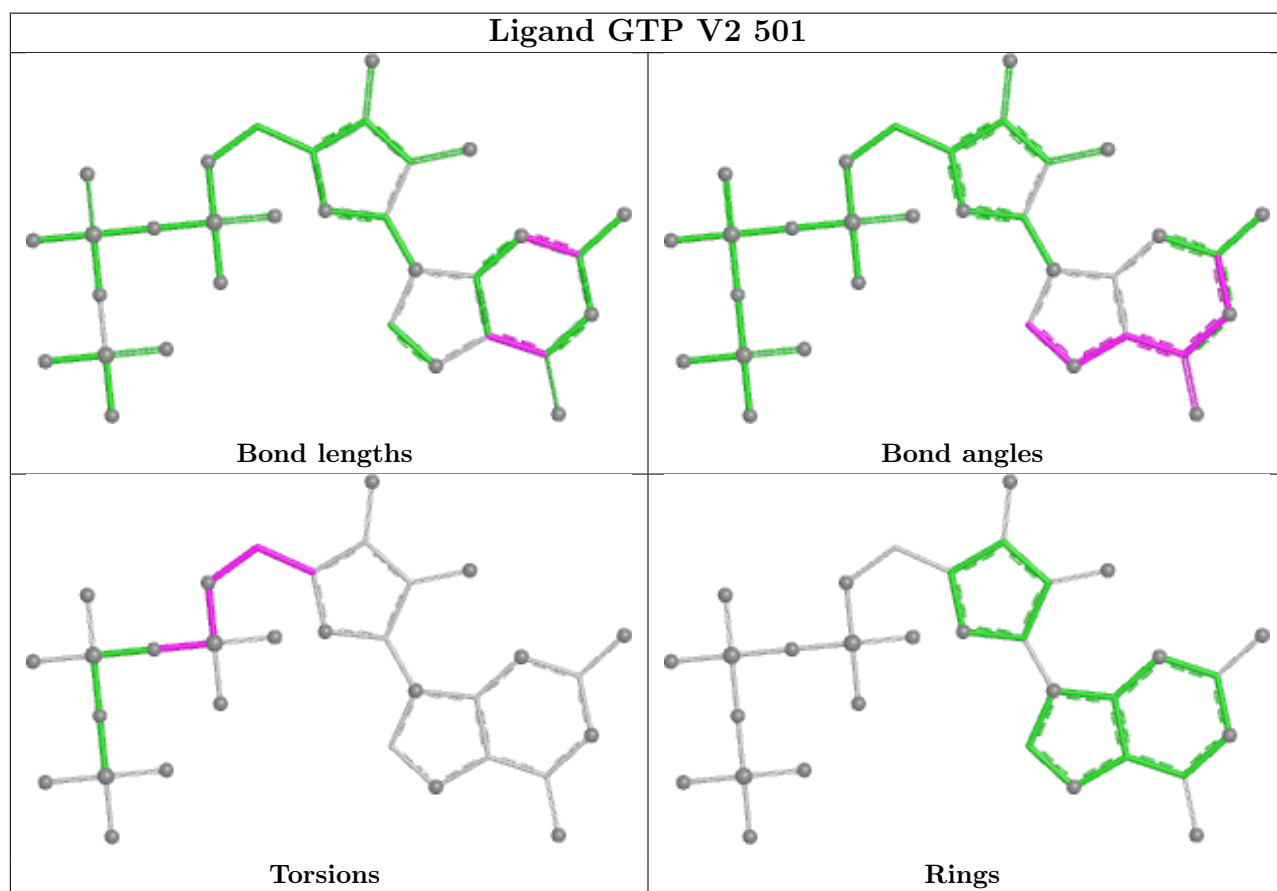
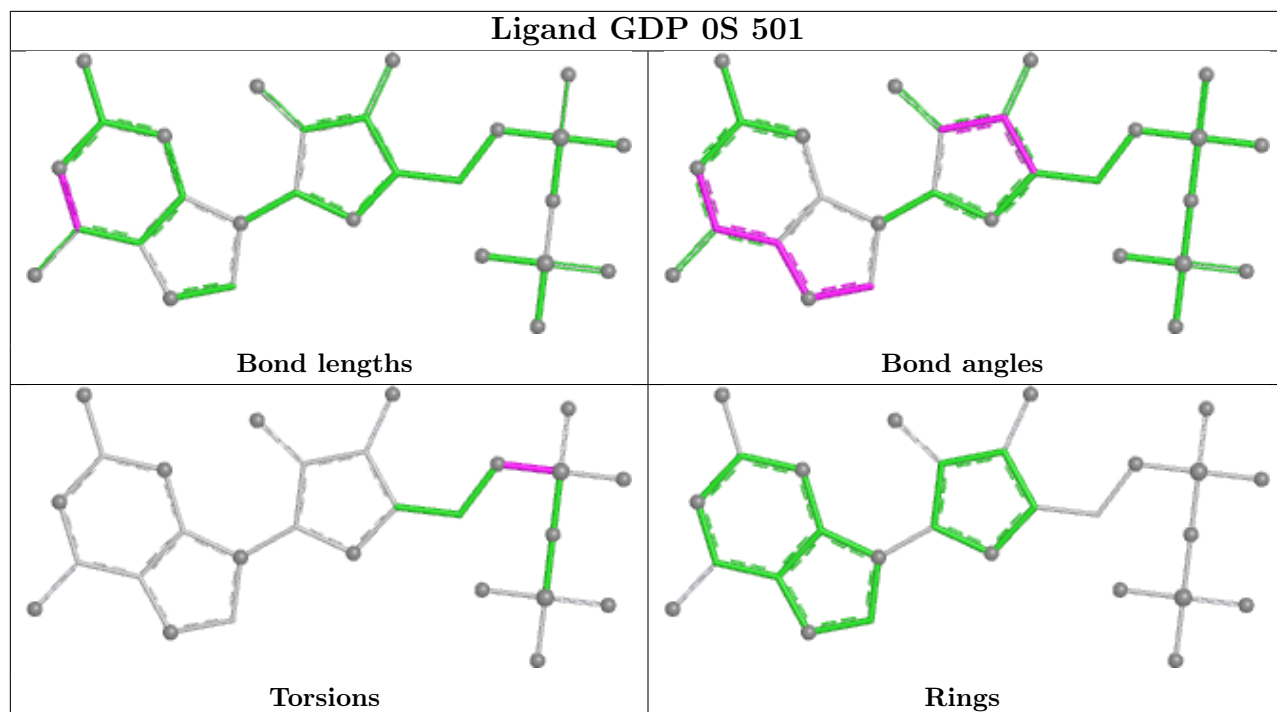


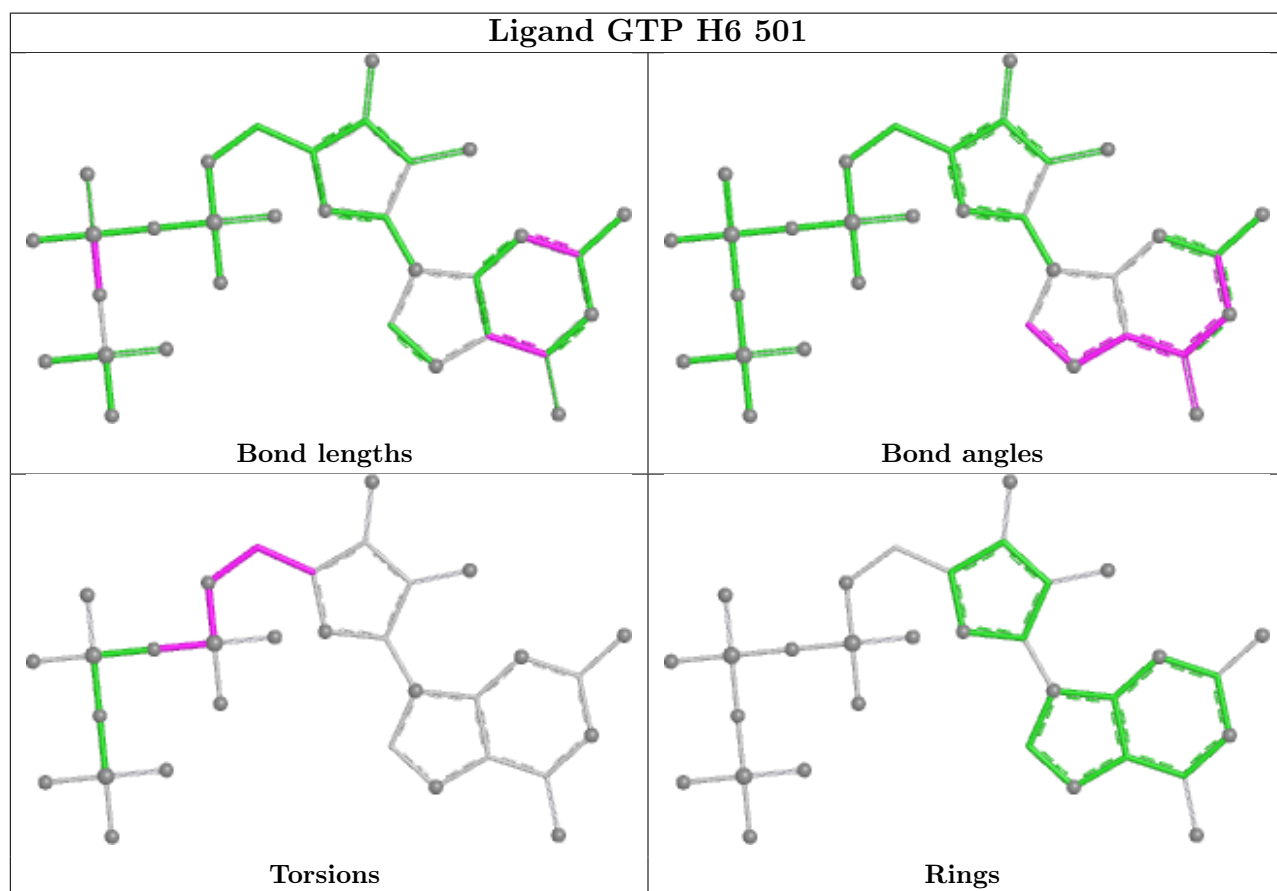
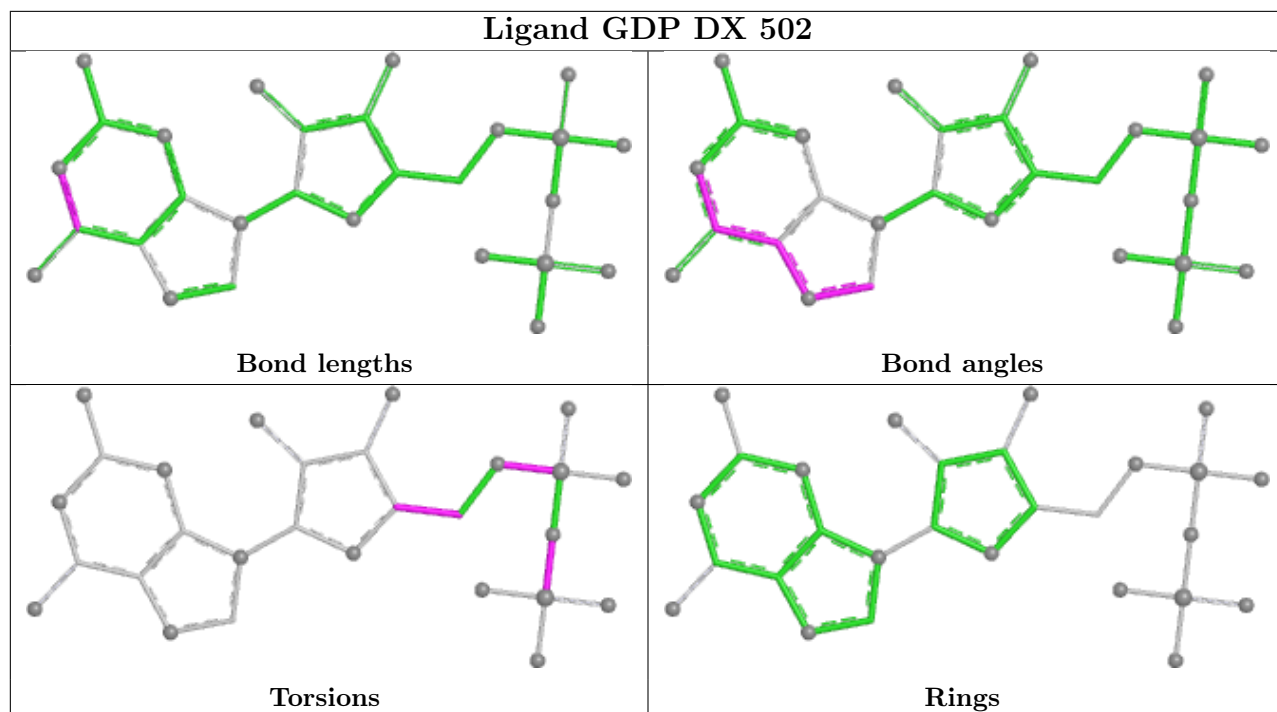


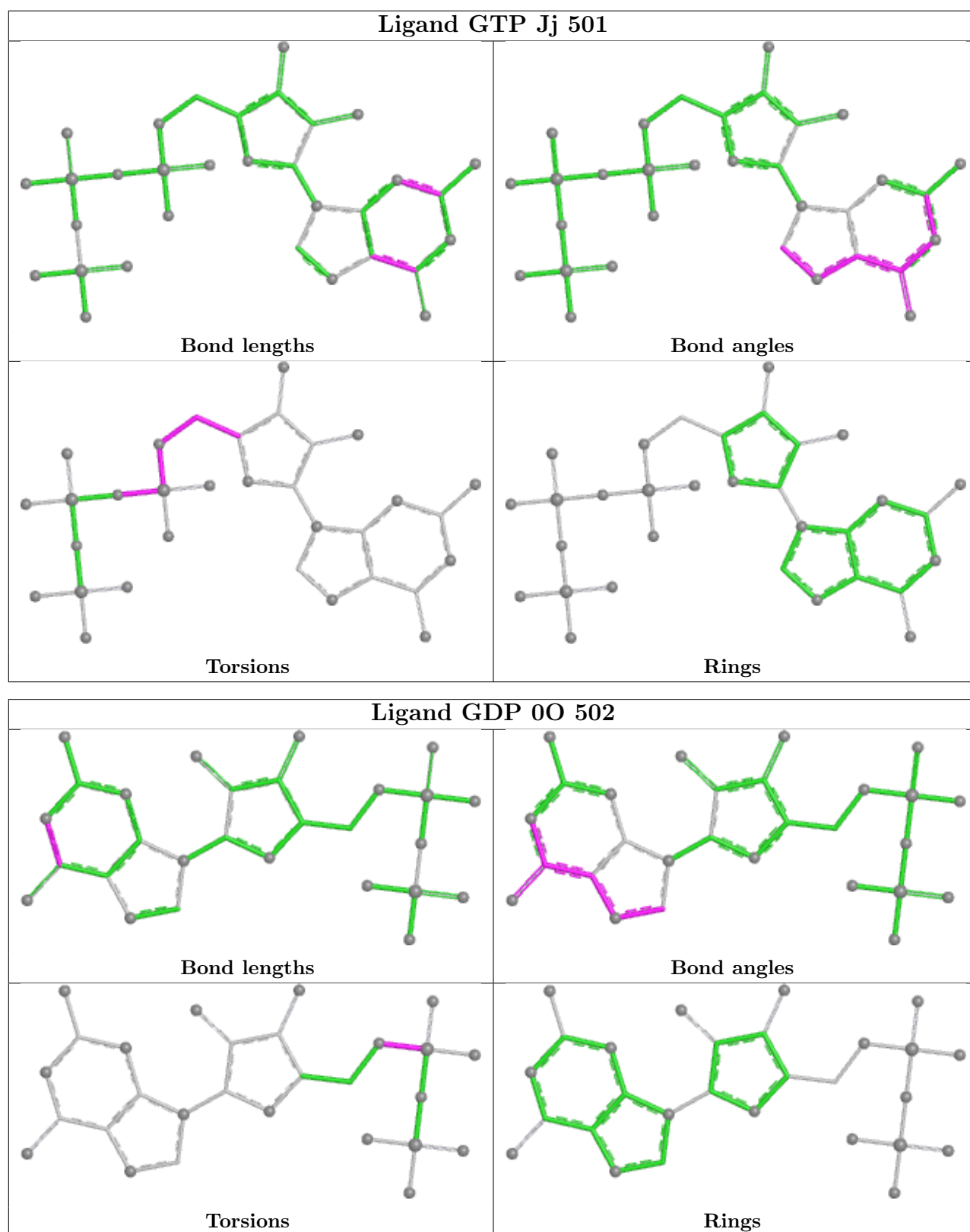


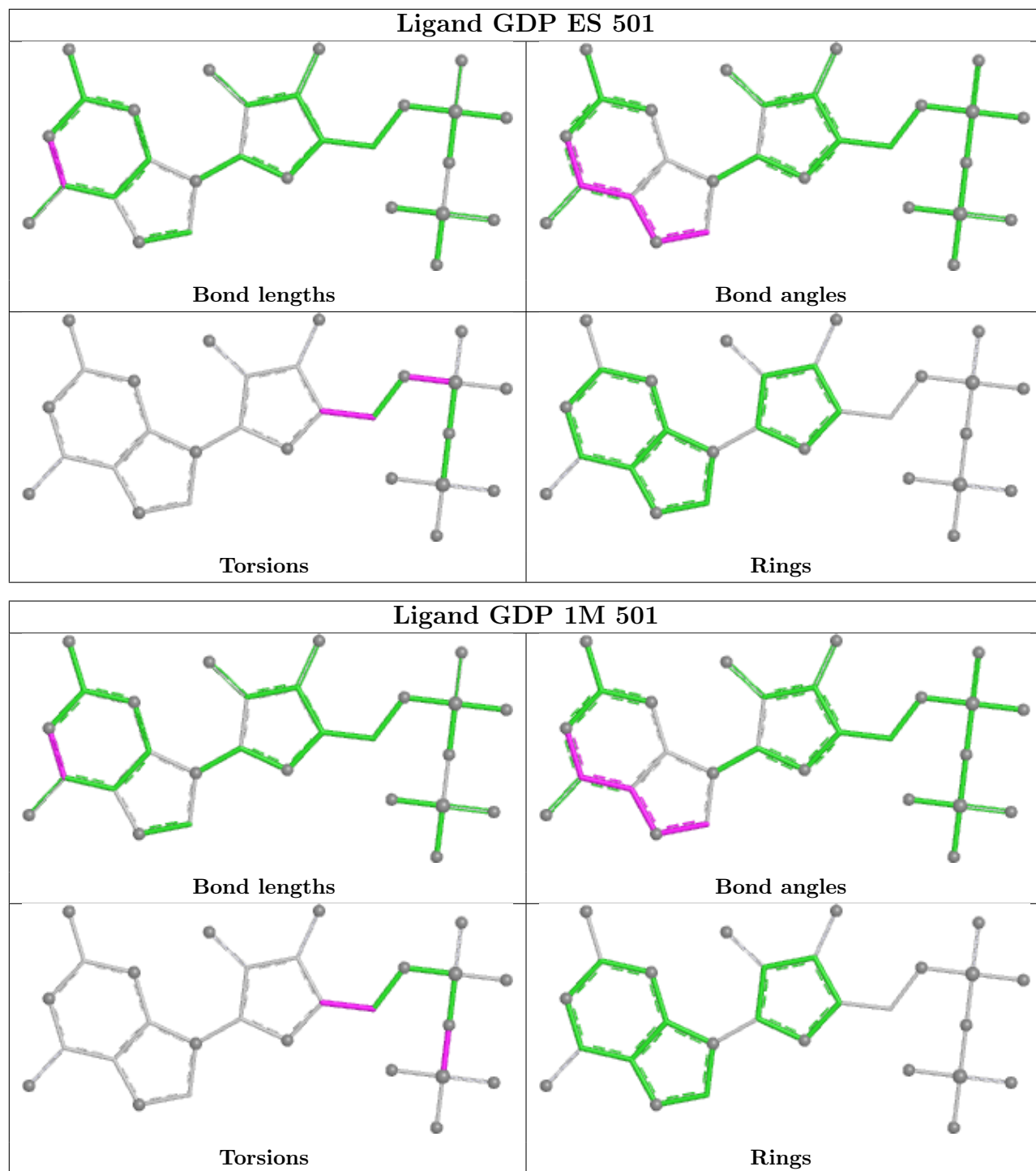


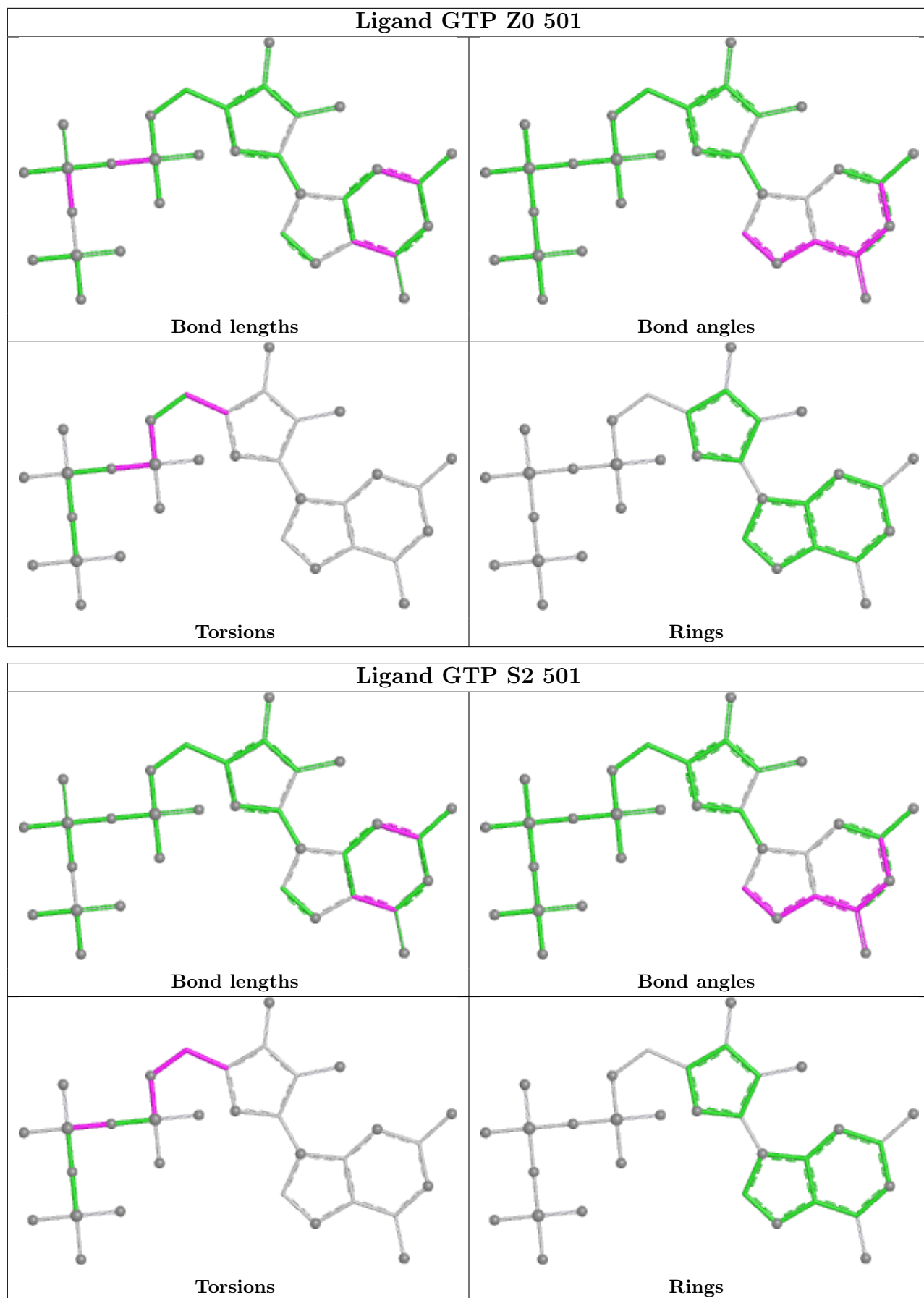


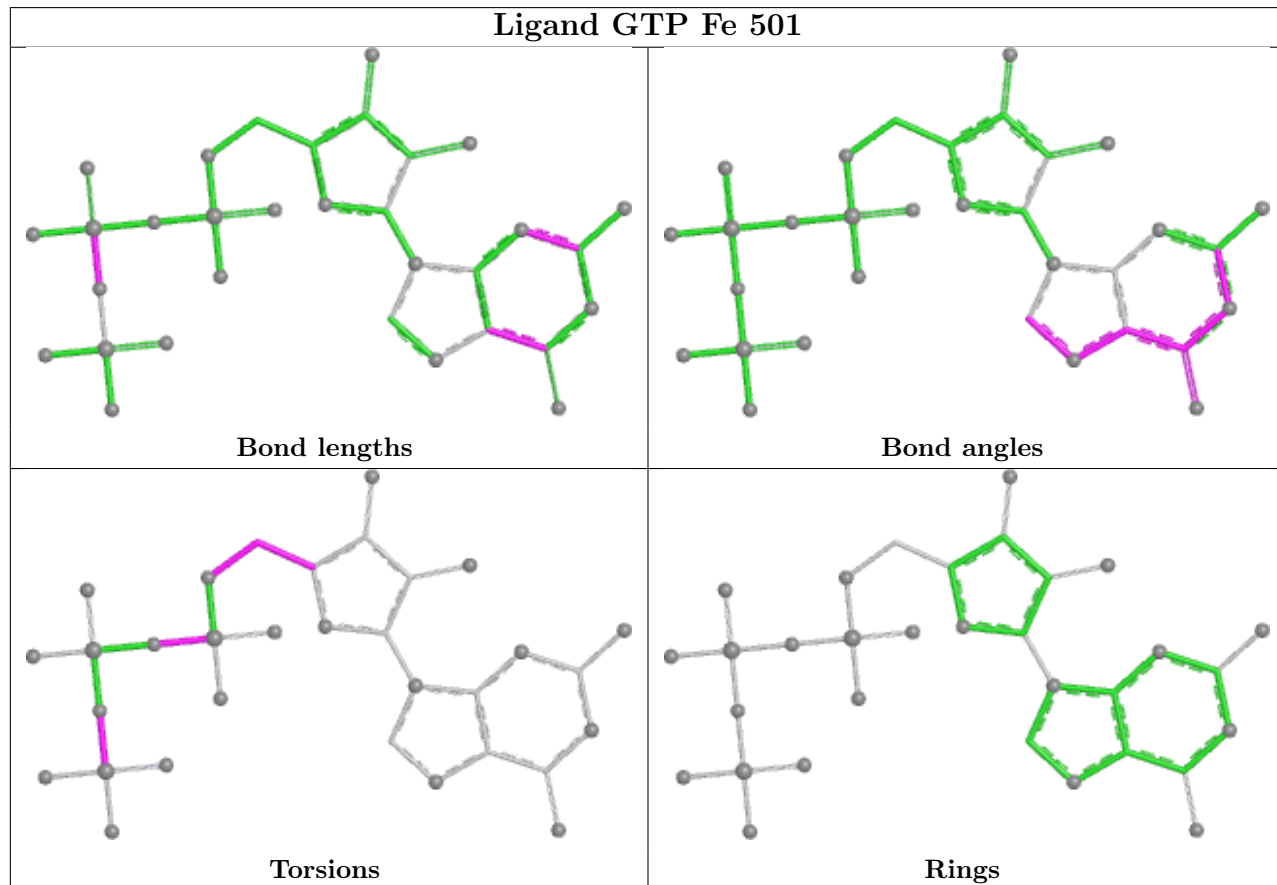
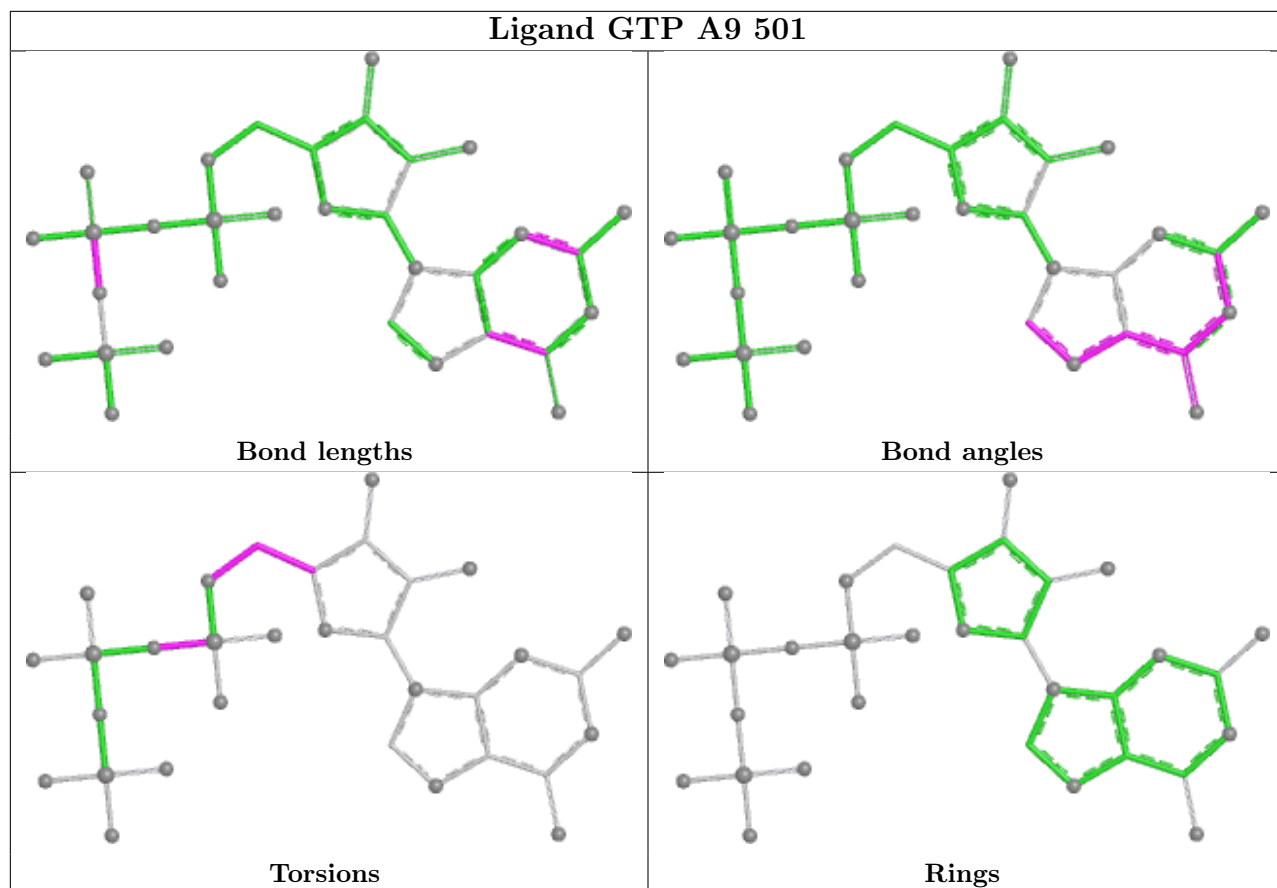


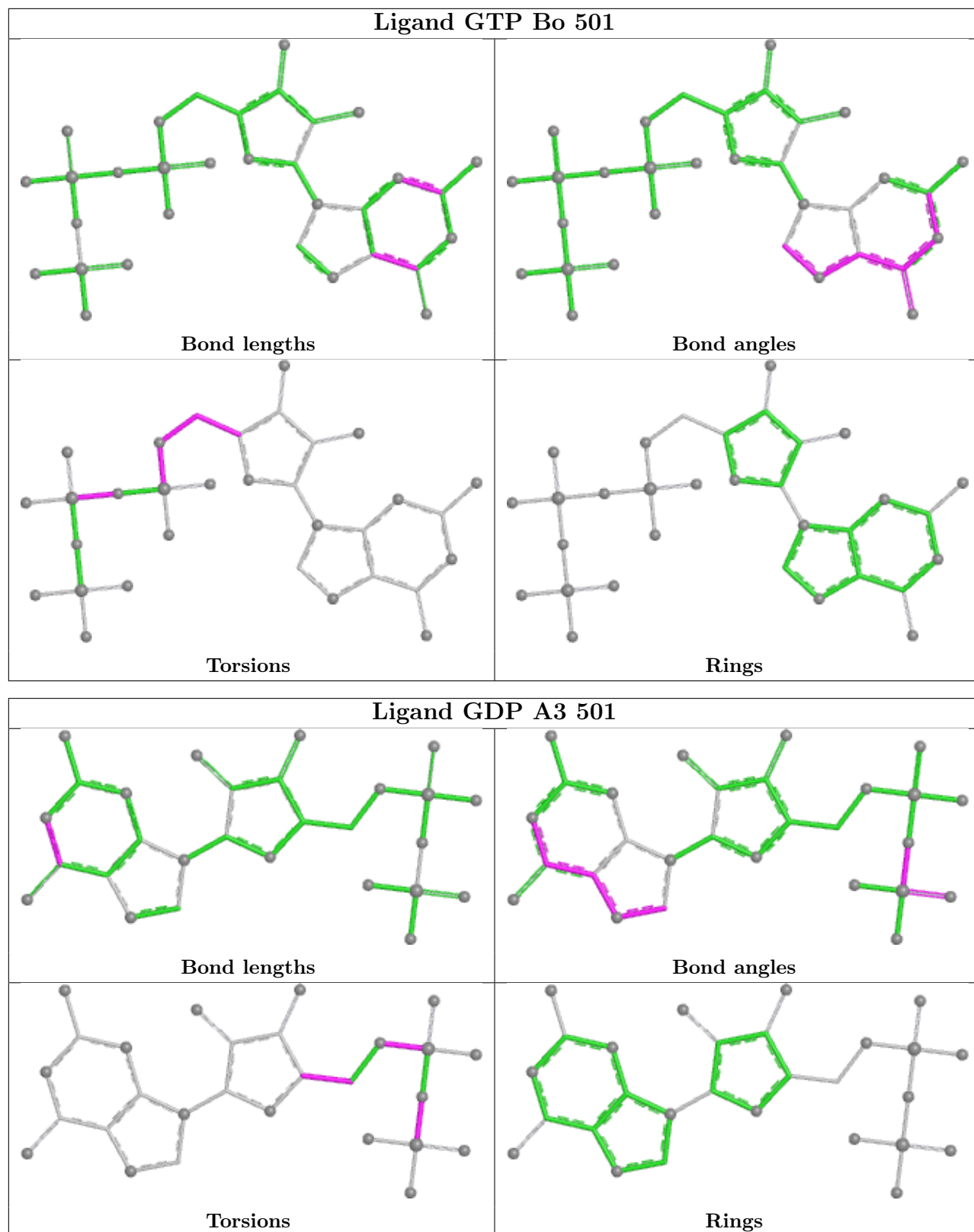


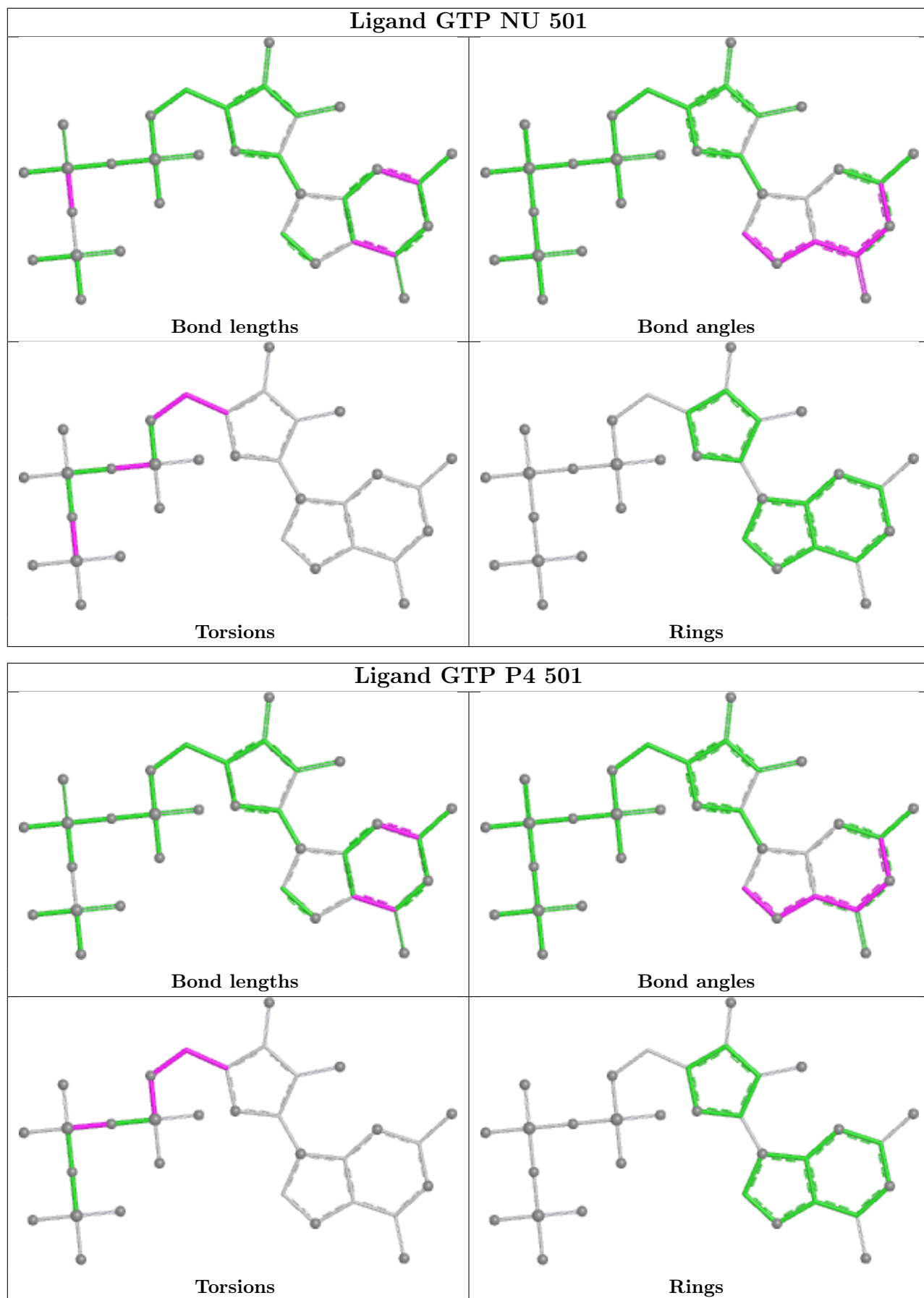


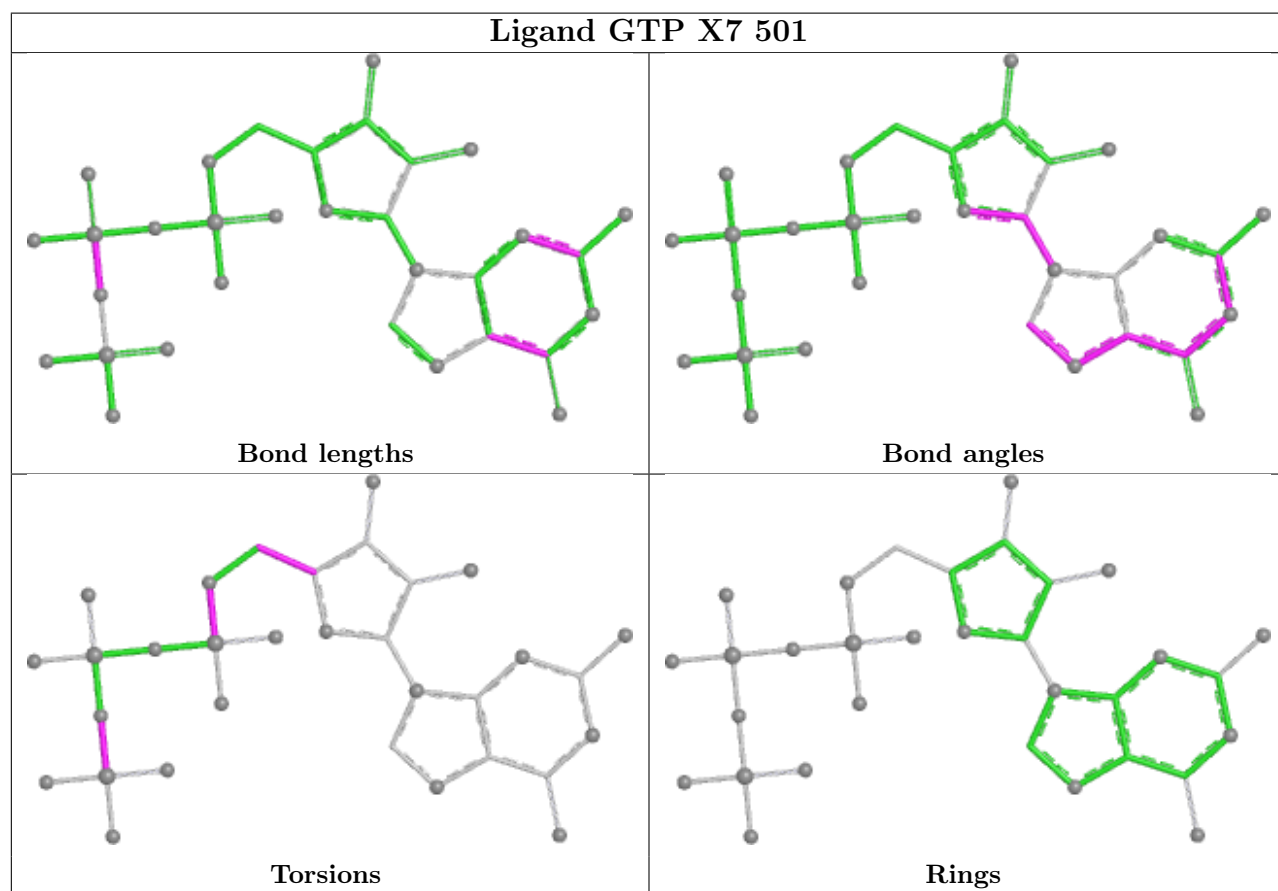
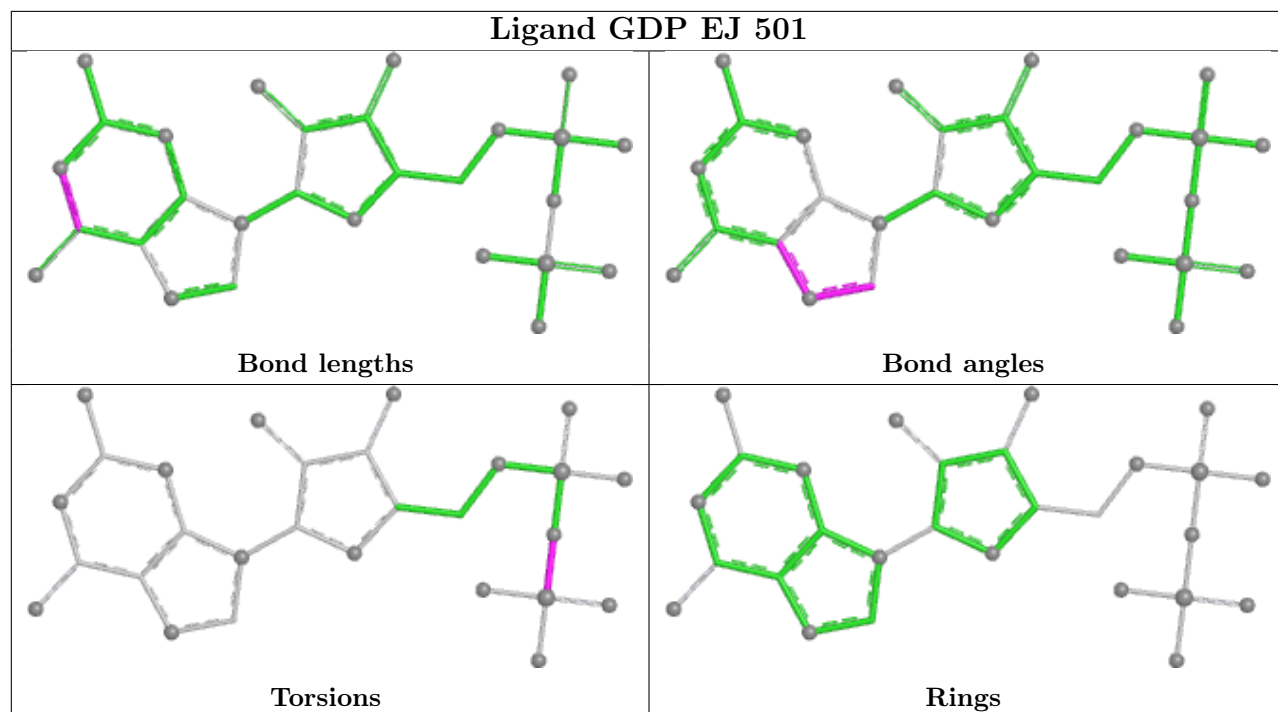


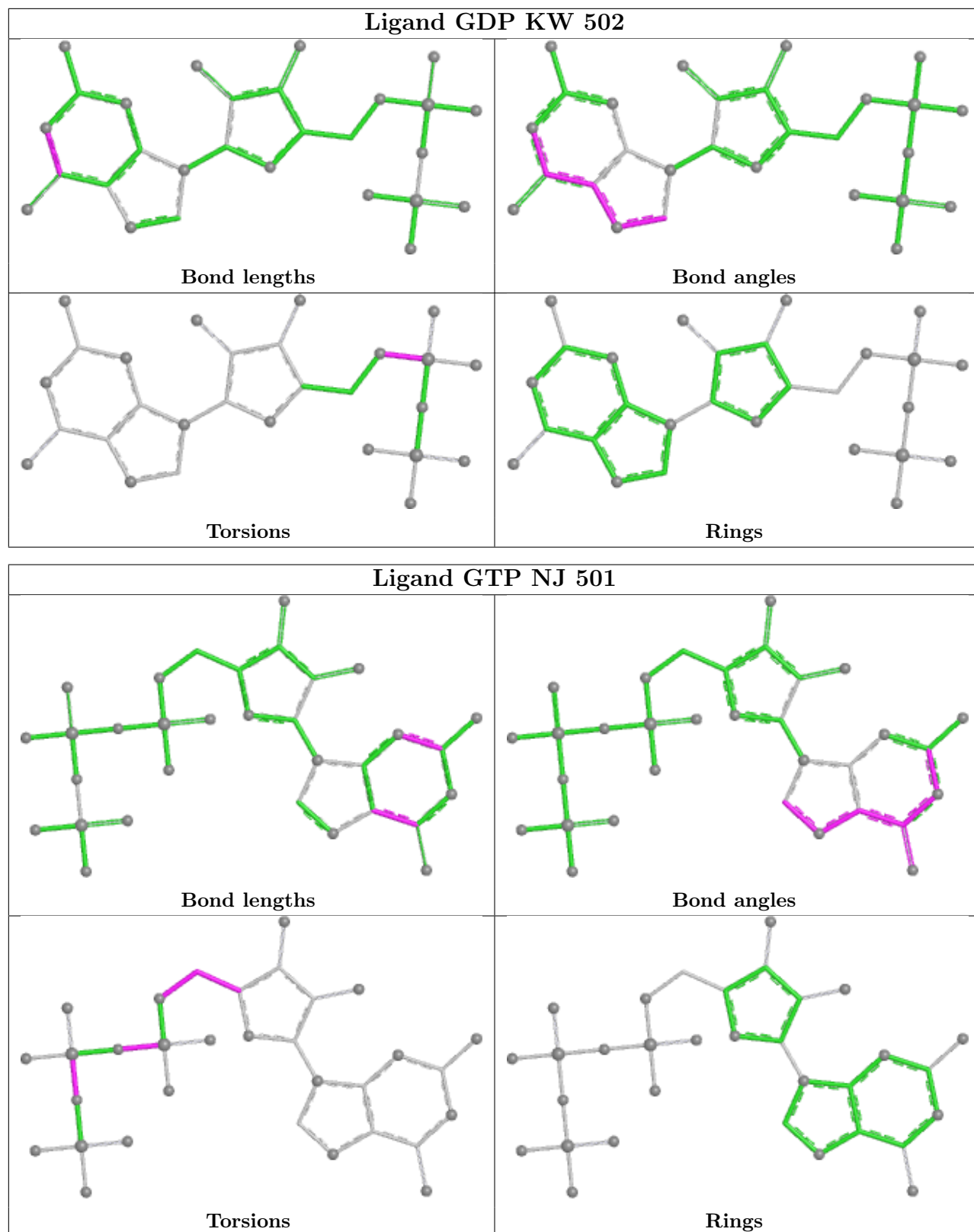


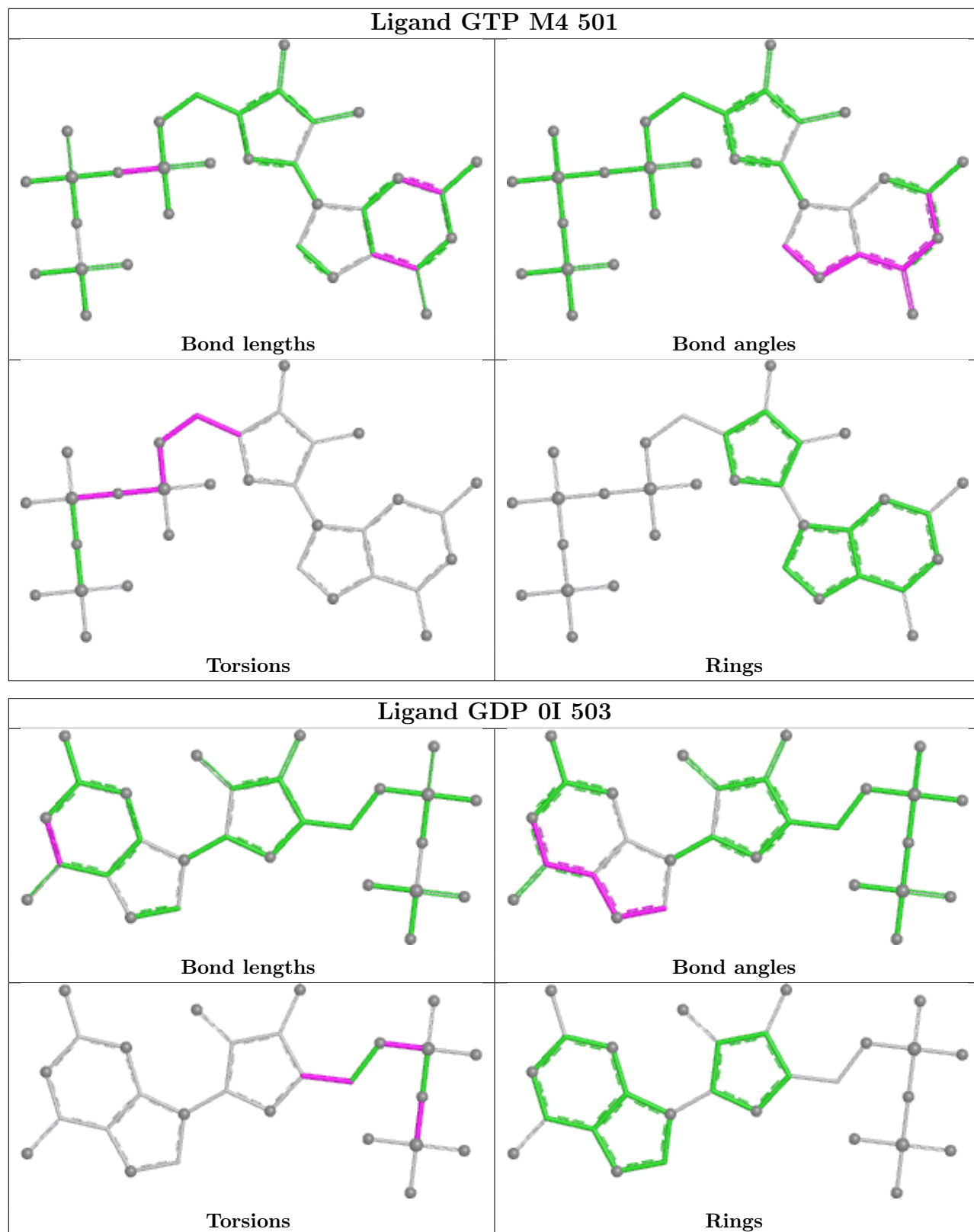


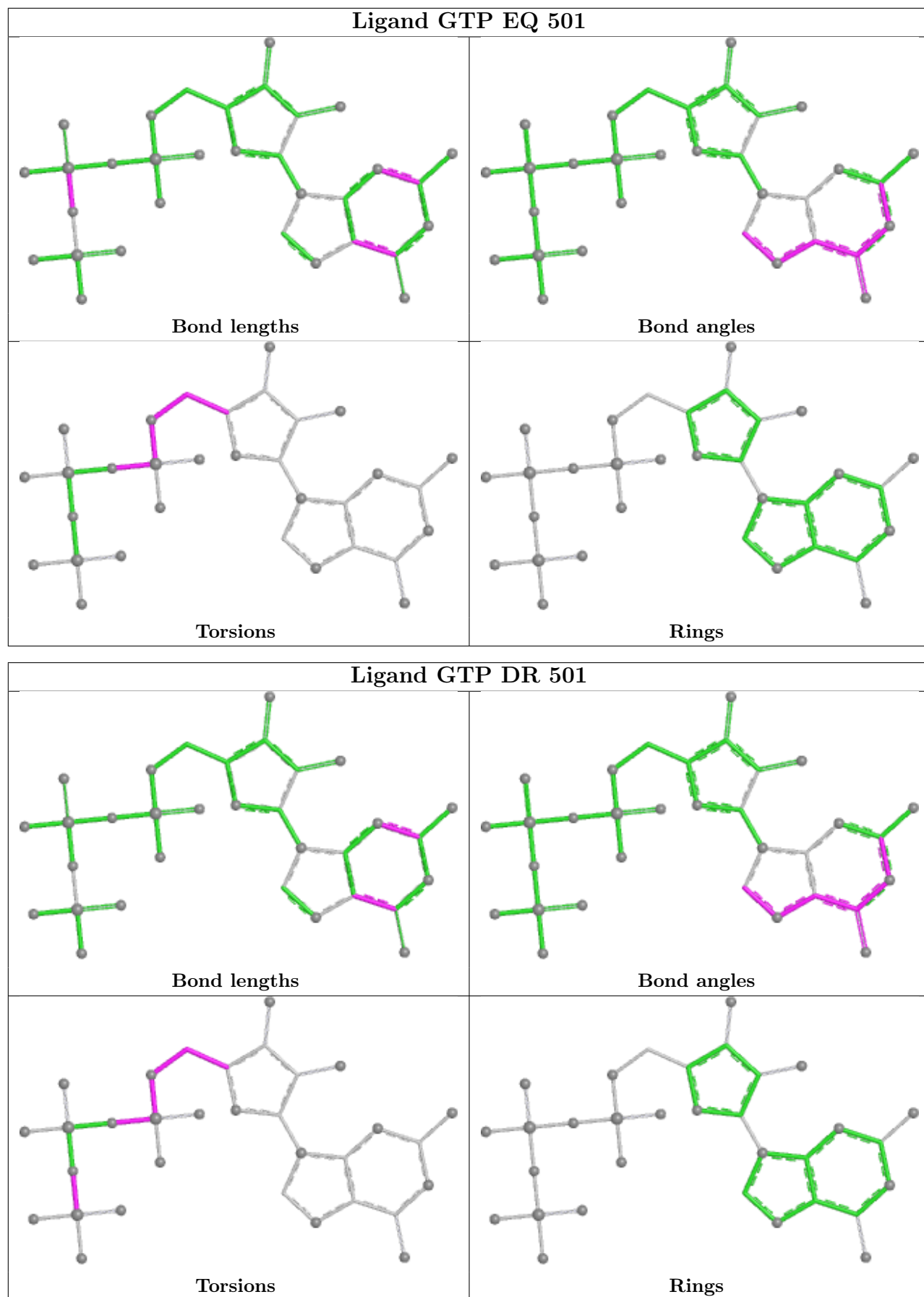


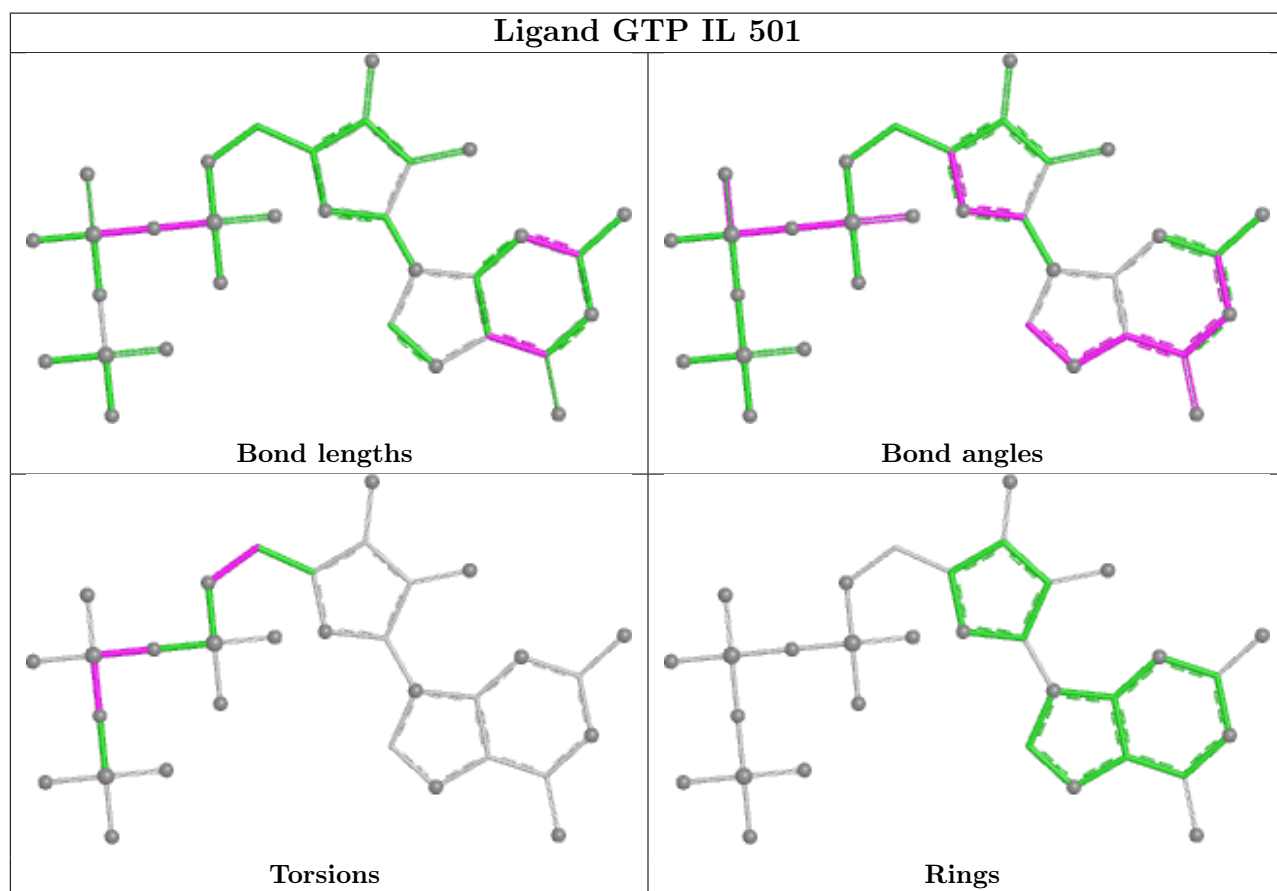
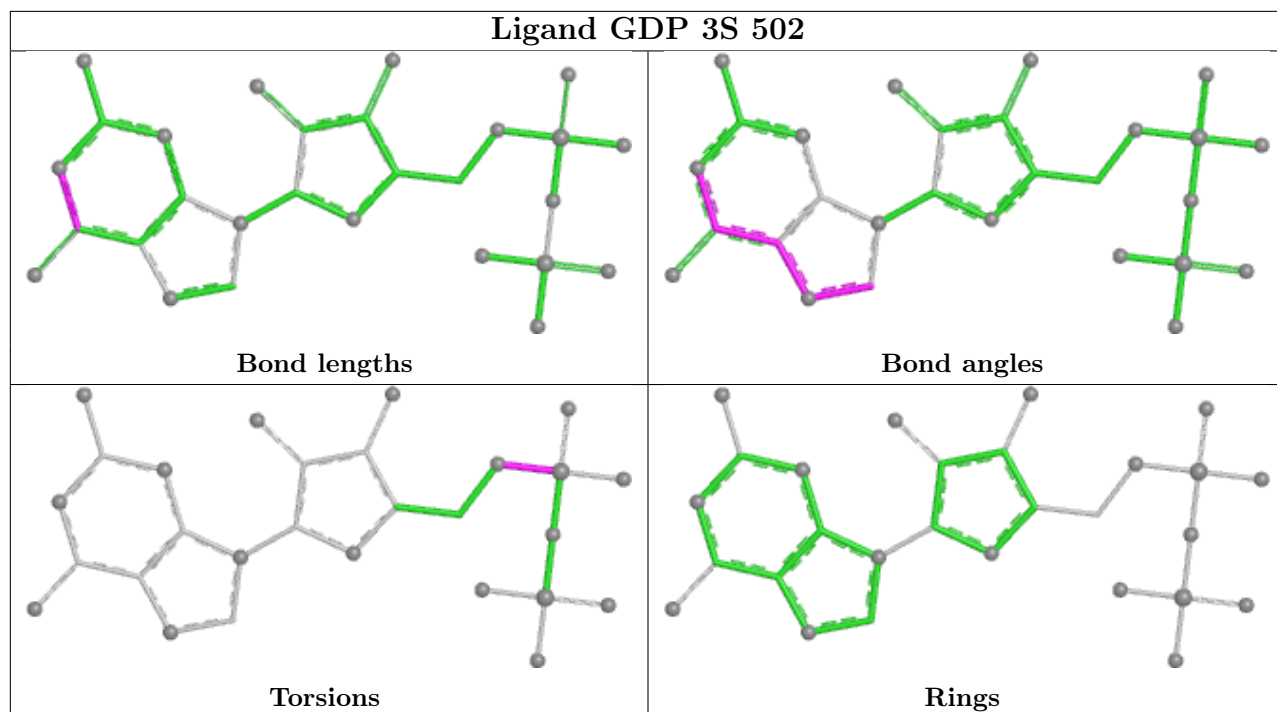


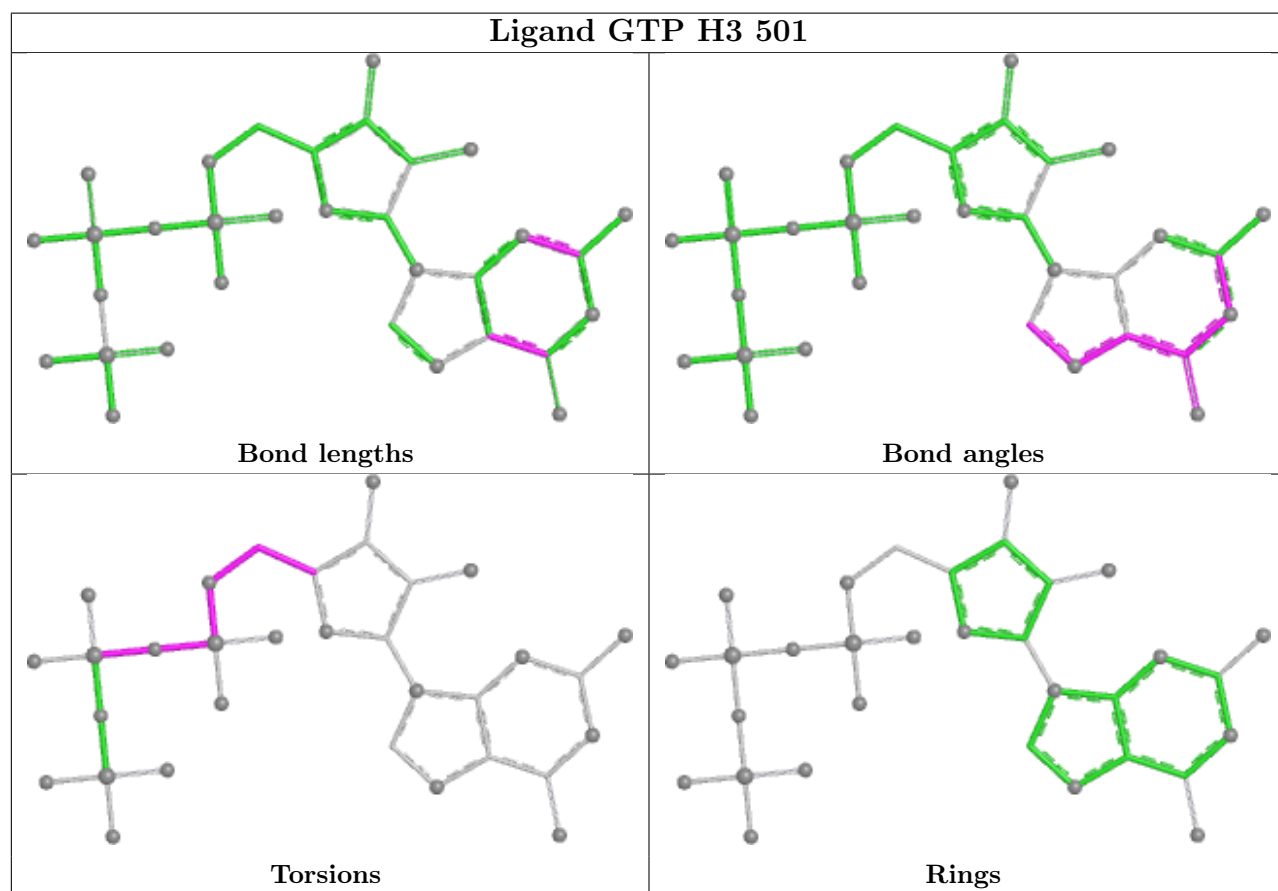
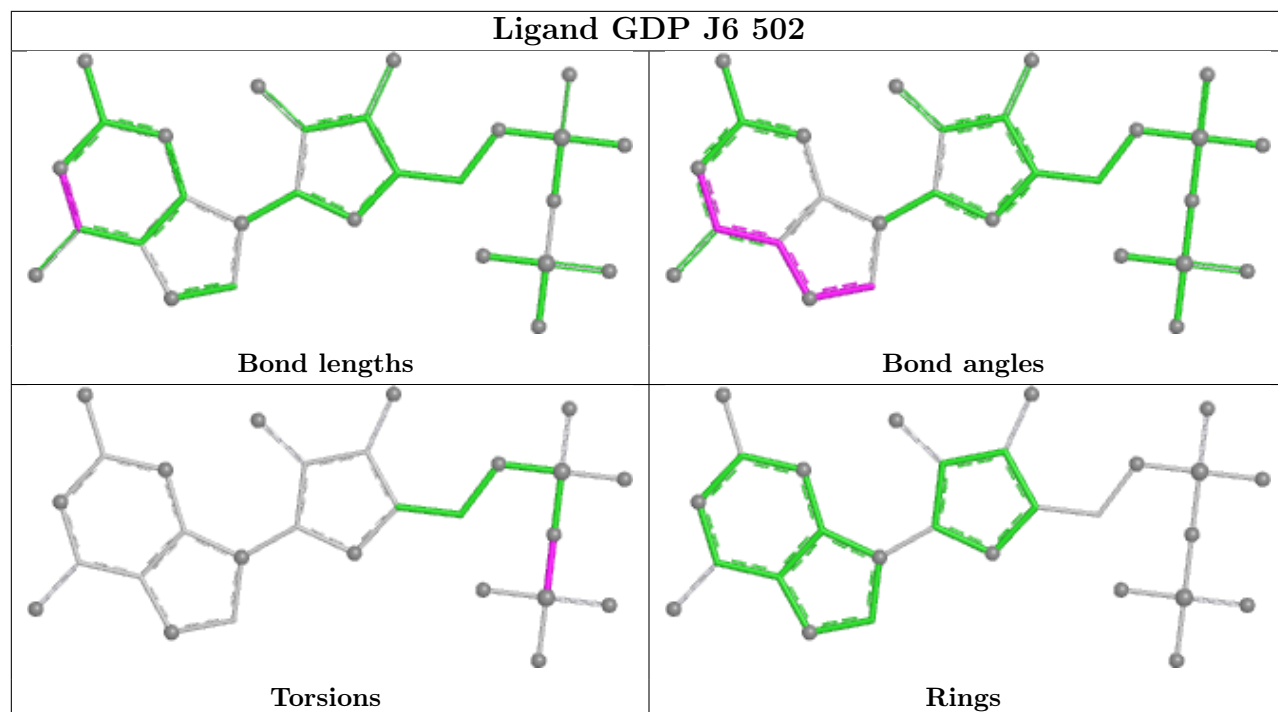


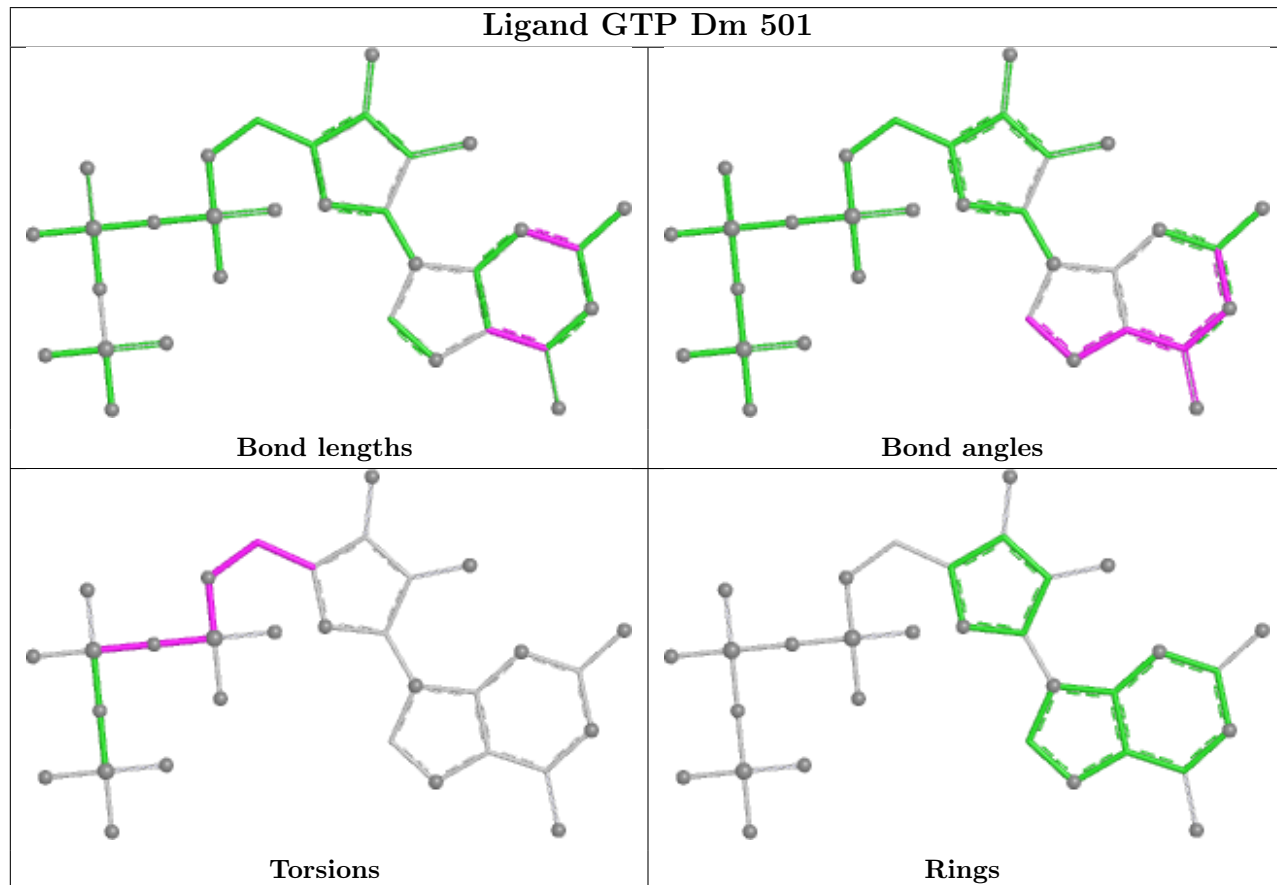
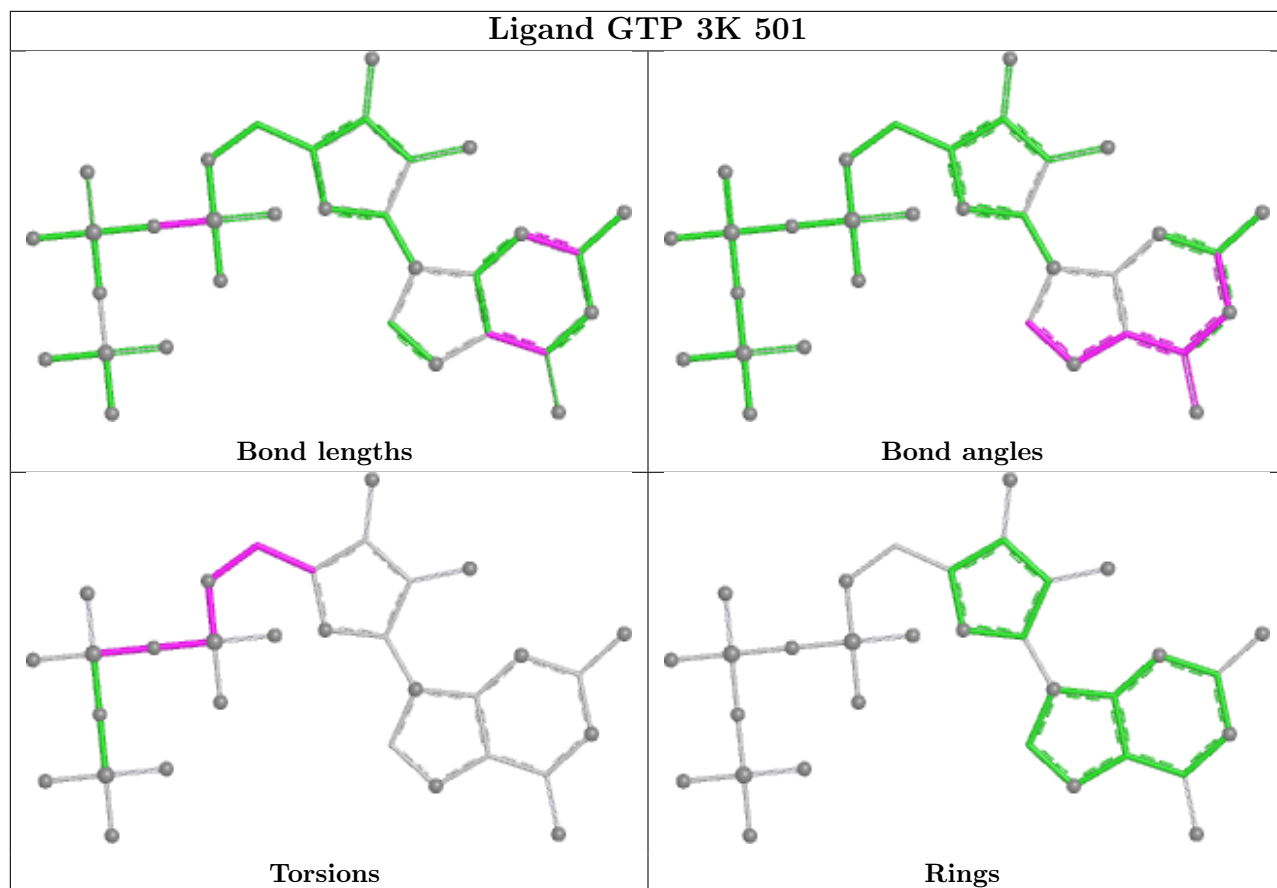


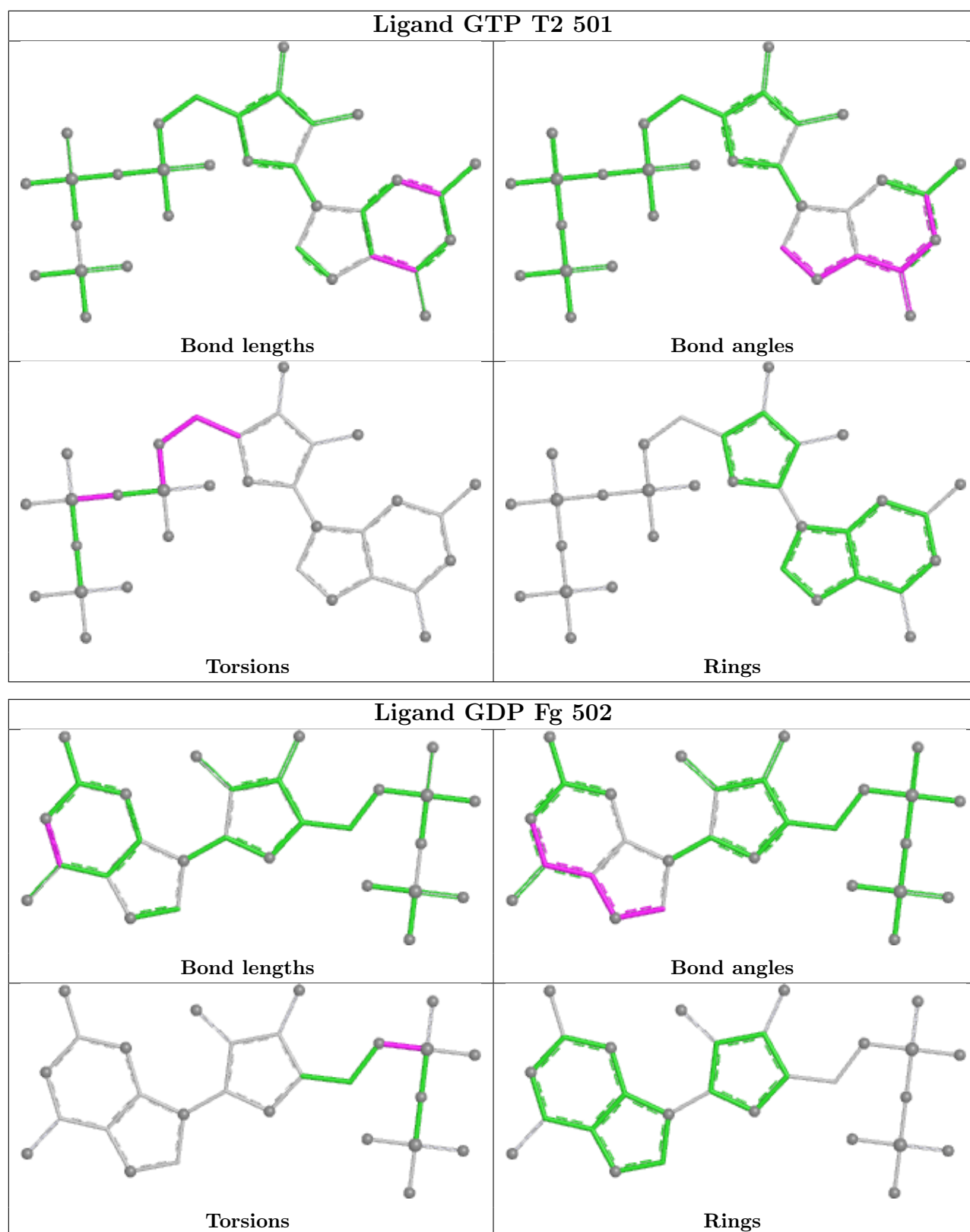


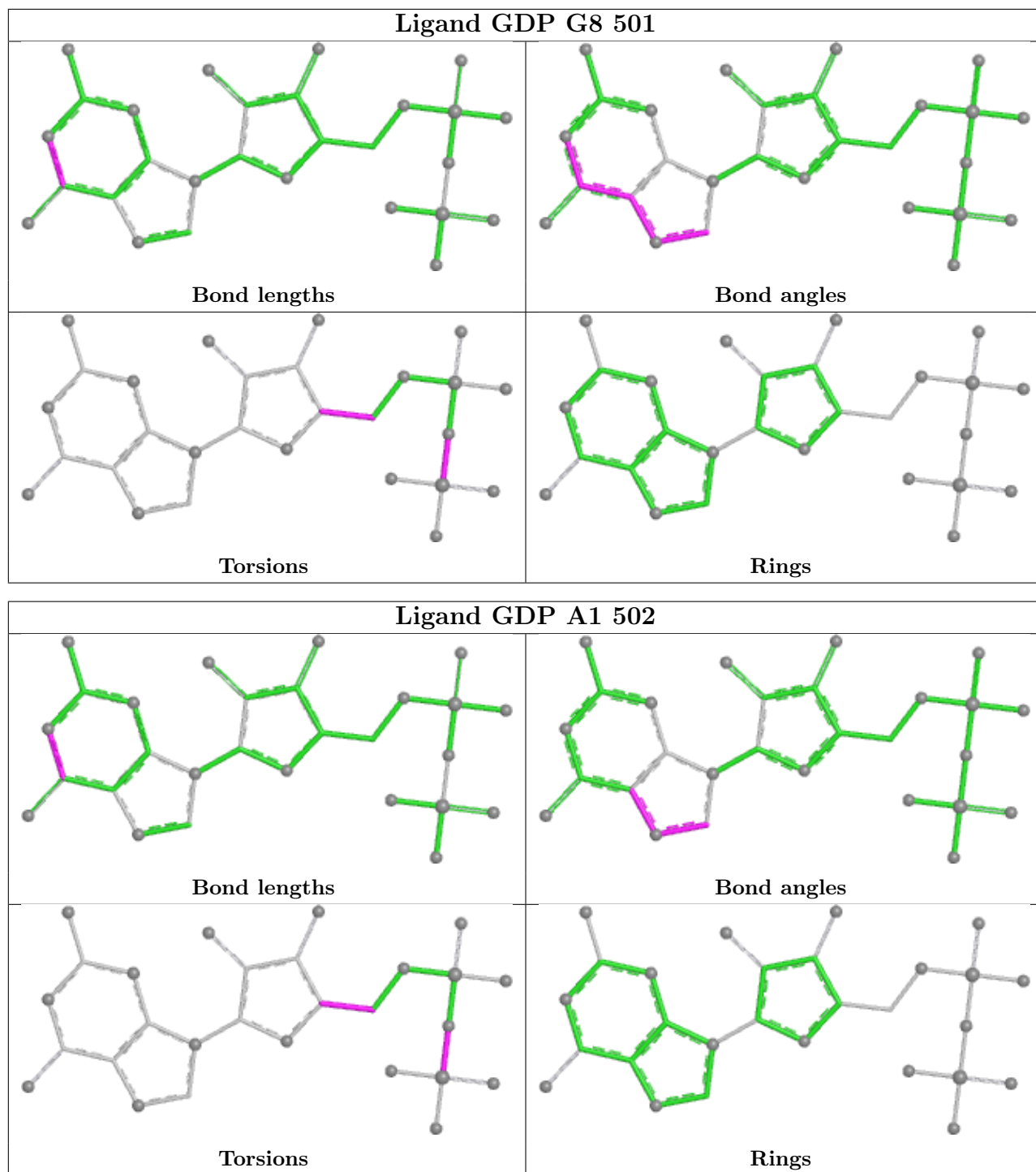


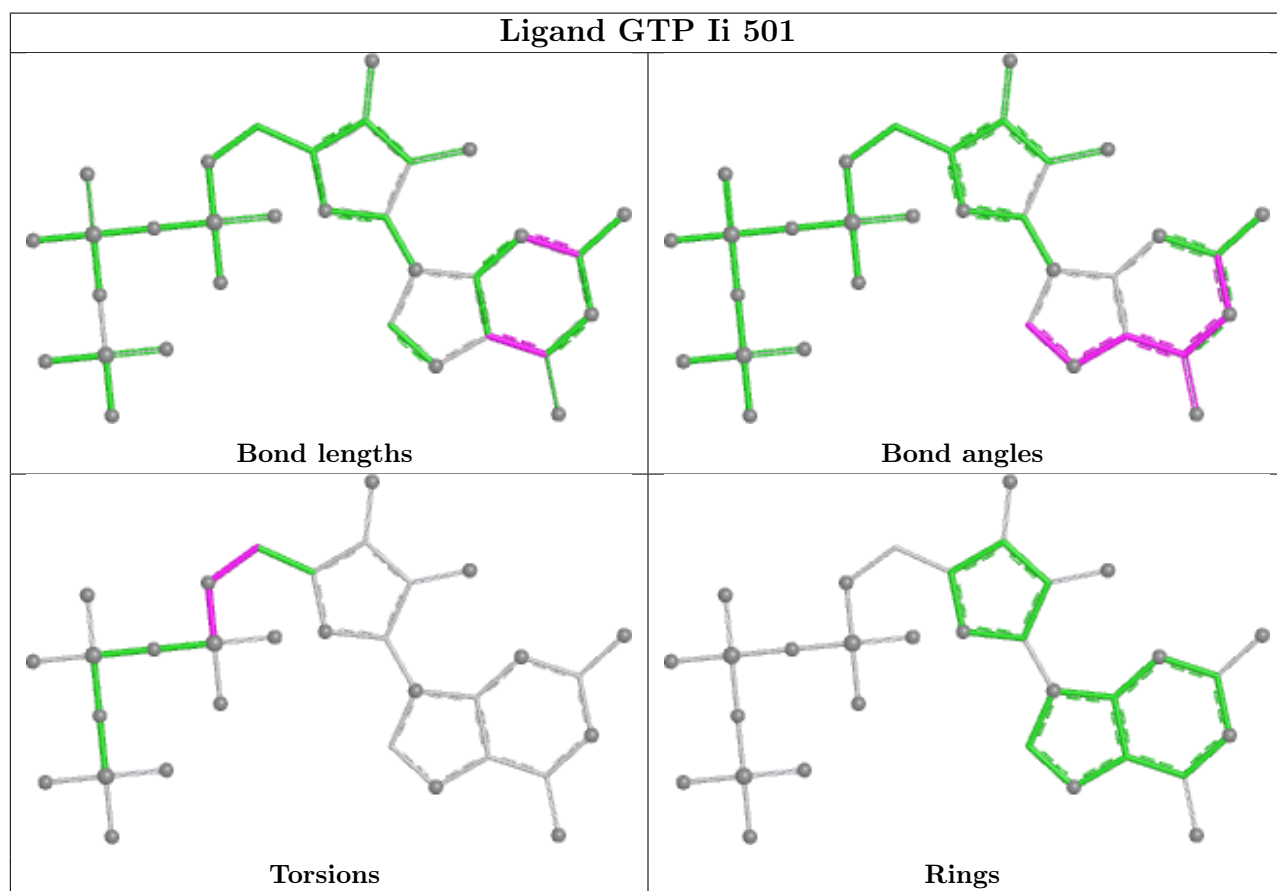
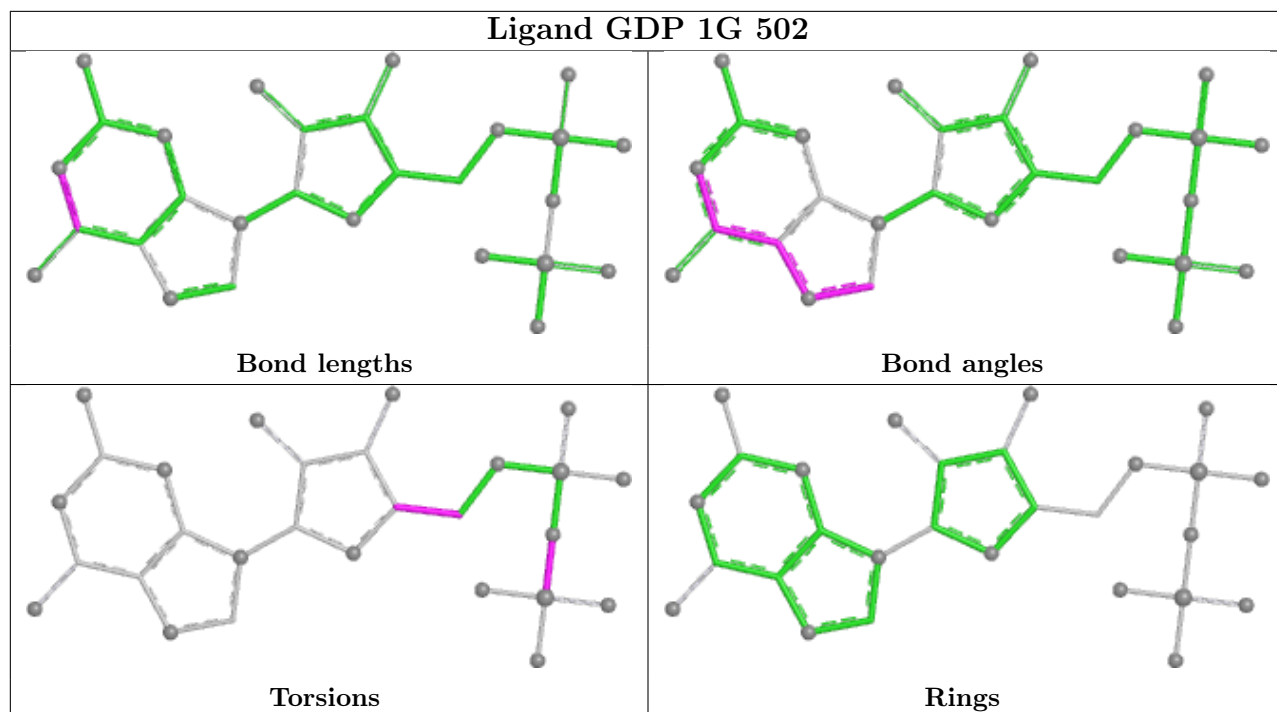


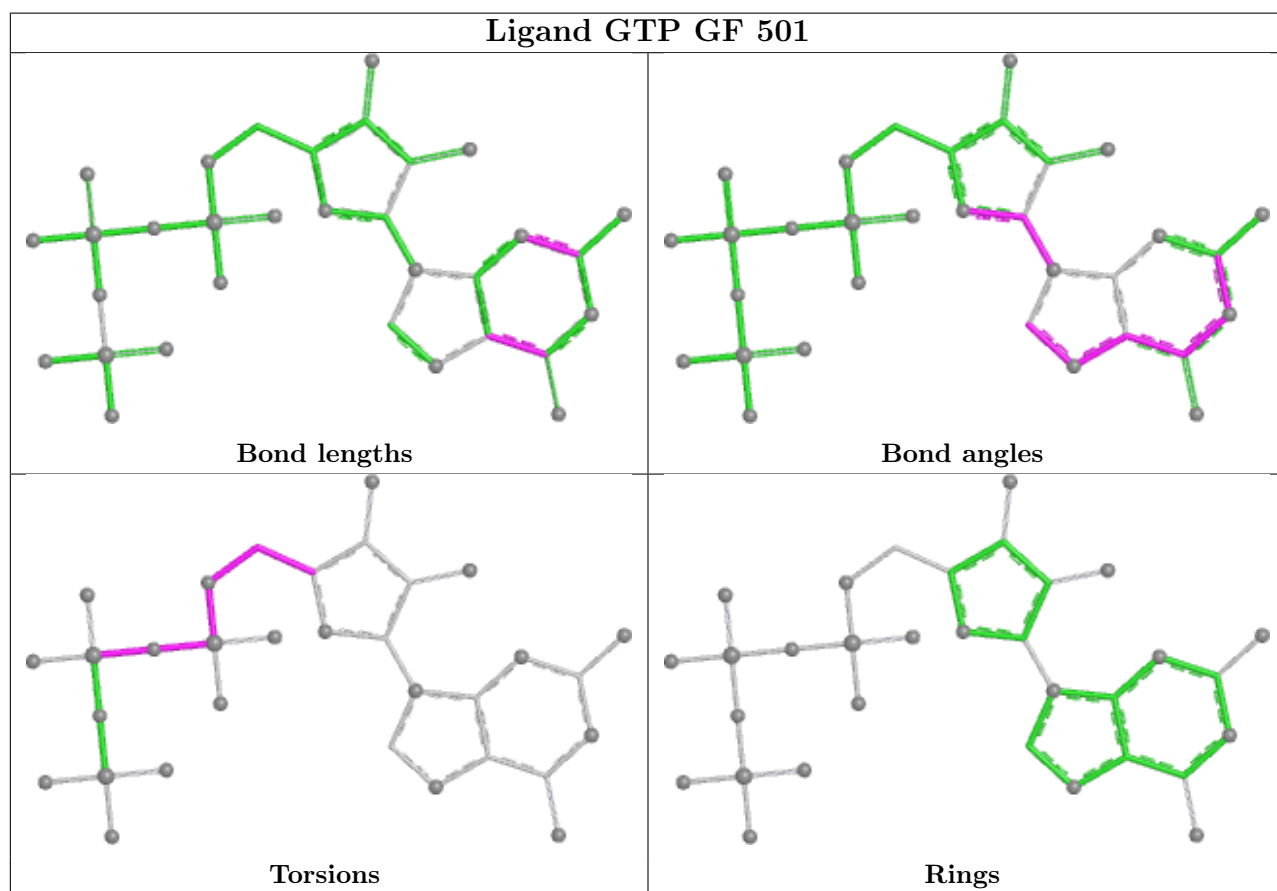
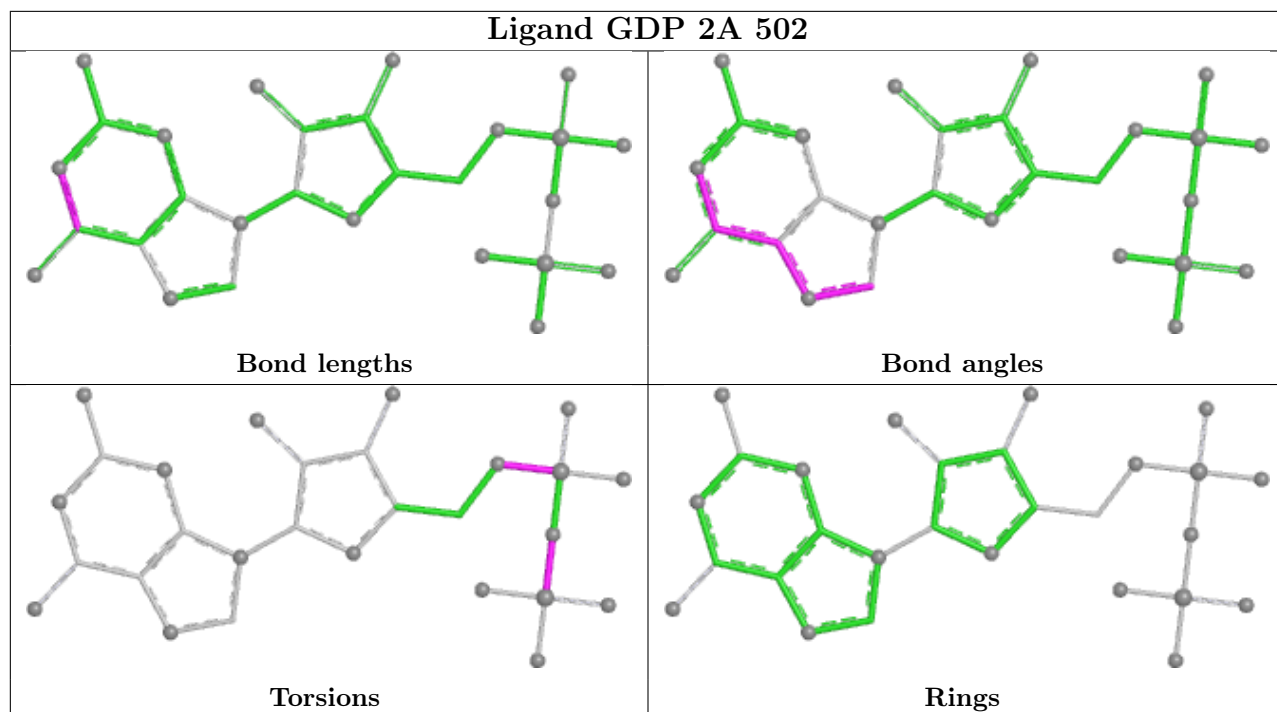


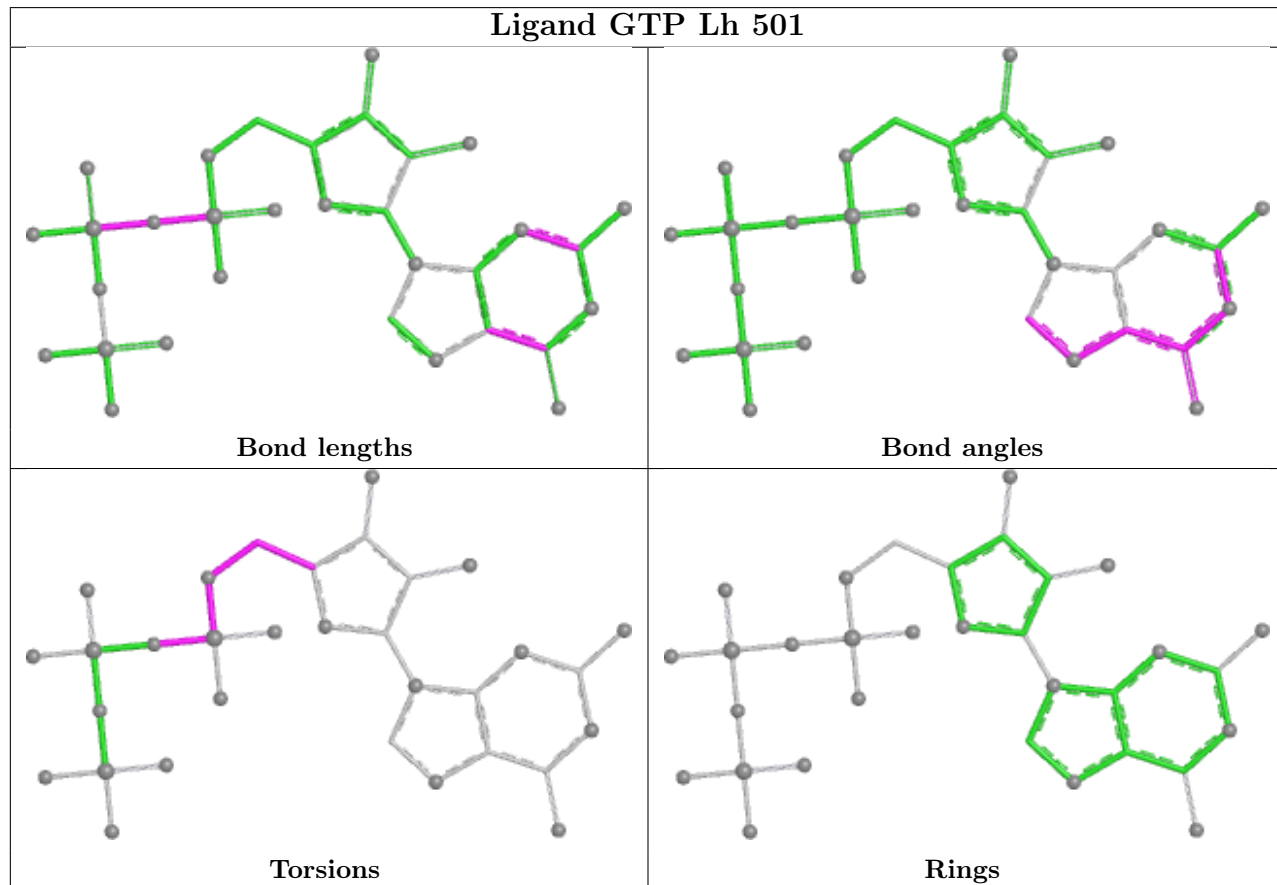
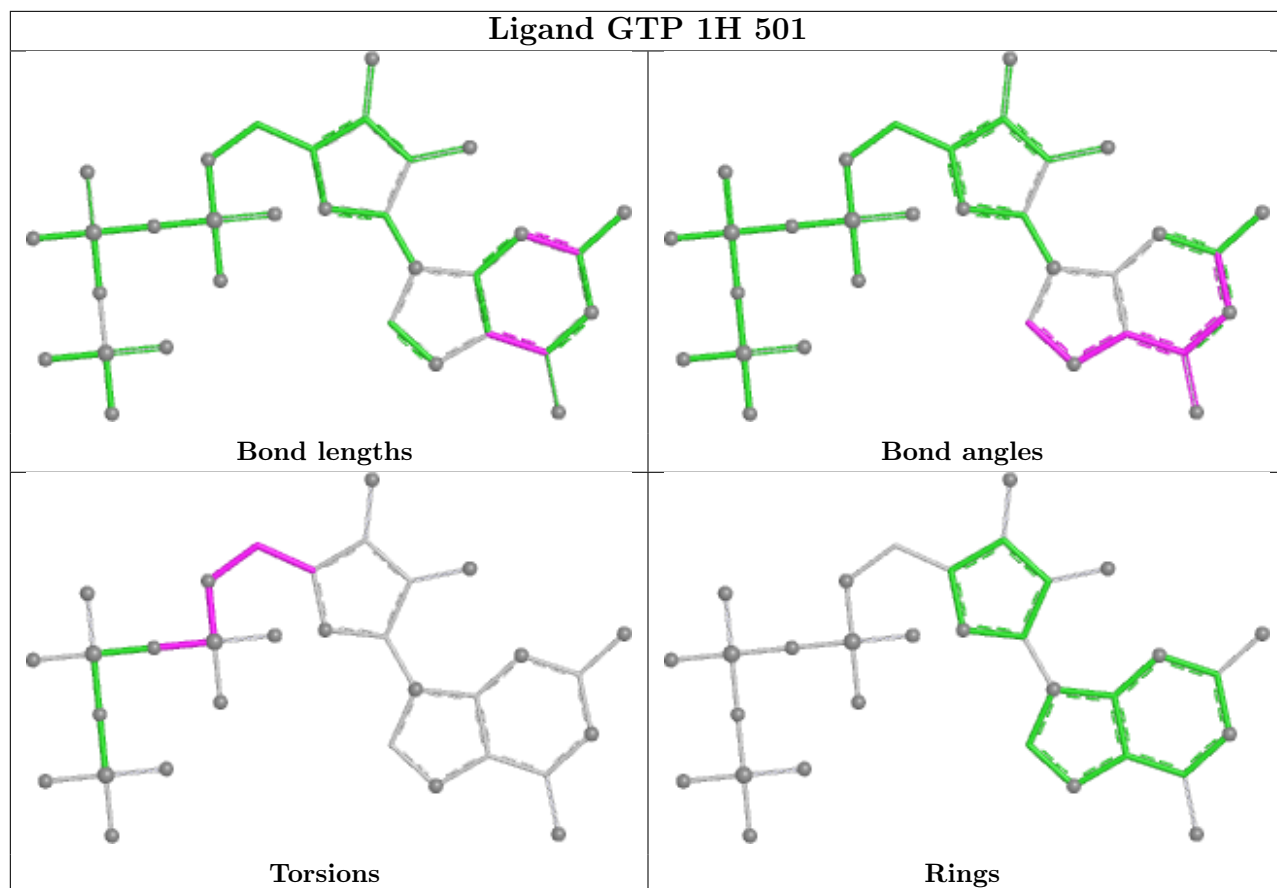


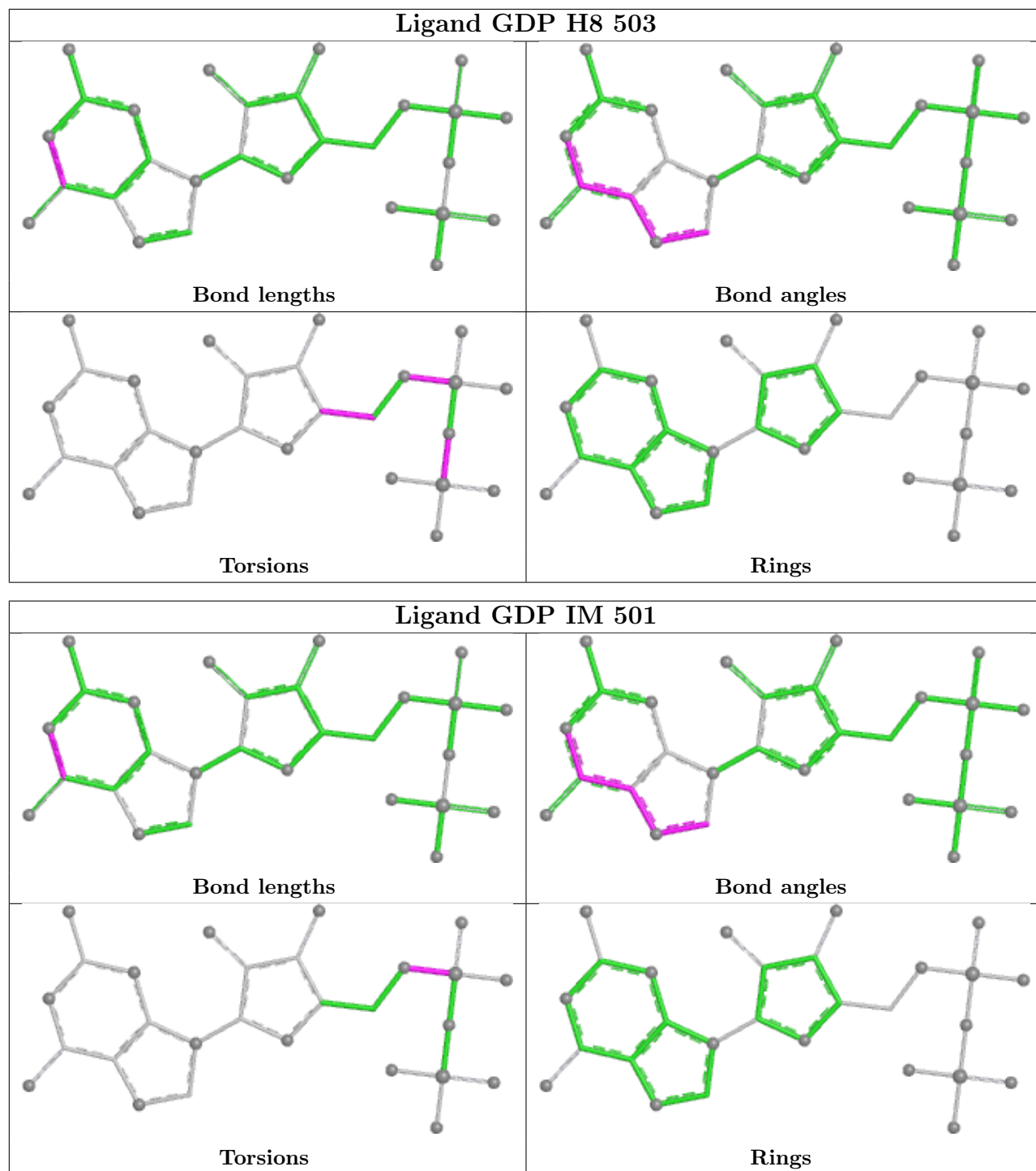


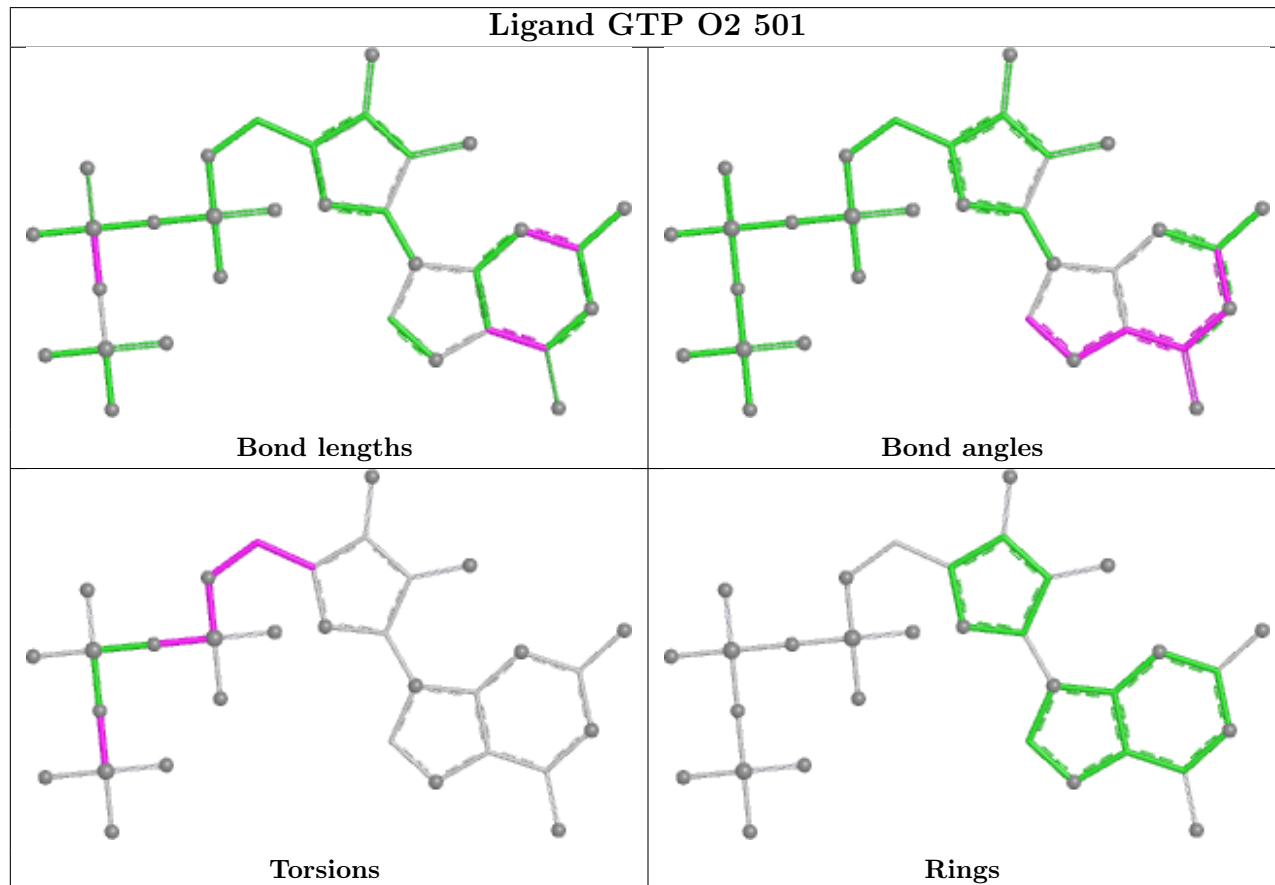
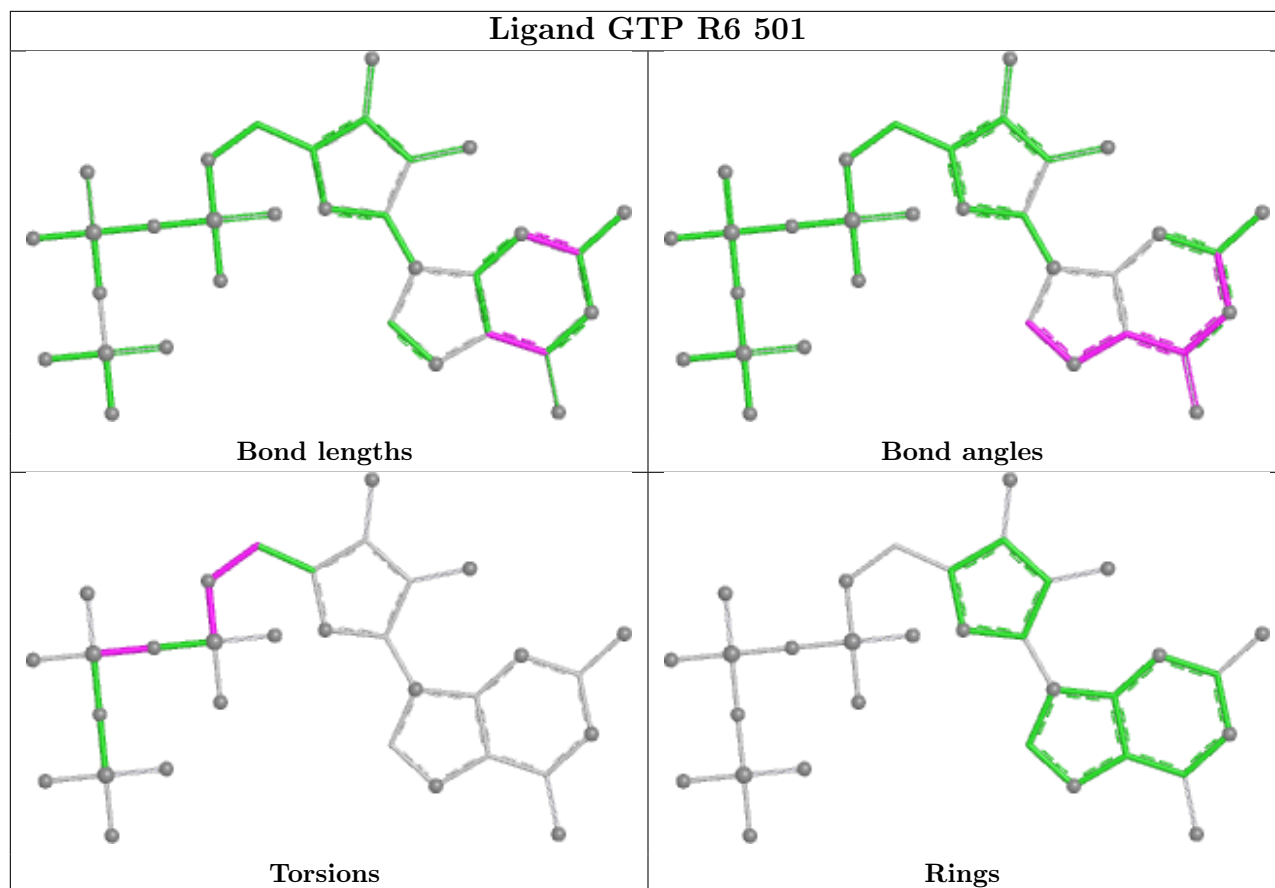


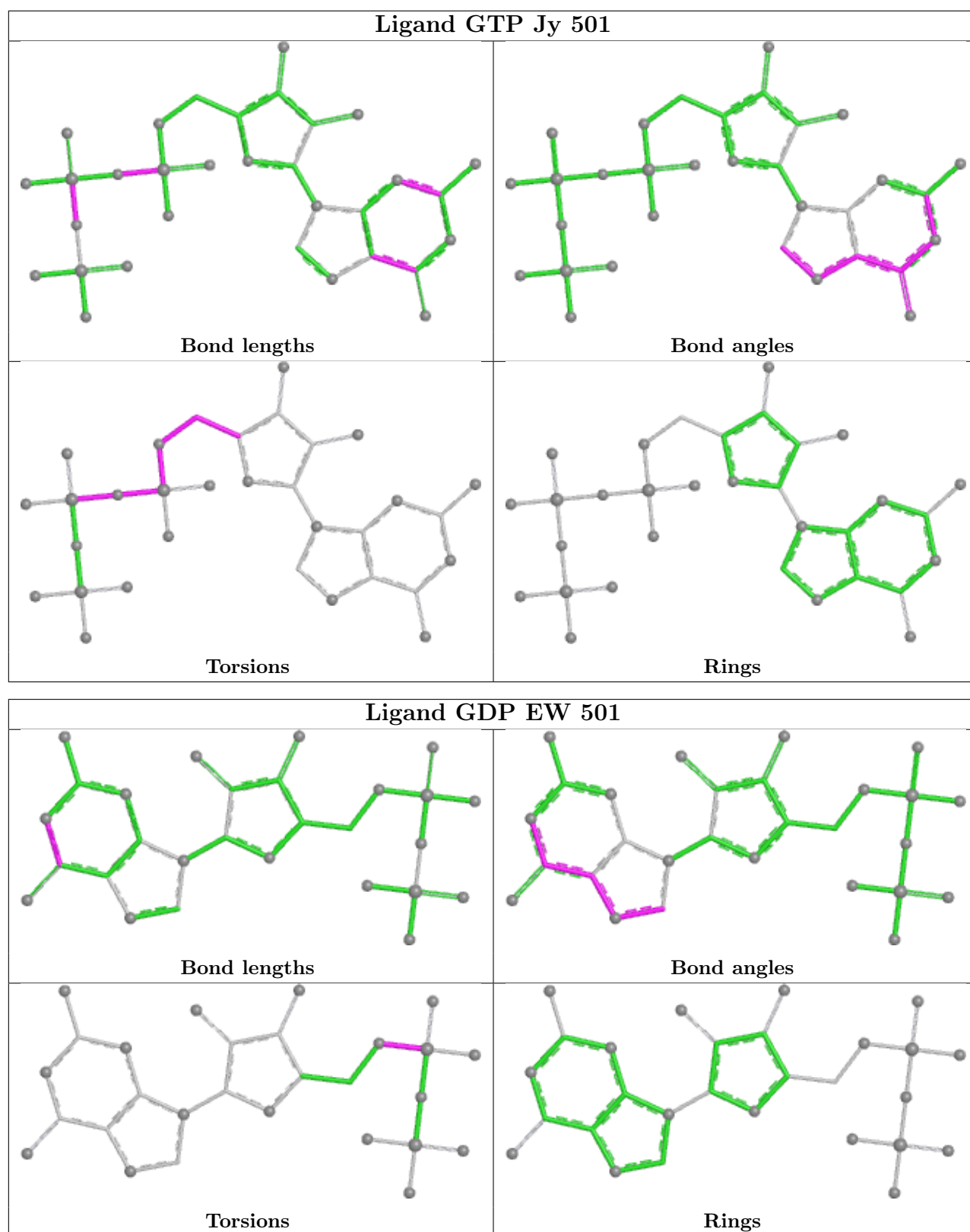


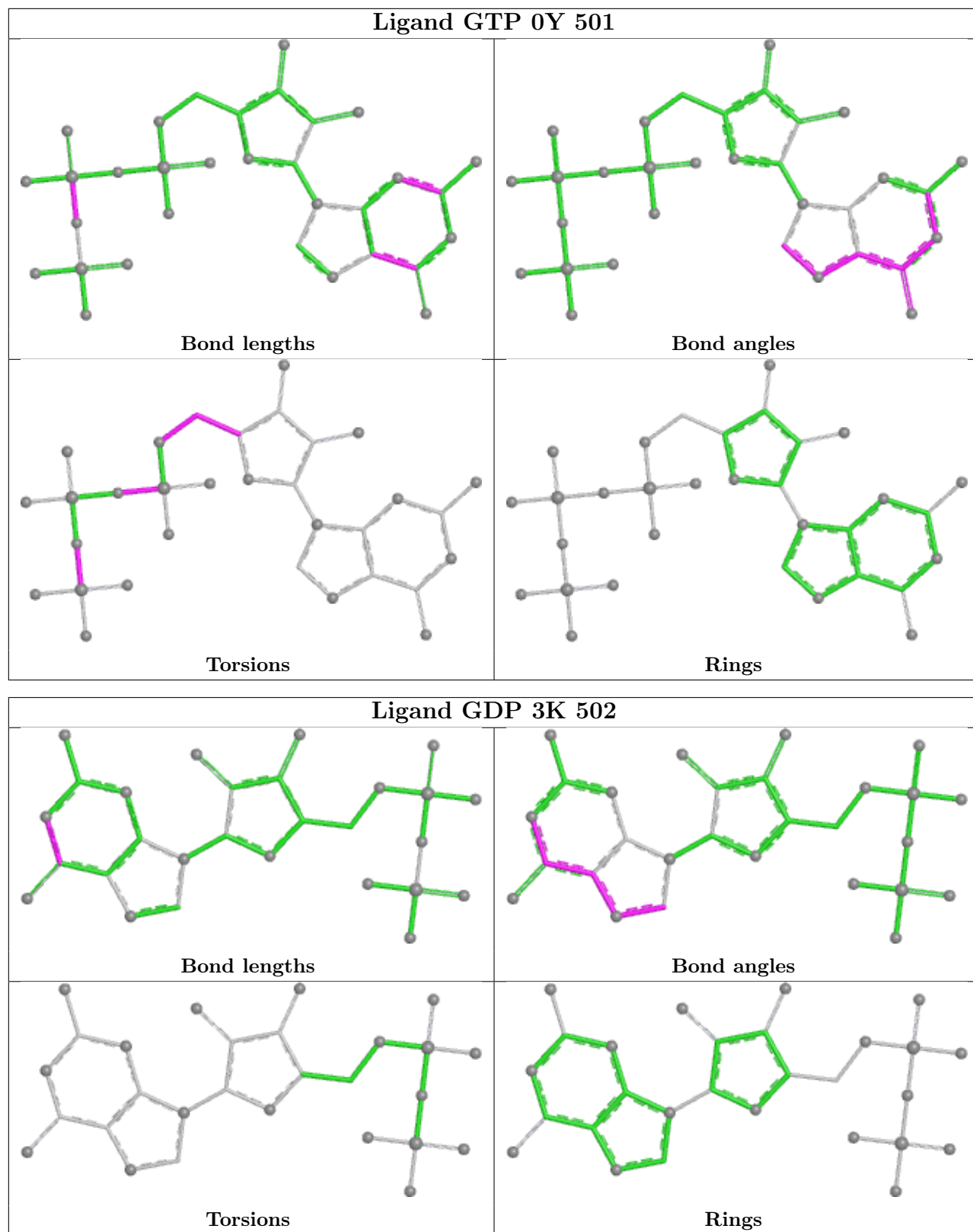


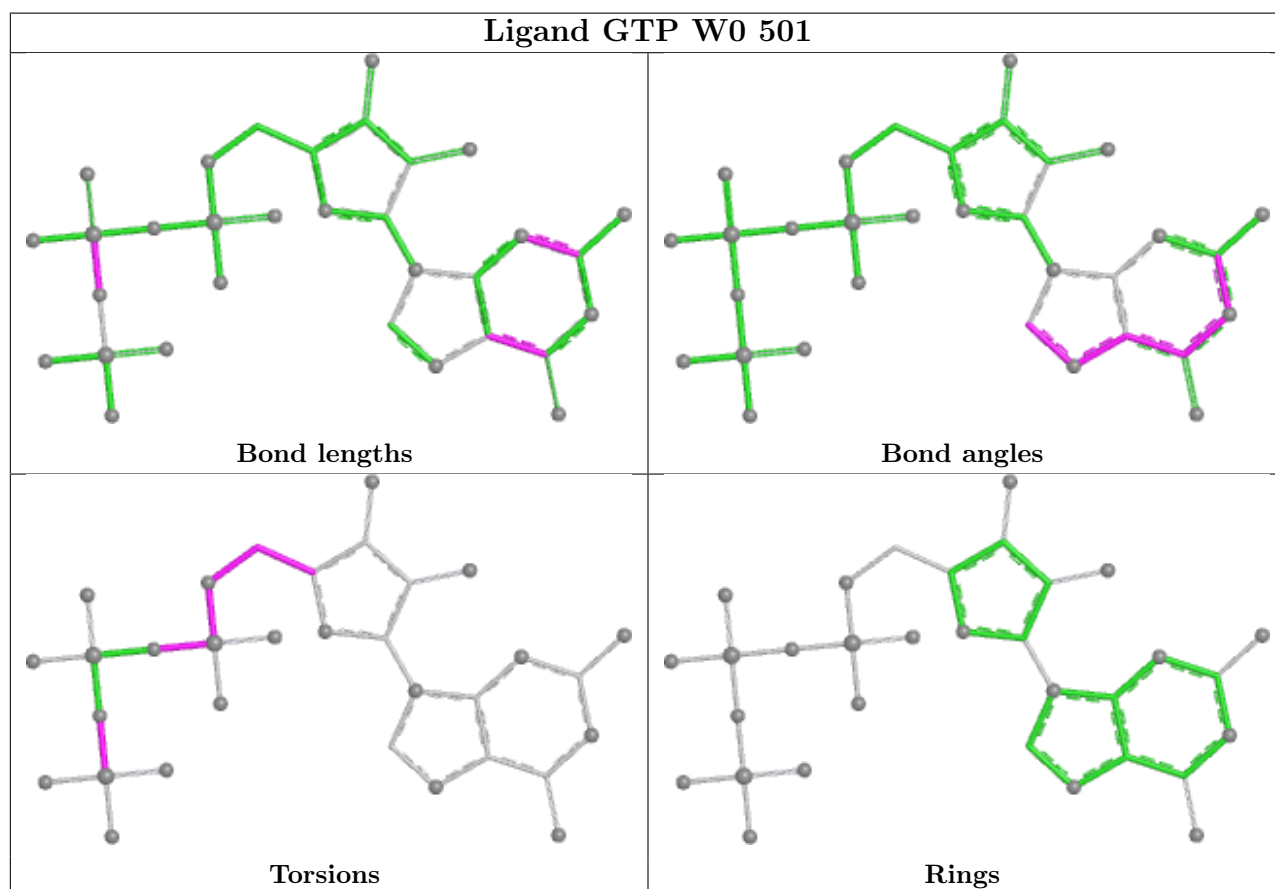
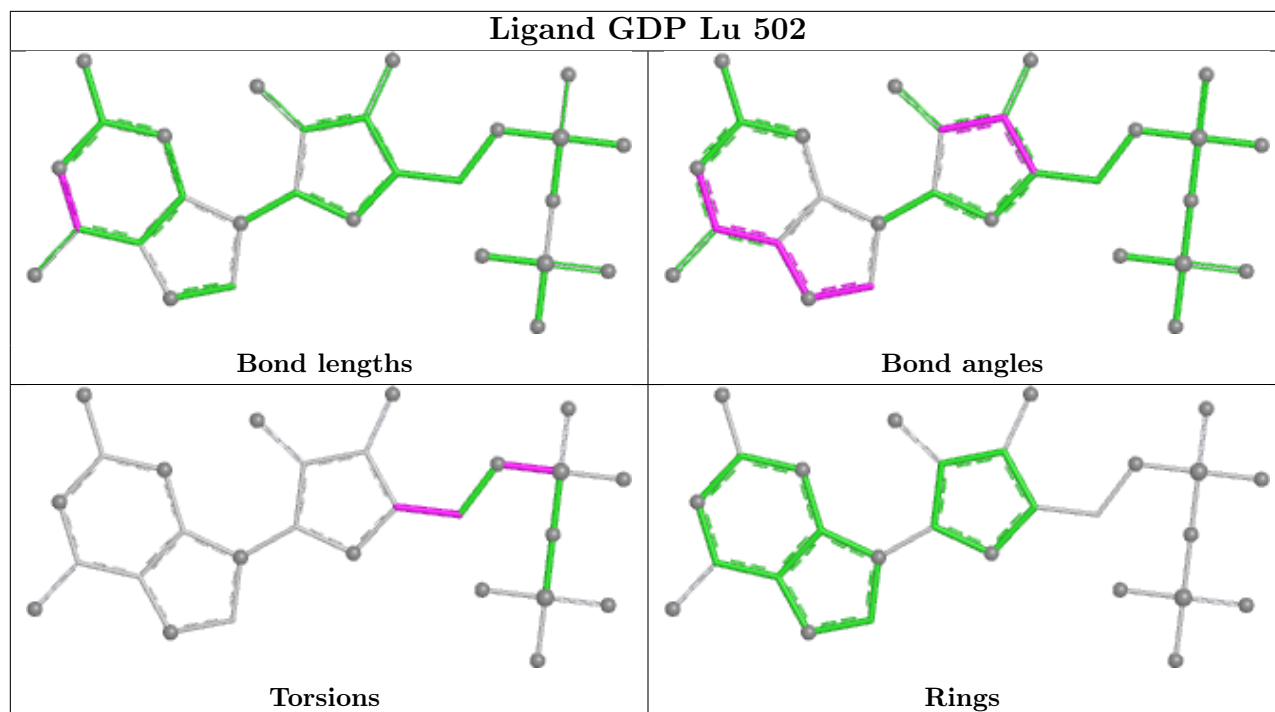


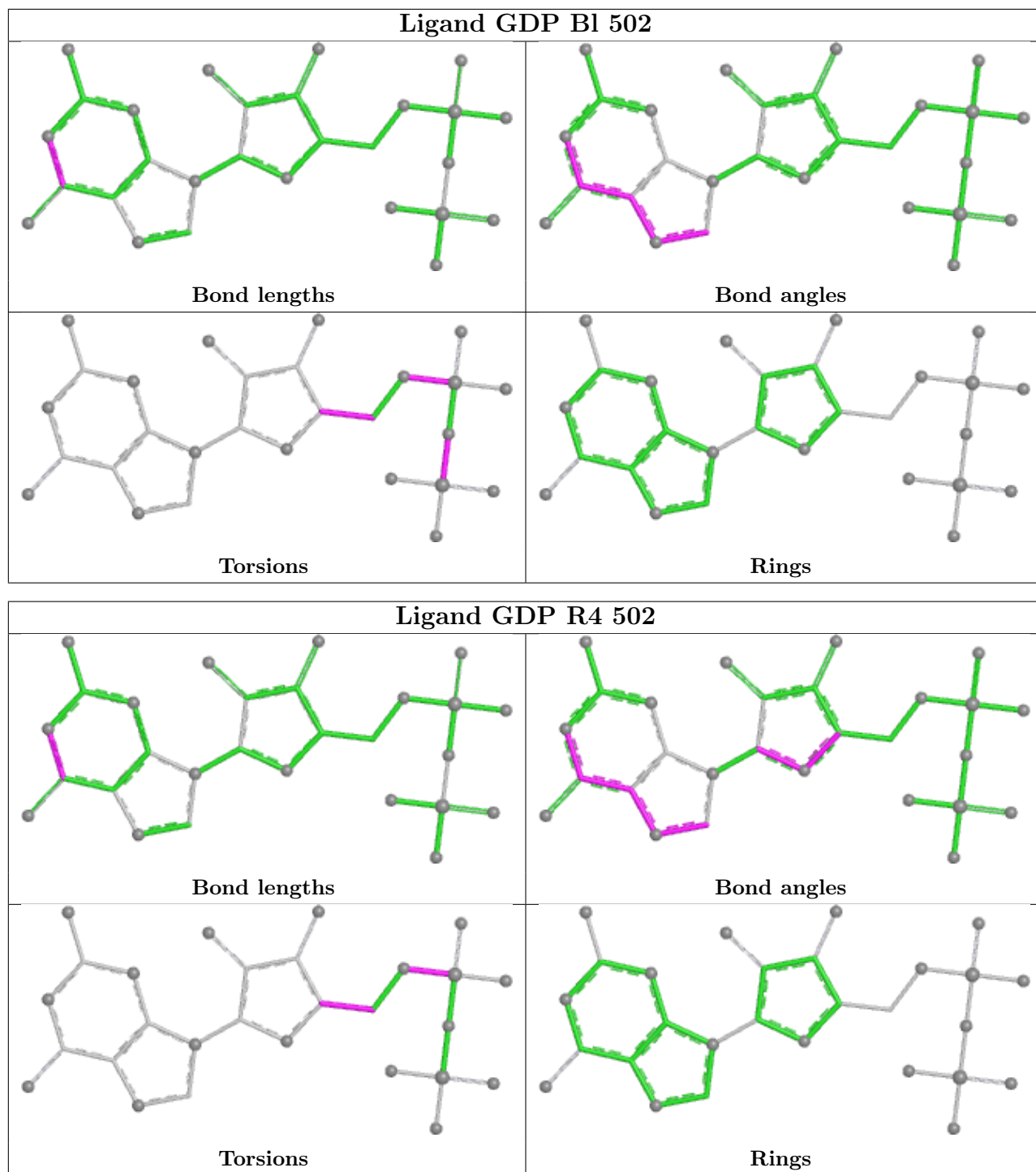


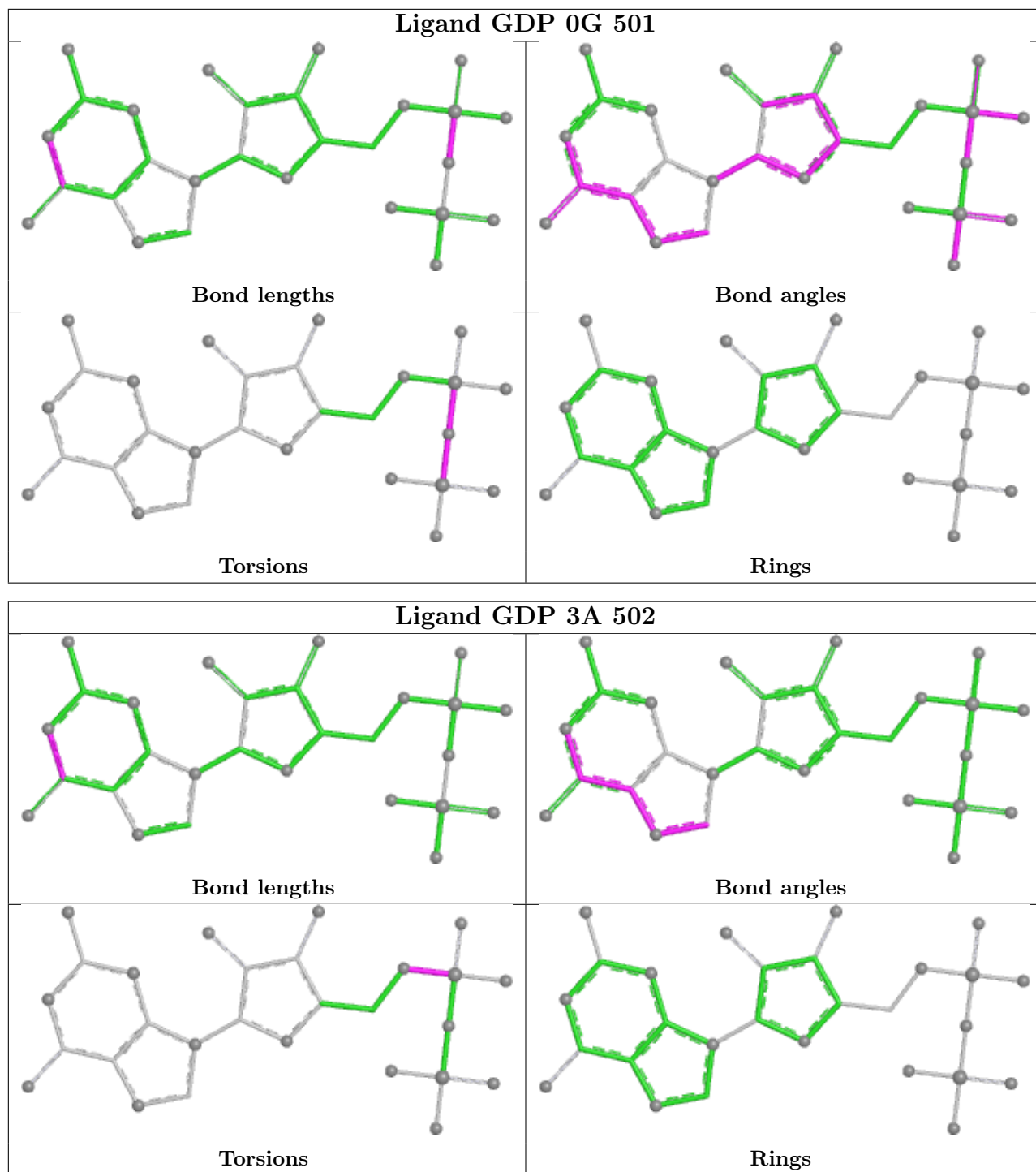


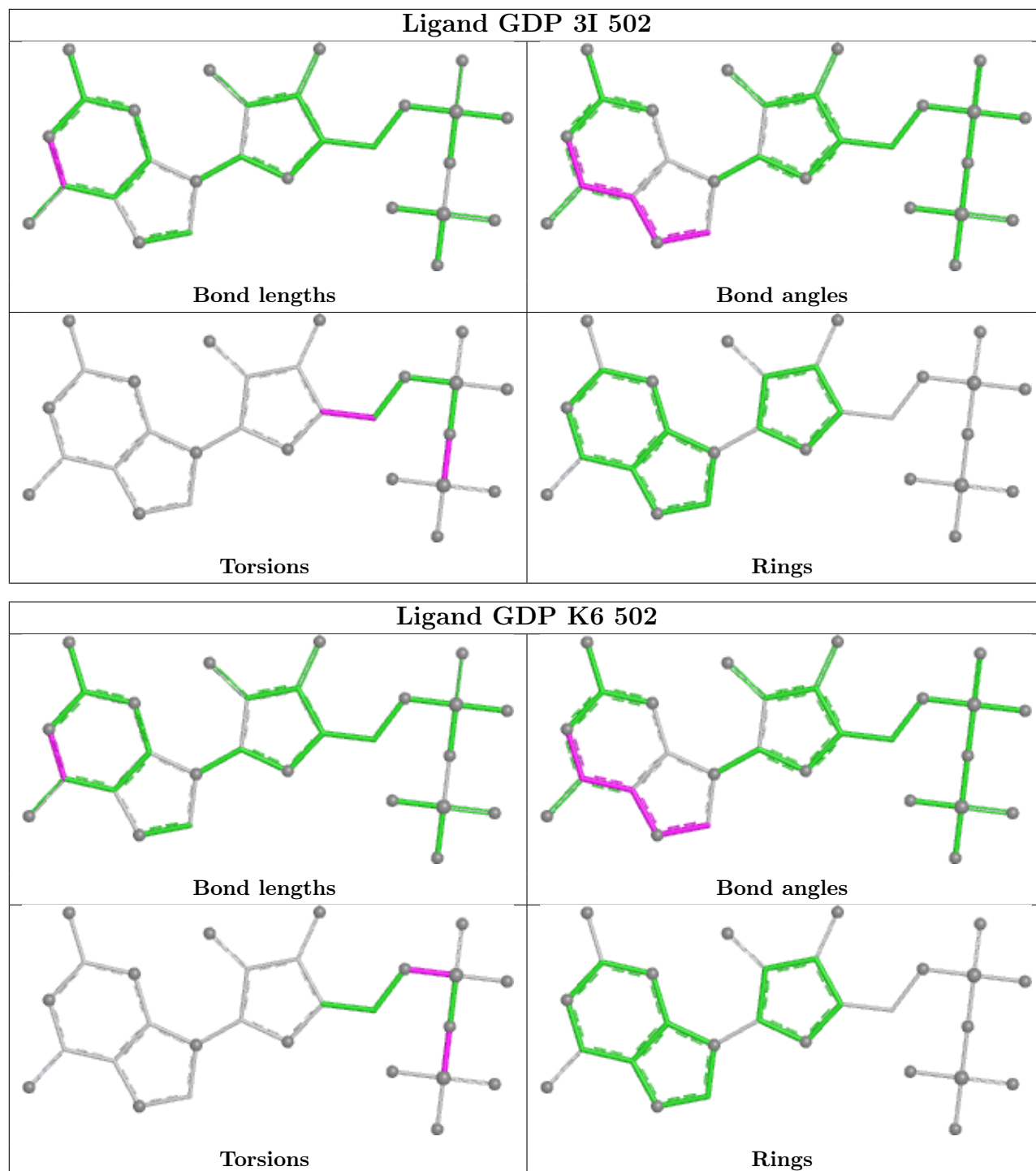


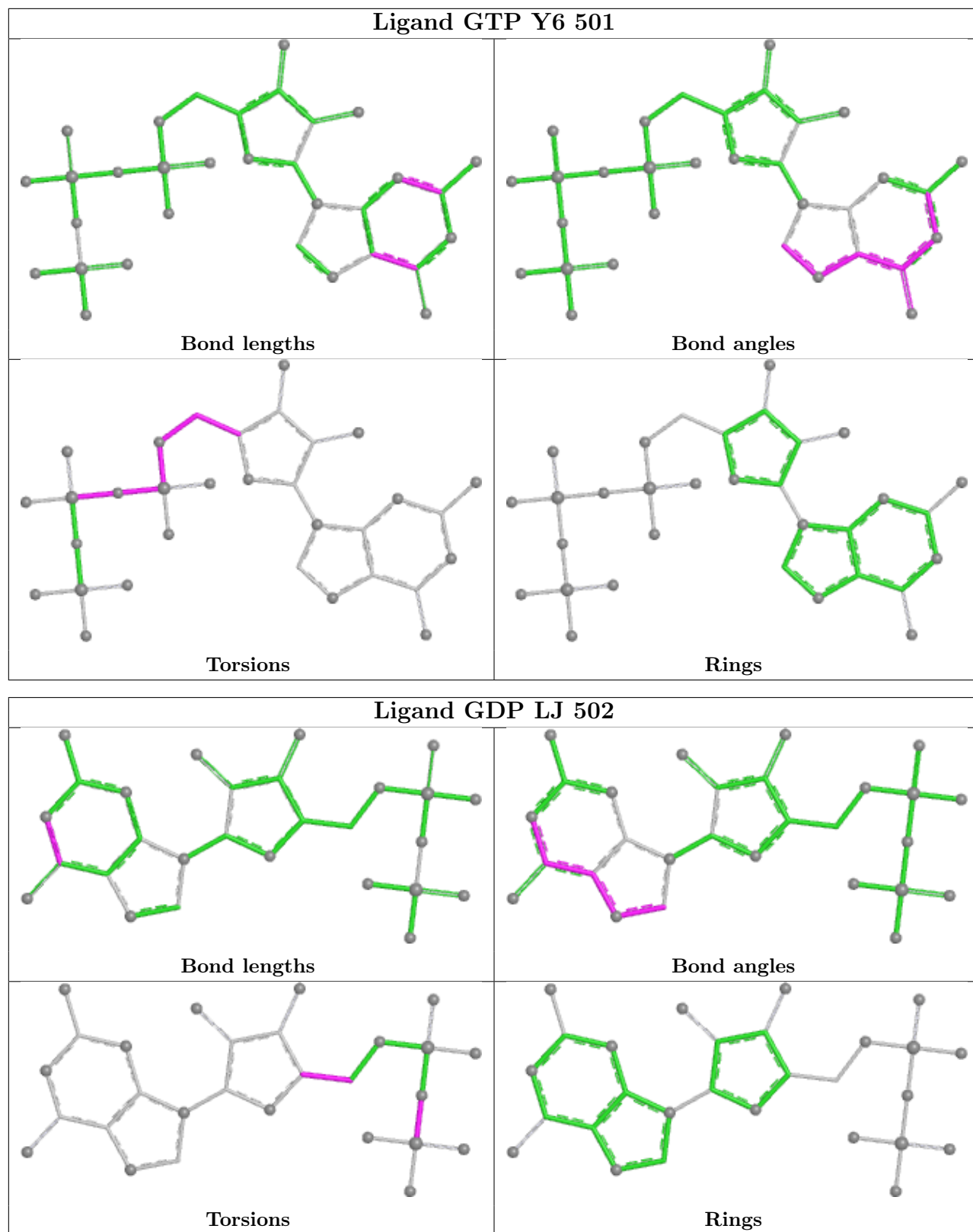


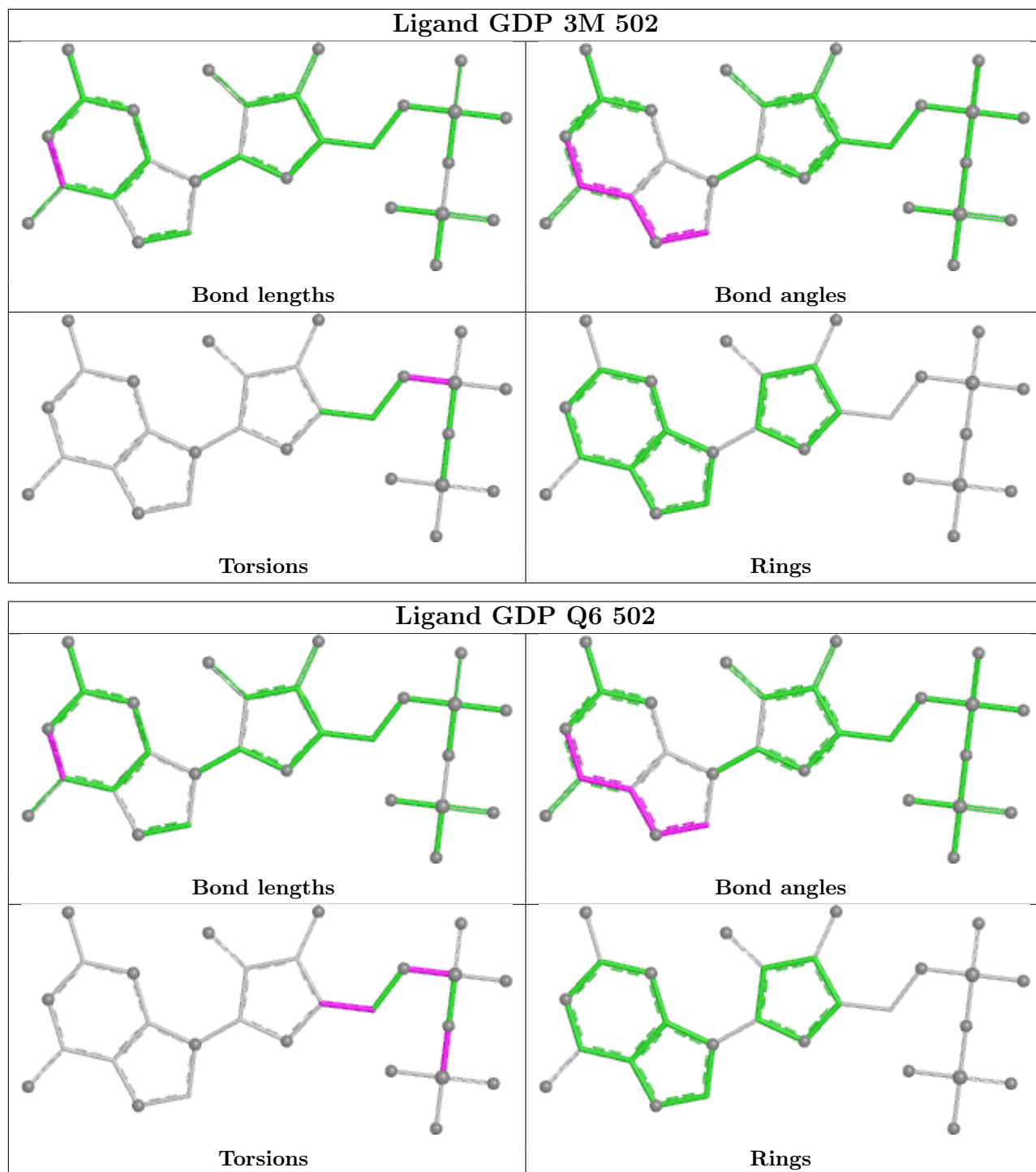




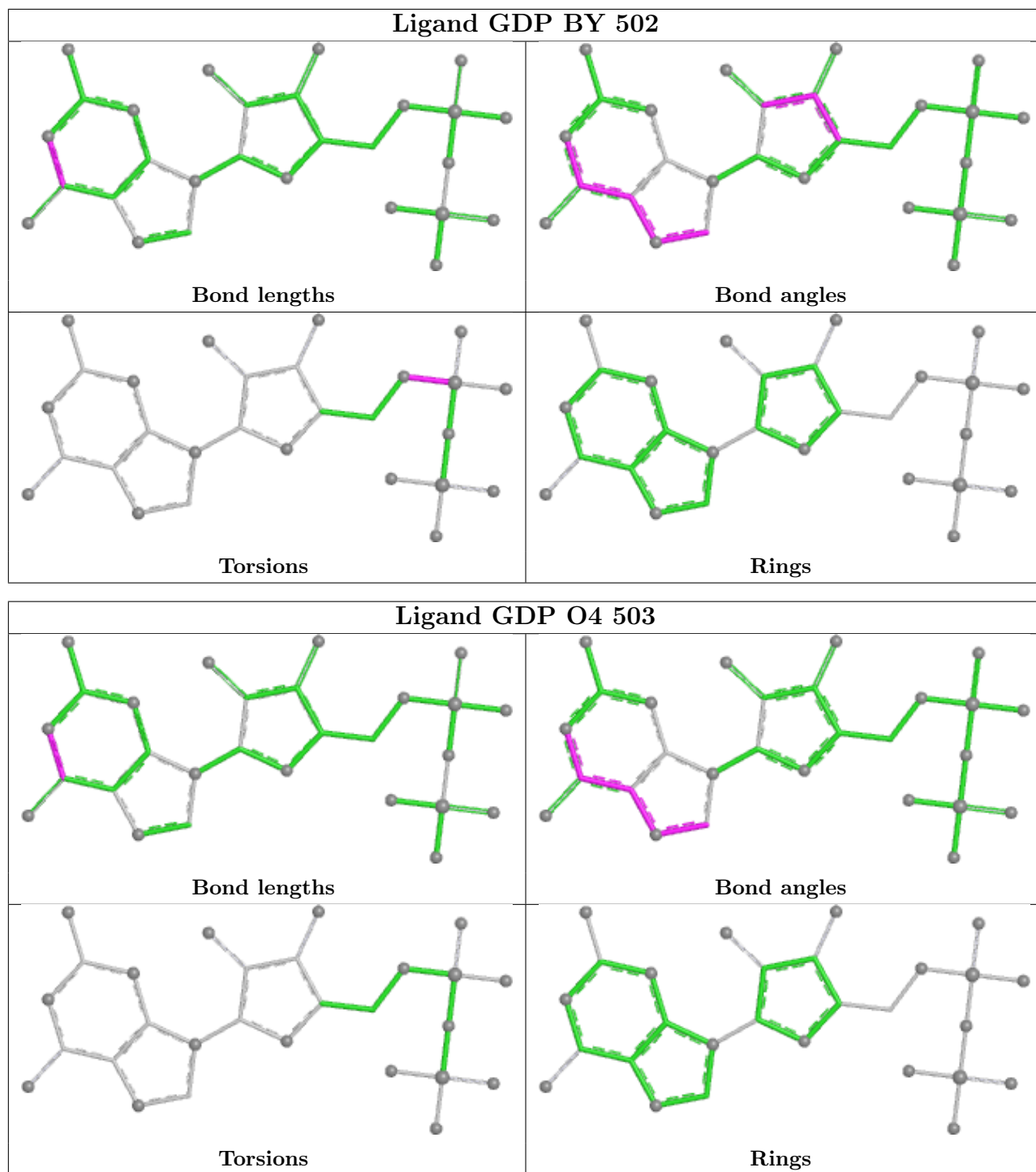


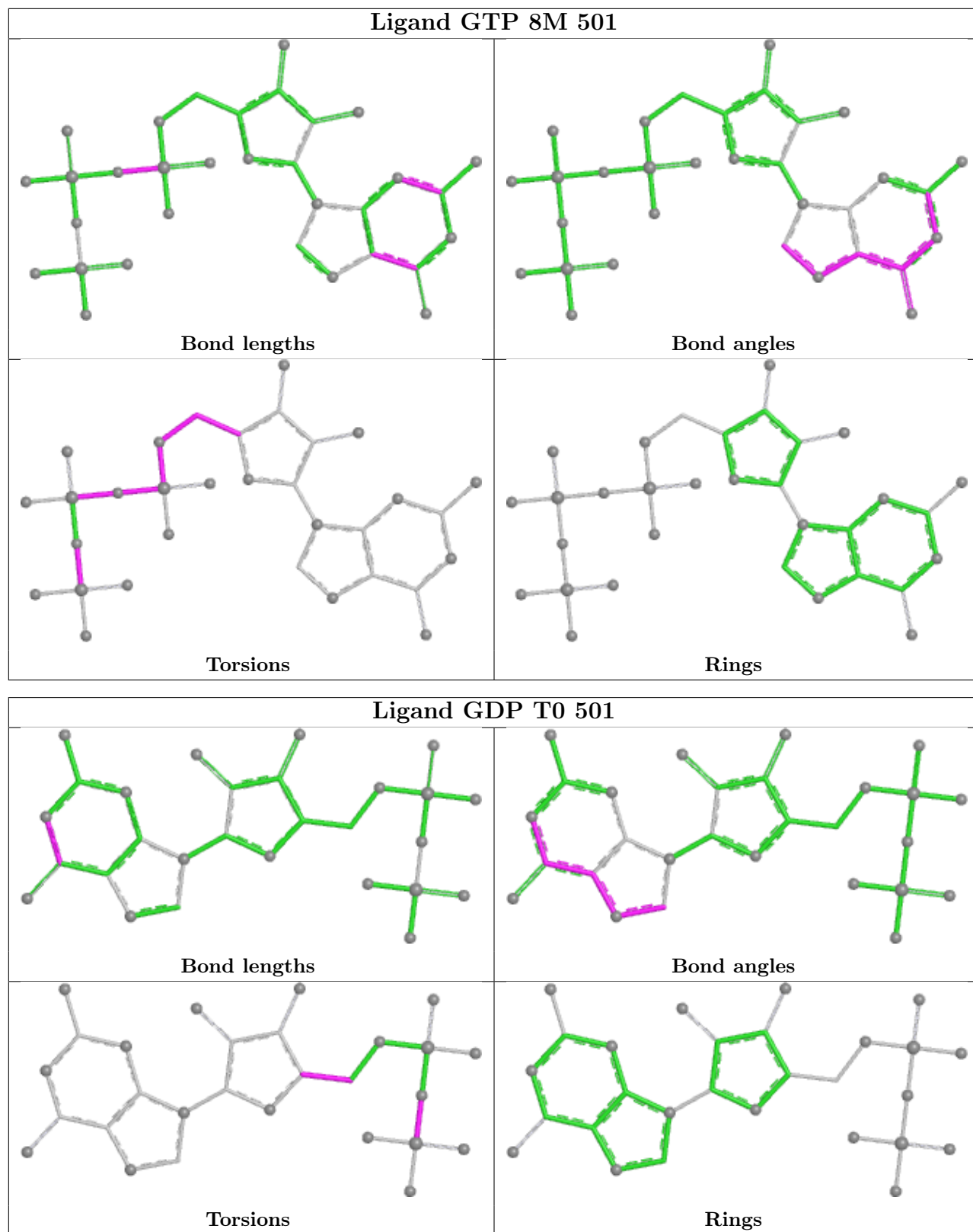


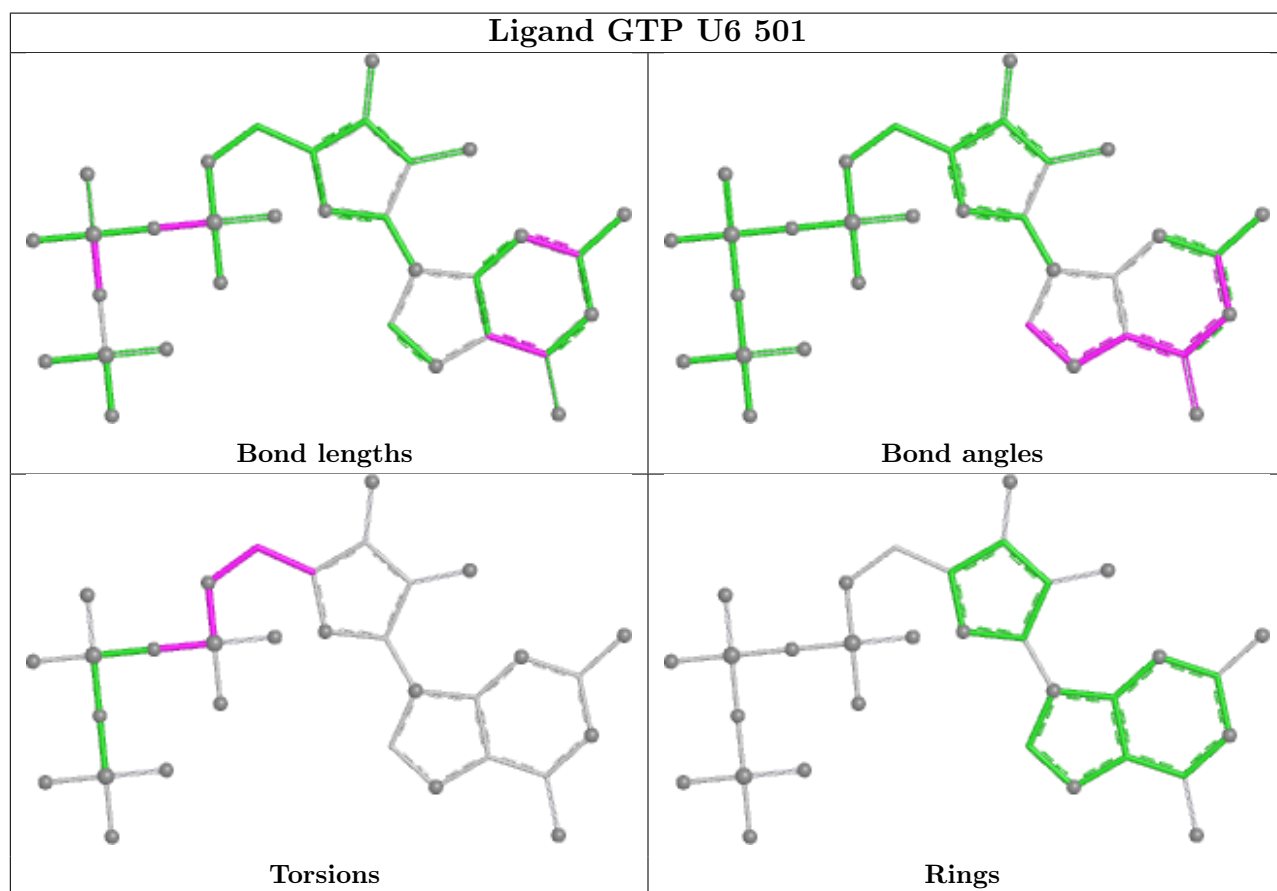
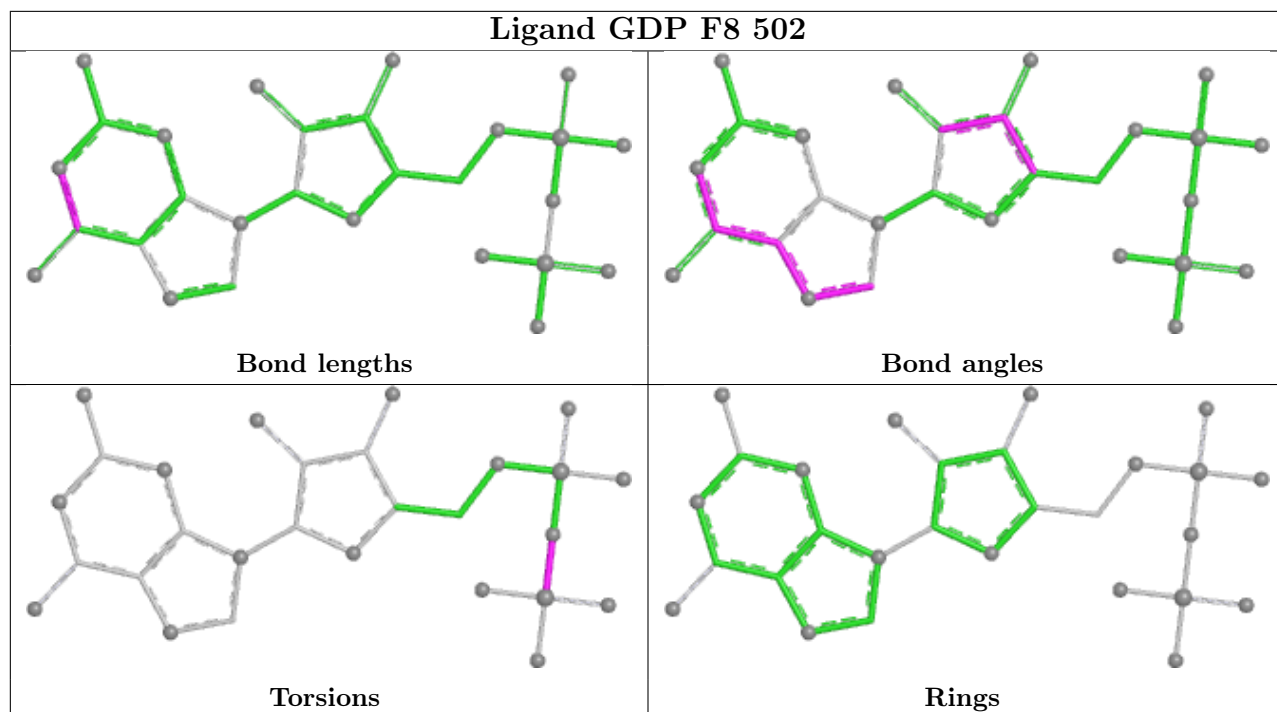


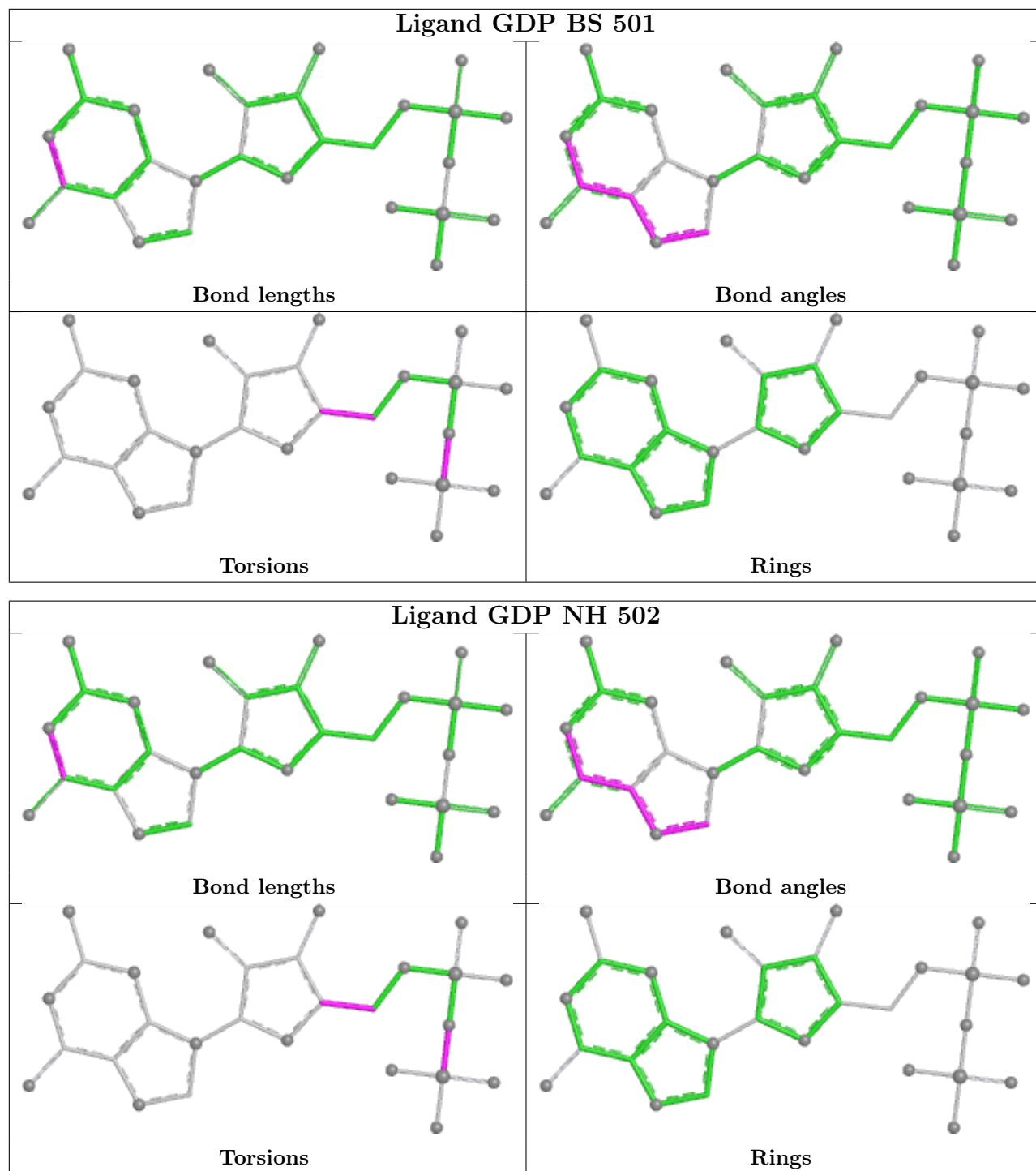


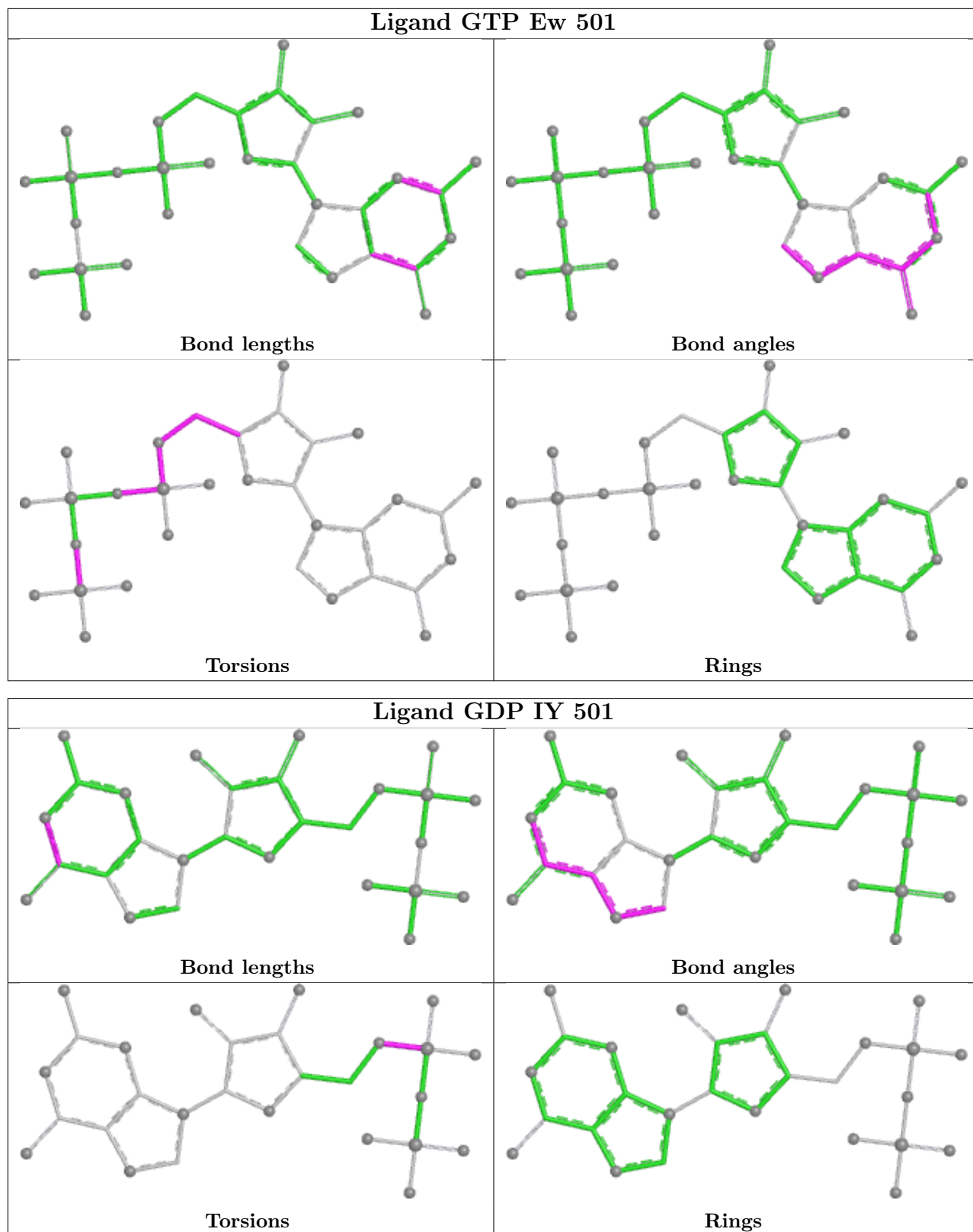


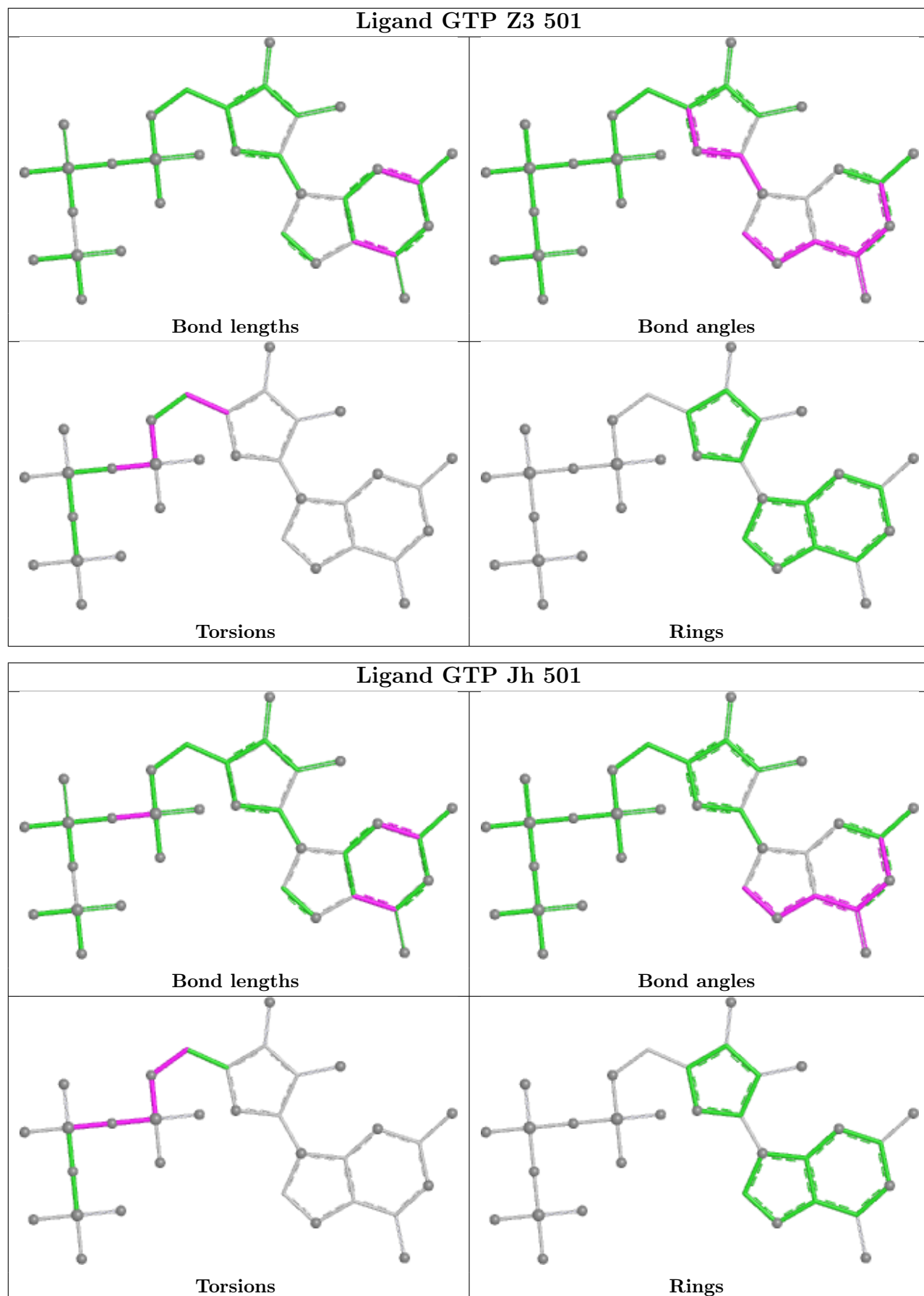


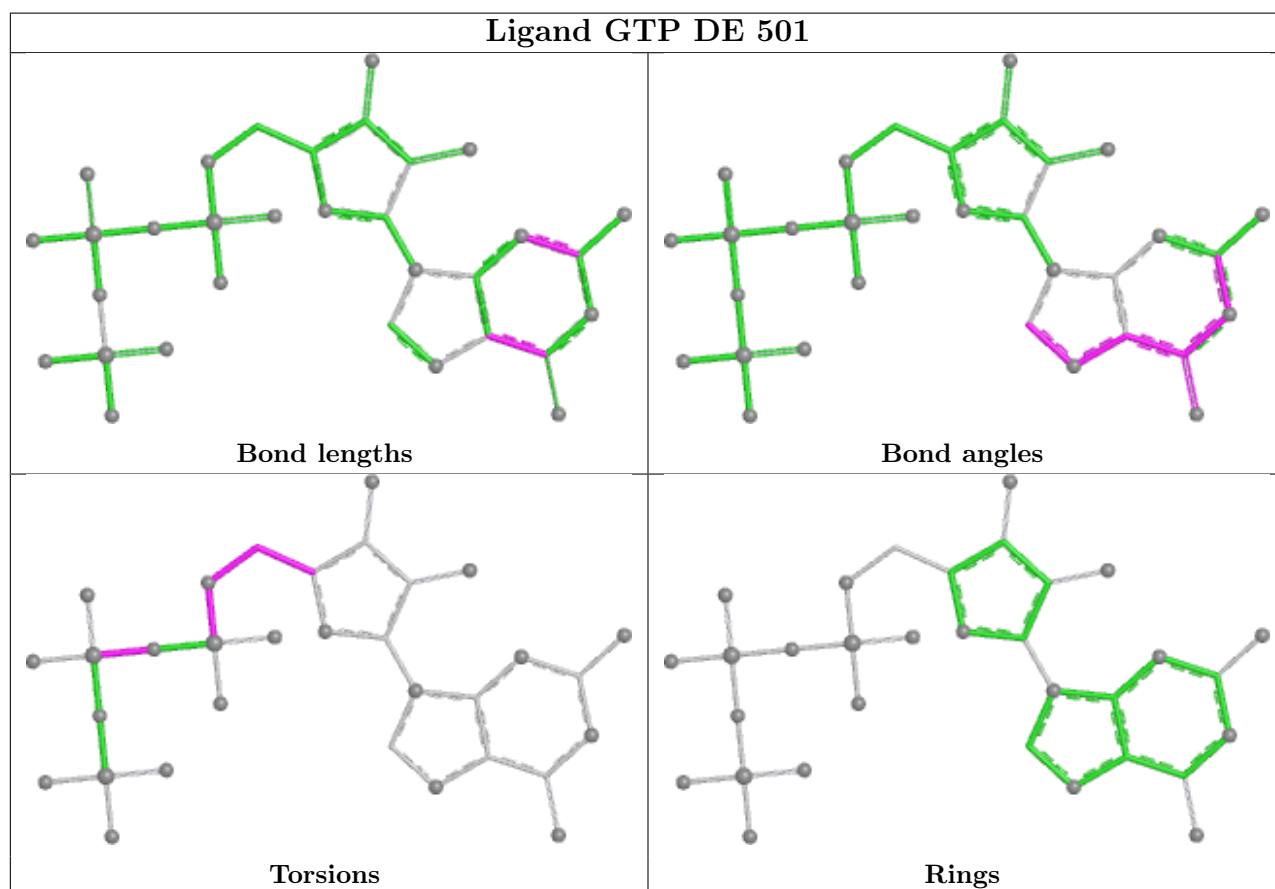
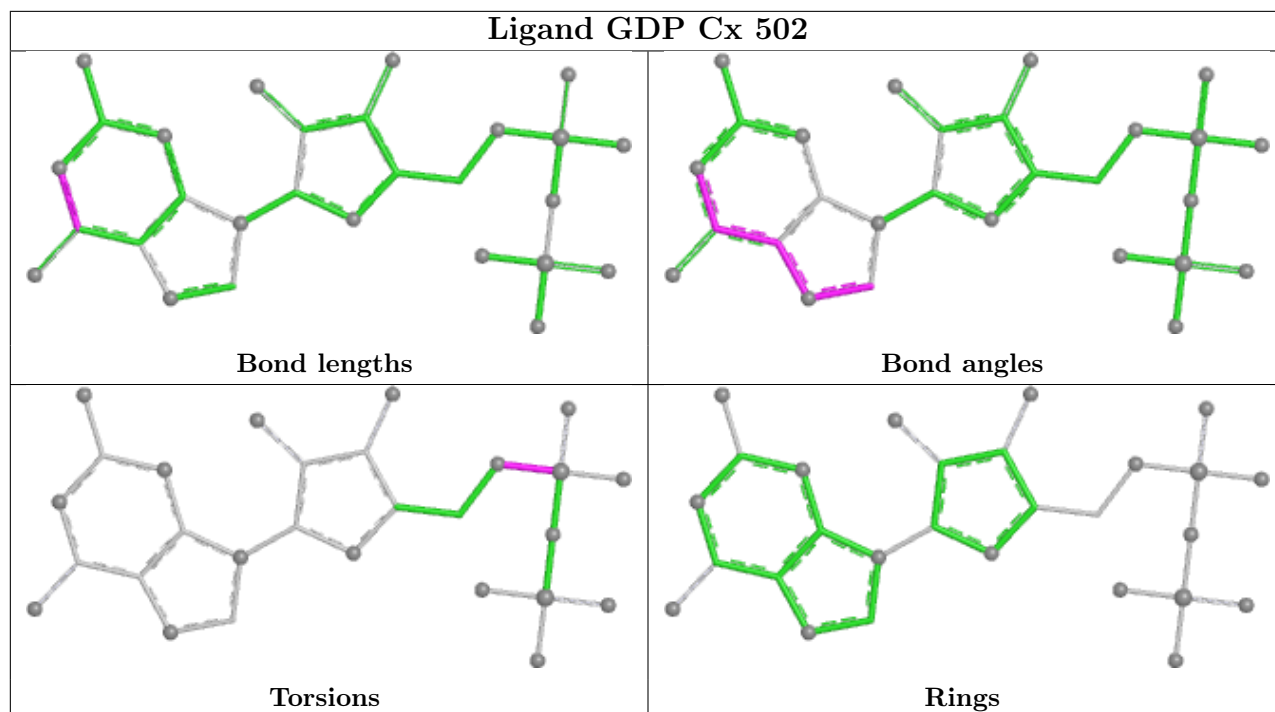


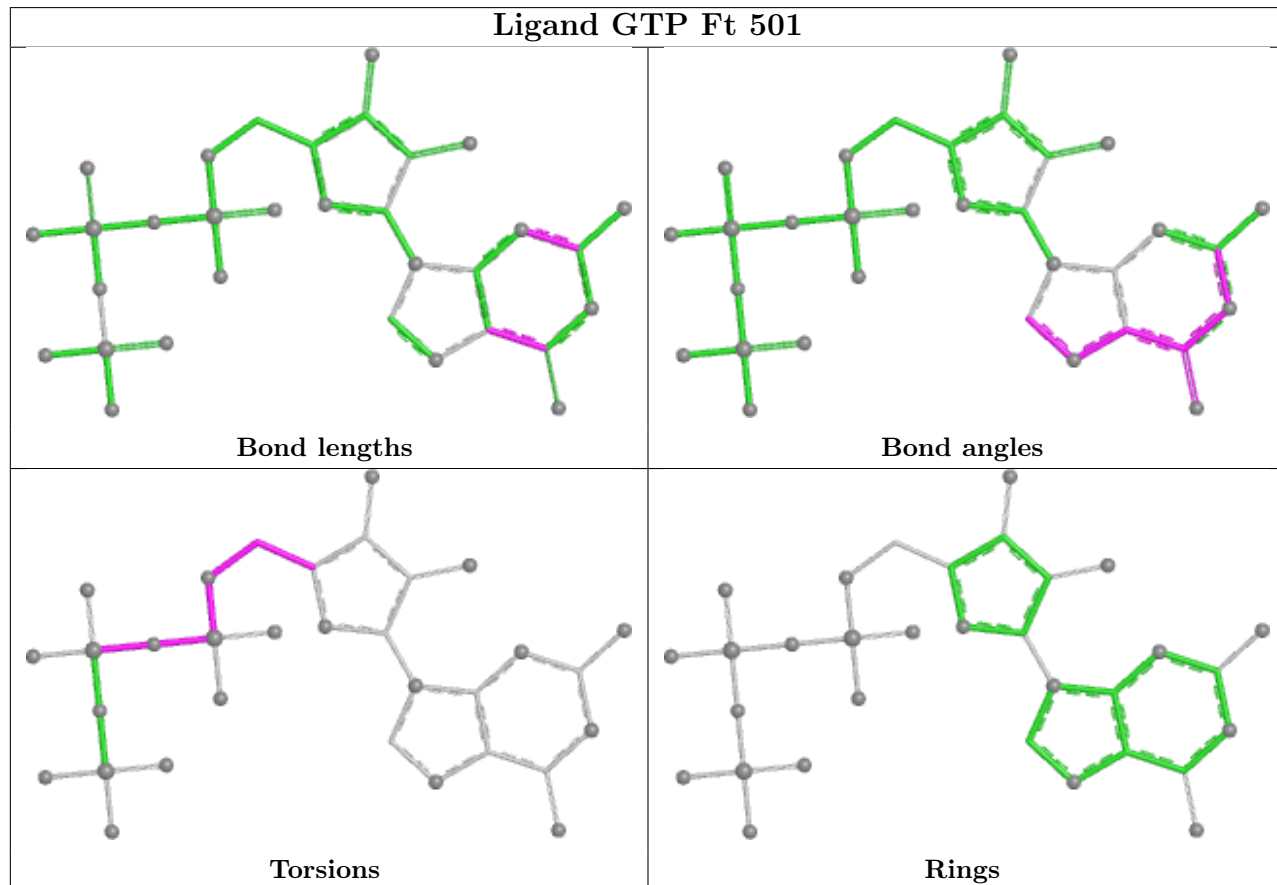
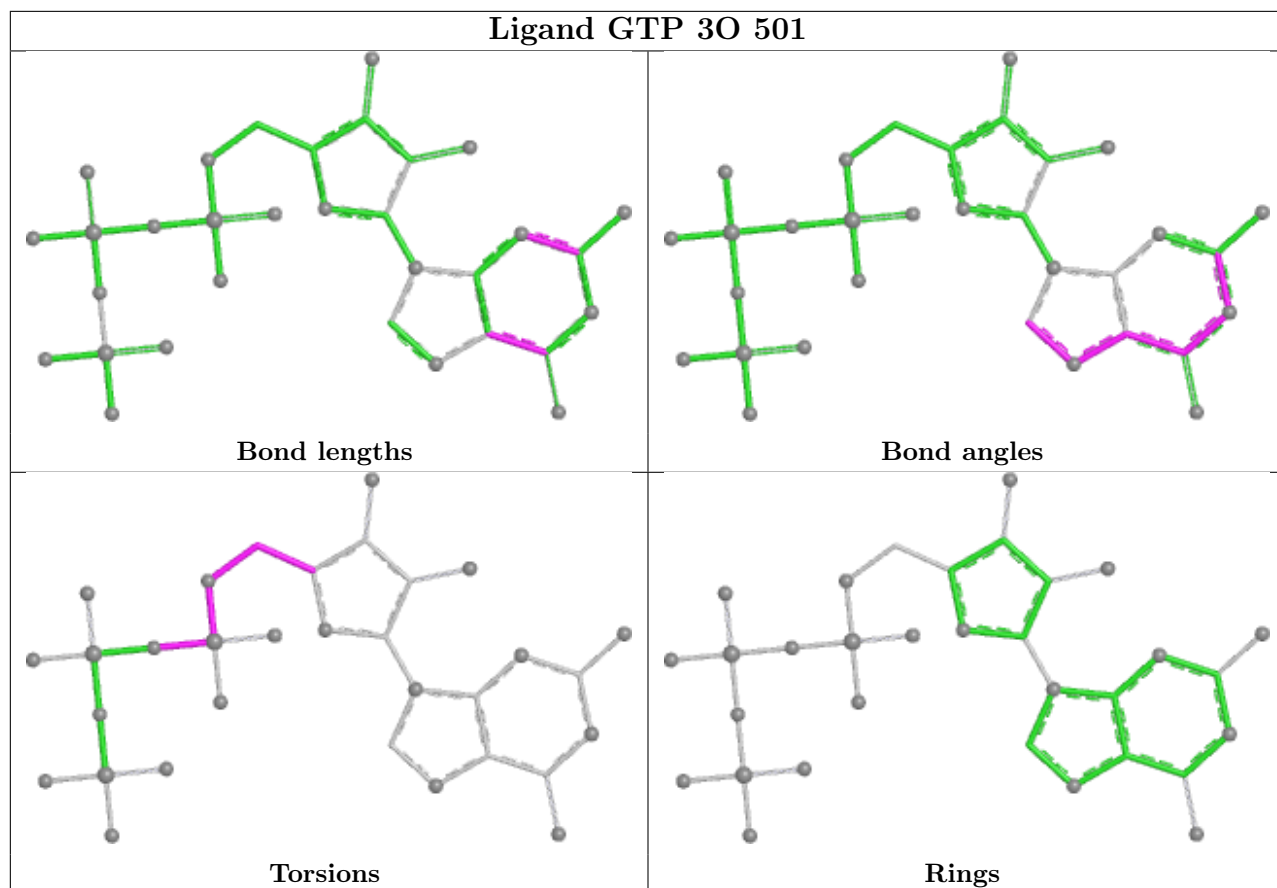


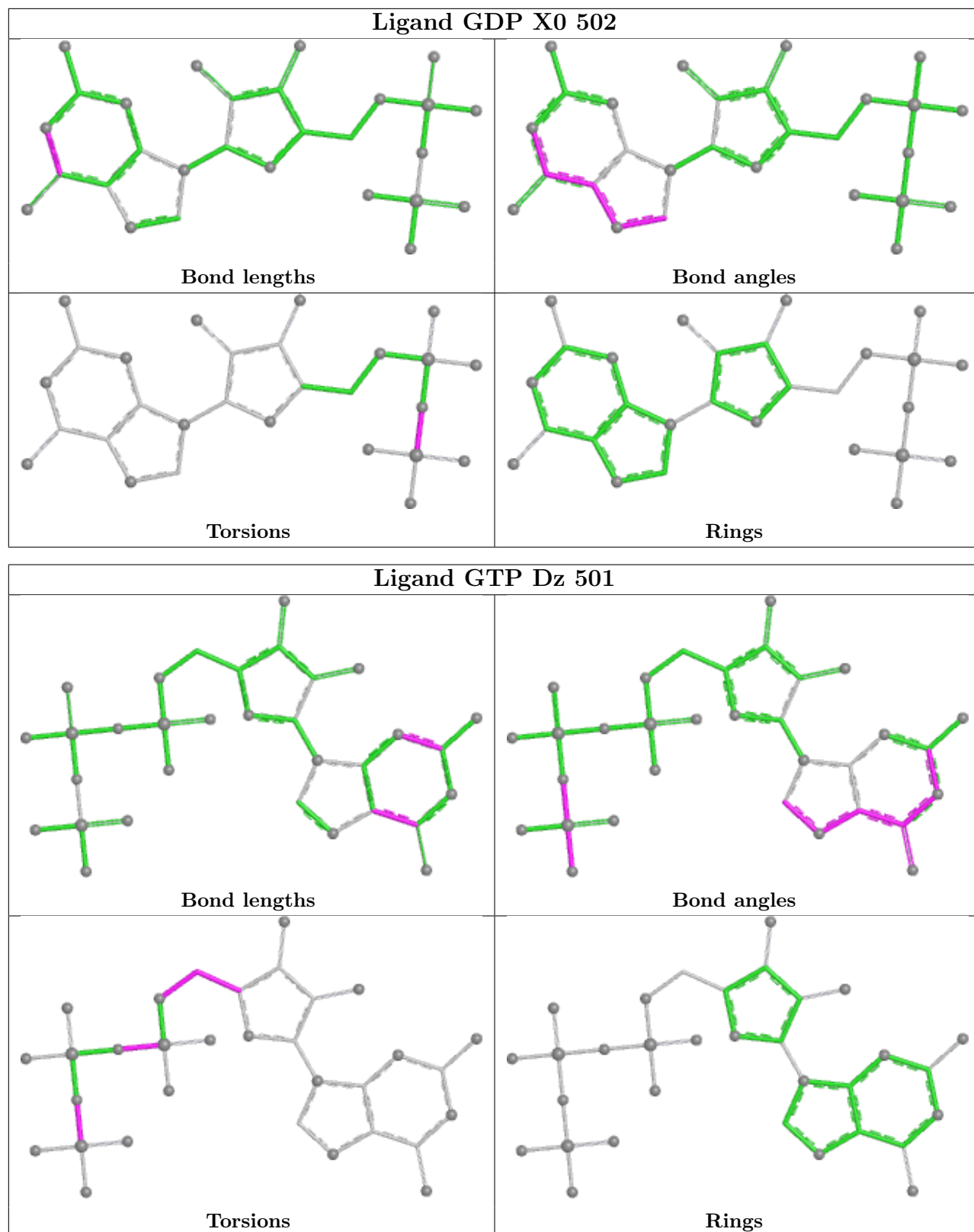


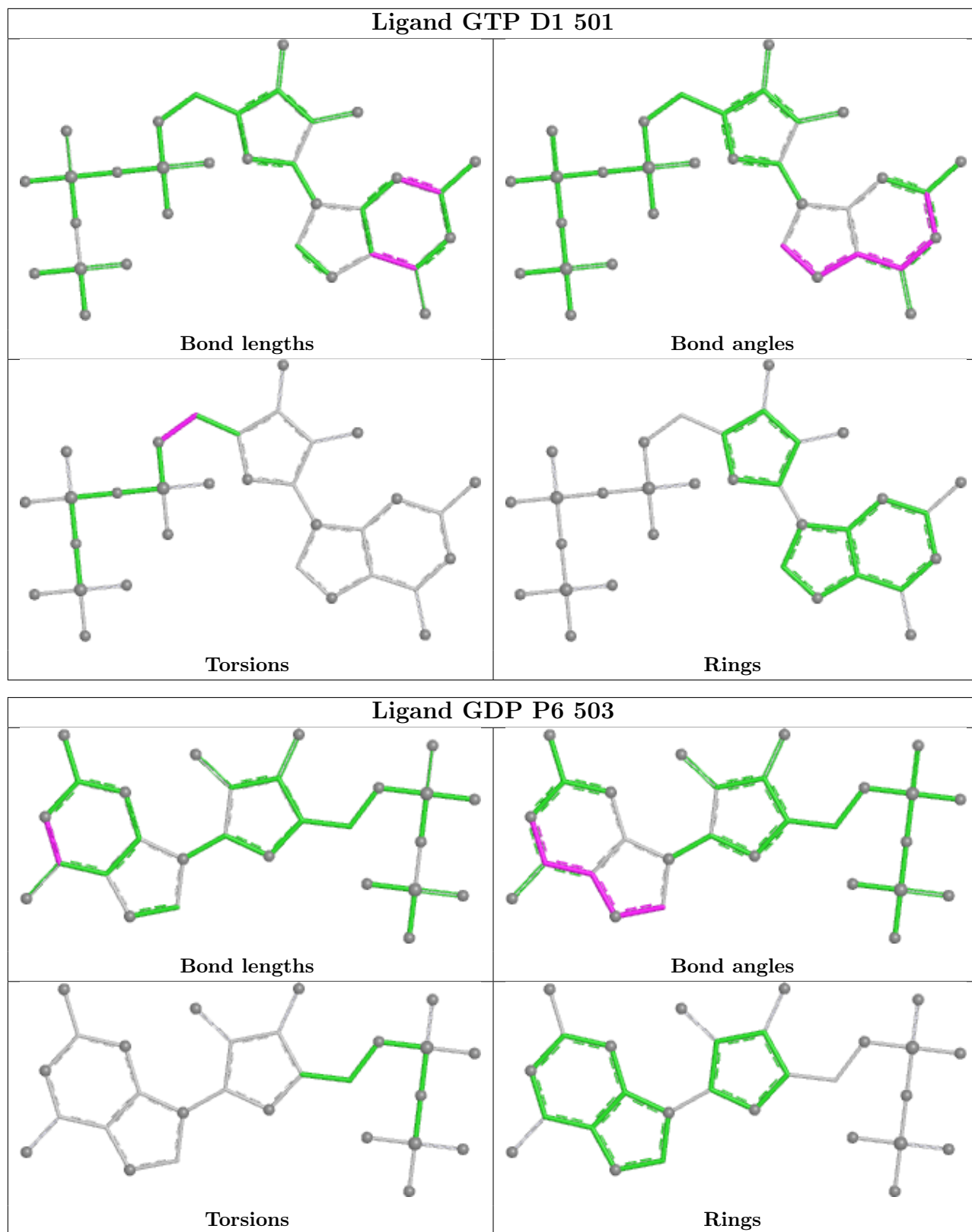


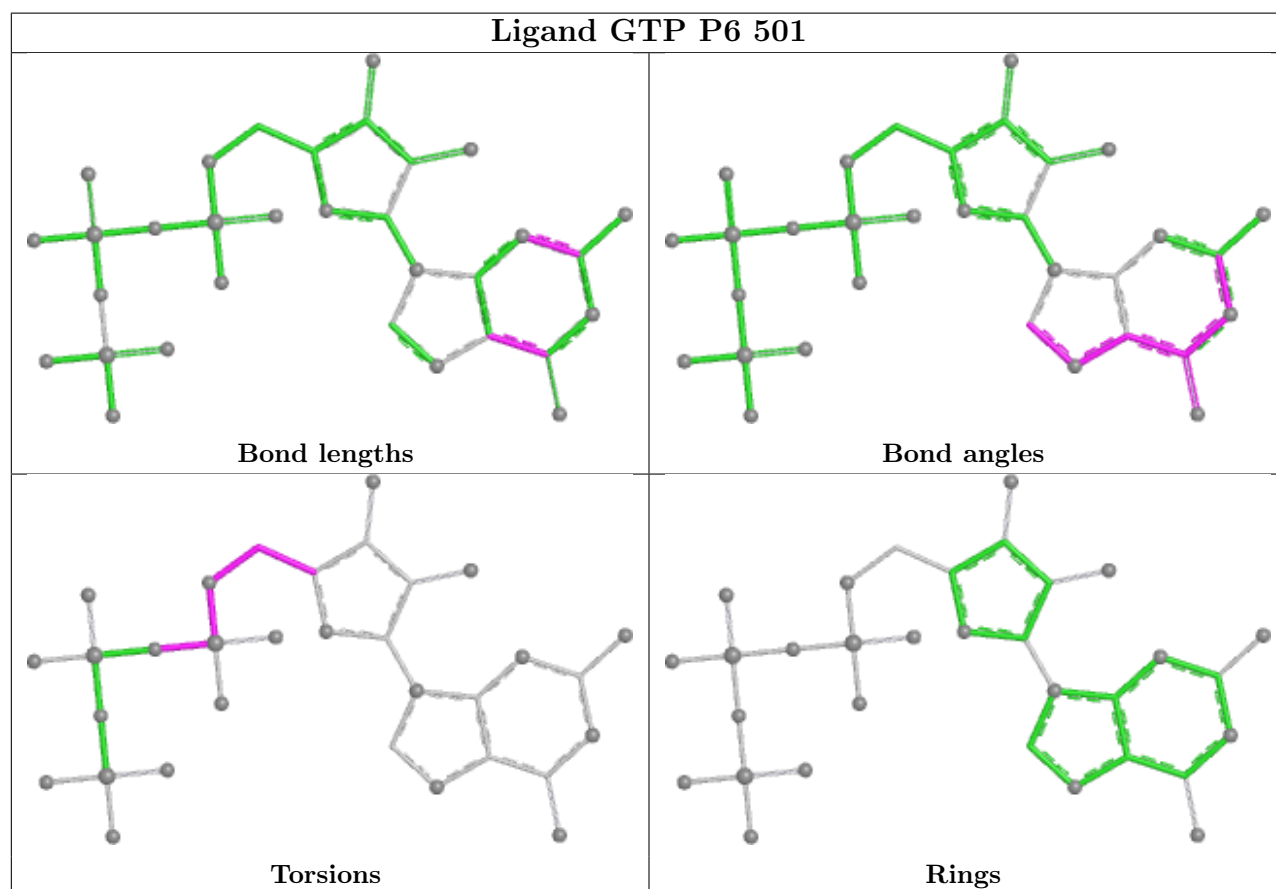
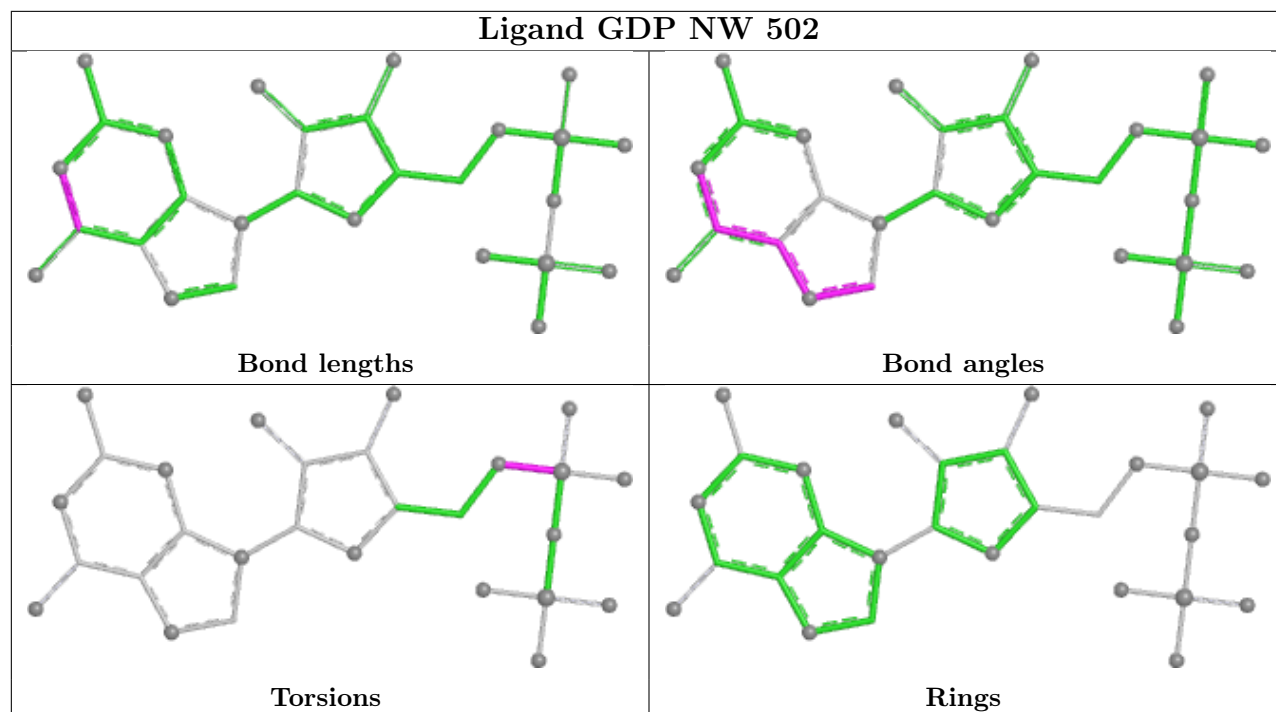


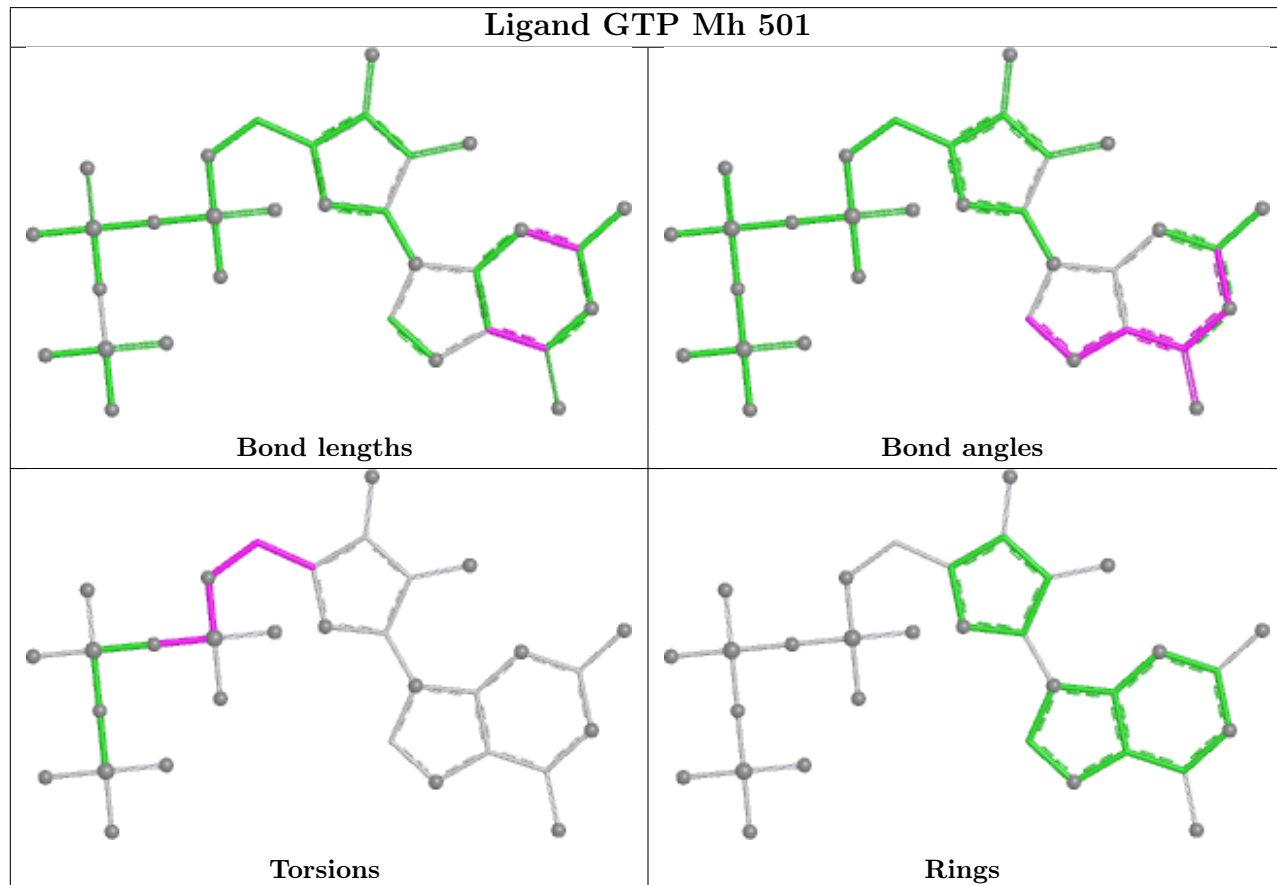
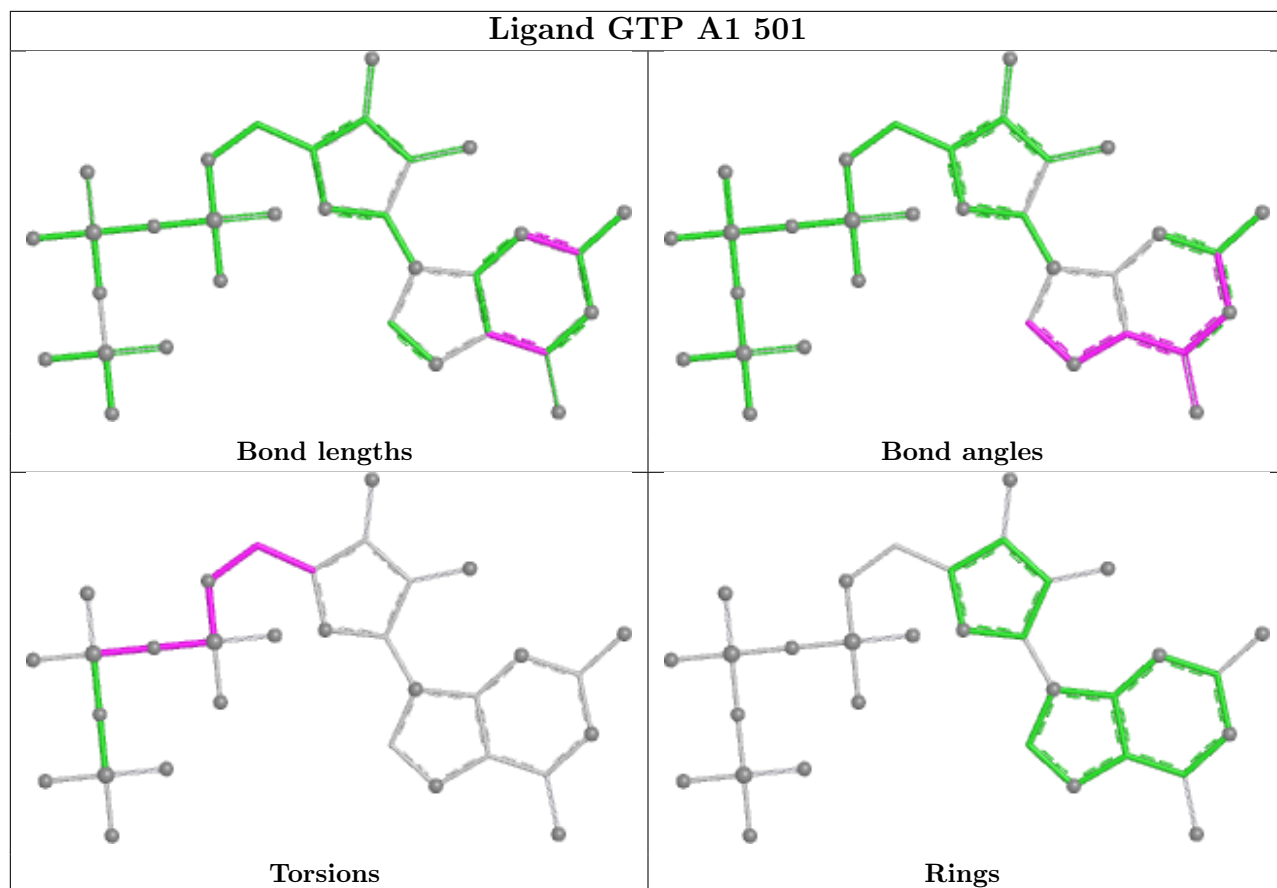


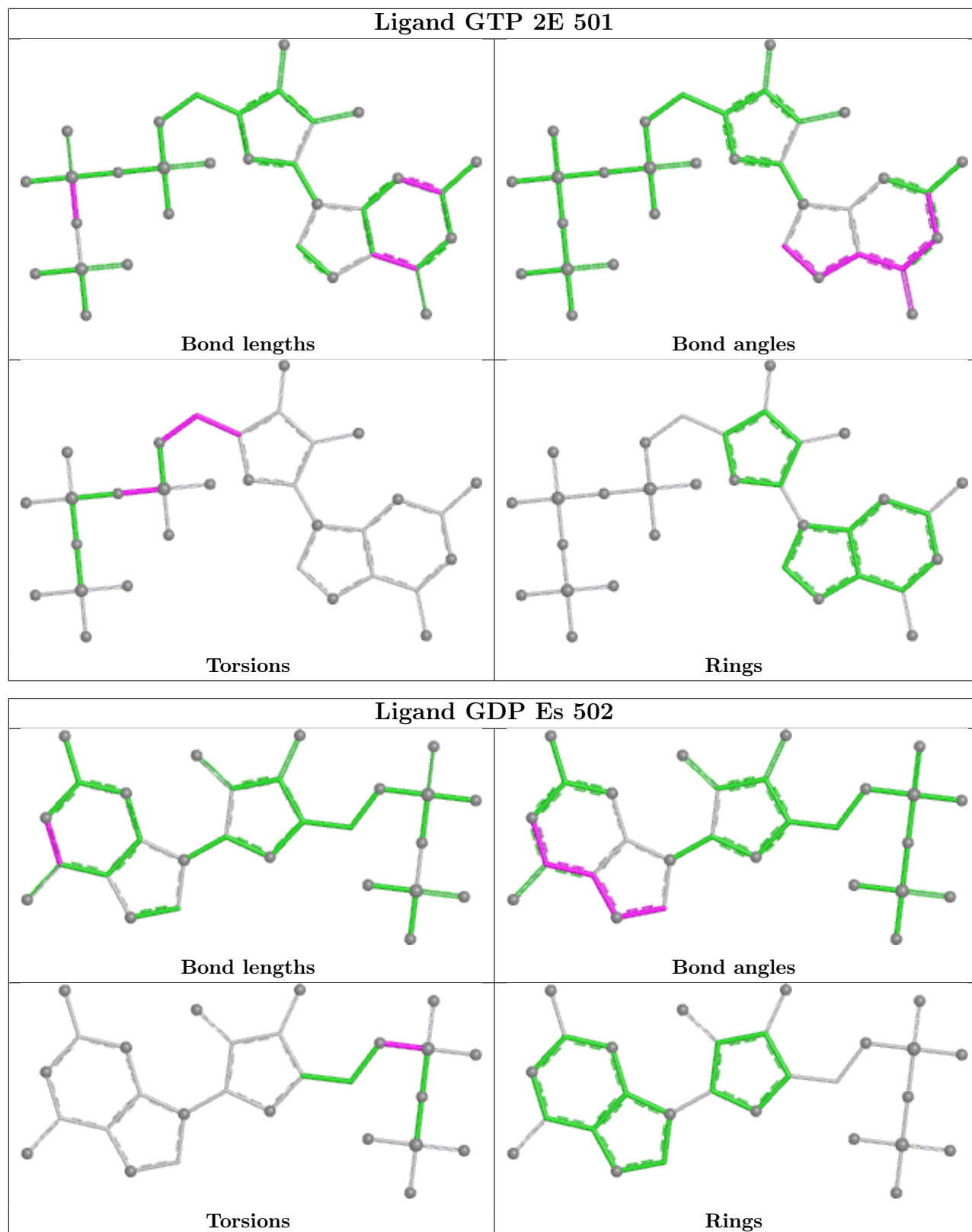


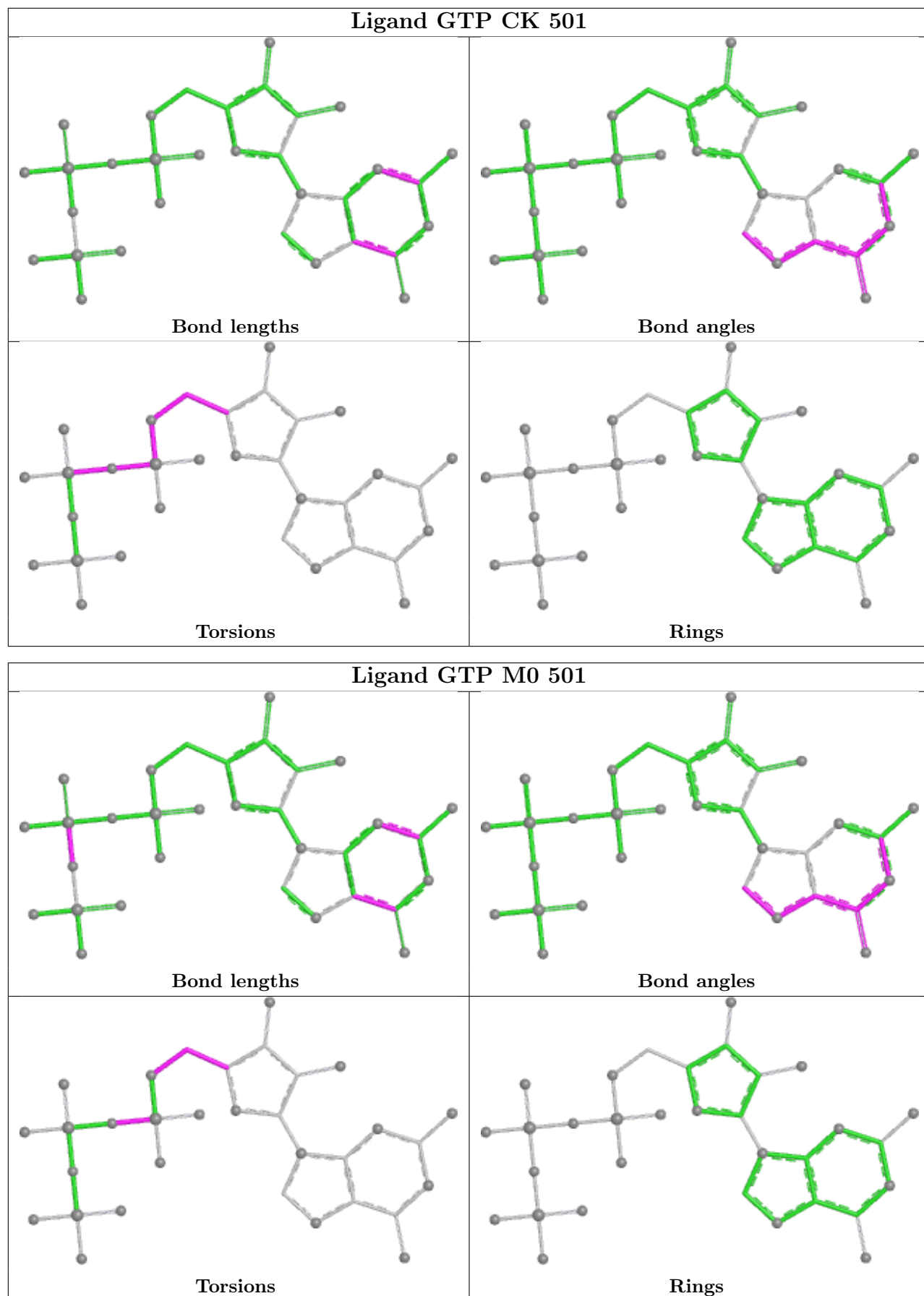


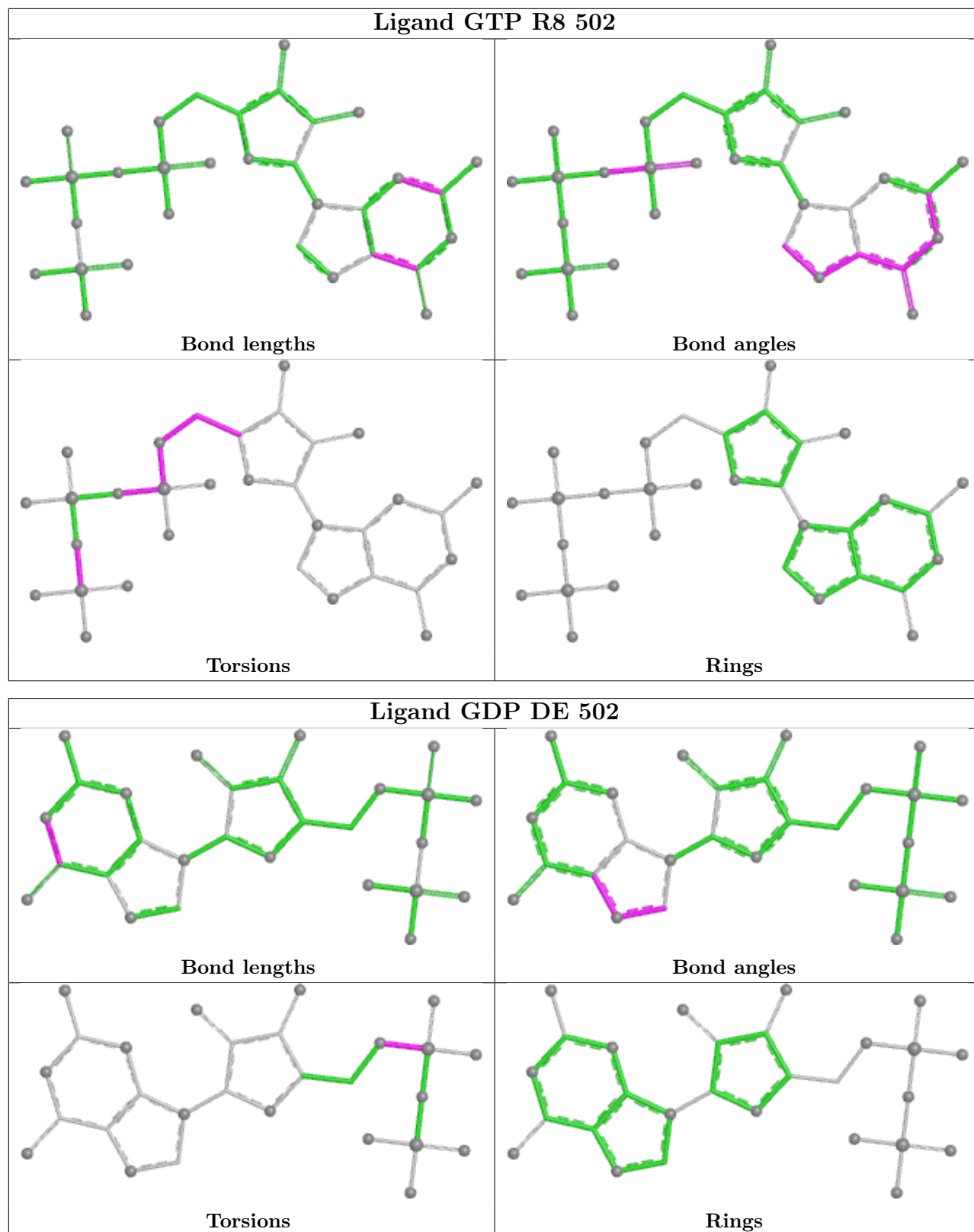


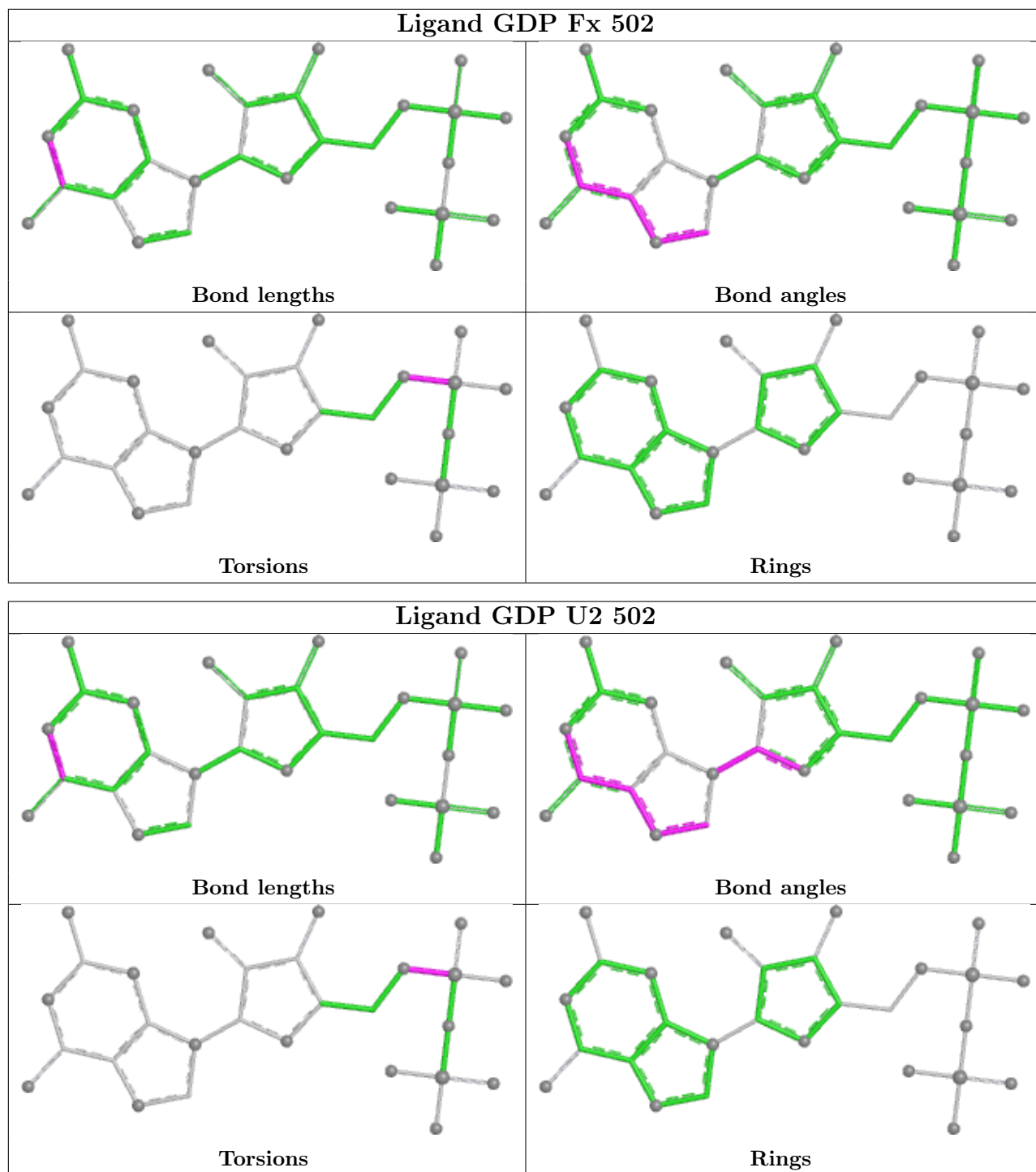


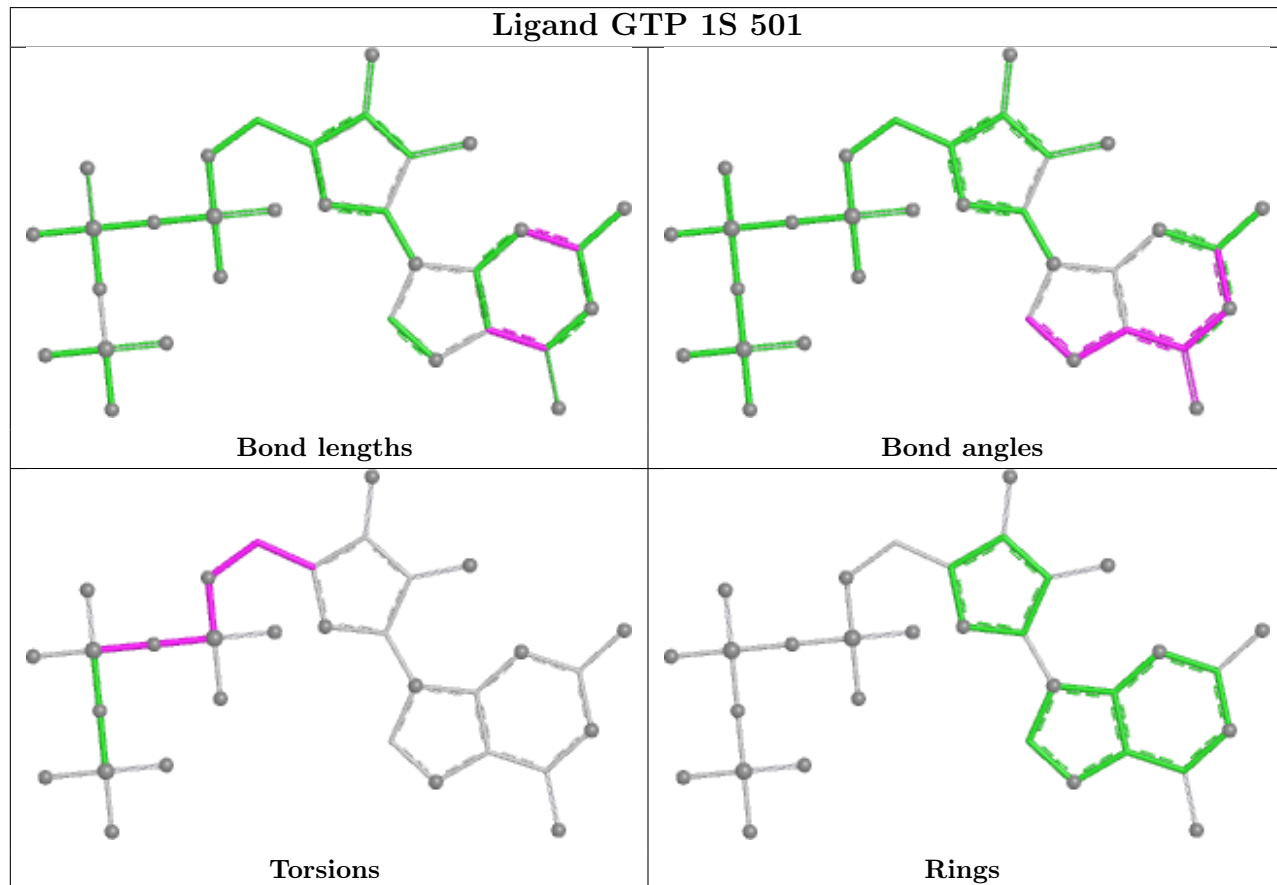
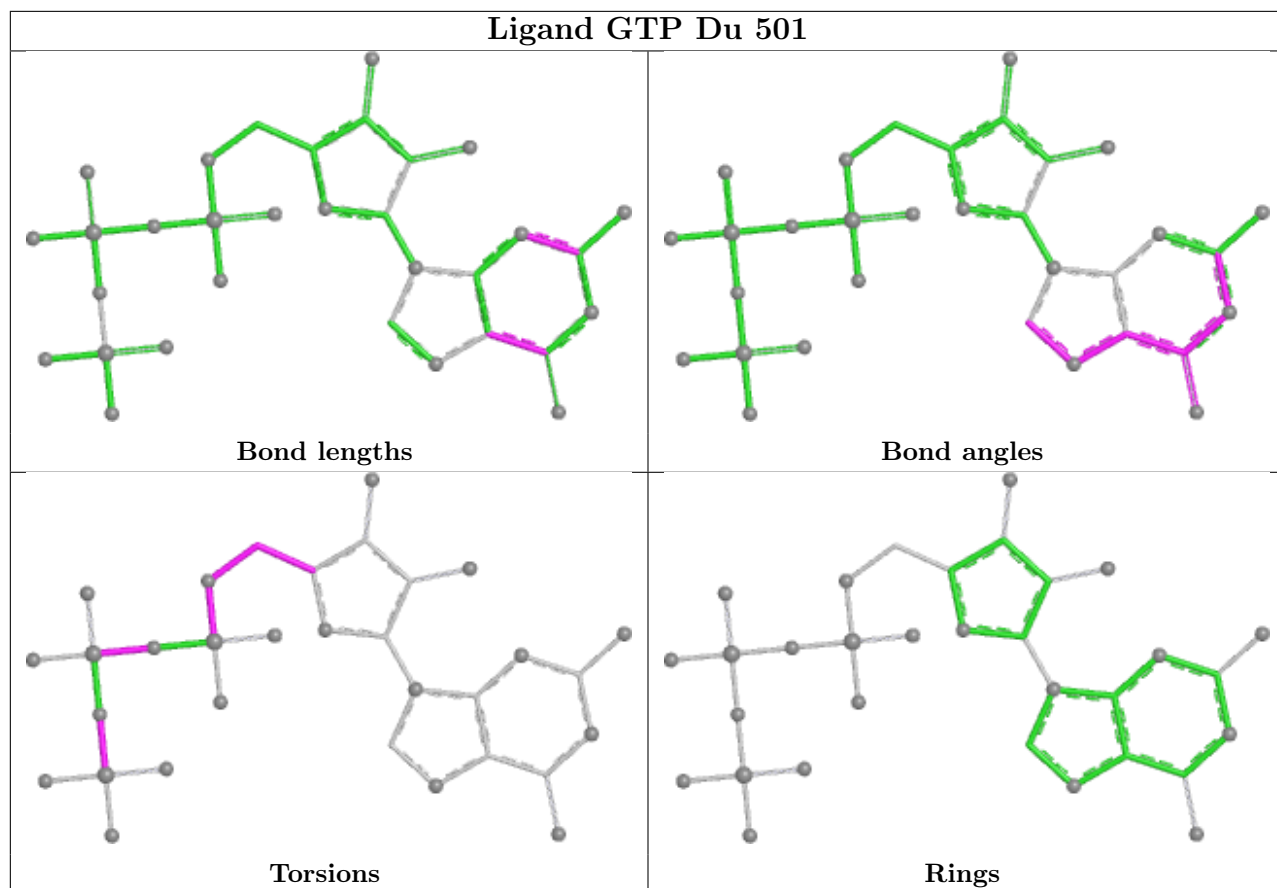


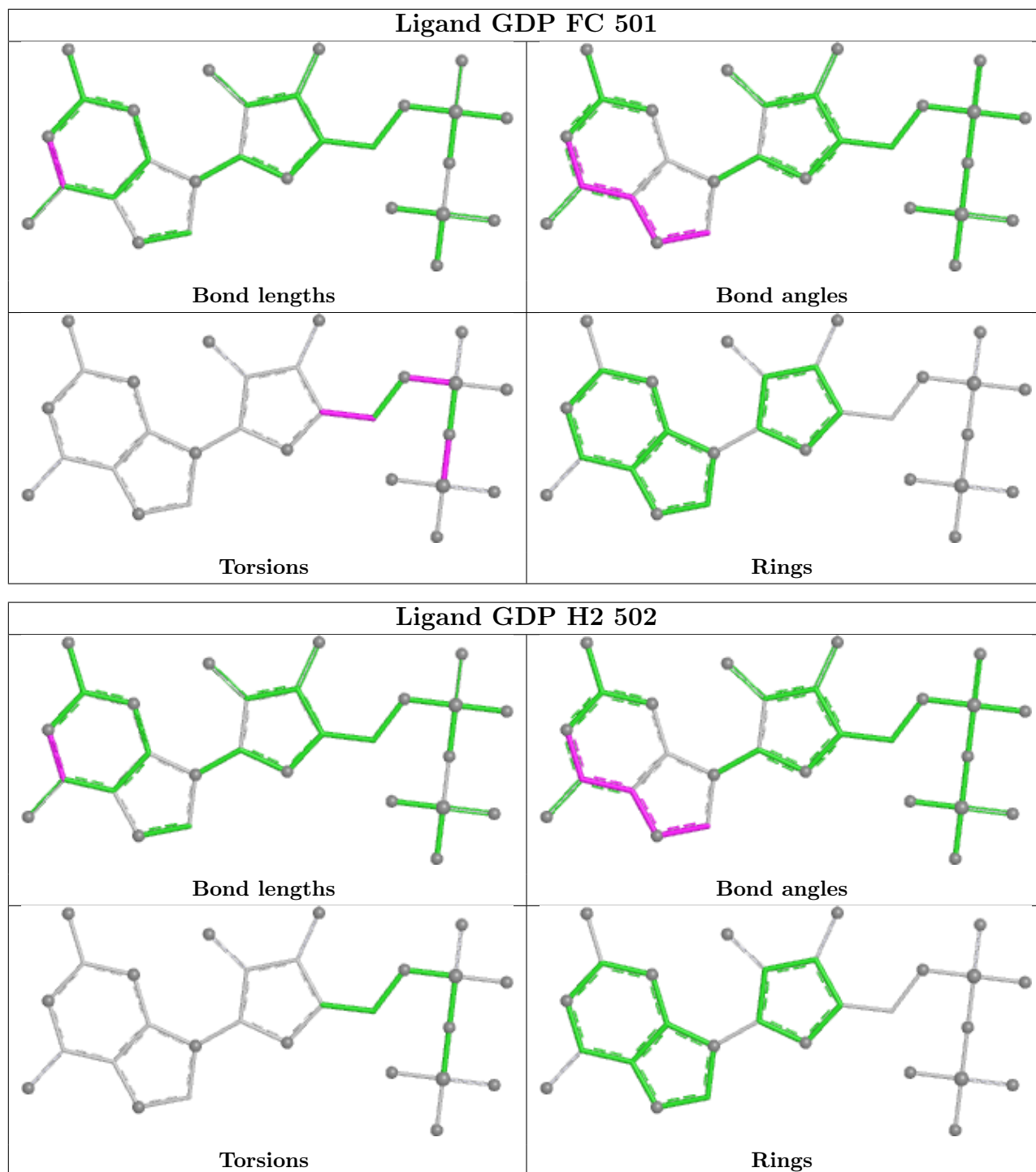


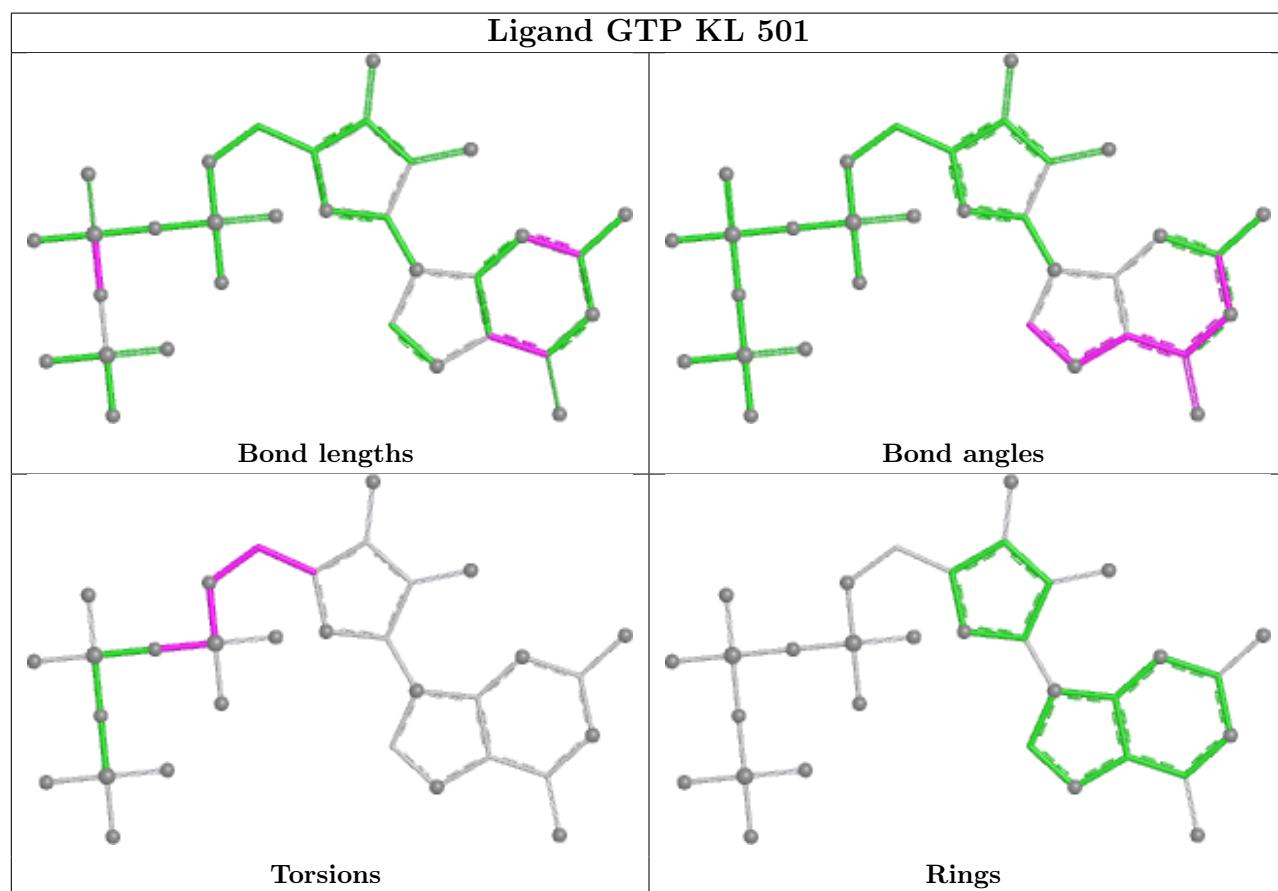
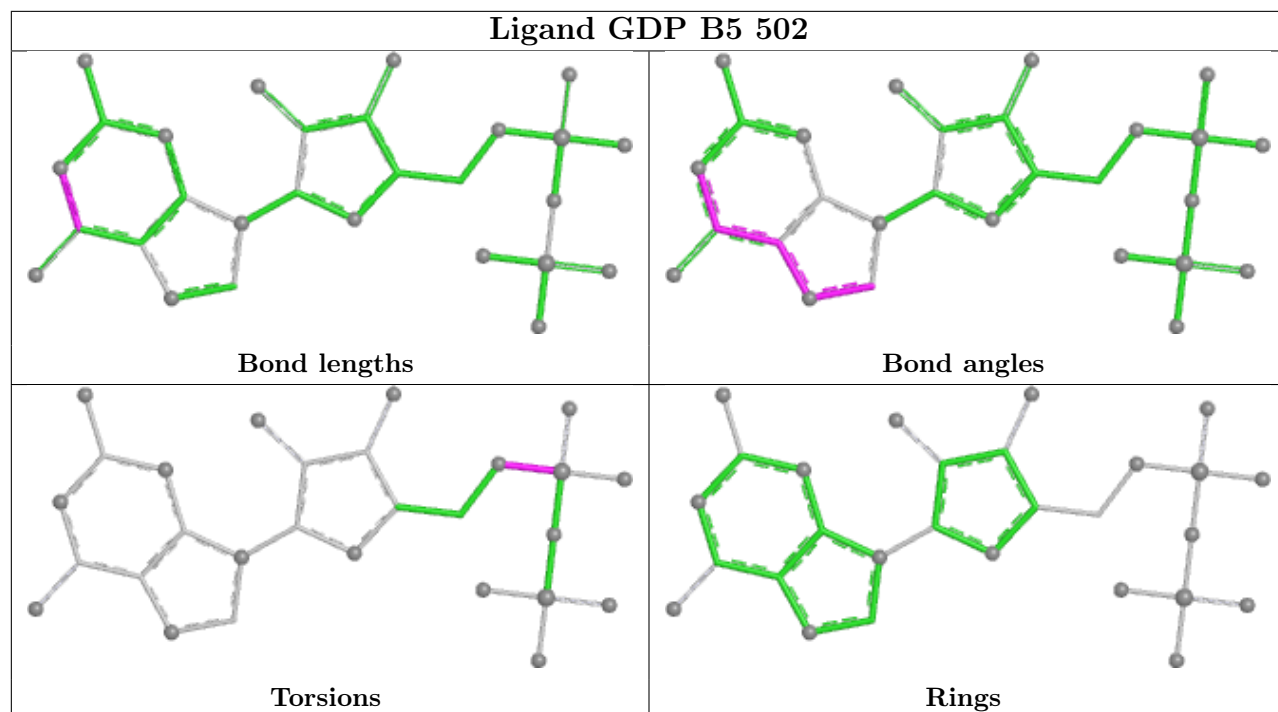


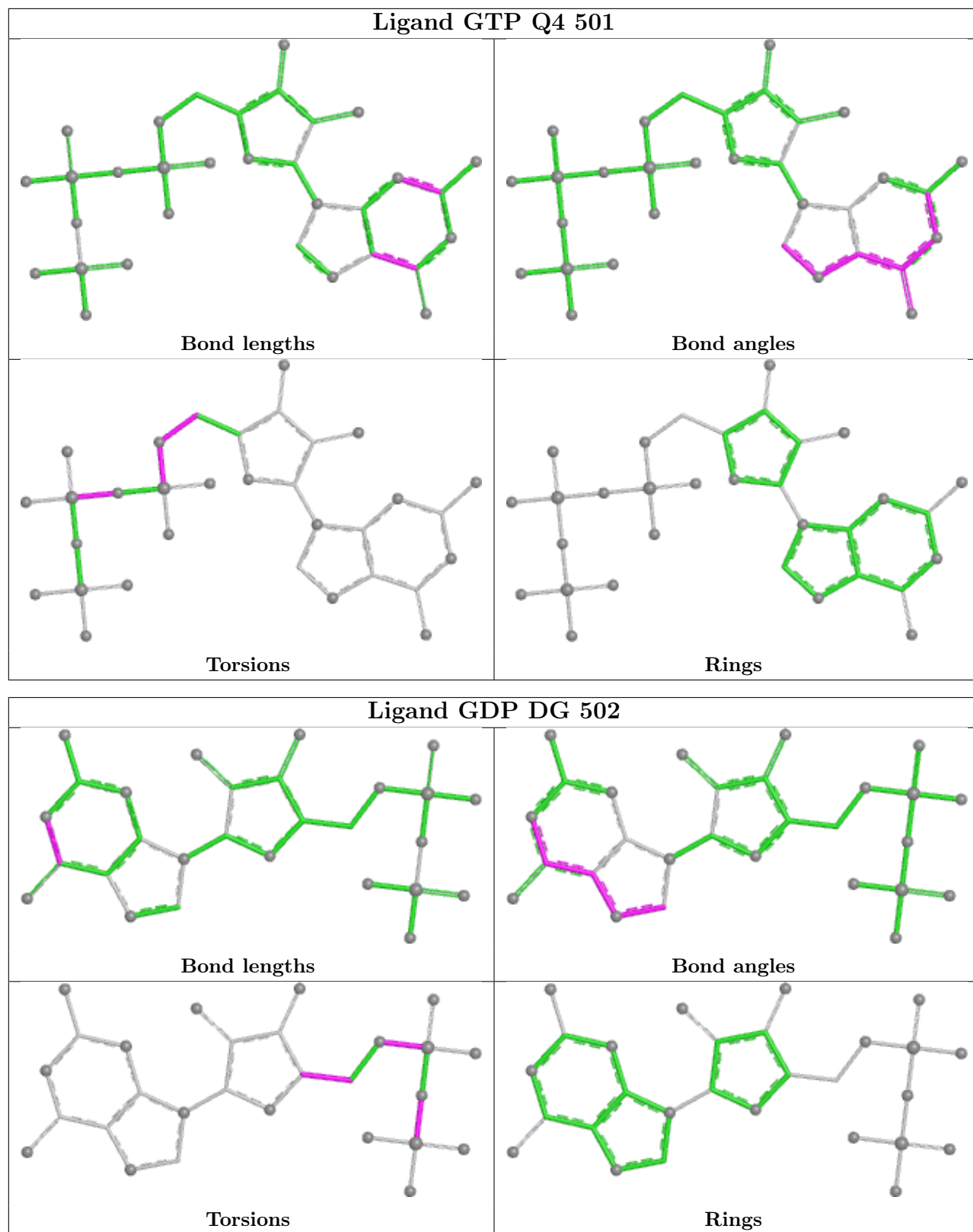


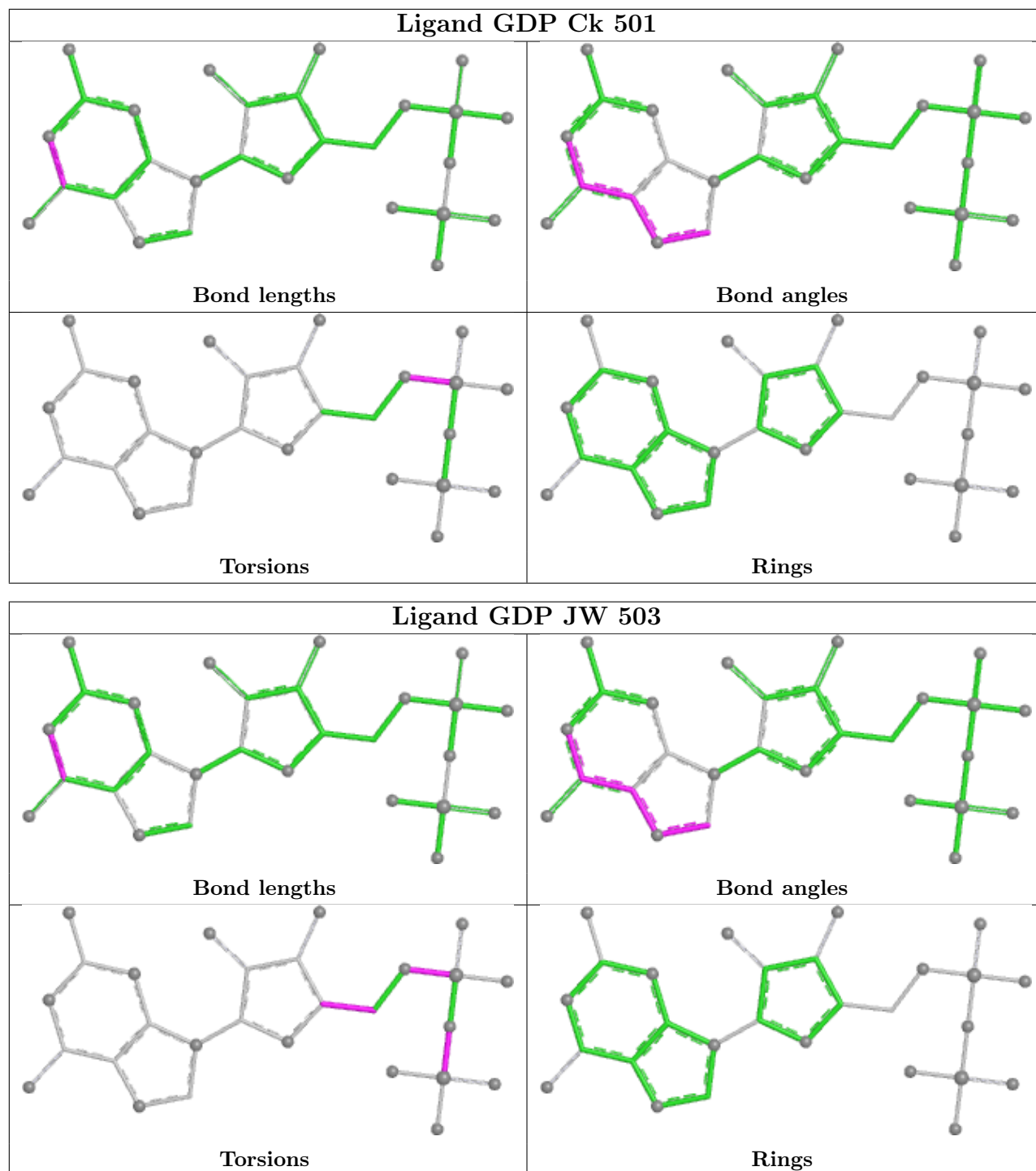


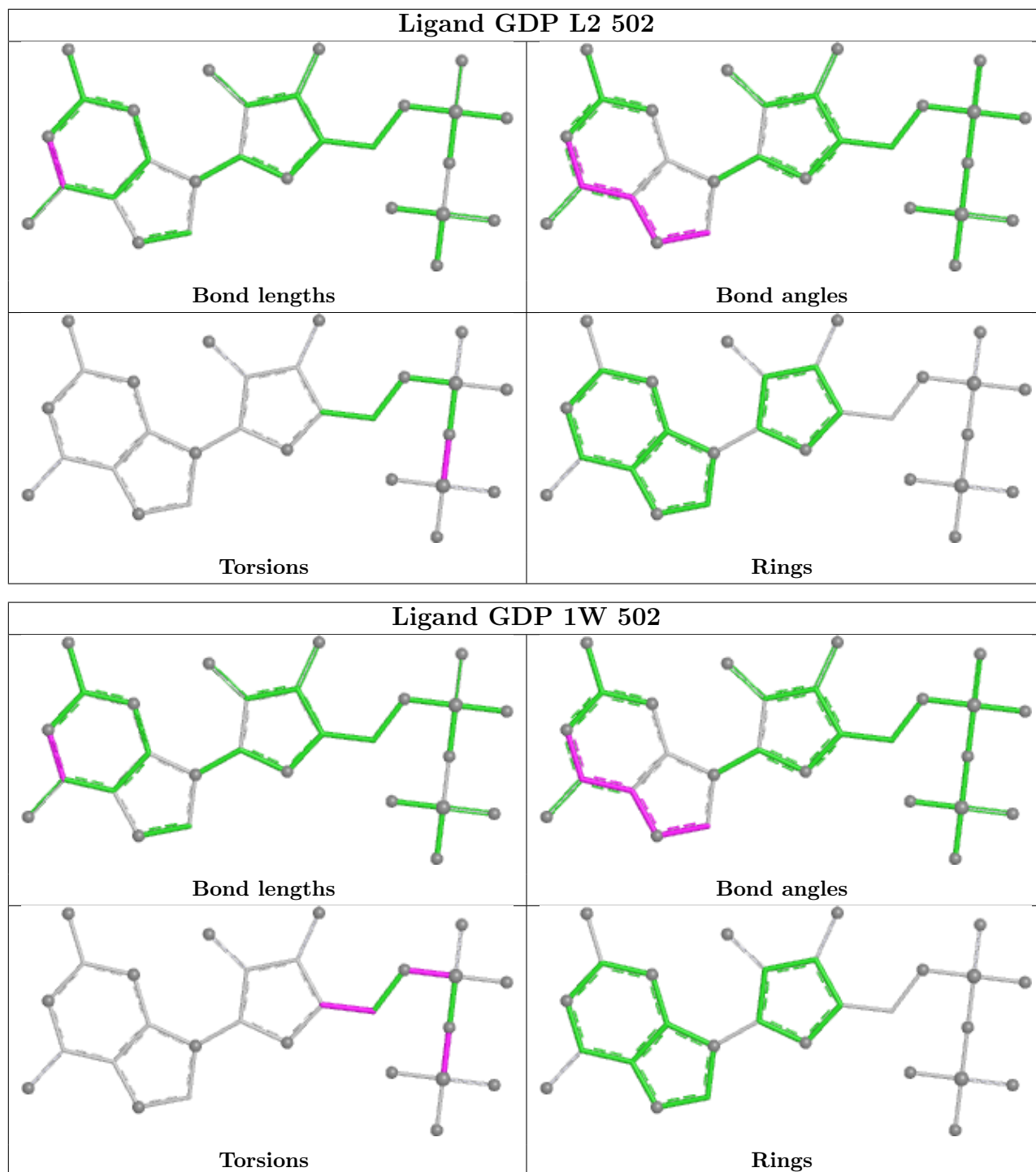


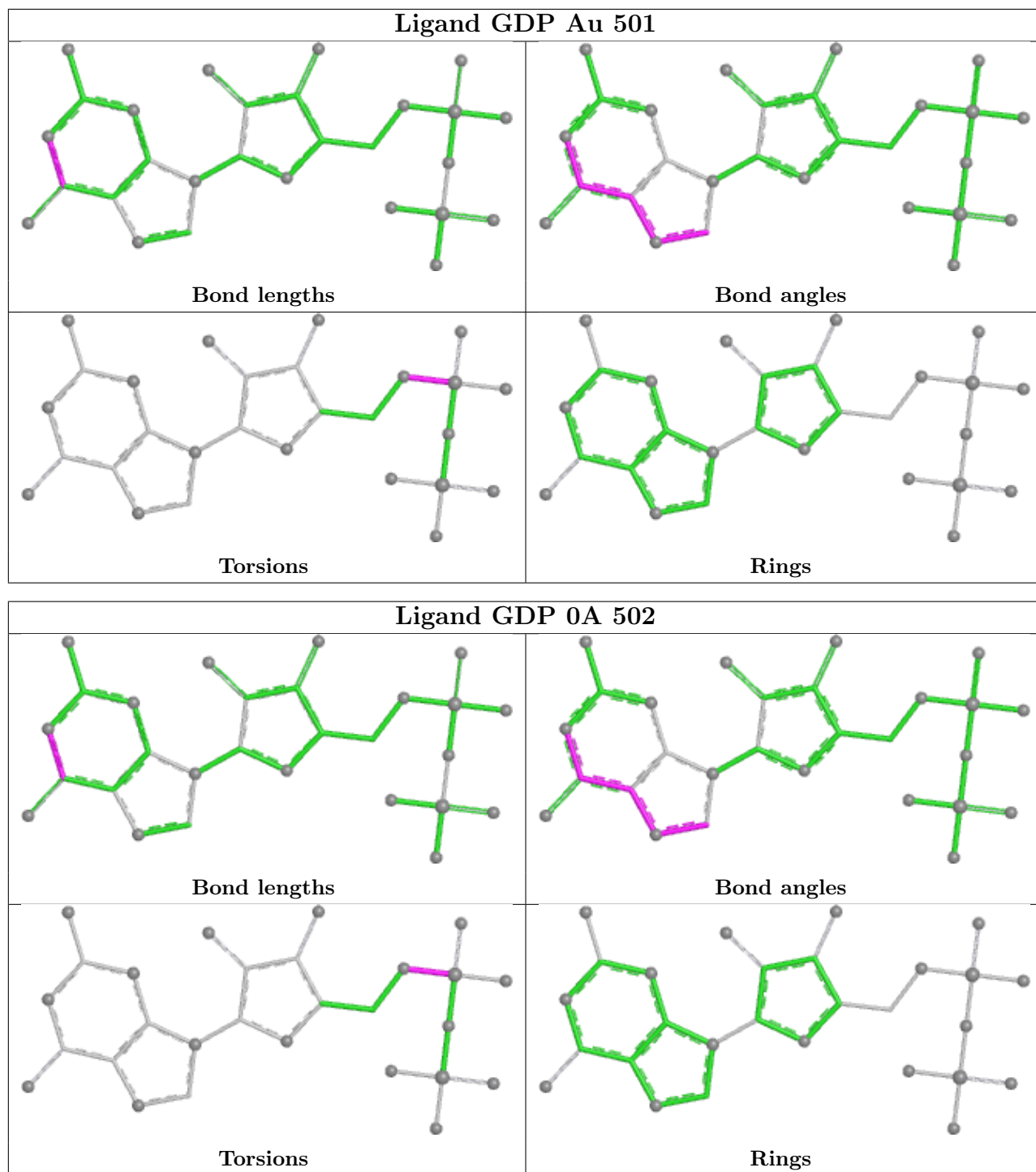


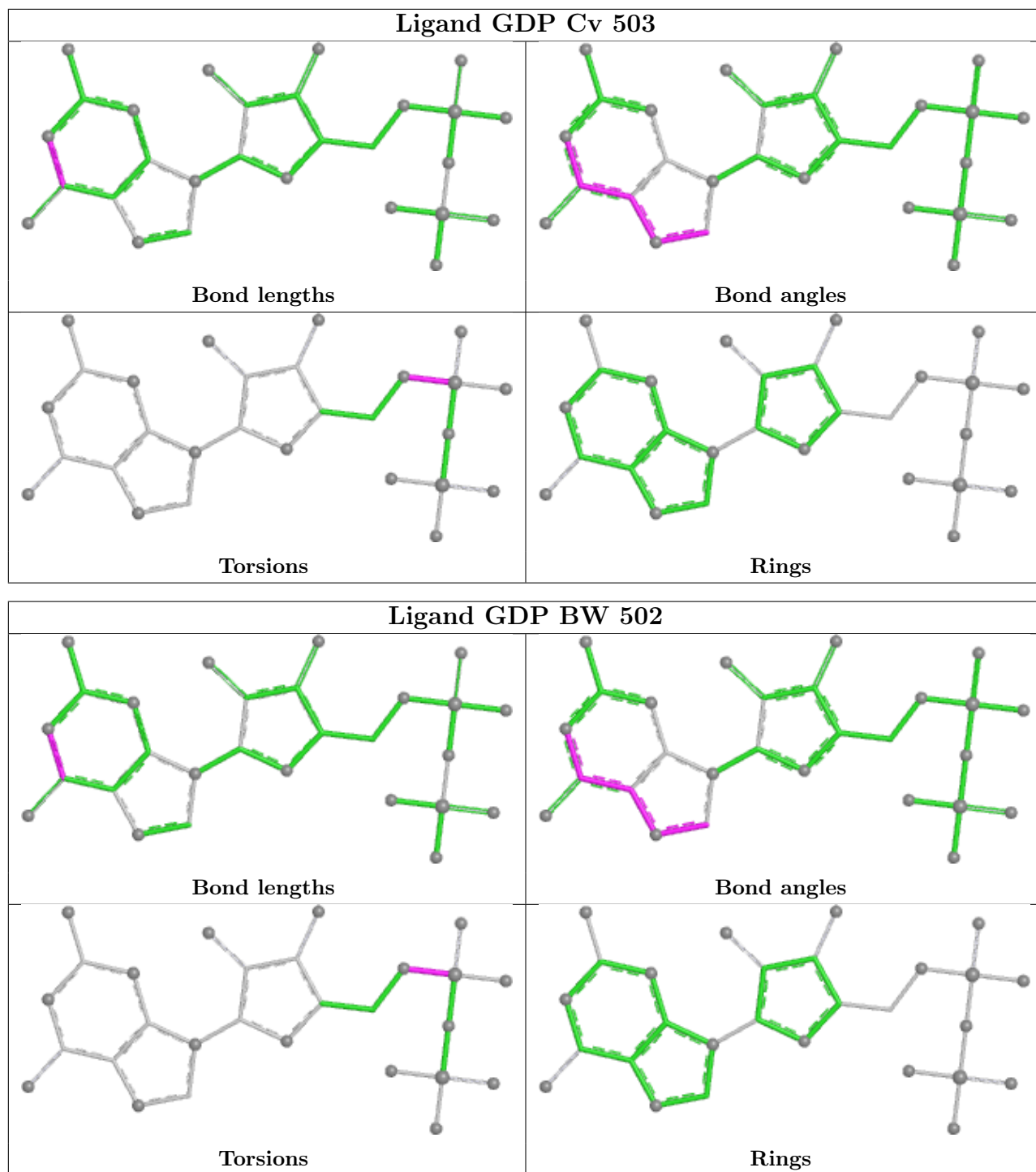


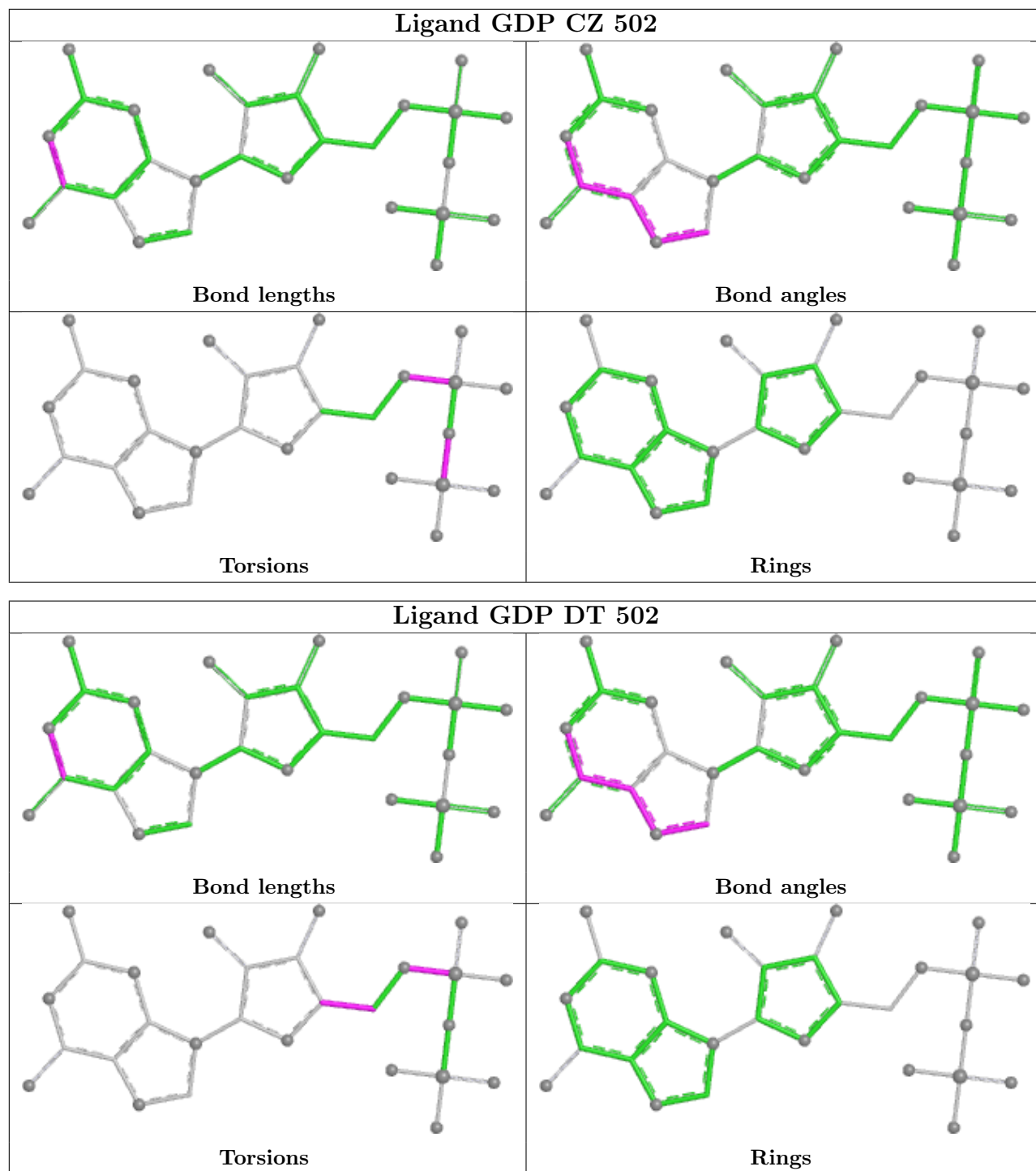


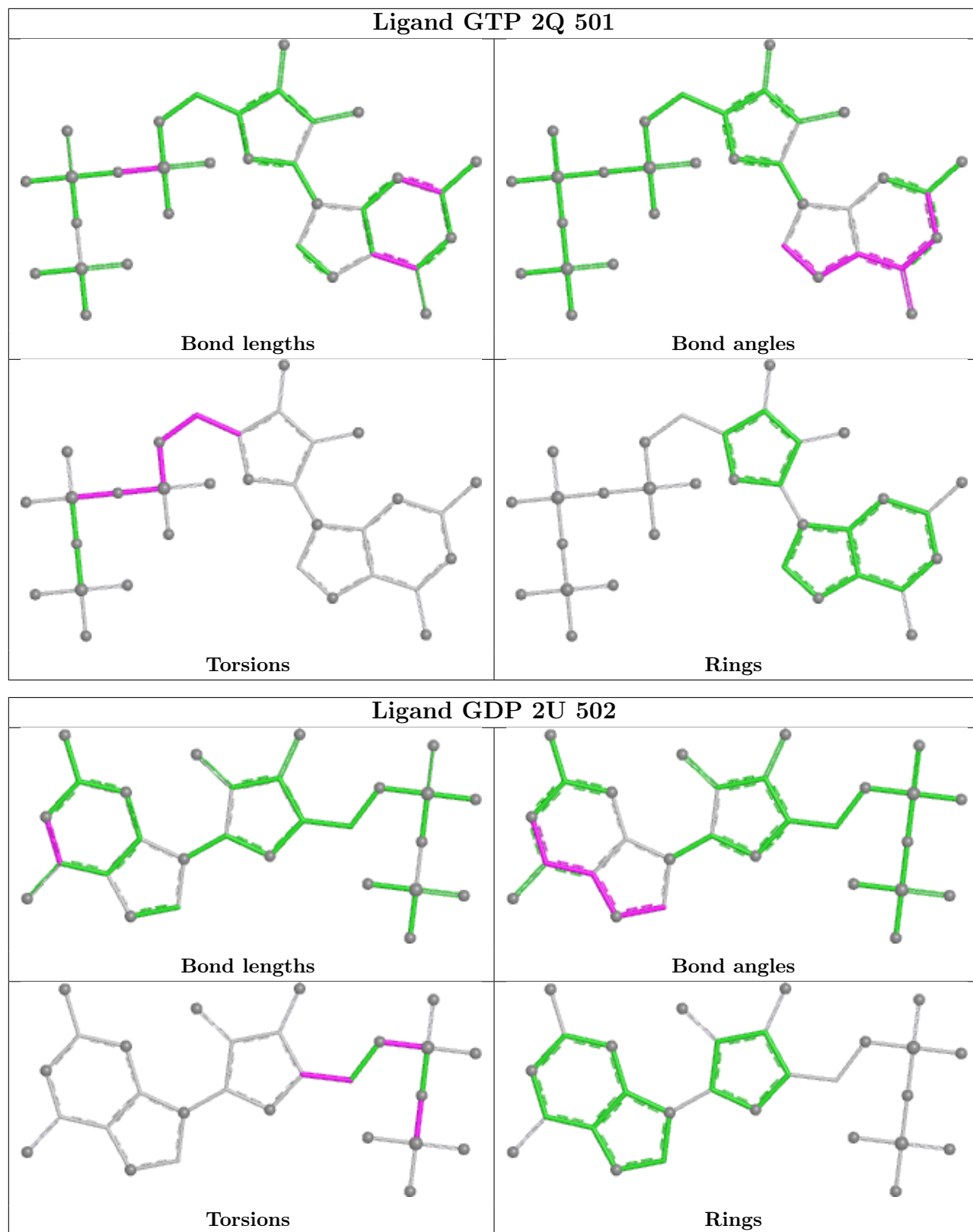


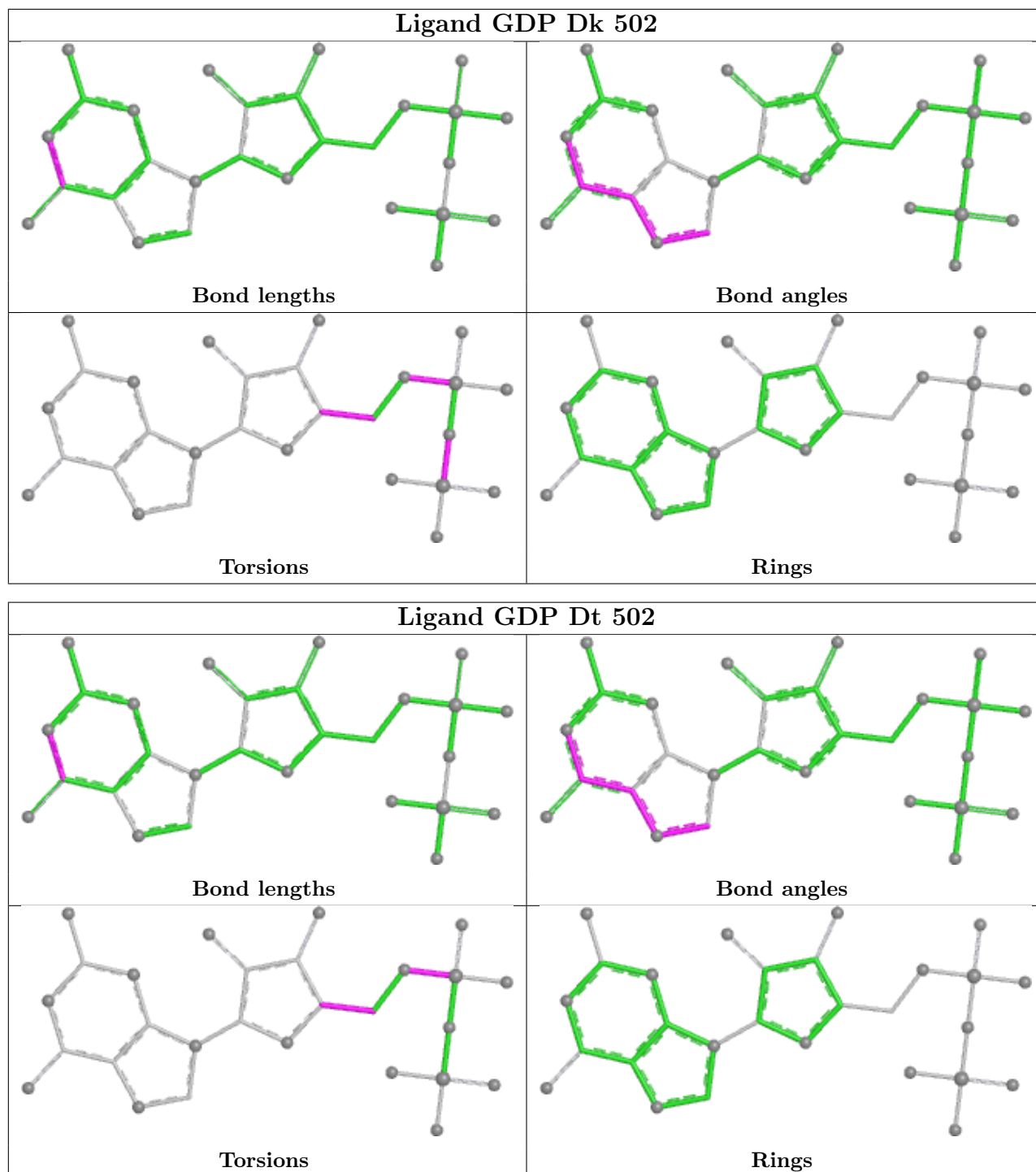


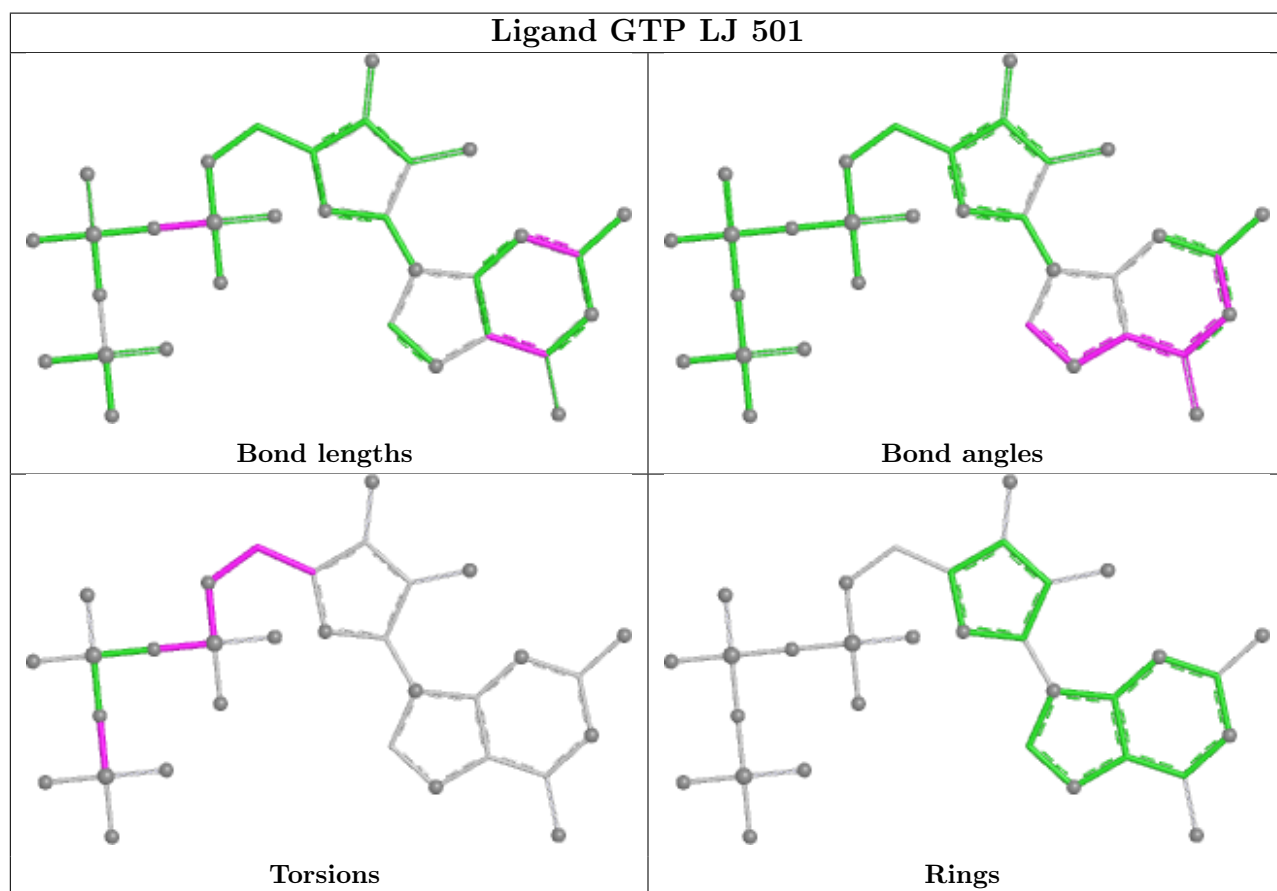
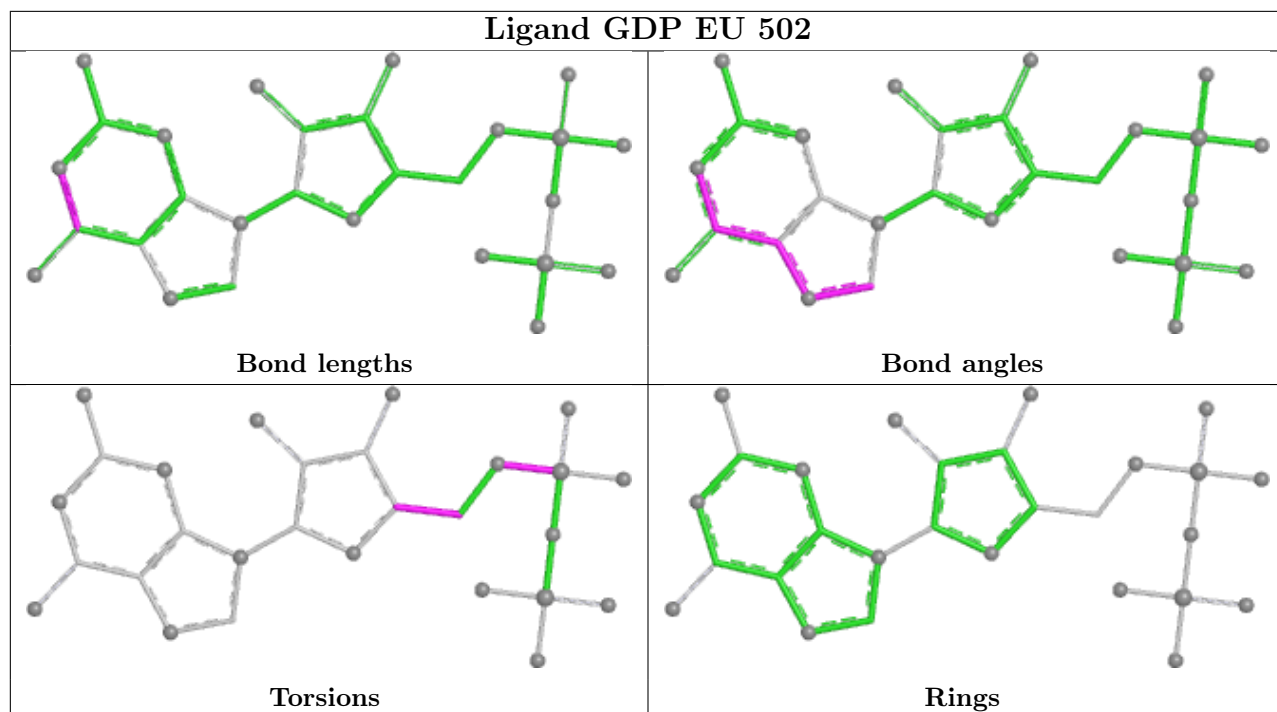


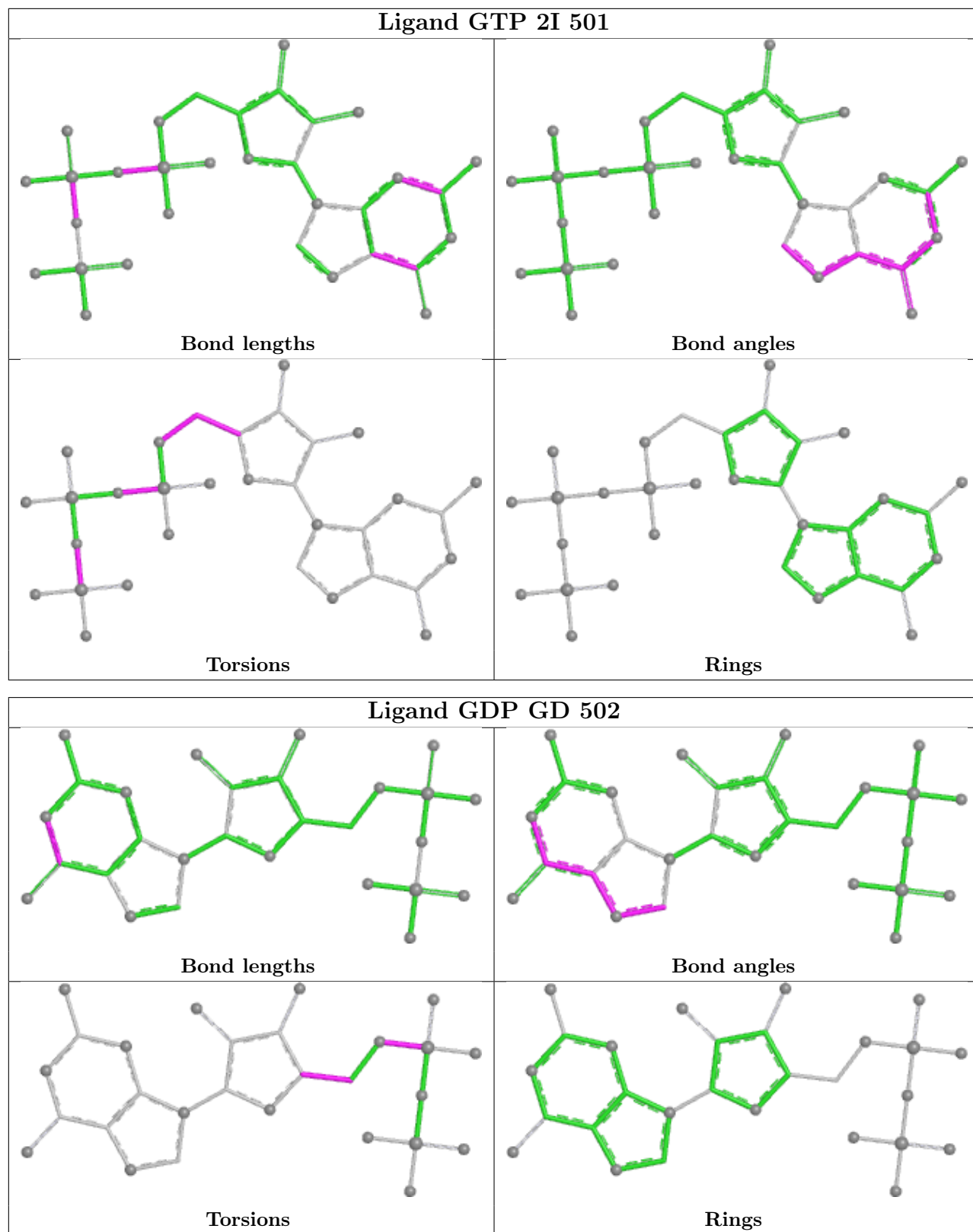


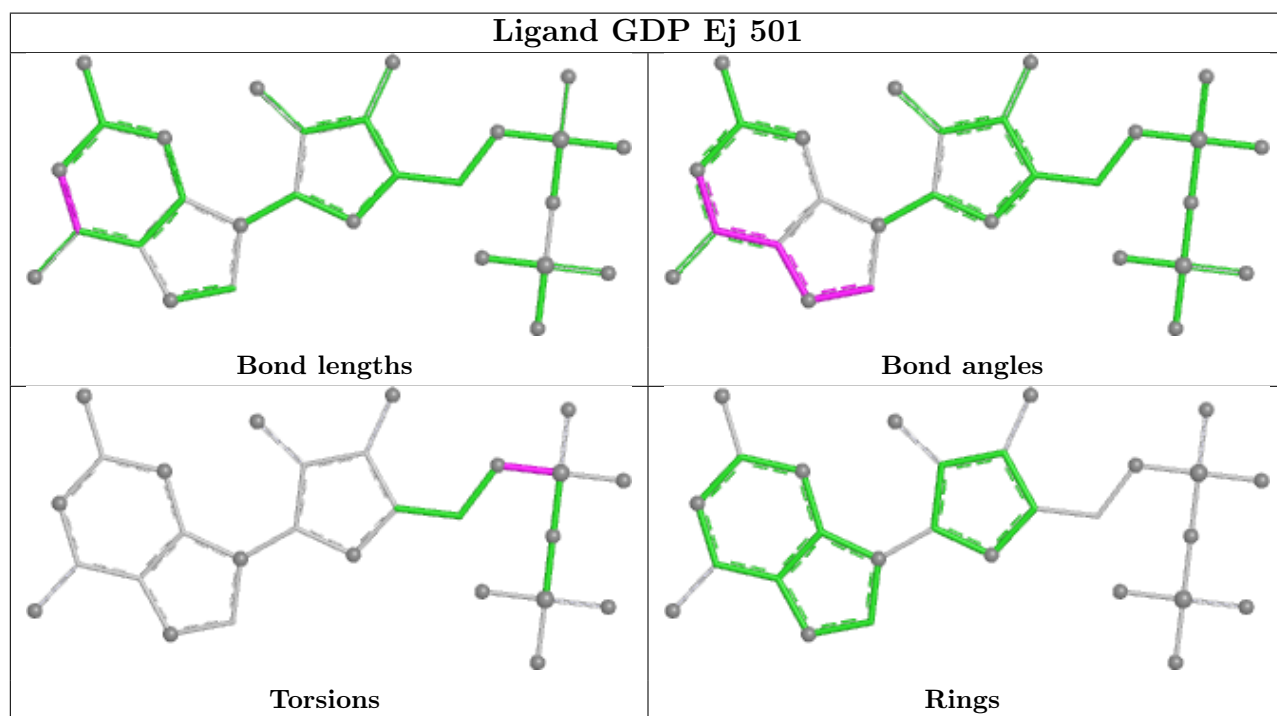
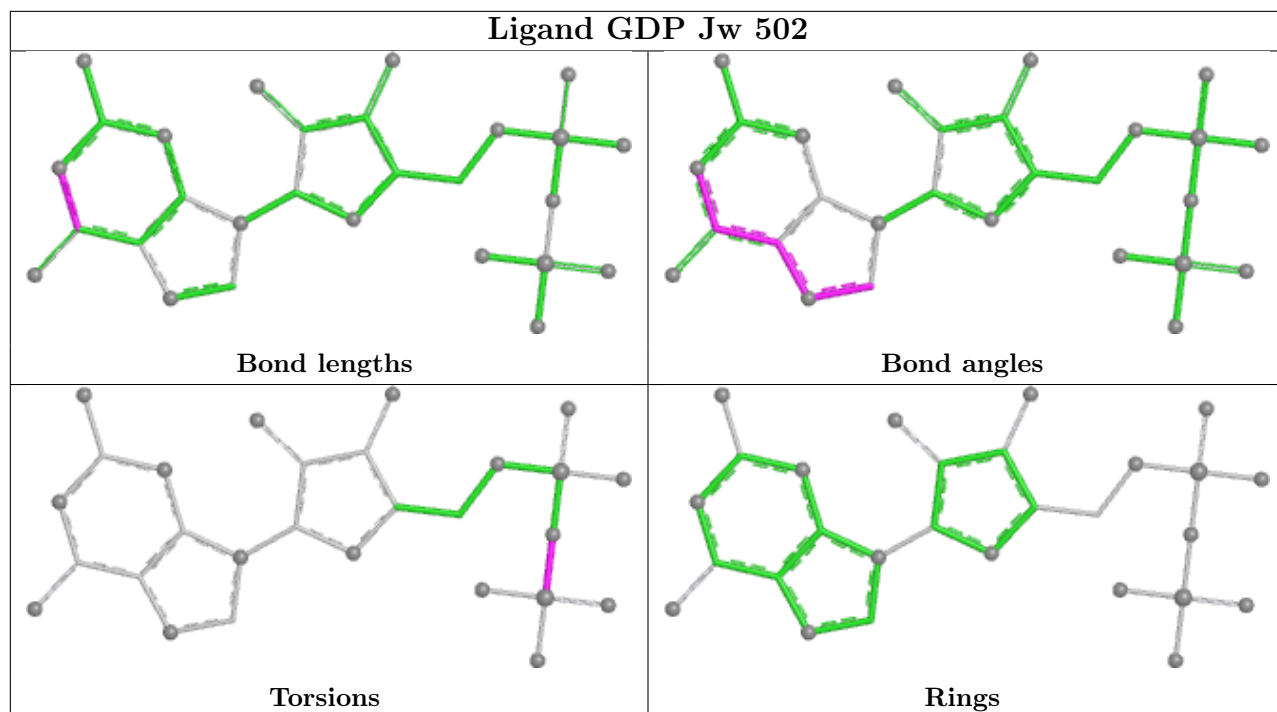


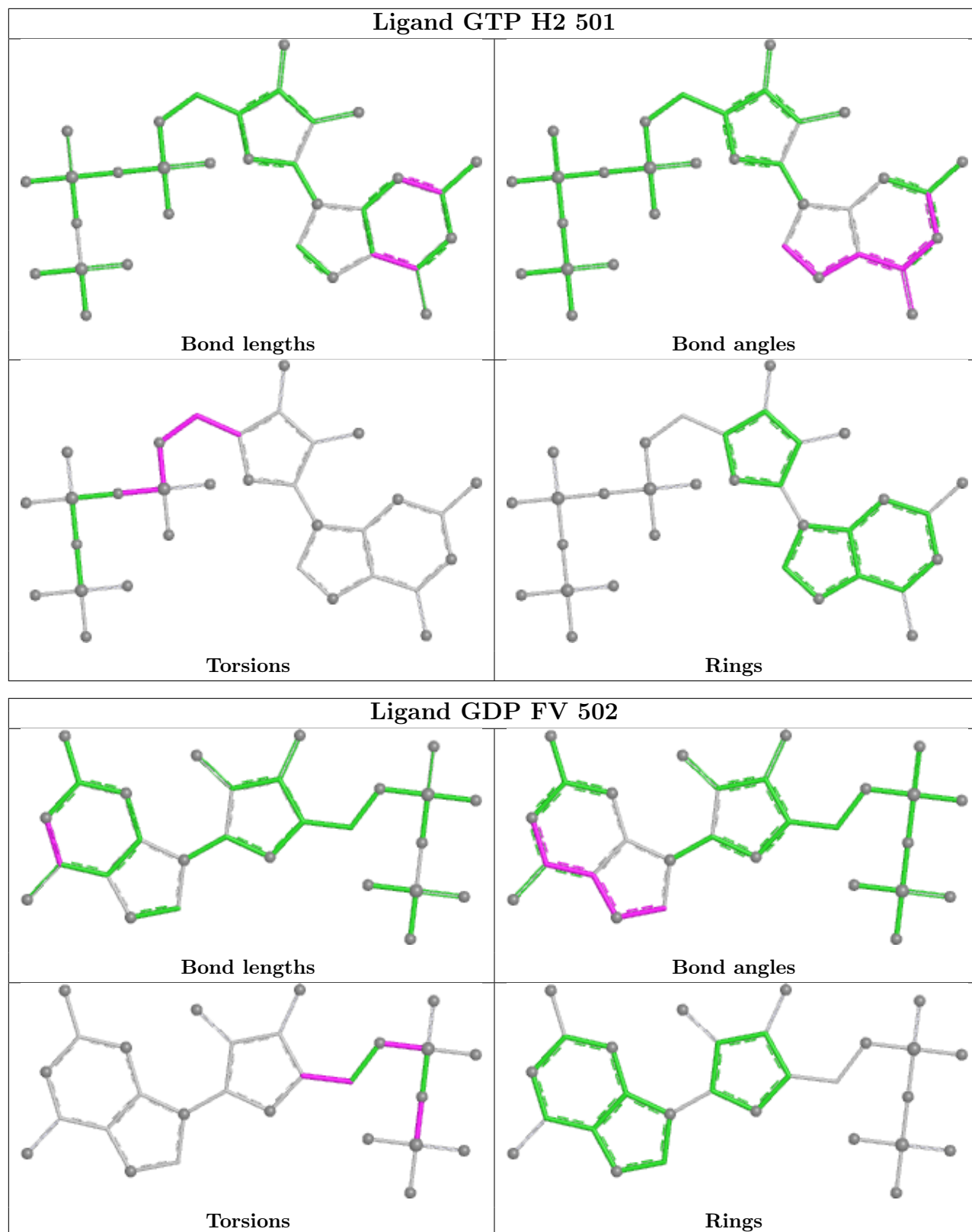


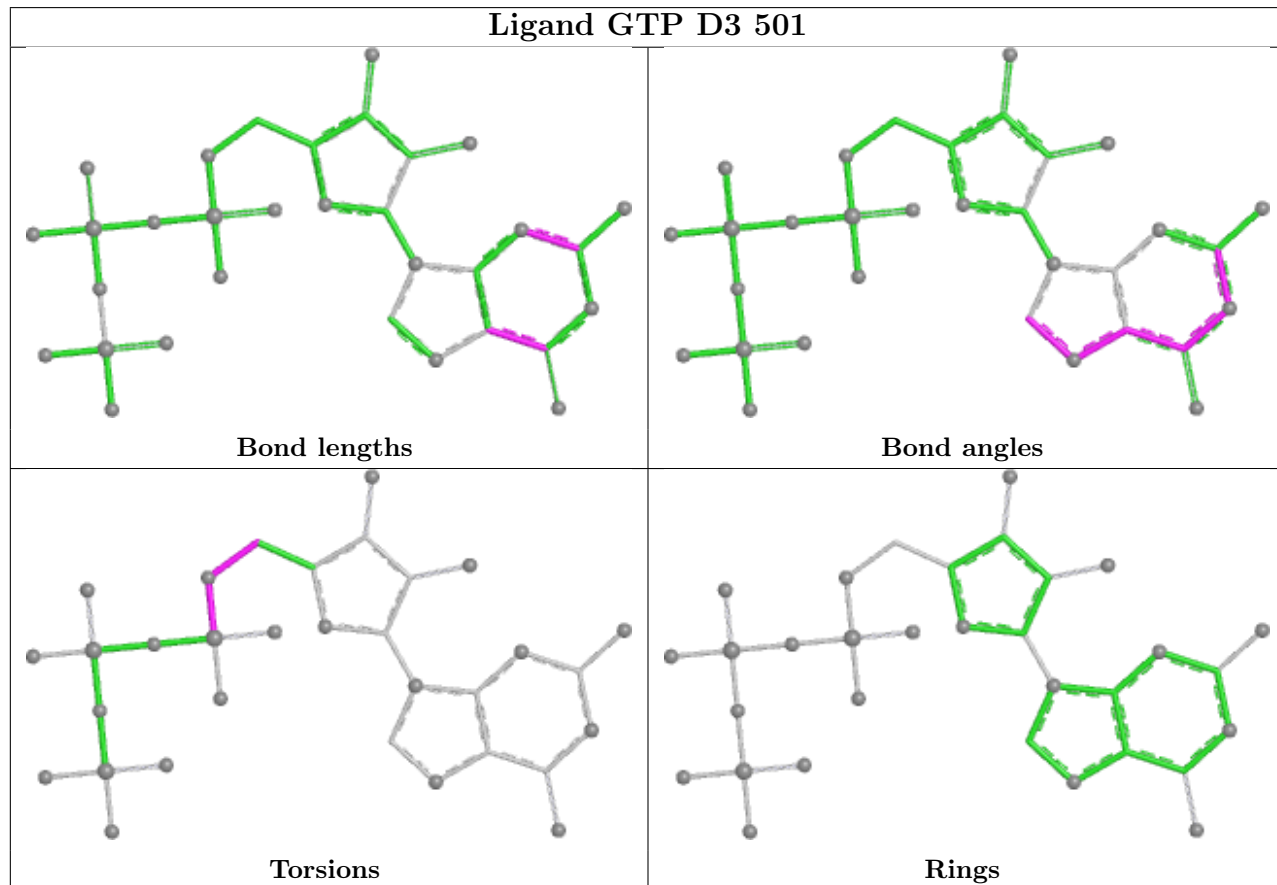
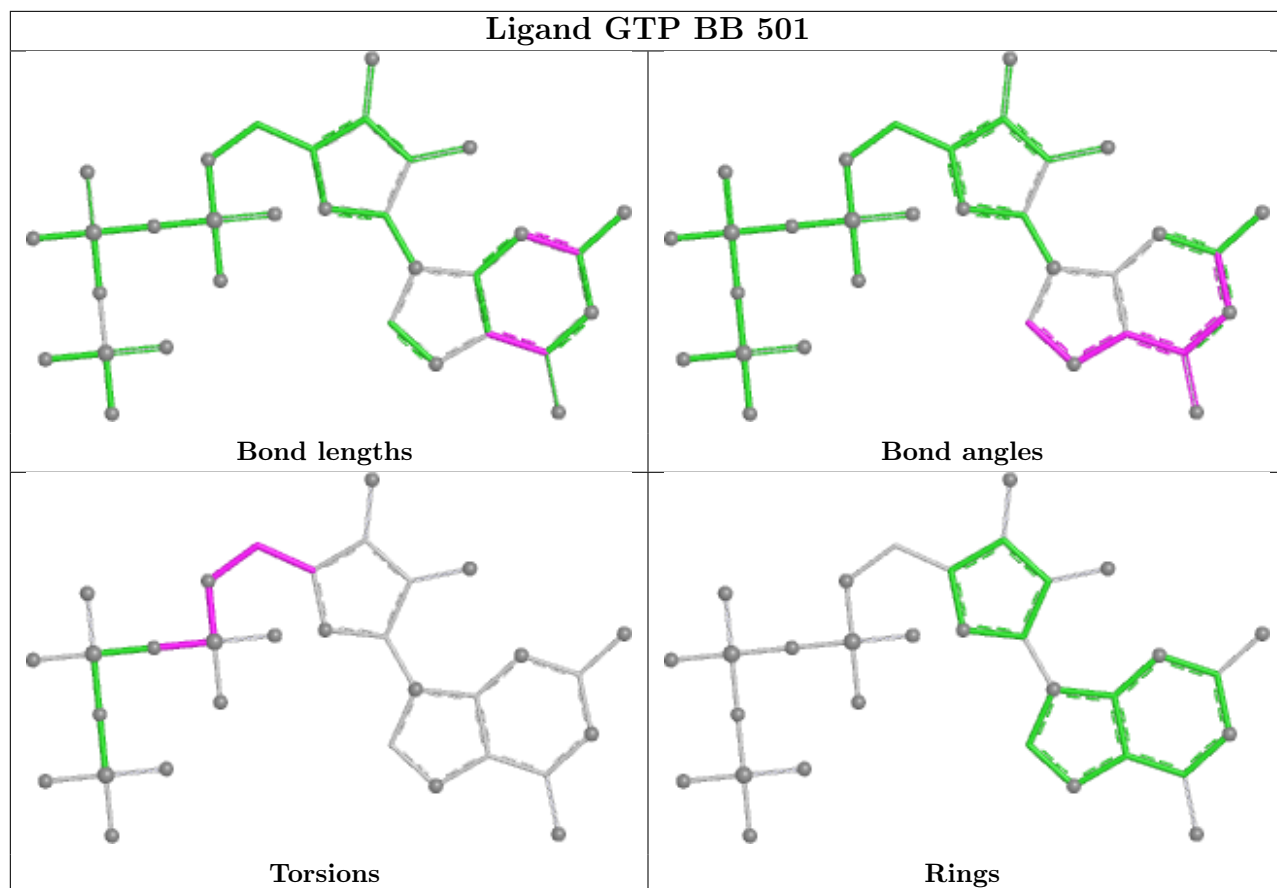


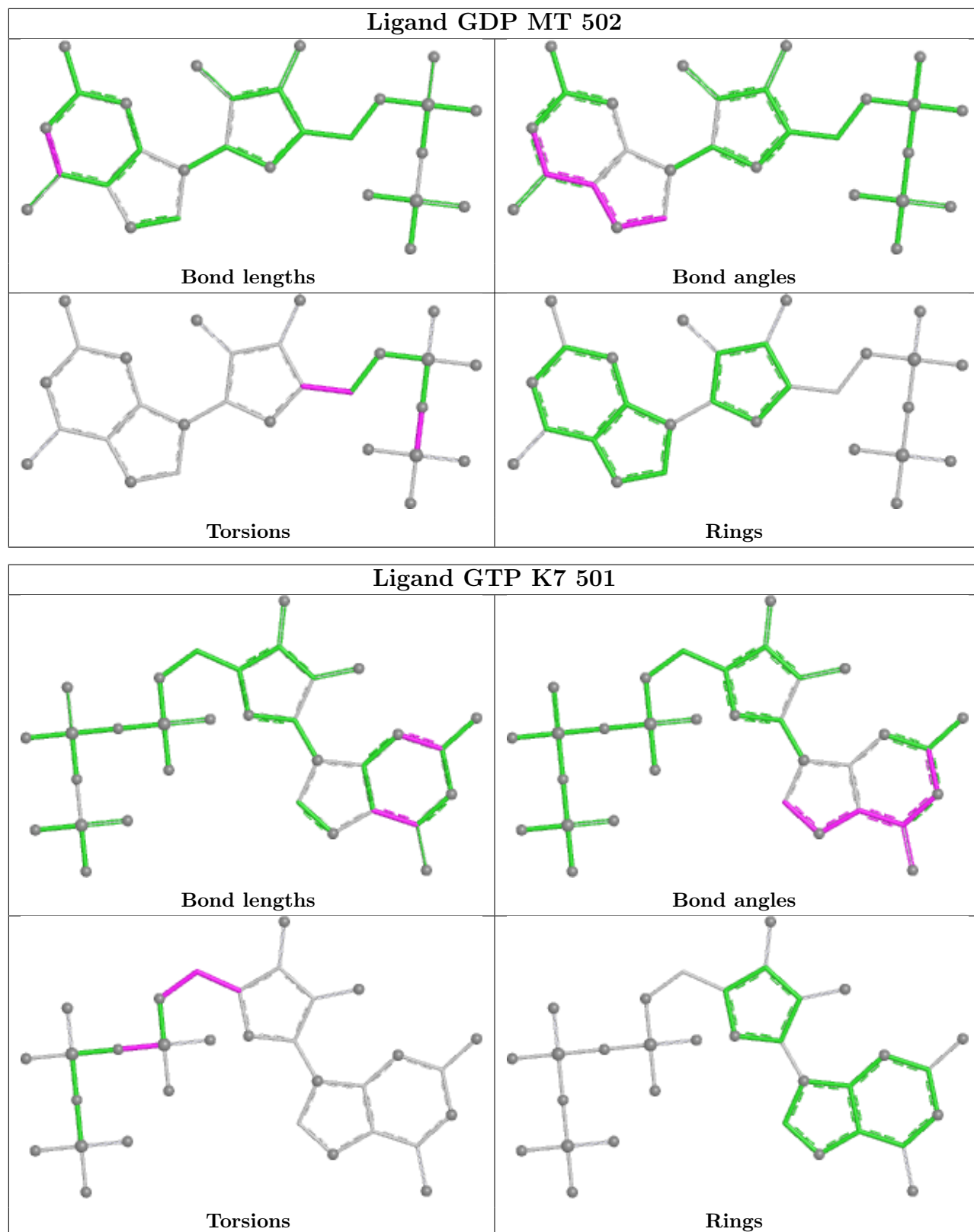


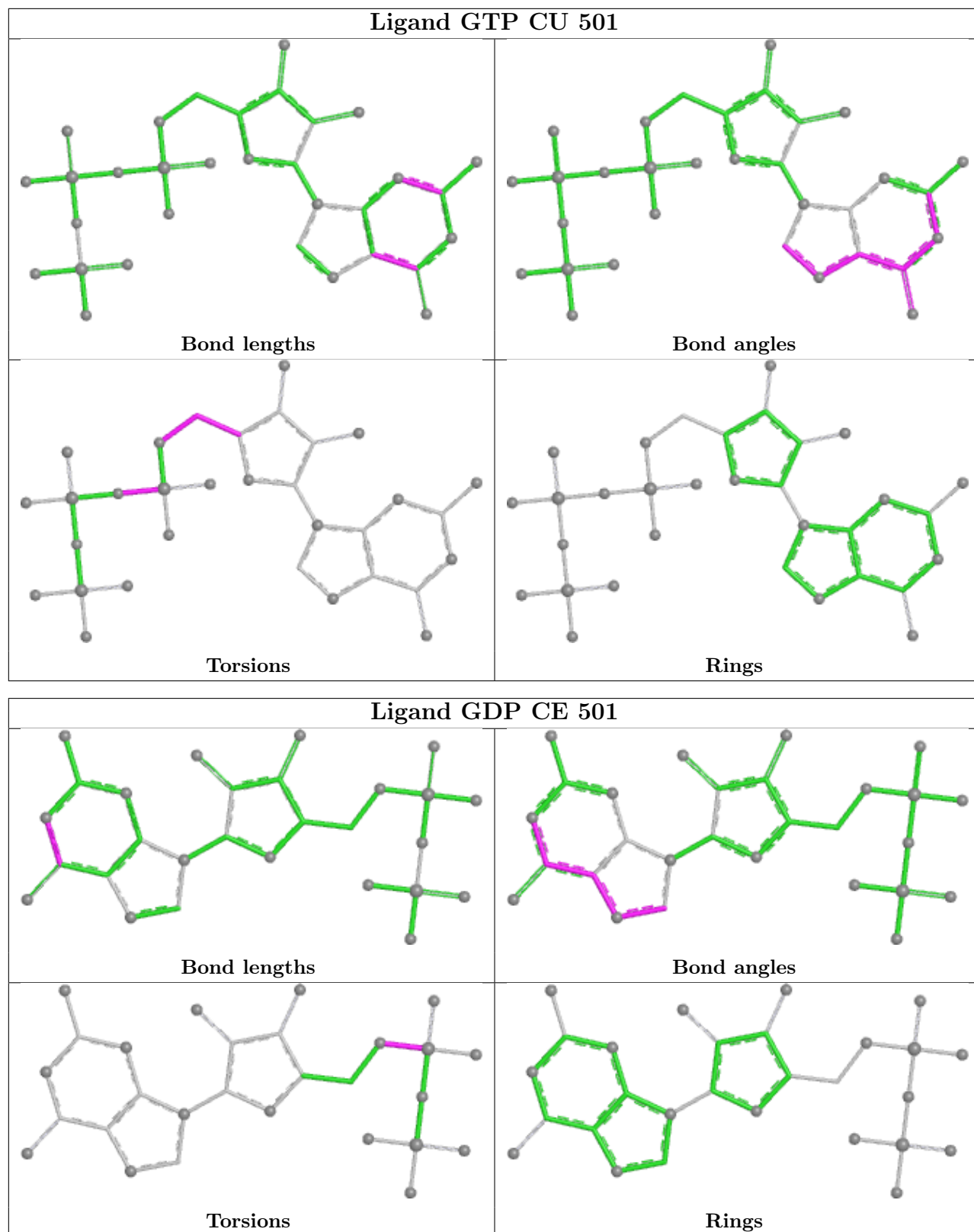


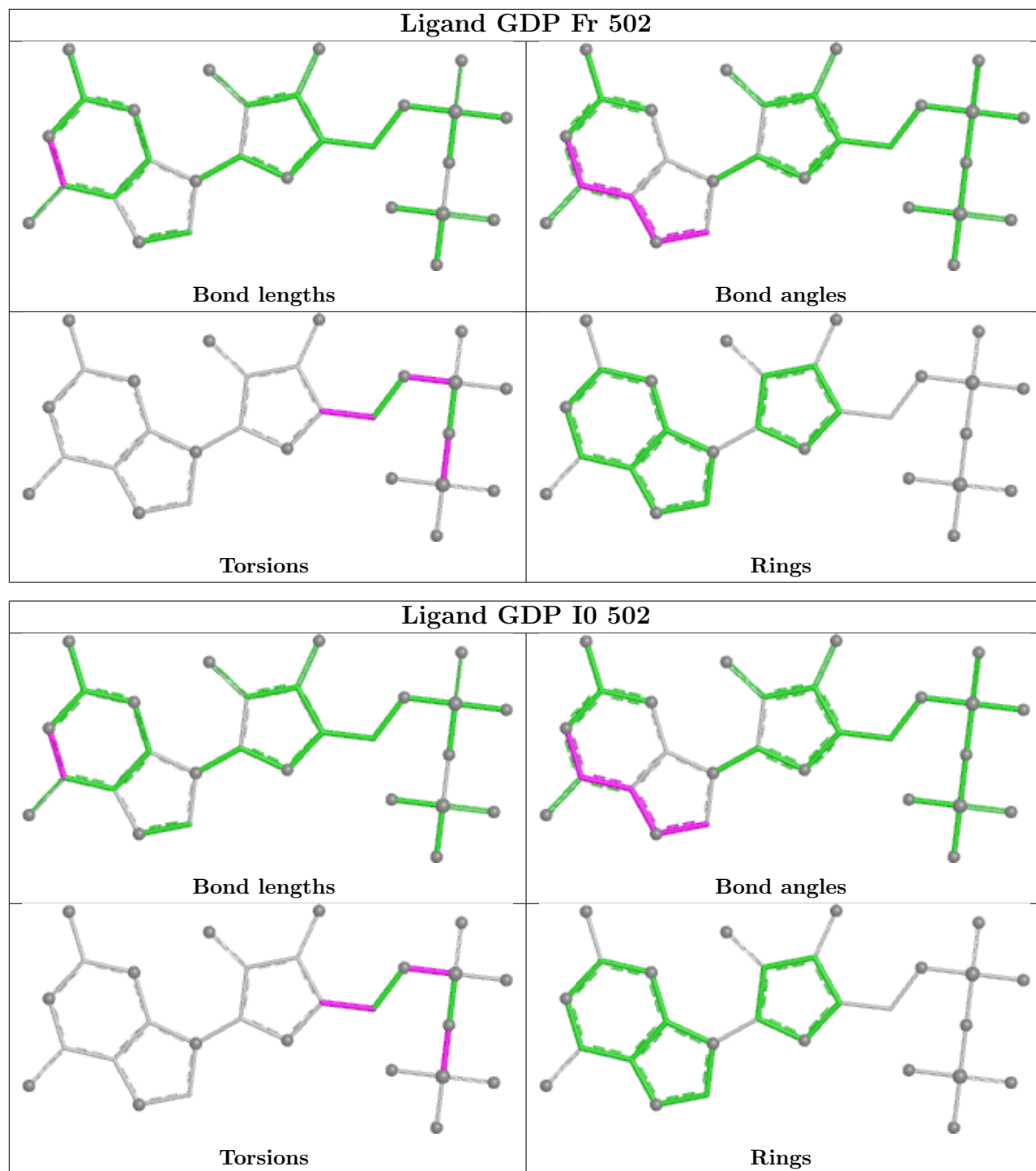


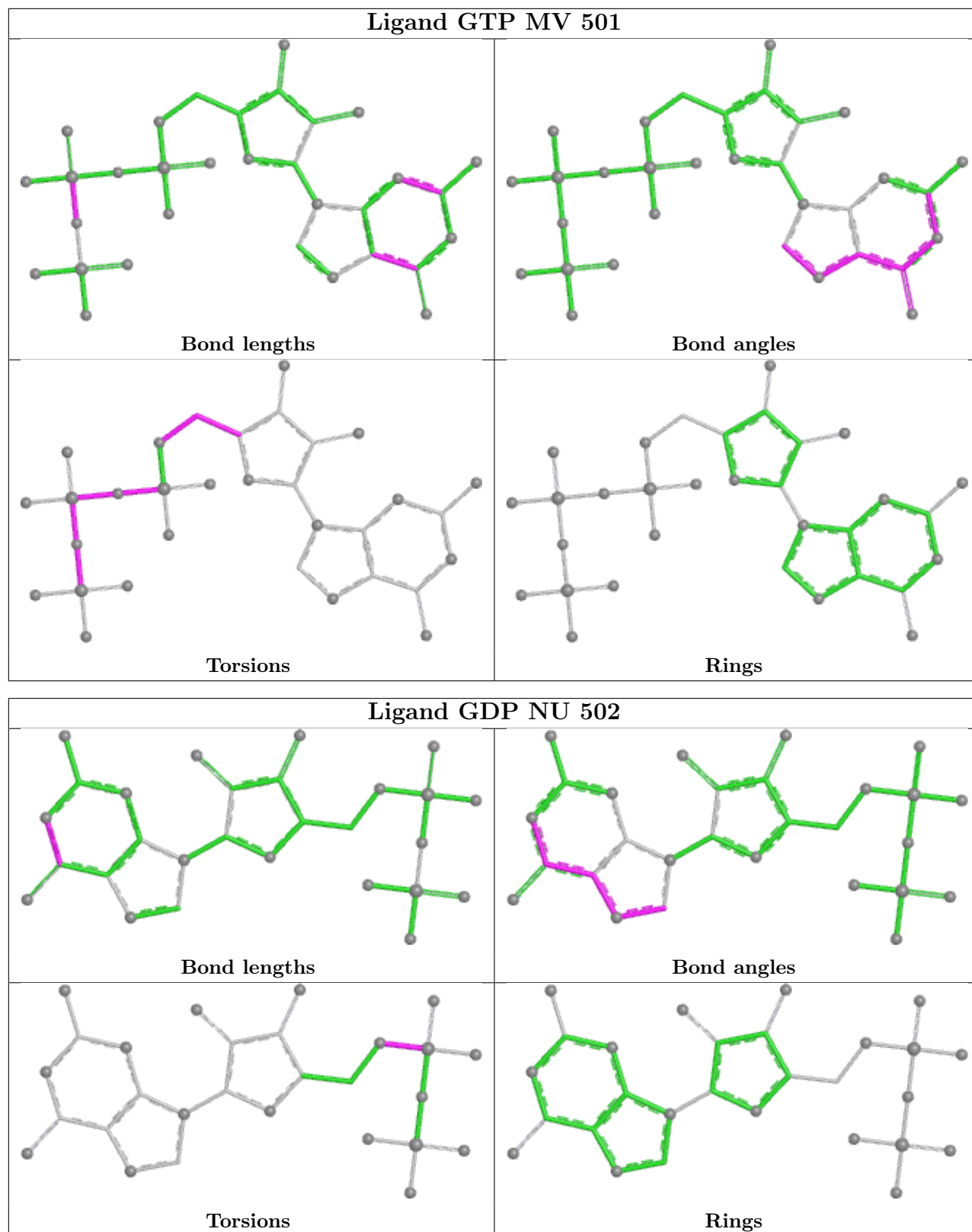


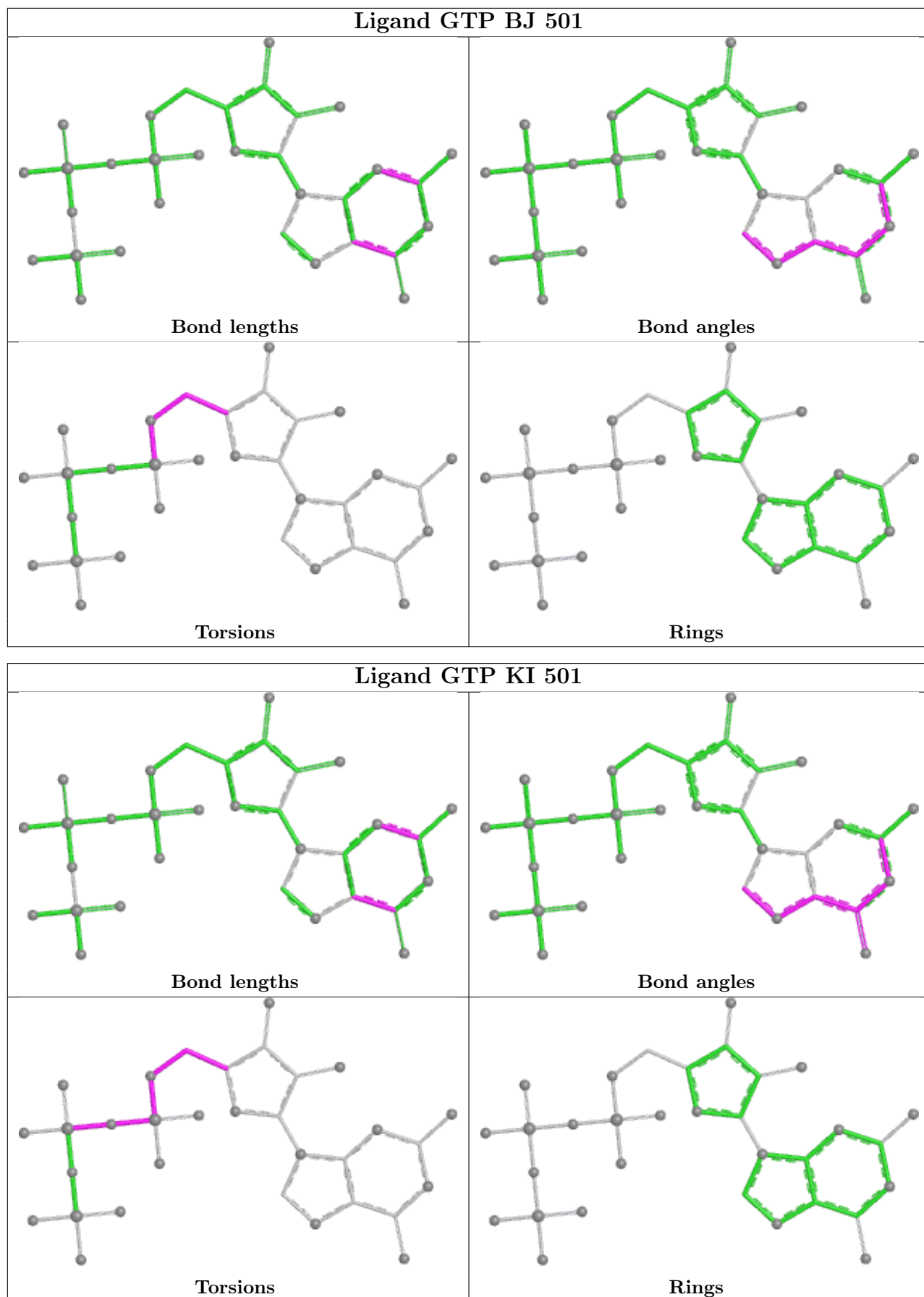


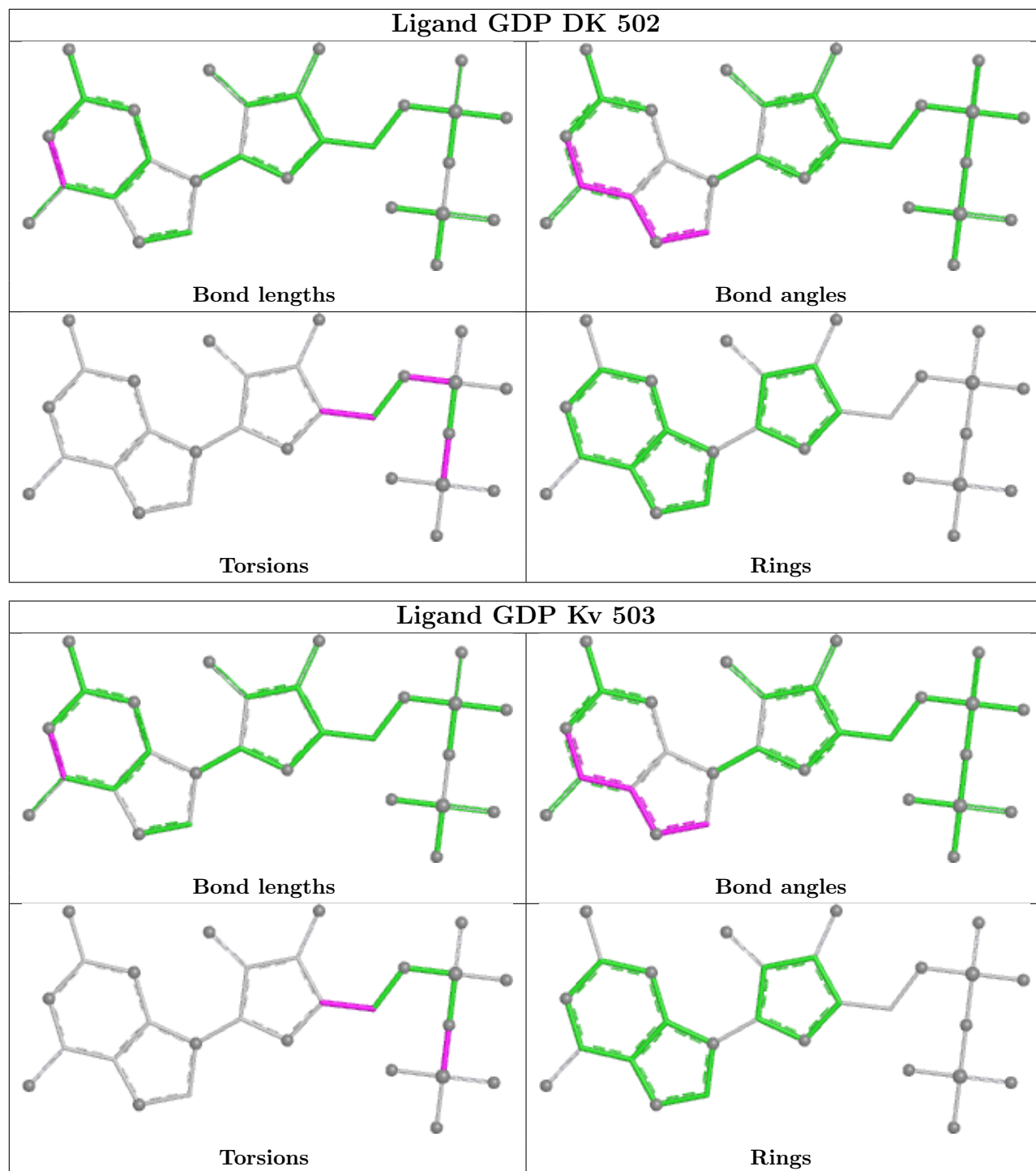


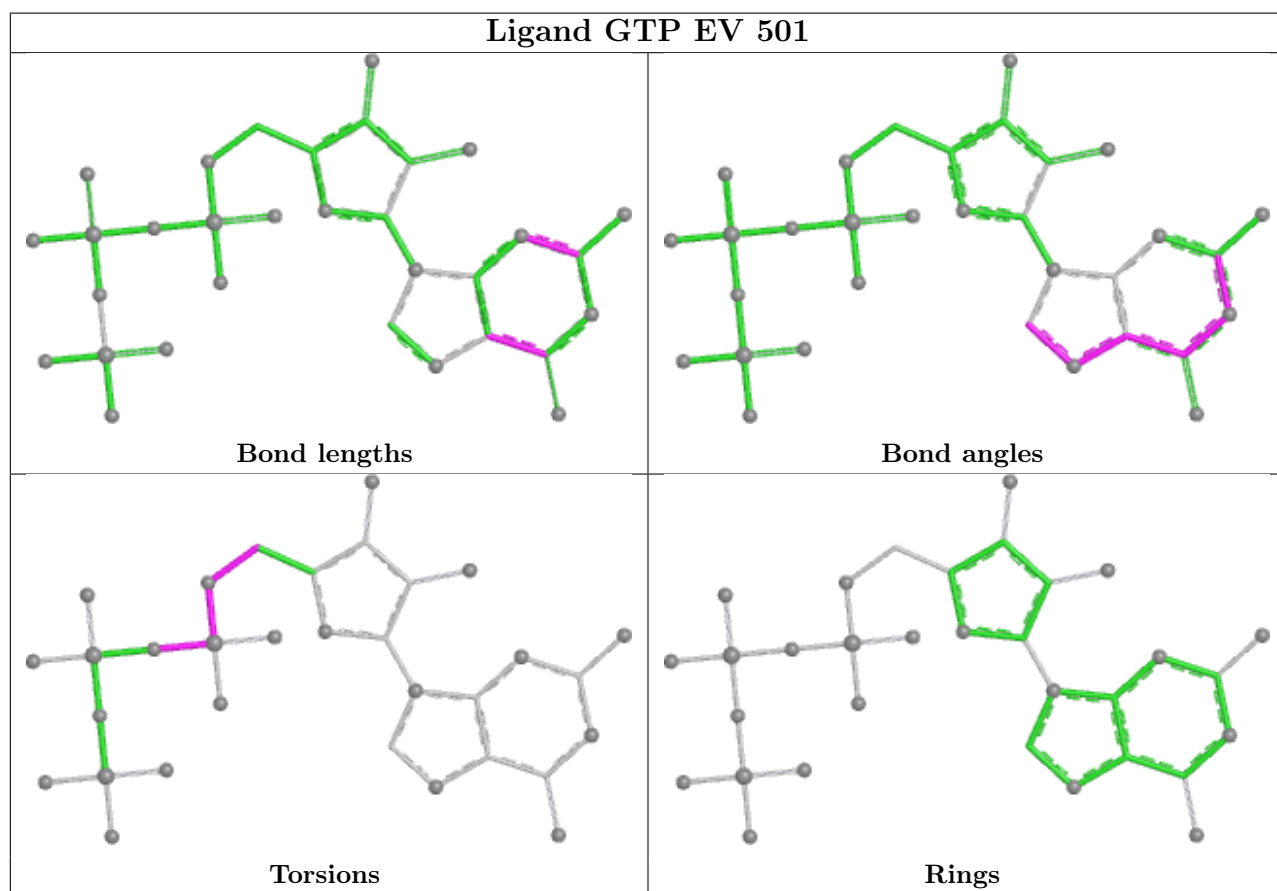
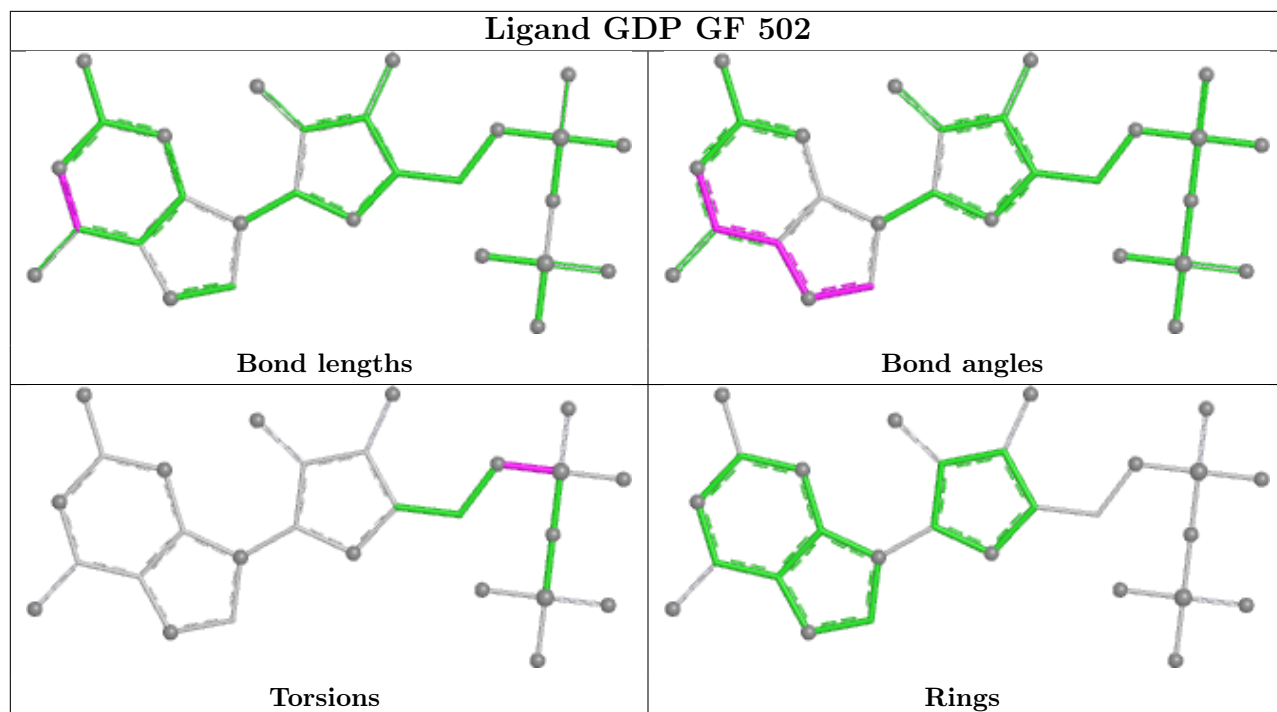


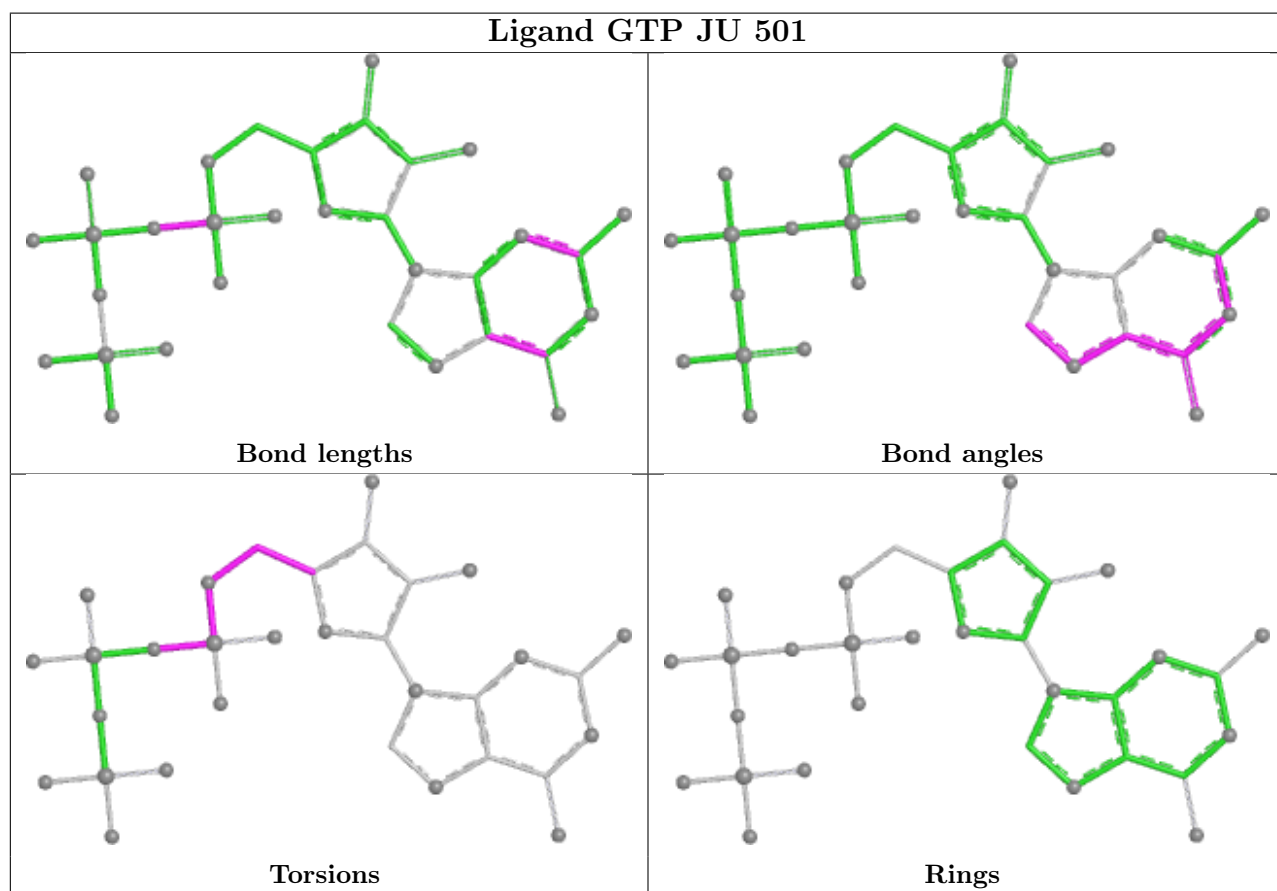
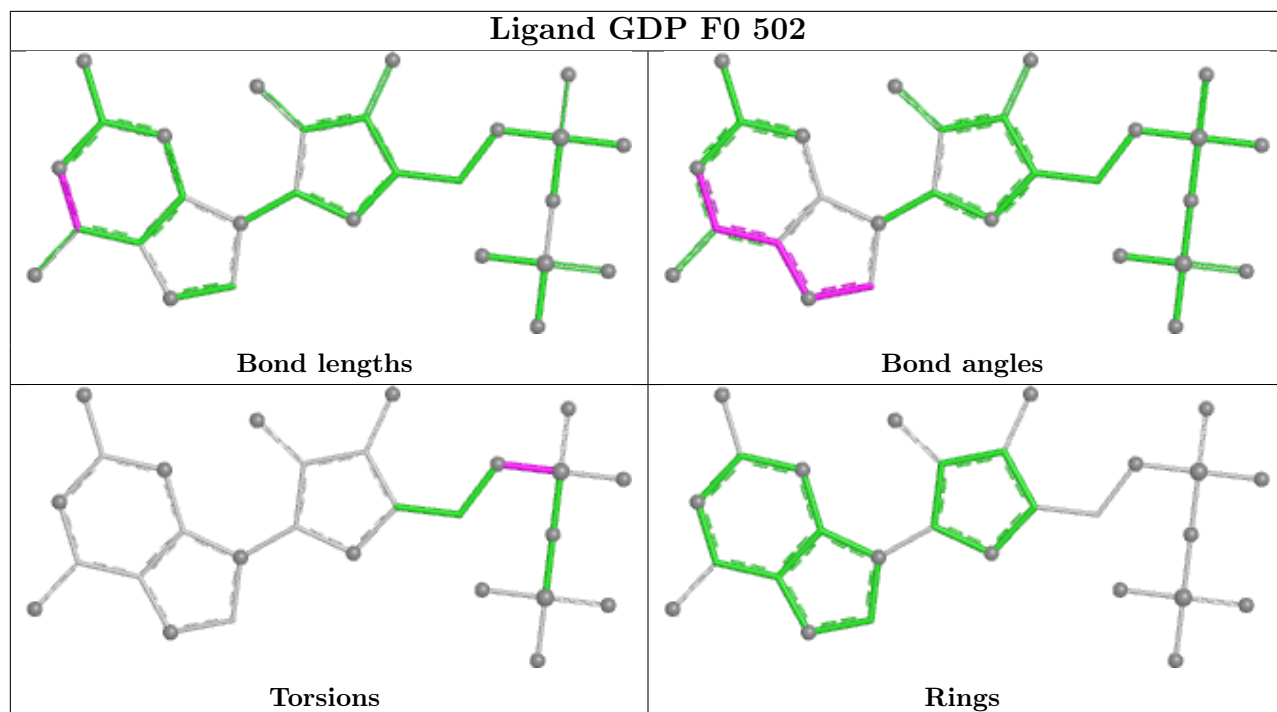


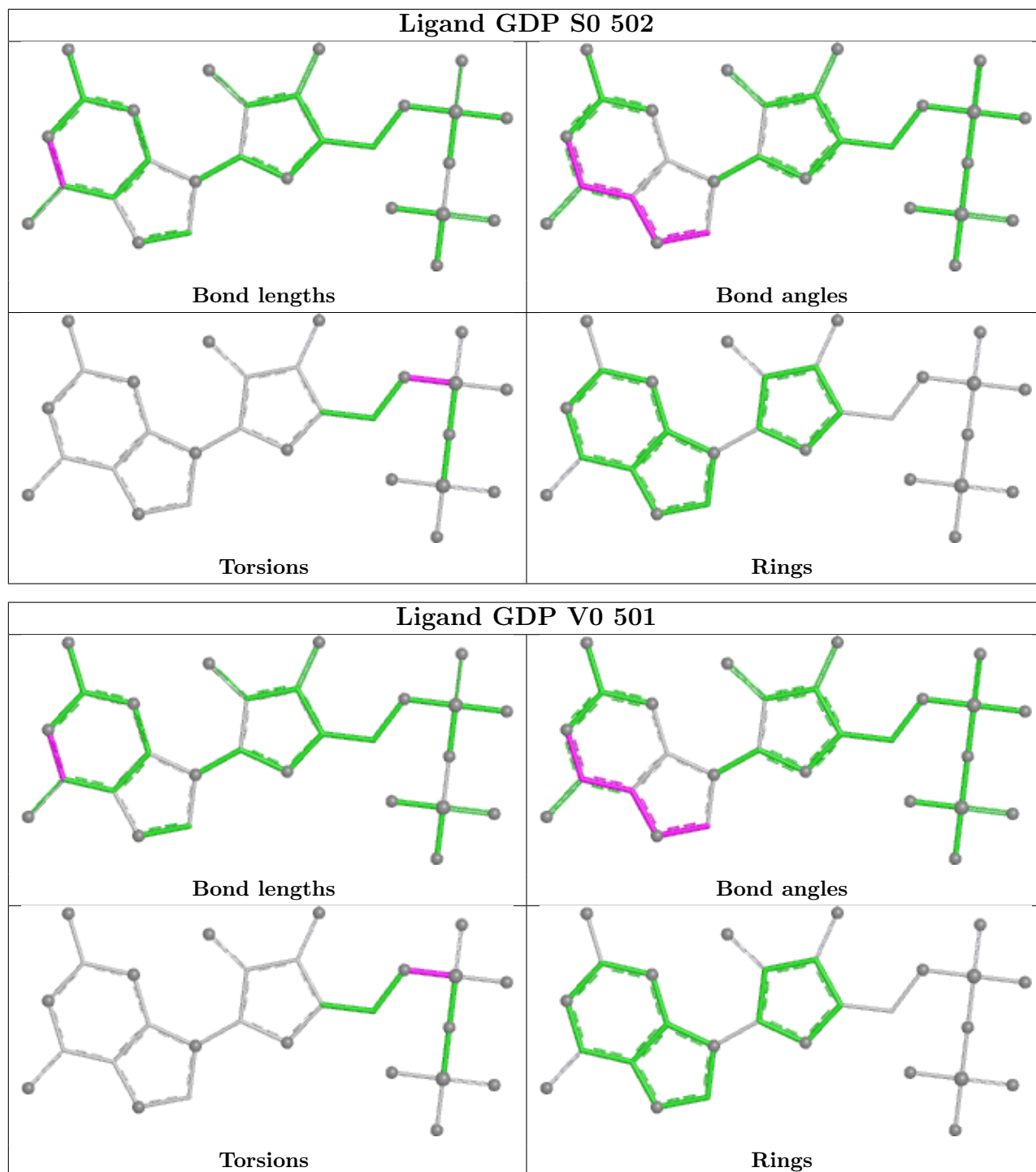


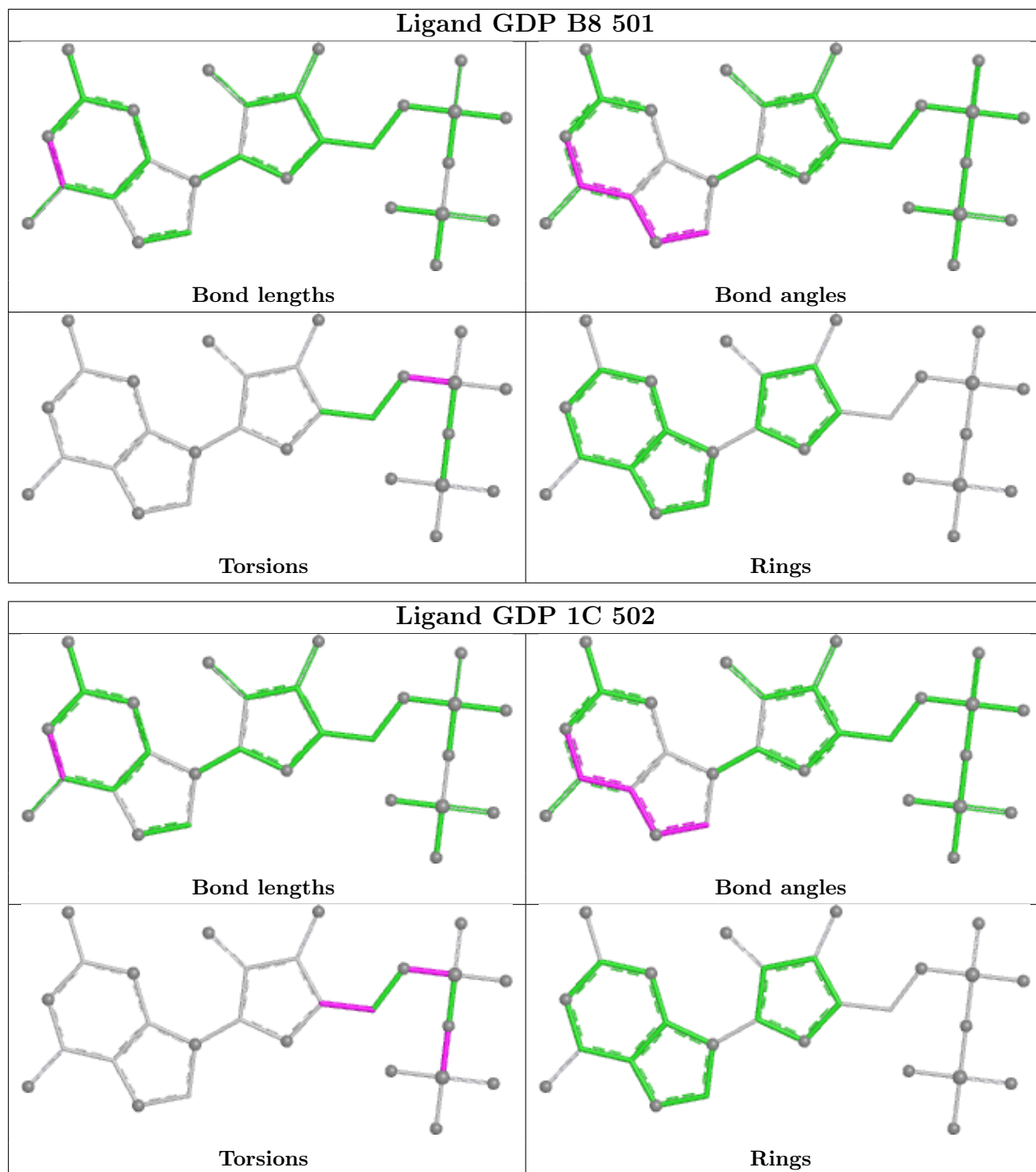


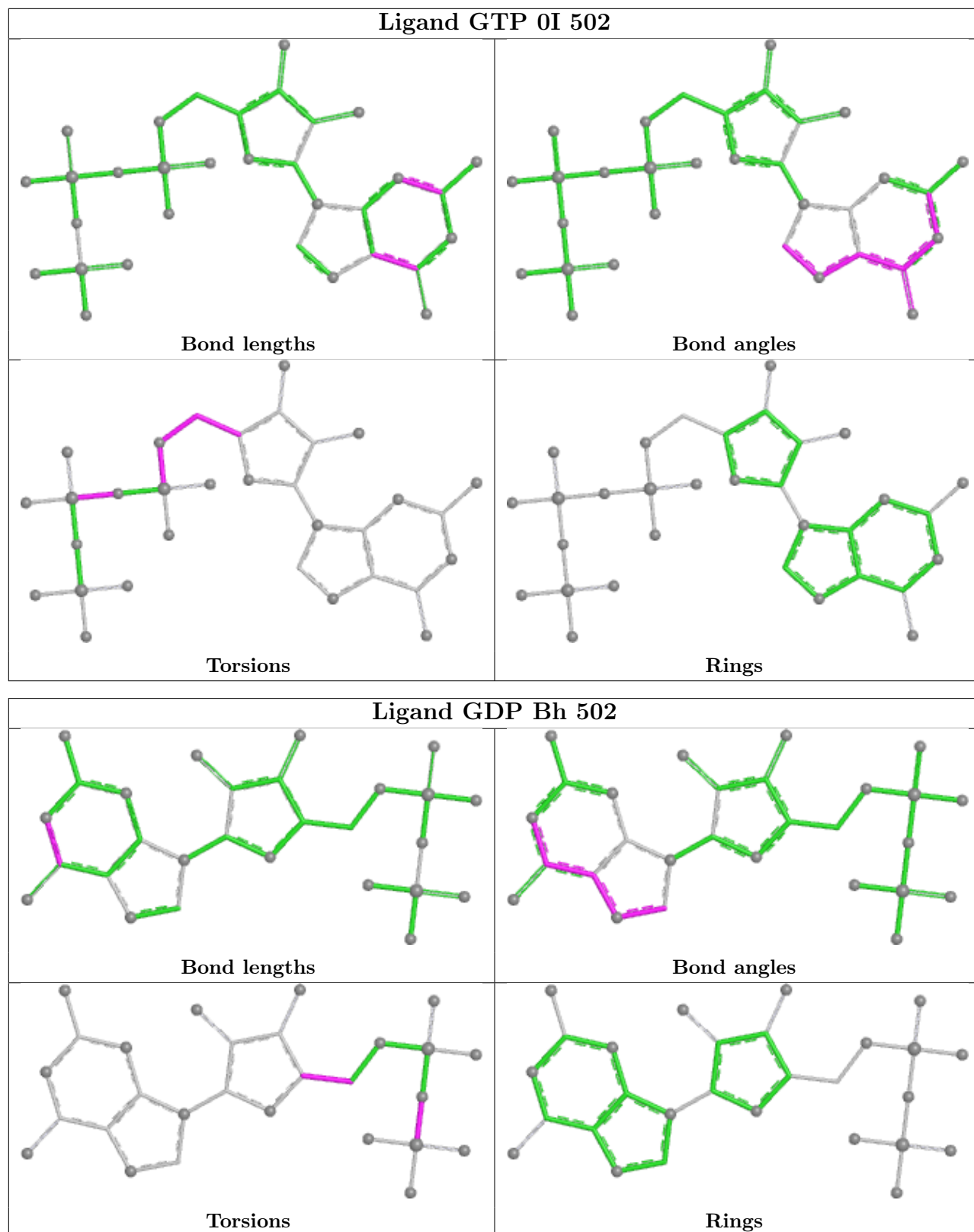


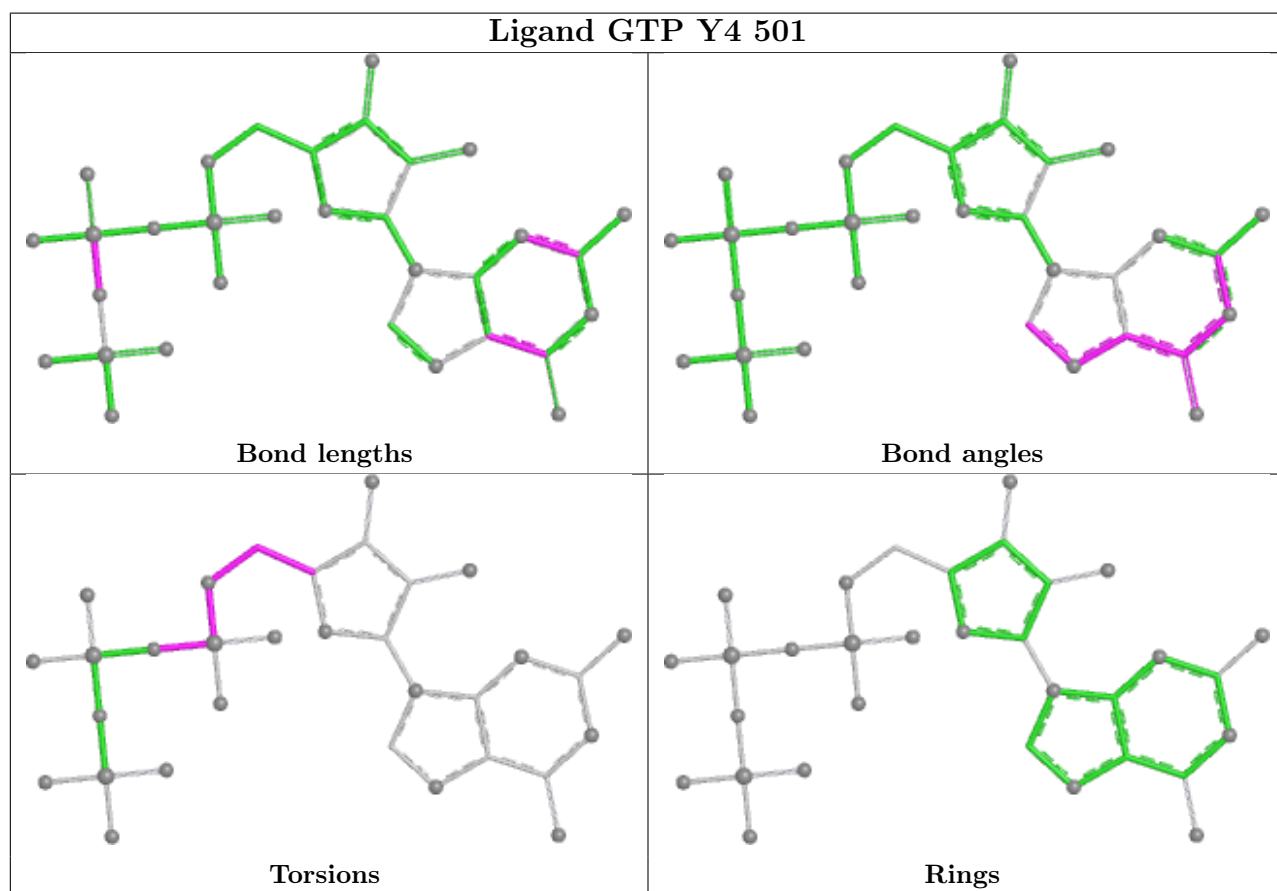
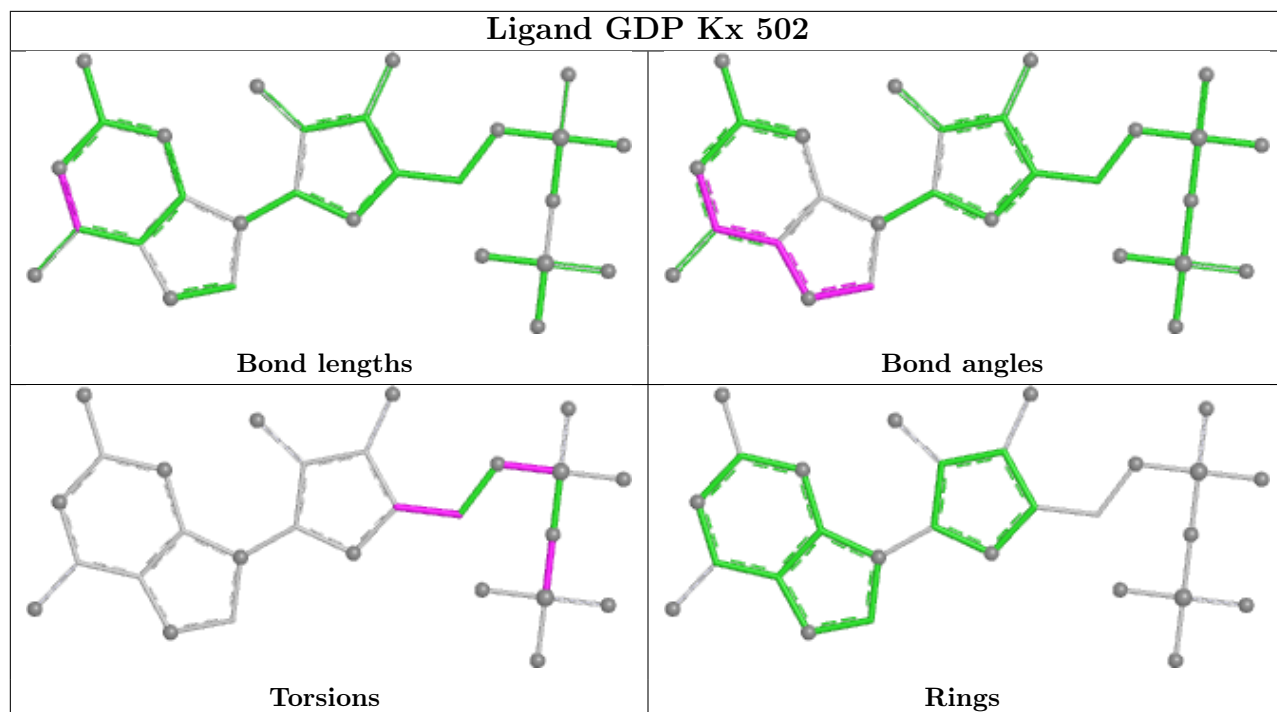


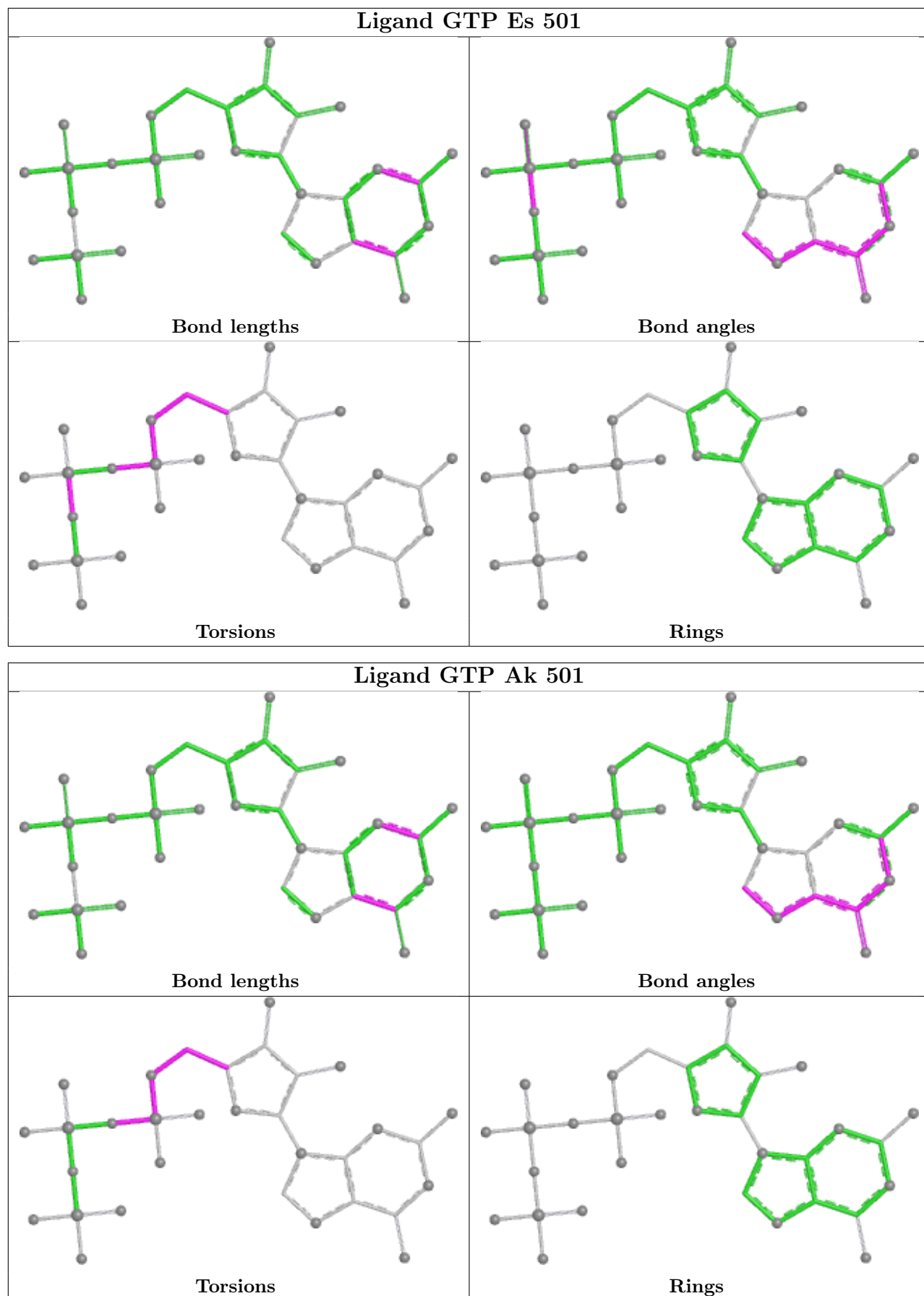


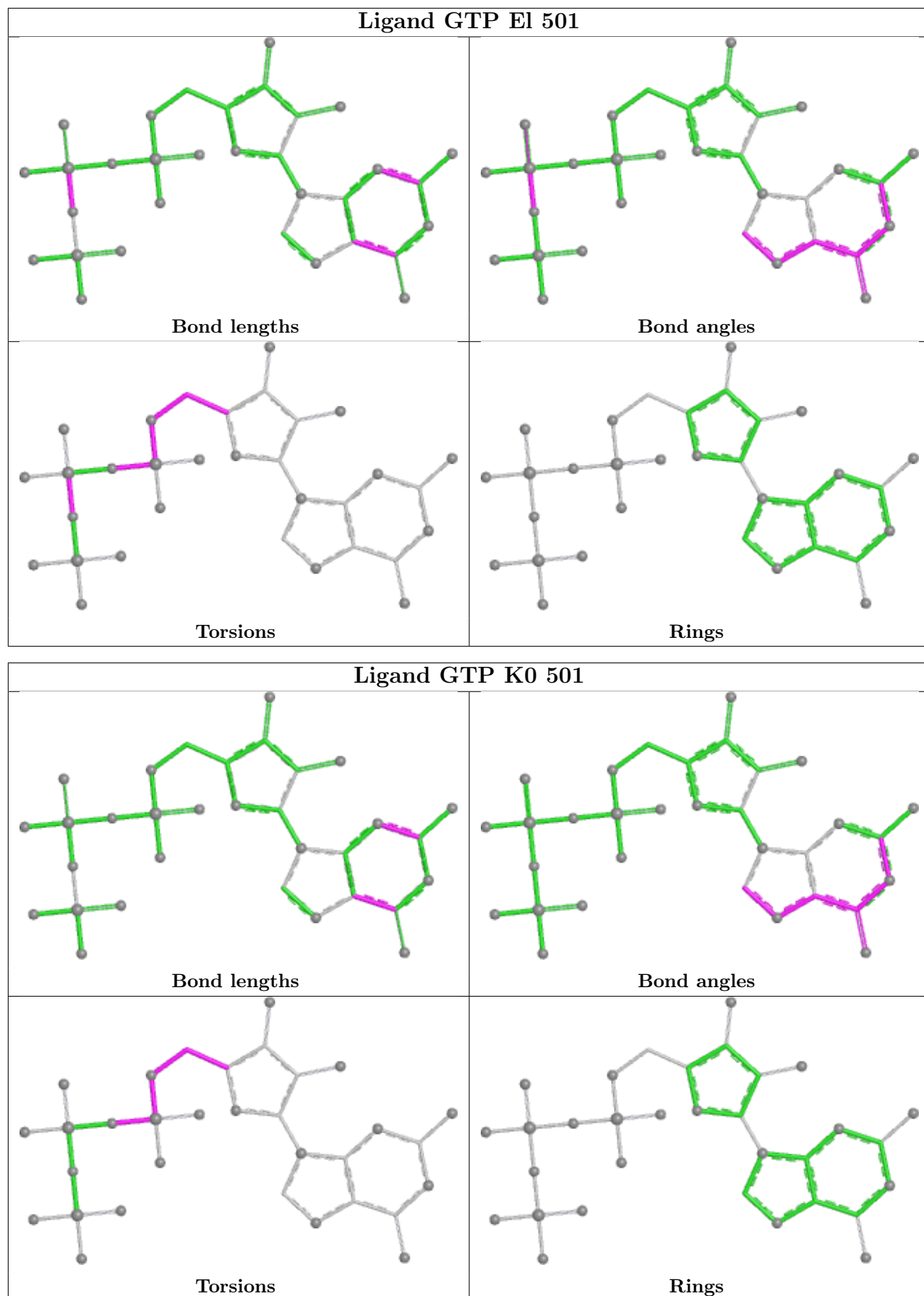


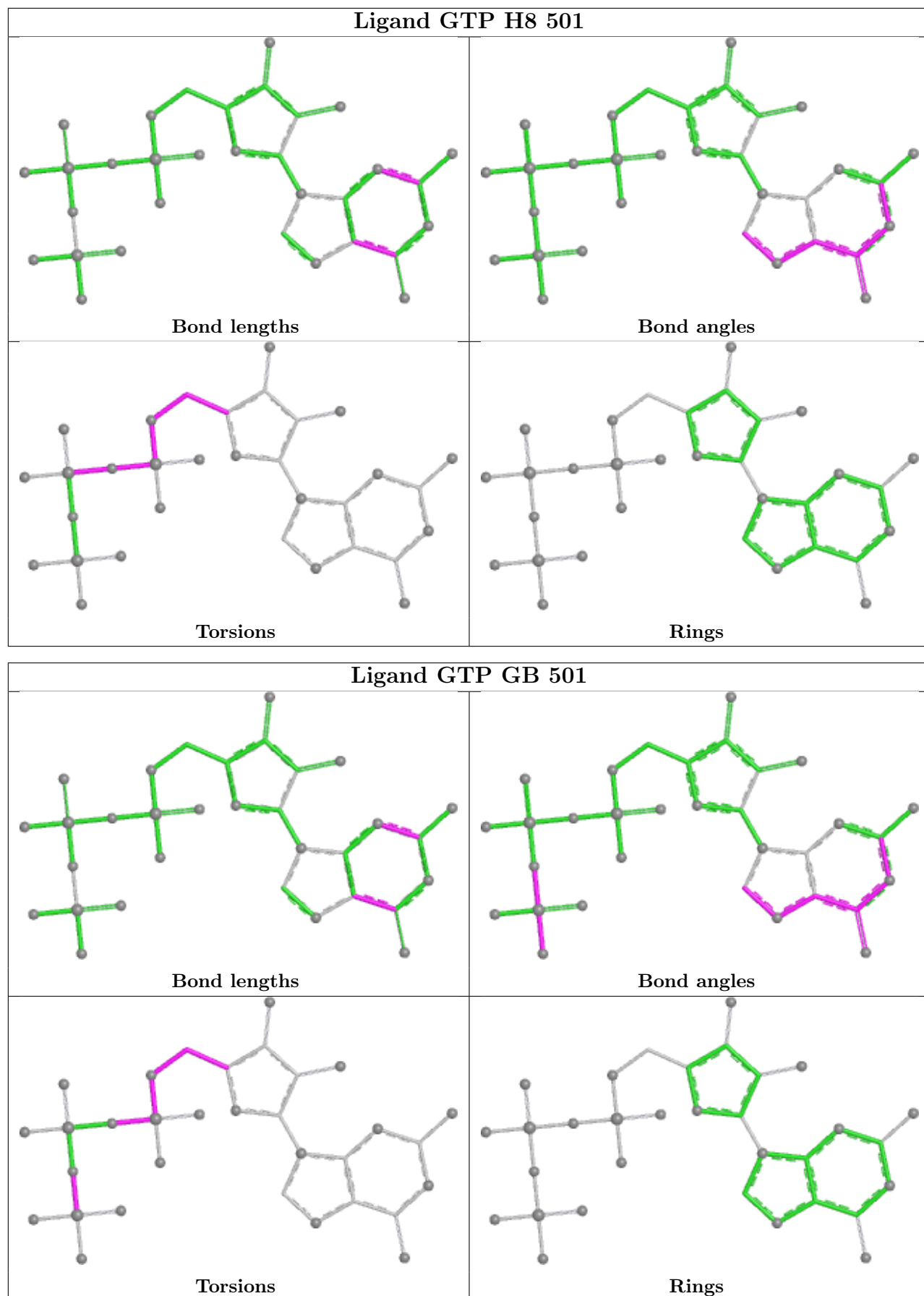


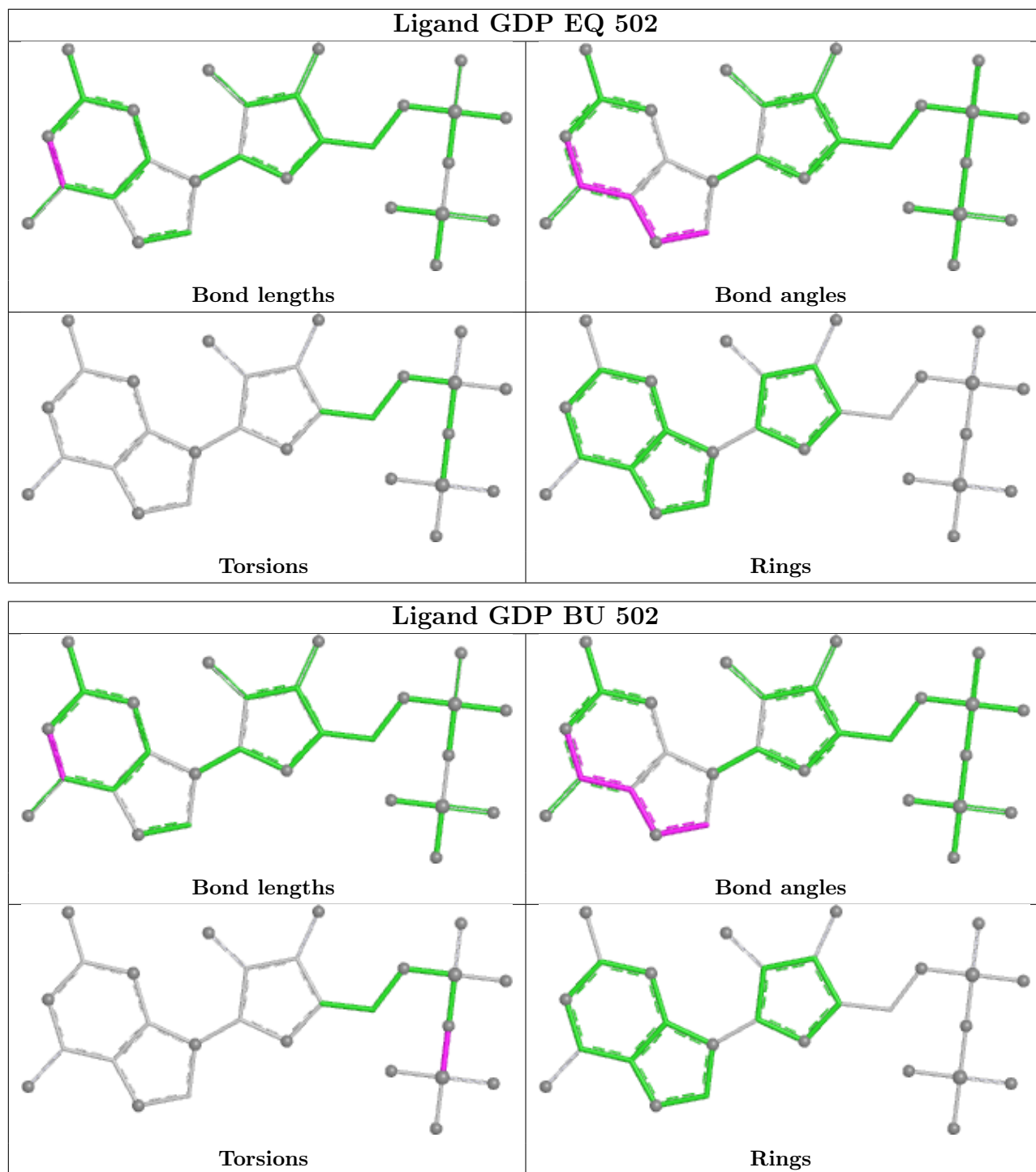


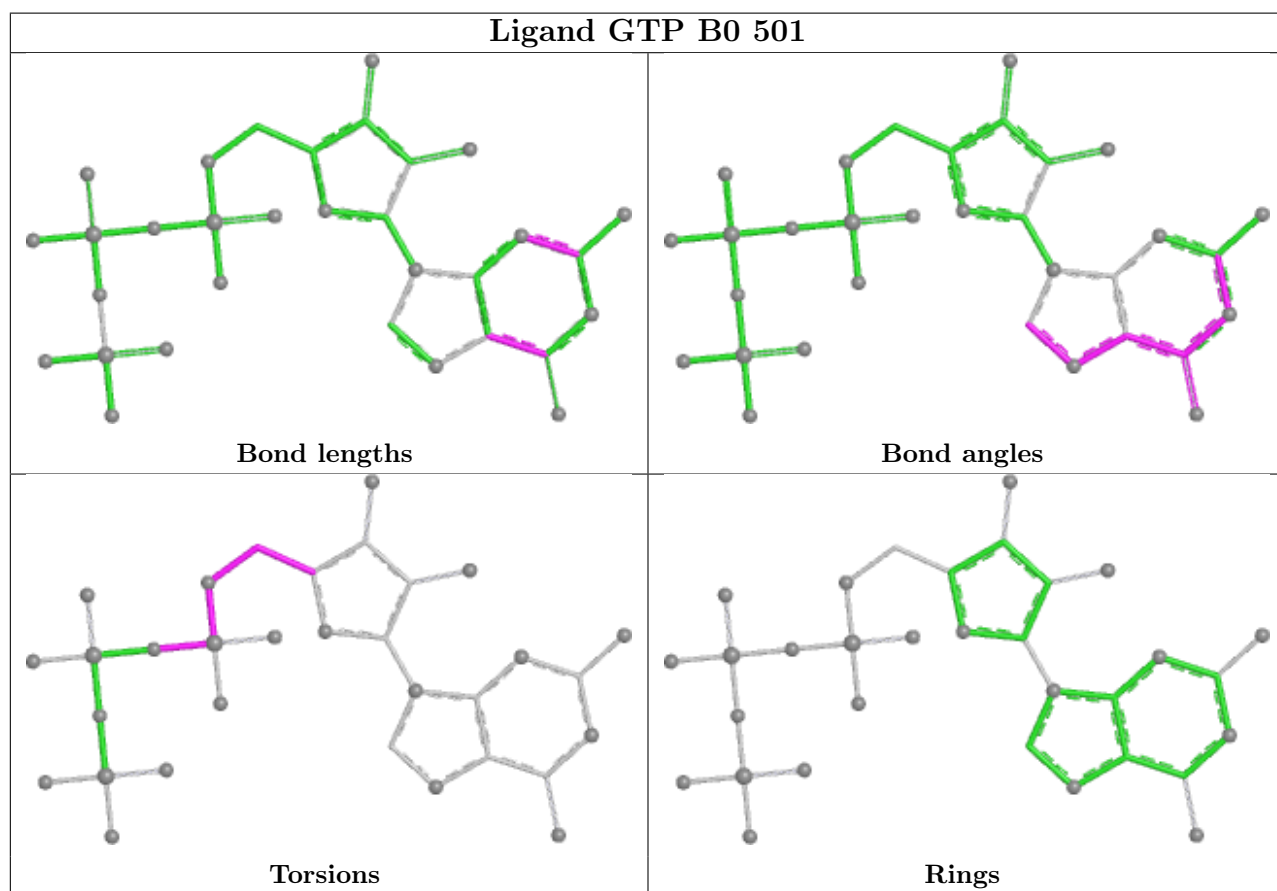
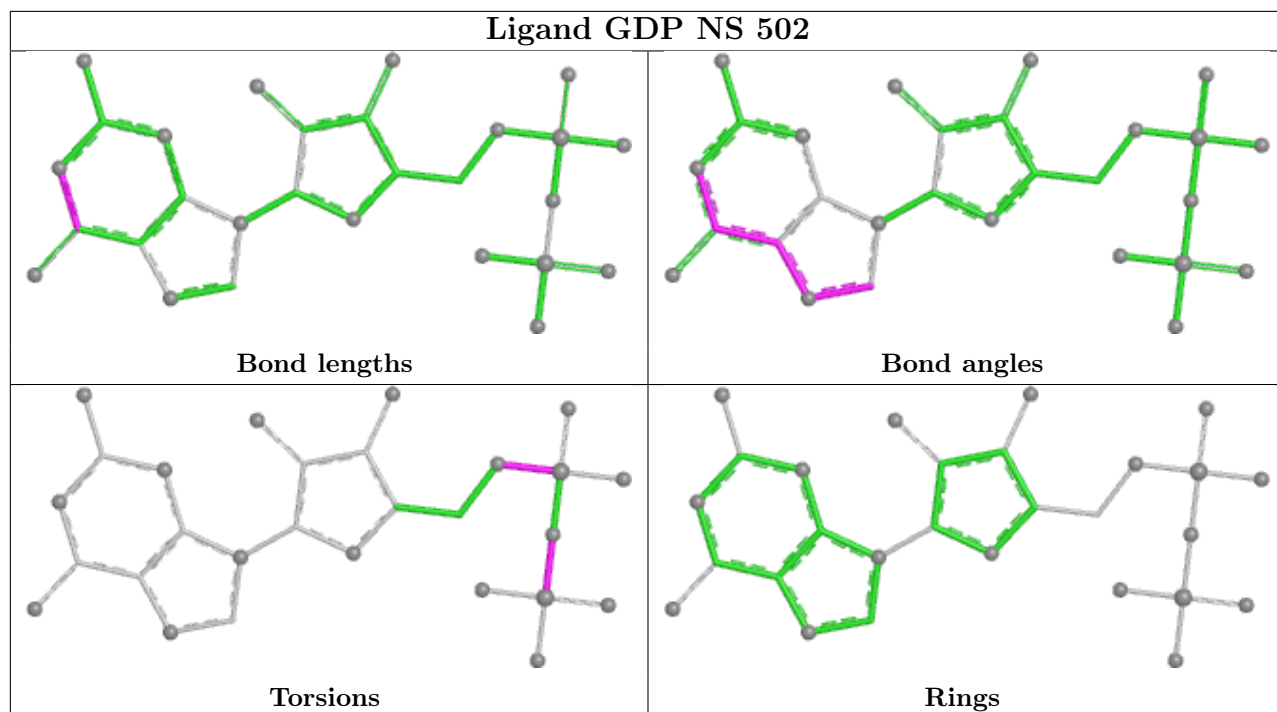


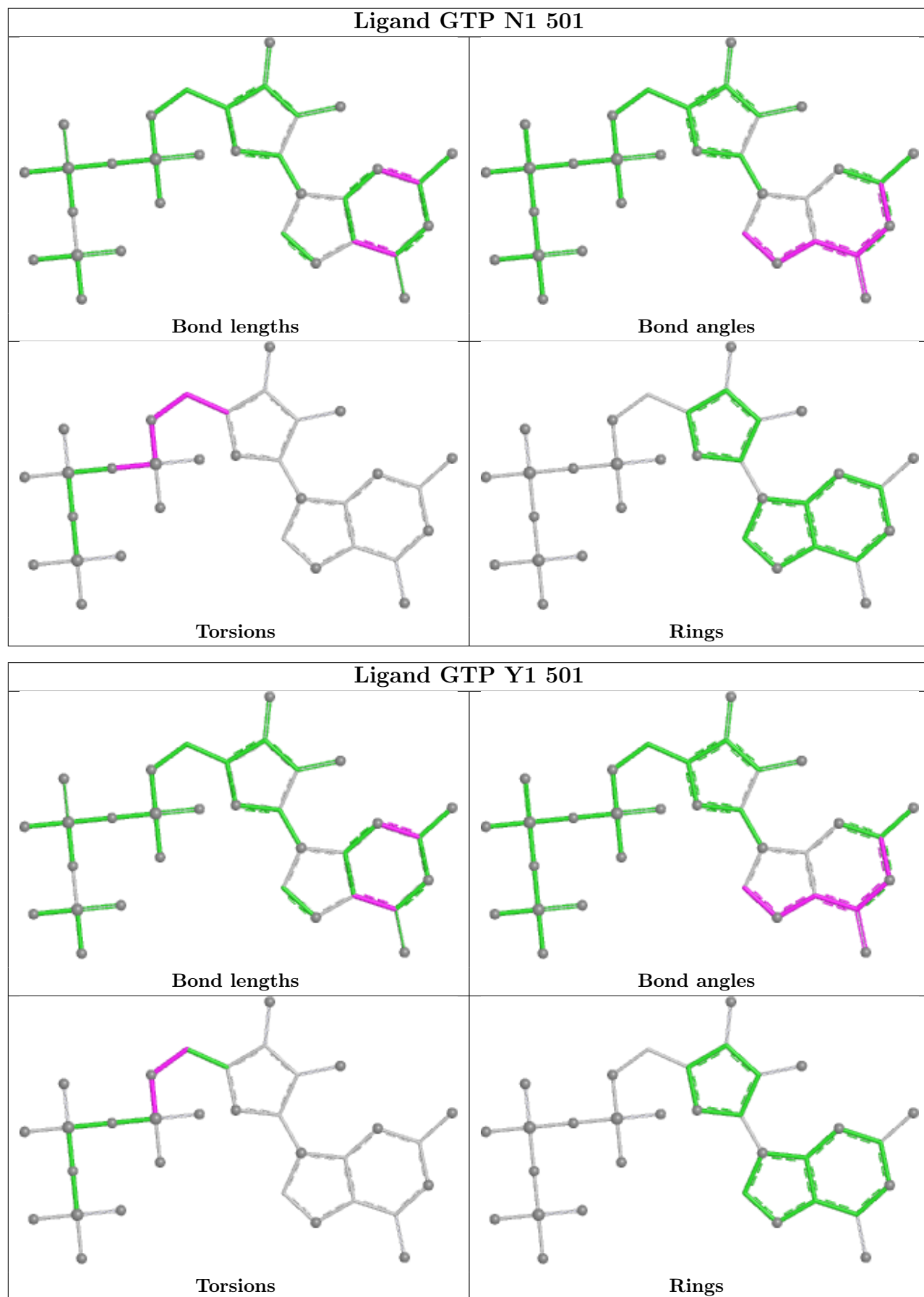


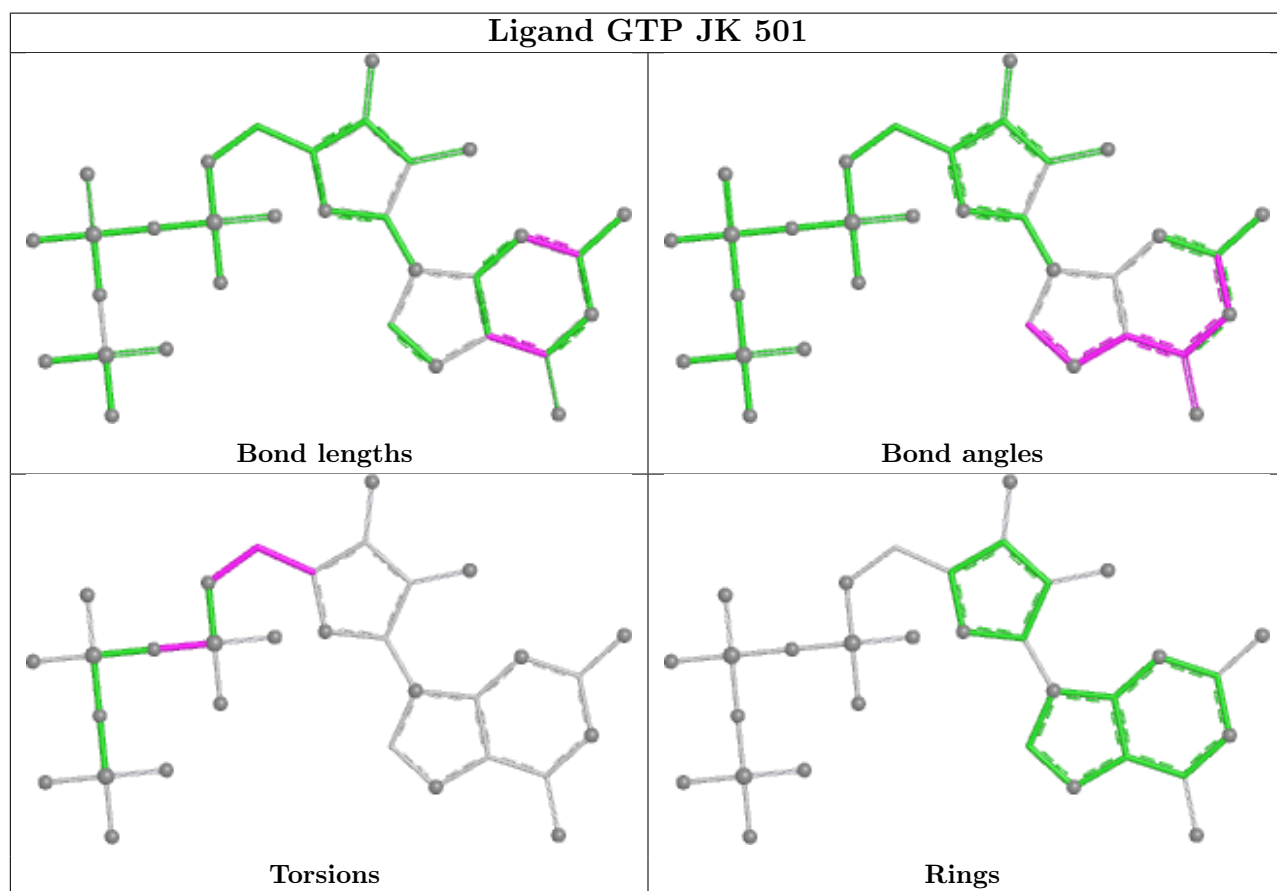
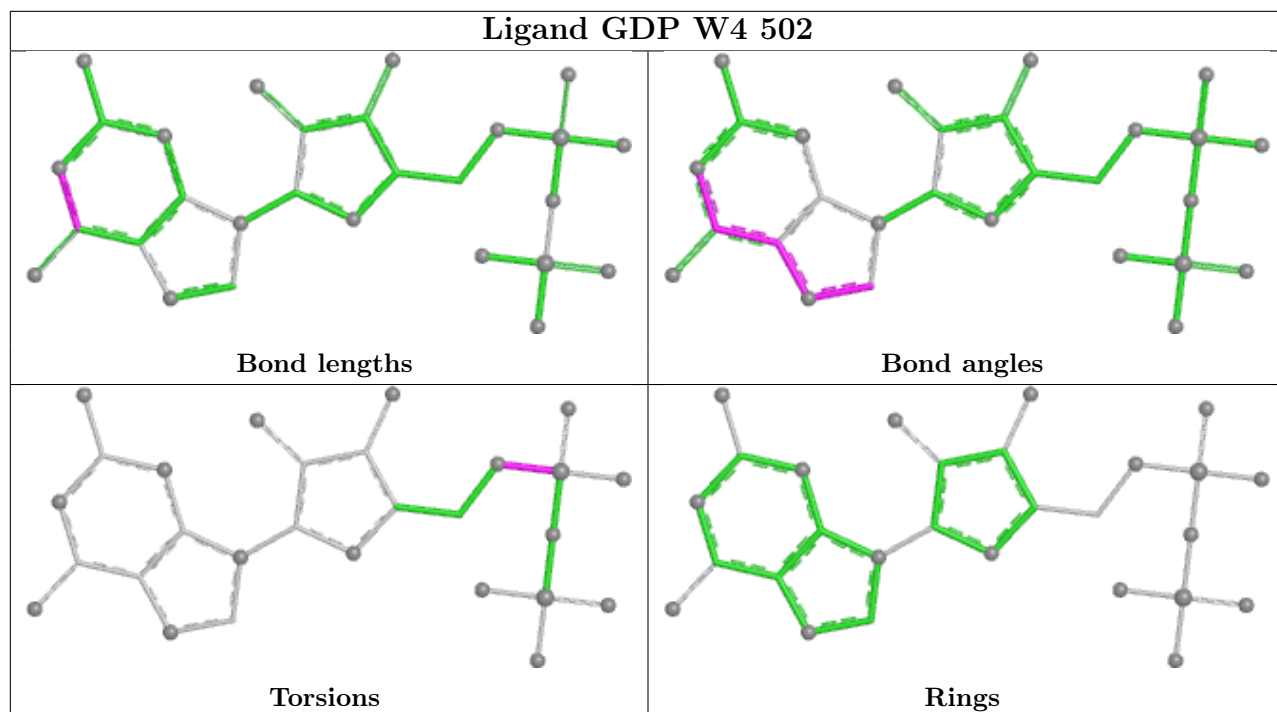


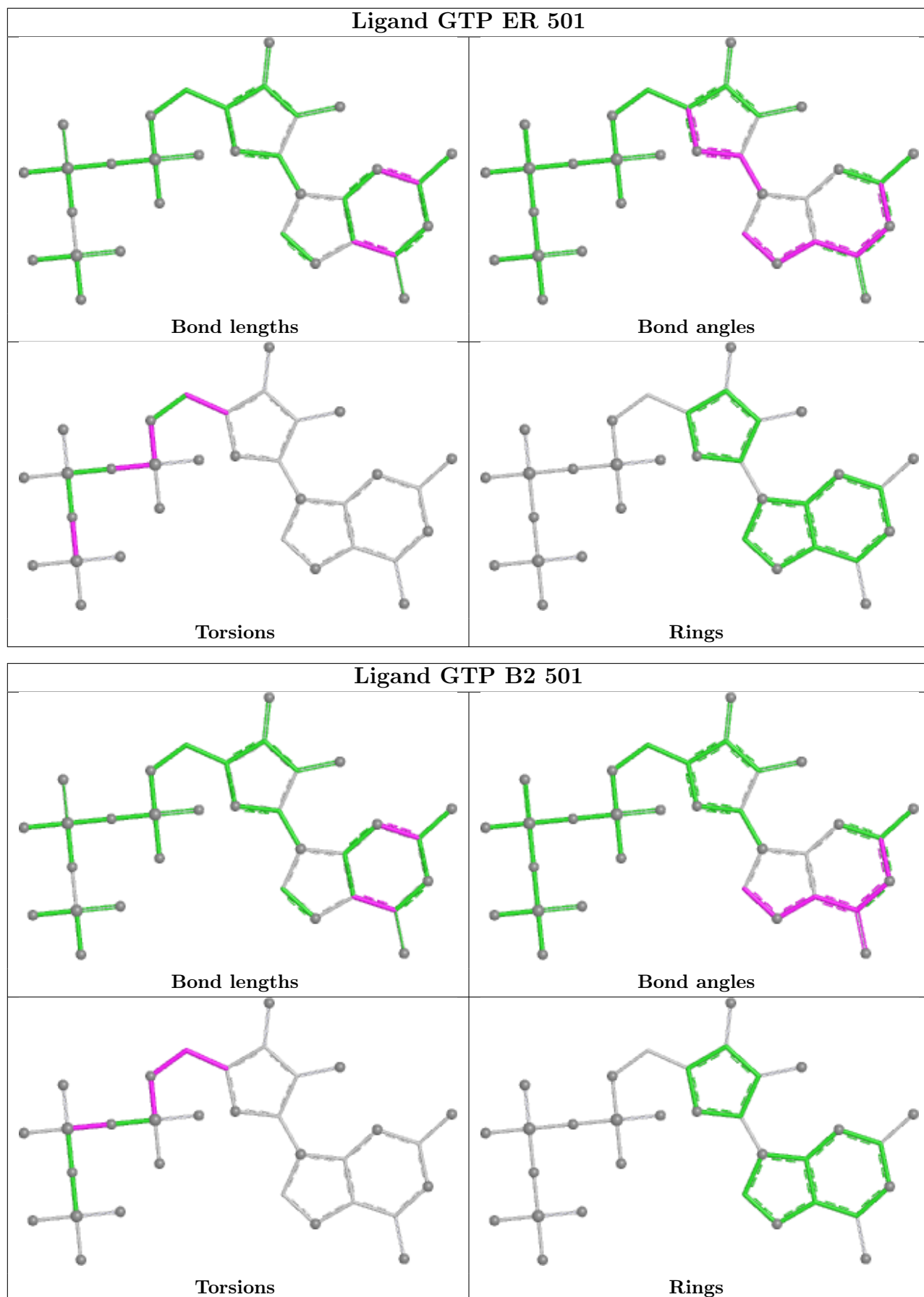


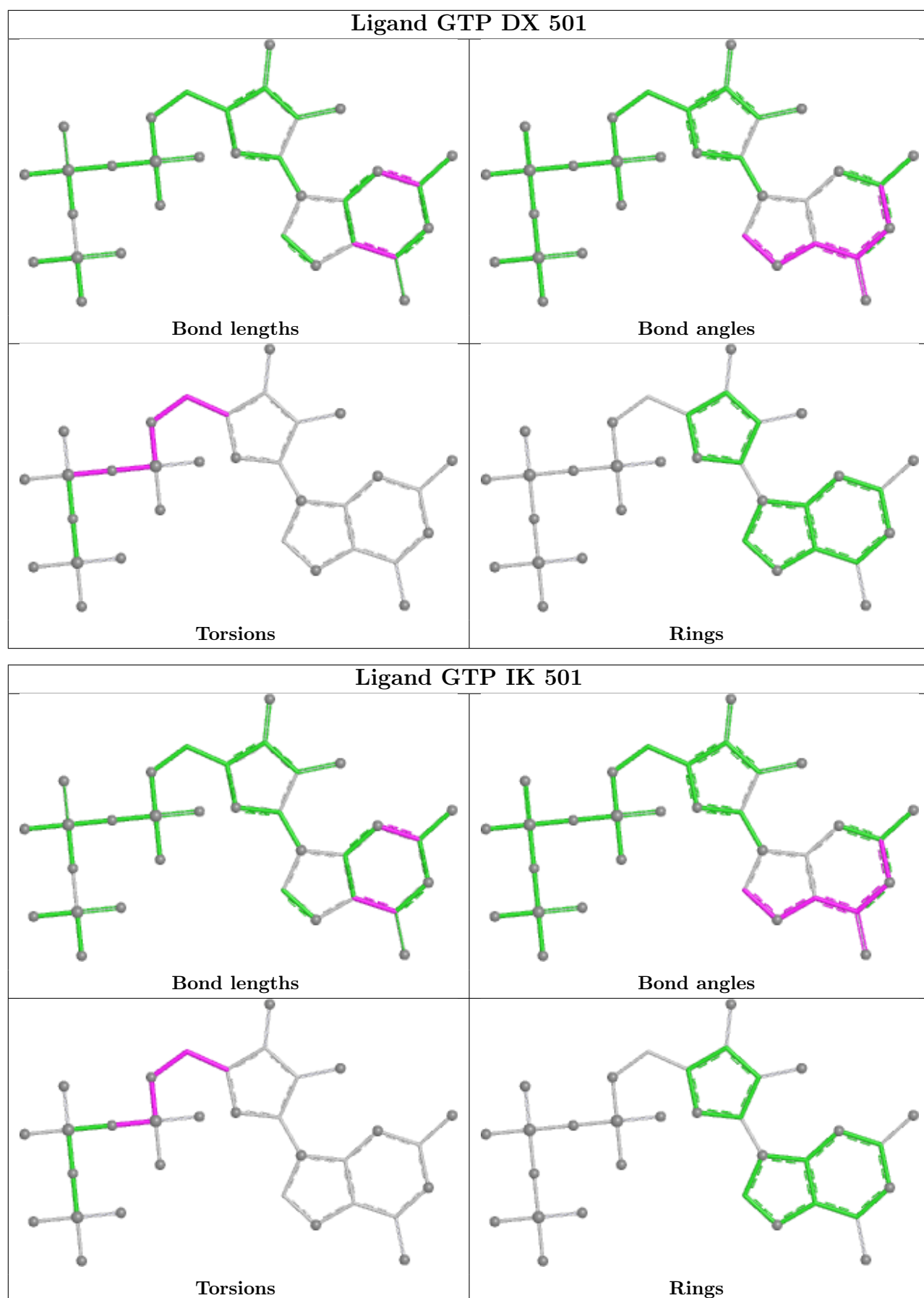


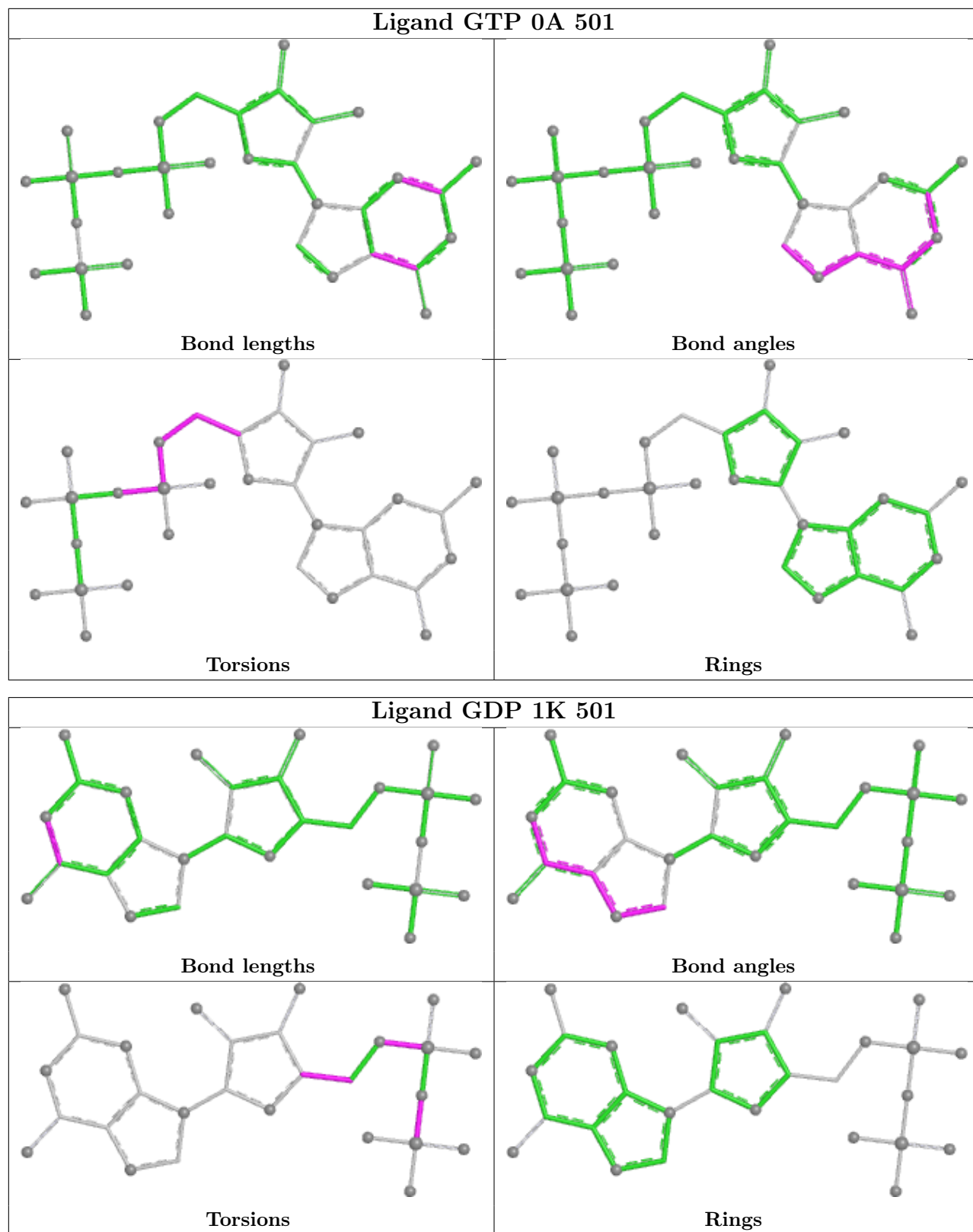


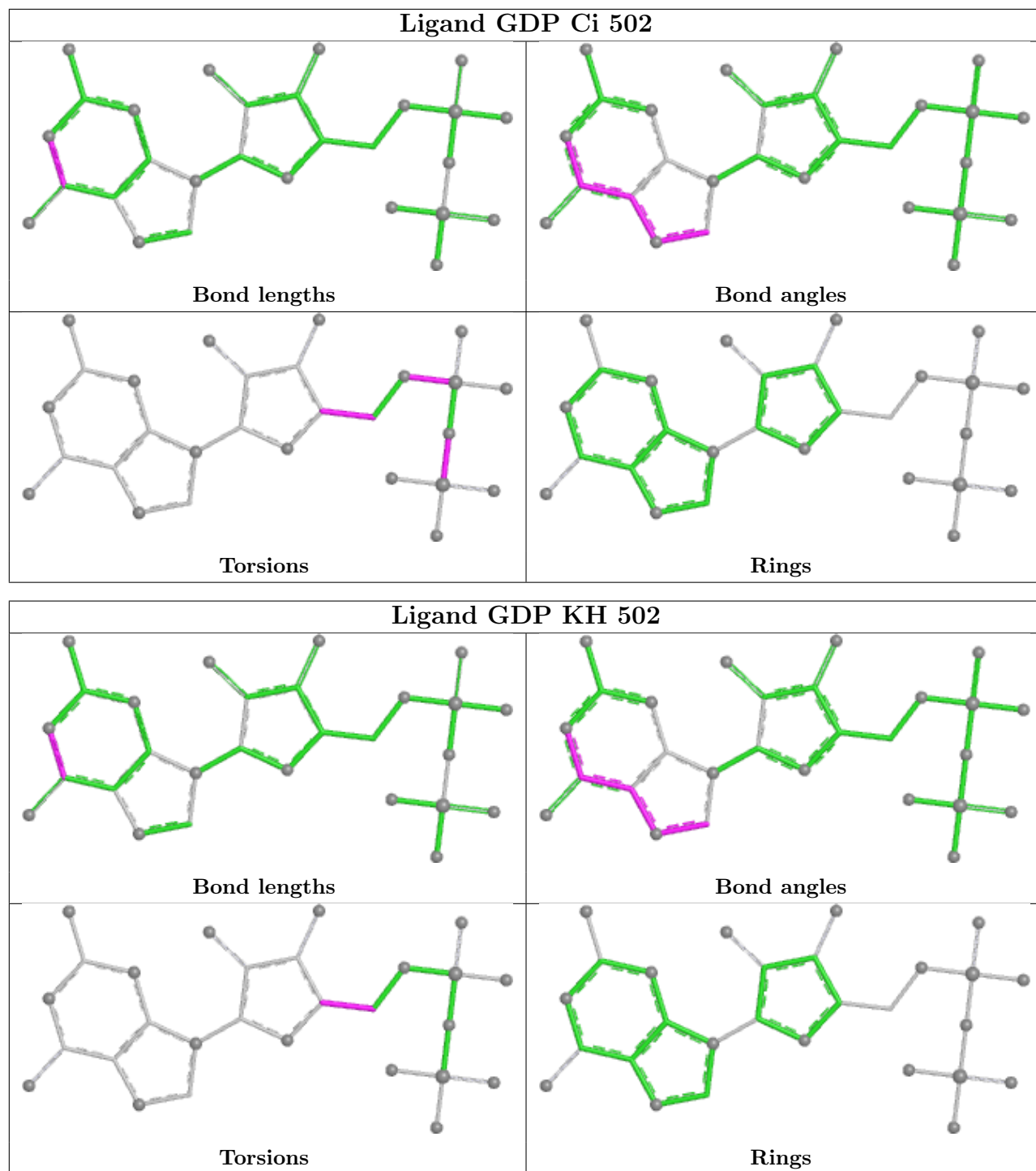


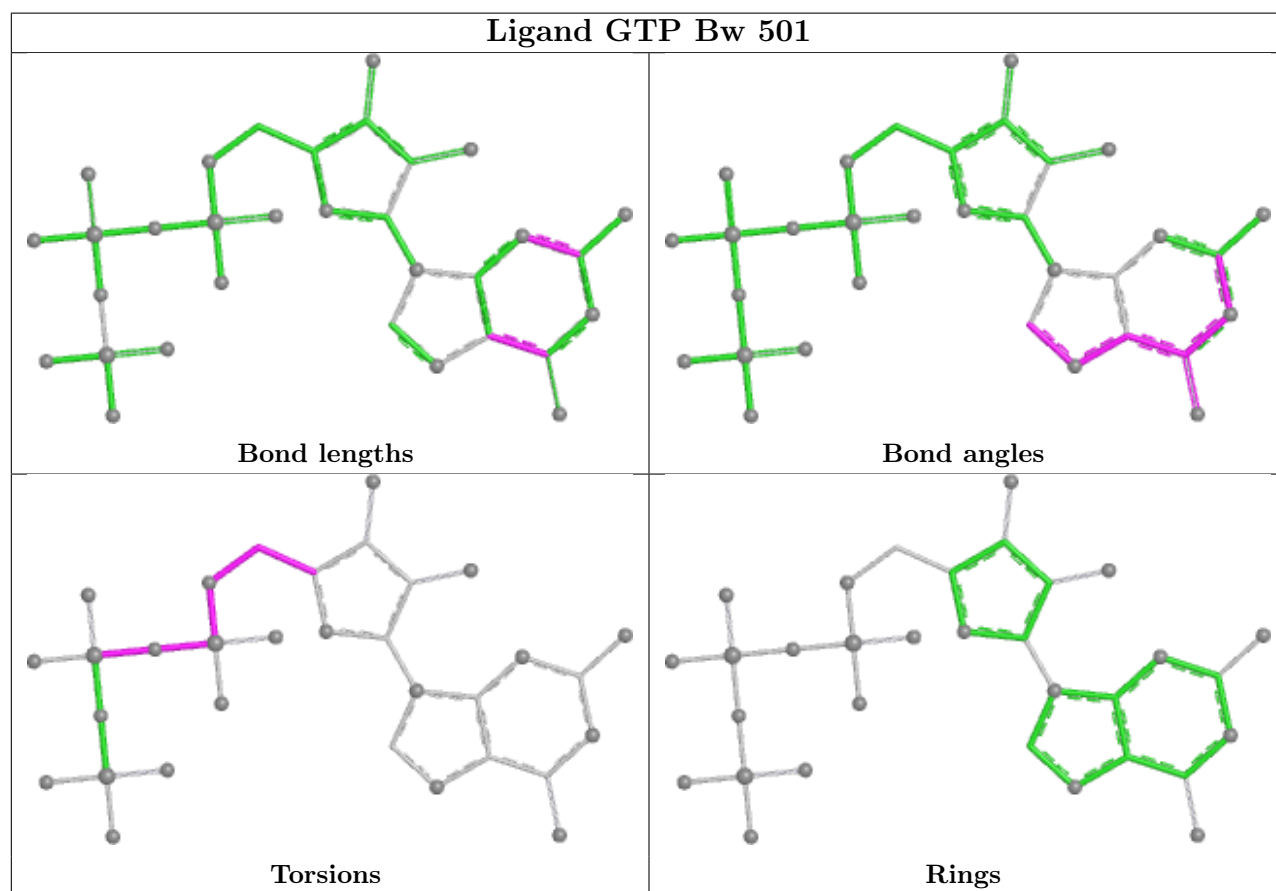
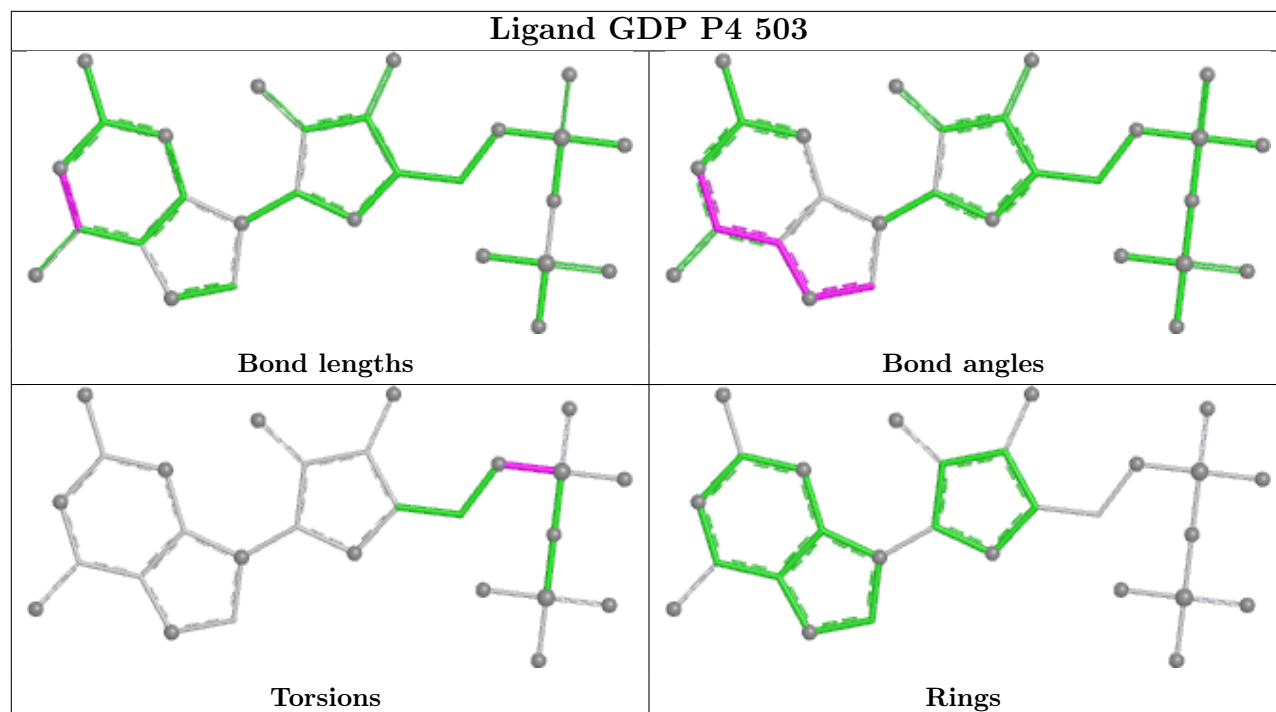


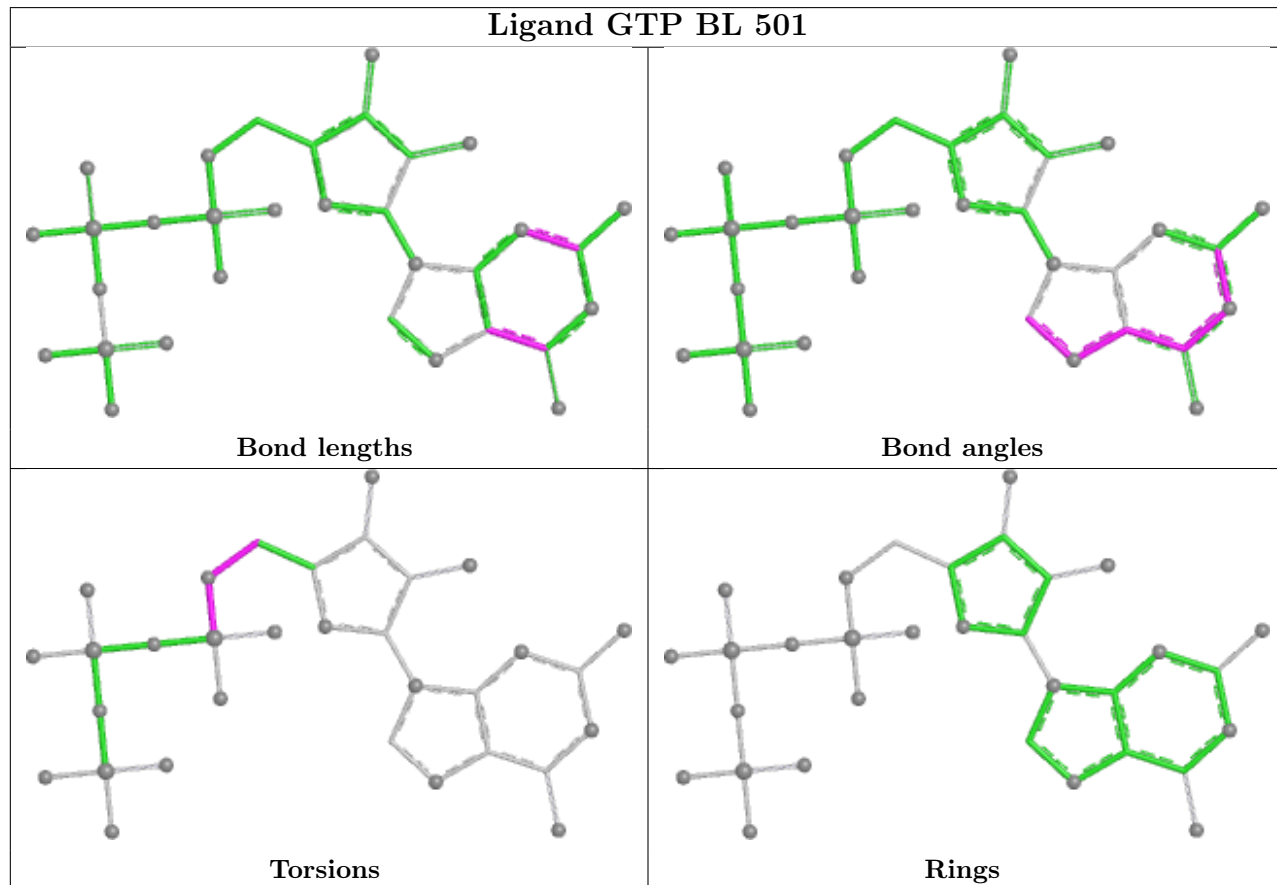
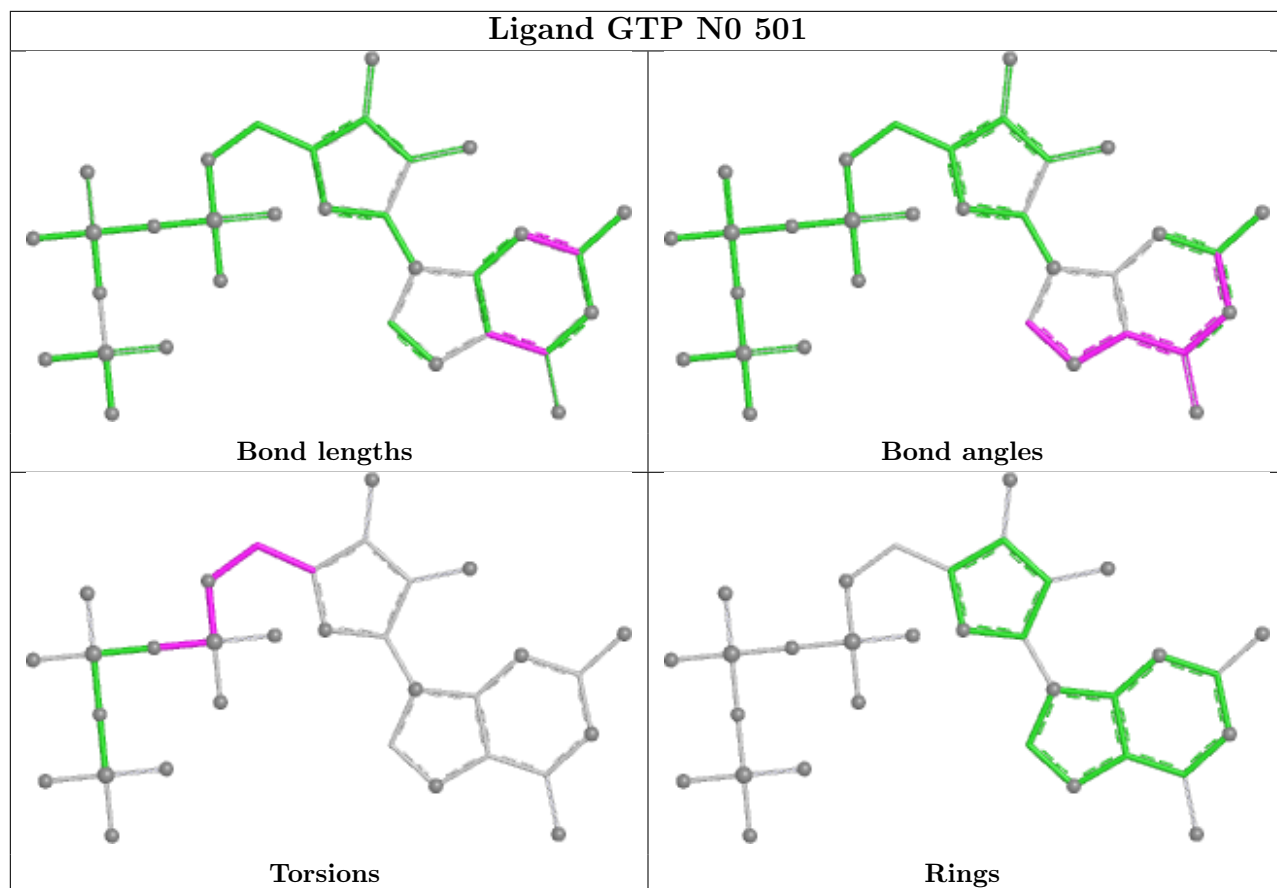


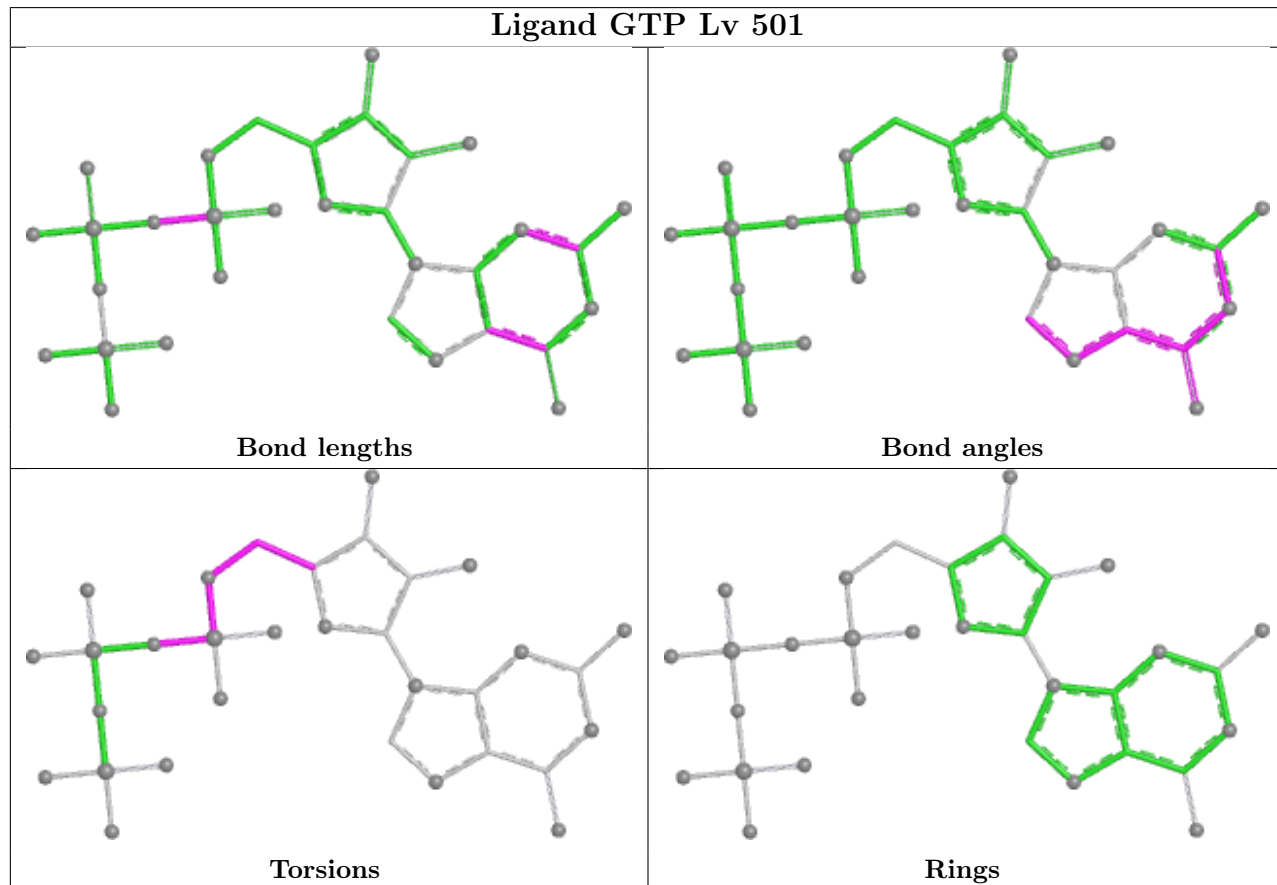
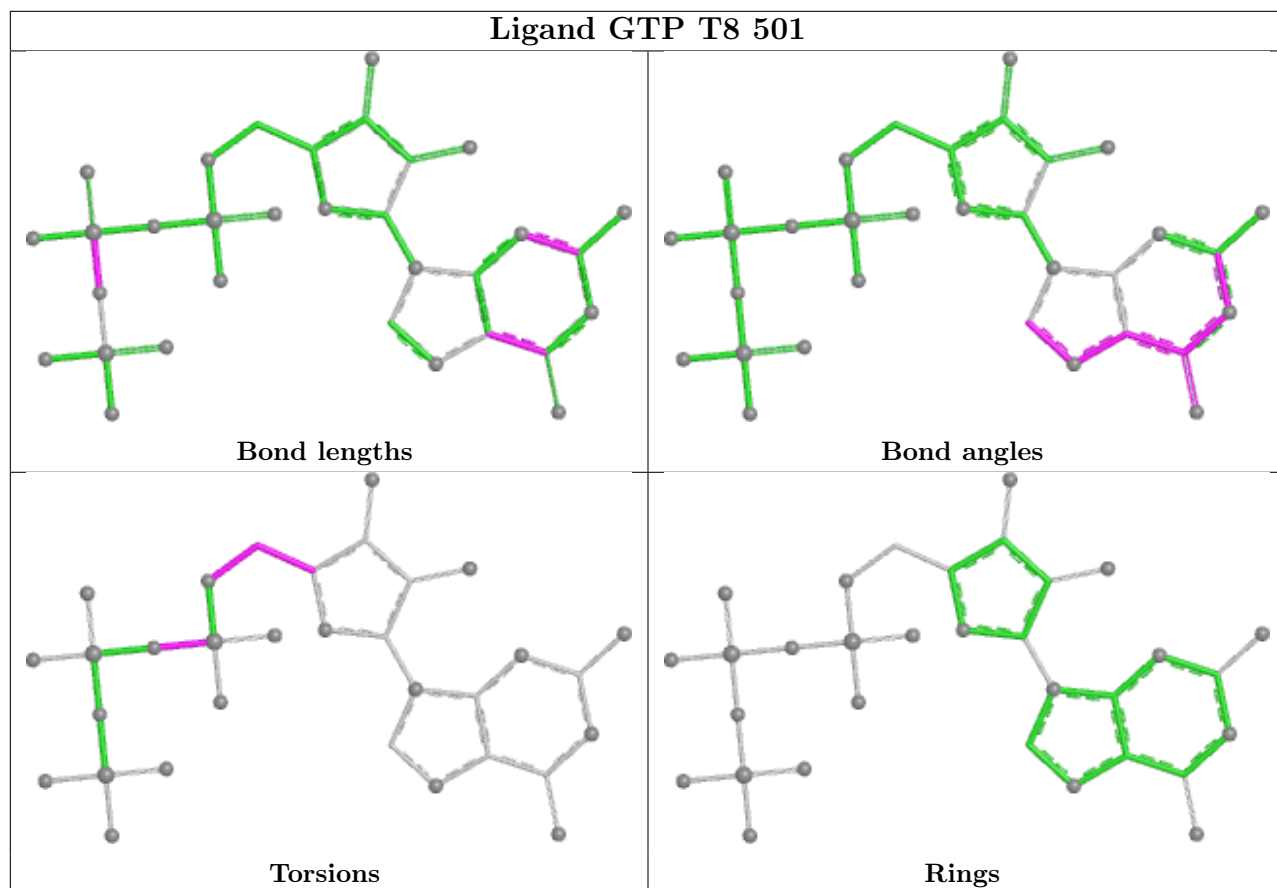


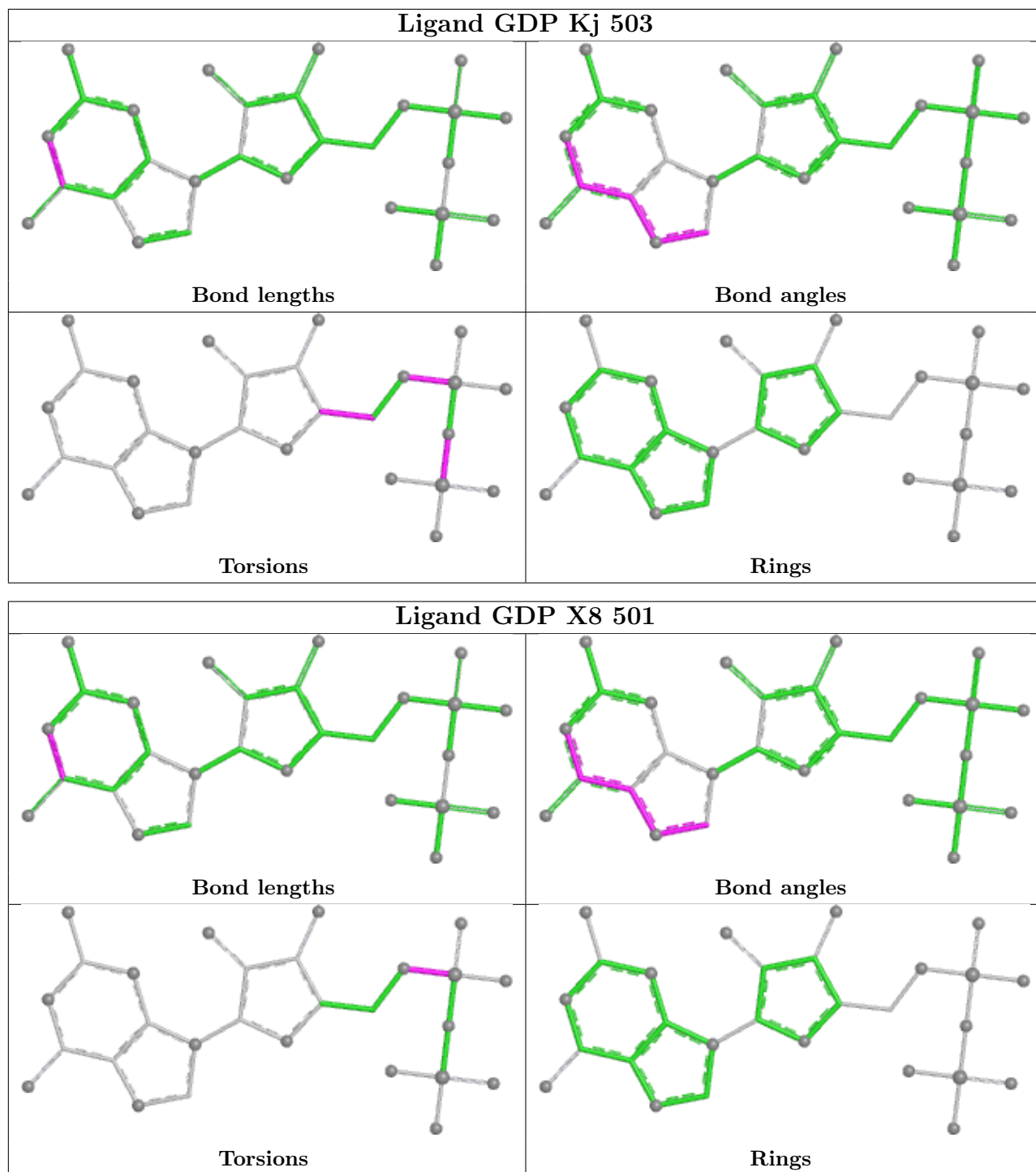


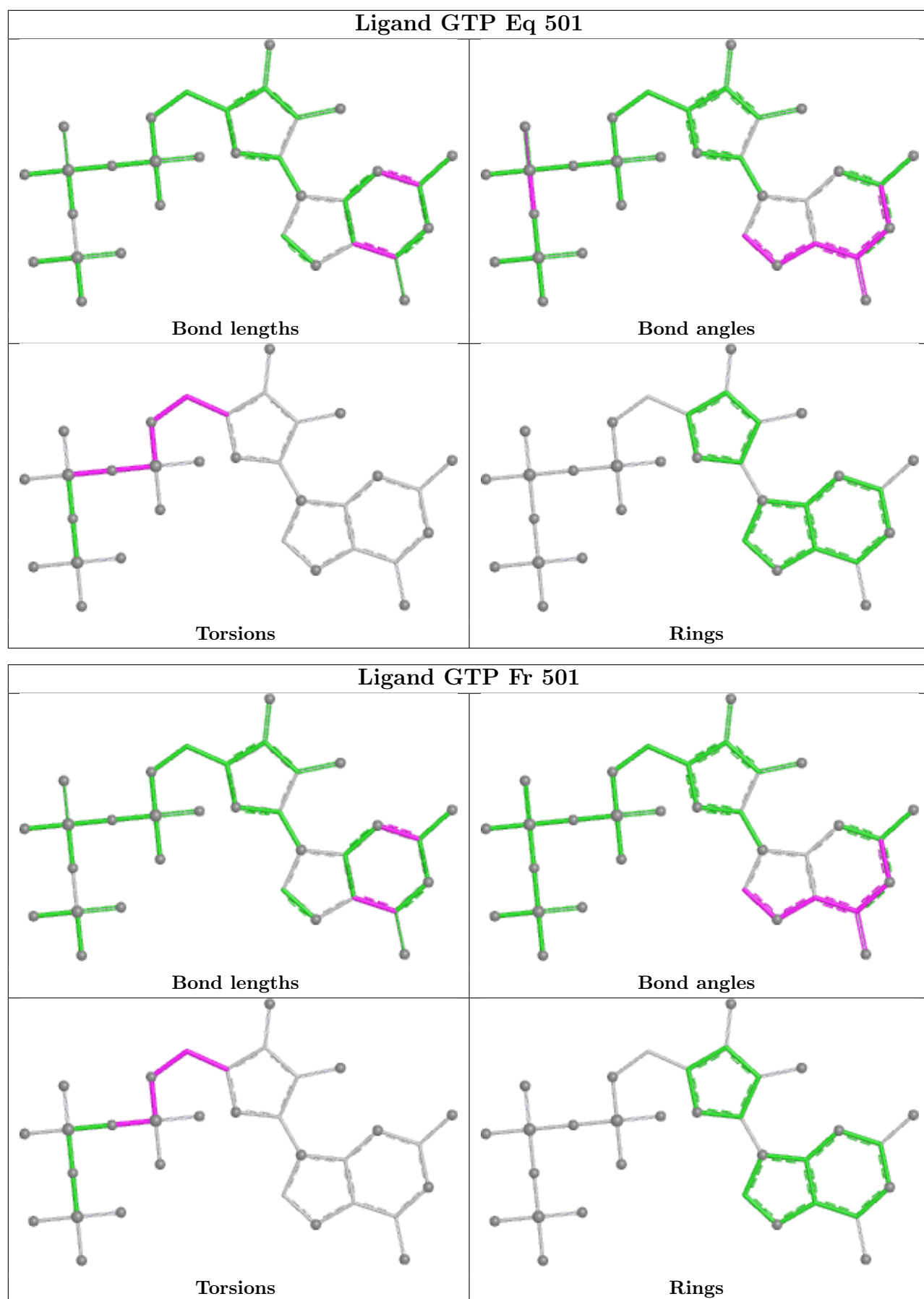


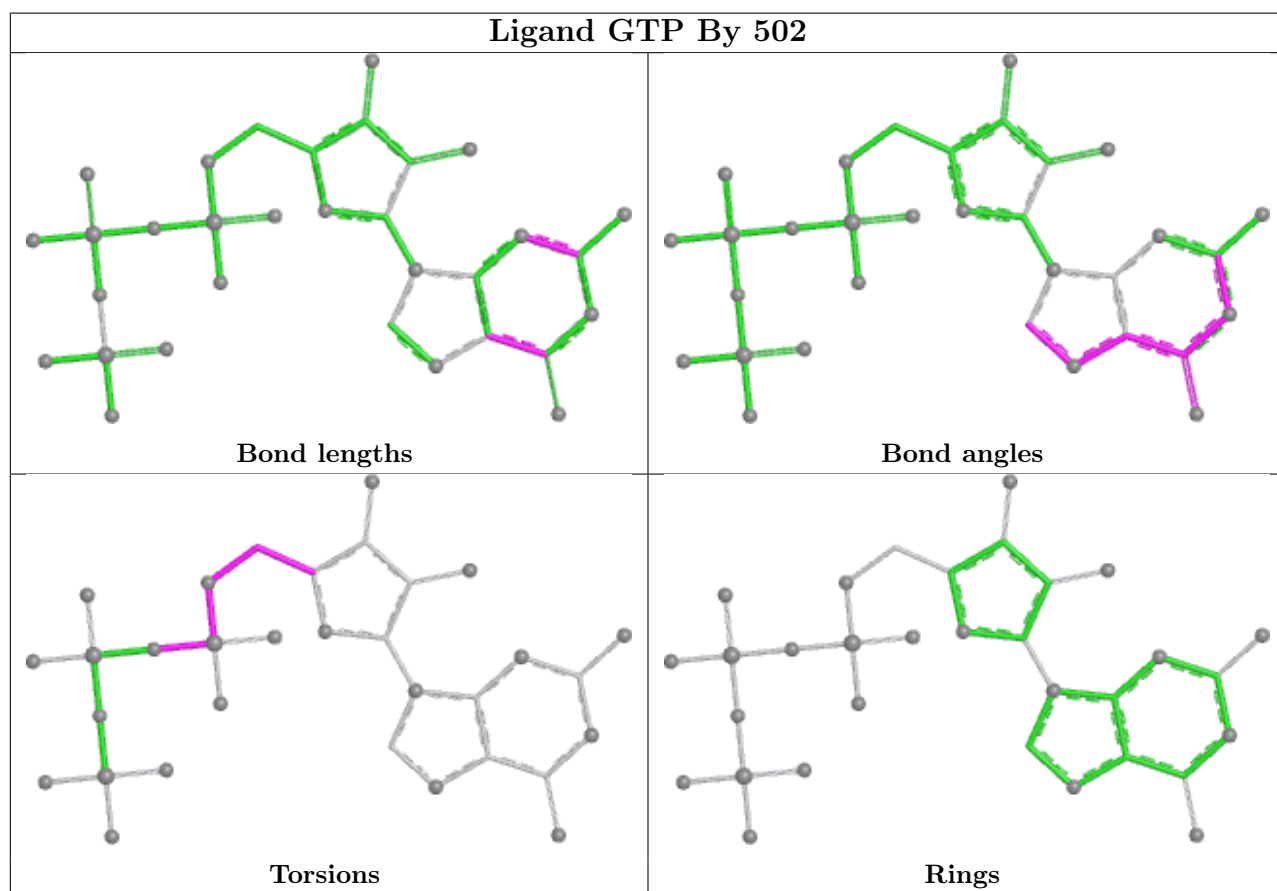
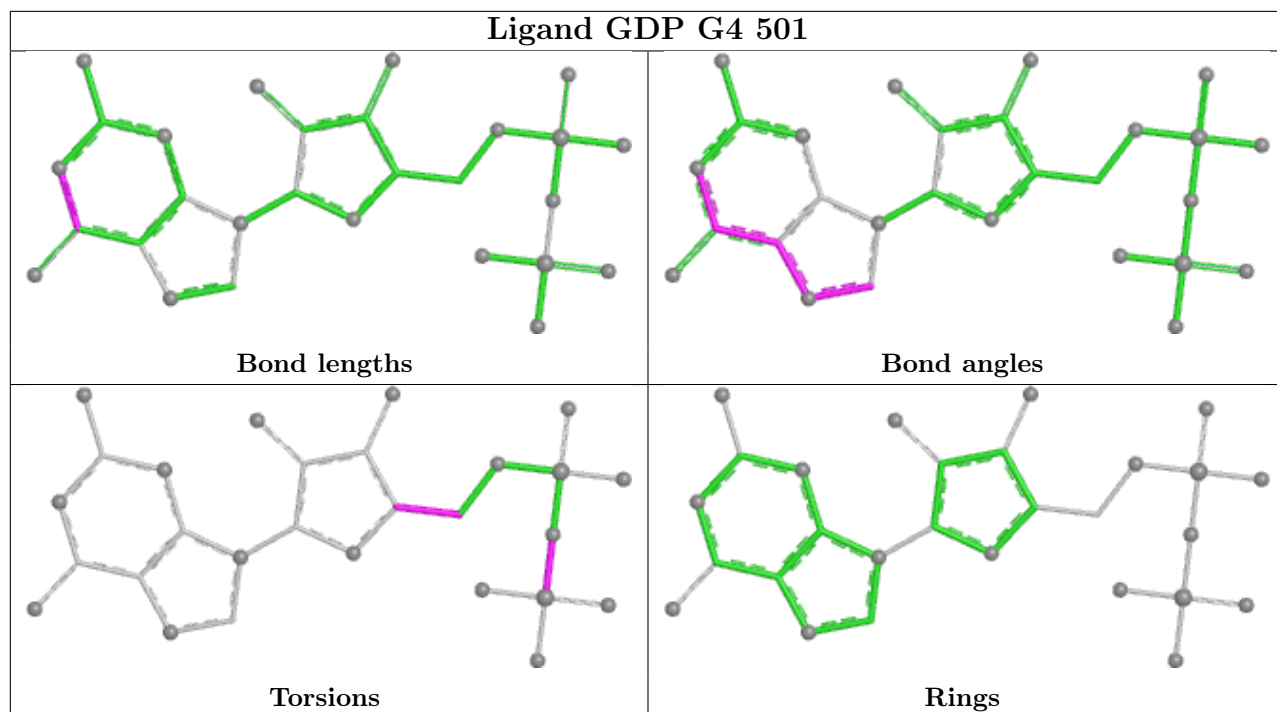


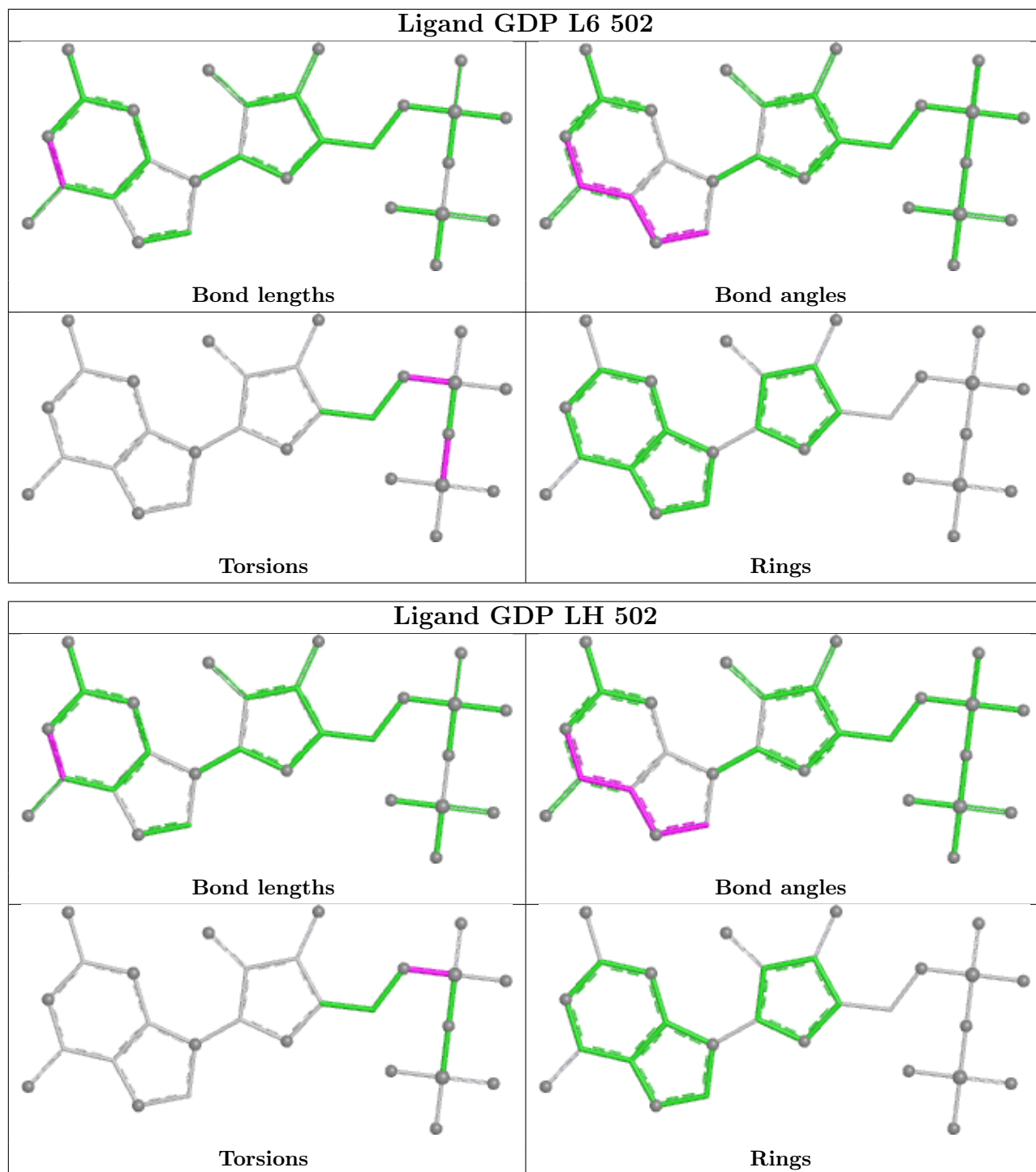


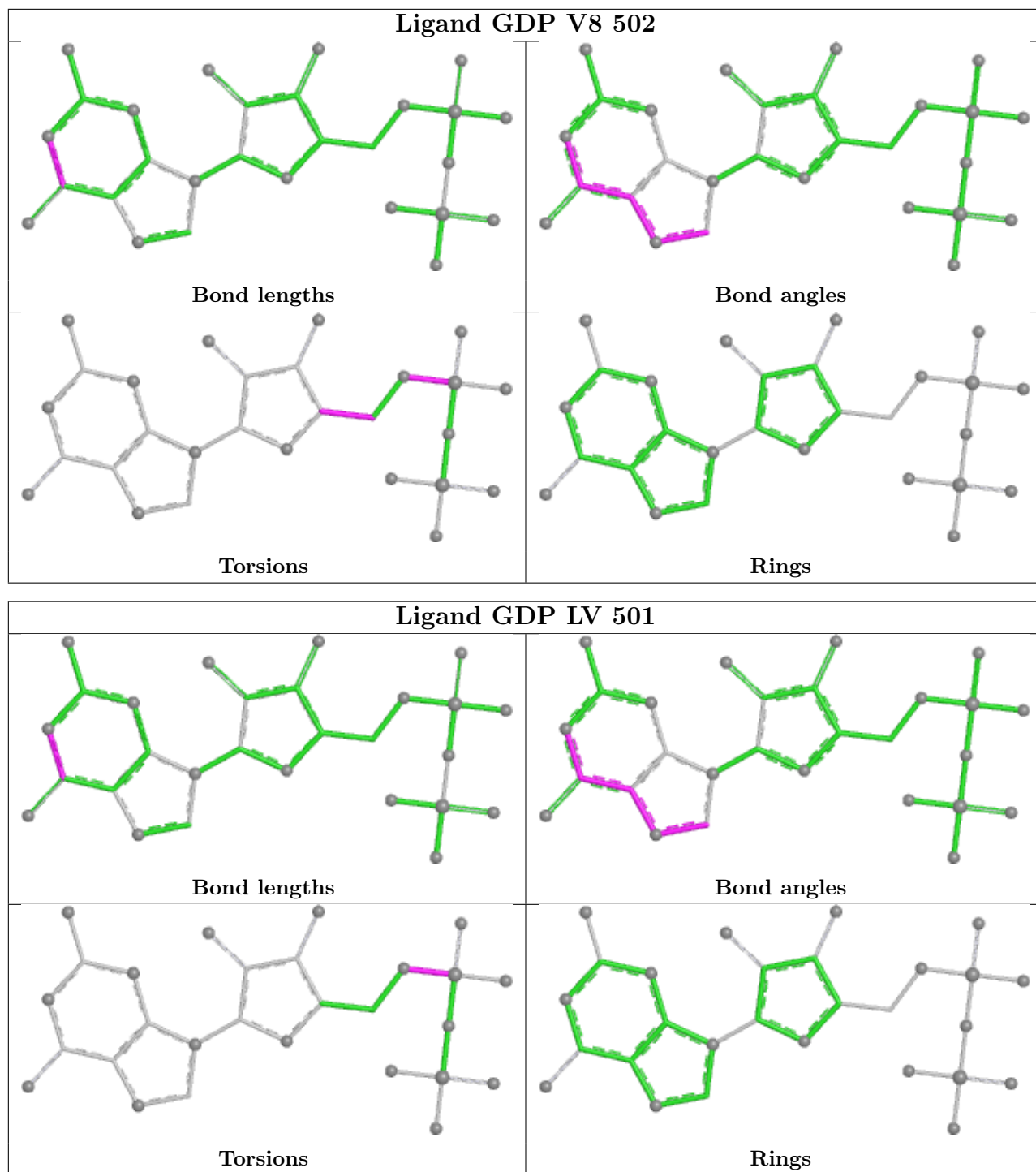


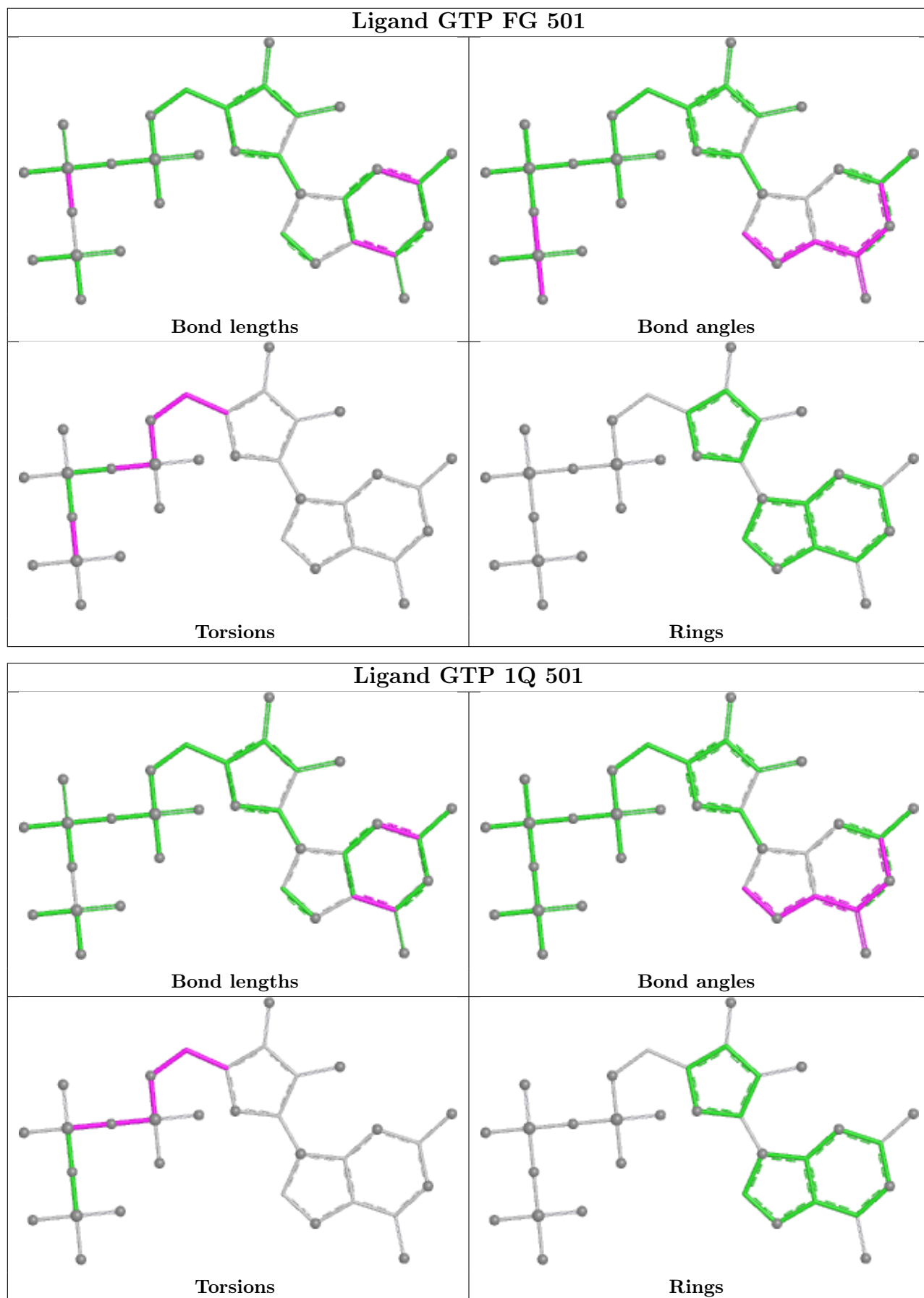


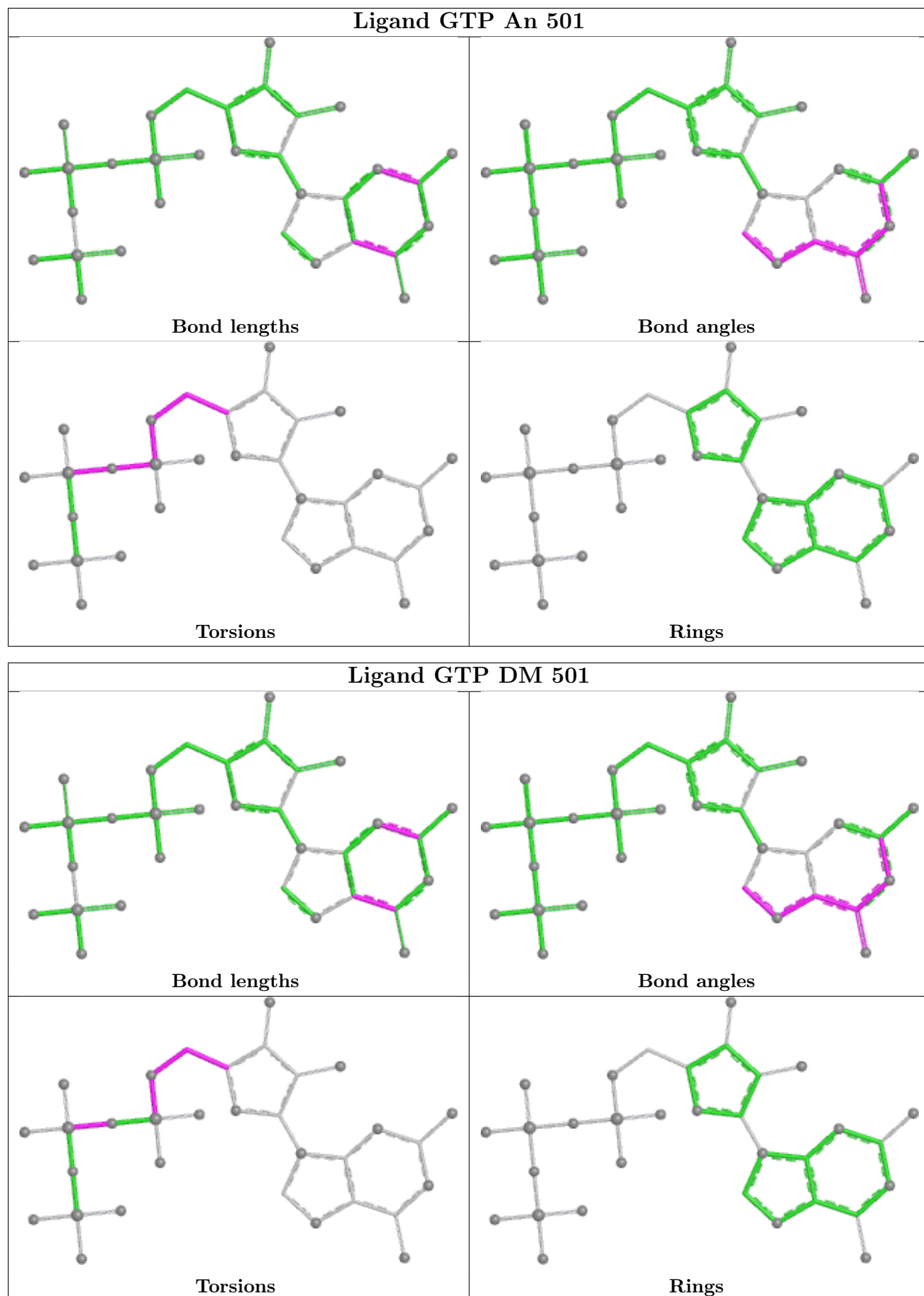


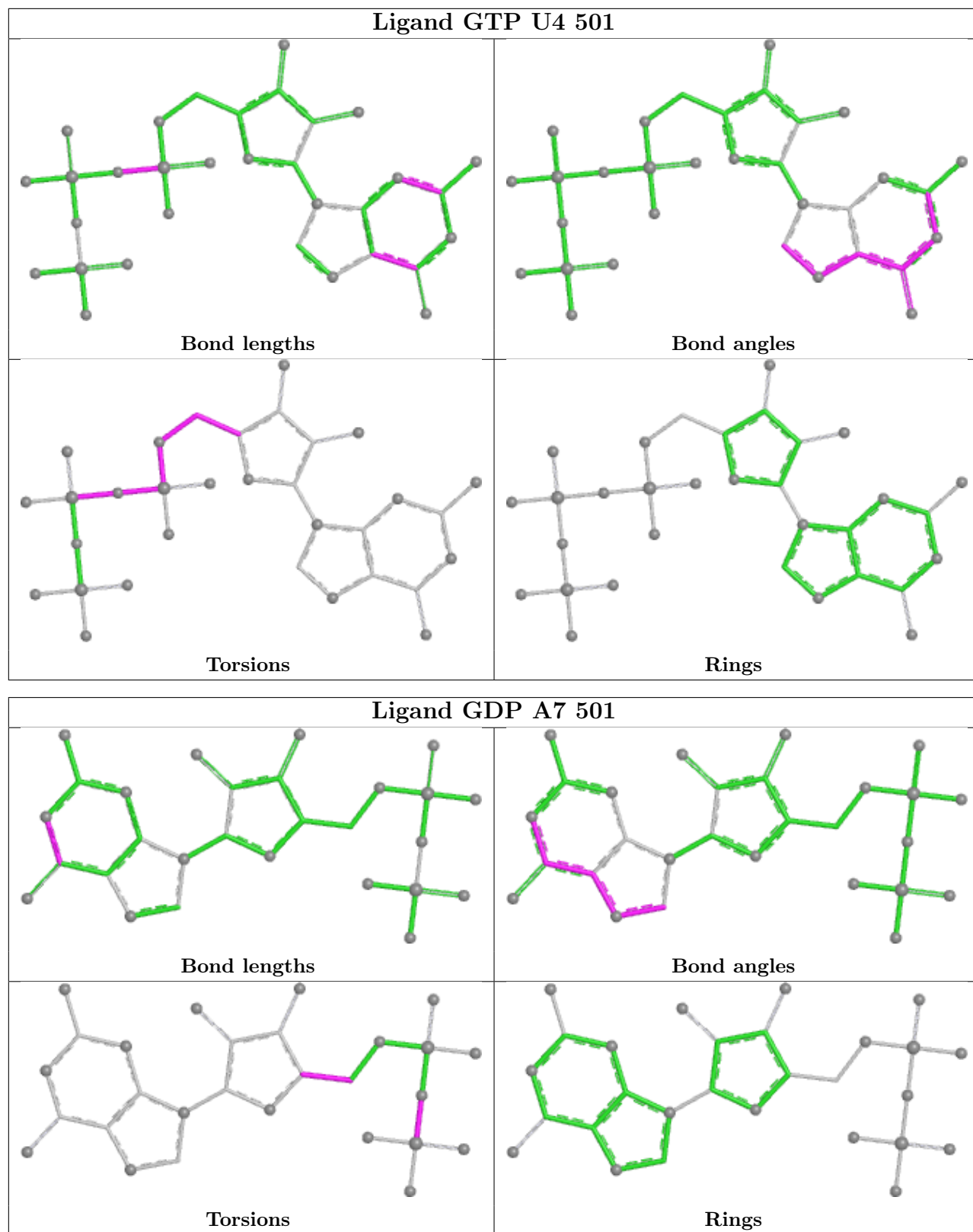


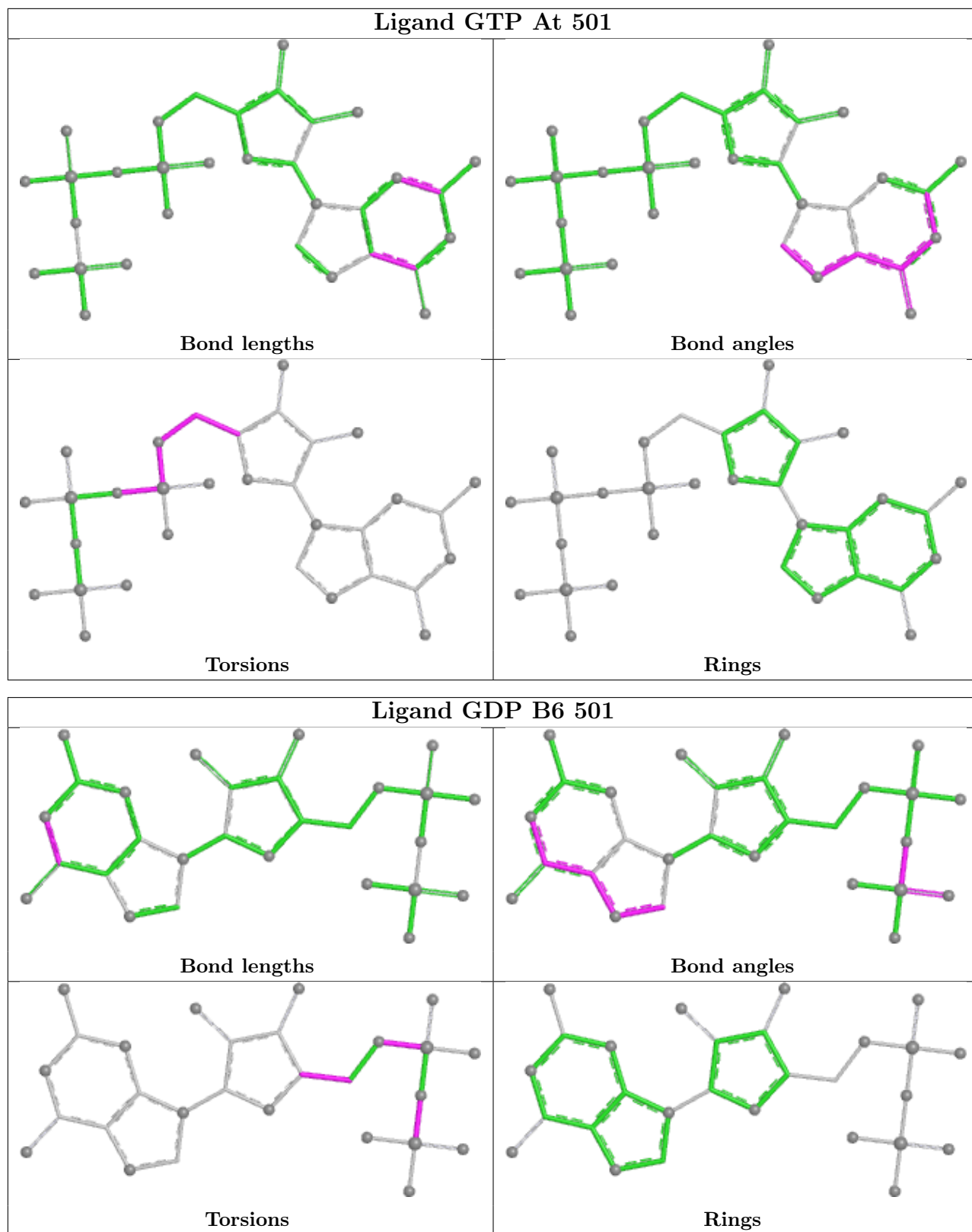


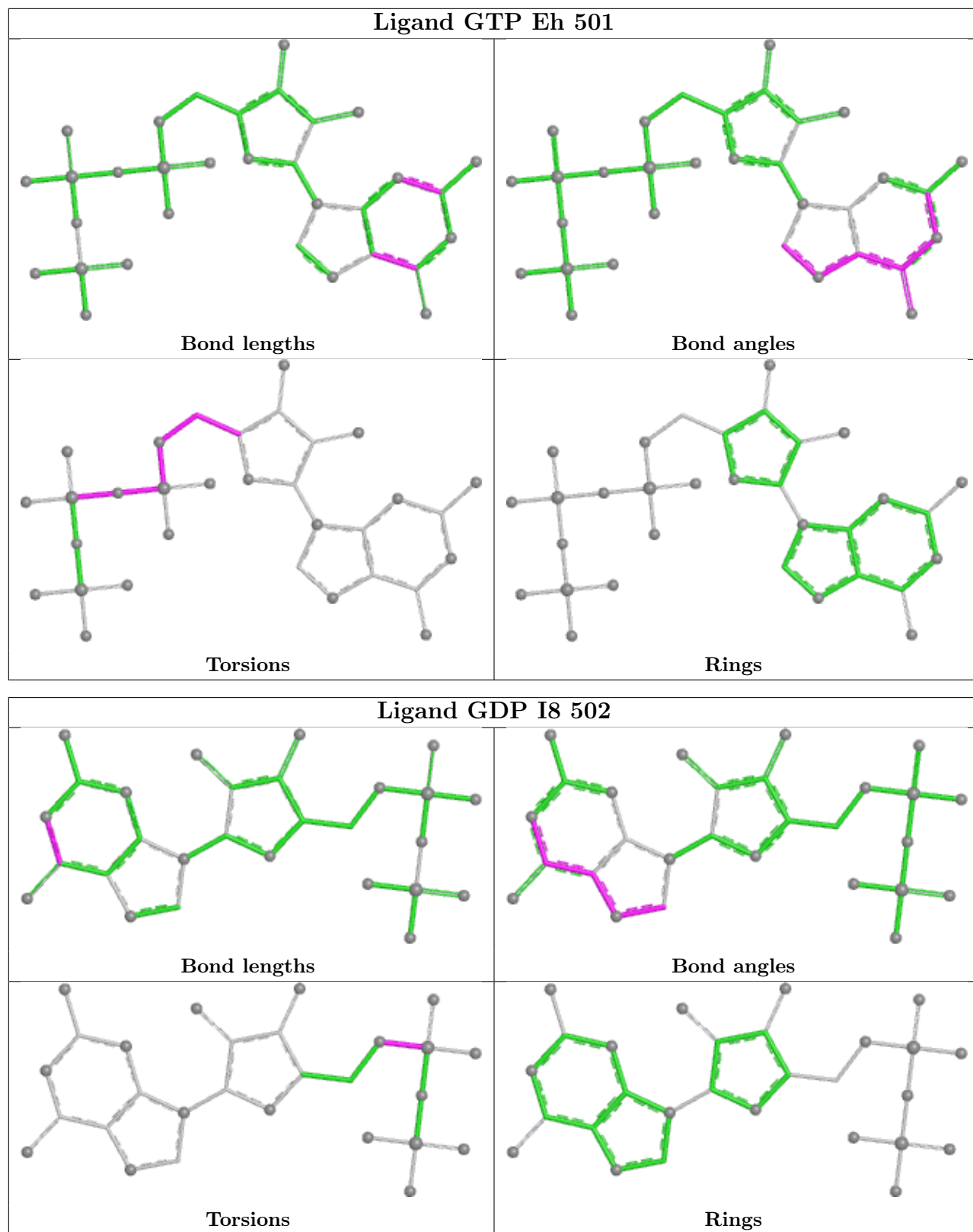


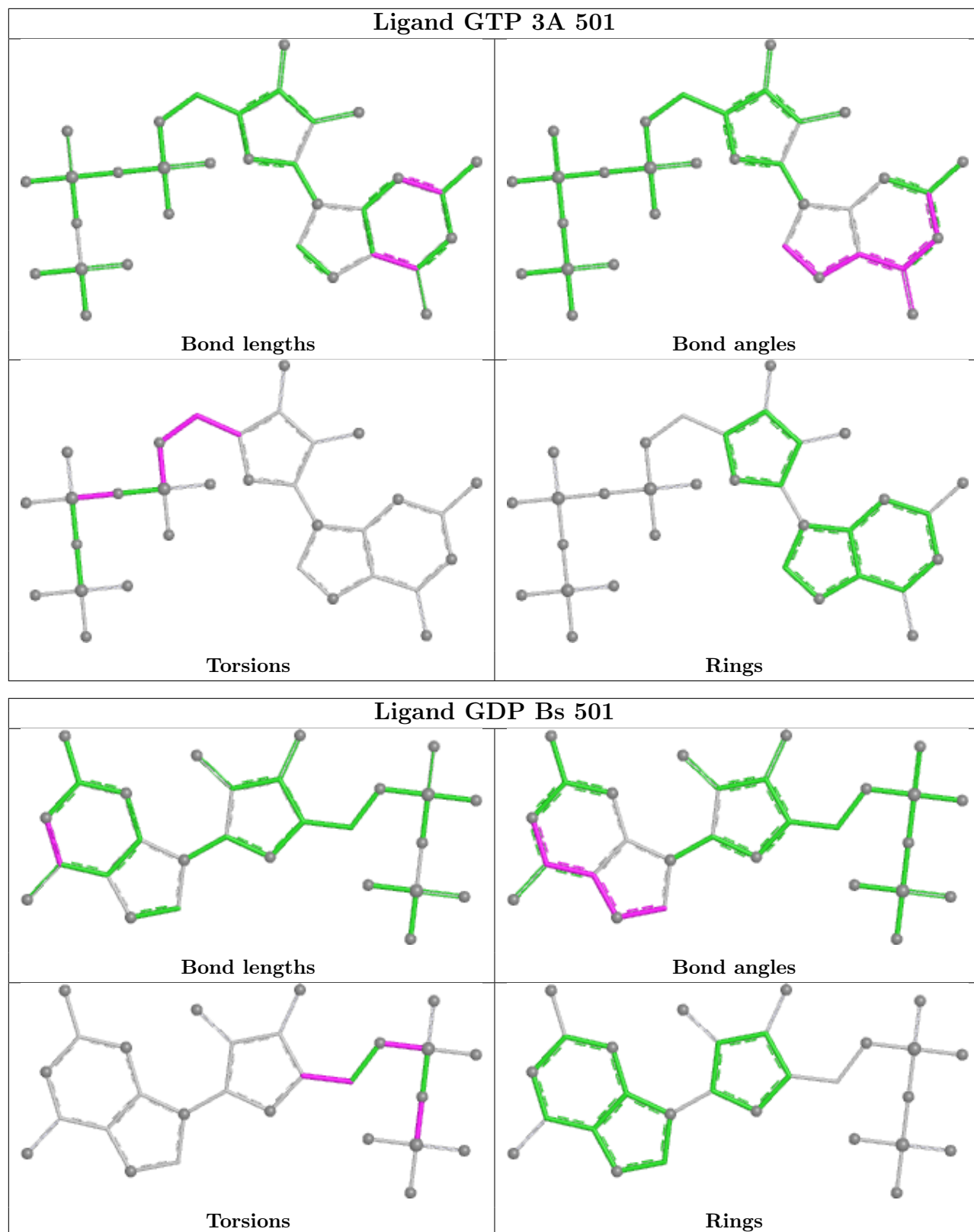


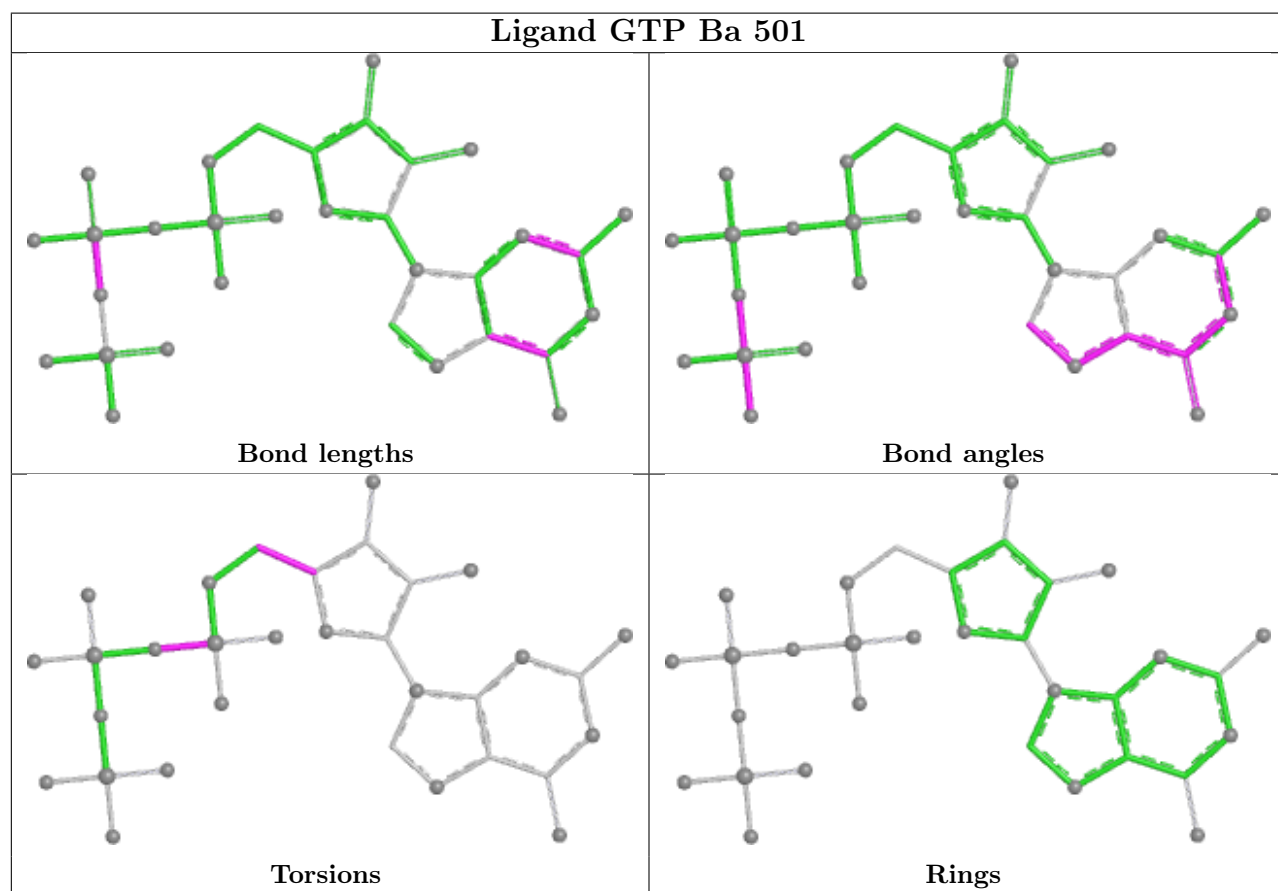
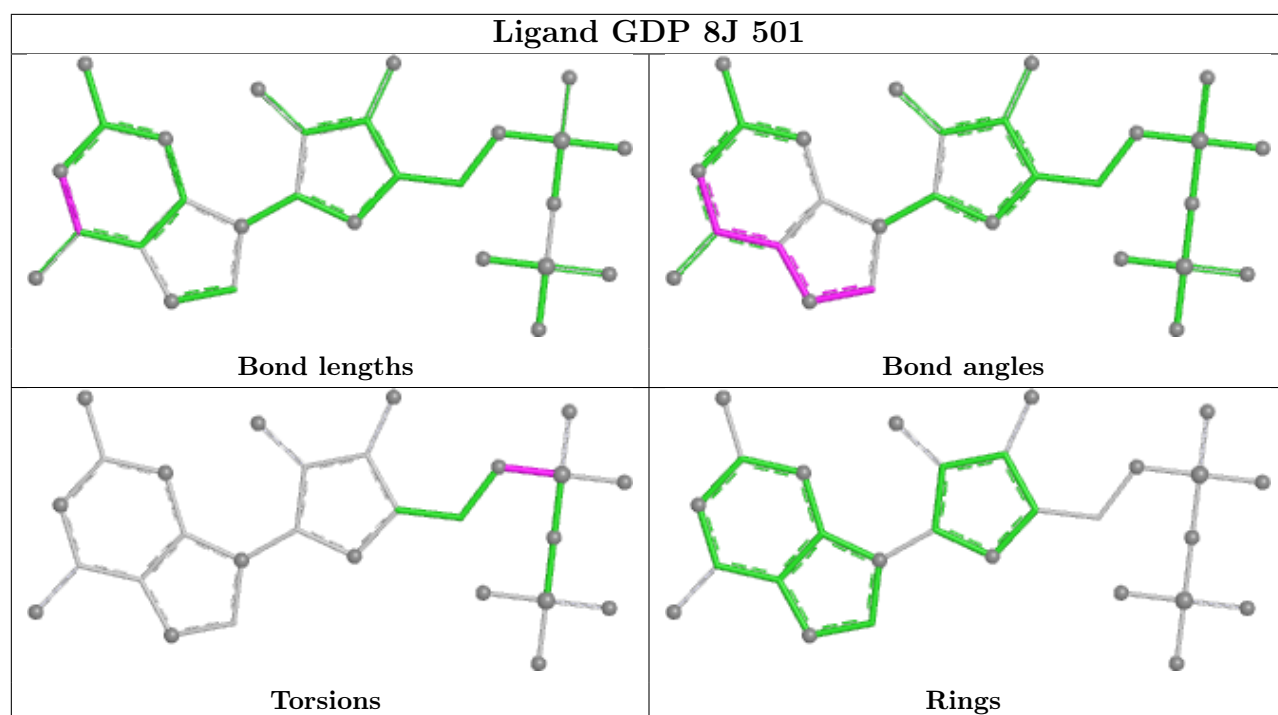


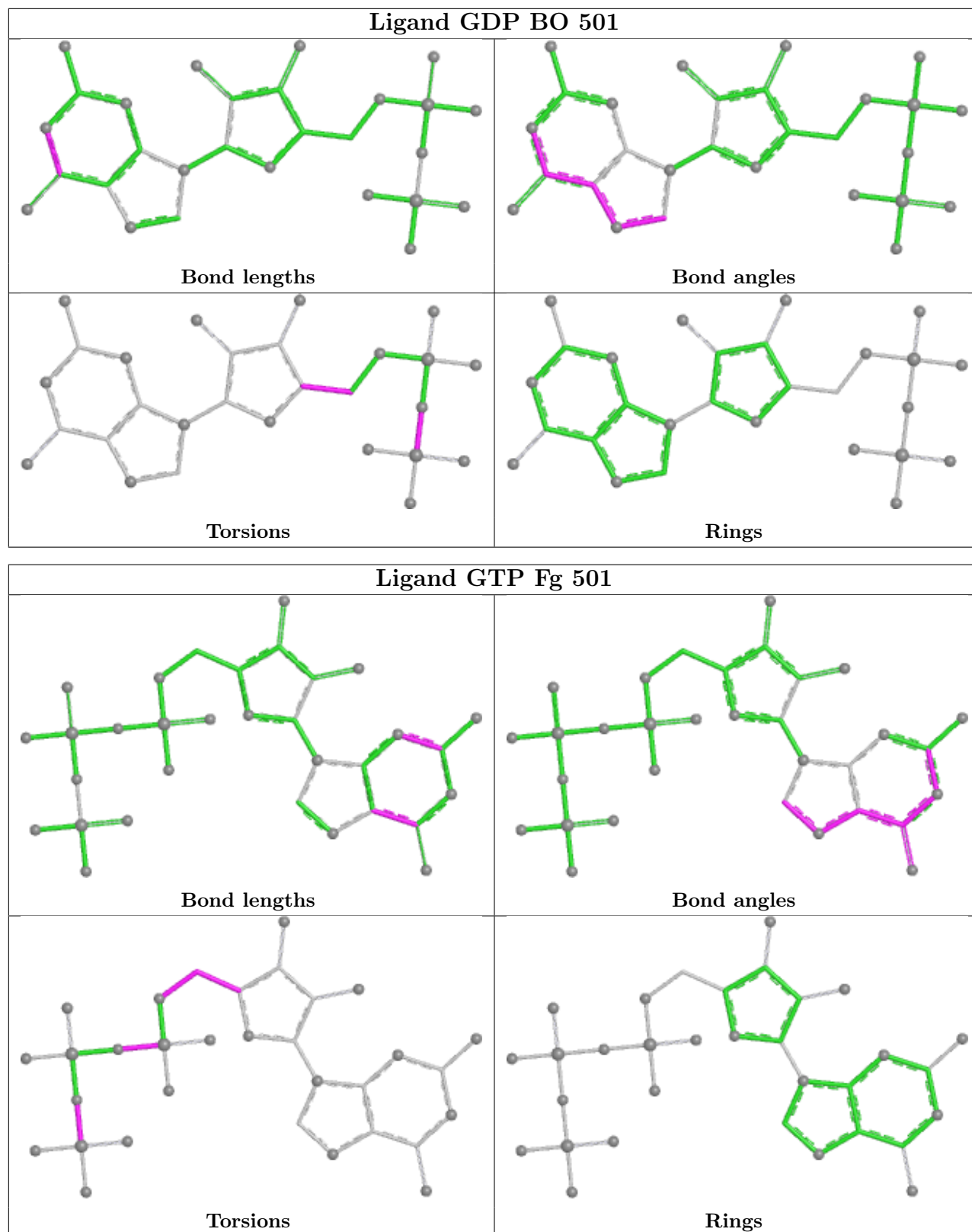


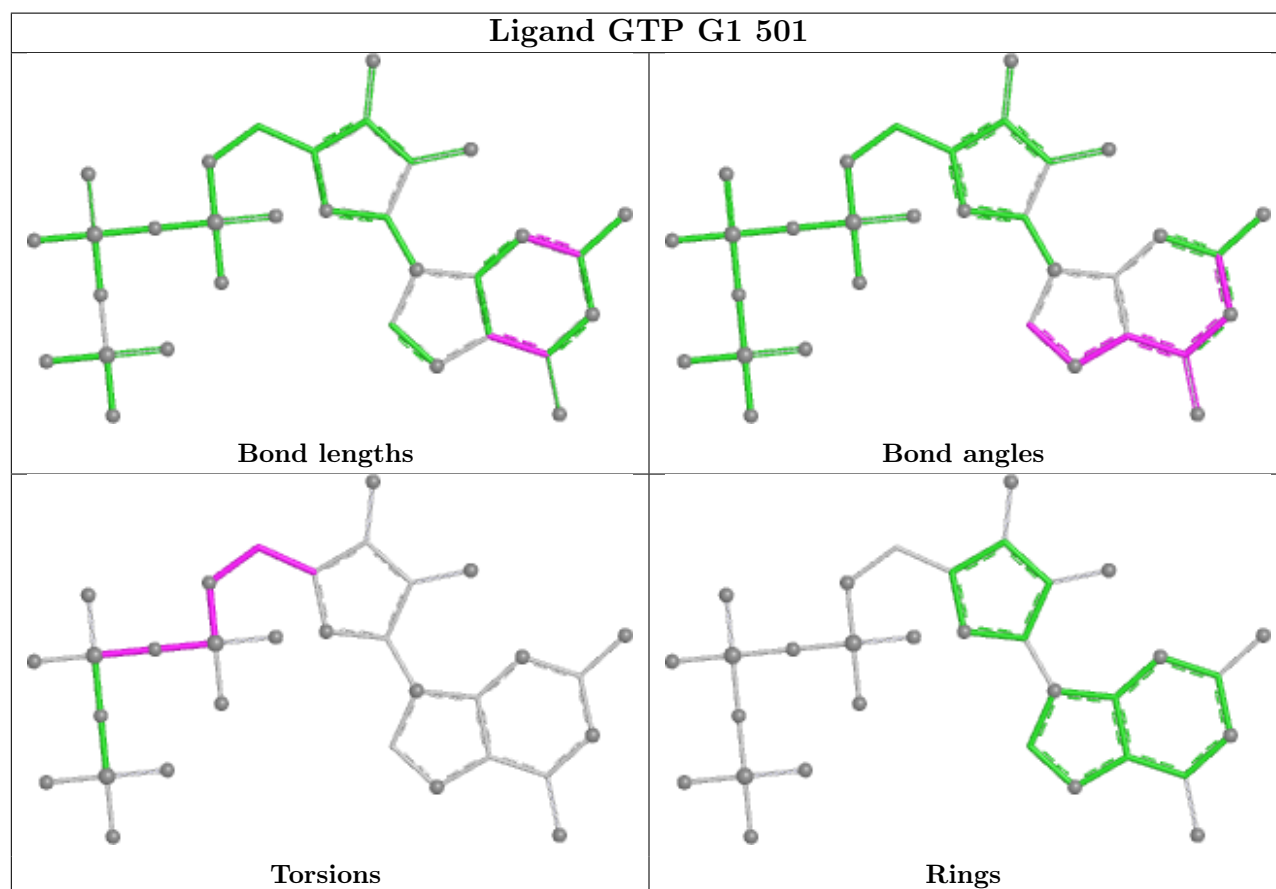
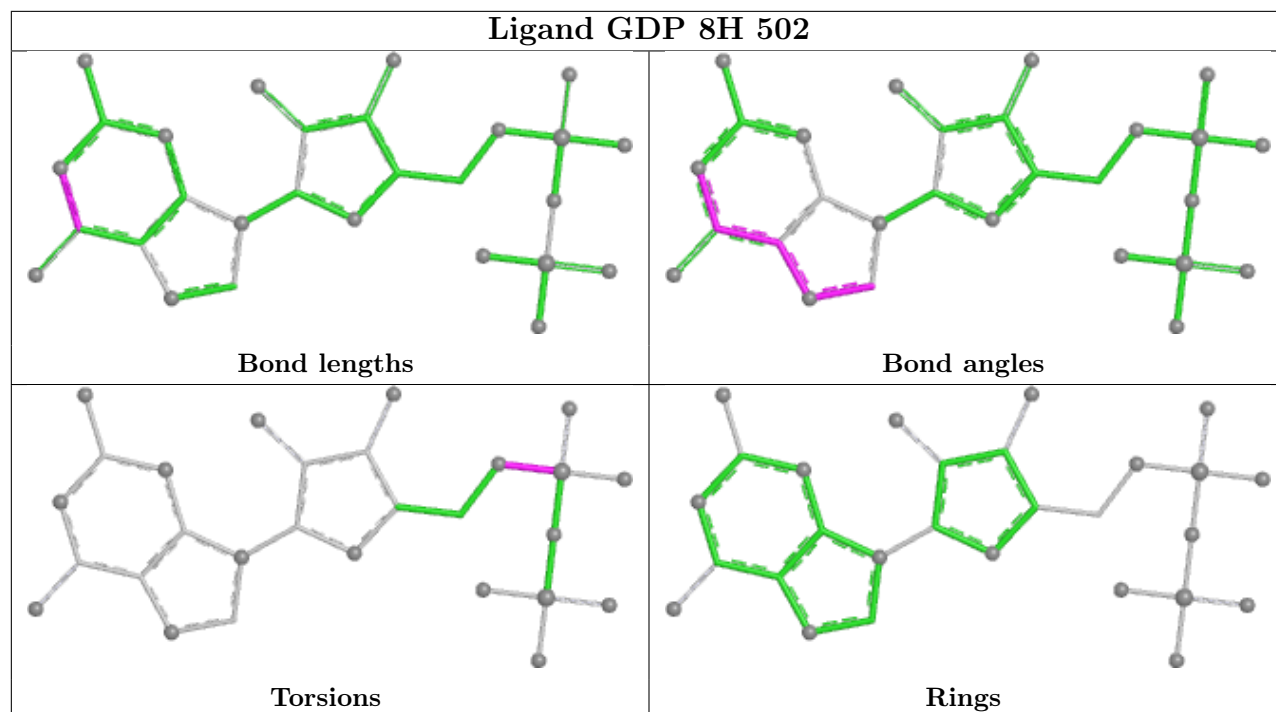


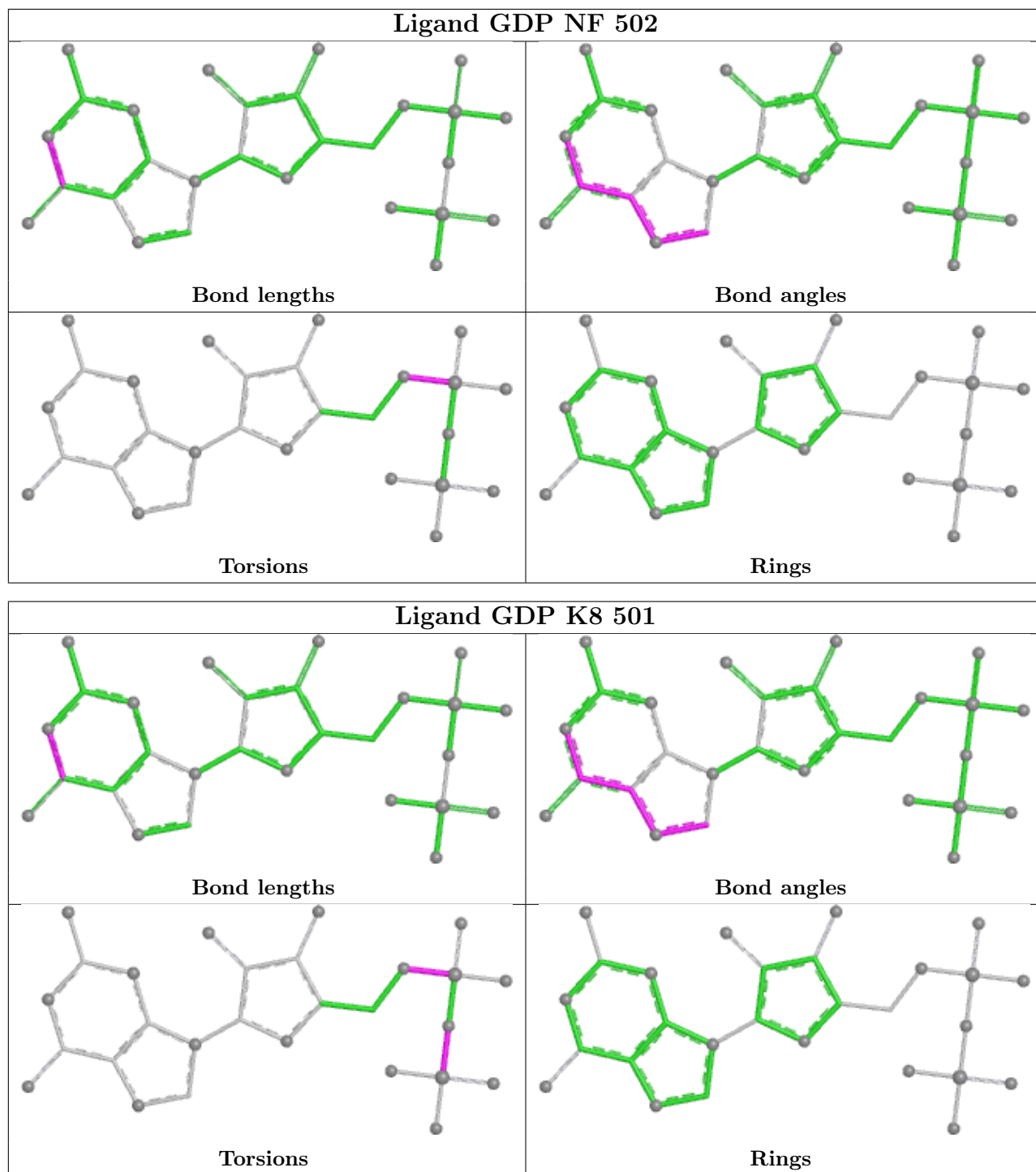


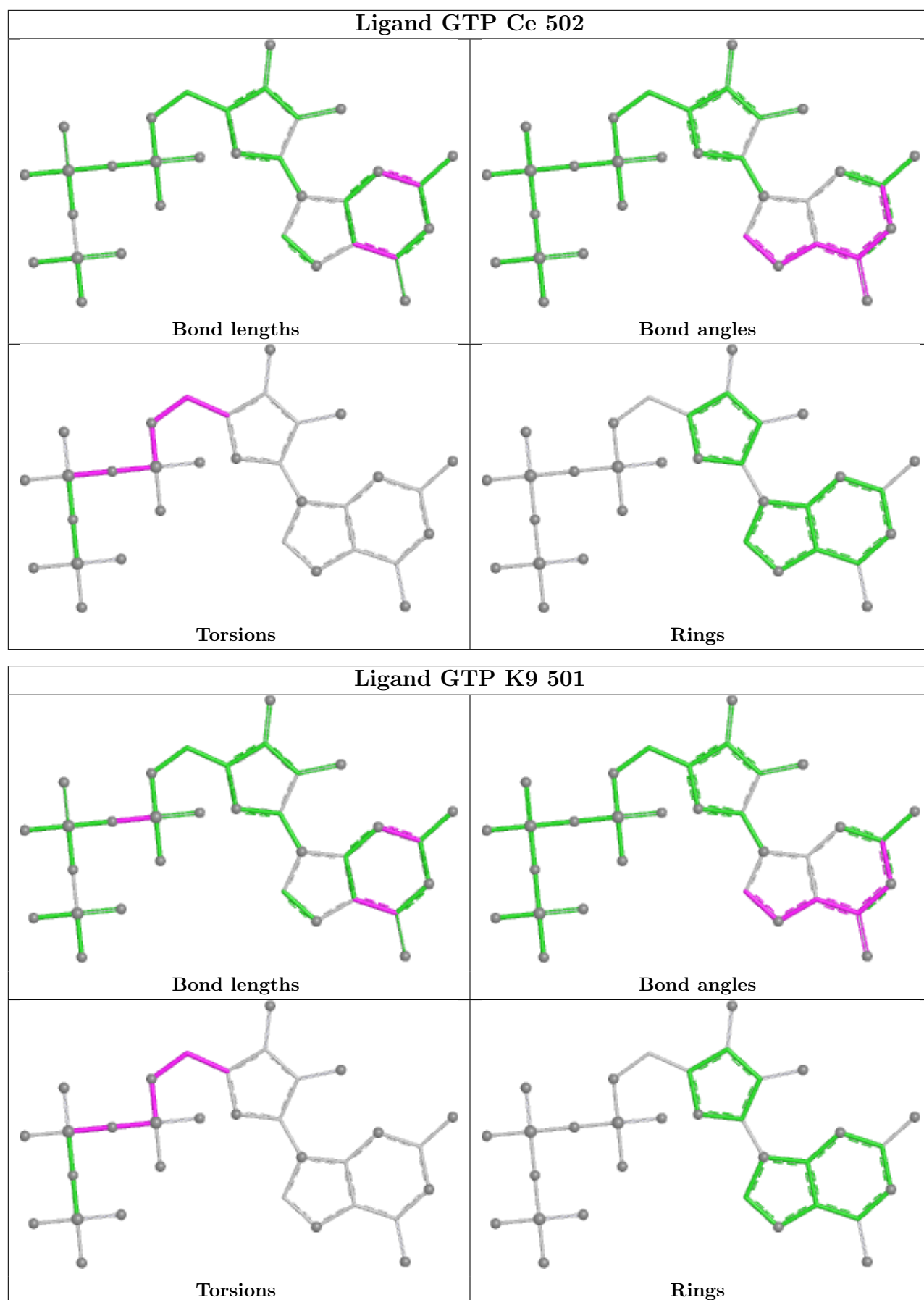


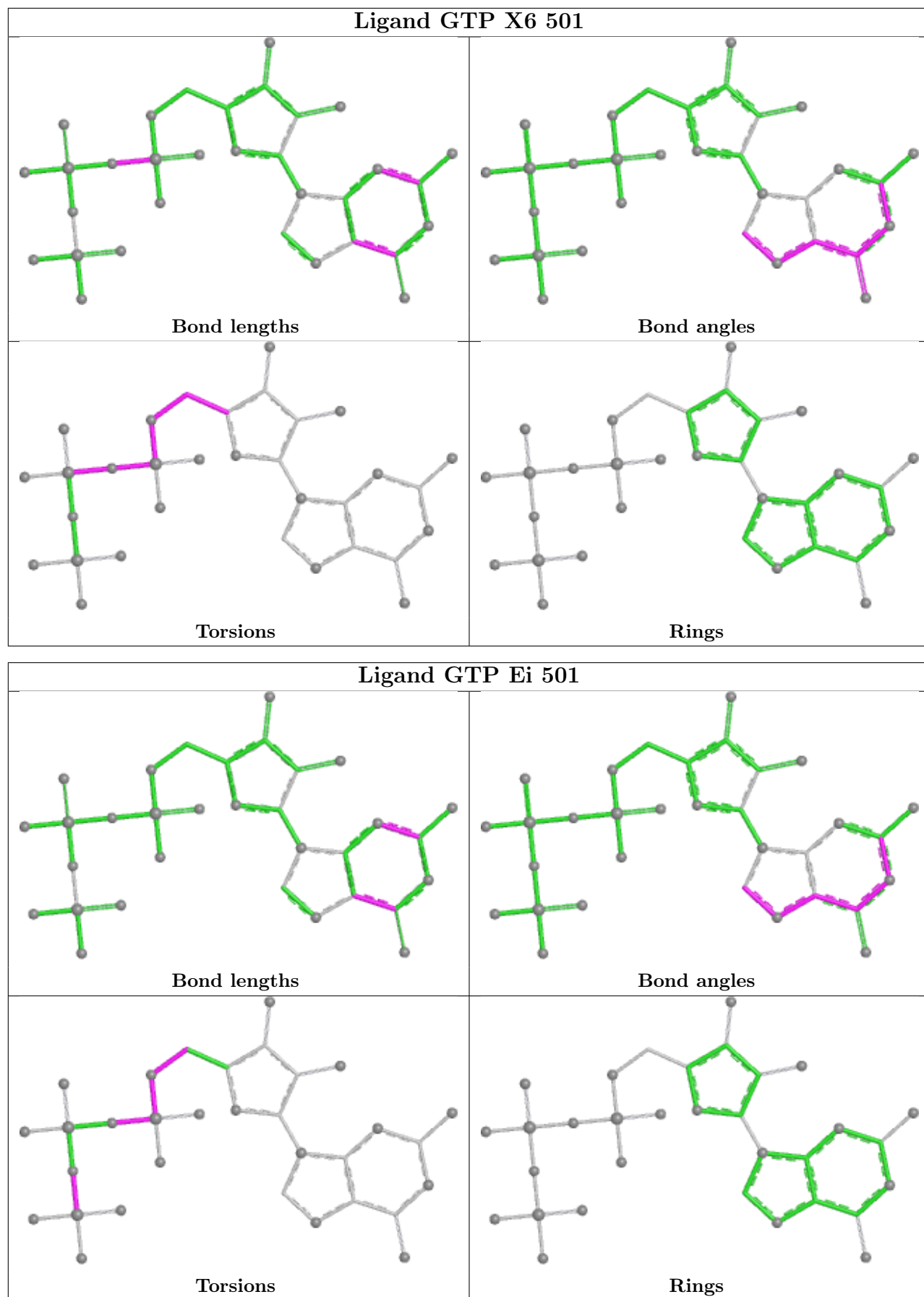


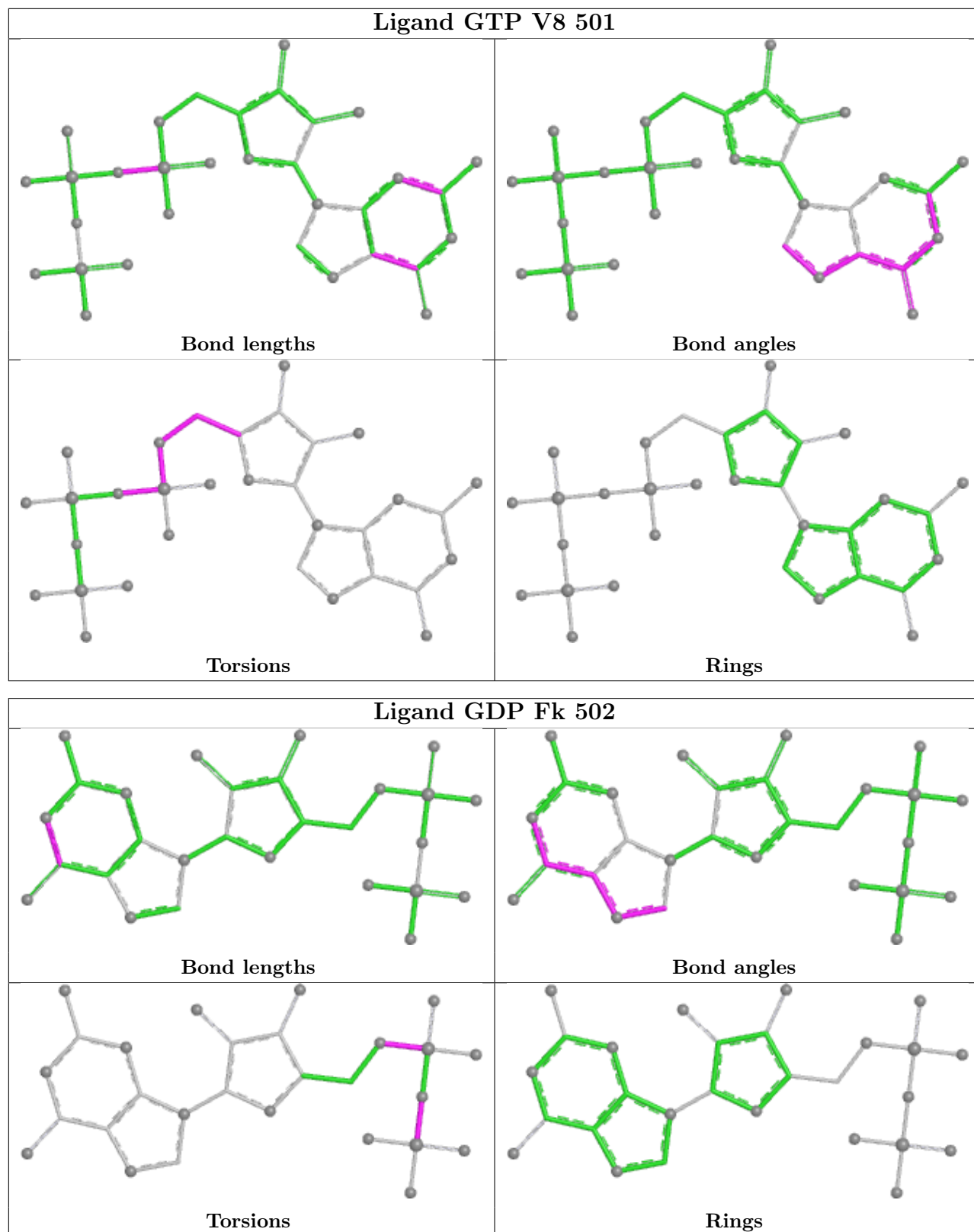


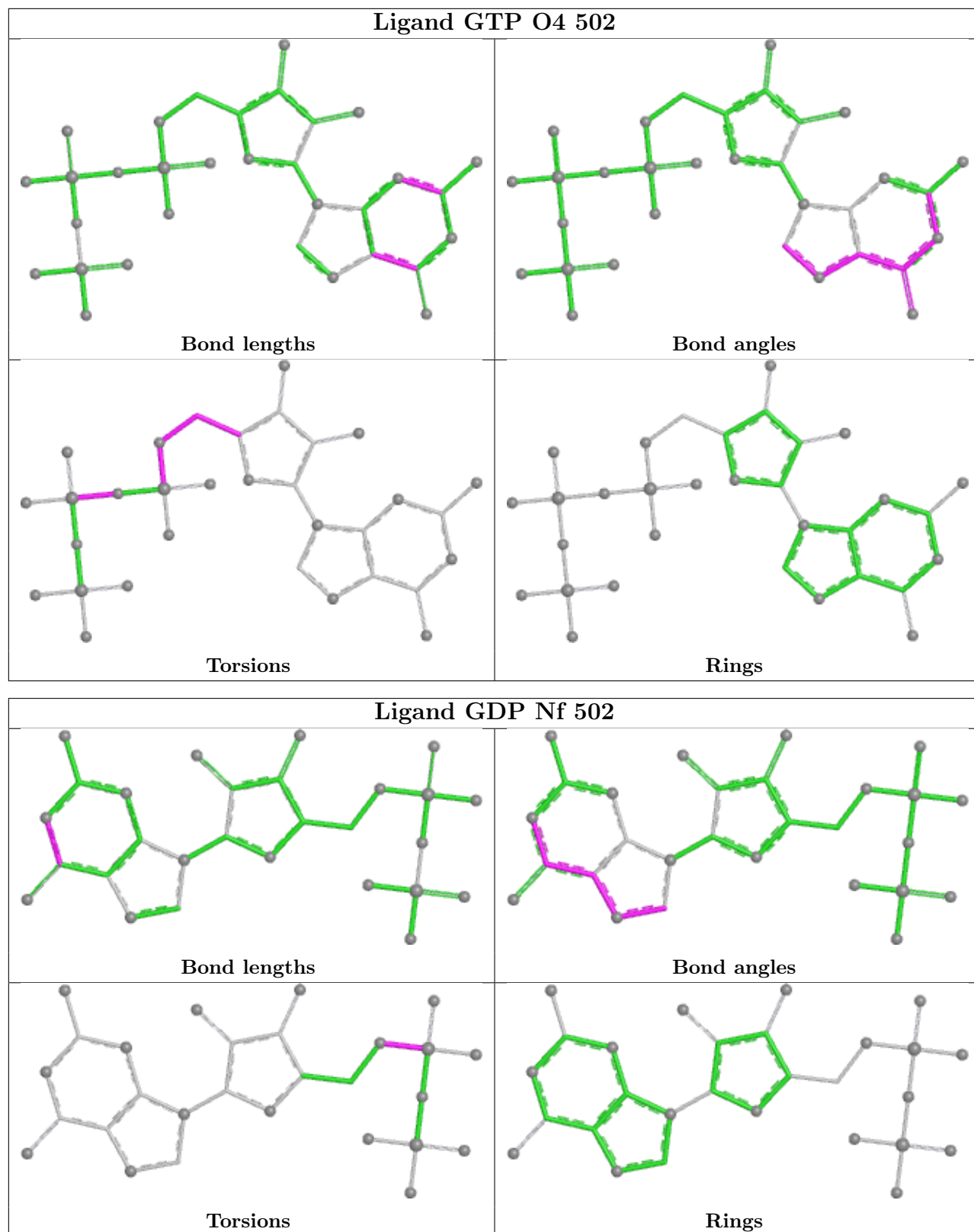


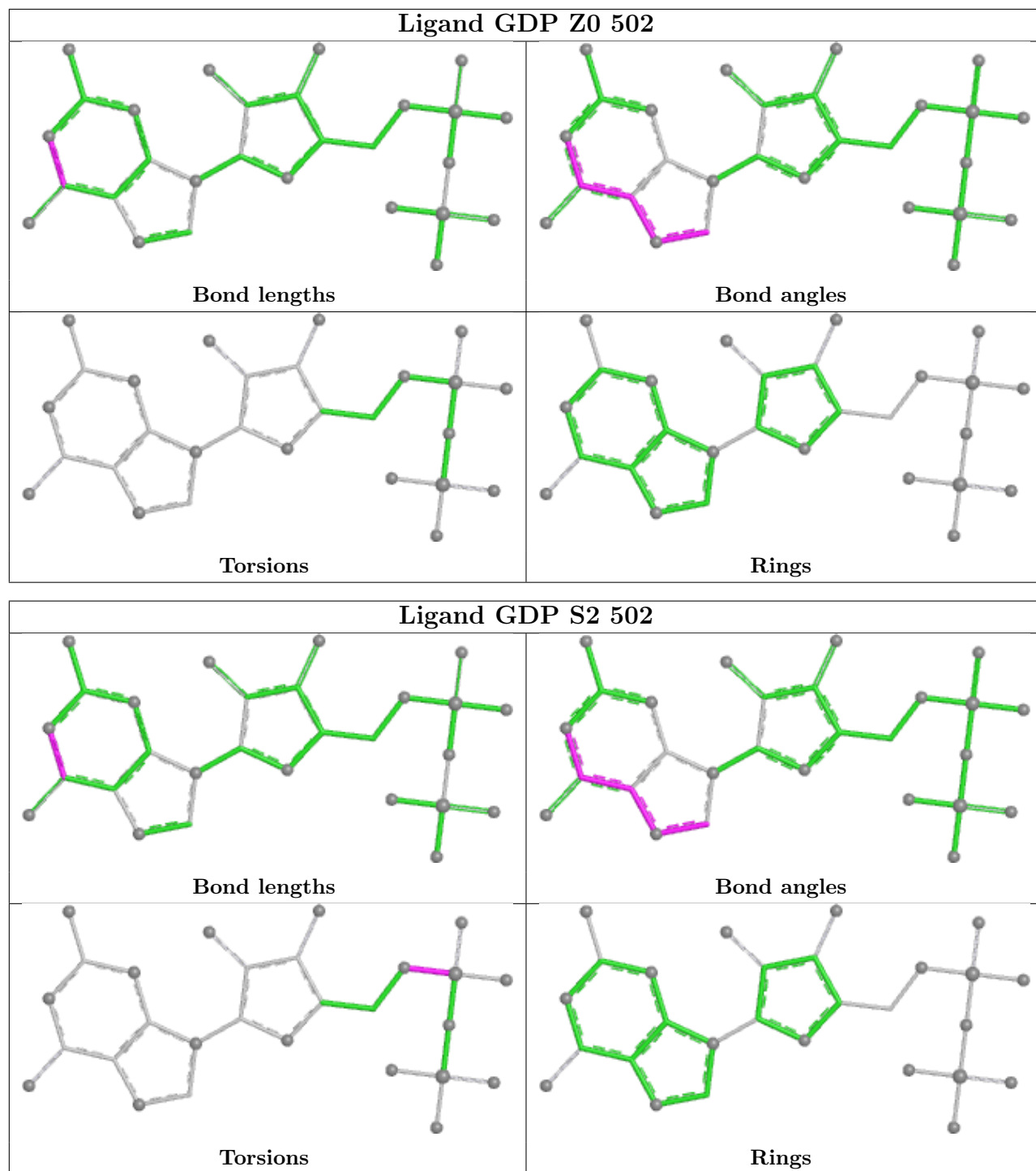


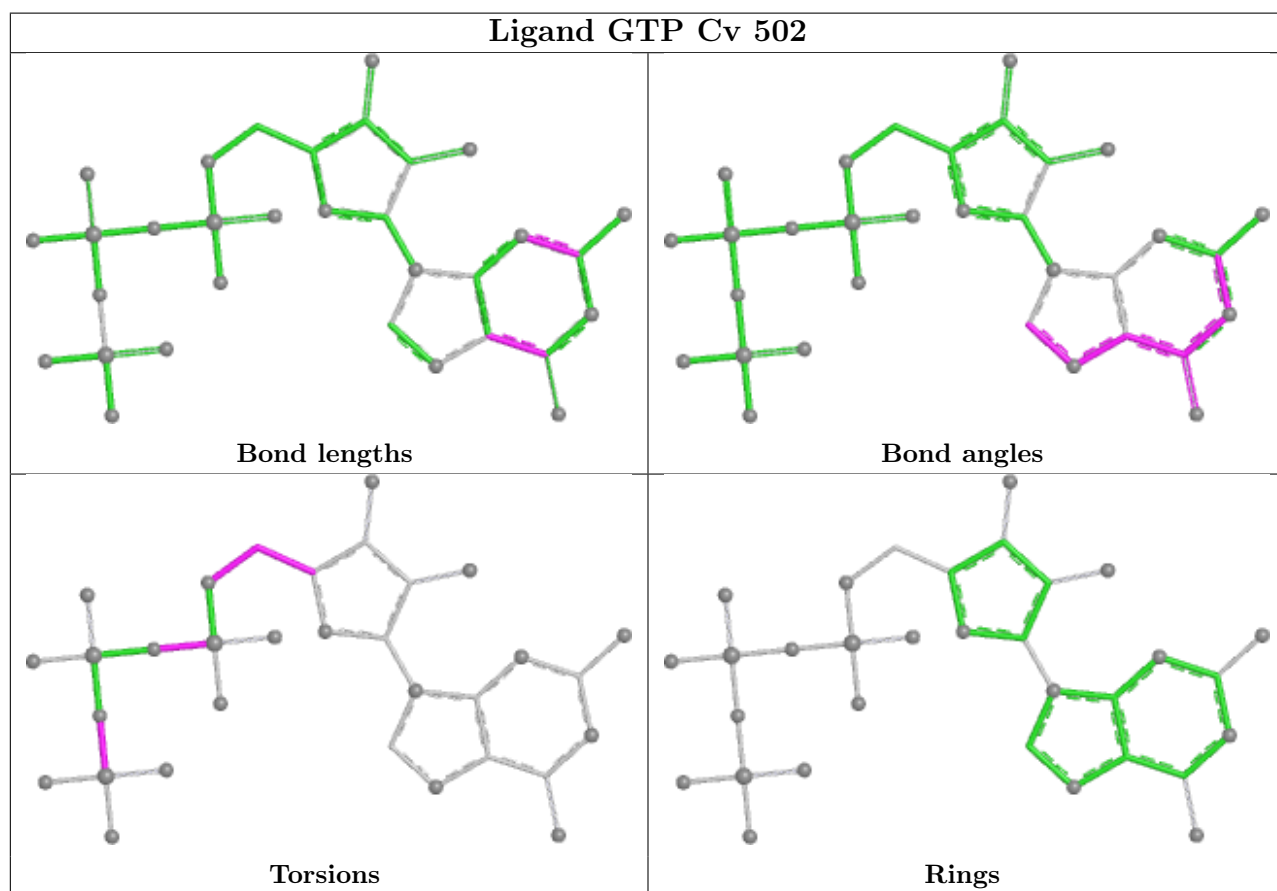
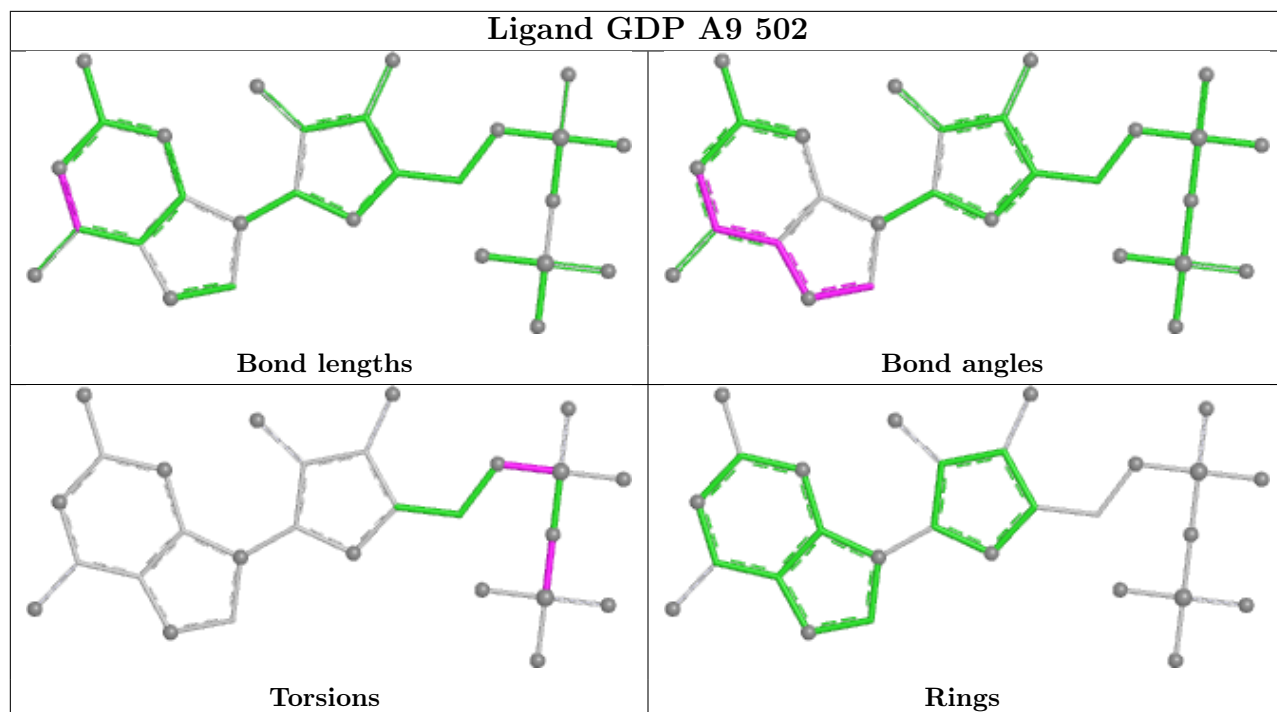


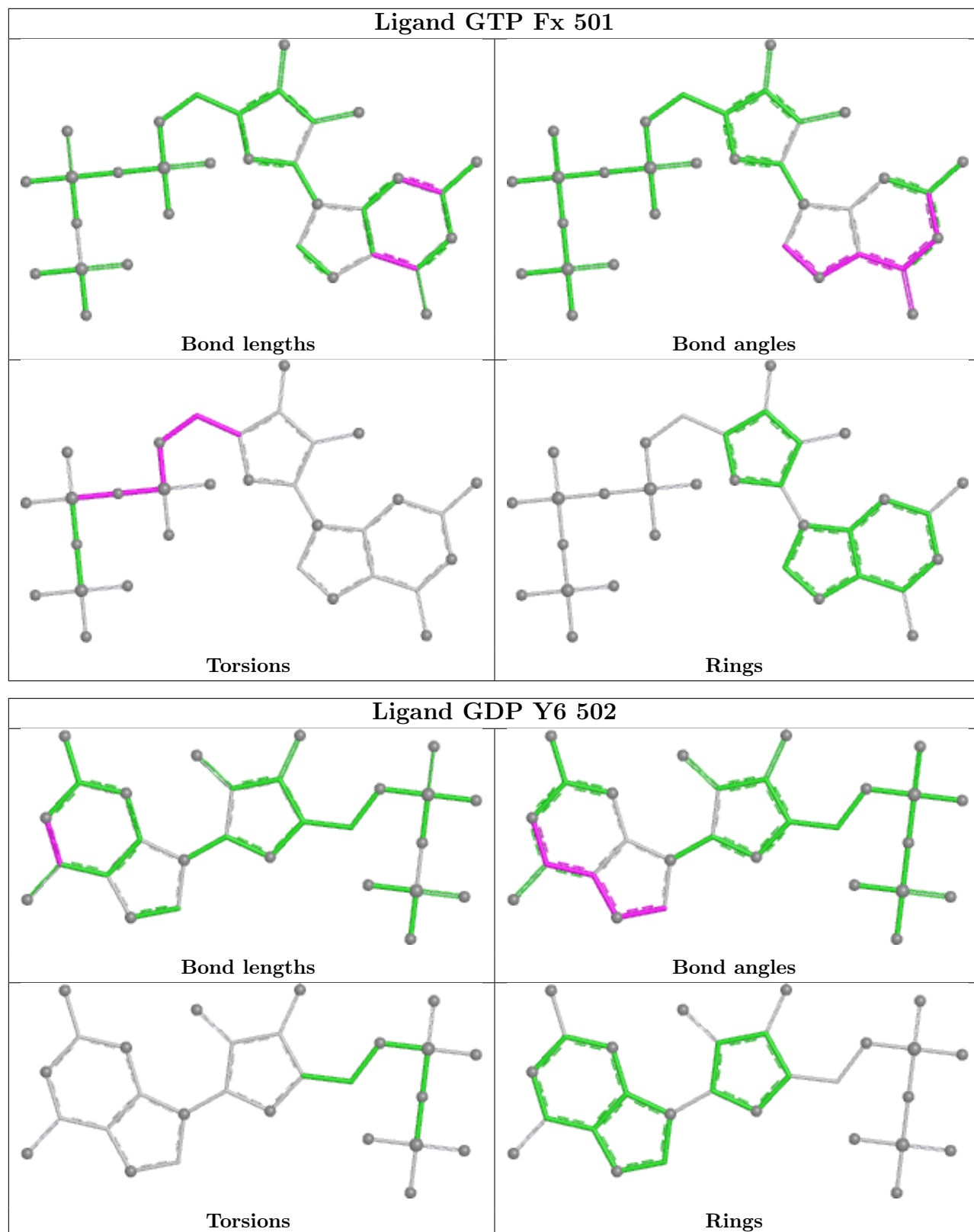


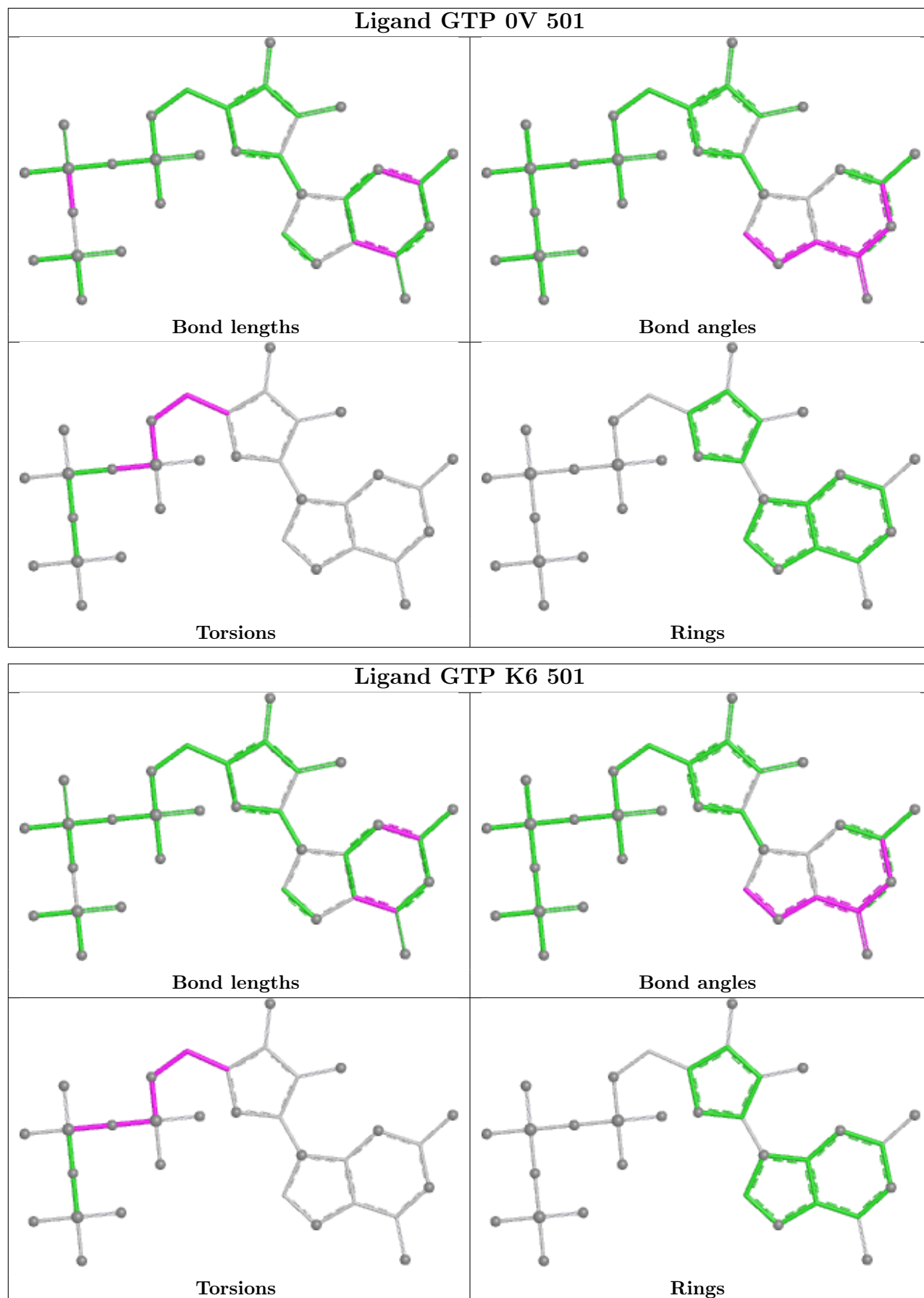


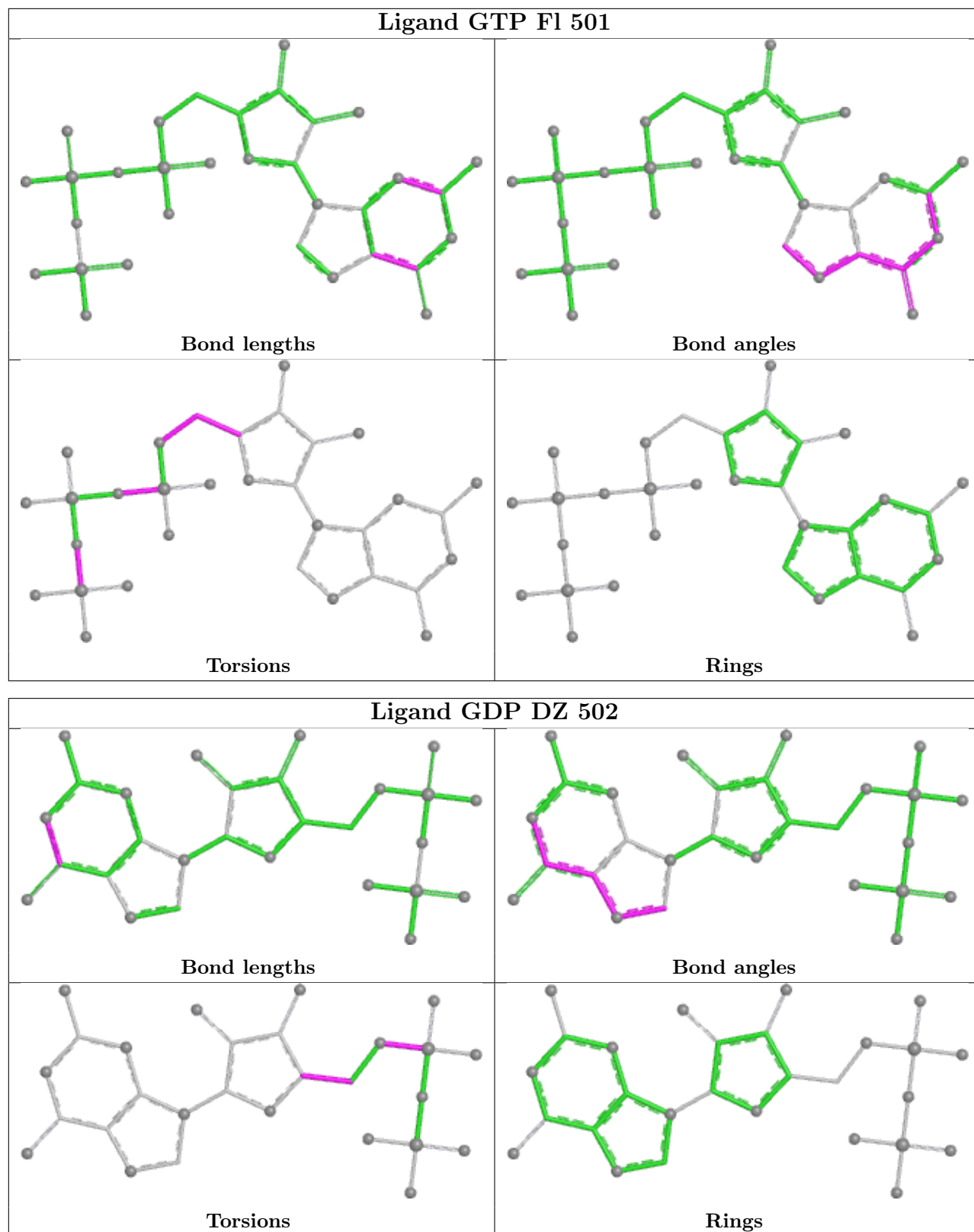


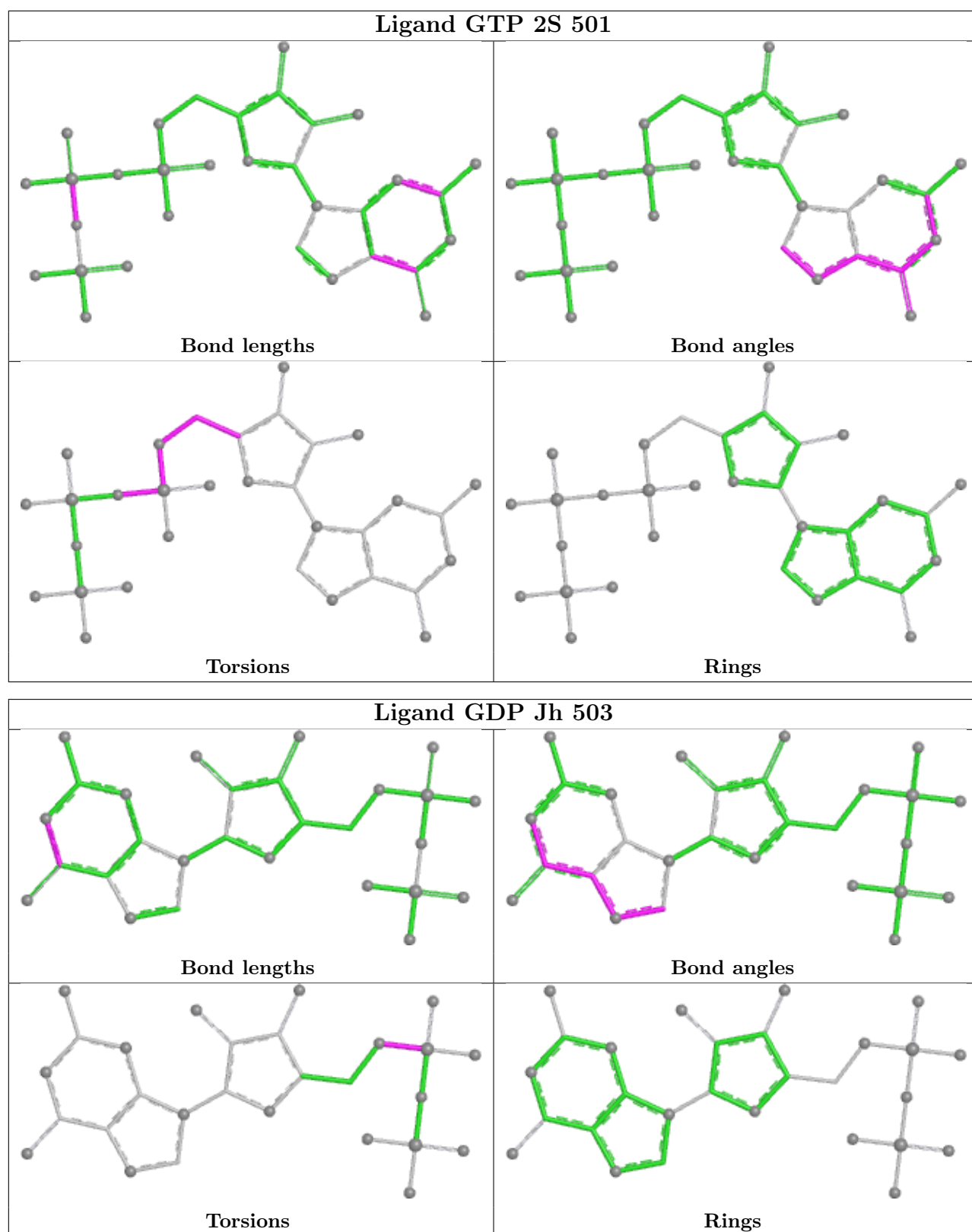


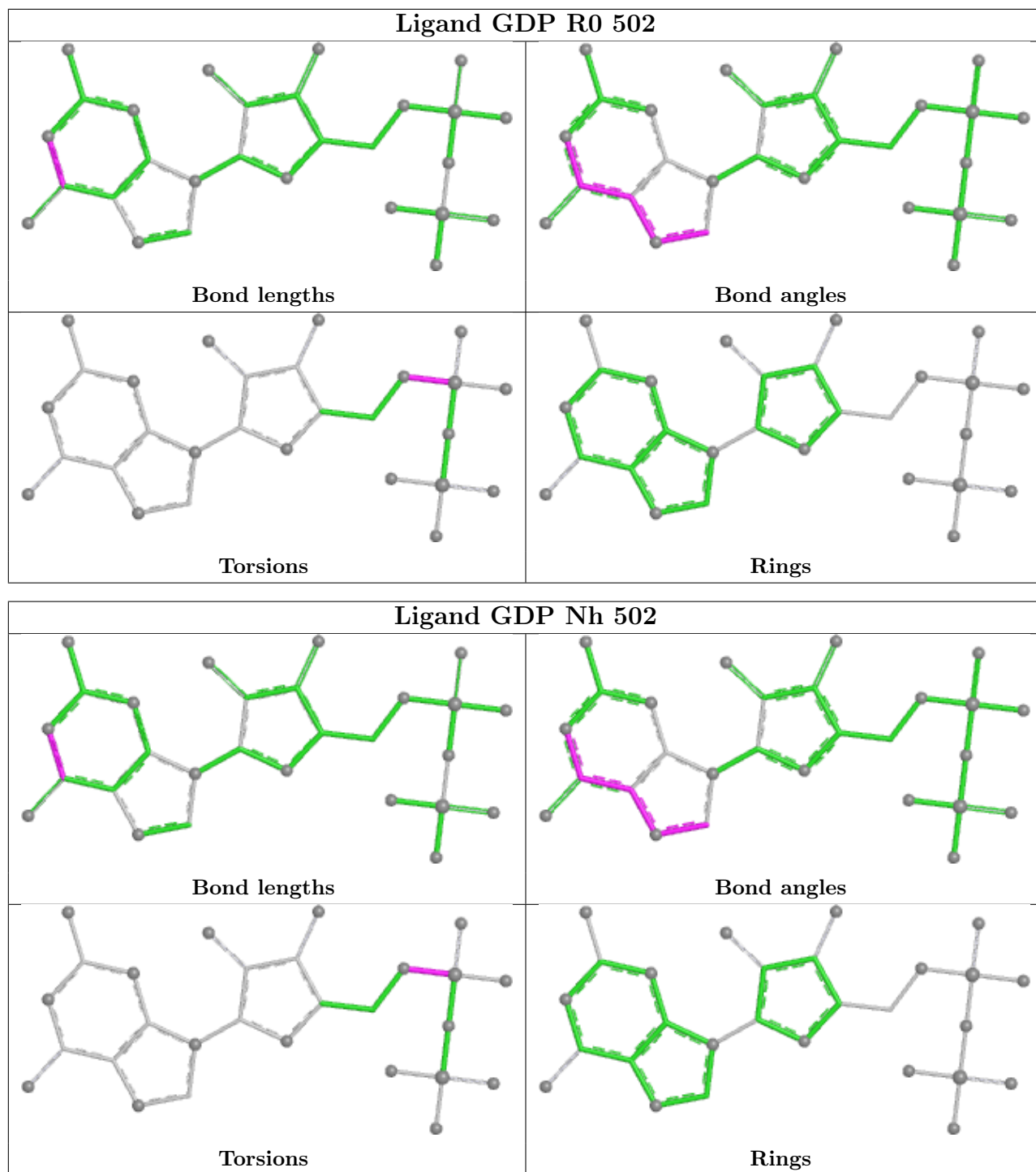


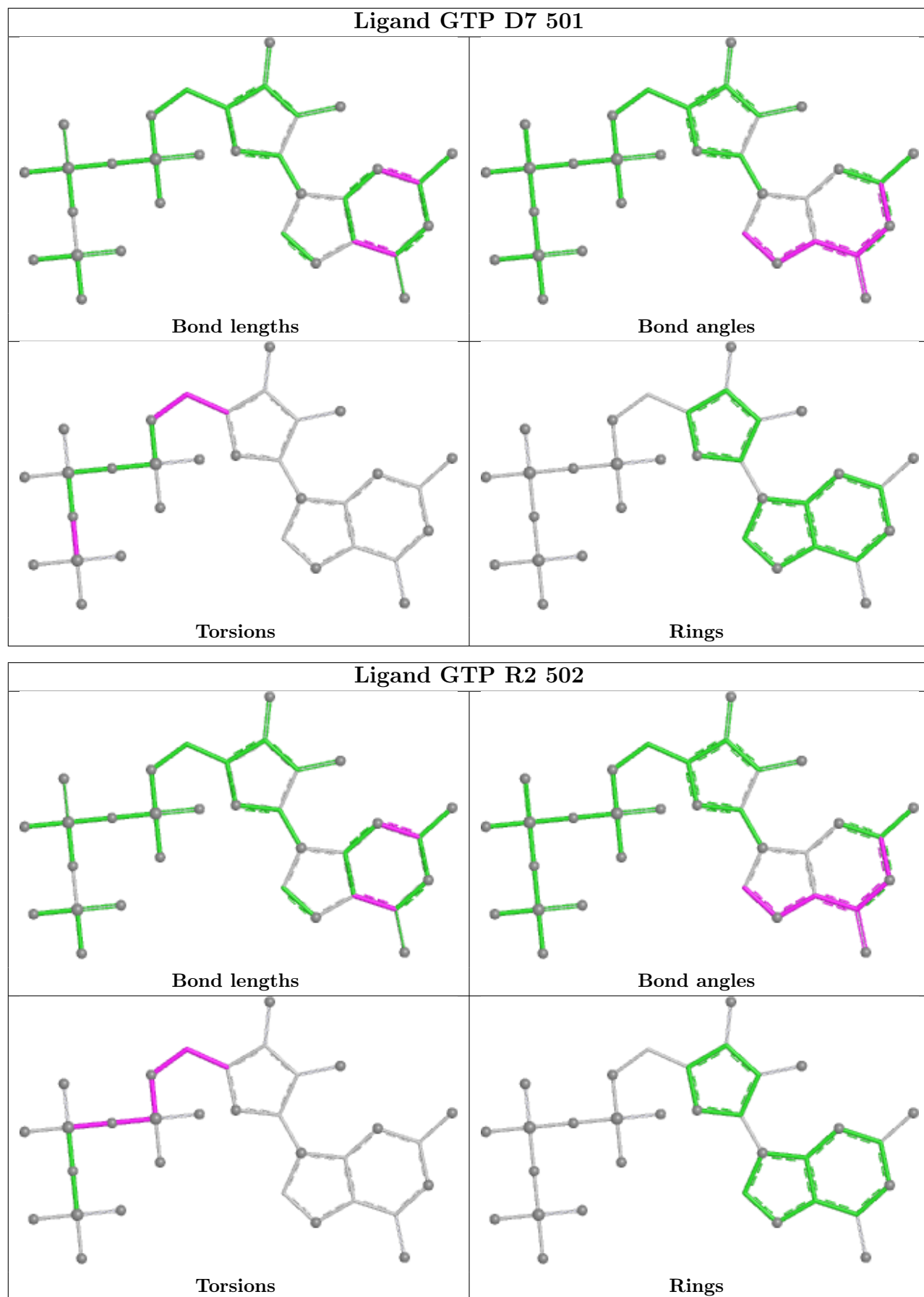


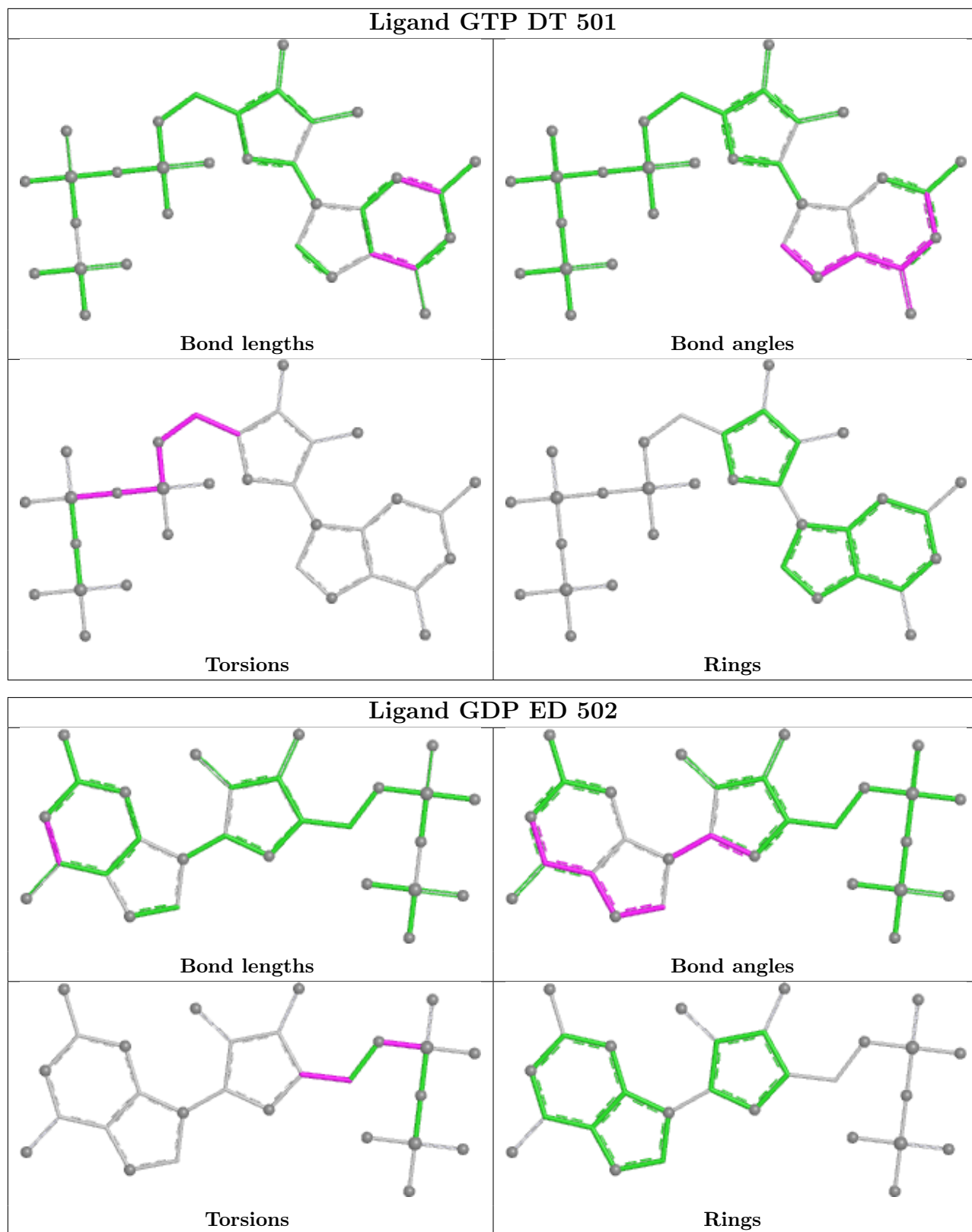


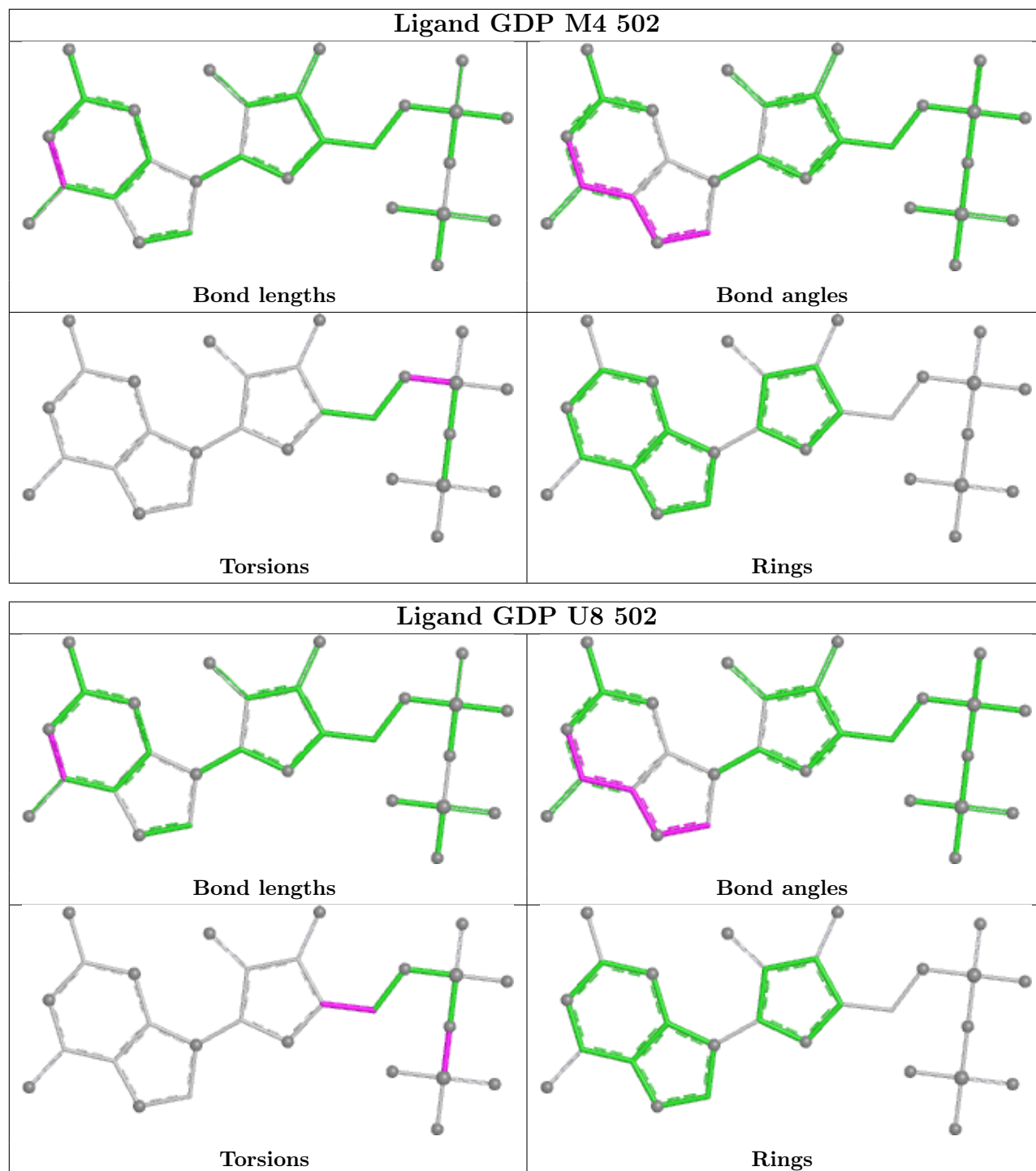


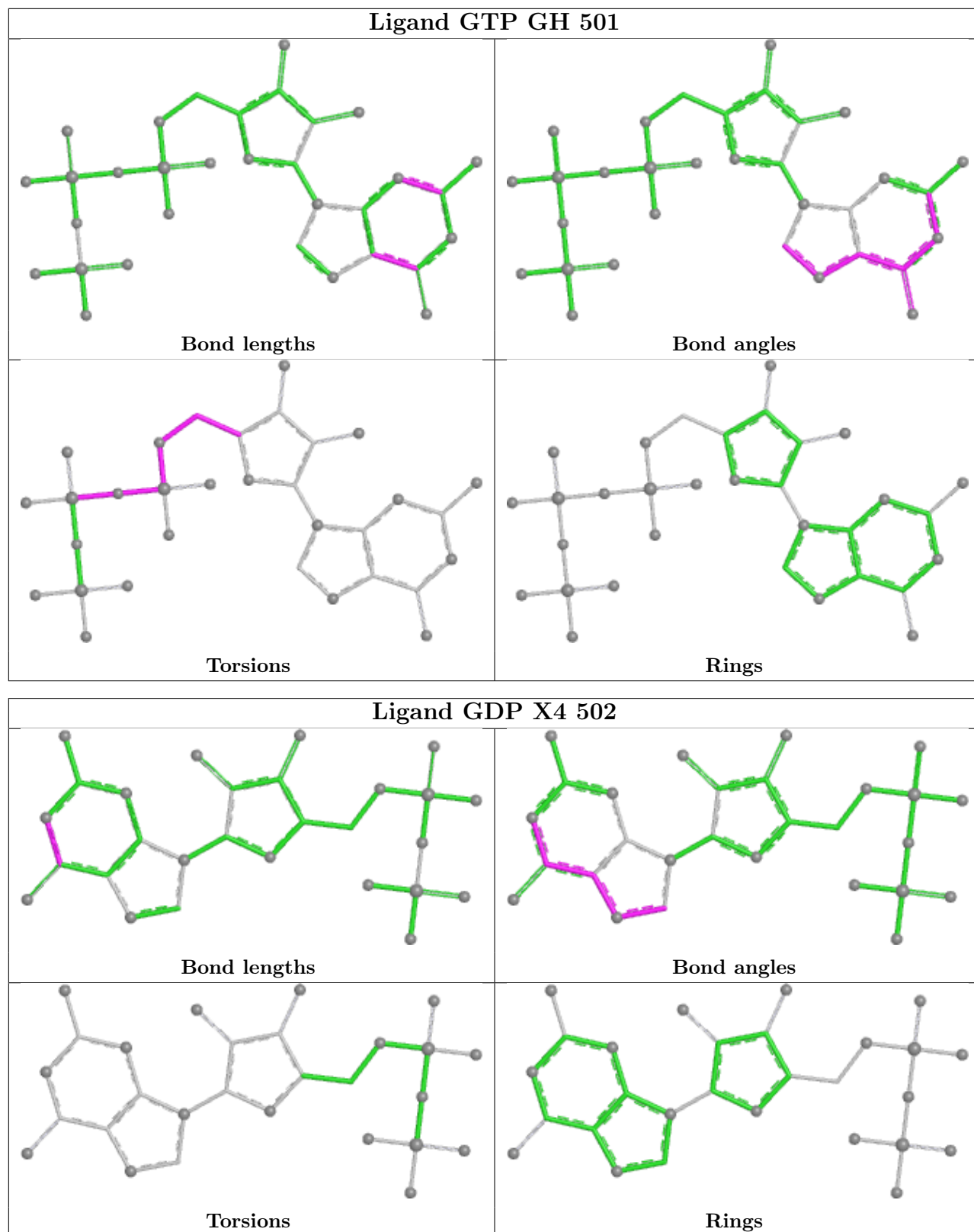


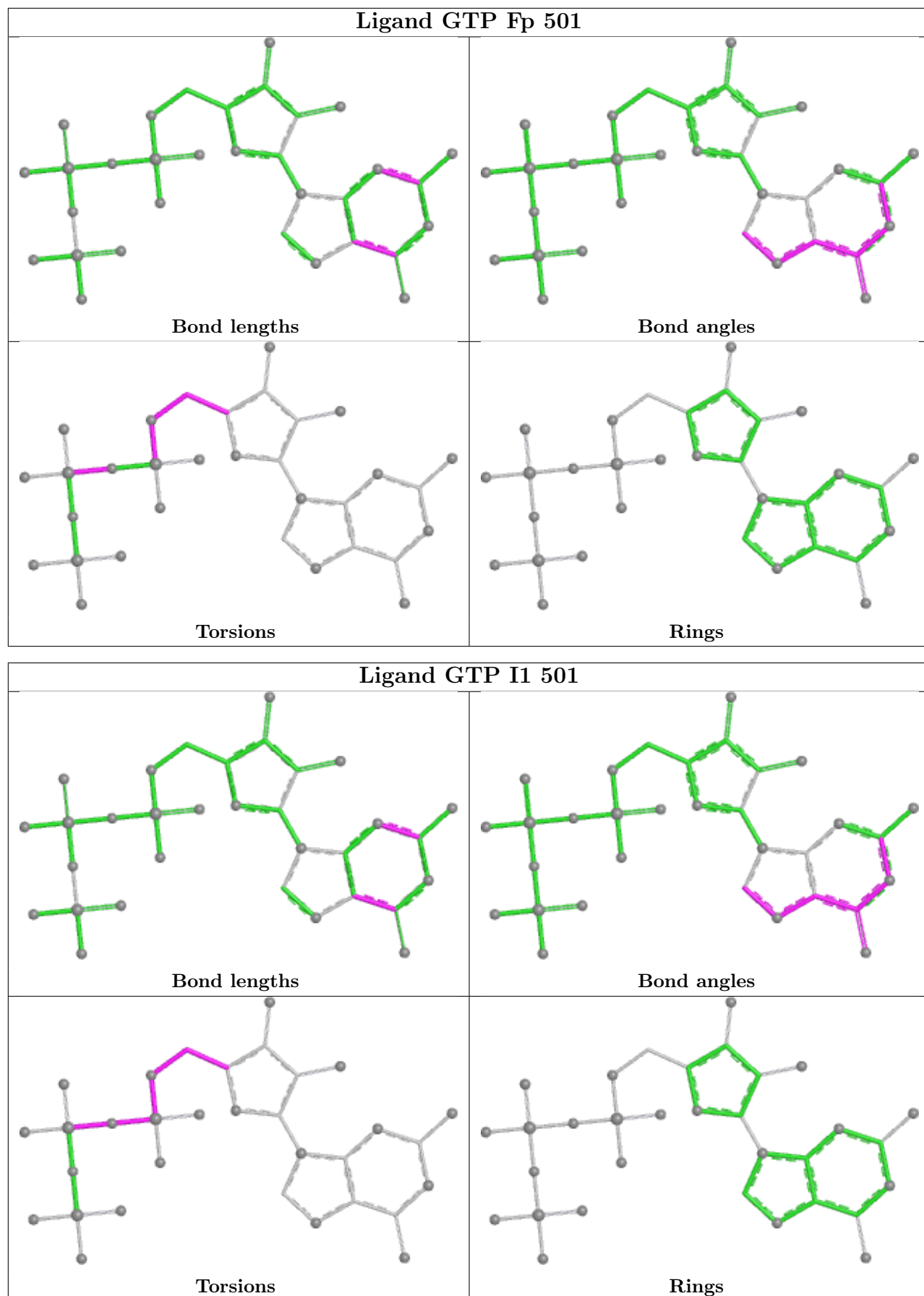


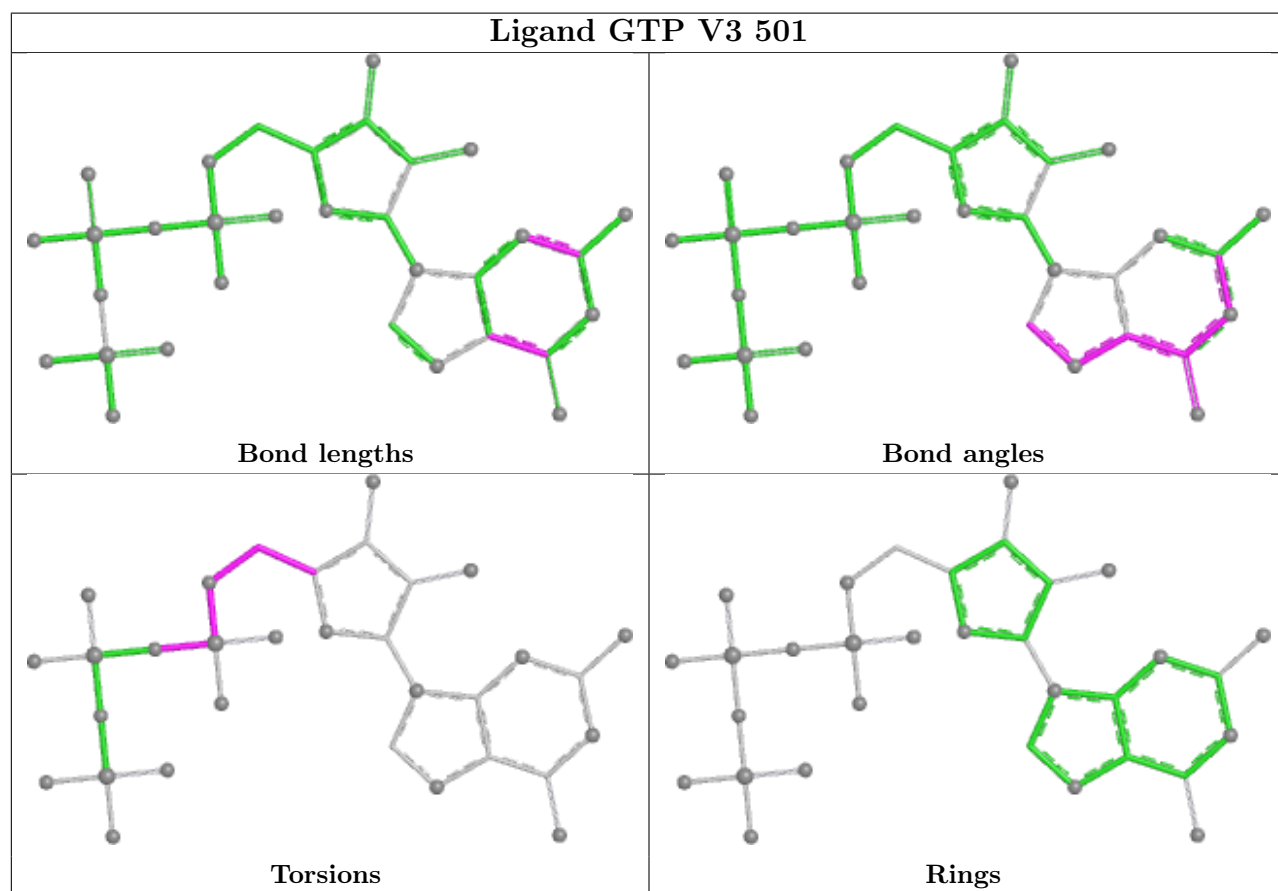
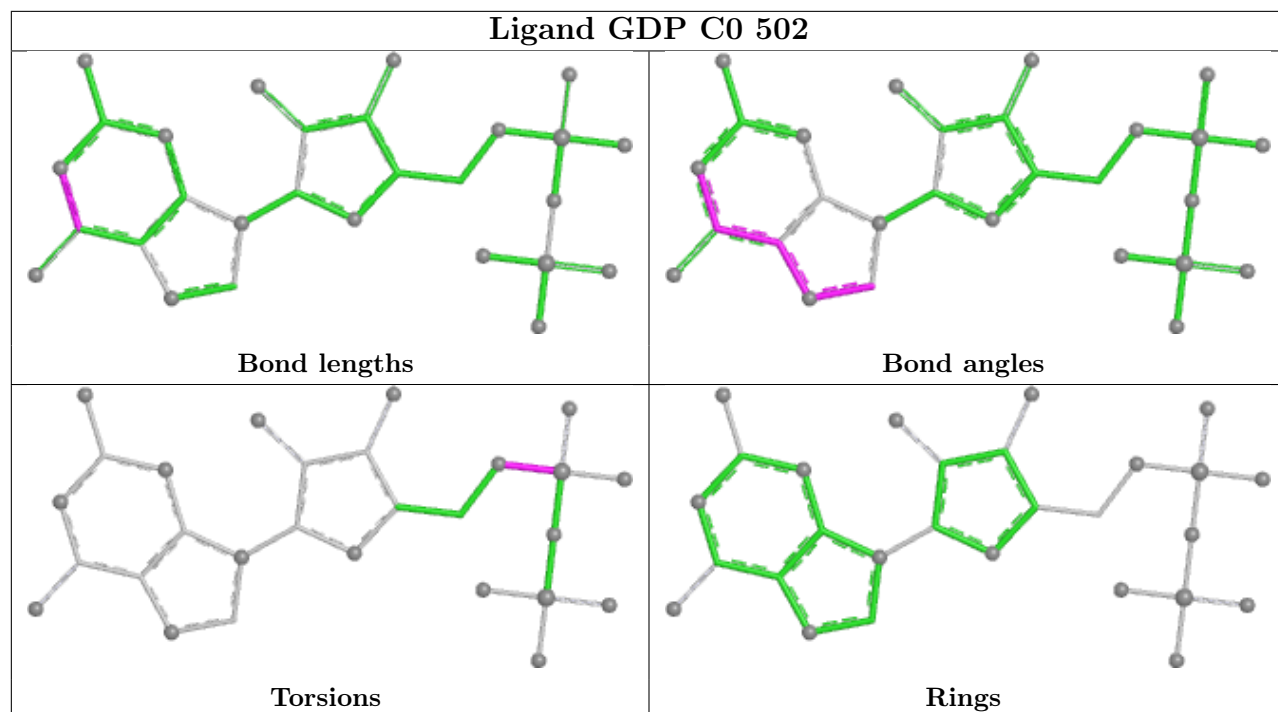


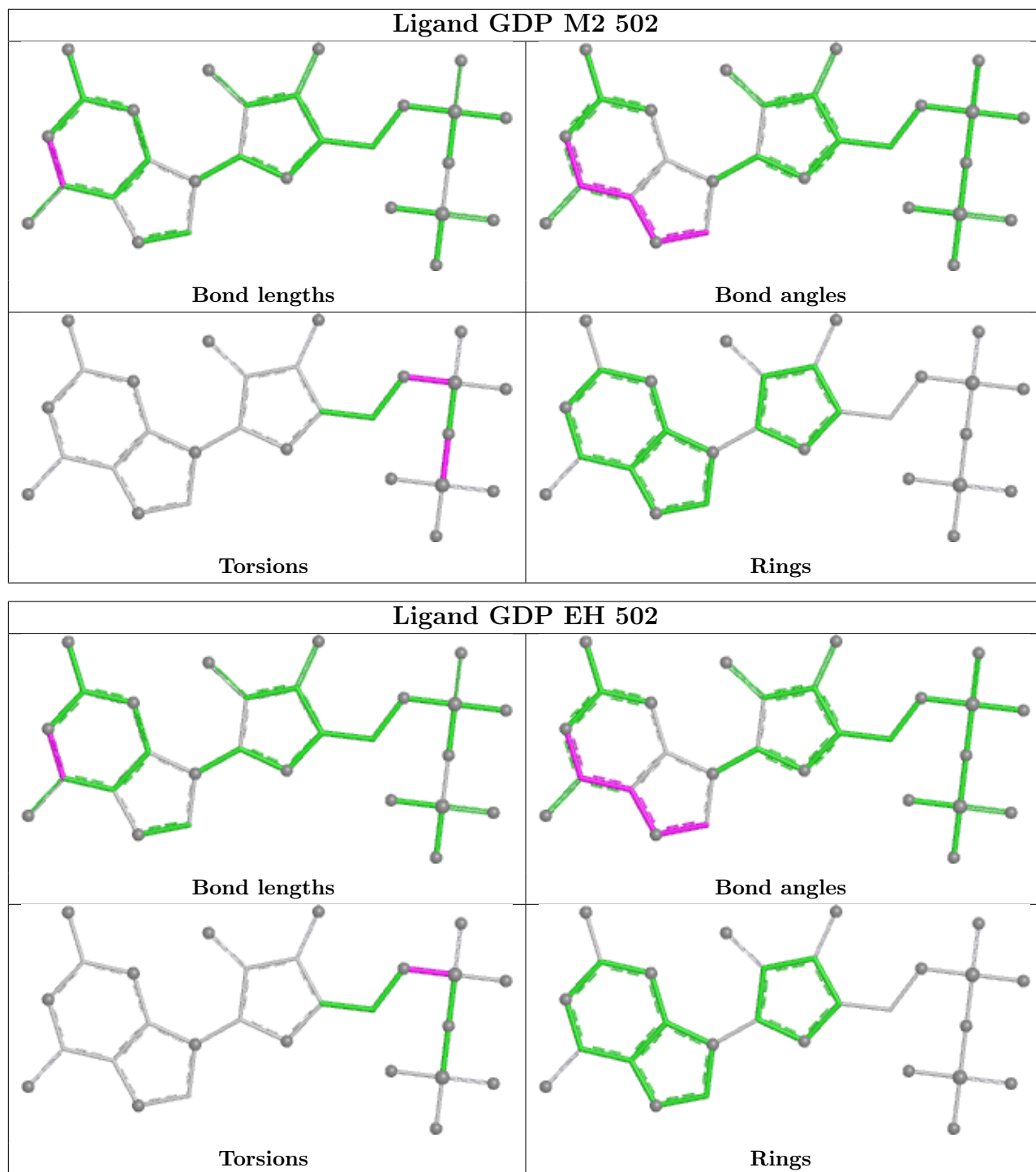


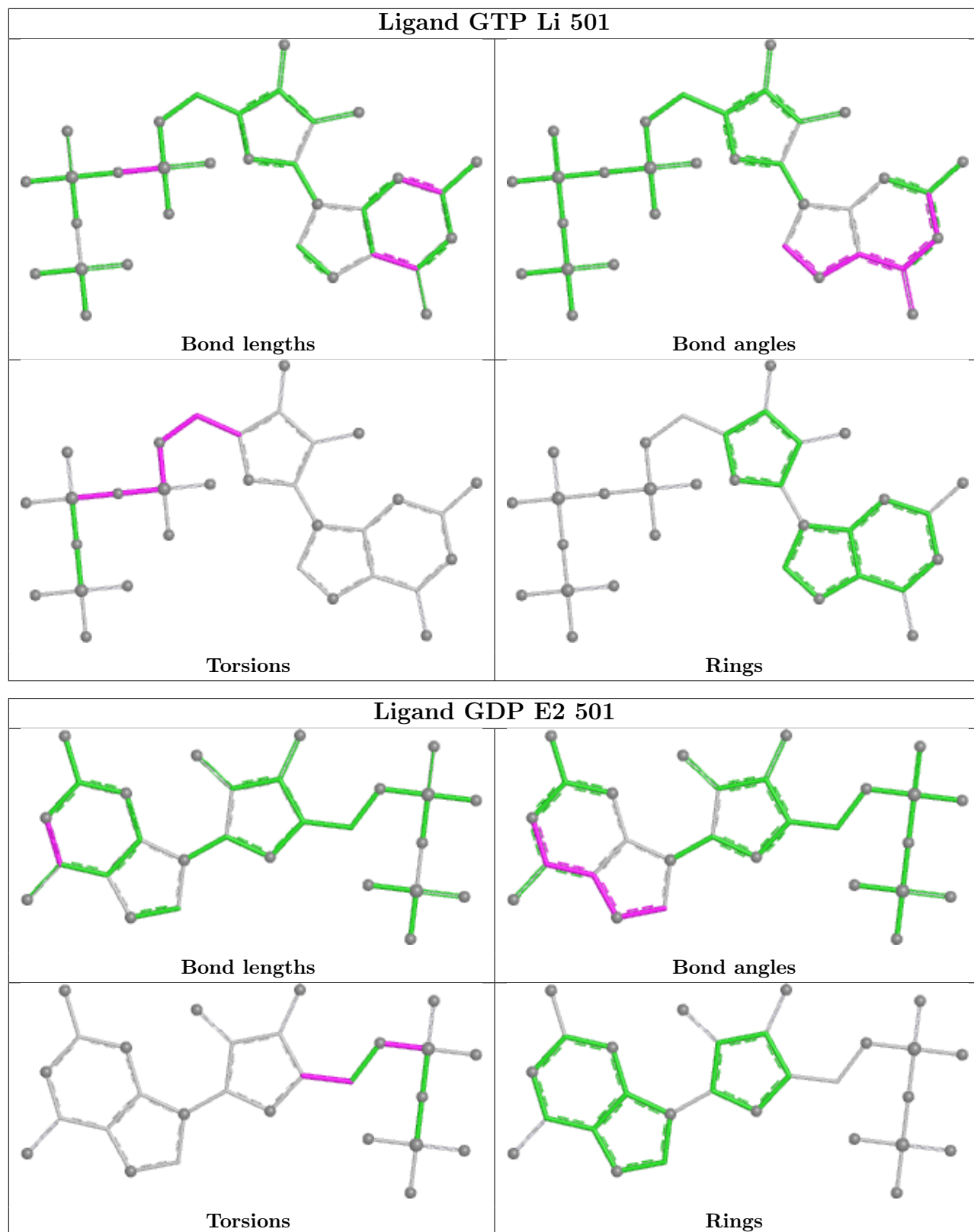


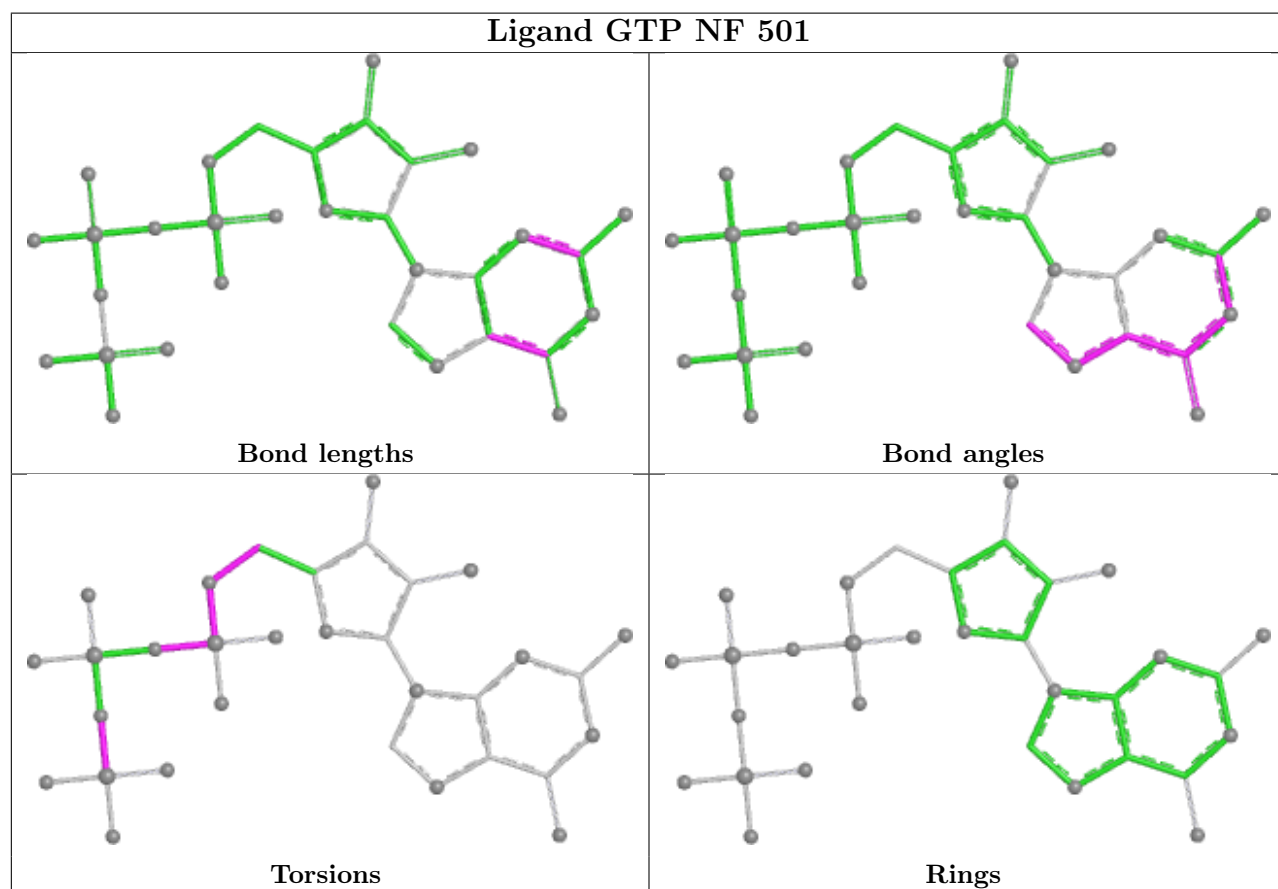
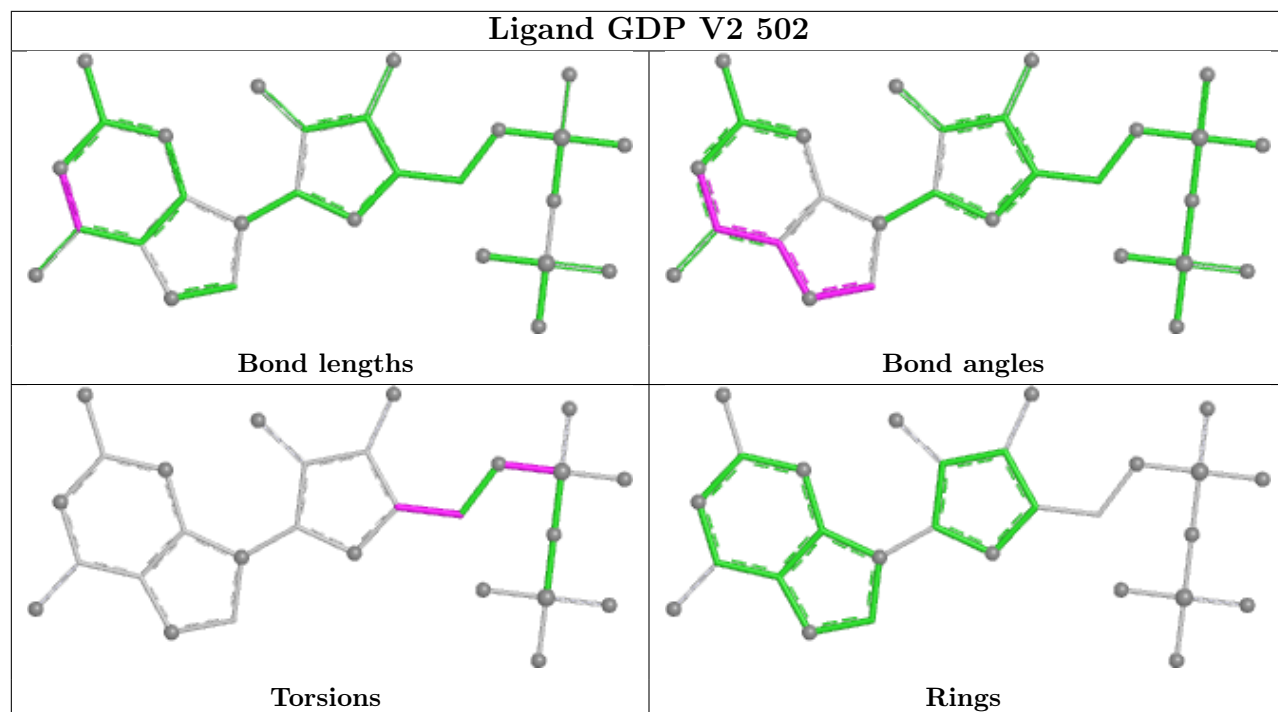


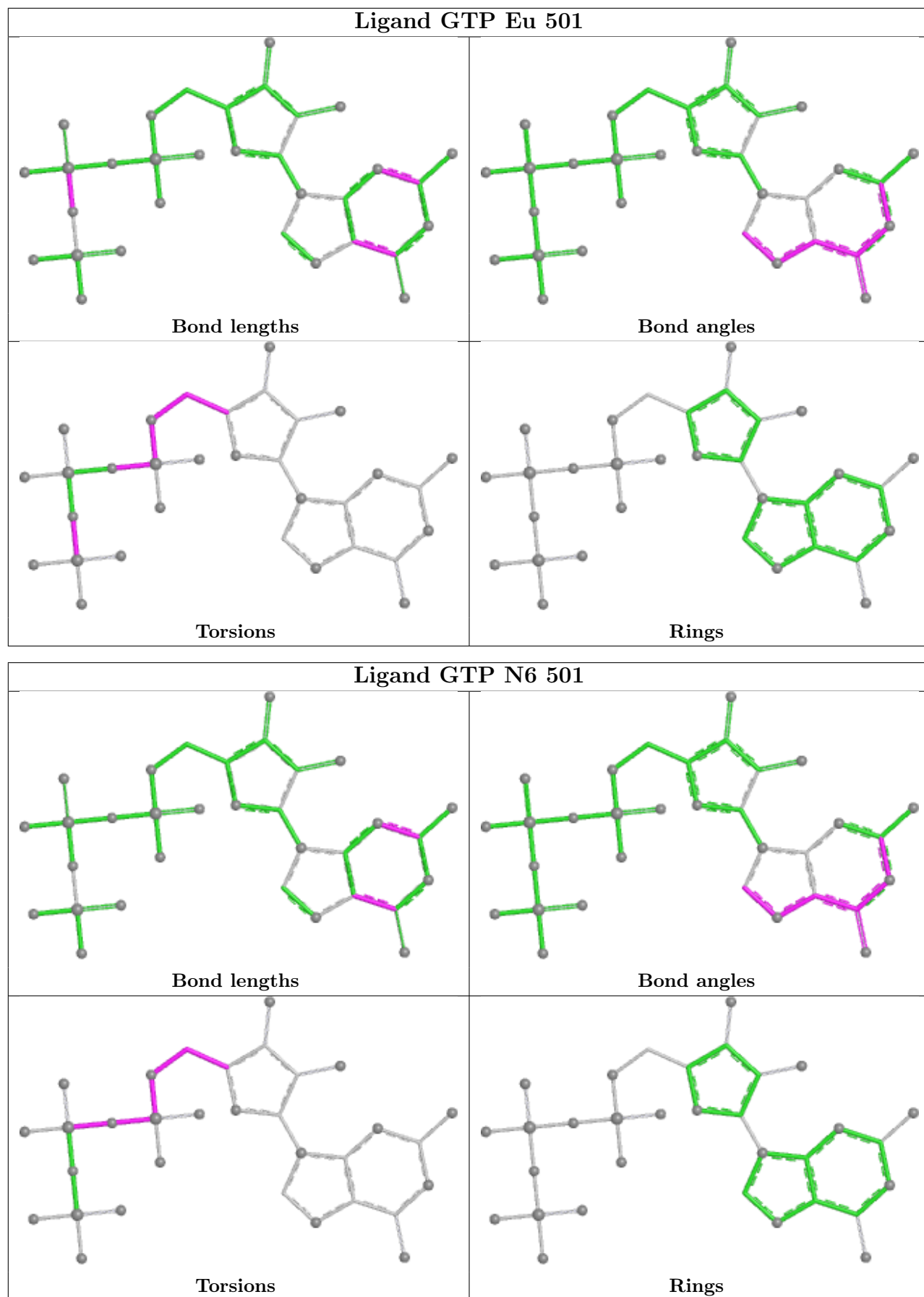


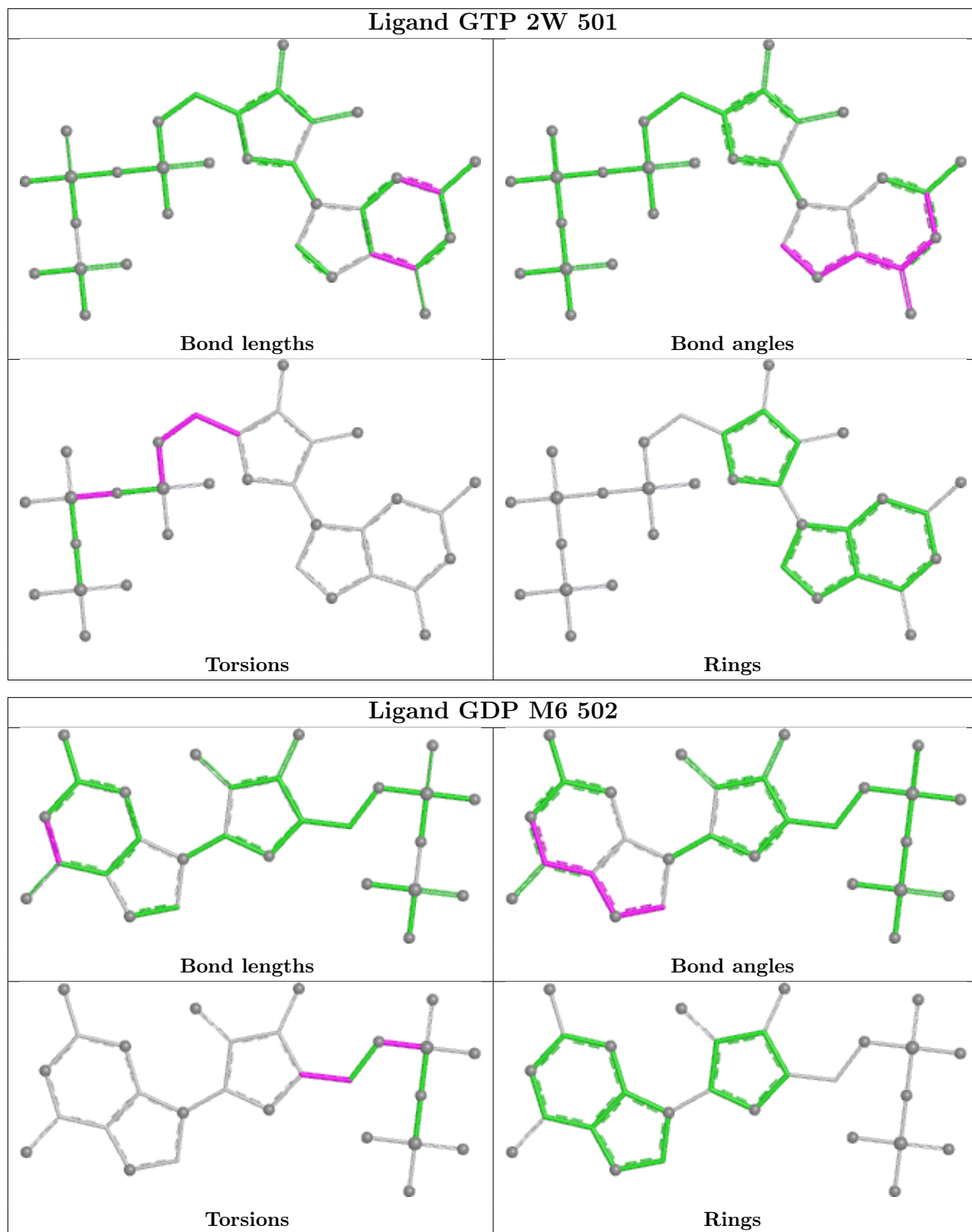


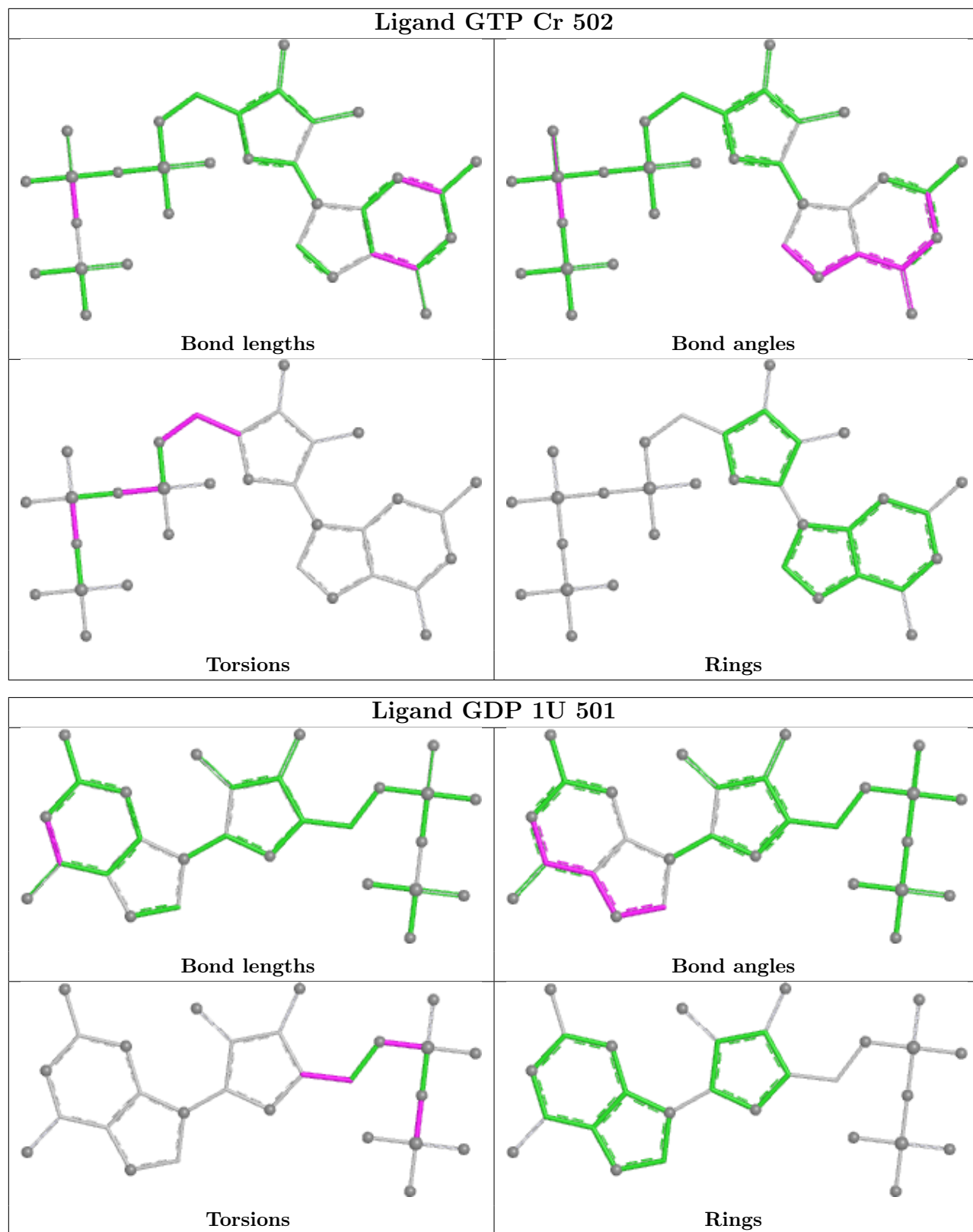


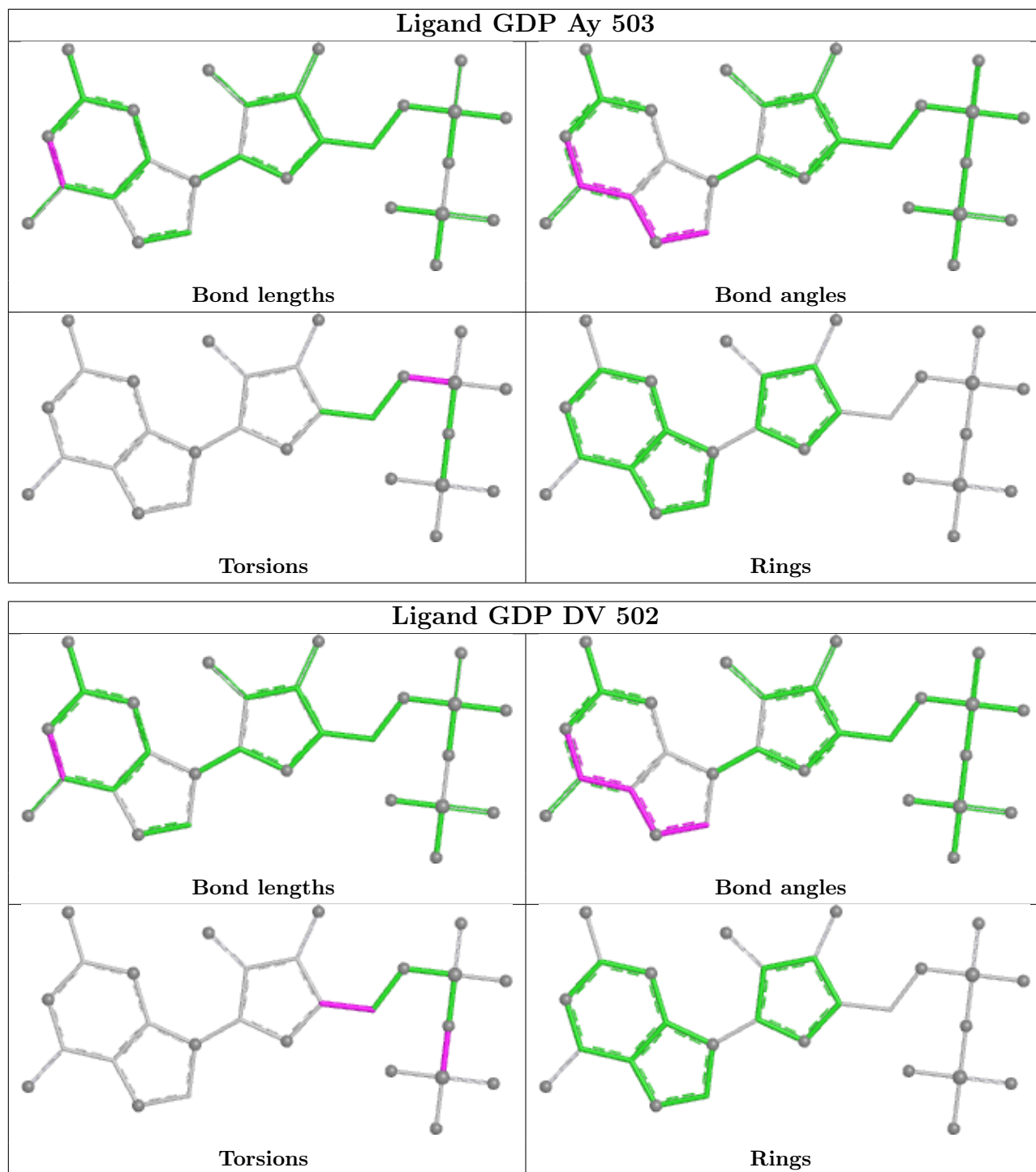


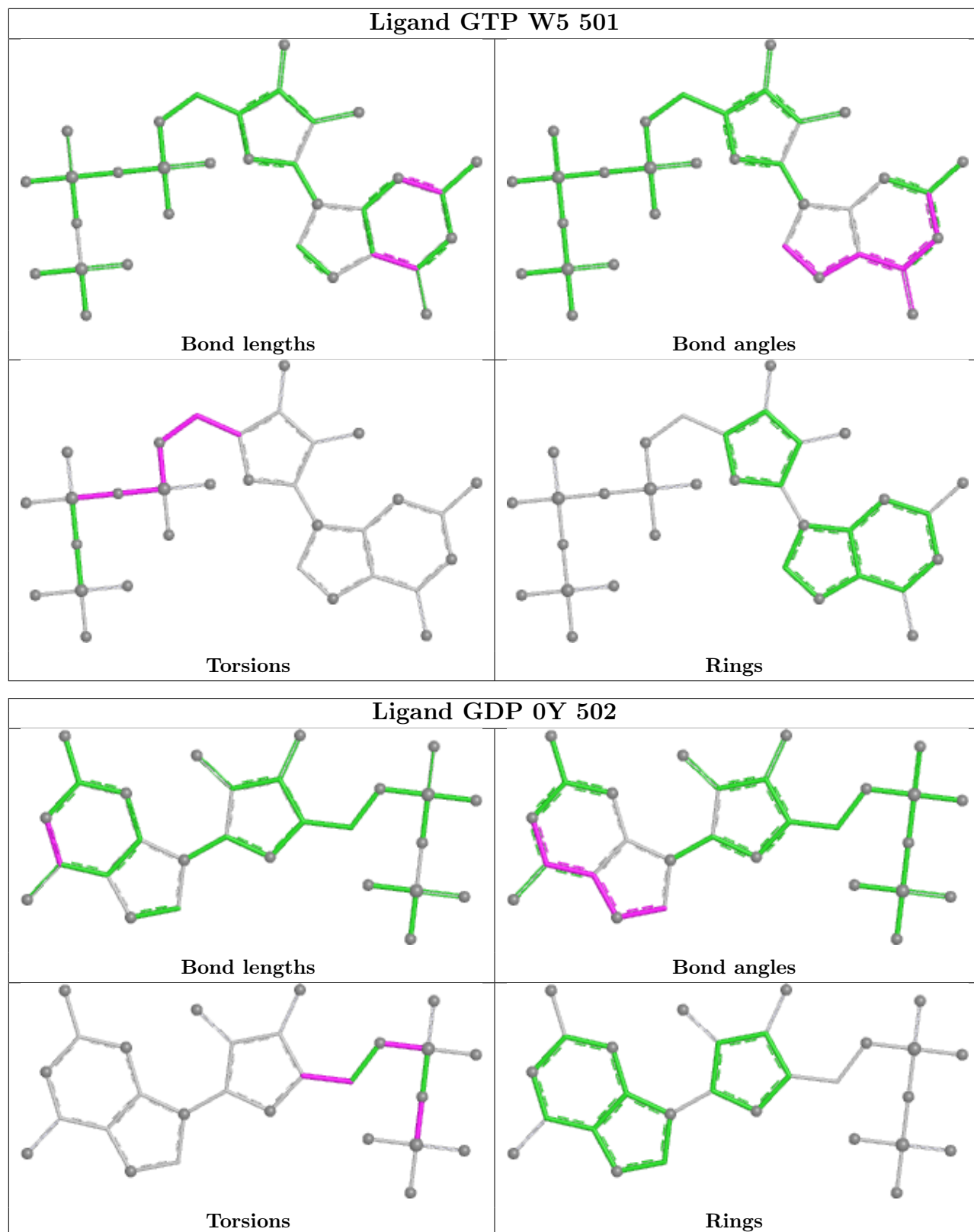


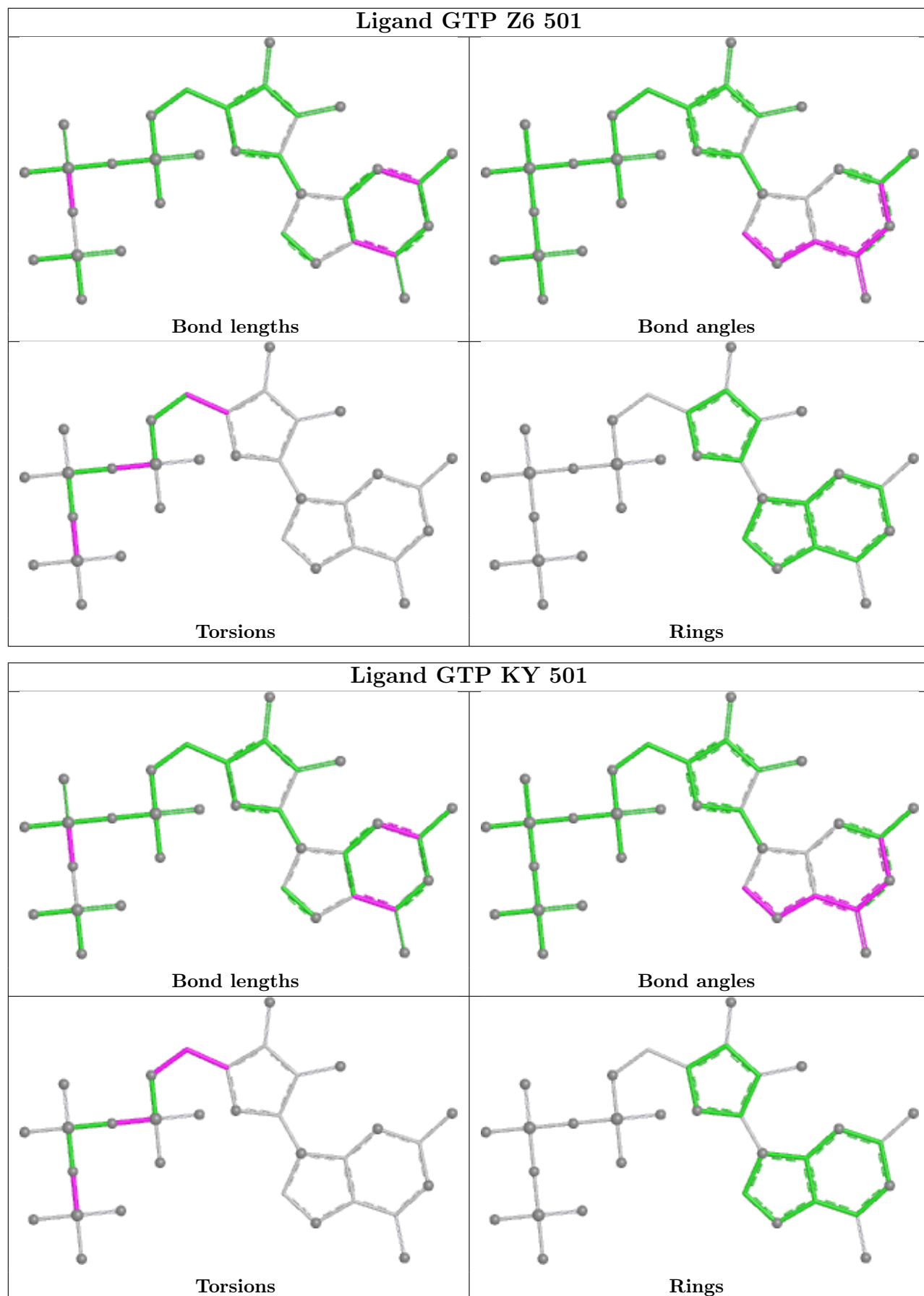


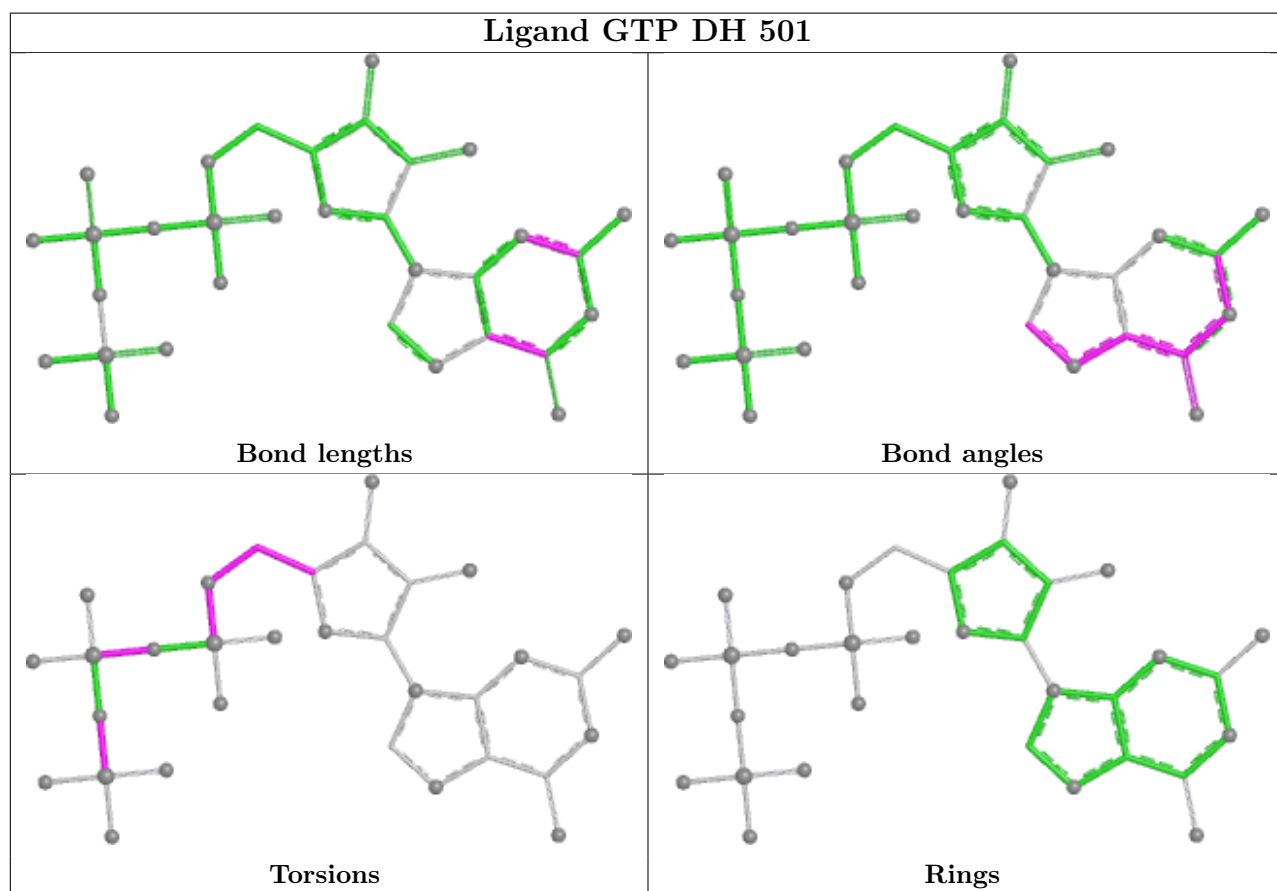
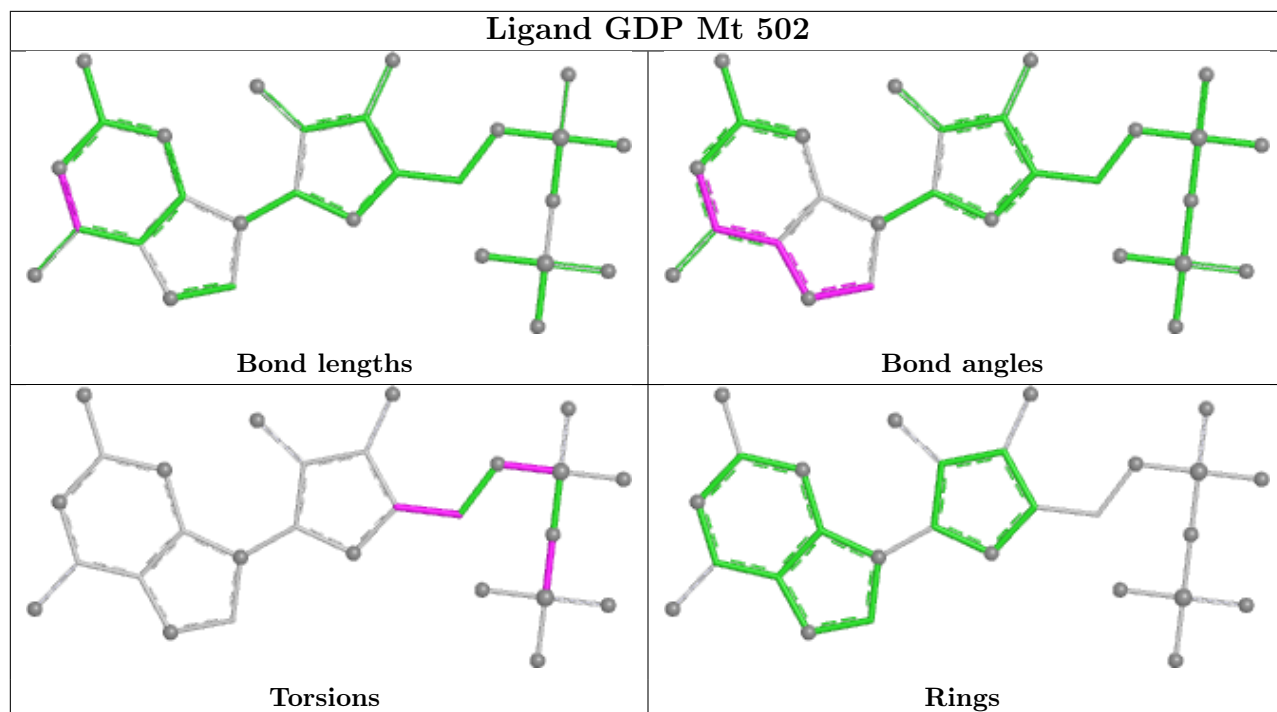


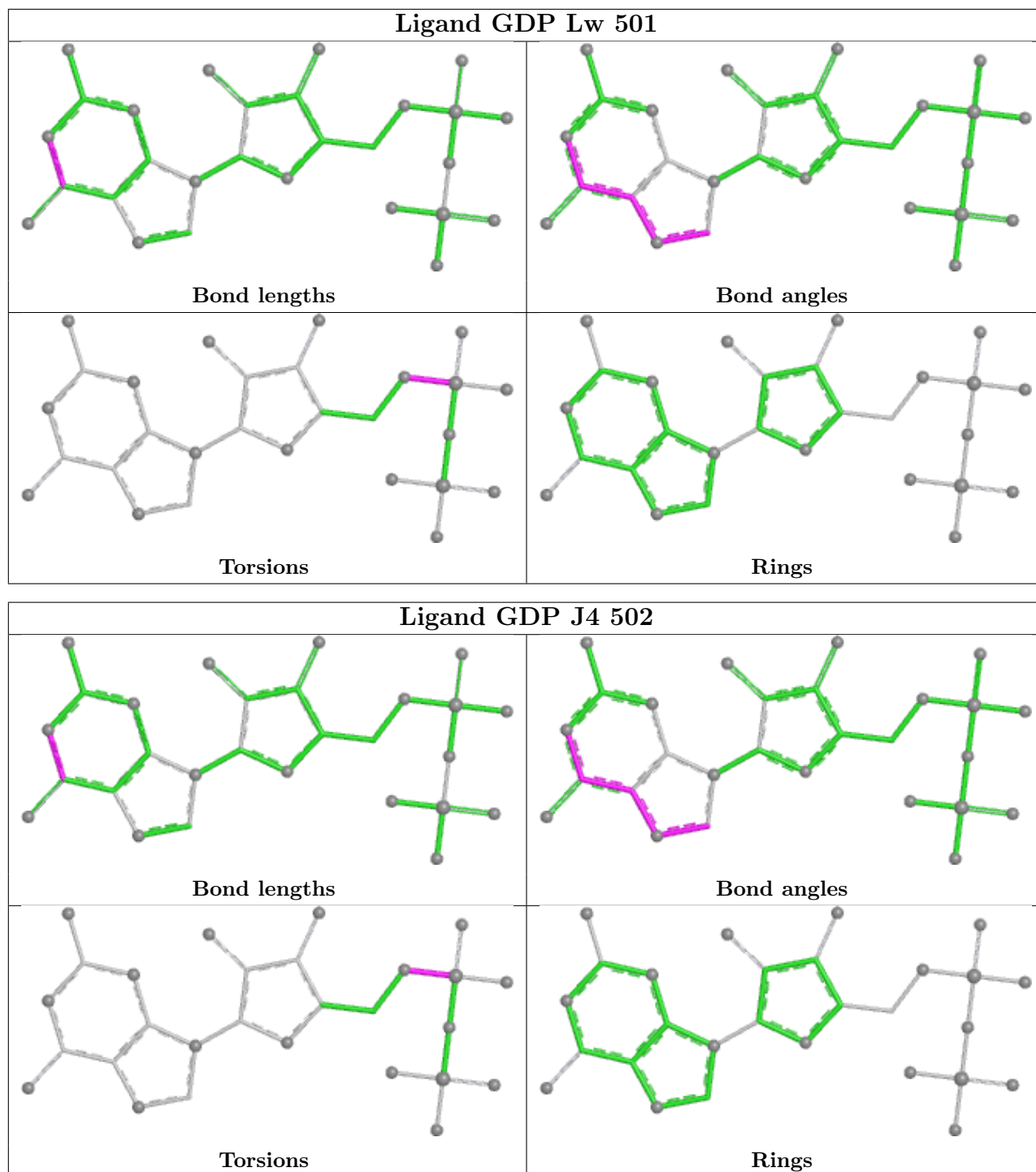


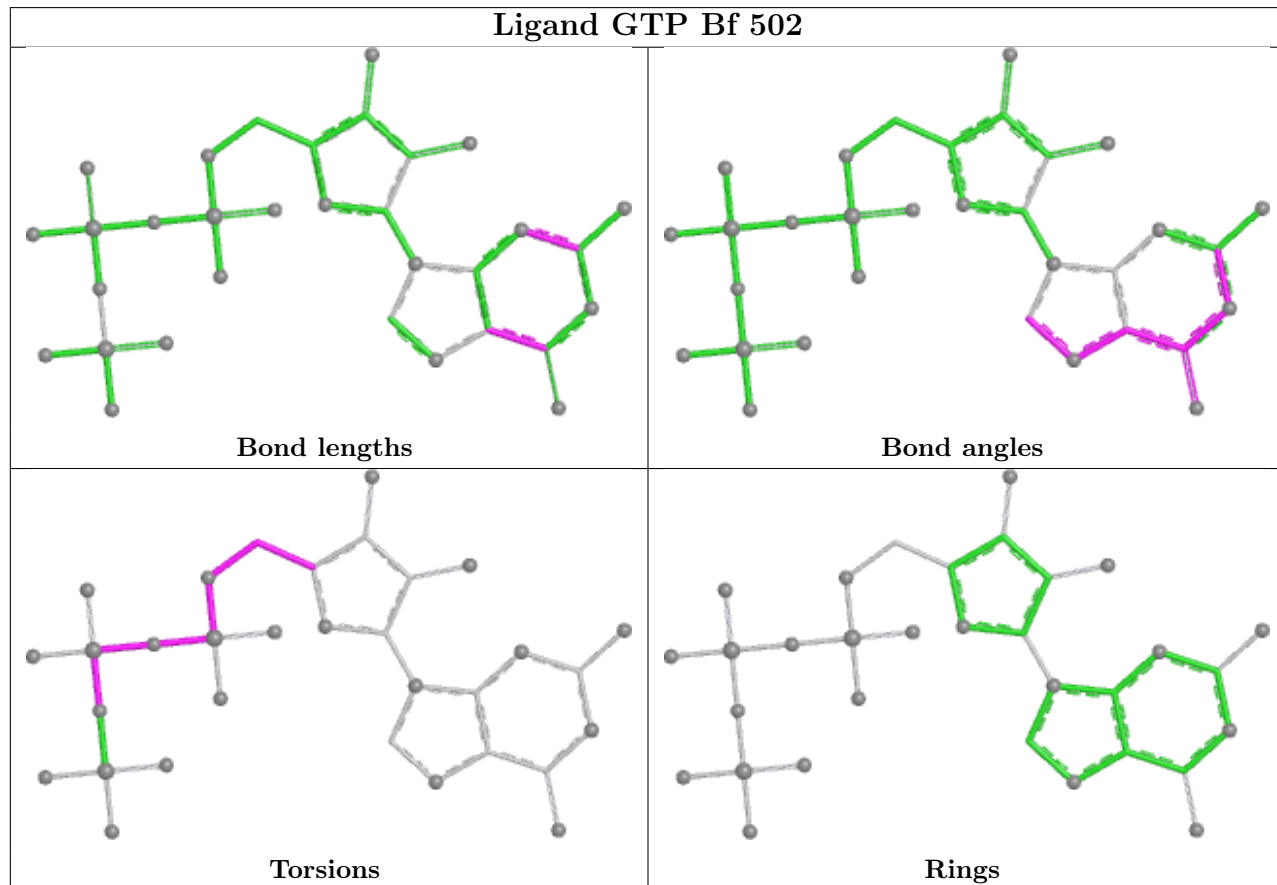
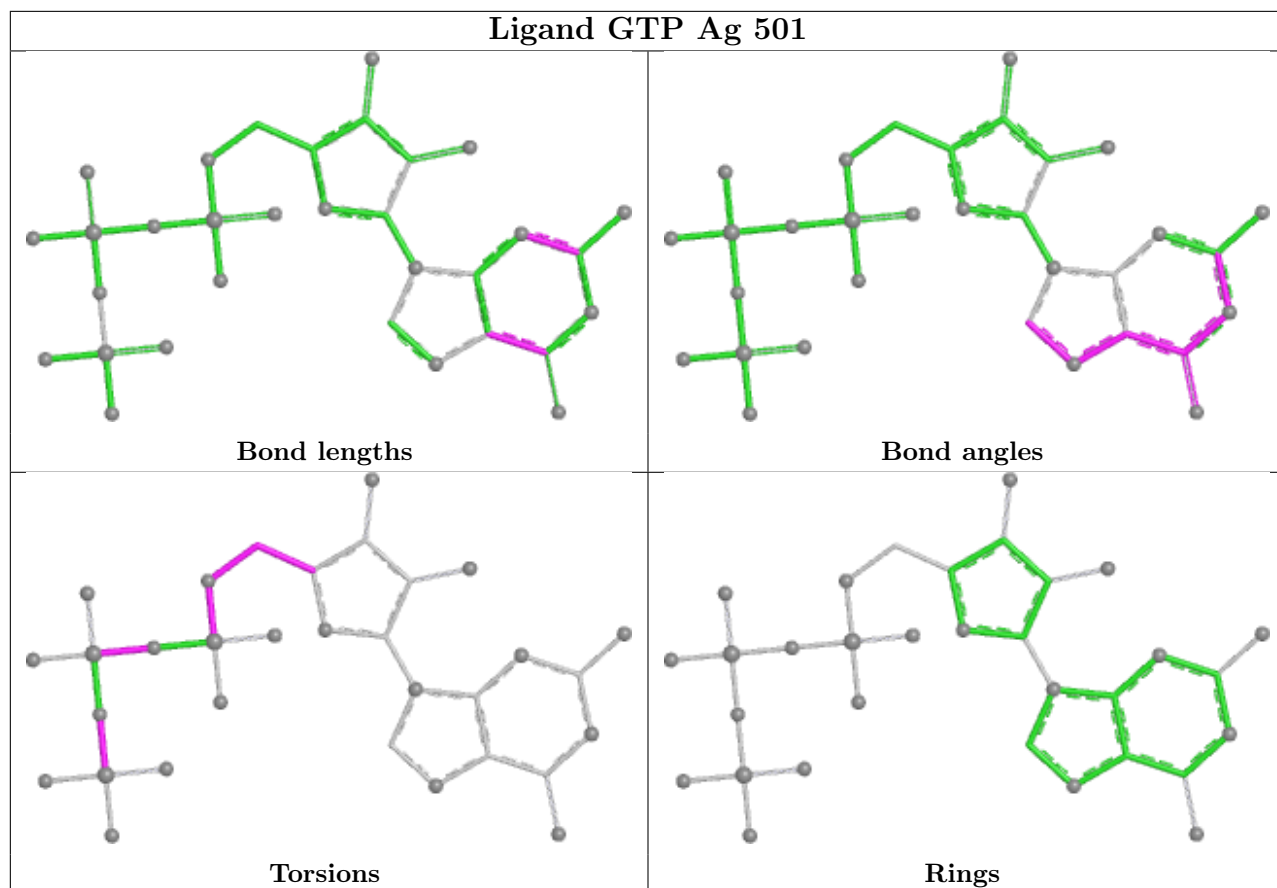


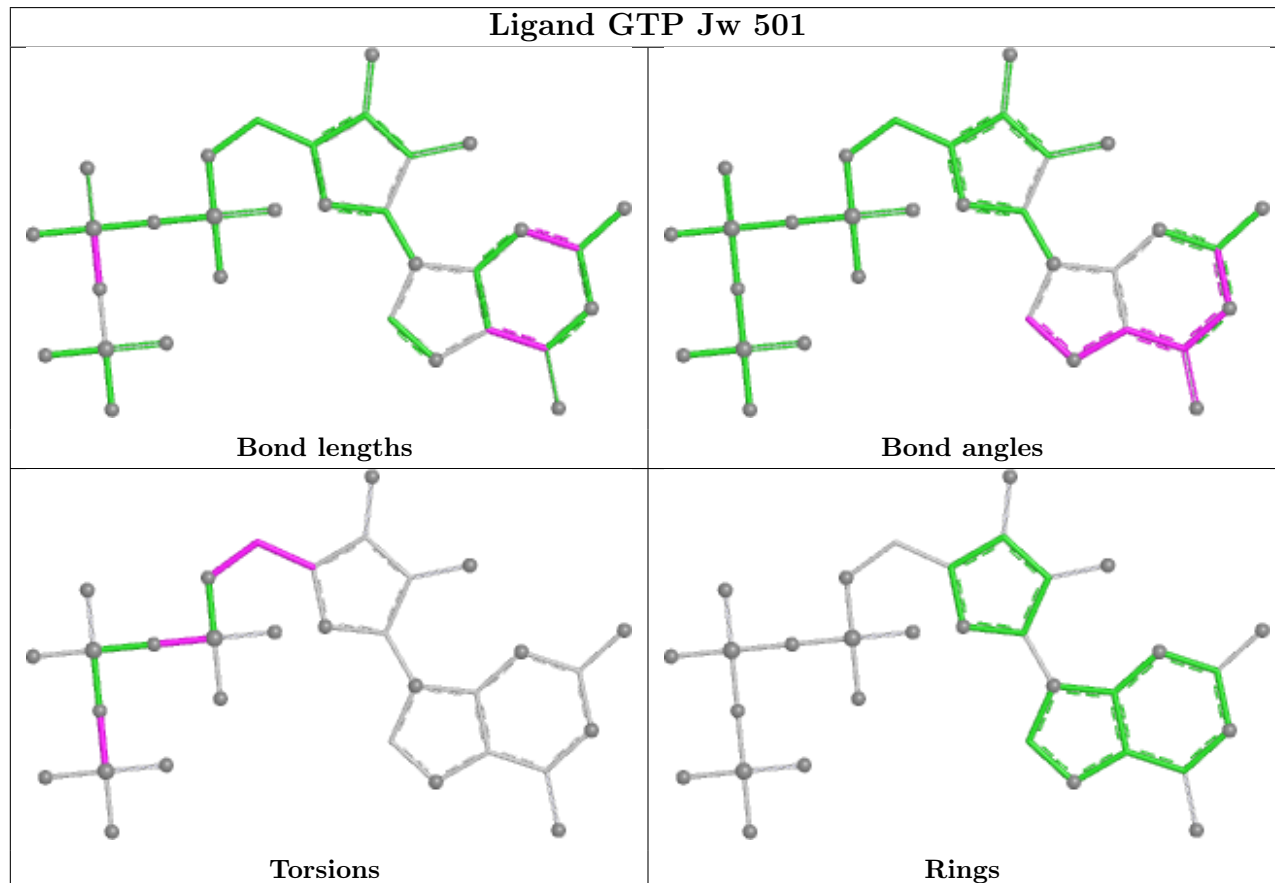
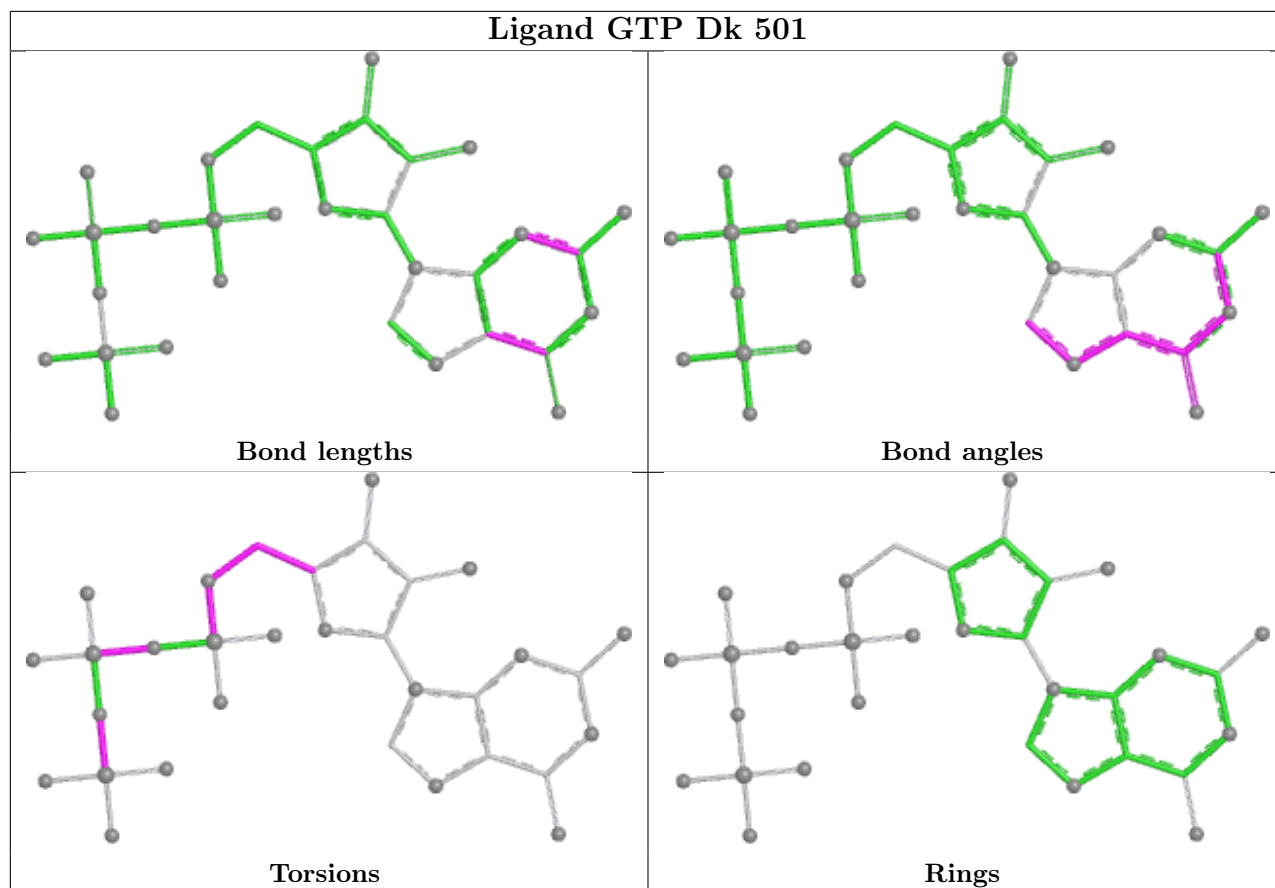


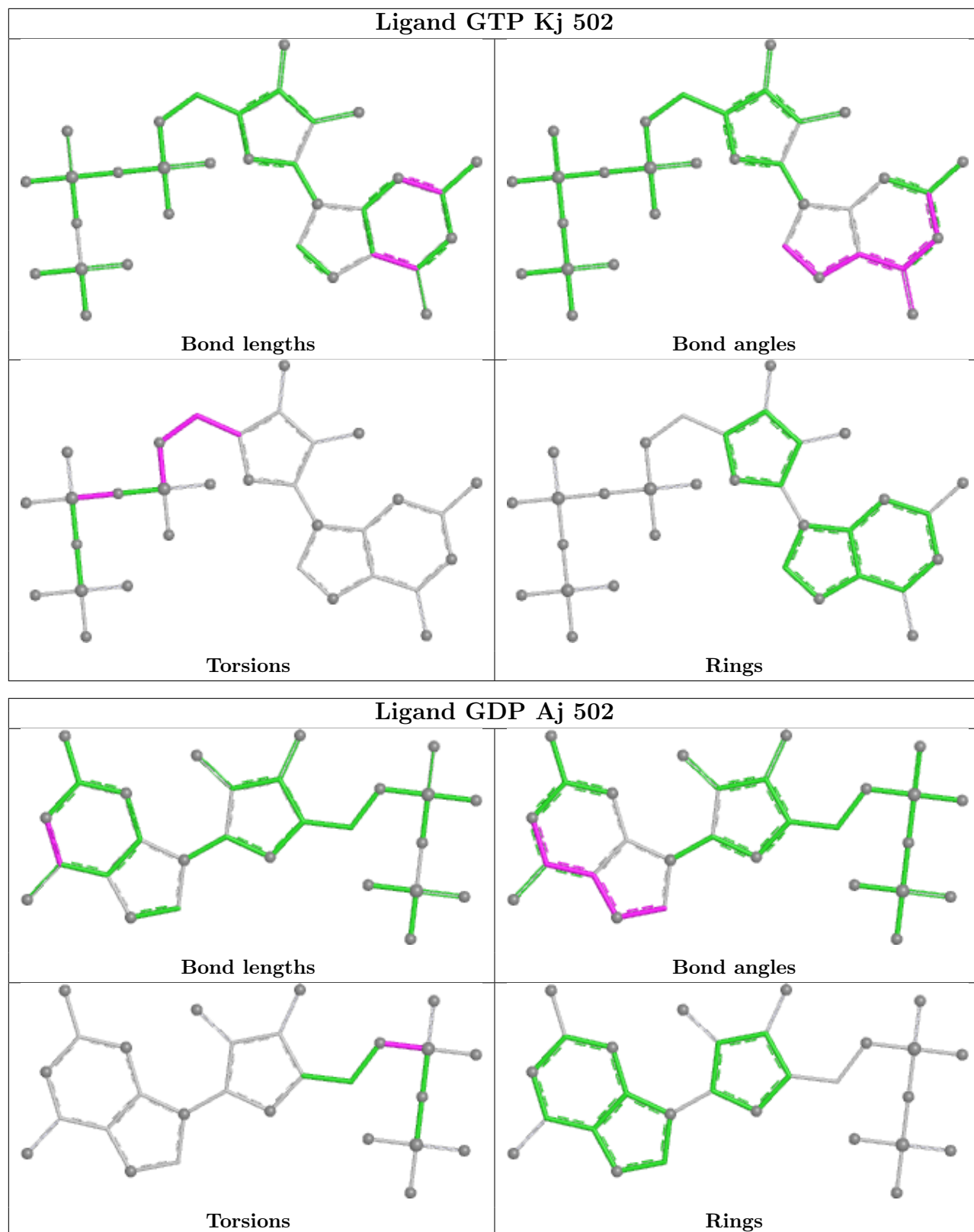


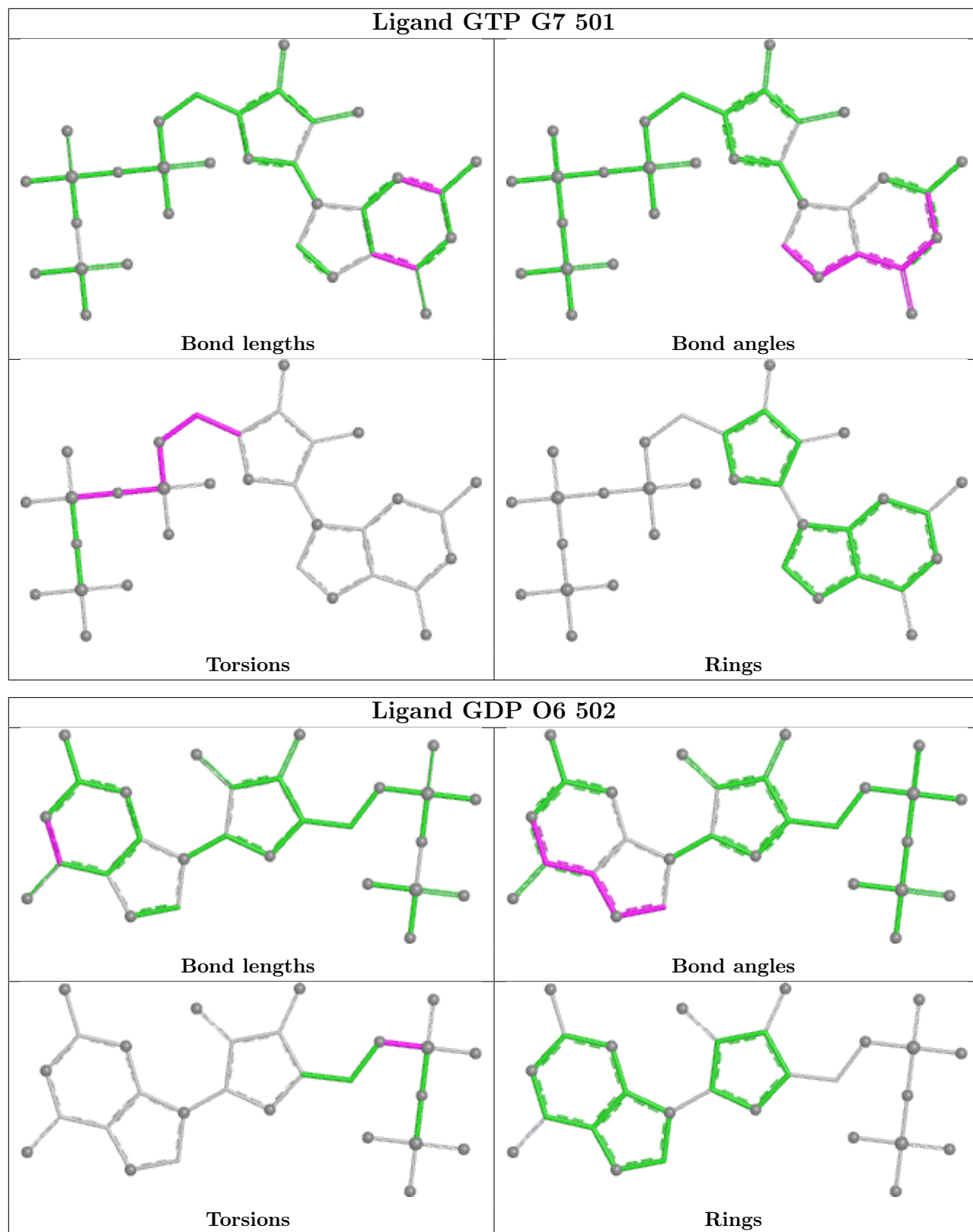


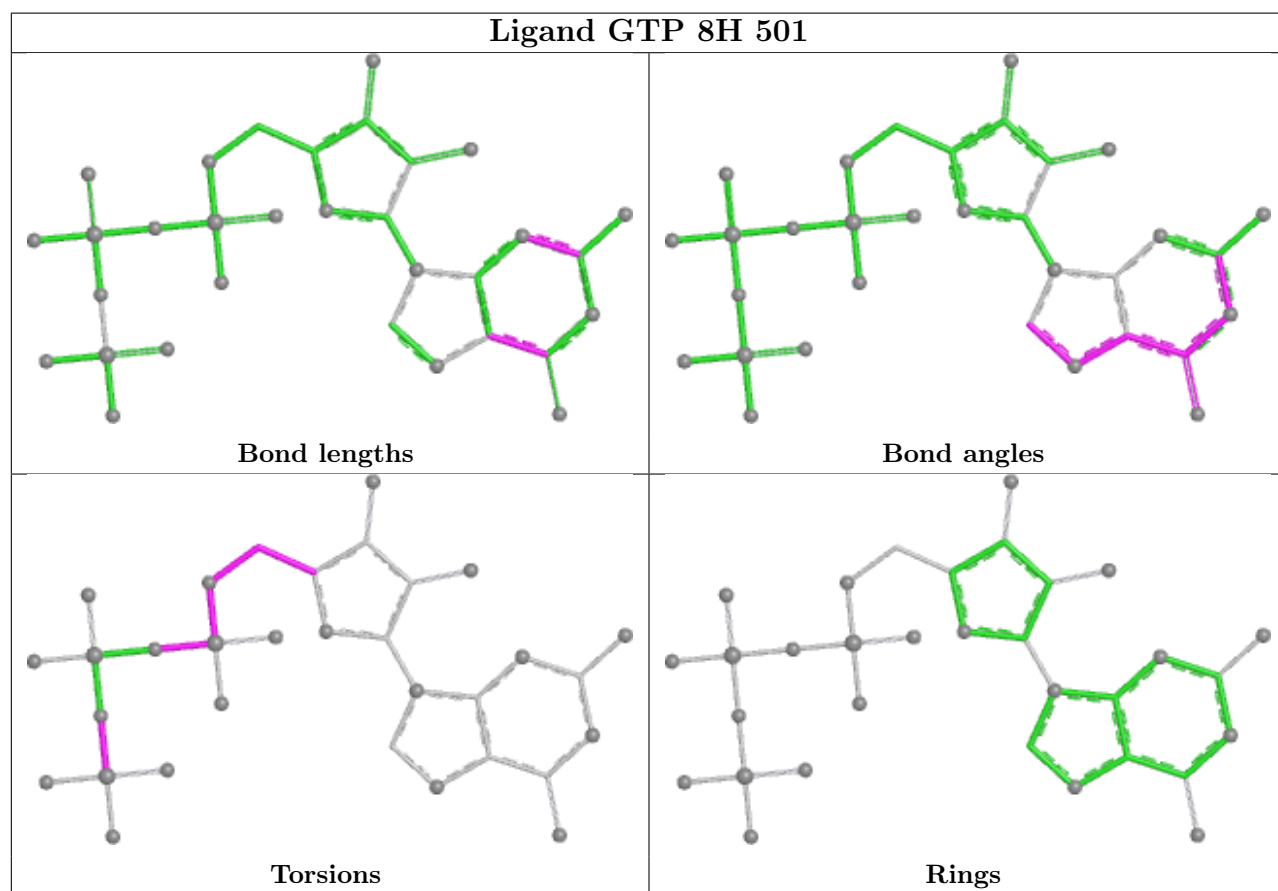
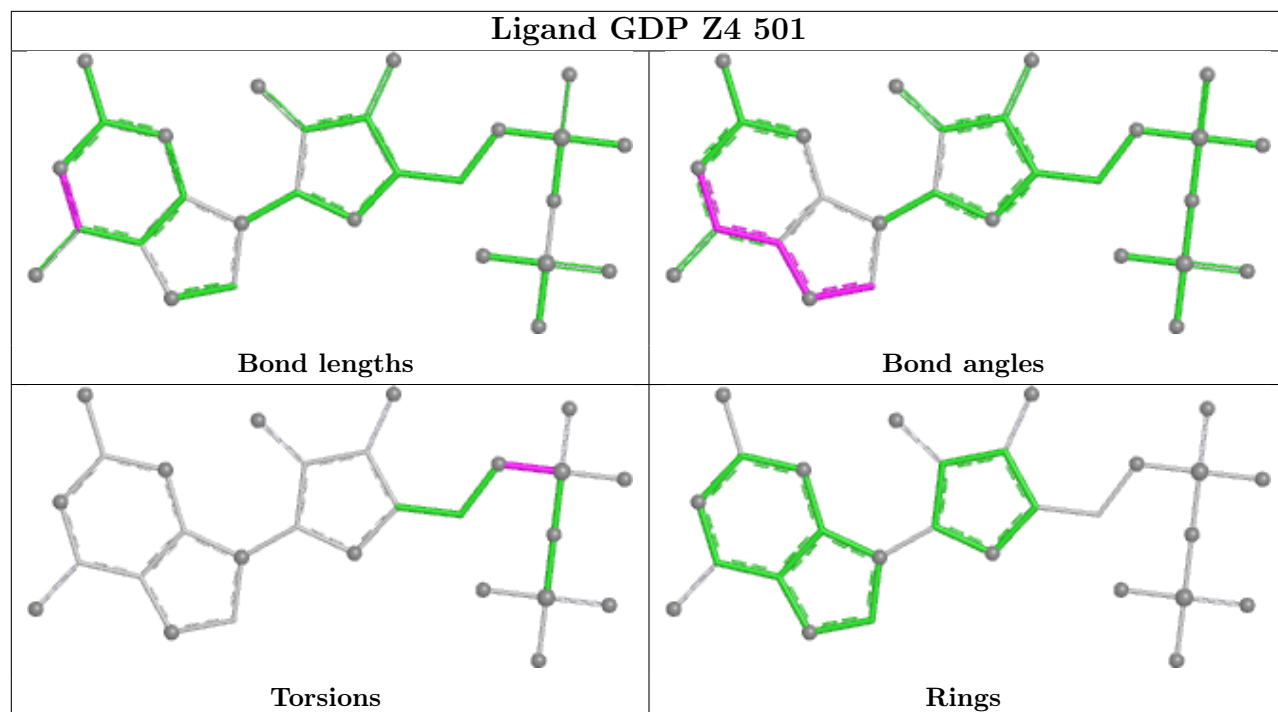


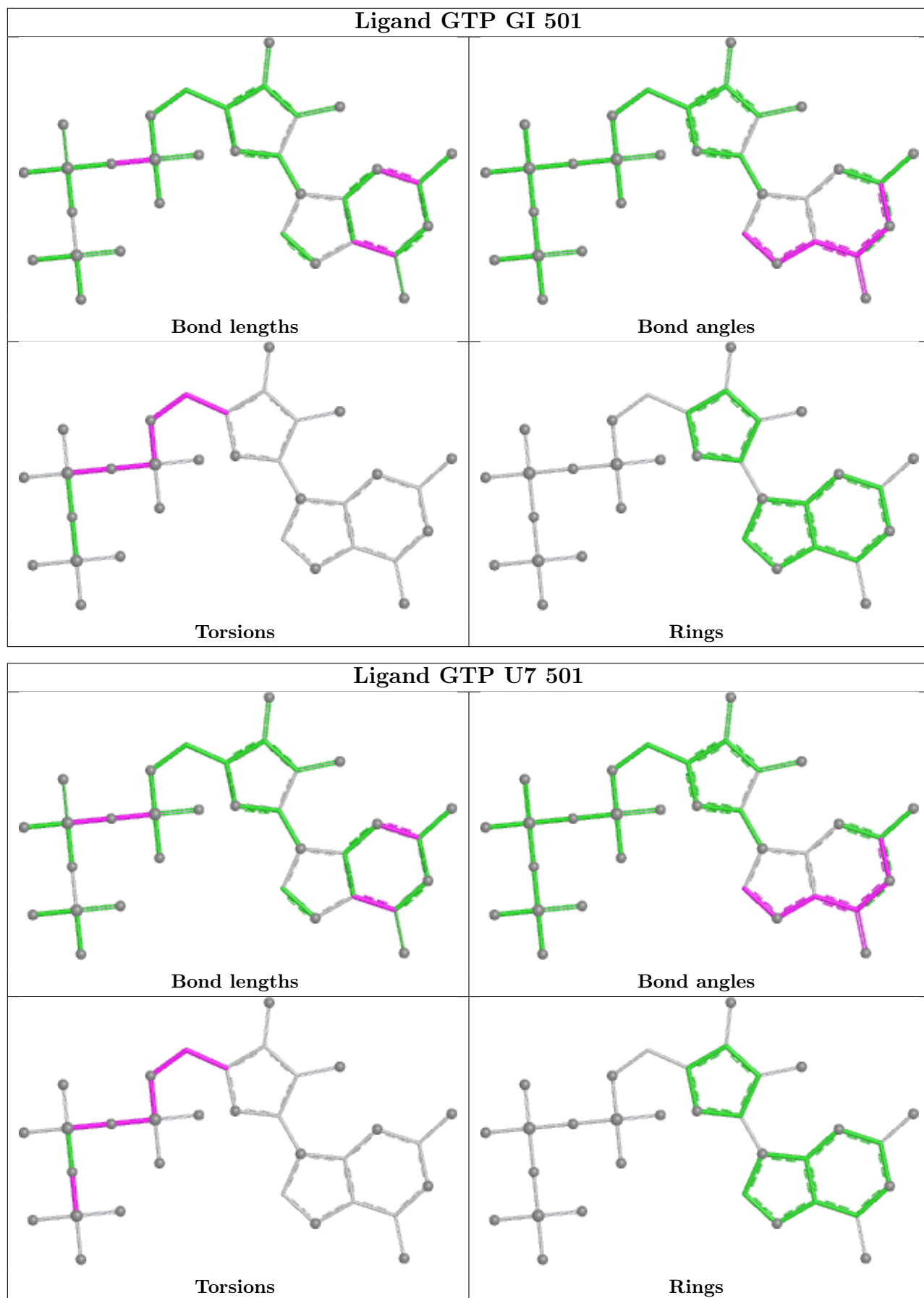


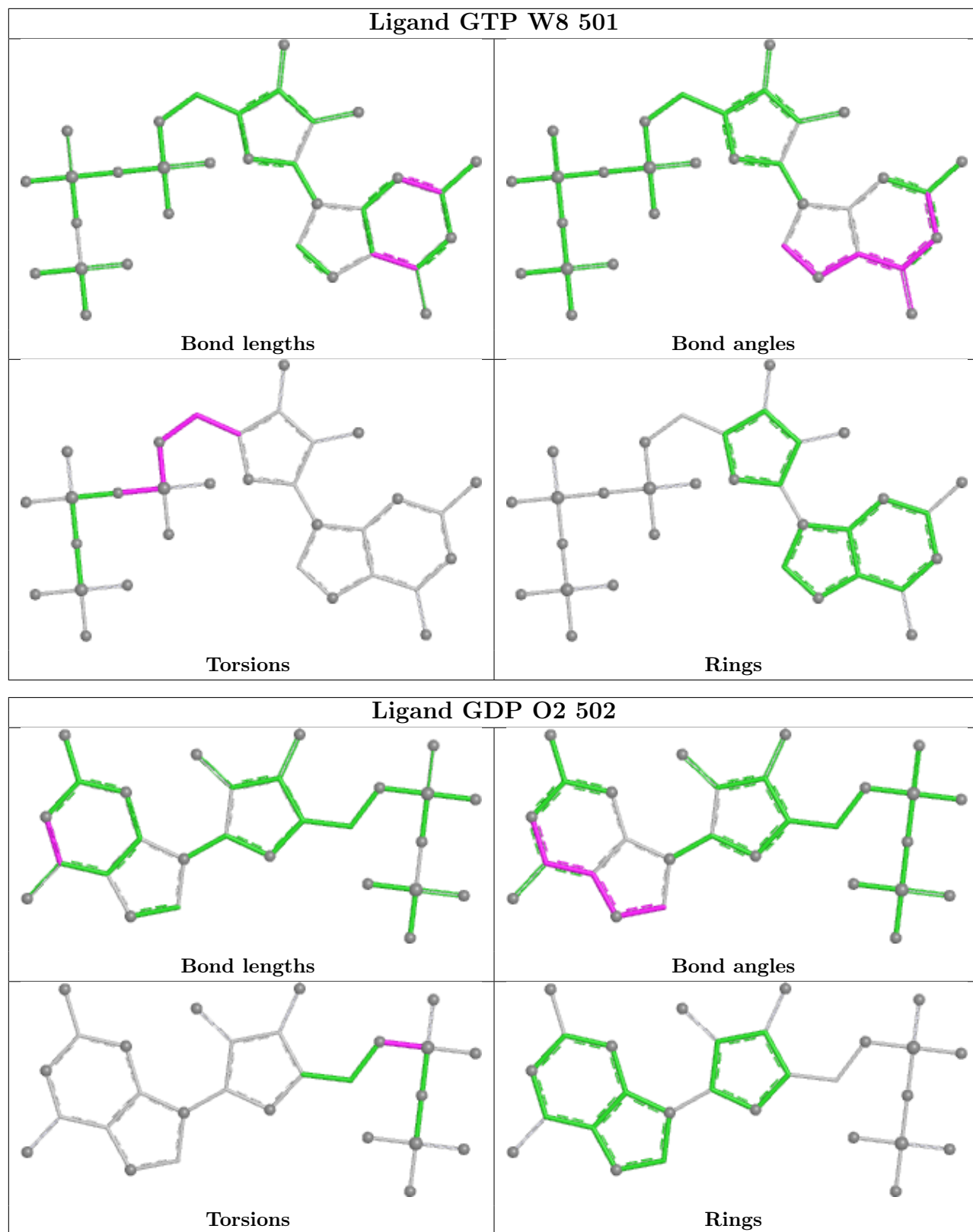


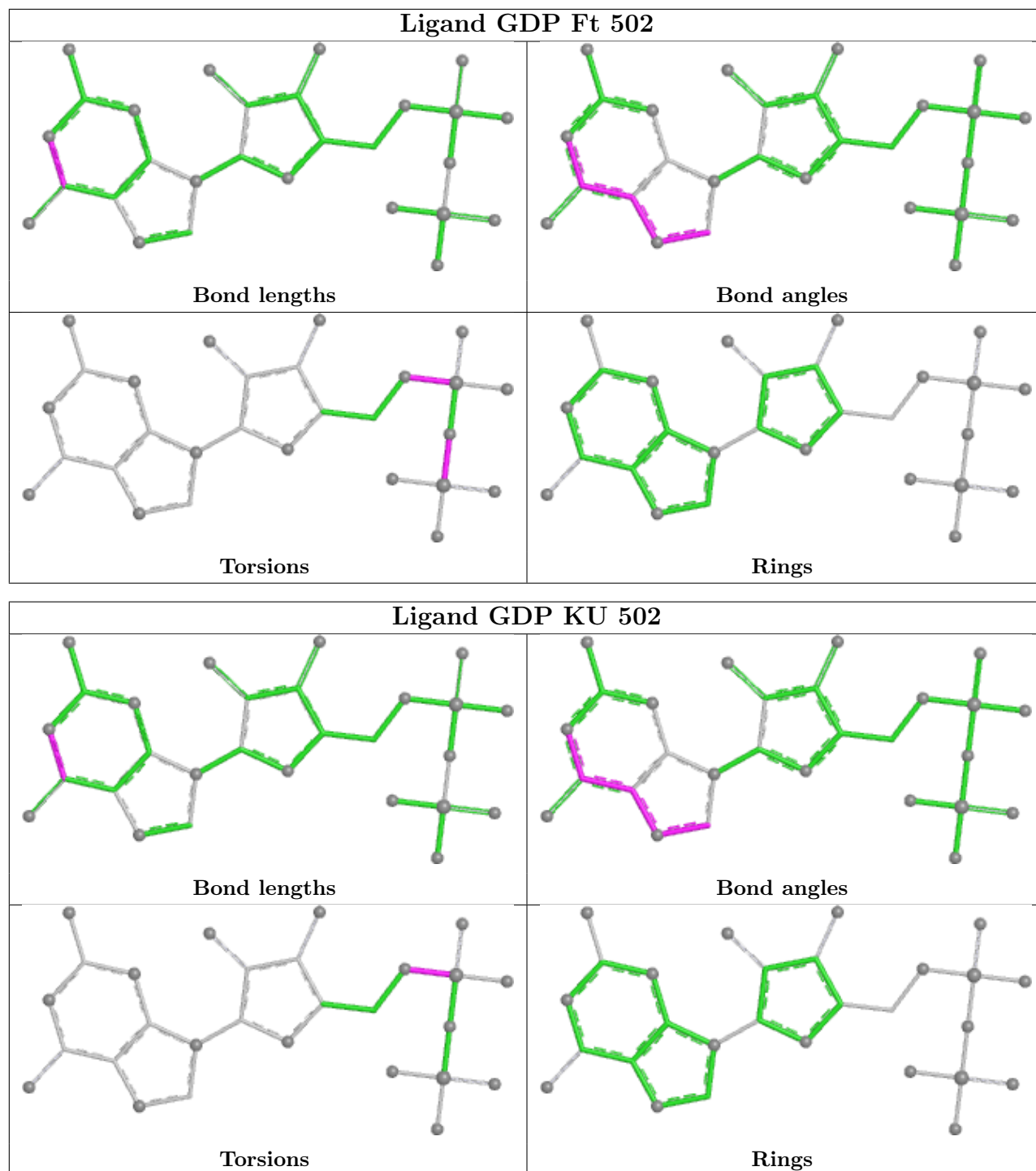


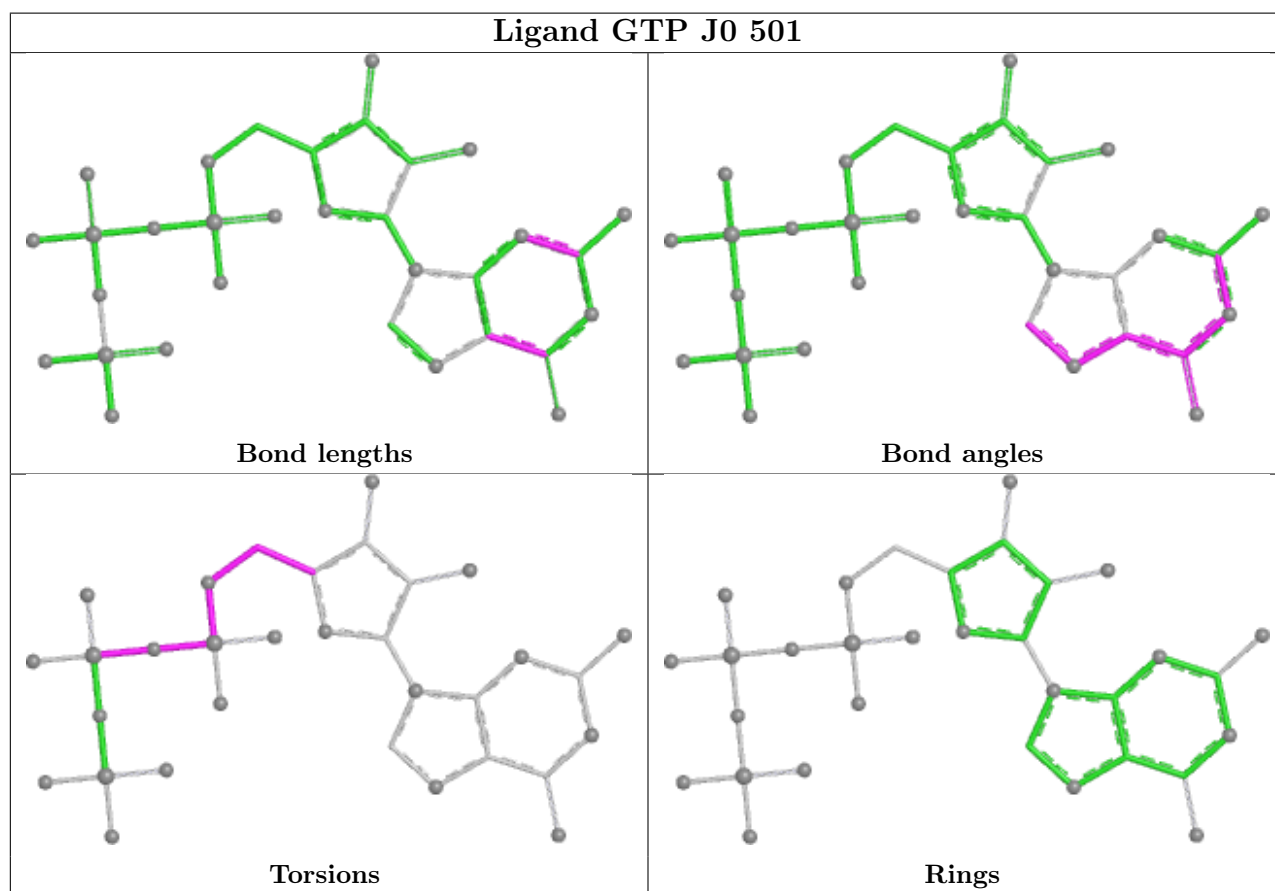
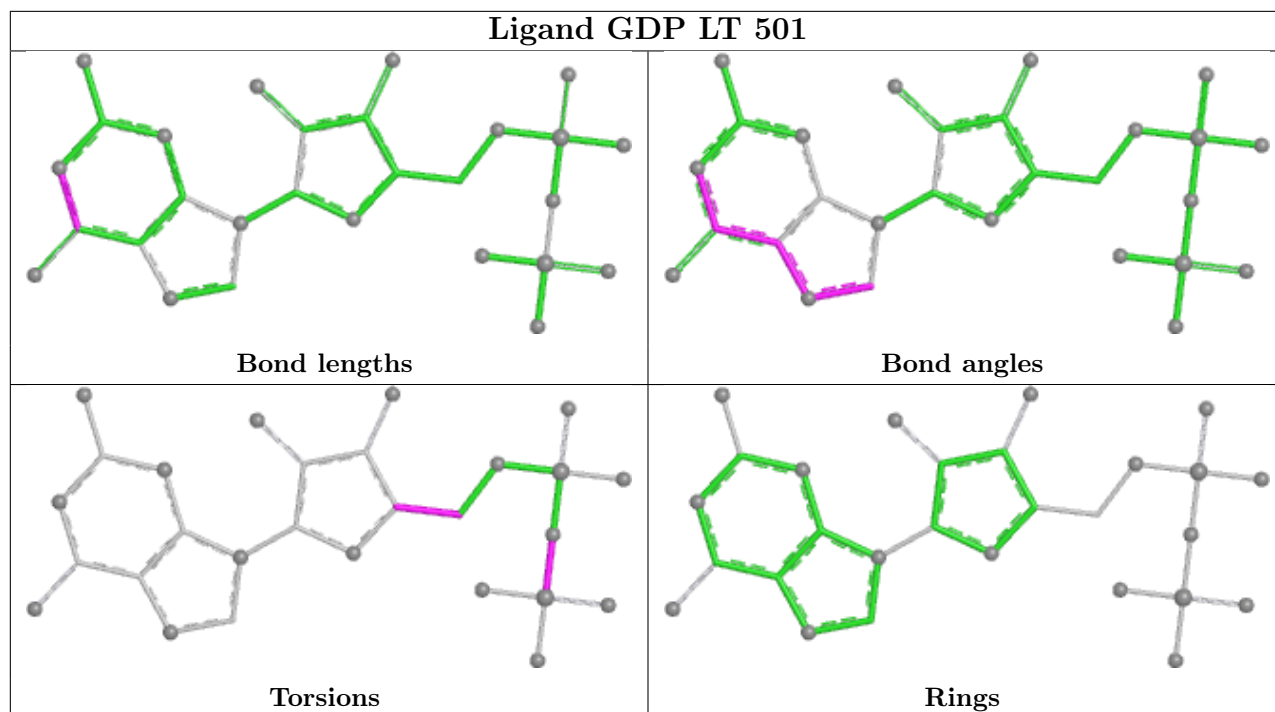


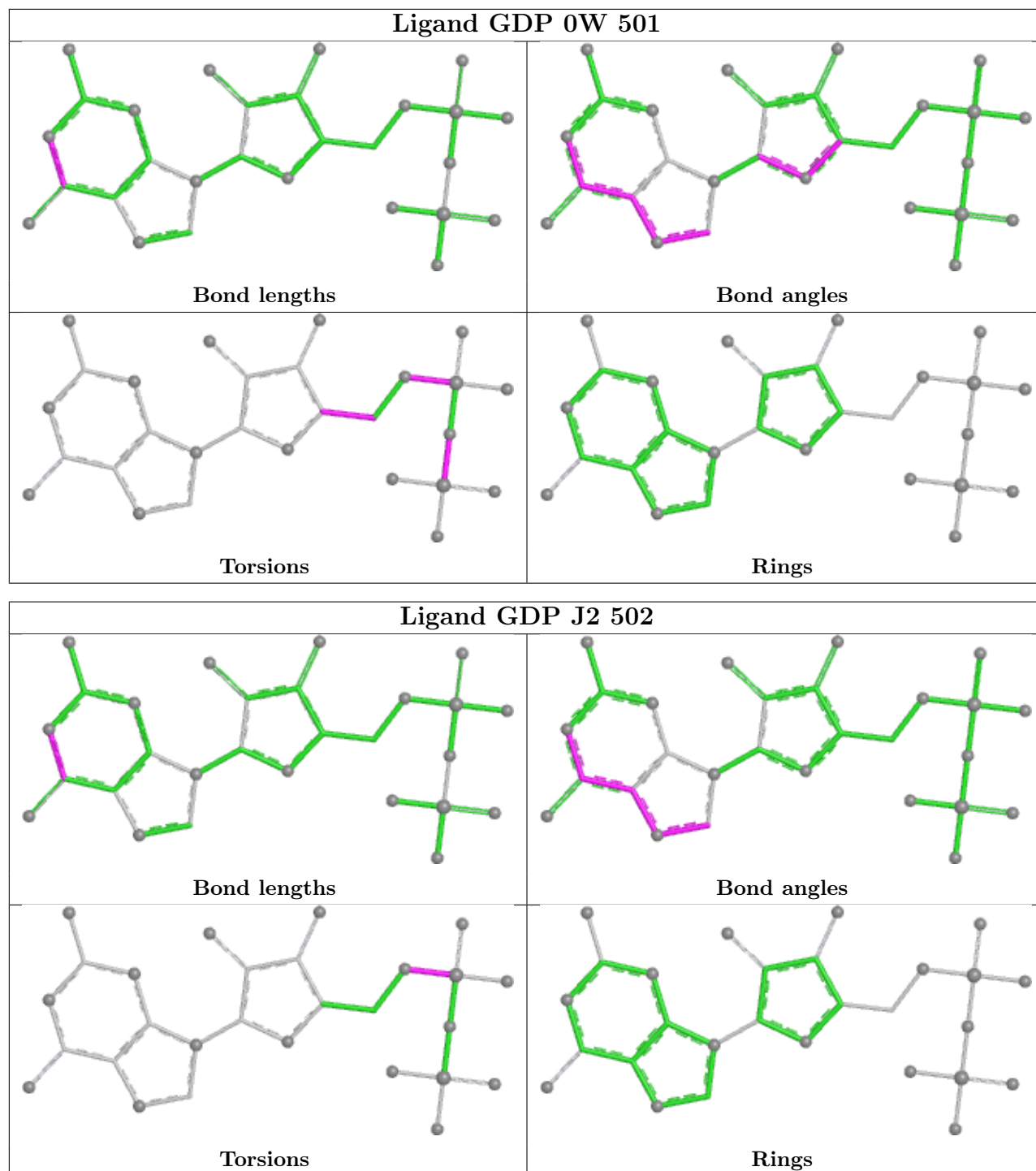


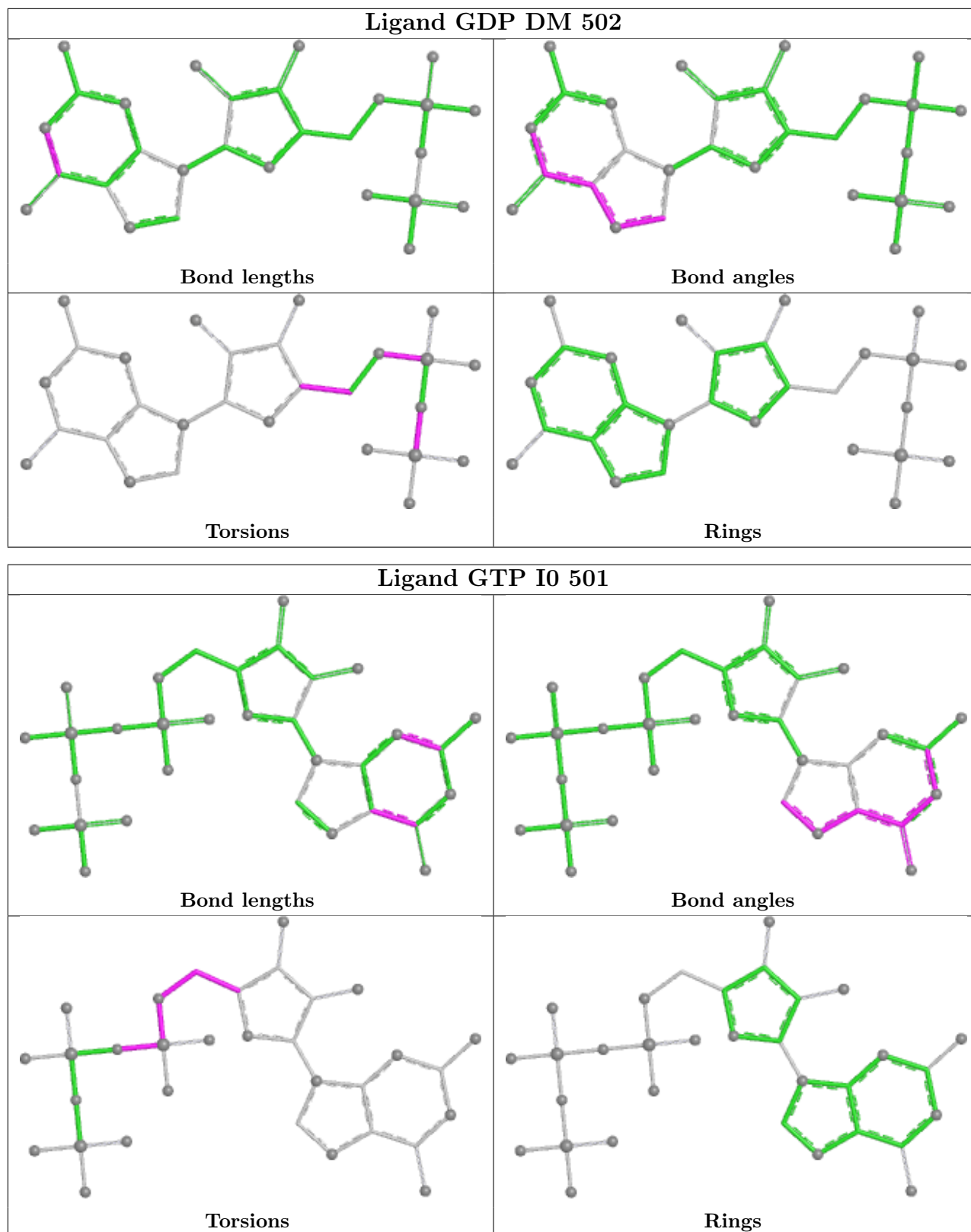


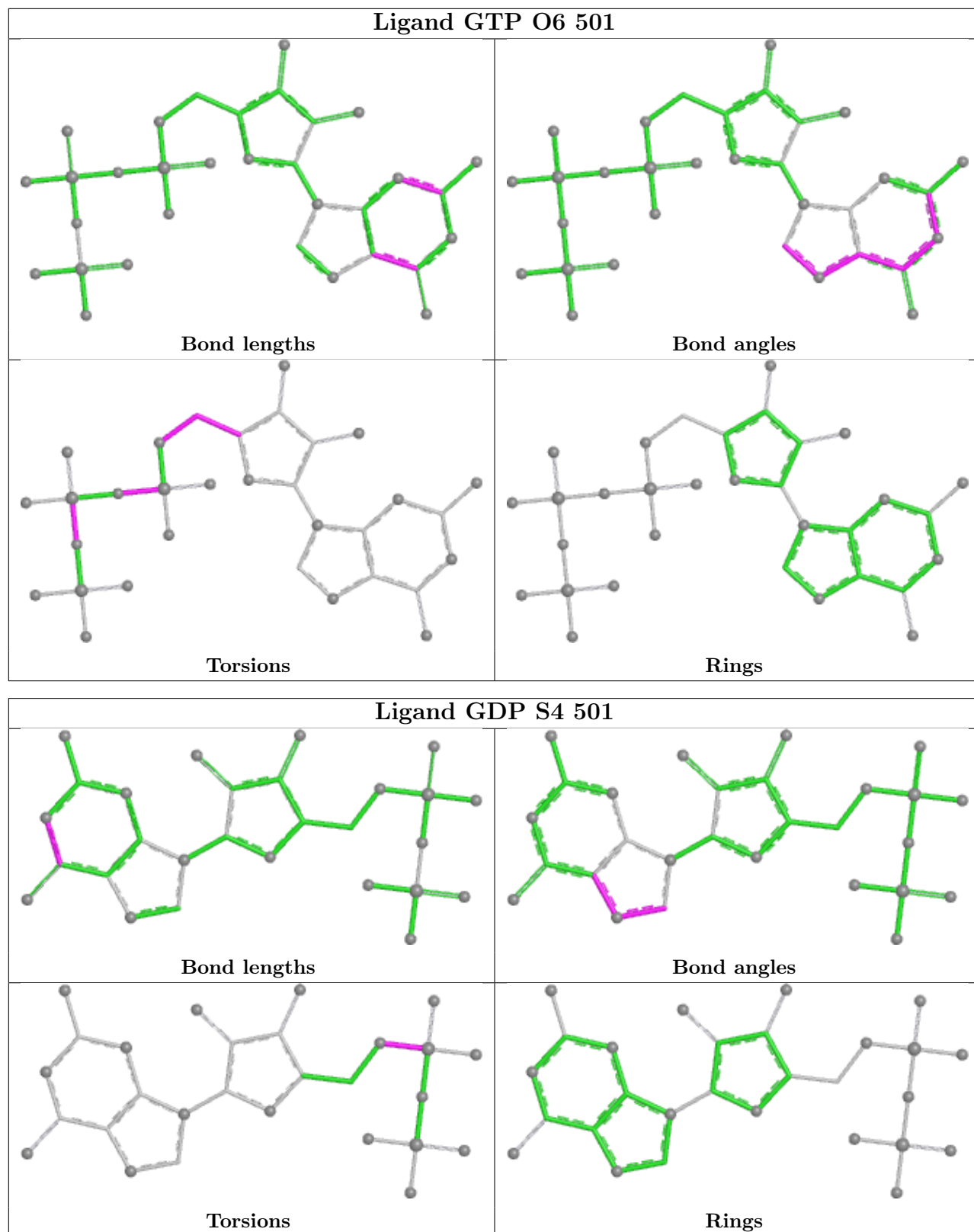


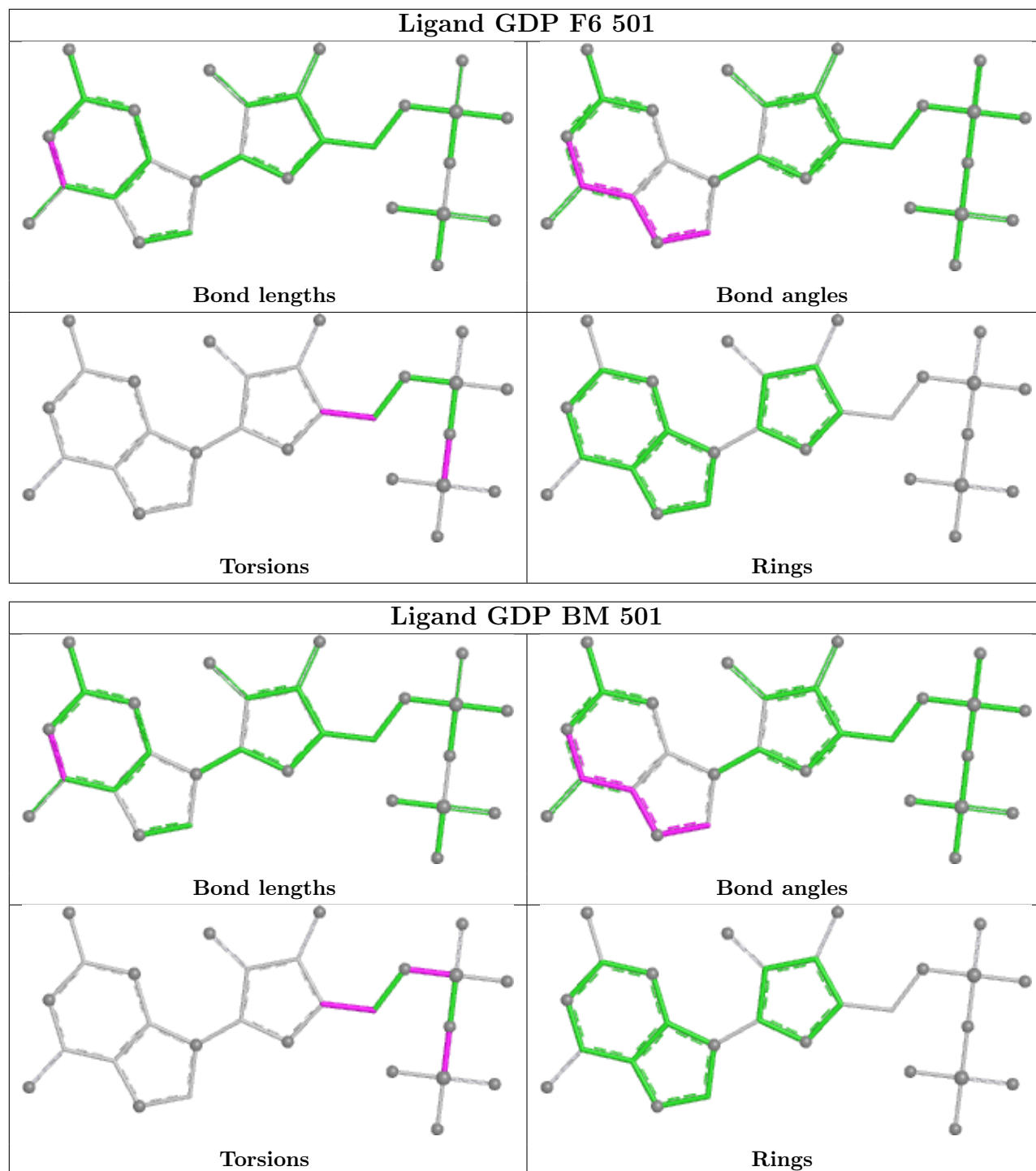


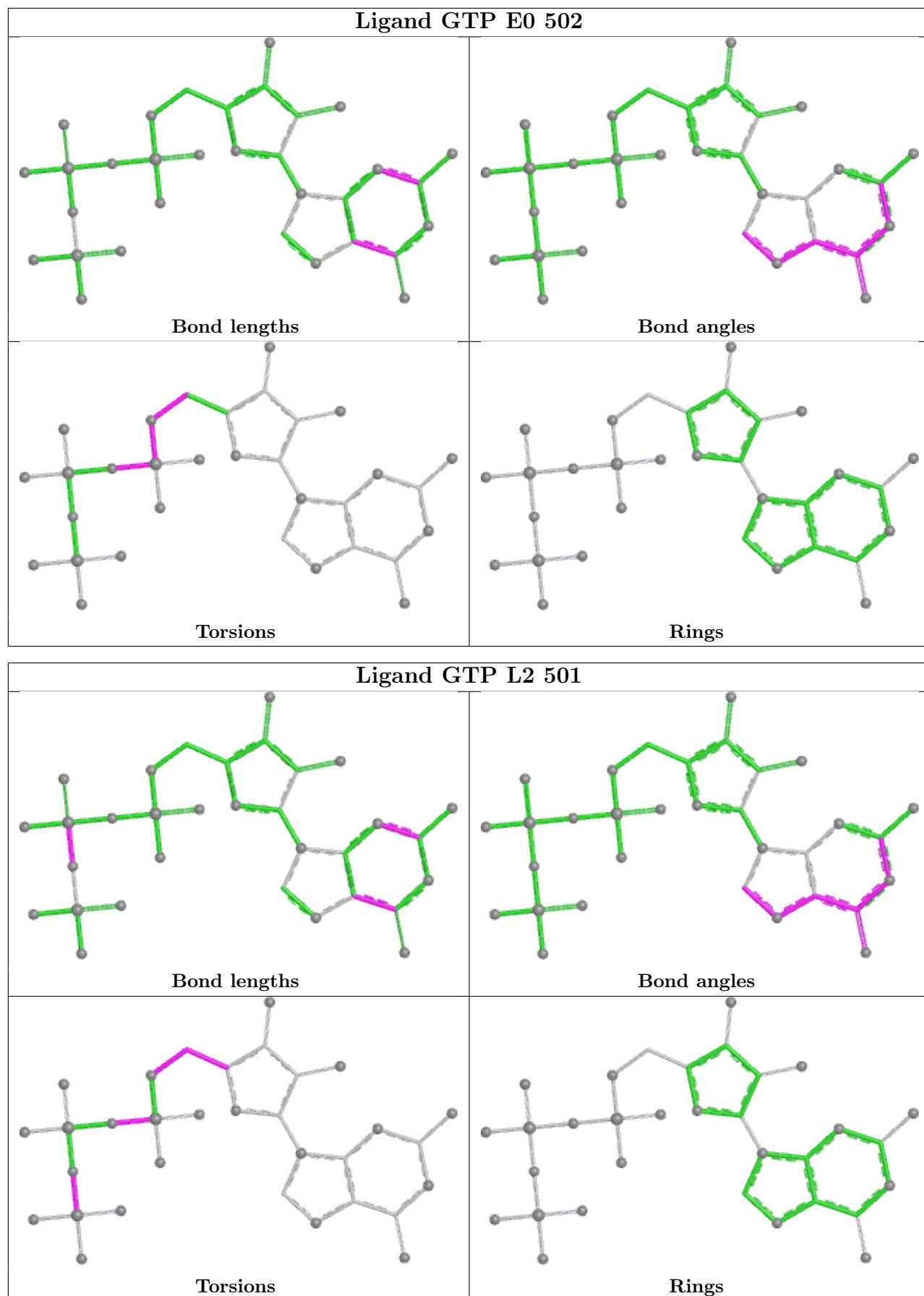


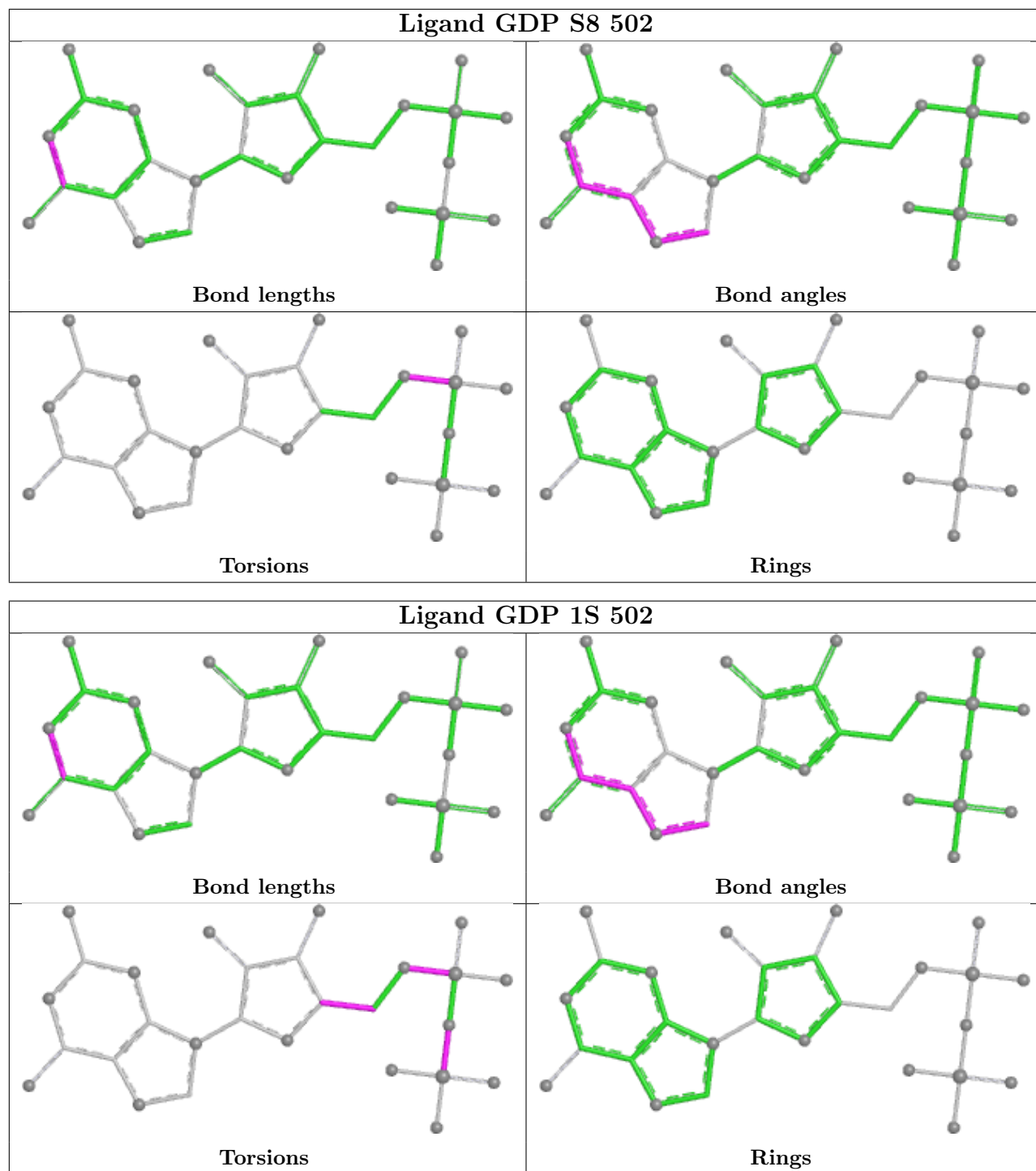


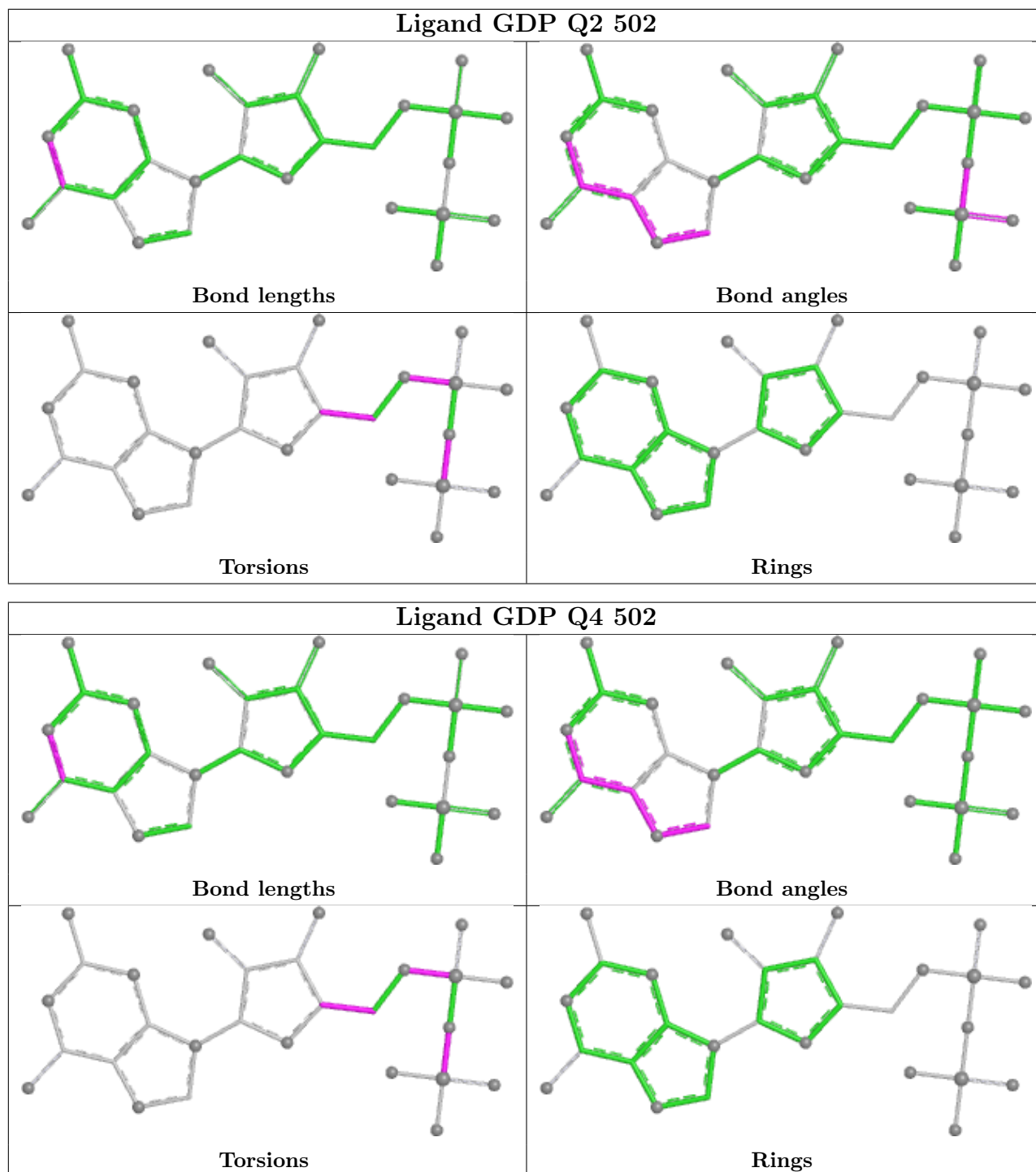


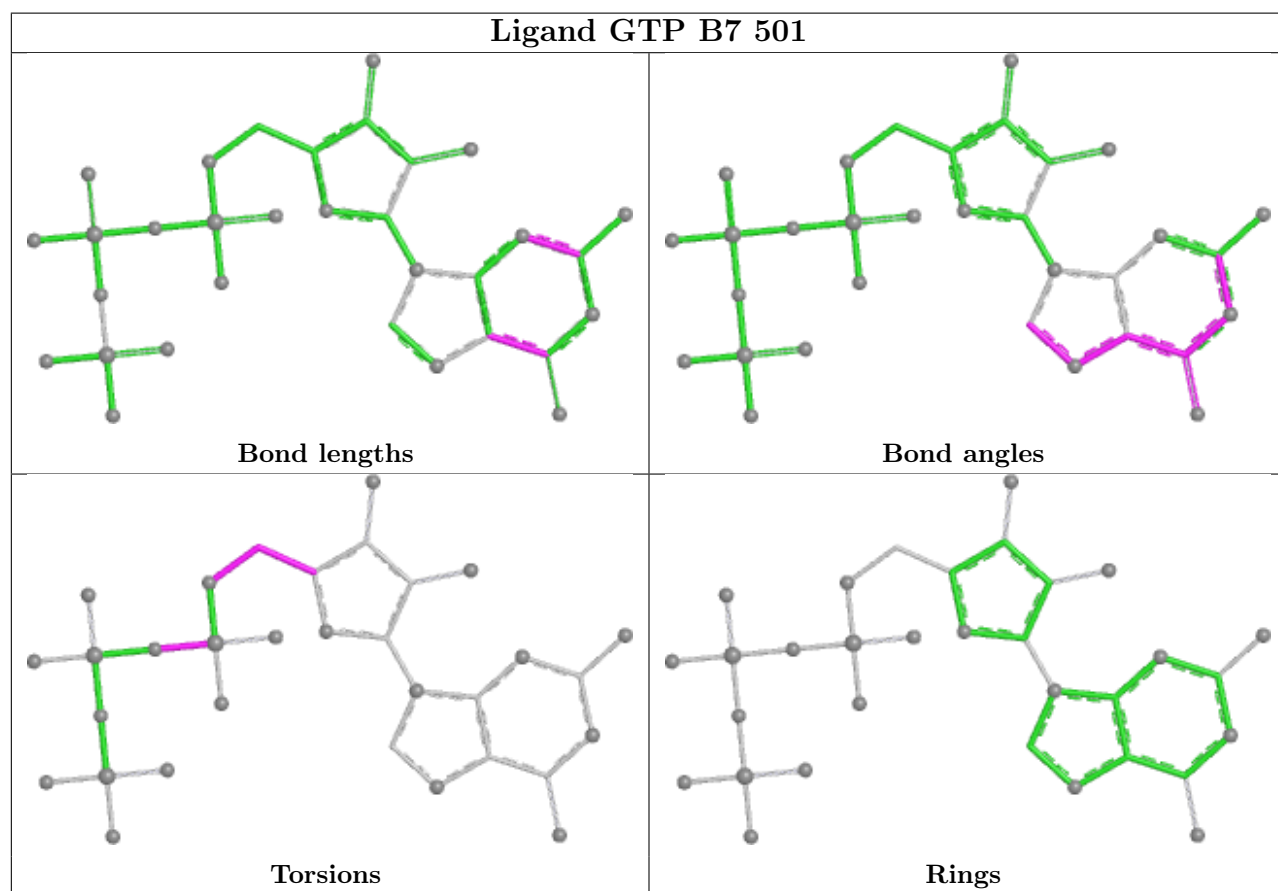
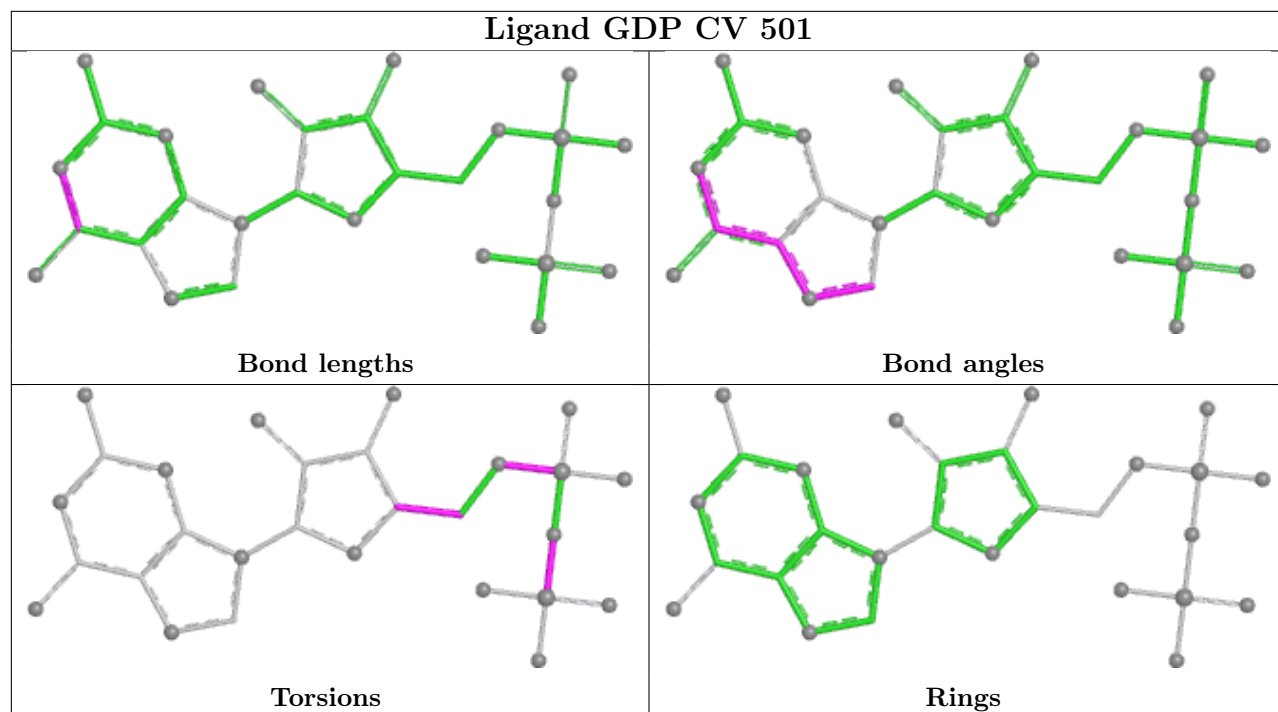


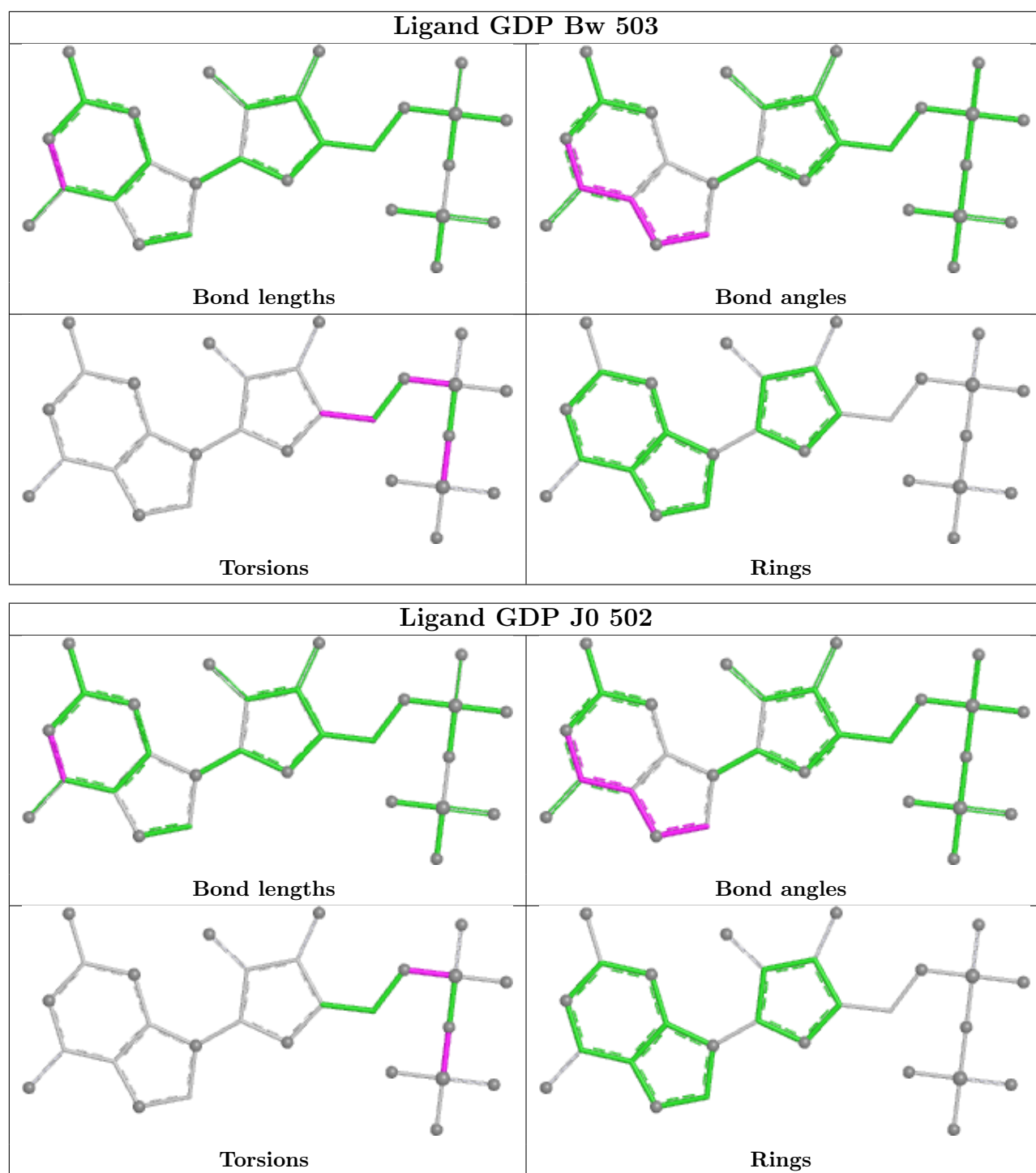


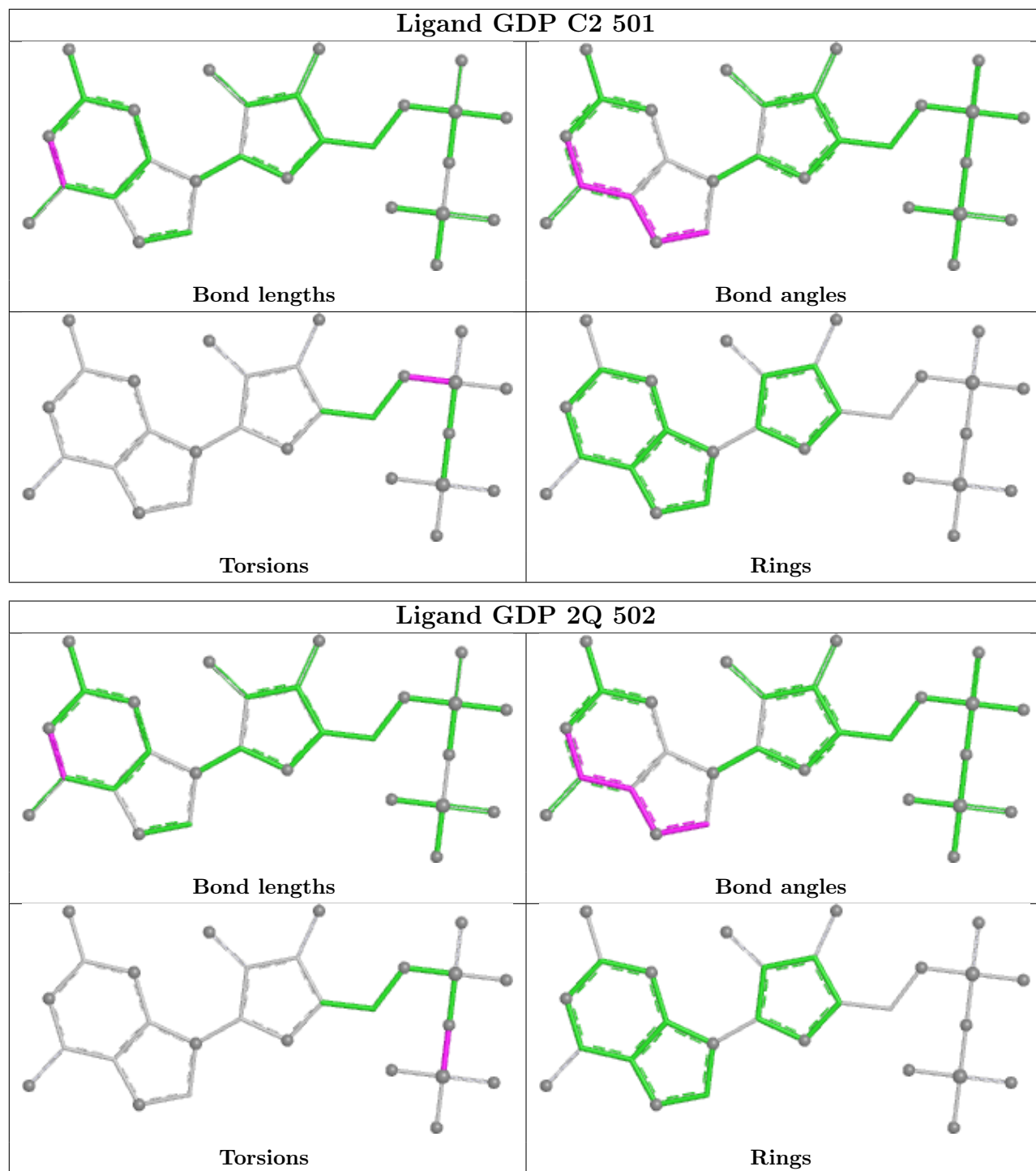


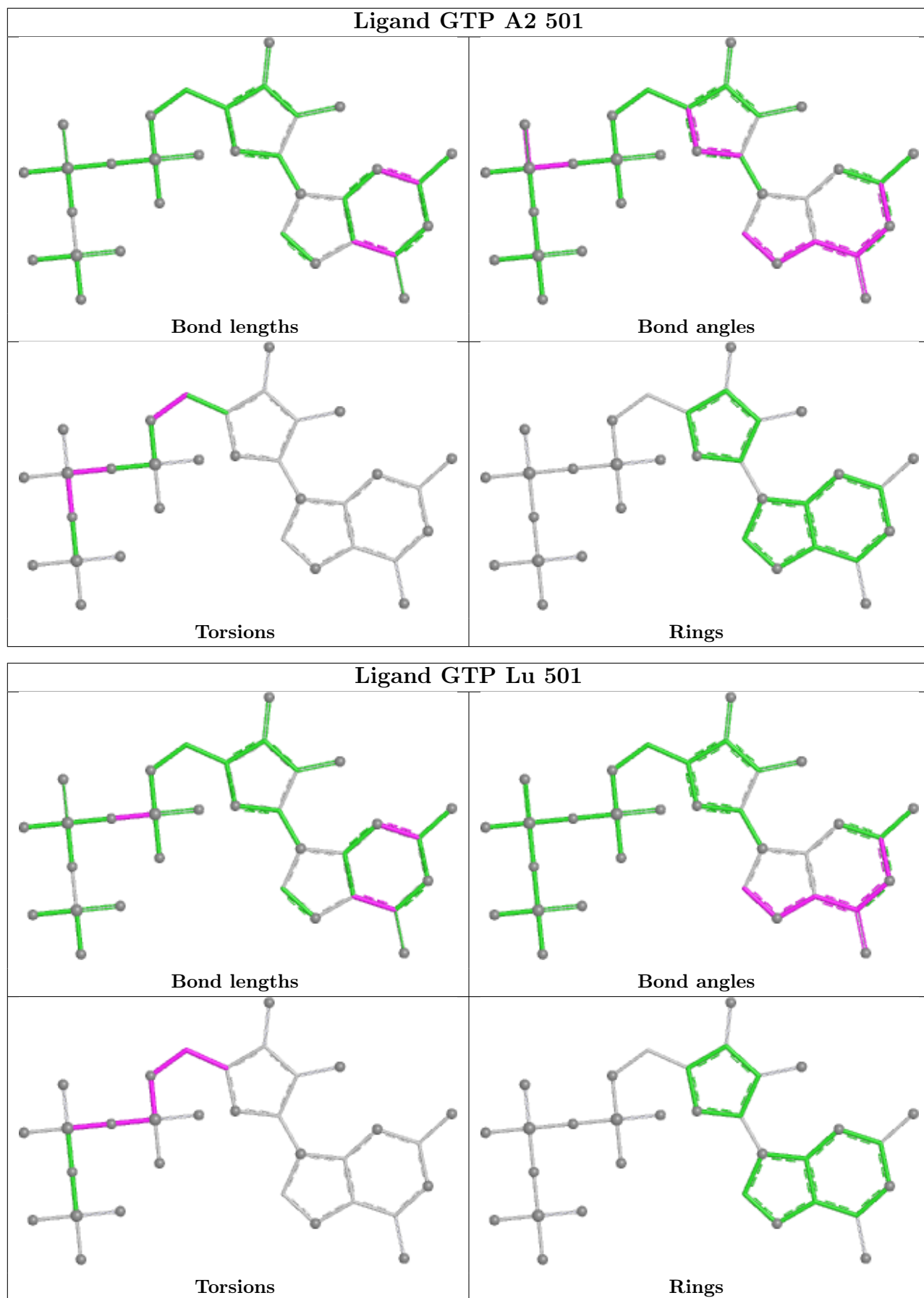


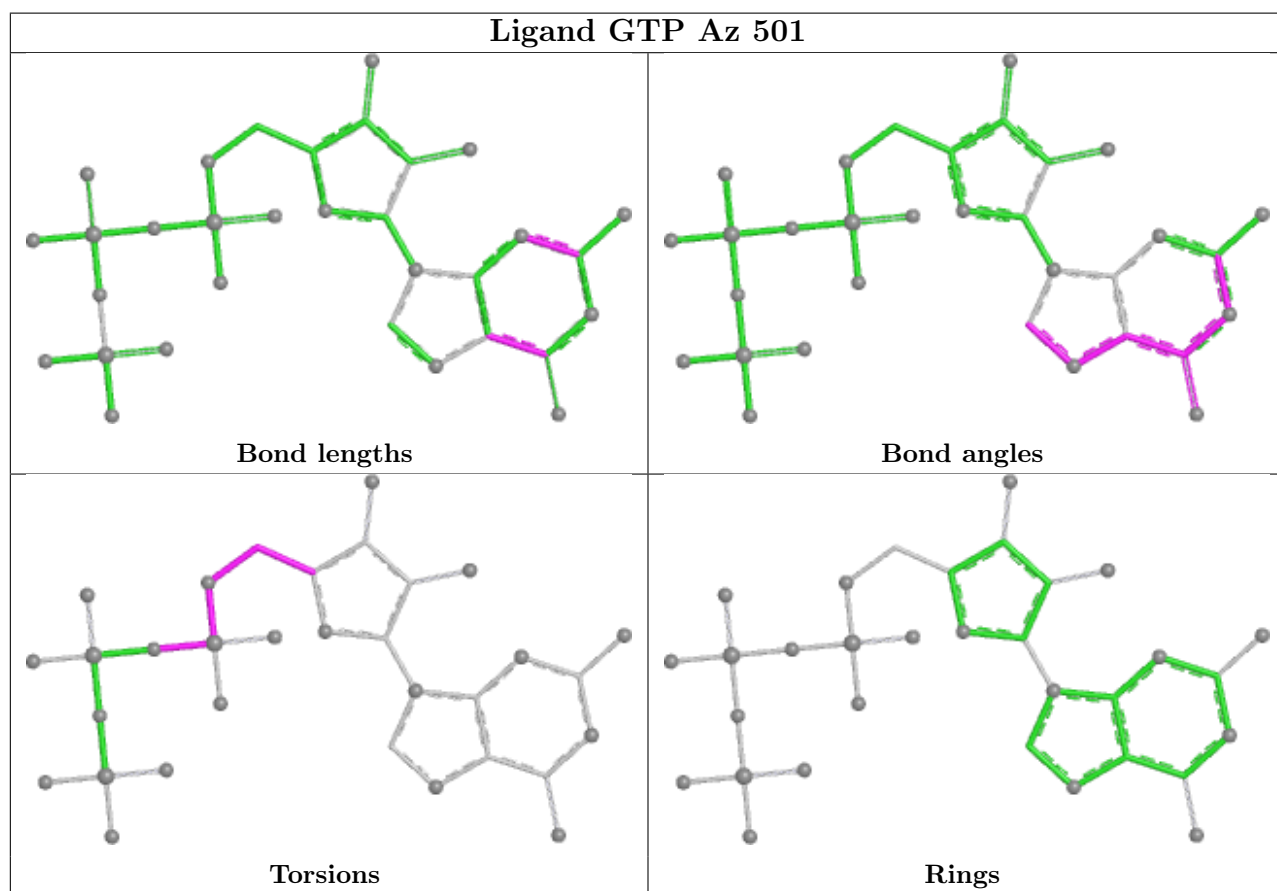
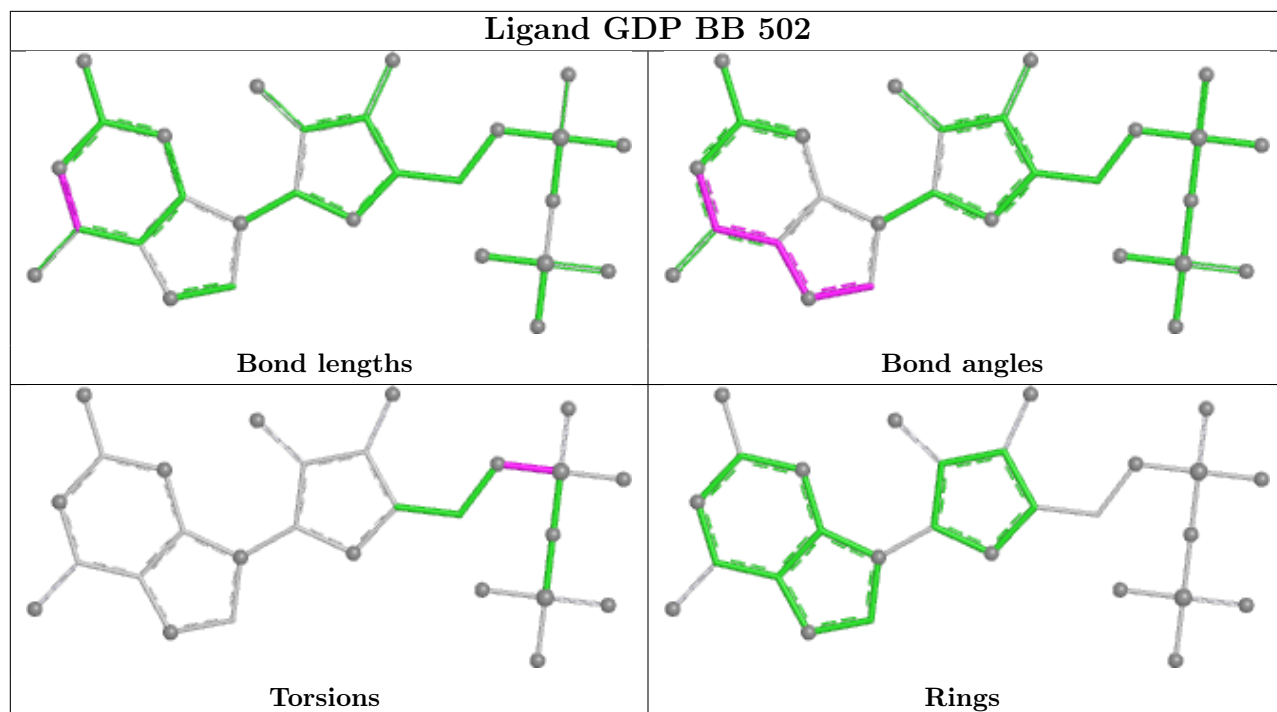


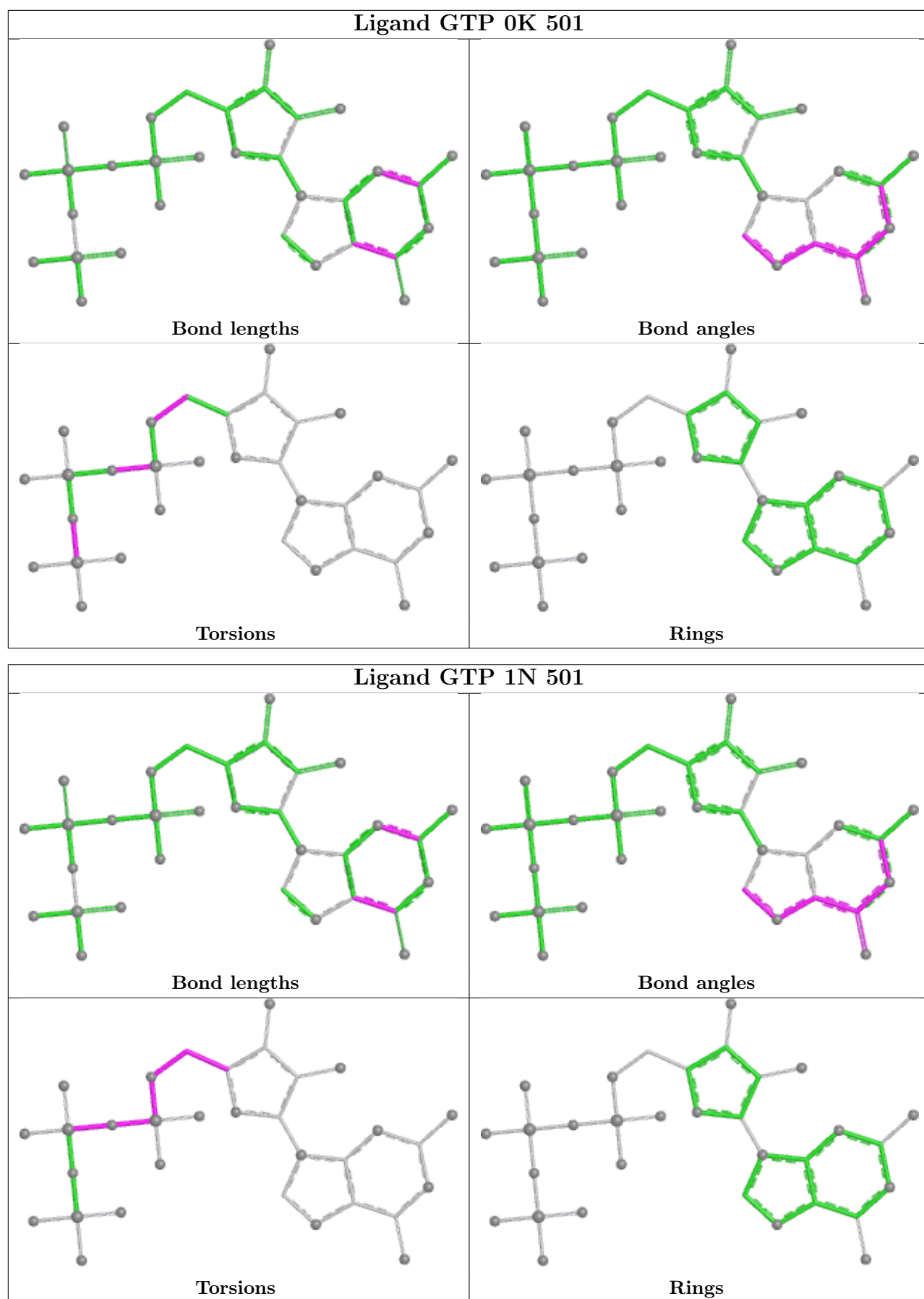


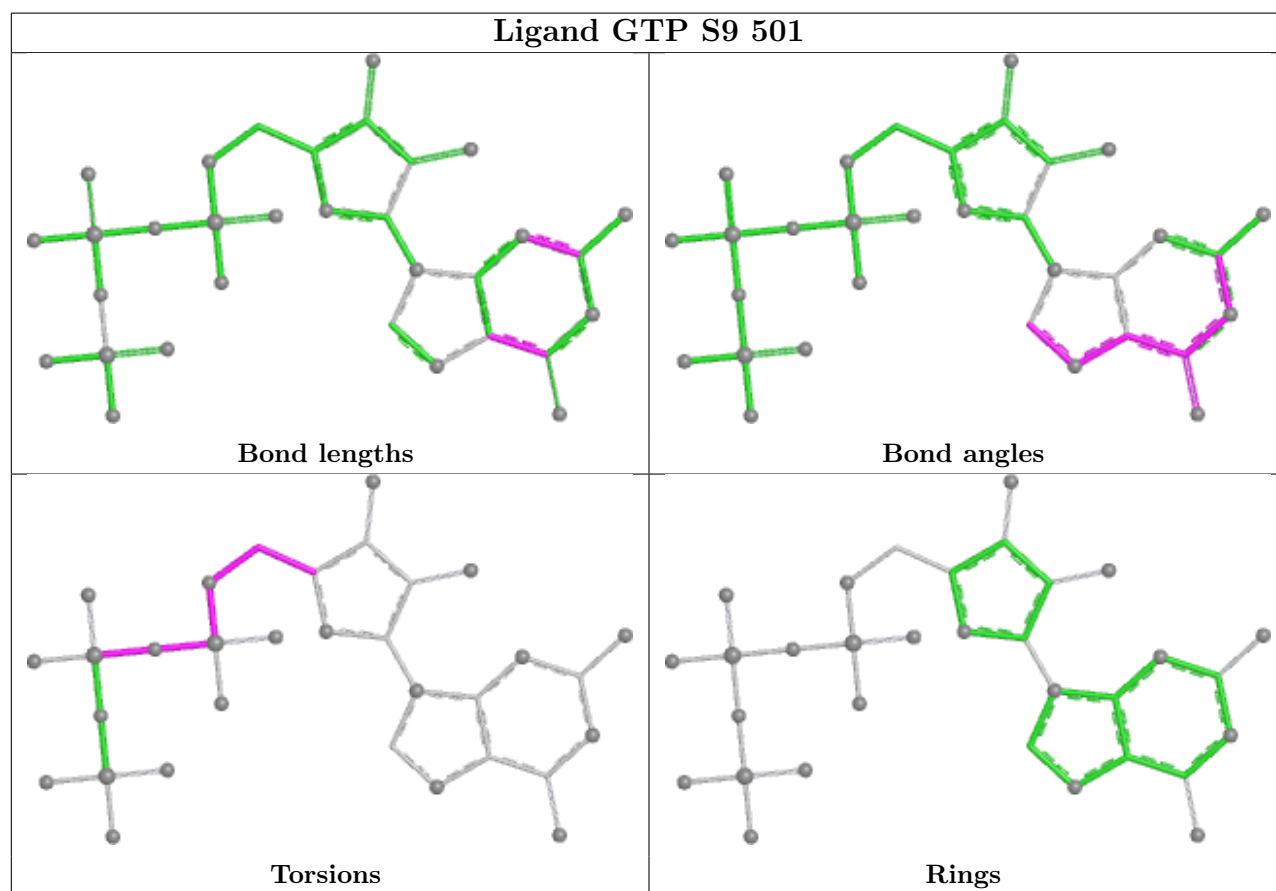
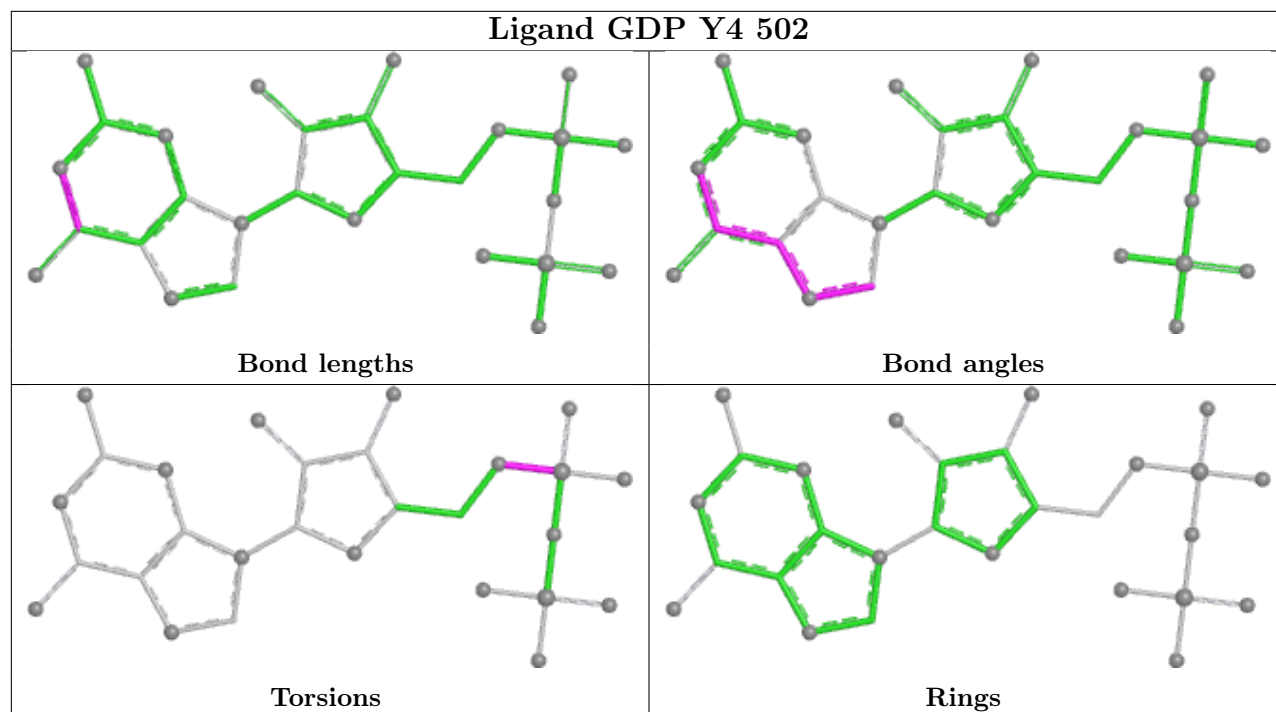


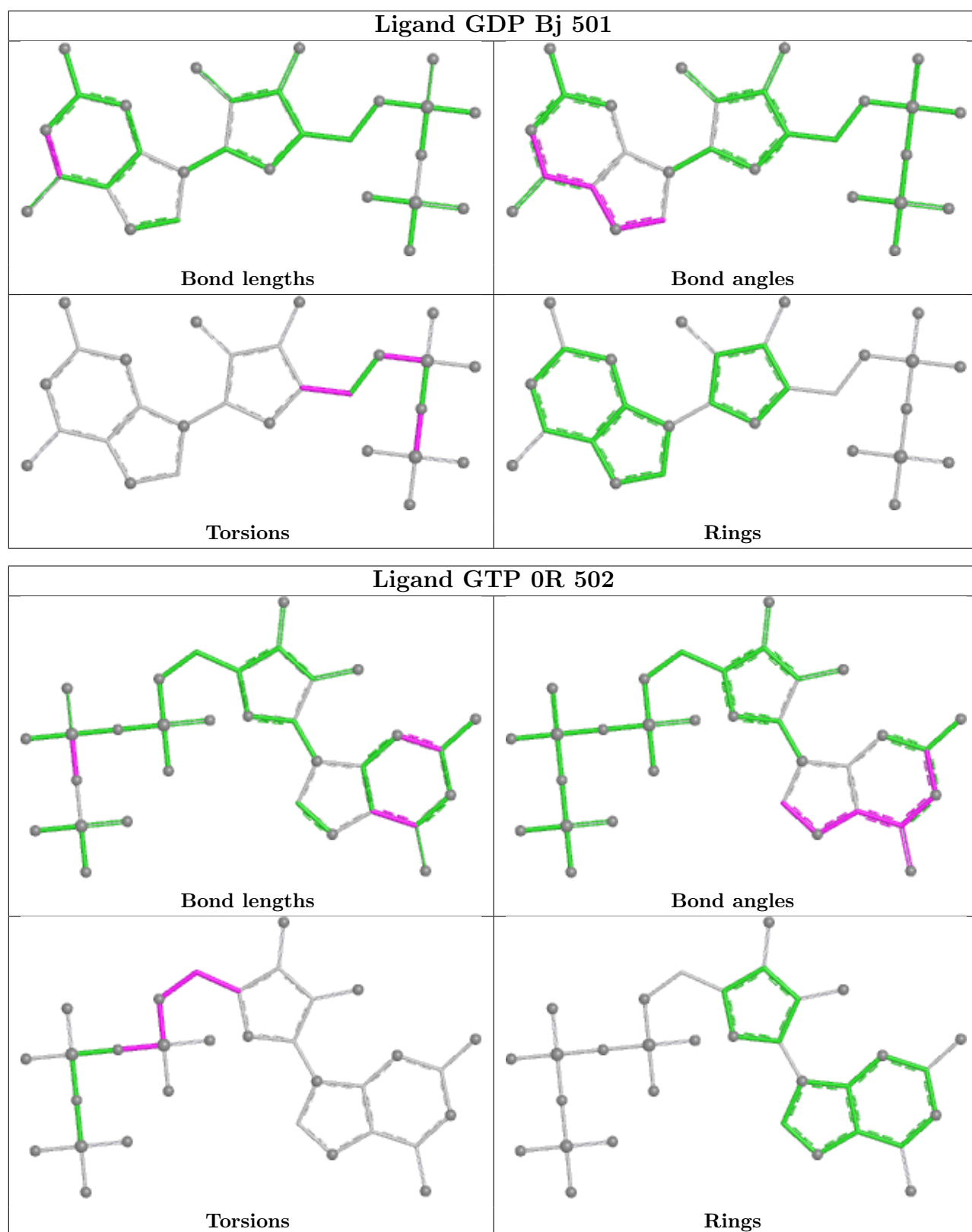


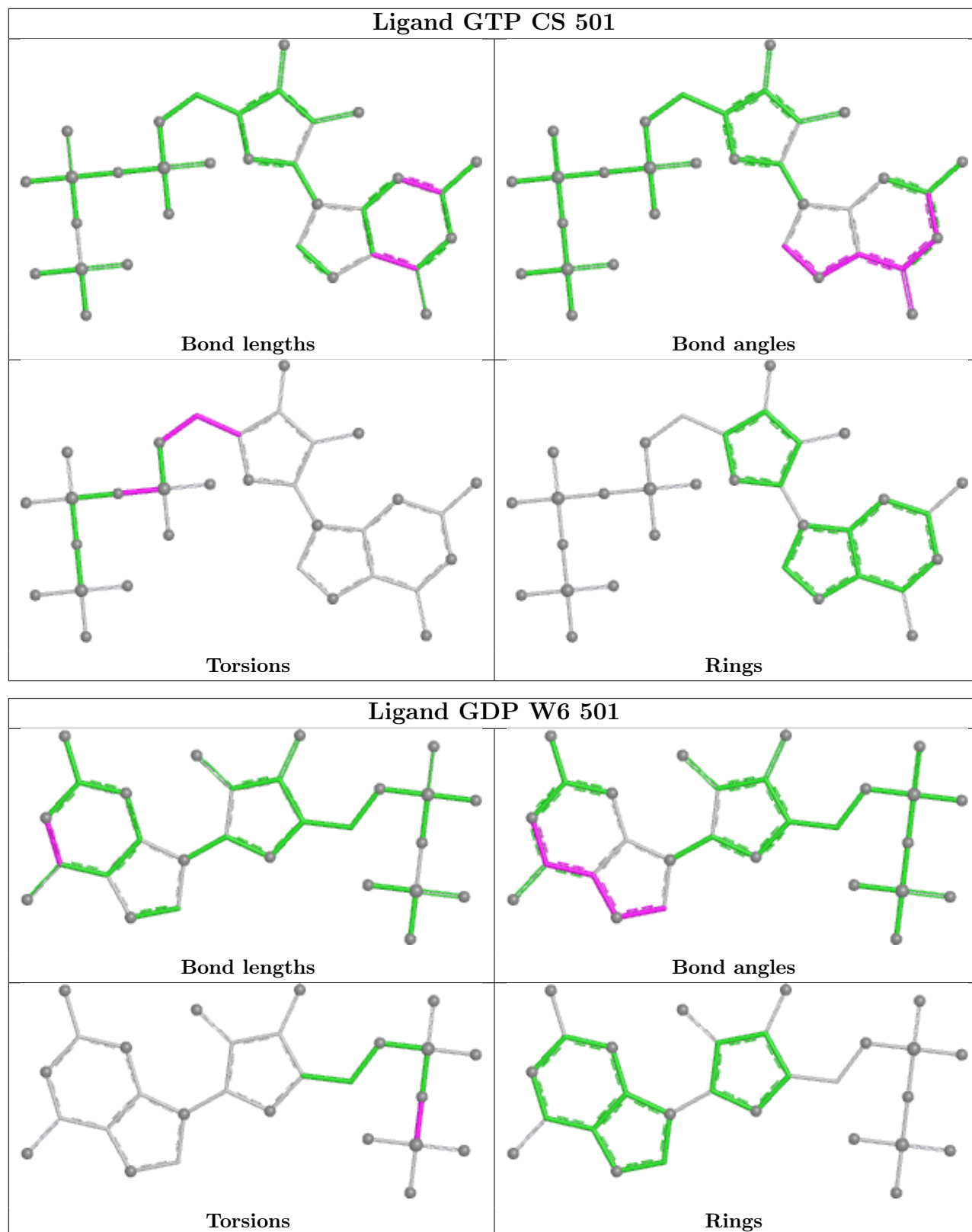


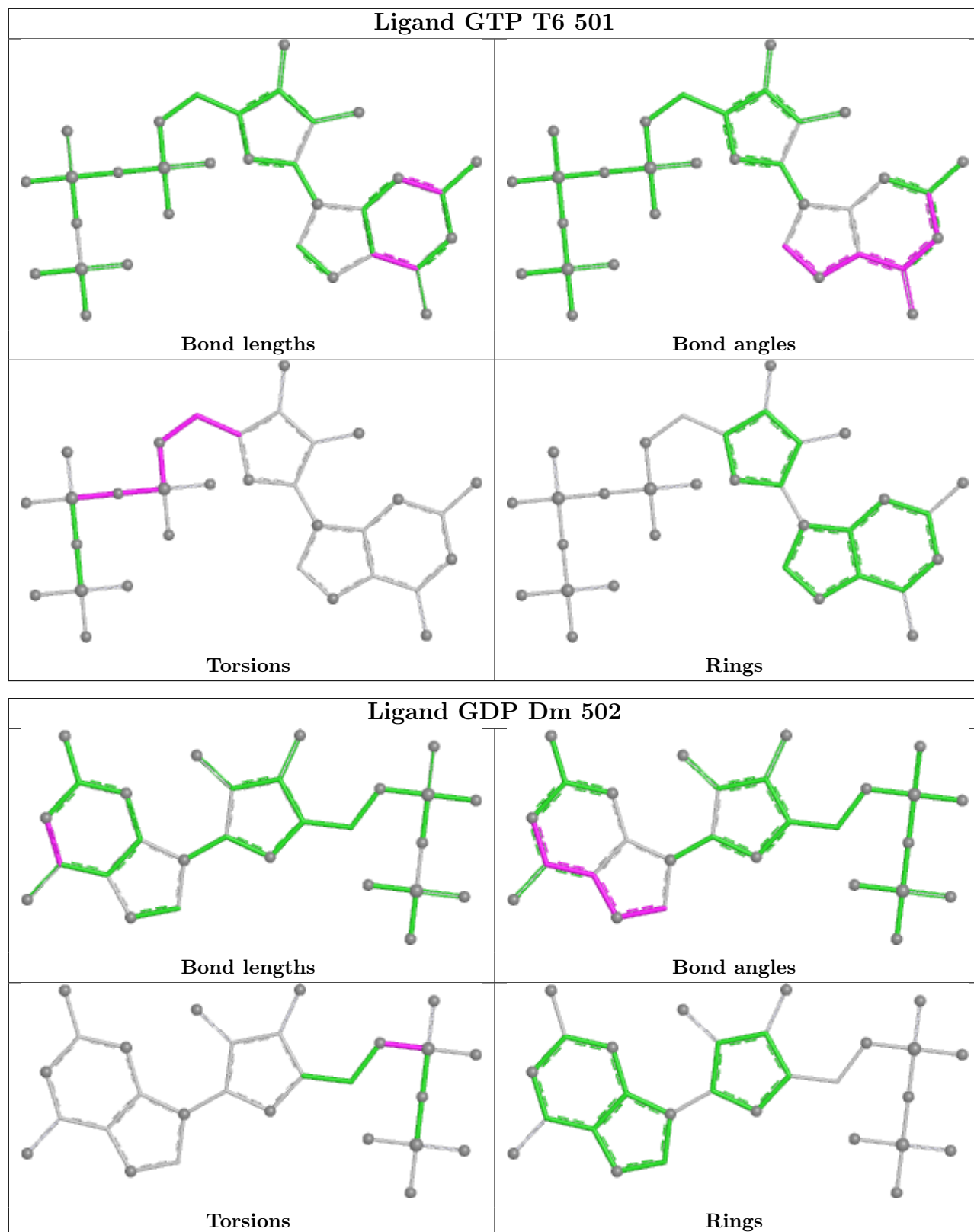


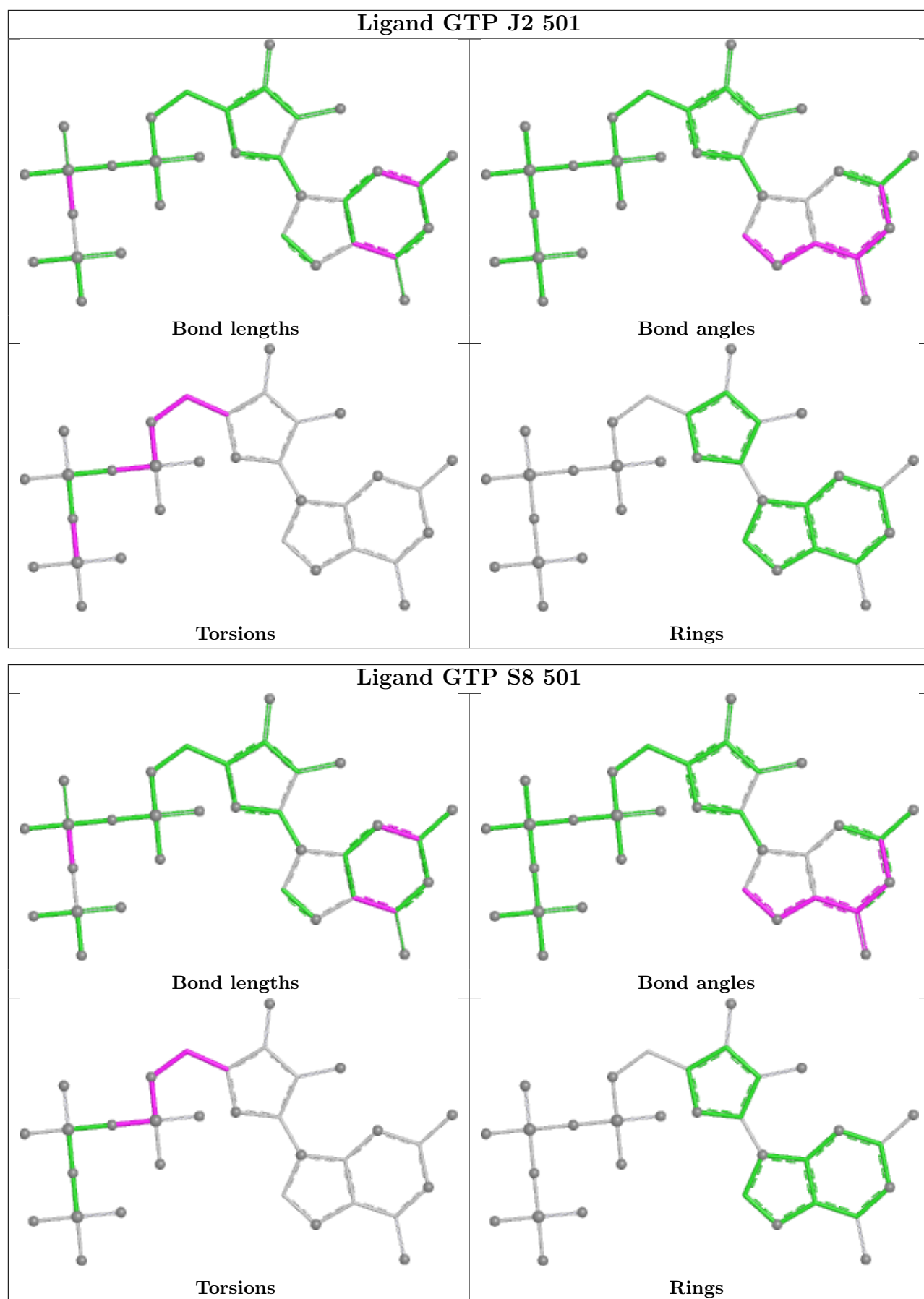


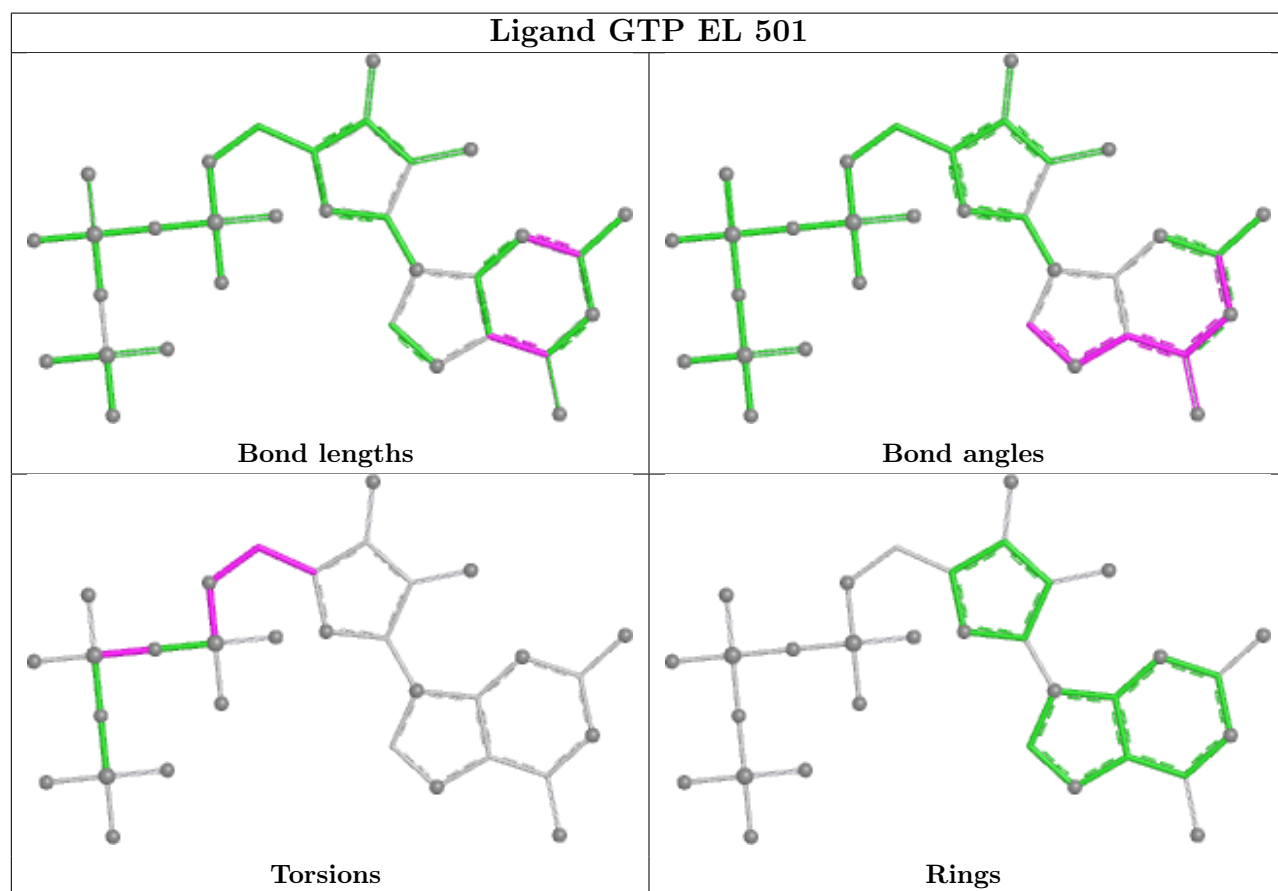
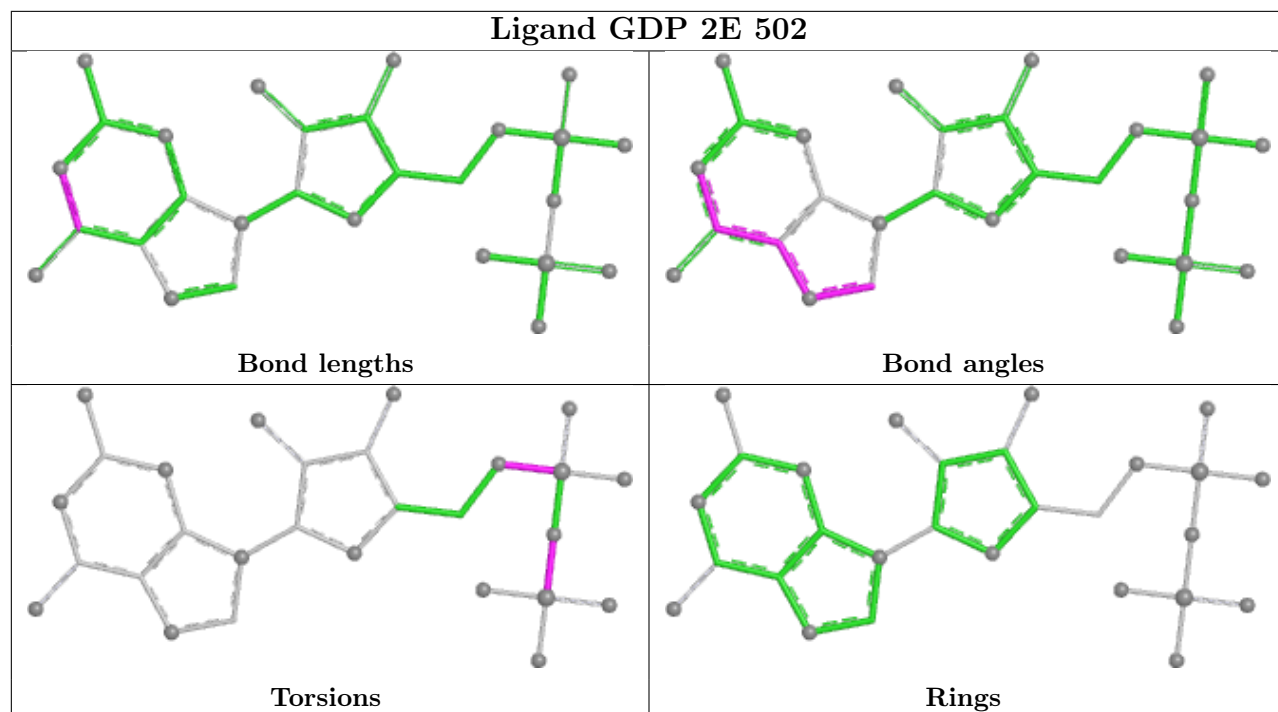


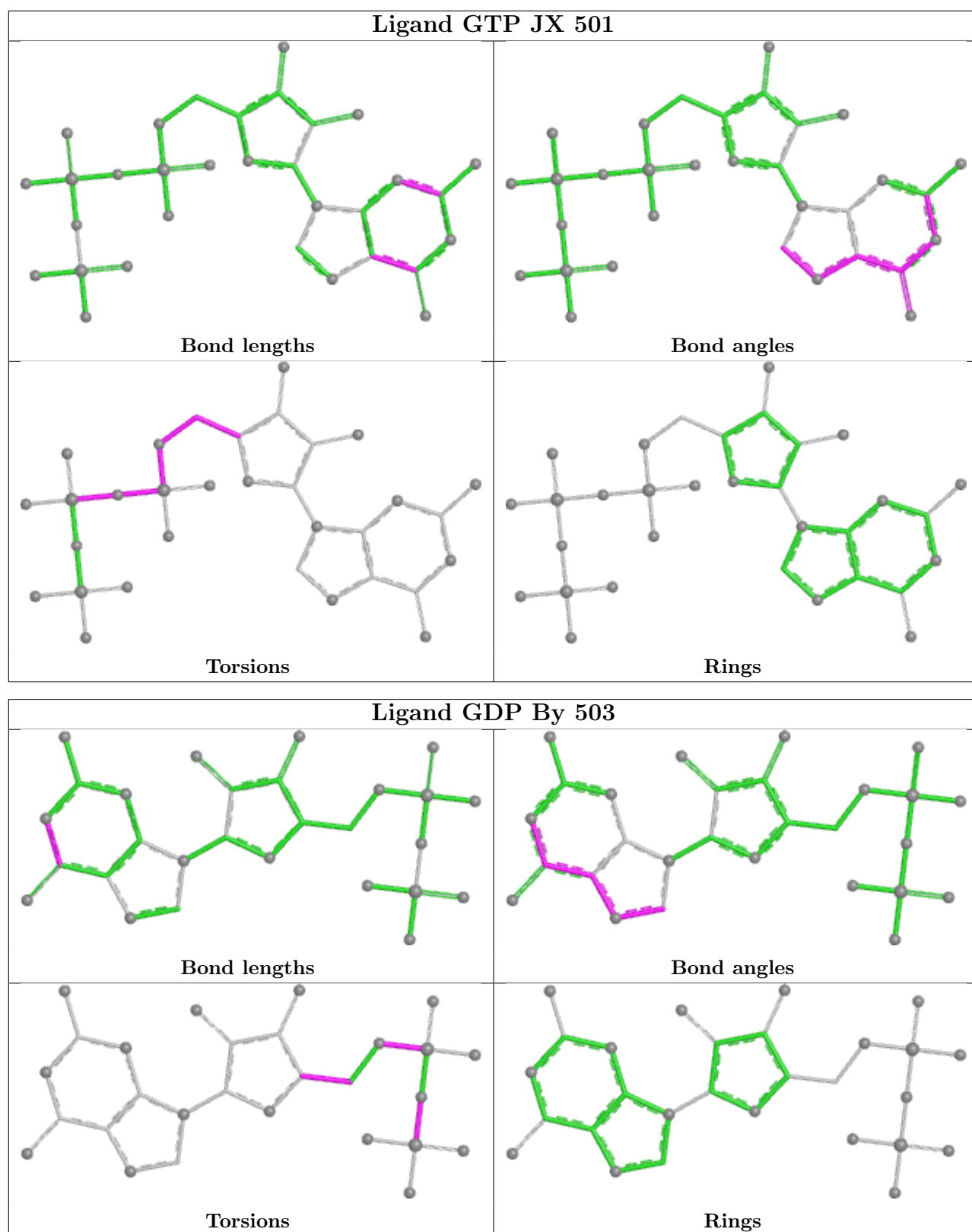


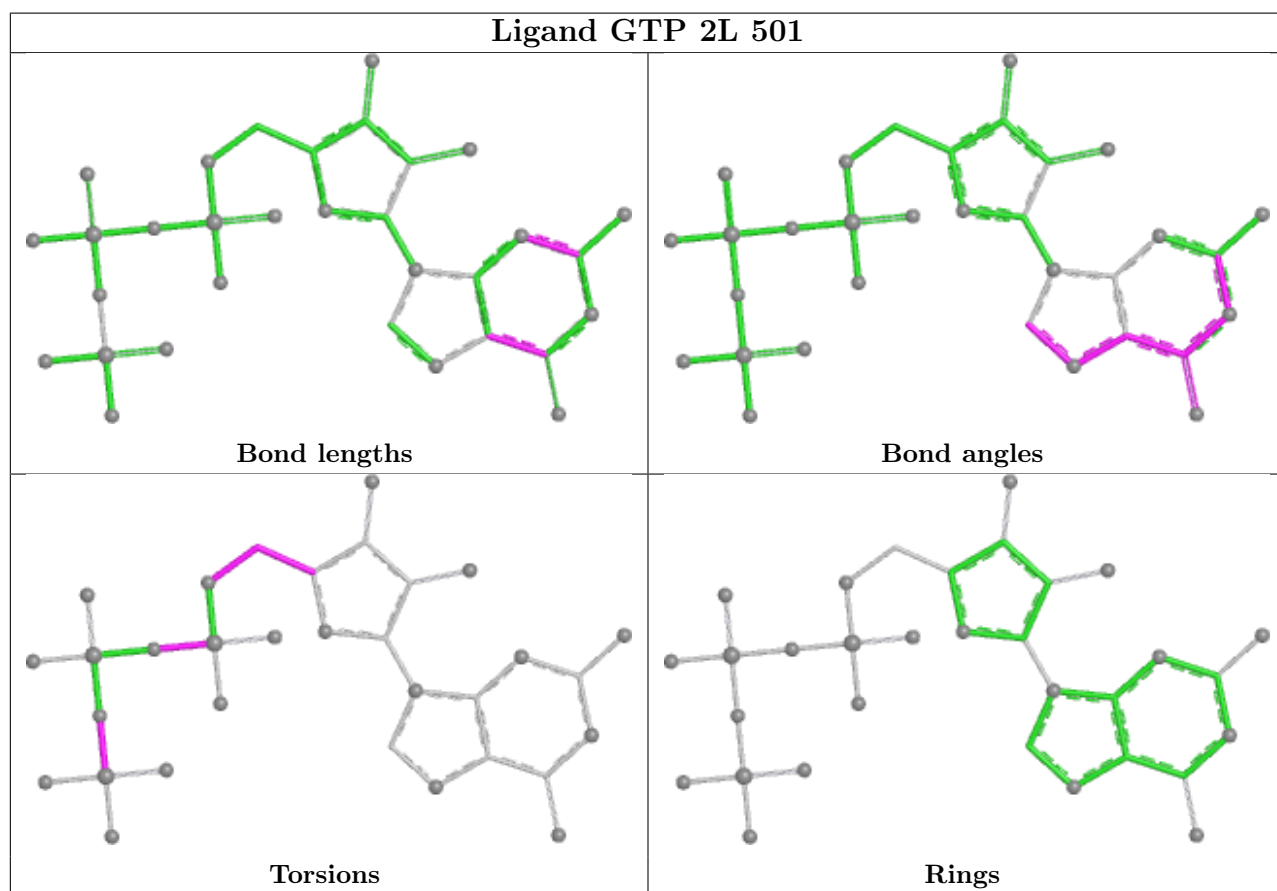
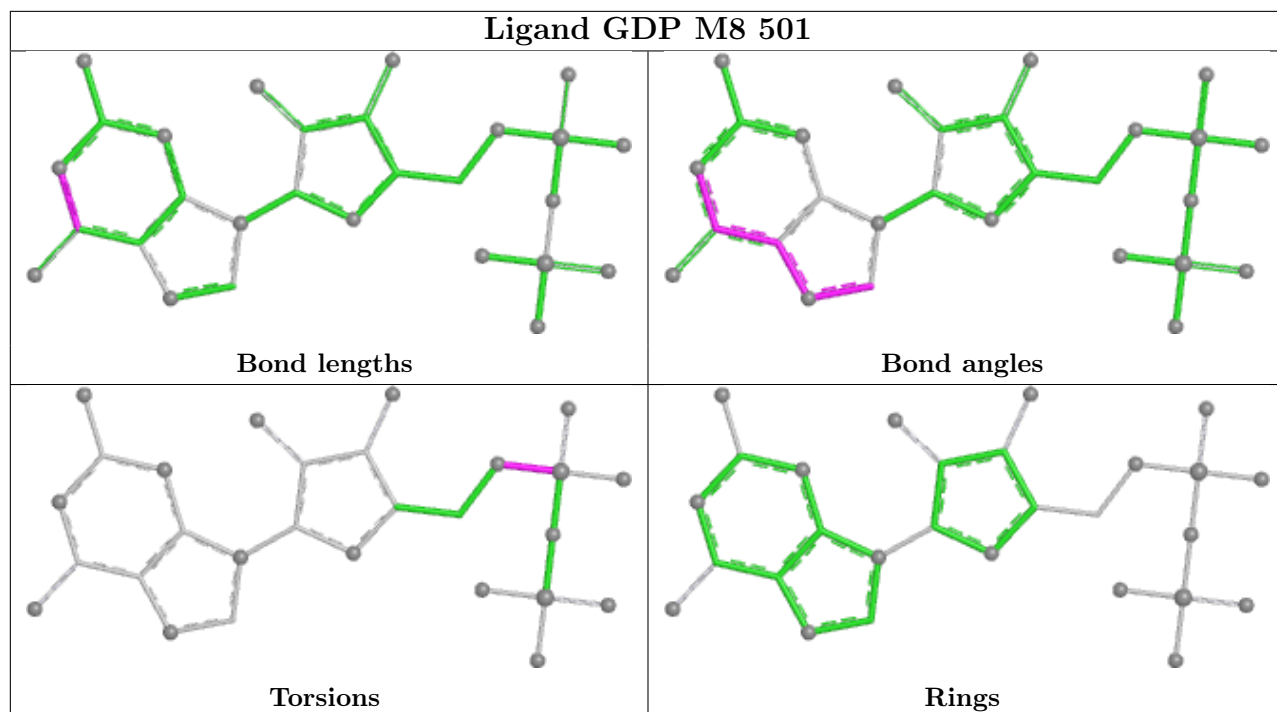


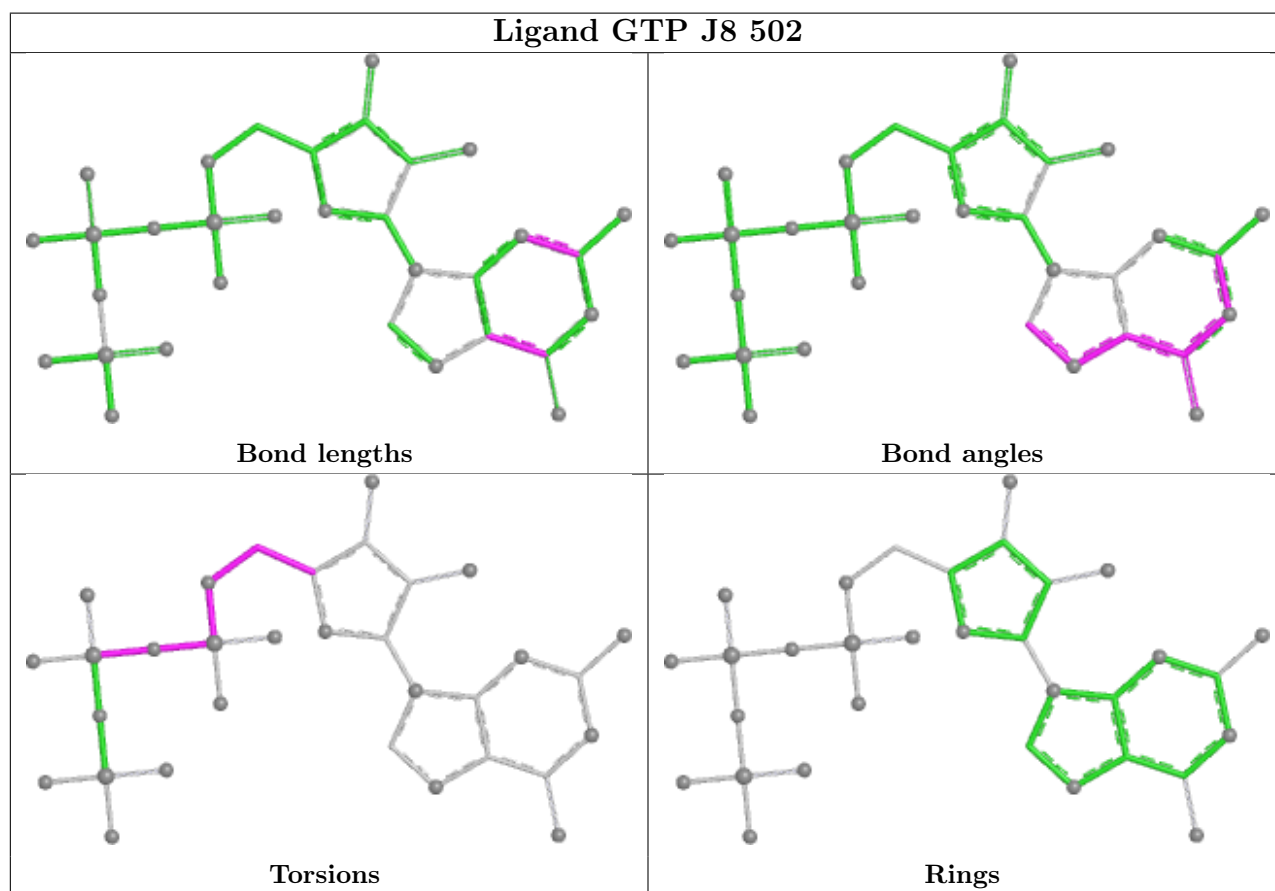
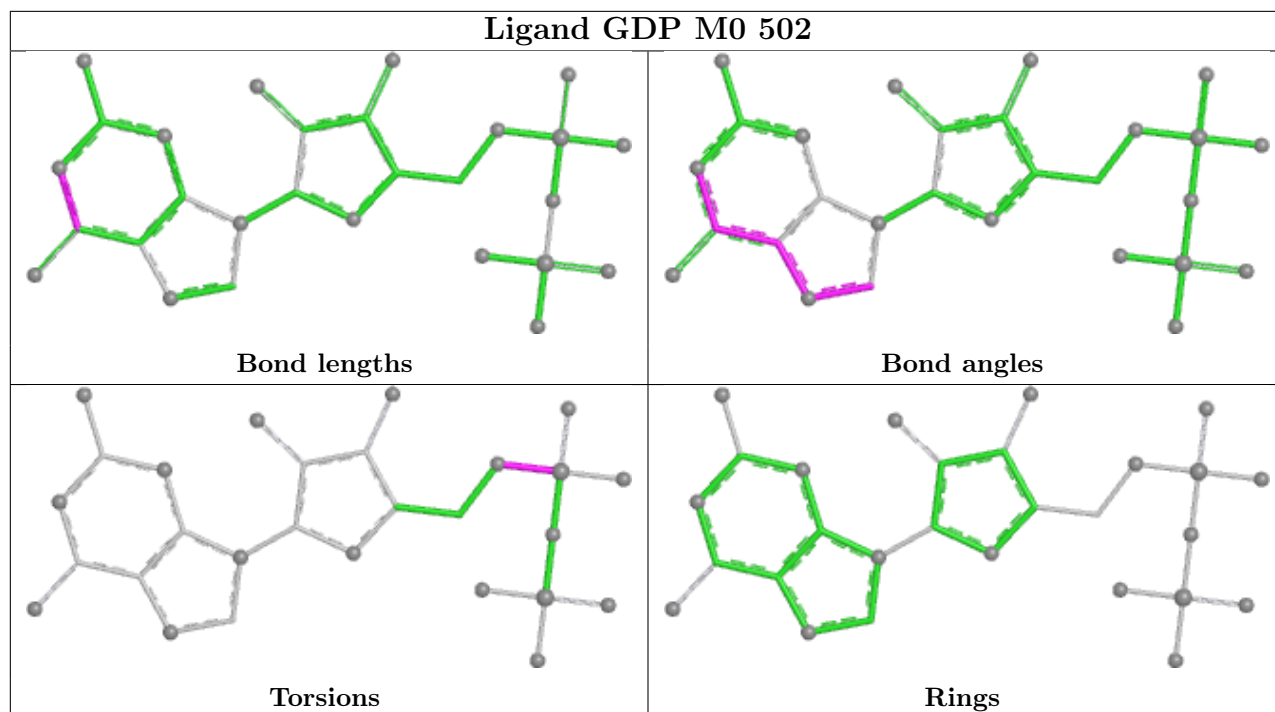


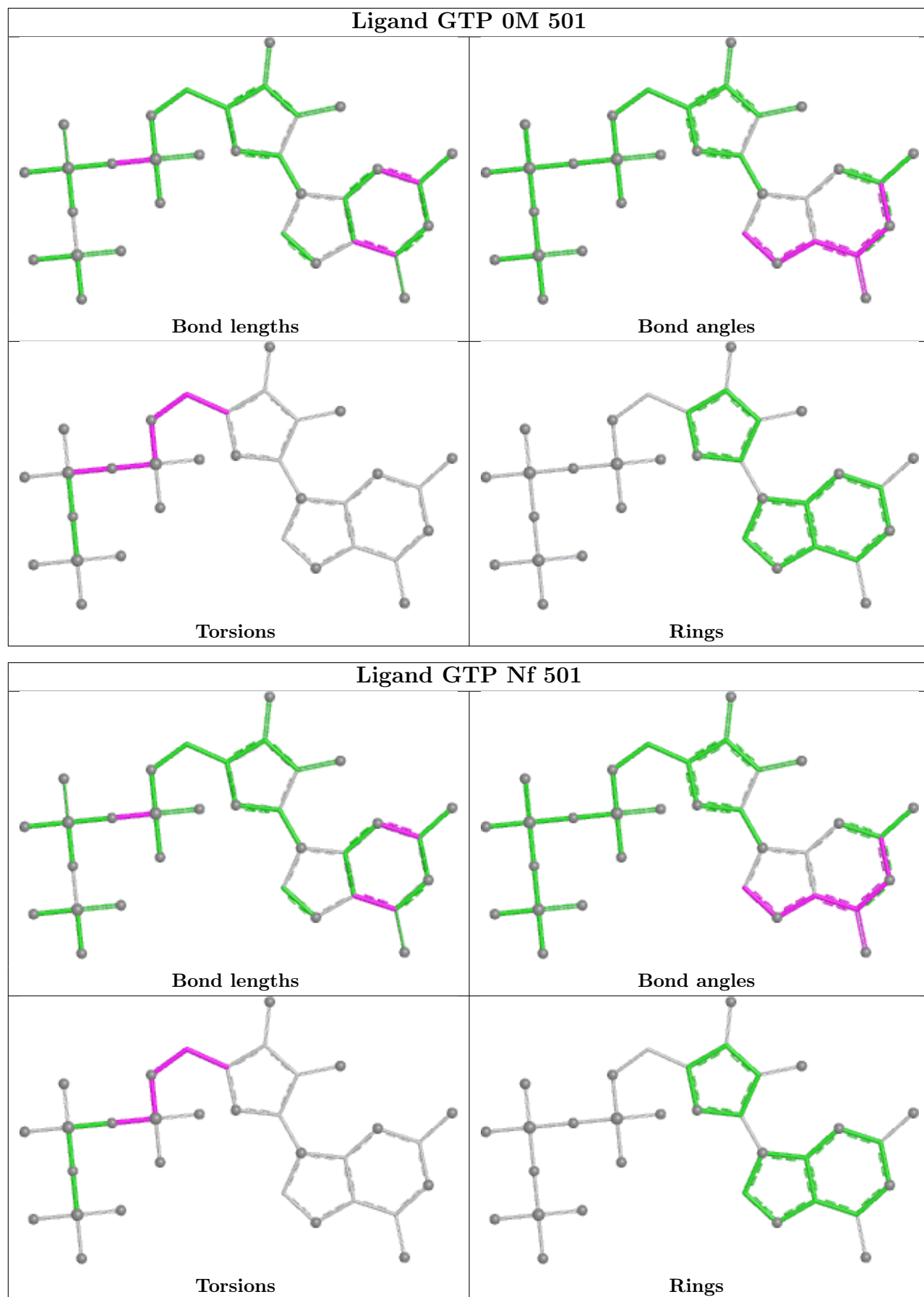


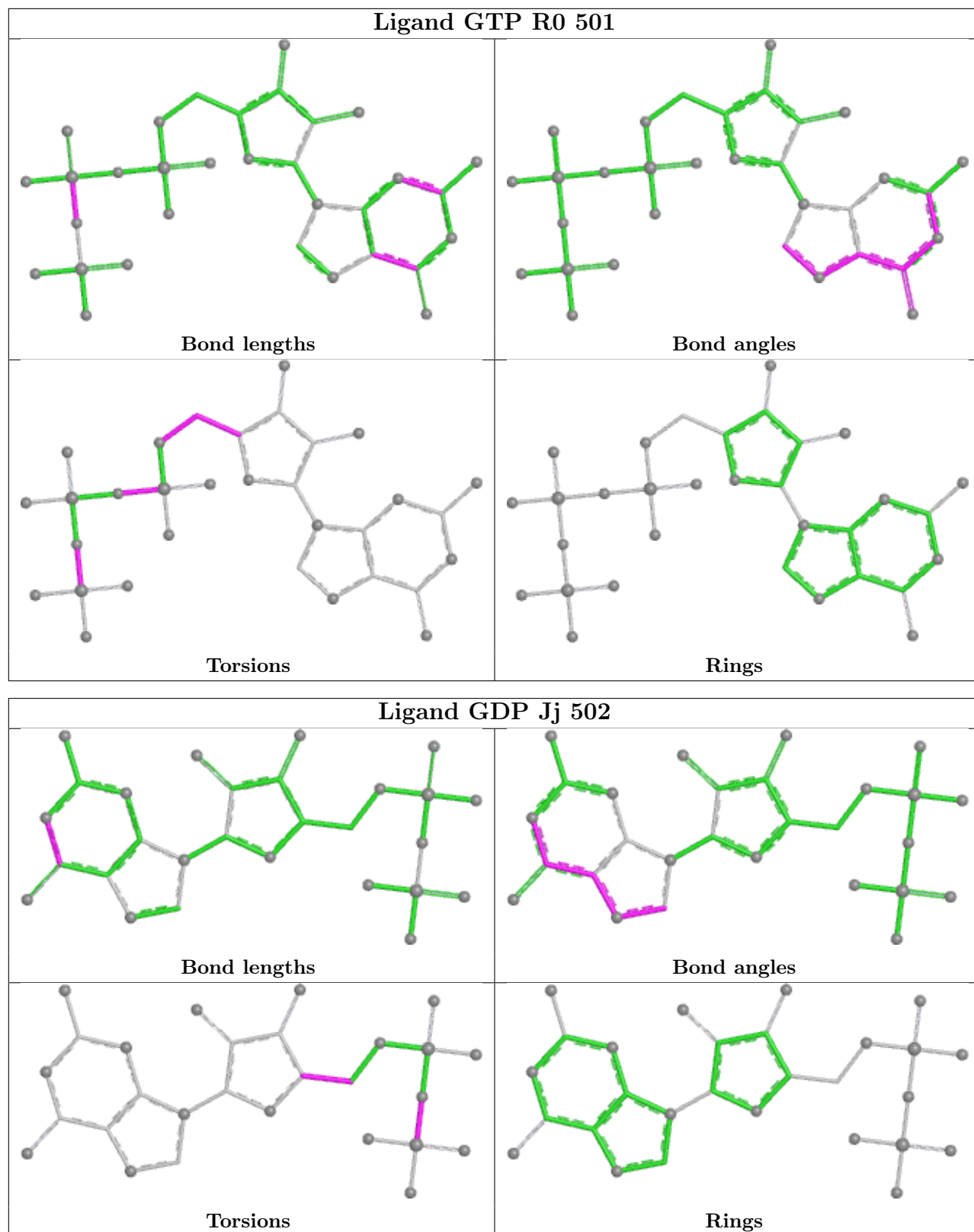


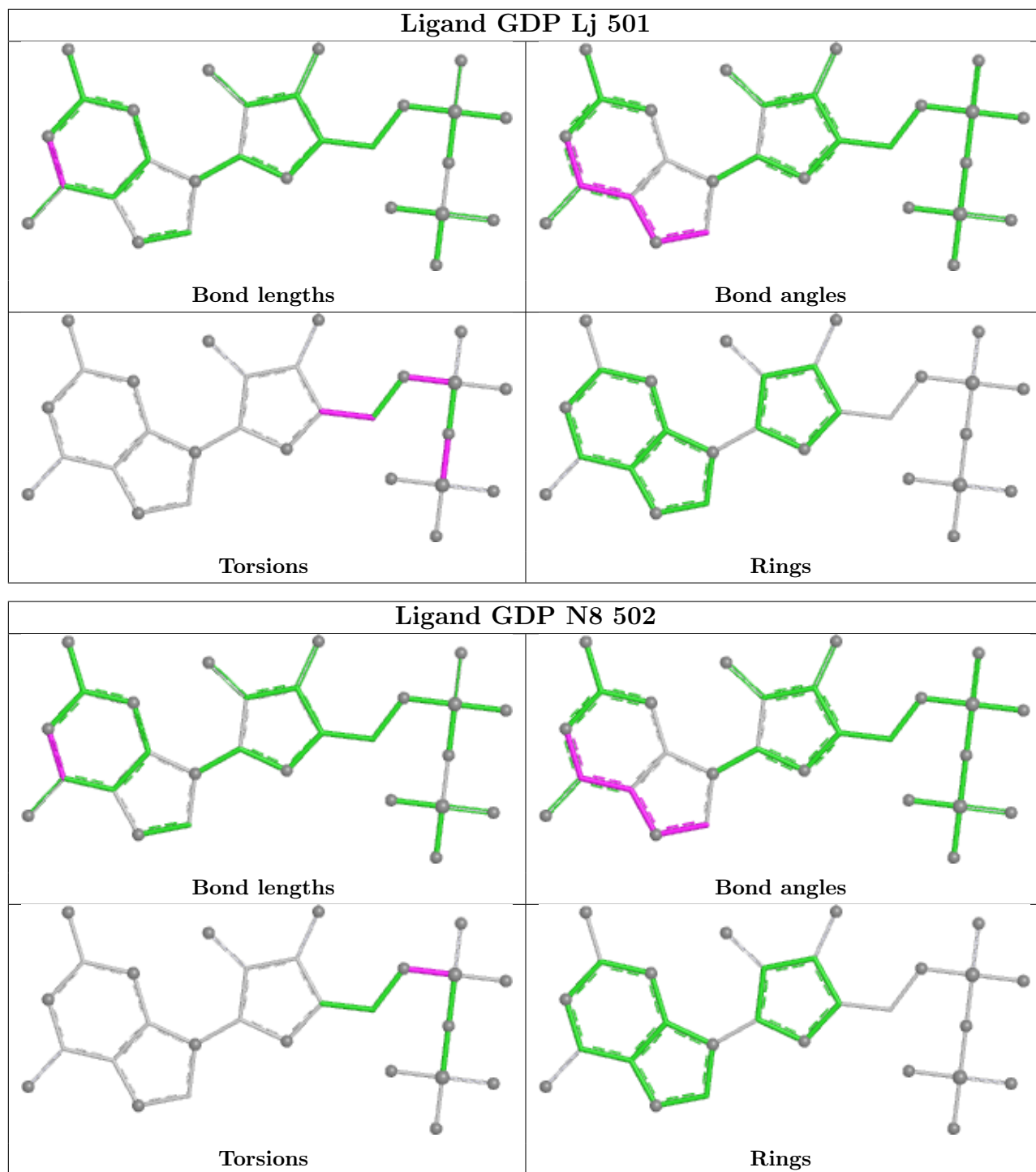


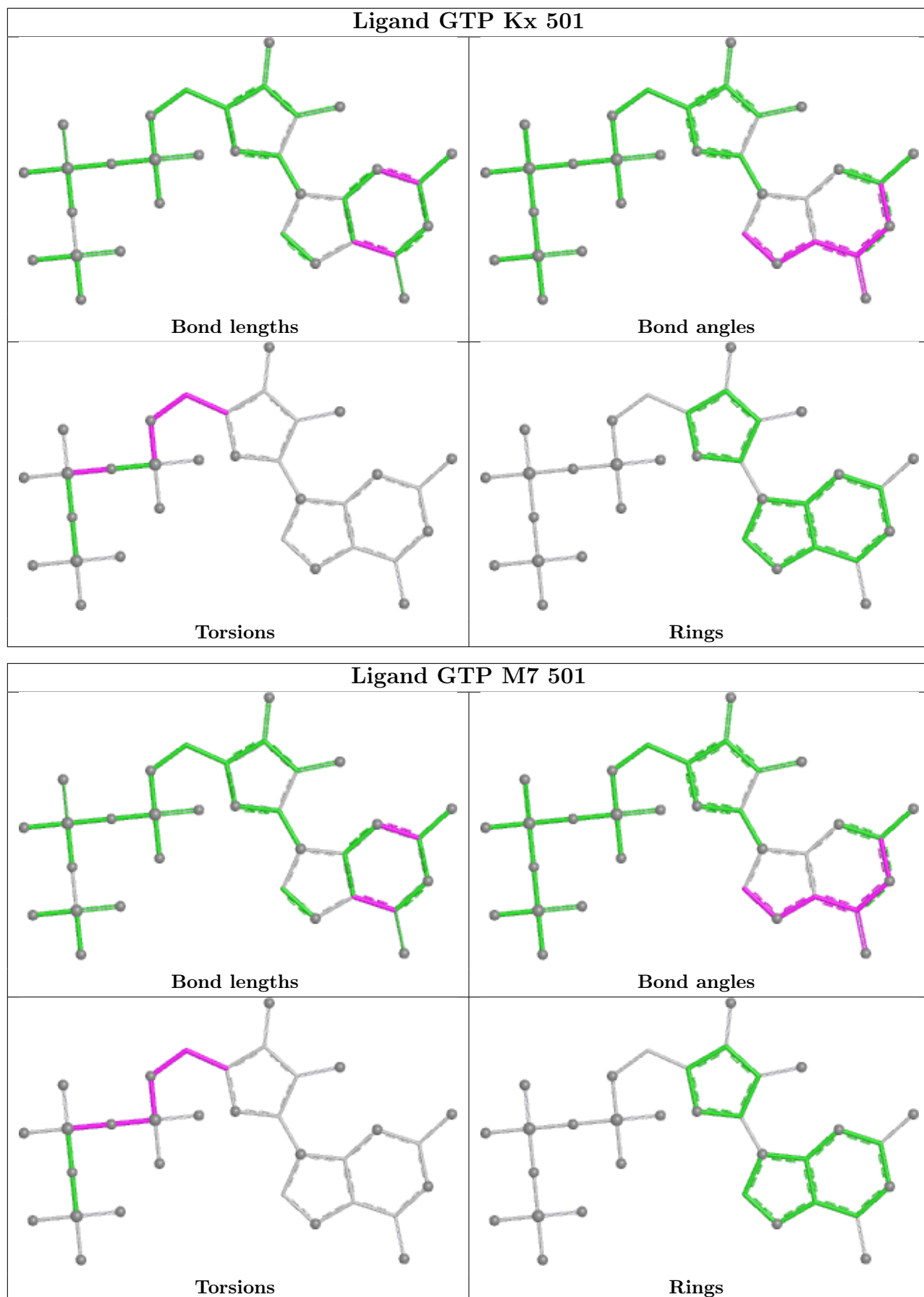


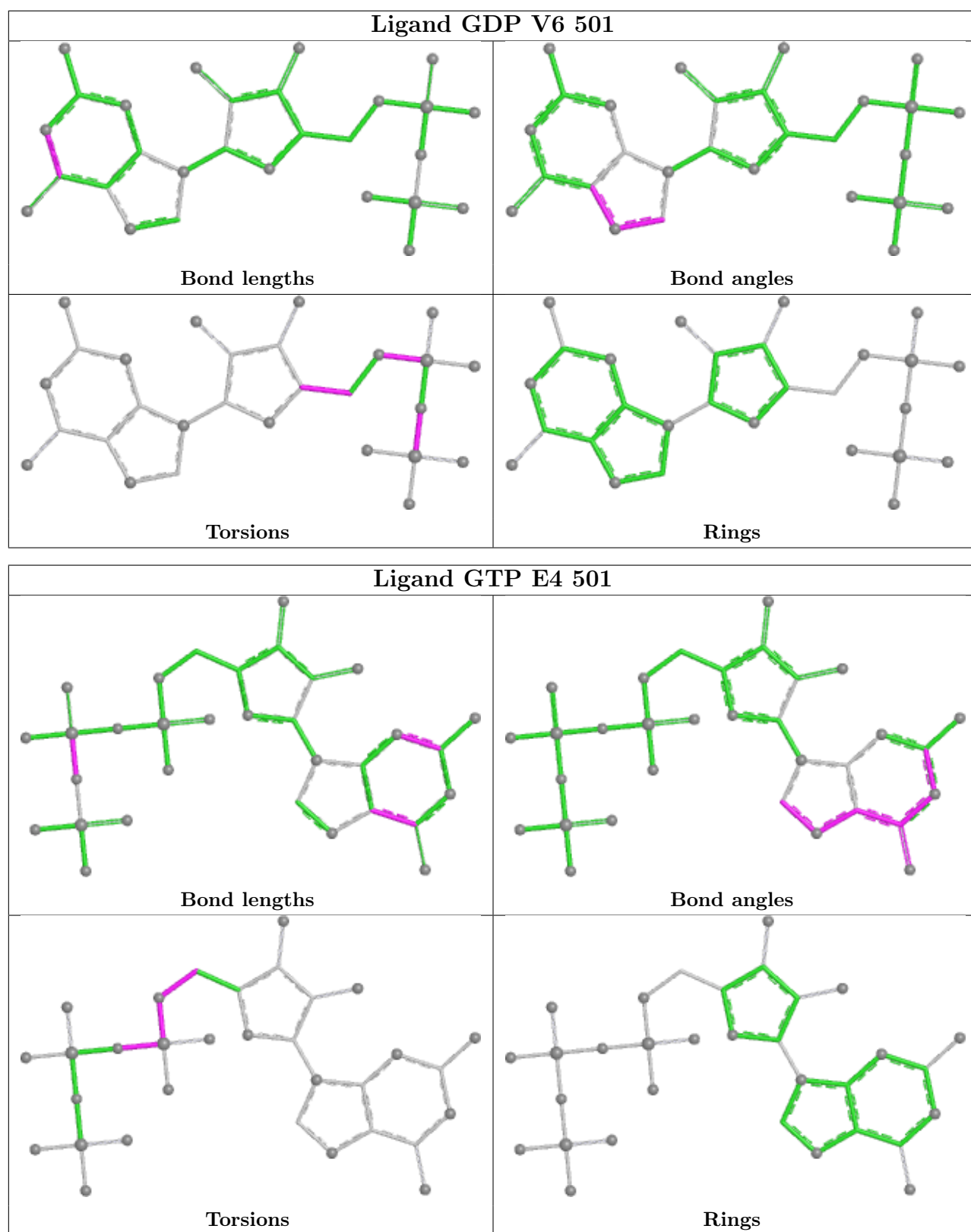


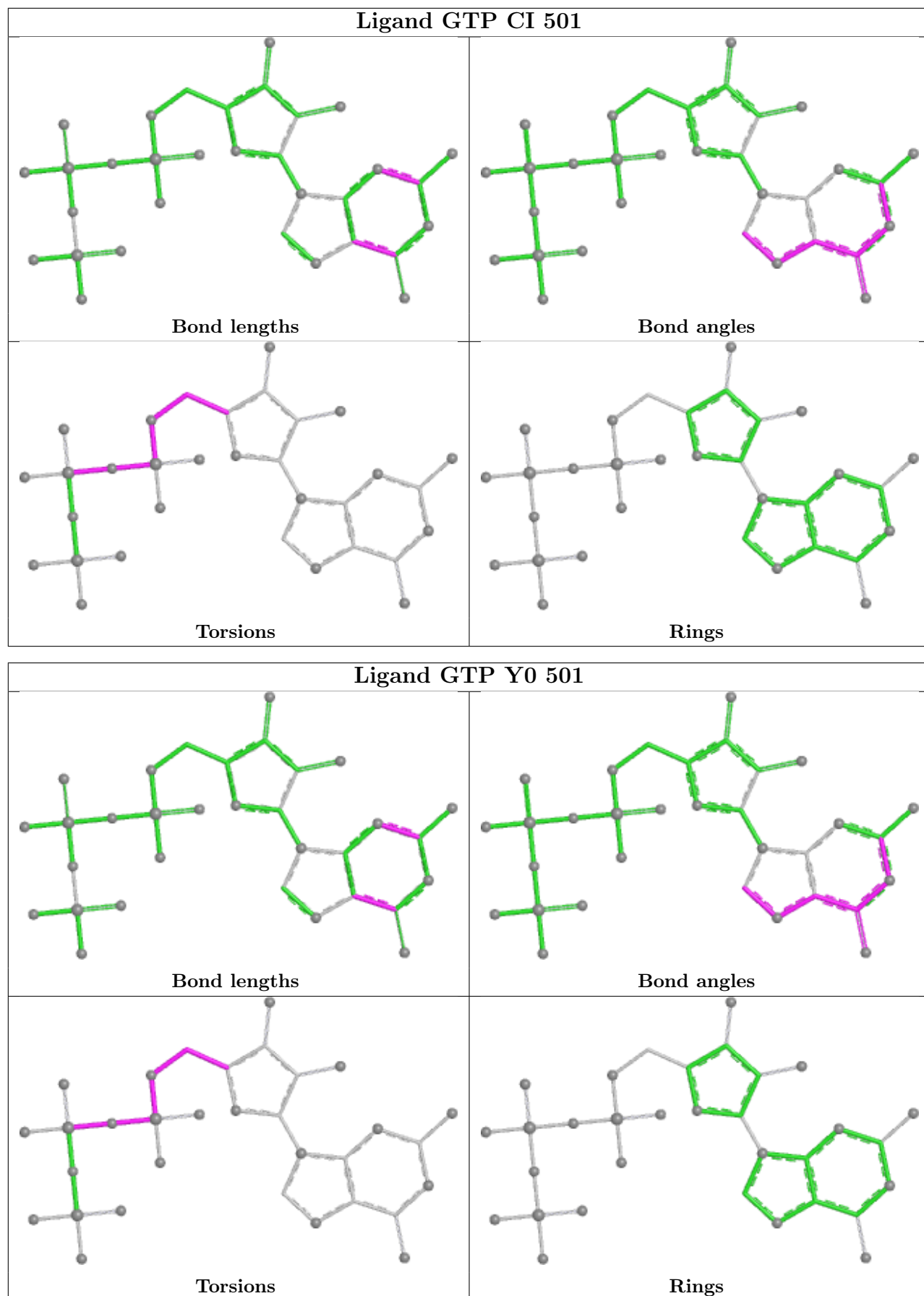


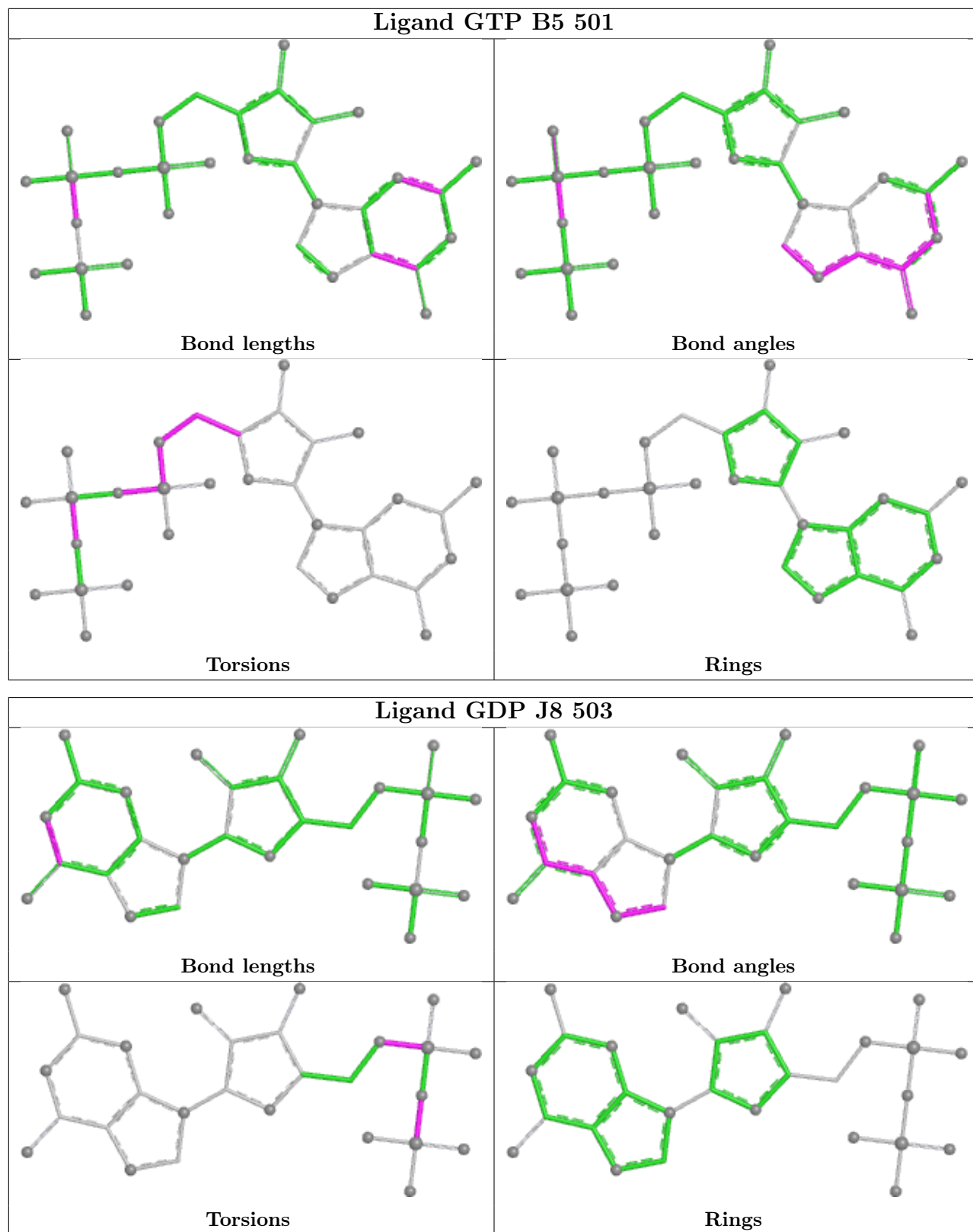


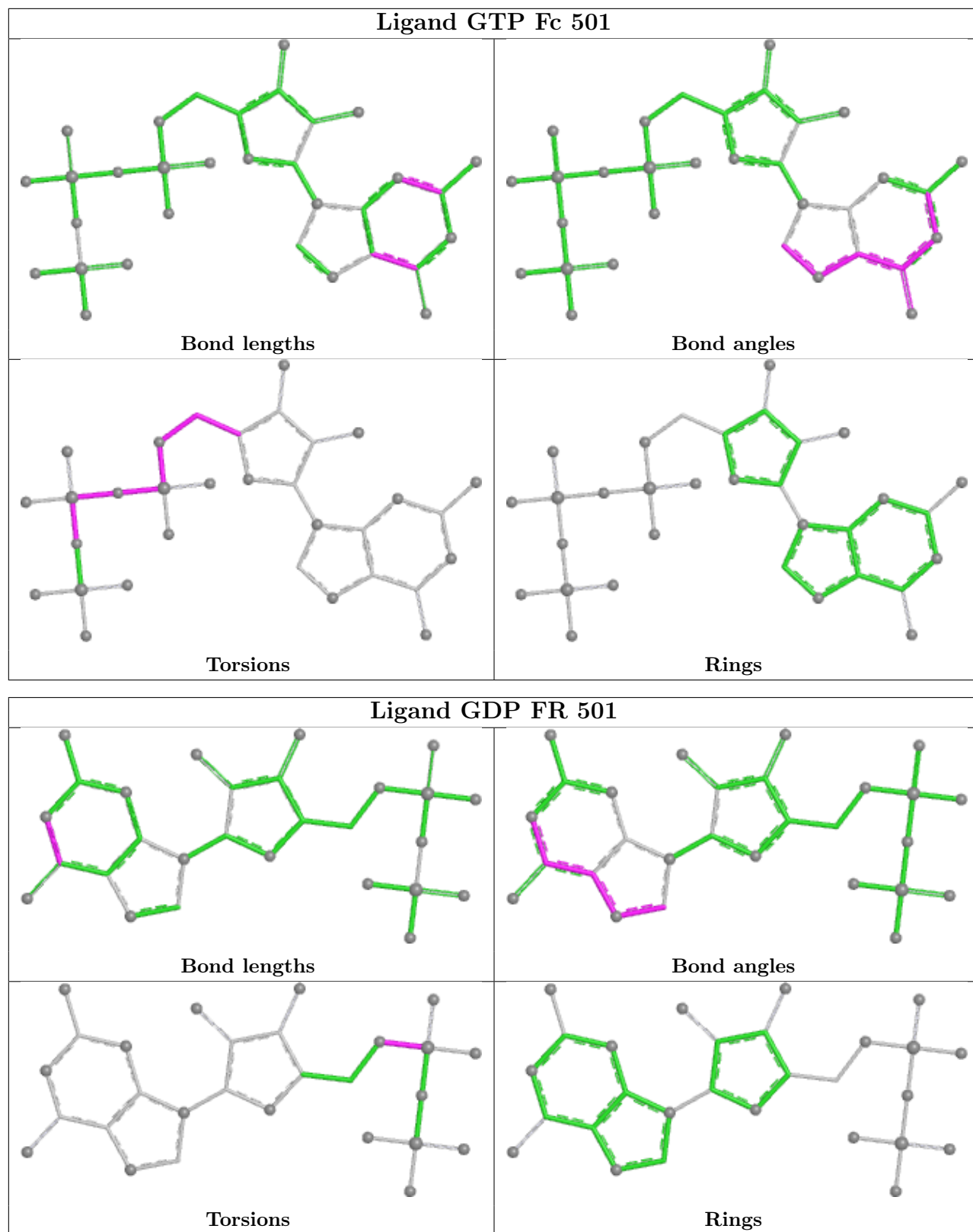


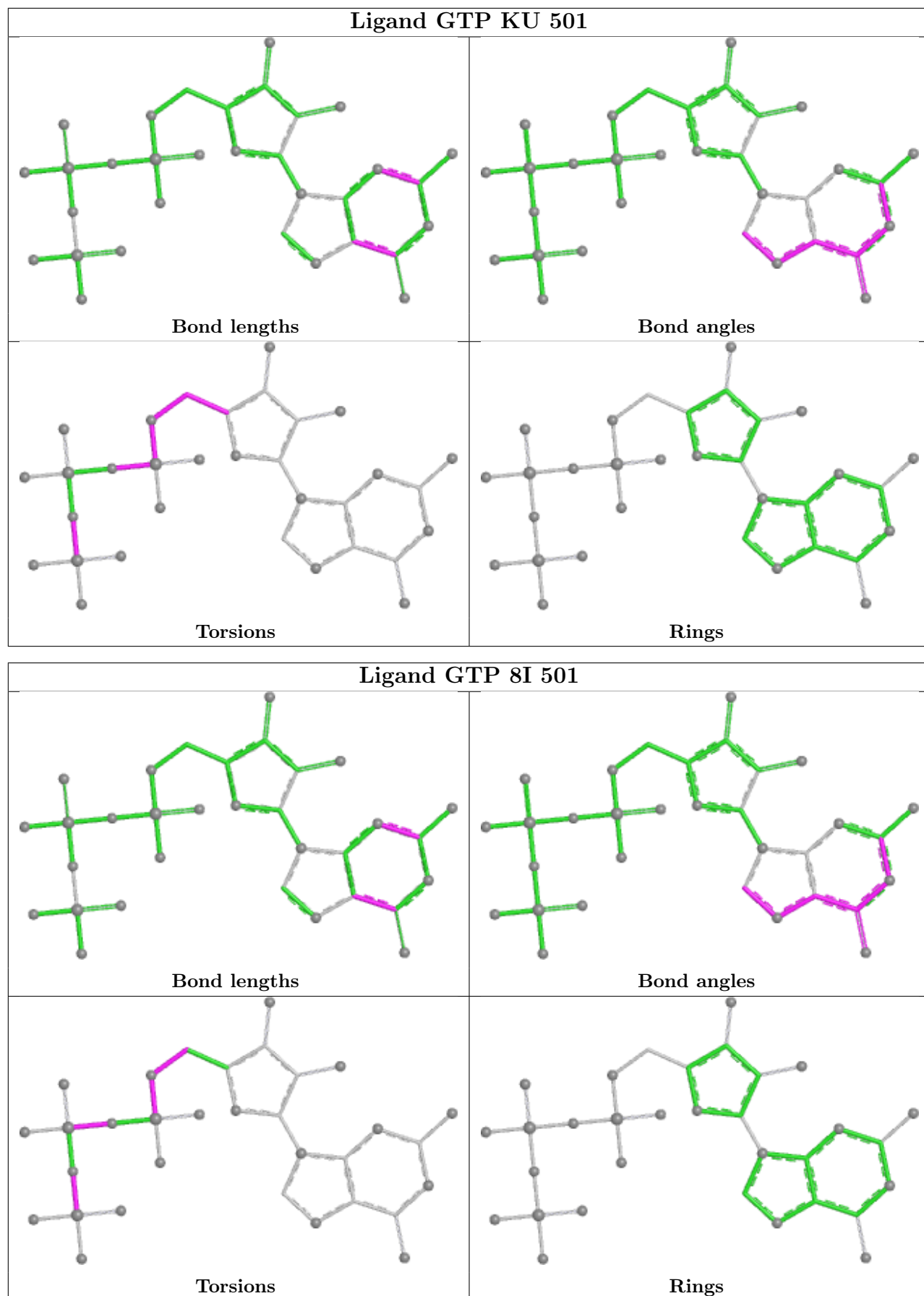


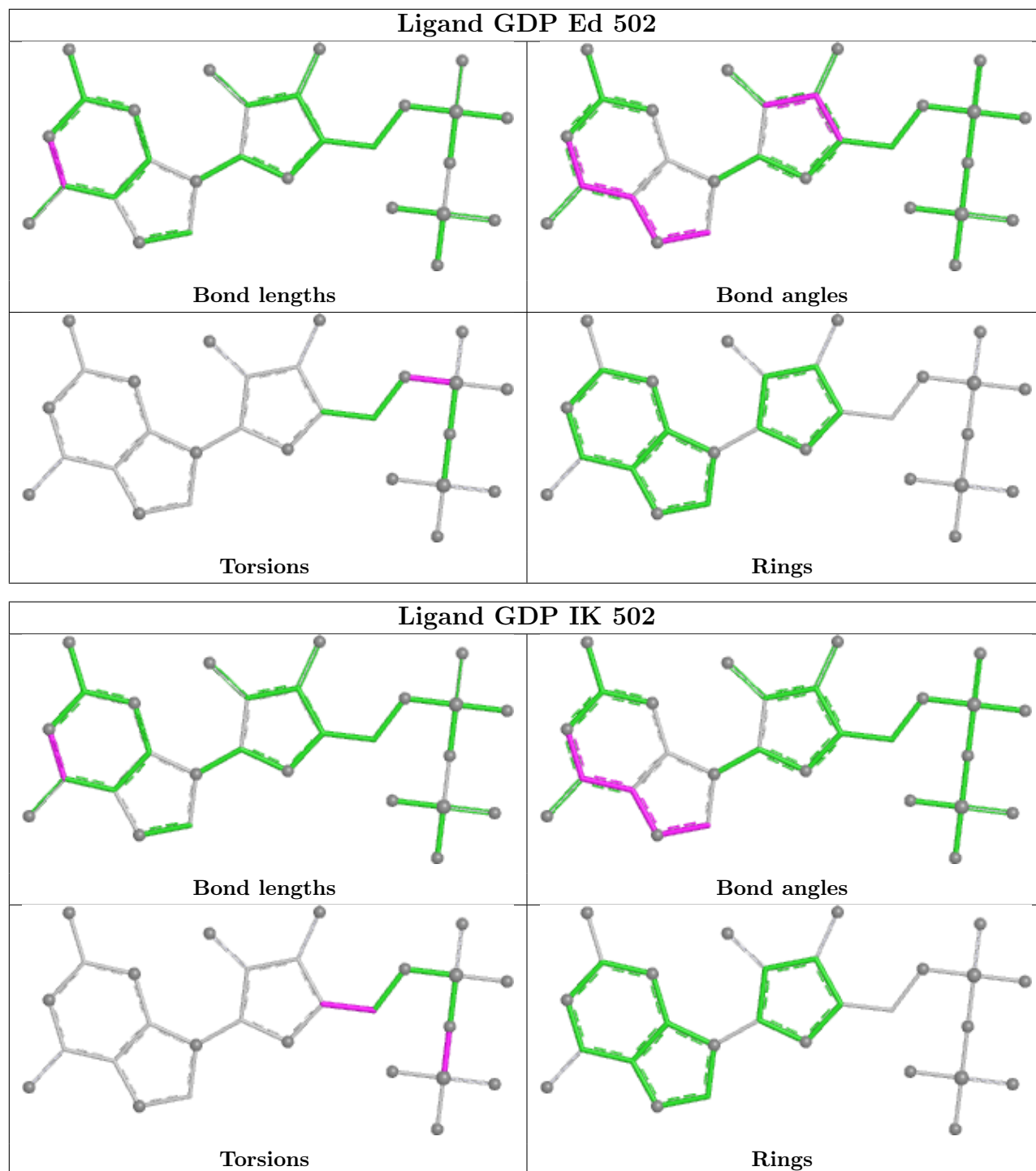


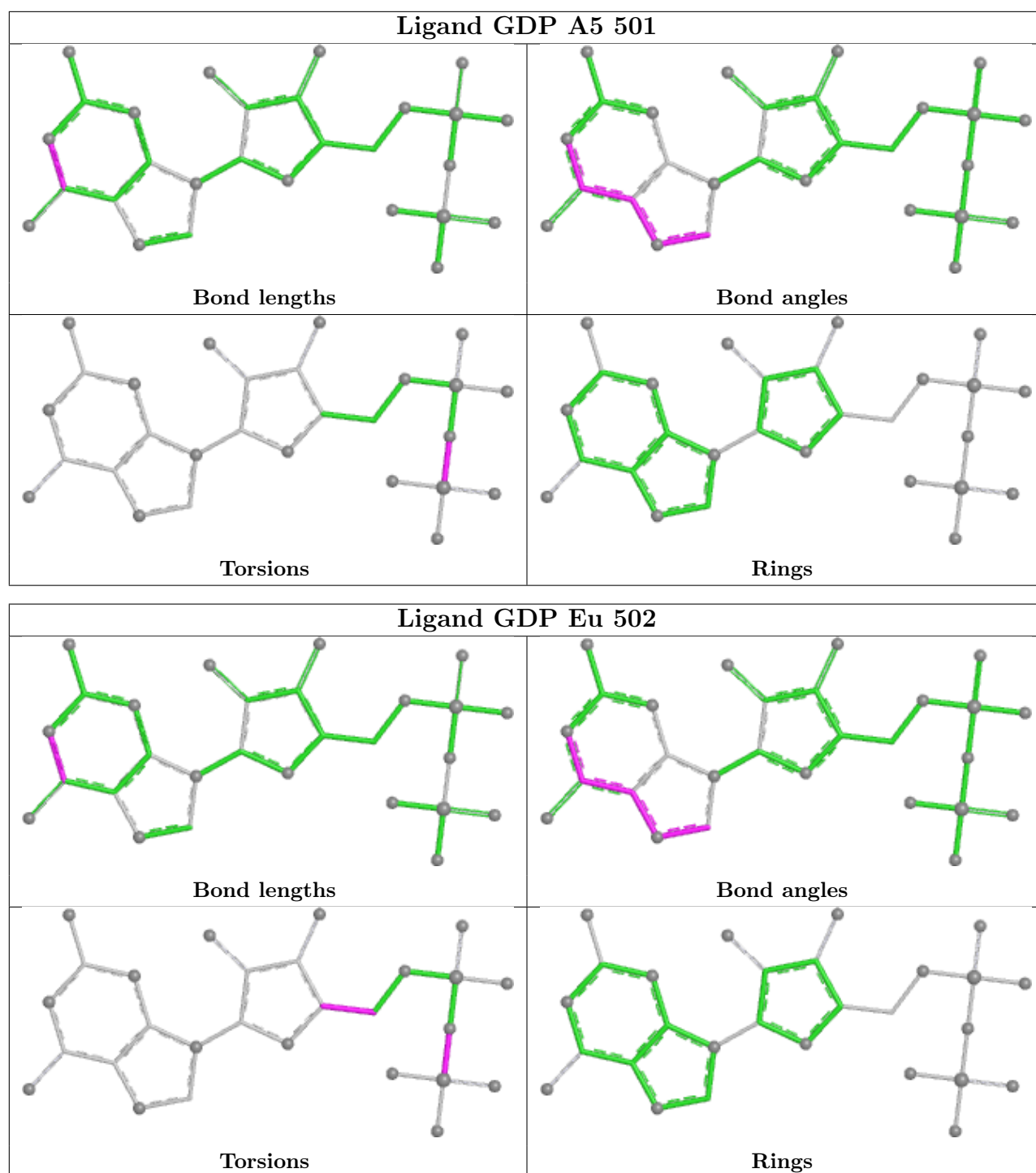


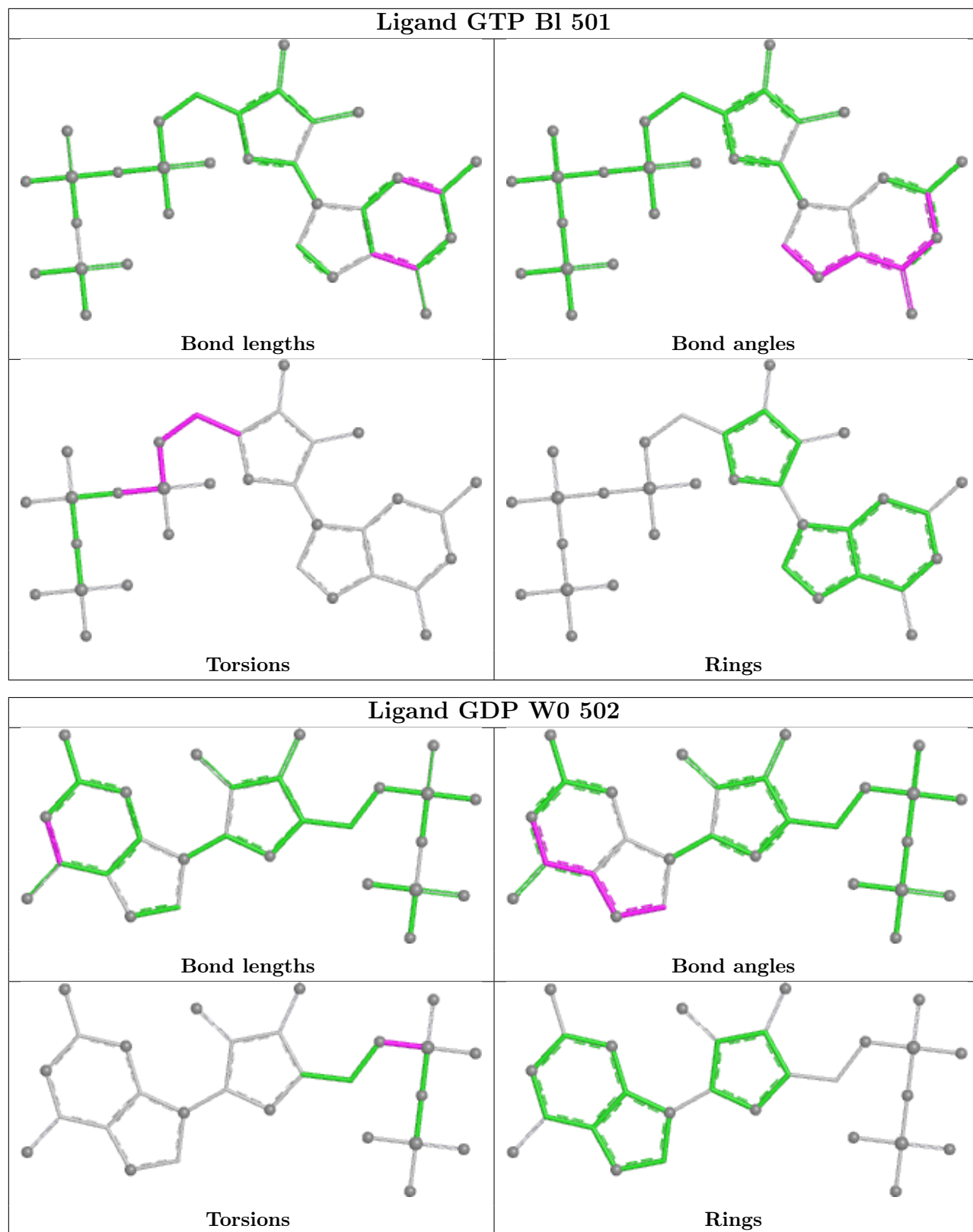


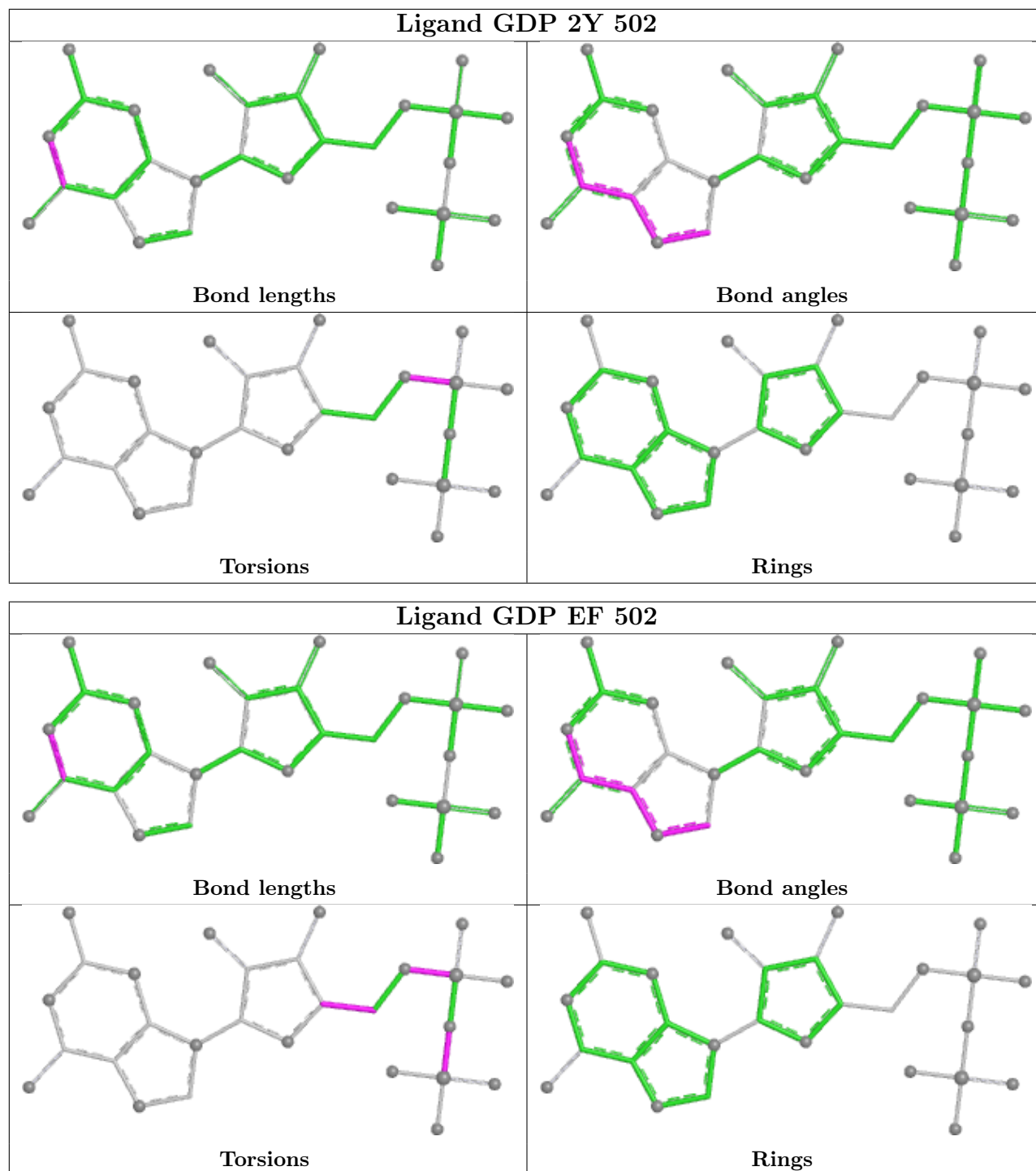


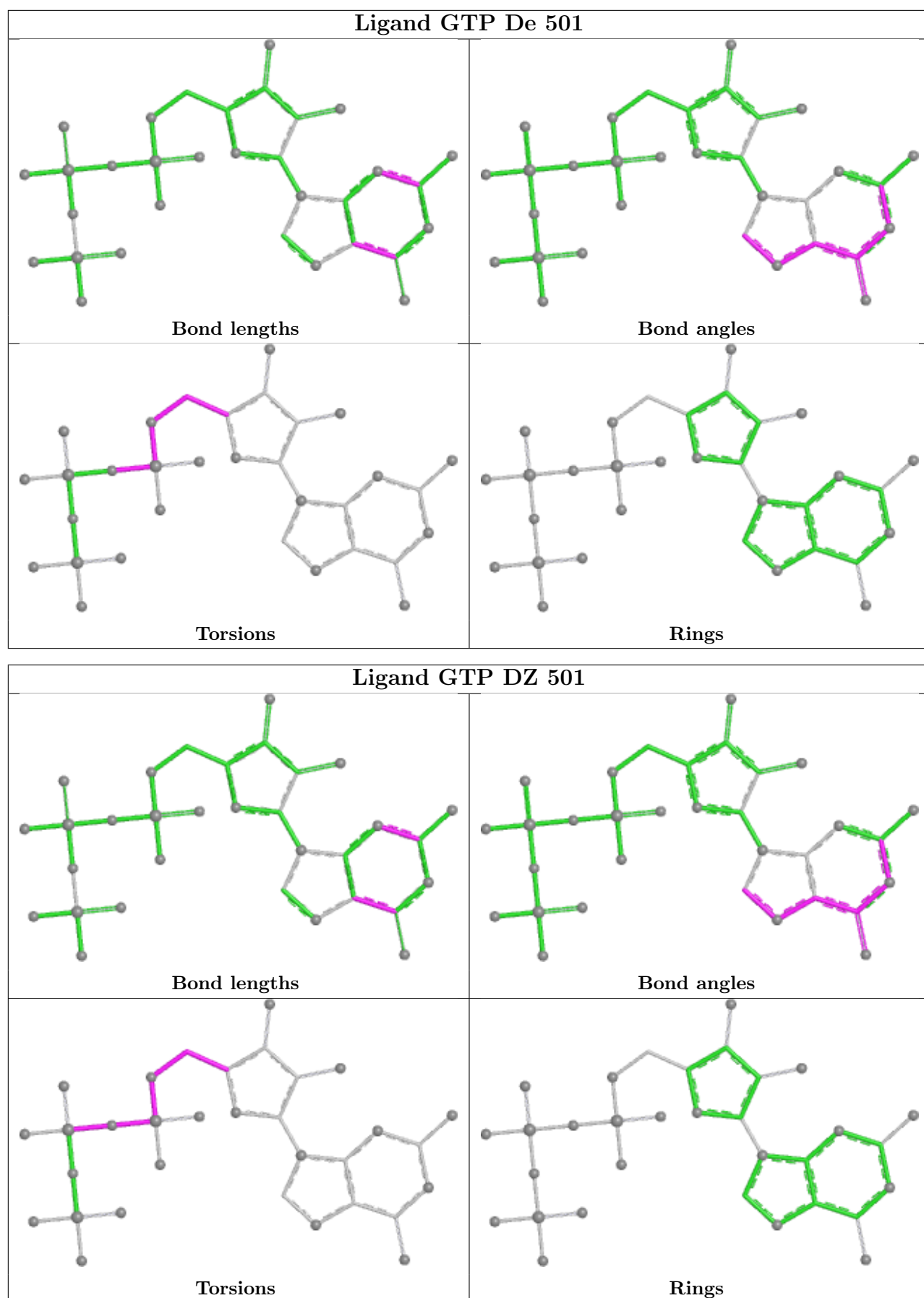


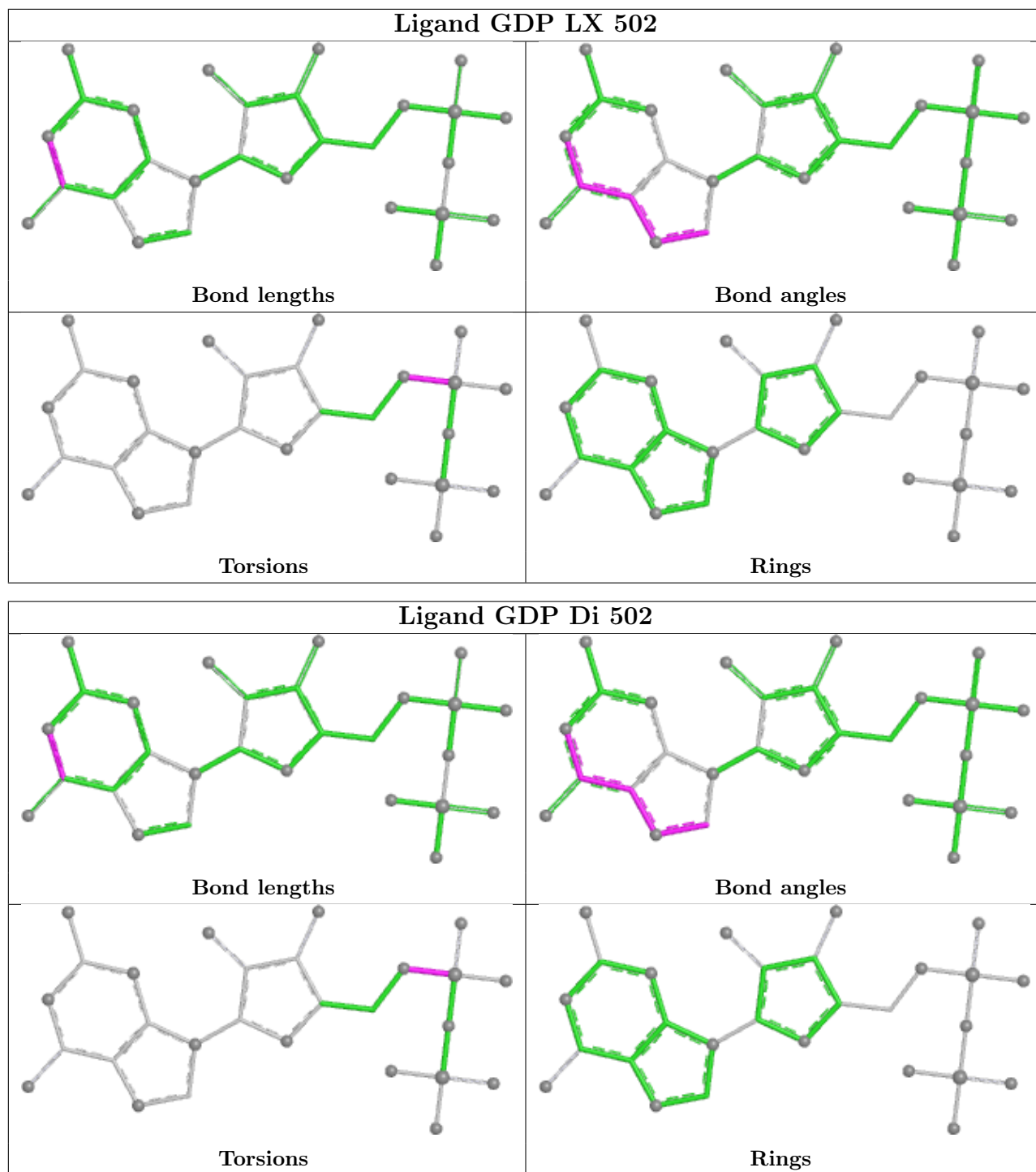


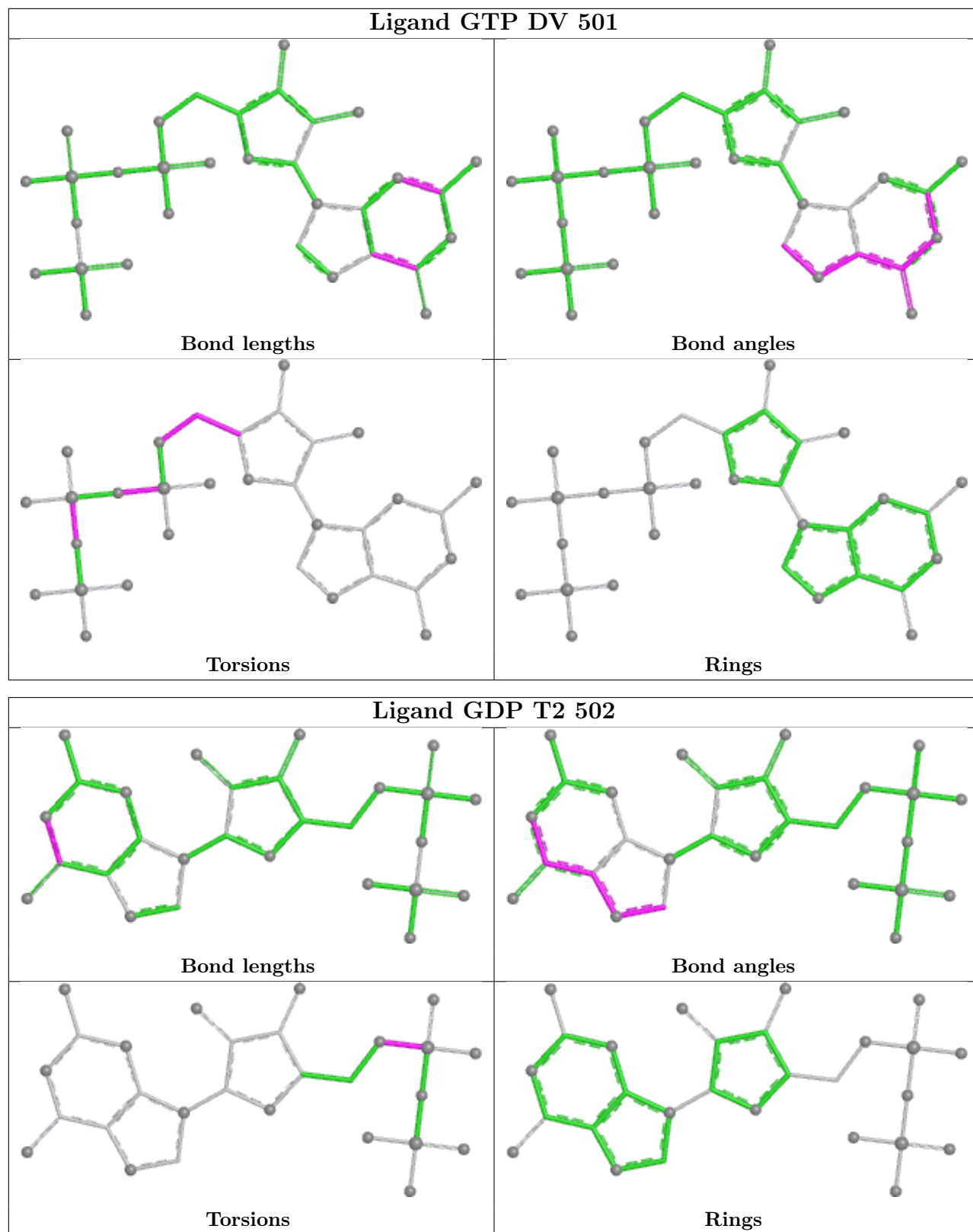


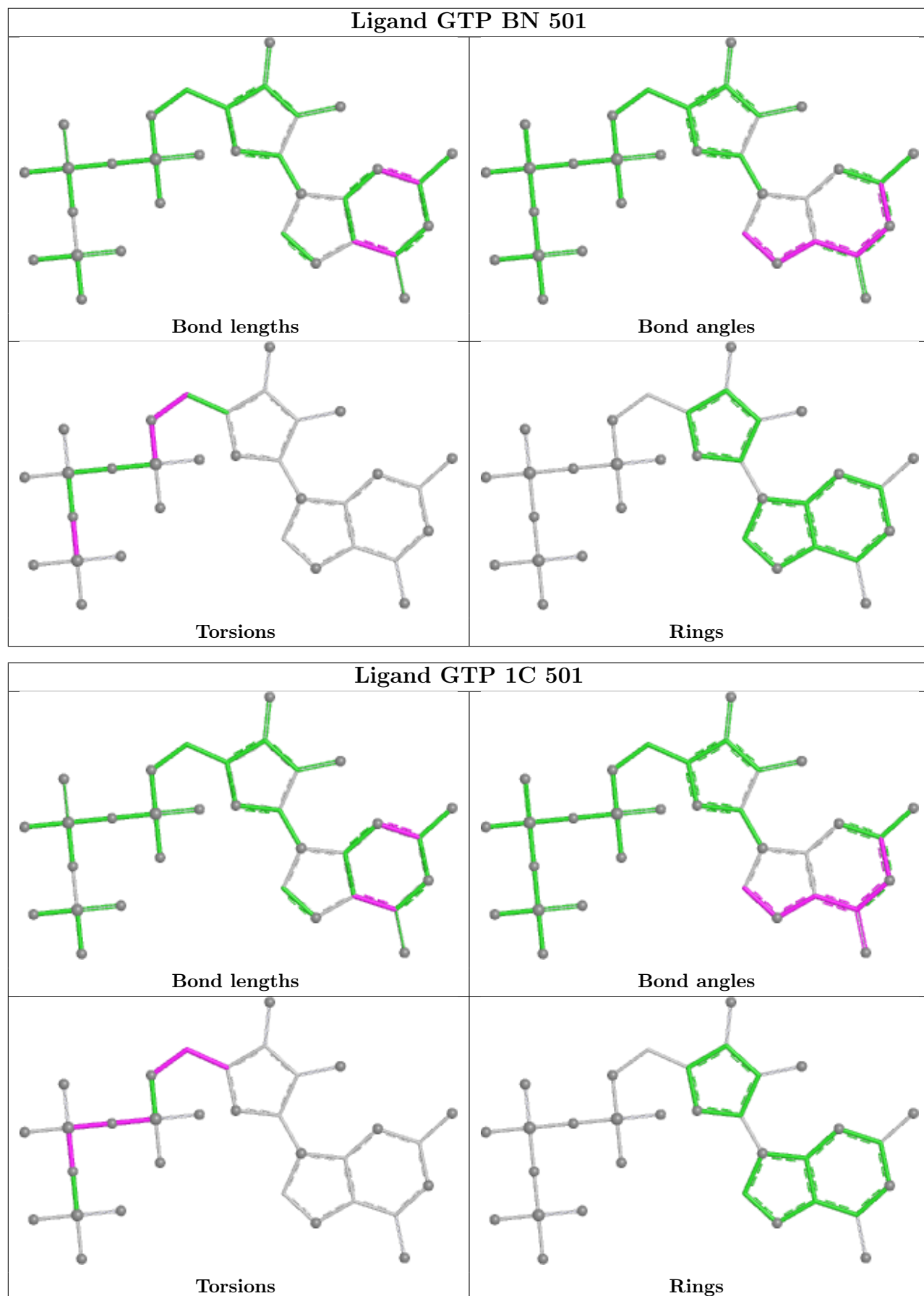


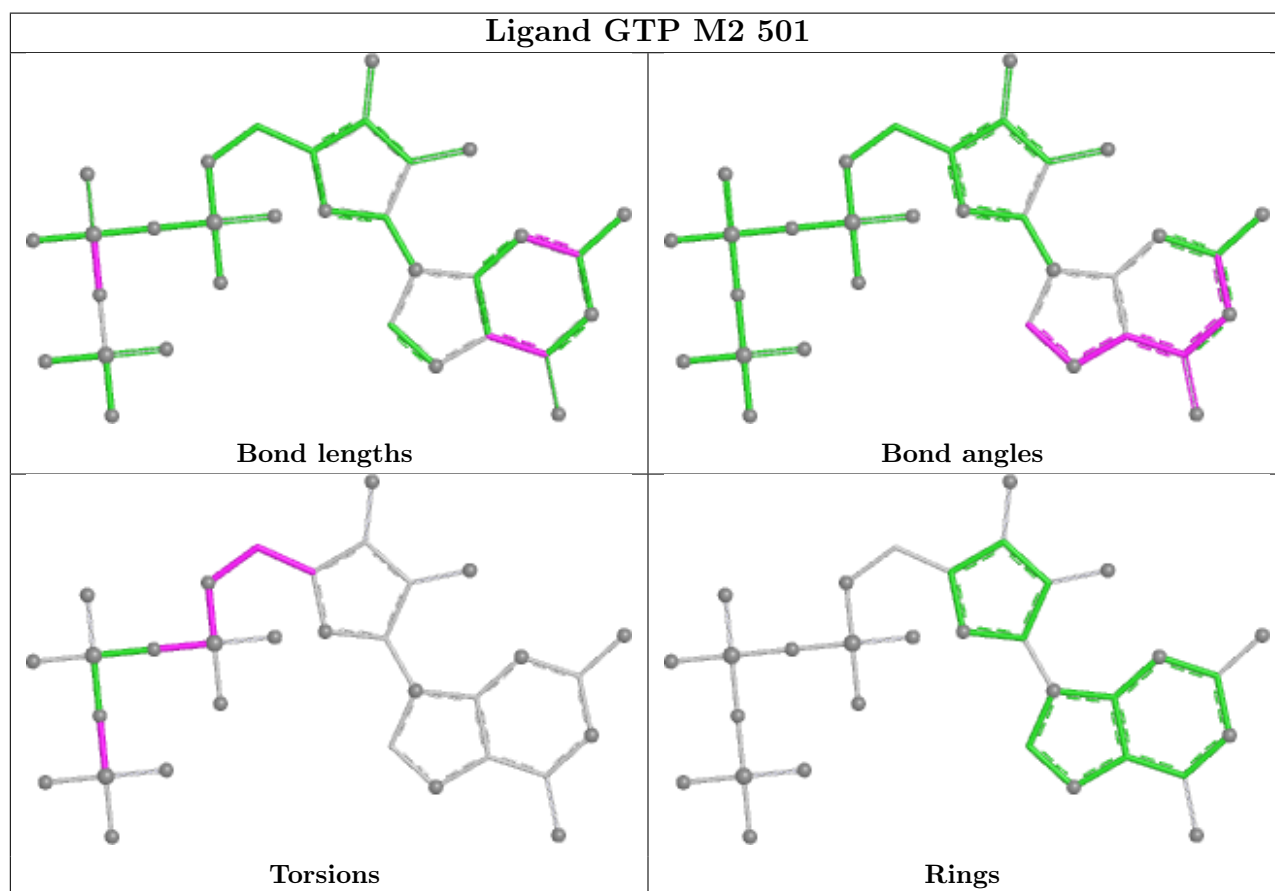
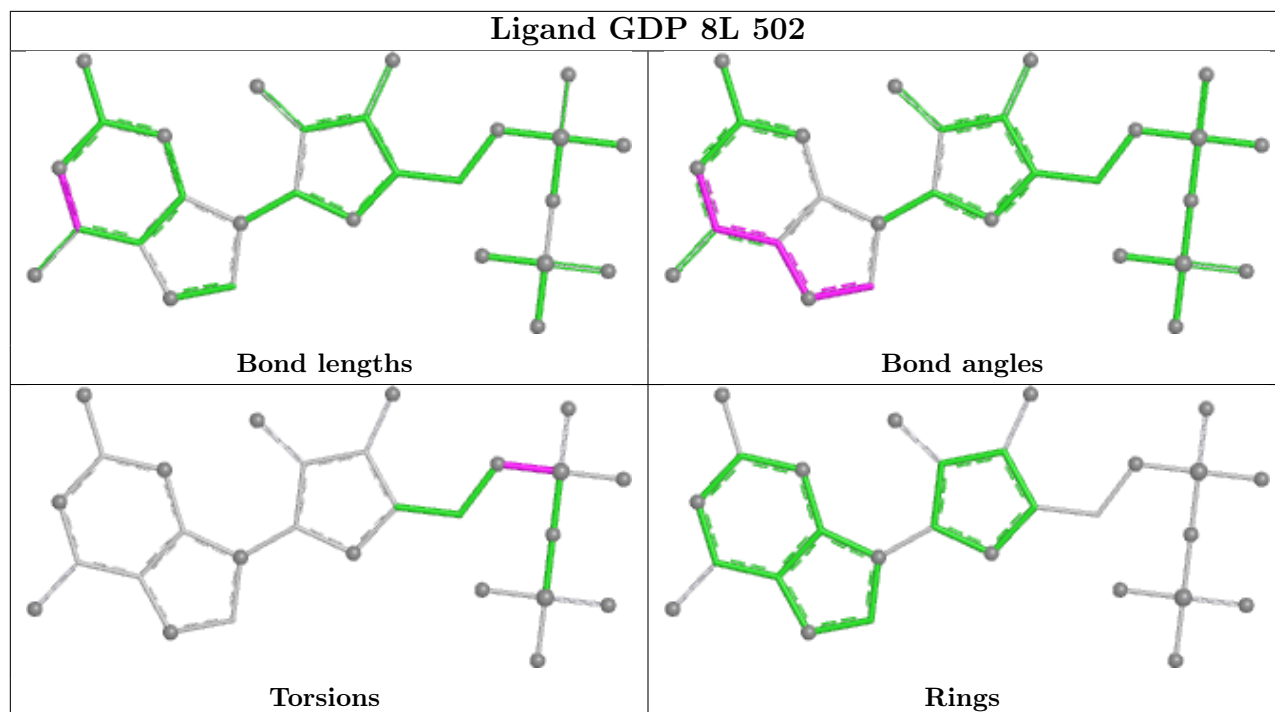


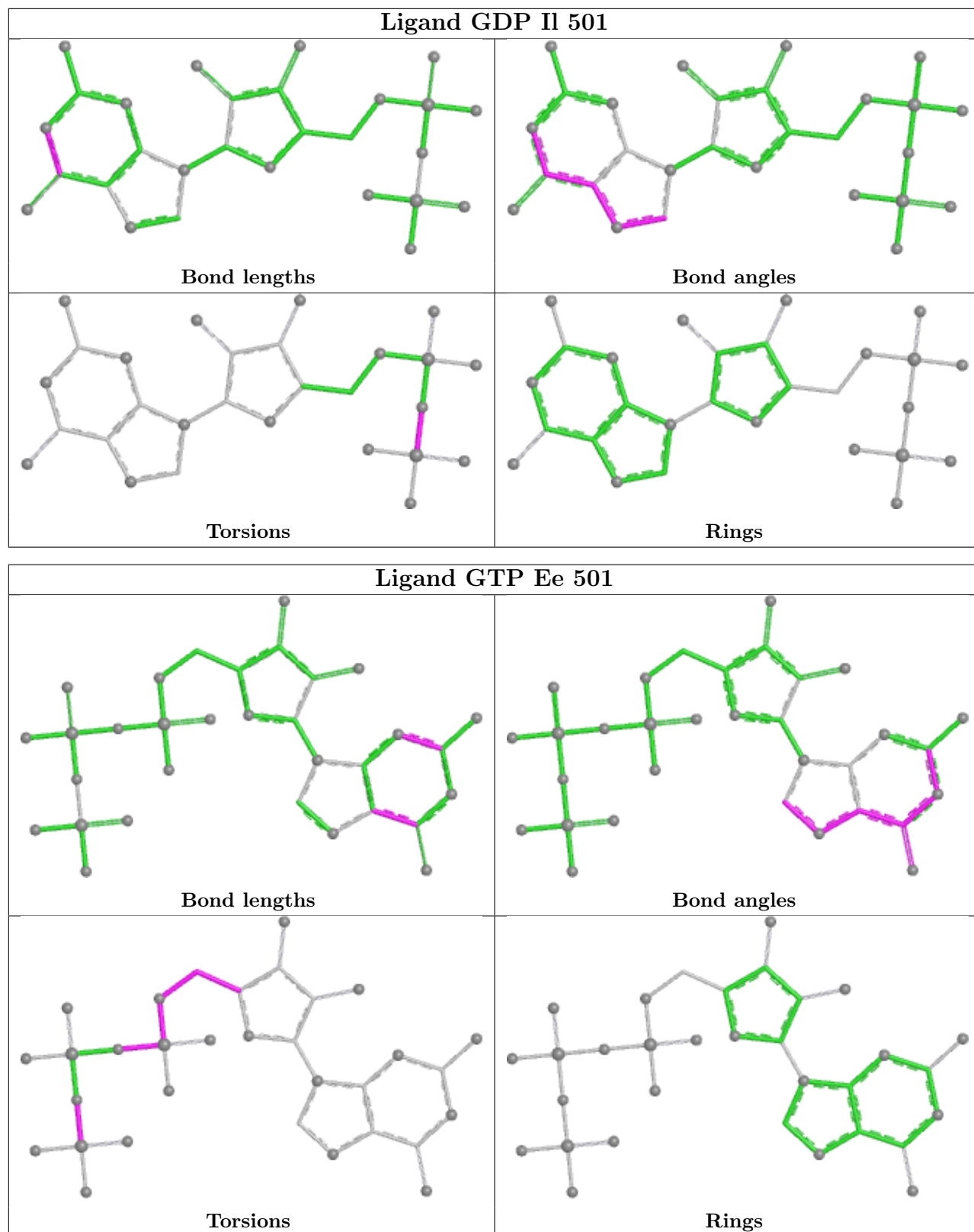


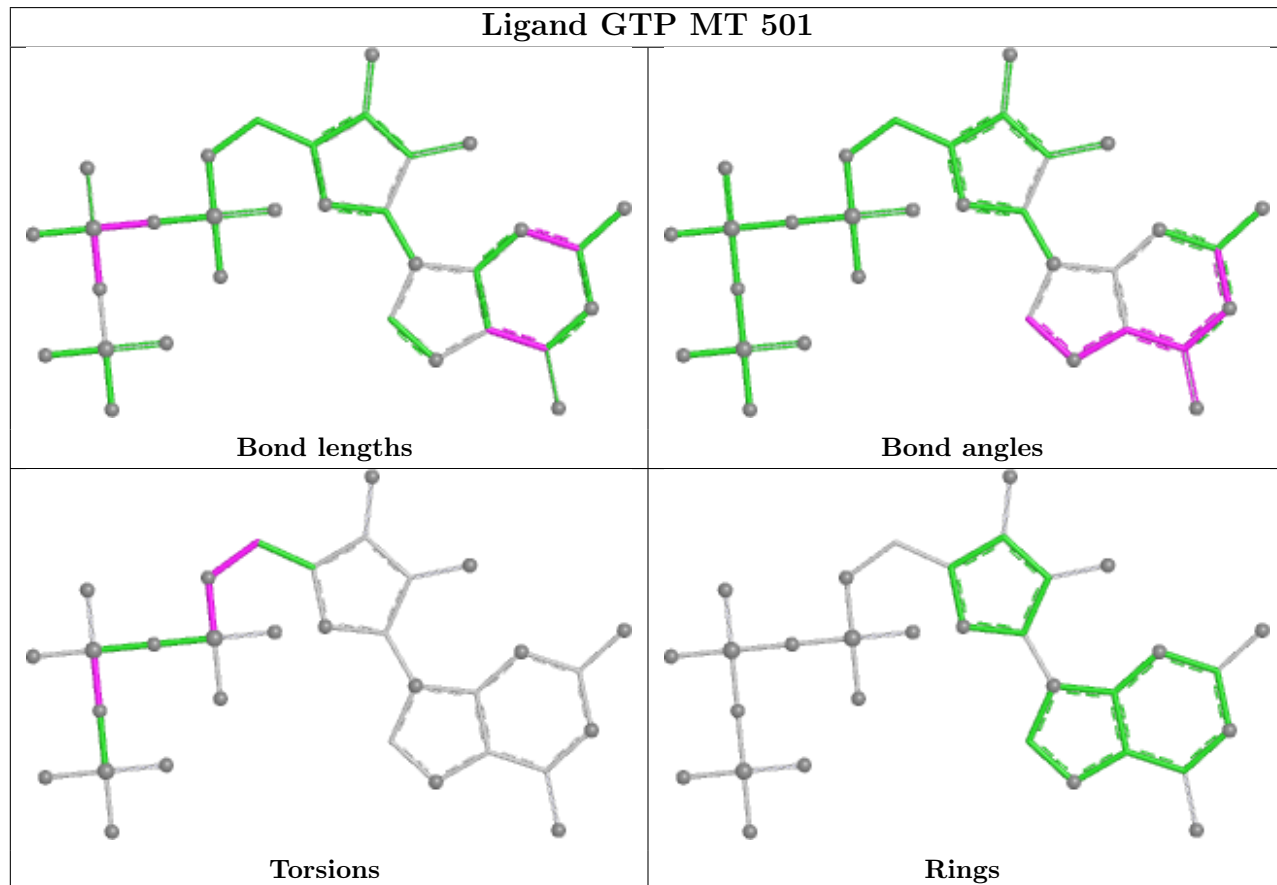
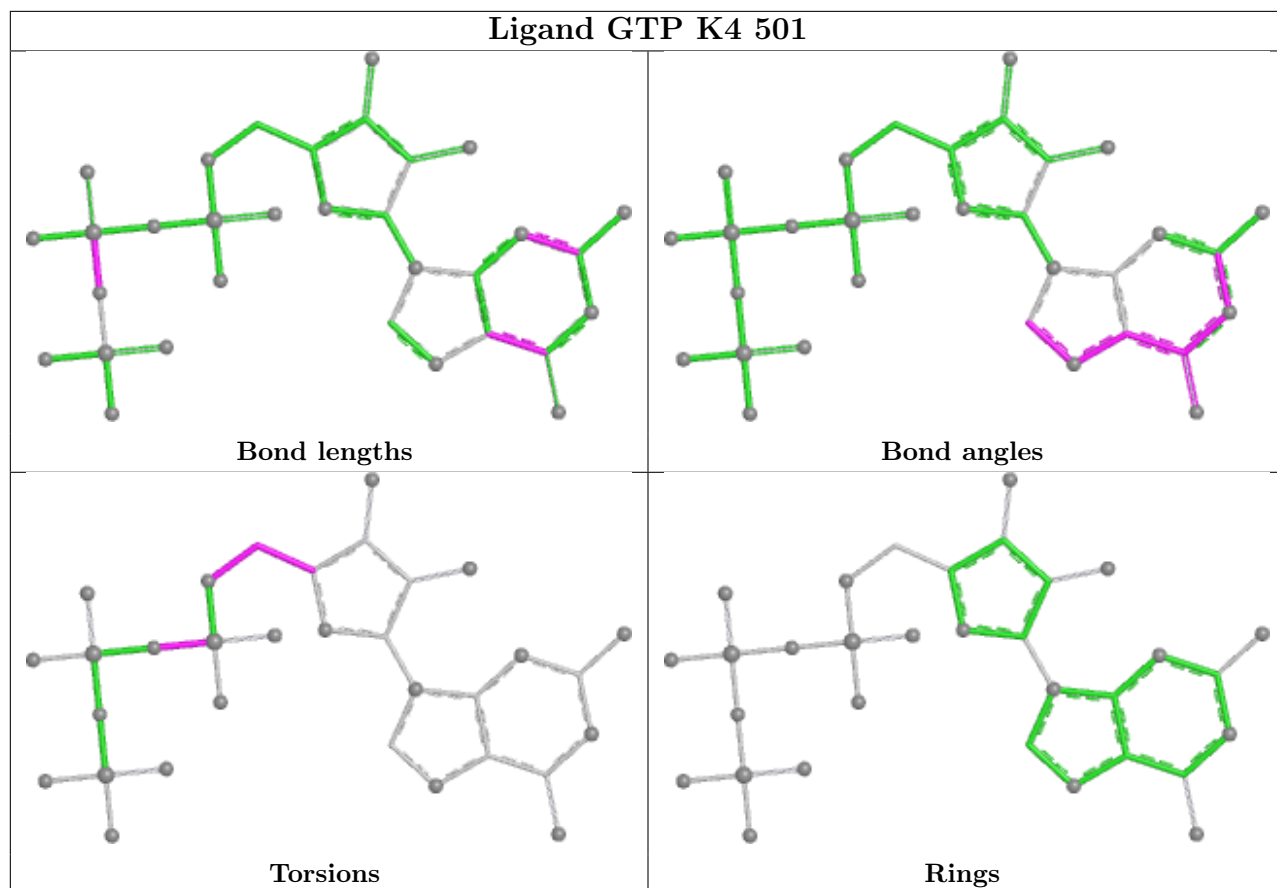


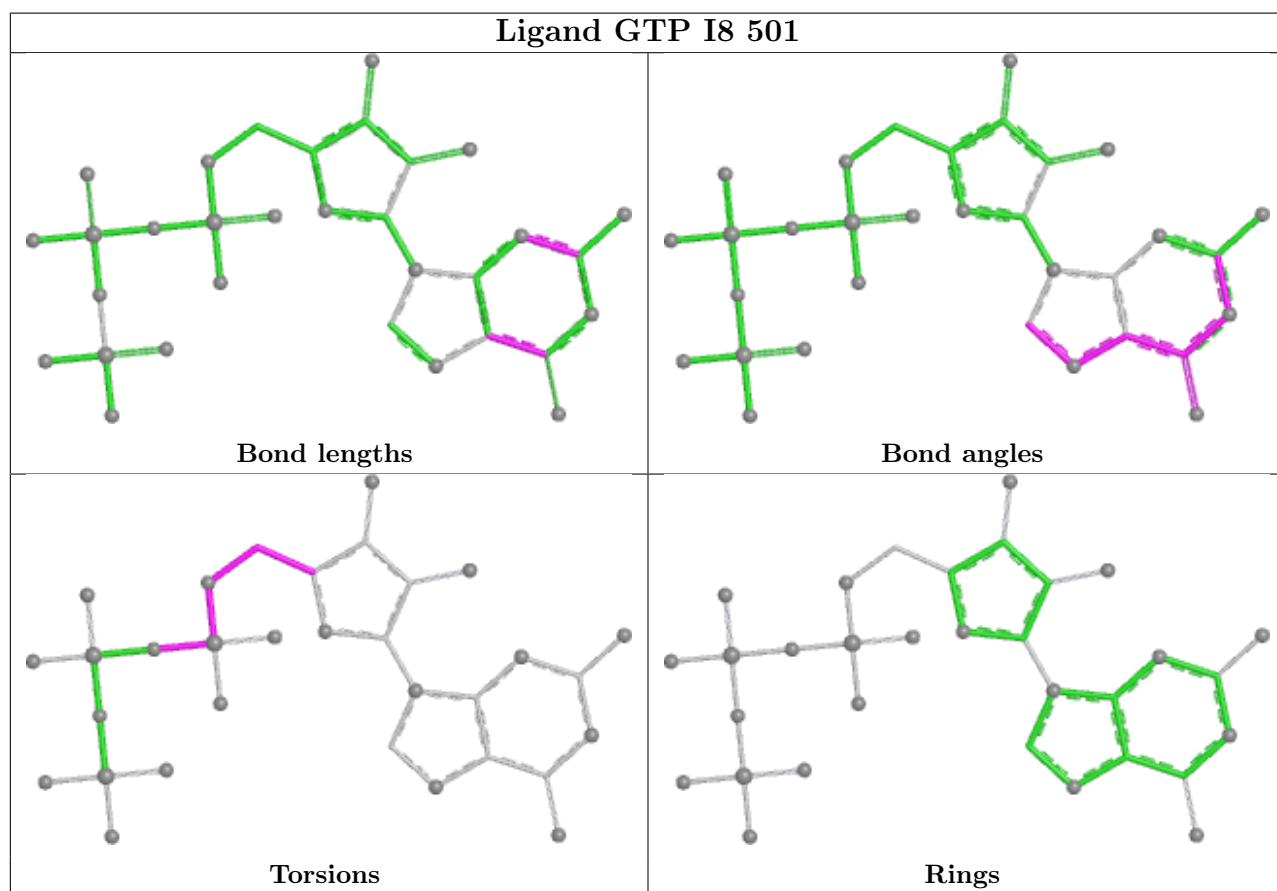
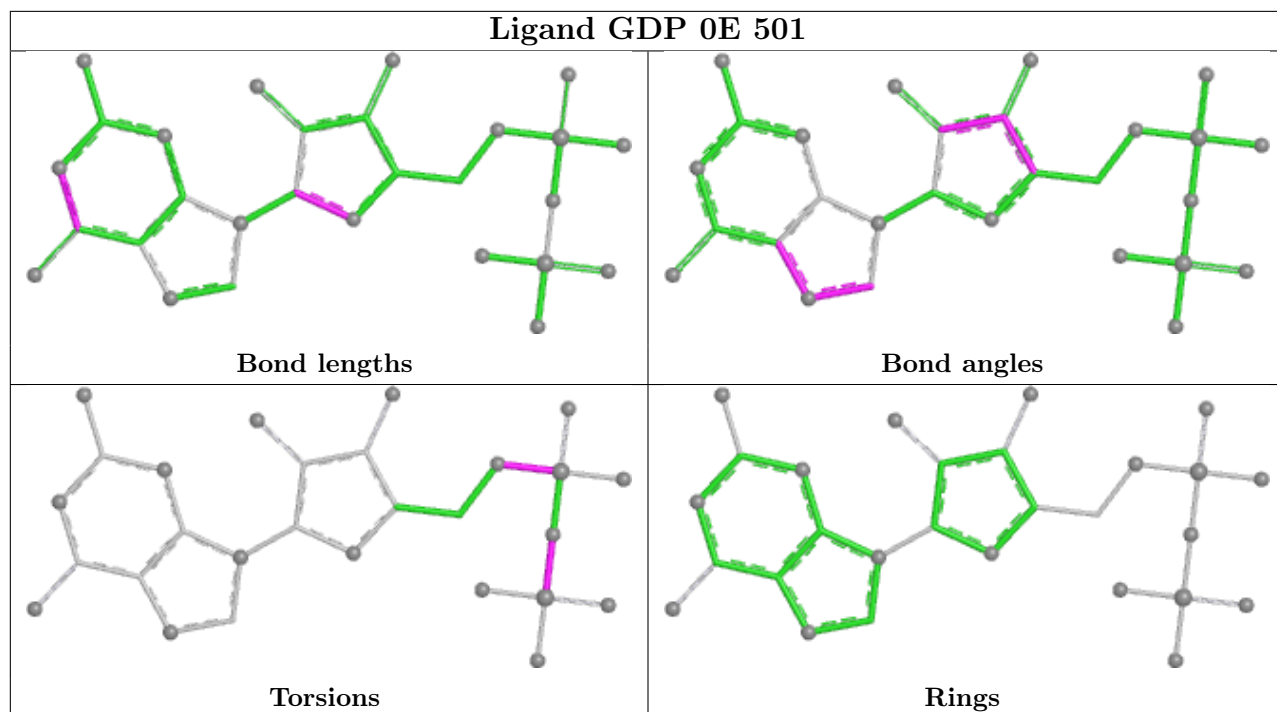


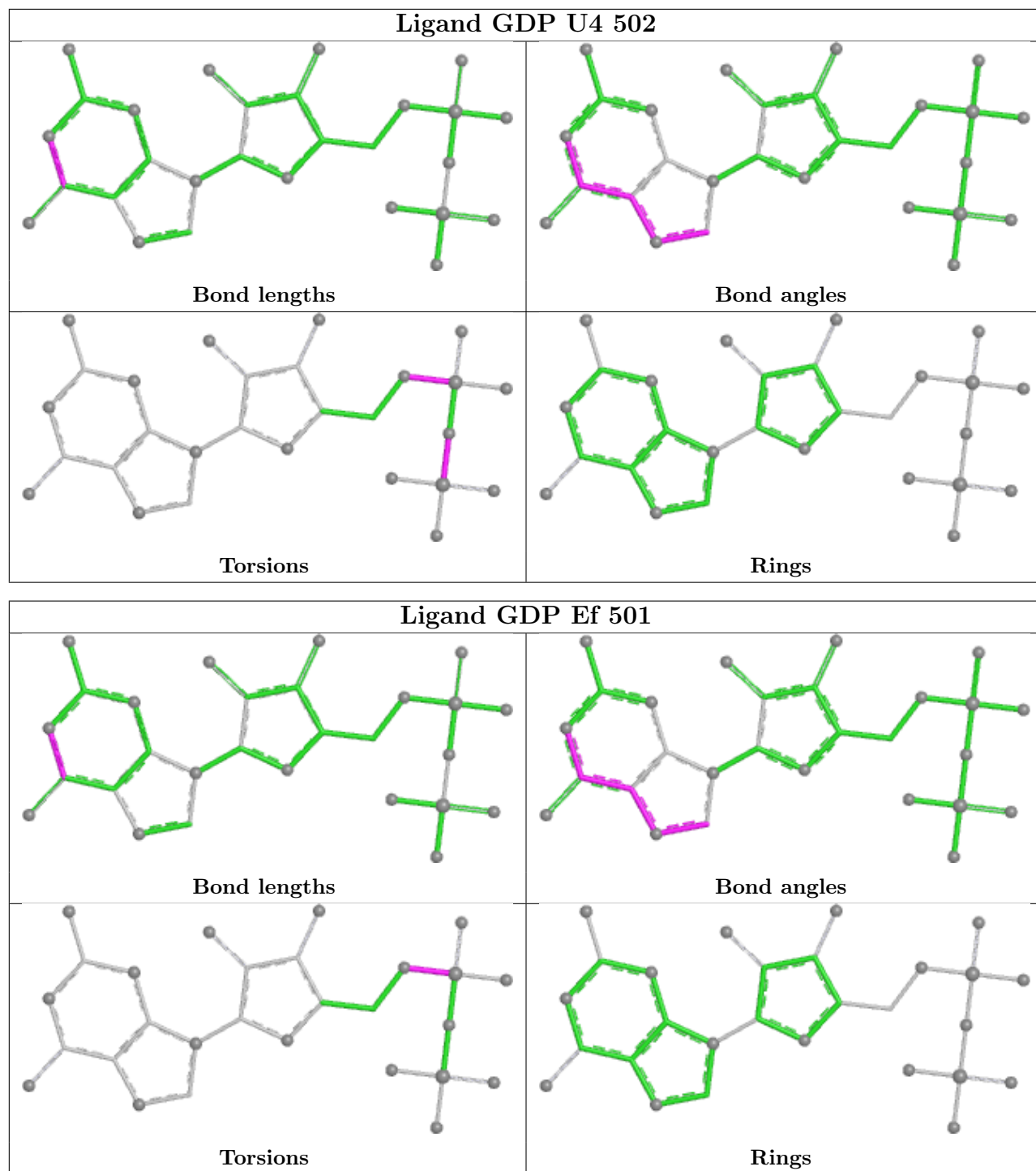


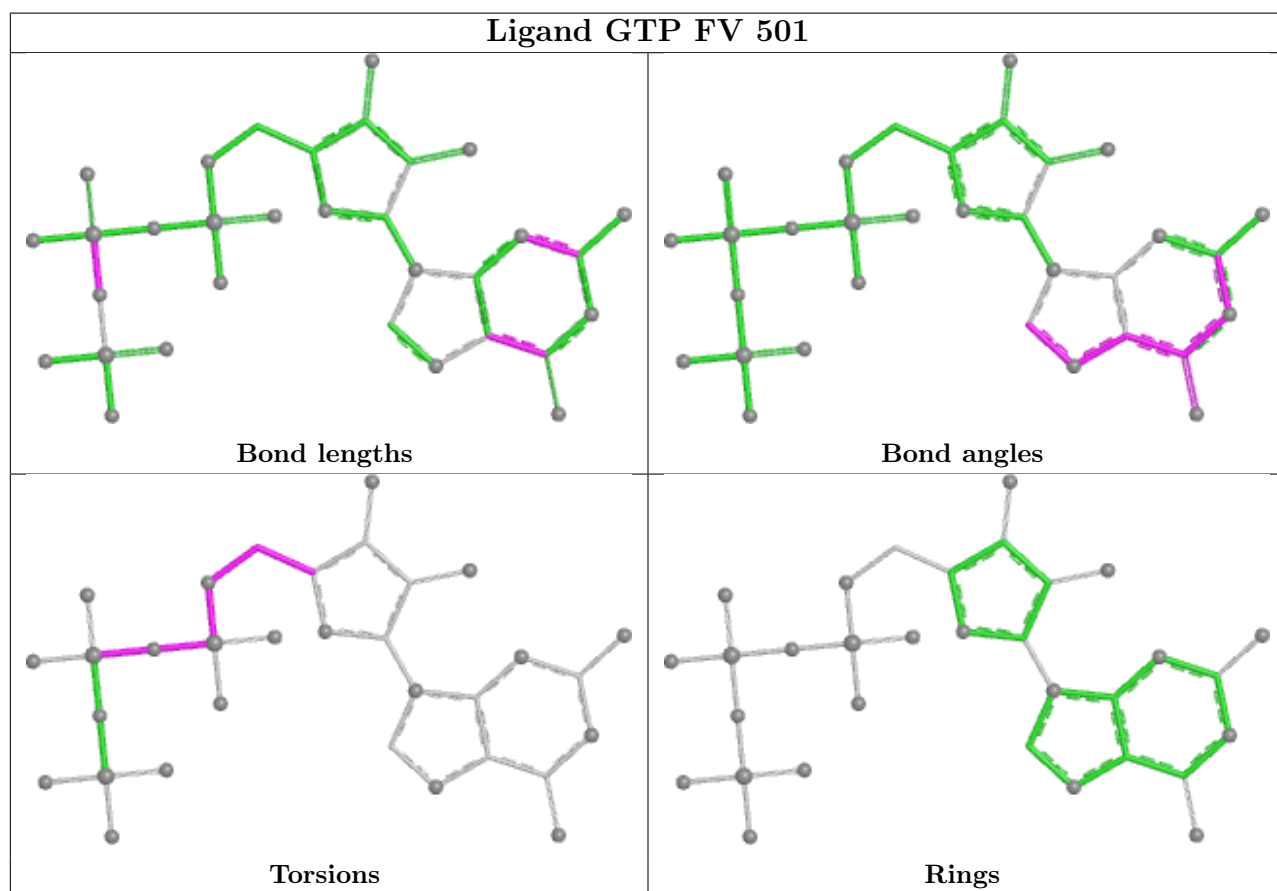
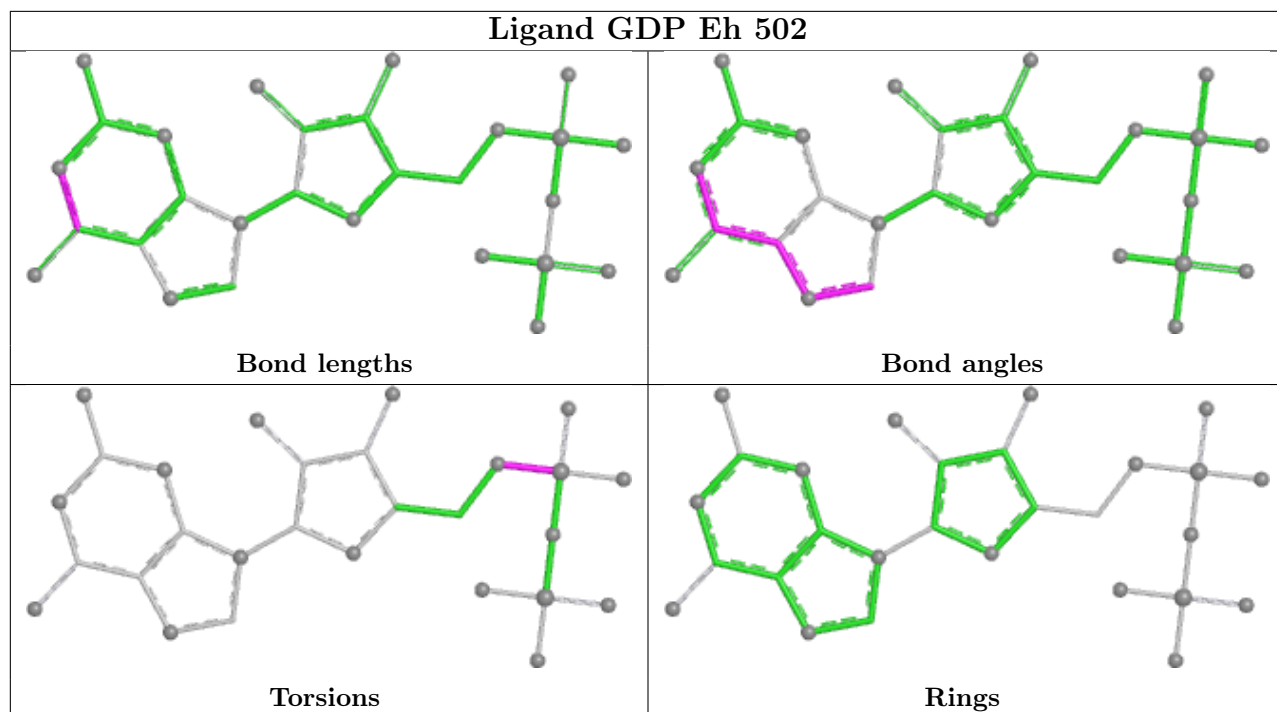


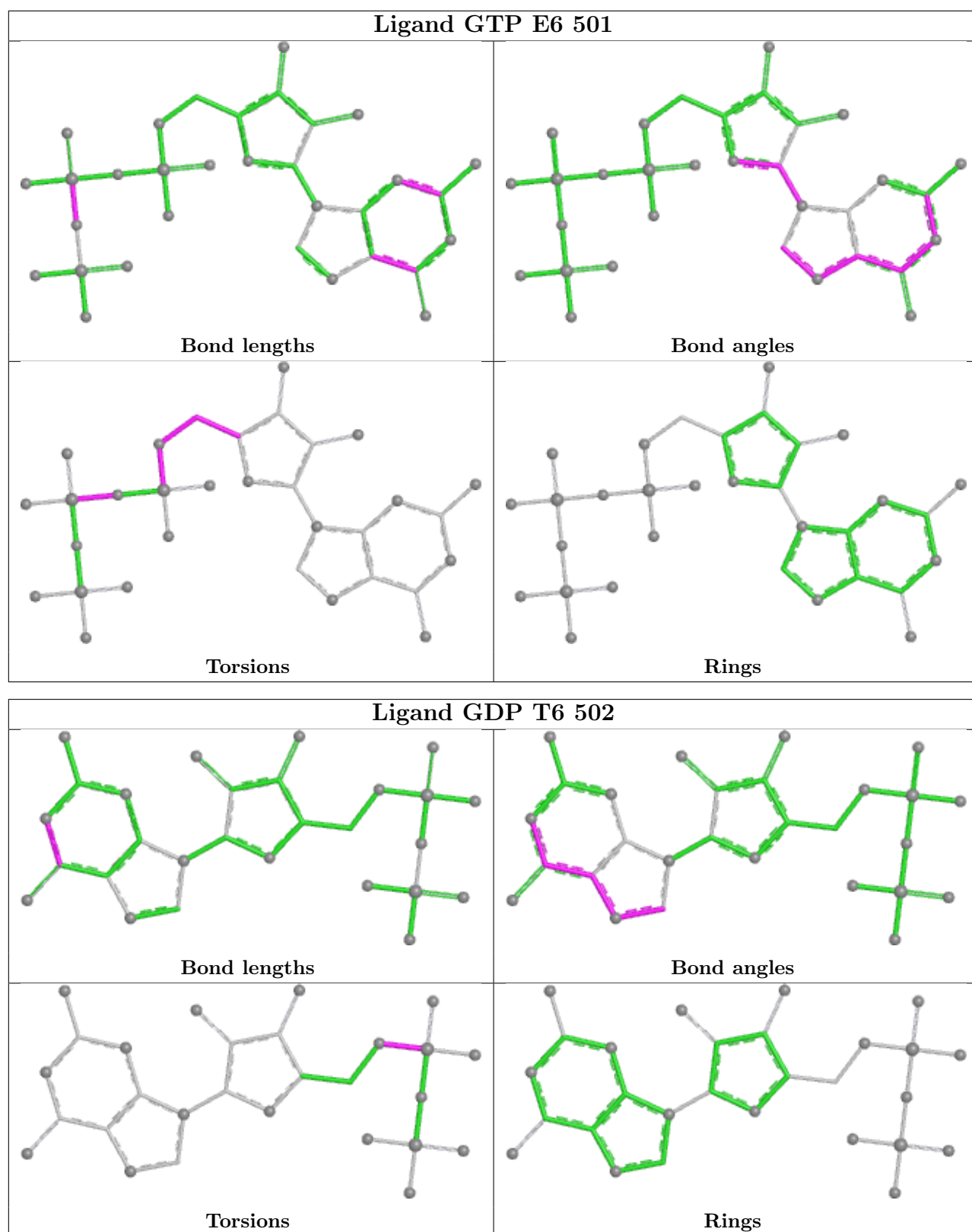


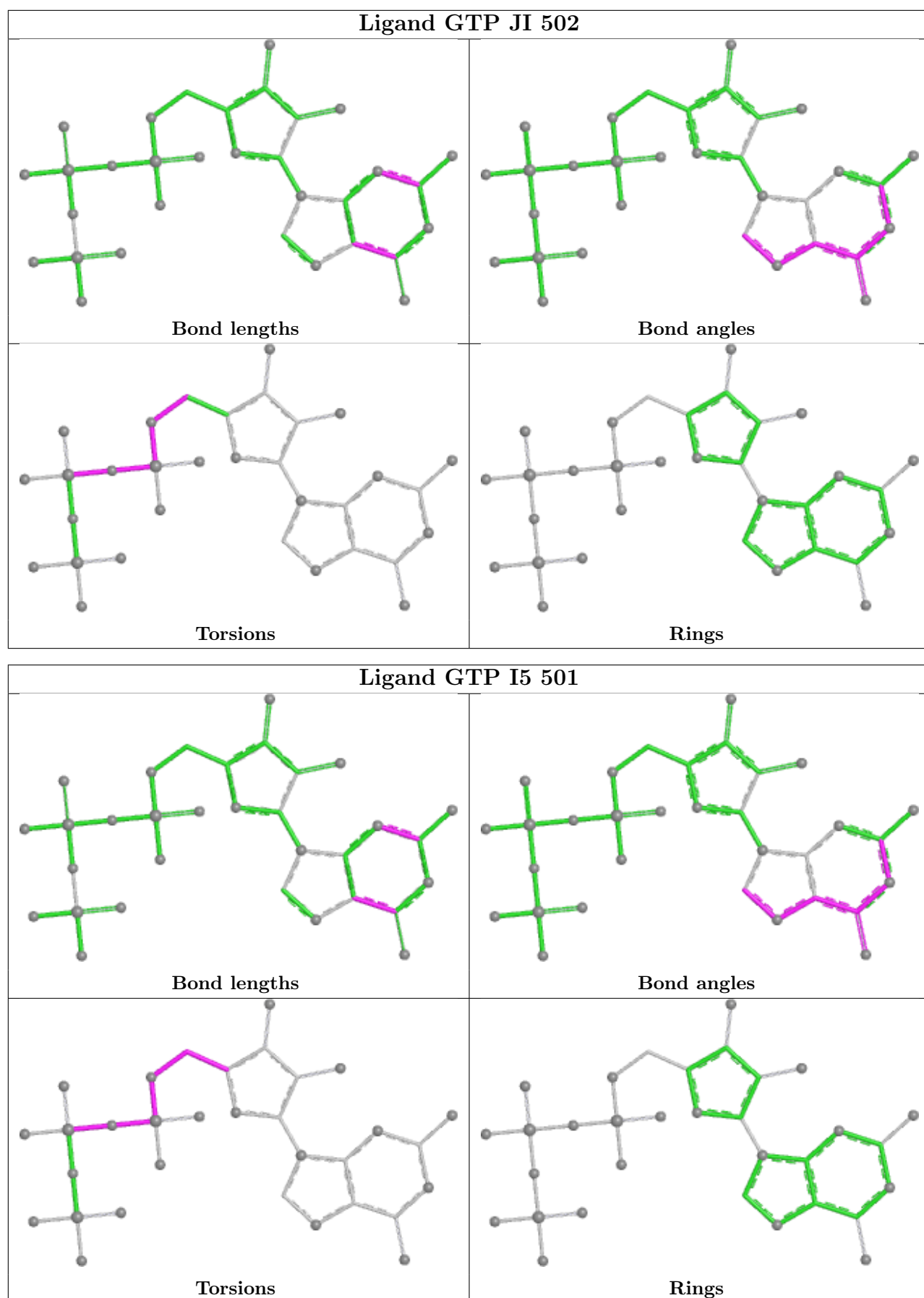


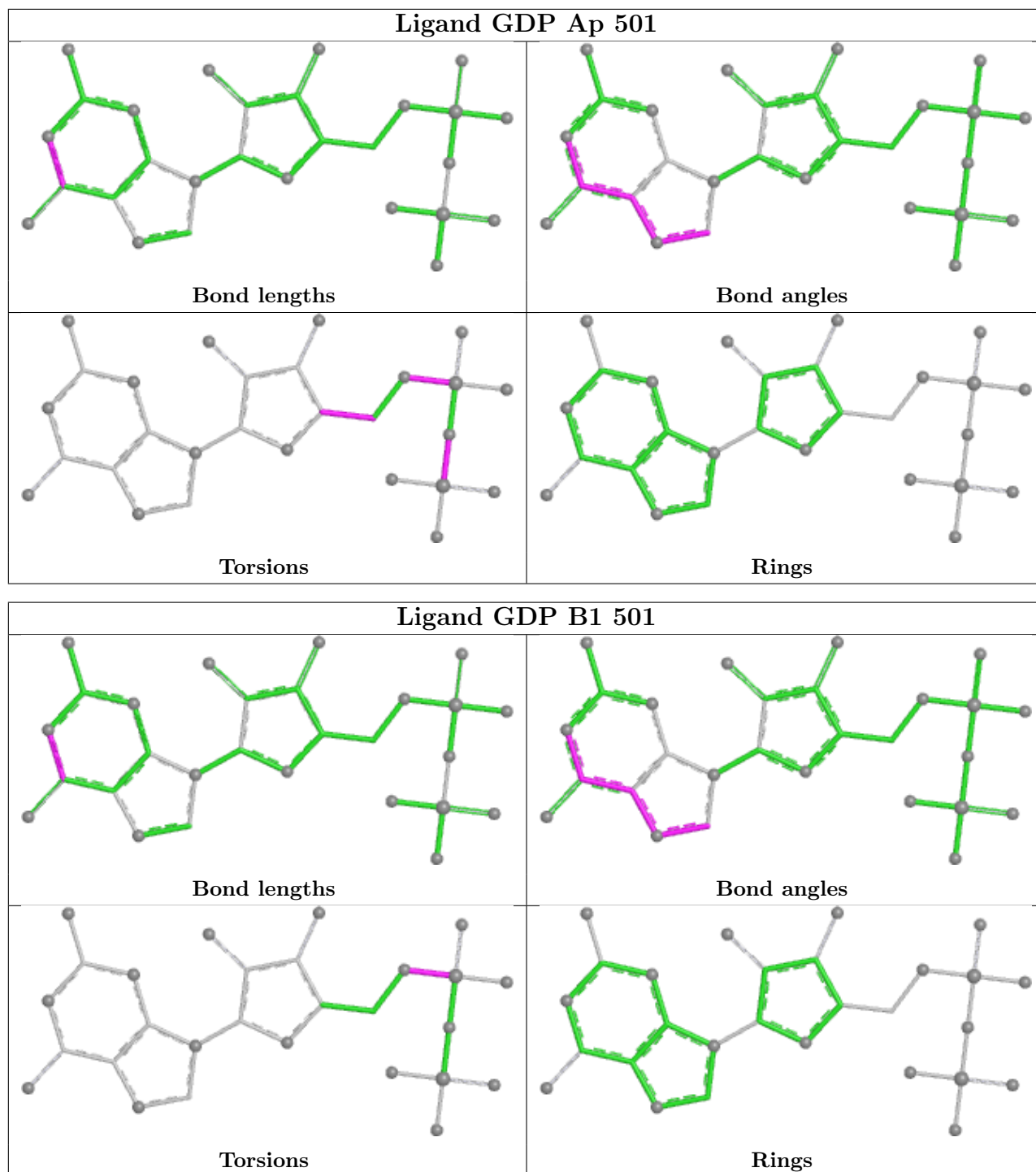


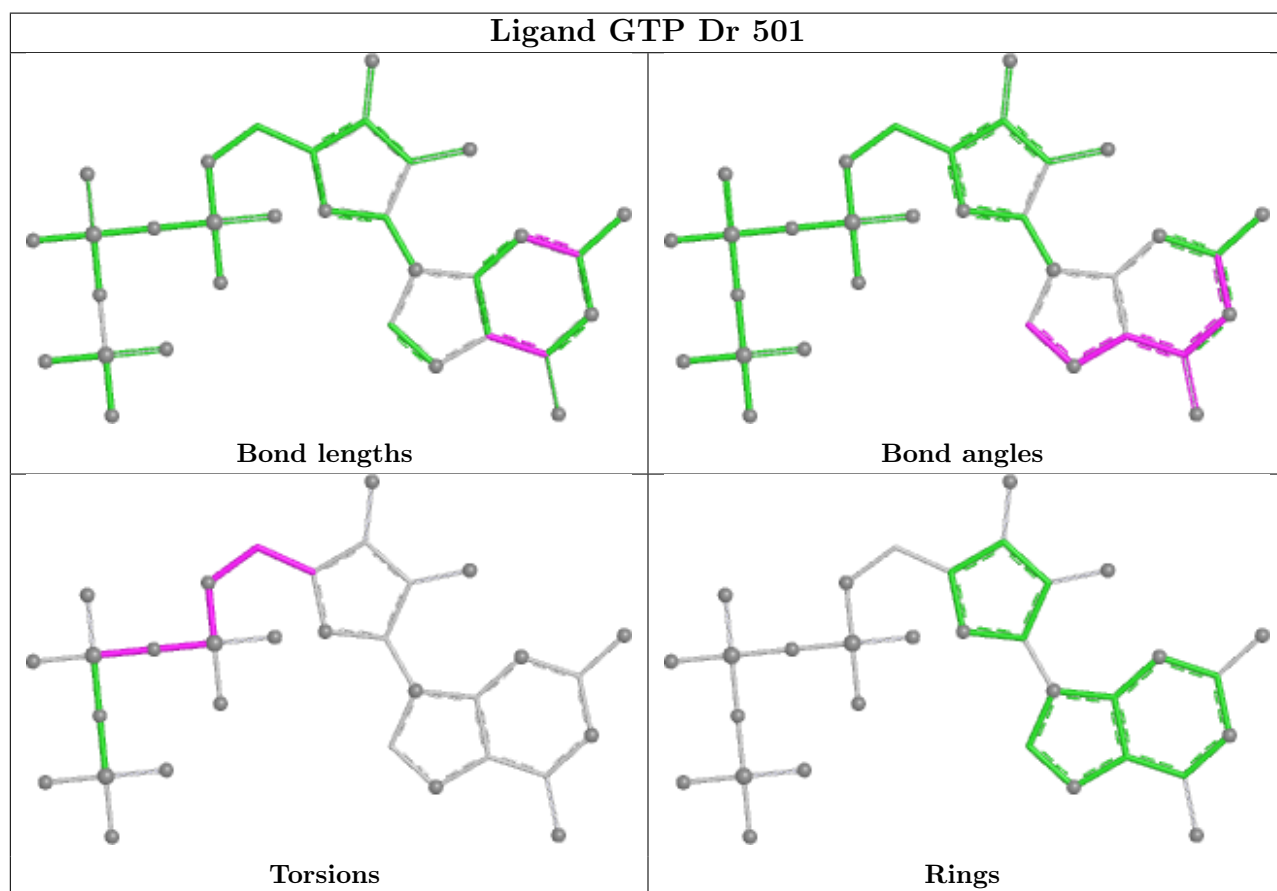
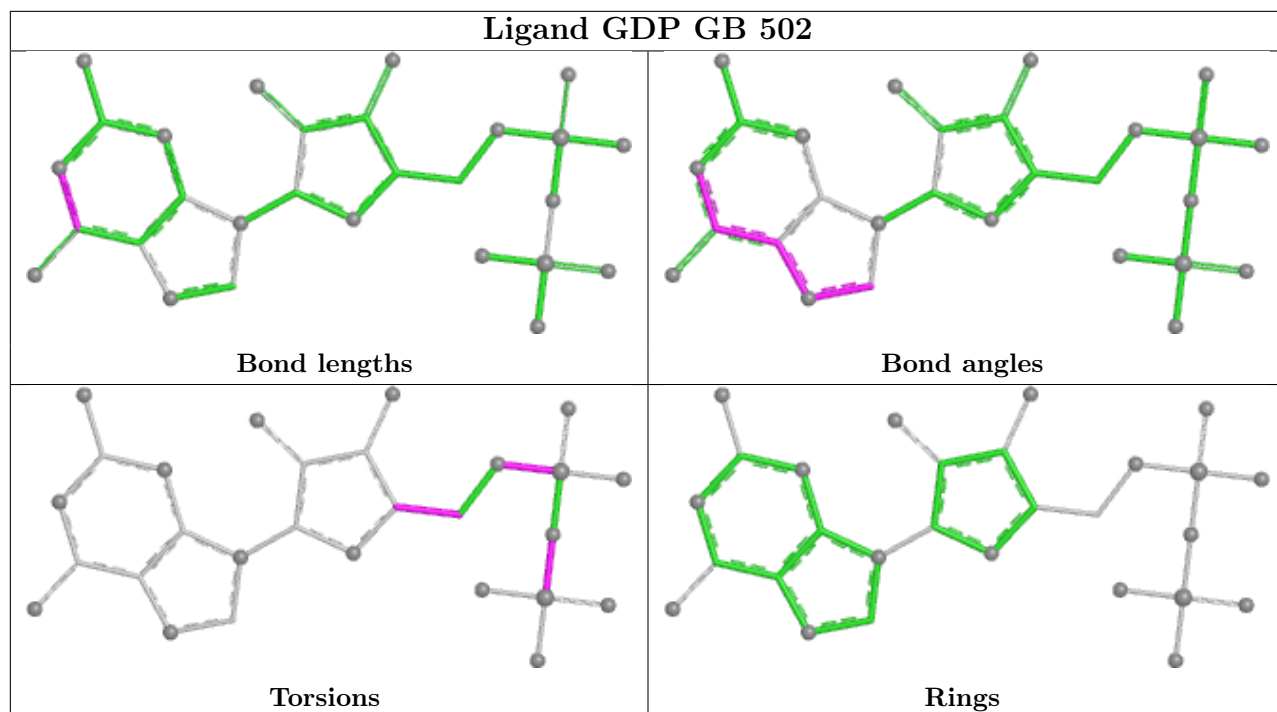


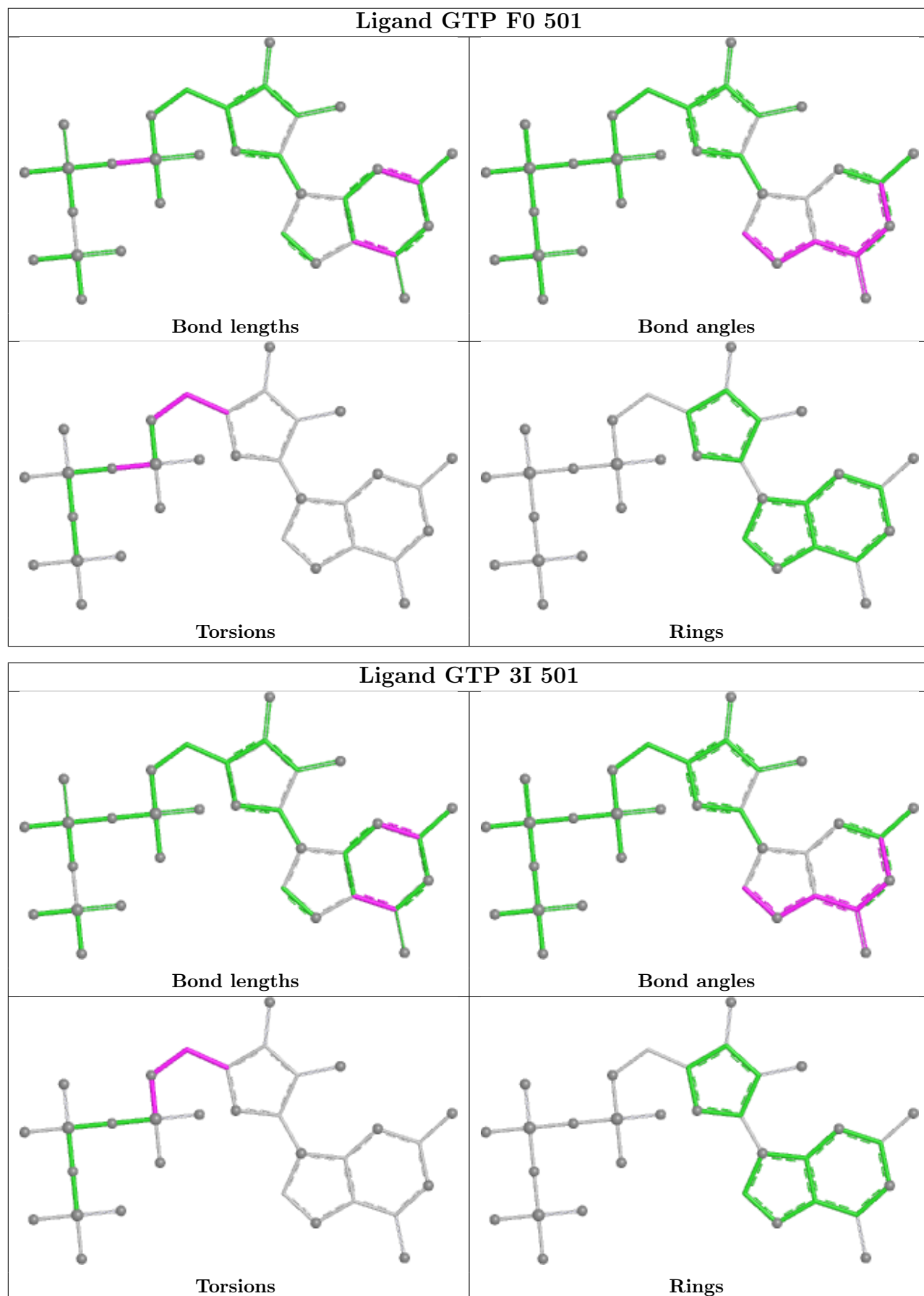


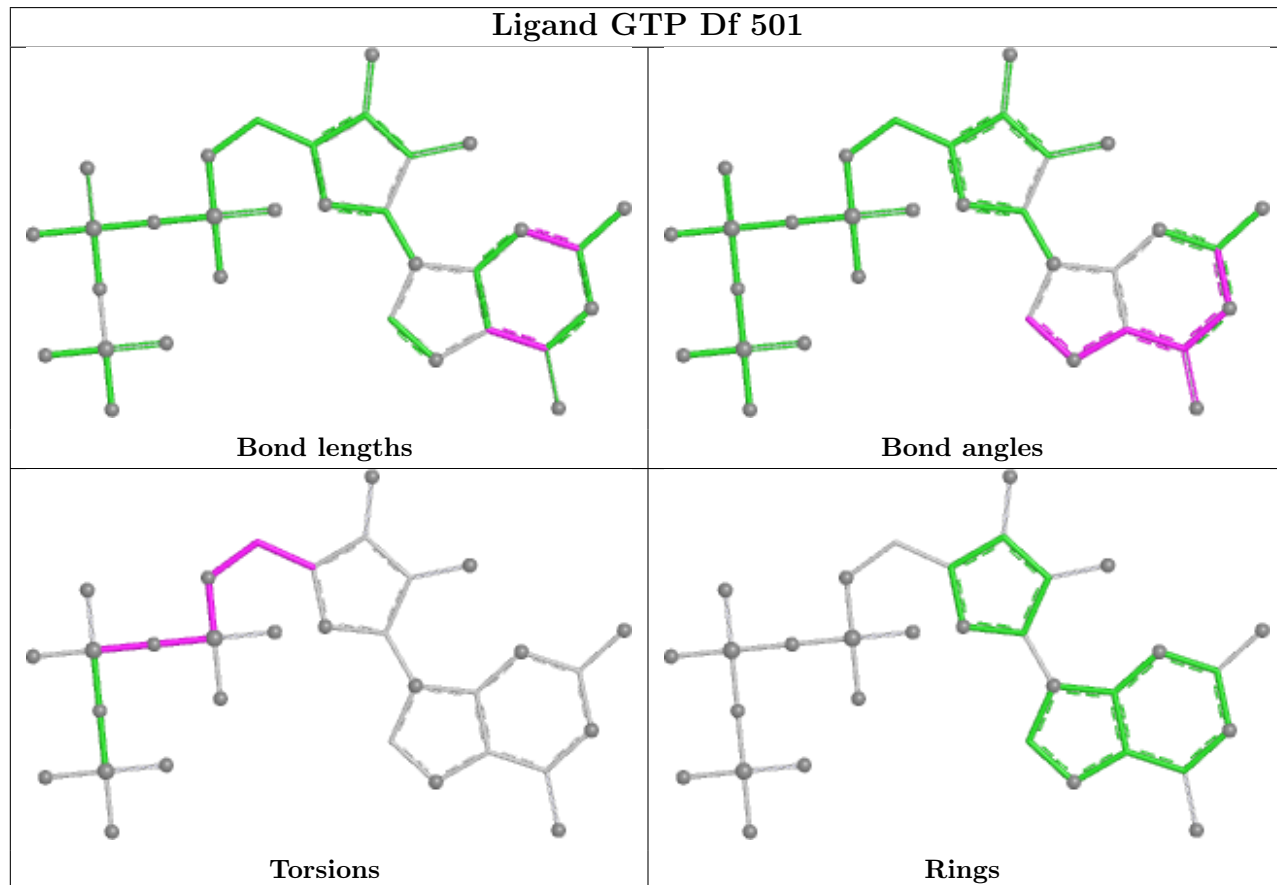
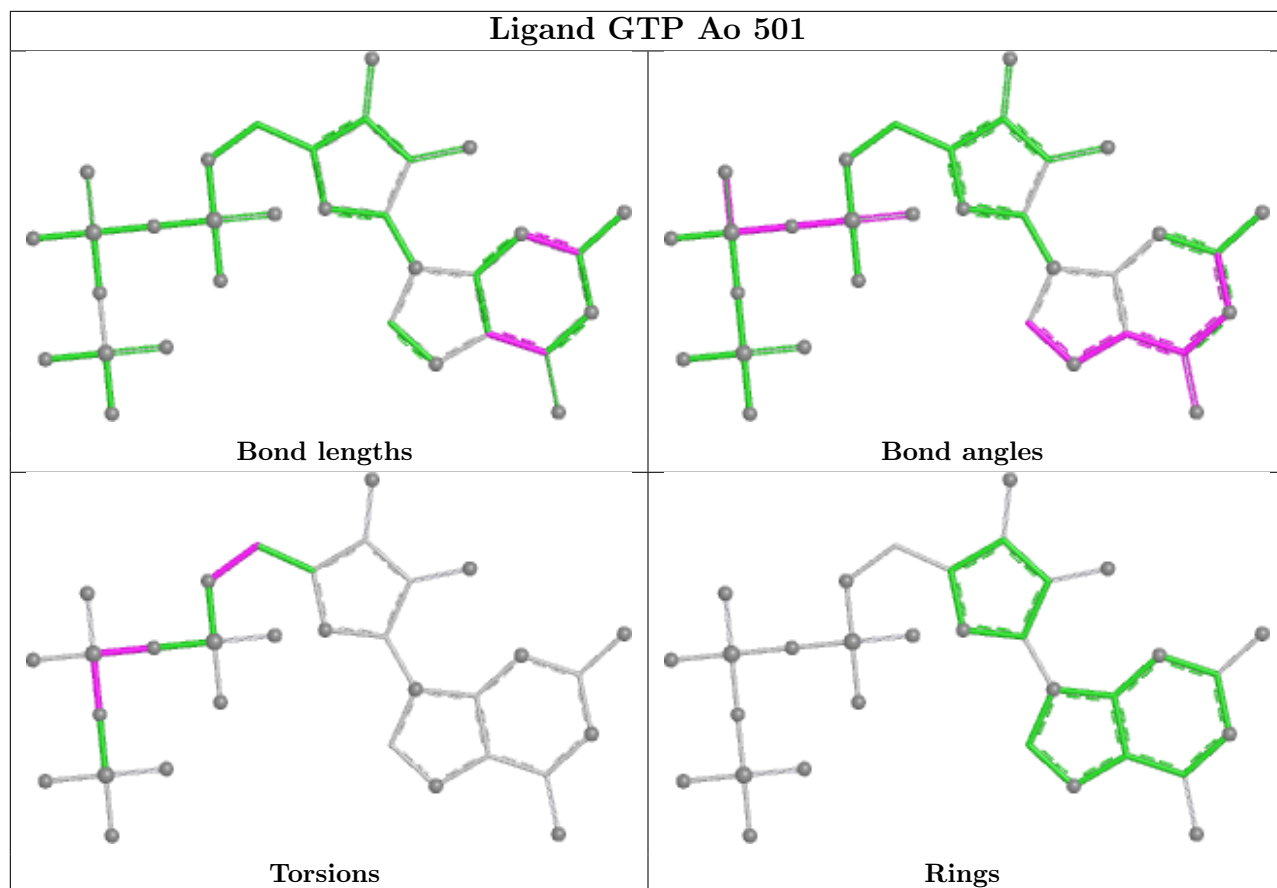


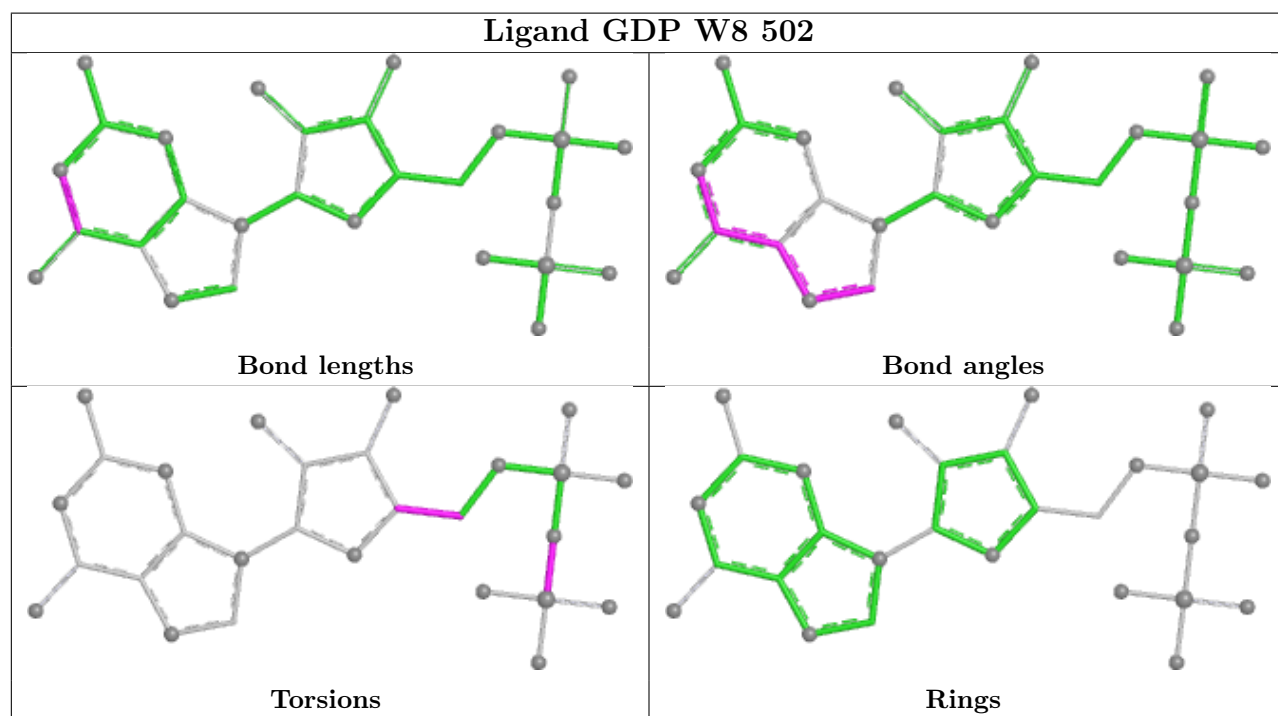
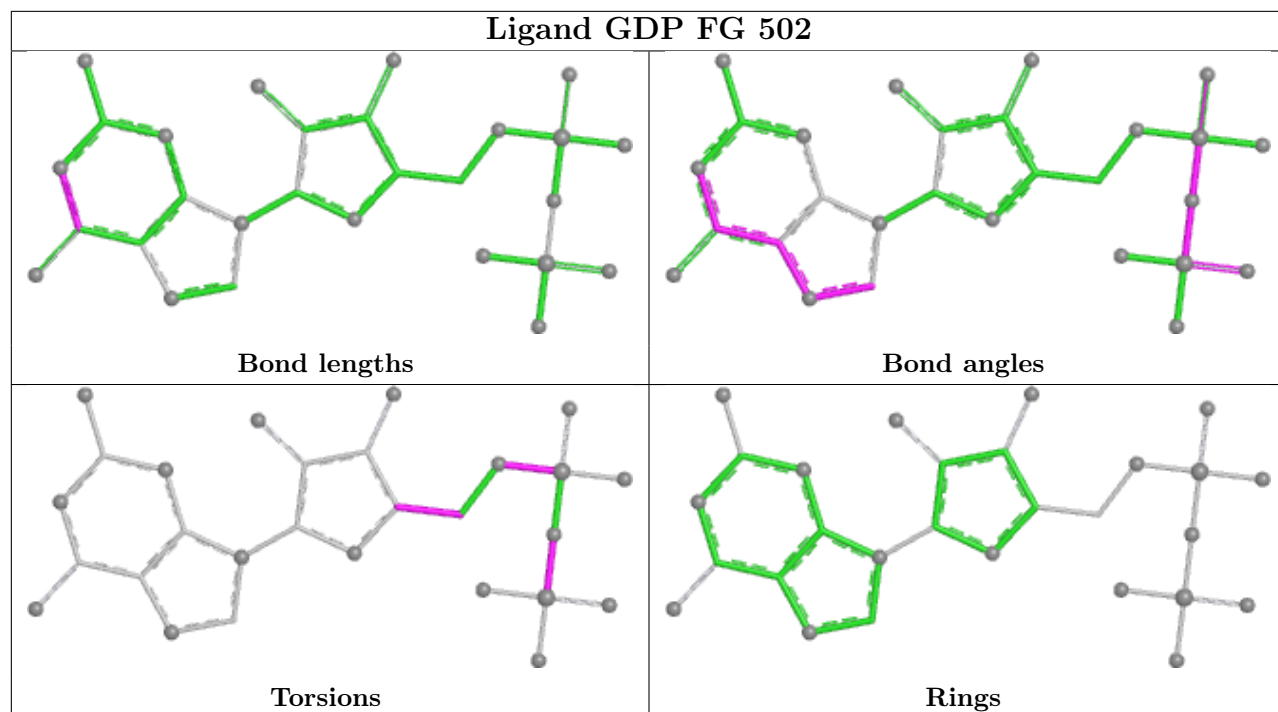


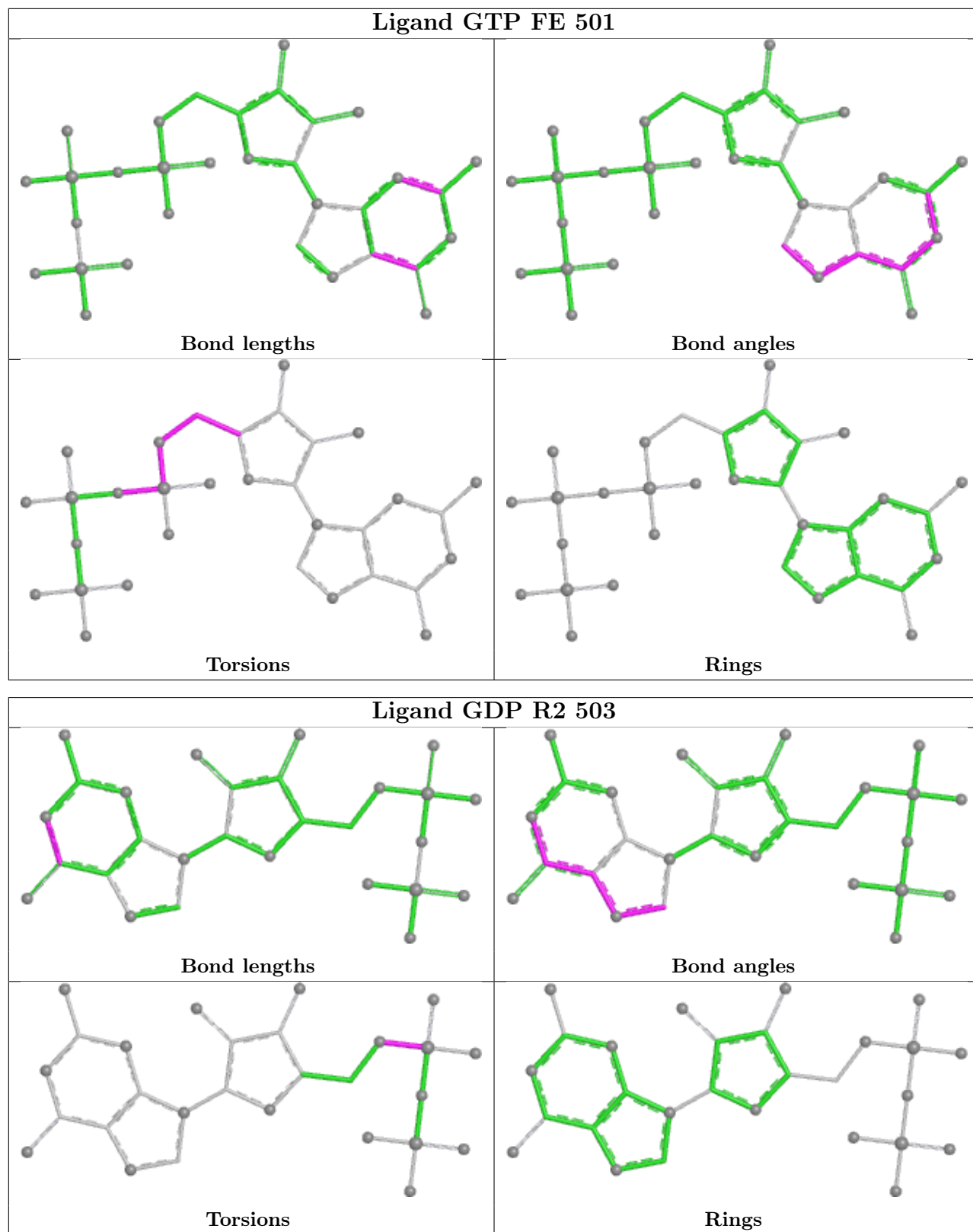


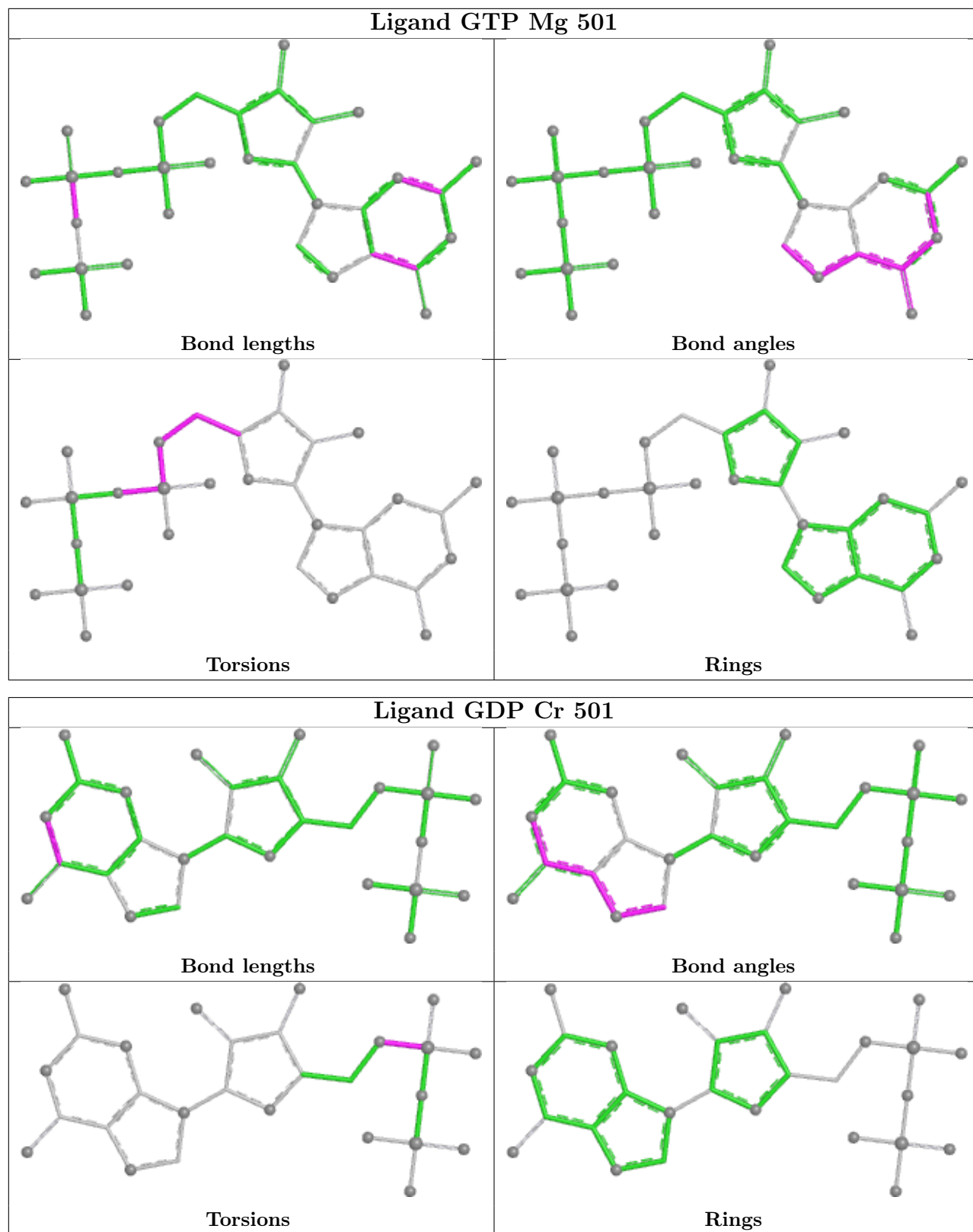


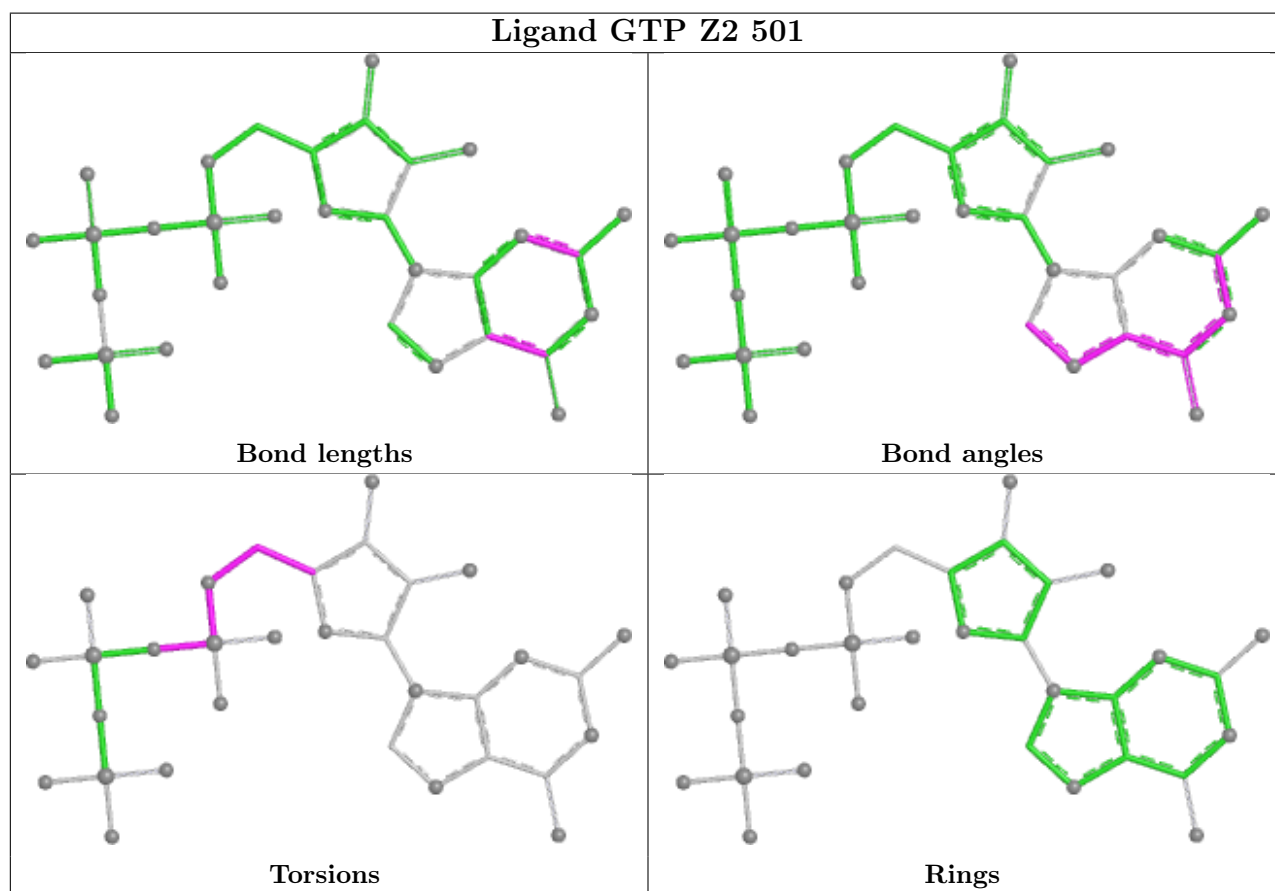
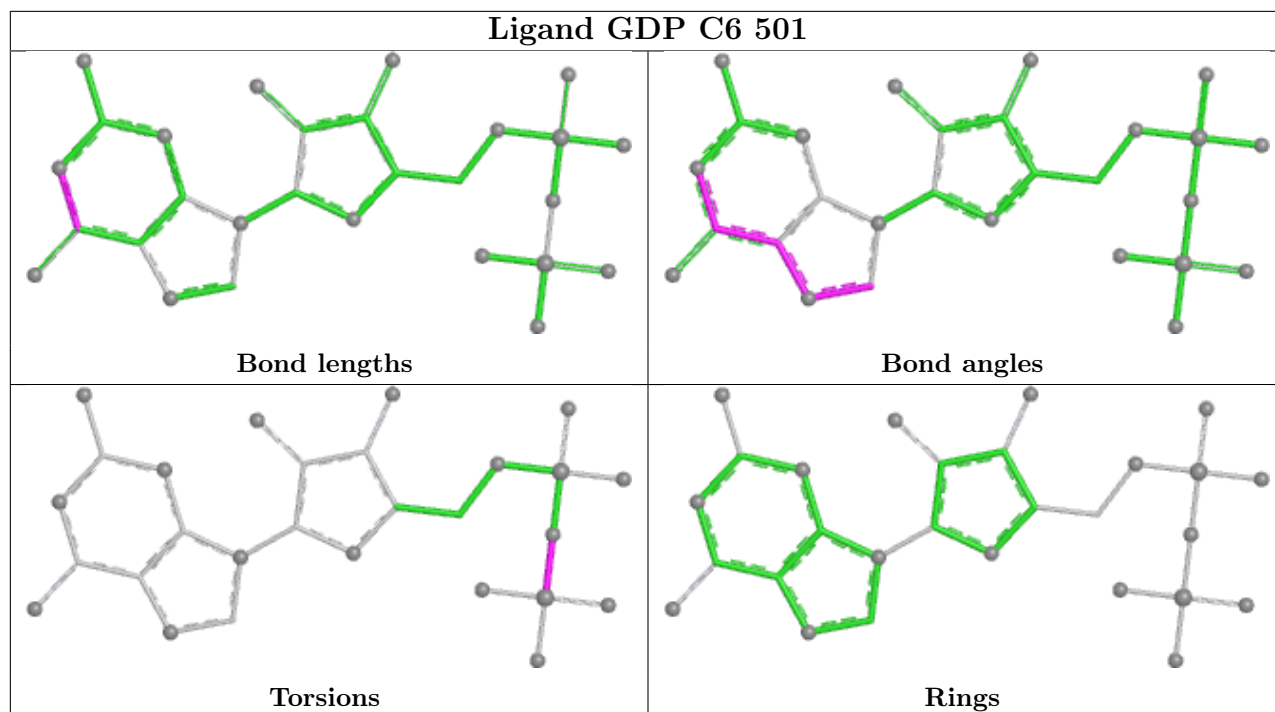


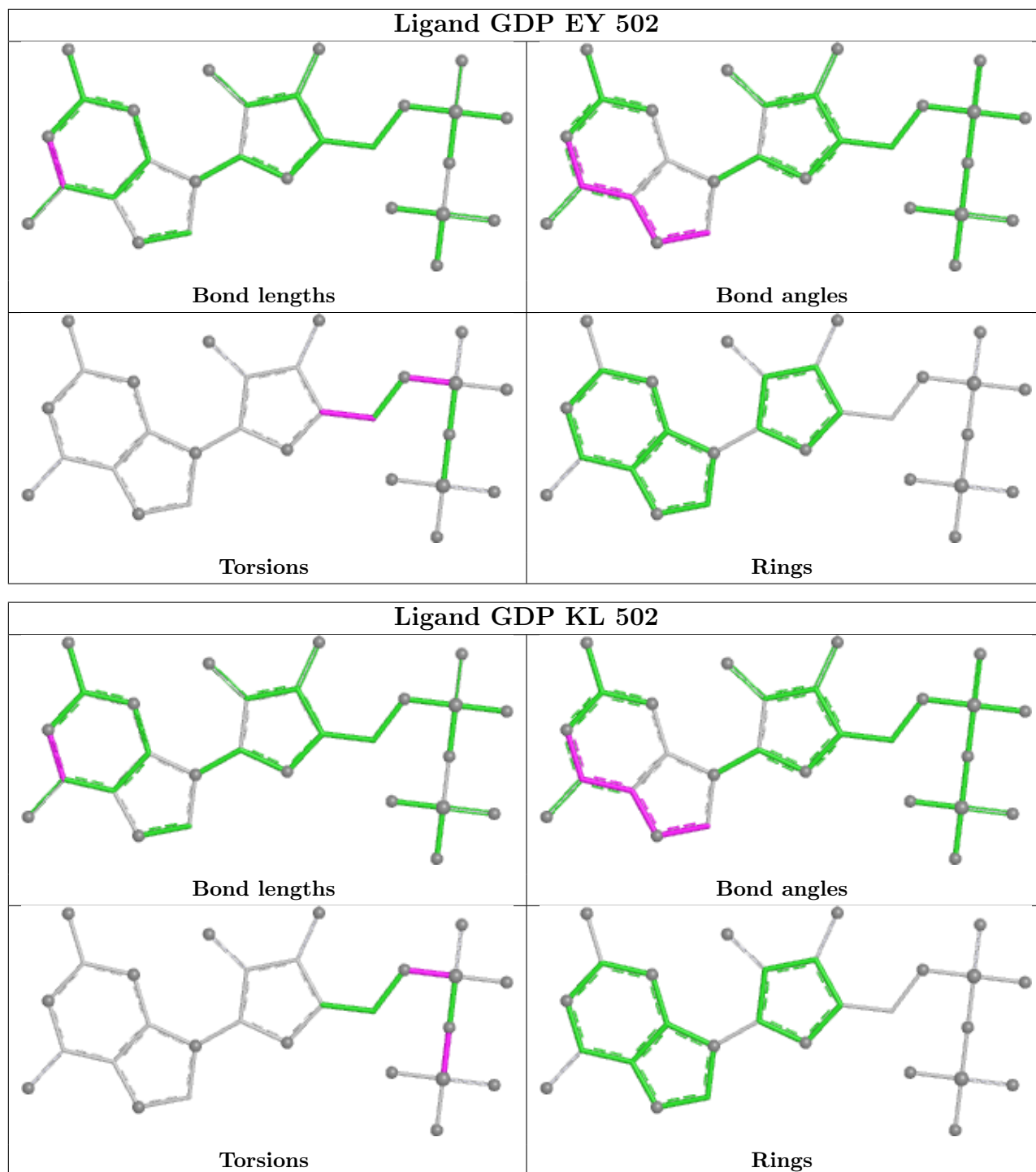


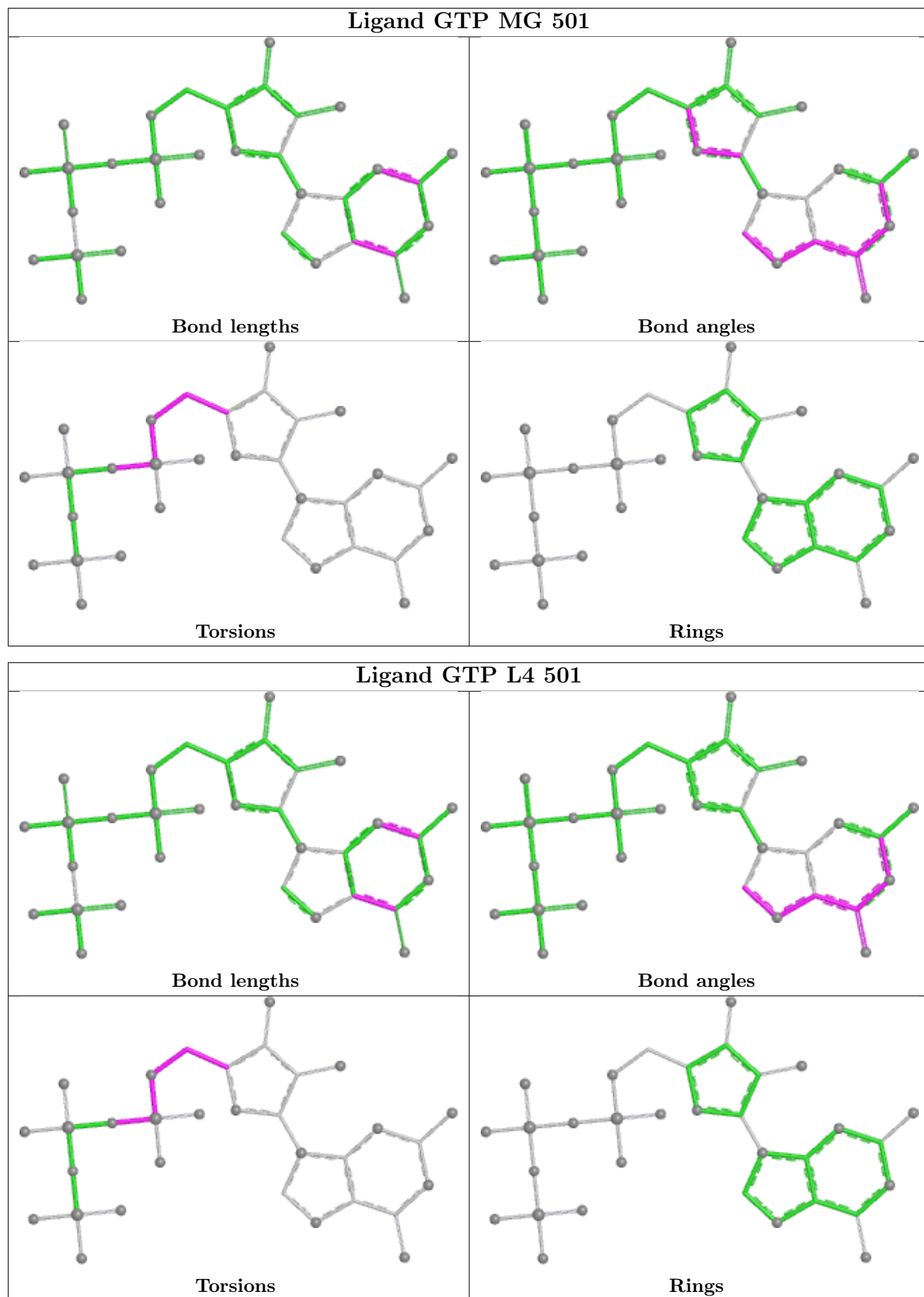


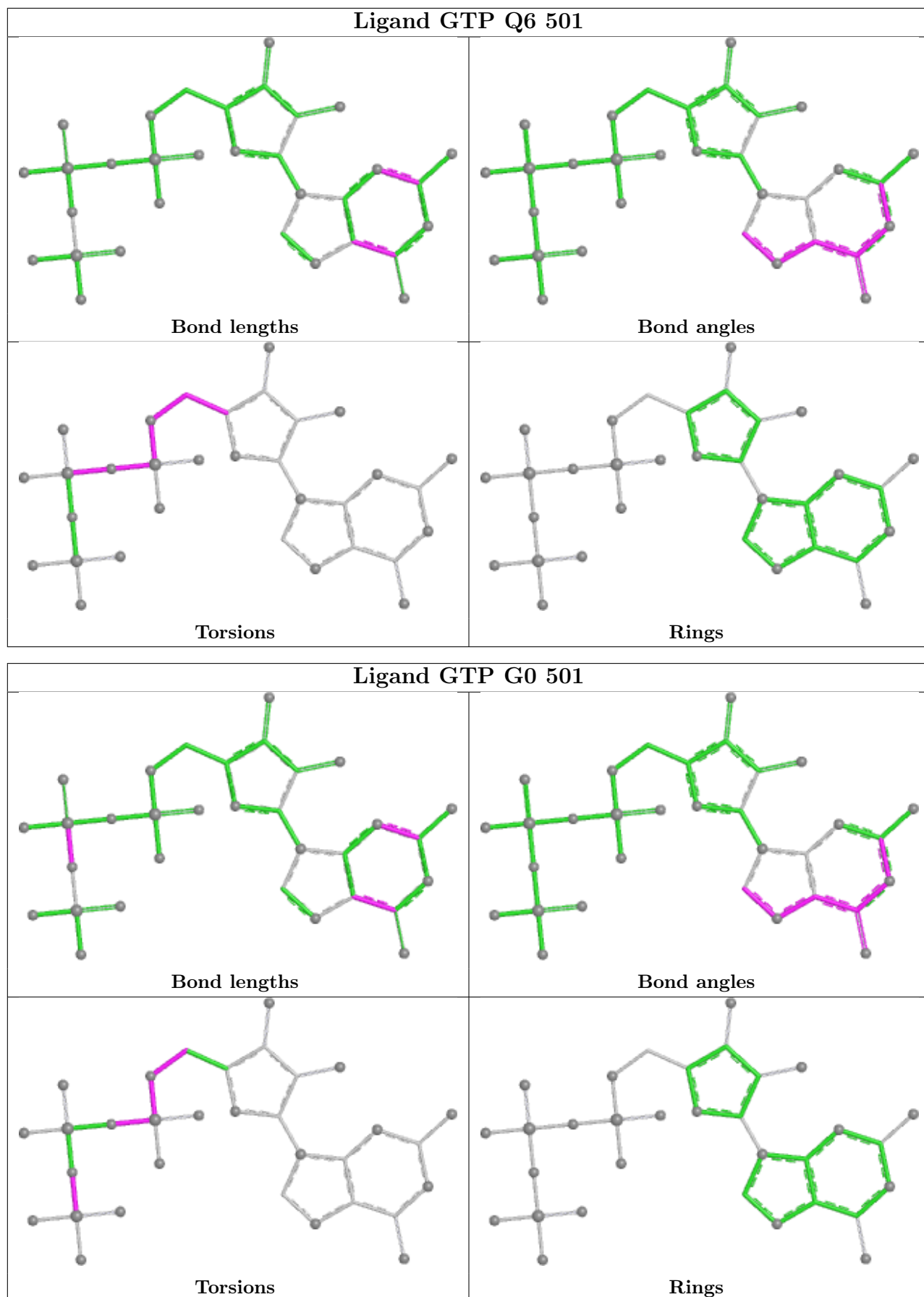


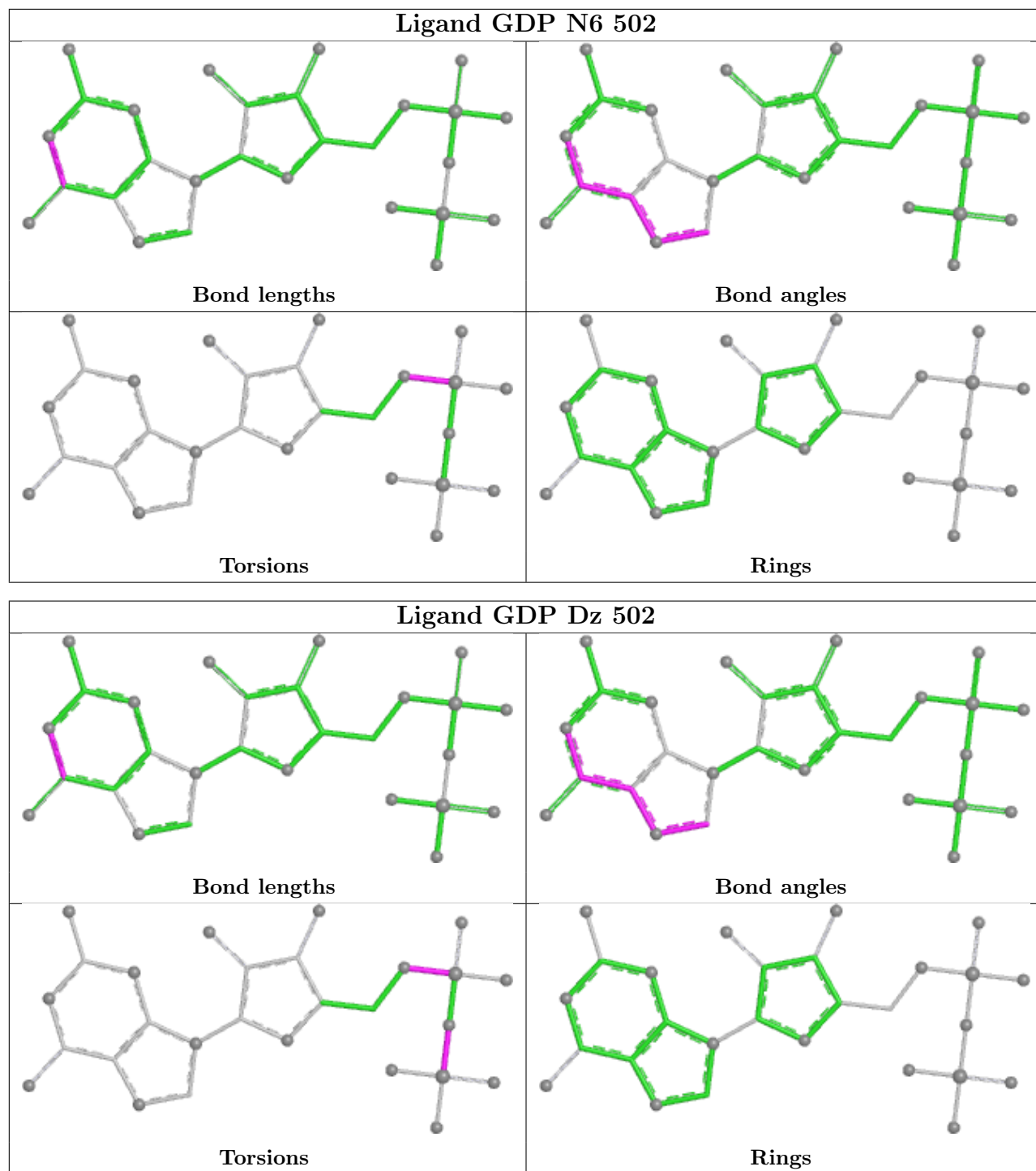


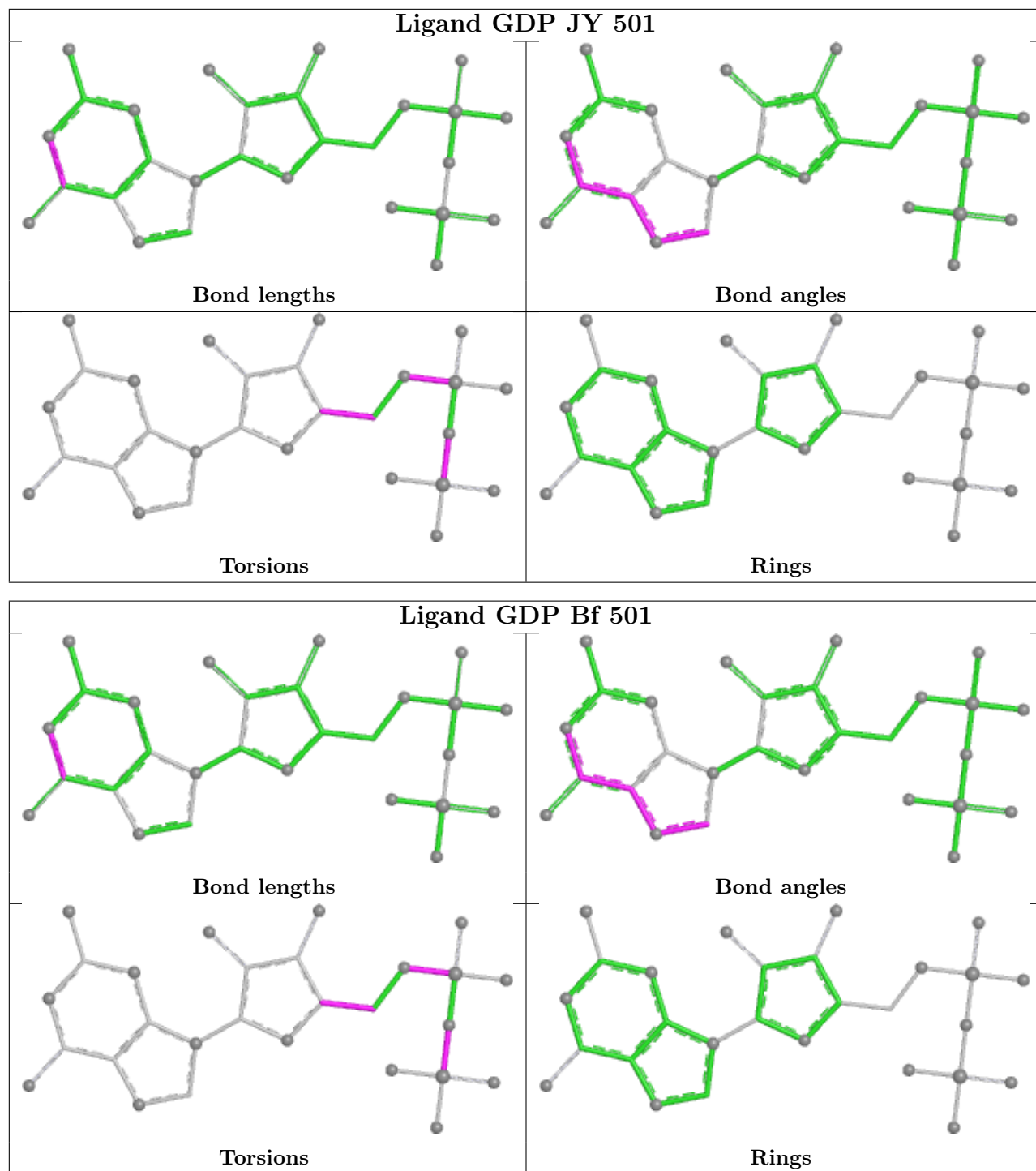


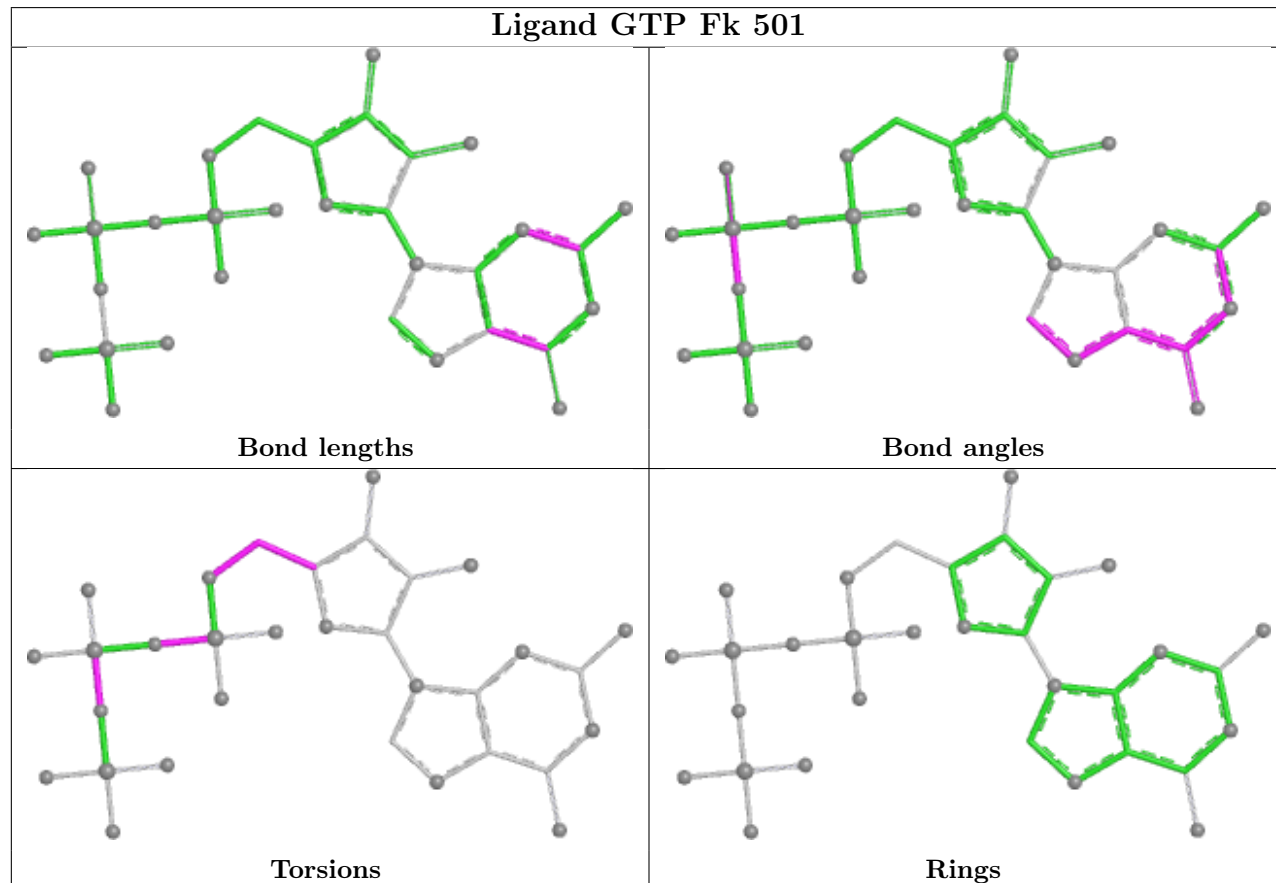
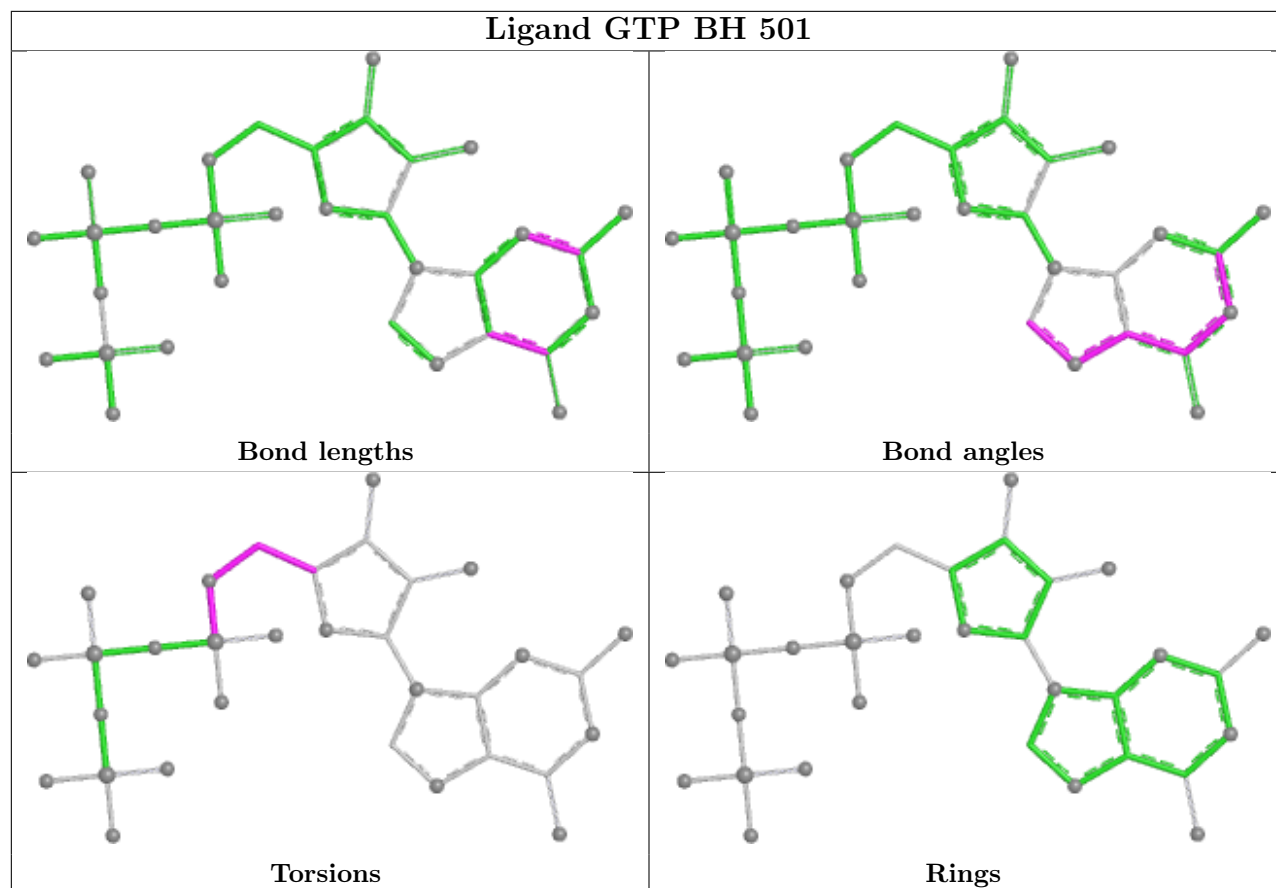


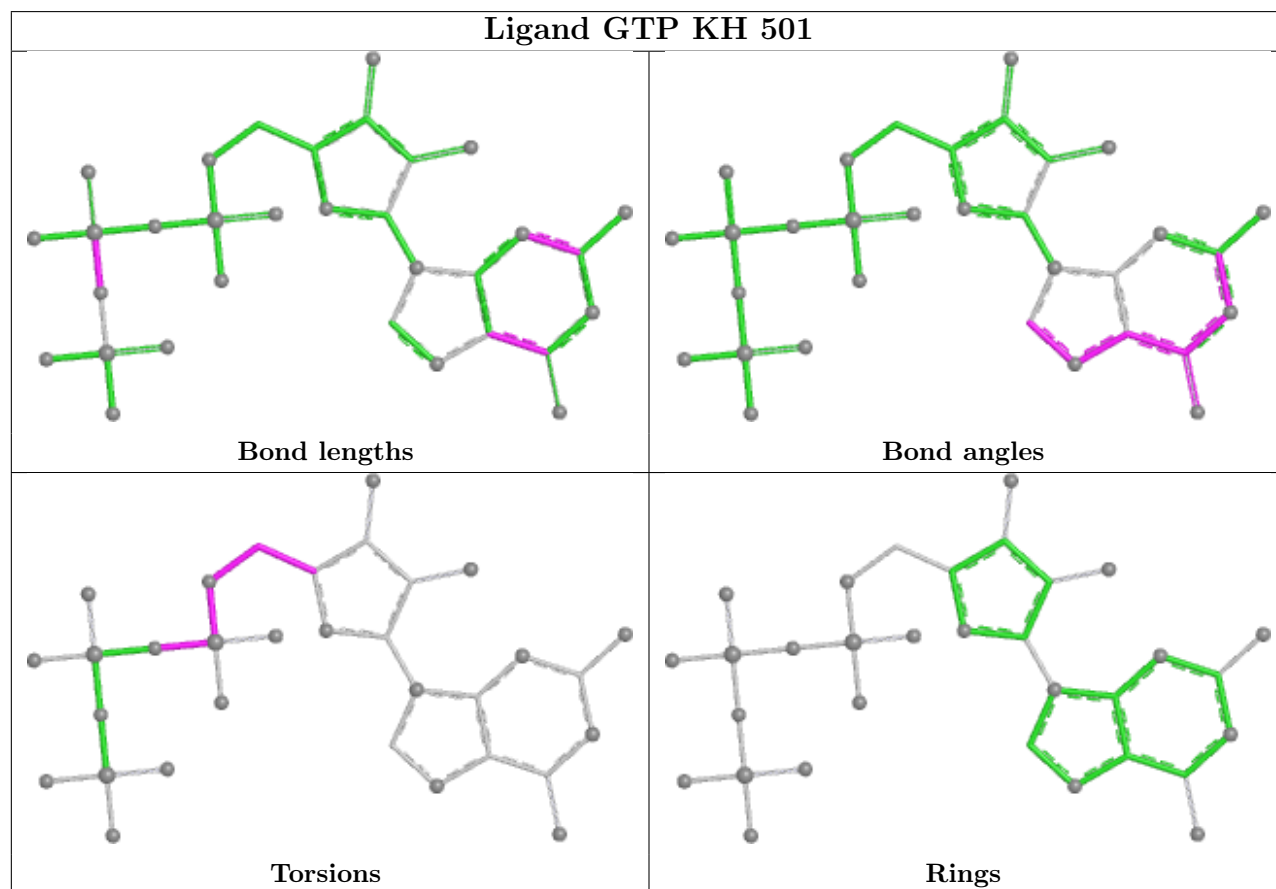
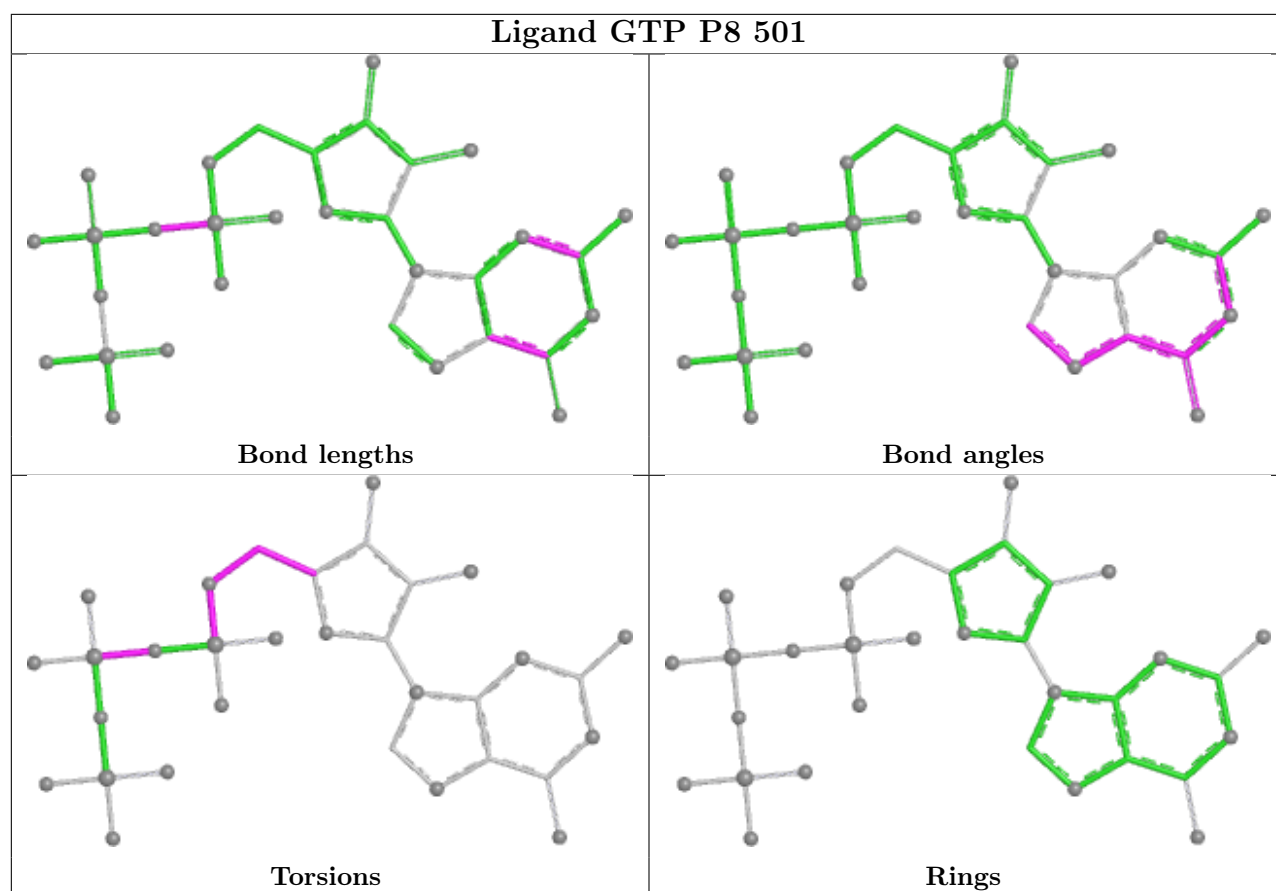


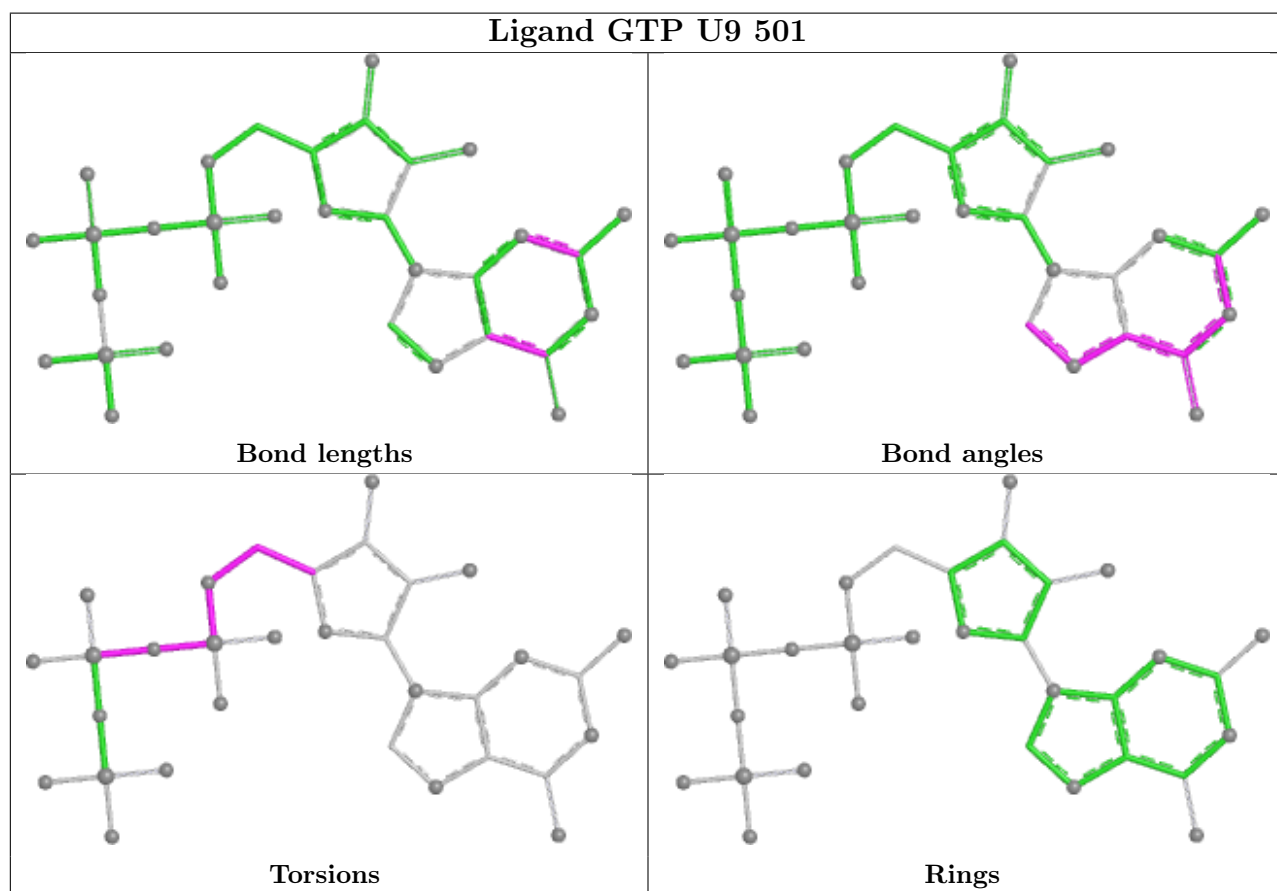
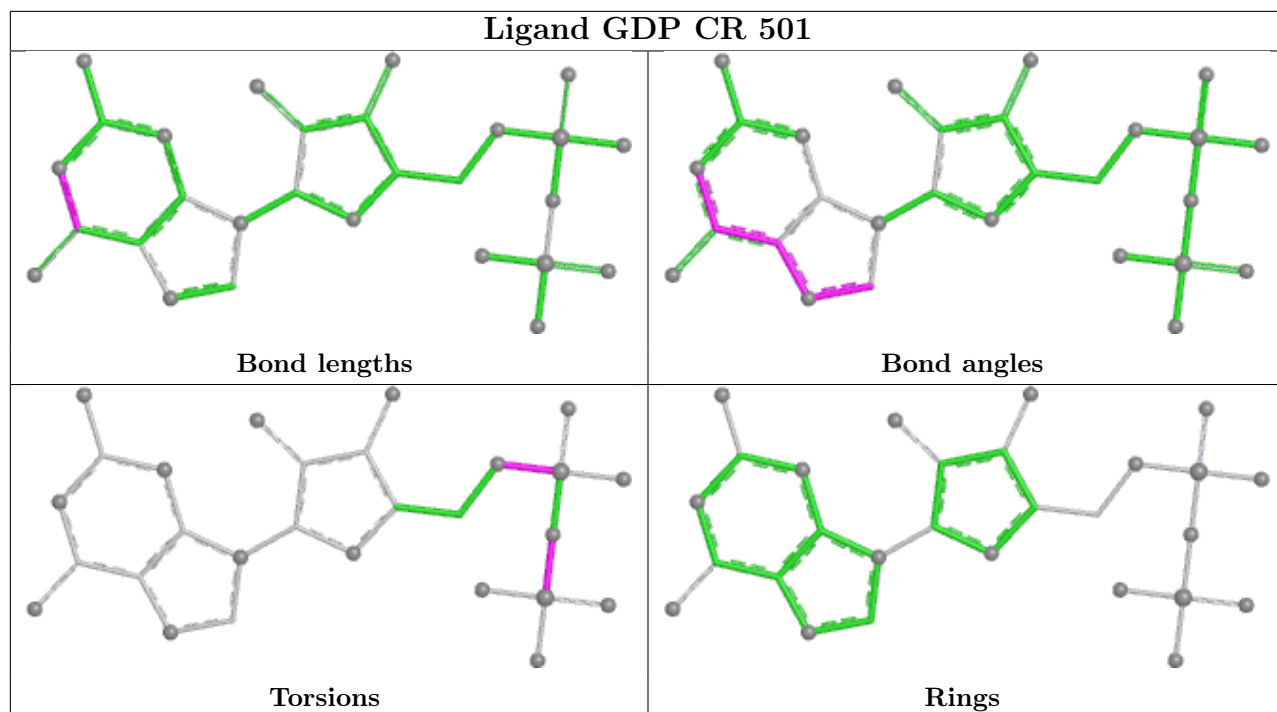


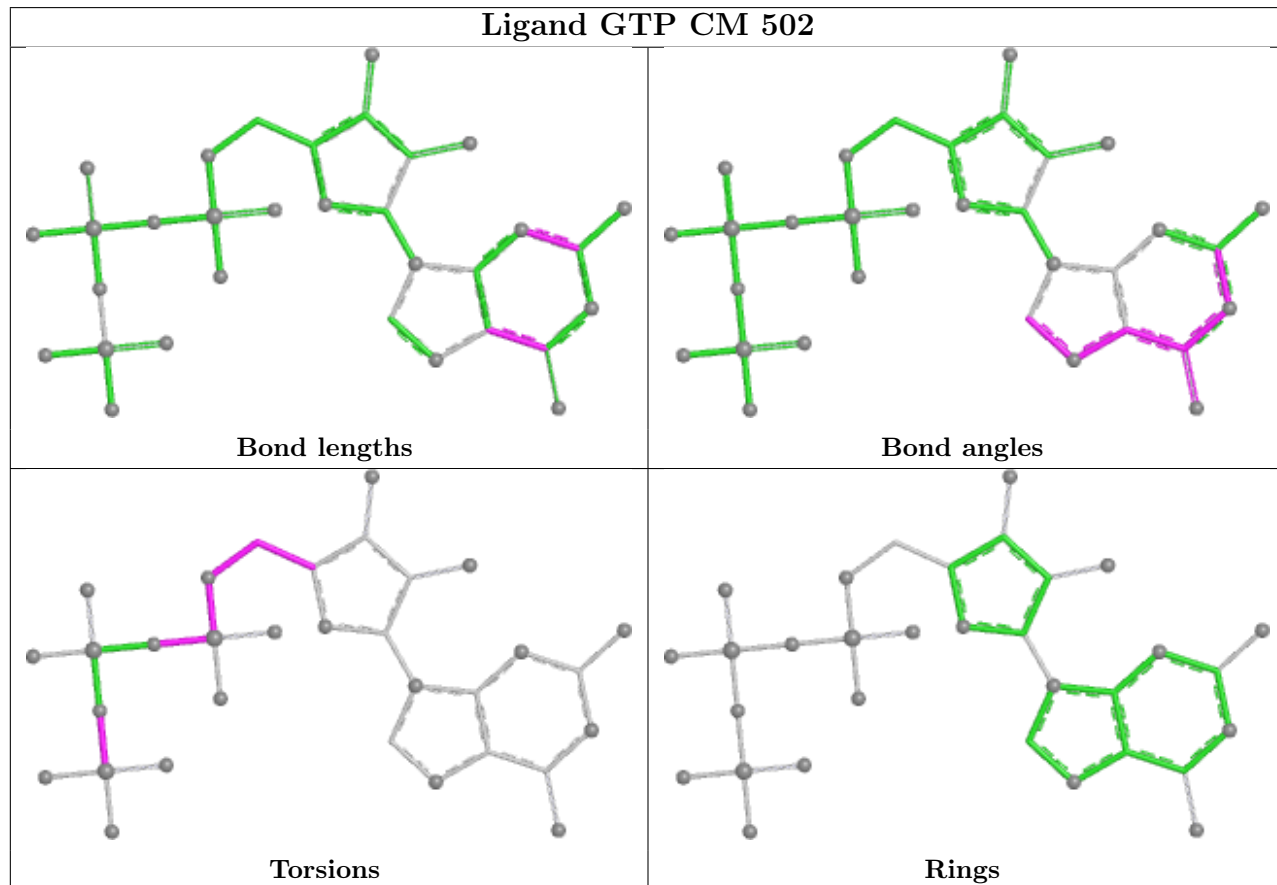
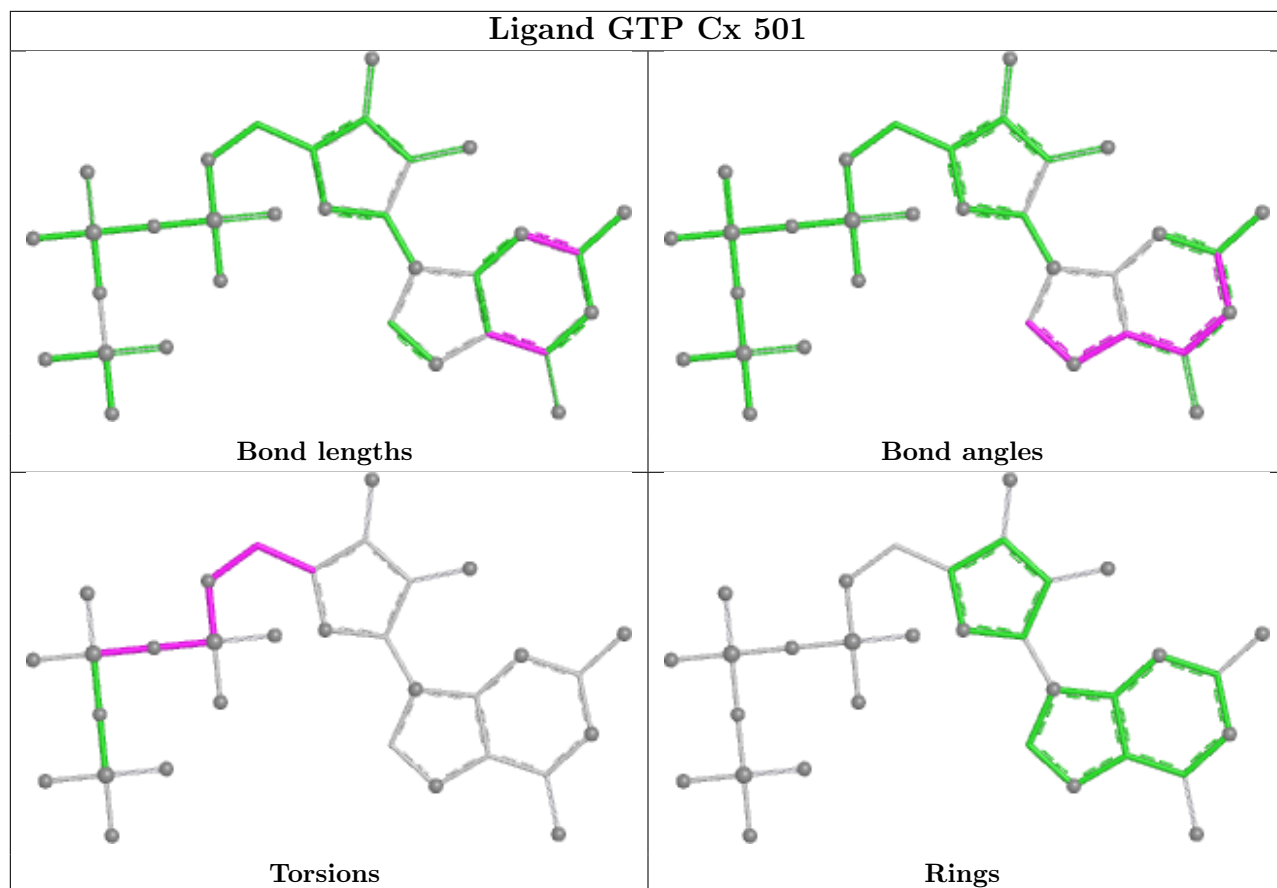


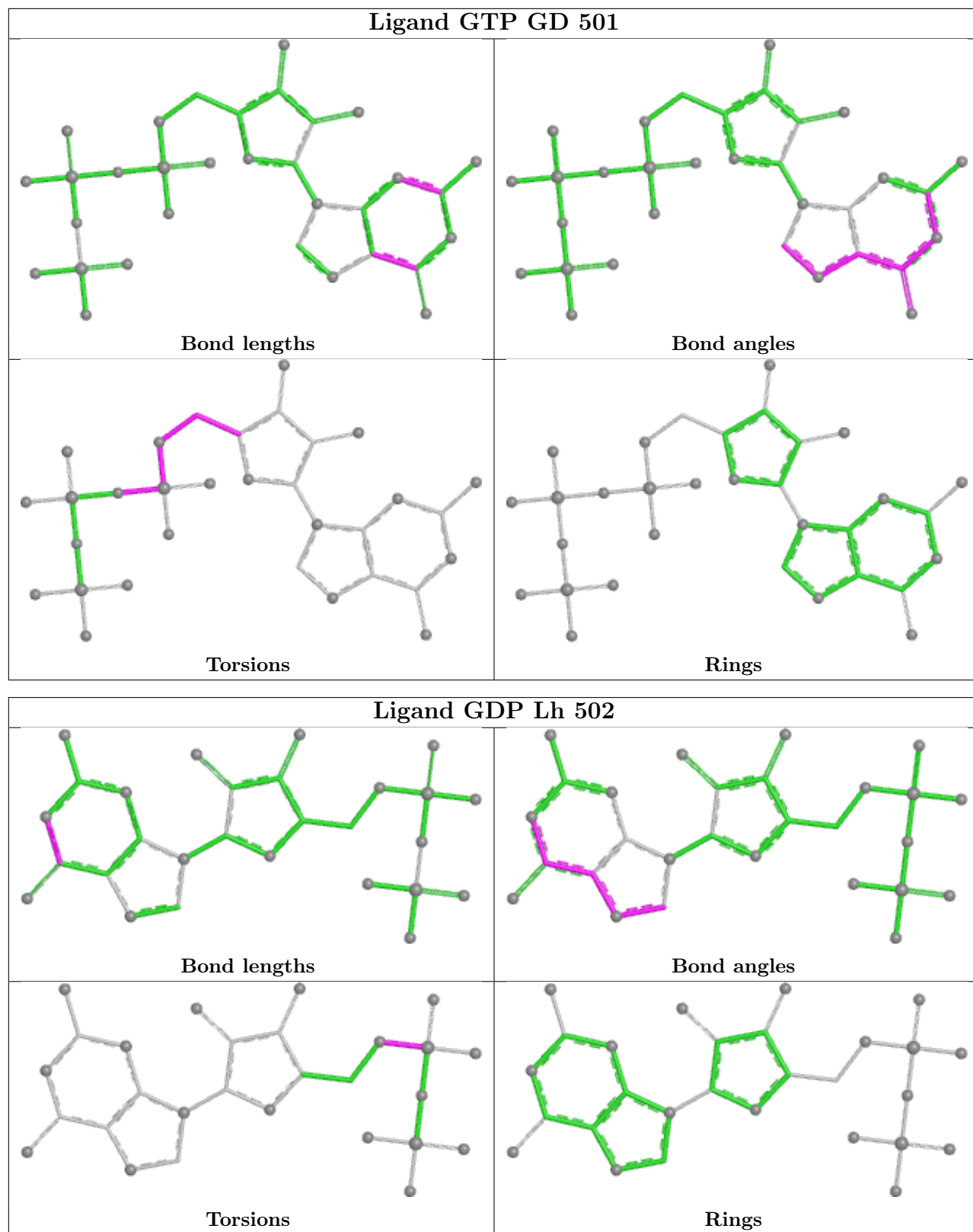


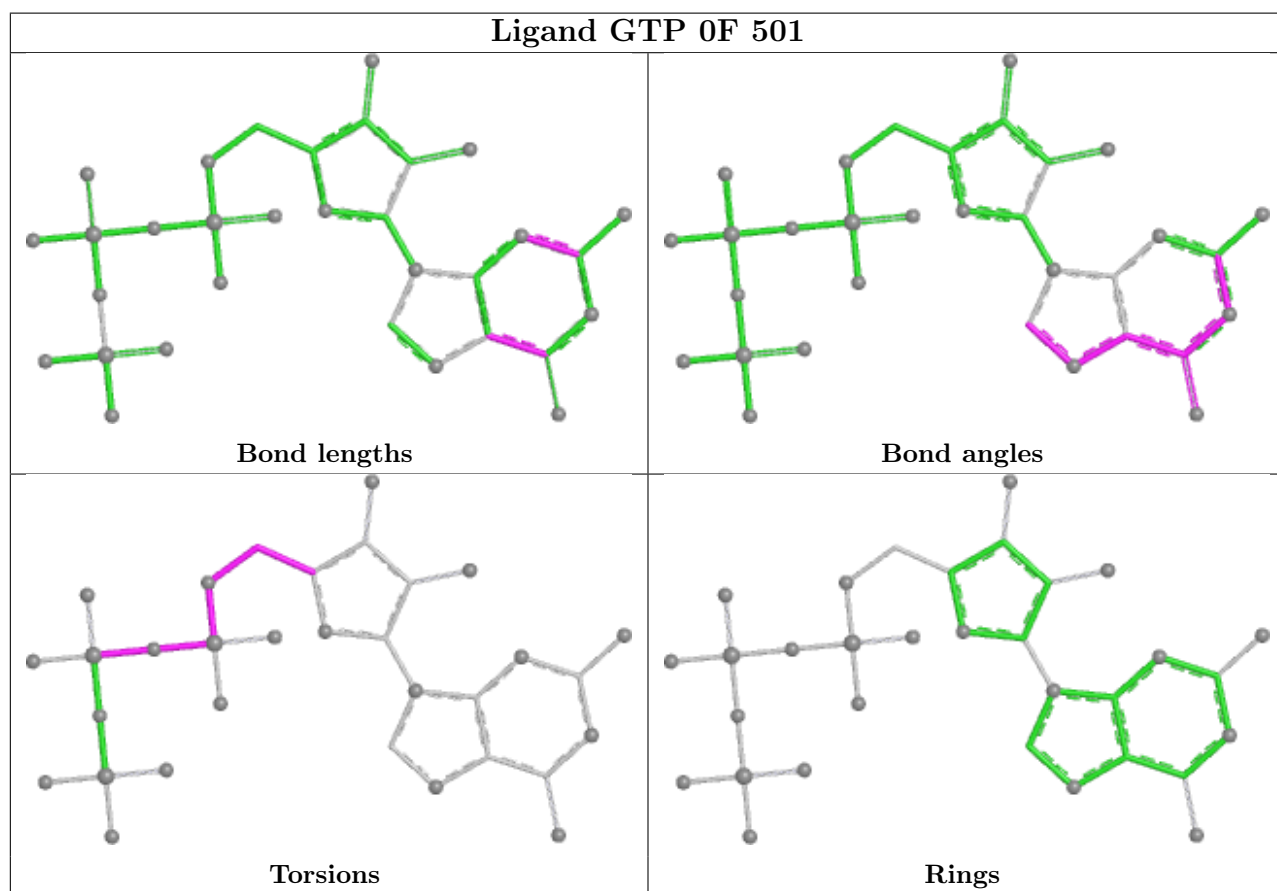
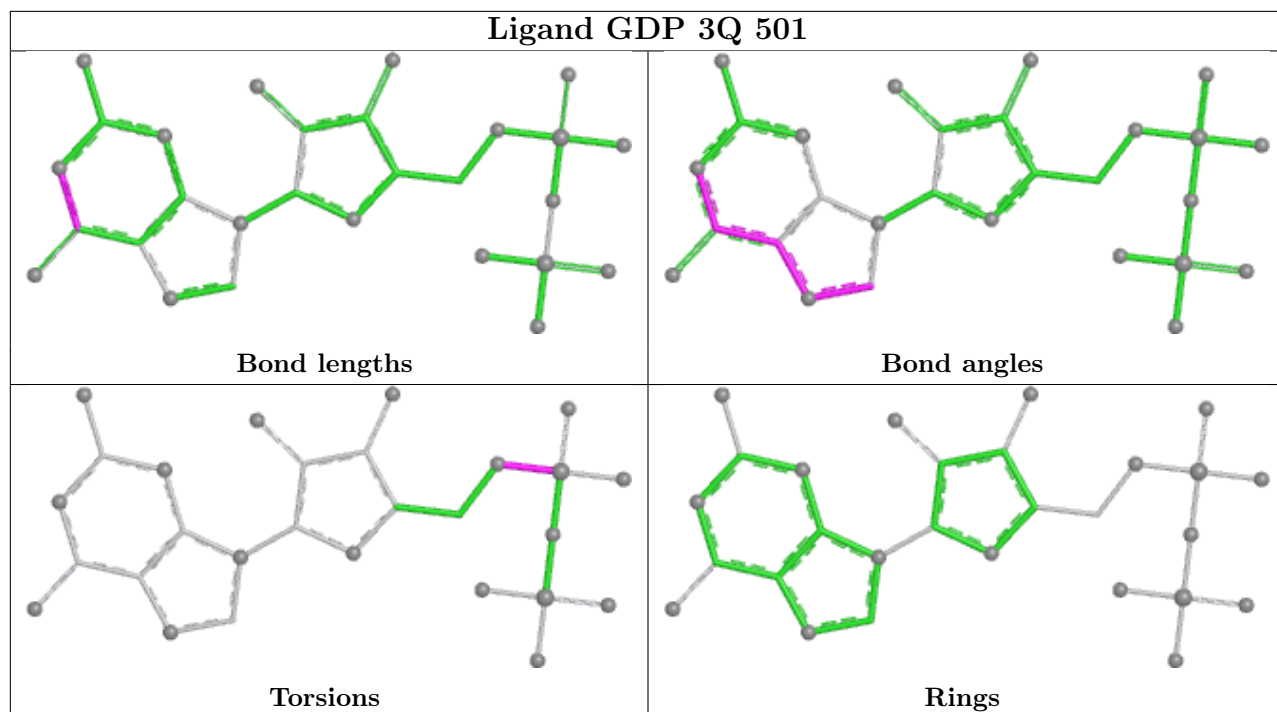


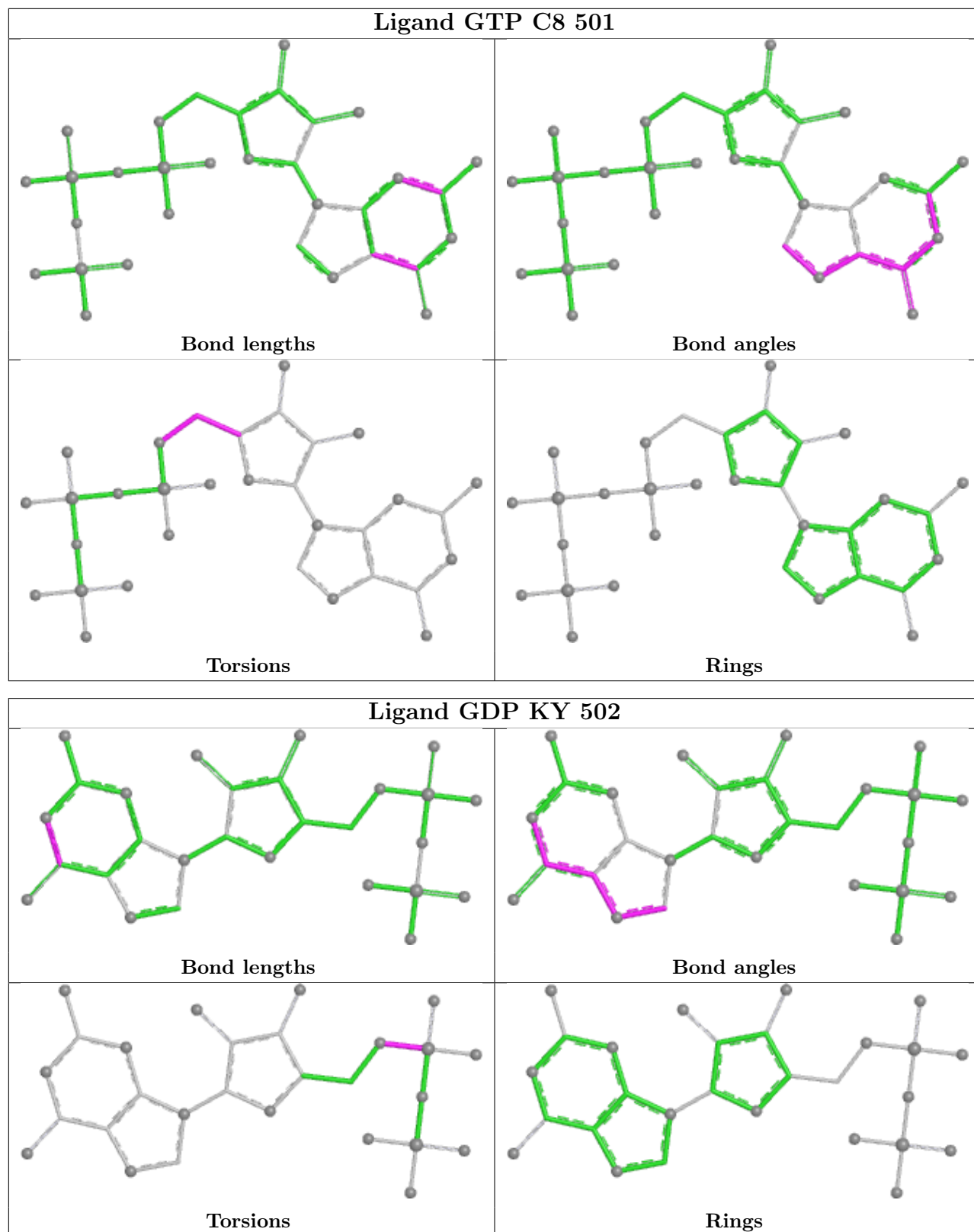


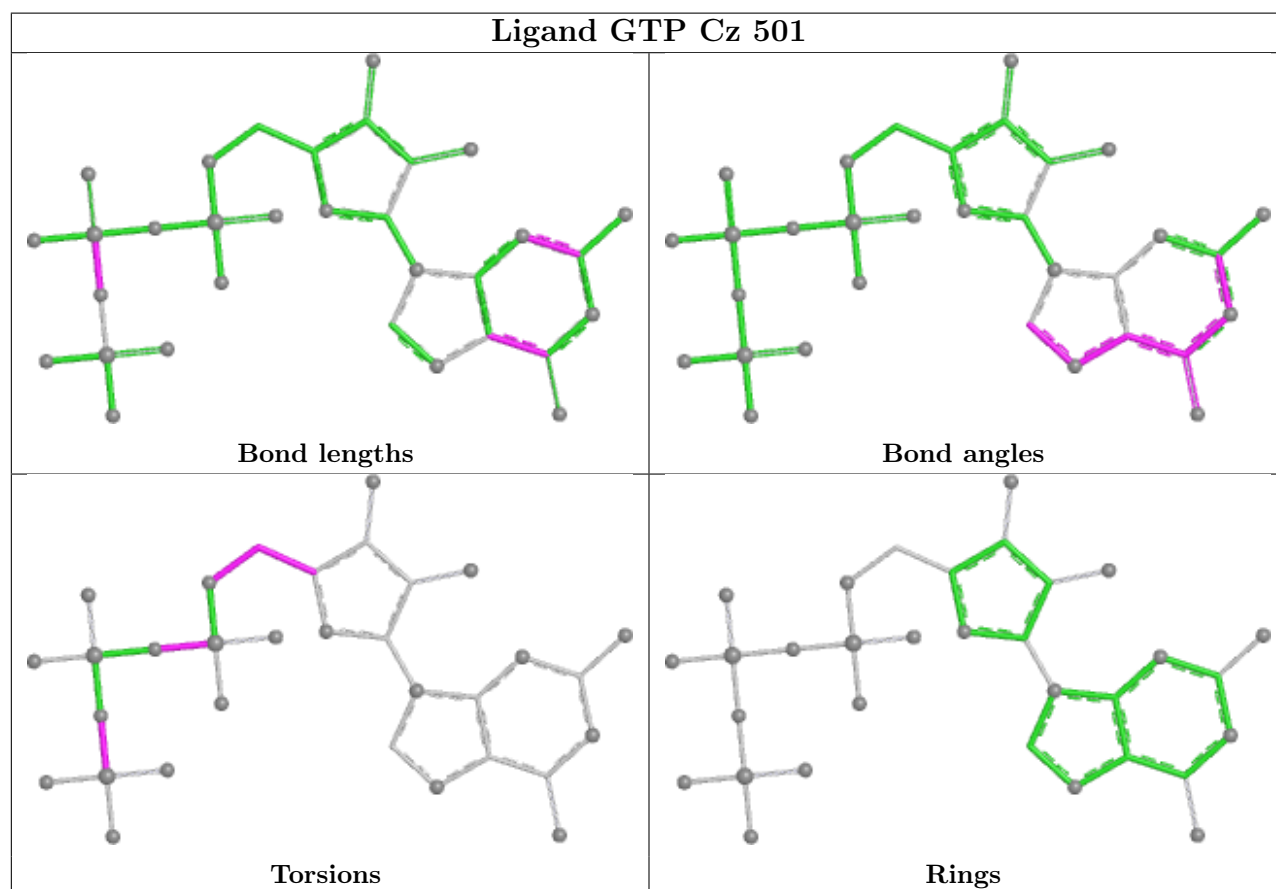
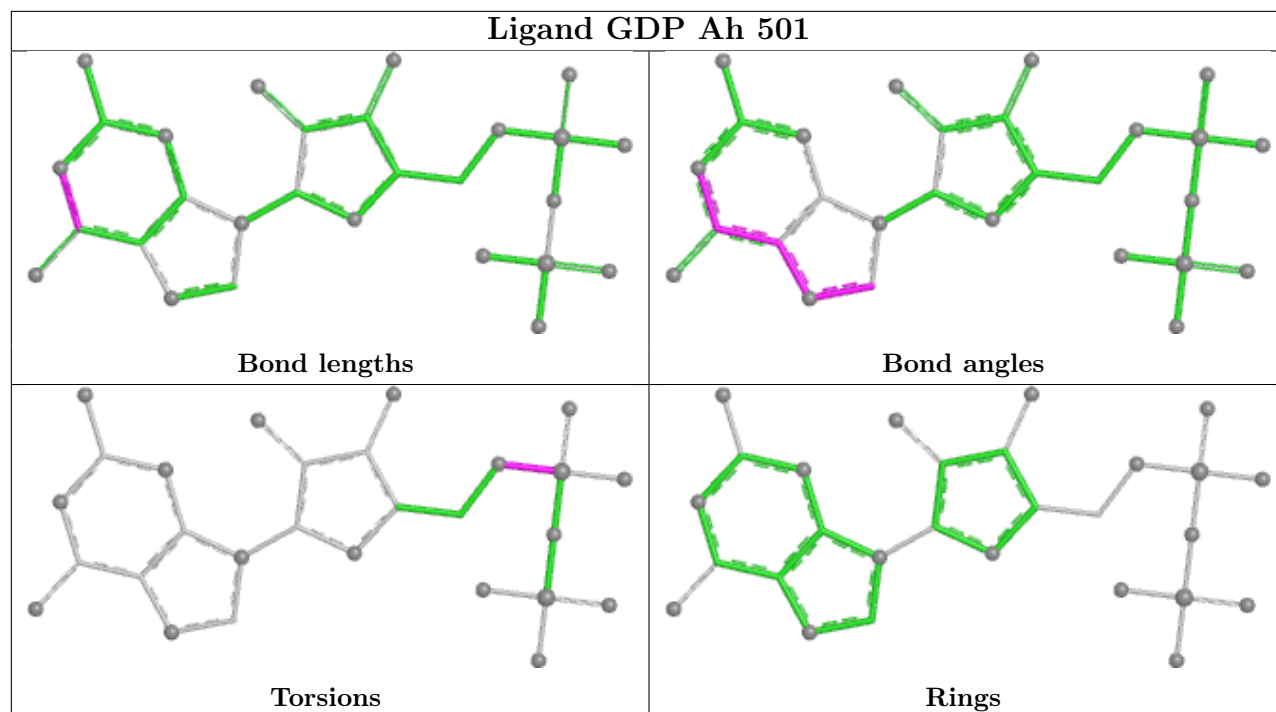


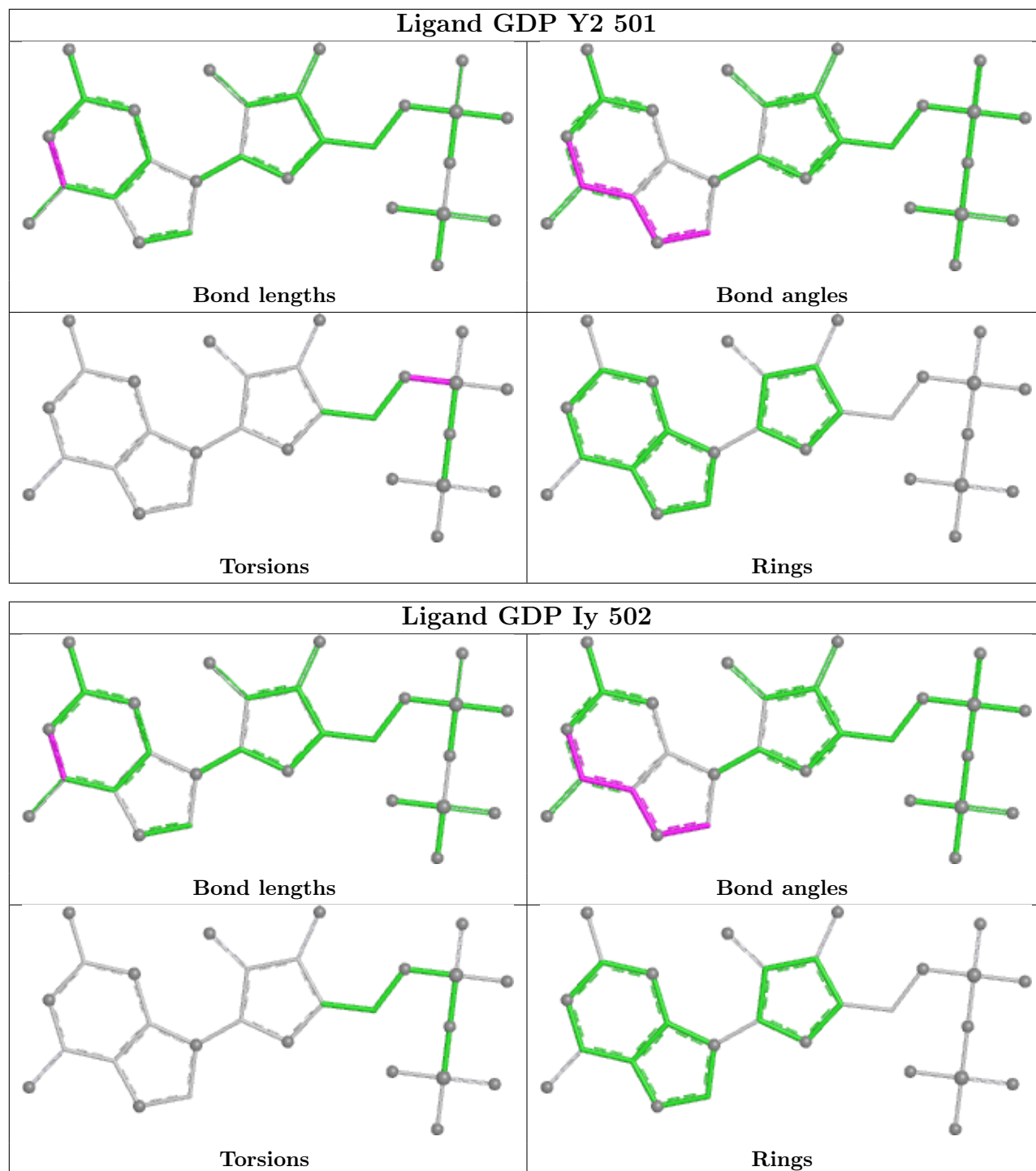


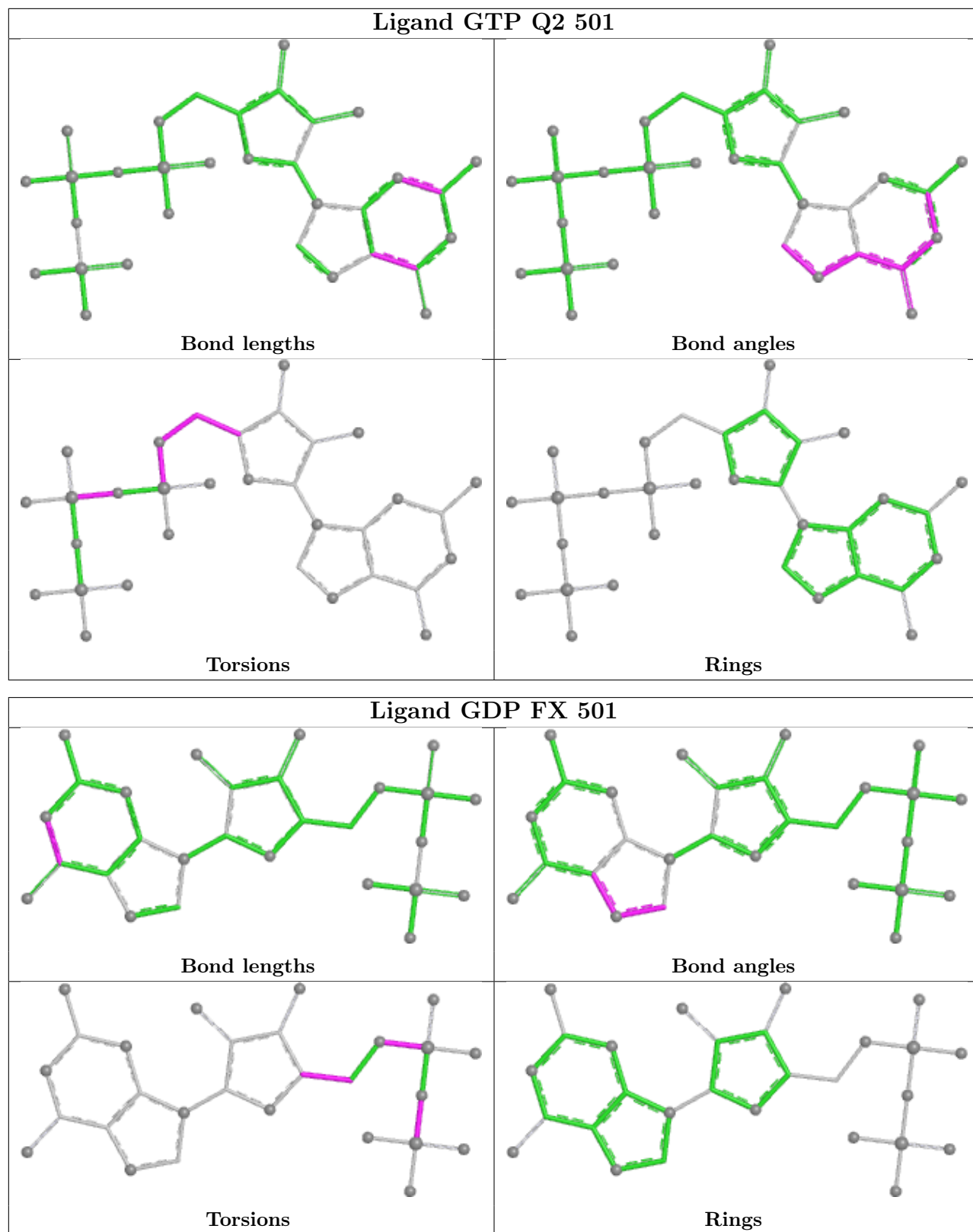


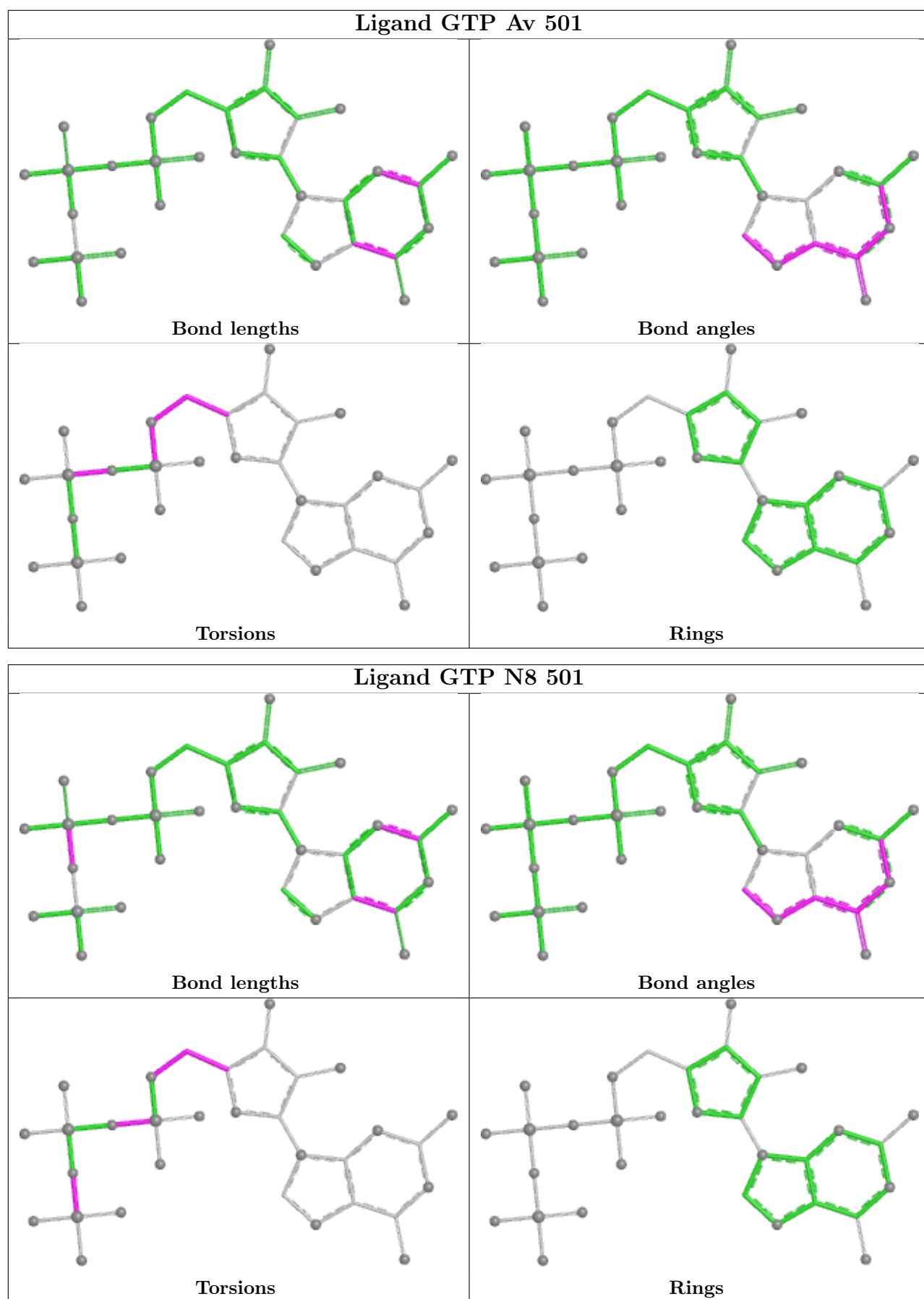


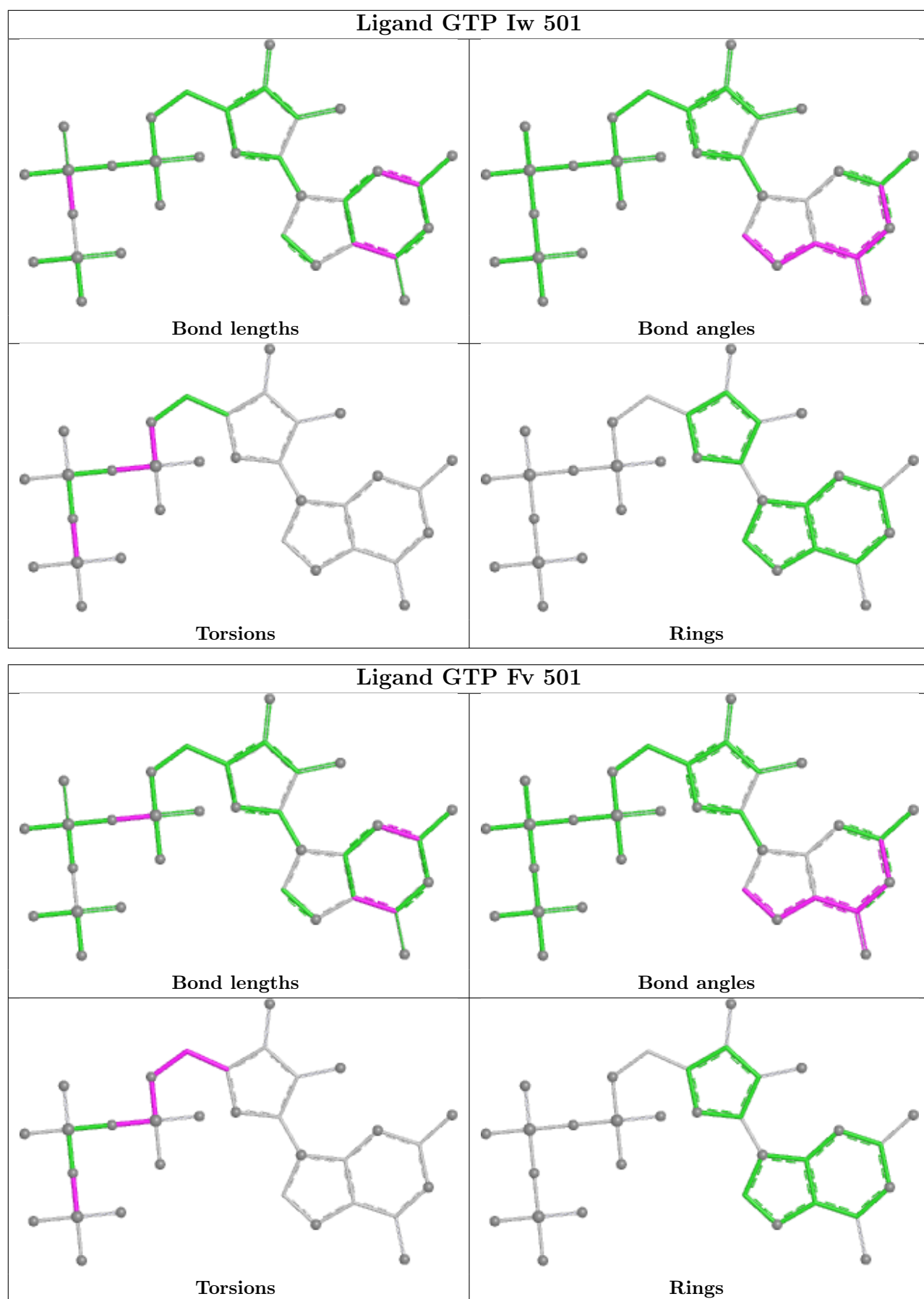


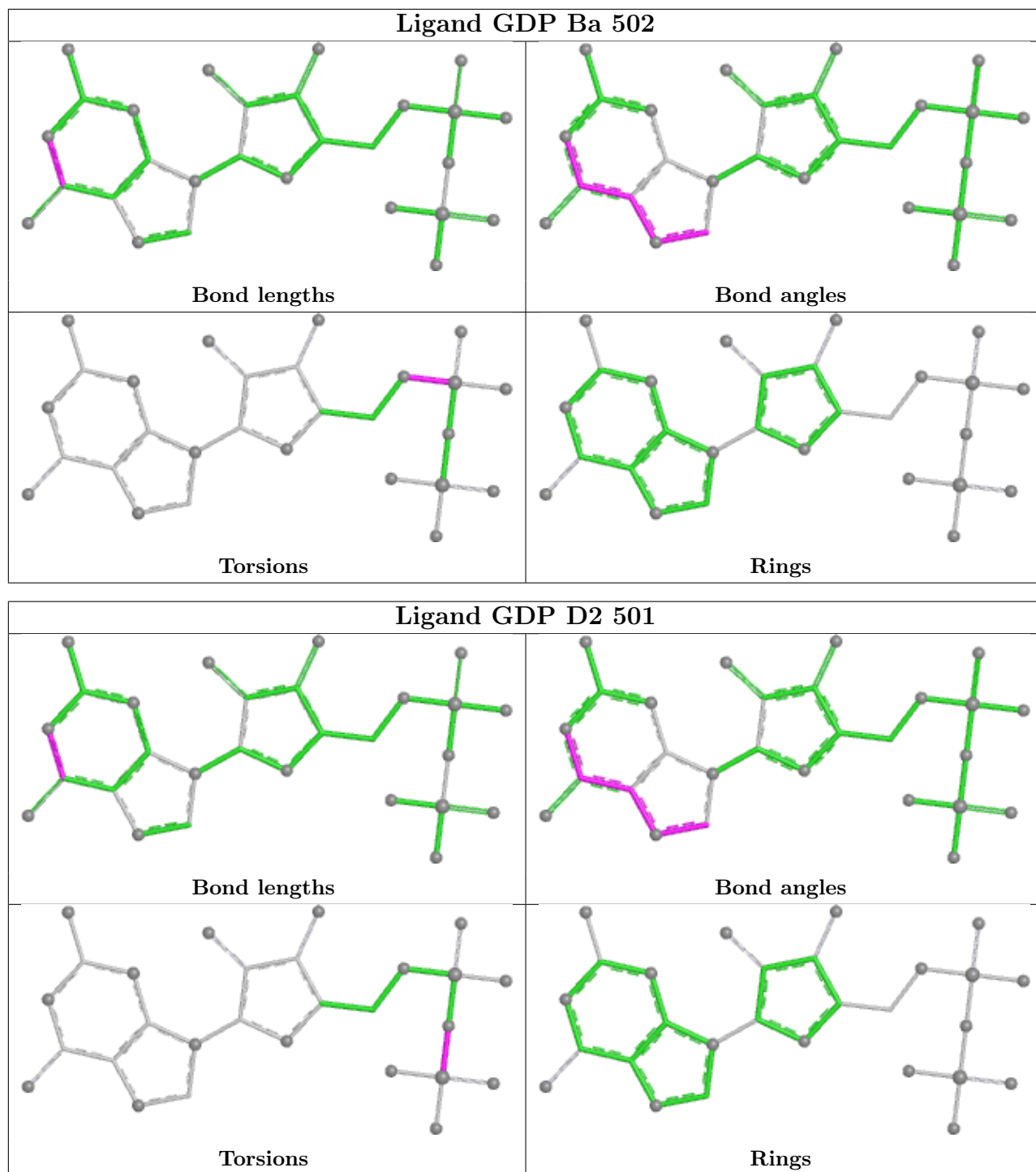


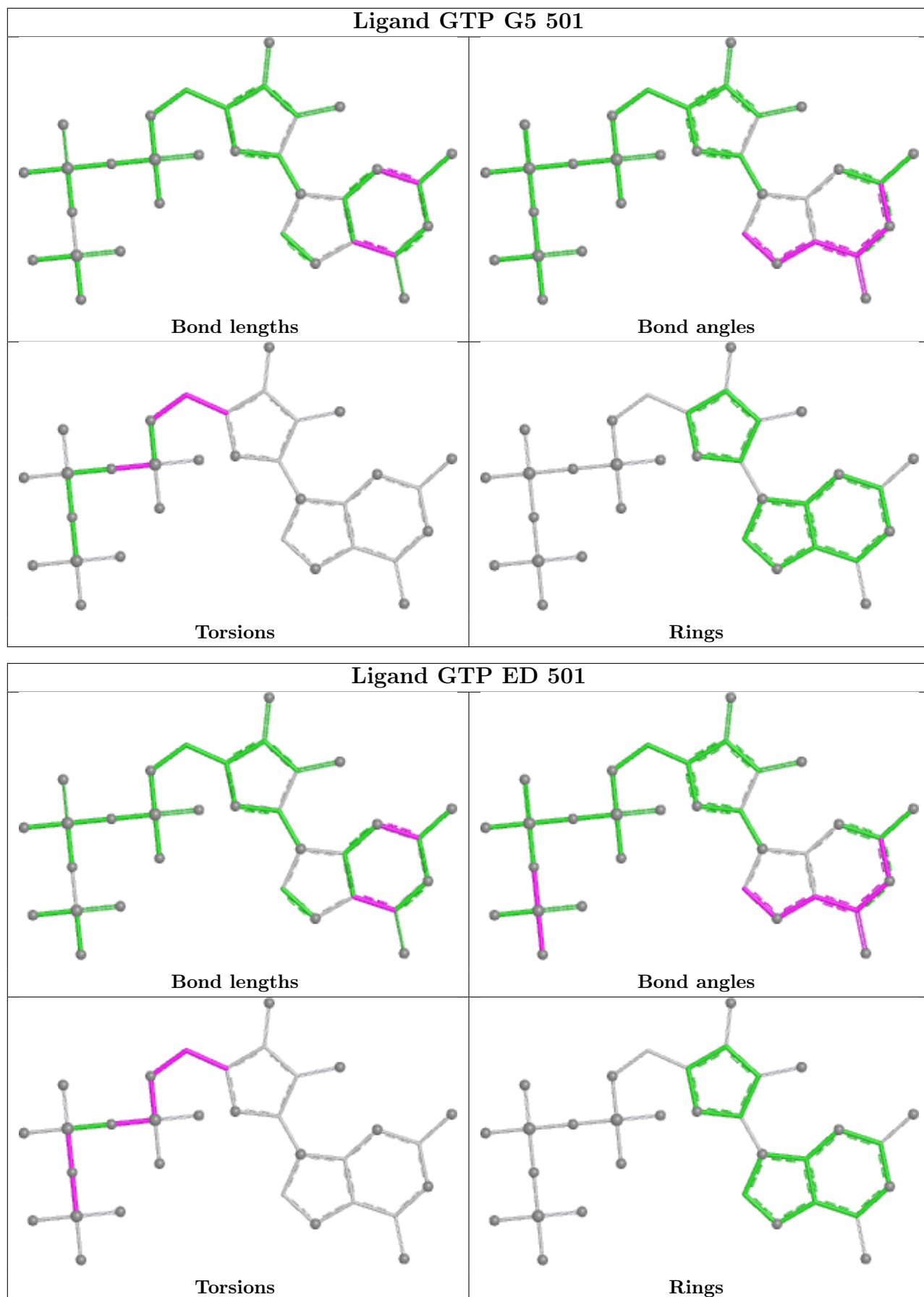


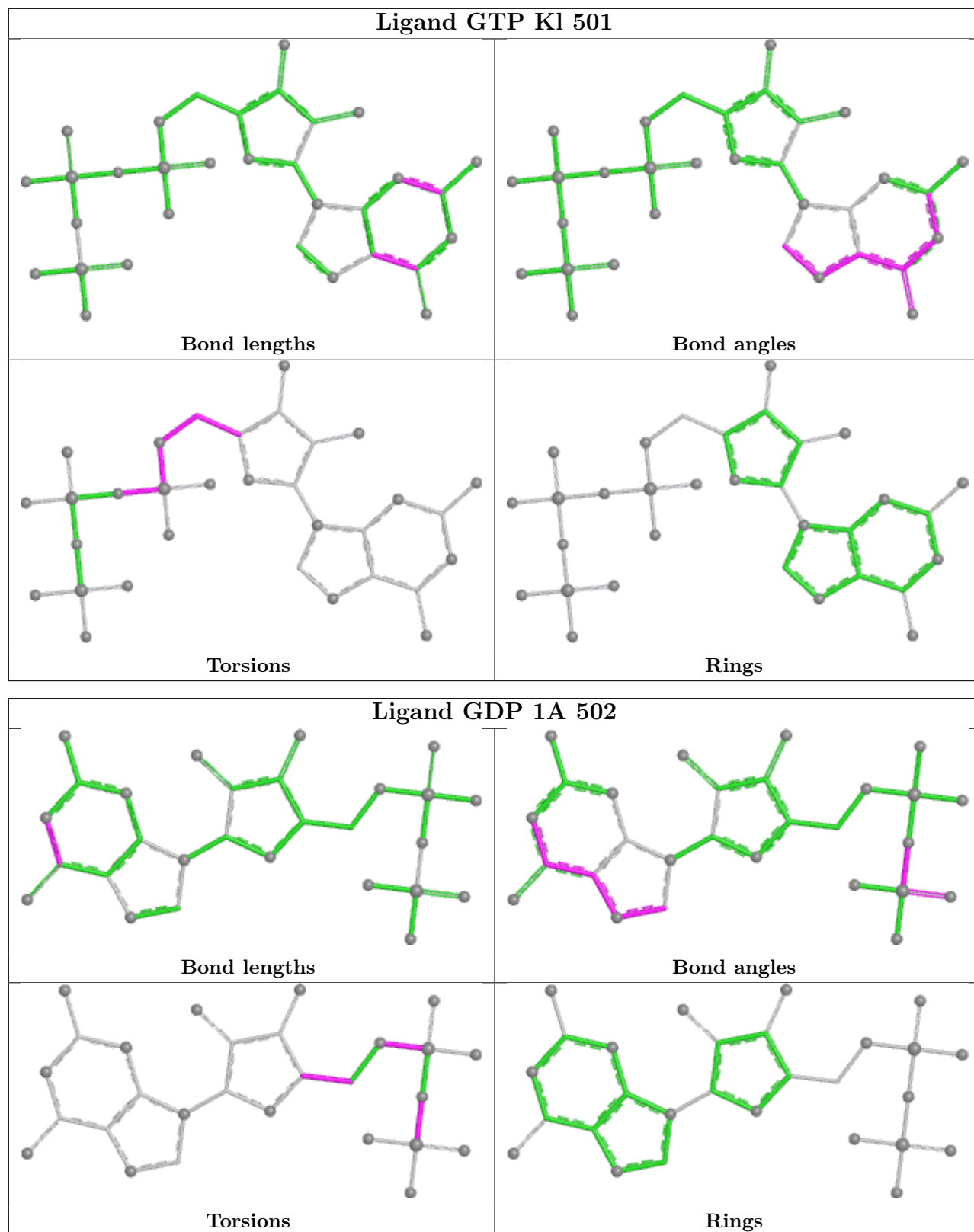


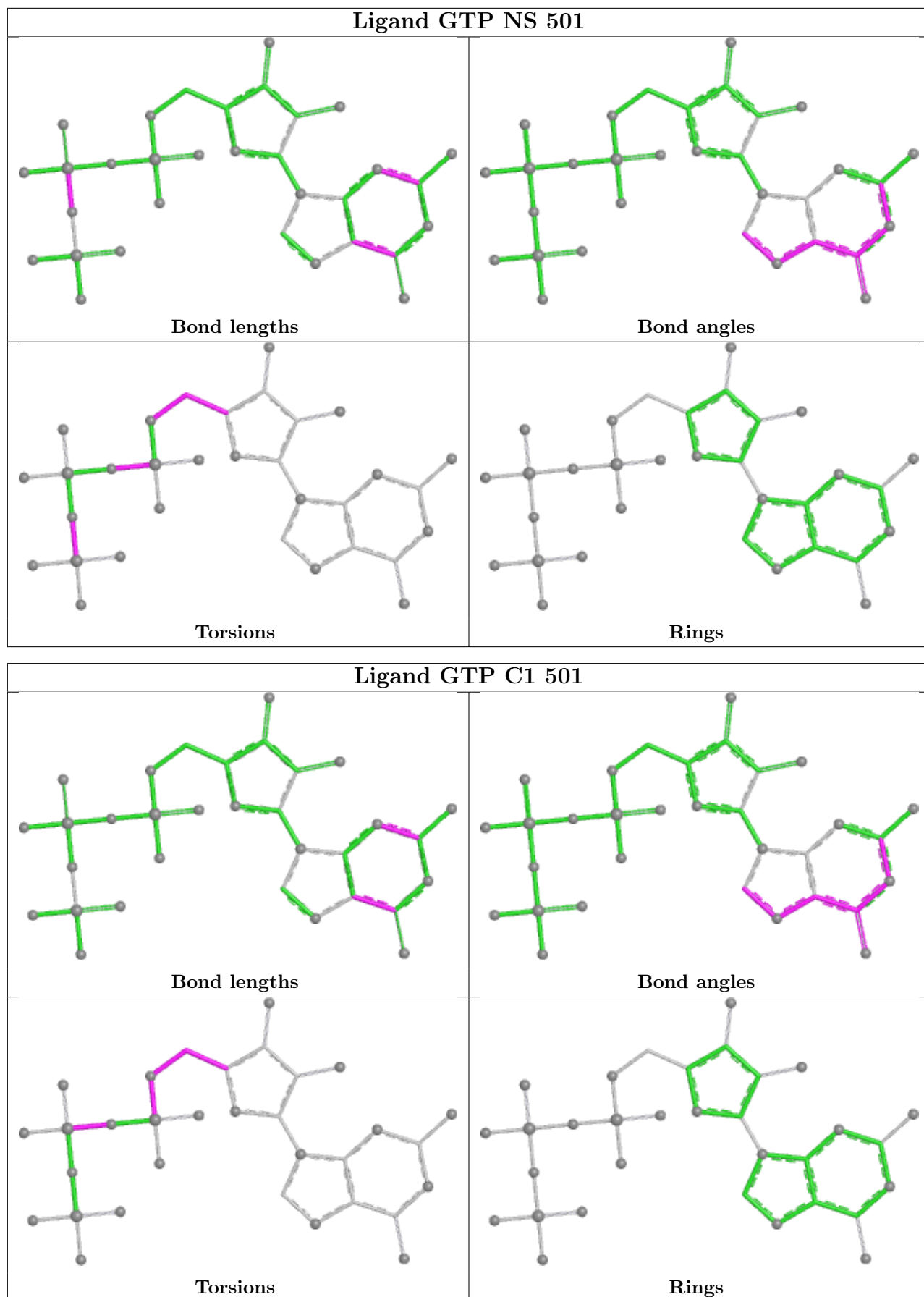


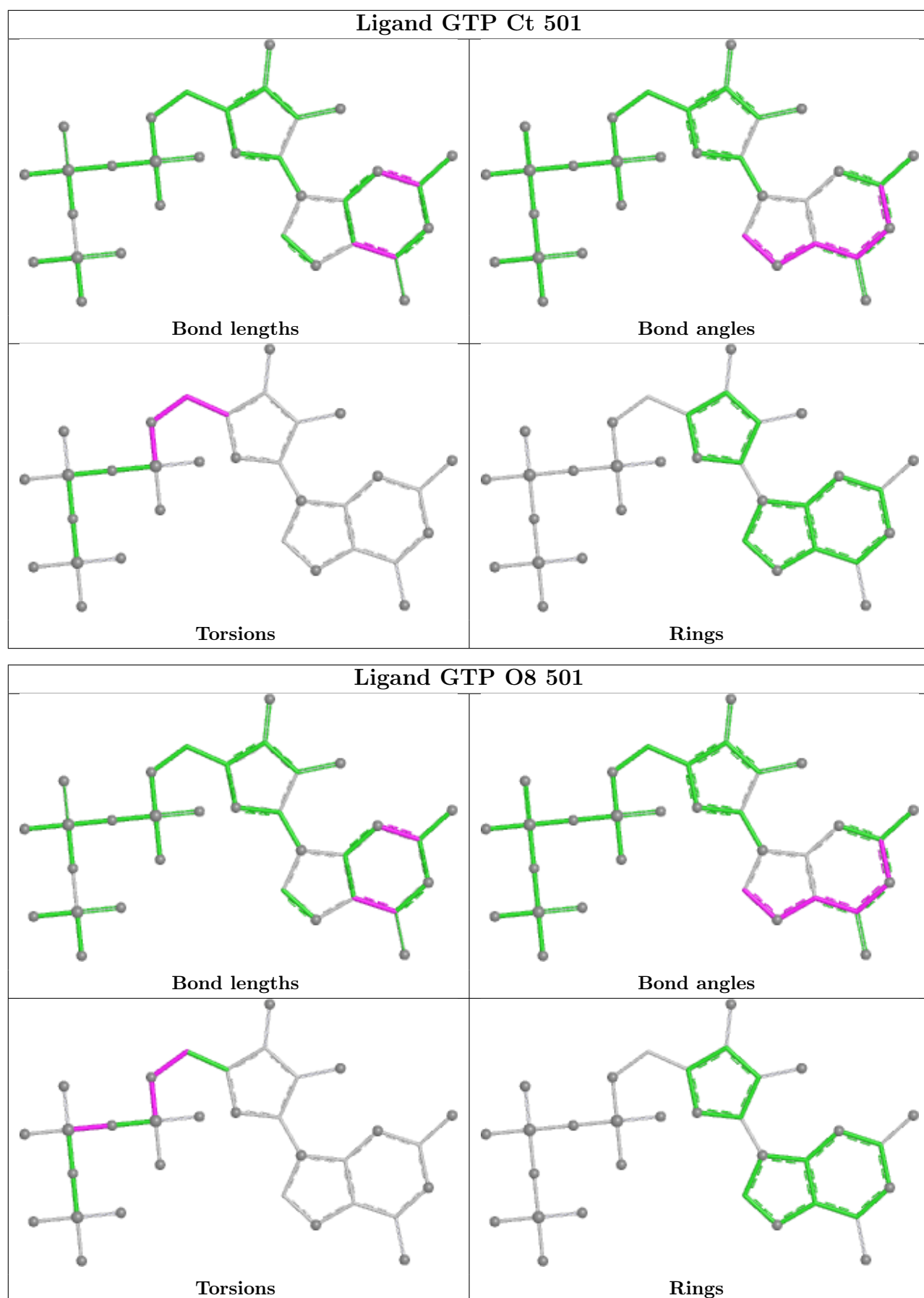


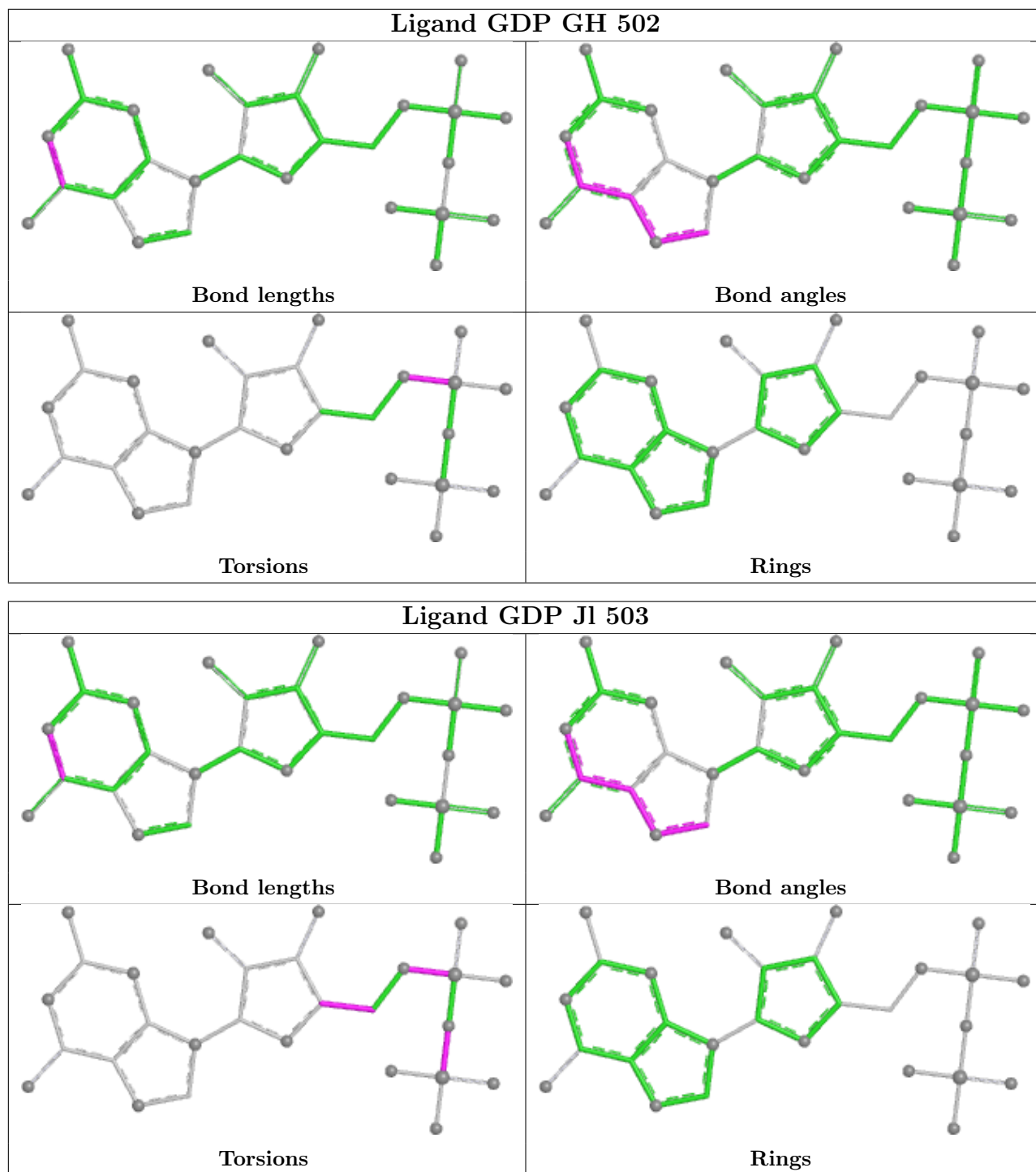


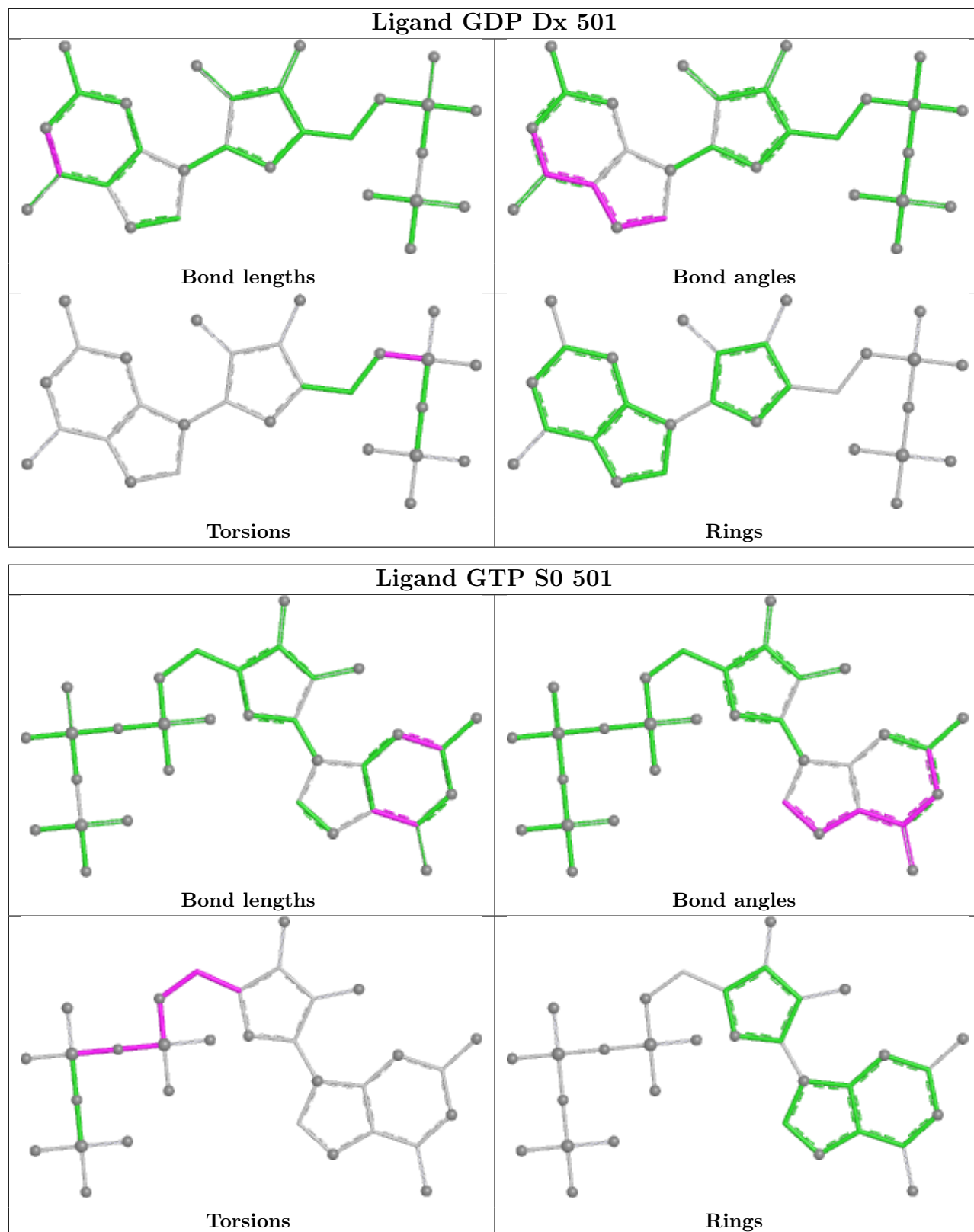


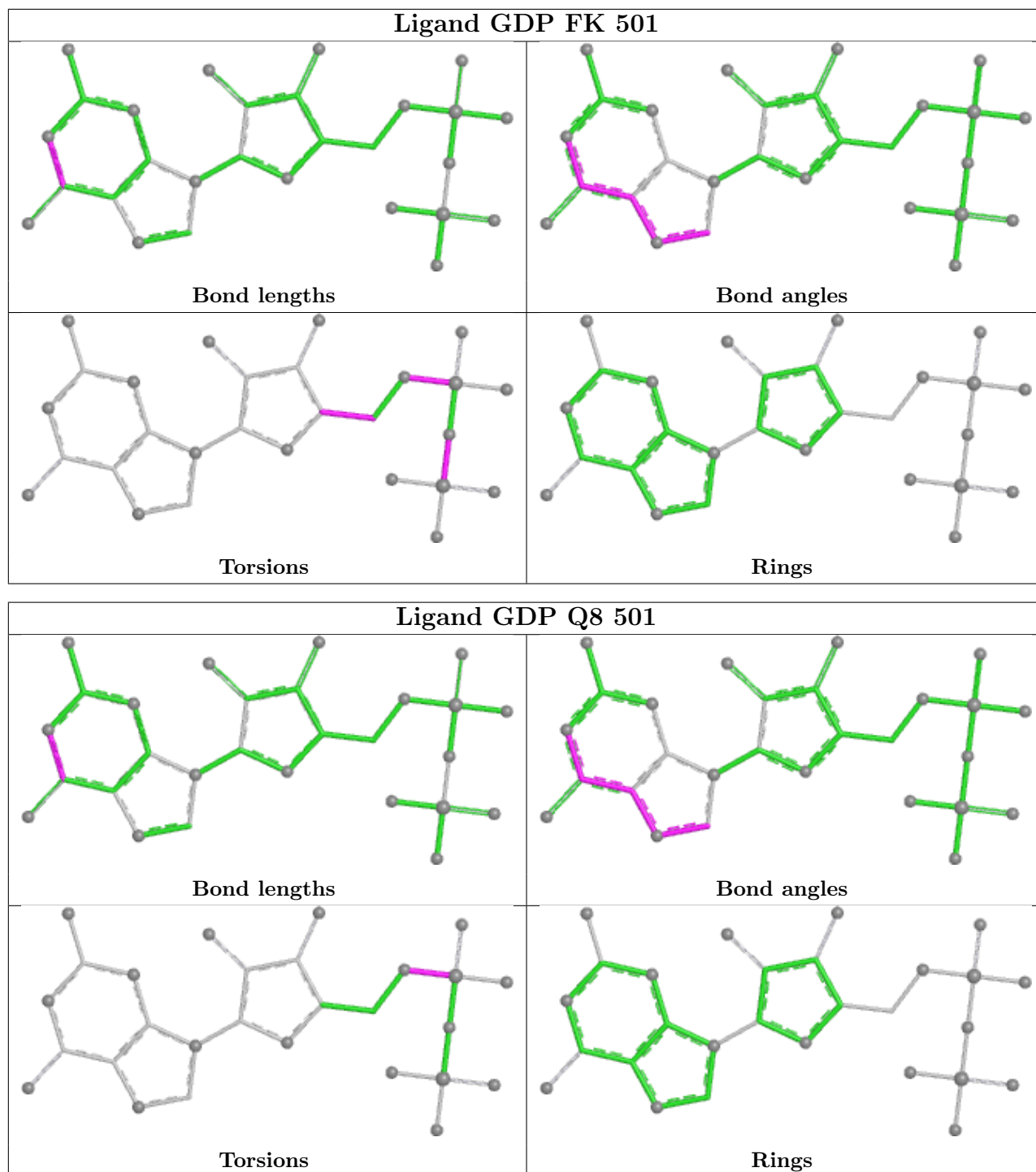


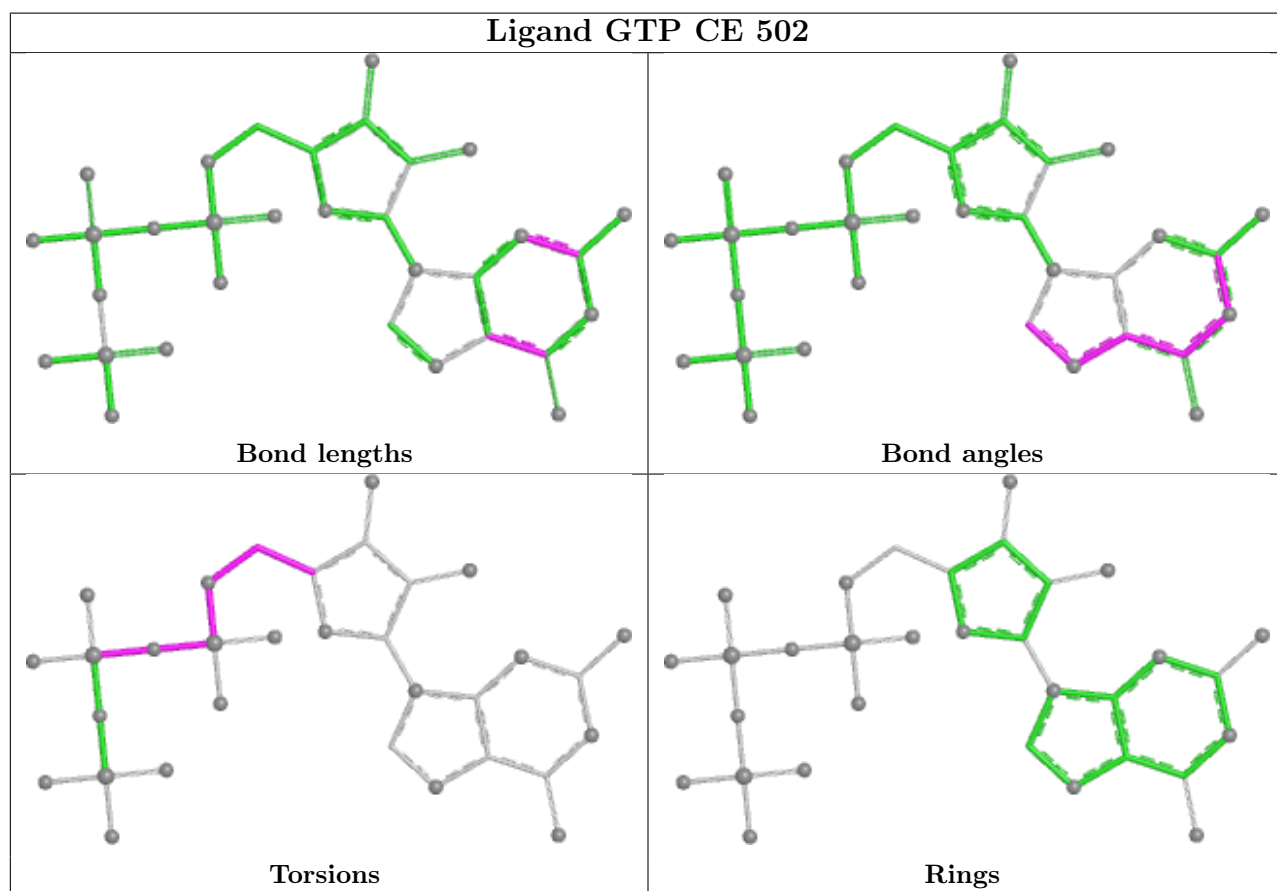
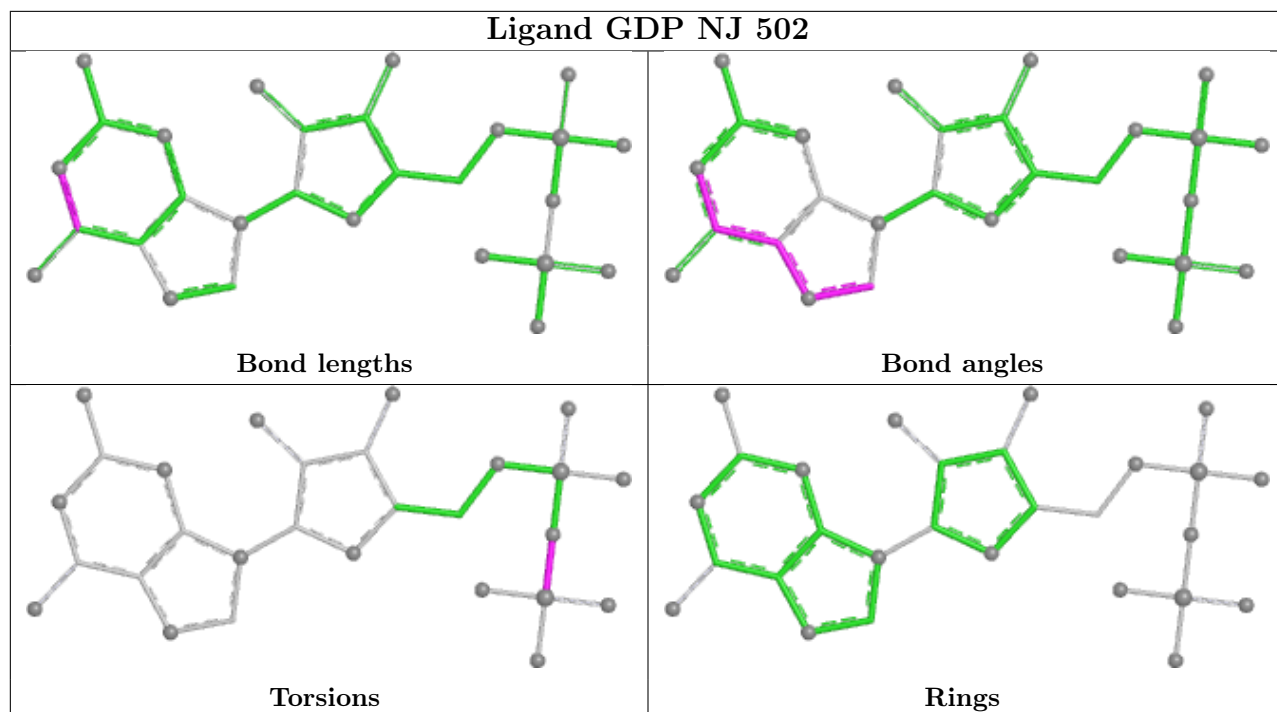


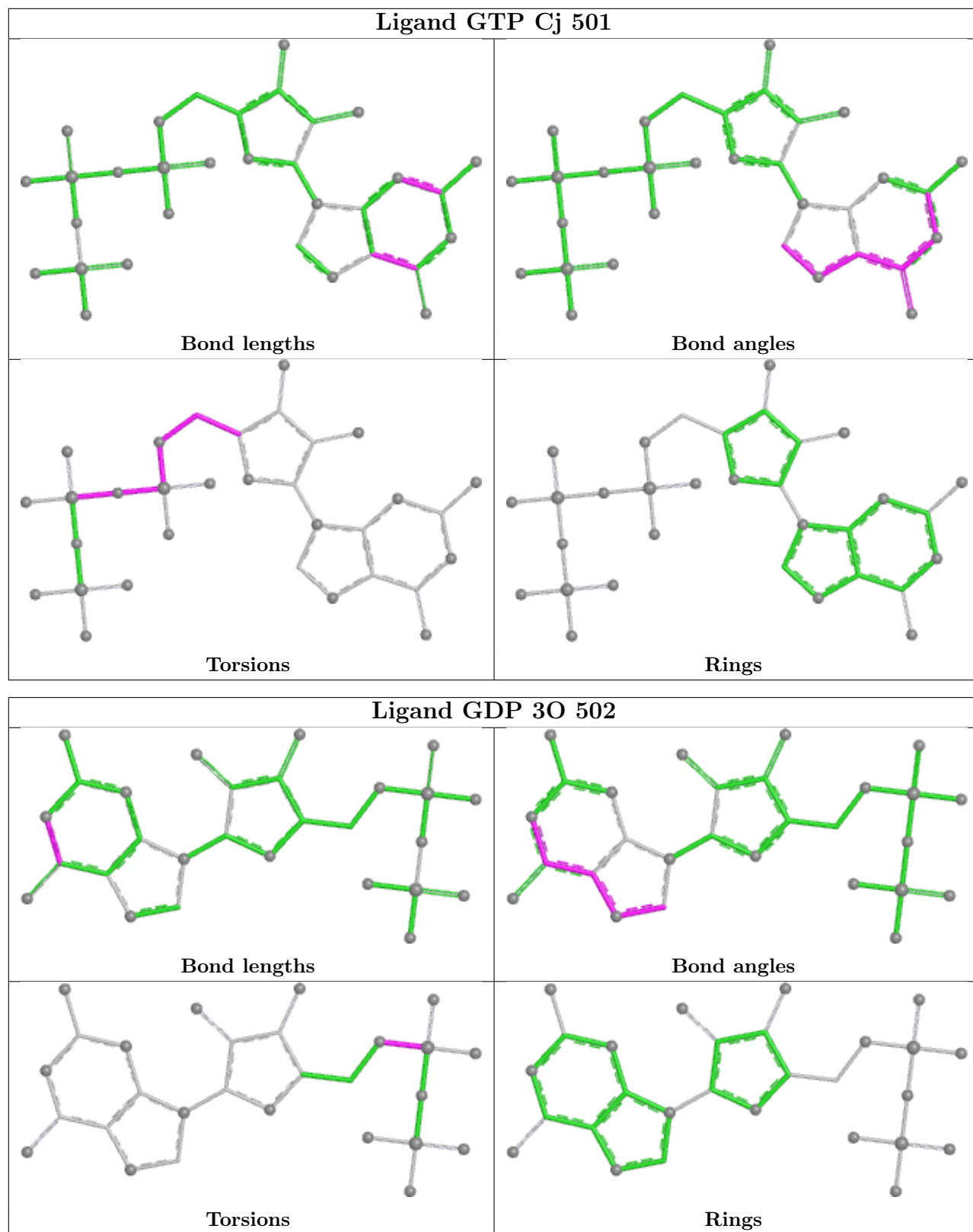


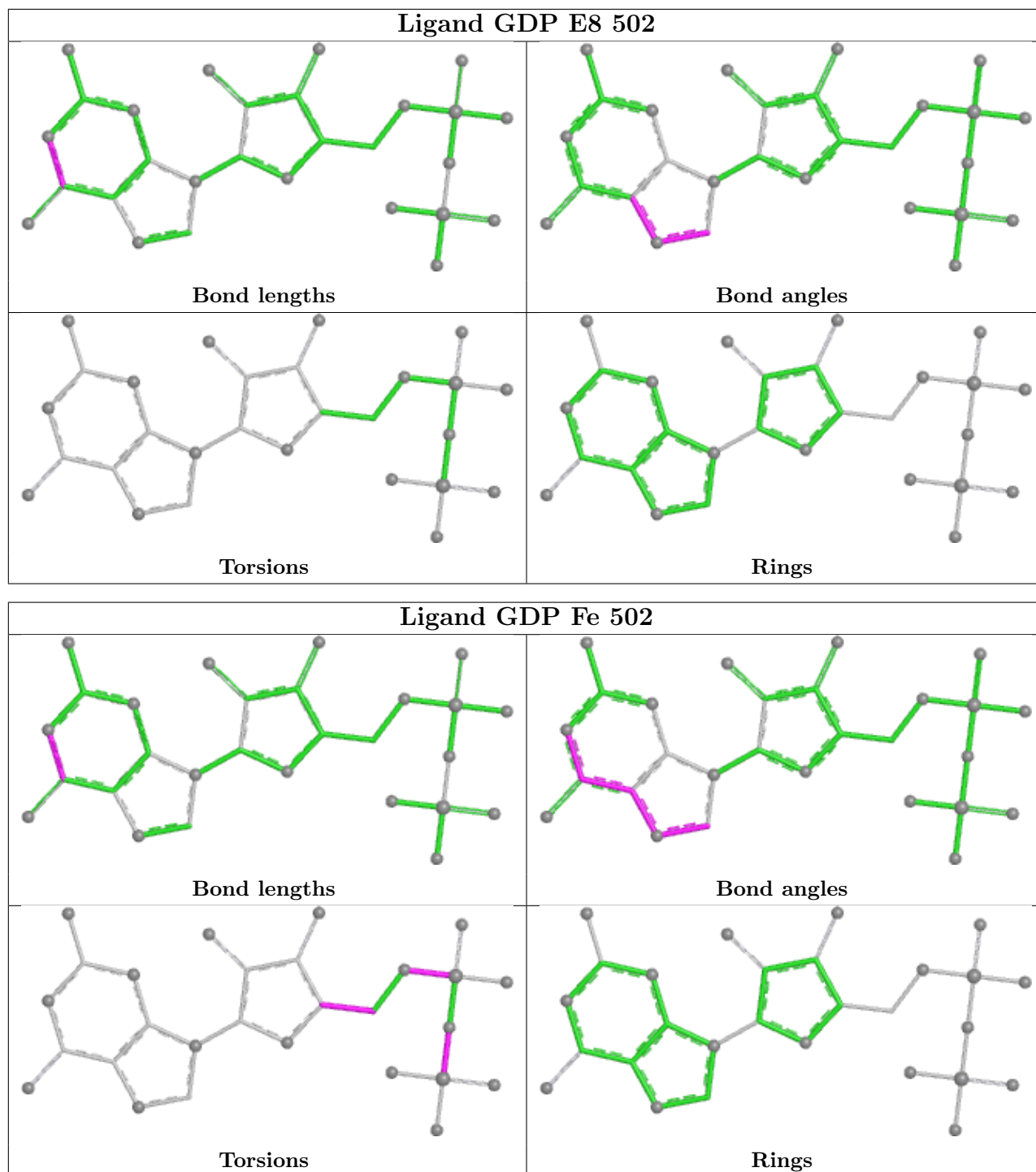


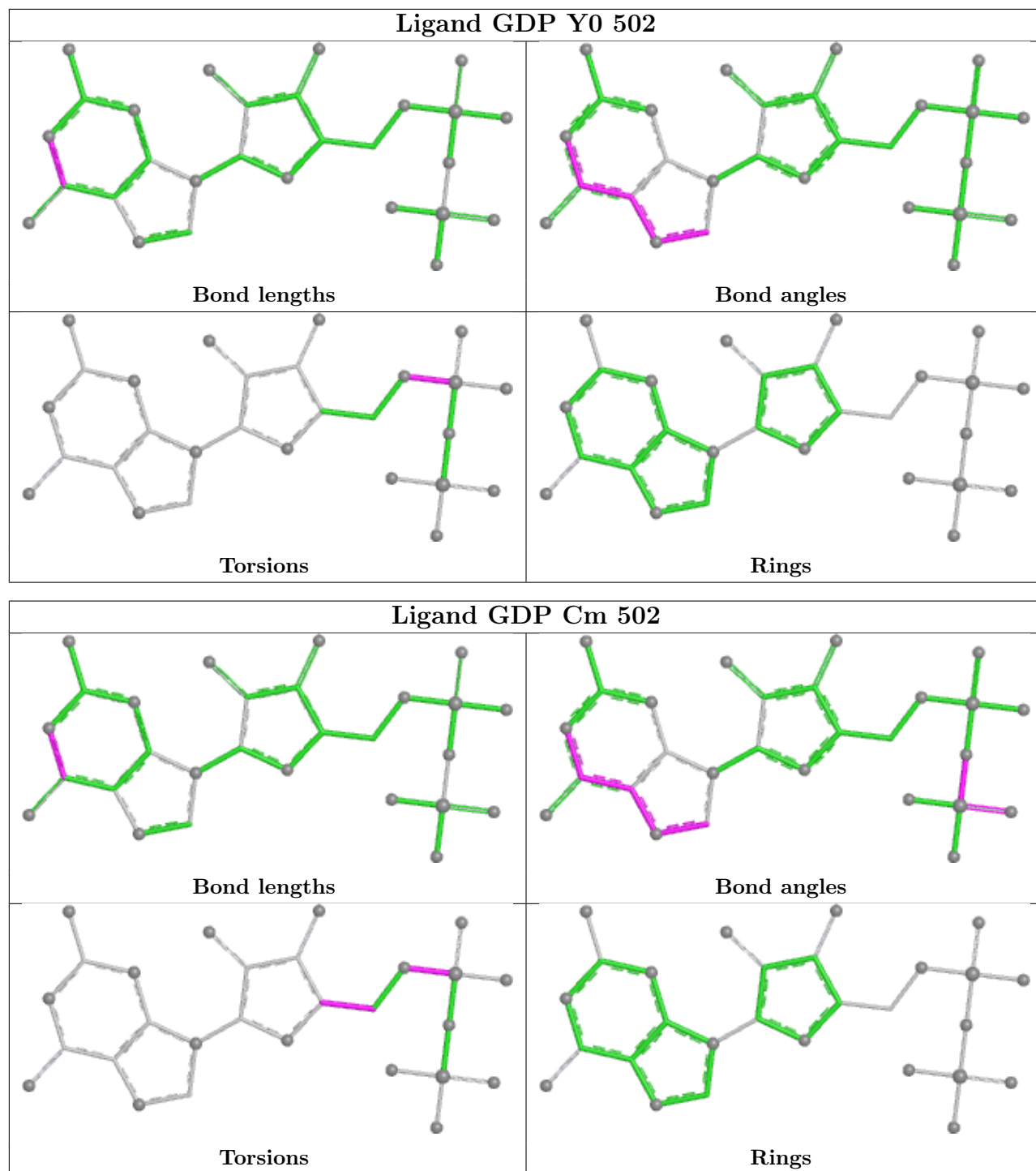


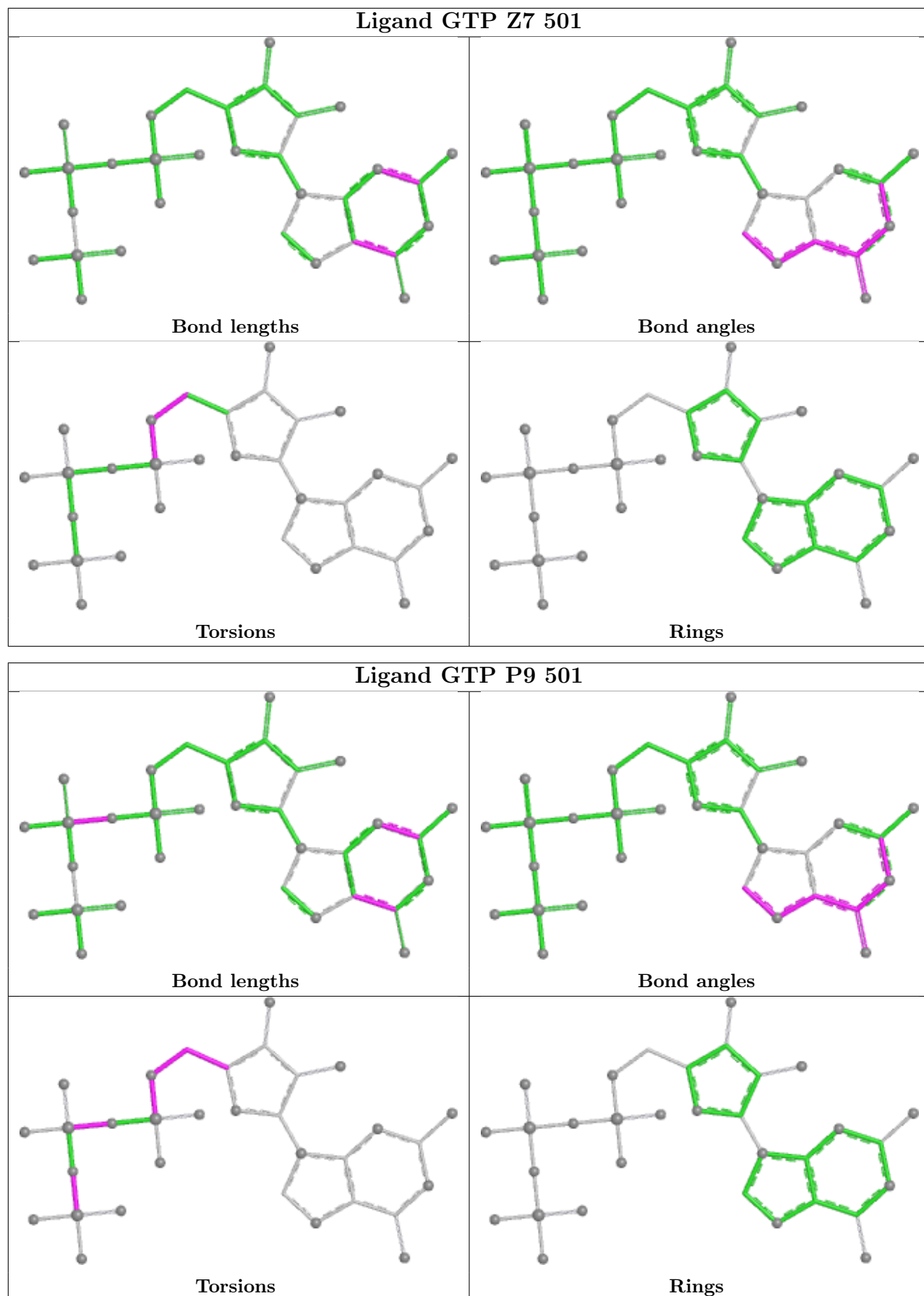


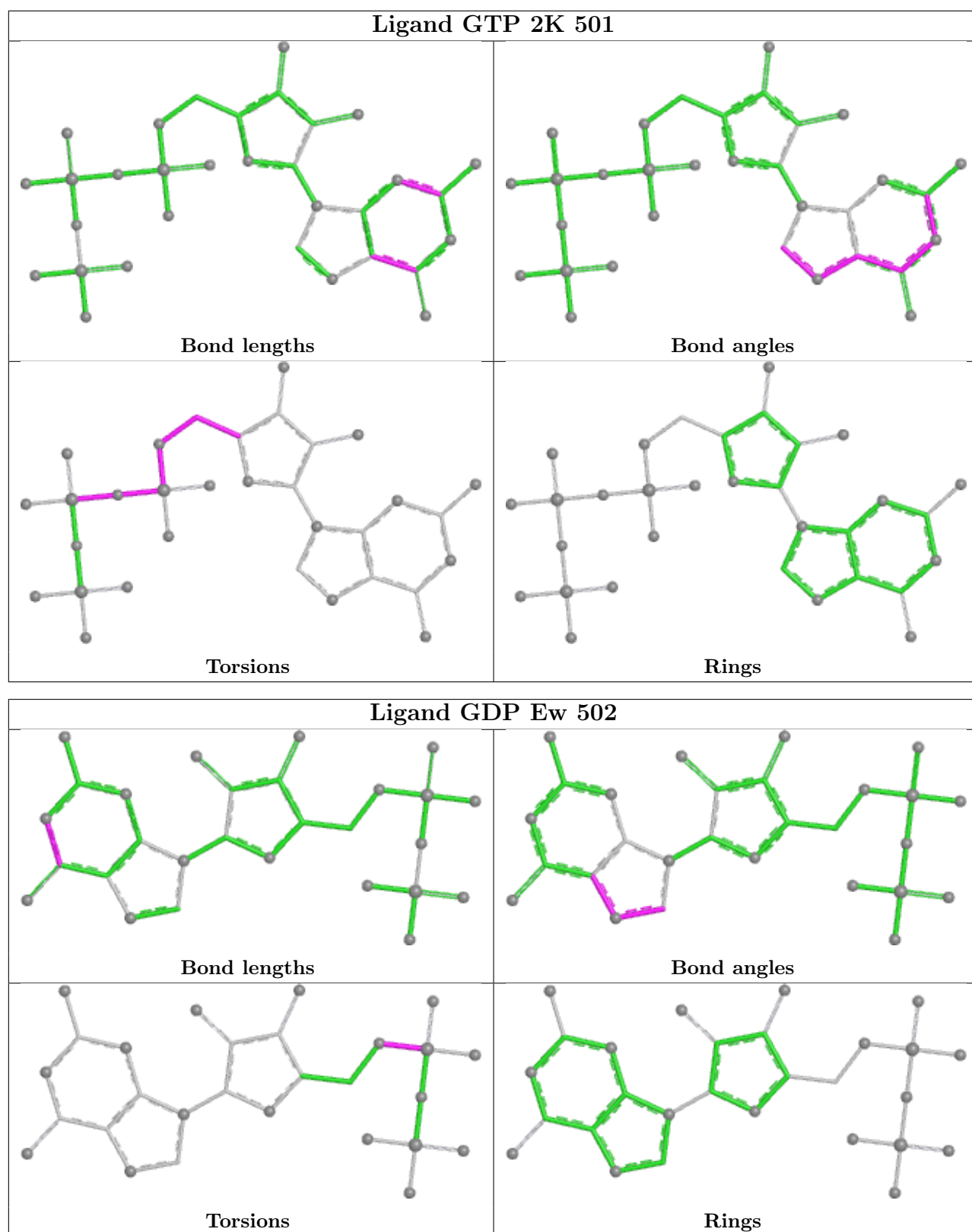


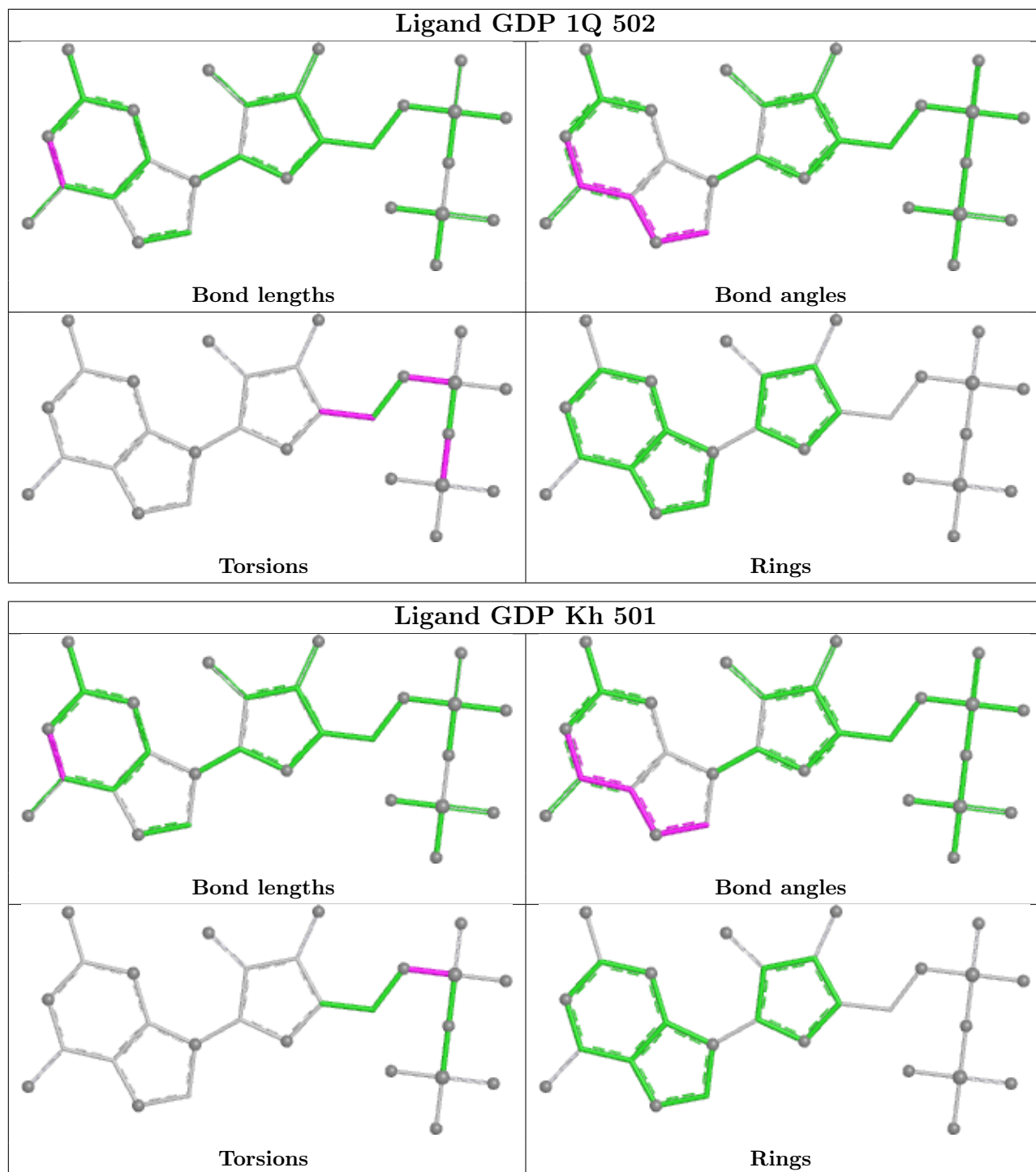


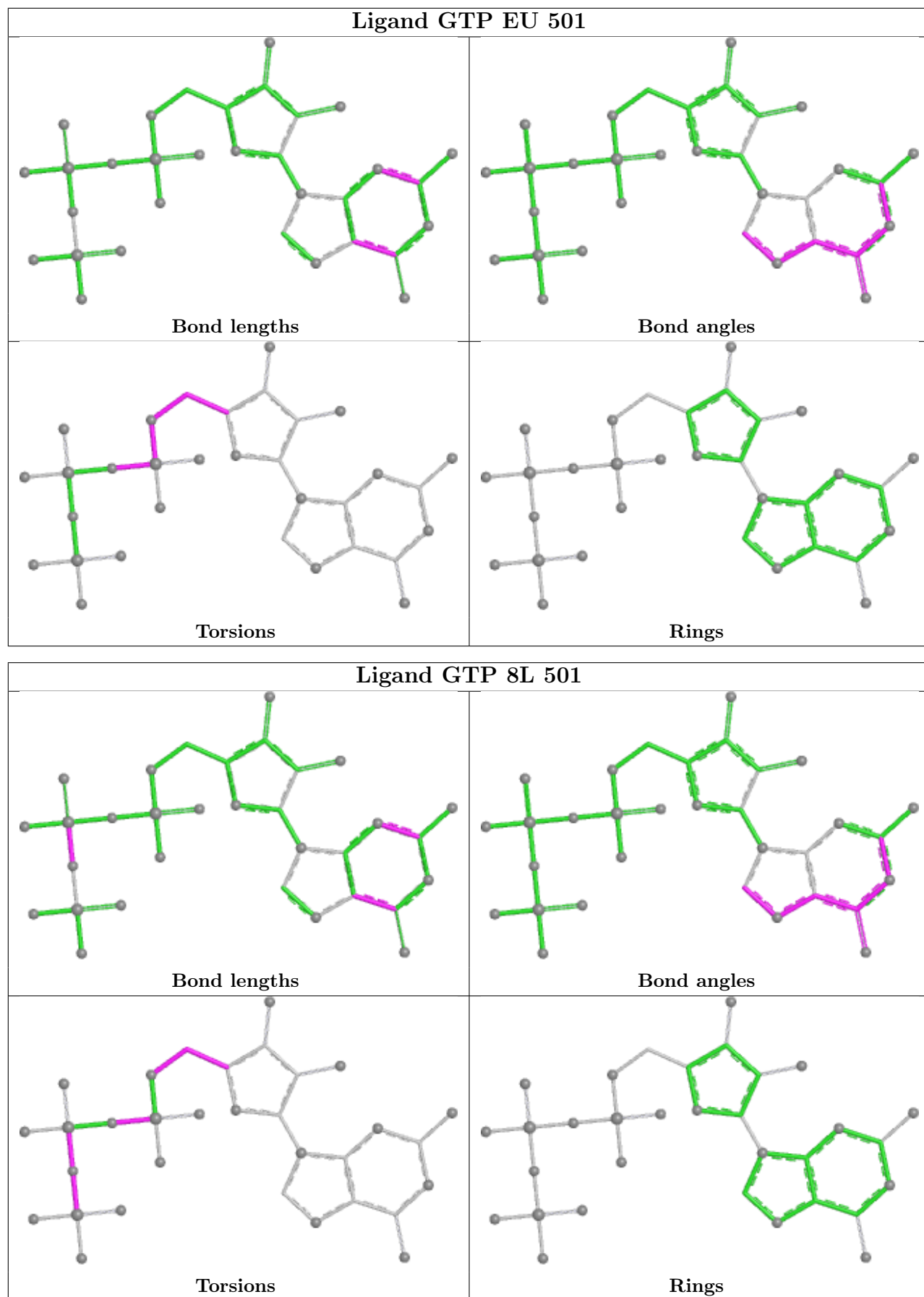












## 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	OA	1
10	7B	1
7	OG	1
59	Cp	1
59	Cq	1
84	OL	1
7	Ga	1
76	Ey	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	OA	445:ARG	C	446:SER	N	3.27
1	7B	97:GLY	C	98:VAL	N	3.16
1	OG	304:HIS	C	305:ASP	N	3.11
1	Cp	669:LEU	C	670:THR	N	3.08
1	Cq	668:GLU	C	669:LEU	N	3.08

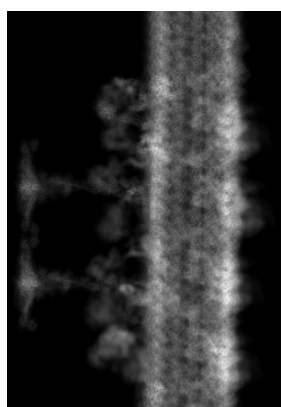
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40220. These allow visual inspection of the internal detail of the map and identification of artifacts.

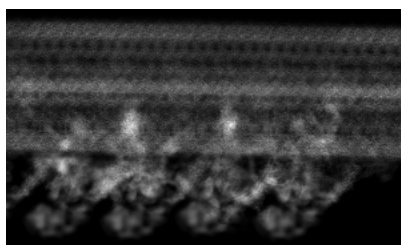
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 5.1 Orthogonal projections [i](#)

#### 5.1.1 Primary map



X



Y

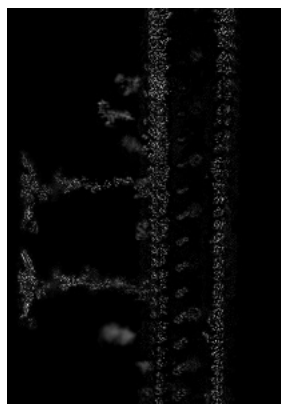


Z

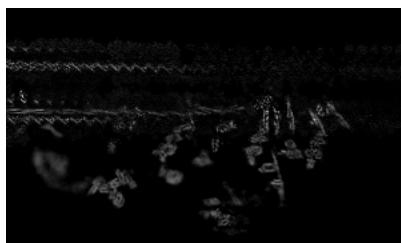
The images above show the map projected in three orthogonal directions.

### 5.2 Central slices [i](#)

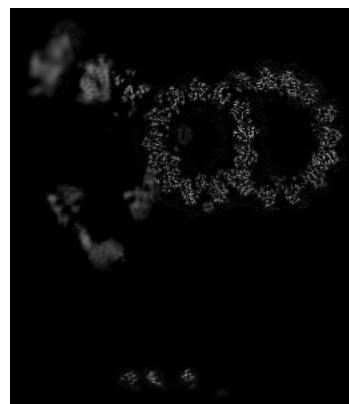
#### 5.2.1 Primary map



X Index: 284



Y Index: 326



Z Index: 476

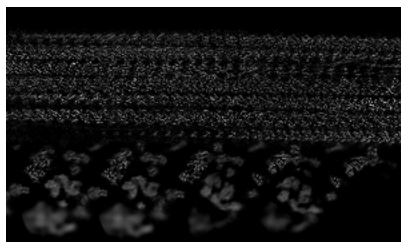
The images above show central slices of the map in three orthogonal directions.

### 5.3 Largest variance slices [\(i\)](#)

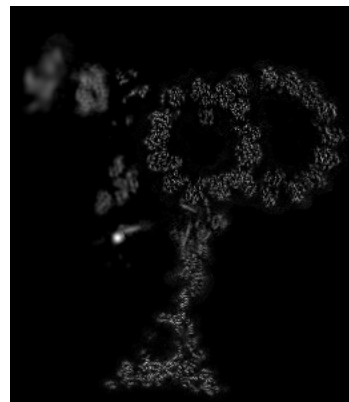
#### 5.3.1 Primary map



X Index: 375



Y Index: 520

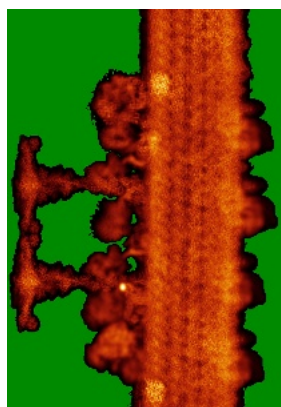


Z Index: 297

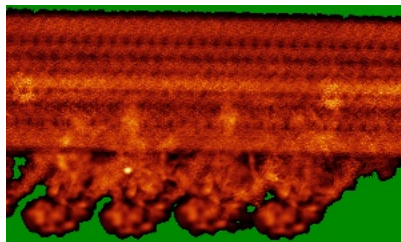
The images above show the largest variance slices of the map in three orthogonal directions.

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

#### 5.4.1 Primary map



X



Y

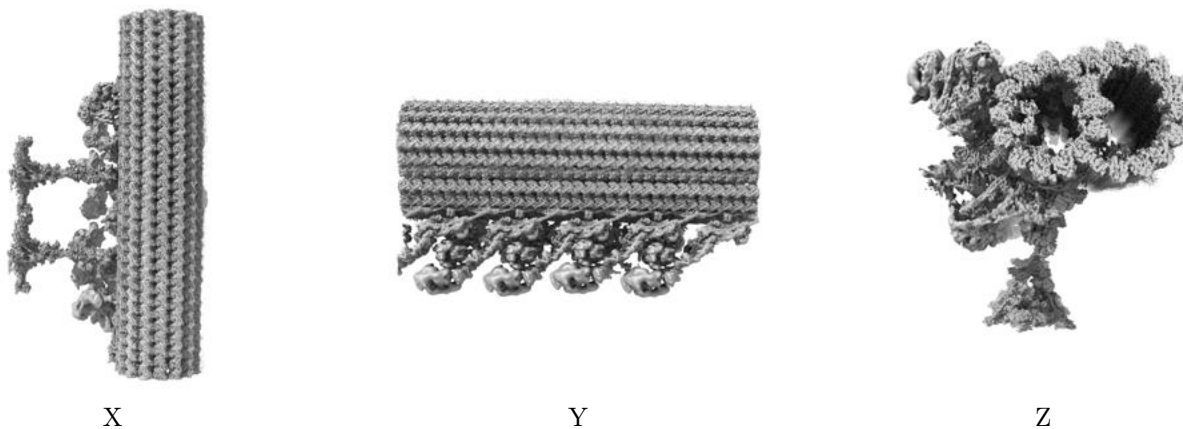


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

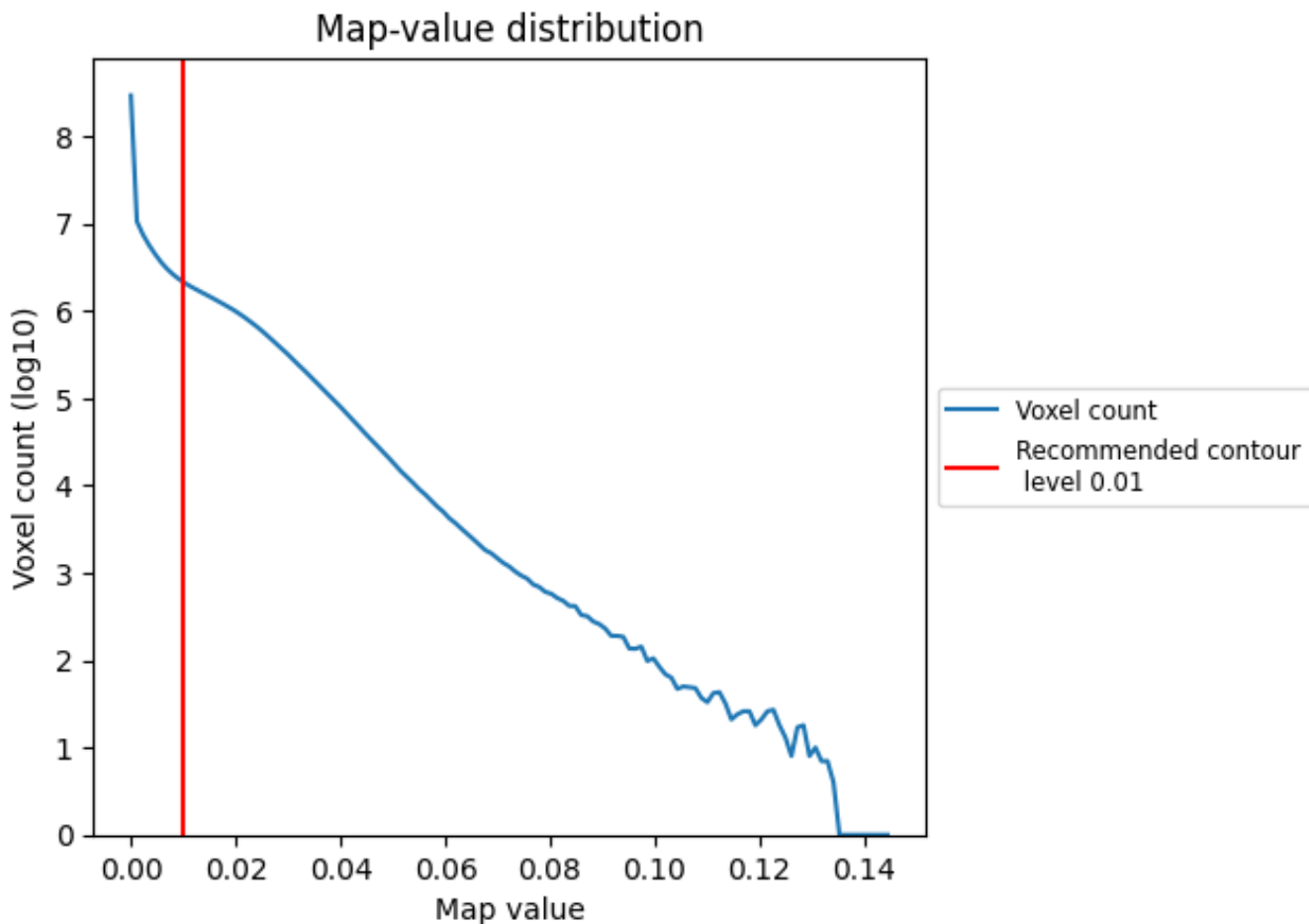
## 5.6 Mask visualisation [i](#)

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

## 6 Map analysis [i](#)

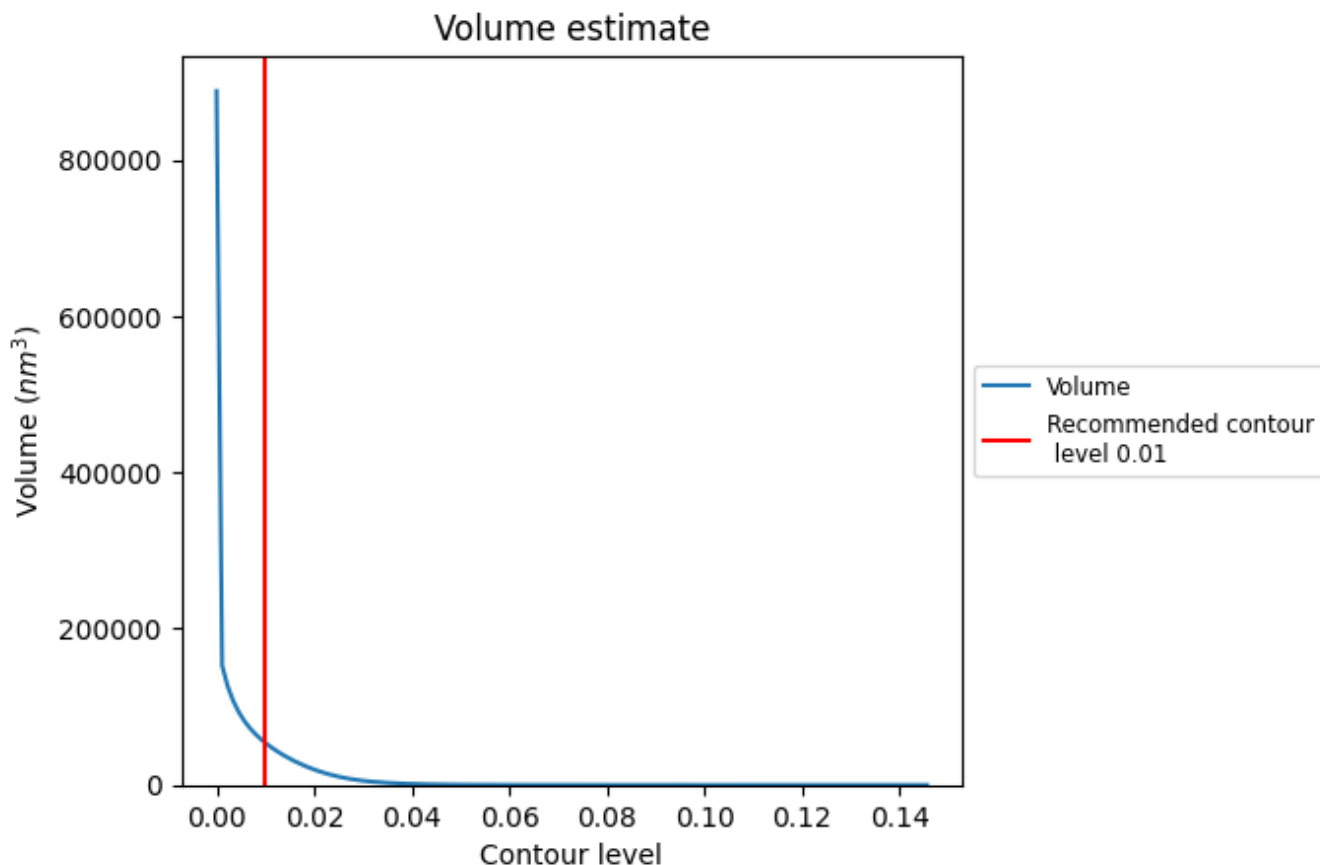
This section contains the results of statistical analysis of the map.

### 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 53940  $\text{nm}^3$ ; this corresponds to an approximate mass of 48725 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.

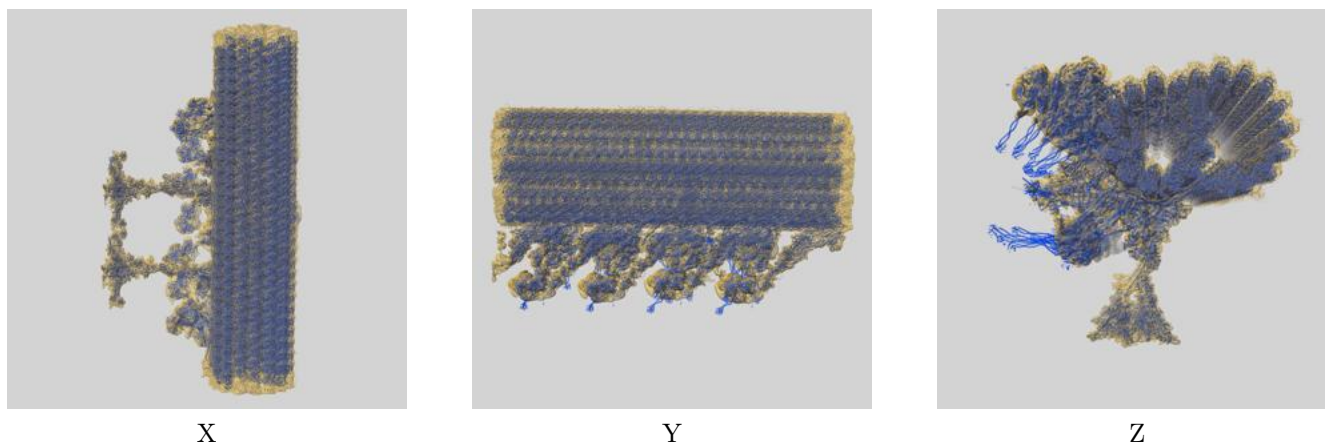
## 7 Fourier-Shell correlation

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-40220 and PDB model 8GLV. Per-residue inclusion information can be found in section ?? on page ??.

### 8.1 Map-model overlay [i](#)

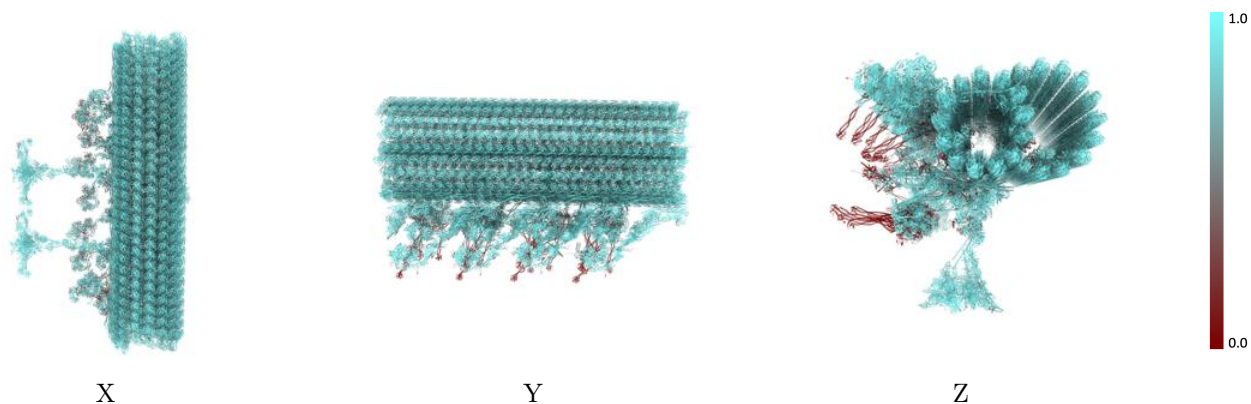


The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

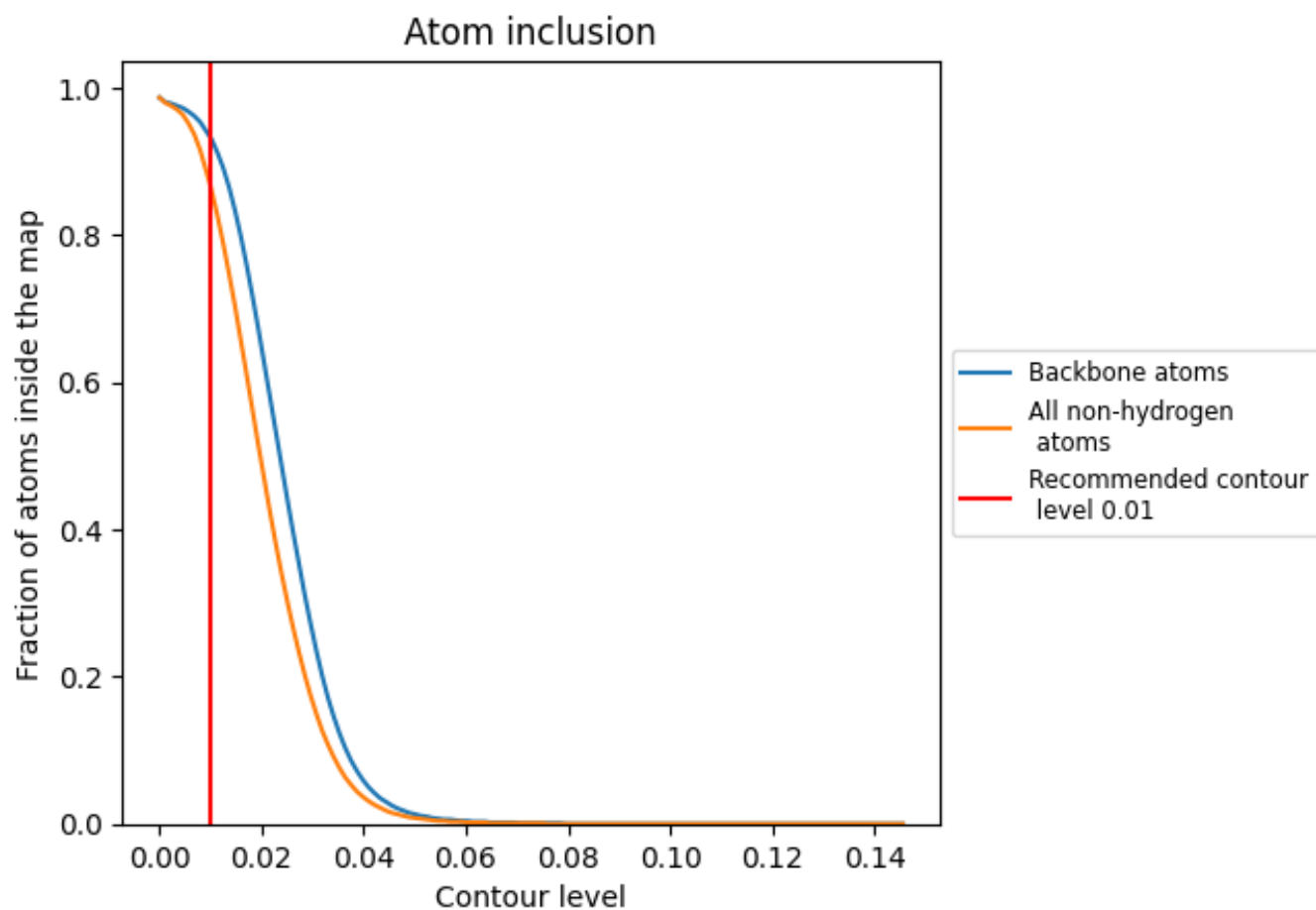
This section was not generated.

## 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 (0.01).




































## 8.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.8670
0A	 0.8380
0B	 0.8100
0C	 0.8150
0E	 0.9060
0F	 0.8810
0G	 0.8870
0H	 0.8840
0I	 0.8910
0J	 0.8750
0K	 0.8950
0L	 0.8710
0M	 0.8480
0N	 0.8440
0O	 0.8610
0P	 0.8450
0Q	 0.8680
0R	 0.8410
0S	 0.8260
0U	 0.9130
0V	 0.8990
0W	 0.9040
0X	 0.8890
0Y	 0.8890
0Z	 0.8800
1A	 0.8920
1B	 0.8770
1C	 0.8660
1D	 0.8840
1E	 0.8750
1F	 0.8660
1G	 0.8760
1H	 0.8530
1K	 0.9480
1L	 0.9410













































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Chain	Atom inclusion
1M	 0.9100
1N	 0.9120
1O	 0.9060
1P	 0.9150
1Q	 0.9200
1R	 0.9050
1S	 0.9180
1T	 0.9330
1U	 0.9290
1V	 0.9320
1W	 0.9260
1X	 0.9230
1Z	 0.8830
2A	 0.8890
2B	 0.9160
2C	 0.9070
2D	 0.8980
2E	 0.9040
2F	 0.8960
2G	 0.9070
2H	 0.8510
2I	 0.8730
2J	 0.8850
2K	 0.8820
2L	 0.8730
2M	 0.8760
2N	 0.8950
2P	 0.8870
2Q	 0.9040
2R	 0.9290
2S	 0.9150
2T	 0.9150
2U	 0.9210
2V	 0.9140
2W	 0.9160
2X	 0.8860
2Y	 0.9030
2Z	 0.9000
3A	 0.9010
3B	 0.8900
3C	 0.8870
3D	 0.9110











































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Chain	Atom inclusion
3F	 0.8790
3G	 0.8730
3H	 0.9250
3I	 0.9050
3J	 0.9040
3K	 0.9080
3L	 0.9080
3M	 0.8950
3N	 0.8910
3O	 0.8900
3P	 0.9010
3Q	 0.8920
3R	 0.8840
3S	 0.8800
3T	 0.9120
3V	 0.7130
3W	 0.9070
3X	 0.7890
3Y	 0.9380
3Z	 0.7850
4A	 0.9210
4B	 0.6510
4C	 0.9250
4D	 0.7970
4E	 0.9220
4F	 0.7570
4G	 0.9200
4H	 0.8060
4I	 0.9290
4J	 0.6730
4O	 0.7900
4Q	 0.8100
4R	 0.9150
4W	 0.7930
4X	 0.7800
5C	 0.6720
5D	 0.7890
5E	 0.9250
5F	 0.9340
5H	 0.9450
5I	 0.9300
5J	 0.9450











































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Chain	Atom inclusion
5K	 0.9480
5L	 0.8530
5M	 0.8570
5N	 0.7990
5O	 0.8070
5P	 0.8630
5Q	 0.8220
5S	 0.8660
5T	 0.8470
5U	 0.8310
5V	 0.8500
5X	 0.9000
5Y	 0.8710
5Z	 0.8520
6A	 0.8440
6B	 0.8420
6C	 0.6850
6D	 0.8710
6E	 0.8790
6F	 0.9200
6G	 0.8750
6H	 0.9050
6I	 0.8630
6J	 0.8730
6K	 0.8500
6L	 0.8480
6M	 0.8720
6N	 0.8480
6O	 0.8430
6P	 0.8510
6Q	 0.6620
6R	 0.6540
6S	 0.3830
6T	 0.8890
6U	 0.8570
6V	 0.8700
6W	 0.8870
6X	 0.8720
6Y	 0.8700
6Z	 0.8550
7B	 0.9510
7C	 0.7870











































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Chain	Atom inclusion
7D	 0.8700
7E	 0.8070
7G	 0.8480
7H	 0.6680
7I	 0.8960
7J	 0.8760
7K	 0.8370
7M	 0.9250
7N	 0.8850
7P	 0.6790
7Q	 0.9270
7X	 0.5600
7Y	 0.5510
8B	 0.5170
8C	 0.6270
8F	 0.9280
8H	 0.9320
8I	 0.9370
8J	 0.9300
8K	 0.9120
8L	 0.9110
8M	 0.9270
8N	 0.9120
A0	 0.9090
A1	 0.9150
A2	 0.9120
A3	 0.9200
A4	 0.9220
A5	 0.9260
A6	 0.9540
A7	 0.9420
A8	 0.9400
A9	 0.9310
AA	 0.0000
AB	 0.8750
AC	 0.8440
AD	 0.6860
AE	 0.9560
AF	 0.9170
AG	 0.8440
AH	 0.8930
AI	 0.9360

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Chain	Atom inclusion
AJ	 0.9490
AK	 0.9500
AL	 0.9340
AM	 0.9780
AN	 0.9610
AO	 0.9830
AP	 0.9870
AQ	 0.9480
AR	 0.9890
AS	 0.9720
AT	 0.9580
AU	 0.9300
AV	 0.9220
AW	 0.9020
AX	 0.7040
AY	 0.9100
AZ	 0.8400
Aa	 0.8780
Ab	 0.8800
Ac	 0.9250
Ad	 0.8620
Ae	 0.8670
Af	 0.8140
Ag	 0.8980
Ah	 0.8920
Ai	 0.9000
Aj	 0.8940
Ak	 0.9520
Al	 0.9600
Am	 0.9590
An	 0.9510
Ao	 0.9380
Ap	 0.9290
Aq	 0.9240
Ar	 0.8830
As	 0.8740
At	 0.9510
Au	 0.9140
Av	 0.9000
Aw	 0.9140
Ax	 0.9540
Ay	 0.9670











































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Chain	Atom inclusion
Az	0.9550
B0	0.9410
B1	0.9350
B2	0.9180
B3	0.9280
B4	0.9240
B5	0.9030
B6	0.9700
B7	0.9160
B8	0.9140
B9	0.9190
BA	0.9400
BB	0.9410
BC	0.8910
BD	0.8970
BE	0.8680
BF	0.9490
BG	0.8870
BH	0.8760
BI	0.9240
BJ	0.9700
BK	0.8770
BL	0.8900
BM	0.9080
BN	0.9250
BO	0.9090
BP	0.8900
BQ	0.9180
BR	0.9320
BS	0.8850
BT	0.8870
BU	0.8850
BV	0.8960
BW	0.9800
BX	0.9690
BY	0.8800
BZ	0.8990
Ba	0.9070
Bb	0.9010
Bc	0.9480
Bd	0.9450
Be	0.9400











































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Chain	Atom inclusion
Bf	 0.9220
Bg	 0.9190
Bh	 0.9260
Bi	 0.9630
Bj	 0.9630
Bk	 0.9610
Bl	 0.9430
Bm	 0.9460
Bn	 0.9460
Bo	 0.9440
Bp	 0.9490
Bq	 0.9290
Br	 0.9300
Bs	 0.9450
Bt	 0.9480
Bu	 0.9470
Bv	 0.9450
Bw	 0.9580
Bx	 0.9400
By	 0.9450
Bz	 0.9600
C0	 0.9260
C1	 0.9140
C2	 0.9460
C3	 0.9570
C4	 0.8890
C5	 0.8690
C6	 0.8980
C7	 0.9200
C8	 0.9130
C9	 0.9310
CA	 0.9550
CB	 0.9290
CC	 0.9530
CD	 0.9310
CE	 0.9380
CF	 0.9460
CG	 0.9400
CH	 0.9370
CI	 0.9500
CJ	 0.9320
CK	 0.9440

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Chain	Atom inclusion
CL	 0.9570
CM	 0.9640
CN	 0.9430
CO	 0.9500
CP	 0.9060
CQ	 0.9210
CR	 0.8830
CS	 0.8960
CT	 0.9060
CU	 0.8960
CV	 0.8920
CW	 0.8870
CX	 0.9100
CY	 0.9270
CZ	 0.9290
Ca	 0.9290
Cb	 0.0000
Cc	 0.9050
Cd	 0.8880
Ce	 0.8760
Cf	 0.8720
Cg	 0.8850
Ch	 0.8840
Ci	 0.8890
Cj	 0.8940
Ck	 0.9070
Cl	 0.9170
Cm	 0.9190
Cn	 0.8620
Co	 0.6060
Cp	 0.8950
Cq	 0.7070
Cr	 0.8730
Cs	 0.8790
Ct	 0.8890
Cu	 0.8720
Cv	 0.8940
Cw	 0.9300
Cx	 0.9320
Cy	 0.9450
Cz	 0.9540
D0	 0.9300











































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Chain	Atom inclusion
D1	0.9190
D2	0.8720
D3	0.9040
D4	0.9030
D5	0.9140
D6	0.8980
D7	0.8900
D8	0.9370
D9	0.8680
DA	0.8530
DB	0.8730
DC	0.9150
DD	0.9060
DE	0.9050
DF	0.9110
DG	0.9050
DH	0.9020
DI	0.9210
DJ	0.9410
DK	0.9410
DL	0.9520
DM	0.9610
DN	0.9600
DO	0.8390
DP	0.8530
DQ	0.9370
DR	0.9350
DS	0.9280
DT	0.9370
DU	0.9220
DV	0.9360
DW	0.9500
DX	0.9530
DY	0.9420
DZ	0.9610
Da	0.9570
Db	0.8740
Dc	0.9150
Dd	0.9000
De	0.9080
Df	0.8930
Dg	0.9000











































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Chain	Atom inclusion
Dh	 0.8950
Di	 0.9170
Dj	 0.9520
Dk	 0.9470
DI	 0.9280
Dm	 0.9220
Dn	 0.8380
Do	 0.8110
Dp	 0.8950
Dq	 0.8370
Dr	 0.8320
Ds	 0.8400
Dt	 0.8300
Du	 0.8410
Dv	 0.8540
Dw	 0.8570
Dx	 0.8560
Dy	 0.8790
Dz	 0.8850
E0	 0.9030
E1	 0.8540
E2	 0.8870
E3	 0.9090
E4	 0.9070
E5	 0.9050
E6	 0.9060
E7	 0.8960
E8	 0.8500
E9	 0.8790
EA	 0.8330
EB	 0.8450
EC	 0.9150
ED	 0.9260
EE	 0.9170
EF	 0.9300
EG	 0.9190
EH	 0.9330
EI	 0.9100
EJ	 0.9210
EK	 0.9170
EL	 0.9310
EM	 0.4730











































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Chain	Atom inclusion
EN	 0.8930
EO	 0.8820
EP	 0.9120
EQ	 0.9140
ER	 0.9170
ES	 0.9190
ET	 0.9160
EU	 0.9120
EV	 0.9010
EW	 0.9040
EX	 0.9130
EY	 0.9090
EZ	 0.5490
Ea	 0.5910
Eb	 0.8140
Ec	 0.8280
Ed	 0.8380
Ee	 0.8240
Ef	 0.8510
Eg	 0.8240
Eh	 0.8390
Ei	 0.8570
Ej	 0.8650
Ek	 0.8660
El	 0.8720
Em	 0.9490
En	 0.7070
Eo	 0.8490
Ep	 0.8320
Eq	 0.8290
Er	 0.8090
Es	 0.8370
Et	 0.8010
Eu	 0.8740
Ev	 0.8850
Ew	 0.8900
Ex	 0.8820
Ey	 0.6010
Ez	 0.9470
F0	 0.9030
F1	 0.8830
F2	 0.8810

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Chain	Atom inclusion
F3	 0.8390
F4	 0.6780
F5	 0.9280
F6	 0.9260
F7	 0.9010
F8	 0.8710
F9	 0.8840
FA	 0.9580
FB	 0.9180
FC	 0.8210
FD	 0.8240
FE	 0.8270
FF	 0.8120
FG	 0.8320
FH	 0.8200
FI	 0.9050
FJ	 0.9120
FK	 0.9130
FL	 0.9110
FM	 0.8930
FN	 0.9290
FO	 0.8430
FP	 0.8720
FQ	 0.8820
FR	 0.8800
FS	 0.8740
FT	 0.8800
FU	 0.8570
FV	 0.9370
FW	 0.9470
FX	 0.9420
FY	 0.9340
FZ	 0.6180
Fa	 0.6520
Fb	 0.9030
Fc	 0.8980
Fd	 0.9020
Fe	 0.9000
Ff	 0.8810
Fg	 0.8950
Fh	 0.8860
Fi	 0.8930

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Chain	Atom inclusion
Fj	0.8990
Fk	0.8960
Fl	0.9010
Fm	0.6760
Fn	0.8600
Fo	0.8840
Fp	0.9040
Fq	0.9150
Fr	0.9050
Fs	0.9040
Ft	0.9070
Fu	0.9000
Fv	0.8970
Fw	0.9150
Fx	0.9180
Fy	0.7180
Fz	0.9270
G0	0.9210
G1	0.9060
G2	0.9160
G3	0.8890
G4	0.8630
G5	0.8900
G6	0.8930
G7	0.8750
G8	0.8780
G9	0.8330
GA	0.8930
GB	0.9100
GC	0.9050
GD	0.9030
GE	0.9000
GF	0.9030
GG	0.8960
GH	0.8930
GI	0.8960
GJ	0.8930
GK	0.9020
GL	0.9010
GM	0.8720
GN	0.9280
GO	0.8940











































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Chain	Atom inclusion
GP	0.7220
GQ	0.8960
GR	0.5780
GS	0.9690
GT	0.7970
GU	0.9300
GV	0.6250
GW	0.9130
GX	0.7320
GY	0.9530
GZ	0.9430
Ga	0.9210
Gb	0.8680
Gc	0.8600
Gd	0.9000
Ge	0.9520
Gf	0.9130
Gg	0.0000
Gh	0.7530
Gi	0.9380
Gj	0.9380
Gk	0.8830
Gl	0.8560
Gm	0.8390
Gn	0.8670
Go	0.7450
Gp	0.7270
Gq	0.7600
Gr	0.9070
Gs	0.9320
Gt	0.8750
Gu	0.8420
Gv	0.9070
Gw	0.9540
Gx	0.9480
Gy	0.8390
Gz	0.8720
H0	0.9710
H1	0.9330
H2	0.9300
H3	0.8890
H4	0.9030

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Chain	Atom inclusion
H5	 0.9180
H6	 0.9350
H7	 0.9200
H8	 0.9250
H9	 0.8580
HA	 0.8580
HB	 0.9160
HD	 0.8320
HE	 0.8410
HF	 0.1610
HG	 0.8320
HH	 0.8130
HI	 0.8060
HJ	 0.8500
HK	 0.8810
HL	 0.7880
HM	 0.2000
HN	 0.9030
HO	 0.9520
HP	 0.9010
HQ	 0.9350
HS	 0.8440
HT	 0.8760
HU	 0.9040
HV	 0.8880
HW	 0.9120
HX	 0.9610
HY	 0.6070
HZ	 0.6690
Ha	 0.3070
Hb	 0.8710
Hc	 0.8620
Hd	 0.8970
He	 0.9080
Hf	 0.9180
Hg	 0.8990
Hh	 0.9620
Hi	 0.9100
Hj	 0.8180
Hk	 0.8030
Hl	 0.7670
Hm	 0.9060











































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Chain	Atom inclusion
Hn	0.8080
Ho	0.9490
Hp	0.9310
Hq	0.8250
Hr	0.9050
Hs	0.9510
Ht	0.9100
Hu	0.9350
Hv	0.8040
Hw	0.9470
Hx	0.9580
Hy	0.9590
Hz	0.9650
I0	0.8740
I1	0.8910
I2	0.8890
I3	0.8780
I4	0.8810
I5	0.9460
I6	0.9830
I7	0.9360
I8	0.9280
I9	0.9180
IA	0.9670
IB	0.9670
IC	0.9480
ID	0.5550
IE	0.9380
IF	0.9880
IG	0.4850
IH	0.6730
II	0.9870
IJ	0.9890
IK	0.9340
IL	0.9120
IM	0.9120
IN	0.9880
IO	0.9870
IP	0.9830
IQ	0.9550
IR	0.9290
IS	0.9560











































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Chain	Atom inclusion
IT	 0.9480
IU	 0.9810
IV	 0.9570
IW	 0.9600
IX	 0.9390
IY	 0.9460
IZ	 0.9280
Ia	 0.9870
Ib	 0.9820
Ic	 0.9590
Id	 0.9640
Ie	 0.9870
If	 0.9760
Ig	 0.9570
Ih	 0.9880
Ii	 0.8740
Ij	 0.8450
Ik	 0.8800
Il	 0.8940
Im	 0.9130
In	 0.9940
Io	 1.0000
Ip	 1.0000
Iq	 1.0000
Ir	 0.9810
Is	 0.9900
It	 1.0000
Iu	 0.9780
Iv	 0.8780
Iw	 0.8410
Ix	 0.8850
Iy	 0.8900
Iz	 0.8940
J0	 0.9190
J1	 0.9390
J2	 0.9340
J3	 0.9300
J4	 0.9310
J5	 0.8690
J6	 0.8780
J7	 0.8950
J8	 0.8960

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Chain	Atom inclusion
J9	 0.8790
JA	 0.8960
JB	 0.9980
JC	 0.9720
JD	 0.9600
JE	 0.7970
JF	 0.8300
JG	 0.7570
JH	 0.9230
JI	 0.9120
JJ	 0.9360
JK	 0.9360
JL	 0.9350
JM	 0.9220
JN	 0.8370
JO	 0.8310
JP	 0.8860
JQ	 0.8870
JR	 0.9230
JS	 0.9200
JT	 0.9320
JU	 0.9440
JV	 0.9270
JW	 0.9360
JX	 0.9410
JY	 0.9460
JZ	 0.9290
Ja	 0.9390
Jb	 0.9410
Jc	 0.9710
Jd	 0.9700
Je	 0.9730
Jf	 0.9700
Jg	 0.9710
Jh	 0.9470
Ji	 0.9340
Jj	 0.9280
Jk	 0.9380
Jl	 0.9550
Jm	 0.9650
Jn	 0.9100
Jo	 0.9530











































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Chain	Atom inclusion
Jp	0.9500
Jq	0.9140
Jr	0.9280
Js	0.9730
Jt	0.9400
Ju	0.8810
Jv	0.8760
Jw	0.8850
Jx	0.9080
Jy	0.9220
Jz	0.9110
K0	0.8680
K1	0.9430
K2	0.8720
K3	0.9110
K4	0.9010
K5	0.8880
K6	0.8810
K7	0.8890
K8	0.8970
K9	0.9010
KA	0.9370
KB	0.9860
KC	0.9830
KD	0.8400
KE	0.8770
KF	0.8290
KG	0.9130
KH	0.8770
KI	0.8940
KJ	0.9010
KK	0.9220
KL	0.9270
KM	0.9420
KN	0.9450
KO	0.9270
KP	0.9290
KQ	0.9630
KR	0.9760
KS	0.9720
KT	0.9680
KU	0.8820











































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Chain	Atom inclusion
KV	 0.9340
KW	 0.9460
KX	 0.9440
KY	 0.9490
KZ	 0.9030
Ka	 0.9180
Kb	 0.9300
Kc	 0.9360
Kd	 0.8790
Ke	 0.8900
Kf	 0.8640
Kg	 0.7150
Kh	 0.9140
Ki	 0.9600
Kj	 0.9540
Kk	 0.9500
Kl	 0.9540
Km	 0.8020
Kn	 0.8330
Ko	 0.8320
Kp	 0.8260
Kq	 0.8290
Kr	 0.9000
Ks	 0.9080
Kt	 0.8630
Ku	 0.9130
Kv	 0.9070
Kw	 0.9500
Kx	 0.9380
Ky	 0.9400
Kz	 0.8400
L0	 0.8990
L1	 0.8780
L2	 0.9000
L3	 0.9130
L4	 0.9110
L5	 0.9080
L6	 0.9090
L7	 0.8740
L8	 0.9240
L9	 0.9220
LA	 0.8500

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Chain	Atom inclusion
LB	 0.9000
LC	 0.9370
LD	 0.9470
LE	 0.8790
LF	 0.9180
LG	 0.9070
LH	 0.9540
LI	 0.9580
LJ	 0.9540
LK	 0.9220
LL	 0.8940
LM	 0.8990
LN	 0.8460
LO	 0.7450
LP	 0.6520
LQ	 0.6720
LR	 0.7830
LS	 0.8050
LT	 0.8360
LU	 0.8610
LV	 0.8530
LW	 0.8750
LX	 0.8900
LY	 0.9380
LZ	 0.6920
La	 0.6680
Lb	 0.8080
Lc	 0.6250
Ld	 0.9340
Le	 0.9340
Lf	 0.8980
Lg	 0.8120
Lh	 0.9320
Li	 0.9060
Lj	 0.9010
Lk	 0.8910
Ll	 0.0000
Lm	 0.8510
Ln	 0.8740
Lo	 0.6830
Lp	 0.8730
Lq	 0.9210

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Chain	Atom inclusion
Lr	0.8800
Ls	0.8380
Lt	0.9080
Lu	0.9100
Lv	0.8900
Lw	0.8860
Lx	0.9000
Ly	0.9140
Lz	0.8740
M0	0.9210
M1	0.8950
M2	0.8880
M3	0.8800
M4	0.8870
M5	0.8930
M6	0.9140
M7	0.8800
M8	0.9010
M9	0.9090
MA	0.9520
MB	0.9460
MC	0.9460
MD	0.9580
ME	0.9440
MF	0.8230
MG	0.8290
MH	0.8370
MI	0.8460
MJ	0.8510
MK	0.9050
ML	0.9320
MM	0.9220
MN	0.9020
MO	0.8680
MP	0.8430
MQ	0.8250
MR	0.9080
MS	0.7880
MT	0.8740
MU	0.8790
MV	0.8960
MW	0.8890

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Chain	Atom inclusion
MX	0.9090
MY	0.9080
MZ	0.9270
Ma	0.8990
Mb	0.9370
Mc	0.9020
Md	0.6640
Me	0.7360
Mf	0.8280
Mg	0.9020
Mh	0.9150
Mi	0.9210
Mj	0.9110
Mk	0.9360
Ml	0.8560
Mm	0.6700
Ms	0.8580
Mt	0.9350
Mu	0.9520
Mv	0.9440
Mw	0.9360
N0	0.9230
N1	0.9080
N2	0.9170
N3	0.8700
N5	0.9420
N6	0.9450
N7	0.9350
N8	0.9140
N9	0.9130
NF	0.8760
NG	0.8630
NH	0.8710
NI	0.9000
NJ	0.9000
NS	0.8950
NT	0.8940
NU	0.8980
NV	0.9320
NW	0.9250
Nf	0.8900
Ng	0.8870











































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Chain	Atom inclusion
Nh	0.8960
Ni	0.9190
Nj	0.9040
Ns	0.9680
Nt	0.8110
Nu	0.9070
Nv	0.5740
Nw	0.8770
Ny	0.9200
Nz	0.7830
O0	0.9040
O1	0.8980
O2	0.9120
O3	0.9100
O4	0.8590
O5	0.8750
O6	0.8820
O7	0.8740
O8	0.8890
O9	0.8730
OA	0.8310
OD	0.7420
OG	0.9190
OL	0.8330
ON	0.8310
OO	0.7770
OQ	0.8720
OV	0.9490
OY	0.8620
OZ	0.8650
Oc	0.8480
Od	0.8180
Oi	0.8460
Oj	0.8530
Ok	0.7370
Om	0.9090
On	0.9340
Op	0.9300
Ot	0.7860
Ou	0.8810
Ov	0.8670
Oy	0.6510











































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Chain	Atom inclusion
Oz	 0.3970
P3	 0.9530
P4	 0.9520
P5	 0.9150
P6	 0.8930
P7	 0.8900
P8	 0.8970
P9	 0.9040
PD	 0.8710
PE	 0.8910
PF	 0.8940
PK	 0.7960
PQ	 0.8370
PV	 0.7830
PW	 0.9470
Pe	 0.6720
Pi	 0.6290
Q0	 0.9270
Q1	 0.9160
Q2	 0.9210
Q3	 0.9330
Q4	 0.9350
Q5	 0.9350
Q6	 0.9310
Q8	 0.9390
Q9	 0.9420
R0	 0.9580
R1	 0.9160
R2	 0.9130
R3	 0.9160
R4	 0.9360
R5	 0.9280
R6	 0.9270
R7	 0.9520
R8	 0.9550
R9	 0.9470
S0	 0.9510
S1	 0.9480
S2	 0.9530
S4	 0.9250
S5	 0.9420
S6	 0.9390











































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Chain	Atom inclusion
S7	 0.9440
S8	 0.9470
S9	 0.9270
T0	 0.9300
T1	 0.9310
T2	 0.9480
T3	 0.9150
T4	 0.9180
T5	 0.9060
T6	 0.9150
T7	 0.9170
T8	 0.9320
U1	 0.8610
U2	 0.8540
U3	 0.8950
U4	 0.8710
U5	 0.8780
U6	 0.8810
U7	 0.8930
U8	 0.8870
U9	 0.8240
V0	 0.8090
V1	 0.8190
V2	 0.8250
V3	 0.8110
V4	 0.8110
V6	 0.9080
V7	 0.8940
V8	 0.9120
V9	 0.9360
W0	 0.9380
W1	 0.9310
W2	 0.9440
W3	 0.9440
W4	 0.9540
W5	 0.9370
W6	 0.9400
W7	 0.9370
W8	 0.9440
W9	 0.9370
X0	 0.9420
X2	 0.9020










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Chain	Atom inclusion
X3	 0.8920
X4	 0.8970
X5	 0.9350
X6	 0.9340
X7	 0.9440
X8	 0.9470
X9	 0.9440
Y0	 0.9400
Y1	 0.9250
Y2	 0.9140
Y3	 0.9310
Y4	 0.9260
Y5	 0.9290
Y6	 0.9170
Y8	 0.8570
Y9	 0.8480
Z0	 0.8830
Z1	 0.8940
Z2	 0.8880
Z3	 0.8890
Z4	 0.9040
Z5	 0.8870
Z6	 0.9010
Z7	 0.8040
Z8	 0.8300
Z9	 0.8170
za	 0.8460
zb	 0.8440
zc	 0.8600
zd	 0.8560
ze	 0.8280
zf	 0.8540
zg	 0.8450
zh	 0.8460
zi	 0.9100
zj	 0.8810
zk	 0.8460
zl	 0.8750
zn	 0.8820
zo	 0.9010
zp	 0.5930
zq	 0.5920

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Chain	Atom inclusion
zr	 0.7730
zs	 0.7710
zt	 0.6550
zu	 0.7040
zv	 0.7280
zw	 0.6180
zx	 0.6340
zy	 0.6770
zz	 0.7040